wwPDB EM Validation Summary Report (i)

Sep 10, 2026 – 07:19 PM JST

PDB ID	:	7Y5E / pdb_00007y5e
EMDB ID	:	EMD-33618
Title	:	In situ single-PBS-PSII-PSI-LHCs megacomplex.
Authors	:	You, X.; Zhang, X.; Cheng, J.; Xiao, Y.N.; Sui, S.F.
Deposited on	:	2022-06-17
Resolution	:	3.30 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

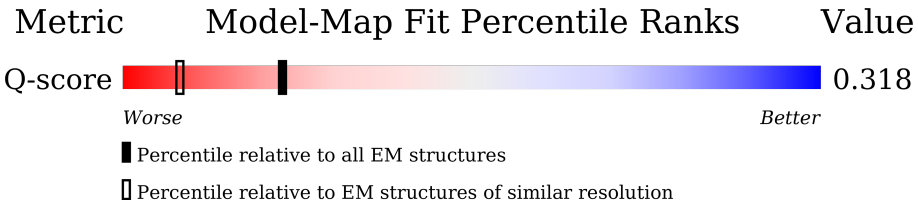
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	FAILED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Q-score	25397	15087 (2.80 - 3.80)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
69	MEN	B3	71	-	X	-	-
69	MEN	D3	71	-	X	-	-
69	MEN	F3	71	-	X	-	-
69	MEN	H3	71	-	X	-	-
69	MEN	I3	71	-	X	-	-
69	MEN	L3	71	-	X	-	-
69	MEN	M3	71	-	X	-	-
69	MEN	Q3	71	-	X	-	-
69	MEN	S3	71	-	X	-	-
69	MEN	U3	71	-	X	-	-
69	MEN	d3	71	-	X	-	-
69	MEN	f3	71	-	X	-	-
69	MEN	h3	71	-	X	-	-
69	MEN	j3	71	-	X	-	-
69	MEN	k3	71	-	X	-	-
69	MEN	n3	71	-	X	-	-
69	MEN	o3	71	-	X	-	-
69	MEN	q3	71	-	X	-	-
69	MEN	s3	71	-	X	-	-
69	MEN	u3	71	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
69	MEN	w3	71	-	X	-	-

2 Entry composition (i)

There are 104 unique types of molecules in this entry. The entry contains 1264616 atoms, of which 2032 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Phycoerythrin alpha subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	CA	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	EA	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	GA	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	IA	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	KA	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	MA	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	OA	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	QA	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	SA	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	UA	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	WA	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	JB	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	TB	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	BD	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	DD	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	FD	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	HD	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	JD	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	LD	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	ND	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	PD	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	RD	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	TD	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	VD	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	XD	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	OE	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	QE	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	SE	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	UE	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	WE	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	ZE	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	AF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	CF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	EF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	GF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	IF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	KF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	MF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	OF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	QF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	SF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	UF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	WF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	YF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	OG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	QG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	SG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	UG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	WG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	ZG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	OH	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	QH	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	SH	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	UH	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	WH	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	ZH	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	AI	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	CI	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	EI	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	GI	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	II	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	KI	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	NI	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	PI	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	RI	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	TI	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	VI	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	XI	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	CJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	EJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	GJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	IJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	KJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	MJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	OJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	QJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	SJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	UJ	164	Total	C	N	O	S	0	0
			1246	776	218	245	7		
1	WJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	YJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	AK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	CK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	EK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	GK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	IK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	KK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	MK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	OK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	QK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	SK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	UK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	WK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	YK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	CM	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	EM	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	GM	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	IM	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	KM	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	MM	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	OM	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	QM	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	SM	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	UM	164	Total	C	N	O	S	0	0
			1246	776	218	245	7		
1	WM	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	YM	164	Total	C	N	O	S	0	0
			1246	776	218	245	7		
1	OO	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	QO	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	SO	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	UO	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	WO	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	ZO	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	AP	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	CP	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	EP	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	GP	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	IP	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	KP	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	MP	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	OP	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	QP	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	SP	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	UP	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	WP	164	Total	C	N	O	S	0	0
			1246	777	219	243	7		
1	BQ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	DQ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	FQ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	HQ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	JQ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	LQ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	NQ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	PQ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	RQ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	TQ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	VQ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	XQ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	O1	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	Q1	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	S1	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	U1	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	W1	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	Z1	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	f1	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	h1	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	j1	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	l1	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	b1	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	d1	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	O4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	Q4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	S4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	U4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	W4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	Z4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	j4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	l4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	b4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	d4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	f4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	h4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	A5	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	C5	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	E5	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	G5	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	I5	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	K5	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	N5	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	P5	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	R5	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	T5	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	V5	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	X5	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	A7	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	C7	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	E7	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	G7	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	I7	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	K7	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	M7	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	O7	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	Q7	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	S7	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	U7	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	W7	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	z8	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	p8	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	r8	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	t8	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	v8	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	x8	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	A9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	C9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	E9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	G9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	I9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	K9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	N9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	P9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	R9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	T9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	V9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	X9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	zC	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	pC	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	rC	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	tC	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	vC	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	xC	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	bE	164	Total	C	N	O	S	0	0
			1243	773	219	244	7		
1	dE	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	fE	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	hE	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	jE	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	lE	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	aF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	cF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	eF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	gF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	iF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	kF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	mF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	oF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	qF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	sF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	uF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	bG	164	Total	C	N	O	S	0	0
			1243	773	219	244	7		
1	dG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	fG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	hG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	jG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	lG	164	Total	C	N	O	S	0	0
			1246	777	219	243	7		
1	fH	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	hH	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	jH	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	lH	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	bH	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	dH	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	aJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	dJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	fJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	hJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	jJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	lJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	aK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	cK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	eK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	gK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	iK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	kK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	mK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	oK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	qK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	sK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	uK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	aM	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	dM	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	fM	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	hM	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	jM	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	lM	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	jO	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	lO	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	bO	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	dO	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	fO	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	hO	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

- Molecule 2 is a protein called B-phycoerythrin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	BA	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	DA	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	FA	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	HA	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	JA	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	LA	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	NA	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	PA	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	RA	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	TA	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	VA	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	XA	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	BB	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	CB	177	Total	C	N	O	S	0	0
			1291	799	225	255	12		
2	DB	146	Total	C	N	O	S	0	0
			1065	654	187	213	11		
2	FB	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	GB	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	HB	174	Total	C	N	O	S	0	0
			1270	785	222	252	11		
2	IB	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	LB	177	Total	C	N	O	S	0	0
			1290	797	224	257	12		
2	MB	177	Total	C	N	O	S	0	0
			1284	793	225	254	12		
2	NB	146	Total	C	N	O	S	0	0
			1062	651	187	213	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	OB	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	PB	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	QB	174	Total	C	N	O	S	0	0
			1270	785	222	252	11		
2	RB	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	SB	177	Total	C	N	O	S	0	0
			1287	794	225	256	12		
2	VB	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	XB	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	YB	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	ZB	152	Total	C	N	O	S	0	0
			1111	687	194	219	11		
2	CD	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	ED	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	GD	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	ID	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	KD	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	MD	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	OD	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	QD	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	SD	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	UD	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	WD	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	YD	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	PE	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	RE	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	TE	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	VE	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	YE	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	BF	177	Total	C	N	O	S	1	0
			1297	802	225	258	12		
2	DF	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	FF	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	HF	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	JF	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	LF	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	NF	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	PF	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	RF	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	TF	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	VF	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	XF	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	ZF	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	PG	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	RG	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	TG	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	VG	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	YG	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	PH	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	RH	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	TH	177	Total	C	N	O	S	0	0
			1288	797	222	257	12		
2	VH	177	Total	C	N	O	S	1	0
			1278	789	225	252	12		
2	YH	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	BI	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	DI	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	FI	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	HI	177	Total	C	N	O	S	1	0
			1297	802	225	258	12		
2	JI	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	LI	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	OI	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	QI	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	SI	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	UI	177	Total	C	N	O	S	1	0
			1297	802	225	258	12		
2	WI	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	YI	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	DJ	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	FJ	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	HJ	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	JJ	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	LJ	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	NJ	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	PJ	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	RJ	177	Total	C	N	O	S	1	0
			1297	802	225	258	12		
2	TJ	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	VJ	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	XJ	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	ZJ	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	BK	177	Total	C	N	O	S	1	0
			1297	802	225	258	12		
2	DK	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	FK	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	HK	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	JK	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	LK	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	NK	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	PK	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	RK	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	TK	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	VK	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	XK	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	ZK	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	DM	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	FM	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	HM	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	JM	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	LM	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	NM	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	PM	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	RM	177	Total	C	N	O	S	1	0
			1297	802	225	258	12		
2	TM	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	VM	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	XM	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	ZM	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	PO	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	RO	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	TO	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	VO	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	YO	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	BP	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	DP	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	FP	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	HP	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	JP	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	LP	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	NP	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	PP	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	RP	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	TP	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	VP	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	XP	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	CQ	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	EQ	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	GQ	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	IQ	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	KQ	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	MQ	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	OQ	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	QQ	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	SQ	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	UQ	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	WQ	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	YQ	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	P1	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	R1	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	T1	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	V1	177	Total	C	N	O	S	2	0
			1291	797	225	257	12		
2	Y1	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	g1	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	i1	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	k1	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	m1	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	a1	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	c1	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	e1	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	P4	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	R4	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	T4	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	V4	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	Y4	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	i4	177	Total	C	N	O	S	1	0
			1297	802	225	258	12		
2	k4	177	Total	C	N	O	S	0	0
			1288	794	225	257	12		
2	m4	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	a4	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	c4	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	e4	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	g4	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	B5	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	D5	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	F5	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	H5	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	J5	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	L5	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	O5	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	Q5	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	S5	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	U5	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	W5	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	Y5	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	B7	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	D7	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	F7	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	H7	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	J7	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	L7	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	N7	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	P7	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	R7	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	T7	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	V7	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	X7	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	y8	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	18	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	q8	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	s8	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	u8	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	w8	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	B9	177	Total	C	N	O	S	0	0
			1291	799	224	256	12		
2	D9	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	F9	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	H9	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	J9	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	L9	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	O9	177	Total	C	N	O	S	0	0
			1291	799	224	256	12		
2	Q9	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	S9	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	U9	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	W9	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	Y9	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	aB	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	bB	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	dB	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	eB	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	gB	152	Total	C	N	O	S	0	0
			1101	679	194	217	11		
2	yC	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	1C	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	qC	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	sC	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	uC	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	wC	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	aE	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	cE	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	eE	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	gE	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	iE	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	kE	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	mE	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	bF	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	dF	177	Total	C	N	O	S	2	0
			1296	802	225	257	12		
2	fF	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	hF	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	jF	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	lF	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	nF	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	pF	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	rF	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	tF	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	vF	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	aG	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	cG	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	eG	177	Total	C	N	O	S	0	0
			1290	797	224	257	12		
2	gG	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	iG	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	kG	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	mG	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	gH	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	iH	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	kH	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	mH	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	aH	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	cH	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	eH	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	cJ	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	eJ	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	gJ	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	iJ	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	kJ	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	mJ	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	bK	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	dK	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	fK	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	hK	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	jK	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	lK	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	nK	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	pK	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	rK	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	tK	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	vK	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	cM	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	eM	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	gM	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	iM	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	kM	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	mM	177	Total	C	N	O	S	3	0
			1303	806	225	260	12		
2	iO	177	Total	C	N	O	S	1	0
			1297	802	225	258	12		
2	kO	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	mO	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	aO	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	cO	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	eO	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	gO	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		

- Molecule 3 is a protein called R-phycoerythrin gamma chain, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	YA	237	Total	C	N	O	S	0	0
			1832	1132	339	346	15		
3	AD	256	Total	C	N	O	S	0	0
			1979	1220	367	377	15		
3	AE	257	Total	C	N	O	S	0	0
			1987	1226	368	378	15		
3	AG	257	Total	C	N	O	S	0	0
			1987	1226	368	378	15		
3	AH	257	Total	C	N	O	S	0	0
			1987	1226	368	378	15		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	AO	257	Total	C	N	O	S	0	0
			1987	1226	368	378	15		
3	AQ	256	Total	C	N	O	S	0	0
			1979	1220	367	377	15		
3	A1	257	Total	C	N	O	S	0	0
			1987	1226	368	378	15		
3	A4	257	Total	C	N	O	S	0	0
			1987	1226	368	378	15		
3	Y7	237	Total	C	N	O	S	0	0
			1832	1132	339	346	15		

- Molecule 4 is a protein called Linker4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AB	103	Total	C	N	O	S	0	0
			781	497	130	150	4		
4	EB	103	Total	C	N	O	S	0	0
			777	492	130	150	5		

- Molecule 5 is a protein called CaRSPs1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	KB	226	Total	C	N	O	S	0	0
			1721	1085	305	322	9		
5	UB	226	Total	C	N	O	S	0	0
			1723	1086	305	323	9		

- Molecule 6 is a protein called CaRSP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	WB	134	Total	C	N	O	S	0	0
			1032	655	176	198	3		
6	cB	139	Total	C	N	O	S	0	0
			1068	675	181	210	2		

- Molecule 7 is a protein called LRH.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	AC	150	Total	C	N	O	0	0
			750	450	150	150		
7	A8	150	Total	C	N	O	0	0
			750	450	150	150		

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Mol	Chain	Residues	Atoms				AltConf	Trace
7	a8	87	Total 435	C 261	N 87	O 87	0	0
7	aC	87	Total 435	C 261	N 87	O 87	0	0

- Molecule 8 is a protein called Phycobilisome rod-core linker polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	BE	231	Total 1897	C 1212	N 332	O 349	S 4	0	0
8	BG	231	Total 1897	C 1212	N 332	O 349	S 4	0	0
8	BH	227	Total 1874	C 1197	N 328	O 345	S 4	0	0
8	BO	230	Total 1889	C 1206	N 331	O 348	S 4	0	0
8	B1	227	Total 1874	C 1197	N 328	O 345	S 4	0	0
8	B4	230	Total 1889	C 1206	N 331	O 348	S 4	0	0

- Molecule 9 is a protein called C-phycocyanin alpha subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	CE	162	Total 1228	C 773	N 209	O 240	S 6	0	0
9	EE	162	Total 1228	C 773	N 209	O 240	S 6	0	0
9	GE	162	Total 1228	C 773	N 209	O 240	S 6	0	0
9	IE	162	Total 1228	C 773	N 209	O 240	S 6	0	0
9	KE	162	Total 1228	C 773	N 209	O 240	S 6	0	0
9	ME	162	Total 1228	C 773	N 209	O 240	S 6	0	0
9	CG	162	Total 1228	C 773	N 209	O 240	S 6	0	0
9	EG	162	Total 1228	C 773	N 209	O 240	S 6	0	0
9	GG	162	Total 1228	C 773	N 209	O 240	S 6	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
9	IG	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
9	KG	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
9	MG	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
9	CH	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
9	EH	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
9	GH	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
9	IH	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
9	KH	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
9	MH	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
9	CO	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
9	EO	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
9	GO	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
9	IO	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
9	KO	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
9	MO	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
9	M1	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
9	C1	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
9	E1	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
9	G1	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
9	I1	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
9	K1	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
9	G4	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
9	I4	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
9	K4	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
9	M4	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
9	C4	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
9	E4	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		

- Molecule 10 is a protein called C-phycocyanin beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	DE	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	FE	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	HE	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	JE	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	LE	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	NE	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	DG	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	FG	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	HG	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	JG	172	Total	C	N	O	S	0	0
			1269	785	224	251	9		
10	LG	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	NG	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	DH	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	FH	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	HH	172	Total	C	N	O	S	0	0
			1262	781	221	251	9		
10	JH	172	Total	C	N	O	S	0	0
			1268	784	224	251	9		
10	LH	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	NH	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	DO	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	FO	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	HO	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	JO	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	LO	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	NO	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	L1	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	N1	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	D1	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	F1	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	H1	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	J1	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	F4	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	H4	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	J4	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	L4	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	N4	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	D4	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		

- Molecule 11 is a protein called Phycobilisome 31.8 kDa linker polypeptide, phycoerythrin-associated, rod.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	XE	324	Total	C	N	O	S	0	0
			2527	1603	431	486	7		
11	XG	324	Total	C	N	O	S	0	0
			2527	1603	431	486	7		
11	XH	324	Total	C	N	O	S	0	0
			2527	1603	431	486	7		
11	XO	324	Total	C	N	O	S	0	0
			2527	1603	431	486	7		
11	X1	324	Total	C	N	O	S	0	0
			2527	1603	431	486	7		
11	X4	324	Total	C	N	O	S	0	0
			2527	1603	431	486	7		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
XE	275	ALA	SER	conflict	UNP A0A5J4YM59
XG	275	ALA	SER	conflict	UNP A0A5J4YM59
XH	275	ALA	SER	conflict	UNP A0A5J4YM59
XO	275	ALA	SER	conflict	UNP A0A5J4YM59
X1	275	ALA	SER	conflict	UNP A0A5J4YM59
X4	275	ALA	SER	conflict	UNP A0A5J4YM59

- Molecule 12 is a protein called Phycobilisome 27.9 kDa linker polypeptide, phycoerythrin-associated, rod.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	MI	265	Total	C	N	O	S	0	0
			2079	1309	364	396	10		
12	ZI	265	Total	C	N	O	S	0	0
			2085	1313	364	398	10		

- Molecule 13 is a protein called R-phycoerythrin gamma chain, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AJ	238	Total	C	N	O	S	0	0
			1814	1122	335	342	15		
13	AM	238	Total	C	N	O	S	0	0
			1814	1122	335	342	15		
13	wF	238	Total	C	N	O	S	0	0
			1814	1122	335	342	15		
13	xF	238	Total	C	N	O	S	0	0
			1814	1122	335	342	15		
13	wK	238	Total	C	N	O	S	0	0
			1814	1122	335	342	15		
13	xK	238	Total	C	N	O	S	0	0
			1814	1122	335	342	15		

- Molecule 14 is a protein called R-phycoerythrin gamma chain, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	BJ	250	Total	C	N	O	S	0	0
			1902	1184	346	358	14		
14	BM	250	Total	C	N	O	S	0	0
			1902	1184	346	358	14		
14	yF	250	Total	C	N	O	S	0	0
			1902	1184	346	358	14		
14	yK	250	Total	C	N	O	S	0	0
			1902	1184	346	358	14		

- Molecule 15 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AL	334	Total	C	N	O	S	0	0
			2571	1683	420	455	13		
15	A6	334	Total	C	N	O	S	0	0
			2565	1678	420	454	13		
15	a6	334	Total	C	N	O	S	0	0
			2565	1678	420	454	13		
15	aL	334	Total	C	N	O	S	0	0
			2571	1683	420	455	13		

- Molecule 16 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	BL	506	Total	C	N	O	S	0	0
			3928	2571	657	688	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
16	B6	506	Total	C	N	O	S	0	0
			3928	2571	657	688	12		
16	b6	506	Total	C	N	O	S	0	0
			3928	2571	657	688	12		
16	bL	506	Total	C	N	O	S	0	0
			3934	2574	660	688	12		

- Molecule 17 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	CL	452	Total	C	N	O	S	0	0
			3474	2274	579	609	12		
17	C6	452	Total	C	N	O	S	0	0
			3474	2274	579	609	12		
17	c6	452	Total	C	N	O	S	0	0
			3474	2274	579	609	12		
17	cL	452	Total	C	N	O	S	0	0
			3474	2274	579	609	12		

- Molecule 18 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	DL	341	Total	C	N	O	S	0	0
			2699	1785	438	464	12		
18	D6	341	Total	C	N	O	S	0	0
			2699	1785	438	464	12		
18	d6	342	Total	C	N	O	S	0	0
			2703	1787	439	465	12		
18	dL	342	Total	C	N	O	S	0	0
			2703	1787	439	465	12		

- Molecule 19 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	EL	78	Total	C	N	O	0	0
			616	402	104	110		
19	E6	78	Total	C	N	O	0	0
			616	402	104	110		
19	e6	79	Total	C	N	O	0	0
			622	404	105	113		
19	eL	79	Total	C	N	O	0	0
			622	404	105	113		

- Molecule 20 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	FL	41	Total	C	N	O	S	0	0
			318	215	51	51	1		
20	F6	41	Total	C	N	O	S	0	0
			318	215	51	51	1		
20	f6	41	Total	C	N	O	S	0	0
			324	218	54	51	1		
20	fL	41	Total	C	N	O	S	0	0
			324	218	54	51	1		

- Molecule 21 is a protein called PSII_Pbs31 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	GL	152	Total	C	N	O	S	0	0
			1161	738	197	224	2		
21	G6	152	Total	C	N	O	S	0	0
			1161	738	197	224	2		
21	g6	145	Total	C	N	O	S	0	0
			1106	702	189	213	2		
21	gL	145	Total	C	N	O	S	0	0
			1106	702	189	213	2		

- Molecule 22 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	HL	66	Total	C	N	O	S	0	0
			508	340	78	88	2		
22	H6	66	Total	C	N	O	S	0	0
			508	340	78	88	2		
22	h6	65	Total	C	N	O	S	0	0
			500	336	76	86	2		
22	hL	65	Total	C	N	O	S	0	0
			500	336	76	86	2		

- Molecule 23 is a protein called Photosystem II reaction center protein I.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	IL	35	Total	C	N	O	S	0	0
			295	201	46	47	1		
23	I6	35	Total	C	N	O	S	0	0
			295	201	46	47	1		
23	i6	35	Total	C	N	O	S	0	0
			295	201	46	47	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
23	iL	35	Total	C	N	O	S	0	0
			295	201	46	47	1		

- Molecule 24 is a protein called Photosystem II reaction center protein J.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	JL	36	Total	C	N	O	0	0
			255	173	40	42		
24	J6	36	Total	C	N	O	0	0
			255	173	40	42		
24	j6	36	Total	C	N	O	0	0
			255	173	40	42		
24	jL	36	Total	C	N	O	0	0
			255	173	40	42		

- Molecule 25 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	KL	37	Total	C	N	O	0	0
			294	209	43	42		
25	K6	37	Total	C	N	O	0	0
			294	209	43	42		
25	k6	37	Total	C	N	O	0	0
			294	209	43	42		
25	kL	37	Total	C	N	O	0	0
			294	209	43	42		

- Molecule 26 is a protein called PsbL.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	LL	37	Total	C	N	O	0	0
			302	204	48	50		
26	L6	37	Total	C	N	O	0	0
			302	204	48	50		
26	l6	37	Total	C	N	O	0	0
			302	204	48	50		
26	lL	37	Total	C	N	O	0	0
			302	204	48	50		

- Molecule 27 is a protein called PsbM.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	ML	42	Total	C	N	O	S	0	0
			306	203	48	54	1		
27	M6	42	Total	C	N	O	S	0	0
			306	203	48	54	1		
27	m6	42	Total	C	N	O	S	0	0
			306	203	48	54	1		
27	mL	42	Total	C	N	O	S	0	0
			306	203	48	54	1		

- Molecule 28 is a protein called Psb34.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	NL	29	Total	C	N	O	0	0
			145	87	29	29		
28	N6	29	Total	C	N	O	0	0
			145	87	29	29		
28	n6	27	Total	C	N	O	0	0
			135	81	27	27		
28	nL	27	Total	C	N	O	0	0
			135	81	27	27		

- Molecule 29 is a protein called Oxygen-evolving enhancer protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	OL	254	Total	C	N	O	S	0	0
			1857	1167	305	376	9		
29	O6	254	Total	C	N	O	S	0	0
			1857	1167	305	376	9		
29	o6	254	Total	C	N	O	S	0	0
			1859	1168	305	377	9		
29	oL	254	Total	C	N	O	S	0	0
			1859	1168	305	377	9		

- Molecule 30 is a protein called PsbQ'.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	QL	141	Total	C	N	O	S	0	0
			1134	702	207	220	5		
30	Q6	141	Total	C	N	O	S	0	0
			1134	702	207	220	5		
30	q6	141	Total	C	N	O	S	0	0
			1134	702	207	220	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
30	qL	141	Total	C	N	O	S	0	0
			1134	702	207	220	5		

- Molecule 31 is a protein called Photosystem II protein Y.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	RL	33	Total	C	N	O	0	0
			263	175	47	41		
31	R6	33	Total	C	N	O	0	0
			263	175	47	41		
31	r6	33	Total	C	N	O	0	0
			263	175	47	41		
31	rL	33	Total	C	N	O	0	0
			263	175	47	41		

- Molecule 32 is a protein called LPP1.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	SL	119	Total	C	N	O	0	0
			595	357	119	119		
32	S6	92	Total	C	N	O	0	0
			460	276	92	92		

- Molecule 33 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	TL	31	Total	C	N	O	S	0	0
			252	177	36	37	2		
33	T6	31	Total	C	N	O	S	0	0
			252	177	36	37	2		
33	t6	31	Total	C	N	O	S	0	0
			252	177	36	37	2		
33	tL	31	Total	C	N	O	S	0	0
			252	177	36	37	2		

- Molecule 34 is a protein called PS II complex 12 kDa extrinsic protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	UL	93	Total	C	N	O	S	0	0
			726	460	120	143	3		
34	U6	93	Total	C	N	O	S	0	0
			726	460	120	143	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
34	u6	93	Total 735	C 466	N 121	O 145	S 3	0	0
34	uL	93	Total 735	C 466	N 121	O 145	S 3	0	0

- Molecule 35 is a protein called Cytochrome c550.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	VL	134	Total 980	C 615	N 168	O 193	S 4	0	0
35	V6	134	Total 980	C 615	N 168	O 193	S 4	0	0
35	v6	134	Total 980	C 615	N 168	O 193	S 4	0	0
35	vL	134	Total 980	C 615	N 168	O 193	S 4	0	0

- Molecule 36 is a protein called PsbW.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	WL	46	Total 230	C 138	N 46	O 46	0	0
36	W6	46	Total 230	C 138	N 46	O 46	0	0
36	w6	46	Total 230	C 138	N 46	O 46	0	0
36	wL	46	Total 230	C 138	N 46	O 46	0	0

- Molecule 37 is a protein called Photosystem II reaction center X protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	XL	39	Total 268	C 177	N 40	O 50	S 1	0	0
37	X6	39	Total 268	C 177	N 40	O 50	S 1	0	0
37	x6	39	Total 278	C 183	N 44	O 50	S 1	0	0
37	xL	39	Total 278	C 183	N 44	O 50	S 1	0	0

- Molecule 38 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	YL	33	Total	C	N	O	S	0	0
			251	172	40	38	1		
38	Y6	33	Total	C	N	O	S	0	0
			251	172	40	38	1		
38	y6	33	Total	C	N	O	S	0	0
			251	172	40	38	1		
38	yL	33	Total	C	N	O	S	0	0
			251	172	40	38	1		

- Molecule 39 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	ZL	59	Total	C	N	O		0	0
			438	294	67	77			
39	Z6	60	Total	C	N	O	S	0	0
			446	299	68	78	1		
39	z6	60	Total	C	N	O	S	0	0
			446	299	68	78	1		
39	zL	59	Total	C	N	O		0	0
			438	294	67	77			

- Molecule 40 is a protein called PsaA.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	AN	745	Total	C	N	O	S	0	0
			5843	3819	1000	997	27		
40	A2	745	Total	C	N	O	S	0	0
			5843	3819	1000	997	27		

- Molecule 41 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	BN	732	Total	C	N	O	S	0	0
			5828	3834	980	996	18		
41	B2	732	Total	C	N	O	S	0	0
			5828	3834	980	996	18		

- Molecule 42 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	CN	80	Total	C	N	O	S	0	0
			595	368	104	114	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
42	C2	80	Total	C	N	O	S	0	0
			595	368	104	114	9		

- Molecule 43 is a protein called Photosystem I reaction center subunit II.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	DN	130	Total	C	N	O	S	0	0
			989	627	170	189	3		
43	D2	130	Total	C	N	O	S	0	0
			989	627	170	189	3		

- Molecule 44 is a protein called Photosystem I reaction center subunit IV.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	EN	58	Total	C	N	O	0	0
			466	295	82	89		
44	E2	58	Total	C	N	O	0	0
			466	295	82	89		

- Molecule 45 is a protein called Photosystem I reaction center subunit III.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	FN	158	Total	C	N	O	S	0	0
			1245	813	207	222	3		
45	F2	158	Total	C	N	O	S	0	0
			1245	813	207	222	3		

- Molecule 46 is a protein called Cytochrome c6.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	GN	84	Total	C	N	O	S	0	0
			620	378	110	127	5		
46	G2	84	Total	C	N	O	S	0	0
			620	378	110	127	5		

- Molecule 47 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	IN	31	Total	C	N	O	S	0	0
			239	168	32	38	1		
47	I2	31	Total	C	N	O	S	0	0
			239	168	32	38	1		

- Molecule 48 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	JN	38	Total	C	N	O	S	0	0
			308	211	45	50	2		
48	J2	38	Total	C	N	O	S	0	0
			308	211	45	50	2		

- Molecule 49 is a protein called Photosystem I reaction center subunit PsaK.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	KN	70	Total	C	N	O	S	0	0
			489	315	82	89	3		
49	K2	70	Total	C	N	O	S	0	0
			489	315	82	89	3		

- Molecule 50 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	LN	140	Total	C	N	O	S	0	0
			1055	689	166	198	2		
50	L2	140	Total	C	N	O	S	0	0
			1055	689	166	198	2		

- Molecule 51 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	MN	30	Total	C	N	O	S	0	0
			223	146	35	41	1		
51	M2	30	Total	C	N	O	S	0	0
			223	146	35	41	1		

- Molecule 52 is a protein called Ferredoxin.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	NN	99	Total	C	N	O	S	0	0
			737	451	114	165	7		
52	N2	99	Total	C	N	O	S	0	0
			737	451	114	165	7		

- Molecule 53 is a protein called Photosystem I subunit O.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	ON	92	Total	C	N	O	S	0	0
			699	462	112	123	2		
53	O2	92	Total	C	N	O	S	0	0
			699	462	112	123	2		

- Molecule 54 is a protein called PsaR.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	RN	78	Total	C	N	O	S	0	0
			582	380	93	108	1		
54	R2	78	Total	C	N	O	S	0	0
			582	380	93	108	1		

- Molecule 55 is a protein called LPS1.

Mol	Chain	Residues	Atoms				AltConf	Trace
55	ZN	66	Total	C	N	O	0	0
			330	198	66	66		
55	Z2	66	Total	C	N	O	0	0
			330	198	66	66		

- Molecule 56 is a protein called Phycobilisome 31.8 kDa linker polypeptide, phycoerythrin-associated, rod.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	YP	372	Total	C	N	O	S	0	0
			2832	1780	483	557	12		
56	bP	372	Total	C	N	O	S	0	0
			2826	1777	480	557	12		

- Molecule 57 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	12	174	Total	C	N	O	S	0	0
			1330	876	208	236	10		
57	1N	174	Total	C	N	O	S	0	0
			1330	876	208	236	10		

- Molecule 58 is a protein called Chlorophyll a-b binding protein of LHCII type III, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	22	166	Total	C	N	O	S	0	0
			1229	811	192	223	3		
58	2N	166	Total	C	N	O	S	0	0
			1229	811	192	223	3		

- Molecule 59 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	32	169	Total	C	N	O	S	0	0
			1256	818	203	225	10		
59	3N	169	Total	C	N	O	S	0	0
			1256	818	203	225	10		

- Molecule 60 is a protein called Chlorophyll a-b binding protein 1B-21, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	42	172	Total	C	N	O	S	0	0
			1332	879	208	233	12		
60	4N	172	Total	C	N	O	S	0	0
			1332	879	208	233	12		

- Molecule 61 is a protein called Chlorophyll a-b binding protein 1B-21, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	52	174	Total	C	N	O	S	0	0
			1328	860	222	236	10		
61	5N	174	Total	C	N	O	S	0	0
			1328	860	222	236	10		

- Molecule 62 is a protein called Chlorophyll a-b binding protein 1B-21, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	62	169	Total	C	N	O	S	0	0
			1314	857	216	233	8		
62	6N	169	Total	C	N	O	S	0	0
			1314	857	216	233	8		

- Molecule 63 is a protein called Fucoxanthin-chlorophyll a-c binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	72	164	Total	C	N	O	S	0	0
			1270	828	209	227	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
63	7N	164	Total	C	N	O	S	0	0
			1270	828	209	227	6		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
72	?	-	LYS	deletion	UNP A0A5J4YKR2
72	?	-	THR	deletion	UNP A0A5J4YKR2
7N	?	-	LYS	deletion	UNP A0A5J4YKR2
7N	?	-	THR	deletion	UNP A0A5J4YKR2

- Molecule 64 is a protein called RedCAP.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	82	180	Total	C	N	O	S	0	0
			1378	896	232	243	7		
64	8N	180	Total	C	N	O	S	0	0
			1378	896	232	243	7		

- Molecule 65 is a protein called Lrc4.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	23	132	Total	C	N	O	S	0	0
			1004	631	179	191	3		
65	Z3	132	Total	C	N	O	S	0	0
			1004	631	179	191	3		

- Molecule 66 is a protein called LRC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	33	253	Total	C	N	O	S	0	0
			1889	1186	325	371	7		
66	a3	253	Total	C	N	O	S	0	0
			1894	1189	325	373	7		

- Molecule 67 is a protein called FAS1 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	43	206	Total	C	N	O	S	0	0
			1528	980	259	284	5		
67	b3	206	Total	C	N	O	S	0	0
			1532	982	259	286	5		

- Molecule 68 is a protein called Allophycocyanin alpha subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	A3	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		
68	C3	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		
68	E3	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		
68	G3	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		
68	J3	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		
68	K3	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		
68	N3	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		
68	P3	160	Total	C	N	O	S	0	0
			1221	766	211	237	7		
68	R3	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		
68	T3	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		
68	c3	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		
68	e3	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		
68	g3	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		
68	i3	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		
68	l3	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		
68	m3	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		
68	p3	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		
68	r3	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		
68	t3	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		
68	v3	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		

- Molecule 69 is a protein called Allophycocyanin beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	B3	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
69	D3	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
69	F3	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
69	H3	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
69	I3	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
69	L3	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
69	M3	161	Total	C	N	O	S	0	0
			1216	764	205	240	7		
69	O3	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
69	Q3	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
69	S3	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
69	U3	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
69	d3	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
69	f3	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
69	h3	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
69	j3	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
69	k3	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
69	n3	161	Total	C	N	O	S	0	0
			1217	766	206	238	7		
69	o3	161	Total	C	N	O	S	0	0
			1216	764	205	240	7		
69	q3	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
69	s3	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
69	u3	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
69	w3	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		

- Molecule 70 is a protein called Allophycocyanin gamma subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	V3	160	Total	C	N	O	S	0	0
			1260	808	207	240	5		
70	x3	160	Total	C	N	O	S	0	0
			1260	808	207	240	5		

- Molecule 71 is a protein called Allophycocyanin beta 18 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	W3	173	Total	C	N	O	S	0	0
			1376	881	230	261	4		
71	y3	173	Total	C	N	O	S	0	0
			1376	881	230	261	4		

- Molecule 72 is a protein called Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	X3	92	Total	C	N	O	S	0	0
			720	453	127	135	5		
72	z3	92	Total	C	N	O	S	0	0
			720	453	127	135	5		

- Molecule 73 is a protein called Phycobiliprotein ApcE.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	63	868	Total	C	N	O	S	0	0
			6933	4434	1198	1286	15		
73	73	865	Total	C	N	O	S	0	0
			6907	4421	1194	1277	15		

- Molecule 74 is a protein called R-phycoerythrin gamma chain, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	M5	238	Total	C	N	O	S	0	0
			1851	1140	348	348	15		
74	Z5	238	Total	C	N	O	S	0	0
			1851	1140	348	348	15		
74	Z9	275	Total	C	N	O	S	0	0
			2148	1327	404	401	16		
74	M9	275	Total	C	N	O	S	0	0
			2142	1324	401	401	16		

- Molecule 75 is a protein called Phycobilisome 31.8 kDa linker polypeptide, phycoerythrin-associated, rod.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	e7	248	Total	C	N	O	S	0	0
			1932	1217	336	369	10		
75	eA	248	Total	C	N	O	S	0	0
			1932	1217	336	369	10		

- Molecule 76 is a protein called FAS1 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	fB	285	Total	C	N	O	S	0	0
			2182	1399	369	404	10		
76	hB	285	Total	C	N	O	S	0	0
			2182	1399	369	404	10		

- Molecule 77 is a protein called Phycobilisome 27.9 kDa linker polypeptide, phycoerythrin-associated, rod.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	dD	285	Total	C	N	O	S	0	0
			2203	1367	390	435	11		
77	dQ	285	Total	C	N	O	S	0	0
			2203	1367	390	435	11		

- Molecule 78 is a protein called Phycobilisome 31.8 kDa linker polypeptide, phycoerythrin-associated, rod.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	zF	462	Total	C	N	O	S	0	0
			3610	2280	636	679	15		
78	zK	463	Total	C	N	O	S	0	0
			3622	2288	637	682	15		

- Molecule 79 is a protein called Phycobilisome 32.1 kDa linker polypeptide, phycocyanin-associated, rod.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	bJ	407	Total	C	N	O	S	0	0
			3083	1946	535	590	12		
79	bM	405	Total	C	N	O	S	0	0
			3082	1943	536	588	15		

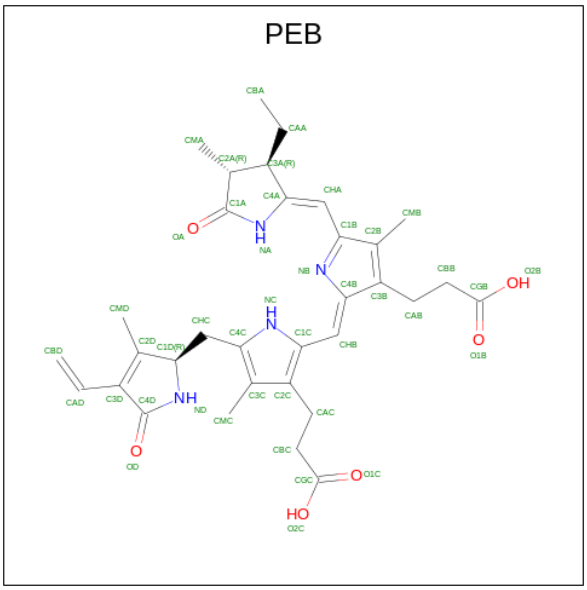
- Molecule 80 is a protein called LPP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	Y3	61	Total	C	N	O	S	0	0
			415	256	77	79	3		
80	53	57	Total	C	N	O	S	0	0
			369	230	70	66	3		

- Molecule 81 is a protein called CNT.

Mol	Chain	Residues	Atoms				AltConf	Trace
81	46	118	Total	C	N	O	0	0
			590	354	118	118		
81	16	118	Total	C	N	O	0	0
			590	354	118	118		
81	4L	118	Total	C	N	O	0	0
			590	354	118	118		
81	1L	118	Total	C	N	O	0	0
			590	354	118	118		

- Molecule 82 is PHYCOERYTHROBILIN (CCD ID: PEB) (formula: $C_{33}H_{40}N_4O_6$).



Mol	Chain	Residues	Atoms				AltConf
82	AA	1	Total	C	N	O	0
			43	33	4	6	
82	AA	1	Total	C	N	O	0
			43	33	4	6	
82	BA	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	BA	1	Total	C	N	O	0
			43	33	4	6	
82	BA	1	Total	C	N	O	0
			43	33	4	6	
82	CA	1	Total	C	N	O	0
			43	33	4	6	
82	CA	1	Total	C	N	O	0
			43	33	4	6	
82	DA	1	Total	C	N	O	0
			43	33	4	6	
82	DA	1	Total	C	N	O	0
			43	33	4	6	
82	DA	1	Total	C	N	O	0
			43	33	4	6	
82	EA	1	Total	C	N	O	0
			43	33	4	6	
82	EA	1	Total	C	N	O	0
			43	33	4	6	
82	FA	1	Total	C	N	O	0
			43	33	4	6	
82	FA	1	Total	C	N	O	0
			43	33	4	6	
82	FA	1	Total	C	N	O	0
			43	33	4	6	
82	GA	1	Total	C	N	O	0
			43	33	4	6	
82	GA	1	Total	C	N	O	0
			43	33	4	6	
82	HA	1	Total	C	N	O	0
			43	33	4	6	
82	HA	1	Total	C	N	O	0
			43	33	4	6	
82	HA	1	Total	C	N	O	0
			43	33	4	6	
82	IA	1	Total	C	N	O	0
			43	33	4	6	
82	IA	1	Total	C	N	O	0
			43	33	4	6	
82	JA	1	Total	C	N	O	0
			43	33	4	6	
82	JA	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	JA	1	Total	C	N	O	0
			43	33	4	6	
82	KA	1	Total	C	N	O	0
			43	33	4	6	
82	KA	1	Total	C	N	O	0
			43	33	4	6	
82	LA	1	Total	C	N	O	0
			43	33	4	6	
82	LA	1	Total	C	N	O	0
			43	33	4	6	
82	LA	1	Total	C	N	O	0
			43	33	4	6	
82	MA	1	Total	C	N	O	0
			43	33	4	6	
82	MA	1	Total	C	N	O	0
			43	33	4	6	
82	NA	1	Total	C	N	O	0
			43	33	4	6	
82	NA	1	Total	C	N	O	0
			43	33	4	6	
82	NA	1	Total	C	N	O	0
			43	33	4	6	
82	OA	1	Total	C	N	O	0
			43	33	4	6	
82	OA	1	Total	C	N	O	0
			43	33	4	6	
82	PA	1	Total	C	N	O	0
			43	33	4	6	
82	PA	1	Total	C	N	O	0
			43	33	4	6	
82	PA	1	Total	C	N	O	0
			43	33	4	6	
82	QA	1	Total	C	N	O	0
			43	33	4	6	
82	QA	1	Total	C	N	O	0
			43	33	4	6	
82	RA	1	Total	C	N	O	0
			43	33	4	6	
82	RA	1	Total	C	N	O	0
			43	33	4	6	
82	RA	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	SA	1	Total	C	N	O	0
			43	33	4	6	
82	SA	1	Total	C	N	O	0
			43	33	4	6	
82	TA	1	Total	C	N	O	0
			43	33	4	6	
82	TA	1	Total	C	N	O	0
			43	33	4	6	
82	TA	1	Total	C	N	O	0
			43	33	4	6	
82	UA	1	Total	C	N	O	0
			43	33	4	6	
82	UA	1	Total	C	N	O	0
			43	33	4	6	
82	VA	1	Total	C	N	O	0
			43	33	4	6	
82	VA	1	Total	C	N	O	0
			43	33	4	6	
82	VA	1	Total	C	N	O	0
			43	33	4	6	
82	WA	1	Total	C	N	O	0
			43	33	4	6	
82	WA	1	Total	C	N	O	0
			43	33	4	6	
82	XA	1	Total	C	N	O	0
			43	33	4	6	
82	XA	1	Total	C	N	O	0
			43	33	4	6	
82	XA	1	Total	C	N	O	0
			43	33	4	6	
82	YA	1	Total	C	N	O	0
			43	33	4	6	
82	YA	1	Total	C	N	O	0
			43	33	4	6	
82	YA	1	Total	C	N	O	0
			43	33	4	6	
82	AB	1	Total	C	N	O	0
			43	33	4	6	
82	BB	1	Total	C	N	O	0
			43	33	4	6	
82	BB	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	BB	1	Total	C	N	O	0
			43	33	4	6	
82	CB	1	Total	C	N	O	0
			43	33	4	6	
82	CB	1	Total	C	N	O	0
			43	33	4	6	
82	DB	1	Total	C	N	O	0
			43	33	4	6	
82	DB	1	Total	C	N	O	0
			43	33	4	6	
82	DB	1	Total	C	N	O	0
			43	33	4	6	
82	EB	1	Total	C	N	O	0
			43	33	4	6	
82	FB	1	Total	C	N	O	0
			43	33	4	6	
82	GB	1	Total	C	N	O	0
			43	33	4	6	
82	GB	1	Total	C	N	O	0
			43	33	4	6	
82	GB	1	Total	C	N	O	0
			43	33	4	6	
82	HB	1	Total	C	N	O	0
			43	33	4	6	
82	HB	1	Total	C	N	O	0
			43	33	4	6	
82	HB	1	Total	C	N	O	0
			43	33	4	6	
82	IB	1	Total	C	N	O	0
			43	33	4	6	
82	IB	1	Total	C	N	O	0
			43	33	4	6	
82	IB	1	Total	C	N	O	0
			43	33	4	6	
82	JB	1	Total	C	N	O	0
			43	33	4	6	
82	JB	1	Total	C	N	O	0
			43	33	4	6	
82	KB	1	Total	C	N	O	0
			43	33	4	6	
82	KB	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	KB	1	Total	C	N	O	0
			43	33	4	6	
82	KB	1	Total	C	N	O	0
			43	33	4	6	
82	LB	1	Total	C	N	O	0
			43	33	4	6	
82	MB	1	Total	C	N	O	0
			43	33	4	6	
82	MB	1	Total	C	N	O	0
			43	33	4	6	
82	NB	1	Total	C	N	O	0
			43	33	4	6	
82	NB	1	Total	C	N	O	0
			43	33	4	6	
82	NB	1	Total	C	N	O	0
			43	33	4	6	
82	OB	1	Total	C	N	O	0
			43	33	4	6	
82	PB	1	Total	C	N	O	0
			43	33	4	6	
82	QB	1	Total	C	N	O	0
			43	33	4	6	
82	QB	1	Total	C	N	O	0
			43	33	4	6	
82	QB	1	Total	C	N	O	0
			43	33	4	6	
82	QB	1	Total	C	N	O	0
			43	33	4	6	
82	RB	1	Total	C	N	O	0
			43	33	4	6	
82	RB	1	Total	C	N	O	0
			43	33	4	6	
82	SB	1	Total	C	N	O	0
			43	33	4	6	
82	SB	1	Total	C	N	O	0
			43	33	4	6	
82	SB	1	Total	C	N	O	0
			43	33	4	6	
82	TB	1	Total	C	N	O	0
			43	33	4	6	
82	TB	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	UB	1	Total	C	N	O	0
			43	33	4	6	
82	UB	1	Total	C	N	O	0
			43	33	4	6	
82	UB	1	Total	C	N	O	0
			43	33	4	6	
82	VB	1	Total	C	N	O	0
			43	33	4	6	
82	VB	1	Total	C	N	O	0
			43	33	4	6	
82	WB	1	Total	C	N	O	0
			43	33	4	6	
82	WB	1	Total	C	N	O	0
			43	33	4	6	
82	XB	1	Total	C	N	O	0
			43	33	4	6	
82	XB	1	Total	C	N	O	0
			43	33	4	6	
82	YB	1	Total	C	N	O	0
			43	33	4	6	
82	YB	1	Total	C	N	O	0
			43	33	4	6	
82	ZB	1	Total	C	N	O	0
			43	33	4	6	
82	ZB	1	Total	C	N	O	0
			43	33	4	6	
82	ZB	1	Total	C	N	O	0
			43	33	4	6	
82	AD	1	Total	C	N	O	0
			43	33	4	6	
82	AD	1	Total	C	N	O	0
			43	33	4	6	
82	AD	1	Total	C	N	O	0
			43	33	4	6	
82	BD	1	Total	C	N	O	0
			43	33	4	6	
82	BD	1	Total	C	N	O	0
			43	33	4	6	
82	BD	1	Total	C	N	O	0
			43	33	4	6	
82	CD	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	CD	1	Total	C	N	O	0
			43	33	4	6	
82	DD	1	Total	C	N	O	0
			43	33	4	6	
82	DD	1	Total	C	N	O	0
			43	33	4	6	
82	DD	1	Total	C	N	O	0
			43	33	4	6	
82	ED	1	Total	C	N	O	0
			43	33	4	6	
82	ED	1	Total	C	N	O	0
			43	33	4	6	
82	FD	1	Total	C	N	O	0
			43	33	4	6	
82	FD	1	Total	C	N	O	0
			43	33	4	6	
82	FD	1	Total	C	N	O	0
			43	33	4	6	
82	GD	1	Total	C	N	O	0
			43	33	4	6	
82	GD	1	Total	C	N	O	0
			43	33	4	6	
82	HD	1	Total	C	N	O	0
			43	33	4	6	
82	HD	1	Total	C	N	O	0
			43	33	4	6	
82	HD	1	Total	C	N	O	0
			43	33	4	6	
82	ID	1	Total	C	N	O	0
			43	33	4	6	
82	ID	1	Total	C	N	O	0
			43	33	4	6	
82	JD	1	Total	C	N	O	0
			43	33	4	6	
82	JD	1	Total	C	N	O	0
			43	33	4	6	
82	JD	1	Total	C	N	O	0
			43	33	4	6	
82	KD	1	Total	C	N	O	0
			43	33	4	6	
82	KD	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	LD	1	Total	C	N	O	0
			43	33	4	6	
82	LD	1	Total	C	N	O	0
			43	33	4	6	
82	LD	1	Total	C	N	O	0
			43	33	4	6	
82	MD	1	Total	C	N	O	0
			43	33	4	6	
82	MD	1	Total	C	N	O	0
			43	33	4	6	
82	ND	1	Total	C	N	O	0
			43	33	4	6	
82	ND	1	Total	C	N	O	0
			43	33	4	6	
82	ND	1	Total	C	N	O	0
			43	33	4	6	
82	OD	1	Total	C	N	O	0
			43	33	4	6	
82	OD	1	Total	C	N	O	0
			43	33	4	6	
82	PD	1	Total	C	N	O	0
			43	33	4	6	
82	PD	1	Total	C	N	O	0
			43	33	4	6	
82	PD	1	Total	C	N	O	0
			43	33	4	6	
82	QD	1	Total	C	N	O	0
			43	33	4	6	
82	QD	1	Total	C	N	O	0
			43	33	4	6	
82	RD	1	Total	C	N	O	0
			43	33	4	6	
82	RD	1	Total	C	N	O	0
			43	33	4	6	
82	RD	1	Total	C	N	O	0
			43	33	4	6	
82	SD	1	Total	C	N	O	0
			43	33	4	6	
82	SD	1	Total	C	N	O	0
			43	33	4	6	
82	TD	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	TD	1	Total	C	N	O	0
			43	33	4	6	
82	TD	1	Total	C	N	O	0
			43	33	4	6	
82	UD	1	Total	C	N	O	0
			43	33	4	6	
82	UD	1	Total	C	N	O	0
			43	33	4	6	
82	VD	1	Total	C	N	O	0
			43	33	4	6	
82	VD	1	Total	C	N	O	0
			43	33	4	6	
82	VD	1	Total	C	N	O	0
			43	33	4	6	
82	WD	1	Total	C	N	O	0
			43	33	4	6	
82	WD	1	Total	C	N	O	0
			43	33	4	6	
82	XD	1	Total	C	N	O	0
			43	33	4	6	
82	XD	1	Total	C	N	O	0
			43	33	4	6	
82	XD	1	Total	C	N	O	0
			43	33	4	6	
82	YD	1	Total	C	N	O	0
			43	33	4	6	
82	YD	1	Total	C	N	O	0
			43	33	4	6	
82	AE	1	Total	C	N	O	0
			43	33	4	6	
82	AE	1	Total	C	N	O	0
			43	33	4	6	
82	DE	1	Total	C	N	O	0
			43	33	4	6	
82	GE	1	Total	C	N	O	0
			43	33	4	6	
82	HE	1	Total	C	N	O	0
			43	33	4	6	
82	KE	1	Total	C	N	O	0
			43	33	4	6	
82	LE	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	NE	1	Total	C	N	O	0
			43	33	4	6	
82	OE	1	Total	C	N	O	0
			43	33	4	6	
82	OE	1	Total	C	N	O	0
			43	33	4	6	
82	OE	1	Total	C	N	O	0
			43	33	4	6	
82	PE	1	Total	C	N	O	0
			43	33	4	6	
82	PE	1	Total	C	N	O	0
			43	33	4	6	
82	QE	1	Total	C	N	O	0
			43	33	4	6	
82	QE	1	Total	C	N	O	0
			43	33	4	6	
82	QE	1	Total	C	N	O	0
			43	33	4	6	
82	RE	1	Total	C	N	O	0
			43	33	4	6	
82	RE	1	Total	C	N	O	0
			43	33	4	6	
82	SE	1	Total	C	N	O	0
			43	33	4	6	
82	SE	1	Total	C	N	O	0
			43	33	4	6	
82	TE	1	Total	C	N	O	0
			43	33	4	6	
82	UE	1	Total	C	N	O	0
			43	33	4	6	
82	UE	1	Total	C	N	O	0
			43	33	4	6	
82	UE	1	Total	C	N	O	0
			43	33	4	6	
82	VE	1	Total	C	N	O	0
			43	33	4	6	
82	VE	1	Total	C	N	O	0
			43	33	4	6	
82	WE	1	Total	C	N	O	0
			43	33	4	6	
82	WE	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	WE	1	Total	C	N	O	0
			43	33	4	6	
82	YE	1	Total	C	N	O	0
			43	33	4	6	
82	YE	1	Total	C	N	O	0
			43	33	4	6	
82	ZE	1	Total	C	N	O	0
			43	33	4	6	
82	ZE	1	Total	C	N	O	0
			43	33	4	6	
82	ZE	1	Total	C	N	O	0
			43	33	4	6	
82	AF	1	Total	C	N	O	0
			43	33	4	6	
82	AF	1	Total	C	N	O	0
			43	33	4	6	
82	BF	1	Total	C	N	O	0
			43	33	4	6	
82	BF	1	Total	C	N	O	0
			43	33	4	6	
82	CF	1	Total	C	N	O	0
			43	33	4	6	
82	CF	1	Total	C	N	O	0
			43	33	4	6	
82	CF	1	Total	C	N	O	0
			43	33	4	6	
82	DF	1	Total	C	N	O	0
			43	33	4	6	
82	DF	1	Total	C	N	O	0
			43	33	4	6	
82	DF	1	Total	C	N	O	0
			43	33	4	6	
82	EF	1	Total	C	N	O	0
			43	33	4	6	
82	EF	1	Total	C	N	O	0
			43	33	4	6	
82	FF	1	Total	C	N	O	0
			43	33	4	6	
82	FF	1	Total	C	N	O	0
			43	33	4	6	
82	GF	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	GF	1	Total	C	N	O	0
			43	33	4	6	
82	GF	1	Total	C	N	O	0
			43	33	4	6	
82	HF	1	Total	C	N	O	0
			43	33	4	6	
82	HF	1	Total	C	N	O	0
			43	33	4	6	
82	IF	1	Total	C	N	O	0
			43	33	4	6	
82	IF	1	Total	C	N	O	0
			43	33	4	6	
82	IF	1	Total	C	N	O	0
			43	33	4	6	
82	JF	1	Total	C	N	O	0
			43	33	4	6	
82	JF	1	Total	C	N	O	0
			43	33	4	6	
82	KF	1	Total	C	N	O	0
			43	33	4	6	
82	KF	1	Total	C	N	O	0
			43	33	4	6	
82	KF	1	Total	C	N	O	0
			43	33	4	6	
82	LF	1	Total	C	N	O	0
			43	33	4	6	
82	LF	1	Total	C	N	O	0
			43	33	4	6	
82	MF	1	Total	C	N	O	0
			43	33	4	6	
82	MF	1	Total	C	N	O	0
			43	33	4	6	
82	MF	1	Total	C	N	O	0
			43	33	4	6	
82	NF	1	Total	C	N	O	0
			43	33	4	6	
82	NF	1	Total	C	N	O	0
			43	33	4	6	
82	OF	1	Total	C	N	O	0
			43	33	4	6	
82	OF	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	OF	1	Total	C	N	O	0
			43	33	4	6	
82	PF	1	Total	C	N	O	0
			43	33	4	6	
82	PF	1	Total	C	N	O	0
			43	33	4	6	
82	QF	1	Total	C	N	O	0
			43	33	4	6	
82	QF	1	Total	C	N	O	0
			43	33	4	6	
82	QF	1	Total	C	N	O	0
			43	33	4	6	
82	RF	1	Total	C	N	O	0
			43	33	4	6	
82	RF	1	Total	C	N	O	0
			43	33	4	6	
82	SF	1	Total	C	N	O	0
			43	33	4	6	
82	SF	1	Total	C	N	O	0
			43	33	4	6	
82	SF	1	Total	C	N	O	0
			43	33	4	6	
82	TF	1	Total	C	N	O	0
			43	33	4	6	
82	TF	1	Total	C	N	O	0
			43	33	4	6	
82	UF	1	Total	C	N	O	0
			43	33	4	6	
82	UF	1	Total	C	N	O	0
			43	33	4	6	
82	VF	1	Total	C	N	O	0
			43	33	4	6	
82	VF	1	Total	C	N	O	0
			43	33	4	6	
82	WF	1	Total	C	N	O	0
			43	33	4	6	
82	WF	1	Total	C	N	O	0
			43	33	4	6	
82	WF	1	Total	C	N	O	0
			43	33	4	6	
82	XF	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	XF	1	Total	C	N	O	0
			43	33	4	6	
82	XF	1	Total	C	N	O	0
			43	33	4	6	
82	YF	1	Total	C	N	O	0
			43	33	4	6	
82	YF	1	Total	C	N	O	0
			43	33	4	6	
82	YF	1	Total	C	N	O	0
			43	33	4	6	
82	ZF	1	Total	C	N	O	0
			43	33	4	6	
82	ZF	1	Total	C	N	O	0
			43	33	4	6	
82	AG	1	Total	C	N	O	0
			43	33	4	6	
82	AG	1	Total	C	N	O	0
			43	33	4	6	
82	DG	1	Total	C	N	O	0
			43	33	4	6	
82	GG	1	Total	C	N	O	0
			43	33	4	6	
82	HG	1	Total	C	N	O	0
			43	33	4	6	
82	KG	1	Total	C	N	O	0
			43	33	4	6	
82	LG	1	Total	C	N	O	0
			43	33	4	6	
82	NG	1	Total	C	N	O	0
			43	33	4	6	
82	OG	1	Total	C	N	O	0
			43	33	4	6	
82	OG	1	Total	C	N	O	0
			43	33	4	6	
82	OG	1	Total	C	N	O	0
			43	33	4	6	
82	PG	1	Total	C	N	O	0
			43	33	4	6	
82	PG	1	Total	C	N	O	0
			43	33	4	6	
82	QG	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	QG	1	Total	C	N	O	0
			43	33	4	6	
82	QG	1	Total	C	N	O	0
			43	33	4	6	
82	RG	1	Total	C	N	O	0
			43	33	4	6	
82	RG	1	Total	C	N	O	0
			43	33	4	6	
82	SG	1	Total	C	N	O	0
			43	33	4	6	
82	SG	1	Total	C	N	O	0
			43	33	4	6	
82	SG	1	Total	C	N	O	0
			43	33	4	6	
82	TG	1	Total	C	N	O	0
			43	33	4	6	
82	UG	1	Total	C	N	O	0
			43	33	4	6	
82	UG	1	Total	C	N	O	0
			43	33	4	6	
82	UG	1	Total	C	N	O	0
			43	33	4	6	
82	VG	1	Total	C	N	O	0
			43	33	4	6	
82	VG	1	Total	C	N	O	0
			43	33	4	6	
82	WG	1	Total	C	N	O	0
			43	33	4	6	
82	WG	1	Total	C	N	O	0
			43	33	4	6	
82	WG	1	Total	C	N	O	0
			43	33	4	6	
82	YG	1	Total	C	N	O	0
			43	33	4	6	
82	YG	1	Total	C	N	O	0
			43	33	4	6	
82	ZG	1	Total	C	N	O	0
			43	33	4	6	
82	ZG	1	Total	C	N	O	0
			43	33	4	6	
82	ZG	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	AH	1	Total	C	N	O	0
			43	33	4	6	
82	AH	1	Total	C	N	O	0
			43	33	4	6	
82	AH	1	Total	C	N	O	0
			43	33	4	6	
82	DH	1	Total	C	N	O	0
			43	33	4	6	
82	FH	1	Total	C	N	O	0
			43	33	4	6	
82	HH	1	Total	C	N	O	0
			43	33	4	6	
82	JH	1	Total	C	N	O	0
			43	33	4	6	
82	LH	1	Total	C	N	O	0
			43	33	4	6	
82	NH	1	Total	C	N	O	0
			43	33	4	6	
82	OH	1	Total	C	N	O	0
			43	33	4	6	
82	OH	1	Total	C	N	O	0
			43	33	4	6	
82	OH	1	Total	C	N	O	0
			43	33	4	6	
82	PH	1	Total	C	N	O	0
			43	33	4	6	
82	PH	1	Total	C	N	O	0
			43	33	4	6	
82	QH	1	Total	C	N	O	0
			43	33	4	6	
82	QH	1	Total	C	N	O	0
			43	33	4	6	
82	QH	1	Total	C	N	O	0
			43	33	4	6	
82	RH	1	Total	C	N	O	0
			43	33	4	6	
82	RH	1	Total	C	N	O	0
			43	33	4	6	
82	SH	1	Total	C	N	O	0
			43	33	4	6	
82	SH	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	SH	1	Total	C	N	O	0
			43	33	4	6	
82	TH	1	Total	C	N	O	0
			43	33	4	6	
82	TH	1	Total	C	N	O	0
			43	33	4	6	
82	UH	1	Total	C	N	O	0
			43	33	4	6	
82	UH	1	Total	C	N	O	0
			43	33	4	6	
82	UH	1	Total	C	N	O	0
			43	33	4	6	
82	VH	1	Total	C	N	O	0
			43	33	4	6	
82	VH	1	Total	C	N	O	0
			43	33	4	6	
82	WH	1	Total	C	N	O	0
			43	33	4	6	
82	WH	1	Total	C	N	O	0
			43	33	4	6	
82	WH	1	Total	C	N	O	0
			43	33	4	6	
82	YH	1	Total	C	N	O	0
			43	33	4	6	
82	YH	1	Total	C	N	O	0
			43	33	4	6	
82	ZH	1	Total	C	N	O	0
			43	33	4	6	
82	ZH	1	Total	C	N	O	0
			43	33	4	6	
82	ZH	1	Total	C	N	O	0
			43	33	4	6	
82	AI	1	Total	C	N	O	0
			43	33	4	6	
82	AI	1	Total	C	N	O	0
			43	33	4	6	
82	AI	1	Total	C	N	O	0
			43	33	4	6	
82	BI	1	Total	C	N	O	0
			43	33	4	6	
82	BI	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	BI	1	Total	C	N	O	0
			43	33	4	6	
82	CI	1	Total	C	N	O	0
			43	33	4	6	
82	CI	1	Total	C	N	O	0
			43	33	4	6	
82	DI	1	Total	C	N	O	0
			43	33	4	6	
82	DI	1	Total	C	N	O	0
			43	33	4	6	
82	EI	1	Total	C	N	O	0
			43	33	4	6	
82	EI	1	Total	C	N	O	0
			43	33	4	6	
82	FI	1	Total	C	N	O	0
			43	33	4	6	
82	FI	1	Total	C	N	O	0
			43	33	4	6	
82	GI	1	Total	C	N	O	0
			43	33	4	6	
82	GI	1	Total	C	N	O	0
			43	33	4	6	
82	GI	1	Total	C	N	O	0
			43	33	4	6	
82	HI	1	Total	C	N	O	0
			43	33	4	6	
82	HI	1	Total	C	N	O	0
			43	33	4	6	
82	HI	1	Total	C	N	O	0
			43	33	4	6	
82	II	1	Total	C	N	O	0
			43	33	4	6	
82	II	1	Total	C	N	O	0
			43	33	4	6	
82	II	1	Total	C	N	O	0
			43	33	4	6	
82	JI	1	Total	C	N	O	0
			43	33	4	6	
82	JI	1	Total	C	N	O	0
			43	33	4	6	
82	KI	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	KI	1	Total	C	N	O	0
			43	33	4	6	
82	KI	1	Total	C	N	O	0
			43	33	4	6	
82	LI	1	Total	C	N	O	0
			43	33	4	6	
82	LI	1	Total	C	N	O	0
			43	33	4	6	
82	MI	1	Total	C	N	O	0
			43	33	4	6	
82	NI	1	Total	C	N	O	0
			43	33	4	6	
82	NI	1	Total	C	N	O	0
			43	33	4	6	
82	NI	1	Total	C	N	O	0
			43	33	4	6	
82	OI	1	Total	C	N	O	0
			43	33	4	6	
82	OI	1	Total	C	N	O	0
			43	33	4	6	
82	OI	1	Total	C	N	O	0
			43	33	4	6	
82	PI	1	Total	C	N	O	0
			43	33	4	6	
82	PI	1	Total	C	N	O	0
			43	33	4	6	
82	QI	1	Total	C	N	O	0
			43	33	4	6	
82	RI	1	Total	C	N	O	0
			43	33	4	6	
82	RI	1	Total	C	N	O	0
			43	33	4	6	
82	RI	1	Total	C	N	O	0
			43	33	4	6	
82	SI	1	Total	C	N	O	0
			43	33	4	6	
82	SI	1	Total	C	N	O	0
			43	33	4	6	
82	TI	1	Total	C	N	O	0
			43	33	4	6	
82	TI	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	TI	1	Total	C	N	O	0
			43	33	4	6	
82	UI	1	Total	C	N	O	0
			43	33	4	6	
82	UI	1	Total	C	N	O	0
			43	33	4	6	
82	VI	1	Total	C	N	O	0
			43	33	4	6	
82	VI	1	Total	C	N	O	0
			43	33	4	6	
82	VI	1	Total	C	N	O	0
			43	33	4	6	
82	WI	1	Total	C	N	O	0
			43	33	4	6	
82	WI	1	Total	C	N	O	0
			43	33	4	6	
82	WI	1	Total	C	N	O	0
			43	33	4	6	
82	XI	1	Total	C	N	O	0
			43	33	4	6	
82	XI	1	Total	C	N	O	0
			43	33	4	6	
82	YI	1	Total	C	N	O	0
			43	33	4	6	
82	YI	1	Total	C	N	O	0
			43	33	4	6	
82	ZI	1	Total	C	N	O	0
			43	33	4	6	
82	AJ	1	Total	C	N	O	0
			43	33	4	6	
82	AJ	1	Total	C	N	O	0
			43	33	4	6	
82	BJ	1	Total	C	N	O	0
			43	33	4	6	
82	CJ	1	Total	C	N	O	0
			43	33	4	6	
82	CJ	1	Total	C	N	O	0
			43	33	4	6	
82	CJ	1	Total	C	N	O	0
			43	33	4	6	
82	DJ	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	DJ	1	Total	C	N	O	0
			43	33	4	6	
82	EJ	1	Total	C	N	O	0
			43	33	4	6	
82	EJ	1	Total	C	N	O	0
			43	33	4	6	
82	EJ	1	Total	C	N	O	0
			43	33	4	6	
82	FJ	1	Total	C	N	O	0
			43	33	4	6	
82	FJ	1	Total	C	N	O	0
			43	33	4	6	
82	GJ	1	Total	C	N	O	0
			43	33	4	6	
82	GJ	1	Total	C	N	O	0
			43	33	4	6	
82	GJ	1	Total	C	N	O	0
			43	33	4	6	
82	HJ	1	Total	C	N	O	0
			43	33	4	6	
82	HJ	1	Total	C	N	O	0
			43	33	4	6	
82	IJ	1	Total	C	N	O	0
			43	33	4	6	
82	IJ	1	Total	C	N	O	0
			43	33	4	6	
82	IJ	1	Total	C	N	O	0
			43	33	4	6	
82	JJ	1	Total	C	N	O	0
			43	33	4	6	
82	JJ	1	Total	C	N	O	0
			43	33	4	6	
82	KJ	1	Total	C	N	O	0
			43	33	4	6	
82	KJ	1	Total	C	N	O	0
			43	33	4	6	
82	KJ	1	Total	C	N	O	0
			43	33	4	6	
82	LJ	1	Total	C	N	O	0
			43	33	4	6	
82	LJ	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	MJ	1	Total	C	N	O	0
			43	33	4	6	
82	MJ	1	Total	C	N	O	0
			43	33	4	6	
82	MJ	1	Total	C	N	O	0
			43	33	4	6	
82	NJ	1	Total	C	N	O	0
			43	33	4	6	
82	NJ	1	Total	C	N	O	0
			43	33	4	6	
82	OJ	1	Total	C	N	O	0
			43	33	4	6	
82	OJ	1	Total	C	N	O	0
			43	33	4	6	
82	OJ	1	Total	C	N	O	0
			43	33	4	6	
82	PJ	1	Total	C	N	O	0
			43	33	4	6	
82	PJ	1	Total	C	N	O	0
			43	33	4	6	
82	QJ	1	Total	C	N	O	0
			43	33	4	6	
82	QJ	1	Total	C	N	O	0
			43	33	4	6	
82	QJ	1	Total	C	N	O	0
			43	33	4	6	
82	RJ	1	Total	C	N	O	0
			43	33	4	6	
82	RJ	1	Total	C	N	O	0
			43	33	4	6	
82	SJ	1	Total	C	N	O	0
			43	33	4	6	
82	SJ	1	Total	C	N	O	0
			43	33	4	6	
82	SJ	1	Total	C	N	O	0
			43	33	4	6	
82	TJ	1	Total	C	N	O	0
			43	33	4	6	
82	TJ	1	Total	C	N	O	0
			43	33	4	6	
82	UJ	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	UJ	1	Total	C	N	O	0
			43	33	4	6	
82	UJ	1	Total	C	N	O	0
			43	33	4	6	
82	VJ	1	Total	C	N	O	0
			43	33	4	6	
82	VJ	1	Total	C	N	O	0
			43	33	4	6	
82	WJ	1	Total	C	N	O	0
			43	33	4	6	
82	WJ	1	Total	C	N	O	0
			43	33	4	6	
82	WJ	1	Total	C	N	O	0
			43	33	4	6	
82	XJ	1	Total	C	N	O	0
			43	33	4	6	
82	XJ	1	Total	C	N	O	0
			43	33	4	6	
82	YJ	1	Total	C	N	O	0
			43	33	4	6	
82	YJ	1	Total	C	N	O	0
			43	33	4	6	
82	YJ	1	Total	C	N	O	0
			43	33	4	6	
82	ZJ	1	Total	C	N	O	0
			43	33	4	6	
82	ZJ	1	Total	C	N	O	0
			43	33	4	6	
82	AK	1	Total	C	N	O	0
			43	33	4	6	
82	AK	1	Total	C	N	O	0
			43	33	4	6	
82	BK	1	Total	C	N	O	0
			43	33	4	6	
82	BK	1	Total	C	N	O	0
			43	33	4	6	
82	CK	1	Total	C	N	O	0
			43	33	4	6	
82	CK	1	Total	C	N	O	0
			43	33	4	6	
82	CK	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	DK	1	Total	C	N	O	0
			43	33	4	6	
82	DK	1	Total	C	N	O	0
			43	33	4	6	
82	DK	1	Total	C	N	O	0
			43	33	4	6	
82	EK	1	Total	C	N	O	0
			43	33	4	6	
82	EK	1	Total	C	N	O	0
			43	33	4	6	
82	FK	1	Total	C	N	O	0
			43	33	4	6	
82	FK	1	Total	C	N	O	0
			43	33	4	6	
82	GK	1	Total	C	N	O	0
			43	33	4	6	
82	GK	1	Total	C	N	O	0
			43	33	4	6	
82	GK	1	Total	C	N	O	0
			43	33	4	6	
82	HK	1	Total	C	N	O	0
			43	33	4	6	
82	HK	1	Total	C	N	O	0
			43	33	4	6	
82	IK	1	Total	C	N	O	0
			43	33	4	6	
82	IK	1	Total	C	N	O	0
			43	33	4	6	
82	IK	1	Total	C	N	O	0
			43	33	4	6	
82	JK	1	Total	C	N	O	0
			43	33	4	6	
82	JK	1	Total	C	N	O	0
			43	33	4	6	
82	KK	1	Total	C	N	O	0
			43	33	4	6	
82	KK	1	Total	C	N	O	0
			43	33	4	6	
82	KK	1	Total	C	N	O	0
			43	33	4	6	
82	LK	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	LK	1	Total	C	N	O	0
			43	33	4	6	
82	MK	1	Total	C	N	O	0
			43	33	4	6	
82	MK	1	Total	C	N	O	0
			43	33	4	6	
82	MK	1	Total	C	N	O	0
			43	33	4	6	
82	NK	1	Total	C	N	O	0
			43	33	4	6	
82	NK	1	Total	C	N	O	0
			43	33	4	6	
82	OK	1	Total	C	N	O	0
			43	33	4	6	
82	OK	1	Total	C	N	O	0
			43	33	4	6	
82	OK	1	Total	C	N	O	0
			43	33	4	6	
82	PK	1	Total	C	N	O	0
			43	33	4	6	
82	PK	1	Total	C	N	O	0
			43	33	4	6	
82	QK	1	Total	C	N	O	0
			43	33	4	6	
82	QK	1	Total	C	N	O	0
			43	33	4	6	
82	QK	1	Total	C	N	O	0
			43	33	4	6	
82	RK	1	Total	C	N	O	0
			43	33	4	6	
82	RK	1	Total	C	N	O	0
			43	33	4	6	
82	SK	1	Total	C	N	O	0
			43	33	4	6	
82	SK	1	Total	C	N	O	0
			43	33	4	6	
82	SK	1	Total	C	N	O	0
			43	33	4	6	
82	TK	1	Total	C	N	O	0
			43	33	4	6	
82	TK	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	UK	1	Total	C	N	O	0
			43	33	4	6	
82	UK	1	Total	C	N	O	0
			43	33	4	6	
82	VK	1	Total	C	N	O	0
			43	33	4	6	
82	VK	1	Total	C	N	O	0
			43	33	4	6	
82	WK	1	Total	C	N	O	0
			43	33	4	6	
82	WK	1	Total	C	N	O	0
			43	33	4	6	
82	WK	1	Total	C	N	O	0
			43	33	4	6	
82	XK	1	Total	C	N	O	0
			43	33	4	6	
82	XK	1	Total	C	N	O	0
			43	33	4	6	
82	XK	1	Total	C	N	O	0
			43	33	4	6	
82	YK	1	Total	C	N	O	0
			43	33	4	6	
82	YK	1	Total	C	N	O	0
			43	33	4	6	
82	YK	1	Total	C	N	O	0
			43	33	4	6	
82	ZK	1	Total	C	N	O	0
			43	33	4	6	
82	ZK	1	Total	C	N	O	0
			43	33	4	6	
82	AM	1	Total	C	N	O	0
			43	33	4	6	
82	AM	1	Total	C	N	O	0
			43	33	4	6	
82	BM	1	Total	C	N	O	0
			43	33	4	6	
82	CM	1	Total	C	N	O	0
			43	33	4	6	
82	CM	1	Total	C	N	O	0
			43	33	4	6	
82	CM	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	DM	1	Total	C	N	O	0
			43	33	4	6	
82	DM	1	Total	C	N	O	0
			43	33	4	6	
82	EM	1	Total	C	N	O	0
			43	33	4	6	
82	EM	1	Total	C	N	O	0
			43	33	4	6	
82	EM	1	Total	C	N	O	0
			43	33	4	6	
82	FM	1	Total	C	N	O	0
			43	33	4	6	
82	FM	1	Total	C	N	O	0
			43	33	4	6	
82	GM	1	Total	C	N	O	0
			43	33	4	6	
82	GM	1	Total	C	N	O	0
			43	33	4	6	
82	GM	1	Total	C	N	O	0
			43	33	4	6	
82	HM	1	Total	C	N	O	0
			43	33	4	6	
82	HM	1	Total	C	N	O	0
			43	33	4	6	
82	IM	1	Total	C	N	O	0
			43	33	4	6	
82	IM	1	Total	C	N	O	0
			43	33	4	6	
82	IM	1	Total	C	N	O	0
			43	33	4	6	
82	JM	1	Total	C	N	O	0
			43	33	4	6	
82	JM	1	Total	C	N	O	0
			43	33	4	6	
82	KM	1	Total	C	N	O	0
			43	33	4	6	
82	KM	1	Total	C	N	O	0
			43	33	4	6	
82	KM	1	Total	C	N	O	0
			43	33	4	6	
82	LM	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	LM	1	Total	C	N	O	0
			43	33	4	6	
82	MM	1	Total	C	N	O	0
			43	33	4	6	
82	MM	1	Total	C	N	O	0
			43	33	4	6	
82	MM	1	Total	C	N	O	0
			43	33	4	6	
82	NM	1	Total	C	N	O	0
			43	33	4	6	
82	NM	1	Total	C	N	O	0
			43	33	4	6	
82	OM	1	Total	C	N	O	0
			43	33	4	6	
82	OM	1	Total	C	N	O	0
			43	33	4	6	
82	OM	1	Total	C	N	O	0
			43	33	4	6	
82	PM	1	Total	C	N	O	0
			43	33	4	6	
82	PM	1	Total	C	N	O	0
			43	33	4	6	
82	QM	1	Total	C	N	O	0
			43	33	4	6	
82	QM	1	Total	C	N	O	0
			43	33	4	6	
82	QM	1	Total	C	N	O	0
			43	33	4	6	
82	RM	1	Total	C	N	O	0
			43	33	4	6	
82	RM	1	Total	C	N	O	0
			43	33	4	6	
82	SM	1	Total	C	N	O	0
			43	33	4	6	
82	SM	1	Total	C	N	O	0
			43	33	4	6	
82	SM	1	Total	C	N	O	0
			43	33	4	6	
82	TM	1	Total	C	N	O	0
			43	33	4	6	
82	TM	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	UM	1	Total	C	N	O	0
			43	33	4	6	
82	UM	1	Total	C	N	O	0
			43	33	4	6	
82	UM	1	Total	C	N	O	0
			43	33	4	6	
82	VM	1	Total	C	N	O	0
			43	33	4	6	
82	VM	1	Total	C	N	O	0
			43	33	4	6	
82	WM	1	Total	C	N	O	0
			43	33	4	6	
82	WM	1	Total	C	N	O	0
			43	33	4	6	
82	WM	1	Total	C	N	O	0
			43	33	4	6	
82	XM	1	Total	C	N	O	0
			43	33	4	6	
82	XM	1	Total	C	N	O	0
			43	33	4	6	
82	YM	1	Total	C	N	O	0
			43	33	4	6	
82	YM	1	Total	C	N	O	0
			43	33	4	6	
82	YM	1	Total	C	N	O	0
			43	33	4	6	
82	ZM	1	Total	C	N	O	0
			43	33	4	6	
82	ZM	1	Total	C	N	O	0
			43	33	4	6	
82	AO	1	Total	C	N	O	0
			43	33	4	6	
82	AO	1	Total	C	N	O	0
			43	33	4	6	
82	AO	1	Total	C	N	O	0
			43	33	4	6	
82	DO	1	Total	C	N	O	0
			43	33	4	6	
82	FO	1	Total	C	N	O	0
			43	33	4	6	
82	HO	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	JO	1	Total	C	N	O	0
			43	33	4	6	
82	LO	1	Total	C	N	O	0
			43	33	4	6	
82	NO	1	Total	C	N	O	0
			43	33	4	6	
82	OO	1	Total	C	N	O	0
			43	33	4	6	
82	OO	1	Total	C	N	O	0
			43	33	4	6	
82	PO	1	Total	C	N	O	0
			43	33	4	6	
82	PO	1	Total	C	N	O	0
			43	33	4	6	
82	PO	1	Total	C	N	O	0
			43	33	4	6	
82	QO	1	Total	C	N	O	0
			43	33	4	6	
82	QO	1	Total	C	N	O	0
			43	33	4	6	
82	RO	1	Total	C	N	O	0
			43	33	4	6	
82	RO	1	Total	C	N	O	0
			43	33	4	6	
82	RO	1	Total	C	N	O	0
			43	33	4	6	
82	SO	1	Total	C	N	O	0
			43	33	4	6	
82	SO	1	Total	C	N	O	0
			43	33	4	6	
82	TO	1	Total	C	N	O	0
			43	33	4	6	
82	TO	1	Total	C	N	O	0
			43	33	4	6	
82	TO	1	Total	C	N	O	0
			43	33	4	6	
82	UO	1	Total	C	N	O	0
			43	33	4	6	
82	UO	1	Total	C	N	O	0
			43	33	4	6	
82	VO	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	VO	1	Total	C	N	O	0
			43	33	4	6	
82	WO	1	Total	C	N	O	0
			43	33	4	6	
82	YO	1	Total	C	N	O	0
			43	33	4	6	
82	YO	1	Total	C	N	O	0
			43	33	4	6	
82	YO	1	Total	C	N	O	0
			43	33	4	6	
82	ZO	1	Total	C	N	O	0
			43	33	4	6	
82	ZO	1	Total	C	N	O	0
			43	33	4	6	
82	AP	1	Total	C	N	O	0
			43	33	4	6	
82	AP	1	Total	C	N	O	0
			43	33	4	6	
82	AP	1	Total	C	N	O	0
			43	33	4	6	
82	BP	1	Total	C	N	O	0
			43	33	4	6	
82	BP	1	Total	C	N	O	0
			43	33	4	6	
82	CP	1	Total	C	N	O	0
			43	33	4	6	
82	CP	1	Total	C	N	O	0
			43	33	4	6	
82	CP	1	Total	C	N	O	0
			43	33	4	6	
82	DP	1	Total	C	N	O	0
			43	33	4	6	
82	DP	1	Total	C	N	O	0
			43	33	4	6	
82	EP	1	Total	C	N	O	0
			43	33	4	6	
82	EP	1	Total	C	N	O	0
			43	33	4	6	
82	EP	1	Total	C	N	O	0
			43	33	4	6	
82	FP	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	FP	1	Total	C	N	O	0
			43	33	4	6	
82	GP	1	Total	C	N	O	0
			43	33	4	6	
82	GP	1	Total	C	N	O	0
			43	33	4	6	
82	GP	1	Total	C	N	O	0
			43	33	4	6	
82	HP	1	Total	C	N	O	0
			43	33	4	6	
82	HP	1	Total	C	N	O	0
			43	33	4	6	
82	IP	1	Total	C	N	O	0
			43	33	4	6	
82	IP	1	Total	C	N	O	0
			43	33	4	6	
82	IP	1	Total	C	N	O	0
			43	33	4	6	
82	JP	1	Total	C	N	O	0
			43	33	4	6	
82	JP	1	Total	C	N	O	0
			43	33	4	6	
82	KP	1	Total	C	N	O	0
			43	33	4	6	
82	KP	1	Total	C	N	O	0
			43	33	4	6	
82	LP	1	Total	C	N	O	0
			43	33	4	6	
82	LP	1	Total	C	N	O	0
			43	33	4	6	
82	MP	1	Total	C	N	O	0
			43	33	4	6	
82	MP	1	Total	C	N	O	0
			43	33	4	6	
82	MP	1	Total	C	N	O	0
			43	33	4	6	
82	NP	1	Total	C	N	O	0
			43	33	4	6	
82	NP	1	Total	C	N	O	0
			43	33	4	6	
82	OP	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	OP	1	Total	C	N	O	0
			43	33	4	6	
82	OP	1	Total	C	N	O	0
			43	33	4	6	
82	PP	1	Total	C	N	O	0
			43	33	4	6	
82	PP	1	Total	C	N	O	0
			43	33	4	6	
82	QP	1	Total	C	N	O	0
			43	33	4	6	
82	QP	1	Total	C	N	O	0
			43	33	4	6	
82	QP	1	Total	C	N	O	0
			43	33	4	6	
82	RP	1	Total	C	N	O	0
			43	33	4	6	
82	RP	1	Total	C	N	O	0
			43	33	4	6	
82	SP	1	Total	C	N	O	0
			43	33	4	6	
82	SP	1	Total	C	N	O	0
			43	33	4	6	
82	SP	1	Total	C	N	O	0
			43	33	4	6	
82	TP	1	Total	C	N	O	0
			43	33	4	6	
82	TP	1	Total	C	N	O	0
			43	33	4	6	
82	UP	1	Total	C	N	O	0
			43	33	4	6	
82	UP	1	Total	C	N	O	0
			43	33	4	6	
82	UP	1	Total	C	N	O	0
			43	33	4	6	
82	VP	1	Total	C	N	O	0
			43	33	4	6	
82	VP	1	Total	C	N	O	0
			43	33	4	6	
82	WP	1	Total	C	N	O	0
			43	33	4	6	
82	WP	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	XP	1	Total	C	N	O	0
			43	33	4	6	
82	XP	1	Total	C	N	O	0
			43	33	4	6	
82	YP	1	Total	C	N	O	0
			43	33	4	6	
82	YP	1	Total	C	N	O	0
			43	33	4	6	
82	YP	1	Total	C	N	O	0
			43	33	4	6	
82	AQ	1	Total	C	N	O	0
			43	33	4	6	
82	AQ	1	Total	C	N	O	0
			43	33	4	6	
82	AQ	1	Total	C	N	O	0
			43	33	4	6	
82	BQ	1	Total	C	N	O	0
			43	33	4	6	
82	BQ	1	Total	C	N	O	0
			43	33	4	6	
82	BQ	1	Total	C	N	O	0
			43	33	4	6	
82	CQ	1	Total	C	N	O	0
			43	33	4	6	
82	CQ	1	Total	C	N	O	0
			43	33	4	6	
82	DQ	1	Total	C	N	O	0
			43	33	4	6	
82	DQ	1	Total	C	N	O	0
			43	33	4	6	
82	DQ	1	Total	C	N	O	0
			43	33	4	6	
82	EQ	1	Total	C	N	O	0
			43	33	4	6	
82	EQ	1	Total	C	N	O	0
			43	33	4	6	
82	FQ	1	Total	C	N	O	0
			43	33	4	6	
82	FQ	1	Total	C	N	O	0
			43	33	4	6	
82	FQ	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	GQ	1	Total	C	N	O	0
			43	33	4	6	
82	GQ	1	Total	C	N	O	0
			43	33	4	6	
82	HQ	1	Total	C	N	O	0
			43	33	4	6	
82	HQ	1	Total	C	N	O	0
			43	33	4	6	
82	HQ	1	Total	C	N	O	0
			43	33	4	6	
82	IQ	1	Total	C	N	O	0
			43	33	4	6	
82	IQ	1	Total	C	N	O	0
			43	33	4	6	
82	JQ	1	Total	C	N	O	0
			43	33	4	6	
82	JQ	1	Total	C	N	O	0
			43	33	4	6	
82	JQ	1	Total	C	N	O	0
			43	33	4	6	
82	KQ	1	Total	C	N	O	0
			43	33	4	6	
82	KQ	1	Total	C	N	O	0
			43	33	4	6	
82	LQ	1	Total	C	N	O	0
			43	33	4	6	
82	LQ	1	Total	C	N	O	0
			43	33	4	6	
82	LQ	1	Total	C	N	O	0
			43	33	4	6	
82	MQ	1	Total	C	N	O	0
			43	33	4	6	
82	MQ	1	Total	C	N	O	0
			43	33	4	6	
82	NQ	1	Total	C	N	O	0
			43	33	4	6	
82	NQ	1	Total	C	N	O	0
			43	33	4	6	
82	NQ	1	Total	C	N	O	0
			43	33	4	6	
82	OQ	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	OQ	1	Total	C	N	O	0
			43	33	4	6	
82	PQ	1	Total	C	N	O	0
			43	33	4	6	
82	PQ	1	Total	C	N	O	0
			43	33	4	6	
82	PQ	1	Total	C	N	O	0
			43	33	4	6	
82	QQ	1	Total	C	N	O	0
			43	33	4	6	
82	QQ	1	Total	C	N	O	0
			43	33	4	6	
82	RQ	1	Total	C	N	O	0
			43	33	4	6	
82	RQ	1	Total	C	N	O	0
			43	33	4	6	
82	RQ	1	Total	C	N	O	0
			43	33	4	6	
82	SQ	1	Total	C	N	O	0
			43	33	4	6	
82	SQ	1	Total	C	N	O	0
			43	33	4	6	
82	TQ	1	Total	C	N	O	0
			43	33	4	6	
82	TQ	1	Total	C	N	O	0
			43	33	4	6	
82	TQ	1	Total	C	N	O	0
			43	33	4	6	
82	UQ	1	Total	C	N	O	0
			43	33	4	6	
82	UQ	1	Total	C	N	O	0
			43	33	4	6	
82	VQ	1	Total	C	N	O	0
			43	33	4	6	
82	VQ	1	Total	C	N	O	0
			43	33	4	6	
82	VQ	1	Total	C	N	O	0
			43	33	4	6	
82	WQ	1	Total	C	N	O	0
			43	33	4	6	
82	WQ	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	XQ	1	Total	C	N	O	0
			43	33	4	6	
82	XQ	1	Total	C	N	O	0
			43	33	4	6	
82	XQ	1	Total	C	N	O	0
			43	33	4	6	
82	YQ	1	Total	C	N	O	0
			43	33	4	6	
82	YQ	1	Total	C	N	O	0
			43	33	4	6	
82	L1	1	Total	C	N	O	0
			43	33	4	6	
82	N1	1	Total	C	N	O	0
			43	33	4	6	
82	O1	1	Total	C	N	O	0
			43	33	4	6	
82	O1	1	Total	C	N	O	0
			43	33	4	6	
82	O1	1	Total	C	N	O	0
			43	33	4	6	
82	P1	1	Total	C	N	O	0
			43	33	4	6	
82	P1	1	Total	C	N	O	0
			43	33	4	6	
82	Q1	1	Total	C	N	O	0
			43	33	4	6	
82	Q1	1	Total	C	N	O	0
			43	33	4	6	
82	Q1	1	Total	C	N	O	0
			43	33	4	6	
82	R1	1	Total	C	N	O	0
			43	33	4	6	
82	R1	1	Total	C	N	O	0
			43	33	4	6	
82	S1	1	Total	C	N	O	0
			43	33	4	6	
82	S1	1	Total	C	N	O	0
			43	33	4	6	
82	T1	1	Total	C	N	O	0
			43	33	4	6	
82	T1	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	U1	1	Total	C	N	O	0
			43	33	4	6	
82	U1	1	Total	C	N	O	0
			43	33	4	6	
82	U1	1	Total	C	N	O	0
			43	33	4	6	
82	A1	1	Total	C	N	O	0
			43	33	4	6	
82	A1	1	Total	C	N	O	0
			43	33	4	6	
82	A1	1	Total	C	N	O	0
			43	33	4	6	
82	D1	1	Total	C	N	O	0
			43	33	4	6	
82	F1	1	Total	C	N	O	0
			43	33	4	6	
82	H1	1	Total	C	N	O	0
			43	33	4	6	
82	J1	1	Total	C	N	O	0
			43	33	4	6	
82	V1	1	Total	C	N	O	0
			43	33	4	6	
82	V1	1	Total	C	N	O	0
			43	33	4	6	
82	V1	1	Total	C	N	O	0
			43	33	4	6	
82	W1	1	Total	C	N	O	0
			43	33	4	6	
82	W1	1	Total	C	N	O	0
			43	33	4	6	
82	W1	1	Total	C	N	O	0
			43	33	4	6	
82	Y1	1	Total	C	N	O	0
			43	33	4	6	
82	Y1	1	Total	C	N	O	0
			43	33	4	6	
82	Z1	1	Total	C	N	O	0
			43	33	4	6	
82	Z1	1	Total	C	N	O	0
			43	33	4	6	
82	Z1	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	f1	1	Total	C	N	O	0
			43	33	4	6	
82	f1	1	Total	C	N	O	0
			43	33	4	6	
82	f1	1	Total	C	N	O	0
			43	33	4	6	
82	g1	1	Total	C	N	O	0
			43	33	4	6	
82	g1	1	Total	C	N	O	0
			43	33	4	6	
82	h1	1	Total	C	N	O	0
			43	33	4	6	
82	h1	1	Total	C	N	O	0
			43	33	4	6	
82	h1	1	Total	C	N	O	0
			43	33	4	6	
82	i1	1	Total	C	N	O	0
			43	33	4	6	
82	i1	1	Total	C	N	O	0
			43	33	4	6	
82	j1	1	Total	C	N	O	0
			43	33	4	6	
82	j1	1	Total	C	N	O	0
			43	33	4	6	
82	j1	1	Total	C	N	O	0
			43	33	4	6	
82	k1	1	Total	C	N	O	0
			43	33	4	6	
82	k1	1	Total	C	N	O	0
			43	33	4	6	
82	l1	1	Total	C	N	O	0
			43	33	4	6	
82	l1	1	Total	C	N	O	0
			43	33	4	6	
82	l1	1	Total	C	N	O	0
			43	33	4	6	
82	m1	1	Total	C	N	O	0
			43	33	4	6	
82	m1	1	Total	C	N	O	0
			43	33	4	6	
82	a1	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	a1	1	Total	C	N	O	0
			43	33	4	6	
82	b1	1	Total	C	N	O	0
			43	33	4	6	
82	b1	1	Total	C	N	O	0
			43	33	4	6	
82	b1	1	Total	C	N	O	0
			43	33	4	6	
82	c1	1	Total	C	N	O	0
			43	33	4	6	
82	c1	1	Total	C	N	O	0
			43	33	4	6	
82	d1	1	Total	C	N	O	0
			43	33	4	6	
82	d1	1	Total	C	N	O	0
			43	33	4	6	
82	d1	1	Total	C	N	O	0
			43	33	4	6	
82	e1	1	Total	C	N	O	0
			43	33	4	6	
82	e1	1	Total	C	N	O	0
			43	33	4	6	
82	F4	1	Total	C	N	O	0
			43	33	4	6	
82	H4	1	Total	C	N	O	0
			43	33	4	6	
82	J4	1	Total	C	N	O	0
			43	33	4	6	
82	L4	1	Total	C	N	O	0
			43	33	4	6	
82	N4	1	Total	C	N	O	0
			43	33	4	6	
82	O4	1	Total	C	N	O	0
			43	33	4	6	
82	O4	1	Total	C	N	O	0
			43	33	4	6	
82	A4	1	Total	C	N	O	0
			43	33	4	6	
82	A4	1	Total	C	N	O	0
			43	33	4	6	
82	A4	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	D4	1	Total	C	N	O	0
			43	33	4	6	
82	P4	1	Total	C	N	O	0
			43	33	4	6	
82	P4	1	Total	C	N	O	0
			43	33	4	6	
82	Q4	1	Total	C	N	O	0
			43	33	4	6	
82	Q4	1	Total	C	N	O	0
			43	33	4	6	
82	R4	1	Total	C	N	O	0
			43	33	4	6	
82	R4	1	Total	C	N	O	0
			43	33	4	6	
82	R4	1	Total	C	N	O	0
			43	33	4	6	
82	S4	1	Total	C	N	O	0
			43	33	4	6	
82	S4	1	Total	C	N	O	0
			43	33	4	6	
82	T4	1	Total	C	N	O	0
			43	33	4	6	
82	T4	1	Total	C	N	O	0
			43	33	4	6	
82	T4	1	Total	C	N	O	0
			43	33	4	6	
82	U4	1	Total	C	N	O	0
			43	33	4	6	
82	U4	1	Total	C	N	O	0
			43	33	4	6	
82	V4	1	Total	C	N	O	0
			43	33	4	6	
82	V4	1	Total	C	N	O	0
			43	33	4	6	
82	W4	1	Total	C	N	O	0
			43	33	4	6	
82	Y4	1	Total	C	N	O	0
			43	33	4	6	
82	Y4	1	Total	C	N	O	0
			43	33	4	6	
82	Y4	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	Z4	1	Total	C	N	O	0
			43	33	4	6	
82	Z4	1	Total	C	N	O	0
			43	33	4	6	
82	i4	1	Total	C	N	O	0
			43	33	4	6	
82	i4	1	Total	C	N	O	0
			43	33	4	6	
82	i4	1	Total	C	N	O	0
			43	33	4	6	
82	j4	1	Total	C	N	O	0
			43	33	4	6	
82	j4	1	Total	C	N	O	0
			43	33	4	6	
82	j4	1	Total	C	N	O	0
			43	33	4	6	
82	k4	1	Total	C	N	O	0
			43	33	4	6	
82	k4	1	Total	C	N	O	0
			43	33	4	6	
82	l4	1	Total	C	N	O	0
			43	33	4	6	
82	l4	1	Total	C	N	O	0
			43	33	4	6	
82	m4	1	Total	C	N	O	0
			43	33	4	6	
82	m4	1	Total	C	N	O	0
			43	33	4	6	
82	m4	1	Total	C	N	O	0
			43	33	4	6	
82	a4	1	Total	C	N	O	0
			43	33	4	6	
82	a4	1	Total	C	N	O	0
			43	33	4	6	
82	a4	1	Total	C	N	O	0
			43	33	4	6	
82	b4	1	Total	C	N	O	0
			43	33	4	6	
82	b4	1	Total	C	N	O	0
			43	33	4	6	
82	c4	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	c4	1	Total	C	N	O	0
			43	33	4	6	
82	c4	1	Total	C	N	O	0
			43	33	4	6	
82	d4	1	Total	C	N	O	0
			43	33	4	6	
82	d4	1	Total	C	N	O	0
			43	33	4	6	
82	e4	1	Total	C	N	O	0
			43	33	4	6	
82	e4	1	Total	C	N	O	0
			43	33	4	6	
82	e4	1	Total	C	N	O	0
			43	33	4	6	
82	f4	1	Total	C	N	O	0
			43	33	4	6	
82	f4	1	Total	C	N	O	0
			43	33	4	6	
82	g4	1	Total	C	N	O	0
			43	33	4	6	
82	g4	1	Total	C	N	O	0
			43	33	4	6	
82	g4	1	Total	C	N	O	0
			43	33	4	6	
82	h4	1	Total	C	N	O	0
			43	33	4	6	
82	h4	1	Total	C	N	O	0
			43	33	4	6	
82	A5	1	Total	C	N	O	0
			43	33	4	6	
82	A5	1	Total	C	N	O	0
			43	33	4	6	
82	B5	1	Total	C	N	O	0
			43	33	4	6	
82	B5	1	Total	C	N	O	0
			43	33	4	6	
82	B5	1	Total	C	N	O	0
			43	33	4	6	
82	C5	1	Total	C	N	O	0
			43	33	4	6	
82	C5	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	D5	1	Total	C	N	O	0
			43	33	4	6	
82	D5	1	Total	C	N	O	0
			43	33	4	6	
82	D5	1	Total	C	N	O	0
			43	33	4	6	
82	E5	1	Total	C	N	O	0
			43	33	4	6	
82	E5	1	Total	C	N	O	0
			43	33	4	6	
82	F5	1	Total	C	N	O	0
			43	33	4	6	
82	F5	1	Total	C	N	O	0
			43	33	4	6	
82	F5	1	Total	C	N	O	0
			43	33	4	6	
82	G5	1	Total	C	N	O	0
			43	33	4	6	
82	G5	1	Total	C	N	O	0
			43	33	4	6	
82	H5	1	Total	C	N	O	0
			43	33	4	6	
82	H5	1	Total	C	N	O	0
			43	33	4	6	
82	H5	1	Total	C	N	O	0
			43	33	4	6	
82	I5	1	Total	C	N	O	0
			43	33	4	6	
82	I5	1	Total	C	N	O	0
			43	33	4	6	
82	J5	1	Total	C	N	O	0
			43	33	4	6	
82	J5	1	Total	C	N	O	0
			43	33	4	6	
82	J5	1	Total	C	N	O	0
			43	33	4	6	
82	K5	1	Total	C	N	O	0
			43	33	4	6	
82	K5	1	Total	C	N	O	0
			43	33	4	6	
82	L5	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	L5	1	Total	C	N	O	0
			43	33	4	6	
82	L5	1	Total	C	N	O	0
			43	33	4	6	
82	M5	1	Total	C	N	O	0
			43	33	4	6	
82	M5	1	Total	C	N	O	0
			43	33	4	6	
82	M5	1	Total	C	N	O	0
			43	33	4	6	
82	N5	1	Total	C	N	O	0
			43	33	4	6	
82	N5	1	Total	C	N	O	0
			43	33	4	6	
82	O5	1	Total	C	N	O	0
			43	33	4	6	
82	O5	1	Total	C	N	O	0
			43	33	4	6	
82	O5	1	Total	C	N	O	0
			43	33	4	6	
82	P5	1	Total	C	N	O	0
			43	33	4	6	
82	P5	1	Total	C	N	O	0
			43	33	4	6	
82	Q5	1	Total	C	N	O	0
			43	33	4	6	
82	Q5	1	Total	C	N	O	0
			43	33	4	6	
82	Q5	1	Total	C	N	O	0
			43	33	4	6	
82	R5	1	Total	C	N	O	0
			43	33	4	6	
82	R5	1	Total	C	N	O	0
			43	33	4	6	
82	S5	1	Total	C	N	O	0
			43	33	4	6	
82	S5	1	Total	C	N	O	0
			43	33	4	6	
82	S5	1	Total	C	N	O	0
			43	33	4	6	
82	T5	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	T5	1	Total	C	N	O	0
			43	33	4	6	
82	U5	1	Total	C	N	O	0
			43	33	4	6	
82	U5	1	Total	C	N	O	0
			43	33	4	6	
82	U5	1	Total	C	N	O	0
			43	33	4	6	
82	V5	1	Total	C	N	O	0
			43	33	4	6	
82	V5	1	Total	C	N	O	0
			43	33	4	6	
82	W5	1	Total	C	N	O	0
			43	33	4	6	
82	W5	1	Total	C	N	O	0
			43	33	4	6	
82	W5	1	Total	C	N	O	0
			43	33	4	6	
82	X5	1	Total	C	N	O	0
			43	33	4	6	
82	X5	1	Total	C	N	O	0
			43	33	4	6	
82	Y5	1	Total	C	N	O	0
			43	33	4	6	
82	Y5	1	Total	C	N	O	0
			43	33	4	6	
82	Y5	1	Total	C	N	O	0
			43	33	4	6	
82	Z5	1	Total	C	N	O	0
			43	33	4	6	
82	Z5	1	Total	C	N	O	0
			43	33	4	6	
82	Z5	1	Total	C	N	O	0
			43	33	4	6	
82	A7	1	Total	C	N	O	0
			43	33	4	6	
82	A7	1	Total	C	N	O	0
			43	33	4	6	
82	B7	1	Total	C	N	O	0
			43	33	4	6	
82	B7	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	B7	1	Total	C	N	O	0
			43	33	4	6	
82	C7	1	Total	C	N	O	0
			43	33	4	6	
82	C7	1	Total	C	N	O	0
			43	33	4	6	
82	D7	1	Total	C	N	O	0
			43	33	4	6	
82	D7	1	Total	C	N	O	0
			43	33	4	6	
82	D7	1	Total	C	N	O	0
			43	33	4	6	
82	E7	1	Total	C	N	O	0
			43	33	4	6	
82	E7	1	Total	C	N	O	0
			43	33	4	6	
82	F7	1	Total	C	N	O	0
			43	33	4	6	
82	F7	1	Total	C	N	O	0
			43	33	4	6	
82	F7	1	Total	C	N	O	0
			43	33	4	6	
82	G7	1	Total	C	N	O	0
			43	33	4	6	
82	G7	1	Total	C	N	O	0
			43	33	4	6	
82	H7	1	Total	C	N	O	0
			43	33	4	6	
82	H7	1	Total	C	N	O	0
			43	33	4	6	
82	H7	1	Total	C	N	O	0
			43	33	4	6	
82	I7	1	Total	C	N	O	0
			43	33	4	6	
82	I7	1	Total	C	N	O	0
			43	33	4	6	
82	J7	1	Total	C	N	O	0
			43	33	4	6	
82	J7	1	Total	C	N	O	0
			43	33	4	6	
82	J7	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	K7	1	Total	C	N	O	0
			43	33	4	6	
82	K7	1	Total	C	N	O	0
			43	33	4	6	
82	L7	1	Total	C	N	O	0
			43	33	4	6	
82	L7	1	Total	C	N	O	0
			43	33	4	6	
82	L7	1	Total	C	N	O	0
			43	33	4	6	
82	M7	1	Total	C	N	O	0
			43	33	4	6	
82	M7	1	Total	C	N	O	0
			43	33	4	6	
82	N7	1	Total	C	N	O	0
			43	33	4	6	
82	N7	1	Total	C	N	O	0
			43	33	4	6	
82	N7	1	Total	C	N	O	0
			43	33	4	6	
82	O7	1	Total	C	N	O	0
			43	33	4	6	
82	O7	1	Total	C	N	O	0
			43	33	4	6	
82	P7	1	Total	C	N	O	0
			43	33	4	6	
82	P7	1	Total	C	N	O	0
			43	33	4	6	
82	P7	1	Total	C	N	O	0
			43	33	4	6	
82	Q7	1	Total	C	N	O	0
			43	33	4	6	
82	Q7	1	Total	C	N	O	0
			43	33	4	6	
82	R7	1	Total	C	N	O	0
			43	33	4	6	
82	R7	1	Total	C	N	O	0
			43	33	4	6	
82	R7	1	Total	C	N	O	0
			43	33	4	6	
82	S7	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	S7	1	Total	C	N	O	0
			43	33	4	6	
82	T7	1	Total	C	N	O	0
			43	33	4	6	
82	T7	1	Total	C	N	O	0
			43	33	4	6	
82	T7	1	Total	C	N	O	0
			43	33	4	6	
82	U7	1	Total	C	N	O	0
			43	33	4	6	
82	U7	1	Total	C	N	O	0
			43	33	4	6	
82	V7	1	Total	C	N	O	0
			43	33	4	6	
82	V7	1	Total	C	N	O	0
			43	33	4	6	
82	V7	1	Total	C	N	O	0
			43	33	4	6	
82	W7	1	Total	C	N	O	0
			43	33	4	6	
82	W7	1	Total	C	N	O	0
			43	33	4	6	
82	X7	1	Total	C	N	O	0
			43	33	4	6	
82	X7	1	Total	C	N	O	0
			43	33	4	6	
82	X7	1	Total	C	N	O	0
			43	33	4	6	
82	Y7	1	Total	C	N	O	0
			43	33	4	6	
82	Y7	1	Total	C	N	O	0
			43	33	4	6	
82	Y7	1	Total	C	N	O	0
			43	33	4	6	
82	e7	1	Total	C	N	O	0
			43	33	4	6	
82	y8	1	Total	C	N	O	0
			43	33	4	6	
82	y8	1	Total	C	N	O	0
			43	33	4	6	
82	y8	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	z8	1	Total	C	N	O	0
			43	33	4	6	
82	z8	1	Total	C	N	O	0
			43	33	4	6	
82	18	1	Total	C	N	O	0
			43	33	4	6	
82	18	1	Total	C	N	O	0
			43	33	4	6	
82	18	1	Total	C	N	O	0
			43	33	4	6	
82	p8	1	Total	C	N	O	0
			43	33	4	6	
82	p8	1	Total	C	N	O	0
			43	33	4	6	
82	q8	1	Total	C	N	O	0
			43	33	4	6	
82	q8	1	Total	C	N	O	0
			43	33	4	6	
82	q8	1	Total	C	N	O	0
			43	33	4	6	
82	r8	1	Total	C	N	O	0
			43	33	4	6	
82	r8	1	Total	C	N	O	0
			43	33	4	6	
82	s8	1	Total	C	N	O	0
			43	33	4	6	
82	s8	1	Total	C	N	O	0
			43	33	4	6	
82	s8	1	Total	C	N	O	0
			43	33	4	6	
82	t8	1	Total	C	N	O	0
			43	33	4	6	
82	t8	1	Total	C	N	O	0
			43	33	4	6	
82	u8	1	Total	C	N	O	0
			43	33	4	6	
82	u8	1	Total	C	N	O	0
			43	33	4	6	
82	u8	1	Total	C	N	O	0
			43	33	4	6	
82	v8	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	v8	1	Total	C	N	O	0
			43	33	4	6	
82	w8	1	Total	C	N	O	0
			43	33	4	6	
82	w8	1	Total	C	N	O	0
			43	33	4	6	
82	w8	1	Total	C	N	O	0
			43	33	4	6	
82	w8	1	Total	C	N	O	0
			43	33	4	6	
82	x8	1	Total	C	N	O	0
			43	33	4	6	
82	x8	1	Total	C	N	O	0
			43	33	4	6	
82	A9	1	Total	C	N	O	0
			43	33	4	6	
82	A9	1	Total	C	N	O	0
			43	33	4	6	
82	B9	1	Total	C	N	O	0
			43	33	4	6	
82	B9	1	Total	C	N	O	0
			43	33	4	6	
82	B9	1	Total	C	N	O	0
			43	33	4	6	
82	C9	1	Total	C	N	O	0
			43	33	4	6	
82	C9	1	Total	C	N	O	0
			43	33	4	6	
82	D9	1	Total	C	N	O	0
			43	33	4	6	
82	D9	1	Total	C	N	O	0
			43	33	4	6	
82	D9	1	Total	C	N	O	0
			43	33	4	6	
82	E9	1	Total	C	N	O	0
			43	33	4	6	
82	E9	1	Total	C	N	O	0
			43	33	4	6	
82	F9	1	Total	C	N	O	0
			43	33	4	6	
82	F9	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	F9	1	Total	C	N	O	0
			43	33	4	6	
82	G9	1	Total	C	N	O	0
			43	33	4	6	
82	G9	1	Total	C	N	O	0
			43	33	4	6	
82	H9	1	Total	C	N	O	0
			43	33	4	6	
82	H9	1	Total	C	N	O	0
			43	33	4	6	
82	H9	1	Total	C	N	O	0
			43	33	4	6	
82	I9	1	Total	C	N	O	0
			43	33	4	6	
82	I9	1	Total	C	N	O	0
			43	33	4	6	
82	J9	1	Total	C	N	O	0
			43	33	4	6	
82	J9	1	Total	C	N	O	0
			43	33	4	6	
82	J9	1	Total	C	N	O	0
			43	33	4	6	
82	K9	1	Total	C	N	O	0
			43	33	4	6	
82	K9	1	Total	C	N	O	0
			43	33	4	6	
82	L9	1	Total	C	N	O	0
			43	33	4	6	
82	L9	1	Total	C	N	O	0
			43	33	4	6	
82	L9	1	Total	C	N	O	0
			43	33	4	6	
82	N9	1	Total	C	N	O	0
			43	33	4	6	
82	N9	1	Total	C	N	O	0
			43	33	4	6	
82	O9	1	Total	C	N	O	0
			43	33	4	6	
82	O9	1	Total	C	N	O	0
			43	33	4	6	
82	O9	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	P9	1	Total	C	N	O	0
			43	33	4	6	
82	P9	1	Total	C	N	O	0
			43	33	4	6	
82	Q9	1	Total	C	N	O	0
			43	33	4	6	
82	Q9	1	Total	C	N	O	0
			43	33	4	6	
82	Q9	1	Total	C	N	O	0
			43	33	4	6	
82	R9	1	Total	C	N	O	0
			43	33	4	6	
82	R9	1	Total	C	N	O	0
			43	33	4	6	
82	S9	1	Total	C	N	O	0
			43	33	4	6	
82	S9	1	Total	C	N	O	0
			43	33	4	6	
82	S9	1	Total	C	N	O	0
			43	33	4	6	
82	T9	1	Total	C	N	O	0
			43	33	4	6	
82	T9	1	Total	C	N	O	0
			43	33	4	6	
82	U9	1	Total	C	N	O	0
			43	33	4	6	
82	U9	1	Total	C	N	O	0
			43	33	4	6	
82	U9	1	Total	C	N	O	0
			43	33	4	6	
82	U9	1	Total	C	N	O	0
			43	33	4	6	
82	V9	1	Total	C	N	O	0
			43	33	4	6	
82	V9	1	Total	C	N	O	0
			43	33	4	6	
82	W9	1	Total	C	N	O	0
			43	33	4	6	
82	W9	1	Total	C	N	O	0
			43	33	4	6	
82	W9	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	X9	1	Total	C	N	O	0
			43	33	4	6	
82	X9	1	Total	C	N	O	0
			43	33	4	6	
82	Y9	1	Total	C	N	O	0
			43	33	4	6	
82	Y9	1	Total	C	N	O	0
			43	33	4	6	
82	Y9	1	Total	C	N	O	0
			43	33	4	6	
82	eA	1	Total	C	N	O	0
			43	33	4	6	
82	fB	1	Total	C	N	O	0
			43	33	4	6	
82	aB	1	Total	C	N	O	0
			43	33	4	6	
82	aB	1	Total	C	N	O	0
			43	33	4	6	
82	bB	1	Total	C	N	O	0
			43	33	4	6	
82	cB	1	Total	C	N	O	0
			43	33	4	6	
82	cB	1	Total	C	N	O	0
			43	33	4	6	
82	cB	1	Total	C	N	O	0
			43	33	4	6	
82	dB	1	Total	C	N	O	0
			43	33	4	6	
82	dB	1	Total	C	N	O	0
			43	33	4	6	
82	eB	1	Total	C	N	O	0
			43	33	4	6	
82	eB	1	Total	C	N	O	0
			43	33	4	6	
82	gB	1	Total	C	N	O	0
			43	33	4	6	
82	gB	1	Total	C	N	O	0
			43	33	4	6	
82	gB	1	Total	C	N	O	0
			43	33	4	6	
82	hB	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	yC	1	Total	C	N	O	0
			43	33	4	6	
82	yC	1	Total	C	N	O	0
			43	33	4	6	
82	yC	1	Total	C	N	O	0
			43	33	4	6	
82	zC	1	Total	C	N	O	0
			43	33	4	6	
82	zC	1	Total	C	N	O	0
			43	33	4	6	
82	1C	1	Total	C	N	O	0
			43	33	4	6	
82	1C	1	Total	C	N	O	0
			43	33	4	6	
82	1C	1	Total	C	N	O	0
			43	33	4	6	
82	pC	1	Total	C	N	O	0
			43	33	4	6	
82	pC	1	Total	C	N	O	0
			43	33	4	6	
82	qC	1	Total	C	N	O	0
			43	33	4	6	
82	qC	1	Total	C	N	O	0
			43	33	4	6	
82	qC	1	Total	C	N	O	0
			43	33	4	6	
82	rC	1	Total	C	N	O	0
			43	33	4	6	
82	rC	1	Total	C	N	O	0
			43	33	4	6	
82	sC	1	Total	C	N	O	0
			43	33	4	6	
82	sC	1	Total	C	N	O	0
			43	33	4	6	
82	sC	1	Total	C	N	O	0
			43	33	4	6	
82	tC	1	Total	C	N	O	0
			43	33	4	6	
82	tC	1	Total	C	N	O	0
			43	33	4	6	
82	uC	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	uC	1	Total	C	N	O	0
			43	33	4	6	
82	uC	1	Total	C	N	O	0
			43	33	4	6	
82	vC	1	Total	C	N	O	0
			43	33	4	6	
82	vC	1	Total	C	N	O	0
			43	33	4	6	
82	wC	1	Total	C	N	O	0
			43	33	4	6	
82	wC	1	Total	C	N	O	0
			43	33	4	6	
82	wC	1	Total	C	N	O	0
			43	33	4	6	
82	wC	1	Total	C	N	O	0
			43	33	4	6	
82	xC	1	Total	C	N	O	0
			43	33	4	6	
82	xC	1	Total	C	N	O	0
			43	33	4	6	
82	dD	1	Total	C	N	O	0
			43	33	4	6	
82	aE	1	Total	C	N	O	0
			43	33	4	6	
82	aE	1	Total	C	N	O	0
			43	33	4	6	
82	bE	1	Total	C	N	O	0
			43	33	4	6	
82	bE	1	Total	C	N	O	0
			43	33	4	6	
82	cE	1	Total	C	N	O	0
			43	33	4	6	
82	cE	1	Total	C	N	O	0
			43	33	4	6	
82	dE	1	Total	C	N	O	0
			43	33	4	6	
82	dE	1	Total	C	N	O	0
			43	33	4	6	
82	dE	1	Total	C	N	O	0
			43	33	4	6	
82	dE	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	eE	1	Total	C	N	O	0
			43	33	4	6	
82	eE	1	Total	C	N	O	0
			43	33	4	6	
82	eE	1	Total	C	N	O	0
			43	33	4	6	
82	fE	1	Total	C	N	O	0
			43	33	4	6	
82	fE	1	Total	C	N	O	0
			43	33	4	6	
82	fE	1	Total	C	N	O	0
			43	33	4	6	
82	gE	1	Total	C	N	O	0
			43	33	4	6	
82	gE	1	Total	C	N	O	0
			43	33	4	6	
82	hE	1	Total	C	N	O	0
			43	33	4	6	
82	hE	1	Total	C	N	O	0
			43	33	4	6	
82	hE	1	Total	C	N	O	0
			43	33	4	6	
82	iE	1	Total	C	N	O	0
			43	33	4	6	
82	iE	1	Total	C	N	O	0
			43	33	4	6	
82	jE	1	Total	C	N	O	0
			43	33	4	6	
82	jE	1	Total	C	N	O	0
			43	33	4	6	
82	kE	1	Total	C	N	O	0
			43	33	4	6	
82	kE	1	Total	C	N	O	0
			43	33	4	6	
82	lE	1	Total	C	N	O	0
			43	33	4	6	
82	lE	1	Total	C	N	O	0
			43	33	4	6	
82	lE	1	Total	C	N	O	0
			43	33	4	6	
82	mE	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	mE	1	Total	C	N	O	0
			43	33	4	6	
82	mE	1	Total	C	N	O	0
			43	33	4	6	
82	aF	1	Total	C	N	O	0
			43	33	4	6	
82	aF	1	Total	C	N	O	0
			43	33	4	6	
82	aF	1	Total	C	N	O	0
			43	33	4	6	
82	bF	1	Total	C	N	O	0
			43	33	4	6	
82	bF	1	Total	C	N	O	0
			43	33	4	6	
82	cF	1	Total	C	N	O	0
			43	33	4	6	
82	cF	1	Total	C	N	O	0
			43	33	4	6	
82	cF	1	Total	C	N	O	0
			43	33	4	6	
82	dF	1	Total	C	N	O	0
			43	33	4	6	
82	dF	1	Total	C	N	O	0
			43	33	4	6	
82	eF	1	Total	C	N	O	0
			43	33	4	6	
82	eF	1	Total	C	N	O	0
			43	33	4	6	
82	eF	1	Total	C	N	O	0
			43	33	4	6	
82	fF	1	Total	C	N	O	0
			43	33	4	6	
82	fF	1	Total	C	N	O	0
			43	33	4	6	
82	gF	1	Total	C	N	O	0
			43	33	4	6	
82	gF	1	Total	C	N	O	0
			43	33	4	6	
82	gF	1	Total	C	N	O	0
			43	33	4	6	
82	hF	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	hF	1	Total	C	N	O	0
			43	33	4	6	
82	iF	1	Total	C	N	O	0
			43	33	4	6	
82	iF	1	Total	C	N	O	0
			43	33	4	6	
82	iF	1	Total	C	N	O	0
			43	33	4	6	
82	jF	1	Total	C	N	O	0
			43	33	4	6	
82	jF	1	Total	C	N	O	0
			43	33	4	6	
82	kF	1	Total	C	N	O	0
			43	33	4	6	
82	kF	1	Total	C	N	O	0
			43	33	4	6	
82	kF	1	Total	C	N	O	0
			43	33	4	6	
82	lF	1	Total	C	N	O	0
			43	33	4	6	
82	lF	1	Total	C	N	O	0
			43	33	4	6	
82	lF	1	Total	C	N	O	0
			43	33	4	6	
82	mF	1	Total	C	N	O	0
			43	33	4	6	
82	mF	1	Total	C	N	O	0
			43	33	4	6	
82	nF	1	Total	C	N	O	0
			43	33	4	6	
82	nF	1	Total	C	N	O	0
			43	33	4	6	
82	oF	1	Total	C	N	O	0
			43	33	4	6	
82	oF	1	Total	C	N	O	0
			43	33	4	6	
82	oF	1	Total	C	N	O	0
			43	33	4	6	
82	pF	1	Total	C	N	O	0
			43	33	4	6	
82	pF	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	qF	1	Total	C	N	O	0
			43	33	4	6	
82	qF	1	Total	C	N	O	0
			43	33	4	6	
82	qF	1	Total	C	N	O	0
			43	33	4	6	
82	rF	1	Total	C	N	O	0
			43	33	4	6	
82	rF	1	Total	C	N	O	0
			43	33	4	6	
82	sF	1	Total	C	N	O	0
			43	33	4	6	
82	sF	1	Total	C	N	O	0
			43	33	4	6	
82	sF	1	Total	C	N	O	0
			43	33	4	6	
82	tF	1	Total	C	N	O	0
			43	33	4	6	
82	tF	1	Total	C	N	O	0
			43	33	4	6	
82	uF	1	Total	C	N	O	0
			43	33	4	6	
82	uF	1	Total	C	N	O	0
			43	33	4	6	
82	uF	1	Total	C	N	O	0
			43	33	4	6	
82	vF	1	Total	C	N	O	0
			43	33	4	6	
82	vF	1	Total	C	N	O	0
			43	33	4	6	
82	wF	1	Total	C	N	O	0
			43	33	4	6	
82	wF	1	Total	C	N	O	0
			43	33	4	6	
82	wF	1	Total	C	N	O	0
			43	33	4	6	
82	xF	1	Total	C	N	O	0
			43	33	4	6	
82	xF	1	Total	C	N	O	0
			43	33	4	6	
82	xF	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	yF	1	Total	C	N	O	0
			43	33	4	6	
82	zF	1	Total	C	N	O	0
			43	33	4	6	
82	aG	1	Total	C	N	O	0
			43	33	4	6	
82	aG	1	Total	C	N	O	0
			43	33	4	6	
82	bG	1	Total	C	N	O	0
			43	33	4	6	
82	cG	1	Total	C	N	O	0
			43	33	4	6	
82	cG	1	Total	C	N	O	0
			43	33	4	6	
82	dG	1	Total	C	N	O	0
			43	33	4	6	
82	dG	1	Total	C	N	O	0
			43	33	4	6	
82	dG	1	Total	C	N	O	0
			43	33	4	6	
82	dG	1	Total	C	N	O	0
			43	33	4	6	
82	eG	1	Total	C	N	O	0
			43	33	4	6	
82	eG	1	Total	C	N	O	0
			43	33	4	6	
82	eG	1	Total	C	N	O	0
			43	33	4	6	
82	fG	1	Total	C	N	O	0
			43	33	4	6	
82	fG	1	Total	C	N	O	0
			43	33	4	6	
82	fG	1	Total	C	N	O	0
			43	33	4	6	
82	gG	1	Total	C	N	O	0
			43	33	4	6	
82	gG	1	Total	C	N	O	0
			43	33	4	6	
82	hG	1	Total	C	N	O	0
			43	33	4	6	
82	hG	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	hG	1	Total	C	N	O	0
			43	33	4	6	
82	iG	1	Total	C	N	O	0
			43	33	4	6	
82	iG	1	Total	C	N	O	0
			43	33	4	6	
82	jG	1	Total	C	N	O	0
			43	33	4	6	
82	jG	1	Total	C	N	O	0
			43	33	4	6	
82	kG	1	Total	C	N	O	0
			43	33	4	6	
82	kG	1	Total	C	N	O	0
			43	33	4	6	
82	lG	1	Total	C	N	O	0
			43	33	4	6	
82	lG	1	Total	C	N	O	0
			43	33	4	6	
82	lG	1	Total	C	N	O	0
			43	33	4	6	
82	mG	1	Total	C	N	O	0
			43	33	4	6	
82	mG	1	Total	C	N	O	0
			43	33	4	6	
82	mG	1	Total	C	N	O	0
			43	33	4	6	
82	fH	1	Total	C	N	O	0
			43	33	4	6	
82	fH	1	Total	C	N	O	0
			43	33	4	6	
82	fH	1	Total	C	N	O	0
			43	33	4	6	
82	gH	1	Total	C	N	O	0
			43	33	4	6	
82	gH	1	Total	C	N	O	0
			43	33	4	6	
82	gH	1	Total	C	N	O	0
			43	33	4	6	
82	hH	1	Total	C	N	O	0
			43	33	4	6	
82	hH	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	iH	1	Total	C	N	O	0
			43	33	4	6	
82	iH	1	Total	C	N	O	0
			43	33	4	6	
82	jH	1	Total	C	N	O	0
			43	33	4	6	
82	jH	1	Total	C	N	O	0
			43	33	4	6	
82	jH	1	Total	C	N	O	0
			43	33	4	6	
82	kH	1	Total	C	N	O	0
			43	33	4	6	
82	kH	1	Total	C	N	O	0
			43	33	4	6	
82	kH	1	Total	C	N	O	0
			43	33	4	6	
82	lH	1	Total	C	N	O	0
			43	33	4	6	
82	lH	1	Total	C	N	O	0
			43	33	4	6	
82	mH	1	Total	C	N	O	0
			43	33	4	6	
82	mH	1	Total	C	N	O	0
			43	33	4	6	
82	aH	1	Total	C	N	O	0
			43	33	4	6	
82	aH	1	Total	C	N	O	0
			43	33	4	6	
82	bH	1	Total	C	N	O	0
			43	33	4	6	
82	bH	1	Total	C	N	O	0
			43	33	4	6	
82	cH	1	Total	C	N	O	0
			43	33	4	6	
82	cH	1	Total	C	N	O	0
			43	33	4	6	
82	dH	1	Total	C	N	O	0
			43	33	4	6	
82	dH	1	Total	C	N	O	0
			43	33	4	6	
82	dH	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	eH	1	Total	C	N	O	0
			43	33	4	6	
82	eH	1	Total	C	N	O	0
			43	33	4	6	
82	eH	1	Total	C	N	O	0
			43	33	4	6	
82	aJ	1	Total	C	N	O	0
			43	33	4	6	
82	aJ	1	Total	C	N	O	0
			43	33	4	6	
82	aJ	1	Total	C	N	O	0
			43	33	4	6	
82	aJ	1	Total	C	N	O	0
			43	33	4	6	
82	cJ	1	Total	C	N	O	0
			43	33	4	6	
82	cJ	1	Total	C	N	O	0
			43	33	4	6	
82	dJ	1	Total	C	N	O	0
			43	33	4	6	
82	dJ	1	Total	C	N	O	0
			43	33	4	6	
82	eJ	1	Total	C	N	O	0
			43	33	4	6	
82	eJ	1	Total	C	N	O	0
			43	33	4	6	
82	fJ	1	Total	C	N	O	0
			43	33	4	6	
82	fJ	1	Total	C	N	O	0
			43	33	4	6	
82	fJ	1	Total	C	N	O	0
			43	33	4	6	
82	gJ	1	Total	C	N	O	0
			43	33	4	6	
82	gJ	1	Total	C	N	O	0
			43	33	4	6	
82	hJ	1	Total	C	N	O	0
			43	33	4	6	
82	hJ	1	Total	C	N	O	0
			43	33	4	6	
82	hJ	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	iJ	1	Total	C	N	O	0
			43	33	4	6	
82	iJ	1	Total	C	N	O	0
			43	33	4	6	
82	jJ	1	Total	C	N	O	0
			43	33	4	6	
82	jJ	1	Total	C	N	O	0
			43	33	4	6	
82	jJ	1	Total	C	N	O	0
			43	33	4	6	
82	kJ	1	Total	C	N	O	0
			43	33	4	6	
82	kJ	1	Total	C	N	O	0
			43	33	4	6	
82	lJ	1	Total	C	N	O	0
			43	33	4	6	
82	lJ	1	Total	C	N	O	0
			43	33	4	6	
82	lJ	1	Total	C	N	O	0
			43	33	4	6	
82	mJ	1	Total	C	N	O	0
			43	33	4	6	
82	mJ	1	Total	C	N	O	0
			43	33	4	6	
82	aK	1	Total	C	N	O	0
			43	33	4	6	
82	aK	1	Total	C	N	O	0
			43	33	4	6	
82	aK	1	Total	C	N	O	0
			43	33	4	6	
82	bK	1	Total	C	N	O	0
			43	33	4	6	
82	bK	1	Total	C	N	O	0
			43	33	4	6	
82	cK	1	Total	C	N	O	0
			43	33	4	6	
82	cK	1	Total	C	N	O	0
			43	33	4	6	
82	cK	1	Total	C	N	O	0
			43	33	4	6	
82	dK	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	dK	1	Total	C	N	O	0
			43	33	4	6	
82	eK	1	Total	C	N	O	0
			43	33	4	6	
82	eK	1	Total	C	N	O	0
			43	33	4	6	
82	eK	1	Total	C	N	O	0
			43	33	4	6	
82	fK	1	Total	C	N	O	0
			43	33	4	6	
82	fK	1	Total	C	N	O	0
			43	33	4	6	
82	gK	1	Total	C	N	O	0
			43	33	4	6	
82	gK	1	Total	C	N	O	0
			43	33	4	6	
82	gK	1	Total	C	N	O	0
			43	33	4	6	
82	hK	1	Total	C	N	O	0
			43	33	4	6	
82	hK	1	Total	C	N	O	0
			43	33	4	6	
82	iK	1	Total	C	N	O	0
			43	33	4	6	
82	iK	1	Total	C	N	O	0
			43	33	4	6	
82	iK	1	Total	C	N	O	0
			43	33	4	6	
82	jK	1	Total	C	N	O	0
			43	33	4	6	
82	jK	1	Total	C	N	O	0
			43	33	4	6	
82	kK	1	Total	C	N	O	0
			43	33	4	6	
82	kK	1	Total	C	N	O	0
			43	33	4	6	
82	kK	1	Total	C	N	O	0
			43	33	4	6	
82	lK	1	Total	C	N	O	0
			43	33	4	6	
82	lK	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	lK	1	Total	C	N	O	0
			43	33	4	6	
82	mK	1	Total	C	N	O	0
			43	33	4	6	
82	mK	1	Total	C	N	O	0
			43	33	4	6	
82	nK	1	Total	C	N	O	0
			43	33	4	6	
82	nK	1	Total	C	N	O	0
			43	33	4	6	
82	oK	1	Total	C	N	O	0
			43	33	4	6	
82	oK	1	Total	C	N	O	0
			43	33	4	6	
82	oK	1	Total	C	N	O	0
			43	33	4	6	
82	pK	1	Total	C	N	O	0
			43	33	4	6	
82	pK	1	Total	C	N	O	0
			43	33	4	6	
82	qK	1	Total	C	N	O	0
			43	33	4	6	
82	qK	1	Total	C	N	O	0
			43	33	4	6	
82	qK	1	Total	C	N	O	0
			43	33	4	6	
82	rK	1	Total	C	N	O	0
			43	33	4	6	
82	rK	1	Total	C	N	O	0
			43	33	4	6	
82	sK	1	Total	C	N	O	0
			43	33	4	6	
82	sK	1	Total	C	N	O	0
			43	33	4	6	
82	sK	1	Total	C	N	O	0
			43	33	4	6	
82	tK	1	Total	C	N	O	0
			43	33	4	6	
82	tK	1	Total	C	N	O	0
			43	33	4	6	
82	tK	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	uK	1	Total	C	N	O	0
			43	33	4	6	
82	uK	1	Total	C	N	O	0
			43	33	4	6	
82	vK	1	Total	C	N	O	0
			43	33	4	6	
82	vK	1	Total	C	N	O	0
			43	33	4	6	
82	wK	1	Total	C	N	O	0
			43	33	4	6	
82	wK	1	Total	C	N	O	0
			43	33	4	6	
82	wK	1	Total	C	N	O	0
			43	33	4	6	
82	xK	1	Total	C	N	O	0
			43	33	4	6	
82	xK	1	Total	C	N	O	0
			43	33	4	6	
82	xK	1	Total	C	N	O	0
			43	33	4	6	
82	yK	1	Total	C	N	O	0
			43	33	4	6	
82	zK	1	Total	C	N	O	0
			43	33	4	6	
82	aM	1	Total	C	N	O	0
			43	33	4	6	
82	aM	1	Total	C	N	O	0
			43	33	4	6	
82	aM	1	Total	C	N	O	0
			43	33	4	6	
82	aM	1	Total	C	N	O	0
			43	33	4	6	
82	cM	1	Total	C	N	O	0
			43	33	4	6	
82	cM	1	Total	C	N	O	0
			43	33	4	6	
82	dM	1	Total	C	N	O	0
			43	33	4	6	
82	dM	1	Total	C	N	O	0
			43	33	4	6	
82	dM	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	eM	1	Total	C	N	O	0
			43	33	4	6	
82	eM	1	Total	C	N	O	0
			43	33	4	6	
82	fM	1	Total	C	N	O	0
			43	33	4	6	
82	fM	1	Total	C	N	O	0
			43	33	4	6	
82	fM	1	Total	C	N	O	0
			43	33	4	6	
82	gM	1	Total	C	N	O	0
			43	33	4	6	
82	gM	1	Total	C	N	O	0
			43	33	4	6	
82	hM	1	Total	C	N	O	0
			43	33	4	6	
82	hM	1	Total	C	N	O	0
			43	33	4	6	
82	hM	1	Total	C	N	O	0
			43	33	4	6	
82	iM	1	Total	C	N	O	0
			43	33	4	6	
82	iM	1	Total	C	N	O	0
			43	33	4	6	
82	jM	1	Total	C	N	O	0
			43	33	4	6	
82	jM	1	Total	C	N	O	0
			43	33	4	6	
82	jM	1	Total	C	N	O	0
			43	33	4	6	
82	kM	1	Total	C	N	O	0
			43	33	4	6	
82	kM	1	Total	C	N	O	0
			43	33	4	6	
82	lM	1	Total	C	N	O	0
			43	33	4	6	
82	lM	1	Total	C	N	O	0
			43	33	4	6	
82	lM	1	Total	C	N	O	0
			43	33	4	6	
82	mM	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
82	mM	1	Total	C	N	O	0
			43	33	4	6	
82	iO	1	Total	C	N	O	0
			43	33	4	6	
82	iO	1	Total	C	N	O	0
			43	33	4	6	
82	iO	1	Total	C	N	O	0
			43	33	4	6	
82	jO	1	Total	C	N	O	0
			43	33	4	6	
82	jO	1	Total	C	N	O	0
			43	33	4	6	
82	kO	1	Total	C	N	O	0
			43	33	4	6	
82	kO	1	Total	C	N	O	0
			43	33	4	6	
82	kO	1	Total	C	N	O	0
			43	33	4	6	
82	lO	1	Total	C	N	O	0
			43	33	4	6	
82	lO	1	Total	C	N	O	0
			43	33	4	6	
82	mO	1	Total	C	N	O	0
			43	33	4	6	
82	mO	1	Total	C	N	O	0
			43	33	4	6	
82	mO	1	Total	C	N	O	0
			43	33	4	6	
82	aO	1	Total	C	N	O	0
			43	33	4	6	
82	aO	1	Total	C	N	O	0
			43	33	4	6	
82	aO	1	Total	C	N	O	0
			43	33	4	6	
82	bO	1	Total	C	N	O	0
			43	33	4	6	
82	bO	1	Total	C	N	O	0
			43	33	4	6	
82	cO	1	Total	C	N	O	0
			43	33	4	6	
82	cO	1	Total	C	N	O	0
			43	33	4	6	

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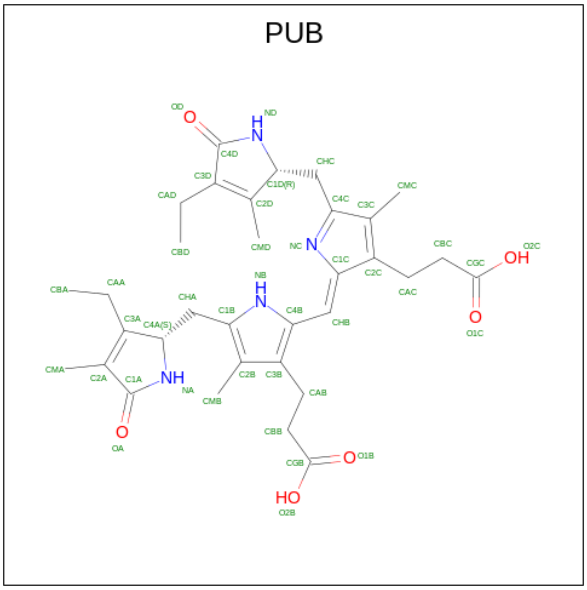
Mol	Chain	Residues	Atoms				AltConf
82	cO	1	Total	C	N	O	0
			43	33	4	6	
82	dO	1	Total	C	N	O	0
			43	33	4	6	
82	dO	1	Total	C	N	O	0
			43	33	4	6	
82	eO	1	Total	C	N	O	0
			43	33	4	6	
82	eO	1	Total	C	N	O	0
			43	33	4	6	
82	eO	1	Total	C	N	O	0
			43	33	4	6	
82	fO	1	Total	C	N	O	0
			43	33	4	6	
82	fO	1	Total	C	N	O	0
			43	33	4	6	
82	gO	1	Total	C	N	O	0
			43	33	4	6	
82	gO	1	Total	C	N	O	0
			43	33	4	6	
82	gO	1	Total	C	N	O	0
			43	33	4	6	
82	hO	1	Total	C	N	O	0
			43	33	4	6	
82	hO	1	Total	C	N	O	0
			43	33	4	6	
82	bP	1	Total	C	N	O	0
			43	33	4	6	
82	bP	1	Total	C	N	O	0
			43	33	4	6	
82	dQ	1	Total	C	N	O	0
			43	33	4	6	
82	Z9	1	Total	C	N	O	0
			43	33	4	6	
82	Z9	1	Total	C	N	O	0
			43	33	4	6	
82	Z9	1	Total	C	N	O	0
			43	33	4	6	
82	M9	1	Total	C	N	O	0
			43	33	4	6	
82	M9	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms	AltConf
82	M9	1	Total C N O 43 33 4 6	0
82	M9	1	Total C N O 43 33 4 6	0

- Molecule 83 is PHYCOUROBILIN (CCD ID: PUB) (formula: $C_{33}H_{42}N_4O_6$).



Mol	Chain	Residues	Atoms	AltConf
83	KA	1	Total C N O 43 33 4 6	0
83	YA	1	Total C N O 43 33 4 6	0
83	AD	1	Total C N O 43 33 4 6	0
83	ND	1	Total C N O 43 33 4 6	0
83	AE	1	Total C N O 43 33 4 6	0
83	AE	1	Total C N O 43 33 4 6	0
83	AG	1	Total C N O 43 33 4 6	0
83	AG	1	Total C N O 43 33 4 6	0
83	AH	1	Total C N O 43 33 4 6	0

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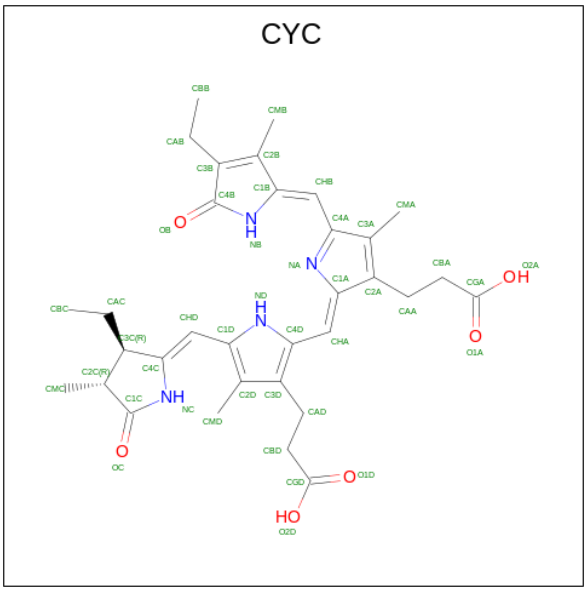
Mol	Chain	Residues	Atoms				AltConf
83	AH	1	Total	C	N	O	0
			43	33	4	6	
83	AJ	1	Total	C	N	O	0
			43	33	4	6	
83	AJ	1	Total	C	N	O	0
			43	33	4	6	
83	BJ	1	Total	C	N	O	0
			43	33	4	6	
83	QJ	1	Total	C	N	O	0
			43	33	4	6	
83	AM	1	Total	C	N	O	0
			43	33	4	6	
83	AM	1	Total	C	N	O	0
			43	33	4	6	
83	BM	1	Total	C	N	O	0
			43	33	4	6	
83	QM	1	Total	C	N	O	0
			43	33	4	6	
83	AO	1	Total	C	N	O	0
			43	33	4	6	
83	AO	1	Total	C	N	O	0
			43	33	4	6	
83	AQ	1	Total	C	N	O	0
			43	33	4	6	
83	NQ	1	Total	C	N	O	0
			43	33	4	6	
83	A1	1	Total	C	N	O	0
			43	33	4	6	
83	A1	1	Total	C	N	O	0
			43	33	4	6	
83	A4	1	Total	C	N	O	0
			43	33	4	6	
83	A4	1	Total	C	N	O	0
			43	33	4	6	
83	M5	1	Total	C	N	O	0
			43	33	4	6	
83	M5	1	Total	C	N	O	0
			43	33	4	6	
83	Z5	1	Total	C	N	O	0
			43	33	4	6	
83	Z5	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
83	K7	1	Total	C	N	O	0
			43	33	4	6	
83	Y7	1	Total	C	N	O	0
			43	33	4	6	
83	wF	1	Total	C	N	O	0
			43	33	4	6	
83	xF	1	Total	C	N	O	0
			43	33	4	6	
83	xF	1	Total	C	N	O	0
			43	33	4	6	
83	xF	1	Total	C	N	O	0
			43	33	4	6	
83	yF	1	Total	C	N	O	0
			43	33	4	6	
83	yF	1	Total	C	N	O	0
			43	33	4	6	
83	wK	1	Total	C	N	O	0
			43	33	4	6	
83	xK	1	Total	C	N	O	0
			43	33	4	6	
83	xK	1	Total	C	N	O	0
			43	33	4	6	
83	xK	1	Total	C	N	O	0
			43	33	4	6	
83	yK	1	Total	C	N	O	0
			43	33	4	6	
83	yK	1	Total	C	N	O	0
			43	33	4	6	
83	Z9	1	Total	C	N	O	0
			43	33	4	6	
83	Z9	1	Total	C	N	O	0
			43	33	4	6	
83	M9	1	Total	C	N	O	0
			43	33	4	6	

- Molecule 84 is PHYCOCYANOBILIN (CCD ID: CYC) (formula: $C_{33}H_{40}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
84	BE	1	Total C N O 43 33 4 6	0
84	BE	1	Total C N O 43 33 4 6	0
84	DE	1	Total C N O 43 33 4 6	0
84	EE	1	Total C N O 43 33 4 6	0
84	FE	1	Total C N O 43 33 4 6	0
84	FE	1	Total C N O 43 33 4 6	0
84	GE	1	Total C N O 43 33 4 6	0
84	HE	1	Total C N O 43 33 4 6	0
84	IE	1	Total C N O 43 33 4 6	0
84	LE	1	Total C N O 43 33 4 6	0
84	ME	1	Total C N O 43 33 4 6	0
84	NE	1	Total C N O 43 33 4 6	0
84	BG	1	Total C N O 43 33 4 6	0
84	BG	1	Total C N O 43 33 4 6	0

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Mol	Chain	Residues	Atoms				AltConf
84	CG	1	Total	C	N	O	0
			43	33	4	6	
84	DG	1	Total	C	N	O	0
			43	33	4	6	
84	EG	1	Total	C	N	O	0
			43	33	4	6	
84	FG	1	Total	C	N	O	0
			43	33	4	6	
84	GG	1	Total	C	N	O	0
			43	33	4	6	
84	HG	1	Total	C	N	O	0
			43	33	4	6	
84	IG	1	Total	C	N	O	0
			43	33	4	6	
84	KG	1	Total	C	N	O	0
			43	33	4	6	
84	LG	1	Total	C	N	O	0
			43	33	4	6	
84	MG	1	Total	C	N	O	0
			43	33	4	6	
84	CH	1	Total	C	N	O	0
			43	33	4	6	
84	DH	1	Total	C	N	O	0
			43	33	4	6	
84	DH	1	Total	C	N	O	0
			43	33	4	6	
84	EH	1	Total	C	N	O	0
			43	33	4	6	
84	FH	1	Total	C	N	O	0
			43	33	4	6	
84	HH	1	Total	C	N	O	0
			43	33	4	6	
84	JH	1	Total	C	N	O	0
			43	33	4	6	
84	JH	1	Total	C	N	O	0
			43	33	4	6	
84	KH	1	Total	C	N	O	0
			43	33	4	6	
84	LH	1	Total	C	N	O	0
			43	33	4	6	
84	LH	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
84	NH	1	Total	C	N	O	0
			43	33	4	6	
84	CO	1	Total	C	N	O	0
			43	33	4	6	
84	DO	1	Total	C	N	O	0
			43	33	4	6	
84	EO	1	Total	C	N	O	0
			43	33	4	6	
84	FO	1	Total	C	N	O	0
			43	33	4	6	
84	GO	1	Total	C	N	O	0
			43	33	4	6	
84	HO	1	Total	C	N	O	0
			43	33	4	6	
84	IO	1	Total	C	N	O	0
			43	33	4	6	
84	JO	1	Total	C	N	O	0
			43	33	4	6	
84	KO	1	Total	C	N	O	0
			43	33	4	6	
84	LO	1	Total	C	N	O	0
			43	33	4	6	
84	MO	1	Total	C	N	O	0
			43	33	4	6	
84	NO	1	Total	C	N	O	0
			43	33	4	6	
84	L1	1	Total	C	N	O	0
			43	33	4	6	
84	M1	1	Total	C	N	O	0
			43	33	4	6	
84	N1	1	Total	C	N	O	0
			43	33	4	6	
84	C1	1	Total	C	N	O	0
			43	33	4	6	
84	D1	1	Total	C	N	O	0
			43	33	4	6	
84	D1	1	Total	C	N	O	0
			43	33	4	6	
84	E1	1	Total	C	N	O	0
			43	33	4	6	
84	F1	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms					AltConf
84	H1	1	Total	C	N	O		0
			43	33	4	6		
84	I1	1	Total	C	N	O		0
			43	33	4	6		
84	J1	1	Total	C	N	O		0
			43	33	4	6		
84	K1	1	Total	C	N	O		0
			43	33	4	6		
84	A3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	B3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	C3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	D3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	E3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	F3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	G3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	H3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	I3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	J3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	K3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	L3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	M3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	N3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	O3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	P3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	Q3	1	Total	C	H	N	O	0
			81	33	38	4	6	

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Mol	Chain	Residues	Atoms					AltConf
84	R3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	S3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	T3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	U3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	V3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	W3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	c3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	d3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	e3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	f3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	g3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	h3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	i3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	j3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	k3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	l3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	m3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	n3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	o3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	p3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	q3	1	Total	C	H	N	O	0
			81	33	38	4	6	

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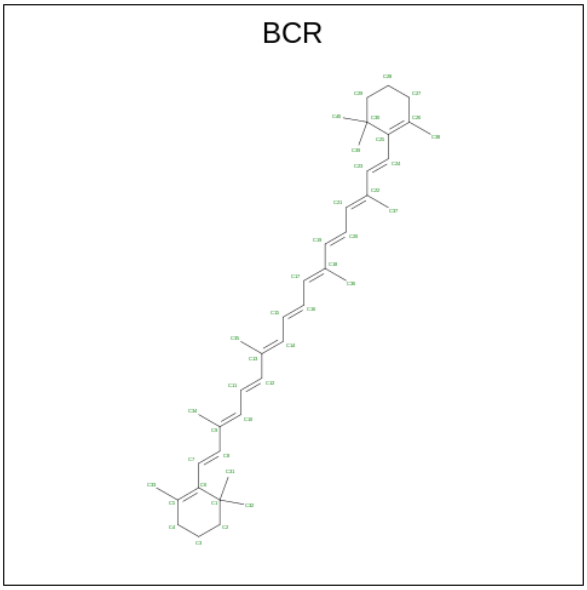
Mol	Chain	Residues	Atoms					AltConf
84	r3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	t3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	u3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	v3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	w3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	x3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	y3	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	63	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	73	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	73	1	Total	C	H	N	O	0
			81	33	38	4	6	
84	F4	1	Total	C	N	O		0
			43	33	4	6		
84	G4	1	Total	C	N	O		0
			43	33	4	6		
84	H4	1	Total	C	N	O		0
			43	33	4	6		
84	I4	1	Total	C	N	O		0
			43	33	4	6		
84	J4	1	Total	C	N	O		0
			43	33	4	6		
84	K4	1	Total	C	N	O		0
			43	33	4	6		
84	L4	1	Total	C	N	O		0
			43	33	4	6		
84	M4	1	Total	C	N	O		0
			43	33	4	6		
84	N4	1	Total	C	N	O		0
			43	33	4	6		
84	C4	1	Total	C	N	O		0
			43	33	4	6		
84	D4	1	Total	C	N	O		0
			43	33	4	6		

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Mol	Chain	Residues	Atoms	AltConf
84	E4	1	Total C N O 43 33 4 6	0

- Molecule 85 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	AltConf
85	AL	1	Total C 40 40	0
85	BL	1	Total C 40 40	0
85	BL	1	Total C 40 40	0
85	BL	1	Total C 40 40	0
85	CL	1	Total C 40 40	0
85	CL	1	Total C 40 40	0
85	CL	1	Total C 40 40	0
85	FL	1	Total C 40 40	0
85	HL	1	Total C 40 40	0
85	KL	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
85	AN	1	Total C 40 40	0
85	AN	1	Total C 40 40	0
85	AN	1	Total C 40 40	0
85	AN	1	Total C 40 40	0
85	AN	1	Total C 40 40	0
85	BN	1	Total C 40 40	0
85	BN	1	Total C 40 40	0
85	BN	1	Total C 40 40	0
85	BN	1	Total C 40 40	0
85	BN	1	Total C 40 40	0
85	BN	1	Total C 40 40	0
85	BN	1	Total C 40 40	0
85	BN	1	Total C 40 40	0
85	FN	1	Total C 40 40	0
85	FN	1	Total C 40 40	0
85	IN	1	Total C 40 40	0
85	JN	1	Total C 40 40	0
85	JN	1	Total C 40 40	0
85	KN	1	Total C 40 40	0
85	KN	1	Total C 40 40	0
85	LN	1	Total C 40 40	0
85	LN	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
85	A2	1	Total C 40 40	0
85	A2	1	Total C 40 40	0
85	A2	1	Total C 40 40	0
85	A2	1	Total C 40 40	0
85	A2	1	Total C 40 40	0
85	B2	1	Total C 40 40	0
85	B2	1	Total C 40 40	0
85	B2	1	Total C 40 40	0
85	B2	1	Total C 40 40	0
85	B2	1	Total C 40 40	0
85	B2	1	Total C 40 40	0
85	B2	1	Total C 40 40	0
85	B2	1	Total C 40 40	0
85	F2	1	Total C 40 40	0
85	F2	1	Total C 40 40	0
85	I2	1	Total C 40 40	0
85	J2	1	Total C 40 40	0
85	J2	1	Total C 40 40	0
85	K2	1	Total C 40 40	0
85	K2	1	Total C 40 40	0
85	L2	1	Total C 40 40	0
85	L2	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
85	A6	1	Total C 40 40	0
85	B6	1	Total C 40 40	0
85	B6	1	Total C 40 40	0
85	B6	1	Total C 40 40	0
85	C6	1	Total C 40 40	0
85	C6	1	Total C 40 40	0
85	F6	1	Total C 40 40	0
85	H6	1	Total C 40 40	0
85	K6	1	Total C 40 40	0
85	Z6	1	Total C 40 40	0
85	a6	1	Total C 40 40	0
85	b6	1	Total C 40 40	0
85	b6	1	Total C 40 40	0
85	b6	1	Total C 40 40	0
85	c6	1	Total C 40 40	0
85	c6	1	Total C 40 40	0
85	c6	1	Total C 40 40	0
85	d6	1	Total C 40 40	0
85	h6	1	Total C 40 40	0
85	k6	1	Total C 40 40	0
85	aL	1	Total C 40 40	0

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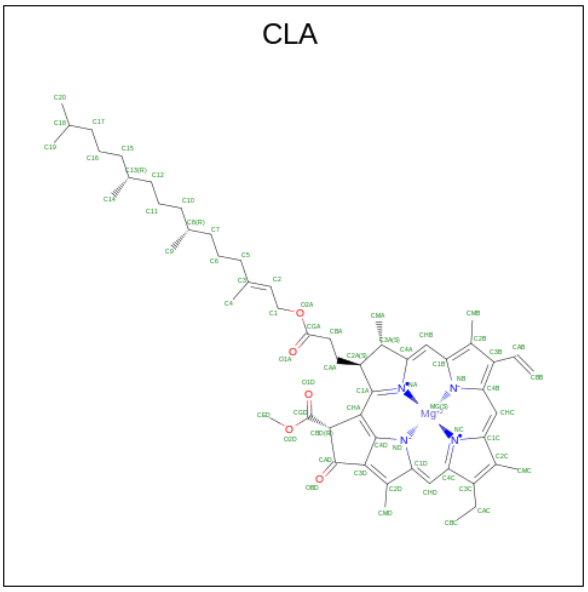
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Mol	Chain	Residues	Atoms	AltConf
85	bL	1	Total C 40 40	0
85	bL	1	Total C 40 40	0
85	bL	1	Total C 40 40	0
85	cL	1	Total C 40 40	0
85	cL	1	Total C 40 40	0
85	cL	1	Total C 40 40	0
85	fL	1	Total C 40 40	0
85	hL	1	Total C 40 40	0
85	kL	1	Total C 40 40	0

- Molecule 86 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	AltConf
86	AL	1	Total Cl 1 1	0
86	C6	1	Total Cl 1 1	0
86	a6	1	Total Cl 1 1	0
86	aL	1	Total Cl 1 1	0

- Molecule 87 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
87	AL	1	Total 65	C 55	Mg 1	N 4	O 5	0
87	AL	1	Total 60	C 50	Mg 1	N 4	O 5	0
87	AL	1	Total 50	C 40	Mg 1	N 4	O 5	0
87	BL	1	Total 65	C 55	Mg 1	N 4	O 5	0
87	BL	1	Total 65	C 55	Mg 1	N 4	O 5	0
87	BL	1	Total 65	C 55	Mg 1	N 4	O 5	0
87	BL	1	Total 59	C 49	Mg 1	N 4	O 5	0
87	BL	1	Total 65	C 55	Mg 1	N 4	O 5	0
87	BL	1	Total 65	C 55	Mg 1	N 4	O 5	0
87	BL	1	Total 65	C 55	Mg 1	N 4	O 5	0
87	BL	1	Total 65	C 55	Mg 1	N 4	O 5	0
87	BL	1	Total 65	C 55	Mg 1	N 4	O 5	0
87	BL	1	Total 65	C 55	Mg 1	N 4	O 5	0
87	BL	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
87	BL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	BL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	CL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	CL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	CL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	CL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	CL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	CL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	CL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	CL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	CL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	CL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	CL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	CL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	CL	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
87	CL	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
87	CL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	CL	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
87	DL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	DL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	DL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	HL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	HL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
87	AN	1	Total	C	Mg	N	O	0
			45	36	1	4	4	
87	AN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
87	AN	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
87	AN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
87	AN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	AN	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	BN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	BN	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
87	BN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	BN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	BN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	BN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	BN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	BN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	BN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	BN	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
87	BN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	BN	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	BN	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
87	BN	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
87	BN	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
87	BN	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
87	BN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	BN	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	BN	1	Total	C	Mg	N	O	0
			43	35	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
87	BN	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
87	BN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	BN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	BN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	BN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	BN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	BN	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	BN	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
87	BN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	BN	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
87	BN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	BN	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
87	BN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	BN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	BN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	FN	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
87	FN	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	FN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	IN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	IN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	JN	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
87	KN	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	KN	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
87	KN	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
87	LN	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
87	LN	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	LN	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
87	LN	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
87	MN	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	ON	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
87	ON	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
87	ON	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	RN	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	RN	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	RN	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
87	RN	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	12	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	12	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	12	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	12	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
87	12	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	12	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
87	12	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
87	12	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
87	12	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
87	12	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	12	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	22	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	22	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	22	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	22	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
87	22	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
87	22	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	22	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	22	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	22	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
87	22	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
87	22	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
87	22	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	32	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	32	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	32	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	32	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
87	32	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
87	32	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	32	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	32	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
87	32	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
87	32	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
87	32	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	32	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	42	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	42	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	42	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	42	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
87	42	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	42	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	42	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	42	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
87	42	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
87	42	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
87	42	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	52	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	52	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
87	52	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	52	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
87	52	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	52	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	52	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
87	52	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
87	52	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
87	52	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	52	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	62	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	62	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	62	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	62	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	62	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
87	62	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	62	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	62	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	62	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
87	62	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
87	62	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
87	62	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
87	62	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	72	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	72	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	72	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	72	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
87	72	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	72	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	72	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
87	72	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
87	72	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
87	72	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	82	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	82	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	82	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	82	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	82	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	82	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
87	82	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
87	82	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			45	36	1	4	4	

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Mol	Chain	Residues	Atoms					AltConf
87	A2	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
87	A2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			51	41	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
87	A2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	A2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
87	B2	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
87	B2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	B2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	B2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	B2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	B2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	B2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	B2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	B2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
87	B2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	B2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	B2	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
87	B2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
87	B2	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
87	B2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
87	B2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	B2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	B2	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
87	B2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
87	B2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	B2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
87	B2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	B2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	B2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	B2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	B2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	B2	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
87	B2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	B2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
87	B2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	B2	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
87	B2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	B2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	B2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	F2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	F2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
87	F2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	I2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	I2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	J2	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
87	K2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	K2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
87	K2	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
87	K2	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
87	L2	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
87	L2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	L2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
87	L2	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
87	M2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	O2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
87	O2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
87	O2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	R2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	R2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	R2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
87	R2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	A6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	A6	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
87	A6	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
87	B6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	B6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	B6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	B6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
87	B6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	B6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	B6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	B6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	B6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	B6	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
87	B6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	B6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	B6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	B6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	C6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	C6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	C6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	C6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	C6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	C6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	C6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	C6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	C6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	C6	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
87	C6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
87	C6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	D6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	D6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	D6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	H6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	H6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	K6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	a6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	a6	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
87	a6	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
87	b6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	b6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	b6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	b6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	b6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	b6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	b6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	b6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	b6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	b6	1	Total	C	Mg	N	O	0
			59	49	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
87	b6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	b6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	b6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	b6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	c6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	c6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	c6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	c6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	c6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	c6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	c6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	c6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	c6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	c6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	c6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	c6	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
87	c6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
87	c6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	d6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	d6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	d6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	aL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
87	aL	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
87	bL	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
87	bL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	bL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	bL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	bL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	bL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	bL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	bL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	bL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	bL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	bL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	bL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	bL	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
87	bL	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
87	bL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	bL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	cL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	cL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	cL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	cL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	cL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
87	cL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	cL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	cL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	cL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	cL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	cL	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
87	cL	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
87	cL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	dL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	dL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	dL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	dL	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
87	nL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	1N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	1N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	1N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	1N	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
87	1N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	1N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	1N	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
87	1N	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
87	1N	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
87	1N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	1N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	2N	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
87	2N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	2N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	2N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	2N	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
87	2N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	2N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	2N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	2N	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
87	2N	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
87	2N	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
87	2N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	3N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	3N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	3N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	3N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	3N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	3N	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
87	3N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	3N	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
87	3N	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
87	3N	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
87	3N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	3N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	4N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	4N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	4N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	4N	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
87	4N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	4N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	4N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	4N	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
87	4N	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
87	4N	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
87	4N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	5N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	5N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	5N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	5N	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

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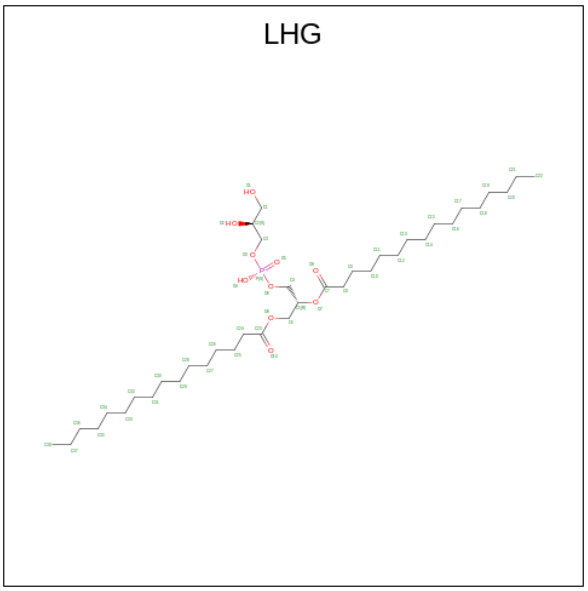
Mol	Chain	Residues	Atoms					AltConf
87	5N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	5N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	5N	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
87	5N	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
87	5N	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
87	5N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	5N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	6N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	6N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	6N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	6N	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
87	6N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	6N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	6N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	6N	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
87	6N	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
87	6N	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
87	6N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	6N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	6N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	7N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
87	7N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	7N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	7N	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
87	7N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	7N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	7N	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
87	7N	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
87	7N	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
87	7N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	8N	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
87	8N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	8N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
87	8N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	8N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	8N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
87	8N	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
87	8N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 88 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



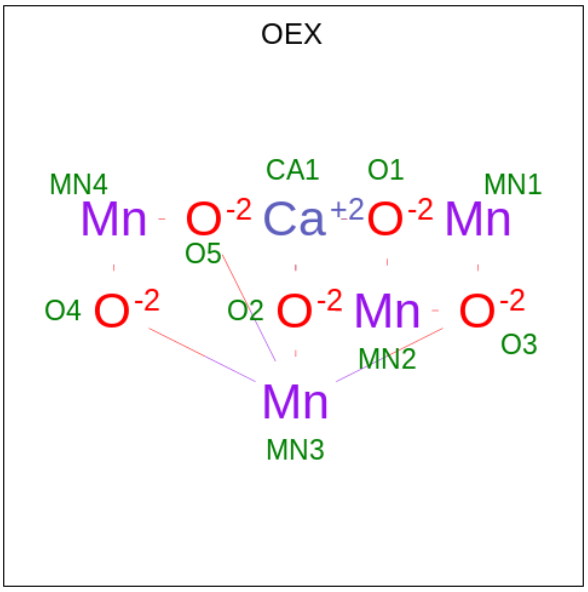
Mol	Chain	Residues	Atoms				AltConf
88	AL	1	Total	C	O	P	0
			49	38	10	1	
88	AL	1	Total	C	O	P	0
			43	32	10	1	
88	BL	1	Total	C	O	P	0
			49	38	10	1	
88	BL	1	Total	C	O	P	0
			41	30	10	1	
88	CL	1	Total	C	O	P	0
			37	26	10	1	
88	CL	1	Total	C	O	P	0
			32	21	10	1	
88	DL	1	Total	C	O	P	0
			49	38	10	1	
88	ML	1	Total	C	O	P	0
			39	28	10	1	
88	AN	1	Total	C	O	P	0
			49	38	10	1	
88	AN	1	Total	C	O	P	0
			40	29	10	1	
88	A2	1	Total	C	O	P	0
			49	38	10	1	
88	A2	1	Total	C	O	P	0
			40	29	10	1	
88	B6	1	Total	C	O	P	0
			49	38	10	1	
88	C6	1	Total	C	O	P	0
			37	26	10	1	

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Mol	Chain	Residues	Atoms	AltConf
88	C6	1	Total C O P 32 21 10 1	0
88	D6	1	Total C O P 43 32 10 1	0
88	D6	1	Total C O P 49 38 10 1	0
88	I6	1	Total C H O P 123 38 74 10 1	0
88	L6	1	Total C O P 49 38 10 1	0
88	M6	1	Total C O P 39 28 10 1	0
88	a6	1	Total C O P 43 32 10 1	0
88	c6	1	Total C O P 32 21 10 1	0
88	d6	1	Total C O P 46 35 10 1	0
88	d6	1	Total C O P 49 38 10 1	0
88	i6	1	Total C H O P 123 38 74 10 1	0
88	l6	1	Total C O P 49 38 10 1	0
88	m6	1	Total C O P 39 28 10 1	0
88	aL	1	Total C O P 43 32 10 1	0
88	bL	1	Total C O P 49 38 10 1	0
88	cL	1	Total C O P 32 21 10 1	0
88	dL	1	Total C O P 49 38 10 1	0
88	dL	1	Total C O P 46 35 10 1	0
88	iL	1	Total C O P 49 38 10 1	0
88	mL	1	Total C O P 39 28 10 1	0

- Molecule 89 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: $CaMn_4O_5$).

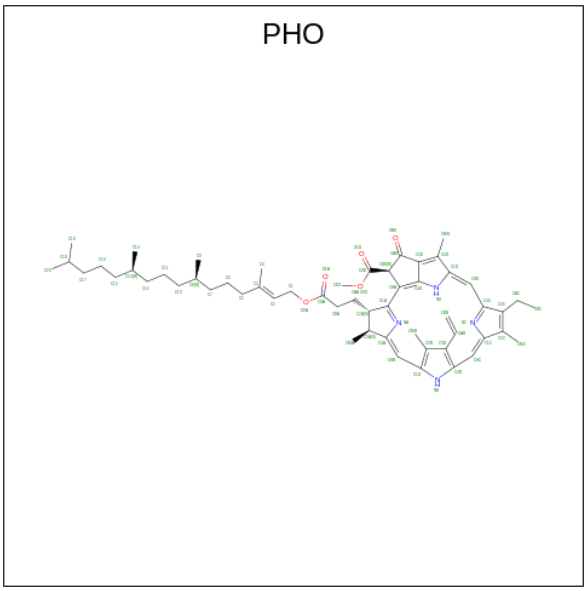


Mol	Chain	Residues	Atoms				AltConf
89	AL	1	Total	Ca	Mn	O	0
			10	1	4	5	
89	A6	1	Total	Ca	Mn	O	0
			10	1	4	5	
89	a6	1	Total	Ca	Mn	O	0
			10	1	4	5	
89	aL	1	Total	Ca	Mn	O	0
			10	1	4	5	

- Molecule 90 is FE (III) ION (CCD ID: FE) (formula: Fe).

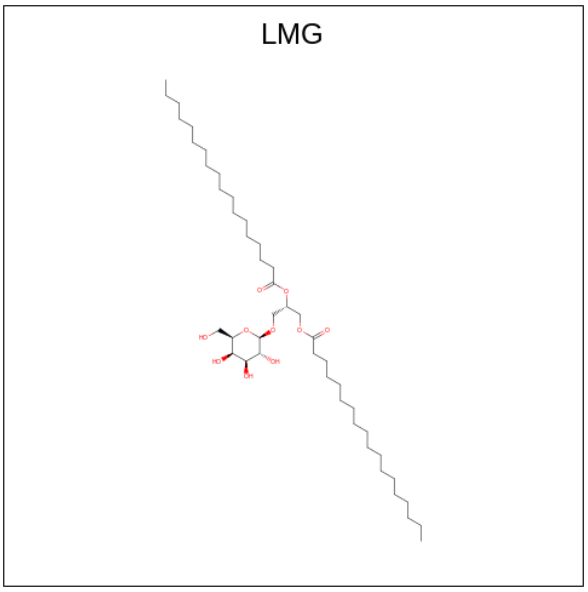
Mol	Chain	Residues	Atoms		AltConf
90	AL	1	Total	Fe	0
			1	1	
90	A6	1	Total	Fe	0
			1	1	
90	a6	1	Total	Fe	0
			1	1	
90	aL	1	Total	Fe	0
			1	1	

- Molecule 91 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



Mol	Chain	Residues	Atoms				AltConf
91	AL	1	Total	C	N	O	0
			64	55	4	5	
91	DL	1	Total	C	N	O	0
			64	55	4	5	
91	A6	1	Total	C	N	O	0
			64	55	4	5	
91	D6	1	Total	C	N	O	0
			64	55	4	5	
91	a6	1	Total	C	N	O	0
			64	55	4	5	
91	d6	1	Total	C	N	O	0
			64	55	4	5	
91	aL	1	Total	C	N	O	0
			64	55	4	5	
91	dL	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 92 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms	AltConf
92	AL	1	Total C O 51 41 10	0
92	BL	1	Total C O 40 30 10	0
92	BL	1	Total C O 39 29 10	0
92	CL	1	Total C O 55 45 10	0
92	DL	1	Total C O 54 44 10	0
92	JL	1	Total C O 43 33 10	0
92	JL	1	Total C O 33 23 10	0
92	ML	1	Total C O 41 31 10	0
92	XL	1	Total C O 50 40 10	0
92	A6	1	Total C O 51 41 10	0
92	B6	1	Total C O 40 30 10	0
92	B6	1	Total C O 39 29 10	0
92	B6	1	Total C O 50 40 10	0
92	C6	1	Total C O 55 45 10	0

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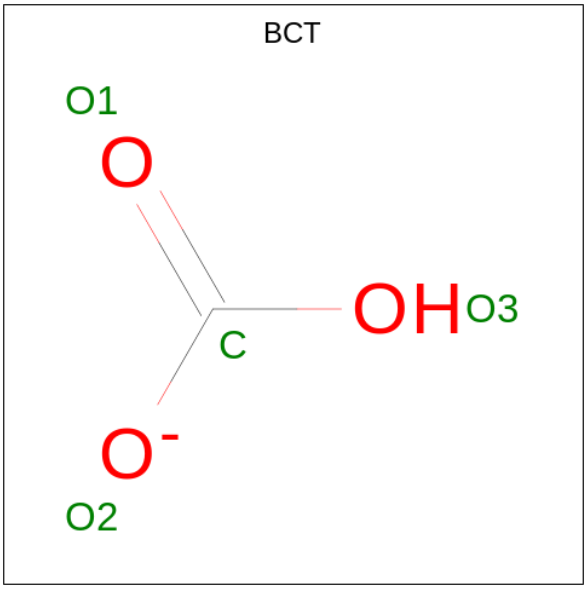
Mol	Chain	Residues	Atoms			AltConf
92	D6	1	Total	C	O	0
			33	23	10	
92	D6	1	Total	C	O	0
			54	44	10	
92	J6	1	Total	C	O	0
			43	33	10	
92	a6	1	Total	C	O	0
			42	32	10	
92	b6	1	Total	C	O	0
			41	31	10	
92	b6	1	Total	C	O	0
			39	29	10	
92	b6	1	Total	C	O	0
			41	31	10	
92	b6	1	Total	C	O	0
			36	26	10	
92	d6	1	Total	C	O	0
			54	44	10	
92	j6	1	Total	C	O	0
			43	33	10	
92	j6	1	Total	C	O	0
			33	23	10	
92	k6	1	Total	C	O	0
			55	45	10	
92	m6	1	Total	C	O	0
			41	31	10	
92	m6	1	Total	C	O	0
			41	31	10	
92	x6	1	Total	C	O	0
			50	40	10	
92	aL	1	Total	C	O	0
			42	32	10	
92	bL	1	Total	C	O	0
			41	31	10	
92	bL	1	Total	C	O	0
			41	31	10	
92	bL	1	Total	C	O	0
			50	40	10	
92	bL	1	Total	C	O	0
			41	31	10	
92	bL	1	Total	C	O	0
			39	29	10	

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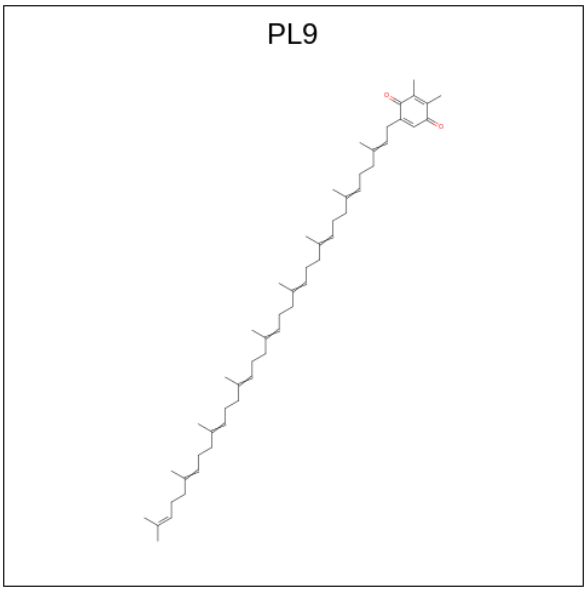
Mol	Chain	Residues	Atoms	AltConf
92	dL	1	Total C O 54 44 10	0
92	jL	1	Total C O 33 23 10	0
92	mL	1	Total C O 41 31 10	0
92	qL	1	Total C O 43 33 10	0
92	yL	1	Total C O 55 45 10	0

- Molecule 93 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



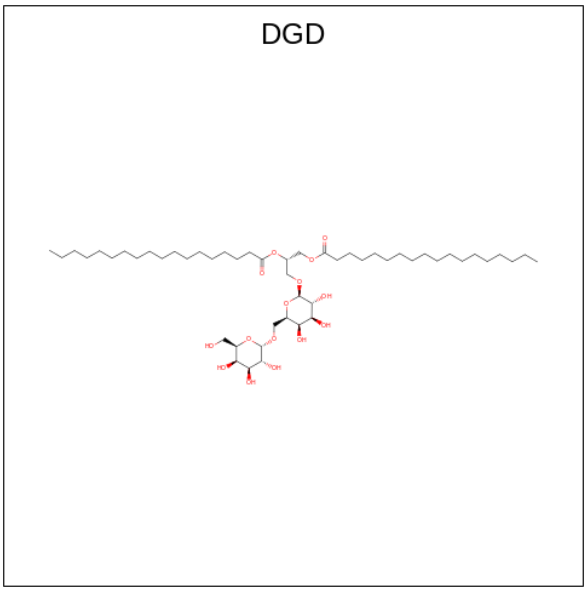
Mol	Chain	Residues	Atoms	AltConf
93	AL	1	Total C O 4 1 3	0
93	A6	1	Total C O 4 1 3	0
93	d6	1	Total C O 4 1 3	0
93	aL	1	Total C O 4 1 3	0

- Molecule 94 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$).



Mol	Chain	Residues	Atoms	AltConf
94	AL	1	Total C O 55 53 2	0
94	DL	1	Total C O 55 53 2	0
94	A6	1	Total C O 55 53 2	0
94	D6	1	Total C O 55 53 2	0
94	a6	1	Total C O 55 53 2	0
94	d6	1	Total C O 55 53 2	0
94	aL	1	Total C O 55 53 2	0
94	dL	1	Total C O 55 53 2	0

- Molecule 95 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms	AltConf
95	AL	1	Total C O 62 47 15	0
95	AL	1	Total C O 40 25 15	0
95	AL	1	Total C O 40 25 15	0
95	BL	1	Total C O 40 25 15	0
95	BL	1	Total C O 40 25 15	0
95	BL	1	Total C O 58 43 15	0
95	CL	1	Total C O 62 47 15	0
95	CL	1	Total C O 42 27 15	0
95	CL	1	Total C O 48 33 15	0
95	DL	1	Total C O 62 47 15	0
95	JL	1	Total C O 62 47 15	0
95	BN	1	Total C O 66 51 15	0
95	B2	1	Total C O 66 51 15	0
95	B6	1	Total C O 58 43 15	0

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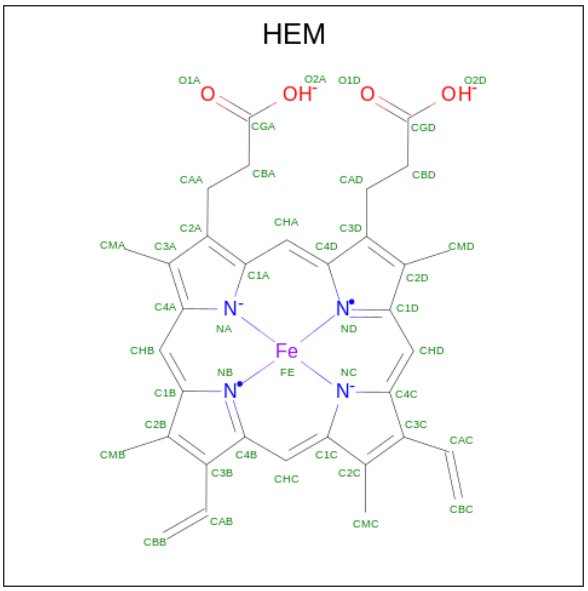
Mol	Chain	Residues	Atoms	AltConf
95	C6	1	Total C O 62 47 15	0
95	C6	1	Total C O 42 27 15	0
95	C6	1	Total C O 42 27 15	0
95	C6	1	Total C O 62 47 15	0
95	C6	1	Total C O 48 33 15	0
95	D6	1	Total C O 62 47 15	0
95	J6	1	Total C O 62 47 15	0
95	L6	1	Total C O 58 43 15	0
95	O6	1	Total C O 40 25 15	0
95	a6	1	Total C O 40 25 15	0
95	a6	1	Total C O 40 25 15	0
95	a6	1	Total C O 53 38 15	0
95	b6	1	Total C O 40 25 15	0
95	b6	1	Total C O 42 27 15	0
95	c6	1	Total C O 62 47 15	0
95	c6	1	Total C O 62 47 15	0
95	c6	1	Total C O 48 33 15	0
95	h6	1	Total C O 62 47 15	0
95	aL	1	Total C O 53 38 15	0
95	cL	1	Total C O 62 47 15	0
95	cL	1	Total C O 62 47 15	0

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Mol	Chain	Residues	Atoms	AltConf
95	cL	1	Total C O 48 33 15	0
95	hL	1	Total C O 62 47 15	0
95	lL	1	Total C O 58 43 15	0

- Molecule 96 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



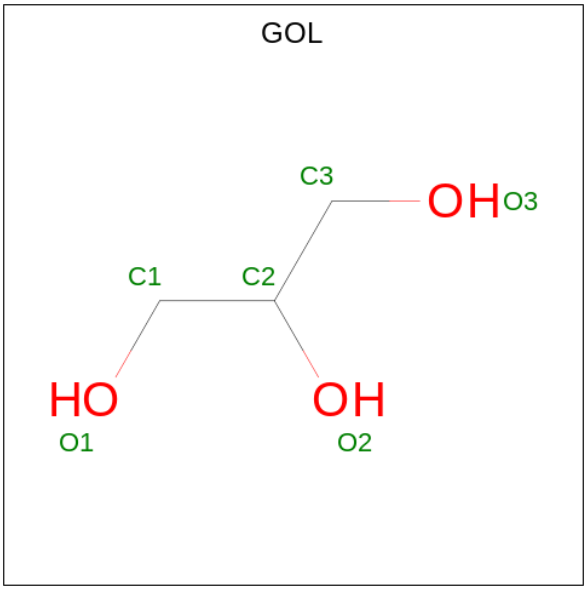
Mol	Chain	Residues	Atoms	AltConf
96	FL	1	Total C Fe N O 43 34 1 4 4	0
96	VL	1	Total C Fe N O 43 34 1 4 4	0
96	GN	1	Total C Fe N O 43 34 1 4 4	0
96	G2	1	Total C Fe N O 43 34 1 4 4	0
96	E6	1	Total C Fe H N O 73 34 1 30 4 4	0
96	V6	1	Total C Fe N O 43 34 1 4 4	0
96	f6	1	Total C Fe H N O 73 34 1 30 4 4	0
96	v6	1	Total C Fe N O 43 34 1 4 4	0

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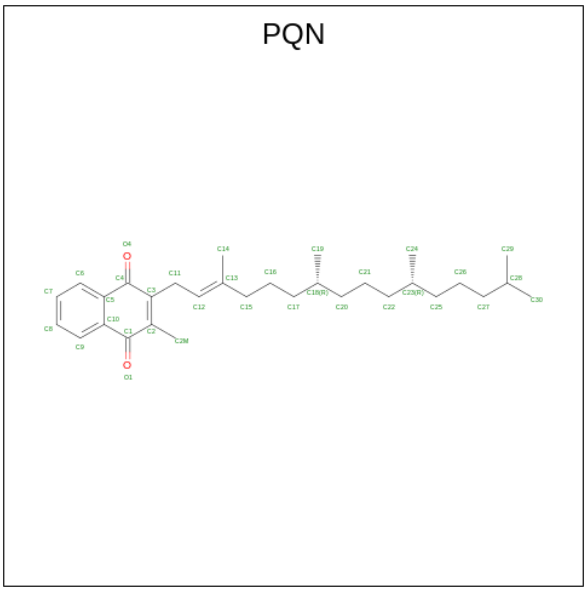
Mol	Chain	Residues	Atoms					AltConf
96	fL	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
96	vL	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 97 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



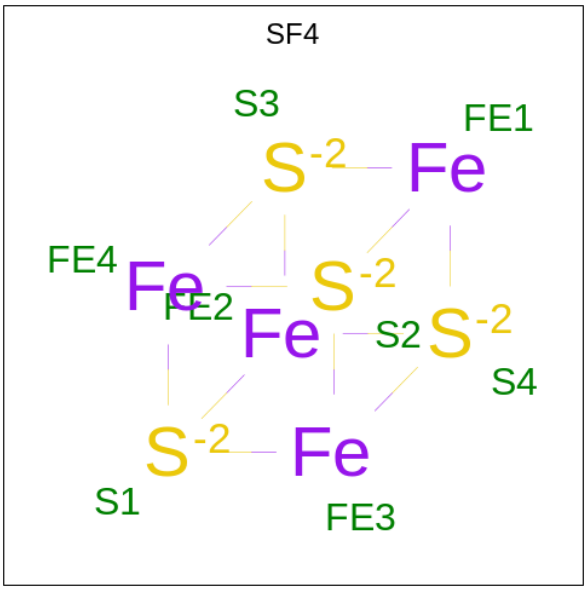
Mol	Chain	Residues	Atoms			AltConf
97	WL	1	Total	C	O	0
			6	3	3	
97	I6	1	Total	C	O	0
			6	3	3	
97	i6	1	Total	C	O	0
			6	3	3	
97	wL	1	Total	C	O	0
			6	3	3	

- Molecule 98 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



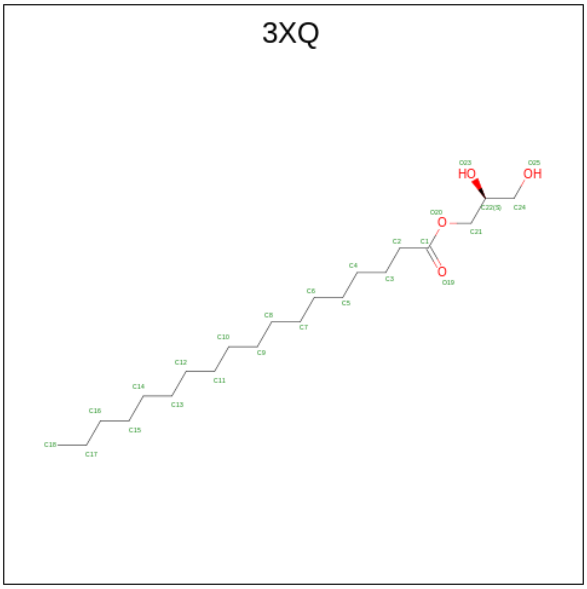
Mol	Chain	Residues	Atoms	AltConf
98	AN	1	Total C O 33 31 2	0
98	BN	1	Total C O 33 31 2	0
98	A2	1	Total C O 33 31 2	0
98	B2	1	Total C O 33 31 2	0

- Molecule 99 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



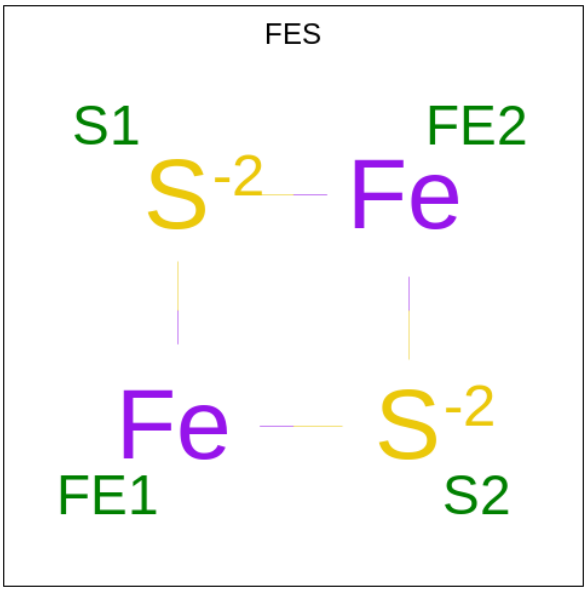
Mol	Chain	Residues	Atoms	AltConf
99	BN	1	Total Fe S 8 4 4	0
99	CN	1	Total Fe S 8 4 4	0
99	CN	1	Total Fe S 8 4 4	0
99	B2	1	Total Fe S 8 4 4	0
99	C2	1	Total Fe S 8 4 4	0
99	C2	1	Total Fe S 8 4 4	0

- Molecule 100 is (2S)-2,3-dihydroxypropyl octadecanoate (CCD ID: 3XQ) (formula: $C_{21}H_{42}O_4$) (labeled as "Ligand of Interest" by depositor).



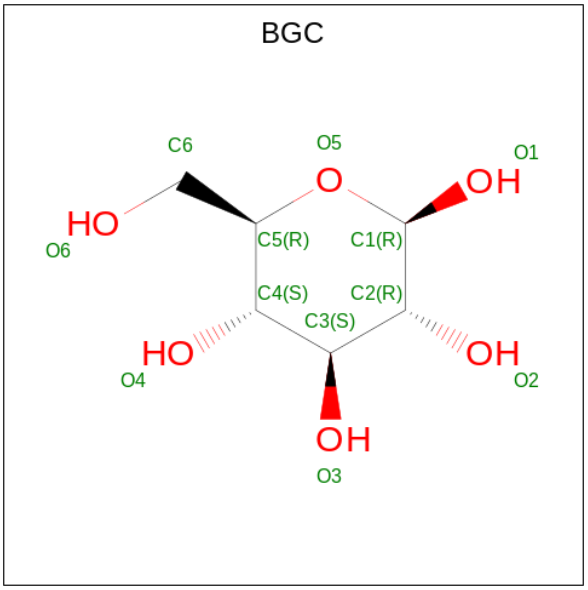
Mol	Chain	Residues	Atoms	AltConf
100	JN	1	Total C O 25 21 4	0
100	J2	1	Total C O 25 21 4	0

- Molecule 101 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



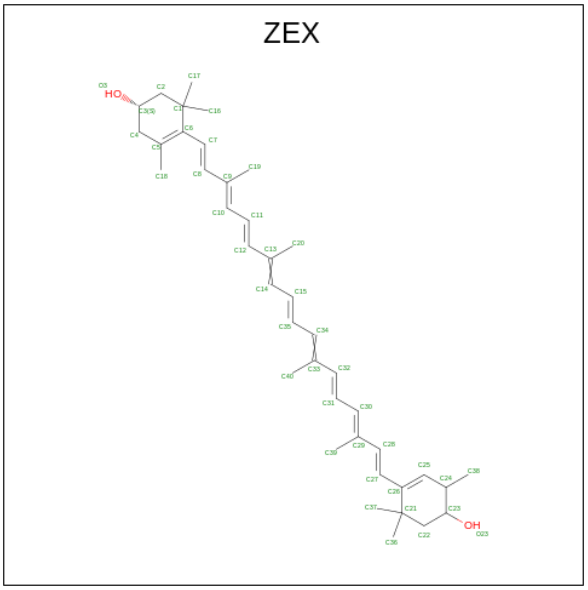
Mol	Chain	Residues	Atoms	AltConf
101	NN	1	Total Fe S 4 2 2	0
101	N2	1	Total Fe S 4 2 2	0

- Molecule 102 is beta-D-glucopyranose (CCD ID: BGC) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	AltConf
102	32	1	Total C O 11 6 5	0
102	3N	1	Total C O 11 6 5	0

- Molecule 103 is (1R,2S)-4-{(1E,3E,5E,7E,9E,11E,13E,15E,17E)-18-[(4S)-4-hydroxy-2,6,6-trimethylcyclohex-1-en-1-yl]-3,7,12,16-tetramethyloctadeca-1,3,5,7,9,11,13,15,17-nonaen-1-yl}-2,5,5-trimethylcyclohex-3-en-1-ol (CCD ID: ZEX) (formula: $C_{40}H_{56}O_2$).



Mol	Chain	Residues	Atoms	AltConf
103	82	1	Total C O 42 40 2	0
103	82	1	Total C O 42 40 2	0
103	8N	1	Total C O 42 40 2	0
103	8N	1	Total C O 42 40 2	0

- Molecule 104 is water.

Mol	Chain	Residues	Atoms	AltConf
104	a6	2	Total O 2 2	0
104	aL	2	Total O 2 2	0

MolProbity failed to run properly - this section is therefore empty.

3 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	215000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	35	Depositor
Minimum defocus (nm)	6000	Depositor
Maximum defocus (nm)	6000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	11.570	Depositor
Minimum map value	-4.947	Depositor
Average map value	0.045	Depositor
Map value standard deviation	0.418	Depositor
Recommended contour level	1	Depositor
Map size (Å)	626.688, 626.688, 626.688	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.632, 1.632, 1.632	Depositor

4 Model quality

4.1 Standard geometry

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles

4.3.1 Protein backbone

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains

346 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	MEN	RB	72	2	7,8,9	0.79	0	6,9,11	1.08	1 (16%)
2	MEN	kG	72	2	7,8,9	0.88	0	6,9,11	1.48	1 (16%)
10	MEN	D1	72	10	7,8,9	0.86	0	6,9,11	1.58	2 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MEN	B9	72	2	7,8,9	1.15	0	6,9,11	1.95	2 (33%)
2	MEN	u8	72	2	7,8,9	0.90	0	6,9,11	1.24	1 (16%)
2	MEN	fF	72	2,82	7,8,9	1.31	1 (14%)	6,9,11	2.30	2 (33%)
2	MEN	XB	72	2	7,8,9	0.66	0	6,9,11	1.14	1 (16%)
2	MEN	YO	72	2	7,8,9	0.83	0	6,9,11	1.46	1 (16%)
2	MEN	dB	72	2	7,8,9	0.69	0	6,9,11	0.88	0
2	MEN	JP	72	2	7,8,9	0.85	0	6,9,11	1.58	1 (16%)
2	MEN	V1	72	2	7,8,9	0.85	0	6,9,11	1.62	2 (33%)
2	MEN	m1	72	2	7,8,9	0.86	0	6,9,11	1.32	1 (16%)
2	MEN	X7	72	2	7,8,9	0.93	0	6,9,11	1.61	2 (33%)
2	MEN	OQ	72	2	7,8,9	0.92	0	6,9,11	1.29	2 (33%)
2	MEN	hK	72	2,82	7,8,9	1.18	1 (14%)	6,9,11	0.88	0
2	MEN	R7	72	2	7,8,9	0.92	0	6,9,11	1.19	0
2	MEN	q8	72	2	7,8,9	0.92	0	6,9,11	1.66	1 (16%)
2	MEN	F7	72	2	7,8,9	1.01	0	6,9,11	1.62	2 (33%)
2	MEN	rK	72	2,82	7,8,9	1.23	1 (14%)	6,9,11	1.00	1 (16%)
2	MEN	VM	72	2	7,8,9	0.86	0	6,9,11	1.65	1 (16%)
10	MEN	LO	72	10	7,8,9	0.85	0	6,9,11	1.84	2 (33%)
2	MEN	W9	72	2	7,8,9	0.92	0	6,9,11	1.32	1 (16%)
2	MEN	J9	72	2	7,8,9	0.96	0	6,9,11	1.26	1 (16%)
2	MEN	iJ	72	2	7,8,9	0.86	0	6,9,11	1.38	1 (16%)
2	MEN	IB	72	2	7,8,9	0.78	0	6,9,11	1.08	1 (16%)
2	MEN	g4	72	2	7,8,9	0.90	0	6,9,11	1.40	1 (16%)
2	MEN	eE	72	2	7,8,9	0.84	0	6,9,11	1.48	1 (16%)
2	MEN	RG	72	2	7,8,9	0.91	0	6,9,11	1.46	1 (16%)
2	MEN	lF	72	2,82	7,8,9	1.04	0	6,9,11	1.70	2 (33%)
2	MEN	DJ	72	2	7,8,9	0.89	0	6,9,11	1.18	0
2	MEN	IQ	72	2	7,8,9	0.87	0	6,9,11	1.67	1 (16%)
2	MEN	HM	72	2	7,8,9	0.87	0	6,9,11	1.62	1 (16%)
10	MEN	HO	72	10	7,8,9	0.87	0	6,9,11	1.66	1 (16%)
69	MEN	S3	71	69	7,8,9	27.44	6 (85%)	6,9,11	17.30	6 (100%)
2	MEN	KQ	72	2	7,8,9	0.88	0	6,9,11	1.41	1 (16%)
2	MEN	VF	72	2,82	7,8,9	1.38	1 (14%)	6,9,11	1.60	1 (16%)
2	MEN	RP	72	2	7,8,9	0.85	0	6,9,11	1.86	2 (33%)
69	MEN	h3	71	69	7,8,9	13.86	3 (42%)	6,9,11	17.17	6 (100%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MEN	VH	72	2	7,8,9	0.86	0	6,9,11	1.63	2 (33%)
2	MEN	aE	72	2	7,8,9	0.86	0	6,9,11	1.68	2 (33%)
2	MEN	k1	72	2	7,8,9	0.91	0	6,9,11	1.08	1 (16%)
2	MEN	dK	72	2,82	7,8,9	1.43	1 (14%)	6,9,11	2.13	1 (16%)
2	MEN	w8	72	2	7,8,9	0.93	0	6,9,11	0.94	0
2	MEN	DA	72	2	7,8,9	0.89	0	6,9,11	1.08	1 (16%)
2	MEN	cM	72	2	7,8,9	0.91	0	6,9,11	1.39	1 (16%)
69	MEN	d3	71	69	7,8,9	13.86	3 (42%)	6,9,11	17.16	6 (100%)
2	MEN	k4	72	2	7,8,9	0.90	0	6,9,11	1.49	1 (16%)
2	MEN	QD	72	2	7,8,9	0.82	0	6,9,11	1.70	2 (33%)
2	MEN	YH	72	2	7,8,9	0.95	0	6,9,11	1.30	1 (16%)
2	MEN	WD	72	2	7,8,9	0.89	0	6,9,11	1.43	1 (16%)
2	MEN	PE	72	2	7,8,9	0.83	0	6,9,11	1.59	1 (16%)
69	MEN	F3	71	69	7,8,9	13.86	3 (42%)	6,9,11	17.17	6 (100%)
2	MEN	QB	72	2	7,8,9	0.83	0	6,9,11	0.86	0
2	MEN	MB	72	2	7,8,9	0.69	0	6,9,11	0.97	0
2	MEN	DF	72	2,82	7,8,9	1.58	1 (14%)	6,9,11	2.43	2 (33%)
2	MEN	JI	72	2	7,8,9	0.89	0	6,9,11	1.61	2 (33%)
2	MEN	VG	72	2	7,8,9	0.82	0	6,9,11	1.51	2 (33%)
2	MEN	R4	72	2	7,8,9	0.88	0	6,9,11	1.43	2 (33%)
10	MEN	DG	72	11,10	7,8,9	0.88	0	6,9,11	1.60	2 (33%)
2	MEN	OB	72	2	7,8,9	0.82	0	6,9,11	1.13	1 (16%)
69	MEN	D3	71	69	7,8,9	13.87	3 (42%)	6,9,11	17.16	6 (100%)
2	MEN	LB	72	2	7,8,9	0.74	0	6,9,11	1.14	1 (16%)
10	MEN	LH	72	10	7,8,9	0.91	0	6,9,11	2.59	2 (33%)
10	MEN	N1	72	10	7,8,9	0.98	0	6,9,11	1.12	0
2	MEN	g1	72	2	7,8,9	0.91	0	6,9,11	1.62	2 (33%)
2	MEN	cE	72	2	7,8,9	0.88	0	6,9,11	1.08	1 (16%)
2	MEN	bF	72	2	7,8,9	0.92	0	6,9,11	1.29	1 (16%)
2	MEN	XA	72	2	7,8,9	0.90	0	6,9,11	1.59	2 (33%)
10	MEN	JH	72	10	7,8,9	0.83	0	6,9,11	1.65	1 (16%)
2	MEN	P1	72	2	7,8,9	0.88	0	6,9,11	1.68	2 (33%)
69	MEN	j3	71	69	7,8,9	13.85	3 (42%)	6,9,11	17.17	6 (100%)
2	MEN	FB	72	2	7,8,9	0.76	0	6,9,11	0.98	0
2	MEN	SQ	72	2	7,8,9	0.95	0	6,9,11	1.34	1 (16%)
2	MEN	TP	72	2	7,8,9	0.88	0	6,9,11	1.46	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MEN	gM	72	2	7,8,9	0.85	0	6,9,11	1.67	2 (33%)
10	MEN	LG	72	10	7,8,9	0.95	0	6,9,11	1.62	2 (33%)
2	MEN	eG	72	2	7,8,9	0.83	0	6,9,11	1.48	1 (16%)
2	MEN	Q5	72	2	7,8,9	0.92	0	6,9,11	1.68	1 (16%)
10	MEN	N4	72	10	7,8,9	0.93	0	6,9,11	1.40	2 (33%)
2	MEN	RA	72	2	7,8,9	0.91	0	6,9,11	1.19	0
2	MEN	YQ	72	2	7,8,9	0.88	0	6,9,11	1.63	1 (16%)
2	MEN	VJ	72	2	7,8,9	0.87	0	6,9,11	1.53	1 (16%)
2	MEN	gE	72	2	7,8,9	0.88	0	6,9,11	1.55	1 (16%)
2	MEN	FM	72	2	7,8,9	0.87	0	6,9,11	1.53	1 (16%)
2	MEN	BF	72	2,82	7,8,9	1.62	1 (14%)	6,9,11	3.01	1 (16%)
2	MEN	D5	72	2	7,8,9	0.86	0	6,9,11	1.50	1 (16%)
2	MEN	H9	72	2	7,8,9	0.92	0	6,9,11	1.49	2 (33%)
69	MEN	M3	71	69	7,8,9	13.85	3 (42%)	6,9,11	17.17	6 (100%)
2	MEN	NJ	72	2	7,8,9	0.94	0	6,9,11	1.54	2 (33%)
2	MEN	nF	72	2,82	7,8,9	1.41	1 (14%)	6,9,11	1.45	1 (16%)
10	MEN	DO	72	10	7,8,9	0.90	0	6,9,11	1.36	2 (33%)
2	MEN	TH	72	2	7,8,9	0.92	0	6,9,11	1.79	2 (33%)
2	MEN	L9	72	2	7,8,9	1.07	0	6,9,11	1.89	2 (33%)
2	MEN	MD	72	2	7,8,9	0.85	0	6,9,11	1.73	2 (33%)
2	MEN	fK	72	2,82	7,8,9	1.28	1 (14%)	6,9,11	2.31	2 (33%)
2	MEN	TE	72	2	7,8,9	0.95	0	6,9,11	1.41	1 (16%)
10	MEN	JO	72	10	7,8,9	0.84	0	6,9,11	1.85	2 (33%)
2	MEN	UI	72	2	7,8,9	0.91	0	6,9,11	1.34	1 (16%)
2	MEN	Y9	72	2	7,8,9	0.96	0	6,9,11	1.26	1 (16%)
2	MEN	jF	72	2,82	7,8,9	1.32	1 (14%)	6,9,11	1.79	2 (33%)
2	MEN	uC	72	2	7,8,9	0.93	0	6,9,11	1.24	1 (16%)
2	MEN	tF	72	2,82	7,8,9	1.18	1 (14%)	6,9,11	1.41	1 (16%)
2	MEN	e1	72	2	7,8,9	0.91	0	6,9,11	1.27	1 (16%)
2	MEN	ZK	72	2	7,8,9	0.91	0	6,9,11	1.41	1 (16%)
2	MEN	GQ	72	2	7,8,9	0.88	0	6,9,11	1.79	2 (33%)
2	MEN	mG	72	2	7,8,9	0.90	0	6,9,11	1.40	1 (16%)
2	MEN	U9	72	2	7,8,9	0.94	0	6,9,11	1.29	2 (33%)
2	MEN	iO	72	2	7,8,9	0.88	0	6,9,11	1.48	1 (16%)
2	MEN	iM	72	2	7,8,9	0.83	0	6,9,11	1.44	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MEN	ZJ	72	2	7,8,9	0.91	0	6,9,11	1.30	1 (16%)
2	MEN	RF	72	2,82	7,8,9	1.77	1 (14%)	6,9,11	3.13	2 (33%)
2	MEN	HI	72	2	7,8,9	0.89	0	6,9,11	1.37	1 (16%)
2	MEN	wC	72	2	7,8,9	0.94	0	6,9,11	0.94	0
2	MEN	LA	72	2	7,8,9	0.89	0	6,9,11	1.18	0
69	MEN	H3	71	69	7,8,9	13.85	3 (42%)	6,9,11	17.17	6 (100%)
2	MEN	1C	72	2	7,8,9	0.90	0	6,9,11	1.46	2 (33%)
2	MEN	cJ	72	2	7,8,9	0.88	0	6,9,11	1.25	1 (16%)
2	MEN	FK	72	2,82	7,8,9	1.91	1 (14%)	6,9,11	3.71	3 (50%)
2	MEN	JM	72	2	7,8,9	0.88	0	6,9,11	1.67	2 (33%)
2	MEN	BK	72	2,82	7,8,9	1.61	1 (14%)	6,9,11	3.01	1 (16%)
2	MEN	s8	72	2	7,8,9	0.88	0	6,9,11	1.41	2 (33%)
2	MEN	NP	72	2	7,8,9	0.89	0	6,9,11	1.53	1 (16%)
2	MEN	FJ	72	2	7,8,9	0.88	0	6,9,11	1.67	1 (16%)
2	MEN	PF	72	2,82	7,8,9	1.54	1 (14%)	6,9,11	2.54	2 (33%)
2	MEN	V4	72	2	7,8,9	0.89	0	6,9,11	1.32	2 (33%)
2	MEN	XK	72	2,82	7,8,9	1.93	1 (14%)	6,9,11	3.18	2 (33%)
2	MEN	T7	72	2,75	7,8,9	0.86	0	6,9,11	3.08	2 (33%)
2	MEN	dF	72	2,82	7,8,9	1.42	1 (14%)	6,9,11	2.13	1 (16%)
2	MEN	BB	72	2	7,8,9	0.80	0	6,9,11	1.25	1 (16%)
69	MEN	L3	71	69	7,8,9	13.86	3 (42%)	6,9,11	17.17	6 (100%)
2	MEN	RO	72	2	7,8,9	0.86	0	6,9,11	1.46	2 (33%)
2	MEN	S5	72	2	7,8,9	0.92	0	6,9,11	1.79	1 (16%)
10	MEN	J4	72	10	7,8,9	0.87	0	6,9,11	1.85	2 (33%)
2	MEN	O9	72	2	7,8,9	0.99	0	6,9,11	1.72	2 (33%)
10	MEN	FH	72	10	7,8,9	0.89	0	6,9,11	1.40	1 (16%)
2	MEN	Y5	72	2	7,8,9	0.86	0	6,9,11	1.86	1 (16%)
2	MEN	D9	72	2	7,8,9	0.96	0	6,9,11	1.31	1 (16%)
10	MEN	NG	72	10	7,8,9	0.86	0	6,9,11	1.51	2 (33%)
2	MEN	T1	72	2	7,8,9	0.95	0	6,9,11	1.81	2 (33%)
69	MEN	f3	71	69	7,8,9	13.86	3 (42%)	6,9,11	17.16	6 (100%)
2	MEN	eJ	72	2	7,8,9	0.91	0	6,9,11	1.50	2 (33%)
2	MEN	bB	72	2	7,8,9	0.68	0	6,9,11	0.75	0
2	MEN	ID	72	2	7,8,9	0.83	0	6,9,11	1.63	1 (16%)
2	MEN	TM	72	2	7,8,9	0.87	0	6,9,11	1.24	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MEN	rF	72	2,82	7,8,9	1.28	1 (14%)	6,9,11	0.98	1 (16%)
2	MEN	UQ	72	2	7,8,9	0.96	0	6,9,11	1.65	1 (16%)
10	MEN	J1	72	10	7,8,9	0.84	0	6,9,11	1.68	1 (16%)
2	MEN	aH	72	2	7,8,9	0.91	0	6,9,11	1.34	1 (16%)
10	MEN	HH	72	10	7,8,9	0.85	0	6,9,11	1.53	1 (16%)
10	MEN	L1	72	10	7,8,9	0.86	0	6,9,11	2.62	2 (33%)
2	MEN	gJ	72	2	7,8,9	0.87	0	6,9,11	1.46	1 (16%)
2	MEN	FF	72	2,82	7,8,9	1.95	1 (14%)	6,9,11	3.67	3 (50%)
10	MEN	JG	72	10	7,8,9	0.88	0	6,9,11	1.53	1 (16%)
2	MEN	TJ	72	2	7,8,9	0.87	0	6,9,11	1.34	1 (16%)
2	MEN	iG	72	2	7,8,9	0.93	0	6,9,11	1.19	1 (16%)
2	MEN	NB	72	2	7,8,9	0.81	0	6,9,11	0.44	0
2	MEN	KD	72	2	7,8,9	0.88	0	6,9,11	1.44	1 (16%)
10	MEN	H4	72	10	7,8,9	0.87	0	6,9,11	1.69	2 (33%)
2	MEN	DM	72	2	7,8,9	0.90	0	6,9,11	1.27	1 (16%)
2	MEN	hF	72	2,82	7,8,9	1.22	1 (14%)	6,9,11	0.85	0
2	MEN	qC	72	2	7,8,9	0.91	0	6,9,11	1.65	1 (16%)
69	MEN	I3	71	69	7,8,9	13.86	3 (42%)	6,9,11	17.16	6 (100%)
2	MEN	c1	72	2	7,8,9	0.83	0	6,9,11	1.84	1 (16%)
2	MEN	HJ	72	2	7,8,9	0.87	0	6,9,11	1.88	1 (16%)
2	MEN	WI	72	2	7,8,9	0.88	0	6,9,11	1.42	1 (16%)
2	MEN	aB	72	2	7,8,9	0.82	0	6,9,11	0.78	0
2	MEN	LF	72	2,82	7,8,9	1.80	1 (14%)	6,9,11	3.80	3 (50%)
2	MEN	DI	72	2	7,8,9	0.97	0	6,9,11	1.24	1 (16%)
2	MEN	CQ	72	2	7,8,9	0.85	0	6,9,11	1.47	2 (33%)
69	MEN	n3	71	69	7,8,9	13.86	3 (42%)	6,9,11	17.17	6 (100%)
2	MEN	FI	72	2	7,8,9	0.93	0	6,9,11	1.52	1 (16%)
2	MEN	gH	72	2	7,8,9	0.91	0	6,9,11	1.63	2 (33%)
2	MEN	kO	72	2	7,8,9	0.85	0	6,9,11	1.50	1 (16%)
2	MEN	TG	72	2	7,8,9	0.95	0	6,9,11	1.44	1 (16%)
69	MEN	O3	71	69	7,8,9	0.68	0	6,9,11	0.78	0
2	MEN	CD	72	2	7,8,9	0.84	0	6,9,11	1.48	2 (33%)
2	MEN	GB	72	2	7,8,9	0.79	0	6,9,11	1.29	1 (16%)
2	MEN	J5	72	2	7,8,9	0.87	0	6,9,11	1.59	2 (33%)
2	MEN	kJ	72	2	7,8,9	0.83	0	6,9,11	1.41	2 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MEN	mH	72	2	7,8,9	0.84	0	6,9,11	1.31	1 (16%)
2	MEN	L7	72	2	7,8,9	0.88	0	6,9,11	1.20	0
2	MEN	PJ	72	2	7,8,9	0.88	0	6,9,11	1.48	1 (16%)
69	MEN	B3	71	69	7,8,9	13.86	3 (42%)	6,9,11	17.17	6 (100%)
2	MEN	B5	72	2	7,8,9	0.81	0	6,9,11	1.89	1 (16%)
2	MEN	B7	72	2	7,8,9	0.95	0	6,9,11	1.13	1 (16%)
2	MEN	RM	72	2	7,8,9	0.88	0	6,9,11	1.29	1 (16%)
2	MEN	YD	72	2	7,8,9	0.91	0	6,9,11	1.66	1 (16%)
2	MEN	WQ	72	2	7,8,9	0.91	0	6,9,11	1.42	1 (16%)
2	MEN	cO	72	2	7,8,9	0.91	0	6,9,11	1.29	1 (16%)
2	MEN	lK	72	2,82	7,8,9	1.02	0	6,9,11	1.69	2 (33%)
2	MEN	FP	72	2	7,8,9	0.88	0	6,9,11	1.70	1 (16%)
2	MEN	PM	72	2	7,8,9	0.88	0	6,9,11	1.56	2 (33%)
10	MEN	NH	72	10	7,8,9	0.97	0	6,9,11	1.13	0
2	MEN	LK	72	2,82	7,8,9	1.80	1 (14%)	6,9,11	3.80	3 (50%)
2	MEN	VO	72	2	7,8,9	0.94	0	6,9,11	1.36	2 (33%)
2	MEN	LP	72	2	7,8,9	0.86	0	6,9,11	1.56	1 (16%)
69	MEN	U3	71	69	7,8,9	27.43	6 (85%)	6,9,11	17.30	6 (100%)
10	MEN	FG	72	10	7,8,9	0.91	0	6,9,11	1.57	1 (16%)
2	MEN	H7	72	2	7,8,9	0.91	0	6,9,11	1.77	1 (16%)
69	MEN	q3	71	69	7,8,9	13.86	3 (42%)	6,9,11	17.17	6 (100%)
2	MEN	mM	72	2	7,8,9	0.87	0	6,9,11	1.65	1 (16%)
2	MEN	VB	72	2	7,8,9	0.77	0	6,9,11	0.90	1 (16%)
2	MEN	CB	72	2	7,8,9	0.71	0	6,9,11	1.14	1 (16%)
2	MEN	HF	72	2,82	7,8,9	1.58	1 (14%)	6,9,11	2.45	2 (33%)
2	MEN	Y1	72	2	7,8,9	0.94	0	6,9,11	1.28	1 (16%)
2	MEN	QI	72	2	7,8,9	1.01	0	6,9,11	1.18	1 (16%)
10	MEN	NO	72	10	7,8,9	0.90	0	6,9,11	1.40	2 (33%)
2	MEN	nK	72	2,82	7,8,9	1.39	1 (14%)	6,9,11	1.50	1 (16%)
2	MEN	YG	72	2	7,8,9	0.94	0	6,9,11	1.32	1 (16%)
2	MEN	Y4	72	2	7,8,9	0.85	0	6,9,11	1.45	1 (16%)
2	MEN	vF	72	2,82	7,8,9	1.40	1 (14%)	6,9,11	1.17	1 (16%)
2	MEN	pK	72	2,82	7,8,9	1.11	0	6,9,11	1.35	1 (16%)
2	MEN	HA	72	2	7,8,9	0.90	0	6,9,11	1.76	1 (16%)
2	MEN	T4	72	2	7,8,9	0.81	0	6,9,11	1.62	2 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MEN	kM	72	2	7,8,9	0.88	0	6,9,11	1.45	1 (16%)
69	MEN	o3	71	69	7,8,9	13.86	3 (42%)	6,9,11	17.16	6 (100%)
2	MEN	yC	72	2	7,8,9	0.99	0	6,9,11	1.22	1 (16%)
2	MEN	pF	72	2,82	7,8,9	1.11	0	6,9,11	1.34	1 (16%)
2	MEN	H5	72	2	7,8,9	0.85	0	6,9,11	1.78	2 (33%)
2	MEN	PA	72	2	7,8,9	0.85	0	6,9,11	1.45	1 (16%)
2	MEN	SD	72	2	7,8,9	0.95	0	6,9,11	1.35	1 (16%)
2	MEN	eH	72	2	7,8,9	0.92	0	6,9,11	1.28	1 (16%)
2	MEN	bK	72	2	7,8,9	0.92	0	6,9,11	1.31	1 (16%)
2	MEN	N7	72	2	7,8,9	0.92	0	6,9,11	1.45	1 (16%)
2	MEN	P7	72	2	7,8,9	0.85	0	6,9,11	1.45	1 (16%)
69	MEN	u3	71	69	7,8,9	27.42	6 (85%)	6,9,11	17.29	6 (100%)
2	MEN	VP	72	2	7,8,9	0.88	0	6,9,11	1.50	1 (16%)
2	MEN	O5	72	2	7,8,9	0.84	0	6,9,11	1.71	1 (16%)
2	MEN	PG	72	2	7,8,9	0.85	0	6,9,11	1.62	1 (16%)
2	MEN	LJ	72	2	7,8,9	0.92	0	6,9,11	1.38	2 (33%)
10	MEN	JE	72	10	7,8,9	0.86	0	6,9,11	1.53	1 (16%)
2	MEN	mE	72	2	7,8,9	0.89	0	6,9,11	1.41	1 (16%)
2	MEN	i4	72	2	7,8,9	0.85	0	6,9,11	1.47	1 (16%)
2	MEN	eB	72	2	7,8,9	0.68	0	6,9,11	1.23	1 (16%)
2	MEN	TO	72	2	7,8,9	0.81	0	6,9,11	1.63	2 (33%)
2	MEN	VA	72	2	7,8,9	0.87	0	6,9,11	1.40	1 (16%)
2	MEN	e4	72	2	7,8,9	0.87	0	6,9,11	1.62	2 (33%)
2	MEN	U5	72	2	7,8,9	0.90	0	6,9,11	1.72	1 (16%)
2	MEN	NA	72	2	7,8,9	0.93	0	6,9,11	1.47	1 (16%)
2	MEN	SB	72	2	7,8,9	0.78	0	6,9,11	0.98	0
2	MEN	c4	72	2	7,8,9	0.87	0	6,9,11	1.29	1 (16%)
2	MEN	F9	72	2	7,8,9	0.88	0	6,9,11	1.68	2 (33%)
2	MEN	gB	72	2	7,8,9	0.65	0	6,9,11	0.75	0
10	MEN	F1	72	10	7,8,9	0.92	0	6,9,11	1.39	1 (16%)
2	MEN	PK	72	2,82	7,8,9	1.57	1 (14%)	6,9,11	2.54	2 (33%)
2	MEN	V7	72	2	7,8,9	0.85	0	6,9,11	1.39	1 (16%)
2	MEN	jK	72	2,82	7,8,9	1.29	1 (14%)	6,9,11	1.81	1 (16%)
10	MEN	D4	72	10	7,8,9	0.87	0	6,9,11	1.34	2 (33%)
2	MEN	y8	72	2	7,8,9	0.99	0	6,9,11	1.24	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
69	MEN	k3	71	69	7,8,9	13.85	3 (42%)	6,9,11	17.17	6 (100%)
2	MEN	NM	72	2	7,8,9	0.87	0	6,9,11	1.42	2 (33%)
2	MEN	BI	72	2	7,8,9	0.87	0	6,9,11	1.49	1 (16%)
2	MEN	P4	72	2	7,8,9	0.89	0	6,9,11	1.25	0
2	MEN	J7	72	2	7,8,9	0.85	0	6,9,11	1.41	1 (16%)
2	MEN	RE	72	2	7,8,9	0.92	0	6,9,11	1.47	1 (16%)
2	MEN	HK	72	2,82	7,8,9	1.57	1 (14%)	6,9,11	2.47	2 (33%)
2	MEN	R1	72	2	7,8,9	0.83	0	6,9,11	1.14	1 (16%)
2	MEN	XP	72	2	7,8,9	0.87	0	6,9,11	1.69	1 (16%)
2	MEN	aG	72	2	7,8,9	0.87	0	6,9,11	1.70	2 (33%)
2	MEN	YB	72	2	7,8,9	0.84	0	6,9,11	1.38	1 (16%)
2	MEN	JA	72	2	7,8,9	0.86	0	6,9,11	1.43	1 (16%)
2	MEN	HB	72	2	7,8,9	0.83	0	6,9,11	1.20	1 (16%)
2	MEN	m4	72	2	7,8,9	0.91	0	6,9,11	1.56	2 (33%)
2	MEN	iE	72	2	7,8,9	0.93	0	6,9,11	1.20	1 (16%)
2	MEN	vK	72	2,82	7,8,9	1.42	1 (14%)	6,9,11	1.13	0
2	MEN	18	72	2	7,8,9	0.90	0	6,9,11	1.46	2 (33%)
2	MEN	F5	72	2	7,8,9	0.87	0	6,9,11	1.70	1 (16%)
2	MEN	gO	72	2	7,8,9	0.90	0	6,9,11	1.39	1 (16%)
2	MEN	PH	72	2	7,8,9	0.88	0	6,9,11	1.68	2 (33%)
2	MEN	DB	72	2	7,8,9	0.83	0	6,9,11	1.23	0
2	MEN	RH	72	2	7,8,9	0.82	0	6,9,11	1.14	1 (16%)
2	MEN	FA	72	2	7,8,9	1.01	0	6,9,11	1.63	2 (33%)
2	MEN	RK	72	2,82	7,8,9	1.77	1 (14%)	6,9,11	3.13	2 (33%)
2	MEN	eO	72	2	7,8,9	0.87	0	6,9,11	1.62	2 (33%)
2	MEN	DP	72	2	7,8,9	0.88	0	6,9,11	1.60	1 (16%)
2	MEN	kH	72	2	7,8,9	0.93	0	6,9,11	1.11	1 (16%)
2	MEN	SI	72	2	7,8,9	0.88	0	6,9,11	1.54	1 (16%)
2	MEN	YE	72	2	7,8,9	0.93	0	6,9,11	1.31	1 (16%)
10	MEN	H1	72	10	7,8,9	0.85	0	6,9,11	1.53	1 (16%)
2	MEN	mO	72	2	7,8,9	0.88	0	6,9,11	1.54	2 (33%)
2	MEN	eM	72	2	7,8,9	0.86	0	6,9,11	1.57	1 (16%)
69	MEN	w3	71	69	7,8,9	27.42	6 (85%)	6,9,11	17.29	6 (100%)
2	MEN	NF	72	2,82	7,8,9	1.50	1 (14%)	6,9,11	2.71	2 (33%)
2	MEN	D7	72	2	7,8,9	0.87	0	6,9,11	1.08	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MEN	YI	72	2	7,8,9	0.97	0	6,9,11	1.38	2 (33%)
2	MEN	EQ	72	2	7,8,9	0.88	0	6,9,11	1.45	1 (16%)
2	MEN	GD	72	2	7,8,9	0.83	0	6,9,11	1.76	2 (33%)
2	MEN	OI	72	2	7,8,9	0.92	0	6,9,11	1.35	1 (16%)
2	MEN	NK	72	2,82	7,8,9	1.52	1 (14%)	6,9,11	2.76	3 (50%)
2	MEN	VE	72	2	7,8,9	0.81	0	6,9,11	1.52	2 (33%)
2	MEN	ZB	72	2	7,8,9	0.65	0	6,9,11	0.55	0
2	MEN	UD	72	2	7,8,9	0.94	0	6,9,11	1.66	1 (16%)
2	MEN	TA	72	2,75	7,8,9	0.86	0	6,9,11	3.06	2 (33%)
2	MEN	LM	72	2	7,8,9	0.86	0	6,9,11	1.44	1 (16%)
2	MEN	cG	72	2	7,8,9	0.90	0	6,9,11	1.10	1 (16%)
2	MEN	tK	72	2,82	7,8,9	1.19	1 (14%)	6,9,11	1.45	1 (16%)
2	MEN	BA	72	2	7,8,9	0.93	0	6,9,11	1.12	1 (16%)
69	MEN	Q3	71	69	7,8,9	27.43	6 (85%)	6,9,11	17.29	6 (100%)
2	MEN	PP	72	2	7,8,9	0.90	0	6,9,11	1.50	1 (16%)
2	MEN	XM	72	2	7,8,9	0.87	0	6,9,11	1.56	2 (33%)
2	MEN	ZM	72	2	7,8,9	0.87	0	6,9,11	1.60	1 (16%)
10	MEN	FE	72	10	7,8,9	0.86	0	6,9,11	1.53	1 (16%)
10	MEN	DH	72	10	7,8,9	0.86	0	6,9,11	1.59	2 (33%)
2	MEN	L5	72	2	7,8,9	0.90	0	6,9,11	1.94	1 (16%)
2	MEN	TK	72	2,82	7,8,9	1.39	1 (14%)	6,9,11	2.25	2 (33%)
69	MEN	s3	71	69	7,8,9	27.44	6 (85%)	6,9,11	17.29	6 (100%)
2	MEN	DK	72	2,82	7,8,9	1.57	1 (14%)	6,9,11	2.45	2 (33%)
10	MEN	FO	72	10	7,8,9	0.89	0	6,9,11	1.55	1 (16%)
2	MEN	ED	72	2	7,8,9	0.82	0	6,9,11	1.44	1 (16%)
2	MEN	mJ	72	2	7,8,9	0.90	0	6,9,11	1.41	1 (16%)
2	MEN	OD	72	2	7,8,9	0.92	0	6,9,11	1.29	2 (33%)
2	MEN	TF	72	2,82	7,8,9	1.39	1 (14%)	6,9,11	2.24	2 (33%)
2	MEN	VK	72	2,82	7,8,9	1.39	1 (14%)	6,9,11	1.60	1 (16%)
2	MEN	BP	72	2	7,8,9	0.87	0	6,9,11	1.54	1 (16%)
10	MEN	HE	72	10	7,8,9	0.89	0	6,9,11	1.39	1 (16%)
2	MEN	RJ	72	2	7,8,9	0.91	0	6,9,11	1.57	1 (16%)
2	MEN	PB	72	2	7,8,9	0.79	0	6,9,11	0.93	0
2	MEN	aO	72	2	7,8,9	0.87	0	6,9,11	1.47	2 (33%)
2	MEN	W5	72	2	7,8,9	0.92	0	6,9,11	1.70	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MEN	HP	72	2	7,8,9	0.87	0	6,9,11	1.50	1 (16%)
2	MEN	Q9	72	2	7,8,9	0.94	0	6,9,11	1.37	2 (33%)
2	MEN	iH	72	2	7,8,9	0.83	0	6,9,11	1.42	1 (16%)
10	MEN	L4	72	10	7,8,9	0.82	0	6,9,11	1.86	2 (33%)
2	MEN	JJ	72	2	7,8,9	0.87	0	6,9,11	1.61	2 (33%)
2	MEN	a1	72	2	7,8,9	0.92	0	6,9,11	1.33	1 (16%)
2	MEN	a4	72	2	7,8,9	0.86	0	6,9,11	1.45	2 (33%)
10	MEN	LE	72	10	7,8,9	0.96	0	6,9,11	1.65	2 (33%)
10	MEN	NE	72	10	7,8,9	0.85	0	6,9,11	1.52	2 (33%)
2	MEN	sC	72	2	7,8,9	0.87	0	6,9,11	1.42	2 (33%)
2	MEN	PO	72	2	7,8,9	0.93	0	6,9,11	1.22	0
2	MEN	ZF	72	2	7,8,9	0.89	0	6,9,11	1.35	1 (16%)
2	MEN	QQ	72	2	7,8,9	0.81	0	6,9,11	1.69	2 (33%)
2	MEN	i1	72	2	7,8,9	0.85	0	6,9,11	1.39	1 (16%)
2	MEN	S9	72	2	7,8,9	0.95	0	6,9,11	1.36	1 (16%)
2	MEN	JK	72	2,82	7,8,9	1.49	1 (14%)	6,9,11	2.15	2 (33%)
2	MEN	LI	72	2	7,8,9	0.97	0	6,9,11	1.68	2 (33%)
10	MEN	DE	72	11,10	7,8,9	0.86	0	6,9,11	1.60	2 (33%)
10	MEN	F4	72	10	7,8,9	0.90	0	6,9,11	1.52	1 (16%)
2	MEN	XF	72	2,82	7,8,9	1.93	1 (14%)	6,9,11	3.17	2 (33%)
2	MEN	XJ	72	2	7,8,9	0.89	0	6,9,11	1.64	2 (33%)
2	MEN	cH	72	2	7,8,9	0.82	0	6,9,11	1.85	1 (16%)
2	MEN	JF	72	2,82	7,8,9	1.46	1 (14%)	6,9,11	2.20	2 (33%)
2	MEN	gG	72	2	7,8,9	0.84	0	6,9,11	1.53	1 (16%)
2	MEN	kE	72	2	7,8,9	0.90	0	6,9,11	1.47	1 (16%)
10	MEN	HG	72	10	7,8,9	0.91	0	6,9,11	1.44	2 (33%)
2	MEN	MQ	72	2	7,8,9	0.89	0	6,9,11	1.74	2 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MEN	RB	72	2	-	7/7/8/10	-
2	MEN	kG	72	2	-	4/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	MEN	D1	72	10	-	4/7/8/10	-
2	MEN	B9	72	2	-	4/7/8/10	-
2	MEN	u8	72	2	-	3/7/8/10	-
2	MEN	fF	72	2,82	-	2/7/8/10	-
2	MEN	XB	72	2	-	5/7/8/10	-
2	MEN	YO	72	2	-	4/7/8/10	-
2	MEN	dB	72	2	-	5/7/8/10	-
2	MEN	JP	72	2	-	4/7/8/10	-
2	MEN	V1	72	2	-	4/7/8/10	-
2	MEN	m1	72	2	-	4/7/8/10	-
2	MEN	X7	72	2	-	4/7/8/10	-
2	MEN	OQ	72	2	-	2/7/8/10	-
2	MEN	hK	72	2,82	-	2/7/8/10	-
2	MEN	R7	72	2	-	4/7/8/10	-
2	MEN	q8	72	2	-	3/7/8/10	-
2	MEN	F7	72	2	-	4/7/8/10	-
2	MEN	rK	72	2,82	-	3/7/8/10	-
2	MEN	VM	72	2	-	4/7/8/10	-
10	MEN	LO	72	10	-	4/7/8/10	-
2	MEN	W9	72	2	-	2/7/8/10	-
2	MEN	J9	72	2	-	2/7/8/10	-
2	MEN	iJ	72	2	-	4/7/8/10	-
2	MEN	IB	72	2	-	4/7/8/10	-
2	MEN	g4	72	2	-	4/7/8/10	-
2	MEN	eE	72	2	-	2/7/8/10	-
2	MEN	RG	72	2	-	3/7/8/10	-
2	MEN	lF	72	2,82	-	4/7/8/10	-
2	MEN	DJ	72	2	-	3/7/8/10	-
2	MEN	IQ	72	2	-	4/7/8/10	-
2	MEN	HM	72	2	-	4/7/8/10	-
10	MEN	HO	72	10	-	2/7/8/10	-
69	MEN	S3	71	69	-	6/7/8/10	-
2	MEN	KQ	72	2	-	4/7/8/10	-
2	MEN	VF	72	2,82	-	4/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MEN	RP	72	2	-	4/7/8/10	-
69	MEN	h3	71	69	-	5/7/8/10	-
2	MEN	VH	72	2	-	4/7/8/10	-
2	MEN	aE	72	2	-	4/7/8/10	-
2	MEN	k1	72	2	-	4/7/8/10	-
2	MEN	dK	72	2,82	-	3/7/8/10	-
2	MEN	w8	72	2	-	2/7/8/10	-
2	MEN	DA	72	2	-	3/7/8/10	-
2	MEN	cM	72	2	-	4/7/8/10	-
69	MEN	d3	71	69	-	5/7/8/10	-
2	MEN	k4	72	2	-	5/7/8/10	-
2	MEN	QD	72	2	-	4/7/8/10	-
2	MEN	YH	72	2	-	4/7/8/10	-
2	MEN	WD	72	2	-	4/7/8/10	-
2	MEN	PE	72	2	-	3/7/8/10	-
69	MEN	F3	71	69	-	4/7/8/10	-
2	MEN	QB	72	2	-	6/7/8/10	-
2	MEN	MB	72	2	-	2/7/8/10	-
2	MEN	DF	72	2,82	-	2/7/8/10	-
2	MEN	JI	72	2	-	5/7/8/10	-
2	MEN	VG	72	2	-	4/7/8/10	-
2	MEN	R4	72	2	-	4/7/8/10	-
10	MEN	DG	72	11,10	-	4/7/8/10	-
2	MEN	OB	72	2	-	4/7/8/10	-
69	MEN	D3	71	69	-	5/7/8/10	-
2	MEN	LB	72	2	-	4/7/8/10	-
10	MEN	LH	72	10	-	2/7/8/10	-
10	MEN	N1	72	10	-	2/7/8/10	-
2	MEN	g1	72	2	-	3/7/8/10	-
2	MEN	cE	72	2	-	3/7/8/10	-
2	MEN	bF	72	2	-	4/7/8/10	-
2	MEN	XA	72	2	-	4/7/8/10	-
10	MEN	JH	72	10	-	1/7/8/10	-
2	MEN	P1	72	2	-	4/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
69	MEN	j3	71	69	-	4/7/8/10	-
2	MEN	FB	72	2	-	3/7/8/10	-
2	MEN	SQ	72	2	-	4/7/8/10	-
2	MEN	TP	72	2	-	4/7/8/10	-
2	MEN	gM	72	2	-	5/7/8/10	-
10	MEN	LG	72	10	-	4/7/8/10	-
2	MEN	eG	72	2	-	2/7/8/10	-
2	MEN	Q5	72	2	-	4/7/8/10	-
10	MEN	N4	72	10	-	3/7/8/10	-
2	MEN	RA	72	2	-	4/7/8/10	-
2	MEN	YQ	72	2	-	4/7/8/10	-
2	MEN	VJ	72	2	-	4/7/8/10	-
2	MEN	gE	72	2	-	4/7/8/10	-
2	MEN	FM	72	2	-	4/7/8/10	-
2	MEN	BF	72	2,82	-	2/7/8/10	-
2	MEN	D5	72	2	-	4/7/8/10	-
2	MEN	H9	72	2	-	2/7/8/10	-
69	MEN	M3	71	69	-	4/7/8/10	-
2	MEN	NJ	72	2	-	5/7/8/10	-
2	MEN	nF	72	2,82	-	3/7/8/10	-
10	MEN	DO	72	10	-	2/7/8/10	-
2	MEN	TH	72	2	-	5/7/8/10	-
2	MEN	L9	72	2	-	2/7/8/10	-
2	MEN	MD	72	2	-	2/7/8/10	-
2	MEN	fK	72	2,82	-	2/7/8/10	-
2	MEN	TE	72	2	-	3/7/8/10	-
10	MEN	JO	72	10	-	2/7/8/10	-
2	MEN	UI	72	2	-	4/7/8/10	-
2	MEN	Y9	72	2	-	2/7/8/10	-
2	MEN	jF	72	2,82	-	4/7/8/10	-
2	MEN	uC	72	2	-	3/7/8/10	-
2	MEN	tF	72	2,82	-	4/7/8/10	-
2	MEN	e1	72	2	-	3/7/8/10	-
2	MEN	ZK	72	2	-	5/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MEN	GQ	72	2	-	4/7/8/10	-
2	MEN	mG	72	2	-	3/7/8/10	-
2	MEN	U9	72	2	-	2/7/8/10	-
2	MEN	iO	72	2	-	4/7/8/10	-
2	MEN	iM	72	2	-	4/7/8/10	-
2	MEN	ZJ	72	2	-	4/7/8/10	-
2	MEN	RF	72	2,82	-	2/7/8/10	-
2	MEN	HI	72	2	-	4/7/8/10	-
2	MEN	wC	72	2	-	2/7/8/10	-
2	MEN	LA	72	2	-	5/7/8/10	-
69	MEN	H3	71	69	-	4/7/8/10	-
2	MEN	1C	72	2	-	4/7/8/10	-
2	MEN	cJ	72	2	-	4/7/8/10	-
2	MEN	FK	72	2,82	-	2/7/8/10	-
2	MEN	JM	72	2	-	4/7/8/10	-
2	MEN	BK	72	2,82	-	2/7/8/10	-
2	MEN	s8	72	2	-	2/7/8/10	-
2	MEN	NP	72	2	-	4/7/8/10	-
2	MEN	FJ	72	2	-	4/7/8/10	-
2	MEN	PF	72	2,82	-	3/7/8/10	-
2	MEN	V4	72	2	-	2/7/8/10	-
2	MEN	XK	72	2,82	-	2/7/8/10	-
2	MEN	T7	72	2,75	-	6/7/8/10	-
2	MEN	dF	72	2,82	-	3/7/8/10	-
2	MEN	BB	72	2	-	5/7/8/10	-
69	MEN	L3	71	69	-	4/7/8/10	-
2	MEN	RO	72	2	-	4/7/8/10	-
2	MEN	S5	72	2	-	4/7/8/10	-
10	MEN	J4	72	10	-	2/7/8/10	-
2	MEN	O9	72	2	-	4/7/8/10	-
10	MEN	FH	72	10	-	2/7/8/10	-
2	MEN	Y5	72	2	-	4/7/8/10	-
2	MEN	D9	72	2	-	2/7/8/10	-
10	MEN	NG	72	10	-	4/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MEN	T1	72	2	-	5/7/8/10	-
69	MEN	f3	71	69	-	4/7/8/10	-
2	MEN	eJ	72	2	-	4/7/8/10	-
2	MEN	bB	72	2	-	4/7/8/10	-
2	MEN	ID	72	2	-	4/7/8/10	-
2	MEN	TM	72	2	-	3/7/8/10	-
2	MEN	rF	72	2,82	-	3/7/8/10	-
2	MEN	UQ	72	2	-	3/7/8/10	-
10	MEN	J1	72	10	-	1/7/8/10	-
2	MEN	aH	72	2	-	3/7/8/10	-
10	MEN	HH	72	10	-	4/7/8/10	-
10	MEN	L1	72	10	-	2/7/8/10	-
2	MEN	gJ	72	2	-	2/7/8/10	-
2	MEN	FF	72	2,82	-	2/7/8/10	-
10	MEN	JG	72	10	-	2/7/8/10	-
2	MEN	TJ	72	2	-	5/7/8/10	-
2	MEN	iG	72	2	-	3/7/8/10	-
2	MEN	NB	72	2	-	3/7/8/10	-
2	MEN	KD	72	2	-	4/7/8/10	-
10	MEN	H4	72	10	-	2/7/8/10	-
2	MEN	DM	72	2	-	5/7/8/10	-
2	MEN	hF	72	2,82	-	2/7/8/10	-
2	MEN	qC	72	2	-	3/7/8/10	-
69	MEN	I3	71	69	-	5/7/8/10	-
2	MEN	c1	72	2	-	4/7/8/10	-
2	MEN	HJ	72	2	-	4/7/8/10	-
2	MEN	WI	72	2	-	5/7/8/10	-
2	MEN	aB	72	2	-	4/7/8/10	-
2	MEN	LF	72	2,82	-	3/7/8/10	-
2	MEN	DI	72	2	-	4/7/8/10	-
2	MEN	CQ	72	2	-	4/7/8/10	-
69	MEN	n3	71	69	-	4/7/8/10	-
2	MEN	FI	72	2	-	5/7/8/10	-
2	MEN	gH	72	2	-	3/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MEN	kO	72	2	-	5/7/8/10	-
2	MEN	TG	72	2	-	3/7/8/10	-
69	MEN	O3	71	69	-	2/7/8/10	-
2	MEN	CD	72	2	-	4/7/8/10	-
2	MEN	GB	72	2	-	6/7/8/10	-
2	MEN	J5	72	2	-	5/7/8/10	-
2	MEN	kJ	72	2	-	4/7/8/10	-
2	MEN	mH	72	2	-	4/7/8/10	-
2	MEN	L7	72	2	-	5/7/8/10	-
2	MEN	PJ	72	2	-	4/7/8/10	-
69	MEN	B3	71	69	-	5/7/8/10	-
2	MEN	B5	72	2	-	4/7/8/10	-
2	MEN	B7	72	2	-	4/7/8/10	-
2	MEN	RM	72	2	-	4/7/8/10	-
2	MEN	YD	72	2	-	4/7/8/10	-
2	MEN	WQ	72	2	-	4/7/8/10	-
2	MEN	cO	72	2	-	2/7/8/10	-
2	MEN	lK	72	2,82	-	4/7/8/10	-
2	MEN	FP	72	2	-	5/7/8/10	-
2	MEN	PM	72	2	-	5/7/8/10	-
10	MEN	NH	72	10	-	2/7/8/10	-
2	MEN	LK	72	2,82	-	3/7/8/10	-
2	MEN	VO	72	2	-	2/7/8/10	-
2	MEN	LP	72	2	-	4/7/8/10	-
69	MEN	U3	71	69	-	6/7/8/10	-
10	MEN	FG	72	10	-	3/7/8/10	-
2	MEN	H7	72	2	-	4/7/8/10	-
69	MEN	q3	71	69	-	5/7/8/10	-
2	MEN	mM	72	2	-	4/7/8/10	-
2	MEN	VB	72	2	-	4/7/8/10	-
2	MEN	CB	72	2	-	2/7/8/10	-
2	MEN	HF	72	2,82	-	2/7/8/10	-
2	MEN	Y1	72	2	-	4/7/8/10	-
2	MEN	QI	72	2	-	4/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	MEN	NO	72	10	-	3/7/8/10	-
2	MEN	nK	72	2,82	-	3/7/8/10	-
2	MEN	YG	72	2	-	5/7/8/10	-
2	MEN	Y4	72	2	-	4/7/8/10	-
2	MEN	vF	72	2,82	-	1/7/8/10	-
2	MEN	pK	72	2,82	-	3/7/8/10	-
2	MEN	HA	72	2	-	4/7/8/10	-
2	MEN	T4	72	2	-	3/7/8/10	-
2	MEN	kM	72	2	-	4/7/8/10	-
69	MEN	o3	71	69	-	5/7/8/10	-
2	MEN	yC	72	2	-	3/7/8/10	-
2	MEN	pF	72	2,82	-	3/7/8/10	-
2	MEN	H5	72	2	-	4/7/8/10	-
2	MEN	PA	72	2	-	4/7/8/10	-
2	MEN	SD	72	2	-	4/7/8/10	-
2	MEN	eH	72	2	-	3/7/8/10	-
2	MEN	bK	72	2	-	4/7/8/10	-
2	MEN	N7	72	2	-	4/7/8/10	-
2	MEN	P7	72	2	-	4/7/8/10	-
69	MEN	u3	71	69	-	6/7/8/10	-
2	MEN	VP	72	2	-	4/7/8/10	-
2	MEN	O5	72	2	-	4/7/8/10	-
2	MEN	PG	72	2	-	3/7/8/10	-
2	MEN	LJ	72	2	-	5/7/8/10	-
10	MEN	JE	72	10	-	2/7/8/10	-
2	MEN	mE	72	2	-	3/7/8/10	-
2	MEN	i4	72	2	-	4/7/8/10	-
2	MEN	eB	72	2	-	3/7/8/10	-
2	MEN	TO	72	2	-	3/7/8/10	-
2	MEN	VA	72	2	-	4/7/8/10	-
2	MEN	e4	72	2	-	5/7/8/10	-
2	MEN	U5	72	2	-	4/7/8/10	-
2	MEN	NA	72	2	-	4/7/8/10	-
2	MEN	SB	72	2	-	3/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MEN	c4	72	2	-	2/7/8/10	-
2	MEN	F9	72	2	-	2/7/8/10	-
2	MEN	gB	72	2	-	5/7/8/10	-
10	MEN	F1	72	10	-	2/7/8/10	-
2	MEN	PK	72	2,82	-	3/7/8/10	-
2	MEN	V7	72	2	-	4/7/8/10	-
2	MEN	jK	72	2,82	-	4/7/8/10	-
10	MEN	D4	72	10	-	2/7/8/10	-
2	MEN	y8	72	2	-	3/7/8/10	-
69	MEN	k3	71	69	-	4/7/8/10	-
2	MEN	NM	72	2	-	4/7/8/10	-
2	MEN	BI	72	2	-	5/7/8/10	-
2	MEN	P4	72	2	-	4/7/8/10	-
2	MEN	J7	72	2	-	1/7/8/10	-
2	MEN	RE	72	2	-	3/7/8/10	-
2	MEN	HK	72	2,82	-	2/7/8/10	-
2	MEN	R1	72	2	-	2/7/8/10	-
2	MEN	XP	72	2	-	4/7/8/10	-
2	MEN	aG	72	2	-	4/7/8/10	-
2	MEN	YB	72	2	-	4/7/8/10	-
2	MEN	JA	72	2	-	1/7/8/10	-
2	MEN	HB	72	2	-	2/7/8/10	-
2	MEN	m4	72	2	-	4/7/8/10	-
2	MEN	iE	72	2	-	3/7/8/10	-
2	MEN	vK	72	2,82	-	1/7/8/10	-
2	MEN	18	72	2	-	4/7/8/10	-
2	MEN	F5	72	2	-	4/7/8/10	-
2	MEN	gO	72	2	-	4/7/8/10	-
2	MEN	PH	72	2	-	4/7/8/10	-
2	MEN	DB	72	2	-	4/7/8/10	-
2	MEN	RH	72	2	-	2/7/8/10	-
2	MEN	FA	72	2	-	4/7/8/10	-
2	MEN	RK	72	2,82	-	2/7/8/10	-
2	MEN	eO	72	2	-	5/7/8/10	-
2	MEN	DP	72	2	-	4/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MEN	kH	72	2	-	4/7/8/10	-
2	MEN	SI	72	2	-	4/7/8/10	-
2	MEN	YE	72	2	-	5/7/8/10	-
10	MEN	H1	72	10	-	4/7/8/10	-
2	MEN	mO	72	2	-	4/7/8/10	-
2	MEN	eM	72	2	-	4/7/8/10	-
69	MEN	w3	71	69	-	6/7/8/10	-
2	MEN	NF	72	2,82	-	2/7/8/10	-
2	MEN	D7	72	2	-	3/7/8/10	-
2	MEN	YI	72	2	-	3/7/8/10	-
2	MEN	EQ	72	2	-	3/7/8/10	-
2	MEN	GD	72	2	-	4/7/8/10	-
2	MEN	OI	72	2	-	5/7/8/10	-
2	MEN	NK	72	2,82	-	2/7/8/10	-
2	MEN	VE	72	2	-	4/7/8/10	-
2	MEN	ZB	72	2	-	6/7/8/10	-
2	MEN	UD	72	2	-	3/7/8/10	-
2	MEN	TA	72	2,75	-	6/7/8/10	-
2	MEN	LM	72	2	-	4/7/8/10	-
2	MEN	cG	72	2	-	3/7/8/10	-
2	MEN	tK	72	2,82	-	4/7/8/10	-
2	MEN	BA	72	2	-	4/7/8/10	-
69	MEN	Q3	71	69	-	6/7/8/10	-
2	MEN	PP	72	2	-	4/7/8/10	-
2	MEN	XM	72	2	-	4/7/8/10	-
2	MEN	ZM	72	2	-	5/7/8/10	-
10	MEN	FE	72	10	-	3/7/8/10	-
10	MEN	DH	72	10	-	4/7/8/10	-
2	MEN	L5	72	2	-	4/7/8/10	-
2	MEN	TK	72	2,82	-	2/7/8/10	-
69	MEN	s3	71	69	-	6/7/8/10	-
2	MEN	DK	72	2,82	-	2/7/8/10	-
10	MEN	FO	72	10	-	3/7/8/10	-
2	MEN	ED	72	2	-	3/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MEN	mJ	72	2	-	4/7/8/10	-
2	MEN	OD	72	2	-	2/7/8/10	-
2	MEN	TF	72	2,82	-	2/7/8/10	-
2	MEN	VK	72	2,82	-	4/7/8/10	-
2	MEN	BP	72	2	-	4/7/8/10	-
10	MEN	HE	72	10	-	4/7/8/10	-
2	MEN	RJ	72	2	-	4/7/8/10	-
2	MEN	PB	72	2	-	4/7/8/10	-
2	MEN	aO	72	2	-	3/7/8/10	-
2	MEN	W5	72	2	-	4/7/8/10	-
2	MEN	HP	72	2	-	4/7/8/10	-
2	MEN	Q9	72	2	-	2/7/8/10	-
2	MEN	iH	72	2	-	4/7/8/10	-
10	MEN	L4	72	10	-	4/7/8/10	-
2	MEN	JJ	72	2	-	3/7/8/10	-
2	MEN	a1	72	2	-	3/7/8/10	-
2	MEN	a4	72	2	-	3/7/8/10	-
10	MEN	LE	72	10	-	4/7/8/10	-
10	MEN	NE	72	10	-	4/7/8/10	-
2	MEN	sC	72	2	-	2/7/8/10	-
2	MEN	PO	72	2	-	4/7/8/10	-
2	MEN	ZF	72	2	-	5/7/8/10	-
2	MEN	QQ	72	2	-	4/7/8/10	-
2	MEN	i1	72	2	-	4/7/8/10	-
2	MEN	S9	72	2	-	2/7/8/10	-
2	MEN	JK	72	2,82	-	2/7/8/10	-
2	MEN	LI	72	2	-	4/7/8/10	-
10	MEN	DE	72	11,10	-	4/7/8/10	-
10	MEN	F4	72	10	-	3/7/8/10	-
2	MEN	XF	72	2,82	-	2/7/8/10	-
2	MEN	XJ	72	2	-	5/7/8/10	-
2	MEN	cH	72	2	-	4/7/8/10	-
2	MEN	JF	72	2,82	-	2/7/8/10	-
2	MEN	gG	72	2	-	4/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MEN	kE	72	2	-	4/7/8/10	-
10	MEN	HG	72	10	-	4/7/8/10	-
2	MEN	MQ	72	2	-	2/7/8/10	-

The worst 5 of 121 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
69	S3	71	MEN	CE2-ND2	67.26	2.65	1.45
69	Q3	71	MEN	CE2-ND2	67.24	2.65	1.45
69	s3	71	MEN	CE2-ND2	67.24	2.65	1.45
69	U3	71	MEN	CE2-ND2	67.22	2.65	1.45
69	w3	71	MEN	CE2-ND2	67.21	2.65	1.45

The worst 5 of 542 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
69	U3	71	MEN	OD1-CG-CB	-38.81	64.66	121.50
69	S3	71	MEN	OD1-CG-CB	-38.79	64.69	121.50
69	s3	71	MEN	OD1-CG-CB	-38.79	64.69	121.50
69	Q3	71	MEN	OD1-CG-CB	-38.78	64.69	121.50
69	w3	71	MEN	OD1-CG-CB	-38.78	64.69	121.50

There are no chirality outliers.

5 of 1235 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	BA	72	MEN	N-CA-CB-CG
2	DA	72	MEN	O-C-CA-CB
2	FA	72	MEN	C-CA-CB-CG
2	LA	72	MEN	O-C-CA-CB
2	LA	72	MEN	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

4.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

4.6 Ligand geometry (i)

Of 2437 ligands modelled in this entry, 8 are monoatomic - leaving 2429 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
82	PEB	rC	201	1	46,46,46	2.63	14 (30%)	54,67,67	2.13	19 (35%)
82	PEB	F5	203	2	46,46,46	2.53	12 (26%)	54,67,67	2.10	19 (35%)
82	PEB	cK	203	1,2	46,46,46	2.60	14 (30%)	54,67,67	2.73	23 (42%)
87	CLA	42	608	60	54,58,73	1.42	10 (18%)	65,95,113	1.77	17 (26%)
87	CLA	I2	102	-	69,73,73	1.22	9 (13%)	83,113,113	1.37	6 (7%)
82	PEB	TH	202	2	46,46,46	2.63	11 (23%)	54,67,67	1.93	16 (29%)
87	CLA	8N	305	-	49,53,73	1.48	8 (16%)	59,89,113	1.52	7 (11%)
82	PEB	RK	202	2	46,46,46	2.66	14 (30%)	54,67,67	2.30	20 (37%)
87	CLA	BN	817	-	63,67,73	1.33	9 (14%)	75,105,113	1.41	11 (14%)
82	PEB	dO	201	1	46,46,46	2.55	11 (23%)	54,67,67	2.21	20 (37%)
87	CLA	BN	834	-	69,73,73	1.28	11 (15%)	83,113,113	1.36	11 (13%)
87	CLA	R2	201	87	49,53,73	1.51	7 (14%)	59,89,113	1.55	7 (11%)
82	PEB	WM	201	1	46,46,46	2.61	12 (26%)	54,67,67	2.18	18 (33%)
82	PEB	dG	202	1,2	46,46,46	2.57	10 (21%)	54,67,67	2.35	21 (38%)
82	PEB	j1	203	1,2	46,46,46	2.71	16 (34%)	54,67,67	2.43	19 (35%)
82	PEB	QD	202	2	46,46,46	2.74	15 (32%)	54,67,67	1.92	16 (29%)
87	CLA	AL	405	15	54,58,73	1.41	10 (18%)	65,95,113	1.61	11 (16%)
82	PEB	YH	202	2	46,46,46	2.72	12 (26%)	54,67,67	2.09	19 (35%)
87	CLA	6N	604	87,62	46,50,73	1.52	8 (17%)	55,85,113	1.45	5 (9%)
82	PEB	fG	202	1	46,46,46	2.66	15 (32%)	54,67,67	1.96	17 (31%)
82	PEB	g4	203	2	46,46,46	2.71	13 (28%)	54,67,67	2.02	15 (27%)
82	PEB	C7	202	1	46,46,46	0.63	0	54,67,67	0.79	1 (1%)
82	PEB	WH	202	1	46,46,46	2.65	13 (28%)	54,67,67	2.33	22 (40%)
82	PEB	iK	201	1,2	46,46,46	2.60	12 (26%)	54,67,67	2.35	18 (33%)
87	CLA	BN	829	-	47,51,73	1.46	9 (19%)	56,86,113	1.57	4 (7%)
82	PEB	CJ	202	1	46,46,46	2.44	13 (28%)	54,67,67	2.09	16 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	SP	202	1	46,46,46	2.61	14 (30%)	54,67,67	2.18	22 (40%)
87	CLA	8N	301	64,103	50,54,73	1.57	12 (24%)	60,90,113	1.73	16 (26%)
84	CYC	H4	1001	10	46,46,46	2.37	17 (36%)	61,67,67	3.00	29 (47%)
82	PEB	z8	201	1	46,46,46	2.71	13 (28%)	54,67,67	2.23	26 (48%)
82	PEB	lM	201	1,2	46,46,46	2.54	13 (28%)	54,67,67	2.32	21 (38%)
87	CLA	2N	312	58	49,53,73	1.50	9 (18%)	59,89,113	1.66	9 (15%)
82	PEB	QF	203	1,2	46,46,46	2.71	14 (30%)	54,67,67	3.06	22 (40%)
87	CLA	dL	401	18	69,73,73	1.25	10 (14%)	83,113,113	1.50	7 (8%)
97	GOL	i6	102	-	5,5,5	0.24	0	5,5,5	0.20	0
84	CYC	V3	1001	-	46,46,46	2.52	15 (32%)	61,67,67	3.07	32 (52%)
82	PEB	lJ	201	1,2	46,46,46	2.51	12 (26%)	54,67,67	2.45	22 (40%)
85	BCR	d6	405	-	41,41,41	0.80	0	56,56,56	2.02	17 (30%)
82	PEB	IM	201	1,2	46,46,46	2.56	12 (26%)	54,67,67	2.42	20 (37%)
87	CLA	B2	804	41	69,73,73	1.29	10 (14%)	83,113,113	1.40	11 (13%)
82	PEB	FM	202	2	46,46,46	2.61	14 (30%)	54,67,67	2.20	19 (35%)
83	PUB	AJ	304	13	45,46,46	2.72	9 (20%)	46,67,67	3.11	23 (50%)
87	CLA	H6	103	22	69,73,73	1.25	10 (14%)	83,113,113	1.26	8 (9%)
87	CLA	1N	601	57	49,53,73	1.47	9 (18%)	59,89,113	1.58	6 (10%)
82	PEB	UM	203	1	46,46,46	2.57	13 (28%)	54,67,67	2.25	18 (33%)
82	PEB	J7	201	3,2	46,46,46	2.67	12 (26%)	54,67,67	2.14	16 (29%)
99	SF4	BN	804	-	0,12,12	-	-	-		
82	PEB	Q9	202	2	46,46,46	2.71	13 (28%)	54,67,67	2.30	23 (42%)
82	PEB	NO	1002	10	46,46,46	2.57	13 (28%)	54,67,67	2.13	19 (35%)
82	PEB	GK	203	1	46,46,46	2.63	13 (28%)	54,67,67	2.45	25 (46%)
82	PEB	HG	1002	10,9	46,46,46	2.58	14 (30%)	54,67,67	2.00	16 (29%)
82	PEB	IA	202	1	46,46,46	2.69	13 (28%)	54,67,67	1.90	17 (31%)
87	CLA	BN	806	41	69,73,73	1.22	8 (11%)	83,113,113	1.41	9 (10%)
82	PEB	XQ	201	1,2	46,46,46	2.59	12 (26%)	54,67,67	2.36	19 (35%)
87	CLA	B2	835	-	69,73,73	1.25	10 (14%)	83,113,113	1.34	7 (8%)
82	PEB	WA	202	1	46,46,46	2.69	13 (28%)	54,67,67	2.06	18 (33%)
82	PEB	YE	202	2	46,46,46	2.62	12 (26%)	54,67,67	2.29	21 (38%)
82	PEB	ID	202	2	46,46,46	2.58	13 (28%)	54,67,67	2.18	21 (38%)
82	PEB	LD	201	1,2	46,46,46	2.54	12 (26%)	54,67,67	2.28	19 (35%)
82	PEB	VK	202	2	46,46,46	2.67	14 (30%)	54,67,67	2.46	22 (40%)
82	PEB	OK	203	1	46,46,46	2.62	11 (23%)	54,67,67	2.08	20 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
87	CLA	D6	403	-	69,73,73	1.24	10 (14%)	83,113,113	1.31	6 (7%)
100	3XQ	JN	104	-	24,24,24	0.20	0	25,25,25	0.23	0
82	PEB	wC	202	2	46,46,46	2.71	12 (26%)	54,67,67	2.41	17 (31%)
92	LMG	B6	619	16	39,39,55	1.03	2 (5%)	47,47,63	1.27	5 (10%)
84	CYC	T3	1001	68	46,46,46	2.66	16 (34%)	61,67,67	2.92	25 (40%)
95	DGD	D6	410	18,22	63,63,67	0.85	2 (3%)	77,77,81	1.10	4 (5%)
87	CLA	12	605	57	49,53,73	1.48	8 (16%)	59,89,113	1.51	6 (10%)
82	PEB	VF	202	2	46,46,46	2.68	13 (28%)	54,67,67	2.46	23 (42%)
87	CLA	d6	406	-	69,73,73	1.24	9 (13%)	83,113,113	1.35	8 (9%)
84	CYC	73	1002	73	46,46,46	2.46	18 (39%)	61,67,67	3.01	29 (47%)
87	CLA	12	606	-	49,53,73	1.47	8 (16%)	59,89,113	1.35	5 (8%)
82	PEB	sF	201	1	46,46,46	2.59	13 (28%)	54,67,67	2.09	16 (29%)
82	PEB	PH	201	11,2	46,46,46	2.60	13 (28%)	54,67,67	2.20	19 (35%)
82	PEB	MB	201	2	46,46,46	2.53	11 (23%)	54,67,67	2.12	18 (33%)
82	PEB	RQ	202	1	46,46,46	2.69	13 (28%)	54,67,67	1.93	16 (29%)
87	CLA	62	307	87	49,53,73	1.50	9 (18%)	59,89,113	1.48	7 (11%)
95	DGD	J6	101	-	63,63,67	0.84	2 (3%)	77,77,81	1.06	5 (6%)
82	PEB	aF	203	1	46,46,46	2.72	11 (23%)	54,67,67	2.27	21 (38%)
82	PEB	RO	201	11,2	46,46,46	2.64	13 (28%)	54,67,67	2.40	16 (29%)
82	PEB	QB	202	2,5	46,46,46	2.61	13 (28%)	54,67,67	2.05	16 (29%)
95	DGD	BL	607	-	41,41,67	1.05	2 (4%)	55,55,81	1.12	4 (7%)
82	PEB	C7	201	1	46,46,46	2.63	14 (30%)	54,67,67	2.52	20 (37%)
82	PEB	B7	202	2	46,46,46	2.65	13 (28%)	54,67,67	2.83	22 (40%)
82	PEB	jF	201	2	46,46,46	2.63	12 (26%)	54,67,67	2.65	22 (40%)
85	BCR	KN	101	40,49	41,41,41	0.78	1 (2%)	56,56,56	2.75	19 (33%)
87	CLA	B6	616	16	69,73,73	1.36	11 (15%)	83,113,113	1.64	6 (7%)
82	PEB	ZB	202	2	46,46,46	2.60	12 (26%)	54,67,67	2.04	14 (25%)
82	PEB	G7	201	1	46,46,46	2.50	9 (19%)	54,67,67	2.31	16 (29%)
82	PEB	RA	202	2	46,46,46	2.50	11 (23%)	54,67,67	2.93	21 (38%)
82	PEB	J7	203	2	46,46,46	2.69	12 (26%)	54,67,67	2.15	19 (35%)
84	CYC	D1	1003	10,9	46,46,46	2.26	15 (32%)	61,67,67	2.88	26 (42%)
82	PEB	NK	201	2	46,46,46	2.59	11 (23%)	54,67,67	2.90	17 (31%)
82	PEB	TF	201	2	46,46,46	2.51	10 (21%)	54,67,67	2.80	17 (31%)
82	PEB	SF	201	1,2	46,46,46	2.55	12 (26%)	54,67,67	2.54	22 (40%)
87	CLA	B2	801	41	62,66,73	1.42	9 (14%)	74,104,113	1.65	15 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	VD	203	1,2	46,46,46	2.70	15 (32%)	54,67,67	2.36	20 (37%)
87	CLA	B2	815	41	59,63,73	1.34	8 (13%)	71,101,113	1.49	7 (9%)
84	CYC	k3	1001	69	46,46,46	2.53	17 (36%)	61,67,67	3.11	28 (45%)
82	PEB	D5	203	2	46,46,46	2.55	11 (23%)	54,67,67	2.00	18 (33%)
87	CLA	A2	813	-	69,73,73	1.21	9 (13%)	83,113,113	1.34	5 (6%)
87	CLA	CL	510	-	69,73,73	1.27	10 (14%)	83,113,113	1.60	13 (15%)
84	CYC	A3	1001	68	46,46,46	2.65	16 (34%)	61,67,67	2.91	26 (42%)
82	PEB	PP	201	2	46,46,46	2.58	12 (26%)	54,67,67	2.09	19 (35%)
87	CLA	FN	205	45	69,73,73	1.36	9 (13%)	83,113,113	1.66	12 (14%)
92	LMG	JL	103	18,24	33,33,55	1.15	2 (6%)	41,41,63	1.22	3 (7%)
85	BCR	A6	401	-	41,41,41	0.74	0	56,56,56	2.25	19 (33%)
82	PEB	fB	301	76,2	46,46,46	2.65	13 (28%)	54,67,67	1.93	16 (29%)
82	PEB	C9	201	1	46,46,46	2.62	15 (32%)	54,67,67	1.97	17 (31%)
82	PEB	MD	202	2	46,46,46	2.60	11 (23%)	54,67,67	2.00	15 (27%)
82	PEB	QG	203	1	46,46,46	2.66	11 (23%)	54,67,67	2.13	19 (35%)
82	PEB	TD	203	1	46,46,46	2.67	11 (23%)	54,67,67	2.12	14 (25%)
82	PEB	MM	203	1	46,46,46	2.44	14 (30%)	54,67,67	2.18	18 (33%)
82	PEB	h4	201	1	46,46,46	2.63	14 (30%)	54,67,67	2.28	22 (40%)
82	PEB	KM	201	1	46,46,46	2.58	12 (26%)	54,67,67	2.08	15 (27%)
87	CLA	CL	514	-	59,63,73	1.36	11 (18%)	71,101,113	1.45	5 (7%)
82	PEB	UP	203	1,2	46,46,46	3.08	13 (28%)	54,67,67	3.08	20 (37%)
84	CYC	S3	1001	69	46,46,46	2.53	17 (36%)	61,67,67	3.11	28 (45%)
87	CLA	cL	509	-	69,73,73	1.24	10 (14%)	83,113,113	1.51	12 (14%)
87	CLA	RN	202	54	49,53,73	1.50	8 (16%)	59,89,113	1.52	8 (13%)
84	CYC	n3	1001	69	46,46,46	2.52	17 (36%)	61,67,67	3.11	28 (45%)
82	PEB	s8	203	2	46,46,46	2.73	12 (26%)	54,67,67	1.89	17 (31%)
82	PEB	cF	201	1	46,46,46	2.63	12 (26%)	54,67,67	2.28	20 (37%)
87	CLA	B2	813	-	49,53,73	1.46	9 (18%)	59,89,113	1.54	5 (8%)
87	CLA	3N	305	59,87	69,73,73	1.35	10 (14%)	83,113,113	1.87	15 (18%)
93	BCT	AL	412	15,90,18	2,3,3	1.16	0	2,3,3	3.89	1 (50%)
103	ZEX	8N	310	64,87	42,43,43	1.78	9 (21%)	55,60,60	3.89	31 (56%)
82	PEB	W9	202	2	46,46,46	2.73	13 (28%)	54,67,67	2.29	20 (37%)
82	PEB	Y9	202	2	46,46,46	2.68	13 (28%)	54,67,67	2.22	18 (33%)
82	PEB	nK	202	2	46,46,46	2.82	15 (32%)	54,67,67	1.97	16 (29%)
84	CYC	D3	1001	73,69	46,46,46	2.53	17 (36%)	61,67,67	3.11	28 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	w8	204	2	46,46,46	2.74	13 (28%)	54,67,67	2.00	16 (29%)
82	PEB	aJ	201	13,1	46,46,46	2.56	13 (28%)	54,67,67	2.09	14 (25%)
82	PEB	Q5	201	74,2	46,46,46	2.56	13 (28%)	54,67,67	2.01	19 (35%)
82	PEB	N7	201	2	46,46,46	2.58	12 (26%)	54,67,67	2.24	20 (37%)
82	PEB	VK	201	2	46,46,46	2.60	11 (23%)	54,67,67	2.43	18 (33%)
82	PEB	hF	201	2	46,46,46	2.61	12 (26%)	54,67,67	2.43	21 (38%)
82	PEB	FO	1002	10	46,46,46	2.57	13 (28%)	54,67,67	2.23	21 (38%)
87	CLA	62	301	62	49,53,73	1.49	10 (20%)	59,89,113	1.39	4 (6%)
82	PEB	IK	201	1	46,46,46	2.53	12 (26%)	54,67,67	3.17	23 (42%)
82	PEB	a4	203	2	46,46,46	2.68	14 (30%)	54,67,67	1.98	17 (31%)
87	CLA	bL	621	-	69,73,73	1.22	8 (11%)	83,113,113	1.42	7 (8%)
87	CLA	c6	607	17	69,73,73	1.23	8 (11%)	83,113,113	1.33	6 (7%)
84	CYC	r3	1001	-	46,46,46	0.79	0	61,67,67	0.76	1 (1%)
82	PEB	IQ	201	2,77	46,46,46	2.69	14 (30%)	54,67,67	2.77	23 (42%)
82	PEB	cH	202	2	46,46,46	2.67	13 (28%)	54,67,67	2.34	21 (38%)
85	BCR	Z6	101	39	41,41,41	0.78	1 (2%)	56,56,56	3.40	25 (44%)
87	CLA	AN	811	-	69,73,73	1.29	11 (15%)	83,113,113	1.56	10 (12%)
84	CYC	I3	1001	69	46,46,46	2.52	17 (36%)	61,67,67	3.11	28 (45%)
93	BCT	A6	409	15,90,18	2,3,3	1.23	0	2,3,3	3.83	2 (100%)
82	PEB	j1	202	1	46,46,46	2.72	14 (30%)	54,67,67	2.20	20 (37%)
85	BCR	F2	204	-	41,41,41	0.72	0	56,56,56	1.94	13 (23%)
83	PUB	Z5	303	1,74	45,46,46	2.79	11 (24%)	46,67,67	3.47	18 (39%)
82	PEB	U7	201	1	46,46,46	2.58	11 (23%)	54,67,67	2.61	18 (33%)
82	PEB	HP	201	56,2	46,46,46	2.65	14 (30%)	54,67,67	2.04	17 (31%)
87	CLA	c6	605	17	69,73,73	1.25	8 (11%)	83,113,113	1.29	6 (7%)
88	LHG	m6	102	-	38,38,48	1.04	2 (5%)	41,44,54	1.09	4 (9%)
88	LHG	CL	521	-	36,36,48	1.08	2 (5%)	39,42,54	1.12	3 (7%)
87	CLA	B2	831	-	64,68,73	1.31	10 (15%)	77,107,113	1.44	9 (11%)
82	PEB	LP	201	2	46,46,46	2.58	13 (28%)	54,67,67	2.01	16 (29%)
92	LMG	J6	102	-	43,43,55	1.01	3 (6%)	51,51,63	2.16	12 (23%)
82	PEB	LF	201	2	46,46,46	2.59	12 (26%)	54,67,67	3.16	21 (38%)
85	BCR	cL	504	17	41,41,41	0.85	1 (2%)	56,56,56	2.32	17 (30%)
88	LHG	d6	402	-	45,45,48	0.96	2 (4%)	48,51,54	1.11	3 (6%)
87	CLA	BN	811	-	69,73,73	1.27	11 (15%)	83,113,113	1.49	7 (8%)
82	PEB	V1	203	2	46,46,46	2.69	13 (28%)	54,67,67	2.14	17 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
95	DGD	h6	101	22	63,63,67	0.91	2 (3%)	77,77,81	1.00	3 (3%)
92	LMG	C6	501	-	55,55,55	0.86	2 (3%)	63,63,63	0.99	2 (3%)
82	PEB	UG	201	1,2	46,46,46	2.59	11 (23%)	54,67,67	2.39	19 (35%)
82	PEB	K5	201	1	46,46,46	2.56	13 (28%)	54,67,67	2.27	20 (37%)
87	CLA	42	603	-	49,53,73	1.47	11 (22%)	59,89,113	1.57	9 (15%)
87	CLA	12	611	-	49,53,73	1.49	9 (18%)	59,89,113	1.49	7 (11%)
82	PEB	fM	202	1	46,46,46	2.60	12 (26%)	54,67,67	2.16	19 (35%)
87	CLA	b6	612	-	69,73,73	1.26	9 (13%)	83,113,113	1.40	10 (12%)
82	PEB	U5	201	74,2	46,46,46	2.77	14 (30%)	54,67,67	2.11	18 (33%)
82	PEB	U7	202	1	46,46,46	2.64	13 (28%)	54,67,67	1.93	16 (29%)
82	PEB	KE	201	10,9	46,46,46	2.60	13 (28%)	54,67,67	2.08	17 (31%)
82	PEB	DA	202	2	46,46,46	2.51	12 (26%)	54,67,67	2.46	21 (38%)
82	PEB	QA	202	1	46,46,46	2.54	12 (26%)	54,67,67	2.02	14 (25%)
82	PEB	BQ	201	1	46,46,46	2.52	12 (26%)	54,67,67	2.31	20 (37%)
82	PEB	IK	203	1,2	46,46,46	2.51	12 (26%)	54,67,67	2.86	24 (44%)
82	PEB	i1	202	2	46,46,46	2.75	12 (26%)	54,67,67	1.88	15 (27%)
82	PEB	V5	201	1	46,46,46	2.56	13 (28%)	54,67,67	2.27	21 (38%)
87	CLA	O2	202	53	54,58,73	1.49	7 (12%)	65,95,113	1.92	13 (20%)
82	PEB	dM	202	1	46,46,46	2.61	13 (28%)	54,67,67	1.98	14 (25%)
87	CLA	6N	611	62	49,53,73	1.44	6 (12%)	59,89,113	1.43	4 (6%)
82	PEB	XM	201	2	46,46,46	2.71	13 (28%)	54,67,67	2.07	19 (35%)
82	PEB	XJ	202	2	46,46,46	2.56	13 (28%)	54,67,67	2.19	22 (40%)
82	PEB	RA	203	2	46,46,46	2.62	13 (28%)	54,67,67	2.40	26 (48%)
82	PEB	CF	203	1	46,46,46	2.62	13 (28%)	54,67,67	2.05	20 (37%)
82	PEB	O1	202	1	46,46,46	2.65	12 (26%)	54,67,67	2.11	18 (33%)
82	PEB	yF	301	14	46,46,46	2.64	13 (28%)	54,67,67	2.13	18 (33%)
87	CLA	HL	101	22	69,73,73	1.24	9 (13%)	83,113,113	1.43	10 (12%)
82	PEB	OE	203	1,2	46,46,46	2.55	13 (28%)	54,67,67	2.23	21 (38%)
88	LHG	BL	610	-	48,48,48	0.92	2 (4%)	51,54,54	1.03	3 (5%)
82	PEB	A9	201	1	46,46,46	2.61	13 (28%)	54,67,67	1.97	17 (31%)
82	PEB	wF	301	13	46,46,46	2.57	12 (26%)	54,67,67	2.18	20 (37%)
85	BCR	FN	202	-	41,41,41	0.72	0	56,56,56	2.11	18 (32%)
82	PEB	PK	202	2	46,46,46	2.87	15 (32%)	54,67,67	2.31	20 (37%)
87	CLA	62	308	62	49,53,73	1.50	9 (18%)	59,89,113	1.54	7 (11%)
82	PEB	WK	203	1	46,46,46	2.70	12 (26%)	54,67,67	1.97	17 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	MQ	201	2	46,46,46	2.66	13 (28%)	54,67,67	2.16	18 (33%)
87	CLA	B2	833	-	51,55,73	1.44	12 (23%)	61,91,113	1.48	12 (19%)
82	PEB	ZO	201	1	46,46,46	2.63	14 (30%)	54,67,67	2.81	23 (42%)
82	PEB	M5	305	74	46,46,46	2.57	13 (28%)	54,67,67	2.36	24 (44%)
82	PEB	E9	202	1	46,46,46	2.73	14 (30%)	54,67,67	2.42	20 (37%)
82	PEB	Q1	203	1	46,46,46	2.61	13 (28%)	54,67,67	2.12	18 (33%)
87	CLA	cL	512	-	69,73,73	1.26	10 (14%)	83,113,113	1.55	12 (14%)
82	PEB	LD	203	1	46,46,46	2.66	10 (21%)	54,67,67	2.06	18 (33%)
87	CLA	cL	506	-	69,73,73	1.28	11 (15%)	83,113,113	1.35	9 (10%)
82	PEB	uF	203	1	46,46,46	2.78	13 (28%)	54,67,67	1.87	17 (31%)
87	CLA	4N	605	60	49,53,73	1.48	9 (18%)	59,89,113	1.99	11 (18%)
82	PEB	qK	203	1	46,46,46	2.76	13 (28%)	54,67,67	2.16	19 (35%)
82	PEB	TK	201	2	46,46,46	2.51	9 (19%)	54,67,67	2.80	17 (31%)
82	PEB	Y1	202	2	46,46,46	2.73	13 (28%)	54,67,67	2.10	19 (35%)
82	PEB	e1	201	2	46,46,46	2.69	13 (28%)	54,67,67	2.09	20 (37%)
95	DGD	CL	520	-	43,43,67	1.08	2 (4%)	57,57,81	1.27	6 (10%)
87	CLA	BN	832	-	69,73,73	1.24	10 (14%)	83,113,113	1.40	8 (9%)
82	PEB	OD	201	3,2,82	46,46,46	2.66	12 (26%)	54,67,67	2.07	16 (29%)
82	PEB	II	201	1	46,46,46	2.58	12 (26%)	54,67,67	2.05	18 (33%)
82	PEB	mG	203	2	46,46,46	2.65	14 (30%)	54,67,67	2.04	14 (25%)
87	CLA	22	611	-	46,50,73	1.49	9 (19%)	55,85,113	1.64	7 (12%)
87	CLA	6N	603	-	49,53,73	1.48	9 (18%)	59,89,113	1.45	4 (6%)
82	PEB	yK	301	14	46,46,46	2.64	13 (28%)	54,67,67	2.12	18 (33%)
87	CLA	4N	606	-	49,53,73	1.49	9 (18%)	59,89,113	1.48	6 (10%)
87	CLA	52	610	-	49,53,73	1.45	9 (18%)	59,89,113	1.50	6 (10%)
82	PEB	GG	1002	10,9	46,46,46	2.55	12 (26%)	54,67,67	2.29	19 (35%)
82	PEB	J7	202	2	46,46,46	2.54	12 (26%)	54,67,67	2.52	20 (37%)
82	PEB	eF	202	1	46,46,46	2.59	12 (26%)	54,67,67	2.32	23 (42%)
82	PEB	lG	201	1,2	46,46,46	2.62	13 (28%)	54,67,67	2.17	17 (31%)
82	PEB	R7	201	2	46,46,46	2.58	13 (28%)	54,67,67	2.19	19 (35%)
84	CYC	F4	1001	10	46,46,46	2.32	15 (32%)	61,67,67	2.90	26 (42%)
82	PEB	Q4	201	1	46,46,46	2.61	13 (28%)	54,67,67	2.77	27 (50%)
82	PEB	HD	201	1,2	46,46,46	2.50	12 (26%)	54,67,67	2.42	20 (37%)
82	PEB	SF	203	1	46,46,46	2.62	12 (26%)	54,67,67	2.15	17 (31%)
82	PEB	FD	202	1	46,46,46	2.70	12 (26%)	54,67,67	1.98	17 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	II	203	1,2	46,46,46	2.29	13 (28%)	54,67,67	3.23	24 (44%)
82	PEB	TJ	202	2	46,46,46	2.59	12 (26%)	54,67,67	2.05	17 (31%)
82	PEB	dE	203	1	46,46,46	2.67	14 (30%)	54,67,67	2.06	20 (37%)
82	PEB	JB	201	1	46,46,46	2.70	13 (28%)	54,67,67	2.77	21 (38%)
85	BCR	C6	507	-	41,41,41	0.82	1 (2%)	56,56,56	2.03	16 (28%)
94	PL9	a6	601	15	55,55,55	0.62	2 (3%)	68,69,69	1.92	22 (32%)
82	PEB	xF	304	13	46,46,46	2.68	11 (23%)	54,67,67	2.07	18 (33%)
82	PEB	sC	203	2	46,46,46	2.73	12 (26%)	54,67,67	1.90	17 (31%)
84	CYC	M3	1001	69	46,46,46	2.52	17 (36%)	61,67,67	3.11	28 (45%)
82	PEB	CK	203	1	46,46,46	2.63	13 (28%)	54,67,67	2.04	20 (37%)
82	PEB	GK	201	1,2	46,46,46	2.54	12 (26%)	54,67,67	2.95	28 (51%)
84	CYC	o3	1001	69	46,46,46	2.53	17 (36%)	61,67,67	3.11	28 (45%)
82	PEB	bH	201	1	46,46,46	2.62	12 (26%)	54,67,67	2.03	18 (33%)
82	PEB	uC	201	2	46,46,46	2.68	15 (32%)	54,67,67	2.32	23 (42%)
82	PEB	S1	202	1	46,46,46	2.69	12 (26%)	54,67,67	2.24	18 (33%)
82	PEB	YK	202	1	46,46,46	2.67	12 (26%)	54,67,67	1.87	16 (29%)
82	PEB	QH	201	1,2	46,46,46	2.53	12 (26%)	54,67,67	2.44	22 (40%)
82	PEB	MJ	202	1	46,46,46	2.47	11 (23%)	54,67,67	2.40	20 (37%)
82	PEB	MA	202	1	46,46,46	2.60	12 (26%)	54,67,67	1.91	13 (24%)
82	PEB	YD	201	2,82	46,46,46	2.71	13 (28%)	54,67,67	1.99	15 (27%)
87	CLA	BN	836	87,41,57	69,73,73	1.23	8 (11%)	83,113,113	1.66	9 (10%)
82	PEB	pF	201	2	46,46,46	2.60	11 (23%)	54,67,67	2.41	22 (40%)
82	PEB	jG	201	1	46,46,46	2.64	13 (28%)	54,67,67	2.08	19 (35%)
87	CLA	B2	827	-	69,73,73	1.32	10 (14%)	83,113,113	1.44	11 (13%)
82	PEB	BI	202	1,2	46,46,46	2.31	12 (26%)	54,67,67	2.80	23 (42%)
87	CLA	AL	403	15	69,73,73	1.29	12 (17%)	83,113,113	1.46	11 (13%)
82	PEB	b4	201	1	46,46,46	2.68	11 (23%)	54,67,67	2.32	22 (40%)
87	CLA	A2	818	-	49,53,73	1.47	9 (18%)	59,89,113	1.48	5 (8%)
82	PEB	OA	201	1	46,46,46	2.55	11 (23%)	54,67,67	2.94	25 (46%)
82	PEB	GM	203	1,2	46,46,46	2.54	12 (26%)	54,67,67	2.39	19 (35%)
82	PEB	w8	202	2	46,46,46	2.70	12 (26%)	54,67,67	2.40	17 (31%)
82	PEB	MB	202	2	46,46,46	2.83	13 (28%)	54,67,67	2.19	22 (40%)
87	CLA	A2	808	-	69,73,73	1.26	11 (15%)	83,113,113	1.38	8 (9%)
82	PEB	YJ	201	1,2	46,46,46	2.55	11 (23%)	54,67,67	2.41	22 (40%)
82	PEB	WG	203	1,2	46,46,46	2.50	11 (23%)	54,67,67	2.32	22 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	qF	203	1	46,46,46	2.74	14 (30%)	54,67,67	2.15	20 (37%)
95	DGD	AL	416	-	41,41,67	1.11	3 (7%)	55,55,81	1.50	8 (14%)
87	CLA	7N	605	-	49,53,73	1.49	9 (18%)	59,89,113	1.52	7 (11%)
82	PEB	UO	202	1	46,46,46	2.53	11 (23%)	54,67,67	1.99	14 (25%)
88	LHG	BL	615	-	40,40,48	0.99	2 (5%)	43,46,54	1.04	3 (6%)
87	CLA	DL	404	-	69,73,73	1.26	10 (14%)	83,113,113	1.30	7 (8%)
91	PHO	A6	407	-	58,69,69	2.61	13 (22%)	56,99,99	2.75	17 (30%)
82	PEB	X5	202	1	46,46,46	2.57	13 (28%)	54,67,67	2.05	18 (33%)
82	PEB	DD	201	1,2	46,46,46	2.49	13 (28%)	54,67,67	2.43	21 (38%)
87	CLA	12	608	57	45,49,73	1.52	8 (17%)	54,84,113	1.52	8 (14%)
82	PEB	YA	304	3,82	46,46,46	2.63	14 (30%)	54,67,67	2.32	18 (33%)
87	CLA	ON	203	53	49,53,73	1.63	11 (22%)	59,89,113	1.47	7 (11%)
82	PEB	AE	304	3	46,46,46	2.60	12 (26%)	54,67,67	2.10	20 (37%)
82	PEB	FK	201	2	46,46,46	2.59	12 (26%)	54,67,67	3.54	18 (33%)
82	PEB	XK	203	2	46,46,46	2.75	15 (32%)	54,67,67	2.27	22 (40%)
82	PEB	lG	203	1	46,46,46	2.64	14 (30%)	54,67,67	1.95	17 (31%)
85	BCR	kL	100	-	41,41,41	0.83	0	56,56,56	2.73	23 (41%)
82	PEB	AG	304	3	46,46,46	2.59	12 (26%)	54,67,67	2.10	19 (35%)
84	CYC	l3	1001	68	46,46,46	2.66	16 (34%)	61,67,67	2.91	26 (42%)
82	PEB	KQ	202	2	46,46,46	2.61	12 (26%)	54,67,67	1.98	18 (33%)
82	PEB	HD	203	1	46,46,46	2.75	12 (26%)	54,67,67	2.07	16 (29%)
82	PEB	YI	202	2	46,46,46	2.55	12 (26%)	54,67,67	2.07	18 (33%)
87	CLA	72	603	-	49,53,73	1.47	8 (16%)	59,89,113	1.53	8 (13%)
82	PEB	kF	201	1	46,46,46	2.72	13 (28%)	54,67,67	2.07	16 (29%)
82	PEB	YK	201	1	46,46,46	2.67	11 (23%)	54,67,67	2.13	19 (35%)
95	DGD	a6	604	15,17	54,54,67	0.91	2 (3%)	68,68,81	1.10	6 (8%)
82	PEB	SE	202	1,2	46,46,46	2.56	11 (23%)	54,67,67	2.49	20 (37%)
87	CLA	B2	822	-	69,73,73	1.27	11 (15%)	83,113,113	1.35	13 (15%)
82	PEB	JI	202	2	46,46,46	2.65	13 (28%)	54,67,67	1.94	17 (31%)
87	CLA	A2	824	40	55,59,73	1.38	8 (14%)	66,96,113	1.57	6 (9%)
87	CLA	8N	308	-	49,53,73	1.49	11 (22%)	59,89,113	2.07	12 (20%)
82	PEB	SD	201	3,2	46,46,46	2.67	13 (28%)	54,67,67	2.10	15 (27%)
82	PEB	Y4	203	2	46,46,46	2.59	12 (26%)	54,67,67	1.97	17 (31%)
82	PEB	BK	202	2	46,46,46	2.73	13 (28%)	54,67,67	2.26	17 (31%)
82	PEB	DD	202	1	46,46,46	2.56	13 (28%)	54,67,67	2.79	24 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	d1	201	1,2	46,46,46	2.60	10 (21%)	54,67,67	2.29	18 (33%)
84	CYC	p3	1001	68	46,46,46	2.65	16 (34%)	61,67,67	2.92	24 (39%)
87	CLA	AN	819	40	66,70,73	1.30	10 (15%)	79,109,113	1.51	9 (11%)
82	PEB	EA	202	1	46,46,46	2.61	14 (30%)	54,67,67	2.00	16 (29%)
82	PEB	GP	201	1,2	46,46,46	3.11	13 (28%)	54,67,67	3.10	20 (37%)
82	PEB	PA	201	2	46,46,46	2.60	12 (26%)	54,67,67	2.15	17 (31%)
82	PEB	QH	202	1	46,46,46	2.58	11 (23%)	54,67,67	2.35	19 (35%)
82	PEB	A4	301	3	46,46,46	2.62	12 (26%)	54,67,67	1.99	17 (31%)
82	PEB	eE	203	2	46,46,46	2.80	14 (30%)	54,67,67	2.41	22 (40%)
82	PEB	I9	202	1	46,46,46	2.74	14 (30%)	54,67,67	2.41	21 (38%)
82	PEB	A1	302	3	46,46,46	2.68	13 (28%)	54,67,67	1.98	16 (29%)
82	PEB	KD	201	2	46,46,46	2.62	13 (28%)	54,67,67	1.95	15 (27%)
82	PEB	QE	201	1,2	46,46,46	2.58	13 (28%)	54,67,67	2.68	24 (44%)
82	PEB	kK	202	1	46,46,46	2.72	12 (26%)	54,67,67	1.79	15 (27%)
82	PEB	BQ	203	1,2	46,46,46	2.34	11 (23%)	54,67,67	2.48	18 (33%)
84	CYC	H3	1001	73,69	46,46,46	2.53	17 (36%)	61,67,67	3.11	28 (45%)
88	LHG	I6	101	-	48,48,48	0.93	2 (4%)	51,54,54	1.13	5 (9%)
87	CLA	AN	807	-	69,73,73	1.25	10 (14%)	83,113,113	1.39	7 (8%)
102	BGC	32	301	-	11,11,12	0.36	0	15,15,17	1.38	1 (6%)
82	PEB	Y7	304	3,82	46,46,46	2.63	14 (30%)	54,67,67	2.32	18 (33%)
82	PEB	Q5	202	2	46,46,46	2.67	12 (26%)	54,67,67	2.50	21 (38%)
82	PEB	aB	201	2	46,46,46	2.54	12 (26%)	54,67,67	2.25	19 (35%)
82	PEB	lK	203	1,2	46,46,46	2.71	16 (34%)	54,67,67	2.49	23 (42%)
87	CLA	AN	840	-	69,73,73	1.25	10 (14%)	83,113,113	1.37	7 (8%)
82	PEB	PJ	201	2	46,46,46	2.68	13 (28%)	54,67,67	2.16	21 (38%)
87	CLA	B6	615	16	69,73,73	1.25	10 (14%)	83,113,113	1.31	7 (8%)
87	CLA	LN	203	85,50,41	69,73,73	1.24	8 (11%)	83,113,113	1.47	6 (7%)
82	PEB	bP	502	2	46,46,46	2.52	11 (23%)	54,67,67	2.16	19 (35%)
84	CYC	LE	1001	10	46,46,46	2.38	18 (39%)	61,67,67	3.02	29 (47%)
95	DGD	c6	620	-	49,49,67	0.95	2 (4%)	63,63,81	1.07	4 (6%)
82	PEB	UJ	201	1,2	46,46,46	2.54	11 (23%)	54,67,67	2.47	24 (44%)
87	CLA	B6	603	-	69,73,73	1.24	10 (14%)	83,113,113	1.28	6 (7%)
84	CYC	f3	1001	69	46,46,46	2.52	17 (36%)	61,67,67	3.11	28 (45%)
87	CLA	bL	620	16,85	60,64,73	1.31	10 (16%)	72,102,113	1.43	6 (8%)
82	PEB	VM	201	2	46,46,46	2.69	13 (28%)	54,67,67	2.15	17 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
87	CLA	FN	203	45	49,53,73	1.53	12 (24%)	59,89,113	1.43	9 (15%)
82	PEB	QJ	202	1,2	46,46,46	2.56	12 (26%)	54,67,67	2.30	21 (38%)
82	PEB	F9	201	74,2	46,46,46	2.73	13 (28%)	54,67,67	2.30	18 (33%)
82	PEB	GM	202	1	46,46,46	2.58	14 (30%)	54,67,67	2.06	16 (29%)
87	CLA	c6	609	-	69,73,73	1.25	10 (14%)	83,113,113	1.28	8 (9%)
87	CLA	AN	826	-	69,73,73	1.27	11 (15%)	83,113,113	1.41	11 (13%)
82	PEB	Q7	201	1	46,46,46	2.56	12 (26%)	54,67,67	2.71	20 (37%)
82	PEB	oK	202	1	46,46,46	2.70	12 (26%)	54,67,67	1.98	18 (33%)
87	CLA	22	608	58	49,53,73	1.52	8 (16%)	59,89,113	1.50	11 (18%)
82	PEB	XI	201	1	46,46,46	2.57	13 (28%)	54,67,67	2.05	20 (37%)
82	PEB	EM	202	1	46,46,46	2.64	11 (23%)	54,67,67	2.10	18 (33%)
82	PEB	UO	201	1	46,46,46	2.52	12 (26%)	54,67,67	2.94	26 (48%)
82	PEB	S4	201	1	46,46,46	2.67	14 (30%)	54,67,67	2.64	25 (46%)
96	HEM	fL	102	-	50,50,50	1.63	9 (18%)	66,82,82	1.68	15 (22%)
95	DGD	CL	517	-	63,63,67	0.84	2 (3%)	77,77,81	1.06	2 (2%)
82	PEB	VA	202	2	46,46,46	2.51	11 (23%)	54,67,67	2.62	23 (42%)
82	PEB	hG	202	1	46,46,46	2.65	14 (30%)	54,67,67	1.99	17 (31%)
82	PEB	rF	202	2	46,46,46	2.80	16 (34%)	54,67,67	2.23	19 (35%)
87	CLA	BN	831	-	64,68,73	1.31	10 (15%)	77,107,113	1.42	9 (11%)
82	PEB	aH	202	2	46,46,46	2.77	13 (28%)	54,67,67	2.00	17 (31%)
82	PEB	O7	201	1	46,46,46	2.55	11 (23%)	54,67,67	2.94	25 (46%)
82	PEB	SG	202	-	46,46,46	0.64	0	54,67,67	0.80	1 (1%)
82	PEB	qK	202	1	46,46,46	2.60	13 (28%)	54,67,67	3.09	23 (42%)
85	BCR	H6	101	-	41,41,41	0.81	2 (4%)	56,56,56	2.14	18 (32%)
84	CYC	K3	1001	68	46,46,46	2.66	16 (34%)	61,67,67	2.92	25 (40%)
87	CLA	nL	101	-	69,73,73	1.24	10 (14%)	83,113,113	1.45	10 (12%)
84	CYC	I4	1001	9	46,46,46	2.31	17 (36%)	61,67,67	2.84	26 (42%)
84	CYC	GO	1001	9	46,46,46	2.40	15 (32%)	61,67,67	2.79	24 (39%)
82	PEB	wC	204	2	46,46,46	2.74	14 (30%)	54,67,67	1.99	15 (27%)
85	BCR	b6	601	-	41,41,41	0.89	2 (4%)	56,56,56	2.10	17 (30%)
87	CLA	B2	830	-	69,73,73	1.23	9 (13%)	83,113,113	1.30	4 (4%)
82	PEB	fF	201	13,2	46,46,46	2.53	10 (21%)	54,67,67	2.92	18 (33%)
82	PEB	fE	202	1	46,46,46	2.67	16 (34%)	54,67,67	1.96	17 (31%)
82	PEB	NJ	201	2	46,46,46	2.65	13 (28%)	54,67,67	2.48	21 (38%)
82	PEB	m4	203	2	46,46,46	2.70	13 (28%)	54,67,67	2.03	20 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	i4	203	2	46,46,46	2.74	13 (28%)	54,67,67	1.86	16 (29%)
87	CLA	BL	606	-	69,73,73	1.24	8 (11%)	83,113,113	1.39	5 (6%)
95	DGD	a6	603	-	41,41,67	1.07	2 (4%)	55,55,81	1.33	5 (9%)
87	CLA	82	306	64,103	50,54,73	1.57	12 (24%)	60,90,113	1.73	16 (26%)
87	CLA	1N	609	-	46,50,73	1.50	9 (19%)	55,85,113	1.66	8 (14%)
82	PEB	mO	202	2	46,46,46	2.61	13 (28%)	54,67,67	2.37	20 (37%)
87	CLA	A2	812	-	59,63,73	1.34	9 (15%)	71,101,113	1.46	5 (7%)
84	CYC	y3	1001	71	46,46,46	2.54	17 (36%)	61,67,67	3.17	31 (50%)
82	PEB	WE	201	1	46,46,46	2.60	14 (30%)	54,67,67	2.36	22 (40%)
82	PEB	cM	201	2	46,46,46	2.69	14 (30%)	54,67,67	2.25	17 (31%)
82	PEB	Y7	303	3,82	46,46,46	2.60	13 (28%)	54,67,67	2.58	22 (40%)
82	PEB	KK	201	1,2	46,46,46	2.48	11 (23%)	54,67,67	2.59	19 (35%)
87	CLA	AN	812	-	59,63,73	1.34	9 (15%)	71,101,113	1.45	6 (8%)
82	PEB	aM	202	1	46,46,46	2.61	12 (26%)	54,67,67	2.05	14 (25%)
95	DGD	AL	415	-	41,41,67	1.07	2 (4%)	55,55,81	1.20	5 (9%)
82	PEB	DM	202	2	46,46,46	2.63	14 (30%)	54,67,67	2.07	20 (37%)
82	PEB	GQ	202	2	46,46,46	2.68	11 (23%)	54,67,67	2.13	21 (38%)
82	PEB	SB	202	2	46,46,46	2.52	13 (28%)	54,67,67	2.12	19 (35%)
87	CLA	C6	519	-	59,63,73	1.34	10 (16%)	71,101,113	1.37	7 (9%)
82	PEB	p8	201	1	46,46,46	2.66	12 (26%)	54,67,67	2.00	18 (33%)
82	PEB	IM	203	1	46,46,46	2.53	12 (26%)	54,67,67	2.11	18 (33%)
82	PEB	JM	202	2	46,46,46	2.65	12 (26%)	54,67,67	2.05	18 (33%)
82	PEB	LQ	202	1	46,46,46	2.61	12 (26%)	54,67,67	2.23	15 (27%)
85	BCR	bL	603	-	41,41,41	0.74	0	56,56,56	1.77	13 (23%)
82	PEB	U9	202	2	46,46,46	2.60	11 (23%)	54,67,67	2.28	20 (37%)
87	CLA	A2	807	-	69,73,73	1.26	10 (14%)	83,113,113	1.39	6 (7%)
82	PEB	RO	202	2	46,46,46	2.59	13 (28%)	54,67,67	2.48	22 (40%)
82	PEB	B9	203	2	46,46,46	2.66	12 (26%)	54,67,67	2.06	14 (25%)
84	CYC	u3	1001	69	46,46,46	2.53	17 (36%)	61,67,67	3.11	28 (45%)
87	CLA	6N	602	62	69,73,73	1.27	9 (13%)	83,113,113	1.28	9 (10%)
87	CLA	72	602	62,63	69,73,73	1.39	10 (14%)	83,113,113	1.79	18 (21%)
82	PEB	FJ	202	2	46,46,46	2.58	13 (28%)	54,67,67	2.21	21 (38%)
94	PL9	A6	410	-	55,55,55	0.61	1 (1%)	68,69,69	2.28	21 (30%)
82	PEB	eB	201	2	46,46,46	2.56	13 (28%)	54,67,67	2.05	16 (29%)
82	PEB	PF	201	2	46,46,46	2.60	11 (23%)	54,67,67	3.03	19 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	OG	203	1,2	46,46,46	2.55	13 (28%)	54,67,67	2.24	21 (38%)
82	PEB	QG	201	1,2	46,46,46	2.58	13 (28%)	54,67,67	2.67	24 (44%)
87	CLA	c6	610	-	69,73,73	1.24	9 (13%)	83,113,113	1.31	7 (8%)
87	CLA	AN	833	-	69,73,73	1.26	9 (13%)	83,113,113	1.33	6 (7%)
82	PEB	TD	202	1	46,46,46	2.66	12 (26%)	54,67,67	2.10	17 (31%)
82	PEB	S9	202	2	46,46,46	2.56	13 (28%)	54,67,67	2.28	22 (40%)
91	PHO	a6	613	-	58,69,69	2.65	13 (22%)	56,99,99	2.69	17 (30%)
95	DGD	cL	502	-	63,63,67	0.84	2 (3%)	77,77,81	1.27	8 (10%)
87	CLA	AN	816	-	49,53,73	1.51	9 (18%)	59,89,113	1.50	6 (10%)
84	CYC	t3	1001	68	46,46,46	2.66	16 (34%)	61,67,67	2.92	25 (40%)
84	CYC	N4	1001	10	46,46,46	2.48	19 (41%)	61,67,67	2.83	27 (44%)
82	PEB	uK	201	1	46,46,46	2.74	13 (28%)	54,67,67	2.05	16 (29%)
82	PEB	PD	201	1,2	46,46,46	2.66	14 (30%)	54,67,67	2.04	18 (33%)
99	SF4	C2	101	42	0,12,12	-	-	-		
92	LMG	BL	611	-	40,40,55	1.01	2 (5%)	48,48,63	1.34	6 (12%)
85	BCR	C6	508	-	41,41,41	0.80	1 (2%)	56,56,56	2.61	22 (39%)
87	CLA	6N	605	62	49,53,73	1.47	8 (16%)	59,89,113	1.54	7 (11%)
82	PEB	HQ	203	1	46,46,46	2.73	13 (28%)	54,67,67	2.08	16 (29%)
82	PEB	xK	304	13	46,46,46	2.72	11 (23%)	54,67,67	2.10	19 (35%)
85	BCR	KL	100	-	41,41,41	0.83	0	56,56,56	2.73	23 (41%)
82	PEB	CP	202	1	46,46,46	2.60	14 (30%)	54,67,67	2.20	20 (37%)
87	CLA	6N	606	87	49,53,73	1.50	9 (18%)	59,89,113	1.48	7 (11%)
82	PEB	VJ	201	2	46,46,46	2.72	13 (28%)	54,67,67	2.19	20 (37%)
82	PEB	R9	202	1	46,46,46	2.73	14 (30%)	54,67,67	2.42	20 (37%)
82	PEB	AA	202	1	46,46,46	2.68	14 (30%)	54,67,67	2.04	16 (29%)
82	PEB	ZE	202	1	46,46,46	2.62	14 (30%)	54,67,67	2.25	19 (35%)
82	PEB	hF	202	2	46,46,46	2.68	12 (26%)	54,67,67	1.97	19 (35%)
82	PEB	F5	201	74,2	46,46,46	2.70	12 (26%)	54,67,67	2.33	24 (44%)
87	CLA	5N	605	61	49,53,73	1.49	9 (18%)	59,89,113	1.51	6 (10%)
82	PEB	JH	1002	10	46,46,46	2.54	13 (28%)	54,67,67	2.20	17 (31%)
82	PEB	J5	203	2	46,46,46	2.54	13 (28%)	54,67,67	2.06	19 (35%)
87	CLA	1N	610	57	49,53,73	1.46	8 (16%)	59,89,113	1.55	7 (11%)
82	PEB	M5	301	74	46,46,46	2.56	12 (26%)	54,67,67	2.22	20 (37%)
82	PEB	KA	202	1	46,46,46	2.67	13 (28%)	54,67,67	1.89	14 (25%)
82	PEB	V1	201	2	46,46,46	2.62	14 (30%)	54,67,67	2.30	20 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	aO	201	2	46,46,46	2.60	12 (26%)	54,67,67	2.29	18 (33%)
87	CLA	cL	507	-	69,73,73	1.26	9 (13%)	83,113,113	1.39	6 (7%)
82	PEB	S7	201	1	46,46,46	2.57	11 (23%)	54,67,67	2.78	21 (38%)
87	CLA	BN	824	-	69,73,73	1.28	11 (15%)	83,113,113	1.47	13 (15%)
82	PEB	hH	202	1	46,46,46	0.64	0	54,67,67	0.79	1 (1%)
82	PEB	T1	201	11,2	46,46,46	2.60	15 (32%)	54,67,67	2.32	24 (44%)
82	PEB	OJ	201	1	46,46,46	2.57	12 (26%)	54,67,67	2.04	18 (33%)
82	PEB	FB	201	2,5	46,46,46	2.49	12 (26%)	54,67,67	2.22	15 (27%)
87	CLA	42	607	60	49,53,73	1.52	10 (20%)	59,89,113	1.65	9 (15%)
82	PEB	tF	201	2	46,46,46	2.68	11 (23%)	54,67,67	2.73	17 (31%)
82	PEB	X9	201	1	46,46,46	2.61	13 (28%)	54,67,67	1.97	17 (31%)
82	PEB	GJ	201	1	46,46,46	2.58	12 (26%)	54,67,67	2.19	20 (37%)
87	CLA	BN	814	-	49,53,73	1.45	9 (18%)	59,89,113	1.54	4 (6%)
82	PEB	TB	201	1	46,46,46	2.70	13 (28%)	54,67,67	2.77	21 (38%)
82	PEB	hB	301	76,2	46,46,46	2.64	12 (26%)	54,67,67	1.93	16 (29%)
82	PEB	pK	202	2	46,46,46	2.77	14 (30%)	54,67,67	2.31	20 (37%)
88	LHG	l6	101	26,16	48,48,48	0.90	2 (4%)	51,54,54	1.13	4 (7%)
82	PEB	dF	202	2	46,46,46	2.92	15 (32%)	54,67,67	2.19	19 (35%)
82	PEB	CF	201	1	46,46,46	2.60	12 (26%)	54,67,67	2.15	17 (31%)
82	PEB	A4	305	3	46,46,46	2.62	12 (26%)	54,67,67	2.02	16 (29%)
87	CLA	KN	105	40,49	53,57,73	1.37	10 (18%)	62,93,113	1.34	10 (16%)
92	LMG	j6	102	18,24	33,33,55	1.12	2 (6%)	41,41,63	1.17	4 (9%)
82	PEB	lF	201	2	46,46,46	2.65	13 (28%)	54,67,67	2.42	17 (31%)
82	PEB	YG	202	2	46,46,46	2.62	13 (28%)	54,67,67	2.29	21 (38%)
87	CLA	AN	820	-	69,73,73	1.28	10 (14%)	83,113,113	1.50	14 (16%)
87	CLA	b6	611	-	69,73,73	1.26	10 (14%)	83,113,113	1.28	6 (7%)
83	PUB	yF	302	14	45,46,46	2.62	8 (17%)	46,67,67	2.96	20 (43%)
95	DGD	C6	521	-	63,63,67	0.84	2 (3%)	77,77,81	1.16	7 (9%)
82	PEB	vK	202	2	46,46,46	2.68	14 (30%)	54,67,67	2.03	19 (35%)
82	PEB	jH	201	1	46,46,46	2.62	12 (26%)	54,67,67	2.21	19 (35%)
87	CLA	4N	603	-	49,53,73	1.47	11 (22%)	59,89,113	1.56	9 (15%)
82	PEB	GF	203	1	46,46,46	2.63	13 (28%)	54,67,67	2.46	26 (48%)
82	PEB	gF	203	1,2	46,46,46	2.54	12 (26%)	54,67,67	2.49	19 (35%)
87	CLA	42	601	60	49,53,73	1.46	9 (18%)	59,89,113	1.55	7 (11%)
84	CYC	FG	1001	10	46,46,46	2.33	15 (32%)	61,67,67	2.90	24 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	FH	1002	10	46,46,46	2.57	13 (28%)	54,67,67	2.17	16 (29%)
87	CLA	22	612	58	49,53,73	1.50	9 (18%)	59,89,113	1.64	9 (15%)
95	DGD	cL	520	-	49,49,67	0.98	2 (4%)	63,63,81	1.12	4 (6%)
82	PEB	hH	201	1	46,46,46	2.67	13 (28%)	54,67,67	2.16	18 (33%)
87	CLA	B2	819	41	49,53,73	1.48	11 (22%)	59,89,113	1.56	7 (11%)
84	CYC	GG	1001	10,9	46,46,46	2.38	15 (32%)	61,67,67	2.87	27 (44%)
82	PEB	BA	202	2	46,46,46	2.65	13 (28%)	54,67,67	2.83	23 (42%)
82	PEB	oF	202	1	46,46,46	2.69	12 (26%)	54,67,67	1.98	17 (31%)
91	PHO	AL	410	-	58,69,69	2.58	13 (22%)	56,99,99	2.58	15 (26%)
82	PEB	KF	202	1	46,46,46	2.66	12 (26%)	54,67,67	2.30	17 (31%)
82	PEB	NP	201	2	46,46,46	2.62	13 (28%)	54,67,67	1.97	18 (33%)
94	PL9	aL	601	15	55,55,55	0.75	3 (5%)	68,69,69	1.97	19 (27%)
87	CLA	b6	618	-	69,73,73	1.24	10 (14%)	83,113,113	1.30	5 (6%)
82	PEB	TE	201	2	46,46,46	2.59	12 (26%)	54,67,67	2.25	19 (35%)
83	PUB	AO	303	3	45,46,46	2.65	9 (20%)	46,67,67	2.86	16 (34%)
83	PUB	NQ	201	1,3	45,46,46	2.85	11 (24%)	46,67,67	3.08	18 (39%)
82	PEB	SH	202	1	46,46,46	2.67	11 (23%)	54,67,67	2.23	18 (33%)
82	PEB	s8	202	2	46,46,46	2.79	13 (28%)	54,67,67	2.34	18 (33%)
87	CLA	DL	406	-	69,73,73	1.22	10 (14%)	83,113,113	1.38	6 (7%)
82	PEB	ZG	201	1,2	46,46,46	2.54	11 (23%)	54,67,67	2.52	23 (42%)
82	PEB	SM	202	1	46,46,46	2.56	13 (28%)	54,67,67	2.05	14 (25%)
82	PEB	dF	201	2	46,46,46	2.62	11 (23%)	54,67,67	2.38	18 (33%)
82	PEB	c4	202	2	46,46,46	2.68	14 (30%)	54,67,67	2.22	17 (31%)
82	PEB	YD	202	2	46,46,46	2.68	13 (28%)	54,67,67	1.94	14 (25%)
82	PEB	LA	203	2	46,46,46	2.66	12 (26%)	54,67,67	1.89	19 (35%)
87	CLA	BL	622	16	69,73,73	1.24	9 (13%)	83,113,113	1.45	7 (8%)
85	BCR	FN	204	-	41,41,41	0.72	0	56,56,56	1.95	13 (23%)
82	PEB	Q1	201	1,2	46,46,46	2.53	12 (26%)	54,67,67	2.43	22 (40%)
82	PEB	KA	201	1	46,46,46	2.73	15 (32%)	54,67,67	2.42	21 (38%)
82	PEB	R4	202	2	46,46,46	2.57	13 (28%)	54,67,67	2.49	22 (40%)
87	CLA	B2	805	41	69,73,73	1.22	8 (11%)	83,113,113	1.41	9 (10%)
82	PEB	EJ	202	1	46,46,46	2.58	11 (23%)	54,67,67	2.07	14 (25%)
87	CLA	5N	604	61	46,50,73	1.48	10 (21%)	55,85,113	1.60	6 (10%)
82	PEB	UF	202	1	46,46,46	2.60	11 (23%)	54,67,67	2.08	16 (29%)
82	PEB	CI	201	1	46,46,46	2.57	13 (28%)	54,67,67	2.05	18 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
87	CLA	cL	510	-	69,73,73	1.27	9 (13%)	83,113,113	1.46	7 (8%)
84	CYC	HE	1001	10	46,46,46	2.27	16 (34%)	61,67,67	3.02	27 (44%)
82	PEB	18	202	2	46,46,46	2.68	14 (30%)	54,67,67	2.16	15 (27%)
85	BCR	A2	846	-	41,41,41	0.76	0	56,56,56	2.75	19 (33%)
82	PEB	DH	1002	10	46,46,46	2.58	13 (28%)	54,67,67	2.06	17 (31%)
82	PEB	vC	201	1	46,46,46	2.69	14 (30%)	54,67,67	2.03	16 (29%)
85	BCR	K2	105	-	41,41,41	0.83	0	56,56,56	2.48	19 (33%)
82	PEB	dE	202	1,2	46,46,46	2.57	12 (26%)	54,67,67	2.35	21 (38%)
82	PEB	GI	201	1,2	46,46,46	2.34	13 (28%)	54,67,67	3.06	24 (44%)
82	PEB	A1	301	3	46,46,46	2.69	11 (23%)	54,67,67	2.02	15 (27%)
82	PEB	PM	201	2	46,46,46	2.70	15 (32%)	54,67,67	2.37	20 (37%)
82	PEB	VQ	201	1	46,46,46	2.52	11 (23%)	54,67,67	2.10	18 (33%)
87	CLA	6N	613	62	49,53,73	1.49	10 (20%)	59,89,113	1.39	4 (6%)
82	PEB	hK	201	2	46,46,46	2.61	13 (28%)	54,67,67	2.44	22 (40%)
82	PEB	NM	202	2	46,46,46	2.62	14 (30%)	54,67,67	2.19	17 (31%)
82	PEB	jM	202	1	46,46,46	2.63	11 (23%)	54,67,67	2.75	18 (33%)
82	PEB	VD	201	1	46,46,46	2.51	11 (23%)	54,67,67	2.10	18 (33%)
82	PEB	KK	203	1	46,46,46	2.63	11 (23%)	54,67,67	2.12	21 (38%)
82	PEB	WB	402	6,2	46,46,46	2.66	12 (26%)	54,67,67	2.33	25 (46%)
82	PEB	L5	201	74,2	46,46,46	2.55	13 (28%)	54,67,67	2.03	18 (33%)
87	CLA	BN	808	-	69,73,73	1.25	10 (14%)	83,113,113	1.35	5 (6%)
82	PEB	JQ	201	1	46,46,46	2.68	12 (26%)	54,67,67	2.11	18 (33%)
87	CLA	6N	601	62	49,53,73	1.47	8 (16%)	59,89,113	1.42	4 (6%)
82	PEB	CJ	201	1	46,46,46	2.50	11 (23%)	54,67,67	2.23	20 (37%)
82	PEB	P1	201	11,2	46,46,46	2.59	13 (28%)	54,67,67	2.21	19 (35%)
82	PEB	D9	202	2	46,46,46	2.66	14 (30%)	54,67,67	2.21	19 (35%)
82	PEB	AO	301	3	46,46,46	2.61	11 (23%)	54,67,67	1.98	17 (31%)
82	PEB	l1	201	1,2	46,46,46	2.65	12 (26%)	54,67,67	2.34	19 (35%)
82	PEB	H7	201	2	46,46,46	2.72	13 (28%)	54,67,67	2.08	17 (31%)
82	PEB	f1	201	1	46,46,46	2.66	14 (30%)	54,67,67	1.93	17 (31%)
82	PEB	eH	203	1,2	46,46,46	2.61	14 (30%)	54,67,67	2.53	18 (33%)
82	PEB	U1	201	1,2	46,46,46	2.64	13 (28%)	54,67,67	2.39	19 (35%)
83	PUB	QJ	201	14,1	45,46,46	2.67	10 (22%)	46,67,67	3.10	21 (45%)
88	LHG	C6	505	-	36,36,48	1.04	2 (5%)	39,42,54	1.23	4 (10%)
82	PEB	LQ	203	1	46,46,46	2.66	10 (21%)	54,67,67	2.06	18 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	NB	201	2	46,46,46	2.53	12 (26%)	54,67,67	2.14	19 (35%)
82	PEB	v8	202	1	46,46,46	2.68	14 (30%)	54,67,67	2.66	22 (40%)
82	PEB	WG	201	1	46,46,46	2.59	13 (28%)	54,67,67	2.37	23 (42%)
87	CLA	B2	832	-	69,73,73	1.24	10 (14%)	83,113,113	1.41	9 (10%)
87	CLA	BL	621	-	69,73,73	1.27	11 (15%)	83,113,113	1.56	10 (12%)
82	PEB	DK	203	2	46,46,46	2.70	14 (30%)	54,67,67	2.07	20 (37%)
82	PEB	BP	202	2	46,46,46	2.65	11 (23%)	54,67,67	2.09	17 (31%)
82	PEB	wK	303	13	46,46,46	2.73	14 (30%)	54,67,67	2.12	20 (37%)
82	PEB	JP	201	2	46,46,46	2.63	14 (30%)	54,67,67	2.01	17 (31%)
87	CLA	2N	310	58	45,49,73	1.48	9 (20%)	54,84,113	1.58	7 (12%)
82	PEB	mH	202	2	46,46,46	2.84	11 (23%)	54,67,67	1.87	15 (27%)
82	PEB	wK	302	13	46,46,46	2.61	12 (26%)	54,67,67	2.05	18 (33%)
82	PEB	hJ	203	1	46,46,46	2.58	12 (26%)	54,67,67	2.19	19 (35%)
82	PEB	IQ	202	2	46,46,46	2.58	13 (28%)	54,67,67	2.18	21 (38%)
84	CYC	P3	1001	68	46,46,46	2.66	16 (34%)	61,67,67	2.91	25 (40%)
87	CLA	cL	511	17	69,73,73	1.23	11 (15%)	83,113,113	1.40	7 (8%)
87	CLA	3N	306	-	49,53,73	1.45	8 (16%)	59,89,113	1.52	8 (13%)
85	BCR	BN	840	41	41,41,41	0.73	0	56,56,56	1.79	16 (28%)
87	CLA	BN	801	-	69,73,73	1.23	12 (17%)	83,113,113	1.33	7 (8%)
82	PEB	WI	202	1,2	46,46,46	2.46	13 (28%)	54,67,67	2.87	21 (38%)
84	CYC	j3	1001	73,69	46,46,46	2.52	17 (36%)	61,67,67	3.11	28 (45%)
94	PL9	DL	401	18,26	55,55,55	0.73	3 (5%)	68,69,69	1.88	15 (22%)
82	PEB	u8	203	2	46,46,46	2.70	13 (28%)	54,67,67	1.98	20 (37%)
87	CLA	HL	102	22	69,73,73	1.24	9 (13%)	83,113,113	1.31	8 (9%)
88	LHG	A2	844	-	39,39,48	1.04	2 (5%)	42,45,54	1.08	2 (4%)
82	PEB	MP	202	1	46,46,46	2.59	12 (26%)	54,67,67	2.05	17 (31%)
82	PEB	oF	203	1	46,46,46	2.68	13 (28%)	54,67,67	2.19	18 (33%)
87	CLA	d6	401	18	69,73,73	1.24	10 (14%)	83,113,113	1.36	8 (9%)
82	PEB	JD	201	1	46,46,46	2.65	14 (30%)	54,67,67	2.11	18 (33%)
87	CLA	A2	810	40	69,73,73	1.18	10 (14%)	83,113,113	1.42	7 (8%)
82	PEB	eB	202	2	46,46,46	2.56	12 (26%)	54,67,67	2.13	19 (35%)
87	CLA	72	607	63	54,58,73	1.45	9 (16%)	65,95,113	1.48	9 (13%)
83	PUB	yF	303	14	45,46,46	2.61	9 (20%)	46,67,67	3.04	19 (41%)
82	PEB	F9	203	2	46,46,46	2.61	11 (23%)	54,67,67	2.14	18 (33%)
82	PEB	sK	202	1	46,46,46	2.72	12 (26%)	54,67,67	1.98	19 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	kO	201	2	46,46,46	2.63	14 (30%)	54,67,67	1.93	14 (25%)
82	PEB	KI	202	1	46,46,46	2.57	13 (28%)	54,67,67	2.05	18 (33%)
82	PEB	L5	203	2	46,46,46	2.52	13 (28%)	54,67,67	2.17	18 (33%)
84	CYC	G3	1001	68	46,46,46	2.65	16 (34%)	61,67,67	2.92	25 (40%)
82	PEB	RB	202	2	46,46,46	2.61	11 (23%)	54,67,67	2.11	20 (37%)
82	PEB	TI	201	1,2	46,46,46	2.37	13 (28%)	54,67,67	2.87	22 (40%)
82	PEB	FA	202	2	46,46,46	2.50	12 (26%)	54,67,67	2.69	22 (40%)
82	PEB	DI	201	12,2	46,46,46	2.70	14 (30%)	54,67,67	2.42	20 (37%)
82	PEB	W5	203	2	46,46,46	2.57	11 (23%)	54,67,67	2.00	17 (31%)
87	CLA	ON	201	-	45,49,73	1.51	8 (17%)	54,84,113	1.54	6 (11%)
82	PEB	I7	202	1	46,46,46	2.69	13 (28%)	54,67,67	1.91	17 (31%)
82	PEB	kJ	201	2	46,46,46	2.70	14 (30%)	54,67,67	2.08	18 (33%)
82	PEB	SI	202	2	46,46,46	2.58	11 (23%)	54,67,67	1.95	15 (27%)
82	PEB	VE	201	2	46,46,46	2.60	14 (30%)	54,67,67	2.10	18 (33%)
82	PEB	ZG	202	1	46,46,46	2.62	13 (28%)	54,67,67	2.25	21 (38%)
82	PEB	M9	305	74	46,46,46	2.53	13 (28%)	54,67,67	2.34	21 (38%)
87	CLA	K2	103	-	49,53,73	1.48	12 (24%)	59,89,113	1.49	7 (11%)
87	CLA	A2	806	-	59,63,73	1.33	10 (16%)	71,101,113	1.49	8 (11%)
82	PEB	IF	202	1	46,46,46	0.64	0	54,67,67	0.78	1 (1%)
82	PEB	mH	201	2	46,46,46	2.73	15 (32%)	54,67,67	2.02	17 (31%)
82	PEB	W1	203	1,2	46,46,46	2.66	14 (30%)	54,67,67	2.25	21 (38%)
87	CLA	a6	607	15	69,73,73	1.25	10 (14%)	83,113,113	1.35	8 (9%)
82	PEB	h1	202	1	46,46,46	2.68	14 (30%)	54,67,67	2.16	18 (33%)
87	CLA	AN	841	-	69,73,73	1.28	11 (15%)	83,113,113	1.43	9 (10%)
85	BCR	cL	518	-	41,41,41	0.69	0	56,56,56	2.99	26 (46%)
87	CLA	c6	615	-	59,63,73	1.34	8 (13%)	71,101,113	1.40	8 (11%)
92	LMG	x6	601	37	50,50,55	0.91	2 (4%)	58,58,63	1.14	4 (6%)
82	PEB	W9	203	2	46,46,46	2.64	12 (26%)	54,67,67	2.00	16 (29%)
87	CLA	BN	825	41	69,73,73	1.30	9 (13%)	83,113,113	1.48	12 (14%)
87	CLA	AN	852	59,40	49,53,73	1.79	11 (22%)	59,89,113	2.61	19 (32%)
87	CLA	62	306	62	49,53,73	1.47	8 (16%)	59,89,113	1.54	7 (11%)
88	LHG	M6	101	-	38,38,48	1.02	2 (5%)	41,44,54	1.27	4 (9%)
82	PEB	pC	202	1	46,46,46	2.81	13 (28%)	54,67,67	2.69	23 (42%)
87	CLA	BL	603	-	69,73,73	1.26	10 (14%)	83,113,113	1.54	10 (12%)
82	PEB	BD	203	1,2	46,46,46	2.34	11 (23%)	54,67,67	2.47	18 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	B5	201	74,2,82	46,46,46	2.63	14 (30%)	54,67,67	2.08	18 (33%)
82	PEB	B7	201	2,82	46,46,46	2.63	13 (28%)	54,67,67	2.21	20 (37%)
88	LHG	A2	843	40	48,48,48	0.93	2 (4%)	51,54,54	0.91	2 (3%)
82	PEB	MP	201	1	46,46,46	2.58	12 (26%)	54,67,67	2.23	22 (40%)
83	PUB	BM	302	14	45,46,46	2.64	9 (20%)	46,67,67	3.02	18 (39%)
82	PEB	IP	202	1	46,46,46	2.64	11 (23%)	54,67,67	2.29	19 (35%)
101	FES	NN	101	-	0,4,4	-	-	-		
82	PEB	RK	201	2	46,46,46	2.50	9 (19%)	54,67,67	3.43	21 (38%)
82	PEB	gO	203	2	46,46,46	2.72	13 (28%)	54,67,67	2.02	16 (29%)
85	BCR	B6	601	-	41,41,41	0.80	1 (2%)	56,56,56	2.08	21 (37%)
82	PEB	YQ	201	2,82	46,46,46	2.72	14 (30%)	54,67,67	1.99	15 (27%)
82	PEB	L7	202	2	46,46,46	2.49	12 (26%)	54,67,67	2.68	22 (40%)
84	CYC	DH	1003	10,9	46,46,46	2.26	15 (32%)	61,67,67	2.89	25 (40%)
85	BCR	L2	201	-	41,41,41	0.75	0	56,56,56	1.87	12 (21%)
87	CLA	c6	612	17	69,73,73	1.26	10 (14%)	83,113,113	1.29	6 (7%)
82	PEB	F9	202	2	46,46,46	2.61	11 (23%)	54,67,67	2.32	22 (40%)
82	PEB	lK	201	2	46,46,46	2.64	14 (30%)	54,67,67	2.41	17 (31%)
82	PEB	AJ	301	13	46,46,46	2.49	12 (26%)	54,67,67	2.14	19 (35%)
82	PEB	lJ	203	1	46,46,46	2.50	13 (28%)	54,67,67	2.16	20 (37%)
82	PEB	fG	201	1	46,46,46	2.60	13 (28%)	54,67,67	2.11	21 (38%)
82	PEB	R5	201	1	46,46,46	2.56	13 (28%)	54,67,67	2.27	21 (38%)
87	CLA	BN	812	-	59,63,73	1.33	10 (16%)	71,101,113	1.47	8 (11%)
82	PEB	IJ	202	1	46,46,46	2.53	13 (28%)	54,67,67	2.33	17 (31%)
87	CLA	AN	818	-	49,53,73	1.48	9 (18%)	59,89,113	1.47	5 (8%)
82	PEB	UH	203	1	46,46,46	2.70	12 (26%)	54,67,67	2.19	19 (35%)
87	CLA	B6	606	-	69,73,73	1.25	9 (13%)	83,113,113	1.43	8 (9%)
82	PEB	AI	202	1	46,46,46	2.53	14 (30%)	54,67,67	2.10	20 (37%)
82	PEB	JK	201	2	46,46,46	2.54	11 (23%)	54,67,67	2.87	19 (35%)
87	CLA	7N	607	63	54,58,73	1.45	9 (16%)	65,95,113	1.48	9 (13%)
82	PEB	d1	202	1	46,46,46	2.67	13 (28%)	54,67,67	2.07	16 (29%)
82	PEB	EI	202	1	46,46,46	2.54	13 (28%)	54,67,67	2.11	20 (37%)
88	LHG	DL	407	18	48,48,48	0.91	2 (4%)	51,54,54	1.04	4 (7%)
82	PEB	C5	201	1	46,46,46	2.56	13 (28%)	54,67,67	2.27	21 (38%)
82	PEB	aM	204	1,2	46,46,46	2.61	12 (26%)	54,67,67	2.26	18 (33%)
83	PUB	Y7	302	3	45,46,46	2.68	11 (24%)	46,67,67	2.93	20 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	XF	203	2	46,46,46	2.75	15 (32%)	54,67,67	2.28	22 (40%)
82	PEB	nK	201	2	46,46,46	2.71	12 (26%)	54,67,67	3.00	20 (37%)
82	PEB	ZH	202	1	46,46,46	2.63	12 (26%)	54,67,67	2.07	17 (31%)
82	PEB	DQ	201	1,2	46,46,46	2.48	13 (28%)	54,67,67	2.42	20 (37%)
82	PEB	dM	203	1	46,46,46	2.62	12 (26%)	54,67,67	2.30	16 (29%)
82	PEB	wC	203	2	46,46,46	2.68	12 (26%)	54,67,67	1.94	15 (27%)
82	PEB	xC	202	1	46,46,46	2.75	13 (28%)	54,67,67	2.68	25 (46%)
87	CLA	3N	313	-	49,53,73	1.49	9 (18%)	59,89,113	1.53	8 (13%)
82	PEB	HP	202	2	46,46,46	2.61	12 (26%)	54,67,67	2.08	17 (31%)
82	PEB	E7	202	1	46,46,46	2.61	14 (30%)	54,67,67	2.01	16 (29%)
84	CYC	JH	1003	10,9	46,46,46	2.30	16 (34%)	61,67,67	2.71	27 (44%)
96	HEM	f6	101	19,20	50,50,50	1.69	9 (18%)	66,82,82	1.58	16 (24%)
82	PEB	MP	203	1,2	46,46,46	3.03	13 (28%)	54,67,67	3.15	20 (37%)
85	BCR	LN	205	50	41,41,41	0.77	0	56,56,56	3.24	24 (42%)
82	PEB	P5	201	1	46,46,46	2.56	13 (28%)	54,67,67	2.26	21 (38%)
82	PEB	GE	1002	10,9	46,46,46	2.54	12 (26%)	54,67,67	2.29	19 (35%)
82	PEB	TM	201	2	46,46,46	2.71	14 (30%)	54,67,67	2.17	18 (33%)
82	PEB	hE	203	1	46,46,46	2.64	11 (23%)	54,67,67	1.98	16 (29%)
84	CYC	H1	1001	10	46,46,46	2.34	17 (36%)	61,67,67	2.88	29 (47%)
82	PEB	P7	201	2	46,46,46	2.61	13 (28%)	54,67,67	2.16	16 (29%)
82	PEB	U9	204	1,2	46,46,46	2.74	13 (28%)	54,67,67	2.16	17 (31%)
85	BCR	k6	102	-	41,41,41	0.73	0	56,56,56	2.76	23 (41%)
82	PEB	DE	1002	10,9	46,46,46	2.58	14 (30%)	54,67,67	2.09	18 (33%)
82	PEB	gJ	202	2	46,46,46	2.69	13 (28%)	54,67,67	2.10	22 (40%)
82	PEB	PQ	203	1	46,46,46	2.70	12 (26%)	54,67,67	2.09	14 (25%)
85	BCR	b6	603	-	41,41,41	0.85	1 (2%)	56,56,56	2.15	18 (32%)
82	PEB	dQ	401	2,77	46,46,46	2.62	12 (26%)	54,67,67	2.24	18 (33%)
82	PEB	YM	201	1,2	46,46,46	2.48	12 (26%)	54,67,67	2.54	22 (40%)
82	PEB	UH	201	1,2	46,46,46	2.63	13 (28%)	54,67,67	2.39	19 (35%)
87	CLA	42	609	60	45,49,73	1.48	8 (17%)	54,84,113	1.68	8 (14%)
92	LMG	BL	612	16	39,39,55	1.06	2 (5%)	47,47,63	1.21	5 (10%)
87	CLA	AN	836	-	49,53,73	1.47	9 (18%)	59,89,113	1.58	6 (10%)
82	PEB	MK	202	1	46,46,46	2.72	12 (26%)	54,67,67	1.93	18 (33%)
91	PHO	aL	610	-	58,69,69	2.62	13 (22%)	56,99,99	2.51	13 (23%)
87	CLA	b6	605	16	69,73,73	1.43	10 (14%)	83,113,113	1.78	11 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	D5	202	2	46,46,46	2.58	12 (26%)	54,67,67	2.17	18 (33%)
82	PEB	R7	203	2	46,46,46	2.63	13 (28%)	54,67,67	2.41	26 (48%)
97	GOL	wL	101	-	5,5,5	0.24	0	5,5,5	0.35	0
100	3XQ	J2	104	-	24,24,24	0.20	0	25,25,25	0.23	0
82	PEB	QQ	202	2	46,46,46	2.73	15 (32%)	54,67,67	1.93	16 (29%)
87	CLA	62	309	62	54,58,73	2.13	12 (22%)	65,95,113	7.24	27 (41%)
82	PEB	OI	202	1,2	46,46,46	2.32	12 (26%)	54,67,67	3.16	24 (44%)
82	PEB	c1	201	2	46,46,46	2.64	13 (28%)	54,67,67	2.15	20 (37%)
82	PEB	lM	203	1	46,46,46	2.56	14 (30%)	54,67,67	2.14	19 (35%)
87	CLA	A2	811	-	69,73,73	1.28	11 (15%)	83,113,113	1.56	10 (12%)
87	CLA	L2	202	50	61,65,73	1.29	8 (13%)	73,103,113	1.31	6 (8%)
87	CLA	bL	608	-	69,73,73	1.27	10 (14%)	83,113,113	1.38	7 (8%)
82	PEB	QB	201	2	46,46,46	2.65	13 (28%)	54,67,67	2.36	18 (33%)
87	CLA	BN	835	-	69,73,73	1.25	9 (13%)	83,113,113	1.34	6 (7%)
82	PEB	J9	202	2	46,46,46	2.68	13 (28%)	54,67,67	2.26	22 (40%)
82	PEB	RI	201	1	46,46,46	2.57	12 (26%)	54,67,67	2.05	18 (33%)
87	CLA	A2	803	40,50,53	56,60,73	1.40	11 (19%)	67,97,113	1.37	7 (10%)
92	LMG	ML	101	-	41,41,55	1.05	3 (7%)	49,49,63	1.65	9 (18%)
84	CYC	FE	1002	10	46,46,46	2.33	16 (34%)	61,67,67	2.90	24 (39%)
83	PUB	AG	302	3	45,46,46	2.70	10 (22%)	46,67,67	3.07	23 (50%)
82	PEB	VE	202	2	46,46,46	2.65	13 (28%)	54,67,67	2.12	17 (31%)
82	PEB	OJ	203	1,2	46,46,46	2.49	12 (26%)	54,67,67	2.60	24 (44%)
82	PEB	M7	202	1	46,46,46	2.60	12 (26%)	54,67,67	1.92	13 (24%)
82	PEB	LH	1003	10	46,46,46	2.46	12 (26%)	54,67,67	2.33	17 (31%)
82	PEB	y8	201	2	46,46,46	0.63	0	54,67,67	0.79	1 (1%)
82	PEB	OB	201	2,5	46,46,46	2.56	12 (26%)	54,67,67	2.24	17 (31%)
82	PEB	FP	201	56,2	46,46,46	2.65	14 (30%)	54,67,67	2.03	18 (33%)
82	PEB	FI	201	2	46,46,46	2.59	14 (30%)	54,67,67	2.06	19 (35%)
82	PEB	KB	303	2	46,46,46	0.63	0	54,67,67	0.79	1 (1%)
82	PEB	OG	201	1	46,46,46	2.59	13 (28%)	54,67,67	2.34	21 (38%)
82	PEB	cF	203	1,2	46,46,46	2.62	13 (28%)	54,67,67	2.73	23 (42%)
87	CLA	62	302	62	49,53,73	1.48	9 (18%)	59,89,113	1.41	4 (6%)
82	PEB	AK	202	1	46,46,46	2.72	13 (28%)	54,67,67	1.82	15 (27%)
82	PEB	PG	201	11,2	46,46,46	2.64	13 (28%)	54,67,67	2.35	22 (40%)
82	PEB	XK	201	2	46,46,46	2.57	10 (21%)	54,67,67	3.43	20 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
87	CLA	AN	815	-	69,73,73	1.26	11 (15%)	83,113,113	1.40	12 (14%)
92	LMG	b6	620	16	39,39,55	1.05	2 (5%)	47,47,63	1.33	5 (10%)
82	PEB	fJ	202	1	46,46,46	2.63	14 (30%)	54,67,67	2.23	19 (35%)
87	CLA	b6	616	-	69,73,73	1.24	9 (13%)	83,113,113	1.34	7 (8%)
83	PUB	xF	306	13	45,46,46	2.74	10 (22%)	46,67,67	2.93	19 (41%)
87	CLA	CL	515	-	69,73,73	1.24	10 (14%)	83,113,113	1.39	6 (7%)
92	LMG	m6	101	85	41,41,55	1.01	2 (4%)	49,49,63	1.15	4 (8%)
82	PEB	AP	203	1,2	46,46,46	3.05	13 (28%)	54,67,67	3.11	19 (35%)
82	PEB	V9	201	1	46,46,46	2.61	13 (28%)	54,67,67	1.97	17 (31%)
82	PEB	SJ	203	1,2	46,46,46	2.55	11 (23%)	54,67,67	2.40	21 (38%)
82	PEB	EF	202	1	46,46,46	2.61	12 (26%)	54,67,67	2.08	20 (37%)
82	PEB	eE	201	2	46,46,46	2.65	13 (28%)	54,67,67	1.91	15 (27%)
82	PEB	Z9	304	74	46,46,46	2.54	14 (30%)	54,67,67	2.34	21 (38%)
88	LHG	mL	102	-	38,38,48	1.05	2 (5%)	41,44,54	1.08	2 (4%)
87	CLA	52	601	61	49,53,73	1.47	8 (16%)	59,89,113	1.59	7 (11%)
87	CLA	A2	840	-	69,73,73	1.24	10 (14%)	83,113,113	1.36	7 (8%)
85	BCR	bL	602	-	41,41,41	0.79	0	56,56,56	2.29	19 (33%)
87	CLA	4N	610	-	46,50,73	1.50	7 (15%)	55,85,113	1.65	7 (12%)
83	PUB	AH	304	3	45,46,46	2.95	11 (24%)	46,67,67	3.30	22 (47%)
82	PEB	QB	203	2	46,46,46	2.57	11 (23%)	54,67,67	2.04	16 (29%)
82	PEB	cE	202	2	46,46,46	2.67	11 (23%)	54,67,67	1.94	15 (27%)
82	PEB	B5	203	2	46,46,46	2.52	12 (26%)	54,67,67	2.02	19 (35%)
82	PEB	B7	203	2	46,46,46	2.66	11 (23%)	54,67,67	2.06	20 (37%)
84	CYC	c3	1001	68	46,46,46	2.65	16 (34%)	61,67,67	2.91	25 (40%)
87	CLA	12	603	-	49,53,73	1.46	9 (18%)	59,89,113	1.49	6 (10%)
82	PEB	fE	201	1	46,46,46	2.62	12 (26%)	54,67,67	2.12	19 (35%)
82	PEB	eG	203	2	46,46,46	2.79	14 (30%)	54,67,67	2.40	22 (40%)
87	CLA	BN	828	41	49,53,73	1.49	11 (22%)	59,89,113	1.49	7 (11%)
82	PEB	qC	201	2	46,46,46	2.73	13 (28%)	54,67,67	2.04	16 (29%)
87	CLA	12	601	57	49,53,73	1.47	9 (18%)	59,89,113	1.58	6 (10%)
82	PEB	aM	201	13,1	46,46,46	2.61	13 (28%)	54,67,67	2.08	16 (29%)
82	PEB	iO	203	2	46,46,46	2.75	12 (26%)	54,67,67	1.85	15 (27%)
82	PEB	VG	202	2	46,46,46	2.66	13 (28%)	54,67,67	2.13	17 (31%)
82	PEB	VI	203	1,2	46,46,46	2.15	10 (21%)	54,67,67	3.09	23 (42%)
87	CLA	b6	610	-	69,73,73	1.26	10 (14%)	83,113,113	1.28	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
87	CLA	AN	849	40	69,73,73	1.25	10 (14%)	83,113,113	1.50	9 (10%)
82	PEB	J4	1002	10	46,46,46	2.65	14 (30%)	54,67,67	2.09	19 (35%)
96	HEM	G2	201	46	50,50,50	1.79	10 (20%)	66,82,82	1.39	7 (10%)
87	CLA	A2	835	-	69,73,73	1.20	10 (14%)	83,113,113	1.38	8 (9%)
82	PEB	lE	203	1	46,46,46	2.64	14 (30%)	54,67,67	1.96	17 (31%)
82	PEB	fJ	201	1	46,46,46	2.61	10 (21%)	54,67,67	1.99	16 (29%)
87	CLA	6N	607	62	49,53,73	1.50	9 (18%)	59,89,113	1.55	7 (11%)
82	PEB	QO	202	1	46,46,46	0.65	0	54,67,67	0.79	1 (1%)
87	CLA	4N	607	60	49,53,73	1.52	9 (18%)	59,89,113	1.66	9 (15%)
82	PEB	DB	201	2	46,46,46	2.62	12 (26%)	54,67,67	2.02	19 (35%)
102	BGC	3N	302	-	11,11,12	0.36	0	15,15,17	1.38	1 (6%)
82	PEB	S5	202	2	46,46,46	2.53	13 (28%)	54,67,67	2.21	16 (29%)
82	PEB	1C	203	2	46,46,46	2.73	10 (21%)	54,67,67	1.84	14 (25%)
85	BCR	F2	203	-	41,41,41	0.73	0	56,56,56	2.11	18 (32%)
87	CLA	72	605	-	49,53,73	1.48	9 (18%)	59,89,113	1.53	7 (11%)
87	CLA	5N	607	61	54,58,73	1.39	8 (14%)	65,95,113	1.57	9 (13%)
87	CLA	3N	309	59	54,58,73	1.36	7 (12%)	65,95,113	1.86	13 (20%)
82	PEB	RD	202	1	46,46,46	2.70	12 (26%)	54,67,67	1.94	16 (29%)
82	PEB	dK	202	2	46,46,46	2.91	15 (32%)	54,67,67	2.19	19 (35%)
84	CYC	EO	1001	9	46,46,46	2.34	18 (39%)	61,67,67	2.88	24 (39%)
82	PEB	dH	202	1	46,46,46	2.68	14 (30%)	54,67,67	2.07	16 (29%)
92	LMG	qL	301	-	43,43,55	0.99	2 (4%)	51,51,63	1.18	6 (11%)
82	PEB	KJ	202	1	46,46,46	2.37	13 (28%)	54,67,67	2.62	20 (37%)
82	PEB	c1	202	2	46,46,46	2.69	13 (28%)	54,67,67	2.35	21 (38%)
87	CLA	72	601	63	49,53,73	1.47	7 (14%)	59,89,113	1.57	6 (10%)
82	PEB	YK	203	1,2	46,46,46	2.68	15 (32%)	54,67,67	2.55	22 (40%)
82	PEB	J9	203	2	46,46,46	2.68	13 (28%)	54,67,67	2.09	16 (29%)
87	CLA	BN	816	41	59,63,73	1.34	7 (11%)	71,101,113	1.48	7 (9%)
82	PEB	aJ	203	1	46,46,46	2.58	12 (26%)	54,67,67	2.14	18 (33%)
82	PEB	R1	201	2	46,46,46	2.61	14 (30%)	54,67,67	2.17	22 (40%)
82	PEB	sF	202	1	46,46,46	2.73	12 (26%)	54,67,67	1.99	19 (35%)
85	BCR	bL	601	87	41,41,41	0.76	0	56,56,56	1.58	11 (19%)
82	PEB	uF	202	1	46,46,46	2.73	12 (26%)	54,67,67	2.03	17 (31%)
82	PEB	QF	201	1	46,46,46	2.50	11 (23%)	54,67,67	2.37	21 (38%)
87	CLA	4N	601	60	49,53,73	1.47	9 (18%)	59,89,113	1.56	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	Z1	202	1	46,46,46	2.66	12 (26%)	54,67,67	2.07	17 (31%)
82	PEB	g4	201	2	46,46,46	2.63	14 (30%)	54,67,67	2.02	17 (31%)
82	PEB	f4	202	1	46,46,46	2.62	13 (28%)	54,67,67	1.96	17 (31%)
82	PEB	PK	201	2	46,46,46	2.59	10 (21%)	54,67,67	3.01	19 (35%)
85	BCR	hL	102	-	41,41,41	0.72	0	56,56,56	1.81	14 (25%)
101	FES	N2	101	-	0,4,4	-	-	-		
82	PEB	TI	203	1	46,46,46	2.53	12 (26%)	54,67,67	2.10	20 (37%)
82	PEB	gG	202	2	46,46,46	2.68	12 (26%)	54,67,67	2.12	19 (35%)
84	CYC	DG	1001	10	46,46,46	2.29	16 (34%)	61,67,67	2.94	28 (45%)
87	CLA	5N	601	61	49,53,73	1.47	7 (14%)	59,89,113	1.61	7 (11%)
82	PEB	WF	202	1	46,46,46	2.71	12 (26%)	54,67,67	2.33	24 (44%)
82	PEB	Y7	301	3	46,46,46	2.87	13 (28%)	54,67,67	2.60	24 (44%)
82	PEB	kE	201	3,2	46,46,46	2.67	13 (28%)	54,67,67	2.30	20 (37%)
87	CLA	2N	302	58	49,53,73	1.45	6 (12%)	59,89,113	1.64	6 (10%)
82	PEB	zK	501	78,2	46,46,46	2.50	11 (23%)	54,67,67	2.41	19 (35%)
87	CLA	BL	605	-	69,73,73	1.23	11 (15%)	83,113,113	1.44	6 (7%)
82	PEB	fJ	203	1,2	46,46,46	2.53	13 (28%)	54,67,67	2.28	19 (35%)
82	PEB	LK	202	2	46,46,46	2.77	14 (30%)	54,67,67	2.54	20 (37%)
84	CYC	i3	1001	68	46,46,46	2.65	16 (34%)	61,67,67	2.92	25 (40%)
82	PEB	lE	202	-	46,46,46	0.63	0	54,67,67	0.78	1 (1%)
82	PEB	TA	201	2	46,46,46	2.66	12 (26%)	54,67,67	2.19	16 (29%)
82	PEB	cE	201	2	46,46,46	2.62	13 (28%)	54,67,67	2.10	18 (33%)
82	PEB	KP	201	1,2	46,46,46	3.00	13 (28%)	54,67,67	3.06	19 (35%)
82	PEB	UM	201	1,2	46,46,46	2.54	12 (26%)	54,67,67	2.40	20 (37%)
87	CLA	F2	201	45	49,53,73	1.52	12 (24%)	59,89,113	1.43	9 (15%)
98	PQN	A2	842	-	34,34,34	1.53	2 (5%)	42,45,45	1.00	2 (4%)
87	CLA	3N	308	59	49,53,73	2.34	6 (12%)	59,89,113	3.49	15 (25%)
82	PEB	u8	202	2	46,46,46	2.59	13 (28%)	54,67,67	2.30	17 (31%)
87	CLA	22	605	58,41	58,62,73	1.45	10 (17%)	73,100,113	1.63	12 (16%)
87	CLA	32	309	59	54,58,73	1.36	7 (12%)	65,95,113	1.86	13 (20%)
82	PEB	WB	401	6,2	46,46,46	2.48	12 (26%)	54,67,67	2.12	19 (35%)
94	PL9	dL	406	18,26	55,55,55	0.70	3 (5%)	68,69,69	1.79	16 (23%)
82	PEB	DA	203	2	46,46,46	2.69	13 (28%)	54,67,67	2.15	20 (37%)
82	PEB	C5	202	1	46,46,46	2.57	13 (28%)	54,67,67	2.05	18 (33%)
87	CLA	JN	101	48	46,50,73	1.52	10 (21%)	55,85,113	1.56	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
85	BCR	AN	848	-	41,41,41	0.83	1 (2%)	56,56,56	2.57	20 (35%)
87	CLA	32	303	59,87	49,53,73	1.53	6 (12%)	59,89,113	1.81	11 (18%)
87	CLA	C6	520	-	69,73,73	1.23	9 (13%)	83,113,113	1.35	5 (6%)
83	PUB	AD	302	1,3	45,46,46	2.72	9 (20%)	46,67,67	3.03	18 (39%)
87	CLA	K2	101	-	69,73,73	1.24	9 (13%)	83,113,113	1.29	5 (6%)
82	PEB	AB	501	2,4	46,46,46	2.52	13 (28%)	54,67,67	2.12	19 (35%)
82	PEB	JA	203	2	46,46,46	2.68	12 (26%)	54,67,67	2.14	20 (37%)
82	PEB	gM	202	2	46,46,46	2.70	11 (23%)	54,67,67	2.06	19 (35%)
87	CLA	B6	613	-	69,73,73	1.24	10 (14%)	83,113,113	1.31	5 (6%)
82	PEB	eM	201	13,2	46,46,46	2.68	14 (30%)	54,67,67	2.26	19 (35%)
87	CLA	B6	605	16	69,73,73	1.23	10 (14%)	83,113,113	1.31	6 (7%)
82	PEB	YB	201	2	46,46,46	2.60	14 (30%)	54,67,67	2.14	17 (31%)
84	CYC	DE	1001	10	46,46,46	2.29	16 (34%)	61,67,67	2.91	28 (45%)
82	PEB	QM	202	1,2	46,46,46	2.54	11 (23%)	54,67,67	2.42	20 (37%)
82	PEB	m1	201	2	46,46,46	2.73	14 (30%)	54,67,67	2.03	18 (33%)
85	BCR	CL	502	17	41,41,41	0.88	0	56,56,56	2.37	18 (32%)
82	PEB	dD	401	2,77	46,46,46	2.61	12 (26%)	54,67,67	2.24	18 (33%)
82	PEB	YP	501	2	46,46,46	2.56	11 (23%)	54,67,67	2.08	16 (29%)
82	PEB	LK	201	2	46,46,46	2.58	12 (26%)	54,67,67	3.15	20 (37%)
82	PEB	H9	202	2	46,46,46	2.56	12 (26%)	54,67,67	2.40	18 (33%)
82	PEB	cK	201	1	46,46,46	2.63	12 (26%)	54,67,67	2.27	19 (35%)
87	CLA	O2	203	53	49,53,73	1.64	11 (22%)	59,89,113	1.48	7 (11%)
85	BCR	FL	101	20	41,41,41	0.74	0	56,56,56	2.39	25 (44%)
87	CLA	7N	608	63	45,49,73	1.52	7 (15%)	54,84,113	1.60	8 (14%)
82	PEB	dH	201	1,2	46,46,46	2.60	12 (26%)	54,67,67	2.29	19 (35%)
82	PEB	bP	501	56,2	46,46,46	2.54	13 (28%)	54,67,67	2.05	17 (31%)
88	LHG	AL	406	-	48,48,48	0.93	2 (4%)	51,54,54	1.06	4 (7%)
82	PEB	F7	202	2	46,46,46	2.49	12 (26%)	54,67,67	2.70	23 (42%)
87	CLA	K2	104	-	46,50,73	1.47	10 (21%)	55,85,113	1.73	8 (14%)
82	PEB	VM	202	2	46,46,46	2.64	13 (28%)	54,67,67	2.04	18 (33%)
82	PEB	GA	202	1	46,46,46	2.65	13 (28%)	54,67,67	1.96	20 (37%)
92	LMG	m6	103	-	41,41,55	1.00	2 (4%)	49,49,63	1.12	5 (10%)
82	PEB	S5	203	2	46,46,46	2.49	13 (28%)	54,67,67	1.99	18 (33%)
82	PEB	SG	201	1	46,46,46	2.55	13 (28%)	54,67,67	2.14	20 (37%)
82	PEB	PI	201	1	46,46,46	2.57	13 (28%)	54,67,67	2.05	18 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	fO	201	1	46,46,46	2.64	11 (23%)	54,67,67	2.24	21 (38%)
82	PEB	BI	201	2	46,46,46	2.66	14 (30%)	54,67,67	2.26	22 (40%)
82	PEB	hM	203	1	46,46,46	2.57	12 (26%)	54,67,67	2.51	18 (33%)
83	PUB	wF	304	13	45,46,46	2.59	10 (22%)	46,67,67	2.96	20 (43%)
82	PEB	UD	202	2	46,46,46	2.73	11 (23%)	54,67,67	1.97	18 (33%)
82	PEB	K5	202	1	46,46,46	2.57	13 (28%)	54,67,67	2.05	18 (33%)
85	BCR	cL	503	-	41,41,41	0.72	0	56,56,56	1.82	14 (25%)
82	PEB	QK	203	1,2	46,46,46	2.69	14 (30%)	54,67,67	3.08	22 (40%)
87	CLA	AN	827	-	59,63,73	1.36	10 (16%)	71,101,113	1.44	13 (18%)
87	CLA	bL	622	-	69,73,73	1.25	11 (15%)	83,113,113	1.38	6 (7%)
82	PEB	lF	203	1,2	46,46,46	2.72	16 (34%)	54,67,67	2.50	23 (42%)
82	PEB	aF	202	1	46,46,46	2.57	12 (26%)	54,67,67	2.15	18 (33%)
82	PEB	R4	201	11,2	46,46,46	2.63	13 (28%)	54,67,67	2.40	17 (31%)
82	PEB	JJ	202	2	46,46,46	2.67	12 (26%)	54,67,67	2.15	19 (35%)
82	PEB	MM	201	1,2	46,46,46	2.48	12 (26%)	54,67,67	2.49	23 (42%)
82	PEB	y8	203	2	46,46,46	2.77	13 (28%)	54,67,67	1.96	17 (31%)
87	CLA	22	604	-	46,50,73	1.49	10 (21%)	55,85,113	1.63	10 (18%)
88	LHG	dL	408	-	45,45,48	0.96	2 (4%)	48,51,54	1.04	3 (6%)
82	PEB	X5	201	1	46,46,46	2.56	13 (28%)	54,67,67	2.26	20 (37%)
85	BCR	HL	103	-	41,41,41	0.73	0	56,56,56	1.70	12 (21%)
82	PEB	JQ	203	1,2	46,46,46	2.48	14 (30%)	54,67,67	2.18	17 (31%)
92	LMG	bL	624	16	39,39,55	1.06	2 (5%)	47,47,63	1.20	3 (6%)
82	PEB	KQ	201	2	46,46,46	2.62	12 (26%)	54,67,67	1.95	15 (27%)
83	PUB	AH	303	3	45,46,46	2.85	10 (22%)	46,67,67	3.03	19 (41%)
87	CLA	B2	809	-	69,73,73	1.25	9 (13%)	83,113,113	1.51	6 (7%)
82	PEB	XM	202	2	46,46,46	2.65	15 (32%)	54,67,67	2.14	19 (35%)
92	LMG	jL	101	18,24	33,33,55	1.16	2 (6%)	41,41,63	1.26	4 (9%)
82	PEB	F7	201	3,2	46,46,46	2.62	9 (19%)	54,67,67	2.07	19 (35%)
82	PEB	SE	201	1	46,46,46	2.55	13 (28%)	54,67,67	2.14	19 (35%)
82	PEB	BD	201	1	46,46,46	2.51	13 (28%)	54,67,67	2.30	19 (35%)
82	PEB	OM	201	1	46,46,46	2.63	12 (26%)	54,67,67	2.20	17 (31%)
82	PEB	AD	304	3,82	46,46,46	2.70	13 (28%)	54,67,67	2.20	18 (33%)
82	PEB	gO	201	2	46,46,46	2.63	13 (28%)	54,67,67	2.02	17 (31%)
82	PEB	a4	201	2	46,46,46	2.59	13 (28%)	54,67,67	2.30	18 (33%)
82	PEB	UJ	203	1	46,46,46	2.54	12 (26%)	54,67,67	2.16	19 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	W5	201	2	46,46,46	2.53	12 (26%)	54,67,67	2.28	20 (37%)
82	PEB	H1	1002	10	46,46,46	2.76	14 (30%)	54,67,67	2.24	19 (35%)
82	PEB	Z4	202	1	46,46,46	2.56	12 (26%)	54,67,67	2.01	14 (25%)
82	PEB	gM	201	2	46,46,46	2.72	13 (28%)	54,67,67	2.07	20 (37%)
87	CLA	AN	822	40	49,53,73	1.47	10 (20%)	59,89,113	1.63	8 (13%)
85	BCR	L2	205	50	41,41,41	0.76	0	56,56,56	3.24	23 (41%)
82	PEB	yC	201	2	46,46,46	0.64	0	54,67,67	0.78	1 (1%)
82	PEB	fK	202	2	46,46,46	2.95	14 (30%)	54,67,67	2.32	22 (40%)
85	BCR	AL	401	-	41,41,41	0.69	0	56,56,56	1.74	11 (19%)
82	PEB	BI	203	2	46,46,46	2.57	11 (23%)	54,67,67	2.18	18 (33%)
82	PEB	LE	1002	10,9	46,46,46	2.71	14 (30%)	54,67,67	2.03	18 (33%)
82	PEB	EK	202	1	46,46,46	2.62	13 (28%)	54,67,67	2.08	20 (37%)
82	PEB	mF	201	1	46,46,46	2.68	11 (23%)	54,67,67	2.01	18 (33%)
82	PEB	WA	201	1	46,46,46	2.44	12 (26%)	54,67,67	2.37	21 (38%)
87	CLA	42	605	60	49,53,73	1.49	9 (18%)	59,89,113	1.99	11 (18%)
84	CYC	K4	1001	9	46,46,46	2.36	16 (34%)	61,67,67	2.84	25 (40%)
82	PEB	HK	202	2	46,46,46	2.66	12 (26%)	54,67,67	2.24	20 (37%)
83	PUB	KA	203	1,3	45,46,46	2.69	9 (20%)	46,67,67	3.07	19 (41%)
82	PEB	jM	201	1	46,46,46	2.69	12 (26%)	54,67,67	2.26	17 (31%)
82	PEB	Z5	304	74,82	46,46,46	2.57	13 (28%)	54,67,67	2.92	22 (40%)
82	PEB	OK	201	1,2	46,46,46	2.55	13 (28%)	54,67,67	2.48	22 (40%)
82	PEB	XD	201	1,2	46,46,46	2.59	11 (23%)	54,67,67	2.36	19 (35%)
82	PEB	KB	302	2,5	46,46,46	2.54	13 (28%)	54,67,67	2.18	16 (29%)
82	PEB	ZM	202	2	46,46,46	2.64	15 (32%)	54,67,67	2.15	17 (31%)
82	PEB	QM	203	1	46,46,46	2.65	12 (26%)	54,67,67	2.03	13 (24%)
82	PEB	SA	202	1	46,46,46	2.50	11 (23%)	54,67,67	2.02	14 (25%)
82	PEB	AE	301	3	46,46,46	2.58	13 (28%)	54,67,67	2.10	19 (35%)
87	CLA	12	610	57	49,53,73	1.46	8 (16%)	59,89,113	1.55	7 (11%)
87	CLA	52	609	61	46,50,73	1.51	8 (17%)	55,85,113	1.68	6 (10%)
82	PEB	IJ	201	1,2	46,46,46	2.52	11 (23%)	54,67,67	2.40	21 (38%)
84	CYC	73	1001	73,69	46,46,46	2.53	17 (36%)	61,67,67	3.11	28 (45%)
82	PEB	DF	202	1,2	46,46,46	2.49	11 (23%)	54,67,67	2.71	23 (42%)
82	PEB	DK	202	1,2	46,46,46	2.48	11 (23%)	54,67,67	2.69	23 (42%)
82	PEB	RQ	201	1	46,46,46	2.66	13 (28%)	54,67,67	1.95	17 (31%)
82	PEB	UE	201	1,2	46,46,46	2.60	11 (23%)	54,67,67	2.39	19 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
87	CLA	8N	306	64	49,53,73	1.57	12 (24%)	59,89,113	1.75	11 (18%)
84	CYC	B3	1001	69	46,46,46	2.53	17 (36%)	61,67,67	3.10	28 (45%)
82	PEB	RA	201	2	46,46,46	2.58	13 (28%)	54,67,67	2.19	19 (35%)
82	PEB	QI	201	2	46,46,46	2.61	12 (26%)	54,67,67	2.01	19 (35%)
82	PEB	RD	203	1,2	46,46,46	2.68	14 (30%)	54,67,67	2.18	20 (37%)
87	CLA	F2	205	45	69,73,73	1.36	9 (13%)	83,113,113	1.67	12 (14%)
95	DGD	O6	301	-	41,41,67	1.05	2 (4%)	55,55,81	1.13	5 (9%)
82	PEB	T1	202	2	46,46,46	2.63	11 (23%)	54,67,67	1.91	15 (27%)
82	PEB	fK	201	13,2	46,46,46	2.56	11 (23%)	54,67,67	2.93	18 (33%)
87	CLA	1N	603	-	49,53,73	1.47	9 (18%)	59,89,113	1.49	6 (10%)
82	PEB	TG	201	2	46,46,46	2.60	12 (26%)	54,67,67	2.25	20 (37%)
85	BCR	B2	841	41	41,41,41	0.77	0	56,56,56	2.31	21 (37%)
87	CLA	DL	403	18	69,73,73	1.25	12 (17%)	83,113,113	1.53	11 (13%)
82	PEB	eK	203	1	46,46,46	2.69	12 (26%)	54,67,67	2.13	17 (31%)
87	CLA	A6	402	15	69,73,73	1.25	9 (13%)	83,113,113	1.40	11 (13%)
87	CLA	D6	402	18	69,73,73	1.23	10 (14%)	83,113,113	1.36	6 (7%)
87	CLA	8N	304	64	49,53,73	1.49	10 (20%)	59,89,113	1.64	11 (18%)
82	PEB	ED	202	2	46,46,46	2.64	12 (26%)	54,67,67	2.10	18 (33%)
82	PEB	PQ	201	1,2	46,46,46	2.67	14 (30%)	54,67,67	2.03	18 (33%)
82	PEB	kK	203	1,2	46,46,46	2.57	13 (28%)	54,67,67	2.41	19 (35%)
82	PEB	SO	201	1	46,46,46	2.68	13 (28%)	54,67,67	2.65	25 (46%)
83	PUB	A1	304	3	45,46,46	2.97	11 (24%)	46,67,67	3.30	22 (47%)
82	PEB	pF	202	2	46,46,46	2.77	14 (30%)	54,67,67	2.29	20 (37%)
92	LMG	aL	611	-	42,42,55	1.05	2 (4%)	50,50,63	1.32	8 (16%)
82	PEB	LM	202	2	46,46,46	2.65	12 (26%)	54,67,67	2.16	21 (38%)
82	PEB	gK	202	1	46,46,46	2.69	13 (28%)	54,67,67	2.04	18 (33%)
82	PEB	HJ	201	2	46,46,46	2.61	12 (26%)	54,67,67	2.28	20 (37%)
82	PEB	PA	203	2	46,46,46	2.59	13 (28%)	54,67,67	2.11	18 (33%)
82	PEB	SA	201	1	46,46,46	2.58	11 (23%)	54,67,67	2.78	22 (40%)
87	CLA	AN	830	-	69,73,73	1.24	12 (17%)	83,113,113	1.35	8 (9%)
84	CYC	E3	1001	68	46,46,46	2.65	16 (34%)	61,67,67	2.91	24 (39%)
82	PEB	HA	202	2	46,46,46	2.58	13 (28%)	54,67,67	2.43	22 (40%)
82	PEB	fH	203	1,2	46,46,46	2.68	13 (28%)	54,67,67	2.00	17 (31%)
82	PEB	NQ	204	1,2	46,46,46	2.73	13 (28%)	54,67,67	2.20	20 (37%)
82	PEB	DK	201	2	46,46,46	2.53	10 (21%)	54,67,67	2.91	20 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	RO	203	2	46,46,46	2.59	11 (23%)	54,67,67	1.88	15 (27%)
82	PEB	z8	202	1	46,46,46	2.72	14 (30%)	54,67,67	2.34	22 (40%)
84	CYC	ME	1001	10,9	46,46,46	2.34	16 (34%)	61,67,67	2.91	25 (40%)
87	CLA	A2	814	40	58,62,73	1.36	10 (17%)	69,99,113	1.43	6 (8%)
82	PEB	B9	202	2	46,46,46	2.63	14 (30%)	54,67,67	2.70	24 (44%)
87	CLA	D6	405	-	69,73,73	1.24	10 (14%)	83,113,113	1.35	8 (9%)
82	PEB	iK	202	1	46,46,46	2.64	12 (26%)	54,67,67	2.29	21 (38%)
82	PEB	dH	203	1	46,46,46	2.69	13 (28%)	54,67,67	2.39	20 (37%)
82	PEB	W1	202	1	46,46,46	2.63	12 (26%)	54,67,67	2.32	21 (38%)
82	PEB	d4	202	1	46,46,46	2.64	14 (30%)	54,67,67	1.93	15 (27%)
82	PEB	YM	202	1	46,46,46	2.61	11 (23%)	54,67,67	2.14	15 (27%)
87	CLA	42	604	60	46,50,73	2.16	10 (21%)	55,85,113	4.30	22 (40%)
82	PEB	cB	401	6,2	46,46,46	2.66	11 (23%)	54,67,67	2.17	16 (29%)
82	PEB	iO	202	2	46,46,46	2.56	12 (26%)	54,67,67	2.30	19 (35%)
82	PEB	mG	201	2	46,46,46	2.69	16 (34%)	54,67,67	1.95	15 (27%)
82	PEB	T5	202	1	46,46,46	2.57	13 (28%)	54,67,67	2.06	18 (33%)
82	PEB	gH	201	2	46,46,46	2.73	13 (28%)	54,67,67	2.00	19 (35%)
82	PEB	ZJ	202	2	46,46,46	2.61	13 (28%)	54,67,67	2.10	17 (31%)
82	PEB	Y4	202	2	46,46,46	2.56	13 (28%)	54,67,67	2.35	22 (40%)
82	PEB	VH	202	2	46,46,46	2.70	13 (28%)	54,67,67	2.12	17 (31%)
82	PEB	AK	201	1	46,46,46	2.61	12 (26%)	54,67,67	2.28	19 (35%)
87	CLA	BL	623	16	69,73,73	1.26	11 (15%)	83,113,113	1.46	8 (9%)
87	CLA	C6	513	-	69,73,73	1.23	10 (14%)	83,113,113	1.33	5 (6%)
82	PEB	VA	203	2	46,46,46	2.70	13 (28%)	54,67,67	1.98	20 (37%)
82	PEB	hG	203	1	46,46,46	2.64	12 (26%)	54,67,67	1.97	16 (29%)
87	CLA	42	602	60	69,73,73	1.28	11 (15%)	83,113,113	1.36	7 (8%)
82	PEB	CA	202	1	46,46,46	0.64	0	54,67,67	0.79	1 (1%)
87	CLA	22	609	58	54,58,73	1.49	10 (18%)	65,95,113	1.89	14 (21%)
82	PEB	e4	202	2	46,46,46	2.62	12 (26%)	54,67,67	2.29	22 (40%)
82	PEB	hM	202	1	46,46,46	2.64	13 (28%)	54,67,67	2.07	16 (29%)
87	CLA	A2	817	-	46,50,73	1.48	9 (19%)	55,85,113	1.58	6 (10%)
82	PEB	WQ	202	2	46,46,46	2.73	15 (32%)	54,67,67	1.92	17 (31%)
84	CYC	IO	1001	9	46,46,46	2.32	17 (36%)	61,67,67	2.83	26 (42%)
87	CLA	32	307	59	49,53,73	2.34	7 (14%)	59,89,113	3.49	14 (23%)
87	CLA	5N	611	61	49,53,73	1.49	8 (16%)	59,89,113	1.60	9 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	cK	202	1	46,46,46	2.66	11 (23%)	54,67,67	2.04	18 (33%)
82	PEB	gH	202	2	46,46,46	2.72	13 (28%)	54,67,67	2.19	16 (29%)
82	PEB	L7	201	2,82	46,46,46	2.69	13 (28%)	54,67,67	2.15	18 (33%)
87	CLA	BL	608	-	69,73,73	1.27	9 (13%)	83,113,113	1.42	8 (9%)
82	PEB	YE	201	2	46,46,46	2.54	13 (28%)	54,67,67	2.59	22 (40%)
82	PEB	dE	201	1,3	46,46,46	2.65	13 (28%)	54,67,67	2.18	19 (35%)
92	LMG	XL	601	37	50,50,55	0.99	2 (4%)	58,58,63	1.25	3 (5%)
82	PEB	fE	203	1,2	46,46,46	2.66	13 (28%)	54,67,67	2.14	16 (29%)
82	PEB	b1	201	1	46,46,46	2.60	12 (26%)	54,67,67	2.03	18 (33%)
82	PEB	MA	201	1	46,46,46	2.54	11 (23%)	54,67,67	2.36	19 (35%)
95	DGD	C6	503	-	43,43,67	1.01	3 (6%)	57,57,81	1.62	11 (19%)
84	CYC	D4	1001	10	46,46,46	2.27	15 (32%)	61,67,67	2.86	26 (42%)
87	CLA	AN	817	-	46,50,73	1.49	9 (19%)	55,85,113	1.57	6 (10%)
82	PEB	Z5	301	74	46,46,46	2.55	13 (28%)	54,67,67	2.22	20 (37%)
82	PEB	SD	202	2	46,46,46	2.67	12 (26%)	54,67,67	2.07	20 (37%)
82	PEB	r8	202	1	46,46,46	2.79	13 (28%)	54,67,67	2.38	20 (37%)
84	CYC	HO	1001	10	46,46,46	2.38	16 (34%)	61,67,67	3.01	29 (47%)
82	PEB	y8	202	2	46,46,46	2.69	11 (23%)	54,67,67	2.30	19 (35%)
87	CLA	82	303	64	49,53,73	1.50	10 (20%)	59,89,113	1.65	11 (18%)
87	CLA	7N	603	-	49,53,73	1.47	9 (18%)	59,89,113	1.53	8 (13%)
82	PEB	X7	201	2,75	46,46,46	2.75	13 (28%)	54,67,67	2.29	20 (37%)
87	CLA	B6	604	-	69,73,73	1.24	10 (14%)	83,113,113	1.34	8 (9%)
82	PEB	OF	201	1,2	46,46,46	2.56	13 (28%)	54,67,67	2.48	22 (40%)
82	PEB	Q1	202	1	46,46,46	2.58	12 (26%)	54,67,67	2.35	19 (35%)
82	PEB	YF	202	1	46,46,46	2.68	12 (26%)	54,67,67	1.89	17 (31%)
82	PEB	DA	201	3,2	46,46,46	2.64	14 (30%)	54,67,67	2.24	17 (31%)
82	PEB	QP	203	1,2	46,46,46	3.07	14 (30%)	54,67,67	3.04	21 (38%)
87	CLA	LN	206	50	60,64,73	1.29	9 (15%)	72,102,113	1.45	9 (12%)
82	PEB	J5	202	2	46,46,46	2.53	12 (26%)	54,67,67	2.15	17 (31%)
82	PEB	RE	202	2	46,46,46	2.62	12 (26%)	54,67,67	2.07	18 (33%)
82	PEB	F1	1002	10	46,46,46	2.57	13 (28%)	54,67,67	2.18	16 (29%)
82	PEB	XF	202	2	46,46,46	2.49	12 (26%)	54,67,67	2.51	20 (37%)
82	PEB	XJ	201	2	46,46,46	2.66	13 (28%)	54,67,67	2.14	19 (35%)
82	PEB	BB	201	2	46,46,46	2.58	12 (26%)	54,67,67	2.09	17 (31%)
87	CLA	A2	820	-	69,73,73	1.28	10 (14%)	83,113,113	1.50	14 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
95	DGD	C6	523	-	49,49,67	0.95	2 (4%)	63,63,81	1.07	4 (6%)
92	LMG	d6	409	18	54,54,55	0.89	2 (3%)	62,62,63	1.00	3 (4%)
82	PEB	Z1	203	1	46,46,46	2.76	13 (28%)	54,67,67	2.22	19 (35%)
87	CLA	C6	514	87	69,73,73	1.25	10 (14%)	83,113,113	1.32	8 (9%)
82	PEB	O1	201	1	46,46,46	2.62	14 (30%)	54,67,67	2.15	21 (38%)
82	PEB	YO	202	2	46,46,46	2.55	12 (26%)	54,67,67	2.35	21 (38%)
82	PEB	q8	202	2	46,46,46	2.61	13 (28%)	54,67,67	2.41	21 (38%)
82	PEB	cO	203	2	46,46,46	2.69	13 (28%)	54,67,67	1.92	14 (25%)
85	BCR	J2	102	-	41,41,41	0.73	0	56,56,56	2.01	16 (28%)
82	PEB	HQ	202	1	46,46,46	2.63	14 (30%)	54,67,67	2.31	20 (37%)
87	CLA	6N	610	-	46,50,73	1.51	9 (19%)	55,85,113	1.70	8 (14%)
82	PEB	fG	203	1,2	46,46,46	2.65	13 (28%)	54,67,67	2.14	16 (29%)
84	CYC	HG	1001	10	46,46,46	2.26	15 (32%)	61,67,67	3.02	27 (44%)
87	CLA	A2	852	59,40	49,53,73	1.79	11 (22%)	59,89,113	2.61	19 (32%)
82	PEB	PJ	202	2	46,46,46	2.62	12 (26%)	54,67,67	2.07	22 (40%)
82	PEB	B5	202	2	46,46,46	2.70	13 (28%)	54,67,67	2.25	20 (37%)
82	PEB	gB	202	2	46,46,46	2.59	12 (26%)	54,67,67	2.09	15 (27%)
82	PEB	iJ	202	2	46,46,46	2.62	12 (26%)	54,67,67	2.21	20 (37%)
82	PEB	WJ	203	1,2	46,46,46	2.45	11 (23%)	54,67,67	2.68	23 (42%)
82	PEB	eG	202	2	46,46,46	2.62	11 (23%)	54,67,67	2.25	20 (37%)
87	CLA	3N	303	59,60	49,53,73	1.57	8 (16%)	59,89,113	2.08	13 (22%)
82	PEB	AH	305	3	46,46,46	2.68	12 (26%)	54,67,67	2.10	16 (29%)
82	PEB	H4	1002	10	46,46,46	2.54	13 (28%)	54,67,67	2.05	16 (29%)
92	LMG	D6	409	18	54,54,55	0.88	2 (3%)	62,62,63	1.01	3 (4%)
82	PEB	mK	202	1	46,46,46	2.68	12 (26%)	54,67,67	2.18	17 (31%)
87	CLA	3N	304	59,87	49,53,73	1.53	6 (12%)	59,89,113	1.81	11 (18%)
82	PEB	H7	203	2	46,46,46	2.70	13 (28%)	54,67,67	2.24	19 (35%)
82	PEB	TP	202	2	46,46,46	2.66	12 (26%)	54,67,67	2.06	20 (37%)
82	PEB	O5	203	2	46,46,46	2.52	12 (26%)	54,67,67	2.11	19 (35%)
82	PEB	hE	202	1	46,46,46	2.65	14 (30%)	54,67,67	1.98	17 (31%)
85	BCR	JN	103	40,48	41,41,41	0.70	0	56,56,56	2.08	16 (28%)
87	CLA	A2	830	-	69,73,73	1.24	12 (17%)	83,113,113	1.36	8 (9%)
82	PEB	CB	202	2	46,46,46	2.73	14 (30%)	54,67,67	2.20	20 (37%)
82	PEB	CM	202	1	46,46,46	2.52	14 (30%)	54,67,67	2.18	20 (37%)
82	PEB	UA	202	1	46,46,46	2.63	13 (28%)	54,67,67	1.94	16 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	gJ	201	2	46,46,46	2.72	14 (30%)	54,67,67	2.25	21 (38%)
87	CLA	BN	820	41	49,53,73	1.47	11 (22%)	59,89,113	1.55	8 (13%)
82	PEB	Y4	201	2	46,46,46	2.61	13 (28%)	54,67,67	2.16	20 (37%)
87	CLA	b6	607	-	69,73,73	1.25	10 (14%)	83,113,113	1.28	6 (7%)
82	PEB	MD	201	2	46,46,46	2.67	13 (28%)	54,67,67	2.17	18 (33%)
82	PEB	AF	202	1	46,46,46	2.70	14 (30%)	54,67,67	1.81	15 (27%)
82	PEB	e4	201	2	46,46,46	2.58	14 (30%)	54,67,67	2.18	17 (31%)
82	PEB	VH	201	2	46,46,46	2.61	14 (30%)	54,67,67	2.28	20 (37%)
82	PEB	KB	301	2,5	46,46,46	2.55	12 (26%)	54,67,67	2.21	23 (42%)
82	PEB	CK	202	1	46,46,46	2.50	9 (19%)	54,67,67	2.41	19 (35%)
82	PEB	iF	202	1	46,46,46	2.65	12 (26%)	54,67,67	2.29	22 (40%)
82	PEB	eA	301	1,75	46,46,46	2.55	12 (26%)	54,67,67	2.03	15 (27%)
87	CLA	RN	201	87	49,53,73	1.50	7 (14%)	59,89,113	1.54	7 (11%)
82	PEB	cB	403	6,2	46,46,46	2.63	12 (26%)	54,67,67	2.26	24 (44%)
82	PEB	dB	201	2	46,46,46	2.54	13 (28%)	54,67,67	2.02	16 (29%)
82	PEB	CQ	201	3,2	46,46,46	2.63	14 (30%)	54,67,67	2.33	21 (38%)
84	CYC	E1	1001	10,9	46,46,46	2.35	17 (36%)	61,67,67	3.17	28 (45%)
82	PEB	iJ	201	13,2	46,46,46	2.69	13 (28%)	54,67,67	2.10	19 (35%)
87	CLA	22	610	58	45,49,73	1.49	9 (20%)	54,84,113	1.58	7 (12%)
82	PEB	P7	203	2	46,46,46	2.60	13 (28%)	54,67,67	2.10	18 (33%)
82	PEB	GQ	201	2	46,46,46	2.69	14 (30%)	54,67,67	2.14	19 (35%)
82	PEB	ZF	201	2	46,46,46	2.67	12 (26%)	54,67,67	2.14	18 (33%)
82	PEB	CP	203	1	46,46,46	2.62	13 (28%)	54,67,67	1.98	19 (35%)
82	PEB	O4	202	1	46,46,46	2.56	14 (30%)	54,67,67	1.94	15 (27%)
82	PEB	k4	202	2	46,46,46	0.63	0	54,67,67	0.79	1 (1%)
82	PEB	xF	302	13	46,46,46	2.71	16 (34%)	54,67,67	2.30	16 (29%)
87	CLA	BN	810	-	69,73,73	1.24	9 (13%)	83,113,113	1.51	6 (7%)
83	PUB	AO	302	3	45,46,46	2.70	9 (20%)	46,67,67	2.90	17 (36%)
87	CLA	4N	604	60	46,50,73	2.15	9 (19%)	55,85,113	4.29	22 (40%)
87	CLA	AN	803	40,50,53	56,60,73	1.40	11 (19%)	67,97,113	1.38	7 (10%)
95	DGD	c6	601	-	63,63,67	1.08	4 (6%)	77,77,81	1.82	16 (20%)
82	PEB	TJ	201	2	46,46,46	2.67	13 (28%)	54,67,67	2.26	20 (37%)
85	BCR	AN	845	40	41,41,41	0.71	0	56,56,56	1.97	12 (21%)
82	PEB	TI	202	1	46,46,46	2.57	12 (26%)	54,67,67	2.05	18 (33%)
82	PEB	SM	203	1,2	46,46,46	2.57	12 (26%)	54,67,67	2.26	19 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	LQ	201	1,2	46,46,46	2.55	12 (26%)	54,67,67	2.28	19 (35%)
87	CLA	32	304	59,87	69,73,73	1.35	10 (14%)	83,113,113	1.87	15 (18%)
87	CLA	A2	821	-	69,73,73	1.24	10 (14%)	83,113,113	1.45	10 (12%)
82	PEB	bO	202	1	46,46,46	2.65	12 (26%)	54,67,67	1.97	15 (27%)
82	PEB	HI	202	1,2	46,46,46	2.32	13 (28%)	54,67,67	3.04	24 (44%)
82	PEB	hO	201	1	46,46,46	2.63	14 (30%)	54,67,67	2.28	21 (38%)
82	PEB	UA	201	1	46,46,46	2.58	11 (23%)	54,67,67	2.61	18 (33%)
87	CLA	BN	813	-	69,73,73	1.26	10 (14%)	83,113,113	1.40	10 (12%)
87	CLA	72	604	63	46,50,73	1.50	10 (21%)	55,85,113	1.60	8 (14%)
87	CLA	3N	310	59,87	45,49,73	1.51	8 (17%)	54,84,113	1.85	9 (16%)
82	PEB	PA	202	2	46,46,46	2.41	12 (26%)	54,67,67	2.67	24 (44%)
82	PEB	PO	202	2	46,46,46	2.58	12 (26%)	54,67,67	2.45	23 (42%)
82	PEB	fH	202	1	46,46,46	2.86	11 (23%)	54,67,67	2.29	19 (35%)
87	CLA	L2	203	85,50,41	69,73,73	1.24	8 (11%)	83,113,113	1.47	6 (7%)
82	PEB	KI	201	1,2	46,46,46	2.45	14 (30%)	54,67,67	2.84	21 (38%)
87	CLA	8N	303	64	69,73,73	1.33	12 (17%)	83,113,113	1.78	14 (16%)
82	PEB	UP	201	1	46,46,46	2.55	12 (26%)	54,67,67	2.25	19 (35%)
84	CYC	NO	1001	10	46,46,46	2.48	19 (41%)	61,67,67	2.84	27 (44%)
82	PEB	FA	201	3,2	46,46,46	2.61	10 (21%)	54,67,67	2.07	19 (35%)
82	PEB	g1	202	2	46,46,46	2.71	13 (28%)	54,67,67	2.20	16 (29%)
85	BCR	K2	102	40,49	41,41,41	0.80	1 (2%)	56,56,56	2.74	19 (33%)
83	PUB	AE	302	3	45,46,46	2.70	10 (22%)	46,67,67	3.07	22 (47%)
82	PEB	OP	201	1,2	46,46,46	3.01	13 (28%)	54,67,67	2.87	20 (37%)
82	PEB	vF	202	2	46,46,46	2.67	13 (28%)	54,67,67	2.01	19 (35%)
82	PEB	kG	201	3,2	46,46,46	2.65	13 (28%)	54,67,67	2.30	19 (35%)
82	PEB	V7	201	2,75	46,46,46	2.58	12 (26%)	54,67,67	2.09	15 (27%)
88	LHG	a6	610	15	42,42,48	0.97	2 (4%)	45,48,54	1.10	2 (4%)
84	CYC	FO	1001	10	46,46,46	2.31	15 (32%)	61,67,67	2.89	26 (42%)
87	CLA	KN	102	-	49,53,73	1.49	12 (24%)	59,89,113	1.49	6 (10%)
82	PEB	W4	201	1	46,46,46	2.56	13 (28%)	54,67,67	2.64	24 (44%)
84	CYC	g3	1001	68	46,46,46	2.65	16 (34%)	61,67,67	2.91	25 (40%)
87	CLA	CL	513	17	64,68,73	1.35	9 (14%)	77,107,113	1.61	16 (20%)
87	CLA	82	305	64	49,53,73	1.57	13 (26%)	59,89,113	1.75	11 (18%)
82	PEB	DB	203	2	46,46,46	2.51	12 (26%)	54,67,67	2.16	18 (33%)
82	PEB	mO	201	2	46,46,46	2.63	12 (26%)	54,67,67	2.14	17 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	H5	202	2	46,46,46	2.56	11 (23%)	54,67,67	2.24	18 (33%)
82	PEB	d1	203	1	46,46,46	2.69	11 (23%)	54,67,67	2.41	20 (37%)
82	PEB	lE	201	1,2	46,46,46	2.61	14 (30%)	54,67,67	2.15	17 (31%)
84	CYC	DH	1001	10	46,46,46	2.37	17 (36%)	61,67,67	2.78	24 (39%)
82	PEB	l4	202	-	46,46,46	2.62	13 (28%)	54,67,67	2.03	18 (33%)
82	PEB	XQ	203	1	46,46,46	2.70	12 (26%)	54,67,67	1.95	14 (25%)
82	PEB	EF	201	1	46,46,46	2.49	11 (23%)	54,67,67	2.37	17 (31%)
84	CYC	JO	1001	10	46,46,46	2.31	18 (39%)	61,67,67	2.95	27 (44%)
82	PEB	GB	201	2	46,46,46	2.60	13 (28%)	54,67,67	2.13	17 (31%)
82	PEB	qF	201	1,2	46,46,46	2.63	13 (28%)	54,67,67	2.51	23 (42%)
92	LMG	dL	407	18	54,54,55	0.92	2 (3%)	62,62,63	1.34	6 (9%)
82	PEB	G5	201	1	46,46,46	2.56	13 (28%)	54,67,67	2.27	20 (37%)
82	PEB	UF	201	1	46,46,46	2.52	11 (23%)	54,67,67	3.22	25 (46%)
82	PEB	t8	201	1	46,46,46	2.72	14 (30%)	54,67,67	1.84	17 (31%)
82	PEB	N7	203	2	46,46,46	2.57	12 (26%)	54,67,67	2.53	22 (40%)
82	PEB	d4	201	1	46,46,46	2.54	11 (23%)	54,67,67	2.22	21 (38%)
82	PEB	OI	203	2	46,46,46	2.61	11 (23%)	54,67,67	1.98	17 (31%)
87	CLA	AN	835	-	69,73,73	1.20	10 (14%)	83,113,113	1.38	8 (9%)
87	CLA	82	302	64	69,73,73	1.33	12 (17%)	83,113,113	1.77	14 (16%)
87	CLA	AN	805	40	69,73,73	1.29	10 (14%)	83,113,113	1.32	8 (9%)
85	BCR	BN	841	41	41,41,41	0.77	0	56,56,56	2.31	21 (37%)
82	PEB	WP	201	1,2	46,46,46	3.07	13 (28%)	54,67,67	3.14	20 (37%)
82	PEB	LO	1002	10	46,46,46	2.56	13 (28%)	54,67,67	2.53	20 (37%)
82	PEB	Y5	201	74,2	46,46,46	2.54	12 (26%)	54,67,67	2.20	19 (35%)
98	PQN	B2	837	41	34,34,34	1.88	4 (11%)	42,45,45	2.53	14 (33%)
87	CLA	c6	606	17	69,73,73	1.25	9 (13%)	83,113,113	1.34	7 (8%)
82	PEB	I5	202	1	46,46,46	2.57	13 (28%)	54,67,67	2.05	18 (33%)
82	PEB	DQ	203	1	46,46,46	2.69	12 (26%)	54,67,67	2.24	17 (31%)
82	PEB	mM	202	2	46,46,46	2.69	15 (32%)	54,67,67	2.16	21 (38%)
92	LMG	k6	101	25	55,55,55	0.89	2 (3%)	63,63,63	0.89	2 (3%)
99	SF4	CN	101	42	0,12,12	-	-	-		
82	PEB	MF	203	1,2	46,46,46	2.59	14 (30%)	54,67,67	2.56	19 (35%)
82	PEB	PP	202	2	46,46,46	2.62	13 (28%)	54,67,67	2.11	17 (31%)
82	PEB	aE	202	2	46,46,46	2.60	14 (30%)	54,67,67	2.09	17 (31%)
82	PEB	DP	201	2	46,46,46	2.59	13 (28%)	54,67,67	2.04	16 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	P4	202	2	46,46,46	2.58	12 (26%)	54,67,67	2.47	23 (42%)
88	LHG	ML	102	-	38,38,48	1.03	2 (5%)	41,44,54	1.09	3 (7%)
87	CLA	BN	805	41	69,73,73	1.29	10 (14%)	83,113,113	1.40	11 (13%)
82	PEB	RM	201	2	46,46,46	2.62	12 (26%)	54,67,67	2.19	18 (33%)
82	PEB	mE	201	2	46,46,46	2.70	16 (34%)	54,67,67	1.95	15 (27%)
82	PEB	OO	201	1	46,46,46	2.60	13 (28%)	54,67,67	2.53	25 (46%)
82	PEB	AQ	301	3	46,46,46	2.61	12 (26%)	54,67,67	2.05	21 (38%)
82	PEB	BP	201	2	46,46,46	2.65	13 (28%)	54,67,67	2.02	19 (35%)
95	DGD	JL	101	-	63,63,67	0.83	2 (3%)	77,77,81	0.94	2 (2%)
87	CLA	8N	307	-	46,50,73	1.48	8 (17%)	55,85,113	1.47	6 (10%)
82	PEB	a1	202	2	46,46,46	2.75	13 (28%)	54,67,67	2.01	16 (29%)
82	PEB	kO	203	2	46,46,46	0.63	0	54,67,67	0.79	1 (1%)
82	PEB	EJ	203	1	46,46,46	2.48	13 (28%)	54,67,67	2.14	18 (33%)
87	CLA	C6	517	-	69,73,73	1.26	10 (14%)	83,113,113	1.34	7 (8%)
82	PEB	D7	202	2	46,46,46	2.52	12 (26%)	54,67,67	2.46	21 (38%)
82	PEB	hJ	202	1	46,46,46	2.60	13 (28%)	54,67,67	1.99	17 (31%)
82	PEB	LI	202	2	46,46,46	2.53	12 (26%)	54,67,67	2.02	16 (29%)
87	CLA	I2	103	47,50	69,73,73	1.25	9 (13%)	83,113,113	1.38	9 (10%)
82	PEB	DD	203	1	46,46,46	2.70	12 (26%)	54,67,67	2.28	17 (31%)
82	PEB	OK	202	1	46,46,46	2.53	11 (23%)	54,67,67	2.26	21 (38%)
87	CLA	AN	809	-	69,73,73	1.24	9 (13%)	83,113,113	1.51	15 (18%)
82	PEB	JO	1002	10	46,46,46	2.65	14 (30%)	54,67,67	2.10	19 (35%)
82	PEB	PE	201	11,2	46,46,46	2.65	13 (28%)	54,67,67	2.35	22 (40%)
82	PEB	RP	201	56,2	46,46,46	2.61	14 (30%)	54,67,67	2.03	17 (31%)
82	PEB	JJ	201	2	46,46,46	2.73	13 (28%)	54,67,67	2.28	18 (33%)
82	PEB	PO	203	2	46,46,46	2.56	11 (23%)	54,67,67	1.86	16 (29%)
87	CLA	A2	849	40	69,73,73	1.26	10 (14%)	83,113,113	1.50	9 (10%)
87	CLA	A2	819	40	66,70,73	1.30	10 (15%)	79,109,113	1.52	9 (11%)
87	CLA	A2	815	-	69,73,73	1.26	11 (15%)	83,113,113	1.40	11 (13%)
82	PEB	QK	201	1	46,46,46	2.49	11 (23%)	54,67,67	2.35	21 (38%)
82	PEB	aH	201	2	46,46,46	2.62	10 (21%)	54,67,67	2.12	19 (35%)
84	CYC	w3	1001	73,69	46,46,46	2.53	17 (36%)	61,67,67	3.11	28 (45%)
92	LMG	bL	623	-	41,41,55	0.98	2 (4%)	49,49,63	1.30	5 (10%)
82	PEB	gF	202	1	46,46,46	2.66	13 (28%)	54,67,67	2.03	18 (33%)
82	PEB	P4	201	2	46,46,46	2.64	12 (26%)	54,67,67	2.19	18 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
87	CLA	bL	617	-	69,73,73	1.28	10 (14%)	83,113,113	1.54	8 (9%)
84	CYC	F1	1001	10	46,46,46	2.34	16 (34%)	61,67,67	2.84	25 (40%)
87	CLA	CL	503	-	69,73,73	1.24	11 (15%)	83,113,113	1.52	10 (12%)
98	PQN	AN	842	-	34,34,34	1.53	2 (5%)	42,45,45	1.01	2 (4%)
82	PEB	HO	1002	10	46,46,46	2.56	13 (28%)	54,67,67	2.05	16 (29%)
89	OEX	AL	408	15	0,14,14	-	-	-		
82	PEB	V4	201	2	46,46,46	2.60	12 (26%)	54,67,67	2.20	19 (35%)
82	PEB	AJ	302	13	46,46,46	2.58	11 (23%)	54,67,67	2.03	15 (27%)
87	CLA	AN	838	-	69,73,73	1.25	11 (15%)	83,113,113	1.38	9 (10%)
87	CLA	B2	818	-	69,73,73	1.26	10 (14%)	83,113,113	1.40	7 (8%)
82	PEB	gB	203	2	46,46,46	2.71	14 (30%)	54,67,67	2.28	22 (40%)
82	PEB	aK	203	1	46,46,46	2.70	10 (21%)	54,67,67	2.27	21 (38%)
82	PEB	QQ	201	3,2	46,46,46	2.72	12 (26%)	54,67,67	2.21	22 (40%)
82	PEB	IB	203	2	46,46,46	2.54	12 (26%)	54,67,67	2.15	18 (33%)
82	PEB	FD	203	1,2	46,46,46	2.82	15 (32%)	54,67,67	2.99	22 (40%)
82	PEB	N9	201	1	46,46,46	2.61	14 (30%)	54,67,67	1.97	17 (31%)
85	BCR	B2	843	-	41,41,41	0.77	0	56,56,56	2.01	18 (32%)
82	PEB	LI	201	12,2	46,46,46	2.59	13 (28%)	54,67,67	2.04	19 (35%)
82	PEB	R1	202	2	46,46,46	2.72	13 (28%)	54,67,67	1.87	14 (25%)
82	PEB	TQ	202	1	46,46,46	2.66	12 (26%)	54,67,67	2.10	18 (33%)
87	CLA	BL	604	-	63,67,73	1.31	11 (17%)	75,105,113	1.28	6 (8%)
82	PEB	G9	202	1	46,46,46	2.73	14 (30%)	54,67,67	2.41	20 (37%)
87	CLA	A2	826	-	69,73,73	1.28	11 (15%)	83,113,113	1.40	11 (13%)
82	PEB	K7	202	1	46,46,46	2.67	13 (28%)	54,67,67	1.89	15 (27%)
82	PEB	SB	201	2	46,46,46	2.53	12 (26%)	54,67,67	2.13	17 (31%)
87	CLA	J2	101	48	46,50,73	1.52	10 (21%)	55,85,113	1.55	8 (14%)
82	PEB	k1	201	2	46,46,46	2.66	13 (28%)	54,67,67	2.06	21 (38%)
82	PEB	PG	202	2	46,46,46	2.64	12 (26%)	54,67,67	2.33	24 (44%)
82	PEB	WI	203	2	46,46,46	2.64	13 (28%)	54,67,67	1.92	17 (31%)
85	BCR	AN	846	-	41,41,41	0.76	0	56,56,56	2.75	19 (33%)
82	PEB	YG	201	2	46,46,46	2.52	12 (26%)	54,67,67	2.58	22 (40%)
87	CLA	b6	604	-	69,73,73	1.25	10 (14%)	83,113,113	1.33	5 (6%)
82	PEB	N9	202	1	46,46,46	2.73	13 (28%)	54,67,67	2.41	20 (37%)
87	CLA	B6	614	-	69,73,73	1.25	10 (14%)	83,113,113	1.33	8 (9%)
82	PEB	tK	202	2	46,46,46	2.81	13 (28%)	54,67,67	2.26	19 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
87	CLA	cL	515	17	64,68,73	1.35	9 (14%)	77,107,113	1.61	14 (18%)
92	LMG	bL	611	37,16	50,50,55	0.98	2 (4%)	58,58,63	1.17	5 (8%)
87	CLA	A2	825	-	59,63,73	1.38	11 (18%)	71,101,113	1.47	9 (12%)
87	CLA	B2	824	41	69,73,73	1.30	9 (13%)	83,113,113	1.47	12 (14%)
82	PEB	HE	1002	10,9	46,46,46	2.58	14 (30%)	54,67,67	1.99	16 (29%)
82	PEB	A7	202	1	46,46,46	2.66	14 (30%)	54,67,67	2.03	16 (29%)
82	PEB	S7	202	1	46,46,46	2.50	12 (26%)	54,67,67	2.02	14 (25%)
82	PEB	NA	202	2	46,46,46	2.40	10 (21%)	54,67,67	3.00	23 (42%)
85	BCR	B2	842	-	41,41,41	0.76	0	56,56,56	2.28	17 (30%)
82	PEB	oF	201	1	46,46,46	2.74	13 (28%)	54,67,67	2.11	19 (35%)
82	PEB	kK	201	1	46,46,46	2.71	12 (26%)	54,67,67	2.06	15 (27%)
82	PEB	BM	301	14	46,46,46	2.63	13 (28%)	54,67,67	2.34	19 (35%)
87	CLA	32	313	-	49,53,73	1.48	9 (18%)	59,89,113	1.52	8 (13%)
87	CLA	6N	612	62	49,53,73	1.66	8 (16%)	59,89,113	2.06	15 (25%)
85	BCR	BN	842	-	41,41,41	0.77	0	56,56,56	2.28	17 (30%)
82	PEB	G9	201	1	46,46,46	2.61	13 (28%)	54,67,67	1.97	17 (31%)
82	PEB	mO	203	2	46,46,46	2.70	14 (30%)	54,67,67	2.03	21 (38%)
82	PEB	RJ	202	2	46,46,46	2.61	13 (28%)	54,67,67	2.20	18 (33%)
87	CLA	A2	832	40	54,58,73	1.41	11 (20%)	65,95,113	1.60	9 (13%)
82	PEB	ND	203	1	46,46,46	2.66	11 (23%)	54,67,67	2.02	16 (29%)
82	PEB	L4	1002	10	46,46,46	2.56	13 (28%)	54,67,67	2.52	20 (37%)
82	PEB	II	202	1	46,46,46	2.54	12 (26%)	54,67,67	2.11	20 (37%)
82	PEB	h1	203	1	46,46,46	0.64	0	54,67,67	0.79	1 (1%)
82	PEB	xK	302	13	46,46,46	2.71	15 (32%)	54,67,67	2.31	16 (29%)
87	CLA	B2	836	87,41,57	69,73,73	1.23	8 (11%)	83,113,113	1.66	9 (10%)
88	LHG	c6	619	17	31,31,48	1.11	2 (6%)	34,37,54	1.31	3 (8%)
84	CYC	J3	1001	68	46,46,46	2.66	16 (34%)	61,67,67	2.92	25 (40%)
96	HEM	vL	201	35	50,50,50	1.67	10 (20%)	66,82,82	1.76	16 (24%)
85	BCR	fL	101	20	41,41,41	0.74	0	56,56,56	2.42	25 (44%)
82	PEB	c4	201	2	46,46,46	2.63	11 (23%)	54,67,67	1.99	14 (25%)
84	CYC	J4	1001	10	46,46,46	2.31	18 (39%)	61,67,67	2.96	28 (45%)
84	CYC	JH	1001	10	46,46,46	2.31	18 (39%)	61,67,67	2.89	30 (49%)
82	PEB	T9	201	1	46,46,46	2.61	14 (30%)	54,67,67	1.97	17 (31%)
82	PEB	eK	201	1,2	46,46,46	2.71	14 (30%)	54,67,67	2.18	19 (35%)
82	PEB	GM	201	1	46,46,46	2.64	12 (26%)	54,67,67	2.08	15 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	jJ	203	1,2	46,46,46	2.54	13 (28%)	54,67,67	2.37	21 (38%)
85	BCR	b6	602	-	41,41,41	0.76	0	56,56,56	2.48	24 (42%)
82	PEB	wF	302	13	46,46,46	2.62	12 (26%)	54,67,67	2.06	18 (33%)
87	CLA	BN	821	54,41	47,51,73	1.43	8 (17%)	56,86,113	1.25	6 (10%)
82	PEB	XA	201	2,75	46,46,46	2.75	13 (28%)	54,67,67	2.29	20 (37%)
82	PEB	QP	202	1	46,46,46	2.61	14 (30%)	54,67,67	2.13	20 (37%)
82	PEB	CP	201	1,2	46,46,46	2.98	14 (30%)	54,67,67	2.95	23 (42%)
87	CLA	L2	206	50	60,64,73	1.29	9 (15%)	72,102,113	1.46	9 (12%)
87	CLA	b6	608	16	69,73,73	1.22	11 (15%)	83,113,113	1.51	10 (12%)
82	PEB	R7	202	2	46,46,46	2.48	12 (26%)	54,67,67	2.93	21 (38%)
82	PEB	JF	202	2	46,46,46	2.78	13 (28%)	54,67,67	2.42	23 (42%)
87	CLA	82	304	-	49,53,73	1.48	8 (16%)	59,89,113	1.52	7 (11%)
82	PEB	ZE	201	1,2	46,46,46	2.53	11 (23%)	54,67,67	2.51	23 (42%)
82	PEB	tC	201	1	46,46,46	2.73	14 (30%)	54,67,67	1.85	17 (31%)
84	CYC	E4	1001	9	46,46,46	2.34	18 (39%)	61,67,67	2.89	24 (39%)
93	BCT	d6	410	15,90,18	2,3,3	1.26	0	2,3,3	4.07	1 (50%)
82	PEB	hG	201	1,2	46,46,46	2.69	14 (30%)	54,67,67	2.26	15 (27%)
82	PEB	H5	201	74,2	46,46,46	2.85	16 (34%)	54,67,67	2.37	17 (31%)
87	CLA	C6	511	-	69,73,73	1.26	9 (13%)	83,113,113	1.33	6 (7%)
82	PEB	18	201	2	46,46,46	2.77	12 (26%)	54,67,67	2.00	17 (31%)
87	CLA	B6	608	16	69,73,73	1.24	9 (13%)	83,113,113	1.30	7 (8%)
82	PEB	YH	201	2	46,46,46	2.74	14 (30%)	54,67,67	2.25	23 (42%)
82	PEB	LF	202	2	46,46,46	2.77	14 (30%)	54,67,67	2.54	20 (37%)
82	PEB	dJ	201	1,2	46,46,46	2.59	13 (28%)	54,67,67	2.29	19 (35%)
89	OEX	A6	405	15	0,14,14	-	-	-		
87	CLA	62	312	62	49,53,73	1.44	6 (12%)	59,89,113	1.44	4 (6%)
82	PEB	uC	202	2	46,46,46	2.59	14 (30%)	54,67,67	2.30	17 (31%)
82	PEB	IP	203	1,2	46,46,46	3.05	13 (28%)	54,67,67	3.09	19 (35%)
82	PEB	KM	202	1	46,46,46	2.48	13 (28%)	54,67,67	2.13	19 (35%)
82	PEB	jG	202	1	46,46,46	2.68	12 (26%)	54,67,67	1.89	14 (25%)
82	PEB	NF	202	2	46,46,46	2.83	14 (30%)	54,67,67	2.40	19 (35%)
87	CLA	cL	513	17	69,73,73	1.28	8 (11%)	83,113,113	1.32	6 (7%)
82	PEB	JD	202	1	46,46,46	2.59	12 (26%)	54,67,67	1.97	14 (25%)
82	PEB	S9	203	2	46,46,46	2.64	12 (26%)	54,67,67	2.08	19 (35%)
84	CYC	M1	201	10,9	46,46,46	2.30	16 (34%)	61,67,67	2.73	27 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	eO	202	2	46,46,46	2.62	12 (26%)	54,67,67	2.30	22 (40%)
84	CYC	C3	1001	68	46,46,46	2.66	16 (34%)	61,67,67	2.92	25 (40%)
87	CLA	A2	816	-	49,53,73	1.51	9 (18%)	59,89,113	1.50	5 (8%)
85	BCR	BL	618	-	41,41,41	0.73	0	56,56,56	1.83	13 (23%)
83	PUB	Z5	302	1,74	45,46,46	2.80	13 (28%)	46,67,67	3.59	25 (54%)
82	PEB	j4	202	1	46,46,46	2.61	14 (30%)	54,67,67	2.02	16 (29%)
82	PEB	ZH	203	1	46,46,46	2.76	13 (28%)	54,67,67	2.22	19 (35%)
82	PEB	VA	201	2,75	46,46,46	2.56	12 (26%)	54,67,67	2.08	15 (27%)
82	PEB	JA	202	2	46,46,46	2.54	12 (26%)	54,67,67	2.52	20 (37%)
82	PEB	NA	201	2	46,46,46	2.58	12 (26%)	54,67,67	2.23	21 (38%)
82	PEB	cM	202	2	46,46,46	2.67	13 (28%)	54,67,67	2.06	19 (35%)
84	CYC	LO	1001	10	46,46,46	2.35	18 (39%)	61,67,67	2.93	28 (45%)
87	CLA	32	302	59,60	49,53,73	1.57	8 (16%)	59,89,113	2.09	12 (20%)
87	CLA	ON	202	53	54,58,73	1.49	7 (12%)	65,95,113	1.93	13 (20%)
82	PEB	rK	202	2	46,46,46	2.80	16 (34%)	54,67,67	2.23	19 (35%)
92	LMG	bL	610	-	41,41,55	0.31	0	49,49,63	0.48	0
82	PEB	Z1	201	1,2	46,46,46	2.64	11 (23%)	54,67,67	2.96	28 (51%)
82	PEB	NI	203	1,2	46,46,46	2.39	13 (28%)	54,67,67	2.66	21 (38%)
82	PEB	dG	204	1	46,46,46	2.68	14 (30%)	54,67,67	1.99	16 (29%)
99	SF4	CN	102	42	0,12,12	-	-	-		
82	PEB	M7	201	1	46,46,46	2.56	11 (23%)	54,67,67	2.36	19 (35%)
87	CLA	b6	617	-	69,73,73	1.25	9 (13%)	83,113,113	1.33	7 (8%)
82	PEB	ZE	203	1,2	46,46,46	2.59	13 (28%)	54,67,67	2.19	18 (33%)
82	PEB	jE	202	1	46,46,46	2.67	12 (26%)	54,67,67	1.89	14 (25%)
87	CLA	1N	611	-	49,53,73	1.50	9 (18%)	59,89,113	1.49	8 (13%)
82	PEB	wC	201	2	46,46,46	2.68	12 (26%)	54,67,67	1.98	17 (31%)
87	CLA	c6	608	85,92	69,73,73	1.24	9 (13%)	83,113,113	1.30	6 (7%)
82	PEB	DJ	202	2	46,46,46	2.58	12 (26%)	54,67,67	2.09	18 (33%)
82	PEB	hJ	201	1,2	46,46,46	2.55	13 (28%)	54,67,67	2.33	20 (37%)
82	PEB	pC	201	1	46,46,46	2.66	12 (26%)	54,67,67	2.00	18 (33%)
87	CLA	cL	516	-	59,63,73	1.35	9 (15%)	71,101,113	1.43	5 (7%)
82	PEB	KF	201	1,2	46,46,46	2.48	11 (23%)	54,67,67	2.59	20 (37%)
82	PEB	YA	301	3	46,46,46	2.87	13 (28%)	54,67,67	2.60	24 (44%)
85	BCR	B6	621	92	41,41,41	0.88	2 (4%)	56,56,56	2.38	19 (33%)
82	PEB	VI	202	1	46,46,46	2.54	13 (28%)	54,67,67	2.11	20 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	TK	202	2	46,46,46	2.77	15 (32%)	54,67,67	2.40	23 (42%)
82	PEB	AG	301	3	46,46,46	2.57	13 (28%)	54,67,67	2.08	18 (33%)
82	PEB	YP	502	2	46,46,46	2.49	13 (28%)	54,67,67	2.05	18 (33%)
82	PEB	SJ	202	1	46,46,46	2.58	13 (28%)	54,67,67	2.07	17 (31%)
95	DGD	AL	414	15	63,63,67	0.83	2 (3%)	77,77,81	1.33	9 (11%)
82	PEB	S9	201	74,2	46,46,46	2.71	14 (30%)	54,67,67	2.45	18 (33%)
82	PEB	OD	202	2	46,46,46	2.73	16 (34%)	54,67,67	1.94	18 (33%)
82	PEB	aO	203	2	46,46,46	2.69	14 (30%)	54,67,67	1.98	17 (31%)
82	PEB	bF	202	2	46,46,46	2.93	14 (30%)	54,67,67	2.54	22 (40%)
82	PEB	I7	201	1	46,46,46	2.60	14 (30%)	54,67,67	2.14	15 (27%)
87	CLA	2N	309	58	54,58,73	1.50	10 (18%)	65,95,113	1.88	14 (21%)
82	PEB	xC	201	1	46,46,46	2.69	12 (26%)	54,67,67	1.87	15 (27%)
87	CLA	aL	605	15	69,73,73	1.26	10 (14%)	83,113,113	1.49	10 (12%)
82	PEB	HF	202	2	46,46,46	2.67	12 (26%)	54,67,67	2.23	19 (35%)
82	PEB	AQ	303	3,82	46,46,46	2.71	14 (30%)	54,67,67	2.11	20 (37%)
94	PL9	d6	408	18,26	55,55,55	0.62	2 (3%)	68,69,69	1.98	21 (30%)
89	OEX	aL	608	15	0,14,14	-	-	-		
87	CLA	CL	505	-	69,73,73	1.27	10 (14%)	83,113,113	1.40	8 (9%)
87	CLA	H6	102	22	69,73,73	1.23	10 (14%)	83,113,113	1.32	8 (9%)
82	PEB	IB	202	2	46,46,46	2.45	13 (28%)	54,67,67	2.14	20 (37%)
87	CLA	BN	819	-	69,73,73	1.27	9 (13%)	83,113,113	1.39	7 (8%)
82	PEB	PB	201	2	46,46,46	2.66	12 (26%)	54,67,67	2.26	19 (35%)
82	PEB	Q4	202	1	46,46,46	0.63	0	54,67,67	0.79	1 (1%)
82	PEB	R9	201	1	46,46,46	2.62	13 (28%)	54,67,67	1.97	17 (31%)
82	PEB	N5	202	1	46,46,46	2.57	13 (28%)	54,67,67	2.06	18 (33%)
82	PEB	iM	202	2	46,46,46	2.65	13 (28%)	54,67,67	2.06	19 (35%)
82	PEB	uK	202	1	46,46,46	2.77	13 (28%)	54,67,67	1.86	17 (31%)
95	DGD	C6	502	-	63,63,67	1.08	4 (6%)	77,77,81	1.82	16 (20%)
84	CYC	D1	1001	10	46,46,46	2.35	15 (32%)	61,67,67	2.79	24 (39%)
82	PEB	uC	203	2	46,46,46	2.71	13 (28%)	54,67,67	1.98	19 (35%)
88	LHG	C6	522	17	31,31,48	1.12	2 (6%)	34,37,54	1.57	4 (11%)
87	CLA	CL	506	-	69,73,73	1.24	11 (15%)	83,113,113	1.63	12 (14%)
95	DGD	cL	519	-	63,63,67	0.84	2 (3%)	77,77,81	0.95	3 (3%)
82	PEB	R4	203	2	46,46,46	2.59	11 (23%)	54,67,67	1.87	14 (25%)
82	PEB	Q9	201	2	46,46,46	2.72	12 (26%)	54,67,67	2.04	15 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
87	CLA	5N	610	-	49,53,73	1.45	9 (18%)	59,89,113	1.50	6 (10%)
82	PEB	BA	203	2	46,46,46	2.65	12 (26%)	54,67,67	2.06	18 (33%)
87	CLA	42	606	-	49,53,73	1.48	9 (18%)	59,89,113	1.47	6 (10%)
87	CLA	A6	404	15	54,58,73	1.38	9 (16%)	65,95,113	1.53	8 (12%)
85	BCR	AN	804	-	41,41,41	0.76	0	56,56,56	2.07	17 (30%)
82	PEB	SH	203	1,2	46,46,46	2.56	12 (26%)	54,67,67	2.41	22 (40%)
82	PEB	NM	201	2	46,46,46	2.67	13 (28%)	54,67,67	2.45	22 (40%)
87	CLA	a6	608	-	64,68,73	1.29	10 (15%)	77,107,113	1.43	11 (14%)
82	PEB	DQ	202	1	46,46,46	2.57	13 (28%)	54,67,67	2.80	26 (48%)
82	PEB	bF	201	2	46,46,46	2.67	13 (28%)	54,67,67	2.07	18 (33%)
82	PEB	lG	202	1	46,46,46	2.59	14 (30%)	54,67,67	1.97	15 (27%)
82	PEB	RD	201	1	46,46,46	2.67	13 (28%)	54,67,67	1.95	16 (29%)
84	CYC	m3	1001	68	46,46,46	2.66	16 (34%)	61,67,67	2.91	25 (40%)
87	CLA	bL	618	-	69,73,73	1.25	11 (15%)	83,113,113	1.53	10 (12%)
82	PEB	ID	201	2,77	46,46,46	2.68	14 (30%)	54,67,67	2.79	23 (42%)
82	PEB	KJ	201	1	46,46,46	2.57	11 (23%)	54,67,67	2.22	18 (33%)
82	PEB	r8	201	1	46,46,46	2.63	13 (28%)	54,67,67	2.14	19 (35%)
87	CLA	BN	833	-	51,55,73	1.44	12 (23%)	61,91,113	1.48	11 (18%)
82	PEB	jJ	202	1	46,46,46	2.68	11 (23%)	54,67,67	2.03	17 (31%)
82	PEB	M9	302	74	46,46,46	2.57	11 (23%)	54,67,67	2.31	22 (40%)
82	PEB	O9	203	2	46,46,46	2.68	14 (30%)	54,67,67	2.08	19 (35%)
88	LHG	bL	612	16	48,48,48	0.94	2 (4%)	51,54,54	1.07	3 (5%)
96	HEM	GN	201	46	50,50,50	1.79	10 (20%)	66,82,82	1.39	7 (10%)
82	PEB	iG	201	2	46,46,46	2.67	13 (28%)	54,67,67	1.96	16 (29%)
82	PEB	VF	201	2	46,46,46	2.58	11 (23%)	54,67,67	2.40	18 (33%)
87	CLA	BL	619	-	69,73,73	1.25	10 (14%)	83,113,113	1.31	8 (9%)
82	PEB	WF	201	1,2	46,46,46	2.54	12 (26%)	54,67,67	2.59	27 (50%)
82	PEB	FQ	202	1	46,46,46	2.70	13 (28%)	54,67,67	1.97	18 (33%)
82	PEB	E7	201	1	46,46,46	2.73	14 (30%)	54,67,67	2.22	17 (31%)
82	PEB	vK	201	2	46,46,46	2.69	12 (26%)	54,67,67	2.74	21 (38%)
82	PEB	QJ	204	1	46,46,46	2.57	13 (28%)	54,67,67	2.12	15 (27%)
82	PEB	jK	202	2	46,46,46	2.71	13 (28%)	54,67,67	2.17	17 (31%)
84	CYC	KG	202	10,9	46,46,46	2.35	16 (34%)	61,67,67	2.78	24 (39%)
82	PEB	mF	202	1	46,46,46	2.68	12 (26%)	54,67,67	2.17	17 (31%)
84	CYC	LH	1001	10,9	46,46,46	2.37	14 (30%)	61,67,67	2.99	28 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
87	CLA	A2	834	-	69,73,73	1.24	10 (14%)	83,113,113	1.43	9 (10%)
82	PEB	cJ	202	2	46,46,46	2.65	12 (26%)	54,67,67	2.25	19 (35%)
87	CLA	7N	601	63	49,53,73	1.48	7 (14%)	59,89,113	1.57	6 (10%)
82	PEB	ZB	201	2	46,46,46	2.62	13 (28%)	54,67,67	1.97	18 (33%)
82	PEB	jO	202	1	46,46,46	2.61	14 (30%)	54,67,67	2.01	16 (29%)
82	PEB	OG	202	1	46,46,46	2.58	12 (26%)	54,67,67	2.08	17 (31%)
87	CLA	RN	204	-	49,53,73	1.46	9 (18%)	59,89,113	1.49	6 (10%)
82	PEB	sK	201	1	46,46,46	2.59	13 (28%)	54,67,67	2.11	16 (29%)
82	PEB	MI	401	-	46,46,46	0.63	0	54,67,67	0.78	1 (1%)
82	PEB	GD	202	2	46,46,46	2.69	12 (26%)	54,67,67	2.14	21 (38%)
87	CLA	cL	508	-	69,73,73	1.25	11 (15%)	83,113,113	1.53	10 (12%)
82	PEB	cO	201	2	46,46,46	2.62	11 (23%)	54,67,67	1.98	14 (25%)
83	PUB	xK	305	13	45,46,46	2.76	9 (20%)	46,67,67	2.88	19 (41%)
84	CYC	N3	1001	68	46,46,46	2.65	16 (34%)	61,67,67	2.91	25 (40%)
82	PEB	SO	202	1,76	46,46,46	2.53	14 (30%)	54,67,67	2.00	16 (29%)
82	PEB	QE	202	1	46,46,46	2.64	13 (28%)	54,67,67	2.05	18 (33%)
82	PEB	YA	303	3,82	46,46,46	2.62	13 (28%)	54,67,67	2.59	22 (40%)
82	PEB	aB	202	2	46,46,46	2.64	12 (26%)	54,67,67	2.01	20 (37%)
82	PEB	KJ	203	1,2	46,46,46	2.45	12 (26%)	54,67,67	2.69	21 (38%)
82	PEB	SP	201	1,2	46,46,46	3.03	13 (28%)	54,67,67	2.94	20 (37%)
87	CLA	1N	604	-	46,50,73	1.49	10 (21%)	55,85,113	1.54	6 (10%)
82	PEB	AP	202	1	46,46,46	2.60	14 (30%)	54,67,67	2.00	17 (31%)
83	PUB	wK	304	13	45,46,46	2.58	11 (24%)	46,67,67	2.96	20 (43%)
84	CYC	L4	1001	10	46,46,46	2.35	18 (39%)	61,67,67	2.93	28 (45%)
82	PEB	T7	201	2	46,46,46	2.65	12 (26%)	54,67,67	2.19	17 (31%)
82	PEB	SM	201	1	46,46,46	2.64	12 (26%)	54,67,67	1.97	14 (25%)
82	PEB	sF	203	1,2	46,46,46	2.75	15 (32%)	54,67,67	2.55	20 (37%)
82	PEB	zC	202	1	46,46,46	2.72	12 (26%)	54,67,67	2.33	22 (40%)
82	PEB	mJ	202	2	46,46,46	2.64	13 (28%)	54,67,67	2.05	18 (33%)
83	PUB	A4	303	3	45,46,46	2.66	9 (20%)	46,67,67	2.86	15 (32%)
84	CYC	BG	1001	10,8	46,46,46	2.44	18 (39%)	61,67,67	2.82	28 (45%)
82	PEB	DF	201	2	46,46,46	2.54	10 (21%)	54,67,67	2.92	21 (38%)
82	PEB	OP	203	1	46,46,46	2.53	12 (26%)	54,67,67	2.39	19 (35%)
82	PEB	T4	203	2	46,46,46	2.60	11 (23%)	54,67,67	1.91	16 (29%)
84	CYC	q3	1001	69	46,46,46	2.53	17 (36%)	61,67,67	3.11	28 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	W9	201	2	46,46,46	2.69	14 (30%)	54,67,67	2.28	18 (33%)
82	PEB	WF	203	1	46,46,46	2.69	13 (28%)	54,67,67	1.97	16 (29%)
84	CYC	G4	1001	9	46,46,46	2.40	16 (34%)	61,67,67	2.79	25 (40%)
87	CLA	BN	827	-	69,73,73	1.32	10 (14%)	83,113,113	1.45	11 (13%)
82	PEB	WK	202	1	46,46,46	2.69	13 (28%)	54,67,67	2.32	24 (44%)
82	PEB	YO	203	2	46,46,46	2.60	12 (26%)	54,67,67	1.97	17 (31%)
82	PEB	qC	202	2	46,46,46	2.62	13 (28%)	54,67,67	2.41	21 (38%)
85	BCR	BL	617	-	41,41,41	0.78	0	56,56,56	2.24	18 (32%)
87	CLA	A2	822	40	49,53,73	1.47	10 (20%)	59,89,113	1.63	8 (13%)
82	PEB	m4	202	2	46,46,46	2.62	13 (28%)	54,67,67	2.37	20 (37%)
82	PEB	CI	202	1	46,46,46	2.53	13 (28%)	54,67,67	2.11	20 (37%)
94	PL9	D6	408	18,26	55,55,55	0.64	2 (3%)	68,69,69	2.02	23 (33%)
82	PEB	cB	402	6,2	46,46,46	2.54	11 (23%)	54,67,67	2.21	19 (35%)
82	PEB	j1	201	1	46,46,46	2.61	12 (26%)	54,67,67	2.22	19 (35%)
82	PEB	GI	202	1	46,46,46	2.57	12 (26%)	54,67,67	2.05	18 (33%)
82	PEB	jH	203	1,2	46,46,46	2.69	16 (34%)	54,67,67	2.42	19 (35%)
87	CLA	AN	828	40	69,73,73	1.36	9 (13%)	83,113,113	1.58	13 (15%)
82	PEB	Y9	203	2	46,46,46	2.60	12 (26%)	54,67,67	2.04	15 (27%)
82	PEB	AO	304	3	46,46,46	2.60	11 (23%)	54,67,67	2.07	17 (31%)
82	PEB	ZG	203	1	46,46,46	2.58	13 (28%)	54,67,67	2.18	18 (33%)
87	CLA	42	611	-	49,53,73	1.46	9 (18%)	59,89,113	1.49	4 (6%)
88	LHG	L6	101	26	48,48,48	0.90	2 (4%)	51,54,54	1.13	4 (7%)
88	LHG	d6	407	18	48,48,48	0.91	2 (4%)	51,54,54	1.05	3 (5%)
82	PEB	gK	201	1	46,46,46	2.63	13 (28%)	54,67,67	2.51	21 (38%)
82	PEB	gF	201	1	46,46,46	2.63	13 (28%)	54,67,67	2.53	21 (38%)
82	PEB	UJ	202	1	46,46,46	2.59	12 (26%)	54,67,67	2.36	21 (38%)
99	SF4	B2	803	-	0,12,12	-	-	-		
82	PEB	NH	1002	10	46,46,46	2.58	13 (28%)	54,67,67	2.03	14 (25%)
82	PEB	mJ	201	13,2	46,46,46	2.73	13 (28%)	54,67,67	2.43	21 (38%)
82	PEB	bO	201	1	46,46,46	2.66	11 (23%)	54,67,67	2.31	21 (38%)
82	PEB	CD	202	2	46,46,46	2.66	12 (26%)	54,67,67	1.99	17 (31%)
82	PEB	WE	202	1,77	46,46,46	2.54	13 (28%)	54,67,67	2.10	17 (31%)
87	CLA	1N	608	57	45,49,73	1.52	8 (17%)	54,84,113	1.52	8 (14%)
87	CLA	A2	841	-	69,73,73	1.28	11 (15%)	83,113,113	1.43	9 (10%)
82	PEB	fM	201	1	46,46,46	2.62	12 (26%)	54,67,67	2.03	14 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
87	CLA	B2	823	-	69,73,73	1.27	11 (15%)	83,113,113	1.46	13 (15%)
82	PEB	T4	202	2	46,46,46	2.61	14 (30%)	54,67,67	2.27	20 (37%)
97	GOL	WL	101	-	5,5,5	0.22	0	5,5,5	0.34	0
82	PEB	QA	201	1	46,46,46	2.55	12 (26%)	54,67,67	2.72	20 (37%)
82	PEB	F4	1002	10	46,46,46	2.57	12 (26%)	54,67,67	2.24	21 (38%)
87	CLA	CL	518	-	50,54,73	1.44	10 (20%)	60,90,113	1.45	6 (10%)
87	CLA	IN	103	47,50	69,73,73	1.25	9 (13%)	83,113,113	1.39	9 (10%)
87	CLA	B6	611	-	69,73,73	1.25	9 (13%)	83,113,113	1.37	7 (8%)
87	CLA	AN	839	-	69,73,73	1.24	8 (11%)	83,113,113	1.41	9 (10%)
87	CLA	O2	201	-	45,49,73	1.50	8 (17%)	54,84,113	1.52	6 (11%)
82	PEB	m4	201	2	46,46,46	2.63	13 (28%)	54,67,67	2.15	17 (31%)
82	PEB	mE	203	2	46,46,46	2.65	14 (30%)	54,67,67	2.04	15 (27%)
87	CLA	c6	614	17	64,68,73	1.30	8 (12%)	77,107,113	1.41	10 (12%)
87	CLA	bL	614	-	69,73,73	1.25	8 (11%)	83,113,113	1.46	9 (10%)
87	CLA	CL	509	17	69,73,73	1.24	10 (14%)	83,113,113	1.41	10 (12%)
85	BCR	aL	604	-	41,41,41	0.70	0	56,56,56	1.72	11 (19%)
87	CLA	BL	620	16	69,73,73	1.28	12 (17%)	83,113,113	1.41	6 (7%)
82	PEB	jM	203	1,2	46,46,46	2.57	13 (28%)	54,67,67	2.32	17 (31%)
82	PEB	AH	301	3	46,46,46	2.70	11 (23%)	54,67,67	2.03	15 (27%)
82	PEB	e7	301	1,75	46,46,46	0.63	0	54,67,67	0.79	1 (1%)
87	CLA	82	308	-	49,53,73	1.49	11 (22%)	59,89,113	2.07	12 (20%)
87	CLA	12	609	-	46,50,73	1.50	9 (19%)	55,85,113	1.67	9 (16%)
82	PEB	X7	203	2	46,46,46	2.61	14 (30%)	54,67,67	2.34	23 (42%)
87	CLA	A2	801	40,45	69,73,73	1.27	9 (13%)	83,113,113	1.43	10 (12%)
82	PEB	L9	203	2	46,46,46	2.64	12 (26%)	54,67,67	2.08	18 (33%)
87	CLA	62	303	62	69,73,73	1.28	8 (11%)	83,113,113	1.29	10 (12%)
82	PEB	MF	202	1	46,46,46	2.71	13 (28%)	54,67,67	1.92	18 (33%)
82	PEB	IJ	203	1	46,46,46	2.53	14 (30%)	54,67,67	2.36	18 (33%)
87	CLA	c6	604	17	69,73,73	1.25	9 (13%)	83,113,113	1.31	6 (7%)
82	PEB	dO	202	1	46,46,46	2.63	14 (30%)	54,67,67	1.92	15 (27%)
82	PEB	fM	203	1,2	46,46,46	2.56	12 (26%)	54,67,67	2.38	20 (37%)
82	PEB	RB	201	6,2	46,46,46	2.75	12 (26%)	54,67,67	2.24	18 (33%)
87	CLA	2N	307	58	49,53,73	1.47	8 (16%)	59,89,113	1.51	9 (15%)
87	CLA	R2	202	54	49,53,73	1.50	8 (16%)	59,89,113	1.54	8 (13%)
84	CYC	v3	1001	68	46,46,46	2.65	16 (34%)	61,67,67	2.92	25 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
97	GOL	I6	102	-	5,5,5	0.24	0	5,5,5	0.21	0
82	PEB	PF	202	2	46,46,46	2.88	15 (32%)	54,67,67	2.31	20 (37%)
82	PEB	WH	201	1	46,46,46	2.57	11 (23%)	54,67,67	2.25	18 (33%)
82	PEB	AI	203	1,2	46,46,46	2.40	14 (30%)	54,67,67	2.83	22 (40%)
95	DGD	aL	603	15	54,54,67	0.91	2 (3%)	68,68,81	1.04	2 (2%)
82	PEB	aJ	204	1,2	46,46,46	2.55	12 (26%)	54,67,67	2.57	22 (40%)
82	PEB	IF	201	1	46,46,46	2.53	12 (26%)	54,67,67	3.18	23 (42%)
82	PEB	1C	201	2	46,46,46	2.78	13 (28%)	54,67,67	2.01	17 (31%)
82	PEB	U9	203	2	46,46,46	2.69	11 (23%)	54,67,67	1.98	15 (27%)
87	CLA	1N	602	57	69,73,73	1.21	6 (8%)	83,113,113	1.44	9 (10%)
82	PEB	M9	304	74	46,46,46	2.69	13 (28%)	54,67,67	2.24	18 (33%)
82	PEB	E5	202	1	46,46,46	2.58	13 (28%)	54,67,67	2.05	18 (33%)
82	PEB	LA	202	2	46,46,46	2.48	12 (26%)	54,67,67	2.69	23 (42%)
92	LMG	B6	622	37,16	50,50,55	0.92	2 (4%)	58,58,63	1.04	4 (6%)
85	BCR	KN	104	-	41,41,41	0.83	0	56,56,56	2.48	19 (33%)
82	PEB	lM	202	1	46,46,46	2.58	11 (23%)	54,67,67	2.16	17 (31%)
82	PEB	SQ	201	3,2	46,46,46	2.67	13 (28%)	54,67,67	2.09	15 (27%)
82	PEB	HK	201	2	46,46,46	2.48	13 (28%)	54,67,67	2.89	27 (50%)
82	PEB	q8	201	2	46,46,46	2.73	13 (28%)	54,67,67	2.04	16 (29%)
83	PUB	AQ	302	1,3	45,46,46	2.73	9 (20%)	46,67,67	3.03	18 (39%)
87	CLA	BN	815	41	46,50,73	1.47	10 (21%)	55,85,113	1.62	8 (14%)
82	PEB	PD	203	1	46,46,46	2.70	12 (26%)	54,67,67	2.10	15 (27%)
85	BCR	JN	102	-	41,41,41	0.74	0	56,56,56	2.00	16 (28%)
82	PEB	AD	301	3	46,46,46	2.63	12 (26%)	54,67,67	2.06	21 (38%)
82	PEB	eF	201	1,2	46,46,46	2.71	14 (30%)	54,67,67	2.19	21 (38%)
85	BCR	K6	102	-	41,41,41	0.73	0	56,56,56	2.77	23 (41%)
82	PEB	P1	202	2	46,46,46	2.69	12 (26%)	54,67,67	2.02	18 (33%)
84	CYC	FE	1001	10,9	46,46,46	2.36	18 (39%)	61,67,67	2.78	25 (40%)
82	PEB	D1	1002	10	46,46,46	2.58	13 (28%)	54,67,67	2.05	17 (31%)
87	CLA	12	604	-	46,50,73	1.49	10 (21%)	55,85,113	1.55	6 (10%)
82	PEB	ED	201	2,77	46,46,46	2.62	14 (30%)	54,67,67	2.36	20 (37%)
82	PEB	IA	201	1	46,46,46	2.60	13 (28%)	54,67,67	2.14	15 (27%)
88	LHG	aL	607	15	42,42,48	0.98	2 (4%)	45,48,54	1.09	2 (4%)
82	PEB	PI	202	1	46,46,46	2.54	14 (30%)	54,67,67	2.11	20 (37%)
82	PEB	CQ	202	2	46,46,46	2.66	12 (26%)	54,67,67	1.96	16 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	IF	203	1,2	46,46,46	2.50	12 (26%)	54,67,67	2.85	24 (44%)
87	CLA	A2	836	-	49,53,73	1.48	9 (18%)	59,89,113	1.57	6 (10%)
82	PEB	aO	202	2	46,46,46	2.59	13 (28%)	54,67,67	2.47	22 (40%)
95	DGD	B2	844	41	67,67,67	0.87	2 (2%)	81,81,81	1.00	4 (4%)
82	PEB	eF	203	1	46,46,46	2.69	12 (26%)	54,67,67	2.14	17 (31%)
82	PEB	OE	202	1	46,46,46	2.57	12 (26%)	54,67,67	2.09	18 (33%)
82	PEB	WJ	202	1	46,46,46	2.47	13 (28%)	54,67,67	2.54	20 (37%)
87	CLA	62	310	-	45,49,73	1.51	8 (17%)	54,84,113	1.54	6 (11%)
82	PEB	AF	201	1	46,46,46	2.60	12 (26%)	54,67,67	2.29	19 (35%)
82	PEB	T7	203	2	46,46,46	2.63	12 (26%)	54,67,67	2.26	21 (38%)
82	PEB	LA	201	2,82	46,46,46	2.67	13 (28%)	54,67,67	2.13	18 (33%)
96	HEM	V6	201	35	50,50,50	1.61	10 (20%)	66,82,82	1.72	18 (27%)
87	CLA	A2	839	-	69,73,73	1.24	9 (13%)	83,113,113	1.41	9 (10%)
82	PEB	DO	1002	10	46,46,46	2.59	12 (26%)	54,67,67	2.16	18 (33%)
82	PEB	ND	204	1,2	46,46,46	2.72	11 (23%)	54,67,67	2.19	19 (35%)
82	PEB	G7	202	1	46,46,46	2.65	12 (26%)	54,67,67	1.97	20 (37%)
95	DGD	BN	844	41	67,67,67	0.87	2 (2%)	81,81,81	0.99	4 (4%)
87	CLA	22	601	58	49,53,73	1.45	6 (12%)	59,89,113	1.63	6 (10%)
88	LHG	CL	522	17	31,31,48	1.11	2 (6%)	34,37,54	1.54	5 (14%)
82	PEB	f1	202	1	46,46,46	2.85	11 (23%)	54,67,67	2.29	19 (35%)
82	PEB	TO	202	2	46,46,46	2.60	13 (28%)	54,67,67	2.26	20 (37%)
82	PEB	ZH	201	1,2	46,46,46	2.63	11 (23%)	54,67,67	2.95	28 (51%)
82	PEB	i1	201	2	46,46,46	2.67	14 (30%)	54,67,67	2.10	16 (29%)
82	PEB	RP	202	2	46,46,46	2.55	11 (23%)	54,67,67	2.09	19 (35%)
84	CYC	O3	1001	69	46,46,46	2.53	17 (36%)	61,67,67	3.10	28 (45%)
87	CLA	72	606	63	49,53,73	1.53	10 (20%)	59,89,113	1.53	7 (11%)
82	PEB	L7	203	2	46,46,46	2.66	12 (26%)	54,67,67	1.89	18 (33%)
82	PEB	oK	201	1	46,46,46	2.72	12 (26%)	54,67,67	2.11	19 (35%)
82	PEB	LJ	202	2	46,46,46	2.63	13 (28%)	54,67,67	2.11	17 (31%)
84	CYC	KO	1001	9	46,46,46	2.36	16 (34%)	61,67,67	2.84	25 (40%)
87	CLA	c6	616	-	69,73,73	1.25	9 (13%)	83,113,113	1.30	7 (8%)
87	CLA	C6	518	-	64,68,73	1.30	10 (15%)	77,107,113	1.35	4 (5%)
87	CLA	bL	606	-	69,73,73	1.27	13 (18%)	83,113,113	1.32	7 (8%)
82	PEB	k4	201	2	46,46,46	2.62	14 (30%)	54,67,67	1.93	14 (25%)
82	PEB	NI	201	1	46,46,46	2.57	13 (28%)	54,67,67	2.05	19 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
87	CLA	7N	610	-	49,53,73	1.48	10 (20%)	59,89,113	1.53	6 (10%)
82	PEB	OH	202	1	46,46,46	2.66	12 (26%)	54,67,67	2.13	18 (33%)
87	CLA	2N	301	58,41	58,62,73	1.45	10 (17%)	73,100,113	1.63	12 (16%)
87	CLA	B2	829	-	47,51,73	1.45	9 (19%)	56,86,113	1.56	4 (7%)
82	PEB	jH	202	1	46,46,46	2.72	13 (28%)	54,67,67	2.20	19 (35%)
82	PEB	OM	202	1	46,46,46	2.58	15 (32%)	54,67,67	2.37	23 (42%)
82	PEB	rC	202	1	46,46,46	2.78	14 (30%)	54,67,67	2.37	21 (38%)
83	PUB	AG	303	3	45,46,46	2.71	9 (20%)	46,67,67	2.85	16 (34%)
82	PEB	DG	1002	10,9	46,46,46	2.58	14 (30%)	54,67,67	2.09	18 (33%)
87	CLA	6N	609	-	45,49,73	1.51	7 (15%)	54,84,113	1.53	6 (11%)
82	PEB	YI	201	12,2	46,46,46	2.51	13 (28%)	54,67,67	2.08	19 (35%)
82	PEB	V7	202	2	46,46,46	2.51	12 (26%)	54,67,67	2.61	23 (42%)
82	PEB	WD	202	2	46,46,46	2.72	15 (32%)	54,67,67	1.92	16 (29%)
87	CLA	R2	203	54,41	50,54,73	1.45	8 (16%)	60,90,113	1.43	5 (8%)
82	PEB	CM	203	1,2	46,46,46	2.53	12 (26%)	54,67,67	2.60	23 (42%)
82	PEB	bK	202	2	46,46,46	2.93	12 (26%)	54,67,67	2.52	21 (38%)
87	CLA	AN	814	40	58,62,73	1.37	10 (17%)	69,99,113	1.44	6 (8%)
82	PEB	BB	203	2	46,46,46	2.60	12 (26%)	54,67,67	2.20	19 (35%)
82	PEB	HB	203	2	46,46,46	2.58	12 (26%)	54,67,67	2.19	17 (31%)
85	BCR	BN	839	-	41,41,41	0.72	0	56,56,56	1.97	14 (25%)
82	PEB	O1	203	1,2	46,46,46	2.56	11 (23%)	54,67,67	2.37	21 (38%)
82	PEB	BK	201	2	46,46,46	2.56	12 (26%)	54,67,67	3.32	19 (35%)
87	CLA	7N	604	63	46,50,73	1.51	10 (21%)	55,85,113	1.59	8 (14%)
82	PEB	gK	203	1,2	46,46,46	2.54	12 (26%)	54,67,67	2.47	19 (35%)
82	PEB	GB	202	2	46,46,46	2.53	11 (23%)	54,67,67	2.06	17 (31%)
82	PEB	M9	301	74,2	46,46,46	2.54	12 (26%)	54,67,67	1.86	16 (29%)
82	PEB	EA	201	1	46,46,46	2.74	14 (30%)	54,67,67	2.23	17 (31%)
82	PEB	18	203	2	46,46,46	2.71	11 (23%)	54,67,67	1.84	14 (25%)
82	PEB	Y1	201	2	46,46,46	2.75	14 (30%)	54,67,67	2.25	23 (42%)
87	CLA	cL	505	-	69,73,73	1.24	9 (13%)	83,113,113	1.49	11 (13%)
93	BCT	aL	612	15,90,18	2,3,3	1.22	0	2,3,3	3.86	1 (50%)
95	DGD	CL	523	-	49,49,67	0.97	2 (4%)	63,63,81	1.12	4 (6%)
88	LHG	dL	405	18	48,48,48	0.90	2 (4%)	51,54,54	1.02	3 (5%)
82	PEB	iK	203	1	46,46,46	2.70	13 (28%)	54,67,67	1.92	16 (29%)
82	PEB	h4	202	1	46,46,46	2.63	12 (26%)	54,67,67	1.95	16 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
87	CLA	B2	806	-	69,73,73	1.26	10 (14%)	83,113,113	1.28	6 (7%)
82	PEB	J1	1002	10	46,46,46	2.53	13 (28%)	54,67,67	2.19	17 (31%)
82	PEB	OH	201	1	46,46,46	2.61	14 (30%)	54,67,67	2.15	21 (38%)
95	DGD	a6	602	-	41,41,67	1.04	2 (4%)	55,55,81	1.16	4 (7%)
82	PEB	J9	201	2	46,46,46	2.76	15 (32%)	54,67,67	2.25	18 (33%)
87	CLA	c6	613	17	69,73,73	1.26	10 (14%)	83,113,113	1.27	7 (8%)
84	CYC	U3	1001	73,69	46,46,46	2.53	17 (36%)	61,67,67	3.11	28 (45%)
82	PEB	TQ	203	1	46,46,46	2.66	11 (23%)	54,67,67	2.13	14 (25%)
82	PEB	lJ	202	1	46,46,46	2.55	13 (28%)	54,67,67	2.44	21 (38%)
82	PEB	eG	201	2	46,46,46	2.66	14 (30%)	54,67,67	1.92	16 (29%)
82	PEB	e4	203	2	46,46,46	2.56	11 (23%)	54,67,67	1.92	13 (24%)
92	LMG	bL	609	-	41,41,55	0.31	0	49,49,63	0.56	0
87	CLA	cL	517	-	69,73,73	1.26	10 (14%)	83,113,113	1.34	6 (7%)
87	CLA	BN	823	-	69,73,73	1.27	11 (15%)	83,113,113	1.34	13 (15%)
87	CLA	LN	204	50	54,58,73	1.46	10 (18%)	65,95,113	1.75	11 (16%)
82	PEB	gH	203	1,74,2	46,46,46	2.62	13 (28%)	54,67,67	2.29	19 (35%)
82	PEB	EM	201	1,2	46,46,46	2.60	13 (28%)	54,67,67	2.33	20 (37%)
82	PEB	CB	201	2,4	46,46,46	2.62	12 (26%)	54,67,67	2.23	20 (37%)
82	PEB	EP	202	1	46,46,46	2.60	12 (26%)	54,67,67	2.04	16 (29%)
82	PEB	VQ	202	1	46,46,46	2.79	12 (26%)	54,67,67	1.94	15 (27%)
84	CYC	R3	1001	68	46,46,46	2.65	16 (34%)	61,67,67	2.91	24 (39%)
87	CLA	bL	615	-	69,73,73	1.23	10 (14%)	83,113,113	1.32	8 (9%)
87	CLA	AN	851	-	69,73,73	1.24	10 (14%)	83,113,113	1.39	8 (9%)
87	CLA	A2	831	-	69,73,73	1.32	11 (15%)	83,113,113	1.50	11 (13%)
95	DGD	b6	621	-	41,41,67	1.10	2 (4%)	55,55,81	1.35	7 (12%)
92	LMG	CL	519	-	55,55,55	0.87	2 (3%)	63,63,63	1.06	4 (6%)
87	CLA	CL	508	87	69,73,73	1.28	10 (14%)	83,113,113	1.48	9 (10%)
82	PEB	VD	202	1	46,46,46	2.78	12 (26%)	54,67,67	1.94	15 (27%)
85	BCR	F6	101	20	41,41,41	0.81	1 (2%)	56,56,56	2.31	17 (30%)
85	BCR	B6	602	-	41,41,41	0.79	0	56,56,56	2.15	17 (30%)
82	PEB	u8	201	2	46,46,46	2.68	15 (32%)	54,67,67	2.31	22 (40%)
82	PEB	XQ	202	1	46,46,46	2.70	14 (30%)	54,67,67	1.90	16 (29%)
83	PUB	QM	201	14,1	45,46,46	2.77	10 (22%)	46,67,67	2.95	20 (43%)
82	PEB	N4	1002	10	46,46,46	2.58	13 (28%)	54,67,67	2.14	20 (37%)
82	PEB	P9	201	1	46,46,46	2.61	14 (30%)	54,67,67	1.97	17 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	YF	203	1,2	46,46,46	2.69	13 (28%)	54,67,67	2.56	22 (40%)
82	PEB	LB	201	2	46,46,46	2.62	12 (26%)	54,67,67	2.20	17 (31%)
87	CLA	AN	813	-	69,73,73	1.20	9 (13%)	83,113,113	1.34	5 (6%)
84	CYC	Q3	1001	73,69	46,46,46	2.52	17 (36%)	61,67,67	3.11	28 (45%)
82	PEB	RH	202	2	46,46,46	2.72	13 (28%)	54,67,67	1.88	15 (27%)
82	PEB	xK	303	13	46,46,46	2.64	12 (26%)	54,67,67	1.88	12 (22%)
82	PEB	FF	202	2	46,46,46	2.66	14 (30%)	54,67,67	2.37	20 (37%)
82	PEB	NB	202	2	46,46,46	2.53	12 (26%)	54,67,67	2.06	16 (29%)
82	PEB	JM	201	2	46,46,46	2.68	13 (28%)	54,67,67	2.06	19 (35%)
82	PEB	L1	1002	10	46,46,46	2.47	12 (26%)	54,67,67	2.33	17 (31%)
82	PEB	U5	202	2	46,46,46	2.58	11 (23%)	54,67,67	2.25	18 (33%)
82	PEB	GP	203	1	46,46,46	2.62	14 (30%)	54,67,67	1.95	16 (29%)
82	PEB	OH	203	1,2	46,46,46	2.55	11 (23%)	54,67,67	2.38	20 (37%)
82	PEB	RG	201	2	46,46,46	2.65	13 (28%)	54,67,67	2.23	20 (37%)
82	PEB	K9	202	1	46,46,46	2.73	13 (28%)	54,67,67	2.42	21 (38%)
82	PEB	SG	203	1,2	46,46,46	2.55	11 (23%)	54,67,67	2.50	20 (37%)
96	HEM	v6	201	35	50,50,50	1.60	10 (20%)	66,82,82	1.72	17 (25%)
82	PEB	V5	202	1	46,46,46	2.57	13 (28%)	54,67,67	2.06	18 (33%)
96	HEM	FL	102	-	50,50,50	1.66	8 (16%)	66,82,82	1.68	15 (22%)
84	CYC	NE	201	10,9	46,46,46	2.35	16 (34%)	61,67,67	2.78	25 (40%)
82	PEB	JA	201	3,2	46,46,46	2.67	13 (28%)	54,67,67	2.14	16 (29%)
82	PEB	W7	202	1	46,46,46	2.68	13 (28%)	54,67,67	2.06	18 (33%)
82	PEB	FA	203	2	46,46,46	2.74	13 (28%)	54,67,67	1.93	21 (38%)
83	PUB	AJ	303	13	45,46,46	2.61	9 (20%)	46,67,67	3.19	21 (45%)
82	PEB	VG	201	2	46,46,46	2.61	14 (30%)	54,67,67	2.11	18 (33%)
87	CLA	A2	805	40	69,73,73	1.28	10 (14%)	83,113,113	1.33	8 (9%)
82	PEB	EP	201	1	46,46,46	2.57	14 (30%)	54,67,67	2.07	17 (31%)
82	PEB	HI	201	2	46,46,46	2.63	14 (30%)	54,67,67	2.12	19 (35%)
82	PEB	bE	201	1	46,46,46	2.65	13 (28%)	54,67,67	2.20	17 (31%)
87	CLA	AN	821	-	69,73,73	1.23	11 (15%)	83,113,113	1.44	10 (12%)
87	CLA	2N	303	58	69,73,73	1.45	6 (8%)	83,113,113	2.61	18 (21%)
87	CLA	b6	613	-	69,73,73	1.24	9 (13%)	83,113,113	1.37	7 (8%)
82	PEB	A9	202	1	46,46,46	2.73	13 (28%)	54,67,67	2.41	20 (37%)
87	CLA	A2	833	-	69,73,73	1.26	9 (13%)	83,113,113	1.33	6 (7%)
82	PEB	WM	203	1,2	46,46,46	2.47	11 (23%)	54,67,67	2.48	20 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	GA	201	1	46,46,46	2.50	11 (23%)	54,67,67	2.32	16 (29%)
87	CLA	C6	512	-	69,73,73	1.23	9 (13%)	83,113,113	1.35	6 (7%)
82	PEB	ZK	202	2	46,46,46	2.82	15 (32%)	54,67,67	2.14	20 (37%)
95	DGD	L6	102	26	59,59,67	0.87	2 (3%)	73,73,81	1.17	7 (9%)
82	PEB	A1	305	3	46,46,46	2.69	14 (30%)	54,67,67	2.09	17 (31%)
87	CLA	52	605	61	49,53,73	1.48	9 (18%)	59,89,113	1.50	6 (10%)
82	PEB	ZO	202	1	46,46,46	2.56	12 (26%)	54,67,67	2.00	13 (24%)
82	PEB	kO	202	2	46,46,46	2.61	13 (28%)	54,67,67	2.35	20 (37%)
82	PEB	XB	202	2	46,46,46	2.69	13 (28%)	54,67,67	2.23	20 (37%)
85	BCR	A2	848	-	41,41,41	0.83	1 (2%)	56,56,56	2.57	20 (35%)
87	CLA	B2	814	41	46,50,73	1.47	10 (21%)	55,85,113	1.63	8 (14%)
82	PEB	b1	202	1	46,46,46	2.76	11 (23%)	54,67,67	2.29	22 (40%)
82	PEB	S5	201	74,2	46,46,46	2.70	14 (30%)	54,67,67	2.22	20 (37%)
82	PEB	TF	202	2	46,46,46	2.76	15 (32%)	54,67,67	2.39	24 (44%)
87	CLA	FN	201	45	45,49,73	1.54	8 (17%)	54,84,113	1.71	8 (14%)
87	CLA	2N	311	-	46,50,73	1.49	9 (19%)	55,85,113	1.65	7 (12%)
82	PEB	hM	201	1,2	46,46,46	2.52	13 (28%)	54,67,67	2.29	19 (35%)
82	PEB	D4	1002	10	46,46,46	2.60	12 (26%)	54,67,67	2.16	18 (33%)
82	PEB	FJ	201	79,2	46,46,46	2.74	12 (26%)	54,67,67	2.50	20 (37%)
82	PEB	kH	201	2	46,46,46	2.66	13 (28%)	54,67,67	2.06	21 (38%)
82	PEB	AO	305	3	46,46,46	2.62	12 (26%)	54,67,67	2.02	17 (31%)
88	LHG	i6	101	-	48,48,48	0.93	2 (4%)	51,54,54	0.77	2 (3%)
82	PEB	Y5	203	2	46,46,46	2.50	12 (26%)	54,67,67	2.15	17 (31%)
82	PEB	uF	201	1,2	46,46,46	2.68	14 (30%)	54,67,67	2.16	15 (27%)
83	PUB	xF	305	13	45,46,46	2.76	9 (20%)	46,67,67	2.88	20 (43%)
87	CLA	AN	810	40	69,73,73	1.19	10 (14%)	83,113,113	1.43	7 (8%)
82	PEB	f4	201	1	46,46,46	2.66	12 (26%)	54,67,67	2.24	21 (38%)
82	PEB	RI	202	1	46,46,46	2.53	13 (28%)	54,67,67	2.11	20 (37%)
82	PEB	IM	202	1	46,46,46	2.59	12 (26%)	54,67,67	2.20	16 (29%)
82	PEB	cF	202	1,10	46,46,46	0.63	0	54,67,67	0.79	1 (1%)
87	CLA	BN	822	-	59,63,73	1.36	10 (16%)	71,101,113	1.42	7 (9%)
82	PEB	eK	202	1	46,46,46	2.60	12 (26%)	54,67,67	2.32	22 (40%)
85	BCR	BN	838	-	41,41,41	0.74	0	56,56,56	2.49	21 (37%)
87	CLA	A2	851	-	69,73,73	1.23	10 (14%)	83,113,113	1.40	8 (9%)
82	PEB	N7	202	2	46,46,46	2.41	10 (21%)	54,67,67	2.99	23 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
87	CLA	b6	615	-	69,73,73	1.23	10 (14%)	83,113,113	1.30	6 (7%)
82	PEB	IK	202	1	46,46,46	0.65	0	54,67,67	0.79	1 (1%)
87	CLA	BN	802	41	62,66,73	1.41	9 (14%)	74,104,113	1.65	14 (18%)
82	PEB	HI	203	2	46,46,46	2.59	12 (26%)	54,67,67	2.06	17 (31%)
82	PEB	VO	202	2	46,46,46	2.55	12 (26%)	54,67,67	2.50	23 (42%)
82	PEB	AQ	304	3,82	46,46,46	2.70	13 (28%)	54,67,67	2.20	18 (33%)
82	PEB	VP	202	2	46,46,46	2.63	13 (28%)	54,67,67	2.12	19 (35%)
82	PEB	AD	303	3,82	46,46,46	2.71	14 (30%)	54,67,67	2.11	20 (37%)
87	CLA	72	610	-	49,53,73	1.48	9 (18%)	59,89,113	1.52	6 (10%)
84	CYC	DO	1001	10	46,46,46	2.27	15 (32%)	61,67,67	2.87	26 (42%)
82	PEB	tK	201	2	46,46,46	2.68	11 (23%)	54,67,67	2.73	19 (35%)
82	PEB	lK	202	2	46,46,46	2.71	13 (28%)	54,67,67	2.11	19 (35%)
82	PEB	FP	202	2	46,46,46	2.55	12 (26%)	54,67,67	2.13	19 (35%)
82	PEB	AA	201	1	46,46,46	2.68	14 (30%)	54,67,67	2.14	22 (40%)
82	PEB	eJ	201	13,2	46,46,46	2.64	13 (28%)	54,67,67	2.16	19 (35%)
87	CLA	4N	608	60	54,58,73	1.42	10 (18%)	65,95,113	1.77	17 (26%)
82	PEB	bB	201	2	46,46,46	2.61	12 (26%)	54,67,67	2.21	19 (35%)
82	PEB	S1	201	1	46,46,46	2.62	13 (28%)	54,67,67	2.27	16 (29%)
82	PEB	aK	202	1	46,46,46	2.58	12 (26%)	54,67,67	2.15	19 (35%)
82	PEB	KP	202	1	46,46,46	2.50	12 (26%)	54,67,67	2.24	19 (35%)
82	PEB	KB	304	2,5	46,46,46	2.49	12 (26%)	54,67,67	2.07	20 (37%)
84	CYC	FH	1001	10	46,46,46	2.34	16 (34%)	61,67,67	2.85	25 (40%)
82	PEB	cG	202	2	46,46,46	2.68	12 (26%)	54,67,67	1.94	15 (27%)
87	CLA	B2	828	41	49,53,73	1.49	11 (22%)	59,89,113	1.49	7 (11%)
87	CLA	dL	404	-	69,73,73	1.23	8 (11%)	83,113,113	1.41	9 (10%)
82	PEB	LP	202	2	46,46,46	2.61	13 (28%)	54,67,67	2.04	17 (31%)
84	CYC	C4	1001	9	46,46,46	2.36	16 (34%)	61,67,67	2.88	28 (45%)
87	CLA	AN	823	40	69,73,73	1.23	11 (15%)	83,113,113	1.45	10 (12%)
87	CLA	B2	820	54,41	47,51,73	1.42	9 (19%)	56,86,113	1.26	6 (10%)
82	PEB	U5	203	2	46,46,46	2.59	13 (28%)	54,67,67	1.96	17 (31%)
87	CLA	BN	807	-	69,73,73	1.26	11 (15%)	83,113,113	1.28	6 (7%)
82	PEB	JK	202	2	46,46,46	2.78	14 (30%)	54,67,67	2.41	23 (42%)
82	PEB	Y5	202	2	46,46,46	2.58	12 (26%)	54,67,67	2.27	18 (33%)
91	PHO	d6	404	-	58,69,69	2.66	13 (22%)	56,99,99	2.72	19 (33%)
82	PEB	ZM	201	2	46,46,46	2.72	14 (30%)	54,67,67	2.23	19 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	H5	203	2	46,46,46	2.60	11 (23%)	54,67,67	1.88	16 (29%)
83	PUB	Z9	305	1,74	45,46,46	2.92	11 (24%)	46,67,67	4.11	25 (54%)
85	BCR	I2	101	-	41,41,41	0.77	0	56,56,56	2.36	15 (26%)
84	CYC	N1	1001	10,8	46,46,46	2.41	18 (39%)	61,67,67	2.74	28 (45%)
87	CLA	b6	614	-	63,67,73	1.30	10 (15%)	75,105,113	1.38	6 (8%)
87	CLA	7N	606	63	49,53,73	1.53	9 (18%)	59,89,113	1.54	7 (11%)
82	PEB	OM	203	1,2	46,46,46	2.63	12 (26%)	54,67,67	2.27	20 (37%)
87	CLA	C6	509	-	69,73,73	1.23	9 (13%)	83,113,113	1.33	6 (7%)
95	DGD	lL	101	26	59,59,67	0.91	2 (3%)	73,73,81	1.58	11 (15%)
82	PEB	YB	202	2	46,46,46	2.58	12 (26%)	54,67,67	2.04	18 (33%)
82	PEB	YO	201	2	46,46,46	2.60	13 (28%)	54,67,67	2.16	20 (37%)
82	PEB	V7	203	2	46,46,46	2.69	13 (28%)	54,67,67	1.97	19 (35%)
87	CLA	32	310	59,87	45,49,73	1.51	9 (20%)	54,84,113	1.84	9 (16%)
82	PEB	QP	201	1	46,46,46	2.61	14 (30%)	54,67,67	2.10	17 (31%)
82	PEB	FM	201	79,2	46,46,46	2.73	13 (28%)	54,67,67	2.31	21 (38%)
82	PEB	pK	201	2	46,46,46	2.60	12 (26%)	54,67,67	2.42	21 (38%)
82	PEB	H9	201	74,2	46,46,46	2.67	13 (28%)	54,67,67	1.97	16 (29%)
95	DGD	b6	622	-	43,43,67	1.06	3 (6%)	57,57,81	1.22	5 (8%)
88	LHG	cL	501	17	31,31,48	1.11	2 (6%)	34,37,54	1.50	5 (14%)
85	BCR	CL	516	-	41,41,41	0.72	0	56,56,56	2.91	21 (37%)
87	CLA	B2	816	-	63,67,73	1.34	10 (15%)	75,105,113	1.42	9 (12%)
82	PEB	P7	202	2	46,46,46	2.43	12 (26%)	54,67,67	2.67	24 (44%)
85	BCR	IN	101	-	41,41,41	0.76	0	56,56,56	2.36	15 (26%)
82	PEB	Z9	301	74	46,46,46	2.58	11 (23%)	54,67,67	2.31	22 (40%)
84	CYC	F3	1001	69	46,46,46	2.53	17 (36%)	61,67,67	3.11	28 (45%)
87	CLA	AN	831	-	69,73,73	1.31	11 (15%)	83,113,113	1.50	11 (13%)
82	PEB	L9	201	2	46,46,46	2.68	14 (30%)	54,67,67	2.00	15 (27%)
82	PEB	MQ	202	2	46,46,46	2.59	11 (23%)	54,67,67	2.00	15 (27%)
82	PEB	iH	202	2	46,46,46	2.76	12 (26%)	54,67,67	1.88	13 (24%)
82	PEB	HA	201	2	46,46,46	2.72	13 (28%)	54,67,67	2.08	17 (31%)
103	ZEX	8N	309	64	42,43,43	0.82	1 (2%)	55,60,60	2.15	16 (29%)
87	CLA	C6	510	-	69,73,73	1.25	10 (14%)	83,113,113	1.29	8 (9%)
84	CYC	CO	1001	9	46,46,46	2.37	16 (34%)	61,67,67	2.87	27 (44%)
82	PEB	kM	202	2	46,46,46	2.65	13 (28%)	54,67,67	2.11	19 (35%)
82	PEB	lH	202	1	46,46,46	2.77	13 (28%)	54,67,67	2.30	19 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
87	CLA	1N	607	57	54,58,73	1.39	8 (14%)	65,95,113	1.53	10 (15%)
82	PEB	yC	203	2	46,46,46	2.77	13 (28%)	54,67,67	1.97	17 (31%)
82	PEB	GP	202	1	46,46,46	2.55	12 (26%)	54,67,67	2.29	18 (33%)
82	PEB	C9	202	1	46,46,46	2.74	13 (28%)	54,67,67	2.42	20 (37%)
82	PEB	kG	202	2	46,46,46	2.63	14 (30%)	54,67,67	2.11	15 (27%)
82	PEB	DF	203	2	46,46,46	2.68	14 (30%)	54,67,67	2.08	20 (37%)
82	PEB	CK	201	1	46,46,46	2.60	13 (28%)	54,67,67	2.15	17 (31%)
82	PEB	A5	202	1	46,46,46	2.56	13 (28%)	54,67,67	2.05	18 (33%)
82	PEB	j4	201	1	46,46,46	2.64	13 (28%)	54,67,67	2.29	22 (40%)
82	PEB	gE	201	2	46,46,46	2.58	12 (26%)	54,67,67	2.09	17 (31%)
82	PEB	P9	202	1	46,46,46	2.74	13 (28%)	54,67,67	2.41	21 (38%)
85	BCR	A2	847	-	41,41,41	0.80	0	56,56,56	1.99	18 (32%)
83	PUB	K7	203	1,3	45,46,46	2.69	9 (20%)	46,67,67	3.07	19 (41%)
82	PEB	AP	201	1	46,46,46	2.51	11 (23%)	54,67,67	2.23	17 (31%)
82	PEB	iO	201	2	46,46,46	2.62	12 (26%)	54,67,67	2.05	18 (33%)
87	CLA	AN	850	40	69,73,73	1.28	9 (13%)	83,113,113	1.36	8 (9%)
87	CLA	BL	601	-	69,73,73	1.25	11 (15%)	83,113,113	1.33	7 (8%)
82	PEB	XD	203	1	46,46,46	2.68	12 (26%)	54,67,67	1.96	15 (27%)
87	CLA	3N	312	59	49,53,73	1.48	9 (18%)	59,89,113	1.50	7 (11%)
82	PEB	qF	202	1	46,46,46	2.59	13 (28%)	54,67,67	3.09	23 (42%)
87	CLA	dL	402	-	69,73,73	1.26	10 (14%)	83,113,113	1.31	9 (10%)
85	BCR	B2	802	87,50,41	41,41,41	0.77	0	56,56,56	3.37	24 (42%)
82	PEB	QF	202	1	46,46,46	2.61	12 (26%)	54,67,67	1.92	17 (31%)
82	PEB	G5	202	1	46,46,46	2.57	13 (28%)	54,67,67	2.05	18 (33%)
82	PEB	M5	304	74,82	46,46,46	2.58	13 (28%)	54,67,67	2.92	22 (40%)
84	CYC	M4	1001	9	46,46,46	2.30	15 (32%)	61,67,67	2.85	22 (36%)
82	PEB	jE	201	1	46,46,46	2.63	13 (28%)	54,67,67	2.08	19 (35%)
87	CLA	4N	602	60	69,73,73	1.28	11 (15%)	83,113,113	1.35	7 (8%)
82	PEB	kE	202	2	46,46,46	2.63	11 (23%)	54,67,67	2.12	17 (31%)
82	PEB	XI	202	1	46,46,46	2.54	12 (26%)	54,67,67	2.12	20 (37%)
82	PEB	WQ	201	3,2	46,46,46	2.63	13 (28%)	54,67,67	2.30	19 (35%)
82	PEB	Z4	201	1	46,46,46	2.63	14 (30%)	54,67,67	2.83	25 (46%)
82	PEB	UI	201	2	46,46,46	2.65	14 (30%)	54,67,67	2.10	21 (38%)
82	PEB	XK	202	2	46,46,46	2.50	12 (26%)	54,67,67	2.51	20 (37%)
82	PEB	UM	202	1	46,46,46	2.60	13 (28%)	54,67,67	2.20	15 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	JB	202	1	46,46,46	2.70	13 (28%)	54,67,67	2.50	20 (37%)
82	PEB	c4	203	2	46,46,46	2.70	13 (28%)	54,67,67	1.92	14 (25%)
87	CLA	F2	202	45	45,49,73	1.54	8 (17%)	54,84,113	1.71	8 (14%)
84	CYC	L1	1001	10	46,46,46	2.53	20 (43%)	61,67,67	3.05	34 (55%)
82	PEB	QB	204	2	46,46,46	2.66	13 (28%)	54,67,67	2.10	17 (31%)
82	PEB	EK	201	1	46,46,46	2.48	11 (23%)	54,67,67	2.37	17 (31%)
82	PEB	GK	202	1	46,46,46	2.49	12 (26%)	54,67,67	3.22	25 (46%)
82	PEB	qK	201	1,2	46,46,46	2.62	13 (28%)	54,67,67	2.49	23 (42%)
82	PEB	UG	203	1	46,46,46	2.64	13 (28%)	54,67,67	2.02	18 (33%)
87	CLA	B2	825	-	69,73,73	1.22	12 (17%)	83,113,113	1.33	7 (8%)
82	PEB	HB	202	2	46,46,46	2.57	12 (26%)	54,67,67	2.12	18 (33%)
82	PEB	XP	202	2	46,46,46	2.67	12 (26%)	54,67,67	2.07	17 (31%)
87	CLA	2N	308	58	49,53,73	1.52	8 (16%)	59,89,113	1.51	11 (18%)
83	PUB	xK	306	13	45,46,46	2.75	10 (22%)	46,67,67	2.93	19 (41%)
87	CLA	5N	609	61	46,50,73	1.50	9 (19%)	55,85,113	1.70	6 (10%)
82	PEB	XF	201	2	46,46,46	2.55	10 (21%)	54,67,67	3.42	20 (37%)
83	PUB	M5	303	1,74	45,46,46	2.80	11 (24%)	46,67,67	3.46	18 (39%)
82	PEB	HF	201	2	46,46,46	2.48	13 (28%)	54,67,67	2.89	28 (51%)
84	CYC	EE	1001	10,9	46,46,46	2.42	19 (41%)	61,67,67	2.80	26 (42%)
83	PUB	YA	302	3	45,46,46	2.67	11 (24%)	46,67,67	2.93	21 (45%)
87	CLA	IN	102	-	69,73,73	1.23	9 (13%)	83,113,113	1.36	6 (7%)
82	PEB	iH	201	2	46,46,46	2.67	14 (30%)	54,67,67	2.10	16 (29%)
82	PEB	EQ	201	2,77	46,46,46	2.61	14 (30%)	54,67,67	2.35	21 (38%)
82	PEB	WP	202	1	46,46,46	2.55	12 (26%)	54,67,67	2.22	18 (33%)
83	PUB	Z9	302	74	45,46,46	2.85	11 (24%)	46,67,67	3.45	20 (43%)
82	PEB	KK	202	1	46,46,46	2.67	12 (26%)	54,67,67	2.30	17 (31%)
87	CLA	AN	834	-	69,73,73	1.24	10 (14%)	83,113,113	1.44	9 (10%)
82	PEB	MK	203	1,2	46,46,46	2.59	14 (30%)	54,67,67	2.55	19 (35%)
82	PEB	xF	303	13	46,46,46	2.64	11 (23%)	54,67,67	1.89	13 (24%)
82	PEB	w8	201	2	46,46,46	2.68	12 (26%)	54,67,67	1.97	17 (31%)
82	PEB	1C	202	2	46,46,46	2.68	14 (30%)	54,67,67	2.16	15 (27%)
82	PEB	PE	202	2	46,46,46	2.63	12 (26%)	54,67,67	2.33	24 (44%)
82	PEB	hO	202	1	46,46,46	2.63	12 (26%)	54,67,67	1.95	16 (29%)
83	PUB	M9	303	74	45,46,46	2.85	11 (24%)	46,67,67	3.45	21 (45%)
82	PEB	mK	201	1	46,46,46	2.68	11 (23%)	54,67,67	2.03	19 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
84	CYC	W3	1001	71	46,46,46	2.54	17 (36%)	61,67,67	3.18	31 (50%)
82	PEB	hE	201	1,2	46,46,46	2.69	15 (32%)	54,67,67	2.26	15 (27%)
82	PEB	kF	202	1	46,46,46	2.72	13 (28%)	54,67,67	1.80	15 (27%)
82	PEB	dB	202	2	46,46,46	2.63	12 (26%)	54,67,67	2.13	16 (29%)
82	PEB	NA	203	2	46,46,46	2.56	12 (26%)	54,67,67	2.53	22 (40%)
82	PEB	CM	201	1	46,46,46	2.55	12 (26%)	54,67,67	2.11	15 (27%)
95	DGD	DL	408	18	63,63,67	0.86	2 (3%)	77,77,81	1.07	4 (5%)
82	PEB	DB	202	2	46,46,46	2.52	13 (28%)	54,67,67	2.10	18 (33%)
82	PEB	HB	201	2	46,46,46	2.70	13 (28%)	54,67,67	2.47	19 (35%)
82	PEB	VP	201	2	46,46,46	2.63	14 (30%)	54,67,67	2.02	19 (35%)
82	PEB	eJ	202	2	46,46,46	2.57	12 (26%)	54,67,67	2.22	23 (42%)
82	PEB	MF	201	1	46,46,46	2.61	11 (23%)	54,67,67	1.95	14 (25%)
87	CLA	bL	604	-	50,54,73	1.44	9 (18%)	60,90,113	1.55	5 (8%)
82	PEB	RQ	203	1,2	46,46,46	2.67	14 (30%)	54,67,67	2.18	20 (37%)
82	PEB	NE	202	10,9	46,46,46	2.61	15 (32%)	54,67,67	2.11	17 (31%)
82	PEB	gE	202	2	46,46,46	2.67	11 (23%)	54,67,67	2.12	19 (35%)
91	PHO	dL	403	-	58,69,69	2.58	13 (22%)	56,99,99	2.75	19 (33%)
82	PEB	q8	203	2	46,46,46	2.67	12 (26%)	54,67,67	2.01	17 (31%)
83	PUB	AE	303	3	45,46,46	2.69	9 (20%)	46,67,67	2.85	16 (34%)
87	CLA	62	304	-	49,53,73	1.48	9 (18%)	59,89,113	1.44	4 (6%)
84	CYC	IE	1001	10,9	46,46,46	2.40	16 (34%)	61,67,67	2.89	25 (40%)
82	PEB	LD	202	1	46,46,46	2.61	12 (26%)	54,67,67	2.23	15 (27%)
85	BCR	a6	605	-	41,41,41	0.81	1 (2%)	56,56,56	1.92	18 (32%)
82	PEB	B9	201	2	46,46,46	2.67	12 (26%)	54,67,67	2.15	16 (29%)
87	CLA	5N	603	-	49,53,73	1.47	9 (18%)	59,89,113	1.42	4 (6%)
82	PEB	TD	201	1,2	46,46,46	2.57	15 (32%)	54,67,67	2.23	16 (29%)
87	CLA	CL	504	-	69,73,73	1.29	10 (14%)	83,113,113	1.34	9 (10%)
82	PEB	F7	203	2	46,46,46	2.75	13 (28%)	54,67,67	1.94	20 (37%)
82	PEB	QG	202	1	46,46,46	2.64	13 (28%)	54,67,67	2.04	18 (33%)
82	PEB	MM	202	1	46,46,46	2.51	13 (28%)	54,67,67	2.24	16 (29%)
82	PEB	SI	201	2	46,46,46	2.54	13 (28%)	54,67,67	2.08	18 (33%)
82	PEB	K7	201	1	46,46,46	2.73	14 (30%)	54,67,67	2.42	20 (37%)
82	PEB	NG	201	10,9	46,46,46	2.60	15 (32%)	54,67,67	2.11	17 (31%)
82	PEB	MJ	203	1	46,46,46	2.34	13 (28%)	54,67,67	2.31	18 (33%)
87	CLA	1N	605	57	49,53,73	1.48	7 (14%)	59,89,113	1.50	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	T5	201	1	46,46,46	2.55	13 (28%)	54,67,67	2.27	20 (37%)
82	PEB	Q9	203	2	46,46,46	2.71	12 (26%)	54,67,67	1.98	19 (35%)
82	PEB	O4	201	1	46,46,46	2.59	12 (26%)	54,67,67	2.54	24 (44%)
82	PEB	Z9	303	74	46,46,46	2.69	13 (28%)	54,67,67	2.25	18 (33%)
82	PEB	i4	202	2	46,46,46	2.56	12 (26%)	54,67,67	2.31	19 (35%)
84	CYC	EG	1001	10,9	46,46,46	2.41	19 (41%)	61,67,67	2.80	26 (42%)
82	PEB	BJ	301	14	46,46,46	2.59	13 (28%)	54,67,67	2.35	19 (35%)
84	CYC	MG	1001	10,9	46,46,46	2.35	18 (39%)	61,67,67	2.91	25 (40%)
87	CLA	M2	101	51,41	49,53,73	1.48	11 (22%)	59,89,113	1.62	11 (18%)
87	CLA	82	301	64	49,53,73	1.52	11 (22%)	59,89,113	1.68	9 (15%)
82	PEB	EQ	202	2	46,46,46	2.64	12 (26%)	54,67,67	2.11	18 (33%)
82	PEB	TQ	201	1,2	46,46,46	2.56	15 (32%)	54,67,67	2.24	16 (29%)
82	PEB	D7	201	3,2	46,46,46	2.65	14 (30%)	54,67,67	2.24	17 (31%)
88	LHG	AL	407	15	42,42,48	0.97	2 (4%)	45,48,54	1.08	2 (4%)
82	PEB	PD	202	1	46,46,46	2.77	12 (26%)	54,67,67	2.16	18 (33%)
87	CLA	7N	602	62,63	69,73,73	1.38	10 (14%)	83,113,113	1.79	18 (21%)
82	PEB	w8	203	2	46,46,46	2.68	12 (26%)	54,67,67	1.94	16 (29%)
82	PEB	PH	202	2	46,46,46	2.69	13 (28%)	54,67,67	2.01	18 (33%)
82	PEB	a4	202	2	46,46,46	2.60	13 (28%)	54,67,67	2.48	23 (42%)
84	CYC	L3	1001	69	46,46,46	2.53	17 (36%)	61,67,67	3.11	28 (45%)
82	PEB	jK	201	2	46,46,46	2.63	11 (23%)	54,67,67	2.66	22 (40%)
82	PEB	Q7	202	1	46,46,46	2.53	12 (26%)	54,67,67	2.02	14 (25%)
85	BCR	h6	102	-	41,41,41	0.80	0	56,56,56	2.08	14 (25%)
82	PEB	QH	203	1	46,46,46	2.61	11 (23%)	54,67,67	2.12	18 (33%)
82	PEB	SP	203	1	46,46,46	2.83	13 (28%)	54,67,67	2.03	17 (31%)
92	LMG	b6	623	-	41,41,55	0.27	0	49,49,63	0.35	0
82	PEB	BF	202	2	46,46,46	2.71	13 (28%)	54,67,67	2.26	18 (33%)
92	LMG	j6	101	-	43,43,55	1.00	3 (6%)	51,51,63	2.16	12 (23%)
82	PEB	yC	202	2	46,46,46	2.70	11 (23%)	54,67,67	2.30	19 (35%)
82	PEB	iE	202	2	46,46,46	2.68	12 (26%)	54,67,67	1.98	18 (33%)
82	PEB	iF	203	1	46,46,46	2.69	12 (26%)	54,67,67	1.93	16 (29%)
82	PEB	WM	202	1	46,46,46	2.52	12 (26%)	54,67,67	2.42	19 (35%)
87	CLA	6N	608	62	54,58,73	2.14	12 (22%)	65,95,113	7.23	27 (41%)
87	CLA	72	608	63	45,49,73	1.52	7 (15%)	54,84,113	1.59	8 (14%)
82	PEB	YJ	203	1	46,46,46	2.36	13 (28%)	54,67,67	2.17	20 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	b4	202	1	46,46,46	2.66	12 (26%)	54,67,67	1.97	15 (27%)
82	PEB	H9	203	2	46,46,46	2.70	13 (28%)	54,67,67	2.06	18 (33%)
82	PEB	GF	202	1	46,46,46	2.49	12 (26%)	54,67,67	3.21	25 (46%)
82	PEB	YF	201	1	46,46,46	2.64	11 (23%)	54,67,67	2.12	19 (35%)
82	PEB	V1	202	1,2	46,46,46	2.55	12 (26%)	54,67,67	2.41	21 (38%)
82	PEB	TH	201	11,2	46,46,46	2.59	15 (32%)	54,67,67	2.31	23 (42%)
82	PEB	NJ	202	2	46,46,46	2.59	12 (26%)	54,67,67	2.28	22 (40%)
82	PEB	J5	201	2	46,46,46	2.63	12 (26%)	54,67,67	2.16	19 (35%)
85	BCR	AN	847	-	41,41,41	0.79	0	56,56,56	1.99	18 (32%)
92	LMG	mL	101	-	41,41,55	1.06	3 (7%)	49,49,63	1.63	8 (16%)
82	PEB	RE	201	2	46,46,46	2.66	13 (28%)	54,67,67	2.23	19 (35%)
82	PEB	QD	201	3,2	46,46,46	2.73	11 (23%)	54,67,67	2.21	23 (42%)
82	PEB	eM	202	2	46,46,46	2.64	13 (28%)	54,67,67	2.09	17 (31%)
82	PEB	aM	203	1	46,46,46	2.59	12 (26%)	54,67,67	2.40	17 (31%)
96	HEM	VL	201	35	50,50,50	1.67	11 (22%)	66,82,82	1.76	16 (24%)
87	CLA	A2	827	-	59,63,73	1.36	10 (16%)	71,101,113	1.43	13 (18%)
82	PEB	HQ	201	1,2	46,46,46	2.51	12 (26%)	54,67,67	2.41	20 (37%)
82	PEB	IB	201	2	46,46,46	2.52	12 (26%)	54,67,67	2.08	16 (29%)
82	PEB	m1	202	2	46,46,46	2.84	12 (26%)	54,67,67	1.86	14 (25%)
87	CLA	4N	611	-	49,53,73	1.47	10 (20%)	59,89,113	1.49	4 (6%)
82	PEB	UE	203	1	46,46,46	2.64	14 (30%)	54,67,67	2.02	18 (33%)
84	CYC	h3	1001	73,69	46,46,46	2.53	17 (36%)	61,67,67	3.11	28 (45%)
82	PEB	aG	201	2	46,46,46	2.62	13 (28%)	54,67,67	2.19	20 (37%)
82	PEB	FD	201	1	46,46,46	2.53	14 (30%)	54,67,67	2.60	22 (40%)
87	CLA	A2	809	-	69,73,73	1.25	9 (13%)	83,113,113	1.52	15 (18%)
82	PEB	TB	202	1	46,46,46	2.69	13 (28%)	54,67,67	2.50	20 (37%)
82	PEB	kF	203	1,2	46,46,46	2.55	12 (26%)	54,67,67	2.40	18 (33%)
82	PEB	UB	301	2,5	46,46,46	2.65	13 (28%)	54,67,67	2.17	18 (33%)
82	PEB	BF	201	2	46,46,46	2.56	12 (26%)	54,67,67	3.30	19 (35%)
82	PEB	CF	202	1	46,46,46	2.52	9 (19%)	54,67,67	2.41	19 (35%)
82	PEB	LG	1002	10,9	46,46,46	2.72	13 (28%)	54,67,67	2.04	19 (35%)
82	PEB	iE	201	2	46,46,46	2.68	13 (28%)	54,67,67	1.96	16 (29%)
82	PEB	WI	201	2	46,46,46	2.71	14 (30%)	54,67,67	2.23	20 (37%)
87	CLA	42	610	-	46,50,73	1.49	7 (15%)	55,85,113	1.64	7 (12%)
92	LMG	AL	411	-	51,51,55	0.95	2 (3%)	59,59,63	1.10	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
87	CLA	BL	609	-	69,73,73	1.25	10 (14%)	83,113,113	1.38	8 (9%)
82	PEB	aE	201	2	46,46,46	2.63	13 (28%)	54,67,67	2.19	20 (37%)
82	PEB	YJ	202	1	46,46,46	2.54	12 (26%)	54,67,67	2.25	20 (37%)
87	CLA	52	603	-	49,53,73	1.47	9 (18%)	59,89,113	1.42	4 (6%)
87	CLA	B6	612	-	63,67,73	1.29	10 (15%)	75,105,113	1.38	6 (8%)
87	CLA	dL	409	-	54,58,73	1.40	9 (16%)	65,95,113	1.55	9 (13%)
82	PEB	BD	202	1	46,46,46	2.61	11 (23%)	54,67,67	1.98	16 (29%)
84	CYC	K1	1001	10,9	46,46,46	2.30	14 (30%)	61,67,67	2.94	28 (45%)
82	PEB	KD	202	2	46,46,46	2.62	13 (28%)	54,67,67	1.97	18 (33%)
84	CYC	BE	1001	10,8	46,46,46	2.43	18 (39%)	61,67,67	2.84	28 (45%)
87	CLA	c6	611	-	69,73,73	1.24	9 (13%)	83,113,113	1.41	10 (12%)
82	PEB	JI	201	2	46,46,46	2.71	14 (30%)	54,67,67	2.06	21 (38%)
82	PEB	RJ	201	2	46,46,46	2.69	13 (28%)	54,67,67	2.30	18 (33%)
83	PUB	BJ	302	14	45,46,46	2.53	8 (17%)	46,67,67	3.02	14 (30%)
92	LMG	A6	408	-	51,51,55	0.93	2 (3%)	59,59,63	1.21	6 (10%)
85	BCR	CL	501	-	41,41,41	0.74	0	56,56,56	1.77	16 (28%)
82	PEB	VJ	202	2	46,46,46	2.65	13 (28%)	54,67,67	2.20	24 (44%)
82	PEB	N1	1002	10	46,46,46	2.60	14 (30%)	54,67,67	2.04	13 (24%)
82	PEB	a1	201	2	46,46,46	2.62	11 (23%)	54,67,67	2.11	19 (35%)
82	PEB	XP	201	2	46,46,46	2.57	13 (28%)	54,67,67	2.06	16 (29%)
98	PQN	BN	837	41	34,34,34	1.88	4 (11%)	42,45,45	2.53	14 (33%)
87	CLA	22	606	58	49,53,73	1.45	7 (14%)	59,89,113	1.57	5 (8%)
82	PEB	mG	202	2	46,46,46	2.64	13 (28%)	54,67,67	2.32	18 (33%)
84	CYC	J1	1001	10	46,46,46	2.32	18 (39%)	61,67,67	2.90	30 (49%)
82	PEB	EJ	201	1,2	46,46,46	2.44	12 (26%)	54,67,67	2.54	22 (40%)
87	CLA	R2	204	-	49,53,73	1.46	10 (20%)	59,89,113	1.50	7 (11%)
92	LMG	b6	624	-	36,36,55	1.16	2 (5%)	44,44,63	1.25	4 (9%)
82	PEB	eH	202	2	46,46,46	2.70	13 (28%)	54,67,67	1.93	16 (29%)
82	PEB	jF	202	2	46,46,46	2.72	13 (28%)	54,67,67	2.15	16 (29%)
87	CLA	12	602	57	69,73,73	1.21	6 (8%)	83,113,113	1.44	9 (10%)
84	CYC	e3	1001	68	46,46,46	2.66	16 (34%)	61,67,67	2.92	25 (40%)
82	PEB	O9	202	2	46,46,46	2.62	13 (28%)	54,67,67	3.12	26 (48%)
96	HEM	E6	101	19	50,50,50	1.69	8 (16%)	66,82,82	1.53	13 (19%)
82	PEB	SF	202	1	46,46,46	2.59	14 (30%)	54,67,67	2.33	18 (33%)
82	PEB	PO	201	2	46,46,46	2.64	12 (26%)	54,67,67	2.18	18 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	nF	202	2	46,46,46	2.81	15 (32%)	54,67,67	1.96	16 (29%)
82	PEB	YM	203	1	46,46,46	2.50	14 (30%)	54,67,67	2.08	16 (29%)
92	LMG	JL	102	-	43,43,55	0.96	2 (4%)	51,51,63	1.28	5 (9%)
82	PEB	EP	203	1,2	46,46,46	3.10	13 (28%)	54,67,67	3.00	19 (35%)
82	PEB	VB	201	2	46,46,46	2.73	14 (30%)	54,67,67	2.20	19 (35%)
84	CYC	IG	1001	10,9	46,46,46	2.41	16 (34%)	61,67,67	2.90	25 (40%)
82	PEB	dM	201	1,2	46,46,46	2.56	13 (28%)	54,67,67	2.46	21 (38%)
87	CLA	C6	515	17	69,73,73	1.24	10 (14%)	83,113,113	1.27	6 (7%)
82	PEB	hK	202	2	46,46,46	2.67	13 (28%)	54,67,67	1.99	20 (37%)
82	PEB	vF	201	2	46,46,46	2.68	12 (26%)	54,67,67	2.75	21 (38%)
87	CLA	C6	516	-	69,73,73	1.24	9 (13%)	83,113,113	1.37	9 (10%)
82	PEB	I9	201	1	46,46,46	2.62	15 (32%)	54,67,67	1.97	17 (31%)
82	PEB	zF	501	78,2	46,46,46	2.50	9 (19%)	54,67,67	2.42	19 (35%)
82	PEB	eO	201	2	46,46,46	2.61	14 (30%)	54,67,67	2.18	17 (31%)
82	PEB	XD	202	1	46,46,46	2.70	13 (28%)	54,67,67	1.92	16 (29%)
82	PEB	X7	202	2	46,46,46	2.43	10 (21%)	54,67,67	2.77	24 (44%)
87	CLA	a6	609	-	54,58,73	1.40	10 (18%)	65,95,113	1.49	8 (12%)
87	CLA	CL	512	-	69,73,73	1.27	10 (14%)	83,113,113	1.32	6 (7%)
82	PEB	EI	201	1	46,46,46	2.57	12 (26%)	54,67,67	2.05	18 (33%)
82	PEB	aK	201	1,2	46,46,46	2.71	14 (30%)	54,67,67	2.29	20 (37%)
82	PEB	QM	204	1	46,46,46	2.55	13 (28%)	54,67,67	1.92	12 (22%)
87	CLA	3N	307	-	46,50,73	1.50	9 (19%)	55,85,113	1.61	8 (14%)
87	CLA	22	603	-	49,53,73	1.47	8 (16%)	59,89,113	1.44	4 (6%)
82	PEB	v8	201	1	46,46,46	2.68	14 (30%)	54,67,67	2.04	16 (29%)
82	PEB	lO	202	1	46,46,46	2.63	13 (28%)	54,67,67	2.05	17 (31%)
82	PEB	GJ	202	1	46,46,46	2.55	12 (26%)	54,67,67	2.01	16 (29%)
83	PUB	xF	301	13	45,46,46	2.66	10 (22%)	46,67,67	3.16	23 (50%)
87	CLA	K2	106	40,49	53,57,73	1.37	10 (18%)	62,93,113	1.34	11 (17%)
99	SF4	C2	102	42	0,12,12	-	-	-		
87	CLA	B2	811	-	59,63,73	1.33	10 (16%)	71,101,113	1.47	8 (11%)
82	PEB	eH	201	2	46,46,46	2.70	14 (30%)	54,67,67	2.09	20 (37%)
82	PEB	WG	202	1,77	46,46,46	2.53	13 (28%)	54,67,67	2.09	17 (31%)
82	PEB	aJ	202	1	46,46,46	2.58	12 (26%)	54,67,67	2.15	19 (35%)
87	CLA	AN	825	-	59,63,73	1.38	11 (18%)	71,101,113	1.47	9 (12%)
82	PEB	sC	202	2	46,46,46	2.78	13 (28%)	54,67,67	2.34	18 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	O9	201	2	46,46,46	2.65	14 (30%)	54,67,67	2.23	19 (35%)
82	PEB	K9	201	1	46,46,46	2.61	14 (30%)	54,67,67	1.97	17 (31%)
82	PEB	t8	202	1	46,46,46	2.75	13 (28%)	54,67,67	2.46	20 (37%)
82	PEB	JP	202	2	46,46,46	2.62	12 (26%)	54,67,67	2.10	17 (31%)
82	PEB	nF	201	2	46,46,46	2.70	12 (26%)	54,67,67	2.98	20 (37%)
82	PEB	UB	303	2,5	46,46,46	2.53	12 (26%)	54,67,67	2.05	17 (31%)
82	PEB	O5	202	2	46,46,46	2.60	13 (28%)	54,67,67	2.33	22 (40%)
82	PEB	HD	202	1	46,46,46	2.64	14 (30%)	54,67,67	2.31	20 (37%)
87	CLA	22	602	58	69,73,73	1.44	6 (8%)	83,113,113	2.60	18 (21%)
82	PEB	I5	201	1	46,46,46	2.56	13 (28%)	54,67,67	2.27	21 (38%)
82	PEB	mM	201	13,2	46,46,46	2.70	14 (30%)	54,67,67	2.12	17 (31%)
87	CLA	B6	607	-	69,73,73	1.26	10 (14%)	83,113,113	1.31	6 (7%)
87	CLA	BN	818	41	64,68,73	1.26	9 (14%)	77,107,113	1.45	9 (11%)
82	PEB	oK	203	1	46,46,46	2.69	13 (28%)	54,67,67	2.19	17 (31%)
82	PEB	AM	302	13	46,46,46	2.59	11 (23%)	54,67,67	1.99	17 (31%)
82	PEB	QE	203	1	46,46,46	2.63	12 (26%)	54,67,67	2.12	19 (35%)
82	PEB	SK	203	1	46,46,46	2.61	11 (23%)	54,67,67	2.15	16 (29%)
82	PEB	ZK	201	2	46,46,46	2.68	12 (26%)	54,67,67	2.14	18 (33%)
82	PEB	U4	202	1	46,46,46	2.53	12 (26%)	54,67,67	1.98	14 (25%)
82	PEB	AH	302	3	46,46,46	2.67	12 (26%)	54,67,67	1.98	16 (29%)
82	PEB	OQ	202	2	46,46,46	2.73	15 (32%)	54,67,67	1.94	16 (29%)
87	CLA	K6	101	25	69,73,73	1.25	9 (13%)	83,113,113	1.37	10 (12%)
82	PEB	bH	202	1	46,46,46	2.76	12 (26%)	54,67,67	2.29	22 (40%)
83	PUB	ND	201	1,3	45,46,46	2.85	11 (24%)	46,67,67	3.07	18 (39%)
82	PEB	HJ	202	2	46,46,46	2.64	12 (26%)	54,67,67	2.13	17 (31%)
82	PEB	WJ	201	1	46,46,46	2.57	12 (26%)	54,67,67	2.27	21 (38%)
87	CLA	A2	838	-	69,73,73	1.25	10 (14%)	83,113,113	1.39	9 (10%)
82	PEB	QO	201	1	46,46,46	2.60	13 (28%)	54,67,67	2.77	27 (50%)
82	PEB	NI	202	1	46,46,46	2.54	12 (26%)	54,67,67	2.12	20 (37%)
84	CYC	BG	1002	10,8	46,46,46	2.43	18 (39%)	61,67,67	2.98	29 (47%)
94	PL9	AL	413	-	55,55,55	0.72	2 (3%)	68,69,69	2.61	17 (25%)
82	PEB	HH	1002	10	46,46,46	2.76	13 (28%)	54,67,67	2.23	19 (35%)
82	PEB	UI	202	2	46,46,46	2.59	12 (26%)	54,67,67	2.11	19 (35%)
82	PEB	RM	202	2	46,46,46	2.66	12 (26%)	54,67,67	2.19	21 (38%)
82	PEB	T4	201	2	46,46,46	2.60	13 (28%)	54,67,67	2.22	19 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	L9	202	2	46,46,46	2.68	12 (26%)	54,67,67	2.23	21 (38%)
84	CYC	GE	1001	10,9	46,46,46	2.39	16 (34%)	61,67,67	2.86	26 (42%)
82	PEB	BQ	202	1	46,46,46	2.61	13 (28%)	54,67,67	1.97	17 (31%)
82	PEB	OA	202	1	46,46,46	2.54	12 (26%)	54,67,67	2.04	19 (35%)
82	PEB	kJ	202	2	46,46,46	2.63	13 (28%)	54,67,67	2.14	21 (38%)
83	PUB	M5	302	1,74	45,46,46	2.80	13 (28%)	46,67,67	3.59	25 (54%)
82	PEB	sC	201	2	46,46,46	2.71	14 (30%)	54,67,67	2.25	18 (33%)
87	CLA	3N	301	59	49,53,73	1.44	9 (18%)	59,89,113	1.48	8 (13%)
82	PEB	OI	201	2	46,46,46	2.68	15 (32%)	54,67,67	2.17	18 (33%)
92	LMG	D6	407	18,24	33,33,55	1.13	2 (6%)	41,41,63	1.51	8 (19%)
92	LMG	DL	402	18	54,54,55	0.92	2 (3%)	62,62,63	1.33	7 (11%)
82	PEB	EB	501	2,4	46,46,46	2.55	11 (23%)	54,67,67	2.07	18 (33%)
82	PEB	h1	201	1,74,2	46,46,46	2.62	13 (28%)	54,67,67	2.29	19 (35%)
87	CLA	LN	202	50	61,65,73	1.30	8 (13%)	73,103,113	1.31	6 (8%)
82	PEB	E9	201	1	46,46,46	2.61	12 (26%)	54,67,67	1.97	17 (31%)
87	CLA	B2	808	-	69,73,73	1.28	11 (15%)	83,113,113	1.35	6 (7%)
82	PEB	dJ	202	1	46,46,46	2.60	13 (28%)	54,67,67	2.07	15 (27%)
82	PEB	HM	202	2	46,46,46	2.70	14 (30%)	54,67,67	2.25	24 (44%)
82	PEB	fH	201	1	46,46,46	2.66	14 (30%)	54,67,67	1.92	16 (29%)
87	CLA	B2	812	-	69,73,73	1.25	10 (14%)	83,113,113	1.40	10 (12%)
87	CLA	5N	606	61	49,53,73	1.43	6 (12%)	59,89,113	1.78	7 (11%)
82	PEB	O5	201	74,2,82	46,46,46	2.56	13 (28%)	54,67,67	2.12	19 (35%)
82	PEB	JF	201	2	46,46,46	2.54	12 (26%)	54,67,67	2.89	19 (35%)
82	PEB	DM	201	14,2	46,46,46	2.70	13 (28%)	54,67,67	2.13	18 (33%)
91	PHO	D6	404	-	58,69,69	2.63	13 (22%)	56,99,99	2.74	19 (33%)
83	PUB	A4	302	3	45,46,46	2.70	9 (20%)	46,67,67	2.89	18 (39%)
82	PEB	cH	201	2	46,46,46	2.63	13 (28%)	54,67,67	2.14	20 (37%)
85	BCR	B2	838	-	41,41,41	0.73	0	56,56,56	2.49	21 (37%)
103	ZEX	82	309	64	42,43,43	0.82	2 (4%)	55,60,60	2.15	16 (29%)
82	PEB	FK	202	2	46,46,46	2.67	13 (28%)	54,67,67	2.37	20 (37%)
82	PEB	NQ	202	1	46,46,46	2.69	14 (30%)	54,67,67	1.89	16 (29%)
82	PEB	U4	201	1	46,46,46	2.51	12 (26%)	54,67,67	2.94	26 (48%)
87	CLA	32	308	59	49,53,73	1.43	9 (18%)	59,89,113	1.47	7 (11%)
87	CLA	52	604	61	46,50,73	1.49	10 (21%)	55,85,113	1.60	6 (10%)
92	LMG	b6	619	-	41,41,55	1.02	2 (4%)	49,49,63	1.21	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	vC	202	1	46,46,46	2.68	14 (30%)	54,67,67	2.66	22 (40%)
82	PEB	cO	202	2	46,46,46	2.68	14 (30%)	54,67,67	2.22	17 (31%)
82	PEB	PM	202	2	46,46,46	2.62	13 (28%)	54,67,67	2.03	20 (37%)
84	CYC	CG	1001	10,9	46,46,46	2.37	18 (39%)	61,67,67	2.77	25 (40%)
82	PEB	WE	203	1,2	46,46,46	2.49	11 (23%)	54,67,67	2.32	22 (40%)
82	PEB	b1	203	1,2	46,46,46	2.62	14 (30%)	54,67,67	2.53	18 (33%)
82	PEB	GJ	203	1,2	46,46,46	2.49	12 (26%)	54,67,67	2.49	22 (40%)
92	LMG	B6	618	-	40,40,55	1.04	2 (5%)	48,48,63	1.36	6 (12%)
82	PEB	W1	201	1	46,46,46	2.55	12 (26%)	54,67,67	2.26	18 (33%)
82	PEB	Q5	203	2	46,46,46	2.53	13 (28%)	54,67,67	2.07	17 (31%)
82	PEB	BB	202	2	46,46,46	2.53	11 (23%)	54,67,67	2.12	18 (33%)
82	PEB	PQ	202	1	46,46,46	2.77	12 (26%)	54,67,67	2.16	19 (35%)
82	PEB	l1	202	1	46,46,46	2.68	12 (26%)	54,67,67	2.02	17 (31%)
82	PEB	H7	202	2	46,46,46	2.59	13 (28%)	54,67,67	2.43	22 (40%)
82	PEB	OQ	201	3,2,82	46,46,46	2.66	12 (26%)	54,67,67	2.07	16 (29%)
84	CYC	LH	1002	10	46,46,46	2.53	20 (43%)	61,67,67	3.04	34 (55%)
85	BCR	BL	616	-	41,41,41	0.80	0	56,56,56	1.59	11 (19%)
87	CLA	62	305	87,62	46,50,73	1.51	8 (17%)	55,85,113	1.45	6 (10%)
87	CLA	aL	606	-	64,68,73	1.44	10 (15%)	77,107,113	2.04	16 (20%)
87	CLA	B2	826	-	69,73,73	1.24	9 (13%)	83,113,113	1.33	8 (9%)
85	BCR	J2	103	40,48	41,41,41	0.71	0	56,56,56	2.09	16 (28%)
82	PEB	O7	202	1	46,46,46	2.54	12 (26%)	54,67,67	2.05	19 (35%)
82	PEB	wF	303	13	46,46,46	2.71	13 (28%)	54,67,67	2.12	19 (35%)
82	PEB	D9	201	2	46,46,46	2.64	13 (28%)	54,67,67	2.16	18 (33%)
82	PEB	NK	202	2	46,46,46	2.84	13 (28%)	54,67,67	2.41	19 (35%)
87	CLA	bL	607	-	69,73,73	1.29	11 (15%)	83,113,113	1.65	12 (14%)
85	BCR	c6	602	-	41,41,41	0.81	0	56,56,56	2.21	22 (39%)
87	CLA	BN	826	-	69,73,73	1.25	11 (15%)	83,113,113	1.34	8 (9%)
82	PEB	TA	203	2	46,46,46	2.62	12 (26%)	54,67,67	2.27	21 (38%)
82	PEB	KM	203	1,2	46,46,46	2.53	12 (26%)	54,67,67	2.55	23 (42%)
87	CLA	32	306	-	46,50,73	1.50	9 (19%)	55,85,113	1.59	8 (14%)
87	CLA	d6	403	-	69,73,73	1.24	10 (14%)	83,113,113	1.33	8 (9%)
87	CLA	AN	802	40,45	69,73,73	1.27	9 (13%)	83,113,113	1.44	10 (12%)
82	PEB	SQ	202	2	46,46,46	2.67	12 (26%)	54,67,67	2.07	20 (37%)
82	PEB	TM	202	2	46,46,46	2.68	13 (28%)	54,67,67	2.15	21 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	jO	201	1	46,46,46	2.65	13 (28%)	54,67,67	2.30	22 (40%)
82	PEB	x8	202	1	46,46,46	2.76	13 (28%)	54,67,67	2.67	25 (46%)
82	PEB	DJ	201	14,2	46,46,46	2.68	13 (28%)	54,67,67	2.23	22 (40%)
85	BCR	BN	843	-	41,41,41	0.77	0	56,56,56	2.01	18 (32%)
87	CLA	52	608	61	45,49,73	1.54	9 (20%)	54,84,113	1.71	9 (16%)
87	CLA	5N	602	61	69,73,73	1.24	9 (13%)	83,113,113	1.37	9 (10%)
82	PEB	HM	201	2	46,46,46	2.70	13 (28%)	54,67,67	2.36	20 (37%)
82	PEB	UQ	202	2	46,46,46	2.73	12 (26%)	54,67,67	1.96	17 (31%)
82	PEB	A7	201	1	46,46,46	2.67	14 (30%)	54,67,67	2.14	21 (38%)
95	DGD	C6	504	-	43,43,67	1.01	3 (6%)	57,57,81	1.53	10 (17%)
103	ZEX	82	310	64,87	42,43,43	1.77	9 (21%)	55,60,60	3.88	30 (54%)
87	CLA	B6	609	-	69,73,73	1.26	10 (14%)	83,113,113	1.29	8 (9%)
84	CYC	MO	1001	9	46,46,46	2.29	15 (32%)	61,67,67	2.87	22 (36%)
87	CLA	2N	304	-	49,53,73	1.48	8 (16%)	59,89,113	1.43	4 (6%)
85	BCR	BN	803	87,50,41	41,41,41	0.76	0	56,56,56	3.37	24 (42%)
82	PEB	e1	202	2	46,46,46	2.70	13 (28%)	54,67,67	1.94	15 (27%)
82	PEB	SJ	201	1	46,46,46	2.57	12 (26%)	54,67,67	2.18	17 (31%)
82	PEB	Z5	305	74	46,46,46	2.57	13 (28%)	54,67,67	2.36	25 (46%)
82	PEB	T7	202	2	46,46,46	2.35	10 (21%)	54,67,67	3.03	27 (50%)
87	CLA	bL	619	-	63,67,73	1.30	10 (15%)	75,105,113	1.35	8 (10%)
82	PEB	UD	201	3,2	46,46,46	2.71	15 (32%)	54,67,67	2.03	19 (35%)
82	PEB	A4	304	3	46,46,46	2.62	13 (28%)	54,67,67	2.06	17 (31%)
82	PEB	DP	202	2	46,46,46	2.63	13 (28%)	54,67,67	2.07	19 (35%)
82	PEB	bG	201	1	46,46,46	2.67	13 (28%)	54,67,67	2.20	16 (29%)
82	PEB	lH	201	1	46,46,46	2.68	14 (30%)	54,67,67	2.02	17 (31%)
87	CLA	A2	823	40	69,73,73	1.23	11 (15%)	83,113,113	1.43	10 (12%)
84	CYC	EH	1001	10,9	46,46,46	2.36	17 (36%)	61,67,67	3.17	28 (45%)
87	CLA	AN	801	-	48,52,73	1.46	10 (20%)	56,87,113	1.70	9 (16%)
82	PEB	QJ	203	1	46,46,46	2.59	12 (26%)	54,67,67	2.03	15 (27%)
87	CLA	b6	606	16	69,73,73	1.24	9 (13%)	83,113,113	1.38	8 (9%)
95	DGD	c6	618	-	63,63,67	0.84	2 (3%)	77,77,81	1.03	4 (5%)
82	PEB	MK	201	1	46,46,46	2.60	11 (23%)	54,67,67	1.95	16 (29%)
82	PEB	bE	202	1	46,46,46	0.63	0	54,67,67	0.79	1 (1%)
82	PEB	iG	202	2	46,46,46	2.67	13 (28%)	54,67,67	1.99	16 (29%)
82	PEB	LJ	201	2	46,46,46	2.67	12 (26%)	54,67,67	2.36	18 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	aF	201	1,2	46,46,46	2.71	13 (28%)	54,67,67	2.28	21 (38%)
95	DGD	BL	613	-	41,41,67	1.11	3 (7%)	55,55,81	1.47	7 (12%)
84	CYC	d3	1001	73,69	46,46,46	2.52	17 (36%)	61,67,67	3.12	28 (45%)
87	CLA	RN	203	54,41	50,54,73	1.46	8 (16%)	60,90,113	1.43	5 (8%)
87	CLA	52	606	61	49,53,73	1.43	7 (14%)	59,89,113	1.79	7 (11%)
82	PEB	ZF	202	2	46,46,46	2.81	15 (32%)	54,67,67	2.12	21 (38%)
82	PEB	WO	201	1	46,46,46	2.57	13 (28%)	54,67,67	2.64	23 (42%)
82	PEB	SH	201	1	46,46,46	2.62	13 (28%)	54,67,67	2.28	16 (29%)
82	PEB	MJ	201	1,2	46,46,46	2.50	11 (23%)	54,67,67	2.55	23 (42%)
84	CYC	C1	1001	10,9	46,46,46	2.35	16 (34%)	61,67,67	2.84	27 (44%)
82	PEB	N5	201	1	46,46,46	2.56	13 (28%)	54,67,67	2.26	21 (38%)
82	PEB	W7	201	1	46,46,46	2.44	12 (26%)	54,67,67	2.39	21 (38%)
82	PEB	D9	203	2	46,46,46	2.70	12 (26%)	54,67,67	1.95	15 (27%)
82	PEB	gG	201	2	46,46,46	2.60	12 (26%)	54,67,67	2.09	17 (31%)
82	PEB	SB	203	2	46,46,46	2.53	11 (23%)	54,67,67	2.13	15 (27%)
83	PUB	A1	303	3	45,46,46	2.83	10 (22%)	46,67,67	3.03	19 (41%)
82	PEB	GI	203	1	46,46,46	2.54	13 (28%)	54,67,67	2.11	20 (37%)
87	CLA	AN	829	-	69,73,73	1.24	9 (13%)	83,113,113	1.52	8 (9%)
82	PEB	UQ	201	3,2	46,46,46	2.70	15 (32%)	54,67,67	2.03	19 (35%)
82	PEB	tC	202	1	46,46,46	2.75	13 (28%)	54,67,67	2.46	20 (37%)
82	PEB	bK	201	2	46,46,46	2.67	13 (28%)	54,67,67	2.08	18 (33%)
82	PEB	AM	301	13	46,46,46	2.58	13 (28%)	54,67,67	2.07	19 (35%)
82	PEB	YQ	202	2	46,46,46	2.67	13 (28%)	54,67,67	1.93	14 (25%)
82	PEB	p8	202	1	46,46,46	2.80	13 (28%)	54,67,67	2.69	22 (40%)
82	PEB	FI	202	2	46,46,46	2.57	11 (23%)	54,67,67	2.08	18 (33%)
82	PEB	NF	201	2	46,46,46	2.59	11 (23%)	54,67,67	2.91	19 (35%)
87	CLA	A2	837	-	55,59,73	1.41	11 (20%)	66,96,113	1.69	15 (22%)
82	PEB	UG	202	1	46,46,46	2.63	13 (28%)	54,67,67	2.06	18 (33%)
87	CLA	L2	204	50	54,58,73	1.46	10 (18%)	65,95,113	1.74	13 (20%)
82	PEB	BA	201	2,82	46,46,46	2.63	13 (28%)	54,67,67	2.21	20 (37%)
82	PEB	Y9	201	2	46,46,46	2.73	14 (30%)	54,67,67	2.11	17 (31%)
82	PEB	JQ	202	1	46,46,46	2.60	11 (23%)	54,67,67	1.99	14 (25%)
82	PEB	OP	202	1	46,46,46	2.53	11 (23%)	54,67,67	2.14	18 (33%)
82	PEB	R5	202	1	46,46,46	2.58	13 (28%)	54,67,67	2.06	18 (33%)
87	CLA	B2	807	-	69,73,73	1.25	10 (14%)	83,113,113	1.35	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	l1	203	1	46,46,46	2.76	14 (30%)	54,67,67	2.29	19 (35%)
82	PEB	NB	203	2	46,46,46	2.56	13 (28%)	54,67,67	2.21	19 (35%)
87	CLA	BN	830	-	69,73,73	1.24	9 (13%)	83,113,113	1.30	4 (4%)
82	PEB	f1	203	1,2	46,46,46	2.70	13 (28%)	54,67,67	2.02	17 (31%)
84	CYC	LG	1001	10	46,46,46	2.40	17 (36%)	61,67,67	3.02	28 (45%)
87	CLA	MN	101	51,41	49,53,73	1.48	11 (22%)	59,89,113	1.63	10 (16%)
82	PEB	TO	203	2	46,46,46	2.59	11 (23%)	54,67,67	1.91	16 (29%)
82	PEB	V4	202	2	46,46,46	2.58	12 (26%)	54,67,67	2.49	22 (40%)
82	PEB	x8	201	1	46,46,46	2.68	12 (26%)	54,67,67	1.87	16 (29%)
82	PEB	NP	202	2	46,46,46	2.63	12 (26%)	54,67,67	2.12	17 (31%)
83	PUB	yK	303	14	45,46,46	2.62	9 (20%)	46,67,67	3.03	19 (41%)
83	PUB	xK	301	13	45,46,46	2.66	10 (22%)	46,67,67	3.18	23 (50%)
85	BCR	c6	617	-	41,41,41	0.76	0	56,56,56	3.02	21 (37%)
82	PEB	dE	204	1	46,46,46	2.67	14 (30%)	54,67,67	1.99	16 (29%)
82	PEB	rK	201	13,2	46,46,46	2.63	12 (26%)	54,67,67	2.17	14 (25%)
82	PEB	sK	203	1,2	46,46,46	2.76	15 (32%)	54,67,67	2.55	20 (37%)
87	CLA	AN	806	-	59,63,73	1.33	9 (15%)	71,101,113	1.49	8 (11%)
87	CLA	A2	850	40	69,73,73	1.27	8 (11%)	83,113,113	1.37	9 (10%)
82	PEB	RF	202	2	46,46,46	2.68	14 (30%)	54,67,67	2.30	21 (38%)
82	PEB	KI	203	1	46,46,46	2.53	13 (28%)	54,67,67	2.11	20 (37%)
87	CLA	62	311	-	46,50,73	1.51	8 (17%)	55,85,113	1.70	8 (14%)
87	CLA	8N	302	64	49,53,73	1.52	11 (22%)	59,89,113	1.67	9 (15%)
82	PEB	FQ	201	1	46,46,46	2.54	12 (26%)	54,67,67	2.61	22 (40%)
87	CLA	A2	802	-	48,52,73	1.46	9 (18%)	56,87,113	1.70	9 (16%)
82	PEB	VO	201	2	46,46,46	2.58	12 (26%)	54,67,67	2.19	19 (35%)
87	CLA	B6	610	-	69,73,73	1.26	10 (14%)	83,113,113	1.38	7 (8%)
87	CLA	82	307	-	46,50,73	1.48	10 (21%)	55,85,113	1.46	6 (10%)
95	DGD	B6	620	16	59,59,67	0.90	2 (3%)	73,73,81	0.98	3 (4%)
82	PEB	JD	203	1,2	46,46,46	2.48	12 (26%)	54,67,67	2.17	16 (29%)
82	PEB	U1	203	1	46,46,46	2.71	11 (23%)	54,67,67	2.19	20 (37%)
82	PEB	XA	203	2	46,46,46	2.60	14 (30%)	54,67,67	2.34	23 (42%)
87	CLA	52	602	61	69,73,73	1.24	9 (13%)	83,113,113	1.37	8 (9%)
87	CLA	AL	404	87	64,68,73	1.26	9 (14%)	77,107,113	1.44	8 (10%)
82	PEB	VB	202	1,2	46,46,46	2.64	12 (26%)	54,67,67	2.04	15 (27%)
82	PEB	S4	202	1,76	46,46,46	2.53	14 (30%)	54,67,67	1.98	16 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
84	CYC	HH	1001	10	46,46,46	2.35	18 (39%)	61,67,67	2.88	29 (47%)
85	BCR	A2	804	-	41,41,41	0.75	0	56,56,56	2.07	17 (30%)
82	PEB	P5	202	1	46,46,46	2.57	13 (28%)	54,67,67	2.05	18 (33%)
82	PEB	D7	203	2	46,46,46	2.68	13 (28%)	54,67,67	2.14	20 (37%)
87	CLA	B2	821	-	59,63,73	1.35	10 (16%)	71,101,113	1.41	6 (8%)
87	CLA	KN	103	-	46,50,73	1.47	10 (21%)	55,85,113	1.74	8 (14%)
82	PEB	ND	202	1	46,46,46	2.67	13 (28%)	54,67,67	1.87	16 (29%)
82	PEB	GB	203	2	46,46,46	2.59	12 (26%)	54,67,67	2.12	18 (33%)
87	CLA	B2	817	41	64,68,73	1.26	9 (14%)	77,107,113	1.45	9 (11%)
87	CLA	2N	306	58	49,53,73	1.46	8 (16%)	59,89,113	1.56	5 (8%)
82	PEB	OE	201	1	46,46,46	2.58	13 (28%)	54,67,67	2.32	21 (38%)
82	PEB	VI	201	1	46,46,46	2.57	12 (26%)	54,67,67	2.05	18 (33%)
82	PEB	GD	201	2	46,46,46	2.69	14 (30%)	54,67,67	2.14	19 (35%)
89	OEX	a6	611	15,17	0,14,14	-	-	-		
84	CYC	BE	1002	10,8	46,46,46	2.43	17 (36%)	61,67,67	2.97	29 (47%)
82	PEB	RH	201	2	46,46,46	2.62	14 (30%)	54,67,67	2.17	22 (40%)
87	CLA	A6	403	87	64,68,73	1.27	10 (15%)	77,107,113	1.41	7 (9%)
82	PEB	mE	202	2	46,46,46	2.64	13 (28%)	54,67,67	2.32	18 (33%)
82	PEB	FF	201	2	46,46,46	2.59	12 (26%)	54,67,67	3.56	17 (31%)
82	PEB	KG	201	10,9	46,46,46	2.58	12 (26%)	54,67,67	2.07	17 (31%)
82	PEB	dG	201	1,3	46,46,46	2.65	12 (26%)	54,67,67	2.18	20 (37%)
84	CYC	CH	1001	10,9	46,46,46	2.35	16 (34%)	61,67,67	2.83	27 (44%)
85	BCR	B2	840	41	41,41,41	0.72	0	56,56,56	1.79	16 (28%)
87	CLA	AN	808	-	69,73,73	1.25	11 (15%)	83,113,113	1.37	8 (9%)
82	PEB	rF	201	13,2	46,46,46	2.62	12 (26%)	54,67,67	2.17	14 (25%)
82	PEB	OF	202	1	46,46,46	2.52	11 (23%)	54,67,67	2.26	21 (38%)
82	PEB	UH	202	1	46,46,46	2.69	15 (32%)	54,67,67	2.02	17 (31%)
87	CLA	A2	829	-	69,73,73	1.24	9 (13%)	83,113,113	1.53	8 (9%)
82	PEB	OJ	202	1	46,46,46	2.56	13 (28%)	54,67,67	2.68	21 (38%)
87	CLA	CL	507	-	69,73,73	1.24	11 (15%)	83,113,113	1.60	11 (13%)
82	PEB	FQ	203	1,2	46,46,46	2.82	15 (32%)	54,67,67	2.98	22 (40%)
82	PEB	U9	201	74,2	46,46,46	2.73	13 (28%)	54,67,67	2.03	15 (27%)
91	PHO	DL	405	-	58,69,69	2.61	13 (22%)	56,99,99	2.81	16 (28%)
82	PEB	WK	201	1,2	46,46,46	2.52	12 (26%)	54,67,67	2.59	27 (50%)
87	CLA	12	607	57	54,58,73	1.39	9 (16%)	65,95,113	1.53	10 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
87	CLA	cL	514	-	69,73,73	1.25	9 (13%)	83,113,113	1.31	6 (7%)
82	PEB	tF	202	2	46,46,46	2.80	14 (30%)	54,67,67	2.26	19 (35%)
87	CLA	BL	602	-	69,73,73	1.29	10 (14%)	83,113,113	1.46	7 (8%)
84	CYC	63	901	73	46,46,46	2.36	17 (36%)	61,67,67	2.98	30 (49%)
82	PEB	iM	201	13,2	46,46,46	2.75	15 (32%)	54,67,67	2.22	19 (35%)
82	PEB	X9	202	1	46,46,46	2.74	14 (30%)	54,67,67	2.42	21 (38%)
82	PEB	g4	202	2	46,46,46	2.56	11 (23%)	54,67,67	2.32	21 (38%)
82	PEB	UE	202	1	46,46,46	2.62	13 (28%)	54,67,67	2.06	17 (31%)
82	PEB	ZJ	201	2	46,46,46	2.69	13 (28%)	54,67,67	2.37	20 (37%)
82	PEB	RF	201	2	46,46,46	2.50	10 (21%)	54,67,67	3.44	21 (38%)
82	PEB	kH	203	1,2	46,46,46	2.64	12 (26%)	54,67,67	2.34	20 (37%)
82	PEB	VQ	203	1,2	46,46,46	2.70	15 (32%)	54,67,67	2.37	19 (35%)
84	CYC	NH	1001	10,8	46,46,46	2.41	18 (39%)	61,67,67	2.75	29 (47%)
82	PEB	UB	302	2,5	46,46,46	2.70	13 (28%)	54,67,67	2.31	21 (38%)
82	PEB	lF	202	2	46,46,46	2.72	13 (28%)	54,67,67	2.12	18 (33%)
87	CLA	AN	824	40	55,59,73	1.38	8 (14%)	66,96,113	1.57	6 (9%)
82	PEB	OO	202	1	46,46,46	2.54	14 (30%)	54,67,67	1.94	14 (25%)
82	PEB	CA	201	1	46,46,46	2.63	14 (30%)	54,67,67	2.54	20 (37%)
82	PEB	NQ	203	1	46,46,46	2.66	11 (23%)	54,67,67	2.02	16 (29%)
82	PEB	XB	201	2	46,46,46	2.55	12 (26%)	54,67,67	2.07	17 (31%)
82	PEB	V9	202	1	46,46,46	2.73	13 (28%)	54,67,67	2.42	21 (38%)
82	PEB	TA	202	2	46,46,46	2.35	10 (21%)	54,67,67	3.04	27 (50%)
82	PEB	s8	201	2	46,46,46	2.72	15 (32%)	54,67,67	2.25	19 (35%)
87	CLA	62	313	62	49,53,73	1.67	8 (16%)	59,89,113	2.06	15 (25%)
82	PEB	UK	202	1	46,46,46	2.61	11 (23%)	54,67,67	2.10	17 (31%)
87	CLA	32	312	59	49,53,73	1.48	10 (20%)	59,89,113	1.51	7 (11%)
87	CLA	B2	810	-	69,73,73	1.27	12 (17%)	83,113,113	1.49	8 (9%)
82	PEB	A5	201	1	46,46,46	2.55	13 (28%)	54,67,67	2.26	21 (38%)
82	PEB	dG	203	1	46,46,46	2.66	14 (30%)	54,67,67	2.07	20 (37%)
82	PEB	jJ	201	1	46,46,46	2.64	11 (23%)	54,67,67	2.14	16 (29%)
87	CLA	2N	305	-	46,50,73	1.49	10 (21%)	55,85,113	1.63	10 (18%)
87	CLA	BN	809	-	69,73,73	1.28	11 (15%)	83,113,113	1.34	6 (7%)
82	PEB	tK	203	1,2	46,46,46	2.70	14 (30%)	54,67,67	2.16	16 (29%)
82	PEB	GF	201	1,2	46,46,46	2.54	12 (26%)	54,67,67	2.96	27 (50%)
87	CLA	3N	311	-	46,50,73	1.51	10 (21%)	55,85,113	1.60	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	WH	203	1,2	46,46,46	2.67	14 (30%)	54,67,67	2.22	21 (38%)
82	PEB	CJ	203	1,2	46,46,46	2.49	11 (23%)	54,67,67	2.53	23 (42%)
82	PEB	k1	202	2	46,46,46	2.71	13 (28%)	54,67,67	2.10	20 (37%)
82	PEB	qC	203	2	46,46,46	2.67	12 (26%)	54,67,67	2.02	17 (31%)
82	PEB	eE	202	2	46,46,46	2.62	10 (21%)	54,67,67	2.25	19 (35%)
82	PEB	QK	202	1	46,46,46	2.60	11 (23%)	54,67,67	1.92	18 (33%)
87	CLA	b6	609	-	69,73,73	1.25	9 (13%)	83,113,113	1.40	9 (10%)
87	CLA	22	607	58	49,53,73	1.47	8 (16%)	59,89,113	1.49	9 (15%)
85	BCR	c6	603	87,17	41,41,41	0.79	0	56,56,56	2.59	25 (44%)
82	PEB	lO	201	1	46,46,46	2.60	12 (26%)	54,67,67	2.30	21 (38%)
95	DGD	BL	614	-	59,59,67	0.94	3 (5%)	73,73,81	1.57	12 (16%)
82	PEB	IP	201	1	46,46,46	2.57	12 (26%)	54,67,67	2.14	18 (33%)
82	PEB	cJ	201	2	46,46,46	2.66	13 (28%)	54,67,67	2.18	18 (33%)
82	PEB	iF	201	1,2	46,46,46	2.61	12 (26%)	54,67,67	2.35	18 (33%)
87	CLA	A2	828	40	69,73,73	1.36	9 (13%)	83,113,113	1.58	13 (15%)
82	PEB	KF	203	1	46,46,46	2.62	12 (26%)	54,67,67	2.11	22 (40%)
88	LHG	iL	101	-	48,48,48	0.96	2 (4%)	51,54,54	0.96	3 (5%)
82	PEB	cG	201	2	46,46,46	2.62	13 (28%)	54,67,67	2.11	18 (33%)
83	PUB	yK	302	14	45,46,46	2.59	8 (17%)	46,67,67	2.96	20 (43%)
87	CLA	bL	613	16	69,73,73	1.26	11 (15%)	83,113,113	1.49	8 (9%)
82	PEB	WD	201	3,2	46,46,46	2.62	14 (30%)	54,67,67	2.30	19 (35%)
87	CLA	32	305	-	49,53,73	1.45	8 (16%)	59,89,113	1.52	8 (13%)
82	PEB	F5	202	2	46,46,46	2.42	12 (26%)	54,67,67	2.47	23 (42%)
85	BCR	LN	201	-	41,41,41	0.75	0	56,56,56	1.87	11 (19%)
87	CLA	B2	834	-	69,73,73	1.28	11 (15%)	83,113,113	1.37	11 (13%)
87	CLA	bL	605	-	69,73,73	1.23	9 (13%)	83,113,113	1.28	7 (8%)
82	PEB	TP	201	56,2	46,46,46	2.68	14 (30%)	54,67,67	2.02	18 (33%)
87	CLA	AN	837	-	55,59,73	1.40	11 (20%)	66,96,113	1.68	15 (22%)
82	PEB	SK	202	1	46,46,46	2.59	14 (30%)	54,67,67	2.33	18 (33%)
88	LHG	AN	844	-	39,39,48	1.03	2 (5%)	42,45,54	1.08	2 (4%)
82	PEB	fO	202	1	46,46,46	2.65	14 (30%)	54,67,67	1.96	17 (31%)
84	CYC	KH	1001	10,9	46,46,46	2.29	13 (28%)	61,67,67	2.93	28 (45%)
82	PEB	LM	201	2	46,46,46	2.68	13 (28%)	54,67,67	2.09	18 (33%)
82	PEB	OF	203	1	46,46,46	2.60	10 (21%)	54,67,67	2.06	20 (37%)
85	BCR	A2	845	40	41,41,41	0.72	0	56,56,56	1.97	12 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	UP	202	1	46,46,46	2.71	14 (30%)	54,67,67	2.33	19 (35%)
82	PEB	L5	202	2	46,46,46	2.59	12 (26%)	54,67,67	2.11	19 (35%)
87	CLA	32	311	-	46,50,73	1.50	10 (21%)	55,85,113	1.58	8 (14%)
82	PEB	E5	201	1	46,46,46	2.56	13 (28%)	54,67,67	2.26	21 (38%)
82	PEB	AI	201	1	46,46,46	2.57	12 (26%)	54,67,67	2.05	18 (33%)
84	CYC	x3	1001	-	46,46,46	2.53	16 (34%)	61,67,67	3.07	32 (52%)
82	PEB	zC	201	1	46,46,46	2.70	13 (28%)	54,67,67	2.23	26 (48%)
82	PEB	RI	203	1,2	46,46,46	2.29	11 (23%)	54,67,67	2.97	22 (40%)
83	PUB	AM	303	13	45,46,46	2.70	10 (22%)	46,67,67	3.06	19 (41%)
82	PEB	YP	503	56,2	46,46,46	2.57	13 (28%)	54,67,67	2.07	16 (29%)
82	PEB	T9	202	1	46,46,46	2.74	13 (28%)	54,67,67	2.41	21 (38%)
82	PEB	RG	202	2	46,46,46	2.60	12 (26%)	54,67,67	2.08	18 (33%)
95	DGD	hL	101	22	63,63,67	0.86	2 (3%)	77,77,81	1.04	5 (6%)
82	PEB	U1	202	1	46,46,46	2.70	14 (30%)	54,67,67	2.02	18 (33%)
87	CLA	52	611	61	49,53,73	1.49	8 (16%)	59,89,113	1.59	9 (15%)
82	PEB	XA	202	2	46,46,46	2.42	10 (21%)	54,67,67	2.76	23 (42%)
82	PEB	eO	203	2	46,46,46	2.55	11 (23%)	54,67,67	1.91	13 (24%)
83	PUB	AM	304	13	45,46,46	2.67	10 (22%)	46,67,67	2.97	18 (39%)
87	CLA	7N	609	-	46,50,73	1.51	9 (19%)	55,85,113	1.59	7 (12%)
82	PEB	UK	201	1	46,46,46	2.53	11 (23%)	54,67,67	3.21	25 (46%)
88	LHG	D6	406	18	48,48,48	0.89	2 (4%)	51,54,54	1.09	3 (5%)
92	LMG	a6	614	87	42,42,55	1.04	2 (4%)	50,50,63	1.22	4 (8%)
82	PEB	i4	201	2	46,46,46	2.61	12 (26%)	54,67,67	2.06	18 (33%)
82	PEB	fF	202	2	46,46,46	2.93	14 (30%)	54,67,67	2.31	22 (40%)
84	CYC	I1	1001	10,9	46,46,46	2.38	14 (30%)	61,67,67	3.00	28 (45%)
82	PEB	j4	203	-	46,46,46	2.60	13 (28%)	54,67,67	2.32	20 (37%)
82	PEB	EM	203	1	46,46,46	2.52	12 (26%)	54,67,67	2.09	15 (27%)
87	CLA	52	607	61	54,58,73	1.38	8 (14%)	65,95,113	1.57	10 (15%)
87	CLA	AN	832	40	54,58,73	1.41	11 (20%)	65,95,113	1.60	9 (13%)
82	PEB	SK	201	1,2	46,46,46	2.53	12 (26%)	54,67,67	2.55	22 (40%)
82	PEB	gO	202	2	46,46,46	2.57	10 (21%)	54,67,67	2.33	21 (38%)
85	BCR	B2	839	-	41,41,41	0.72	0	56,56,56	1.97	14 (25%)
82	PEB	W5	202	2	46,46,46	2.61	13 (28%)	54,67,67	2.20	20 (37%)
87	CLA	1N	606	-	49,53,73	1.48	9 (18%)	59,89,113	1.36	5 (8%)
82	PEB	kM	201	2	46,46,46	2.73	14 (30%)	54,67,67	2.16	19 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	PEB	ZB	203	2	46,46,46	2.76	12 (26%)	54,67,67	2.16	17 (31%)
87	CLA	CL	511	-	69,73,73	1.25	10 (14%)	83,113,113	1.47	12 (14%)
82	PEB	HA	203	2	46,46,46	2.72	14 (30%)	54,67,67	2.25	19 (35%)
88	LHG	AN	843	40	48,48,48	0.93	2 (4%)	51,54,54	0.91	2 (3%)
82	PEB	CD	201	3,2	46,46,46	2.63	14 (30%)	54,67,67	2.34	21 (38%)
87	CLA	5N	608	61	45,49,73	1.53	9 (20%)	54,84,113	1.72	9 (16%)
82	PEB	g1	201	2	46,46,46	2.74	13 (28%)	54,67,67	2.00	19 (35%)
87	CLA	bL	616	-	69,73,73	1.26	11 (15%)	83,113,113	1.34	9 (10%)
87	CLA	4N	609	60	45,49,73	1.49	8 (17%)	54,84,113	1.69	8 (14%)
82	PEB	TO	201	2	46,46,46	2.58	13 (28%)	54,67,67	2.22	19 (35%)
82	PEB	DI	202	2	46,46,46	2.59	11 (23%)	54,67,67	2.00	15 (27%)
82	PEB	wK	301	13	46,46,46	2.54	12 (26%)	54,67,67	2.17	22 (40%)
82	PEB	D5	201	74,2	46,46,46	2.55	13 (28%)	54,67,67	2.17	20 (37%)
82	PEB	dK	201	2	46,46,46	2.62	11 (23%)	54,67,67	2.38	19 (35%)
82	PEB	kH	202	2	46,46,46	2.71	13 (28%)	54,67,67	2.11	20 (37%)
82	PEB	l4	201	1	46,46,46	2.59	13 (28%)	54,67,67	2.29	21 (38%)
82	PEB	aG	202	2	46,46,46	2.61	13 (28%)	54,67,67	2.09	17 (31%)
82	PEB	ZI	401	12,2	46,46,46	2.79	16 (34%)	54,67,67	3.04	22 (40%)
87	CLA	72	609	-	46,50,73	1.51	8 (17%)	55,85,113	1.57	7 (12%)
88	LHG	B6	617	-	48,48,48	0.92	2 (4%)	51,54,54	1.00	2 (3%)
88	LHG	D6	401	-	42,42,48	0.97	2 (4%)	45,48,54	1.10	2 (4%)
92	LMG	yL	101	-	55,55,55	0.34	0	63,63,63	0.53	0
82	PEB	gB	201	2	46,46,46	2.63	13 (28%)	54,67,67	2.08	14 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	rC	201	1	-	9/26/74/74	0/4/4/4
82	PEB	F5	203	2	-	12/26/74/74	0/4/4/4
82	PEB	cK	203	1,2	-	6/26/74/74	0/4/4/4
87	CLA	42	608	60	-	11/21/97/115	-
87	CLA	I2	102	-	-	12/39/115/115	-
82	PEB	TH	202	2	-	15/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	CLA	8N	305	-	-	7/15/91/115	-
82	PEB	RK	202	2	-	13/26/74/74	0/4/4/4
87	CLA	BN	817	-	-	8/32/108/115	-
82	PEB	dO	201	1	-	9/26/74/74	0/4/4/4
87	CLA	BN	834	-	-	15/39/115/115	-
87	CLA	R2	201	87	-	7/15/91/115	-
82	PEB	WM	201	1	-	7/26/74/74	0/4/4/4
82	PEB	dG	202	1,2	-	6/26/74/74	0/4/4/4
82	PEB	j1	203	1,2	-	9/26/74/74	0/4/4/4
82	PEB	QD	202	2	-	11/26/74/74	0/4/4/4
87	CLA	AL	405	15	-	8/21/97/115	-
82	PEB	YH	202	2	-	8/26/74/74	0/4/4/4
87	CLA	6N	604	87,62	-	9/12/88/115	-
82	PEB	fG	202	1	-	8/26/74/74	0/4/4/4
82	PEB	g4	203	2	-	11/26/74/74	0/4/4/4
82	PEB	C7	202	1	-	13/26/74/74	0/4/4/4
82	PEB	WH	202	1	-	9/26/74/74	0/4/4/4
82	PEB	iK	201	1,2	-	9/26/74/74	0/4/4/4
87	CLA	BN	829	-	-	7/13/89/115	-
82	PEB	CJ	202	1	-	10/26/74/74	0/4/4/4
82	PEB	SP	202	1	-	4/26/74/74	0/4/4/4
87	CLA	8N	301	64,103	-	10/17/93/115	-
84	CYC	H4	1001	10	-	8/26/74/74	0/4/4/4
82	PEB	z8	201	1	-	10/26/74/74	0/4/4/4
82	PEB	lM	201	1,2	-	8/26/74/74	0/4/4/4
87	CLA	2N	312	58	-	7/15/91/115	-
82	PEB	QF	203	1,2	-	7/26/74/74	0/4/4/4
87	CLA	dL	401	18	-	14/39/115/115	-
97	GOL	i6	102	-	-	0/4/4/4	-
84	CYC	V3	1001	-	-	10/26/74/74	0/4/4/4
82	PEB	lJ	201	1,2	-	8/26/74/74	0/4/4/4
85	BCR	d6	405	-	-	12/29/63/63	0/2/2/2
82	PEB	IM	201	1,2	-	6/26/74/74	0/4/4/4
87	CLA	B2	804	41	-	8/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	FM	202	2	-	9/26/74/74	0/4/4/4
83	PUB	AJ	304	13	-	8/26/74/74	0/4/4/4
87	CLA	H6	103	22	-	19/39/115/115	-
87	CLA	1N	601	57	-	12/15/91/115	-
82	PEB	UM	203	1	-	9/26/74/74	0/4/4/4
82	PEB	J7	201	3,2	-	4/26/74/74	0/4/4/4
99	SF4	BN	804	-	-	-	0/6/5/5
82	PEB	Q9	202	2	-	7/26/74/74	0/4/4/4
82	PEB	NO	1002	10	-	8/26/74/74	0/4/4/4
82	PEB	GK	203	1	-	9/26/74/74	0/4/4/4
82	PEB	HG	1002	10,9	-	8/26/74/74	0/4/4/4
82	PEB	IA	202	1	-	11/26/74/74	0/4/4/4
87	CLA	BN	806	41	-	18/39/115/115	-
82	PEB	XQ	201	1,2	-	9/26/74/74	0/4/4/4
87	CLA	B2	835	-	-	22/39/115/115	-
82	PEB	WA	202	1	-	12/26/74/74	0/4/4/4
82	PEB	YE	202	2	-	11/26/74/74	0/4/4/4
82	PEB	ID	202	2	-	7/26/74/74	0/4/4/4
82	PEB	LD	201	1,2	-	9/26/74/74	0/4/4/4
82	PEB	VK	202	2	-	12/26/74/74	0/4/4/4
82	PEB	OK	203	1	-	9/26/74/74	0/4/4/4
87	CLA	D6	403	-	-	19/39/115/115	-
100	3XQ	JN	104	-	-	17/24/24/24	-
82	PEB	wC	202	2	-	5/26/74/74	0/4/4/4
92	LMG	B6	619	16	-	7/34/54/70	0/1/1/1
84	CYC	T3	1001	68	-	8/26/74/74	0/4/4/4
95	DGD	D6	410	18,22	-	12/51/91/95	0/2/2/2
87	CLA	12	605	57	-	9/15/91/115	-
82	PEB	VF	202	2	-	12/26/74/74	0/4/4/4
87	CLA	d6	406	-	-	21/39/115/115	-
84	CYC	73	1002	73	-	6/26/74/74	0/4/4/4
87	CLA	12	606	-	-	8/15/91/115	-
82	PEB	sF	201	1	-	12/26/74/74	0/4/4/4
82	PEB	PH	201	11,2	-	6/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	MB	201	2	-	3/26/74/74	0/4/4/4
82	PEB	RQ	202	1	-	10/26/74/74	0/4/4/4
87	CLA	62	307	87	-	8/15/91/115	-
95	DGD	J6	101	-	-	13/51/91/95	0/2/2/2
82	PEB	aF	203	1	-	12/26/74/74	0/4/4/4
82	PEB	RO	201	11,2	-	3/26/74/74	0/4/4/4
82	PEB	QB	202	2,5	-	9/26/74/74	0/4/4/4
95	DGD	BL	607	-	-	5/29/69/95	0/2/2/2
82	PEB	C7	201	1	-	7/26/74/74	0/4/4/4
82	PEB	B7	202	2	-	8/26/74/74	0/4/4/4
82	PEB	jF	201	2	-	7/26/74/74	0/4/4/4
85	BCR	KN	101	40,49	-	13/29/63/63	0/2/2/2
87	CLA	B6	616	16	-	16/39/115/115	-
82	PEB	ZB	202	2	-	10/26/74/74	0/4/4/4
82	PEB	G7	201	1	-	6/26/74/74	0/4/4/4
82	PEB	RA	202	2	-	10/26/74/74	0/4/4/4
82	PEB	J7	203	2	-	16/26/74/74	0/4/4/4
84	CYC	D1	1003	10,9	-	10/26/74/74	0/4/4/4
82	PEB	NK	201	2	-	7/26/74/74	0/4/4/4
82	PEB	TF	201	2	-	7/26/74/74	0/4/4/4
82	PEB	SF	201	1,2	-	4/26/74/74	0/4/4/4
87	CLA	B2	801	41	-	13/31/107/115	-
82	PEB	VD	203	1,2	-	14/26/74/74	0/4/4/4
87	CLA	B2	815	41	-	8/27/103/115	-
84	CYC	k3	1001	69	-	4/26/74/74	0/4/4/4
82	PEB	D5	203	2	-	12/26/74/74	0/4/4/4
87	CLA	A2	813	-	-	13/39/115/115	-
87	CLA	CL	510	-	-	11/39/115/115	-
84	CYC	A3	1001	68	-	8/26/74/74	0/4/4/4
82	PEB	PP	201	2	-	7/26/74/74	0/4/4/4
87	CLA	FN	205	45	-	19/39/115/115	-
92	LMG	JL	103	18,24	-	6/28/48/70	0/1/1/1
85	BCR	A6	401	-	-	4/29/63/63	0/2/2/2
82	PEB	fB	301	76,2	-	10/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	C9	201	1	-	7/26/74/74	0/4/4/4
82	PEB	MD	202	2	-	9/26/74/74	0/4/4/4
82	PEB	QG	203	1	-	10/26/74/74	0/4/4/4
82	PEB	TD	203	1	-	13/26/74/74	0/4/4/4
82	PEB	MM	203	1	-	10/26/74/74	0/4/4/4
82	PEB	h4	201	1	-	10/26/74/74	0/4/4/4
82	PEB	KM	201	1	-	9/26/74/74	0/4/4/4
87	CLA	CL	514	-	-	11/27/103/115	-
82	PEB	UP	203	1,2	-	11/26/74/74	0/4/4/4
84	CYC	S3	1001	69	-	4/26/74/74	0/4/4/4
87	CLA	cL	509	-	-	21/39/115/115	-
87	CLA	RN	202	54	-	9/15/91/115	-
84	CYC	n3	1001	69	-	4/26/74/74	0/4/4/4
82	PEB	s8	203	2	-	7/26/74/74	0/4/4/4
82	PEB	cF	201	1	-	10/26/74/74	0/4/4/4
87	CLA	B2	813	-	-	4/15/91/115	-
87	CLA	3N	305	59,87	-	15/39/115/115	-
103	ZEX	8N	310	64,87	-	11/29/67/67	0/2/2/2
82	PEB	W9	202	2	-	12/26/74/74	0/4/4/4
82	PEB	Y9	202	2	-	7/26/74/74	0/4/4/4
82	PEB	nK	202	2	-	11/26/74/74	0/4/4/4
84	CYC	D3	1001	73,69	-	4/26/74/74	0/4/4/4
82	PEB	w8	204	2	-	8/26/74/74	0/4/4/4
82	PEB	aJ	201	13,1	-	12/26/74/74	0/4/4/4
82	PEB	Q5	201	74,2	-	8/26/74/74	0/4/4/4
82	PEB	N7	201	2	-	3/26/74/74	0/4/4/4
82	PEB	VK	201	2	-	10/26/74/74	0/4/4/4
82	PEB	hF	201	2	-	8/26/74/74	0/4/4/4
82	PEB	FO	1002	10	-	9/26/74/74	0/4/4/4
87	CLA	62	301	62	-	6/15/91/115	-
82	PEB	IK	201	1	-	9/26/74/74	0/4/4/4
82	PEB	a4	203	2	-	11/26/74/74	0/4/4/4
87	CLA	bL	621	-	-	8/39/115/115	-
87	CLA	c6	607	17	-	17/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	CYC	r3	1001	-	-	12/26/74/74	0/4/4/4
82	PEB	IQ	201	2,77	-	7/26/74/74	0/4/4/4
82	PEB	cH	202	2	-	11/26/74/74	0/4/4/4
85	BCR	Z6	101	39	-	3/29/63/63	0/2/2/2
87	CLA	AN	811	-	-	21/39/115/115	-
84	CYC	I3	1001	69	-	4/26/74/74	0/4/4/4
82	PEB	j1	202	1	-	8/26/74/74	0/4/4/4
85	BCR	F2	204	-	-	6/29/63/63	0/2/2/2
83	PUB	Z5	303	1,74	-	8/26/74/74	0/4/4/4
82	PEB	U7	201	1	-	4/26/74/74	0/4/4/4
82	PEB	HP	201	56,2	-	7/26/74/74	0/4/4/4
87	CLA	c6	605	17	-	17/39/115/115	-
88	LHG	m6	102	-	-	19/43/43/53	-
88	LHG	CL	521	-	-	14/41/41/53	-
87	CLA	B2	831	-	-	17/33/109/115	-
82	PEB	LP	201	2	-	7/26/74/74	0/4/4/4
92	LMG	J6	102	-	-	17/38/58/70	0/1/1/1
82	PEB	LF	201	2	-	9/26/74/74	0/4/4/4
85	BCR	cL	504	17	-	5/29/63/63	0/2/2/2
88	LHG	d6	402	-	-	17/50/50/53	-
87	CLA	BN	811	-	-	20/39/115/115	-
82	PEB	V1	203	2	-	7/26/74/74	0/4/4/4
95	DGD	h6	101	22	-	12/51/91/95	0/2/2/2
92	LMG	C6	501	-	-	17/50/70/70	0/1/1/1
82	PEB	UG	201	1,2	-	5/26/74/74	0/4/4/4
82	PEB	K5	201	1	-	11/26/74/74	0/4/4/4
87	CLA	42	603	-	-	5/15/91/115	-
87	CLA	12	611	-	-	8/15/91/115	-
82	PEB	fM	202	1	-	13/26/74/74	0/4/4/4
87	CLA	b6	612	-	-	17/39/115/115	-
82	PEB	U5	201	74,2	-	11/26/74/74	0/4/4/4
82	PEB	U7	202	1	-	10/26/74/74	0/4/4/4
82	PEB	KE	201	10,9	-	6/26/74/74	0/4/4/4
82	PEB	DA	202	2	-	12/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	QA	202	1	-	9/26/74/74	0/4/4/4
82	PEB	BQ	201	1	-	9/26/74/74	0/4/4/4
82	PEB	IK	203	1,2	-	5/26/74/74	0/4/4/4
82	PEB	i1	202	2	-	9/26/74/74	0/4/4/4
82	PEB	V5	201	1	-	11/26/74/74	0/4/4/4
87	CLA	O2	202	53	-	10/21/97/115	-
82	PEB	dM	202	1	-	10/26/74/74	0/4/4/4
87	CLA	6N	611	62	-	10/15/91/115	-
82	PEB	XM	201	2	-	9/26/74/74	0/4/4/4
82	PEB	XJ	202	2	-	8/26/74/74	0/4/4/4
82	PEB	RA	203	2	-	10/26/74/74	0/4/4/4
82	PEB	CF	203	1	-	10/26/74/74	0/4/4/4
82	PEB	O1	202	1	-	7/26/74/74	0/4/4/4
82	PEB	yF	301	14	-	8/26/74/74	0/4/4/4
87	CLA	HL	101	22	-	10/39/115/115	-
82	PEB	OE	203	1,2	-	6/26/74/74	0/4/4/4
88	LHG	BL	610	-	-	13/53/53/53	-
82	PEB	A9	201	1	-	7/26/74/74	0/4/4/4
82	PEB	wF	301	13	-	11/26/74/74	0/4/4/4
85	BCR	FN	202	-	-	6/29/63/63	0/2/2/2
82	PEB	PK	202	2	-	14/26/74/74	0/4/4/4
87	CLA	62	308	62	-	5/15/91/115	-
82	PEB	WK	203	1	-	13/26/74/74	0/4/4/4
82	PEB	MQ	201	2	-	7/26/74/74	0/4/4/4
87	CLA	B2	833	-	-	8/18/94/115	-
82	PEB	ZO	201	1	-	7/26/74/74	0/4/4/4
82	PEB	M5	305	74	-	13/26/74/74	0/4/4/4
82	PEB	E9	202	1	-	15/26/74/74	0/4/4/4
82	PEB	Q1	203	1	-	9/26/74/74	0/4/4/4
87	CLA	cL	512	-	-	8/39/115/115	-
82	PEB	LD	203	1	-	12/26/74/74	0/4/4/4
87	CLA	cL	506	-	-	16/39/115/115	-
82	PEB	uF	203	1	-	10/26/74/74	0/4/4/4
87	CLA	4N	605	60	-	9/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	qK	203	1	-	10/26/74/74	0/4/4/4
82	PEB	TK	201	2	-	7/26/74/74	0/4/4/4
82	PEB	Y1	202	2	-	8/26/74/74	0/4/4/4
82	PEB	e1	201	2	-	8/26/74/74	0/4/4/4
95	DGD	CL	520	-	-	5/31/71/95	0/2/2/2
87	CLA	BN	832	-	-	12/39/115/115	-
82	PEB	OD	201	3,2,82	-	8/26/74/74	0/4/4/4
82	PEB	II	201	1	-	9/26/74/74	0/4/4/4
82	PEB	mG	203	2	-	8/26/74/74	0/4/4/4
87	CLA	22	611	-	-	7/12/88/115	-
87	CLA	6N	603	-	-	9/15/91/115	-
82	PEB	yK	301	14	-	8/26/74/74	0/4/4/4
87	CLA	4N	606	-	-	8/15/91/115	-
87	CLA	52	610	-	-	5/15/91/115	-
82	PEB	GG	1002	10,9	-	9/26/74/74	0/4/4/4
82	PEB	J7	202	2	-	8/26/74/74	0/4/4/4
82	PEB	eF	202	1	-	8/26/74/74	0/4/4/4
82	PEB	lG	201	1,2	-	9/26/74/74	0/4/4/4
82	PEB	R7	201	2	-	5/26/74/74	0/4/4/4
84	CYC	F4	1001	10	-	11/26/74/74	0/4/4/4
82	PEB	Q4	201	1	-	8/26/74/74	0/4/4/4
82	PEB	HD	201	1,2	-	12/26/74/74	0/4/4/4
82	PEB	SF	203	1	-	9/26/74/74	0/4/4/4
82	PEB	FD	202	1	-	10/26/74/74	0/4/4/4
82	PEB	II	203	1,2	-	10/26/74/74	0/4/4/4
82	PEB	TJ	202	2	-	9/26/74/74	0/4/4/4
82	PEB	dE	203	1	-	8/26/74/74	0/4/4/4
82	PEB	JB	201	1	-	8/26/74/74	0/4/4/4
85	BCR	C6	507	-	-	1/29/63/63	0/2/2/2
94	PL9	a6	601	15	-	11/53/73/73	0/1/1/1
82	PEB	xF	304	13	-	8/26/74/74	0/4/4/4
82	PEB	sC	203	2	-	7/26/74/74	0/4/4/4
84	CYC	M3	1001	69	-	4/26/74/74	0/4/4/4
82	PEB	CK	203	1	-	10/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	GK	201	1,2	-	8/26/74/74	0/4/4/4
84	CYC	o3	1001	69	-	4/26/74/74	0/4/4/4
82	PEB	bH	201	1	-	10/26/74/74	0/4/4/4
82	PEB	uC	201	2	-	10/26/74/74	0/4/4/4
82	PEB	S1	202	1	-	9/26/74/74	0/4/4/4
82	PEB	YK	202	1	-	10/26/74/74	0/4/4/4
82	PEB	QH	201	1,2	-	9/26/74/74	0/4/4/4
82	PEB	MJ	202	1	-	5/26/74/74	0/4/4/4
82	PEB	MA	202	1	-	13/26/74/74	0/4/4/4
82	PEB	YD	201	2,82	-	7/26/74/74	0/4/4/4
87	CLA	BN	836	87,41,57	-	18/39/115/115	-
82	PEB	pF	201	2	-	8/26/74/74	0/4/4/4
82	PEB	jG	201	1	-	9/26/74/74	0/4/4/4
87	CLA	B2	827	-	-	15/39/115/115	-
82	PEB	BI	202	1,2	-	10/26/74/74	0/4/4/4
87	CLA	AL	403	15	-	12/39/115/115	-
82	PEB	b4	201	1	-	9/26/74/74	0/4/4/4
87	CLA	A2	818	-	-	8/15/91/115	-
82	PEB	OA	201	1	-	7/26/74/74	0/4/4/4
82	PEB	GM	203	1,2	-	8/26/74/74	0/4/4/4
82	PEB	w8	202	2	-	5/26/74/74	0/4/4/4
82	PEB	MB	202	2	-	9/26/74/74	0/4/4/4
87	CLA	A2	808	-	-	17/39/115/115	-
82	PEB	YJ	201	1,2	-	6/26/74/74	0/4/4/4
82	PEB	WG	203	1,2	-	7/26/74/74	0/4/4/4
82	PEB	qF	203	1	-	10/26/74/74	0/4/4/4
95	DGD	AL	416	-	-	8/29/69/95	0/2/2/2
87	CLA	7N	605	-	-	8/15/91/115	-
82	PEB	UO	202	1	-	10/26/74/74	0/4/4/4
88	LHG	BL	615	-	-	17/45/45/53	-
87	CLA	DL	404	-	-	15/39/115/115	-
91	PHO	A6	407	-	3/3/17/22	11/37/103/103	0/5/6/6
82	PEB	X5	202	1	-	11/26/74/74	0/4/4/4
82	PEB	DD	201	1,2	-	11/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	CLA	12	608	57	-	7/10/86/115	-
82	PEB	YA	304	3,82	-	13/26/74/74	0/4/4/4
87	CLA	ON	203	53	-	10/15/91/115	-
82	PEB	AE	304	3	-	5/26/74/74	0/4/4/4
82	PEB	FK	201	2	-	5/26/74/74	0/4/4/4
82	PEB	XK	203	2	-	11/26/74/74	0/4/4/4
82	PEB	lG	203	1	-	7/26/74/74	0/4/4/4
85	BCR	kL	100	-	-	13/29/63/63	0/2/2/2
82	PEB	AG	304	3	-	5/26/74/74	0/4/4/4
84	CYC	l3	1001	68	-	8/26/74/74	0/4/4/4
82	PEB	KQ	202	2	-	12/26/74/74	0/4/4/4
82	PEB	HD	203	1	-	12/26/74/74	0/4/4/4
82	PEB	YI	202	2	-	5/26/74/74	0/4/4/4
87	CLA	72	603	-	-	7/15/91/115	-
82	PEB	kF	201	1	-	12/26/74/74	0/4/4/4
82	PEB	YK	201	1	-	7/26/74/74	0/4/4/4
95	DGD	a6	604	15,17	-	4/42/82/95	0/2/2/2
82	PEB	SE	202	1,2	-	7/26/74/74	0/4/4/4
87	CLA	B2	822	-	-	16/39/115/115	-
82	PEB	JI	202	2	-	9/26/74/74	0/4/4/4
87	CLA	A2	824	40	-	10/23/99/115	-
87	CLA	8N	308	-	-	12/15/91/115	-
82	PEB	SD	201	3,2	-	4/26/74/74	0/4/4/4
82	PEB	Y4	203	2	-	11/26/74/74	0/4/4/4
82	PEB	BK	202	2	-	13/26/74/74	0/4/4/4
82	PEB	DD	202	1	-	9/26/74/74	0/4/4/4
82	PEB	d1	201	1,2	-	5/26/74/74	0/4/4/4
84	CYC	p3	1001	68	-	8/26/74/74	0/4/4/4
87	CLA	AN	819	40	-	12/36/112/115	-
82	PEB	EA	202	1	-	11/26/74/74	0/4/4/4
82	PEB	GP	201	1,2	-	11/26/74/74	0/4/4/4
82	PEB	PA	201	2	-	4/26/74/74	0/4/4/4
82	PEB	QH	202	1	-	12/26/74/74	0/4/4/4
82	PEB	A4	301	3	-	7/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	eE	203	2	-	13/26/74/74	0/4/4/4
82	PEB	I9	202	1	-	15/26/74/74	0/4/4/4
82	PEB	A1	302	3	-	11/26/74/74	0/4/4/4
82	PEB	KD	201	2	-	9/26/74/74	0/4/4/4
82	PEB	QE	201	1,2	-	9/26/74/74	0/4/4/4
82	PEB	kK	202	1	-	10/26/74/74	0/4/4/4
82	PEB	BQ	203	1,2	-	12/26/74/74	0/4/4/4
84	CYC	H3	1001	73,69	-	4/26/74/74	0/4/4/4
88	LHG	I6	101	-	-	21/53/53/53	-
87	CLA	AN	807	-	-	12/39/115/115	-
102	BGC	32	301	-	-	0/2/19/22	0/1/1/1
82	PEB	Y7	304	3,82	-	13/26/74/74	0/4/4/4
82	PEB	Q5	202	2	-	10/26/74/74	0/4/4/4
82	PEB	aB	201	2	-	2/26/74/74	0/4/4/4
82	PEB	lK	203	1,2	-	10/26/74/74	0/4/4/4
87	CLA	AN	840	-	-	14/39/115/115	-
82	PEB	PJ	201	2	-	6/26/74/74	0/4/4/4
87	CLA	B6	615	16	-	20/39/115/115	-
87	CLA	LN	203	85,50,41	-	22/39/115/115	-
82	PEB	bP	502	2	-	9/26/74/74	0/4/4/4
84	CYC	LE	1001	10	-	11/26/74/74	0/4/4/4
95	DGD	c6	620	-	-	13/37/77/95	0/2/2/2
82	PEB	UJ	201	1,2	-	8/26/74/74	0/4/4/4
87	CLA	B6	603	-	-	13/39/115/115	-
84	CYC	f3	1001	69	-	4/26/74/74	0/4/4/4
87	CLA	bL	620	16,85	-	11/29/105/115	-
82	PEB	VM	201	2	-	6/26/74/74	0/4/4/4
87	CLA	FN	203	45	-	10/15/91/115	-
82	PEB	QJ	202	1,2	-	8/26/74/74	0/4/4/4
82	PEB	F9	201	74,2	-	12/26/74/74	0/4/4/4
82	PEB	GM	202	1	-	12/26/74/74	0/4/4/4
87	CLA	c6	609	-	-	19/39/115/115	-
87	CLA	AN	826	-	-	11/39/115/115	-
82	PEB	Q7	201	1	-	5/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	oK	202	1	-	10/26/74/74	0/4/4/4
87	CLA	22	608	58	-	7/15/91/115	-
82	PEB	XI	201	1	-	9/26/74/74	0/4/4/4
82	PEB	EM	202	1	-	8/26/74/74	0/4/4/4
82	PEB	UO	201	1	-	7/26/74/74	0/4/4/4
82	PEB	S4	201	1	-	10/26/74/74	0/4/4/4
96	HEM	fL	102	-	-	7/14/54/54	-
95	DGD	CL	517	-	-	5/51/91/95	0/2/2/2
82	PEB	VA	202	2	-	10/26/74/74	0/4/4/4
82	PEB	hG	202	1	-	11/26/74/74	0/4/4/4
82	PEB	rF	202	2	-	13/26/74/74	0/4/4/4
87	CLA	BN	831	-	-	17/33/109/115	-
82	PEB	aH	202	2	-	10/26/74/74	0/4/4/4
82	PEB	O7	201	1	-	7/26/74/74	0/4/4/4
82	PEB	SG	202	-	-	10/26/74/74	0/4/4/4
82	PEB	qK	202	1	-	17/26/74/74	0/4/4/4
85	BCR	H6	101	-	-	3/29/63/63	0/2/2/2
84	CYC	K3	1001	68	-	8/26/74/74	0/4/4/4
87	CLA	nL	101	-	-	18/39/115/115	-
84	CYC	I4	1001	9	-	11/26/74/74	0/4/4/4
84	CYC	GO	1001	9	-	8/26/74/74	0/4/4/4
82	PEB	wC	204	2	-	8/26/74/74	0/4/4/4
85	BCR	b6	601	-	-	2/29/63/63	0/2/2/2
87	CLA	B2	830	-	-	15/39/115/115	-
82	PEB	fF	201	13,2	-	10/26/74/74	0/4/4/4
82	PEB	fE	202	1	-	8/26/74/74	0/4/4/4
82	PEB	NJ	201	2	-	8/26/74/74	0/4/4/4
82	PEB	m4	203	2	-	7/26/74/74	0/4/4/4
82	PEB	i4	203	2	-	10/26/74/74	0/4/4/4
87	CLA	BL	606	-	-	2/39/115/115	-
95	DGD	a6	603	-	-	10/29/69/95	0/2/2/2
87	CLA	82	306	64,103	-	10/17/93/115	-
87	CLA	1N	609	-	-	6/12/88/115	-
82	PEB	mO	202	2	-	8/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	CLA	A2	812	-	-	11/27/103/115	-
84	CYC	y3	1001	71	-	10/26/74/74	0/4/4/4
82	PEB	WE	201	1	-	7/26/74/74	0/4/4/4
82	PEB	cM	201	2	-	10/26/74/74	0/4/4/4
82	PEB	Y7	303	3,82	-	13/26/74/74	0/4/4/4
82	PEB	KK	201	1,2	-	7/26/74/74	0/4/4/4
87	CLA	AN	812	-	-	11/27/103/115	-
82	PEB	aM	202	1	-	7/26/74/74	0/4/4/4
95	DGD	AL	415	-	-	1/29/69/95	0/2/2/2
82	PEB	DM	202	2	-	9/26/74/74	0/4/4/4
82	PEB	GQ	202	2	-	13/26/74/74	0/4/4/4
82	PEB	SB	202	2	-	7/26/74/74	0/4/4/4
87	CLA	C6	519	-	-	11/27/103/115	-
82	PEB	p8	201	1	-	12/26/74/74	0/4/4/4
82	PEB	IM	203	1	-	9/26/74/74	0/4/4/4
82	PEB	JM	202	2	-	10/26/74/74	0/4/4/4
82	PEB	LQ	202	1	-	9/26/74/74	0/4/4/4
85	BCR	bL	603	-	-	4/29/63/63	0/2/2/2
82	PEB	U9	202	2	-	11/26/74/74	0/4/4/4
87	CLA	A2	807	-	-	12/39/115/115	-
82	PEB	RO	202	2	-	10/26/74/74	0/4/4/4
82	PEB	B9	203	2	-	7/26/74/74	0/4/4/4
84	CYC	u3	1001	69	-	4/26/74/74	0/4/4/4
87	CLA	6N	602	62	-	18/39/115/115	-
87	CLA	72	602	62,63	-	14/39/115/115	-
82	PEB	FJ	202	2	-	7/26/74/74	0/4/4/4
94	PL9	A6	410	-	-	17/53/73/73	0/1/1/1
82	PEB	eB	201	2	-	6/26/74/74	0/4/4/4
82	PEB	PF	201	2	-	7/26/74/74	0/4/4/4
82	PEB	OG	203	1,2	-	6/26/74/74	0/4/4/4
82	PEB	QG	201	1,2	-	9/26/74/74	0/4/4/4
87	CLA	c6	610	-	-	11/39/115/115	-
87	CLA	AN	833	-	-	13/39/115/115	-
82	PEB	TD	202	1	-	9/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	S9	202	2	-	9/26/74/74	0/4/4/4
91	PHO	a6	613	-	3/3/17/22	11/37/103/103	0/5/6/6
95	DGD	cL	502	-	-	12/51/91/95	0/2/2/2
87	CLA	AN	816	-	-	8/15/91/115	-
84	CYC	t3	1001	68	-	8/26/74/74	0/4/4/4
84	CYC	N4	1001	10	-	13/26/74/74	0/4/4/4
82	PEB	uK	201	1	-	10/26/74/74	0/4/4/4
82	PEB	PD	201	1,2	-	8/26/74/74	0/4/4/4
99	SF4	C2	101	42	-	-	0/6/5/5
92	LMG	BL	611	-	-	12/35/55/70	0/1/1/1
85	BCR	C6	508	-	-	10/29/63/63	0/2/2/2
87	CLA	6N	605	62	-	8/15/91/115	-
82	PEB	HQ	203	1	-	12/26/74/74	0/4/4/4
82	PEB	xK	304	13	-	8/26/74/74	0/4/4/4
85	BCR	KL	100	-	-	13/29/63/63	0/2/2/2
82	PEB	CP	202	1	-	6/26/74/74	0/4/4/4
87	CLA	6N	606	87	-	8/15/91/115	-
82	PEB	VJ	201	2	-	6/26/74/74	0/4/4/4
82	PEB	R9	202	1	-	15/26/74/74	0/4/4/4
82	PEB	AA	202	1	-	13/26/74/74	0/4/4/4
82	PEB	ZE	202	1	-	9/26/74/74	0/4/4/4
82	PEB	hF	202	2	-	9/26/74/74	0/4/4/4
82	PEB	F5	201	74,2	-	11/26/74/74	0/4/4/4
87	CLA	5N	605	61	-	6/15/91/115	-
82	PEB	JH	1002	10	-	10/26/74/74	0/4/4/4
82	PEB	J5	203	2	-	12/26/74/74	0/4/4/4
87	CLA	1N	610	57	-	8/15/91/115	-
82	PEB	M5	301	74	-	8/26/74/74	0/4/4/4
82	PEB	KA	202	1	-	11/26/74/74	0/4/4/4
82	PEB	V1	201	2	-	2/26/74/74	0/4/4/4
82	PEB	aO	201	2	-	2/26/74/74	0/4/4/4
87	CLA	cL	507	-	-	12/39/115/115	-
82	PEB	S7	201	1	-	4/26/74/74	0/4/4/4
87	CLA	BN	824	-	-	8/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	hH	202	1	-	11/26/74/74	0/4/4/4
82	PEB	T1	201	11,2	-	9/26/74/74	0/4/4/4
82	PEB	OJ	201	1	-	5/26/74/74	0/4/4/4
82	PEB	FB	201	2,5	-	12/26/74/74	0/4/4/4
87	CLA	42	607	60	-	8/15/91/115	-
82	PEB	tF	201	2	-	7/26/74/74	0/4/4/4
82	PEB	X9	201	1	-	7/26/74/74	0/4/4/4
82	PEB	GJ	201	1	-	6/26/74/74	0/4/4/4
87	CLA	BN	814	-	-	4/15/91/115	-
82	PEB	TB	201	1	-	8/26/74/74	0/4/4/4
82	PEB	hB	301	76,2	-	10/26/74/74	0/4/4/4
82	PEB	pK	202	2	-	11/26/74/74	0/4/4/4
88	LHG	l6	101	26,16	-	18/53/53/53	-
82	PEB	dF	202	2	-	14/26/74/74	0/4/4/4
82	PEB	CF	201	1	-	6/26/74/74	0/4/4/4
82	PEB	A4	305	3	-	11/26/74/74	0/4/4/4
87	CLA	KN	105	40,49	-	11/20/96/115	-
92	LMG	j6	102	18,24	-	10/28/48/70	0/1/1/1
82	PEB	lF	201	2	-	11/26/74/74	0/4/4/4
82	PEB	YG	202	2	-	12/26/74/74	0/4/4/4
87	CLA	AN	820	-	-	12/39/115/115	-
87	CLA	b6	611	-	-	19/39/115/115	-
83	PUB	yF	302	14	-	3/26/74/74	0/4/4/4
95	DGD	C6	521	-	-	14/51/91/95	0/2/2/2
82	PEB	vK	202	2	-	9/26/74/74	0/4/4/4
82	PEB	jH	201	1	-	9/26/74/74	0/4/4/4
87	CLA	4N	603	-	-	5/15/91/115	-
82	PEB	GF	203	1	-	9/26/74/74	0/4/4/4
82	PEB	gF	203	1,2	-	9/26/74/74	0/4/4/4
87	CLA	42	601	60	-	8/15/91/115	-
84	CYC	FG	1001	10	-	7/26/74/74	0/4/4/4
82	PEB	FH	1002	10	-	11/26/74/74	0/4/4/4
87	CLA	22	612	58	-	7/15/91/115	-
95	DGD	cL	520	-	-	11/37/77/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	hH	201	1	-	11/26/74/74	0/4/4/4
87	CLA	B2	819	41	-	8/15/91/115	-
84	CYC	GG	1001	10,9	-	9/26/74/74	0/4/4/4
82	PEB	BA	202	2	-	8/26/74/74	0/4/4/4
82	PEB	oF	202	1	-	10/26/74/74	0/4/4/4
91	PHO	AL	410	-	3/3/17/22	14/37/103/103	0/5/6/6
82	PEB	KF	202	1	-	4/26/74/74	0/4/4/4
82	PEB	NP	201	2	-	8/26/74/74	0/4/4/4
94	PL9	aL	601	15	-	10/53/73/73	0/1/1/1
87	CLA	b6	618	-	-	19/39/115/115	-
82	PEB	TE	201	2	-	3/26/74/74	0/4/4/4
83	PUB	AO	303	3	-	6/26/74/74	0/4/4/4
83	PUB	NQ	201	1,3	-	1/26/74/74	0/4/4/4
82	PEB	SH	202	1	-	9/26/74/74	0/4/4/4
82	PEB	s8	202	2	-	8/26/74/74	0/4/4/4
87	CLA	DL	406	-	-	18/39/115/115	-
82	PEB	ZG	201	1,2	-	7/26/74/74	0/4/4/4
82	PEB	SM	202	1	-	11/26/74/74	0/4/4/4
82	PEB	dF	201	2	-	9/26/74/74	0/4/4/4
82	PEB	c4	202	2	-	11/26/74/74	0/4/4/4
82	PEB	YD	202	2	-	8/26/74/74	0/4/4/4
82	PEB	LA	203	2	-	10/26/74/74	0/4/4/4
87	CLA	BL	622	16	-	9/39/115/115	-
85	BCR	FN	204	-	-	6/29/63/63	0/2/2/2
82	PEB	Q1	201	1,2	-	9/26/74/74	0/4/4/4
82	PEB	KA	201	1	-	7/26/74/74	0/4/4/4
82	PEB	R4	202	2	-	10/26/74/74	0/4/4/4
87	CLA	B2	805	41	-	18/39/115/115	-
82	PEB	EJ	202	1	-	5/26/74/74	0/4/4/4
87	CLA	5N	604	61	-	6/12/88/115	-
82	PEB	UF	202	1	-	10/26/74/74	0/4/4/4
82	PEB	CI	201	1	-	9/26/74/74	0/4/4/4
87	CLA	cL	510	-	-	23/39/115/115	-
84	CYC	HE	1001	10	-	9/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	18	202	2	-	6/26/74/74	0/4/4/4
85	BCR	A2	846	-	-	10/29/63/63	0/2/2/2
82	PEB	DH	1002	10	-	11/26/74/74	0/4/4/4
82	PEB	vC	201	1	-	10/26/74/74	0/4/4/4
85	BCR	K2	105	-	-	8/29/63/63	0/2/2/2
82	PEB	dE	202	1,2	-	6/26/74/74	0/4/4/4
82	PEB	GI	201	1,2	-	10/26/74/74	0/4/4/4
82	PEB	A1	301	3	-	7/26/74/74	0/4/4/4
82	PEB	PM	201	2	-	10/26/74/74	0/4/4/4
82	PEB	VQ	201	1	-	12/26/74/74	0/4/4/4
87	CLA	6N	613	62	-	6/15/91/115	-
82	PEB	hK	201	2	-	8/26/74/74	0/4/4/4
82	PEB	NM	202	2	-	10/26/74/74	0/4/4/4
82	PEB	jM	202	1	-	12/26/74/74	0/4/4/4
82	PEB	VD	201	1	-	12/26/74/74	0/4/4/4
82	PEB	KK	203	1	-	8/26/74/74	0/4/4/4
82	PEB	WB	402	6,2	-	6/26/74/74	0/4/4/4
82	PEB	L5	201	74,2	-	10/26/74/74	0/4/4/4
87	CLA	BN	808	-	-	11/39/115/115	-
82	PEB	JQ	201	1	-	12/26/74/74	0/4/4/4
87	CLA	6N	601	62	-	7/15/91/115	-
82	PEB	CJ	201	1	-	4/26/74/74	0/4/4/4
82	PEB	P1	201	11,2	-	6/26/74/74	0/4/4/4
82	PEB	D9	202	2	-	9/26/74/74	0/4/4/4
82	PEB	AO	301	3	-	7/26/74/74	0/4/4/4
82	PEB	l1	201	1,2	-	9/26/74/74	0/4/4/4
82	PEB	H7	201	2	-	5/26/74/74	0/4/4/4
82	PEB	f1	201	1	-	9/26/74/74	0/4/4/4
82	PEB	eH	203	1,2	-	7/26/74/74	0/4/4/4
82	PEB	U1	201	1,2	-	9/26/74/74	0/4/4/4
83	PUB	QJ	201	14,1	-	5/26/74/74	0/4/4/4
88	LHG	C6	505	-	-	14/41/41/53	-
82	PEB	LQ	203	1	-	12/26/74/74	0/4/4/4
82	PEB	NB	201	2	-	6/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	v8	202	1	-	15/26/74/74	0/4/4/4
82	PEB	WG	201	1	-	7/26/74/74	0/4/4/4
87	CLA	B2	832	-	-	12/39/115/115	-
87	CLA	BL	621	-	-	15/39/115/115	-
82	PEB	DK	203	2	-	12/26/74/74	0/4/4/4
82	PEB	BP	202	2	-	6/26/74/74	0/4/4/4
82	PEB	wK	303	13	-	7/26/74/74	0/4/4/4
82	PEB	JP	201	2	-	6/26/74/74	0/4/4/4
87	CLA	2N	310	58	-	5/10/86/115	-
82	PEB	mH	202	2	-	10/26/74/74	0/4/4/4
82	PEB	wK	302	13	-	10/26/74/74	0/4/4/4
82	PEB	hJ	203	1	-	14/26/74/74	0/4/4/4
82	PEB	IQ	202	2	-	7/26/74/74	0/4/4/4
84	CYC	P3	1001	68	-	8/26/74/74	0/4/4/4
87	CLA	cL	511	17	-	13/39/115/115	-
87	CLA	3N	306	-	-	8/15/91/115	-
85	BCR	BN	840	41	-	7/29/63/63	0/2/2/2
87	CLA	BN	801	-	-	17/39/115/115	-
82	PEB	WI	202	1,2	-	9/26/74/74	0/4/4/4
84	CYC	j3	1001	73,69	-	4/26/74/74	0/4/4/4
94	PL9	DL	401	18,26	-	12/53/73/73	0/1/1/1
82	PEB	u8	203	2	-	2/26/74/74	0/4/4/4
87	CLA	HL	102	22	-	15/39/115/115	-
88	LHG	A2	844	-	-	17/44/44/53	-
82	PEB	MP	202	1	-	9/26/74/74	0/4/4/4
82	PEB	oF	203	1	-	15/26/74/74	0/4/4/4
87	CLA	d6	401	18	-	17/39/115/115	-
82	PEB	JD	201	1	-	12/26/74/74	0/4/4/4
87	CLA	A2	810	40	-	23/39/115/115	-
82	PEB	eB	202	2	-	5/26/74/74	0/4/4/4
87	CLA	72	607	63	-	9/21/97/115	-
83	PUB	yF	303	14	-	4/26/74/74	0/4/4/4
82	PEB	F9	203	2	-	9/26/74/74	0/4/4/4
82	PEB	sK	202	1	-	10/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	kO	201	2	-	8/26/74/74	0/4/4/4
82	PEB	KI	202	1	-	9/26/74/74	0/4/4/4
82	PEB	L5	203	2	-	12/26/74/74	0/4/4/4
84	CYC	G3	1001	68	-	8/26/74/74	0/4/4/4
82	PEB	RB	202	2	-	11/26/74/74	0/4/4/4
82	PEB	TI	201	1,2	-	10/26/74/74	0/4/4/4
82	PEB	FA	202	2	-	10/26/74/74	0/4/4/4
82	PEB	DI	201	12,2	-	6/26/74/74	0/4/4/4
82	PEB	W5	203	2	-	12/26/74/74	0/4/4/4
87	CLA	ON	201	-	-	7/10/86/115	-
82	PEB	I7	202	1	-	11/26/74/74	0/4/4/4
82	PEB	kJ	201	2	-	9/26/74/74	0/4/4/4
82	PEB	SI	202	2	-	9/26/74/74	0/4/4/4
82	PEB	VE	201	2	-	8/26/74/74	0/4/4/4
82	PEB	ZG	202	1	-	9/26/74/74	0/4/4/4
82	PEB	M9	305	74	-	10/26/74/74	0/4/4/4
87	CLA	K2	103	-	-	5/15/91/115	-
87	CLA	A2	806	-	-	9/27/103/115	-
82	PEB	IF	202	1	-	15/26/74/74	0/4/4/4
82	PEB	mH	201	2	-	8/26/74/74	0/4/4/4
82	PEB	W1	203	1,2	-	8/26/74/74	0/4/4/4
87	CLA	a6	607	15	-	13/39/115/115	-
82	PEB	h1	202	1	-	11/26/74/74	0/4/4/4
87	CLA	AN	841	-	-	14/39/115/115	-
85	BCR	cL	518	-	-	4/29/63/63	0/2/2/2
87	CLA	c6	615	-	-	10/27/103/115	-
92	LMG	x6	601	37	-	8/45/65/70	0/1/1/1
82	PEB	W9	203	2	-	6/26/74/74	0/4/4/4
87	CLA	BN	825	41	-	20/39/115/115	-
87	CLA	AN	852	59,40	-	8/15/91/115	-
87	CLA	62	306	62	-	8/15/91/115	-
88	LHG	M6	101	-	-	13/43/43/53	-
82	PEB	pC	202	1	-	16/26/74/74	0/4/4/4
87	CLA	BL	603	-	-	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	BD	203	1,2	-	12/26/74/74	0/4/4/4
82	PEB	B5	201	74,2,82	-	11/26/74/74	0/4/4/4
82	PEB	B7	201	2,82	-	8/26/74/74	0/4/4/4
88	LHG	A2	843	40	-	16/53/53/53	-
82	PEB	MP	201	1	-	5/26/74/74	0/4/4/4
83	PUB	BM	302	14	-	9/26/74/74	0/4/4/4
82	PEB	IP	202	1	-	11/26/74/74	0/4/4/4
101	FES	NN	101	-	-	-	0/1/1/1
82	PEB	RK	201	2	-	8/26/74/74	0/4/4/4
82	PEB	gO	203	2	-	11/26/74/74	0/4/4/4
85	BCR	B6	601	-	-	0/29/63/63	0/2/2/2
82	PEB	YQ	201	2,82	-	7/26/74/74	0/4/4/4
82	PEB	L7	202	2	-	9/26/74/74	0/4/4/4
84	CYC	DH	1003	10,9	-	10/26/74/74	0/4/4/4
85	BCR	L2	201	-	-	13/29/63/63	0/2/2/2
87	CLA	c6	612	17	-	19/39/115/115	-
82	PEB	F9	202	2	-	8/26/74/74	0/4/4/4
82	PEB	lK	201	2	-	11/26/74/74	0/4/4/4
82	PEB	AJ	301	13	-	12/26/74/74	0/4/4/4
82	PEB	lJ	203	1	-	11/26/74/74	0/4/4/4
82	PEB	fG	201	1	-	10/26/74/74	0/4/4/4
82	PEB	R5	201	1	-	11/26/74/74	0/4/4/4
87	CLA	BN	812	-	-	7/27/103/115	-
82	PEB	IJ	202	1	-	7/26/74/74	0/4/4/4
87	CLA	AN	818	-	-	8/15/91/115	-
82	PEB	UH	203	1	-	9/26/74/74	0/4/4/4
87	CLA	B6	606	-	-	13/39/115/115	-
82	PEB	AI	202	1	-	10/26/74/74	0/4/4/4
82	PEB	JK	201	2	-	8/26/74/74	0/4/4/4
87	CLA	7N	607	63	-	9/21/97/115	-
82	PEB	d1	202	1	-	10/26/74/74	0/4/4/4
82	PEB	EI	202	1	-	10/26/74/74	0/4/4/4
88	LHG	DL	407	18	-	16/53/53/53	-
82	PEB	C5	201	1	-	11/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	aM	204	1,2	-	9/26/74/74	0/4/4/4
83	PUB	Y7	302	3	-	3/26/74/74	0/4/4/4
82	PEB	XF	203	2	-	11/26/74/74	0/4/4/4
82	PEB	nK	201	2	-	7/26/74/74	0/4/4/4
82	PEB	ZH	202	1	-	9/26/74/74	0/4/4/4
82	PEB	DQ	201	1,2	-	11/26/74/74	0/4/4/4
82	PEB	dM	203	1	-	13/26/74/74	0/4/4/4
82	PEB	wC	203	2	-	6/26/74/74	0/4/4/4
82	PEB	xC	202	1	-	15/26/74/74	0/4/4/4
87	CLA	3N	313	-	-	8/15/91/115	-
82	PEB	HP	202	2	-	6/26/74/74	0/4/4/4
82	PEB	E7	202	1	-	11/26/74/74	0/4/4/4
84	CYC	JH	1003	10,9	-	11/26/74/74	0/4/4/4
96	HEM	f6	101	19,20	-	2/14/54/54	-
82	PEB	MP	203	1,2	-	13/26/74/74	0/4/4/4
85	BCR	LN	205	50	-	11/29/63/63	0/2/2/2
82	PEB	P5	201	1	-	11/26/74/74	0/4/4/4
82	PEB	GE	1002	10,9	-	9/26/74/74	0/4/4/4
82	PEB	TM	201	2	-	7/26/74/74	0/4/4/4
82	PEB	hE	203	1	-	7/26/74/74	0/4/4/4
84	CYC	H1	1001	10	-	8/26/74/74	0/4/4/4
82	PEB	P7	201	2	-	4/26/74/74	0/4/4/4
82	PEB	U9	204	1,2	-	8/26/74/74	0/4/4/4
85	BCR	k6	102	-	-	12/29/63/63	0/2/2/2
82	PEB	DE	1002	10,9	-	8/26/74/74	0/4/4/4
82	PEB	gJ	202	2	-	10/26/74/74	0/4/4/4
82	PEB	PQ	203	1	-	12/26/74/74	0/4/4/4
85	BCR	b6	603	-	-	2/29/63/63	0/2/2/2
82	PEB	dQ	401	2,77	-	12/26/74/74	0/4/4/4
82	PEB	YM	201	1,2	-	7/26/74/74	0/4/4/4
82	PEB	UH	201	1,2	-	9/26/74/74	0/4/4/4
87	CLA	42	609	60	-	5/10/86/115	-
92	LMG	BL	612	16	-	5/34/54/70	0/1/1/1
87	CLA	AN	836	-	-	7/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
91	PHO	aL	610	-	3/3/17/22	14/37/103/103	0/5/6/6
82	PEB	MK	202	1	-	10/26/74/74	0/4/4/4
87	CLA	b6	605	16	-	15/39/115/115	-
82	PEB	D5	202	2	-	11/26/74/74	0/4/4/4
82	PEB	R7	203	2	-	10/26/74/74	0/4/4/4
97	GOL	wL	101	-	-	2/4/4/4	-
100	3XQ	J2	104	-	-	14/24/24/24	-
82	PEB	QQ	202	2	-	11/26/74/74	0/4/4/4
87	CLA	62	309	62	-	10/21/97/115	-
82	PEB	OI	202	1,2	-	10/26/74/74	0/4/4/4
82	PEB	c1	201	2	-	7/26/74/74	0/4/4/4
82	PEB	lM	203	1	-	12/26/74/74	0/4/4/4
87	CLA	A2	811	-	-	21/39/115/115	-
87	CLA	L2	202	50	-	16/30/106/115	-
87	CLA	bL	608	-	-	10/39/115/115	-
82	PEB	QB	201	2	-	15/26/74/74	0/4/4/4
87	CLA	BN	835	-	-	22/39/115/115	-
82	PEB	J9	202	2	-	8/26/74/74	0/4/4/4
82	PEB	RI	201	1	-	9/26/74/74	0/4/4/4
87	CLA	A2	803	40,50,53	-	13/24/100/115	-
92	LMG	ML	101	-	-	11/36/56/70	0/1/1/1
84	CYC	FE	1002	10	-	7/26/74/74	0/4/4/4
83	PUB	AG	302	3	-	9/26/74/74	0/4/4/4
82	PEB	VE	202	2	-	10/26/74/74	0/4/4/4
82	PEB	OJ	203	1,2	-	7/26/74/74	0/4/4/4
82	PEB	M7	202	1	-	13/26/74/74	0/4/4/4
82	PEB	LH	1003	10	-	8/26/74/74	0/4/4/4
82	PEB	y8	201	2	-	16/26/74/74	0/4/4/4
82	PEB	OB	201	2,5	-	11/26/74/74	0/4/4/4
82	PEB	FP	201	56,2	-	7/26/74/74	0/4/4/4
82	PEB	FI	201	2	-	12/26/74/74	0/4/4/4
82	PEB	KB	303	2	-	12/26/74/74	0/4/4/4
82	PEB	OG	201	1	-	9/26/74/74	0/4/4/4
82	PEB	cF	203	1,2	-	6/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	CLA	62	302	62	-	7/15/91/115	-
82	PEB	AK	202	1	-	11/26/74/74	0/4/4/4
82	PEB	PG	201	11,2	-	6/26/74/74	0/4/4/4
82	PEB	XK	201	2	-	9/26/74/74	0/4/4/4
87	CLA	AN	815	-	-	20/39/115/115	-
92	LMG	b6	620	16	-	12/34/54/70	0/1/1/1
82	PEB	fJ	202	1	-	10/26/74/74	0/4/4/4
87	CLA	b6	616	-	-	12/39/115/115	-
83	PUB	xF	306	13	-	6/26/74/74	0/4/4/4
87	CLA	CL	515	-	-	8/39/115/115	-
92	LMG	m6	101	85	-	16/36/56/70	0/1/1/1
82	PEB	AP	203	1,2	-	12/26/74/74	0/4/4/4
82	PEB	V9	201	1	-	7/26/74/74	0/4/4/4
82	PEB	SJ	203	1,2	-	9/26/74/74	0/4/4/4
82	PEB	EF	202	1	-	10/26/74/74	0/4/4/4
82	PEB	eE	201	2	-	9/26/74/74	0/4/4/4
82	PEB	Z9	304	74	-	10/26/74/74	0/4/4/4
88	LHG	mL	102	-	-	17/43/43/53	-
87	CLA	52	601	61	-	11/15/91/115	-
87	CLA	A2	840	-	-	14/39/115/115	-
85	BCR	bL	602	-	-	1/29/63/63	0/2/2/2
87	CLA	4N	610	-	-	7/12/88/115	-
83	PUB	AH	304	3	-	15/26/74/74	0/4/4/4
82	PEB	QB	203	2	-	9/26/74/74	0/4/4/4
82	PEB	cE	202	2	-	10/26/74/74	0/4/4/4
82	PEB	B5	203	2	-	12/26/74/74	0/4/4/4
82	PEB	B7	203	2	-	12/26/74/74	0/4/4/4
84	CYC	c3	1001	68	-	8/26/74/74	0/4/4/4
87	CLA	12	603	-	-	4/15/91/115	-
82	PEB	fE	201	1	-	10/26/74/74	0/4/4/4
82	PEB	eG	203	2	-	13/26/74/74	0/4/4/4
87	CLA	BN	828	41	-	7/15/91/115	-
82	PEB	qC	201	2	-	5/26/74/74	0/4/4/4
87	CLA	12	601	57	-	12/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	aM	201	13,1	-	10/26/74/74	0/4/4/4
82	PEB	iO	203	2	-	10/26/74/74	0/4/4/4
82	PEB	VG	202	2	-	10/26/74/74	0/4/4/4
82	PEB	VI	203	1,2	-	10/26/74/74	0/4/4/4
87	CLA	b6	610	-	-	17/39/115/115	-
87	CLA	AN	849	40	-	11/39/115/115	-
82	PEB	J4	1002	10	-	11/26/74/74	0/4/4/4
96	HEM	G2	201	46	-	6/14/54/54	-
87	CLA	A2	835	-	-	16/39/115/115	-
82	PEB	lE	203	1	-	7/26/74/74	0/4/4/4
82	PEB	fJ	201	1	-	5/26/74/74	0/4/4/4
87	CLA	6N	607	62	-	5/15/91/115	-
82	PEB	QO	202	1	-	8/26/74/74	0/4/4/4
87	CLA	4N	607	60	-	8/15/91/115	-
82	PEB	DB	201	2	-	8/26/74/74	0/4/4/4
102	BGC	3N	302	-	-	0/2/19/22	0/1/1/1
82	PEB	S5	202	2	-	11/26/74/74	0/4/4/4
82	PEB	1C	203	2	-	6/26/74/74	0/4/4/4
85	BCR	F2	203	-	-	6/29/63/63	0/2/2/2
87	CLA	72	605	-	-	8/15/91/115	-
87	CLA	5N	607	61	-	8/21/97/115	-
87	CLA	3N	309	59	-	14/21/97/115	-
82	PEB	RD	202	1	-	10/26/74/74	0/4/4/4
82	PEB	dK	202	2	-	14/26/74/74	0/4/4/4
84	CYC	EO	1001	9	-	10/26/74/74	0/4/4/4
82	PEB	dH	202	1	-	10/26/74/74	0/4/4/4
92	LMG	qL	301	-	-	10/38/58/70	0/1/1/1
82	PEB	KJ	202	1	-	16/26/74/74	0/4/4/4
82	PEB	c1	202	2	-	11/26/74/74	0/4/4/4
87	CLA	72	601	63	-	12/15/91/115	-
82	PEB	YK	203	1,2	-	8/26/74/74	0/4/4/4
82	PEB	J9	203	2	-	9/26/74/74	0/4/4/4
87	CLA	BN	816	41	-	8/27/103/115	-
82	PEB	aJ	203	1	-	12/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	R1	201	2	-	7/26/74/74	0/4/4/4
82	PEB	sF	202	1	-	10/26/74/74	0/4/4/4
85	BCR	bL	601	87	-	8/29/63/63	0/2/2/2
82	PEB	uF	202	1	-	10/26/74/74	0/4/4/4
82	PEB	QF	201	1	-	7/26/74/74	0/4/4/4
87	CLA	4N	601	60	-	8/15/91/115	-
82	PEB	Z1	202	1	-	9/26/74/74	0/4/4/4
82	PEB	g4	201	2	-	4/26/74/74	0/4/4/4
82	PEB	f4	202	1	-	11/26/74/74	0/4/4/4
82	PEB	PK	201	2	-	7/26/74/74	0/4/4/4
85	BCR	hL	102	-	-	3/29/63/63	0/2/2/2
101	FES	N2	101	-	-	-	0/1/1/1
82	PEB	TI	203	1	-	10/26/74/74	0/4/4/4
82	PEB	gG	202	2	-	11/26/74/74	0/4/4/4
84	CYC	DG	1001	10	-	13/26/74/74	0/4/4/4
87	CLA	5N	601	61	-	11/15/91/115	-
82	PEB	WF	202	1	-	8/26/74/74	0/4/4/4
82	PEB	Y7	301	3	-	18/26/74/74	0/4/4/4
82	PEB	kE	201	3,2	-	9/26/74/74	0/4/4/4
87	CLA	2N	302	58	-	7/15/91/115	-
82	PEB	zK	501	78,2	-	7/26/74/74	0/4/4/4
87	CLA	BL	605	-	-	16/39/115/115	-
82	PEB	fJ	203	1,2	-	8/26/74/74	0/4/4/4
82	PEB	LK	202	2	-	14/26/74/74	0/4/4/4
84	CYC	i3	1001	68	-	8/26/74/74	0/4/4/4
82	PEB	lE	202	-	-	13/26/74/74	0/4/4/4
82	PEB	TA	201	2	-	5/26/74/74	0/4/4/4
82	PEB	cE	201	2	-	6/26/74/74	0/4/4/4
82	PEB	KP	201	1,2	-	12/26/74/74	0/4/4/4
82	PEB	UM	201	1,2	-	6/26/74/74	0/4/4/4
87	CLA	F2	201	45	-	10/15/91/115	-
98	PQN	A2	842	-	-	6/23/43/43	0/2/2/2
87	CLA	3N	308	59	-	5/15/91/115	-
82	PEB	u8	202	2	-	7/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	CLA	22	605	58,41	-	11/25/101/115	-
87	CLA	32	309	59	-	14/21/97/115	-
82	PEB	WB	401	6,2	-	10/26/74/74	0/4/4/4
94	PL9	dL	406	18,26	-	13/53/73/73	0/1/1/1
82	PEB	DA	203	2	-	11/26/74/74	0/4/4/4
82	PEB	C5	202	1	-	11/26/74/74	0/4/4/4
87	CLA	JN	101	48	-	5/12/88/115	-
85	BCR	AN	848	-	-	16/29/63/63	0/2/2/2
87	CLA	32	303	59,87	-	8/15/91/115	-
87	CLA	C6	520	-	-	15/39/115/115	-
83	PUB	AD	302	1,3	-	8/26/74/74	0/4/4/4
87	CLA	K2	101	-	-	12/39/115/115	-
82	PEB	AB	501	2,4	-	10/26/74/74	0/4/4/4
82	PEB	JA	203	2	-	16/26/74/74	0/4/4/4
82	PEB	gM	202	2	-	10/26/74/74	0/4/4/4
87	CLA	B6	613	-	-	17/39/115/115	-
82	PEB	eM	201	13,2	-	6/26/74/74	0/4/4/4
87	CLA	B6	605	16	-	16/39/115/115	-
82	PEB	YB	201	2	-	5/26/74/74	0/4/4/4
84	CYC	DE	1001	10	-	13/26/74/74	0/4/4/4
82	PEB	QM	202	1,2	-	7/26/74/74	0/4/4/4
82	PEB	m1	201	2	-	8/26/74/74	0/4/4/4
85	BCR	CL	502	17	-	5/29/63/63	0/2/2/2
82	PEB	dD	401	2,77	-	12/26/74/74	0/4/4/4
82	PEB	YP	501	2	-	4/26/74/74	0/4/4/4
82	PEB	LK	201	2	-	9/26/74/74	0/4/4/4
82	PEB	H9	202	2	-	8/26/74/74	0/4/4/4
82	PEB	cK	201	1	-	10/26/74/74	0/4/4/4
87	CLA	O2	203	53	-	10/15/91/115	-
85	BCR	FL	101	20	-	8/29/63/63	0/2/2/2
87	CLA	7N	608	63	-	6/10/86/115	-
82	PEB	dH	201	1,2	-	5/26/74/74	0/4/4/4
82	PEB	bP	501	56,2	-	10/26/74/74	0/4/4/4
88	LHG	AL	406	-	-	22/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	F7	202	2	-	10/26/74/74	0/4/4/4
87	CLA	K2	104	-	-	4/12/88/115	-
82	PEB	VM	202	2	-	9/26/74/74	0/4/4/4
82	PEB	GA	202	1	-	12/26/74/74	0/4/4/4
92	LMG	m6	103	-	-	10/36/56/70	0/1/1/1
82	PEB	S5	203	2	-	12/26/74/74	0/4/4/4
82	PEB	SG	201	1	-	10/26/74/74	0/4/4/4
82	PEB	PI	201	1	-	9/26/74/74	0/4/4/4
82	PEB	fO	201	1	-	11/26/74/74	0/4/4/4
82	PEB	BI	201	2	-	9/26/74/74	0/4/4/4
82	PEB	hM	203	1	-	11/26/74/74	0/4/4/4
83	PUB	wF	304	13	-	7/26/74/74	0/4/4/4
82	PEB	UD	202	2	-	7/26/74/74	0/4/4/4
82	PEB	K5	202	1	-	11/26/74/74	0/4/4/4
85	BCR	cL	503	-	-	2/29/63/63	0/2/2/2
82	PEB	QK	203	1,2	-	8/26/74/74	0/4/4/4
87	CLA	AN	827	-	-	9/27/103/115	-
87	CLA	bL	622	-	-	15/39/115/115	-
82	PEB	lF	203	1,2	-	10/26/74/74	0/4/4/4
82	PEB	aF	202	1	-	9/26/74/74	0/4/4/4
82	PEB	R4	201	11,2	-	3/26/74/74	0/4/4/4
82	PEB	JJ	202	2	-	8/26/74/74	0/4/4/4
82	PEB	MM	201	1,2	-	7/26/74/74	0/4/4/4
82	PEB	y8	203	2	-	9/26/74/74	0/4/4/4
87	CLA	22	604	-	-	3/12/88/115	-
88	LHG	dL	408	-	-	12/50/50/53	-
82	PEB	X5	201	1	-	11/26/74/74	0/4/4/4
85	BCR	HL	103	-	-	4/29/63/63	0/2/2/2
82	PEB	JQ	203	1,2	-	14/26/74/74	0/4/4/4
92	LMG	bL	624	16	-	7/34/54/70	0/1/1/1
82	PEB	KQ	201	2	-	9/26/74/74	0/4/4/4
83	PUB	AH	303	3	-	5/26/74/74	0/4/4/4
87	CLA	B2	809	-	-	11/39/115/115	-
82	PEB	XM	202	2	-	9/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
92	LMG	jL	101	18,24	-	8/28/48/70	0/1/1/1
82	PEB	F7	201	3,2	-	5/26/74/74	0/4/4/4
82	PEB	SE	201	1	-	10/26/74/74	0/4/4/4
82	PEB	BD	201	1	-	9/26/74/74	0/4/4/4
82	PEB	OM	201	1	-	7/26/74/74	0/4/4/4
82	PEB	AD	304	3,82	-	11/26/74/74	0/4/4/4
82	PEB	gO	201	2	-	4/26/74/74	0/4/4/4
82	PEB	a4	201	2	-	2/26/74/74	0/4/4/4
82	PEB	UJ	203	1	-	9/26/74/74	0/4/4/4
82	PEB	W5	201	2	-	7/26/74/74	0/4/4/4
82	PEB	H1	1002	10	-	8/26/74/74	0/4/4/4
82	PEB	Z4	202	1	-	9/26/74/74	0/4/4/4
82	PEB	gM	201	2	-	8/26/74/74	0/4/4/4
87	CLA	AN	822	40	-	8/15/91/115	-
85	BCR	L2	205	50	-	11/29/63/63	0/2/2/2
82	PEB	yC	201	2	-	12/26/74/74	0/4/4/4
82	PEB	fK	202	2	-	13/26/74/74	0/4/4/4
85	BCR	AL	401	-	-	5/29/63/63	0/2/2/2
82	PEB	BI	203	2	-	7/26/74/74	0/4/4/4
82	PEB	LE	1002	10,9	-	11/26/74/74	0/4/4/4
82	PEB	EK	202	1	-	10/26/74/74	0/4/4/4
82	PEB	mF	201	1	-	6/26/74/74	0/4/4/4
82	PEB	WA	201	1	-	7/26/74/74	0/4/4/4
87	CLA	42	605	60	-	9/15/91/115	-
84	CYC	K4	1001	9	-	9/26/74/74	0/4/4/4
82	PEB	HK	202	2	-	12/26/74/74	0/4/4/4
83	PUB	KA	203	1,3	-	6/26/74/74	0/4/4/4
82	PEB	jM	201	1	-	10/26/74/74	0/4/4/4
82	PEB	Z5	304	74,82	-	8/26/74/74	0/4/4/4
82	PEB	OK	201	1,2	-	7/26/74/74	0/4/4/4
82	PEB	XD	201	1,2	-	9/26/74/74	0/4/4/4
82	PEB	KB	302	2,5	-	7/26/74/74	0/4/4/4
82	PEB	ZM	202	2	-	10/26/74/74	0/4/4/4
82	PEB	QM	203	1	-	10/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	SA	202	1	-	8/26/74/74	0/4/4/4
82	PEB	AE	301	3	-	10/26/74/74	0/4/4/4
87	CLA	12	610	57	-	8/15/91/115	-
87	CLA	52	609	61	-	6/12/88/115	-
82	PEB	IJ	201	1,2	-	6/26/74/74	0/4/4/4
84	CYC	73	1001	73,69	-	4/26/74/74	0/4/4/4
82	PEB	DF	202	1,2	-	12/26/74/74	0/4/4/4
82	PEB	DK	202	1,2	-	12/26/74/74	0/4/4/4
82	PEB	RQ	201	1	-	11/26/74/74	0/4/4/4
82	PEB	UE	201	1,2	-	5/26/74/74	0/4/4/4
87	CLA	8N	306	64	-	9/15/91/115	-
84	CYC	B3	1001	69	-	4/26/74/74	0/4/4/4
82	PEB	RA	201	2	-	5/26/74/74	0/4/4/4
82	PEB	QI	201	2	-	6/26/74/74	0/4/4/4
82	PEB	RD	203	1,2	-	10/26/74/74	0/4/4/4
87	CLA	F2	205	45	-	19/39/115/115	-
95	DGD	O6	301	-	-	7/29/69/95	0/2/2/2
82	PEB	T1	202	2	-	15/26/74/74	0/4/4/4
82	PEB	fK	201	13,2	-	10/26/74/74	0/4/4/4
87	CLA	1N	603	-	-	4/15/91/115	-
82	PEB	TG	201	2	-	3/26/74/74	0/4/4/4
85	BCR	B2	841	41	-	4/29/63/63	0/2/2/2
87	CLA	DL	403	18	-	10/39/115/115	-
82	PEB	eK	203	1	-	8/26/74/74	0/4/4/4
87	CLA	A6	402	15	-	22/39/115/115	-
87	CLA	D6	402	18	-	17/39/115/115	-
87	CLA	8N	304	64	-	8/15/91/115	-
82	PEB	ED	202	2	-	7/26/74/74	0/4/4/4
82	PEB	PQ	201	1,2	-	8/26/74/74	0/4/4/4
82	PEB	kK	203	1,2	-	9/26/74/74	0/4/4/4
82	PEB	SO	201	1	-	10/26/74/74	0/4/4/4
83	PUB	A1	304	3	-	15/26/74/74	0/4/4/4
82	PEB	pF	202	2	-	11/26/74/74	0/4/4/4
92	LMG	aL	611	-	-	9/37/57/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	LM	202	2	-	10/26/74/74	0/4/4/4
82	PEB	gK	202	1	-	11/26/74/74	0/4/4/4
82	PEB	HJ	201	2	-	6/26/74/74	0/4/4/4
82	PEB	PA	203	2	-	8/26/74/74	0/4/4/4
82	PEB	SA	201	1	-	4/26/74/74	0/4/4/4
87	CLA	AN	830	-	-	14/39/115/115	-
84	CYC	E3	1001	68	-	8/26/74/74	0/4/4/4
82	PEB	HA	202	2	-	8/26/74/74	0/4/4/4
82	PEB	fH	203	1,2	-	12/26/74/74	0/4/4/4
82	PEB	NQ	204	1,2	-	13/26/74/74	0/4/4/4
82	PEB	DK	201	2	-	7/26/74/74	0/4/4/4
82	PEB	RO	203	2	-	7/26/74/74	0/4/4/4
82	PEB	z8	202	1	-	11/26/74/74	0/4/4/4
84	CYC	ME	1001	10,9	-	9/26/74/74	0/4/4/4
87	CLA	A2	814	40	-	10/26/102/115	-
82	PEB	B9	202	2	-	8/26/74/74	0/4/4/4
87	CLA	D6	405	-	-	13/39/115/115	-
82	PEB	iK	202	1	-	11/26/74/74	0/4/4/4
82	PEB	dH	203	1	-	10/26/74/74	0/4/4/4
82	PEB	W1	202	1	-	9/26/74/74	0/4/4/4
82	PEB	d4	202	1	-	8/26/74/74	0/4/4/4
82	PEB	YM	202	1	-	8/26/74/74	0/4/4/4
87	CLA	42	604	60	-	7/12/88/115	-
82	PEB	cB	401	6,2	-	6/26/74/74	0/4/4/4
82	PEB	iO	202	2	-	8/26/74/74	0/4/4/4
82	PEB	mG	201	2	-	6/26/74/74	0/4/4/4
82	PEB	T5	202	1	-	11/26/74/74	0/4/4/4
82	PEB	gH	201	2	-	9/26/74/74	0/4/4/4
82	PEB	ZJ	202	2	-	9/26/74/74	0/4/4/4
82	PEB	Y4	202	2	-	6/26/74/74	0/4/4/4
82	PEB	VH	202	2	-	7/26/74/74	0/4/4/4
82	PEB	AK	201	1	-	9/26/74/74	0/4/4/4
87	CLA	BL	623	16	-	11/39/115/115	-
87	CLA	C6	513	-	-	21/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	VA	203	2	-	7/26/74/74	0/4/4/4
82	PEB	hG	203	1	-	7/26/74/74	0/4/4/4
87	CLA	42	602	60	-	16/39/115/115	-
82	PEB	CA	202	1	-	13/26/74/74	0/4/4/4
87	CLA	22	609	58	-	11/21/97/115	-
82	PEB	e4	202	2	-	10/26/74/74	0/4/4/4
82	PEB	hM	202	1	-	11/26/74/74	0/4/4/4
87	CLA	A2	817	-	-	7/12/88/115	-
82	PEB	WQ	202	2	-	8/26/74/74	0/4/4/4
84	CYC	IO	1001	9	-	11/26/74/74	0/4/4/4
87	CLA	32	307	59	-	5/15/91/115	-
87	CLA	5N	611	61	-	10/15/91/115	-
82	PEB	cK	202	1	-	13/26/74/74	0/4/4/4
82	PEB	gH	202	2	-	5/26/74/74	0/4/4/4
82	PEB	L7	201	2,82	-	7/26/74/74	0/4/4/4
87	CLA	BL	608	-	-	17/39/115/115	-
82	PEB	YE	201	2	-	11/26/74/74	0/4/4/4
82	PEB	dE	201	1,3	-	11/26/74/74	0/4/4/4
92	LMG	XL	601	37	-	15/45/65/70	0/1/1/1
82	PEB	fE	203	1,2	-	9/26/74/74	0/4/4/4
82	PEB	b1	201	1	-	10/26/74/74	0/4/4/4
82	PEB	MA	201	1	-	8/26/74/74	0/4/4/4
95	DGD	C6	503	-	-	13/31/71/95	0/2/2/2
84	CYC	D4	1001	10	-	10/26/74/74	0/4/4/4
87	CLA	AN	817	-	-	7/12/88/115	-
82	PEB	Z5	301	74	-	8/26/74/74	0/4/4/4
82	PEB	SD	202	2	-	10/26/74/74	0/4/4/4
82	PEB	r8	202	1	-	16/26/74/74	0/4/4/4
84	CYC	HO	1001	10	-	8/26/74/74	0/4/4/4
82	PEB	y8	202	2	-	9/26/74/74	0/4/4/4
87	CLA	82	303	64	-	8/15/91/115	-
87	CLA	7N	603	-	-	7/15/91/115	-
82	PEB	X7	201	2,75	-	5/26/74/74	0/4/4/4
87	CLA	B6	604	-	-	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	OF	201	1,2	-	7/26/74/74	0/4/4/4
82	PEB	Q1	202	1	-	12/26/74/74	0/4/4/4
82	PEB	YF	202	1	-	10/26/74/74	0/4/4/4
82	PEB	DA	201	3,2	-	11/26/74/74	0/4/4/4
82	PEB	QP	203	1,2	-	12/26/74/74	0/4/4/4
87	CLA	LN	206	50	-	5/29/105/115	-
82	PEB	J5	202	2	-	11/26/74/74	0/4/4/4
82	PEB	RE	202	2	-	12/26/74/74	0/4/4/4
82	PEB	F1	1002	10	-	11/26/74/74	0/4/4/4
82	PEB	XF	202	2	-	6/26/74/74	0/4/4/4
82	PEB	XJ	201	2	-	5/26/74/74	0/4/4/4
82	PEB	BB	201	2	-	3/26/74/74	0/4/4/4
87	CLA	A2	820	-	-	12/39/115/115	-
95	DGD	C6	523	-	-	13/37/77/95	0/2/2/2
92	LMG	d6	409	18	-	17/49/69/70	0/1/1/1
82	PEB	Z1	203	1	-	7/26/74/74	0/4/4/4
87	CLA	C6	514	87	-	24/39/115/115	-
82	PEB	O1	201	1	-	11/26/74/74	0/4/4/4
82	PEB	YO	202	2	-	6/26/74/74	0/4/4/4
82	PEB	q8	202	2	-	9/26/74/74	0/4/4/4
82	PEB	cO	203	2	-	11/26/74/74	0/4/4/4
85	BCR	J2	102	-	-	7/29/63/63	0/2/2/2
82	PEB	HQ	202	1	-	12/26/74/74	0/4/4/4
87	CLA	6N	610	-	-	5/12/88/115	-
82	PEB	fG	203	1,2	-	9/26/74/74	0/4/4/4
84	CYC	HG	1001	10	-	9/26/74/74	0/4/4/4
87	CLA	A2	852	59,40	-	8/15/91/115	-
82	PEB	PJ	202	2	-	8/26/74/74	0/4/4/4
82	PEB	B5	202	2	-	9/26/74/74	0/4/4/4
82	PEB	gB	202	2	-	8/26/74/74	0/4/4/4
82	PEB	iJ	202	2	-	10/26/74/74	0/4/4/4
82	PEB	WJ	203	1,2	-	7/26/74/74	0/4/4/4
82	PEB	eG	202	2	-	7/26/74/74	0/4/4/4
87	CLA	3N	303	59,60	-	9/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	AH	305	3	-	12/26/74/74	0/4/4/4
82	PEB	H4	1002	10	-	8/26/74/74	0/4/4/4
92	LMG	D6	409	18	-	16/49/69/70	0/1/1/1
82	PEB	mK	202	1	-	11/26/74/74	0/4/4/4
87	CLA	3N	304	59,87	-	8/15/91/115	-
82	PEB	H7	203	2	-	12/26/74/74	0/4/4/4
82	PEB	TP	202	2	-	8/26/74/74	0/4/4/4
82	PEB	O5	203	2	-	14/26/74/74	0/4/4/4
82	PEB	hE	202	1	-	11/26/74/74	0/4/4/4
85	BCR	JN	103	40,48	-	13/29/63/63	0/2/2/2
87	CLA	A2	830	-	-	14/39/115/115	-
82	PEB	CB	202	2	-	9/26/74/74	0/4/4/4
82	PEB	CM	202	1	-	11/26/74/74	0/4/4/4
82	PEB	UA	202	1	-	10/26/74/74	0/4/4/4
82	PEB	gJ	201	2	-	9/26/74/74	0/4/4/4
87	CLA	BN	820	41	-	8/15/91/115	-
82	PEB	Y4	201	2	-	4/26/74/74	0/4/4/4
87	CLA	b6	607	-	-	15/39/115/115	-
82	PEB	MD	201	2	-	7/26/74/74	0/4/4/4
82	PEB	AF	202	1	-	11/26/74/74	0/4/4/4
82	PEB	e4	201	2	-	5/26/74/74	0/4/4/4
82	PEB	VH	201	2	-	2/26/74/74	0/4/4/4
82	PEB	KB	301	2,5	-	9/26/74/74	0/4/4/4
82	PEB	CK	202	1	-	7/26/74/74	0/4/4/4
82	PEB	iF	202	1	-	11/26/74/74	0/4/4/4
82	PEB	eA	301	1,75	-	9/26/74/74	0/4/4/4
87	CLA	RN	201	87	-	7/15/91/115	-
82	PEB	cB	403	6,2	-	6/26/74/74	0/4/4/4
82	PEB	dB	201	2	-	9/26/74/74	0/4/4/4
82	PEB	CQ	201	3,2	-	4/26/74/74	0/4/4/4
84	CYC	E1	1001	10,9	-	9/26/74/74	0/4/4/4
82	PEB	iJ	201	13,2	-	5/26/74/74	0/4/4/4
87	CLA	22	610	58	-	5/10/86/115	-
82	PEB	P7	203	2	-	8/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	GQ	201	2	-	4/26/74/74	0/4/4/4
82	PEB	ZF	201	2	-	9/26/74/74	0/4/4/4
82	PEB	CP	203	1	-	9/26/74/74	0/4/4/4
82	PEB	O4	202	1	-	6/26/74/74	0/4/4/4
82	PEB	k4	202	2	-	12/26/74/74	0/4/4/4
82	PEB	xF	302	13	-	13/26/74/74	0/4/4/4
87	CLA	BN	810	-	-	11/39/115/115	-
83	PUB	AO	302	3	-	2/26/74/74	0/4/4/4
87	CLA	4N	604	60	-	7/12/88/115	-
87	CLA	AN	803	40,50,53	-	13/24/100/115	-
95	DGD	c6	601	-	-	26/51/91/95	0/2/2/2
82	PEB	TJ	201	2	-	7/26/74/74	0/4/4/4
85	BCR	AN	845	40	-	11/29/63/63	0/2/2/2
82	PEB	TI	202	1	-	9/26/74/74	0/4/4/4
82	PEB	SM	203	1,2	-	8/26/74/74	0/4/4/4
82	PEB	LQ	201	1,2	-	9/26/74/74	0/4/4/4
87	CLA	32	304	59,87	-	15/39/115/115	-
87	CLA	A2	821	-	-	18/39/115/115	-
82	PEB	bO	202	1	-	8/26/74/74	0/4/4/4
82	PEB	HI	202	1,2	-	10/26/74/74	0/4/4/4
82	PEB	hO	201	1	-	10/26/74/74	0/4/4/4
82	PEB	UA	201	1	-	4/26/74/74	0/4/4/4
87	CLA	BN	813	-	-	28/39/115/115	-
87	CLA	72	604	63	-	7/12/88/115	-
87	CLA	3N	310	59,87	-	5/10/86/115	-
82	PEB	PA	202	2	-	7/26/74/74	0/4/4/4
82	PEB	PO	202	2	-	6/26/74/74	0/4/4/4
82	PEB	fH	202	1	-	10/26/74/74	0/4/4/4
87	CLA	L2	203	85,50,41	-	22/39/115/115	-
82	PEB	KI	201	1,2	-	10/26/74/74	0/4/4/4
87	CLA	8N	303	64	-	19/39/115/115	-
82	PEB	UP	201	1	-	4/26/74/74	0/4/4/4
84	CYC	NO	1001	10	-	13/26/74/74	0/4/4/4
82	PEB	FA	201	3,2	-	5/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	g1	202	2	-	5/26/74/74	0/4/4/4
85	BCR	K2	102	40,49	-	13/29/63/63	0/2/2/2
83	PUB	AE	302	3	-	9/26/74/74	0/4/4/4
82	PEB	OP	201	1,2	-	10/26/74/74	0/4/4/4
82	PEB	vF	202	2	-	9/26/74/74	0/4/4/4
82	PEB	kG	201	3,2	-	9/26/74/74	0/4/4/4
82	PEB	V7	201	2,75	-	11/26/74/74	0/4/4/4
88	LHG	a6	610	15	-	14/47/47/53	-
84	CYC	FO	1001	10	-	11/26/74/74	0/4/4/4
87	CLA	KN	102	-	-	5/15/91/115	-
82	PEB	W4	201	1	-	6/26/74/74	0/4/4/4
84	CYC	g3	1001	68	-	8/26/74/74	0/4/4/4
87	CLA	CL	513	17	-	16/33/109/115	-
87	CLA	82	305	64	-	9/15/91/115	-
82	PEB	DB	203	2	-	15/26/74/74	0/4/4/4
82	PEB	mO	201	2	-	9/26/74/74	0/4/4/4
82	PEB	H5	202	2	-	8/26/74/74	0/4/4/4
82	PEB	d1	203	1	-	10/26/74/74	0/4/4/4
82	PEB	lE	201	1,2	-	9/26/74/74	0/4/4/4
84	CYC	DH	1001	10	-	8/26/74/74	0/4/4/4
82	PEB	l4	202	-	-	10/26/74/74	0/4/4/4
82	PEB	XQ	203	1	-	10/26/74/74	0/4/4/4
82	PEB	EF	201	1	-	9/26/74/74	0/4/4/4
84	CYC	JO	1001	10	-	11/26/74/74	0/4/4/4
82	PEB	GB	201	2	-	6/26/74/74	0/4/4/4
82	PEB	qF	201	1,2	-	9/26/74/74	0/4/4/4
92	LMG	dL	407	18	-	23/49/69/70	0/1/1/1
82	PEB	G5	201	1	-	11/26/74/74	0/4/4/4
82	PEB	UF	201	1	-	8/26/74/74	0/4/4/4
82	PEB	t8	201	1	-	9/26/74/74	0/4/4/4
82	PEB	N7	203	2	-	8/26/74/74	0/4/4/4
82	PEB	d4	201	1	-	9/26/74/74	0/4/4/4
82	PEB	OI	203	2	-	8/26/74/74	0/4/4/4
87	CLA	AN	835	-	-	16/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	CLA	82	302	64	-	19/39/115/115	-
87	CLA	AN	805	40	-	23/39/115/115	-
85	BCR	BN	841	41	-	4/29/63/63	0/2/2/2
82	PEB	WP	201	1,2	-	12/26/74/74	0/4/4/4
82	PEB	LO	1002	10	-	8/26/74/74	0/4/4/4
82	PEB	Y5	201	74,2	-	10/26/74/74	0/4/4/4
98	PQN	B2	837	41	-	5/23/43/43	0/2/2/2
87	CLA	c6	606	17	-	16/39/115/115	-
82	PEB	I5	202	1	-	11/26/74/74	0/4/4/4
82	PEB	DQ	203	1	-	10/26/74/74	0/4/4/4
82	PEB	mM	202	2	-	9/26/74/74	0/4/4/4
92	LMG	k6	101	25	-	15/50/70/70	0/1/1/1
99	SF4	CN	101	42	-	-	0/6/5/5
82	PEB	MF	203	1,2	-	7/26/74/74	0/4/4/4
82	PEB	PP	202	2	-	6/26/74/74	0/4/4/4
82	PEB	aE	202	2	-	14/26/74/74	0/4/4/4
82	PEB	DP	201	2	-	6/26/74/74	0/4/4/4
82	PEB	P4	202	2	-	6/26/74/74	0/4/4/4
88	LHG	ML	102	-	-	15/43/43/53	-
87	CLA	BN	805	41	-	8/39/115/115	-
82	PEB	RM	201	2	-	7/26/74/74	0/4/4/4
82	PEB	mE	201	2	-	6/26/74/74	0/4/4/4
82	PEB	OO	201	1	-	8/26/74/74	0/4/4/4
82	PEB	AQ	301	3	-	11/26/74/74	0/4/4/4
82	PEB	BP	201	2	-	9/26/74/74	0/4/4/4
95	DGD	JL	101	-	-	8/51/91/95	0/2/2/2
87	CLA	8N	307	-	-	5/12/88/115	-
82	PEB	a1	202	2	-	10/26/74/74	0/4/4/4
82	PEB	kO	203	2	-	12/26/74/74	0/4/4/4
82	PEB	EJ	203	1	-	11/26/74/74	0/4/4/4
87	CLA	C6	517	-	-	13/39/115/115	-
82	PEB	D7	202	2	-	12/26/74/74	0/4/4/4
82	PEB	hJ	202	1	-	6/26/74/74	0/4/4/4
82	PEB	LI	202	2	-	6/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	CLA	I2	103	47,50	-	20/39/115/115	-
82	PEB	DD	203	1	-	10/26/74/74	0/4/4/4
82	PEB	OK	202	1	-	9/26/74/74	0/4/4/4
87	CLA	AN	809	-	-	15/39/115/115	-
82	PEB	JO	1002	10	-	11/26/74/74	0/4/4/4
82	PEB	PE	201	11,2	-	6/26/74/74	0/4/4/4
82	PEB	RP	201	56,2	-	9/26/74/74	0/4/4/4
82	PEB	JJ	201	2	-	6/26/74/74	0/4/4/4
82	PEB	PO	203	2	-	6/26/74/74	0/4/4/4
87	CLA	A2	849	40	-	11/39/115/115	-
87	CLA	A2	819	40	-	12/36/112/115	-
87	CLA	A2	815	-	-	20/39/115/115	-
82	PEB	QK	201	1	-	7/26/74/74	0/4/4/4
82	PEB	aH	201	2	-	6/26/74/74	0/4/4/4
84	CYC	w3	1001	73,69	-	4/26/74/74	0/4/4/4
92	LMG	bL	623	-	-	11/36/56/70	0/1/1/1
82	PEB	gF	202	1	-	11/26/74/74	0/4/4/4
82	PEB	P4	201	2	-	5/26/74/74	0/4/4/4
87	CLA	bL	617	-	-	13/39/115/115	-
84	CYC	F1	1001	10	-	8/26/74/74	0/4/4/4
87	CLA	CL	503	-	-	22/39/115/115	-
98	PQN	AN	842	-	-	6/23/43/43	0/2/2/2
82	PEB	HO	1002	10	-	8/26/74/74	0/4/4/4
82	PEB	V4	201	2	-	4/26/74/74	0/4/4/4
82	PEB	AJ	302	13	-	8/26/74/74	0/4/4/4
87	CLA	AN	838	-	-	15/39/115/115	-
87	CLA	B2	818	-	-	16/39/115/115	-
82	PEB	gB	203	2	-	14/26/74/74	0/4/4/4
82	PEB	aK	203	1	-	12/26/74/74	0/4/4/4
82	PEB	QQ	201	3,2	-	3/26/74/74	0/4/4/4
82	PEB	IB	203	2	-	8/26/74/74	0/4/4/4
82	PEB	FD	203	1,2	-	9/26/74/74	0/4/4/4
82	PEB	N9	201	1	-	7/26/74/74	0/4/4/4
85	BCR	B2	843	-	-	6/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	LI	201	12,2	-	10/26/74/74	0/4/4/4
82	PEB	R1	202	2	-	12/26/74/74	0/4/4/4
82	PEB	TQ	202	1	-	9/26/74/74	0/4/4/4
87	CLA	BL	604	-	-	7/32/108/115	-
82	PEB	G9	202	1	-	15/26/74/74	0/4/4/4
87	CLA	A2	826	-	-	11/39/115/115	-
82	PEB	K7	202	1	-	11/26/74/74	0/4/4/4
82	PEB	SB	201	2	-	4/26/74/74	0/4/4/4
87	CLA	J2	101	48	-	5/12/88/115	-
82	PEB	k1	201	2	-	8/26/74/74	0/4/4/4
82	PEB	PG	202	2	-	13/26/74/74	0/4/4/4
82	PEB	WI	203	2	-	6/26/74/74	0/4/4/4
85	BCR	AN	846	-	-	10/29/63/63	0/2/2/2
82	PEB	YG	201	2	-	11/26/74/74	0/4/4/4
87	CLA	b6	604	-	-	16/39/115/115	-
82	PEB	N9	202	1	-	15/26/74/74	0/4/4/4
87	CLA	B6	614	-	-	8/39/115/115	-
82	PEB	tK	202	2	-	11/26/74/74	0/4/4/4
87	CLA	cL	515	17	-	17/33/109/115	-
92	LMG	bL	611	37,16	-	14/45/65/70	0/1/1/1
87	CLA	A2	825	-	-	7/27/103/115	-
87	CLA	B2	824	41	-	20/39/115/115	-
82	PEB	HE	1002	10,9	-	8/26/74/74	0/4/4/4
82	PEB	A7	202	1	-	13/26/74/74	0/4/4/4
82	PEB	S7	202	1	-	8/26/74/74	0/4/4/4
82	PEB	NA	202	2	-	9/26/74/74	0/4/4/4
85	BCR	B2	842	-	-	13/29/63/63	0/2/2/2
82	PEB	oF	201	1	-	13/26/74/74	0/4/4/4
82	PEB	kK	201	1	-	12/26/74/74	0/4/4/4
82	PEB	BM	301	14	-	13/26/74/74	0/4/4/4
87	CLA	32	313	-	-	8/15/91/115	-
87	CLA	6N	612	62	-	9/15/91/115	-
85	BCR	BN	842	-	-	13/29/63/63	0/2/2/2
82	PEB	G9	201	1	-	7/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	mO	203	2	-	7/26/74/74	0/4/4/4
82	PEB	RJ	202	2	-	9/26/74/74	0/4/4/4
87	CLA	A2	832	40	-	10/21/97/115	-
82	PEB	ND	203	1	-	12/26/74/74	0/4/4/4
82	PEB	L4	1002	10	-	8/26/74/74	0/4/4/4
82	PEB	II	202	1	-	10/26/74/74	0/4/4/4
82	PEB	h1	203	1	-	11/26/74/74	0/4/4/4
82	PEB	xK	302	13	-	13/26/74/74	0/4/4/4
87	CLA	B2	836	87,41,57	-	18/39/115/115	-
88	LHG	c6	619	17	-	11/36/36/53	-
84	CYC	J3	1001	68	-	8/26/74/74	0/4/4/4
96	HEM	vL	201	35	-	2/14/54/54	-
85	BCR	fL	101	20	-	8/29/63/63	0/2/2/2
82	PEB	c4	201	2	-	7/26/74/74	0/4/4/4
84	CYC	J4	1001	10	-	11/26/74/74	0/4/4/4
84	CYC	JH	1001	10	-	7/26/74/74	0/4/4/4
82	PEB	T9	201	1	-	7/26/74/74	0/4/4/4
82	PEB	eK	201	1,2	-	12/26/74/74	0/4/4/4
82	PEB	GM	201	1	-	8/26/74/74	0/4/4/4
82	PEB	jJ	203	1,2	-	7/26/74/74	0/4/4/4
85	BCR	b6	602	-	-	1/29/63/63	0/2/2/2
82	PEB	wF	302	13	-	10/26/74/74	0/4/4/4
87	CLA	BN	821	54,41	-	2/13/89/115	-
82	PEB	XA	201	2,75	-	6/26/74/74	0/4/4/4
82	PEB	QP	202	1	-	11/26/74/74	0/4/4/4
82	PEB	CP	201	1,2	-	13/26/74/74	0/4/4/4
87	CLA	L2	206	50	-	5/29/105/115	-
87	CLA	b6	608	16	-	17/39/115/115	-
82	PEB	R7	202	2	-	10/26/74/74	0/4/4/4
82	PEB	JF	202	2	-	15/26/74/74	0/4/4/4
87	CLA	82	304	-	-	7/15/91/115	-
82	PEB	ZE	201	1,2	-	8/26/74/74	0/4/4/4
82	PEB	tC	201	1	-	9/26/74/74	0/4/4/4
84	CYC	E4	1001	9	-	10/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	hG	201	1,2	-	9/26/74/74	0/4/4/4
82	PEB	H5	201	74,2	-	11/26/74/74	0/4/4/4
87	CLA	C6	511	-	-	15/39/115/115	-
82	PEB	18	201	2	-	11/26/74/74	0/4/4/4
87	CLA	B6	608	16	-	16/39/115/115	-
82	PEB	YH	201	2	-	6/26/74/74	0/4/4/4
82	PEB	LF	202	2	-	14/26/74/74	0/4/4/4
82	PEB	dJ	201	1,2	-	9/26/74/74	0/4/4/4
87	CLA	62	312	62	-	10/15/91/115	-
82	PEB	uC	202	2	-	7/26/74/74	0/4/4/4
82	PEB	IP	203	1,2	-	13/26/74/74	0/4/4/4
82	PEB	KM	202	1	-	14/26/74/74	0/4/4/4
82	PEB	jG	202	1	-	7/26/74/74	0/4/4/4
82	PEB	NF	202	2	-	12/26/74/74	0/4/4/4
87	CLA	cL	513	17	-	9/39/115/115	-
82	PEB	JD	202	1	-	12/26/74/74	0/4/4/4
82	PEB	S9	203	2	-	11/26/74/74	0/4/4/4
84	CYC	M1	201	10,9	-	11/26/74/74	0/4/4/4
82	PEB	eO	202	2	-	10/26/74/74	0/4/4/4
84	CYC	C3	1001	68	-	8/26/74/74	0/4/4/4
87	CLA	A2	816	-	-	8/15/91/115	-
85	BCR	BL	618	-	-	4/29/63/63	0/2/2/2
83	PUB	Z5	302	1,74	-	7/26/74/74	0/4/4/4
82	PEB	j4	202	1	-	7/26/74/74	0/4/4/4
82	PEB	ZH	203	1	-	7/26/74/74	0/4/4/4
82	PEB	VA	201	2,75	-	11/26/74/74	0/4/4/4
82	PEB	JA	202	2	-	8/26/74/74	0/4/4/4
82	PEB	NA	201	2	-	3/26/74/74	0/4/4/4
82	PEB	cM	202	2	-	10/26/74/74	0/4/4/4
84	CYC	LO	1001	10	-	6/26/74/74	0/4/4/4
87	CLA	32	302	59,60	-	9/15/91/115	-
87	CLA	ON	202	53	-	10/21/97/115	-
82	PEB	rK	202	2	-	13/26/74/74	0/4/4/4
92	LMG	bL	610	-	-	17/36/56/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	Z1	201	1,2	-	11/26/74/74	0/4/4/4
82	PEB	NI	203	1,2	-	10/26/74/74	0/4/4/4
82	PEB	dG	204	1	-	12/26/74/74	0/4/4/4
99	SF4	CN	102	42	-	-	0/6/5/5
82	PEB	M7	201	1	-	8/26/74/74	0/4/4/4
87	CLA	b6	617	-	-	17/39/115/115	-
82	PEB	ZE	203	1,2	-	8/26/74/74	0/4/4/4
82	PEB	jE	202	1	-	7/26/74/74	0/4/4/4
87	CLA	1N	611	-	-	8/15/91/115	-
82	PEB	wC	201	2	-	12/26/74/74	0/4/4/4
87	CLA	c6	608	85,92	-	23/39/115/115	-
82	PEB	DJ	202	2	-	11/26/74/74	0/4/4/4
82	PEB	hJ	201	1,2	-	7/26/74/74	0/4/4/4
82	PEB	pC	201	1	-	13/26/74/74	0/4/4/4
87	CLA	cL	516	-	-	10/27/103/115	-
82	PEB	KF	201	1,2	-	6/26/74/74	0/4/4/4
82	PEB	YA	301	3	-	18/26/74/74	0/4/4/4
85	BCR	B6	621	92	-	0/29/63/63	0/2/2/2
82	PEB	VI	202	1	-	10/26/74/74	0/4/4/4
82	PEB	TK	202	2	-	17/26/74/74	0/4/4/4
82	PEB	AG	301	3	-	10/26/74/74	0/4/4/4
82	PEB	YP	502	2	-	12/26/74/74	0/4/4/4
82	PEB	SJ	202	1	-	12/26/74/74	0/4/4/4
95	DGD	AL	414	15	-	17/51/91/95	0/2/2/2
82	PEB	S9	201	74,2	-	12/26/74/74	0/4/4/4
82	PEB	OD	202	2	-	14/26/74/74	0/4/4/4
82	PEB	aO	203	2	-	11/26/74/74	0/4/4/4
82	PEB	bF	202	2	-	11/26/74/74	0/4/4/4
82	PEB	I7	201	1	-	13/26/74/74	0/4/4/4
87	CLA	2N	309	58	-	11/21/97/115	-
82	PEB	xC	201	1	-	11/26/74/74	0/4/4/4
87	CLA	aL	605	15	-	12/39/115/115	-
82	PEB	HF	202	2	-	12/26/74/74	0/4/4/4
82	PEB	AQ	303	3,82	-	11/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
94	PL9	d6	408	18,26	-	15/53/73/73	0/1/1/1
87	CLA	CL	505	-	-	16/39/115/115	-
87	CLA	H6	102	22	-	8/39/115/115	-
82	PEB	IB	202	2	-	8/26/74/74	0/4/4/4
87	CLA	BN	819	-	-	16/39/115/115	-
82	PEB	PB	201	2	-	5/26/74/74	0/4/4/4
82	PEB	Q4	202	1	-	8/26/74/74	0/4/4/4
82	PEB	R9	201	1	-	7/26/74/74	0/4/4/4
82	PEB	N5	202	1	-	11/26/74/74	0/4/4/4
82	PEB	iM	202	2	-	10/26/74/74	0/4/4/4
82	PEB	uK	202	1	-	9/26/74/74	0/4/4/4
95	DGD	C6	502	-	-	26/51/91/95	0/2/2/2
84	CYC	D1	1001	10	-	8/26/74/74	0/4/4/4
82	PEB	uC	203	2	-	2/26/74/74	0/4/4/4
88	LHG	C6	522	17	-	13/36/36/53	-
87	CLA	CL	506	-	-	17/39/115/115	-
95	DGD	cL	519	-	-	7/51/91/95	0/2/2/2
82	PEB	R4	203	2	-	7/26/74/74	0/4/4/4
82	PEB	Q9	201	2	-	10/26/74/74	0/4/4/4
87	CLA	5N	610	-	-	5/15/91/115	-
82	PEB	BA	203	2	-	12/26/74/74	0/4/4/4
87	CLA	42	606	-	-	8/15/91/115	-
87	CLA	A6	404	15	-	4/21/97/115	-
85	BCR	AN	804	-	-	2/29/63/63	0/2/2/2
82	PEB	SH	203	1,2	-	8/26/74/74	0/4/4/4
82	PEB	NM	201	2	-	9/26/74/74	0/4/4/4
87	CLA	a6	608	-	-	13/33/109/115	-
82	PEB	DQ	202	1	-	9/26/74/74	0/4/4/4
82	PEB	bF	201	2	-	4/26/74/74	0/4/4/4
82	PEB	lG	202	1	-	14/26/74/74	0/4/4/4
82	PEB	RD	201	1	-	11/26/74/74	0/4/4/4
84	CYC	m3	1001	68	-	8/26/74/74	0/4/4/4
87	CLA	bL	618	-	-	11/39/115/115	-
82	PEB	ID	201	2,77	-	7/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	KJ	201	1	-	6/26/74/74	0/4/4/4
82	PEB	r8	201	1	-	9/26/74/74	0/4/4/4
87	CLA	BN	833	-	-	8/18/94/115	-
82	PEB	jJ	202	1	-	11/26/74/74	0/4/4/4
82	PEB	M9	302	74	-	16/26/74/74	0/4/4/4
82	PEB	O9	203	2	-	7/26/74/74	0/4/4/4
88	LHG	bL	612	16	-	17/53/53/53	-
96	HEM	GN	201	46	-	6/14/54/54	-
82	PEB	iG	201	2	-	10/26/74/74	0/4/4/4
82	PEB	VF	201	2	-	10/26/74/74	0/4/4/4
87	CLA	BL	619	-	-	6/39/115/115	-
82	PEB	WF	201	1,2	-	7/26/74/74	0/4/4/4
82	PEB	FQ	202	1	-	10/26/74/74	0/4/4/4
82	PEB	E7	201	1	-	7/26/74/74	0/4/4/4
82	PEB	vK	201	2	-	7/26/74/74	0/4/4/4
82	PEB	QJ	204	1	-	10/26/74/74	0/4/4/4
82	PEB	jK	202	2	-	12/26/74/74	0/4/4/4
84	CYC	KG	202	10,9	-	11/26/74/74	0/4/4/4
82	PEB	mF	202	1	-	11/26/74/74	0/4/4/4
84	CYC	LH	1001	10,9	-	9/26/74/74	0/4/4/4
87	CLA	A2	834	-	-	20/39/115/115	-
82	PEB	cJ	202	2	-	10/26/74/74	0/4/4/4
87	CLA	7N	601	63	-	12/15/91/115	-
82	PEB	ZB	201	2	-	10/26/74/74	0/4/4/4
82	PEB	jO	202	1	-	7/26/74/74	0/4/4/4
82	PEB	OG	202	1	-	10/26/74/74	0/4/4/4
87	CLA	RN	204	-	-	11/15/91/115	-
82	PEB	sK	201	1	-	12/26/74/74	0/4/4/4
82	PEB	MI	401	-	-	10/26/74/74	0/4/4/4
82	PEB	GD	202	2	-	13/26/74/74	0/4/4/4
87	CLA	cL	508	-	-	18/39/115/115	-
82	PEB	cO	201	2	-	7/26/74/74	0/4/4/4
83	PUB	xK	305	13	-	8/26/74/74	0/4/4/4
84	CYC	N3	1001	68	-	8/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	SO	202	1,76	-	10/26/74/74	0/4/4/4
82	PEB	QE	202	1	-	9/26/74/74	0/4/4/4
82	PEB	YA	303	3,82	-	13/26/74/74	0/4/4/4
82	PEB	aB	202	2	-	6/26/74/74	0/4/4/4
82	PEB	KJ	203	1,2	-	8/26/74/74	0/4/4/4
82	PEB	SP	201	1,2	-	11/26/74/74	0/4/4/4
87	CLA	1N	604	-	-	3/12/88/115	-
82	PEB	AP	202	1	-	9/26/74/74	0/4/4/4
83	PUB	wK	304	13	-	7/26/74/74	0/4/4/4
84	CYC	L4	1001	10	-	6/26/74/74	0/4/4/4
82	PEB	T7	201	2	-	5/26/74/74	0/4/4/4
82	PEB	SM	201	1	-	10/26/74/74	0/4/4/4
82	PEB	sF	203	1,2	-	6/26/74/74	0/4/4/4
82	PEB	zC	202	1	-	11/26/74/74	0/4/4/4
82	PEB	mJ	202	2	-	7/26/74/74	0/4/4/4
83	PUB	A4	303	3	-	6/26/74/74	0/4/4/4
84	CYC	BG	1001	10,8	-	13/26/74/74	0/4/4/4
82	PEB	DF	201	2	-	7/26/74/74	0/4/4/4
82	PEB	OP	203	1	-	12/26/74/74	0/4/4/4
82	PEB	T4	203	2	-	10/26/74/74	0/4/4/4
84	CYC	q3	1001	69	-	4/26/74/74	0/4/4/4
82	PEB	W9	201	2	-	12/26/74/74	0/4/4/4
82	PEB	WF	203	1	-	13/26/74/74	0/4/4/4
84	CYC	G4	1001	9	-	8/26/74/74	0/4/4/4
87	CLA	BN	827	-	-	15/39/115/115	-
82	PEB	WK	202	1	-	8/26/74/74	0/4/4/4
82	PEB	YO	203	2	-	11/26/74/74	0/4/4/4
82	PEB	qC	202	2	-	9/26/74/74	0/4/4/4
85	BCR	BL	617	-	-	3/29/63/63	0/2/2/2
87	CLA	A2	822	40	-	8/15/91/115	-
82	PEB	m4	202	2	-	8/26/74/74	0/4/4/4
82	PEB	CI	202	1	-	10/26/74/74	0/4/4/4
94	PL9	D6	408	18,26	-	12/53/73/73	0/1/1/1
82	PEB	cB	402	6,2	-	12/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	j1	201	1	-	9/26/74/74	0/4/4/4
82	PEB	GI	202	1	-	9/26/74/74	0/4/4/4
82	PEB	jH	203	1,2	-	9/26/74/74	0/4/4/4
87	CLA	AN	828	40	-	13/39/115/115	-
82	PEB	Y9	203	2	-	7/26/74/74	0/4/4/4
82	PEB	AO	304	3	-	9/26/74/74	0/4/4/4
82	PEB	ZG	203	1	-	8/26/74/74	0/4/4/4
87	CLA	42	611	-	-	6/15/91/115	-
88	LHG	L6	101	26	-	18/53/53/53	-
88	LHG	d6	407	18	-	15/53/53/53	-
82	PEB	gK	201	1	-	6/26/74/74	0/4/4/4
82	PEB	gF	201	1	-	6/26/74/74	0/4/4/4
82	PEB	UJ	202	1	-	5/26/74/74	0/4/4/4
99	SF4	B2	803	-	-	-	0/6/5/5
82	PEB	NH	1002	10	-	10/26/74/74	0/4/4/4
82	PEB	mJ	201	13,2	-	8/26/74/74	0/4/4/4
82	PEB	bO	201	1	-	9/26/74/74	0/4/4/4
82	PEB	CD	202	2	-	7/26/74/74	0/4/4/4
82	PEB	WE	202	1,77	-	7/26/74/74	0/4/4/4
87	CLA	1N	608	57	-	7/10/86/115	-
87	CLA	A2	841	-	-	14/39/115/115	-
82	PEB	fM	201	1	-	6/26/74/74	0/4/4/4
87	CLA	B2	823	-	-	8/39/115/115	-
82	PEB	T4	202	2	-	5/26/74/74	0/4/4/4
97	GOL	WL	101	-	-	2/4/4/4	-
82	PEB	QA	201	1	-	5/26/74/74	0/4/4/4
82	PEB	F4	1002	10	-	9/26/74/74	0/4/4/4
87	CLA	CL	518	-	-	12/17/93/115	-
87	CLA	IN	103	47,50	-	20/39/115/115	-
87	CLA	B6	611	-	-	19/39/115/115	-
87	CLA	AN	839	-	-	9/39/115/115	-
87	CLA	O2	201	-	-	7/10/86/115	-
82	PEB	m4	201	2	-	9/26/74/74	0/4/4/4
82	PEB	mE	203	2	-	8/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	CLA	c6	614	17	-	12/33/109/115	-
87	CLA	bL	614	-	-	11/39/115/115	-
87	CLA	CL	509	17	-	14/39/115/115	-
85	BCR	aL	604	-	-	6/29/63/63	0/2/2/2
87	CLA	BL	620	16	-	11/39/115/115	-
82	PEB	jM	203	1,2	-	6/26/74/74	0/4/4/4
82	PEB	AH	301	3	-	7/26/74/74	0/4/4/4
82	PEB	e7	301	1,75	-	9/26/74/74	0/4/4/4
87	CLA	82	308	-	-	12/15/91/115	-
87	CLA	12	609	-	-	6/12/88/115	-
82	PEB	X7	203	2	-	12/26/74/74	0/4/4/4
87	CLA	A2	801	40,45	-	16/39/115/115	-
82	PEB	L9	203	2	-	7/26/74/74	0/4/4/4
87	CLA	62	303	62	-	18/39/115/115	-
82	PEB	MF	202	1	-	10/26/74/74	0/4/4/4
82	PEB	IJ	203	1	-	10/26/74/74	0/4/4/4
87	CLA	c6	604	17	-	27/39/115/115	-
82	PEB	dO	202	1	-	8/26/74/74	0/4/4/4
82	PEB	fM	203	1,2	-	7/26/74/74	0/4/4/4
82	PEB	RB	201	6,2	-	6/26/74/74	0/4/4/4
87	CLA	2N	307	58	-	8/15/91/115	-
87	CLA	R2	202	54	-	9/15/91/115	-
84	CYC	v3	1001	68	-	8/26/74/74	0/4/4/4
97	GOL	I6	102	-	-	0/4/4/4	-
82	PEB	PF	202	2	-	14/26/74/74	0/4/4/4
82	PEB	WH	201	1	-	8/26/74/74	0/4/4/4
82	PEB	AI	203	1,2	-	10/26/74/74	0/4/4/4
95	DGD	aL	603	15	-	7/42/82/95	0/2/2/2
82	PEB	aJ	204	1,2	-	6/26/74/74	0/4/4/4
82	PEB	IF	201	1	-	9/26/74/74	0/4/4/4
82	PEB	1C	201	2	-	11/26/74/74	0/4/4/4
82	PEB	U9	203	2	-	7/26/74/74	0/4/4/4
87	CLA	1N	602	57	-	15/39/115/115	-
82	PEB	M9	304	74	-	11/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	E5	202	1	-	11/26/74/74	0/4/4/4
82	PEB	LA	202	2	-	9/26/74/74	0/4/4/4
92	LMG	B6	622	37,16	-	12/45/65/70	0/1/1/1
85	BCR	KN	104	-	-	8/29/63/63	0/2/2/2
82	PEB	lM	202	1	-	6/26/74/74	0/4/4/4
82	PEB	SQ	201	3,2	-	4/26/74/74	0/4/4/4
82	PEB	HK	201	2	-	7/26/74/74	0/4/4/4
82	PEB	q8	201	2	-	5/26/74/74	0/4/4/4
83	PUB	AQ	302	1,3	-	8/26/74/74	0/4/4/4
87	CLA	BN	815	41	-	5/12/88/115	-
82	PEB	PD	203	1	-	12/26/74/74	0/4/4/4
85	BCR	JN	102	-	-	7/29/63/63	0/2/2/2
82	PEB	AD	301	3	-	11/26/74/74	0/4/4/4
82	PEB	eF	201	1,2	-	12/26/74/74	0/4/4/4
85	BCR	K6	102	-	-	12/29/63/63	0/2/2/2
82	PEB	P1	202	2	-	8/26/74/74	0/4/4/4
84	CYC	FE	1001	10,9	-	10/26/74/74	0/4/4/4
82	PEB	D1	1002	10	-	11/26/74/74	0/4/4/4
87	CLA	12	604	-	-	3/12/88/115	-
82	PEB	ED	201	2,77	-	12/26/74/74	0/4/4/4
82	PEB	IA	201	1	-	13/26/74/74	0/4/4/4
88	LHG	aL	607	15	-	18/47/47/53	-
82	PEB	PI	202	1	-	10/26/74/74	0/4/4/4
82	PEB	CQ	202	2	-	7/26/74/74	0/4/4/4
82	PEB	IF	203	1,2	-	5/26/74/74	0/4/4/4
87	CLA	A2	836	-	-	7/15/91/115	-
82	PEB	aO	202	2	-	7/26/74/74	0/4/4/4
95	DGD	B2	844	41	-	19/55/95/95	0/2/2/2
82	PEB	eF	203	1	-	8/26/74/74	0/4/4/4
82	PEB	OE	202	1	-	10/26/74/74	0/4/4/4
82	PEB	WJ	202	1	-	14/26/74/74	0/4/4/4
87	CLA	62	310	-	-	5/10/86/115	-
82	PEB	AF	201	1	-	9/26/74/74	0/4/4/4
82	PEB	T7	203	2	-	7/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	LA	201	2,82	-	6/26/74/74	0/4/4/4
96	HEM	V6	201	35	-	2/14/54/54	-
87	CLA	A2	839	-	-	9/39/115/115	-
82	PEB	DO	1002	10	-	10/26/74/74	0/4/4/4
82	PEB	ND	204	1,2	-	13/26/74/74	0/4/4/4
82	PEB	G7	202	1	-	12/26/74/74	0/4/4/4
95	DGD	BN	844	41	-	19/55/95/95	0/2/2/2
87	CLA	22	601	58	-	7/15/91/115	-
88	LHG	CL	522	17	-	10/36/36/53	-
82	PEB	f1	202	1	-	10/26/74/74	0/4/4/4
82	PEB	TO	202	2	-	5/26/74/74	0/4/4/4
82	PEB	ZH	201	1,2	-	11/26/74/74	0/4/4/4
82	PEB	i1	201	2	-	7/26/74/74	0/4/4/4
82	PEB	RP	202	2	-	6/26/74/74	0/4/4/4
84	CYC	O3	1001	69	-	4/26/74/74	0/4/4/4
87	CLA	72	606	63	-	7/15/91/115	-
82	PEB	L7	203	2	-	10/26/74/74	0/4/4/4
82	PEB	oK	201	1	-	13/26/74/74	0/4/4/4
82	PEB	LJ	202	2	-	10/26/74/74	0/4/4/4
84	CYC	KO	1001	9	-	9/26/74/74	0/4/4/4
87	CLA	c6	616	-	-	12/39/115/115	-
87	CLA	C6	518	-	-	14/33/109/115	-
87	CLA	bL	606	-	-	11/39/115/115	-
82	PEB	k4	201	2	-	8/26/74/74	0/4/4/4
82	PEB	NI	201	1	-	9/26/74/74	0/4/4/4
87	CLA	7N	610	-	-	5/15/91/115	-
82	PEB	OH	202	1	-	7/26/74/74	0/4/4/4
87	CLA	2N	301	58,41	-	11/25/101/115	-
87	CLA	B2	829	-	-	7/13/89/115	-
82	PEB	jH	202	1	-	8/26/74/74	0/4/4/4
82	PEB	OM	202	1	-	9/26/74/74	0/4/4/4
82	PEB	rC	202	1	-	16/26/74/74	0/4/4/4
83	PUB	AG	303	3	-	9/26/74/74	0/4/4/4
82	PEB	DG	1002	10,9	-	8/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	CLA	6N	609	-	-	5/10/86/115	-
82	PEB	YI	201	12,2	-	10/26/74/74	0/4/4/4
82	PEB	V7	202	2	-	10/26/74/74	0/4/4/4
82	PEB	WD	202	2	-	8/26/74/74	0/4/4/4
87	CLA	R2	203	54,41	-	8/17/93/115	-
82	PEB	CM	203	1,2	-	6/26/74/74	0/4/4/4
82	PEB	bK	202	2	-	11/26/74/74	0/4/4/4
87	CLA	AN	814	40	-	10/26/102/115	-
82	PEB	BB	203	2	-	8/26/74/74	0/4/4/4
82	PEB	HB	203	2	-	12/26/74/74	0/4/4/4
85	BCR	BN	839	-	-	6/29/63/63	0/2/2/2
82	PEB	O1	203	1,2	-	10/26/74/74	0/4/4/4
82	PEB	BK	201	2	-	9/26/74/74	0/4/4/4
87	CLA	7N	604	63	-	7/12/88/115	-
82	PEB	gK	203	1,2	-	9/26/74/74	0/4/4/4
82	PEB	GB	202	2	-	9/26/74/74	0/4/4/4
82	PEB	M9	301	74,2	-	6/26/74/74	0/4/4/4
82	PEB	EA	201	1	-	7/26/74/74	0/4/4/4
82	PEB	18	203	2	-	6/26/74/74	0/4/4/4
82	PEB	Y1	201	2	-	6/26/74/74	0/4/4/4
87	CLA	cL	505	-	-	23/39/115/115	-
95	DGD	CL	523	-	-	11/37/77/95	0/2/2/2
88	LHG	dL	405	18	-	15/53/53/53	-
82	PEB	iK	203	1	-	13/26/74/74	0/4/4/4
82	PEB	h4	202	1	-	8/26/74/74	0/4/4/4
87	CLA	B2	806	-	-	20/39/115/115	-
82	PEB	J1	1002	10	-	10/26/74/74	0/4/4/4
82	PEB	OH	201	1	-	11/26/74/74	0/4/4/4
95	DGD	a6	602	-	-	10/29/69/95	0/2/2/2
82	PEB	J9	201	2	-	12/26/74/74	0/4/4/4
87	CLA	c6	613	17	-	14/39/115/115	-
84	CYC	U3	1001	73,69	-	4/26/74/74	0/4/4/4
82	PEB	TQ	203	1	-	13/26/74/74	0/4/4/4
82	PEB	lJ	202	1	-	7/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	eG	201	2	-	9/26/74/74	0/4/4/4
82	PEB	e4	203	2	-	6/26/74/74	0/4/4/4
92	LMG	bL	609	-	3/3/8/8	21/36/56/70	0/1/1/1
87	CLA	cL	517	-	-	10/39/115/115	-
87	CLA	BN	823	-	-	16/39/115/115	-
87	CLA	LN	204	50	-	13/21/97/115	-
82	PEB	gH	203	1,74,2	-	9/26/74/74	0/4/4/4
82	PEB	EM	201	1,2	-	6/26/74/74	0/4/4/4
82	PEB	CB	201	2,4	-	3/26/74/74	0/4/4/4
82	PEB	EP	202	1	-	11/26/74/74	0/4/4/4
82	PEB	VQ	202	1	-	12/26/74/74	0/4/4/4
84	CYC	R3	1001	68	-	8/26/74/74	0/4/4/4
87	CLA	bL	615	-	-	15/39/115/115	-
87	CLA	AN	851	-	-	22/39/115/115	-
87	CLA	A2	831	-	-	13/39/115/115	-
95	DGD	b6	621	-	-	9/29/69/95	0/2/2/2
92	LMG	CL	519	-	-	22/50/70/70	0/1/1/1
87	CLA	CL	508	87	-	23/39/115/115	-
82	PEB	VD	202	1	-	12/26/74/74	0/4/4/4
85	BCR	F6	101	20	-	9/29/63/63	0/2/2/2
85	BCR	B6	602	-	-	2/29/63/63	0/2/2/2
82	PEB	u8	201	2	-	10/26/74/74	0/4/4/4
82	PEB	XQ	202	1	-	12/26/74/74	0/4/4/4
83	PUB	QM	201	14,1	-	7/26/74/74	0/4/4/4
82	PEB	N4	1002	10	-	8/26/74/74	0/4/4/4
82	PEB	P9	201	1	-	7/26/74/74	0/4/4/4
82	PEB	YF	203	1,2	-	8/26/74/74	0/4/4/4
82	PEB	LB	201	2	-	10/26/74/74	0/4/4/4
87	CLA	AN	813	-	-	13/39/115/115	-
84	CYC	Q3	1001	73,69	-	4/26/74/74	0/4/4/4
82	PEB	RH	202	2	-	12/26/74/74	0/4/4/4
82	PEB	xK	303	13	-	12/26/74/74	0/4/4/4
82	PEB	FF	202	2	-	11/26/74/74	0/4/4/4
82	PEB	NB	202	2	-	8/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	JM	201	2	-	6/26/74/74	0/4/4/4
82	PEB	L1	1002	10	-	8/26/74/74	0/4/4/4
82	PEB	U5	202	2	-	11/26/74/74	0/4/4/4
82	PEB	GP	203	1	-	10/26/74/74	0/4/4/4
82	PEB	OH	203	1,2	-	10/26/74/74	0/4/4/4
82	PEB	RG	201	2	-	8/26/74/74	0/4/4/4
82	PEB	K9	202	1	-	15/26/74/74	0/4/4/4
82	PEB	SG	203	1,2	-	7/26/74/74	0/4/4/4
96	HEM	v6	201	35	-	2/14/54/54	-
82	PEB	V5	202	1	-	11/26/74/74	0/4/4/4
96	HEM	FL	102	-	-	6/14/54/54	-
84	CYC	NE	201	10,9	-	10/26/74/74	0/4/4/4
82	PEB	JA	201	3,2	-	4/26/74/74	0/4/4/4
82	PEB	W7	202	1	-	12/26/74/74	0/4/4/4
82	PEB	FA	203	2	-	11/26/74/74	0/4/4/4
83	PUB	AJ	303	13	-	13/26/74/74	0/4/4/4
82	PEB	VG	201	2	-	8/26/74/74	0/4/4/4
87	CLA	A2	805	40	-	23/39/115/115	-
82	PEB	EP	201	1	-	7/26/74/74	0/4/4/4
82	PEB	HI	201	2	-	8/26/74/74	0/4/4/4
82	PEB	bE	201	1	-	6/26/74/74	0/4/4/4
87	CLA	AN	821	-	-	18/39/115/115	-
87	CLA	2N	303	58	-	16/39/115/115	-
87	CLA	b6	613	-	-	17/39/115/115	-
82	PEB	A9	202	1	-	15/26/74/74	0/4/4/4
87	CLA	A2	833	-	-	13/39/115/115	-
82	PEB	WM	203	1,2	-	7/26/74/74	0/4/4/4
82	PEB	GA	201	1	-	6/26/74/74	0/4/4/4
87	CLA	C6	512	-	-	13/39/115/115	-
82	PEB	ZK	202	2	-	10/26/74/74	0/4/4/4
95	DGD	L6	102	26	-	24/47/87/95	0/2/2/2
82	PEB	A1	305	3	-	12/26/74/74	0/4/4/4
87	CLA	52	605	61	-	6/15/91/115	-
82	PEB	ZO	202	1	-	9/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	kO	202	2	-	13/26/74/74	0/4/4/4
82	PEB	XB	202	2	-	10/26/74/74	0/4/4/4
85	BCR	A2	848	-	-	16/29/63/63	0/2/2/2
87	CLA	B2	814	41	-	5/12/88/115	-
82	PEB	b1	202	1	-	10/26/74/74	0/4/4/4
82	PEB	S5	201	74,2	-	11/26/74/74	0/4/4/4
82	PEB	TF	202	2	-	17/26/74/74	0/4/4/4
87	CLA	FN	201	45	-	5/10/86/115	-
87	CLA	2N	311	-	-	7/12/88/115	-
82	PEB	hM	201	1,2	-	8/26/74/74	0/4/4/4
82	PEB	D4	1002	10	-	10/26/74/74	0/4/4/4
82	PEB	FJ	201	79,2	-	7/26/74/74	0/4/4/4
82	PEB	kH	201	2	-	8/26/74/74	0/4/4/4
82	PEB	AO	305	3	-	11/26/74/74	0/4/4/4
88	LHG	i6	101	-	-	17/53/53/53	-
82	PEB	Y5	203	2	-	12/26/74/74	0/4/4/4
82	PEB	uF	201	1,2	-	11/26/74/74	0/4/4/4
83	PUB	xF	305	13	-	8/26/74/74	0/4/4/4
87	CLA	AN	810	40	-	23/39/115/115	-
82	PEB	f4	201	1	-	11/26/74/74	0/4/4/4
82	PEB	RI	202	1	-	10/26/74/74	0/4/4/4
82	PEB	IM	202	1	-	7/26/74/74	0/4/4/4
82	PEB	cF	202	1,10	-	9/26/74/74	0/4/4/4
87	CLA	BN	822	-	-	13/27/103/115	-
82	PEB	eK	202	1	-	8/26/74/74	0/4/4/4
85	BCR	BN	838	-	-	5/29/63/63	0/2/2/2
87	CLA	A2	851	-	-	22/39/115/115	-
82	PEB	N7	202	2	-	9/26/74/74	0/4/4/4
87	CLA	b6	615	-	-	17/39/115/115	-
82	PEB	IK	202	1	-	15/26/74/74	0/4/4/4
87	CLA	BN	802	41	-	13/31/107/115	-
82	PEB	HI	203	2	-	6/26/74/74	0/4/4/4
82	PEB	VO	202	2	-	12/26/74/74	0/4/4/4
82	PEB	AQ	304	3,82	-	11/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	VP	202	2	-	7/26/74/74	0/4/4/4
82	PEB	AD	303	3,82	-	11/26/74/74	0/4/4/4
87	CLA	72	610	-	-	5/15/91/115	-
84	CYC	DO	1001	10	-	10/26/74/74	0/4/4/4
82	PEB	tK	201	2	-	7/26/74/74	0/4/4/4
82	PEB	lK	202	2	-	13/26/74/74	0/4/4/4
82	PEB	FP	202	2	-	7/26/74/74	0/4/4/4
82	PEB	AA	201	1	-	11/26/74/74	0/4/4/4
82	PEB	eJ	201	13,2	-	6/26/74/74	0/4/4/4
87	CLA	4N	608	60	-	11/21/97/115	-
82	PEB	bB	201	2	-	11/26/74/74	0/4/4/4
82	PEB	S1	201	1	-	7/26/74/74	0/4/4/4
82	PEB	aK	202	1	-	9/26/74/74	0/4/4/4
82	PEB	KP	202	1	-	4/26/74/74	0/4/4/4
82	PEB	KB	304	2,5	-	9/26/74/74	0/4/4/4
84	CYC	FH	1001	10	-	8/26/74/74	0/4/4/4
82	PEB	cG	202	2	-	10/26/74/74	0/4/4/4
87	CLA	B2	828	41	-	7/15/91/115	-
87	CLA	dL	404	-	-	17/39/115/115	-
82	PEB	LP	202	2	-	6/26/74/74	0/4/4/4
84	CYC	C4	1001	9	-	11/26/74/74	0/4/4/4
87	CLA	AN	823	40	-	20/39/115/115	-
87	CLA	B2	820	54,41	-	2/13/89/115	-
82	PEB	U5	203	2	-	12/26/74/74	0/4/4/4
87	CLA	BN	807	-	-	20/39/115/115	-
82	PEB	JK	202	2	-	15/26/74/74	0/4/4/4
91	PHO	d6	404	-	3/3/17/22	3/37/103/103	0/5/6/6
82	PEB	Y5	202	2	-	12/26/74/74	0/4/4/4
82	PEB	ZM	201	2	-	8/26/74/74	0/4/4/4
82	PEB	H5	203	2	-	12/26/74/74	0/4/4/4
83	PUB	Z9	305	1,74	-	14/26/74/74	0/4/4/4
85	BCR	I2	101	-	-	12/29/63/63	0/2/2/2
84	CYC	N1	1001	10,8	-	10/26/74/74	0/4/4/4
87	CLA	b6	614	-	-	10/32/108/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	CLA	7N	606	63	-	7/15/91/115	-
82	PEB	OM	203	1,2	-	6/26/74/74	0/4/4/4
87	CLA	C6	509	-	-	19/39/115/115	-
95	DGD	lL	101	26	-	20/47/87/95	0/2/2/2
82	PEB	YB	202	2	-	8/26/74/74	0/4/4/4
82	PEB	YO	201	2	-	3/26/74/74	0/4/4/4
82	PEB	V7	203	2	-	7/26/74/74	0/4/4/4
87	CLA	32	310	59,87	-	5/10/86/115	-
82	PEB	QP	201	1	-	7/26/74/74	0/4/4/4
82	PEB	FM	201	79,2	-	6/26/74/74	0/4/4/4
82	PEB	pK	201	2	-	8/26/74/74	0/4/4/4
82	PEB	H9	201	74,2	-	10/26/74/74	0/4/4/4
95	DGD	b6	622	-	-	10/31/71/95	0/2/2/2
88	LHG	cL	501	17	-	7/36/36/53	-
85	BCR	CL	516	-	-	5/29/63/63	0/2/2/2
87	CLA	B2	816	-	-	8/32/108/115	-
82	PEB	P7	202	2	-	7/26/74/74	0/4/4/4
85	BCR	IN	101	-	-	12/29/63/63	0/2/2/2
82	PEB	Z9	301	74	-	16/26/74/74	0/4/4/4
84	CYC	F3	1001	69	-	4/26/74/74	0/4/4/4
87	CLA	AN	831	-	-	14/39/115/115	-
82	PEB	L9	201	2	-	10/26/74/74	0/4/4/4
82	PEB	MQ	202	2	-	9/26/74/74	0/4/4/4
82	PEB	iH	202	2	-	9/26/74/74	0/4/4/4
82	PEB	HA	201	2	-	5/26/74/74	0/4/4/4
103	ZEX	8N	309	64	-	11/29/67/67	0/2/2/2
87	CLA	C6	510	-	-	17/39/115/115	-
84	CYC	CO	1001	9	-	11/26/74/74	0/4/4/4
82	PEB	kM	202	2	-	9/26/74/74	0/4/4/4
82	PEB	lH	202	1	-	13/26/74/74	0/4/4/4
87	CLA	1N	607	57	-	11/21/97/115	-
82	PEB	yC	203	2	-	9/26/74/74	0/4/4/4
82	PEB	GP	202	1	-	4/26/74/74	0/4/4/4
82	PEB	C9	202	1	-	15/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	kG	202	2	-	11/26/74/74	0/4/4/4
82	PEB	DF	203	2	-	12/26/74/74	0/4/4/4
82	PEB	CK	201	1	-	6/26/74/74	0/4/4/4
82	PEB	A5	202	1	-	11/26/74/74	0/4/4/4
82	PEB	j4	201	1	-	10/26/74/74	0/4/4/4
82	PEB	gE	201	2	-	6/26/74/74	0/4/4/4
82	PEB	P9	202	1	-	15/26/74/74	0/4/4/4
85	BCR	A2	847	-	-	8/29/63/63	0/2/2/2
83	PUB	K7	203	1,3	-	6/26/74/74	0/4/4/4
82	PEB	AP	201	1	-	4/26/74/74	0/4/4/4
82	PEB	iO	201	2	-	7/26/74/74	0/4/4/4
87	CLA	AN	850	40	-	6/39/115/115	-
87	CLA	BL	601	-	-	15/39/115/115	-
82	PEB	XD	203	1	-	10/26/74/74	0/4/4/4
87	CLA	3N	312	59	-	9/15/91/115	-
82	PEB	qF	202	1	-	17/26/74/74	0/4/4/4
87	CLA	dL	402	-	-	8/39/115/115	-
85	BCR	B2	802	87,50,41	-	11/29/63/63	0/2/2/2
82	PEB	QF	202	1	-	7/26/74/74	0/4/4/4
82	PEB	G5	202	1	-	11/26/74/74	0/4/4/4
82	PEB	M5	304	74,82	-	8/26/74/74	0/4/4/4
84	CYC	M4	1001	9	-	10/26/74/74	0/4/4/4
82	PEB	jE	201	1	-	9/26/74/74	0/4/4/4
87	CLA	4N	602	60	-	16/39/115/115	-
82	PEB	kE	202	2	-	11/26/74/74	0/4/4/4
82	PEB	XI	202	1	-	10/26/74/74	0/4/4/4
82	PEB	WQ	201	3,2	-	4/26/74/74	0/4/4/4
82	PEB	Z4	201	1	-	7/26/74/74	0/4/4/4
82	PEB	UI	201	2	-	7/26/74/74	0/4/4/4
82	PEB	XK	202	2	-	6/26/74/74	0/4/4/4
82	PEB	UM	202	1	-	4/26/74/74	0/4/4/4
82	PEB	JB	202	1	-	11/26/74/74	0/4/4/4
82	PEB	c4	203	2	-	11/26/74/74	0/4/4/4
87	CLA	F2	202	45	-	5/10/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	CYC	L1	1001	10	-	12/26/74/74	0/4/4/4
82	PEB	QB	204	2	-	11/26/74/74	0/4/4/4
82	PEB	EK	201	1	-	9/26/74/74	0/4/4/4
82	PEB	GK	202	1	-	7/26/74/74	0/4/4/4
82	PEB	qK	201	1,2	-	9/26/74/74	0/4/4/4
82	PEB	UG	203	1	-	12/26/74/74	0/4/4/4
87	CLA	B2	825	-	-	17/39/115/115	-
82	PEB	HB	202	2	-	10/26/74/74	0/4/4/4
82	PEB	XP	202	2	-	8/26/74/74	0/4/4/4
87	CLA	2N	308	58	-	7/15/91/115	-
83	PUB	xK	306	13	-	6/26/74/74	0/4/4/4
87	CLA	5N	609	61	-	6/12/88/115	-
82	PEB	XF	201	2	-	10/26/74/74	0/4/4/4
83	PUB	M5	303	1,74	-	8/26/74/74	0/4/4/4
82	PEB	HF	201	2	-	7/26/74/74	0/4/4/4
84	CYC	EE	1001	10,9	-	8/26/74/74	0/4/4/4
83	PUB	YA	302	3	-	3/26/74/74	0/4/4/4
87	CLA	IN	102	-	-	11/39/115/115	-
82	PEB	iH	201	2	-	7/26/74/74	0/4/4/4
82	PEB	EQ	201	2,77	-	12/26/74/74	0/4/4/4
82	PEB	WP	202	1	-	4/26/74/74	0/4/4/4
83	PUB	Z9	302	74	-	7/26/74/74	0/4/4/4
82	PEB	KK	202	1	-	4/26/74/74	0/4/4/4
87	CLA	AN	834	-	-	20/39/115/115	-
82	PEB	MK	203	1,2	-	7/26/74/74	0/4/4/4
82	PEB	xF	303	13	-	12/26/74/74	0/4/4/4
82	PEB	w8	201	2	-	12/26/74/74	0/4/4/4
82	PEB	1C	202	2	-	6/26/74/74	0/4/4/4
82	PEB	PE	202	2	-	13/26/74/74	0/4/4/4
82	PEB	hO	202	1	-	8/26/74/74	0/4/4/4
83	PUB	M9	303	74	-	7/26/74/74	0/4/4/4
82	PEB	mK	201	1	-	6/26/74/74	0/4/4/4
84	CYC	W3	1001	71	-	10/26/74/74	0/4/4/4
82	PEB	hE	201	1,2	-	9/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	kF	202	1	-	10/26/74/74	0/4/4/4
82	PEB	dB	202	2	-	10/26/74/74	0/4/4/4
82	PEB	NA	203	2	-	8/26/74/74	0/4/4/4
82	PEB	CM	201	1	-	8/26/74/74	0/4/4/4
95	DGD	DL	408	18	-	9/51/91/95	0/2/2/2
82	PEB	DB	202	2	-	10/26/74/74	0/4/4/4
82	PEB	HB	201	2	-	15/26/74/74	0/4/4/4
82	PEB	VP	201	2	-	7/26/74/74	0/4/4/4
82	PEB	eJ	202	2	-	11/26/74/74	0/4/4/4
82	PEB	MF	201	1	-	6/26/74/74	0/4/4/4
87	CLA	bL	604	-	-	8/17/93/115	-
82	PEB	RQ	203	1,2	-	10/26/74/74	0/4/4/4
82	PEB	NE	202	10,9	-	9/26/74/74	0/4/4/4
91	PHO	dL	403	-	3/3/17/22	8/37/103/103	0/5/6/6
82	PEB	gE	202	2	-	11/26/74/74	0/4/4/4
82	PEB	q8	203	2	-	6/26/74/74	0/4/4/4
83	PUB	AE	303	3	-	9/26/74/74	0/4/4/4
87	CLA	62	304	-	-	9/15/91/115	-
84	CYC	IE	1001	10,9	-	10/26/74/74	0/4/4/4
82	PEB	LD	202	1	-	9/26/74/74	0/4/4/4
85	BCR	a6	605	-	-	6/29/63/63	0/2/2/2
82	PEB	B9	201	2	-	10/26/74/74	0/4/4/4
87	CLA	5N	603	-	-	8/15/91/115	-
82	PEB	TD	201	1,2	-	13/26/74/74	0/4/4/4
87	CLA	CL	504	-	-	18/39/115/115	-
82	PEB	F7	203	2	-	11/26/74/74	0/4/4/4
82	PEB	QG	202	1	-	9/26/74/74	0/4/4/4
82	PEB	MM	202	1	-	6/26/74/74	0/4/4/4
82	PEB	SI	201	2	-	12/26/74/74	0/4/4/4
82	PEB	K7	201	1	-	7/26/74/74	0/4/4/4
82	PEB	NG	201	10,9	-	9/26/74/74	0/4/4/4
82	PEB	MJ	203	1	-	9/26/74/74	0/4/4/4
87	CLA	1N	605	57	-	9/15/91/115	-
82	PEB	T5	201	1	-	11/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	Q9	203	2	-	7/26/74/74	0/4/4/4
82	PEB	O4	201	1	-	8/26/74/74	0/4/4/4
82	PEB	Z9	303	74	-	11/26/74/74	0/4/4/4
82	PEB	i4	202	2	-	8/26/74/74	0/4/4/4
84	CYC	EG	1001	10,9	-	8/26/74/74	0/4/4/4
82	PEB	BJ	301	14	-	9/26/74/74	0/4/4/4
84	CYC	MG	1001	10,9	-	9/26/74/74	0/4/4/4
87	CLA	M2	101	51,41	-	10/15/91/115	-
87	CLA	82	301	64	-	10/15/91/115	-
82	PEB	EQ	202	2	-	7/26/74/74	0/4/4/4
82	PEB	TQ	201	1,2	-	13/26/74/74	0/4/4/4
82	PEB	D7	201	3,2	-	11/26/74/74	0/4/4/4
88	LHG	AL	407	15	-	16/47/47/53	-
82	PEB	PD	202	1	-	9/26/74/74	0/4/4/4
87	CLA	7N	602	62,63	-	14/39/115/115	-
82	PEB	w8	203	2	-	6/26/74/74	0/4/4/4
82	PEB	PH	202	2	-	8/26/74/74	0/4/4/4
82	PEB	a4	202	2	-	7/26/74/74	0/4/4/4
84	CYC	L3	1001	69	-	4/26/74/74	0/4/4/4
82	PEB	jK	201	2	-	7/26/74/74	0/4/4/4
82	PEB	Q7	202	1	-	9/26/74/74	0/4/4/4
85	BCR	h6	102	-	-	3/29/63/63	0/2/2/2
82	PEB	QH	203	1	-	9/26/74/74	0/4/4/4
82	PEB	SP	203	1	-	11/26/74/74	0/4/4/4
92	LMG	b6	623	-	-	21/36/56/70	0/1/1/1
82	PEB	BF	202	2	-	13/26/74/74	0/4/4/4
92	LMG	j6	101	-	-	17/38/58/70	0/1/1/1
82	PEB	yC	202	2	-	9/26/74/74	0/4/4/4
82	PEB	iE	202	2	-	10/26/74/74	0/4/4/4
82	PEB	iF	203	1	-	13/26/74/74	0/4/4/4
82	PEB	WM	202	1	-	12/26/74/74	0/4/4/4
87	CLA	6N	608	62	-	10/21/97/115	-
87	CLA	72	608	63	-	6/10/86/115	-
82	PEB	YJ	203	1	-	9/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	b4	202	1	-	8/26/74/74	0/4/4/4
82	PEB	H9	203	2	-	9/26/74/74	0/4/4/4
82	PEB	GF	202	1	-	7/26/74/74	0/4/4/4
82	PEB	YF	201	1	-	7/26/74/74	0/4/4/4
82	PEB	V1	202	1,2	-	8/26/74/74	0/4/4/4
82	PEB	TH	201	11,2	-	9/26/74/74	0/4/4/4
82	PEB	NJ	202	2	-	10/26/74/74	0/4/4/4
82	PEB	J5	201	2	-	9/26/74/74	0/4/4/4
85	BCR	AN	847	-	-	8/29/63/63	0/2/2/2
92	LMG	mL	101	-	-	8/36/56/70	0/1/1/1
82	PEB	RE	201	2	-	8/26/74/74	0/4/4/4
82	PEB	QD	201	3,2	-	3/26/74/74	0/4/4/4
82	PEB	eM	202	2	-	10/26/74/74	0/4/4/4
82	PEB	aM	203	1	-	15/26/74/74	0/4/4/4
96	HEM	VL	201	35	-	2/14/54/54	-
87	CLA	A2	827	-	-	9/27/103/115	-
82	PEB	HQ	201	1,2	-	12/26/74/74	0/4/4/4
82	PEB	IB	201	2	-	7/26/74/74	0/4/4/4
82	PEB	m1	202	2	-	10/26/74/74	0/4/4/4
87	CLA	4N	611	-	-	6/15/91/115	-
82	PEB	UE	203	1	-	12/26/74/74	0/4/4/4
84	CYC	h3	1001	73,69	-	4/26/74/74	0/4/4/4
82	PEB	aG	201	2	-	5/26/74/74	0/4/4/4
82	PEB	FD	201	1	-	11/26/74/74	0/4/4/4
87	CLA	A2	809	-	-	15/39/115/115	-
82	PEB	TB	202	1	-	11/26/74/74	0/4/4/4
82	PEB	kF	203	1,2	-	10/26/74/74	0/4/4/4
82	PEB	UB	301	2,5	-	9/26/74/74	0/4/4/4
82	PEB	BF	201	2	-	9/26/74/74	0/4/4/4
82	PEB	CF	202	1	-	7/26/74/74	0/4/4/4
82	PEB	LG	1002	10,9	-	11/26/74/74	0/4/4/4
82	PEB	iE	201	2	-	10/26/74/74	0/4/4/4
82	PEB	WI	201	2	-	8/26/74/74	0/4/4/4
87	CLA	42	610	-	-	7/12/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
92	LMG	AL	411	-	-	12/46/66/70	0/1/1/1
87	CLA	BL	609	-	-	18/39/115/115	-
82	PEB	aE	201	2	-	5/26/74/74	0/4/4/4
82	PEB	YJ	202	1	-	6/26/74/74	0/4/4/4
87	CLA	52	603	-	-	8/15/91/115	-
87	CLA	B6	612	-	-	14/32/108/115	-
87	CLA	dL	409	-	-	8/21/97/115	-
82	PEB	BD	202	1	-	10/26/74/74	0/4/4/4
84	CYC	K1	1001	10,9	-	10/26/74/74	0/4/4/4
82	PEB	KD	202	2	-	12/26/74/74	0/4/4/4
84	CYC	BE	1001	10,8	-	13/26/74/74	0/4/4/4
87	CLA	c6	611	-	-	10/39/115/115	-
82	PEB	JI	201	2	-	8/26/74/74	0/4/4/4
82	PEB	RJ	201	2	-	6/26/74/74	0/4/4/4
83	PUB	BJ	302	14	-	7/26/74/74	0/4/4/4
92	LMG	A6	408	-	-	8/46/66/70	0/1/1/1
85	BCR	CL	501	-	-	1/29/63/63	0/2/2/2
82	PEB	VJ	202	2	-	8/26/74/74	0/4/4/4
82	PEB	N1	1002	10	-	10/26/74/74	0/4/4/4
82	PEB	a1	201	2	-	6/26/74/74	0/4/4/4
82	PEB	XP	201	2	-	6/26/74/74	0/4/4/4
98	PQN	BN	837	41	-	5/23/43/43	0/2/2/2
87	CLA	22	606	58	-	9/15/91/115	-
82	PEB	mG	202	2	-	8/26/74/74	0/4/4/4
84	CYC	J1	1001	10	-	6/26/74/74	0/4/4/4
82	PEB	EJ	201	1,2	-	7/26/74/74	0/4/4/4
87	CLA	R2	204	-	-	11/15/91/115	-
92	LMG	b6	624	-	-	11/31/51/70	0/1/1/1
82	PEB	eH	202	2	-	11/26/74/74	0/4/4/4
82	PEB	jF	202	2	-	12/26/74/74	0/4/4/4
87	CLA	12	602	57	-	15/39/115/115	-
84	CYC	e3	1001	68	-	8/26/74/74	0/4/4/4
82	PEB	O9	202	2	-	8/26/74/74	0/4/4/4
96	HEM	E6	101	19	-	2/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	SF	202	1	-	8/26/74/74	0/4/4/4
82	PEB	PO	201	2	-	5/26/74/74	0/4/4/4
82	PEB	nF	202	2	-	11/26/74/74	0/4/4/4
82	PEB	YM	203	1	-	13/26/74/74	0/4/4/4
92	LMG	JL	102	-	-	16/38/58/70	0/1/1/1
82	PEB	EP	203	1,2	-	13/26/74/74	0/4/4/4
82	PEB	VB	201	2	-	10/26/74/74	0/4/4/4
84	CYC	IG	1001	10,9	-	10/26/74/74	0/4/4/4
82	PEB	dM	201	1,2	-	7/26/74/74	0/4/4/4
87	CLA	C6	515	17	-	13/39/115/115	-
82	PEB	hK	202	2	-	9/26/74/74	0/4/4/4
82	PEB	vF	201	2	-	7/26/74/74	0/4/4/4
87	CLA	C6	516	-	-	10/39/115/115	-
82	PEB	I9	201	1	-	7/26/74/74	0/4/4/4
82	PEB	zF	501	78,2	-	7/26/74/74	0/4/4/4
82	PEB	eO	201	2	-	5/26/74/74	0/4/4/4
82	PEB	XD	202	1	-	12/26/74/74	0/4/4/4
82	PEB	X7	202	2	-	9/26/74/74	0/4/4/4
87	CLA	a6	609	-	-	6/21/97/115	-
87	CLA	CL	512	-	-	6/39/115/115	-
82	PEB	EI	201	1	-	9/26/74/74	0/4/4/4
82	PEB	aK	201	1,2	-	9/26/74/74	0/4/4/4
82	PEB	QM	204	1	-	10/26/74/74	0/4/4/4
87	CLA	3N	307	-	-	4/12/88/115	-
87	CLA	22	603	-	-	9/15/91/115	-
82	PEB	v8	201	1	-	10/26/74/74	0/4/4/4
82	PEB	lO	202	1	-	10/26/74/74	0/4/4/4
82	PEB	GJ	202	1	-	6/26/74/74	0/4/4/4
83	PUB	xF	301	13	-	6/26/74/74	0/4/4/4
87	CLA	K2	106	40,49	-	10/20/96/115	-
99	SF4	C2	102	42	-	-	0/6/5/5
87	CLA	B2	811	-	-	7/27/103/115	-
82	PEB	eH	201	2	-	8/26/74/74	0/4/4/4
82	PEB	WG	202	1,77	-	7/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	aJ	202	1	-	7/26/74/74	0/4/4/4
87	CLA	AN	825	-	-	7/27/103/115	-
82	PEB	sC	202	2	-	8/26/74/74	0/4/4/4
82	PEB	O9	201	2	-	12/26/74/74	0/4/4/4
82	PEB	K9	201	1	-	7/26/74/74	0/4/4/4
82	PEB	t8	202	1	-	18/26/74/74	0/4/4/4
82	PEB	JP	202	2	-	6/26/74/74	0/4/4/4
82	PEB	nF	201	2	-	7/26/74/74	0/4/4/4
82	PEB	UB	303	2,5	-	8/26/74/74	0/4/4/4
82	PEB	O5	202	2	-	11/26/74/74	0/4/4/4
82	PEB	HD	202	1	-	12/26/74/74	0/4/4/4
87	CLA	22	602	58	-	16/39/115/115	-
82	PEB	I5	201	1	-	11/26/74/74	0/4/4/4
82	PEB	mM	201	13,2	-	7/26/74/74	0/4/4/4
87	CLA	B6	607	-	-	16/39/115/115	-
87	CLA	BN	818	41	-	12/33/109/115	-
82	PEB	oK	203	1	-	15/26/74/74	0/4/4/4
82	PEB	AM	302	13	-	8/26/74/74	0/4/4/4
82	PEB	QE	203	1	-	10/26/74/74	0/4/4/4
82	PEB	SK	203	1	-	9/26/74/74	0/4/4/4
82	PEB	ZK	201	2	-	9/26/74/74	0/4/4/4
82	PEB	U4	202	1	-	10/26/74/74	0/4/4/4
82	PEB	AH	302	3	-	11/26/74/74	0/4/4/4
82	PEB	OQ	202	2	-	14/26/74/74	0/4/4/4
87	CLA	K6	101	25	-	14/39/115/115	-
82	PEB	bH	202	1	-	10/26/74/74	0/4/4/4
83	PUB	ND	201	1,3	-	1/26/74/74	0/4/4/4
82	PEB	HJ	202	2	-	9/26/74/74	0/4/4/4
82	PEB	WJ	201	1	-	4/26/74/74	0/4/4/4
87	CLA	A2	838	-	-	15/39/115/115	-
82	PEB	QO	201	1	-	8/26/74/74	0/4/4/4
82	PEB	NI	202	1	-	10/26/74/74	0/4/4/4
84	CYC	BG	1002	10,8	-	7/26/74/74	0/4/4/4
94	PL9	AL	413	-	-	13/53/73/73	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	HH	1002	10	-	8/26/74/74	0/4/4/4
82	PEB	UI	202	2	-	6/26/74/74	0/4/4/4
82	PEB	RM	202	2	-	11/26/74/74	0/4/4/4
82	PEB	T4	201	2	-	5/26/74/74	0/4/4/4
82	PEB	L9	202	2	-	8/26/74/74	0/4/4/4
84	CYC	GE	1001	10,9	-	9/26/74/74	0/4/4/4
82	PEB	BQ	202	1	-	10/26/74/74	0/4/4/4
82	PEB	OA	202	1	-	10/26/74/74	0/4/4/4
82	PEB	kJ	202	2	-	7/26/74/74	0/4/4/4
83	PUB	M5	302	1,74	-	7/26/74/74	0/4/4/4
82	PEB	sC	201	2	-	7/26/74/74	0/4/4/4
87	CLA	3N	301	59	-	5/15/91/115	-
82	PEB	OI	201	2	-	8/26/74/74	0/4/4/4
92	LMG	D6	407	18,24	-	7/28/48/70	0/1/1/1
92	LMG	DL	402	18	-	18/49/69/70	0/1/1/1
82	PEB	EB	501	2,4	-	10/26/74/74	0/4/4/4
82	PEB	h1	201	1,74,2	-	9/26/74/74	0/4/4/4
87	CLA	LN	202	50	-	16/30/106/115	-
82	PEB	E9	201	1	-	7/26/74/74	0/4/4/4
87	CLA	B2	808	-	-	14/39/115/115	-
82	PEB	dJ	202	1	-	6/26/74/74	0/4/4/4
82	PEB	HM	202	2	-	11/26/74/74	0/4/4/4
82	PEB	fH	201	1	-	9/26/74/74	0/4/4/4
87	CLA	B2	812	-	-	28/39/115/115	-
87	CLA	5N	606	61	-	6/15/91/115	-
82	PEB	O5	201	74,2,82	-	9/26/74/74	0/4/4/4
82	PEB	JF	201	2	-	8/26/74/74	0/4/4/4
91	PHO	D6	404	-	3/3/17/22	7/37/103/103	0/5/6/6
82	PEB	DM	201	14,2	-	10/26/74/74	0/4/4/4
83	PUB	A4	302	3	-	2/26/74/74	0/4/4/4
82	PEB	cH	201	2	-	7/26/74/74	0/4/4/4
85	BCR	B2	838	-	-	5/29/63/63	0/2/2/2
103	ZEX	82	309	64	-	11/29/67/67	0/2/2/2
82	PEB	FK	202	2	-	11/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	NQ	202	1	-	11/26/74/74	0/4/4/4
82	PEB	U4	201	1	-	8/26/74/74	0/4/4/4
87	CLA	32	308	59	-	5/15/91/115	-
87	CLA	52	604	61	-	6/12/88/115	-
92	LMG	b6	619	-	-	5/36/56/70	0/1/1/1
82	PEB	vC	202	1	-	15/26/74/74	0/4/4/4
82	PEB	cO	202	2	-	11/26/74/74	0/4/4/4
82	PEB	PM	202	2	-	7/26/74/74	0/4/4/4
84	CYC	CG	1001	10,9	-	10/26/74/74	0/4/4/4
82	PEB	WE	203	1,2	-	7/26/74/74	0/4/4/4
82	PEB	b1	203	1,2	-	7/26/74/74	0/4/4/4
82	PEB	GJ	203	1,2	-	8/26/74/74	0/4/4/4
92	LMG	B6	618	-	-	10/35/55/70	0/1/1/1
82	PEB	W1	201	1	-	8/26/74/74	0/4/4/4
82	PEB	Q5	203	2	-	12/26/74/74	0/4/4/4
82	PEB	BB	202	2	-	7/26/74/74	0/4/4/4
82	PEB	PQ	202	1	-	9/26/74/74	0/4/4/4
82	PEB	l1	202	1	-	10/26/74/74	0/4/4/4
82	PEB	H7	202	2	-	8/26/74/74	0/4/4/4
82	PEB	OQ	201	3,2,82	-	8/26/74/74	0/4/4/4
84	CYC	LH	1002	10	-	12/26/74/74	0/4/4/4
85	BCR	BL	616	-	-	4/29/63/63	0/2/2/2
87	CLA	62	305	87,62	-	9/12/88/115	-
87	CLA	aL	606	-	1/1/14/20	10/33/109/115	-
87	CLA	B2	826	-	-	18/39/115/115	-
85	BCR	J2	103	40,48	-	13/29/63/63	0/2/2/2
82	PEB	O7	202	1	-	10/26/74/74	0/4/4/4
82	PEB	wF	303	13	-	7/26/74/74	0/4/4/4
82	PEB	D9	201	2	-	10/26/74/74	0/4/4/4
82	PEB	NK	202	2	-	12/26/74/74	0/4/4/4
87	CLA	bL	607	-	-	16/39/115/115	-
85	BCR	c6	602	-	-	3/29/63/63	0/2/2/2
87	CLA	BN	826	-	-	18/39/115/115	-
82	PEB	TA	203	2	-	7/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	KM	203	1,2	-	6/26/74/74	0/4/4/4
87	CLA	32	306	-	-	4/12/88/115	-
87	CLA	d6	403	-	-	18/39/115/115	-
87	CLA	AN	802	40,45	-	16/39/115/115	-
82	PEB	SQ	202	2	-	10/26/74/74	0/4/4/4
82	PEB	TM	202	2	-	7/26/74/74	0/4/4/4
82	PEB	jO	201	1	-	10/26/74/74	0/4/4/4
82	PEB	x8	202	1	-	15/26/74/74	0/4/4/4
82	PEB	DJ	201	14,2	-	8/26/74/74	0/4/4/4
85	BCR	BN	843	-	-	6/29/63/63	0/2/2/2
87	CLA	52	608	61	-	6/10/86/115	-
87	CLA	5N	602	61	-	12/39/115/115	-
82	PEB	HM	201	2	-	7/26/74/74	0/4/4/4
82	PEB	UQ	202	2	-	7/26/74/74	0/4/4/4
82	PEB	A7	201	1	-	11/26/74/74	0/4/4/4
95	DGD	C6	504	-	-	12/31/71/95	0/2/2/2
103	ZEX	82	310	64,87	-	10/29/67/67	0/2/2/2
87	CLA	B6	609	-	-	14/39/115/115	-
84	CYC	MO	1001	9	-	10/26/74/74	0/4/4/4
87	CLA	2N	304	-	-	9/15/91/115	-
85	BCR	BN	803	87,50,41	-	11/29/63/63	0/2/2/2
82	PEB	e1	202	2	-	11/26/74/74	0/4/4/4
82	PEB	SJ	201	1	-	8/26/74/74	0/4/4/4
82	PEB	Z5	305	74	-	13/26/74/74	0/4/4/4
82	PEB	T7	202	2	-	9/26/74/74	0/4/4/4
87	CLA	bL	619	-	-	8/32/108/115	-
82	PEB	UD	201	3,2	-	9/26/74/74	0/4/4/4
82	PEB	A4	304	3	-	9/26/74/74	0/4/4/4
82	PEB	DP	202	2	-	6/26/74/74	0/4/4/4
82	PEB	bG	201	1	-	6/26/74/74	0/4/4/4
82	PEB	lH	201	1	-	10/26/74/74	0/4/4/4
87	CLA	A2	823	40	-	20/39/115/115	-
84	CYC	EH	1001	10,9	-	9/26/74/74	0/4/4/4
87	CLA	AN	801	-	-	9/13/90/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	QJ	203	1	-	7/26/74/74	0/4/4/4
87	CLA	b6	606	16	-	10/39/115/115	-
95	DGD	c6	618	-	-	10/51/91/95	0/2/2/2
82	PEB	MK	201	1	-	6/26/74/74	0/4/4/4
82	PEB	bE	202	1	-	12/26/74/74	0/4/4/4
82	PEB	iG	202	2	-	10/26/74/74	0/4/4/4
82	PEB	LJ	201	2	-	6/26/74/74	0/4/4/4
82	PEB	aF	201	1,2	-	9/26/74/74	0/4/4/4
95	DGD	BL	613	-	-	7/29/69/95	0/2/2/2
84	CYC	d3	1001	73,69	-	4/26/74/74	0/4/4/4
87	CLA	RN	203	54,41	-	8/17/93/115	-
87	CLA	52	606	61	-	6/15/91/115	-
82	PEB	ZF	202	2	-	10/26/74/74	0/4/4/4
82	PEB	WO	201	1	-	6/26/74/74	0/4/4/4
82	PEB	SH	201	1	-	7/26/74/74	0/4/4/4
82	PEB	MJ	201	1,2	-	7/26/74/74	0/4/4/4
84	CYC	C1	1001	10,9	-	8/26/74/74	0/4/4/4
82	PEB	N5	201	1	-	11/26/74/74	0/4/4/4
82	PEB	W7	201	1	-	7/26/74/74	0/4/4/4
82	PEB	D9	203	2	-	7/26/74/74	0/4/4/4
82	PEB	gG	201	2	-	6/26/74/74	0/4/4/4
82	PEB	SB	203	2	-	8/26/74/74	0/4/4/4
83	PUB	A1	303	3	-	5/26/74/74	0/4/4/4
82	PEB	GI	203	1	-	10/26/74/74	0/4/4/4
87	CLA	AN	829	-	-	17/39/115/115	-
82	PEB	UQ	201	3,2	-	9/26/74/74	0/4/4/4
82	PEB	tC	202	1	-	18/26/74/74	0/4/4/4
82	PEB	bK	201	2	-	4/26/74/74	0/4/4/4
82	PEB	AM	301	13	-	12/26/74/74	0/4/4/4
82	PEB	YQ	202	2	-	8/26/74/74	0/4/4/4
82	PEB	p8	202	1	-	16/26/74/74	0/4/4/4
82	PEB	FI	202	2	-	9/26/74/74	0/4/4/4
82	PEB	NF	201	2	-	7/26/74/74	0/4/4/4
87	CLA	A2	837	-	-	8/23/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	UG	202	1	-	9/26/74/74	0/4/4/4
87	CLA	L2	204	50	-	13/21/97/115	-
82	PEB	BA	201	2,82	-	8/26/74/74	0/4/4/4
82	PEB	Y9	201	2	-	10/26/74/74	0/4/4/4
82	PEB	JQ	202	1	-	12/26/74/74	0/4/4/4
82	PEB	OP	202	1	-	4/26/74/74	0/4/4/4
82	PEB	R5	202	1	-	11/26/74/74	0/4/4/4
87	CLA	B2	807	-	-	11/39/115/115	-
82	PEB	l1	203	1	-	13/26/74/74	0/4/4/4
82	PEB	NB	203	2	-	13/26/74/74	0/4/4/4
87	CLA	BN	830	-	-	15/39/115/115	-
82	PEB	f1	203	1,2	-	12/26/74/74	0/4/4/4
84	CYC	LG	1001	10	-	11/26/74/74	0/4/4/4
87	CLA	MN	101	51,41	-	10/15/91/115	-
82	PEB	TO	203	2	-	10/26/74/74	0/4/4/4
82	PEB	V4	202	2	-	12/26/74/74	0/4/4/4
82	PEB	x8	201	1	-	11/26/74/74	0/4/4/4
82	PEB	NP	202	2	-	6/26/74/74	0/4/4/4
83	PUB	yK	303	14	-	5/26/74/74	0/4/4/4
83	PUB	xK	301	13	-	6/26/74/74	0/4/4/4
85	BCR	c6	617	-	-	9/29/63/63	0/2/2/2
82	PEB	dE	204	1	-	12/26/74/74	0/4/4/4
82	PEB	rK	201	13,2	-	11/26/74/74	0/4/4/4
82	PEB	sK	203	1,2	-	6/26/74/74	0/4/4/4
87	CLA	AN	806	-	-	9/27/103/115	-
87	CLA	A2	850	40	-	6/39/115/115	-
82	PEB	RF	202	2	-	13/26/74/74	0/4/4/4
82	PEB	KI	203	1	-	10/26/74/74	0/4/4/4
87	CLA	62	311	-	-	5/12/88/115	-
87	CLA	8N	302	64	-	10/15/91/115	-
82	PEB	FQ	201	1	-	11/26/74/74	0/4/4/4
87	CLA	A2	802	-	-	9/13/90/115	-
82	PEB	VO	201	2	-	4/26/74/74	0/4/4/4
87	CLA	B6	610	-	-	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	CLA	82	307	-	-	5/12/88/115	-
95	DGD	B6	620	16	-	12/47/87/95	0/2/2/2
82	PEB	JD	203	1,2	-	14/26/74/74	0/4/4/4
82	PEB	U1	203	1	-	9/26/74/74	0/4/4/4
82	PEB	XA	203	2	-	12/26/74/74	0/4/4/4
87	CLA	52	602	61	-	12/39/115/115	-
87	CLA	AL	404	87	-	6/33/109/115	-
82	PEB	VB	202	1,2	-	10/26/74/74	0/4/4/4
82	PEB	S4	202	1,76	-	10/26/74/74	0/4/4/4
84	CYC	HH	1001	10	-	8/26/74/74	0/4/4/4
85	BCR	A2	804	-	-	2/29/63/63	0/2/2/2
82	PEB	P5	202	1	-	11/26/74/74	0/4/4/4
82	PEB	D7	203	2	-	11/26/74/74	0/4/4/4
87	CLA	B2	821	-	-	13/27/103/115	-
87	CLA	KN	103	-	-	4/12/88/115	-
82	PEB	ND	202	1	-	11/26/74/74	0/4/4/4
82	PEB	GB	203	2	-	12/26/74/74	0/4/4/4
87	CLA	B2	817	41	-	12/33/109/115	-
87	CLA	2N	306	58	-	9/15/91/115	-
82	PEB	OE	201	1	-	9/26/74/74	0/4/4/4
82	PEB	VI	201	1	-	9/26/74/74	0/4/4/4
82	PEB	GD	201	2	-	4/26/74/74	0/4/4/4
84	CYC	BE	1002	10,8	-	7/26/74/74	0/4/4/4
82	PEB	RH	201	2	-	7/26/74/74	0/4/4/4
87	CLA	A6	403	87	-	9/33/109/115	-
82	PEB	mE	202	2	-	8/26/74/74	0/4/4/4
82	PEB	FF	201	2	-	5/26/74/74	0/4/4/4
82	PEB	KG	201	10,9	-	6/26/74/74	0/4/4/4
82	PEB	dG	201	1,3	-	10/26/74/74	0/4/4/4
84	CYC	CH	1001	10,9	-	8/26/74/74	0/4/4/4
85	BCR	B2	840	41	-	7/29/63/63	0/2/2/2
87	CLA	AN	808	-	-	17/39/115/115	-
82	PEB	rF	201	13,2	-	11/26/74/74	0/4/4/4
82	PEB	OF	202	1	-	9/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	UH	202	1	-	7/26/74/74	0/4/4/4
87	CLA	A2	829	-	-	17/39/115/115	-
82	PEB	OJ	202	1	-	16/26/74/74	0/4/4/4
87	CLA	CL	507	-	-	19/39/115/115	-
82	PEB	FQ	203	1,2	-	9/26/74/74	0/4/4/4
82	PEB	U9	201	74,2	-	10/26/74/74	0/4/4/4
91	PHO	DL	405	-	3/3/17/22	8/37/103/103	0/5/6/6
82	PEB	WK	201	1,2	-	7/26/74/74	0/4/4/4
87	CLA	12	607	57	-	11/21/97/115	-
87	CLA	cL	514	-	-	6/39/115/115	-
82	PEB	tF	202	2	-	11/26/74/74	0/4/4/4
87	CLA	BL	602	-	-	16/39/115/115	-
84	CYC	63	901	73	-	7/26/74/74	0/4/4/4
82	PEB	iM	201	13,2	-	8/26/74/74	0/4/4/4
82	PEB	X9	202	1	-	15/26/74/74	0/4/4/4
82	PEB	g4	202	2	-	8/26/74/74	0/4/4/4
82	PEB	UE	202	1	-	9/26/74/74	0/4/4/4
82	PEB	ZJ	201	2	-	5/26/74/74	0/4/4/4
82	PEB	RF	201	2	-	8/26/74/74	0/4/4/4
82	PEB	kH	203	1,2	-	9/26/74/74	0/4/4/4
82	PEB	VQ	203	1,2	-	14/26/74/74	0/4/4/4
84	CYC	NH	1001	10,8	-	10/26/74/74	0/4/4/4
82	PEB	UB	302	2,5	-	9/26/74/74	0/4/4/4
82	PEB	lF	202	2	-	13/26/74/74	0/4/4/4
87	CLA	AN	824	40	-	10/23/99/115	-
82	PEB	OO	202	1	-	6/26/74/74	0/4/4/4
82	PEB	CA	201	1	-	7/26/74/74	0/4/4/4
82	PEB	NQ	203	1	-	12/26/74/74	0/4/4/4
82	PEB	XB	201	2	-	9/26/74/74	0/4/4/4
82	PEB	V9	202	1	-	15/26/74/74	0/4/4/4
82	PEB	TA	202	2	-	9/26/74/74	0/4/4/4
82	PEB	s8	201	2	-	7/26/74/74	0/4/4/4
87	CLA	62	313	62	-	9/15/91/115	-
82	PEB	UK	202	1	-	10/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	CLA	32	312	59	-	9/15/91/115	-
87	CLA	B2	810	-	-	20/39/115/115	-
82	PEB	A5	201	1	-	11/26/74/74	0/4/4/4
82	PEB	dG	203	1	-	8/26/74/74	0/4/4/4
82	PEB	jJ	201	1	-	6/26/74/74	0/4/4/4
87	CLA	2N	305	-	-	3/12/88/115	-
87	CLA	BN	809	-	-	14/39/115/115	-
82	PEB	tK	203	1,2	-	11/26/74/74	0/4/4/4
82	PEB	GF	201	1,2	-	8/26/74/74	0/4/4/4
87	CLA	3N	311	-	-	9/12/88/115	-
82	PEB	WH	203	1,2	-	8/26/74/74	0/4/4/4
82	PEB	CJ	203	1,2	-	8/26/74/74	0/4/4/4
82	PEB	k1	202	2	-	8/26/74/74	0/4/4/4
82	PEB	qC	203	2	-	6/26/74/74	0/4/4/4
82	PEB	eE	202	2	-	7/26/74/74	0/4/4/4
82	PEB	QK	202	1	-	7/26/74/74	0/4/4/4
87	CLA	b6	609	-	-	19/39/115/115	-
87	CLA	22	607	58	-	8/15/91/115	-
85	BCR	c6	603	87,17	-	10/29/63/63	0/2/2/2
82	PEB	lO	201	1	-	8/26/74/74	0/4/4/4
95	DGD	BL	614	-	-	15/47/87/95	0/2/2/2
82	PEB	IP	201	1	-	5/26/74/74	0/4/4/4
82	PEB	cJ	201	2	-	6/26/74/74	0/4/4/4
82	PEB	iF	201	1,2	-	9/26/74/74	0/4/4/4
87	CLA	A2	828	40	-	13/39/115/115	-
82	PEB	KF	203	1	-	8/26/74/74	0/4/4/4
88	LHG	iL	101	-	-	16/53/53/53	-
82	PEB	cG	201	2	-	6/26/74/74	0/4/4/4
83	PUB	yK	302	14	-	3/26/74/74	0/4/4/4
87	CLA	bL	613	16	-	13/39/115/115	-
82	PEB	WD	201	3,2	-	4/26/74/74	0/4/4/4
87	CLA	32	305	-	-	8/15/91/115	-
82	PEB	F5	202	2	-	10/26/74/74	0/4/4/4
85	BCR	LN	201	-	-	12/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	CLA	B2	834	-	-	15/39/115/115	-
87	CLA	bL	605	-	-	8/39/115/115	-
82	PEB	TP	201	56,2	-	7/26/74/74	0/4/4/4
87	CLA	AN	837	-	-	8/23/99/115	-
82	PEB	SK	202	1	-	8/26/74/74	0/4/4/4
88	LHG	AN	844	-	-	17/44/44/53	-
82	PEB	fO	202	1	-	11/26/74/74	0/4/4/4
84	CYC	KH	1001	10,9	-	10/26/74/74	0/4/4/4
82	PEB	LM	201	2	-	4/26/74/74	0/4/4/4
82	PEB	OF	203	1	-	9/26/74/74	0/4/4/4
85	BCR	A2	845	40	-	11/29/63/63	0/2/2/2
82	PEB	UP	202	1	-	10/26/74/74	0/4/4/4
82	PEB	L5	202	2	-	10/26/74/74	0/4/4/4
87	CLA	32	311	-	-	9/12/88/115	-
82	PEB	E5	201	1	-	11/26/74/74	0/4/4/4
82	PEB	AI	201	1	-	9/26/74/74	0/4/4/4
84	CYC	x3	1001	-	-	10/26/74/74	0/4/4/4
82	PEB	zC	201	1	-	10/26/74/74	0/4/4/4
82	PEB	RI	203	1,2	-	10/26/74/74	0/4/4/4
83	PUB	AM	303	13	-	11/26/74/74	0/4/4/4
82	PEB	YP	503	56,2	-	7/26/74/74	0/4/4/4
82	PEB	T9	202	1	-	15/26/74/74	0/4/4/4
82	PEB	RG	202	2	-	12/26/74/74	0/4/4/4
95	DGD	hL	101	22	-	18/51/91/95	0/2/2/2
82	PEB	U1	202	1	-	7/26/74/74	0/4/4/4
87	CLA	52	611	61	-	10/15/91/115	-
82	PEB	XA	202	2	-	9/26/74/74	0/4/4/4
82	PEB	eO	203	2	-	6/26/74/74	0/4/4/4
83	PUB	AM	304	13	-	8/26/74/74	0/4/4/4
87	CLA	7N	609	-	-	7/12/88/115	-
82	PEB	UK	201	1	-	8/26/74/74	0/4/4/4
88	LHG	D6	406	18	-	11/53/53/53	-
92	LMG	a6	614	87	-	3/37/57/70	0/1/1/1
82	PEB	i4	201	2	-	7/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	fF	202	2	-	13/26/74/74	0/4/4/4
84	CYC	I1	1001	10,9	-	9/26/74/74	0/4/4/4
82	PEB	j4	203	-	-	13/26/74/74	0/4/4/4
82	PEB	EM	203	1	-	12/26/74/74	0/4/4/4
87	CLA	52	607	61	-	8/21/97/115	-
87	CLA	AN	832	40	-	10/21/97/115	-
82	PEB	SK	201	1,2	-	4/26/74/74	0/4/4/4
82	PEB	gO	202	2	-	8/26/74/74	0/4/4/4
85	BCR	B2	839	-	-	6/29/63/63	0/2/2/2
82	PEB	W5	202	2	-	11/26/74/74	0/4/4/4
87	CLA	1N	606	-	-	8/15/91/115	-
82	PEB	kM	201	2	-	7/26/74/74	0/4/4/4
82	PEB	ZB	203	2	-	11/26/74/74	0/4/4/4
87	CLA	CL	511	-	-	11/39/115/115	-
82	PEB	HA	203	2	-	12/26/74/74	0/4/4/4
88	LHG	AN	843	40	-	16/53/53/53	-
82	PEB	CD	201	3,2	-	4/26/74/74	0/4/4/4
87	CLA	5N	608	61	-	6/10/86/115	-
82	PEB	g1	201	2	-	9/26/74/74	0/4/4/4
87	CLA	bL	616	-	-	16/39/115/115	-
87	CLA	4N	609	60	-	5/10/86/115	-
82	PEB	TO	201	2	-	5/26/74/74	0/4/4/4
82	PEB	DI	202	2	-	6/26/74/74	0/4/4/4
82	PEB	wK	301	13	-	11/26/74/74	0/4/4/4
82	PEB	D5	201	74,2	-	6/26/74/74	0/4/4/4
82	PEB	dK	201	2	-	9/26/74/74	0/4/4/4
82	PEB	kH	202	2	-	8/26/74/74	0/4/4/4
82	PEB	l4	201	1	-	8/26/74/74	0/4/4/4
82	PEB	aG	202	2	-	14/26/74/74	0/4/4/4
82	PEB	ZI	401	12,2	-	7/26/74/74	0/4/4/4
87	CLA	72	609	-	-	7/12/88/115	-
88	LHG	B6	617	-	-	15/53/53/53	-
88	LHG	D6	401	-	-	16/47/47/53	-
92	LMG	yL	101	-	-	29/50/70/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEB	gB	201	2	-	11/26/74/74	0/4/4/4

The worst 5 of 26459 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	A1	304	PUB	C3A-C2A	13.51	1.49	1.34
83	AH	304	PUB	C3A-C2A	13.34	1.49	1.34
83	M9	303	PUB	C3A-C2A	12.80	1.49	1.34
83	Z9	302	PUB	C3A-C2A	12.78	1.48	1.34
82	WP	201	PEB	C4C-C3C	12.62	1.56	1.37

The worst 5 of 38864 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	62	309	CLA	CHB-C4A-NA	-41.83	66.67	124.51
87	6N	608	CLA	CHB-C4A-NA	-41.80	66.71	124.51
87	62	309	CLA	C4A-NA-C1A	23.13	117.10	106.71
87	6N	608	CLA	C4A-NA-C1A	22.99	117.04	106.71
87	42	604	CLA	C4D-C3D-CAD	-21.59	82.65	108.10

5 of 28 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
87	aL	606	CLA	C8
91	AL	410	PHO	C13
91	AL	410	PHO	C2A
91	AL	410	PHO	C8
91	DL	405	PHO	C13

5 of 23196 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
82	AA	201	PEB	ND-C1D-CHC-C4C
82	AA	201	PEB	C2D-C1D-CHC-C4C
82	AA	201	PEB	NB-C1B-CHA-C4A
82	AA	201	PEB	C2B-C1B-CHA-C4A
82	AA	202	PEB	ND-C1D-CHC-C4C

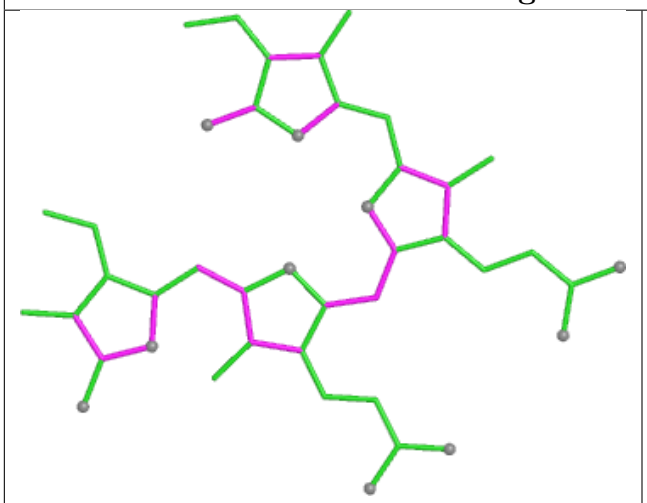
There are no ring outliers.

No monomer is involved in short contacts.

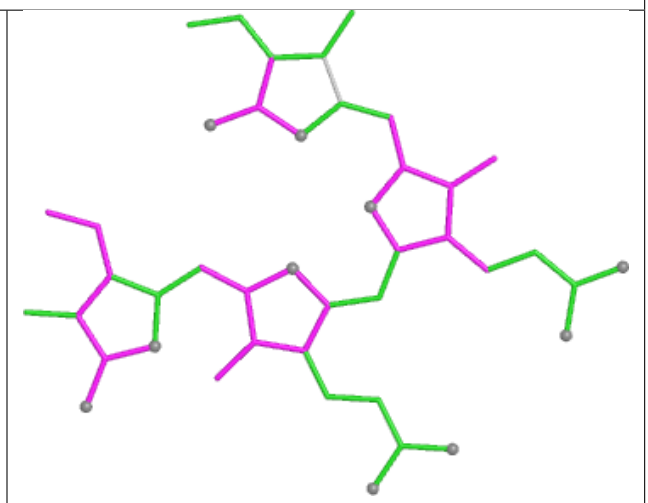
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

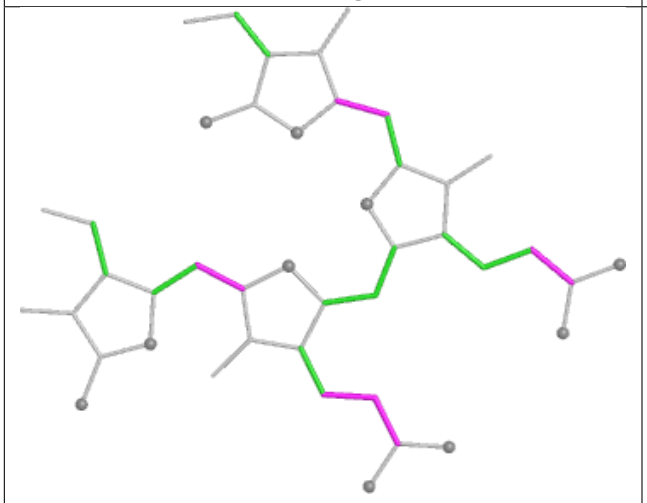
Ligand PEB rC 201



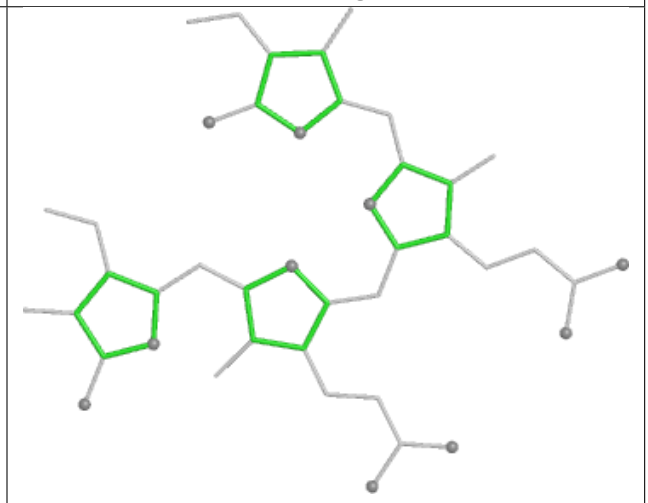
Bond lengths



Bond angles

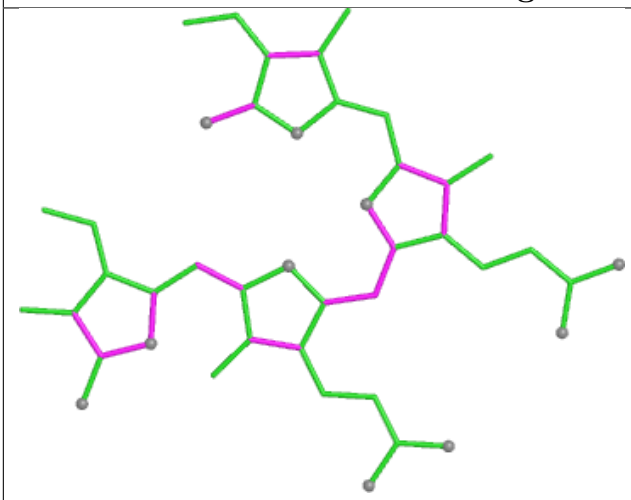


Torsions

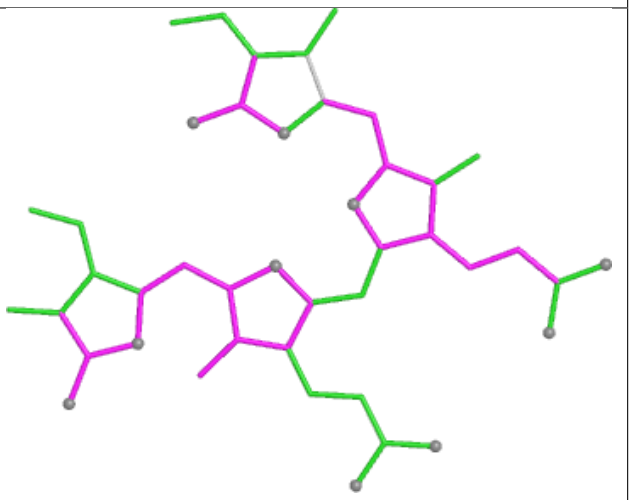


Rings

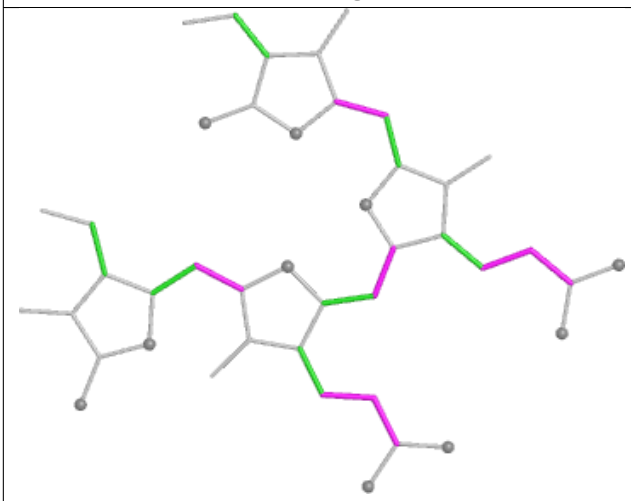
Ligand PEB F5 203



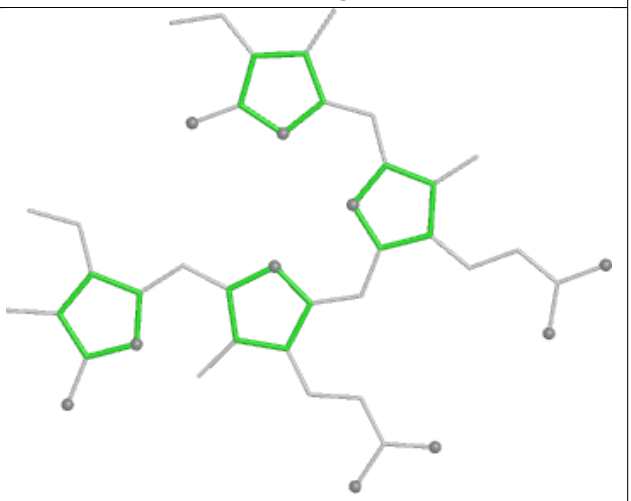
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Bond angles

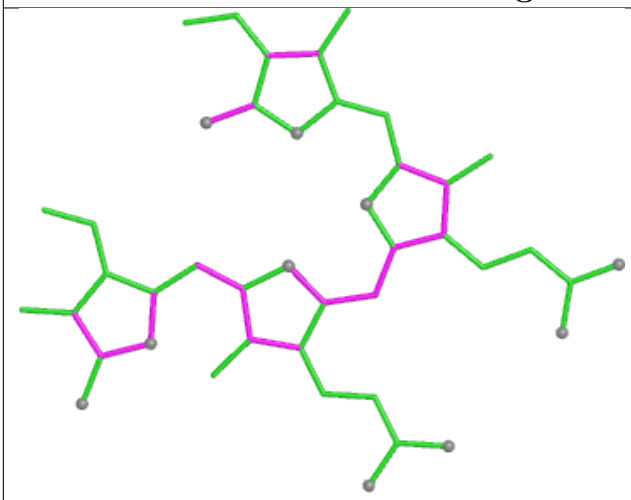


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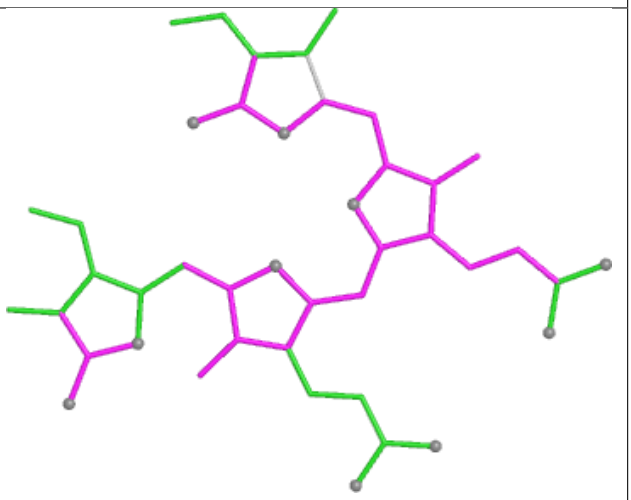


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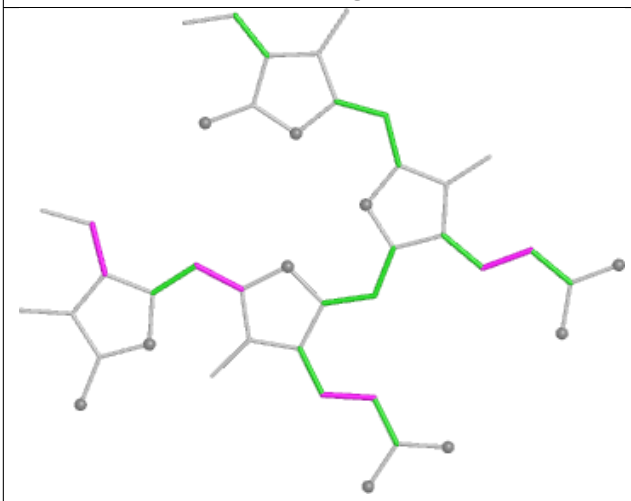
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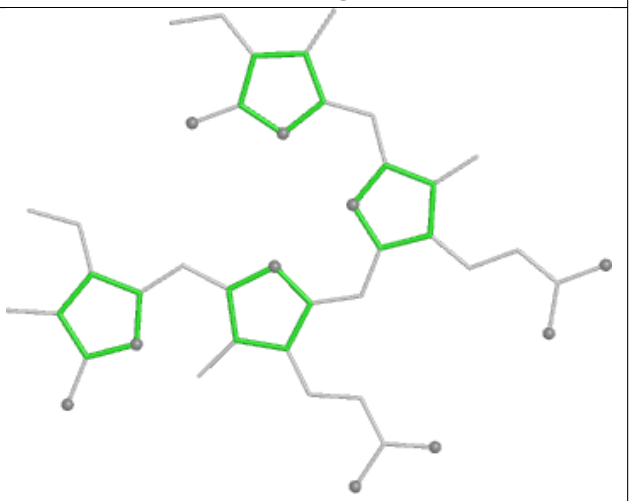
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Bond angles

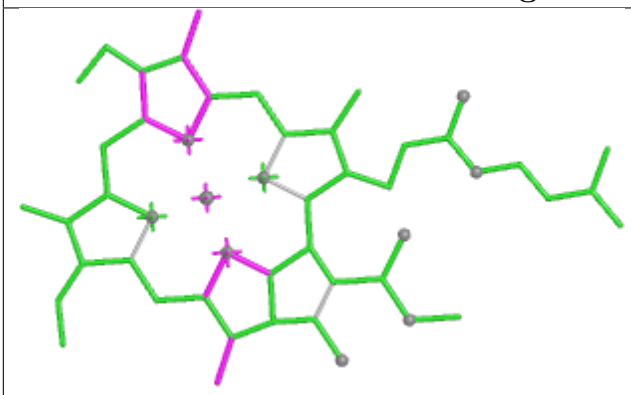


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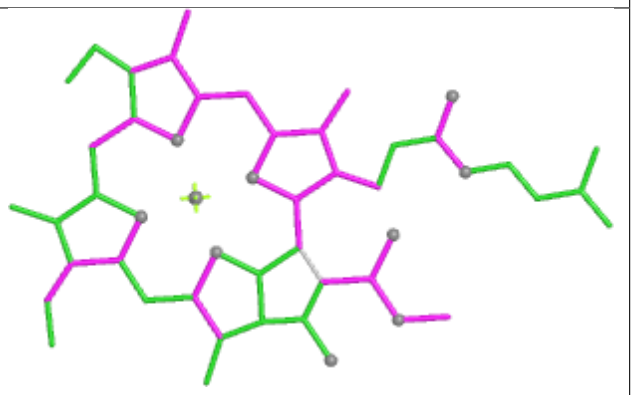


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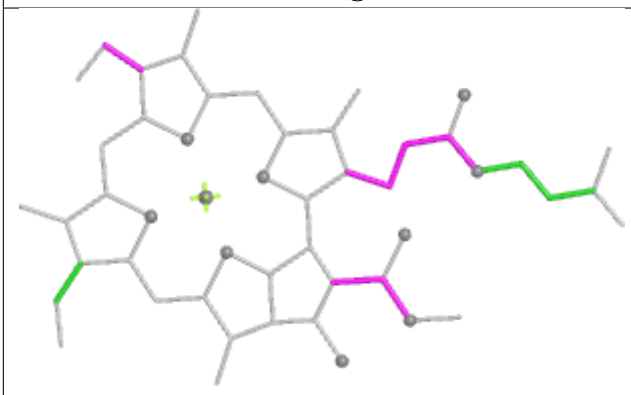
Ligand CLA 42 608



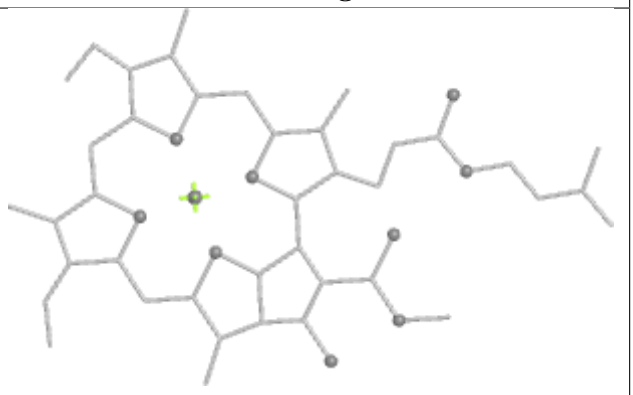
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Bond angles

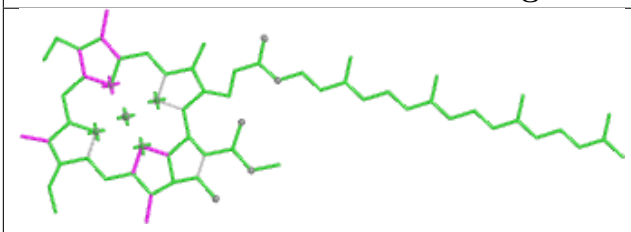


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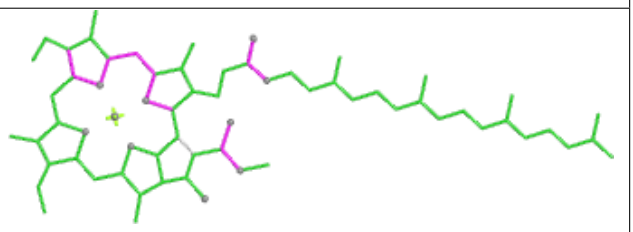


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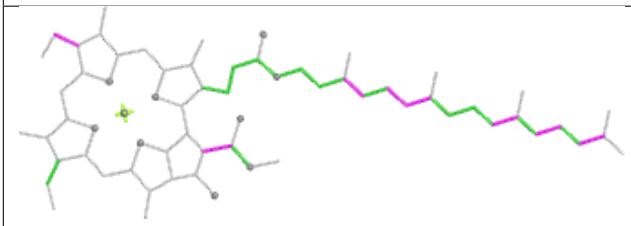
Ligand CLA I2 102



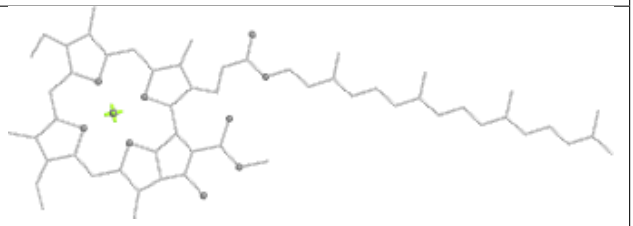
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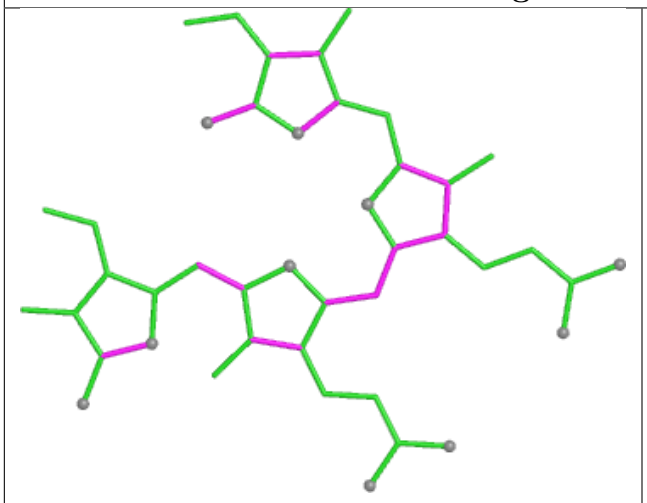


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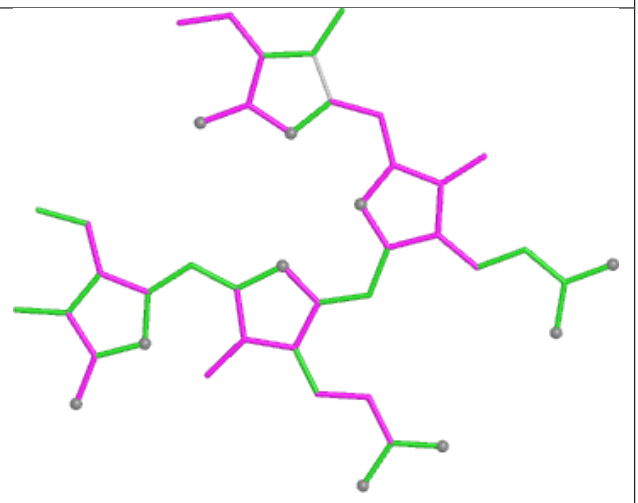


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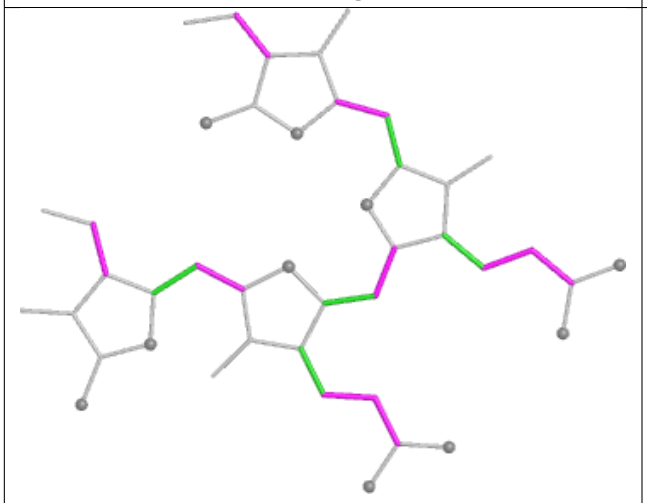
Ligand PEB TH 202



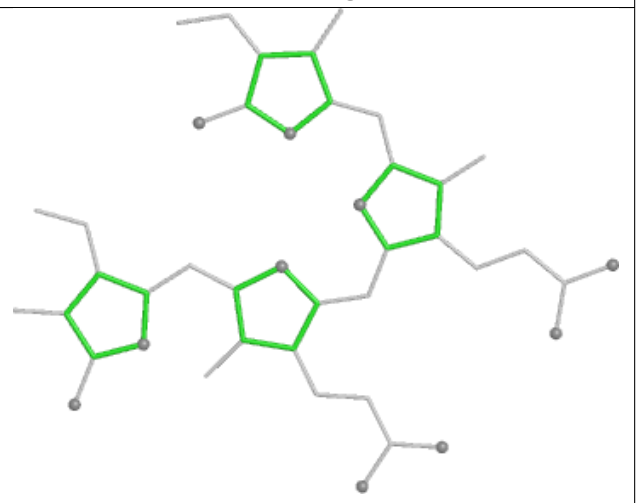
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Bond angles

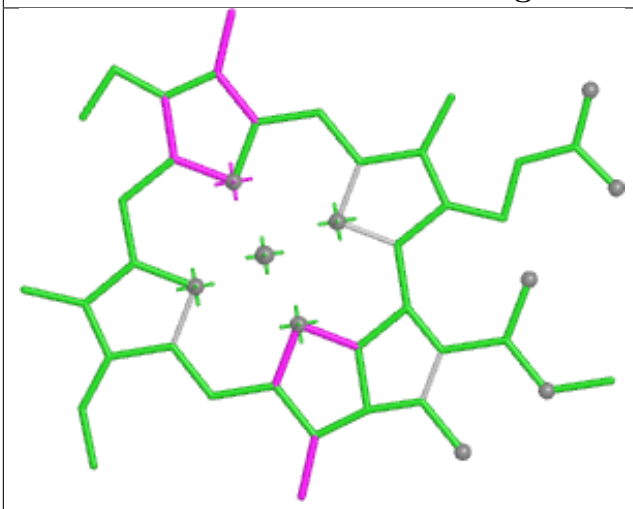


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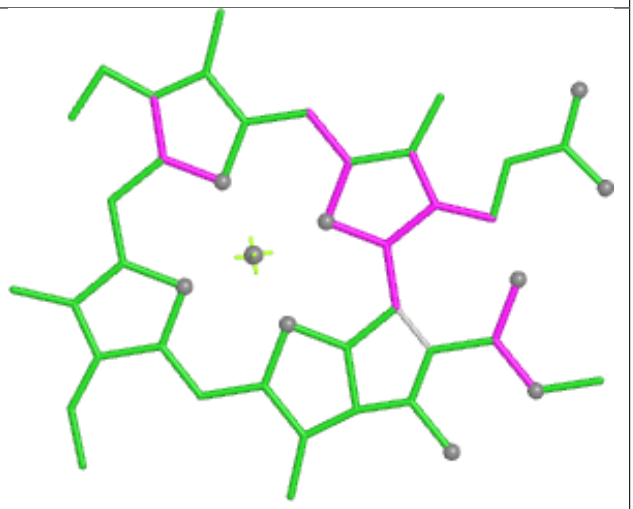


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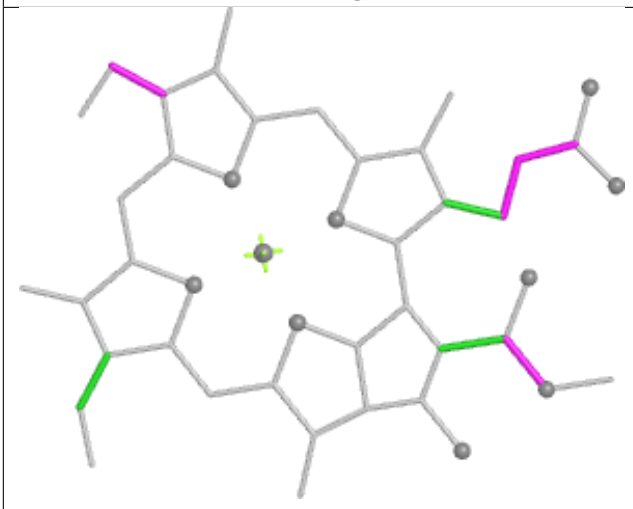
Ligand CLA 8N 305



Bond lengths



Bond angles

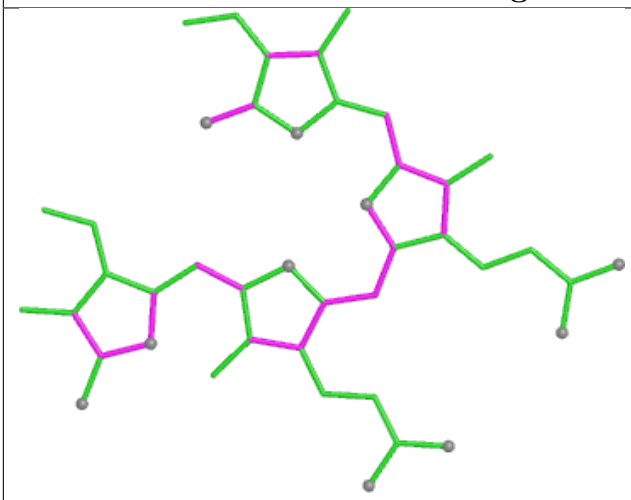


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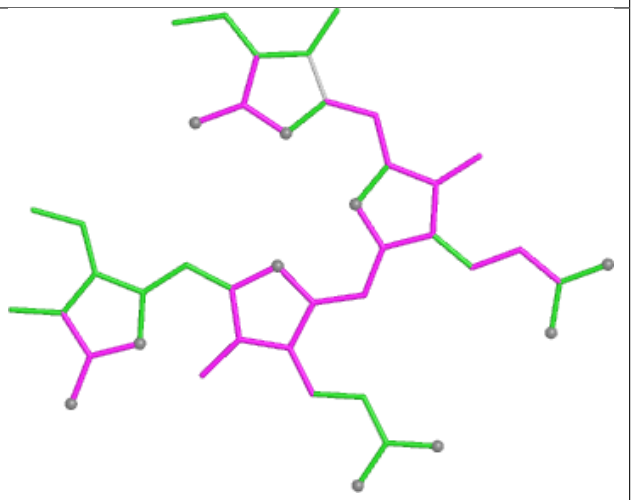


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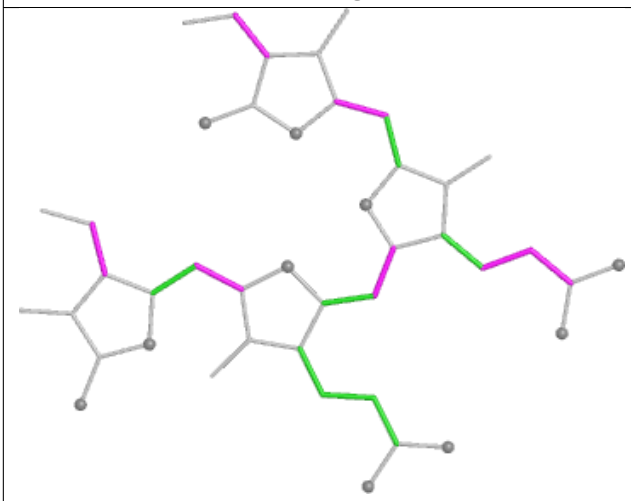
Ligand PEB RK 202



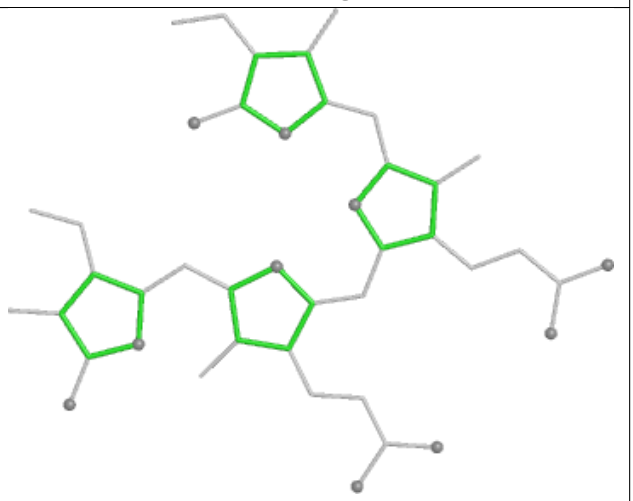
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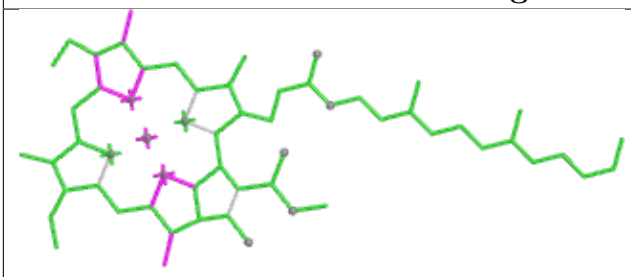


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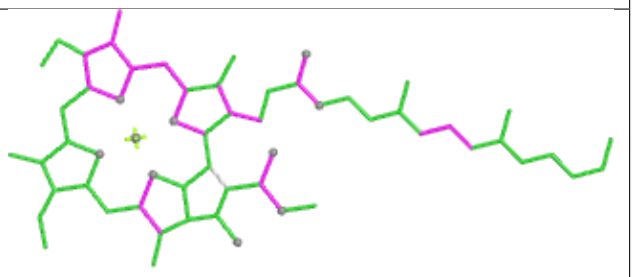


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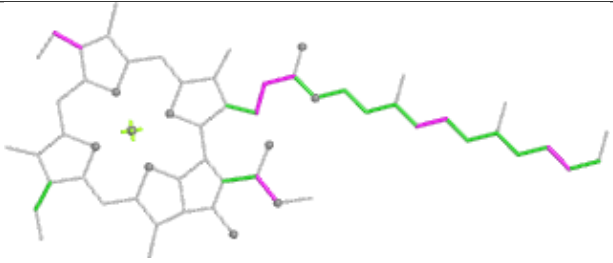
Ligand CLA BN 817



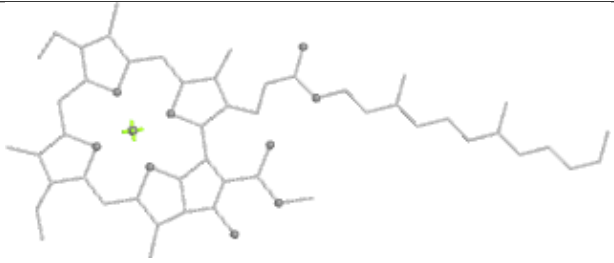
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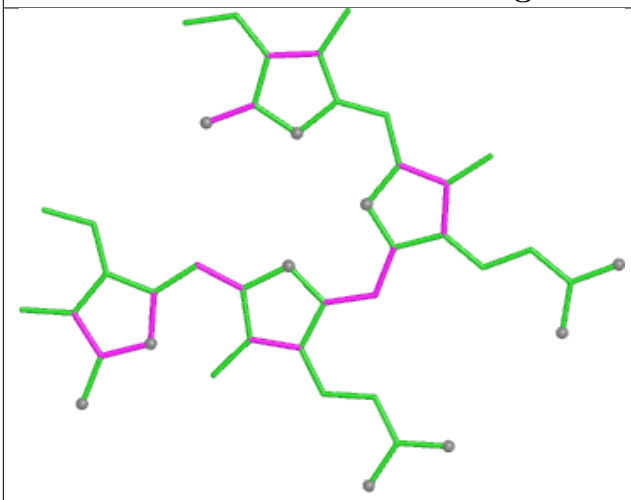


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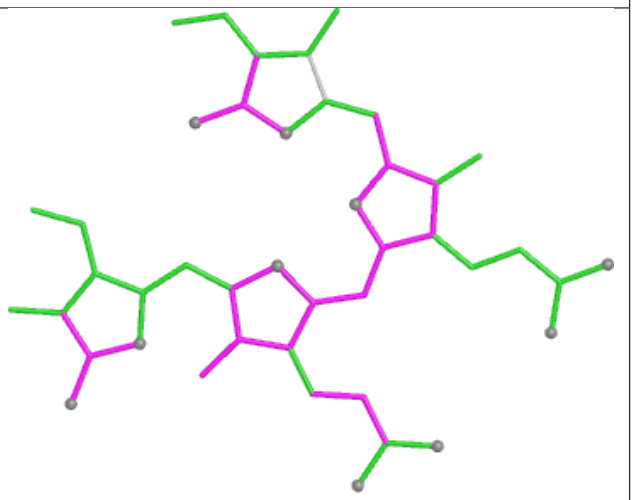


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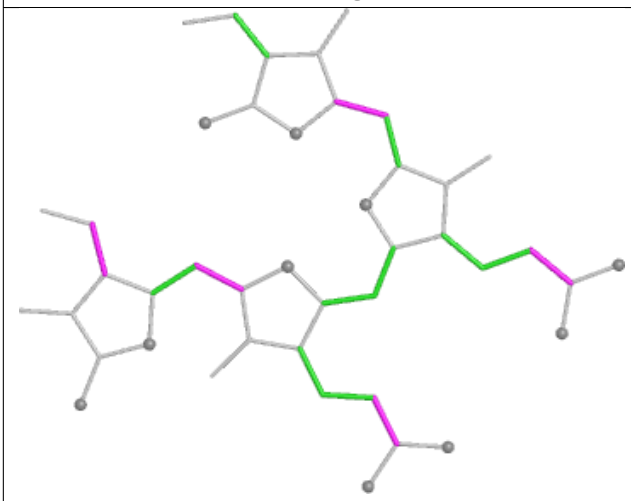
Ligand PEB dO 201



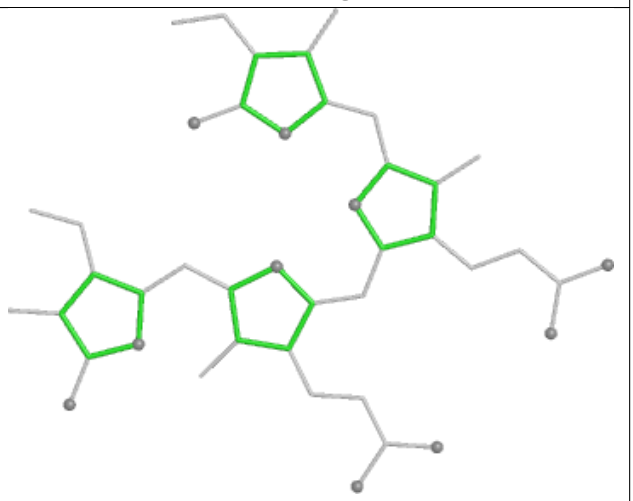
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Bond angles

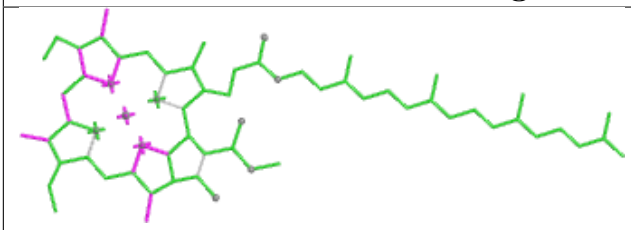


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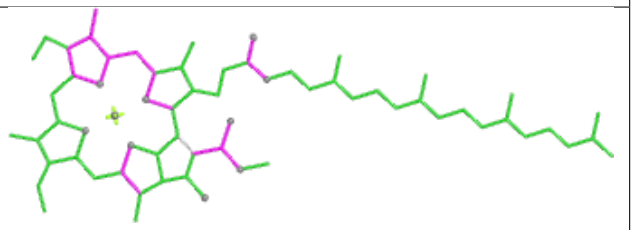


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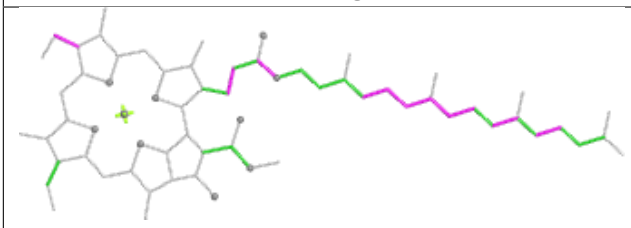
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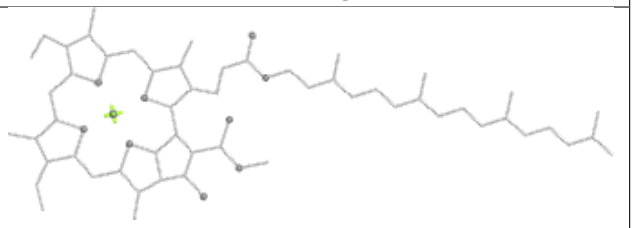
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Bond angles

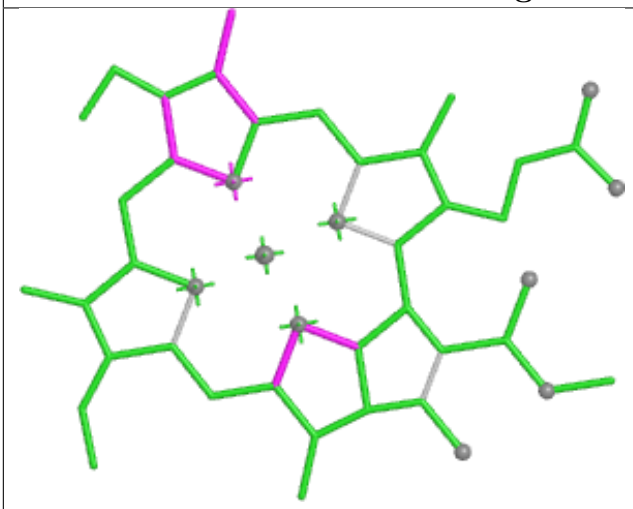


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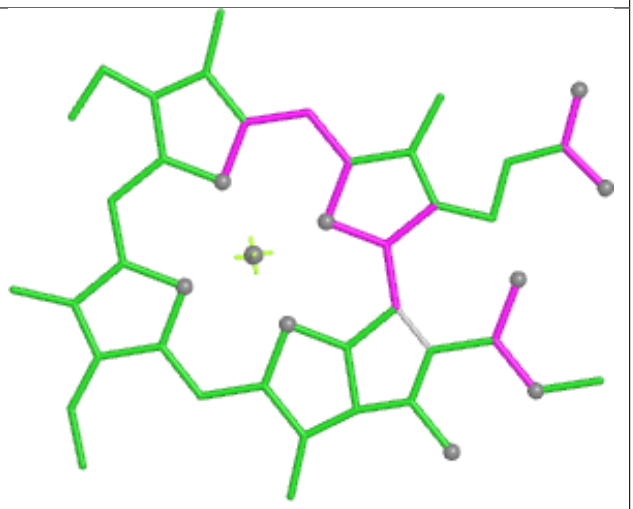


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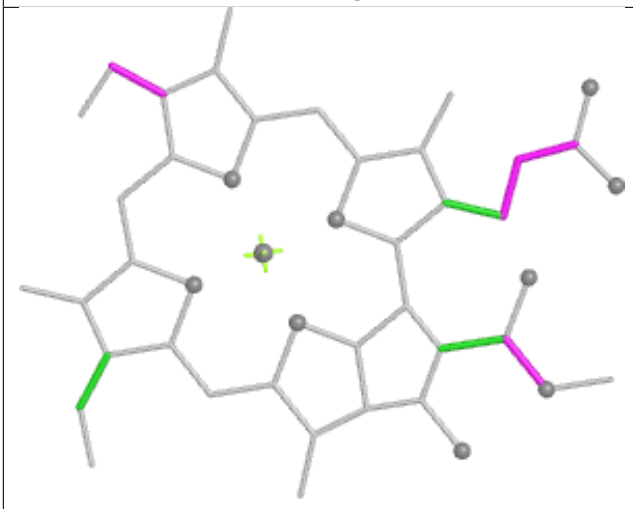
Ligand CLA R2 201



Bond lengths



Bond angles

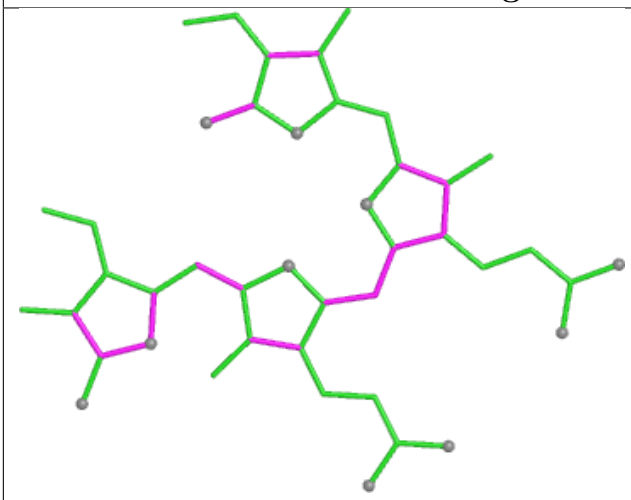


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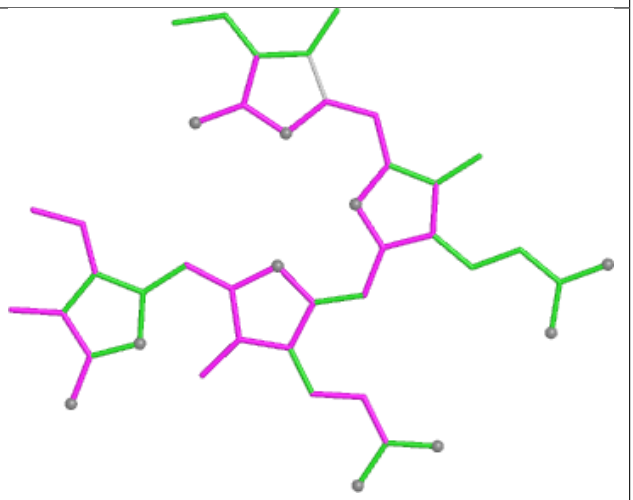


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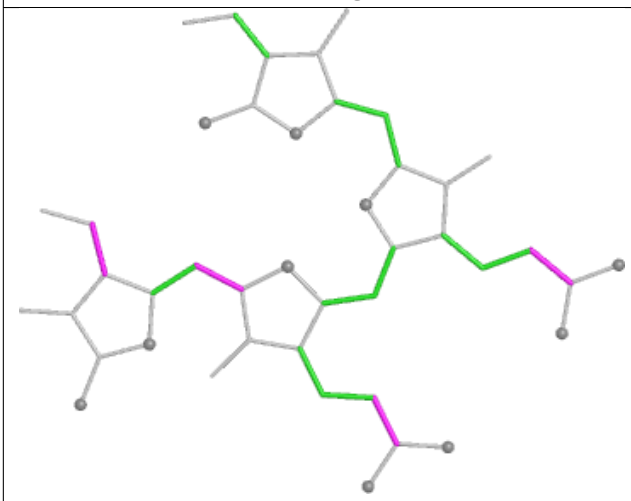
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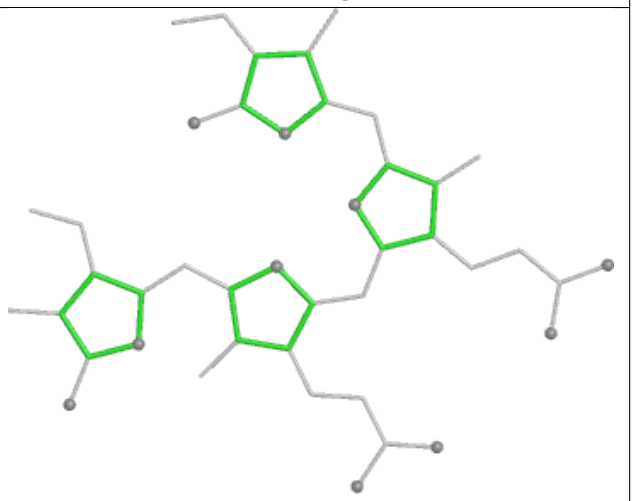
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Bond angles

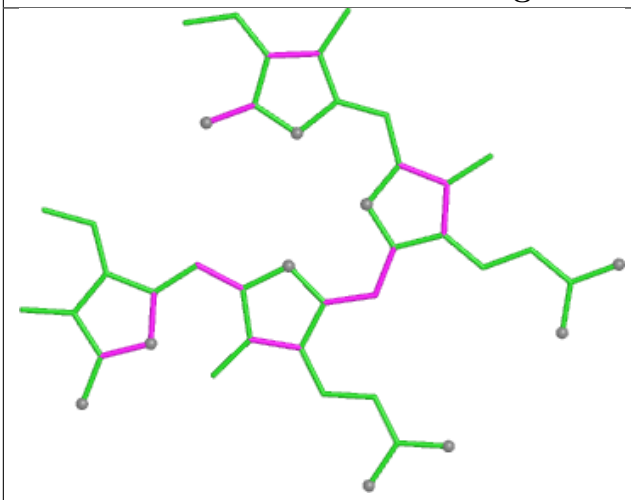


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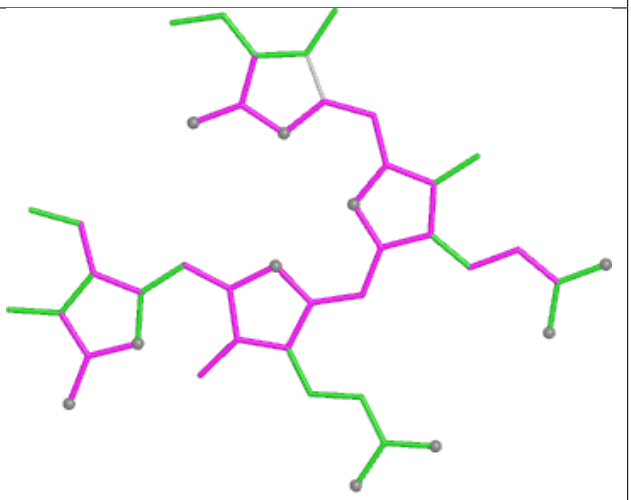


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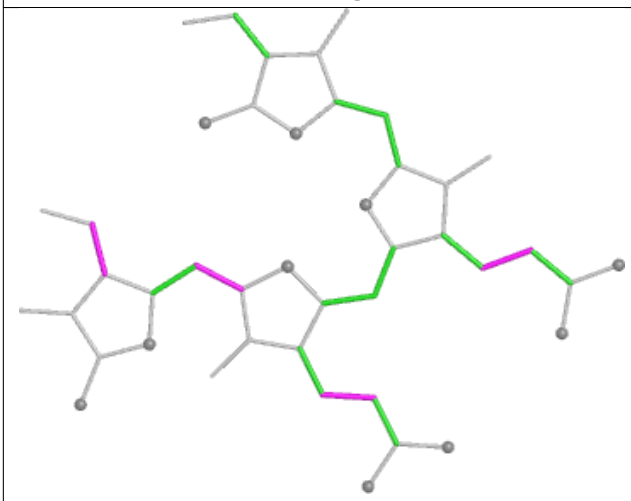
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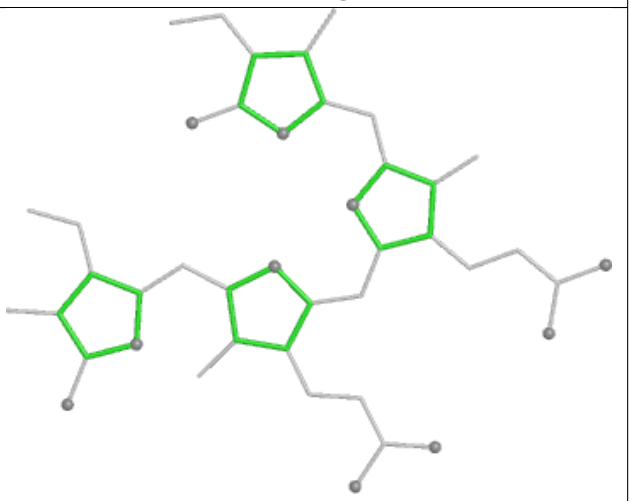
Bond lengths



Bond angles

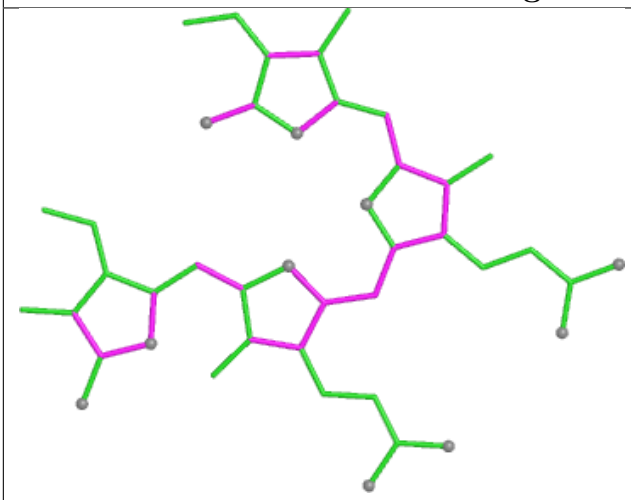


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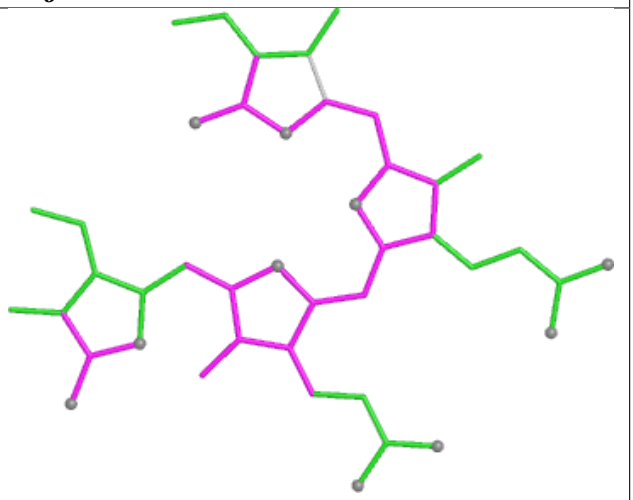


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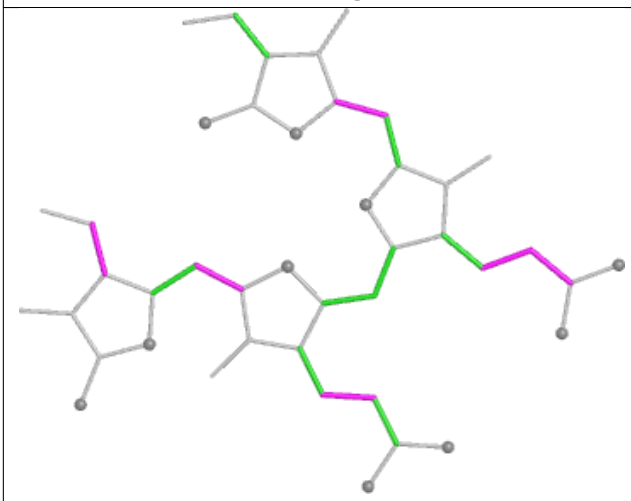
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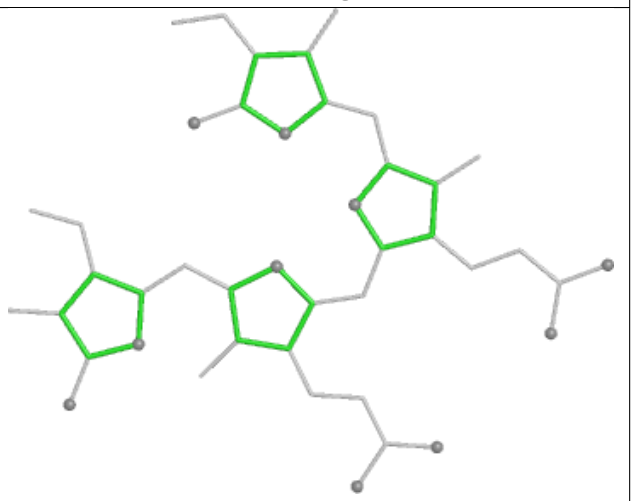
Bond lengths



Bond angles

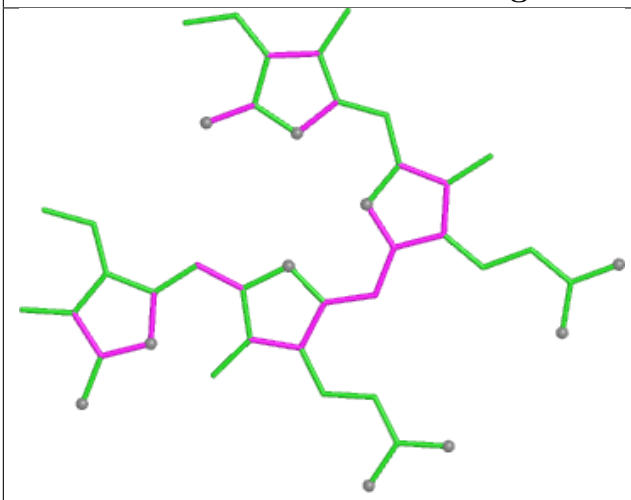


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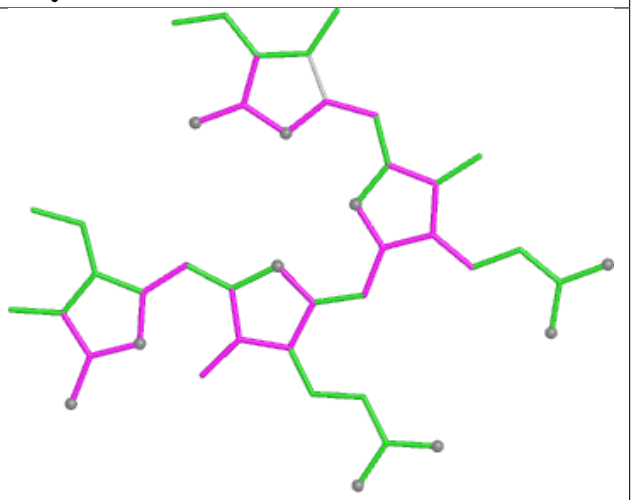


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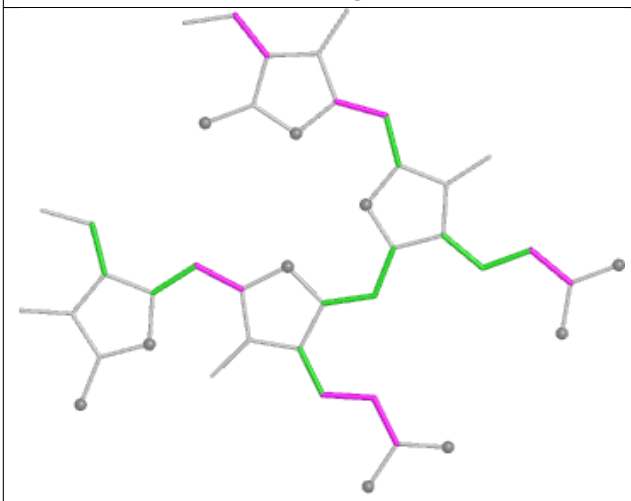
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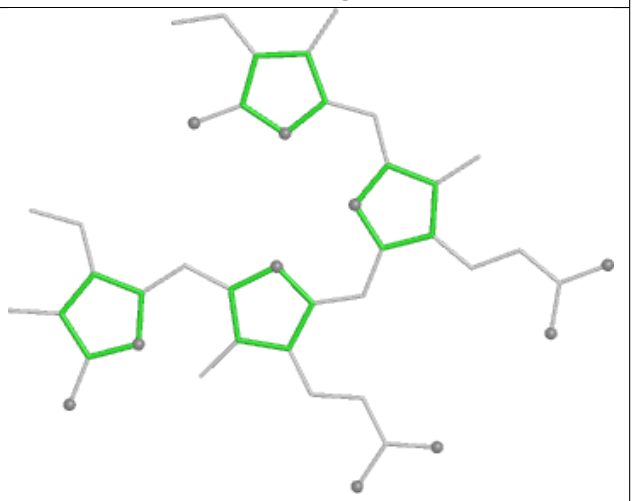
Bond lengths



Bond angles

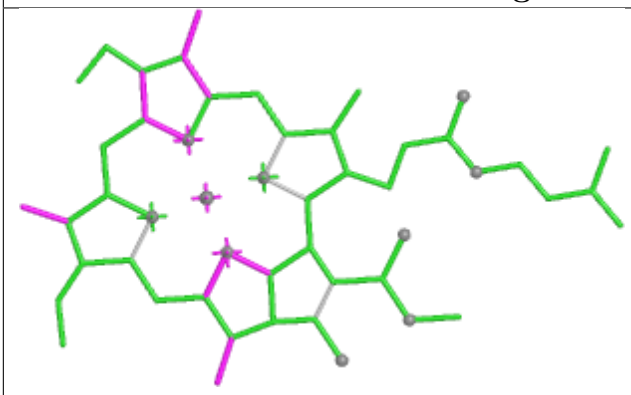


Torsions

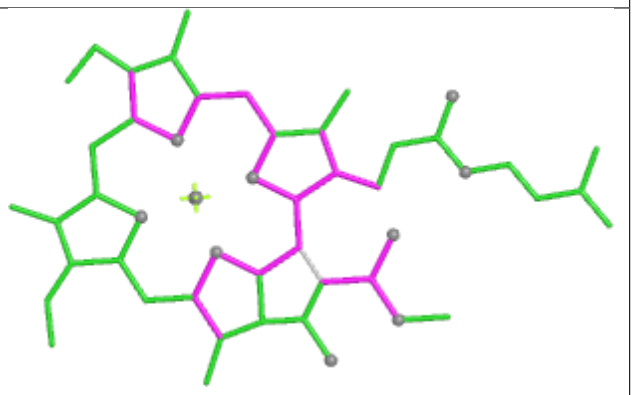


Rings

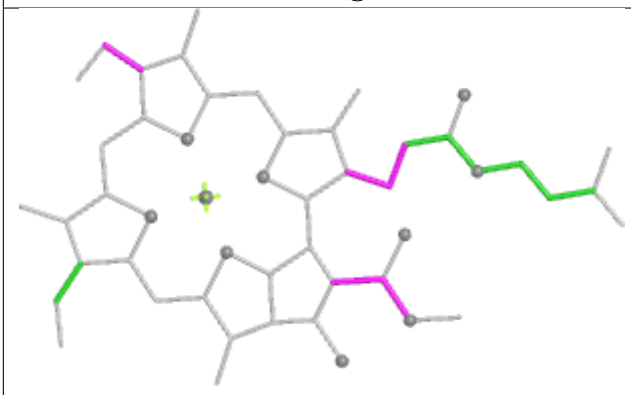
Ligand CLA AL 405



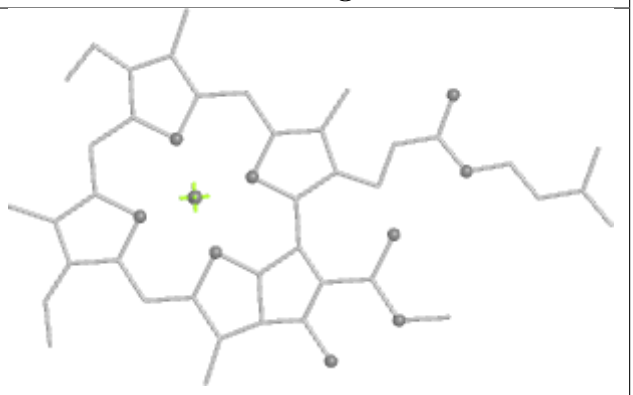
Bond lengths



Bond angles

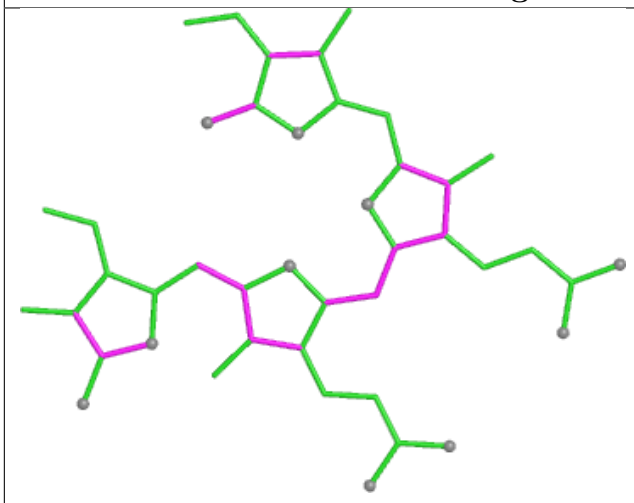


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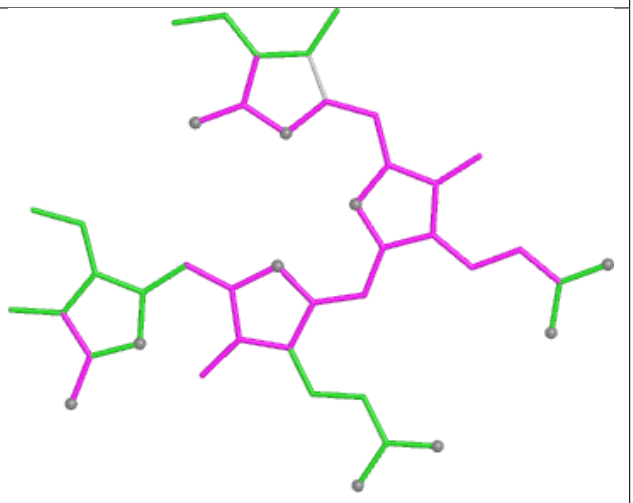


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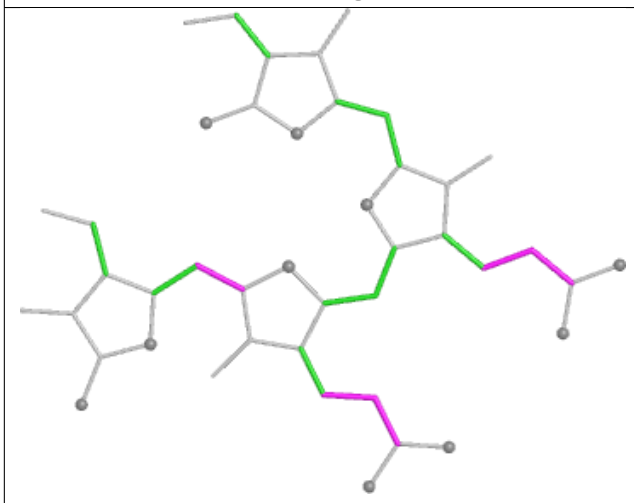
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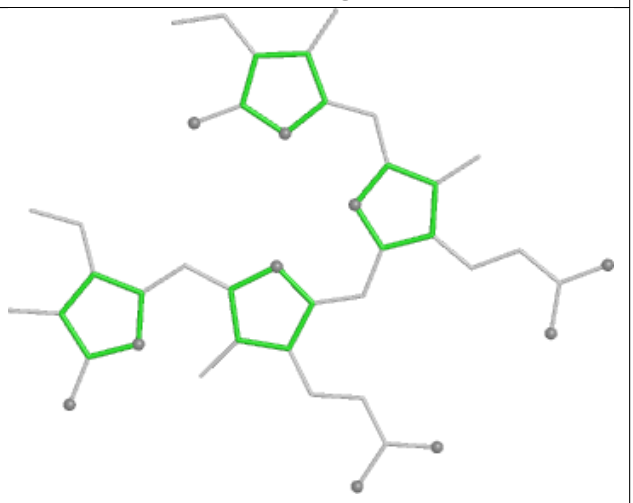
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Bond angles

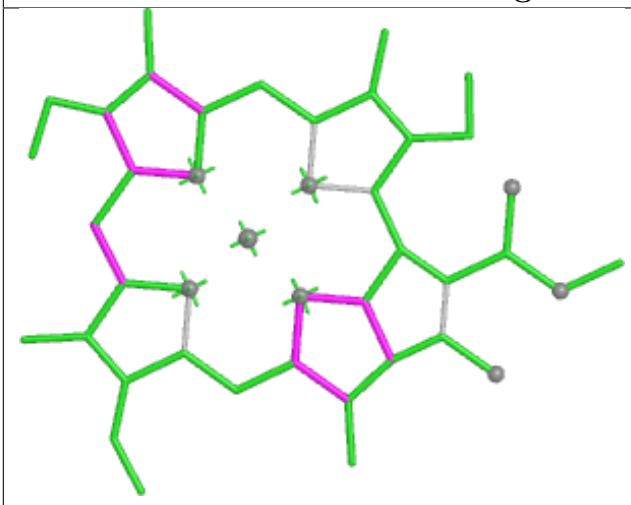


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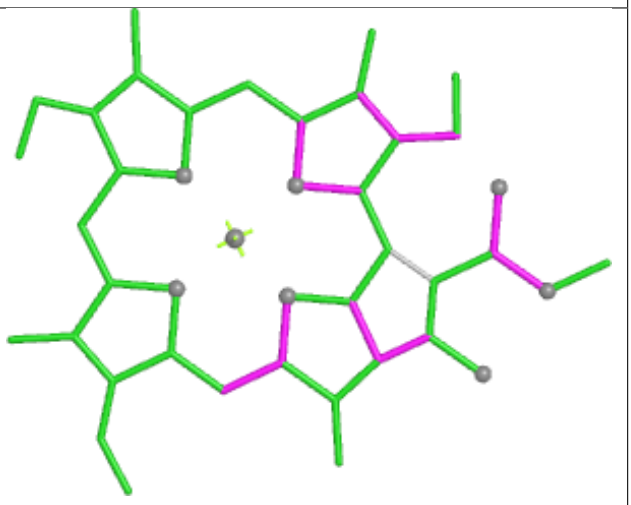


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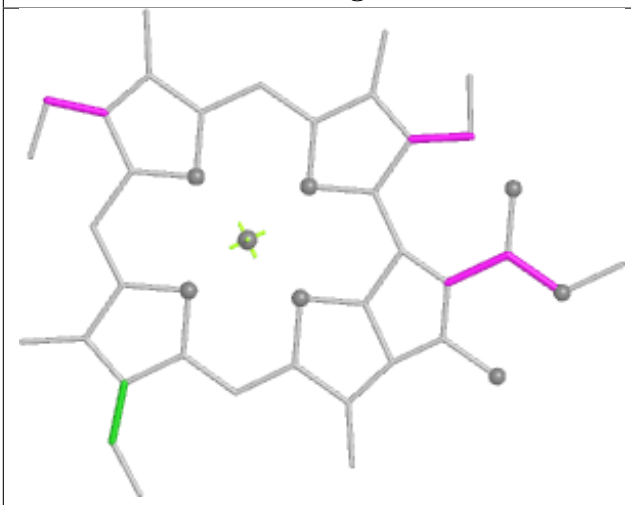
Ligand CLA 6N 604



Bond lengths



Bond angles

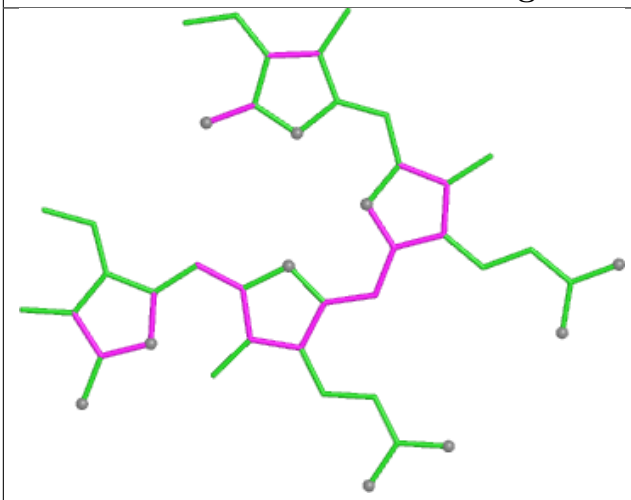


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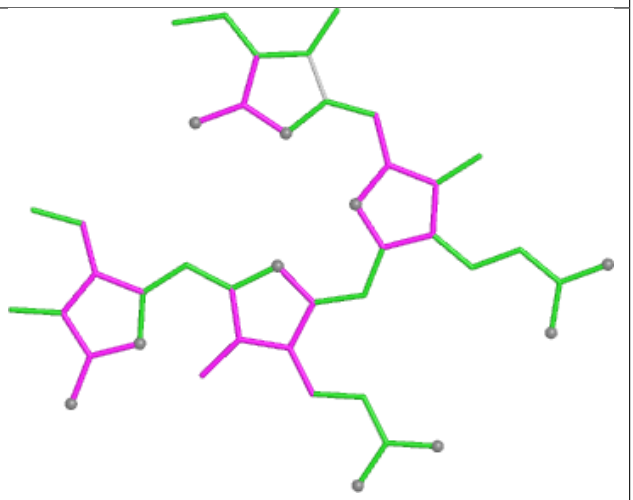


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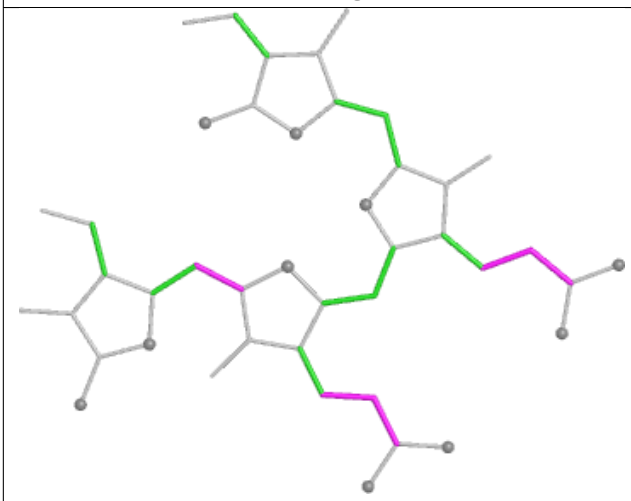
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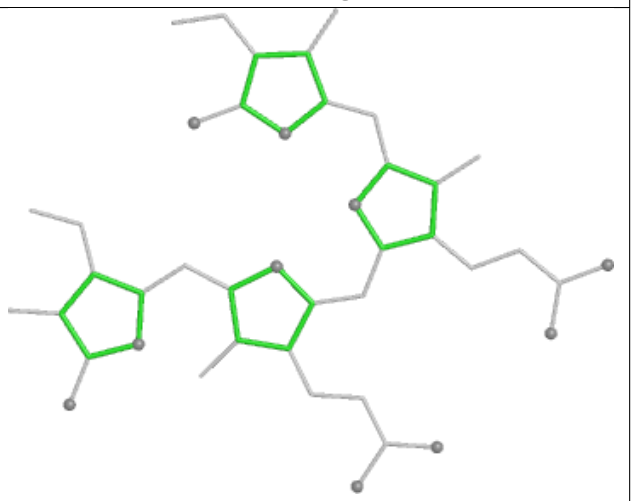
Bond lengths



Bond angles

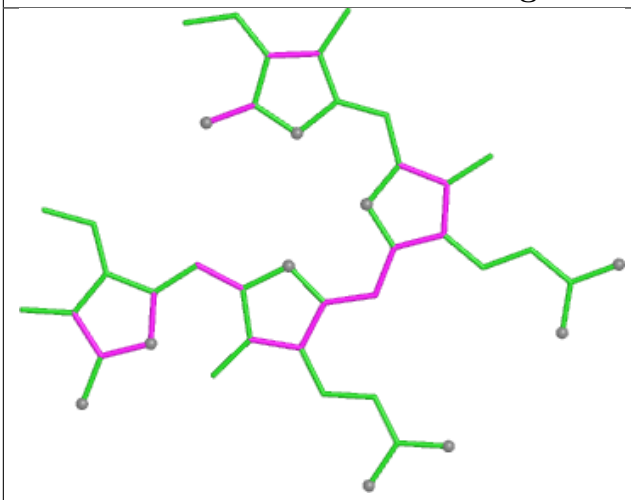


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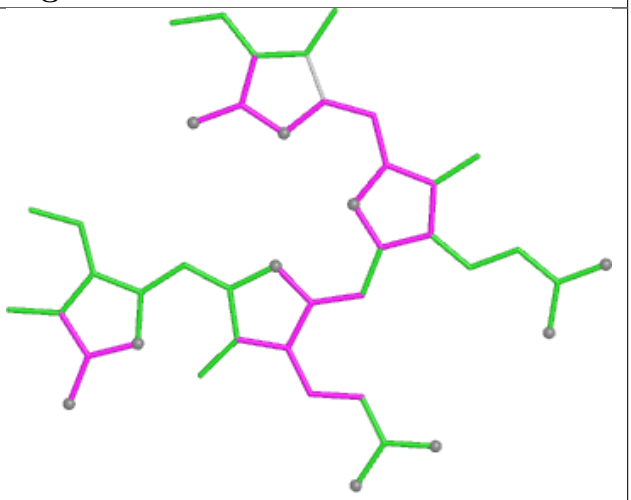


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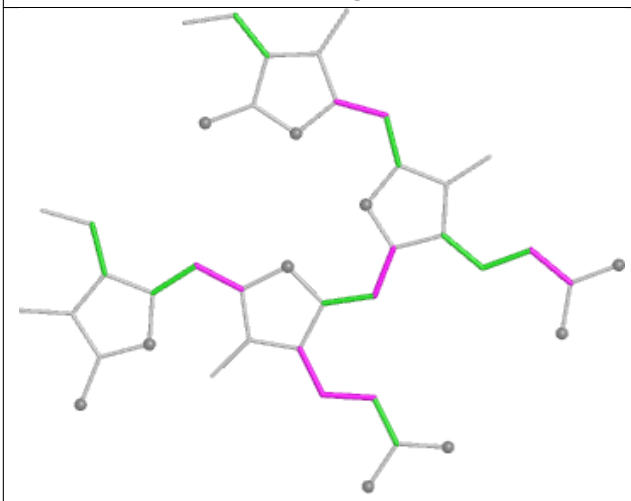
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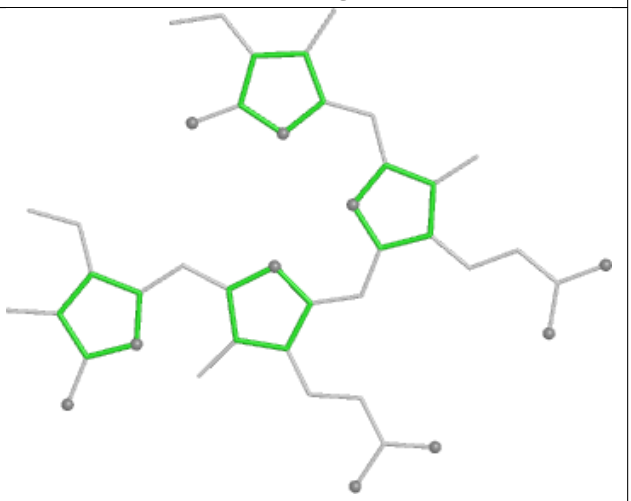
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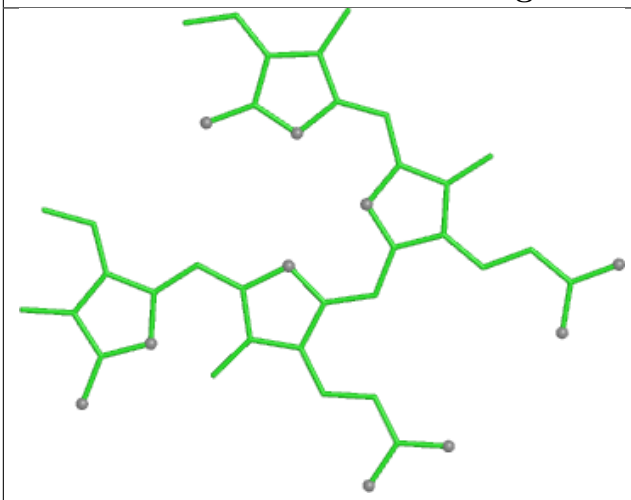


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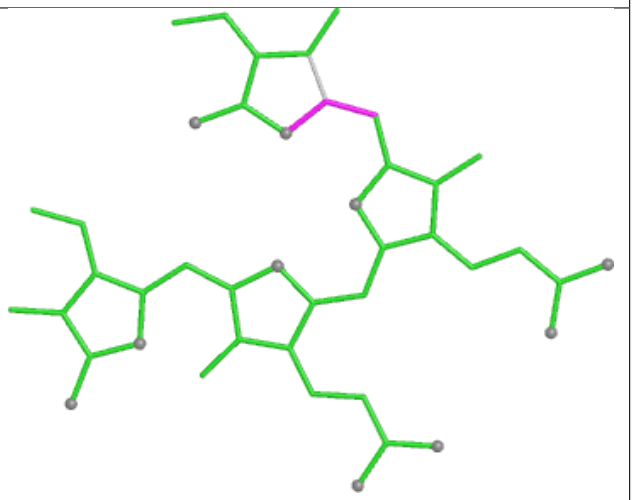


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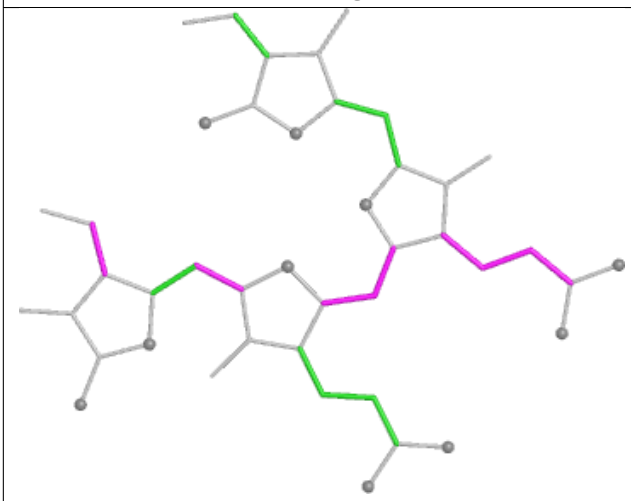
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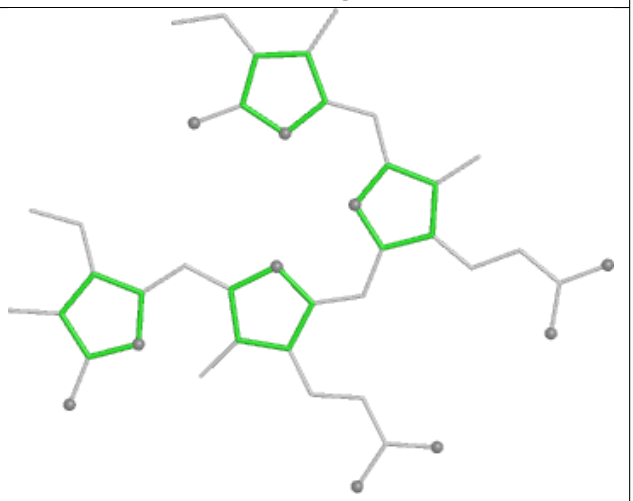
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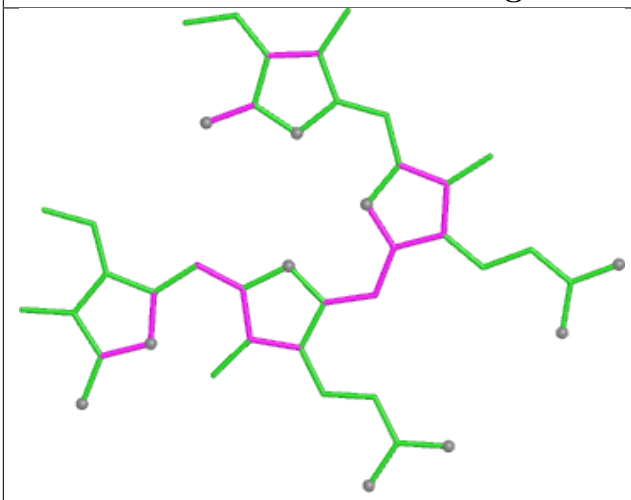


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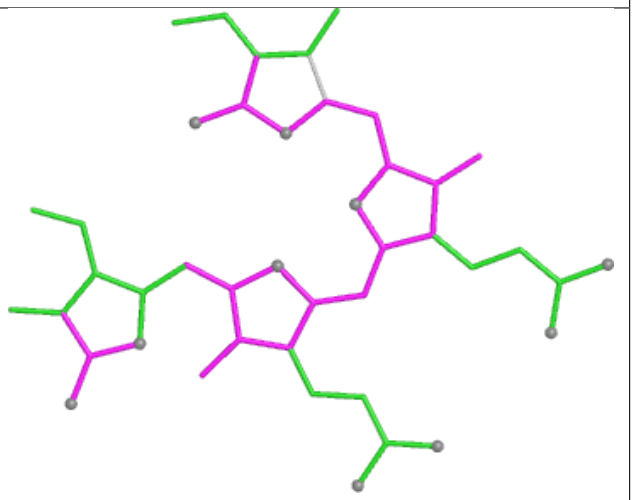


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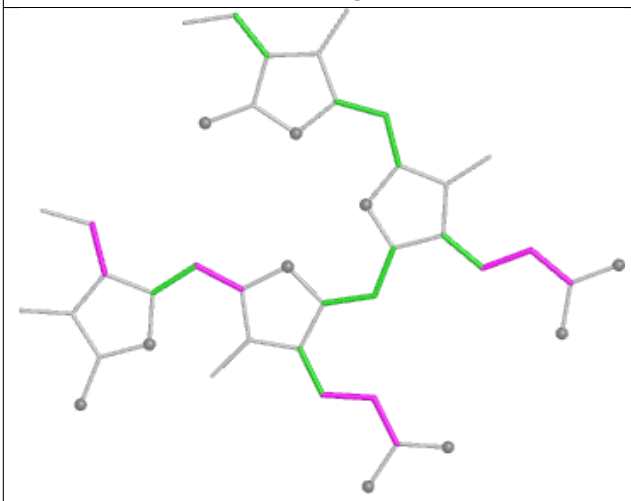
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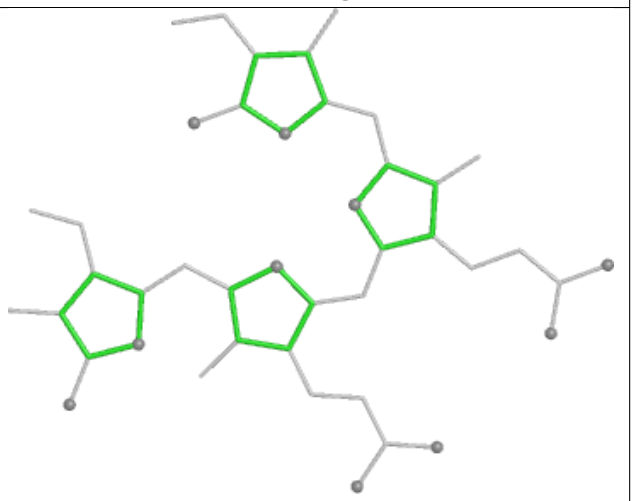
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Bond angles

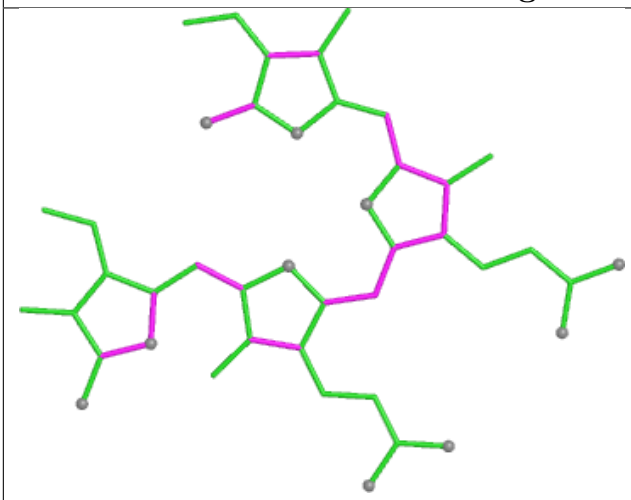


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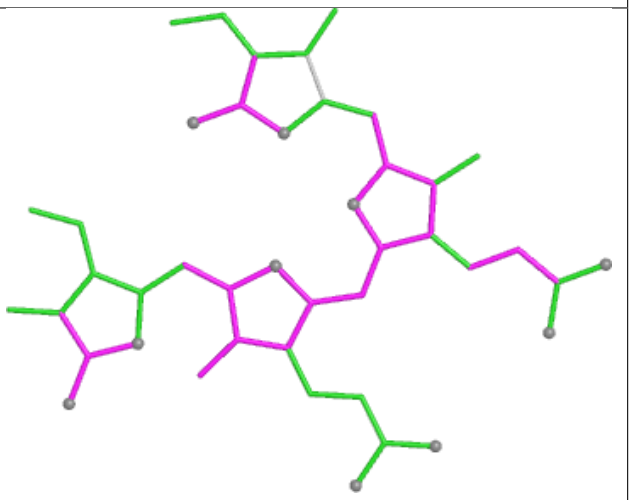


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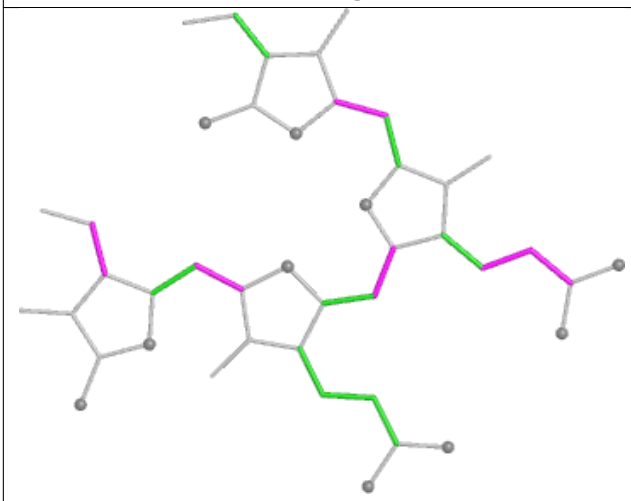
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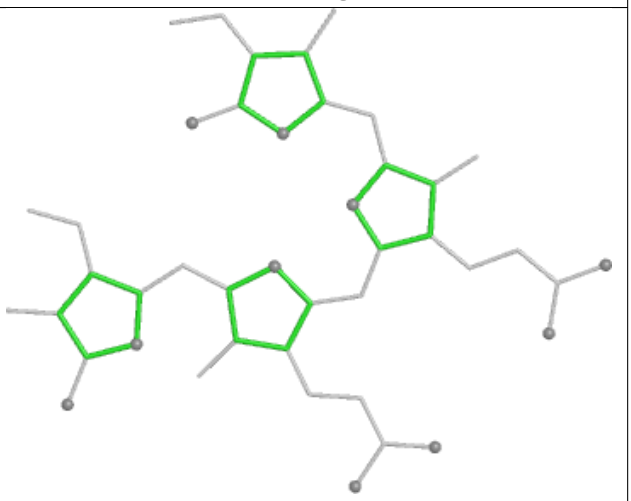
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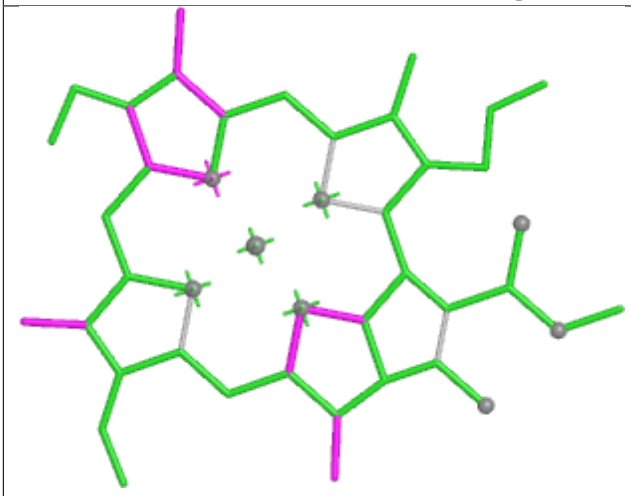


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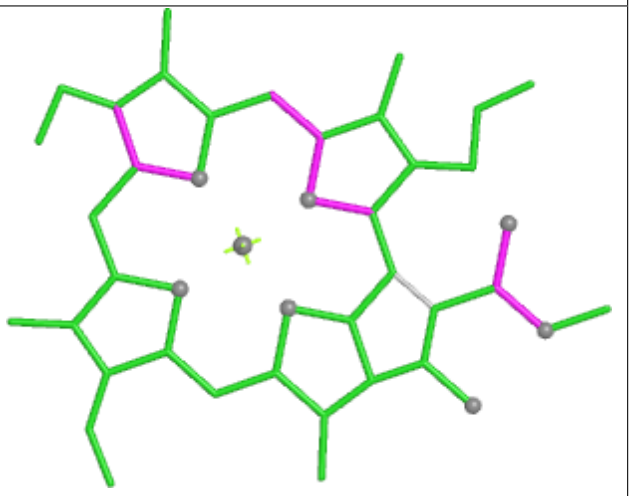


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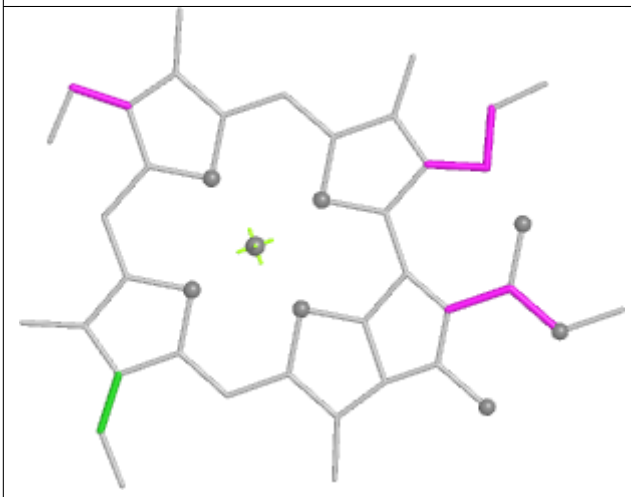
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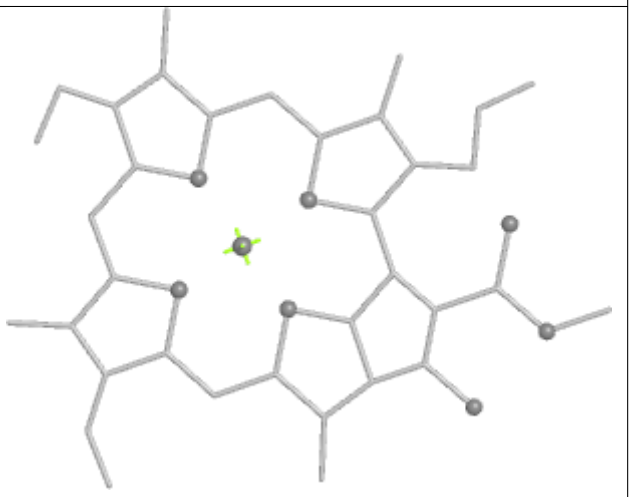
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Bond angles

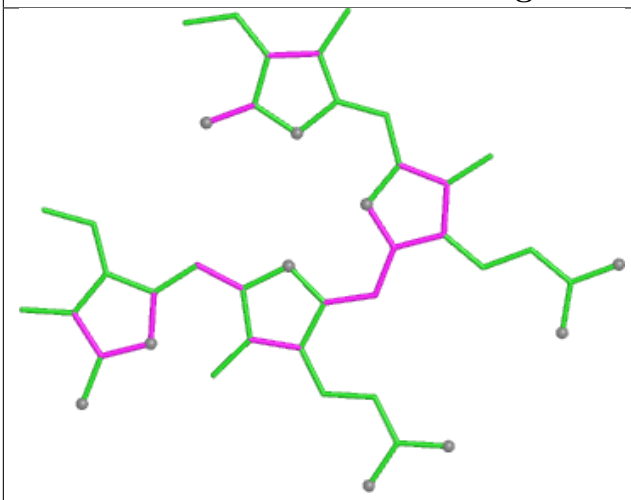


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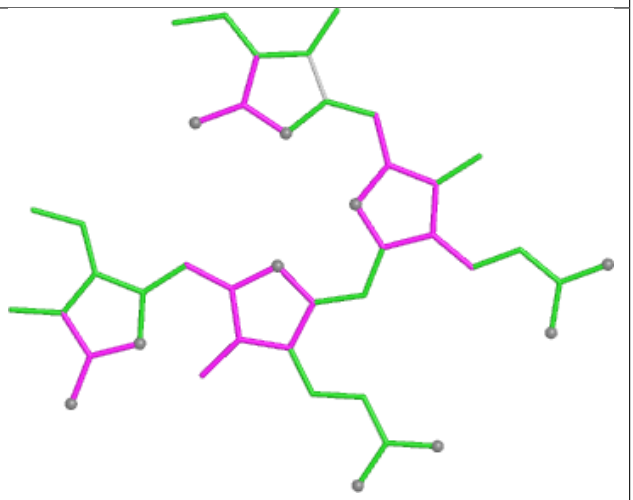


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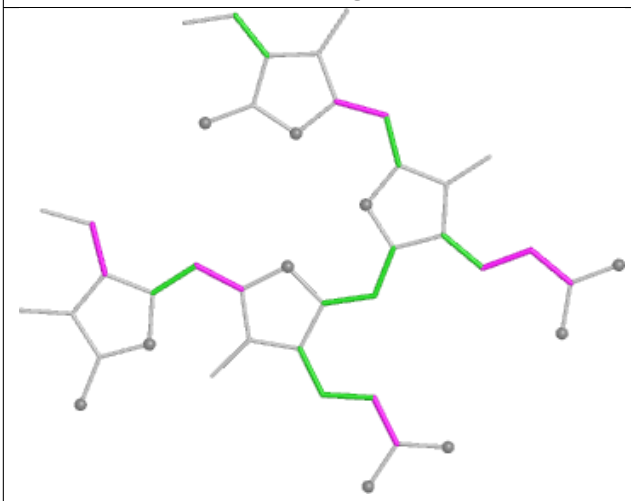
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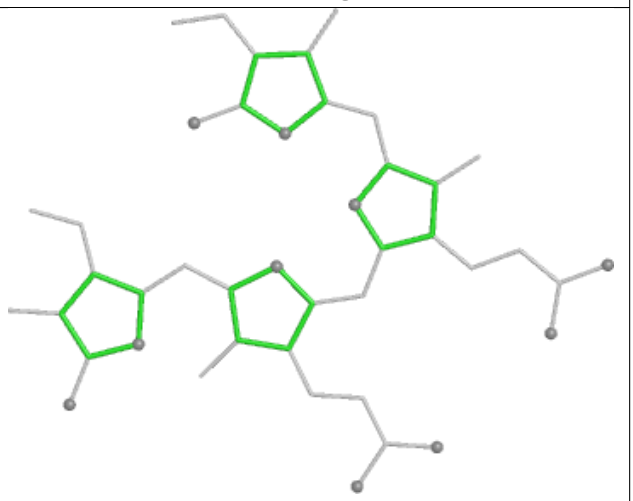
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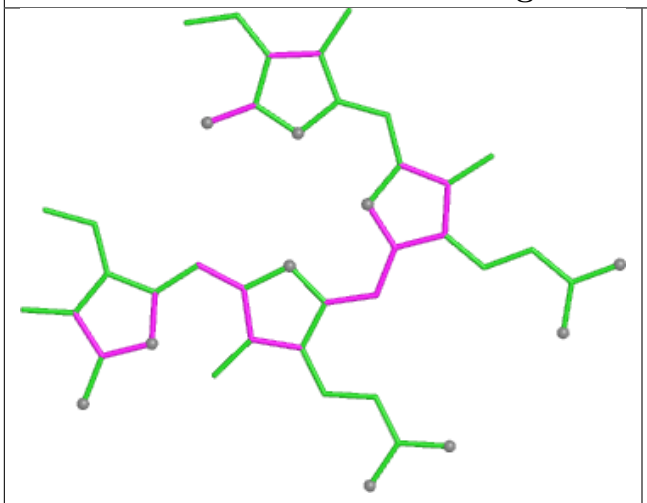


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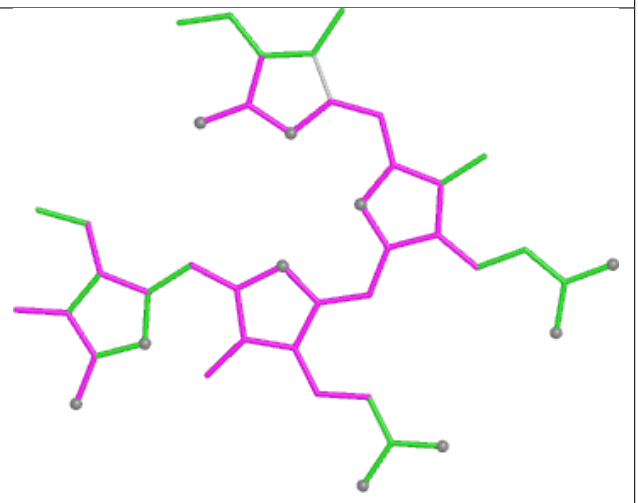


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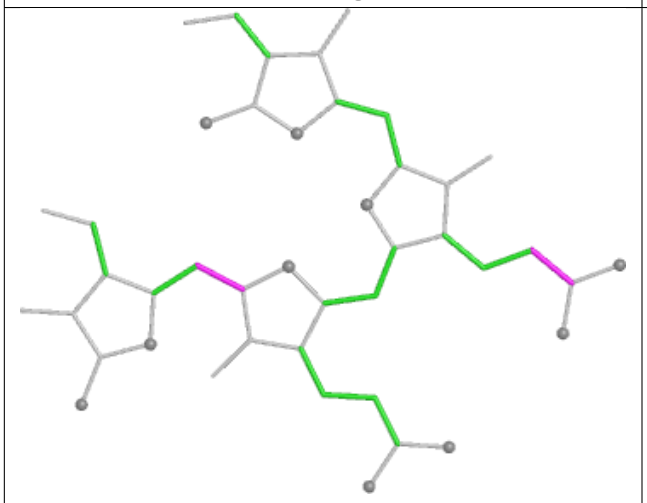
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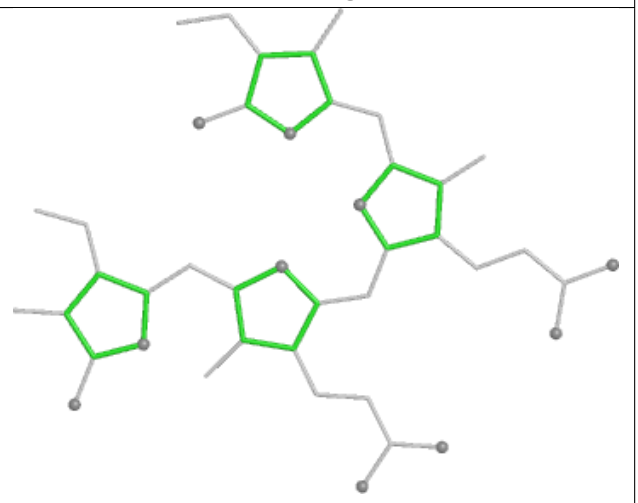
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Bond angles

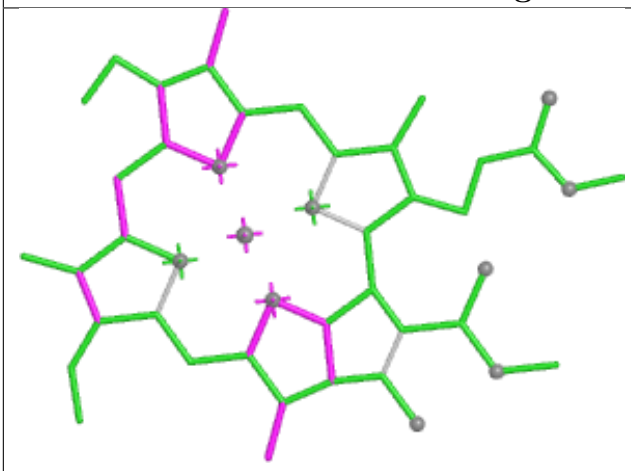


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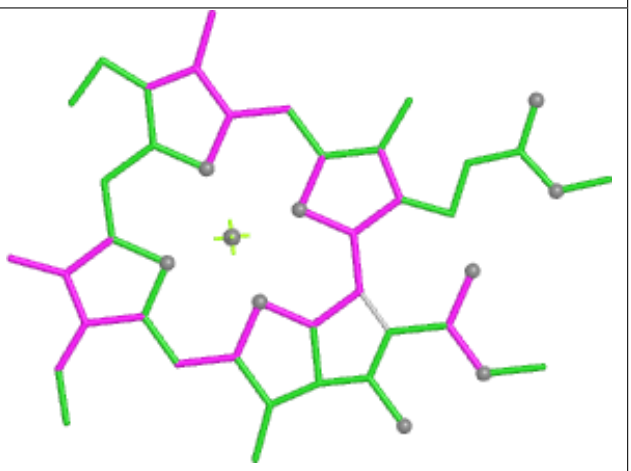


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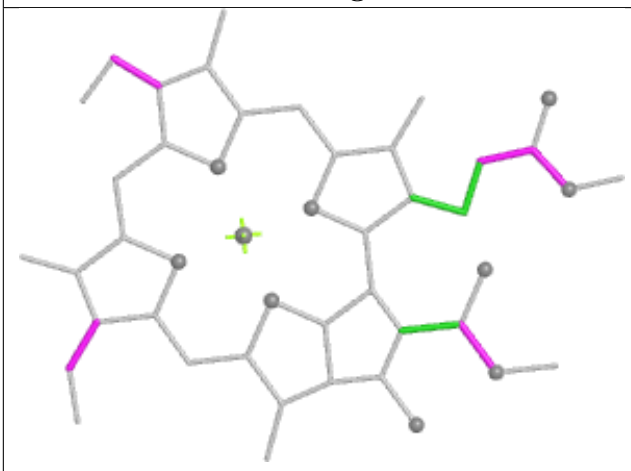
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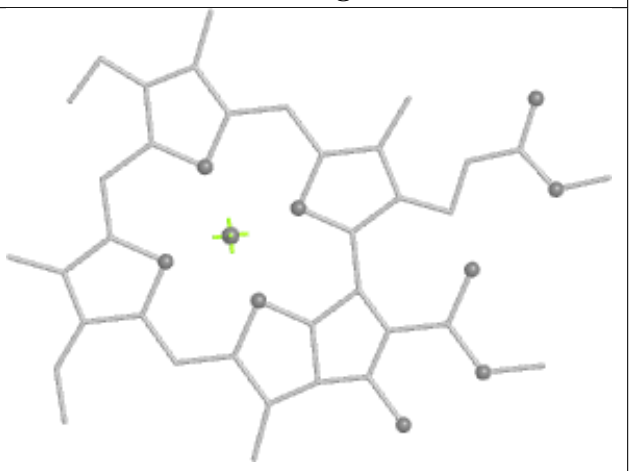
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Bond angles

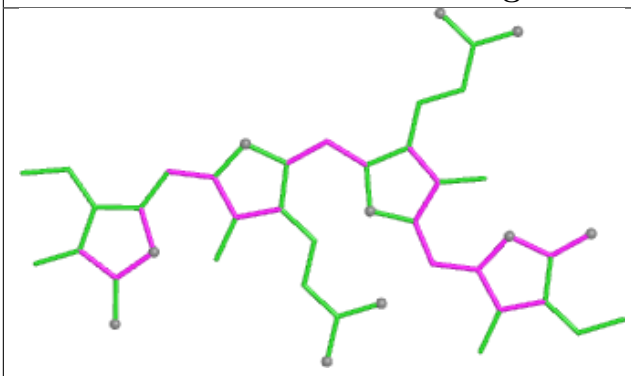


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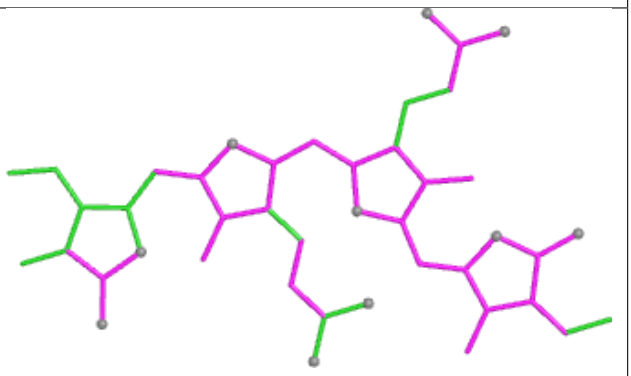


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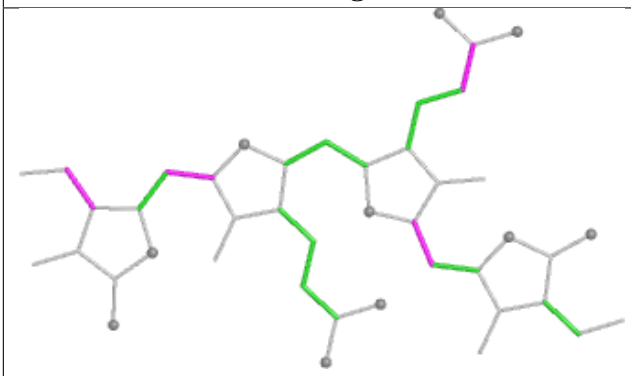
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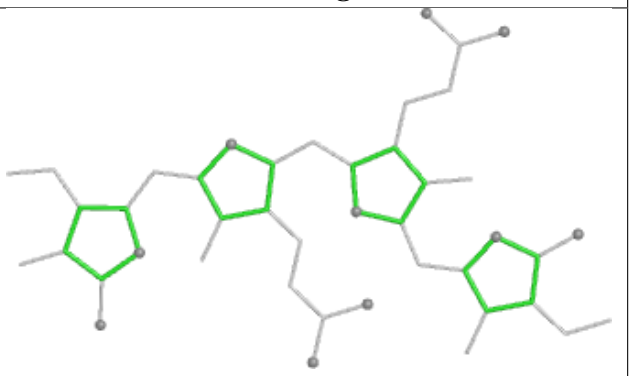
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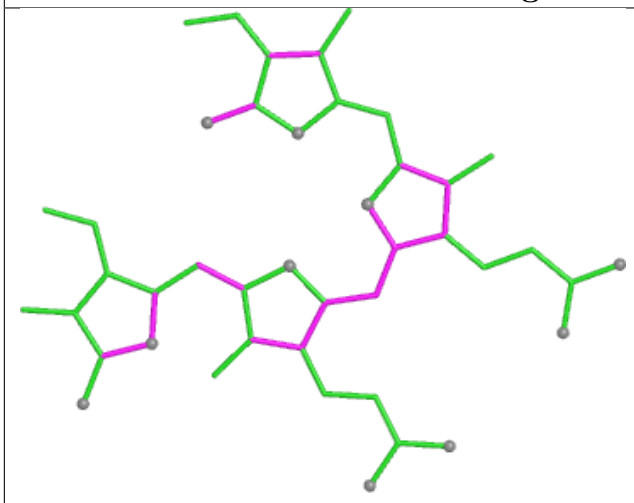


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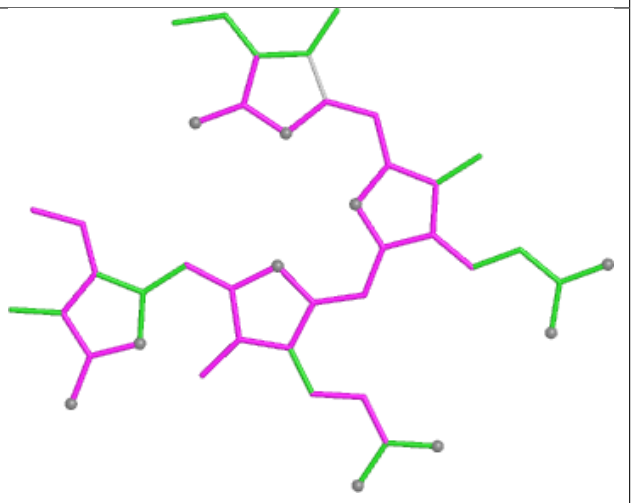


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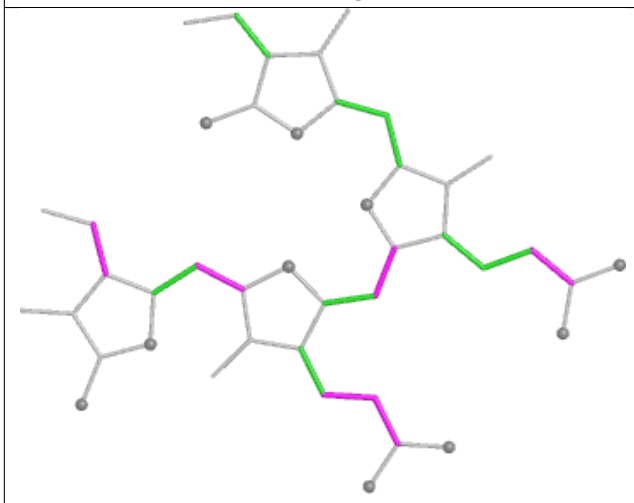
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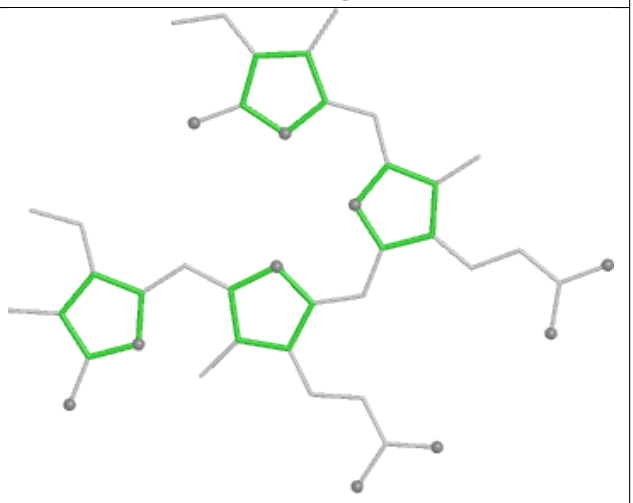
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Bond angles

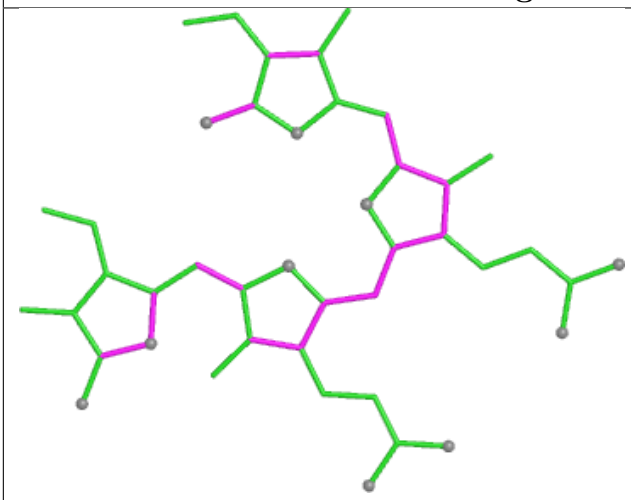


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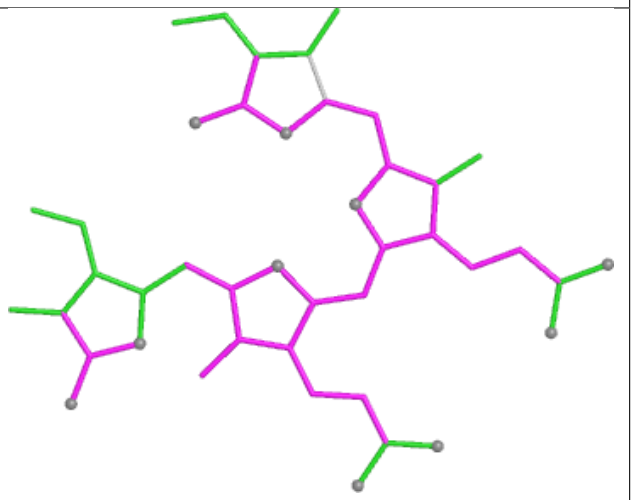


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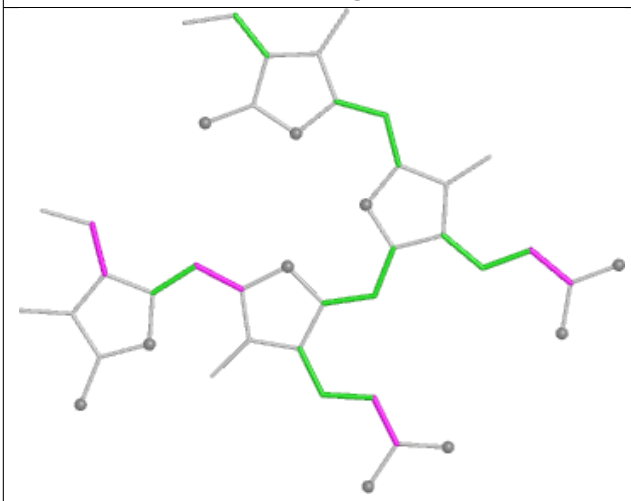
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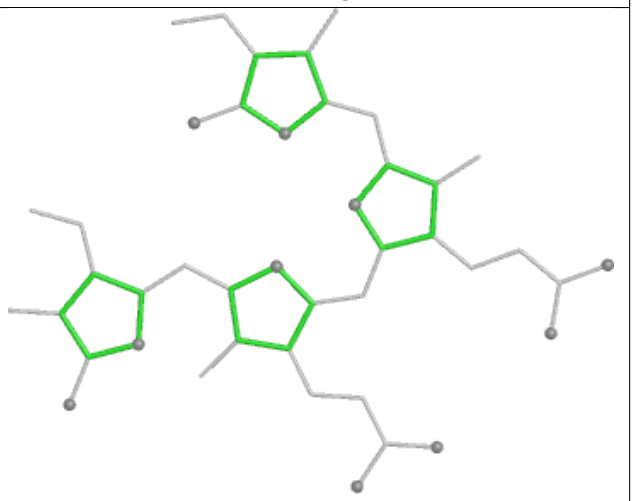
Bond lengths



Bond angles

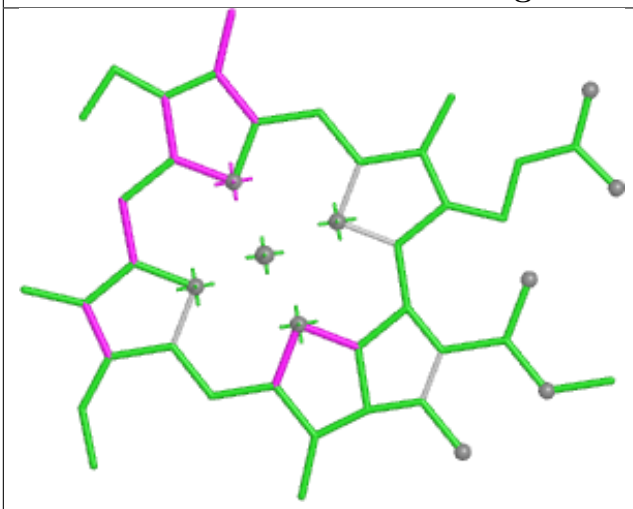


Torsions

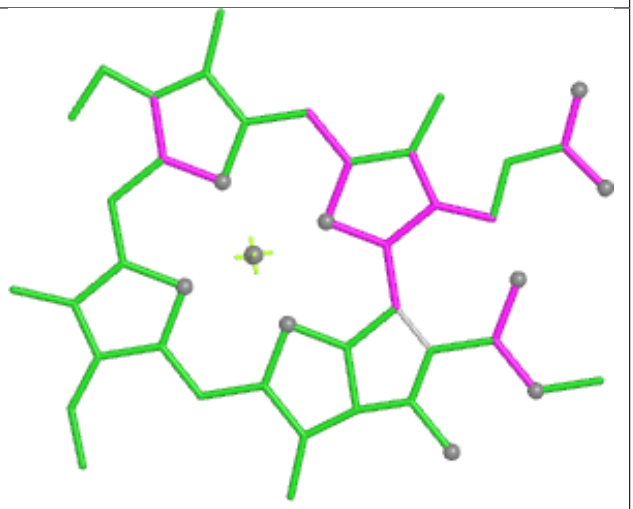


Rings

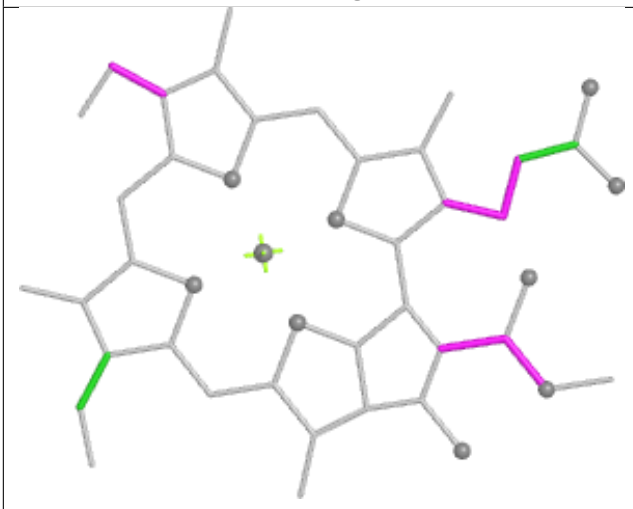
Ligand CLA 2N 312



Bond lengths



Bond angles

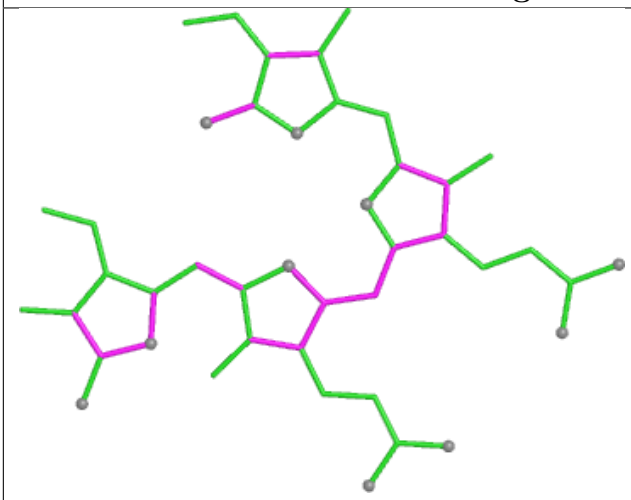


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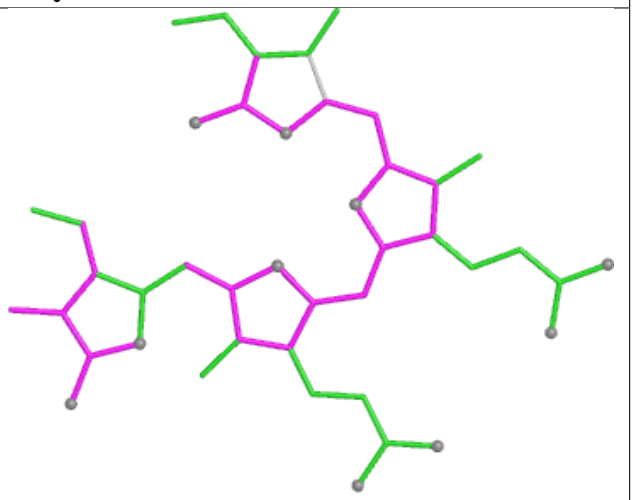


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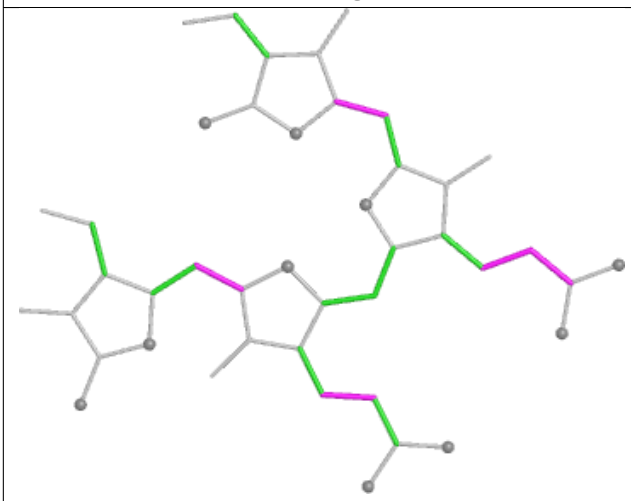
Ligand PEB QF 203



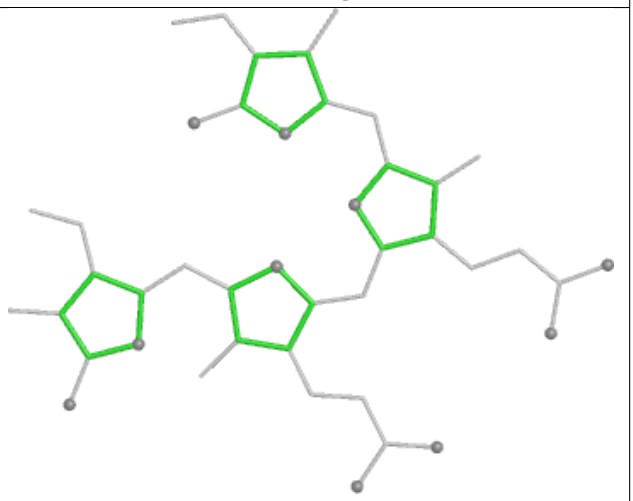
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Bond angles

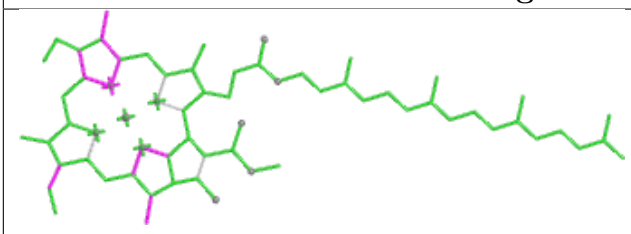


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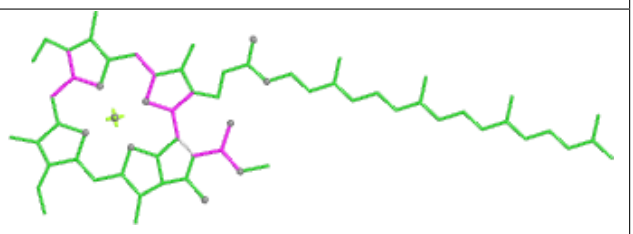


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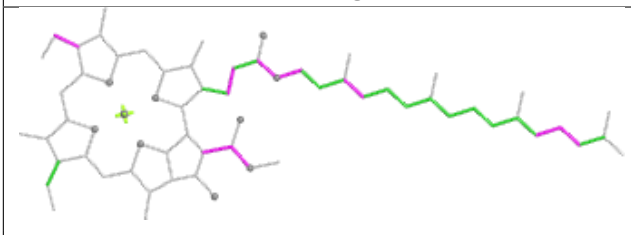
Ligand CLA dL 401



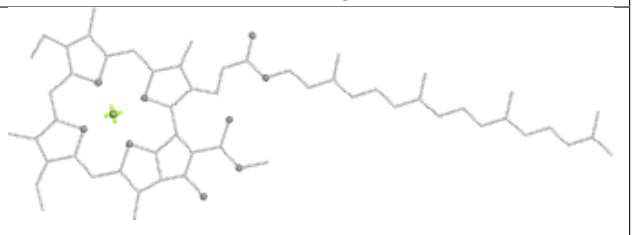
Bond lengths



Bond angles

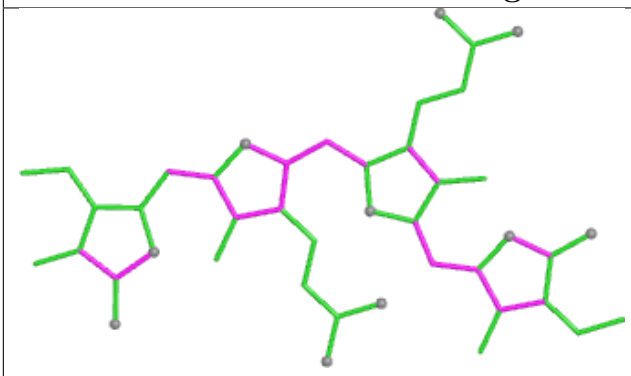


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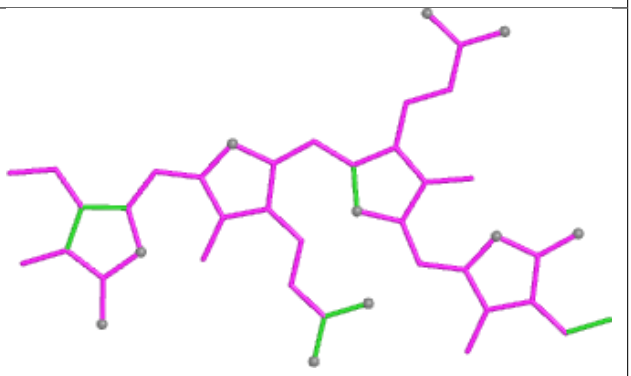


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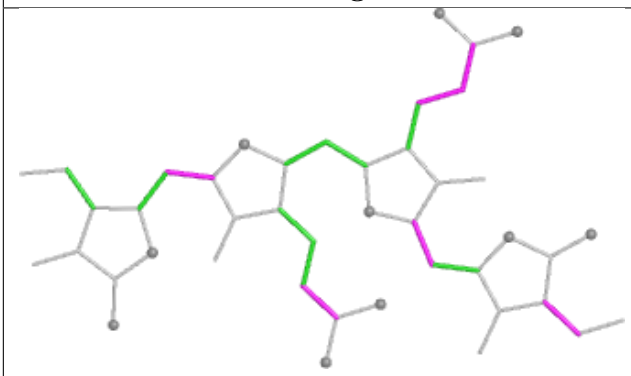
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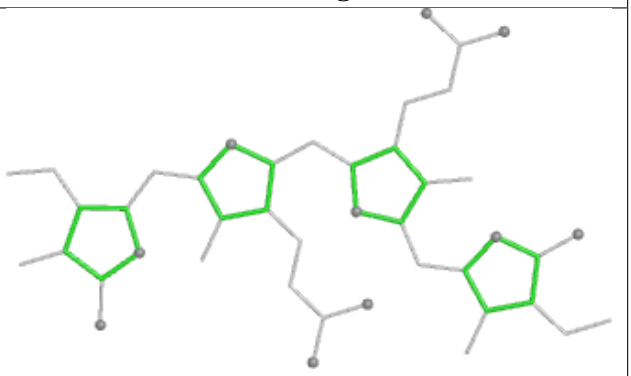
Bond lengths



Bond angles

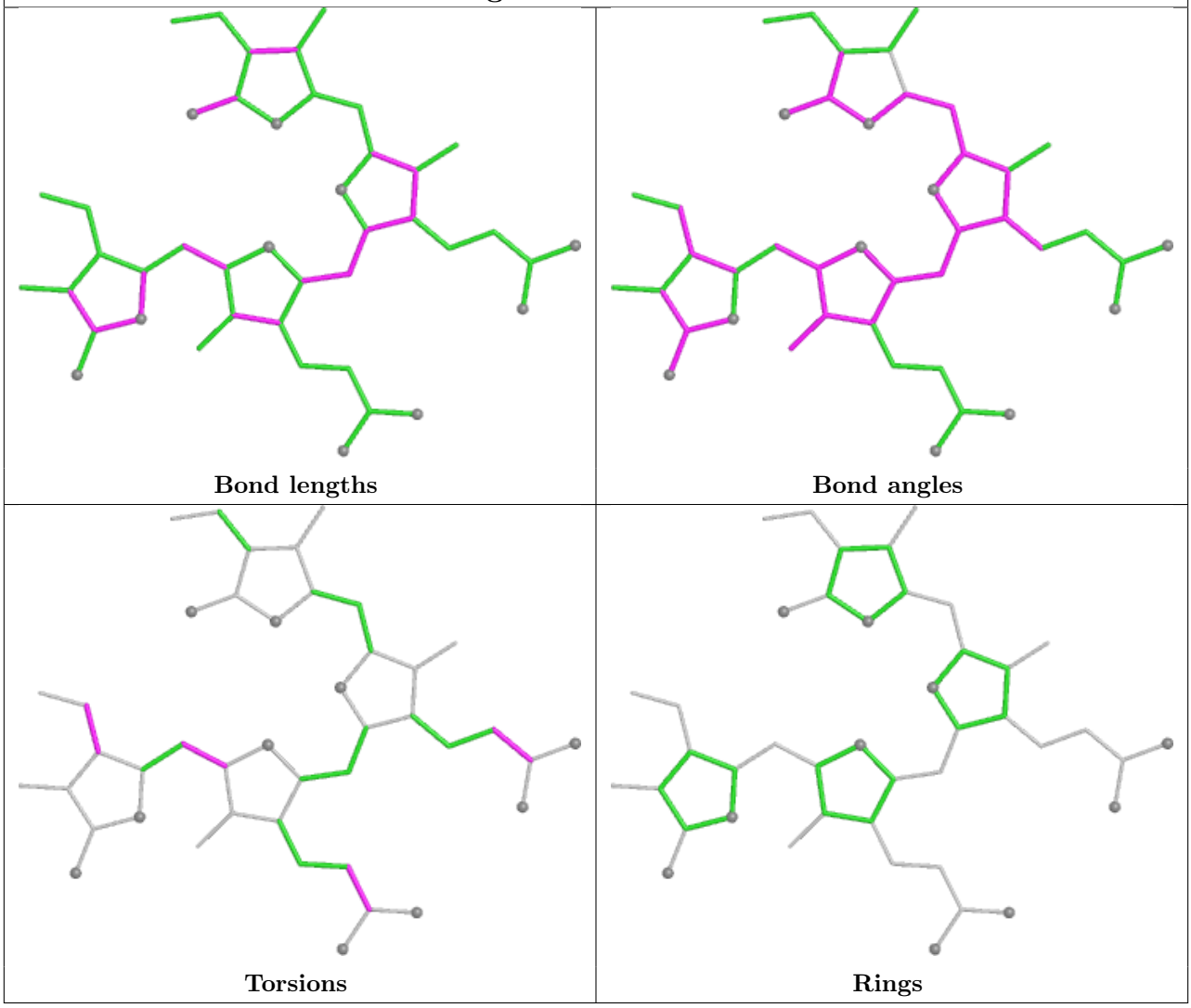


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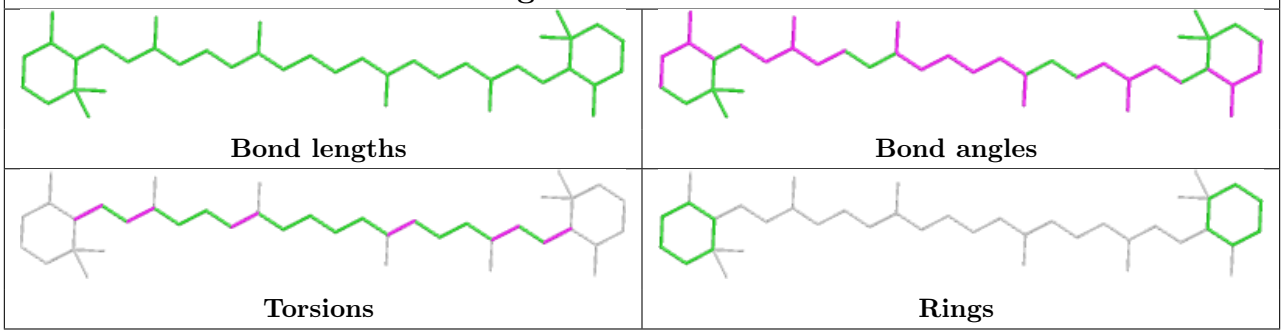


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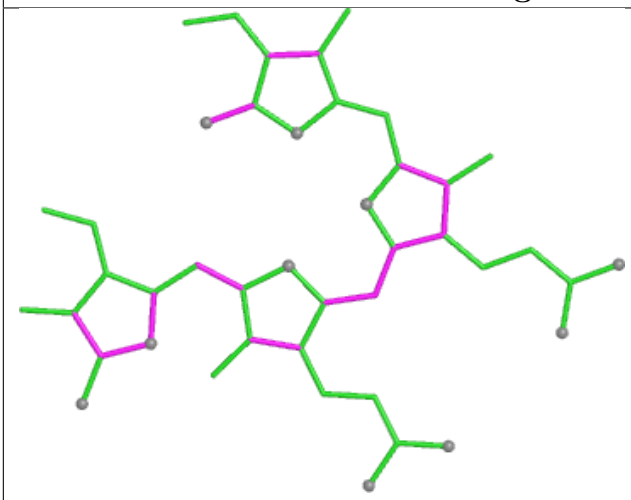
Ligand PEB lJ 201



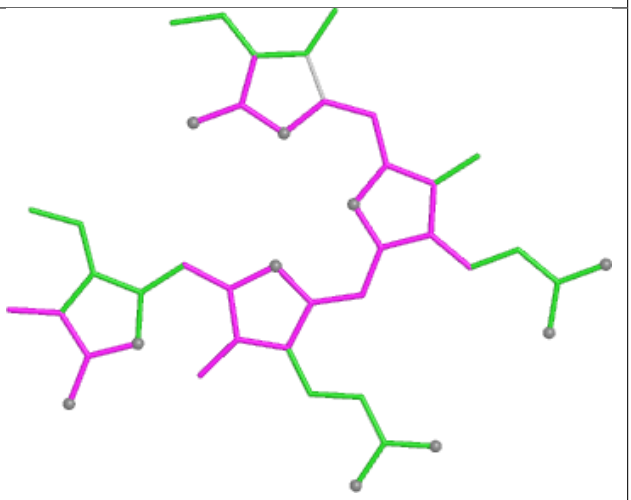
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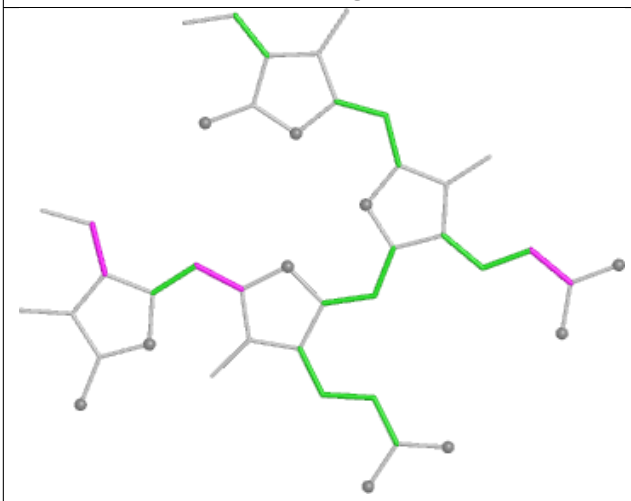
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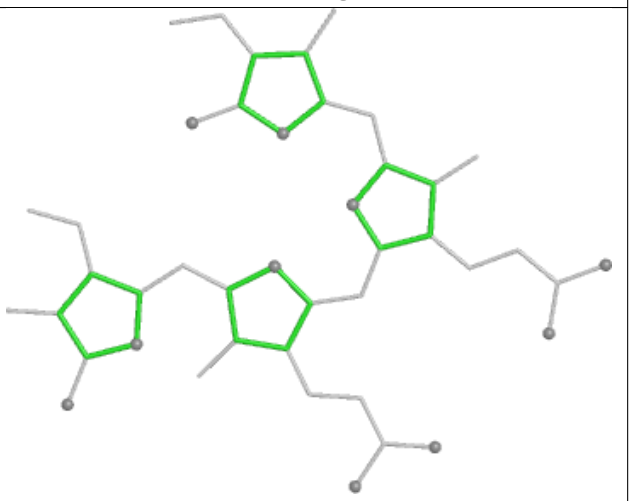
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Bond angles

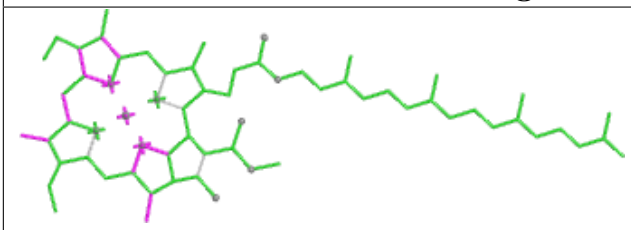


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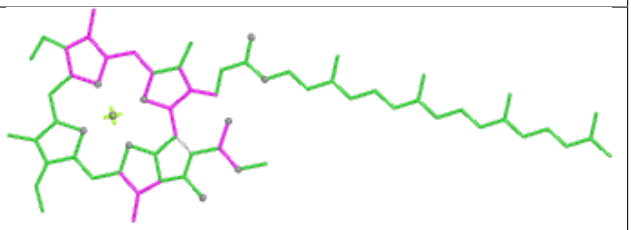


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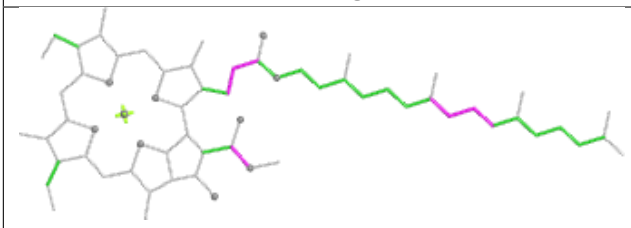
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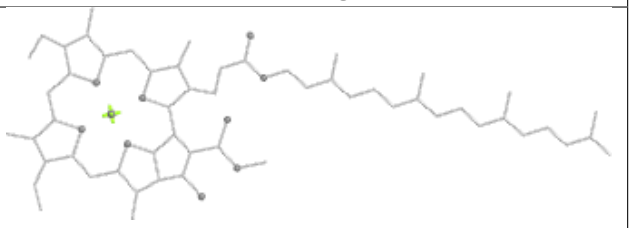
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Bond angles

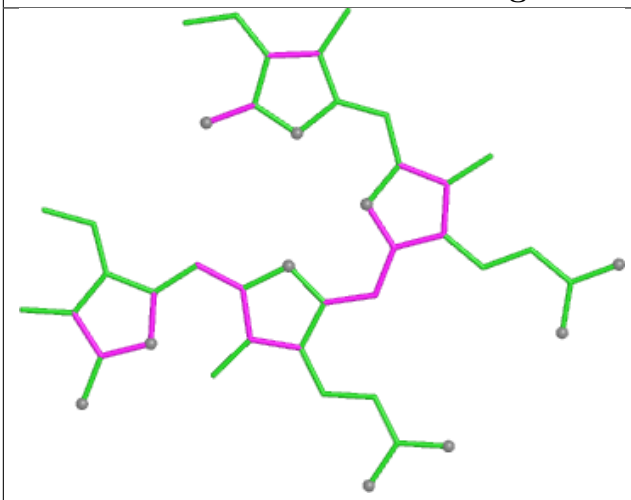


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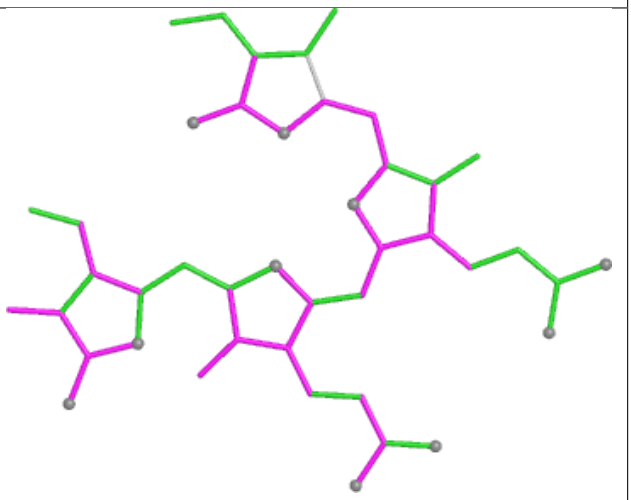


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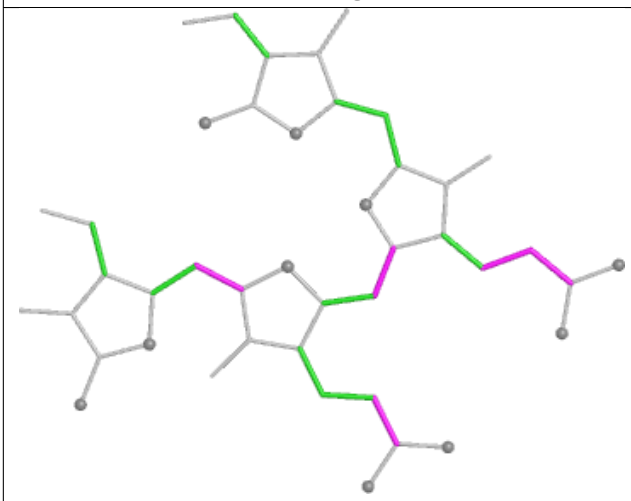
Ligand PEB FM 202



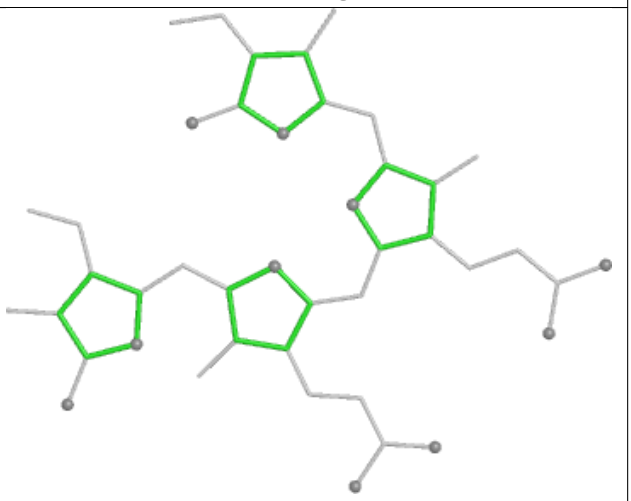
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Bond angles

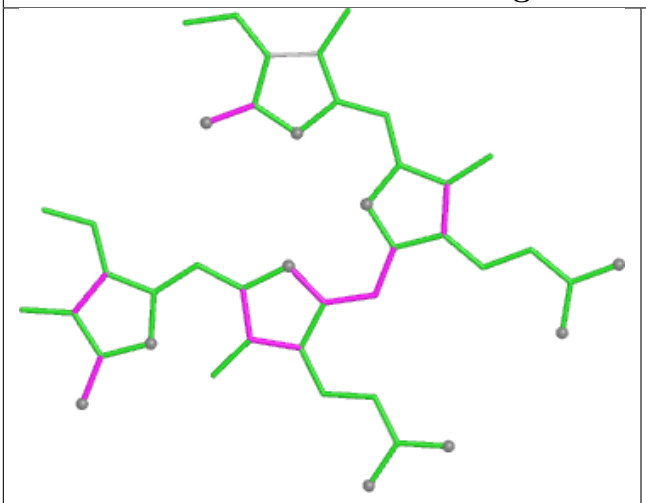


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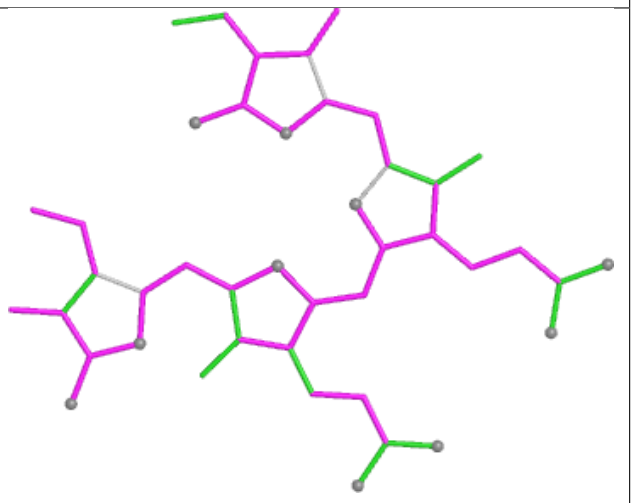


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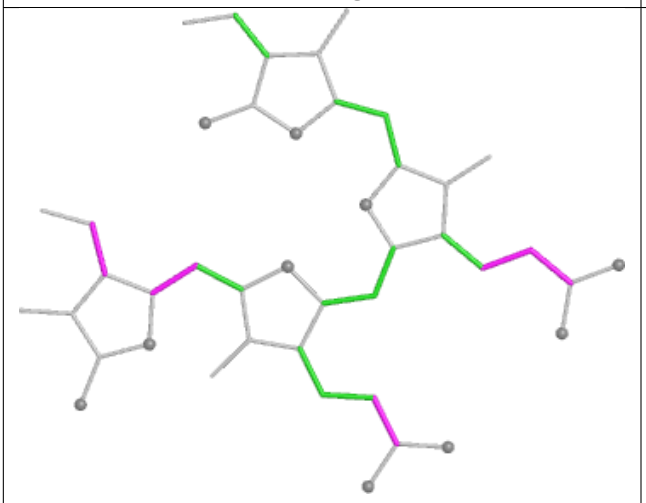
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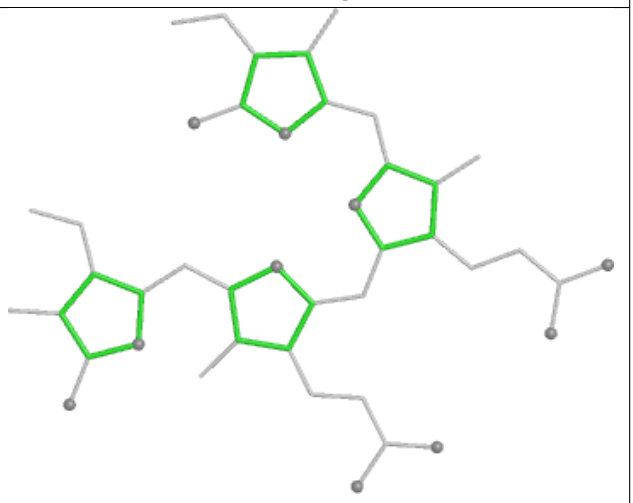
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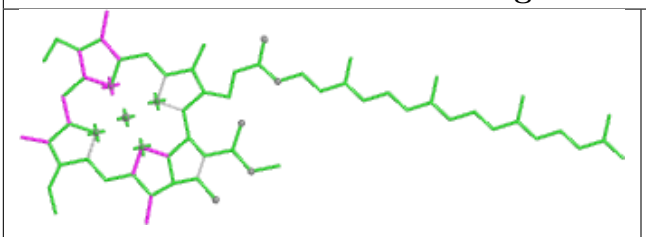


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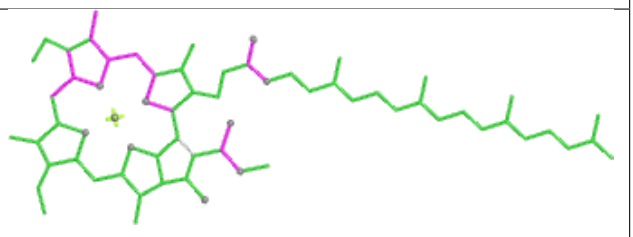


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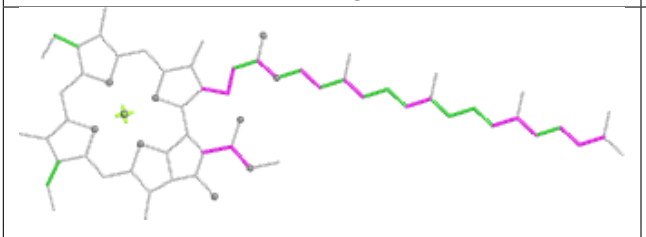
Ligand CLA H6 103



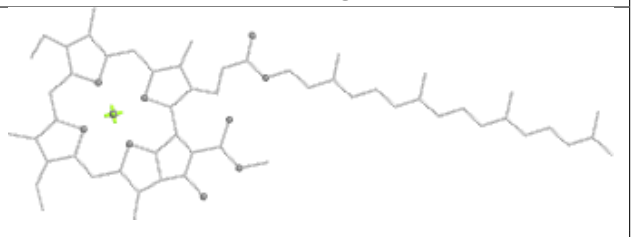
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Bond angles

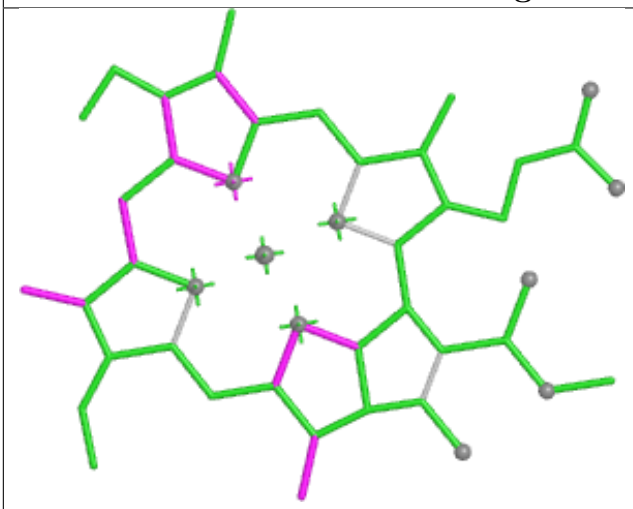


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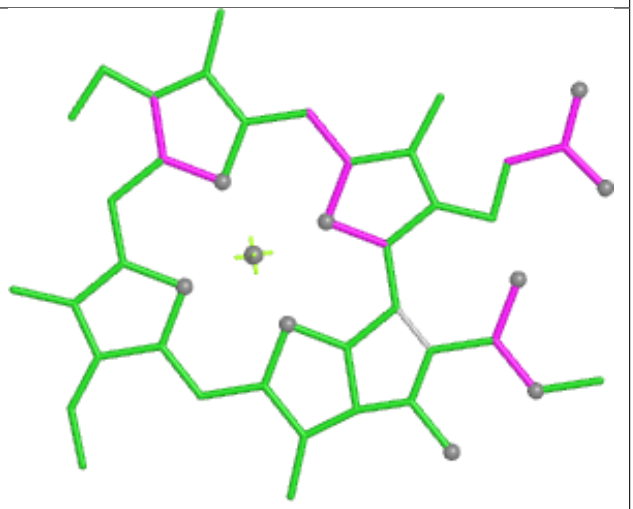


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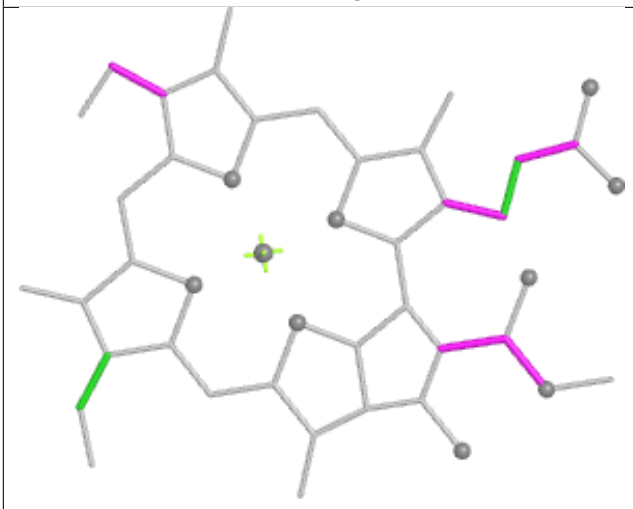
Ligand CLA 1N 601



Bond lengths



Bond angles

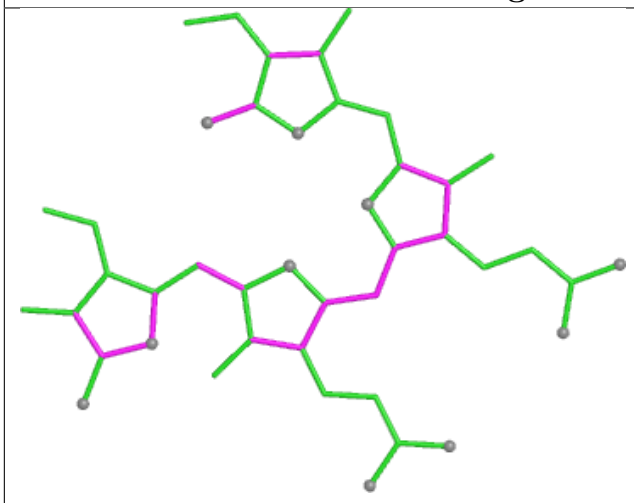


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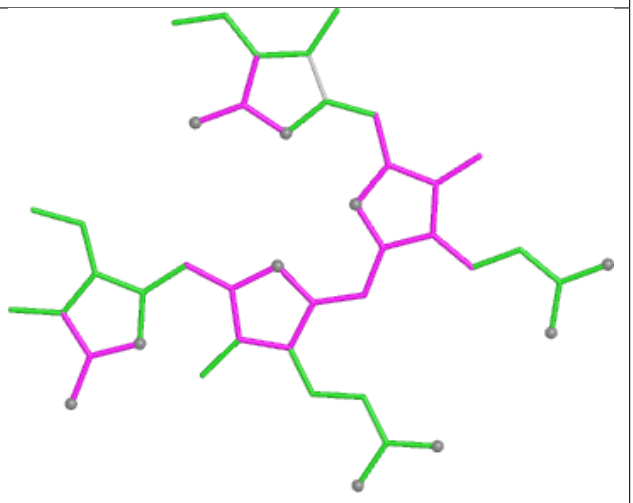


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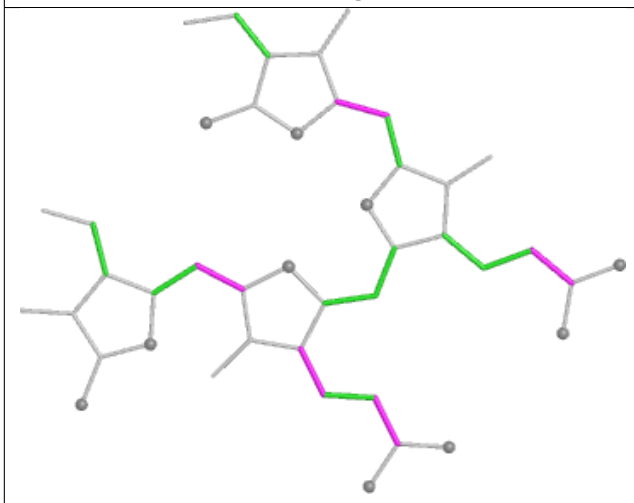
Ligand PEB UM 203



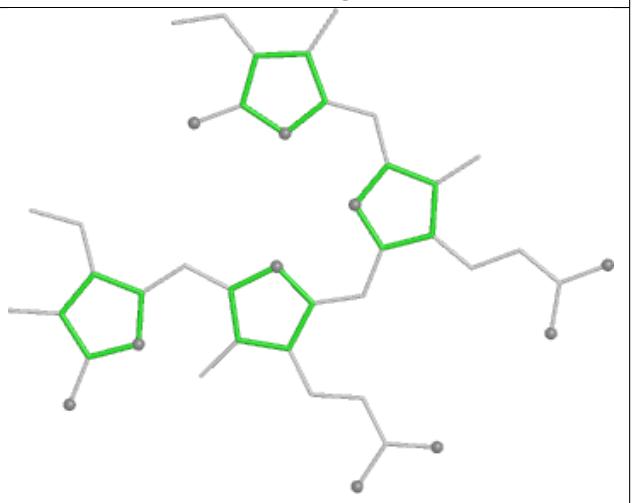
Bond lengths



Bond angles

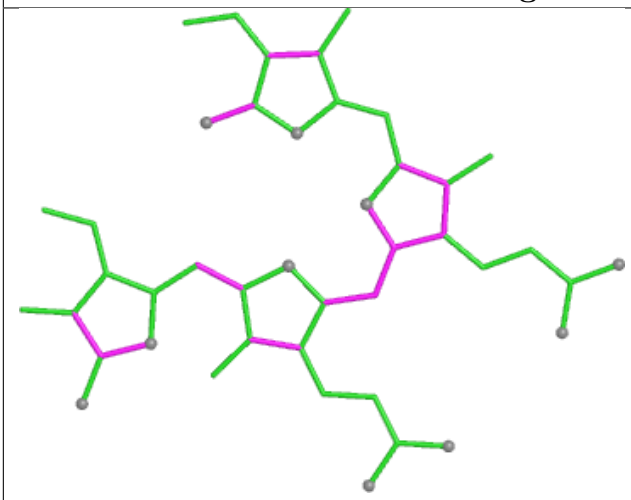


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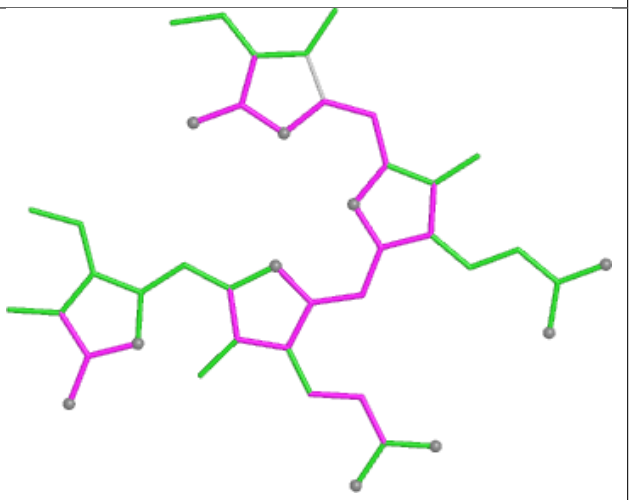


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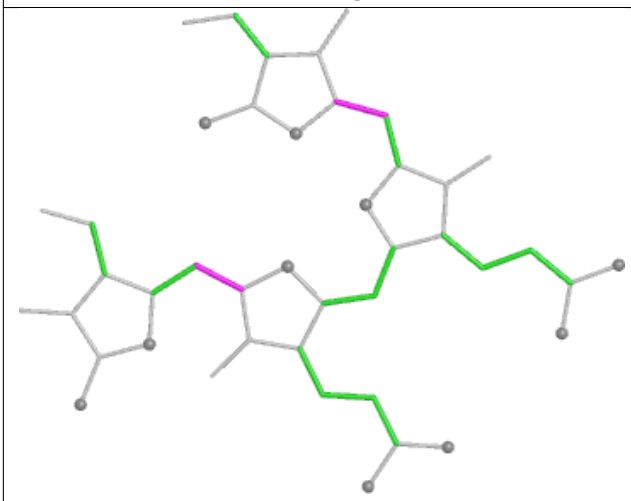
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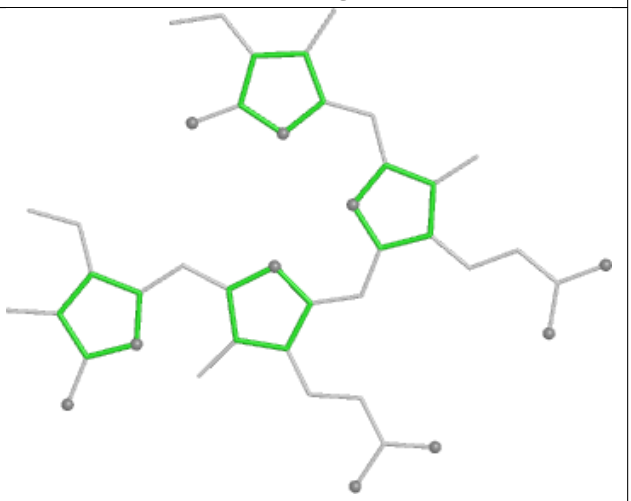
Bond lengths



Bond angles

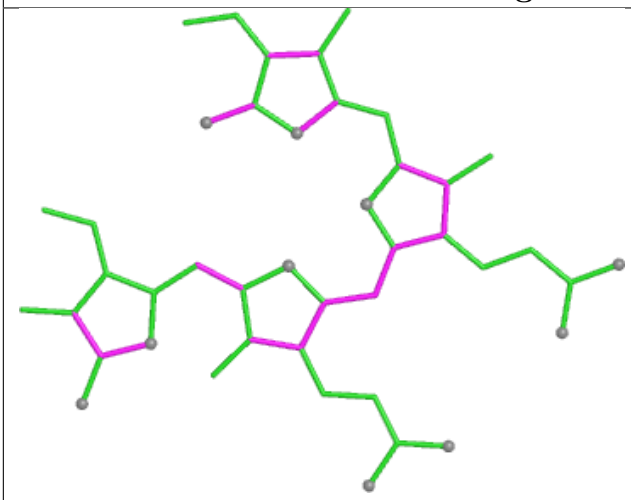


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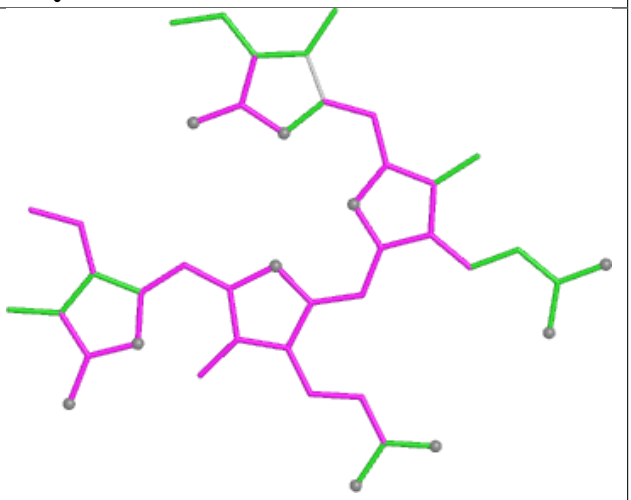


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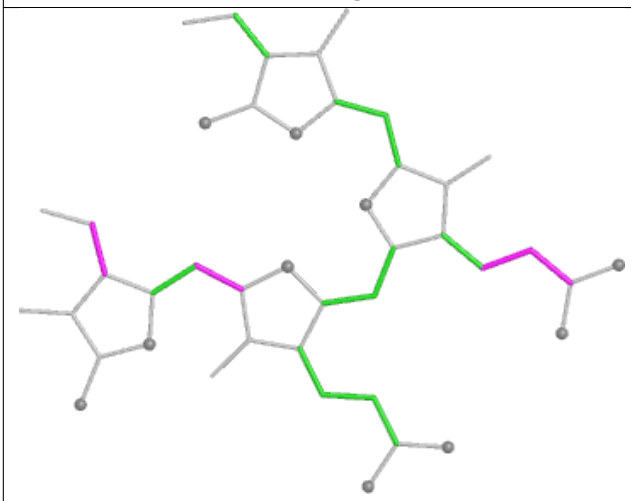
Ligand PEB Q9 202



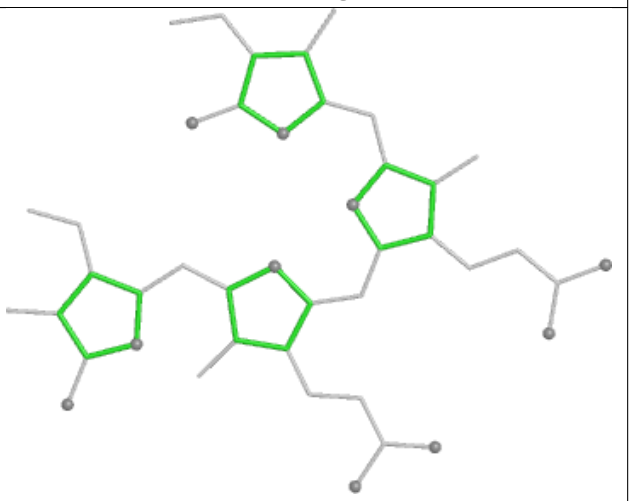
Bond lengths



Bond angles

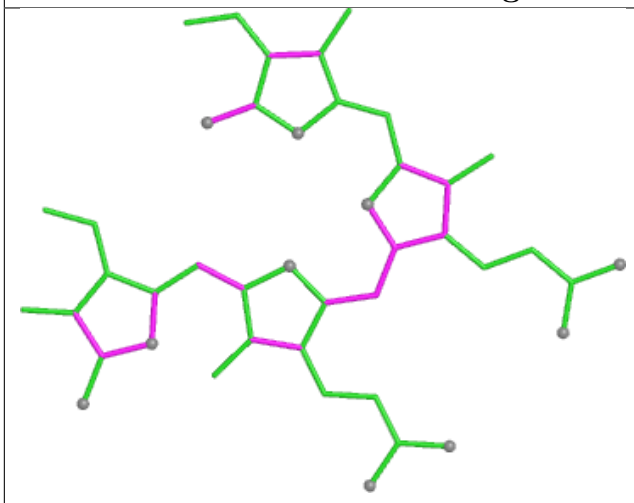


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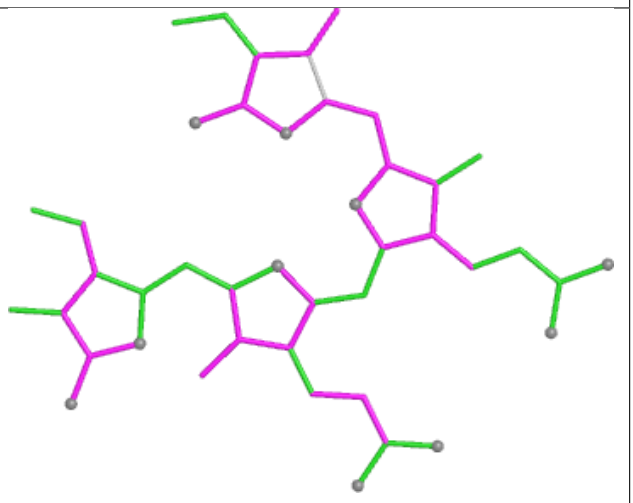


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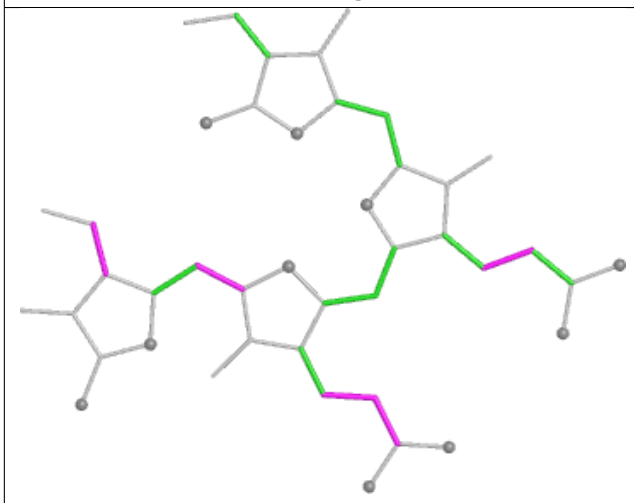
Ligand PEB NO 1002



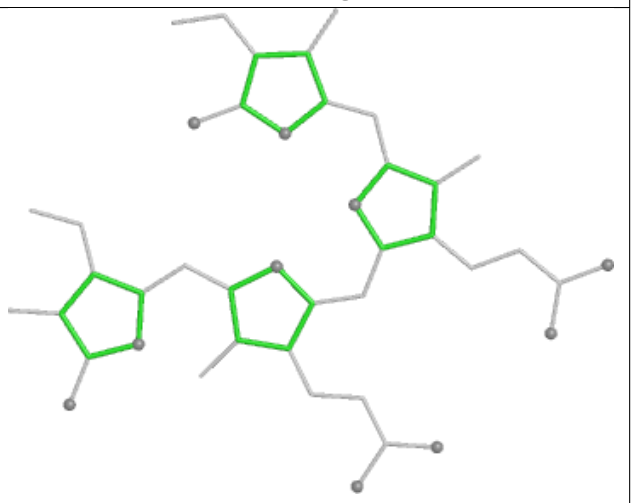
Bond lengths



Bond angles

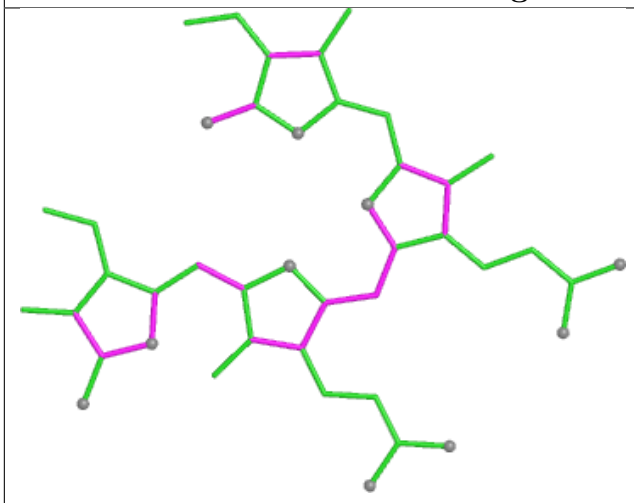


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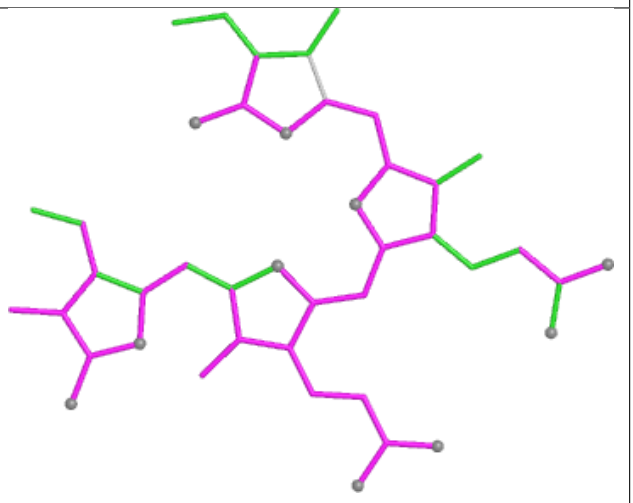


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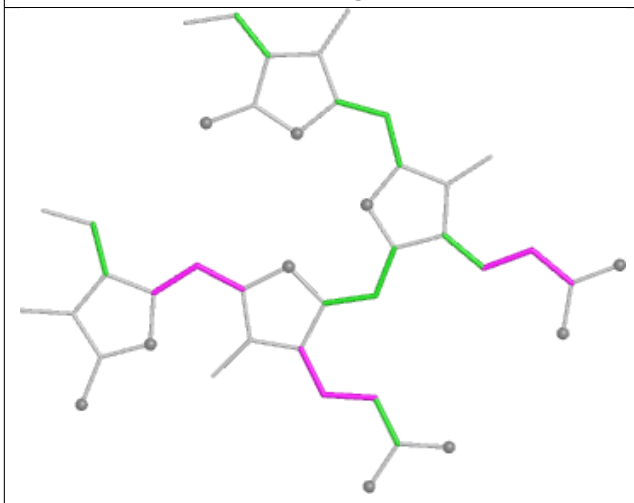
Ligand PEB GK 203



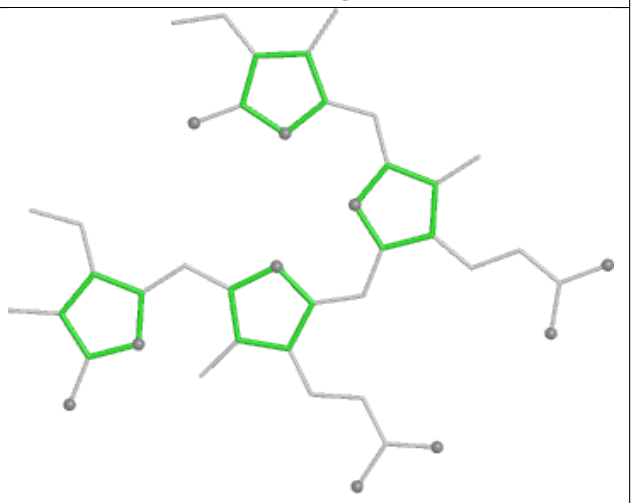
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Bond angles

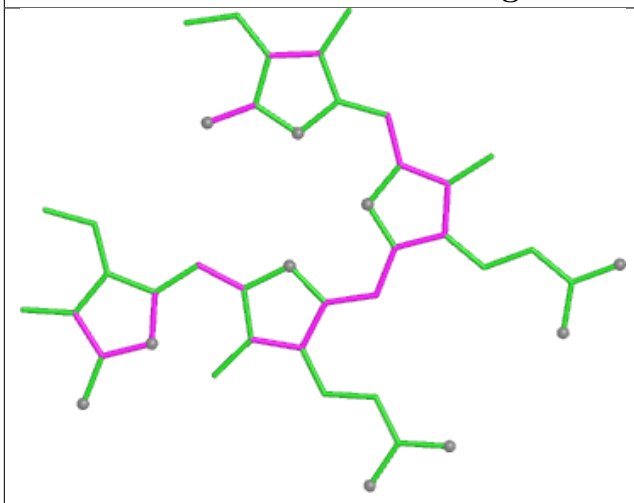


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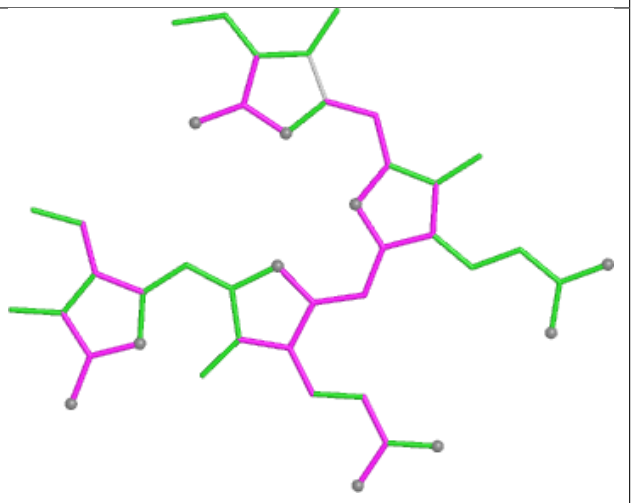


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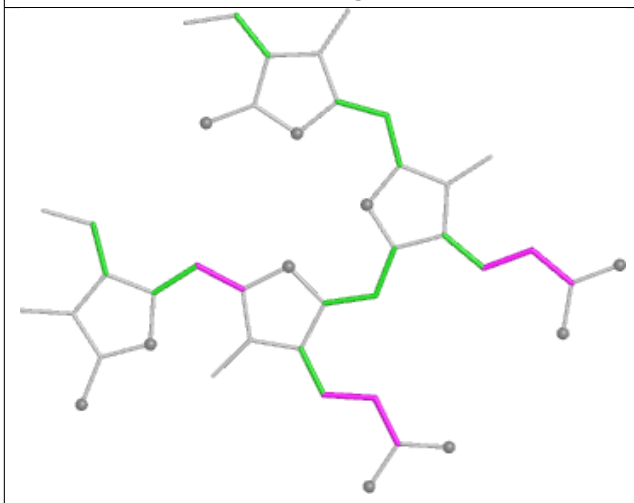
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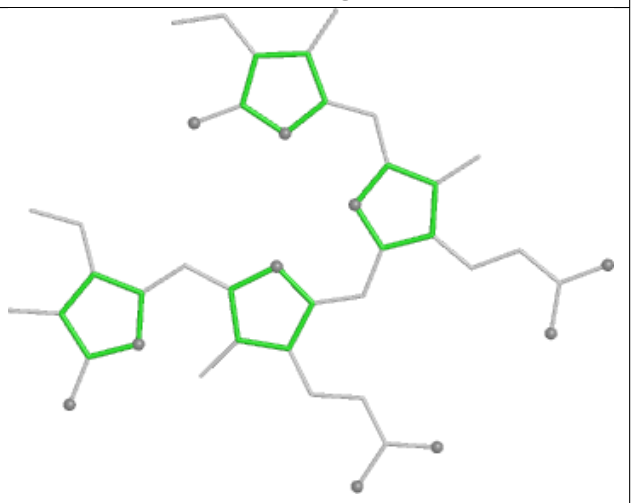
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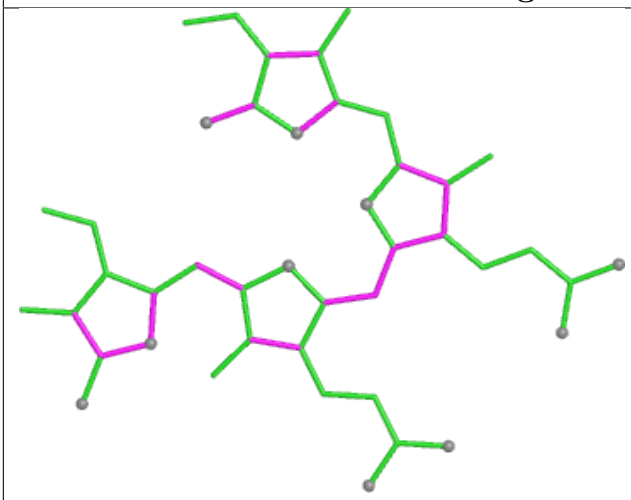


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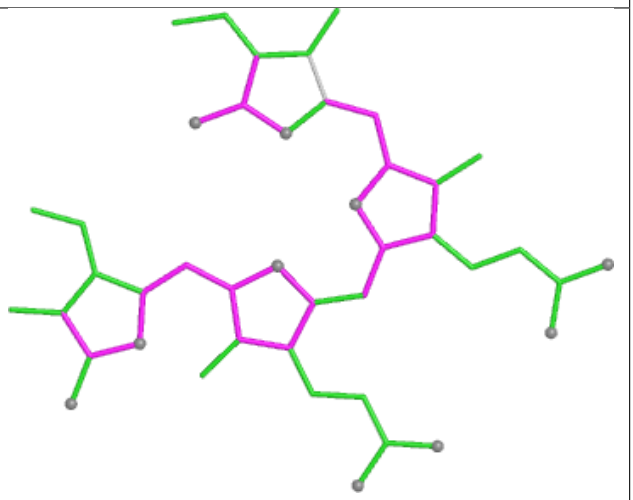


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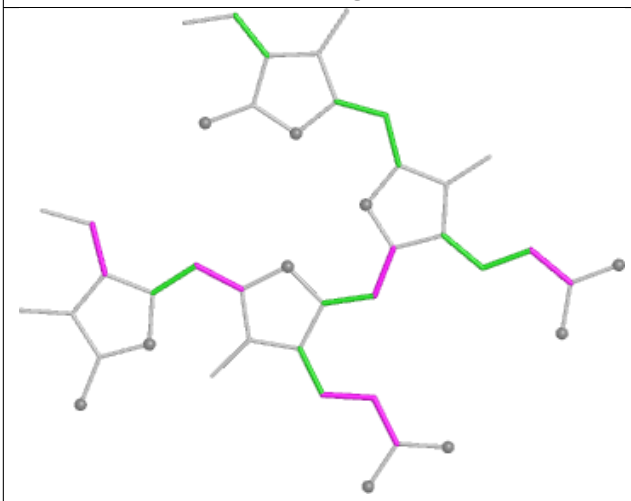
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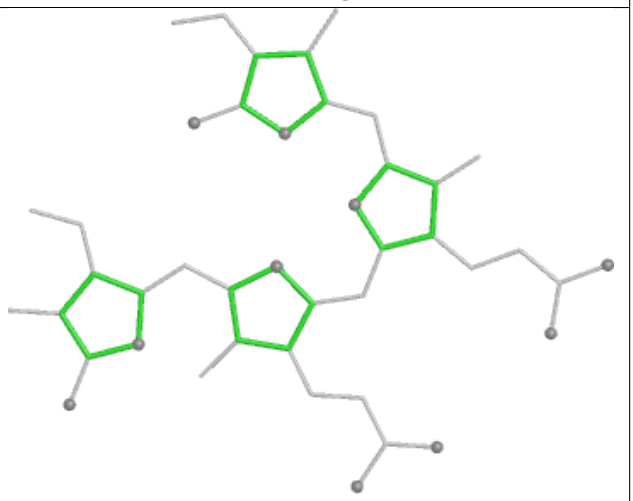
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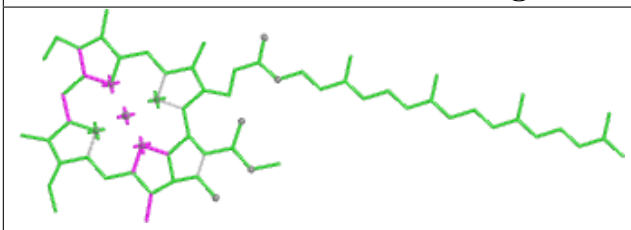


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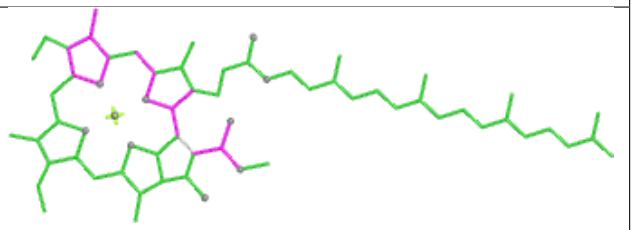


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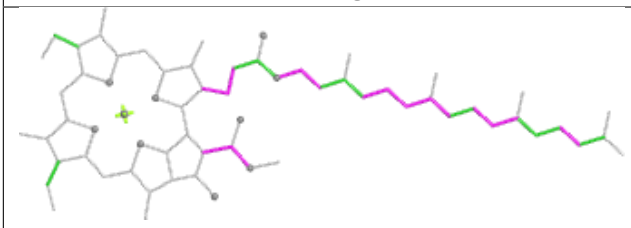
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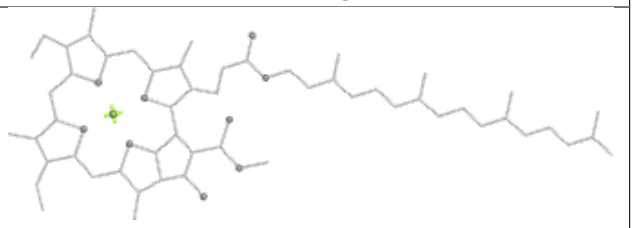
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Bond angles

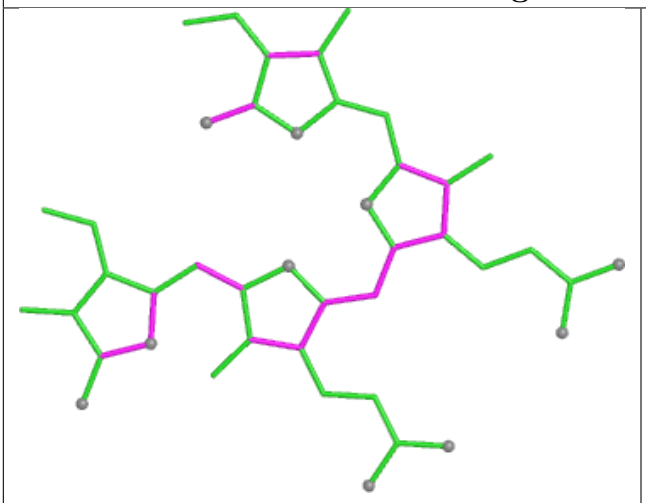


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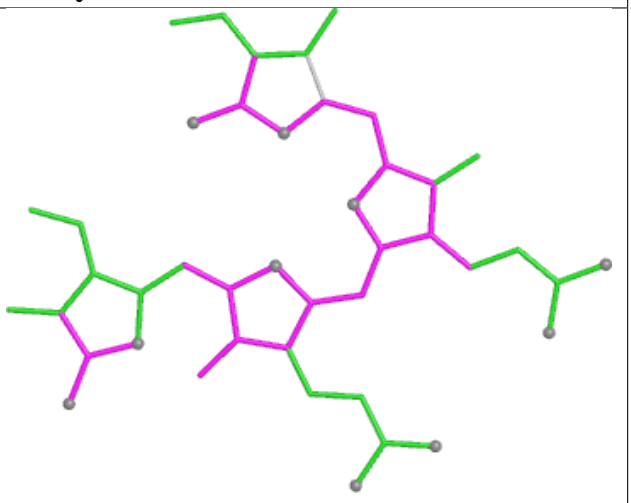


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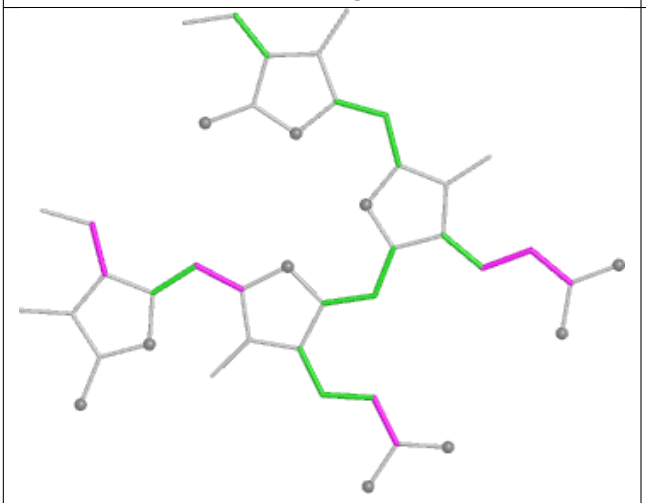
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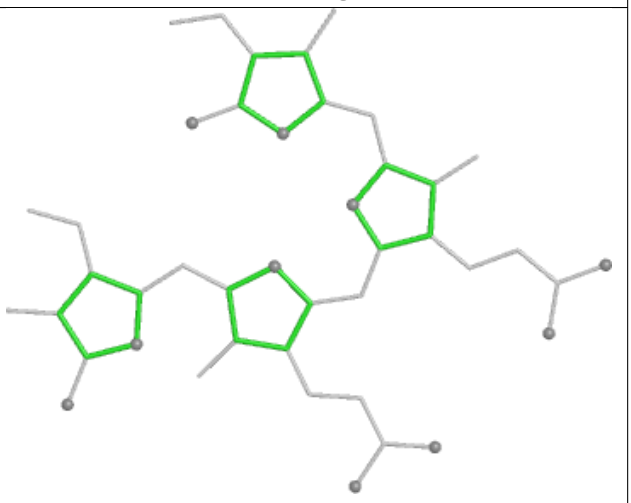
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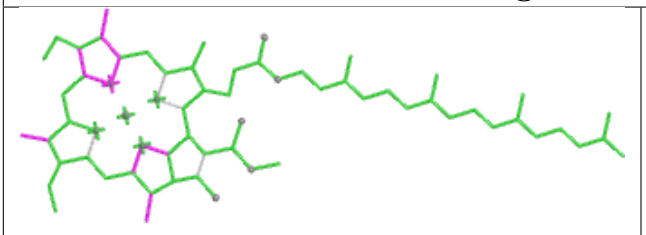


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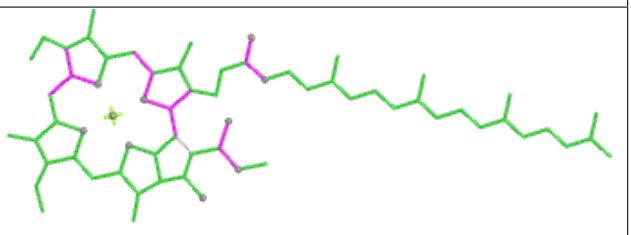


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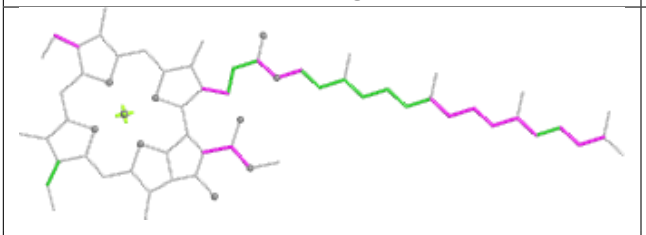
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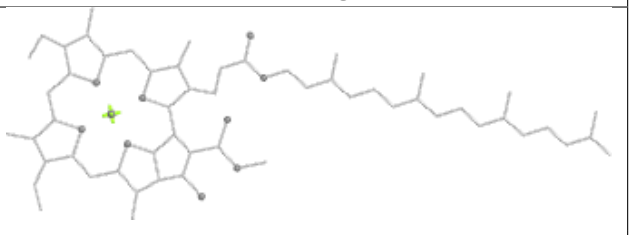
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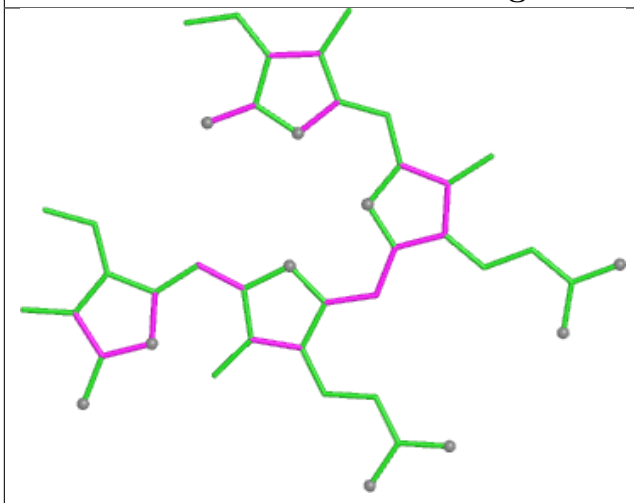


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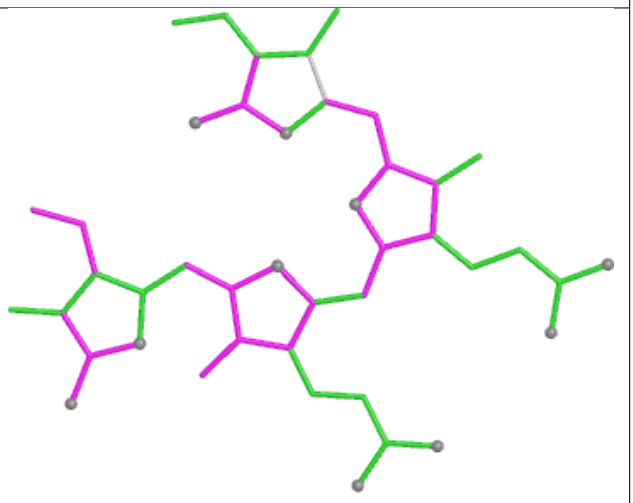


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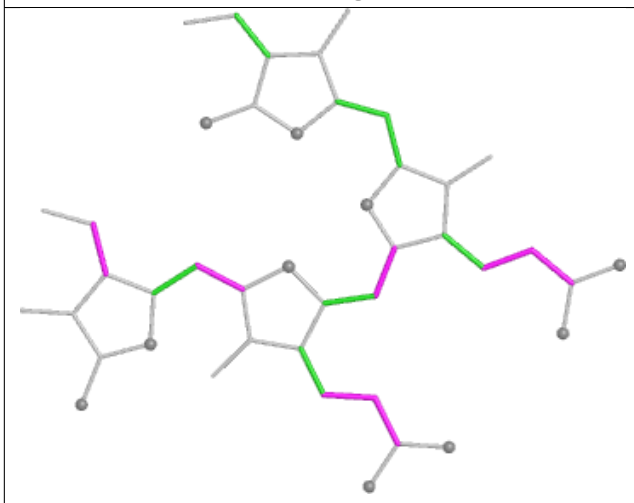
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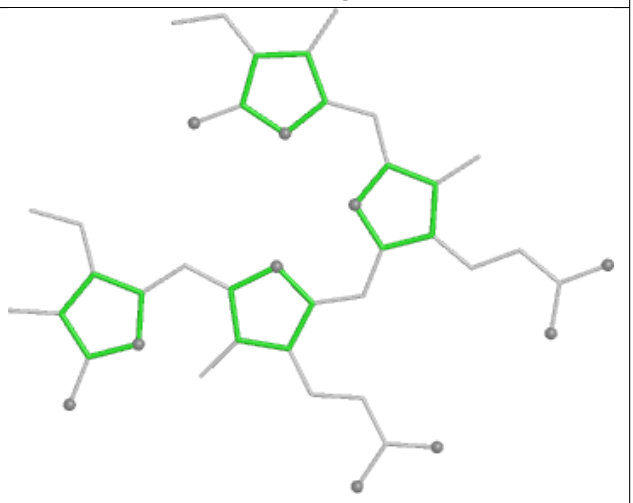
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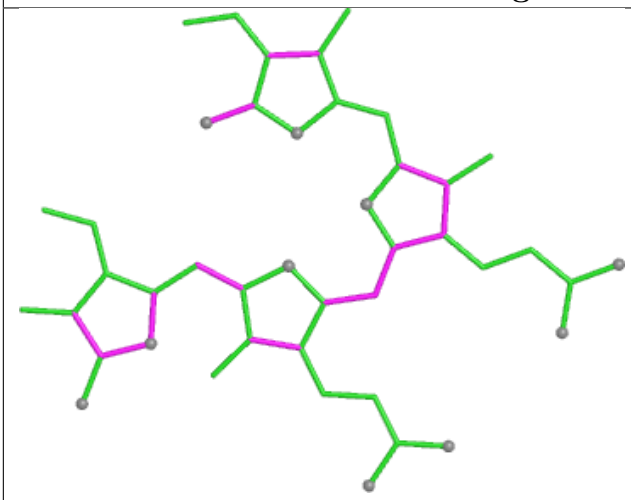


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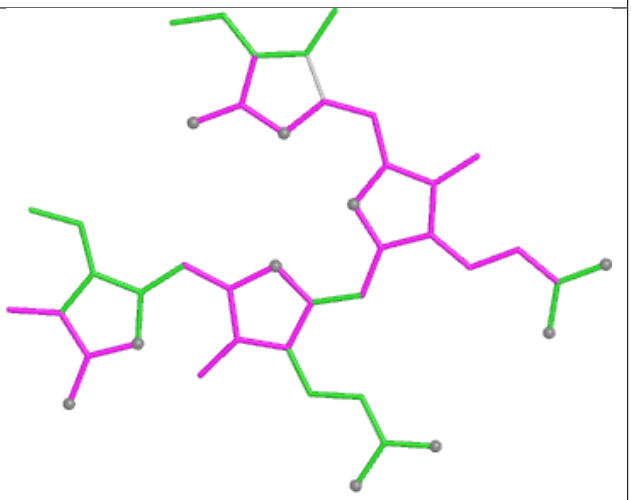


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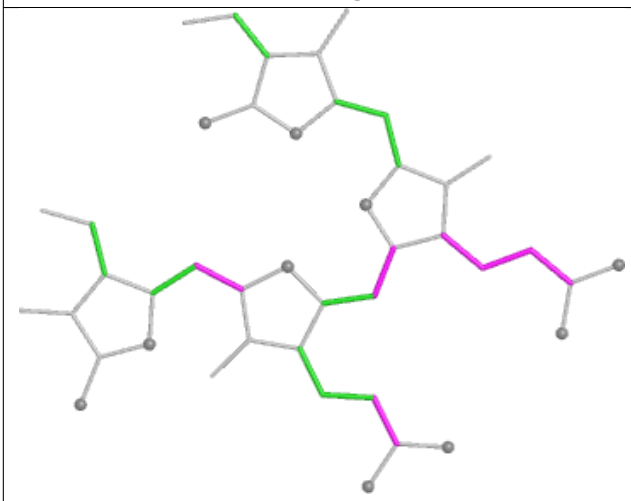
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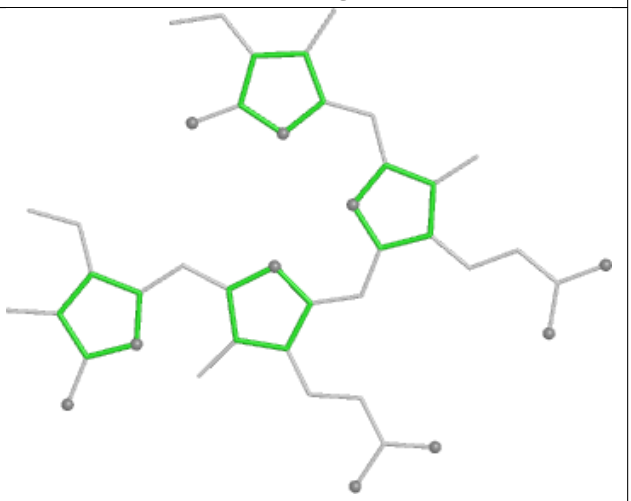
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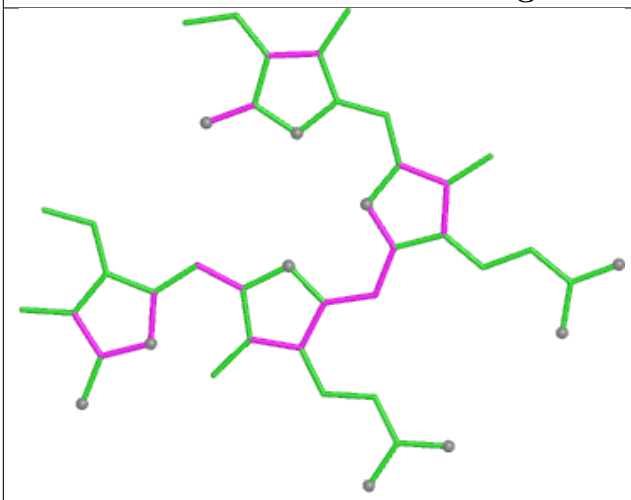


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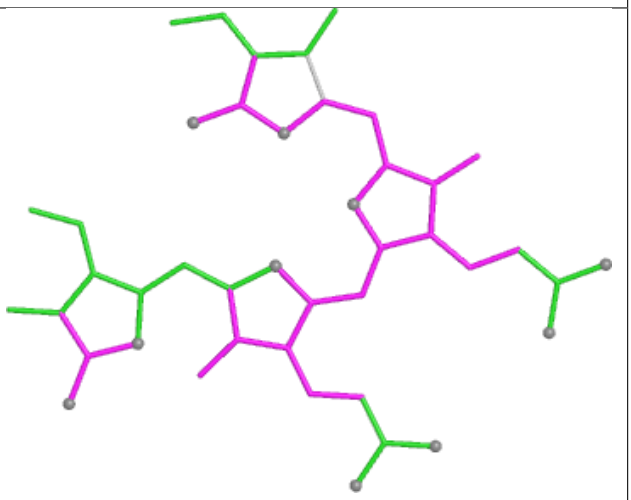


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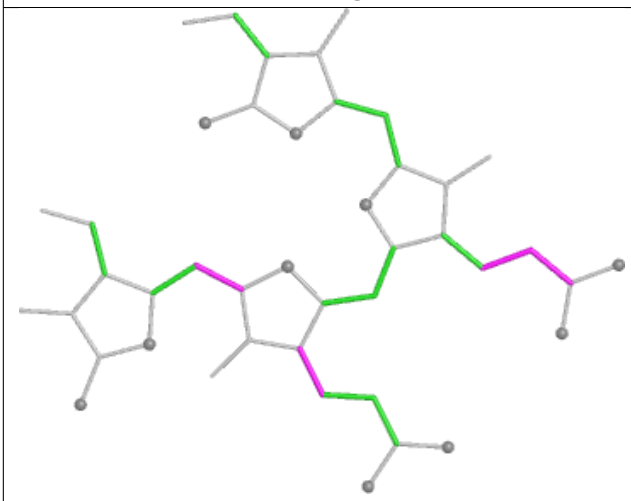
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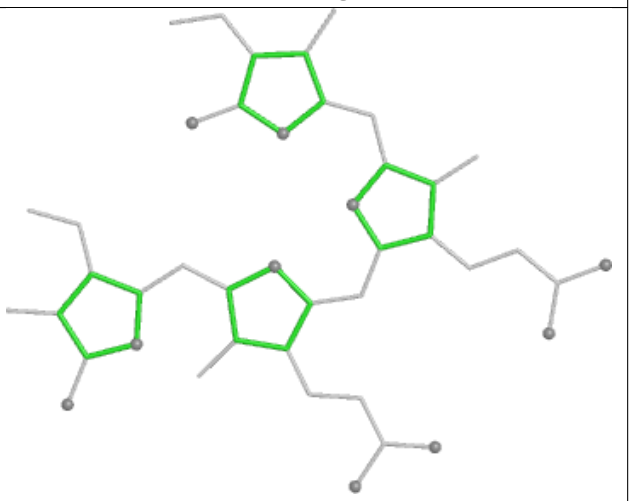
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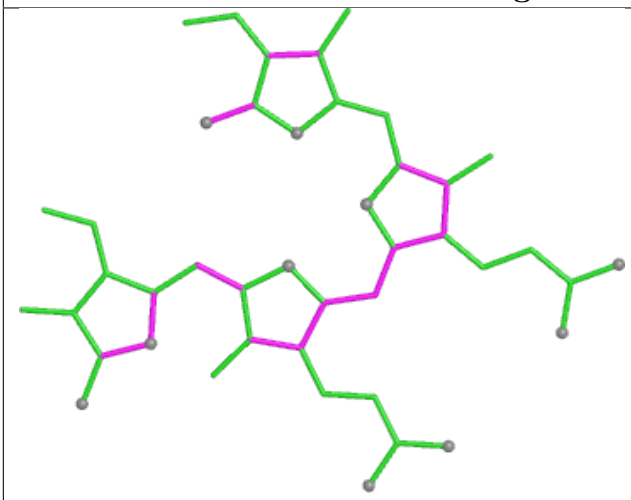


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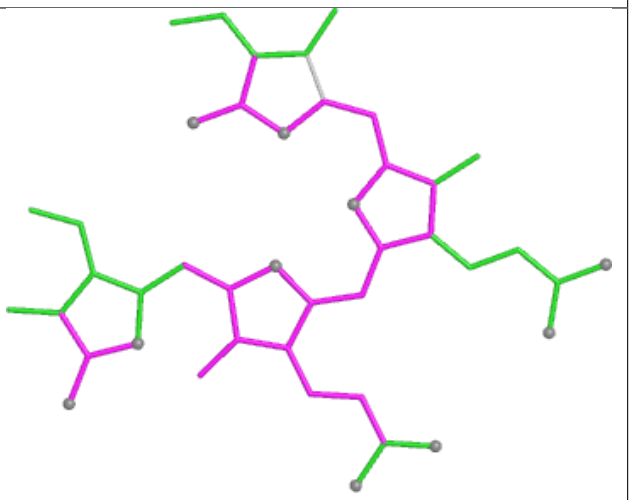


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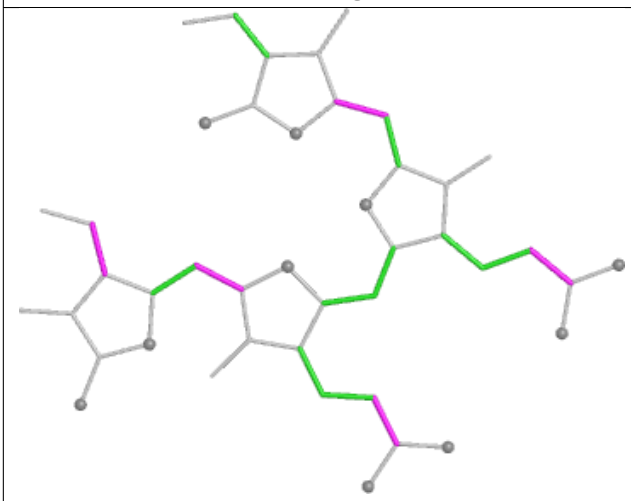
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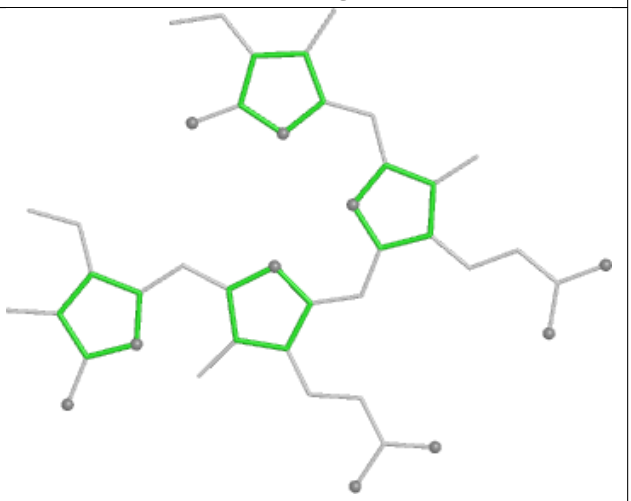
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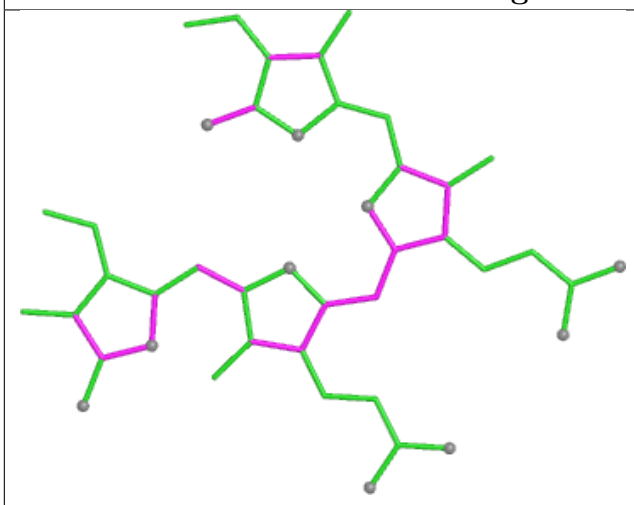


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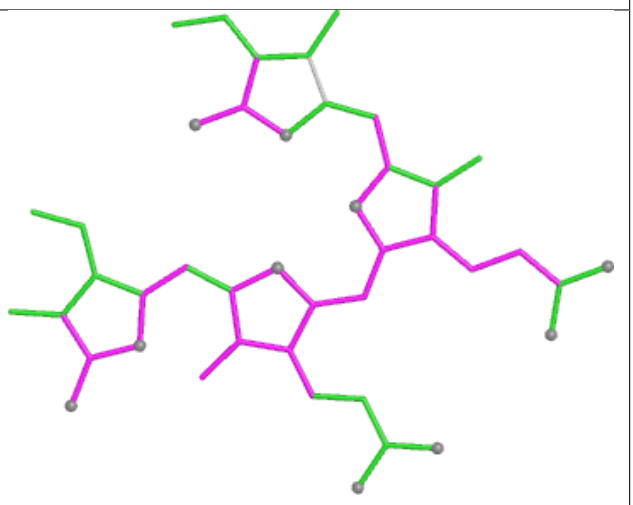


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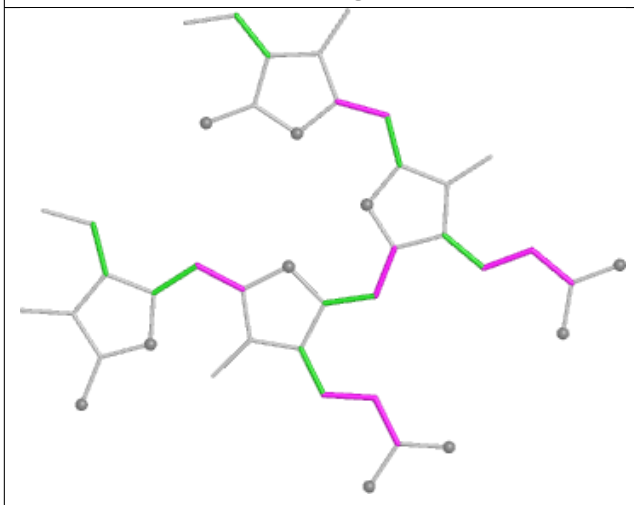
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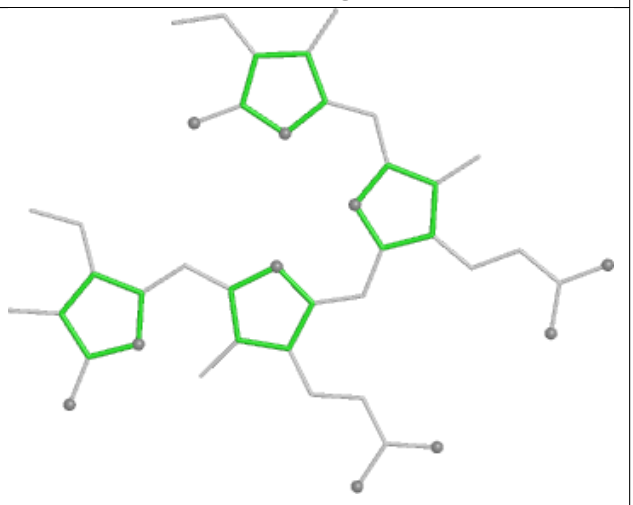
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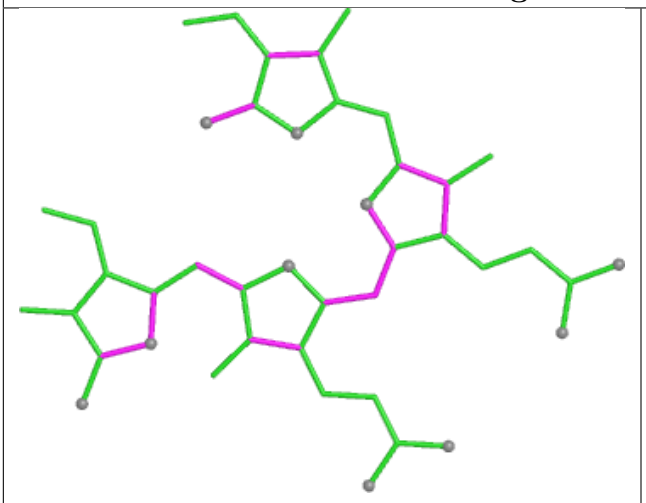


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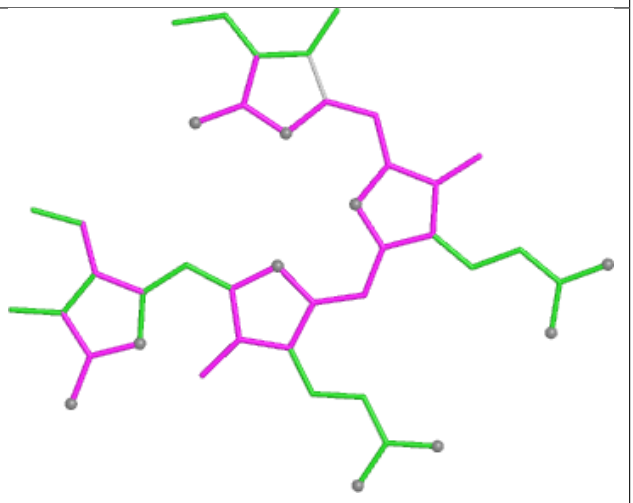


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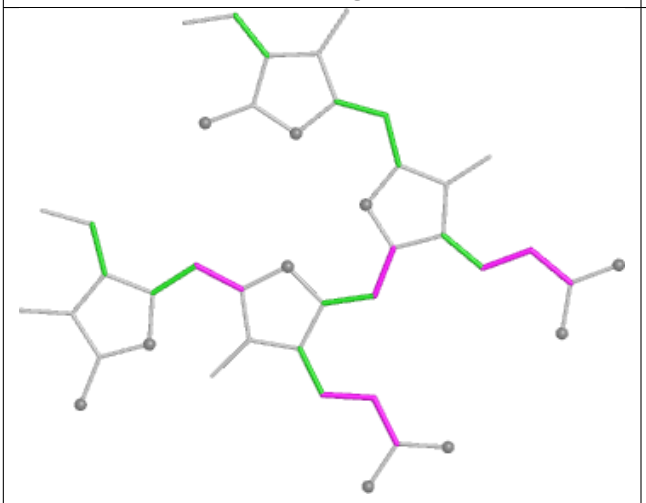
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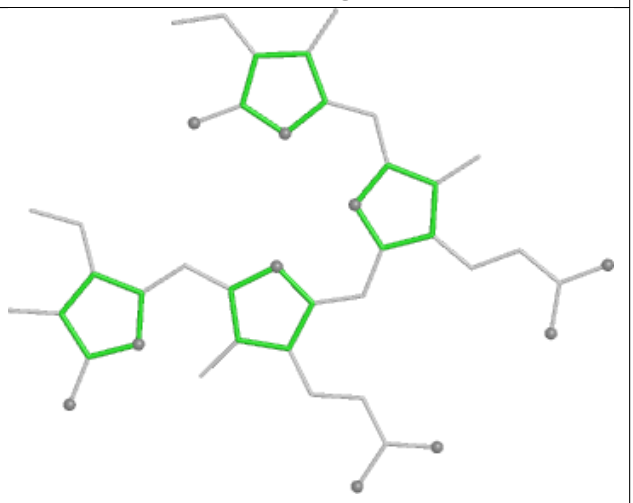
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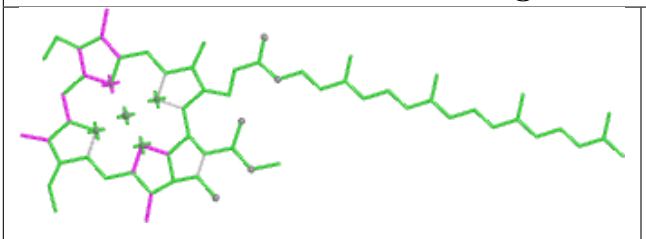


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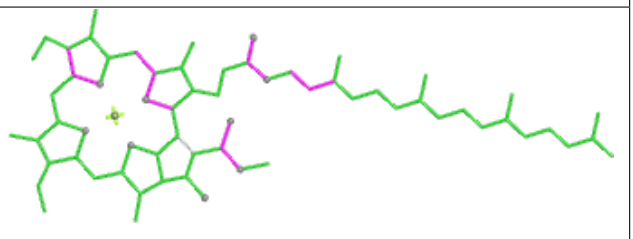


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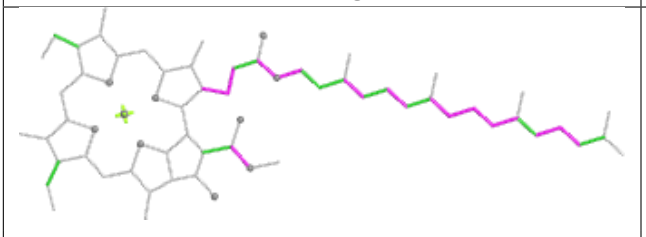
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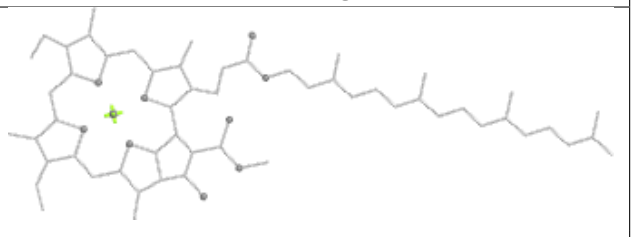
Bond lengths



Bond angles

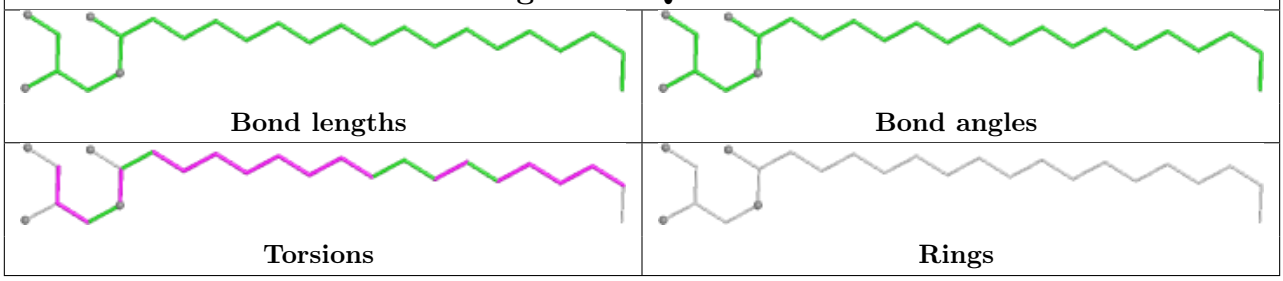


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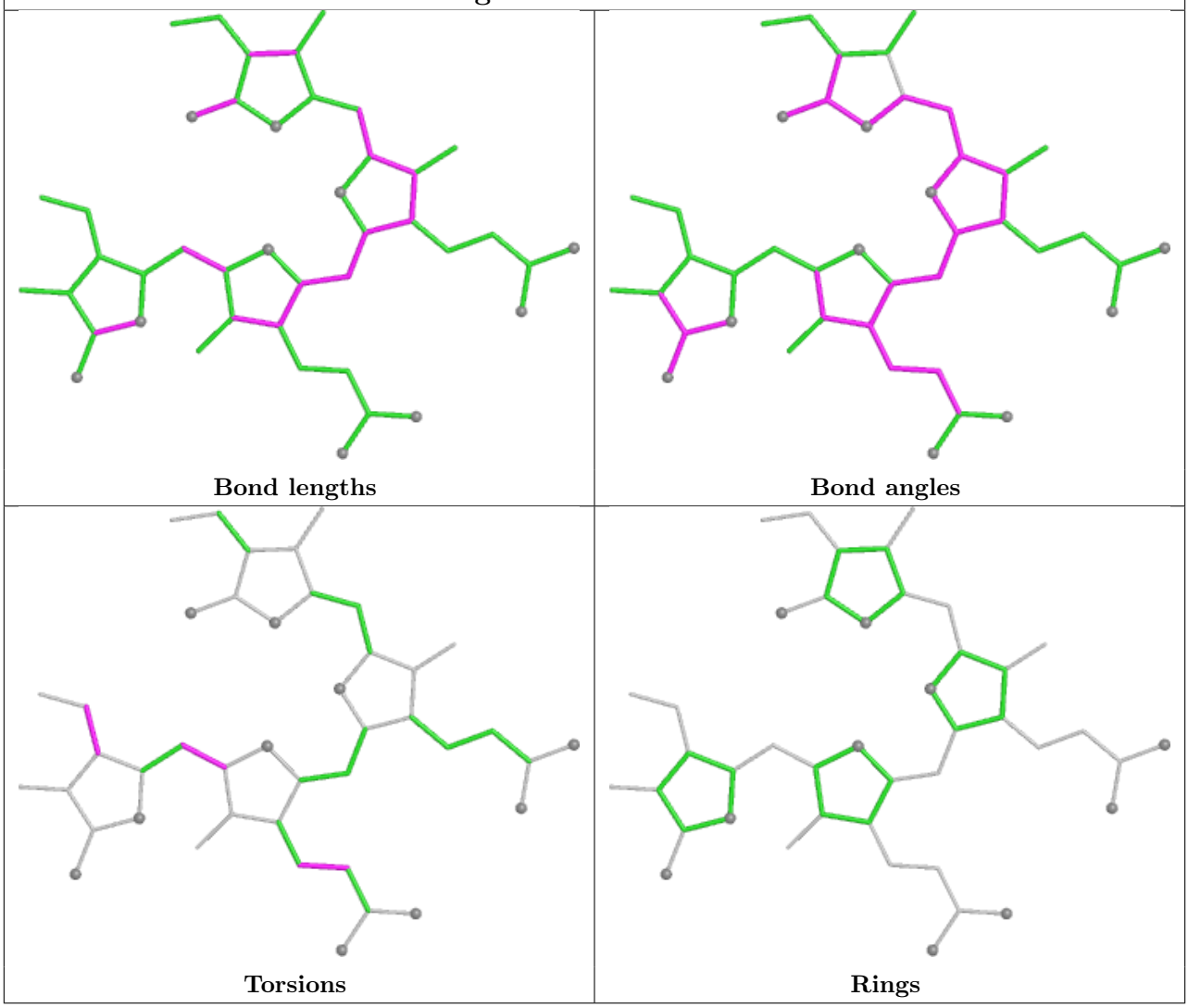


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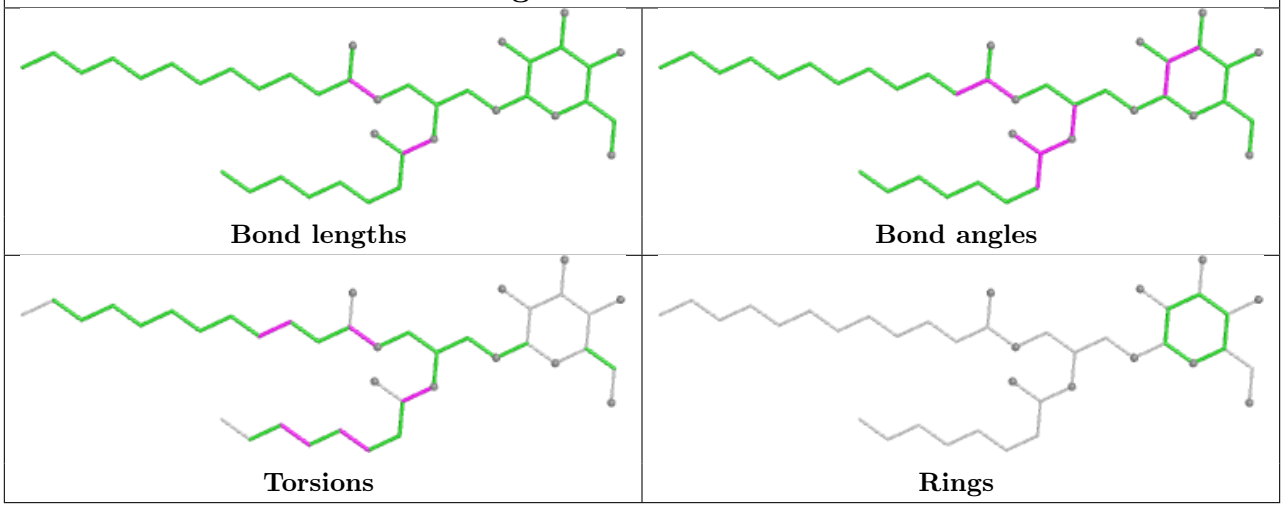
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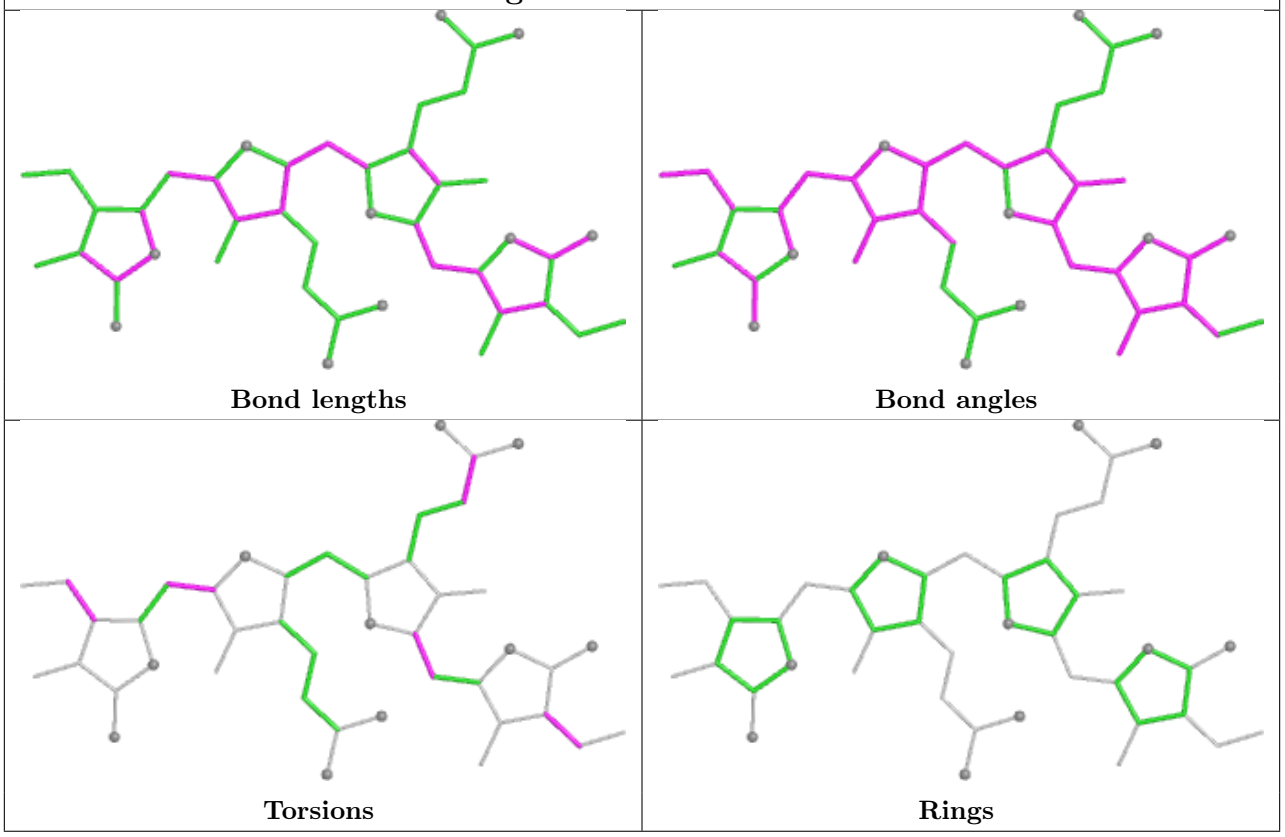
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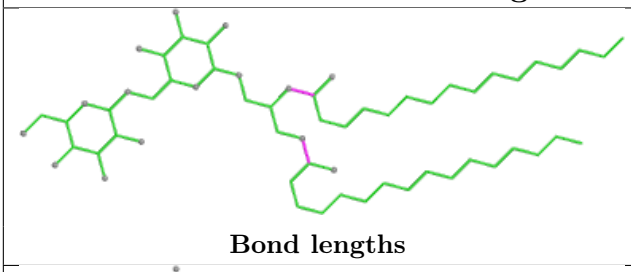
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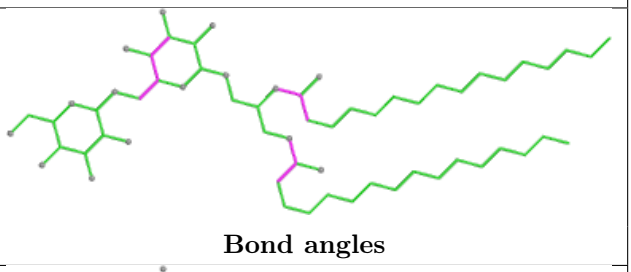
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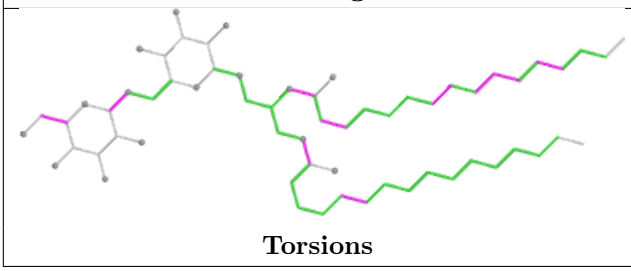
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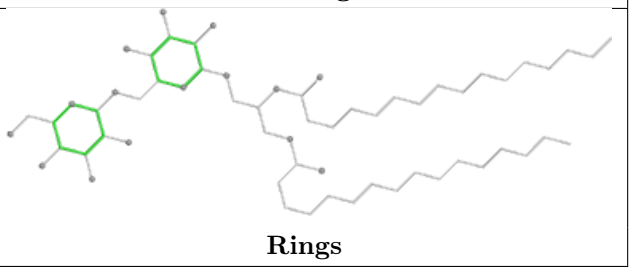
Bond lengths



Bond angles

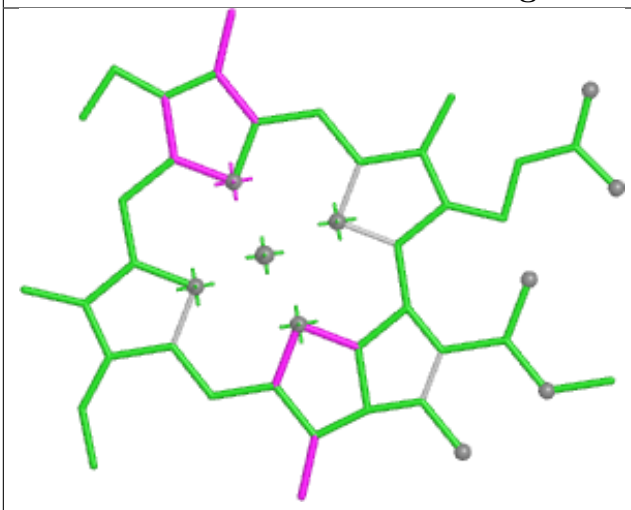


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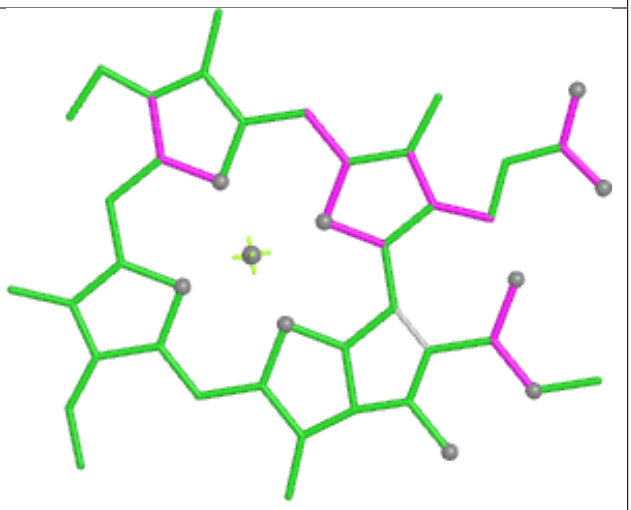


Rings

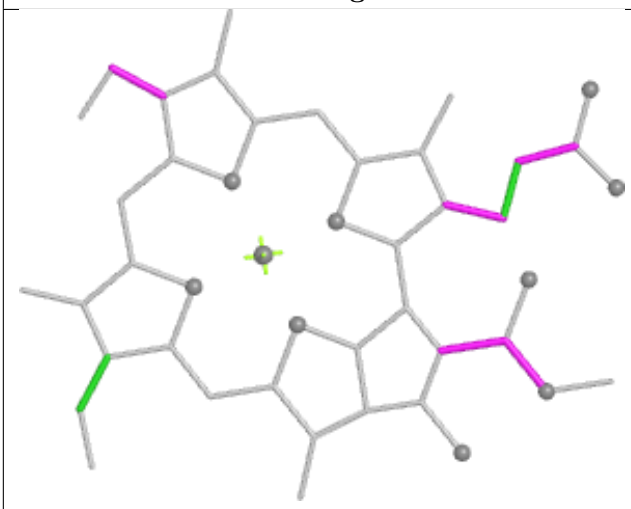
Ligand CLA 12 605



Bond lengths



Bond angles

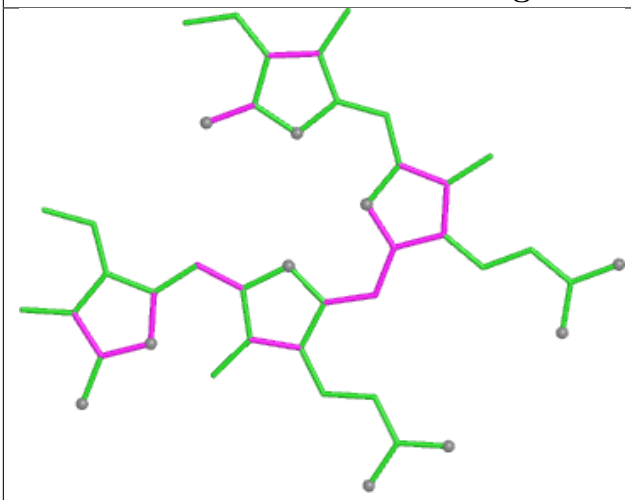


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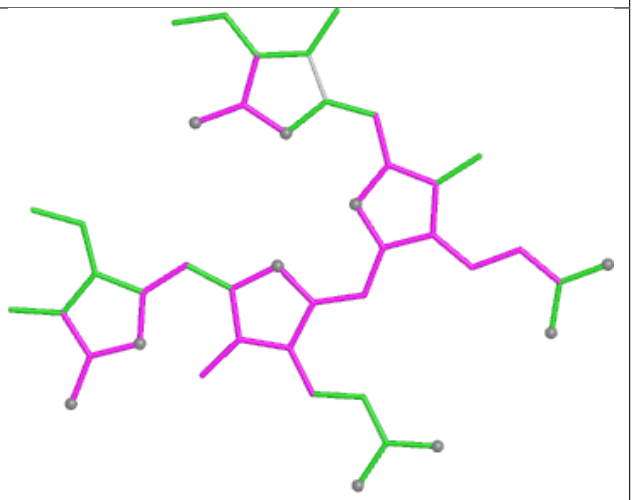


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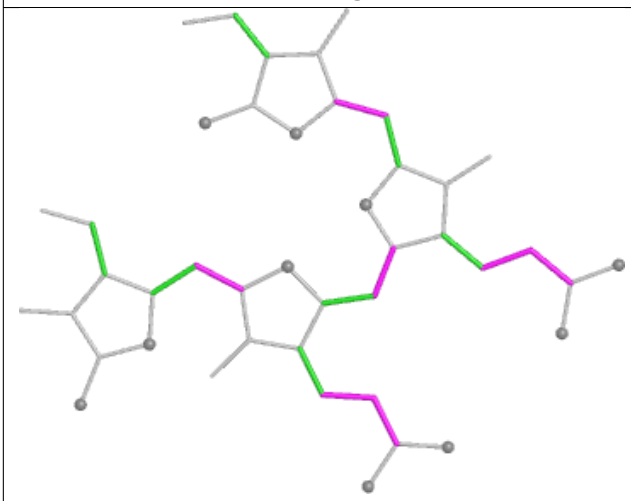
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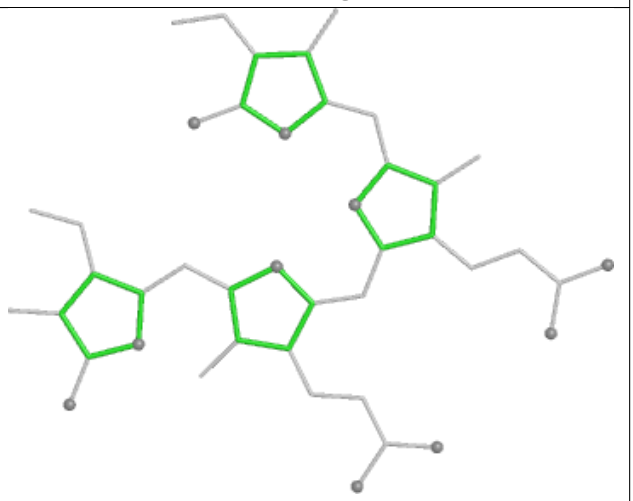
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Bond angles

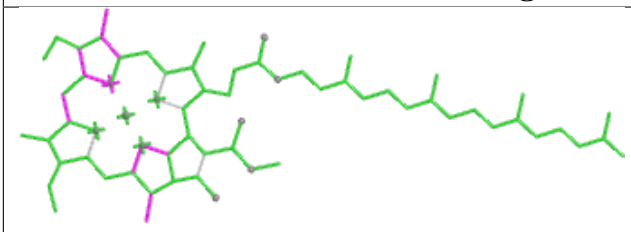


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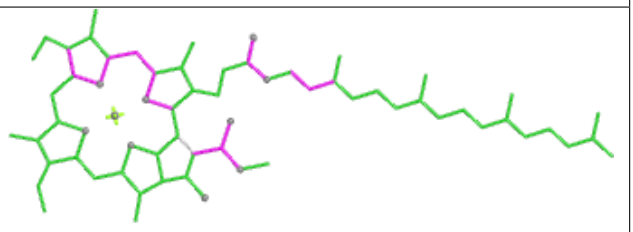


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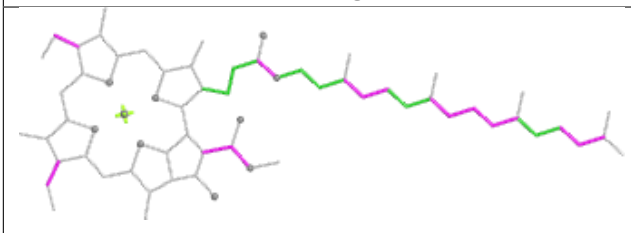
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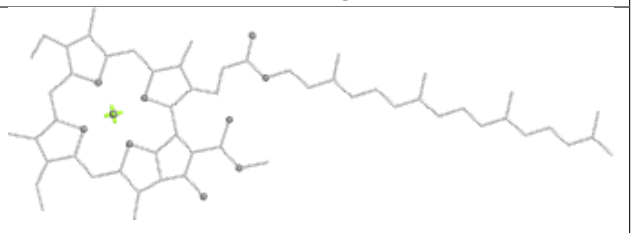
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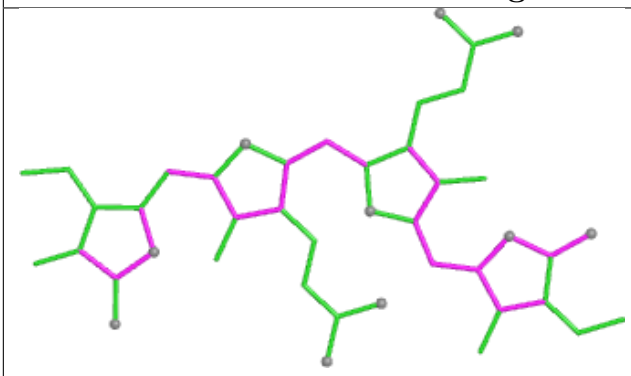


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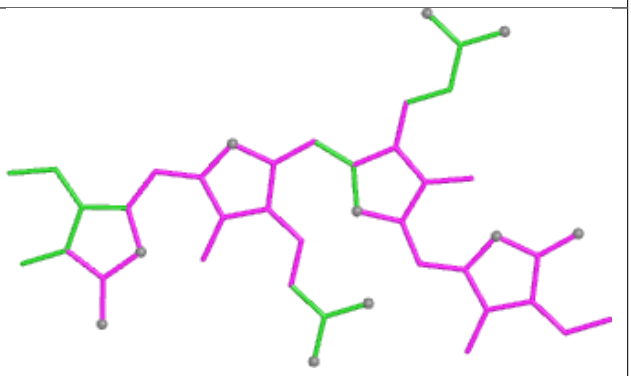


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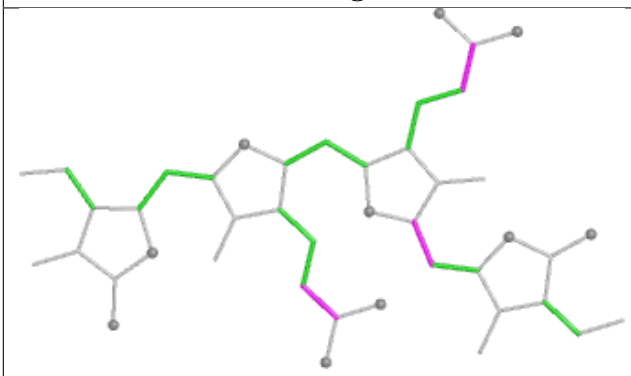
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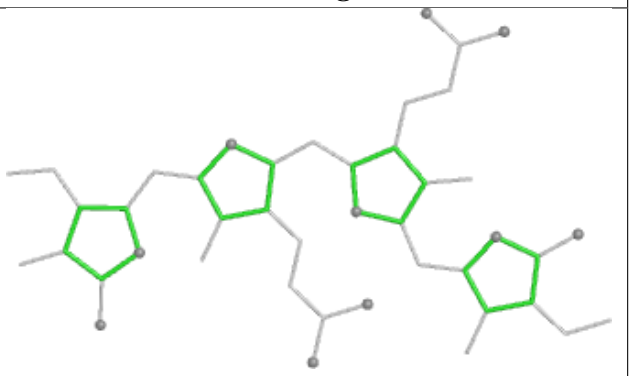
Bond lengths



Bond angles

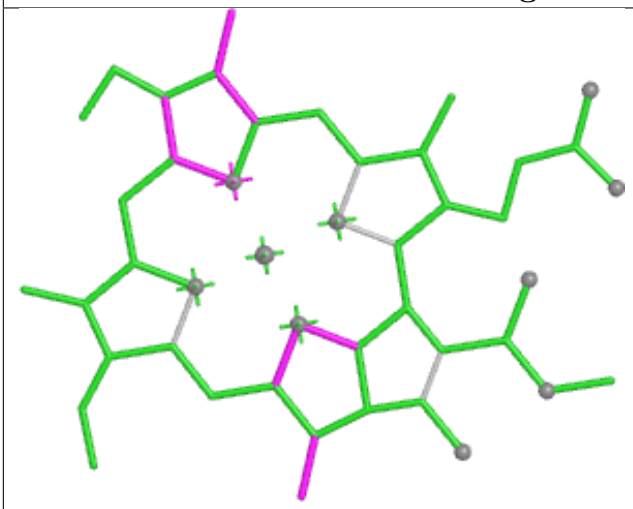


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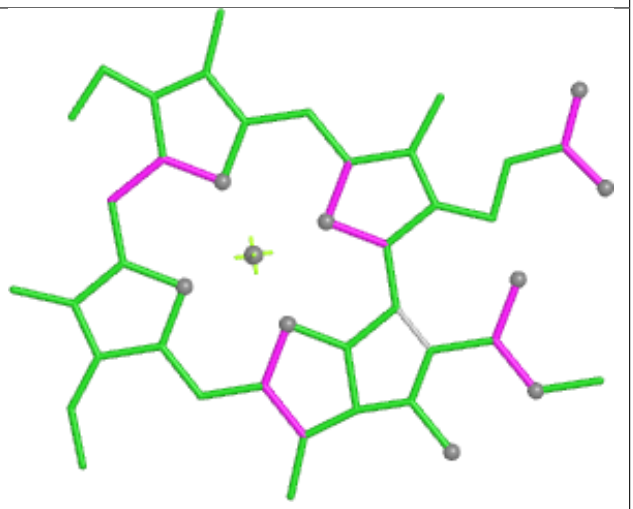


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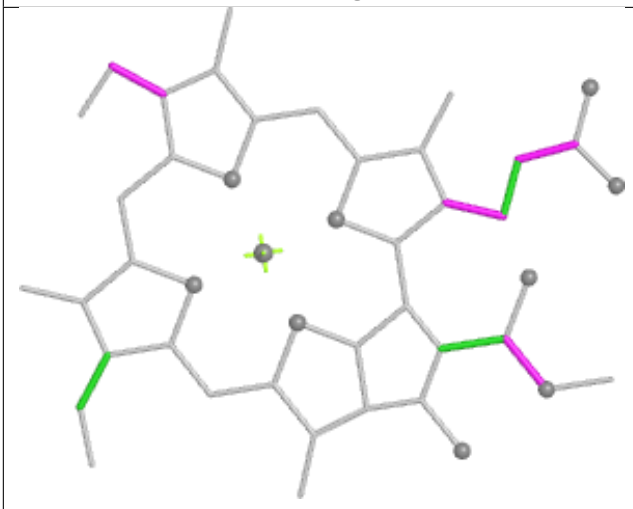
Ligand CLA 12 606



Bond lengths



Bond angles

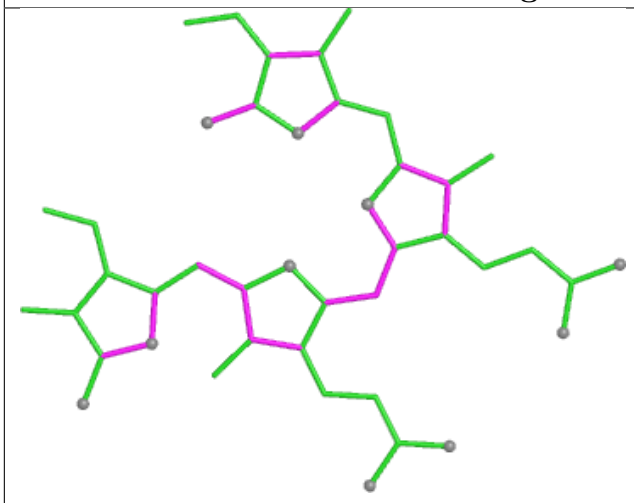


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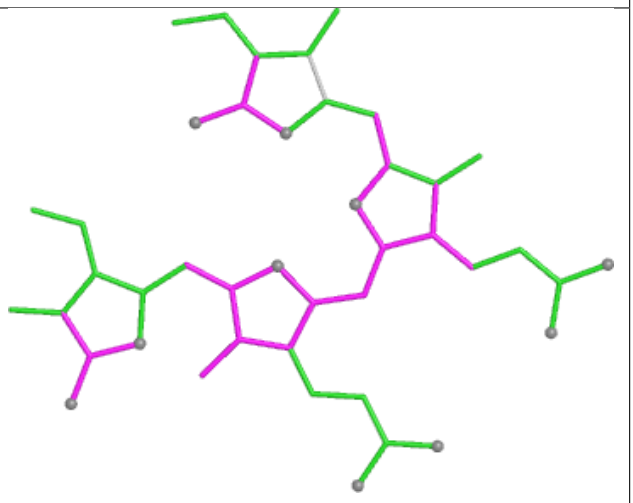


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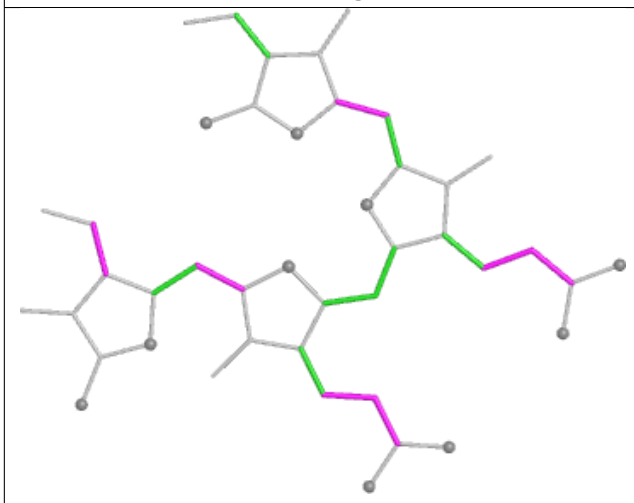
Ligand PEB sF 201



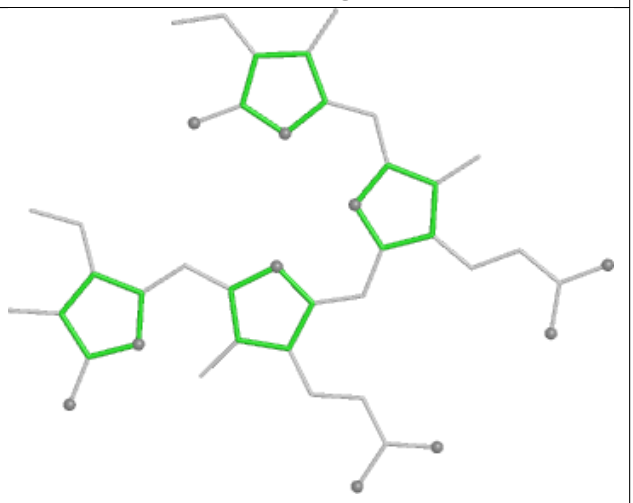
Bond lengths



Bond angles

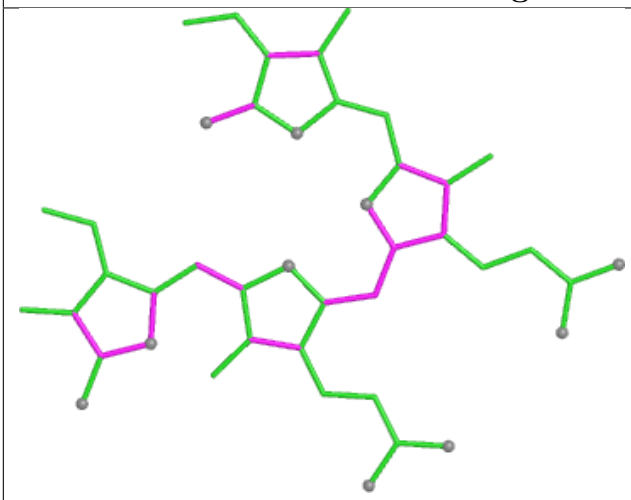


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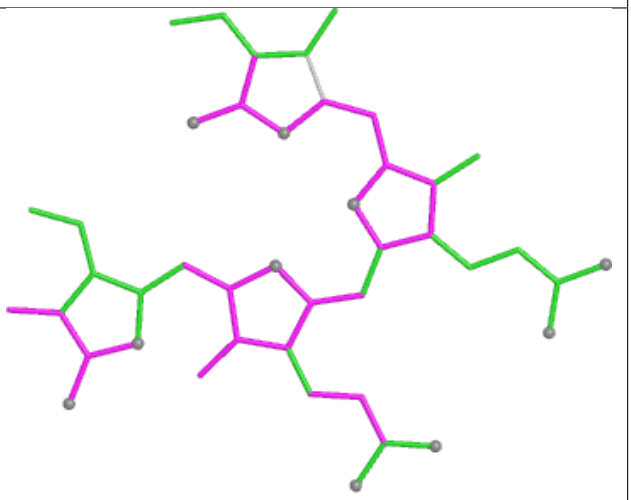


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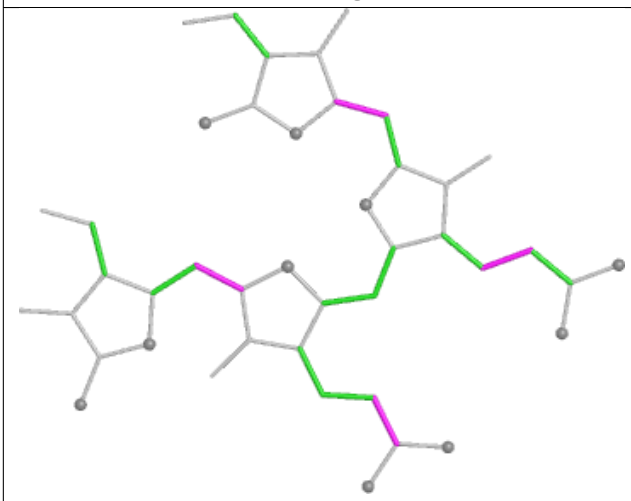
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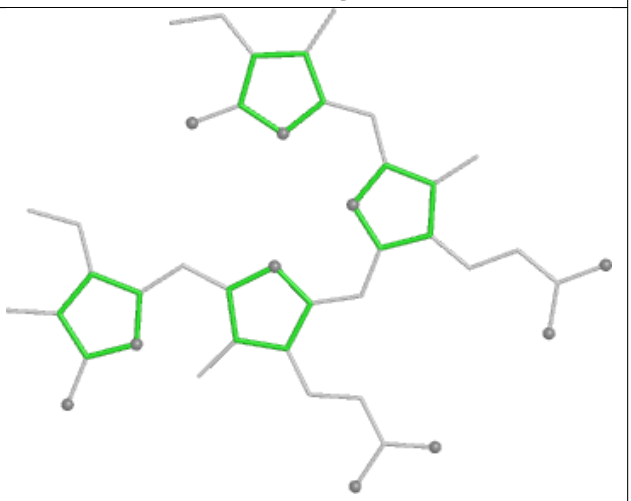
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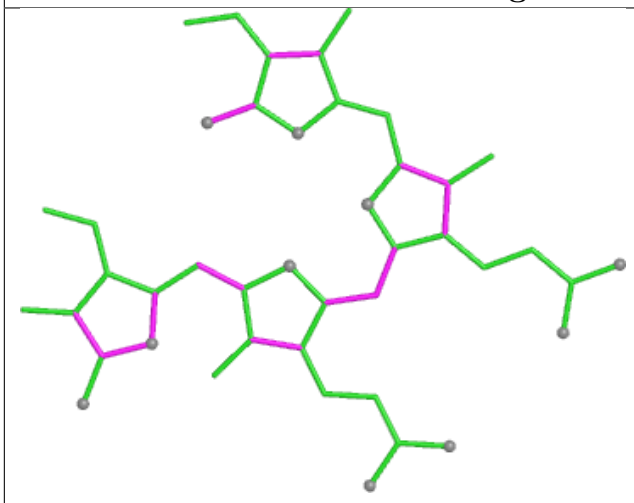


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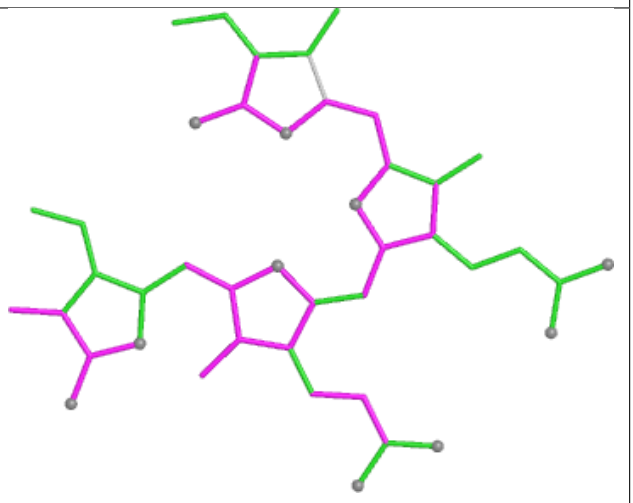


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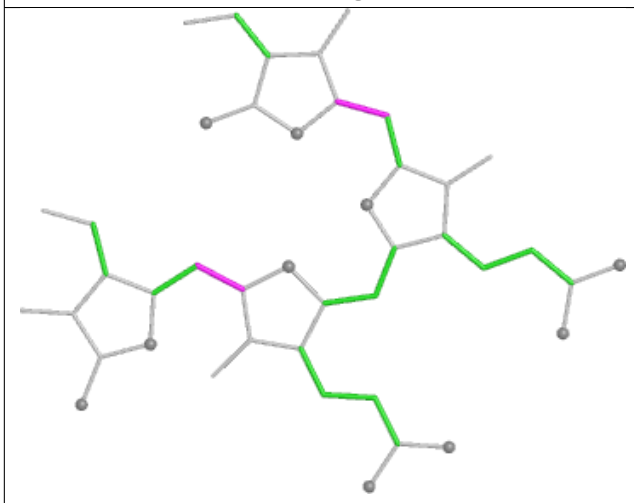
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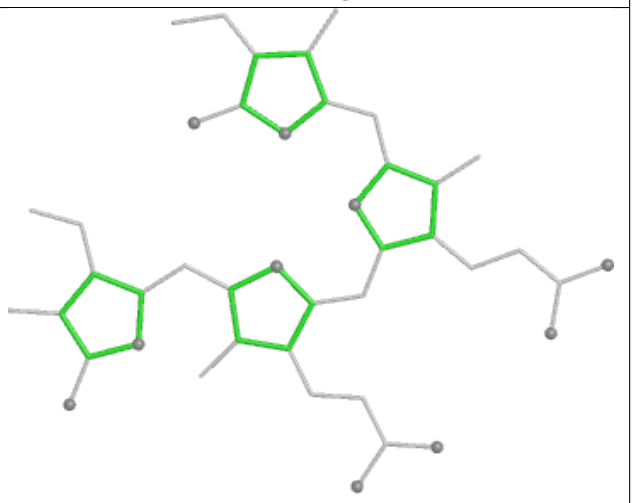
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Bond angles

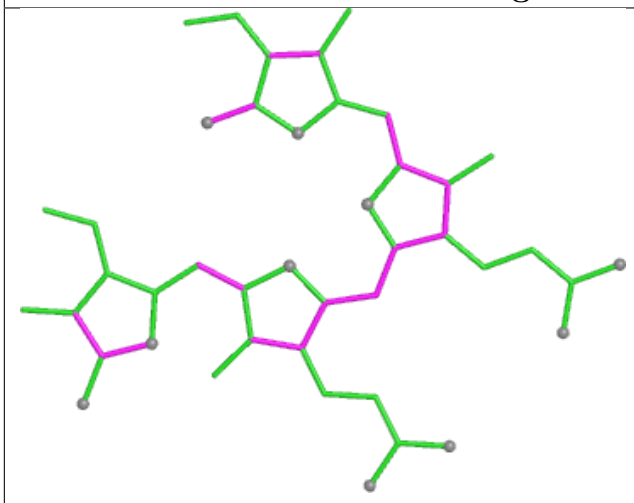


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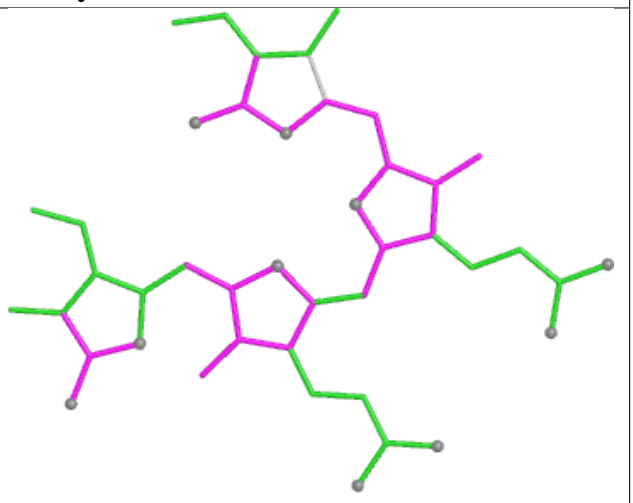


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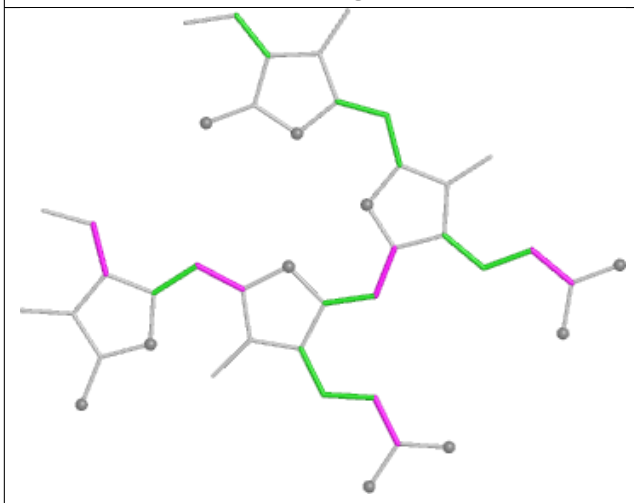
Ligand PEB RQ 202



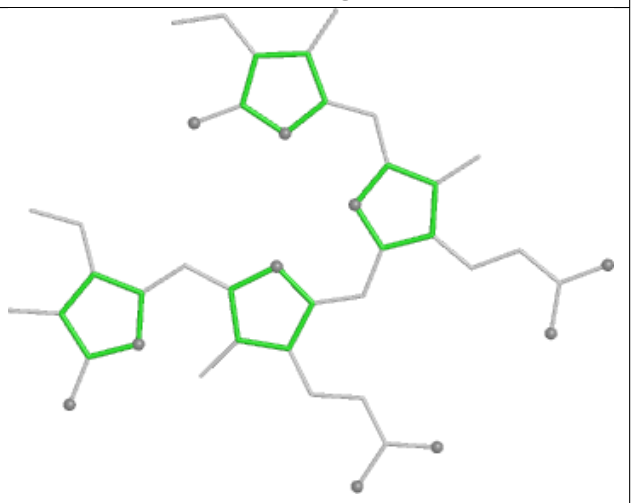
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Bond angles

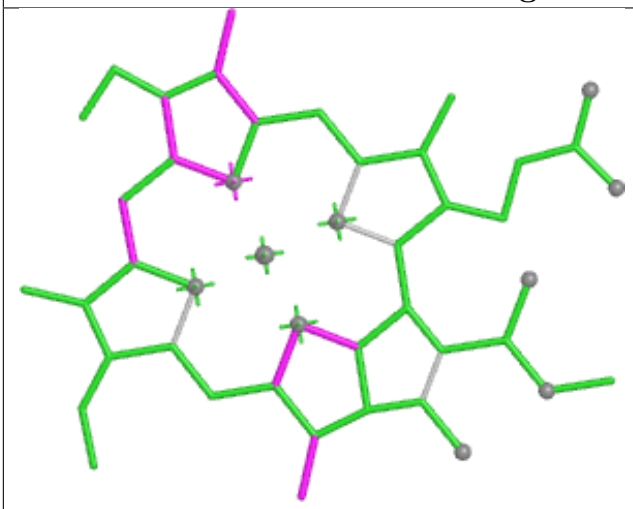


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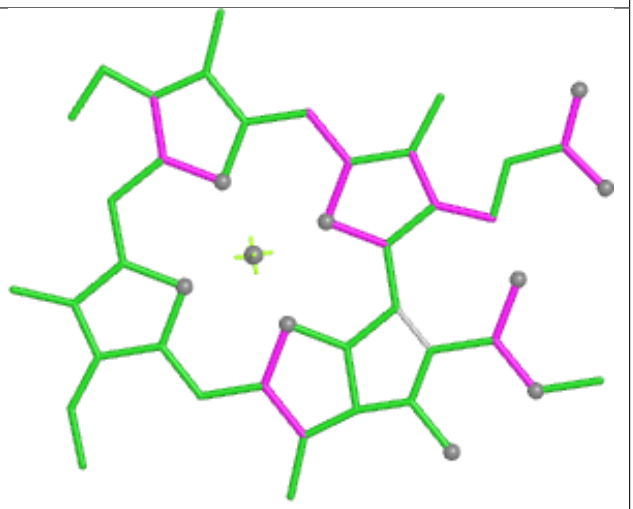


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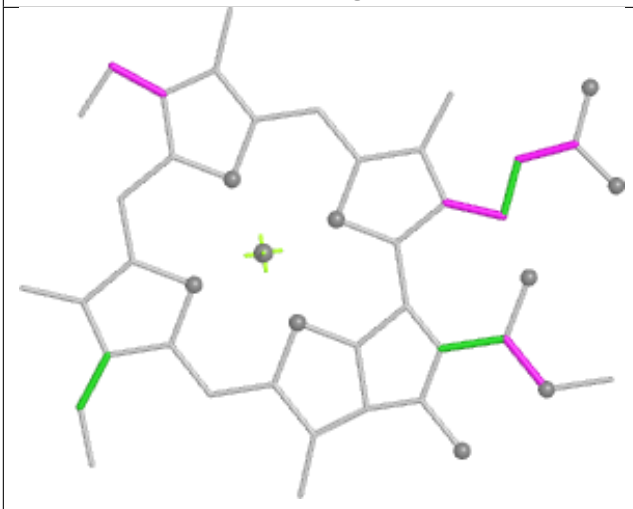
Ligand CLA 62 307



Bond lengths



Bond angles

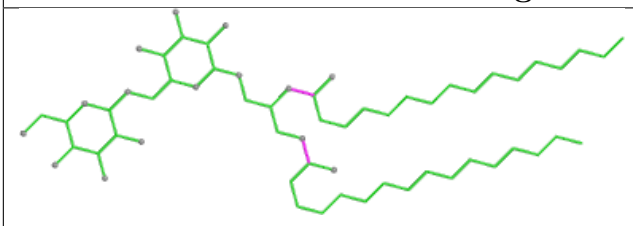


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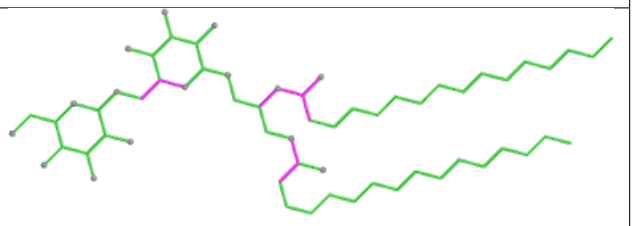


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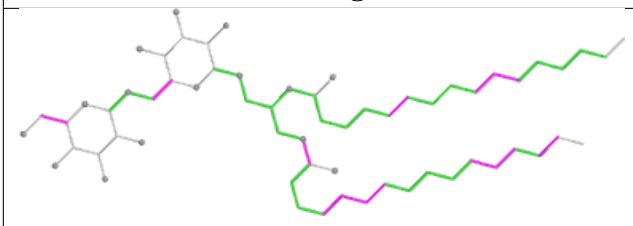
Ligand DGD J6 101



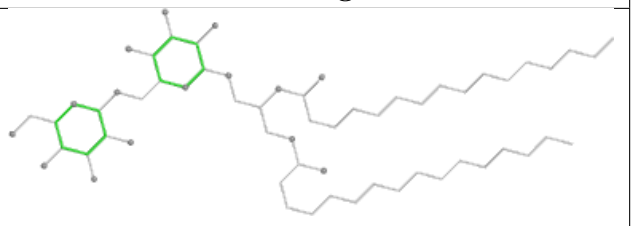
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Bond angles

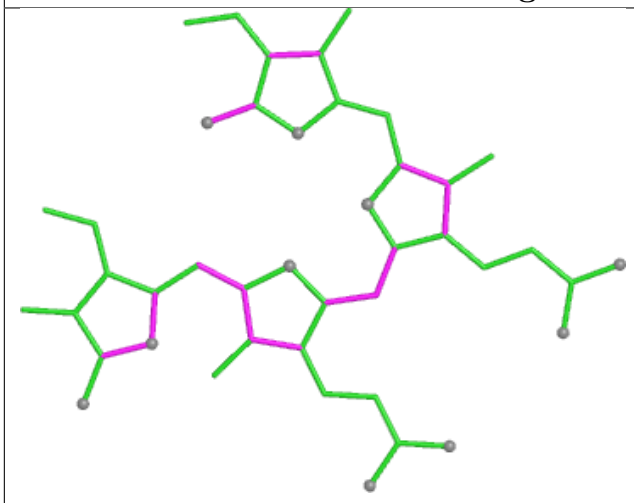


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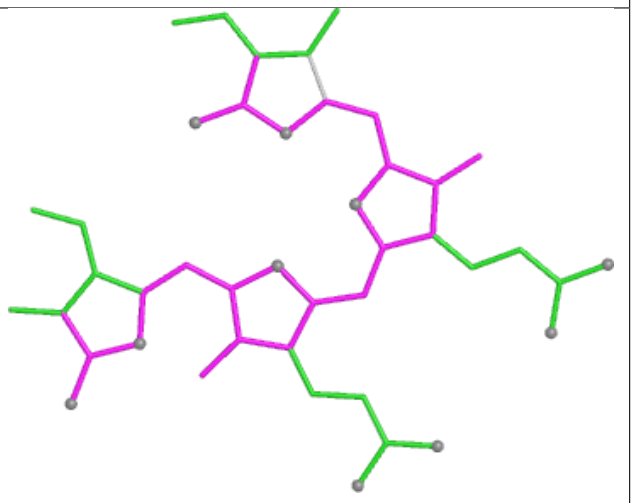


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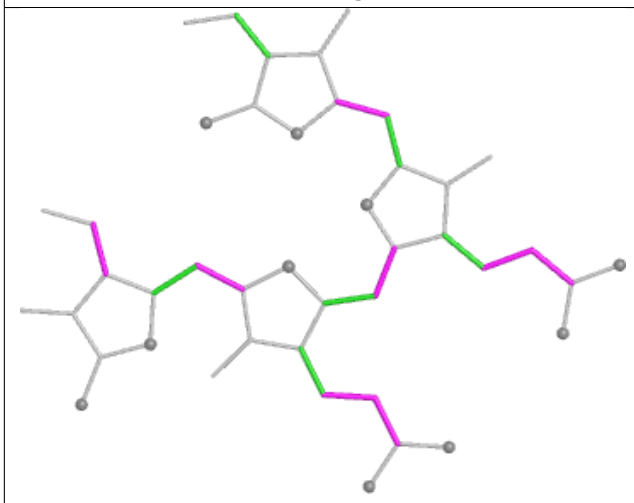
Ligand PEB aF 203



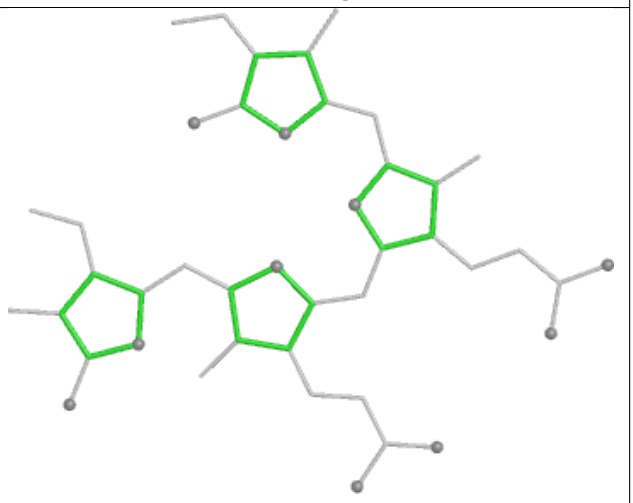
Bond lengths



Bond angles

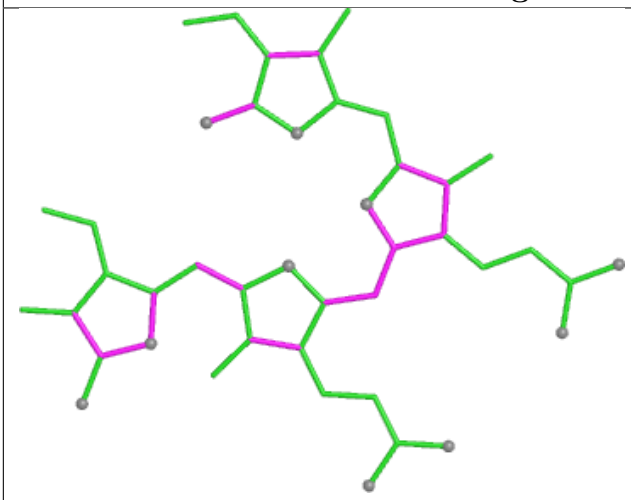


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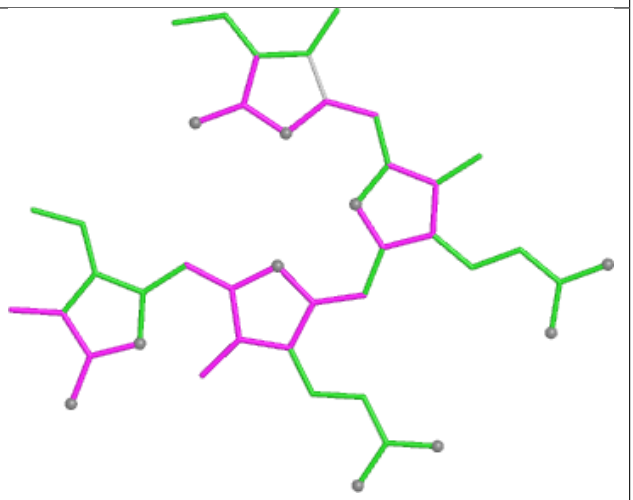


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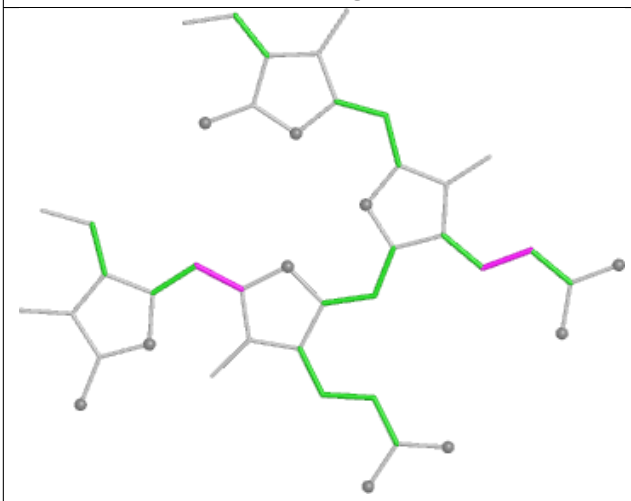
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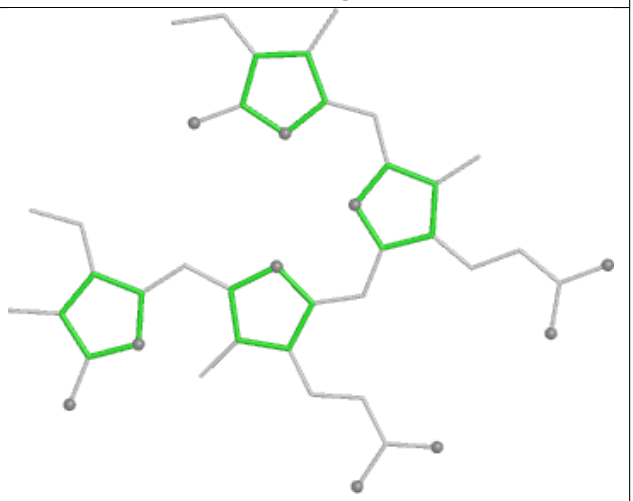
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Bond angles

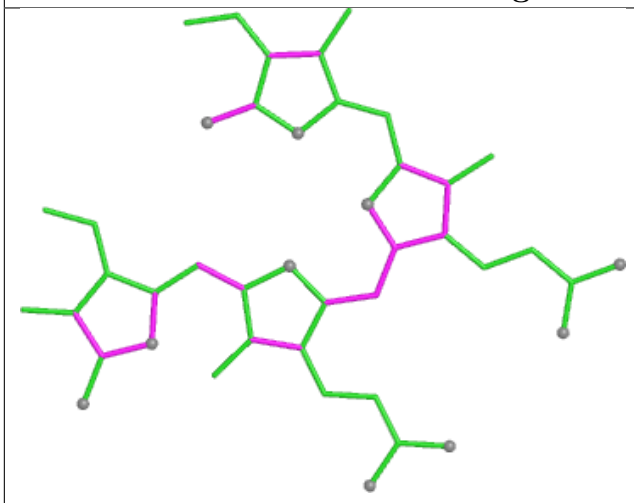


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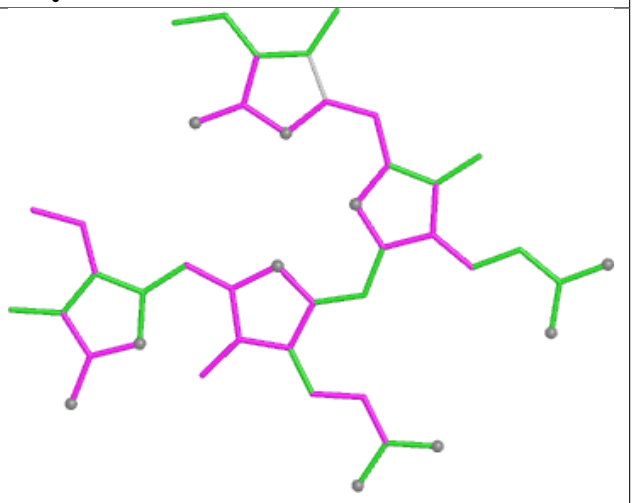


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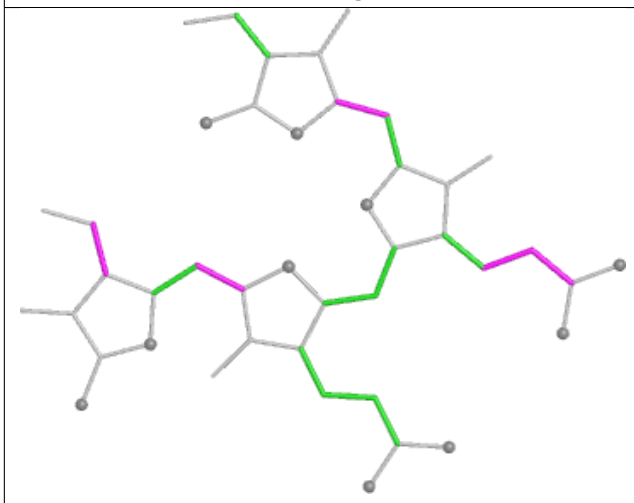
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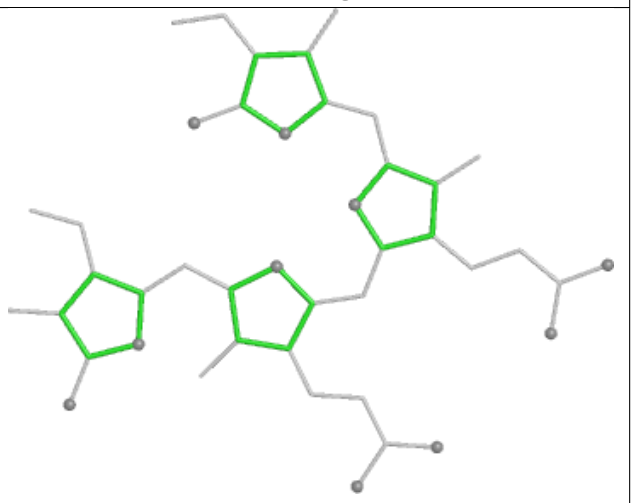
Bond lengths



Bond angles

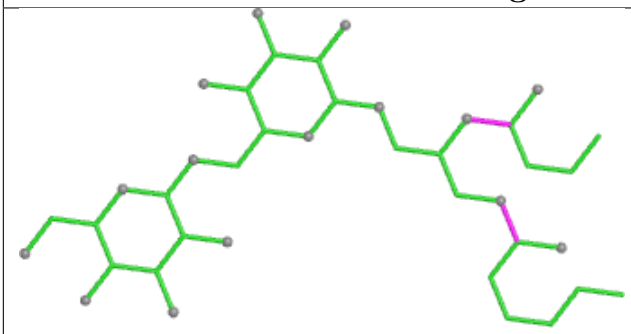


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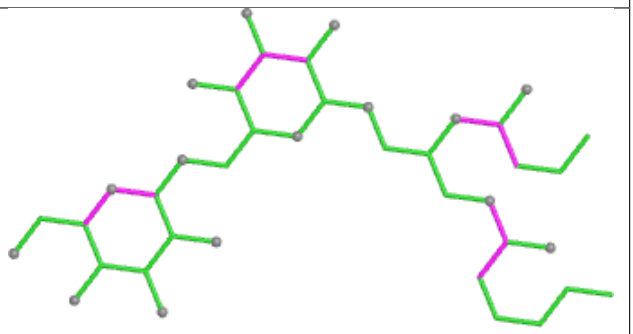


Rings

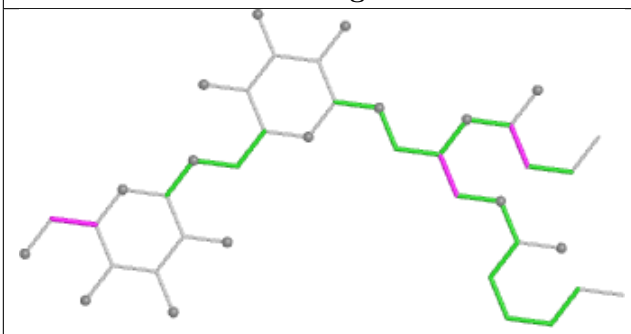
Ligand DGD BL 607



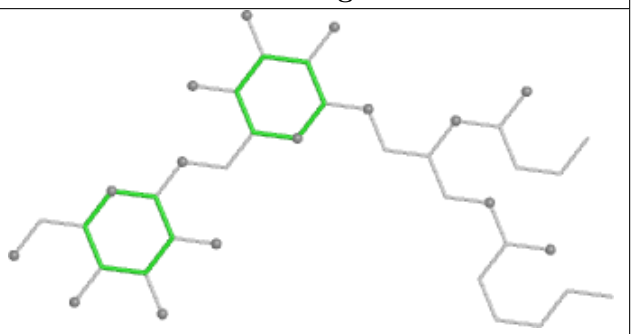
Bond lengths



Bond angles

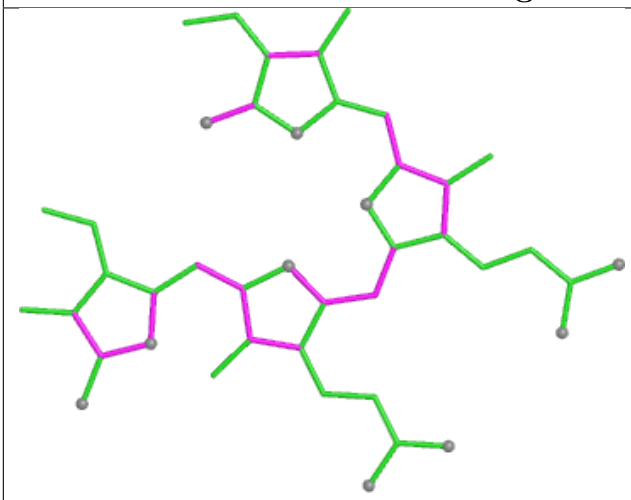


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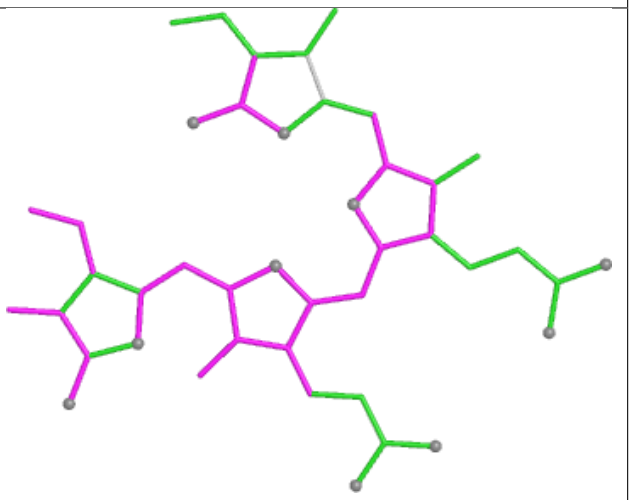


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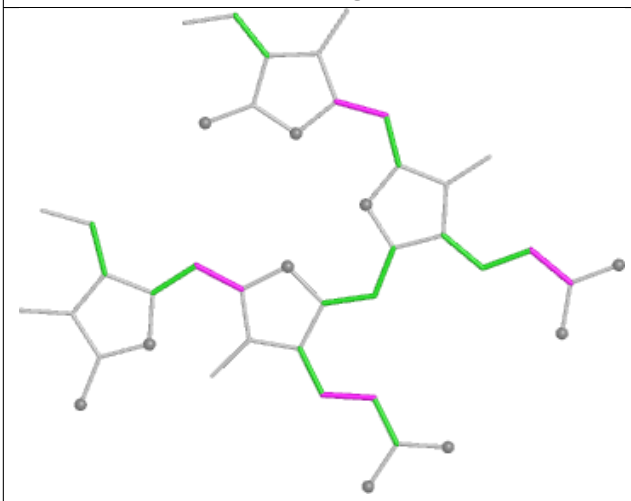
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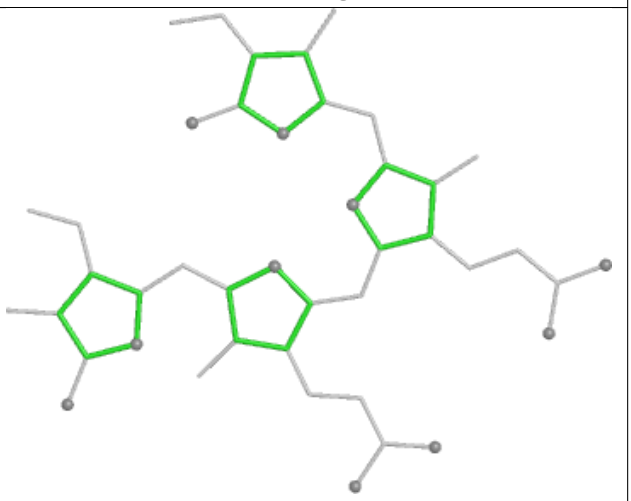
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Bond angles

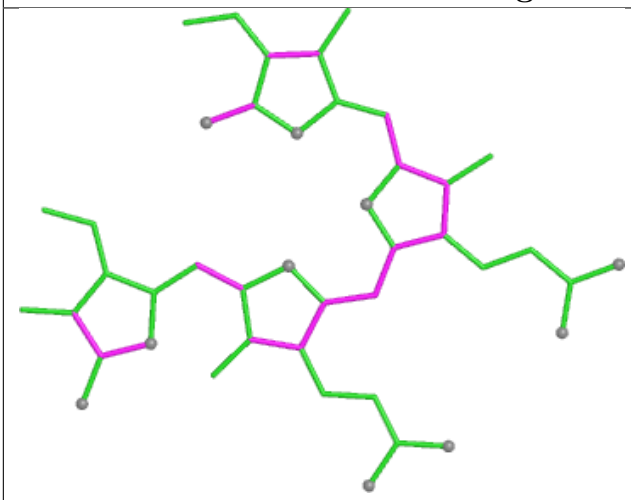


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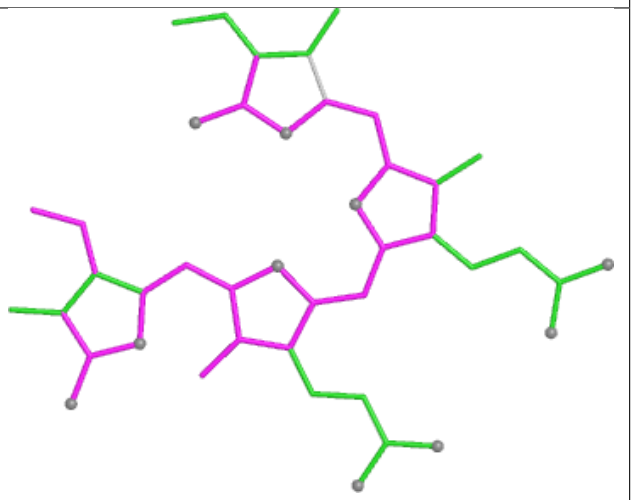


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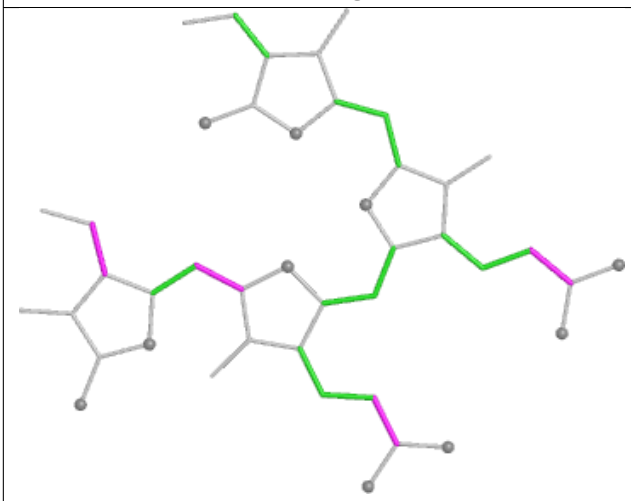
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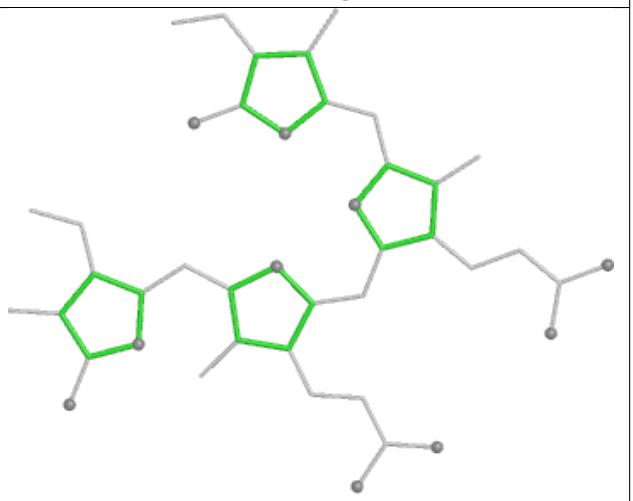
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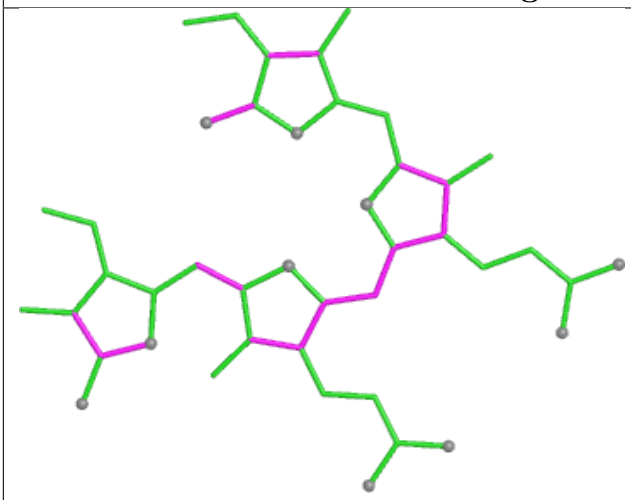


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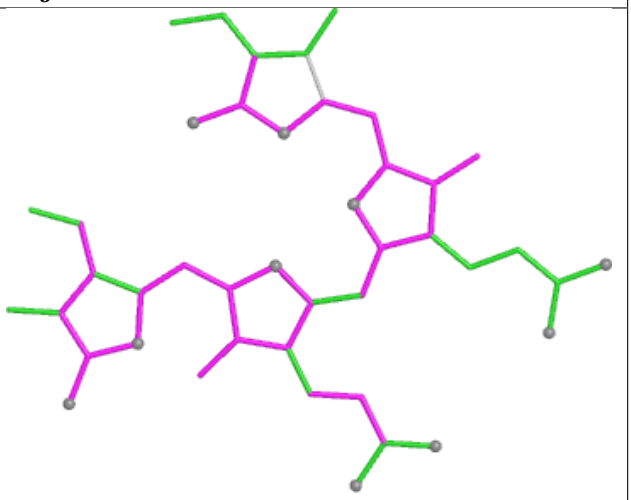


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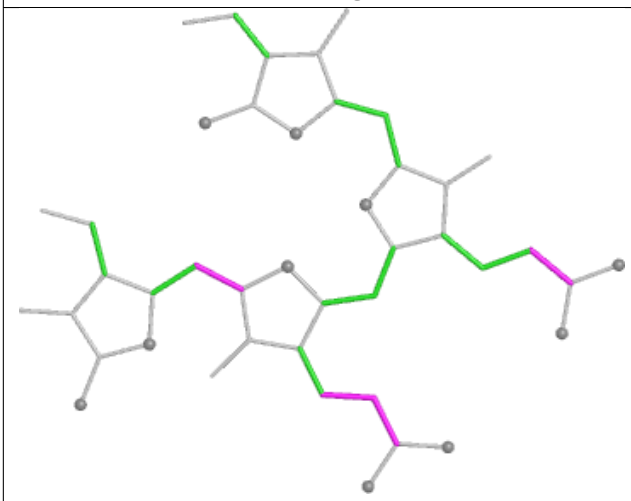
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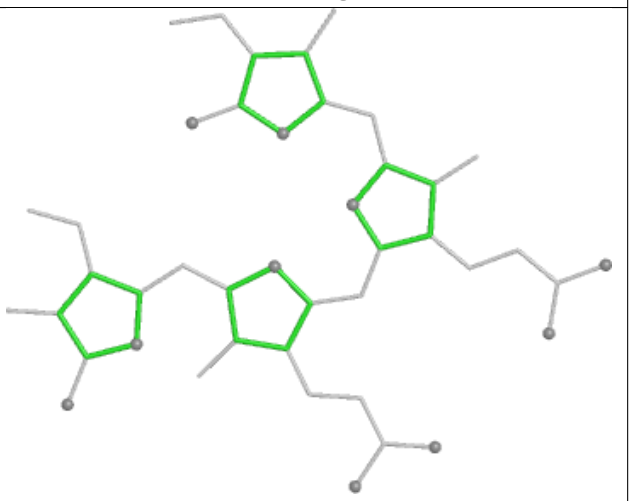
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Bond angles

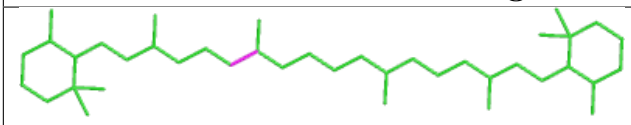


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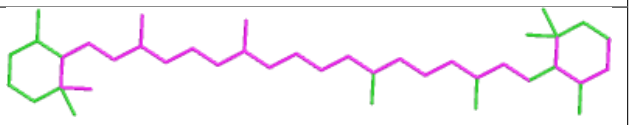


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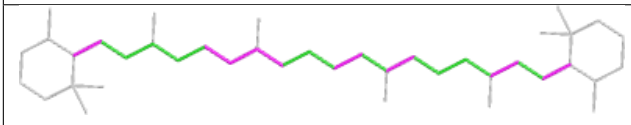
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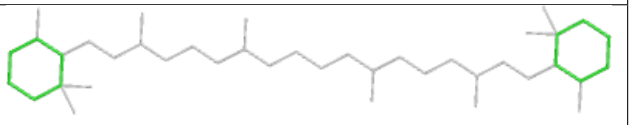
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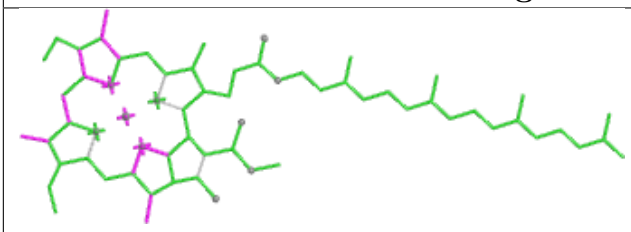


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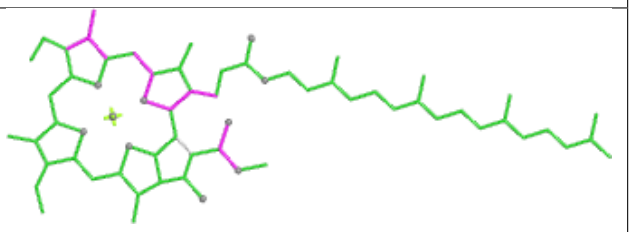


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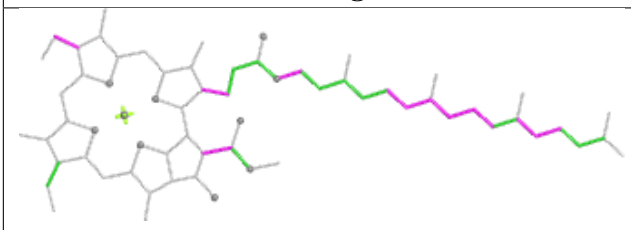
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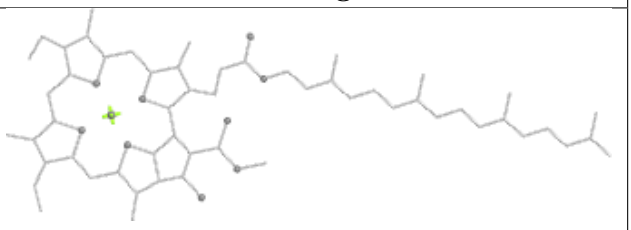
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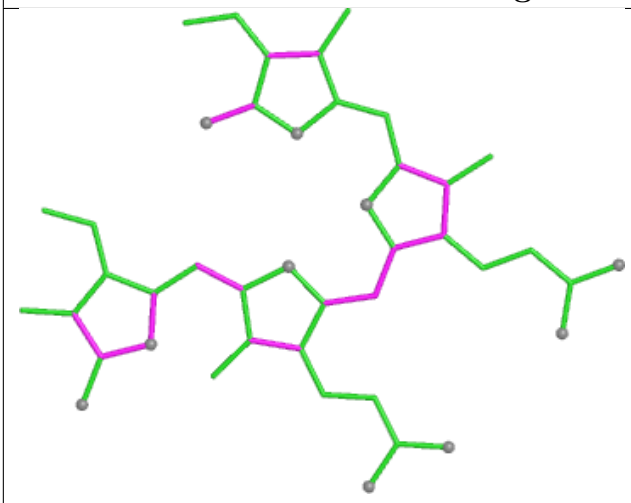


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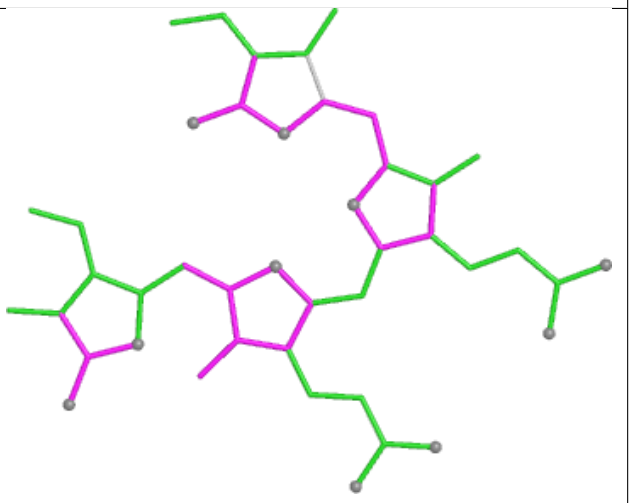


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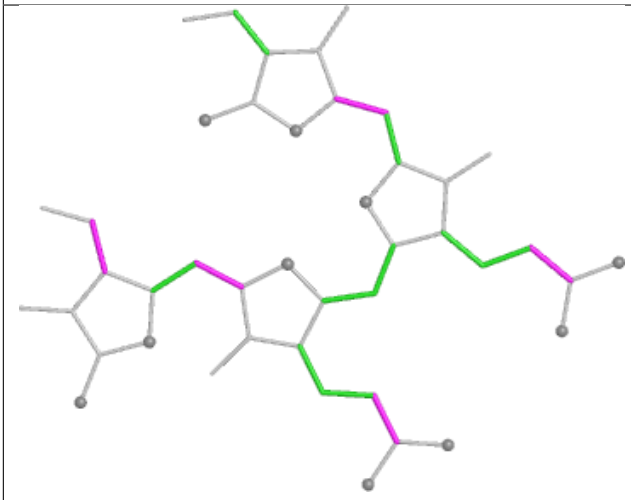
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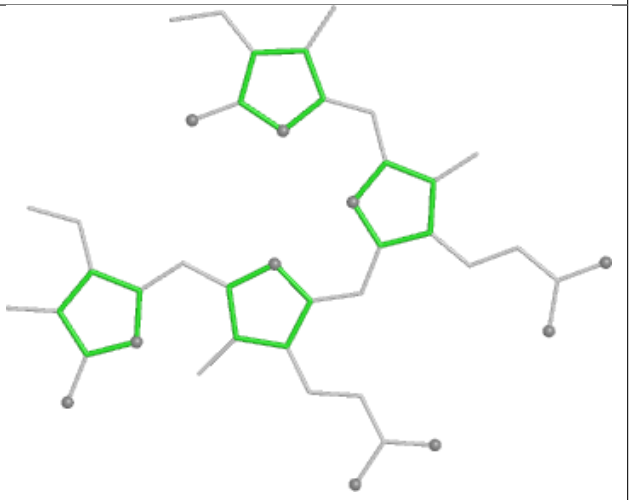
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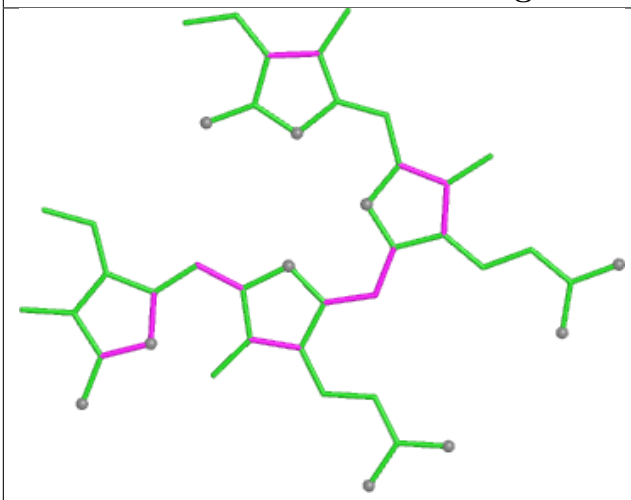


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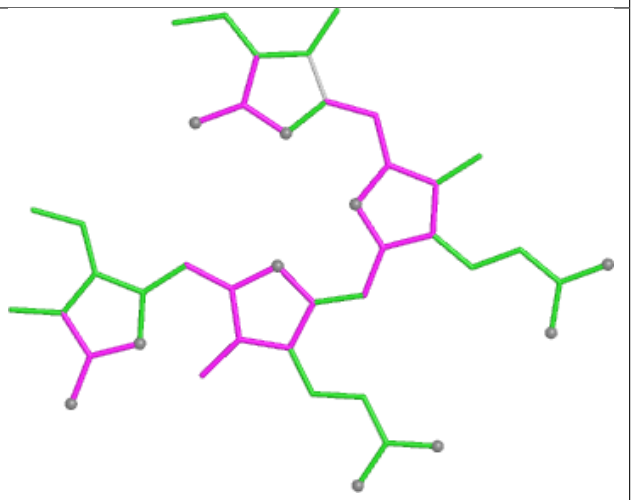


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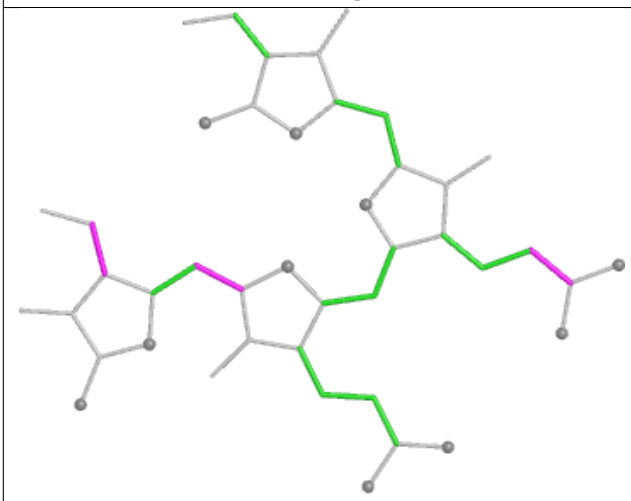
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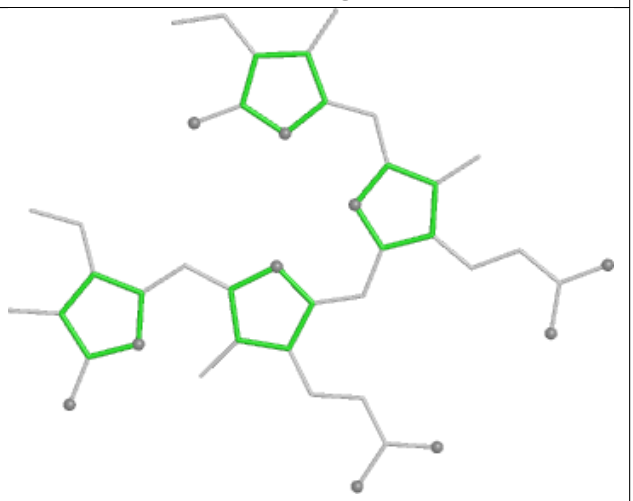
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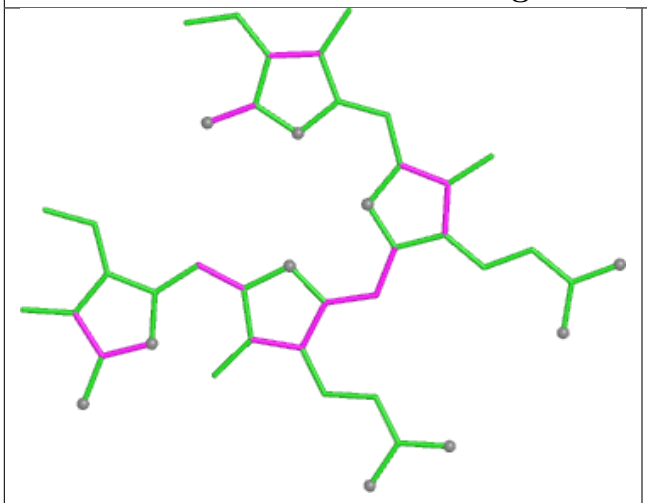


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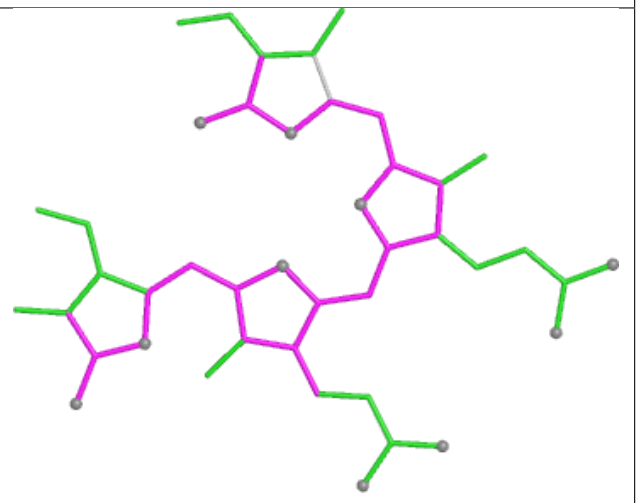


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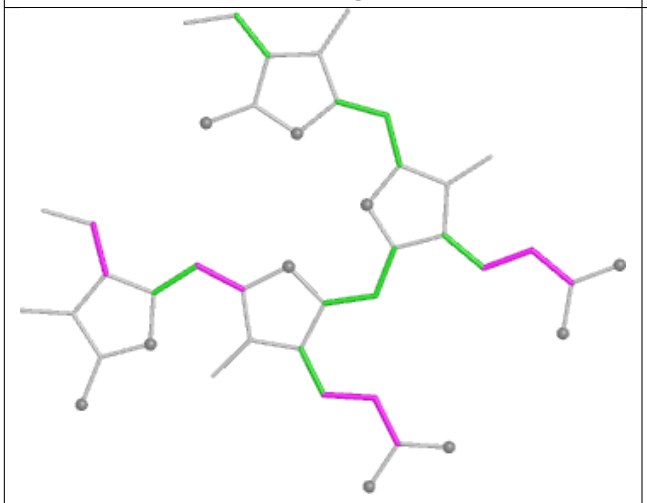
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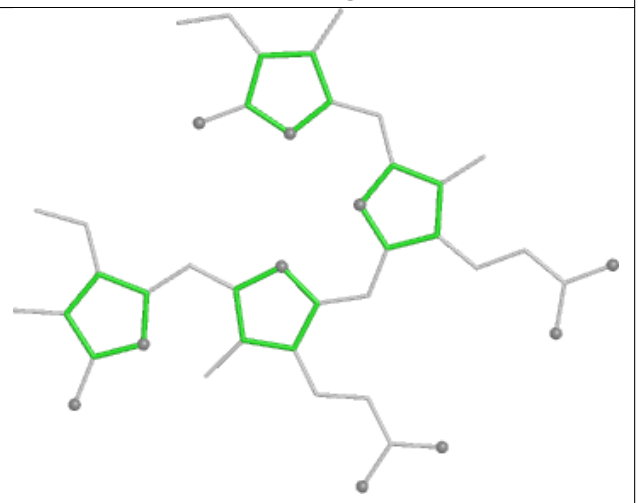
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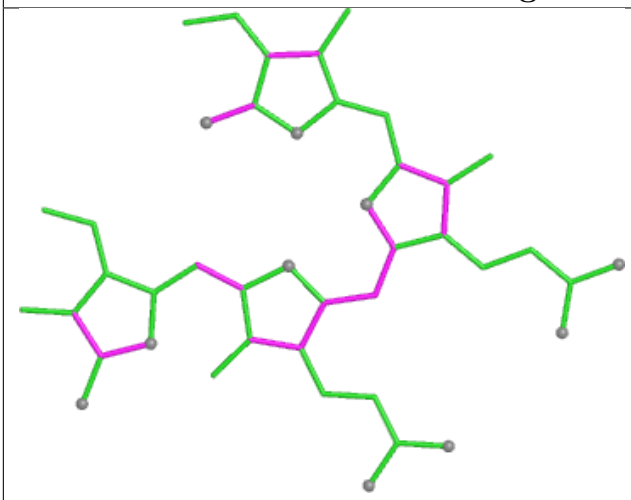


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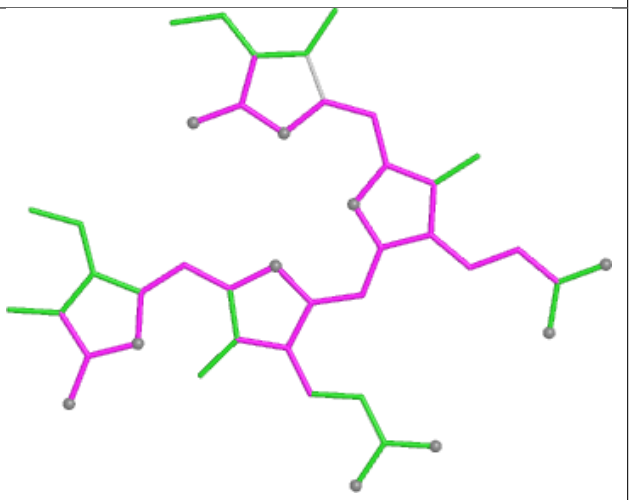


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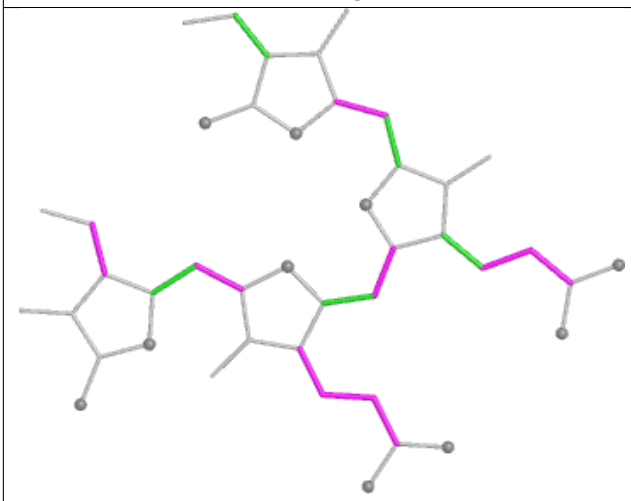
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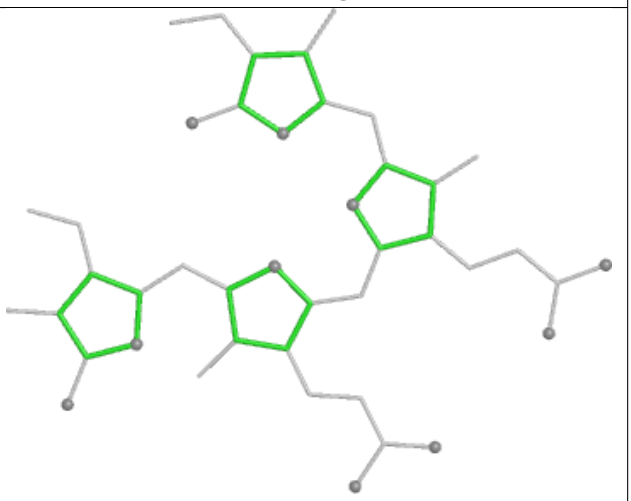
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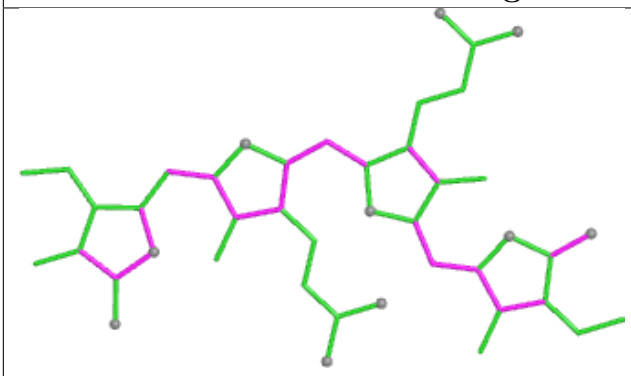


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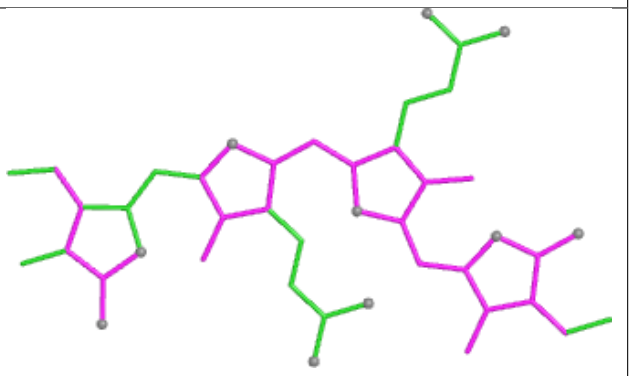


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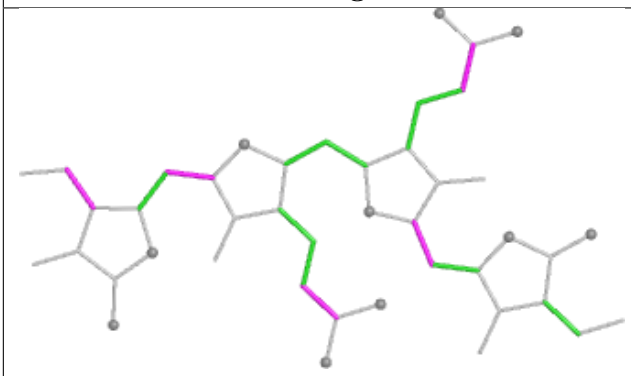
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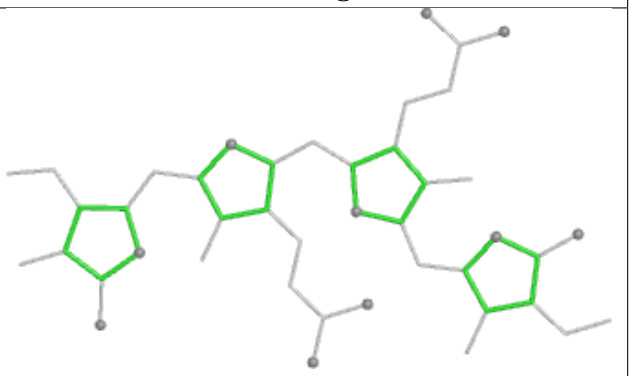
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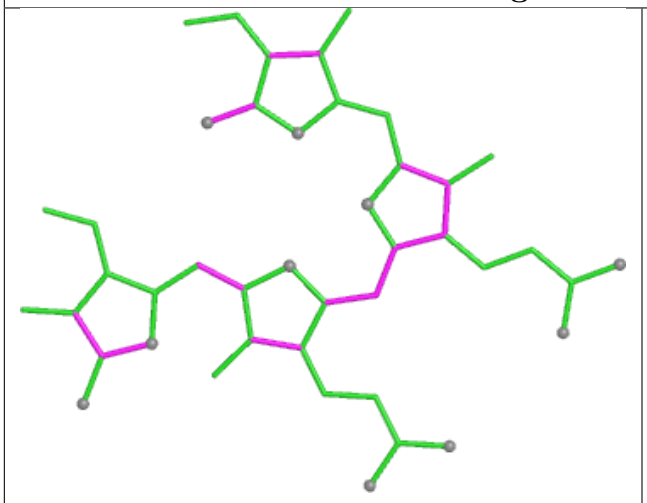


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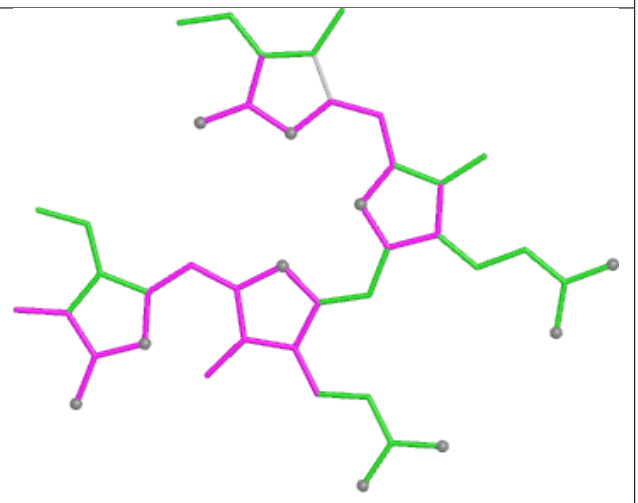


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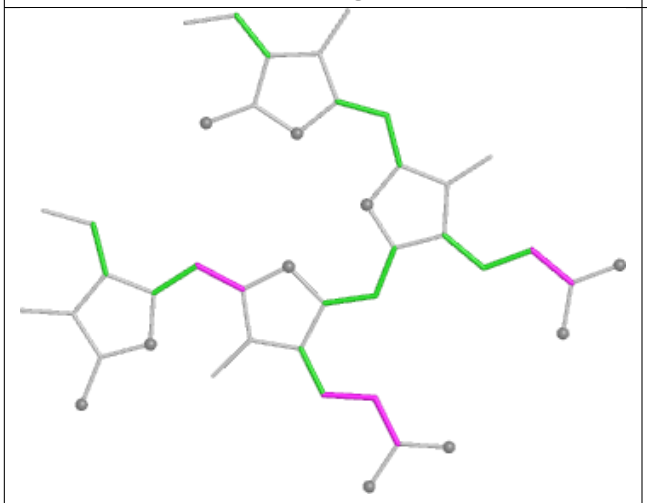
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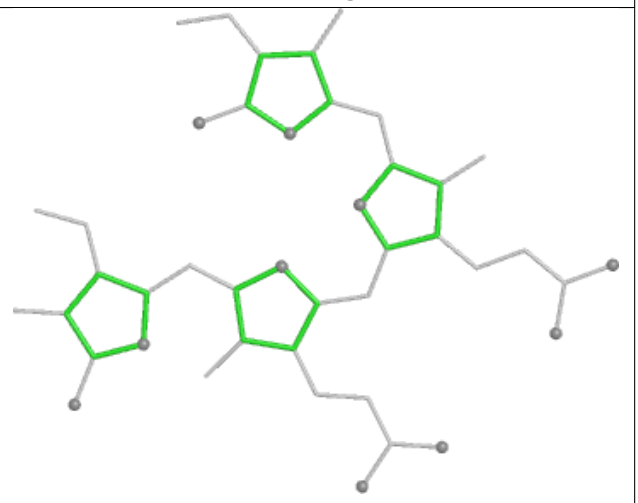
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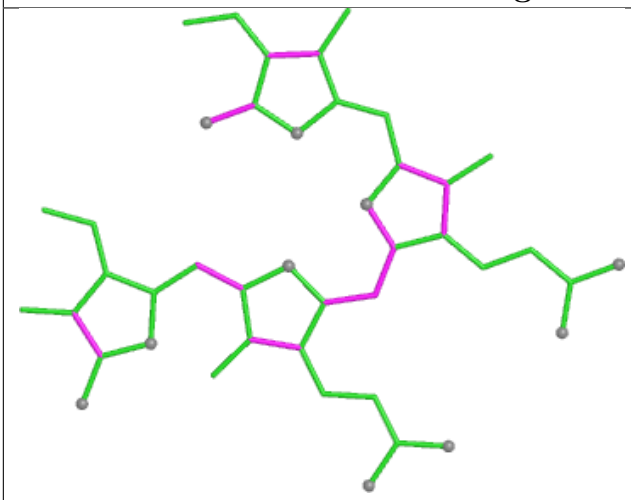


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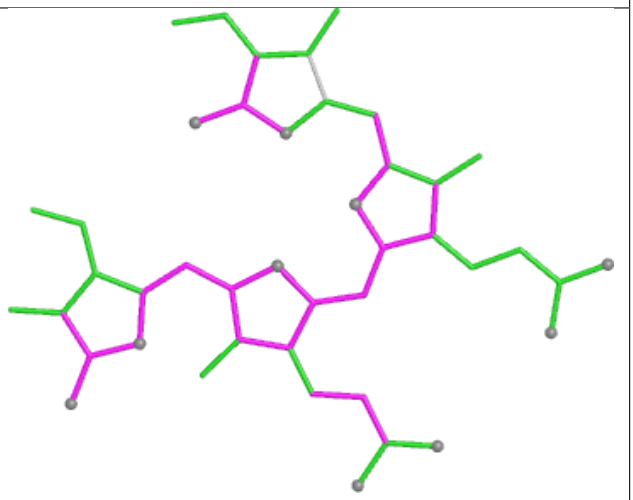


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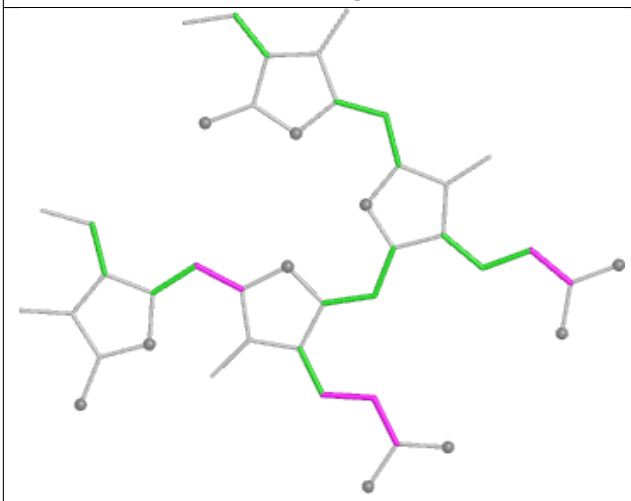
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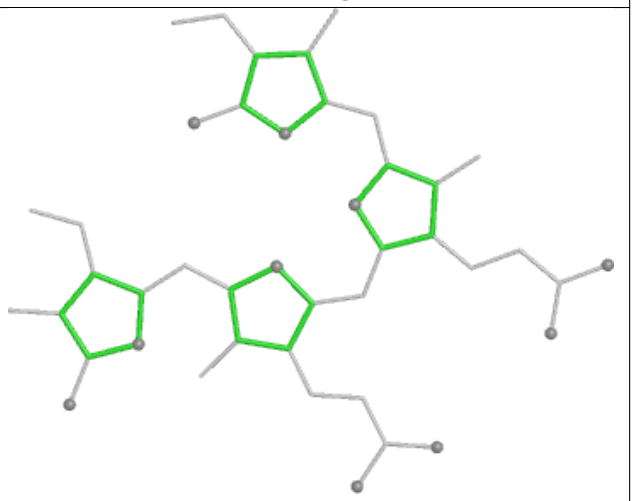
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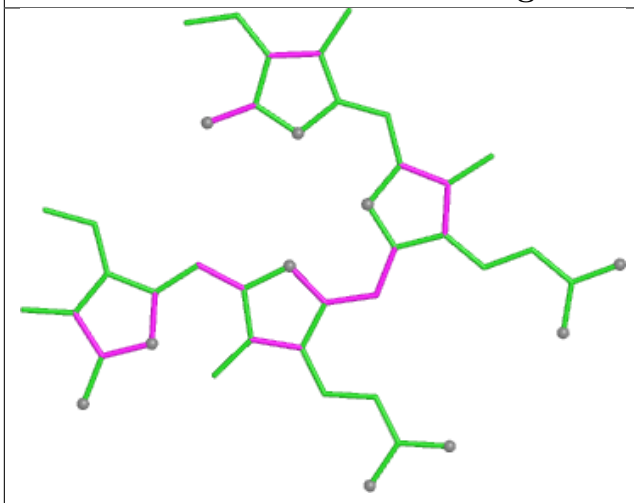


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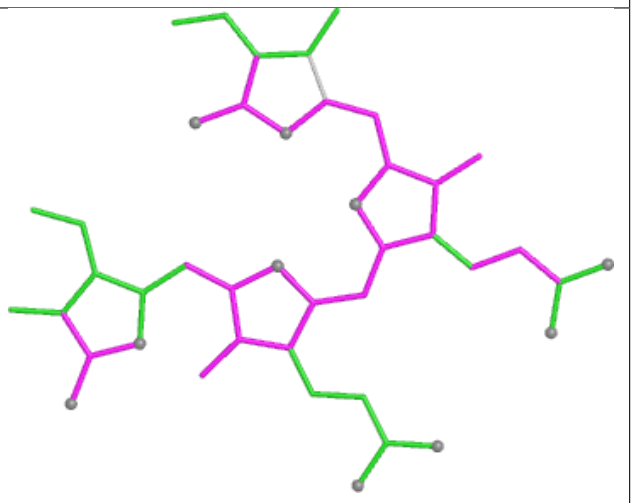


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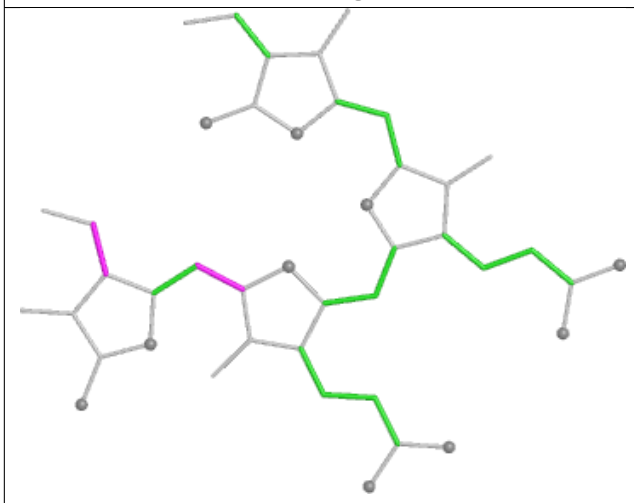
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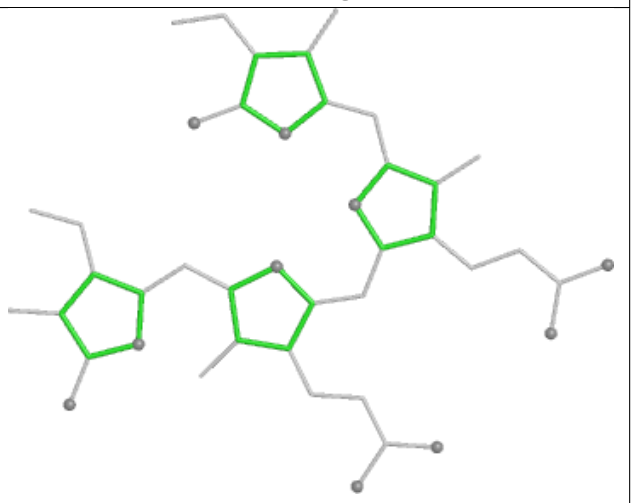
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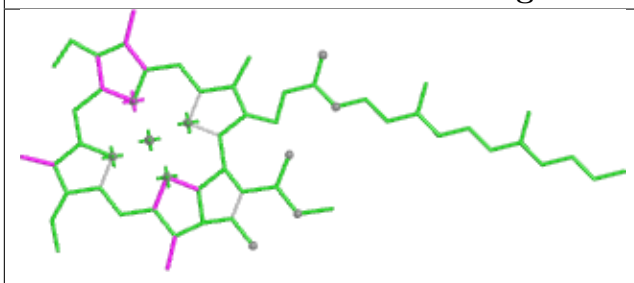


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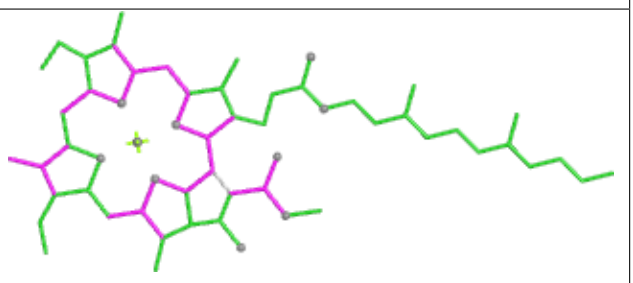


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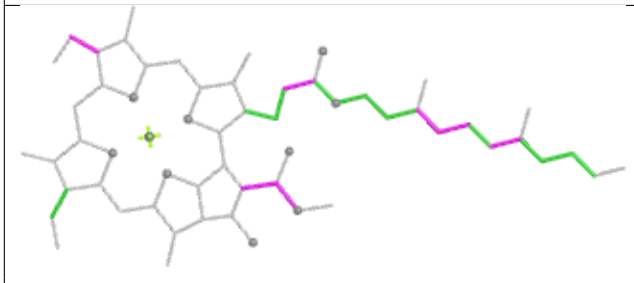
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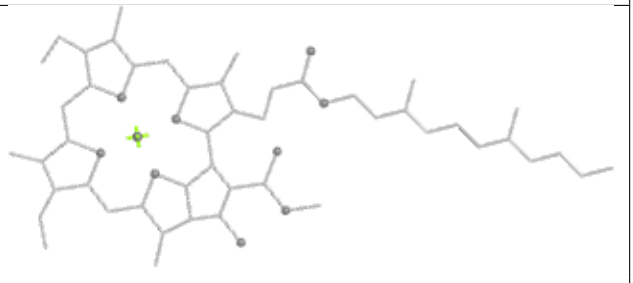
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Bond angles

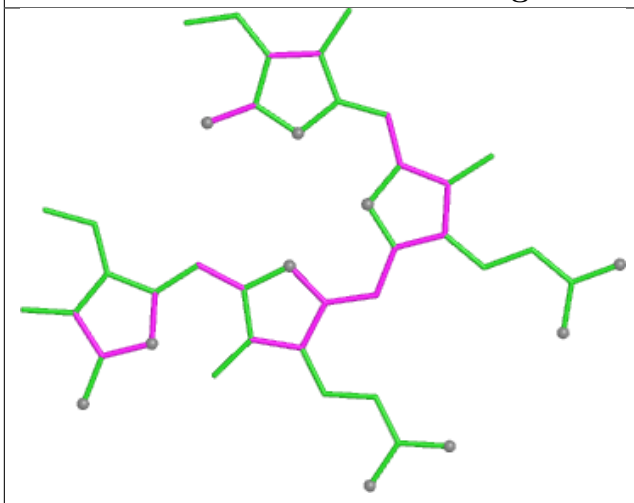


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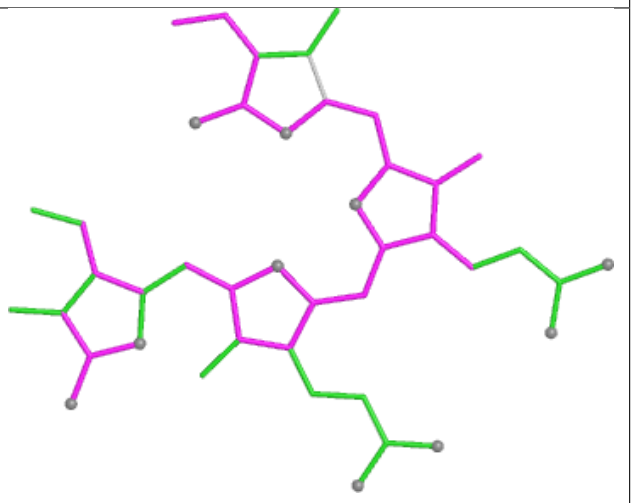


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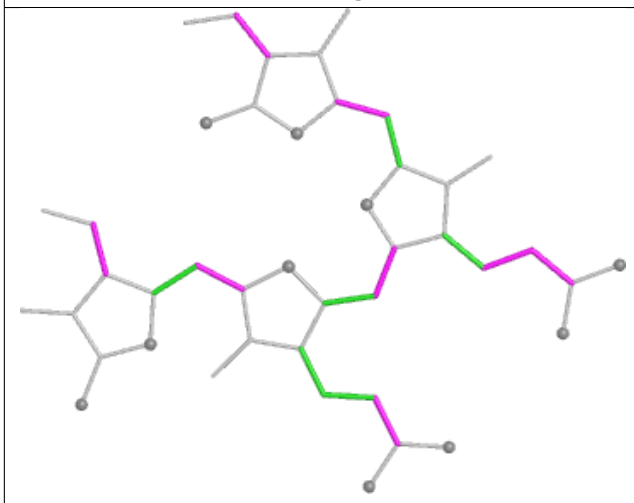
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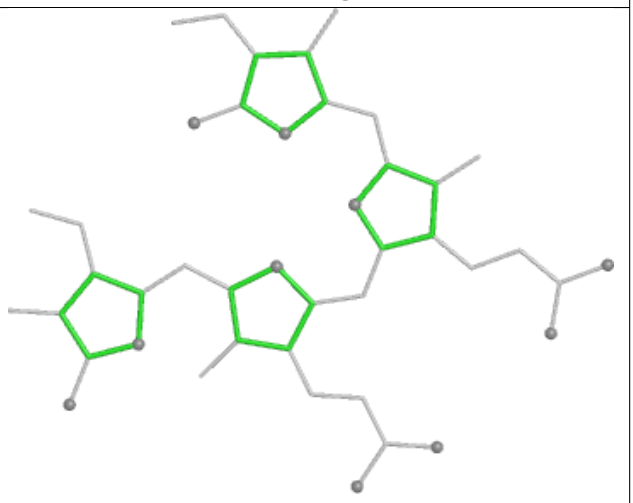
Bond lengths



Bond angles

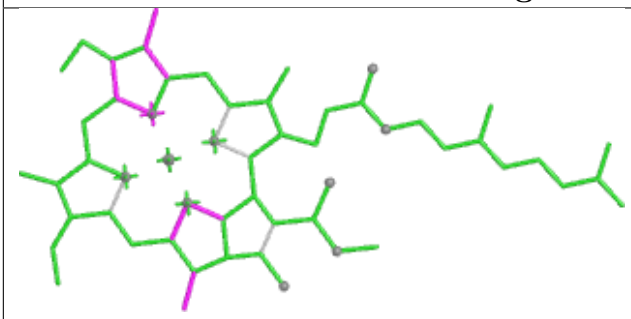


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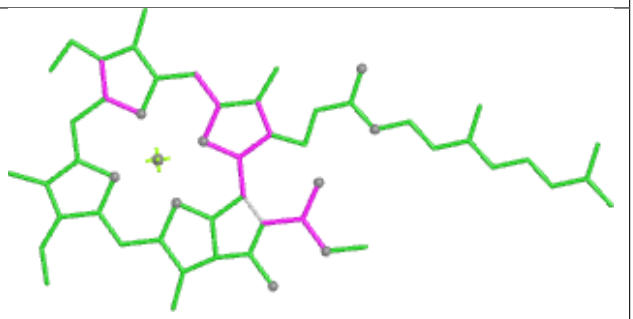


Rings

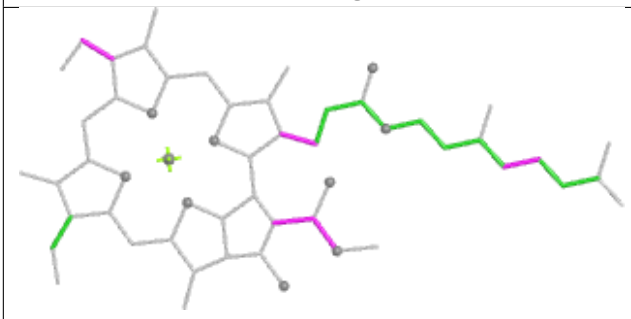
Ligand CLA B2 815



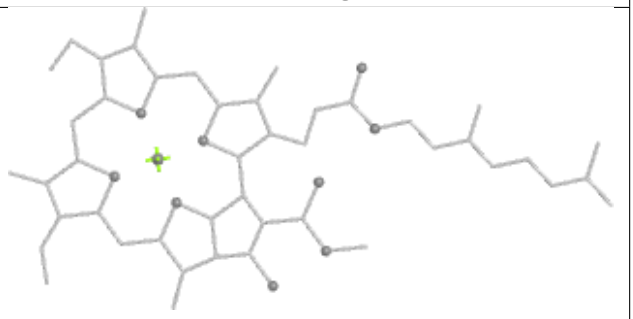
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Bond angles

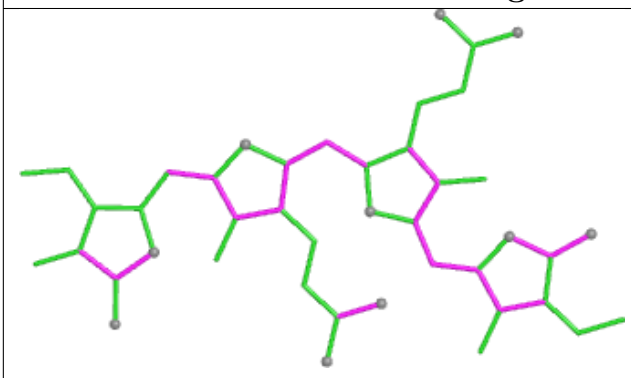


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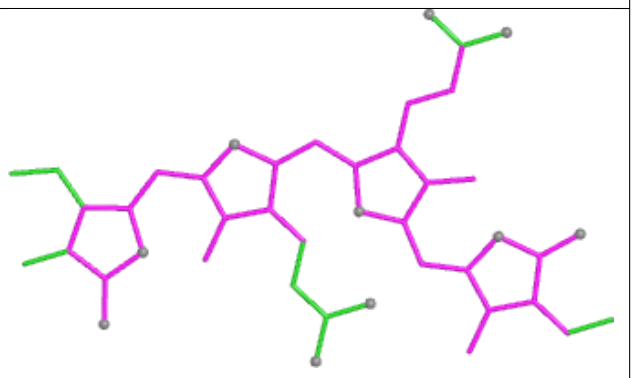


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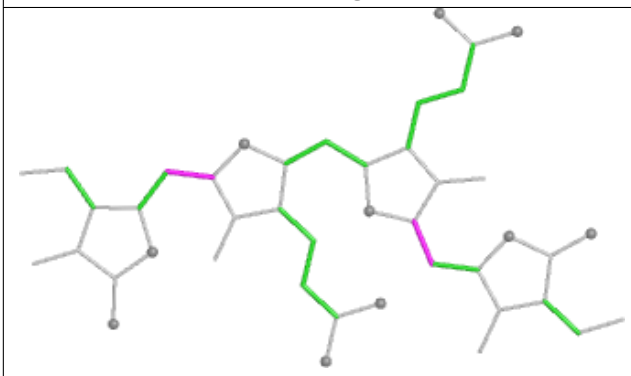
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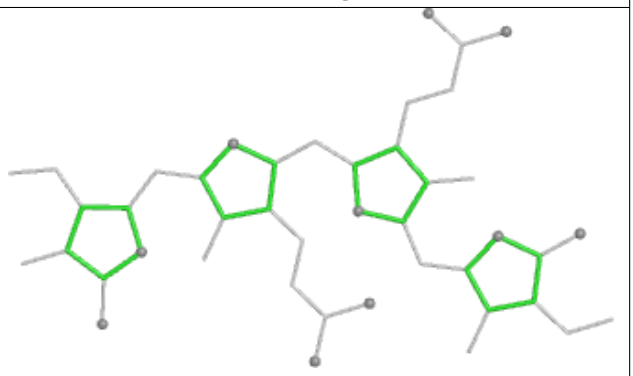
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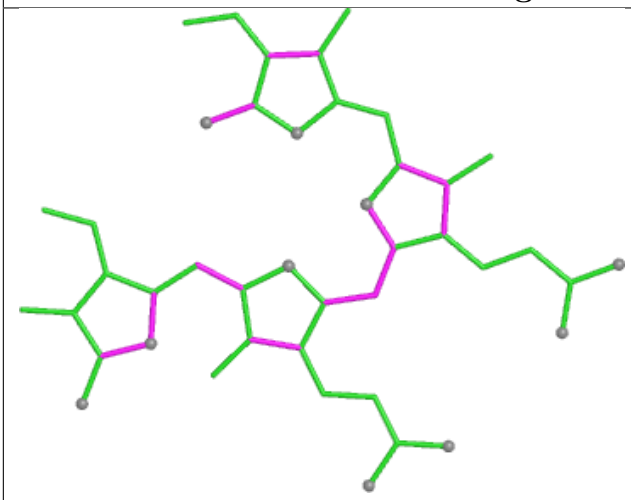


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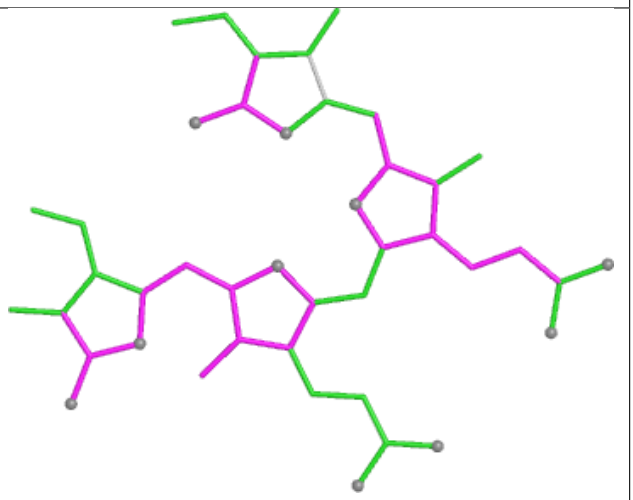


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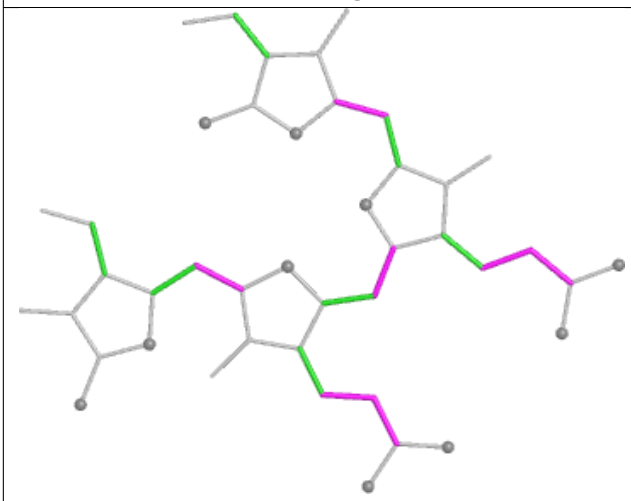
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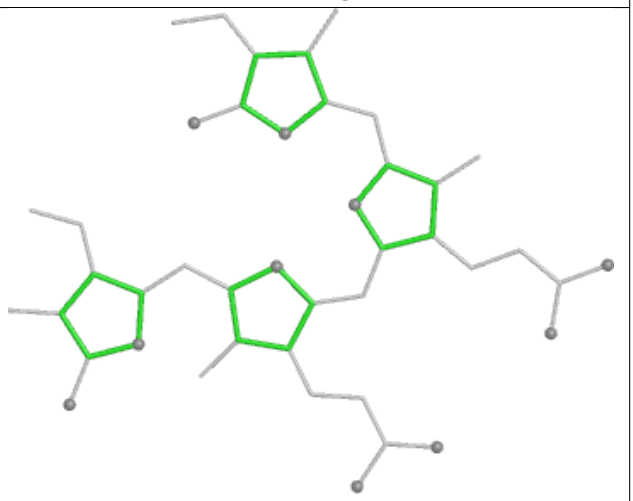
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Bond angles

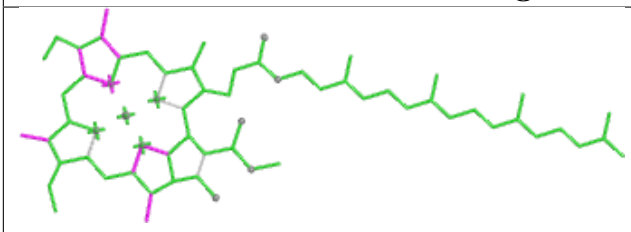


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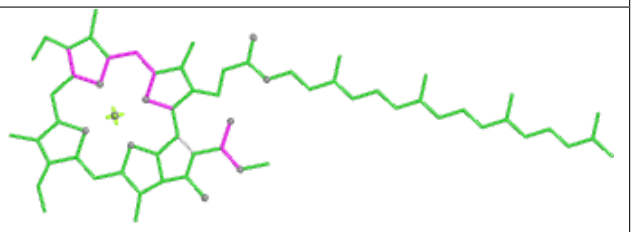


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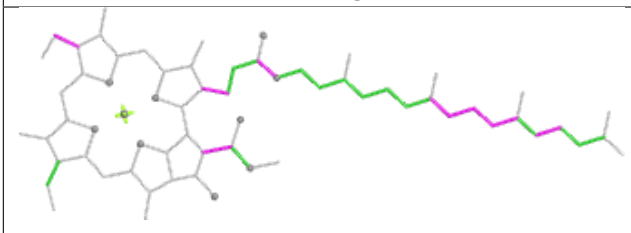
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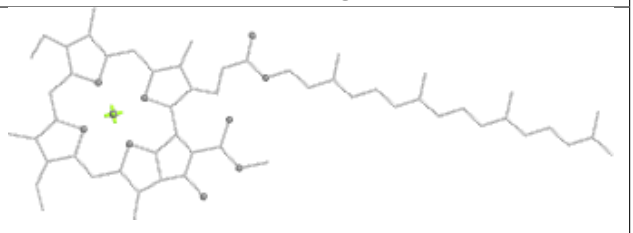
Bond lengths



Bond angles

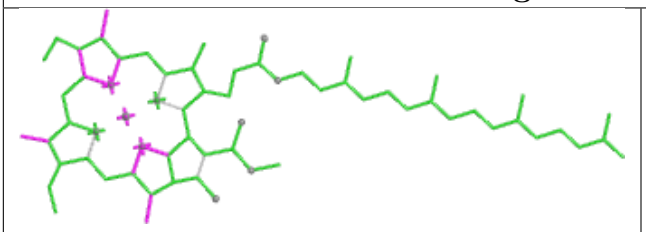


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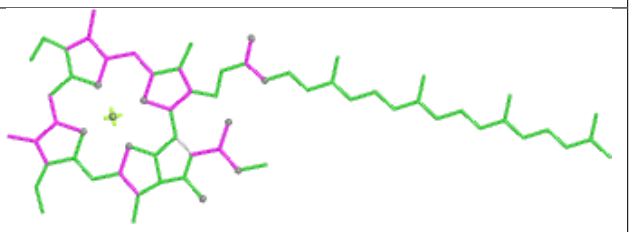


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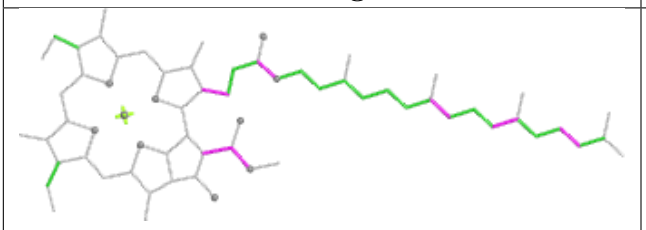
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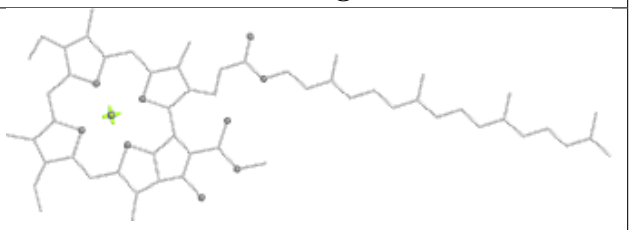
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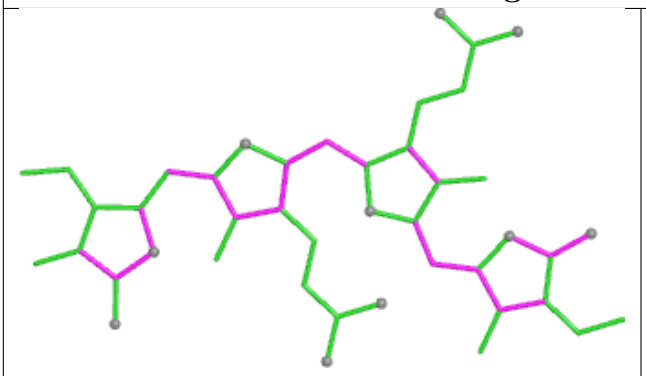


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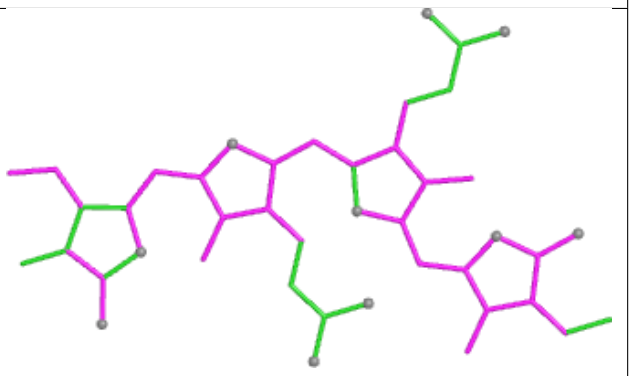


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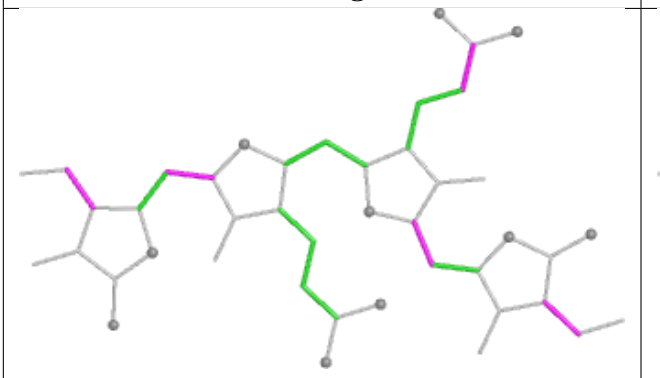
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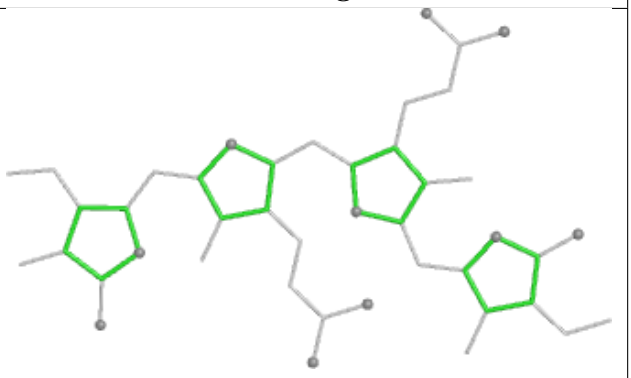
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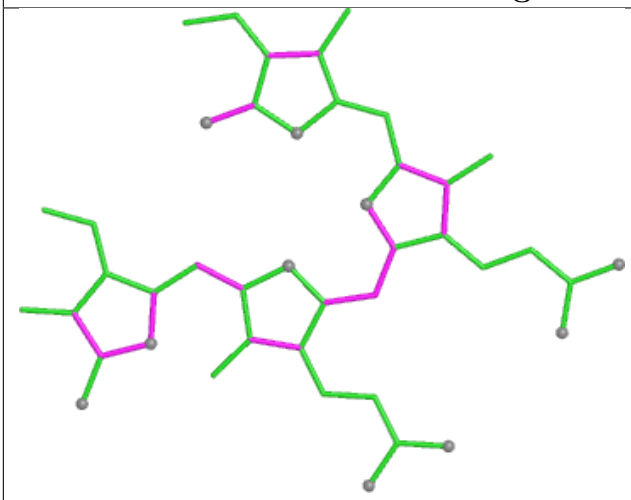


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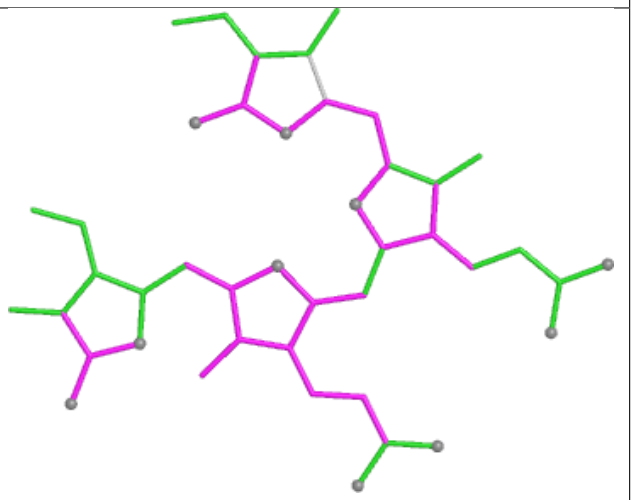


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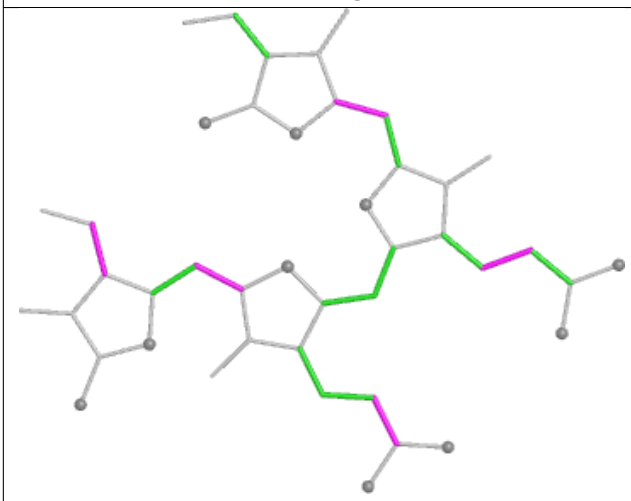
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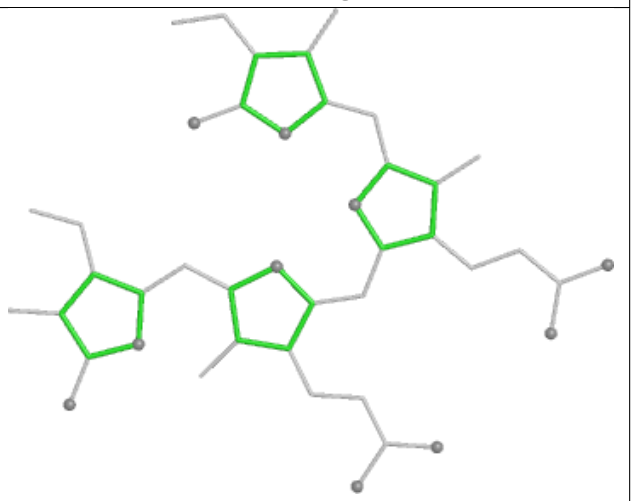
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Bond angles

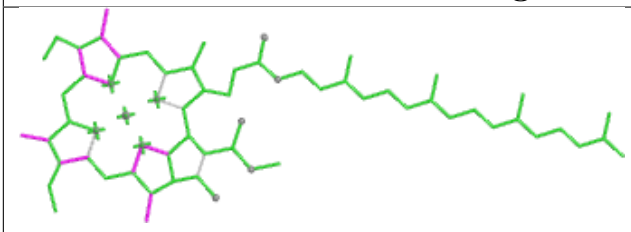


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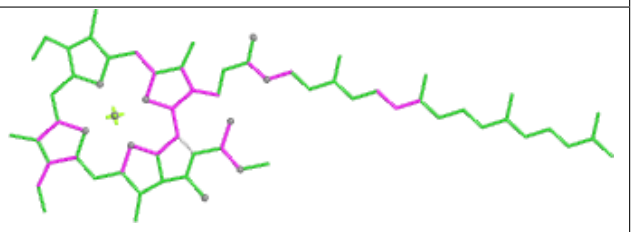


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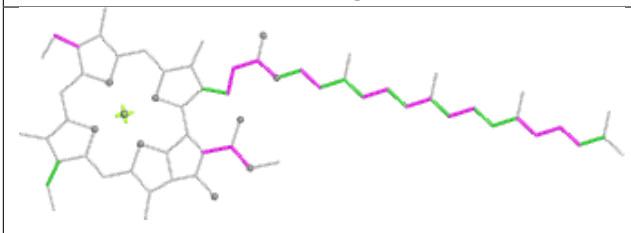
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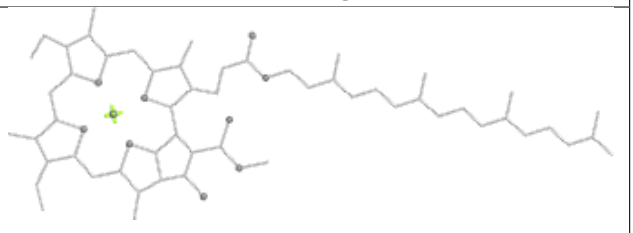
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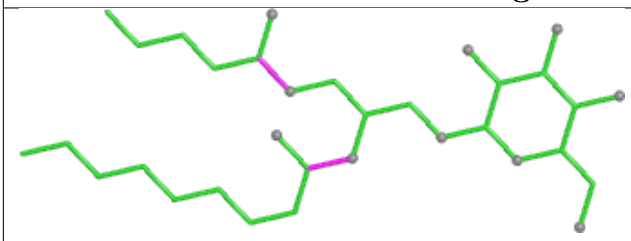


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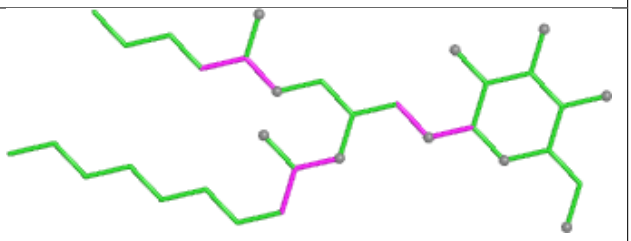


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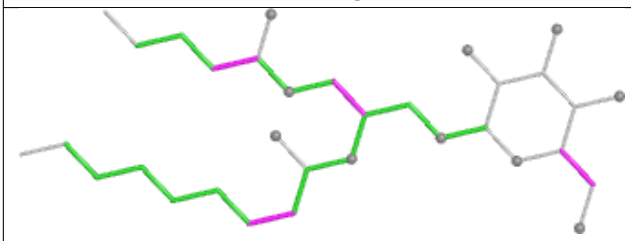
Ligand LMG JL 103



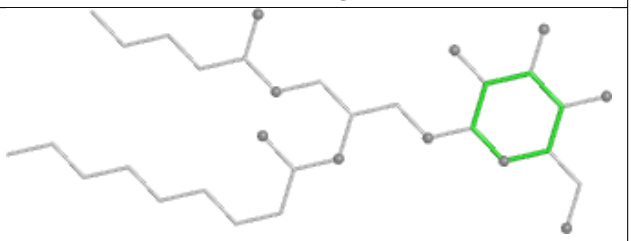
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Bond angles

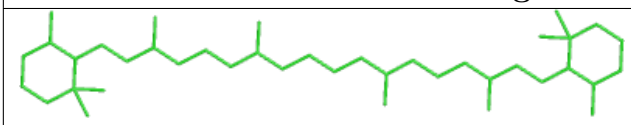


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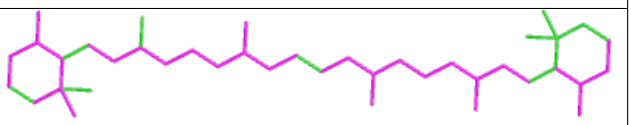


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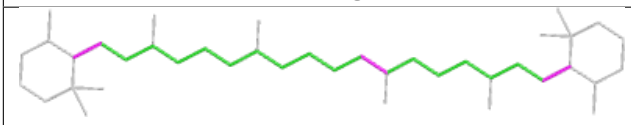
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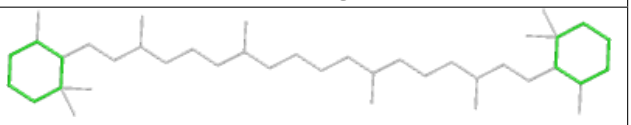
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Bond angles

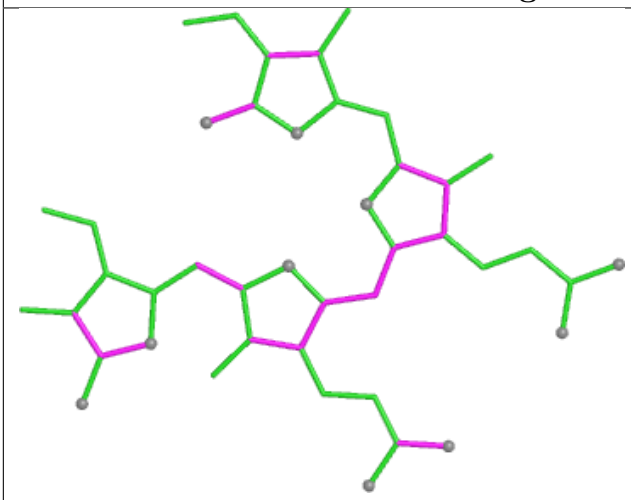


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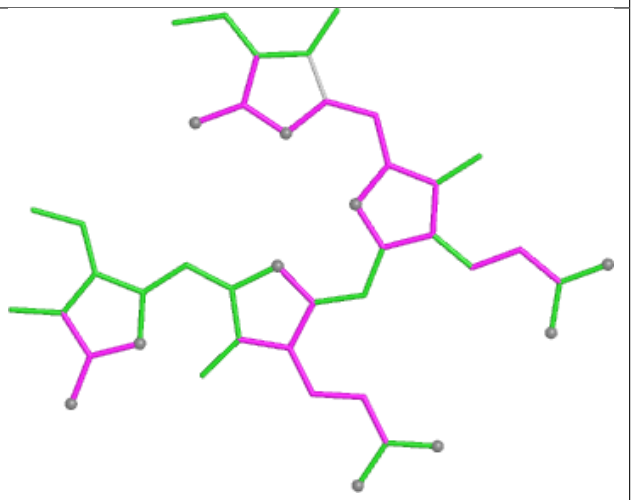


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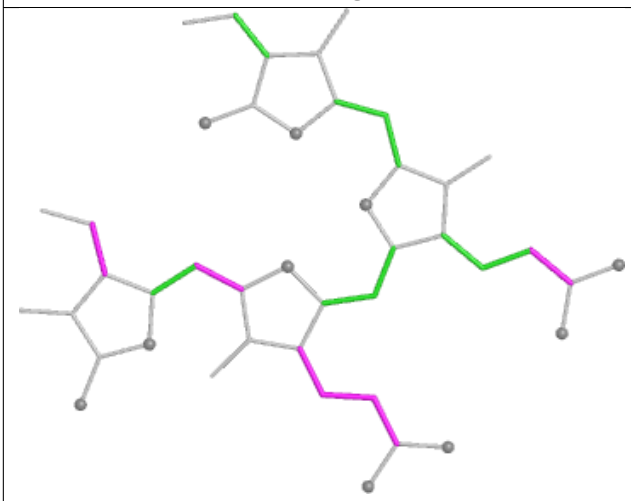
Ligand PEB fB 301



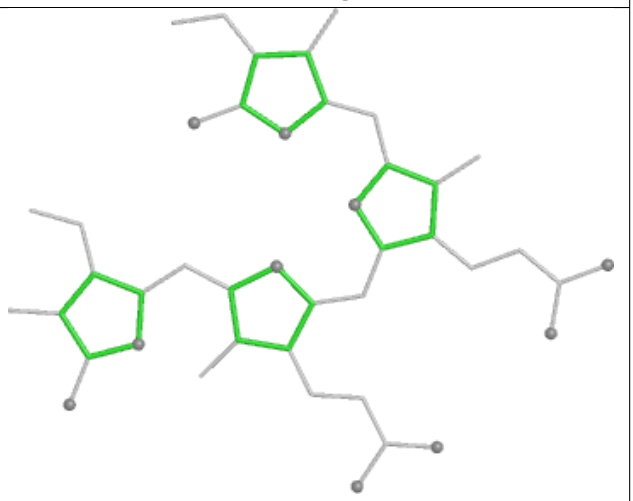
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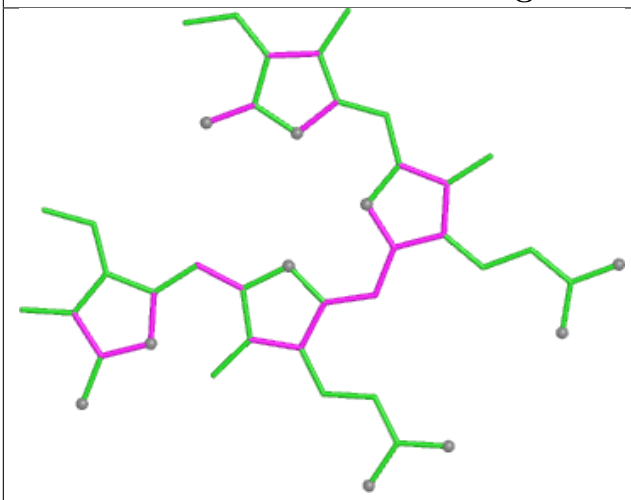


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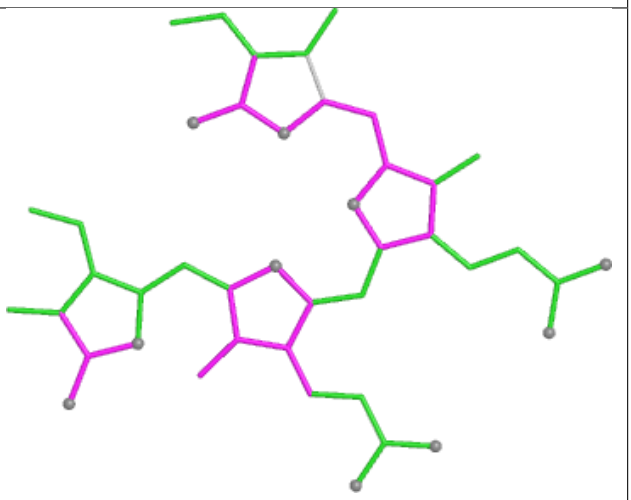


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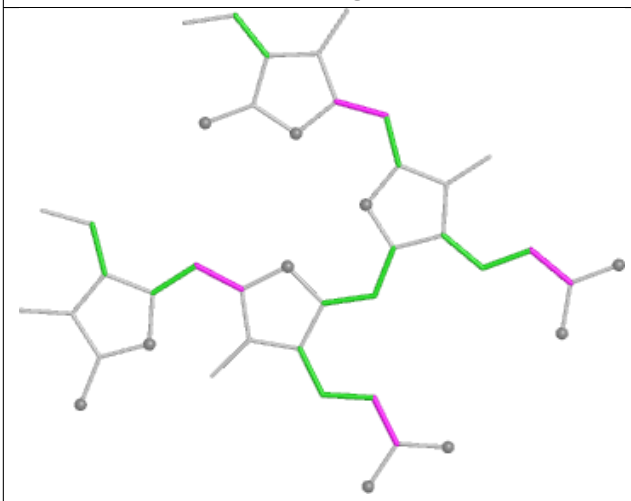
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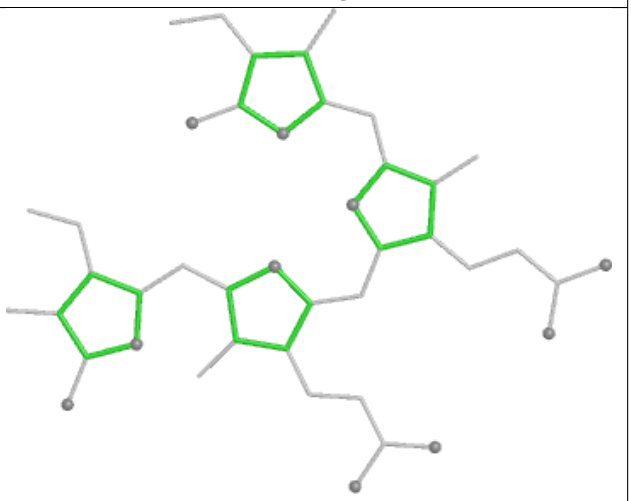
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Bond angles

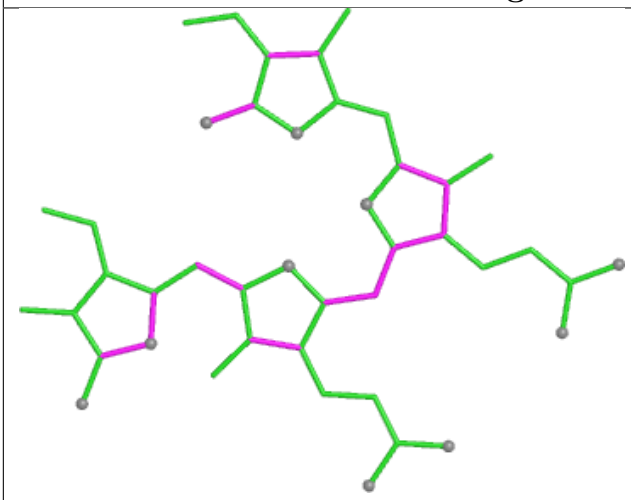


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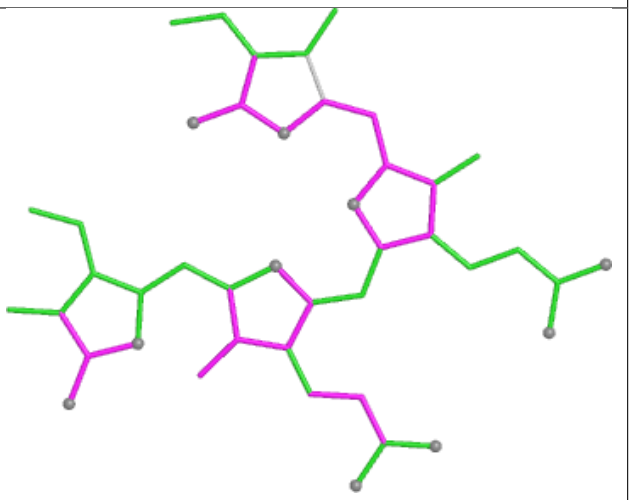


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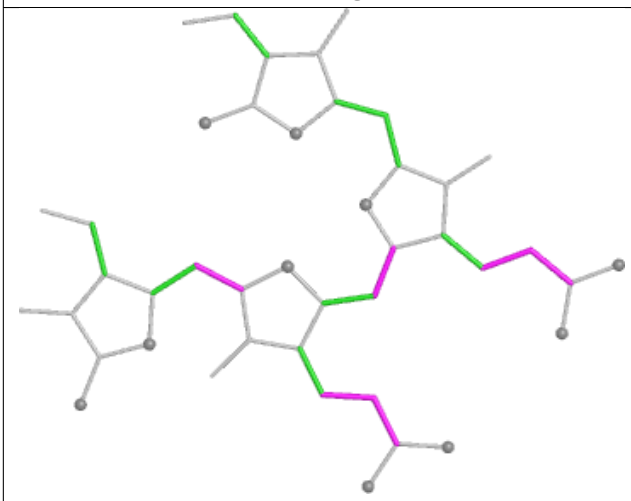
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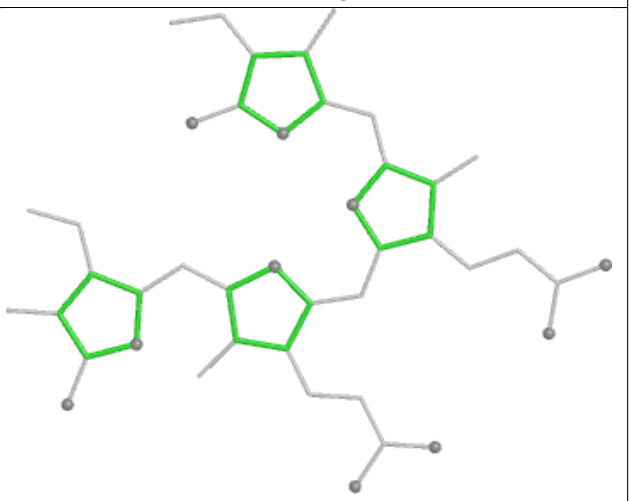
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Bond angles

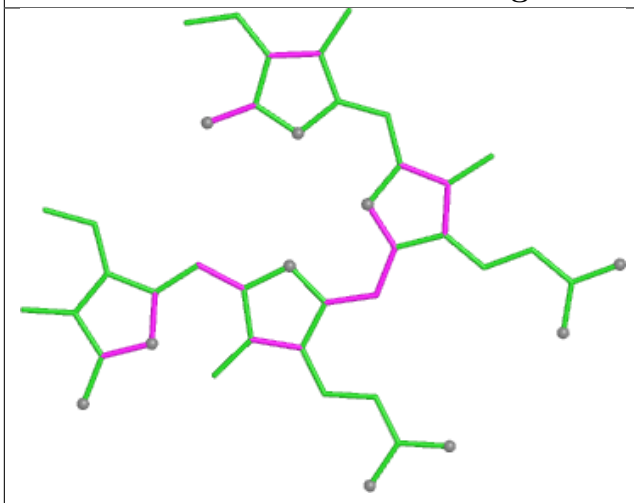


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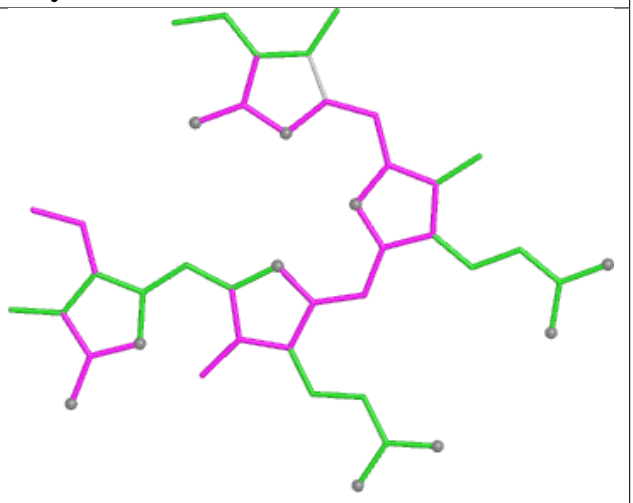


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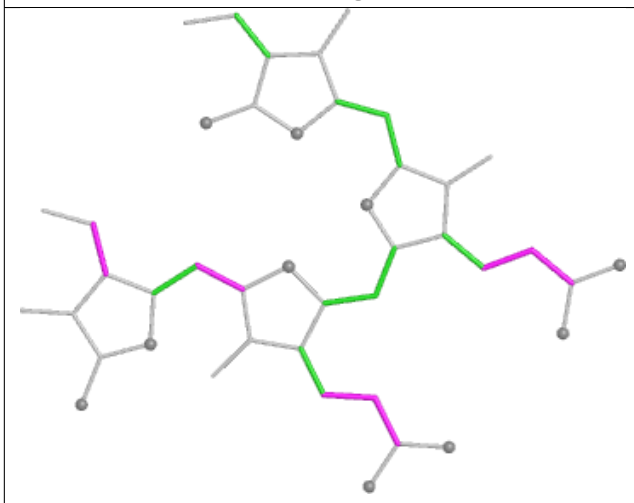
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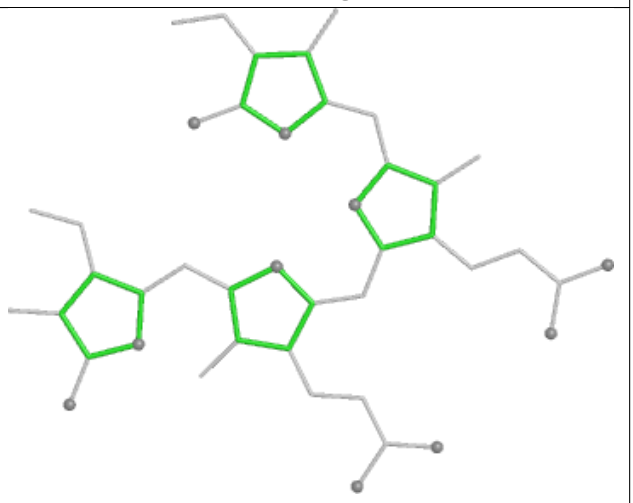
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Bond angles

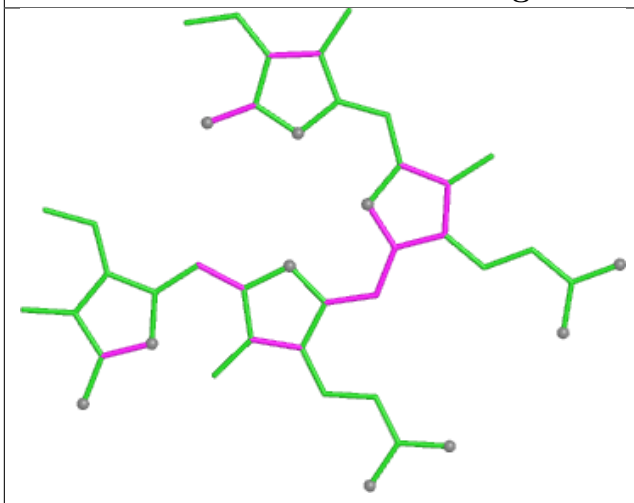


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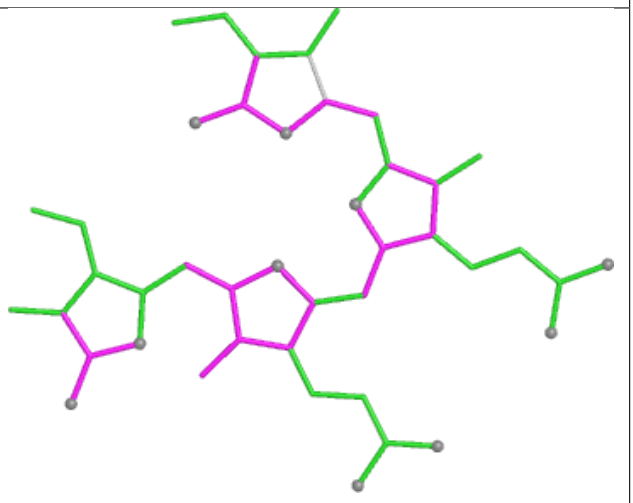


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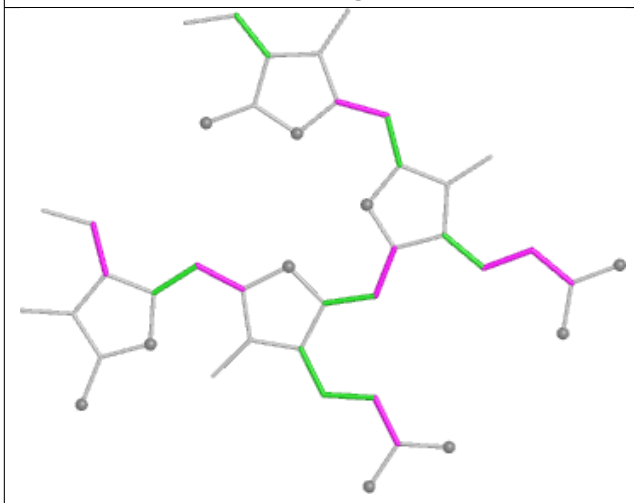
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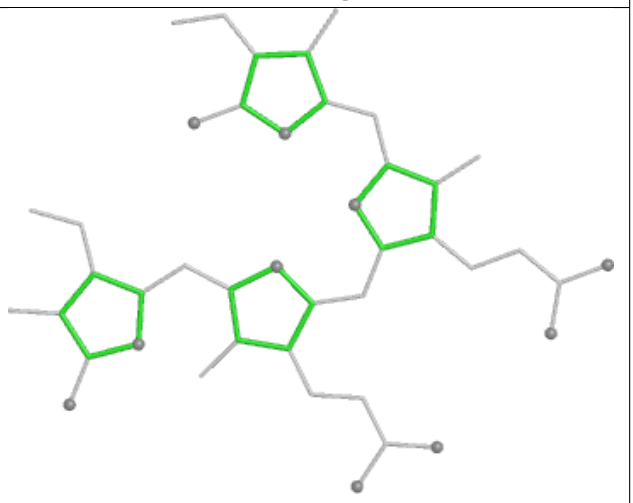
Bond lengths



Bond angles

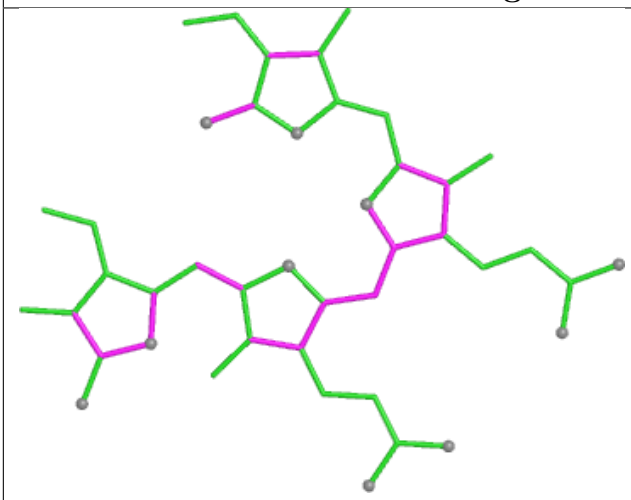


Torsions

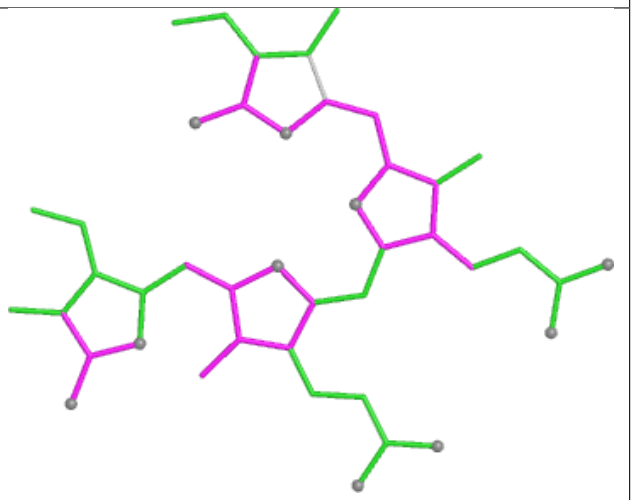


Rings

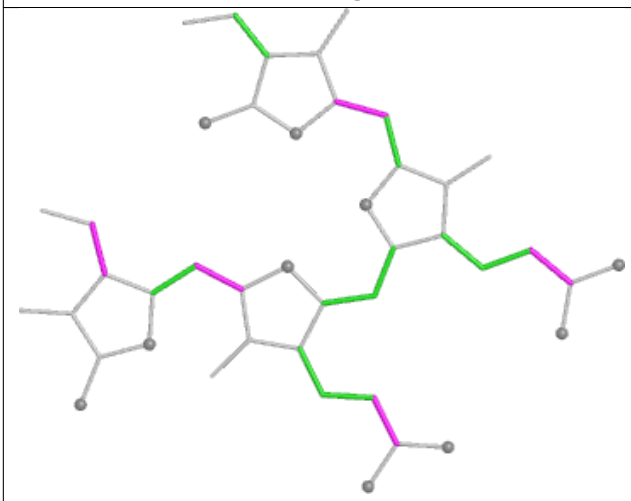
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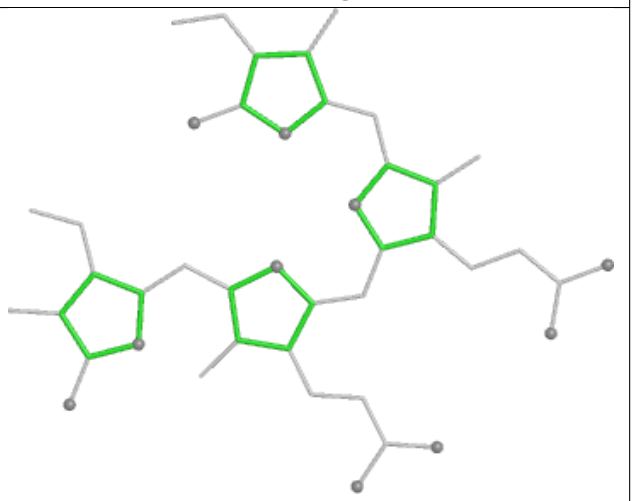
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Bond angles

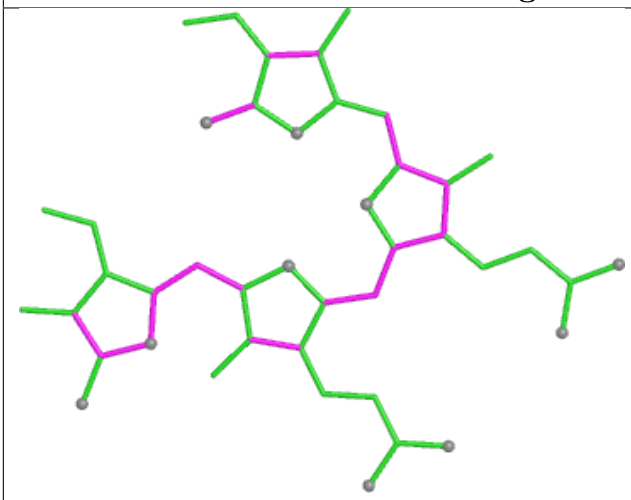


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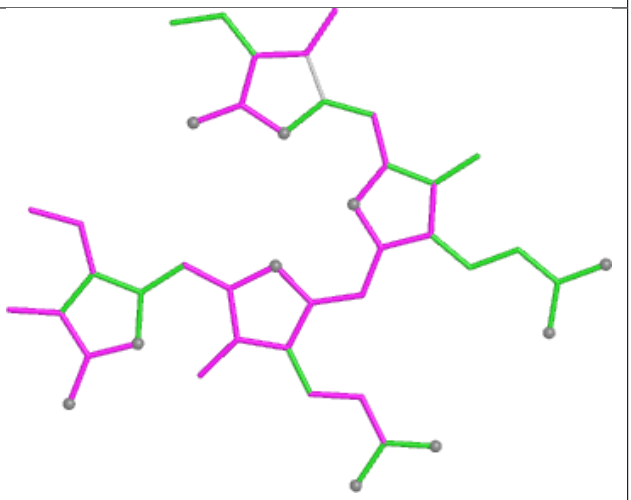


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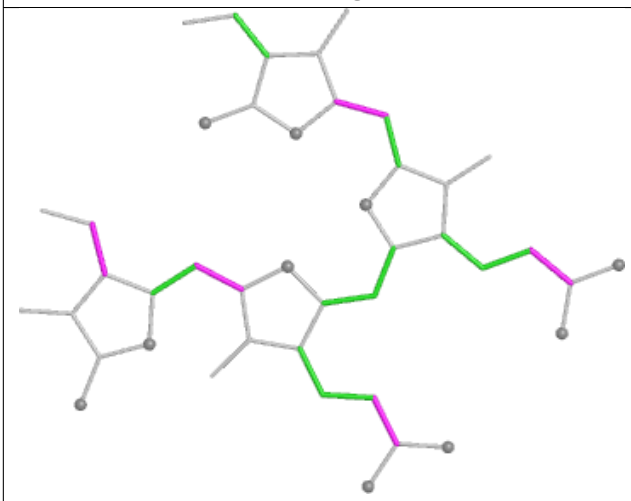
Ligand PEB h4 201



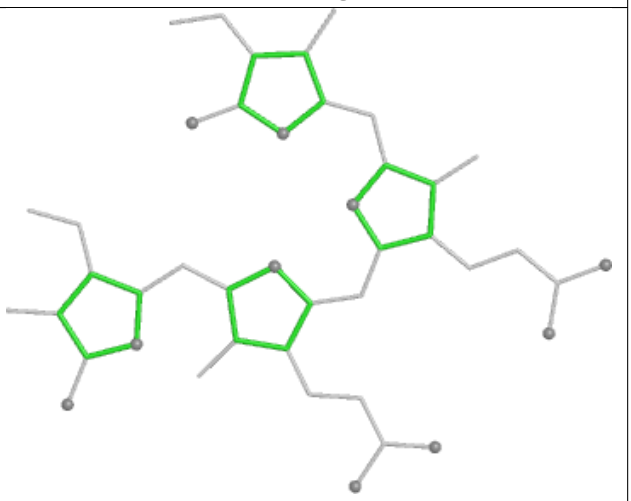
Bond lengths



Bond angles

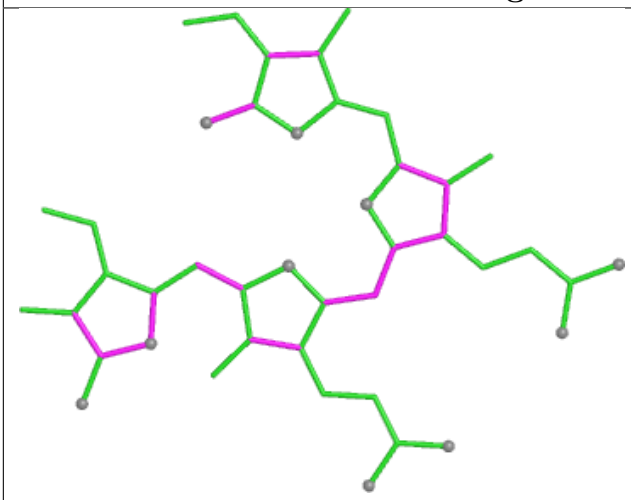


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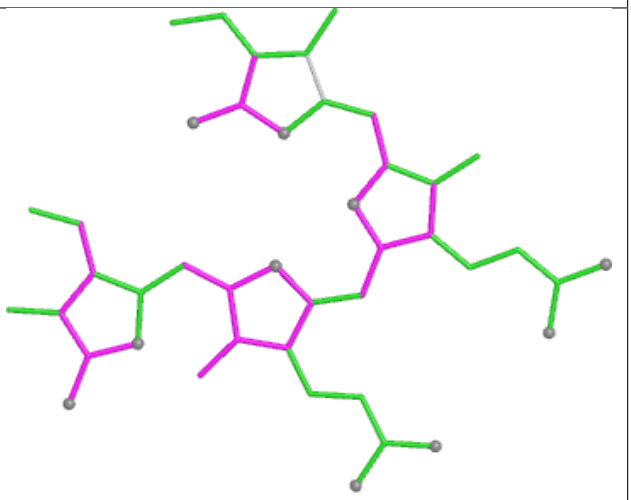


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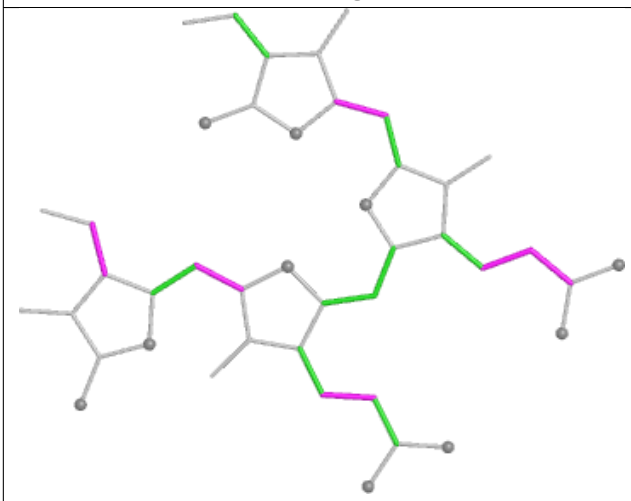
Ligand PEB KM 201



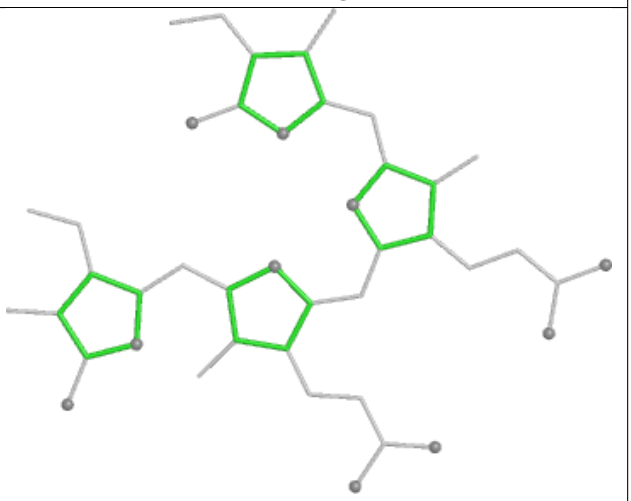
Bond lengths



Bond angles

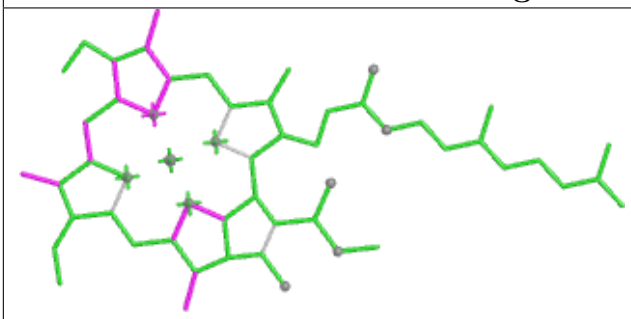


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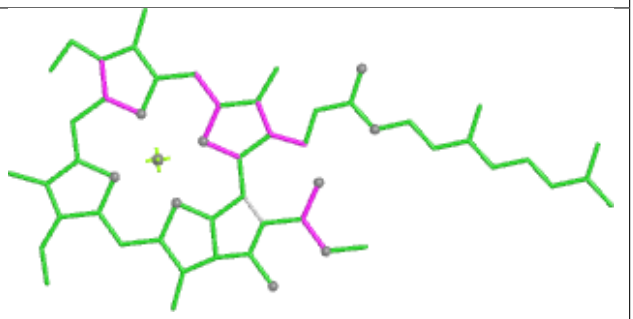


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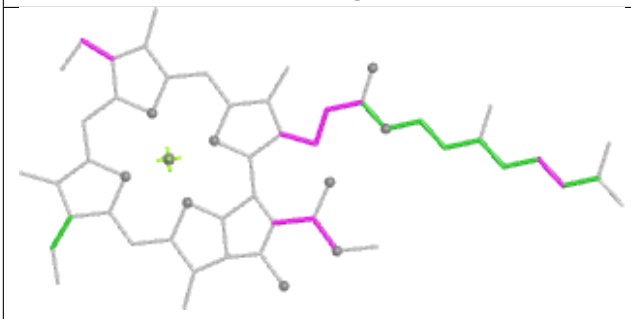
Ligand CLA CL 514



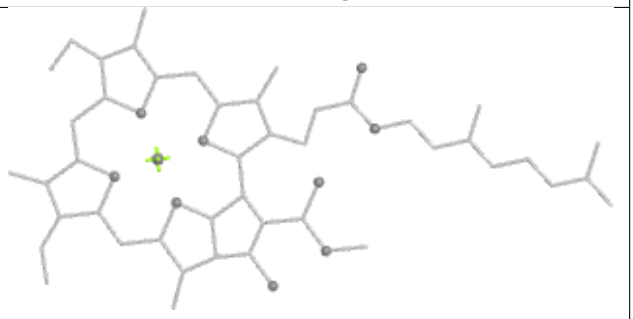
Bond lengths



Bond angles

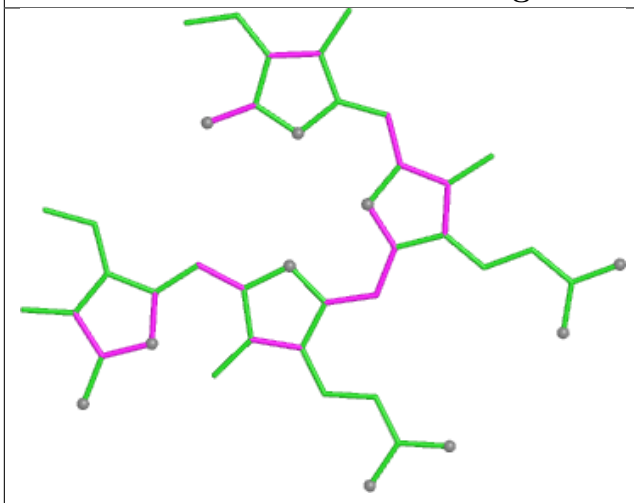


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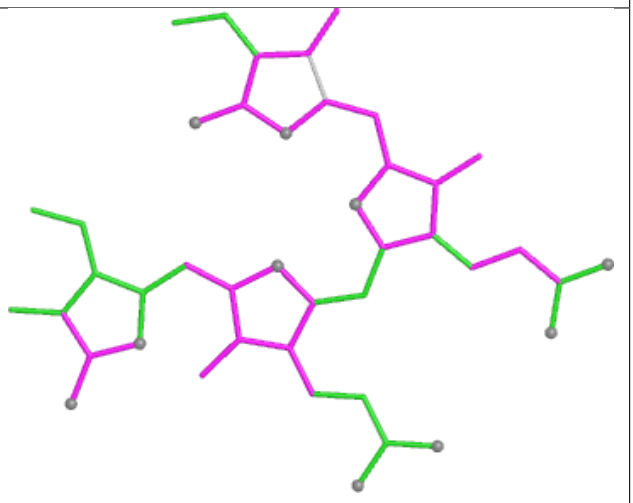


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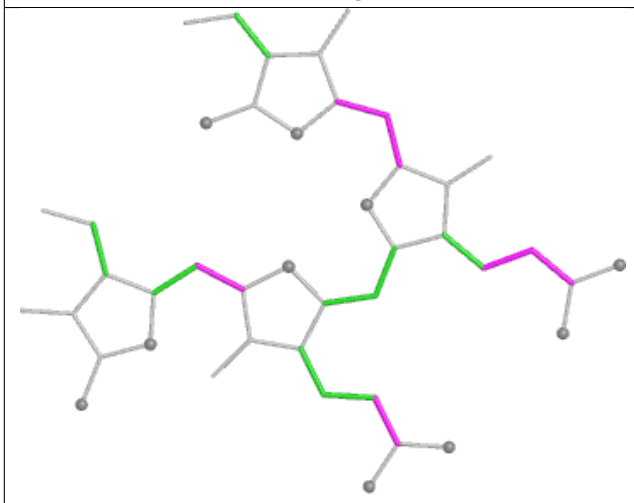
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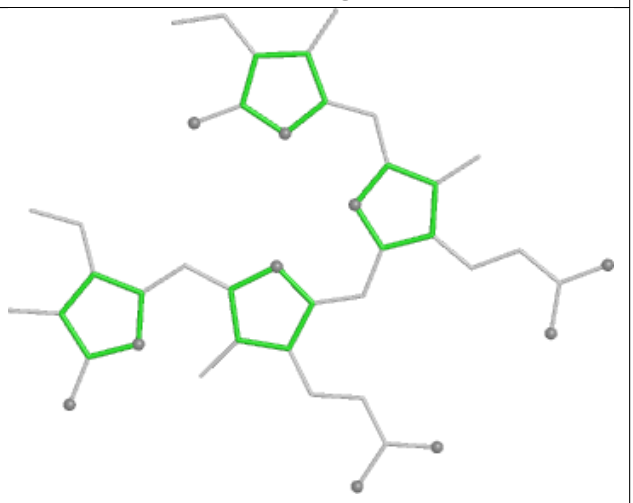
Bond lengths



Bond angles

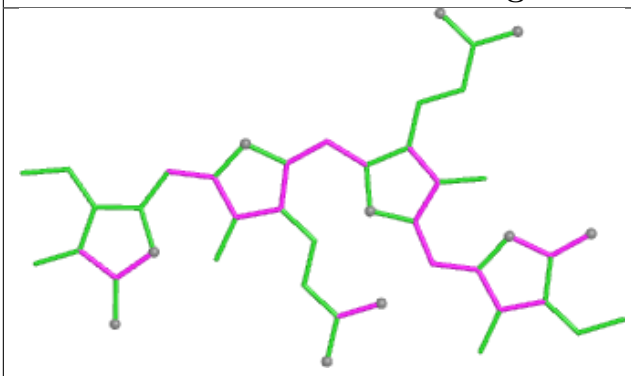


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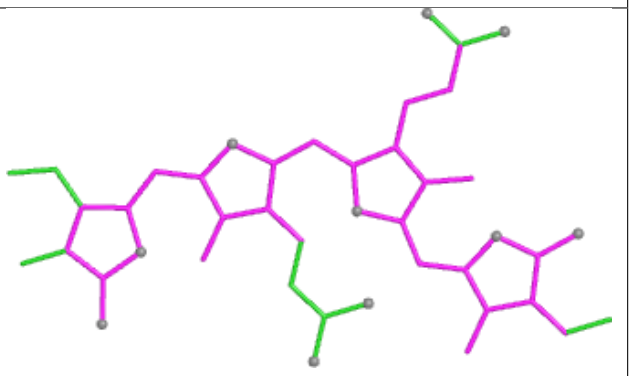


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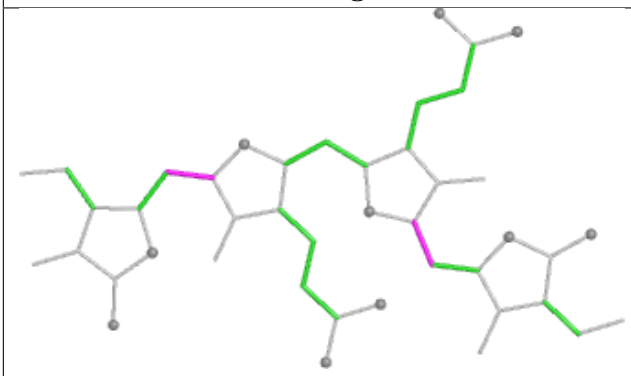
Ligand CYC S3 1001



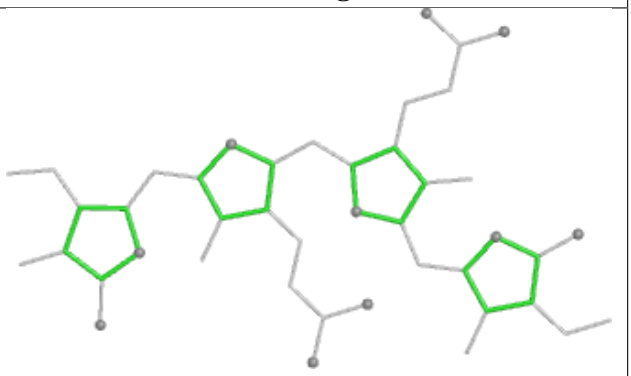
Bond lengths



Bond angles

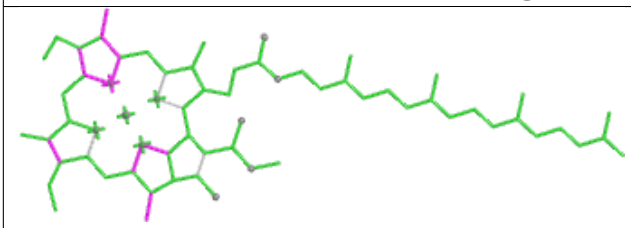


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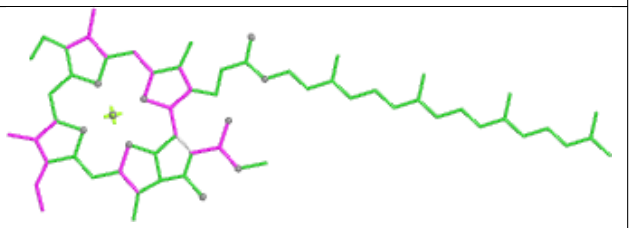


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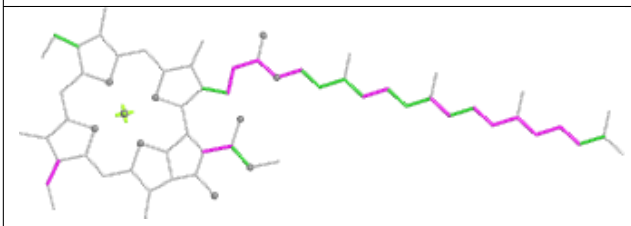
Ligand CLA cL 509



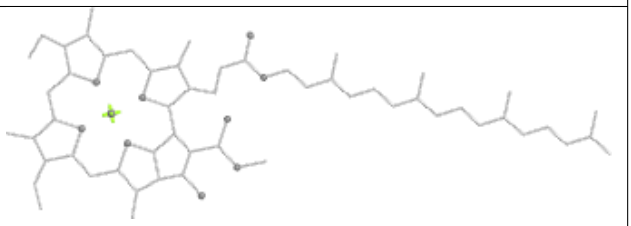
Bond lengths



Bond angles

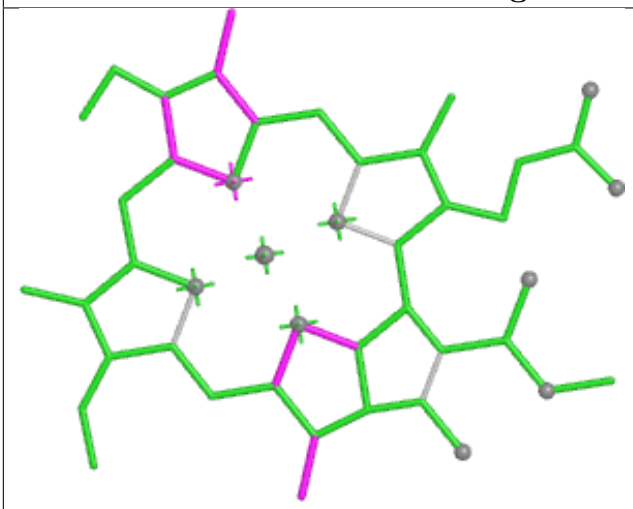


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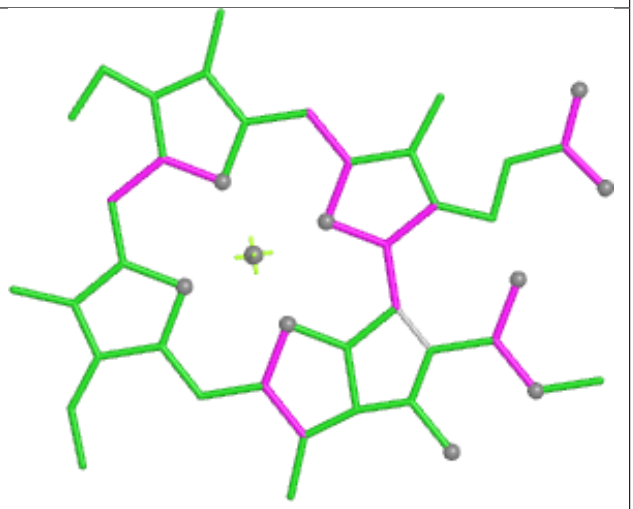


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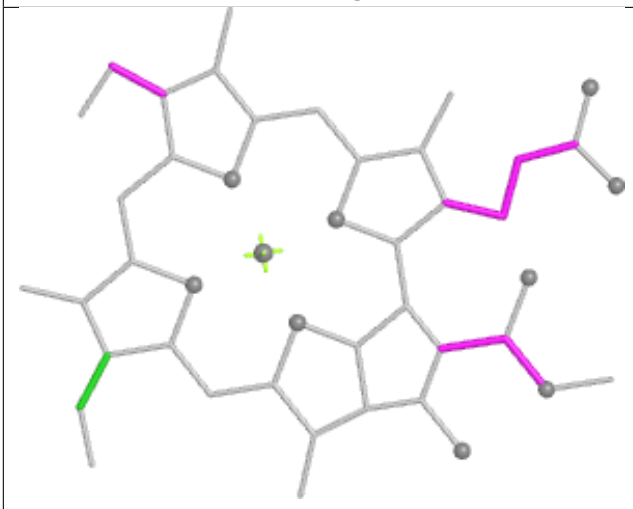
Ligand CLA RN 202



Bond lengths



Bond angles

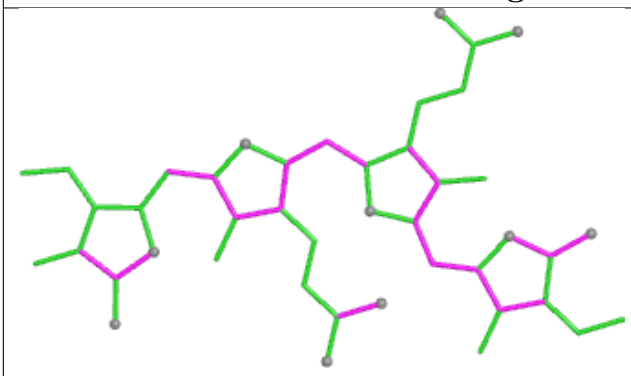


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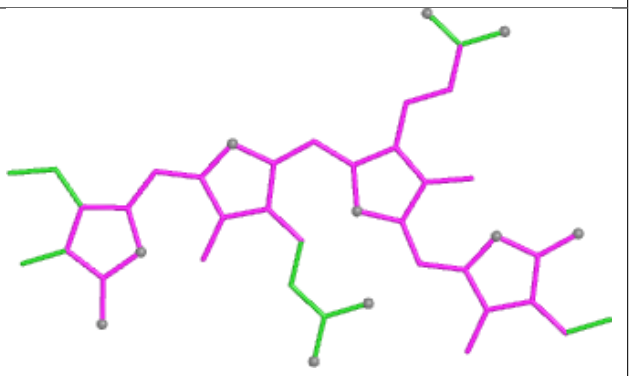


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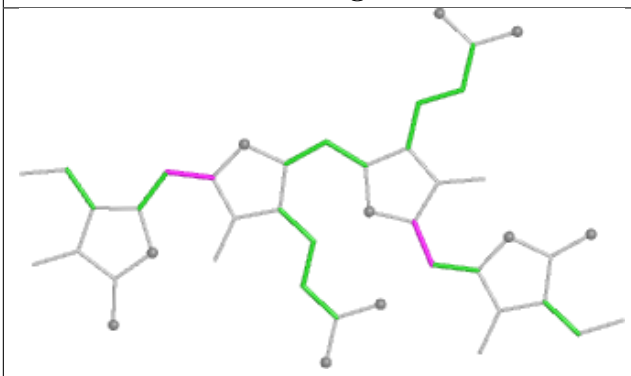
Ligand CYC n3 1001



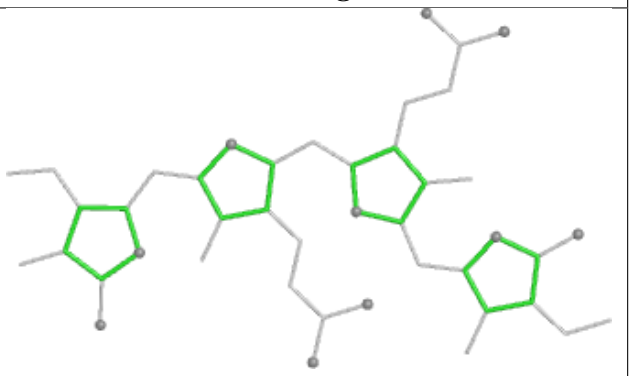
Bond lengths



Bond angles

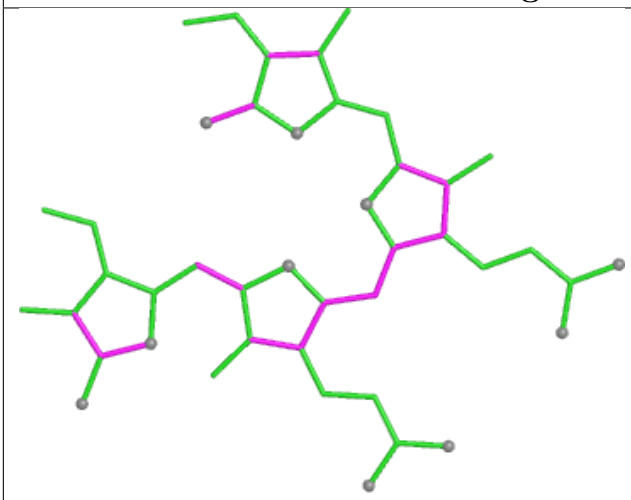


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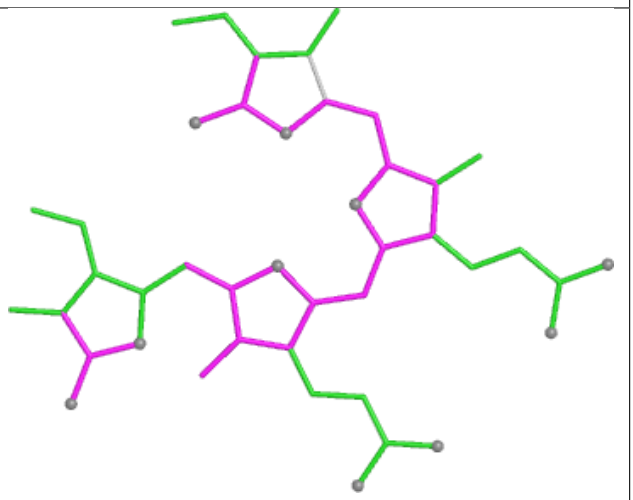


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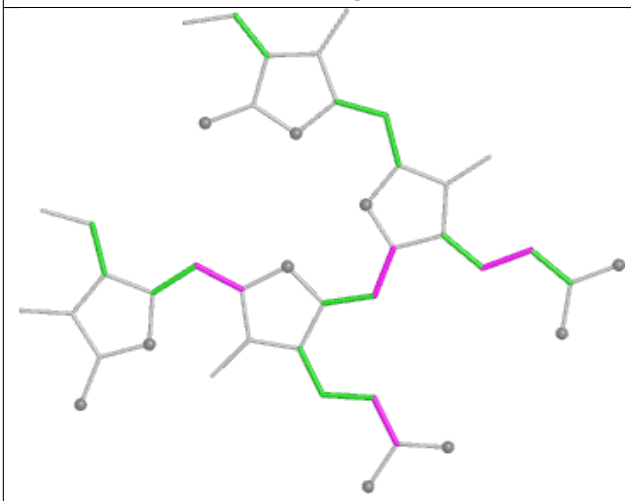
Ligand PEB s8 203



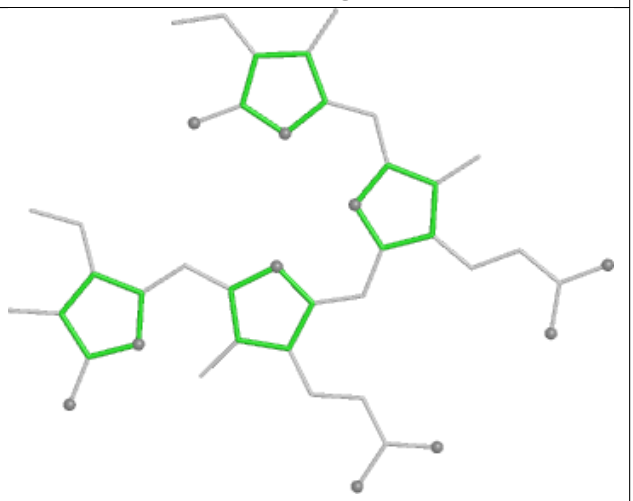
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Bond angles

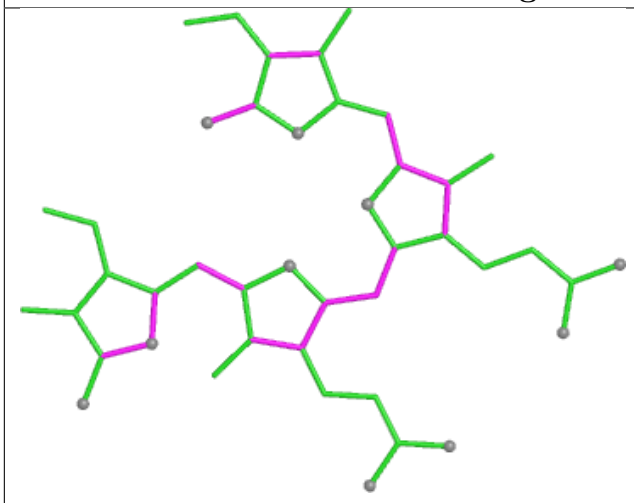


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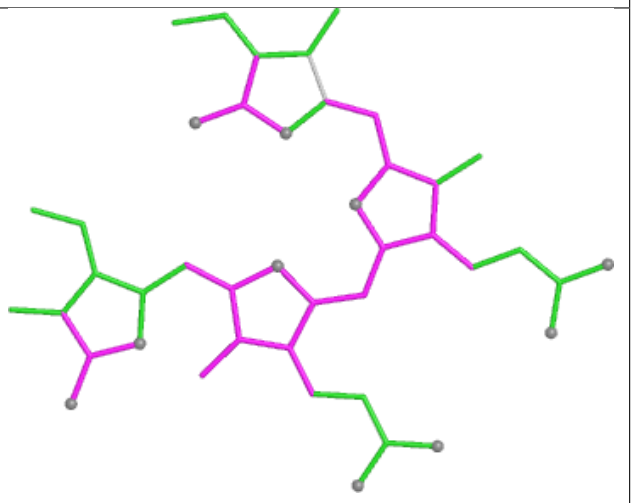


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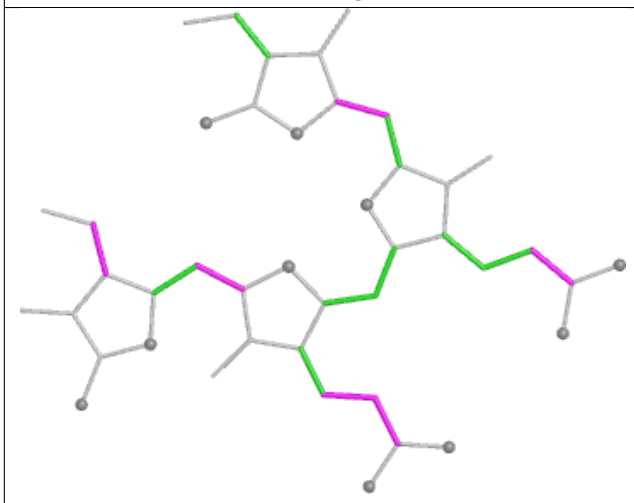
Ligand PEB cF 201



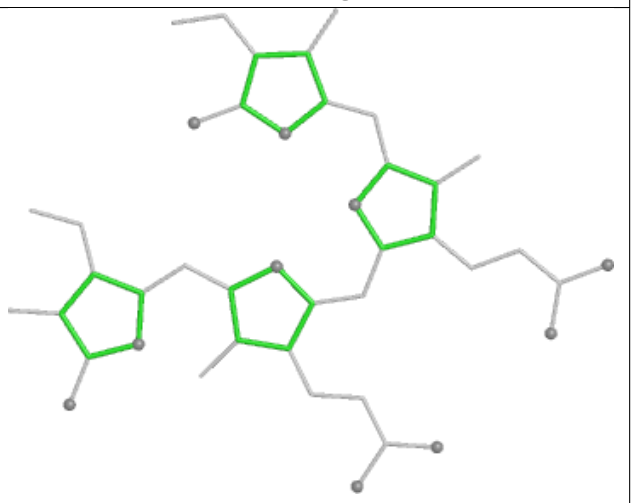
Bond lengths



Bond angles

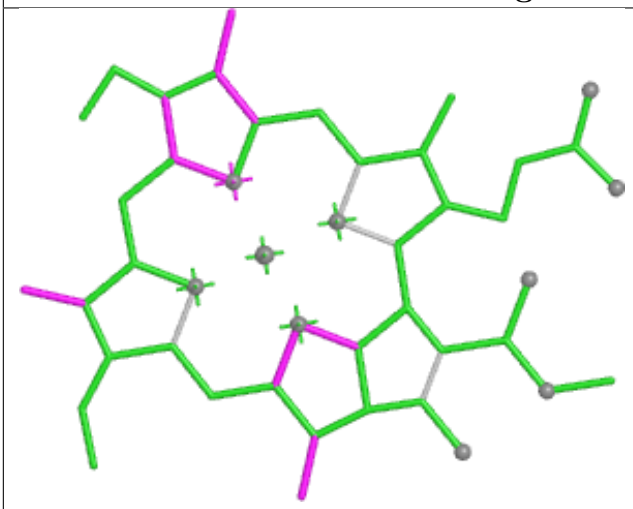


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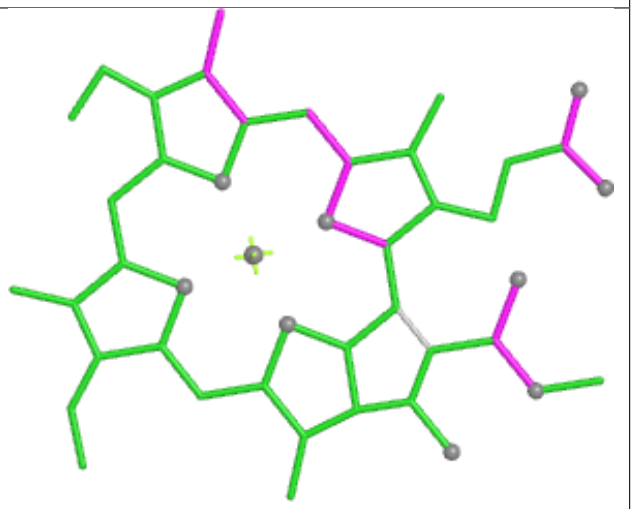


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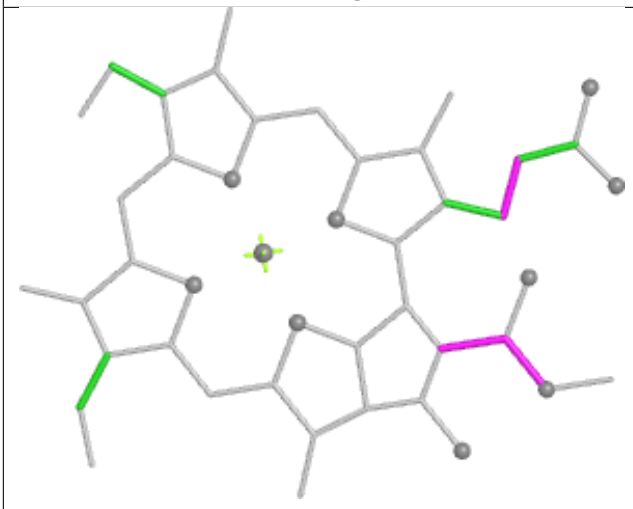
Ligand CLA B2 813



Bond lengths



Bond angles

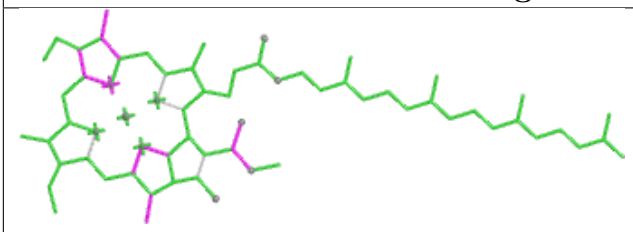


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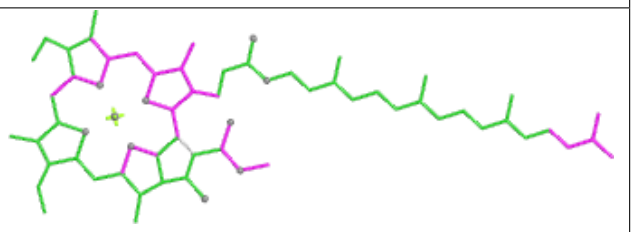


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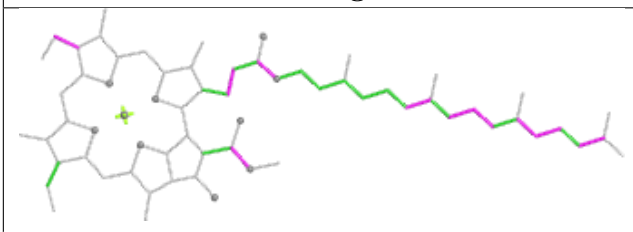
Ligand CLA 3N 305



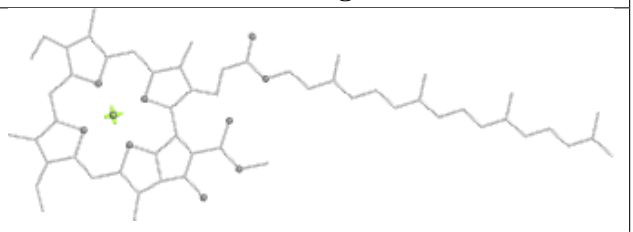
Bond lengths



Bond angles

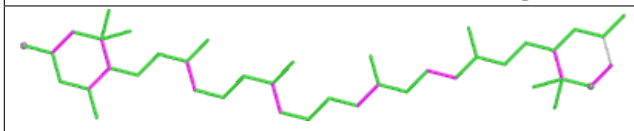


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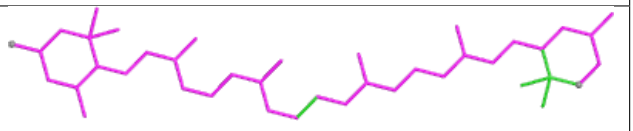


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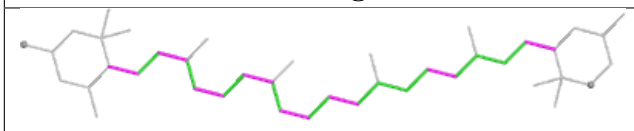
Ligand ZEX 8N 310



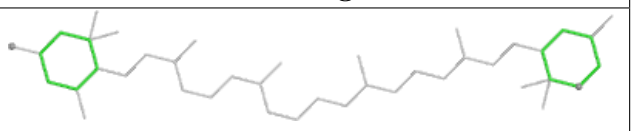
Bond lengths



Bond angles

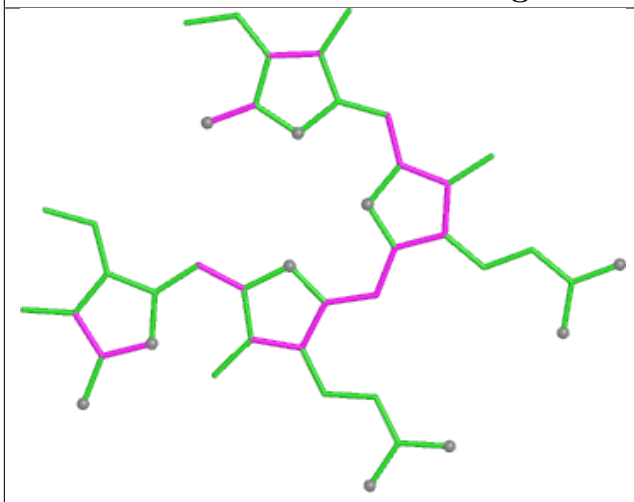


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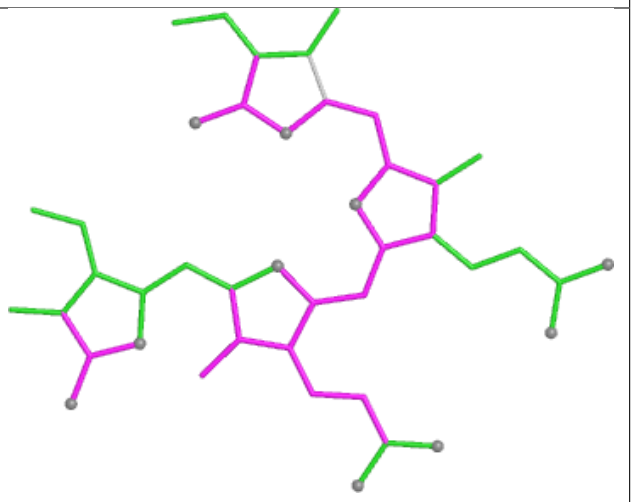


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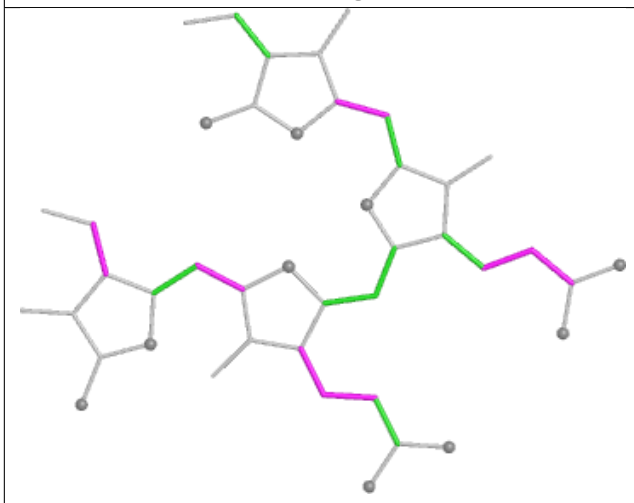
Ligand PEB W9 202



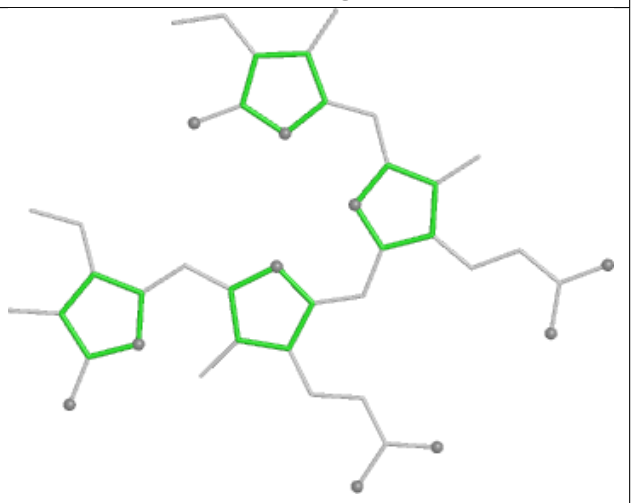
Bond lengths



Bond angles

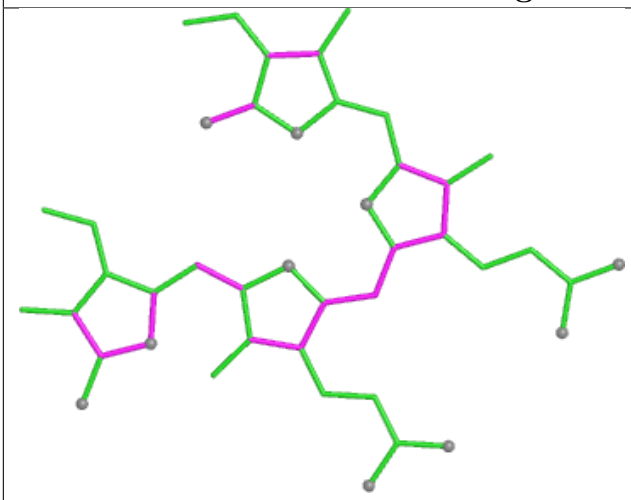


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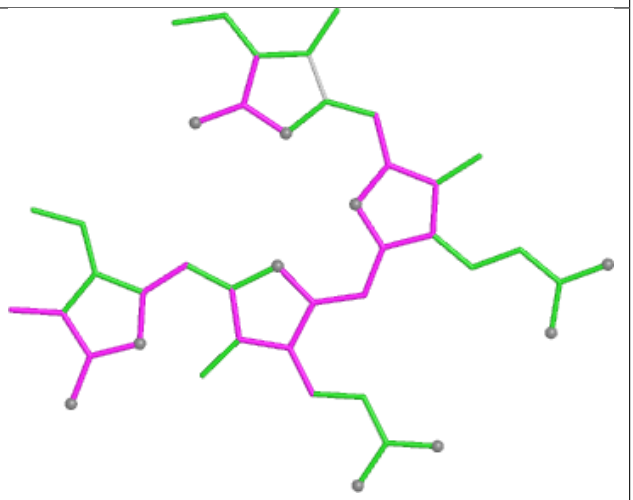


Rings

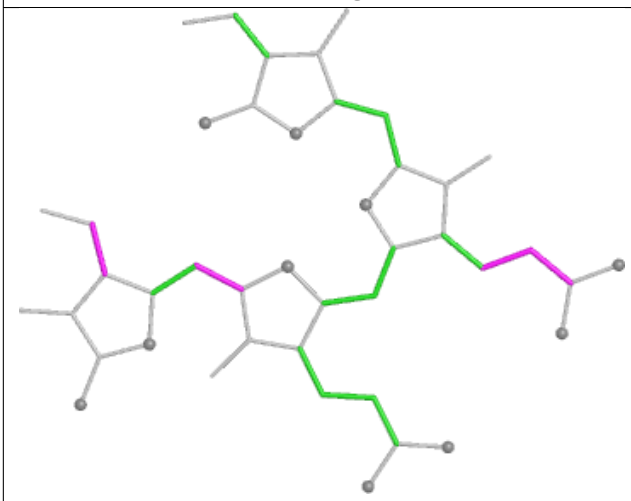
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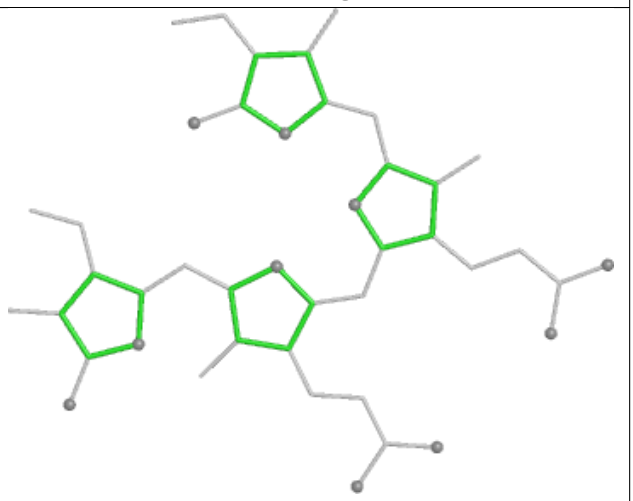
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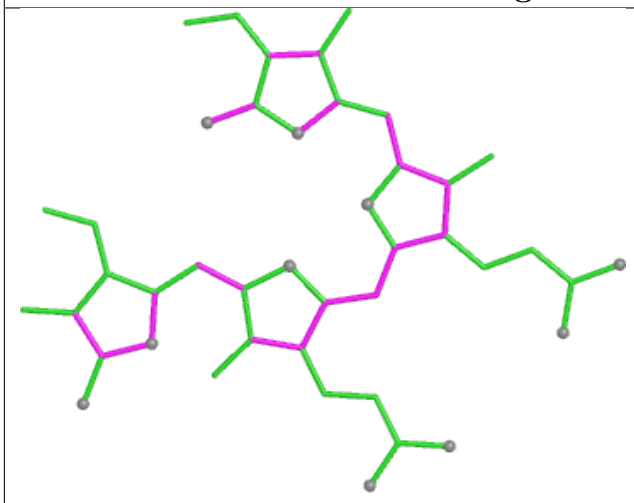


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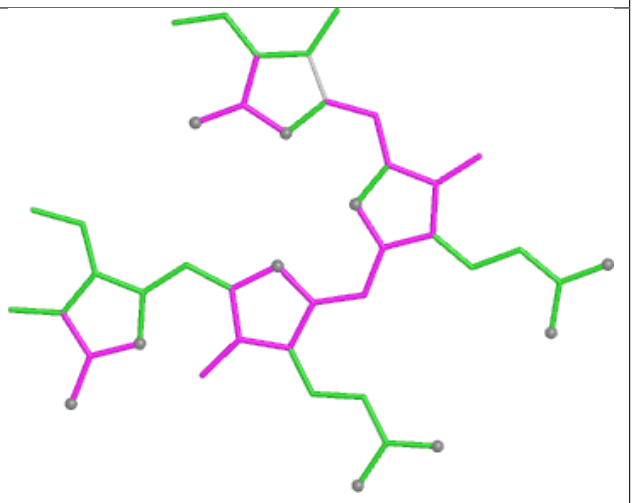


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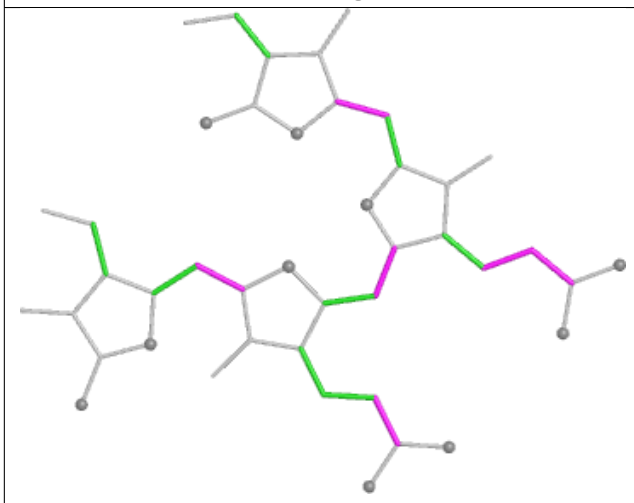
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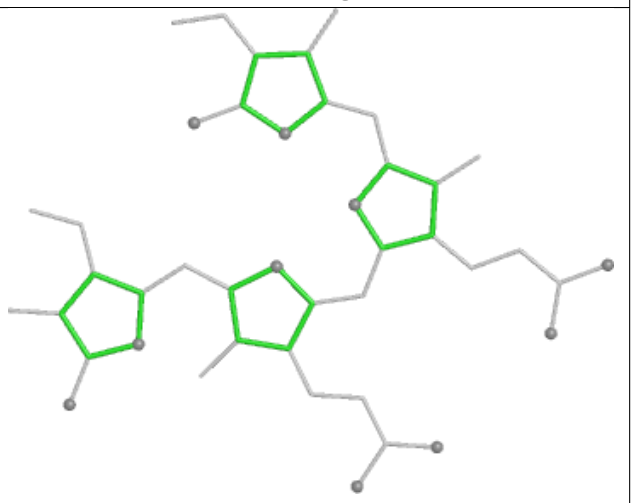
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Bond angles

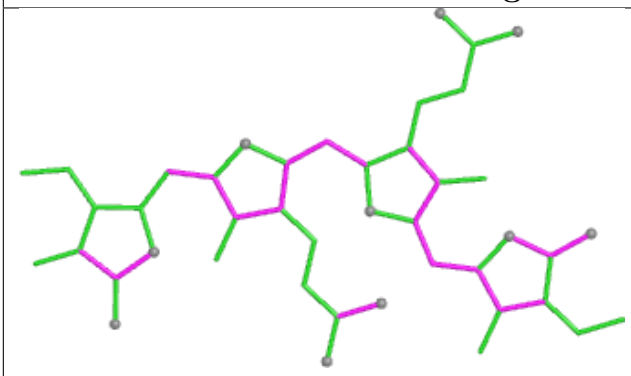


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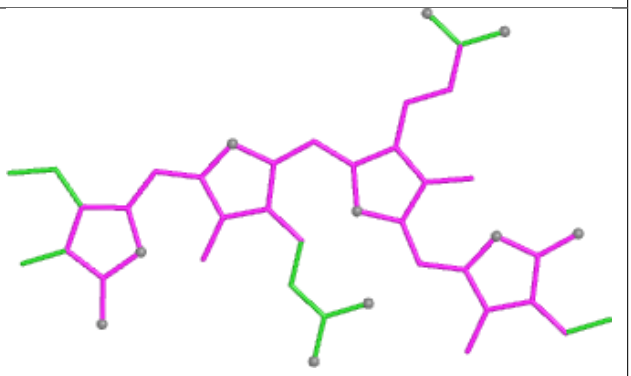


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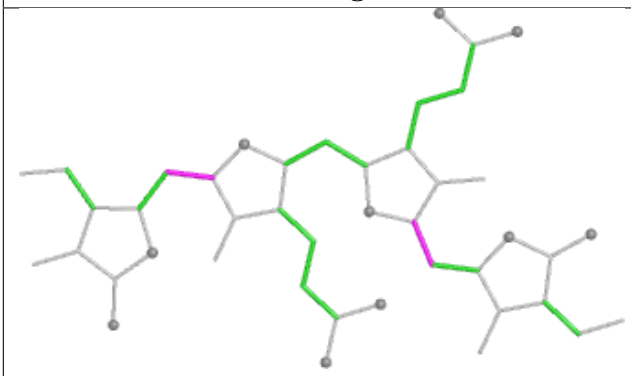
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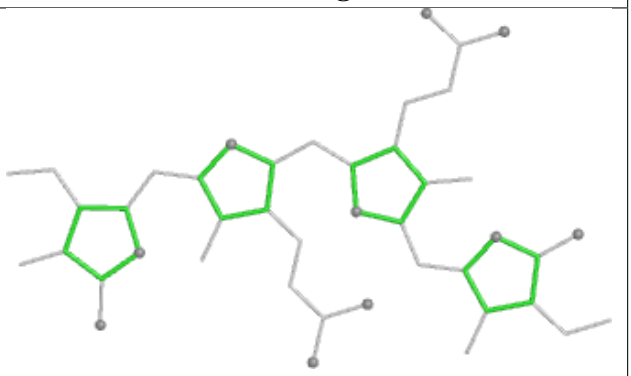
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Bond angles

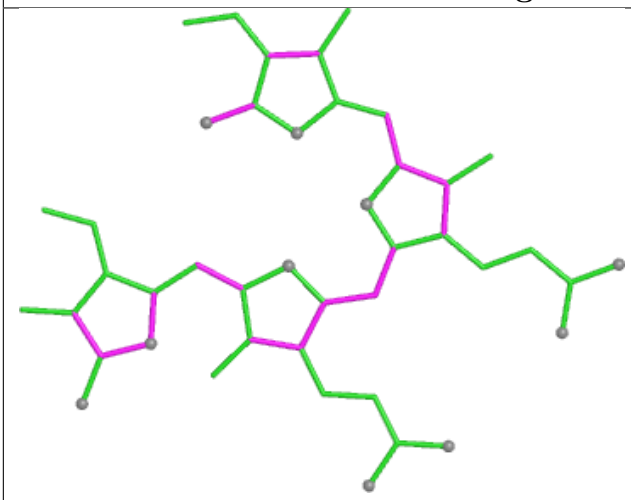


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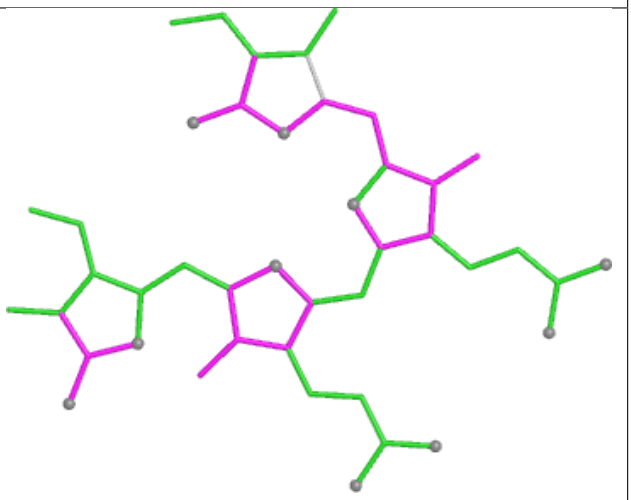


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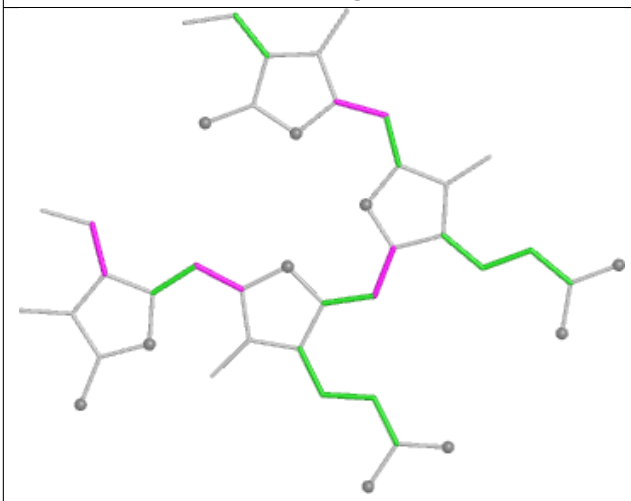
Ligand PEB w8 204



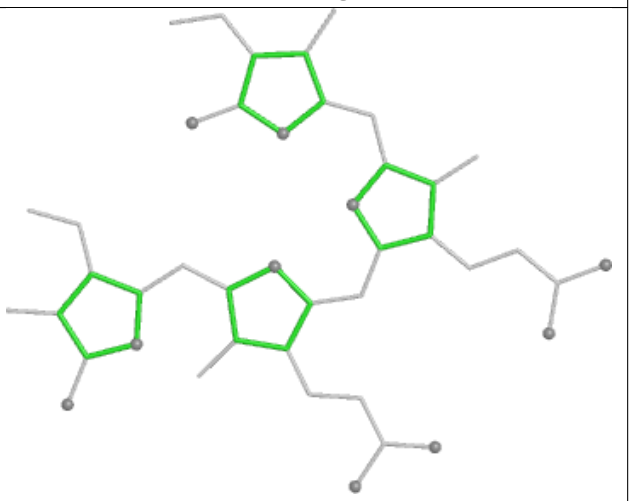
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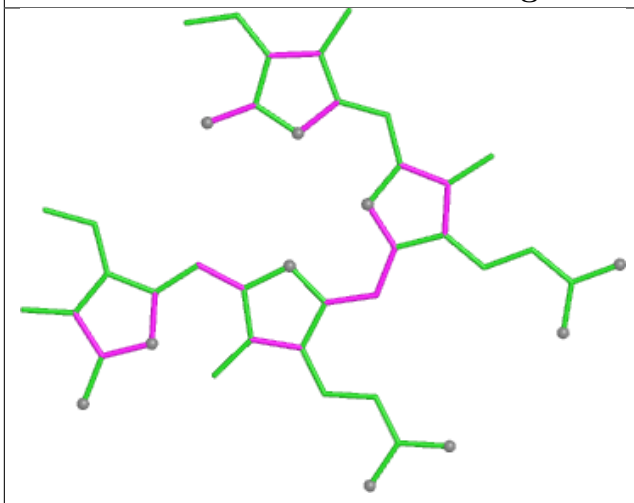


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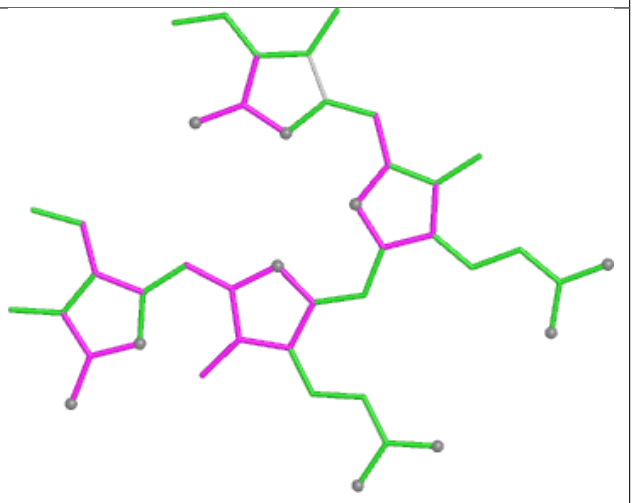


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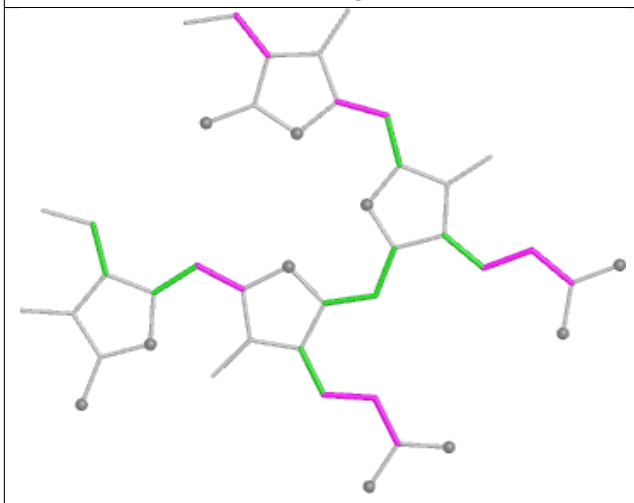
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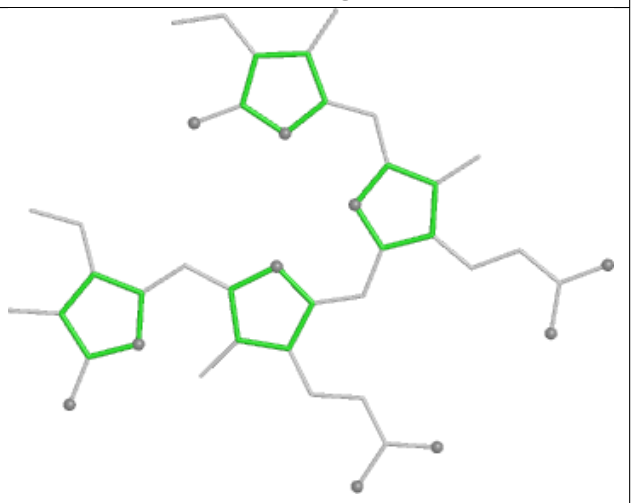
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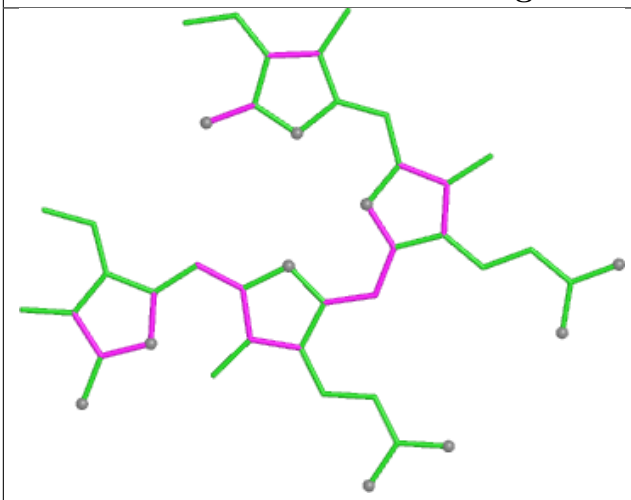


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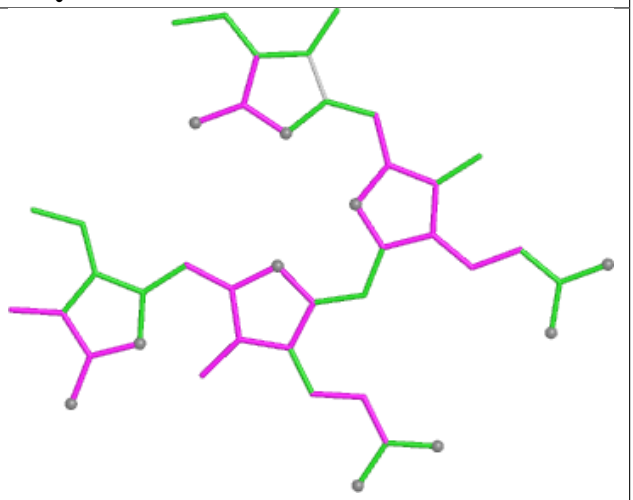


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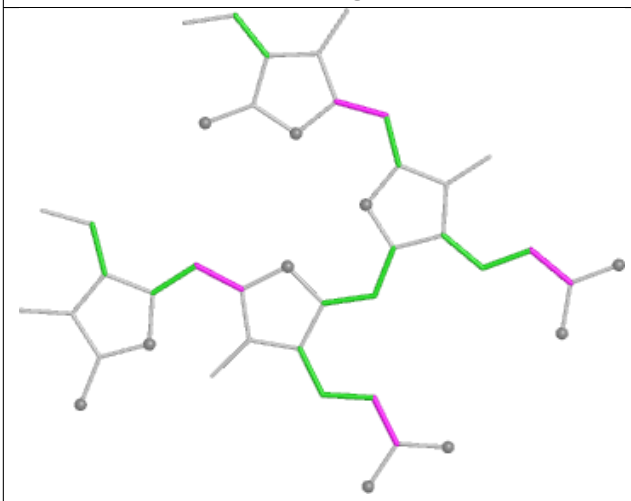
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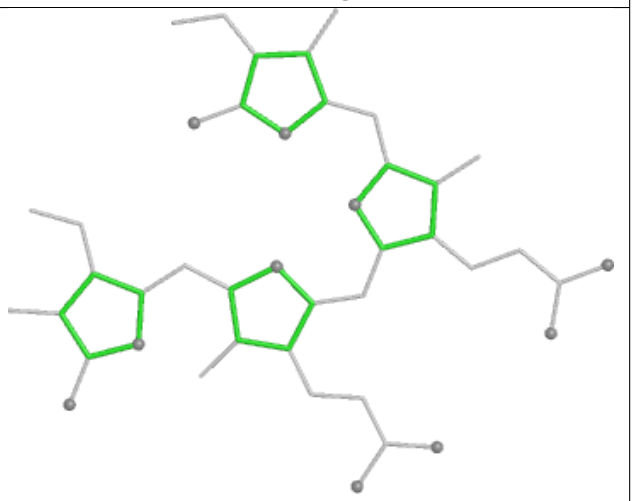
Bond lengths



Bond angles

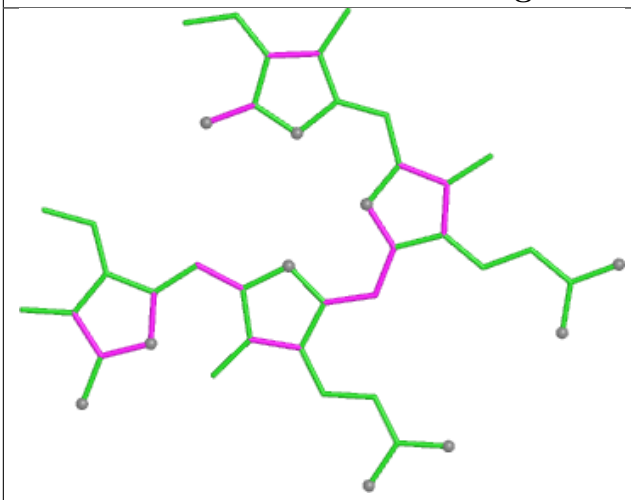


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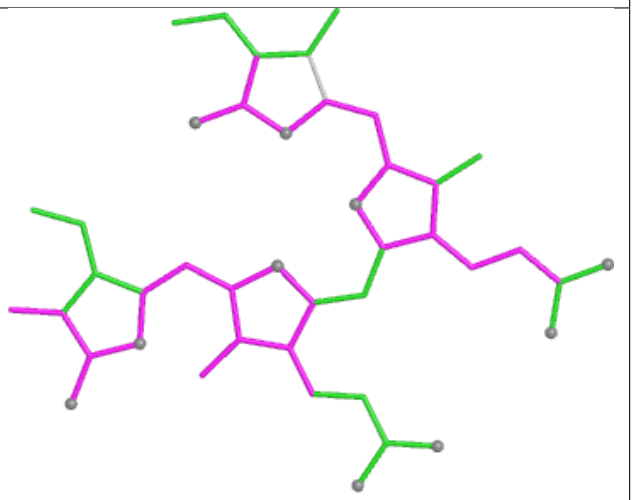


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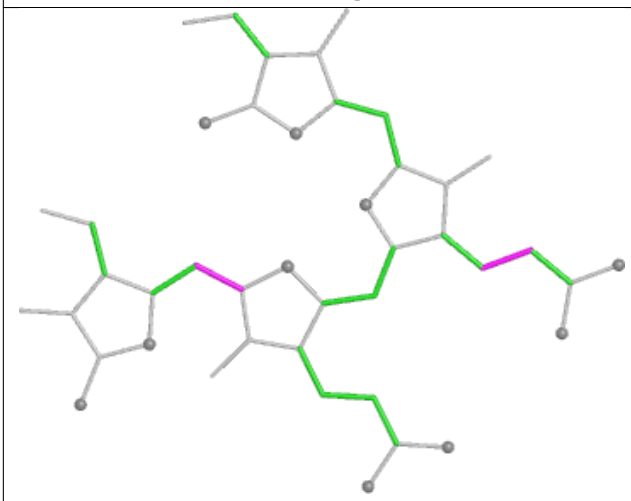
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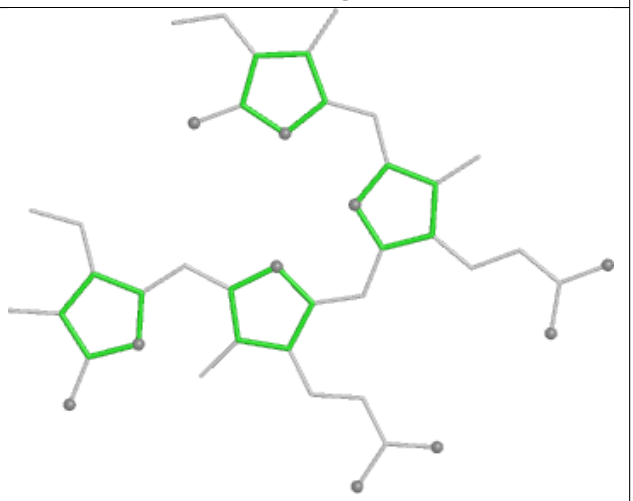
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Bond angles

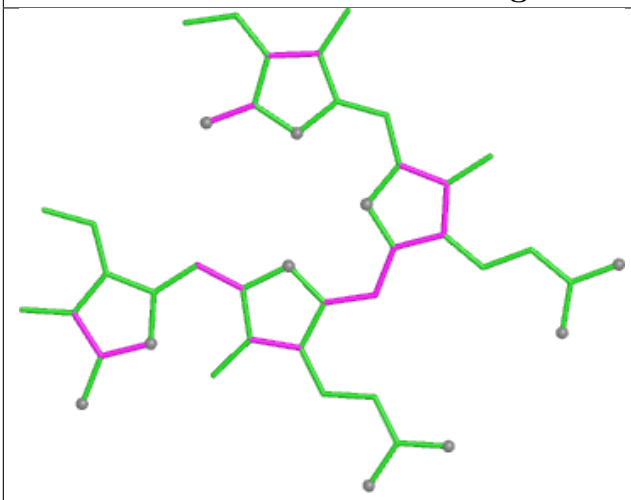


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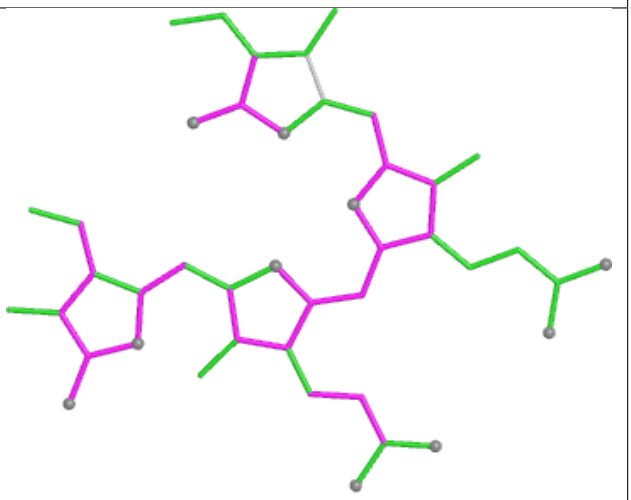


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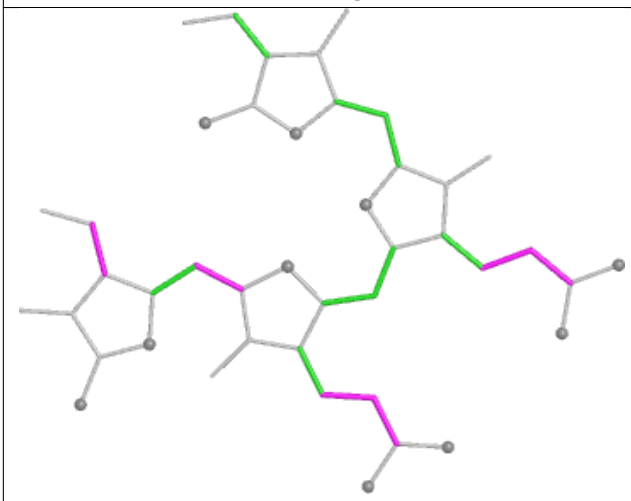
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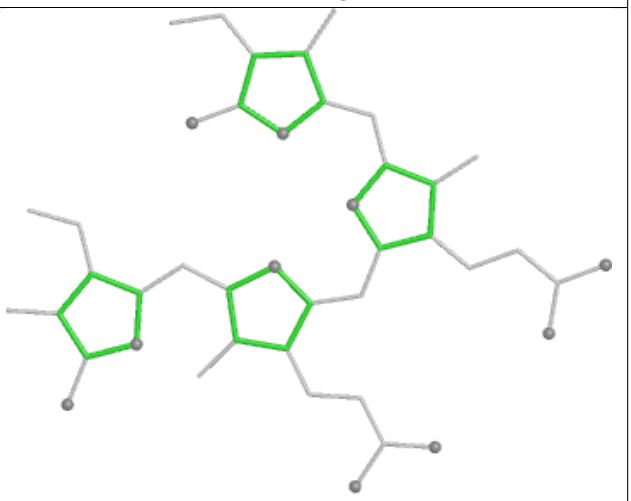
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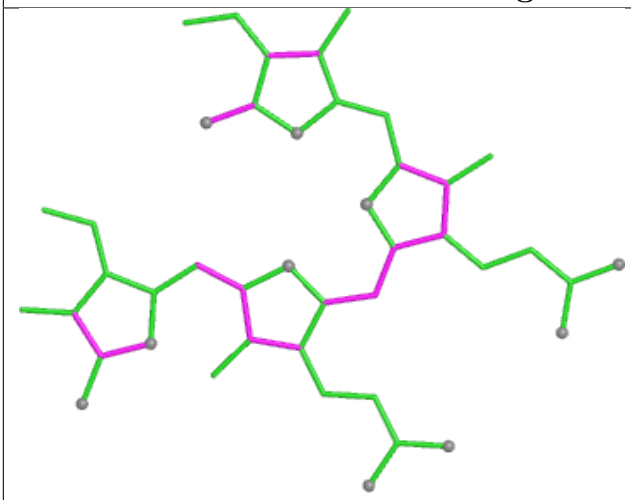


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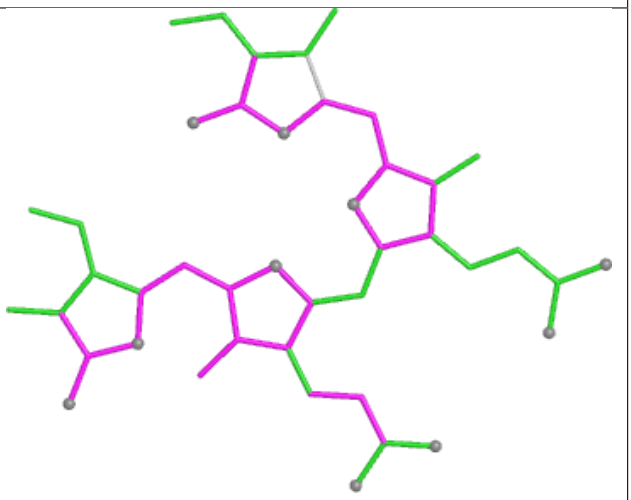


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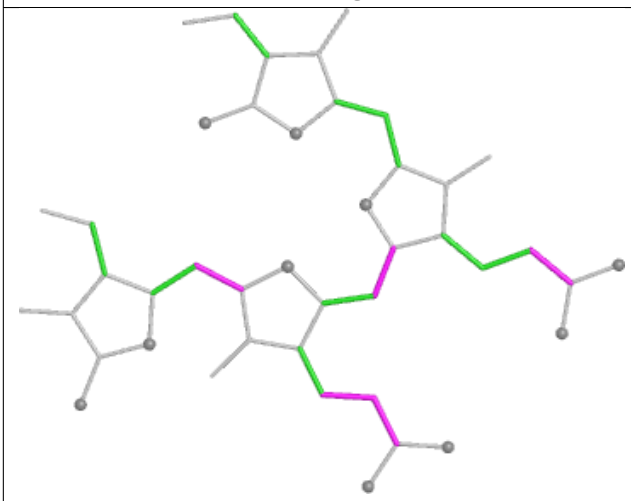
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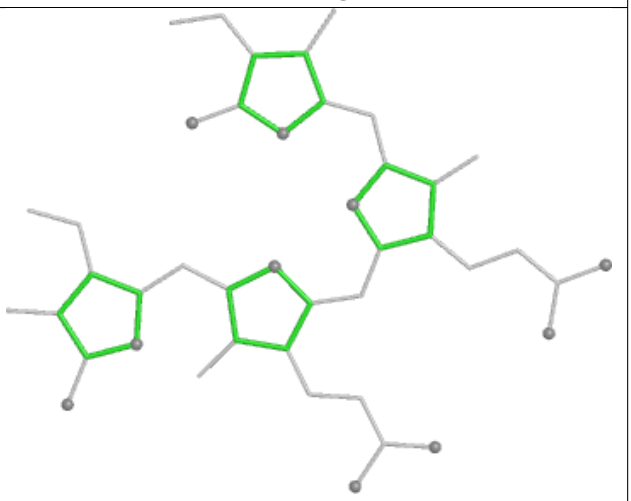
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Bond angles

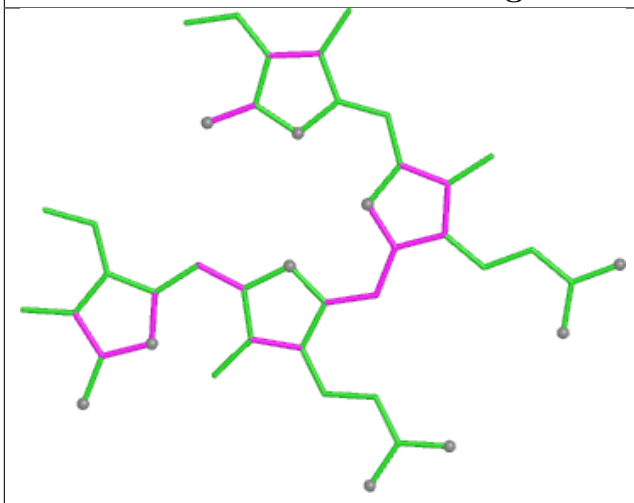


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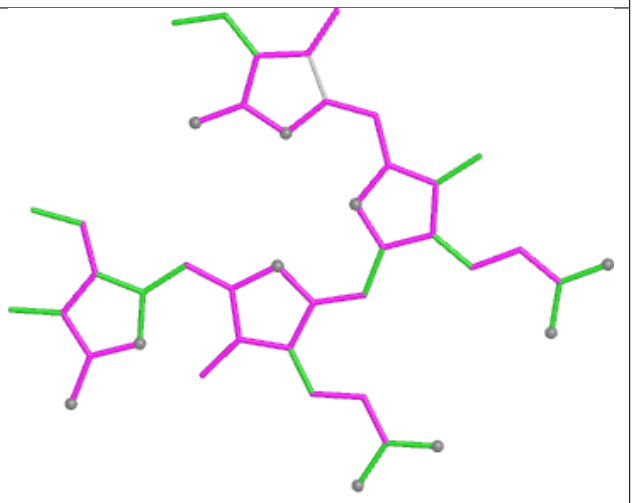


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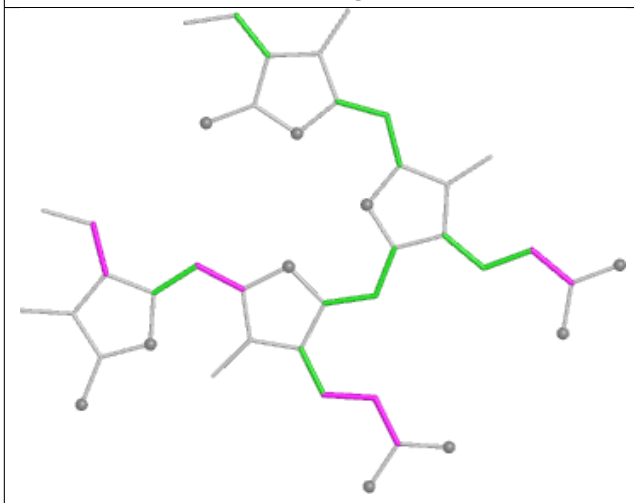
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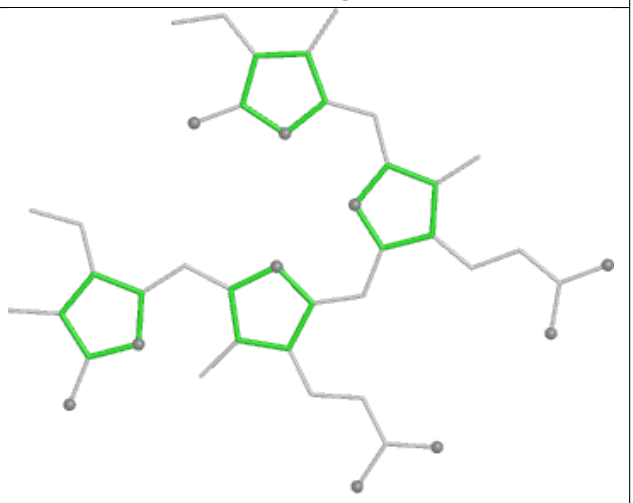
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Bond angles

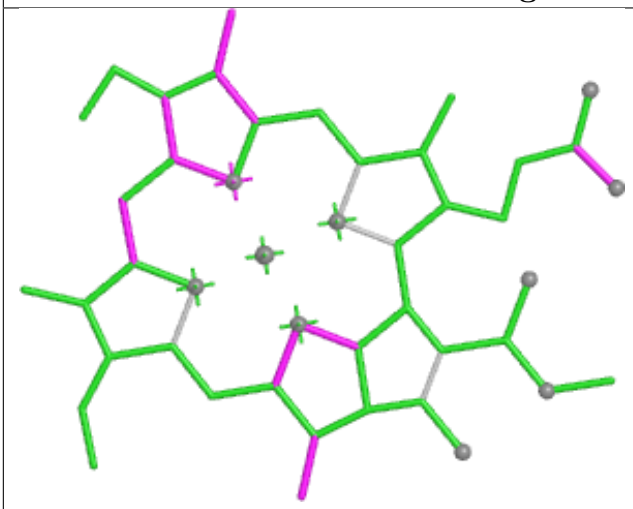


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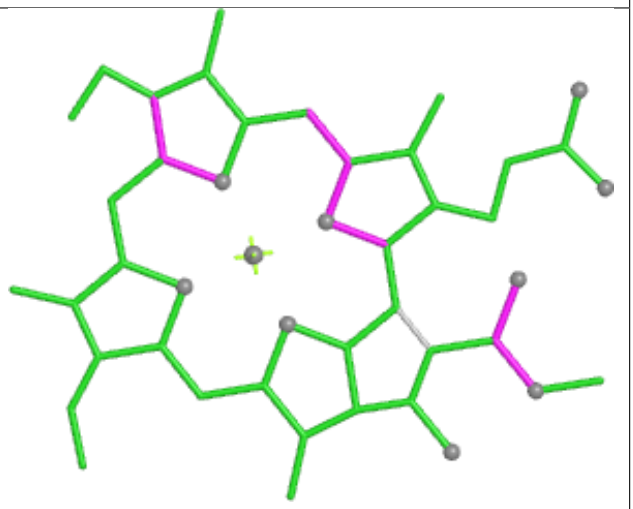


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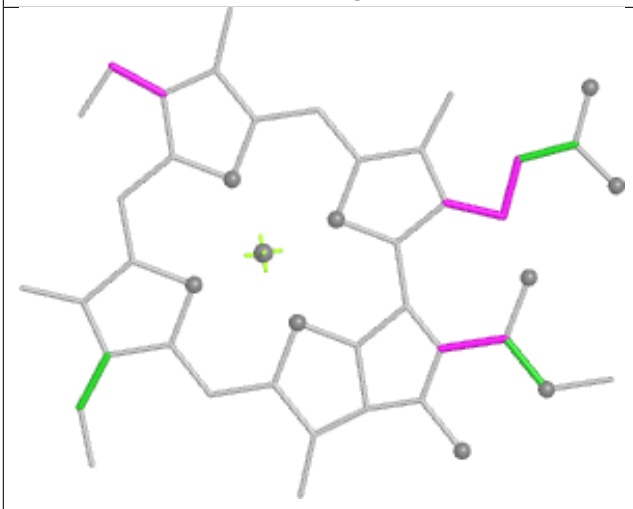
Ligand CLA 62 301



Bond lengths



Bond angles

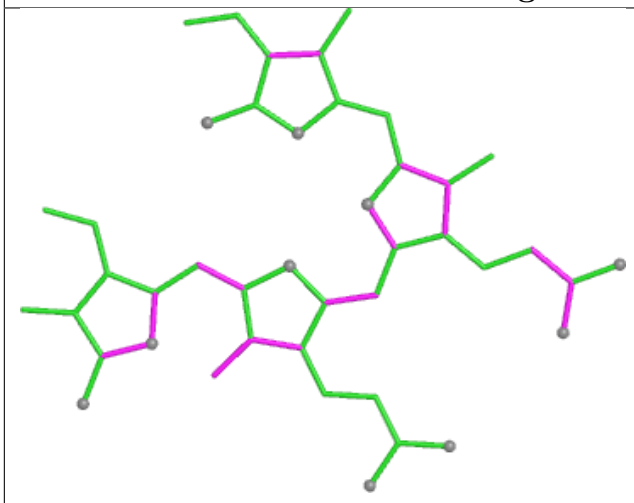


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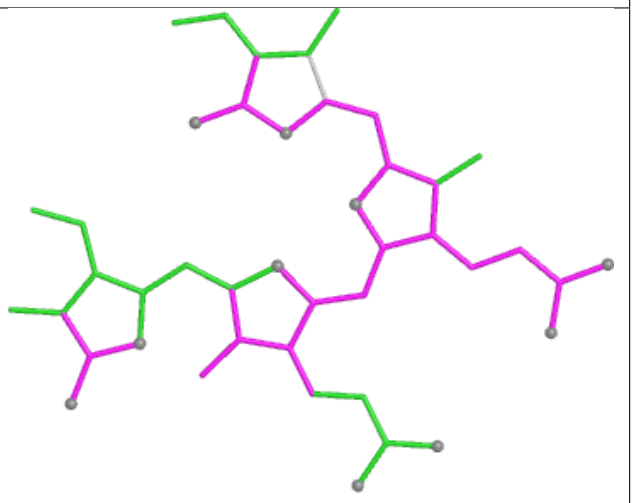


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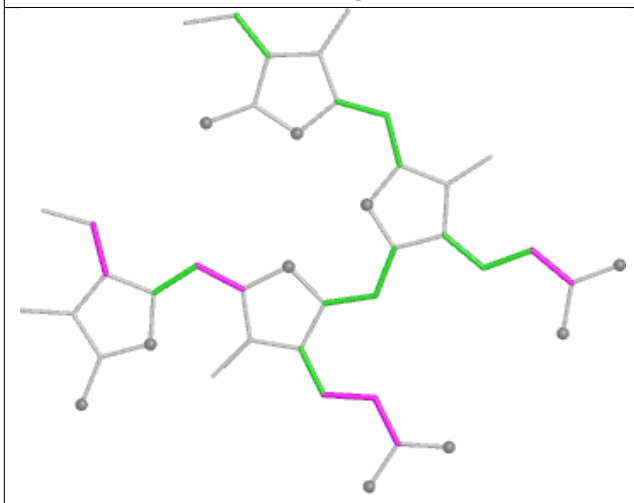
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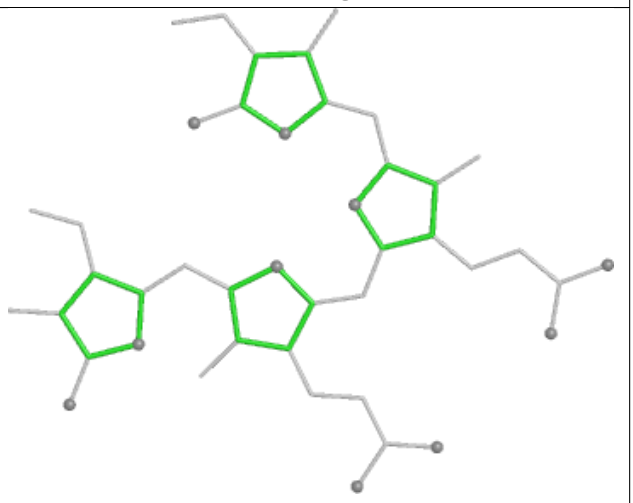
Bond lengths



Bond angles

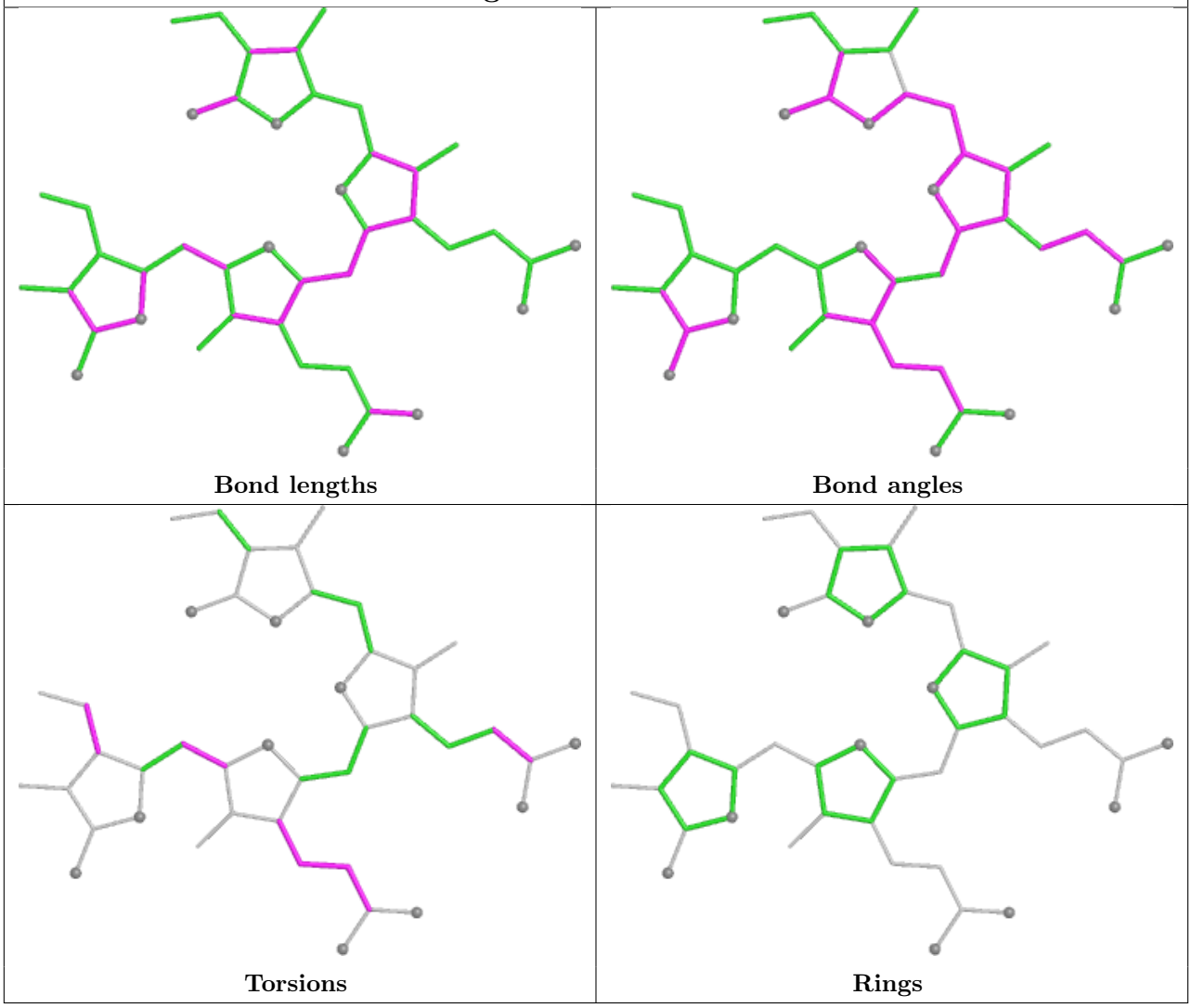


Torsions



Rings

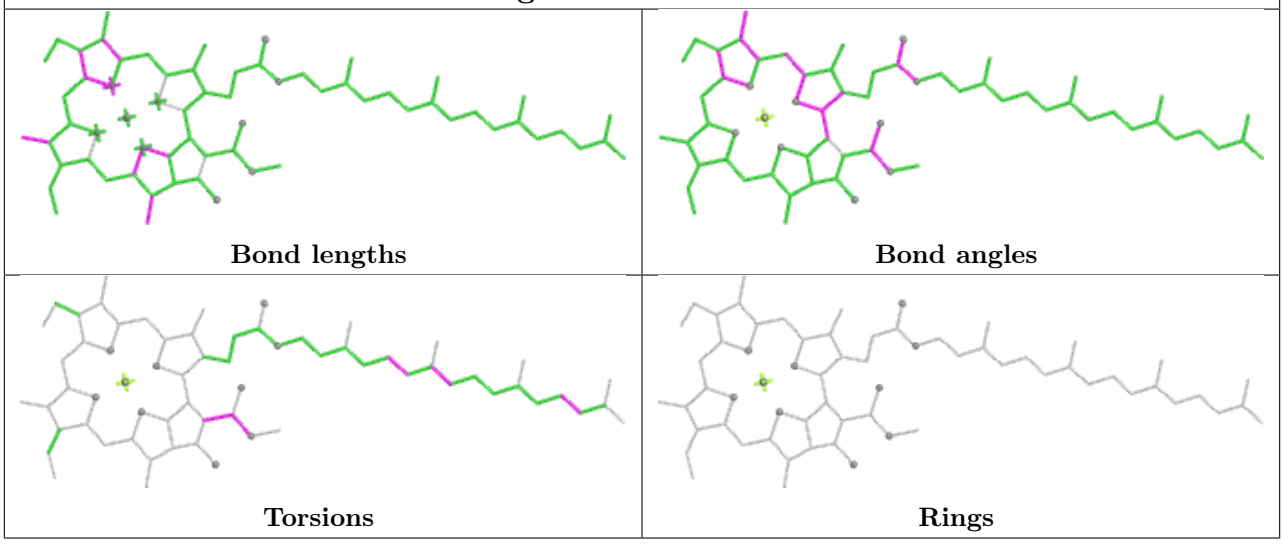
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Bond lengths | Bond angles

Torsions | Rings

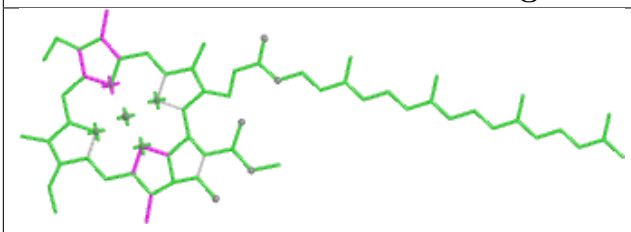
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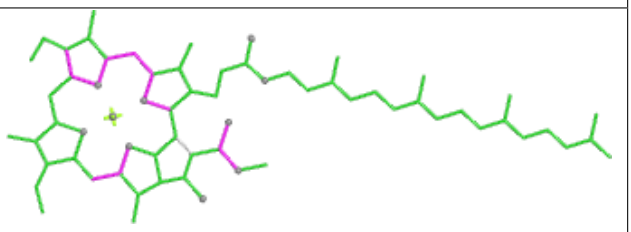
Bond lengths | Bond angles

Torsions | Rings

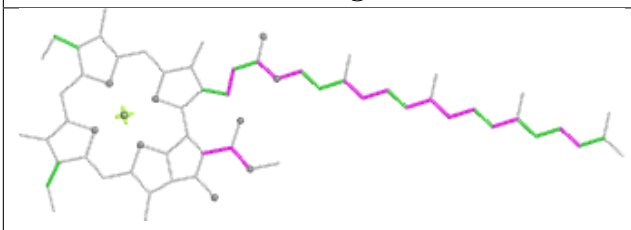
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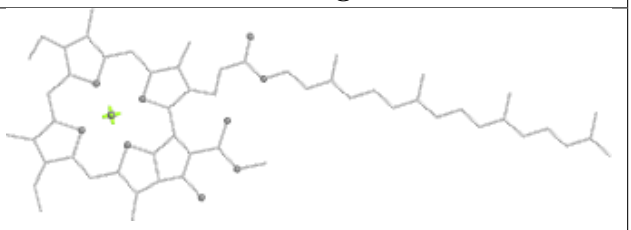
Bond lengths



Bond angles

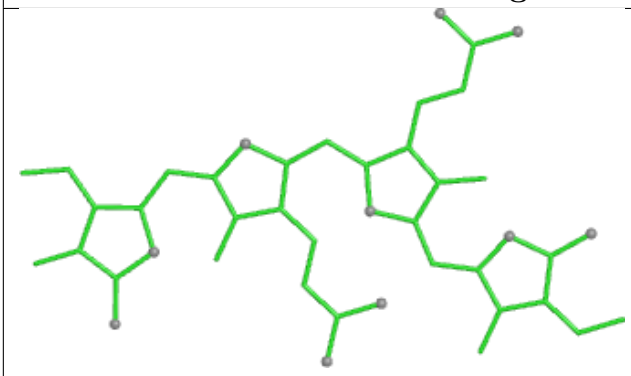


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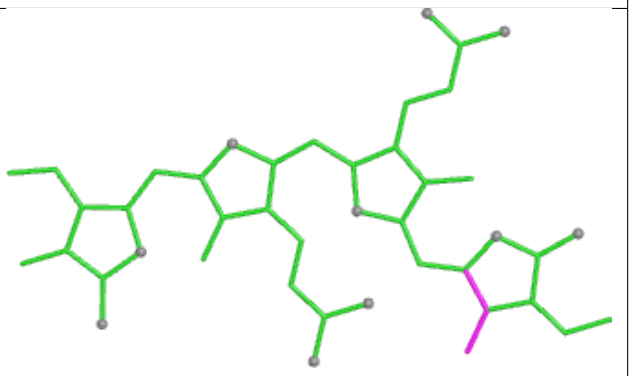


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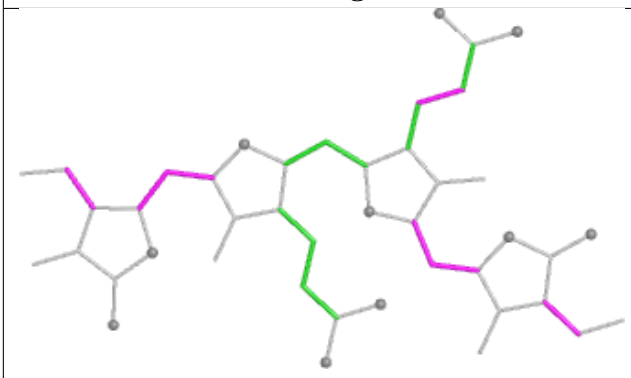
Ligand CYC r3 1001



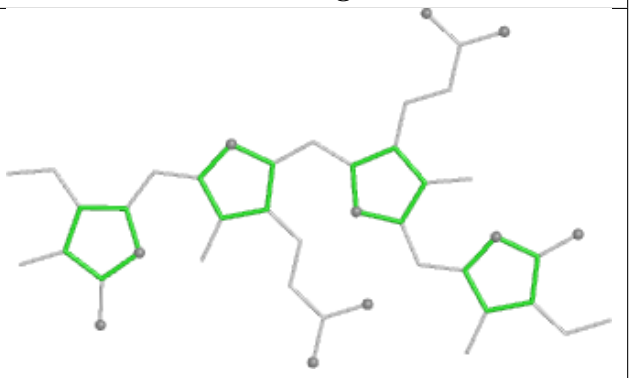
Bond lengths



Bond angles

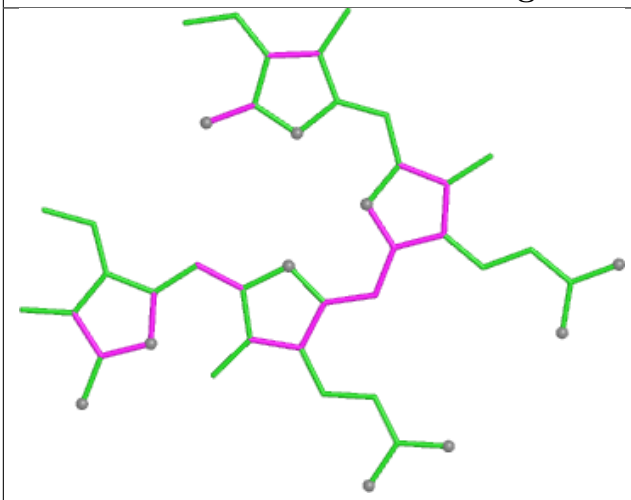


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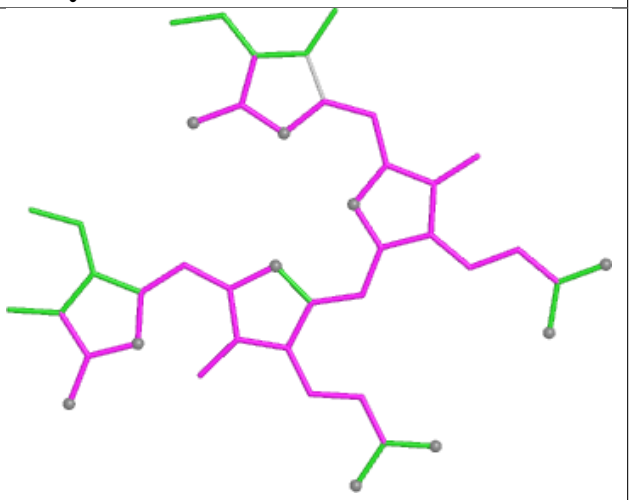


Rings

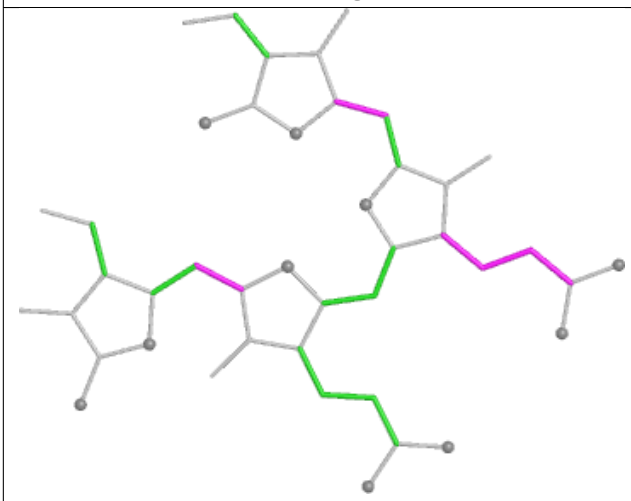
Ligand PEB IQ 201



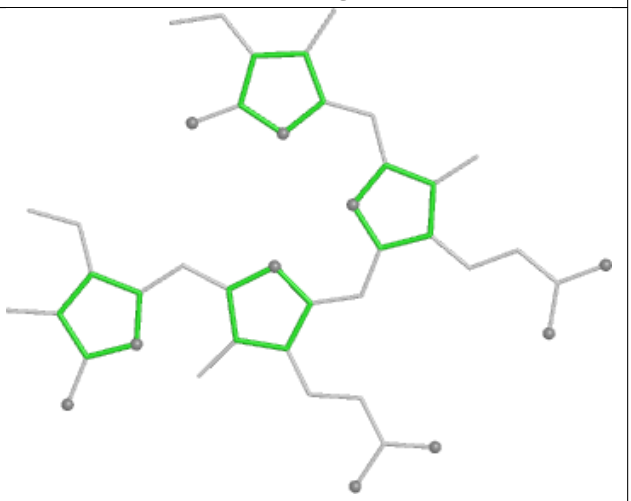
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Bond angles

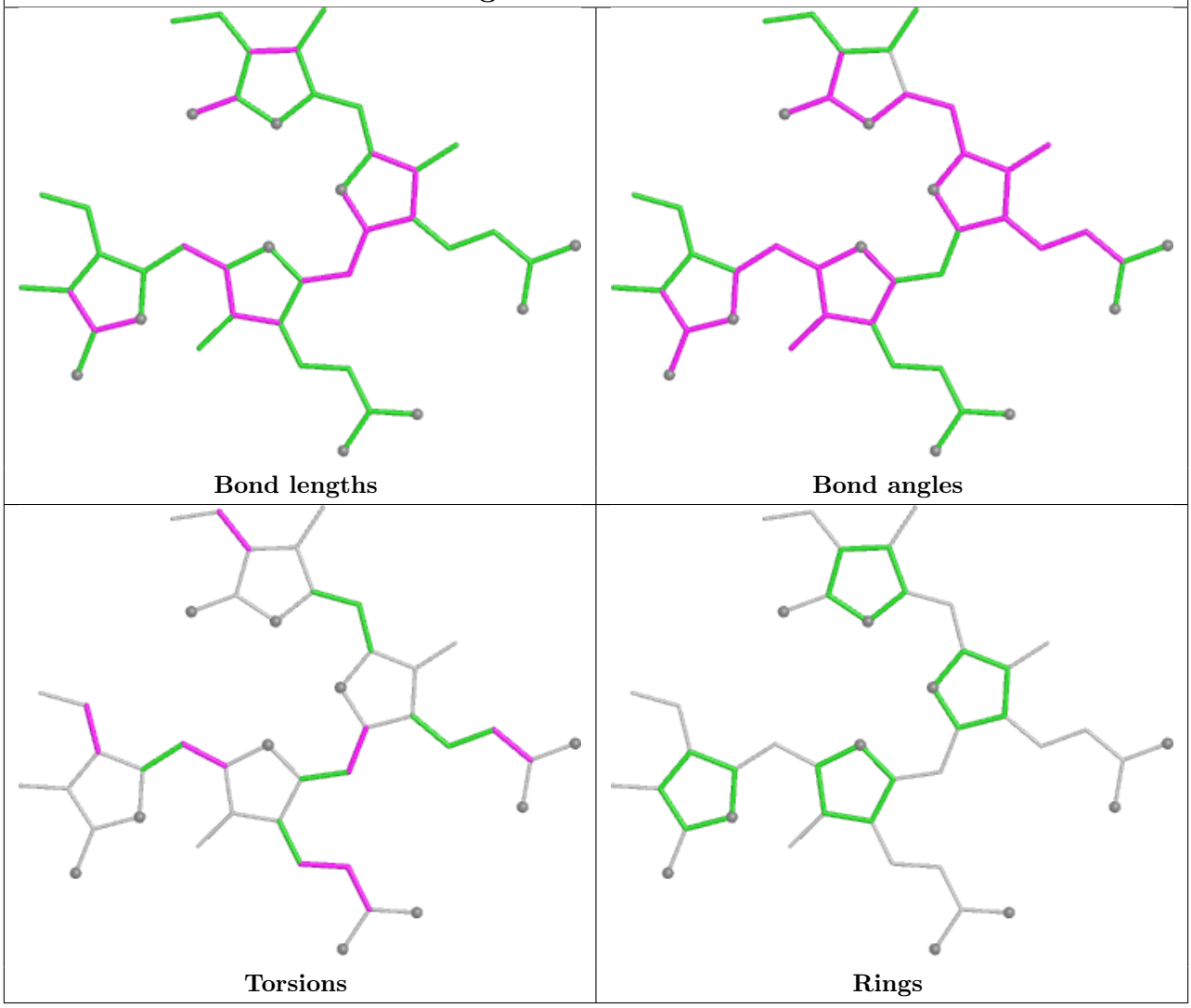


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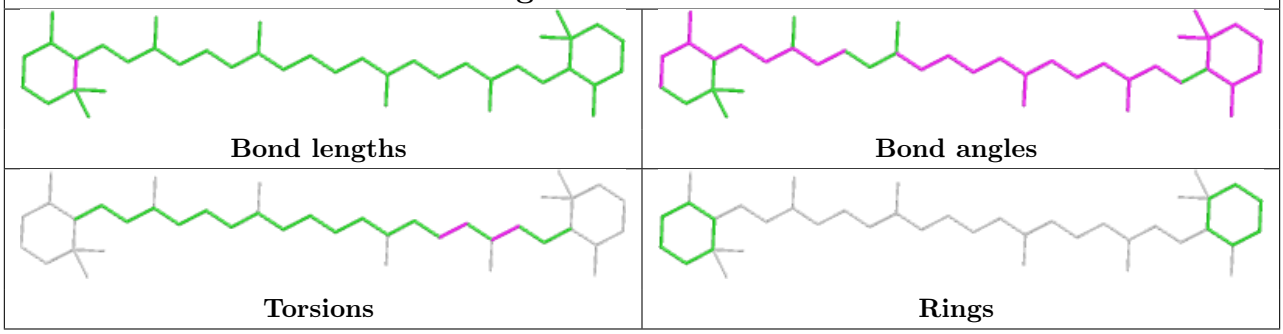


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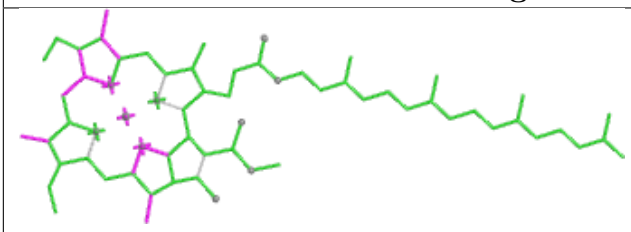
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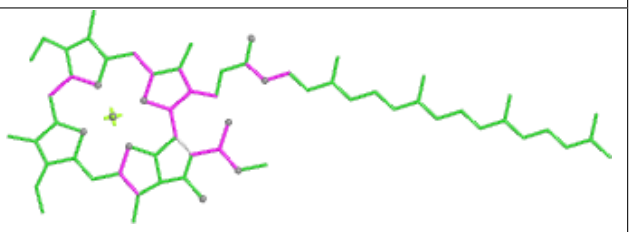
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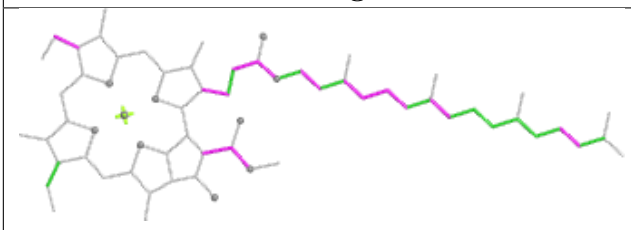
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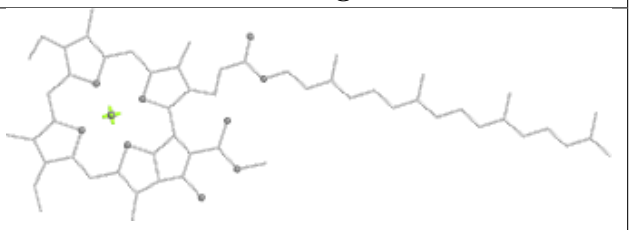
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Bond angles

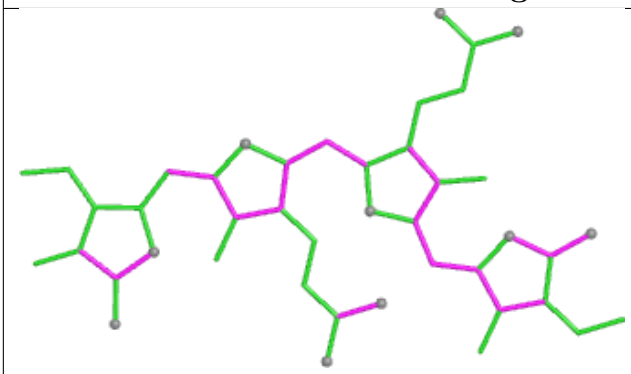


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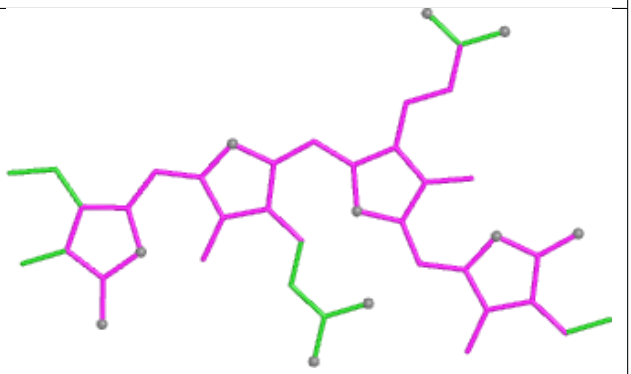


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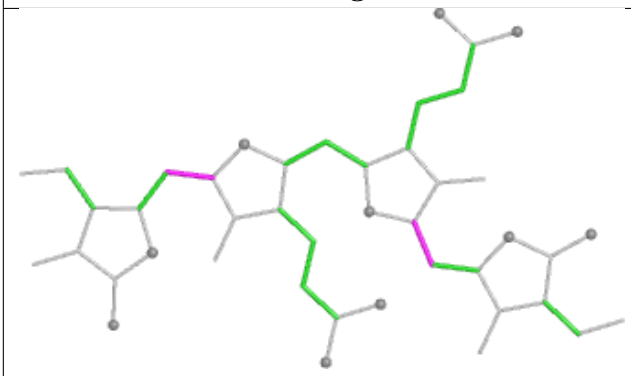
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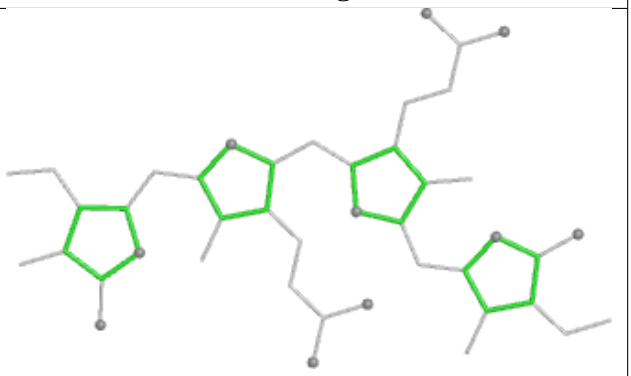
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Bond angles

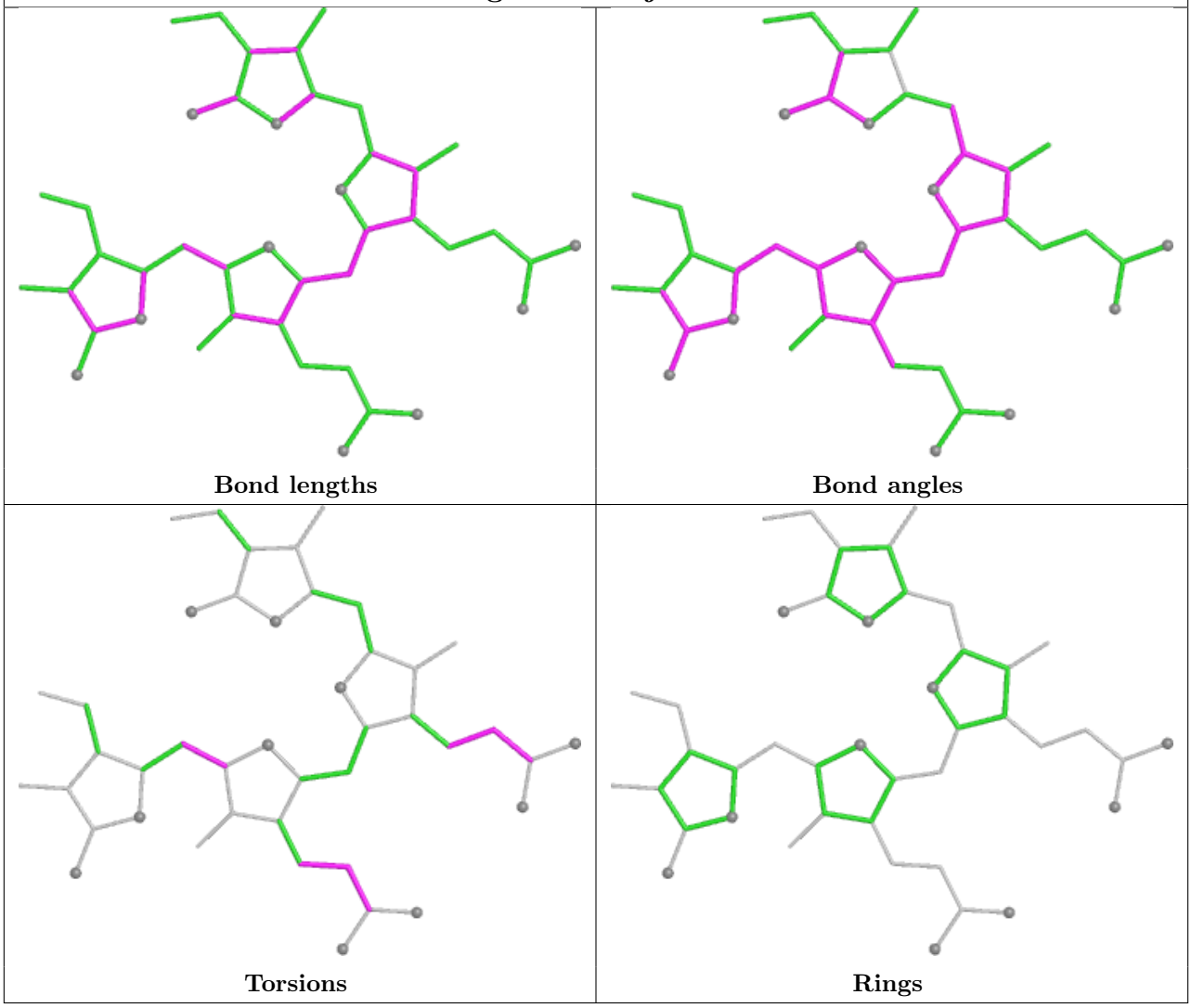


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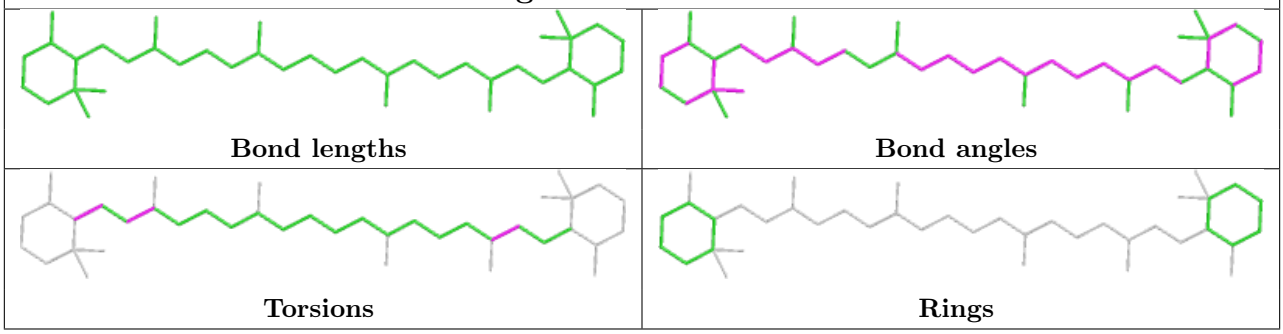


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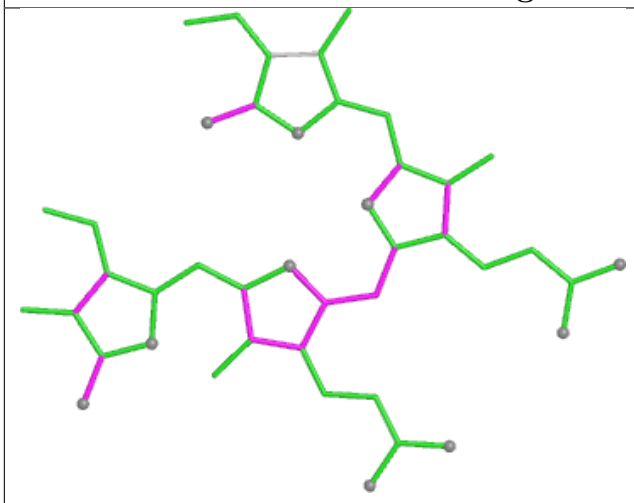
Ligand PEB j1 202



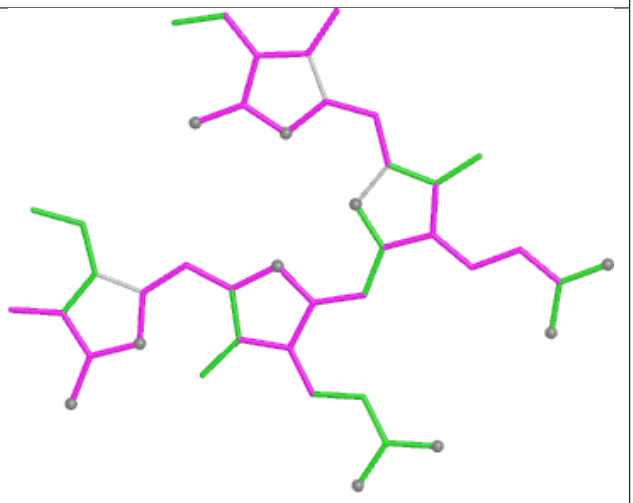
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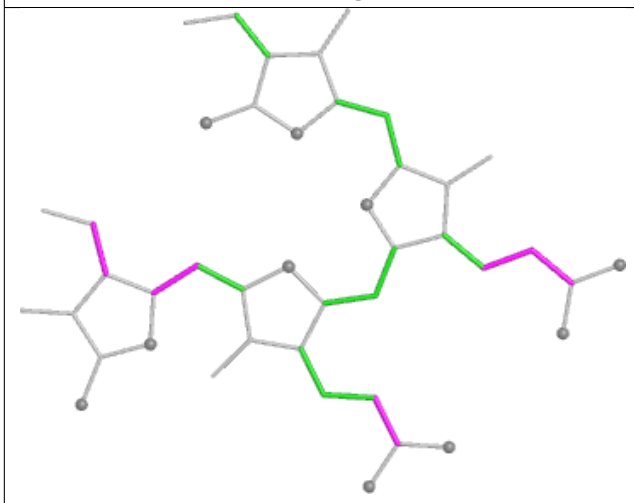
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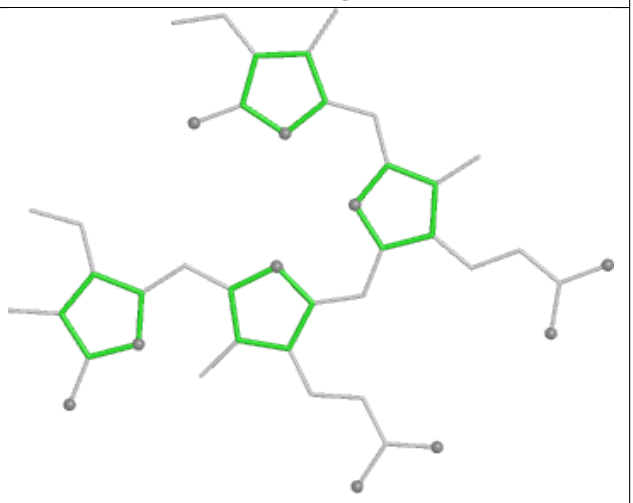
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Bond angles

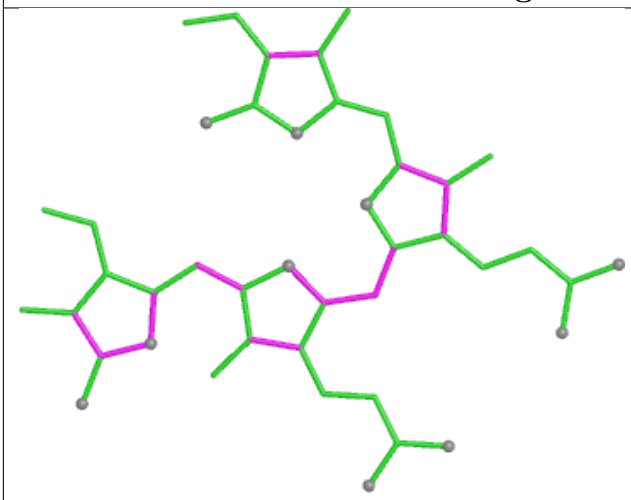


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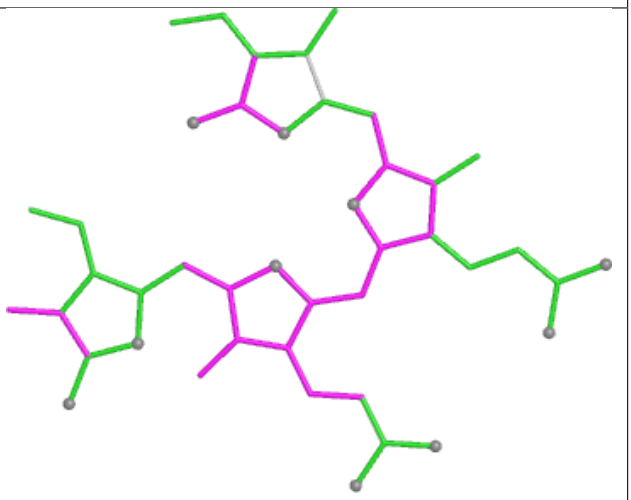


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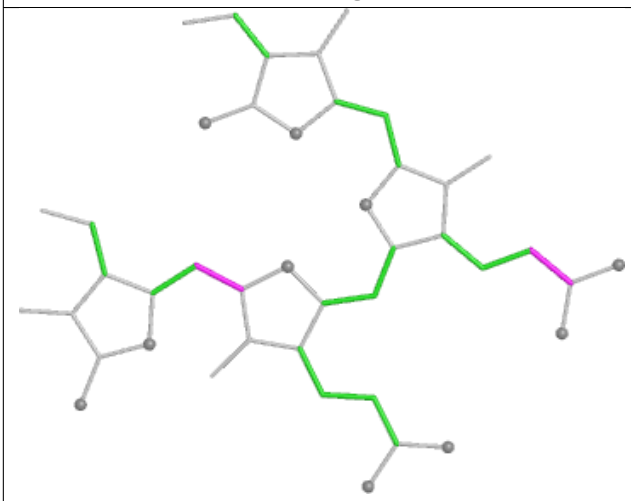
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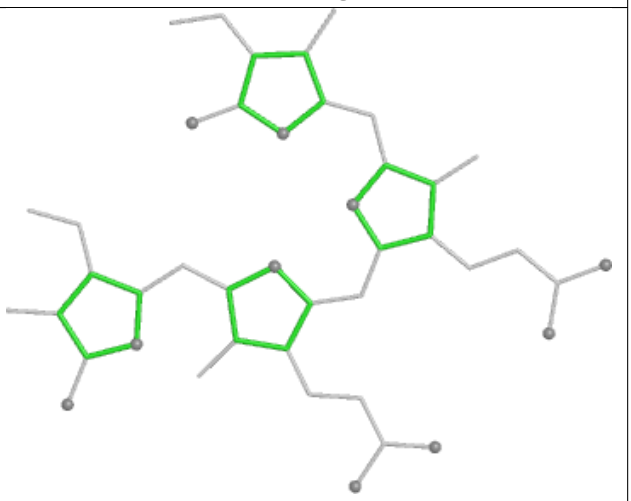
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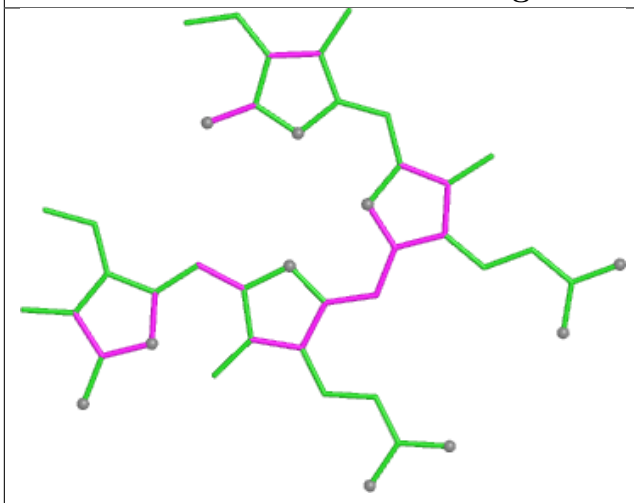


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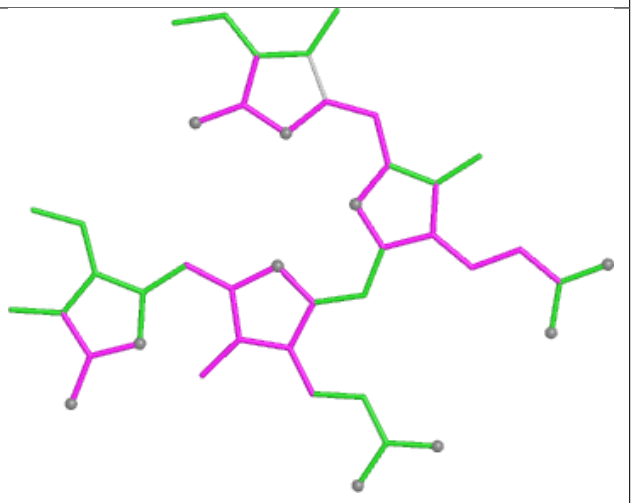


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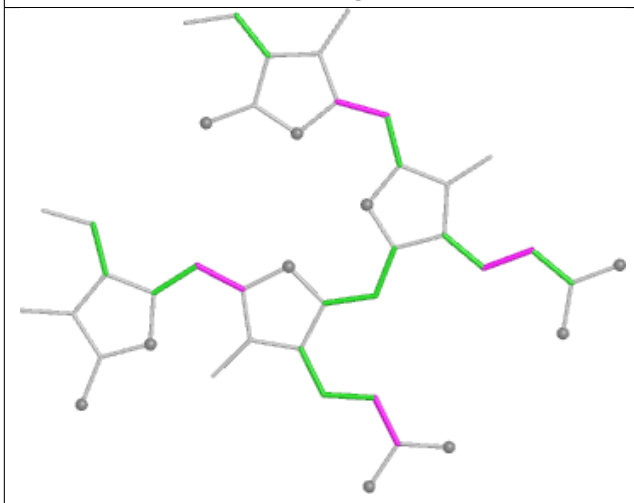
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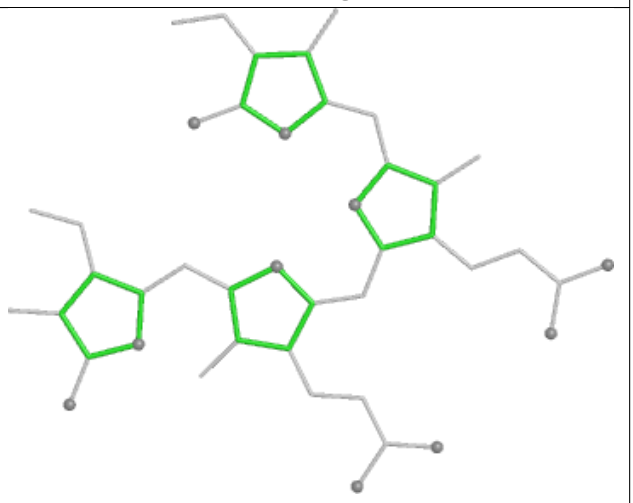
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Bond angles

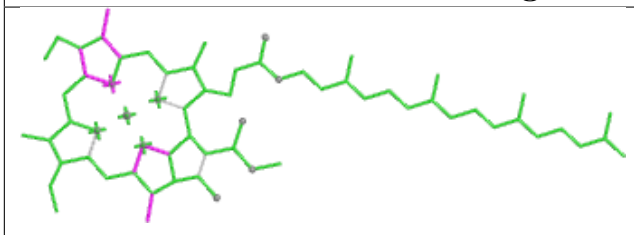


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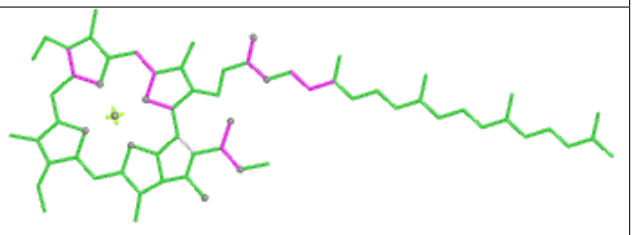


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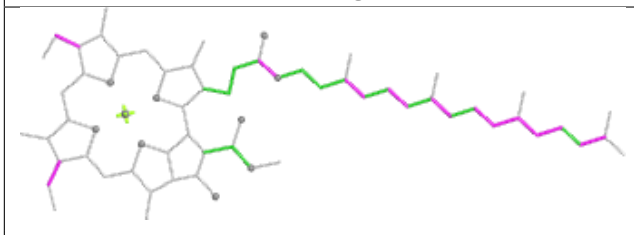
Ligand CLA c6 605



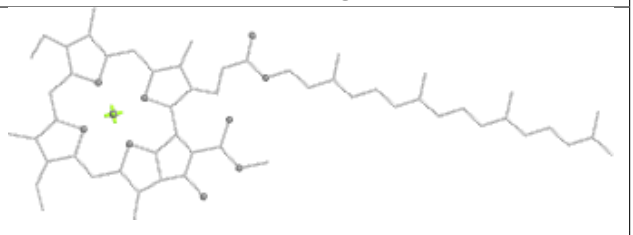
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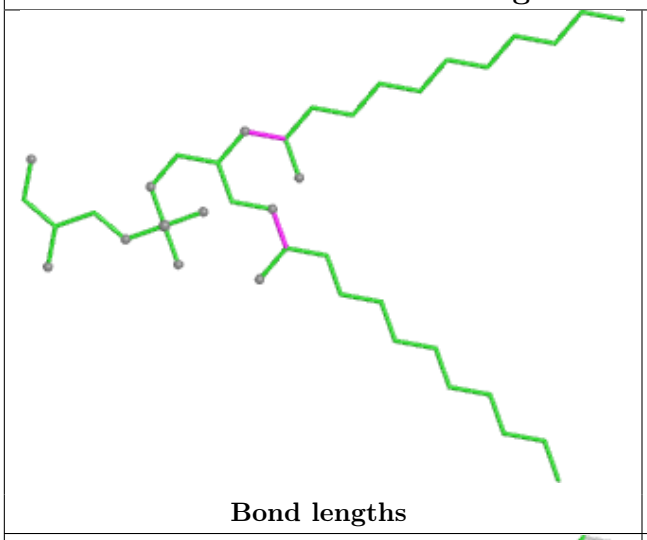


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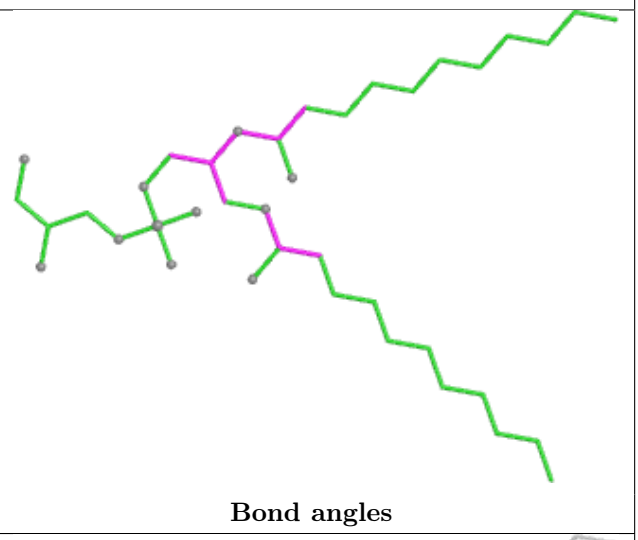


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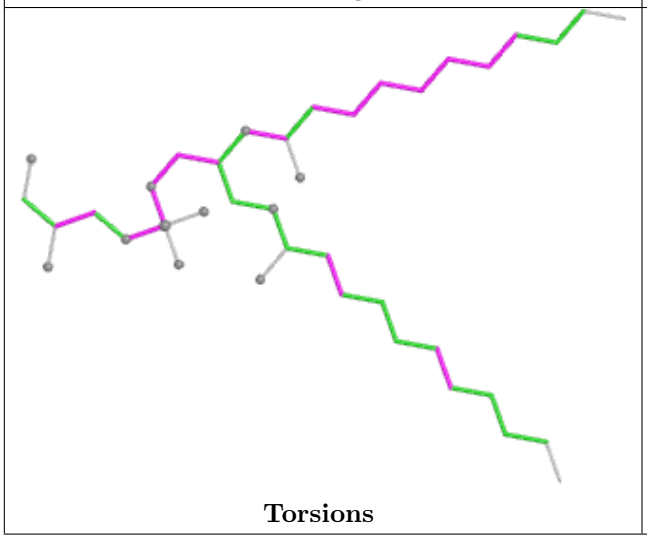
Ligand LHG m6 102



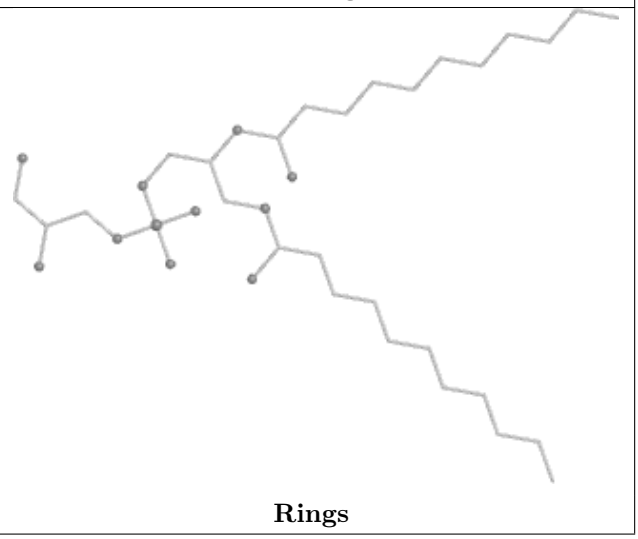
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Bond angles

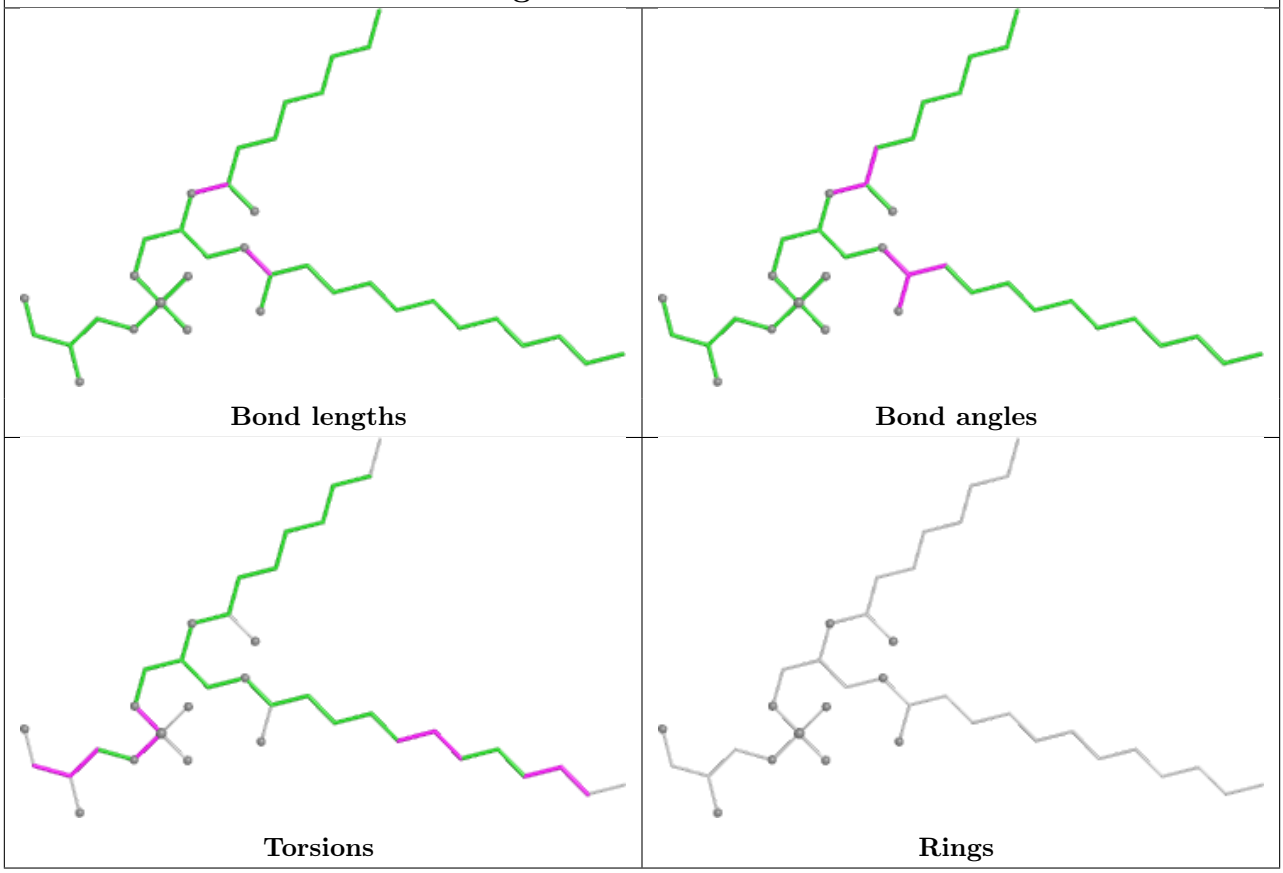


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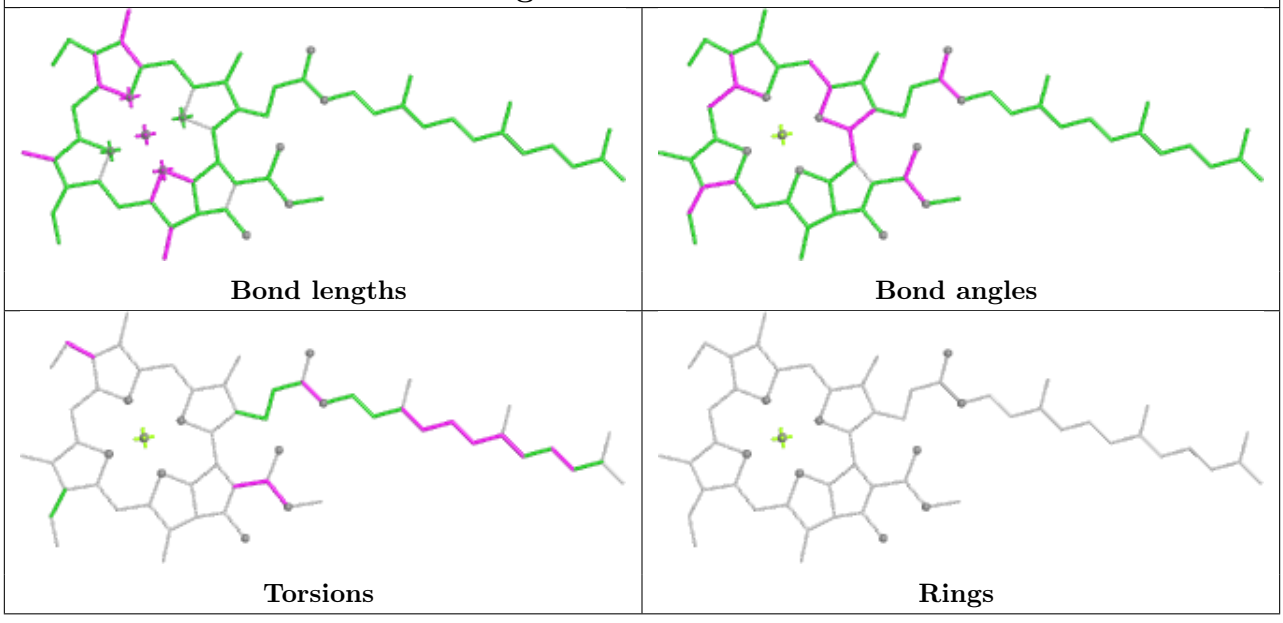


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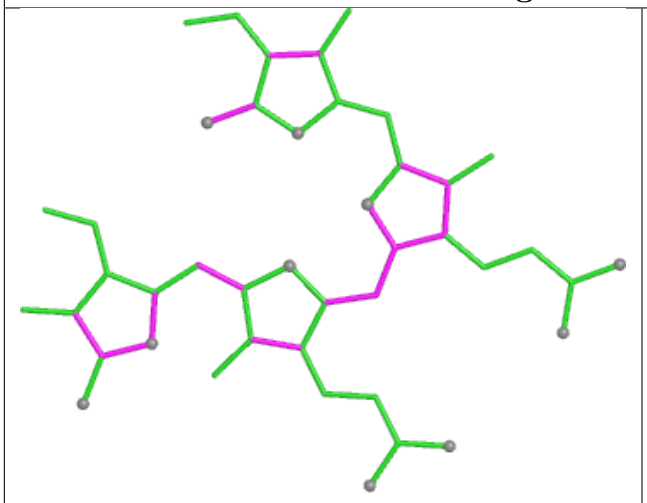
Ligand LHG CL 521



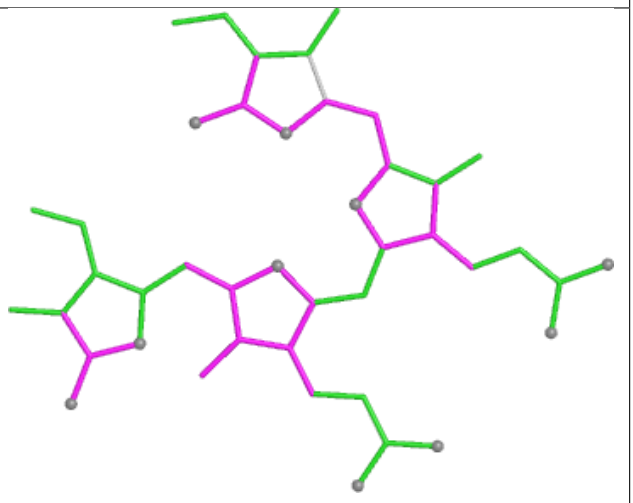
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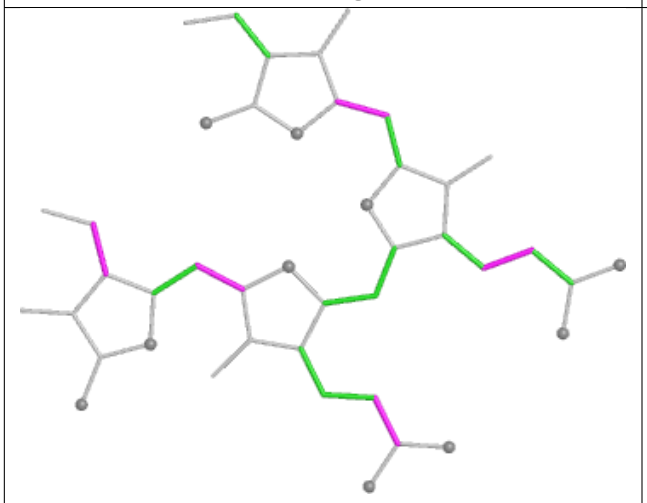
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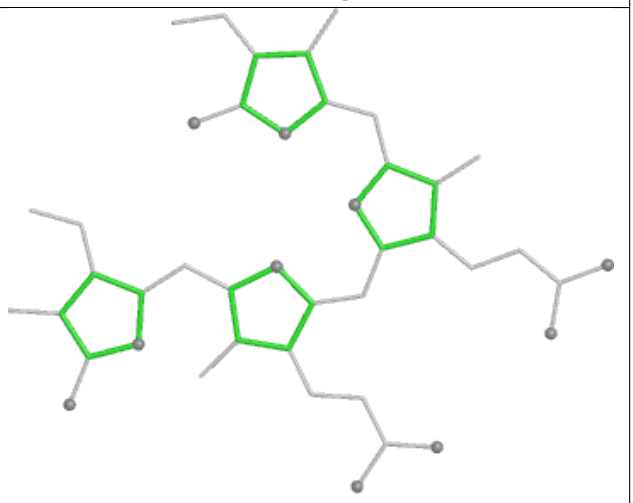
Bond lengths



Bond angles

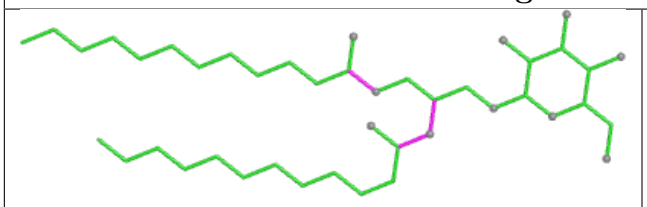


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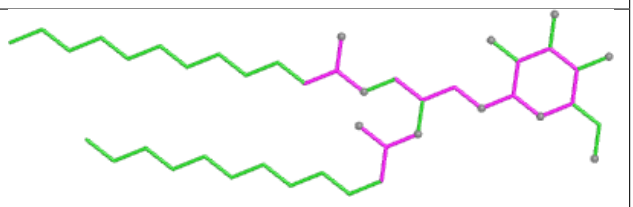


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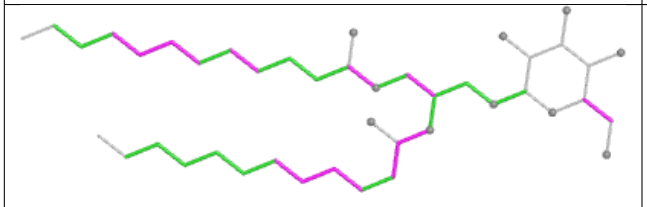
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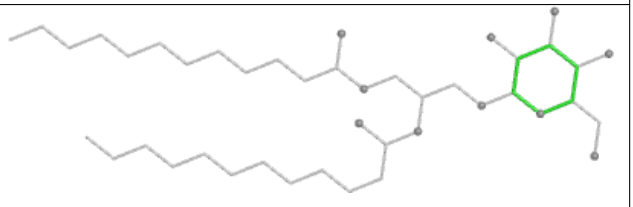
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Bond angles

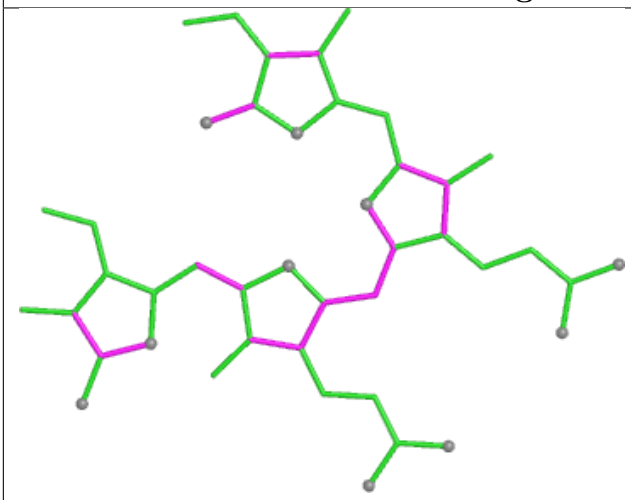


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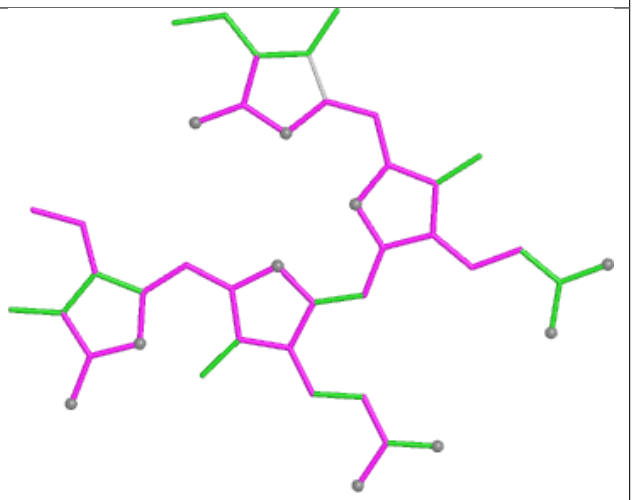


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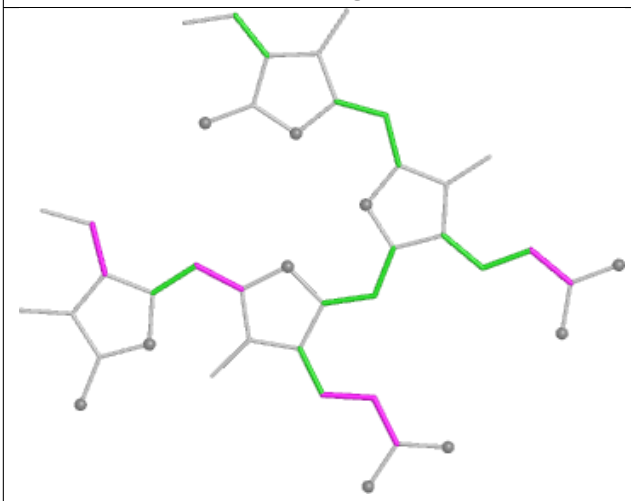
Ligand PEB LF 201



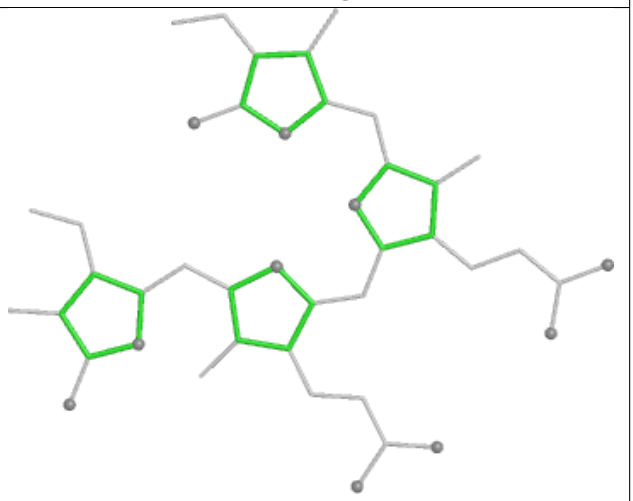
Bond lengths



Bond angles



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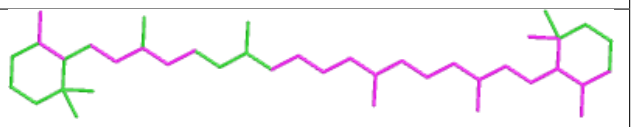


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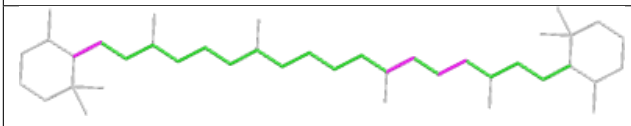
Ligand BCR cL 504



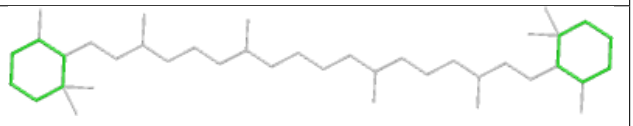
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Bond angles

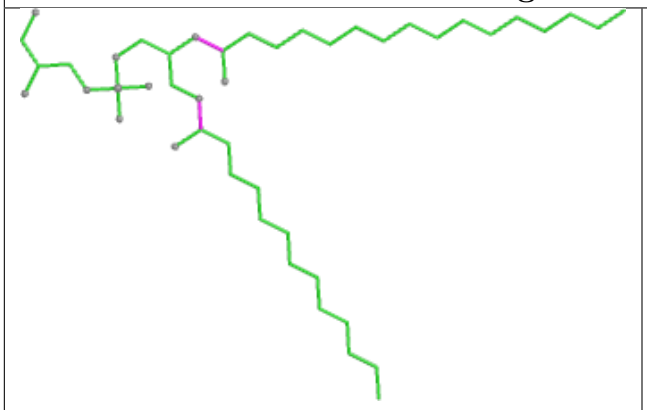


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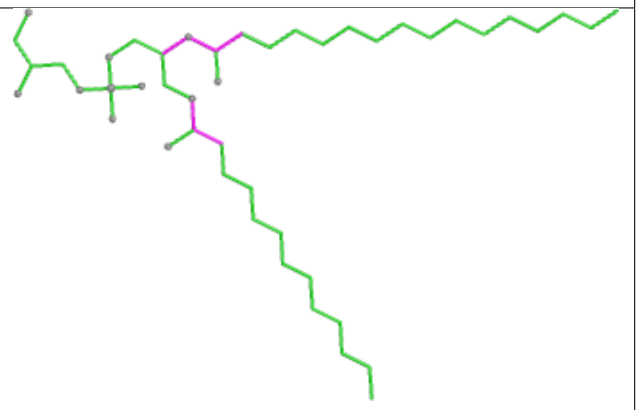


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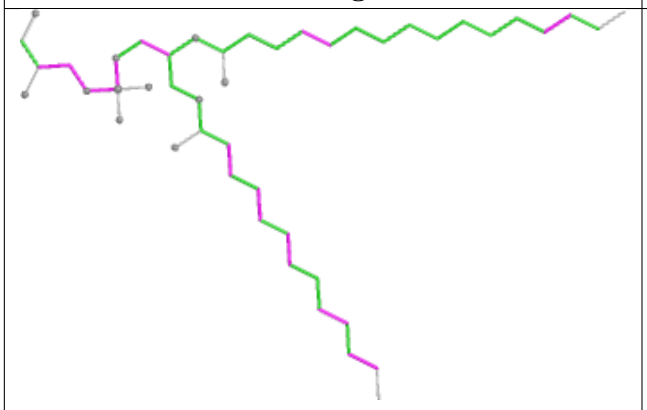
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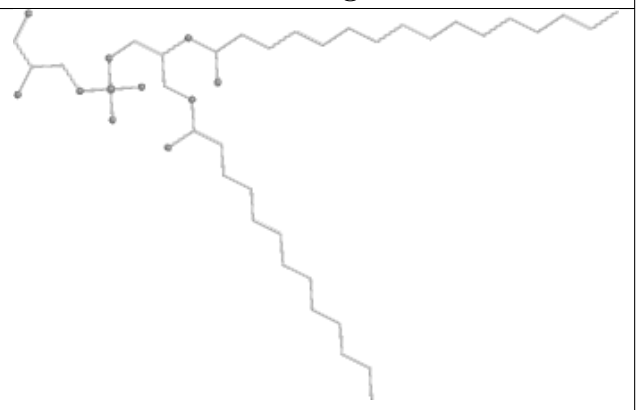
Bond lengths



Bond angles

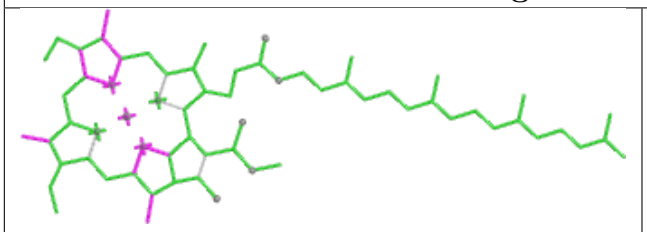


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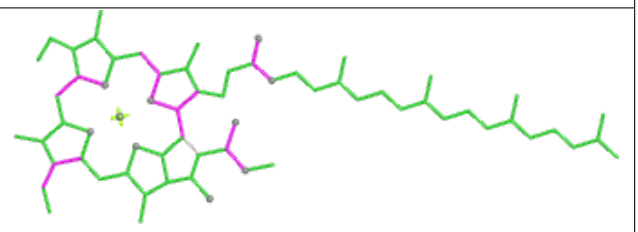


Rings

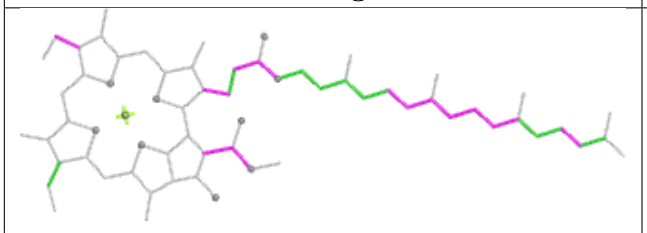
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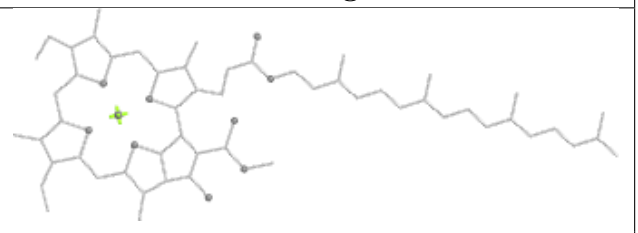
Bond lengths



Bond angles

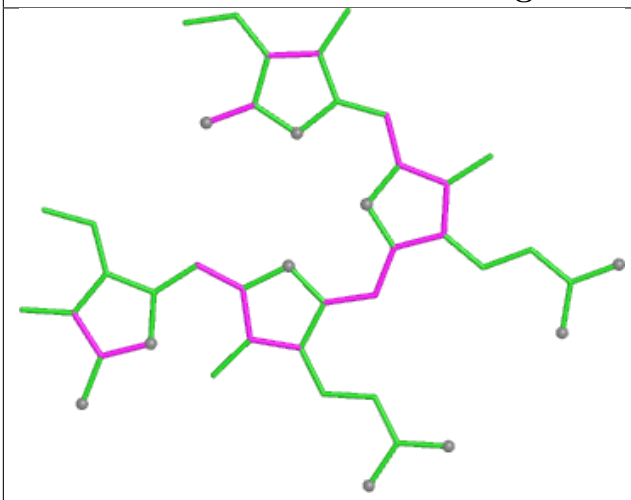


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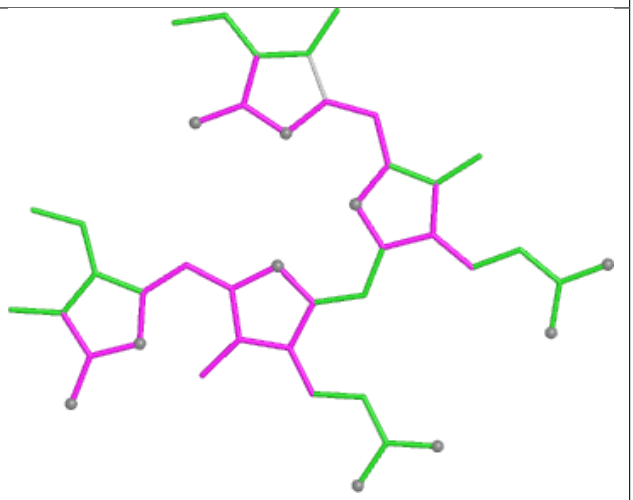


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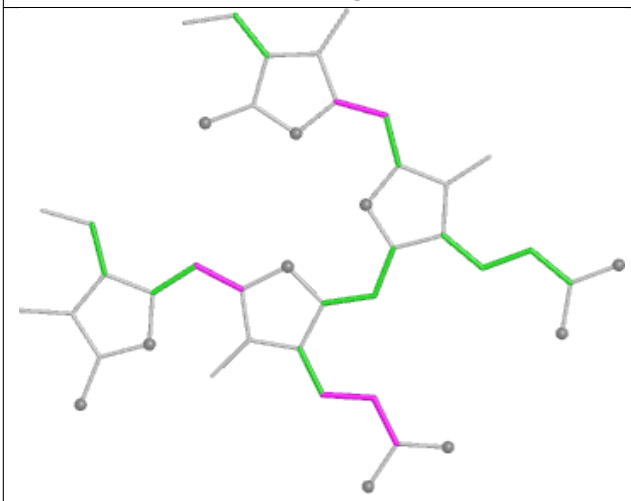
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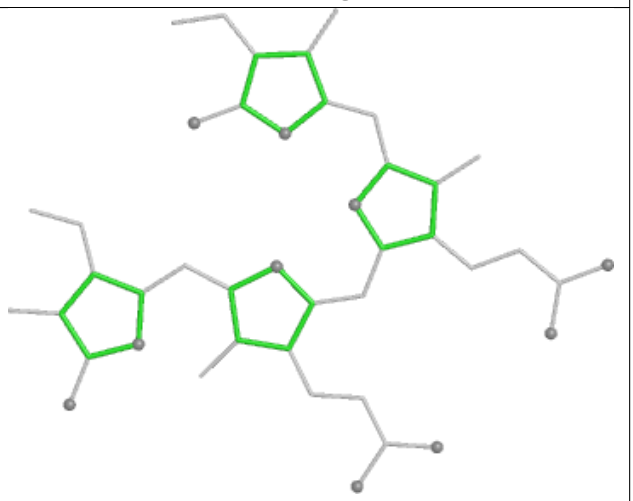
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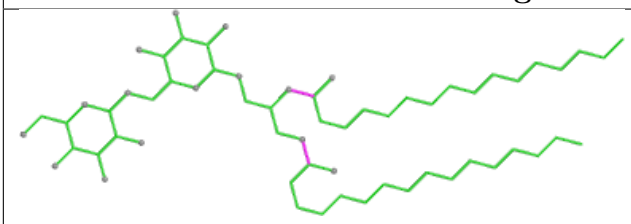


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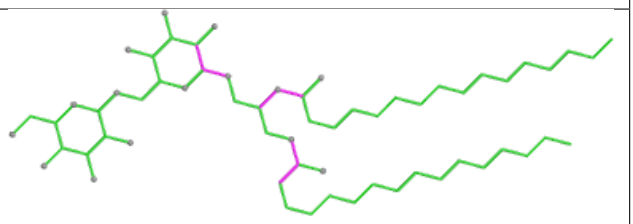


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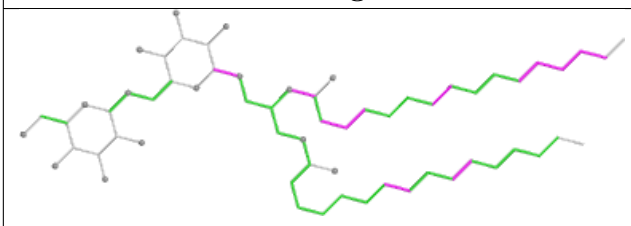
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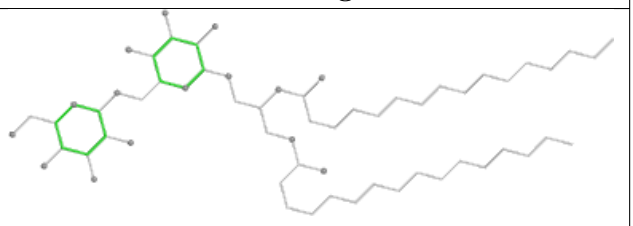
Bond lengths



Bond angles

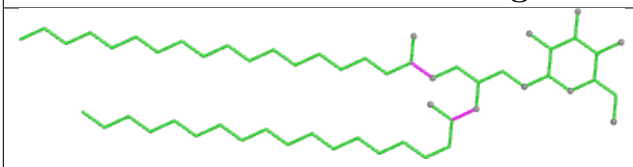


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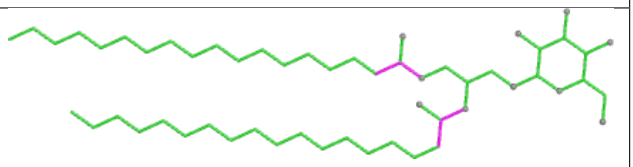


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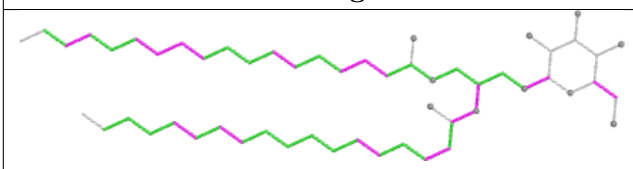
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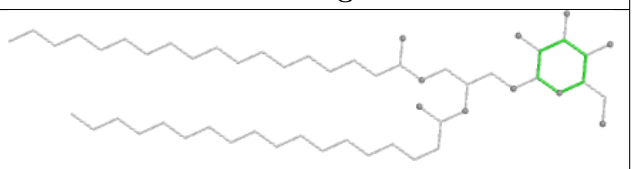
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Bond angles

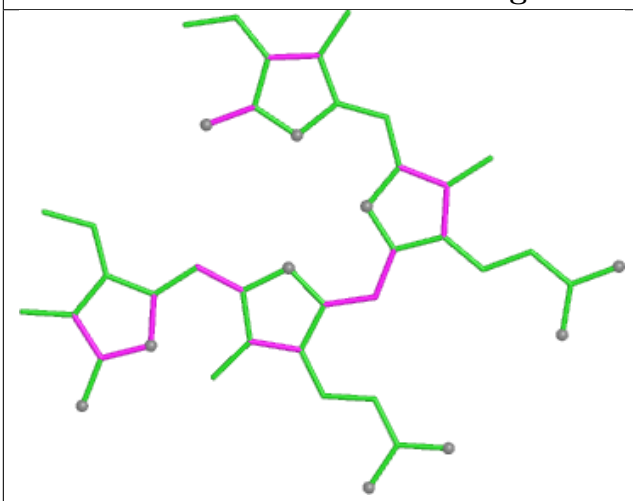


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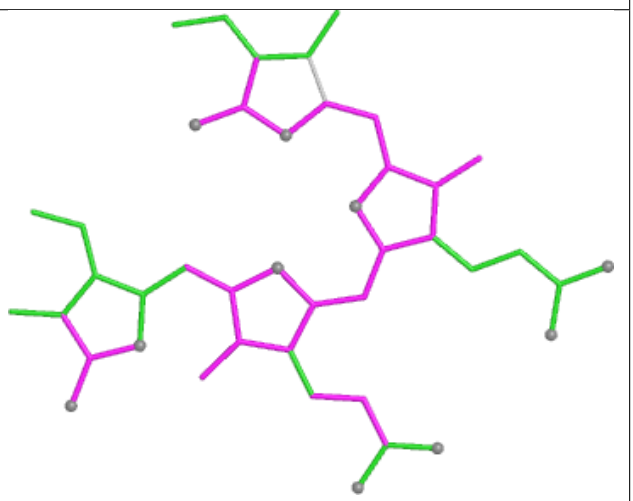


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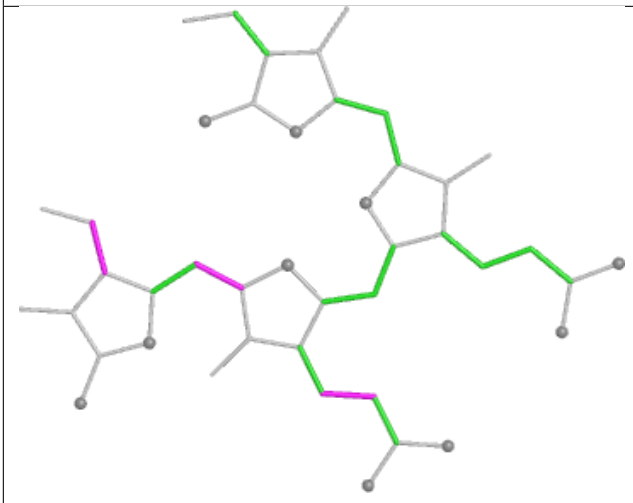
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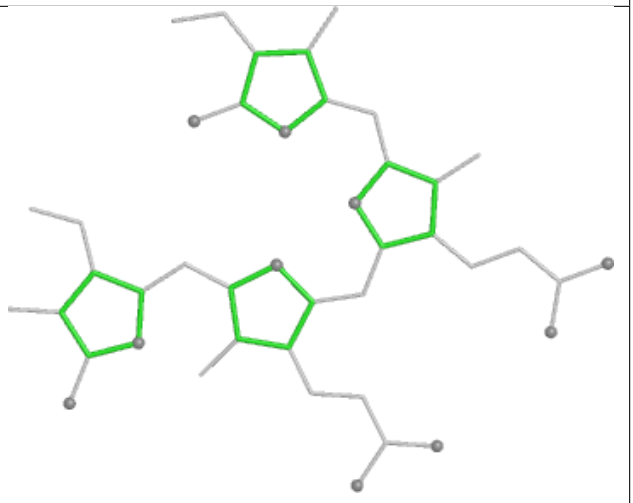
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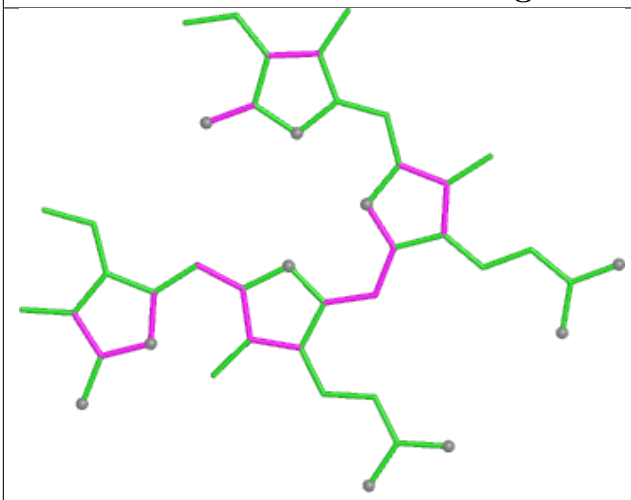


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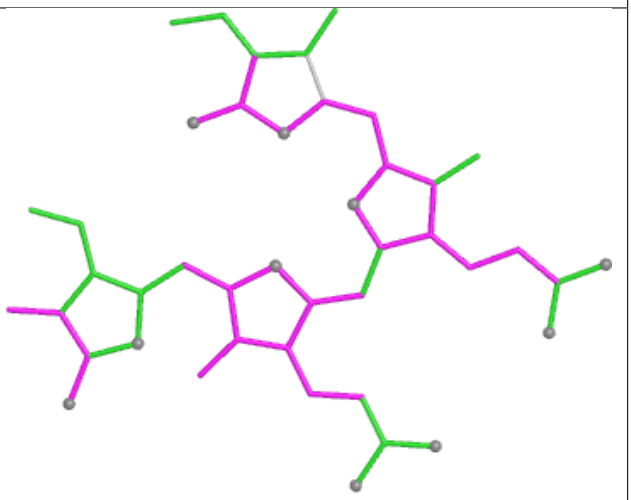


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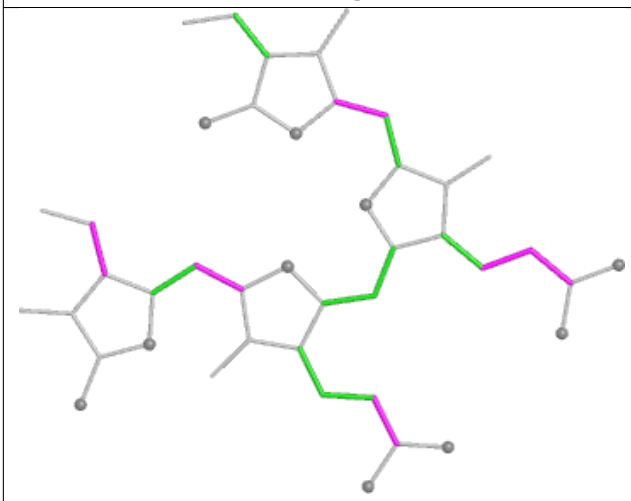
Ligand PEB K5 201



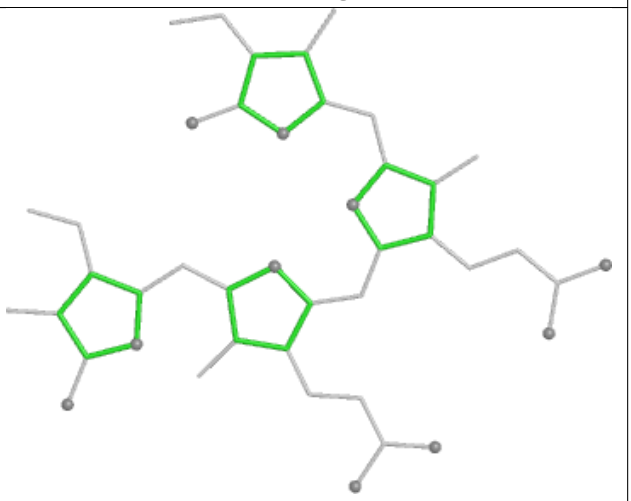
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Bond angles

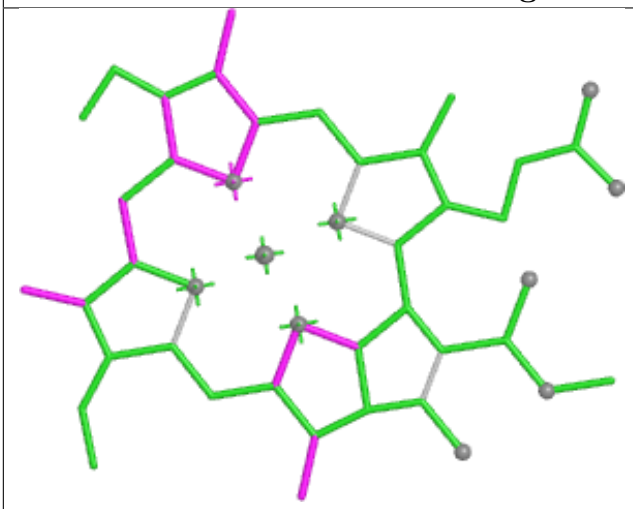


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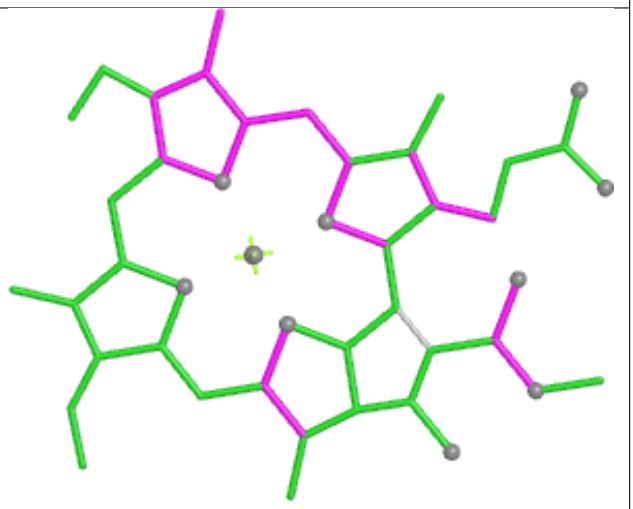


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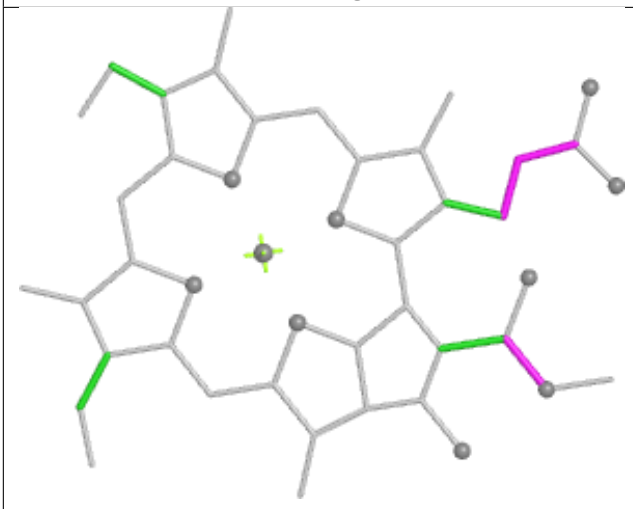
Ligand CLA 42 603



Bond lengths



Bond angles

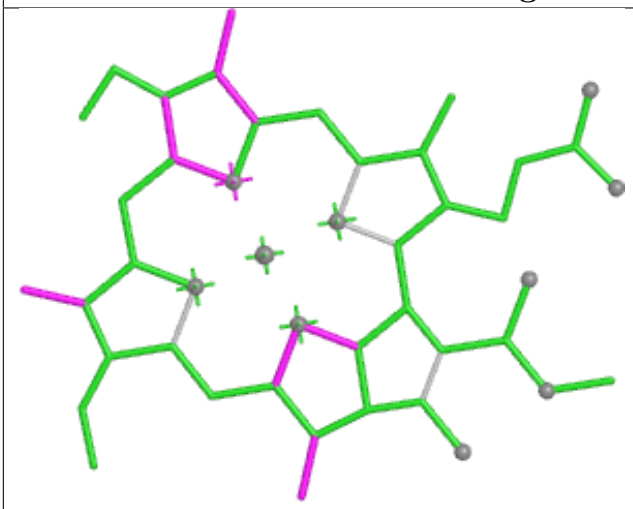


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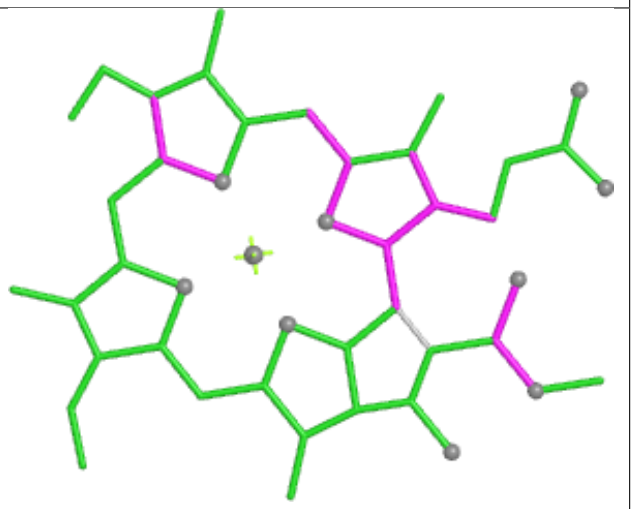


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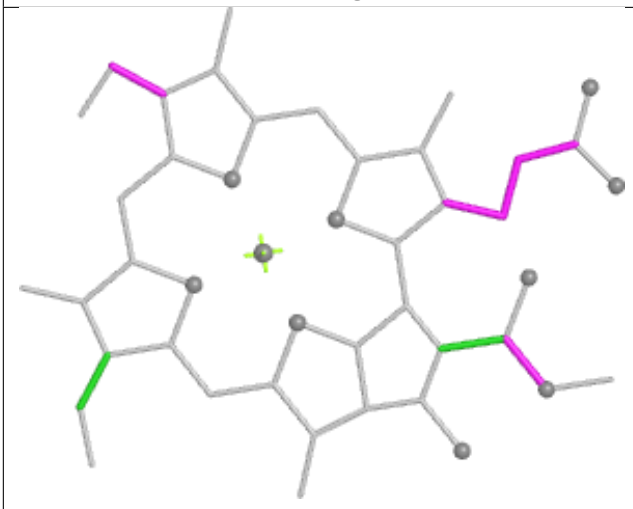
Ligand CLA 12 611



Bond lengths



Bond angles

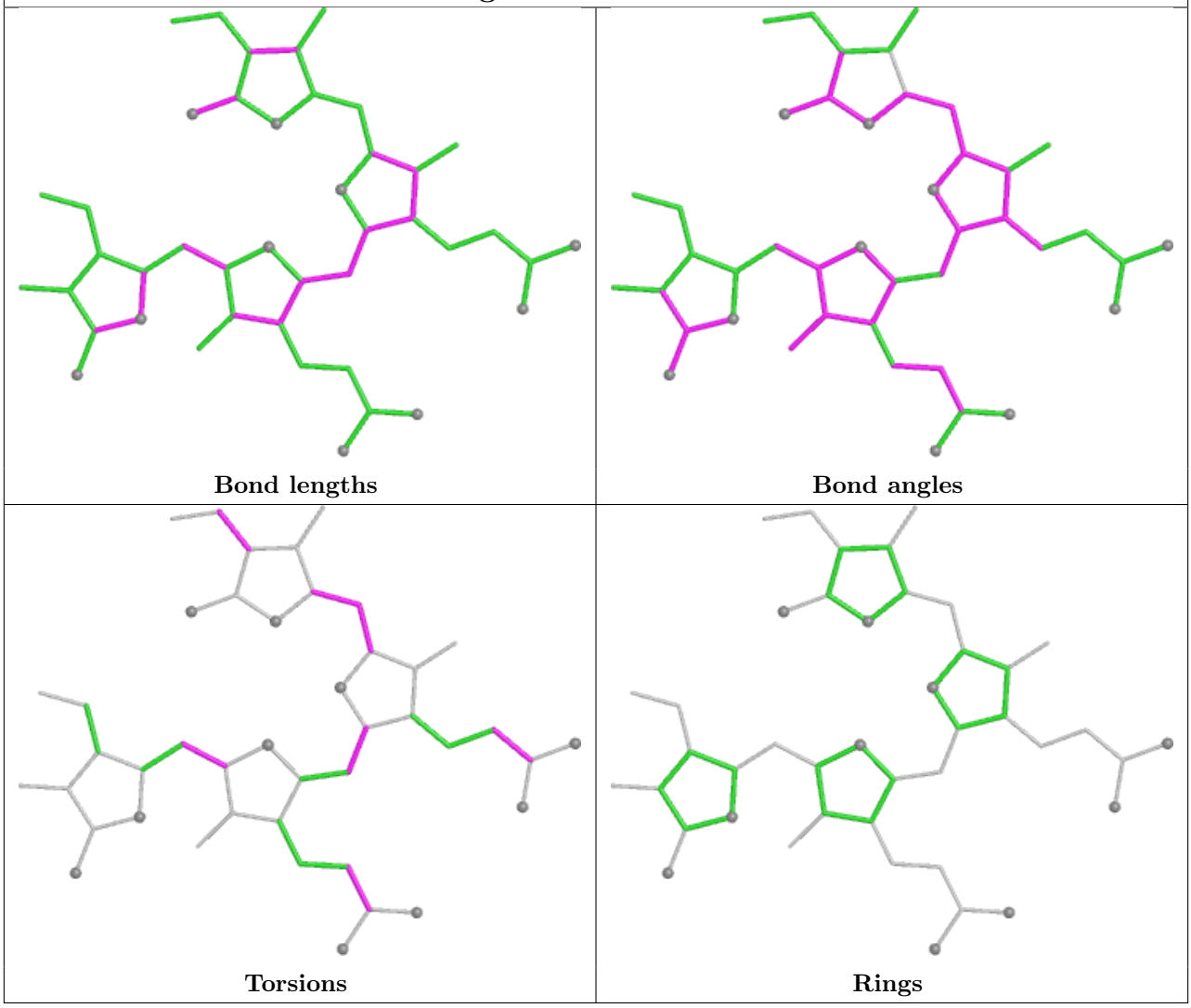


Torsions



Rings

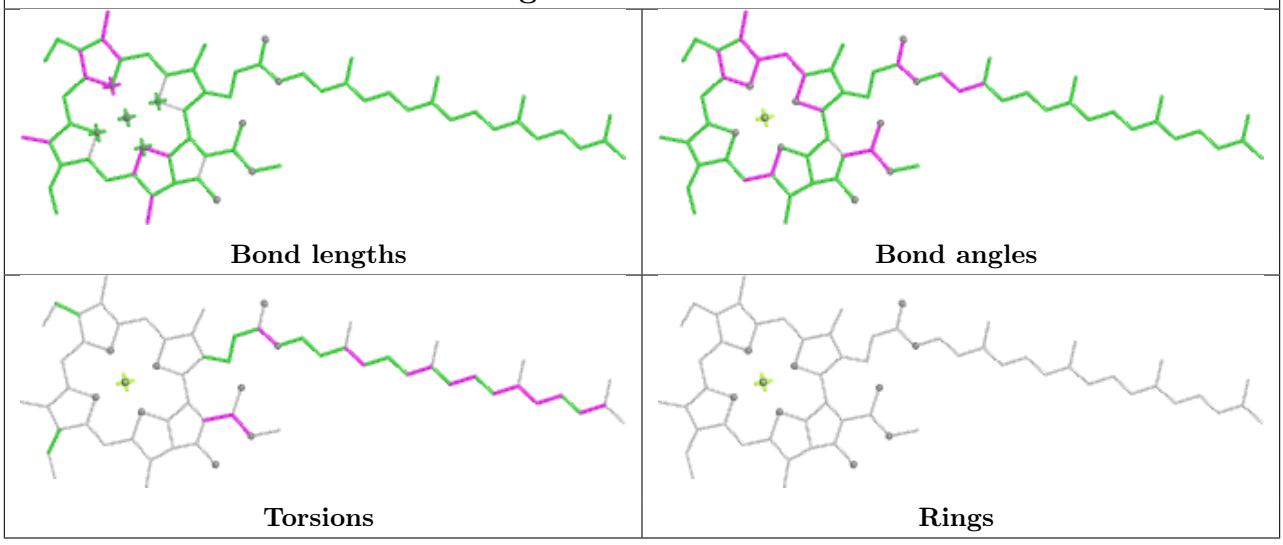
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Bond lengths | Bond angles

Torsions | Rings

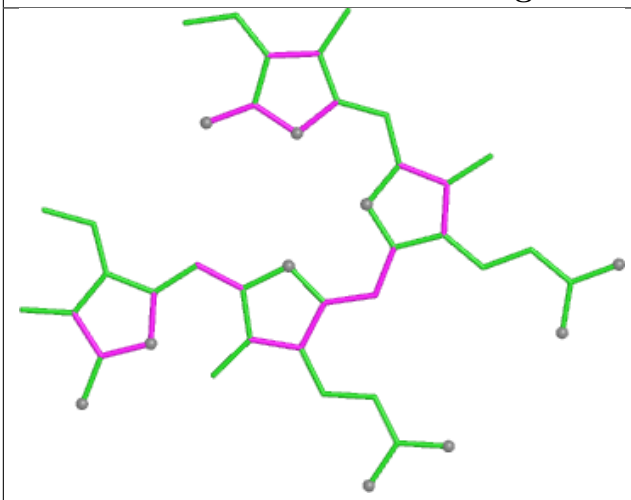
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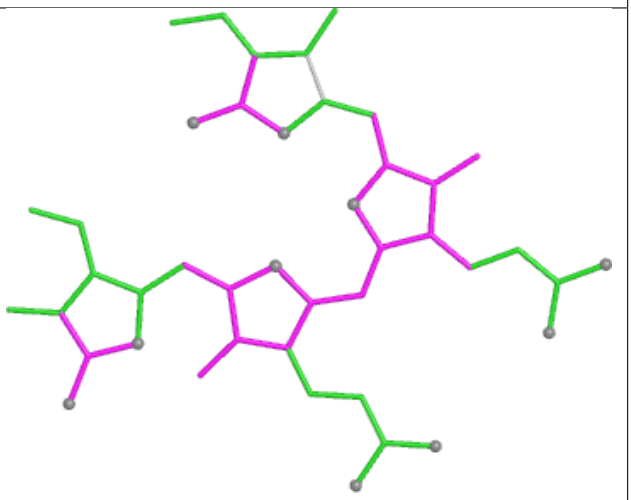
Bond lengths | Bond angles

Torsions | Rings

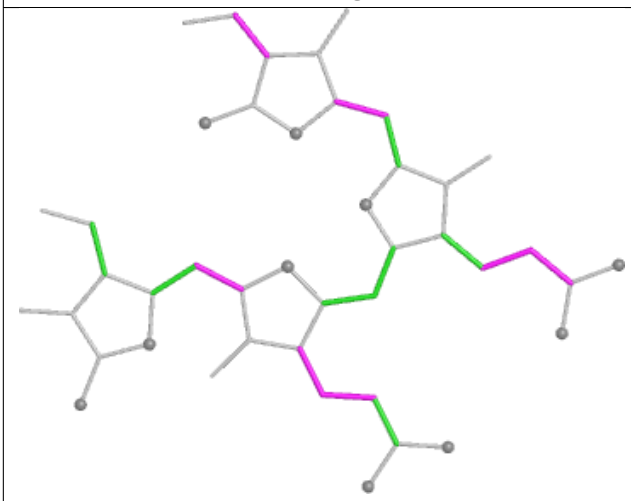
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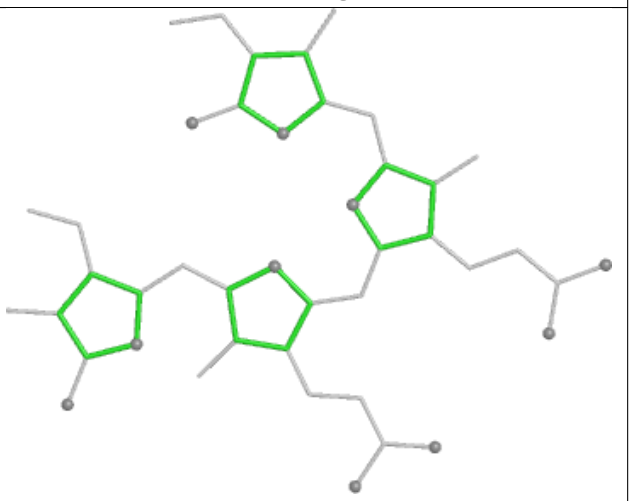
Bond lengths



Bond angles

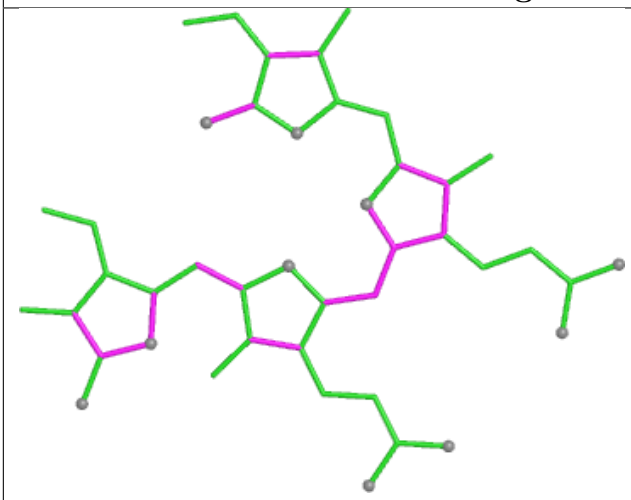


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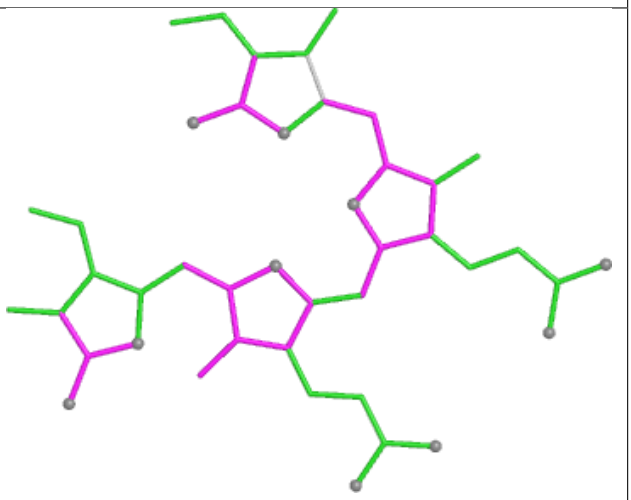


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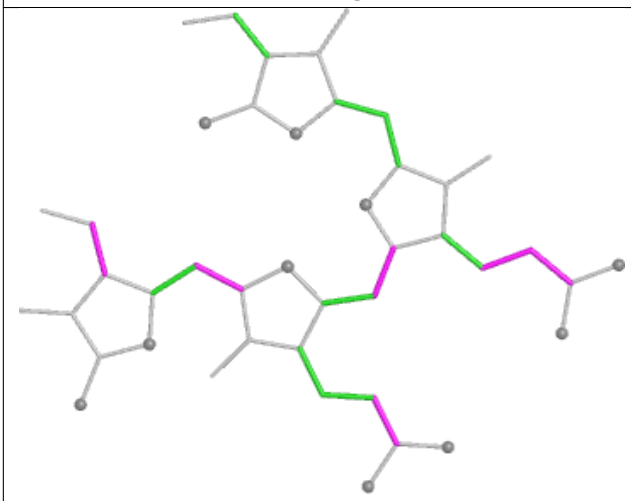
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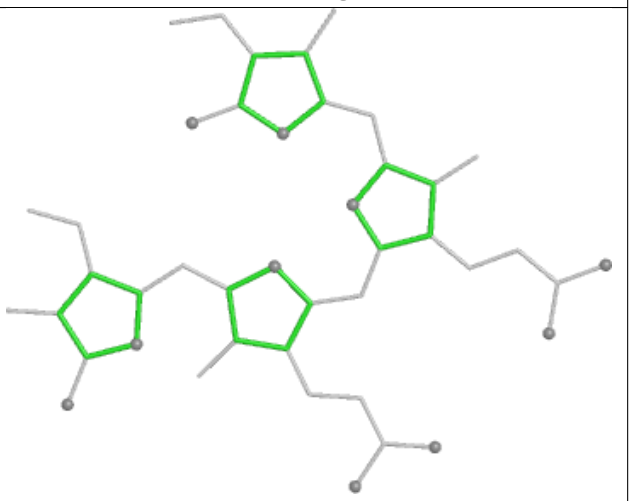
Bond lengths



Bond angles

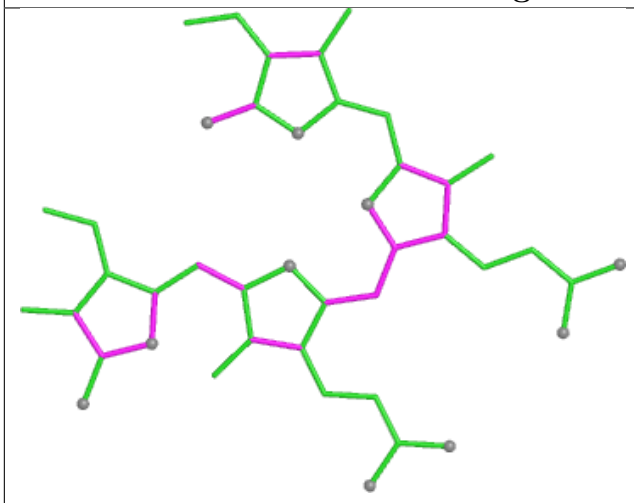


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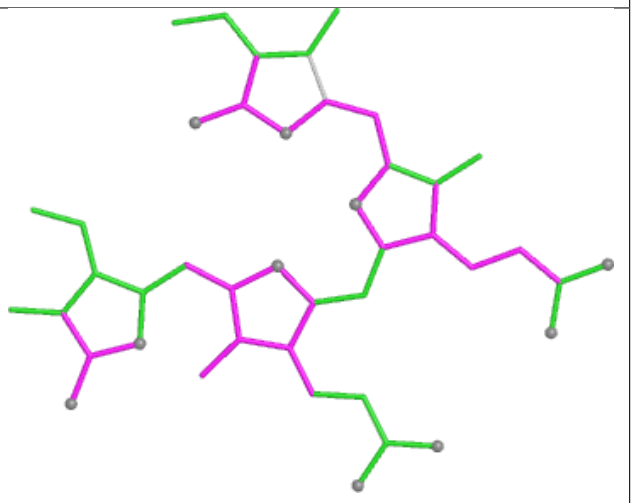


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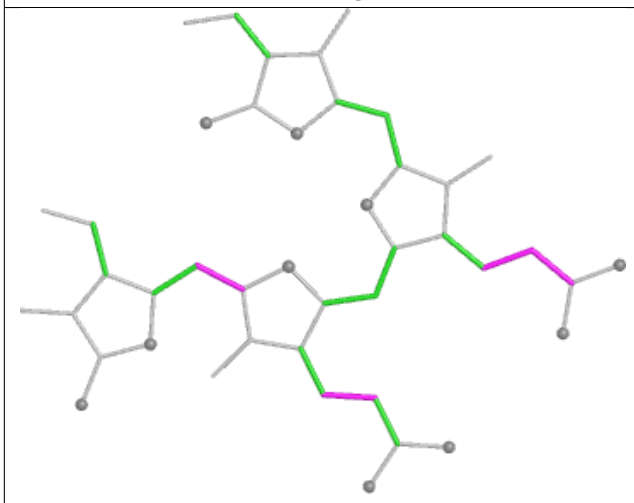
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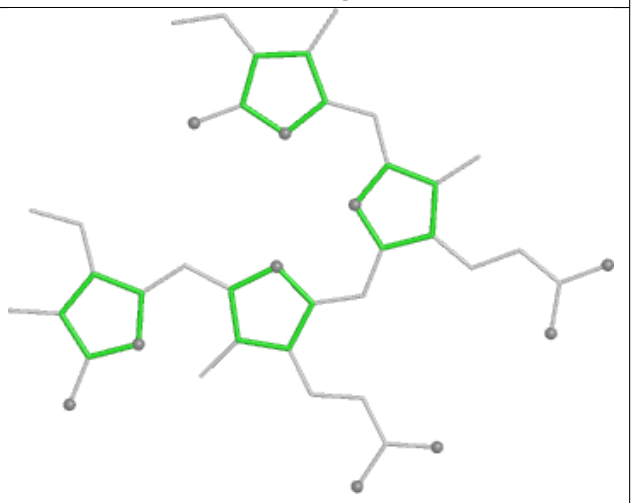
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Bond angles

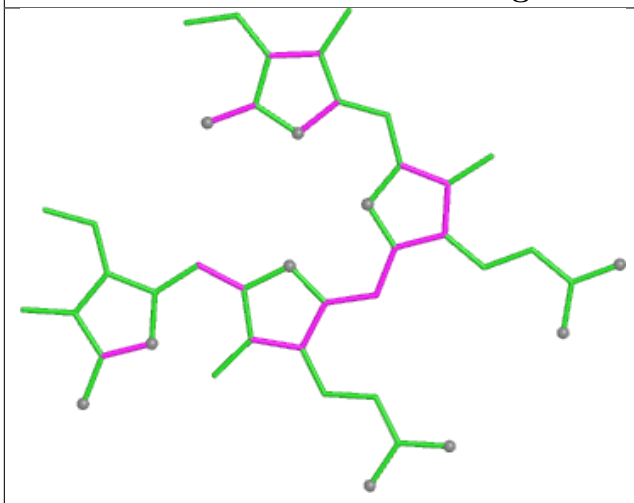


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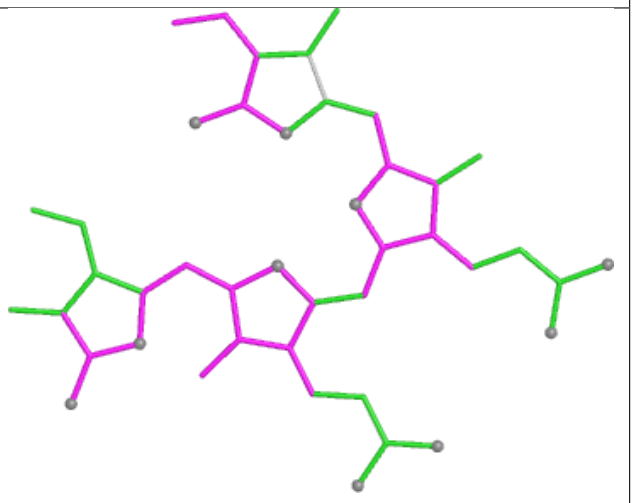


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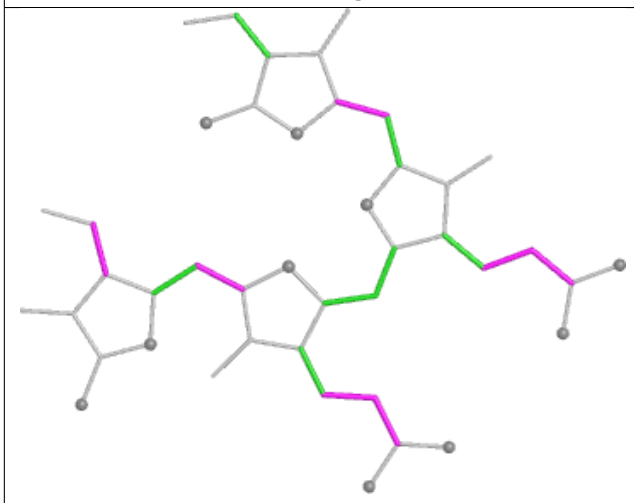
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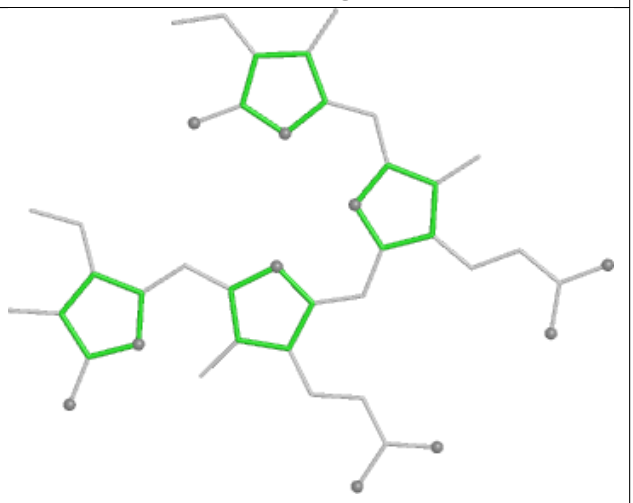
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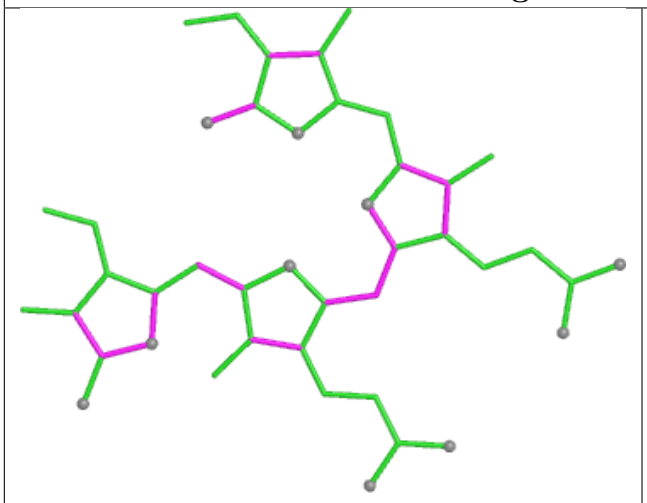


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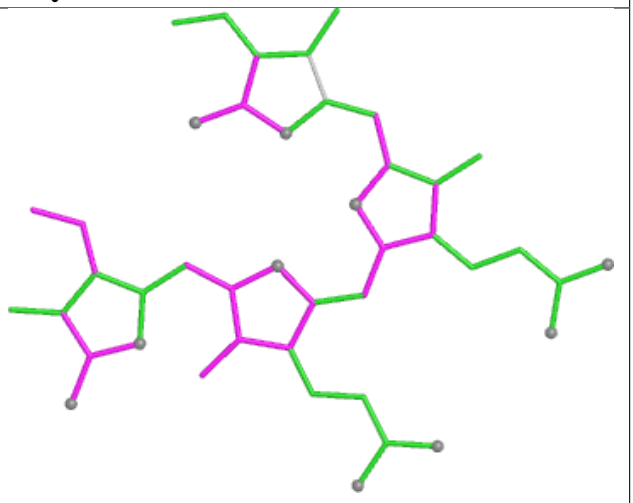


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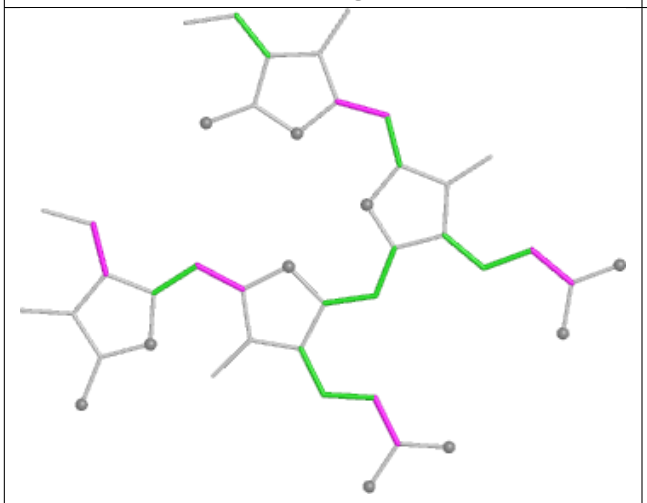
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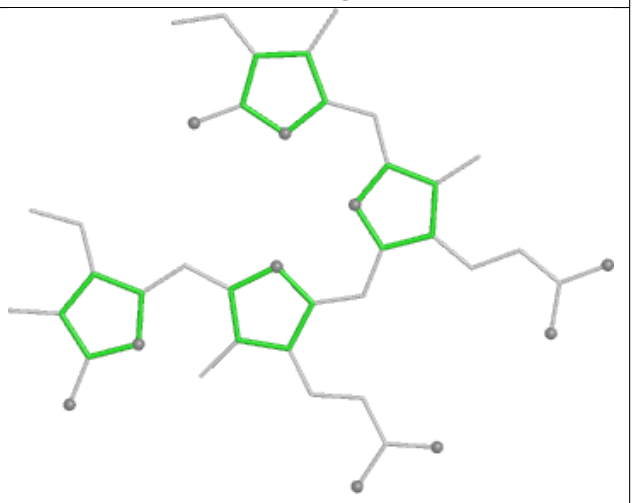
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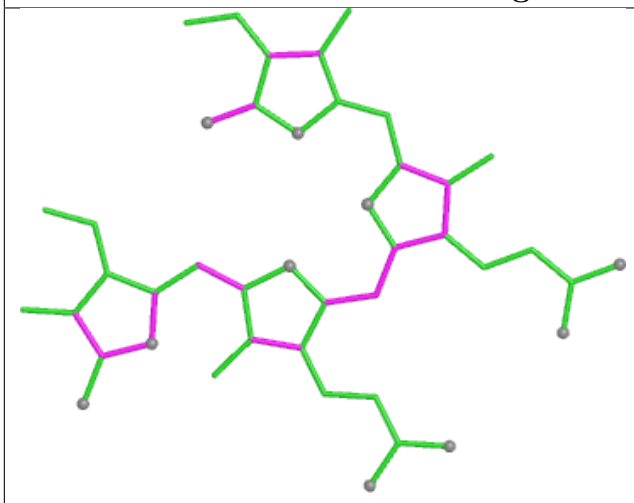


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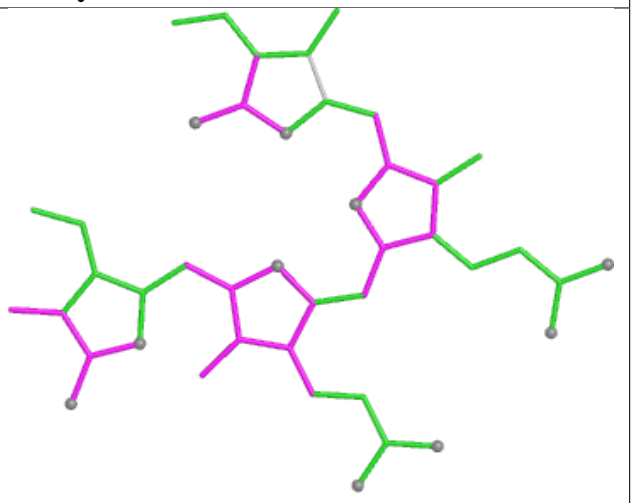


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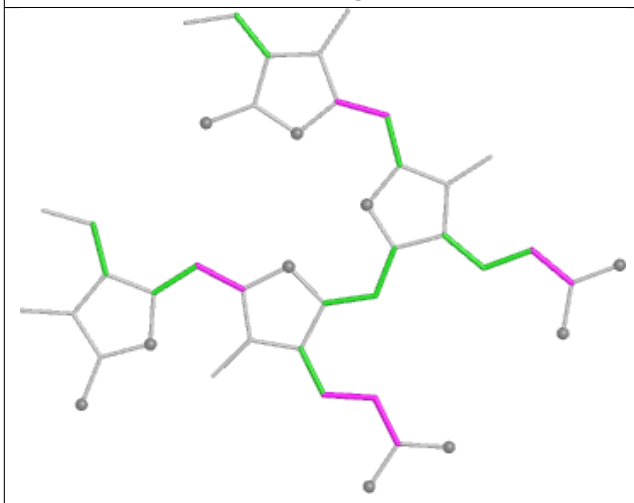
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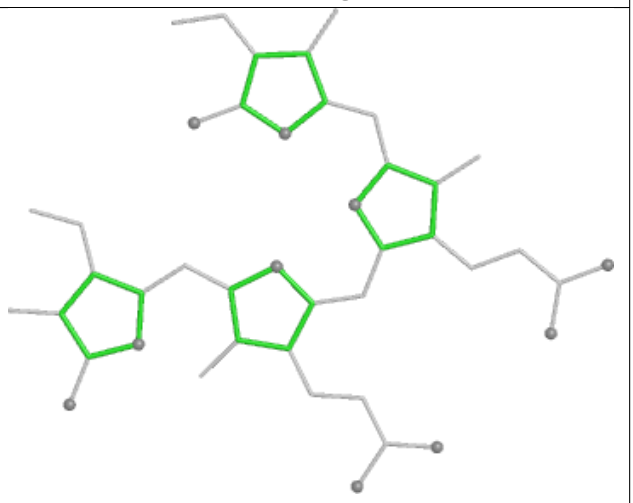
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Bond angles

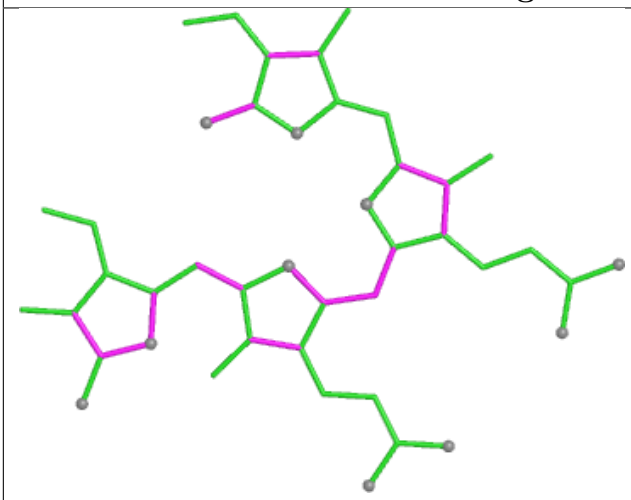


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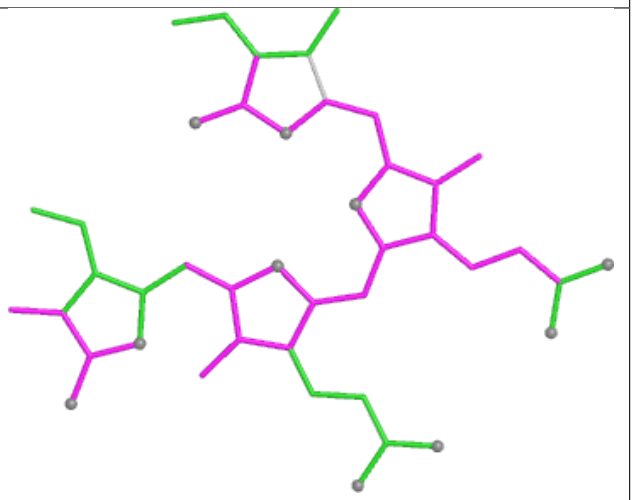


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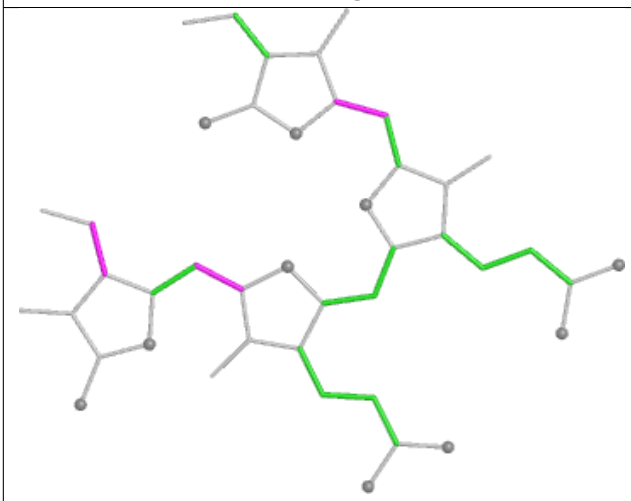
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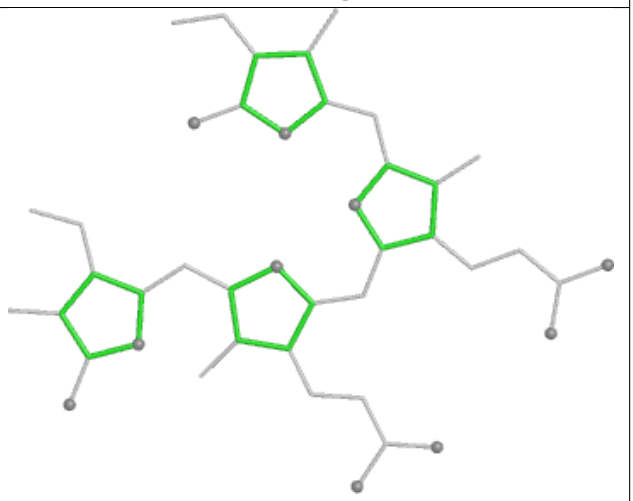
Bond lengths



Bond angles

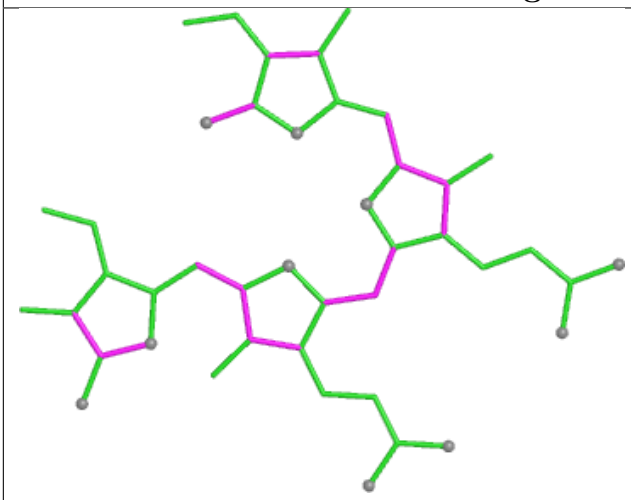


Torsions

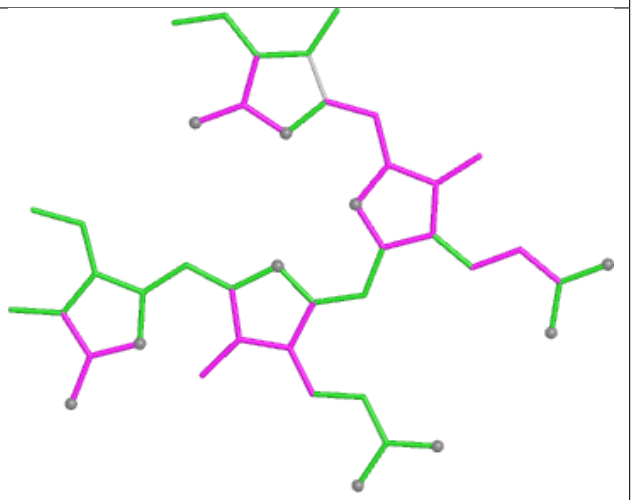


Rings

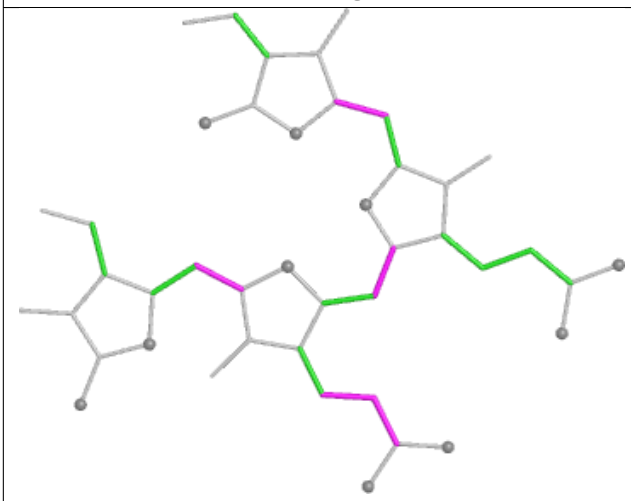
Ligand PEB i1 202



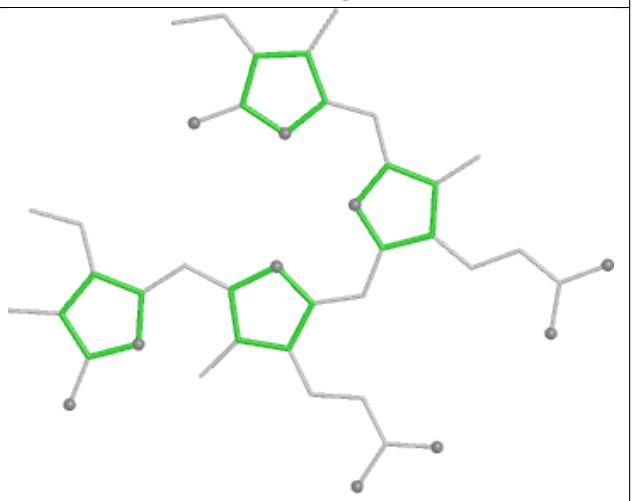
Bond lengths



Bond angles

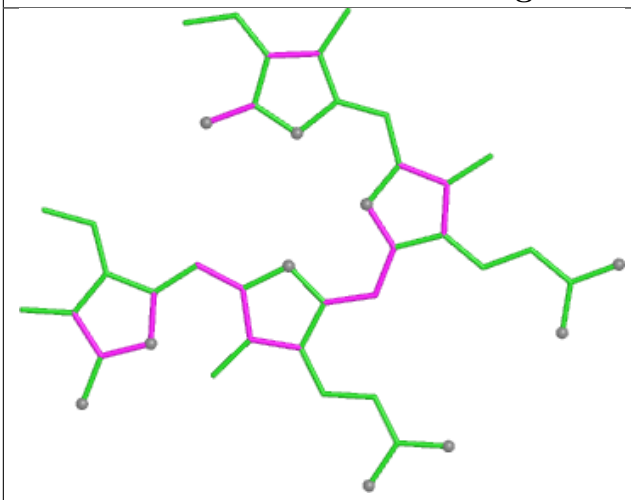


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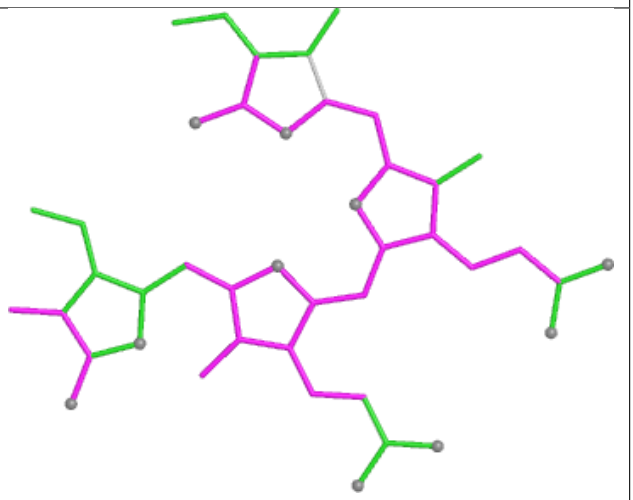


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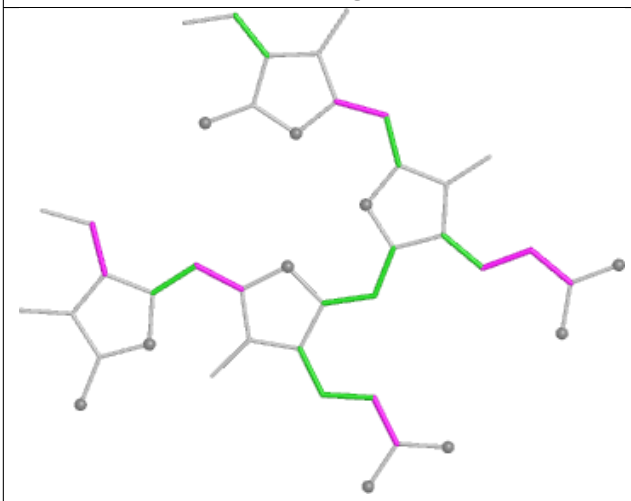
Ligand PEB V5 201



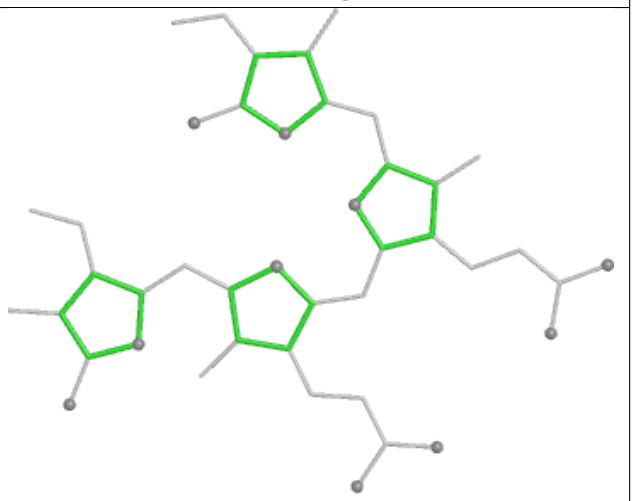
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Bond angles

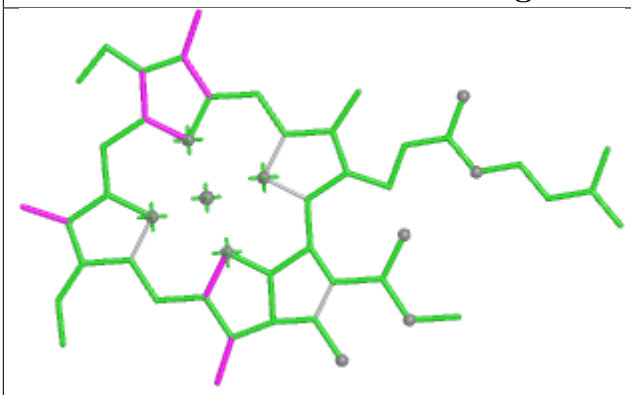


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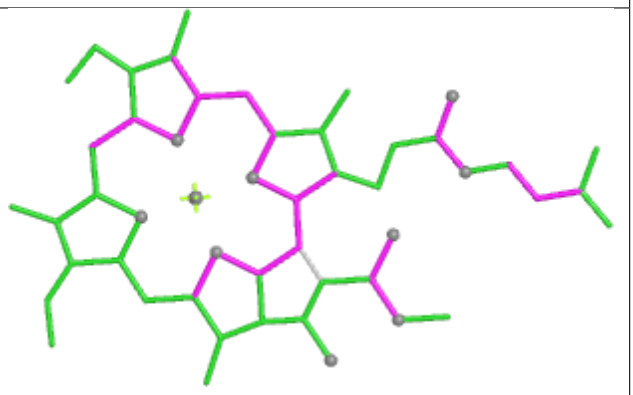


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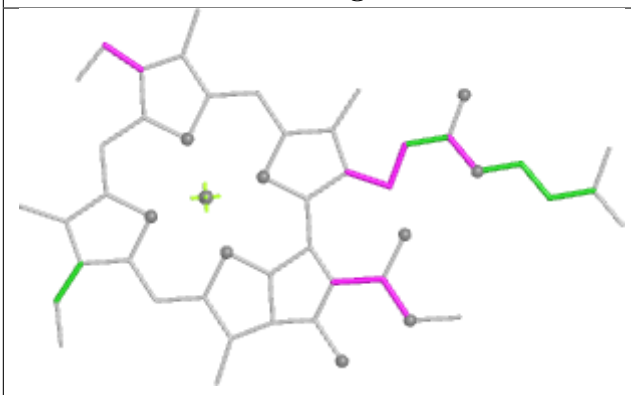
Ligand CLA O2 202



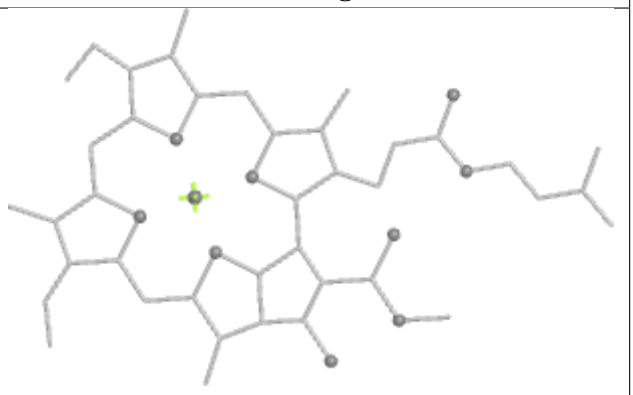
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Bond angles

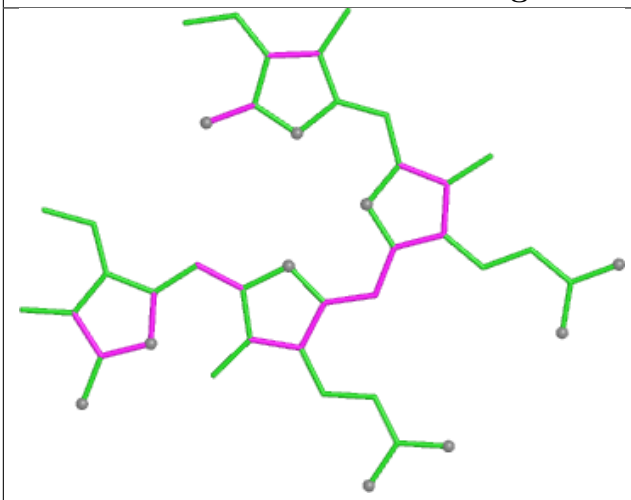


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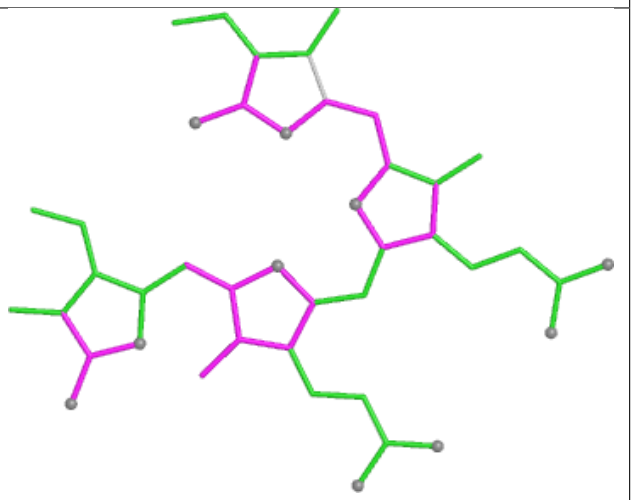


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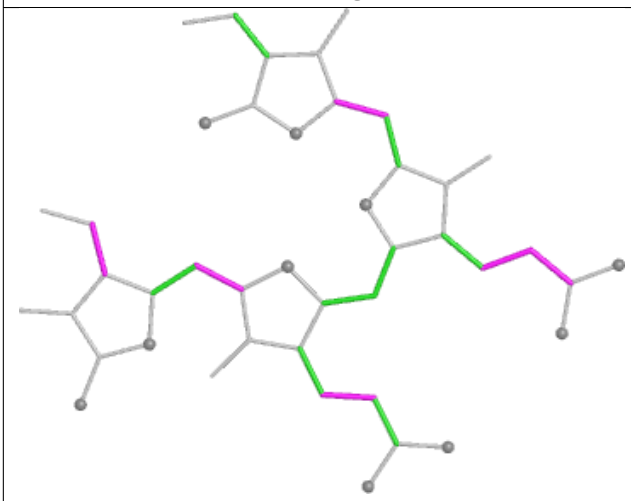
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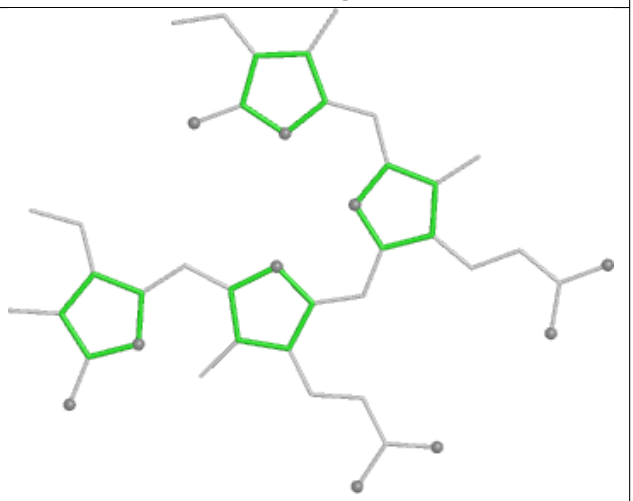
Bond lengths



Bond angles

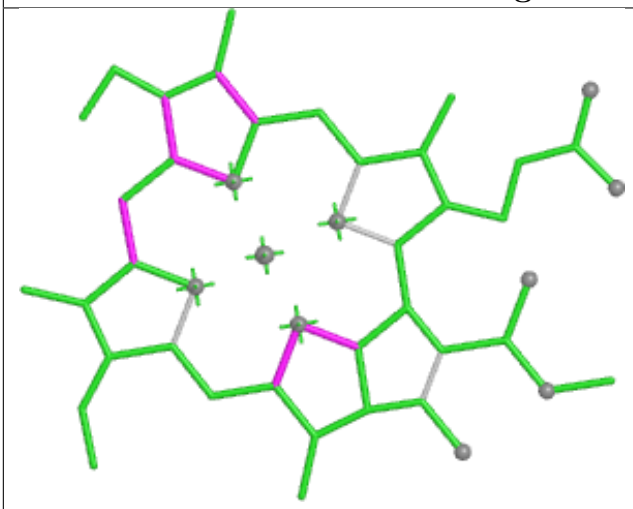


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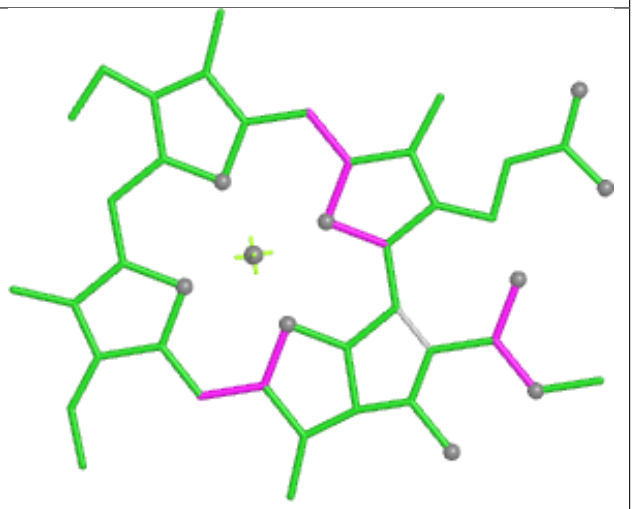


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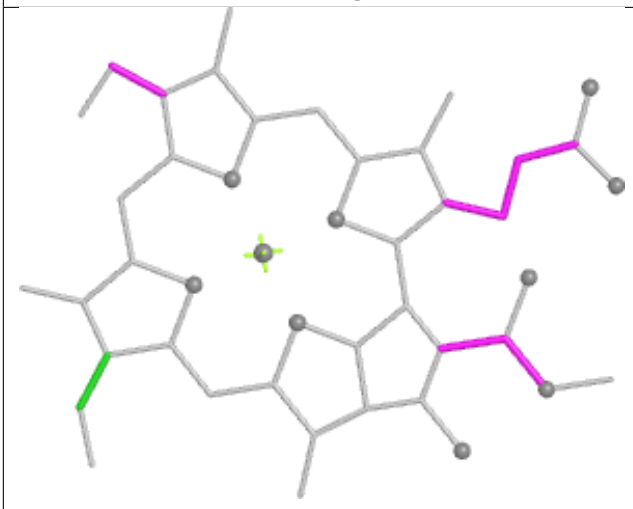
Ligand CLA 6N 611



Bond lengths



Bond angles

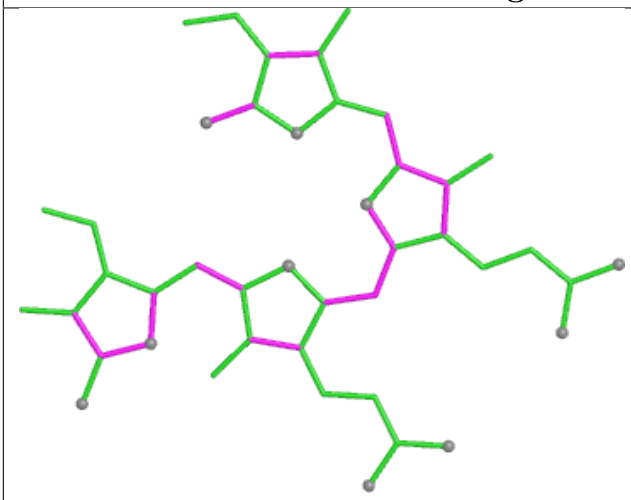


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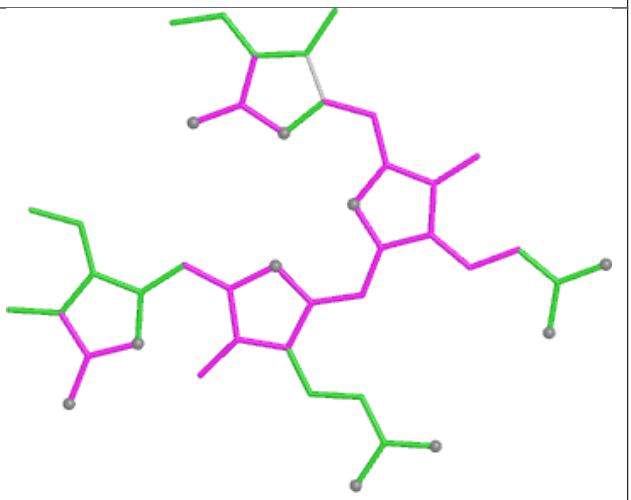


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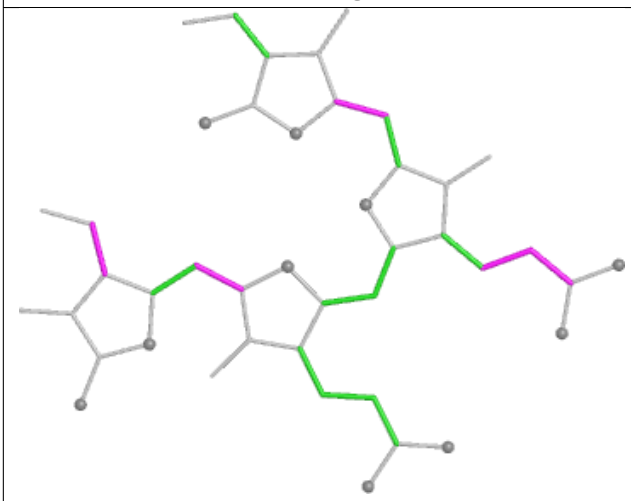
Ligand PEB XM 201



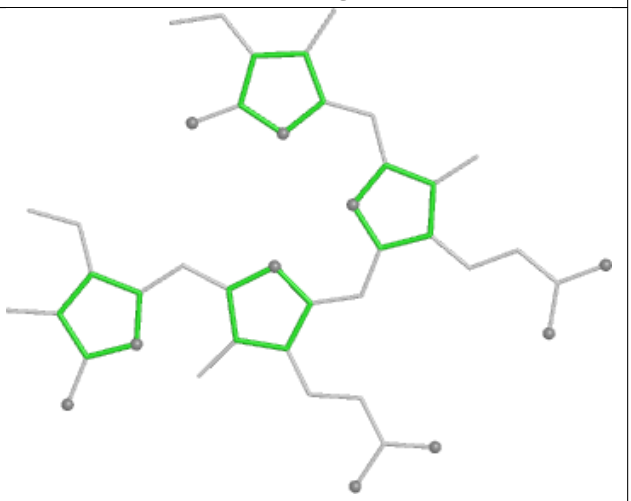
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Bond angles

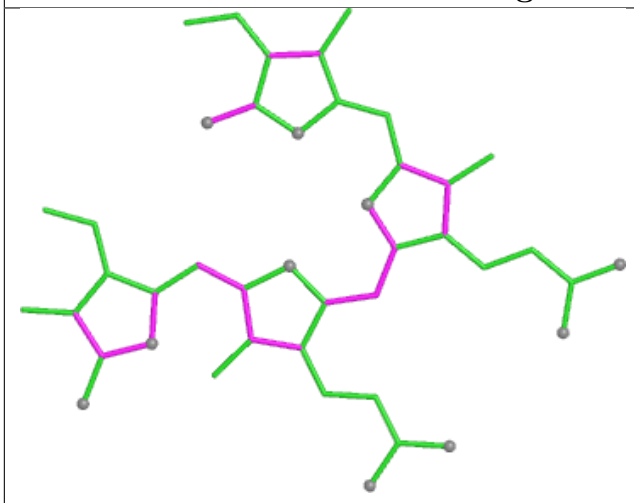


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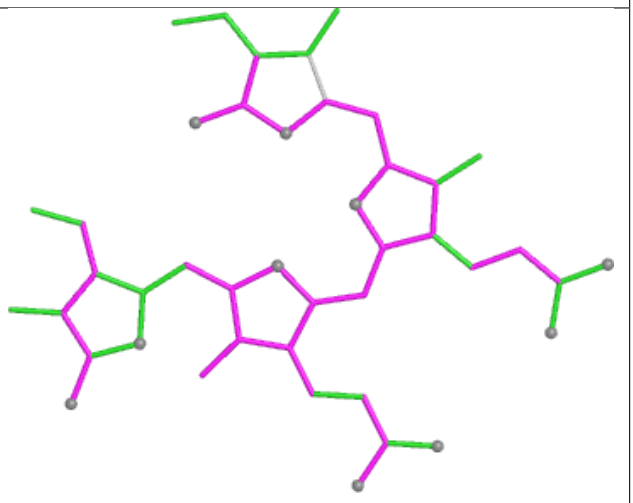


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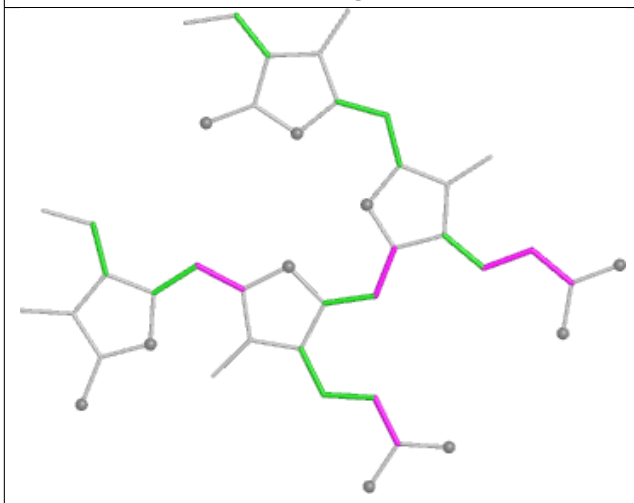
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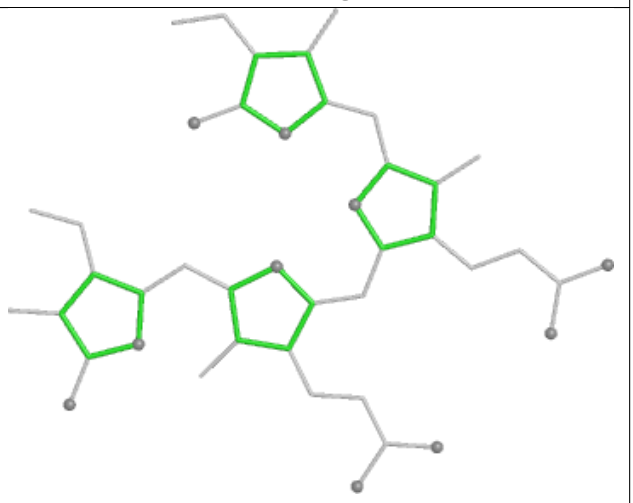
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Bond angles

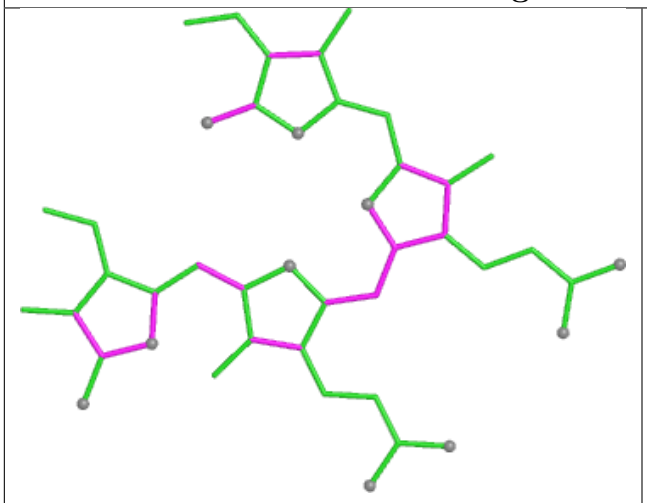


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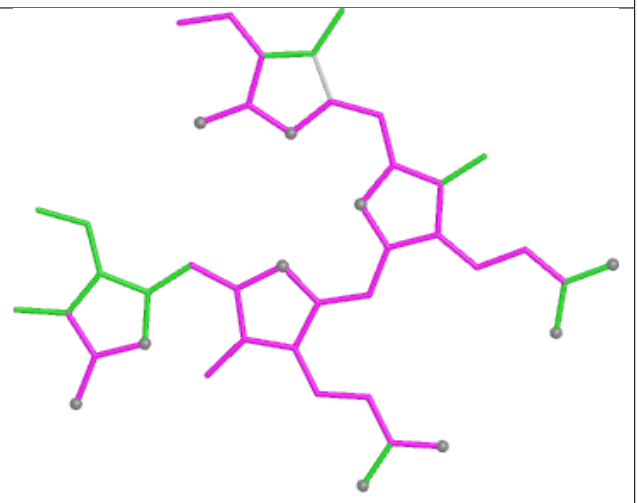


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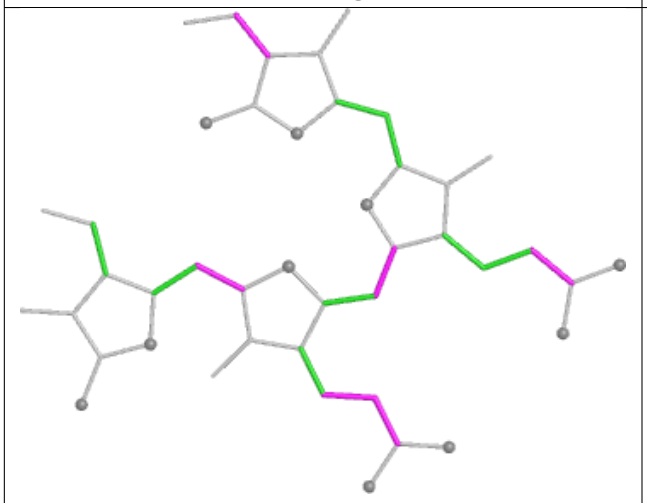
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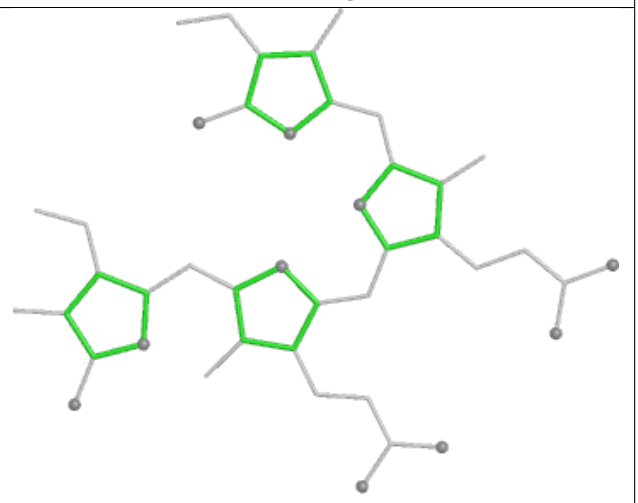
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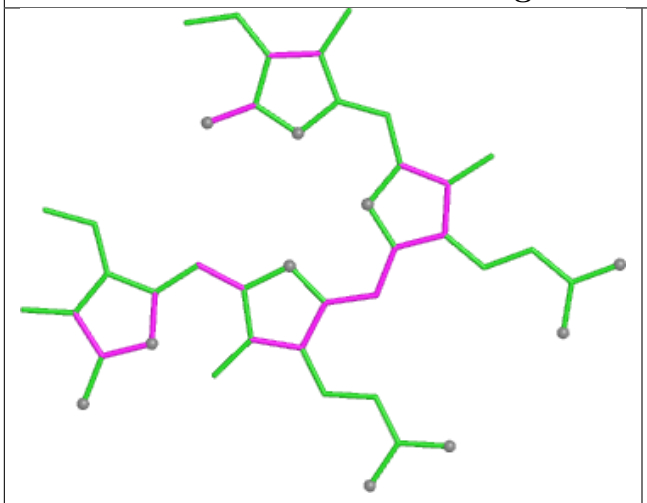


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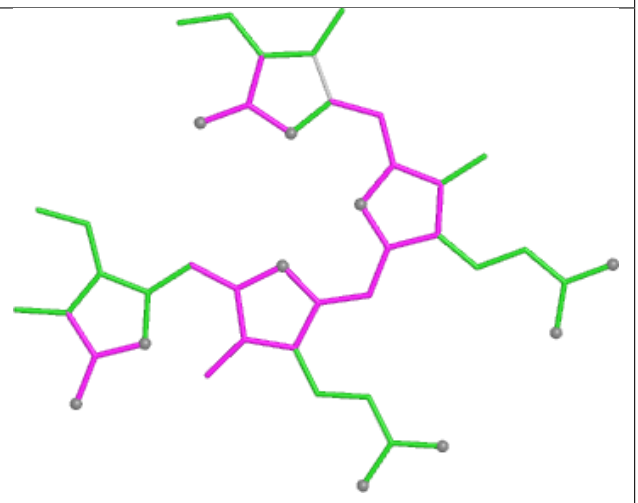


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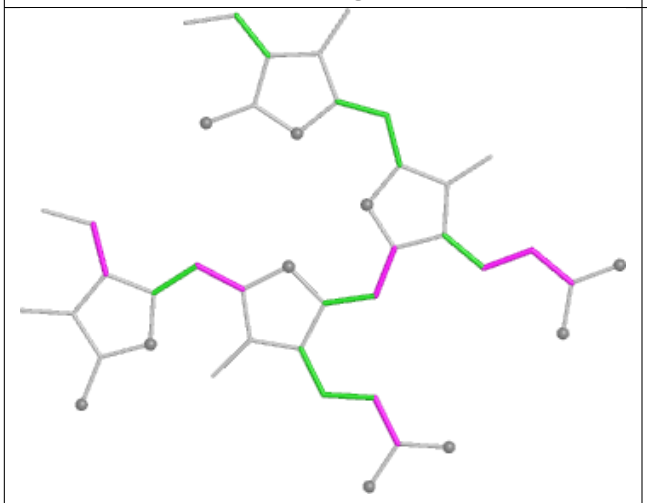
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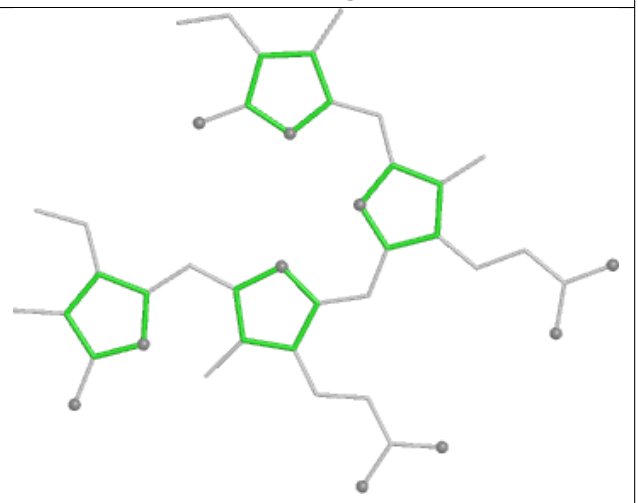
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Bond angles

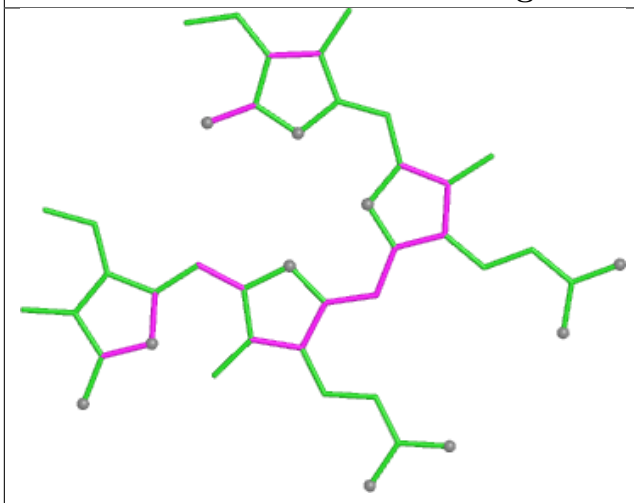


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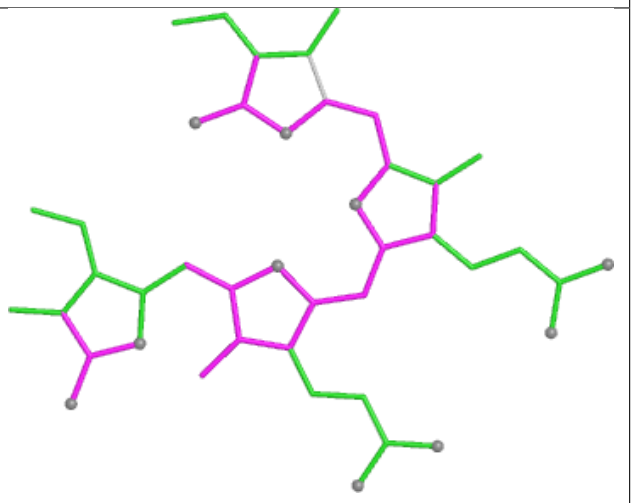


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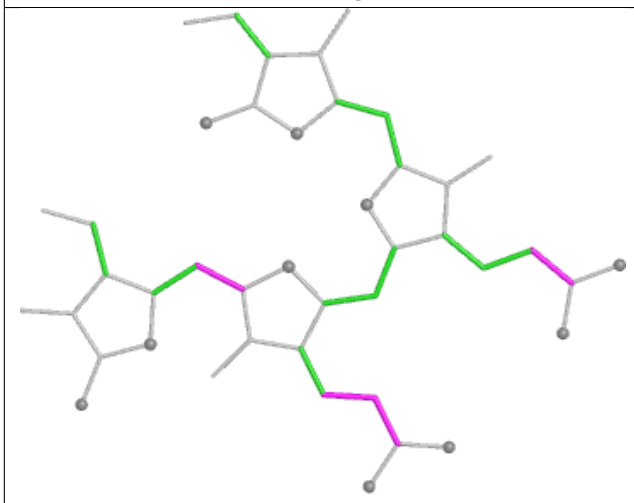
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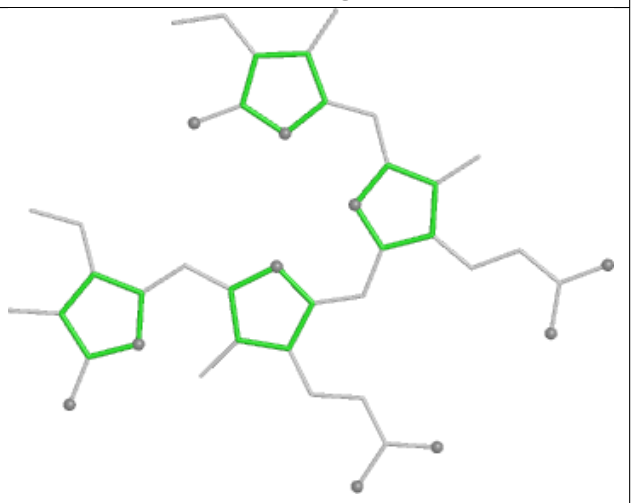
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Bond angles

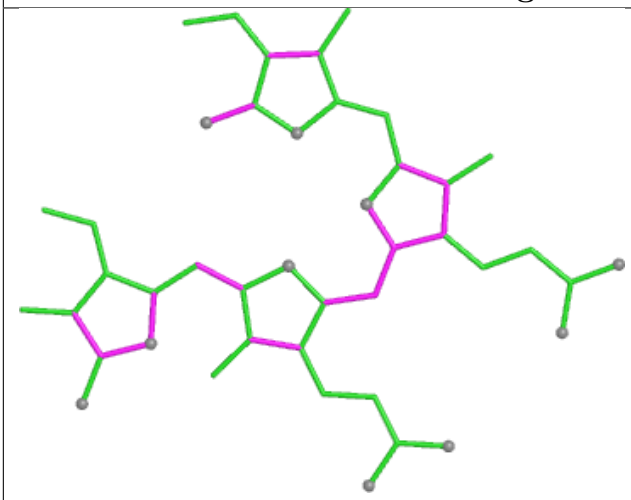


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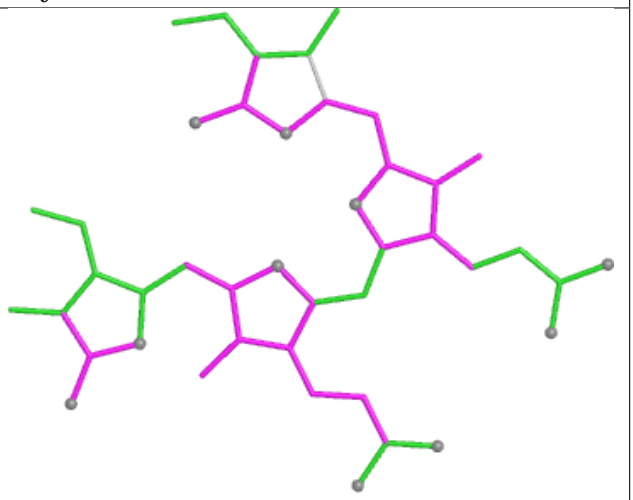


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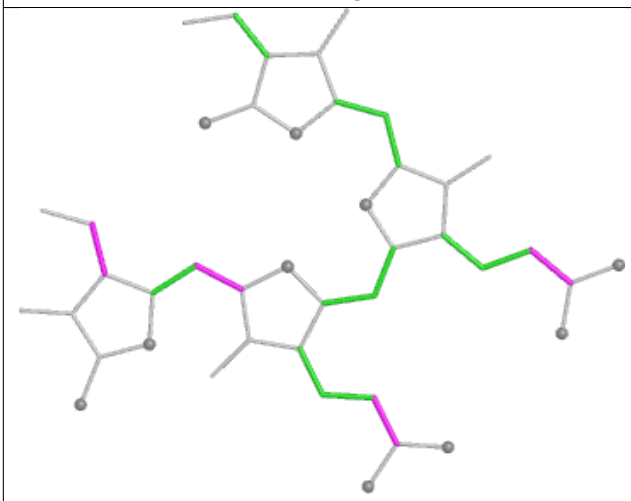
Ligand PEB yF 301



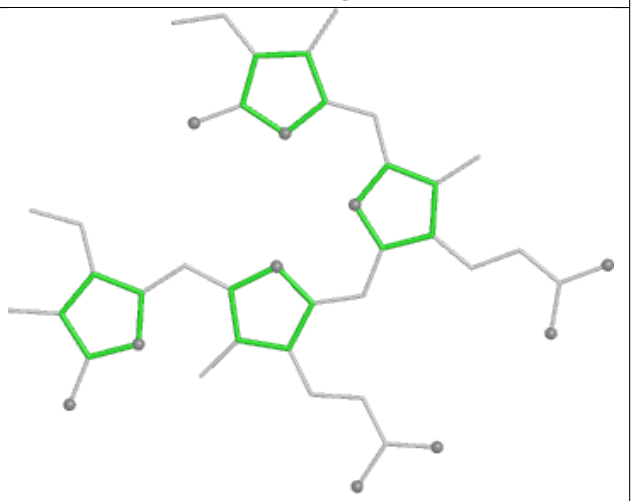
Bond lengths



Bond angles

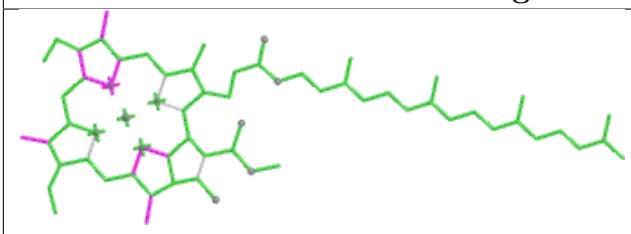


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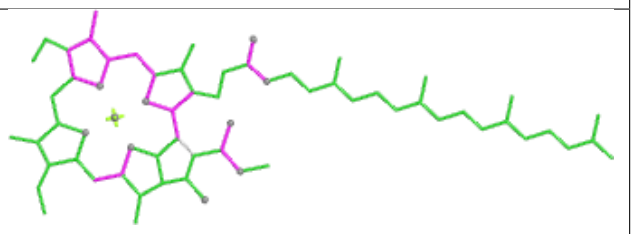


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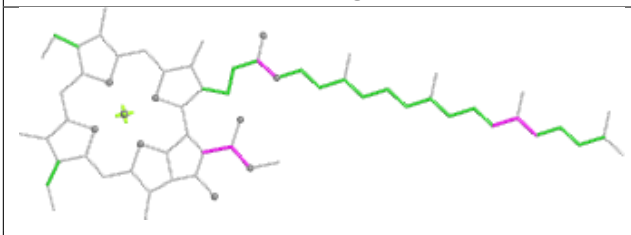
Ligand CLA HL 101



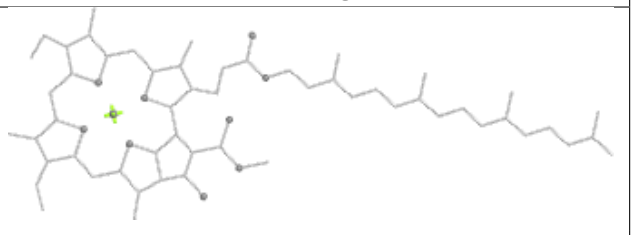
Bond lengths



Bond angles

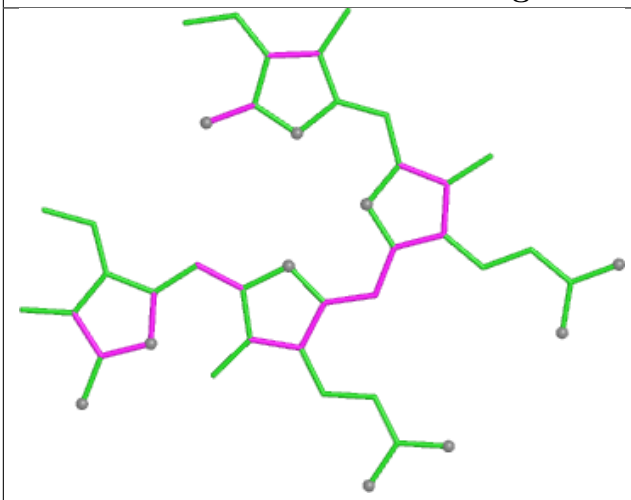


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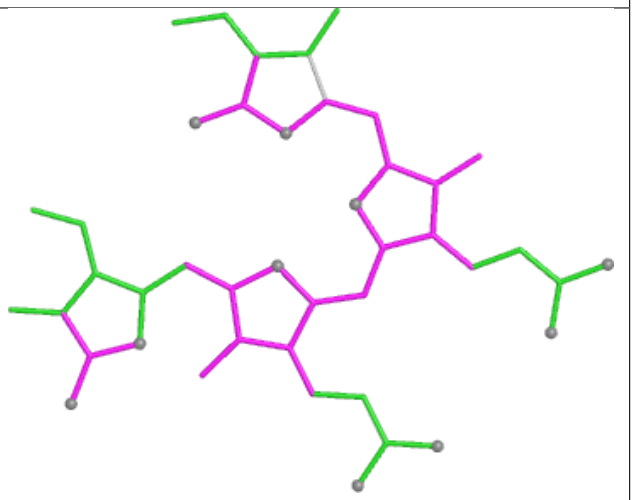


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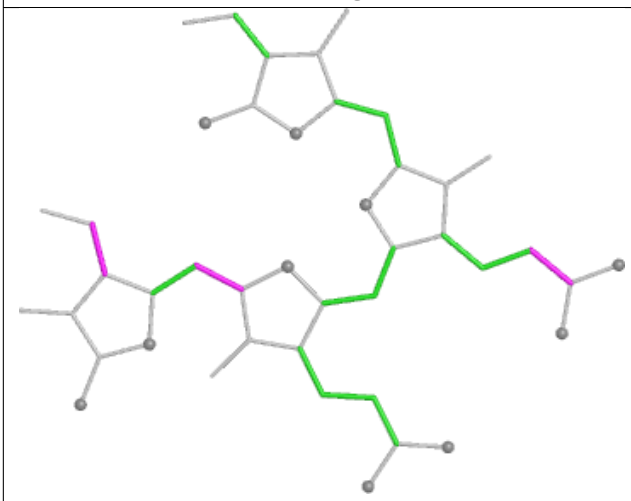
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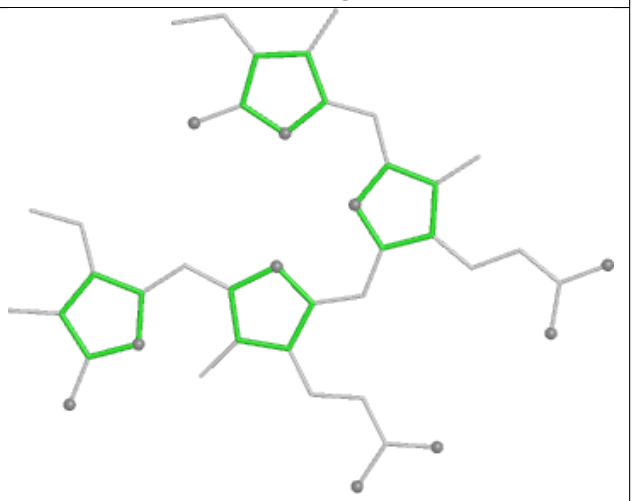
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Bond angles

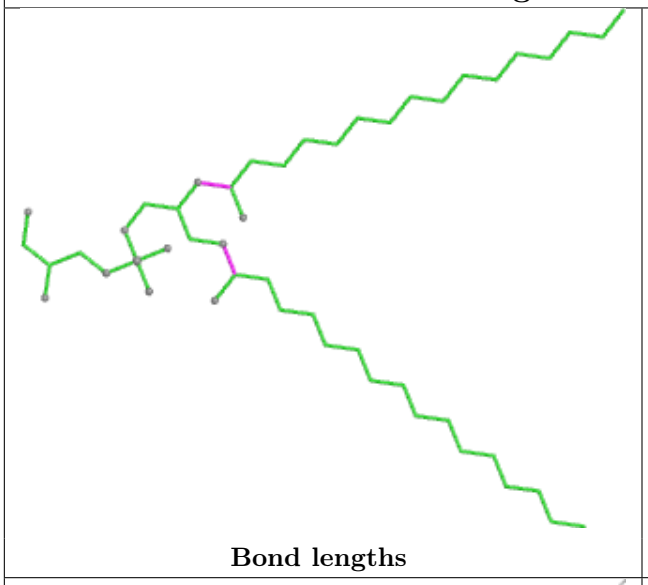


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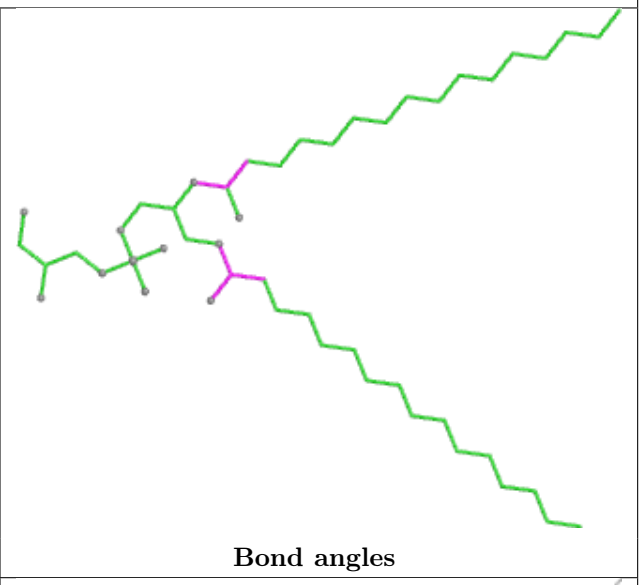


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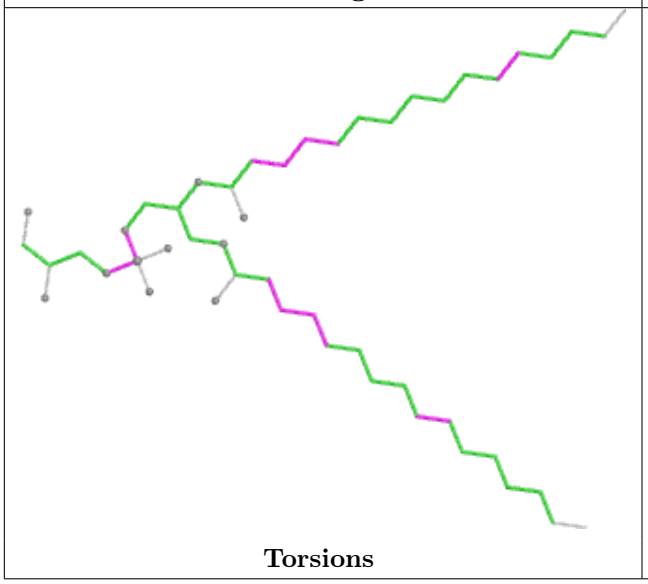
Ligand LHG BL 610



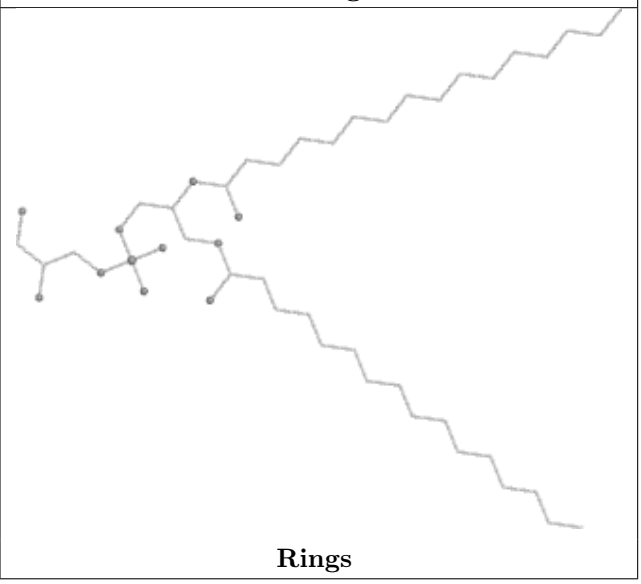
Bond lengths



Bond angles

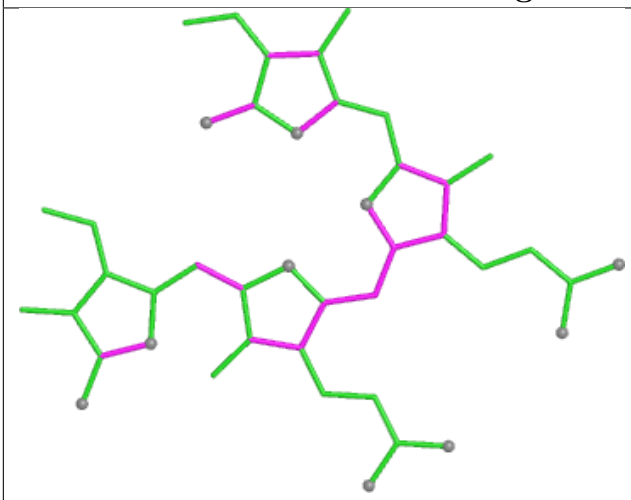


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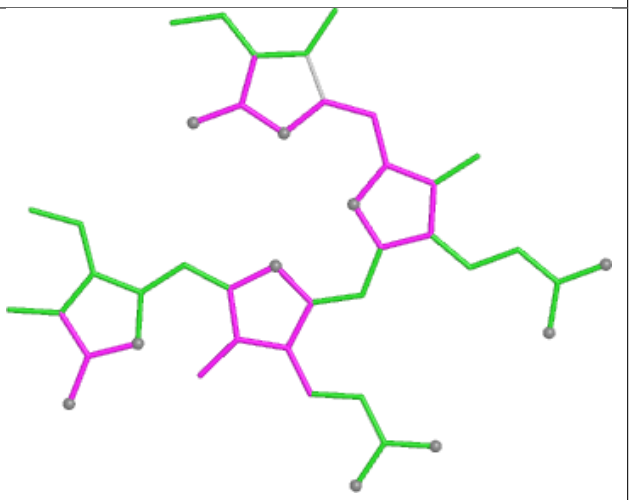


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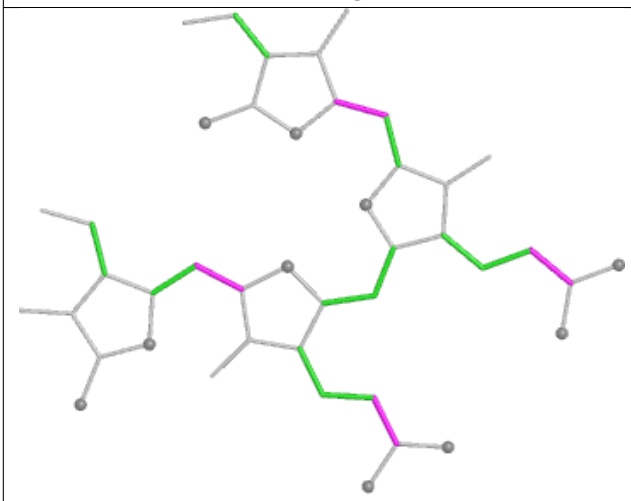
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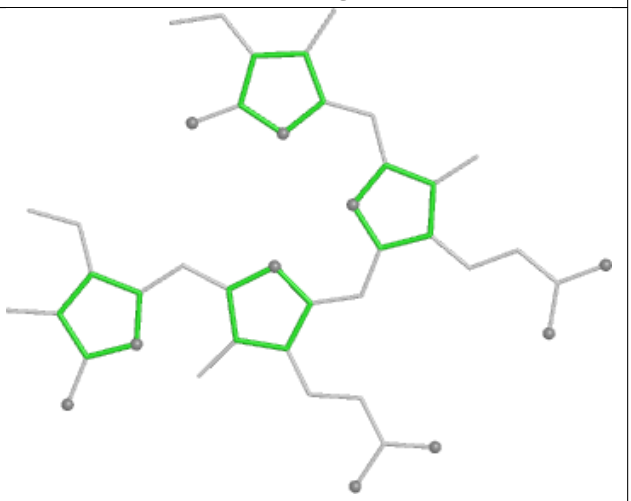
Bond lengths



Bond angles

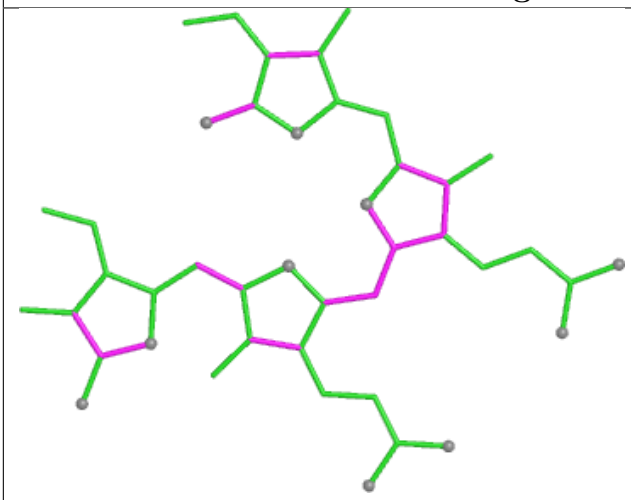


Torsions

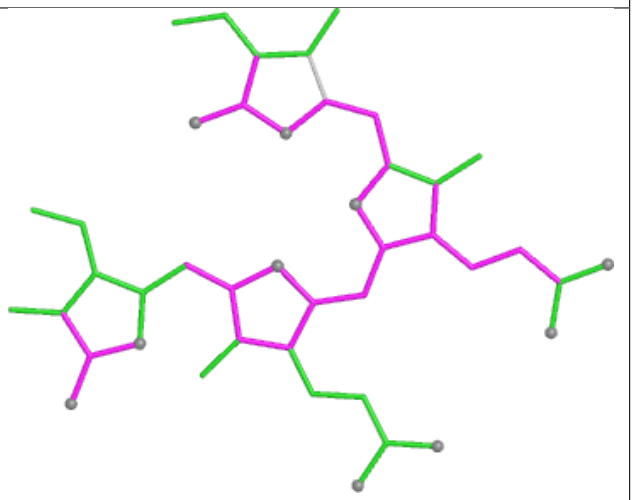


Rings

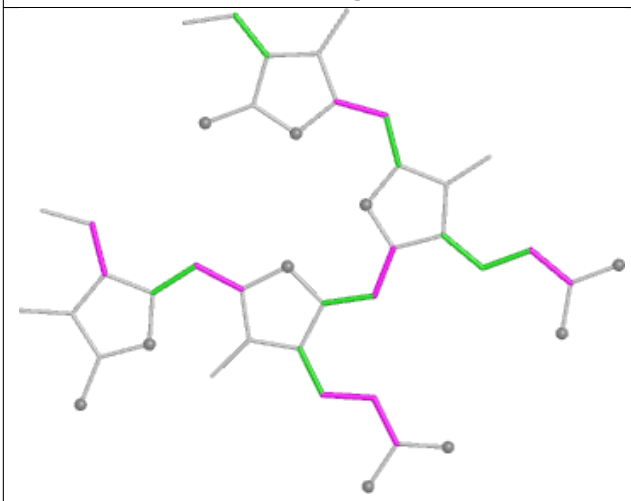
Ligand PEB wF 301



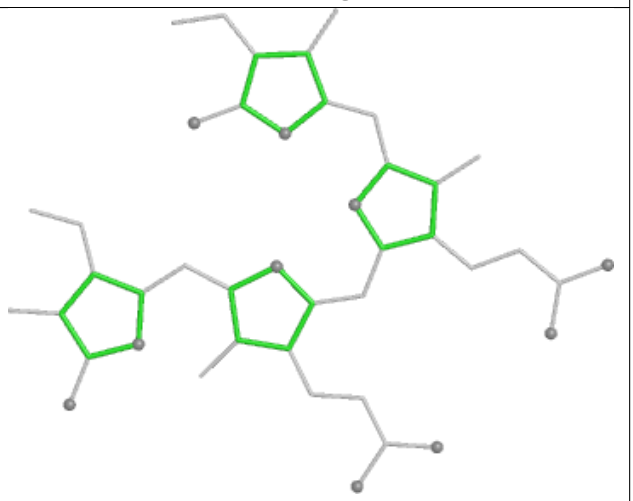
Bond lengths



Bond angles

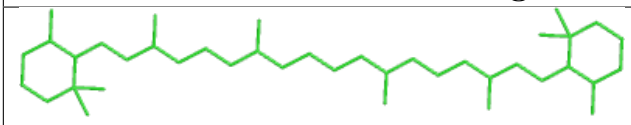


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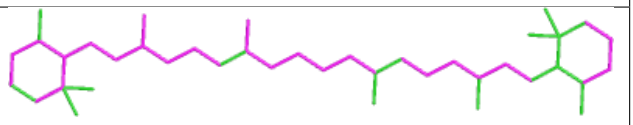


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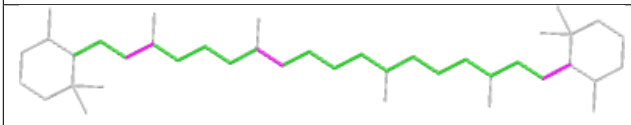
Ligand BCR FN 202



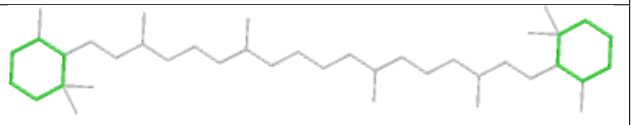
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Bond angles

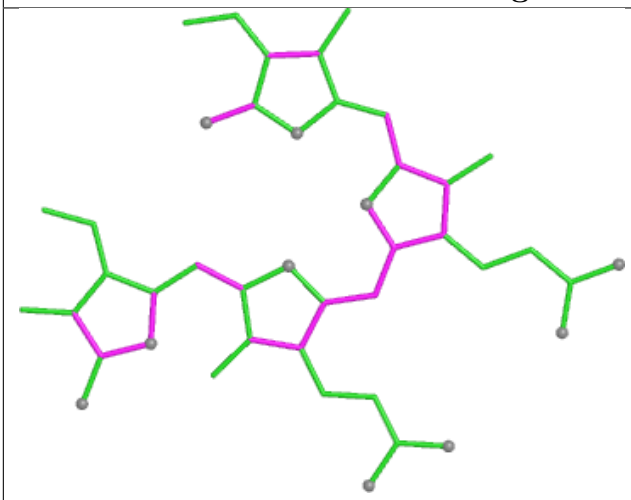


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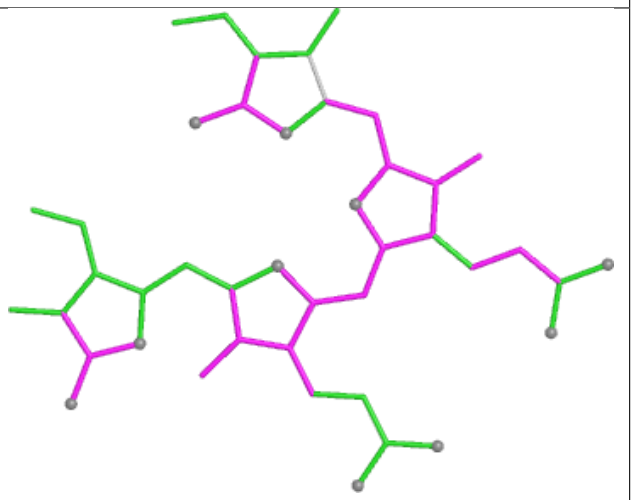


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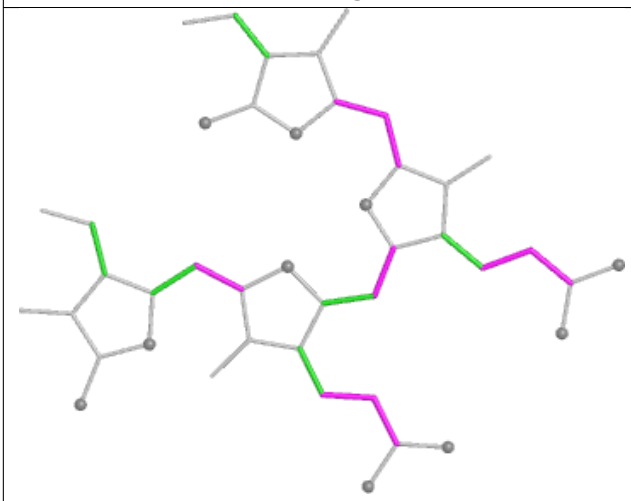
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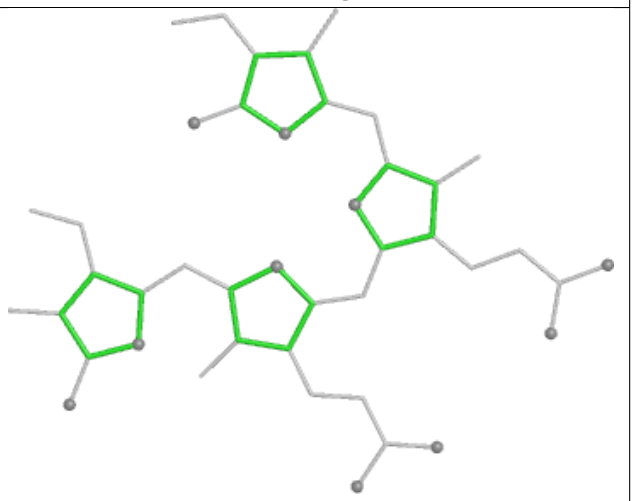
Bond lengths



Bond angles

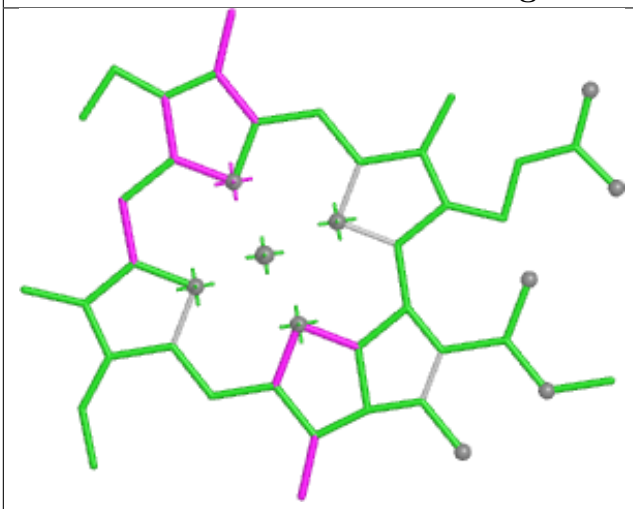


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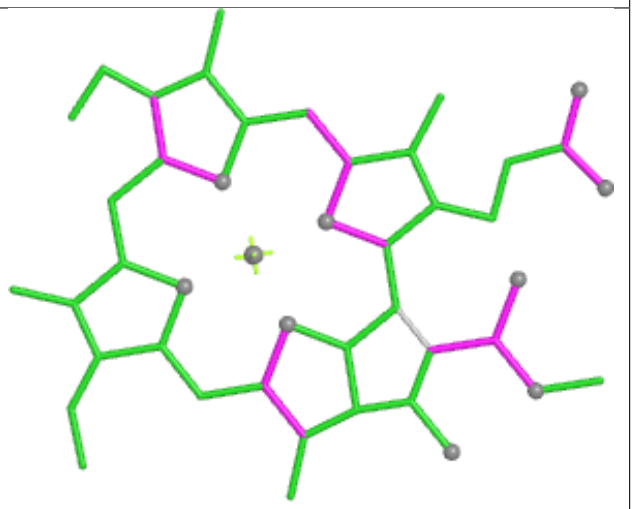


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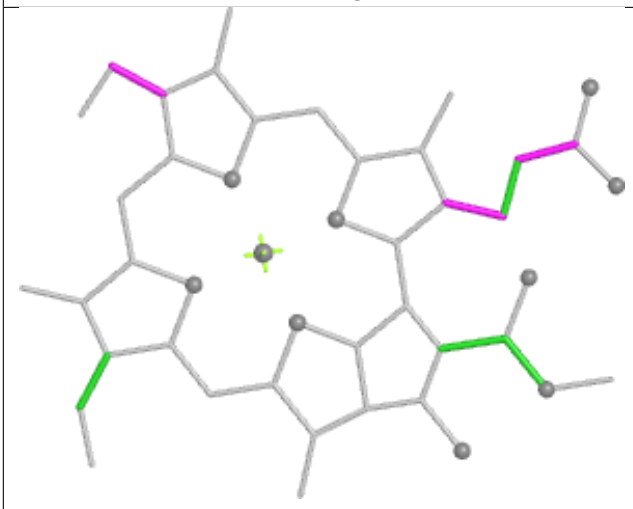
Ligand CLA 62 308



Bond lengths



Bond angles

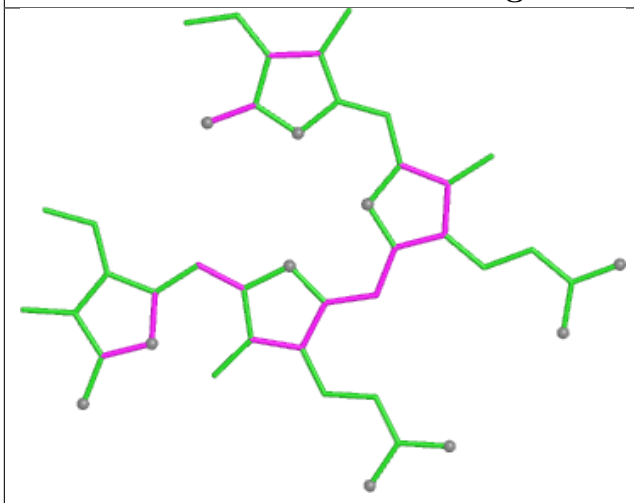


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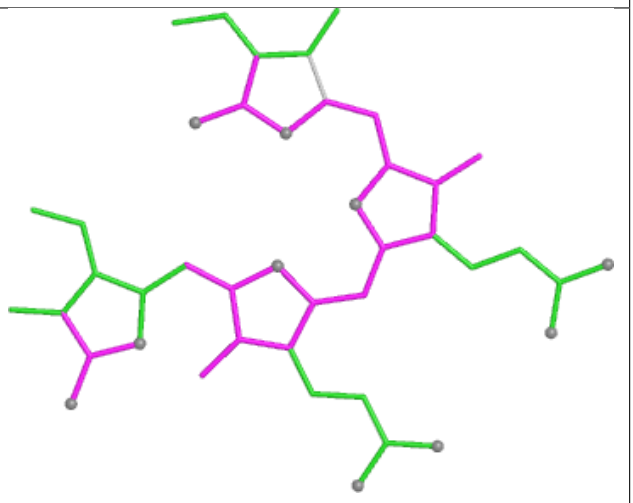


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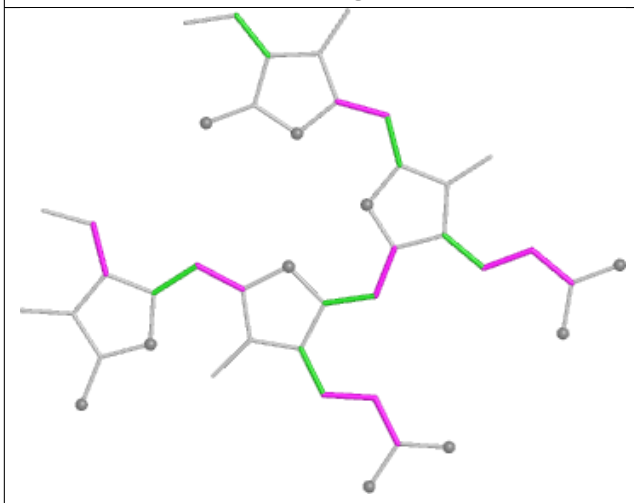
Ligand PEB WK 203



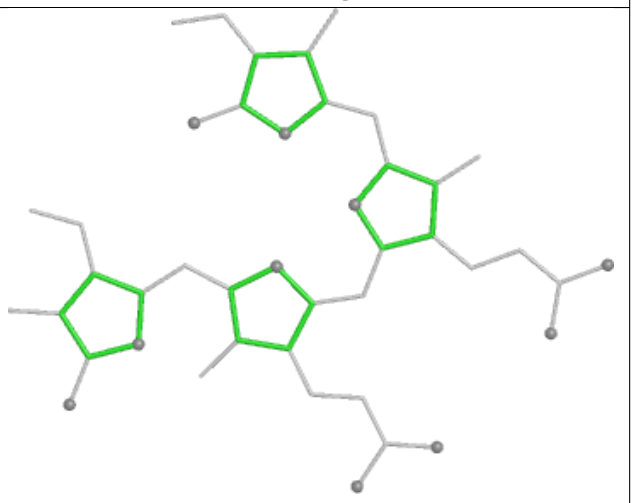
Bond lengths



Bond angles

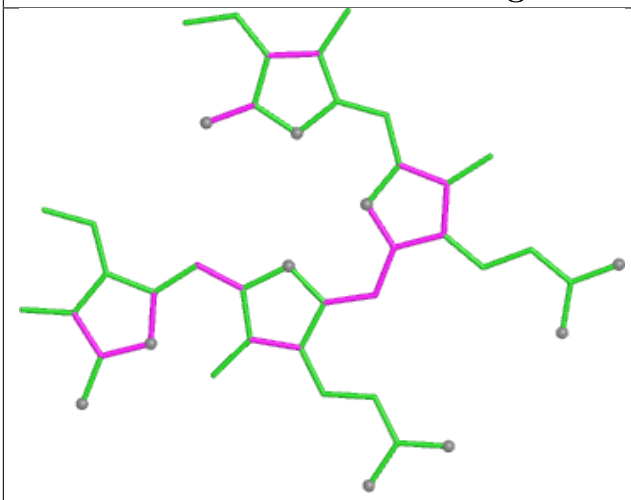


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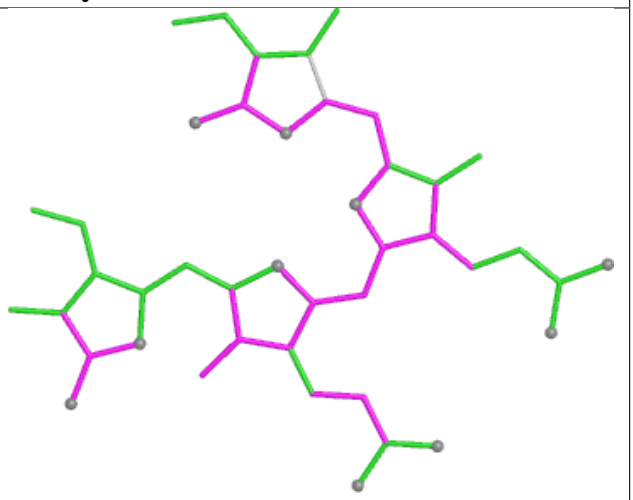


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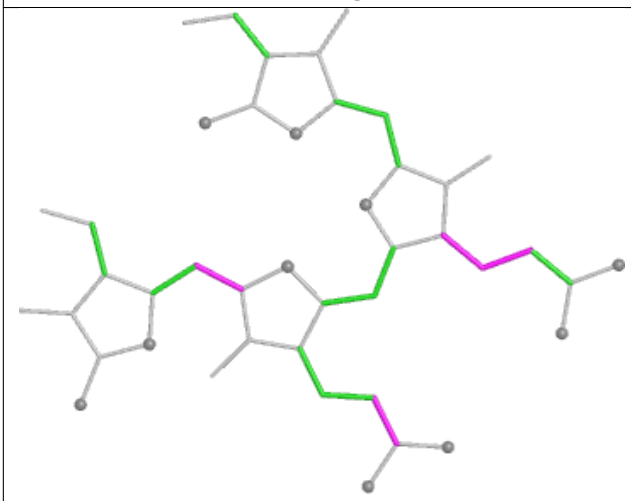
Ligand PEB MQ 201



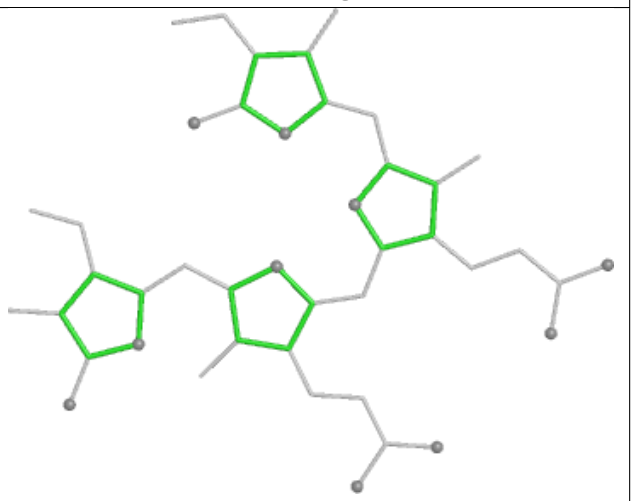
Bond lengths



Bond angles

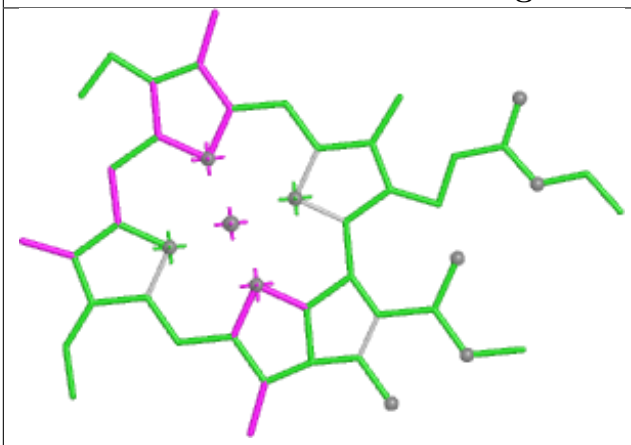


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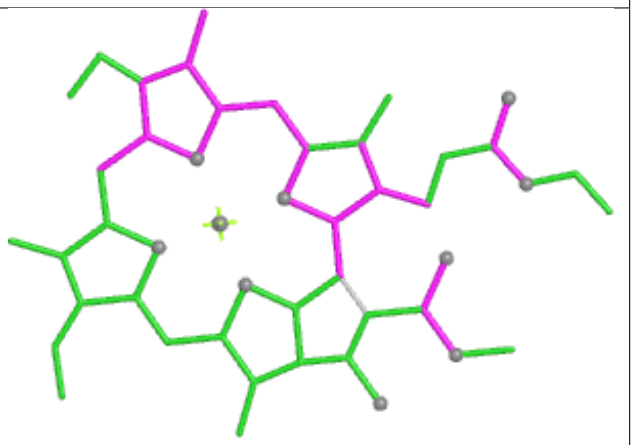


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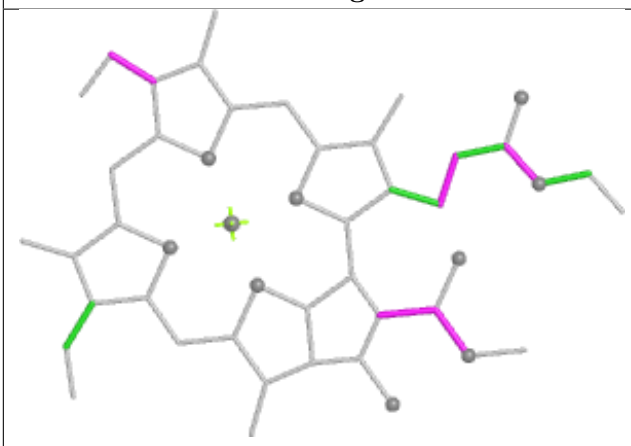
Ligand CLA B2 833



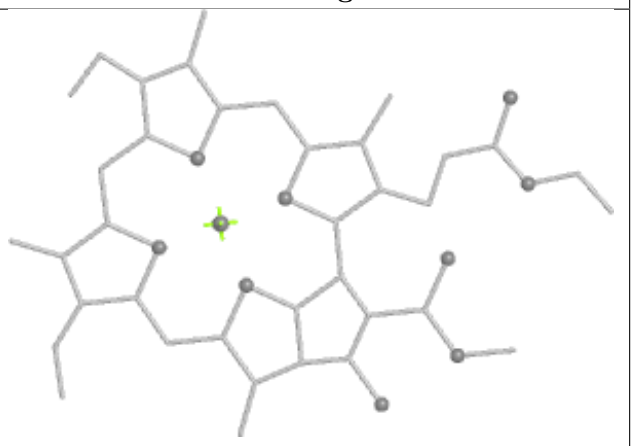
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Bond angles

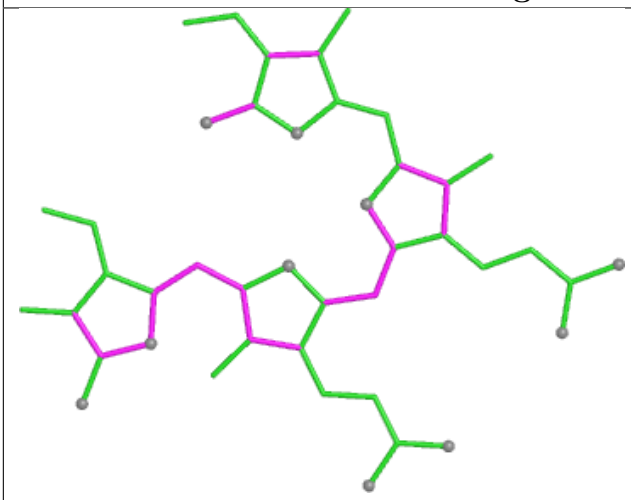


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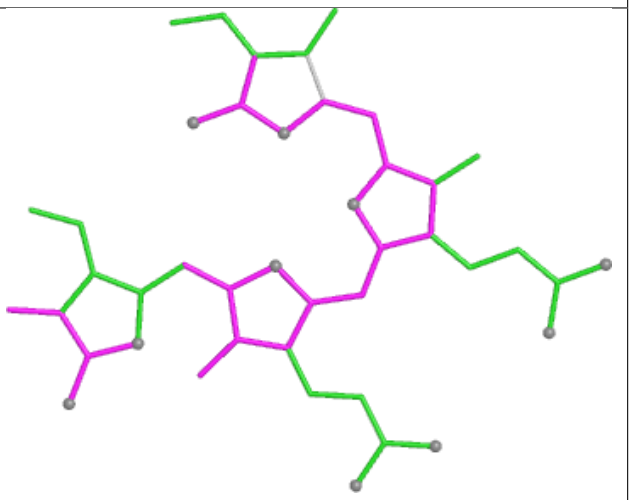


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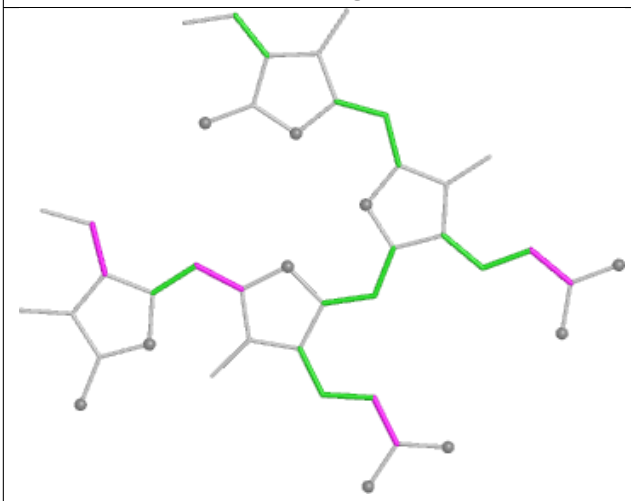
Ligand PEB ZO 201



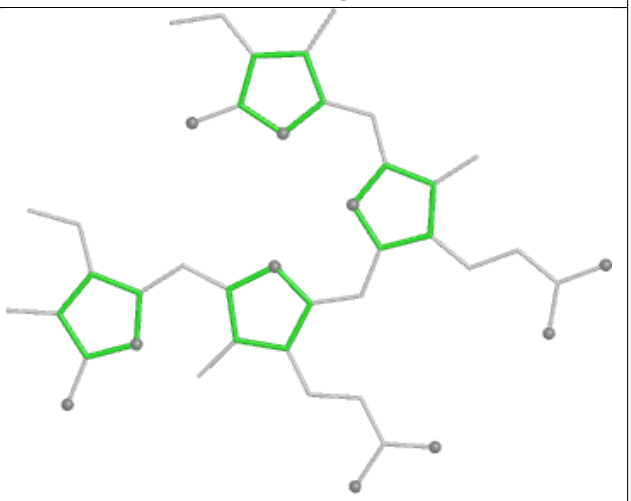
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Bond angles

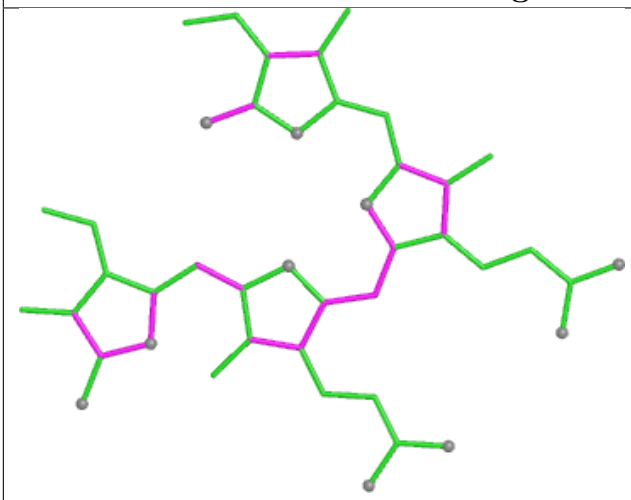


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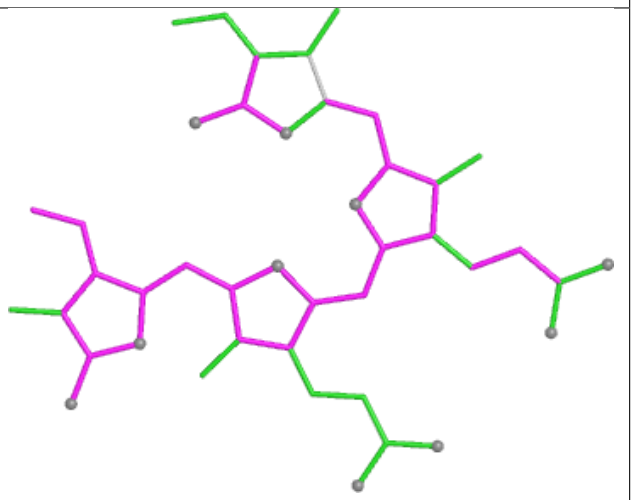


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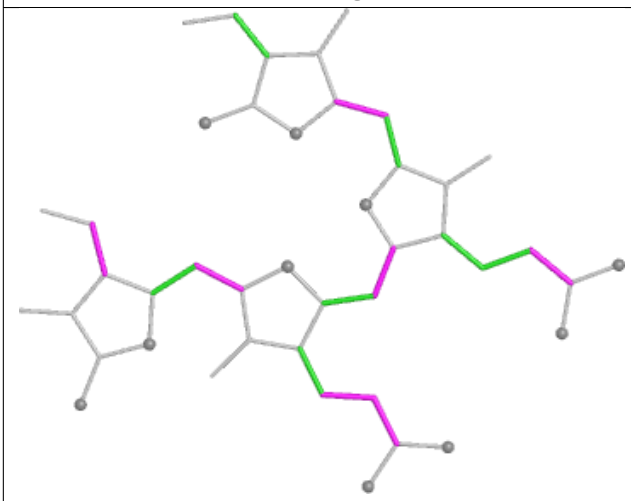
Ligand PEB M5 305



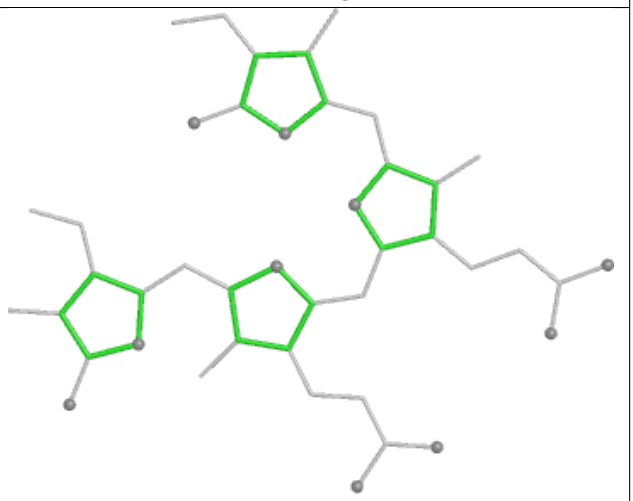
Bond lengths



Bond angles

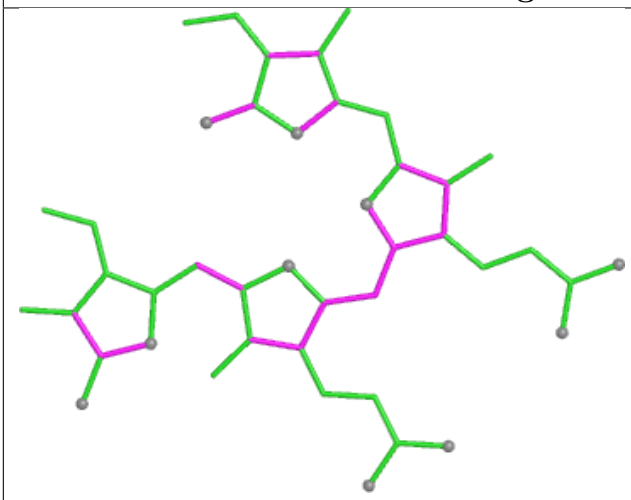


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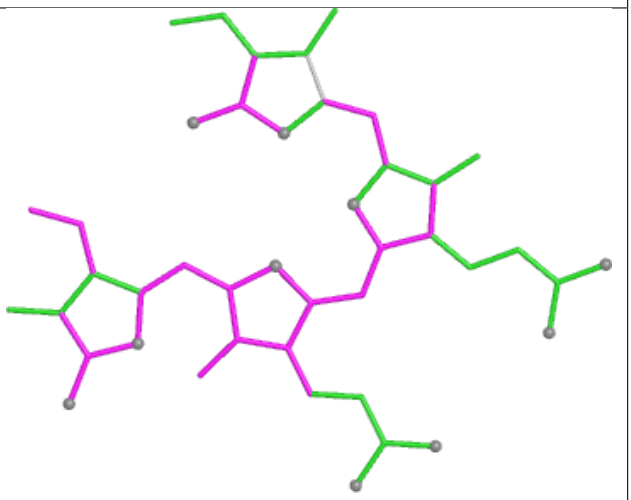


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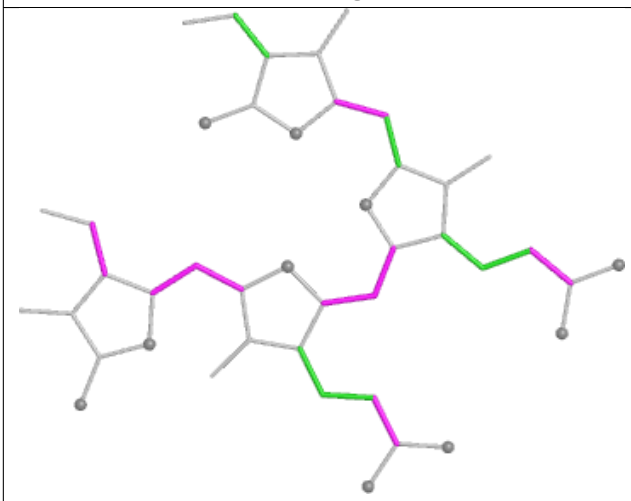
Ligand PEB E9 202



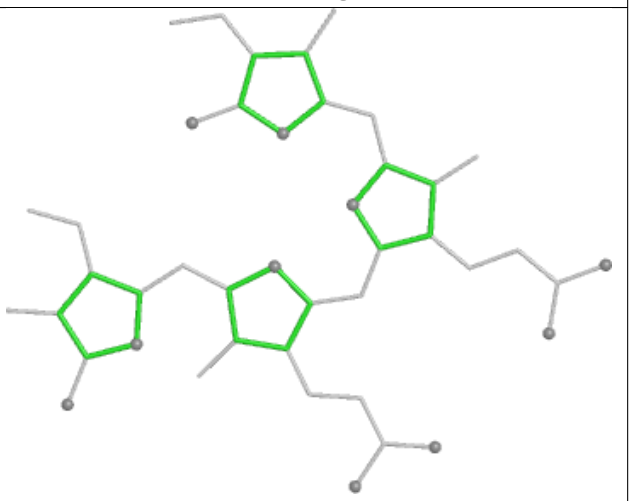
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Bond angles

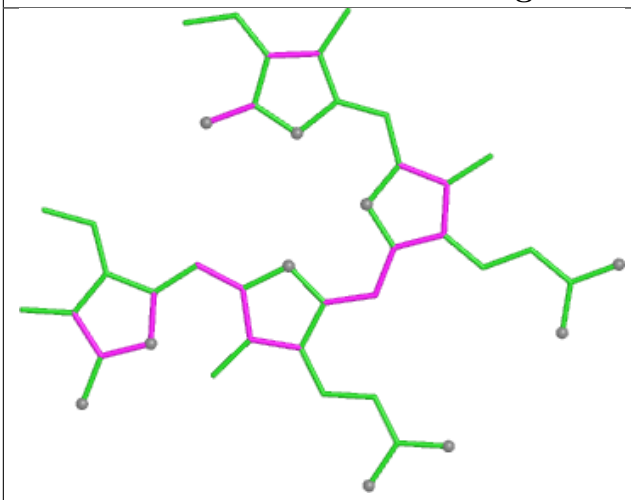


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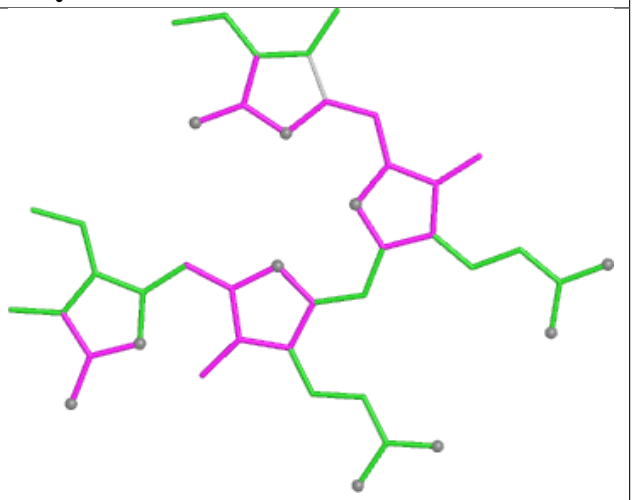


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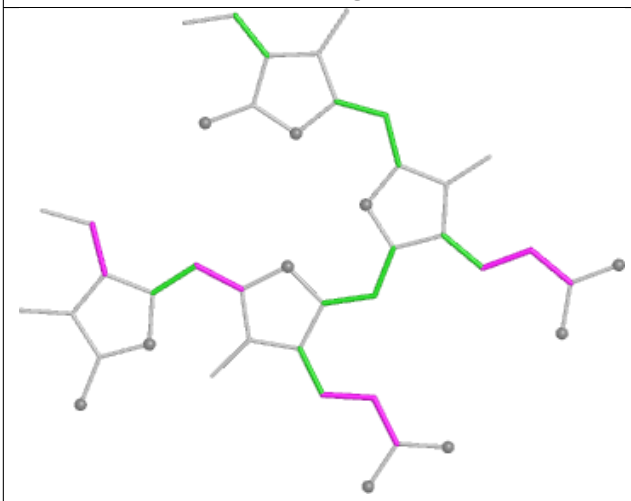
Ligand PEB Q1 203



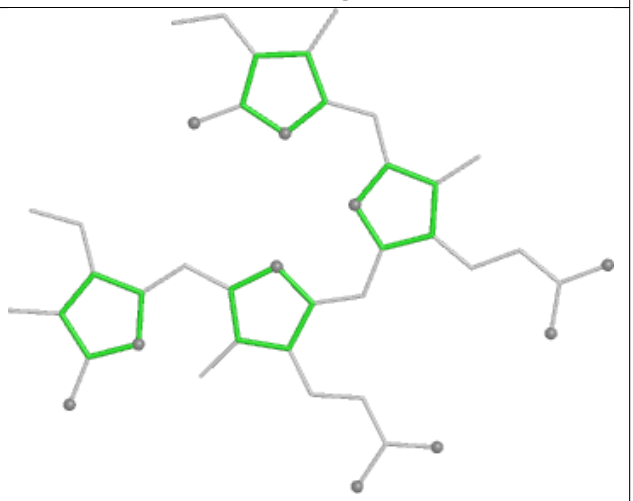
Bond lengths



Bond angles

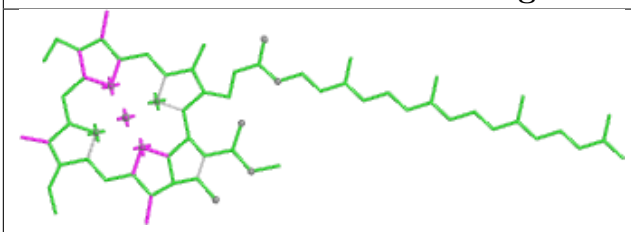


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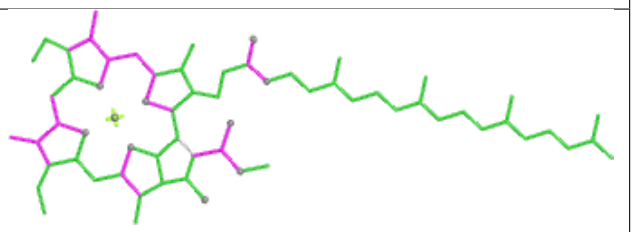


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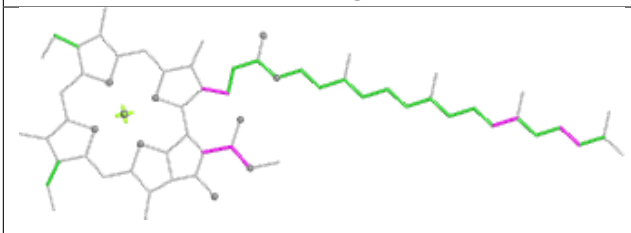
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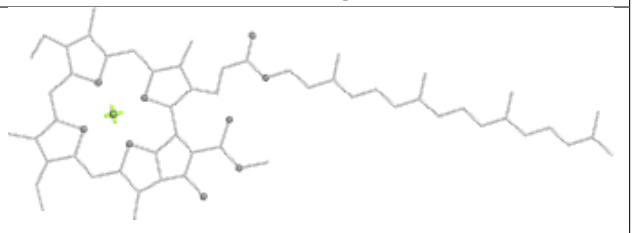
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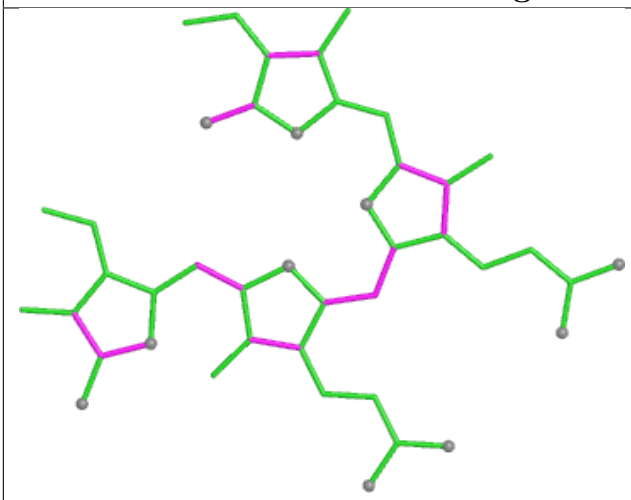


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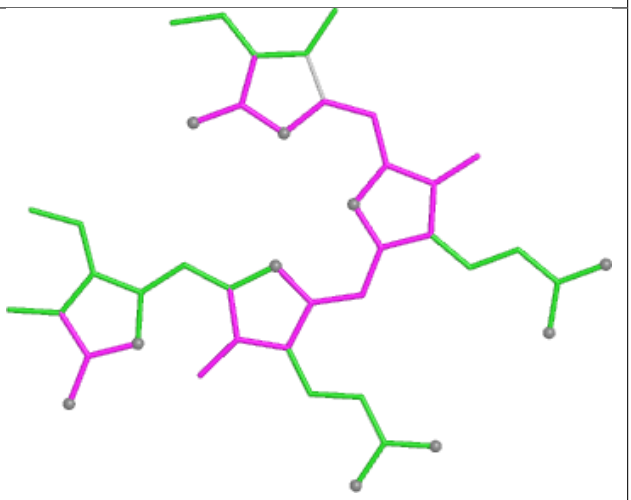


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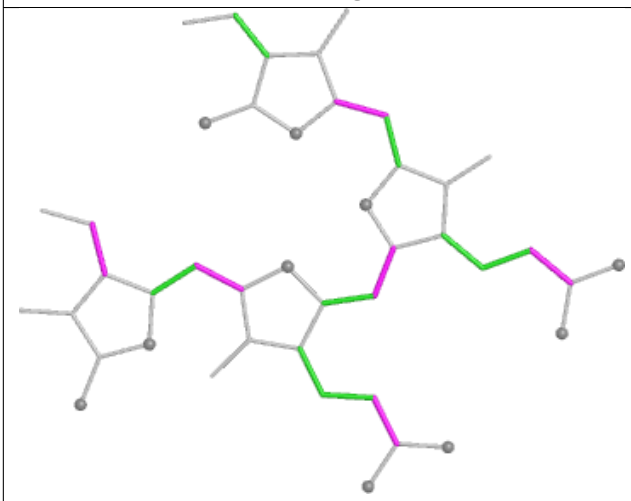
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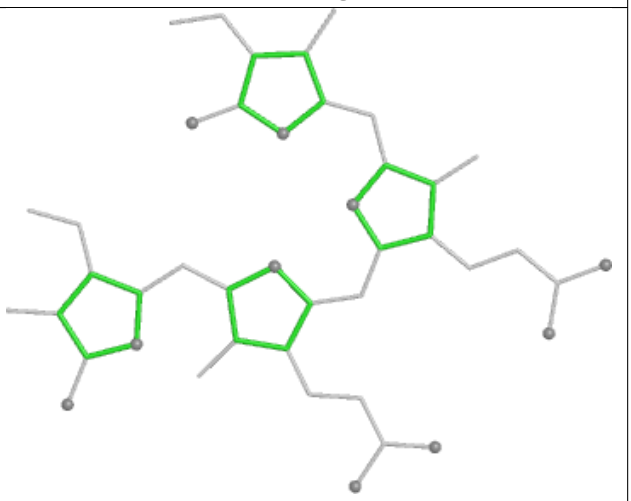
Bond lengths



Bond angles

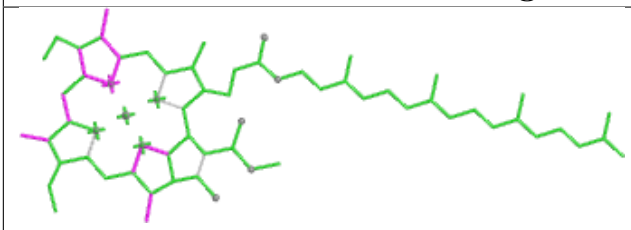


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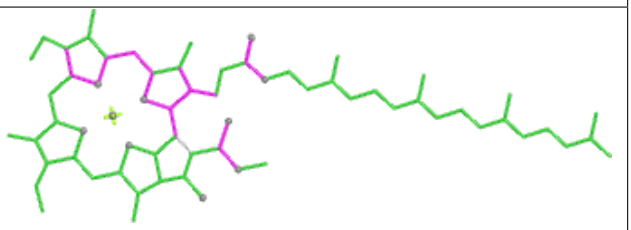


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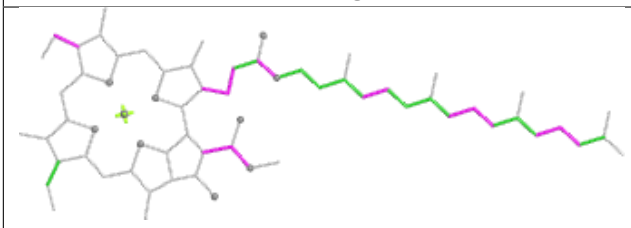
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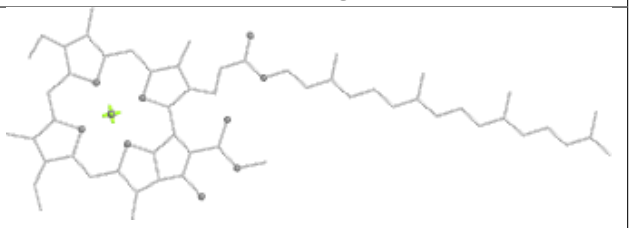
Bond lengths



Bond angles

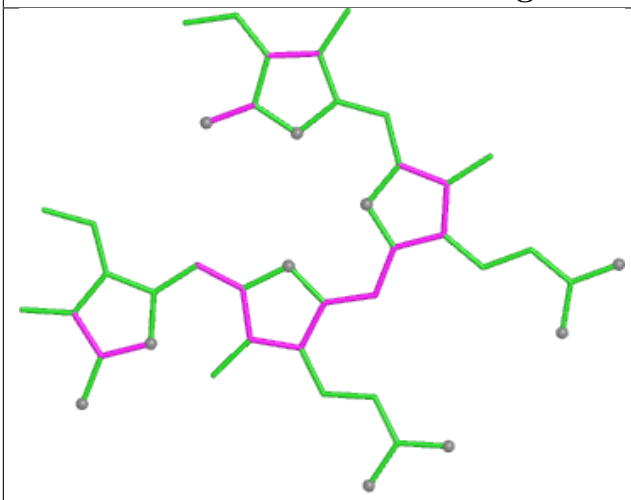


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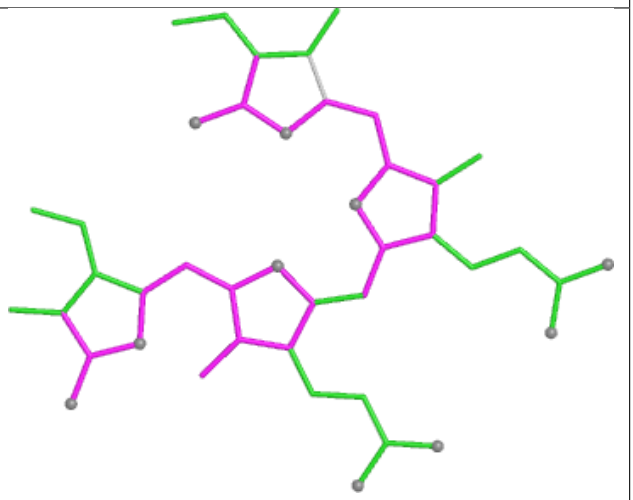


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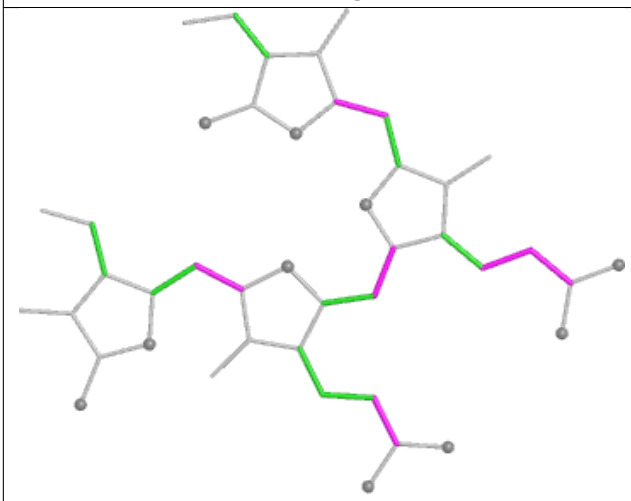
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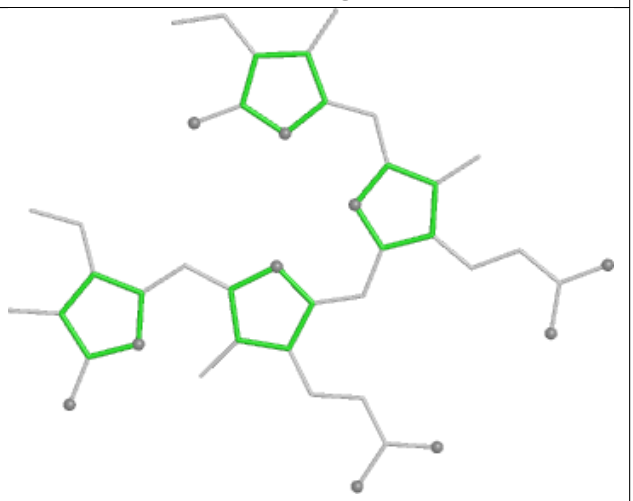
Bond lengths



Bond angles

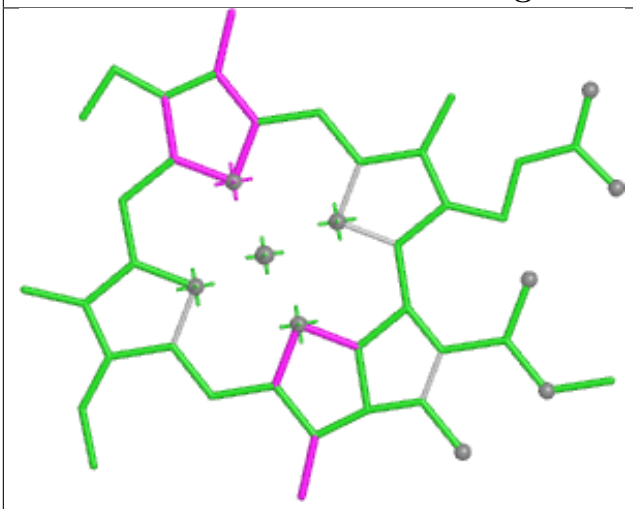


Torsions

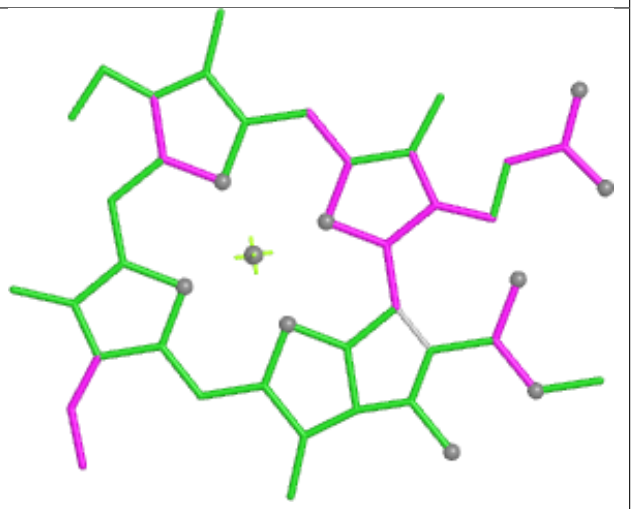


Rings

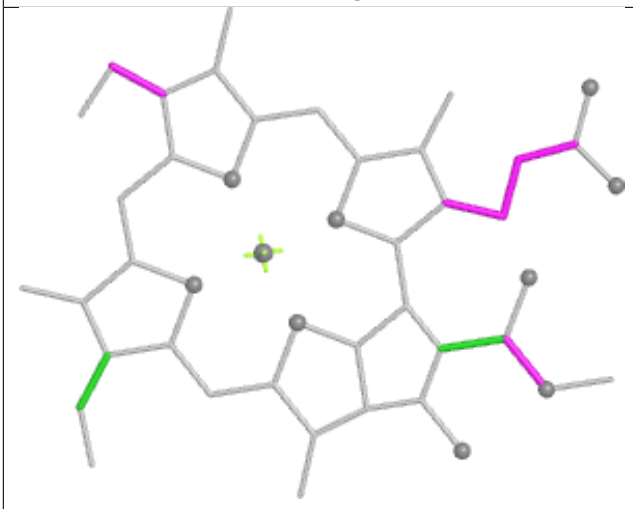
Ligand CLA 4N 605



Bond lengths



Bond angles

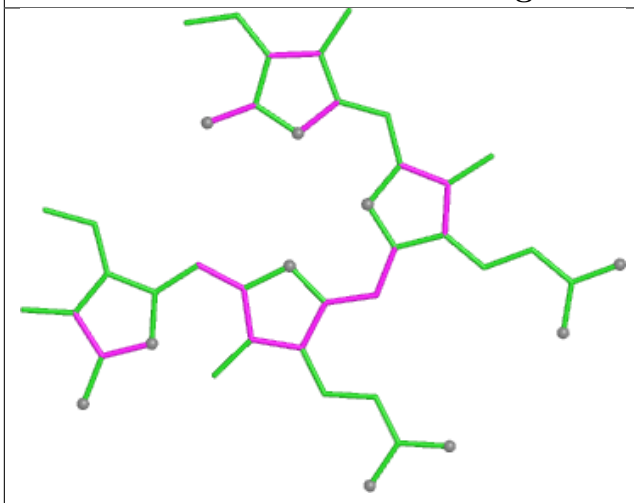


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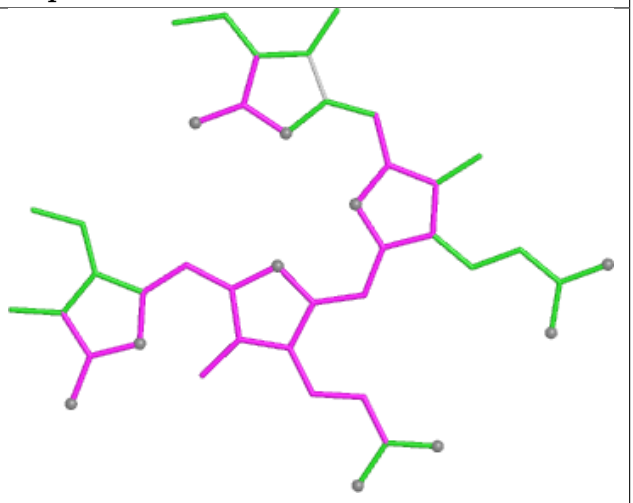


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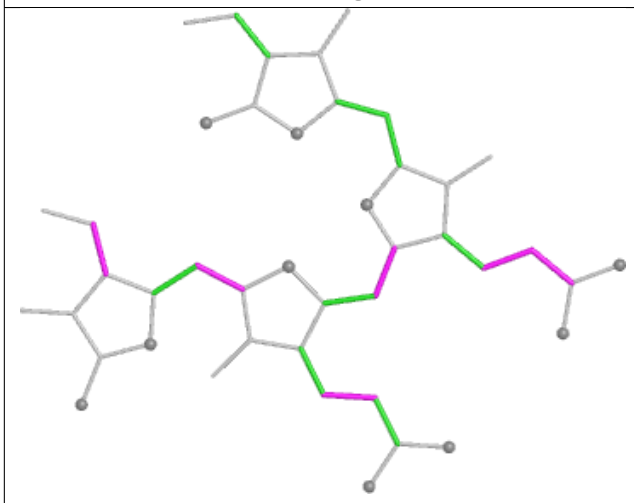
Ligand PEB qK 203



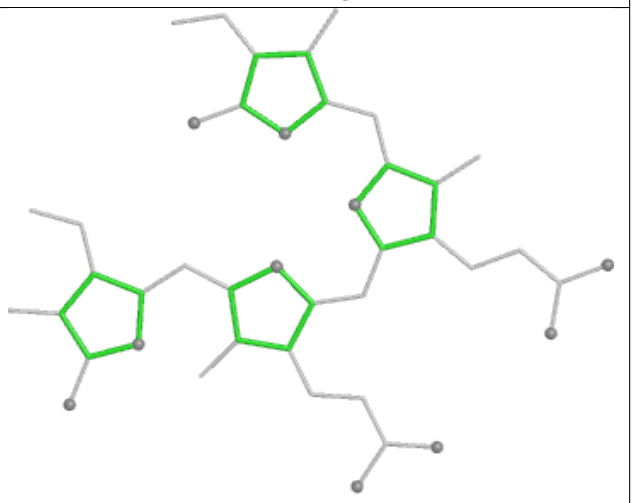
Bond lengths



Bond angles

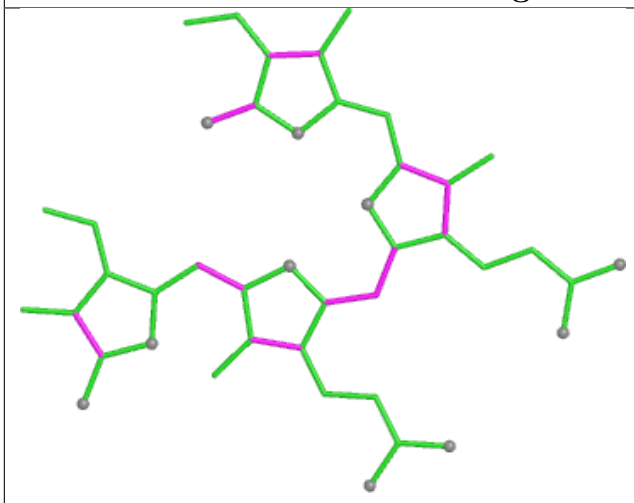


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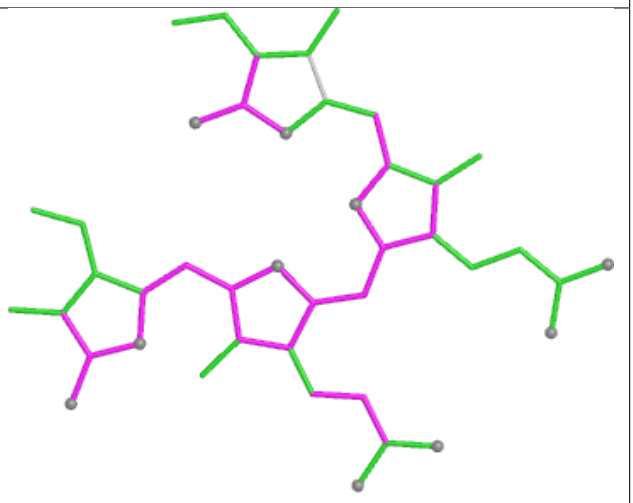


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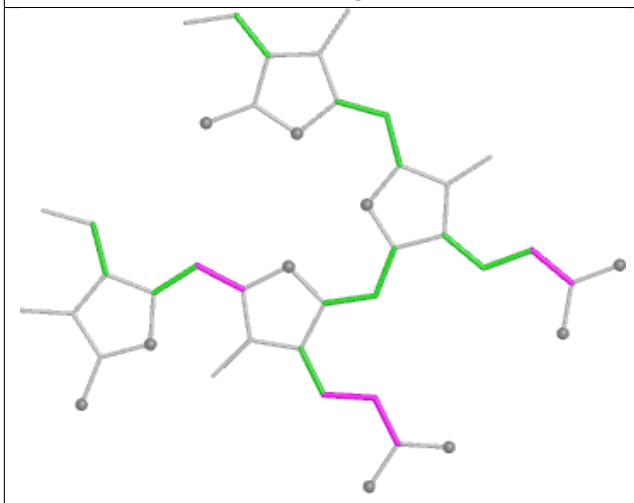
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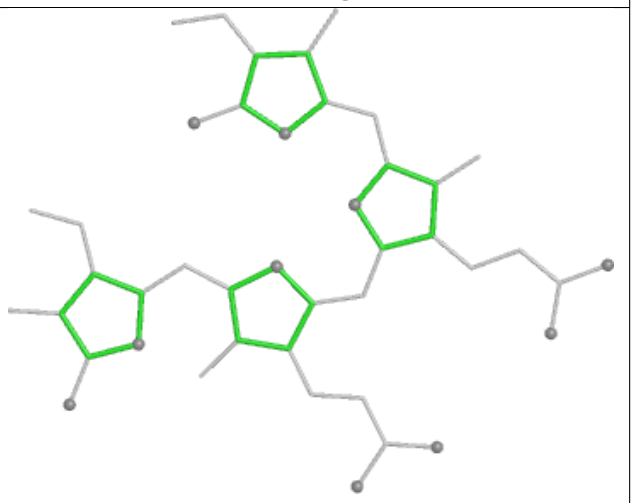
Bond lengths



Bond angles

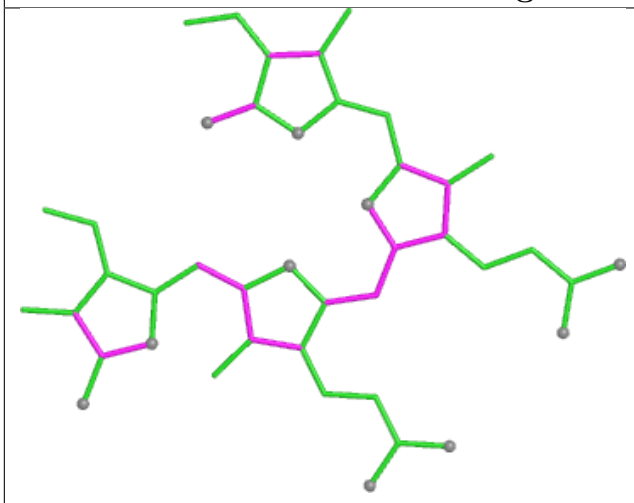


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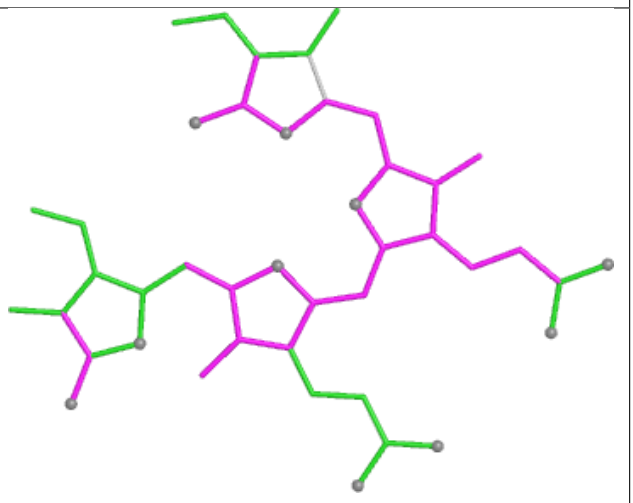


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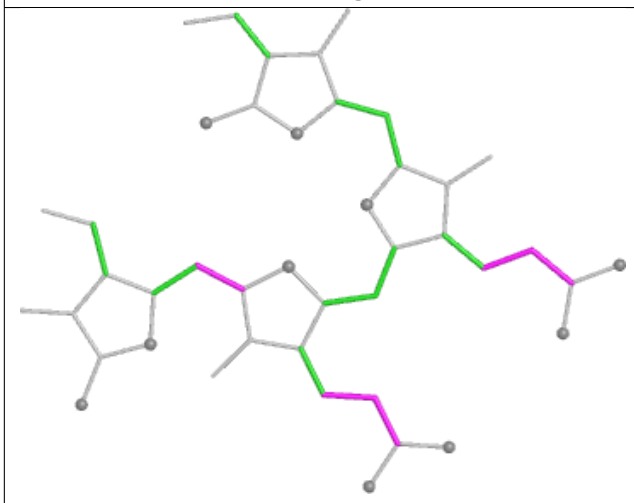
Ligand PEB Y1 202



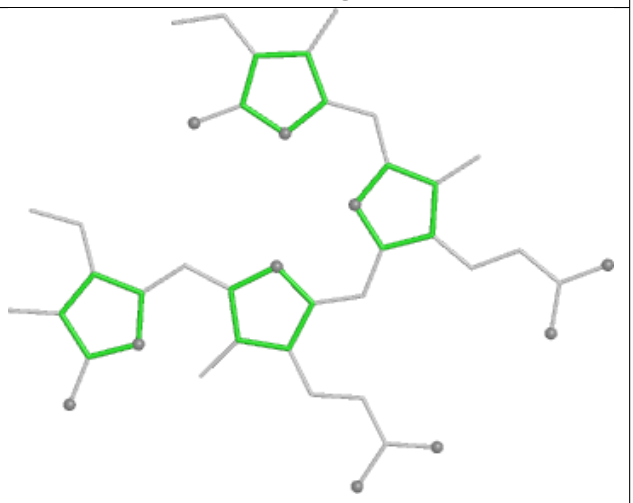
Bond lengths



Bond angles

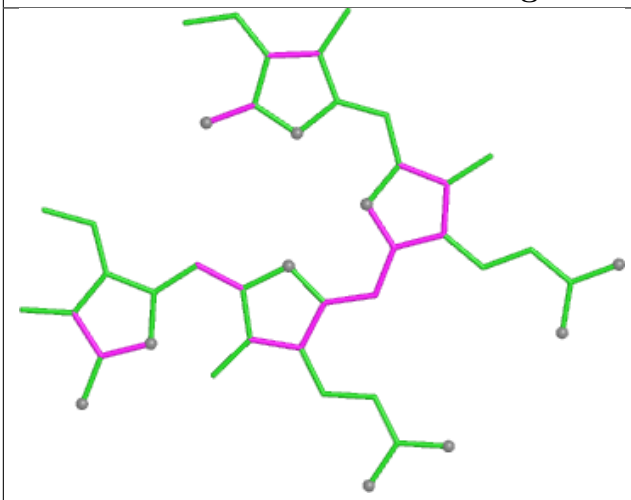


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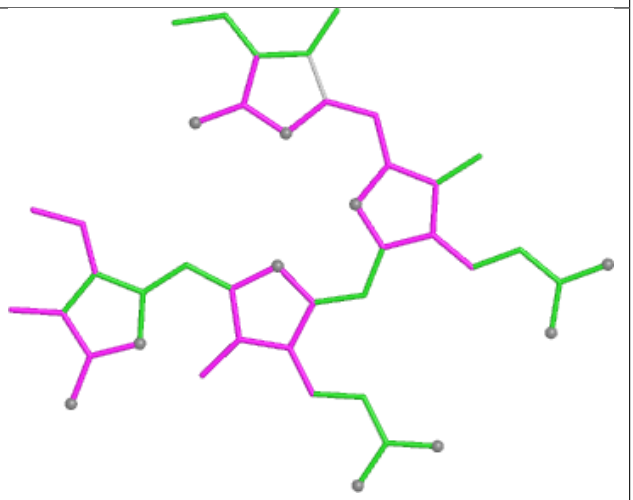


Rings

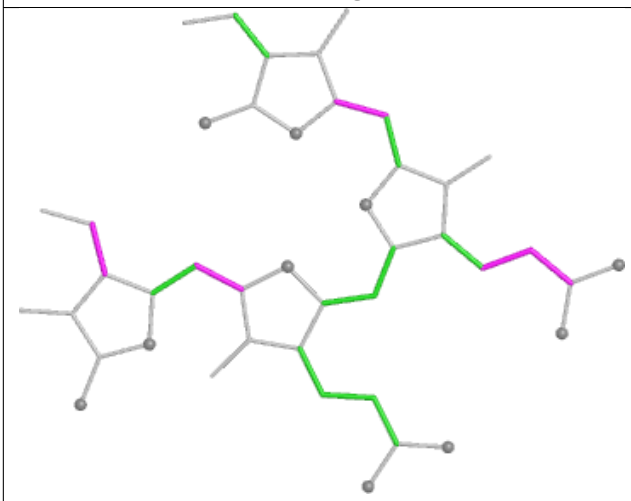
Ligand PEB e1 201



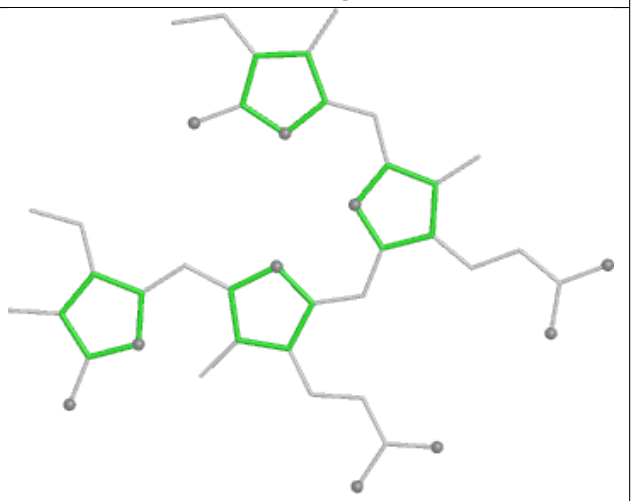
Bond lengths



Bond angles

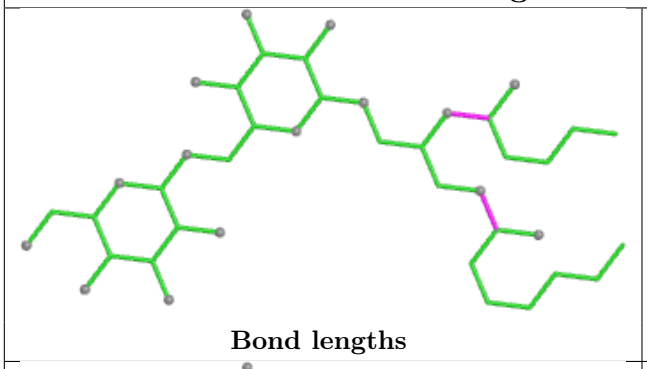


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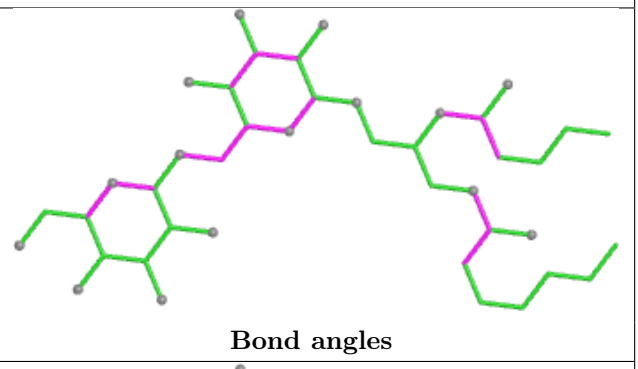


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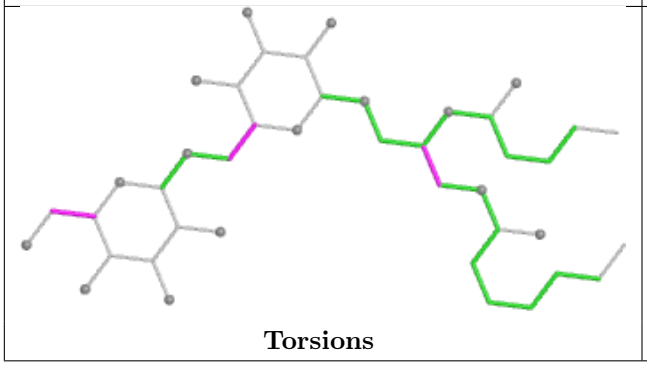
Ligand DGD CL 520



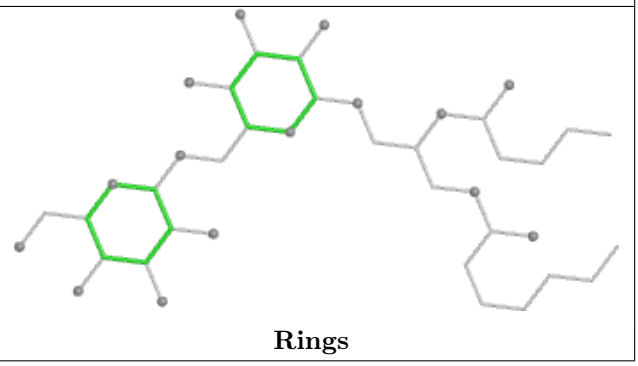
Bond lengths



Bond angles

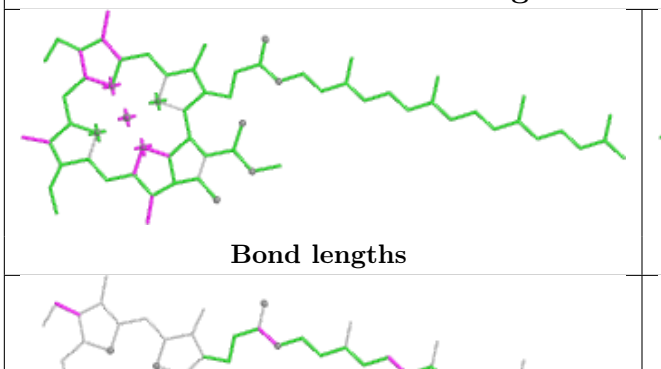


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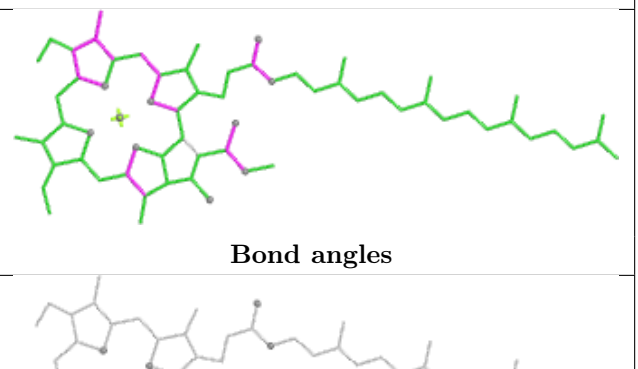


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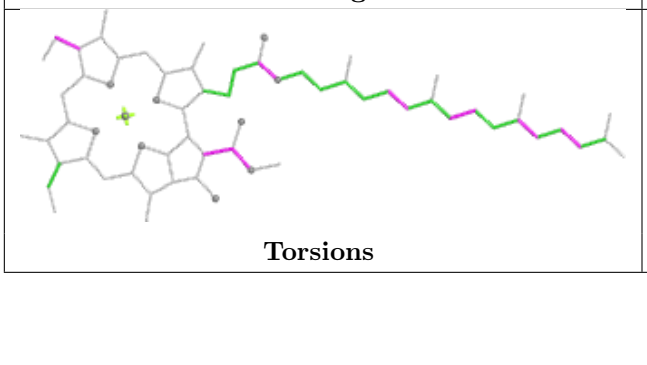
Ligand CLA BN 832



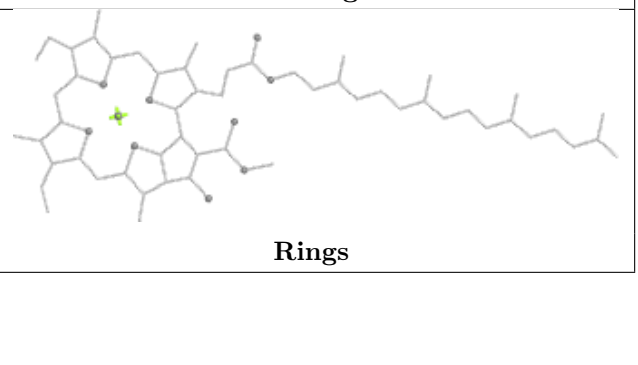
Bond lengths



Bond angles

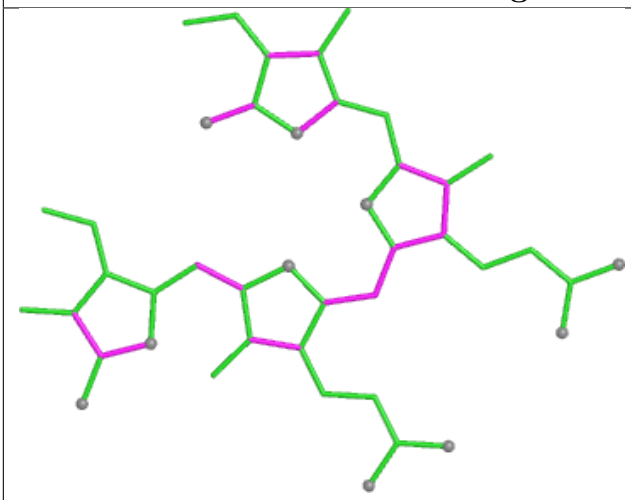


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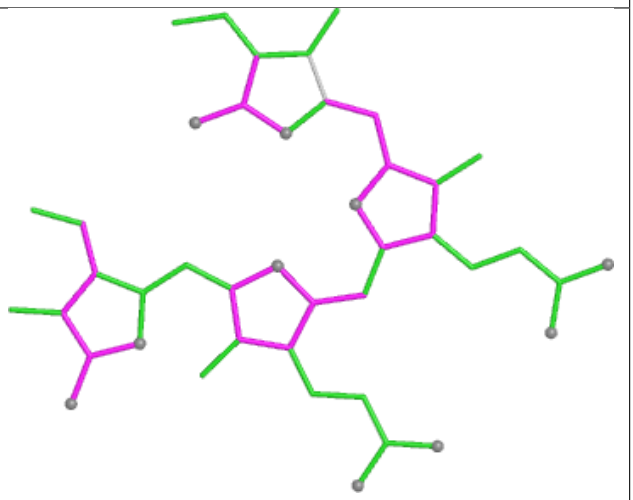


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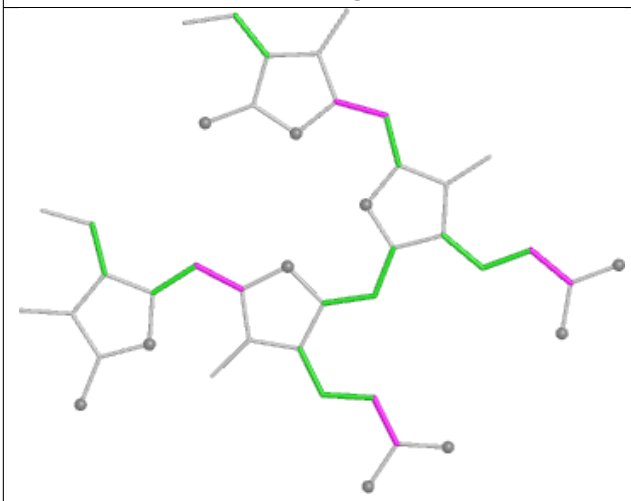
Ligand PEB OD 201



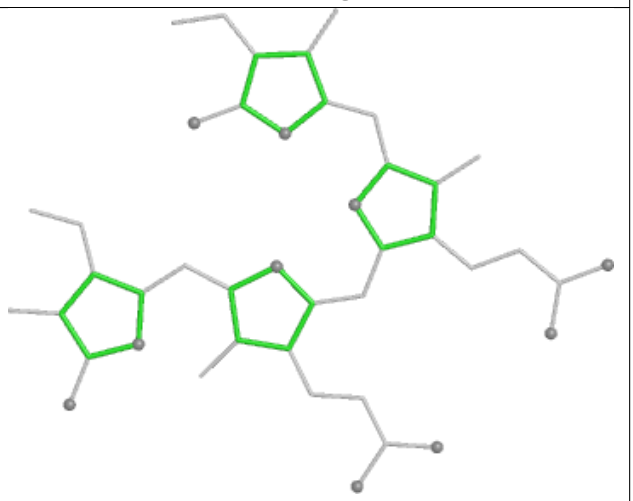
Bond lengths



Bond angles

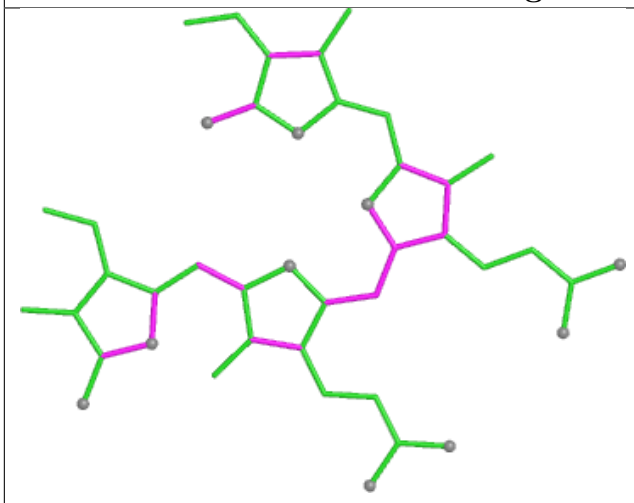


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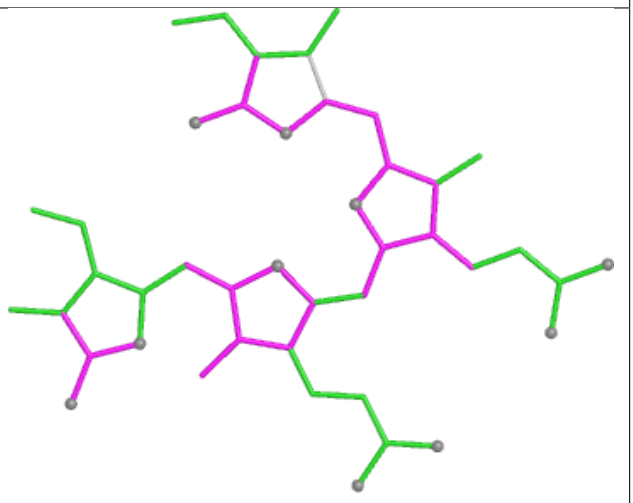


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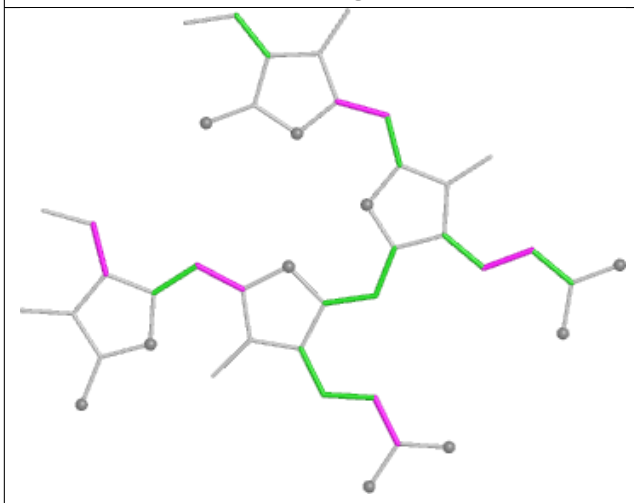
Ligand PEB II 201



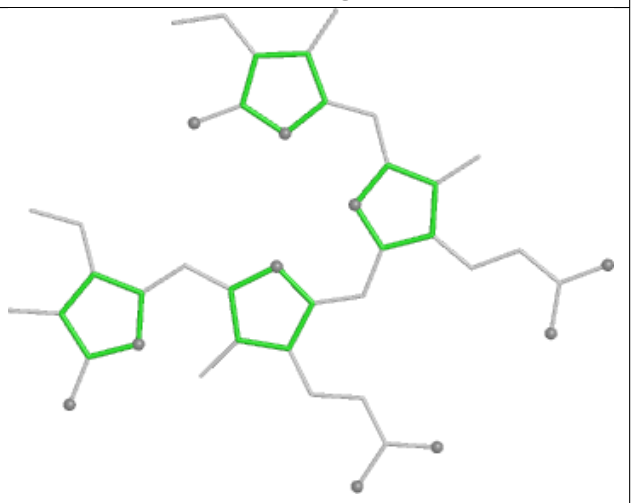
Bond lengths



Bond angles

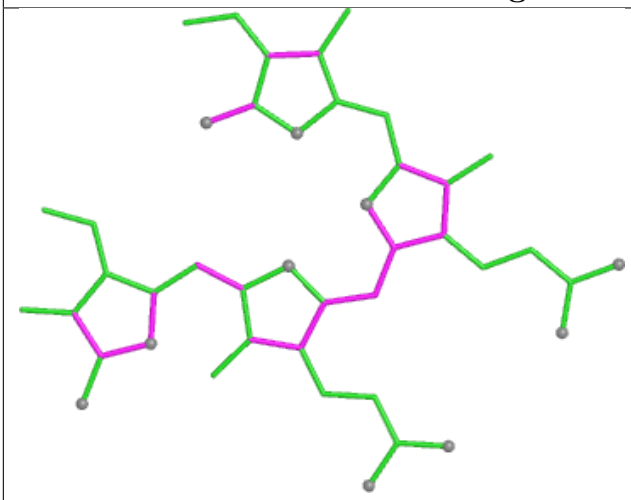


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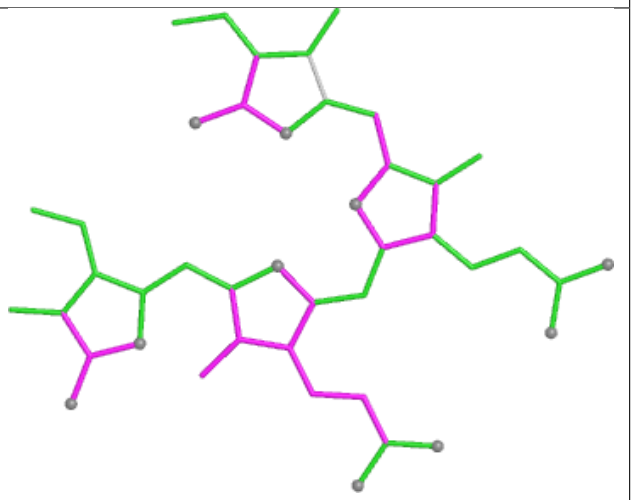


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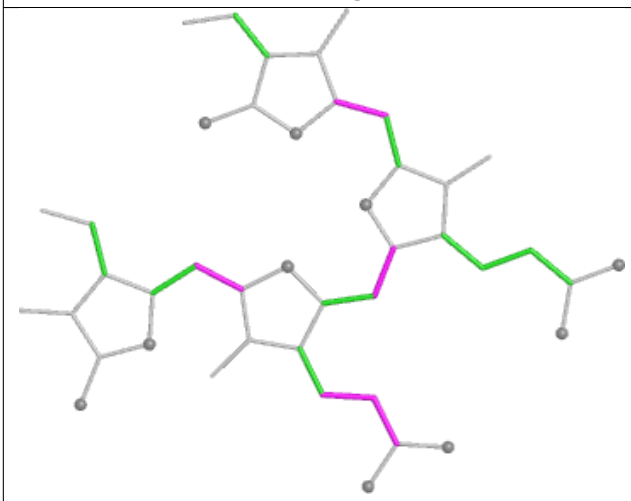
Ligand PEB mG 203



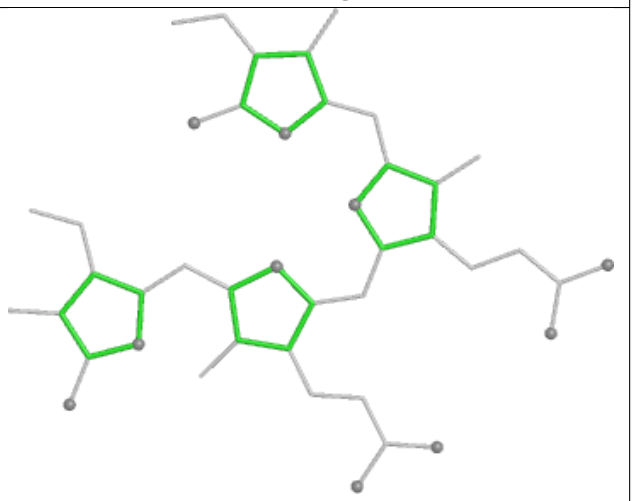
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Bond angles

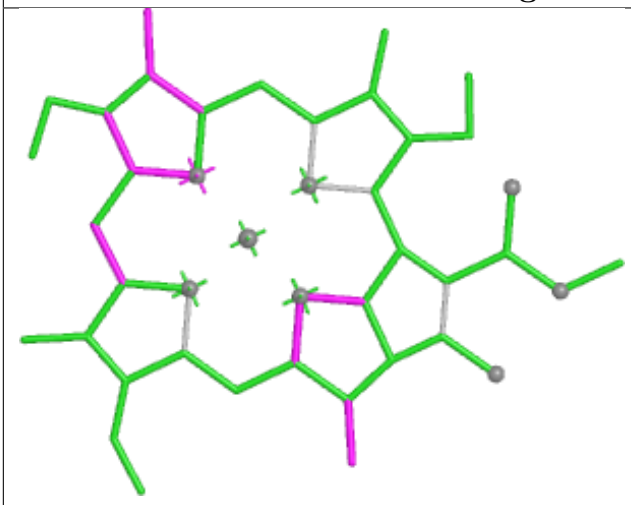


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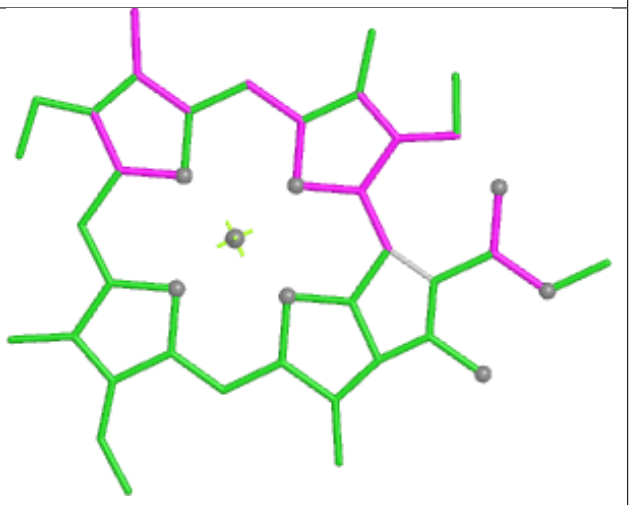


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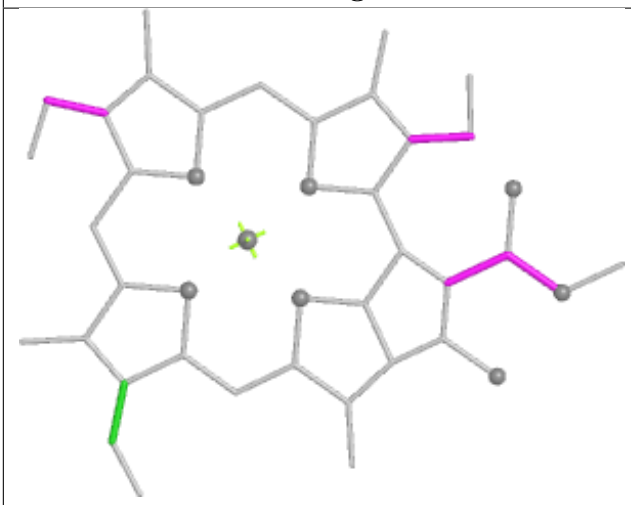
Ligand CLA 22 611



Bond lengths



Bond angles

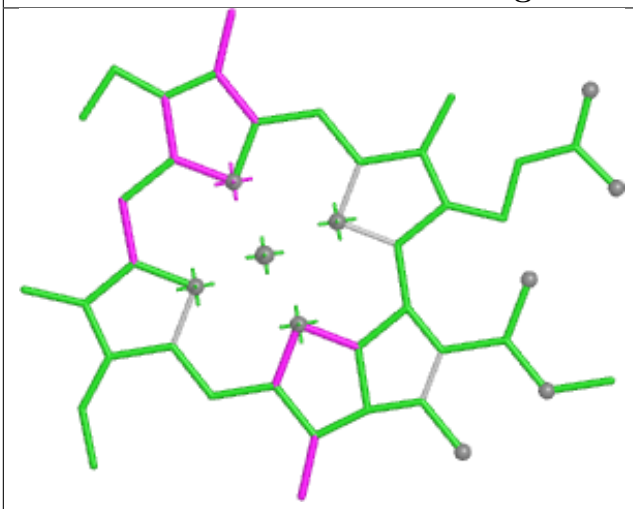


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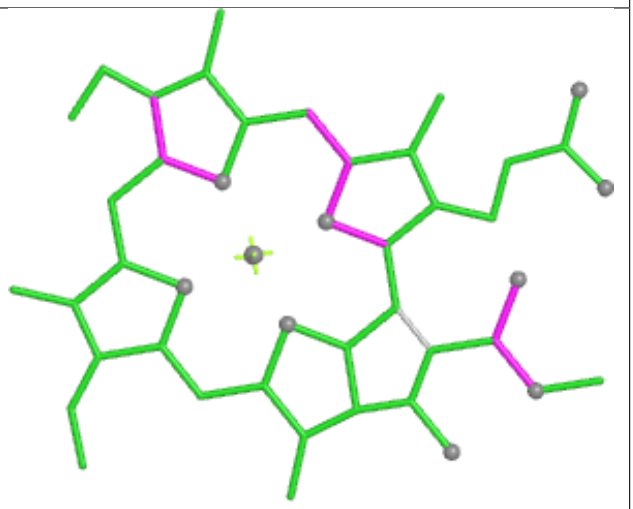


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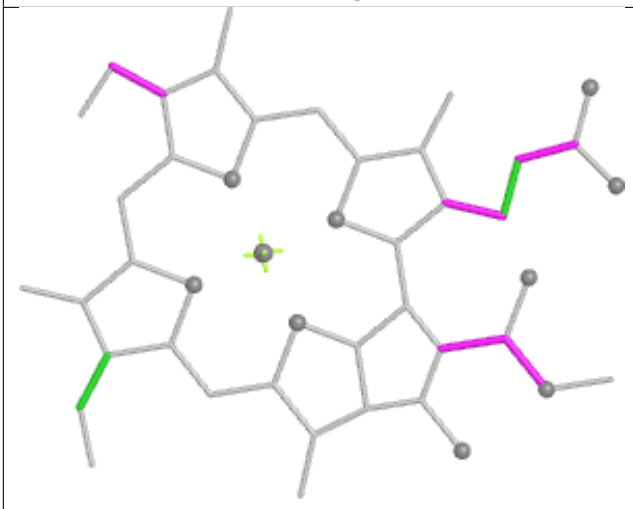
Ligand CLA 6N 603



Bond lengths



Bond angles

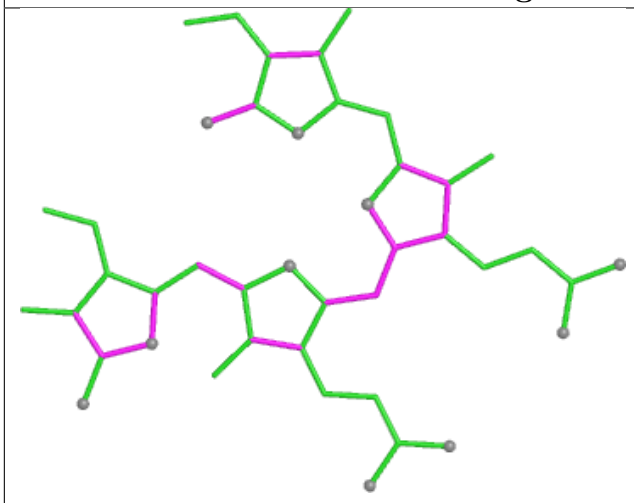


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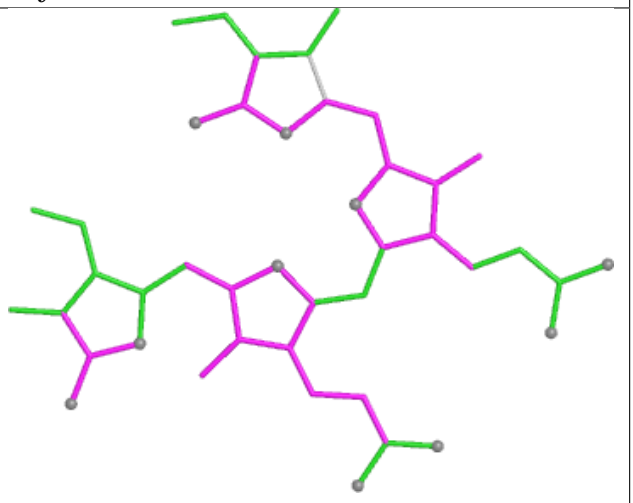


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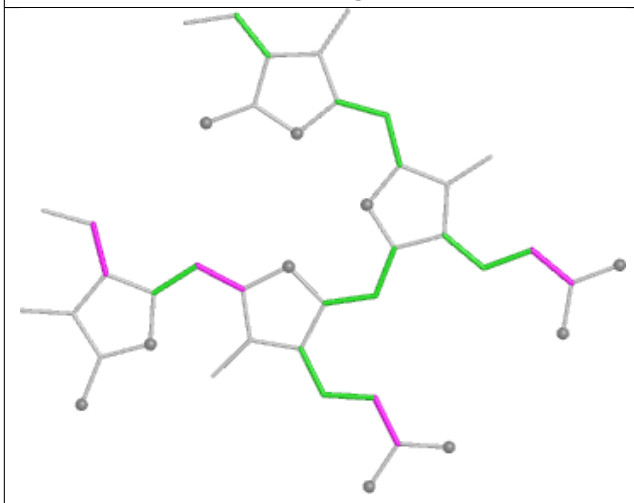
Ligand PEB yK 301



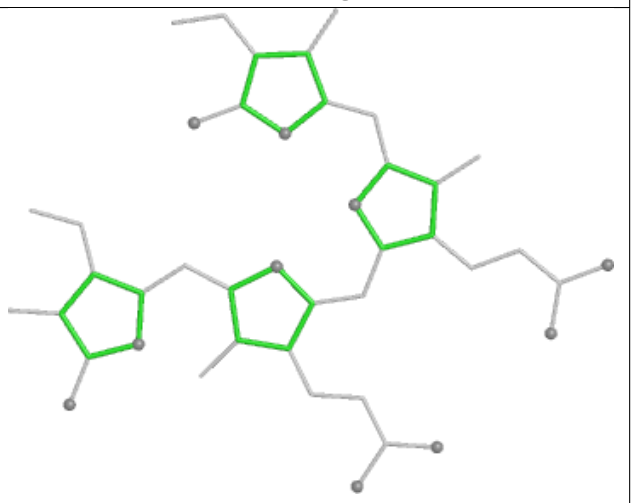
Bond lengths



Bond angles

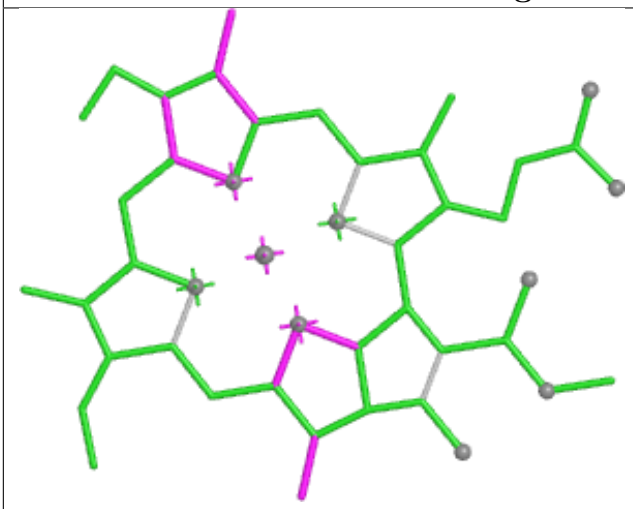


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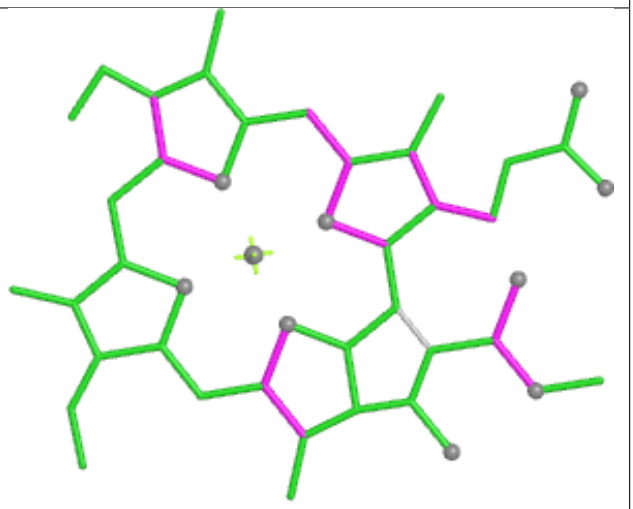


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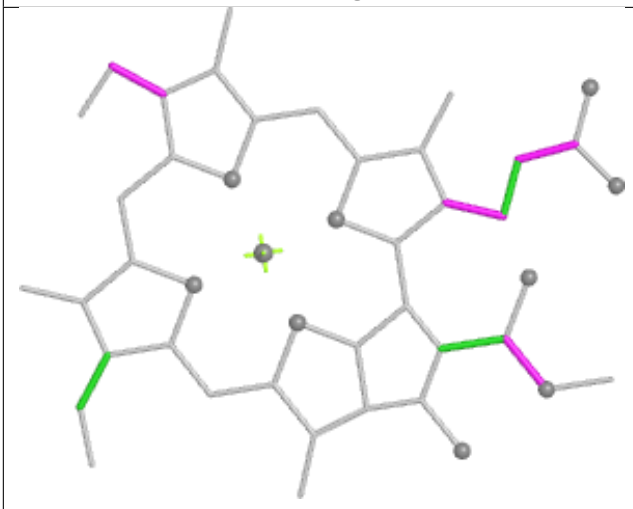
Ligand CLA 4N 606



Bond lengths



Bond angles

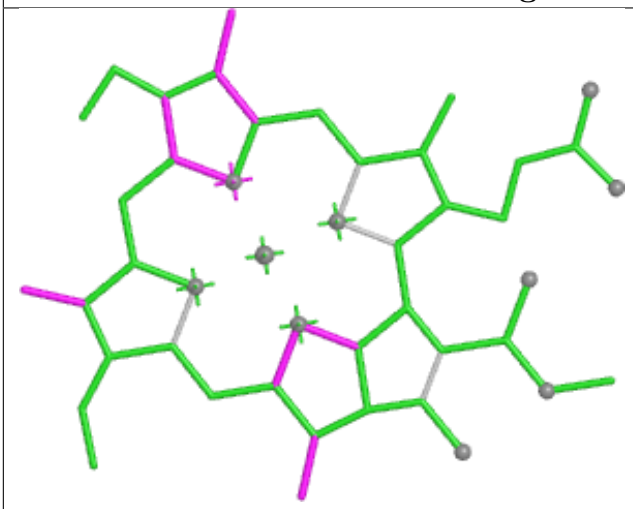


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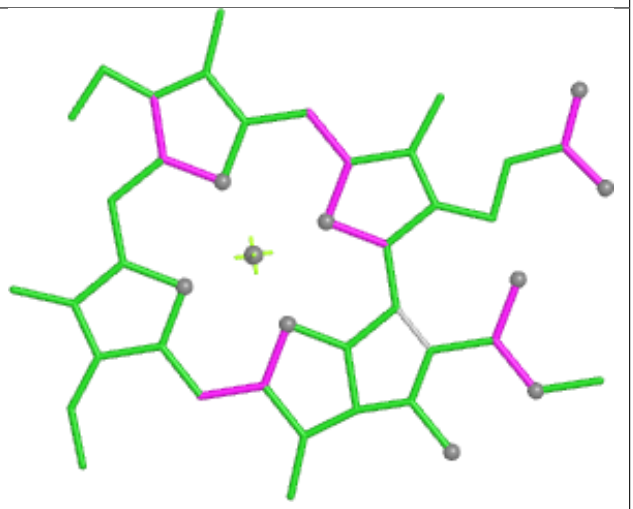


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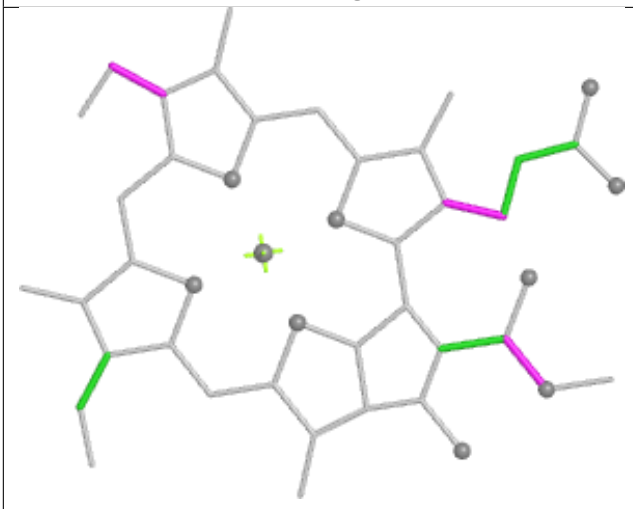
Ligand CLA 52 610



Bond lengths



Bond angles

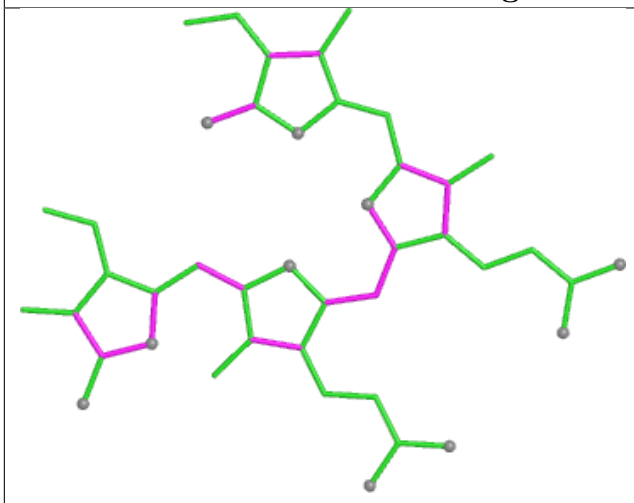


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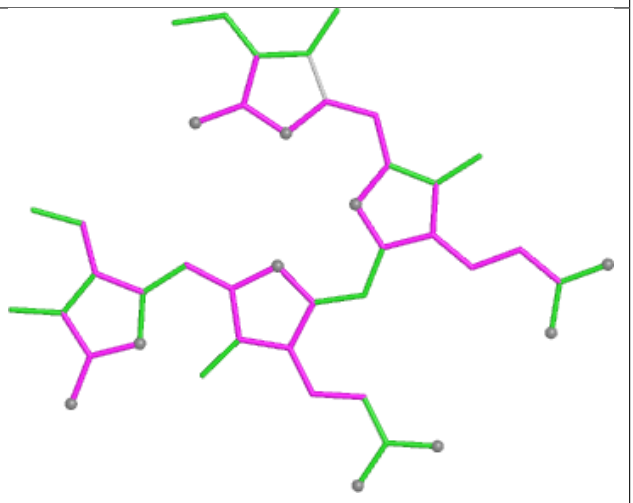


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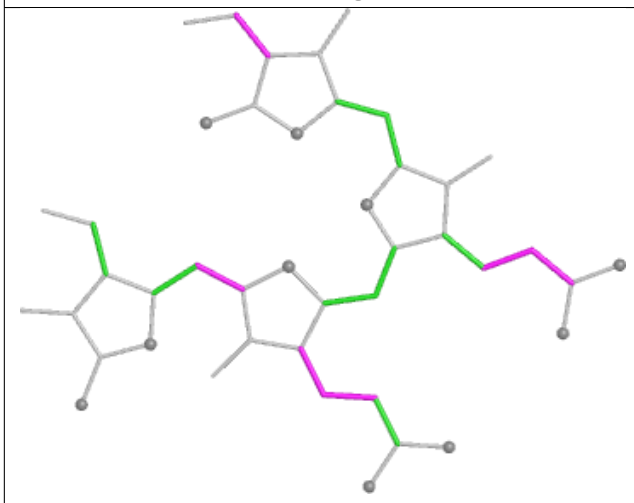
Ligand PEB GG 1002



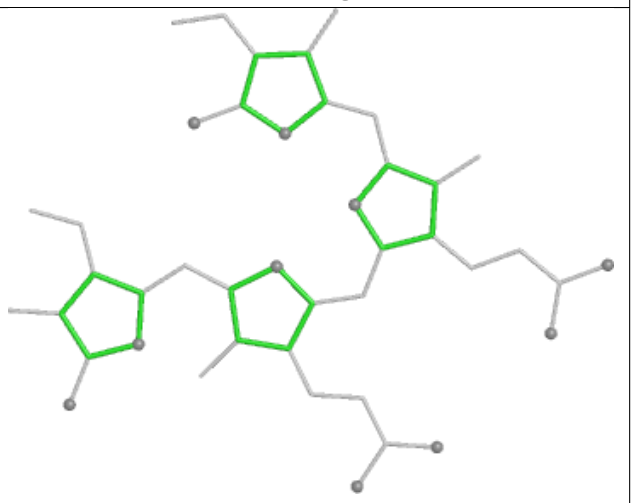
Bond lengths



Bond angles

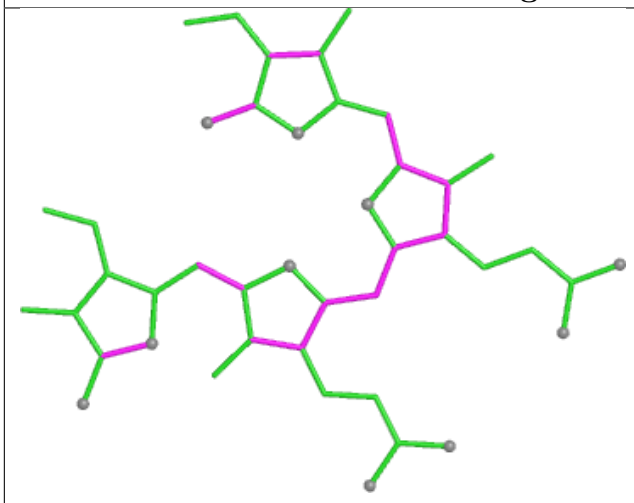


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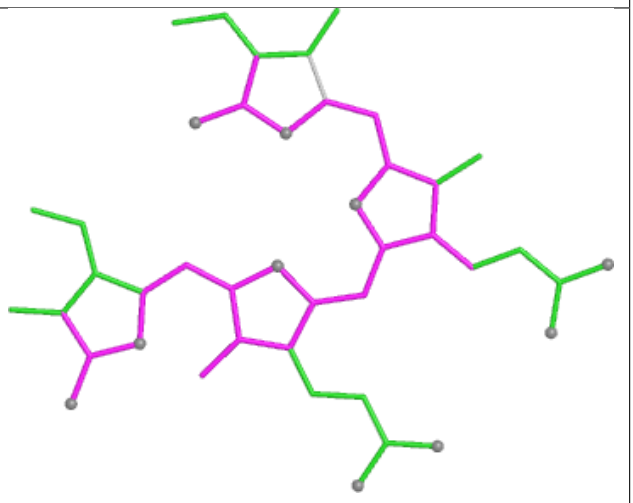


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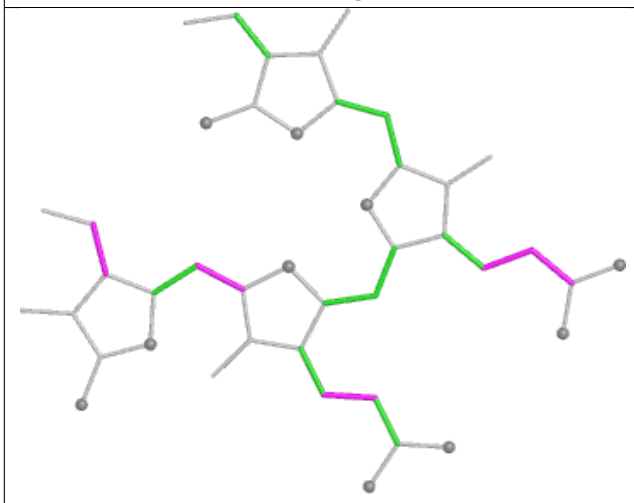
Ligand PEB J7 202



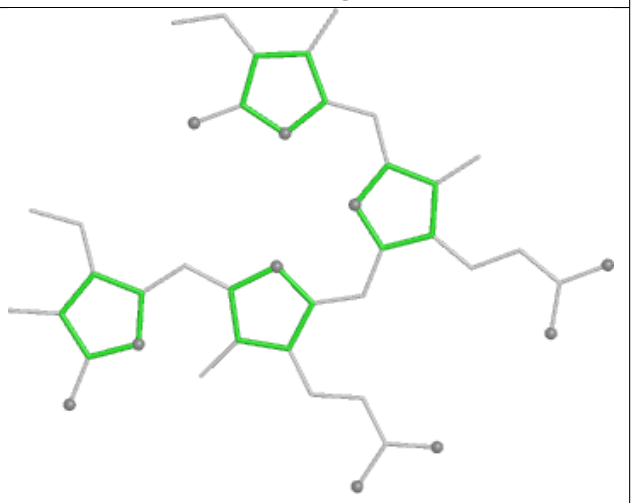
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Bond angles

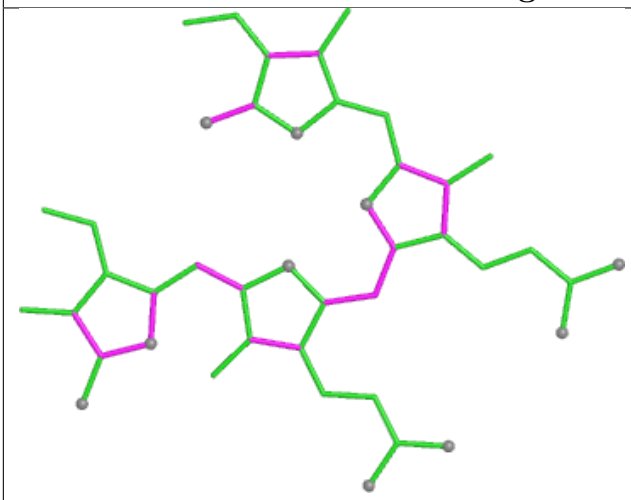


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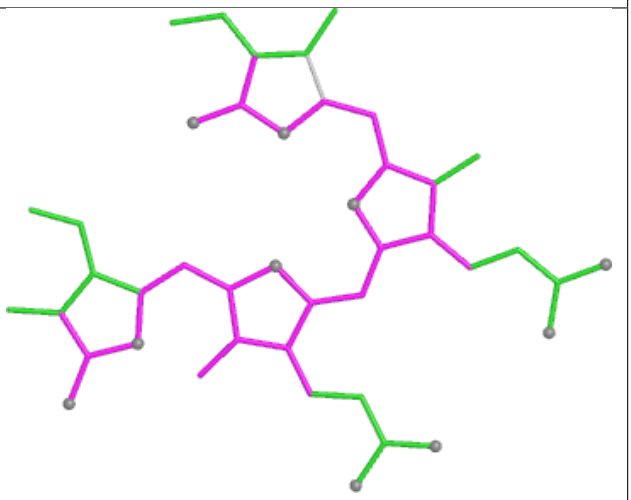


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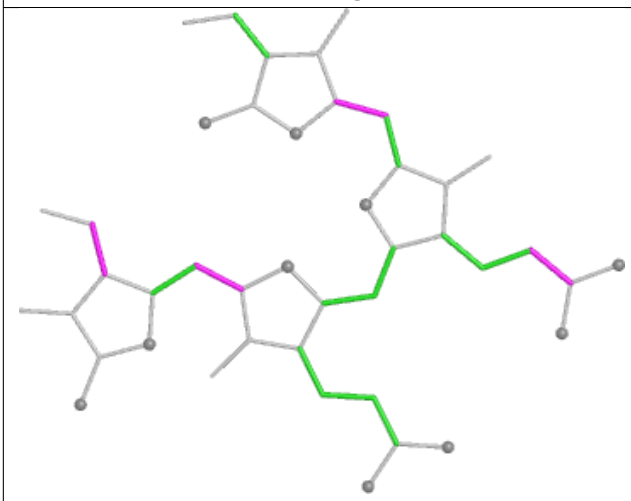
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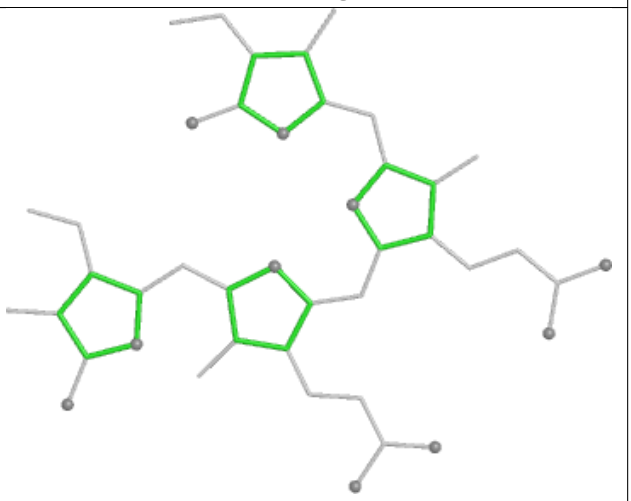
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Bond angles

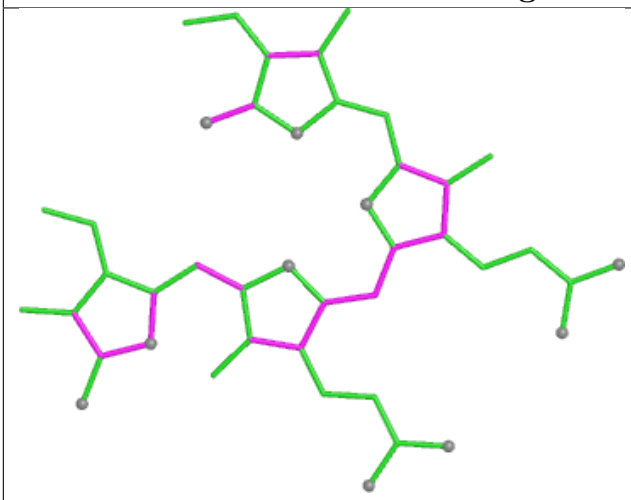


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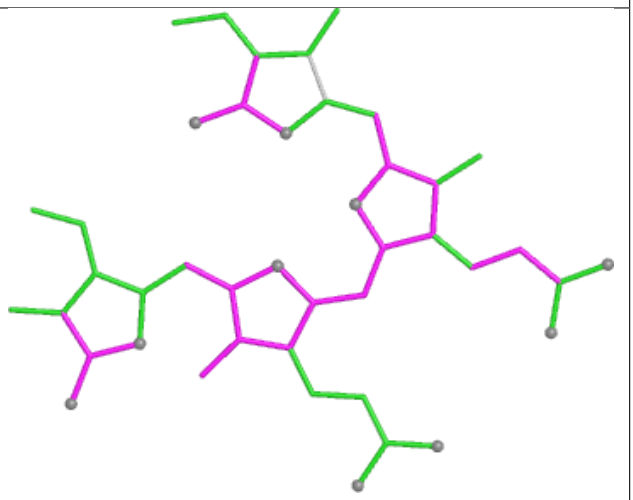


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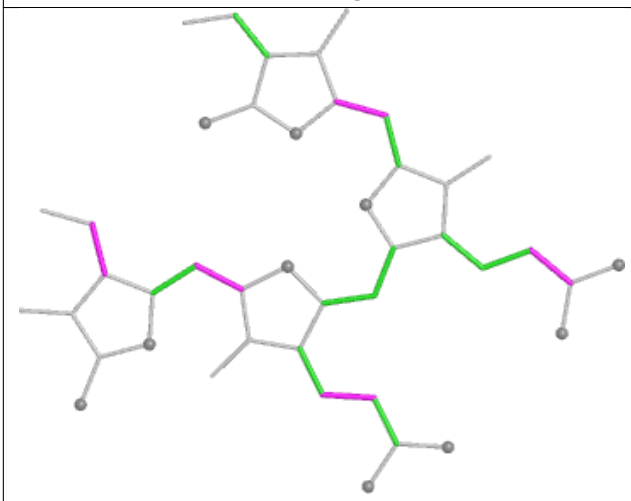
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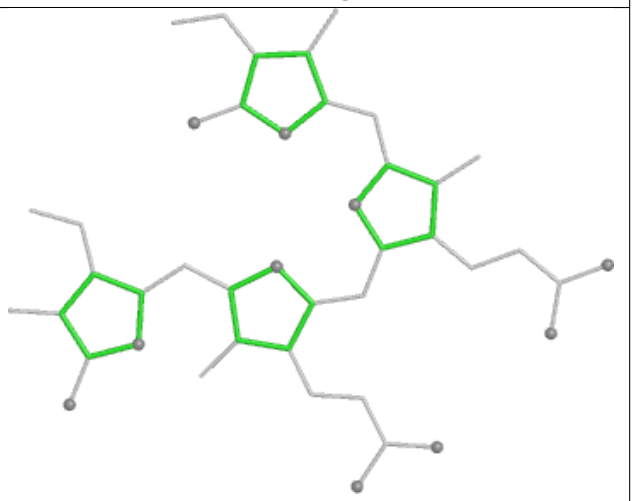
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Bond angles

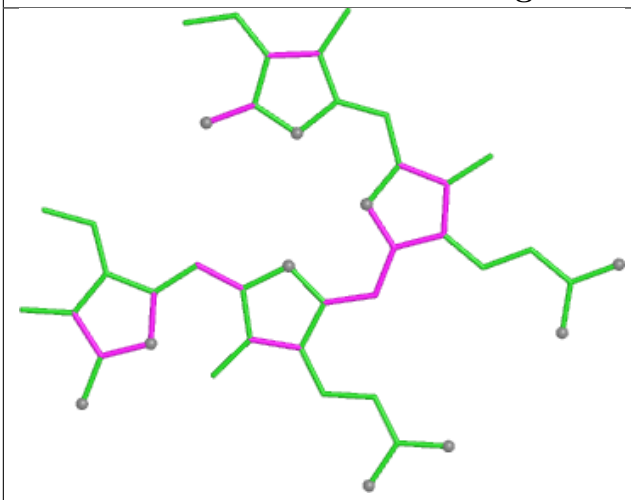


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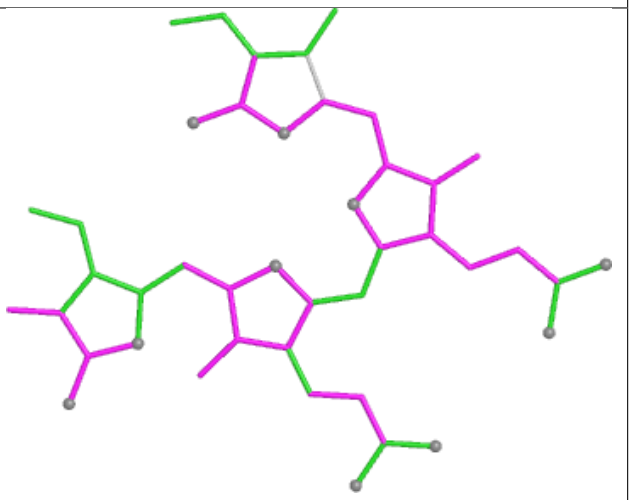


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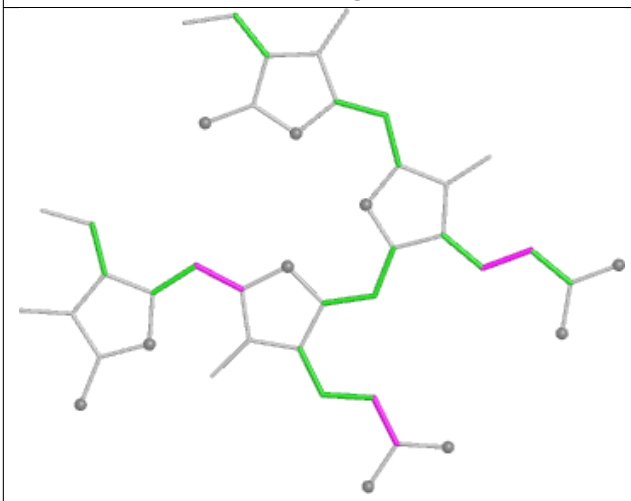
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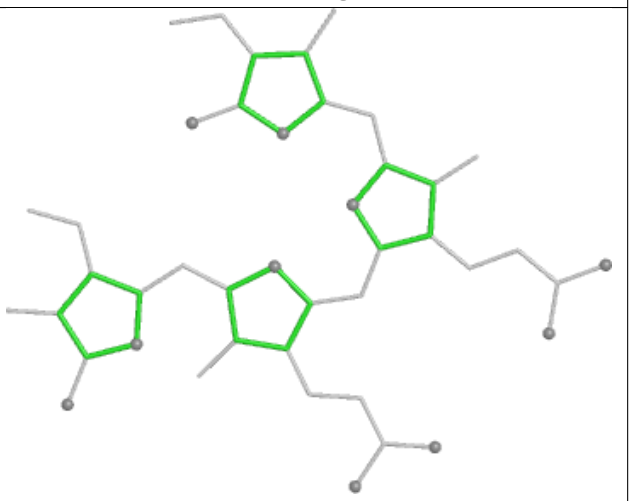
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Bond angles

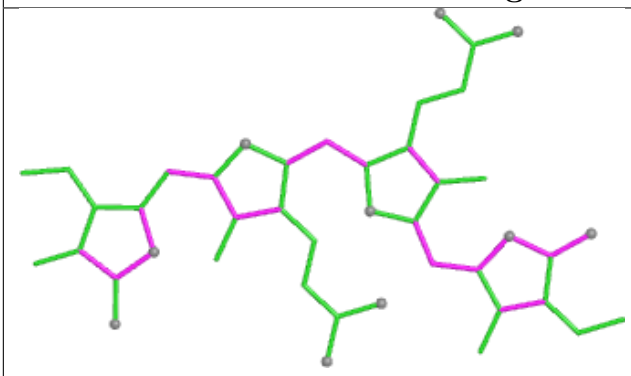


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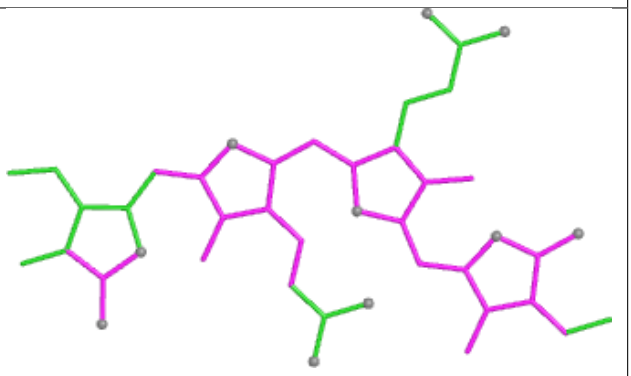


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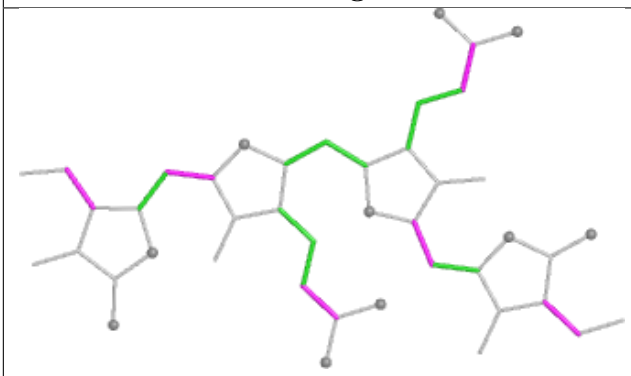
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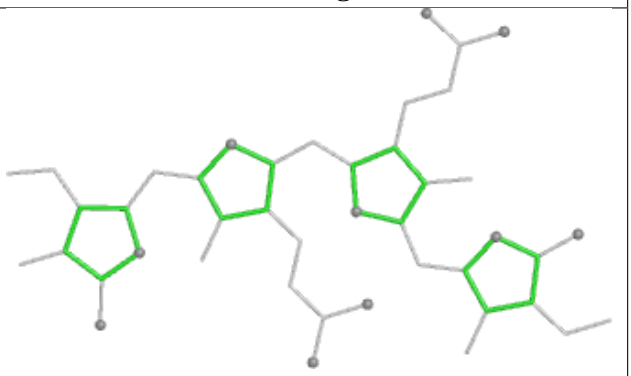
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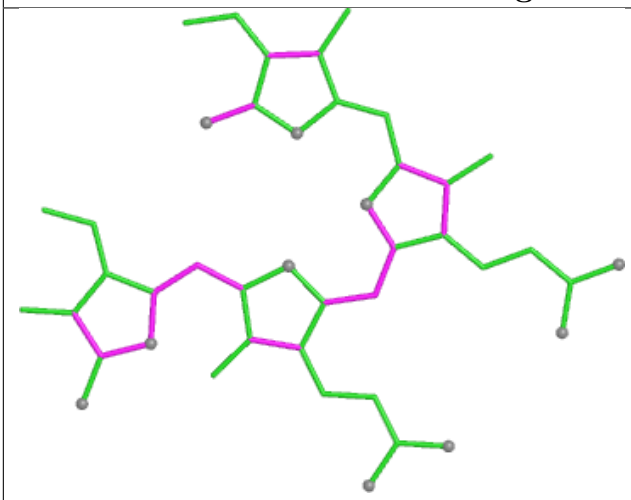


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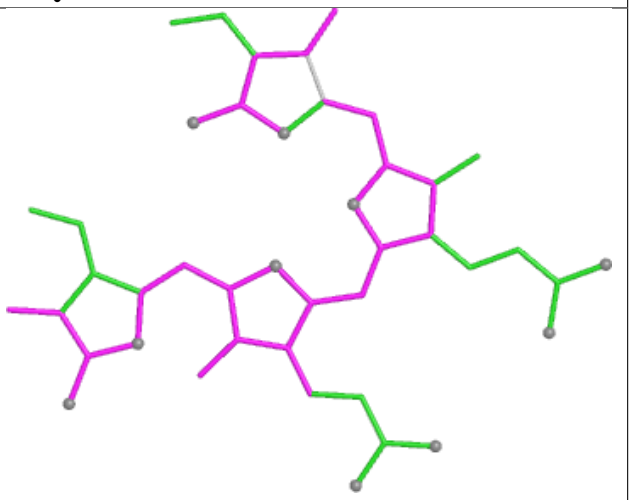


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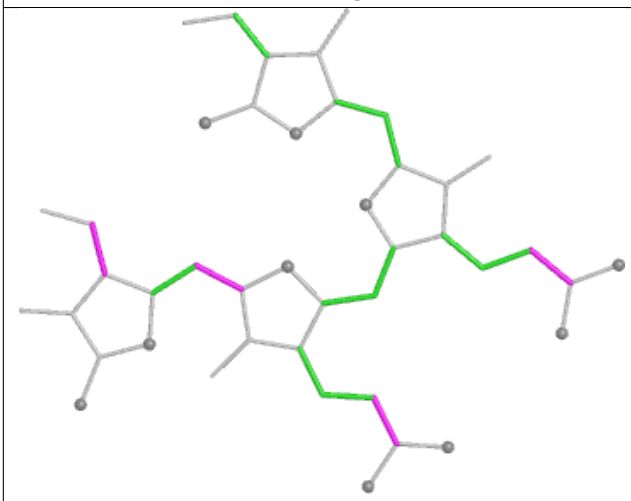
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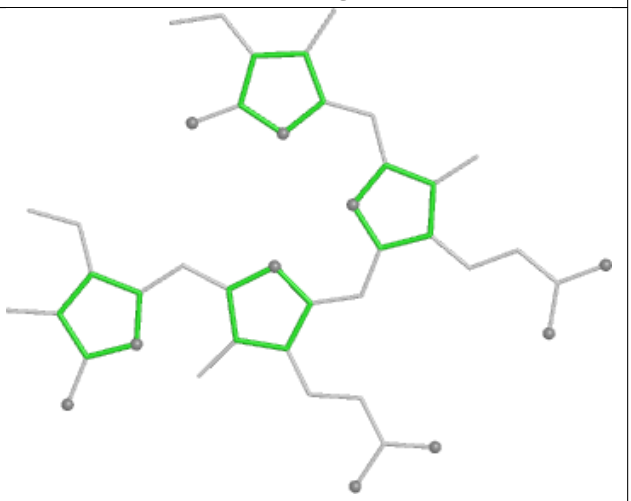
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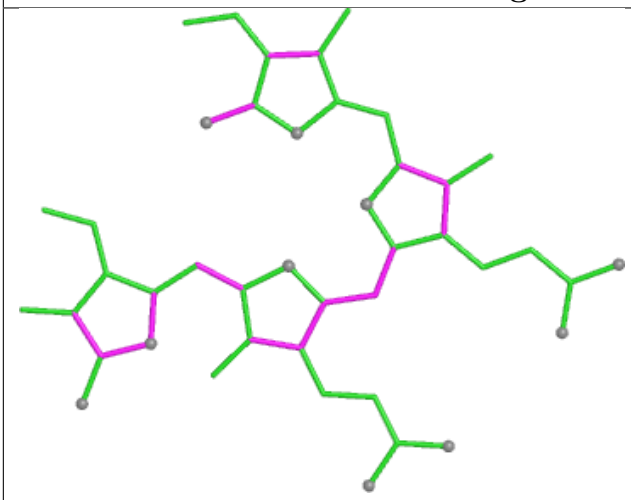


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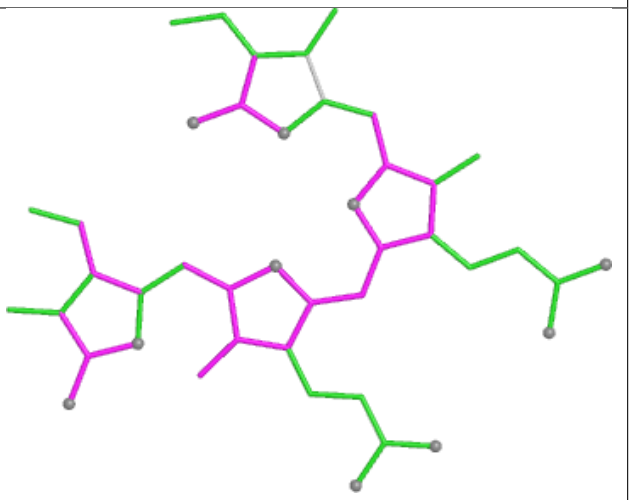


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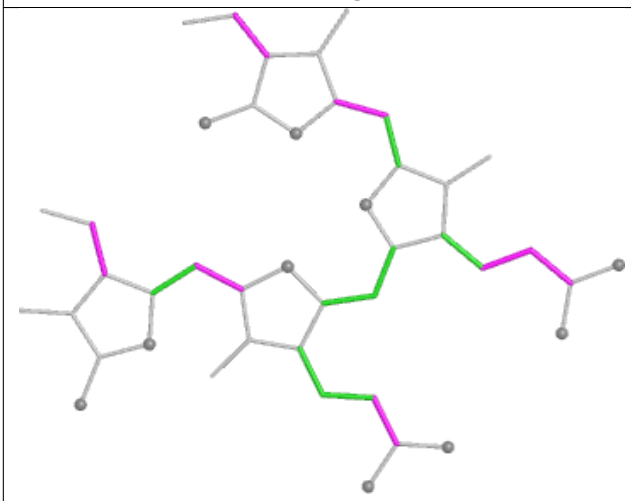
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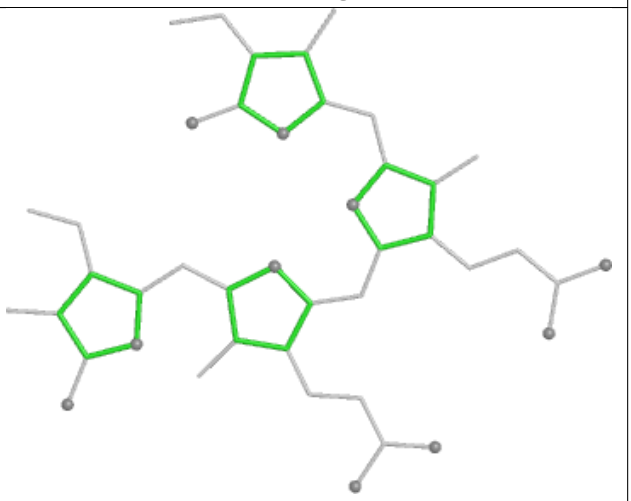
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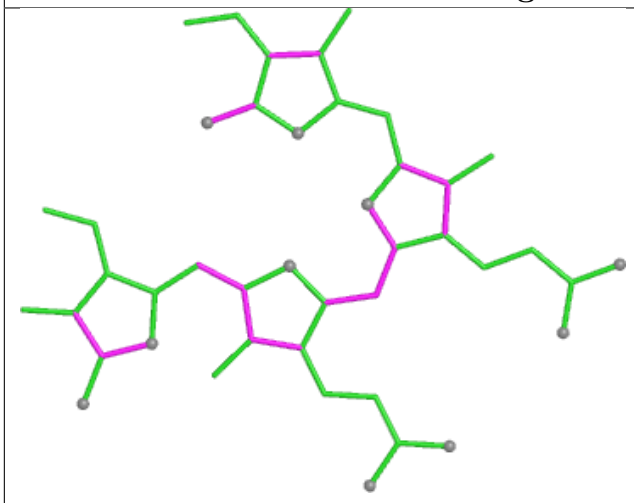


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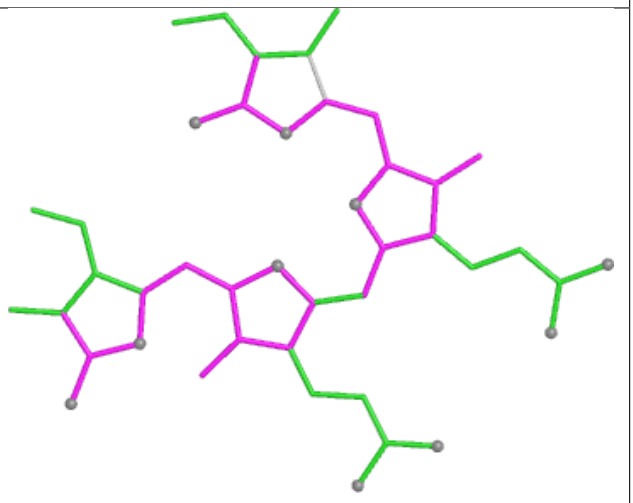


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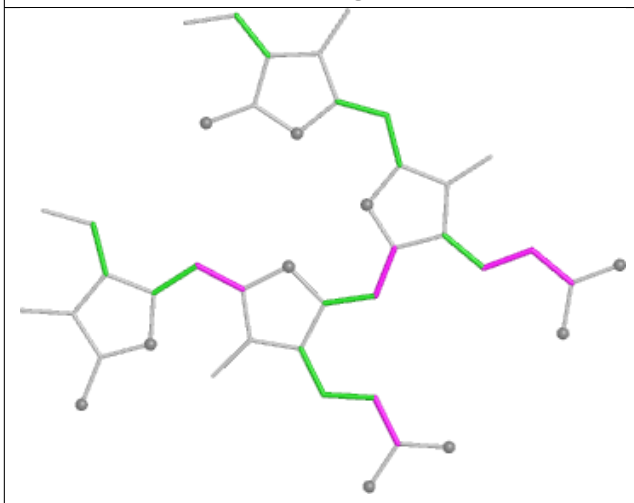
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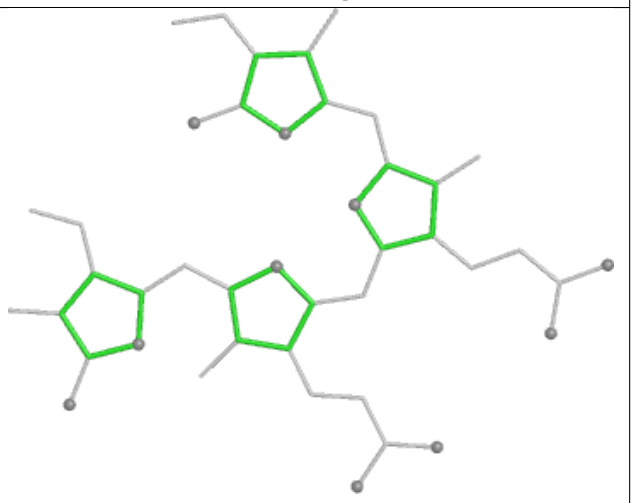
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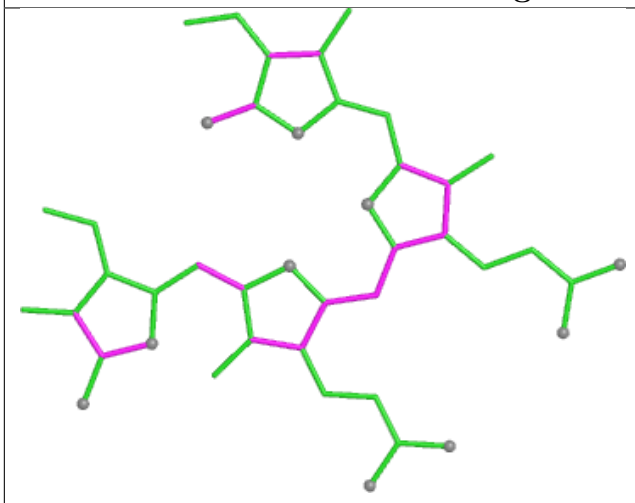


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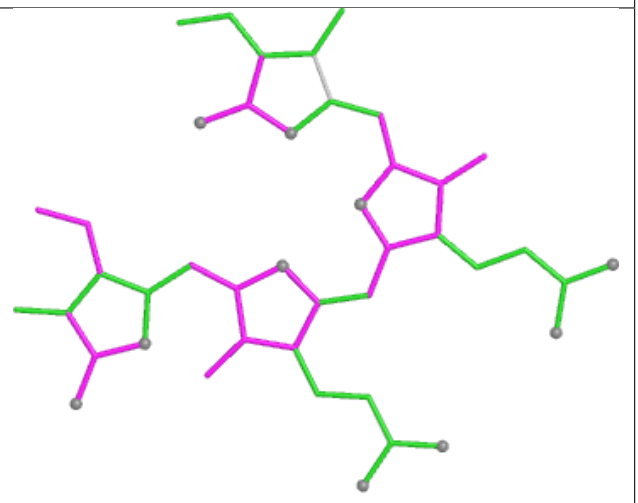


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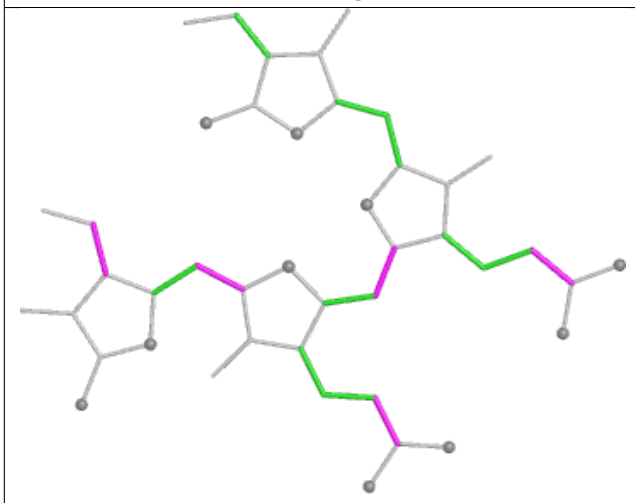
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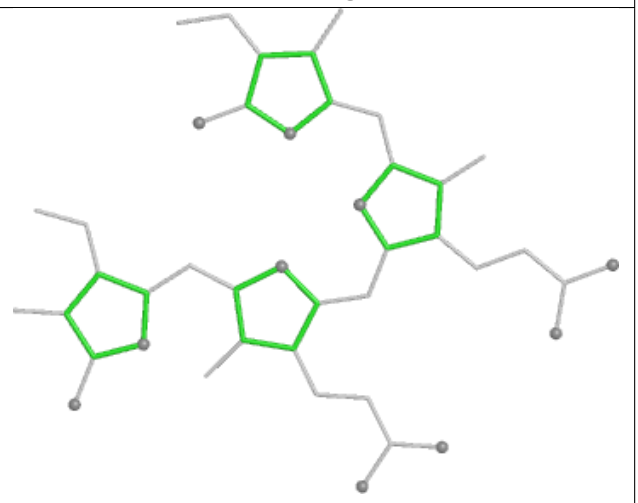
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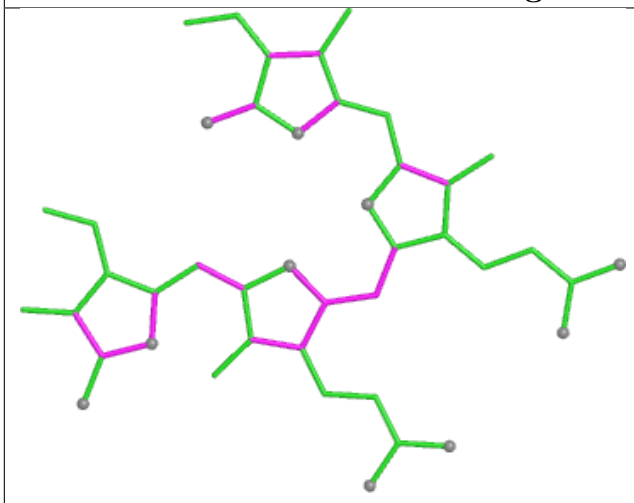


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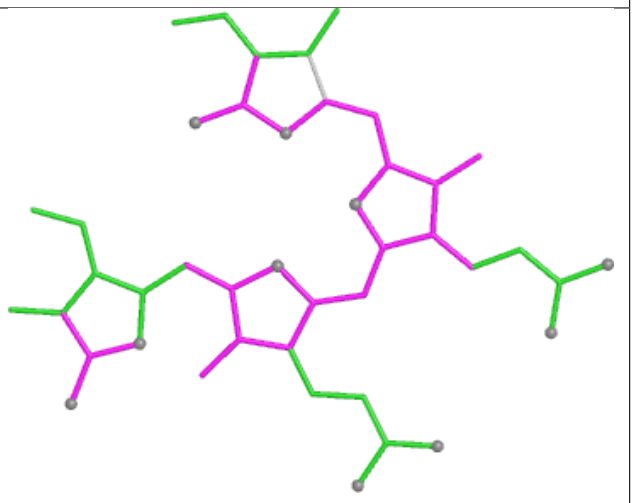


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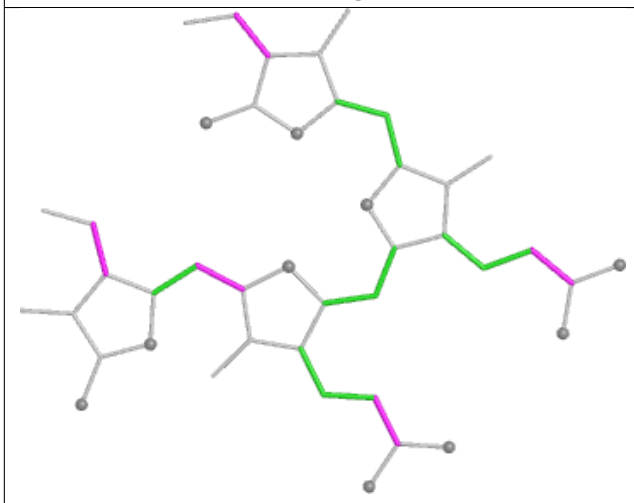
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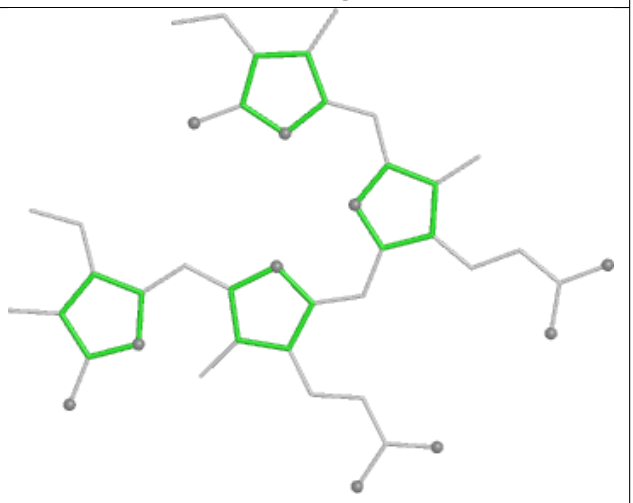
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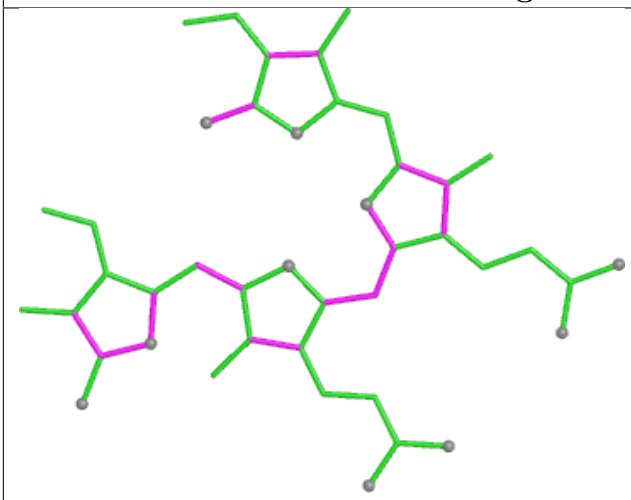


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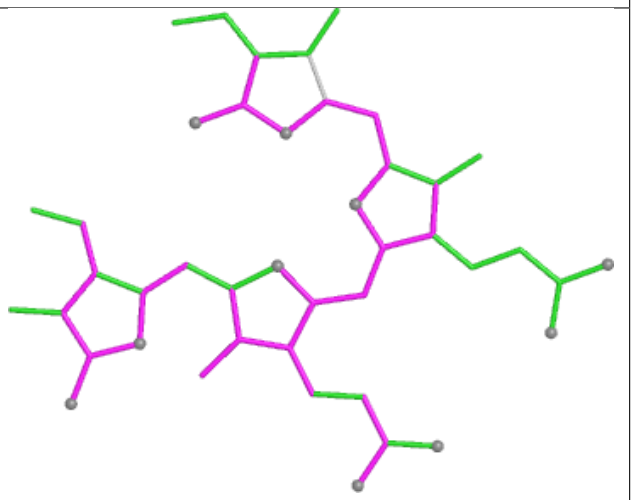


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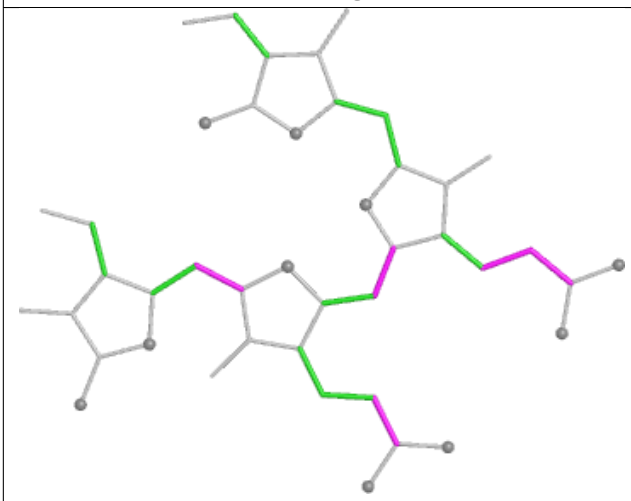
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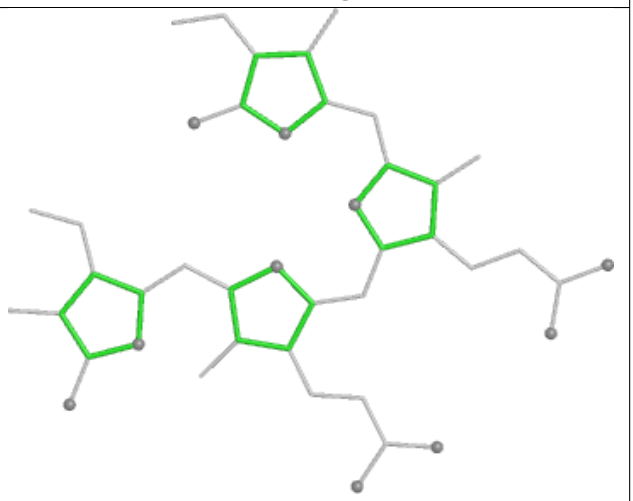
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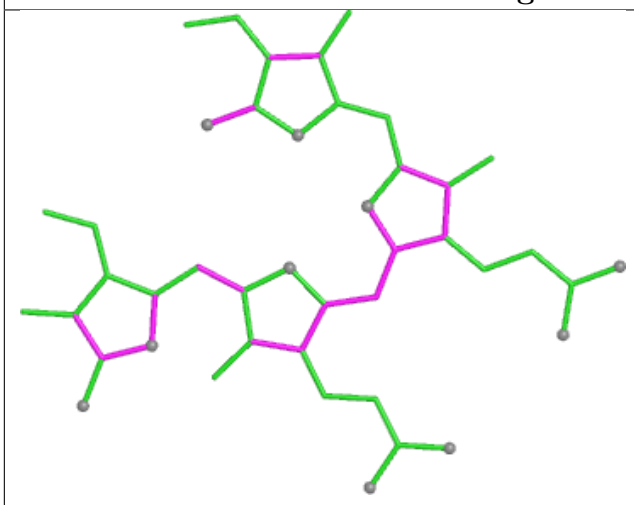


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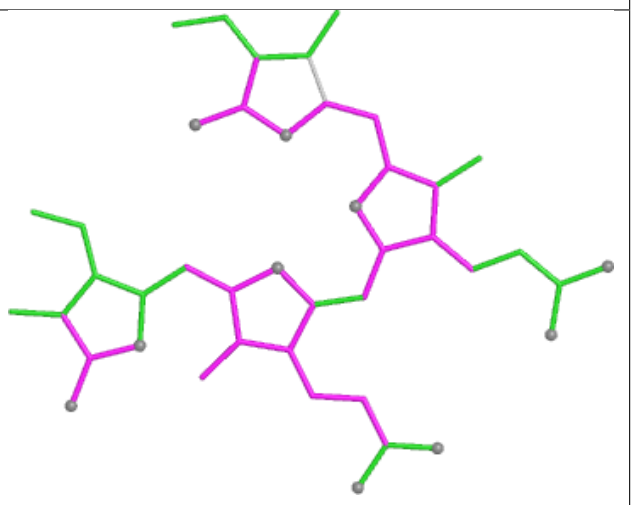


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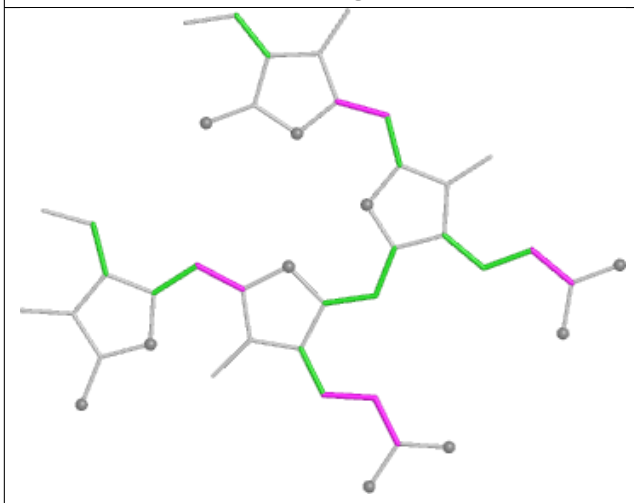
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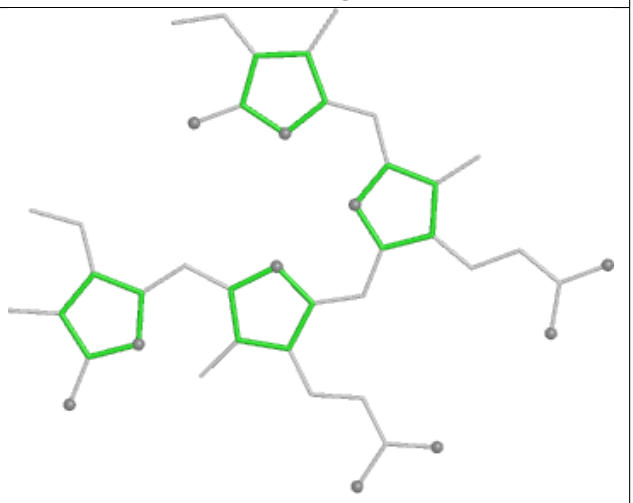
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Bond angles

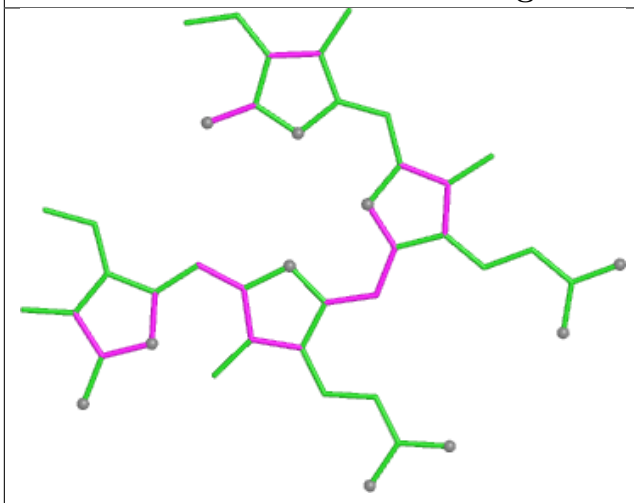


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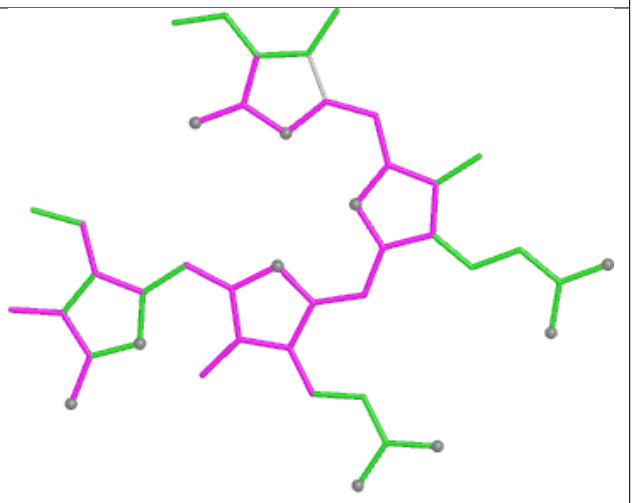


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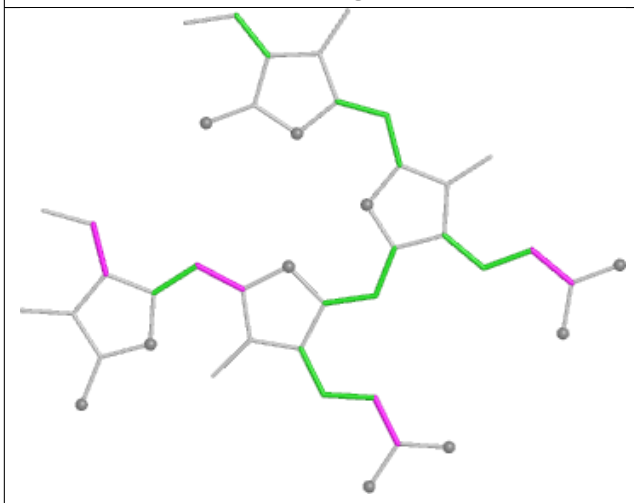
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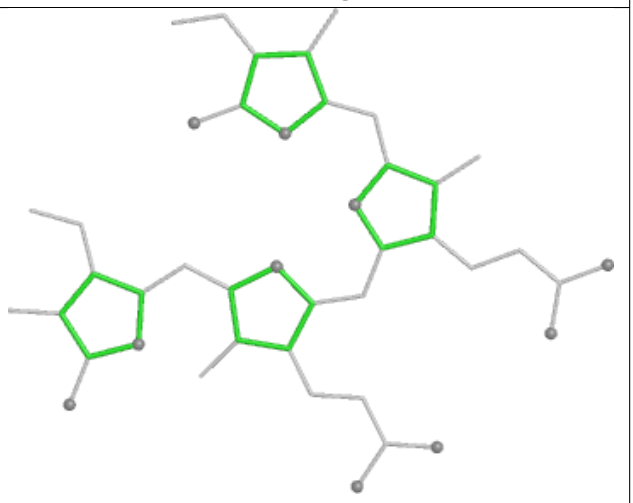
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Bond angles



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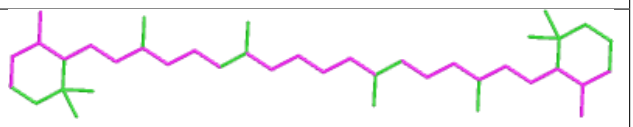


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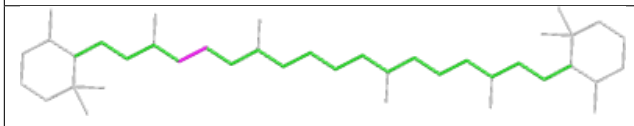
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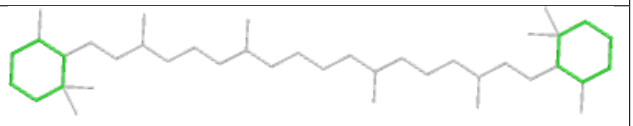
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Bond angles

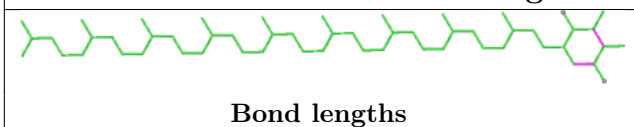


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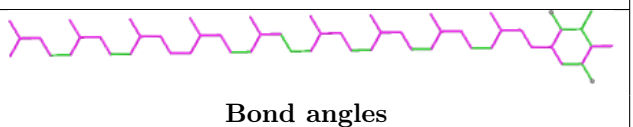


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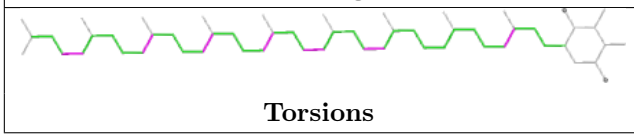
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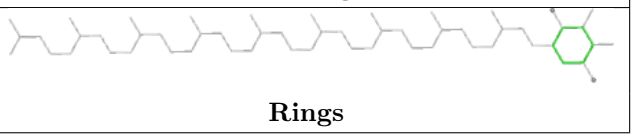
Bond lengths



Bond angles

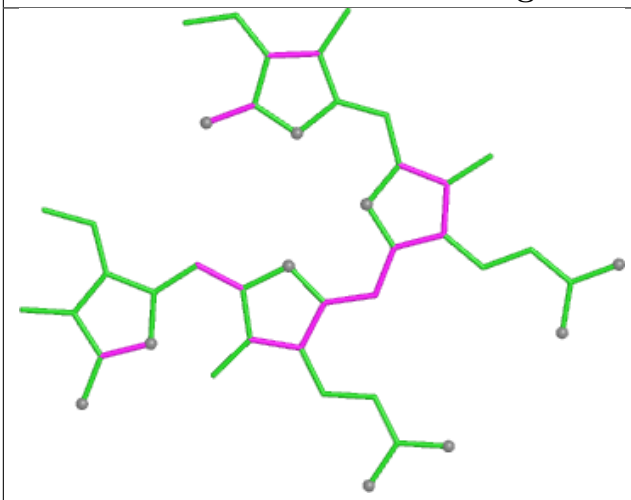


Torsions

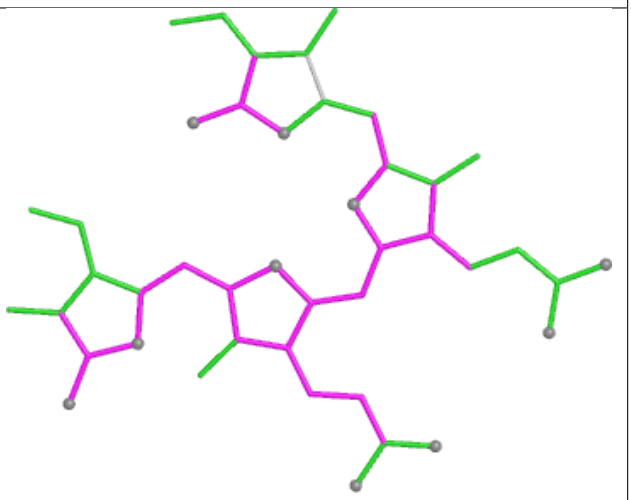


Rings

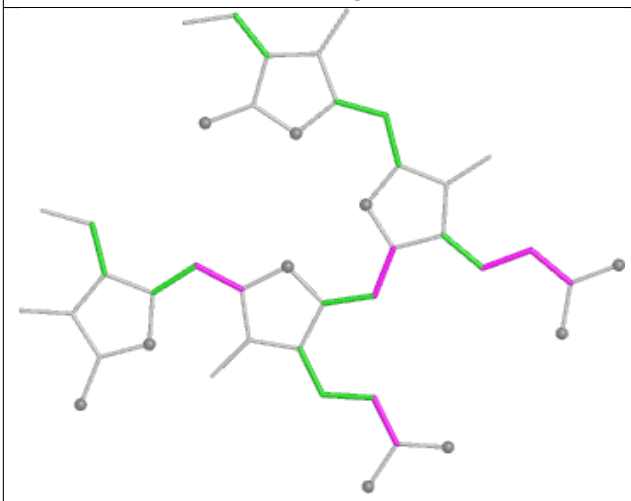
Ligand PEB xF 304



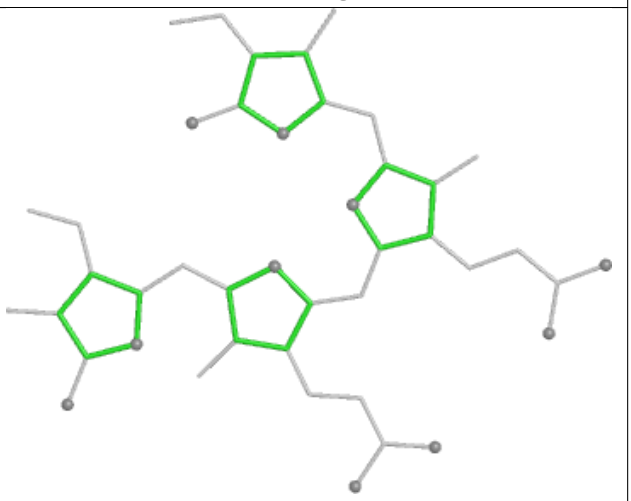
Bond lengths



Bond angles

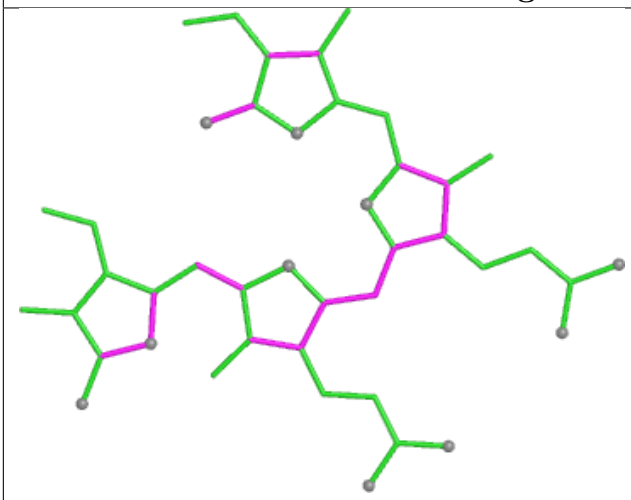


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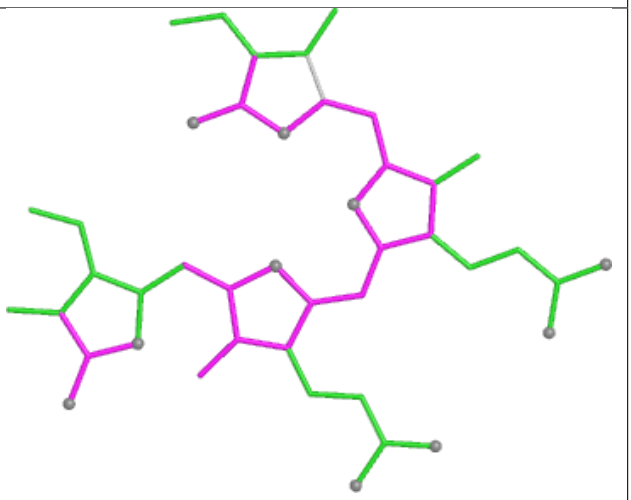


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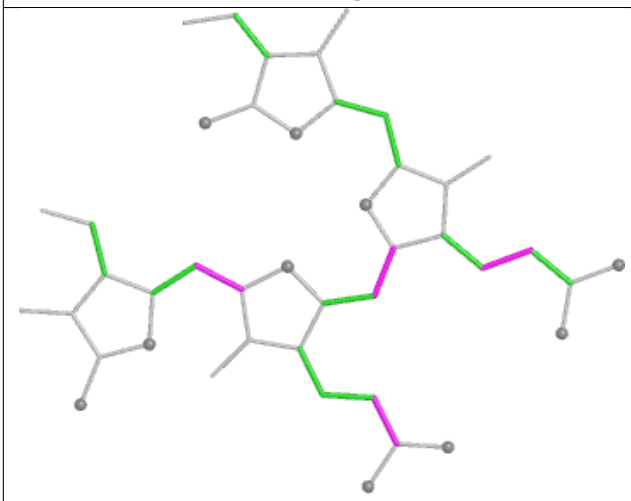
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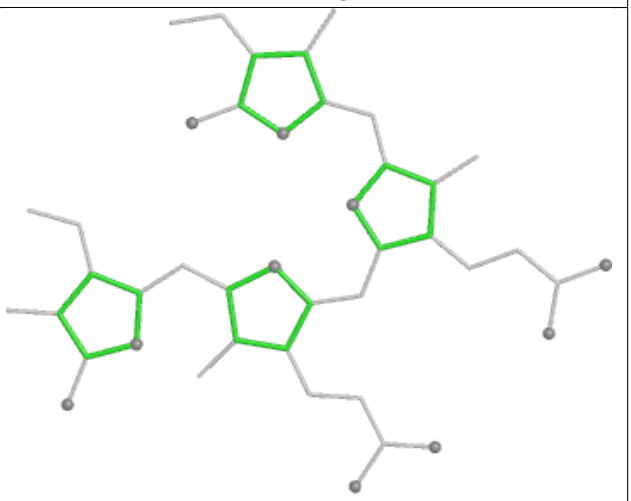
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Bond angles

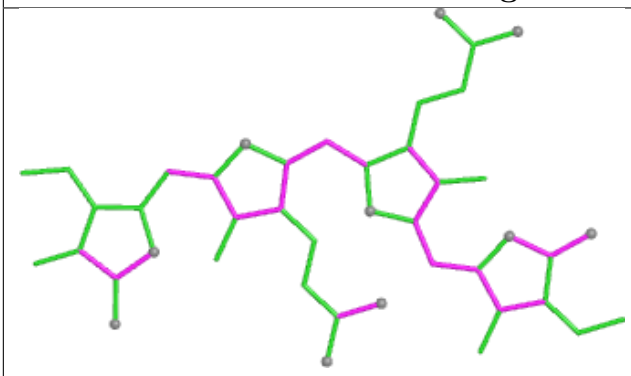


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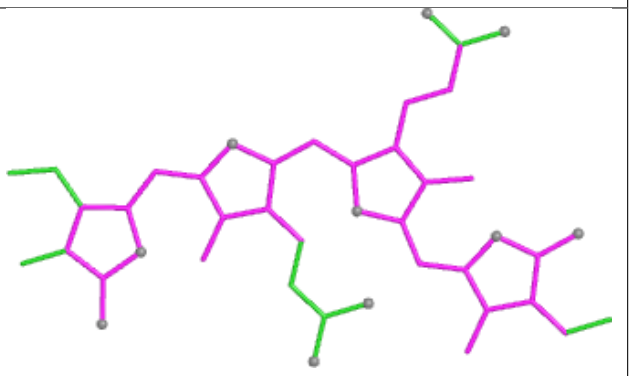


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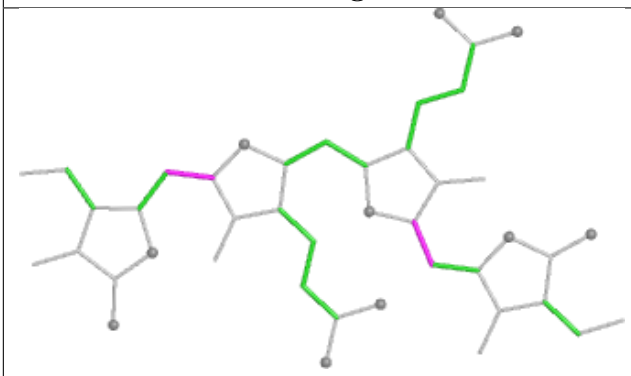
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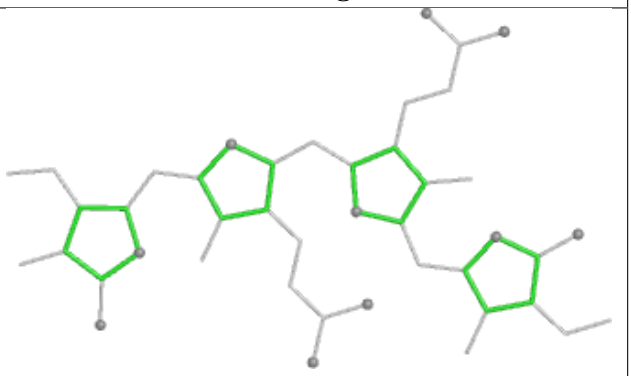
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Bond angles

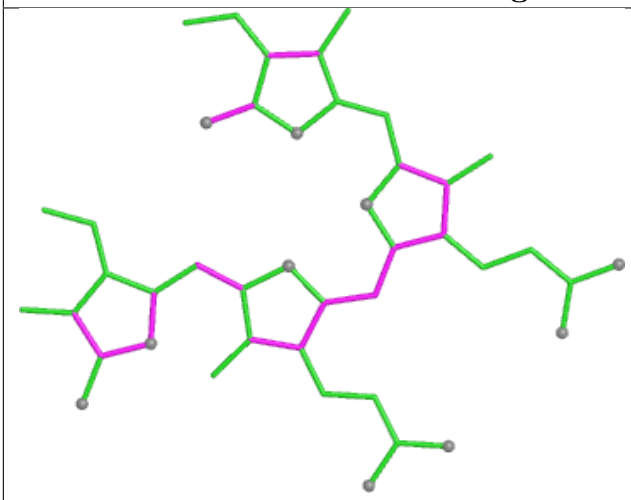


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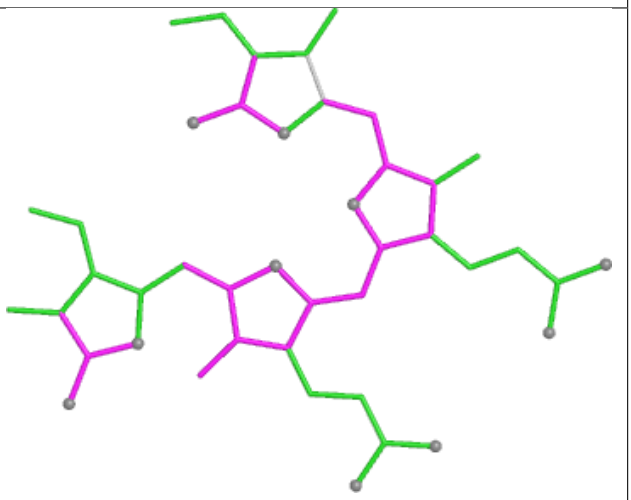


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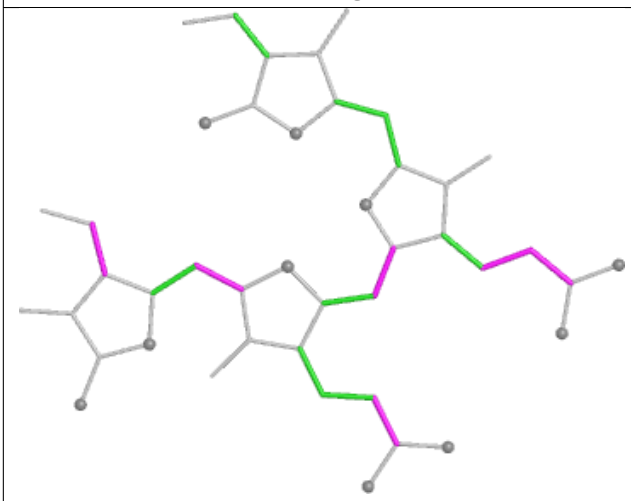
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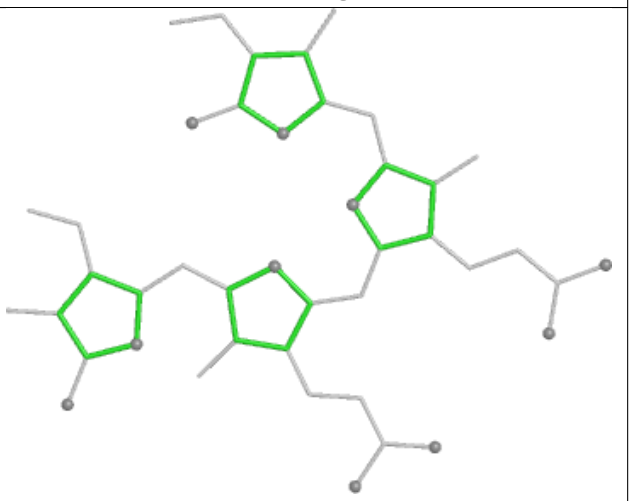
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Bond angles

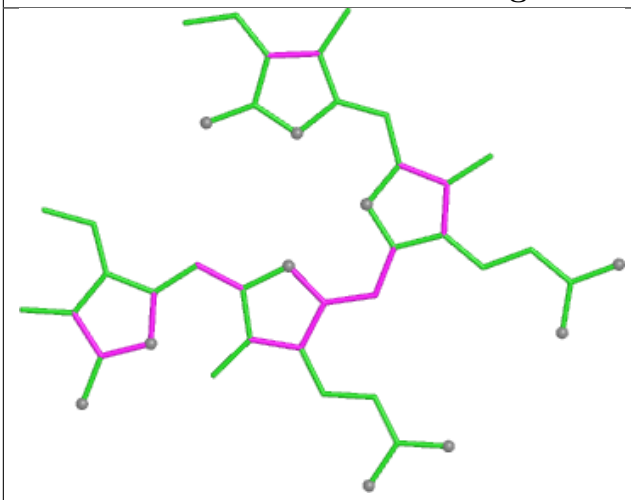


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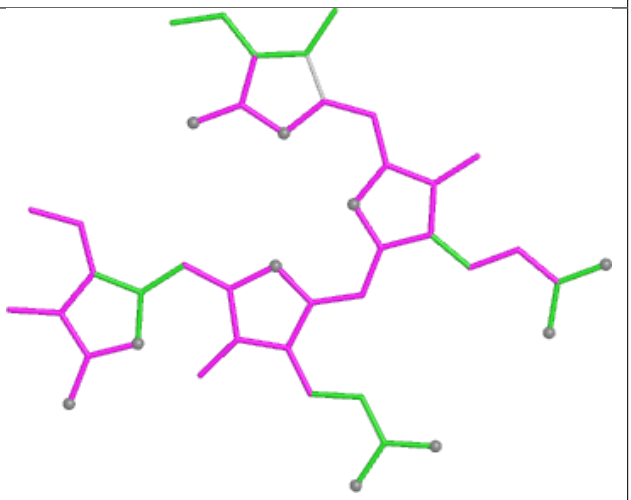


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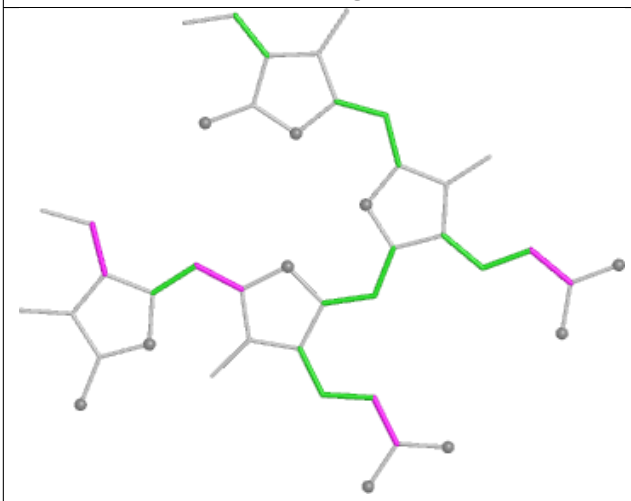
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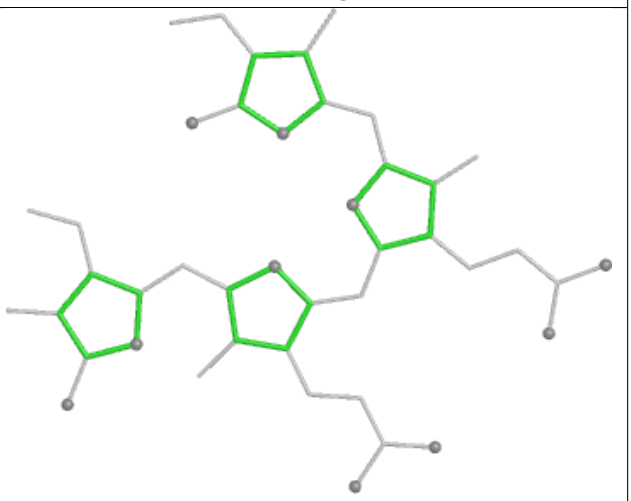
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Bond angles

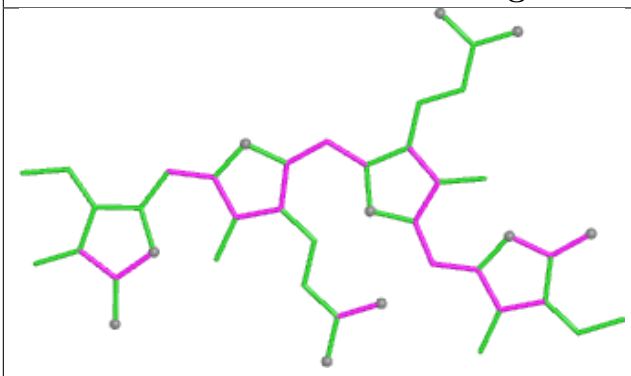


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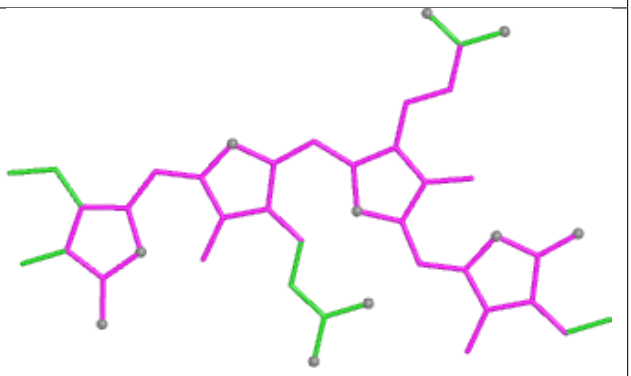


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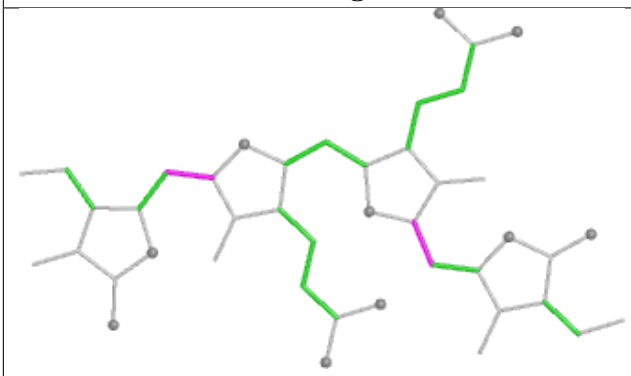
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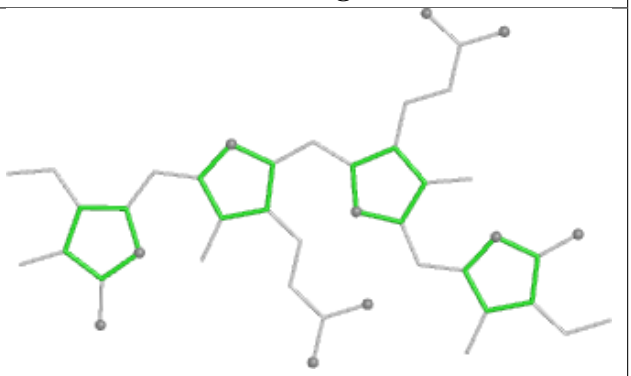
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Bond angles

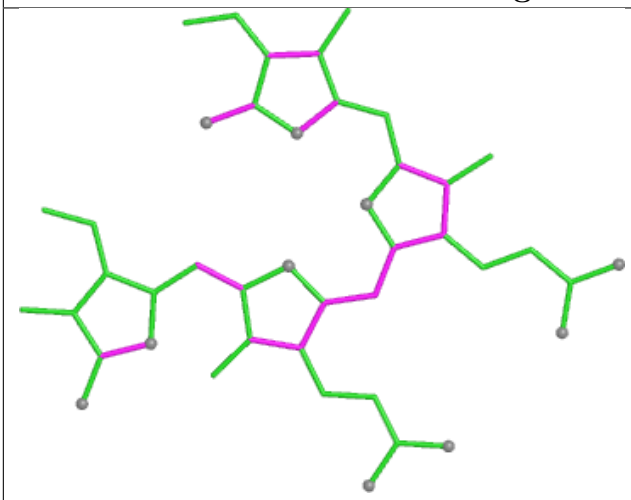


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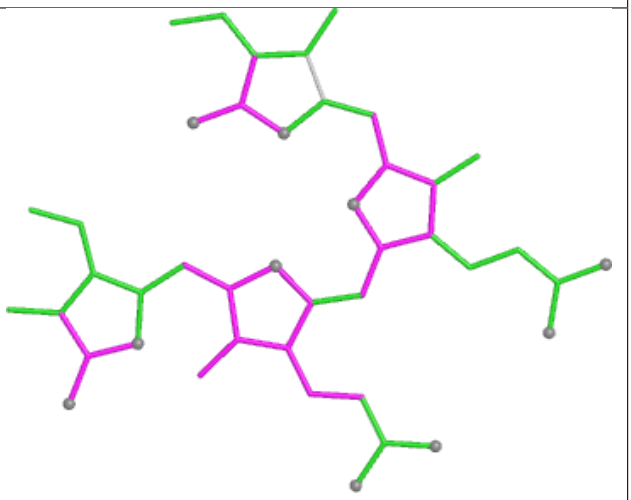


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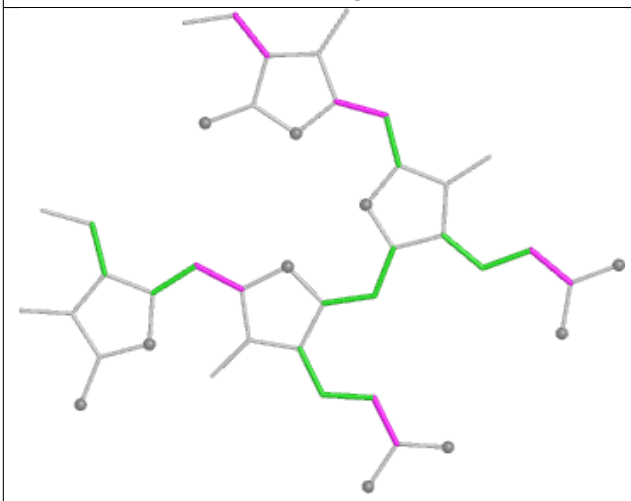
Ligand PEB bH 201



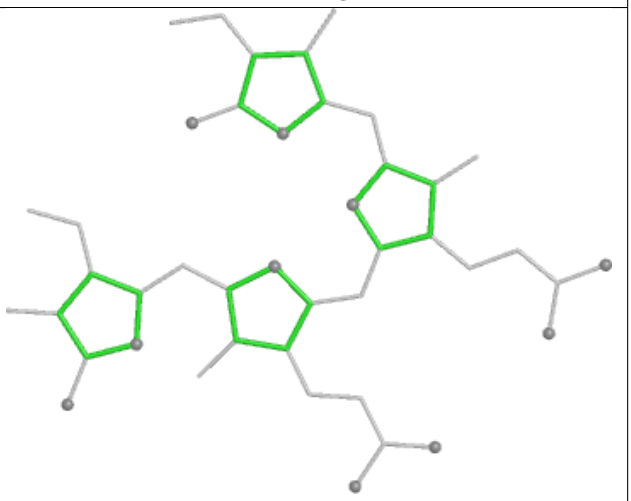
Bond lengths



Bond angles

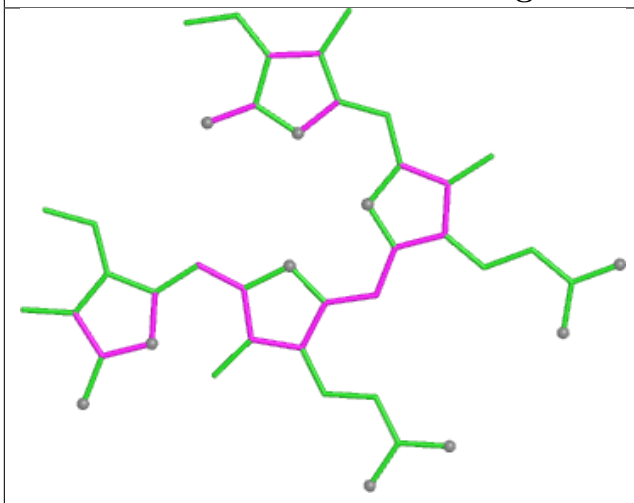


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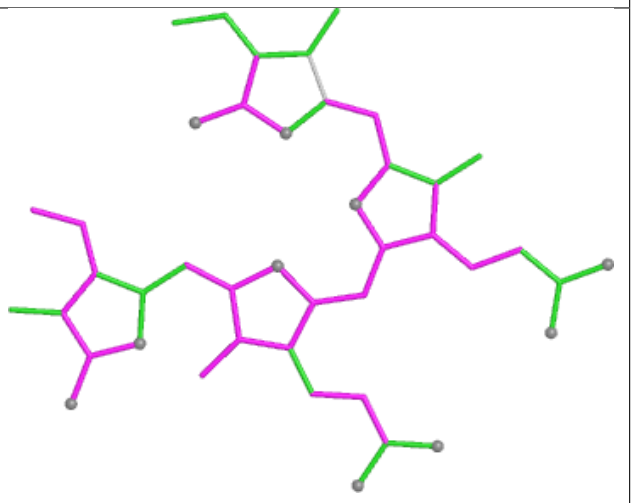


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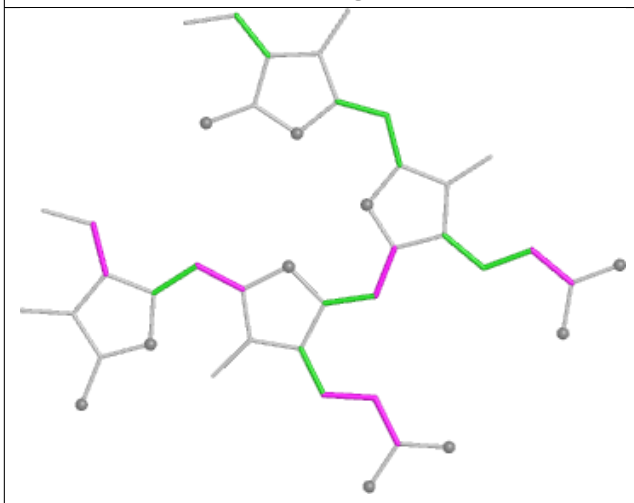
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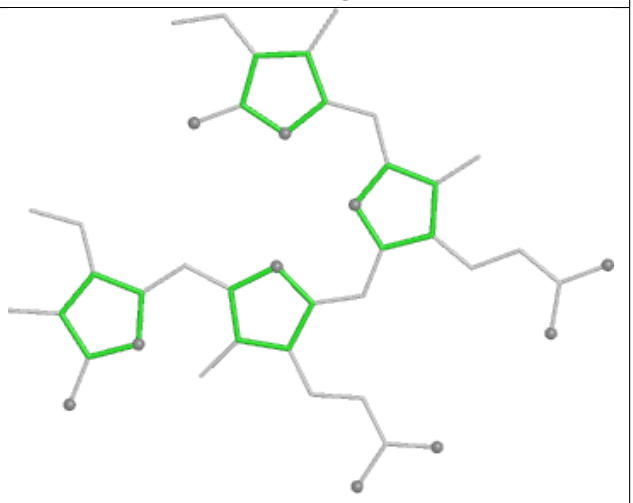
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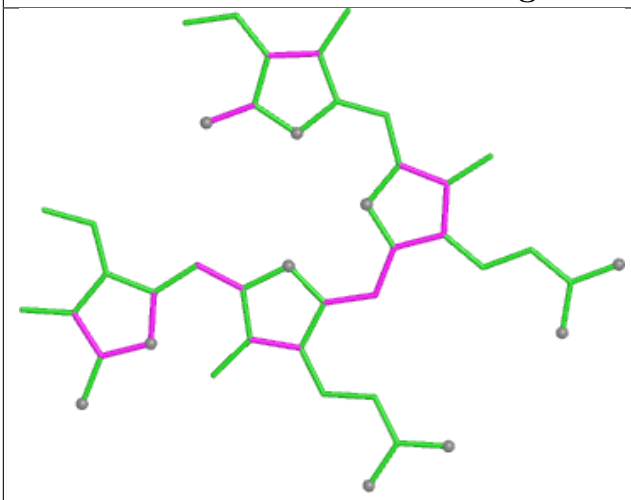


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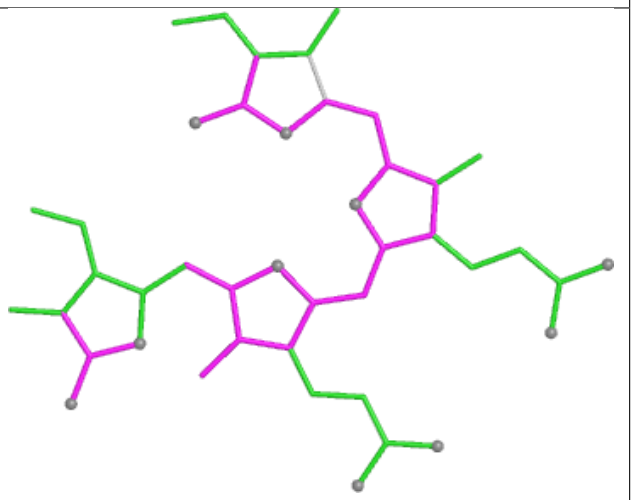


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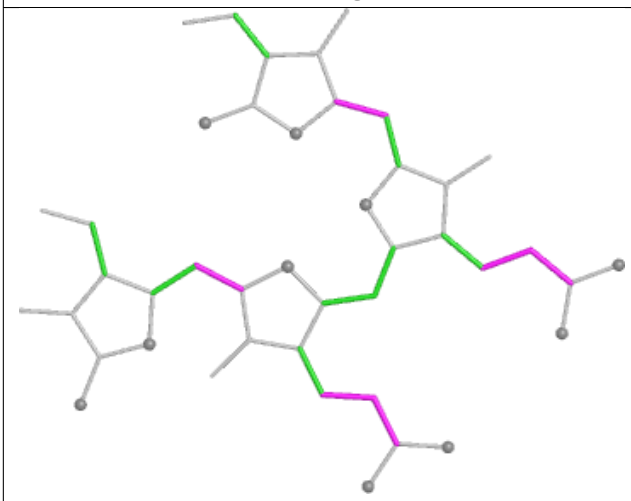
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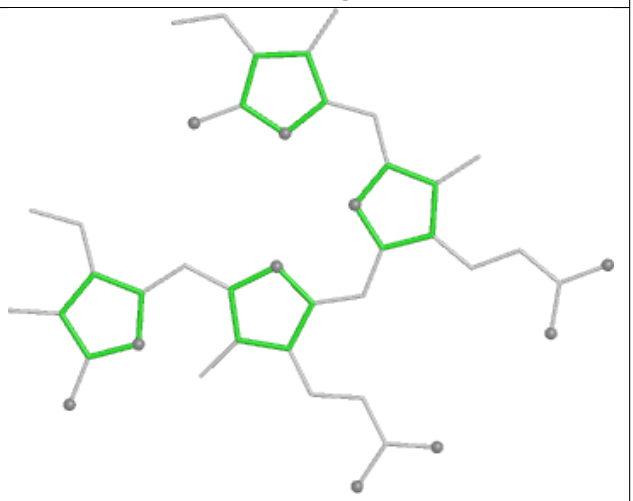
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Bond angles

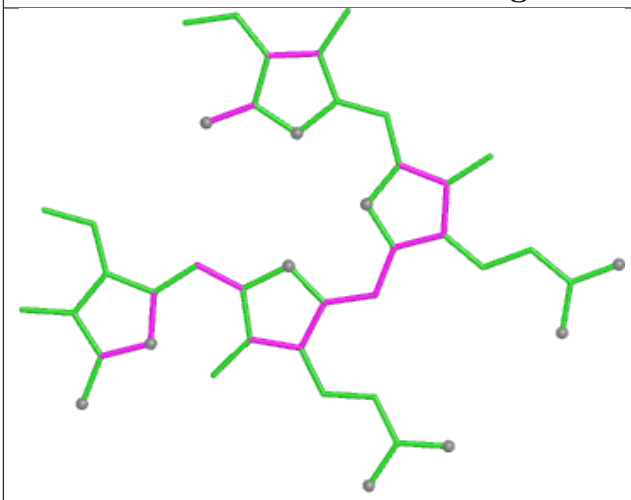


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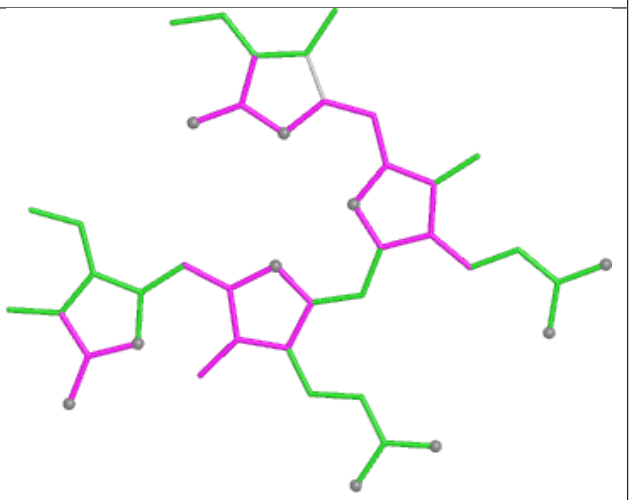


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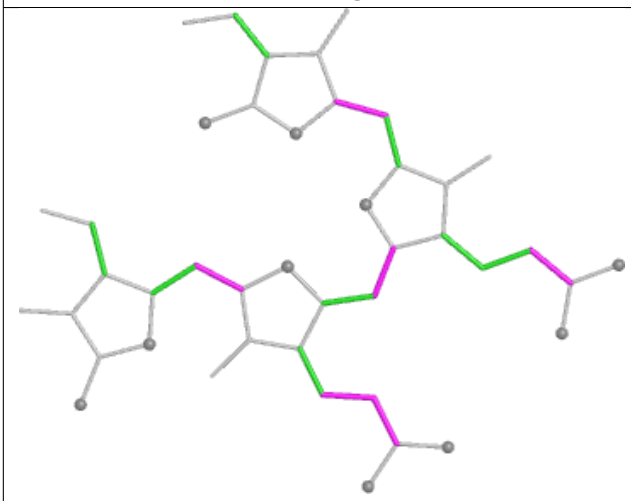
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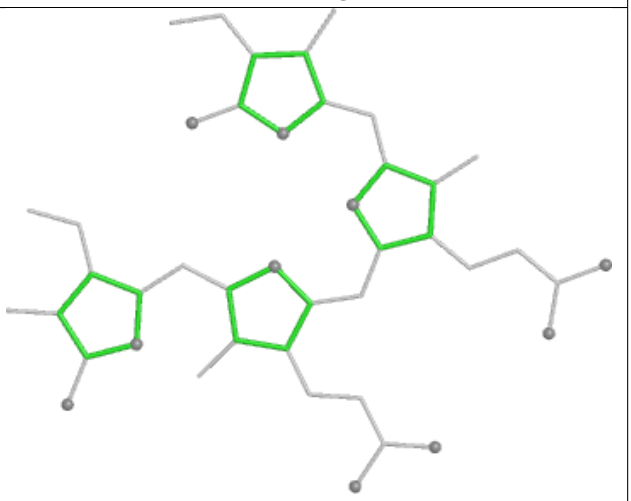
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Bond angles

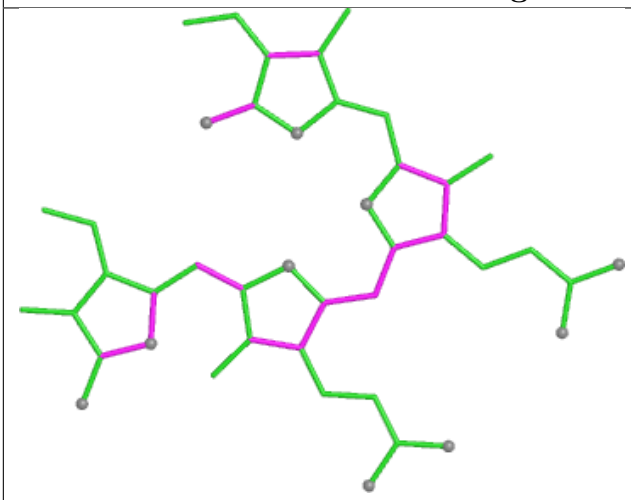


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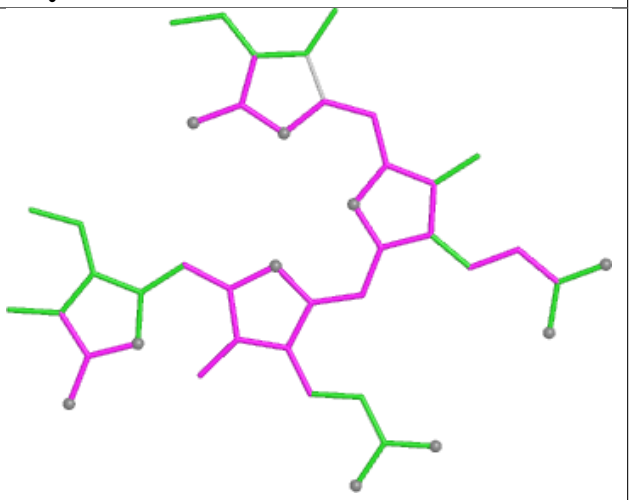


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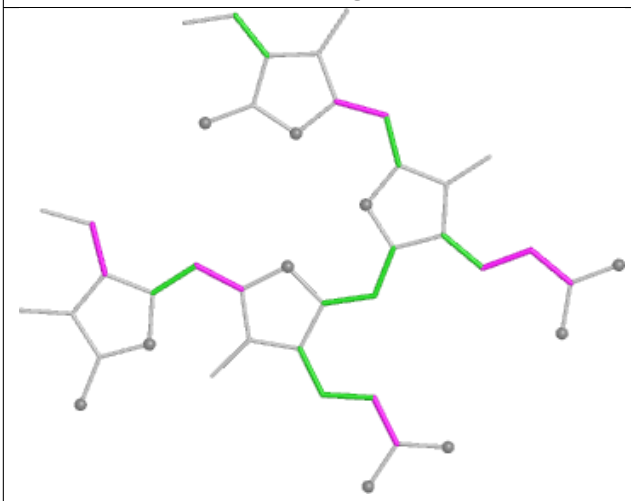
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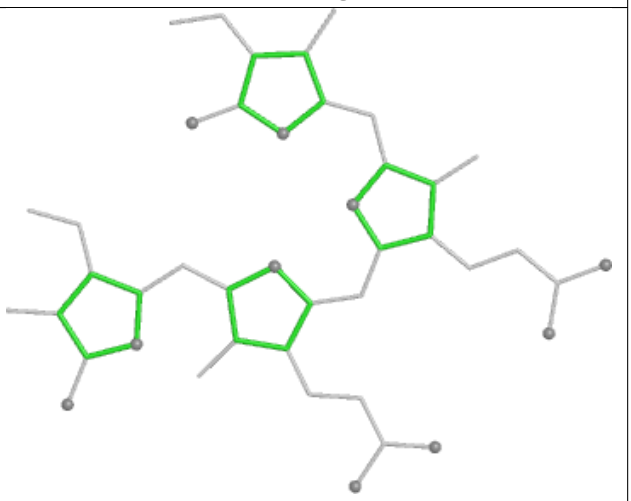
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Bond angles

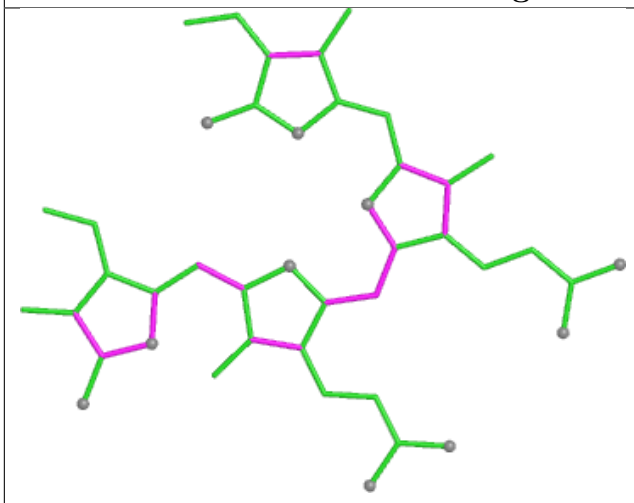


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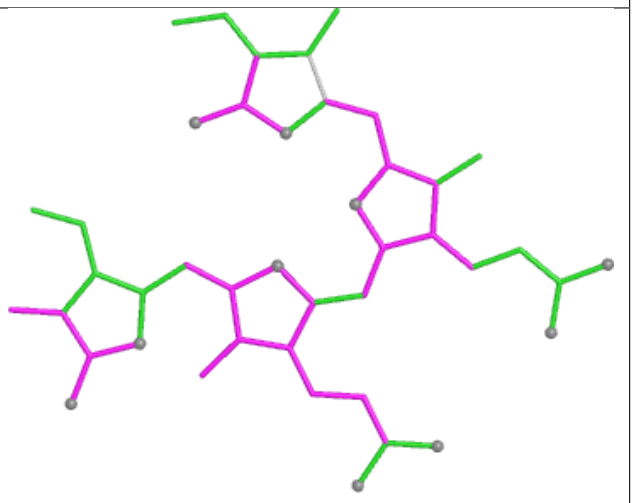


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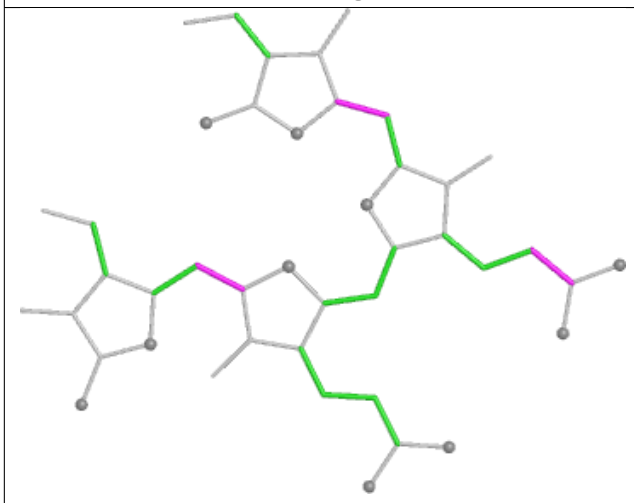
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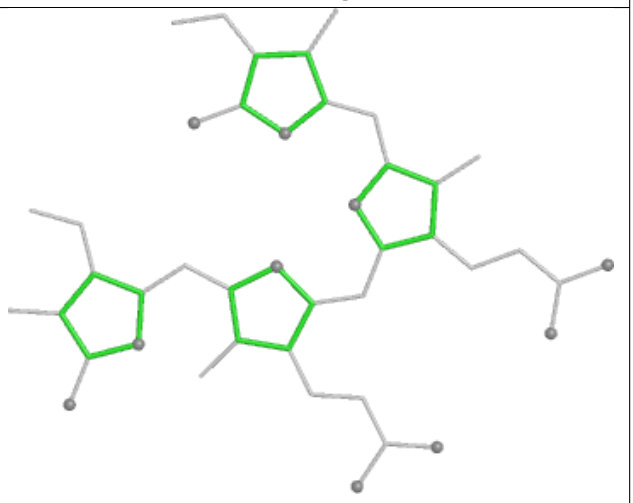
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Bond angles

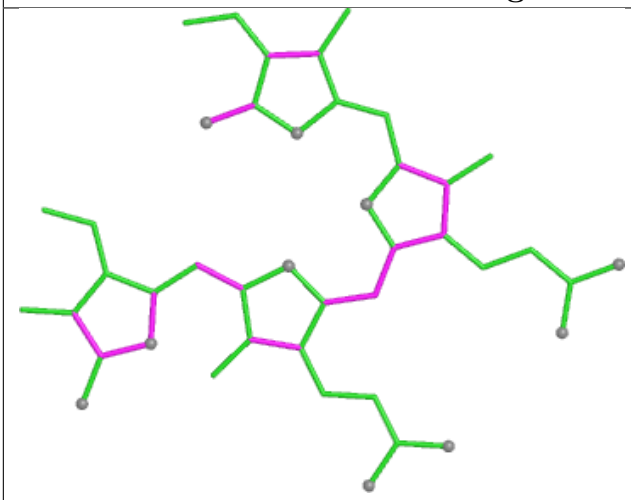


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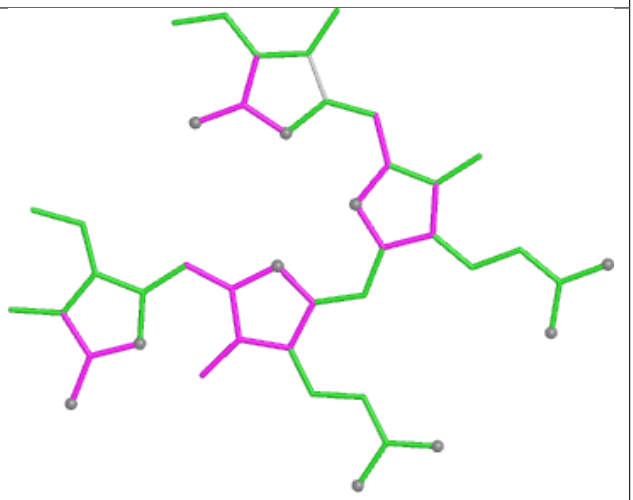


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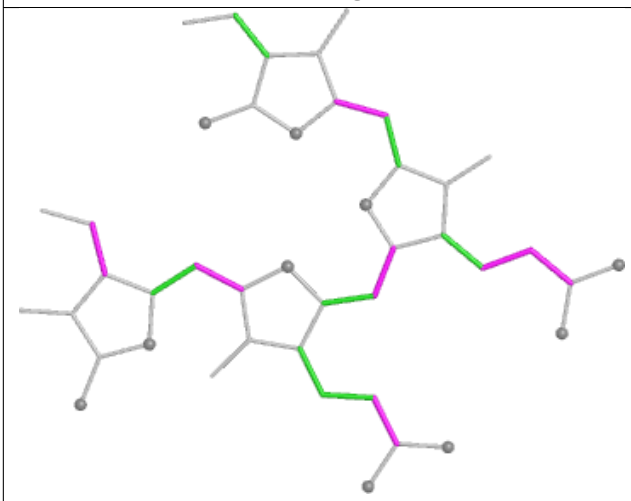
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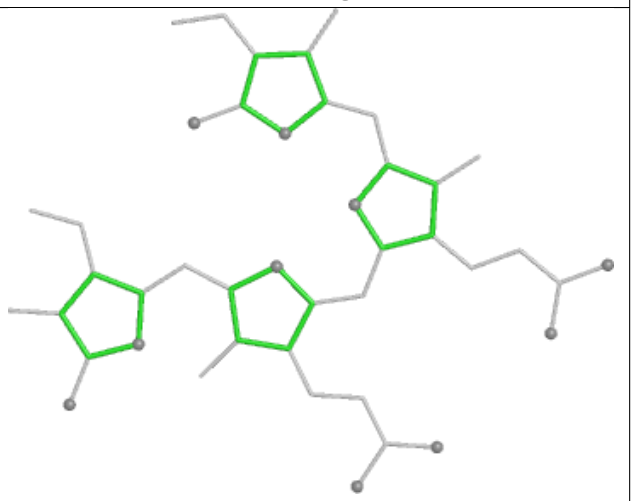
Bond lengths



Bond angles

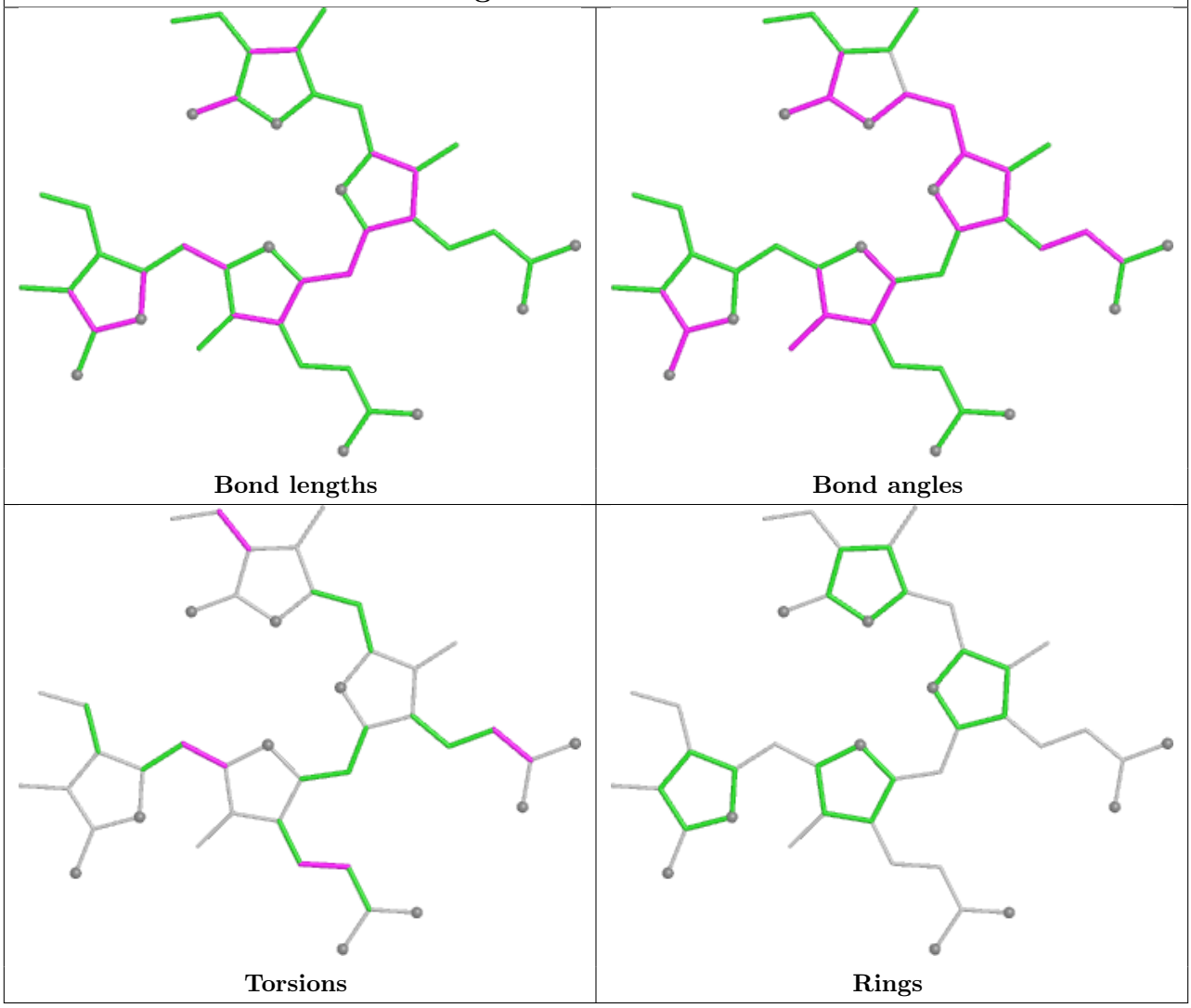


Torsions



Rings

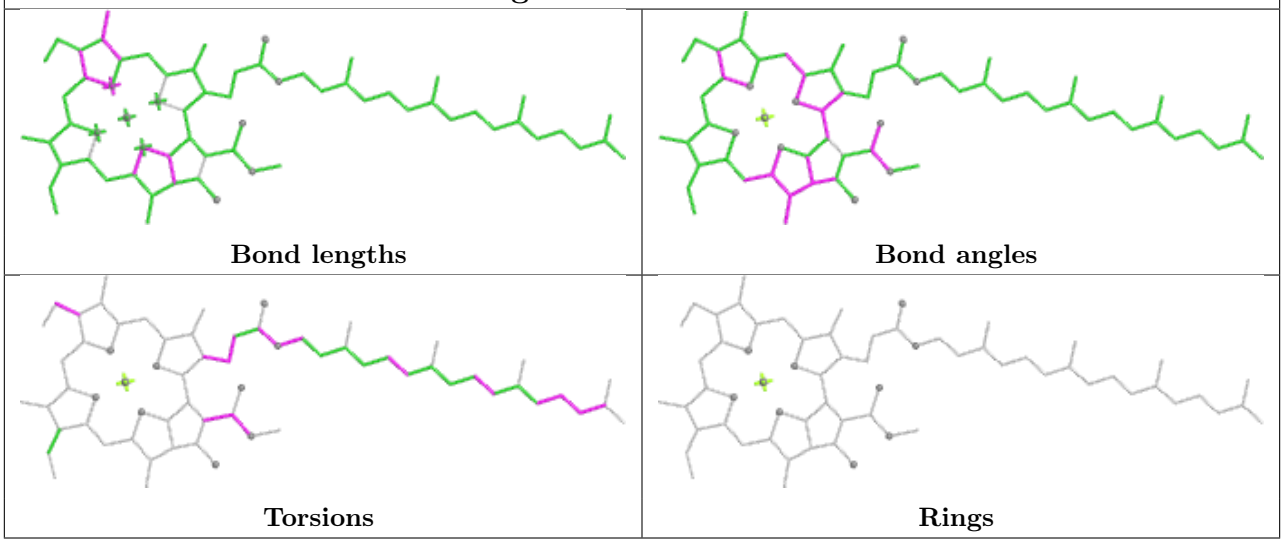
Ligand PEB YD 201



Bond lengths | Bond angles

Torsions | Rings

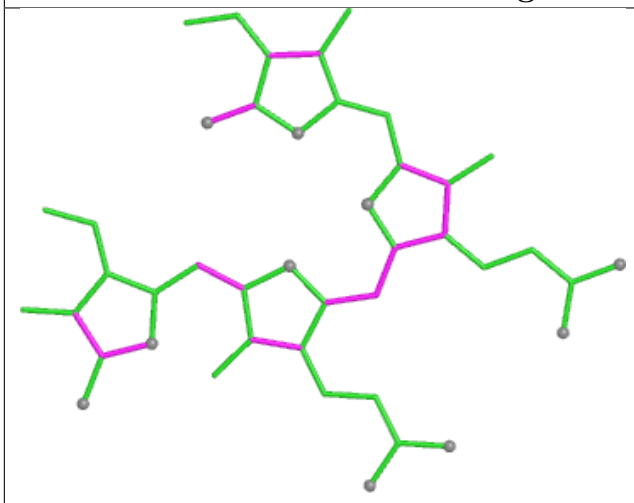
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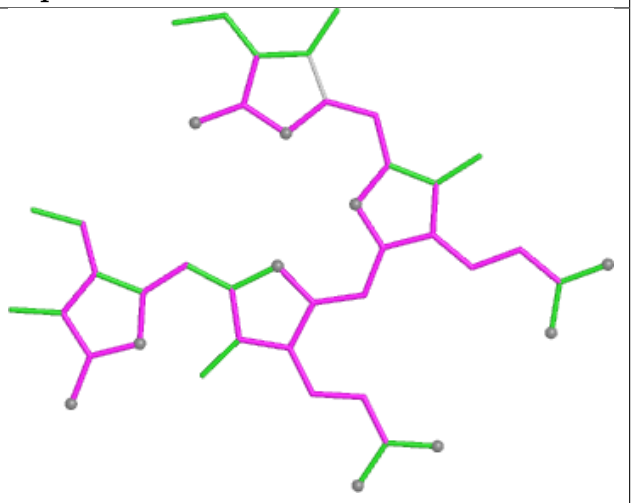
Bond lengths | Bond angles

Torsions | Rings

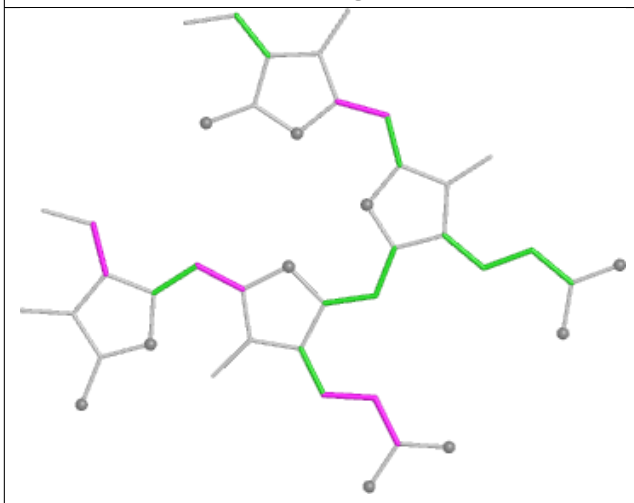
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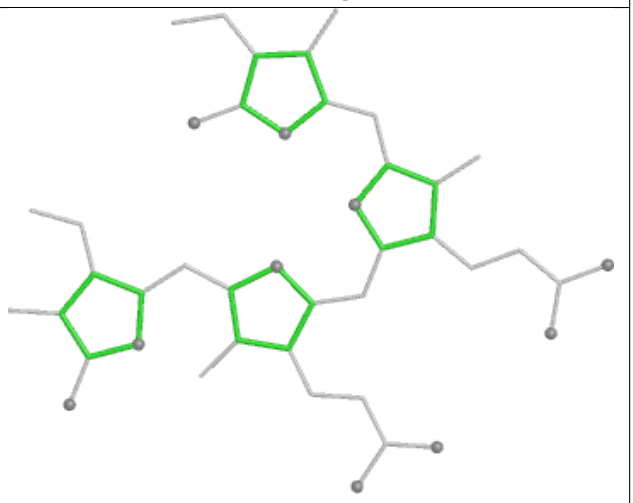
Bond lengths



Bond angles

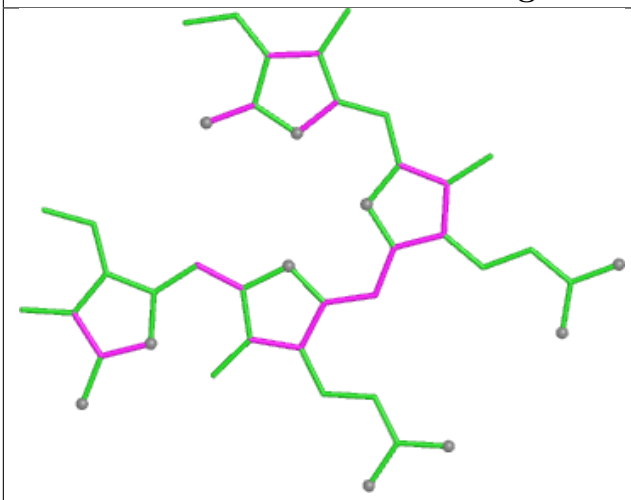


Torsions

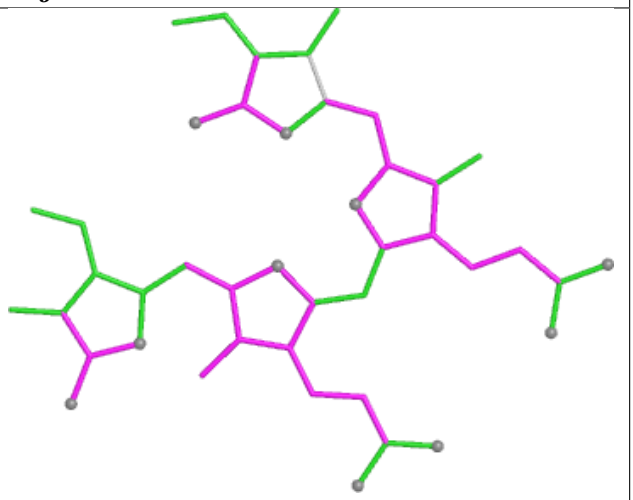


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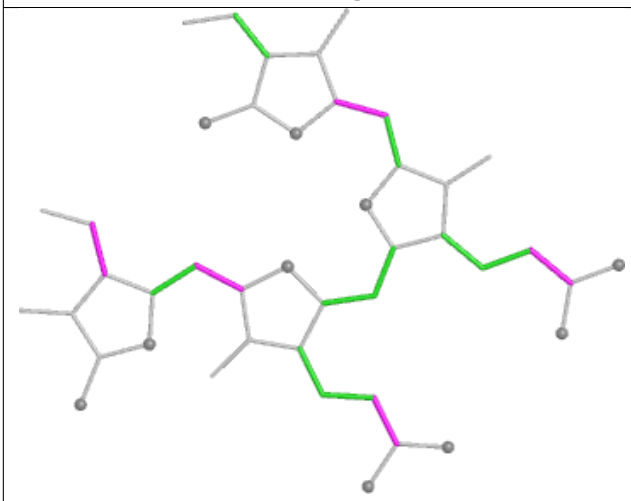
Ligand PEB jG 201



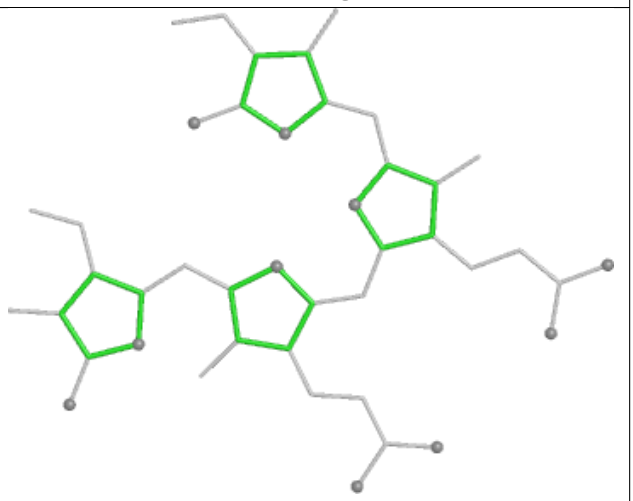
Bond lengths



Bond angles

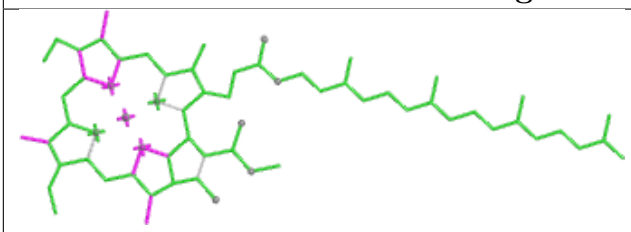


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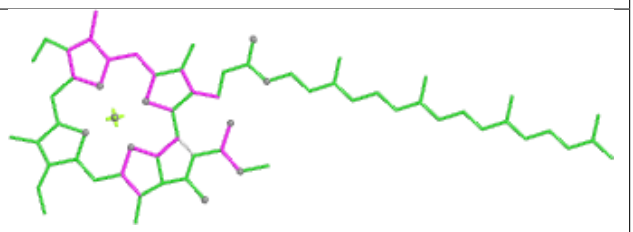


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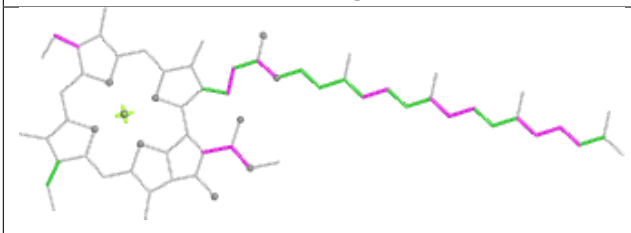
Ligand CLA B2 827



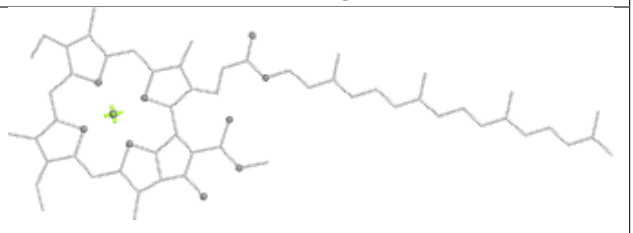
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Bond angles

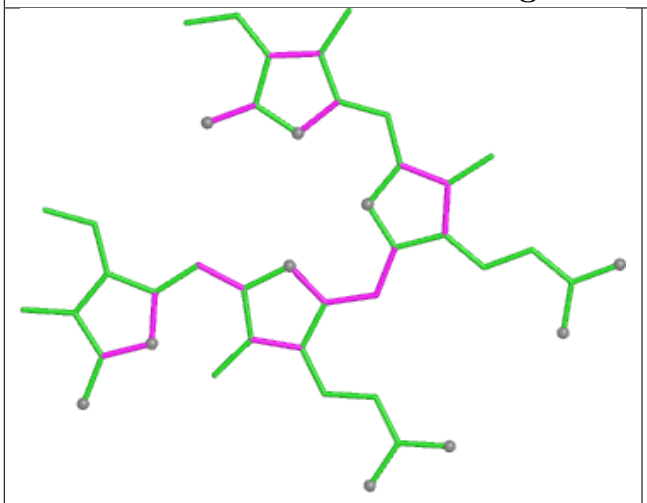


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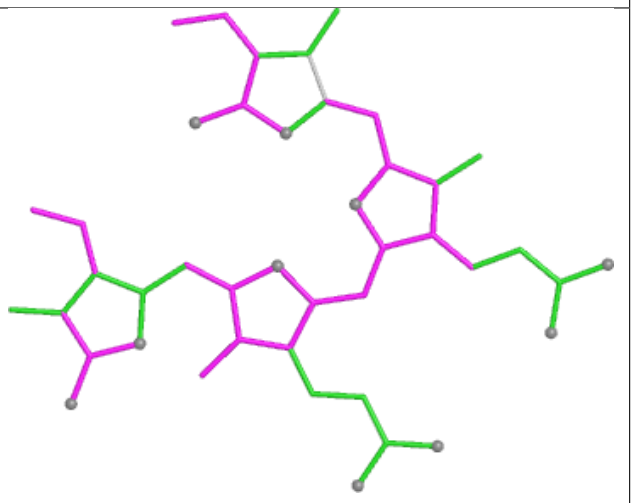


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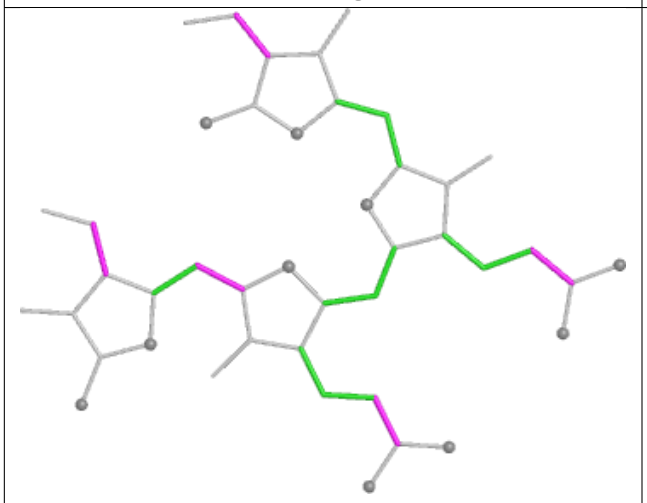
Ligand PEB BI 202



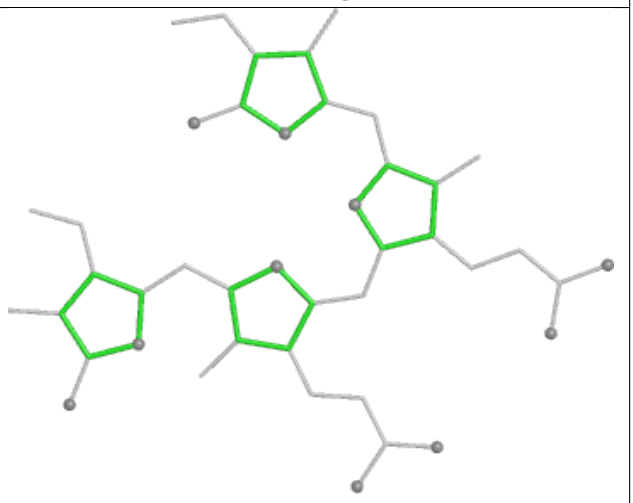
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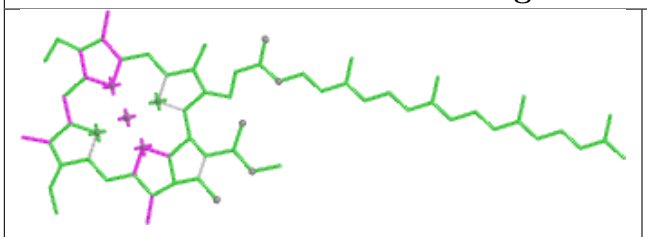


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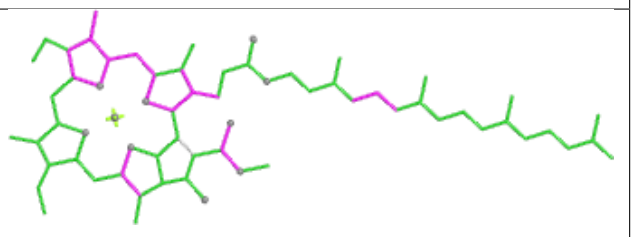


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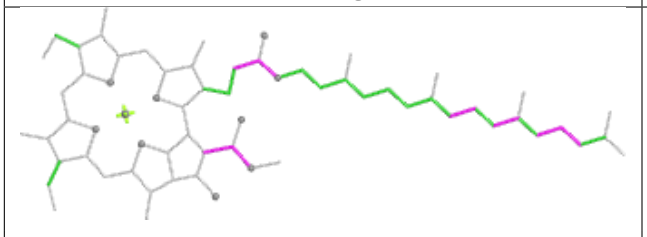
Ligand CLA AL 403



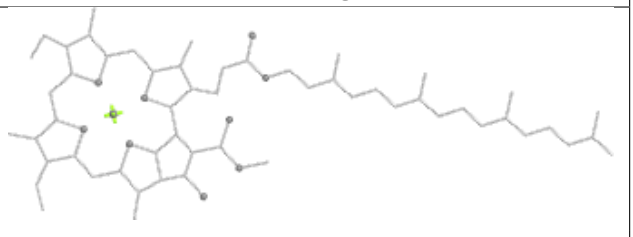
Bond lengths



Bond angles

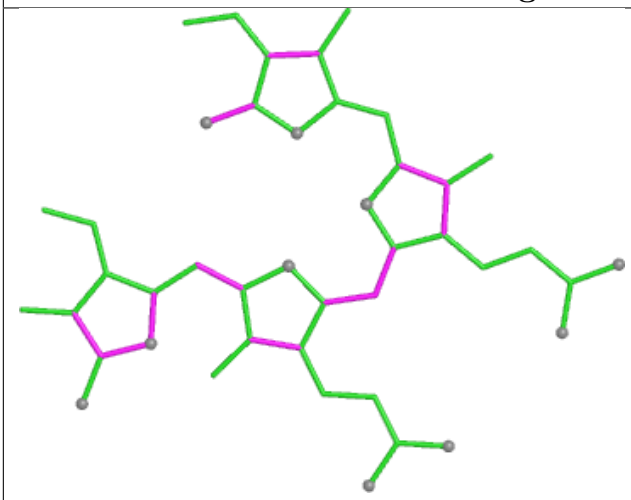


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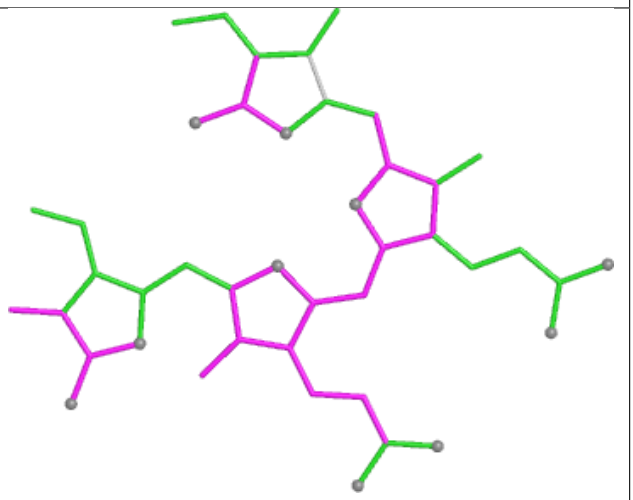


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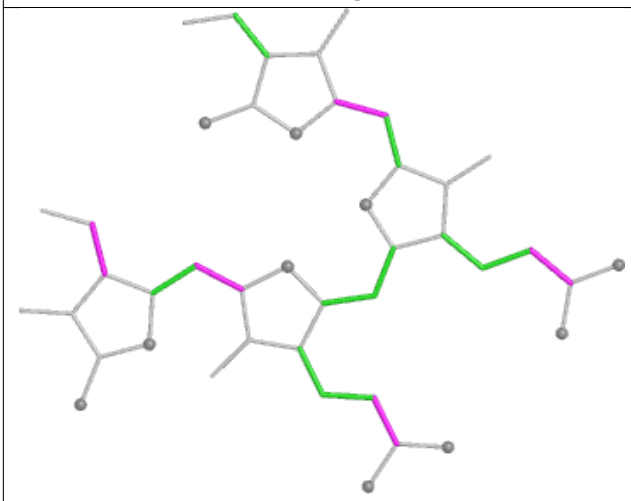
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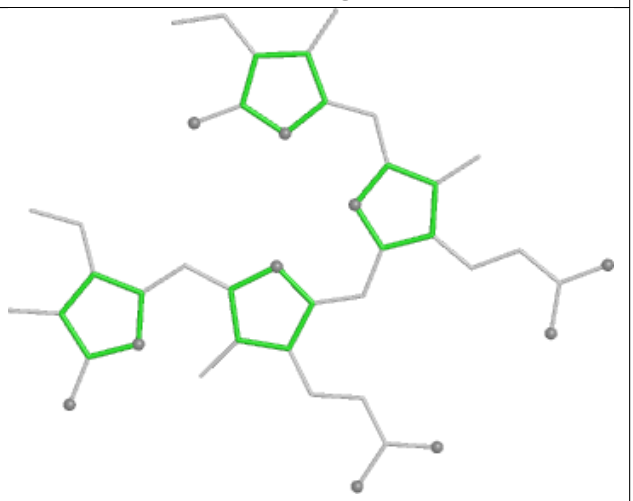
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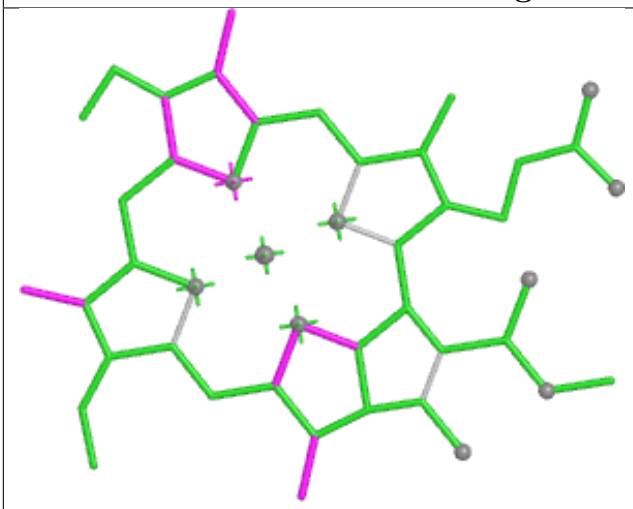


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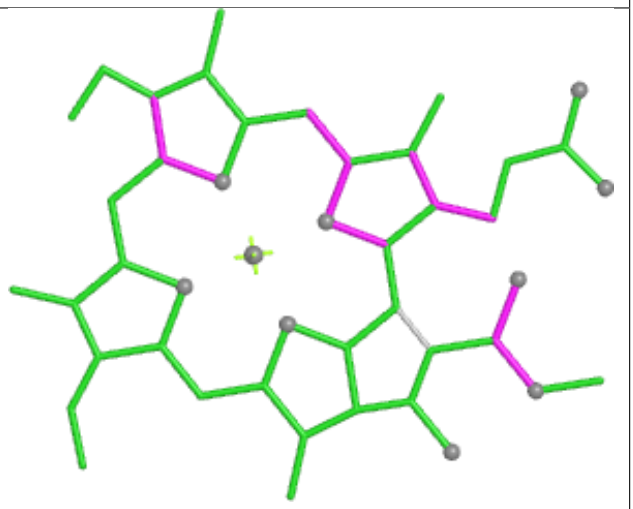


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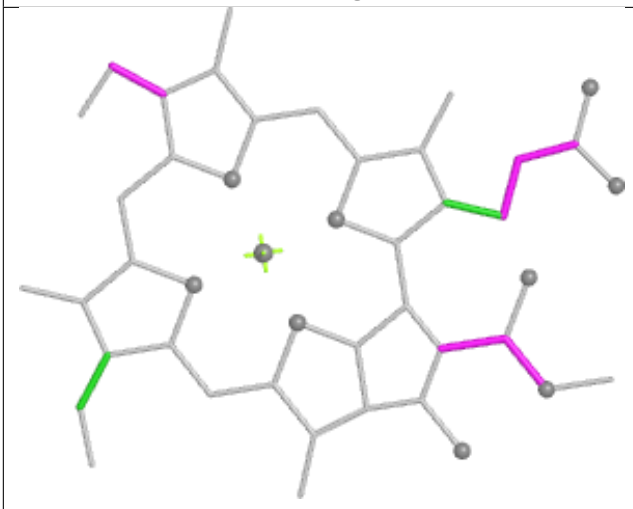
Ligand CLA A2 818



Bond lengths



Bond angles

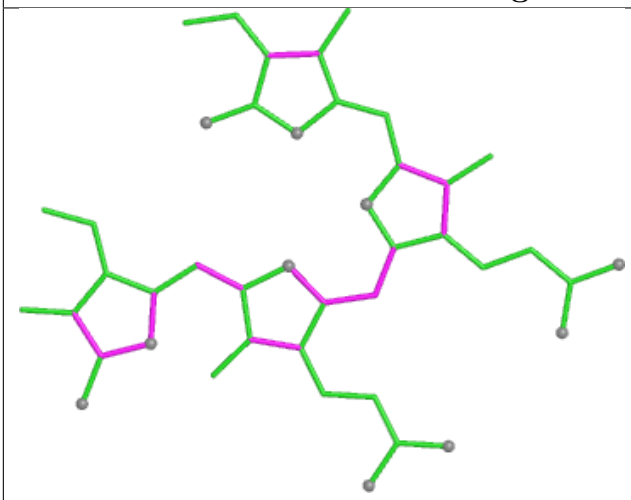


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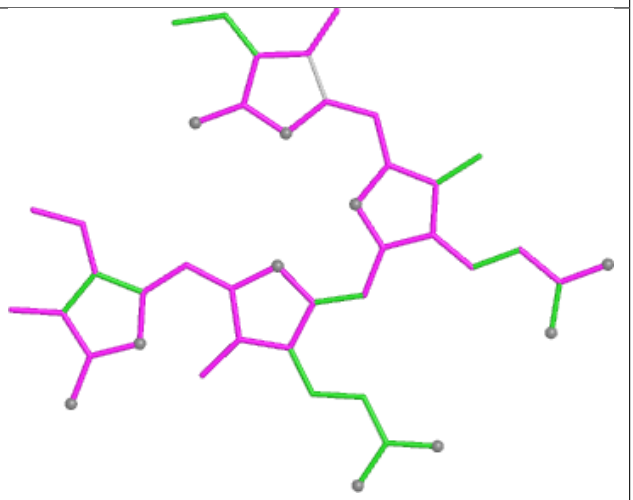


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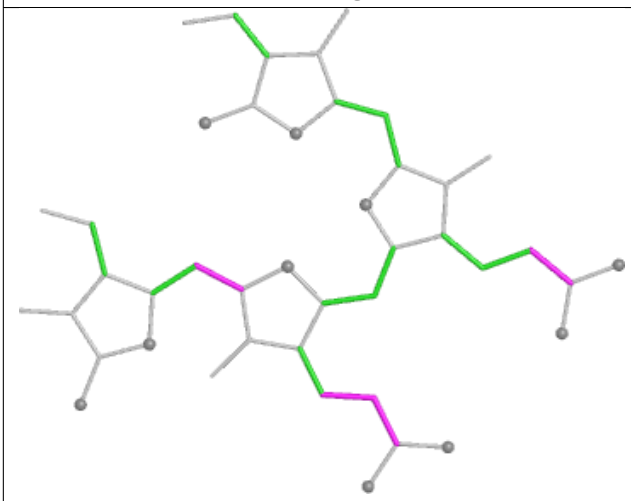
Ligand PEB OA 201



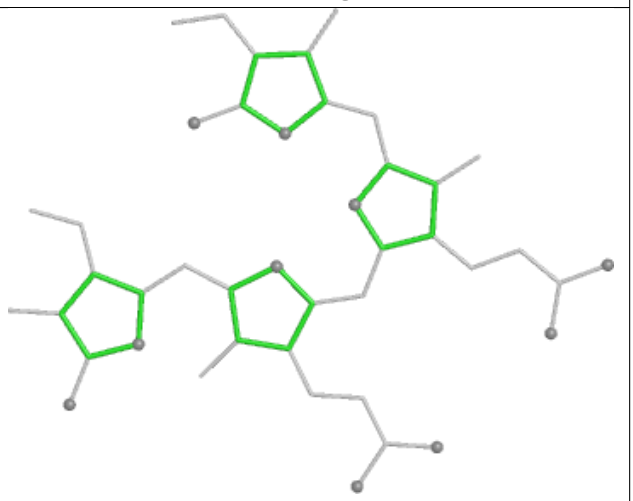
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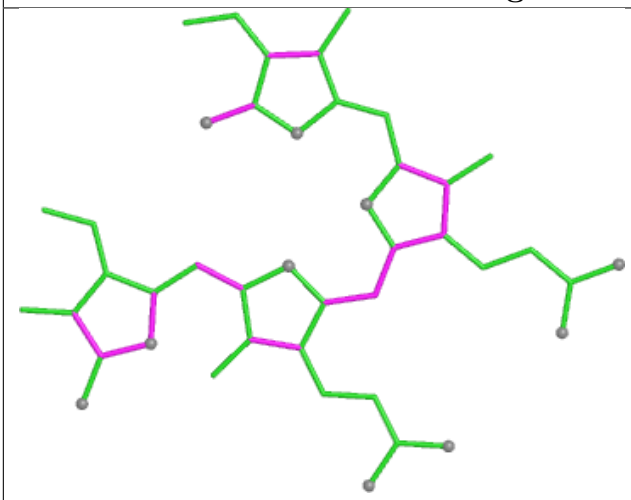


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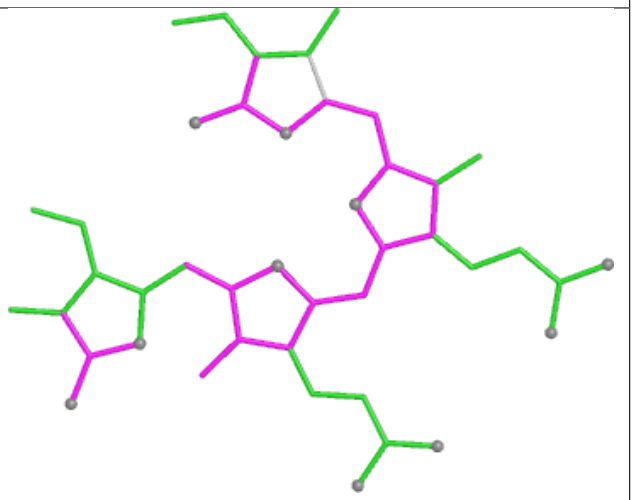


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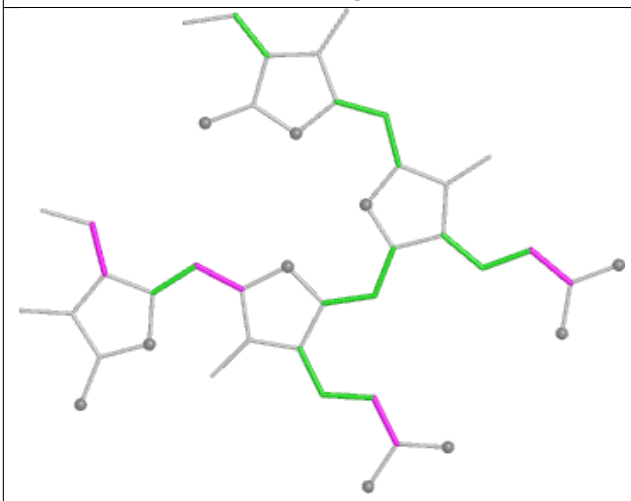
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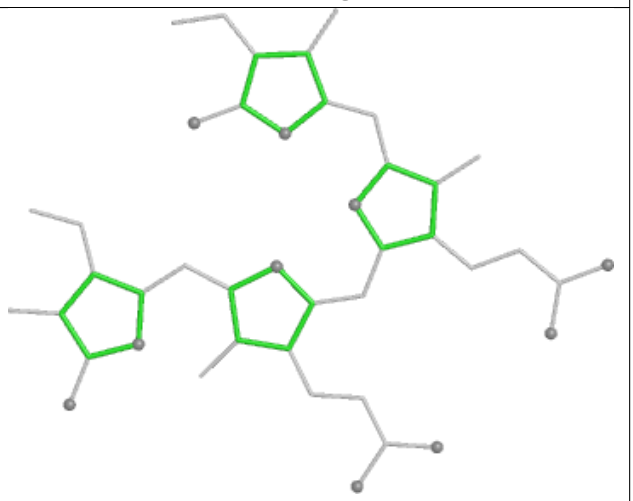
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Bond angles

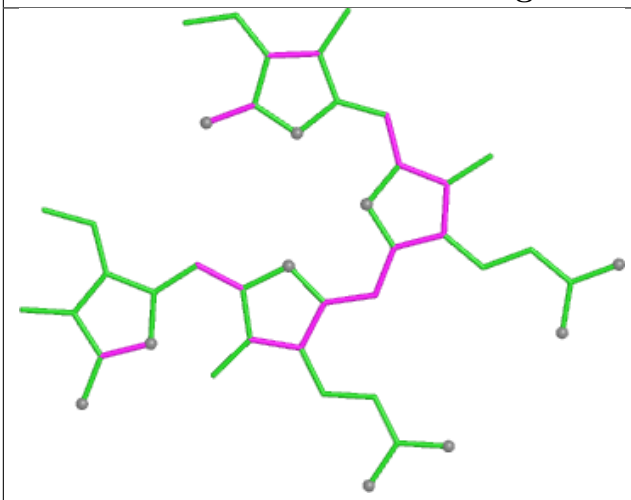


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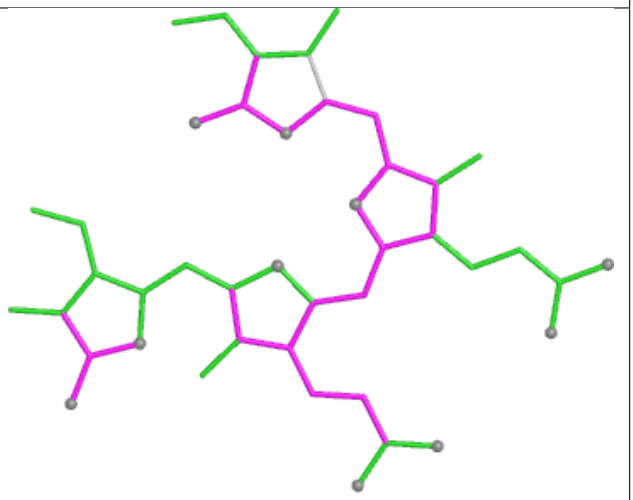


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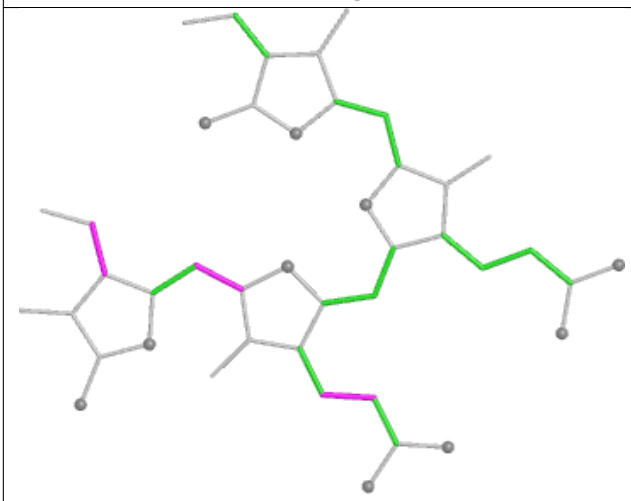
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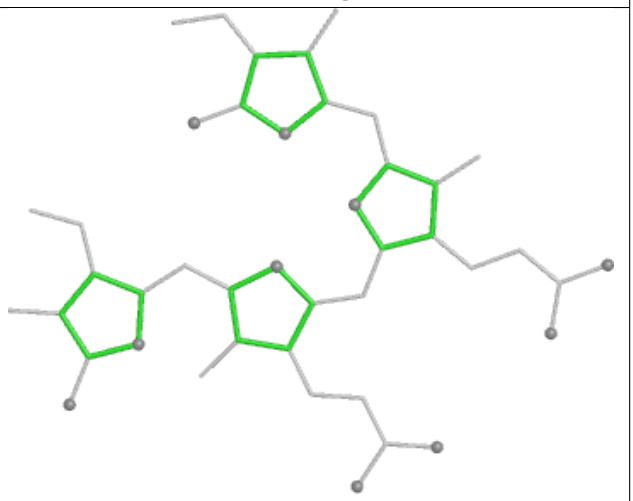
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Bond angles

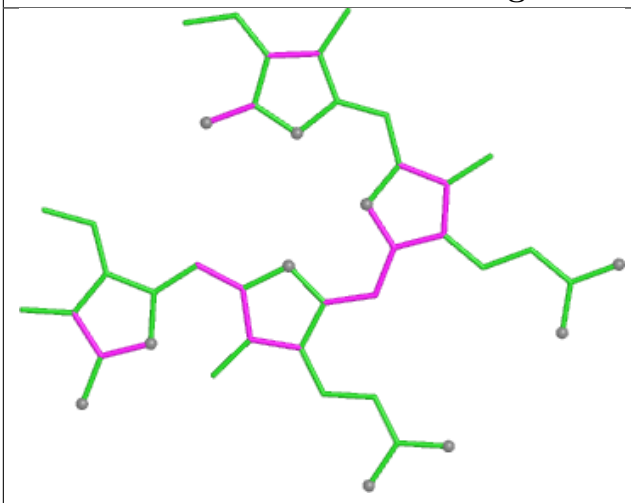


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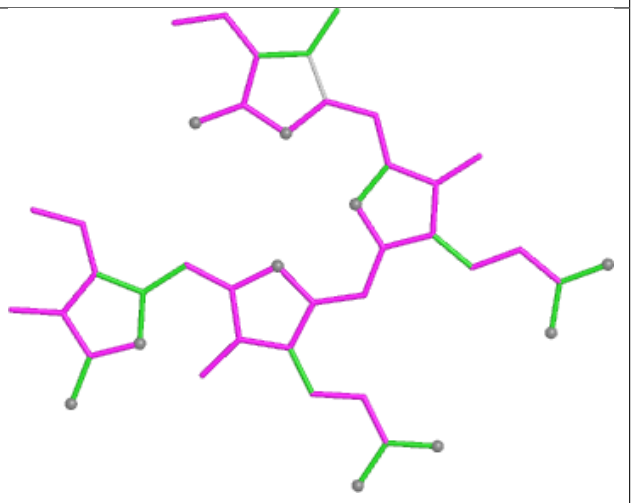


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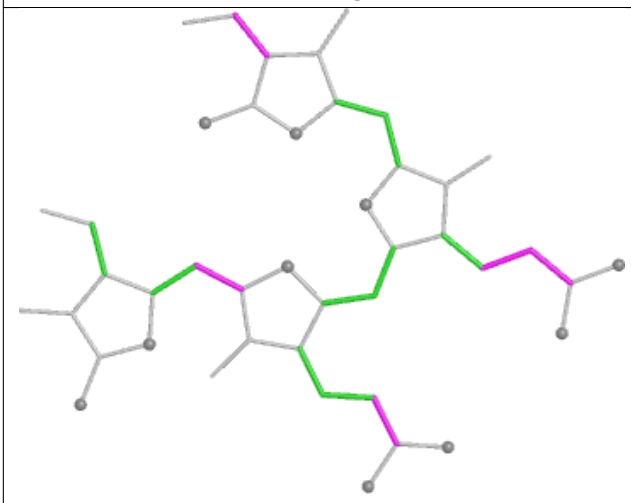
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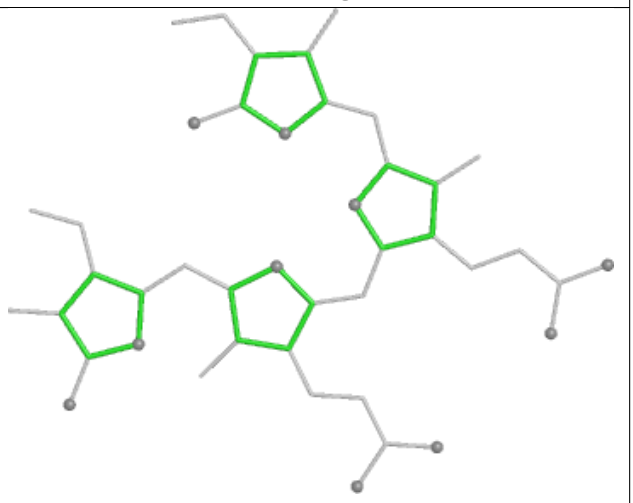
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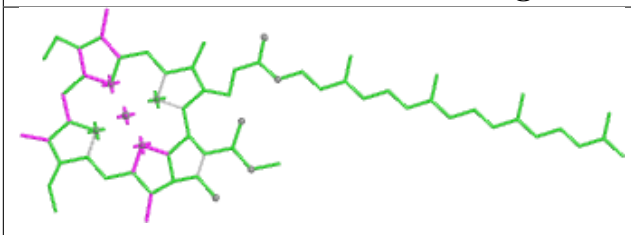


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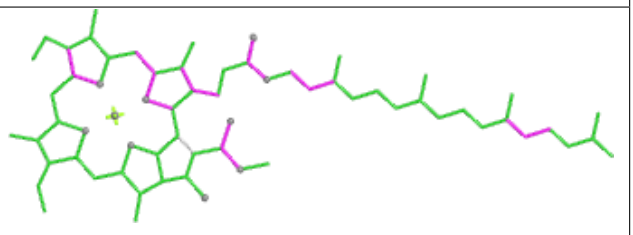


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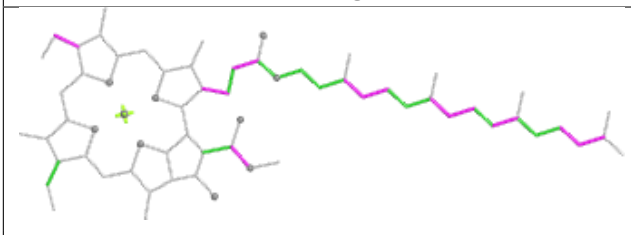
Ligand CLA A2 808



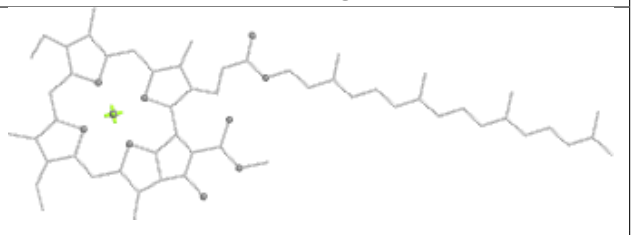
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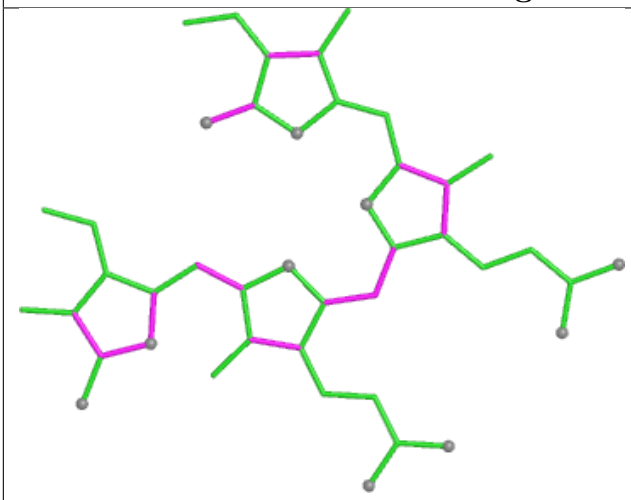


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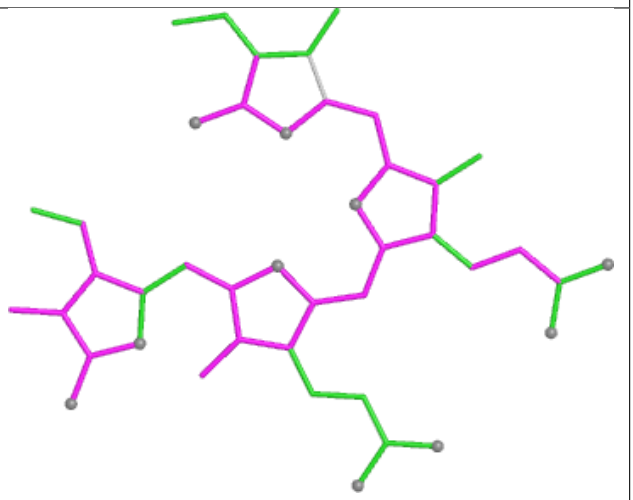


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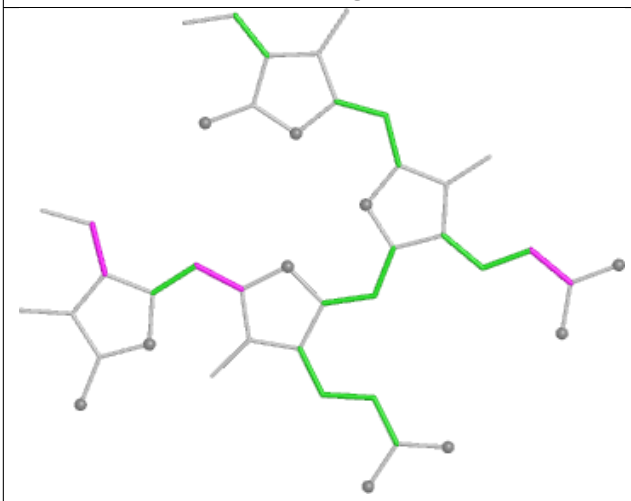
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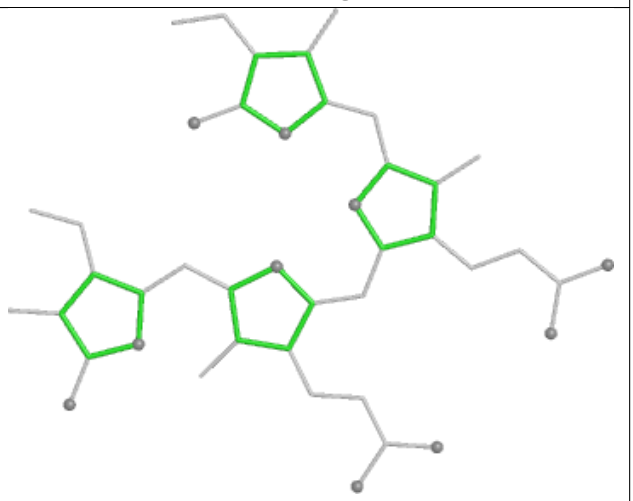
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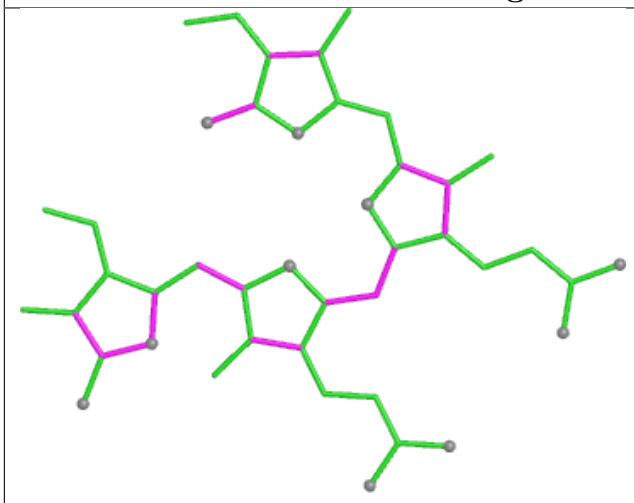


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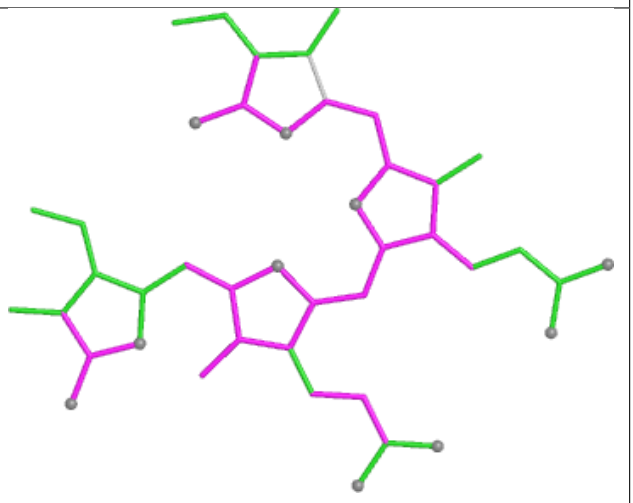


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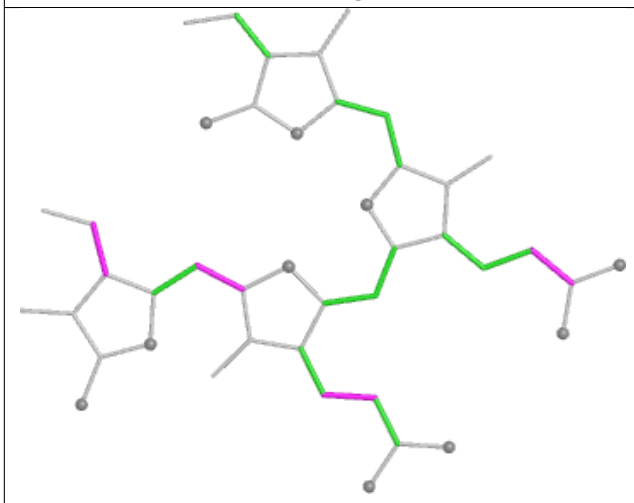
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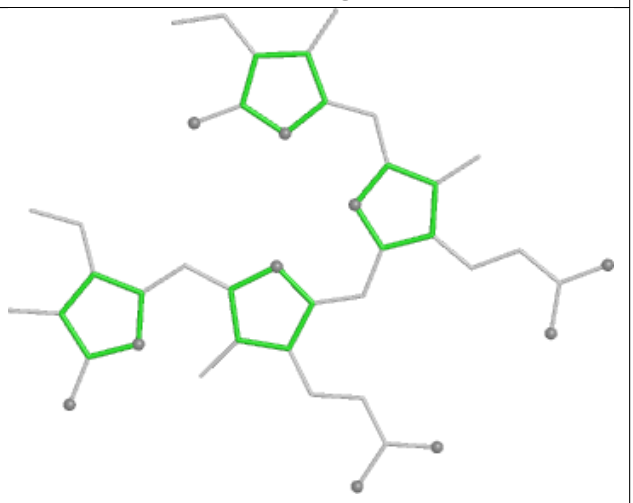
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Bond angles

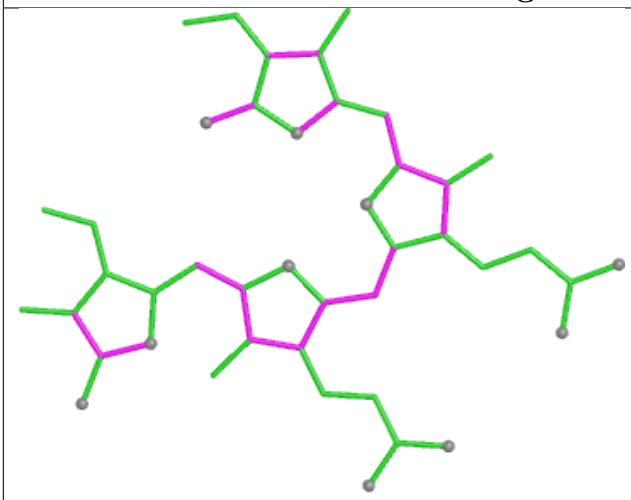


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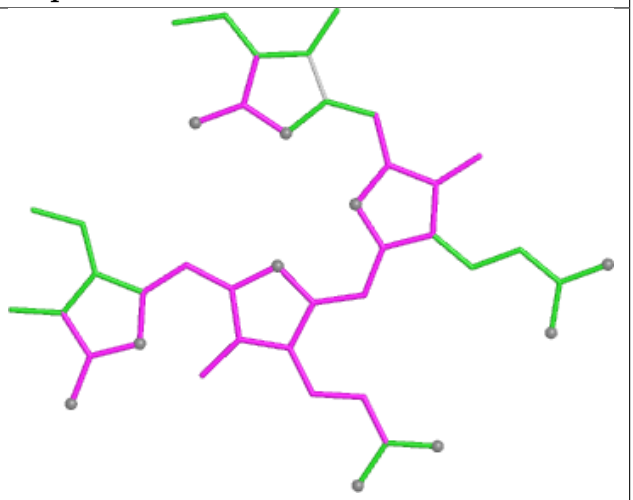


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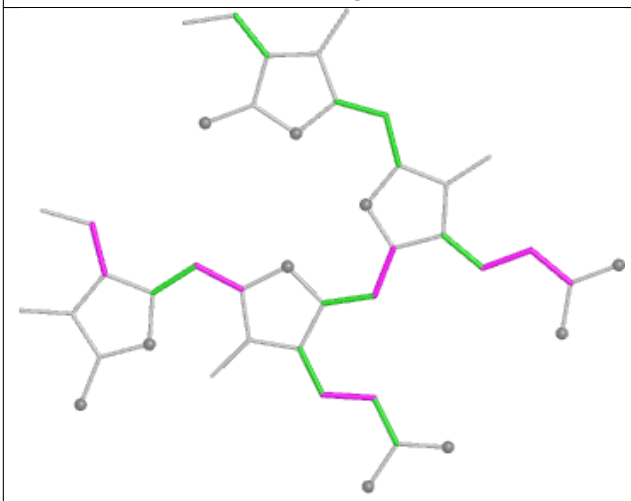
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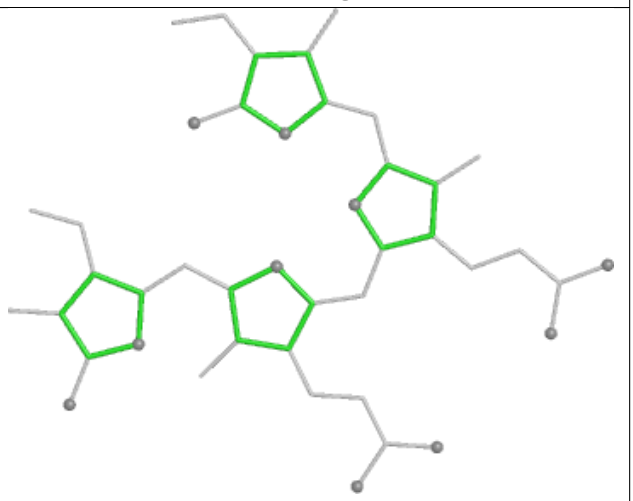
Bond lengths



Bond angles

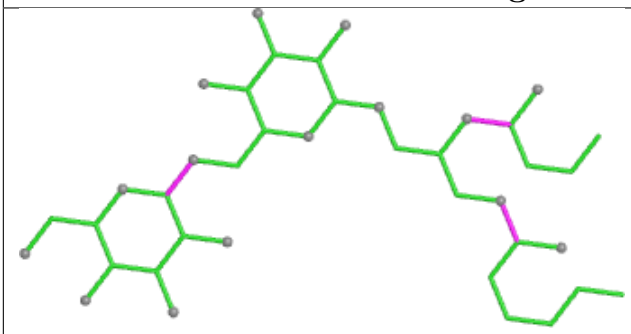


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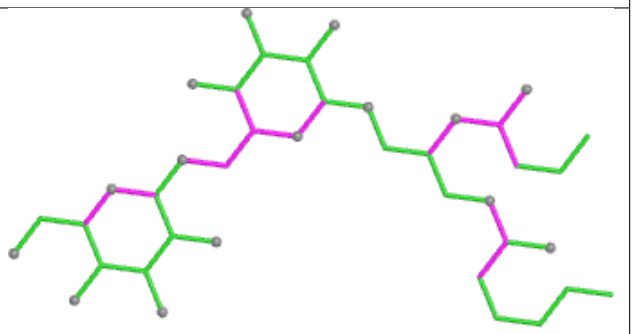


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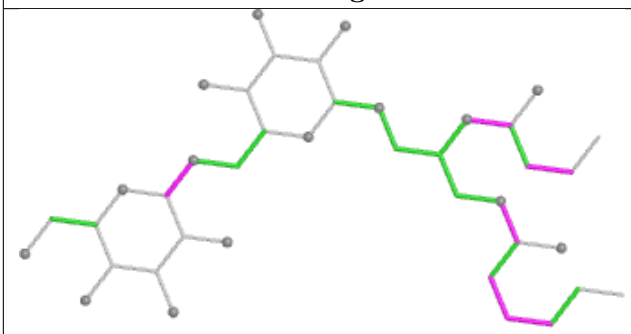
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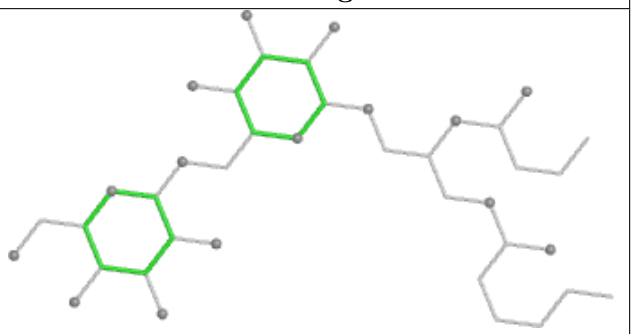
Bond lengths



Bond angles

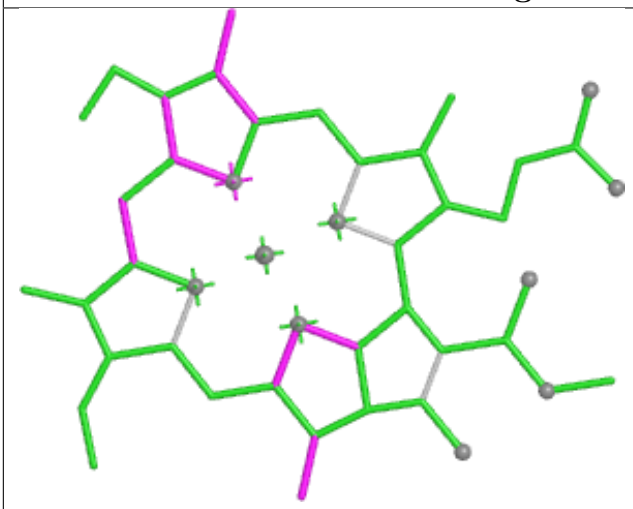


Torsions

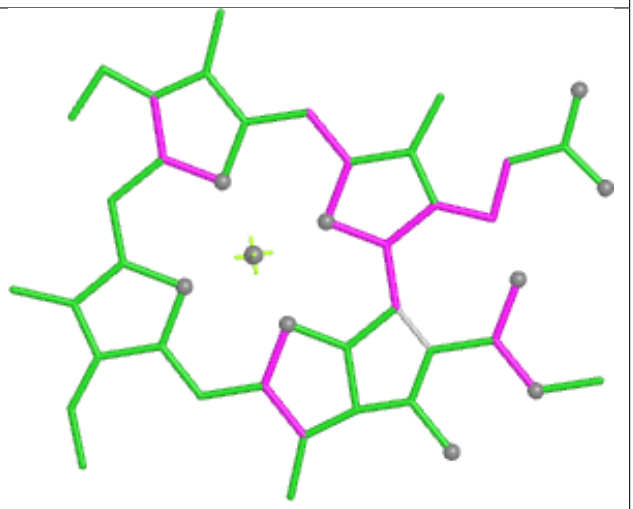


Rings

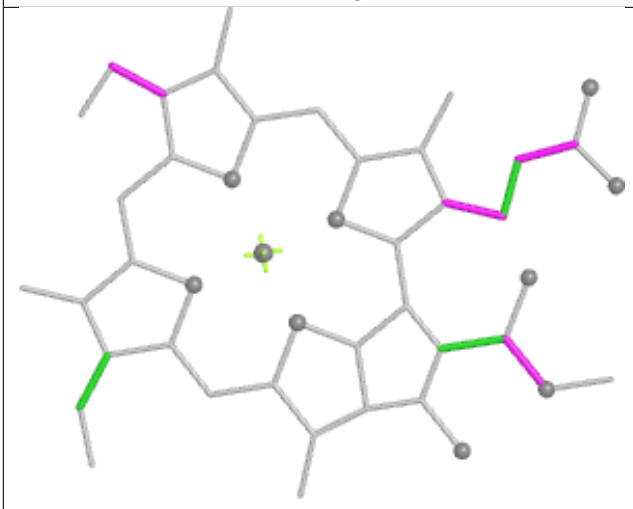
Ligand CLA 7N 605



Bond lengths



Bond angles

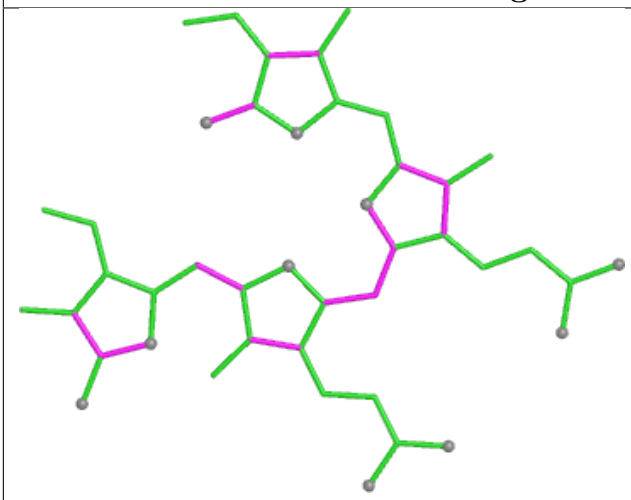


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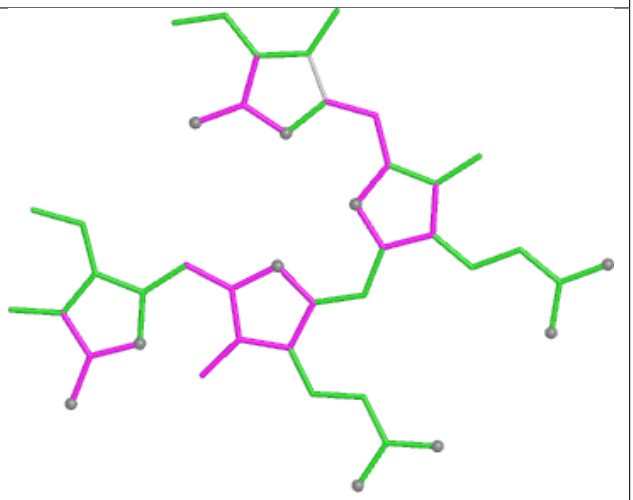


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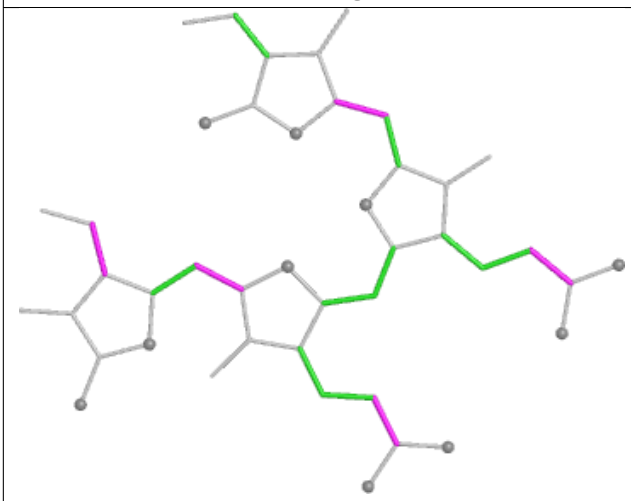
Ligand PEB UO 202



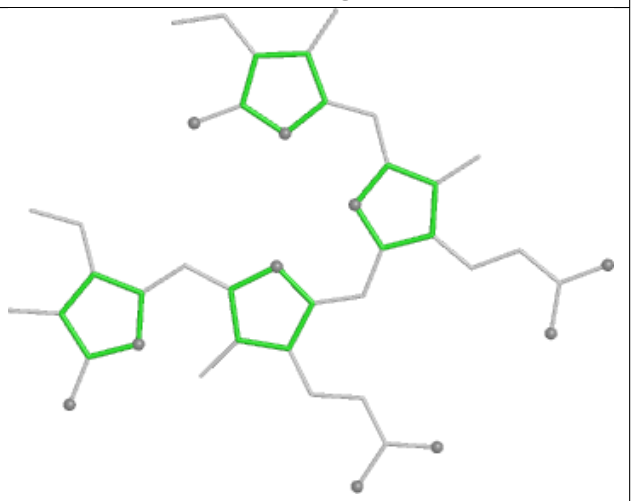
Bond lengths



Bond angles

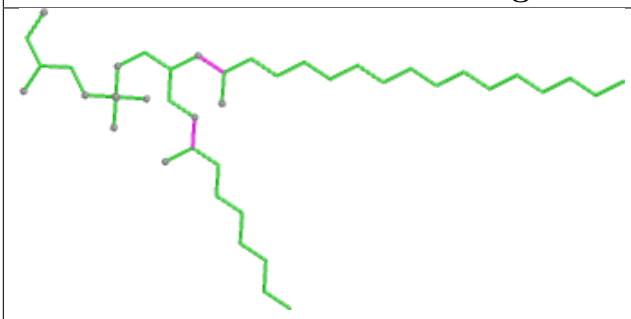


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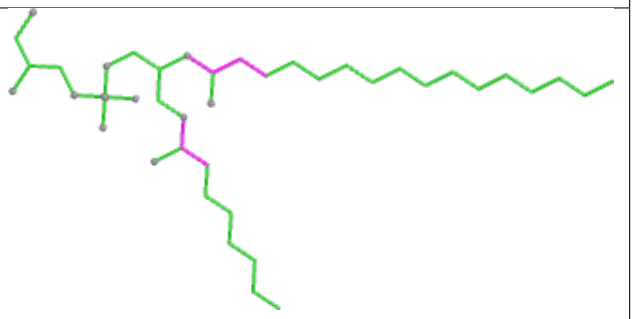


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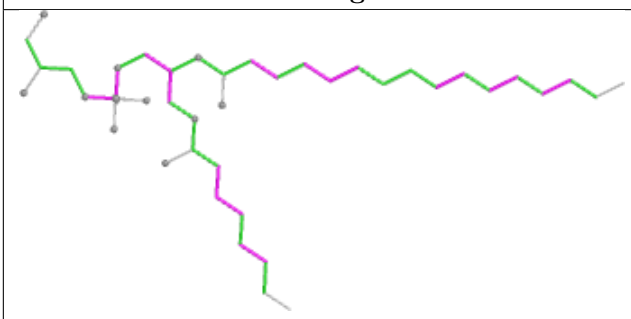
Ligand LHG BL 615



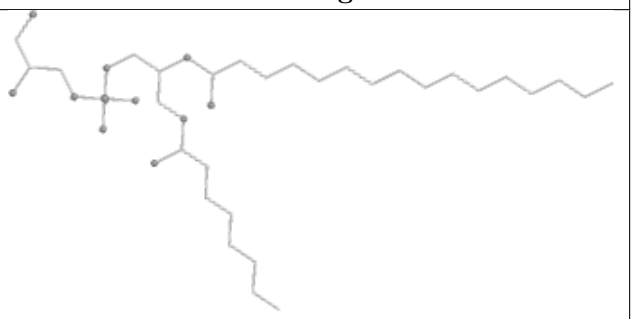
Bond lengths



Bond angles

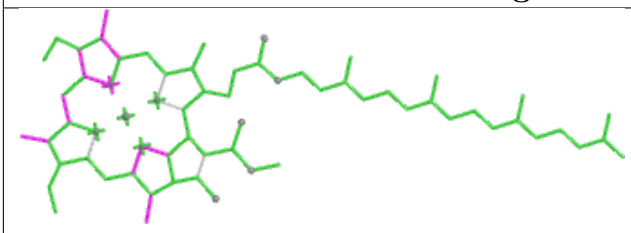


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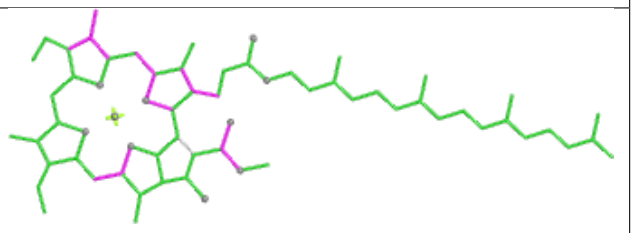


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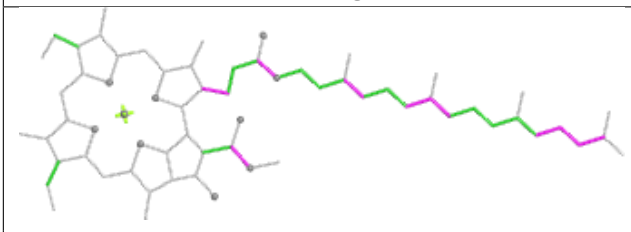
Ligand CLA DL 404



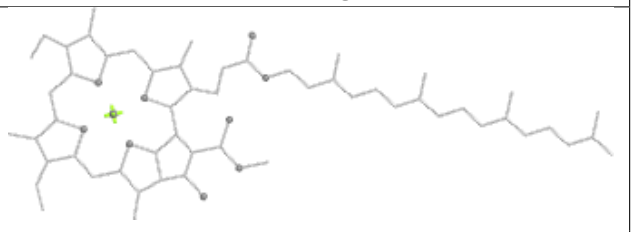
Bond lengths



Bond angles

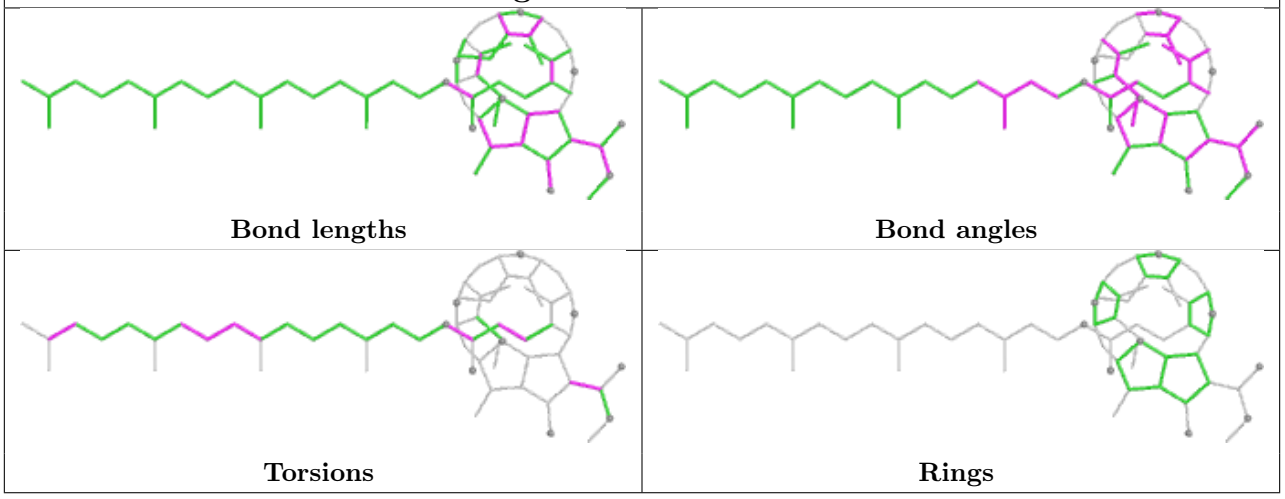


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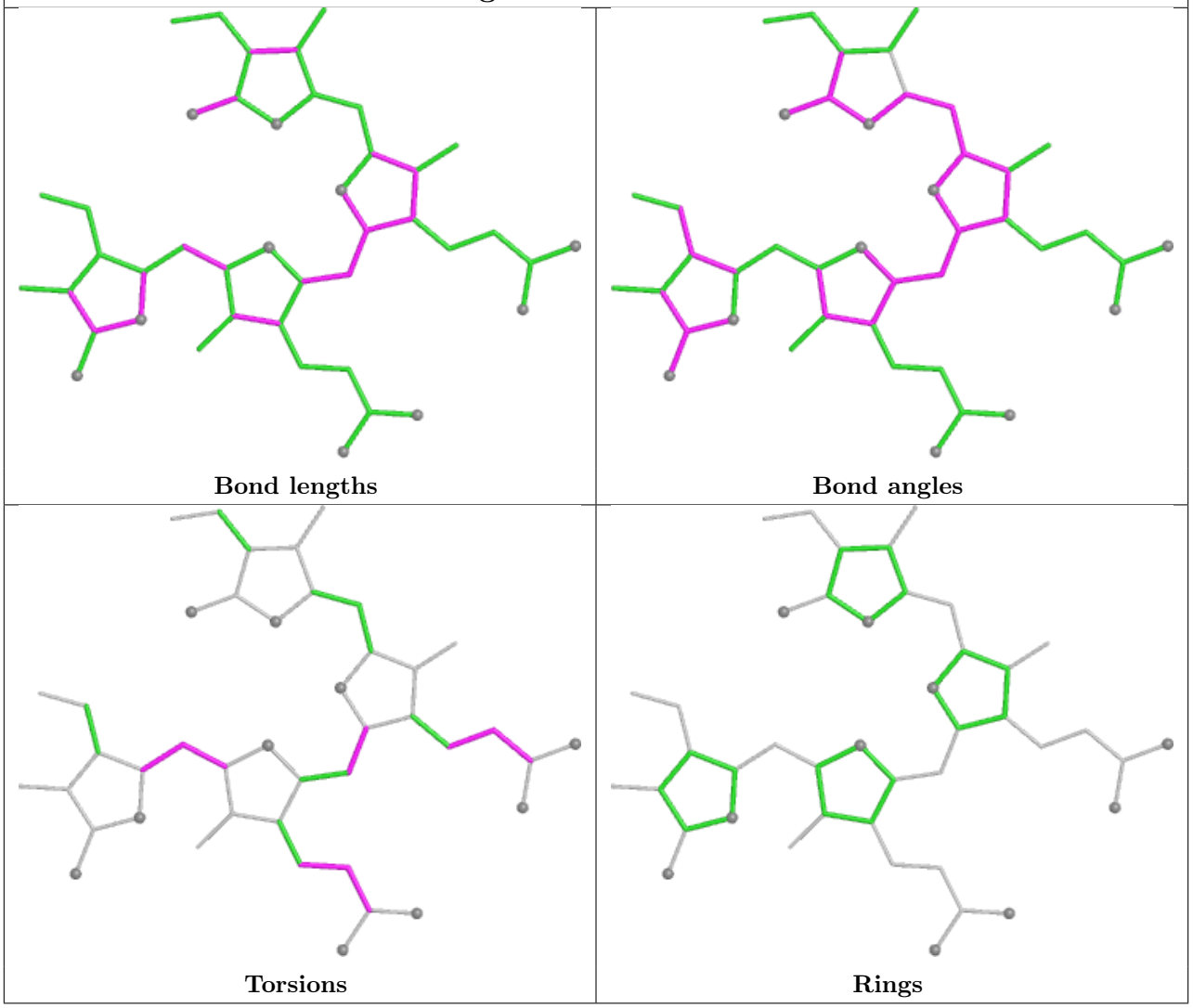


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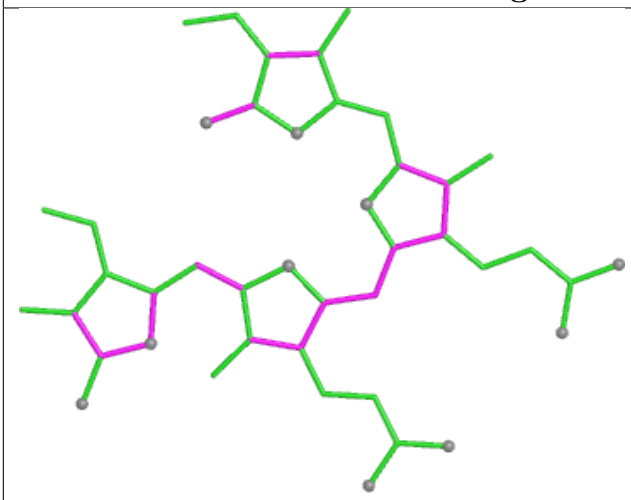
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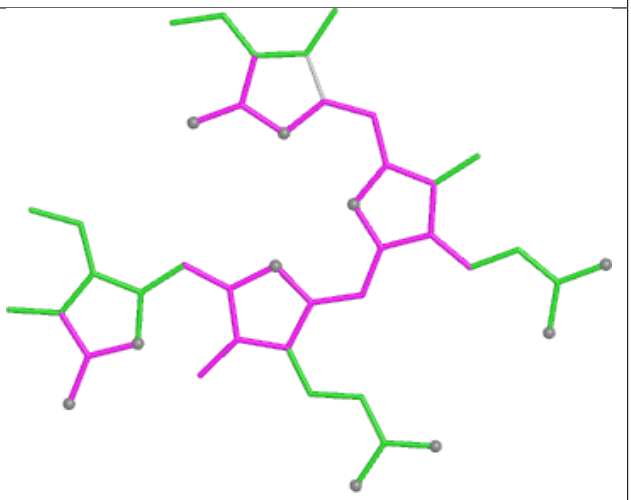
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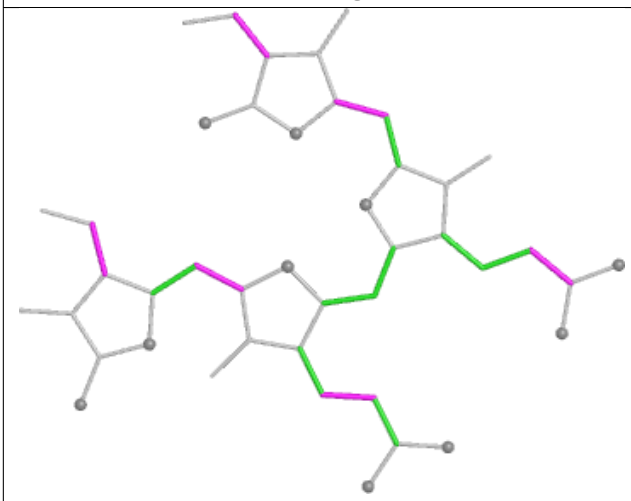
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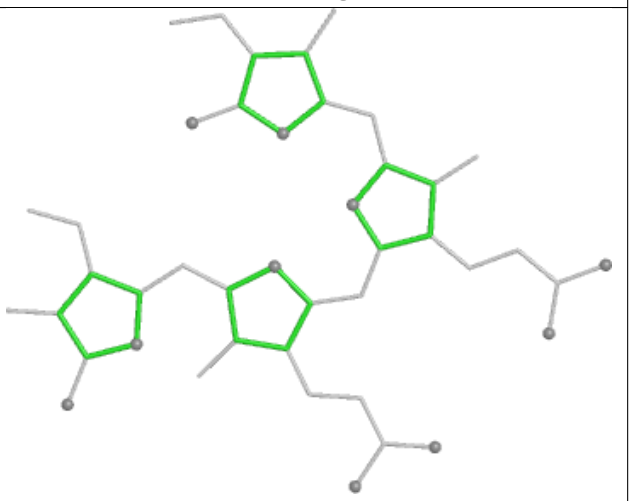
Bond lengths



Bond angles

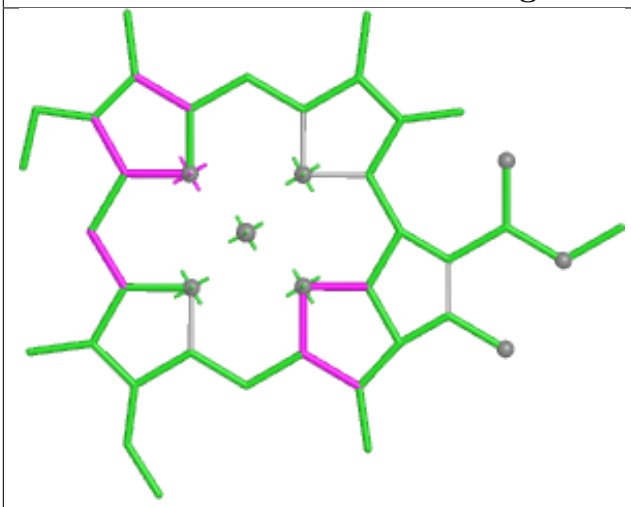


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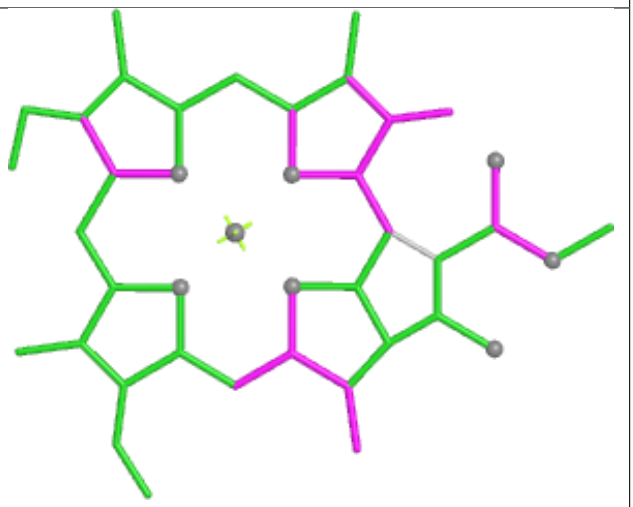


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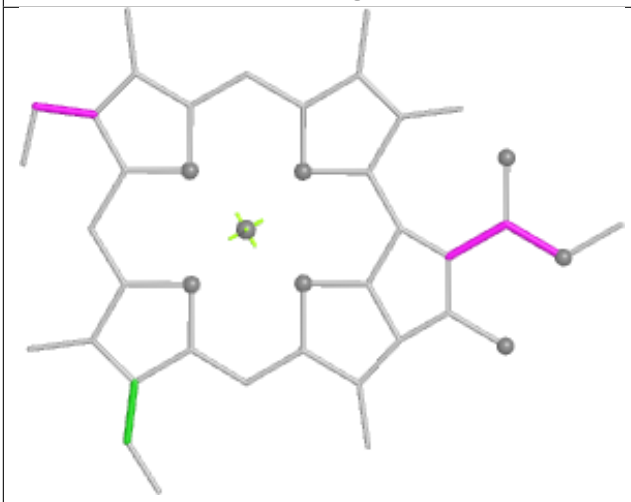
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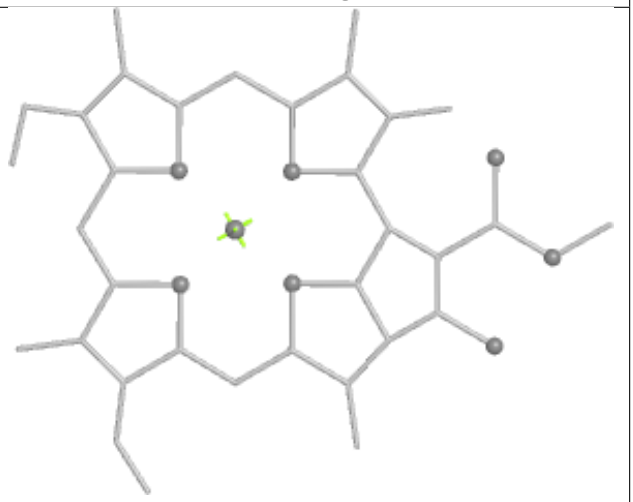
Bond lengths



Bond angles

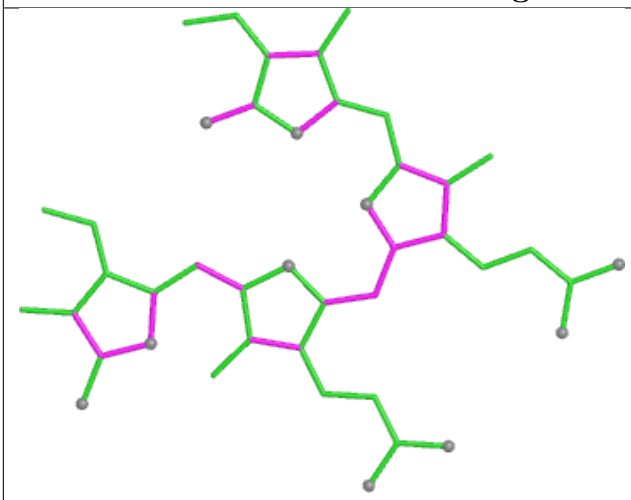


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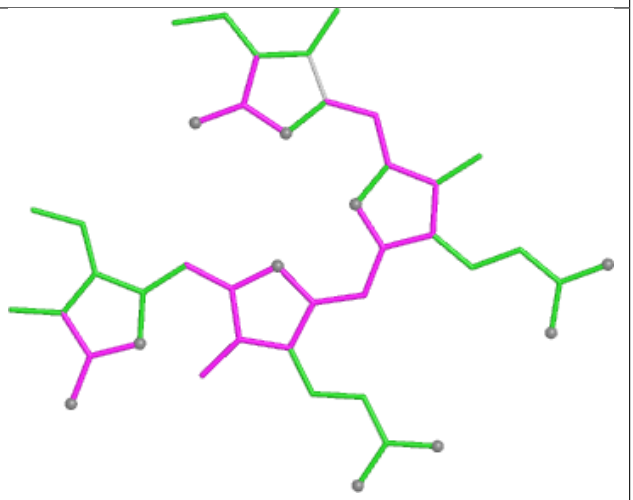


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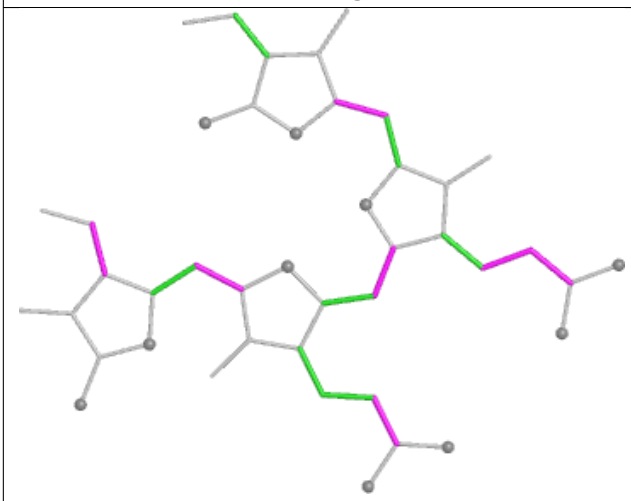
Ligand PEB YA 304



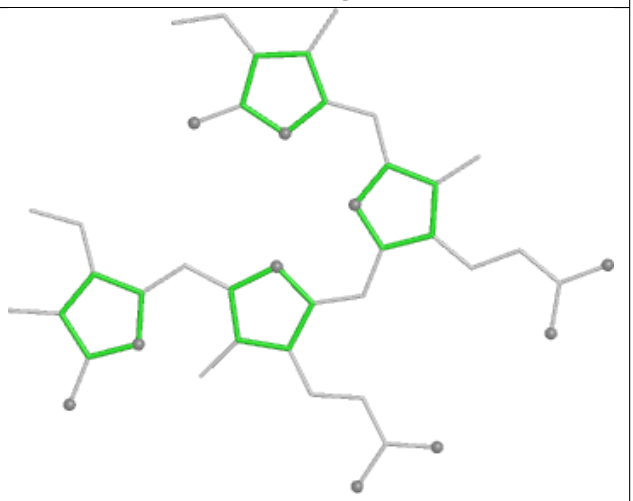
Bond lengths



Bond angles

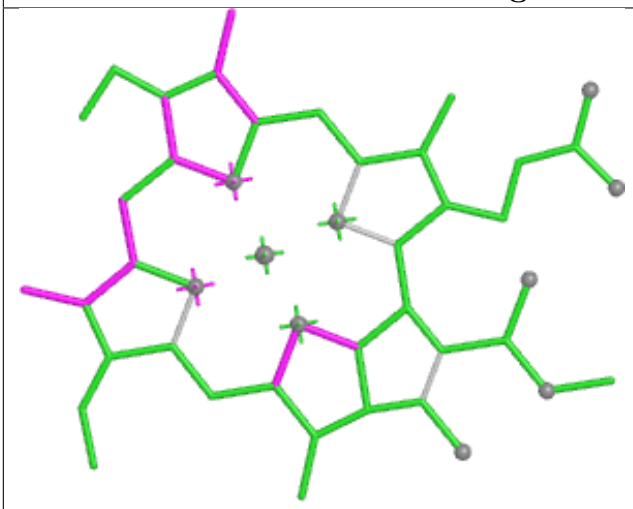


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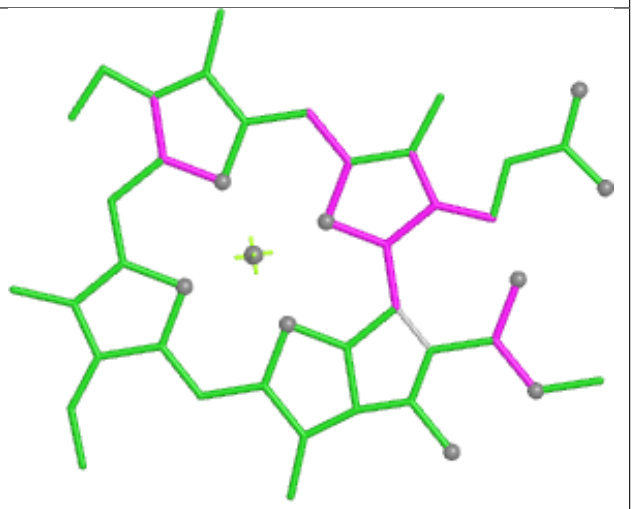


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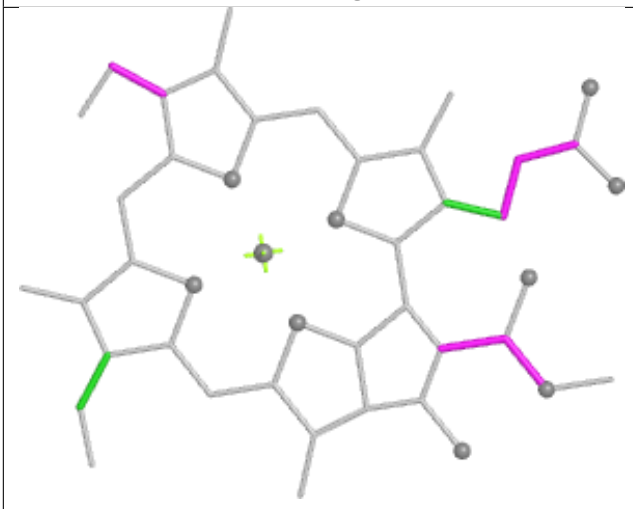
Ligand CLA ON 203



Bond lengths



Bond angles

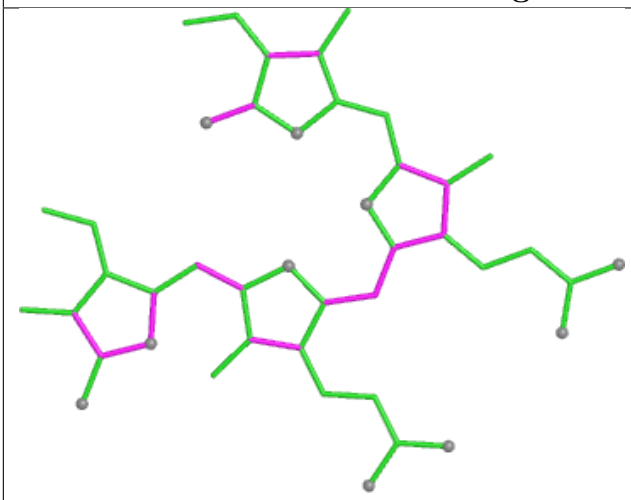


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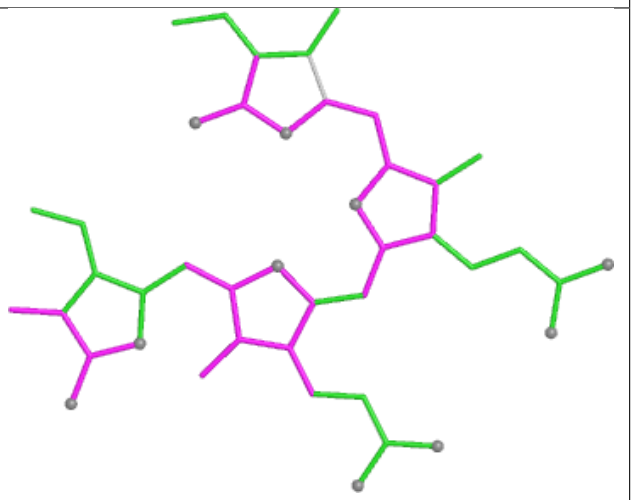


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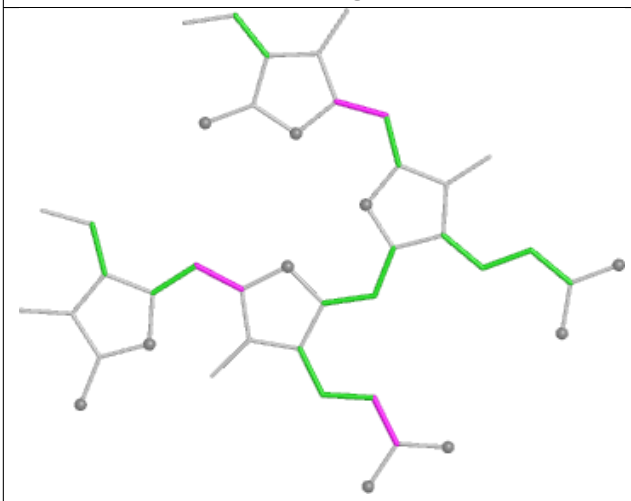
Ligand PEB AE 304



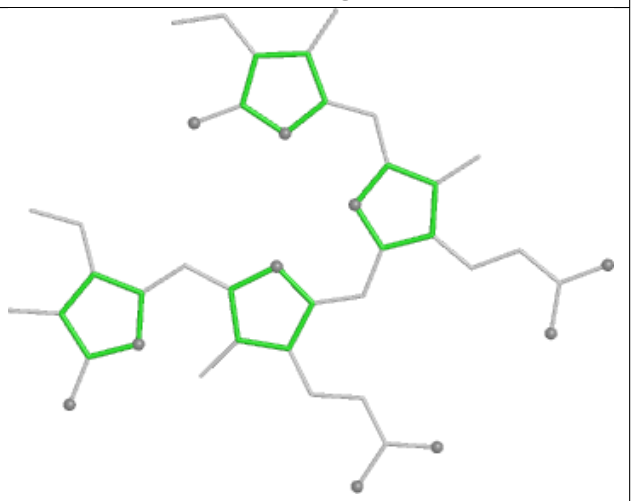
Bond lengths



Bond angles

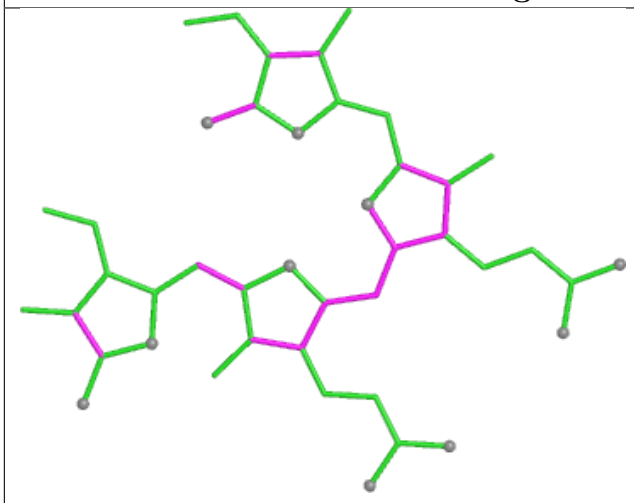


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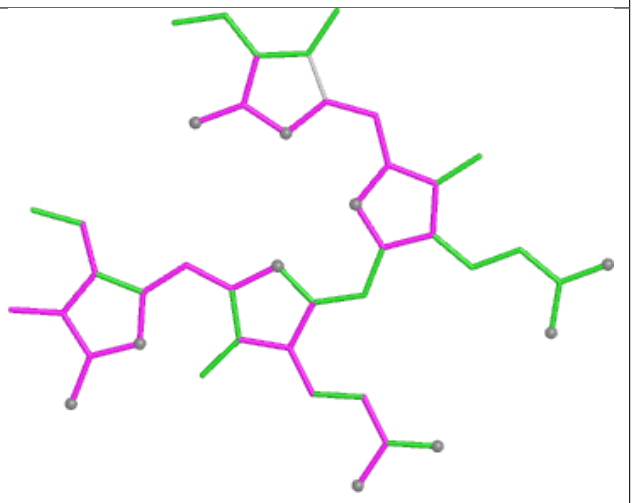


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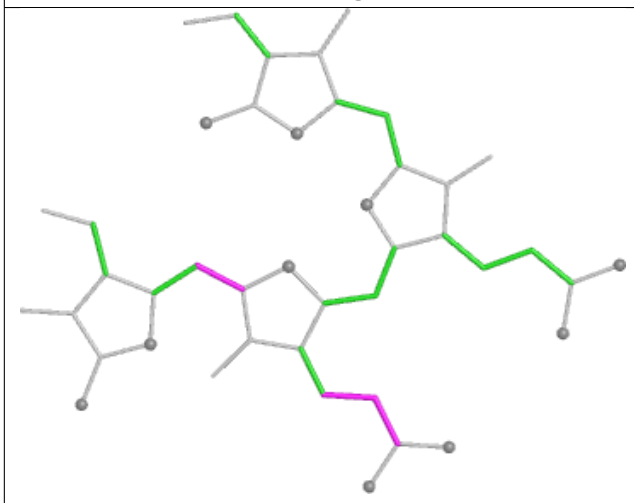
Ligand PEB FK 201



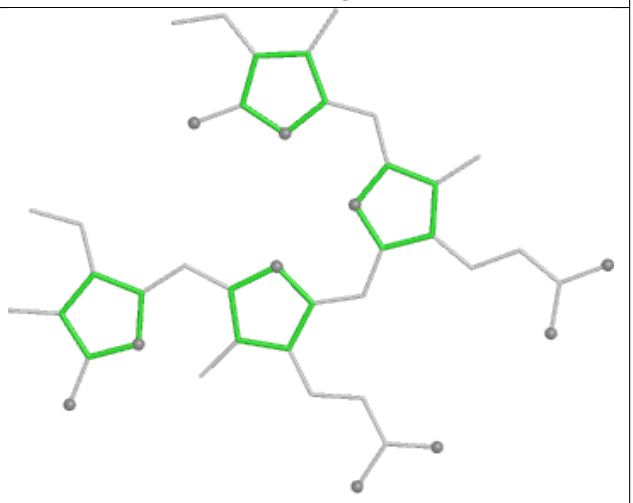
Bond lengths



Bond angles

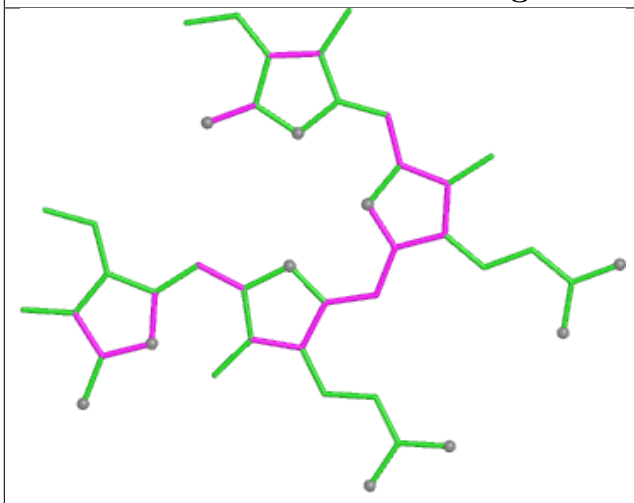


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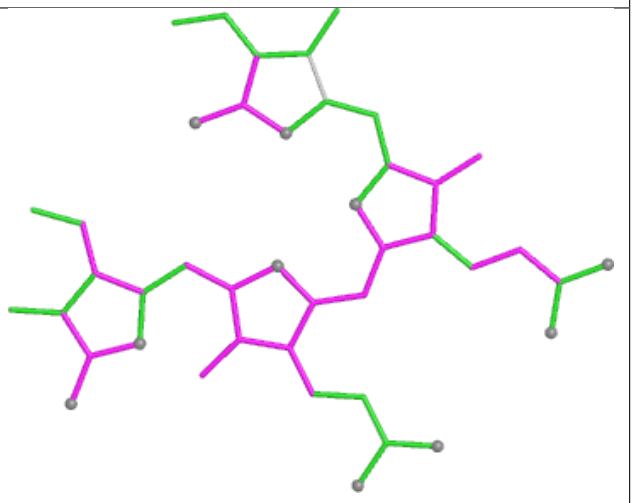


Rings

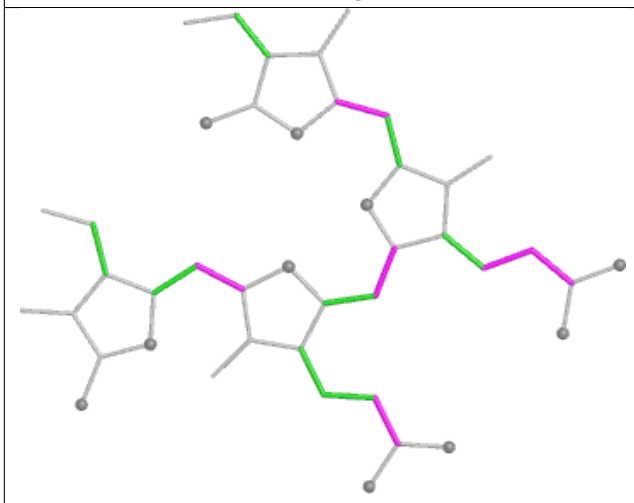
Ligand PEB XK 203



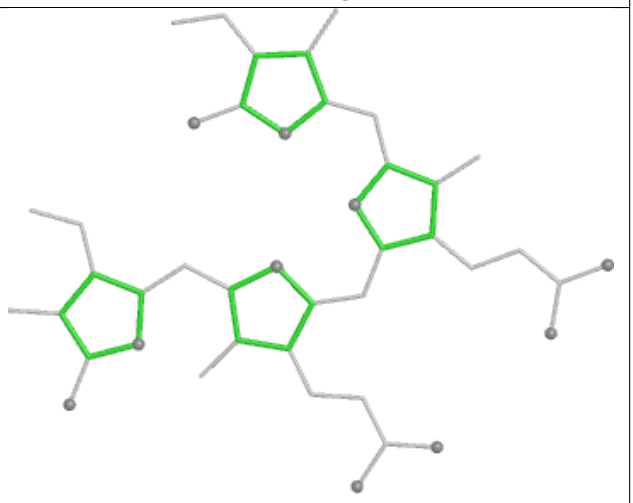
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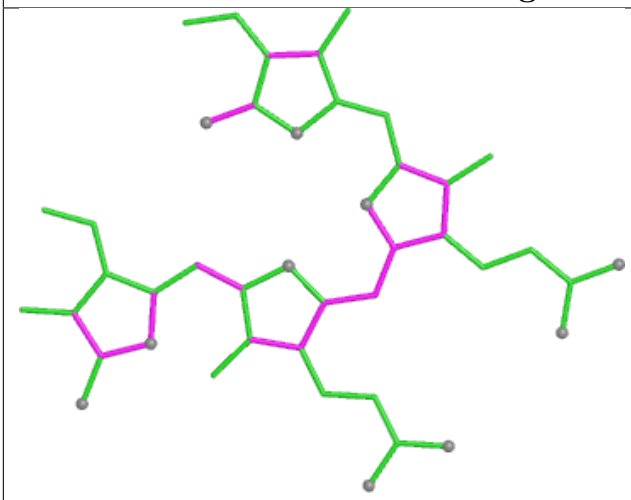
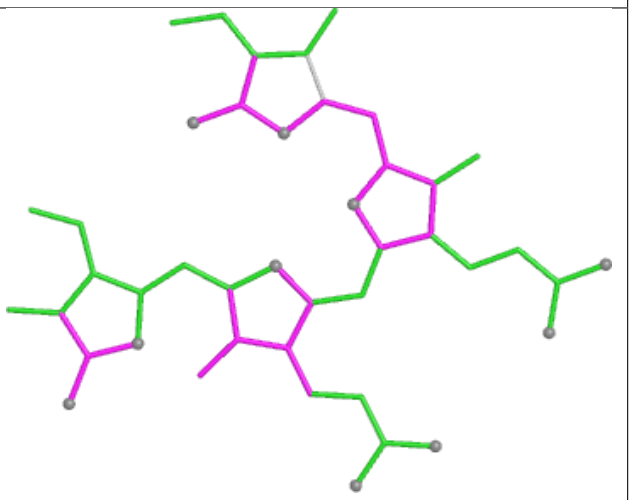
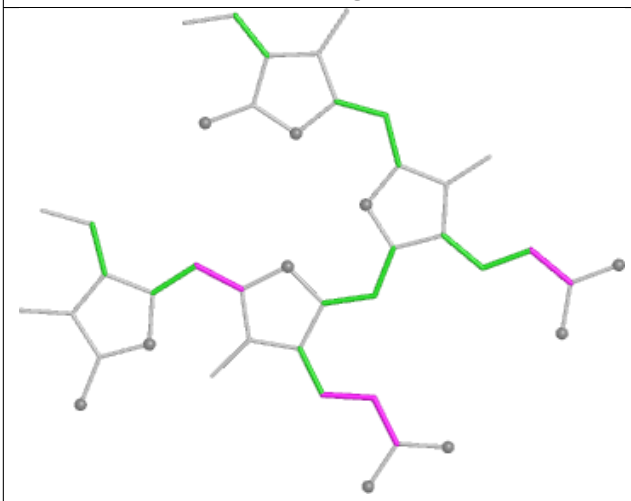
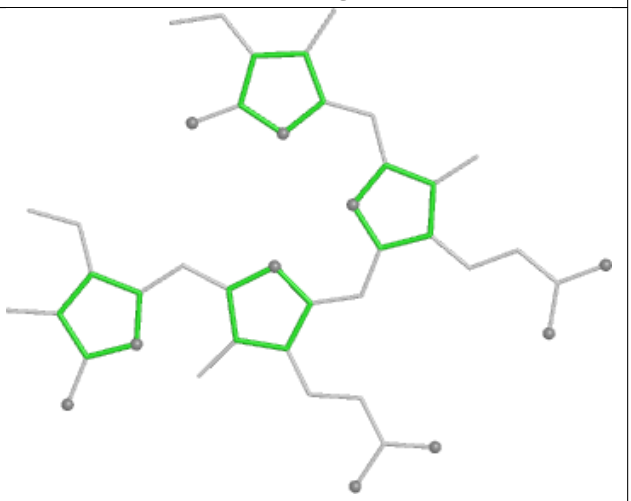
Bond angles

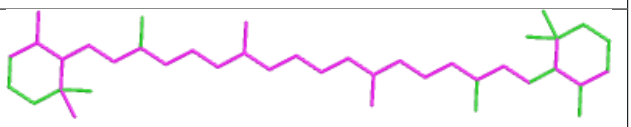
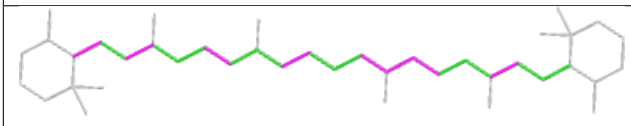
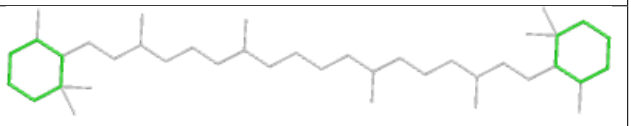


Torsions

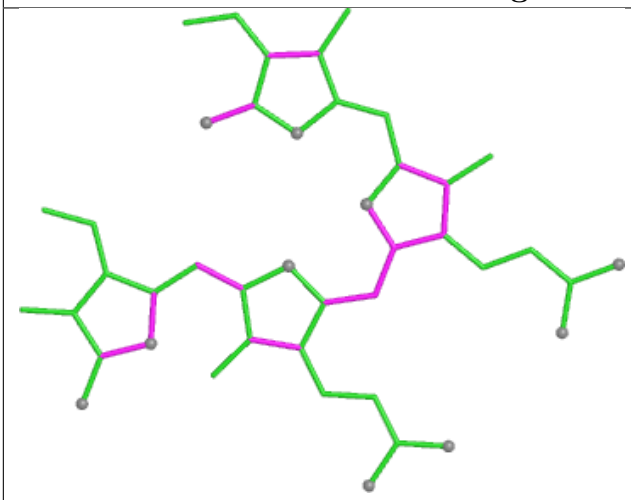


Rings

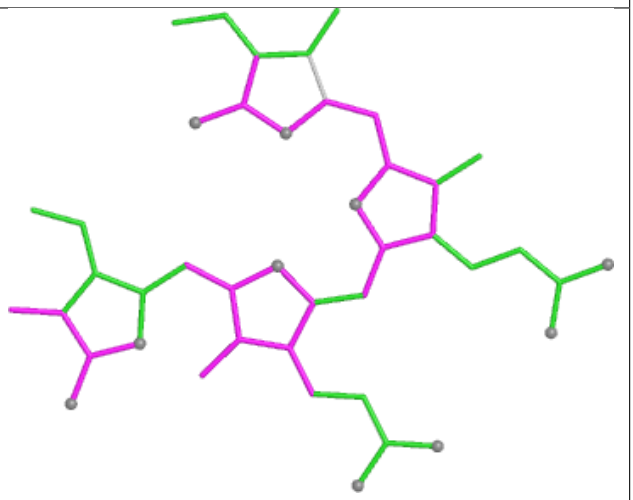
Ligand PEB lG 203	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR kL 100	
	
Bond lengths	Bond angles
	
Torsions	Rings

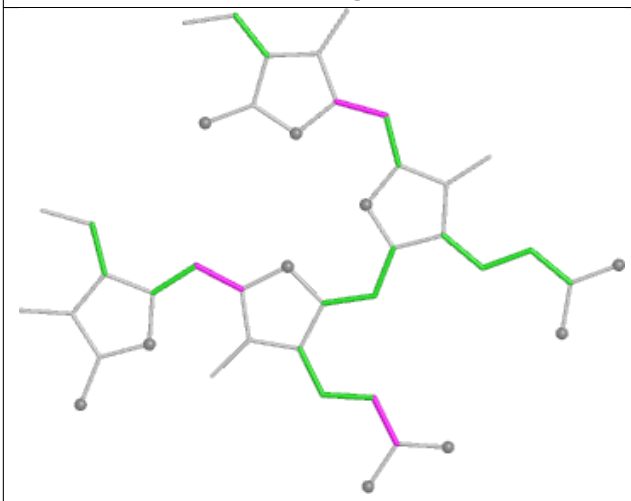
Ligand PEB AG 304



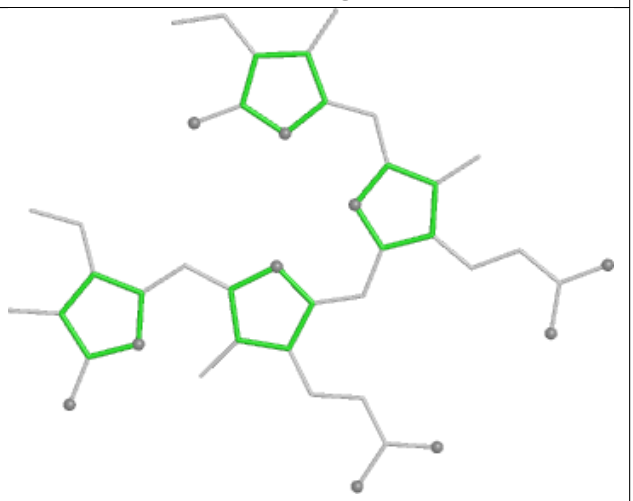
Bond lengths



Bond angles

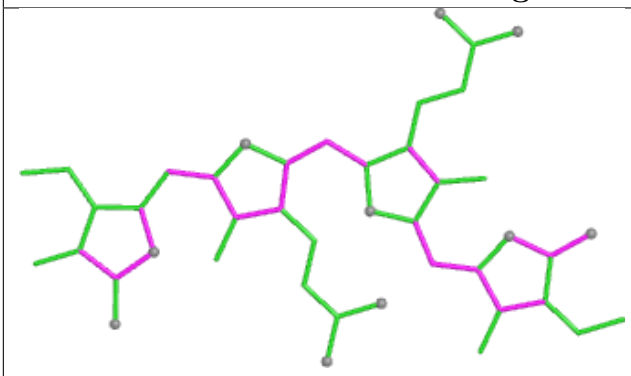


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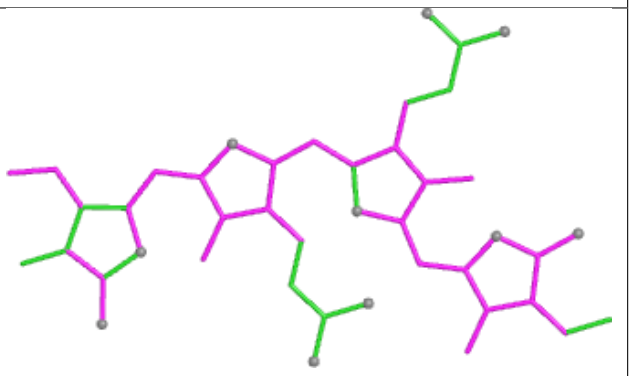


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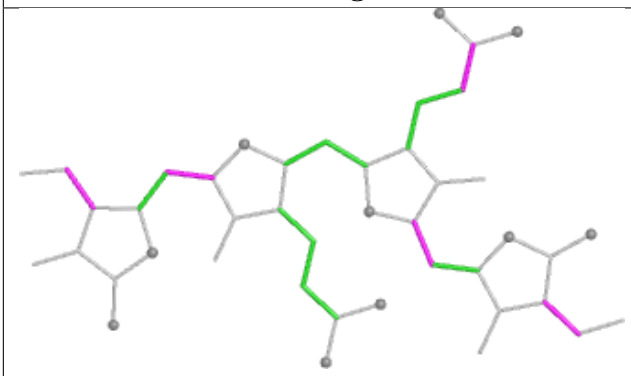
Ligand CYC l3 1001



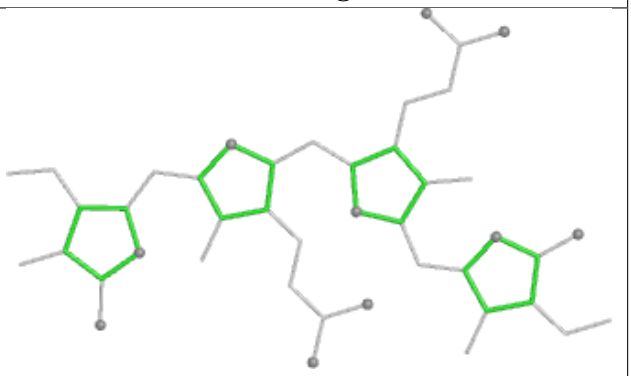
Bond lengths



Bond angles

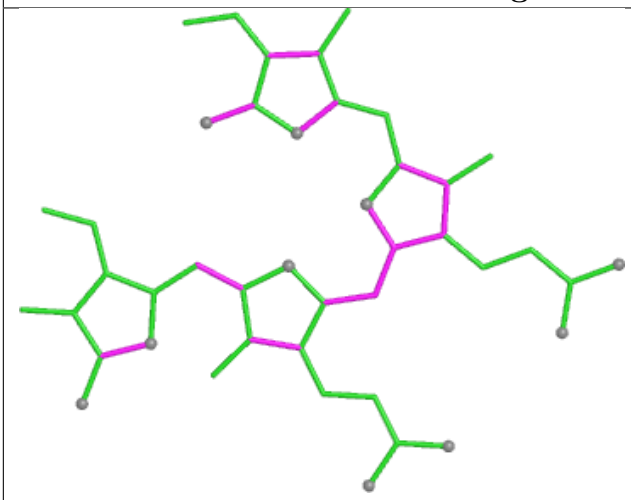


Torsions

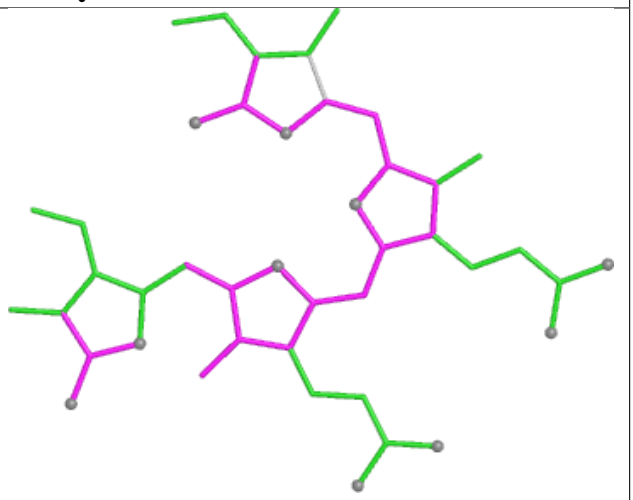


Rings

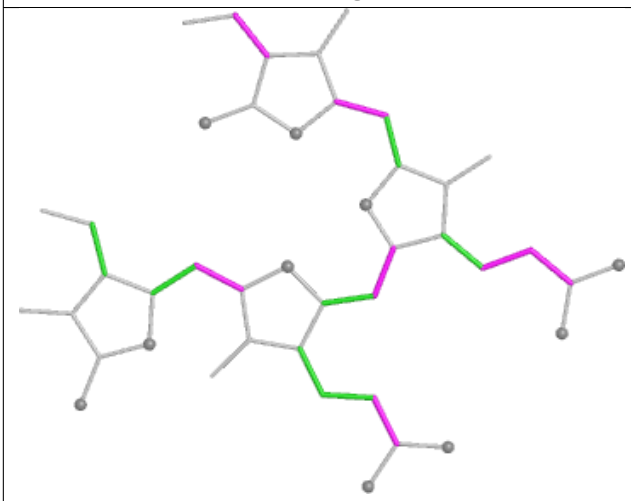
Ligand PEB KQ 202



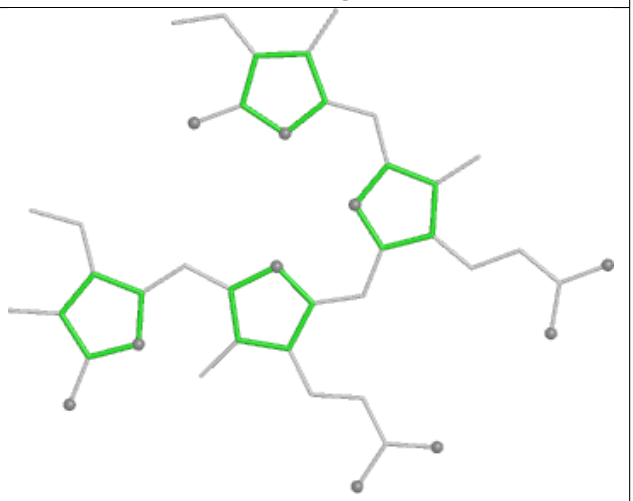
Bond lengths



Bond angles

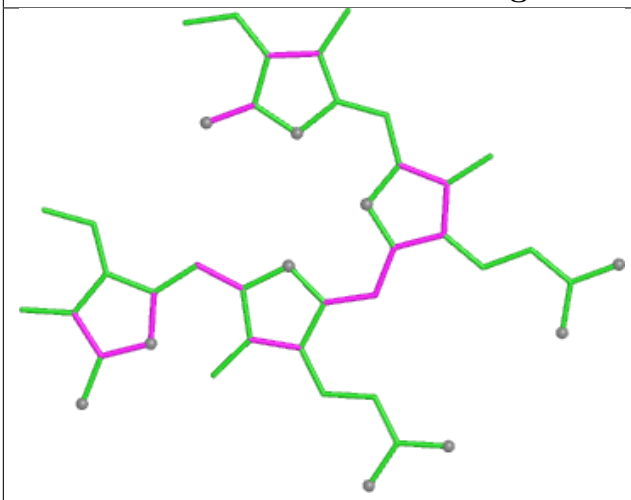


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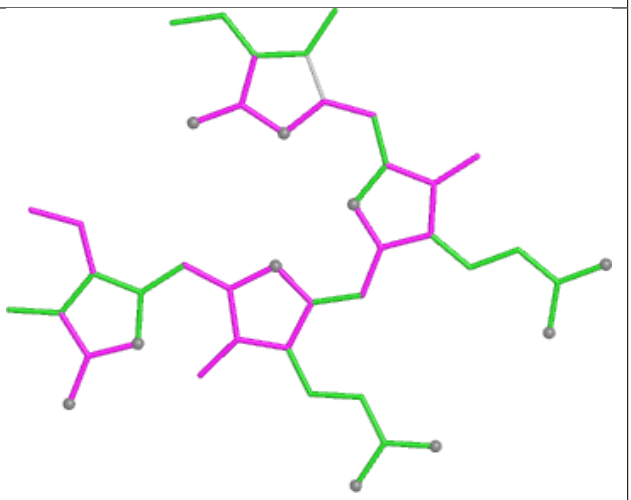


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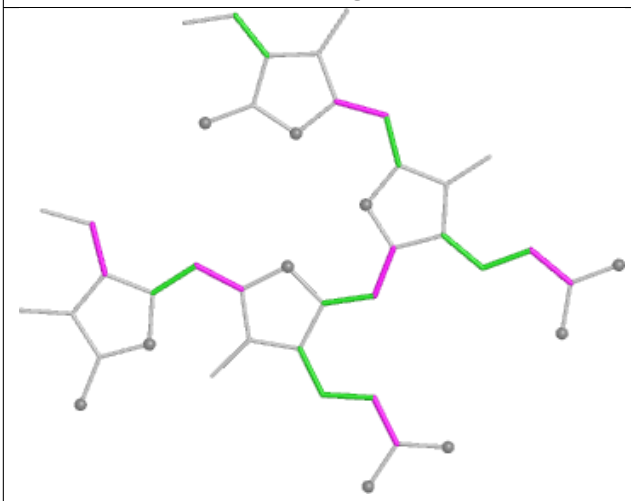
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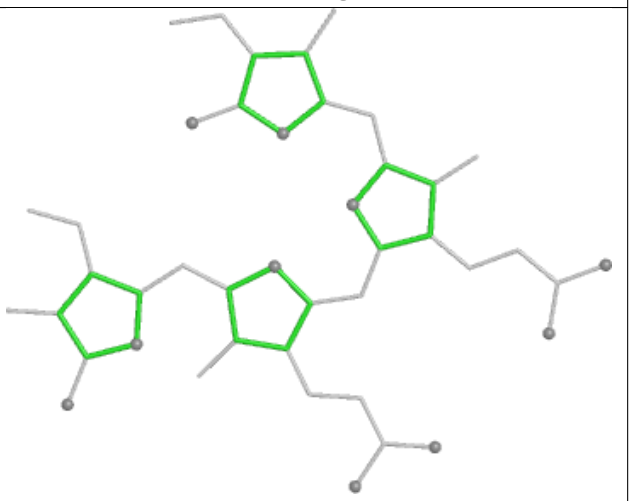
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Bond angles

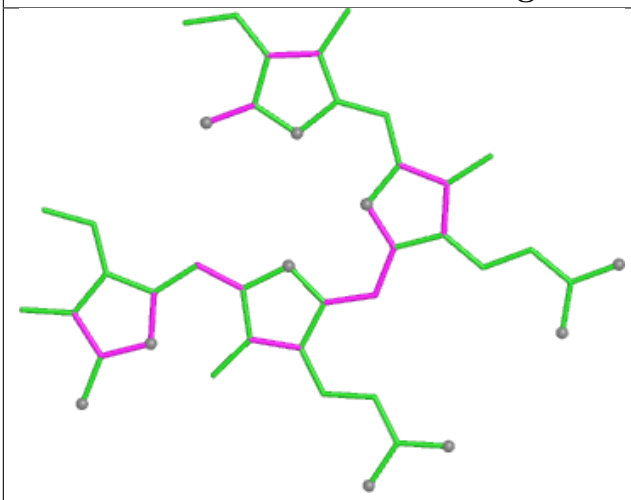


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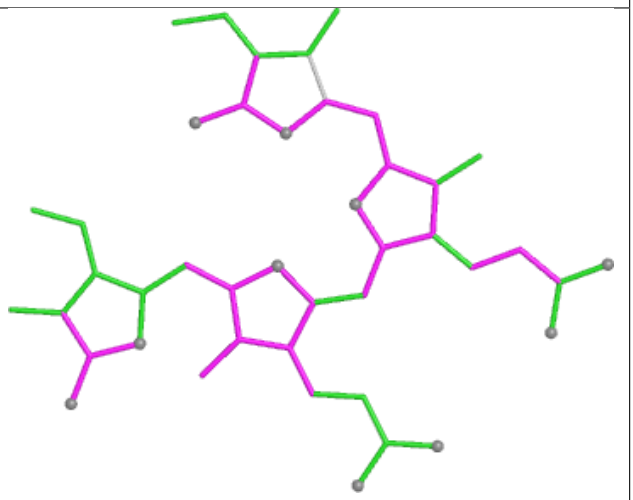


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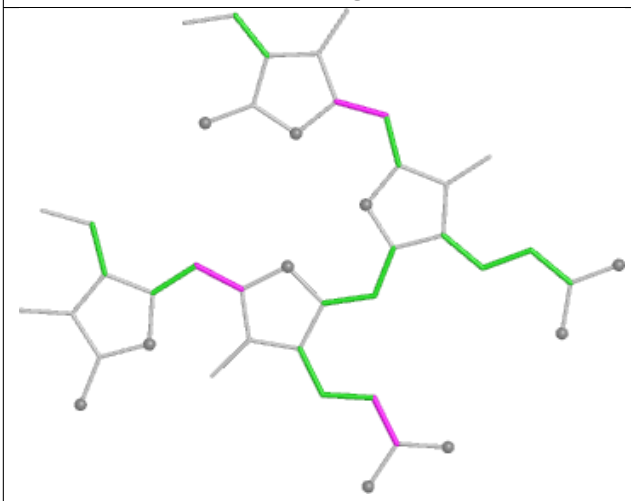
Ligand PEB YI 202



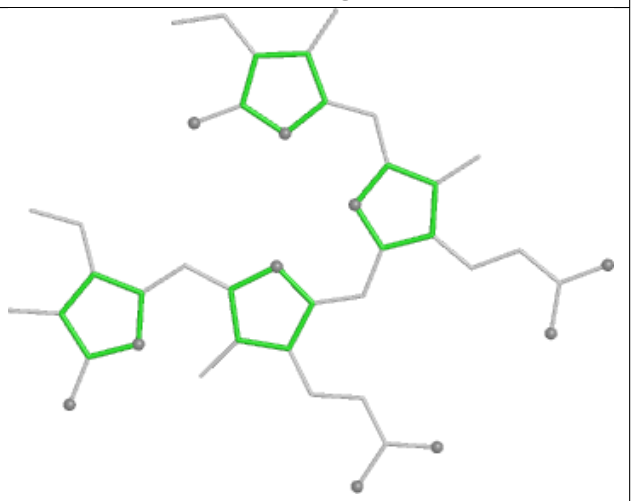
Bond lengths



Bond angles

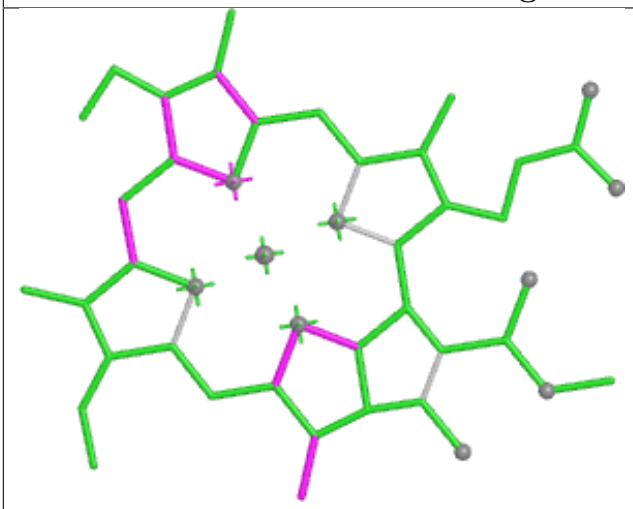


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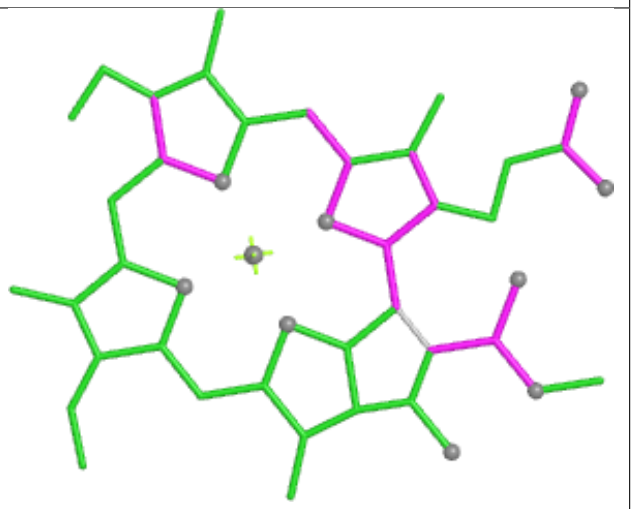


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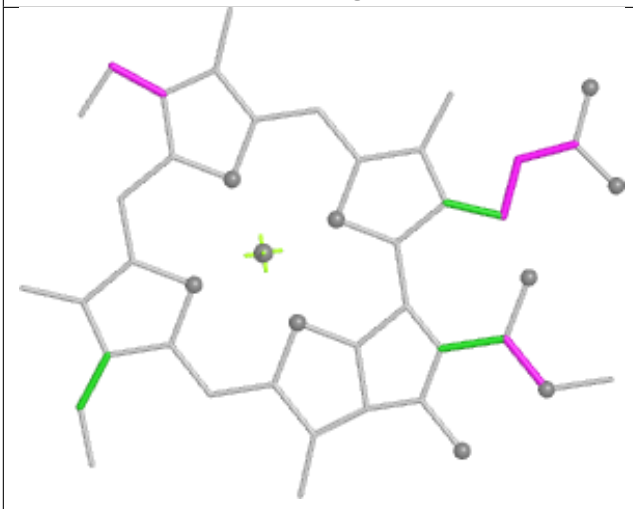
Ligand CLA 72 603



Bond lengths



Bond angles

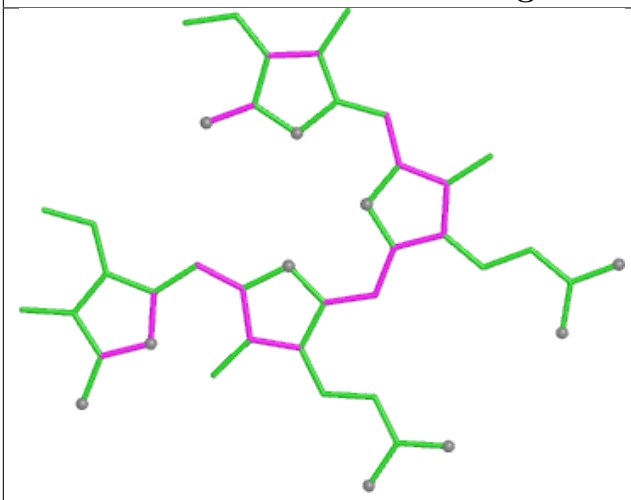


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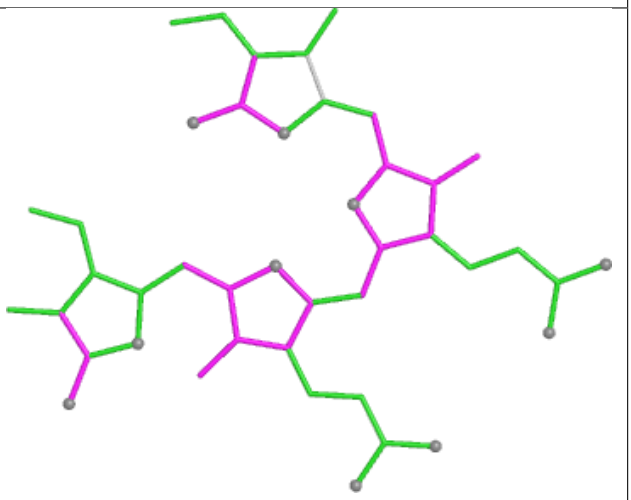


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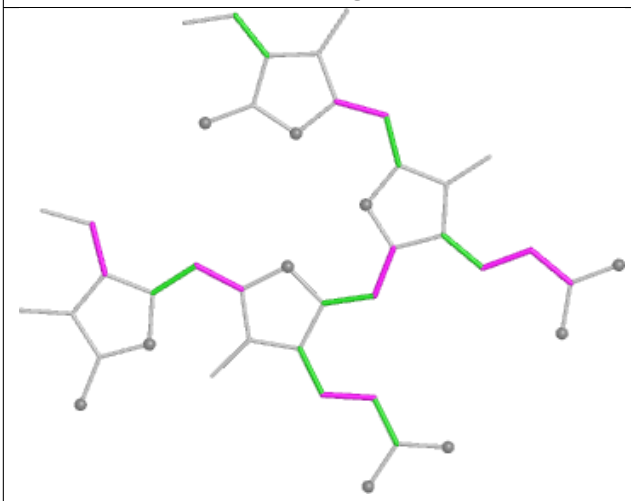
Ligand PEB kF 201



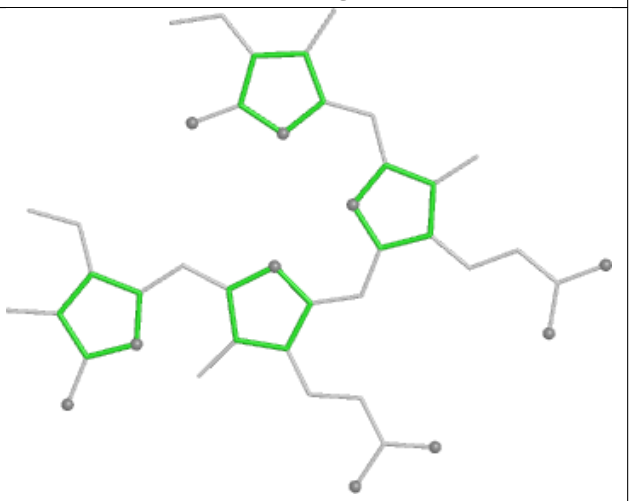
Bond lengths



Bond angles

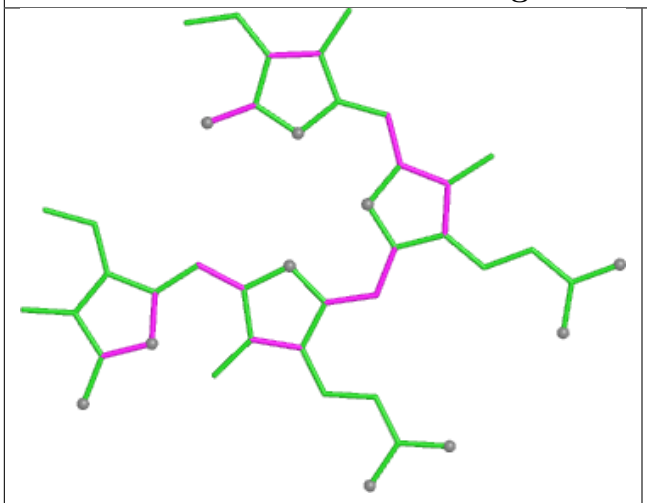


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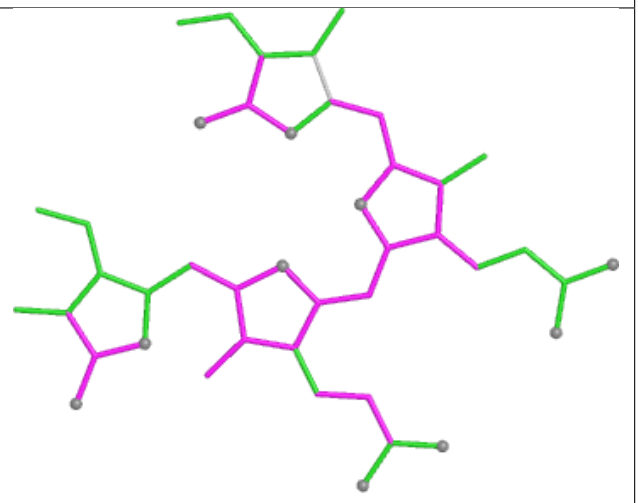


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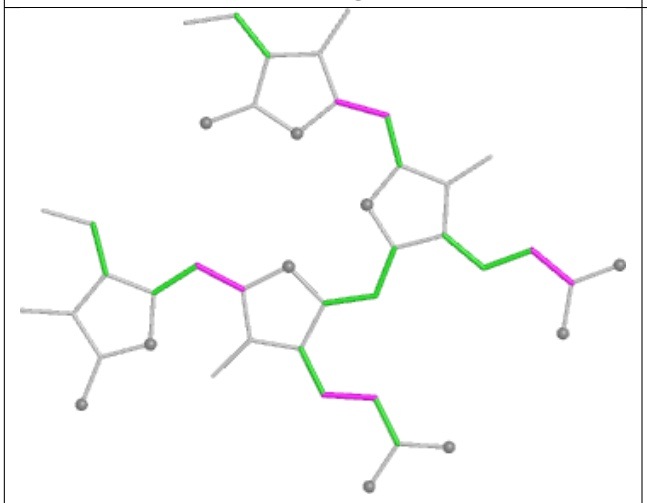
Ligand PEB YK 201



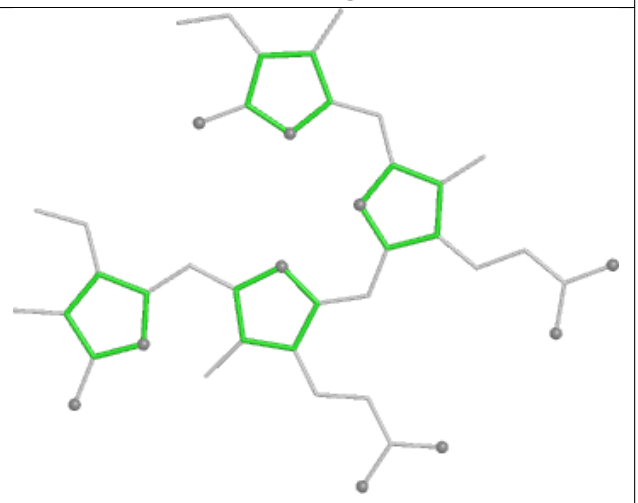
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Bond angles

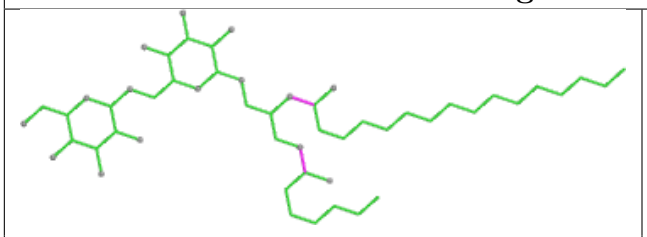


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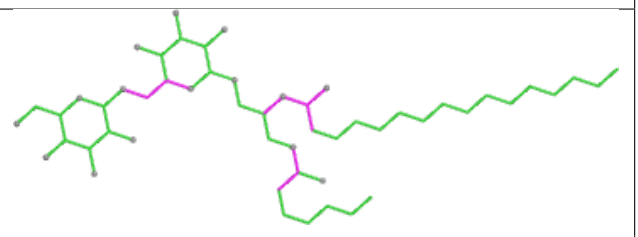


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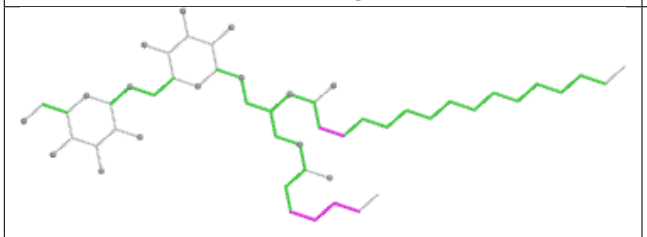
Ligand DGD a6 604



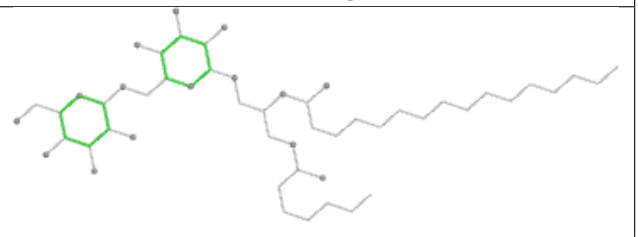
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Bond angles

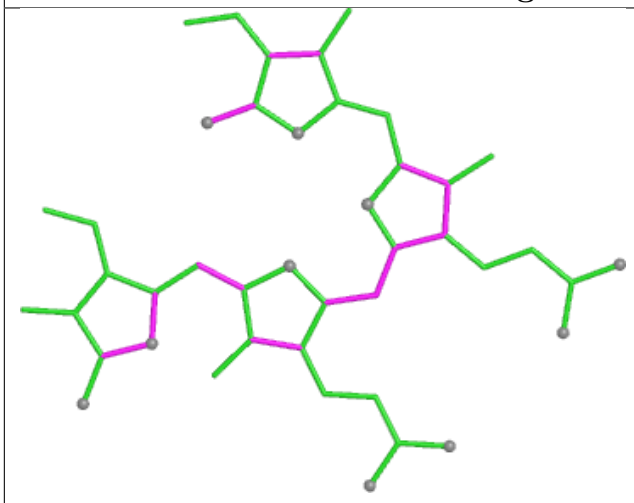


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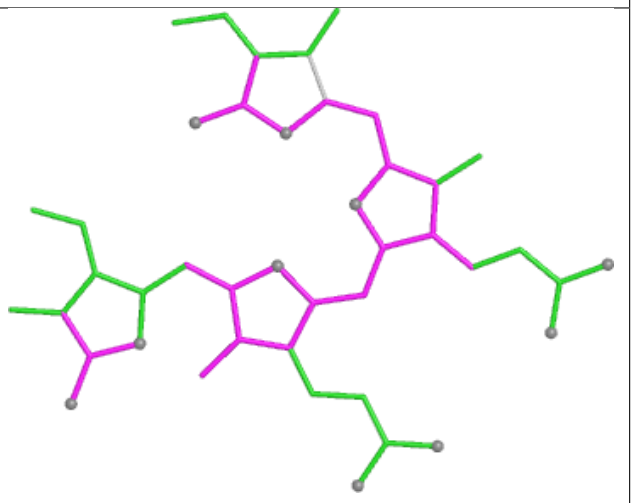


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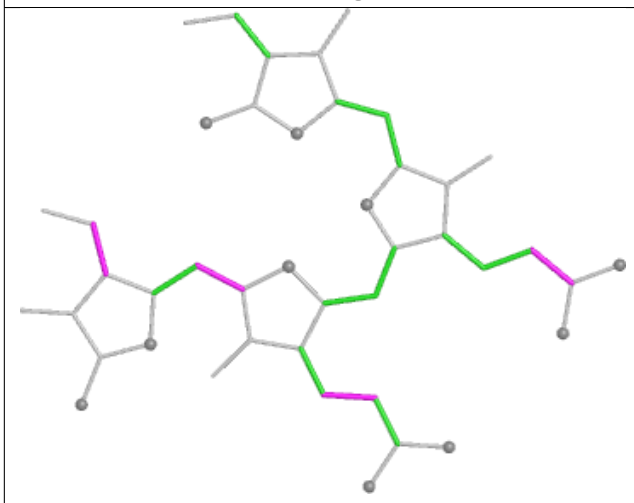
Ligand PEB SE 202



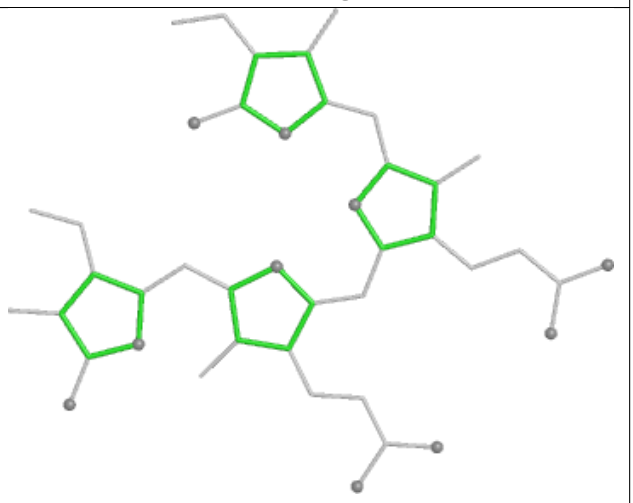
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Bond angles

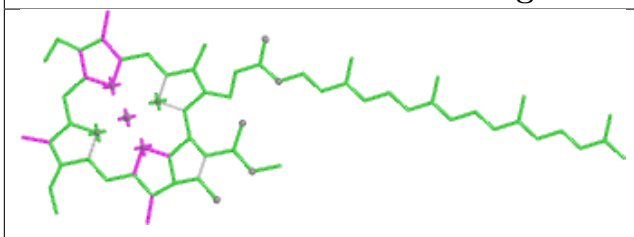


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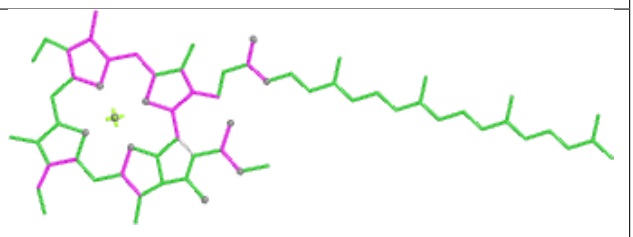


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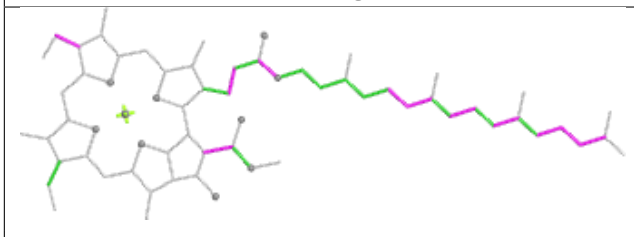
Ligand CLA B2 822



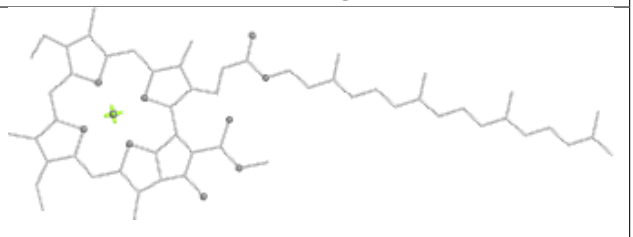
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Bond angles

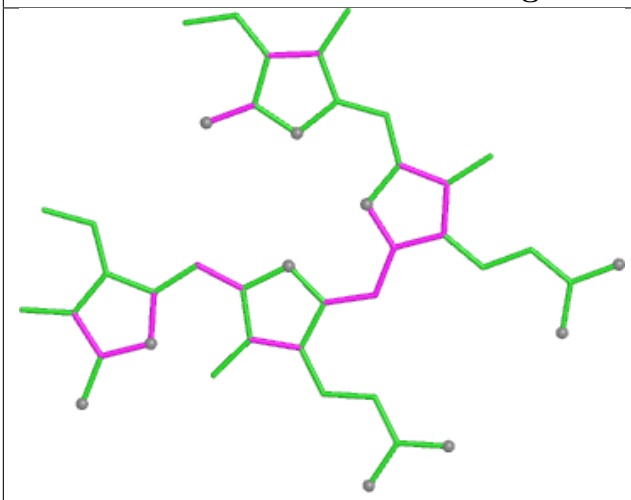


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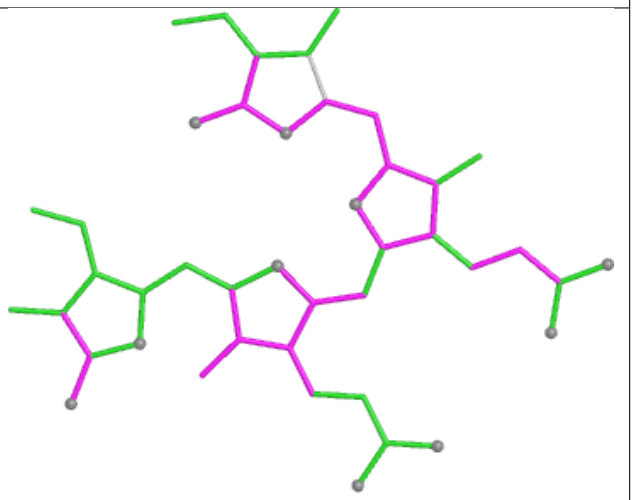


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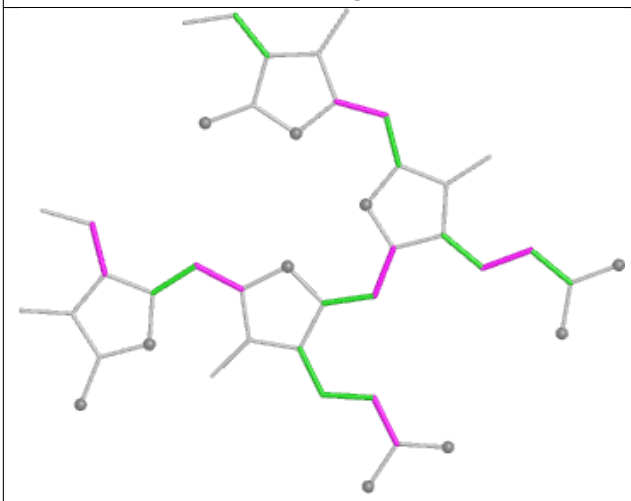
Ligand PEB JI 202



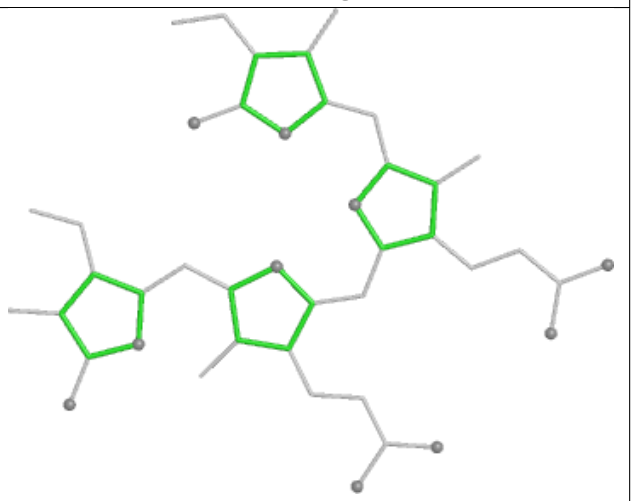
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Bond angles

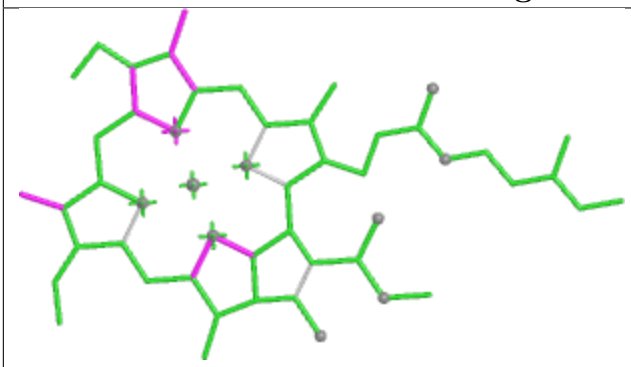


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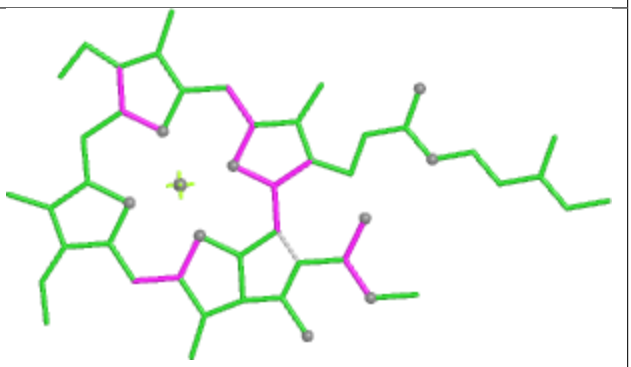


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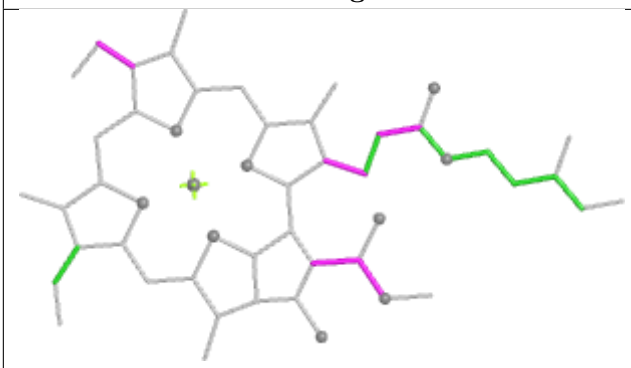
Ligand CLA A2 824



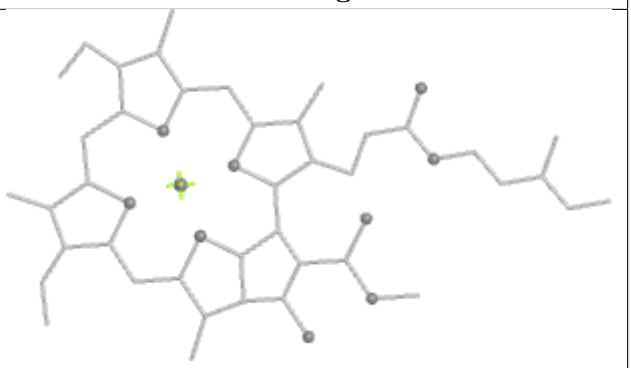
Bond lengths



Bond angles

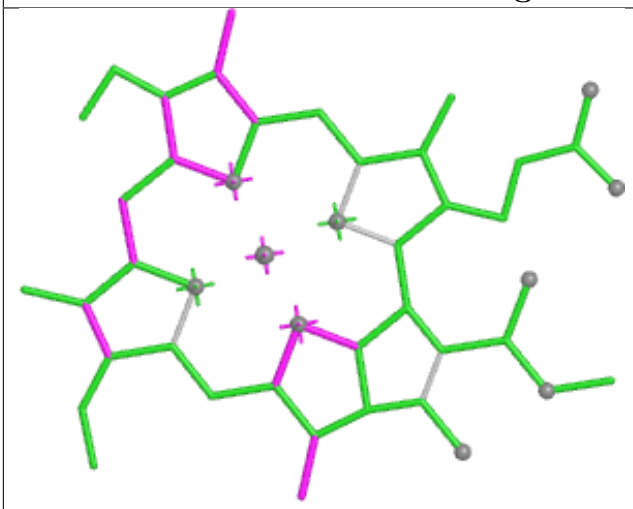


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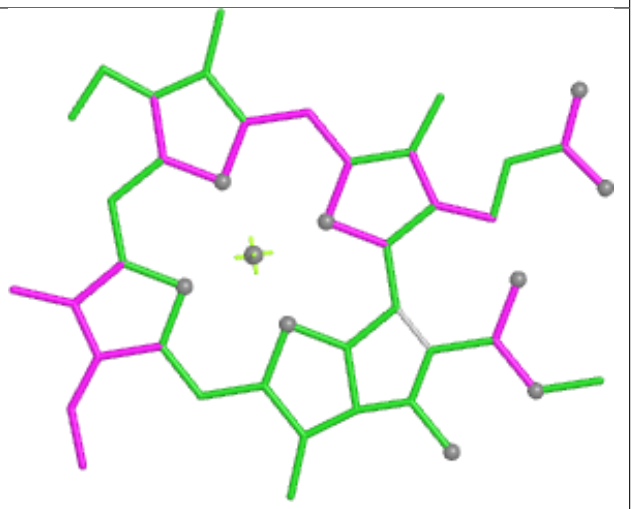


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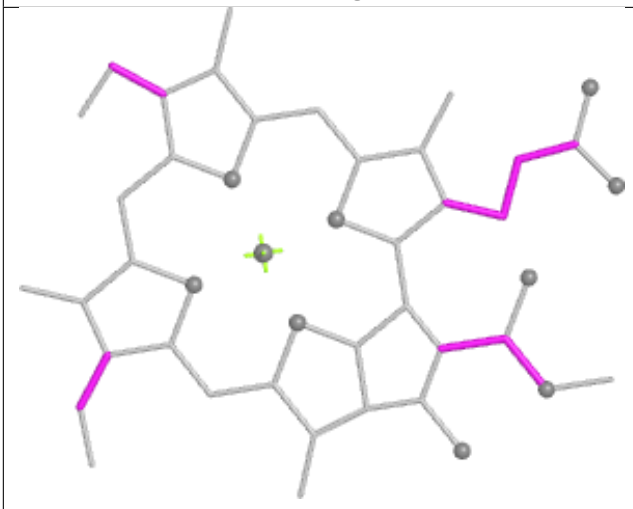
Ligand CLA 8N 308



Bond lengths



Bond angles

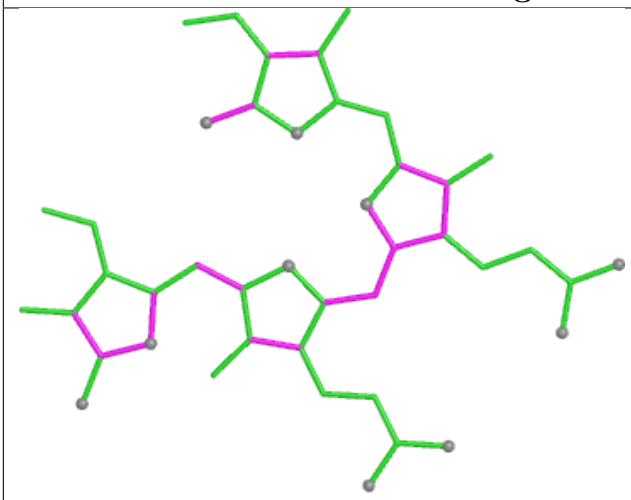


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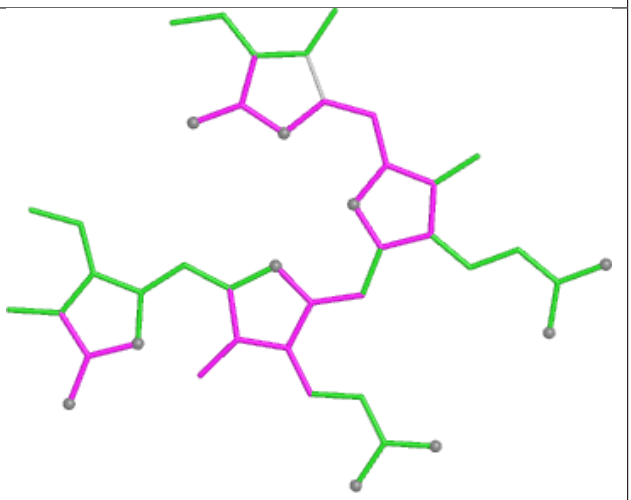


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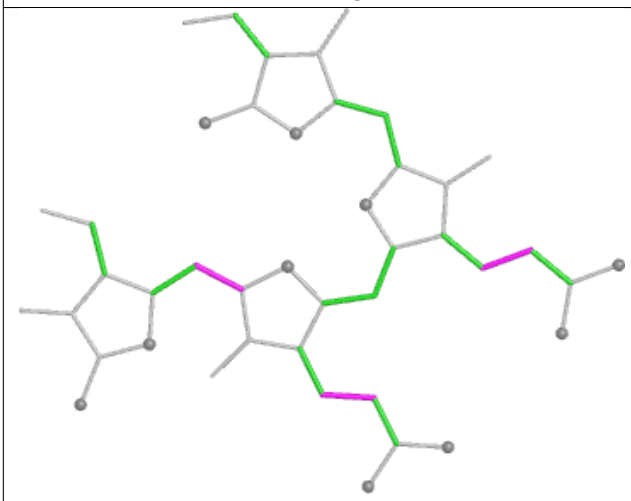
Ligand PEB SD 201



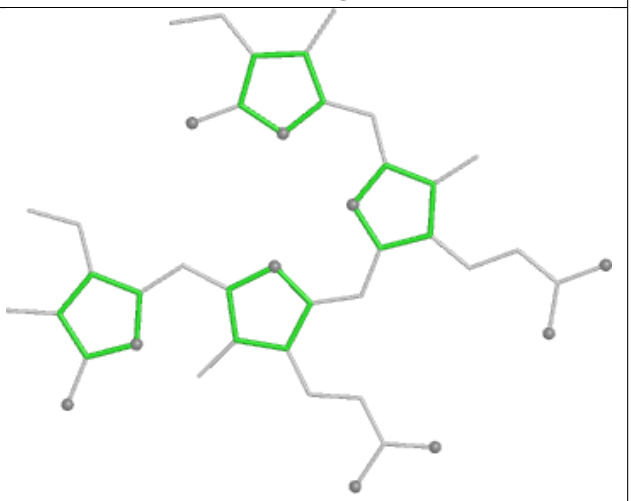
Bond lengths



Bond angles

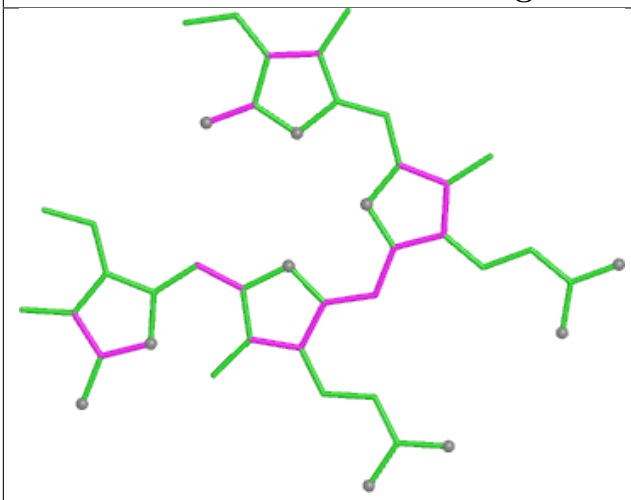


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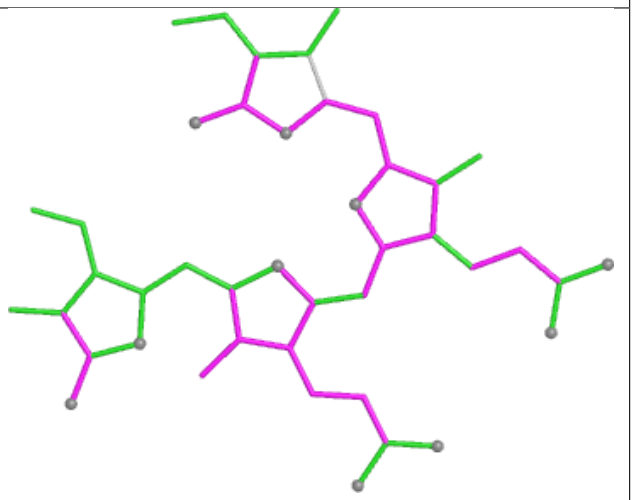


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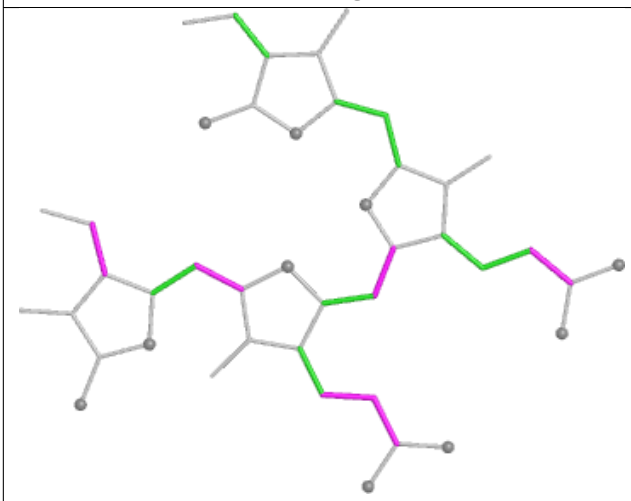
Ligand PEB Y4 203



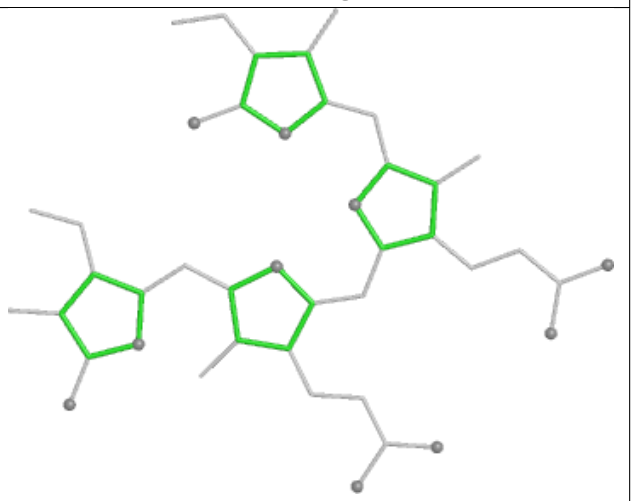
Bond lengths



Bond angles

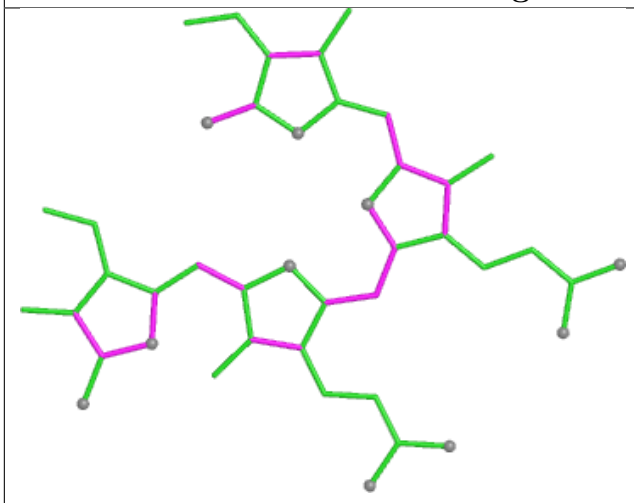


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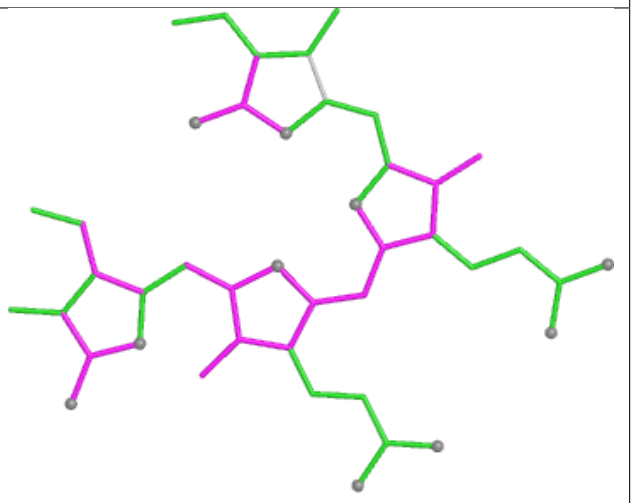


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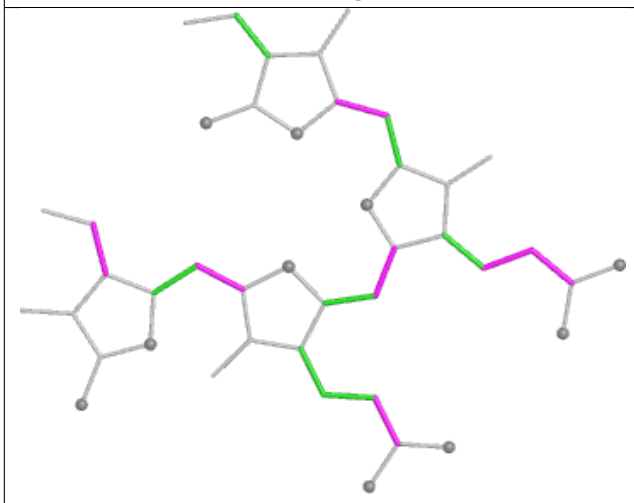
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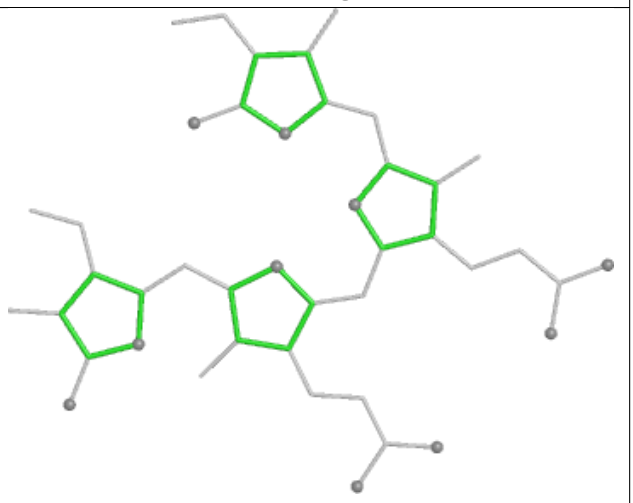
Bond lengths



Bond angles

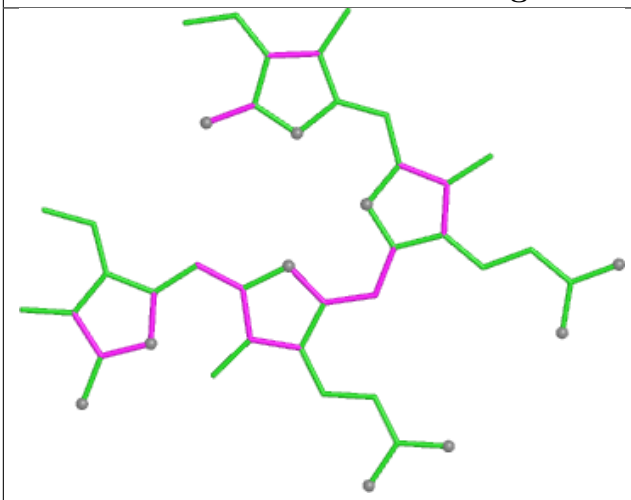


Torsions

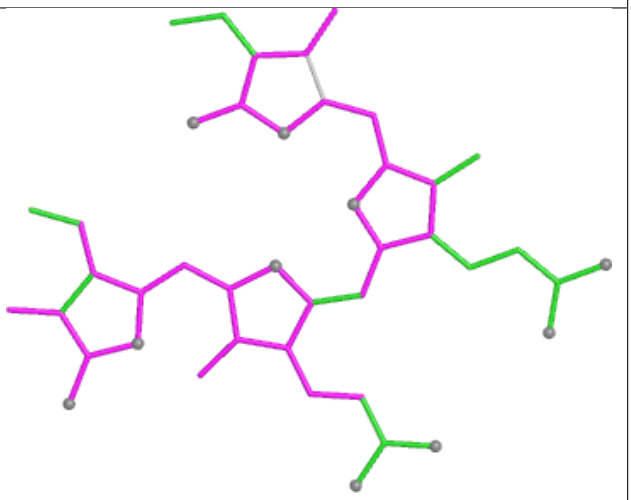


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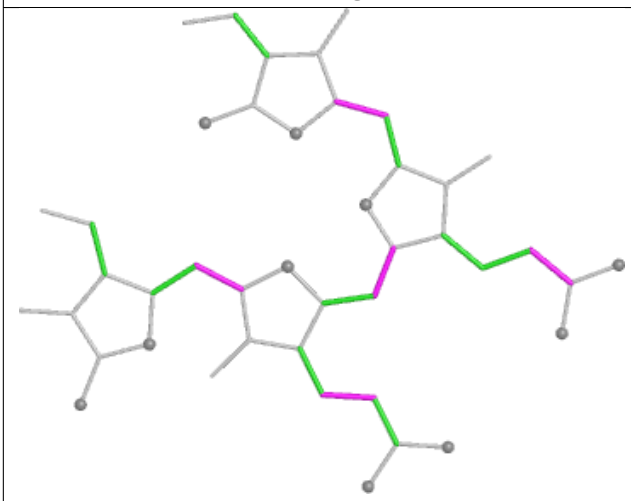
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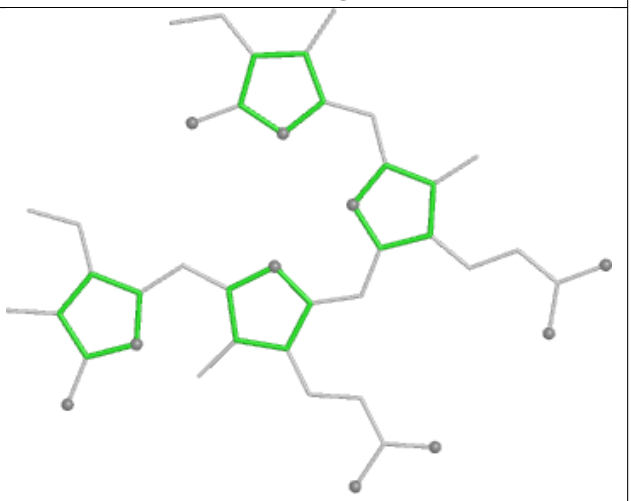
Bond lengths



Bond angles

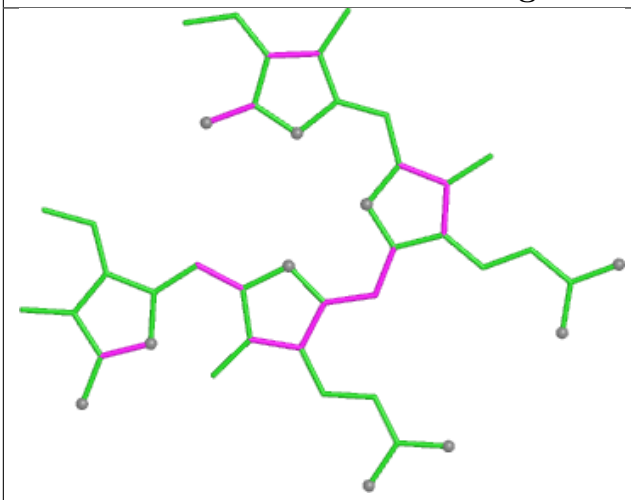


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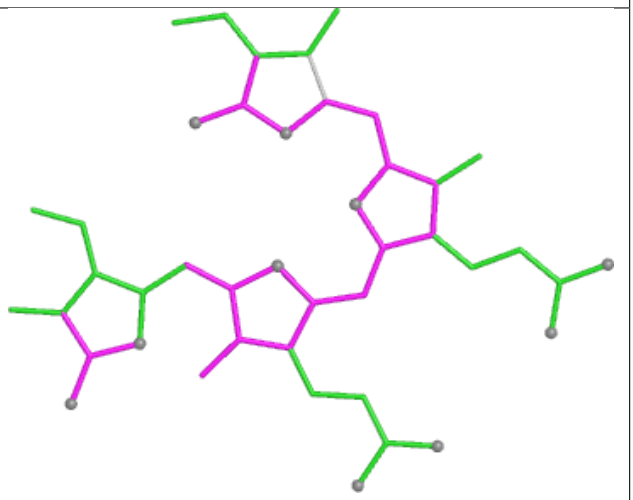


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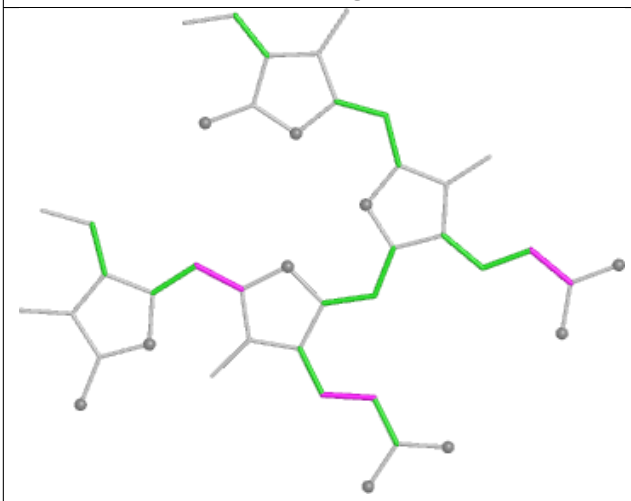
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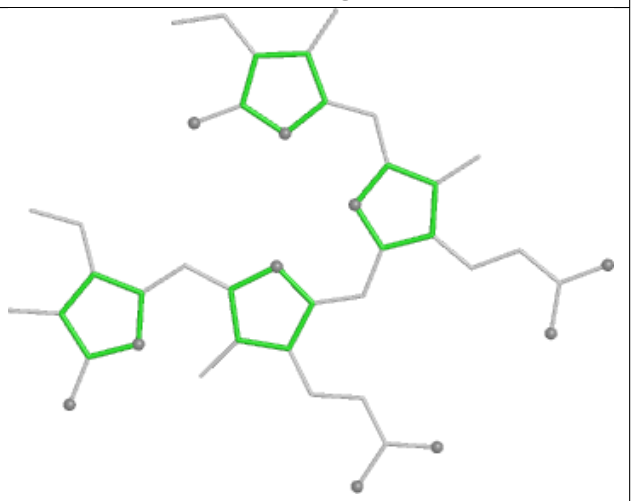
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Bond angles

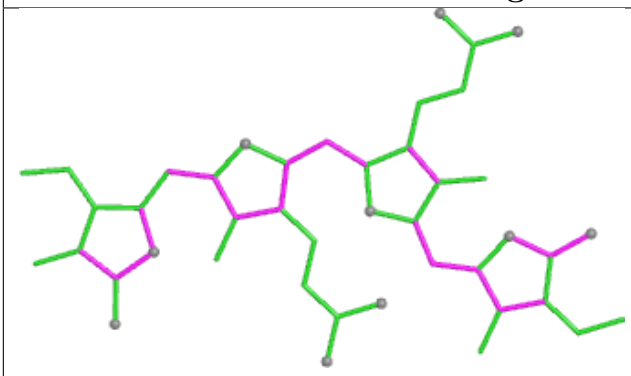


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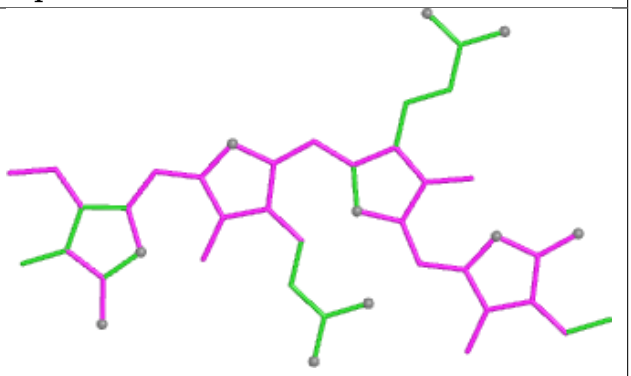


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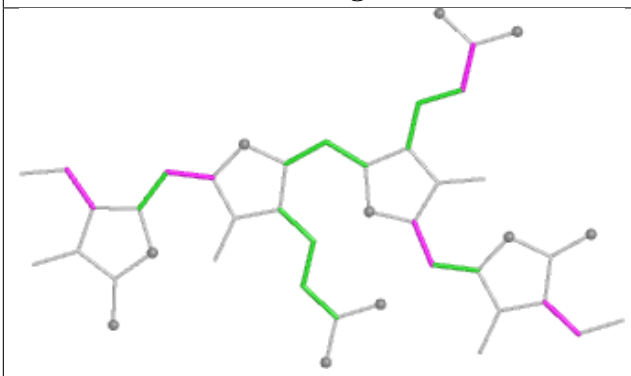
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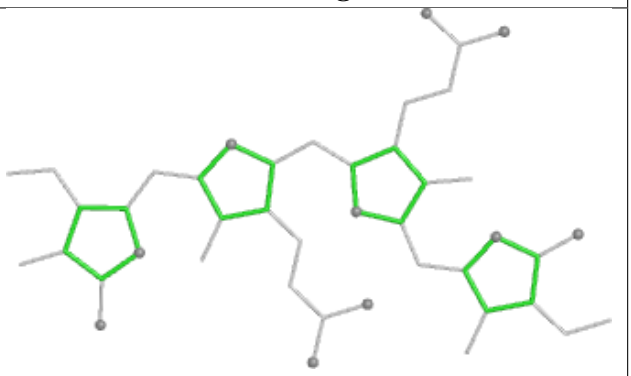
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Bond angles

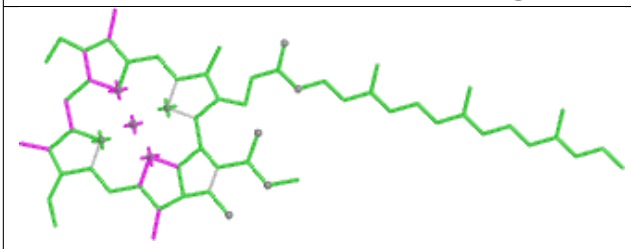


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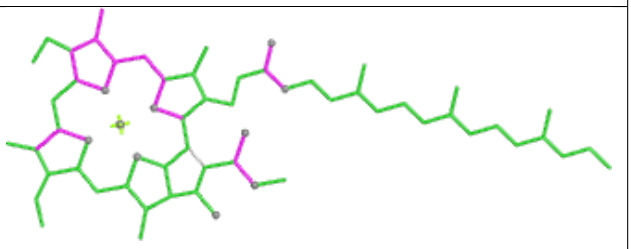


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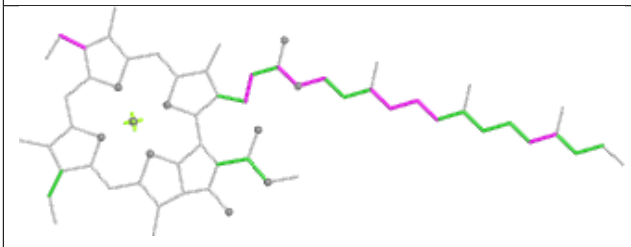
Ligand CLA AN 819



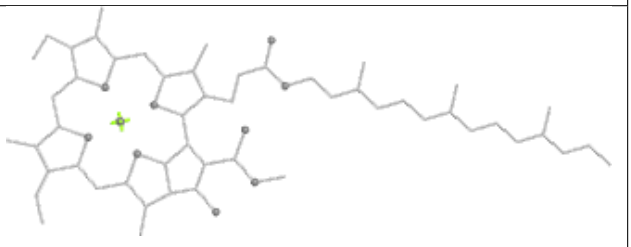
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Bond angles

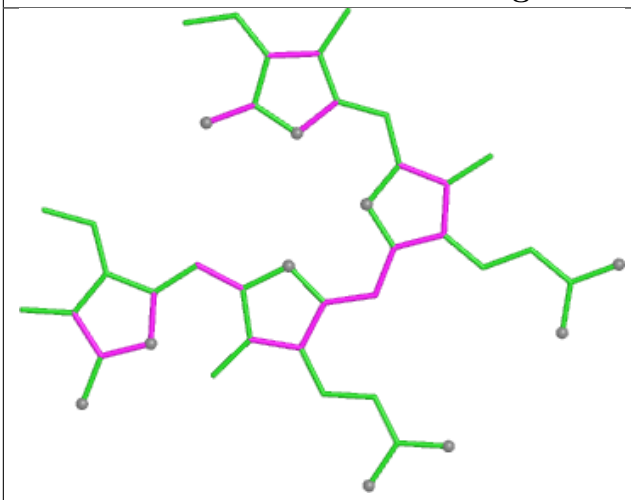


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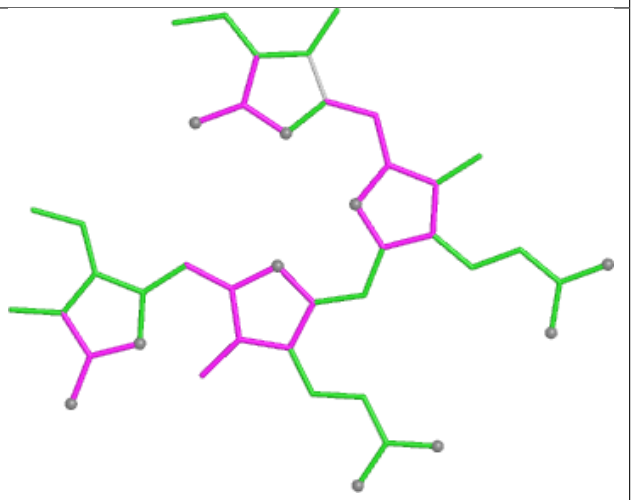


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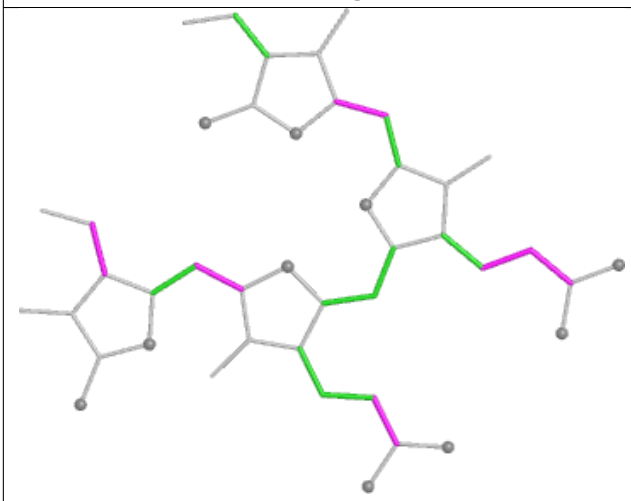
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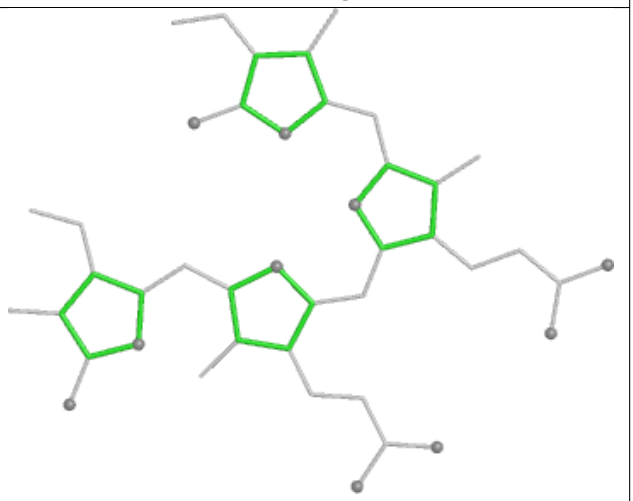
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Bond angles

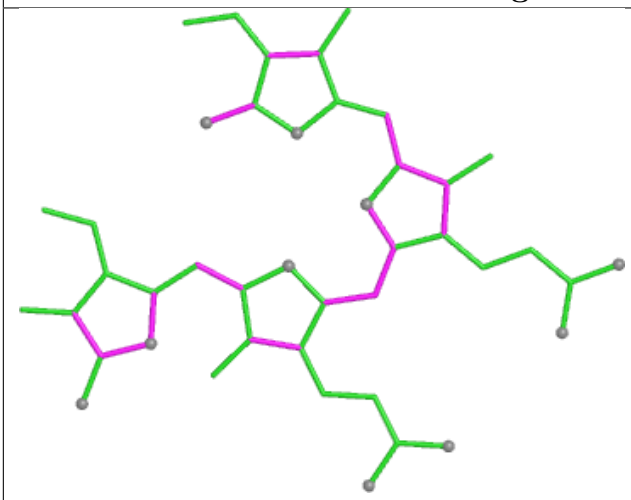


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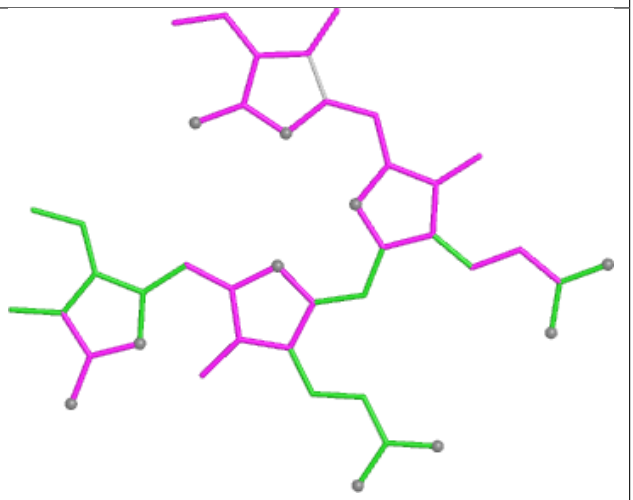


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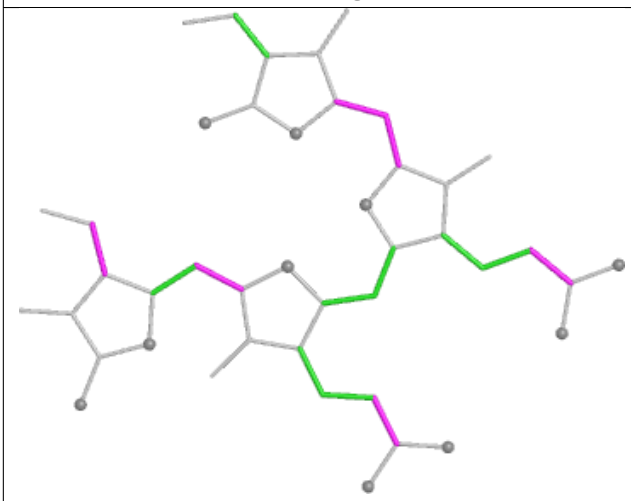
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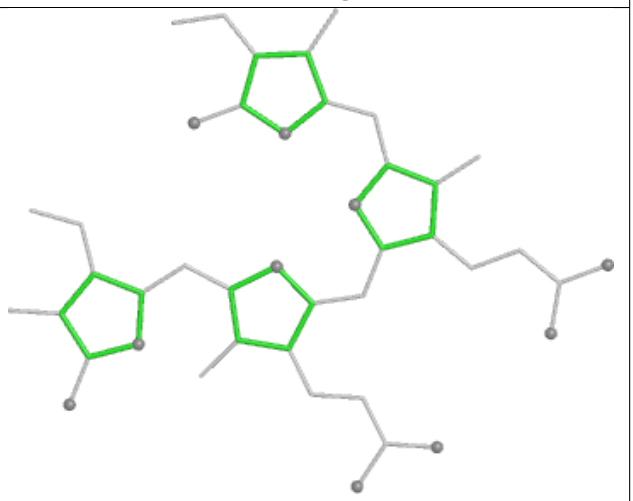
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Bond angles

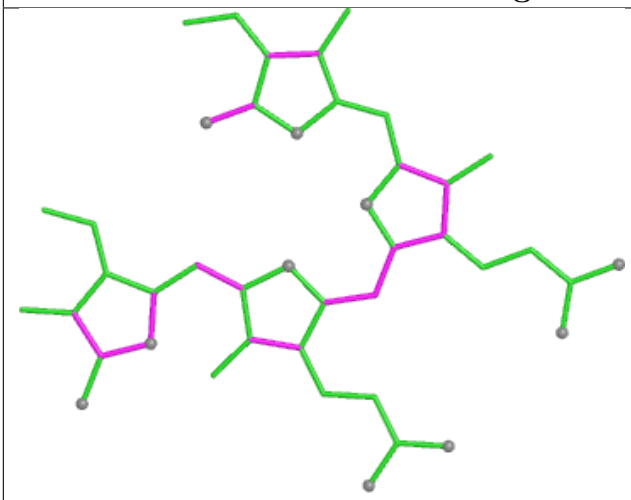


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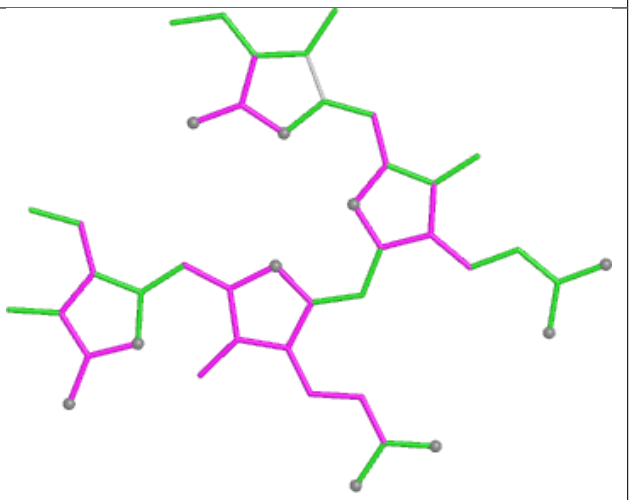


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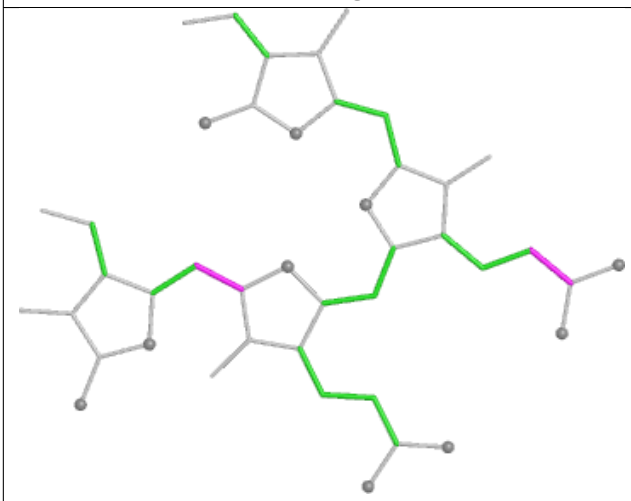
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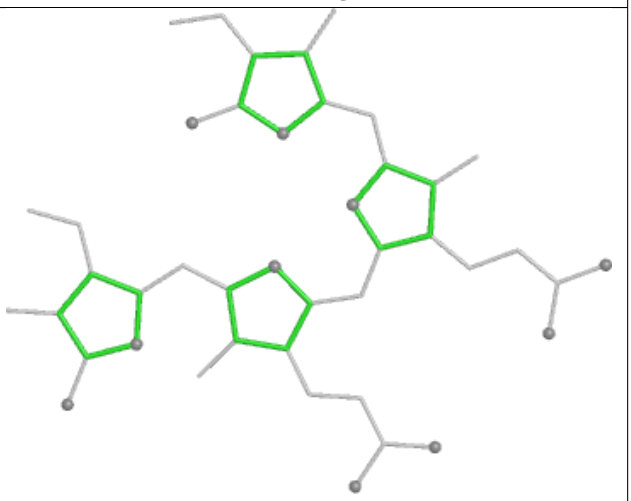
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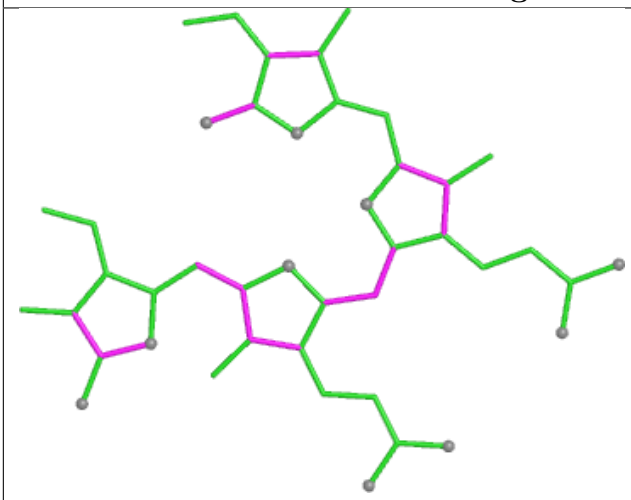


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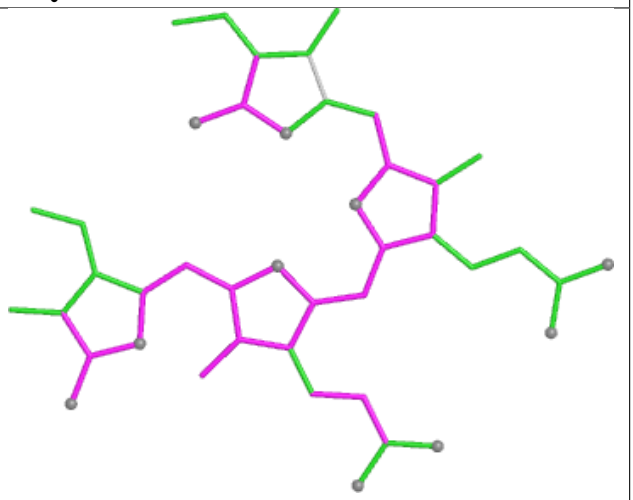


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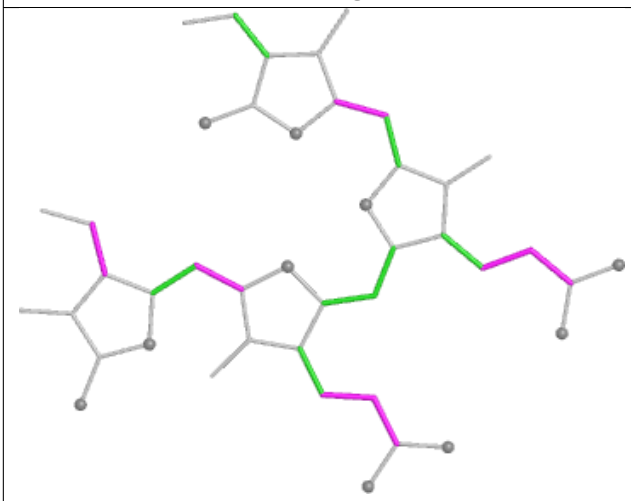
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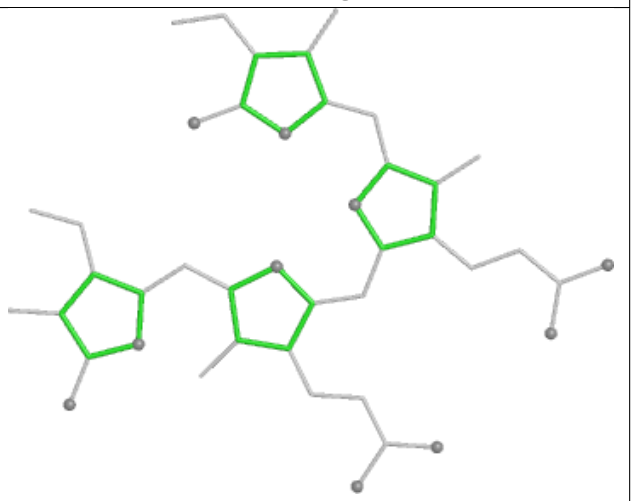
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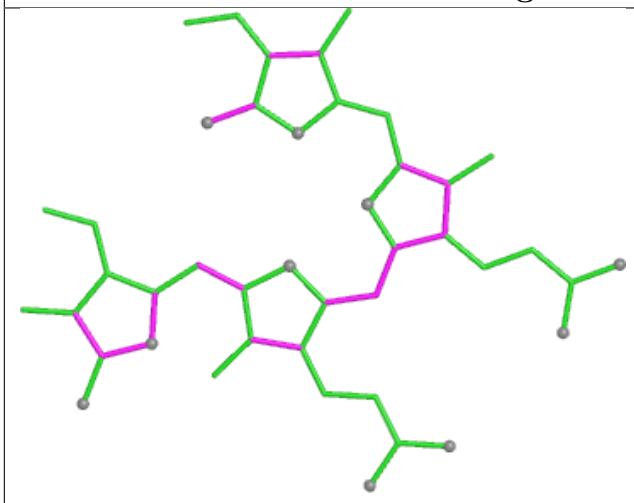


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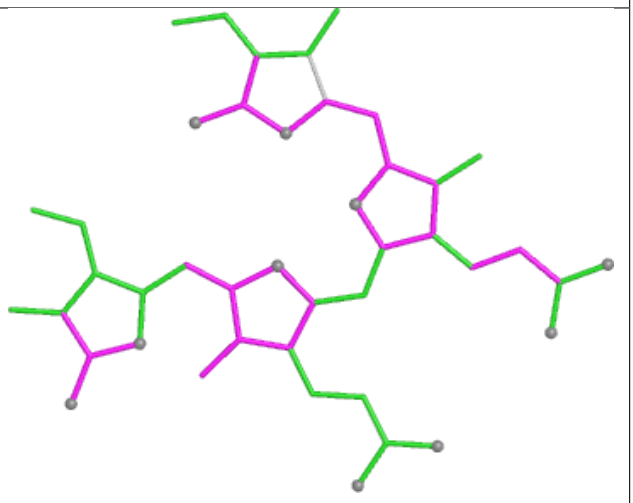


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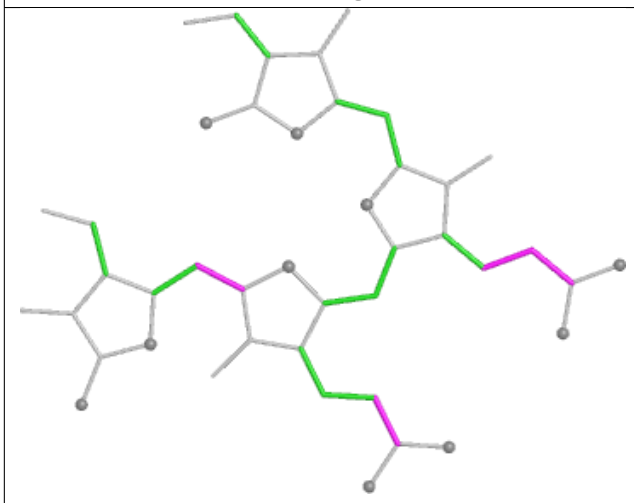
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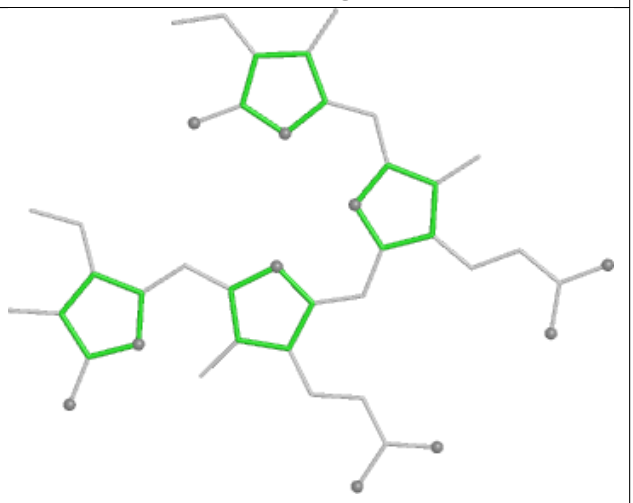
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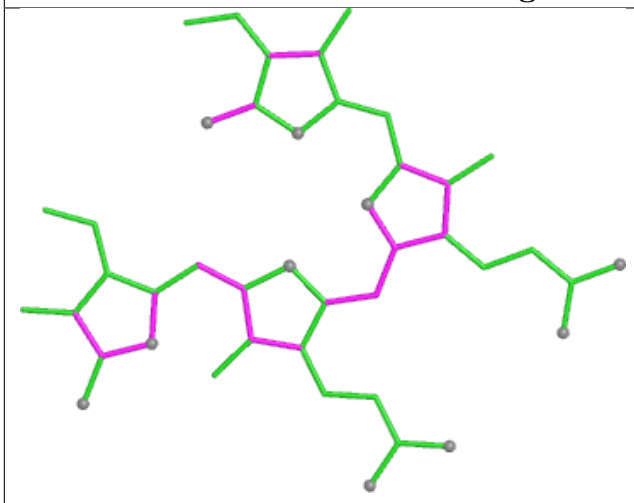


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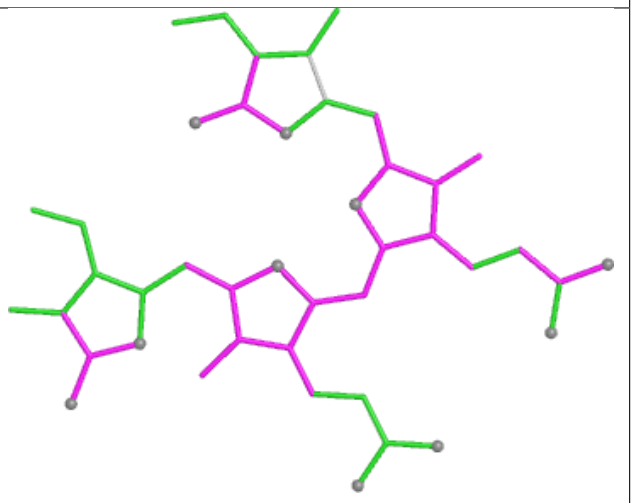


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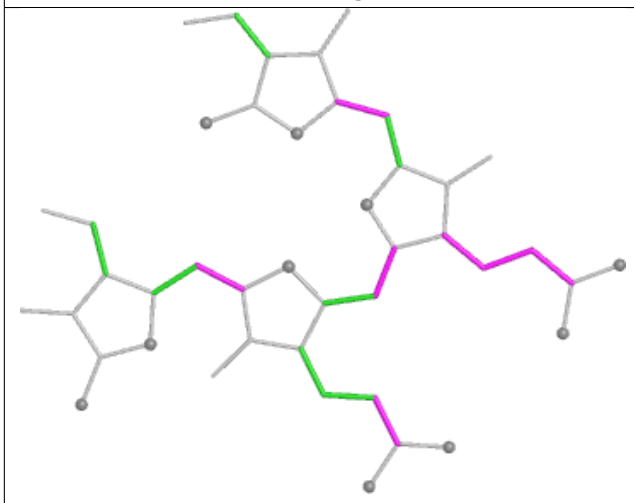
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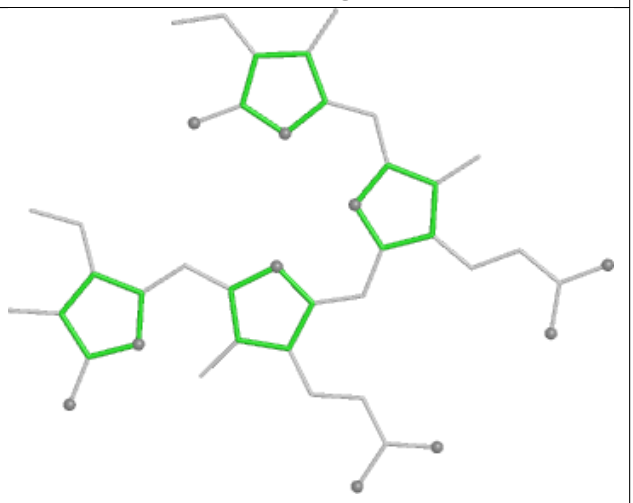
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Bond angles

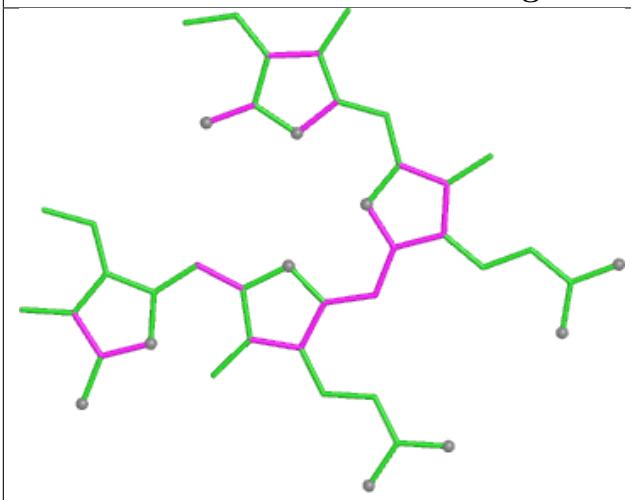


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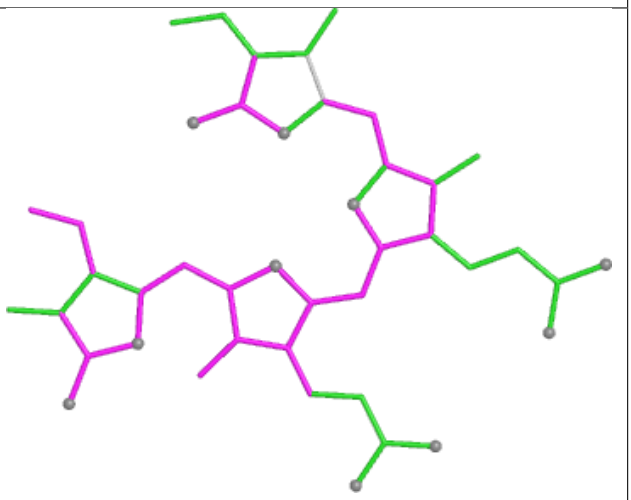


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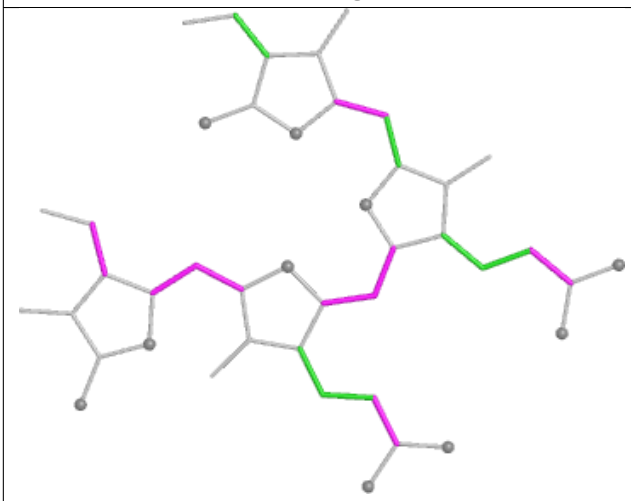
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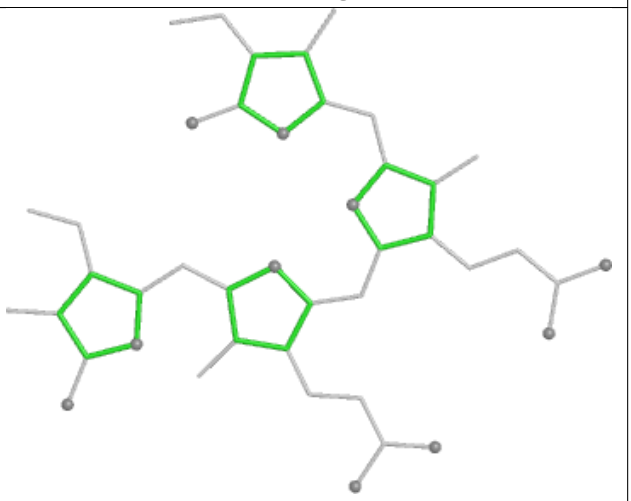
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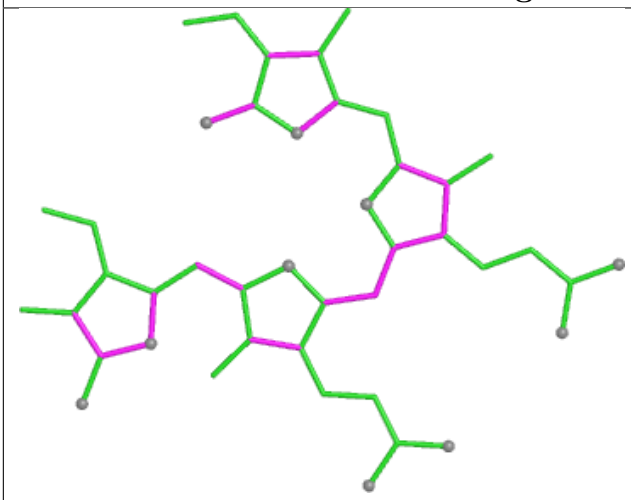


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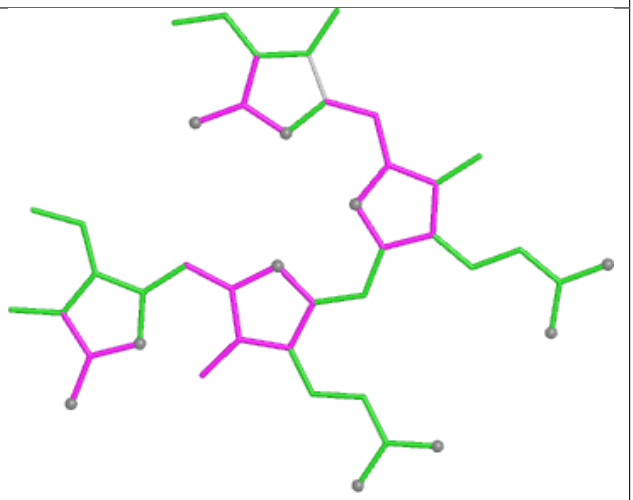


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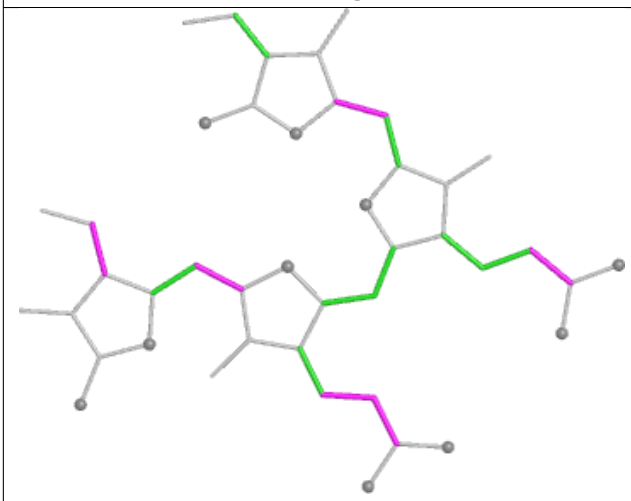
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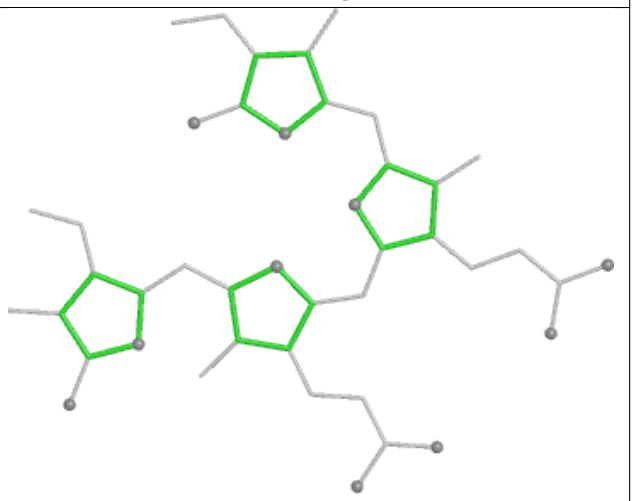
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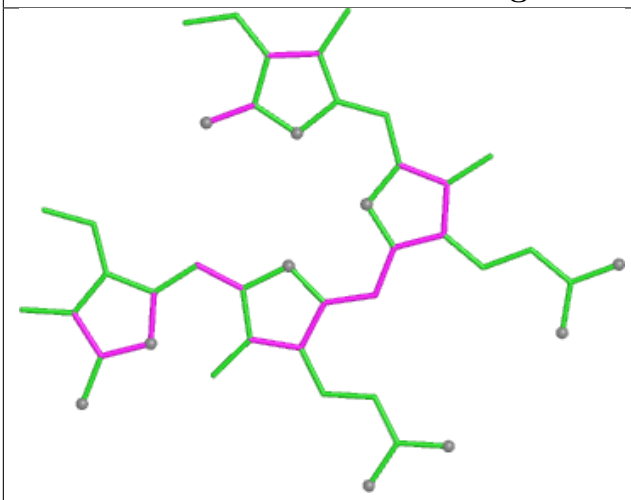


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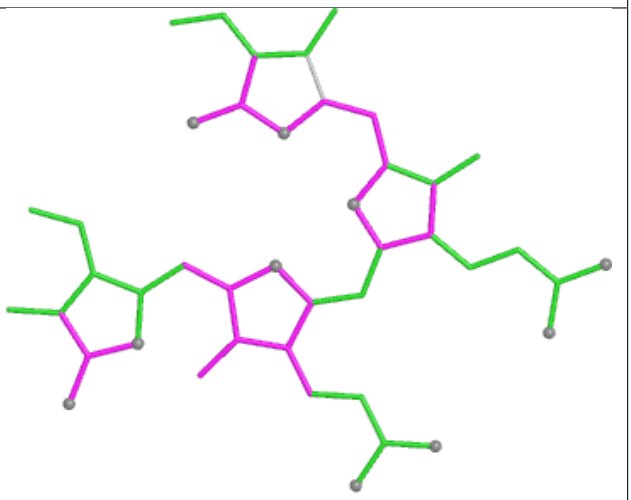


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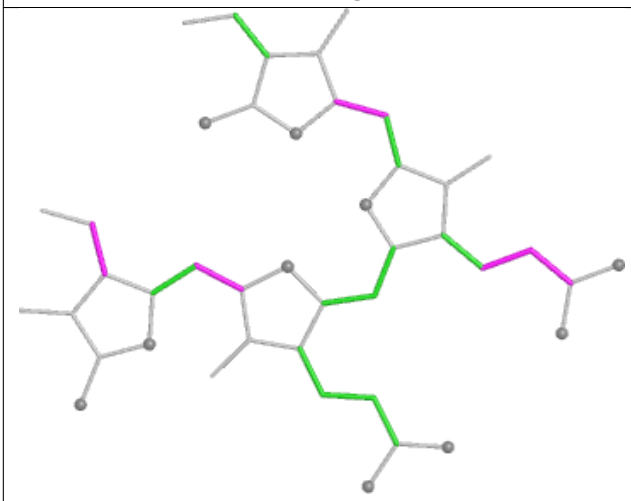
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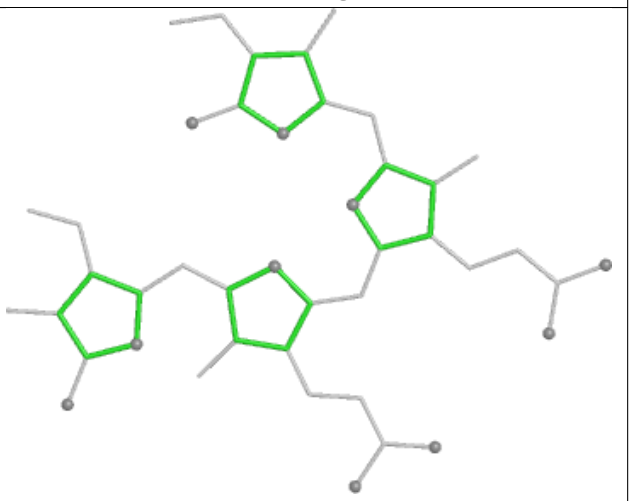
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Bond angles

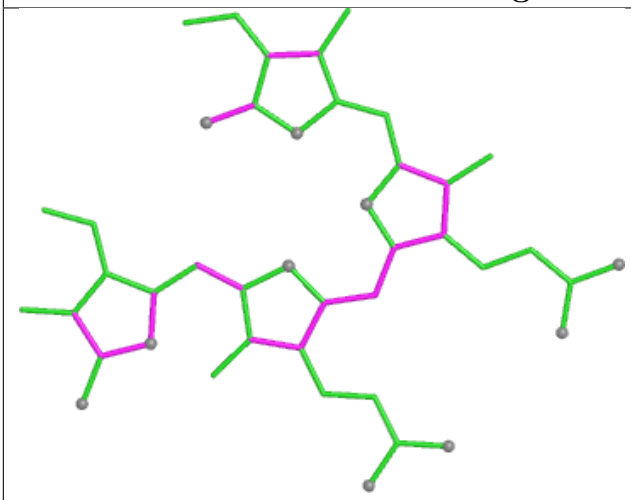


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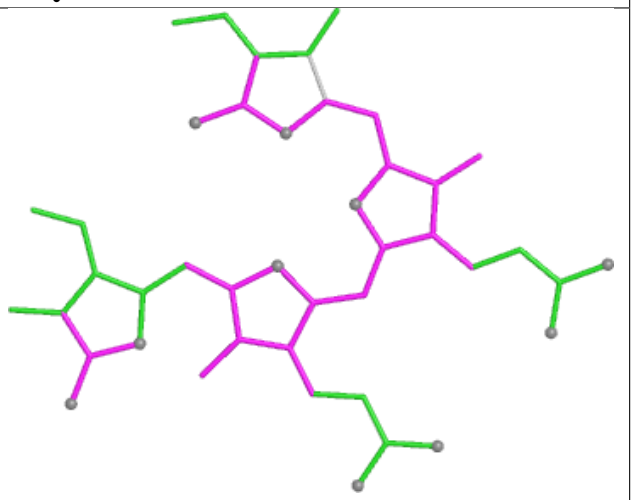


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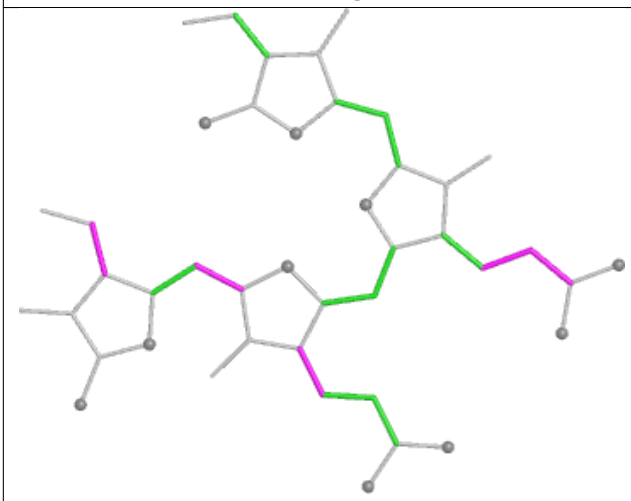
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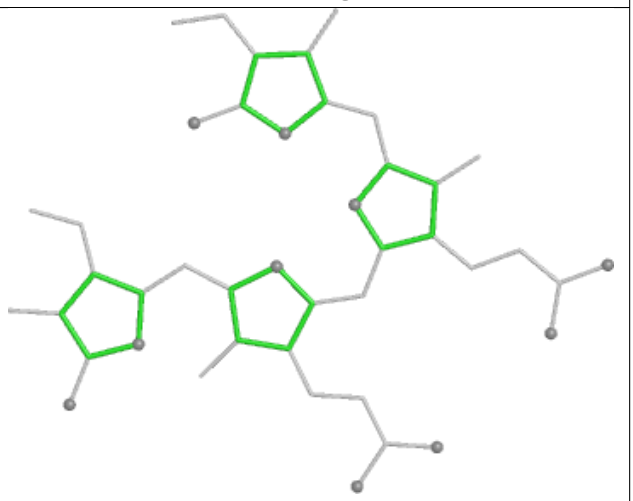
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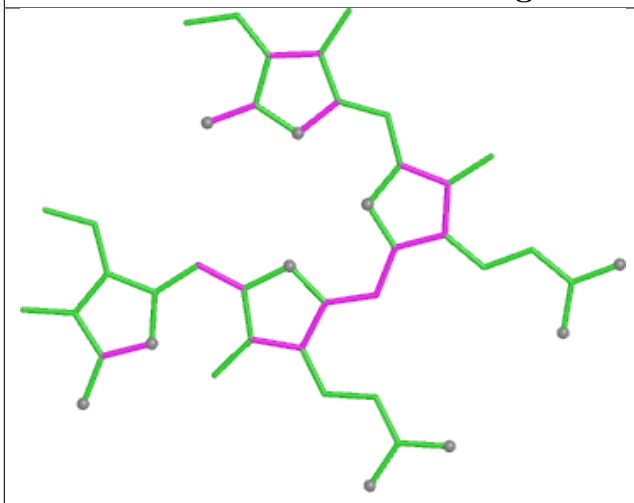


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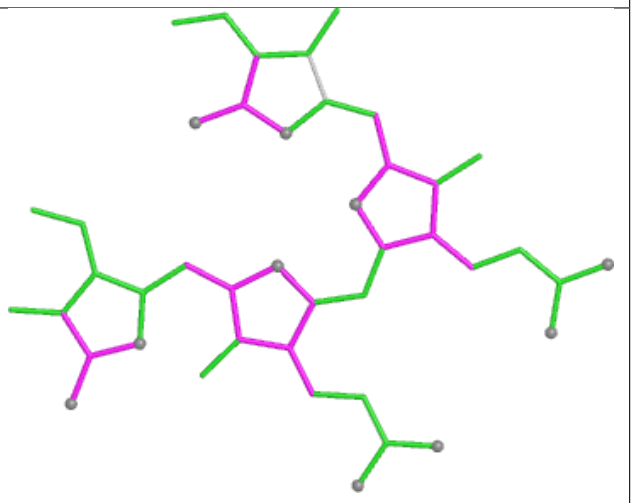


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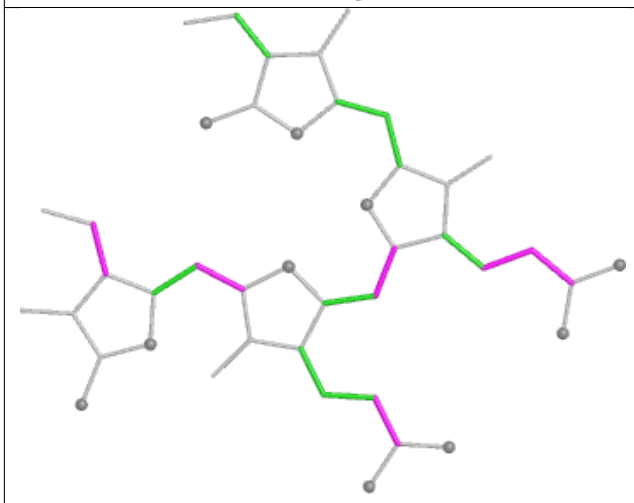
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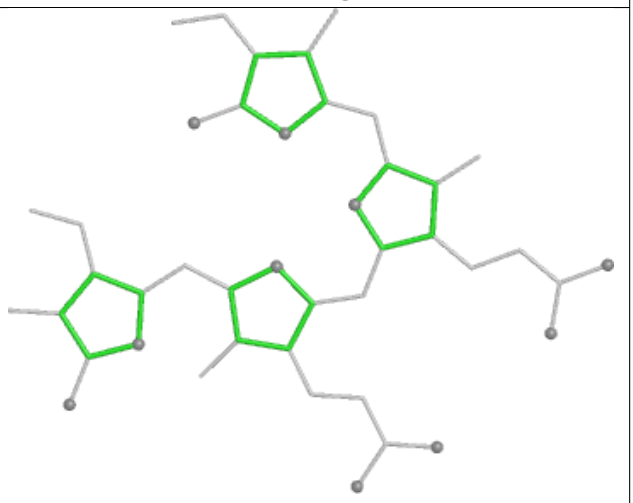
Bond lengths



Bond angles

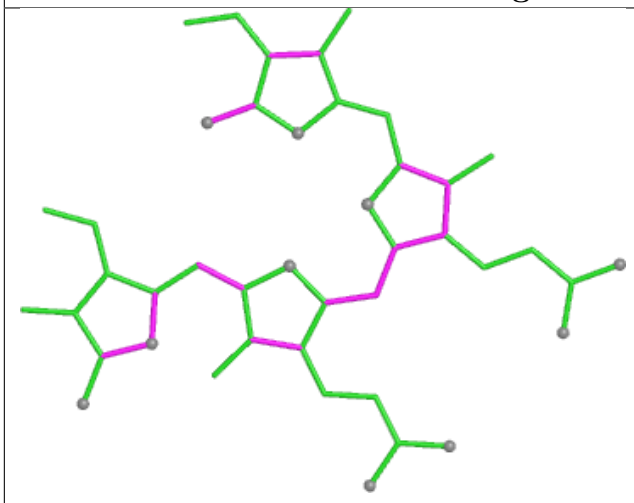


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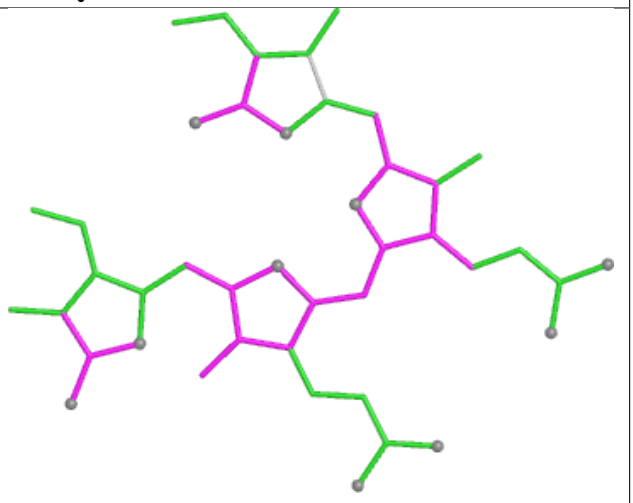


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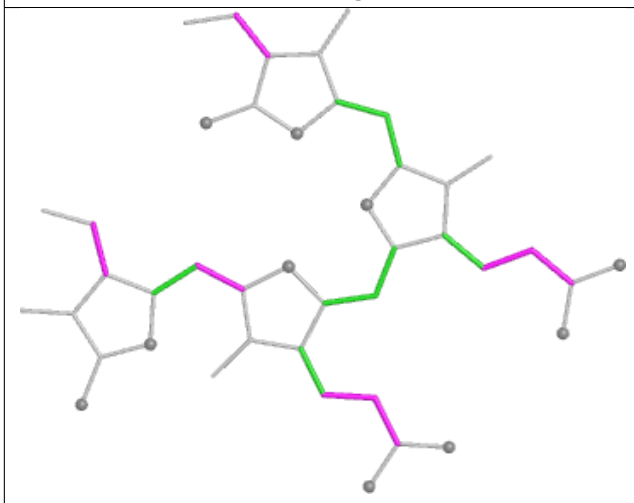
Ligand PEB BQ 203



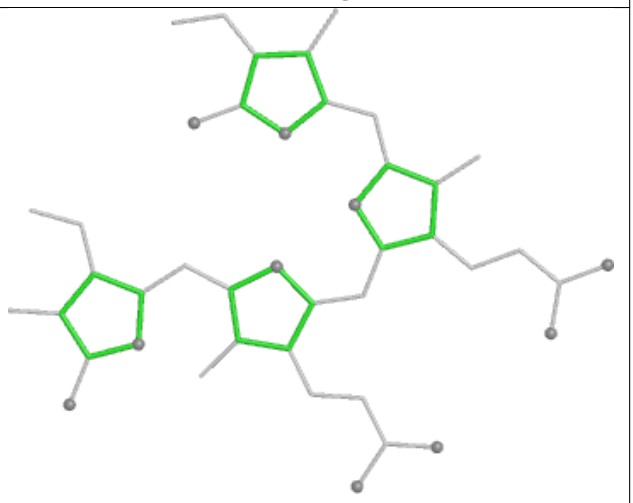
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Bond angles

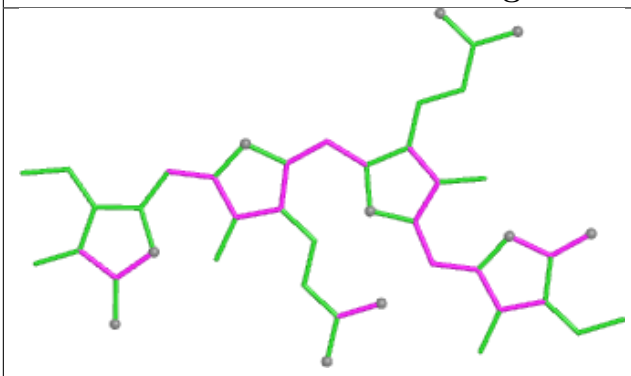


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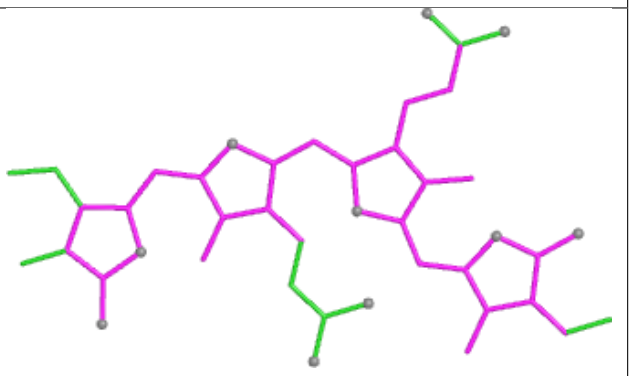


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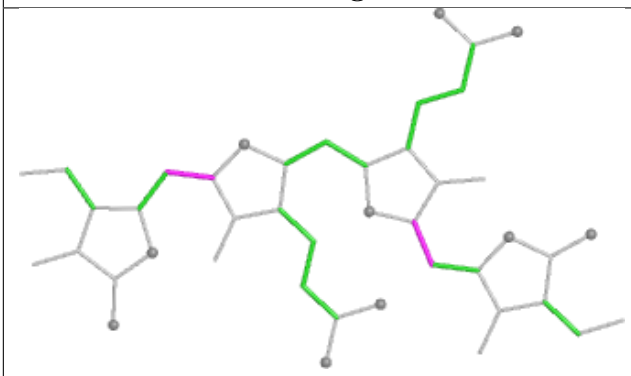
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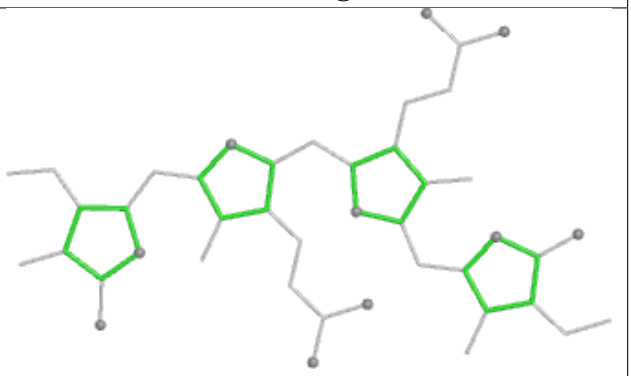
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Bond angles

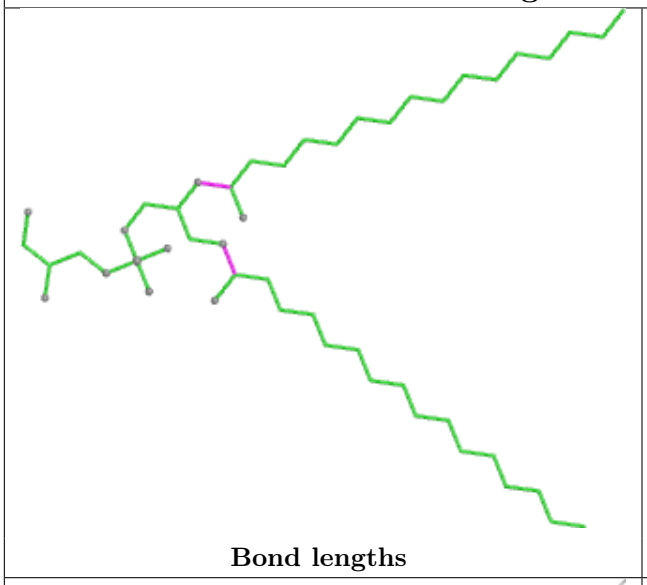


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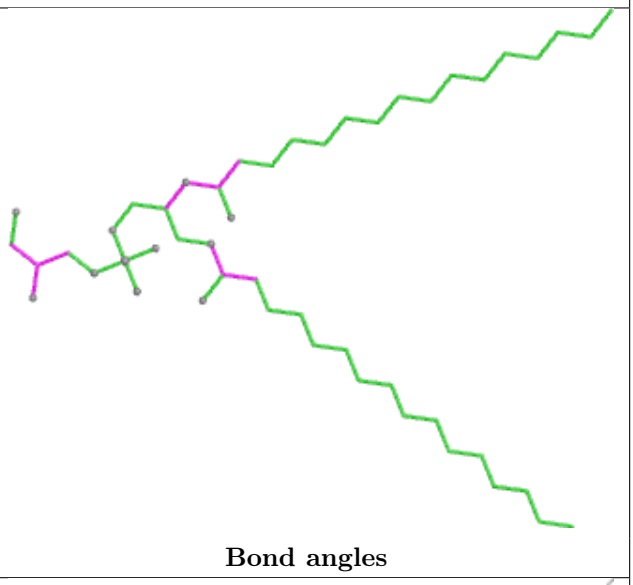


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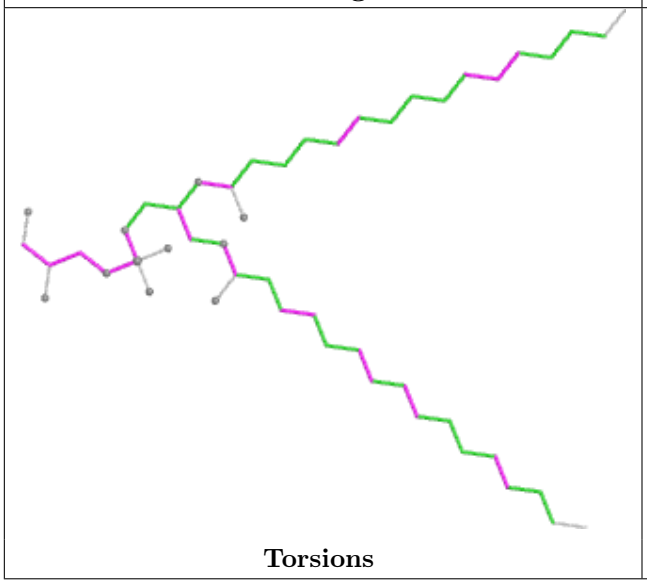
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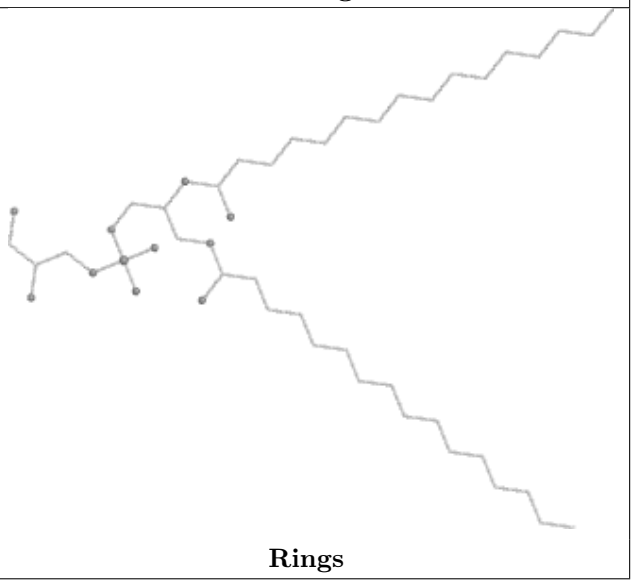
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Bond angles

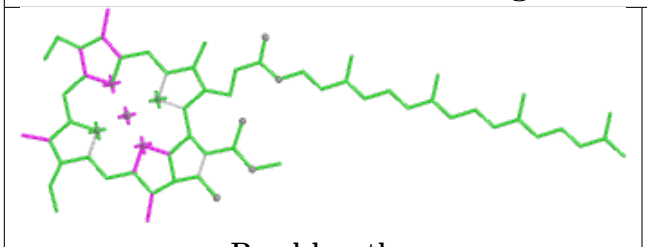


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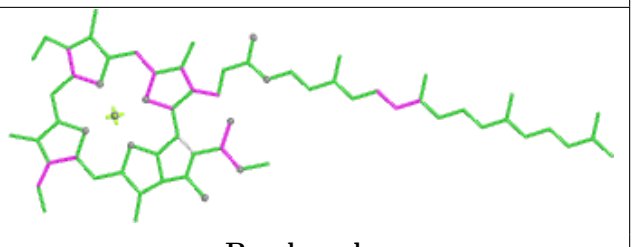


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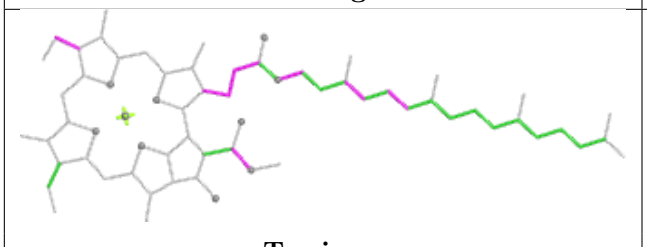
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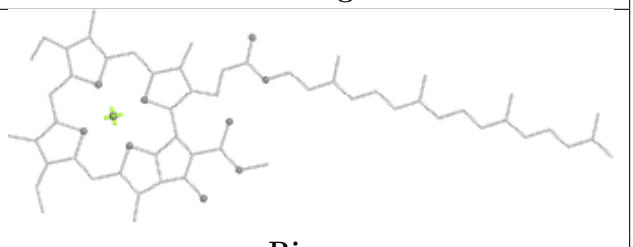
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Bond angles

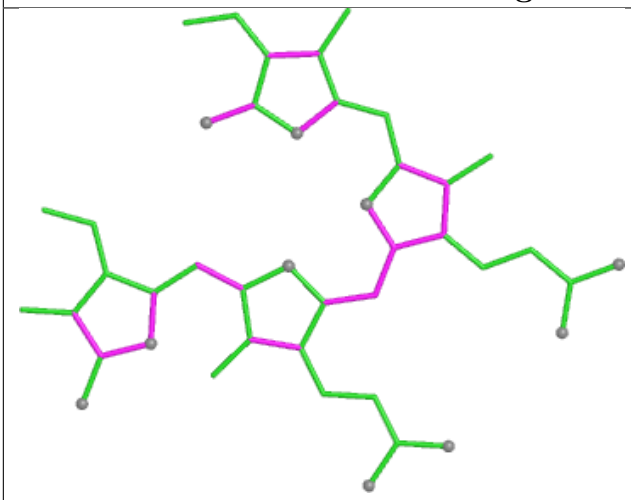


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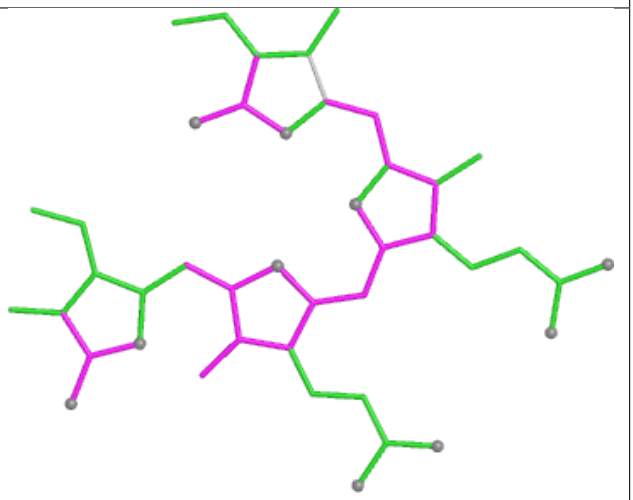


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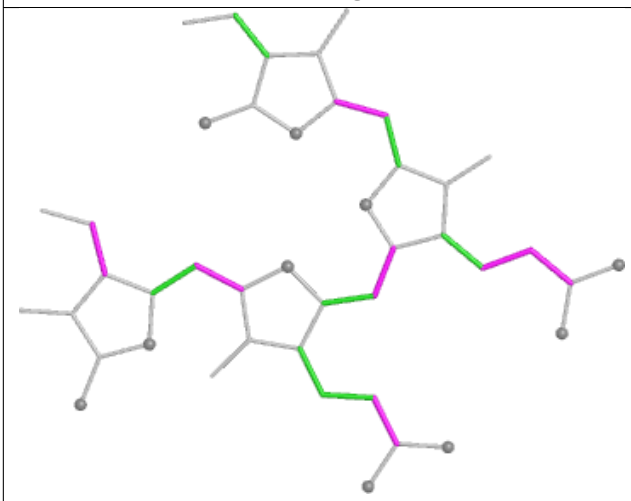
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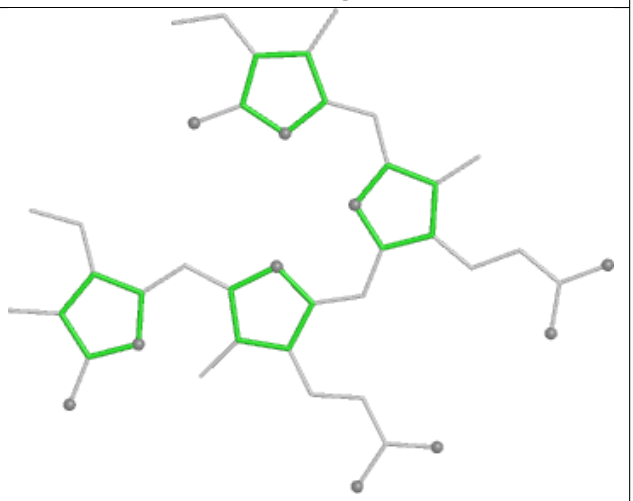
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Bond angles

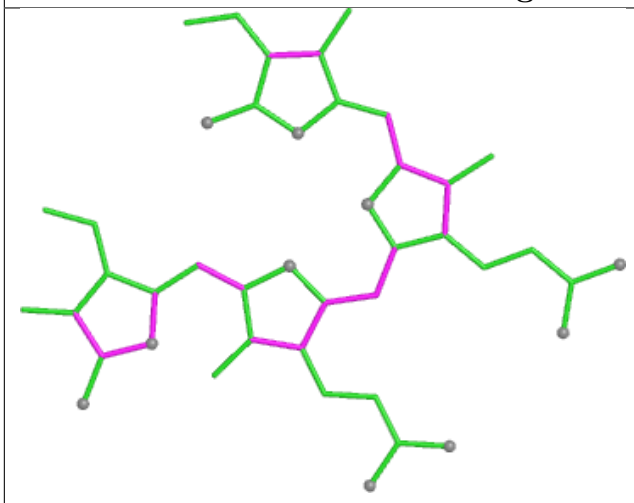


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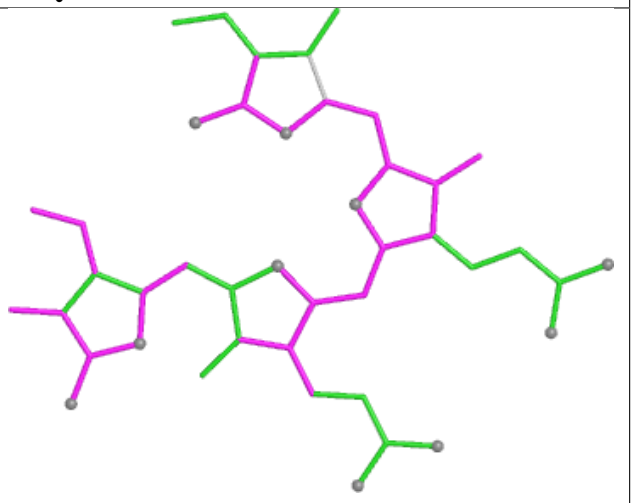


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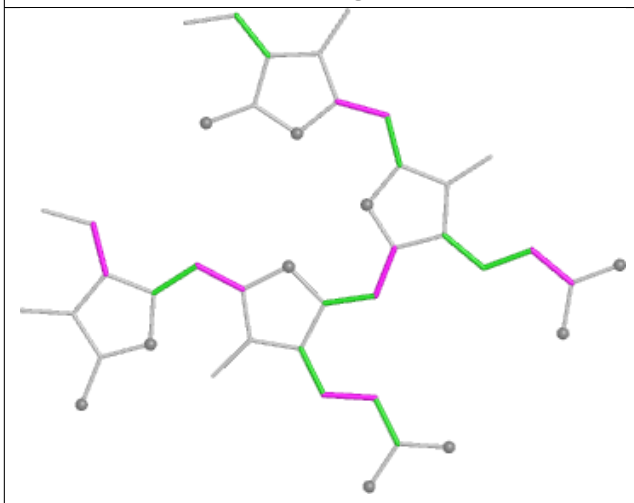
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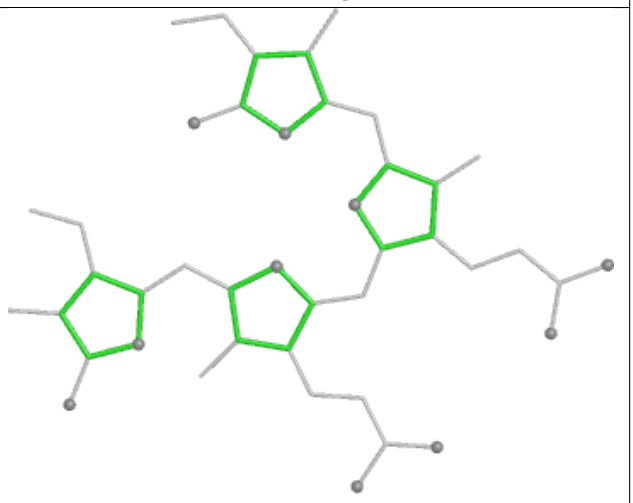
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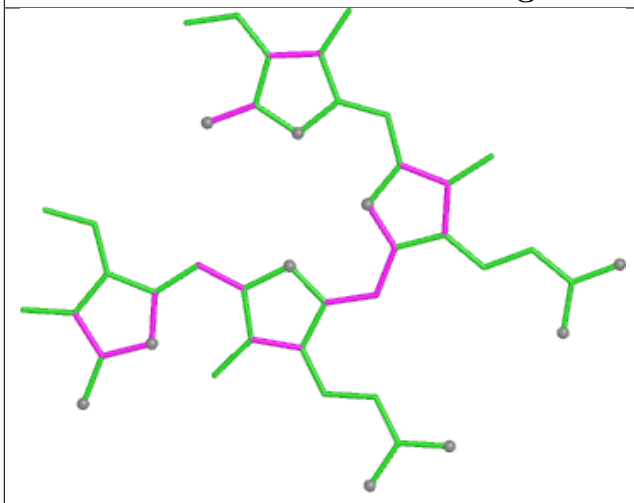


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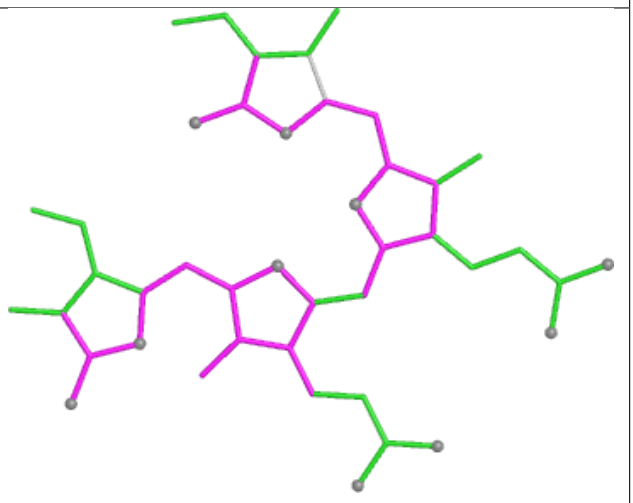


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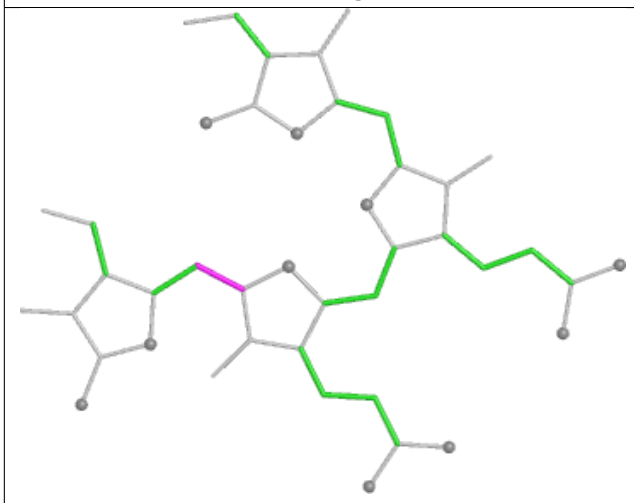
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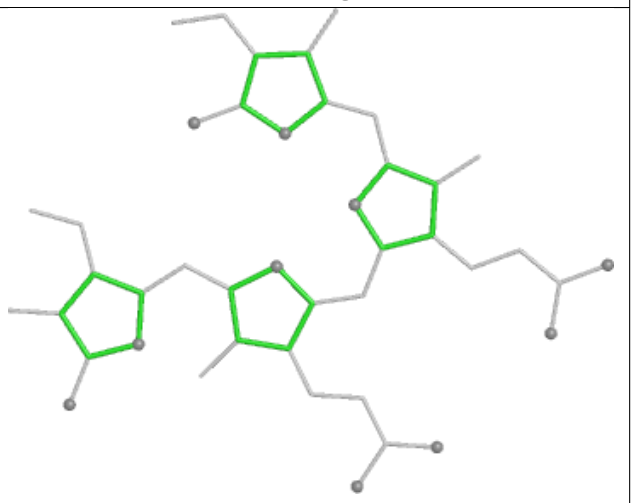
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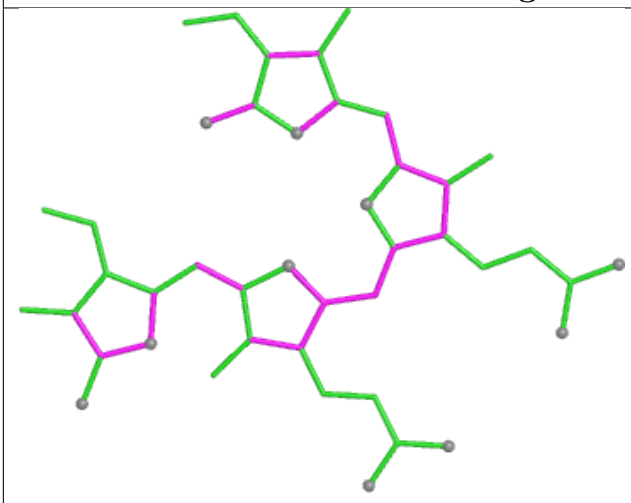


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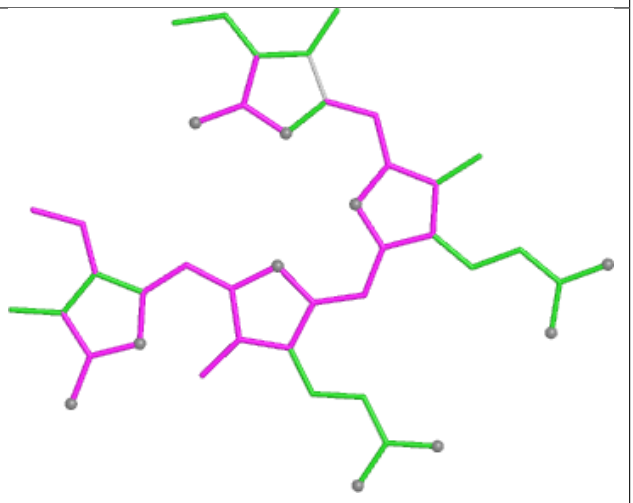


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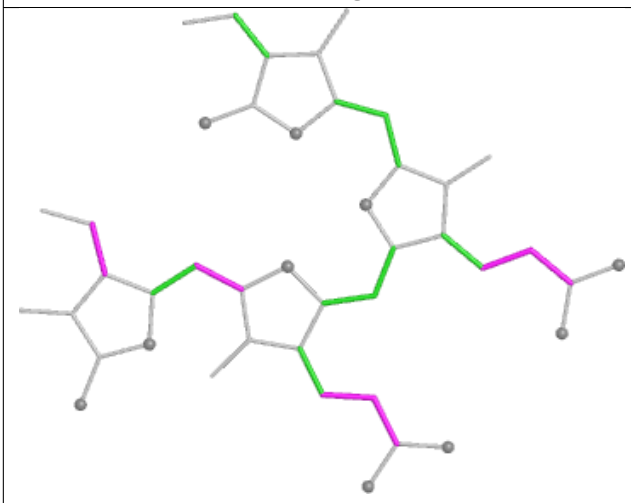
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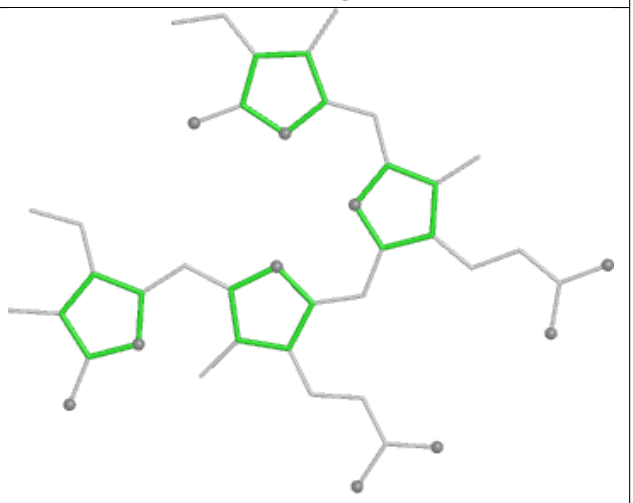
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Bond angles

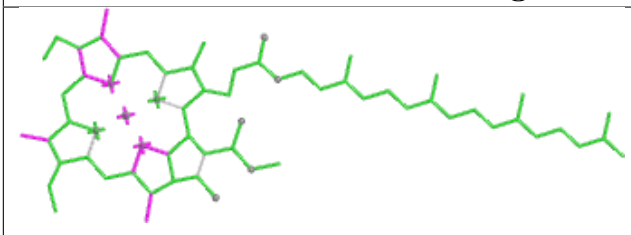


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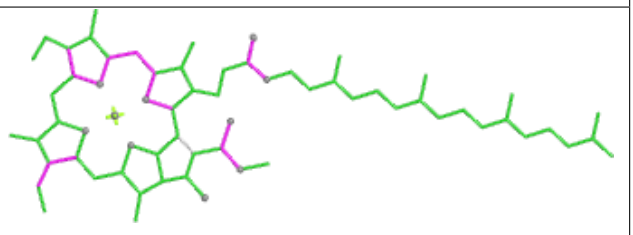


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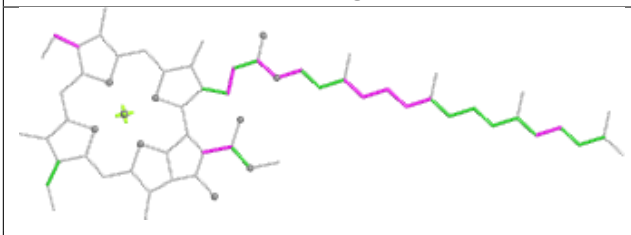
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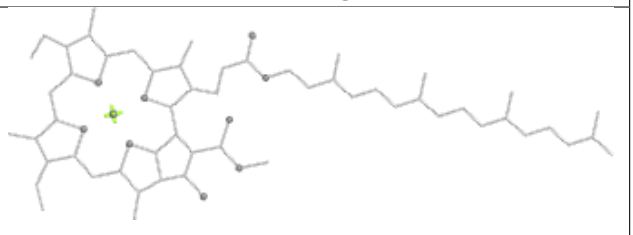
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Bond angles

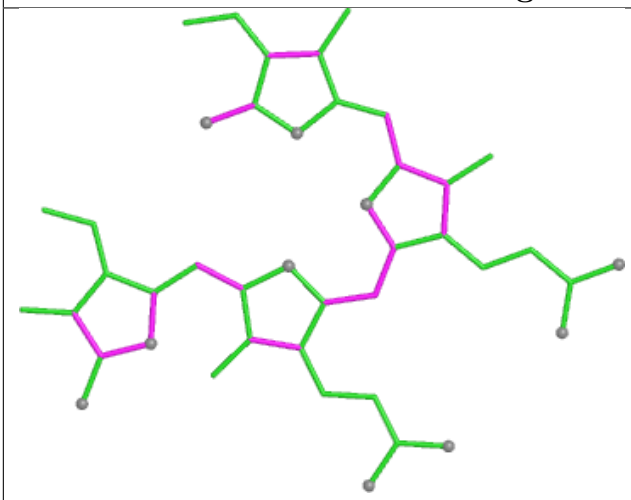


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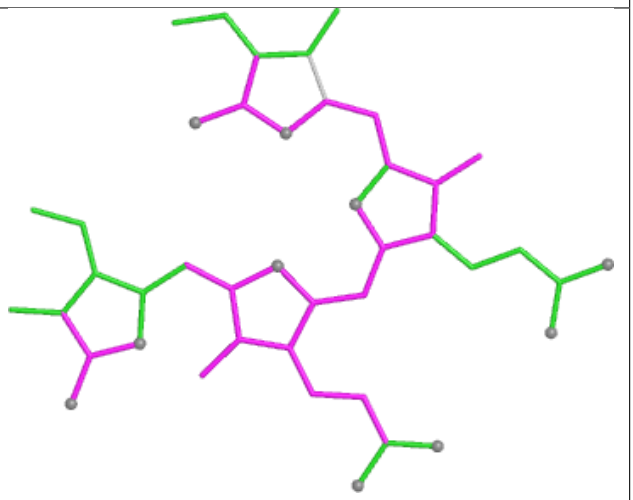


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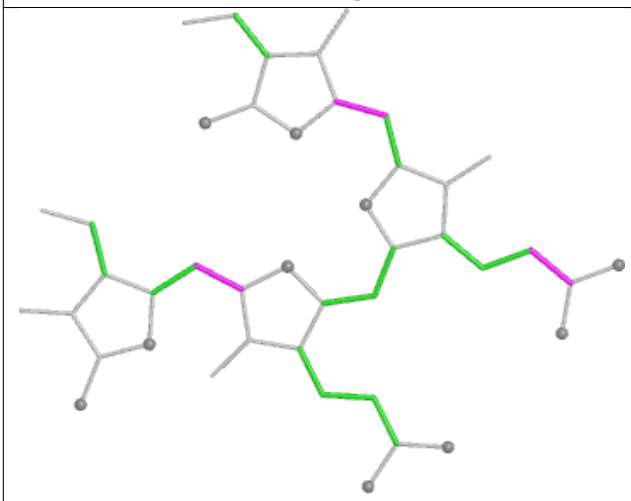
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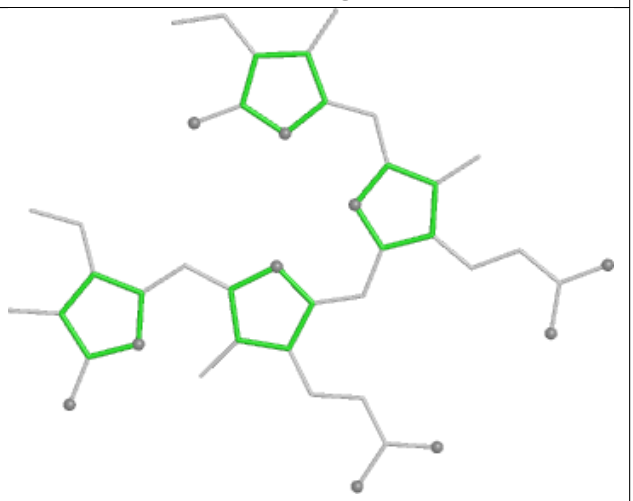
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Bond angles

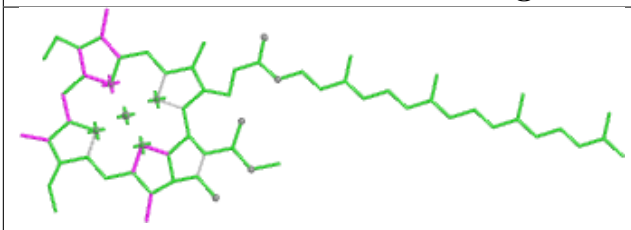


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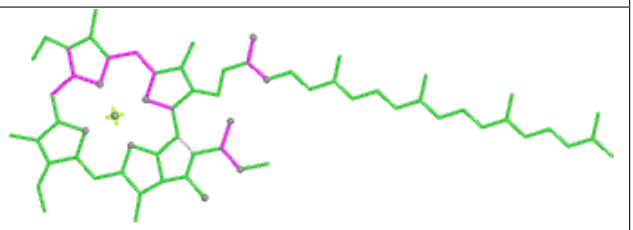


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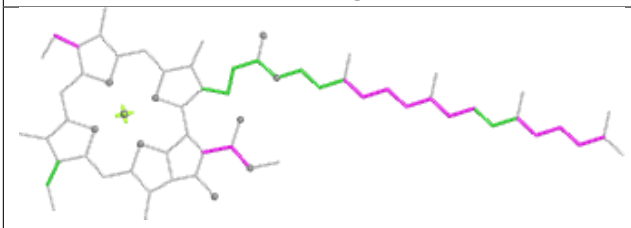
Ligand CLA B6 615



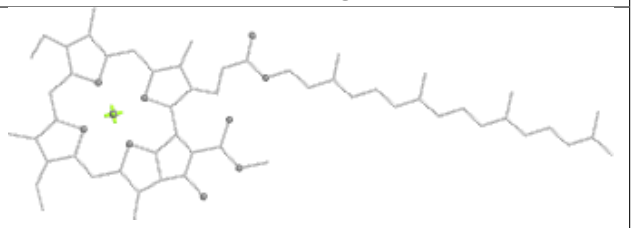
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Bond angles

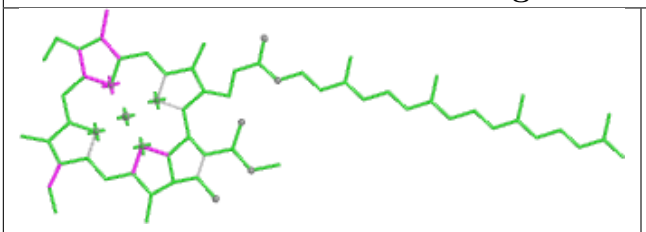


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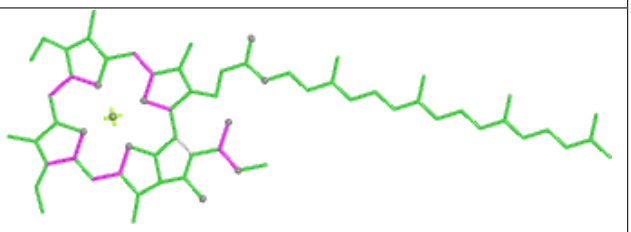


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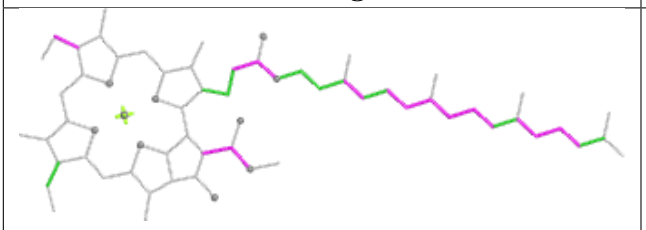
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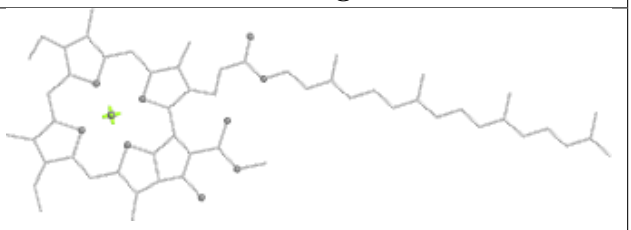
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Bond angles

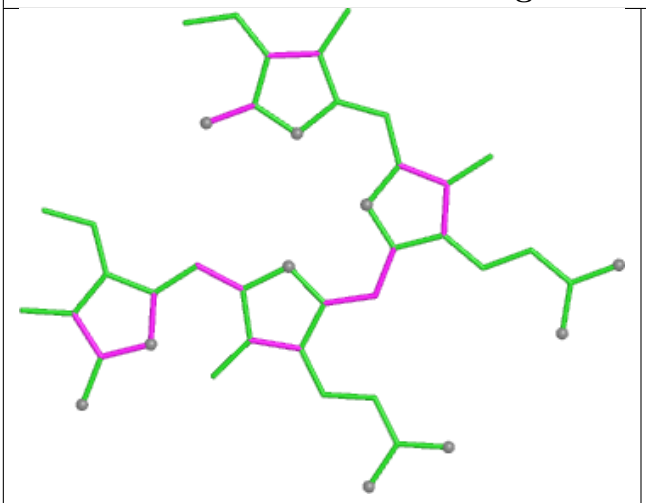


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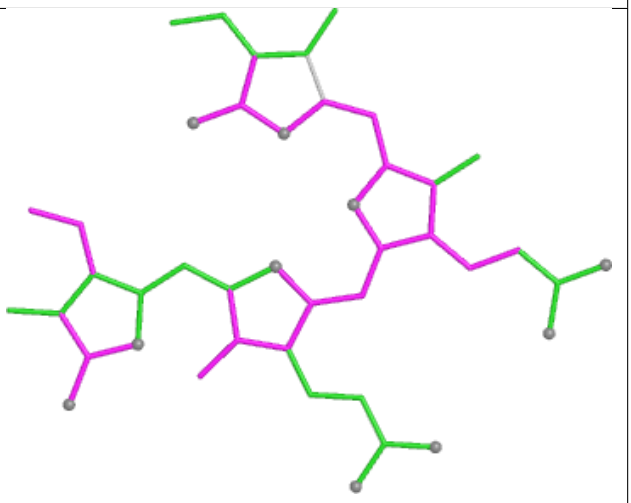


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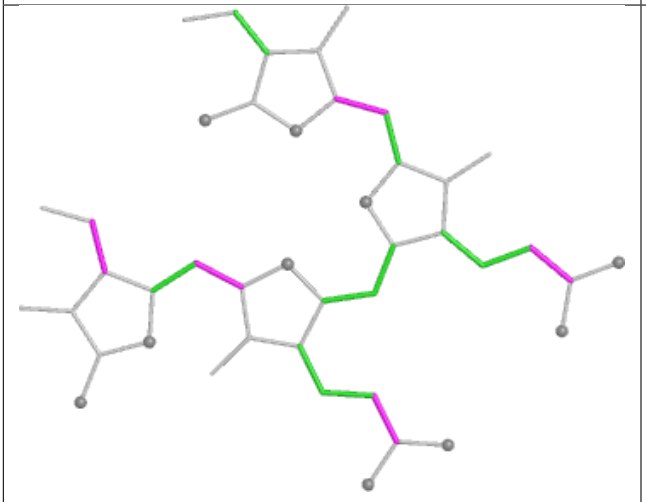
Ligand PEB bP 502



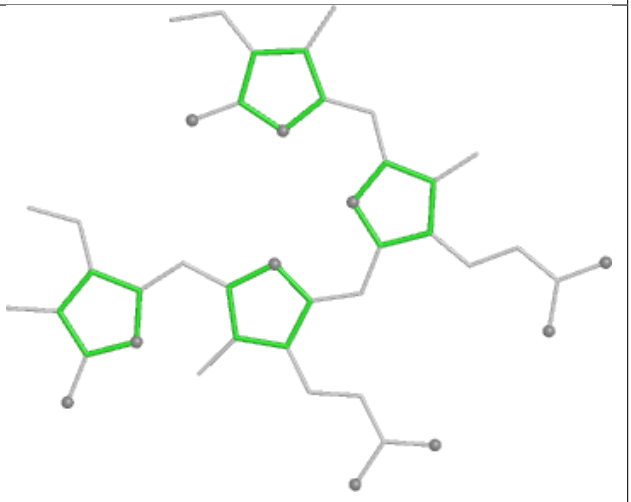
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Bond angles

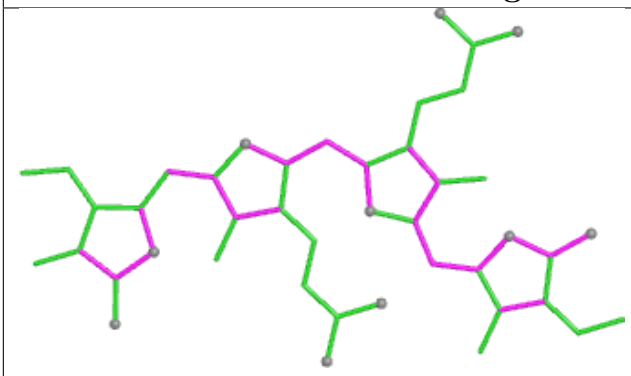


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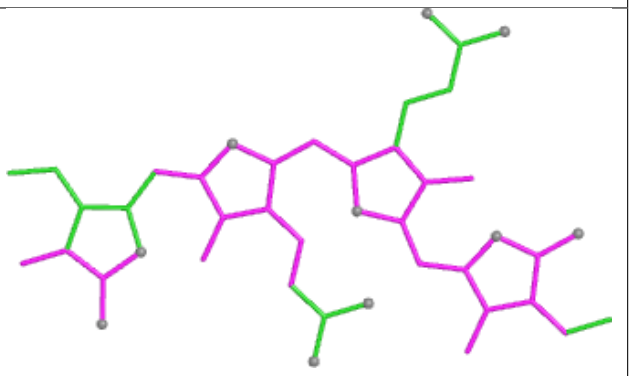


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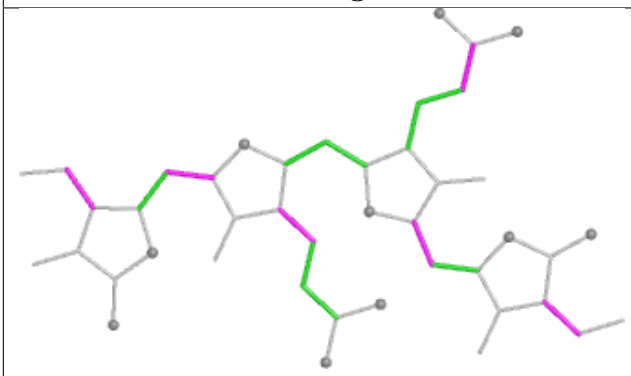
Ligand CYC LE 1001



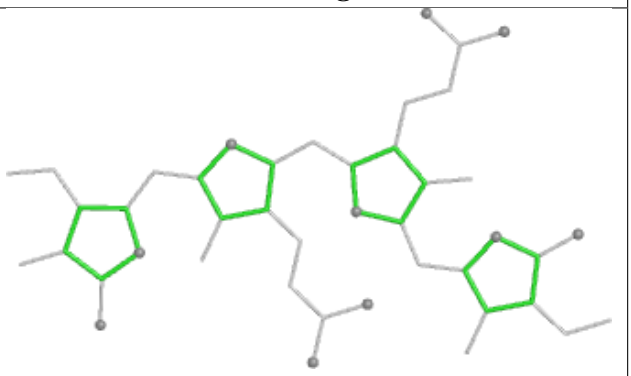
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Bond angles

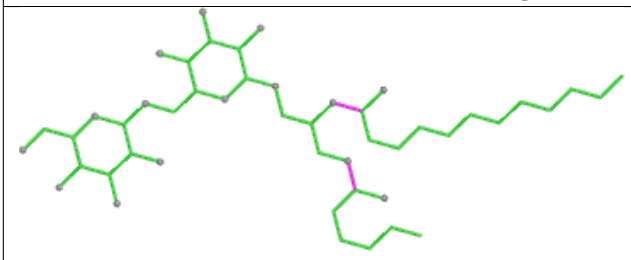


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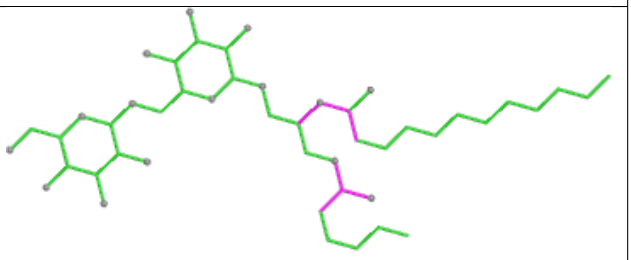


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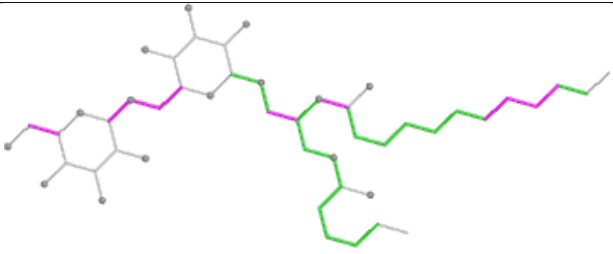
Ligand DGD c6 620



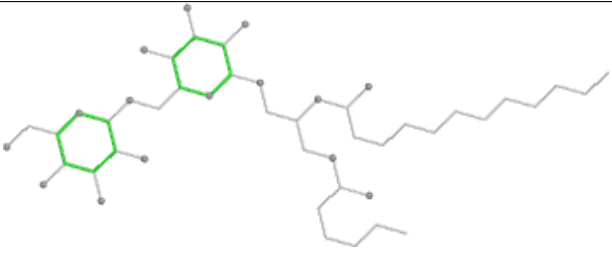
Bond lengths



Bond angles

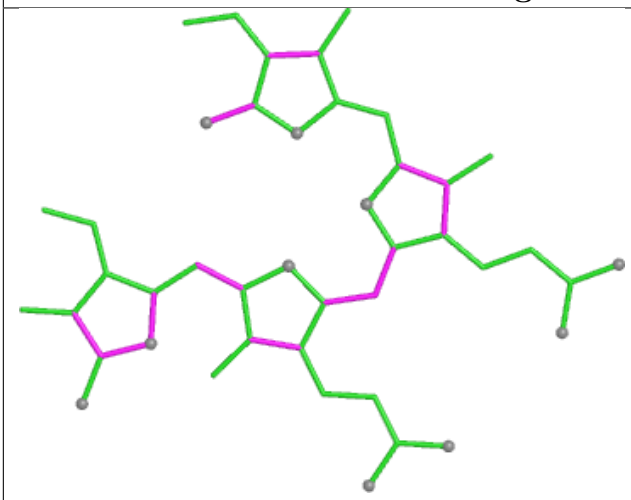


Torsions

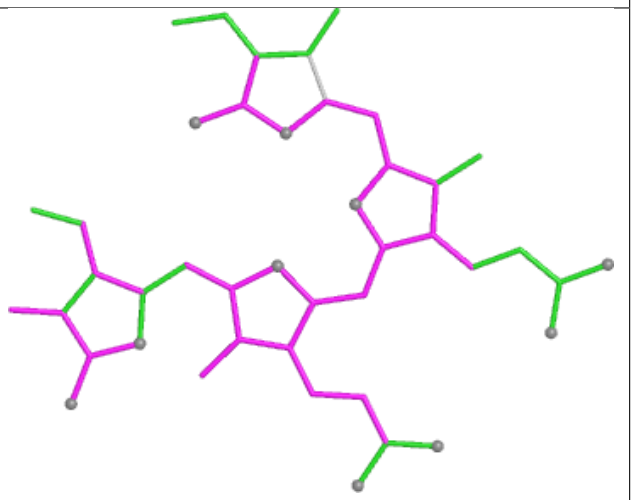


Rings

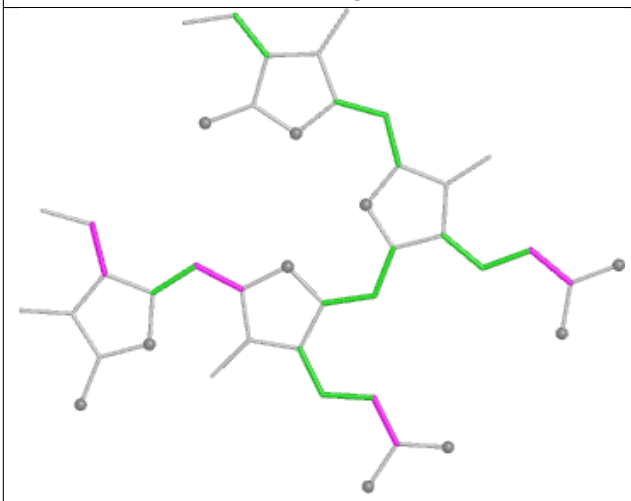
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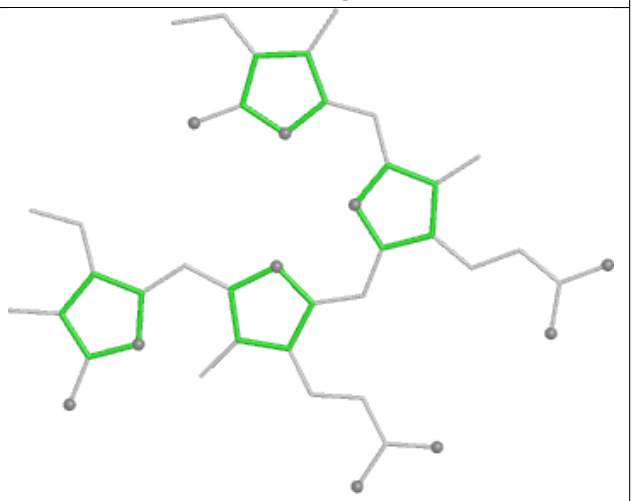
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Bond angles

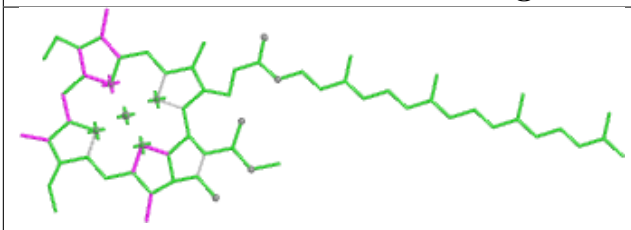


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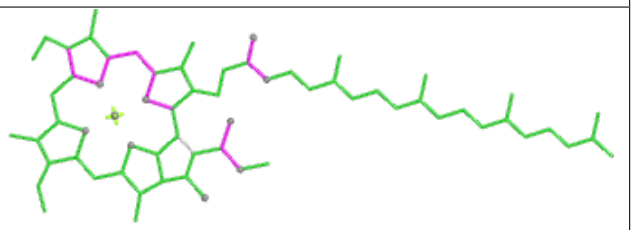


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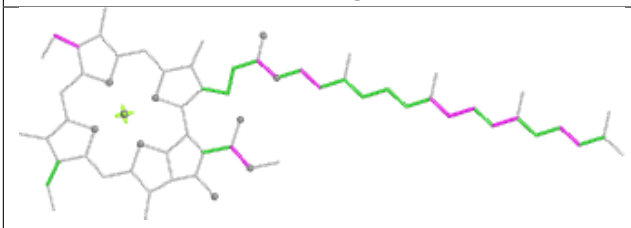
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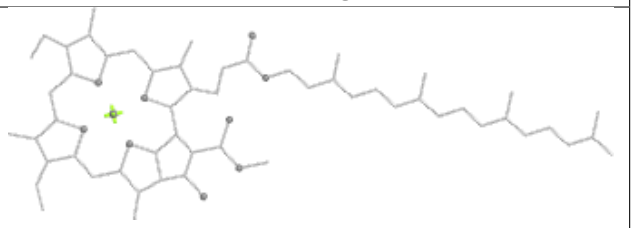
Bond lengths



Bond angles

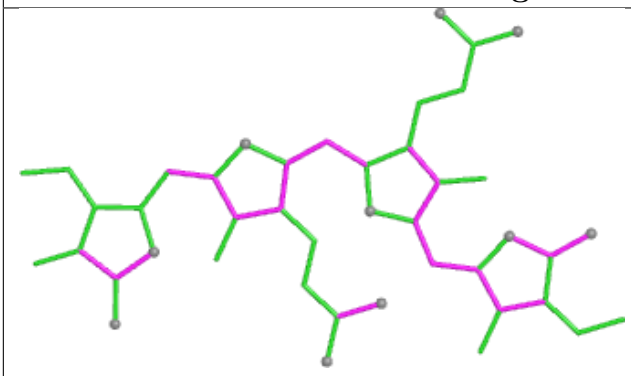


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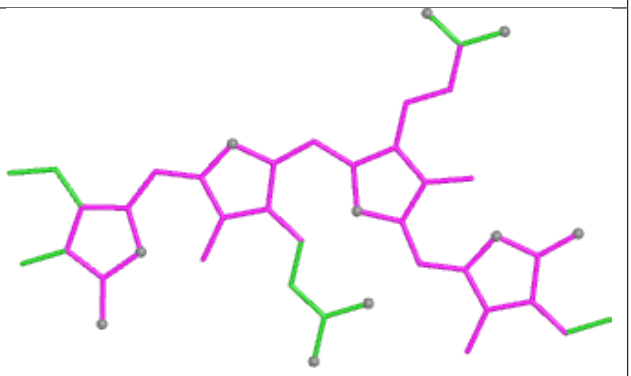


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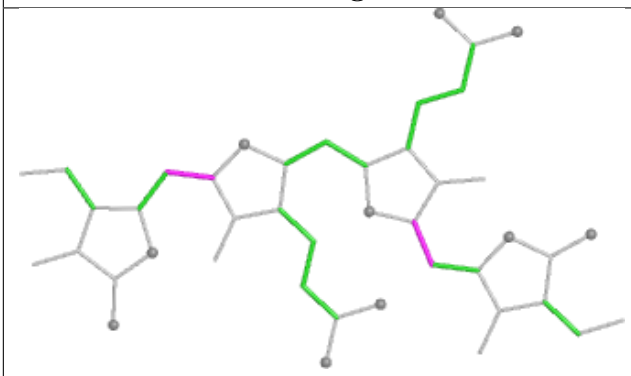
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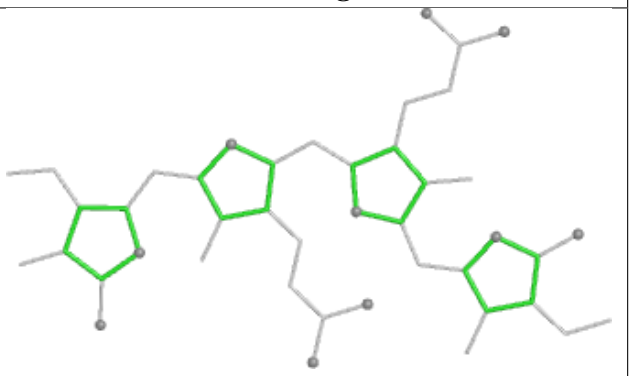
Bond lengths



Bond angles

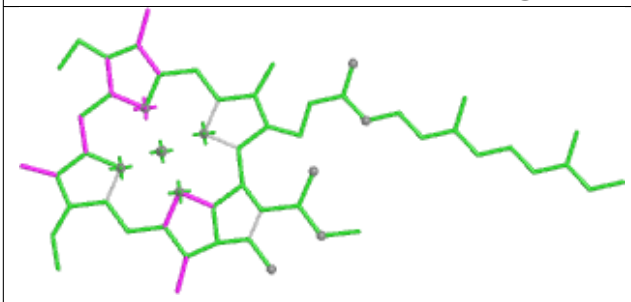


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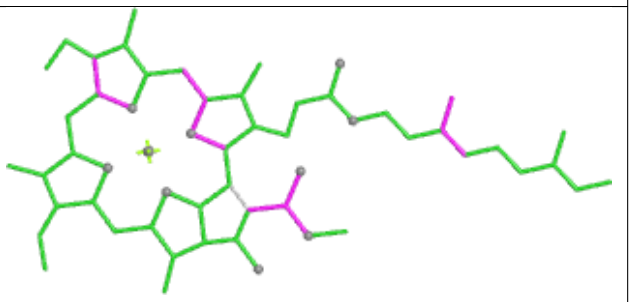


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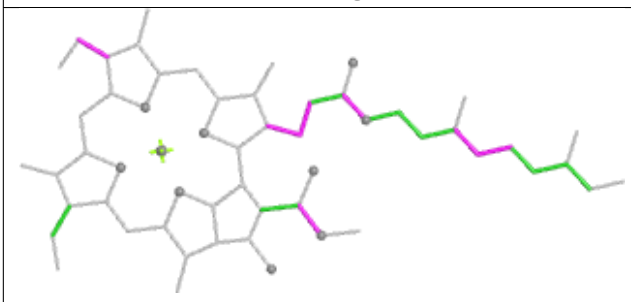
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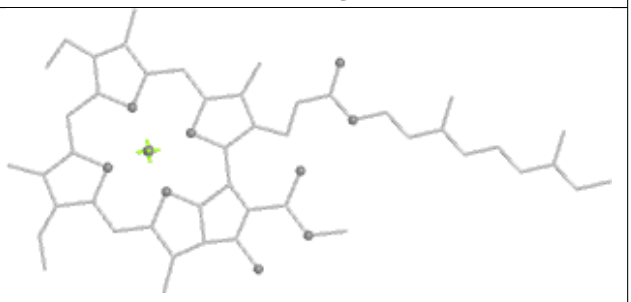
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Bond angles

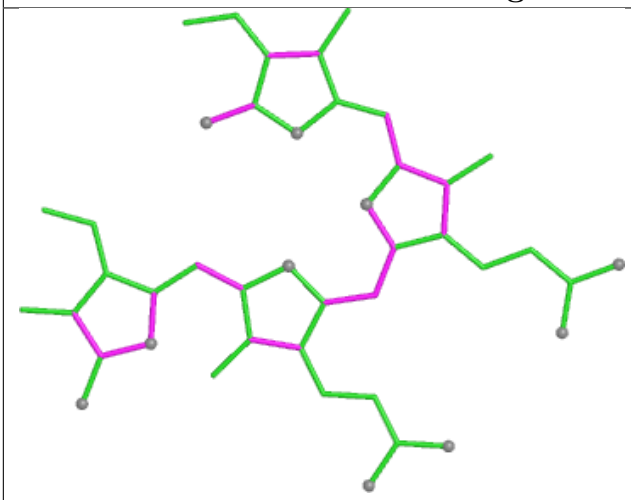


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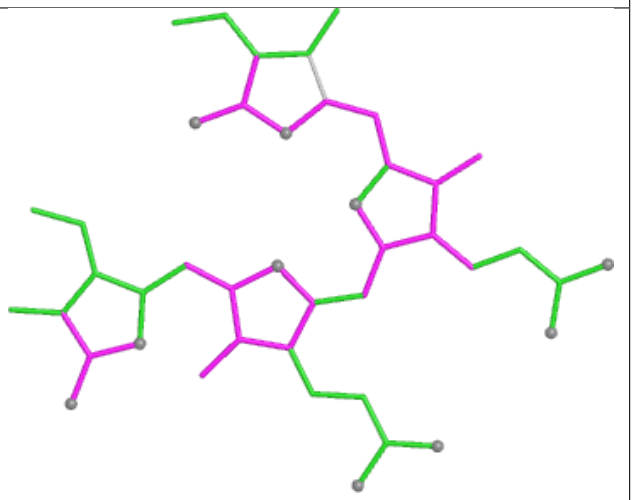


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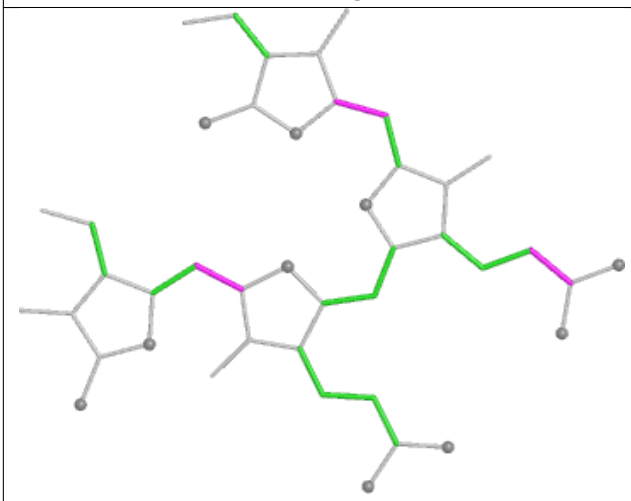
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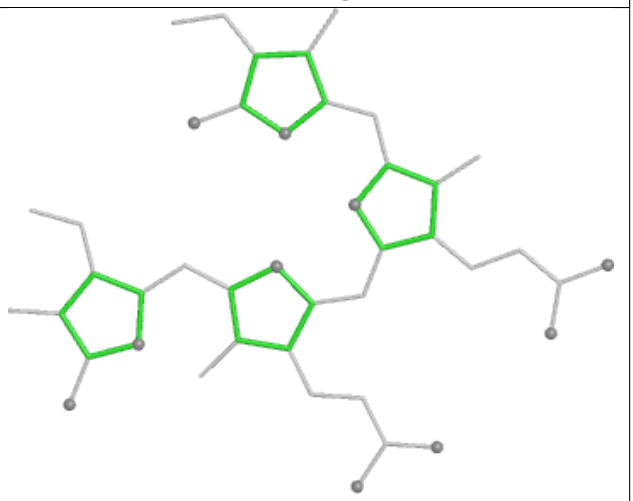
Bond lengths



Bond angles

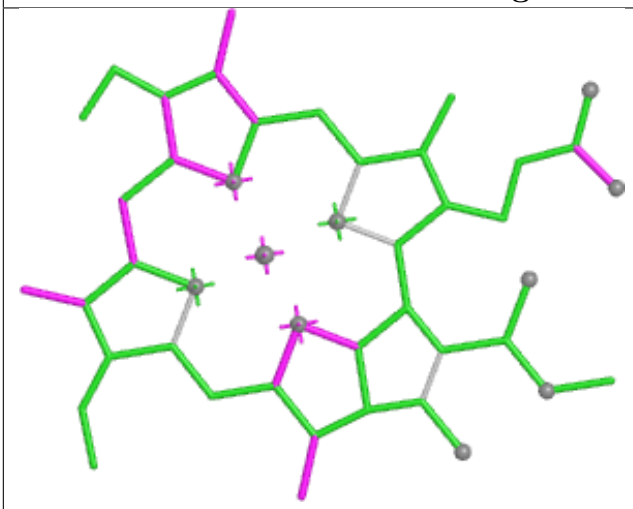


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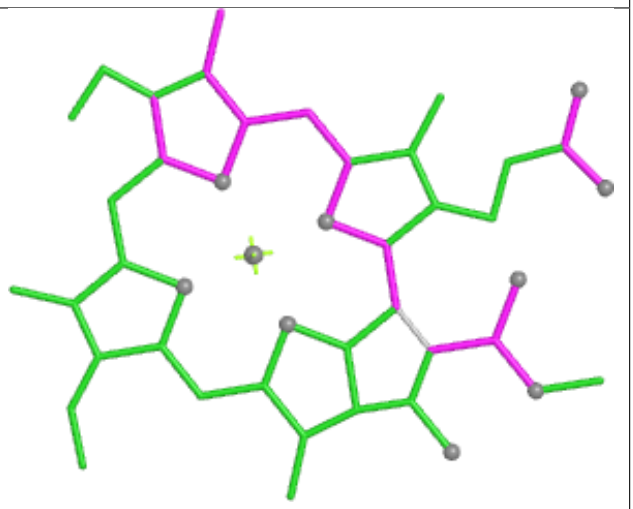


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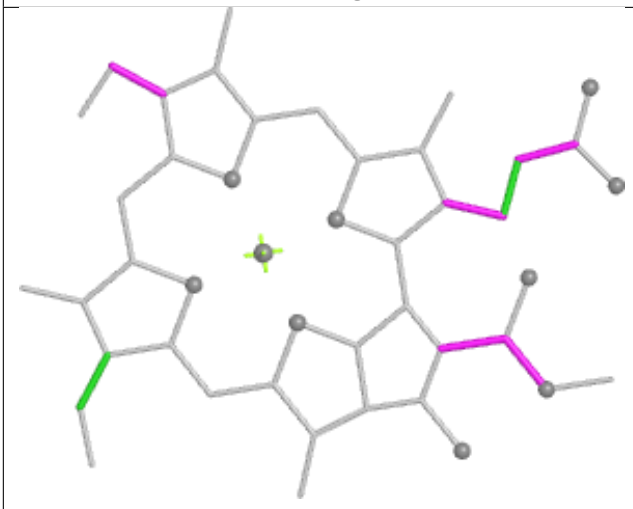
Ligand CLA FN 203



Bond lengths



Bond angles

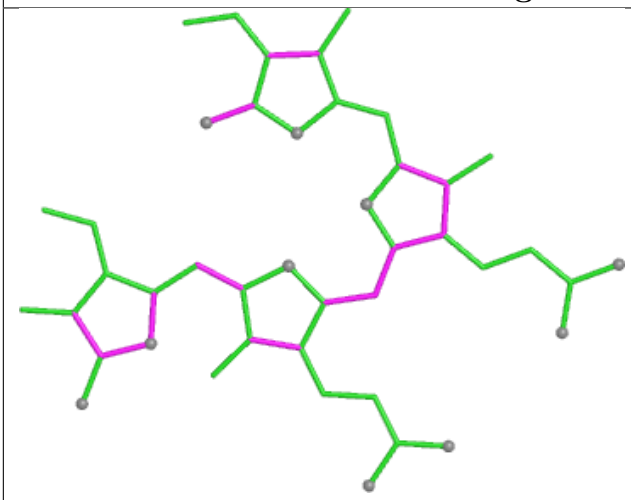


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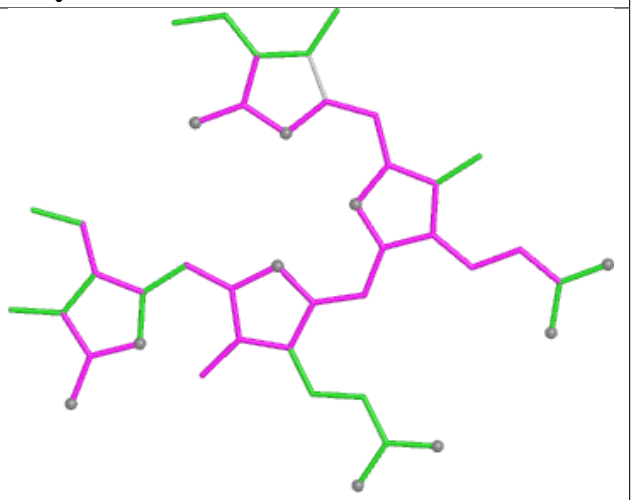


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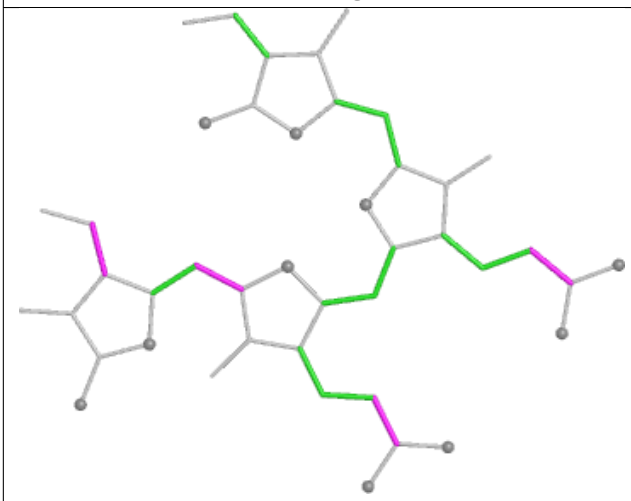
Ligand PEB QJ 202



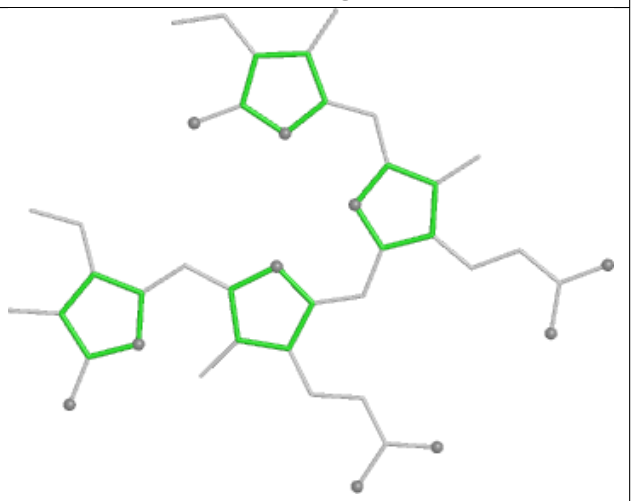
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Bond angles

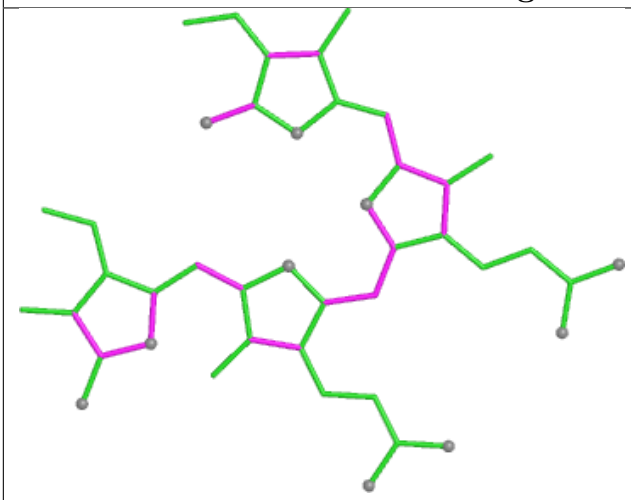


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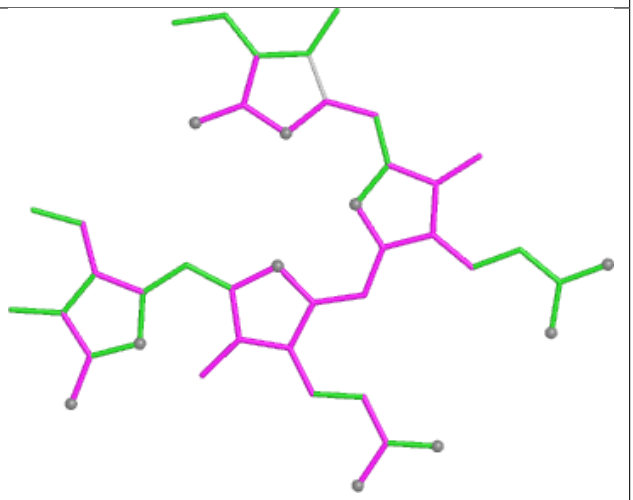


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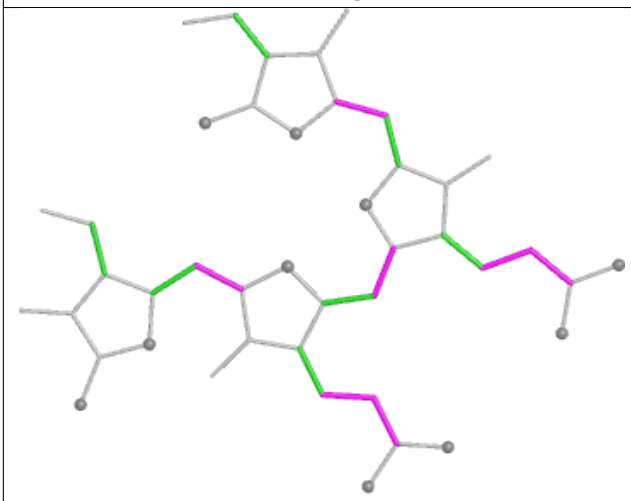
Ligand PEB F9 201



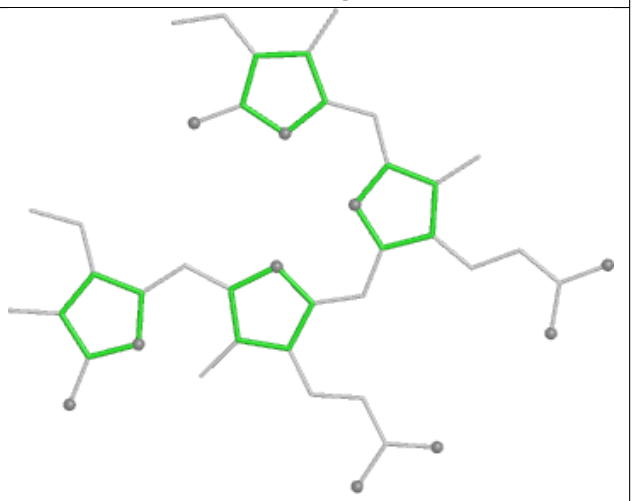
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Bond angles

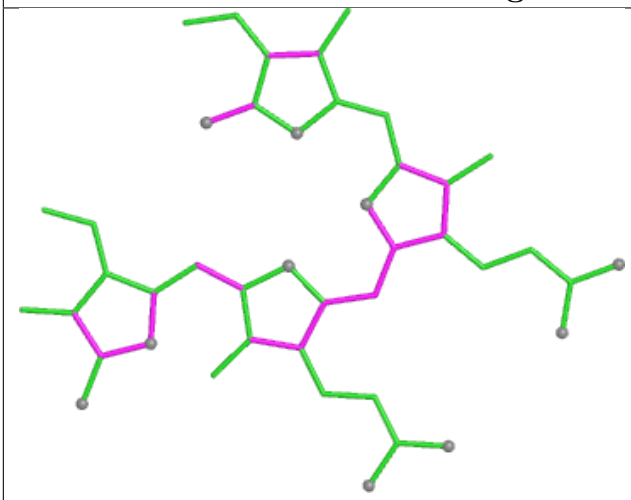


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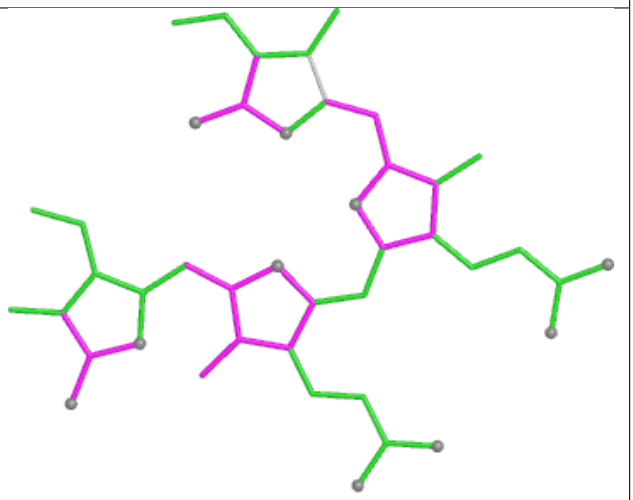


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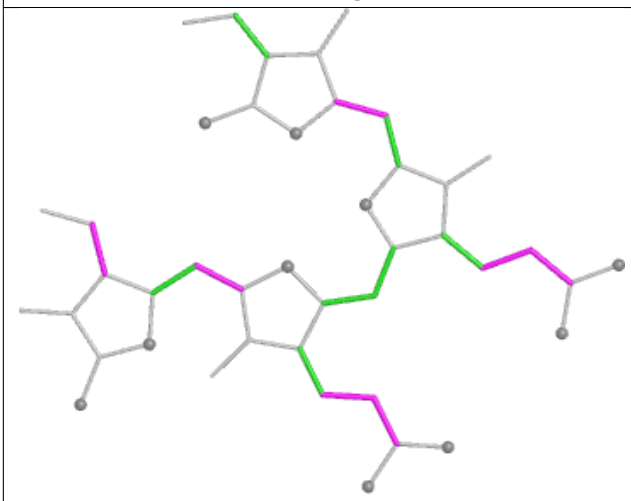
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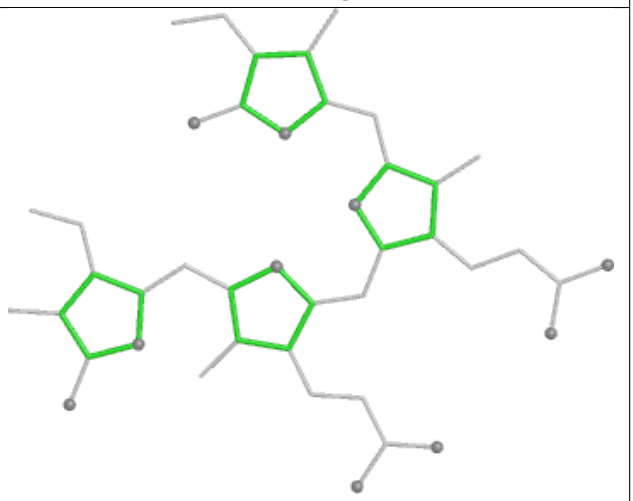
Bond lengths



Bond angles

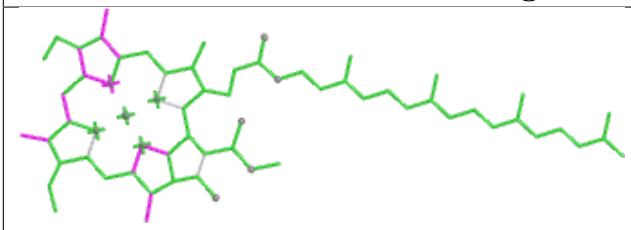


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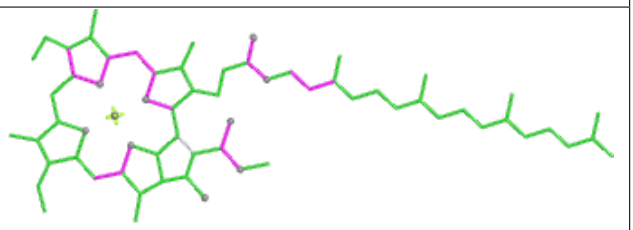


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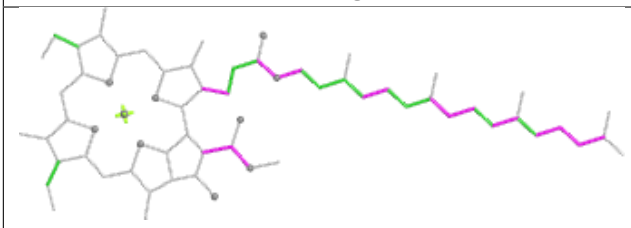
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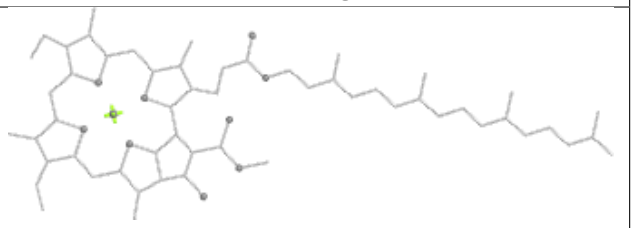
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Bond angles

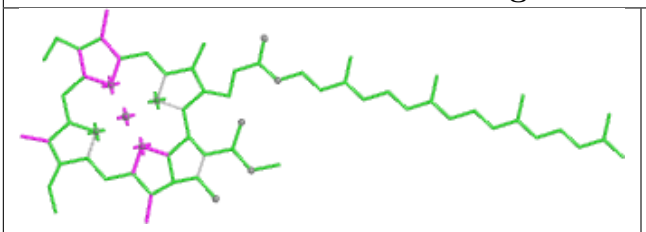


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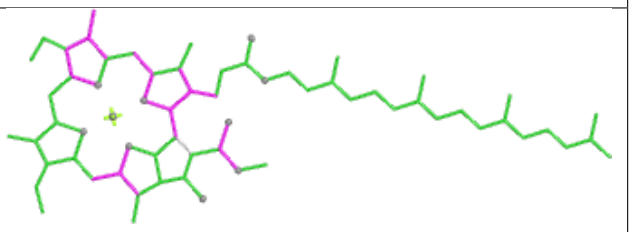


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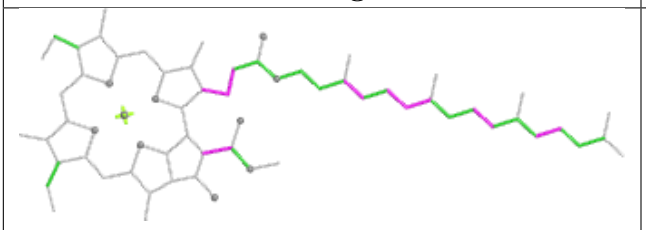
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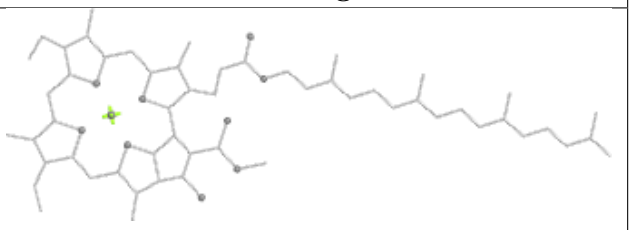
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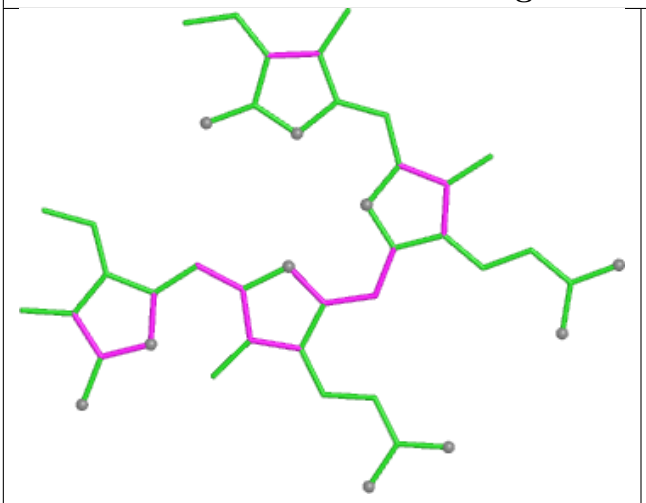


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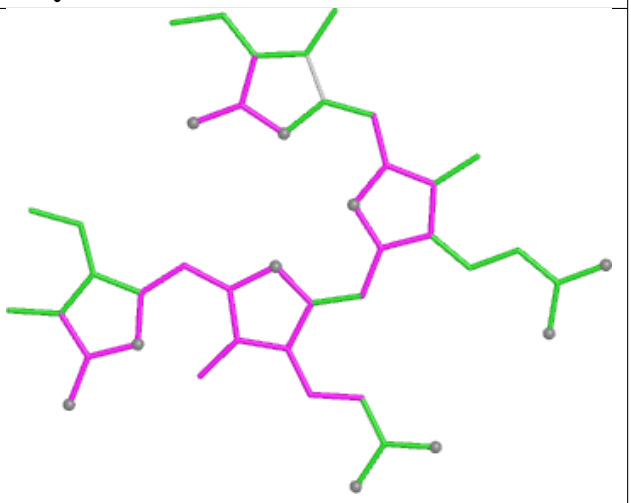


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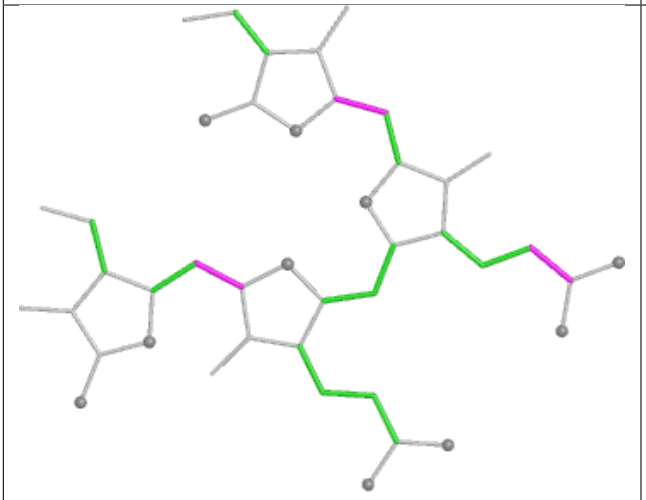
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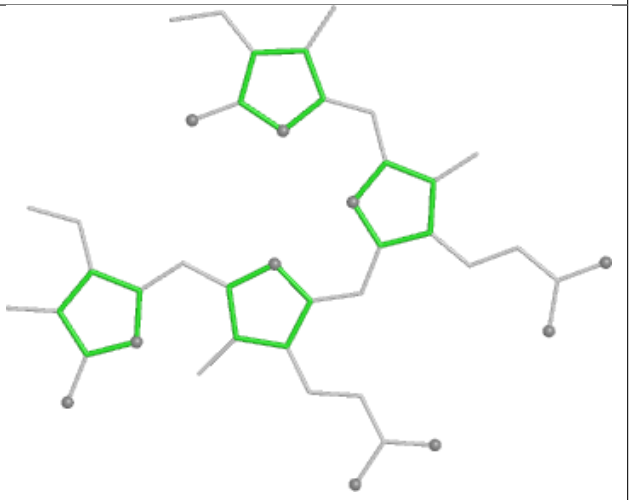
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Bond angles

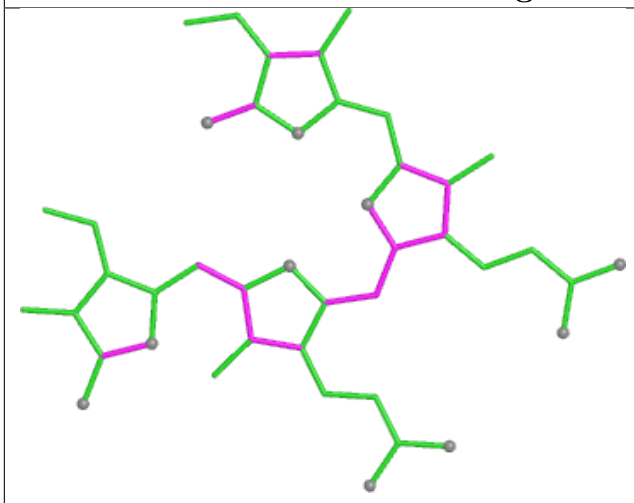


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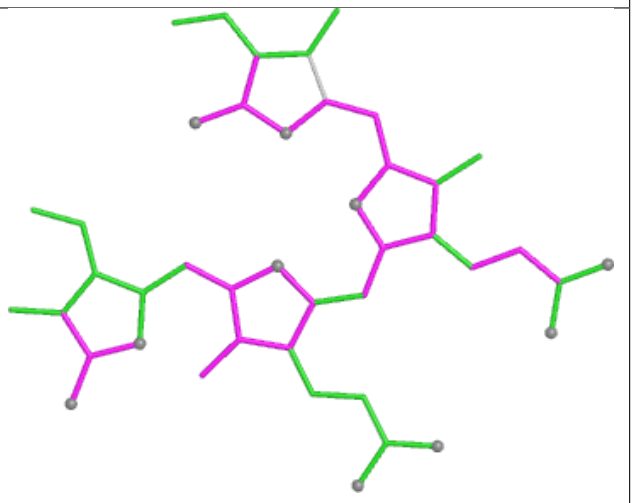


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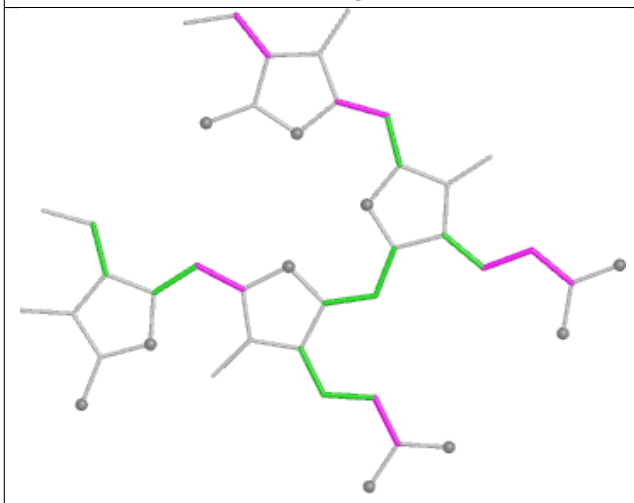
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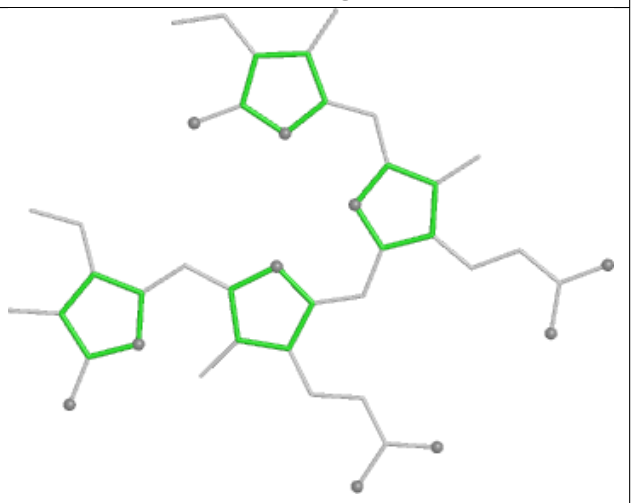
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Bond angles

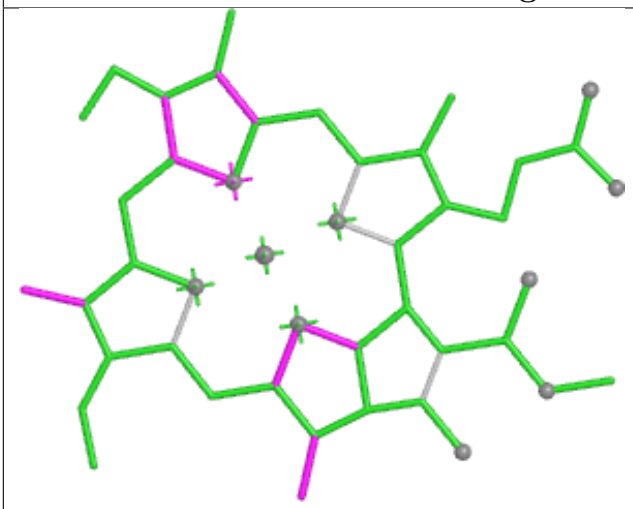


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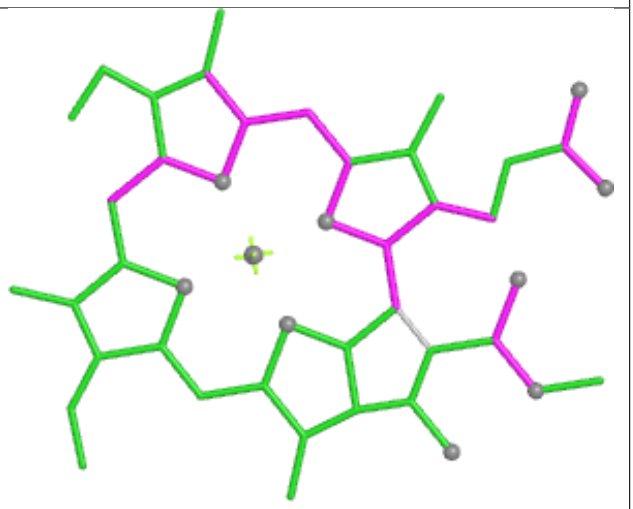


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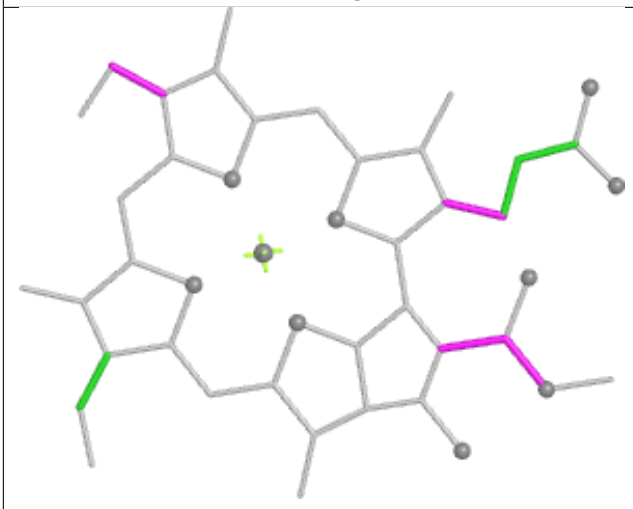
Ligand CLA 22 608



Bond lengths



Bond angles

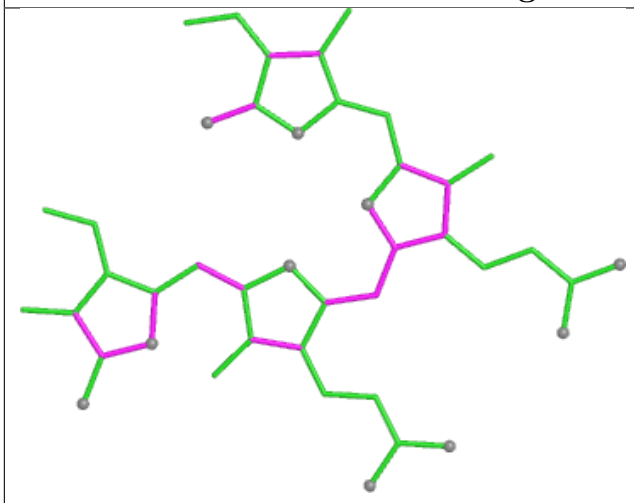


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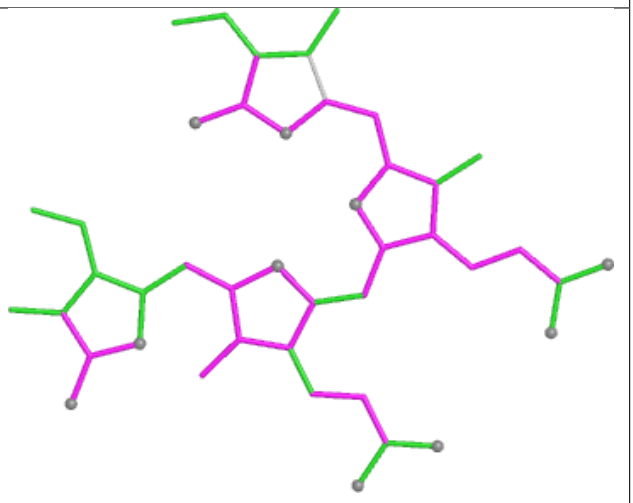


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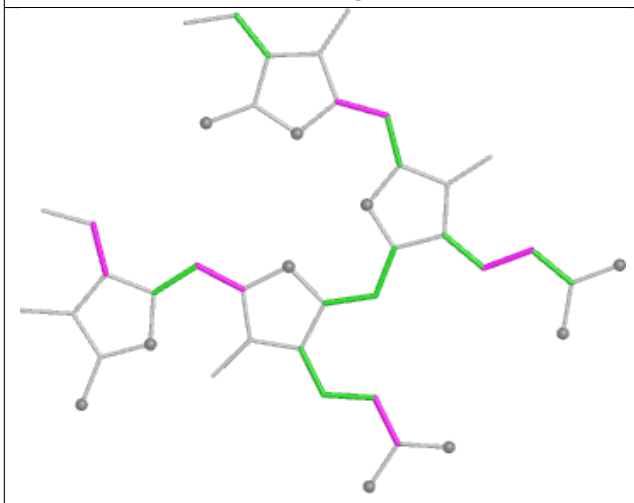
Ligand PEB XI 201



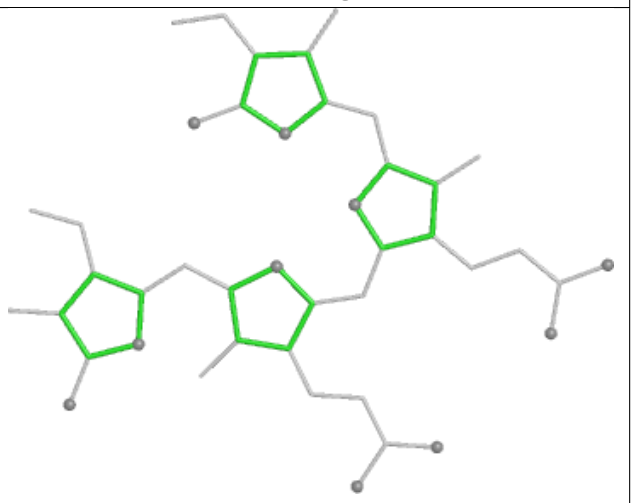
Bond lengths



Bond angles

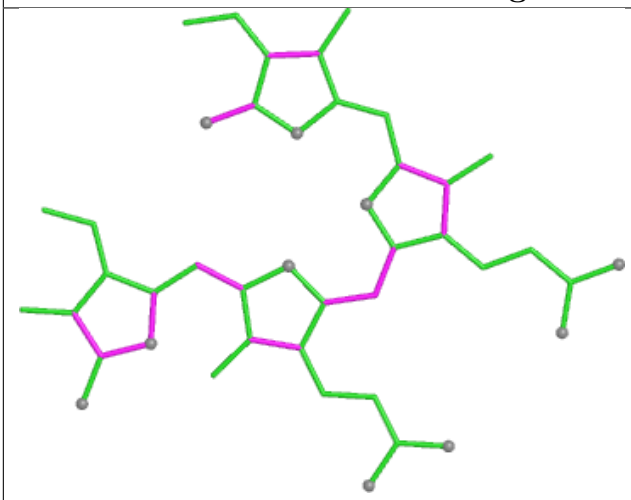


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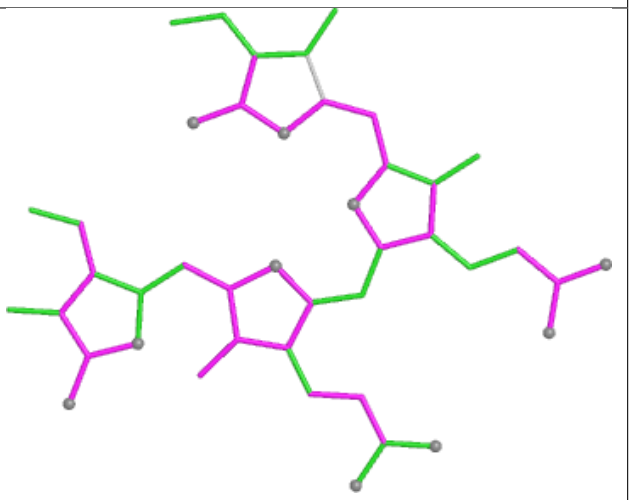


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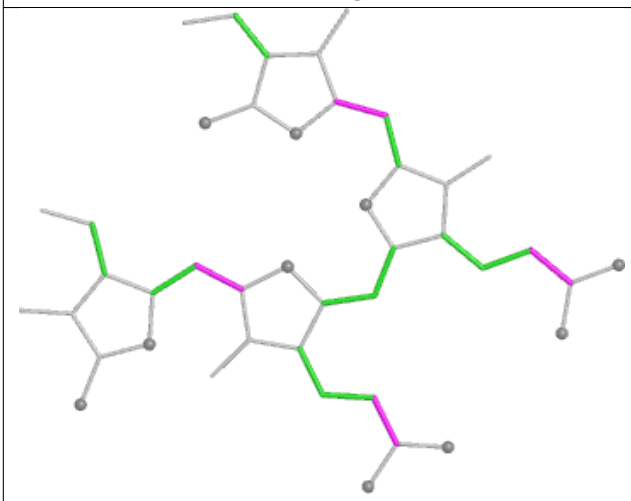
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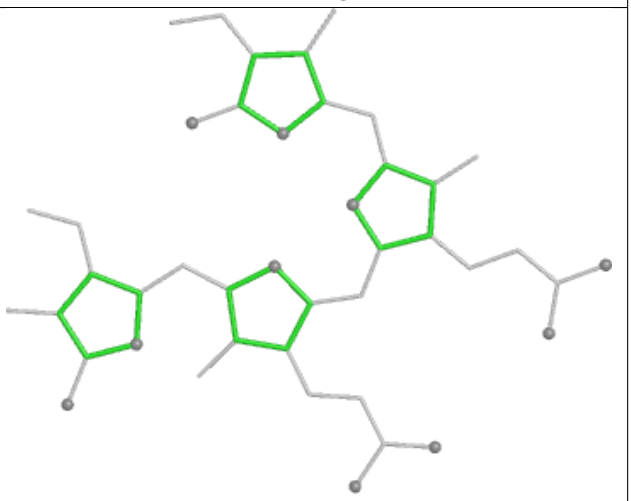
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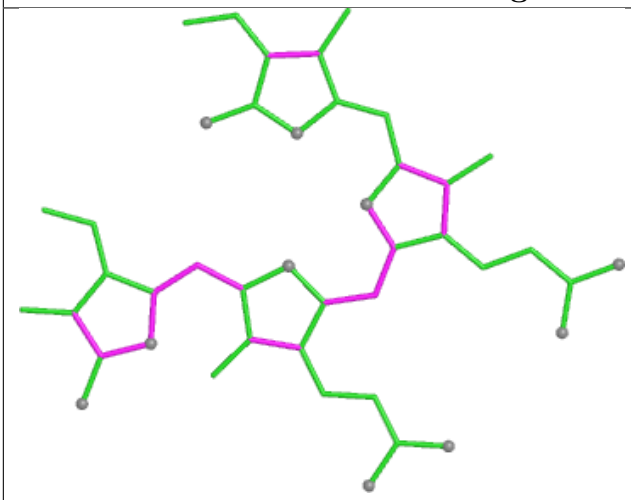


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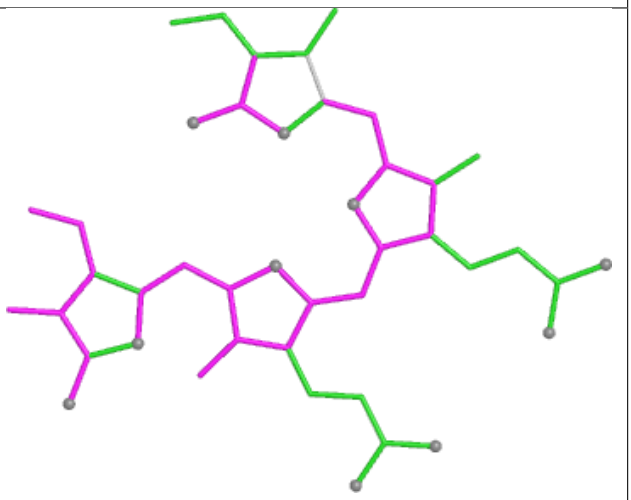


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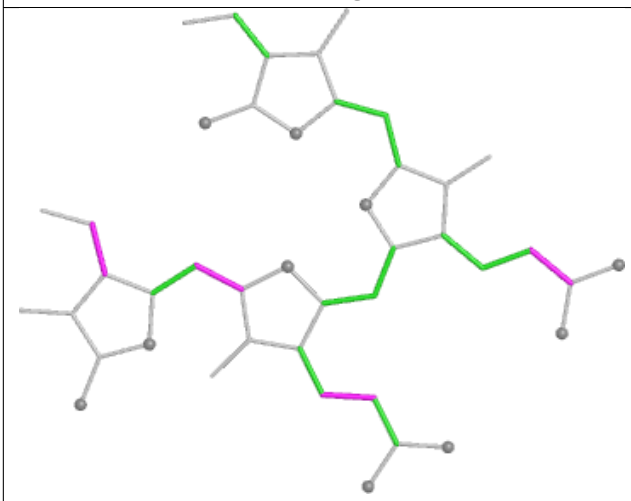
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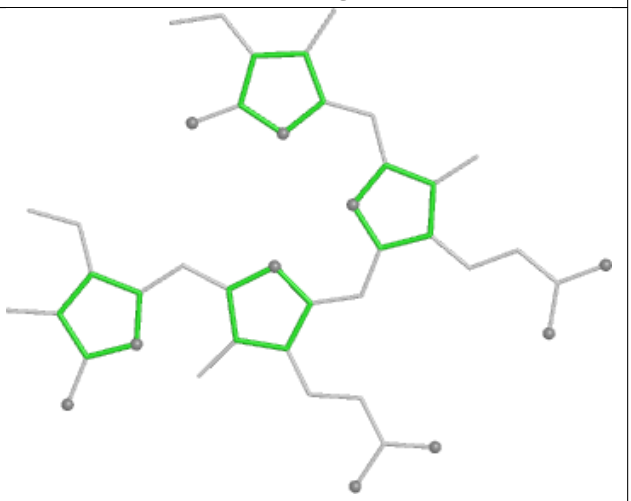
Bond lengths



Bond angles

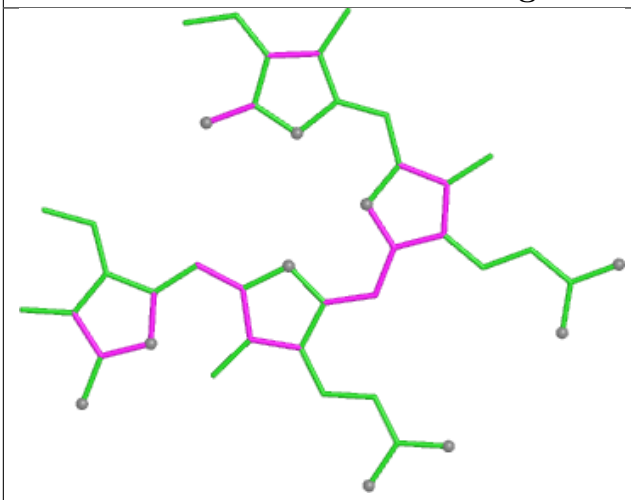


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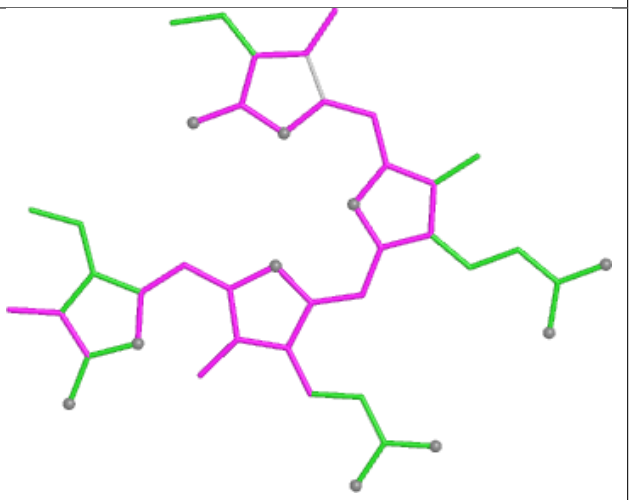


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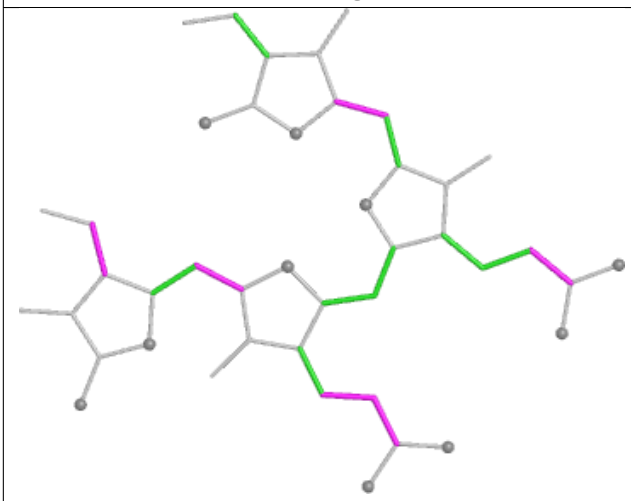
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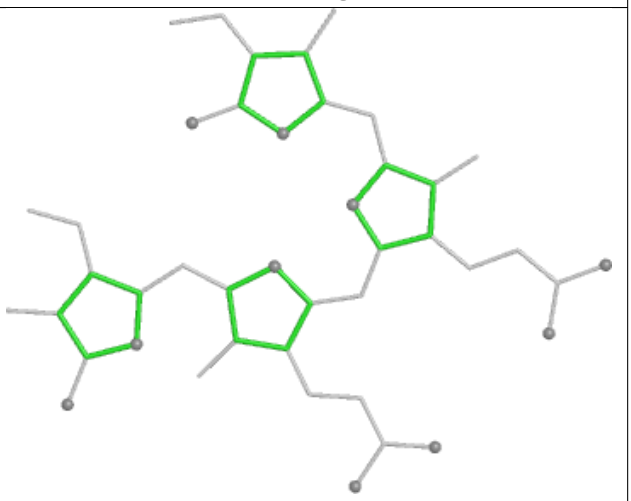
Bond lengths



Bond angles

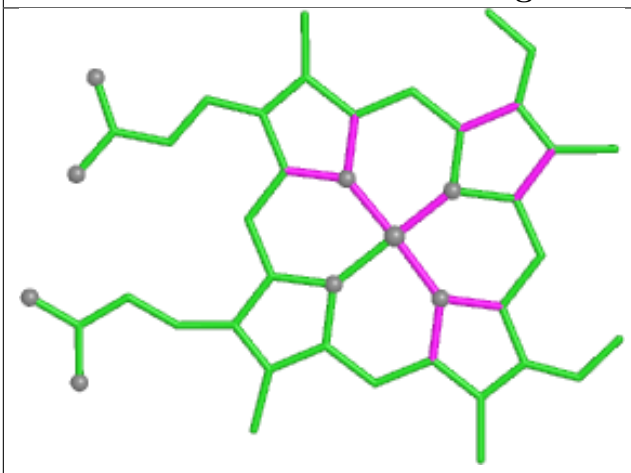


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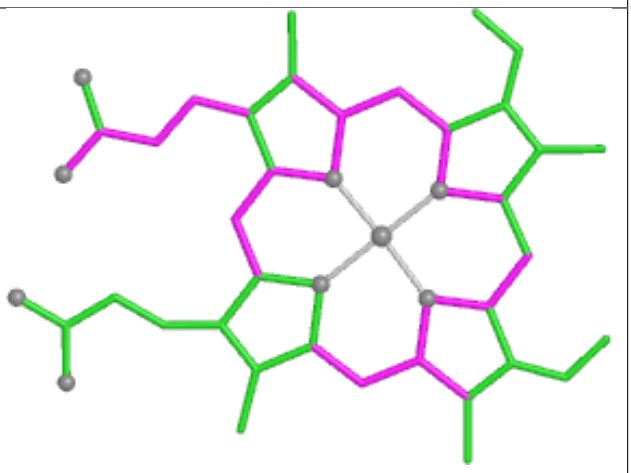


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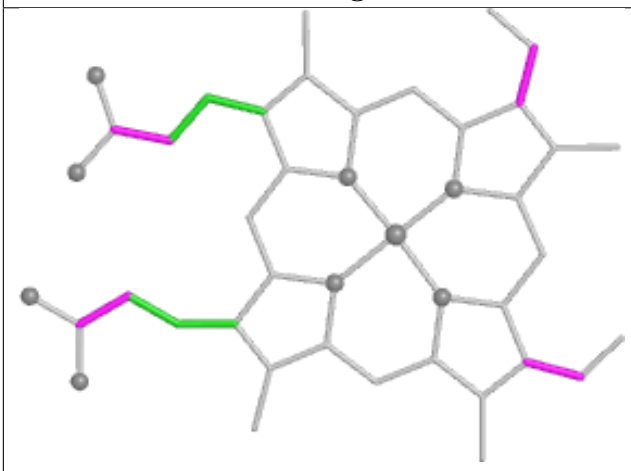
Ligand HEM fL 102



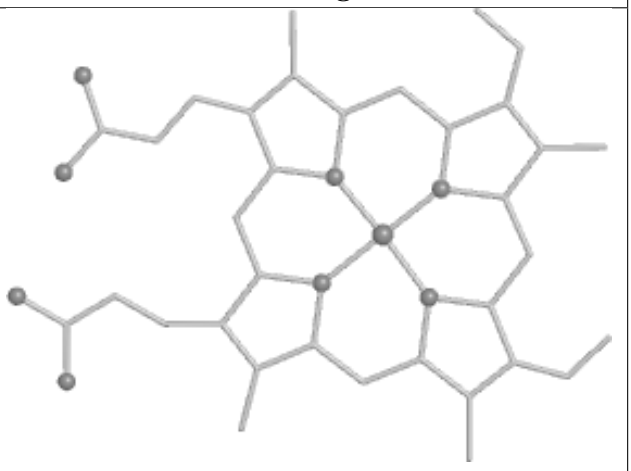
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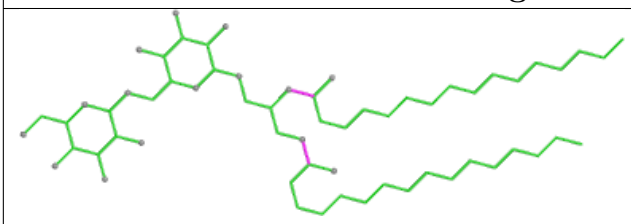


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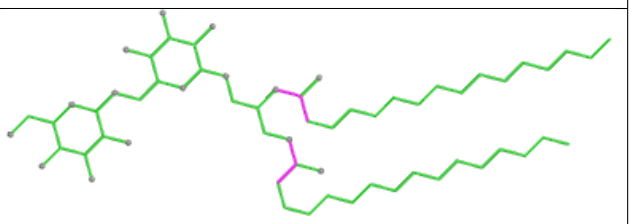


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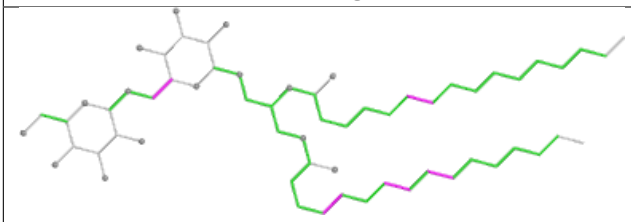
Ligand DGD CL 517



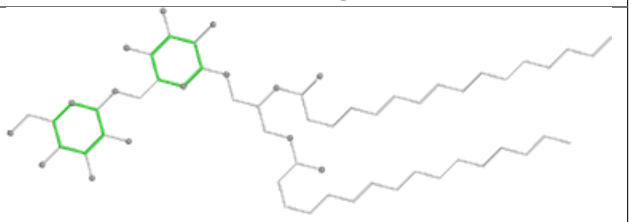
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Bond angles

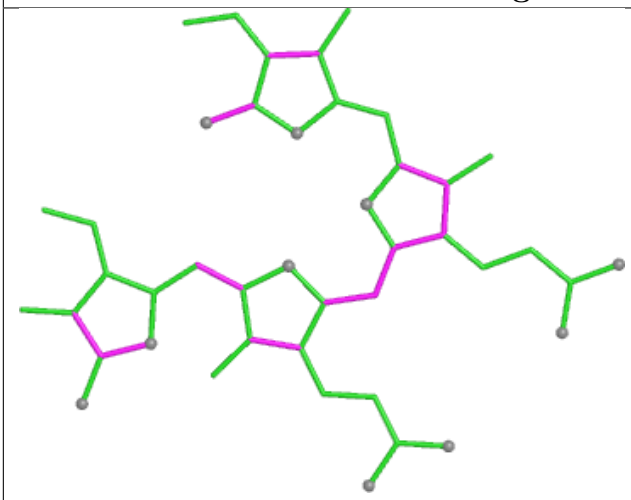


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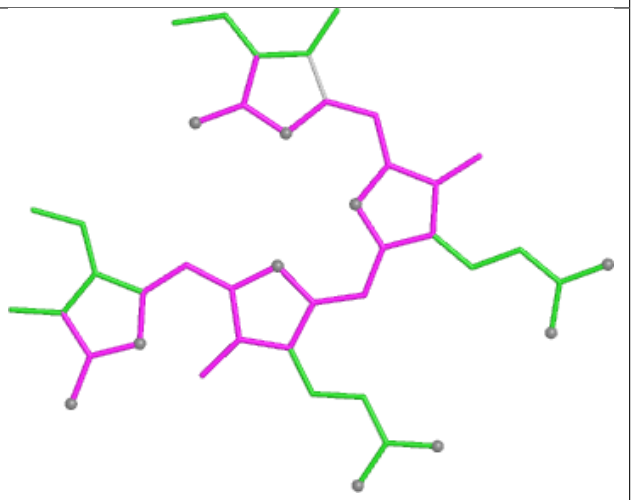


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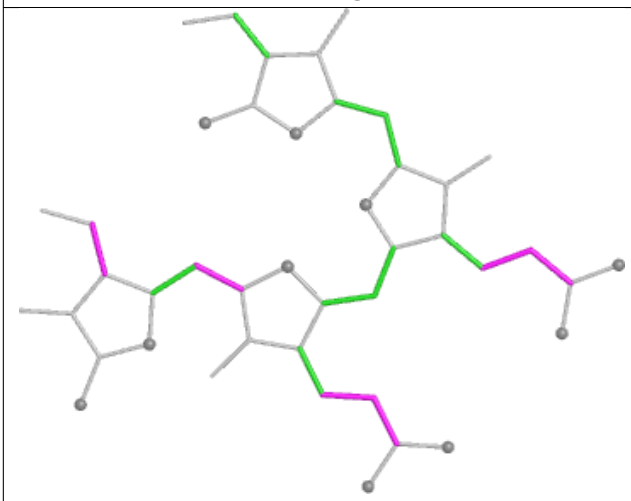
Ligand PEB VA 202



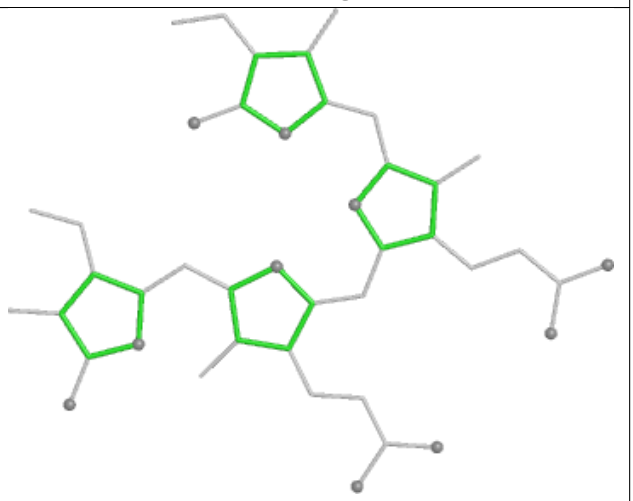
Bond lengths



Bond angles

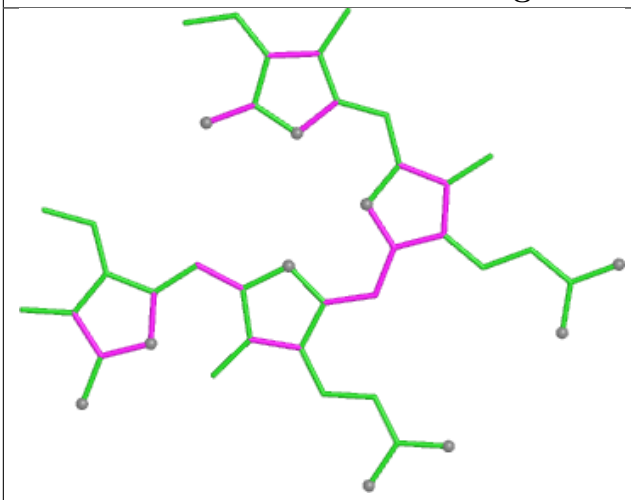


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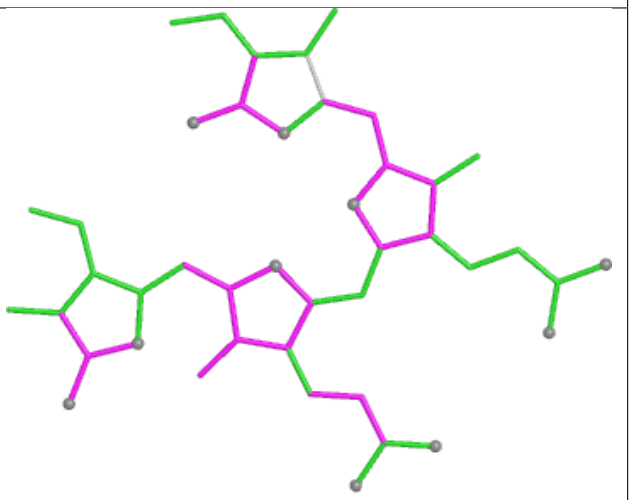


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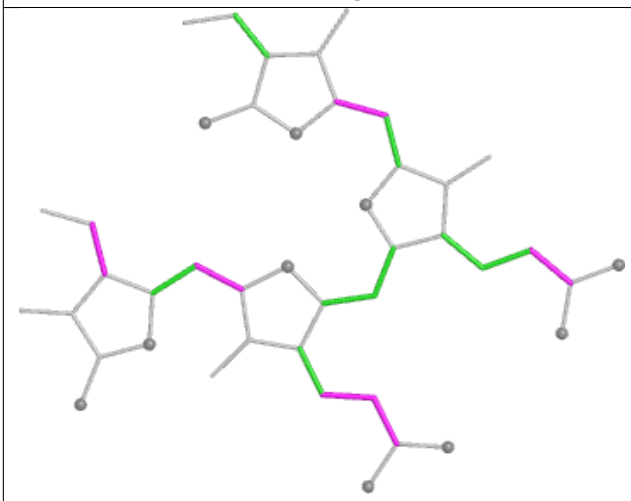
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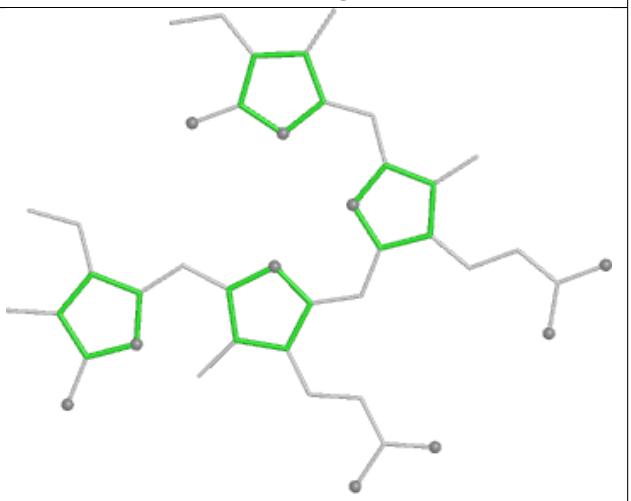
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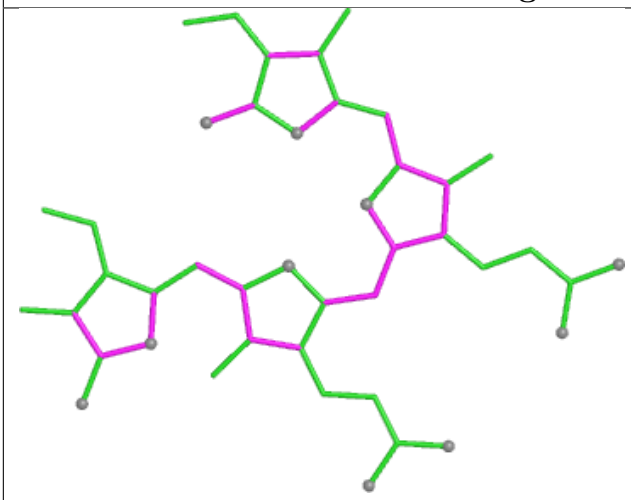


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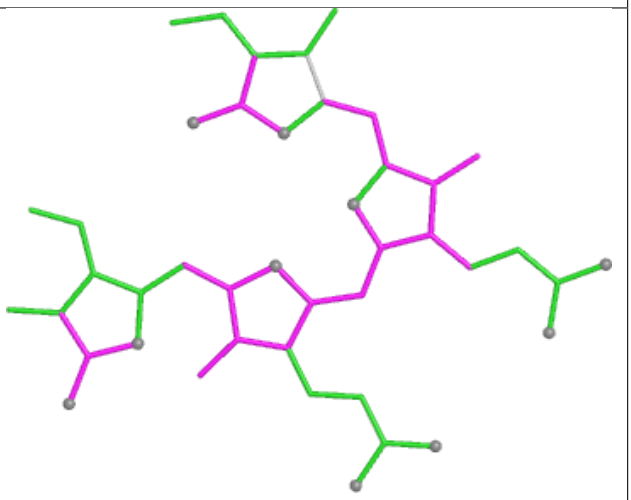


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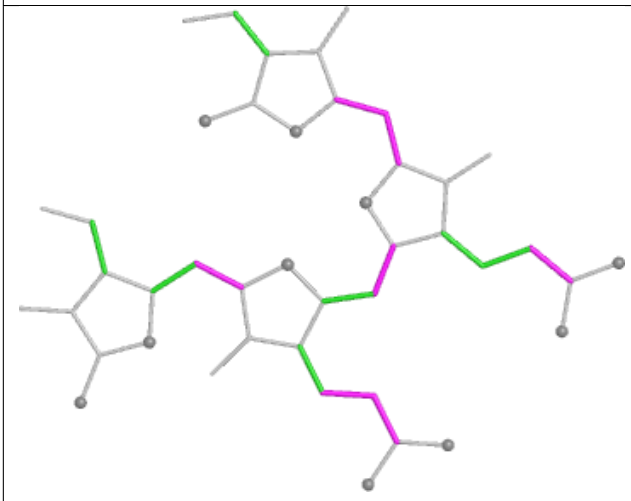
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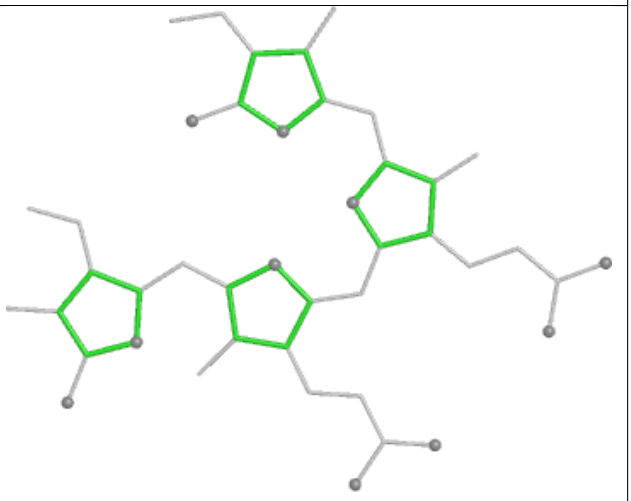
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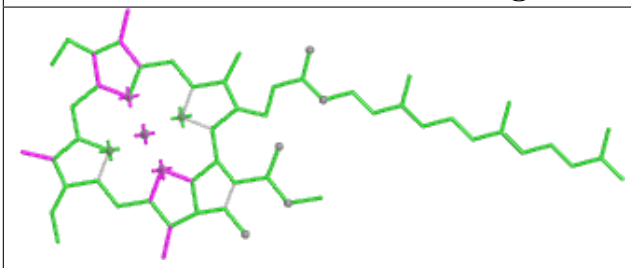


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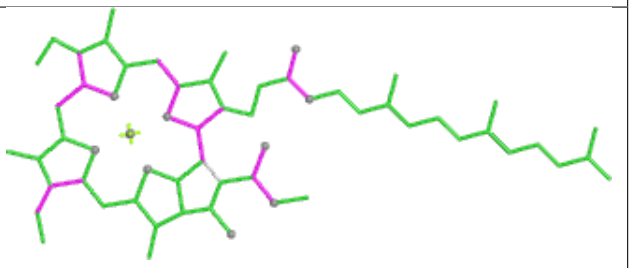


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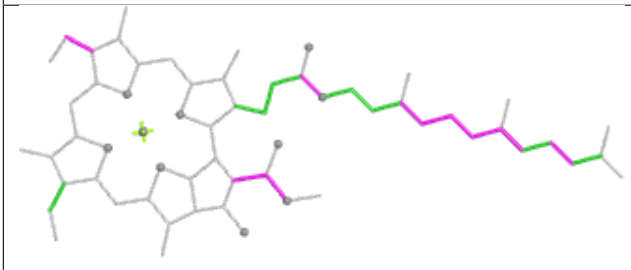
Ligand CLA BN 831



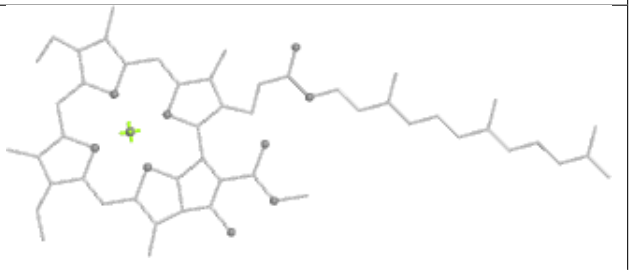
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Bond angles

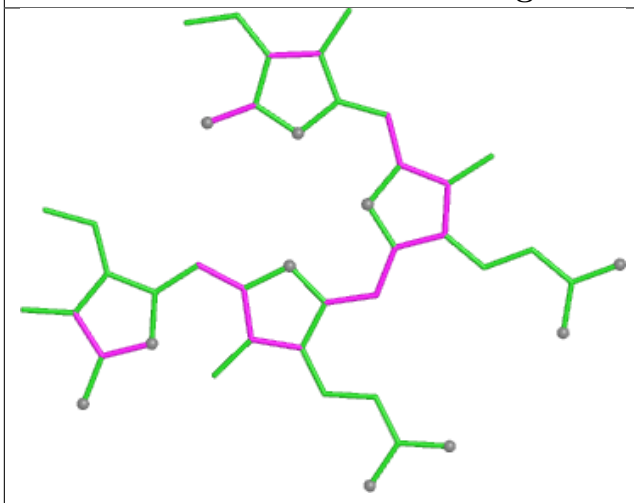


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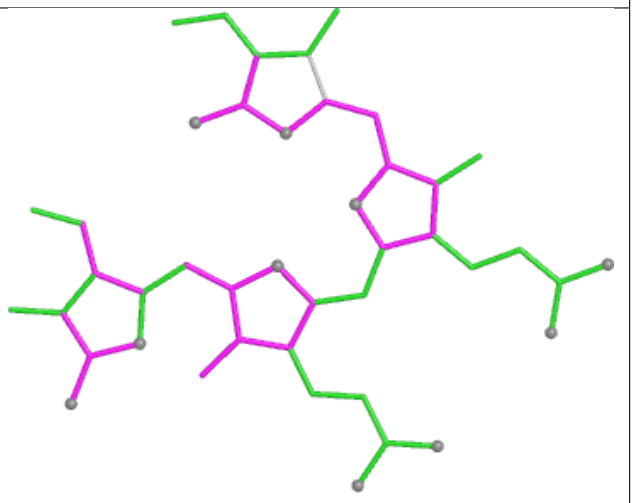


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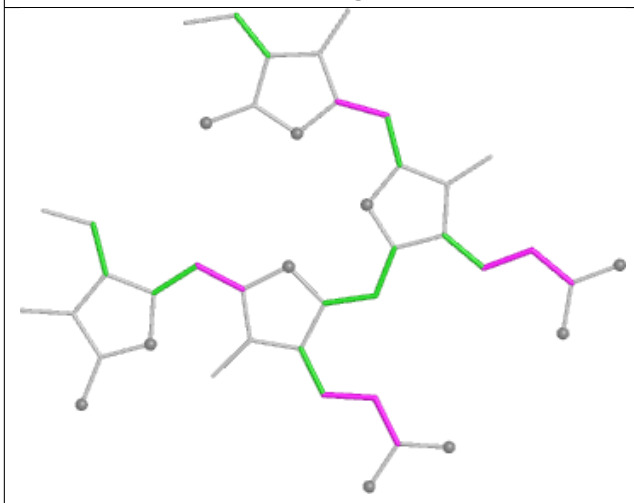
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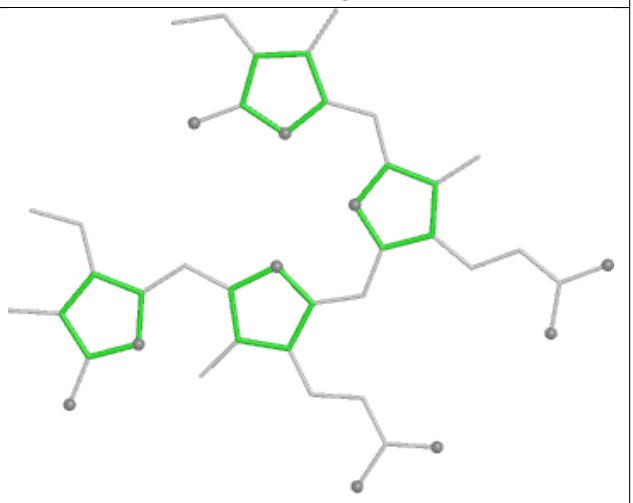
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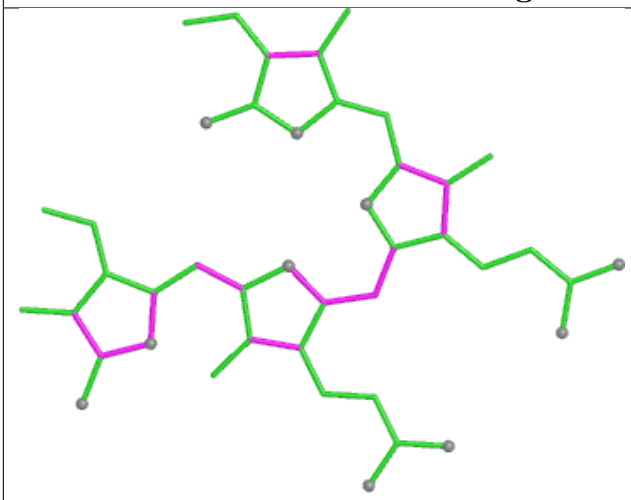


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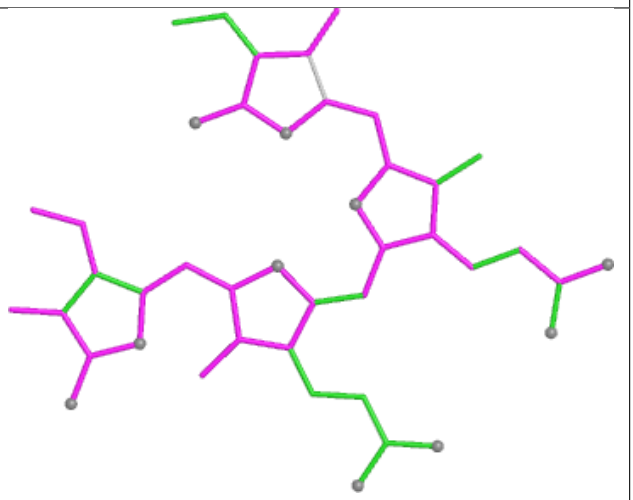


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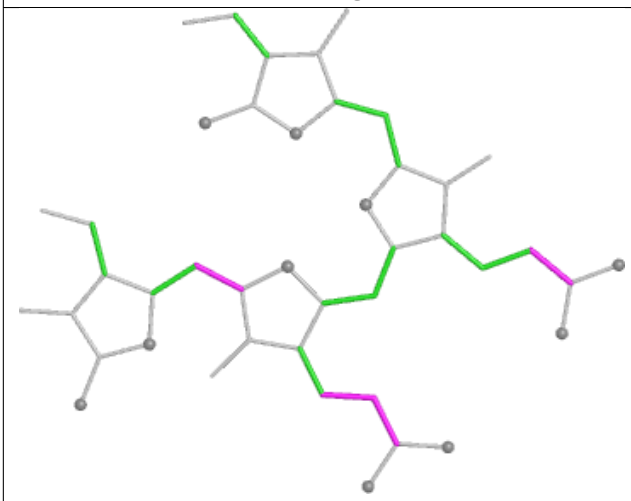
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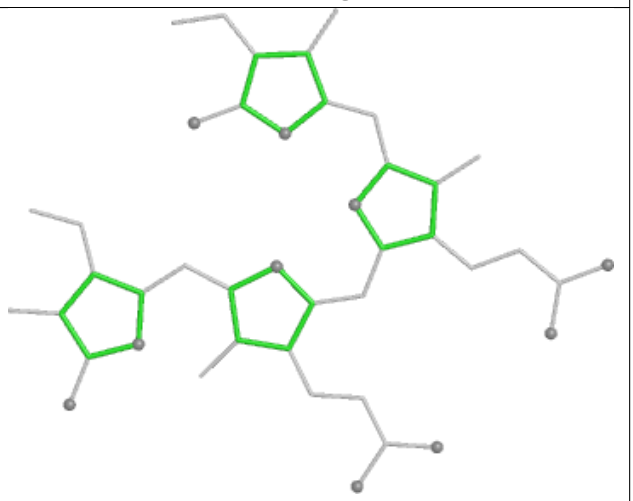
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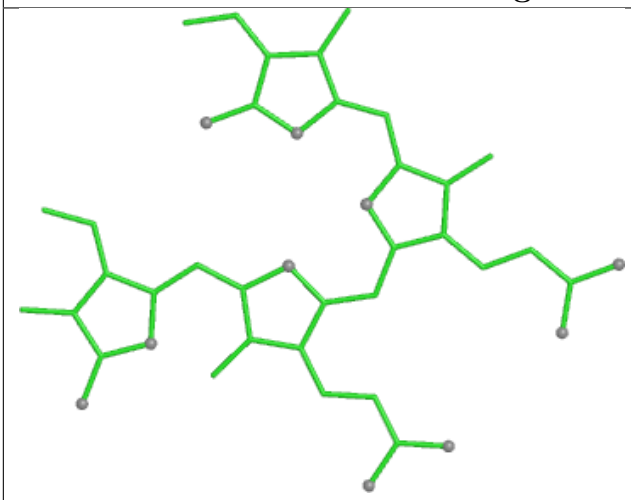


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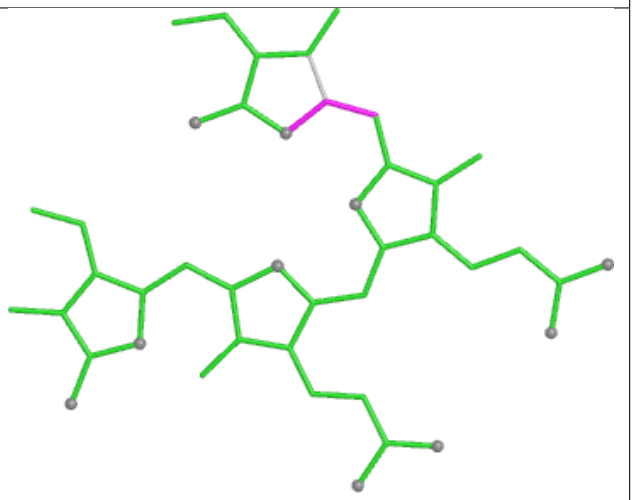


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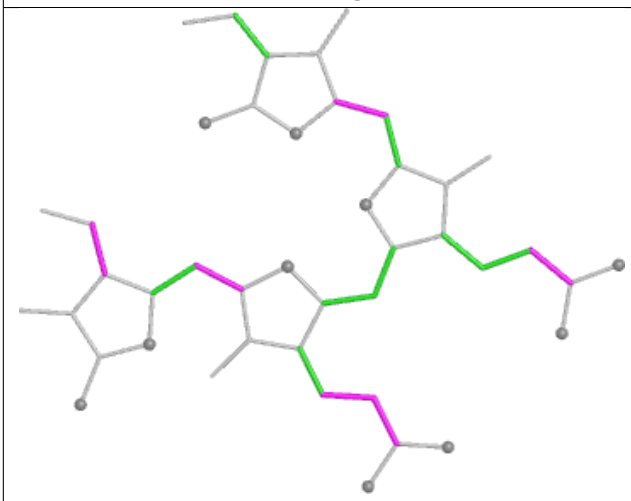
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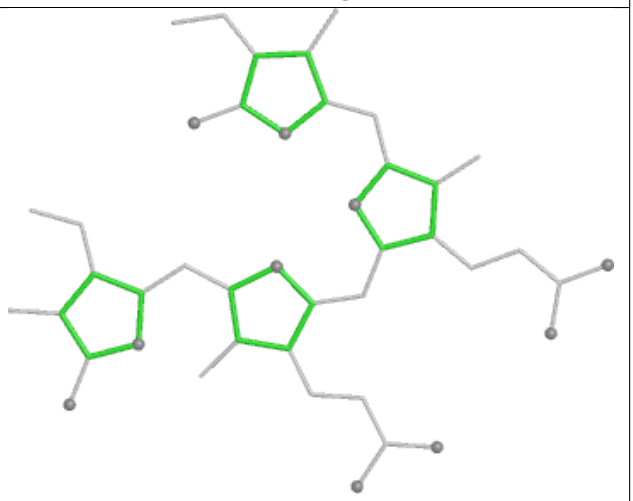
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Bond angles

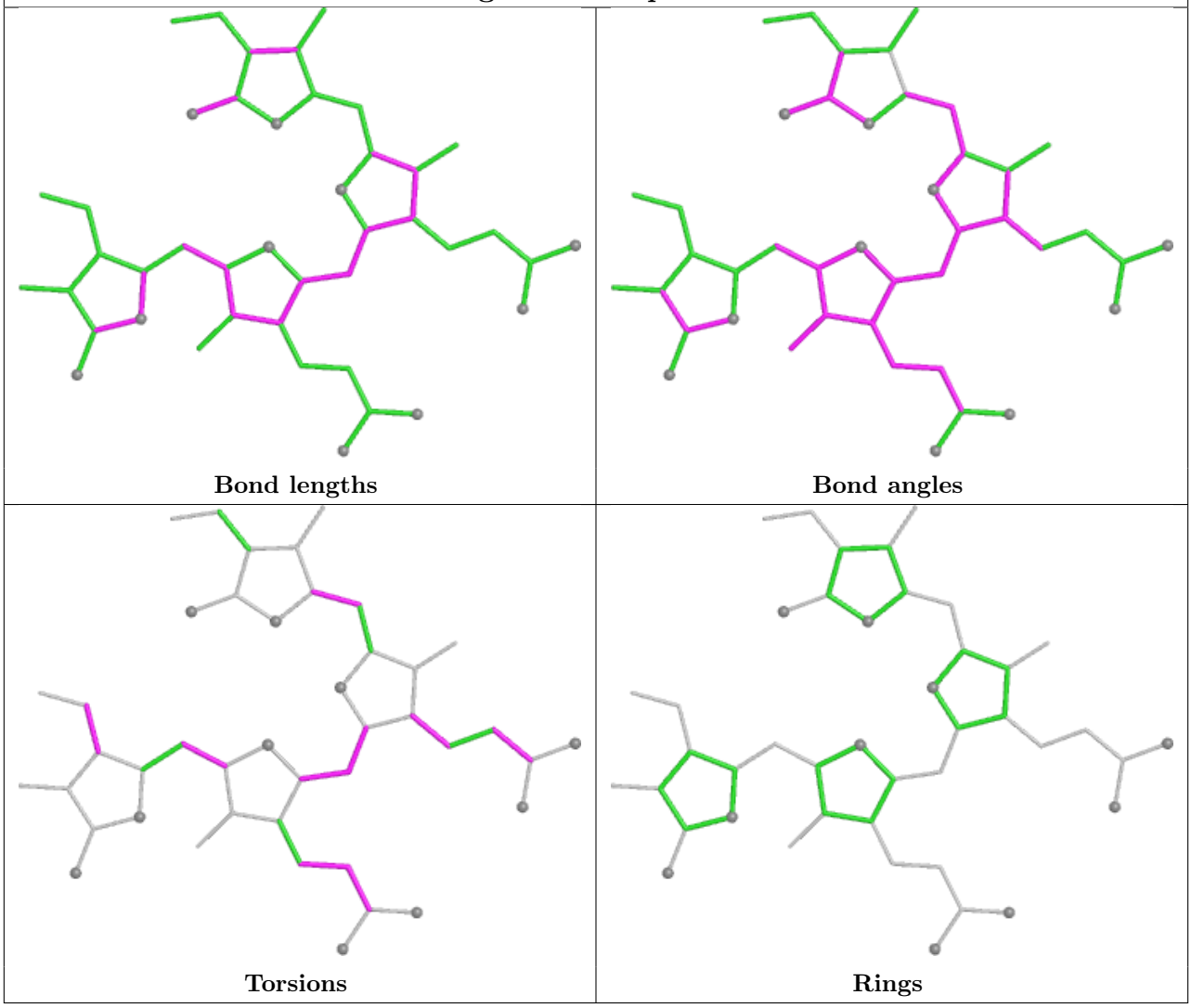


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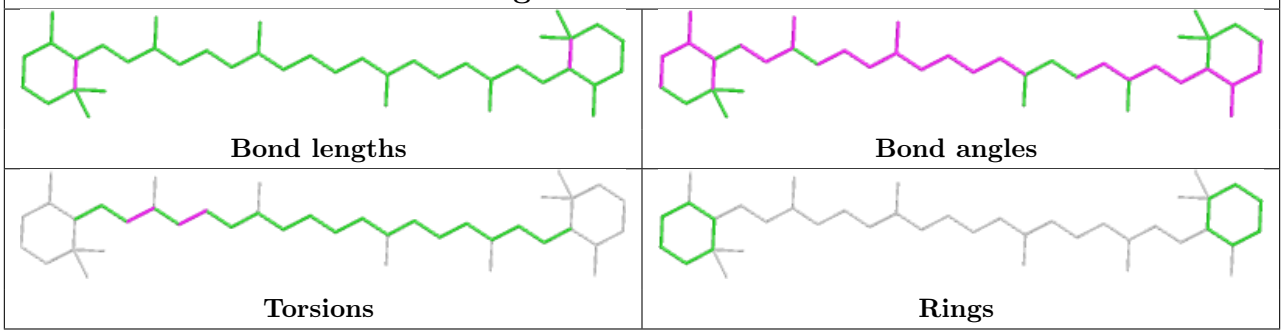


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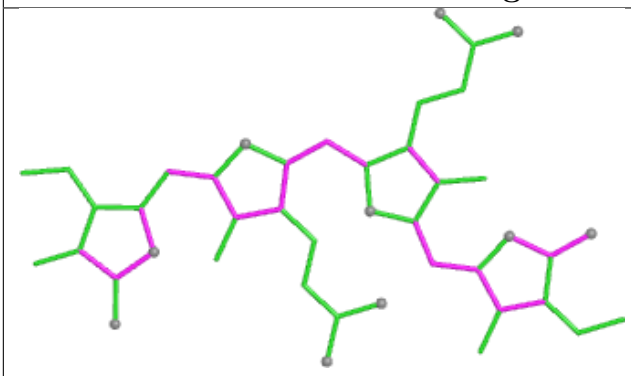
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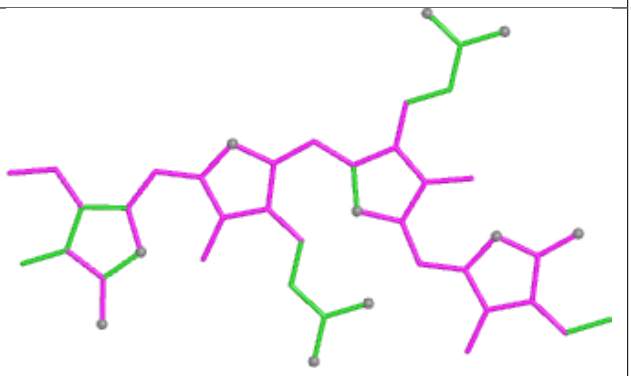
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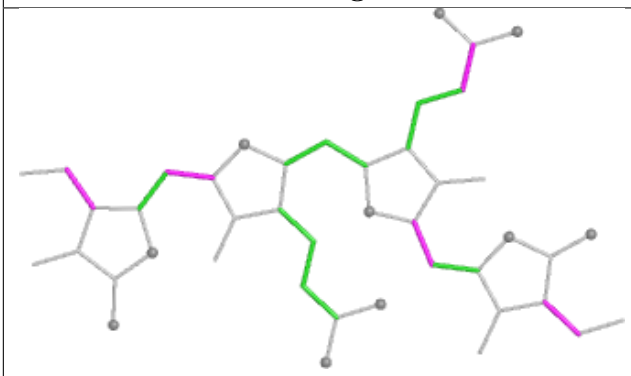
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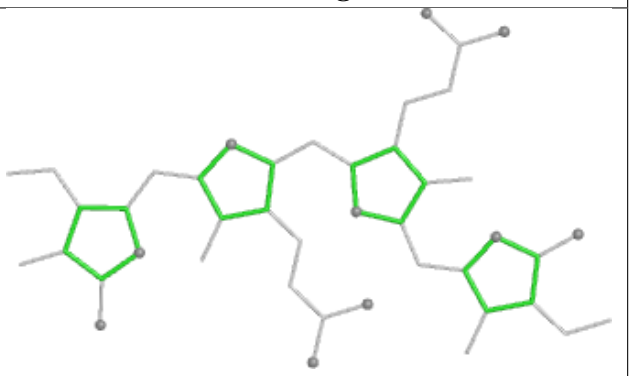
Bond lengths



Bond angles

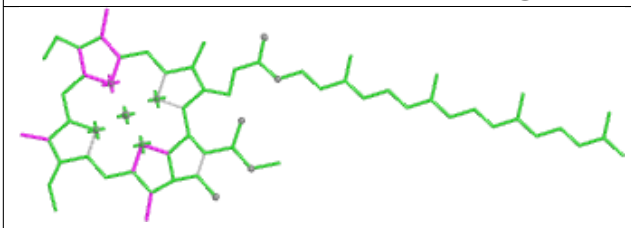


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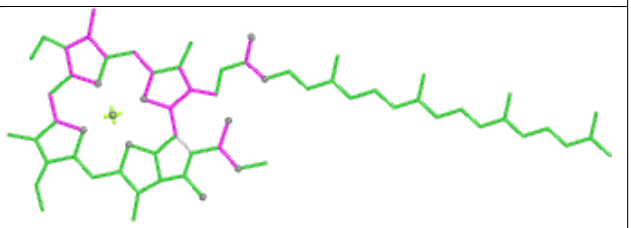


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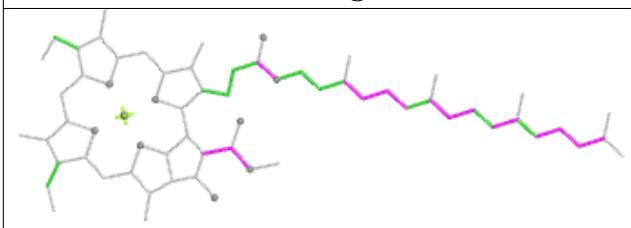
Ligand CLA nL 101



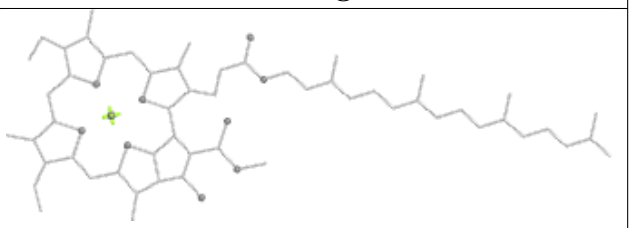
Bond lengths



Bond angles

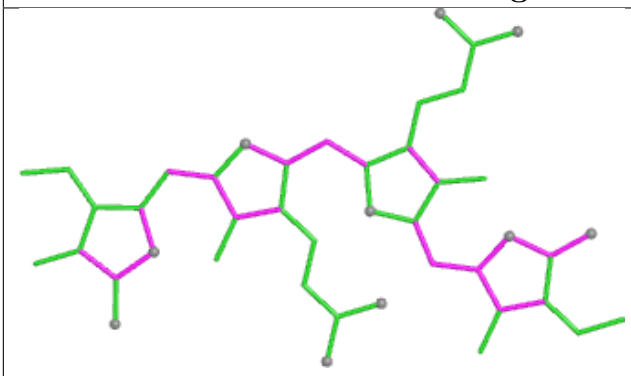


Torsions

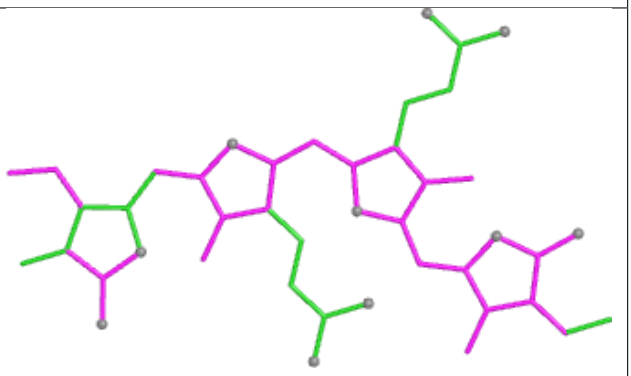


Rings

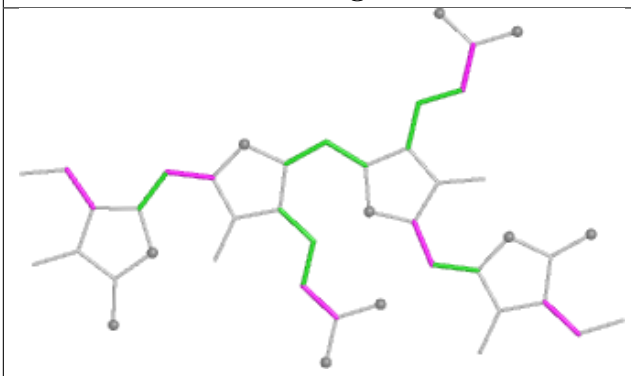
Ligand CYC I4 1001



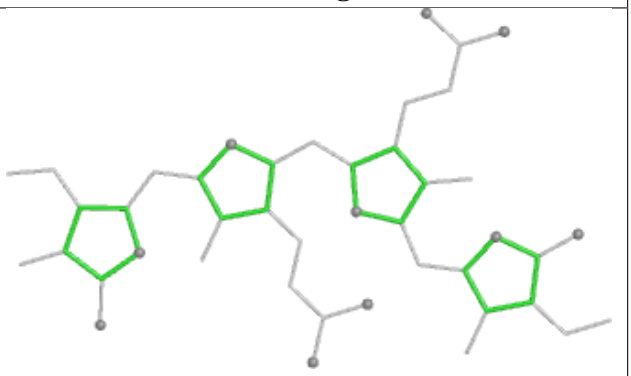
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Bond angles

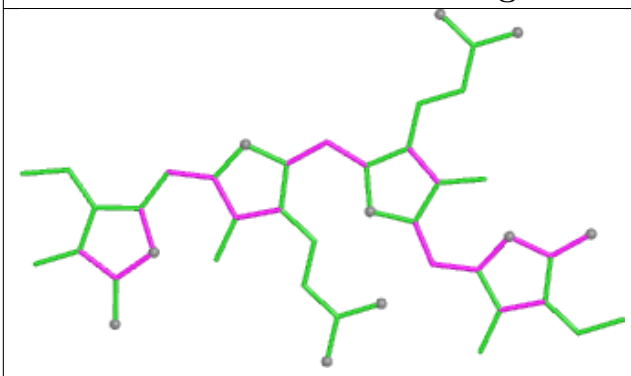


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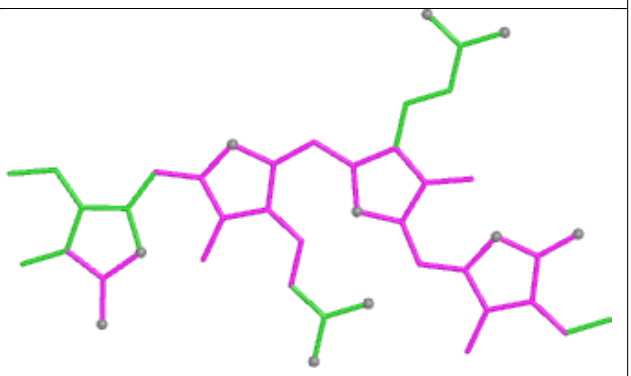


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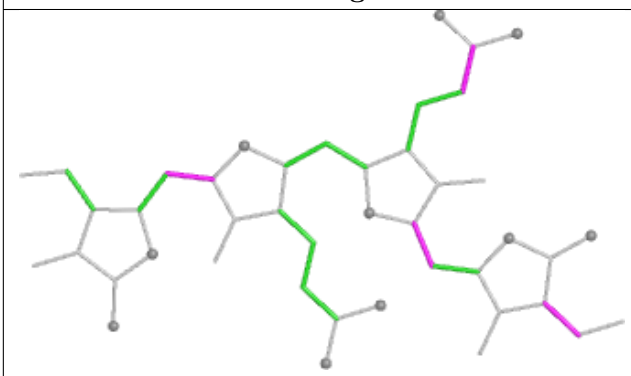
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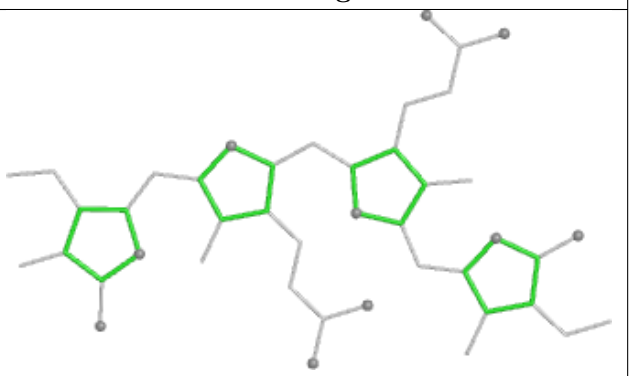
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Bond angles

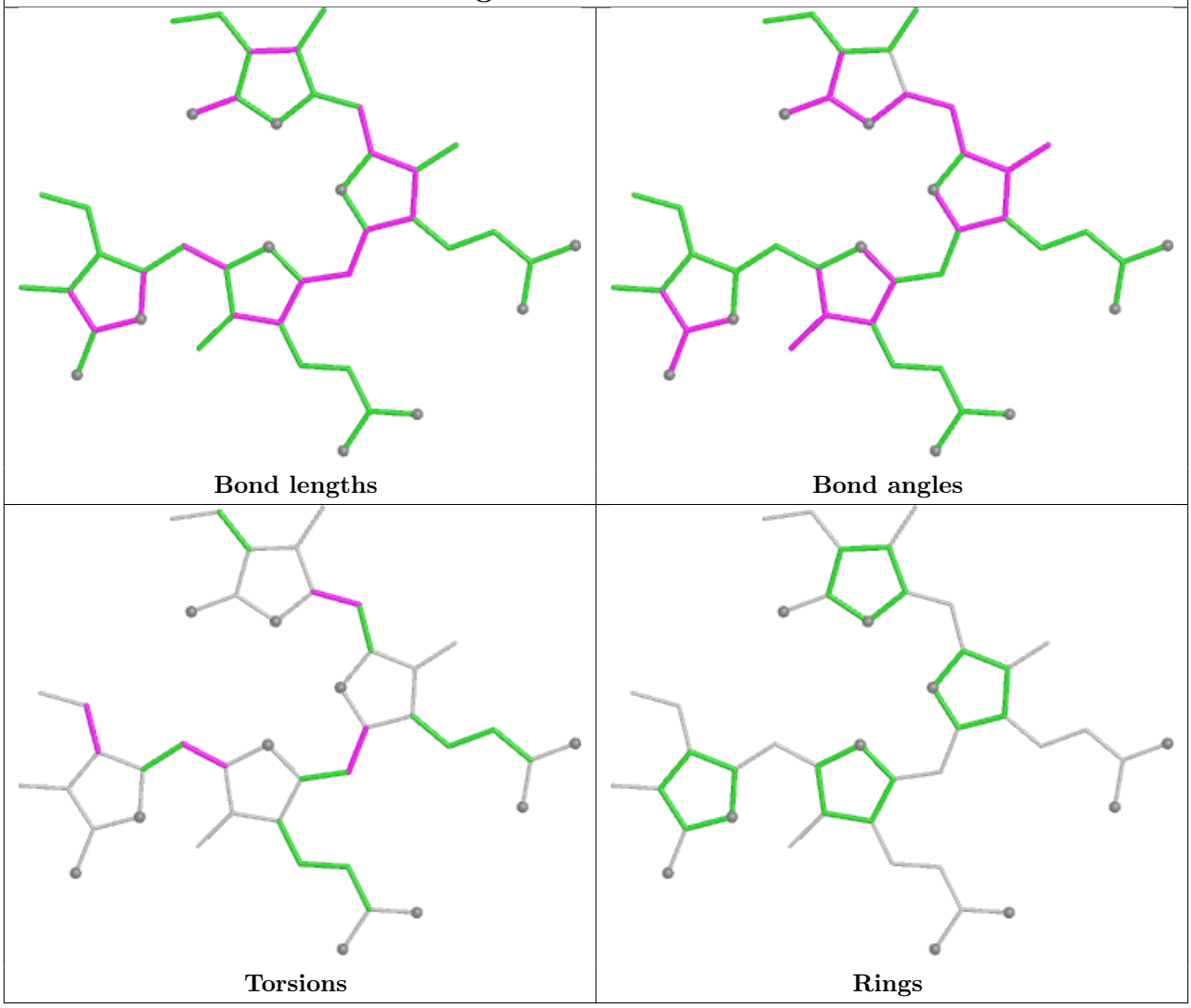


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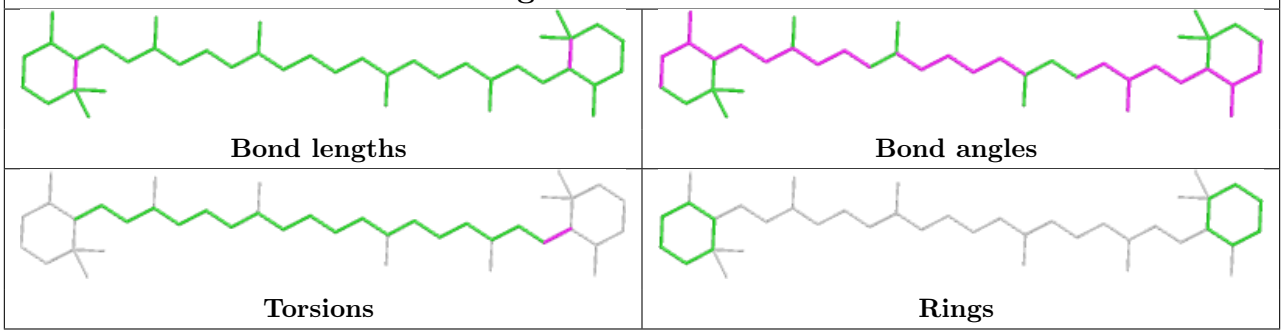


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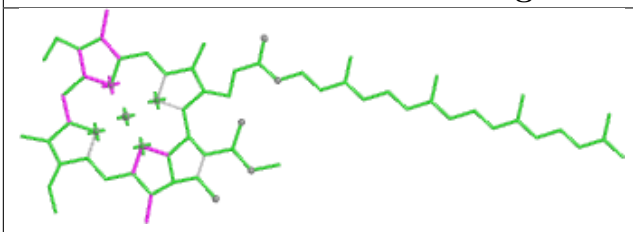
Ligand PEB wC 204



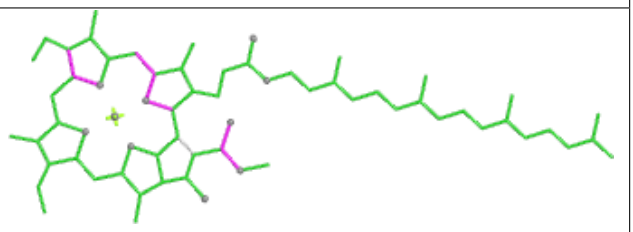
Ligand BCR b6 601



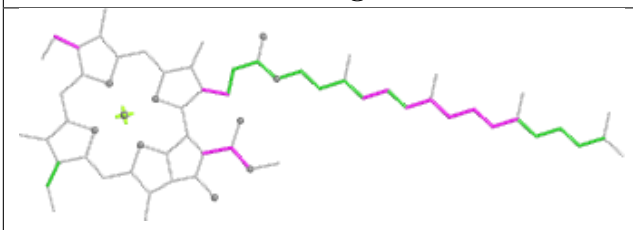
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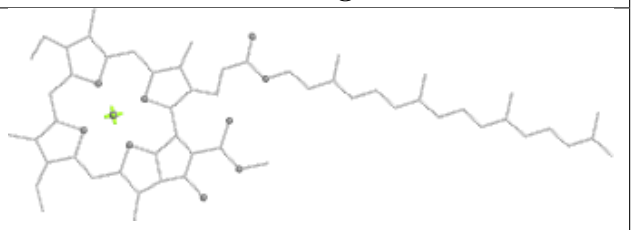
Bond lengths



Bond angles

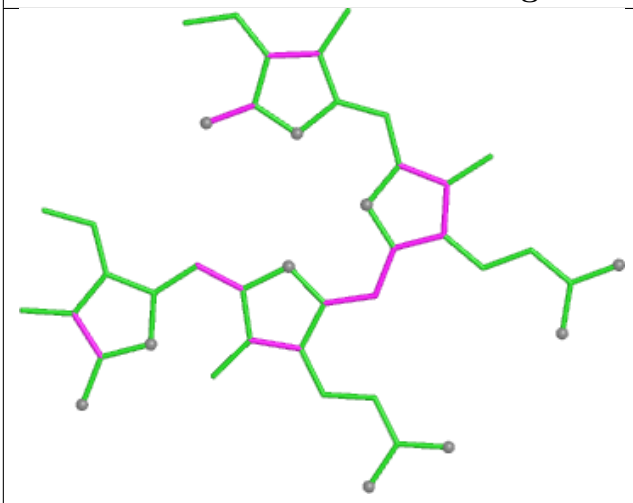


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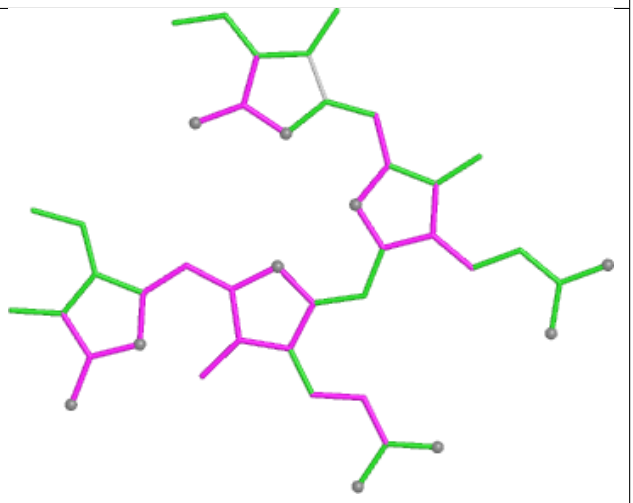


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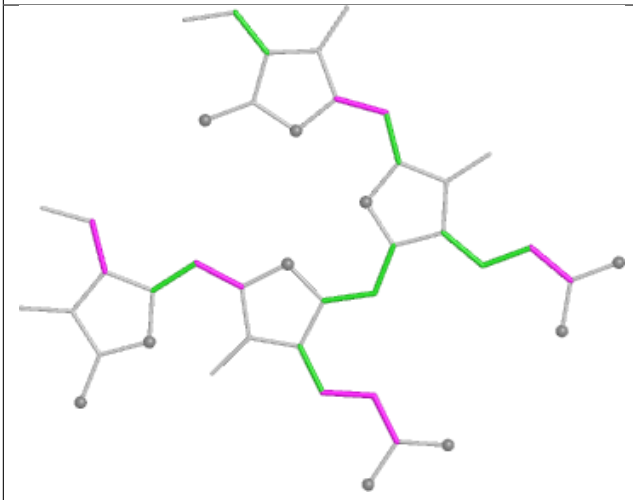
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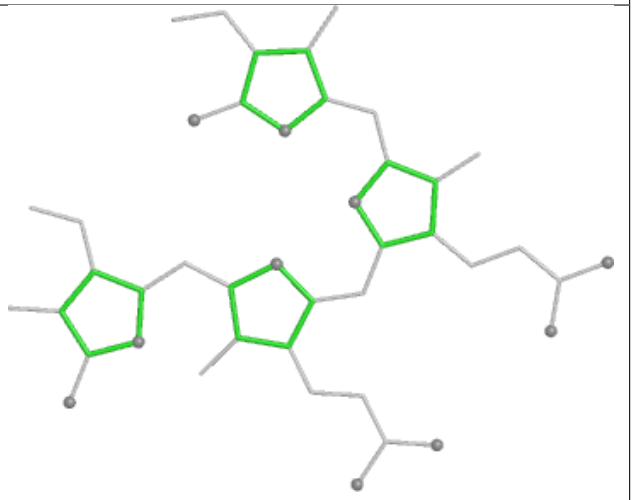
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Bond angles

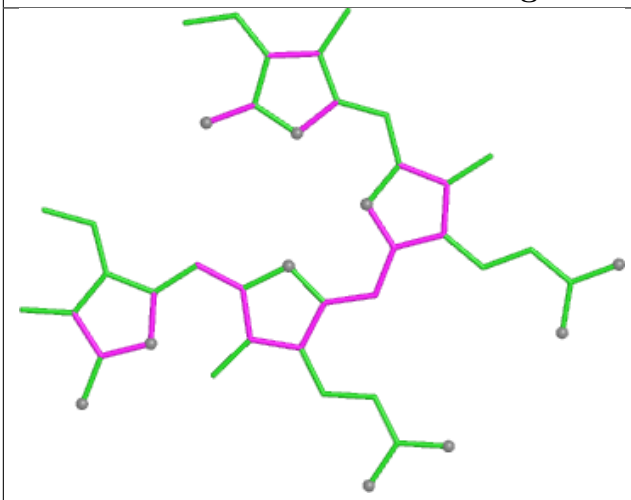


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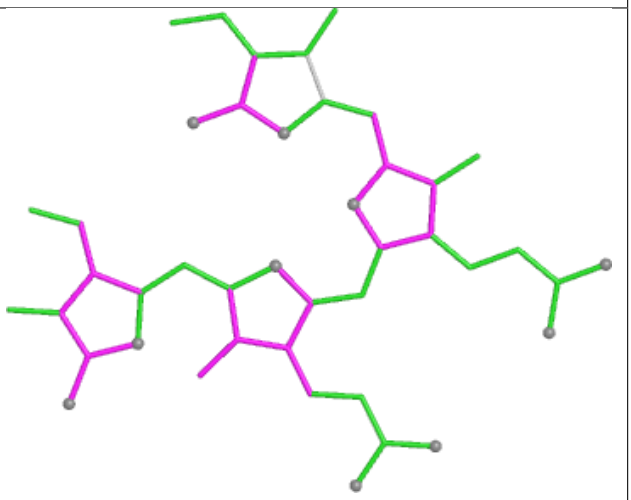


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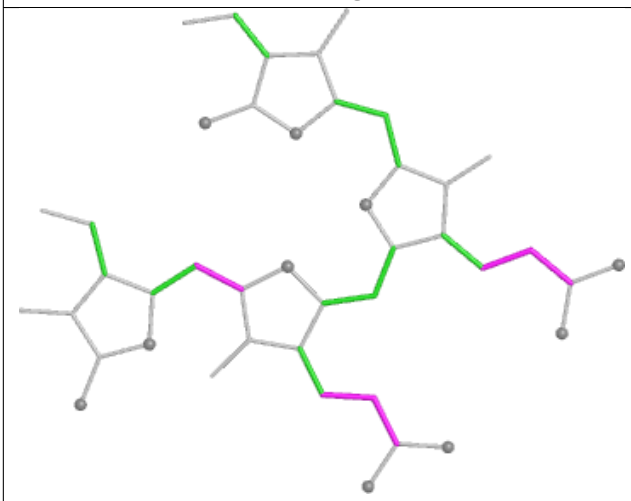
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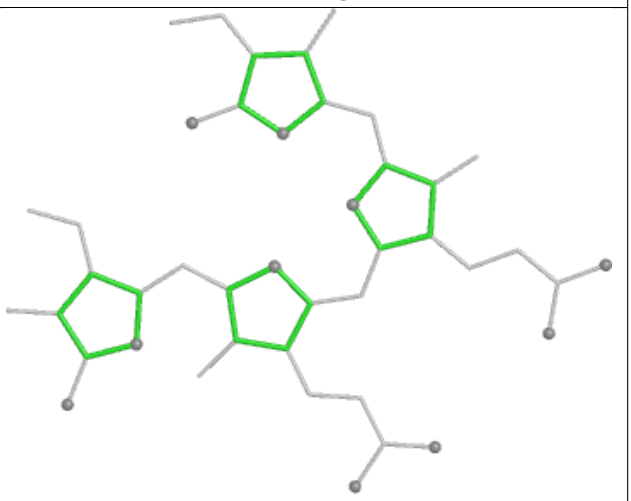
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Bond angles

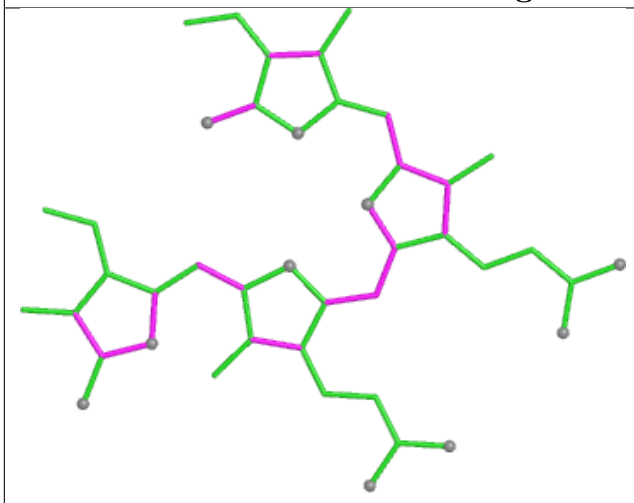


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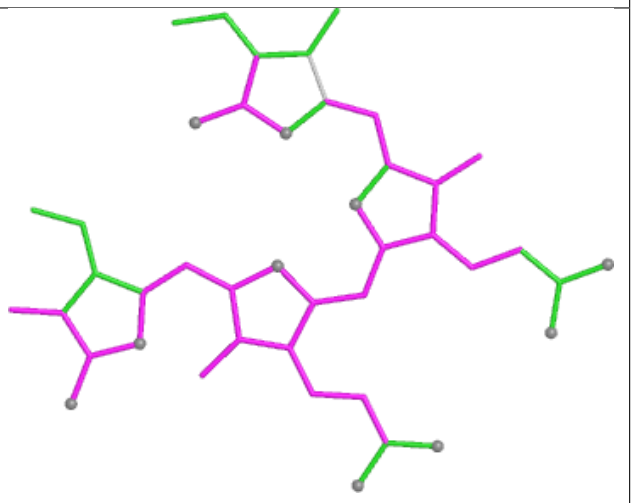


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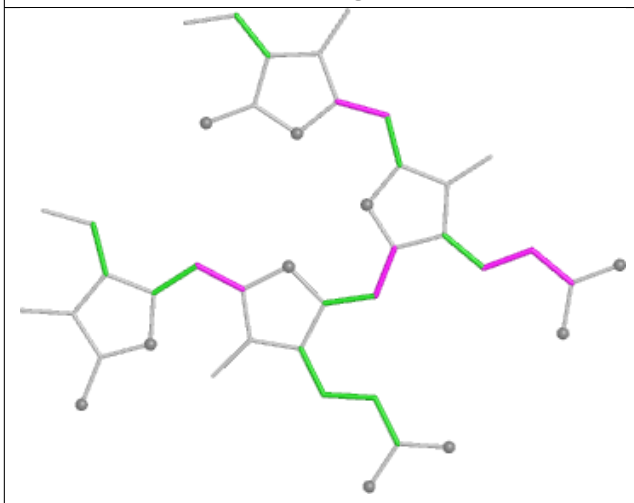
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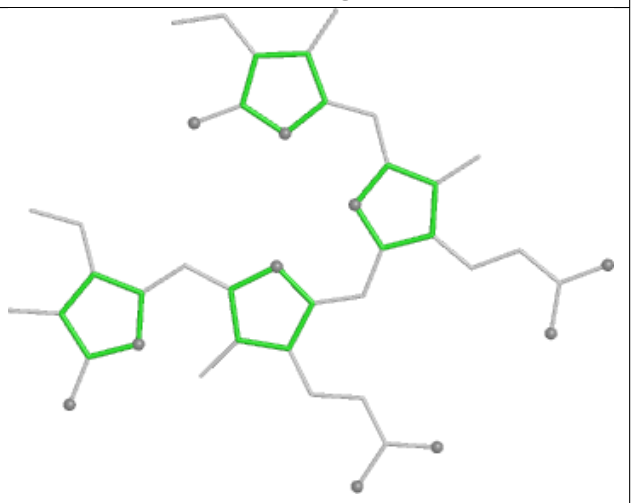
Bond lengths



Bond angles

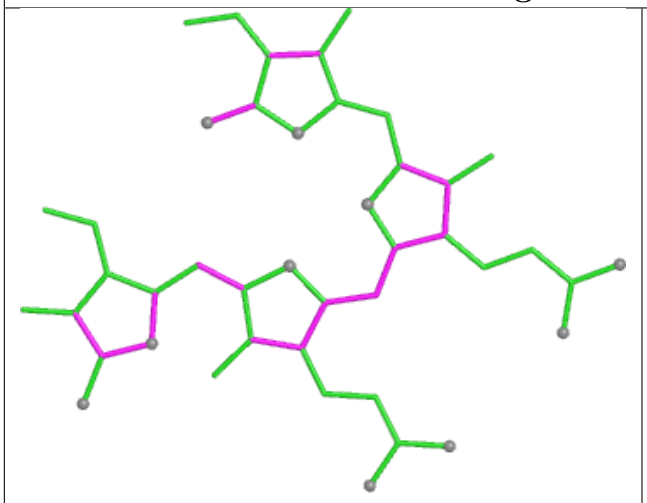


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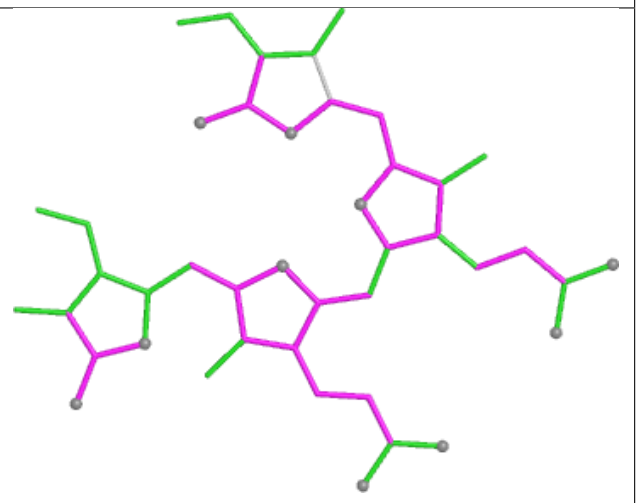


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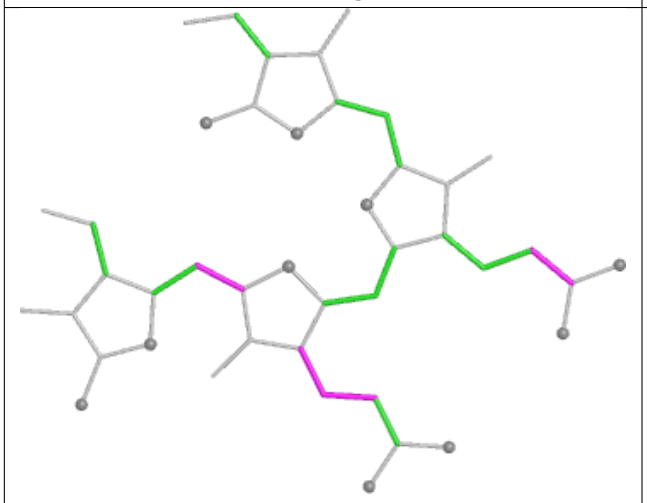
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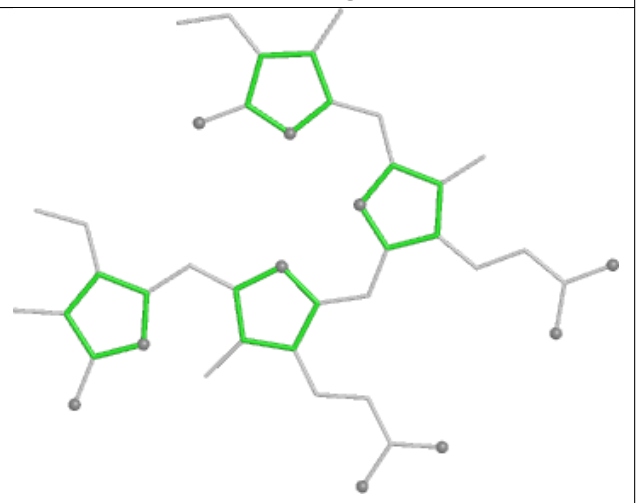
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Bond angles

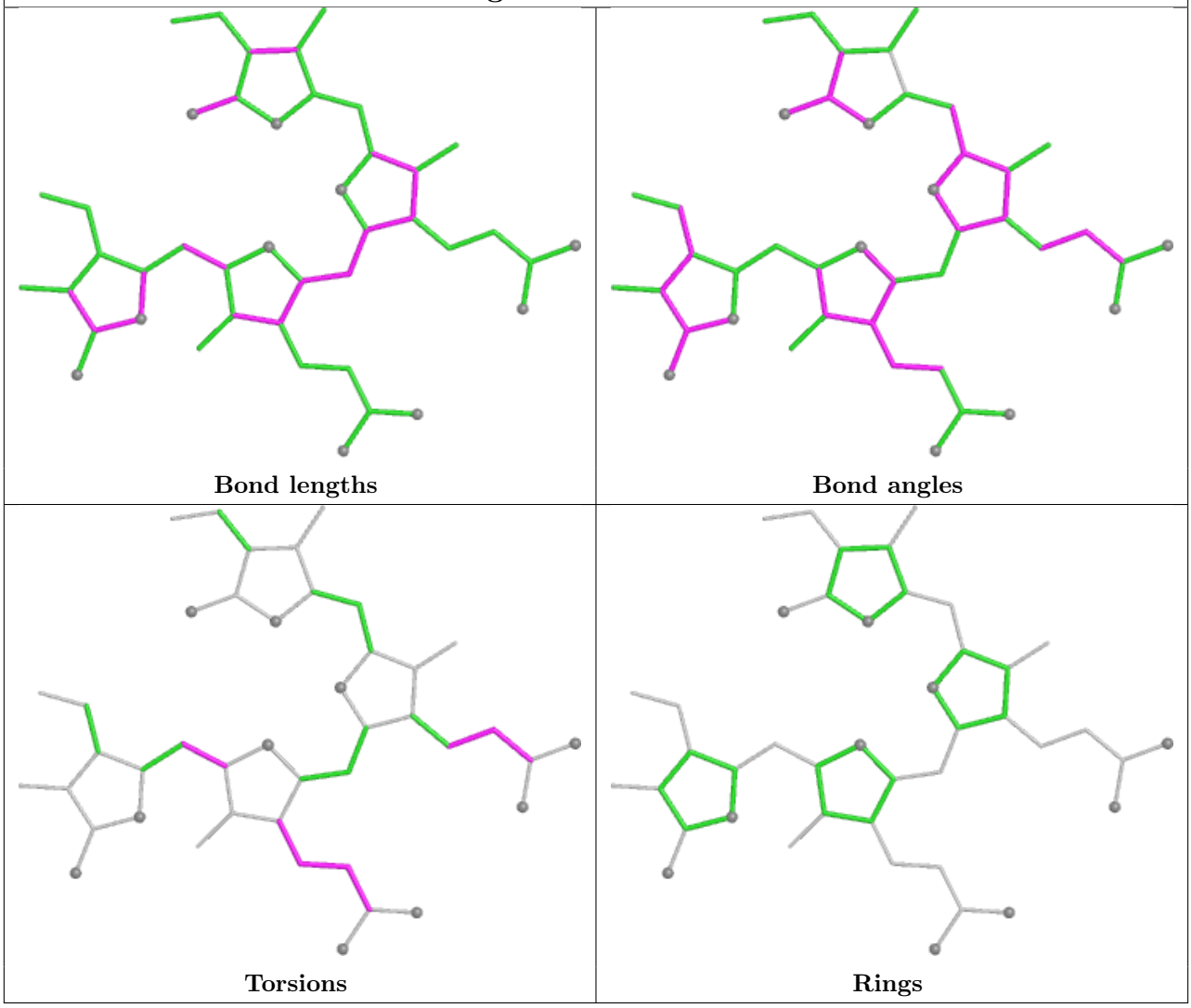


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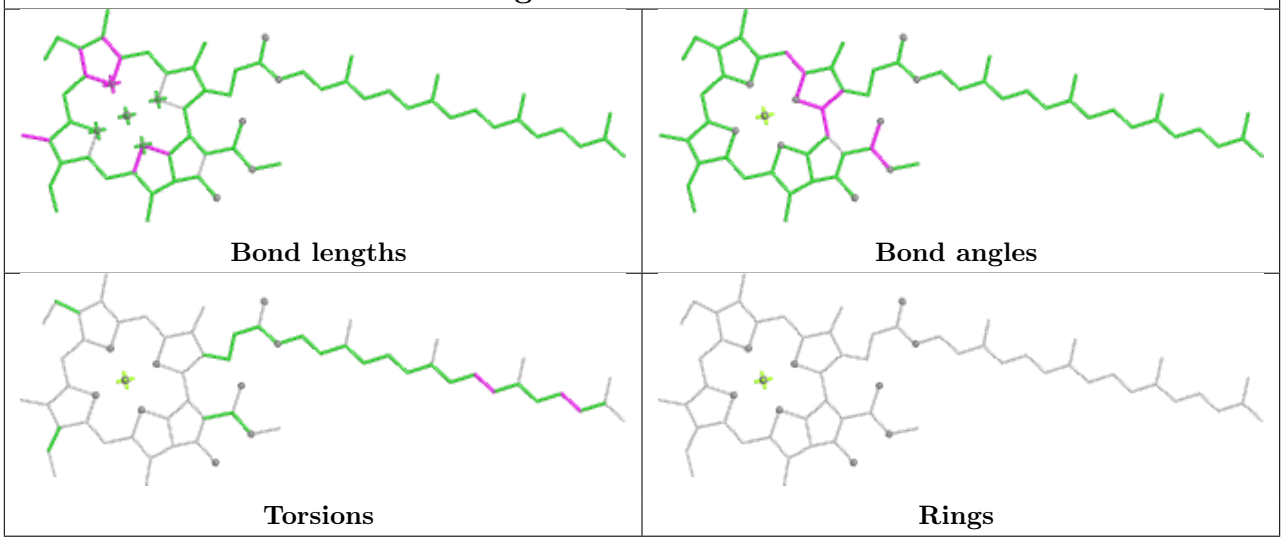


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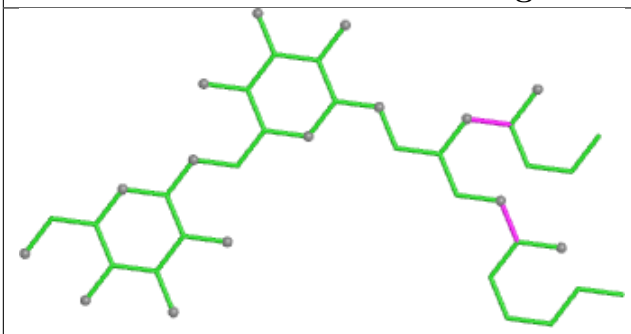
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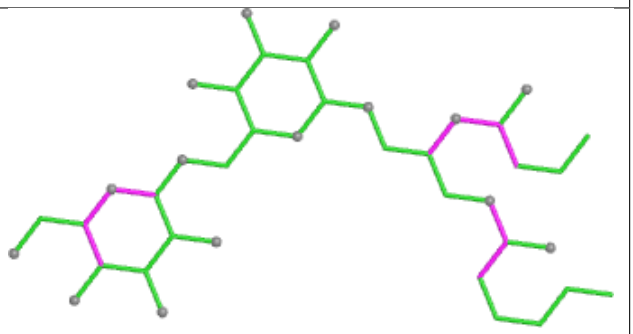
Ligand CLA BL 606



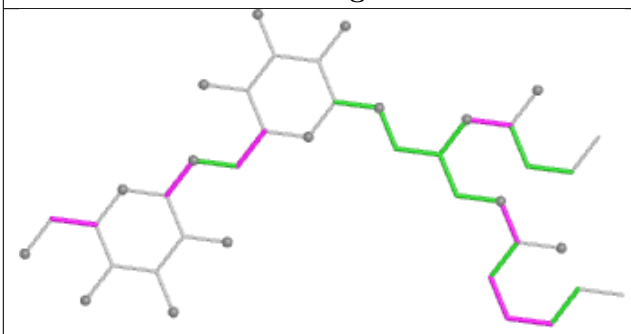
Ligand DGD a6 603



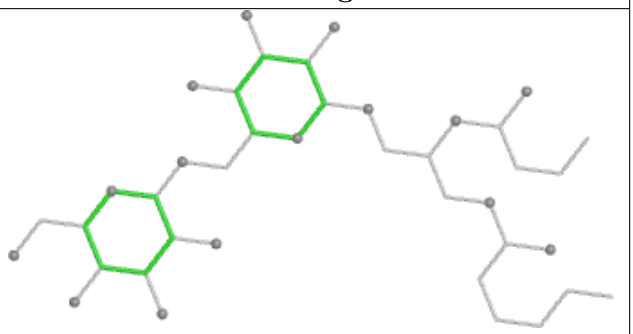
Bond lengths



Bond angles

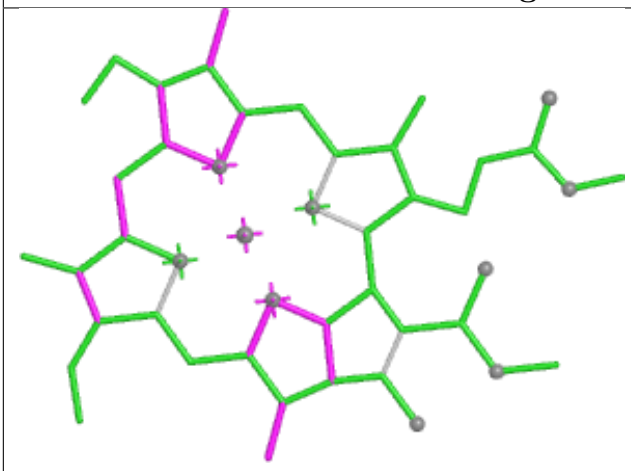


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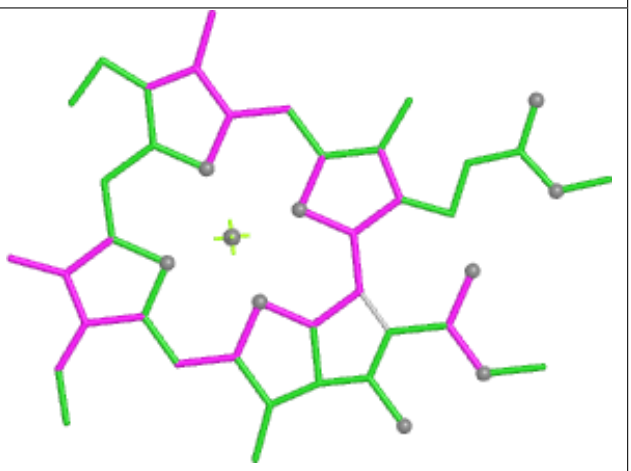


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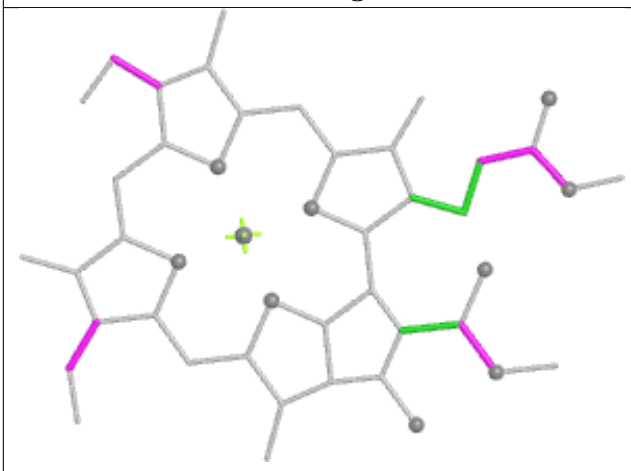
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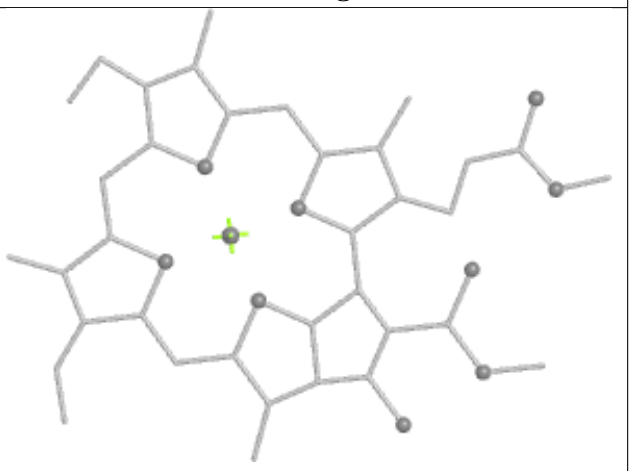
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Bond angles

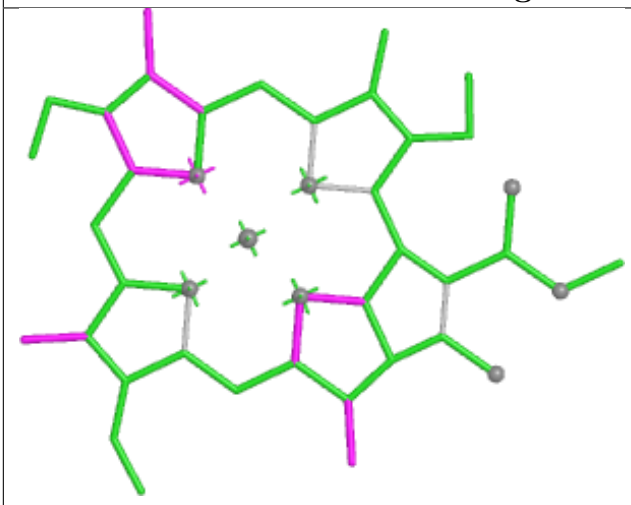


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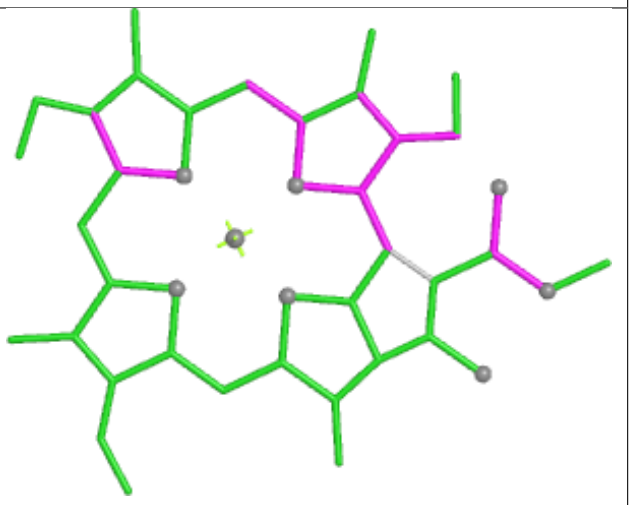


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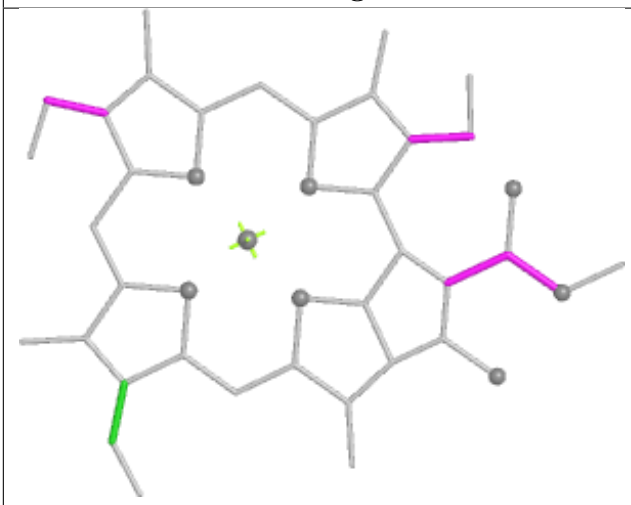
Ligand CLA 1N 609



Bond lengths



Bond angles

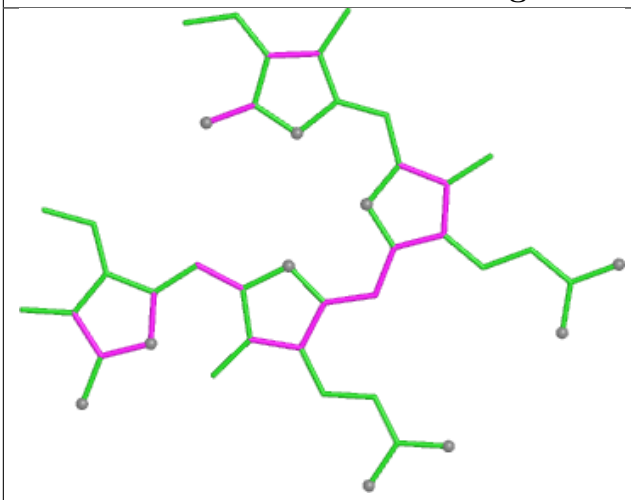


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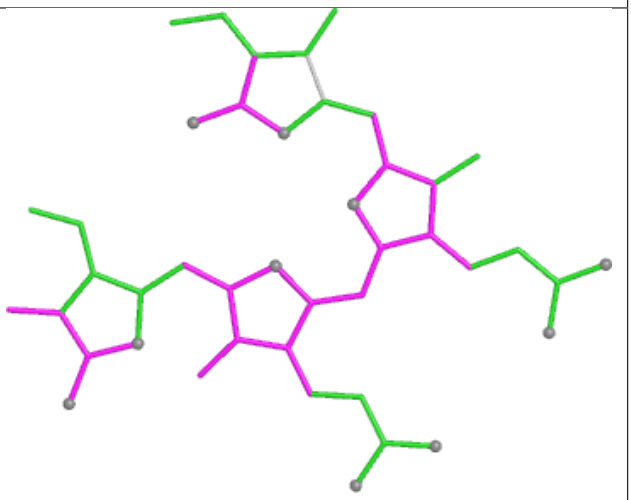


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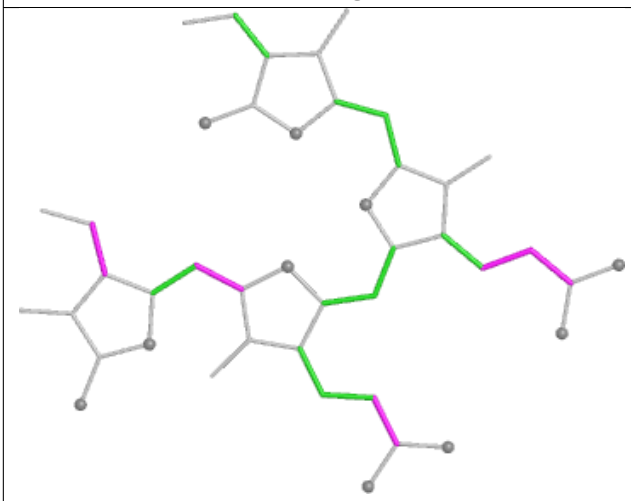
Ligand PEB mO 202



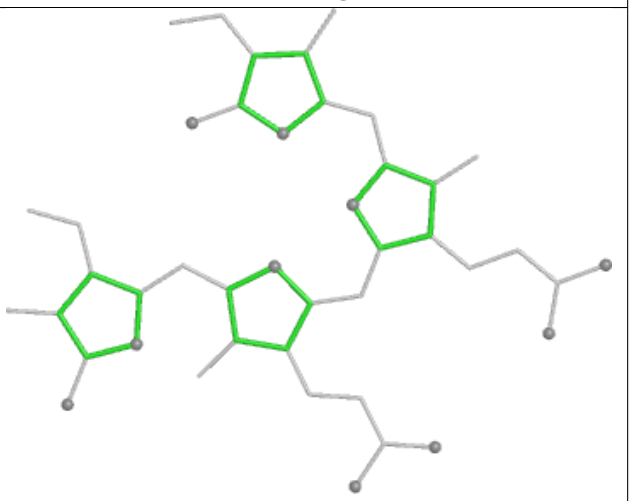
Bond lengths



Bond angles

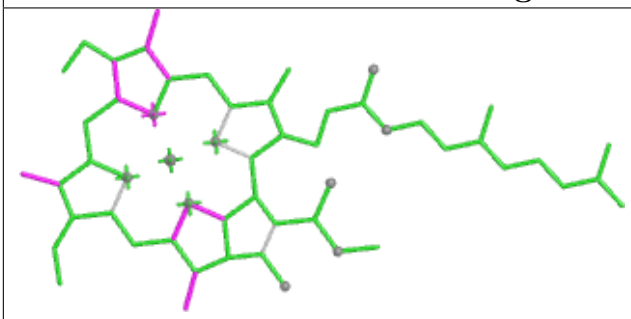


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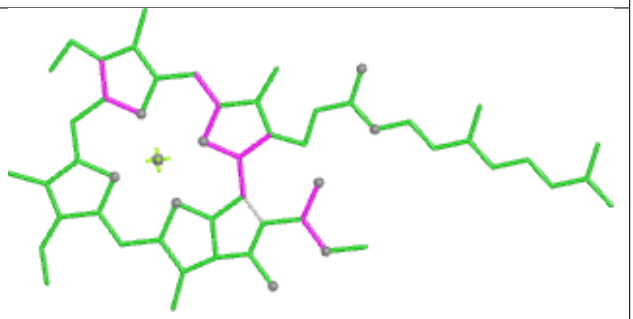


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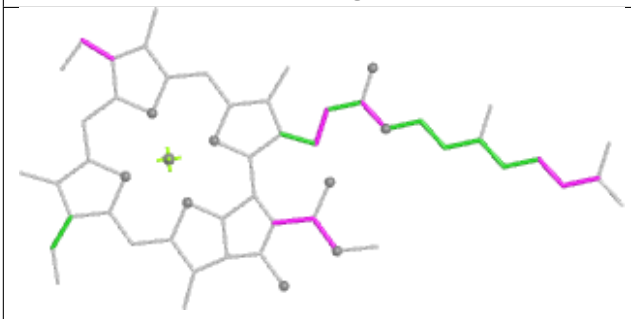
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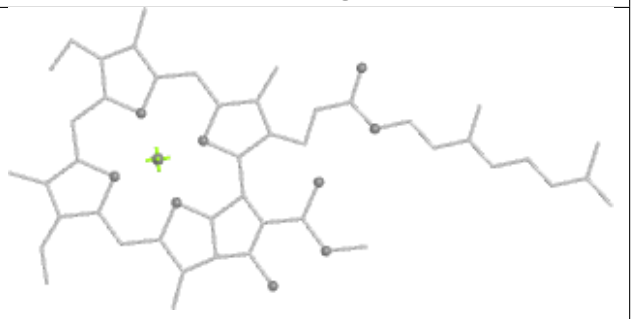
Bond lengths



Bond angles

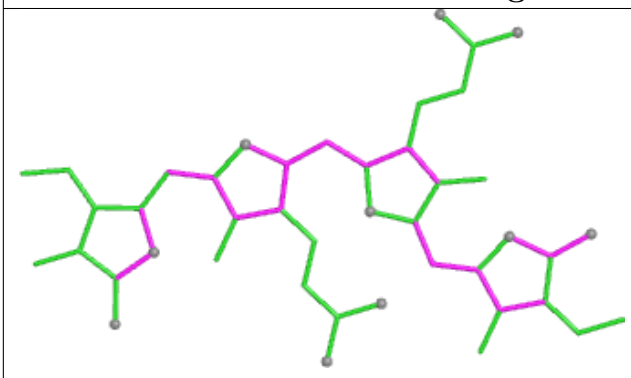


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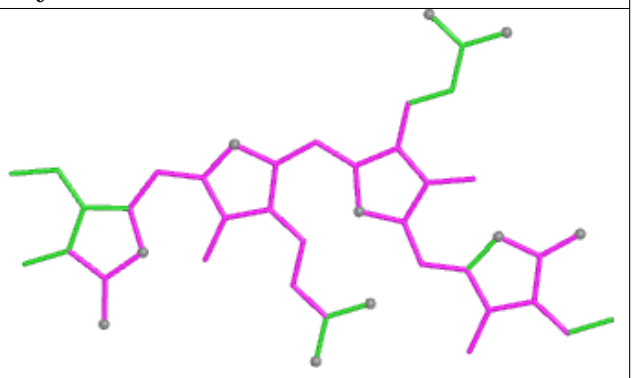


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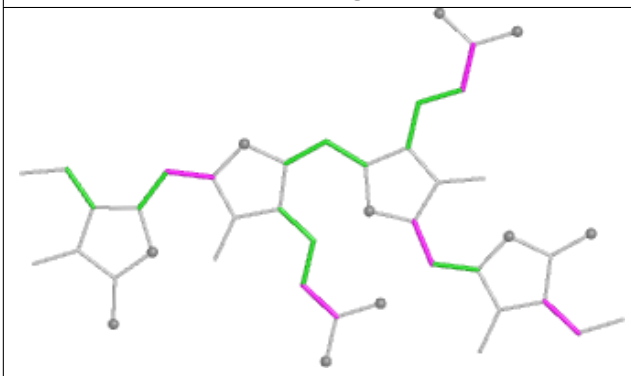
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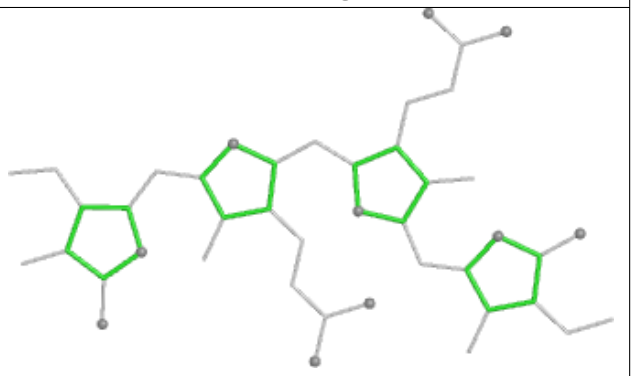
Bond lengths



Bond angles

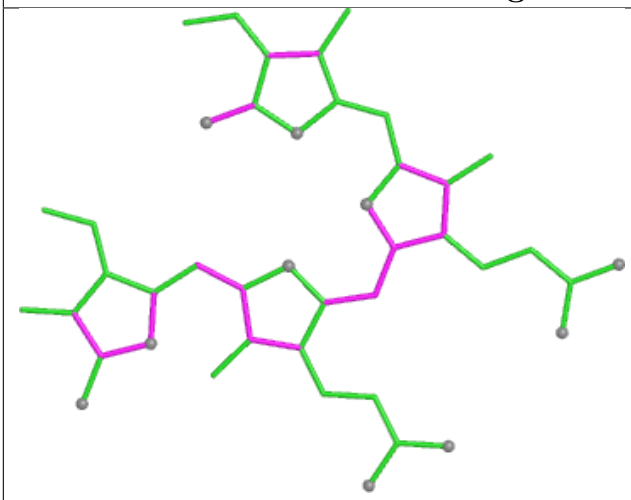


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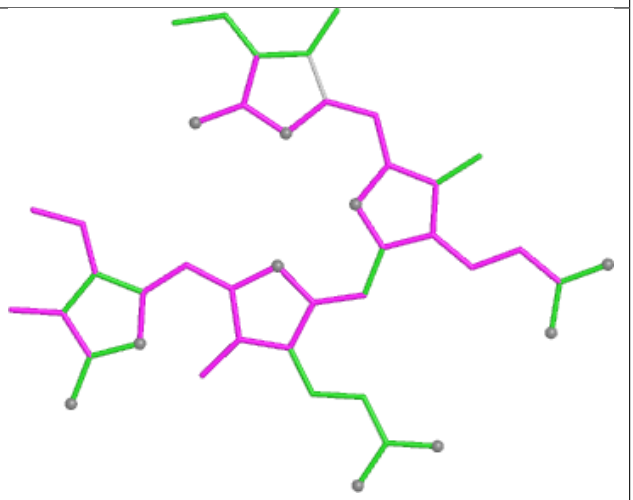


Rings

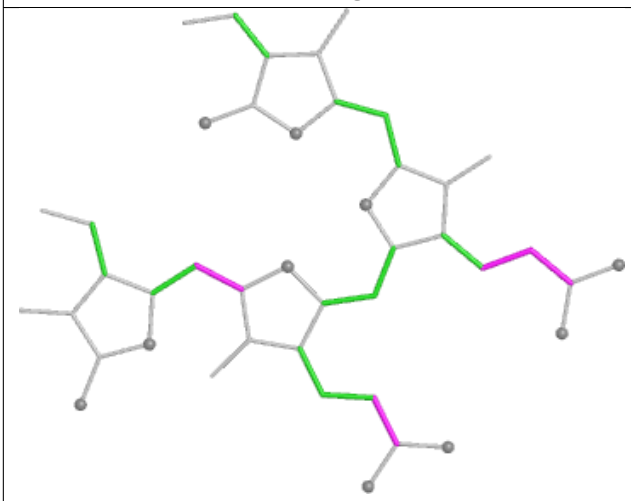
Ligand PEB WE 201



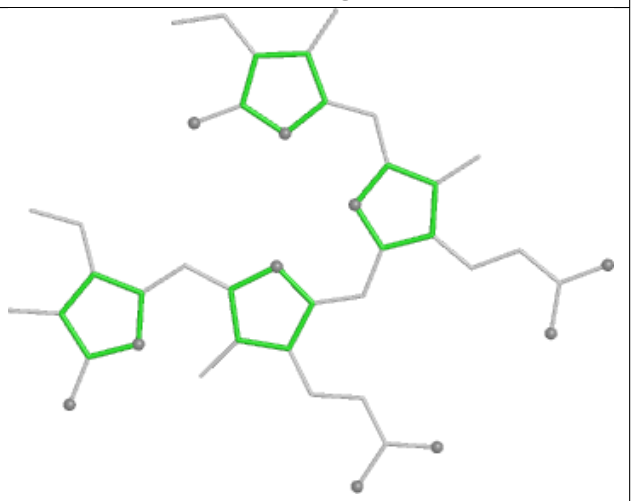
Bond lengths



Bond angles

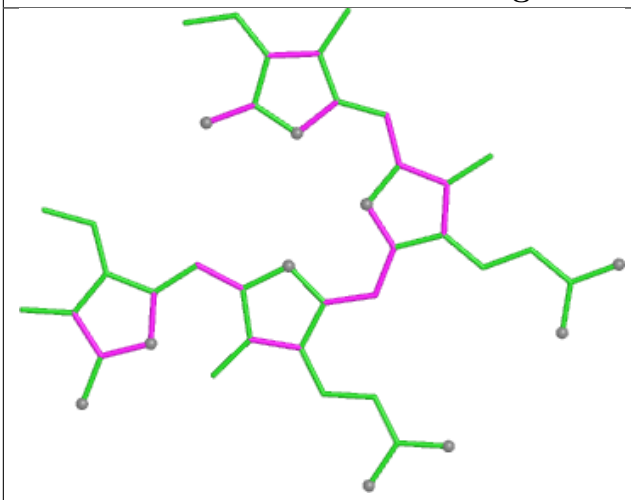


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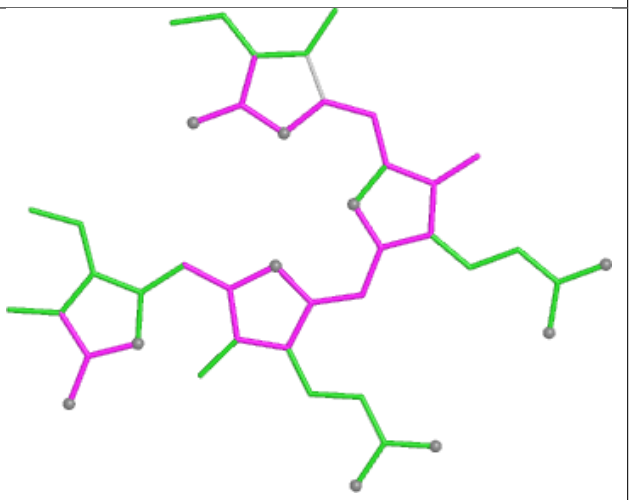


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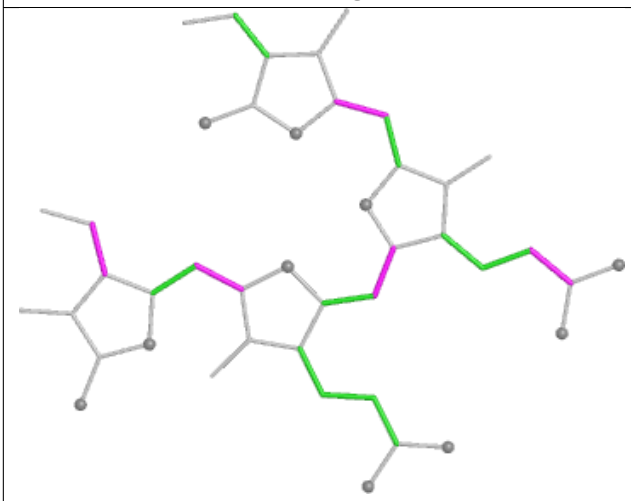
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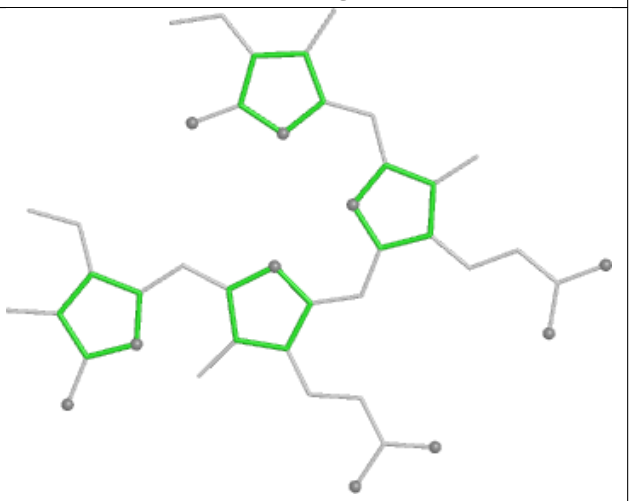
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Bond angles

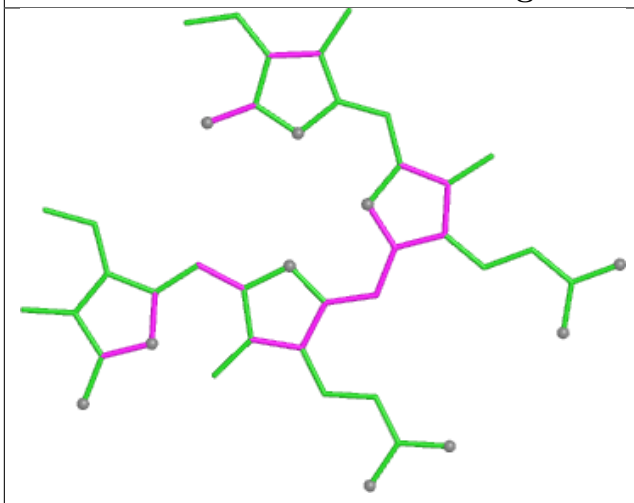


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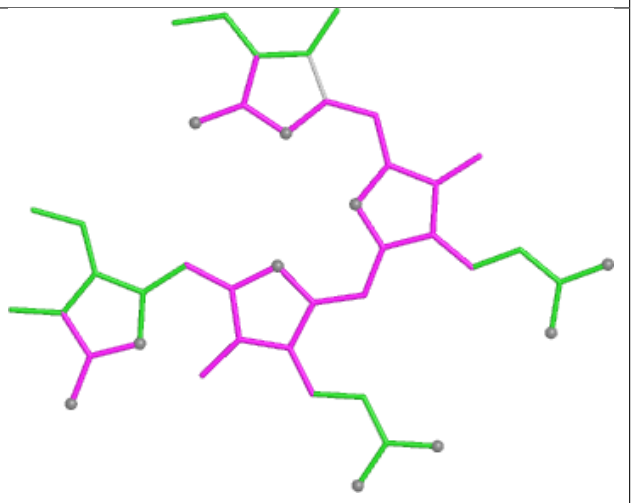


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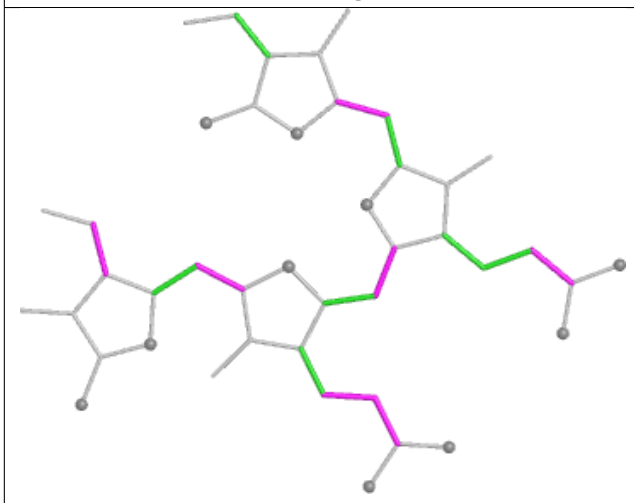
Ligand PEB Y7 303



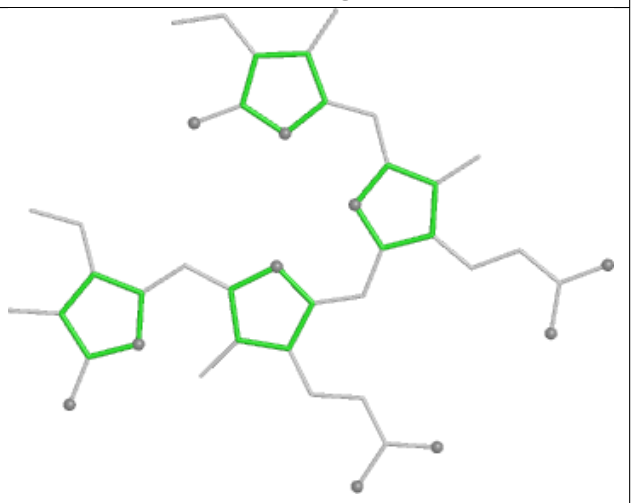
Bond lengths



Bond angles

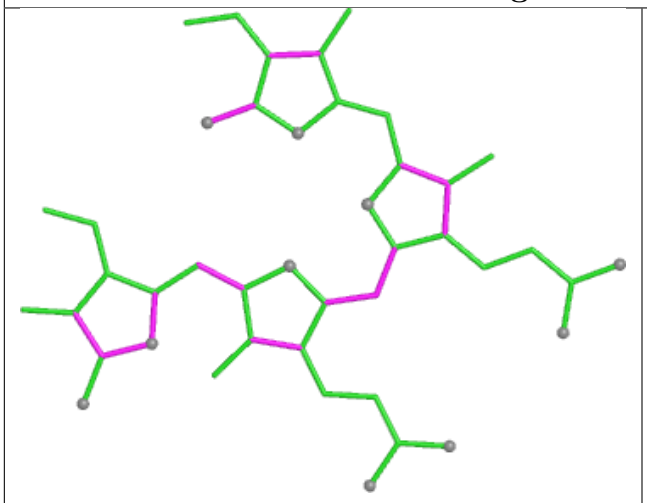


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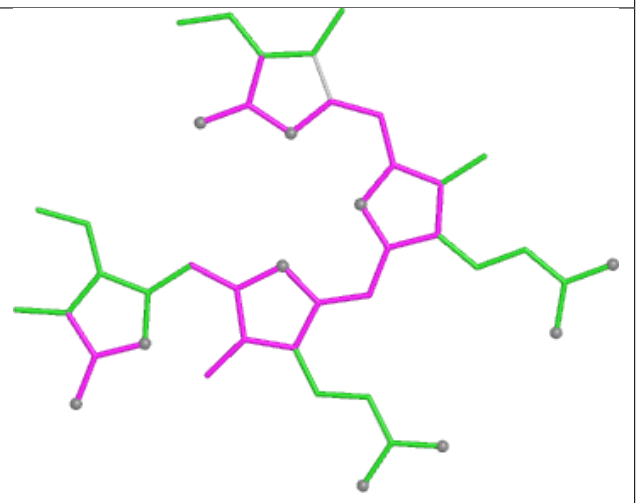


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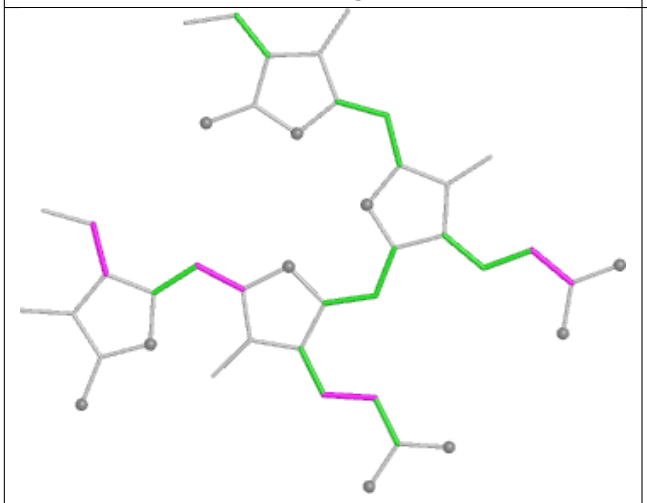
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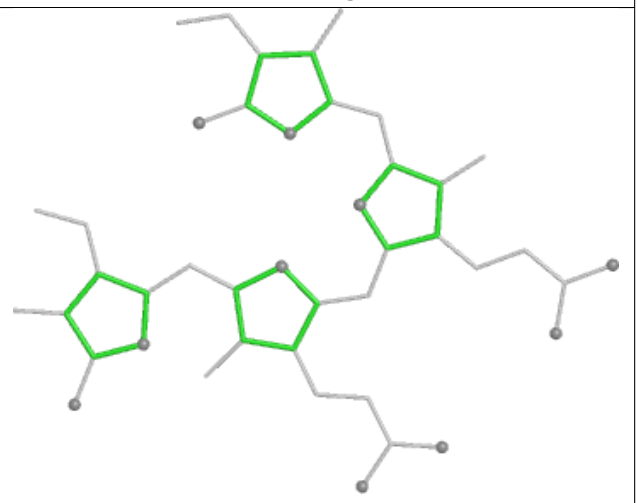
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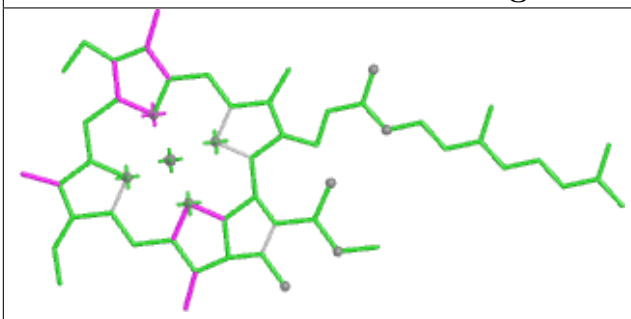
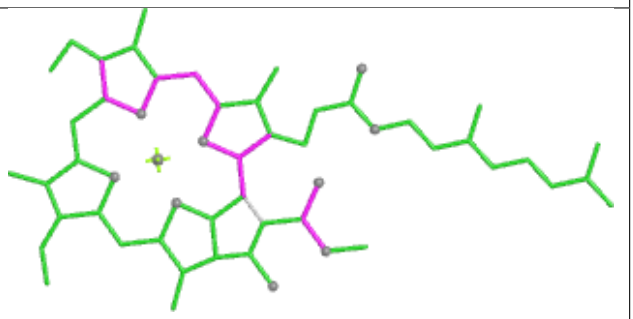
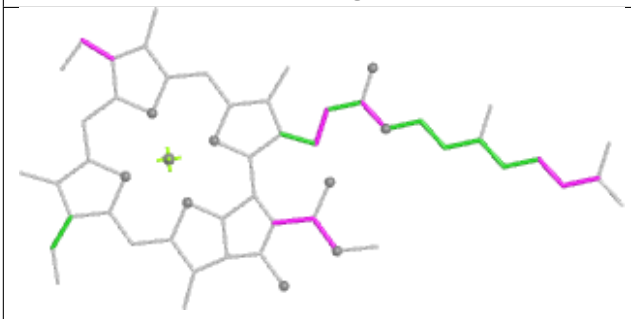
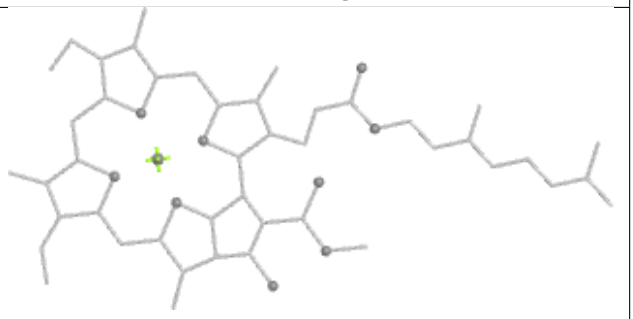
Bond angles



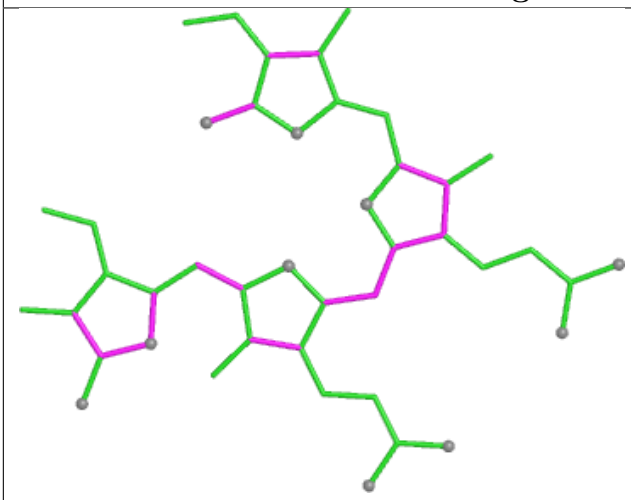
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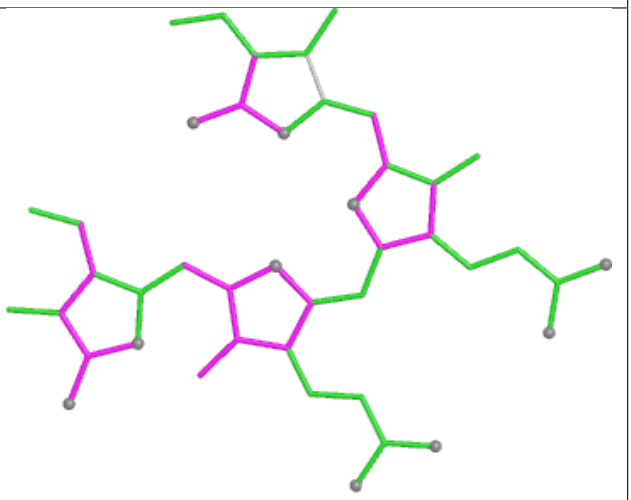
Rings

Ligand CLA AN 812	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

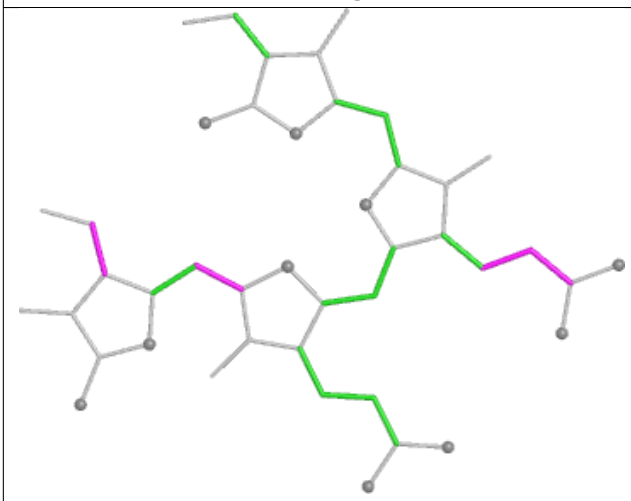
Ligand PEB aM 202



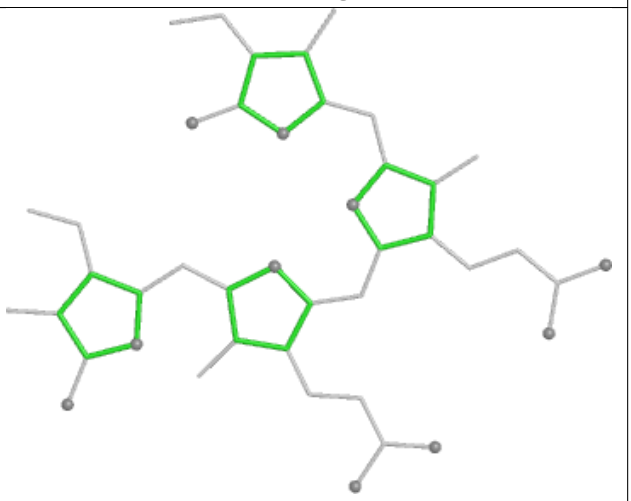
Bond lengths



Bond angles

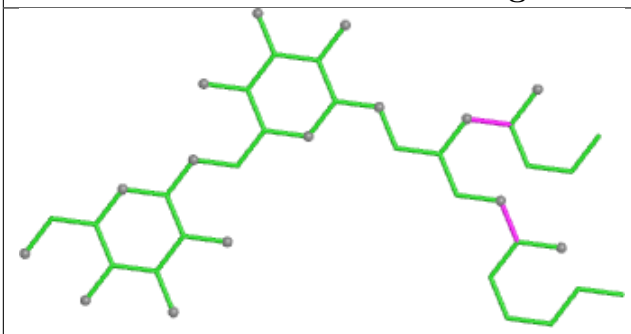


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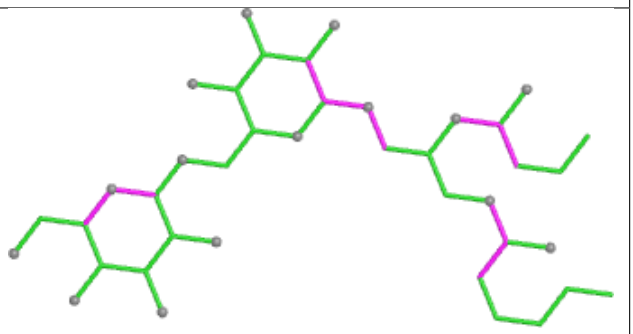


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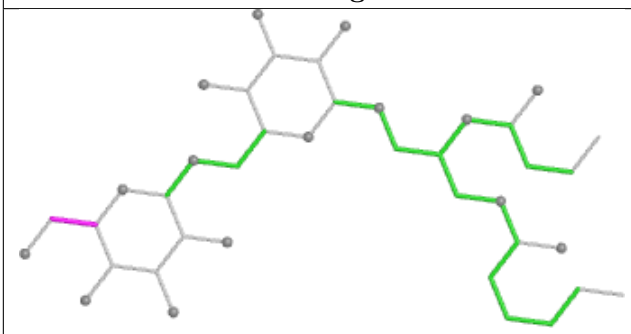
Ligand DGD AL 415



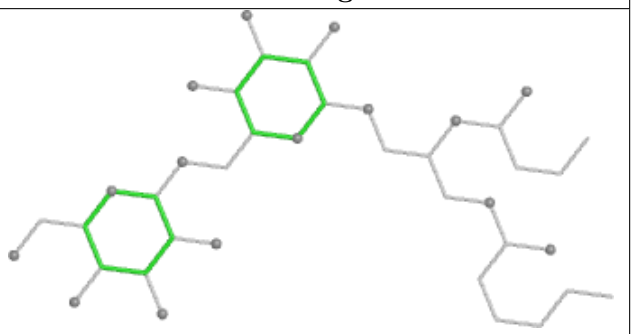
Bond lengths



Bond angles

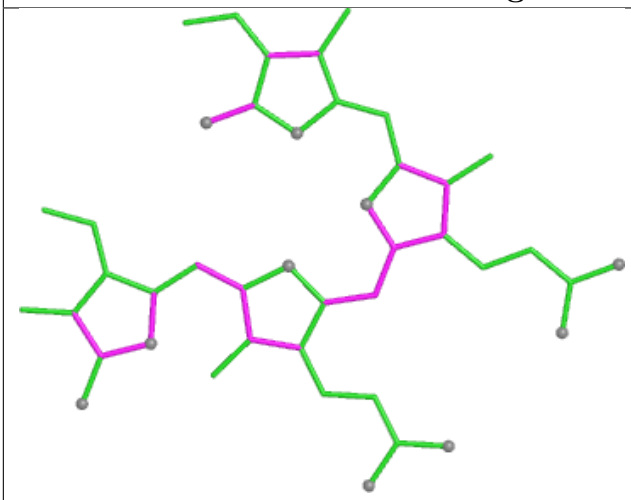


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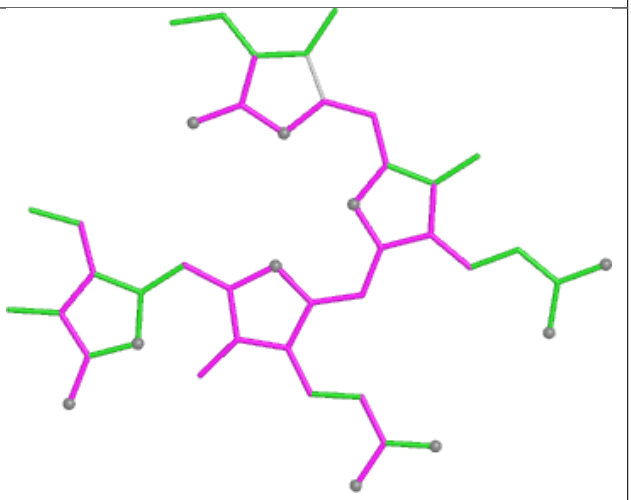


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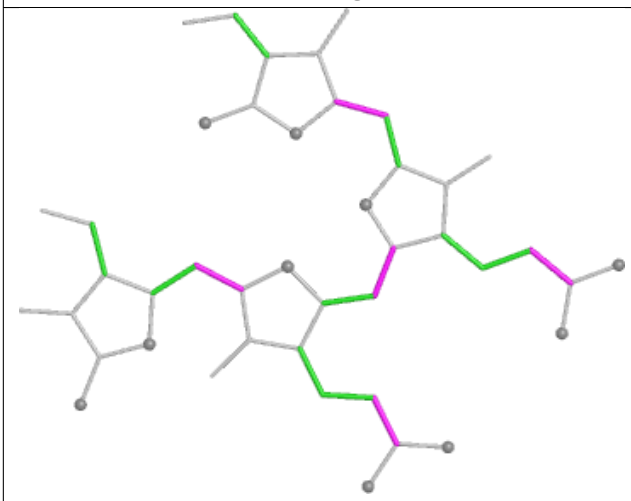
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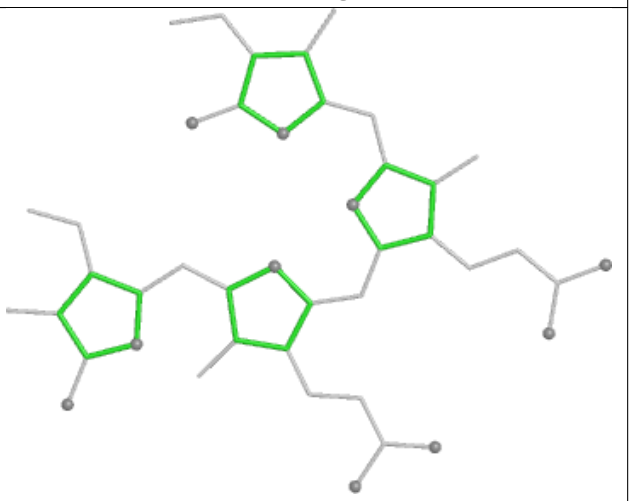
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Bond angles

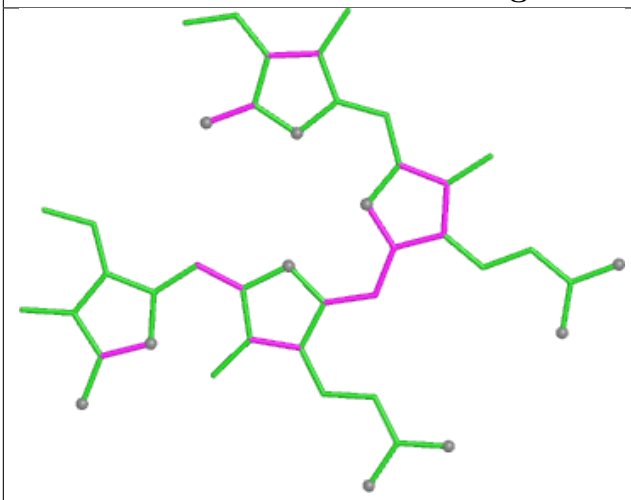


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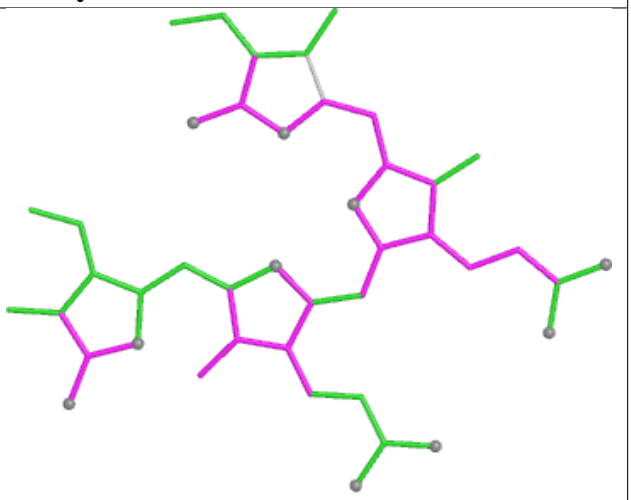


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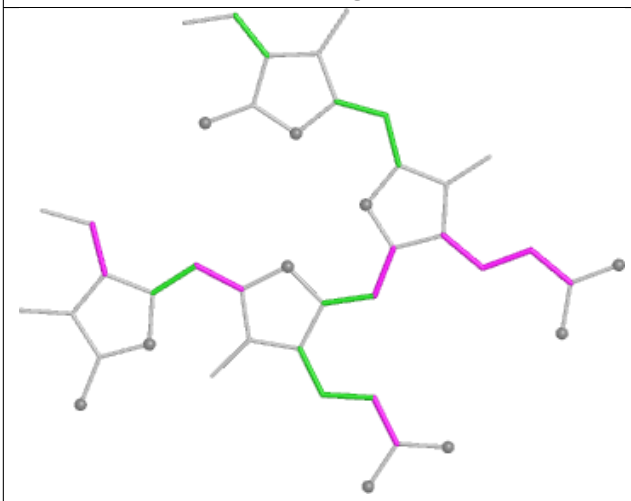
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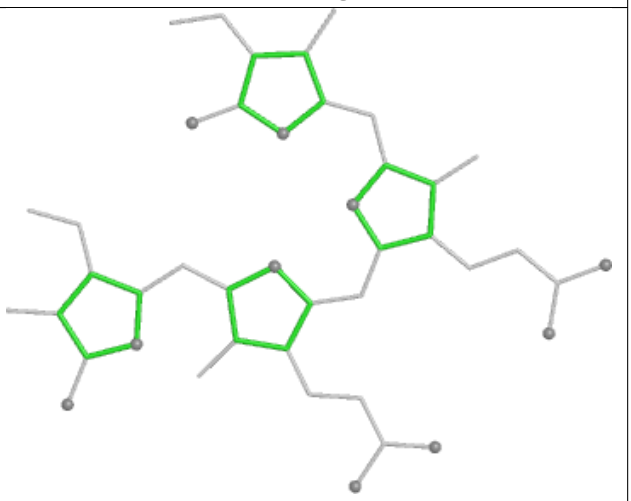
Bond lengths



Bond angles

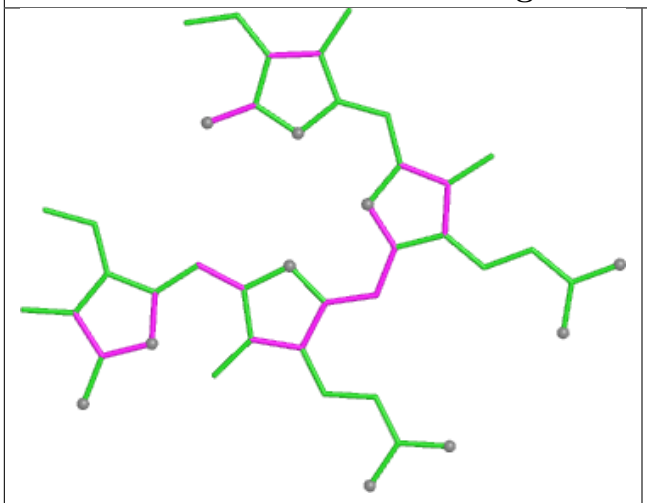


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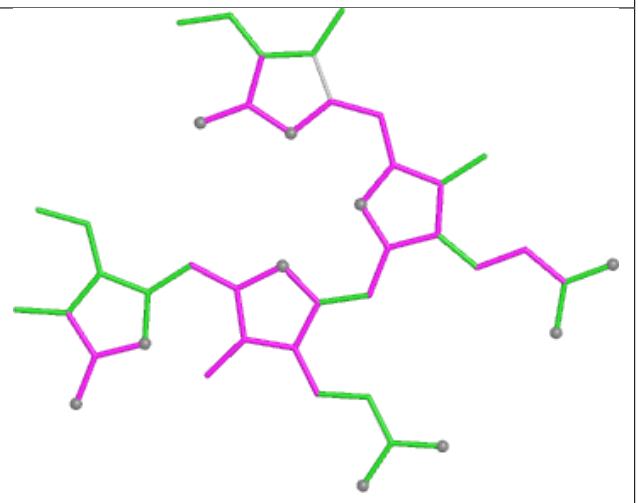


Rings

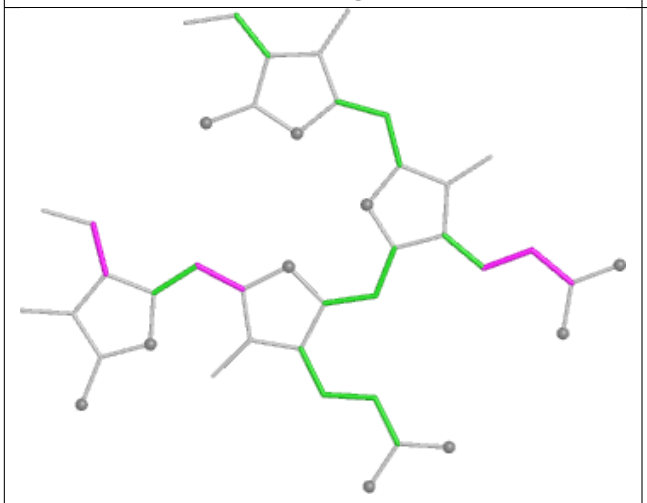
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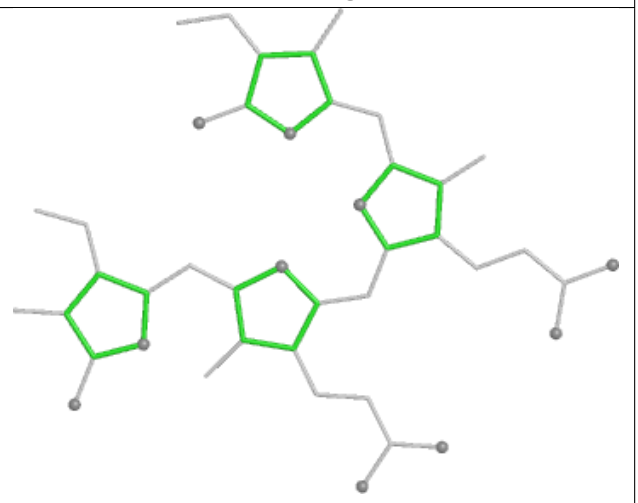
Bond lengths



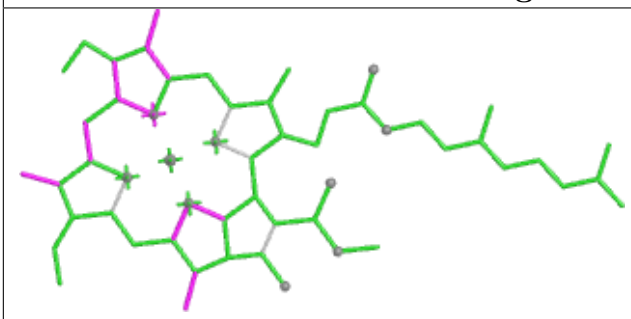
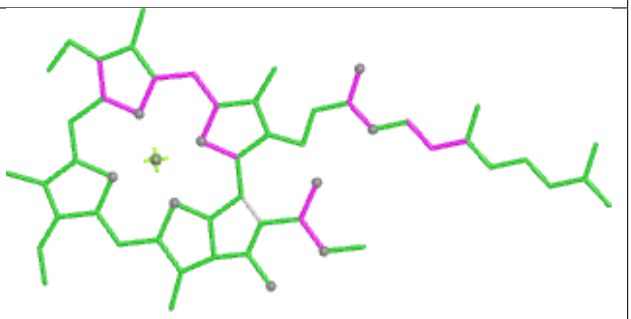
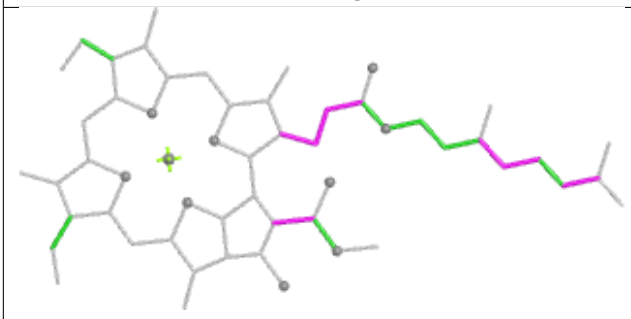
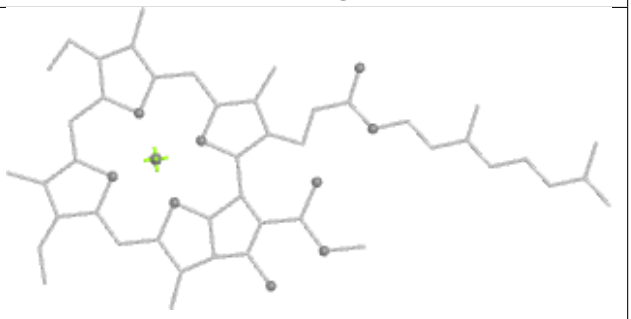
Bond angles



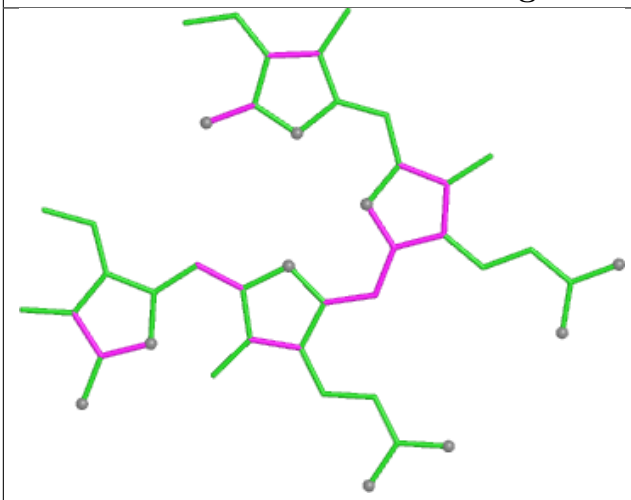
Torsions



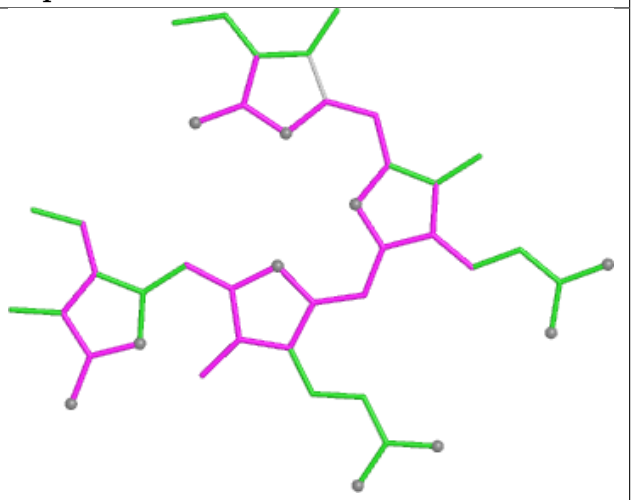
Rings

Ligand CLA C6 519	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

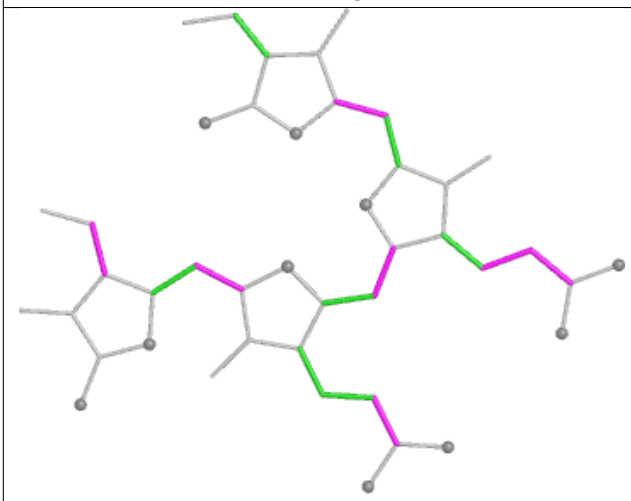
Ligand PEB p8 201



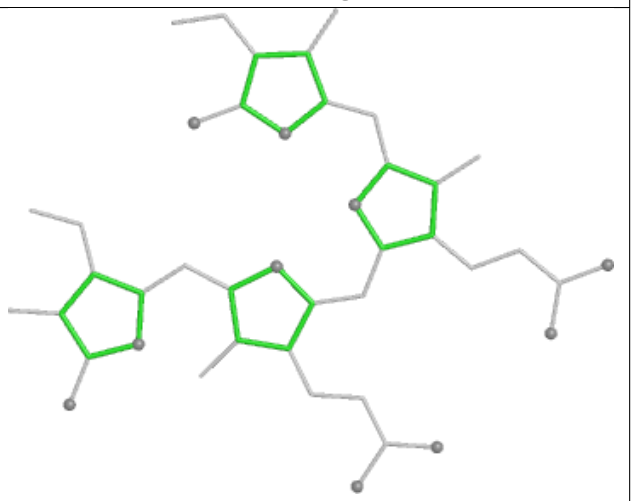
Bond lengths



Bond angles

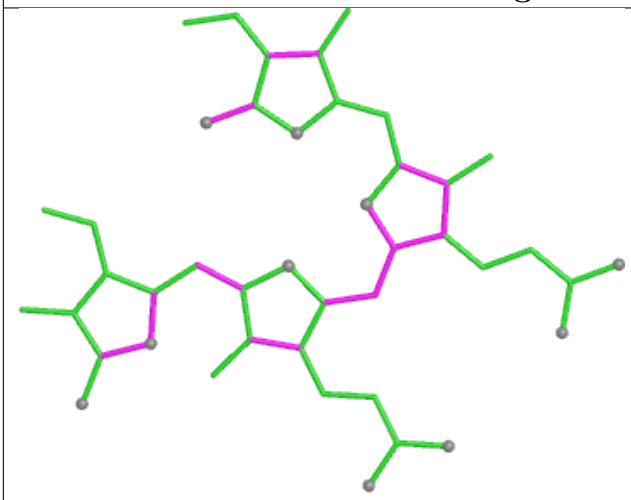


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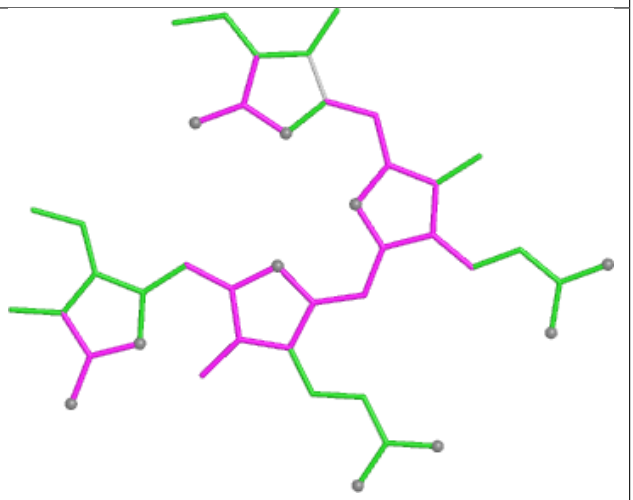


Rings

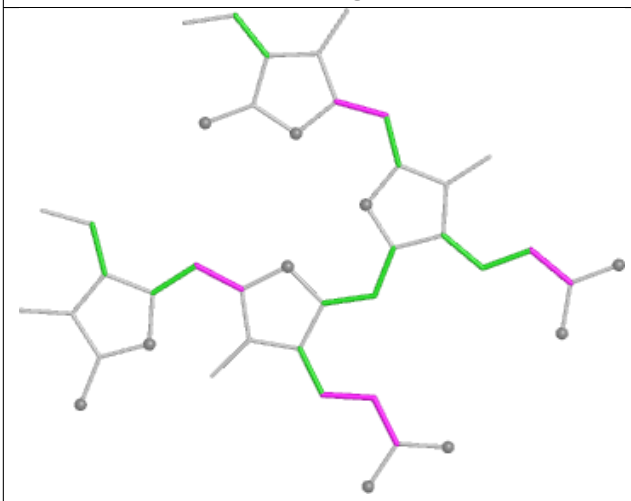
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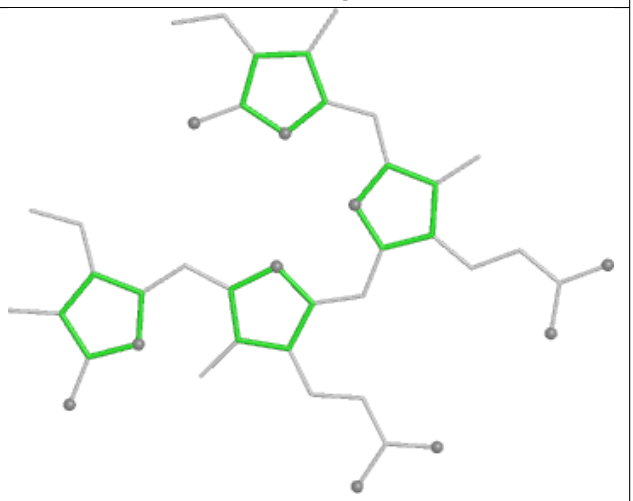
Bond lengths



Bond angles

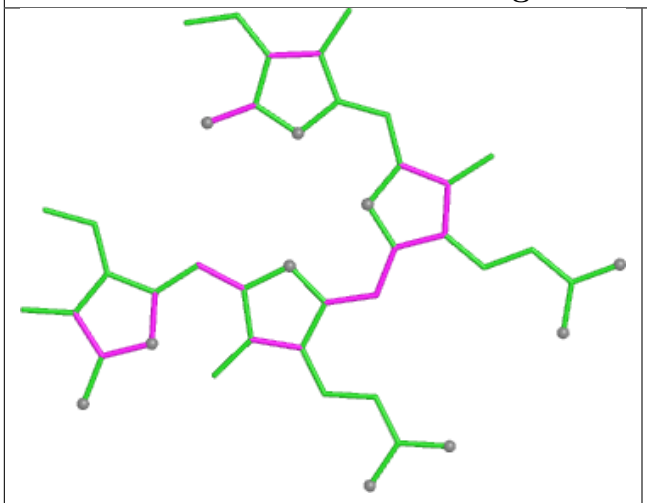


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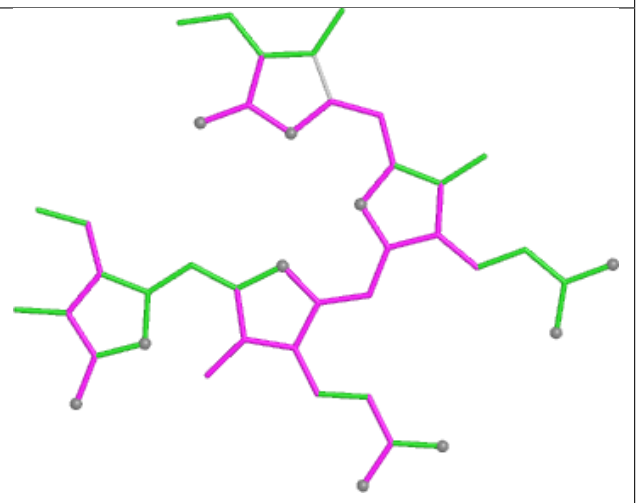


Rings

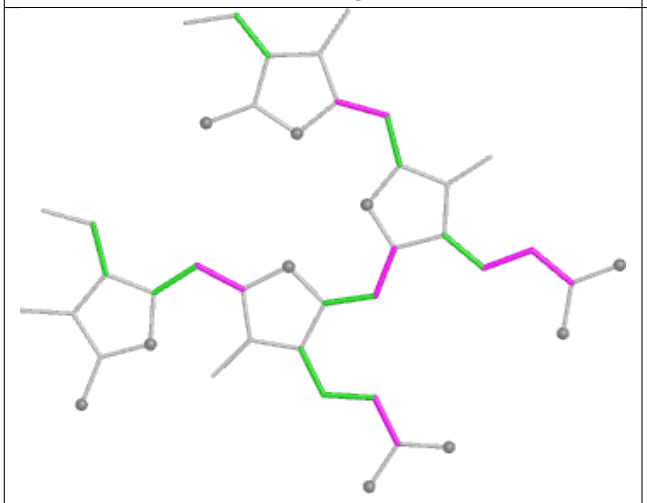
Ligand PEB JM 202



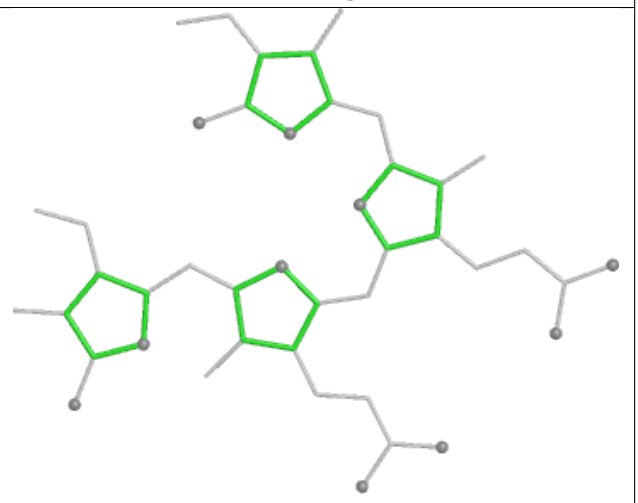
Bond lengths



Bond angles

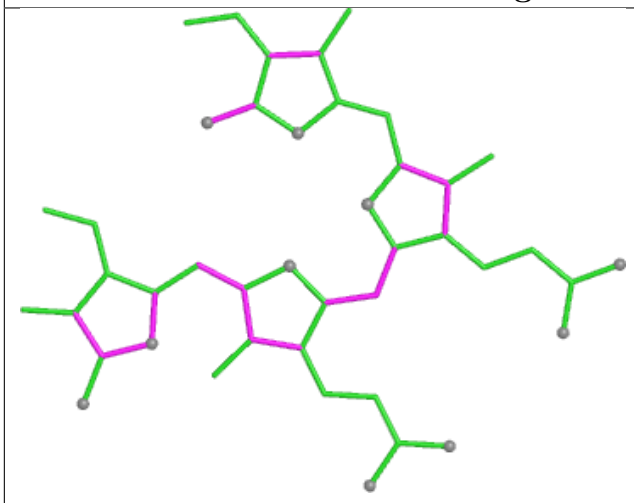


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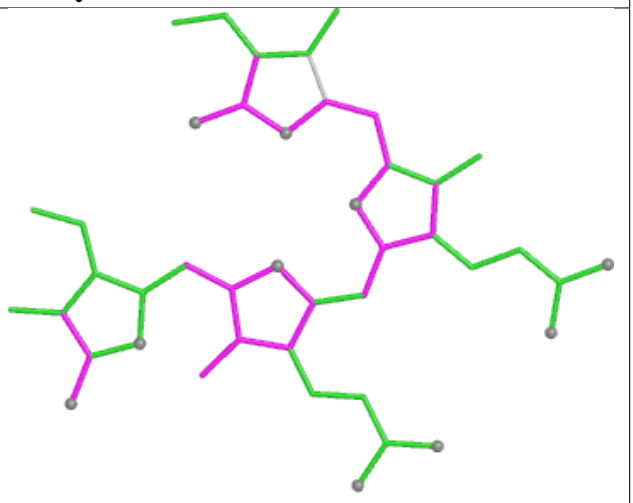


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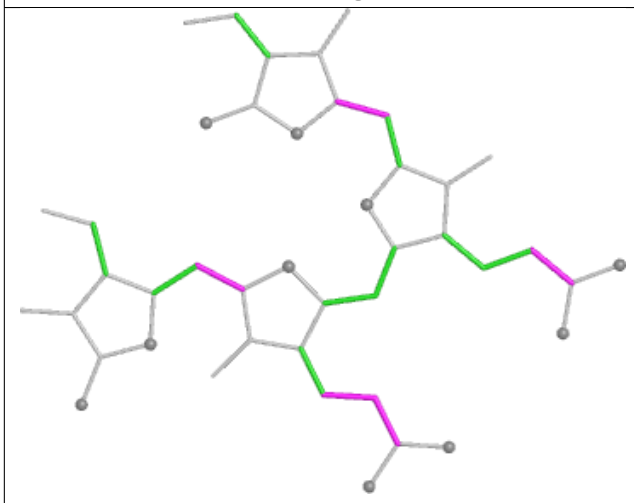
Ligand PEB LQ 202



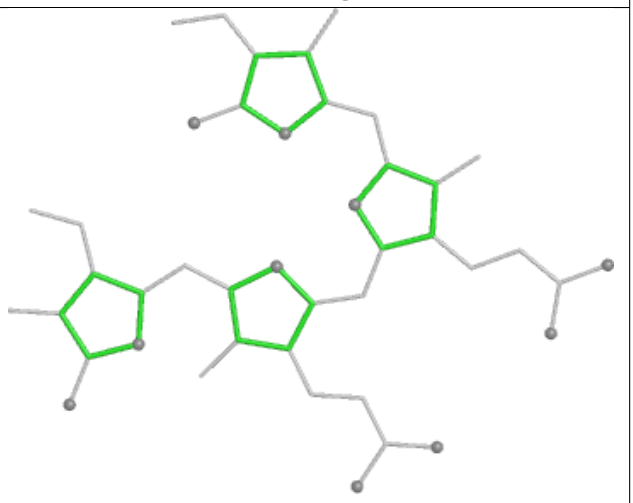
Bond lengths



Bond angles



Torsions

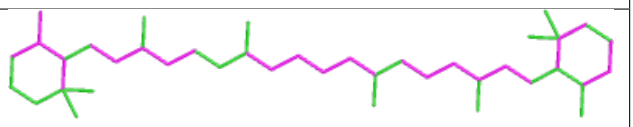


Rings

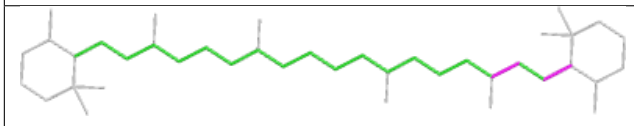
Ligand BCR bL 603



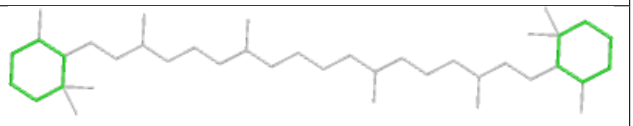
Bond lengths



Bond angles

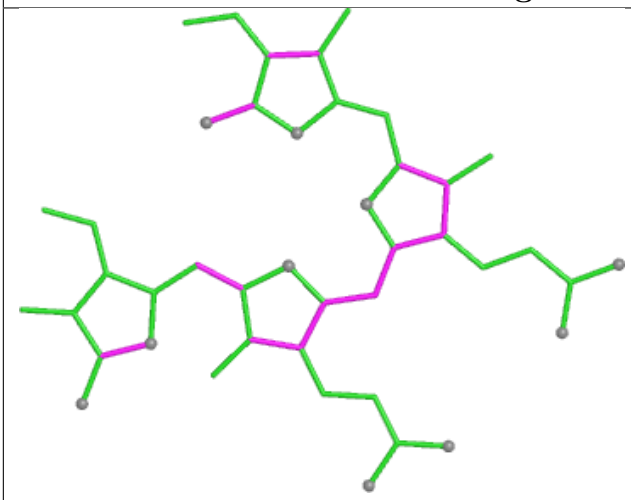


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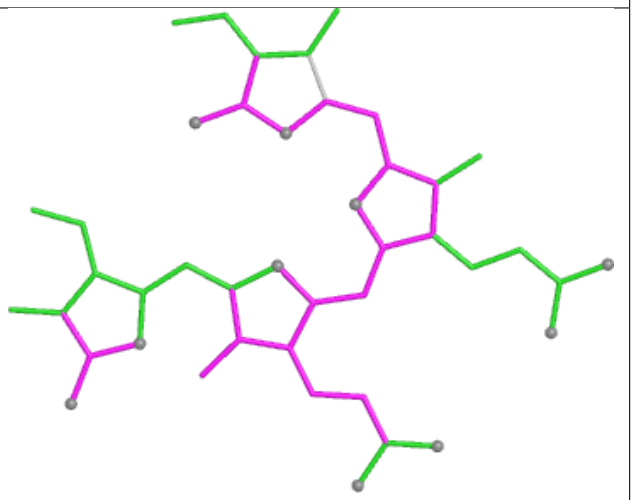


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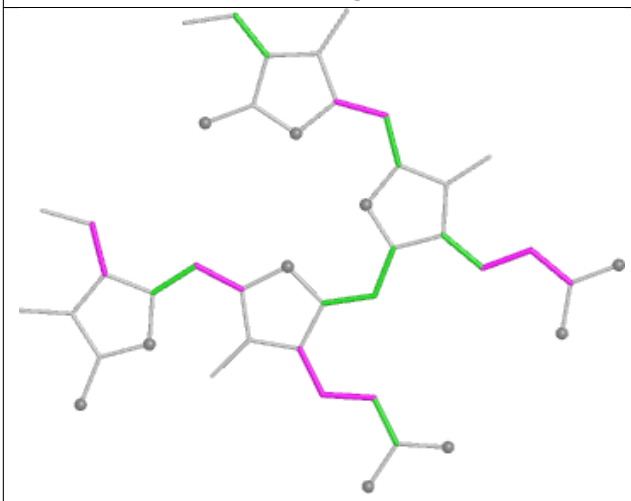
Ligand PEB U9 202



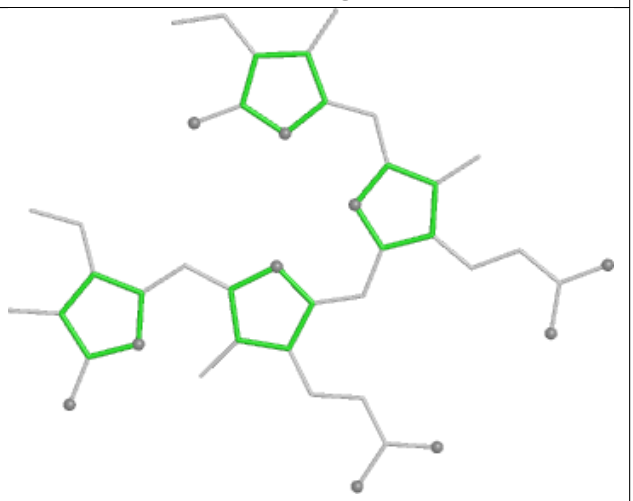
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Bond angles

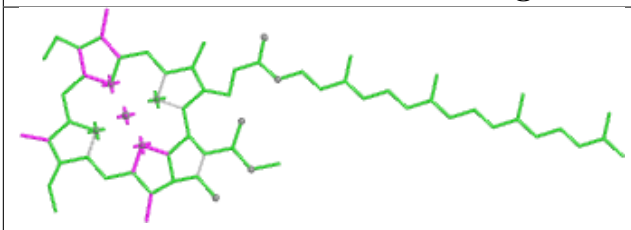


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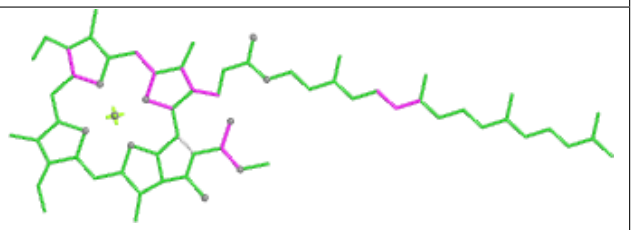


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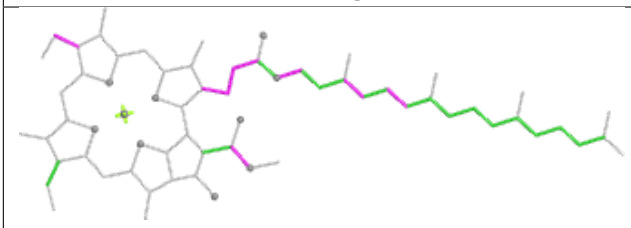
Ligand CLA A2 807



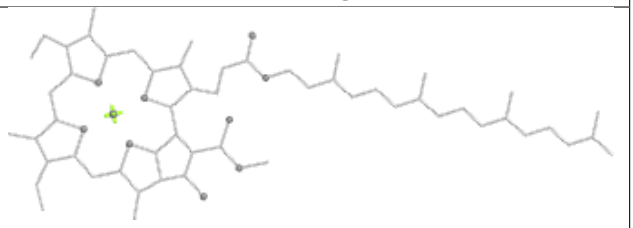
Bond lengths



Bond angles

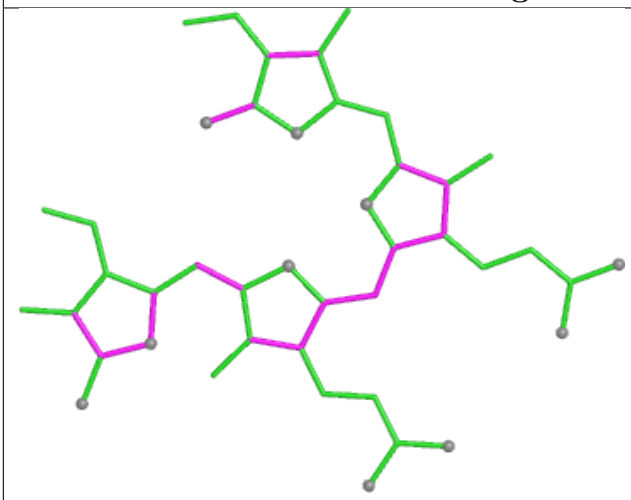


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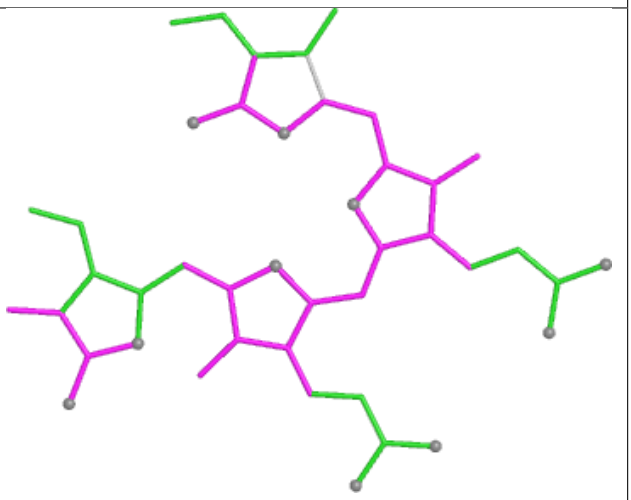


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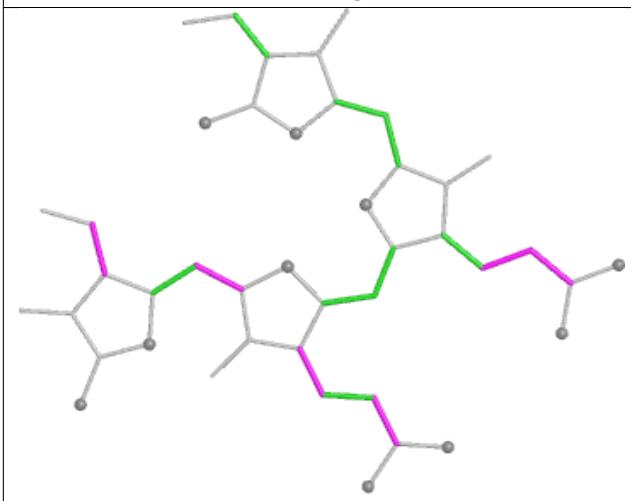
Ligand PEB RO 202



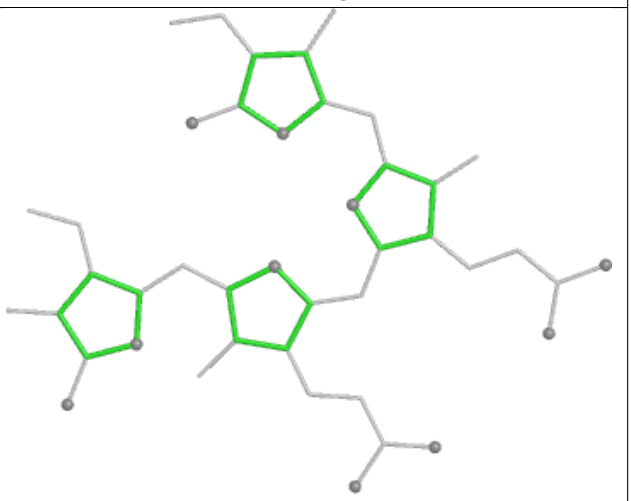
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Bond angles

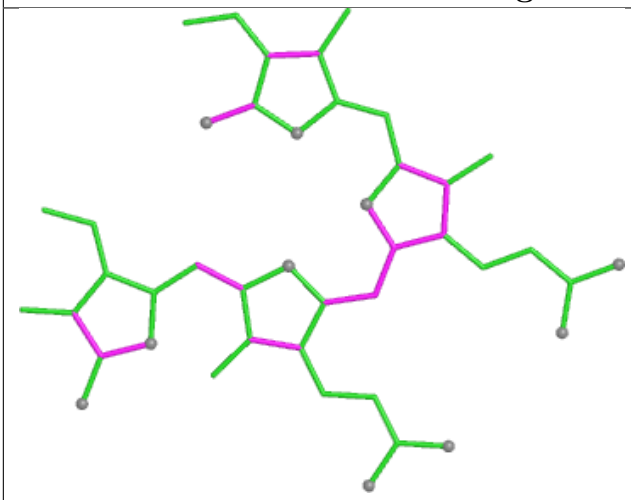


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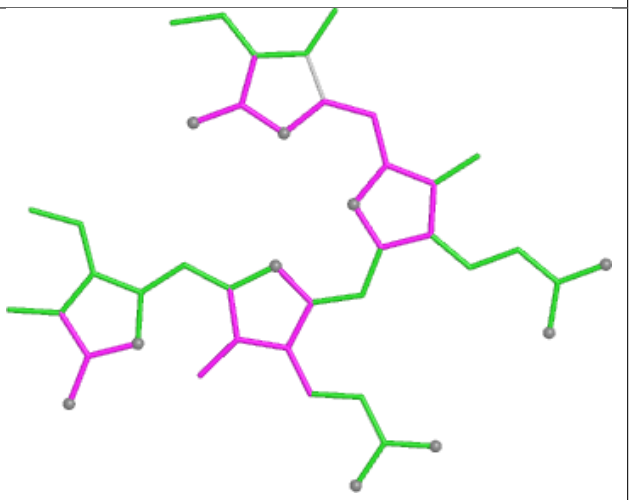


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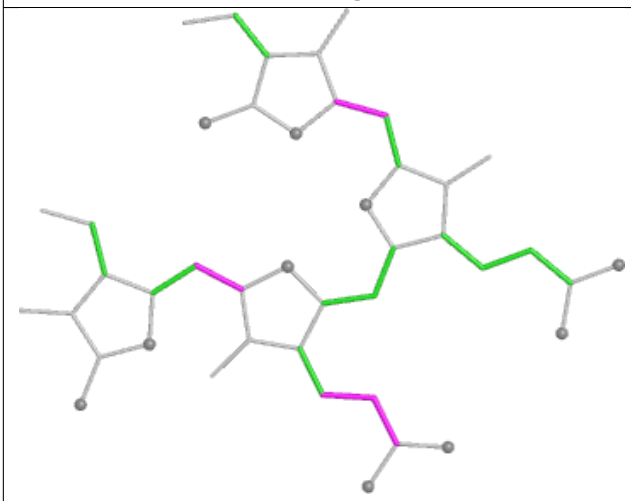
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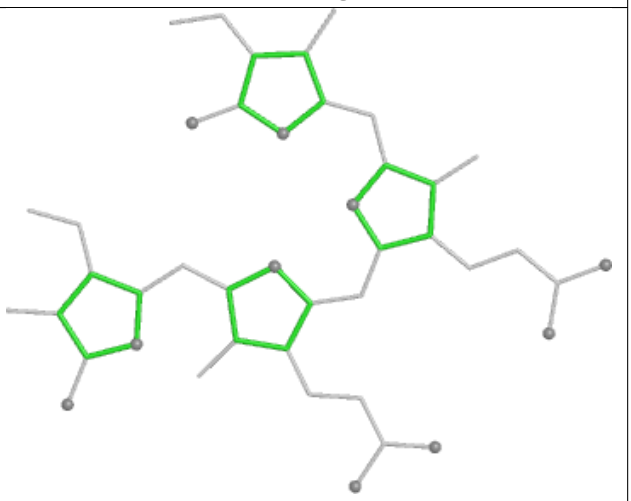
Bond lengths



Bond angles

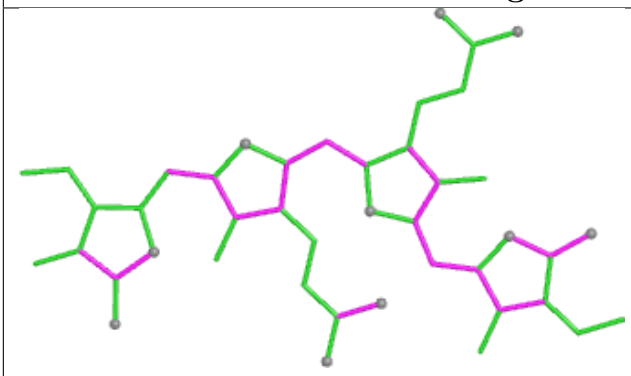


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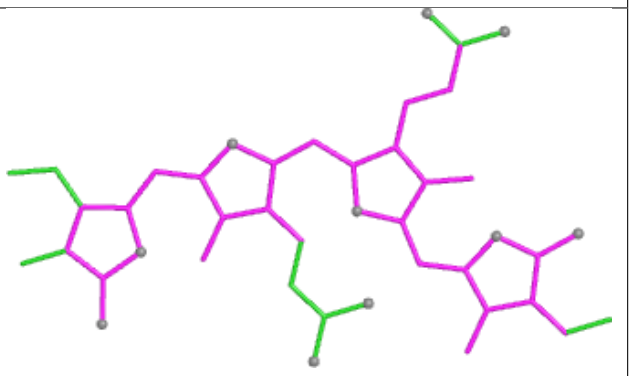


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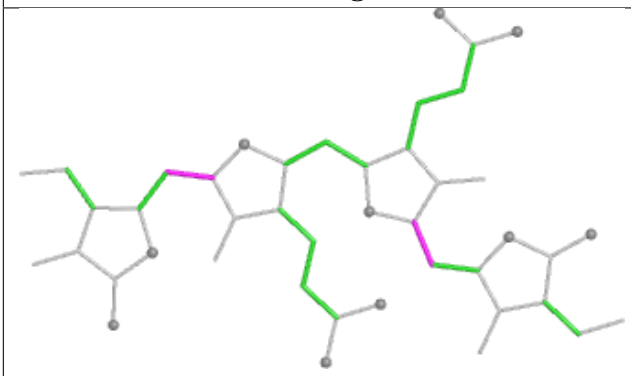
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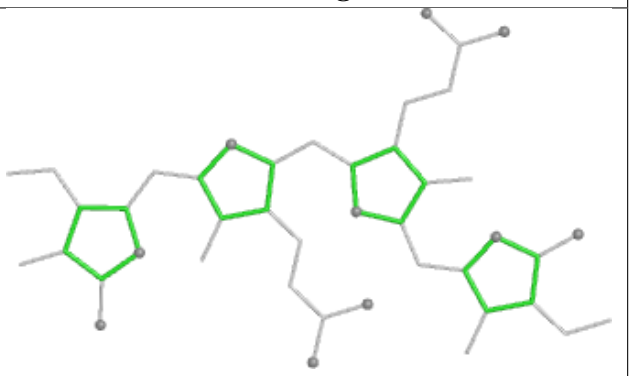
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Bond angles

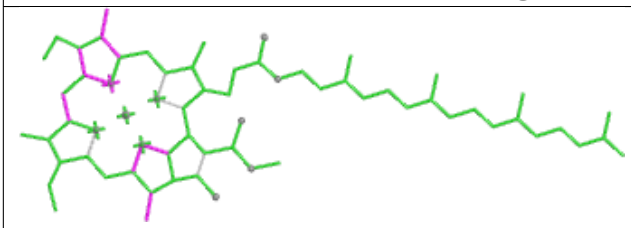


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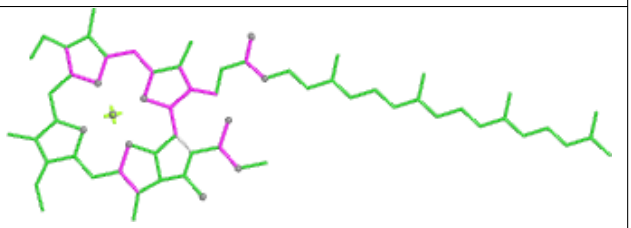


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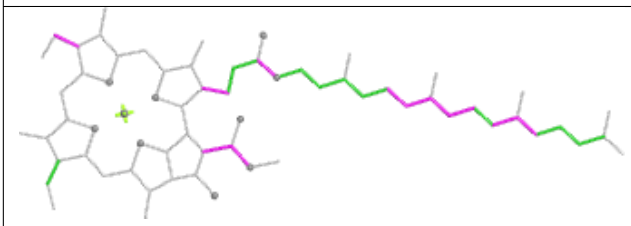
Ligand CLA 6N 602



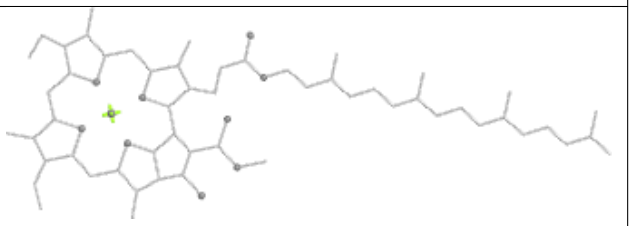
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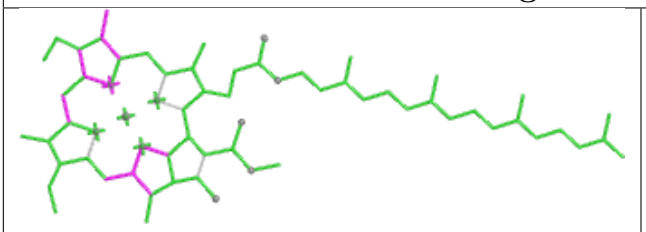


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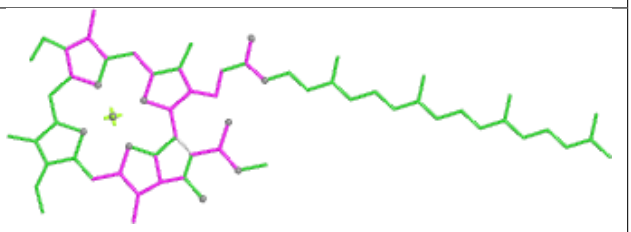


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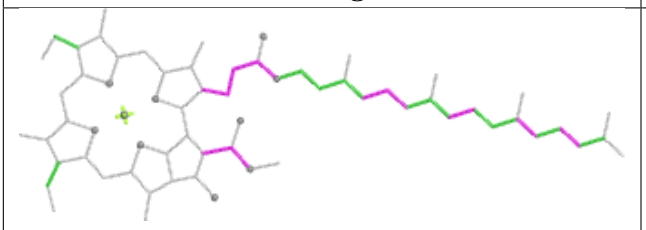
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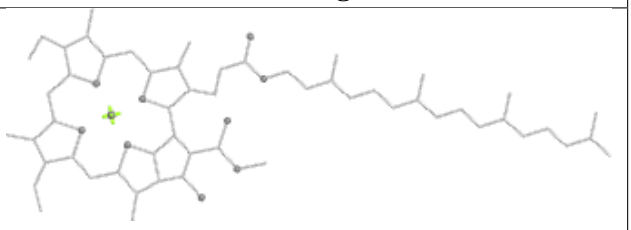
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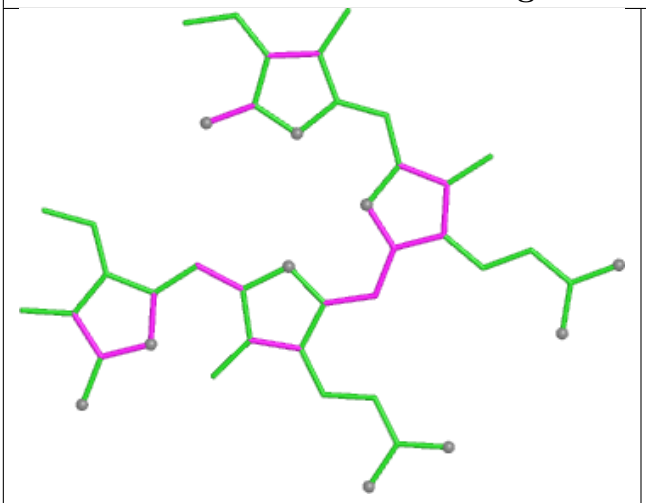


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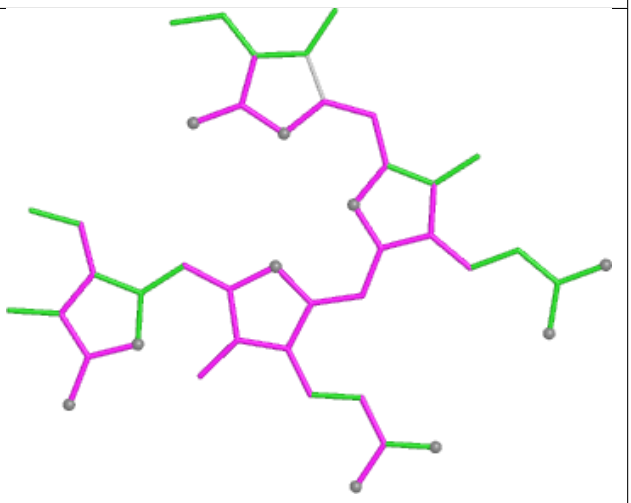


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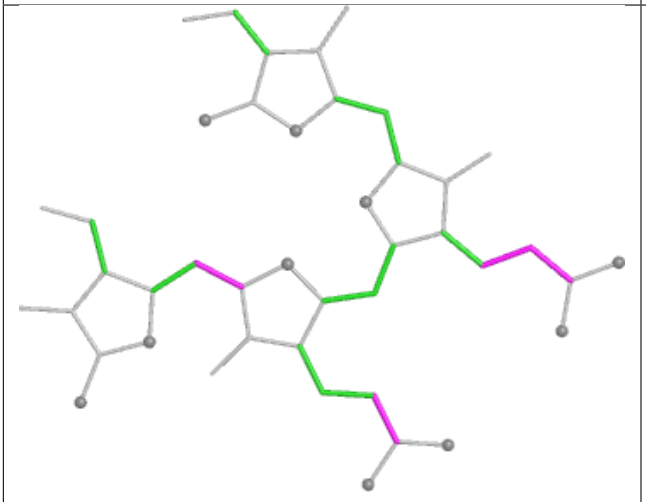
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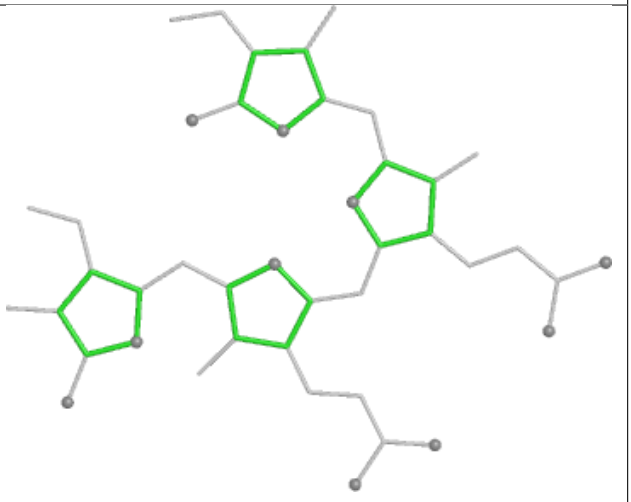
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Bond angles



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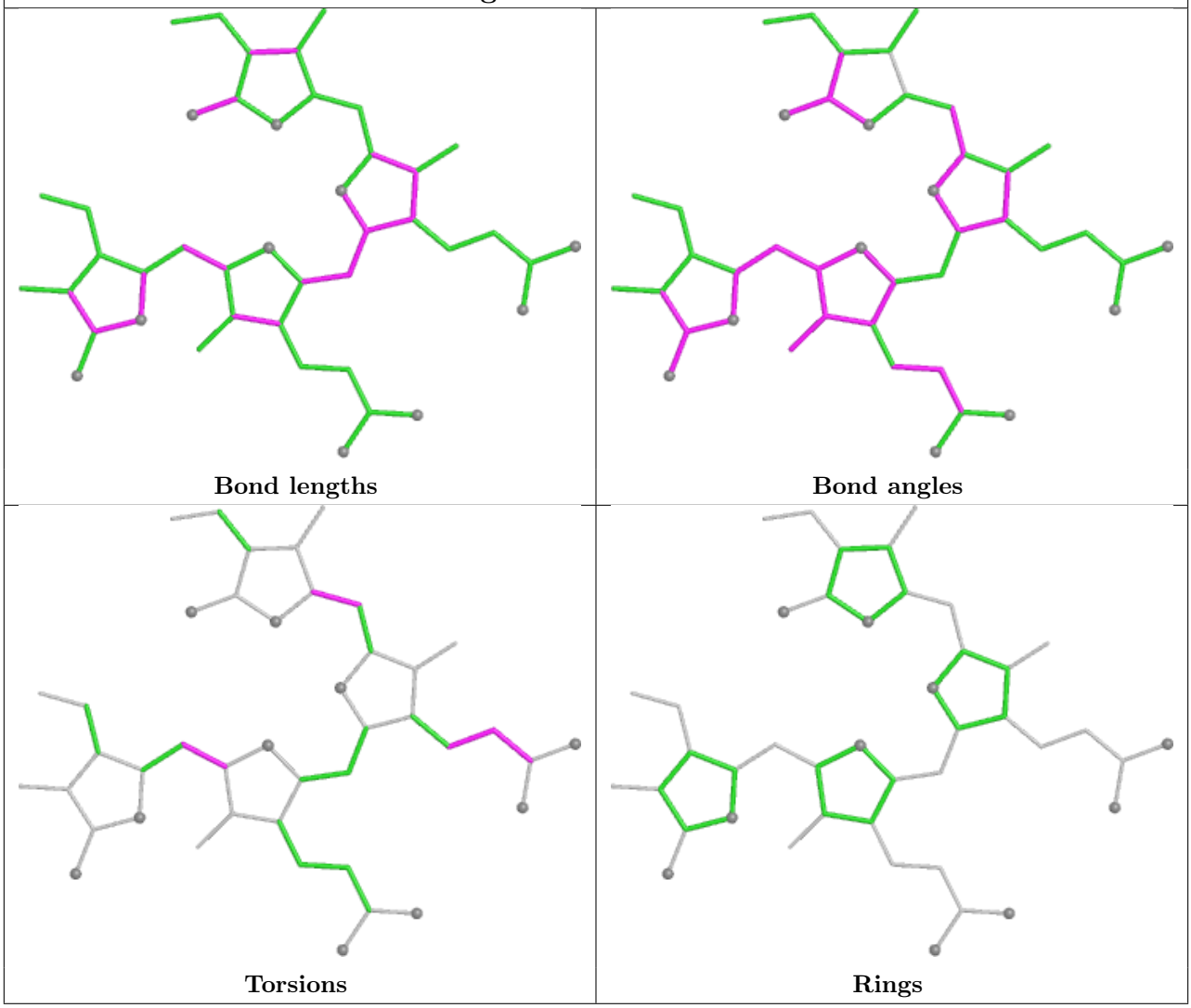


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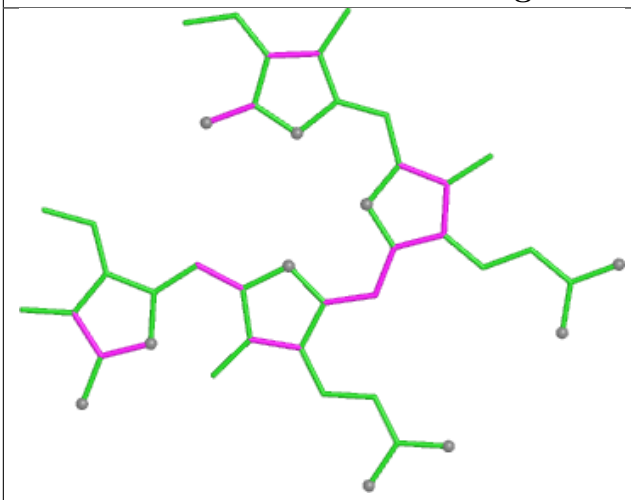
Ligand PL9 A6 410



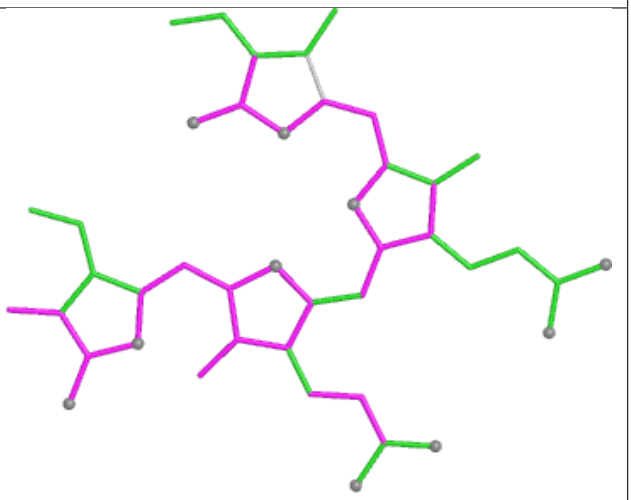
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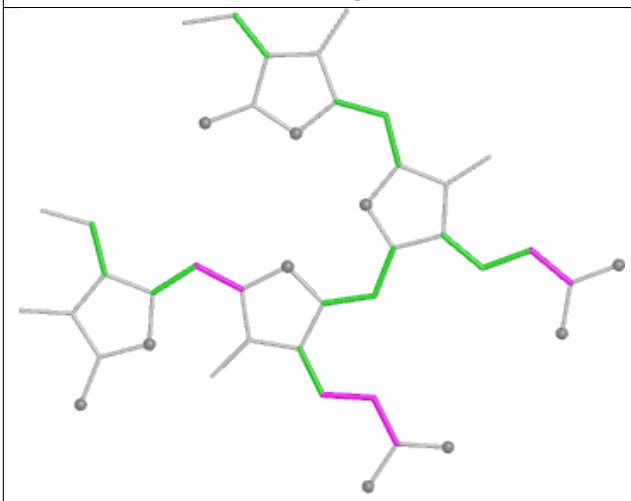
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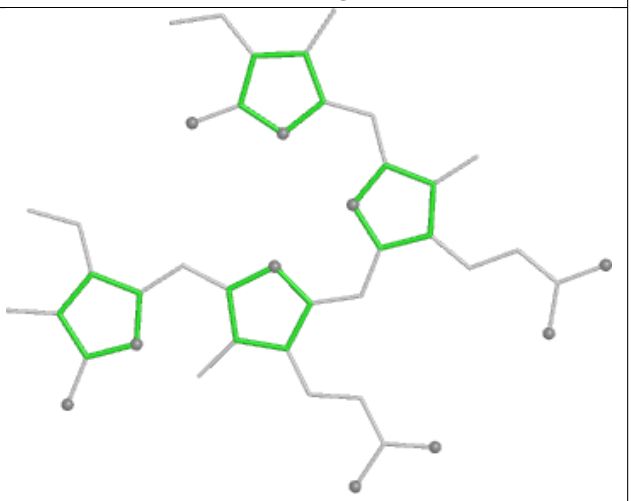
Bond lengths



Bond angles

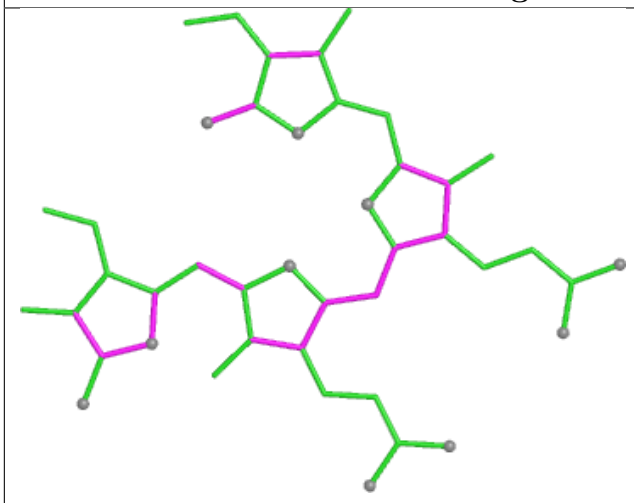


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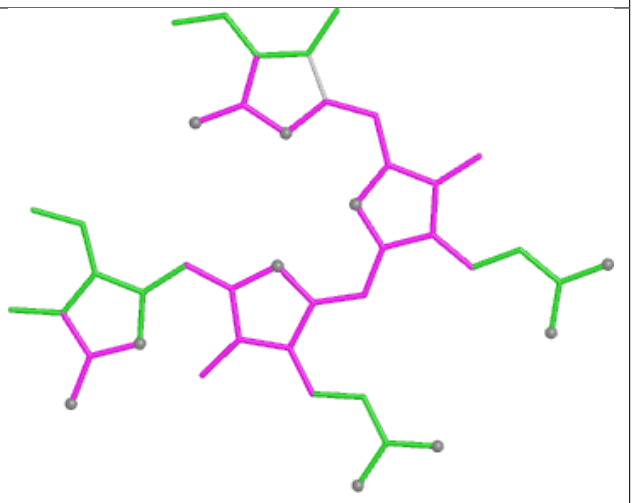


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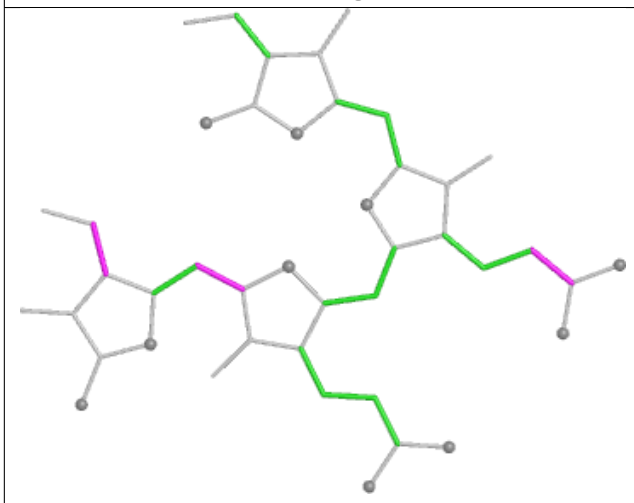
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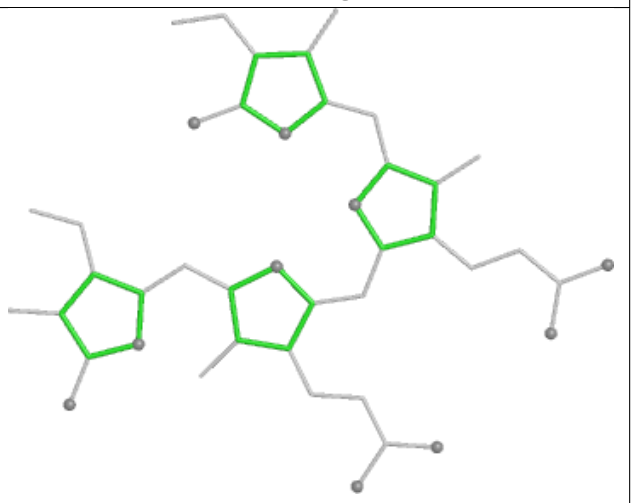
Bond lengths



Bond angles

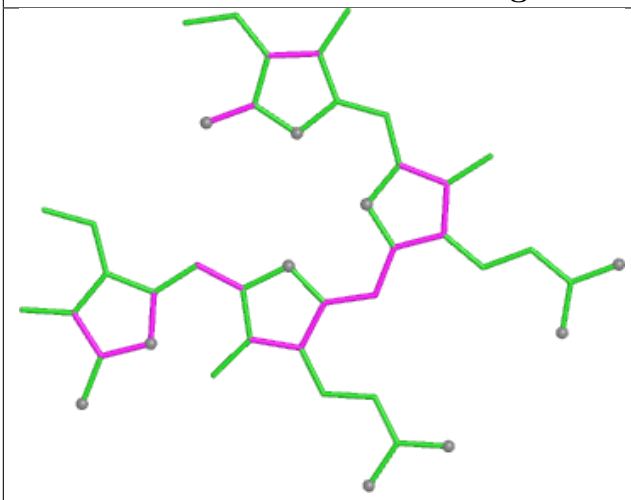


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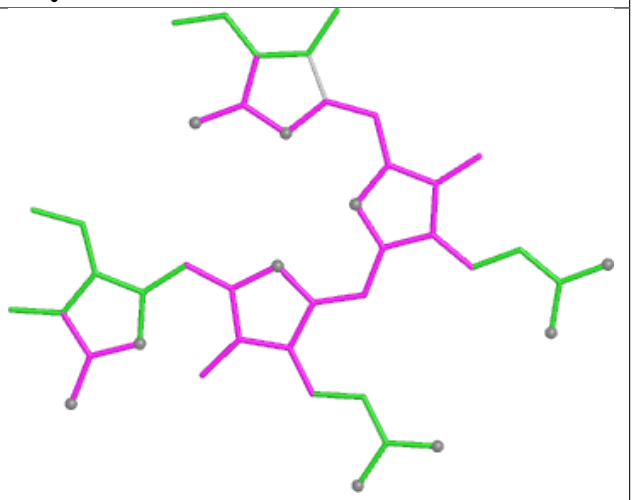


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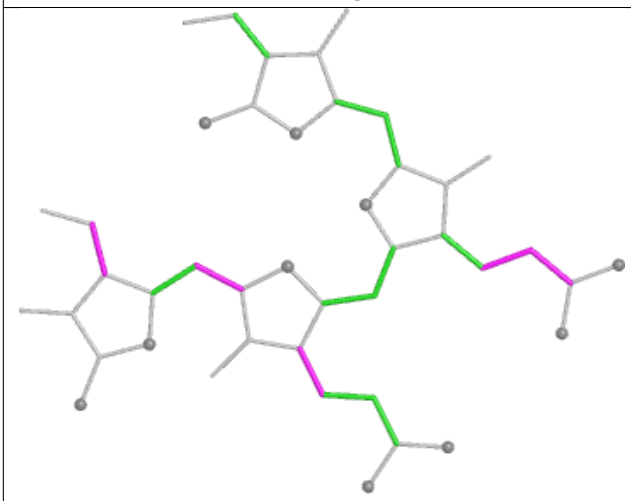
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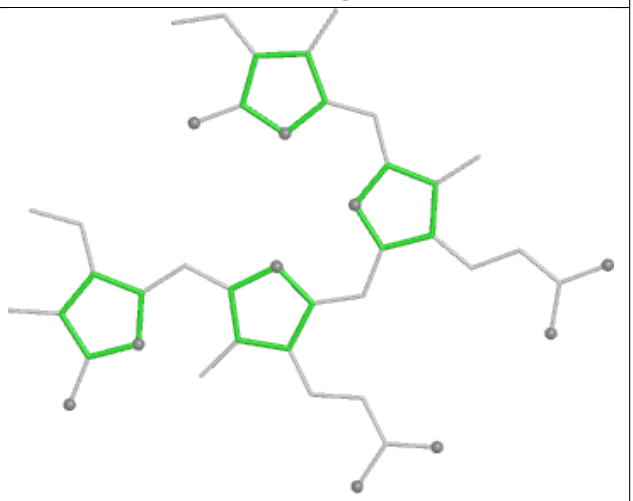
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Bond angles

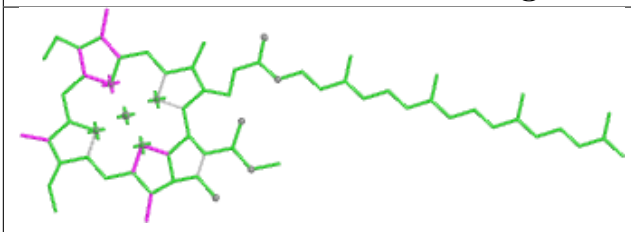


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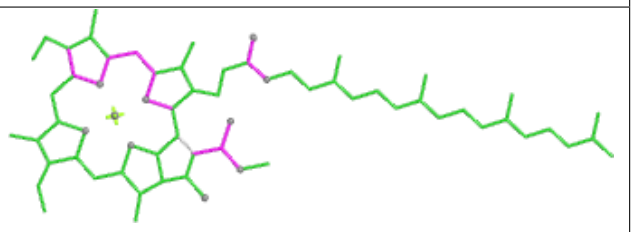


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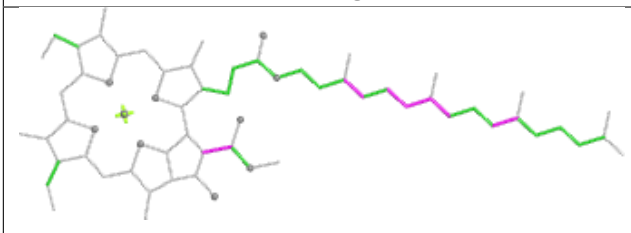
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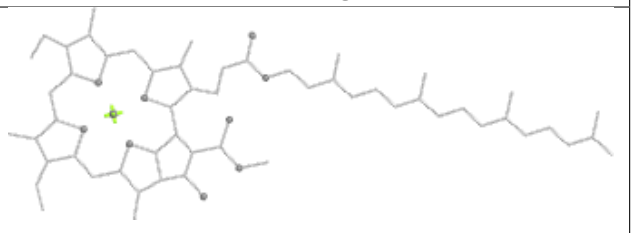
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Bond angles

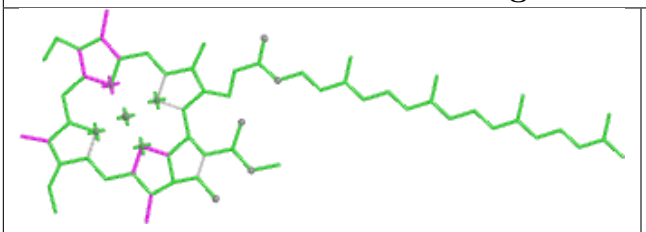


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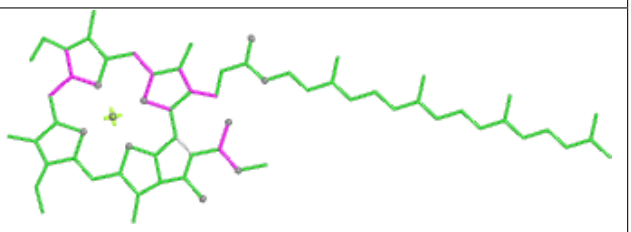


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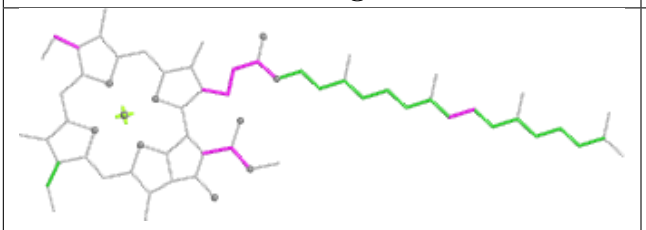
Ligand CLA AN 833



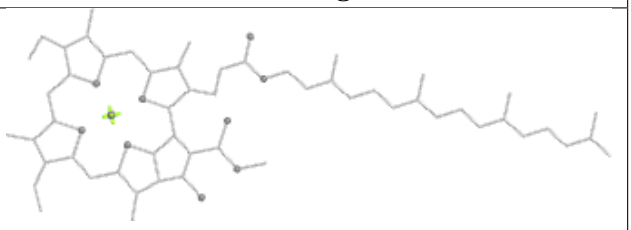
Bond lengths



Bond angles

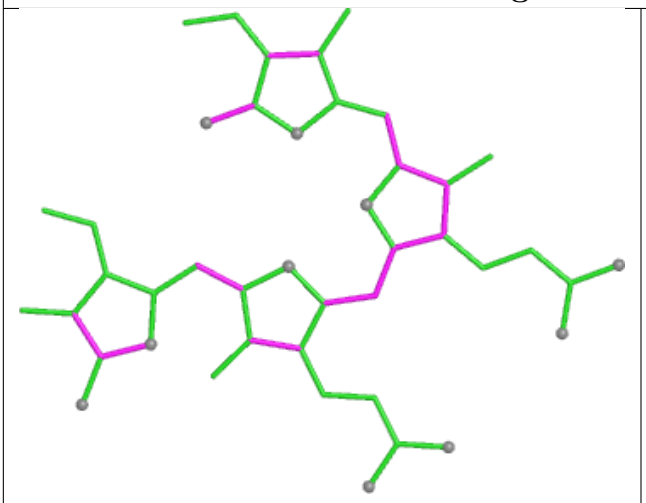


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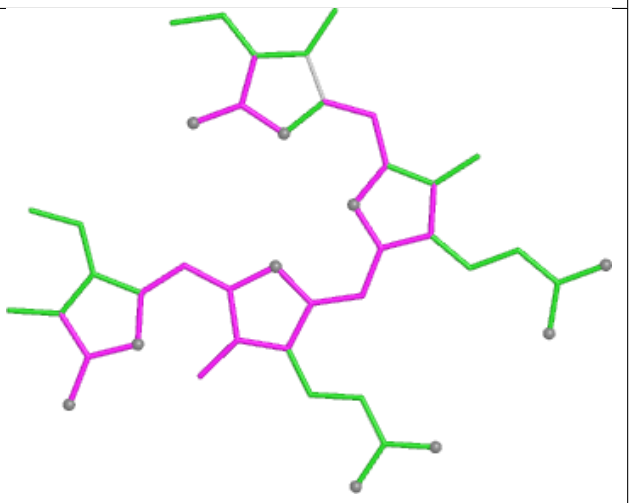


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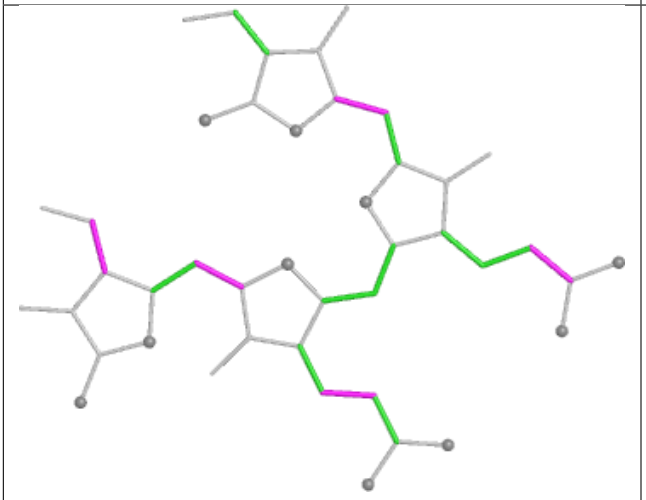
Ligand PEB TD 202



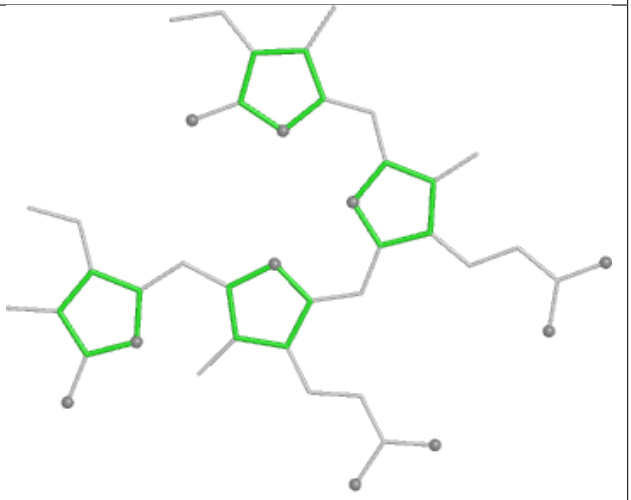
Bond lengths



Bond angles

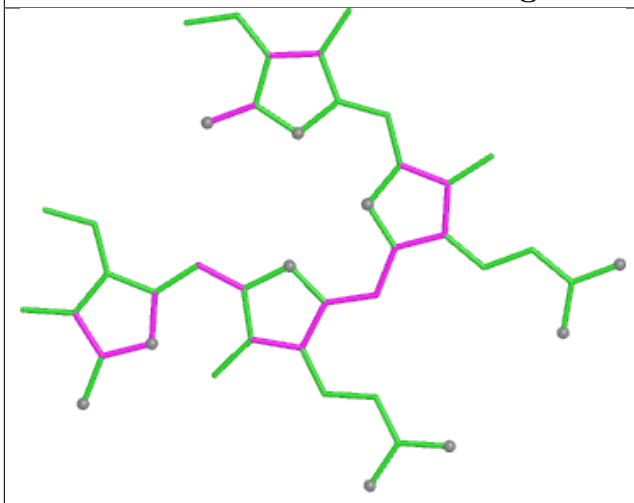


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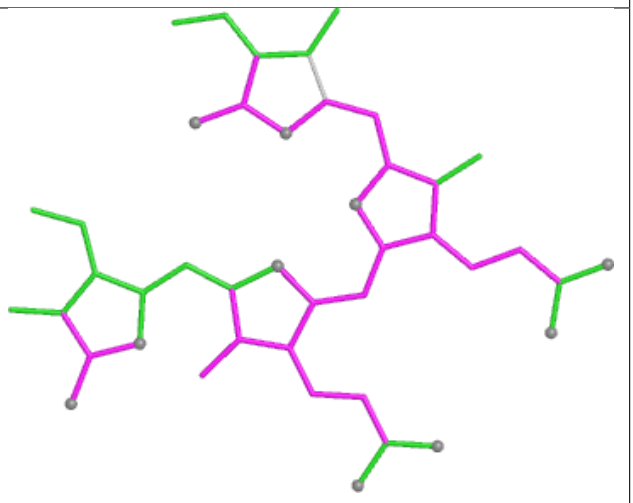


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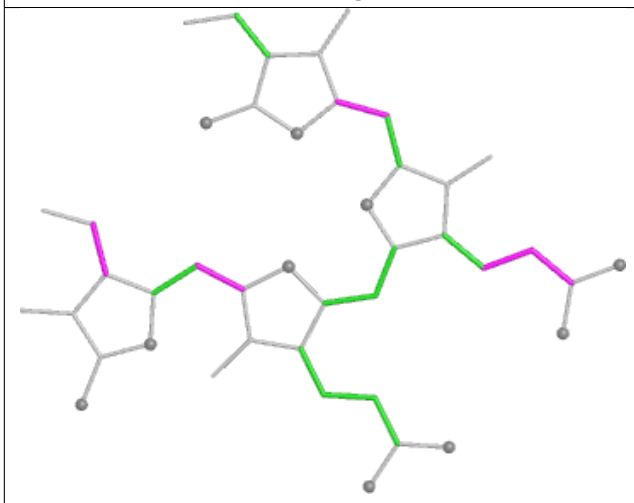
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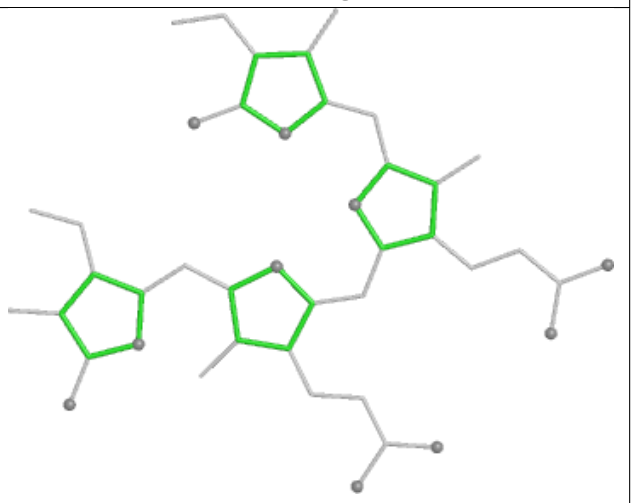
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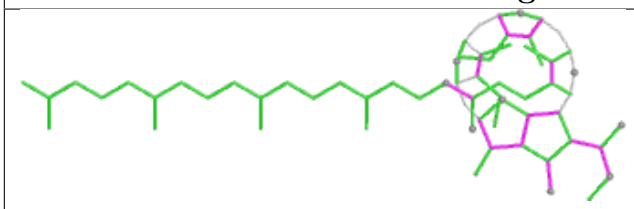


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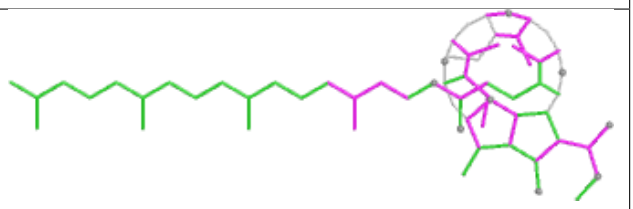


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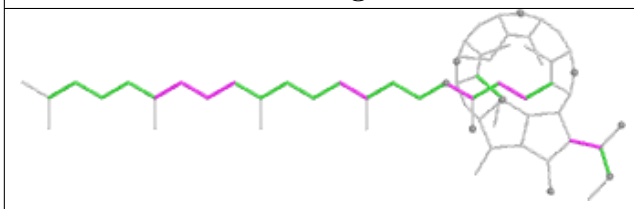
Ligand PHO a6 613



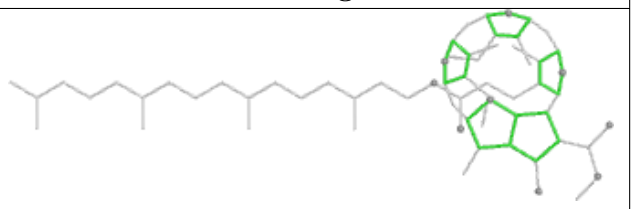
Bond lengths



Bond angles

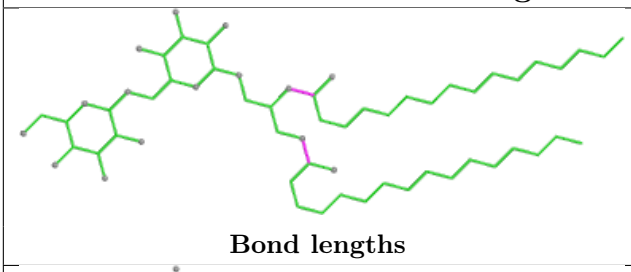


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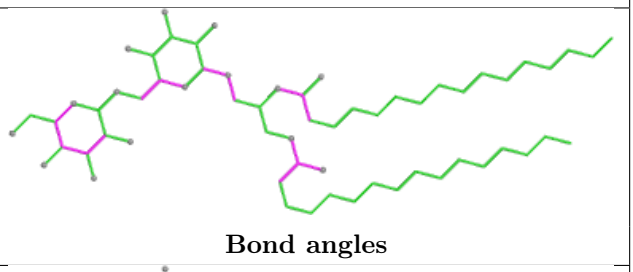


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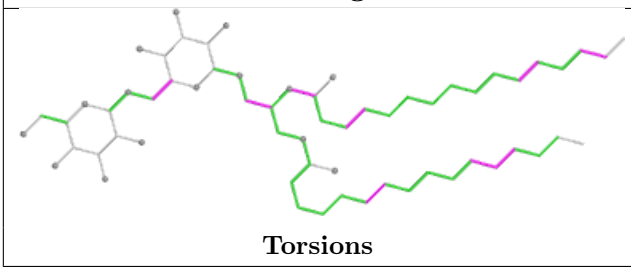
Ligand DGD cL 502



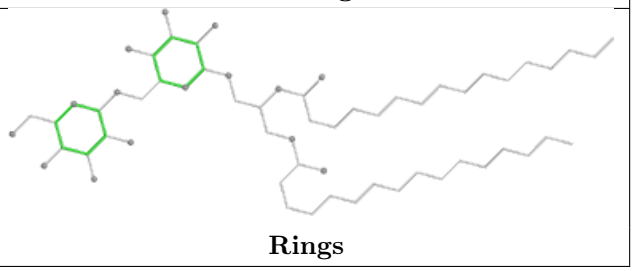
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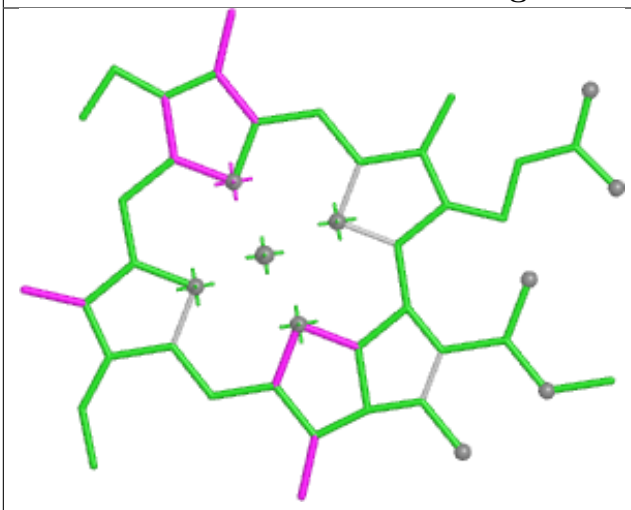


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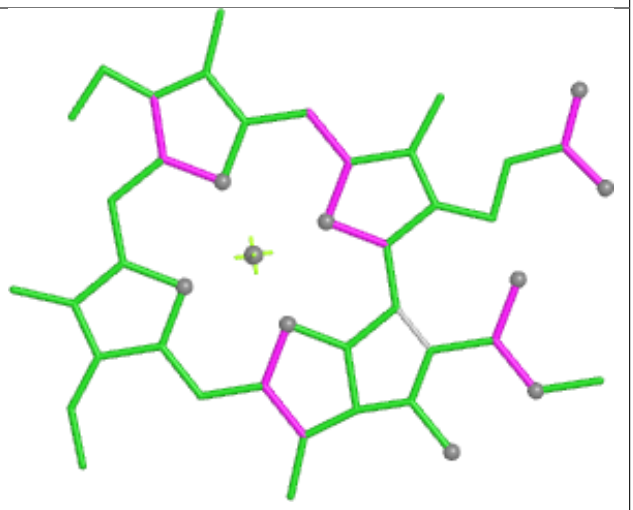


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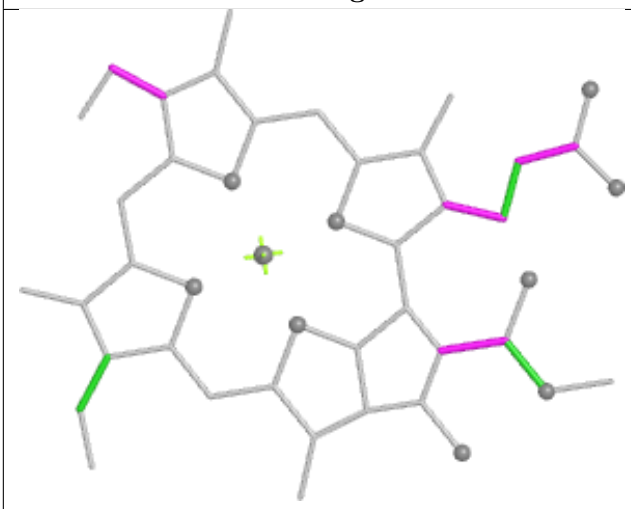
Ligand CLA AN 816



Bond lengths



Bond angles

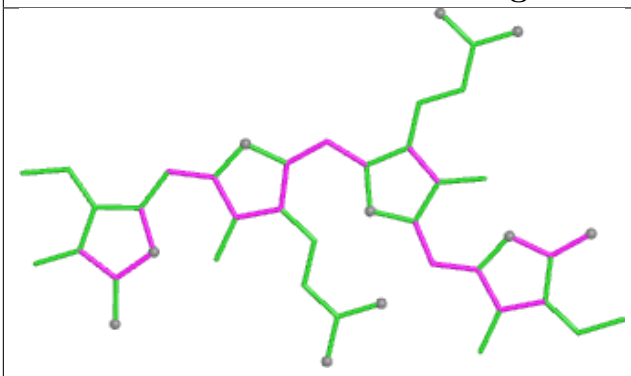


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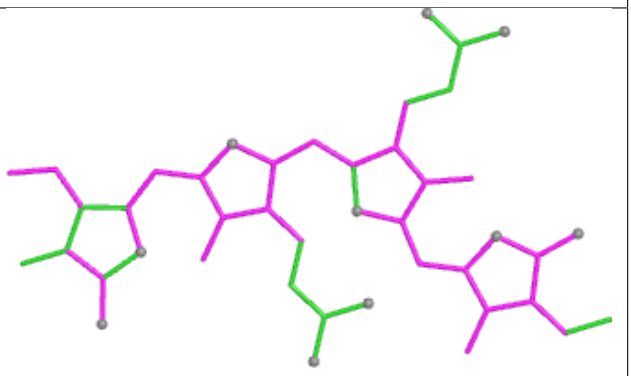


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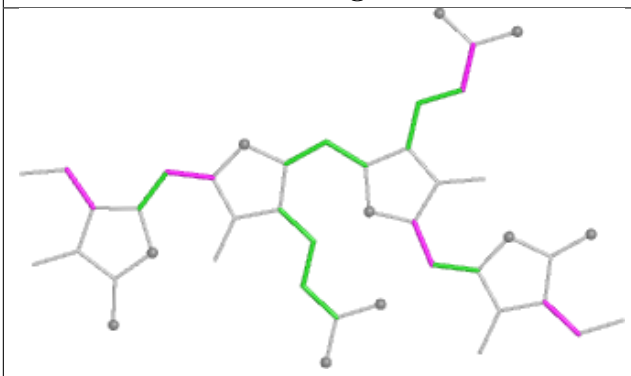
Ligand CYC t3 1001



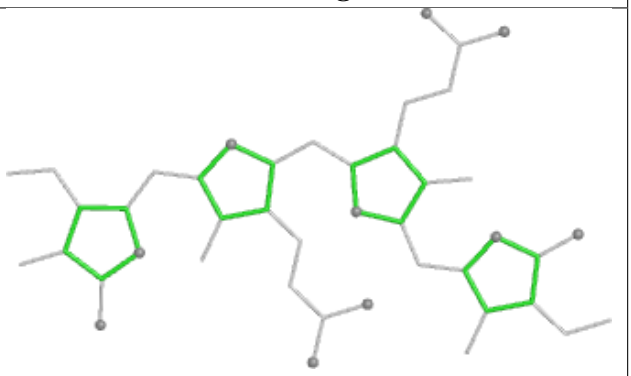
Bond lengths



Bond angles

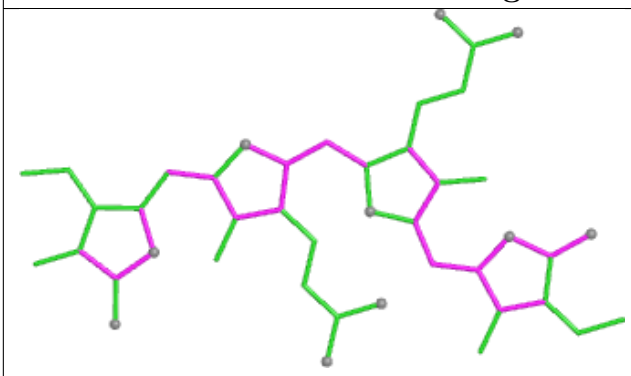


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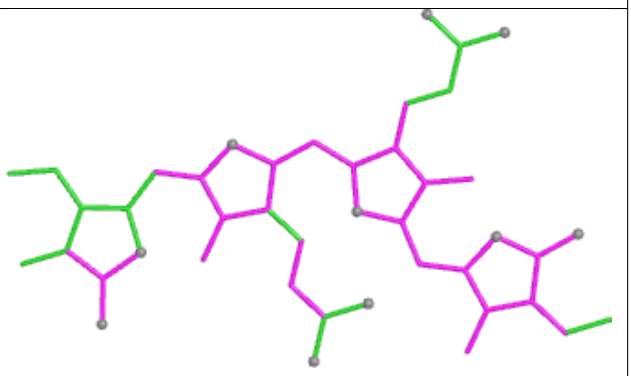


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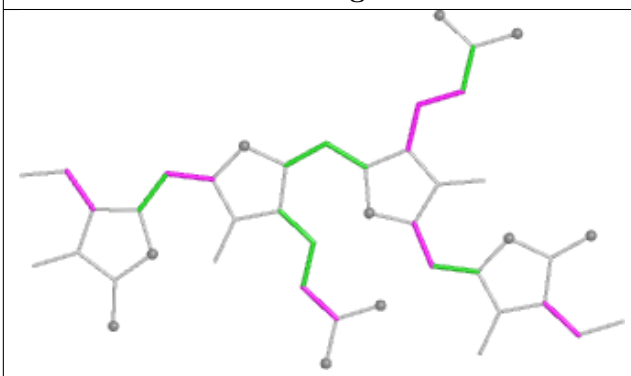
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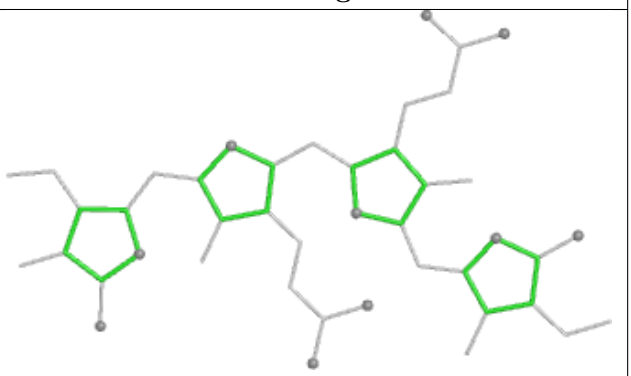
Bond lengths



Bond angles

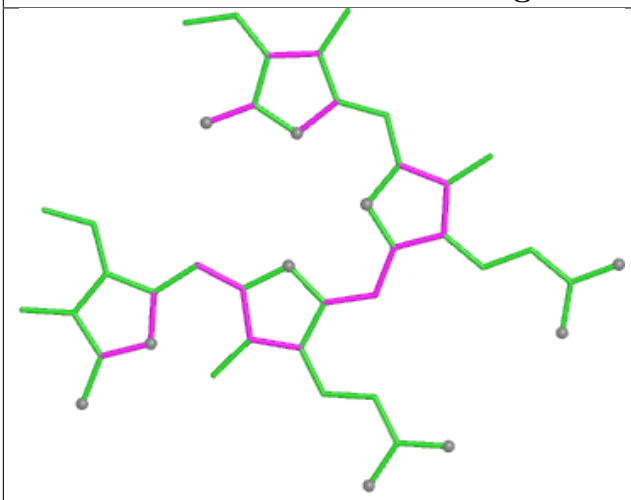


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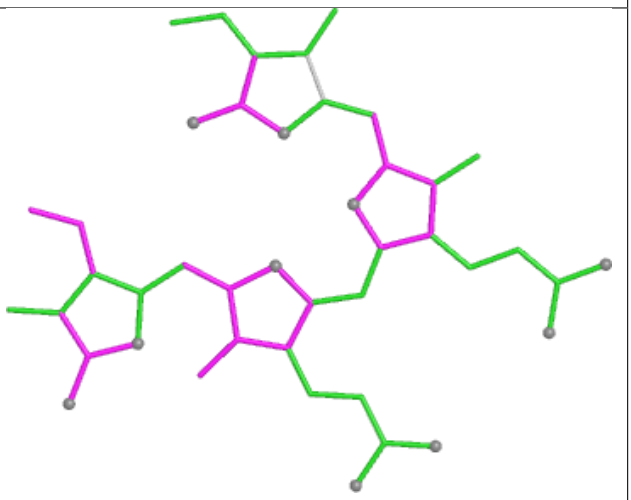


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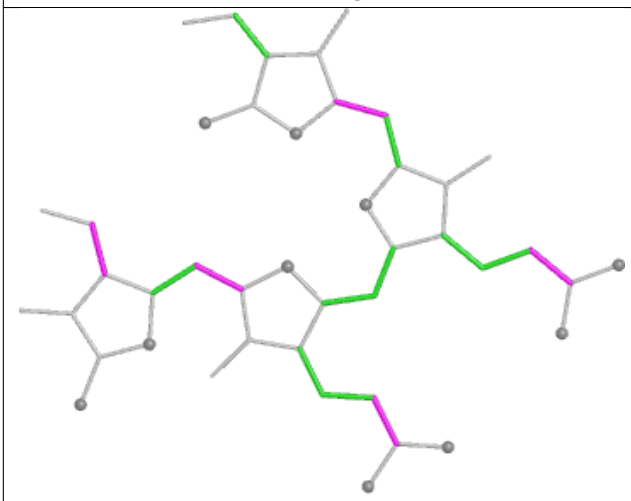
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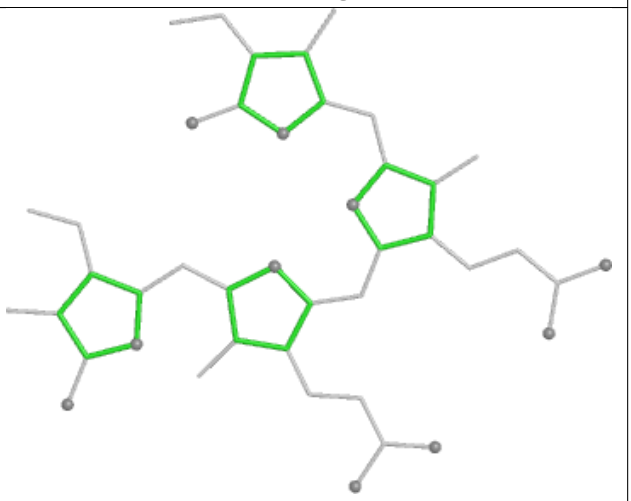
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Bond angles

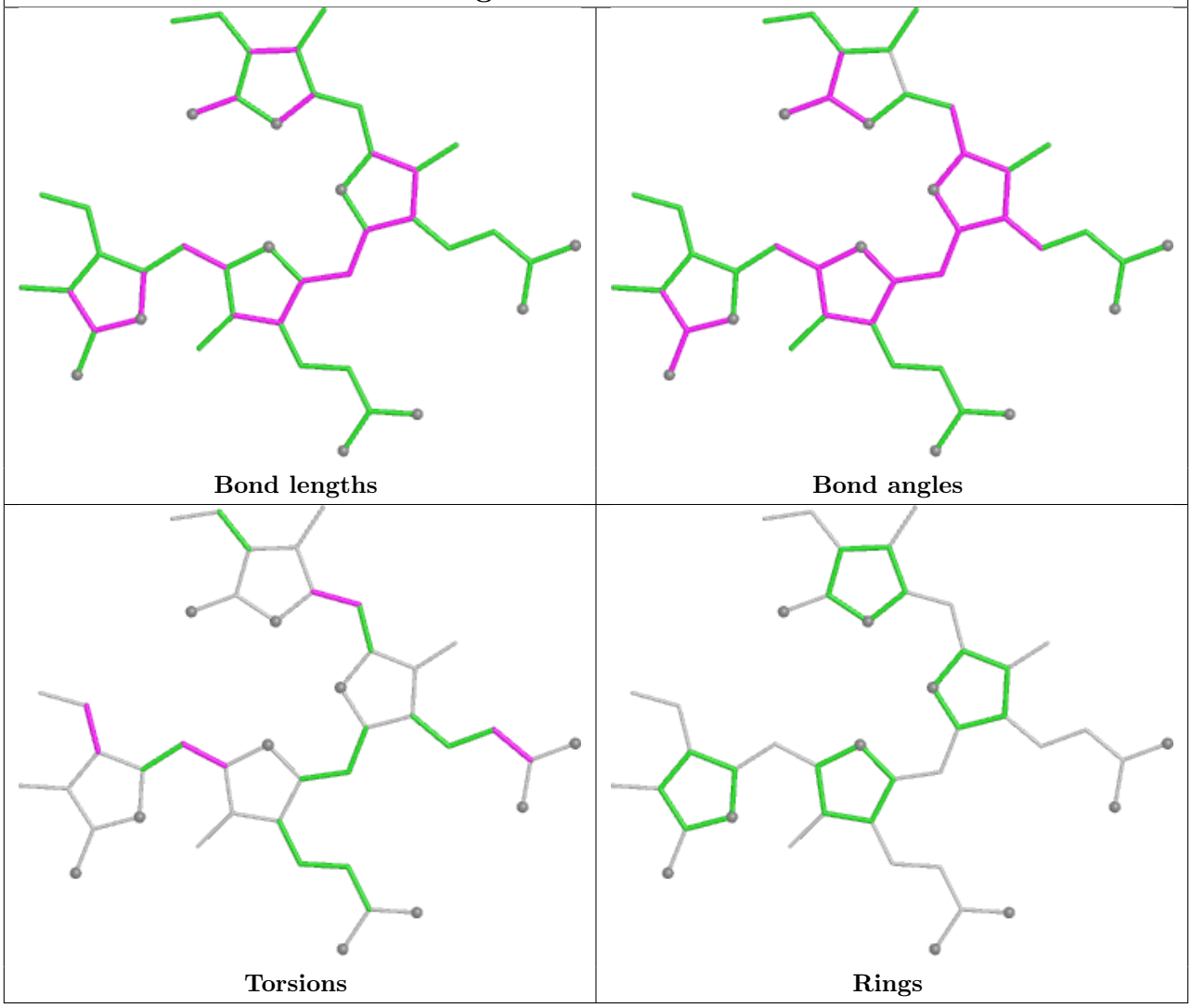


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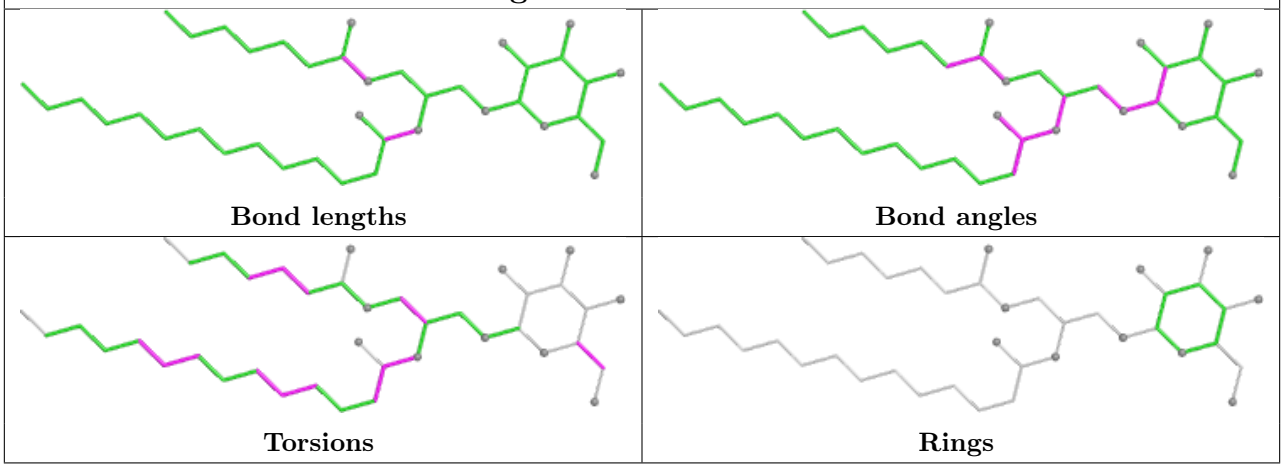


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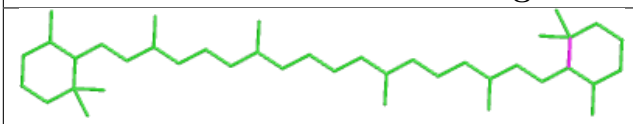
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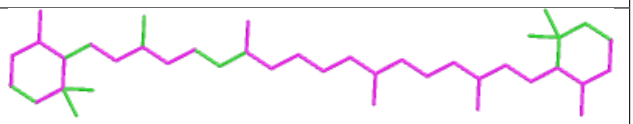
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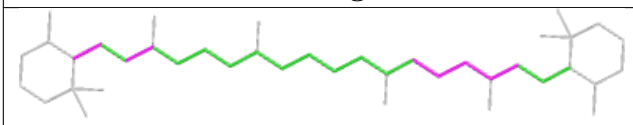
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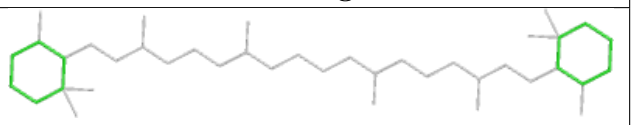
Bond lengths



Bond angles

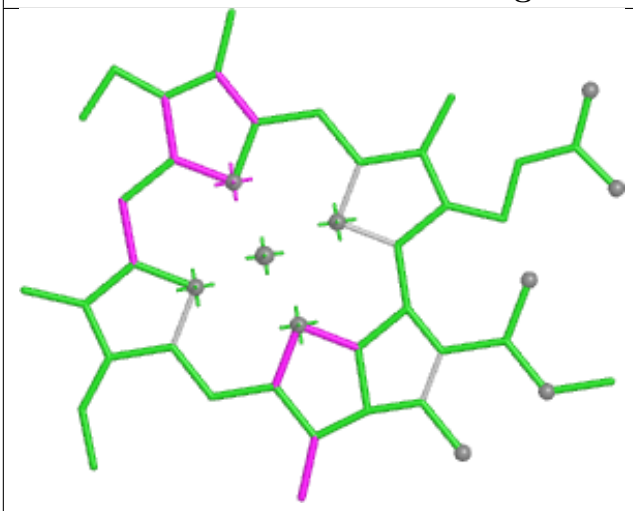


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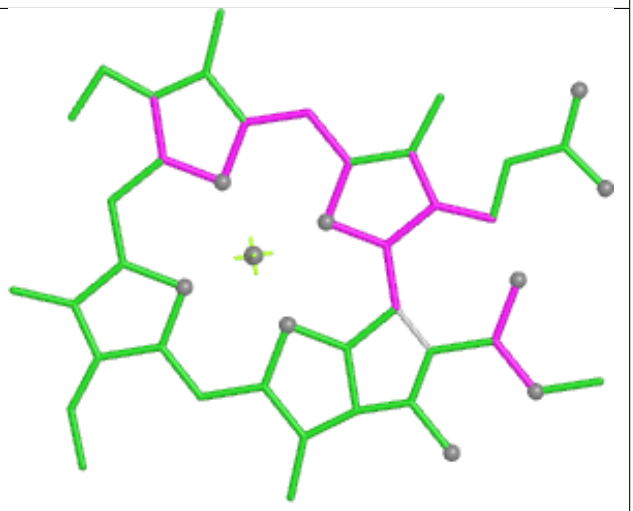


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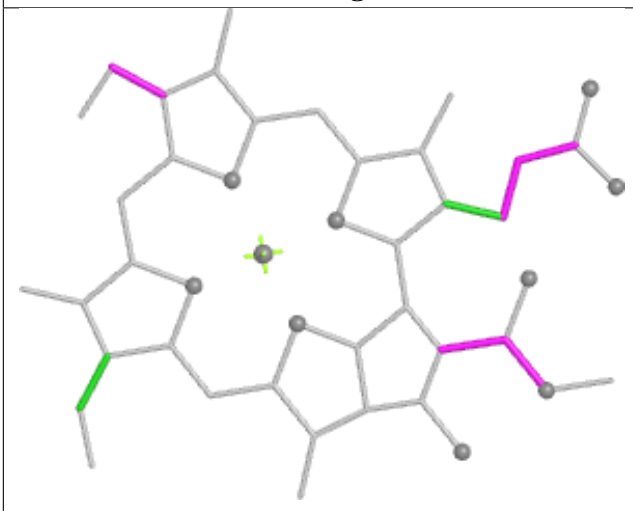
Ligand CLA 6N 605



Bond lengths



Bond angles

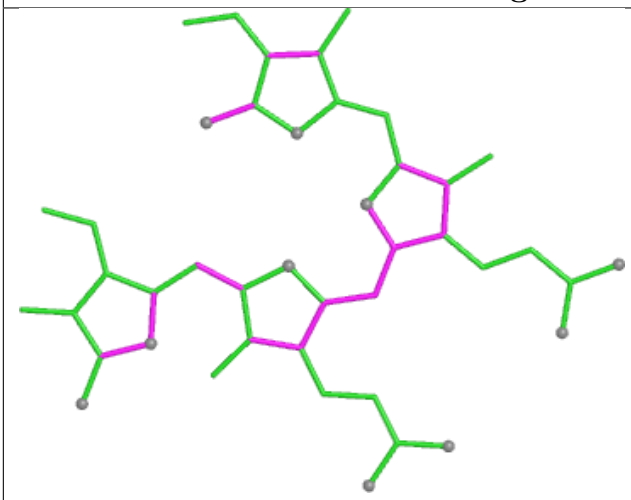


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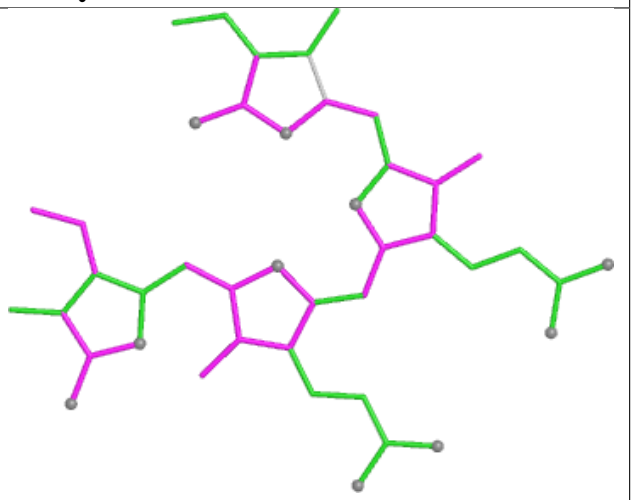


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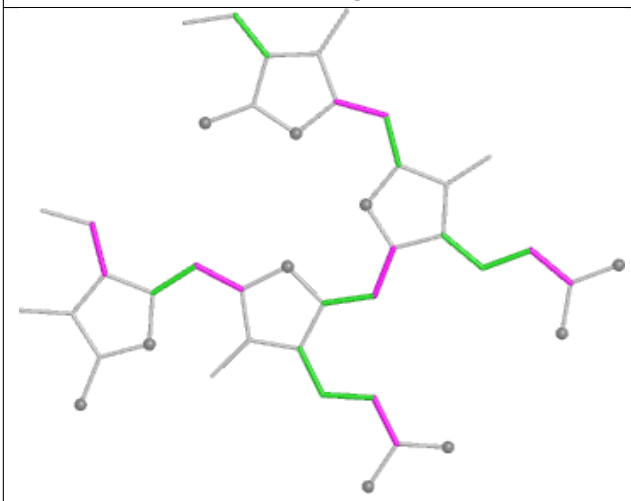
Ligand PEB HQ 203



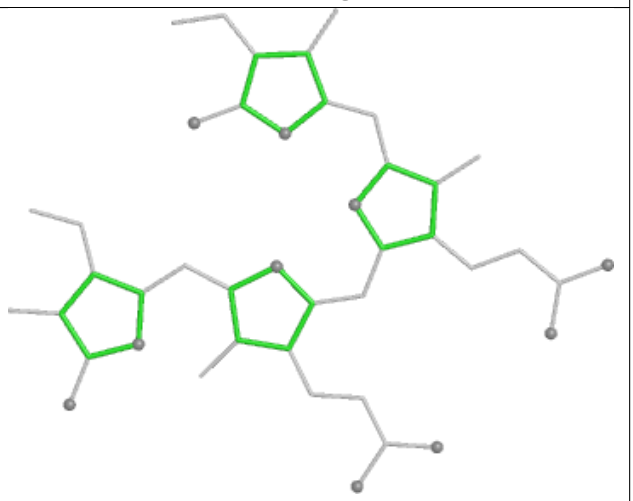
Bond lengths



Bond angles

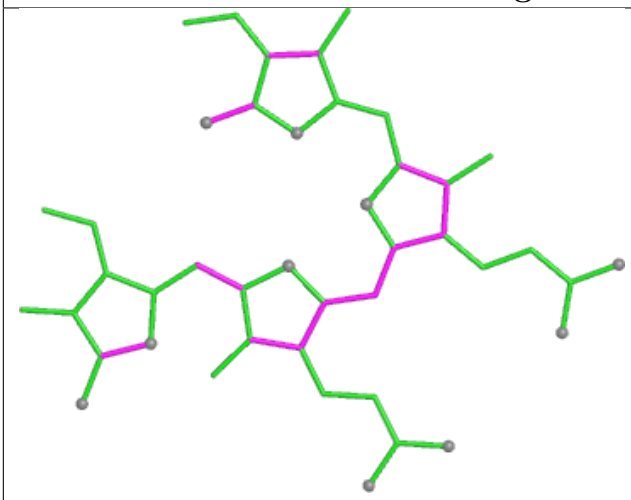


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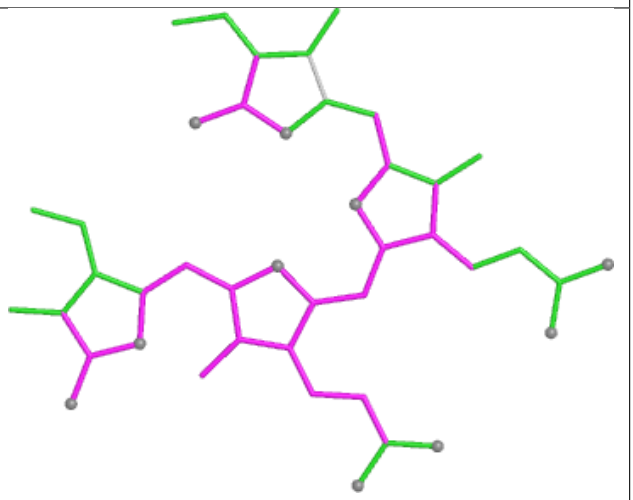


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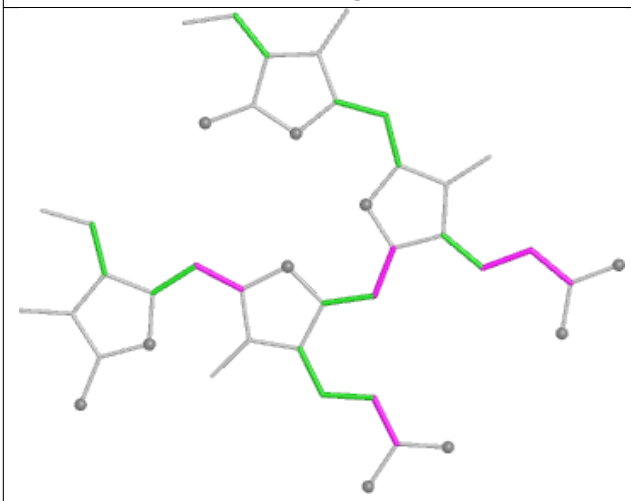
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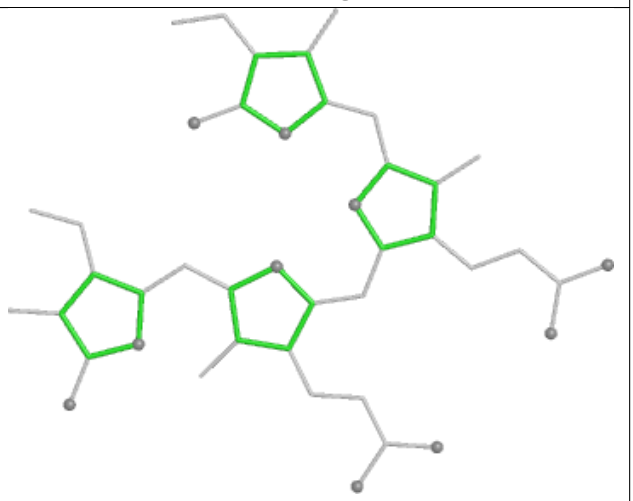
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Bond angles

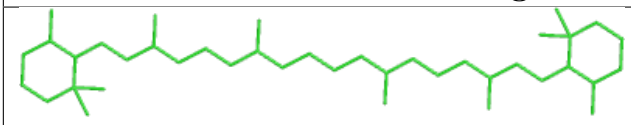


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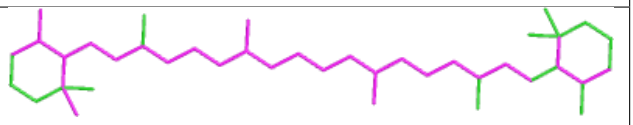


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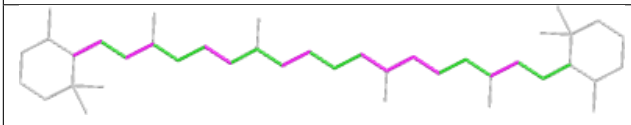
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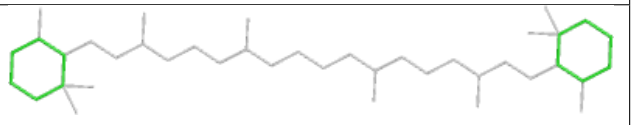
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Bond angles

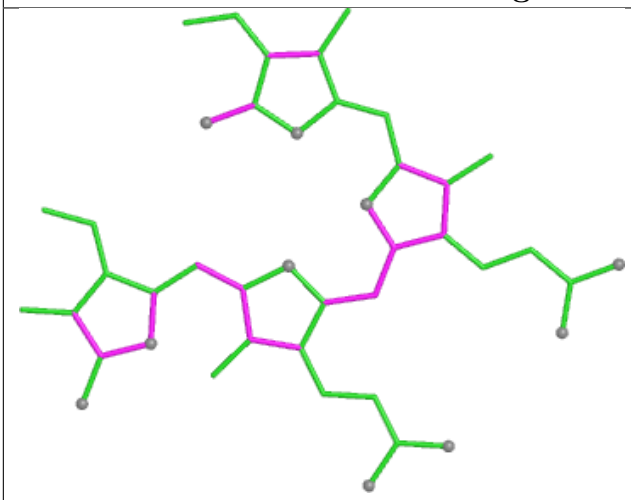


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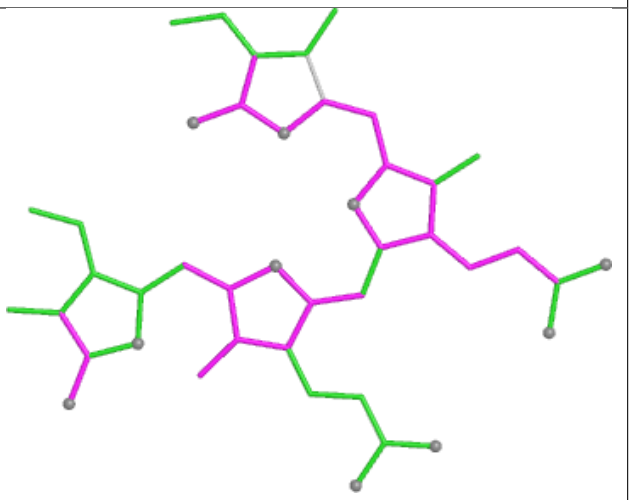


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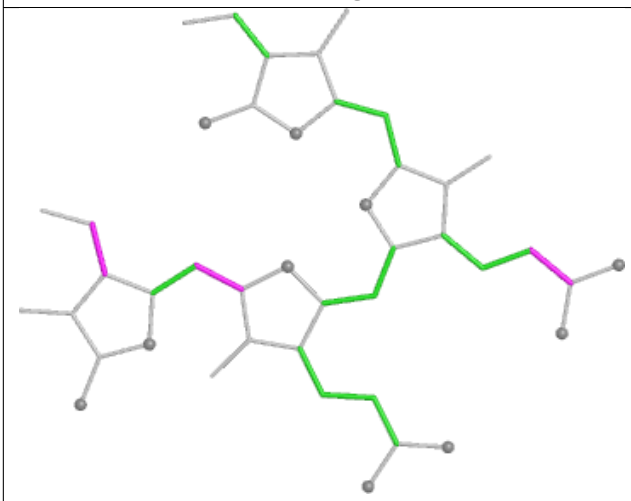
Ligand PEB CP 202



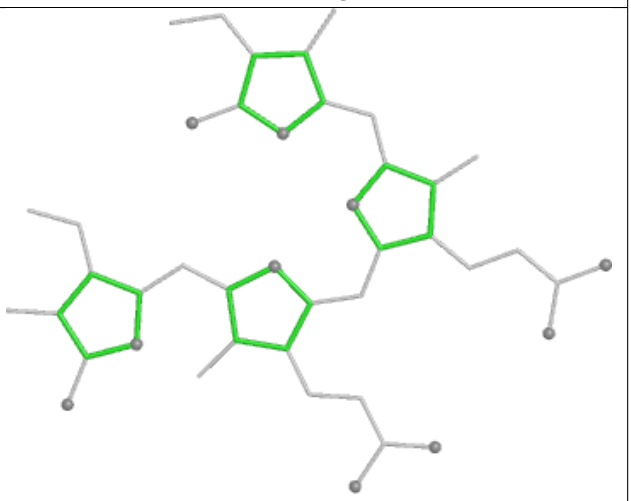
Bond lengths



Bond angles

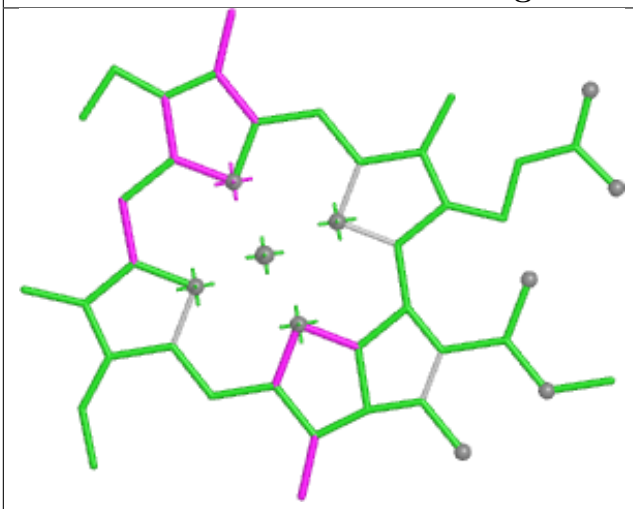


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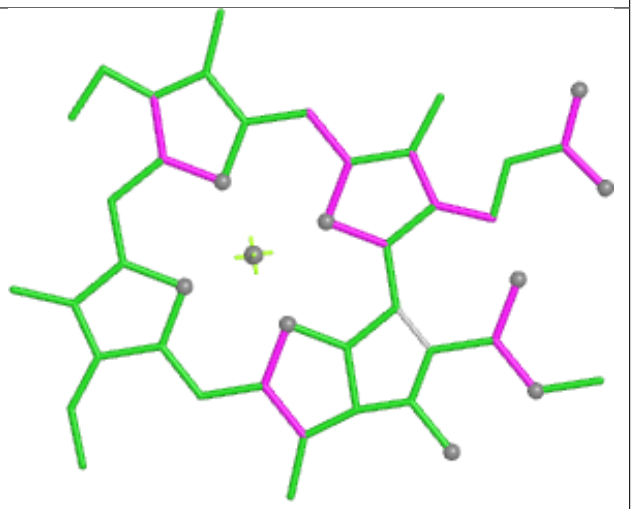


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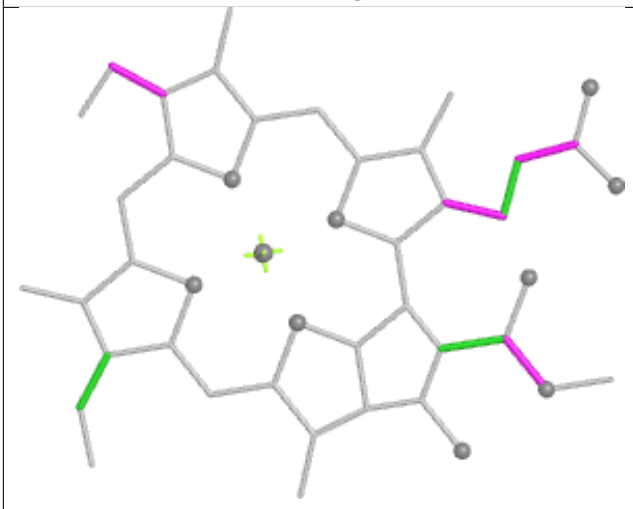
Ligand CLA 6N 606



Bond lengths



Bond angles

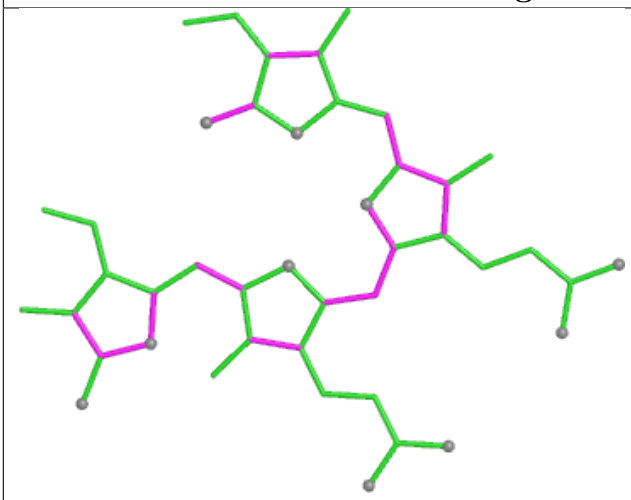


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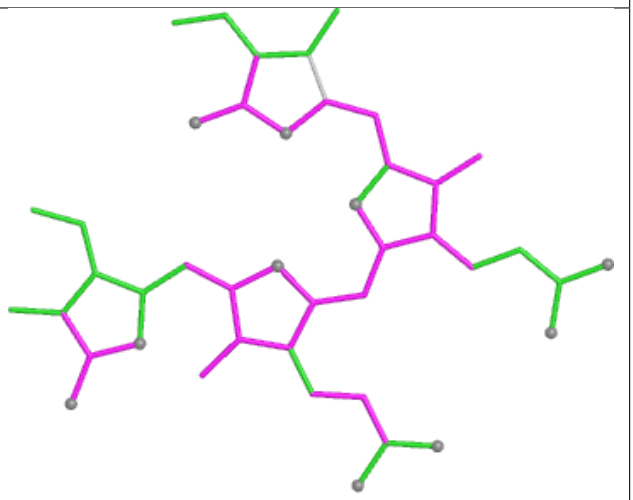


Rings

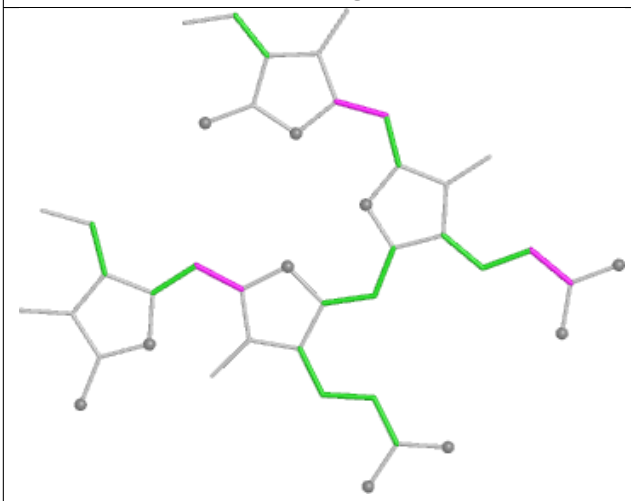
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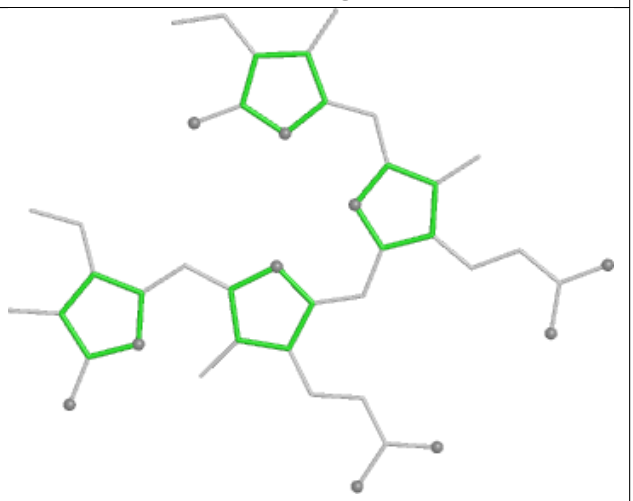
Bond lengths



Bond angles

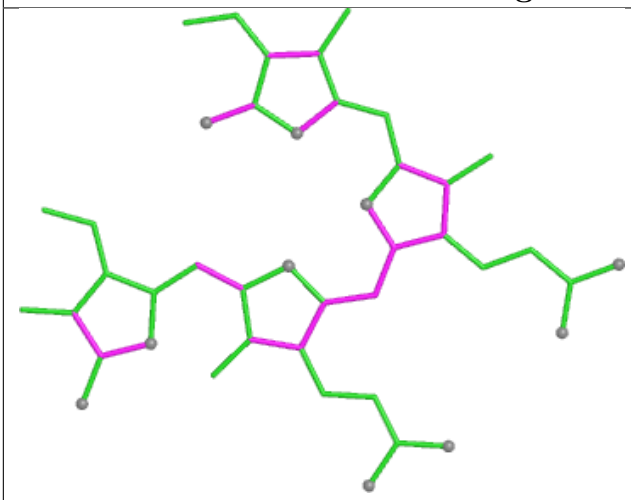


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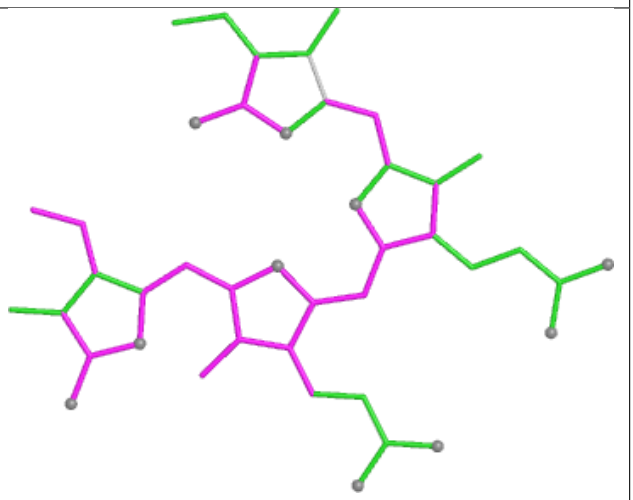


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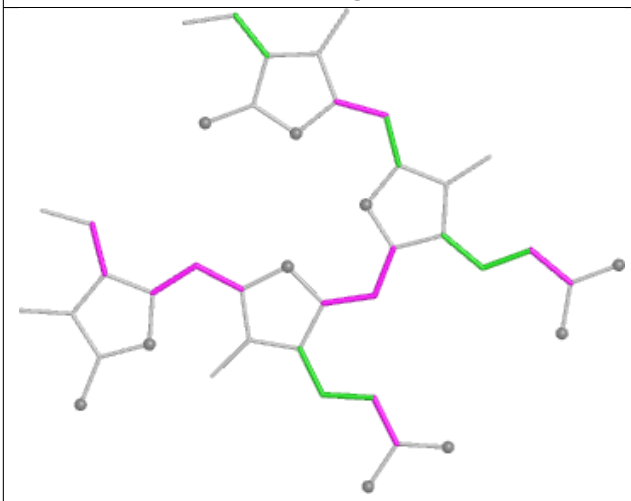
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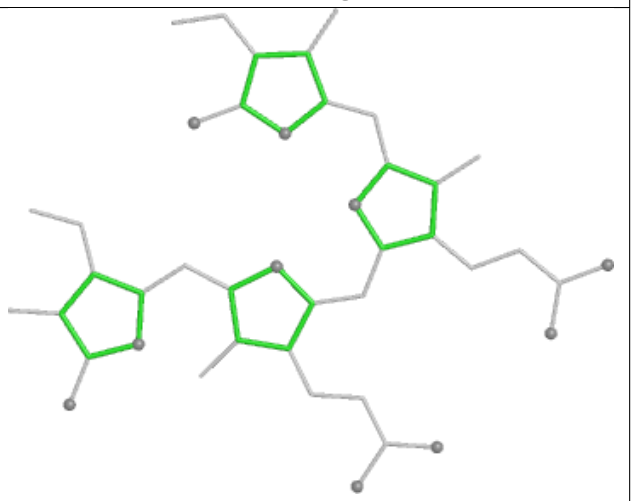
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Bond angles

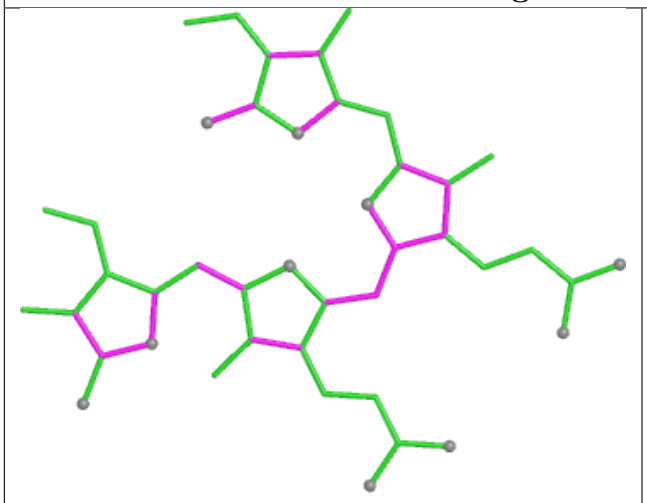


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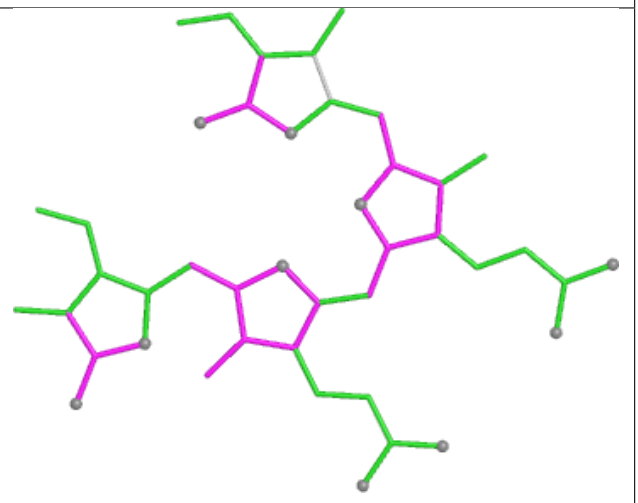


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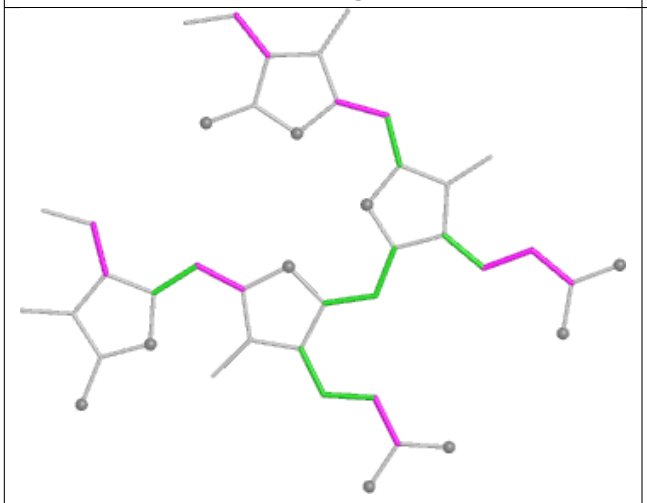
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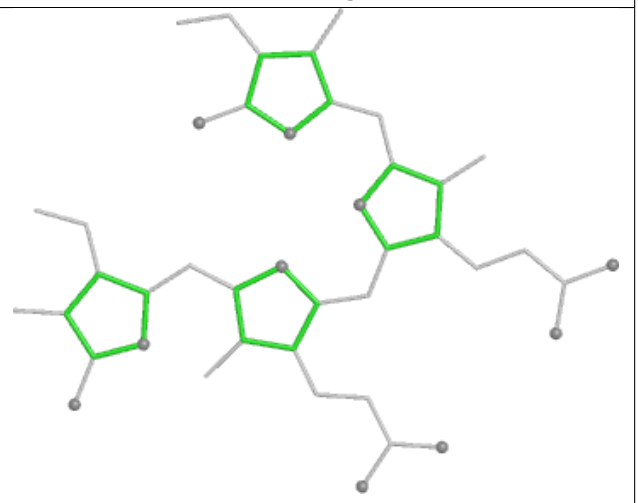
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Bond angles

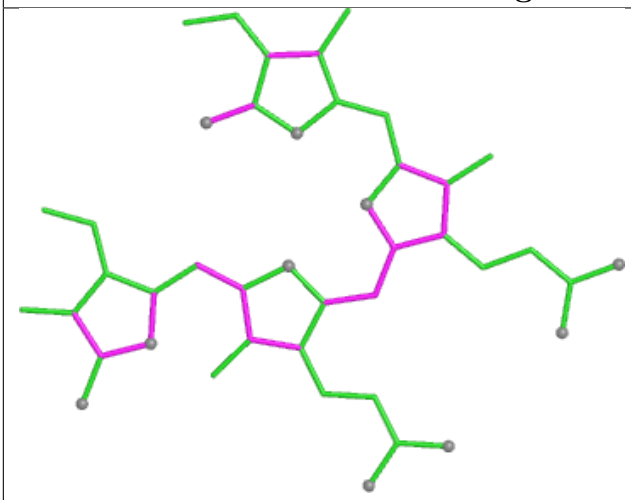


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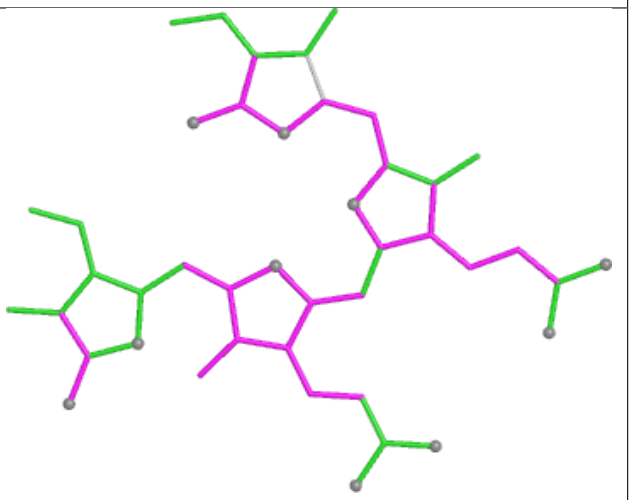


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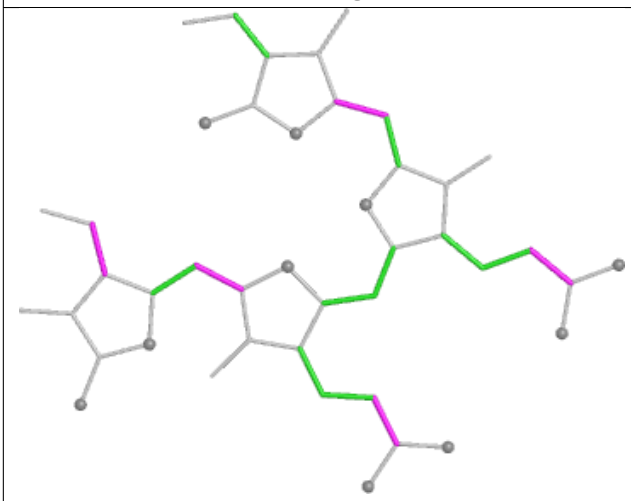
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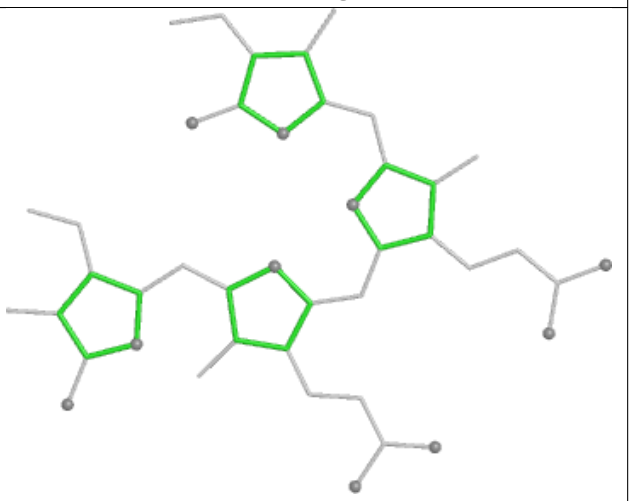
Bond lengths



Bond angles

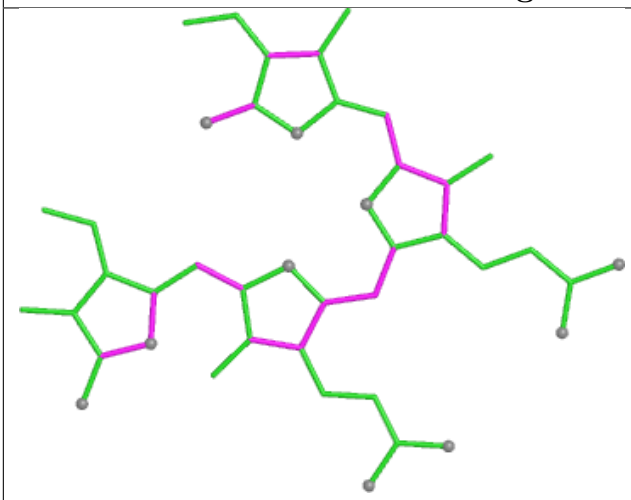


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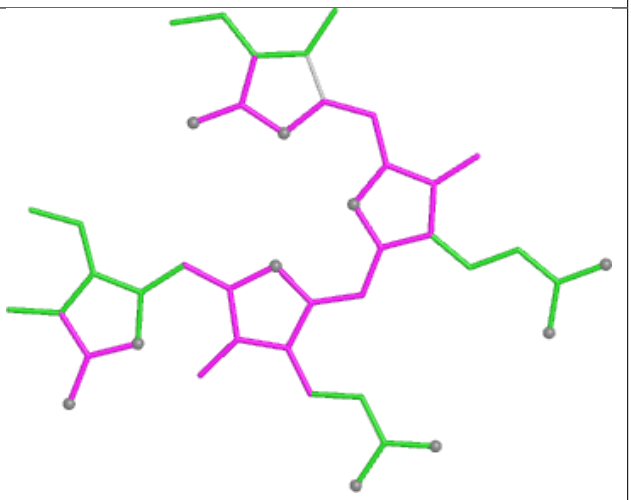


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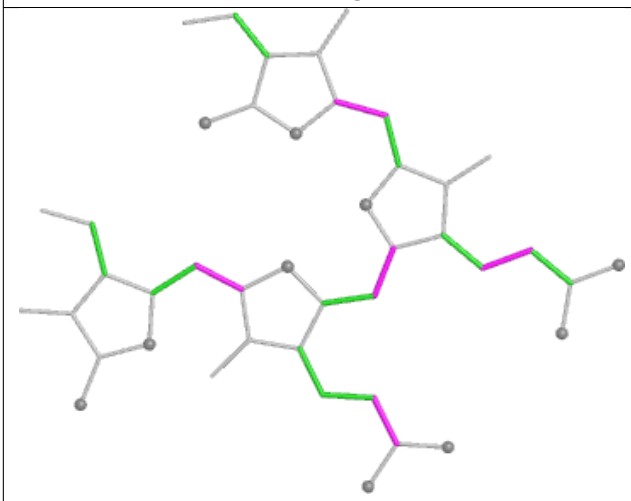
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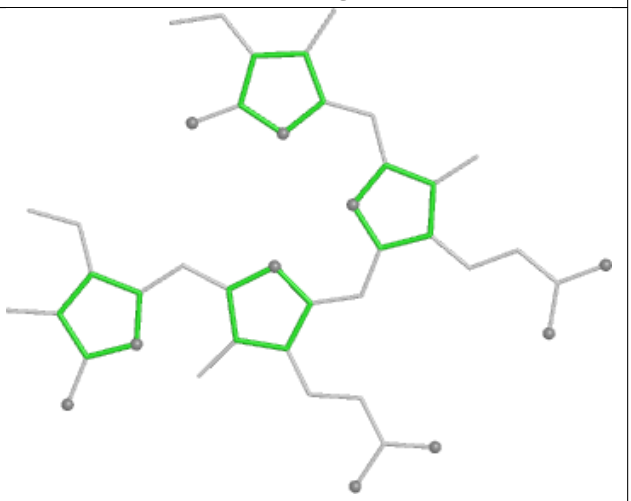
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Bond angles

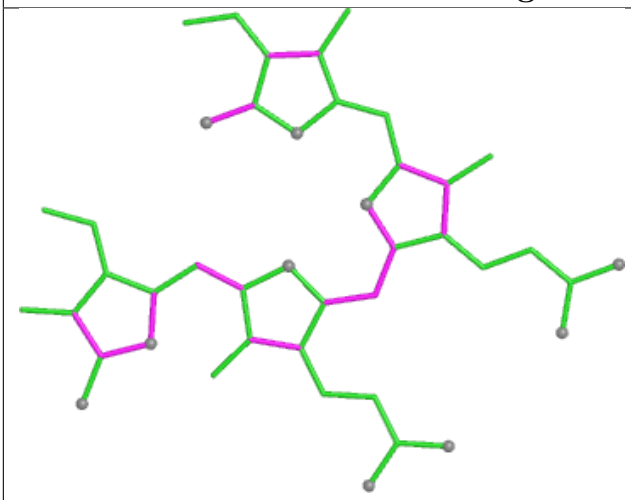


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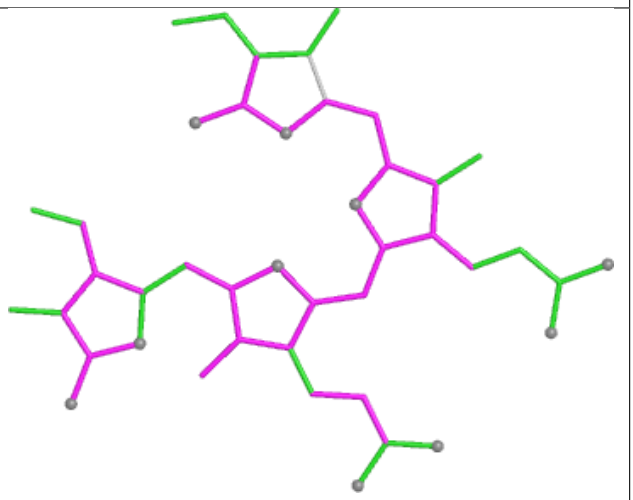


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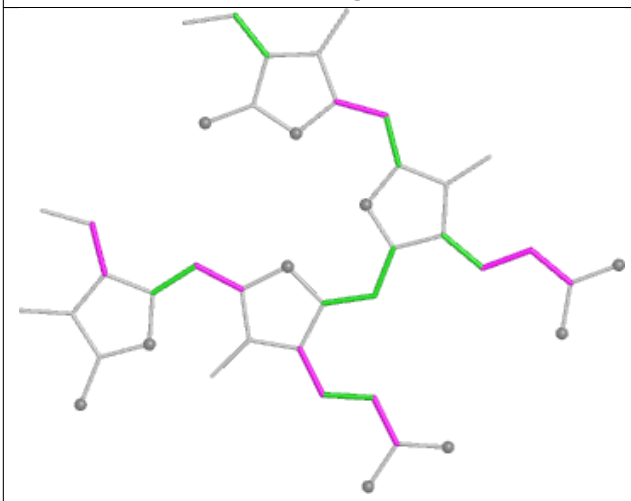
Ligand PEB F5 201



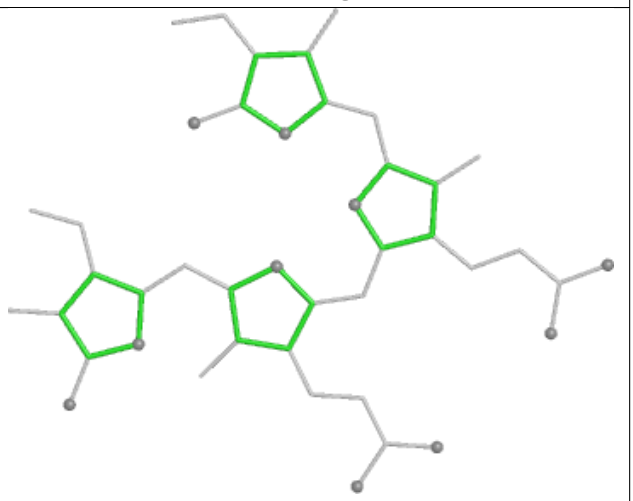
Bond lengths



Bond angles

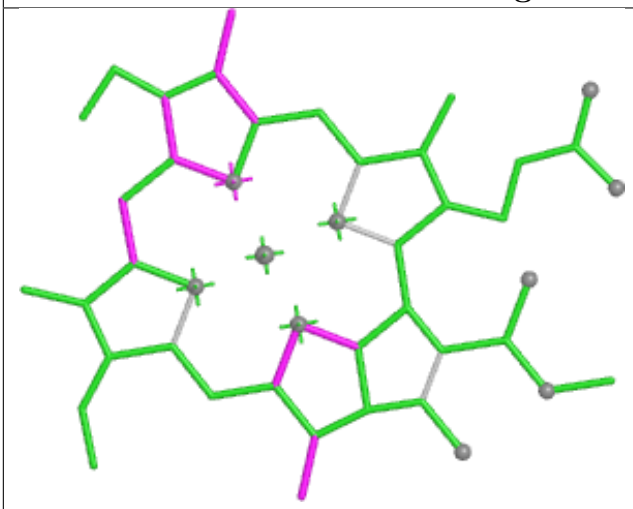


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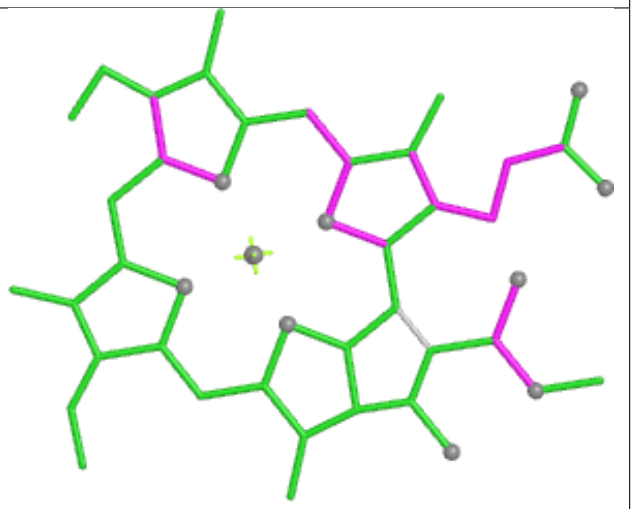


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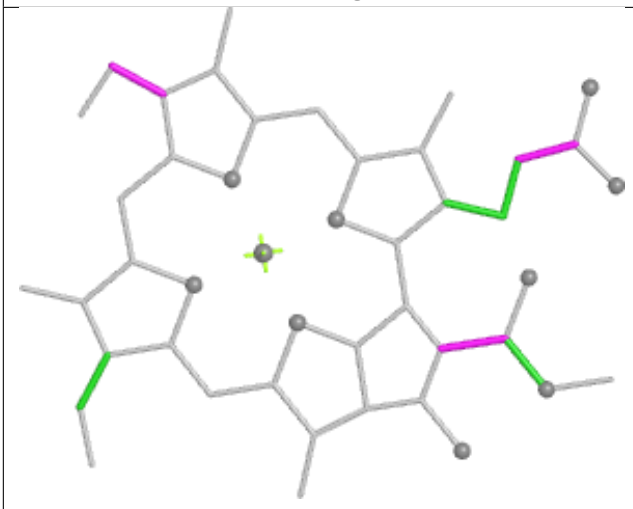
Ligand CLA 5N 605



Bond lengths



Bond angles

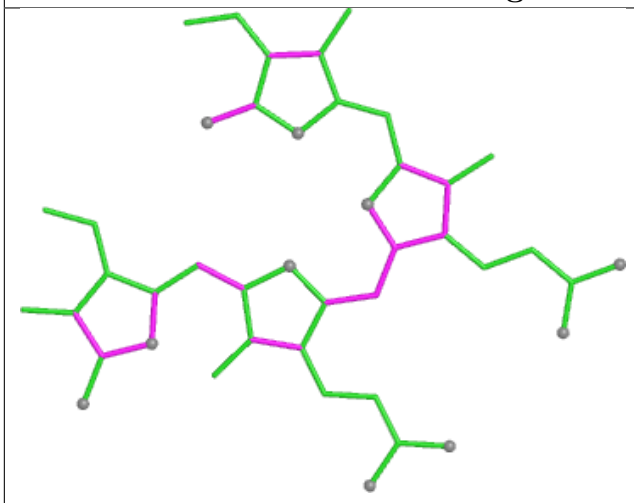


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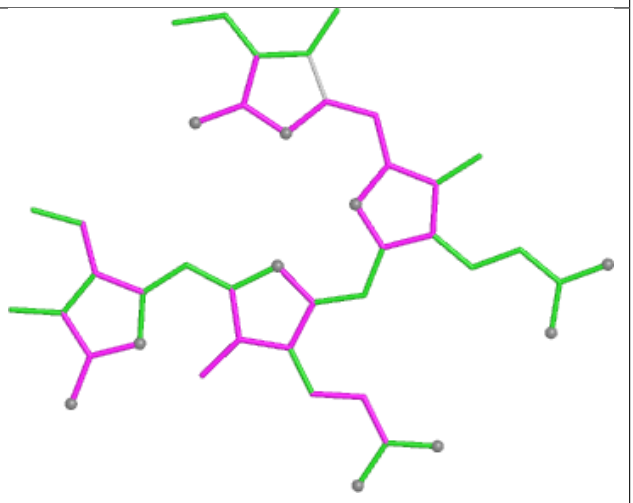


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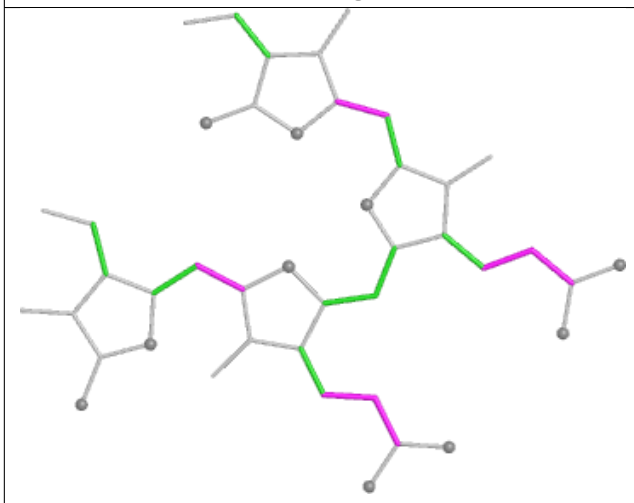
Ligand PEB JH 1002



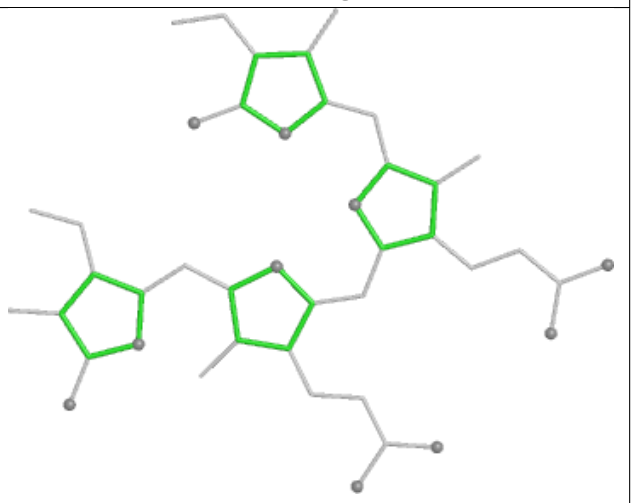
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Bond angles

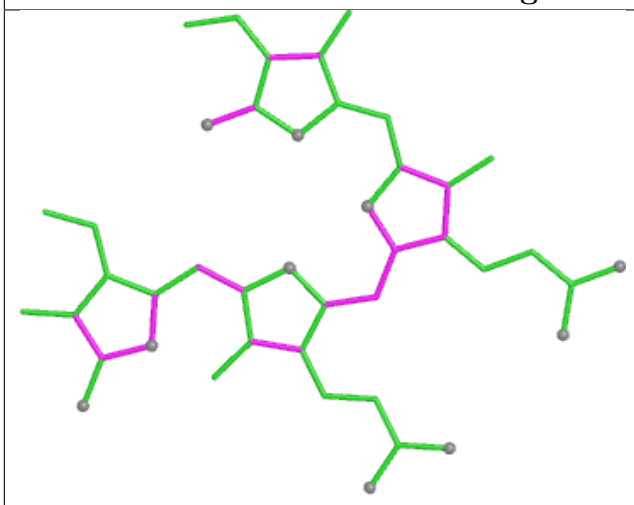


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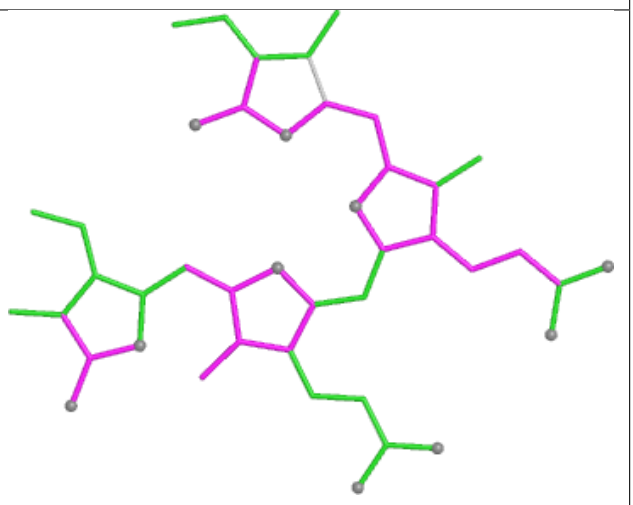


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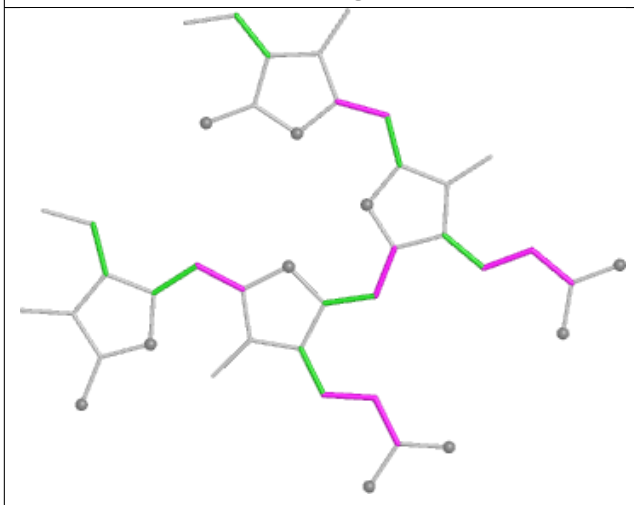
Ligand PEB J5 203



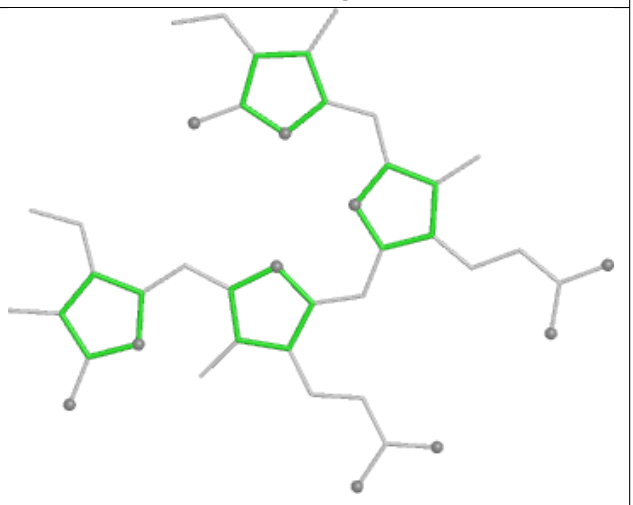
Bond lengths



Bond angles

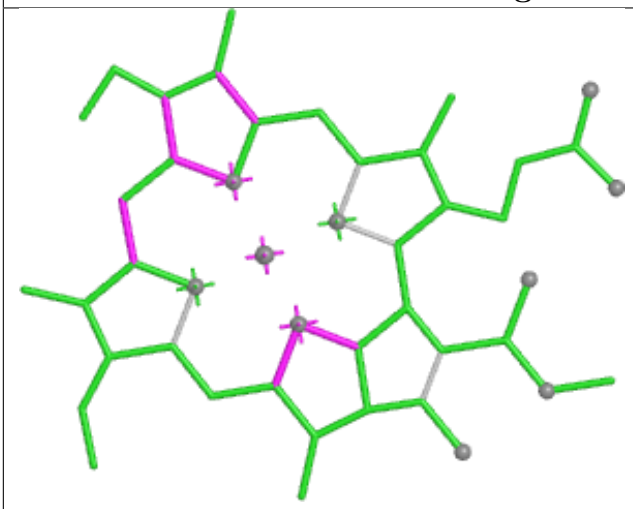


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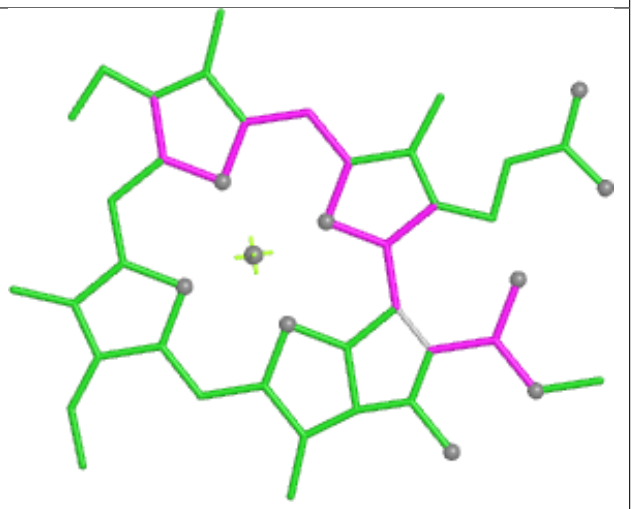


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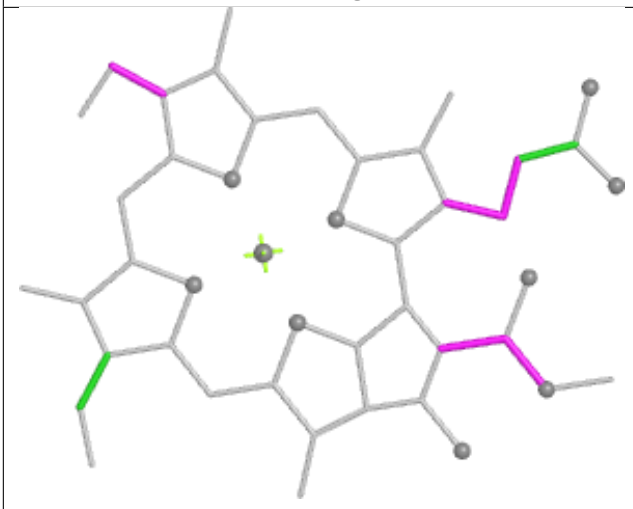
Ligand CLA 1N 610



Bond lengths



Bond angles

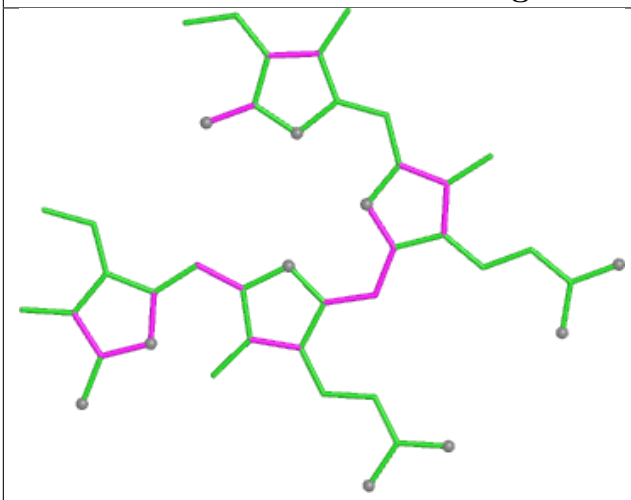


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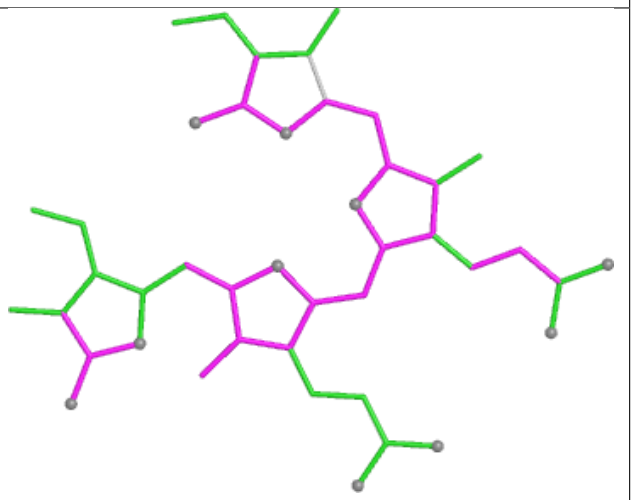


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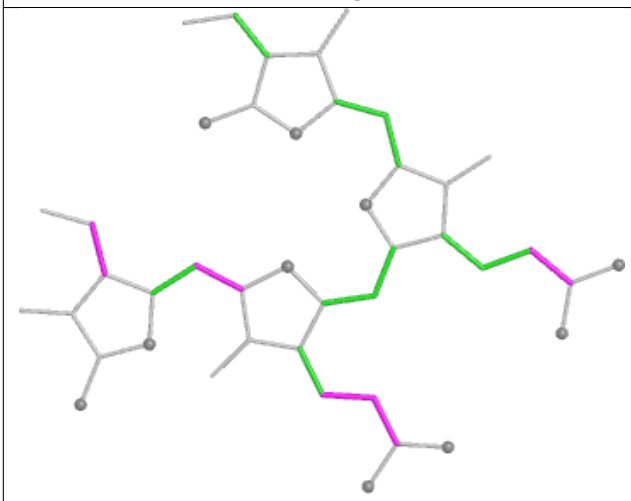
Ligand PEB M5 301



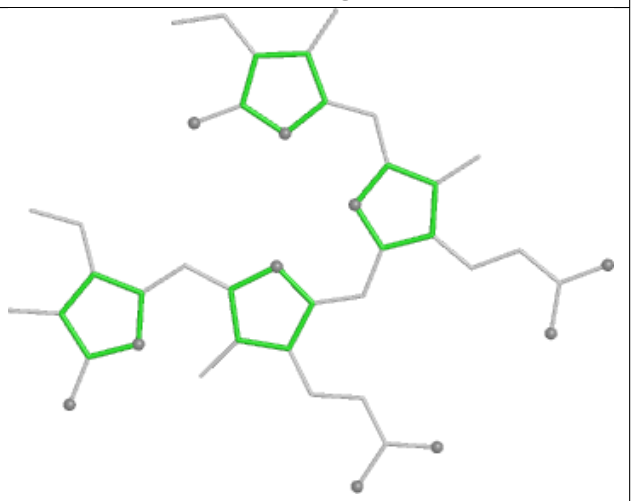
Bond lengths



Bond angles

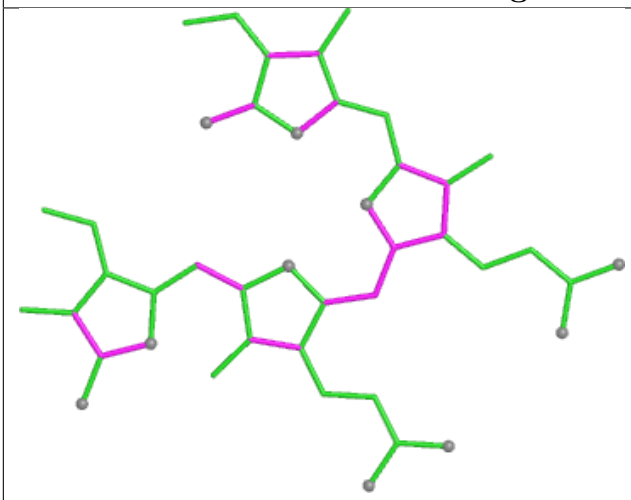


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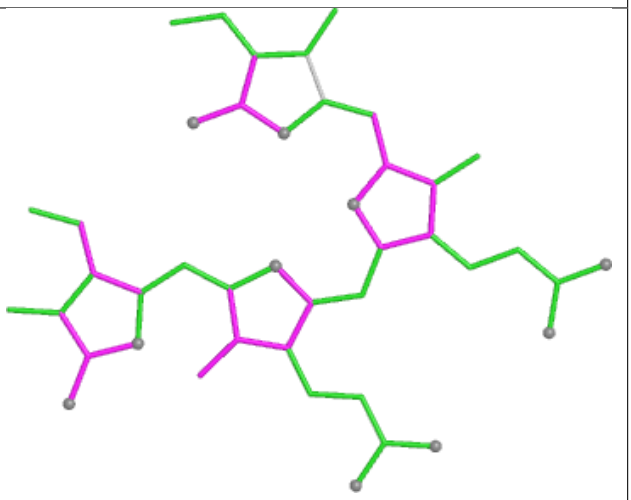


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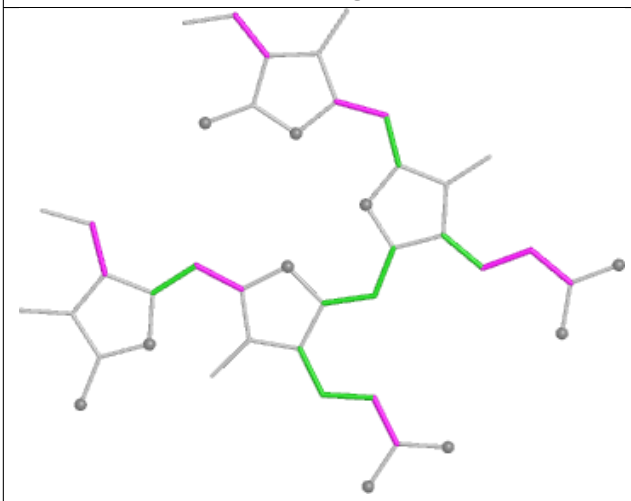
Ligand PEB KA 202



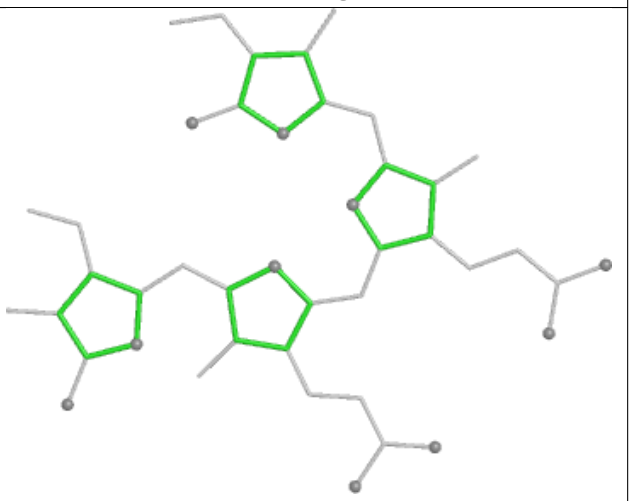
Bond lengths



Bond angles

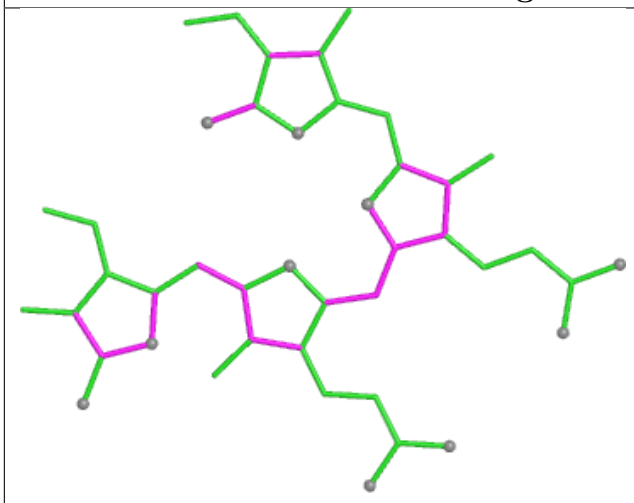


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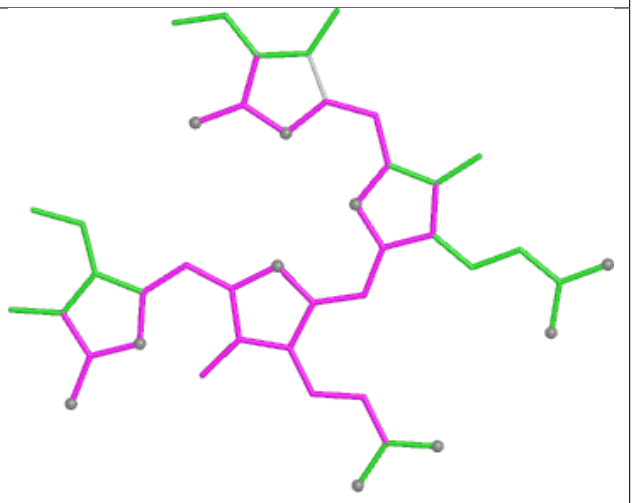


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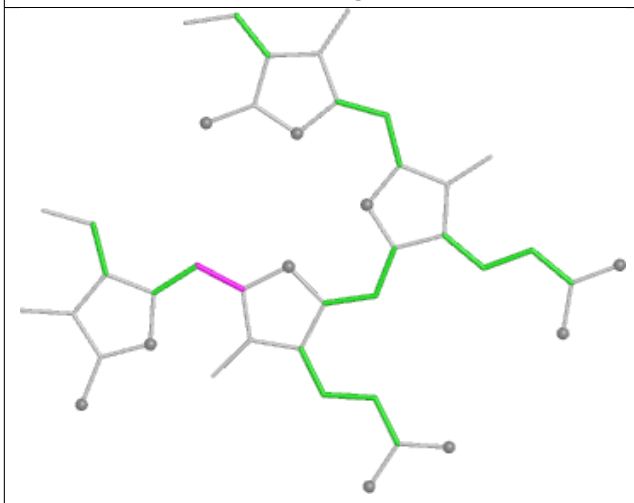
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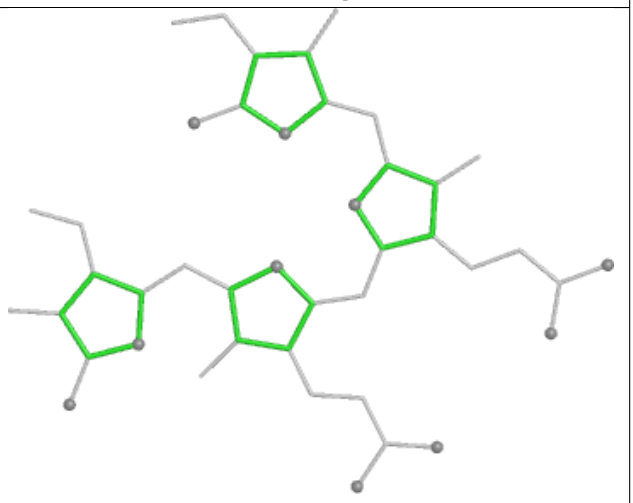
Bond lengths



Bond angles

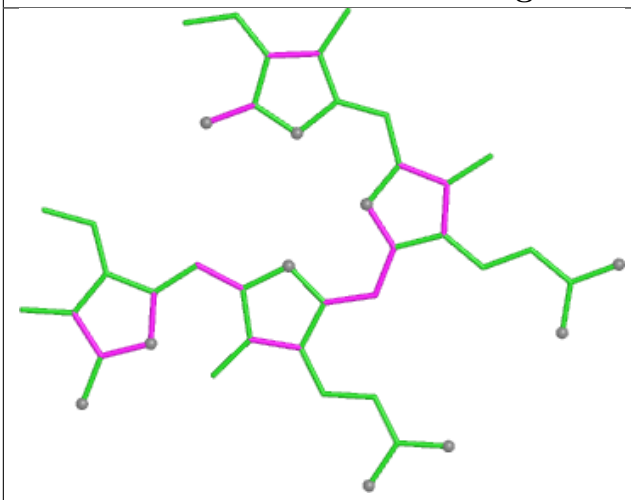


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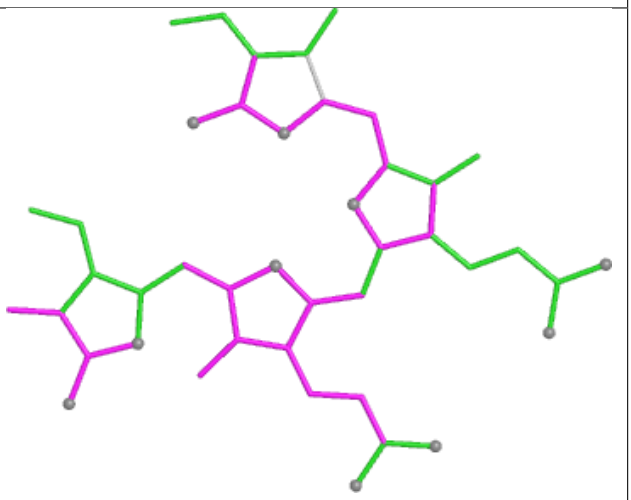


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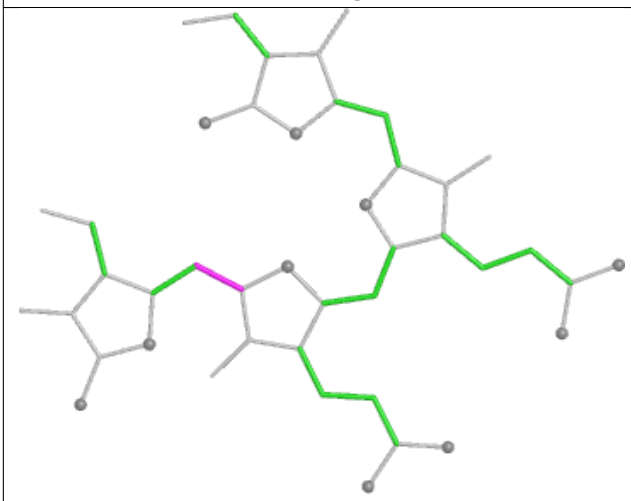
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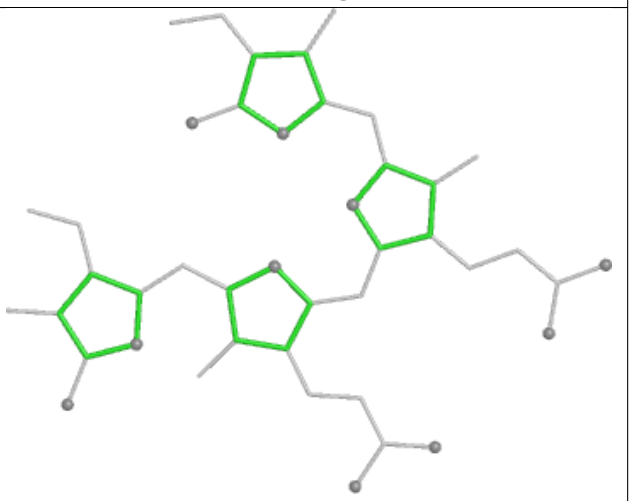
Bond lengths



Bond angles

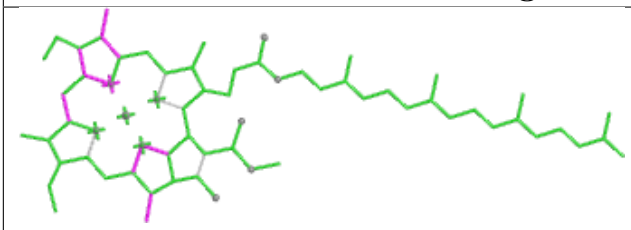


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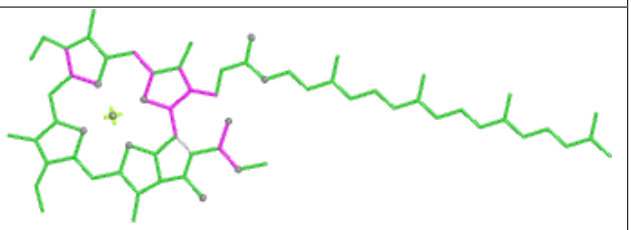


Rings

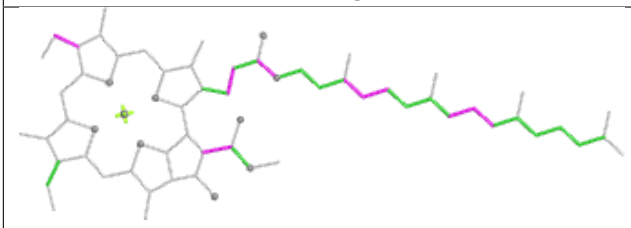
Ligand CLA cL 507



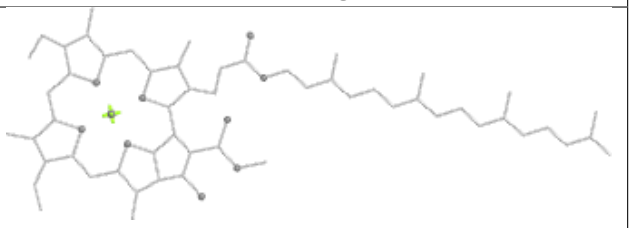
Bond lengths



Bond angles

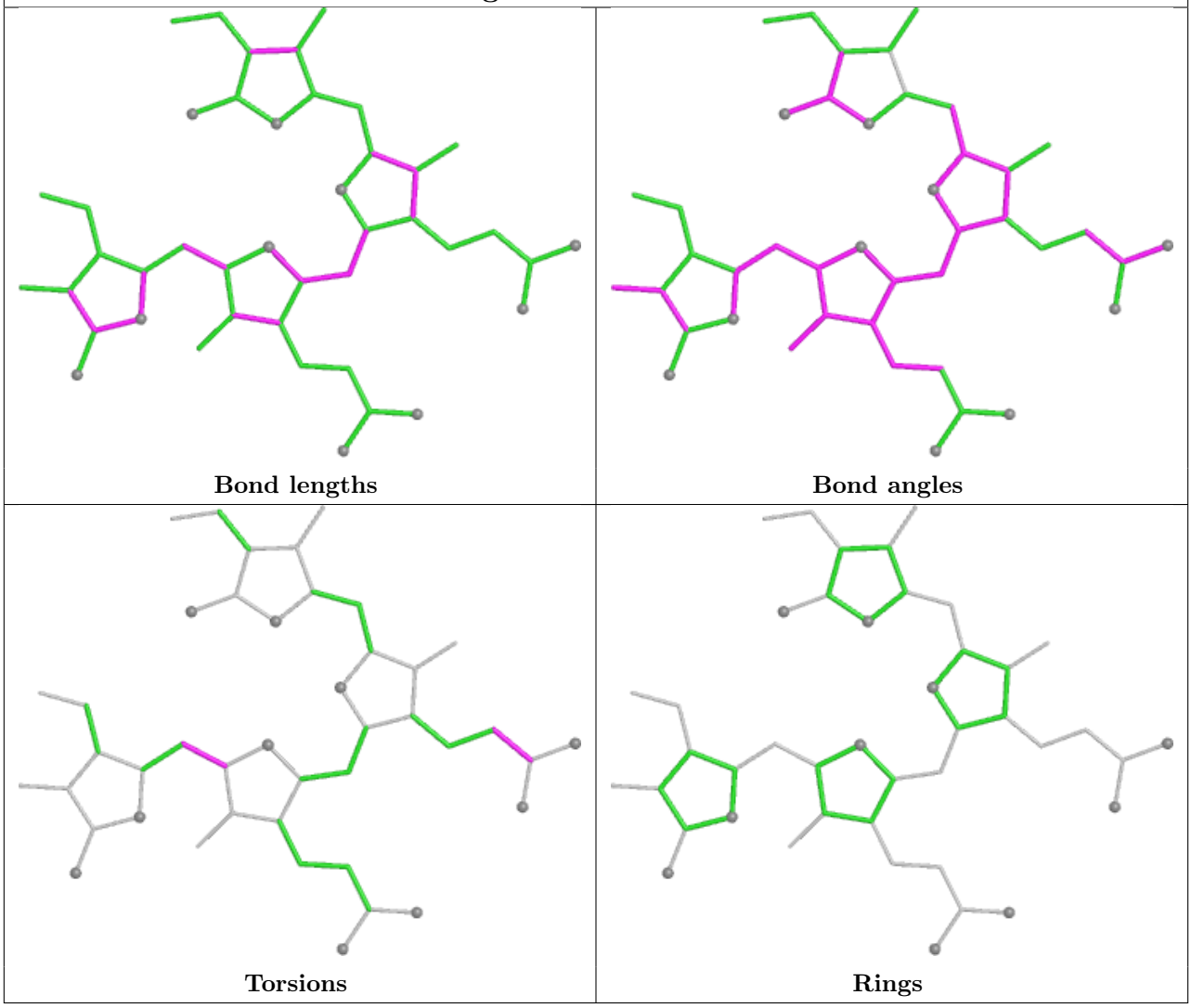


Torsions



Rings

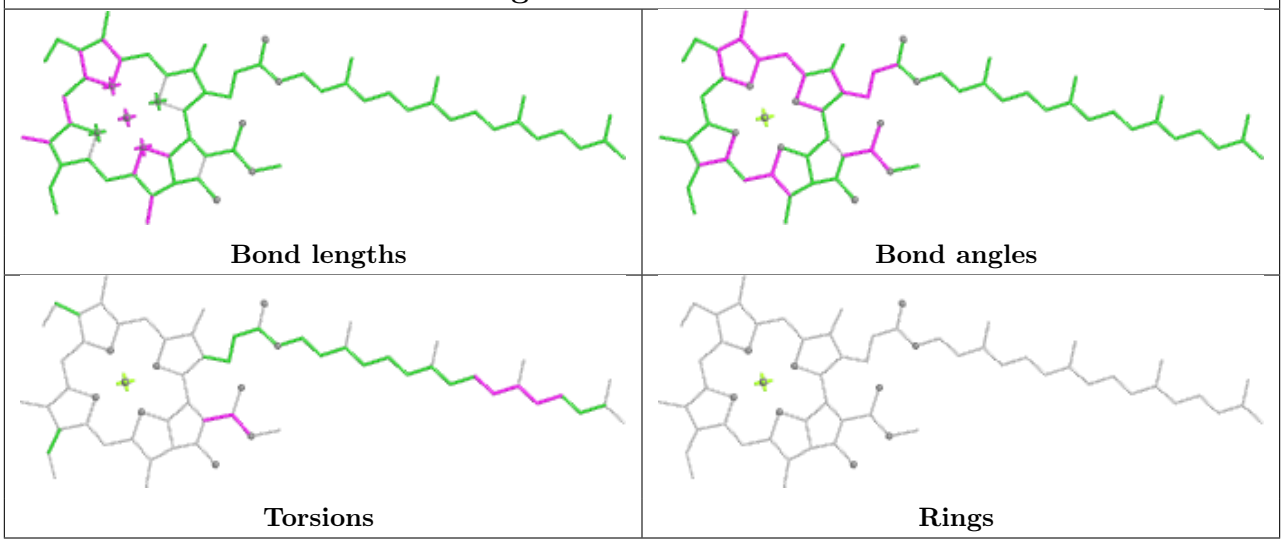
Ligand PEB S7 201



Bond lengths | Bond angles

Torsions | Rings

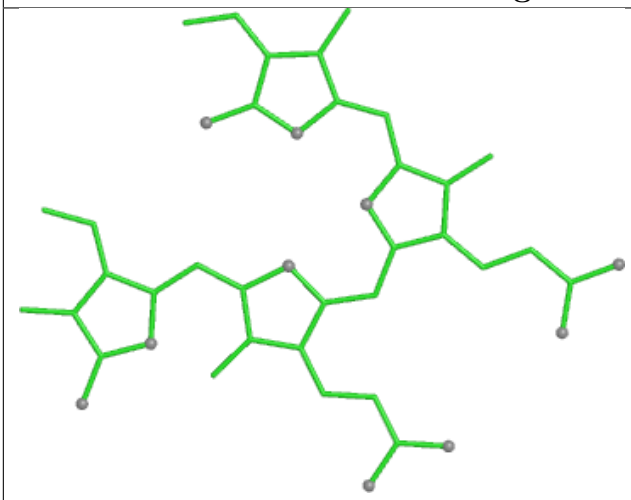
Ligand CLA BN 824



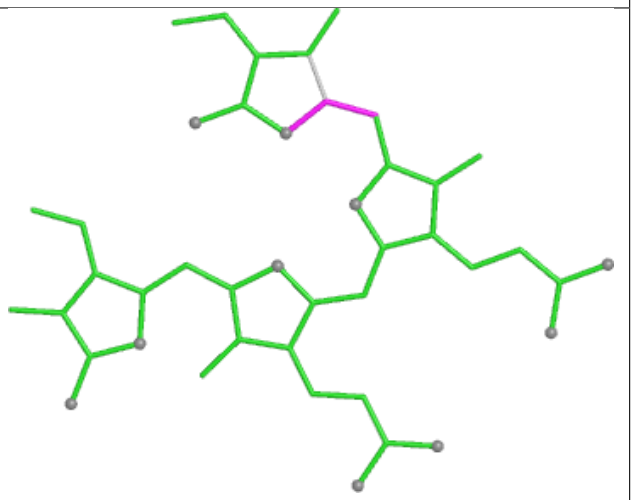
Bond lengths | Bond angles

Torsions | Rings

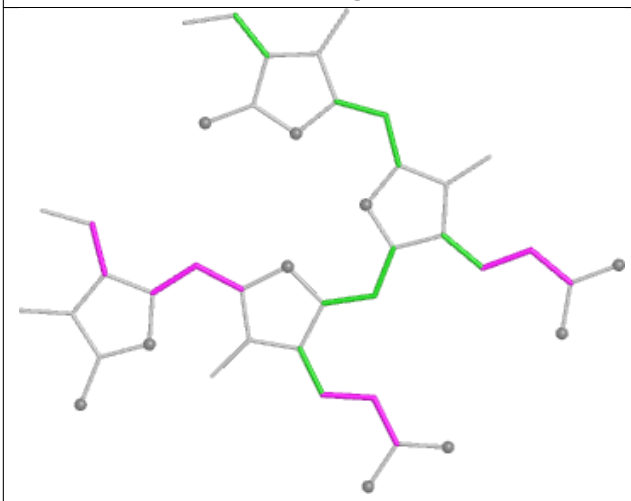
Ligand PEB hH 202



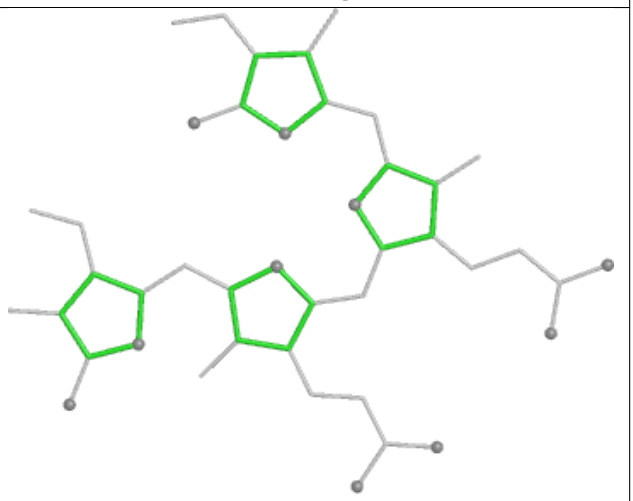
Bond lengths



Bond angles

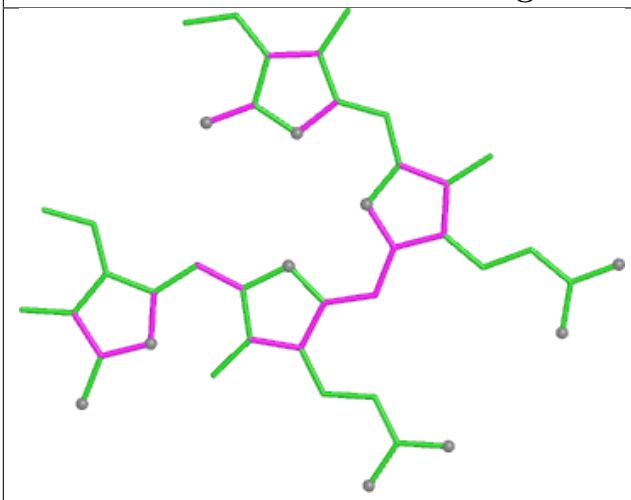


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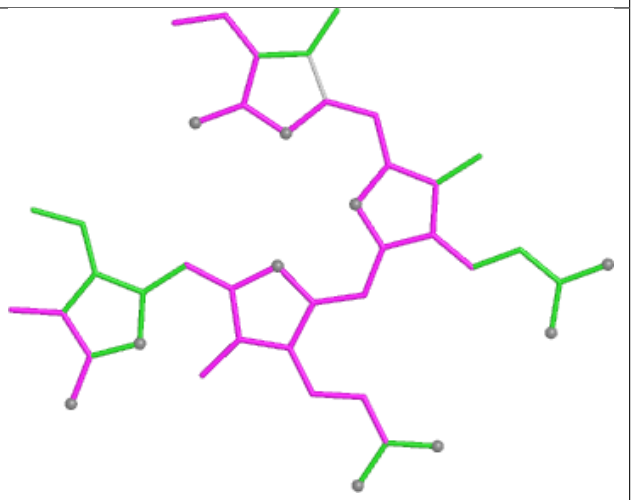


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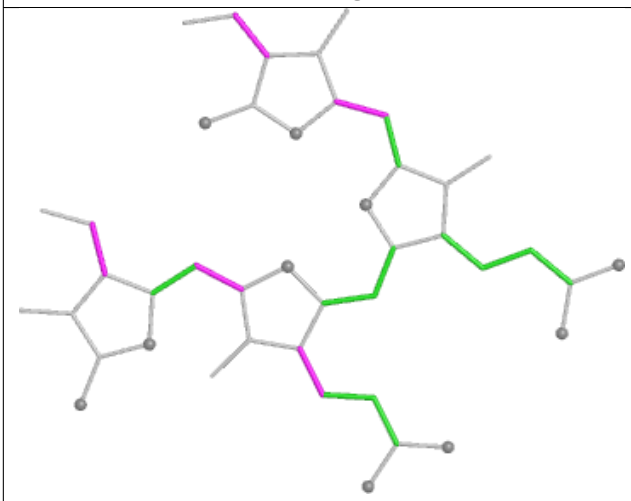
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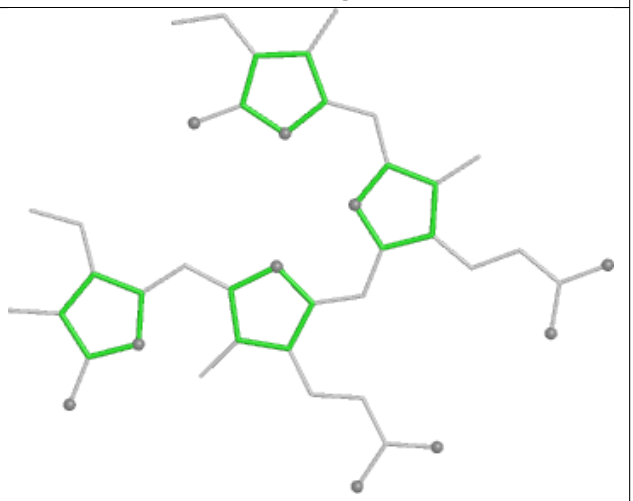
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Bond angles

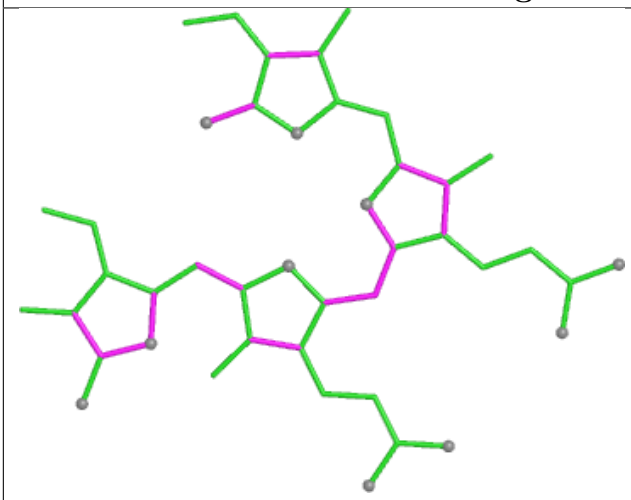


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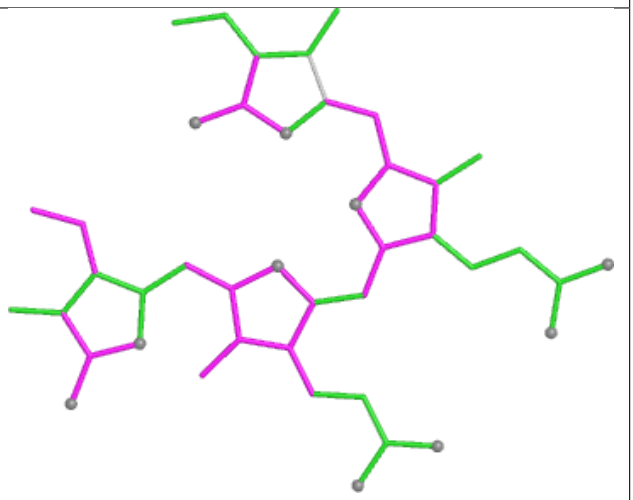


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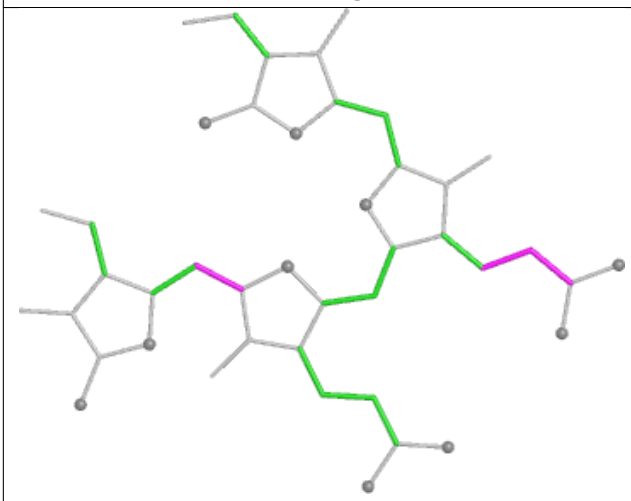
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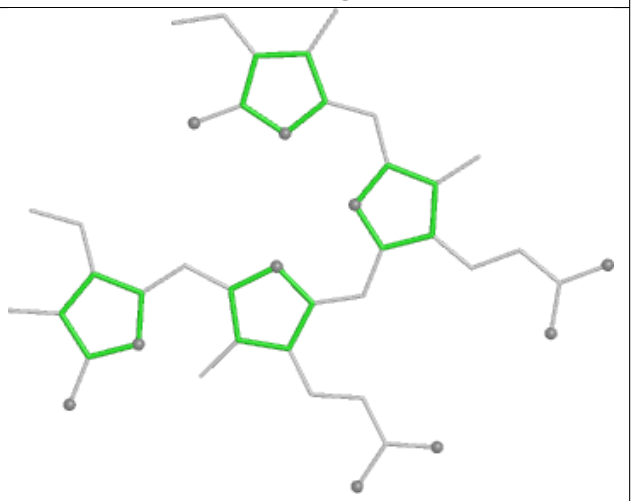
Bond lengths



Bond angles

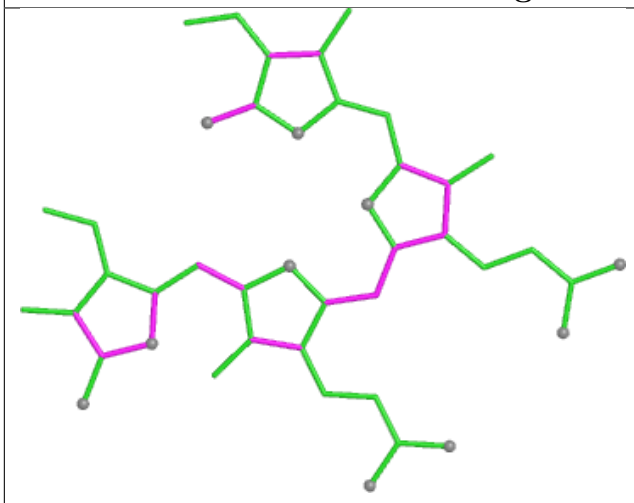


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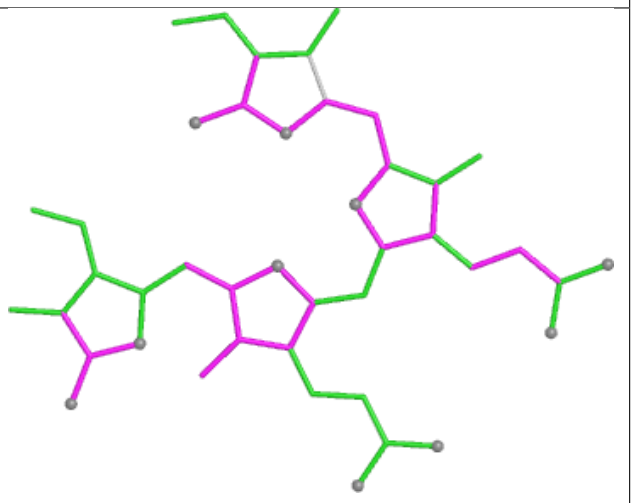


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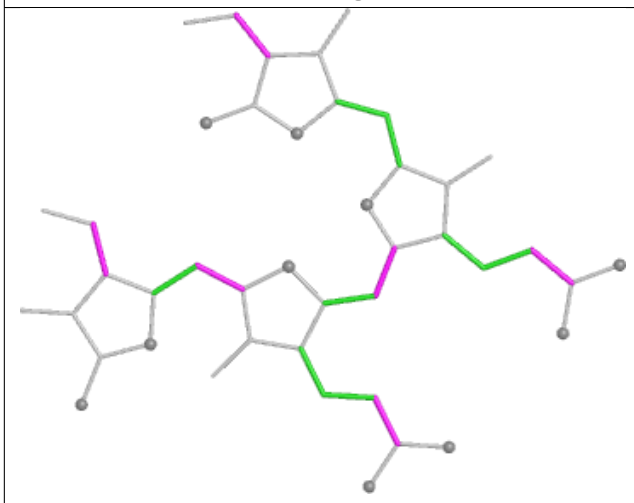
Ligand PEB FB 201



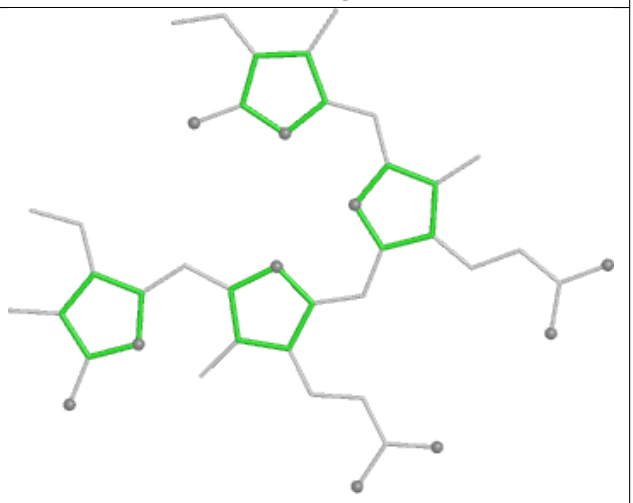
Bond lengths



Bond angles

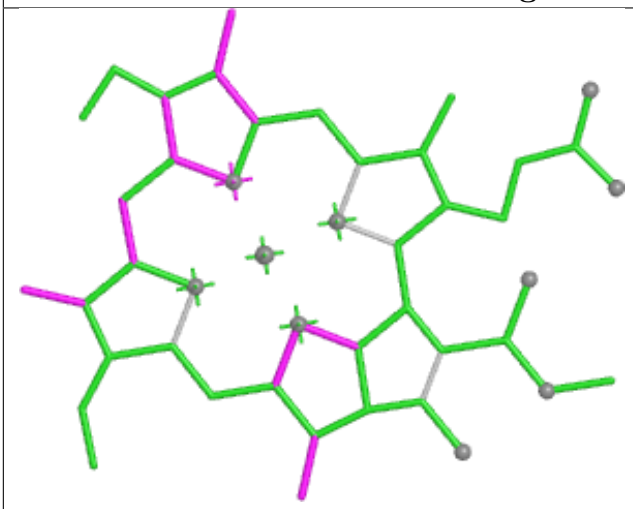


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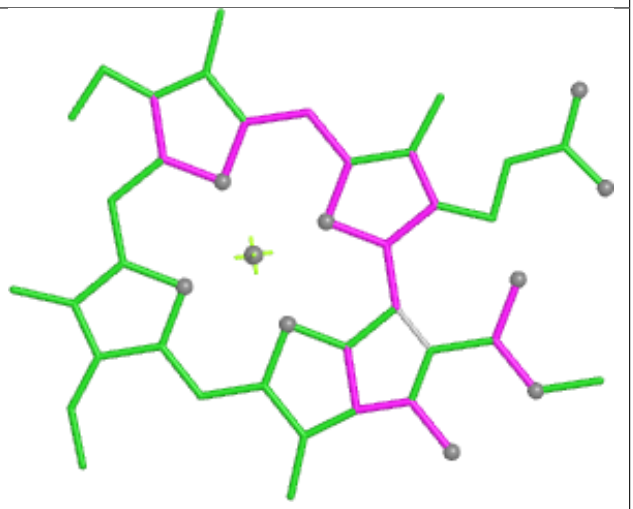


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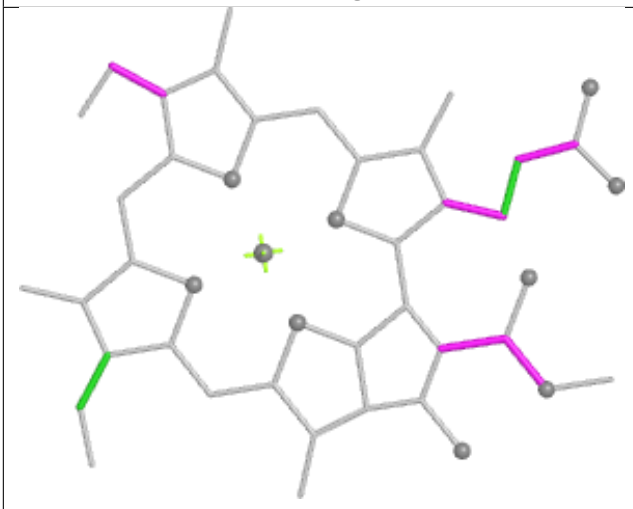
Ligand CLA 42 607



Bond lengths



Bond angles

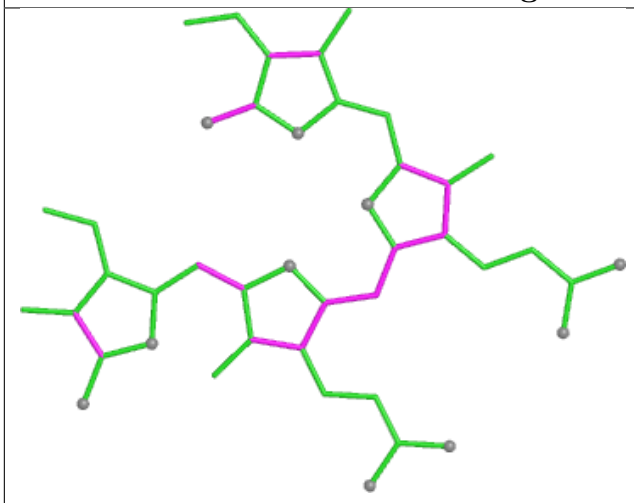


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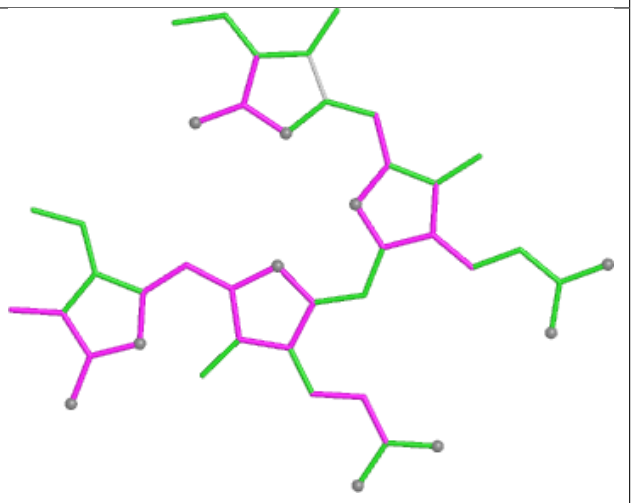


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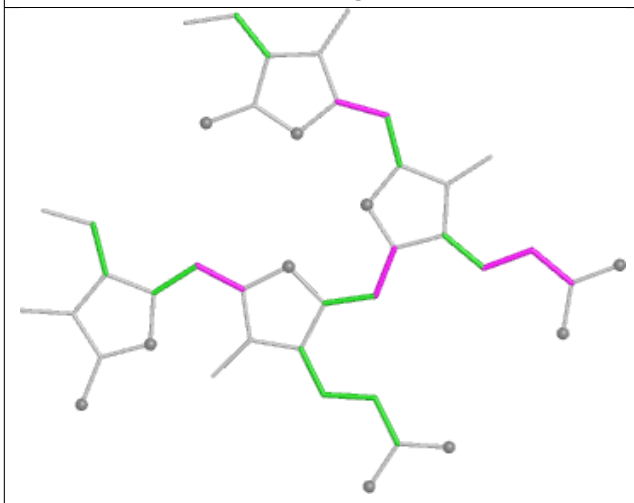
Ligand PEB tF 201



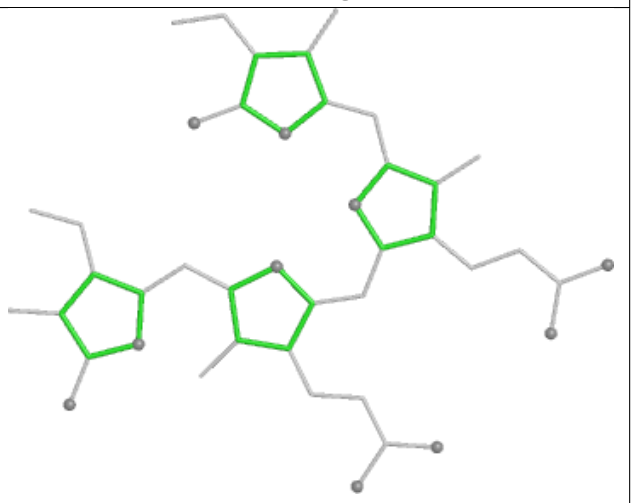
Bond lengths



Bond angles

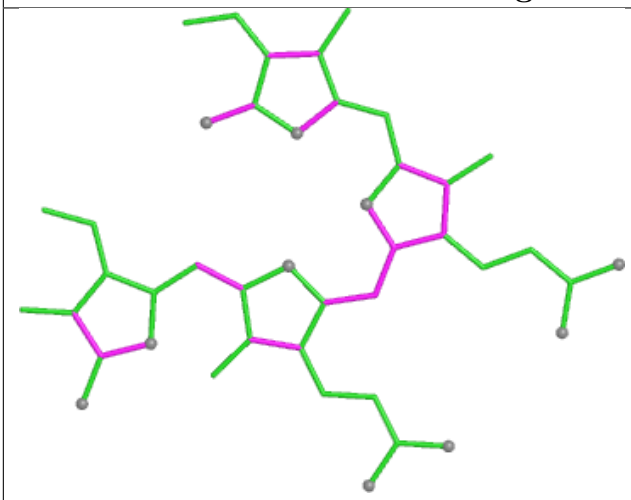


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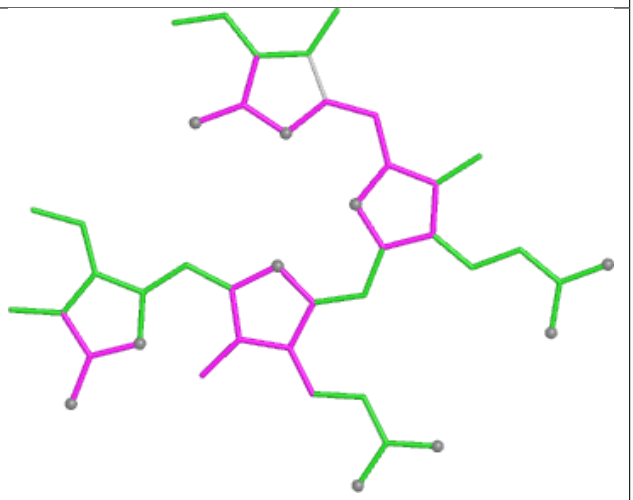


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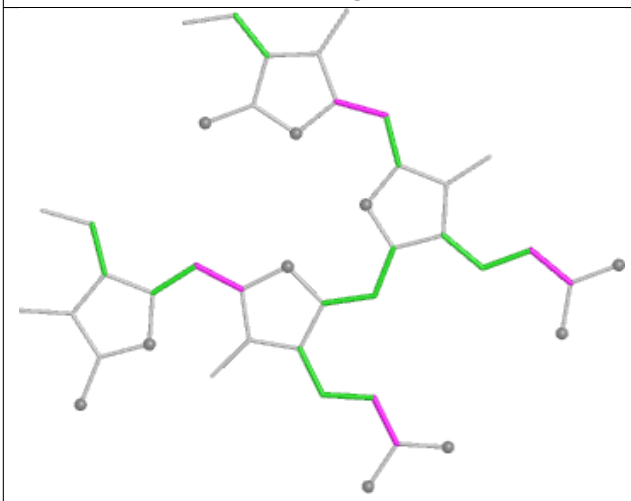
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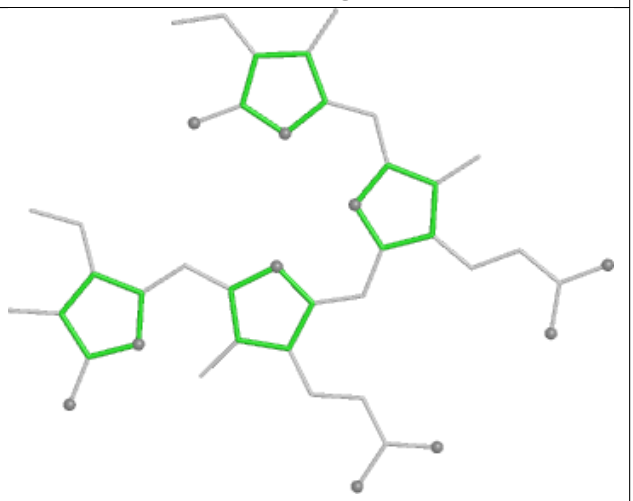
Bond lengths



Bond angles

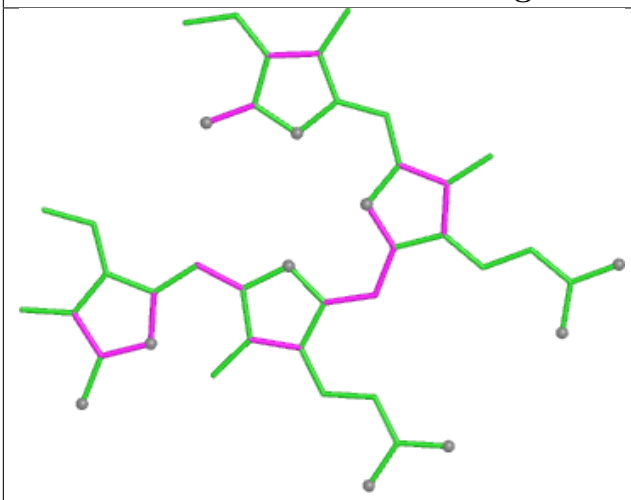


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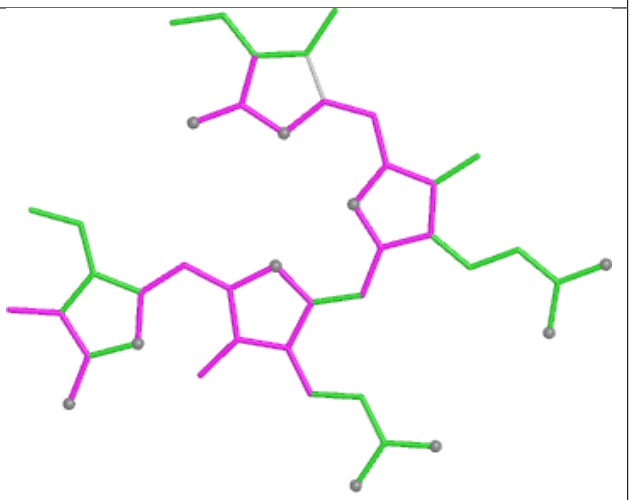


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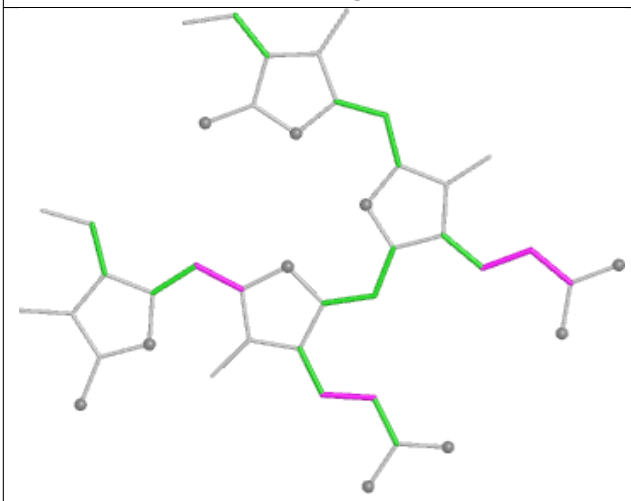
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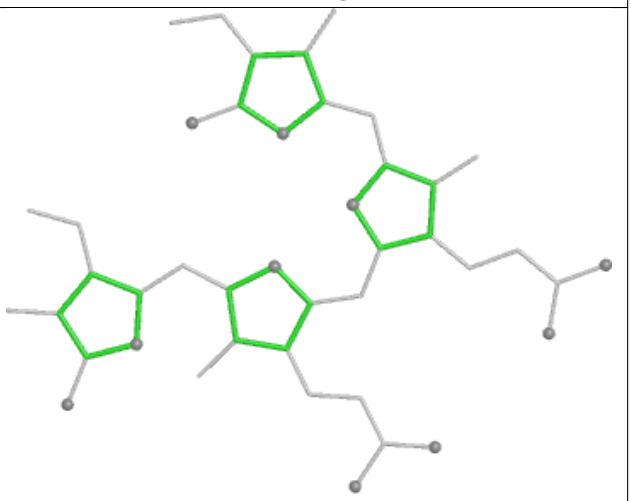
Bond lengths



Bond angles

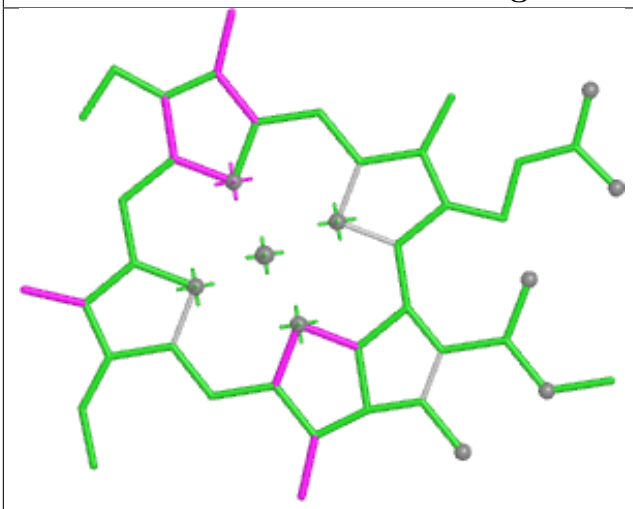


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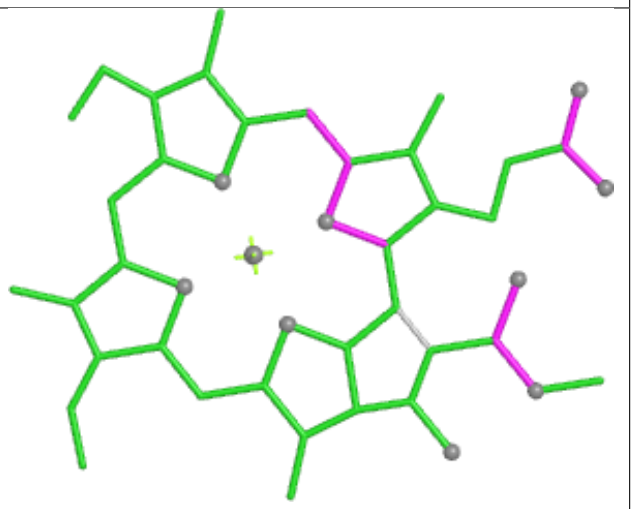


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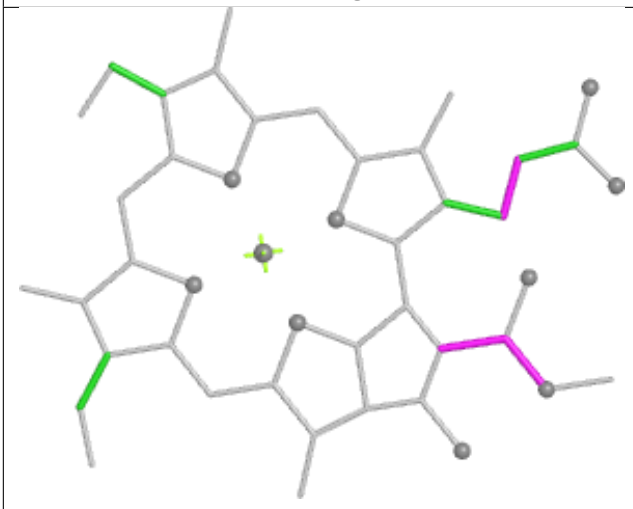
Ligand CLA BN 814



Bond lengths



Bond angles

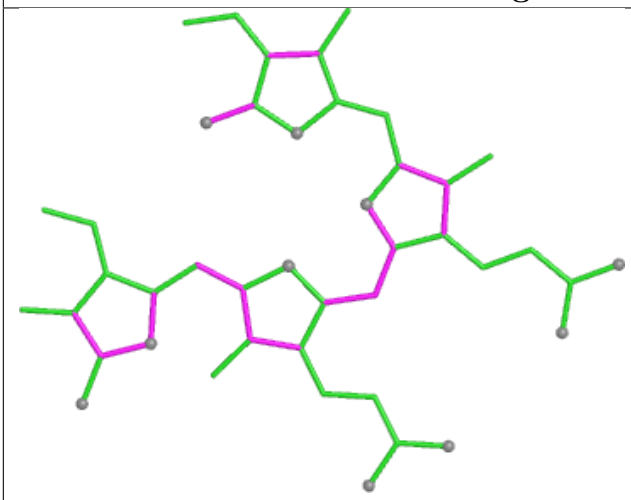


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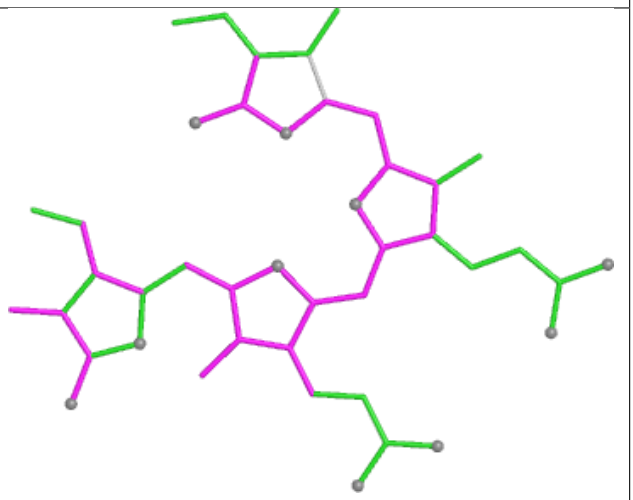


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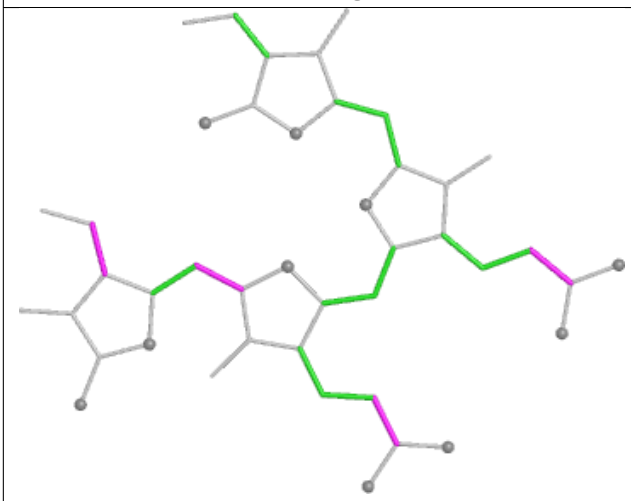
Ligand PEB TB 201



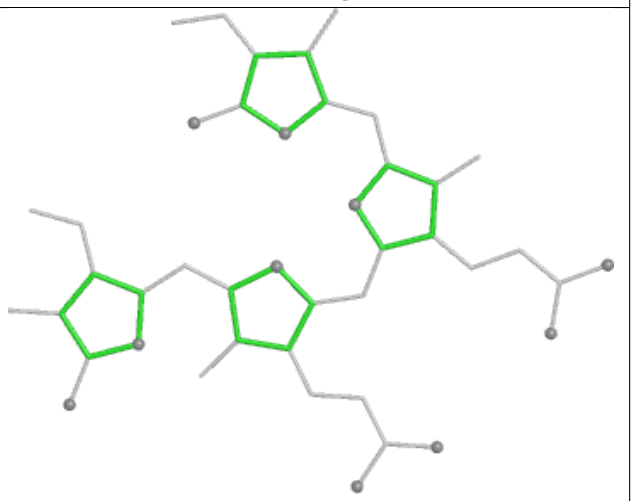
Bond lengths



Bond angles

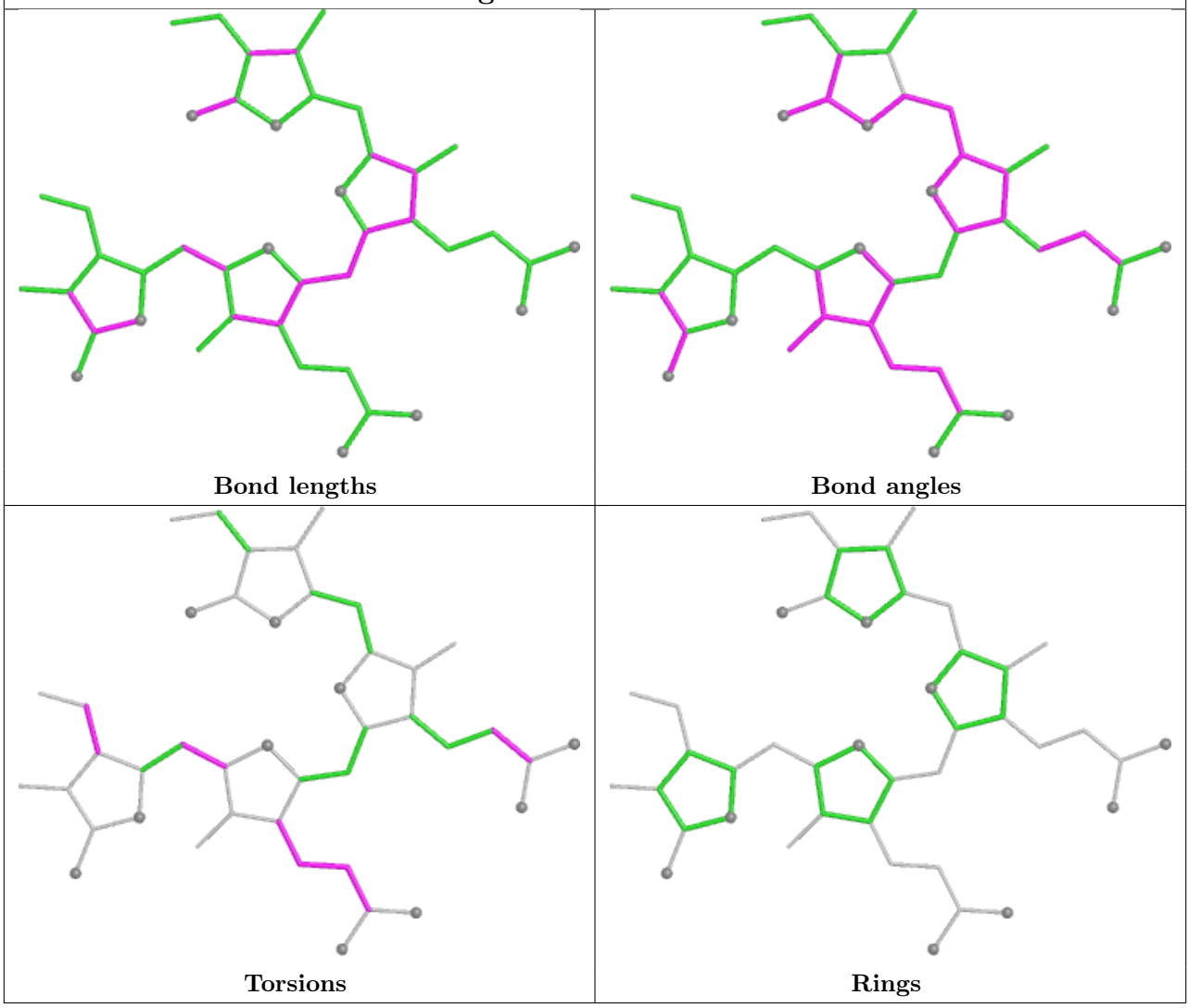


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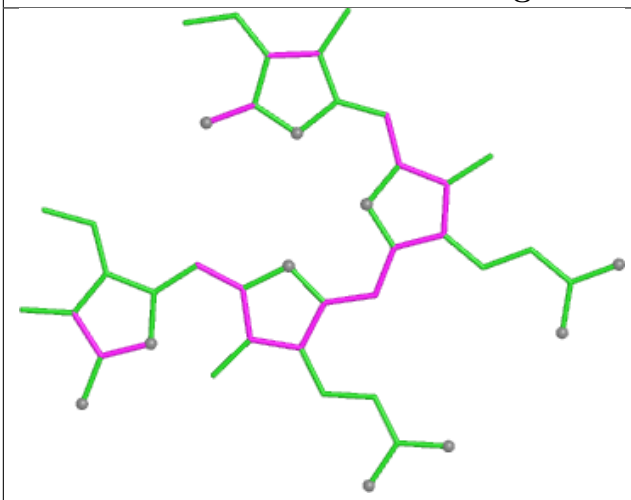


Rings

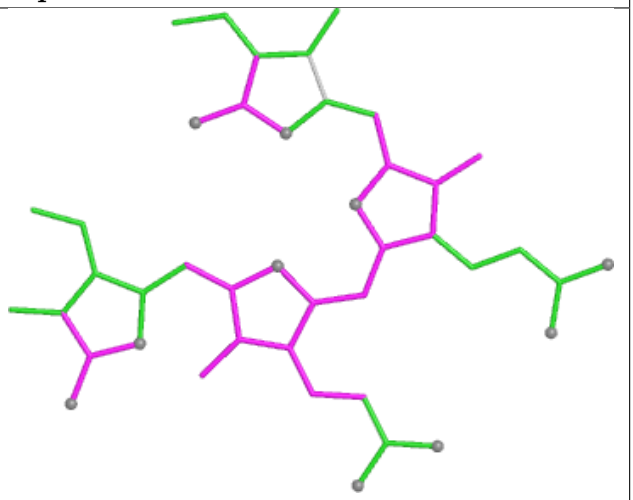
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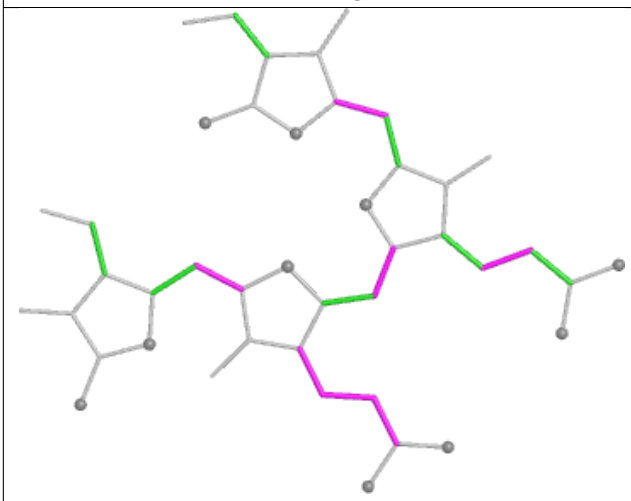
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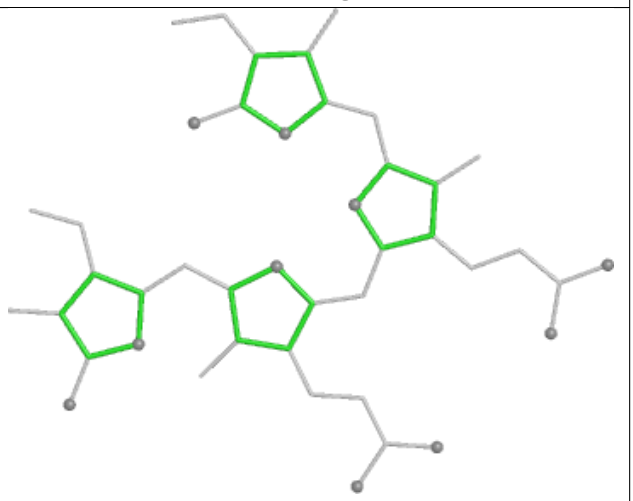
Bond lengths



Bond angles

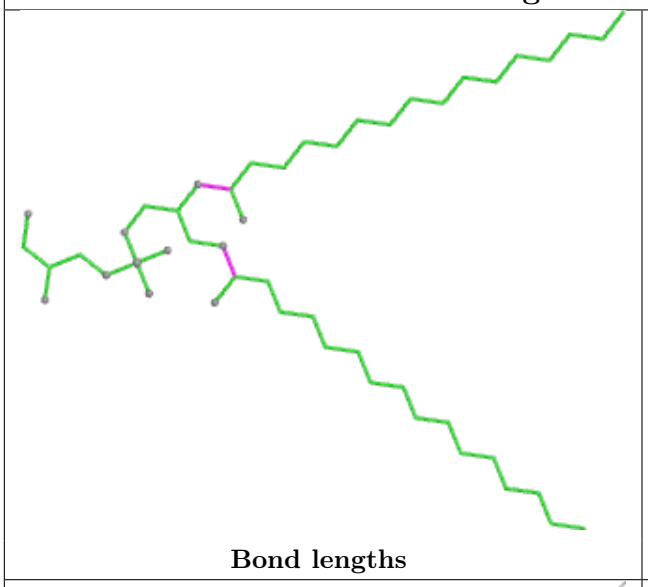


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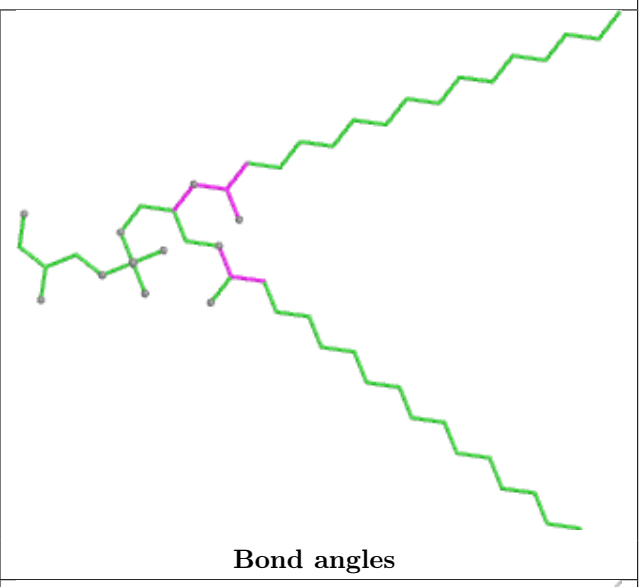


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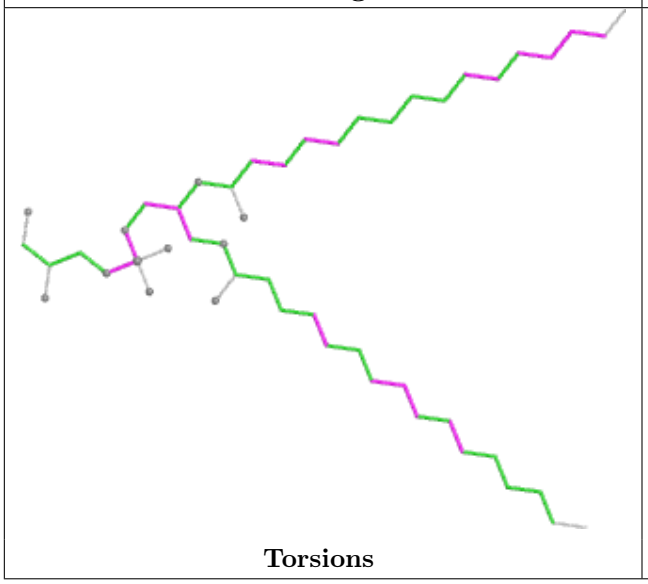
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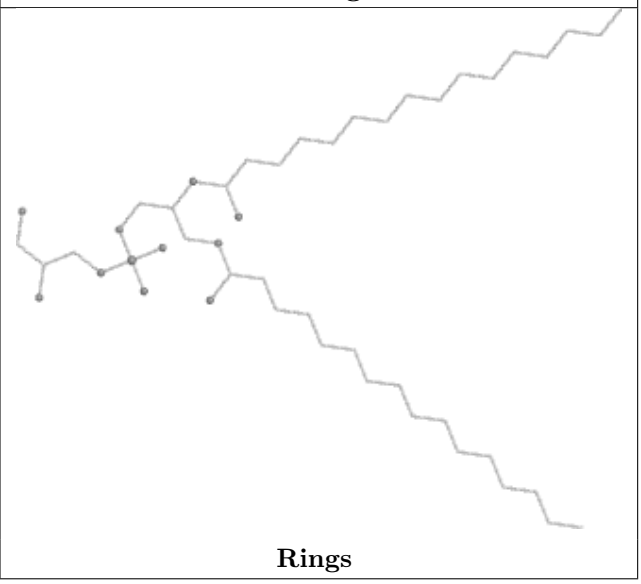
Bond lengths



Bond angles

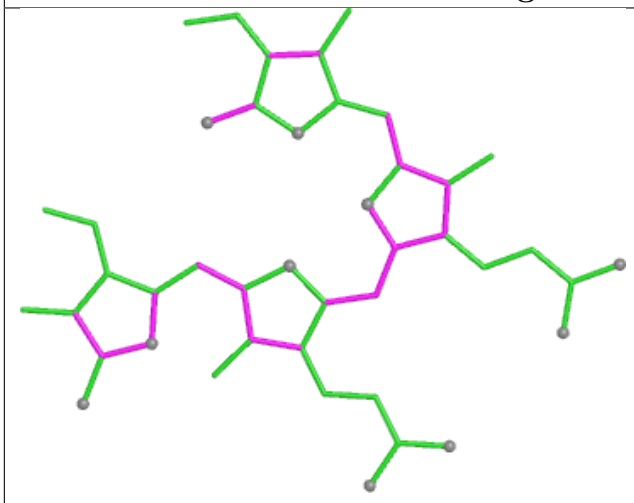


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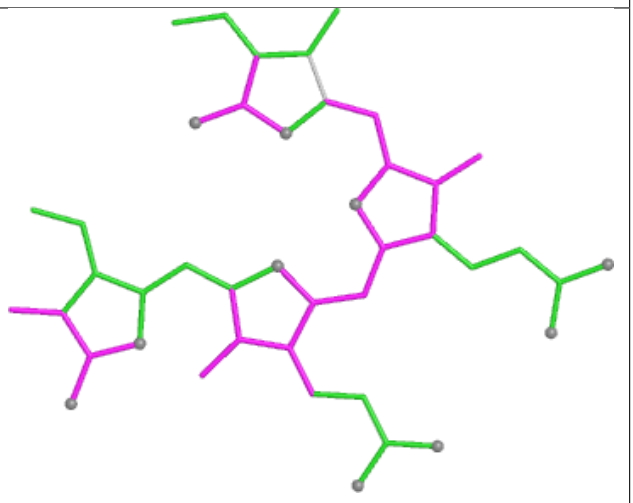


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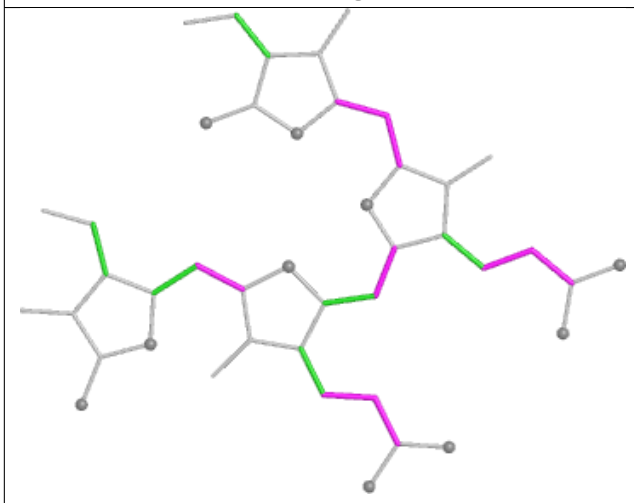
Ligand PEB dF 202



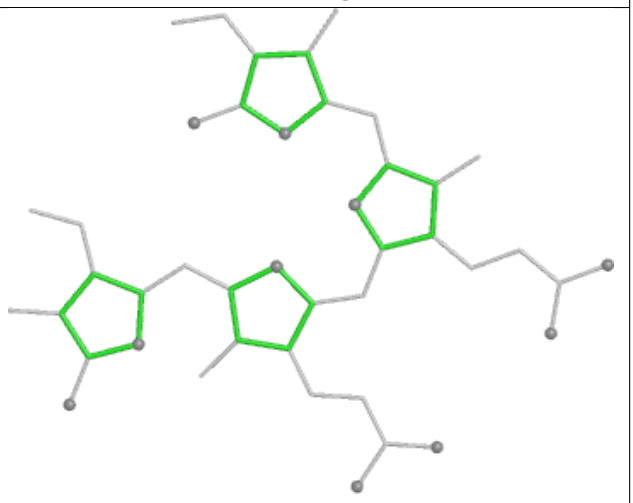
Bond lengths



Bond angles

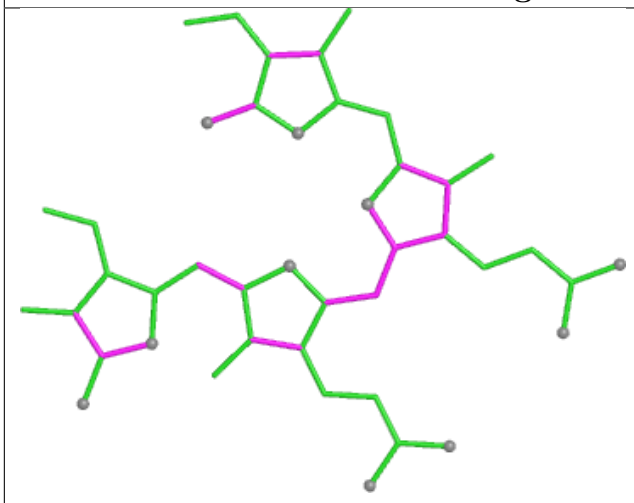


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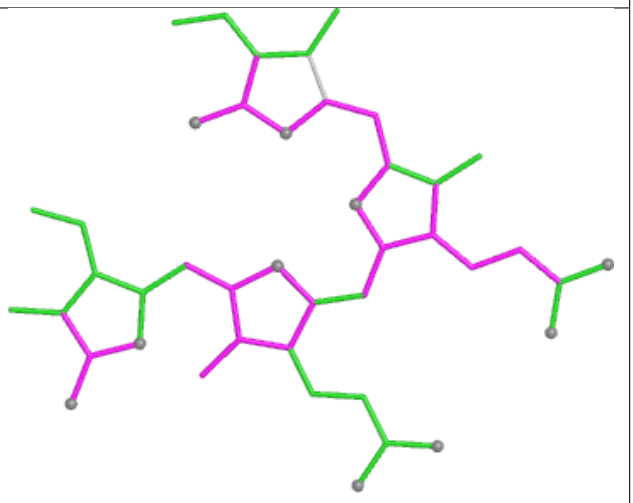


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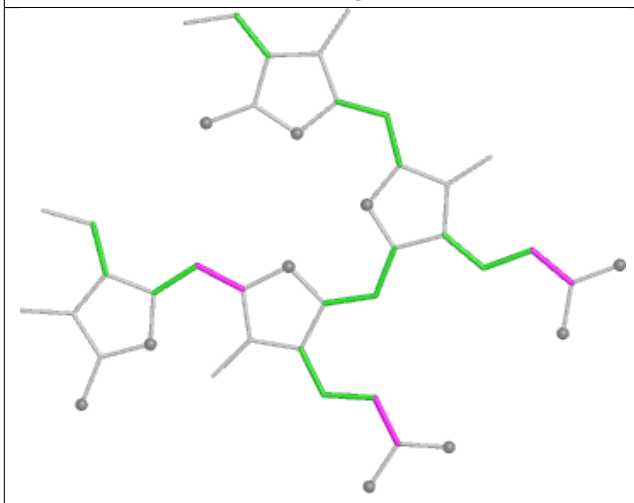
Ligand PEB CF 201



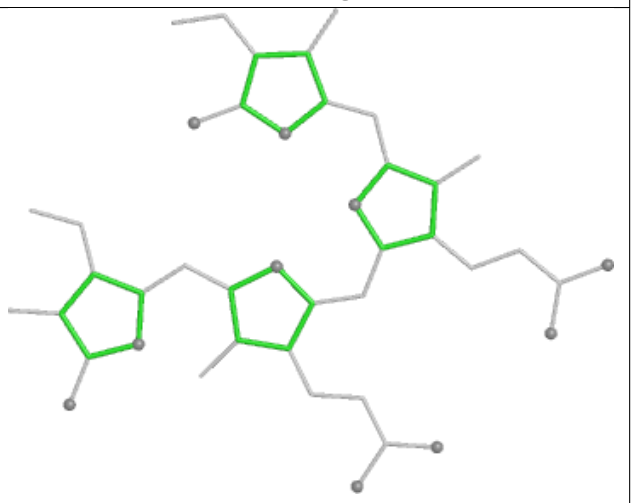
Bond lengths



Bond angles

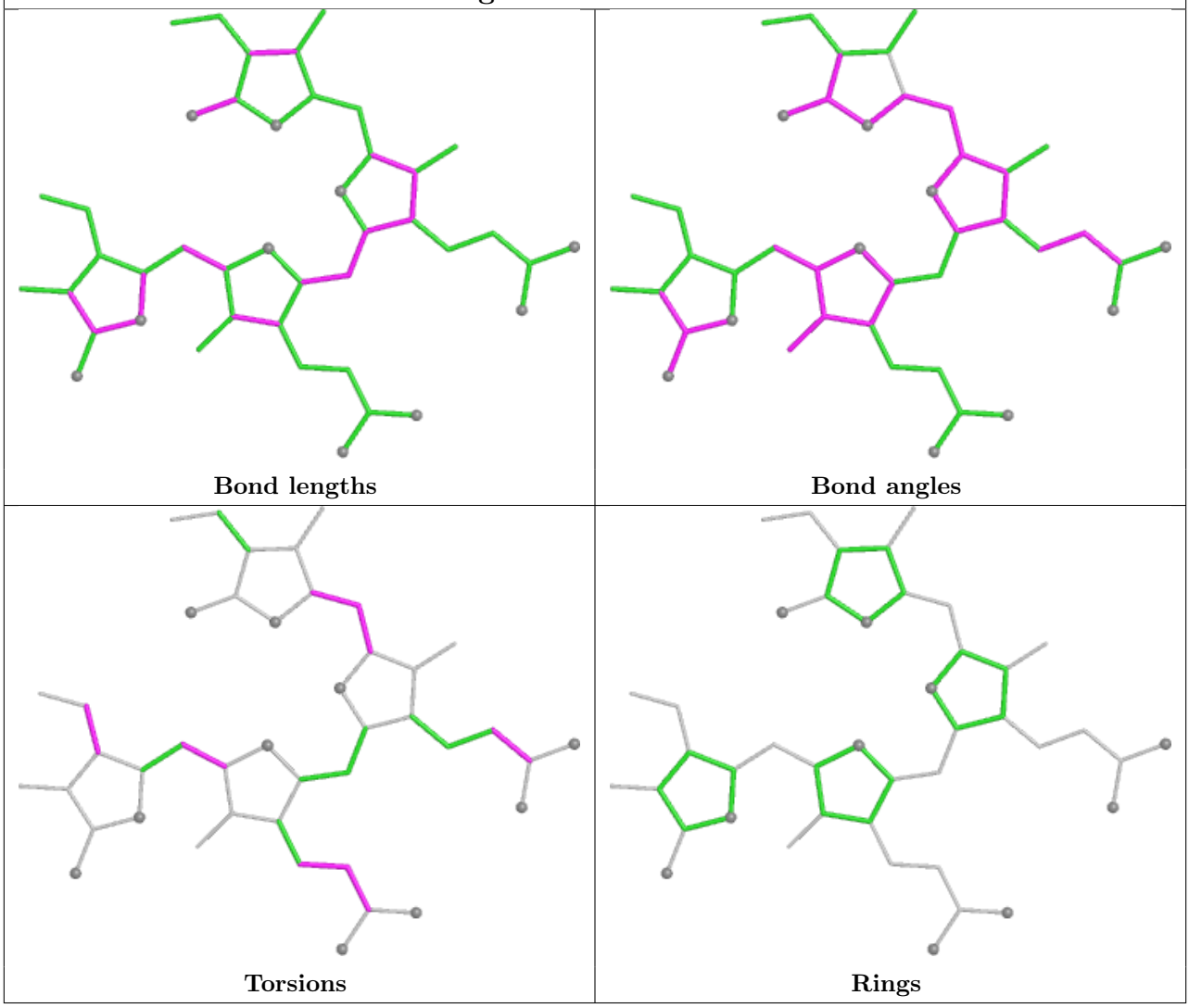


Torsions



Rings

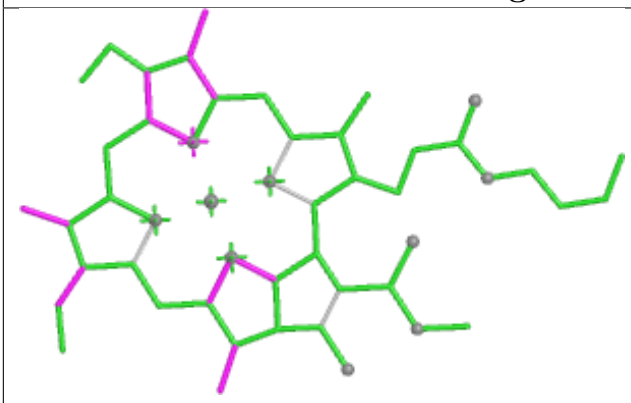
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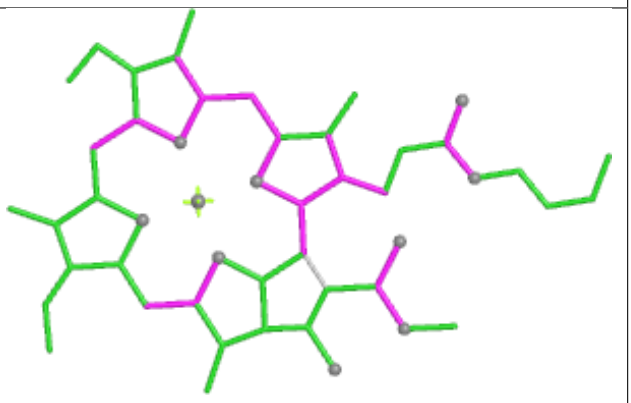
Bond lengths | Bond angles

Torsions | Rings

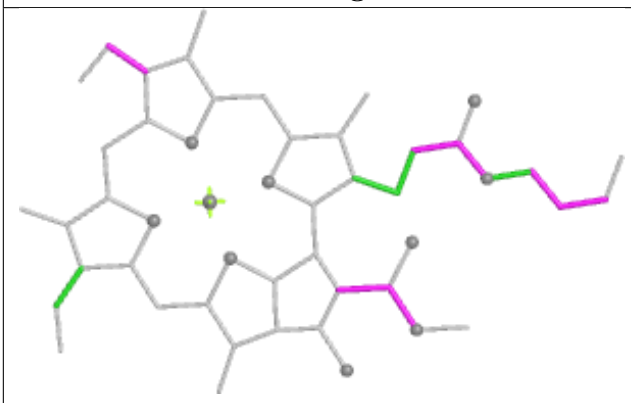
Ligand CLA KN 105



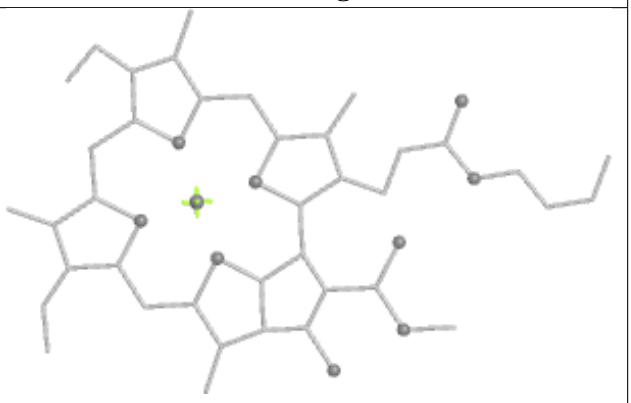
Bond lengths



Bond angles

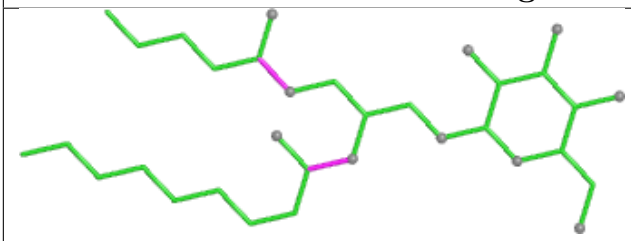


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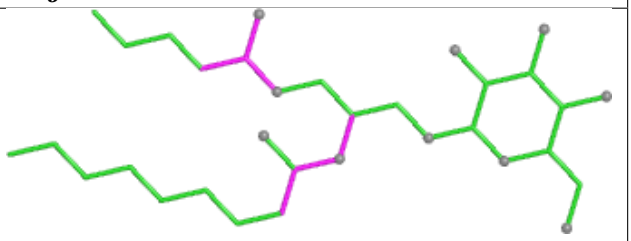


Rings

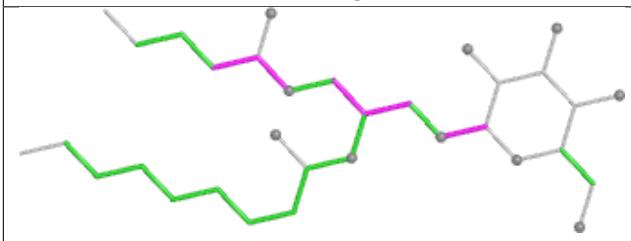
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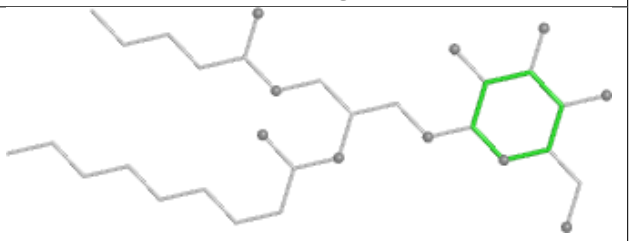
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Bond angles

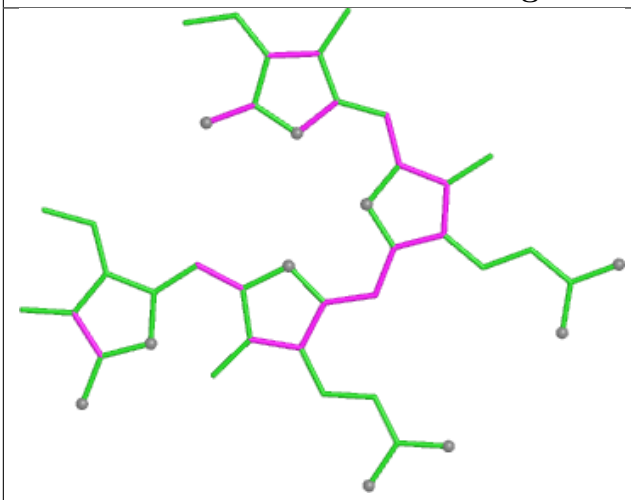


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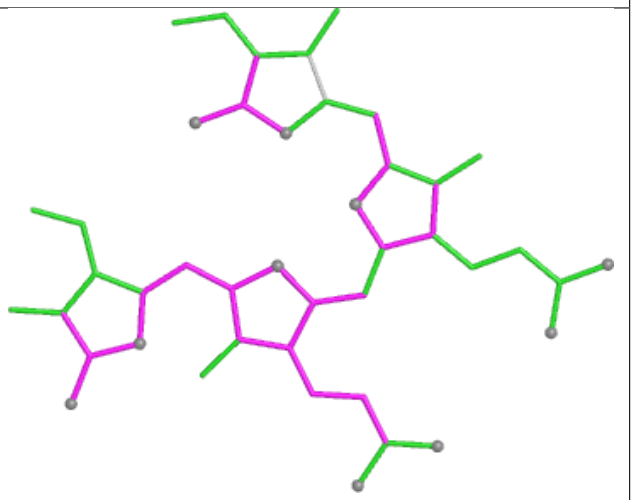


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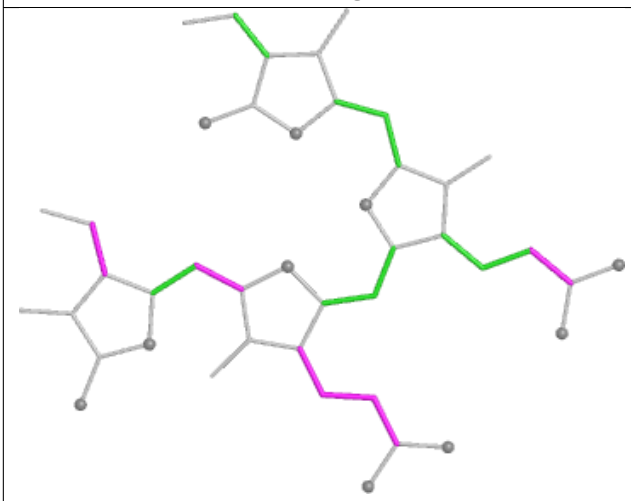
Ligand PEB lF 201



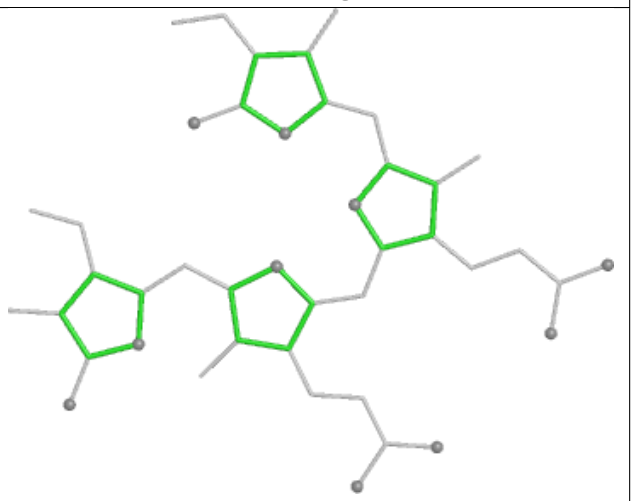
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Bond angles

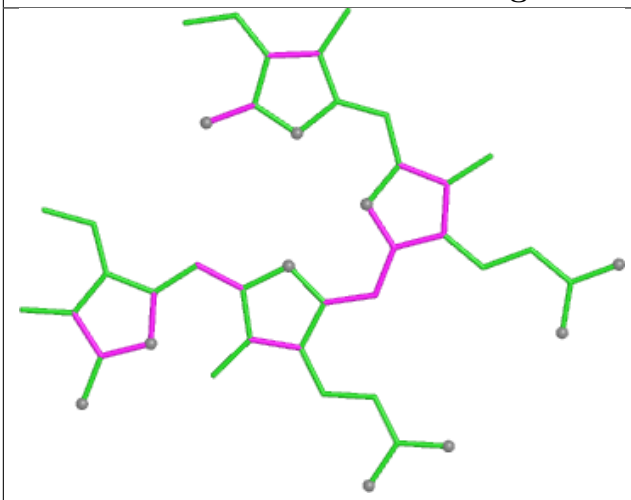


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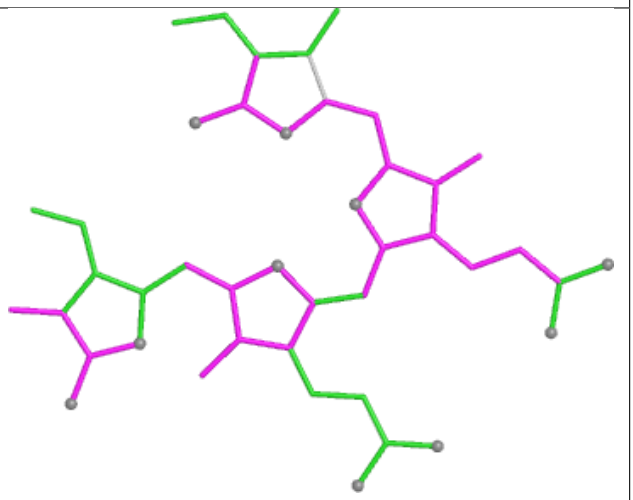


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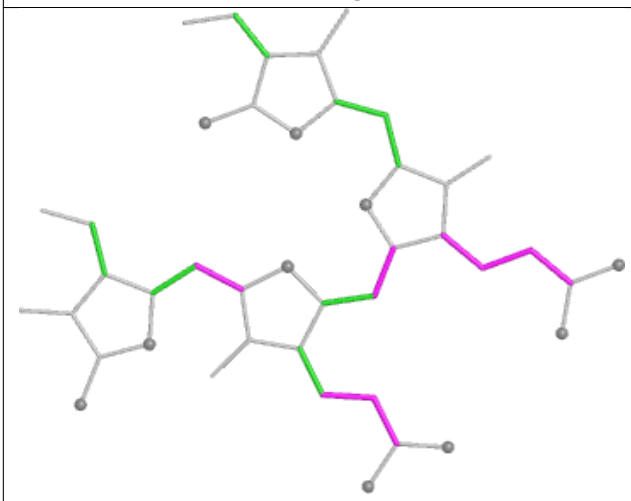
Ligand PEB YG 202



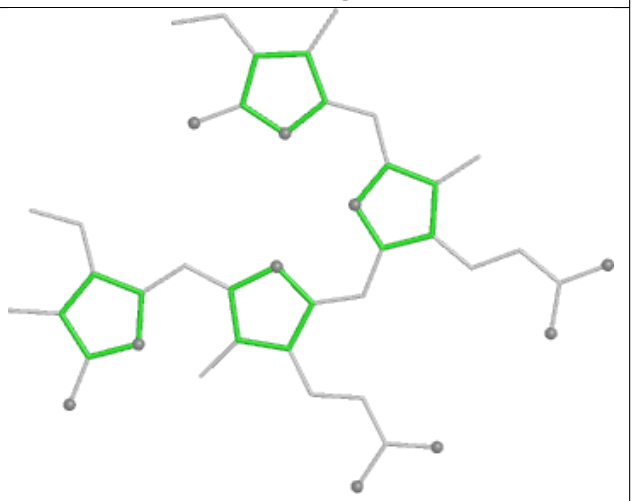
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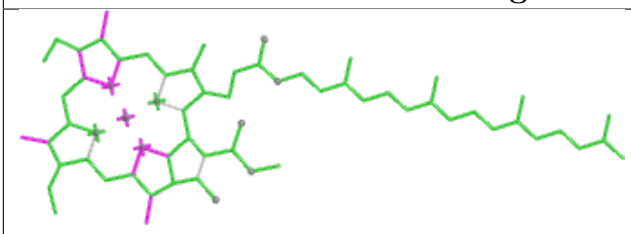


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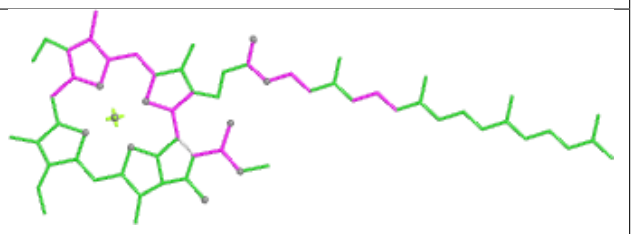


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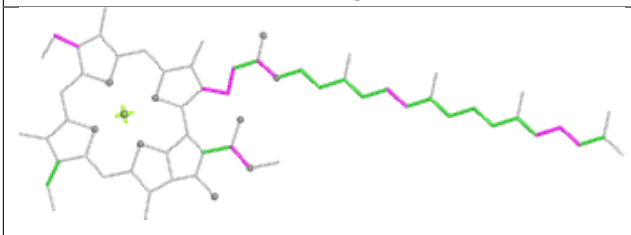
Ligand CLA AN 820



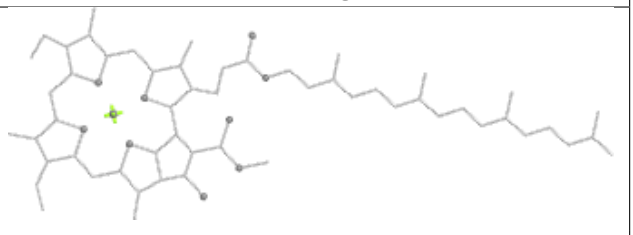
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Bond angles

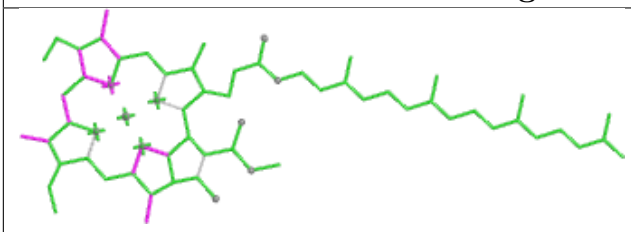


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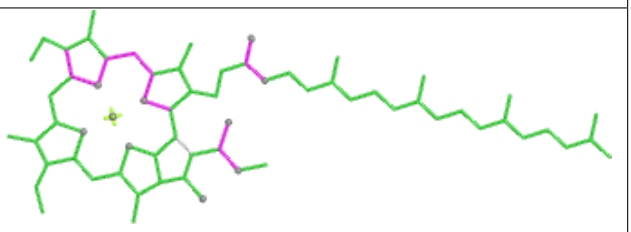


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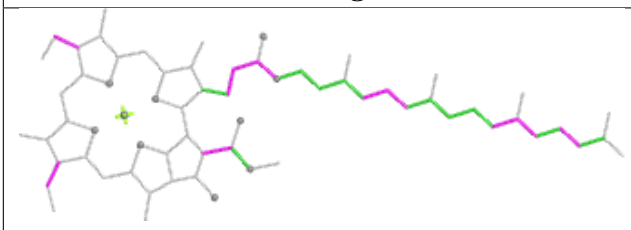
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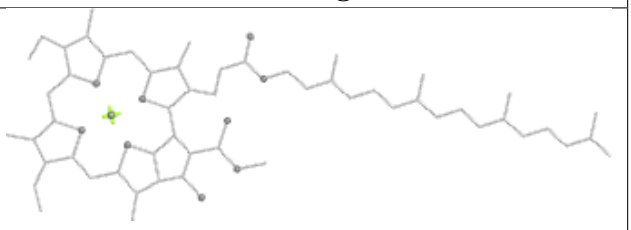
Bond lengths



Bond angles

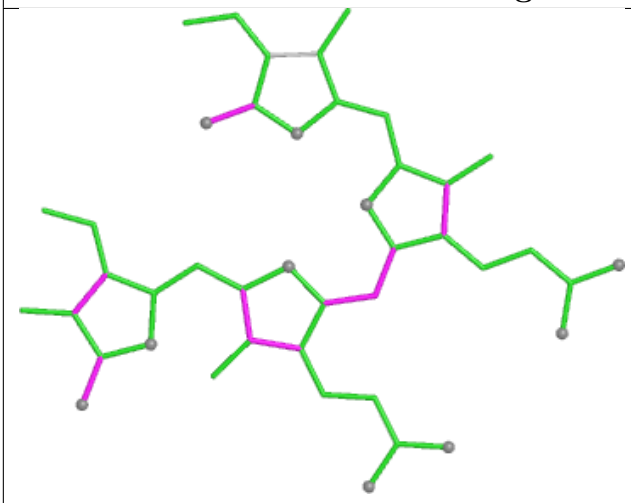


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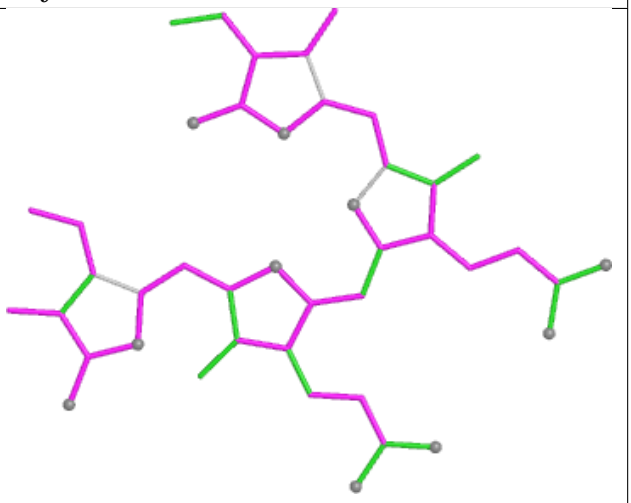


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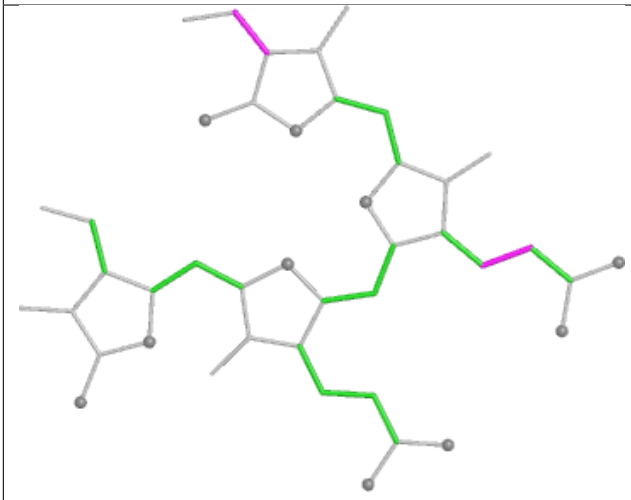
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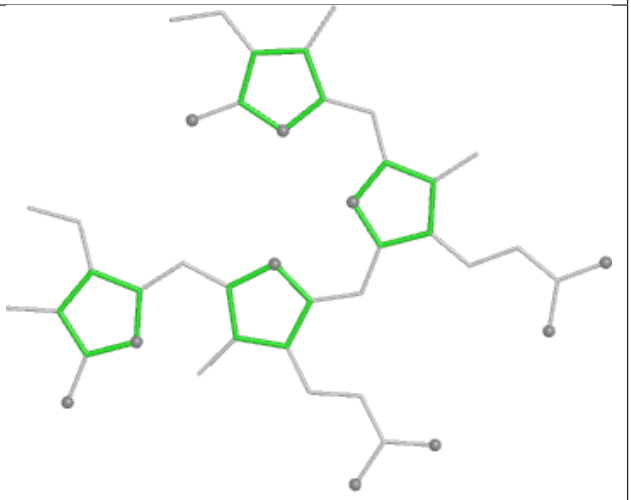
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Bond angles

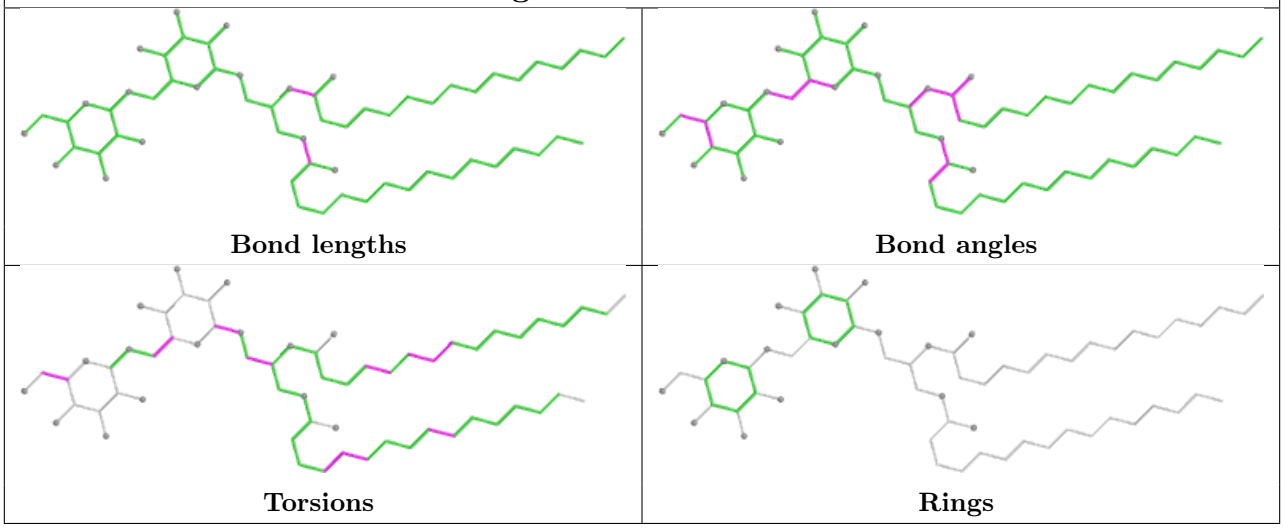


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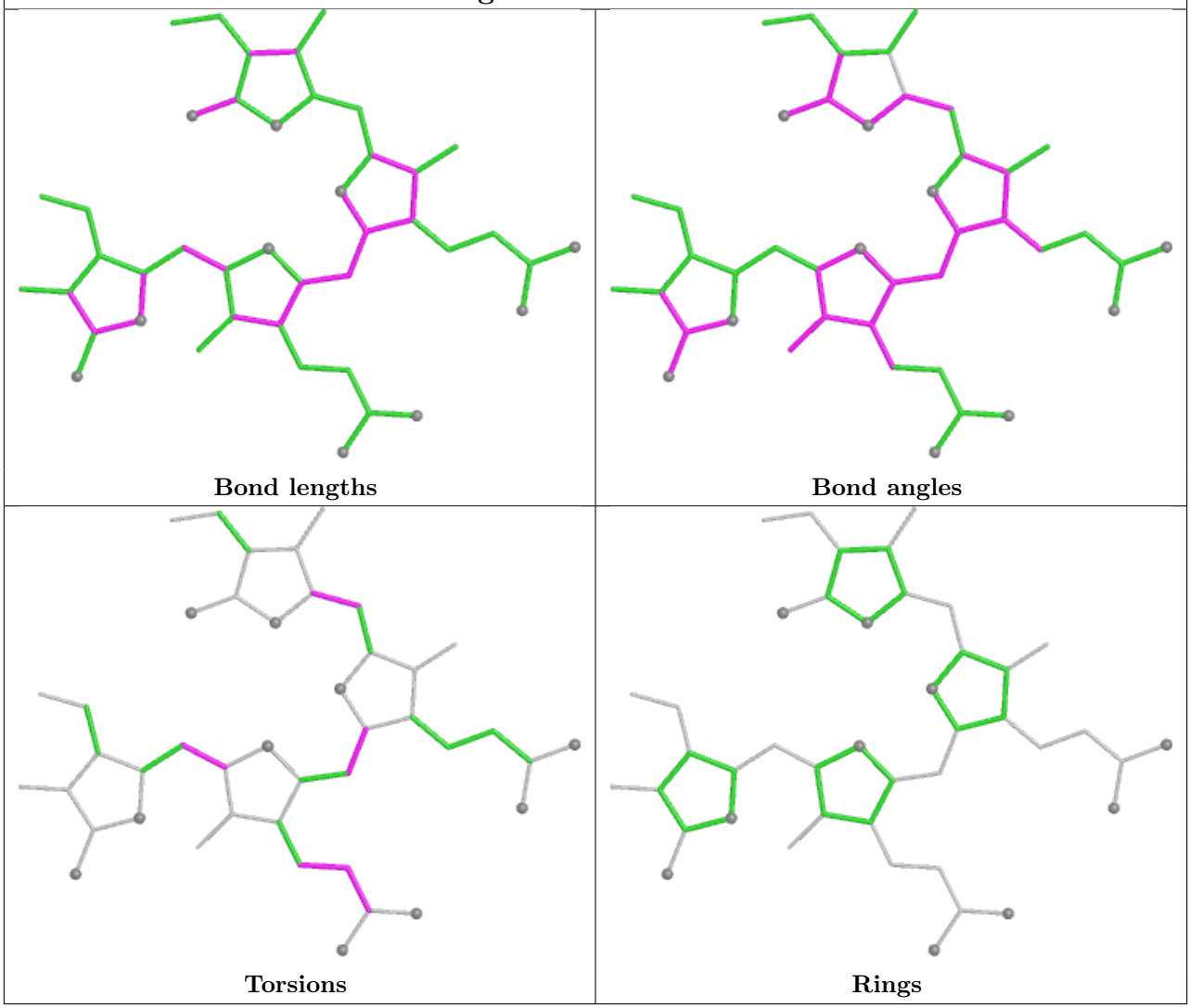


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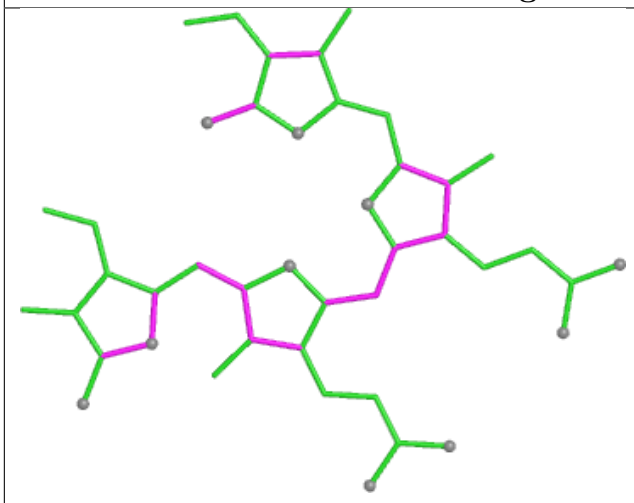
Ligand DGD C6 521



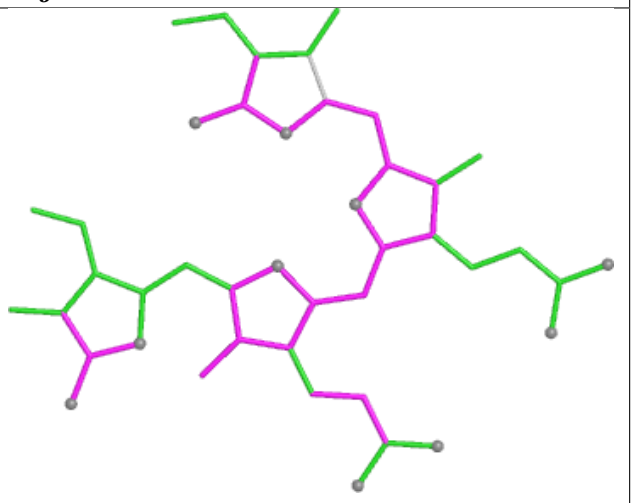
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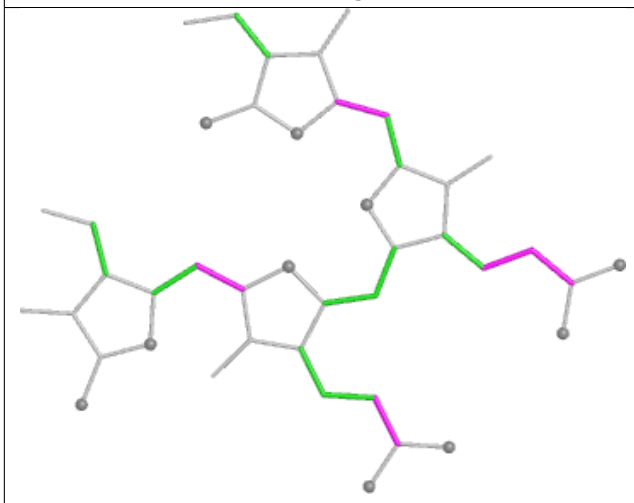
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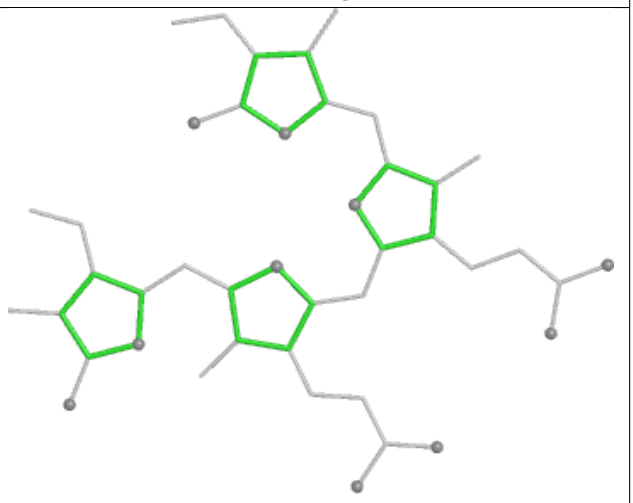
Bond lengths



Bond angles

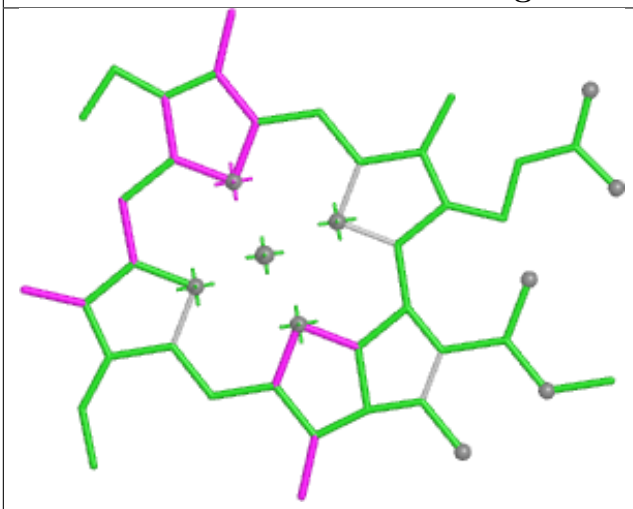


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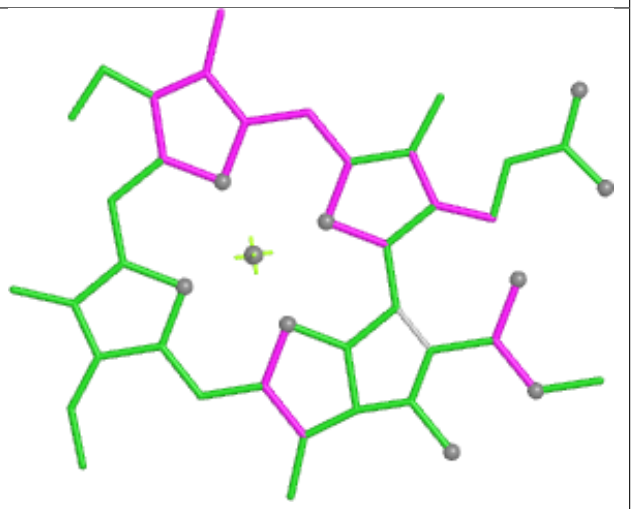


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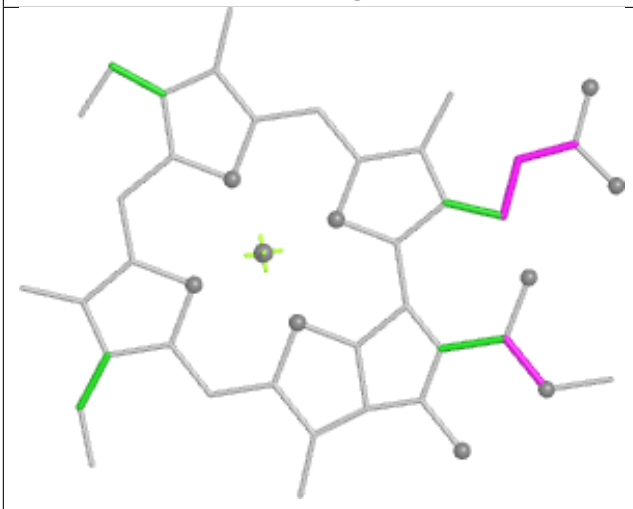
Ligand CLA 4N 603



Bond lengths



Bond angles

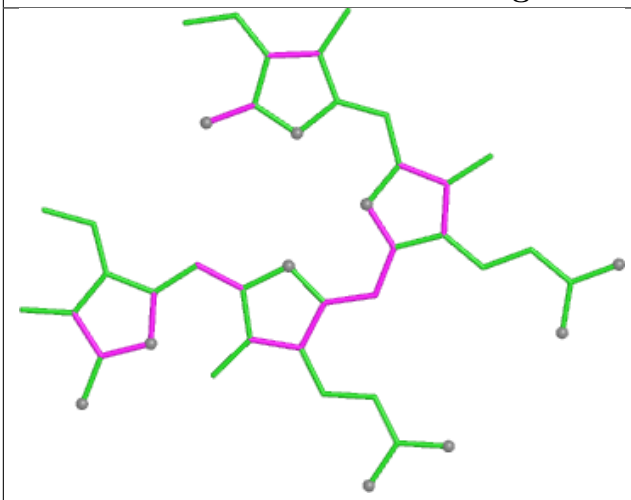


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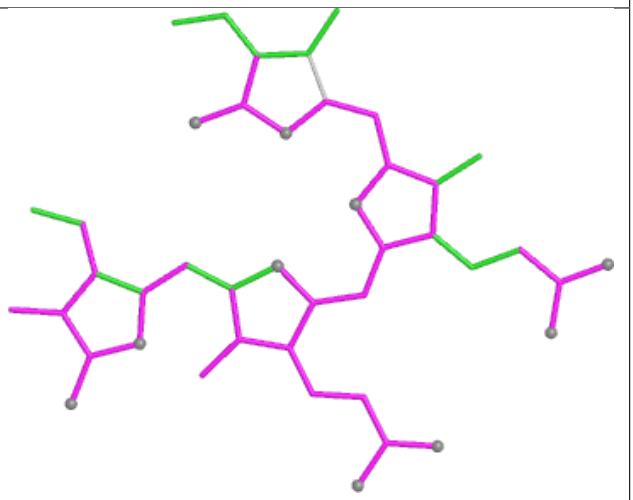


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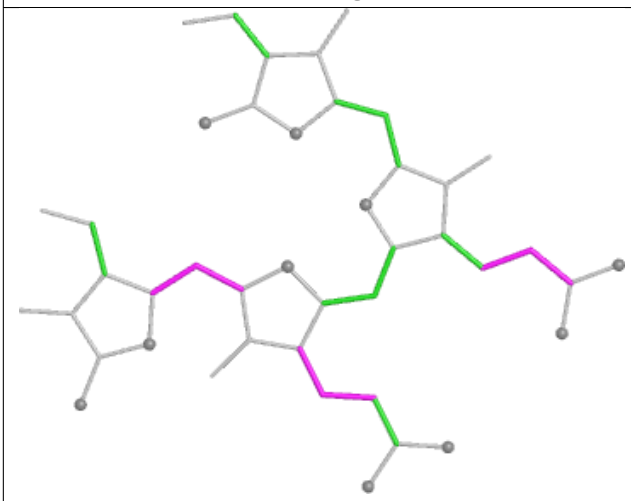
Ligand PEB GF 203



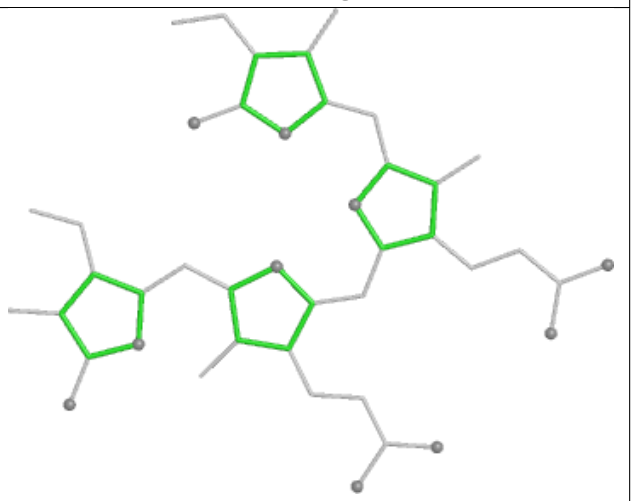
Bond lengths



Bond angles

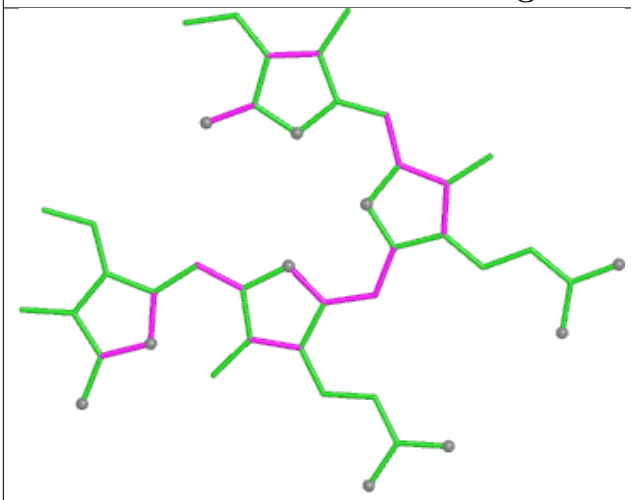


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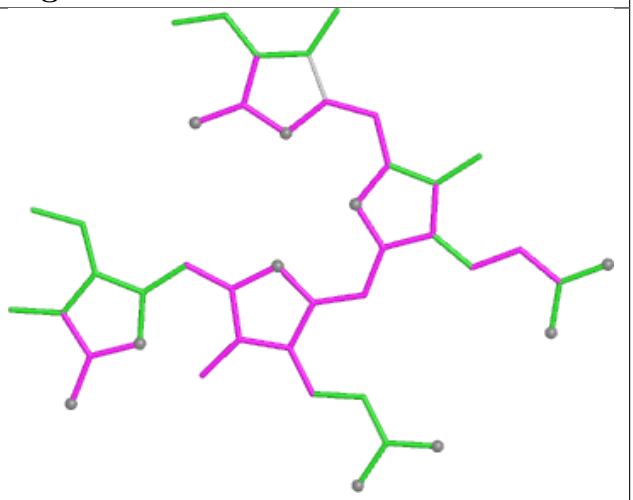


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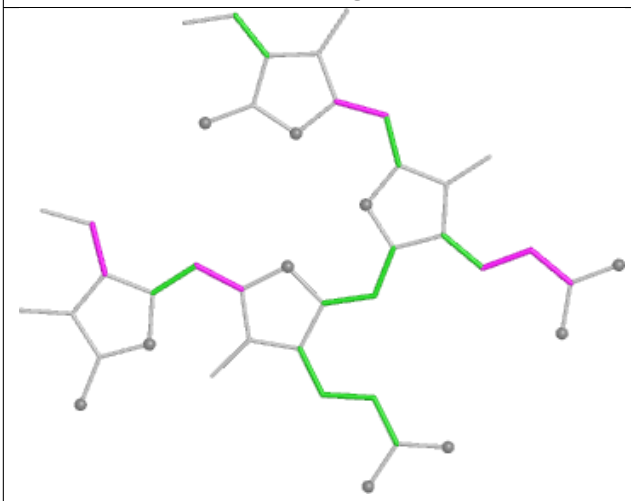
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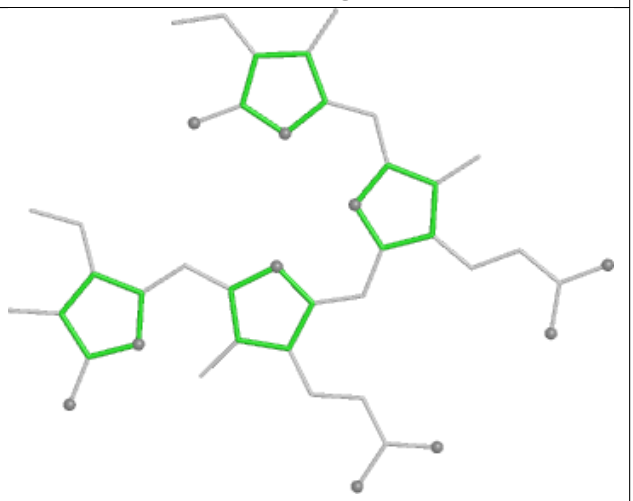
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Bond angles

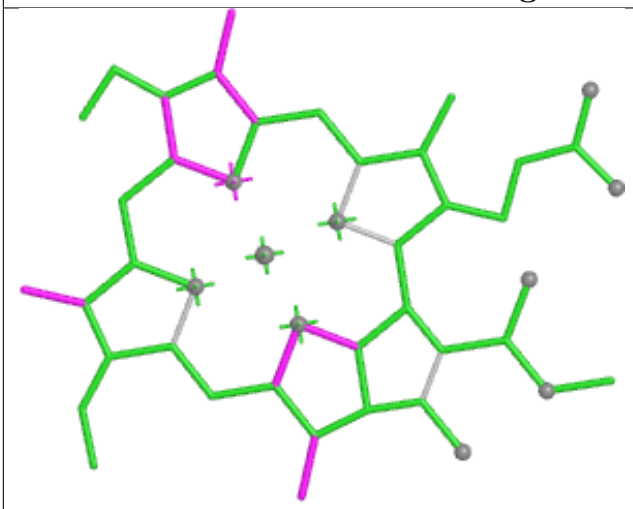


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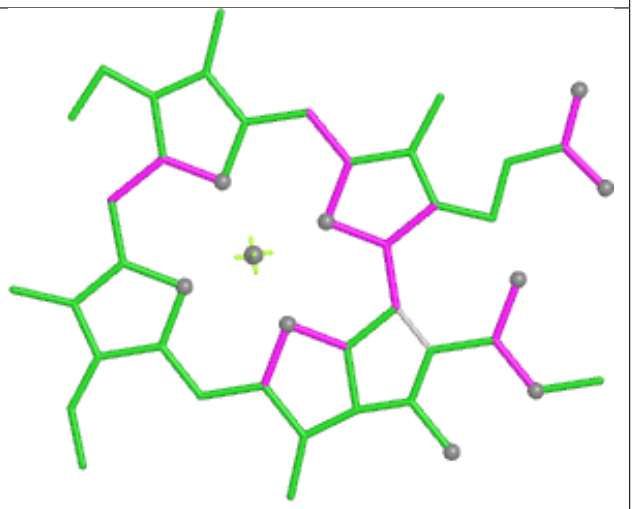


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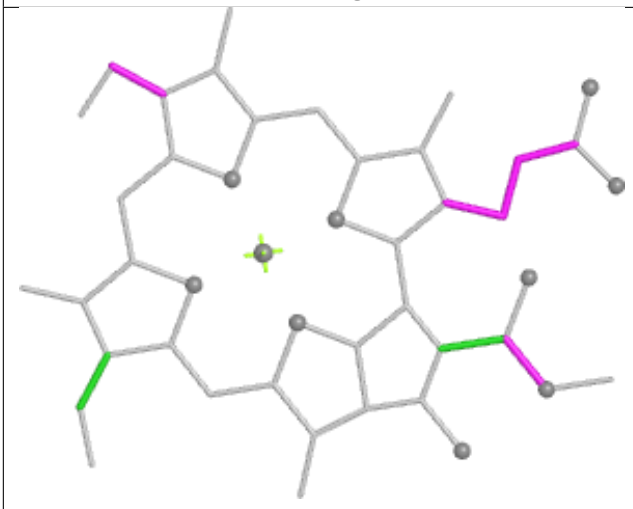
Ligand CLA 42 601



Bond lengths



Bond angles

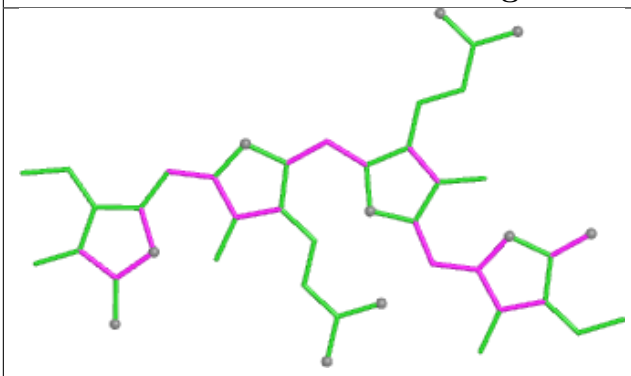


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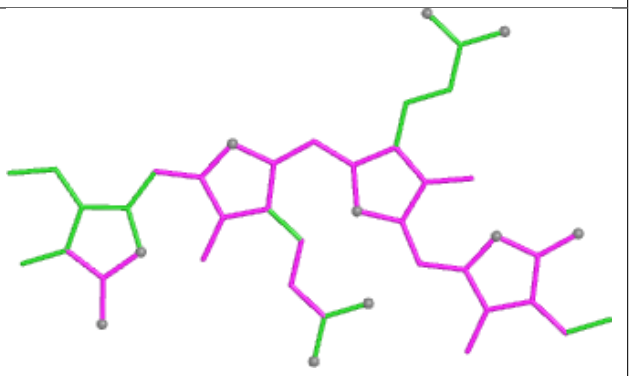


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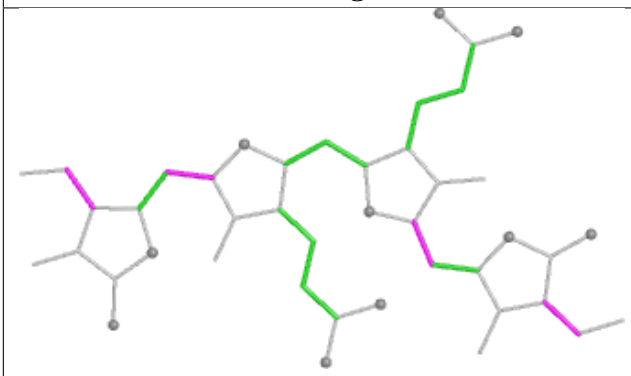
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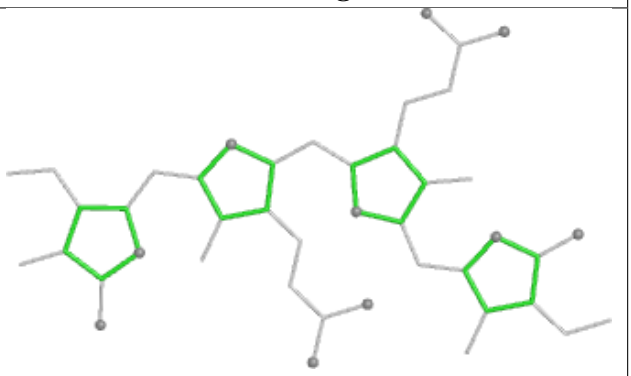
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Bond angles

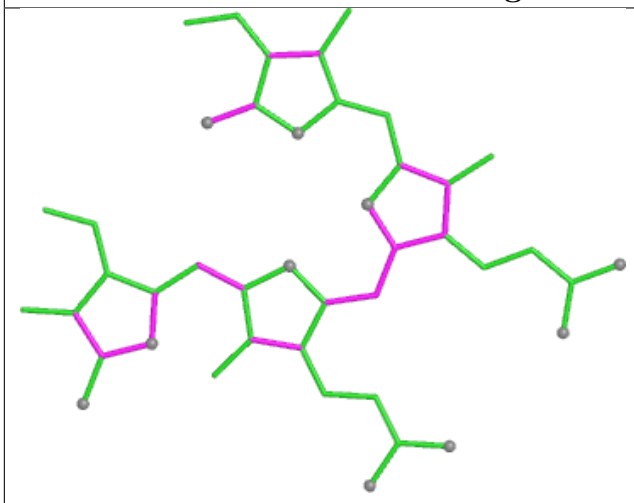


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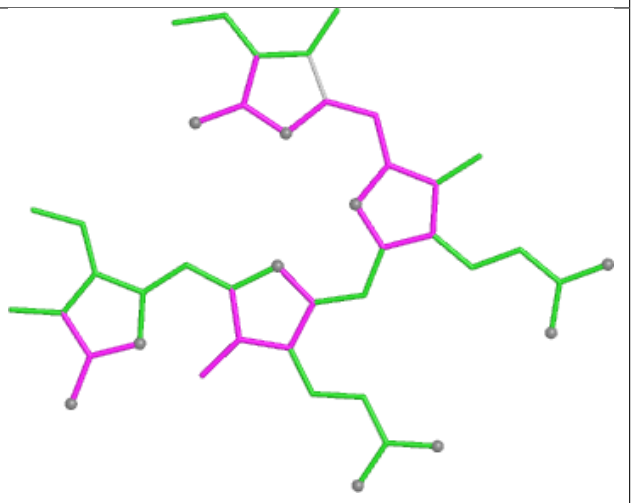


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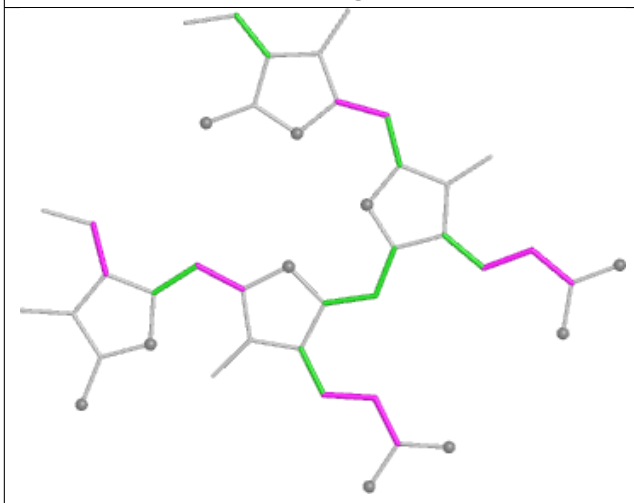
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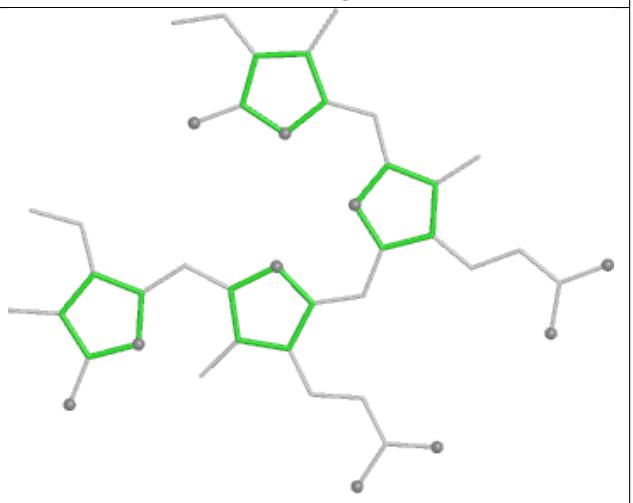
Bond lengths



Bond angles

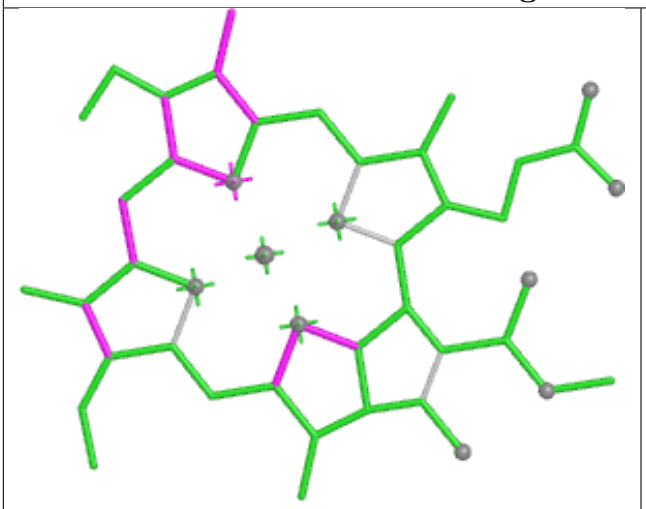


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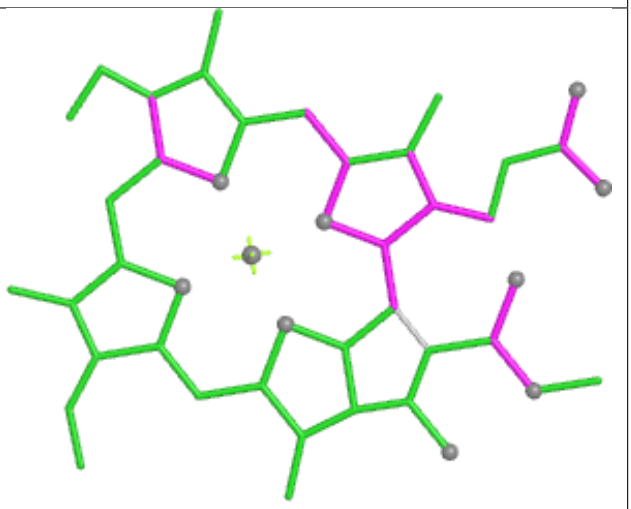


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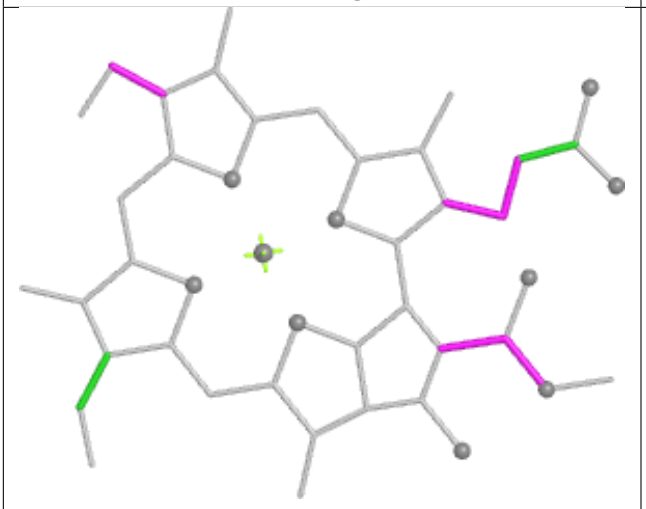
Ligand CLA 22 612



Bond lengths



Bond angles

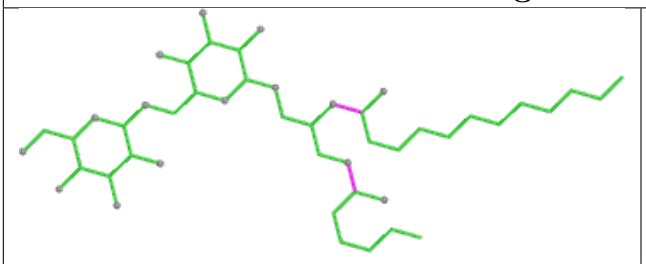


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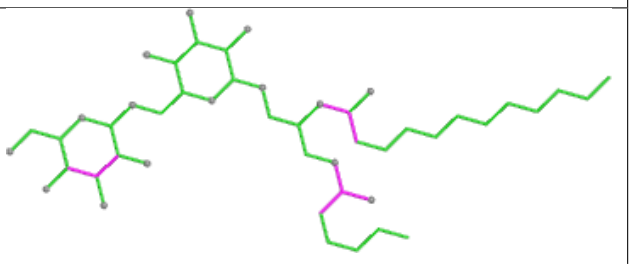


Rings

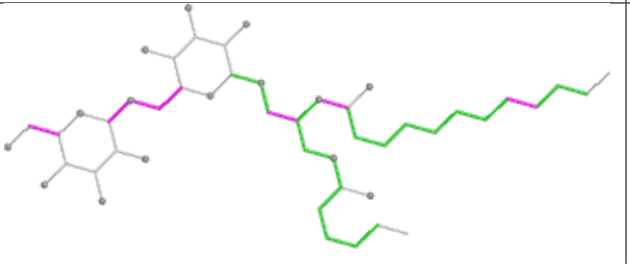
Ligand DGD cL 520



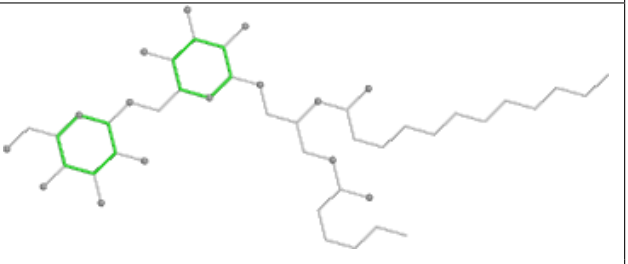
Bond lengths



Bond angles

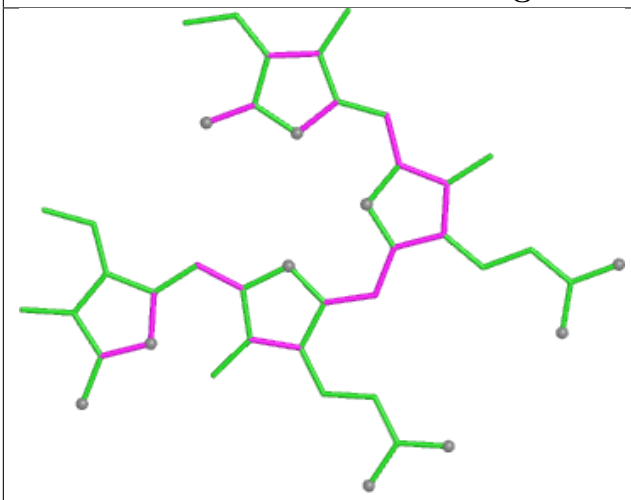


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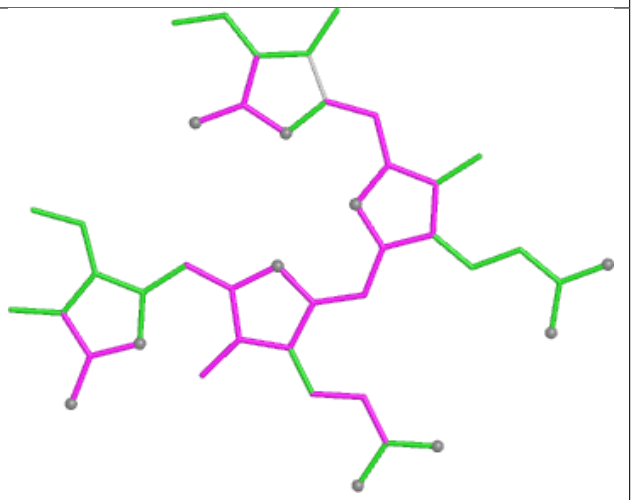


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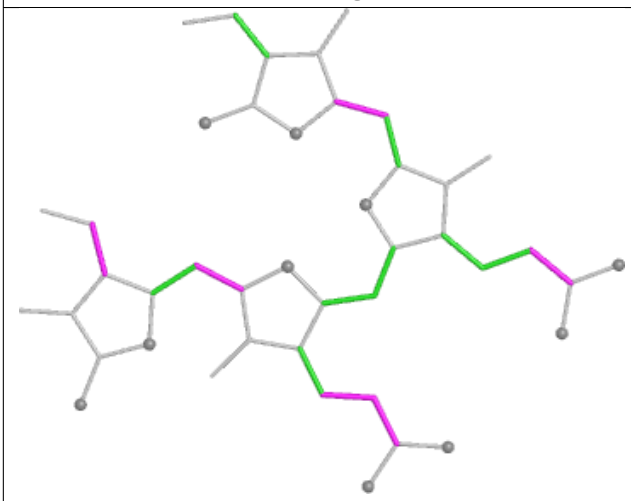
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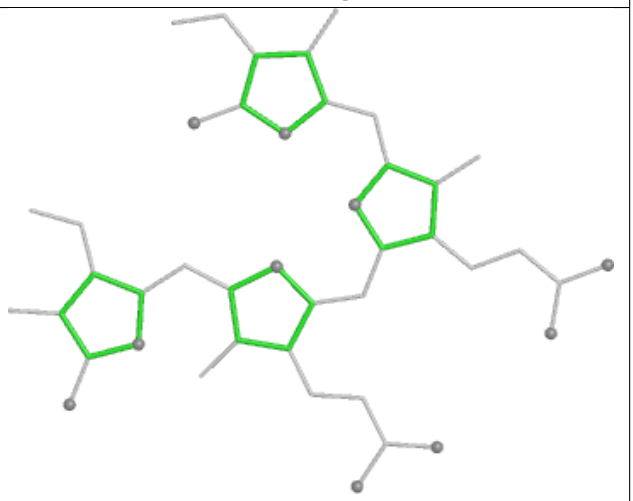
Bond lengths



Bond angles

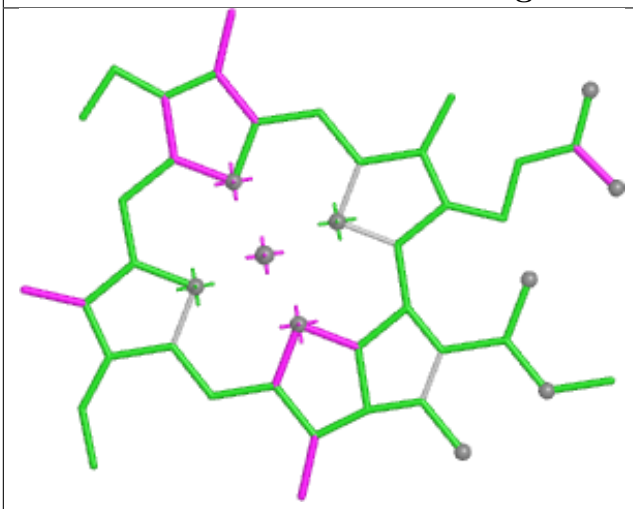


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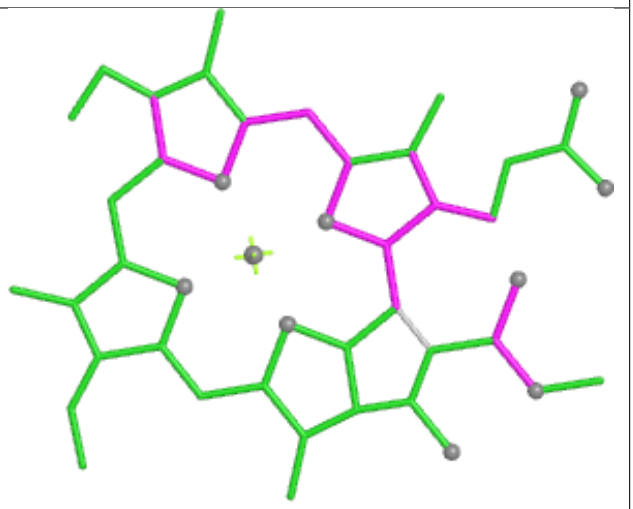


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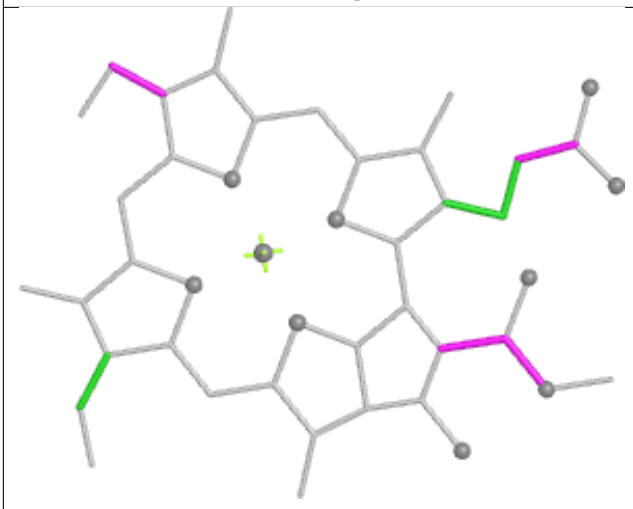
Ligand CLA B2 819



Bond lengths



Bond angles

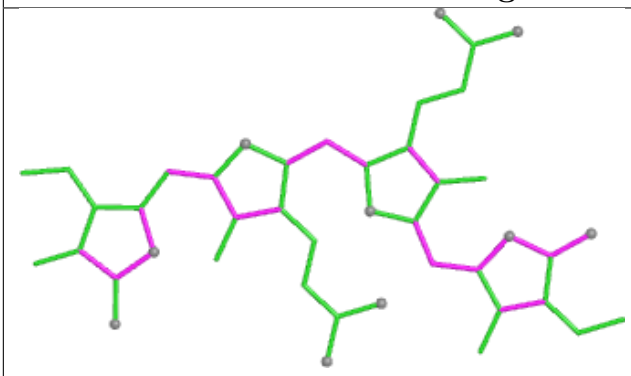


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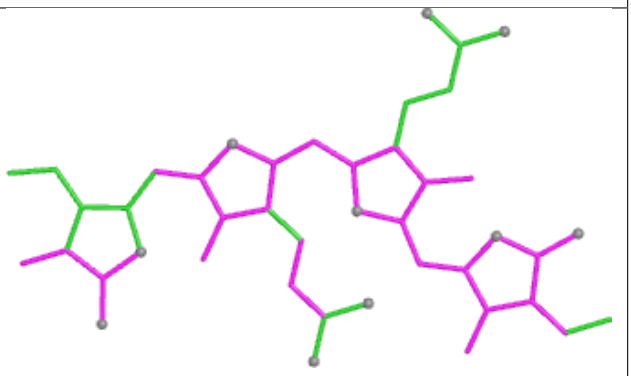


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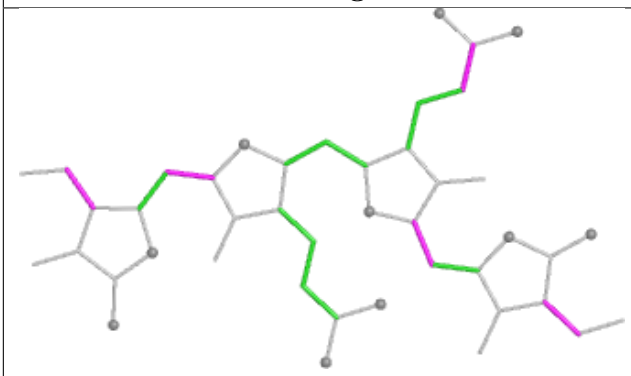
Ligand CYC GG 1001



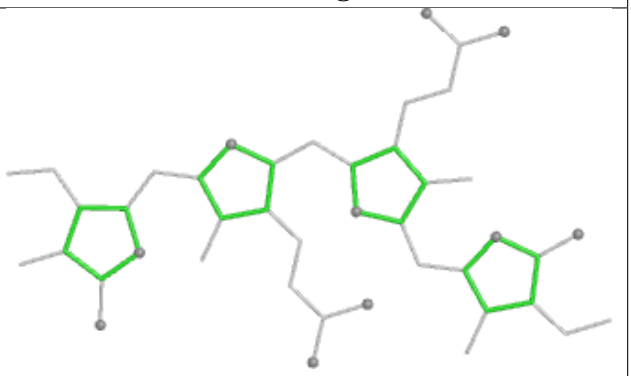
Bond lengths



Bond angles

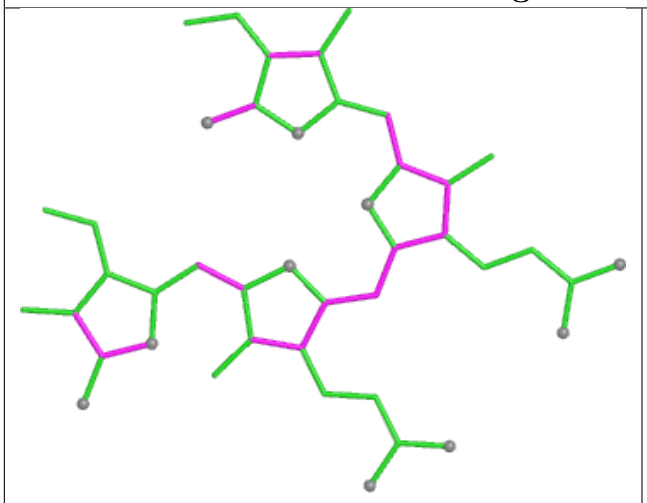


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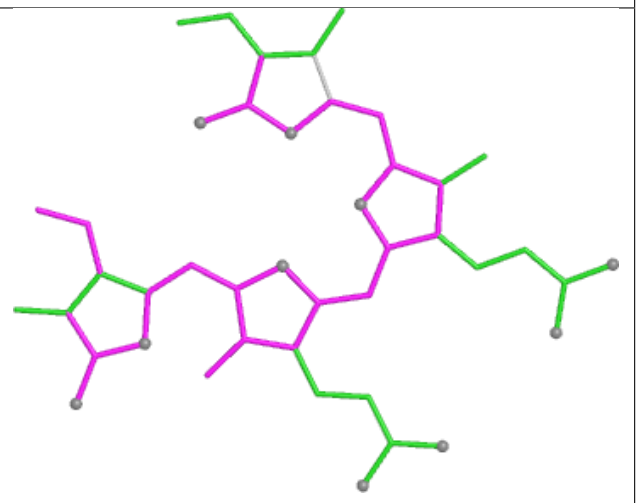


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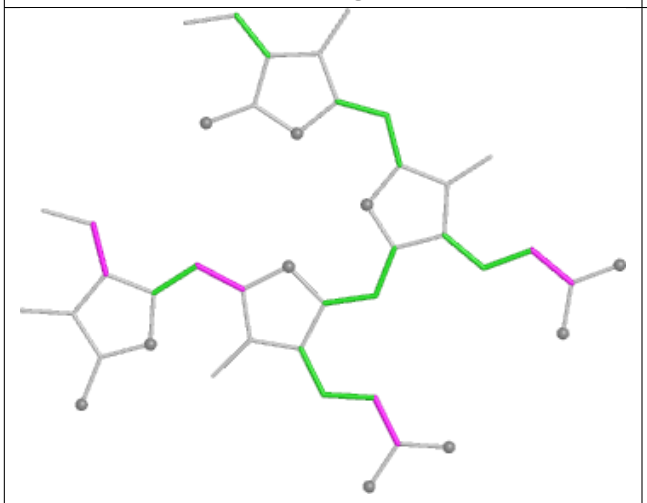
Ligand PEB BA 202



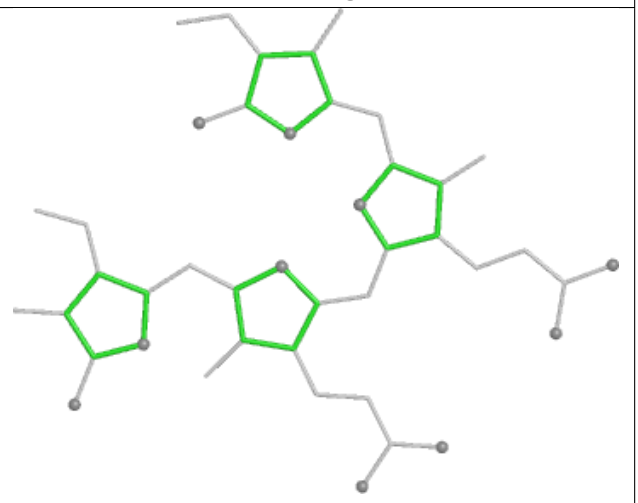
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Bond angles

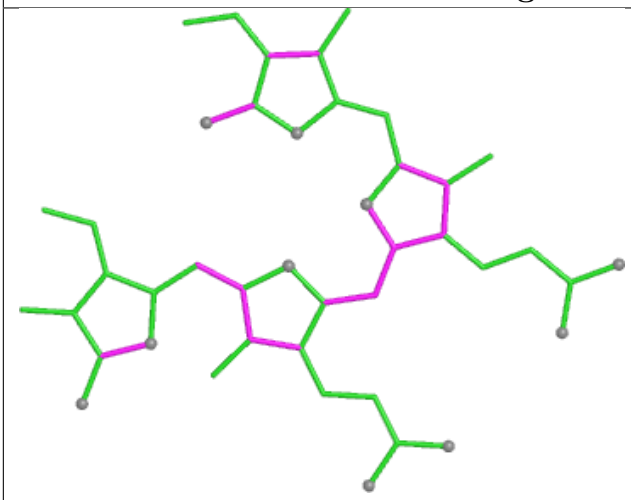


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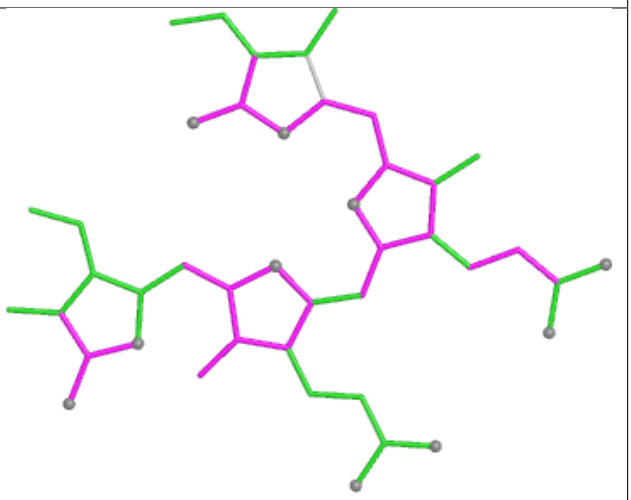


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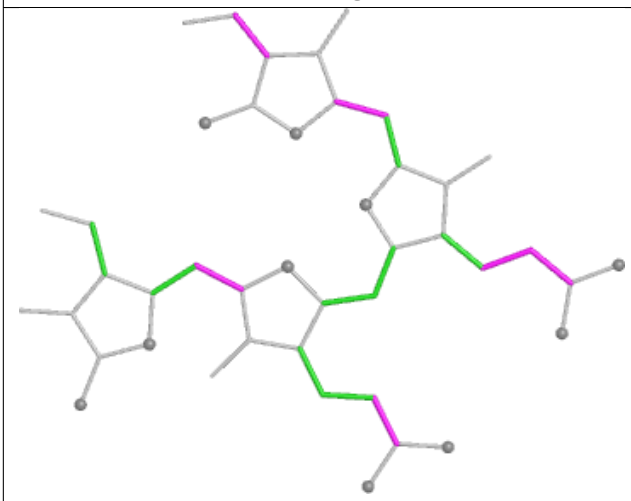
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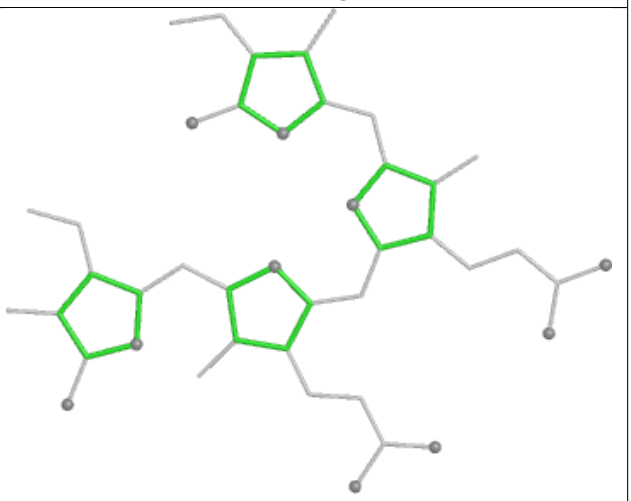
Bond lengths



Bond angles

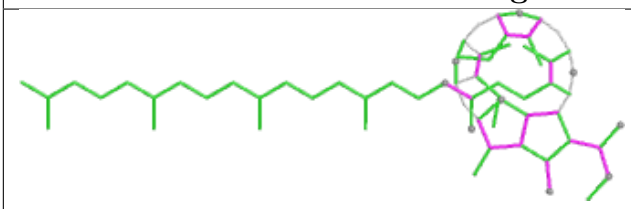


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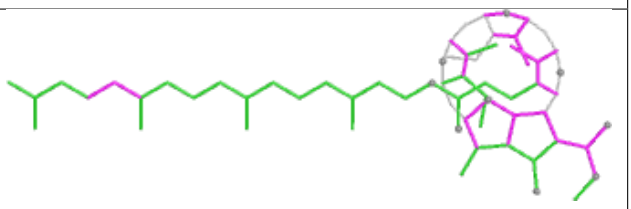


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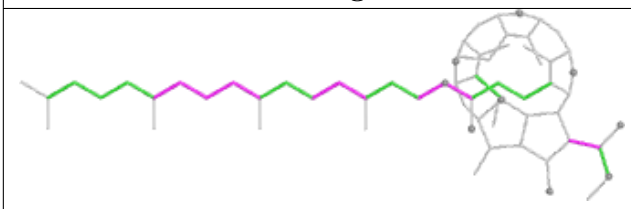
Ligand PHO AL 410



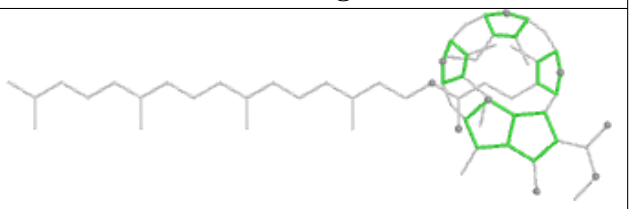
Bond lengths



Bond angles

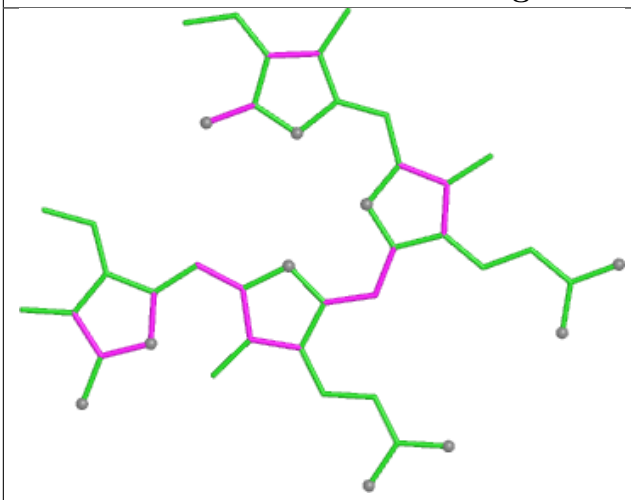


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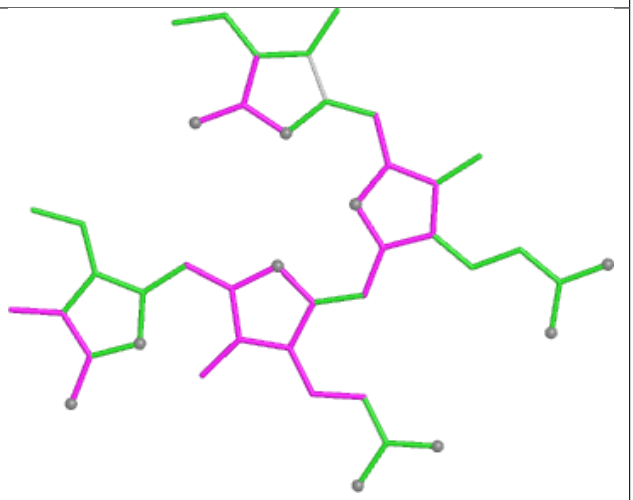


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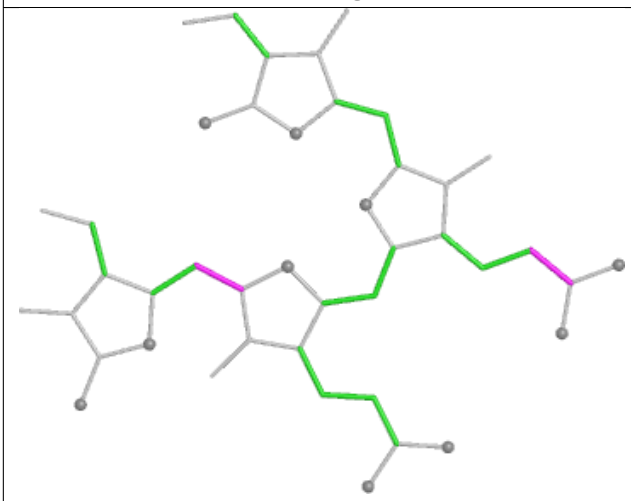
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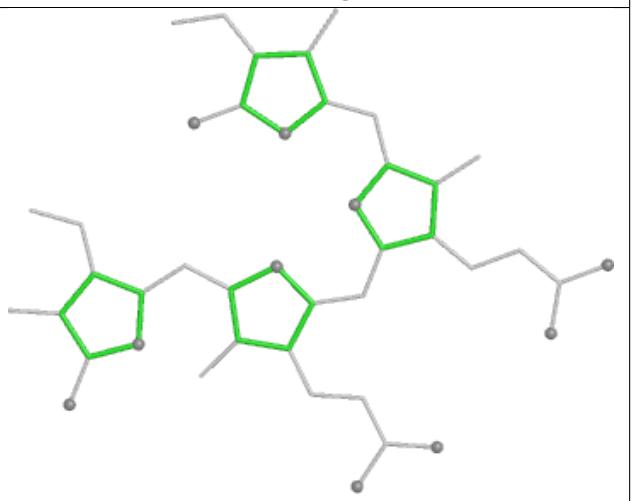
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Bond angles

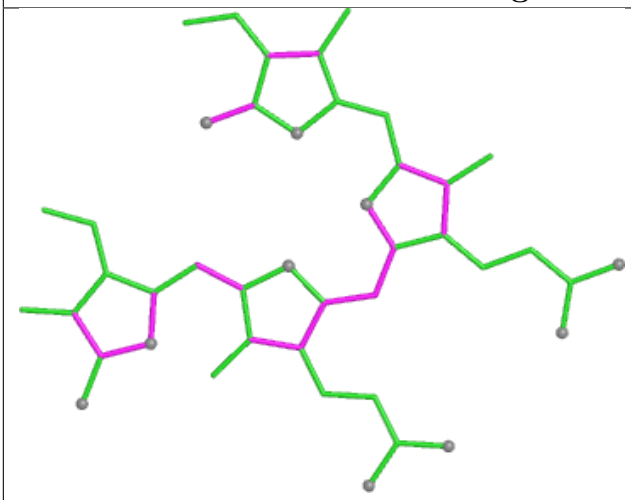


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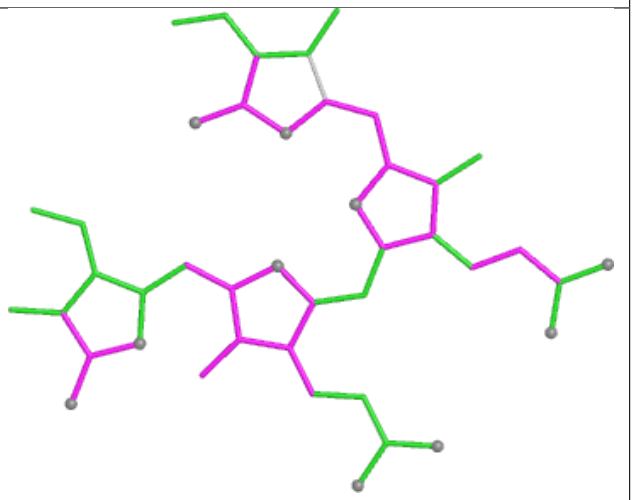


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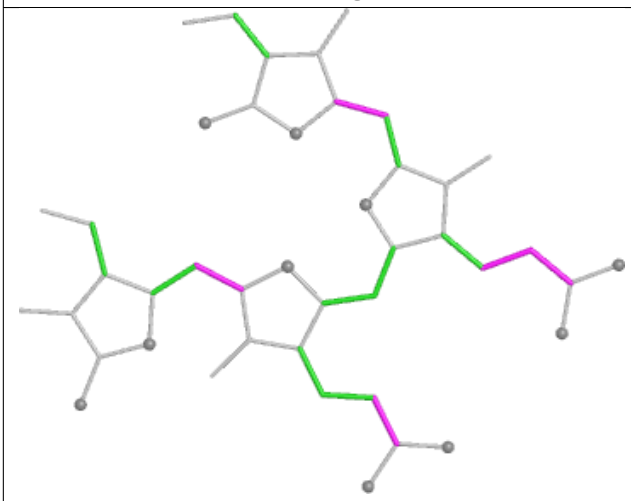
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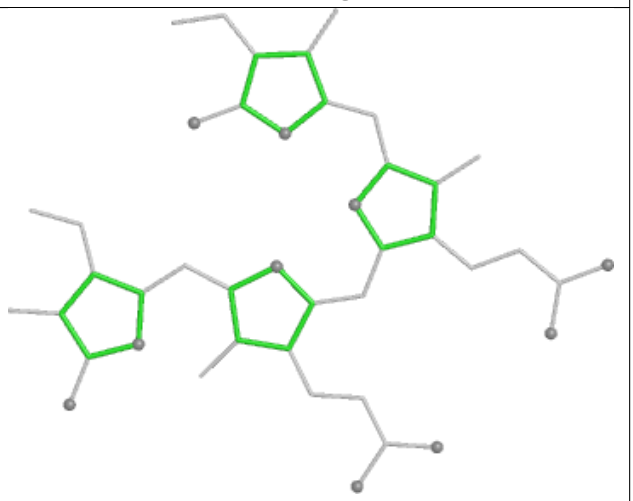
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Bond angles

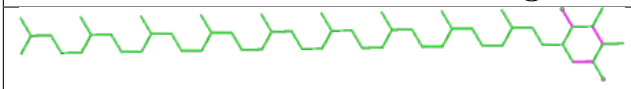


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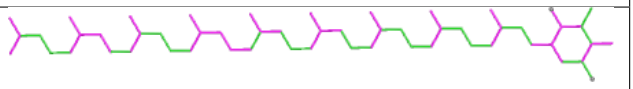


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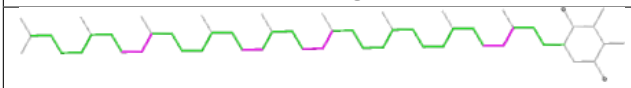
Ligand PL9 aL 601



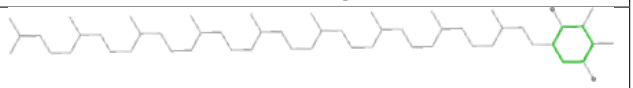
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Bond angles

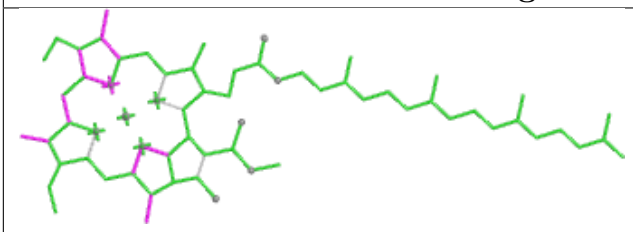


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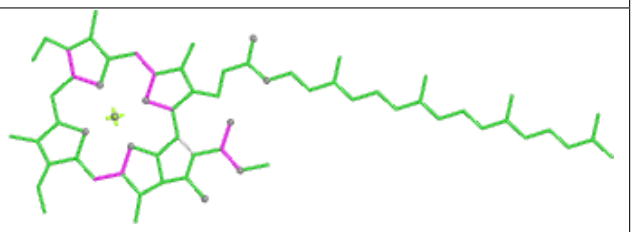


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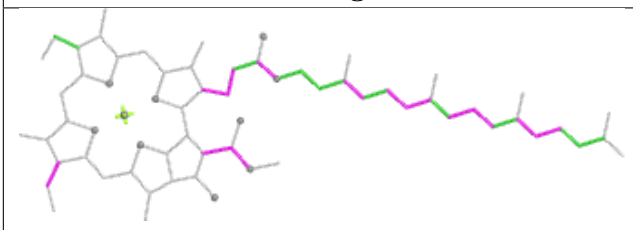
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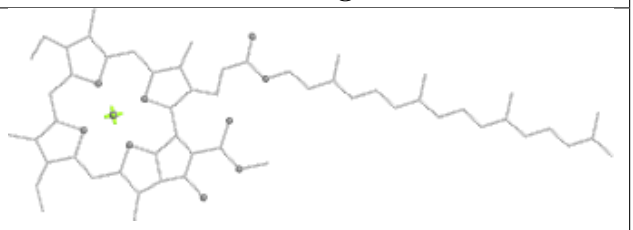
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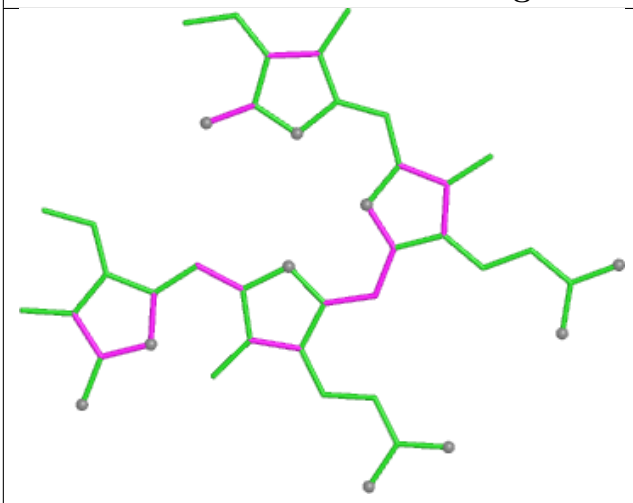


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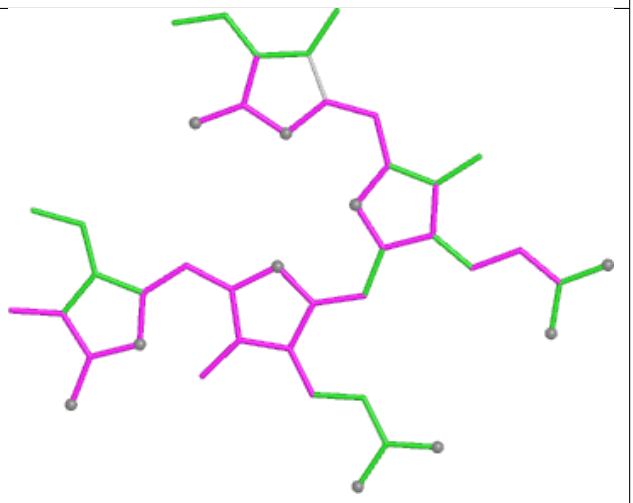


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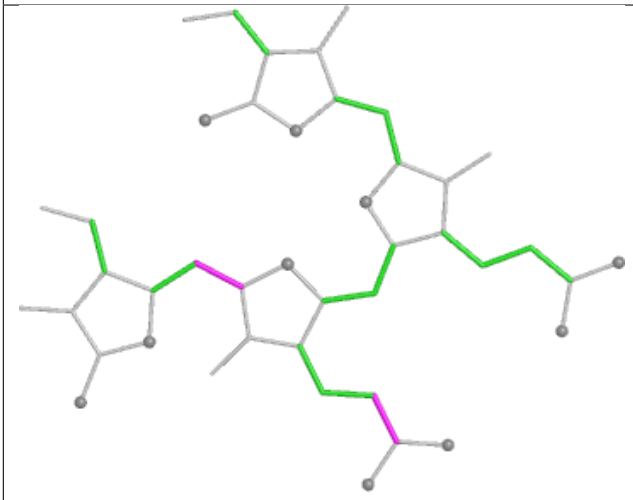
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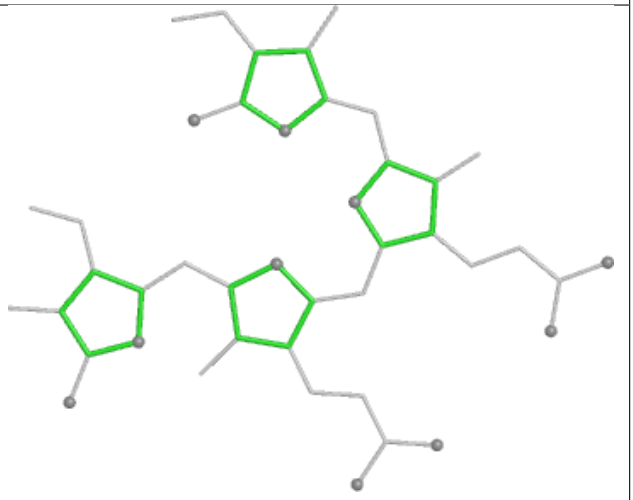
Bond lengths



Bond angles

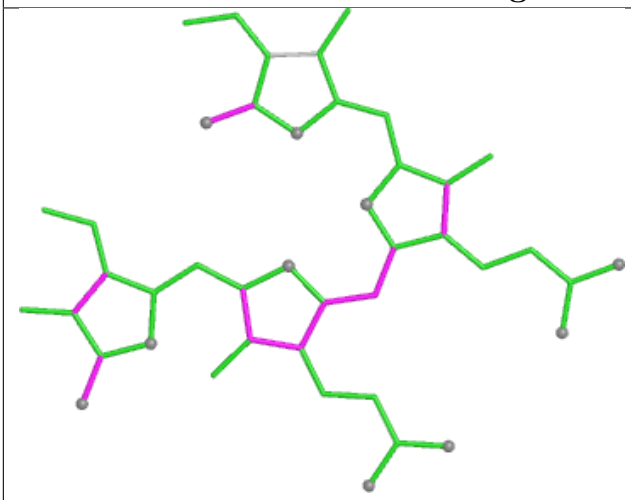


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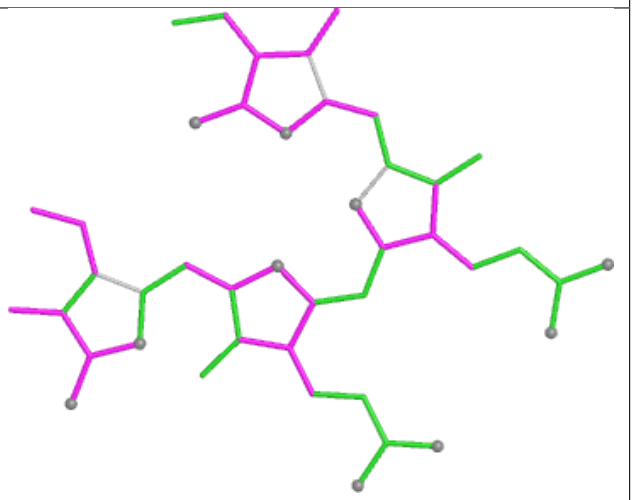


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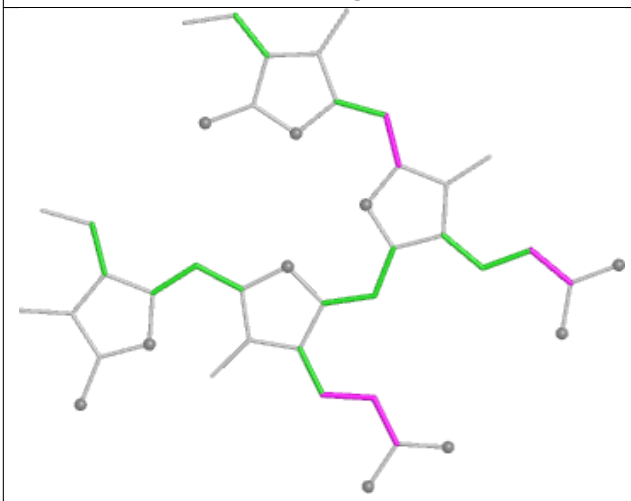
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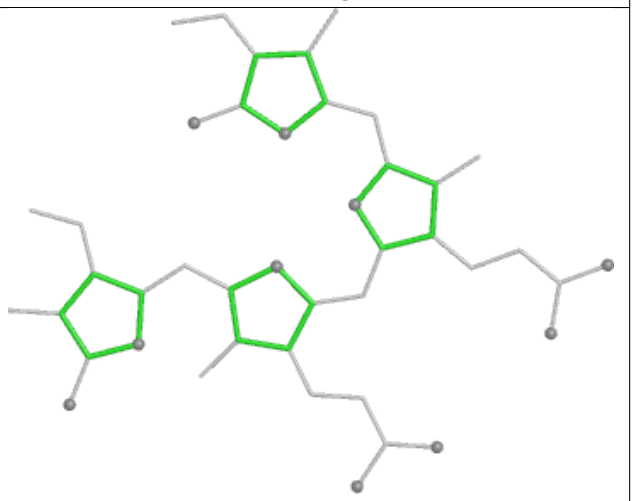
Bond lengths



Bond angles

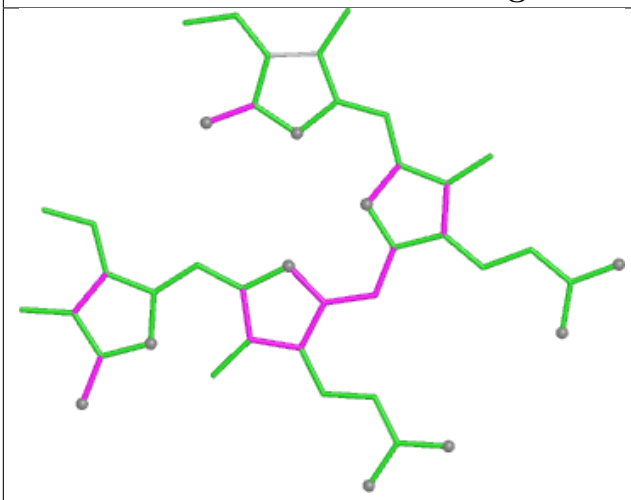


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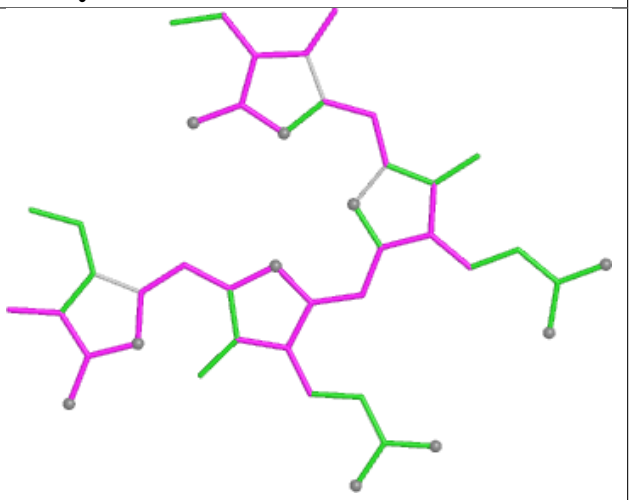


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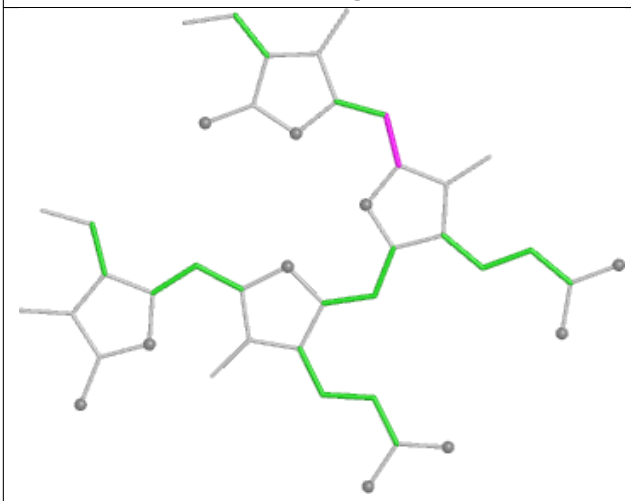
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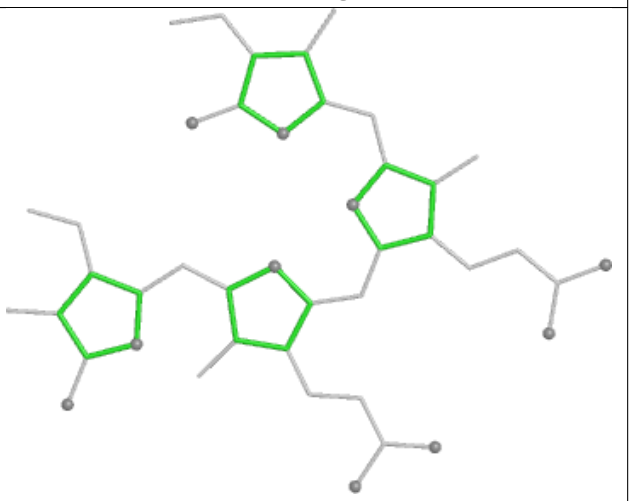
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Bond angles

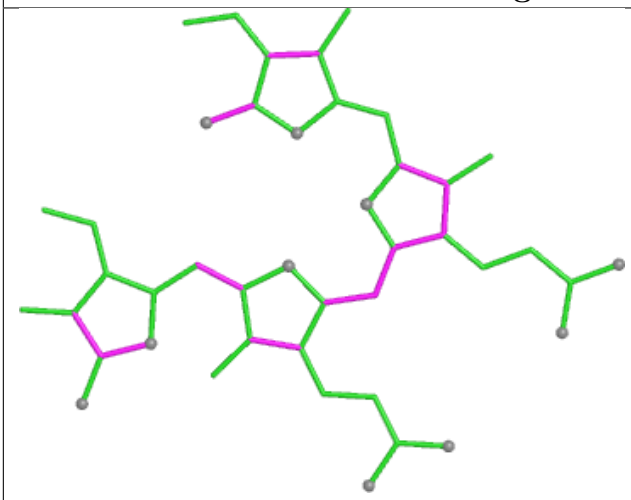


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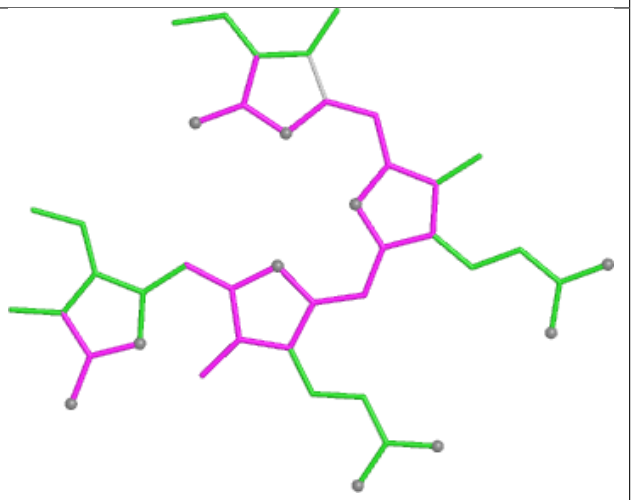


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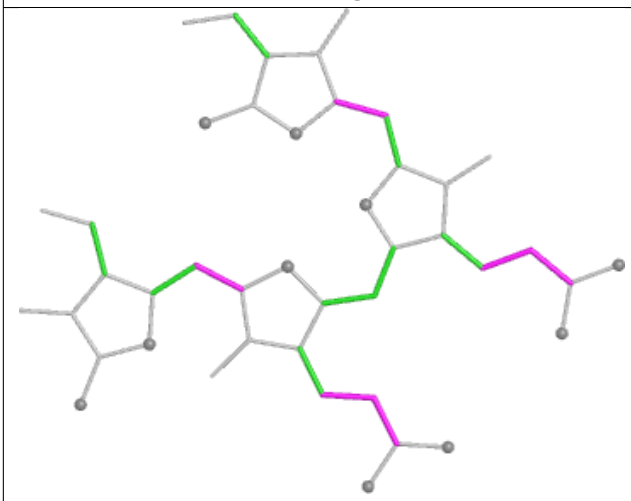
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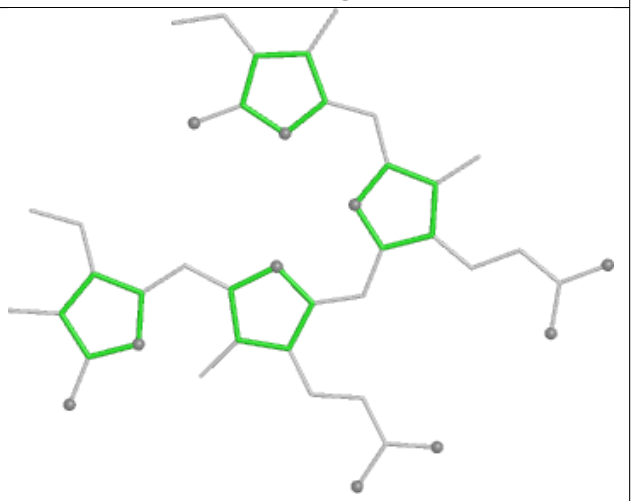
Bond lengths



Bond angles

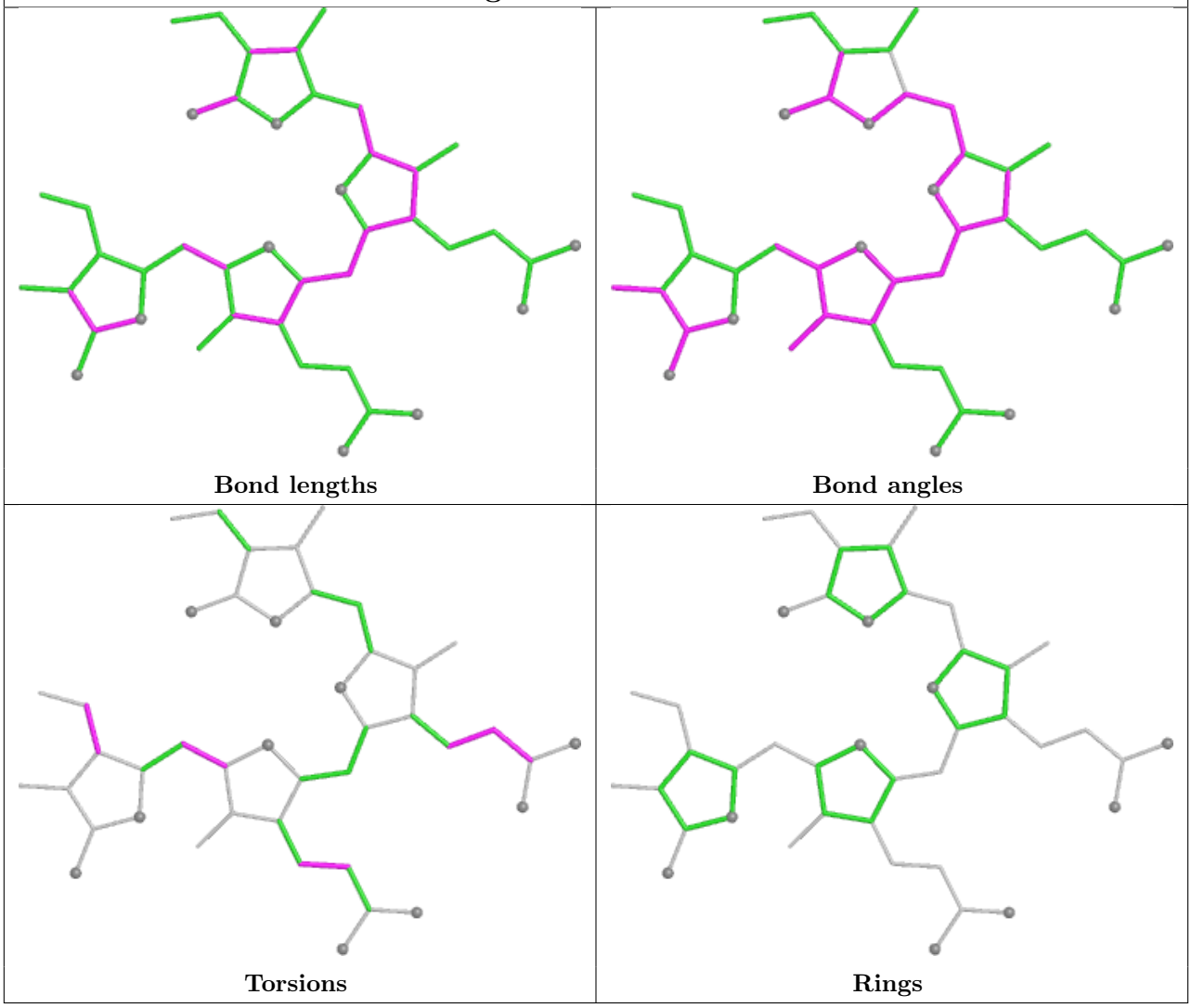


Torsions

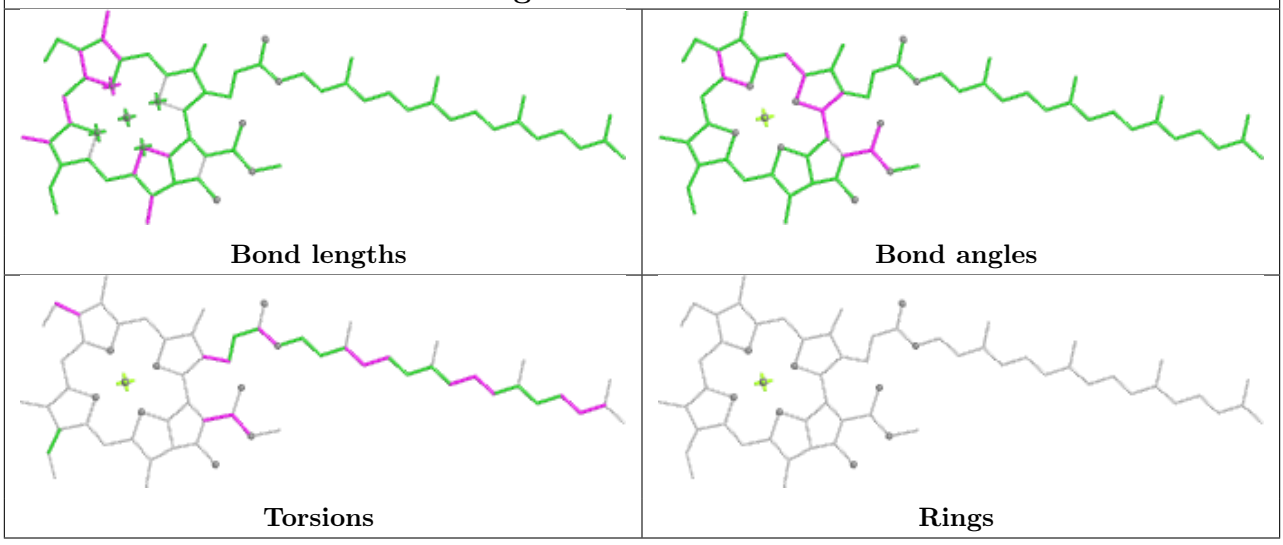


Rings

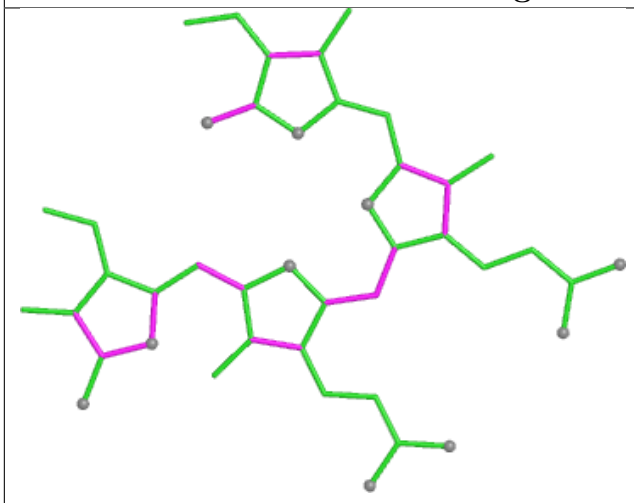
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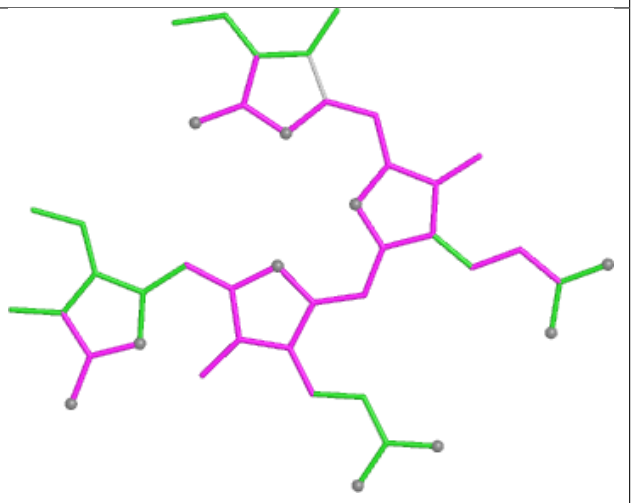
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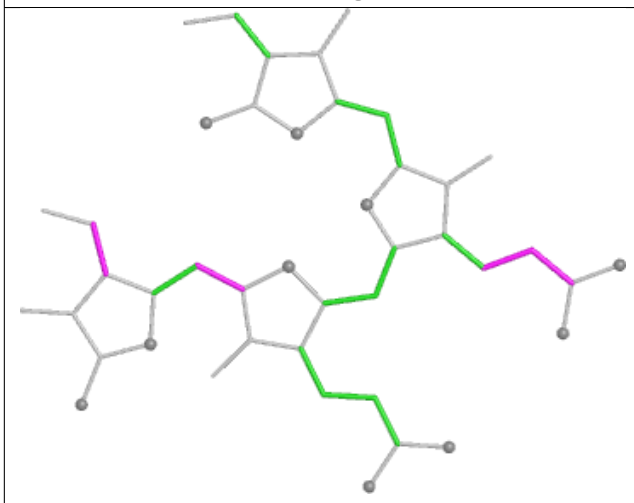
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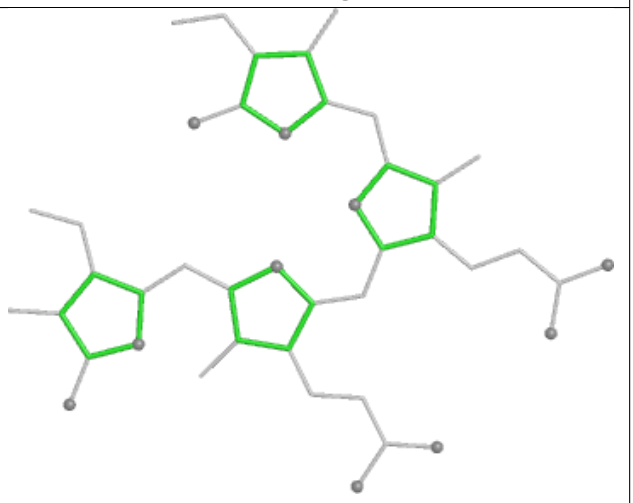
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Bond angles

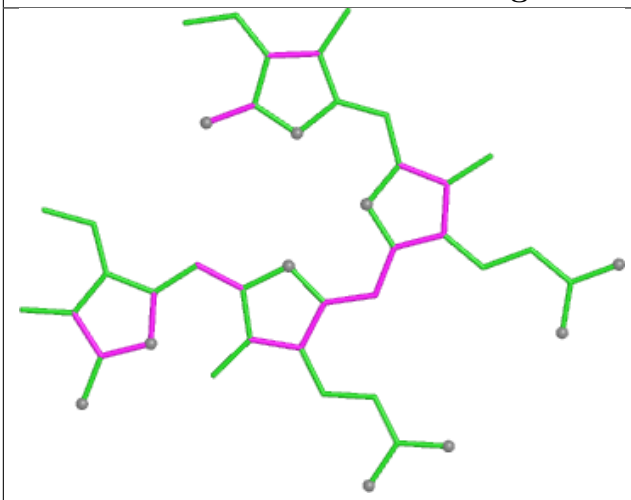


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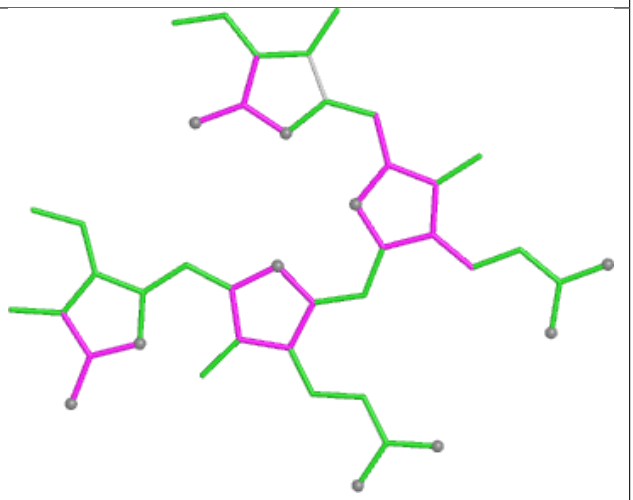


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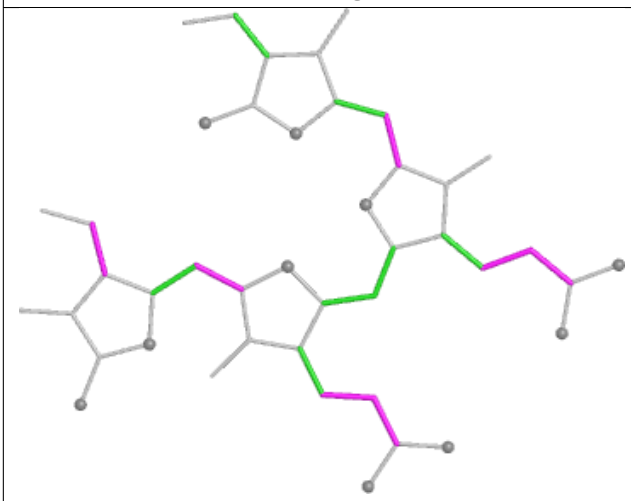
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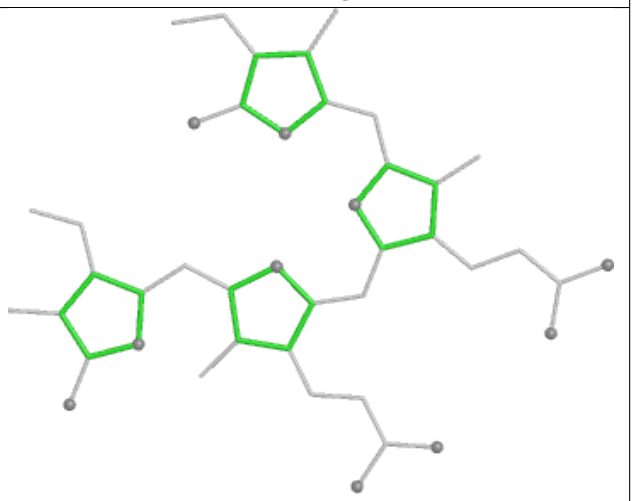
Bond lengths



Bond angles

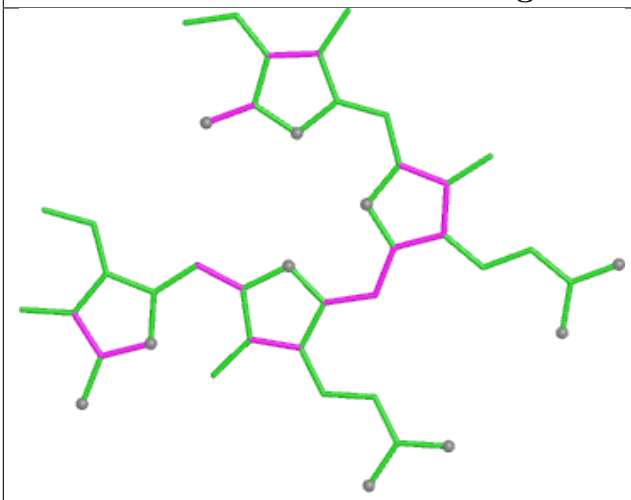


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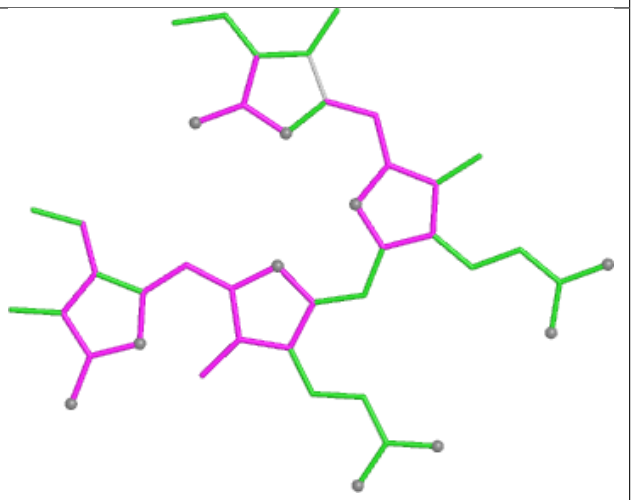


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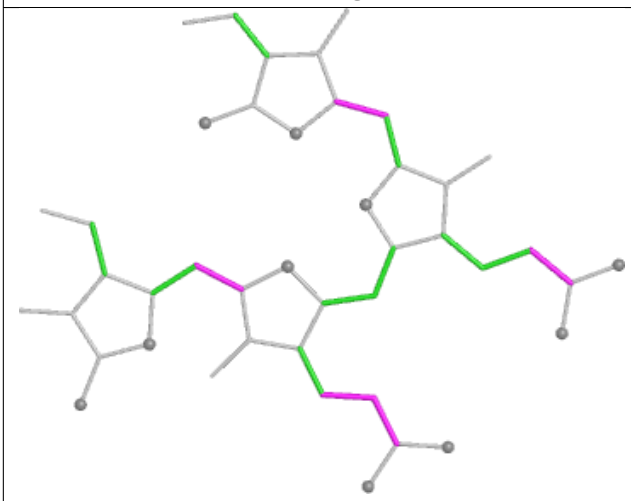
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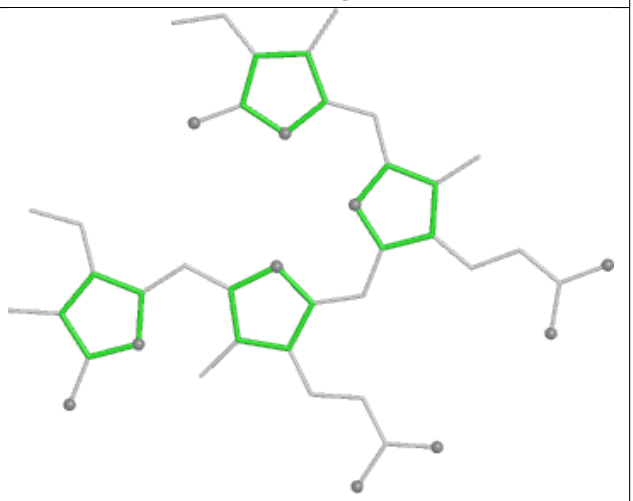
Bond lengths



Bond angles

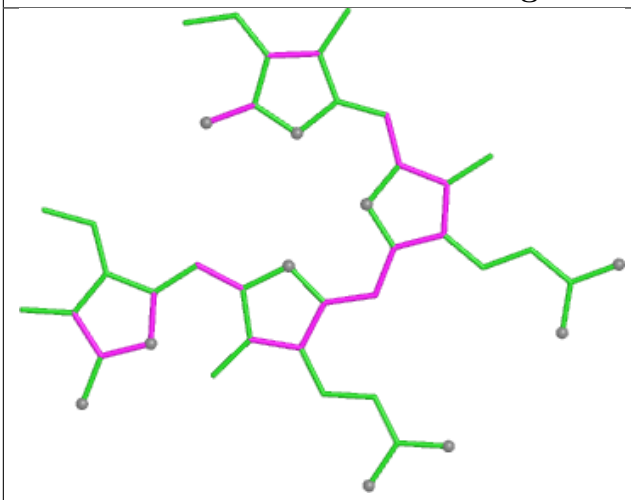


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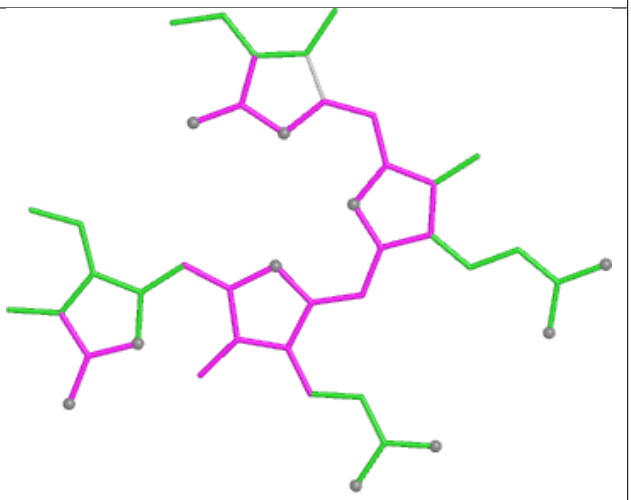


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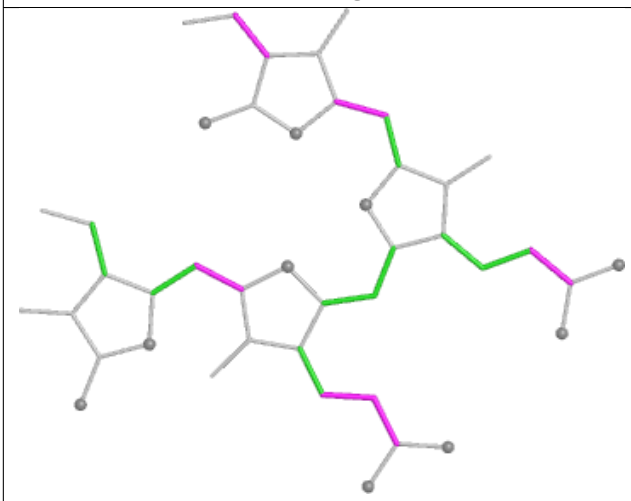
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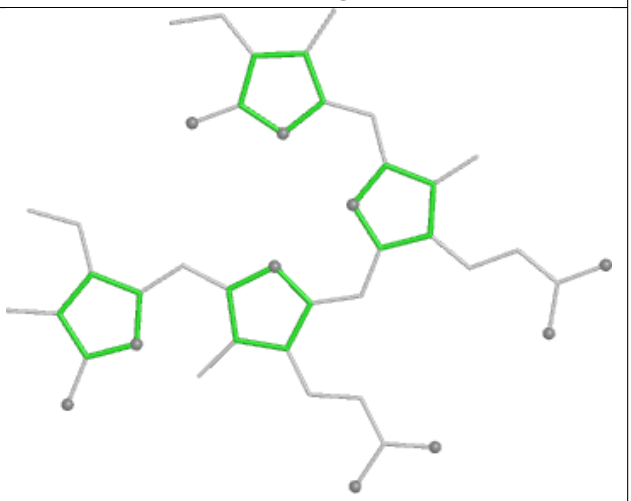
Bond lengths



Bond angles

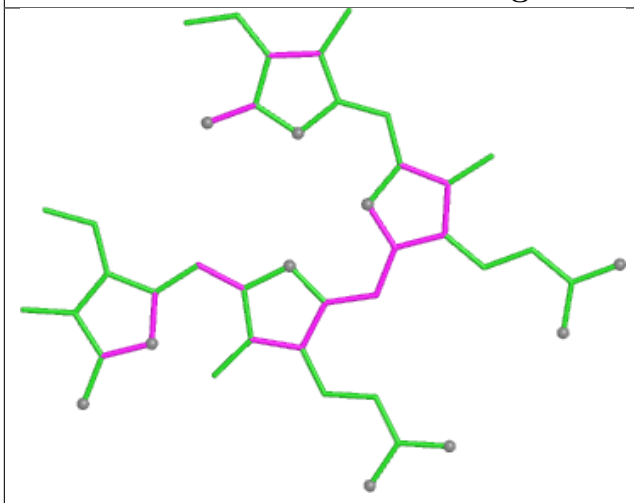


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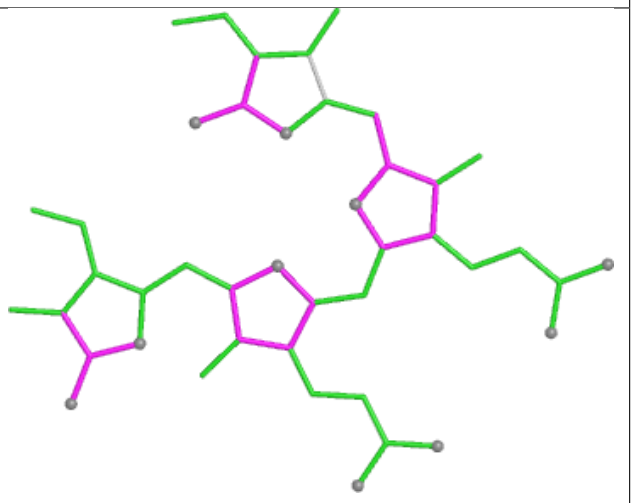


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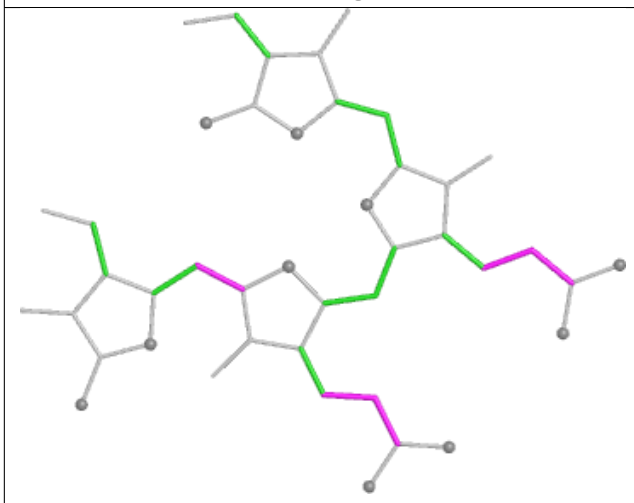
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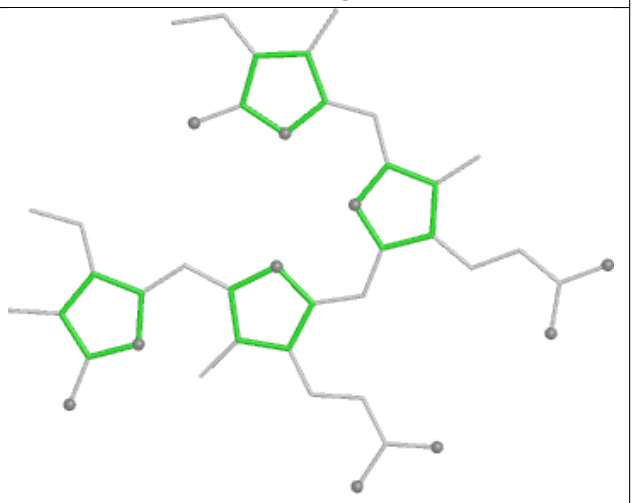
Bond lengths



Bond angles

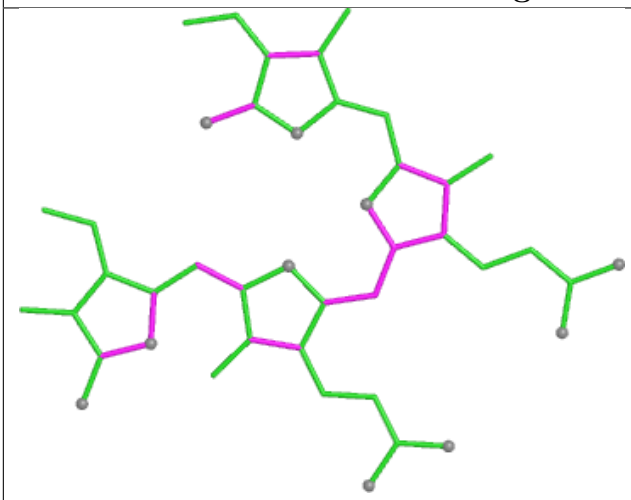


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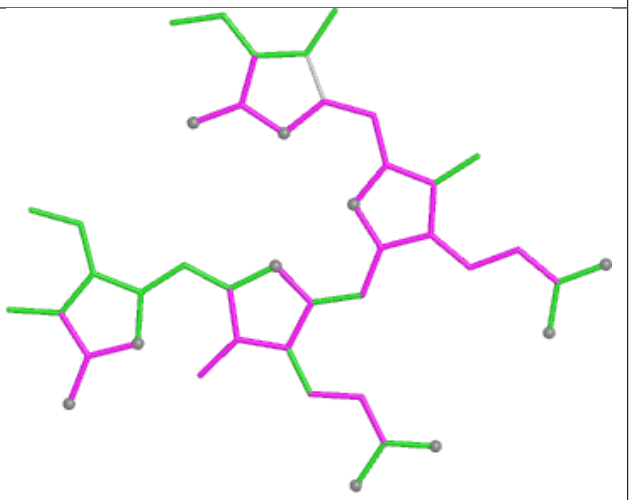


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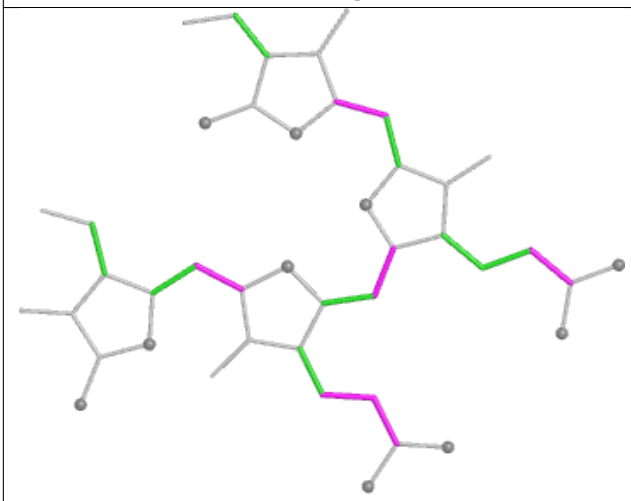
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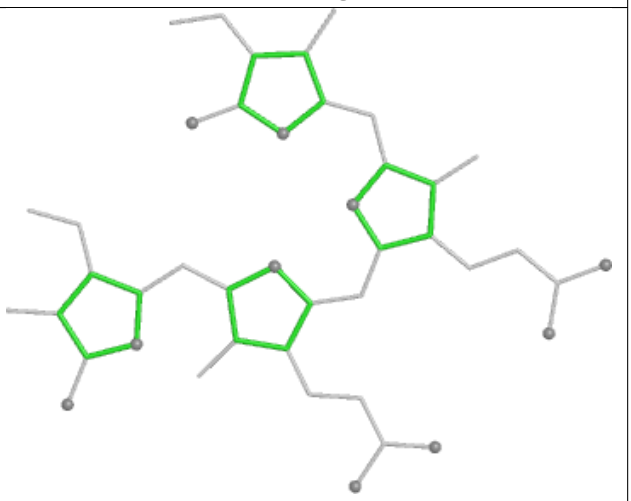
Bond lengths



Bond angles

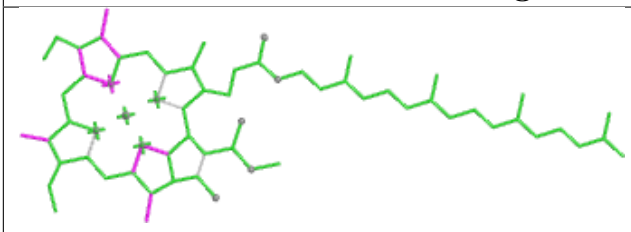


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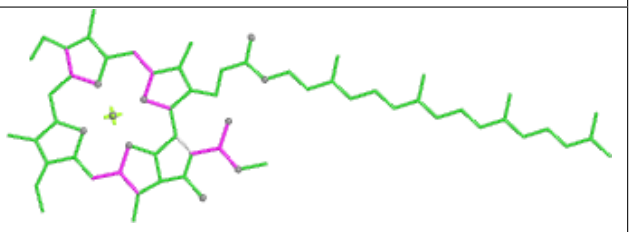


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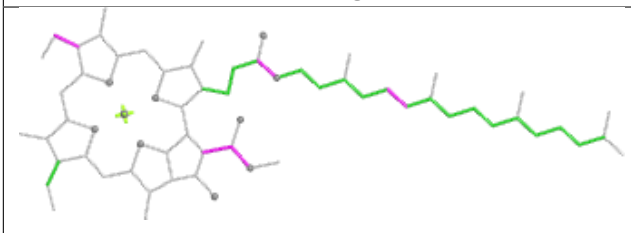
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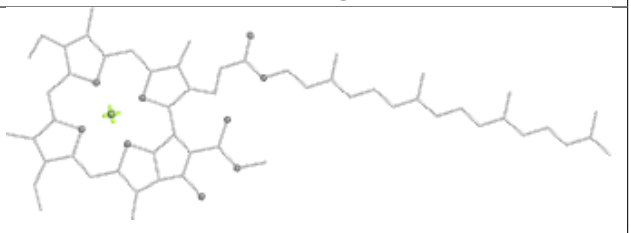
Bond lengths



Bond angles

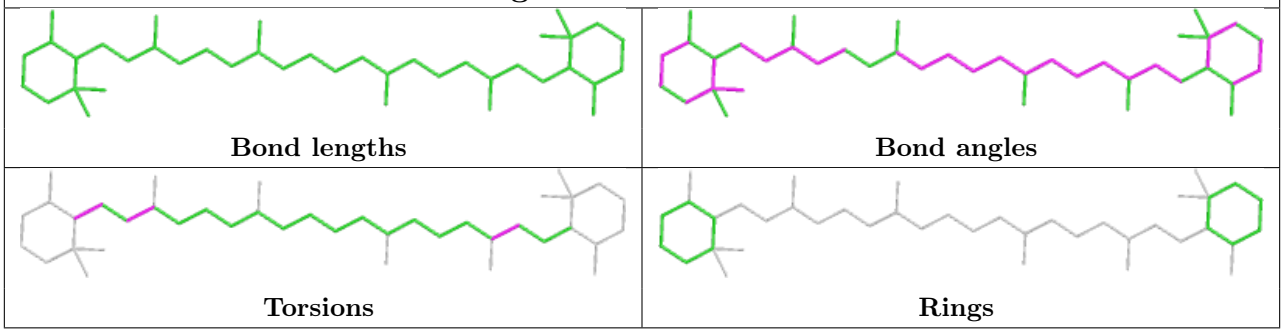


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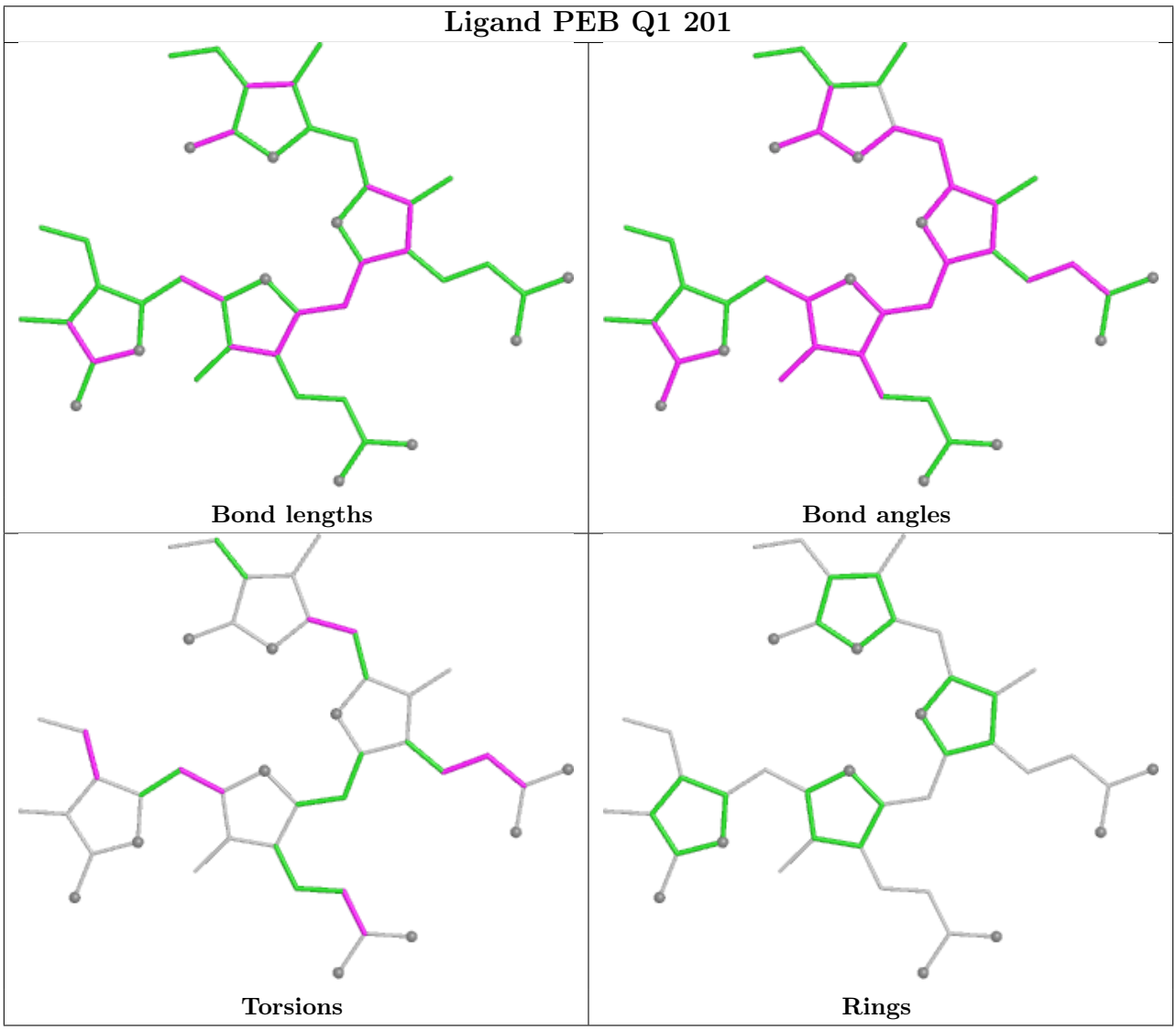


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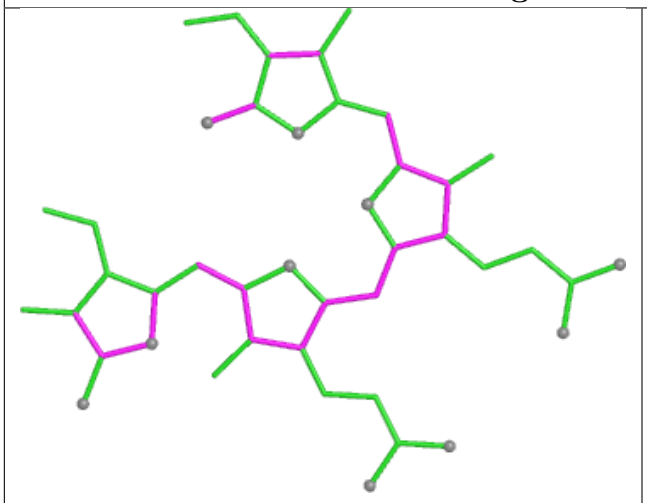
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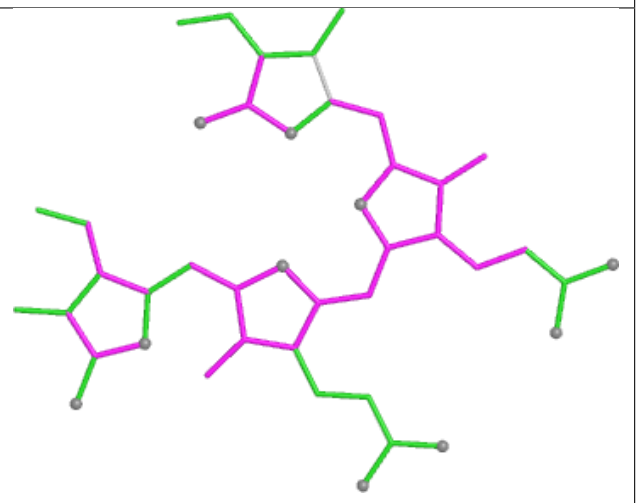
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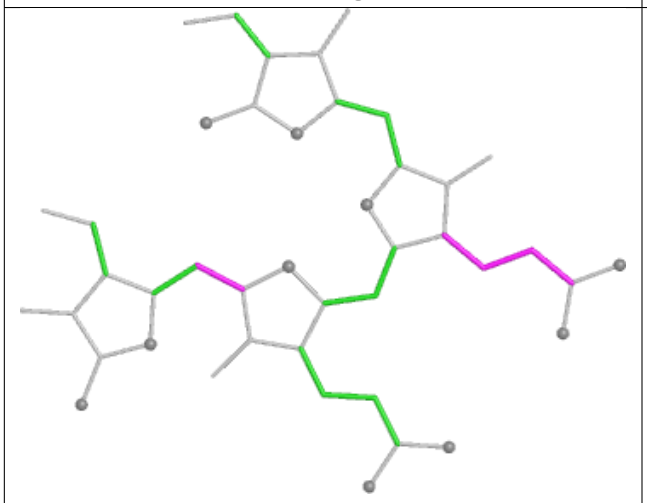
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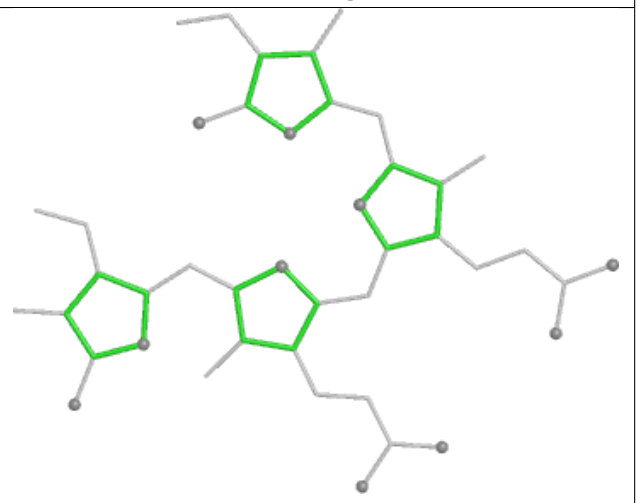
Bond lengths



Bond angles

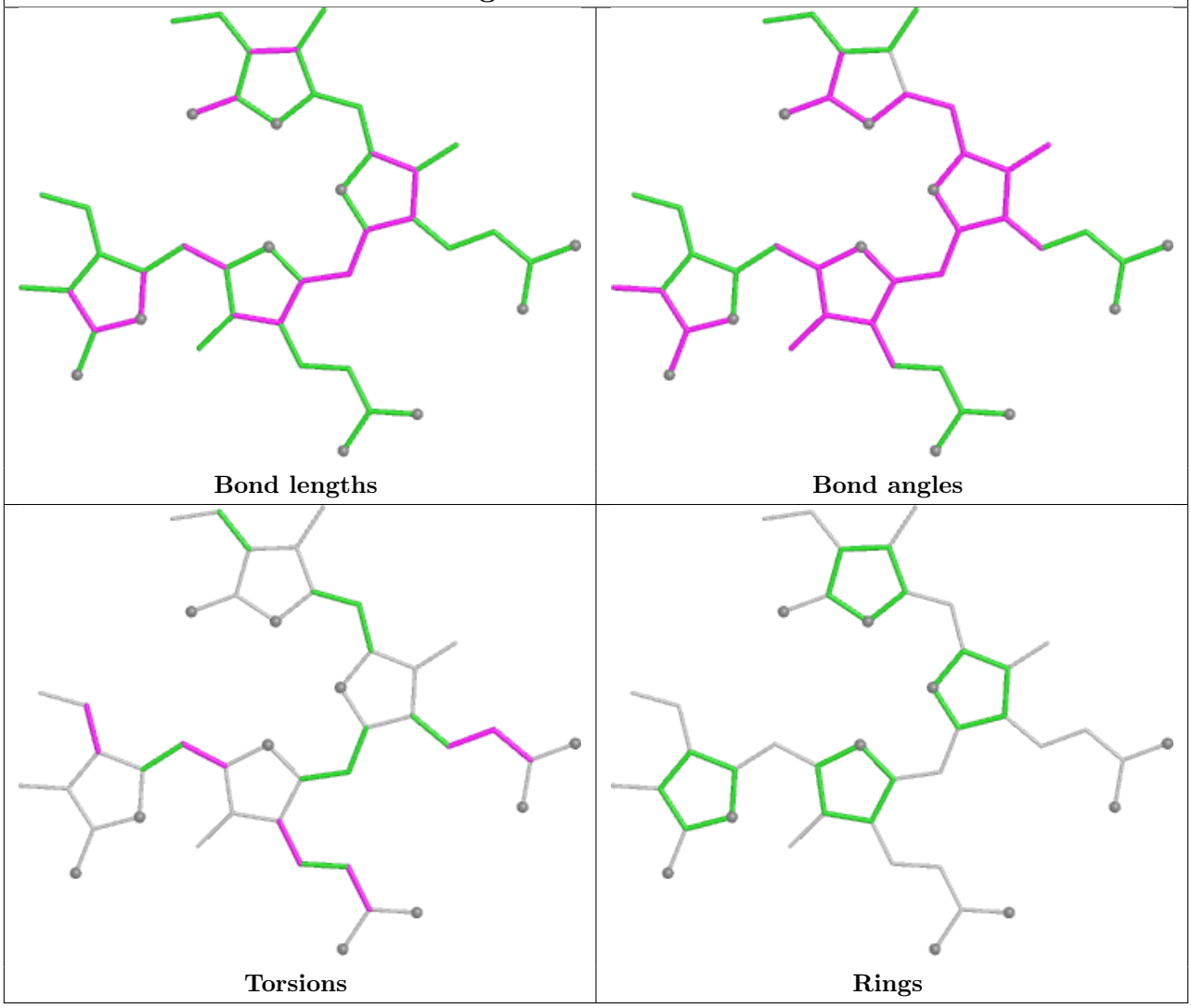


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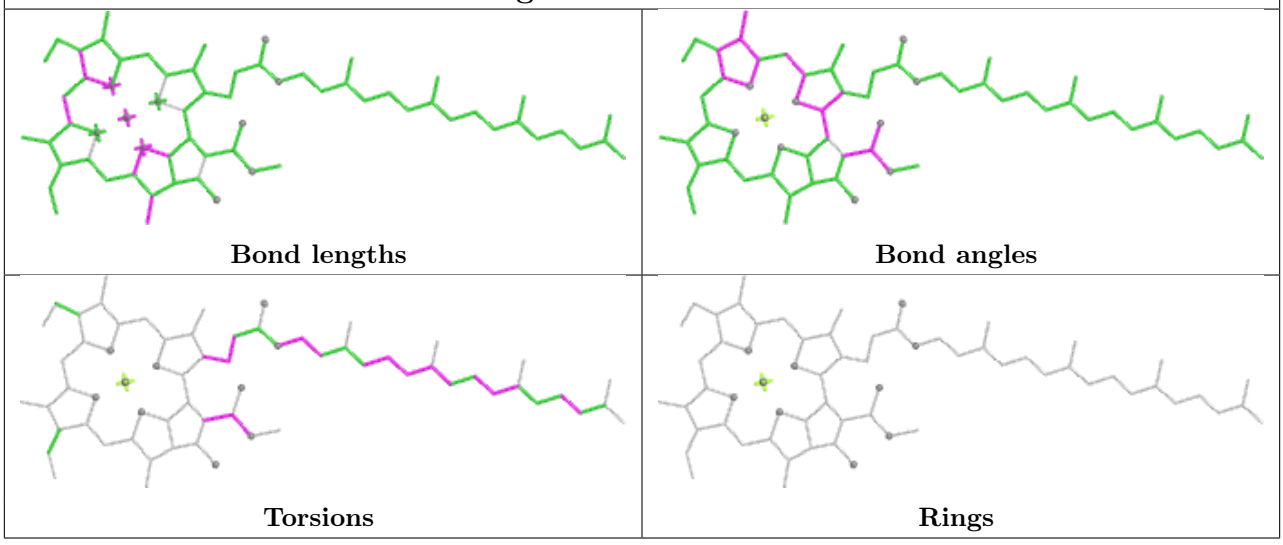


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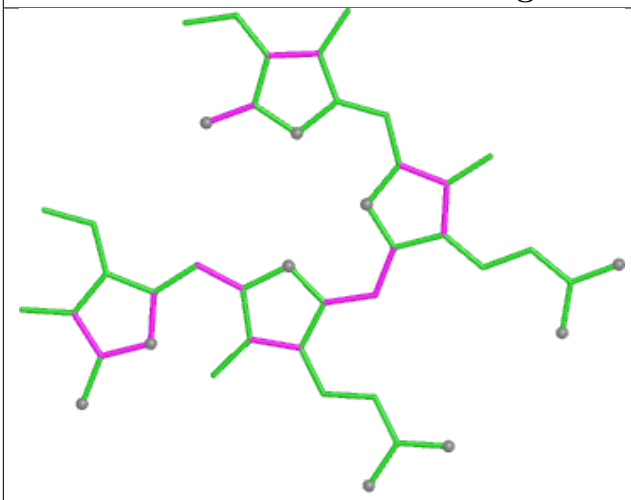
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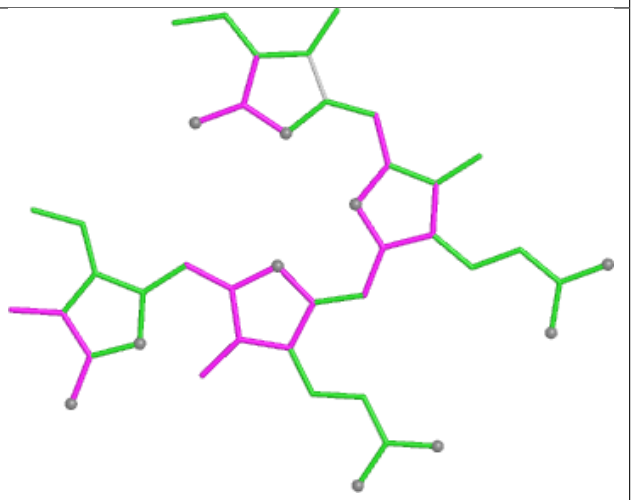
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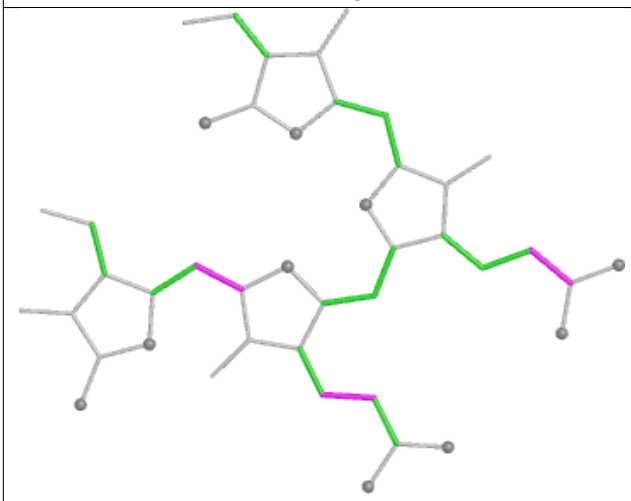
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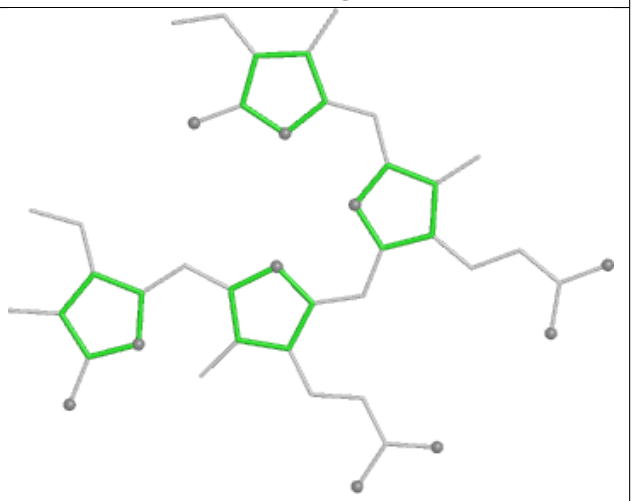
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Bond angles

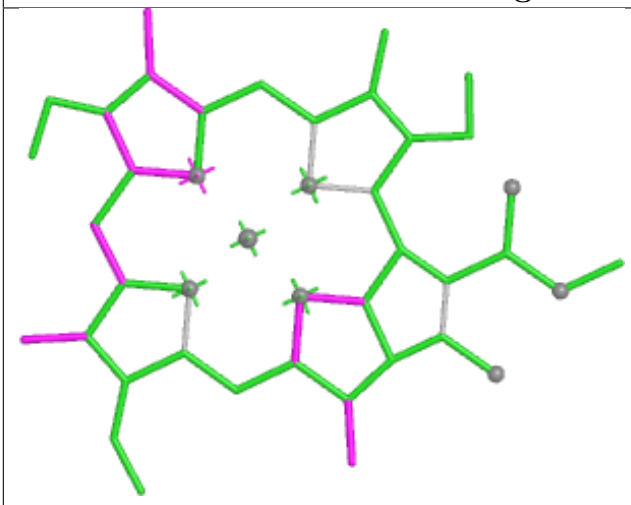


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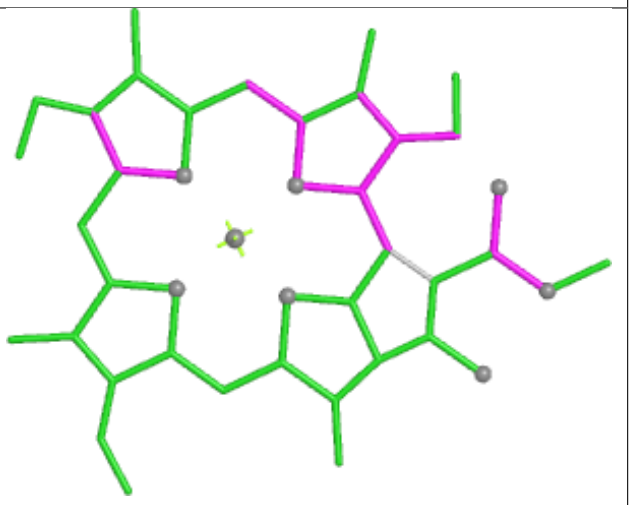


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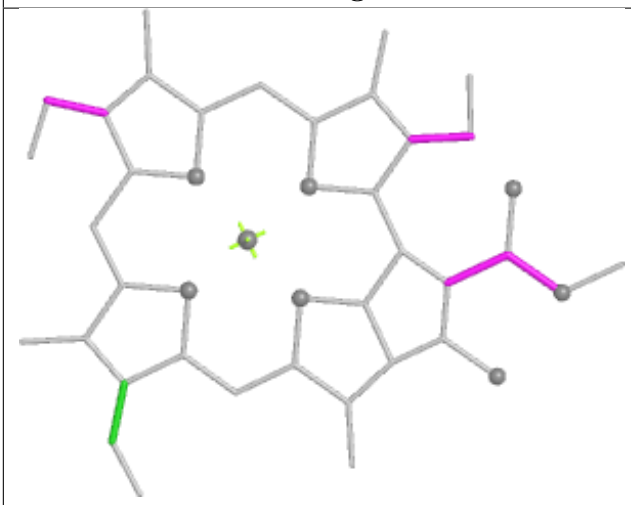
Ligand CLA 5N 604



Bond lengths



Bond angles

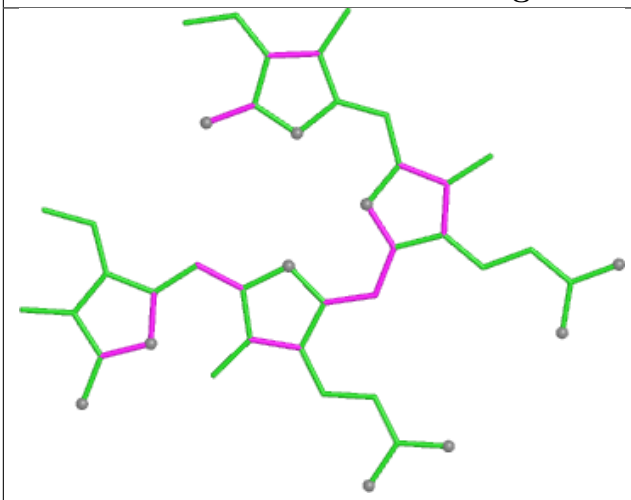


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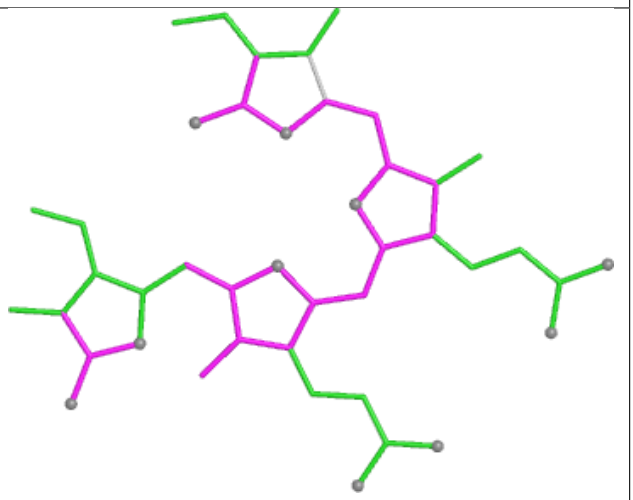


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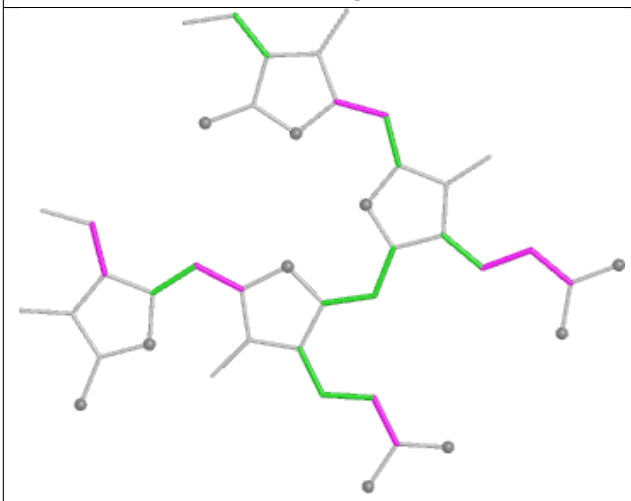
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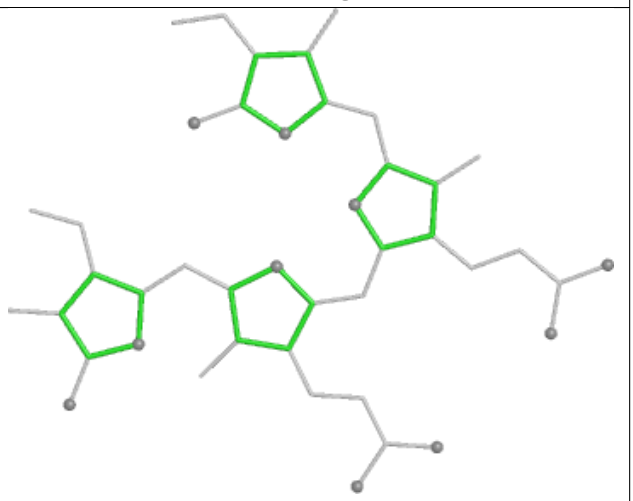
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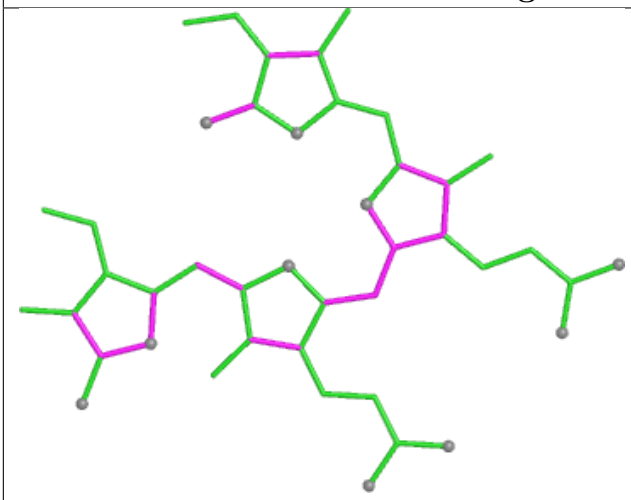


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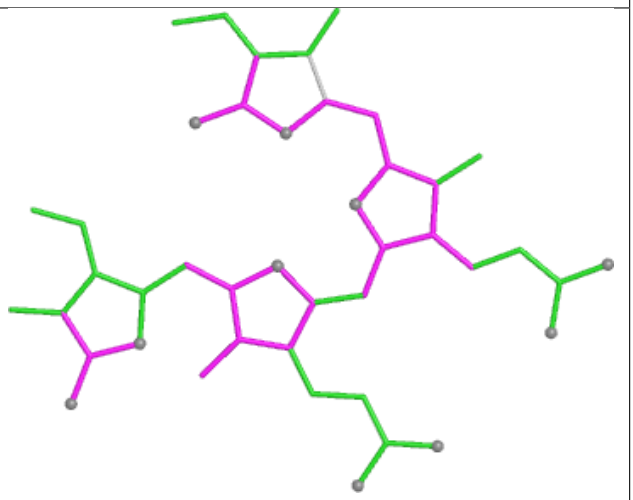


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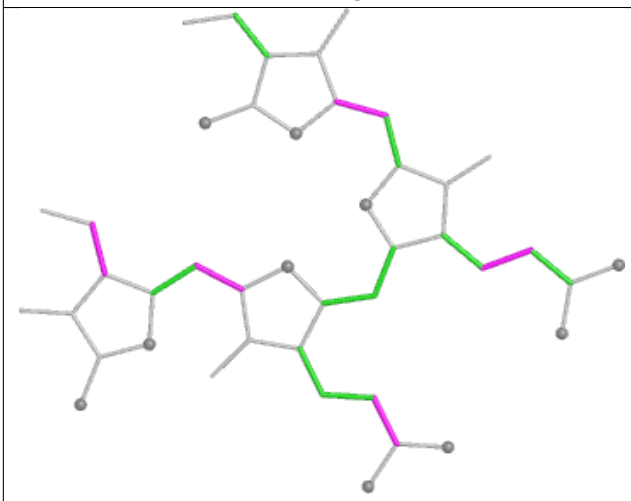
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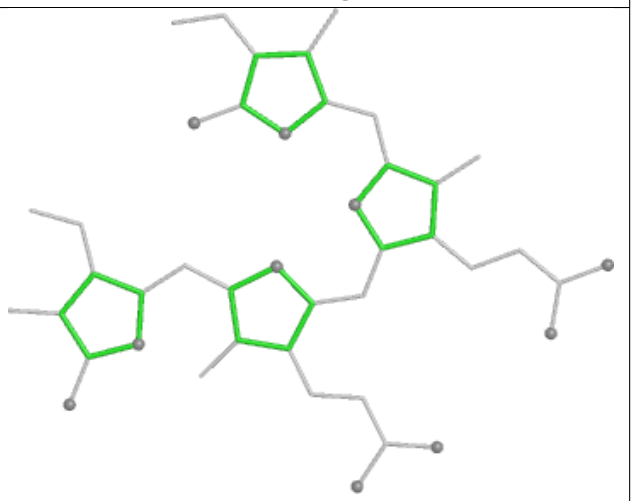
Bond lengths



Bond angles

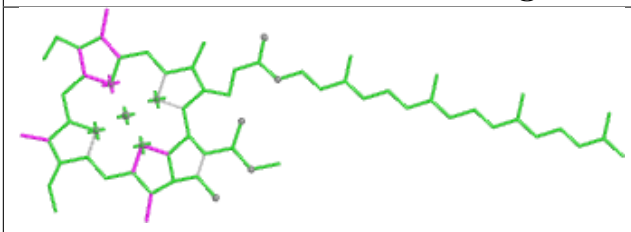


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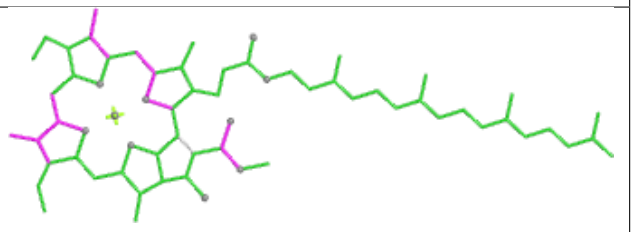


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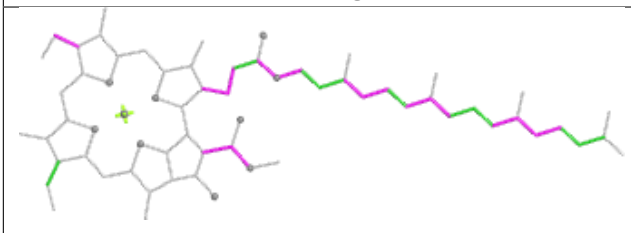
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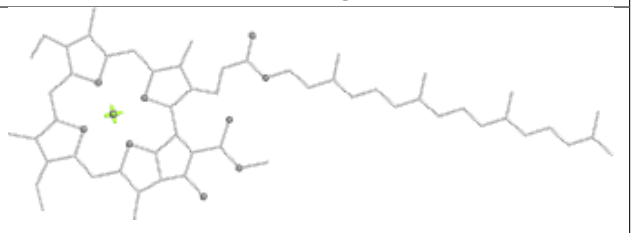
Bond lengths



Bond angles

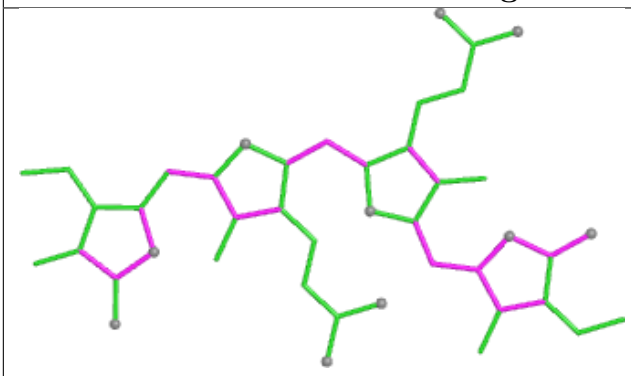


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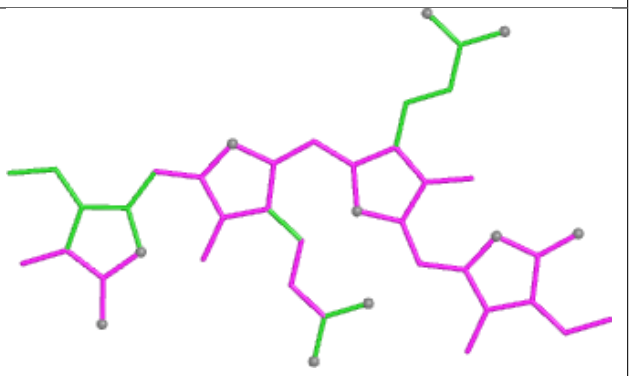


Rings

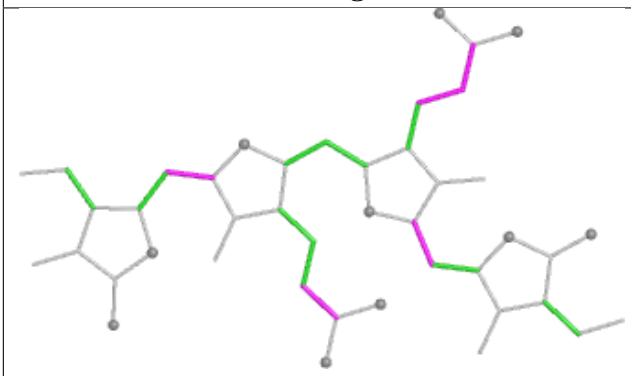
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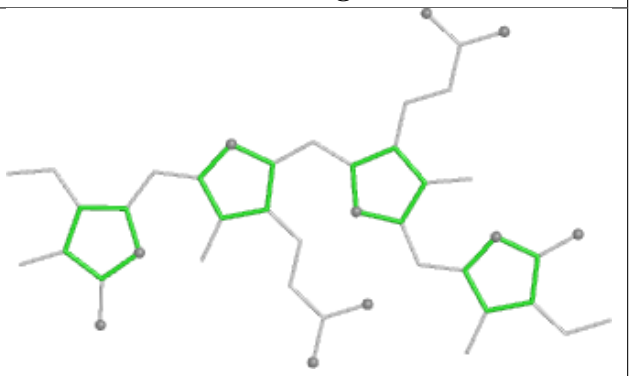
Bond lengths



Bond angles

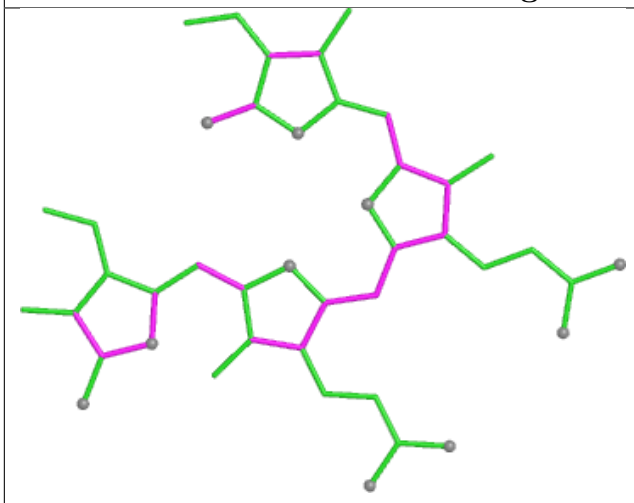


Torsions

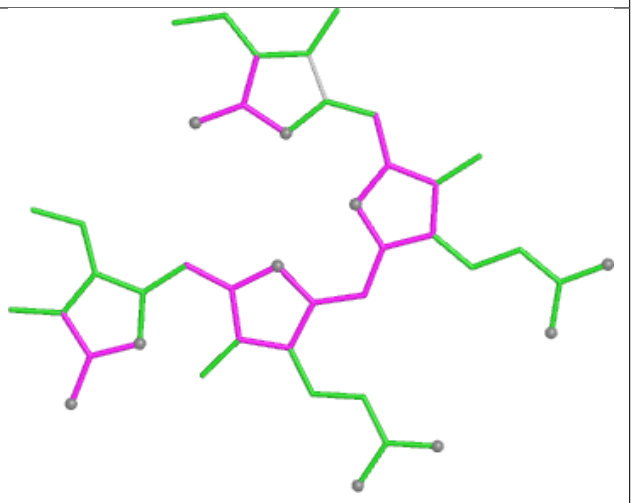


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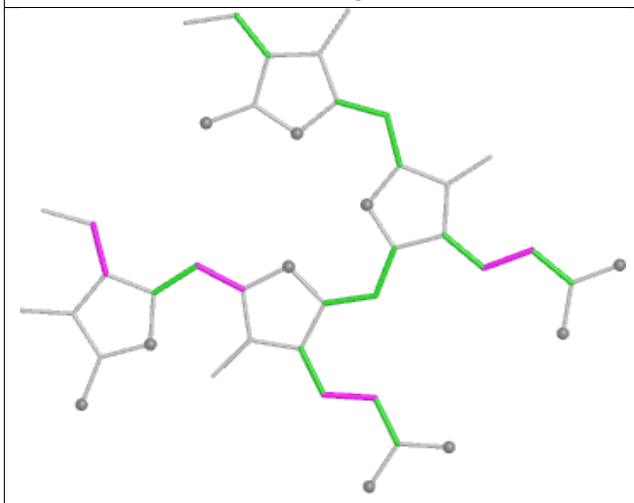
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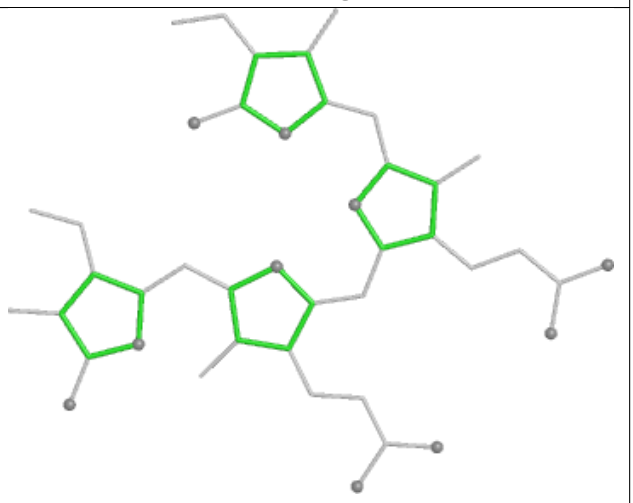
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Bond angles



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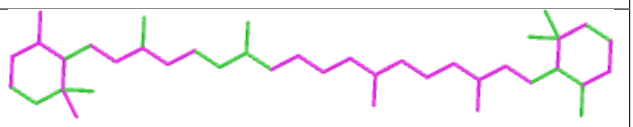


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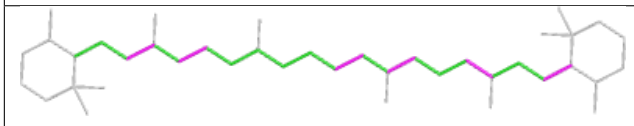
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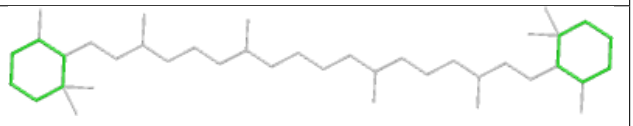
Bond lengths



Bond angles

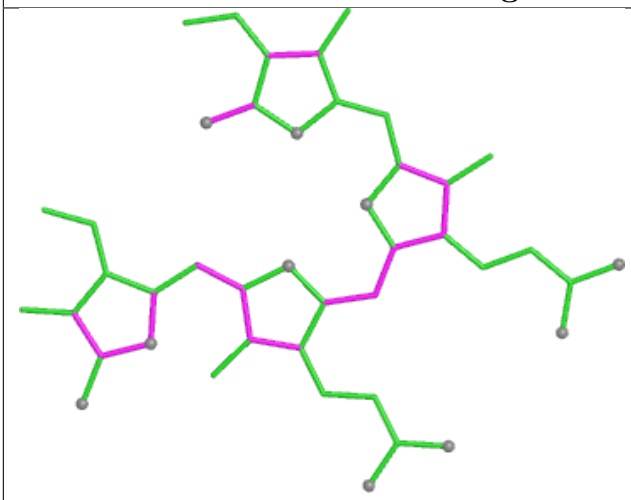


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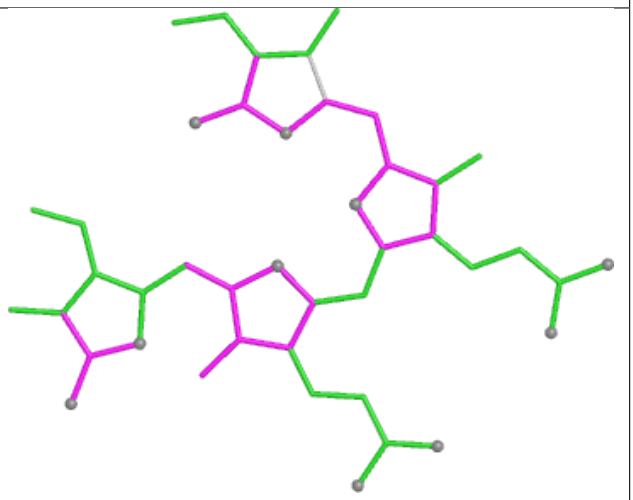


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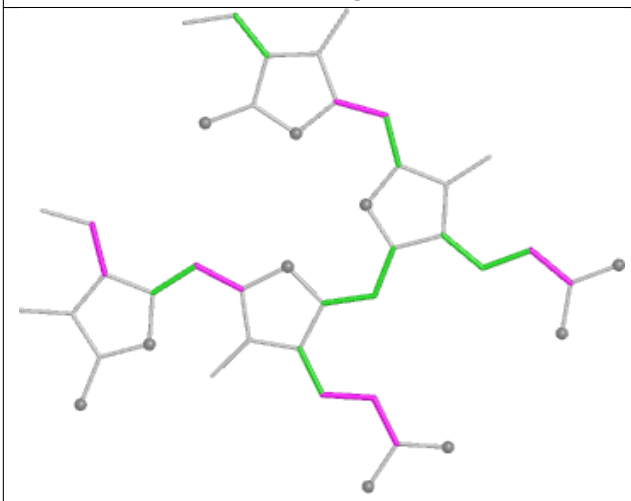
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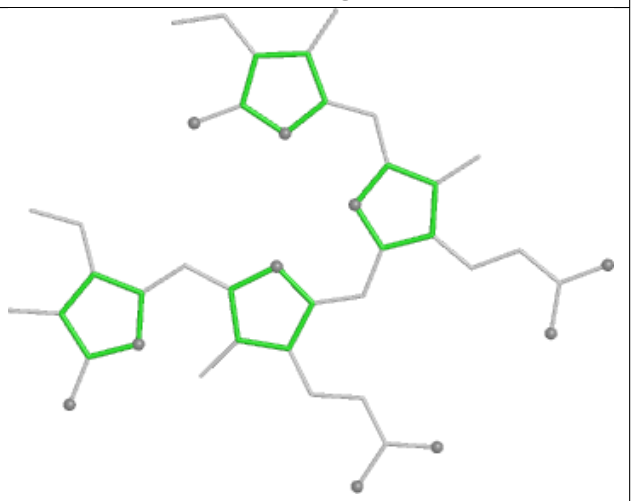
Bond lengths



Bond angles

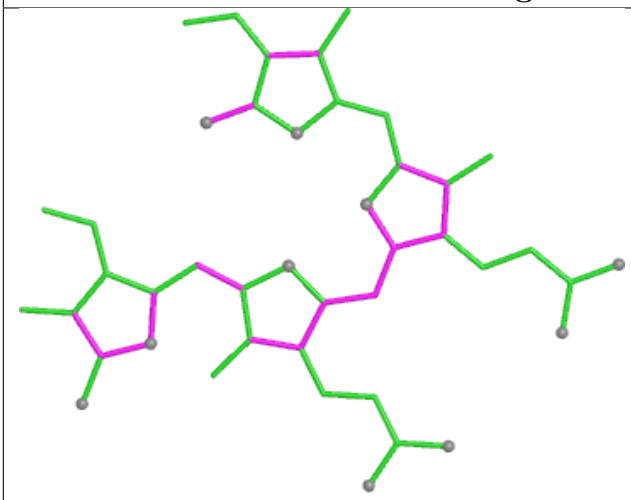


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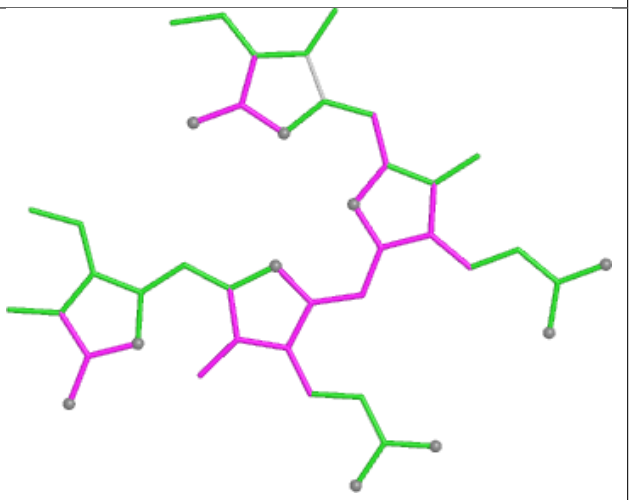


Rings

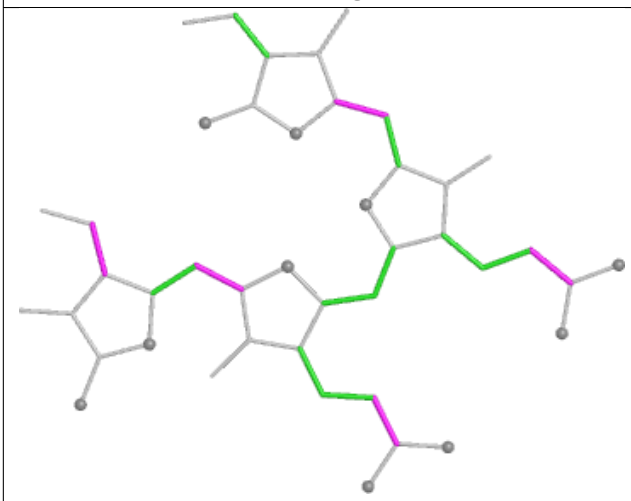
Ligand PEB vC 201



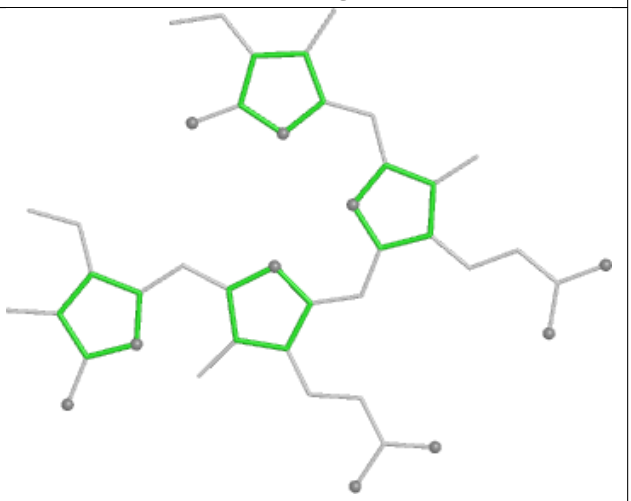
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Bond angles

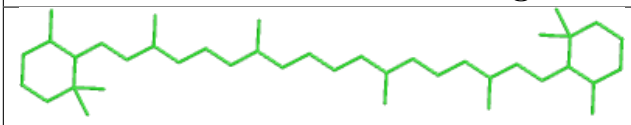


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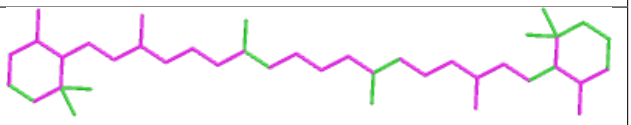


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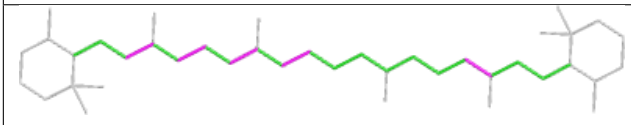
Ligand BCR K2 105



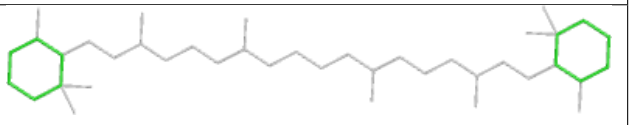
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Bond angles

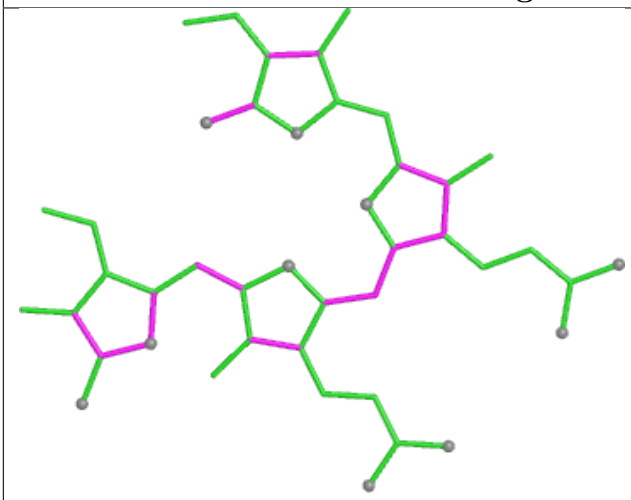


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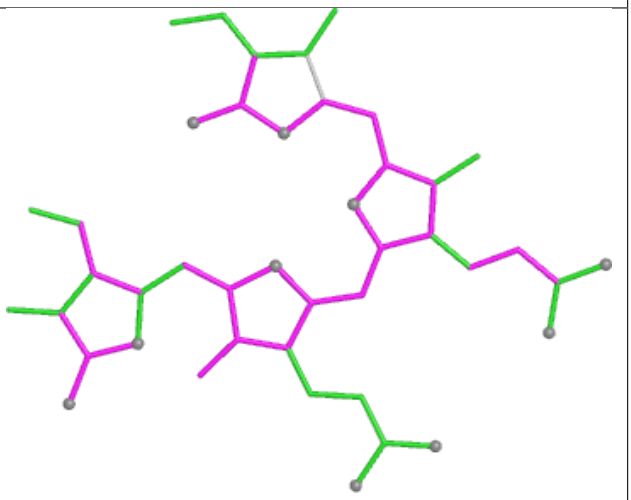


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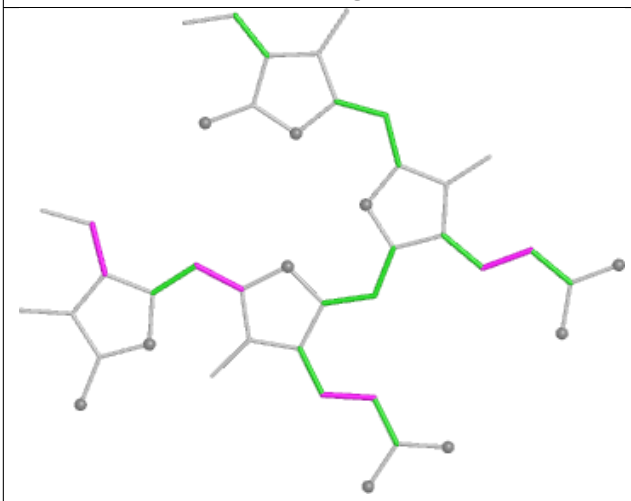
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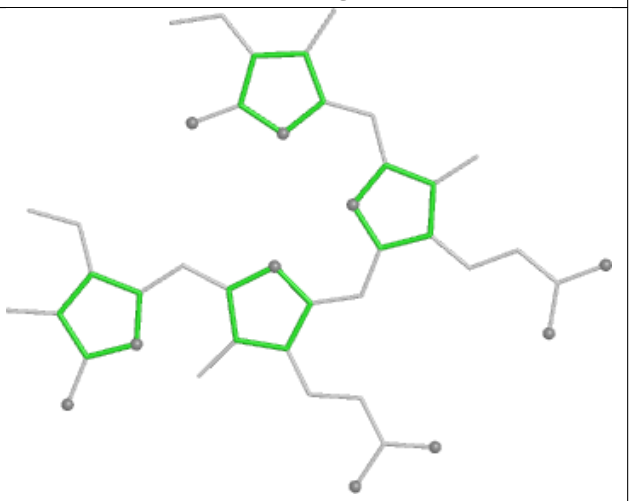
Bond lengths



Bond angles

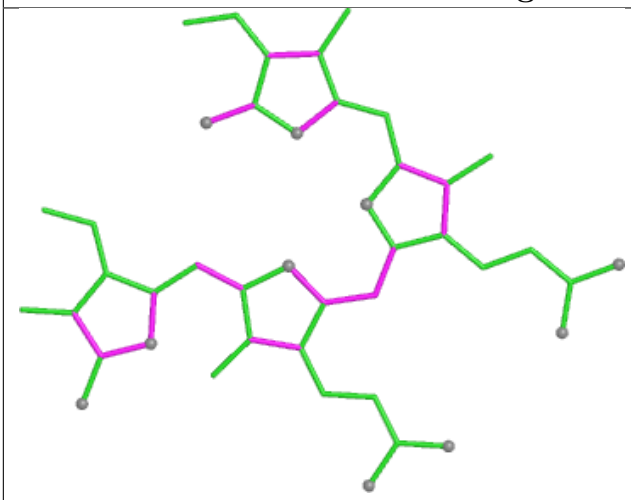


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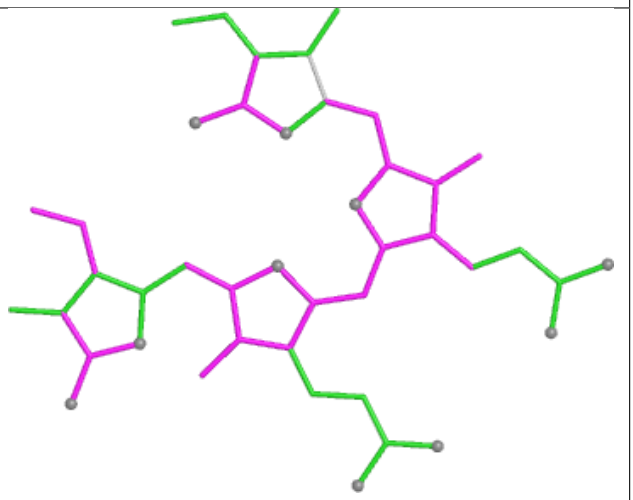


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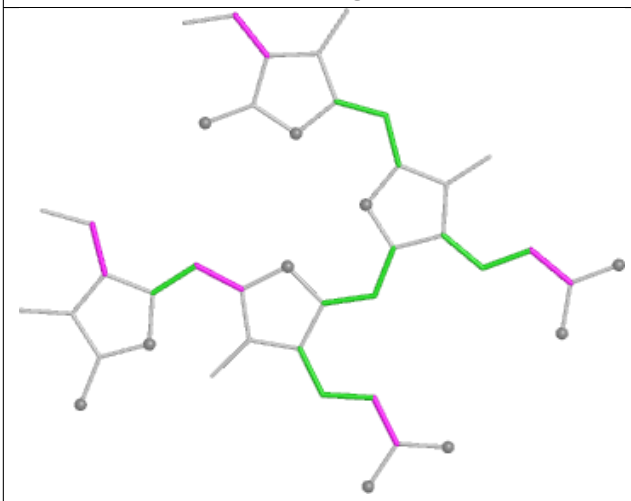
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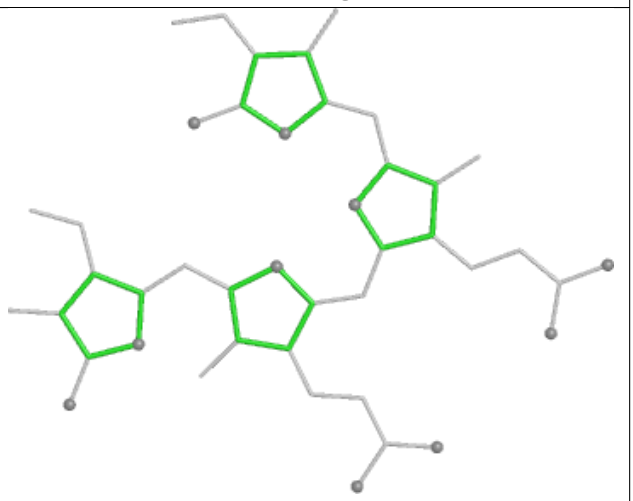
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Bond angles

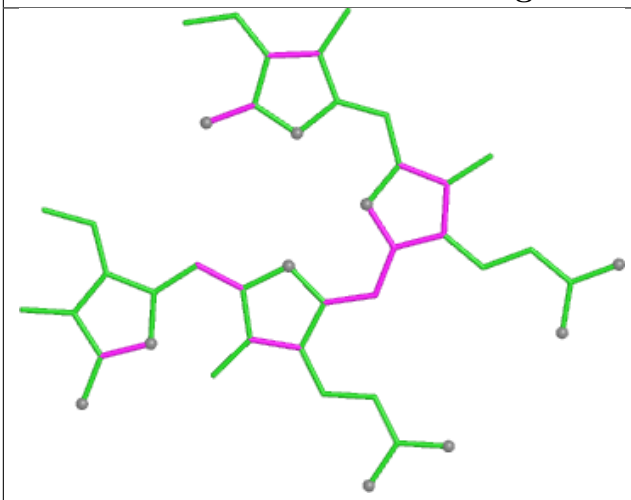


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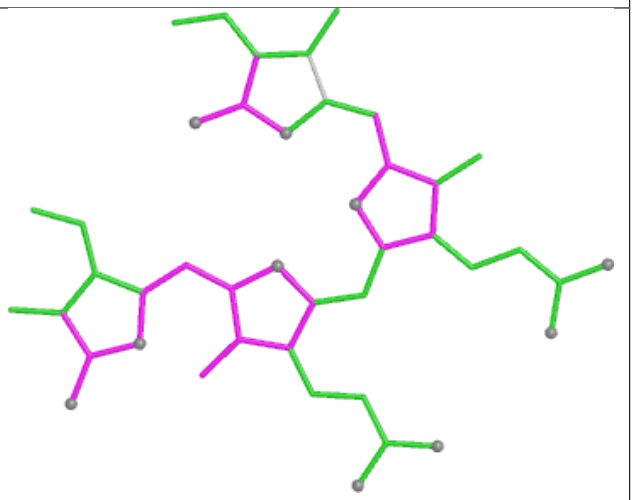


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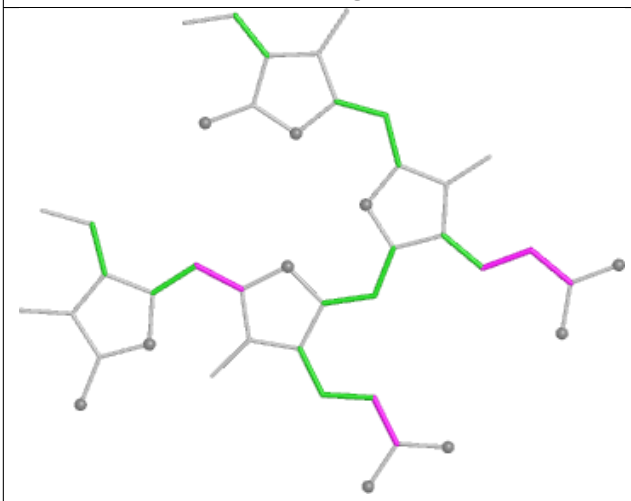
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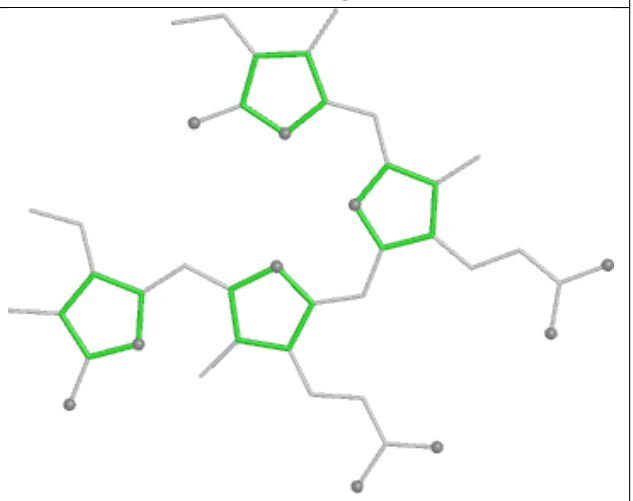
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Bond angles

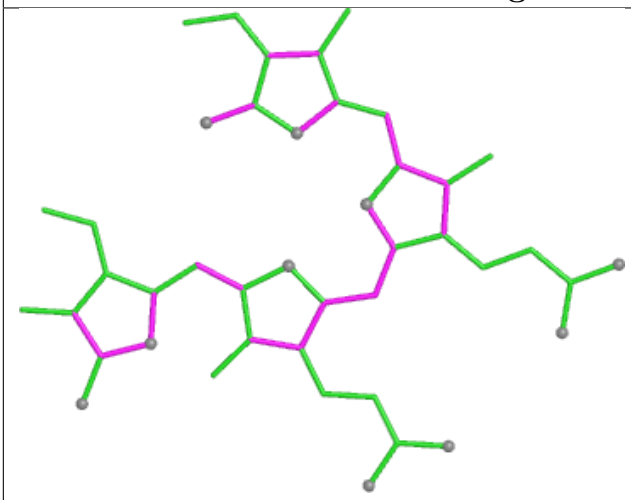


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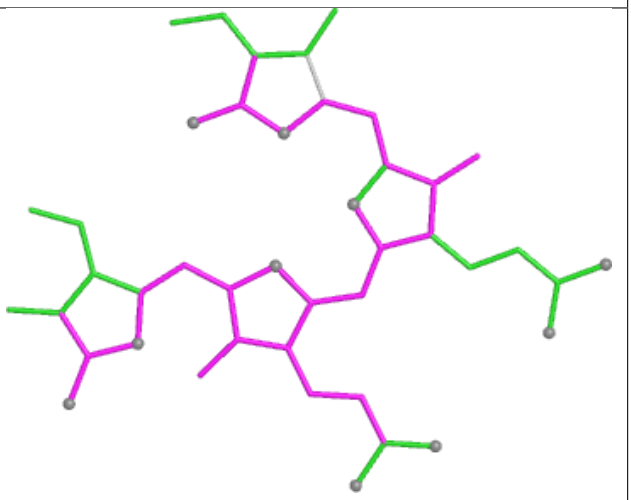


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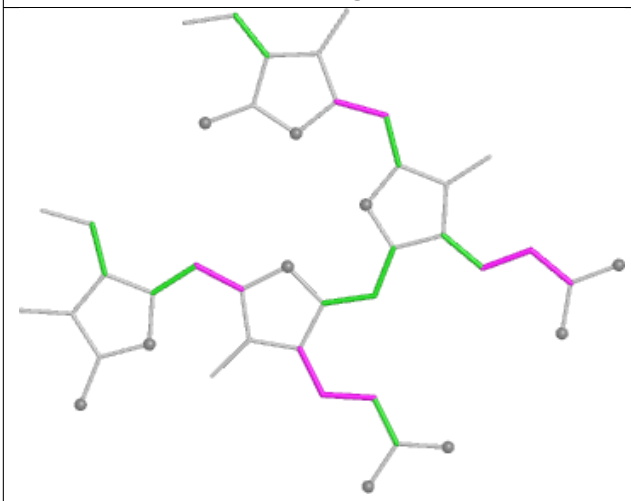
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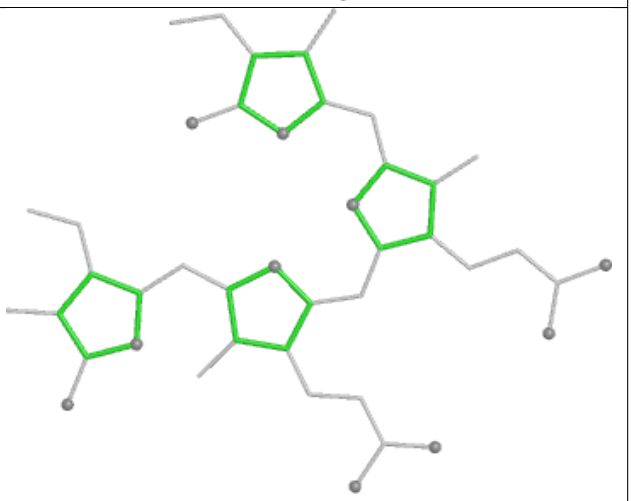
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Bond angles

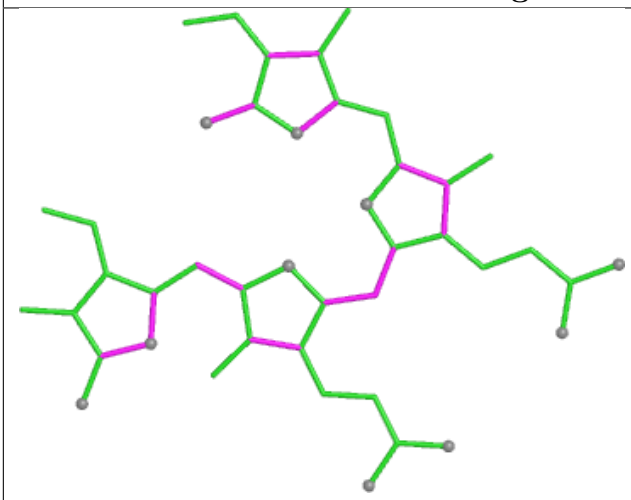


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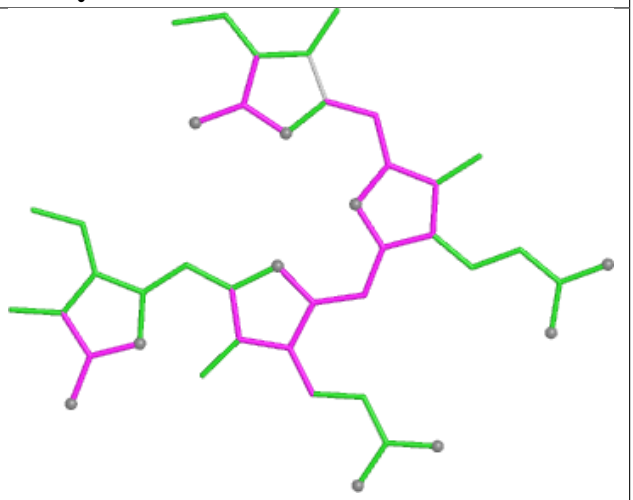


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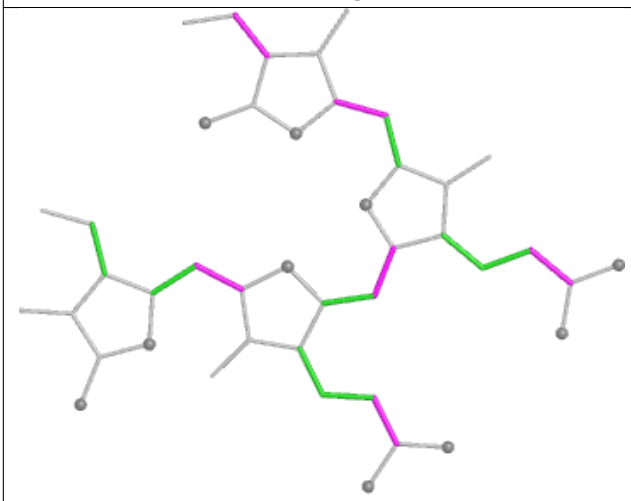
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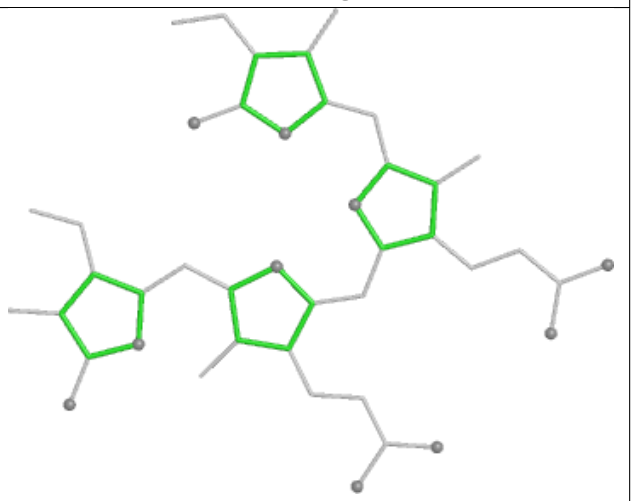
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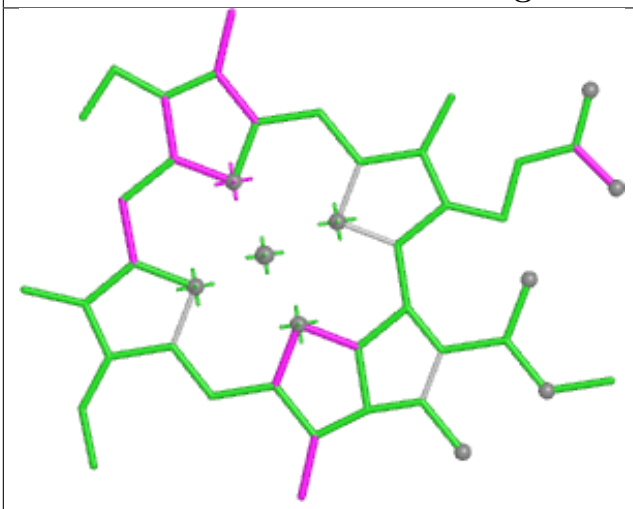


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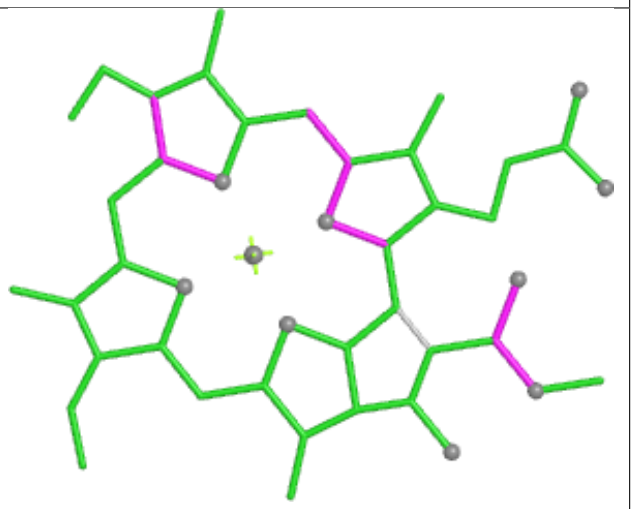


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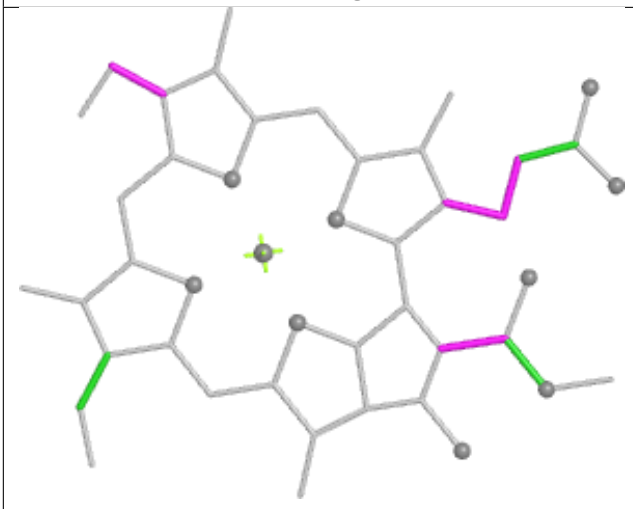
Ligand CLA 6N 613



Bond lengths



Bond angles

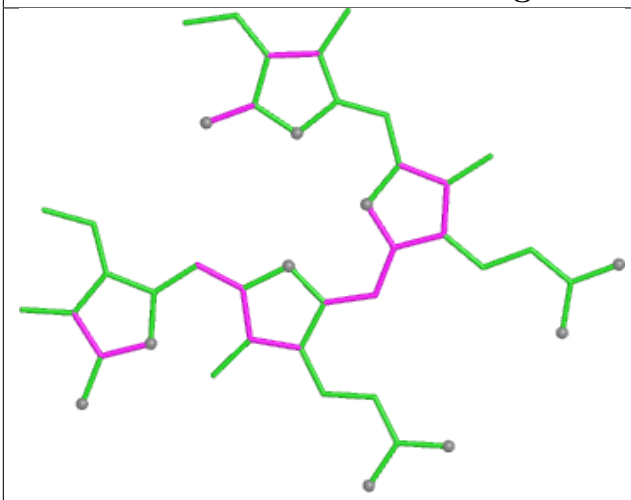


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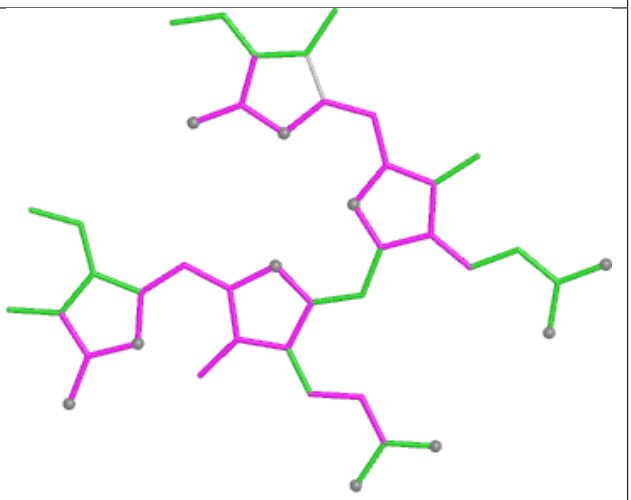


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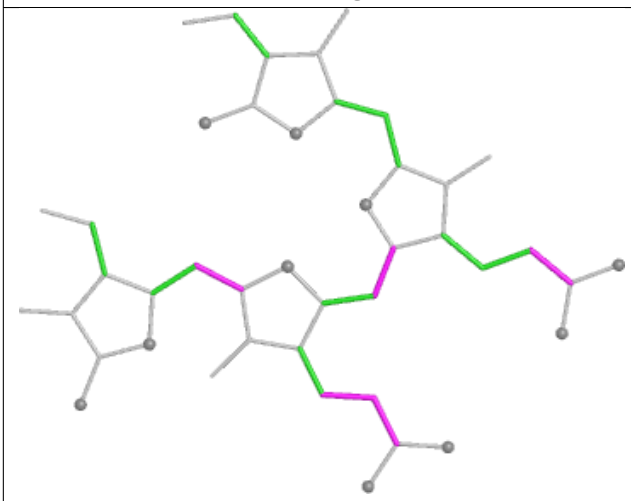
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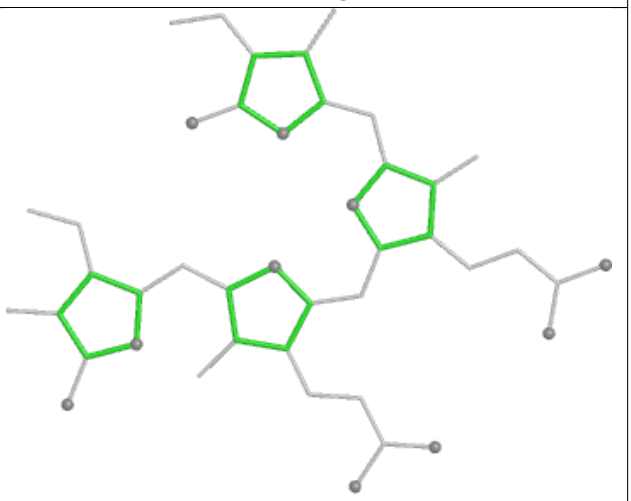
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Bond angles

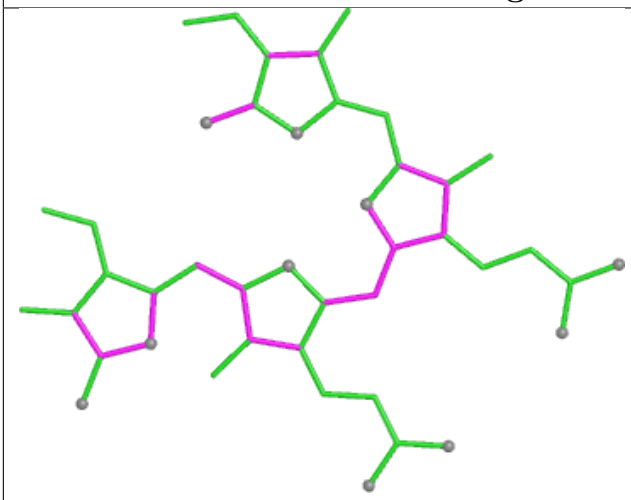


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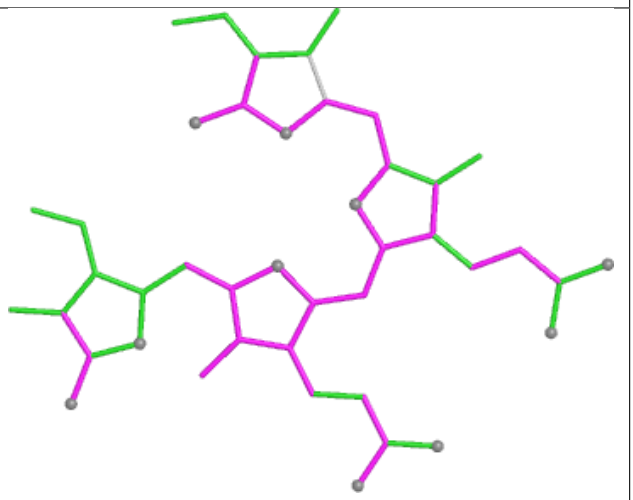


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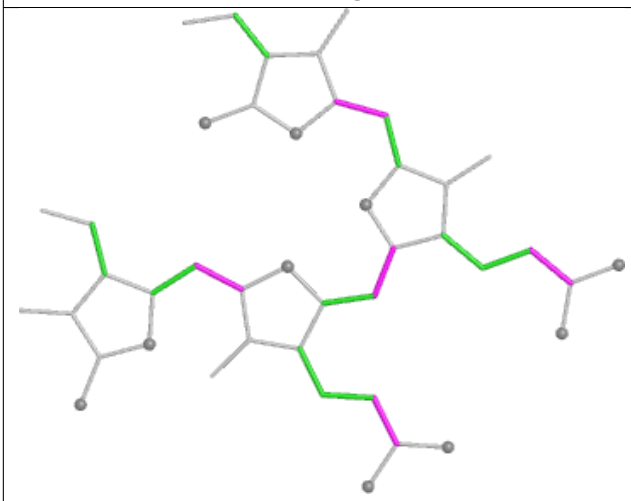
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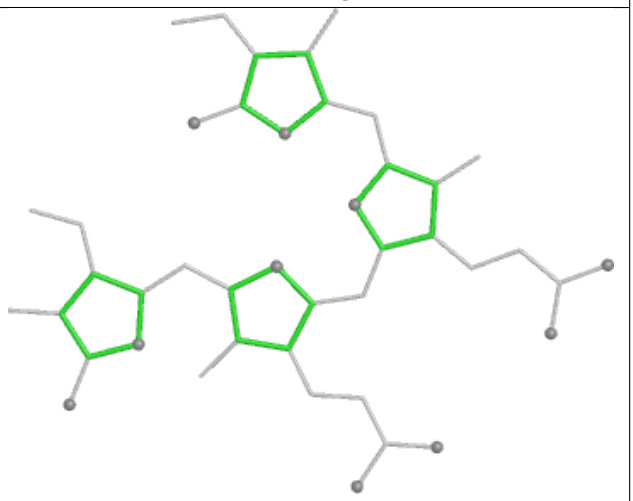
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Bond angles

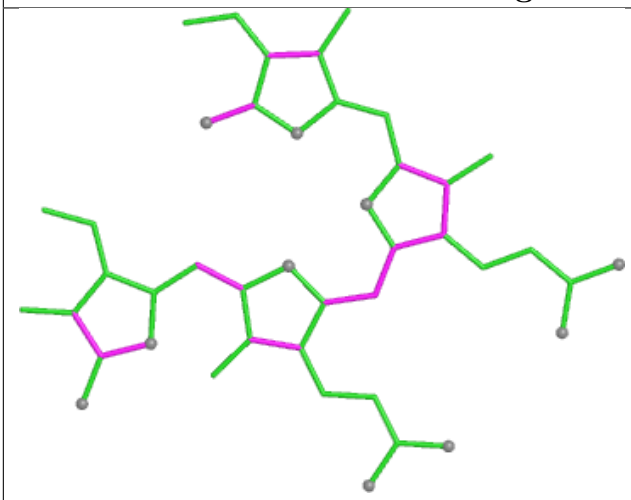


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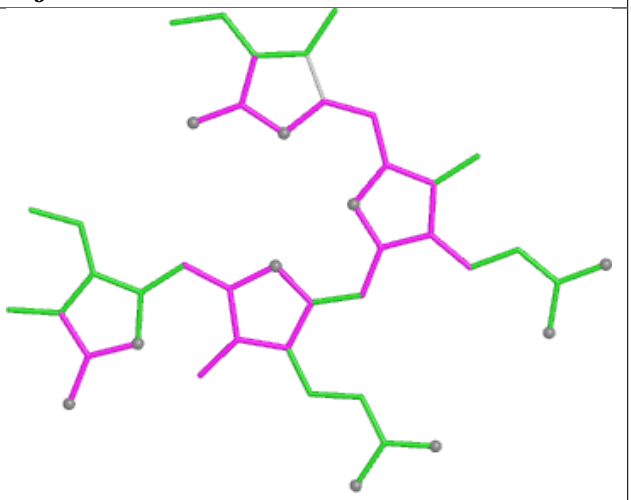


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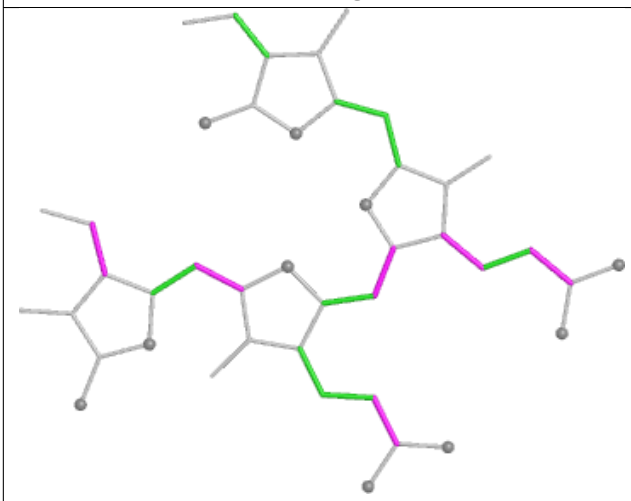
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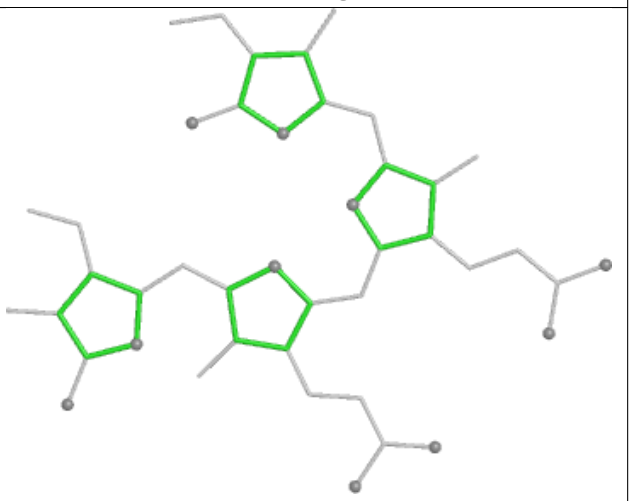
Bond lengths



Bond angles

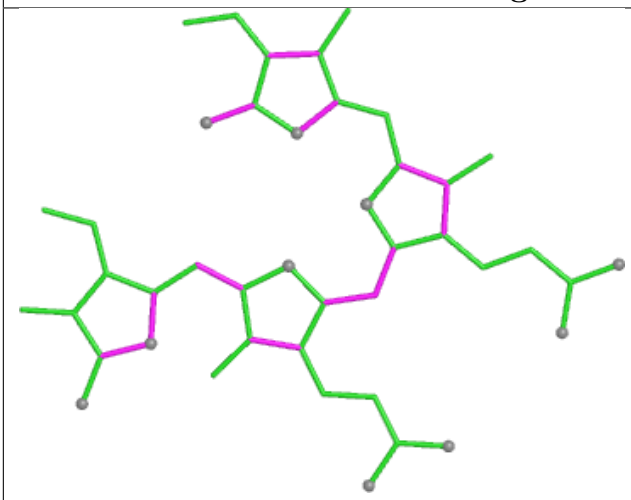


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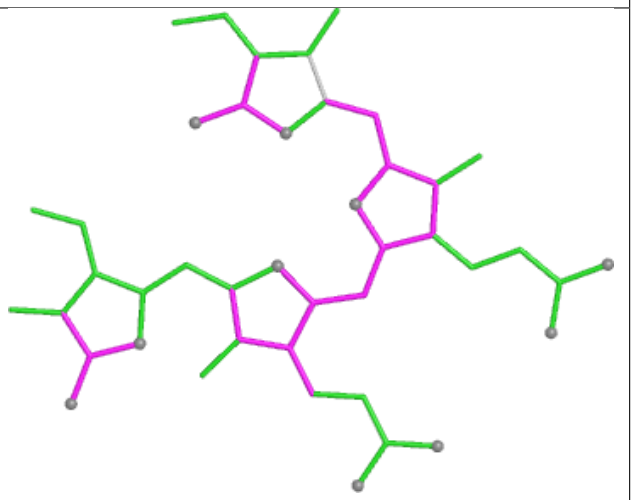


Rings

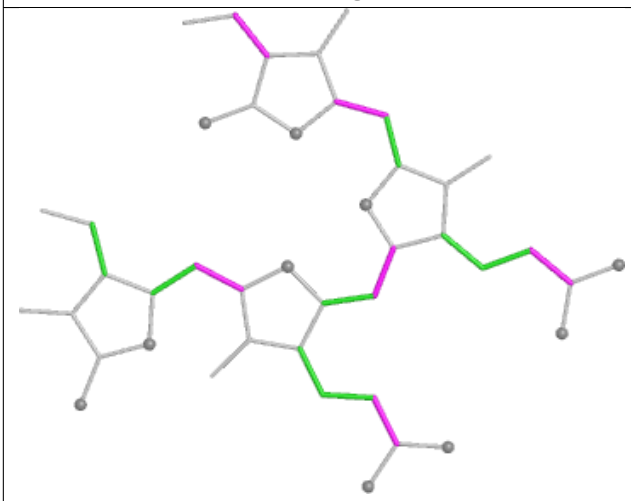
Ligand PEB VD 201



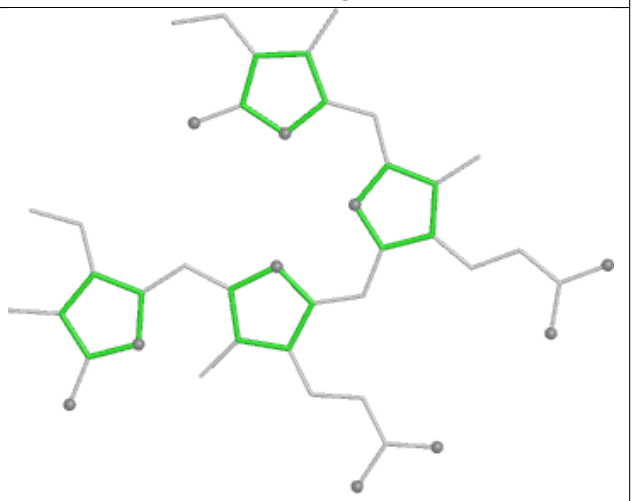
Bond lengths



Bond angles

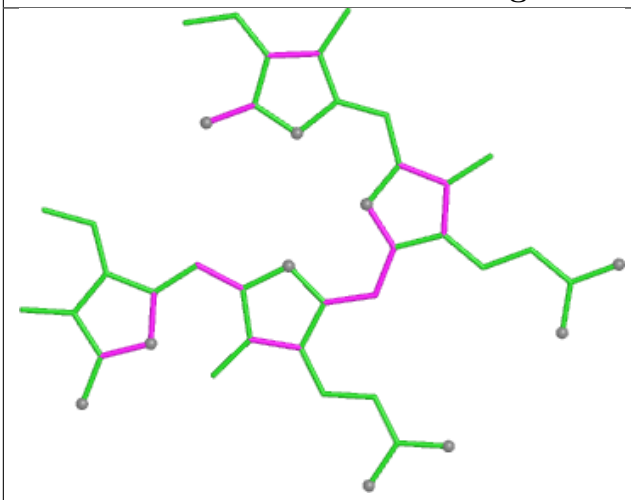


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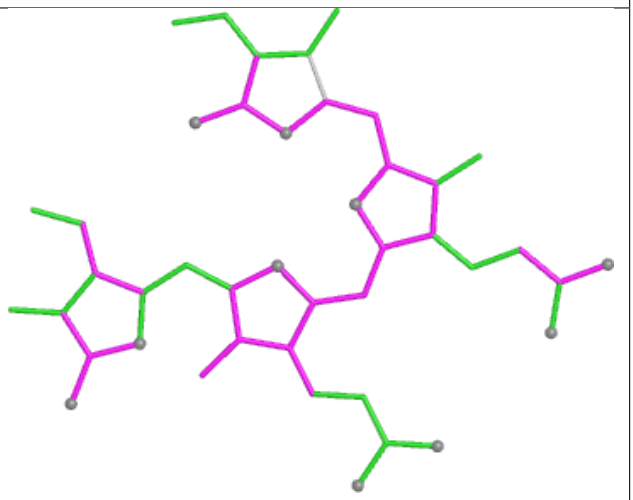


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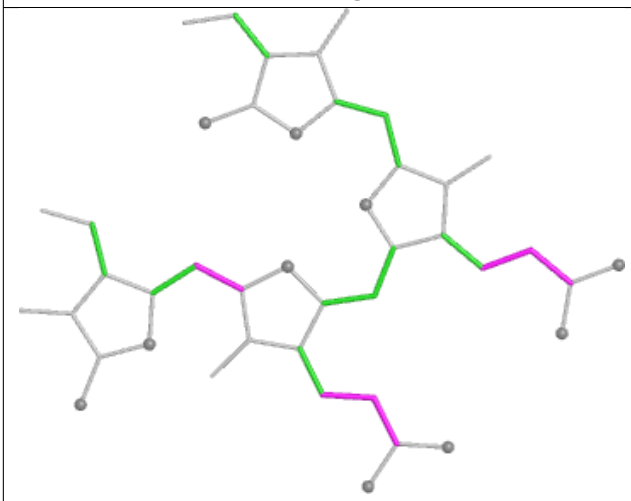
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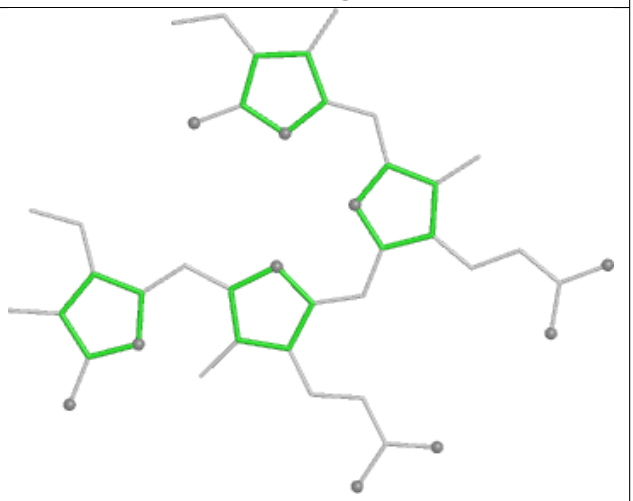
Bond lengths



Bond angles

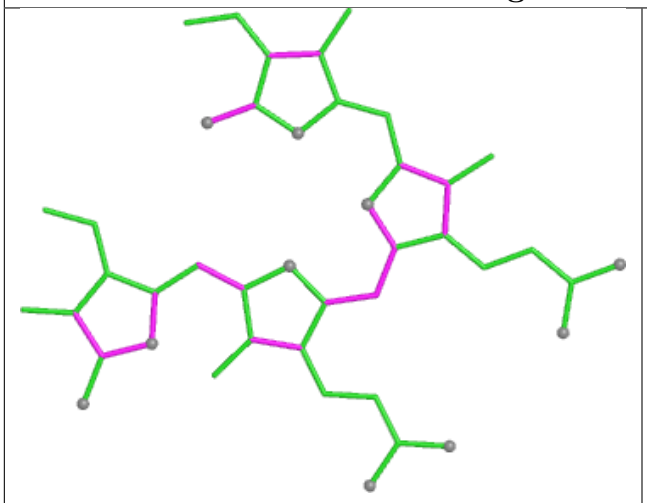


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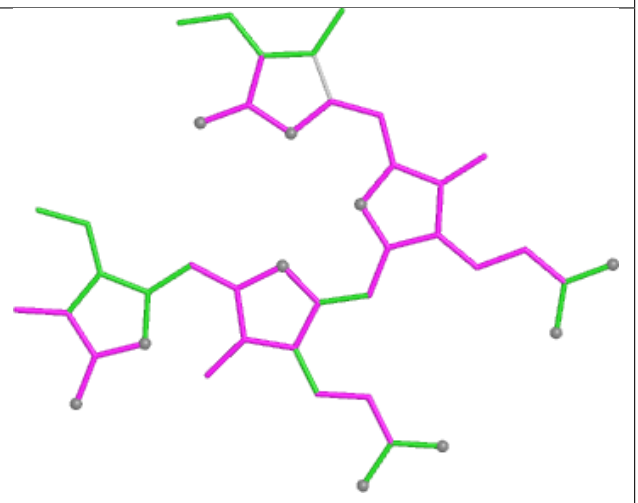


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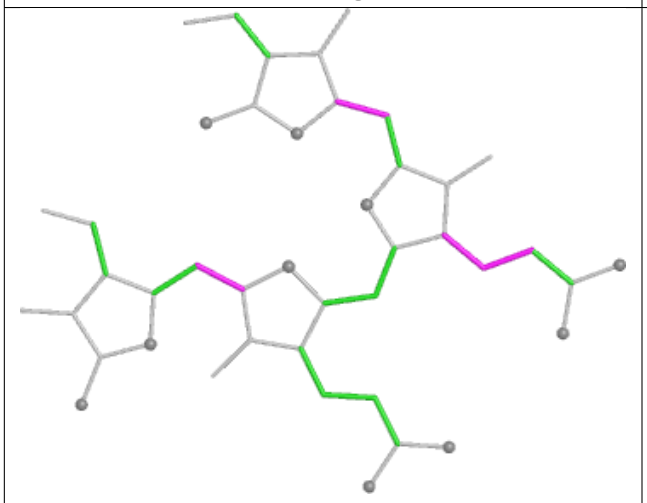
Ligand PEB WB 402



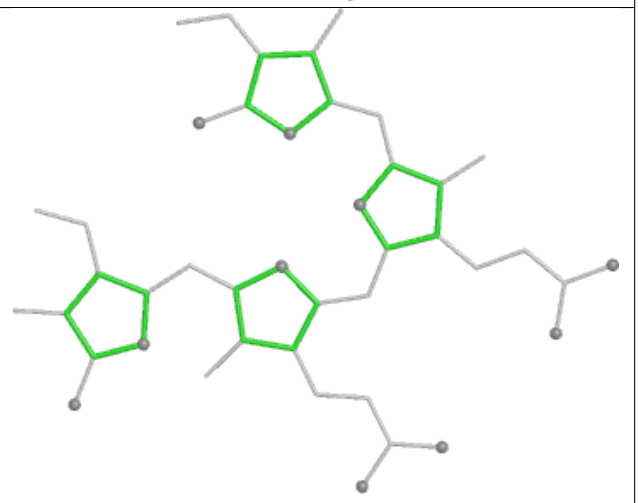
Bond lengths



Bond angles

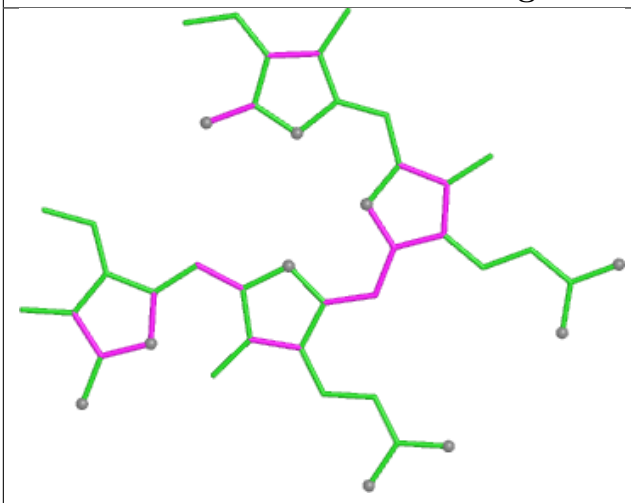


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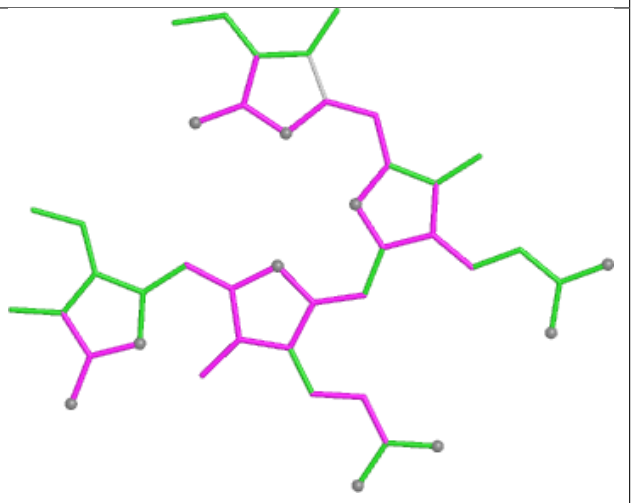


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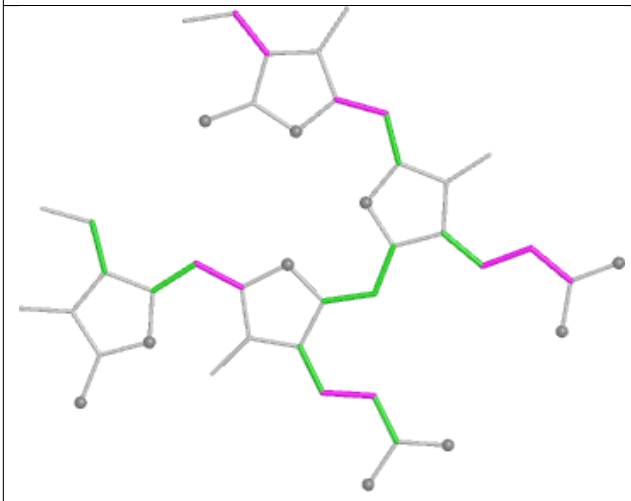
Ligand PEB L5 201



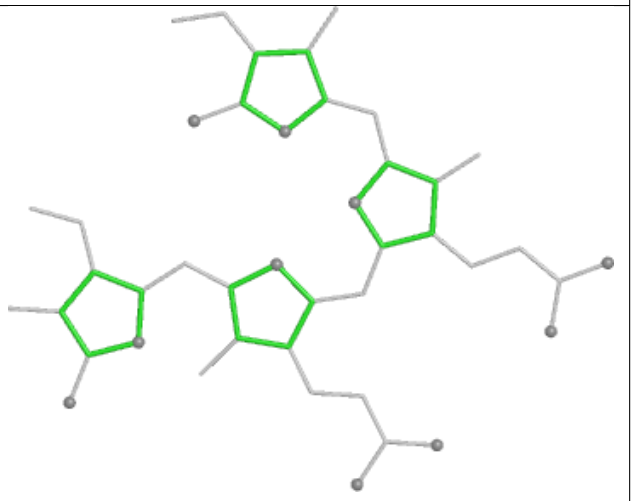
Bond lengths



Bond angles

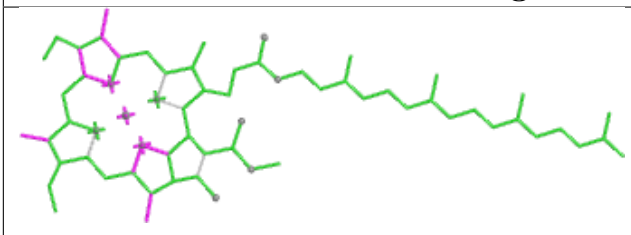


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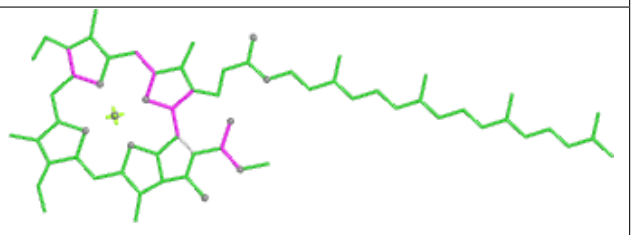


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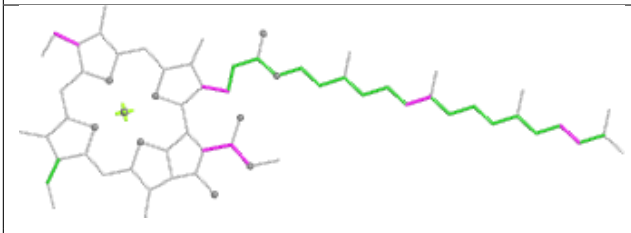
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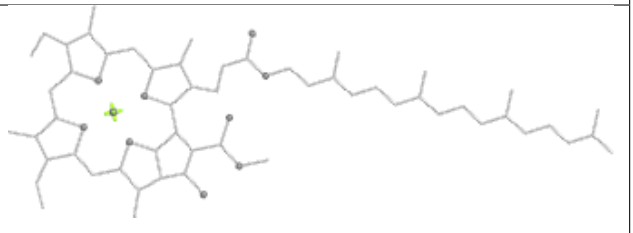
Bond lengths



Bond angles

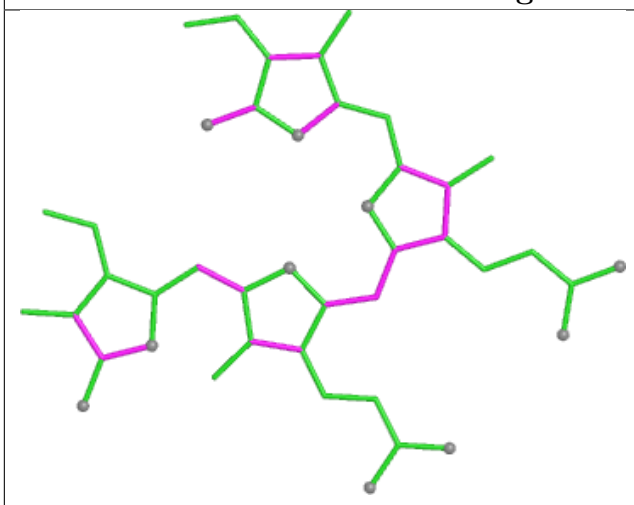


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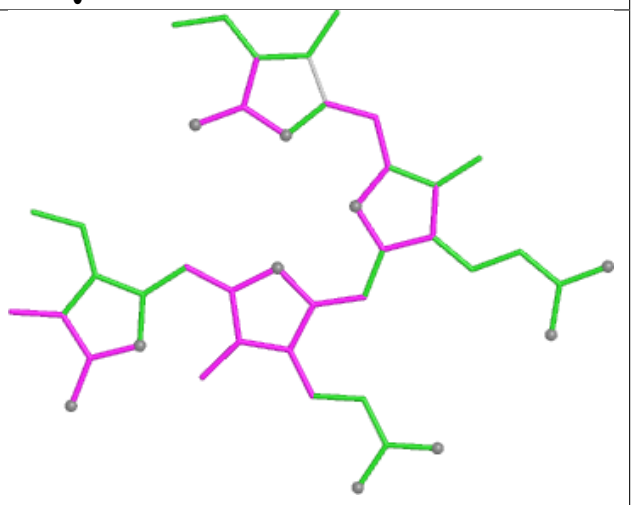


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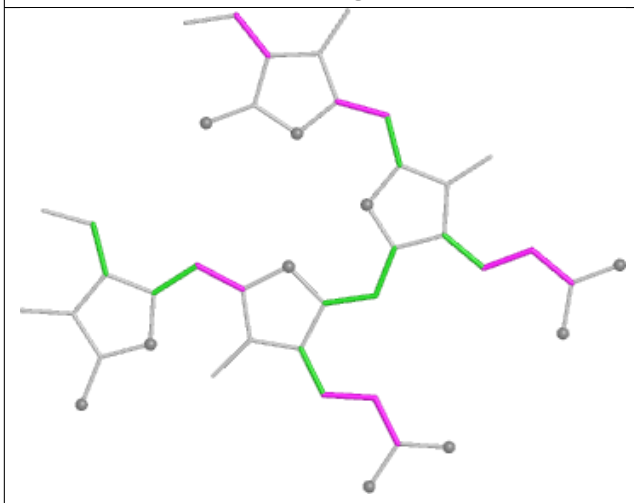
Ligand PEB JQ 201



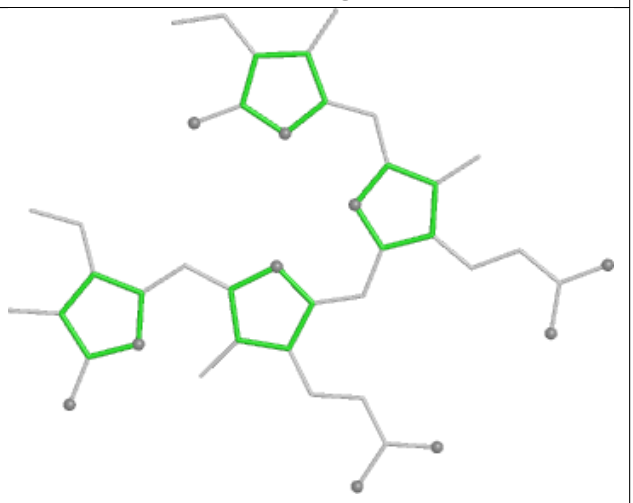
Bond lengths



Bond angles

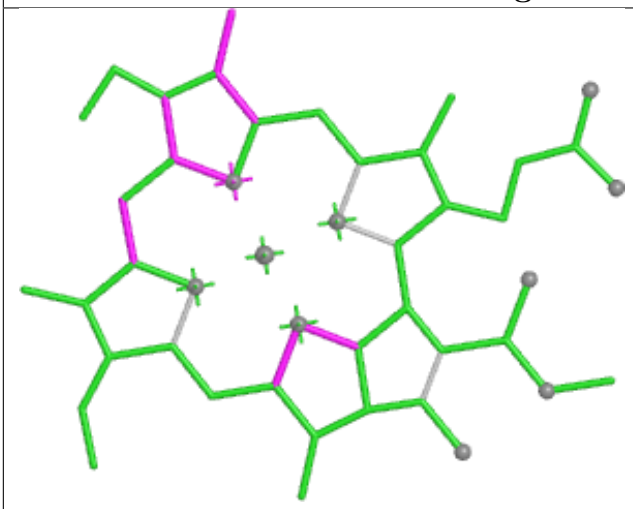


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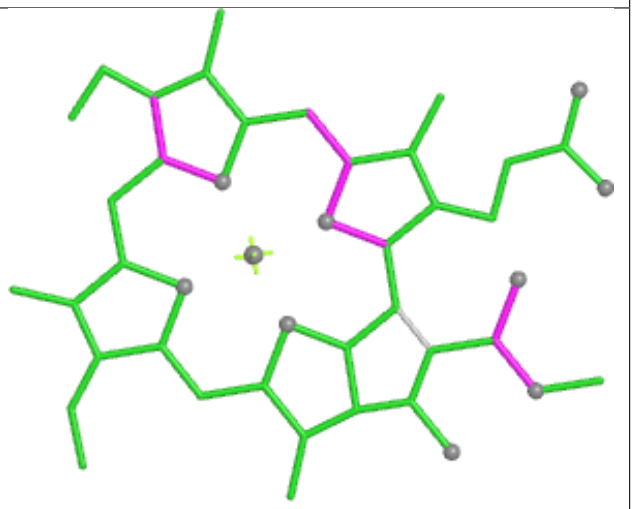


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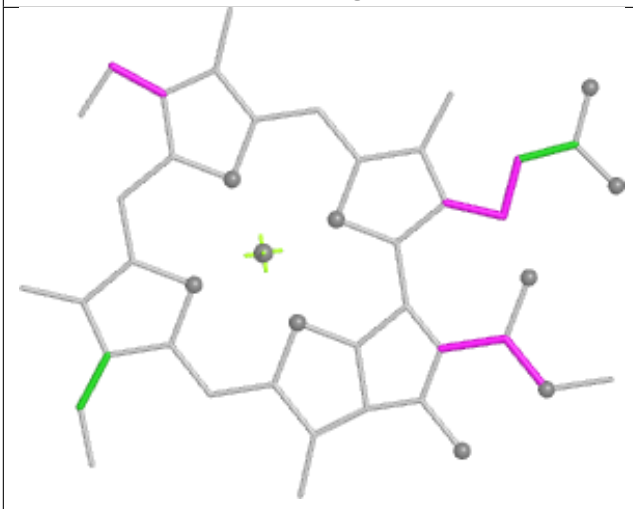
Ligand CLA 6N 601



Bond lengths



Bond angles

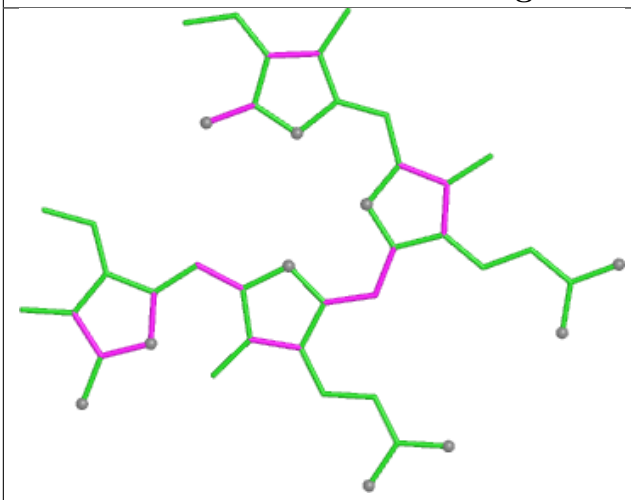


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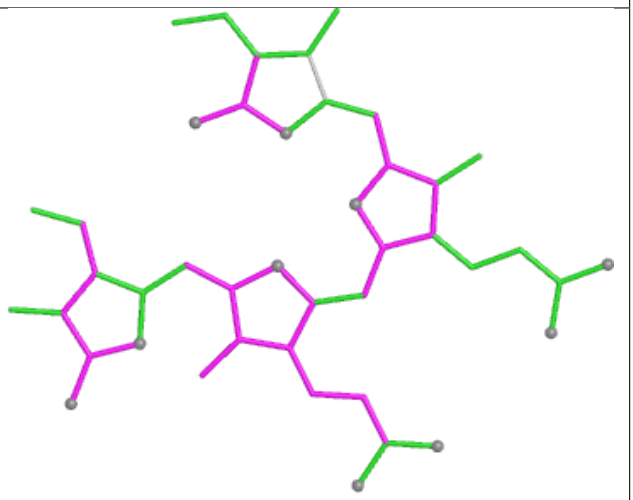


Rings

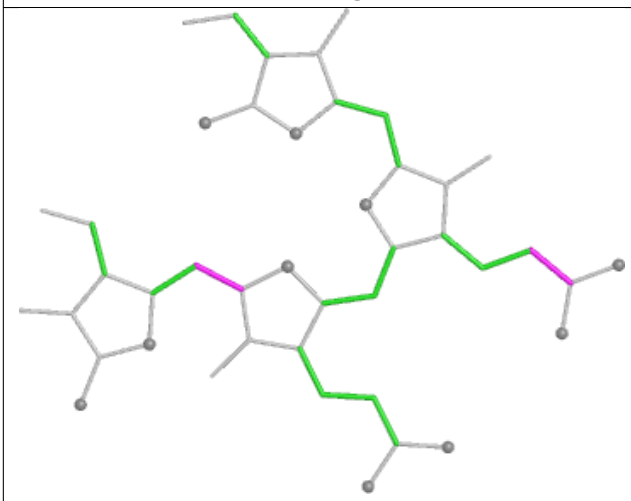
Ligand PEB CJ 201



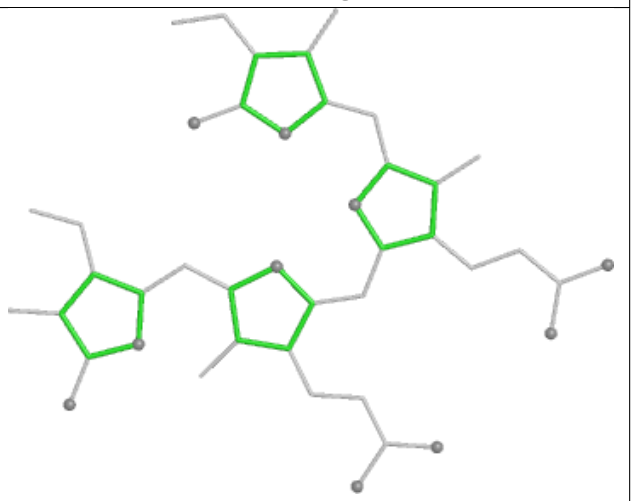
Bond lengths



Bond angles

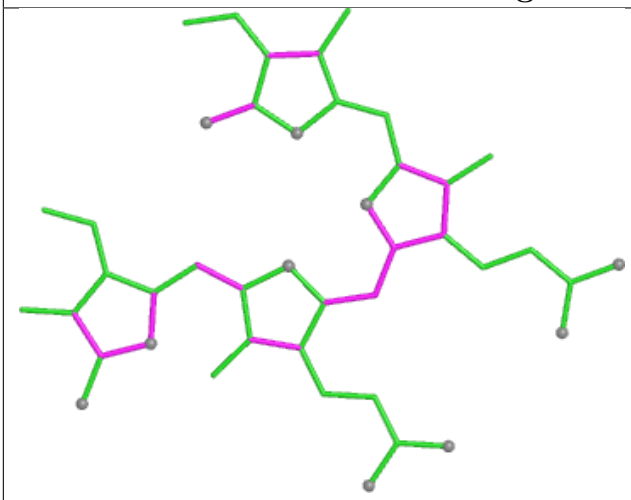


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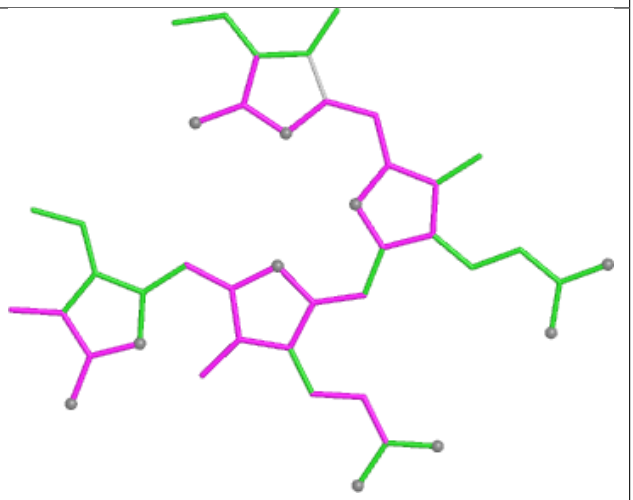


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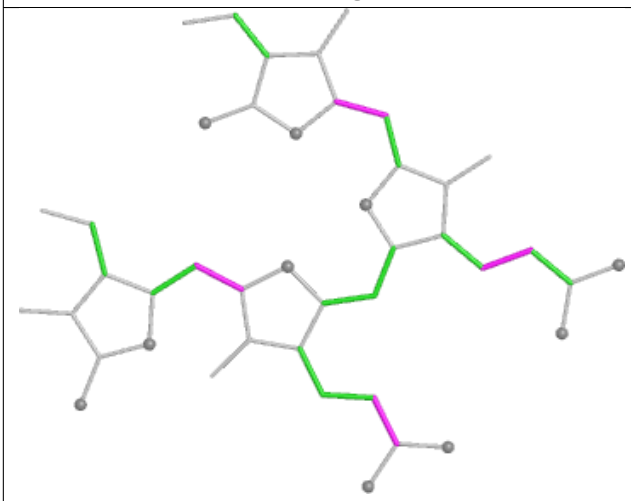
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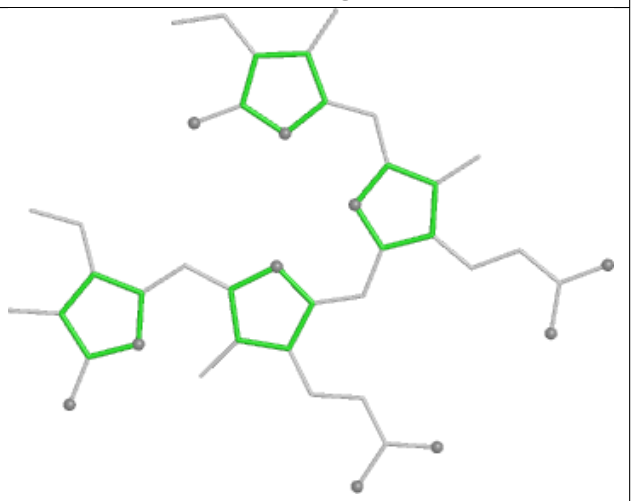
Bond lengths



Bond angles

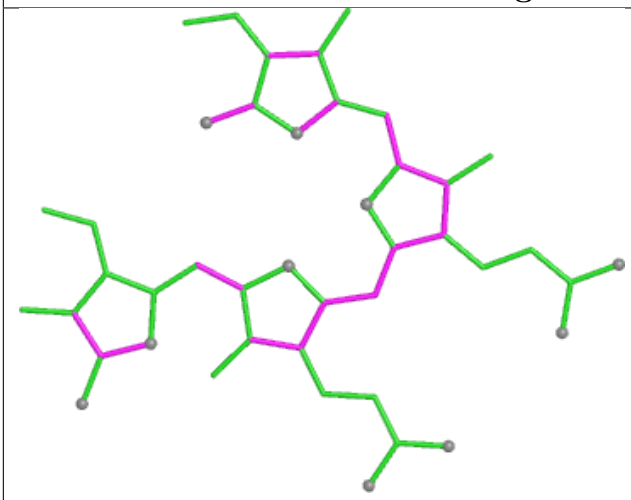


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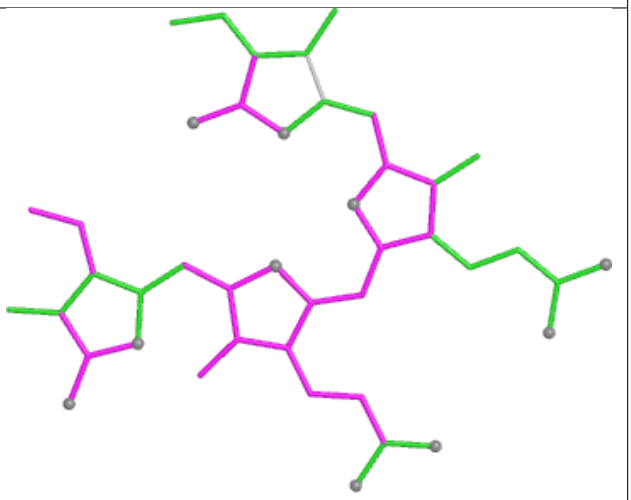


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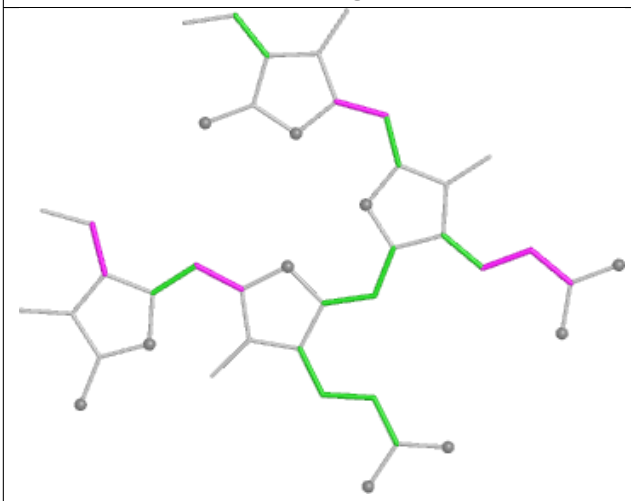
Ligand PEB D9 202



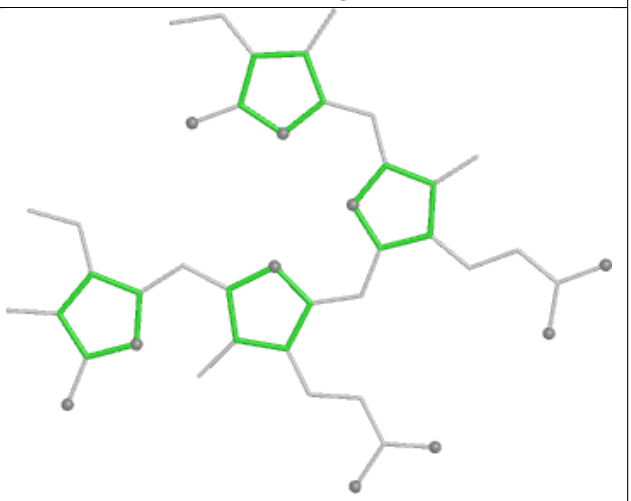
Bond lengths



Bond angles

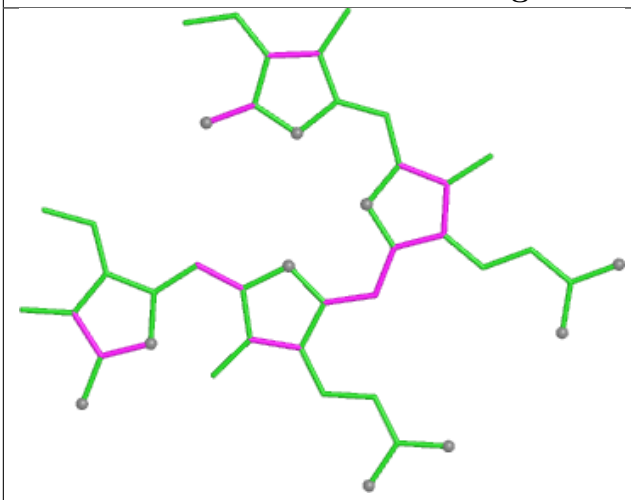


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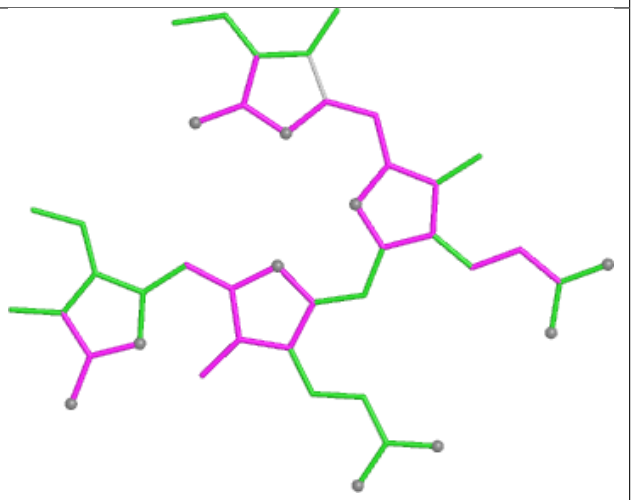


Rings

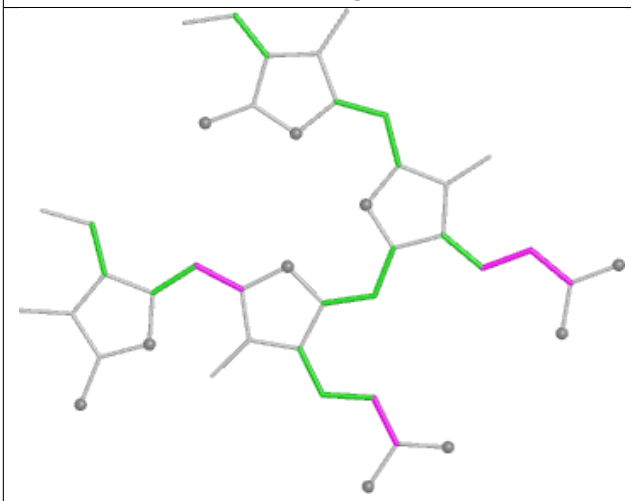
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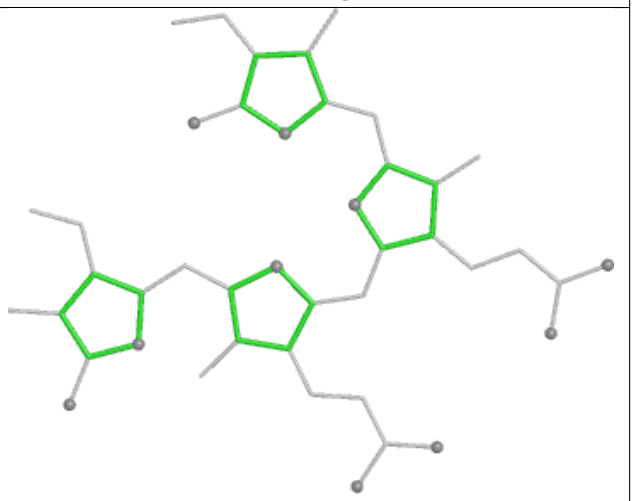
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Bond angles

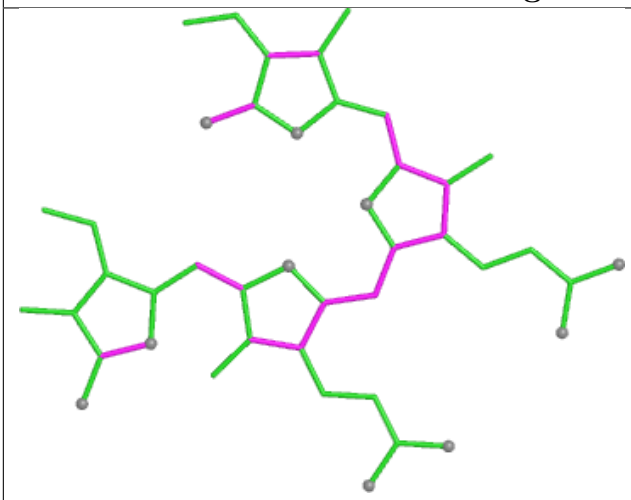


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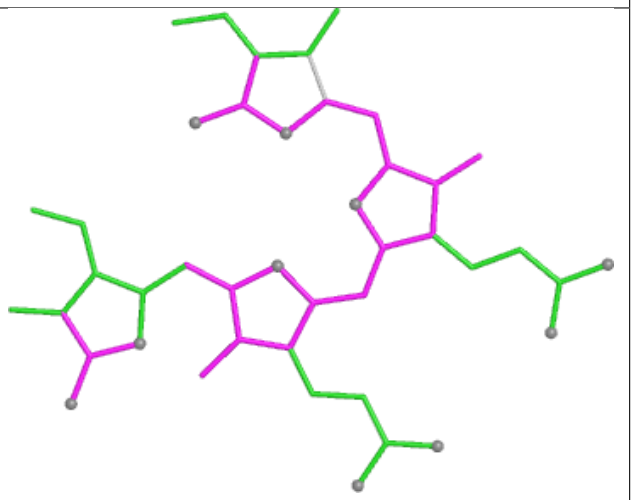


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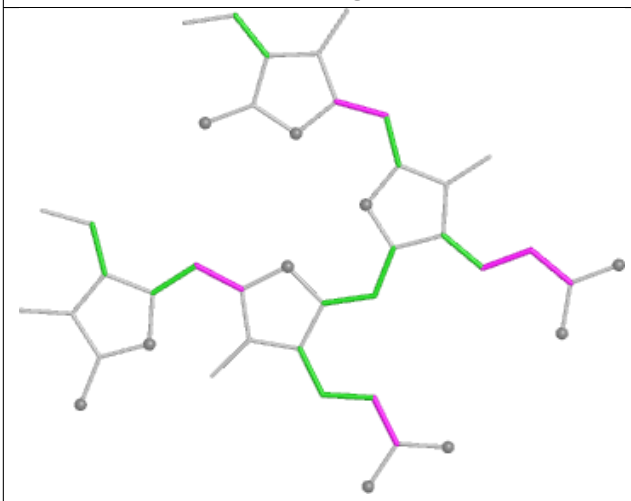
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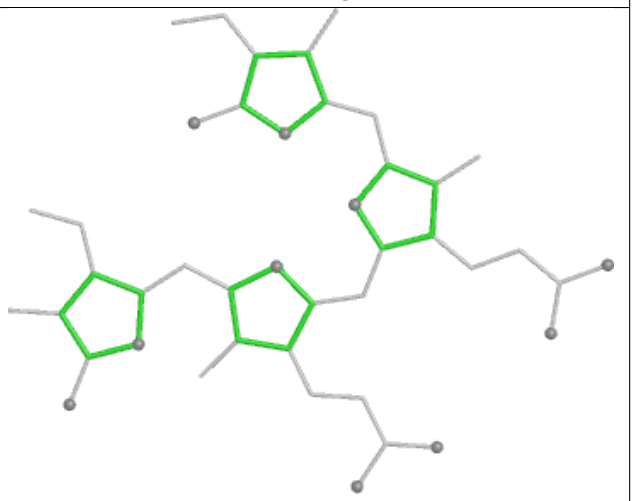
Bond lengths



Bond angles

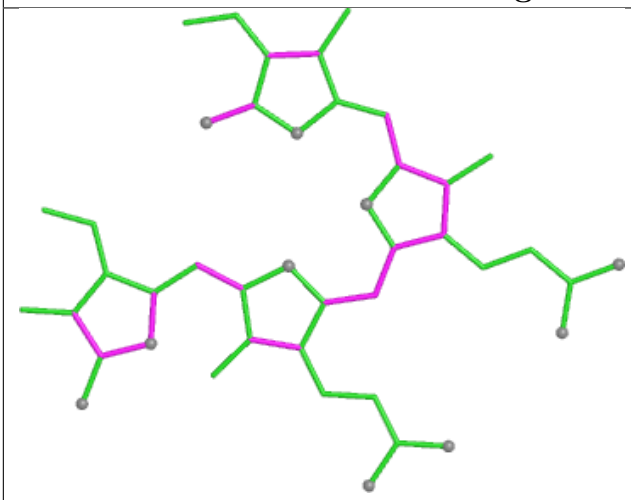


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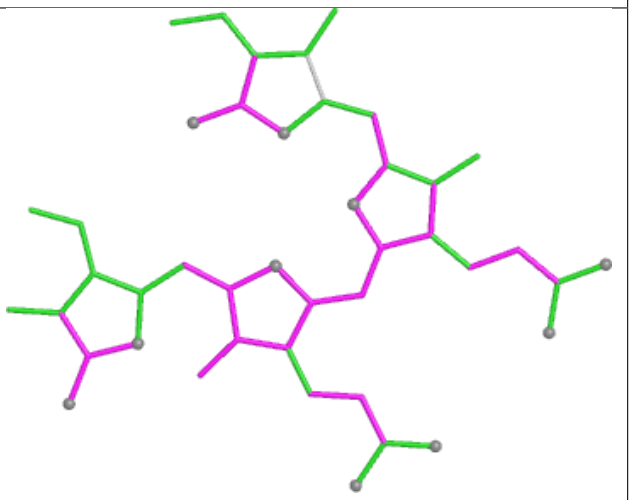


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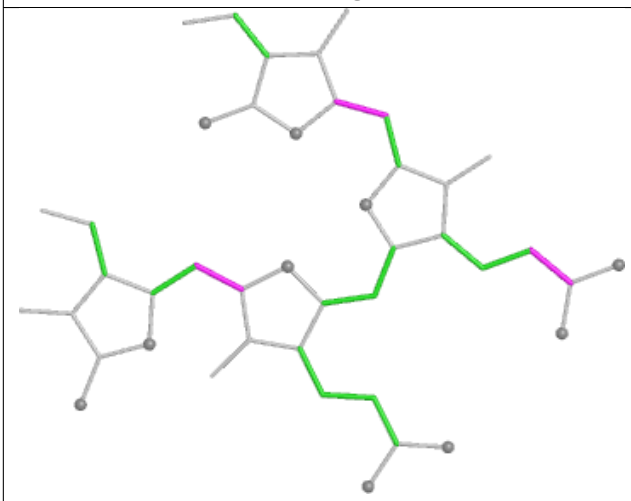
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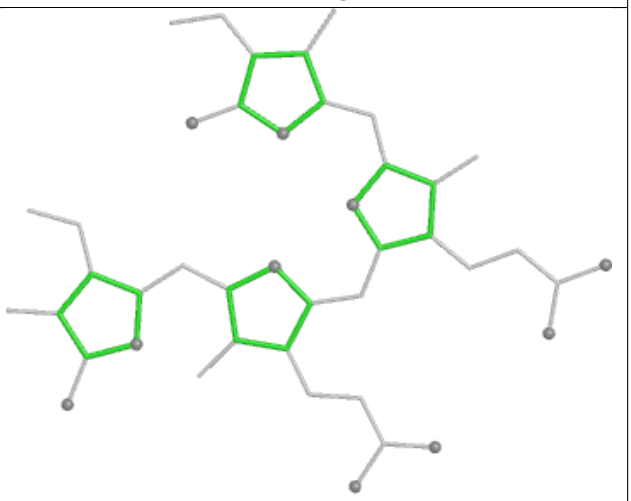
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Bond angles

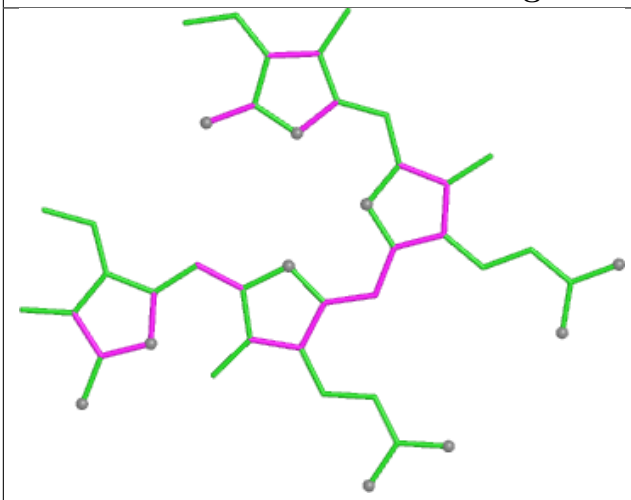


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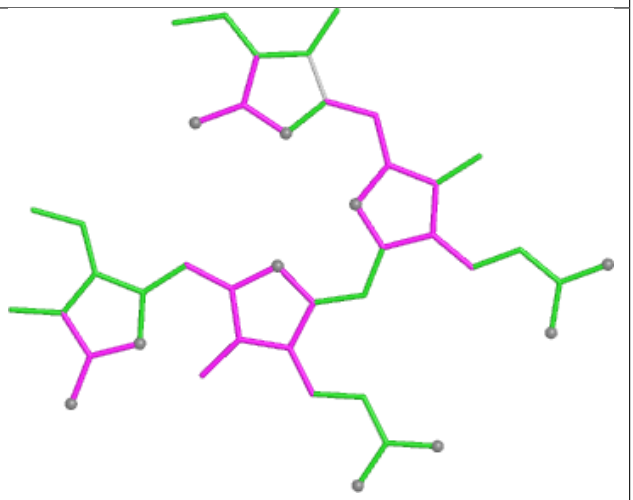


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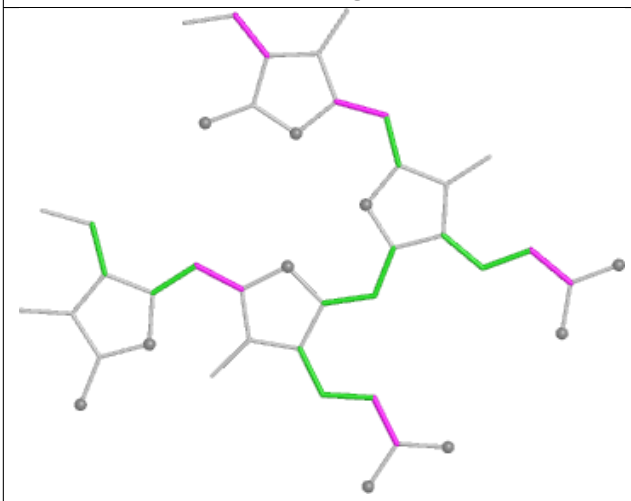
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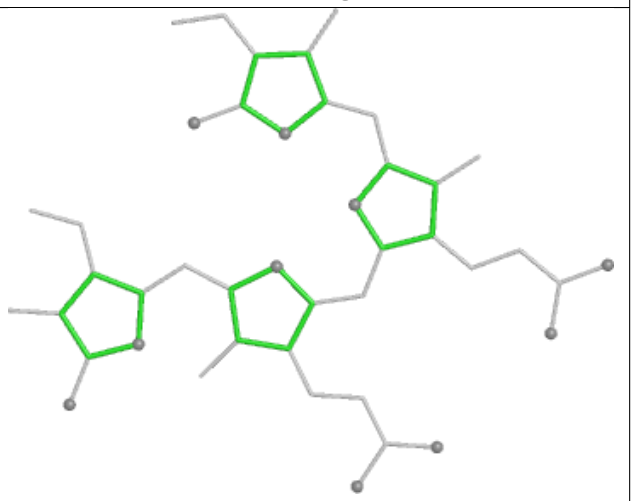
Bond lengths



Bond angles

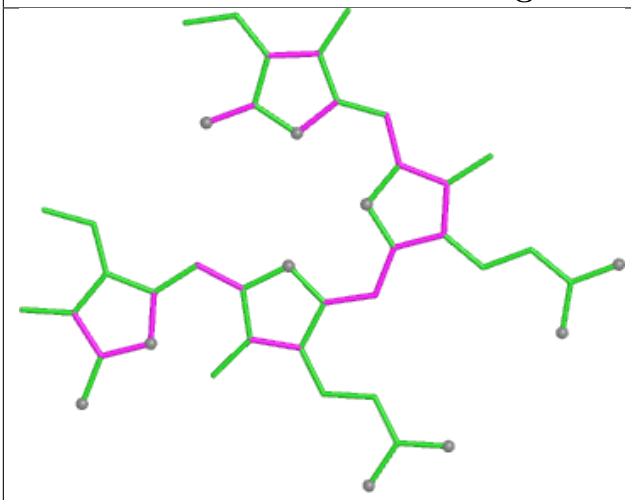


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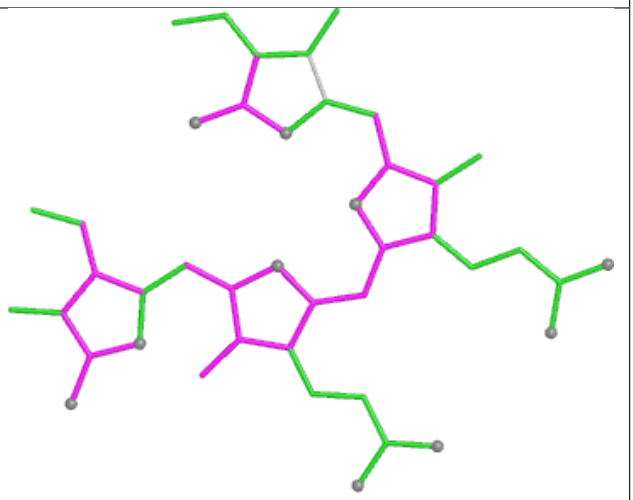


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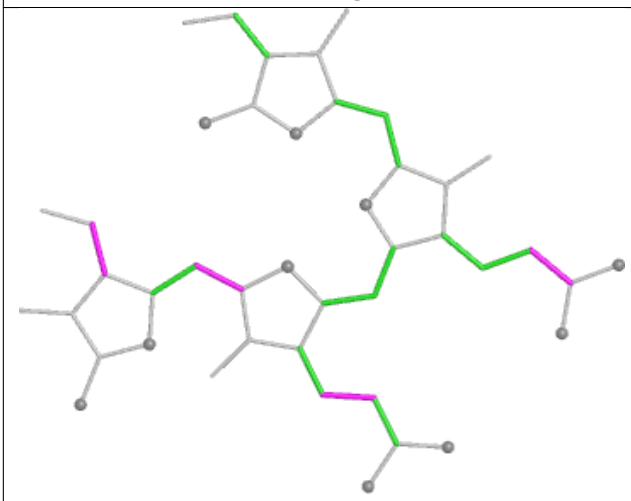
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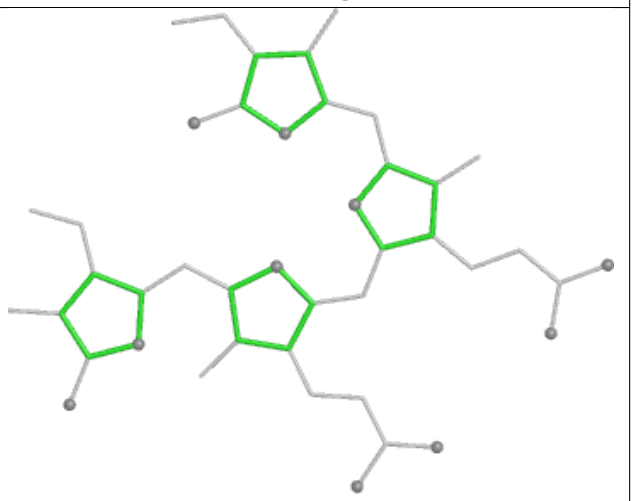
Bond lengths



Bond angles

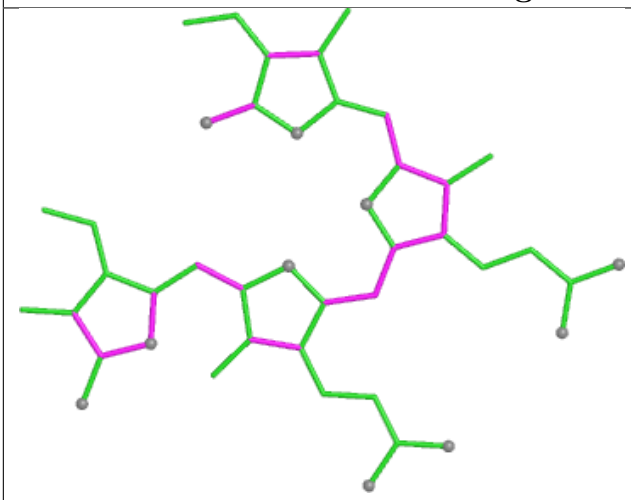


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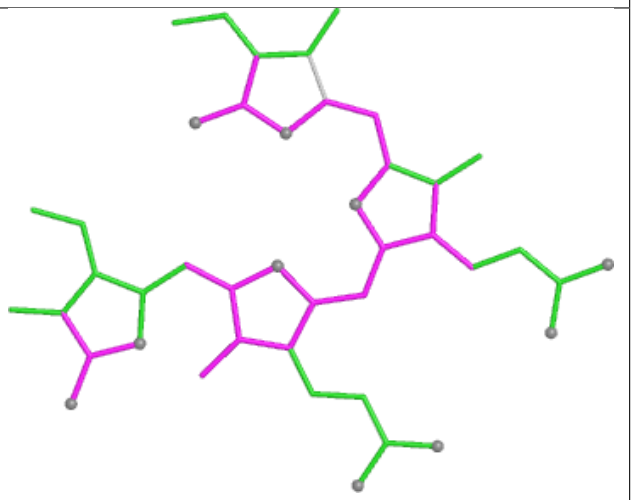


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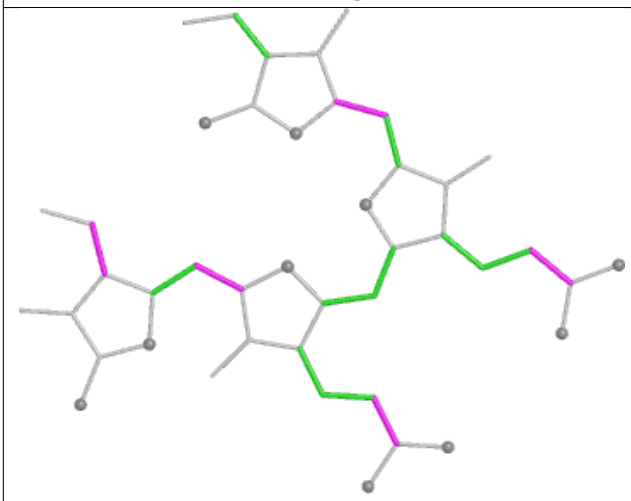
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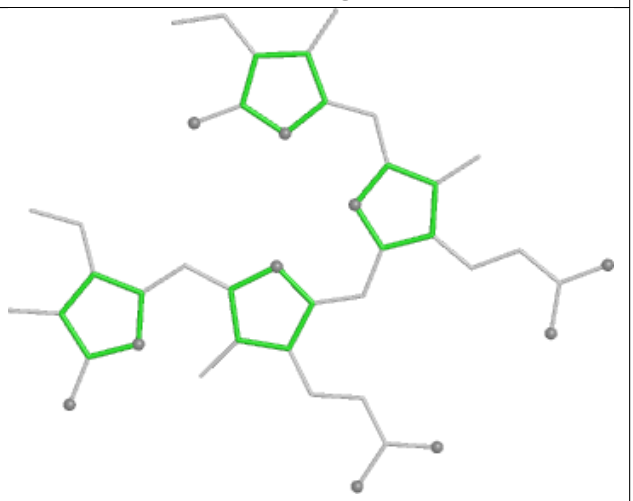
Bond lengths



Bond angles

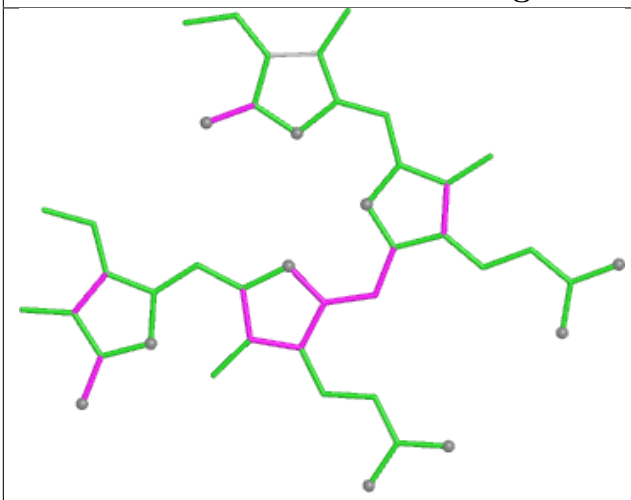


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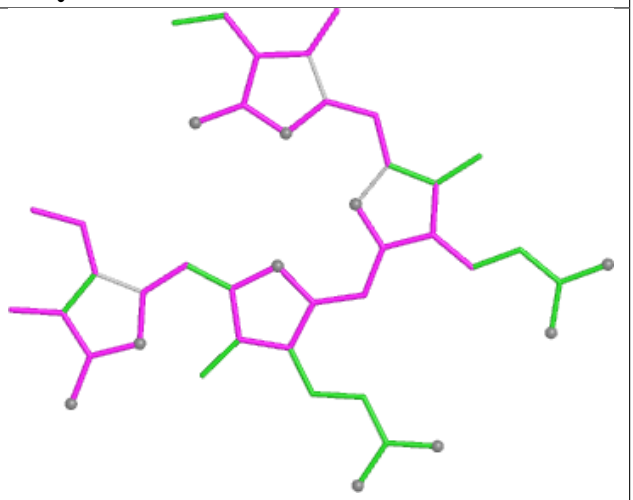


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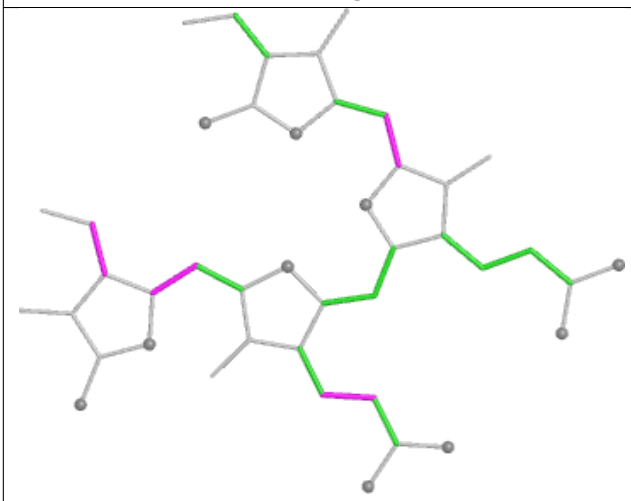
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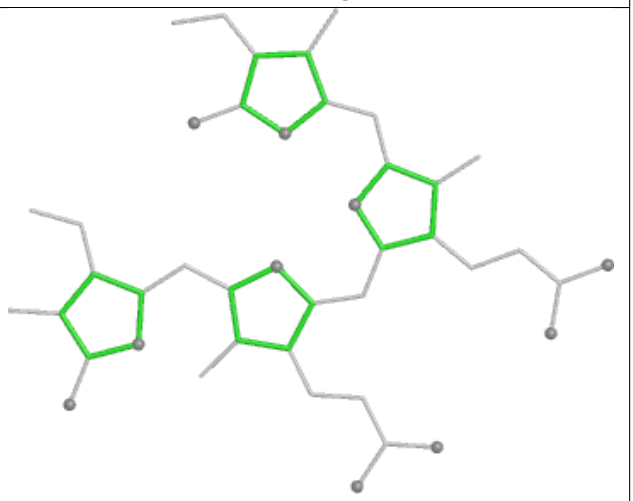
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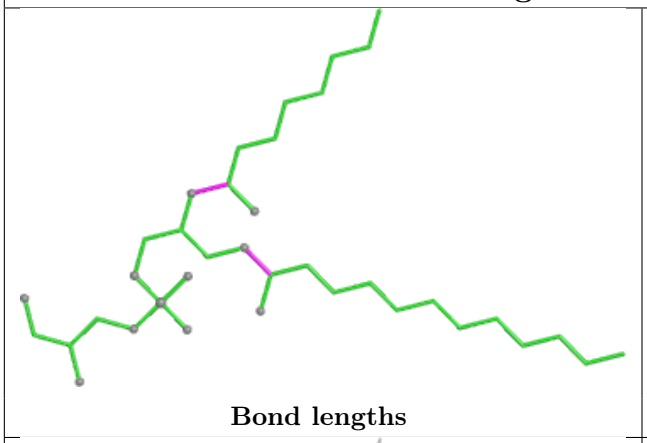


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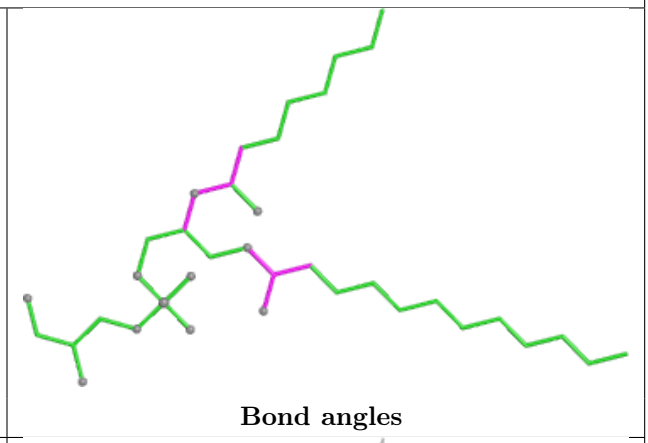


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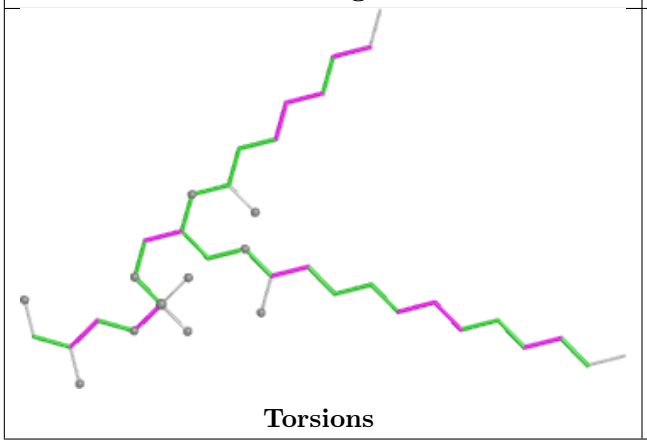
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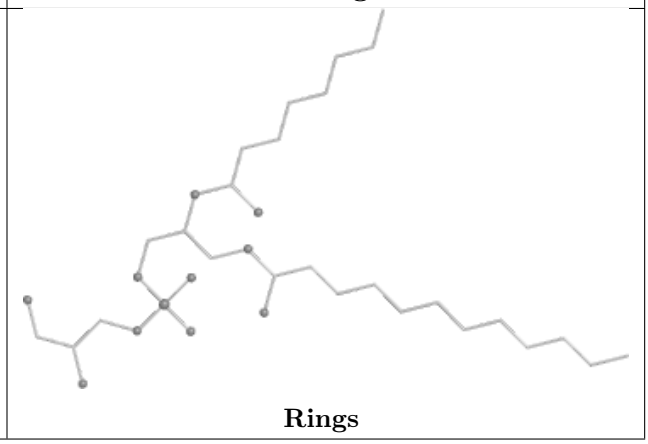
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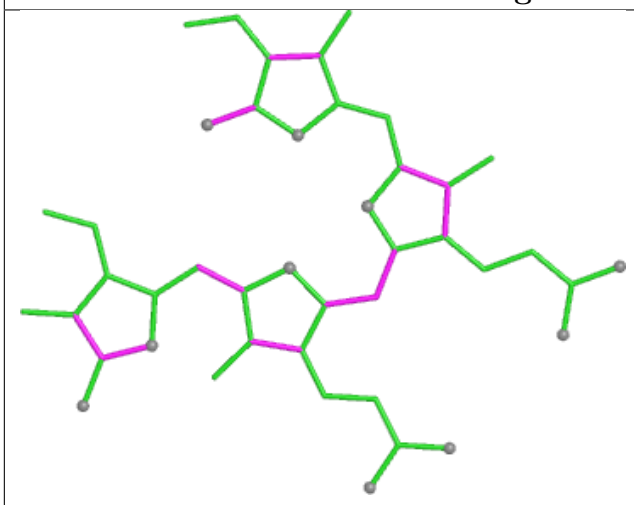


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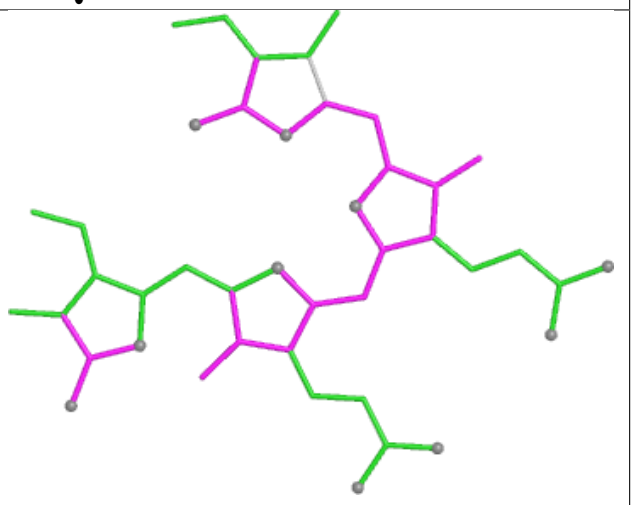


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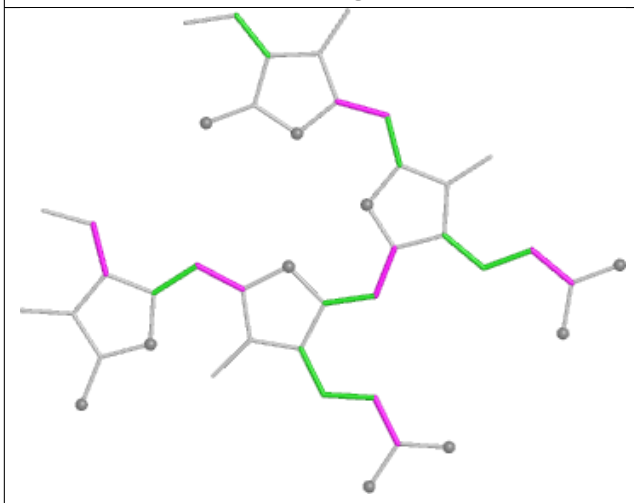
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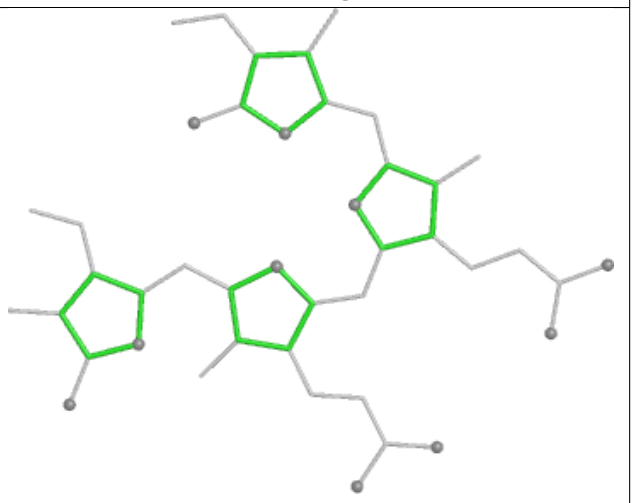
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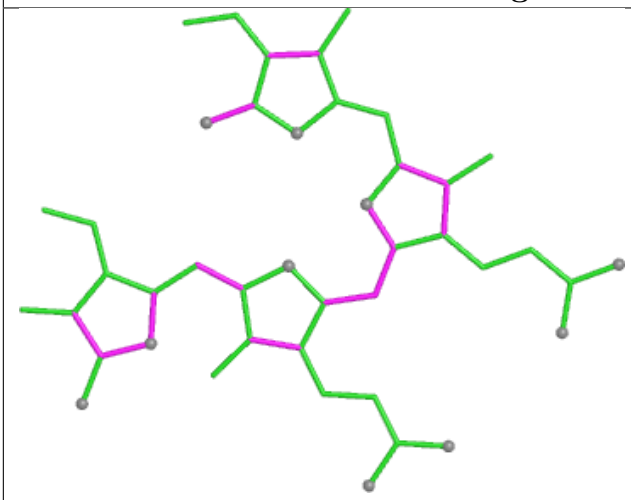


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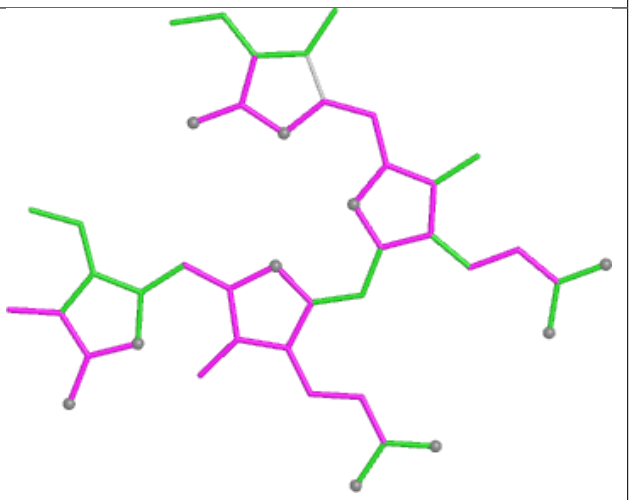


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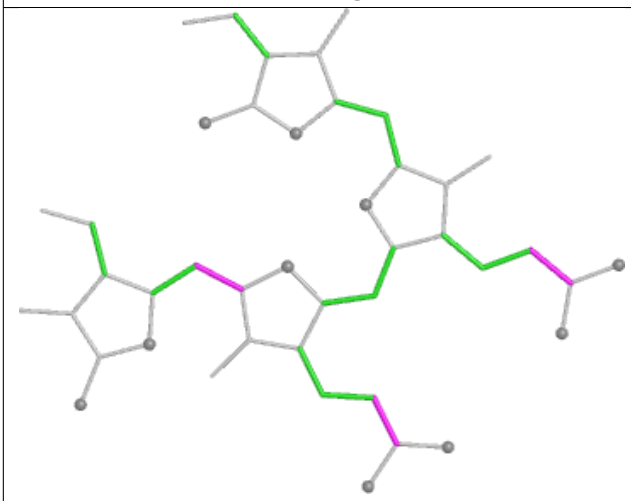
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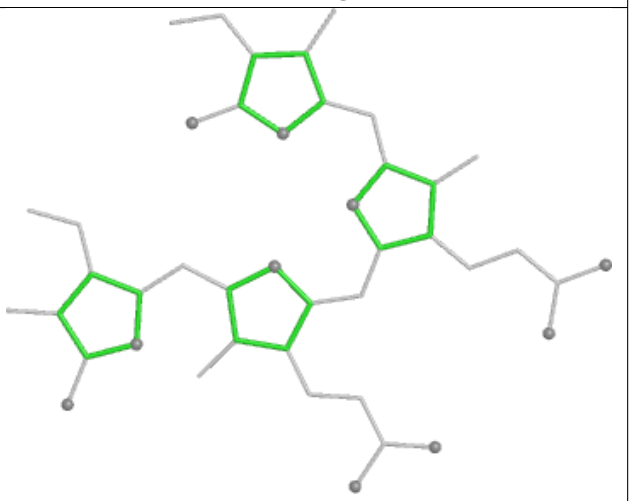
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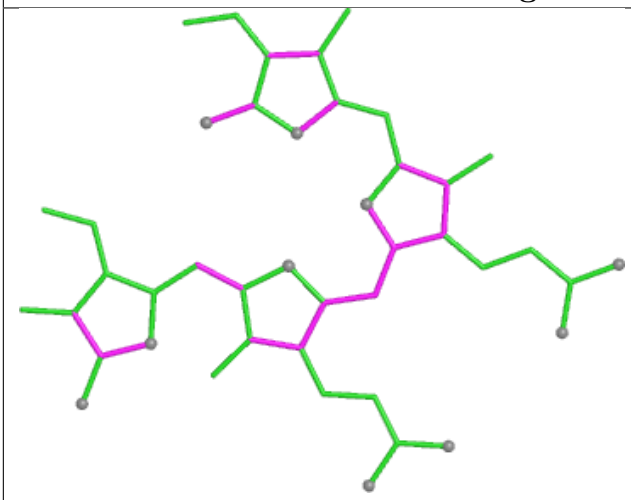


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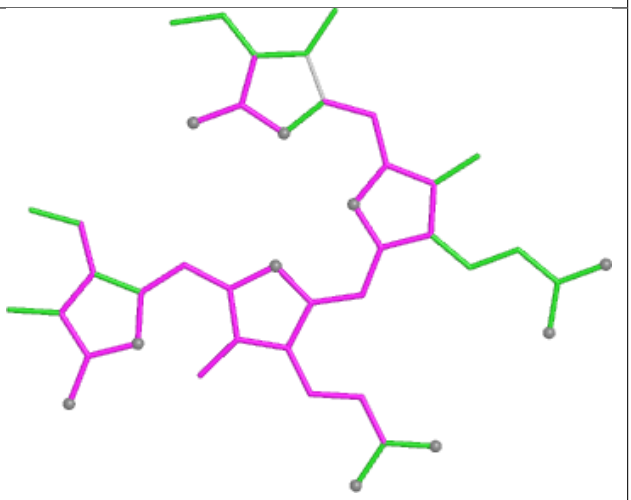


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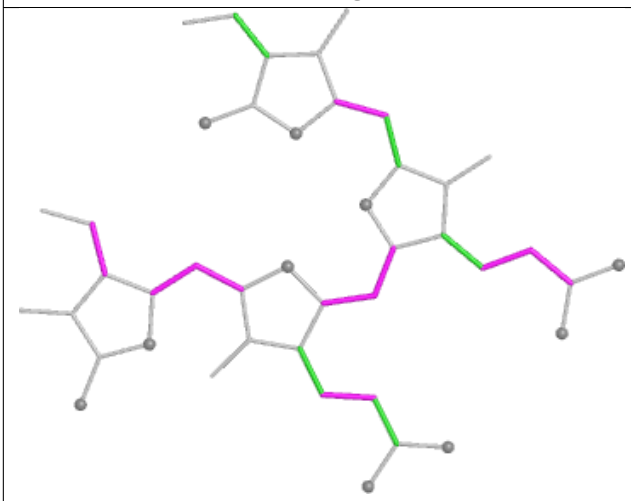
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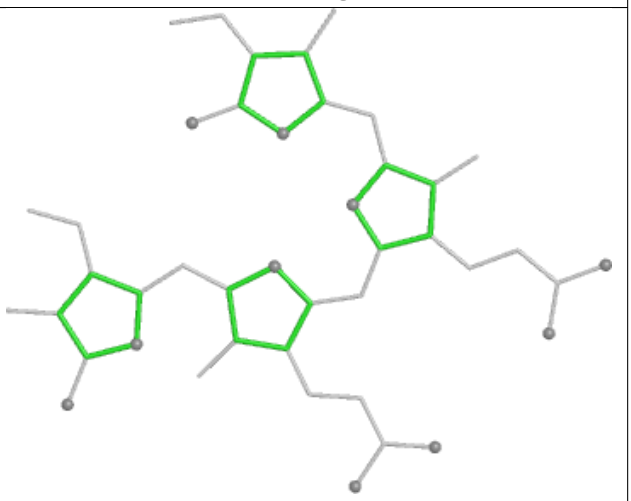
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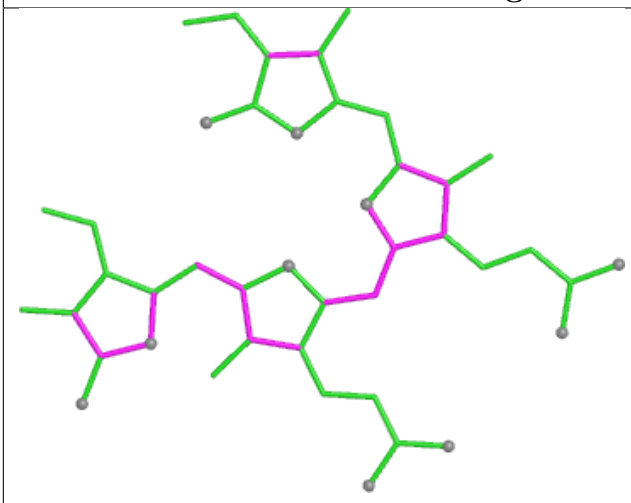


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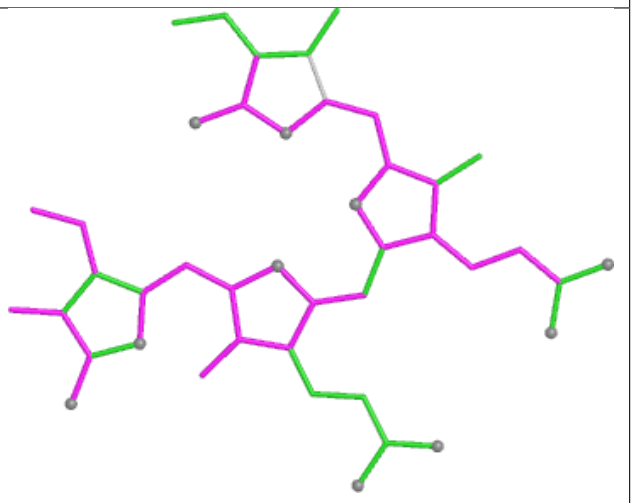


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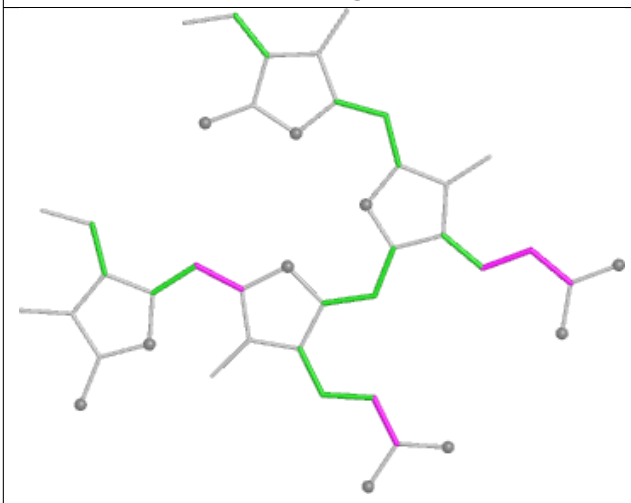
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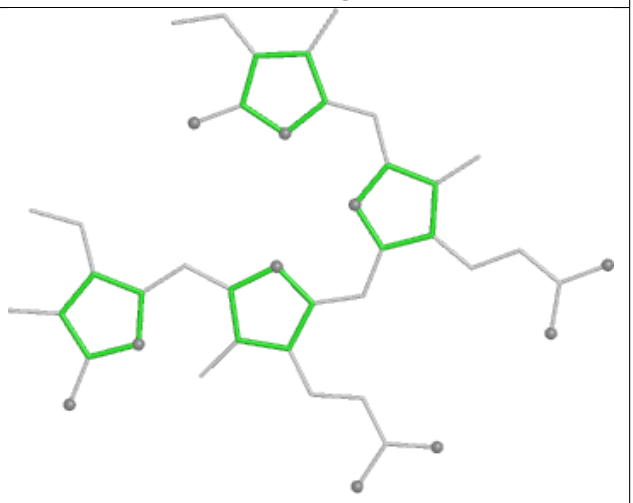
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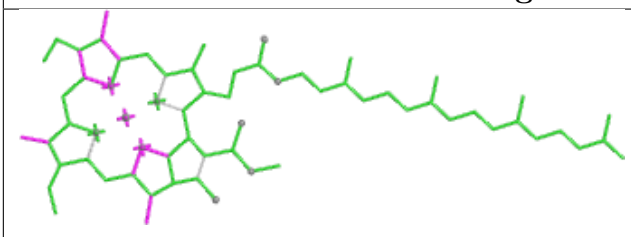


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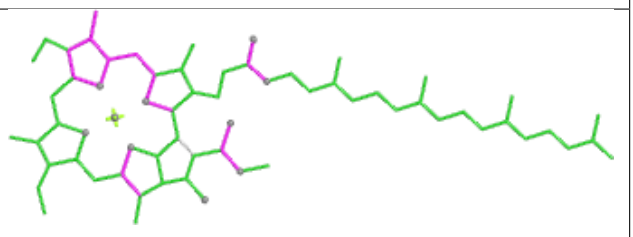


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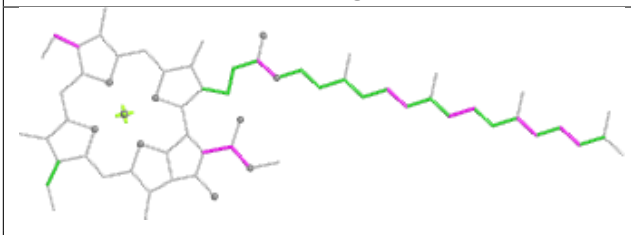
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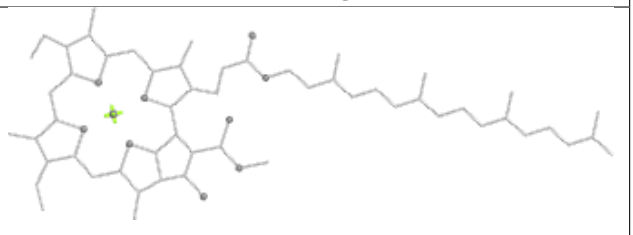
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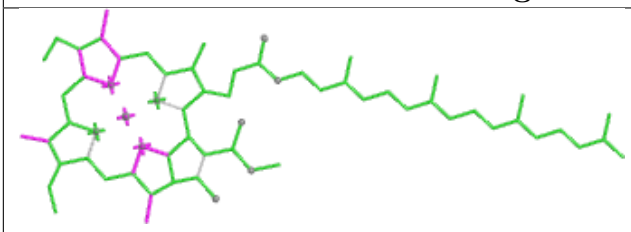


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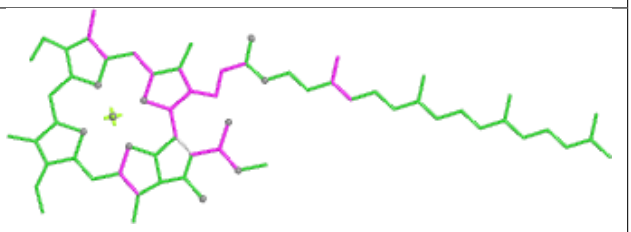


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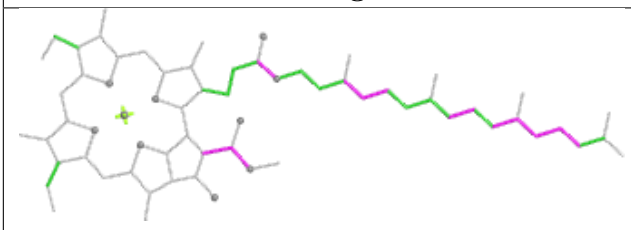
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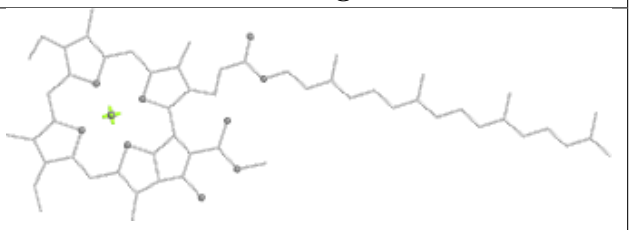
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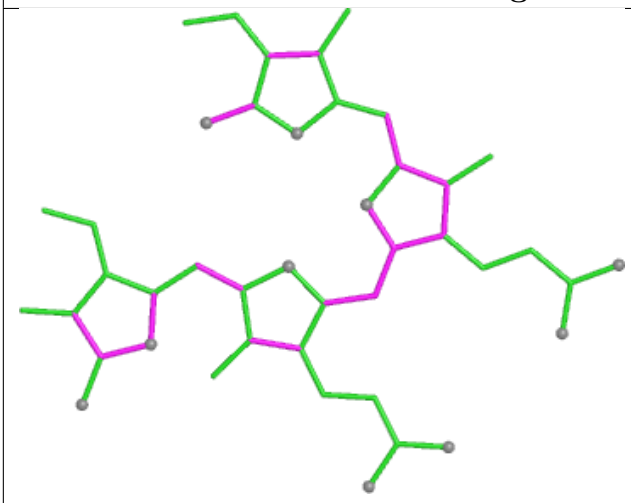


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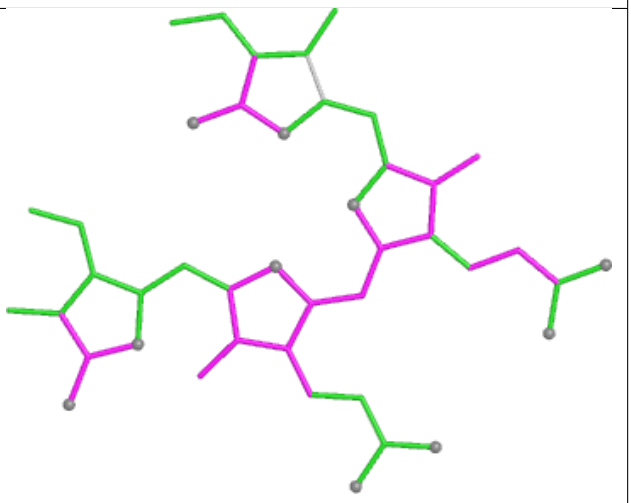


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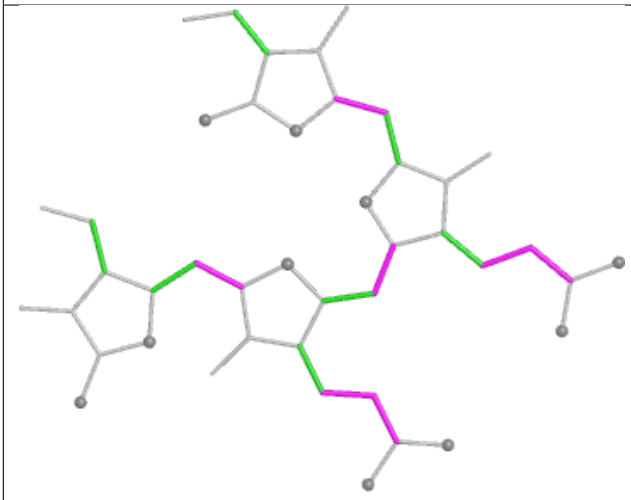
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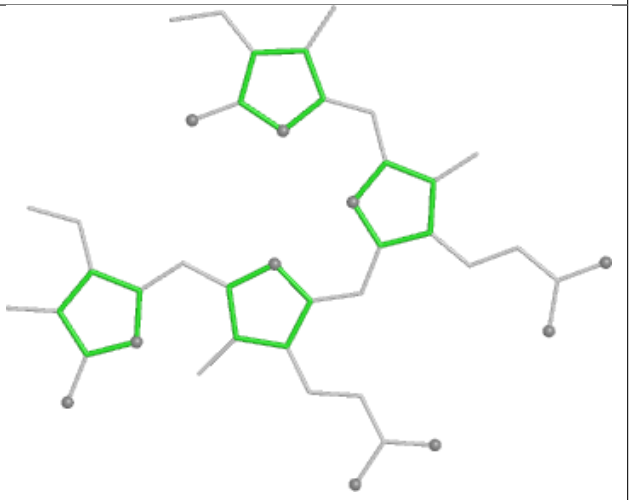
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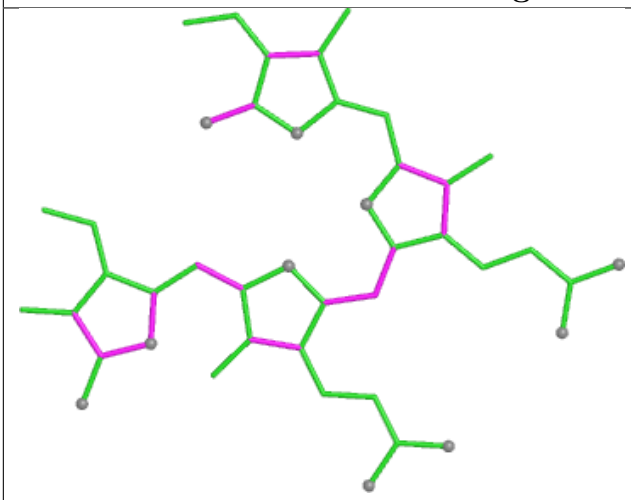


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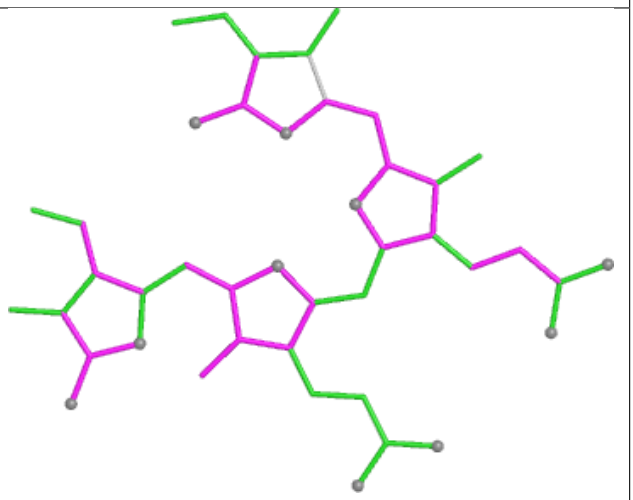


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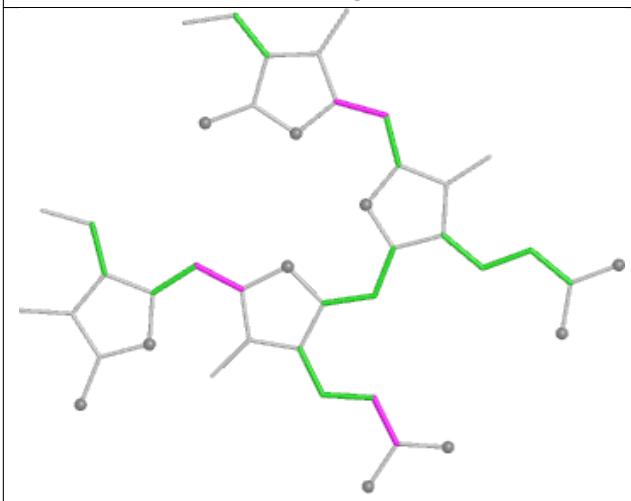
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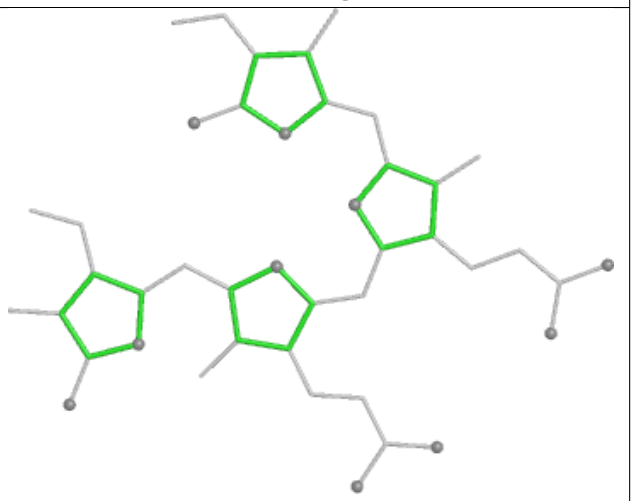
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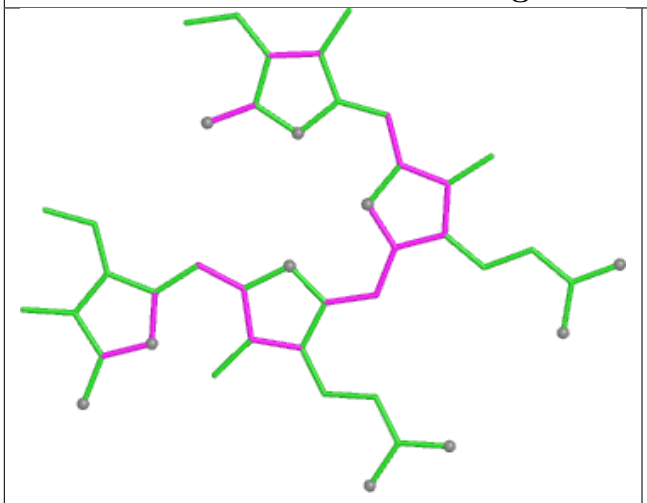


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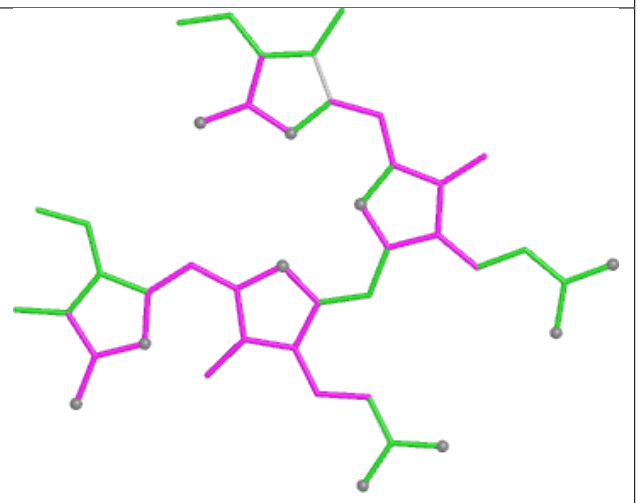


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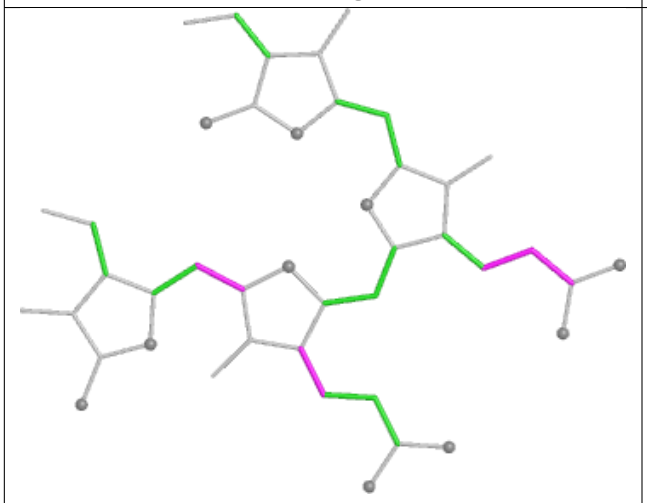
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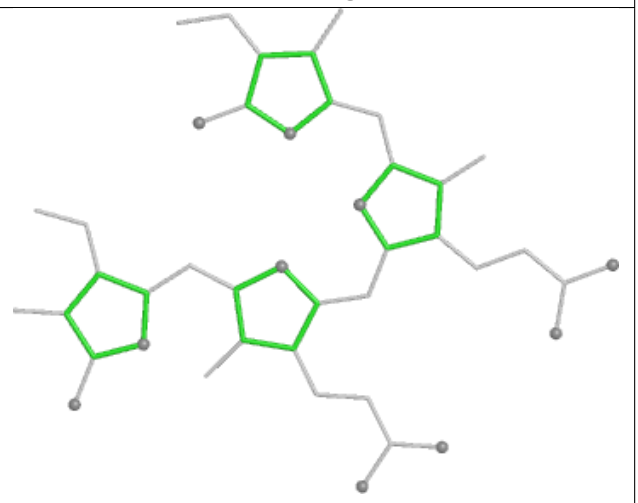
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Bond angles

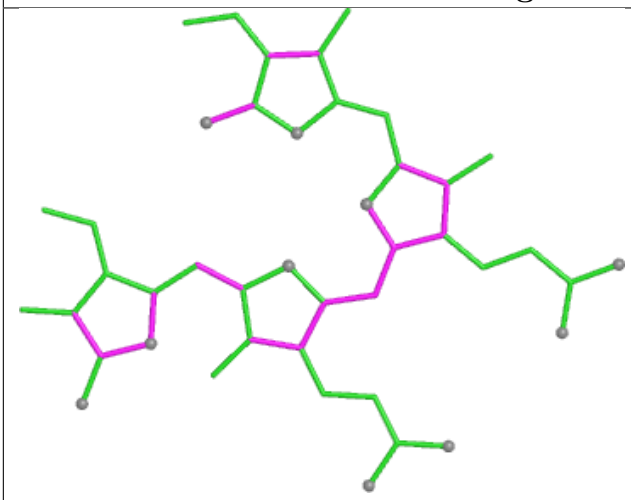


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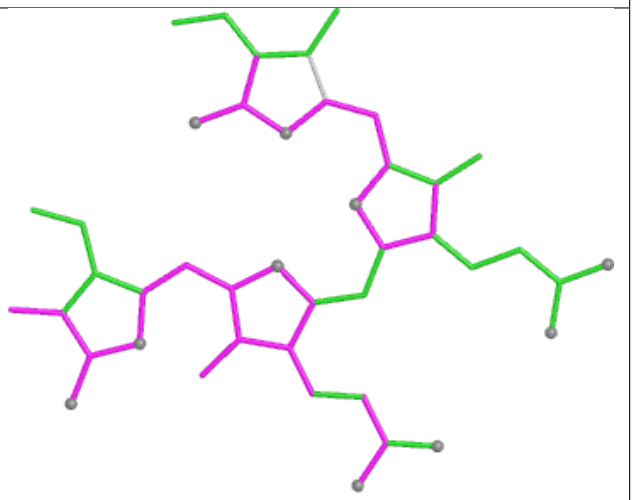


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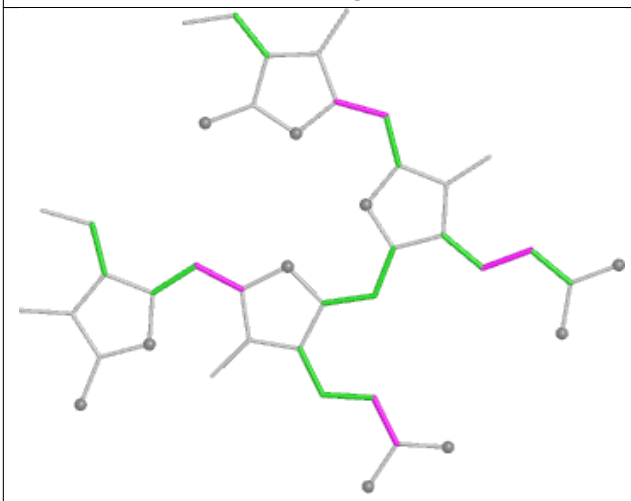
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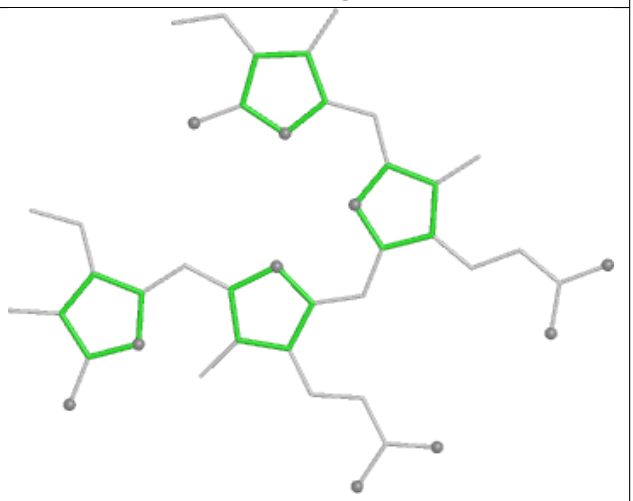
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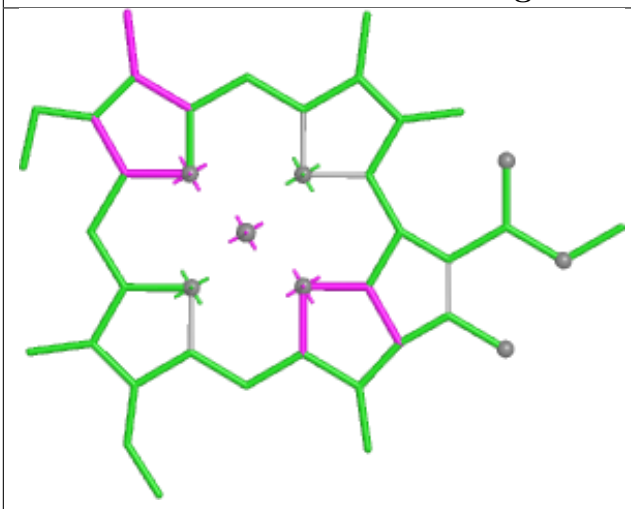


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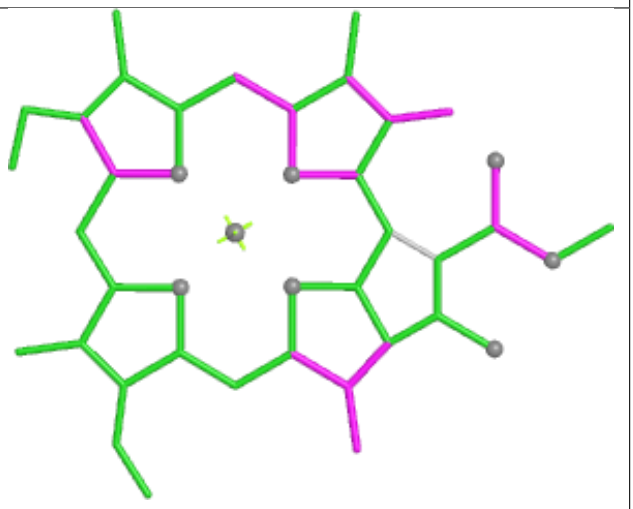


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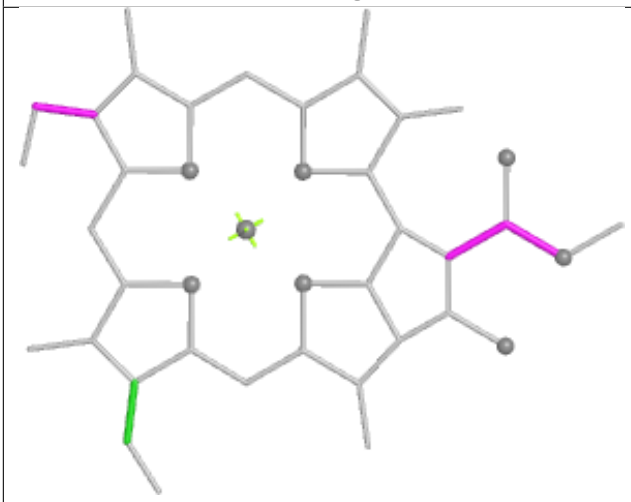
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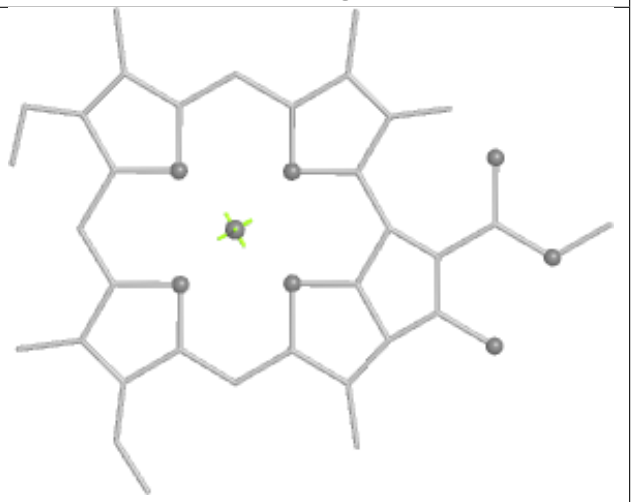
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Bond angles

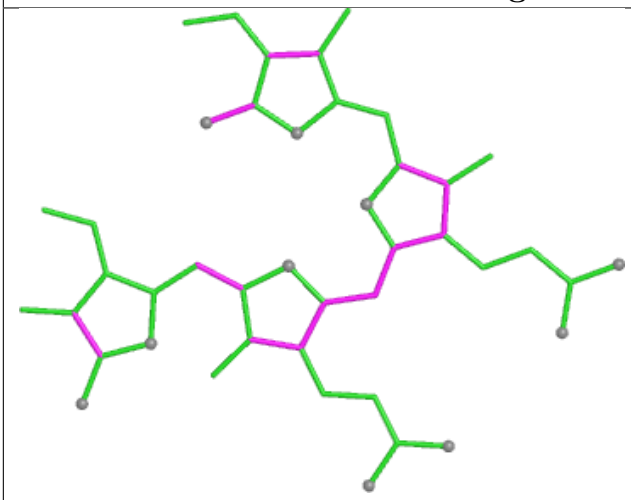


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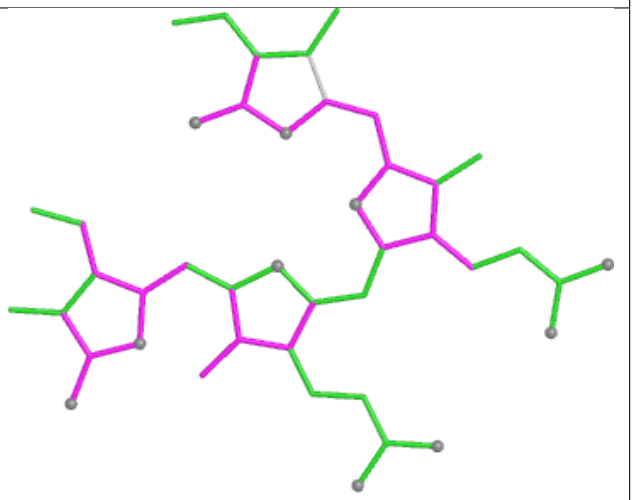


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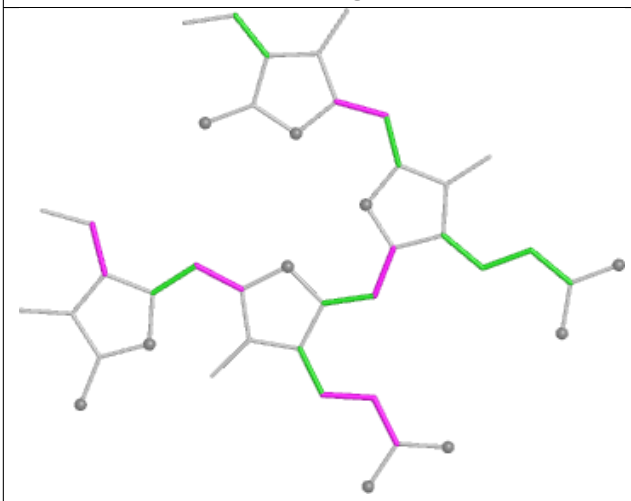
Ligand PEB mH 202



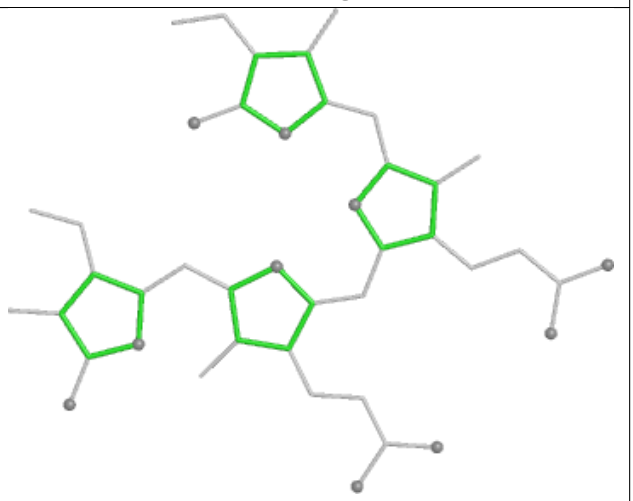
Bond lengths



Bond angles

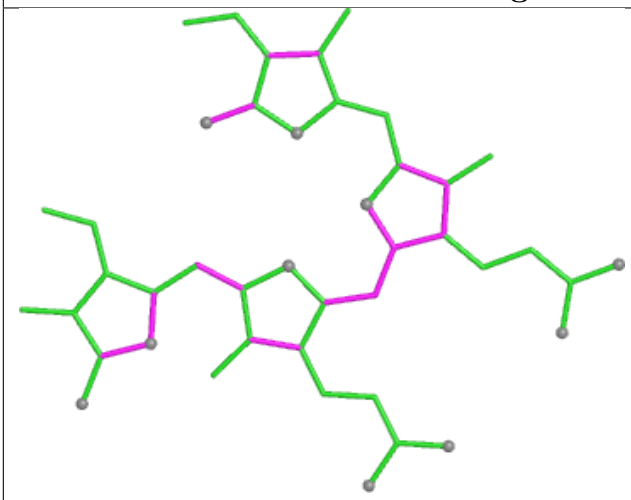


Torsions

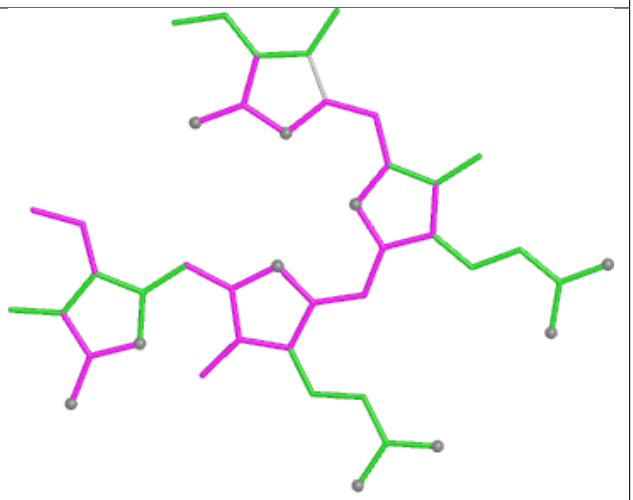


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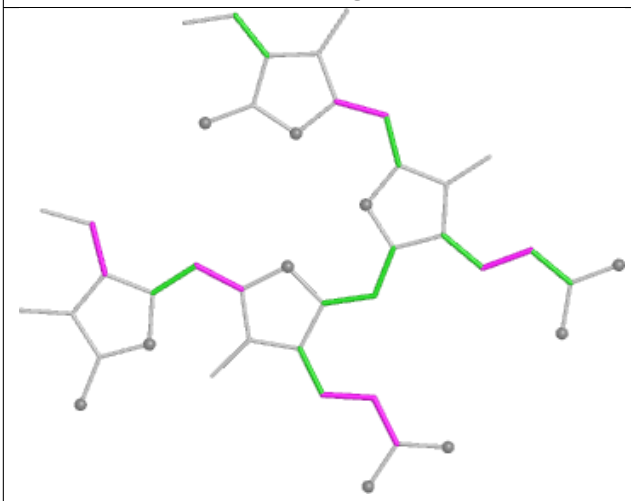
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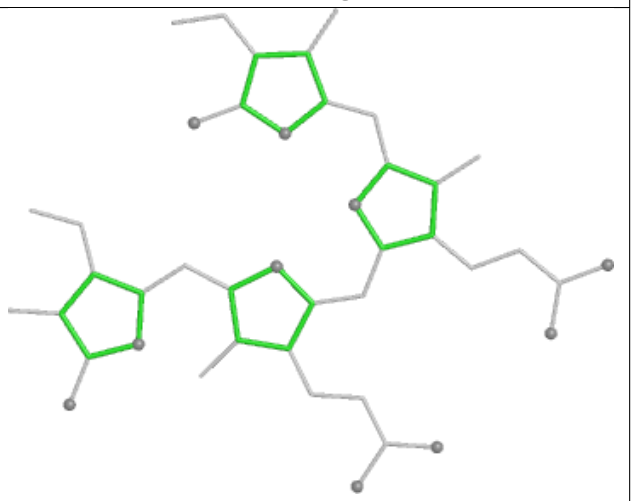
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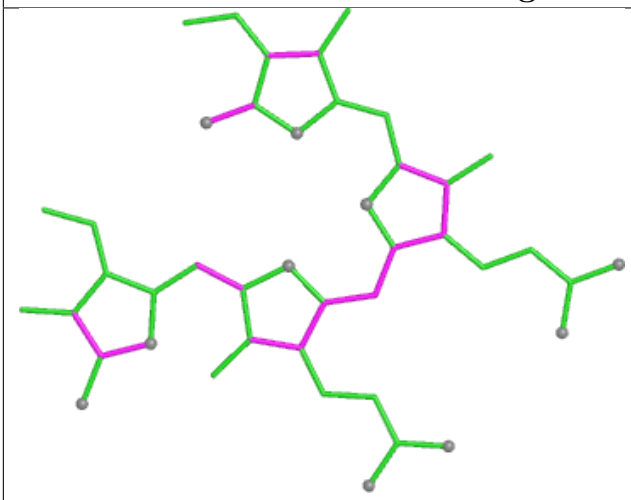


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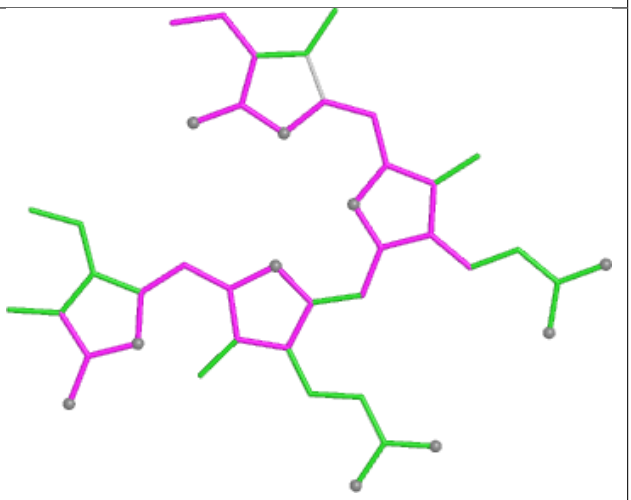


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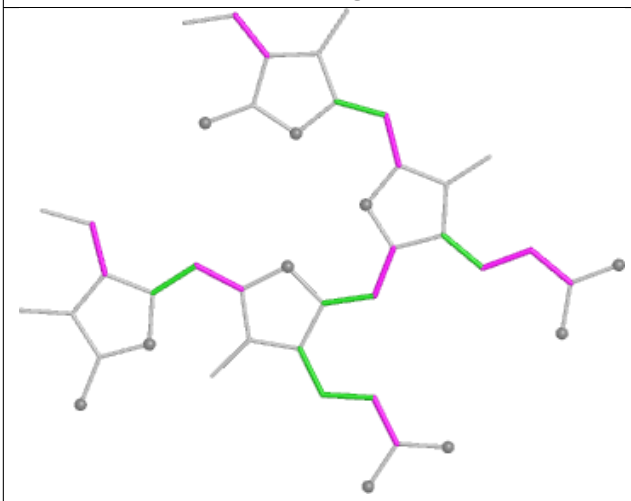
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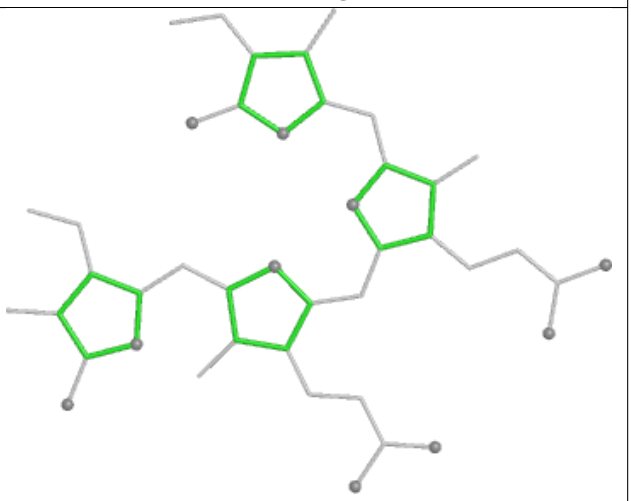
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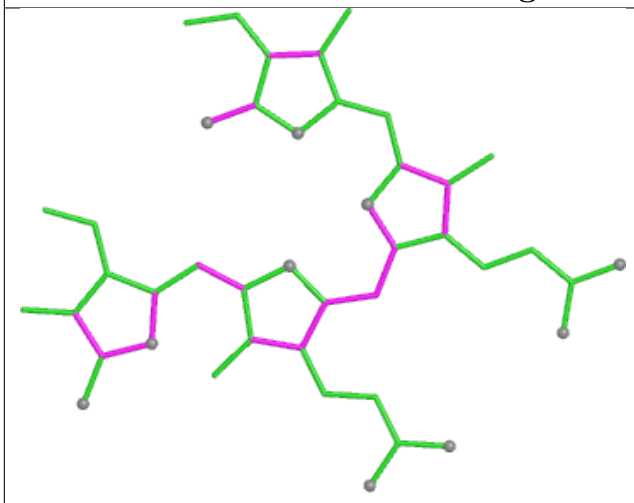


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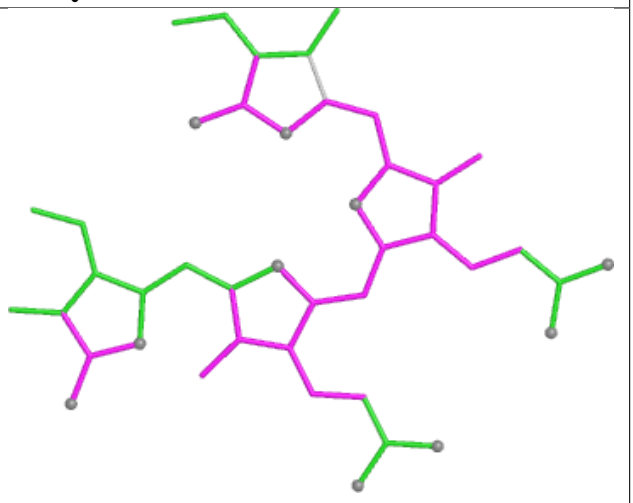


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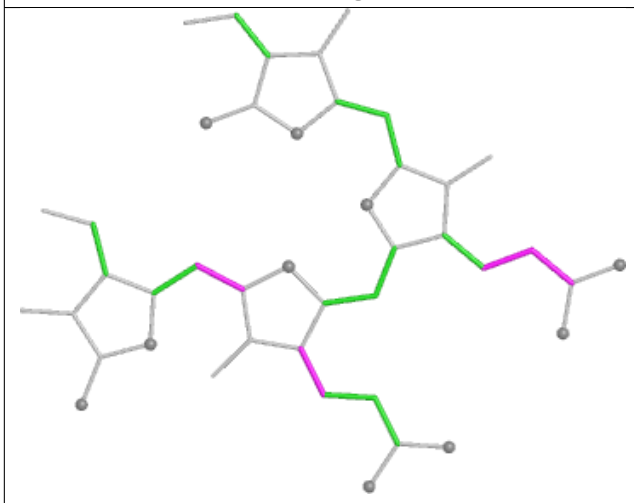
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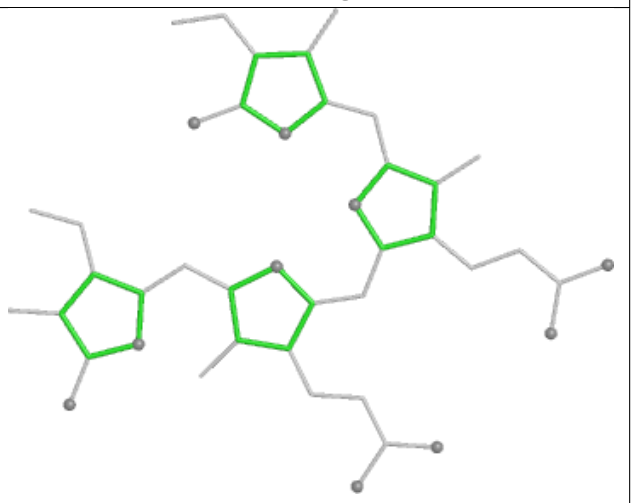
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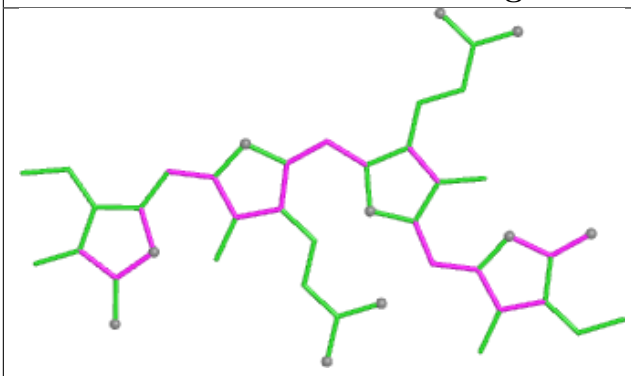


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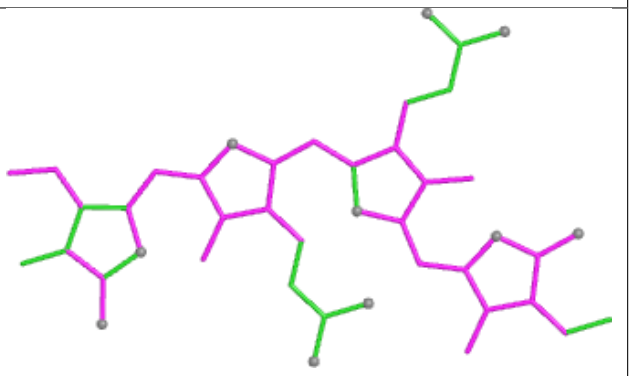


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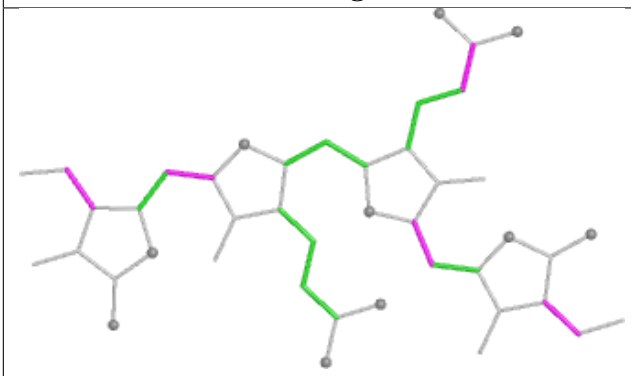
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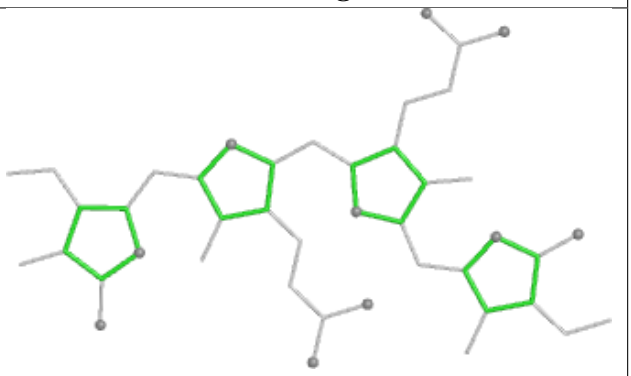
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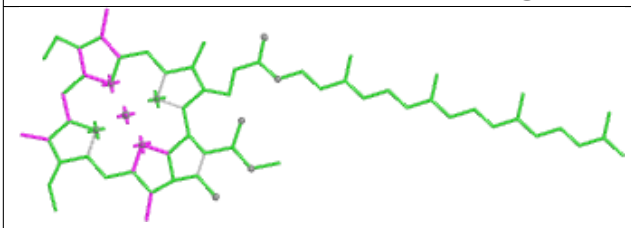


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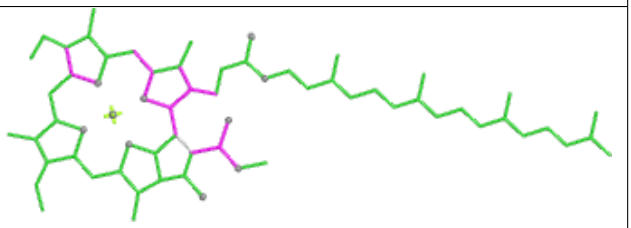


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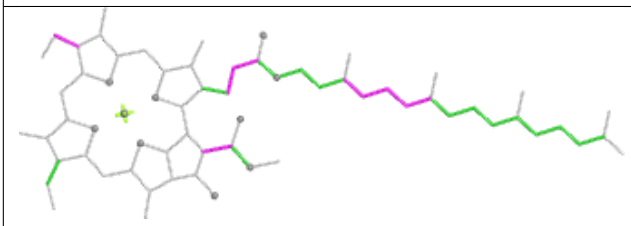
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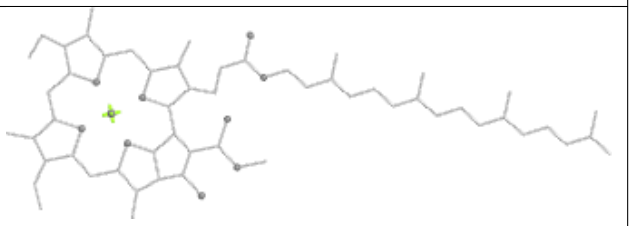
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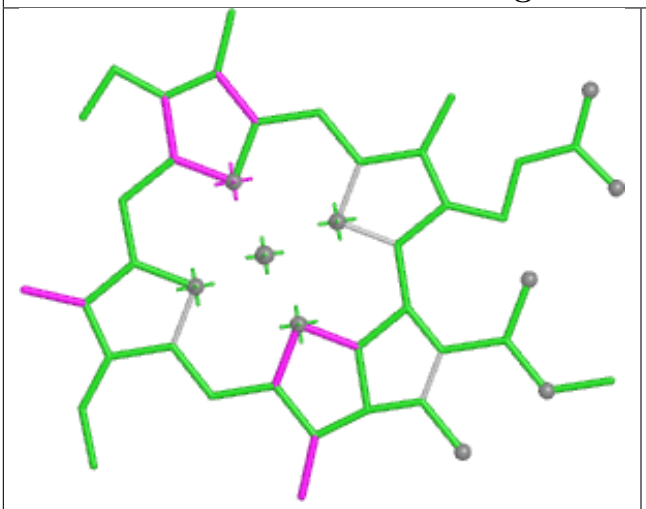


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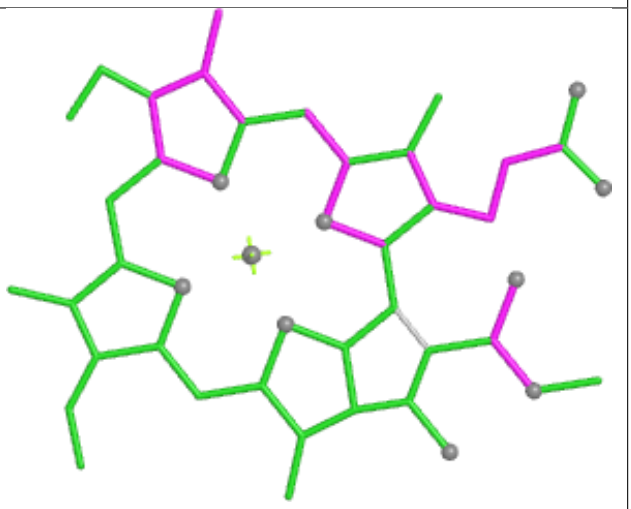


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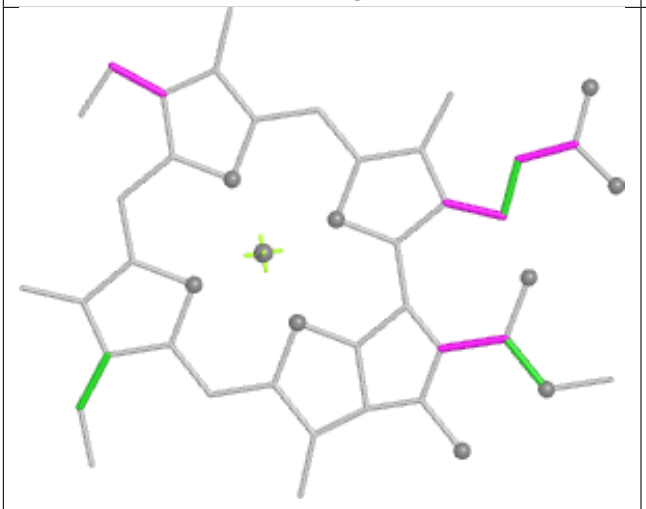
Ligand CLA 3N 306



Bond lengths



Bond angles

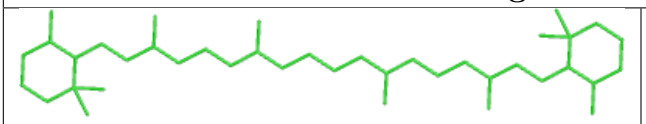


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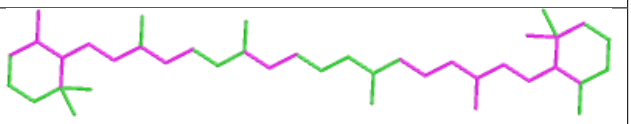


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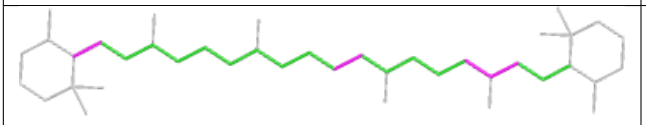
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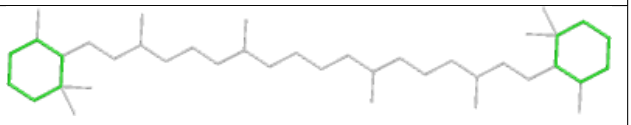
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Bond angles

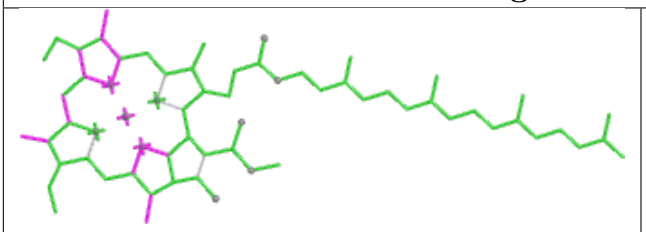


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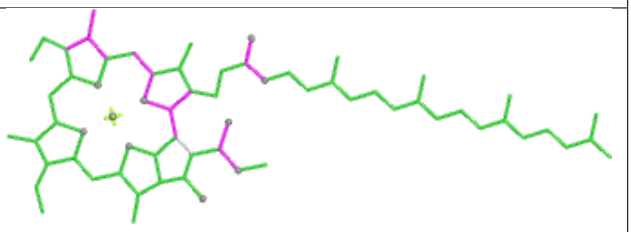


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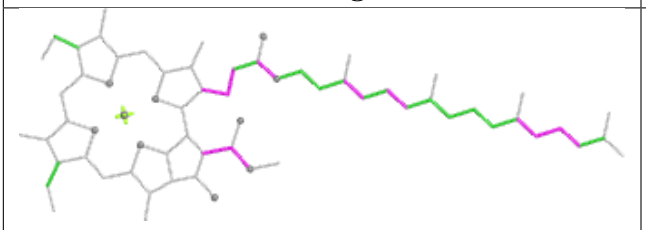
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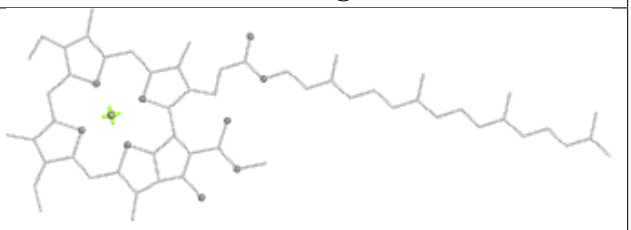
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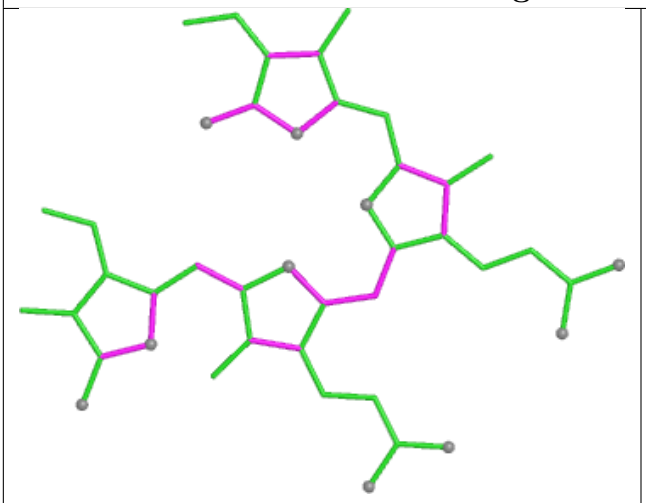


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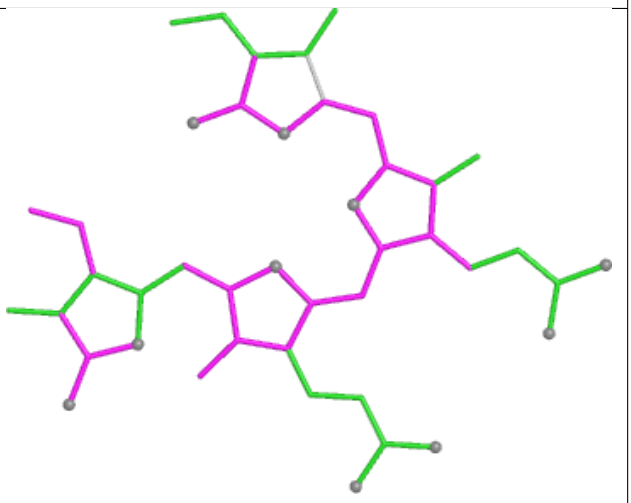


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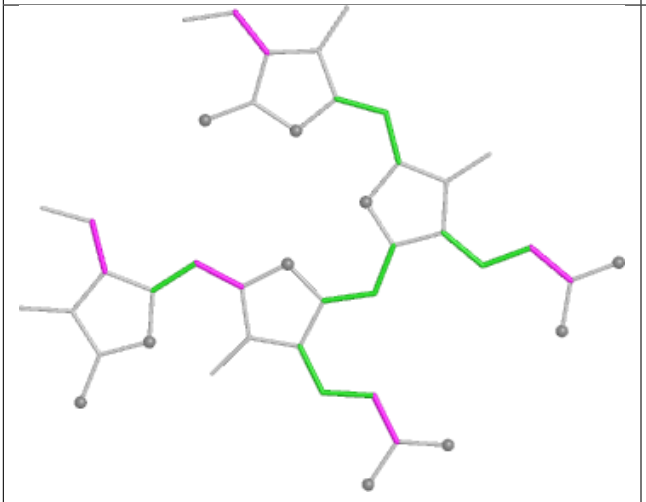
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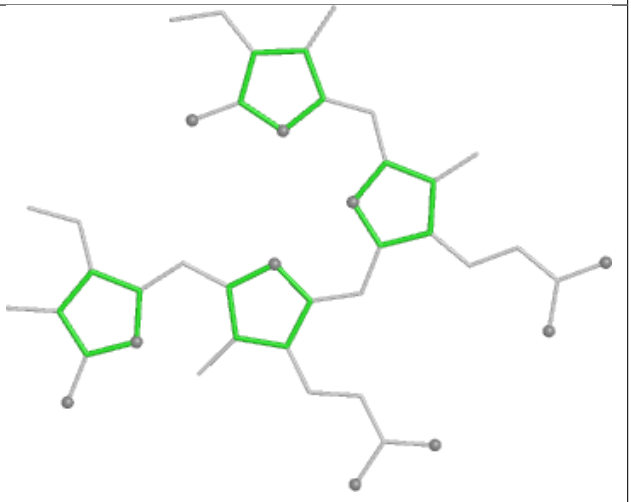
Bond lengths



Bond angles

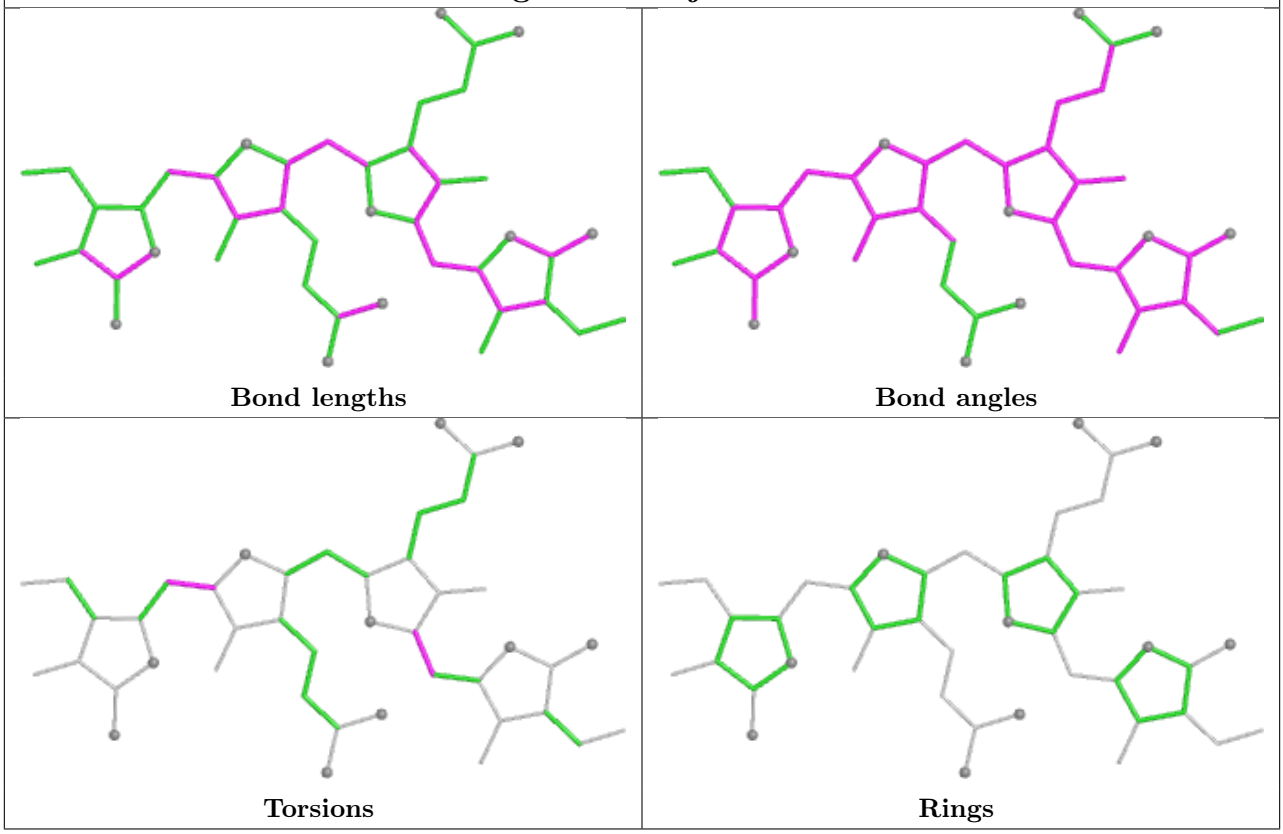


Torsions



Rings

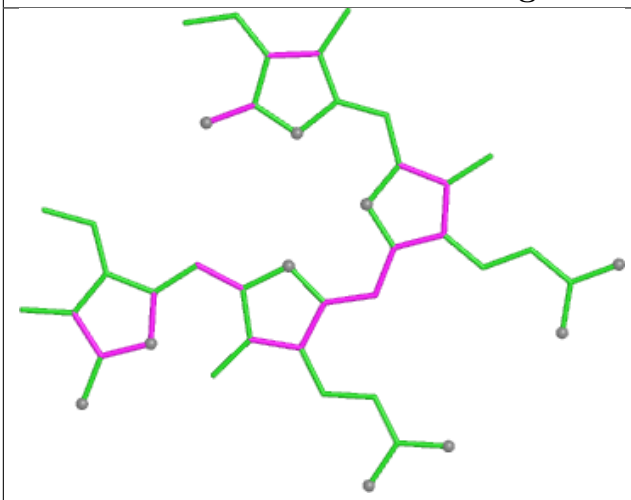
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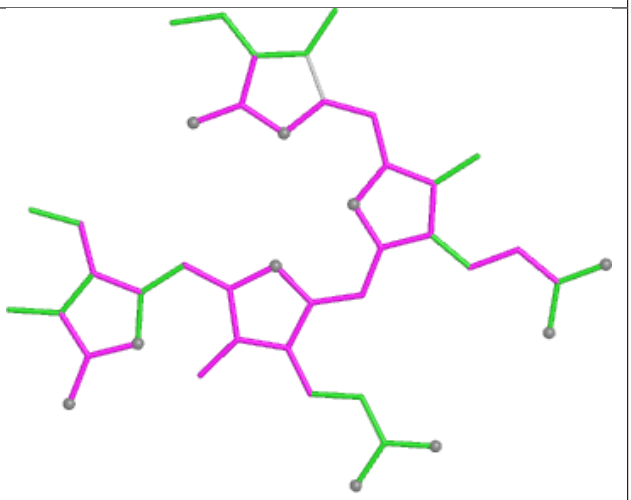
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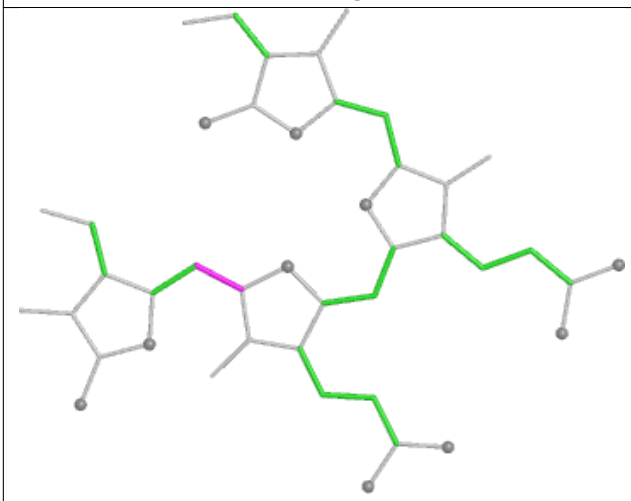
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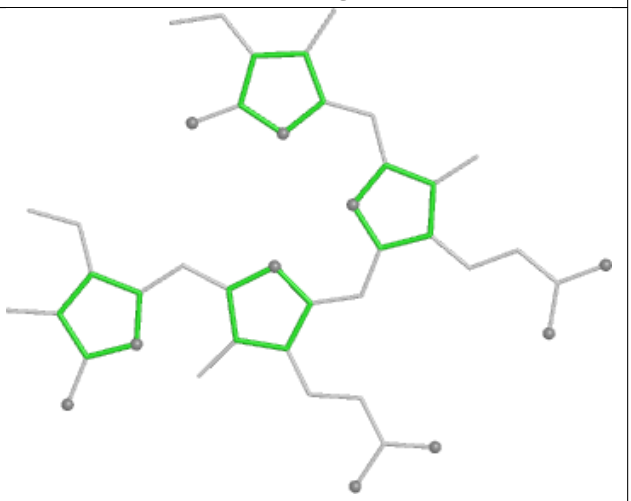
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Bond angles

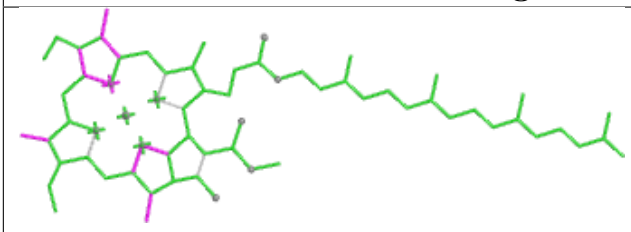


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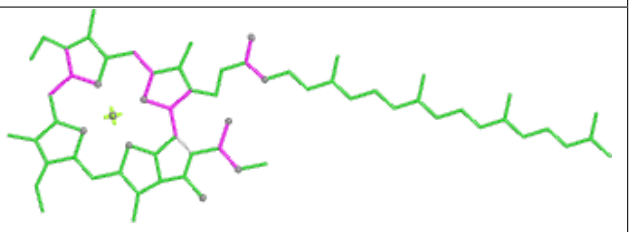


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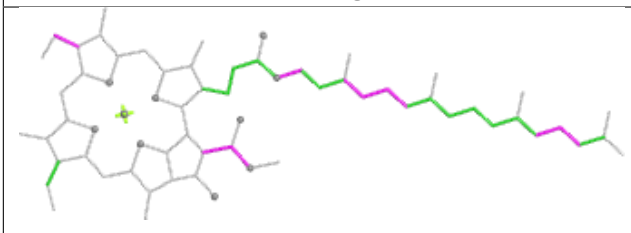
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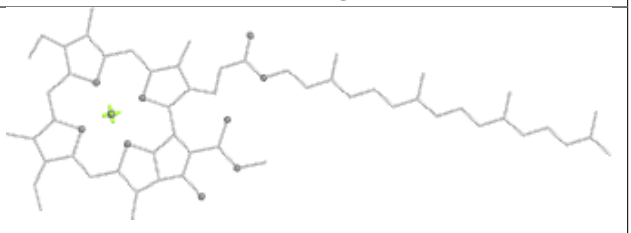
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Bond angles

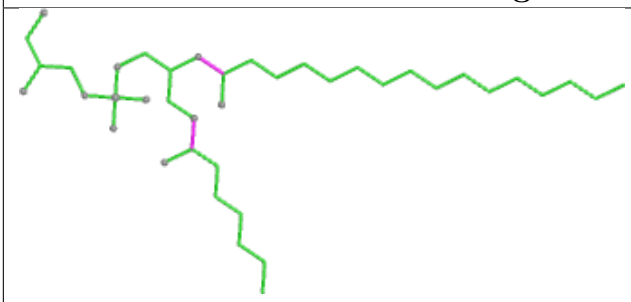


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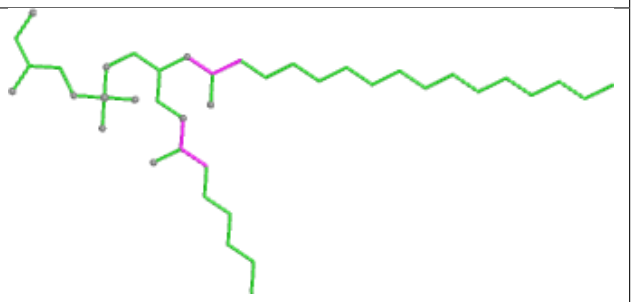


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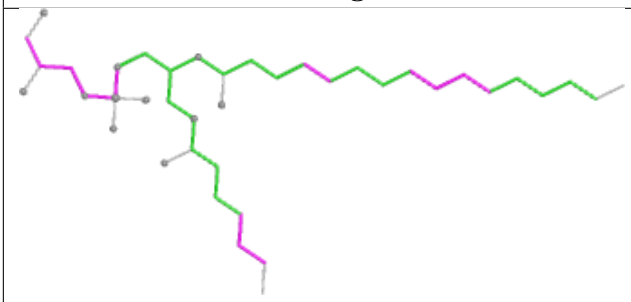
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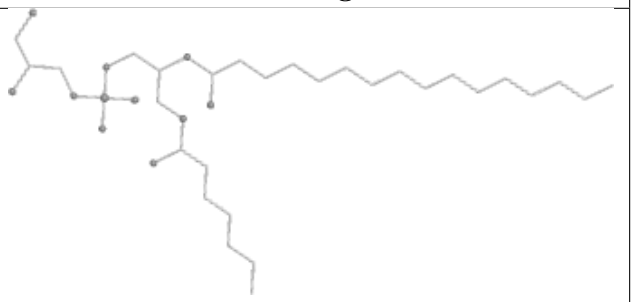
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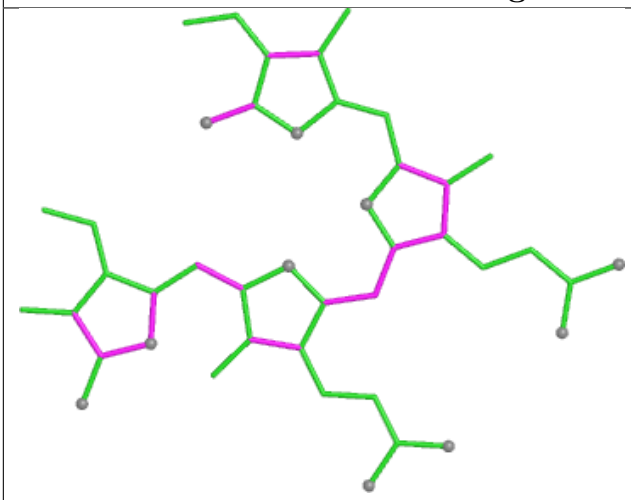


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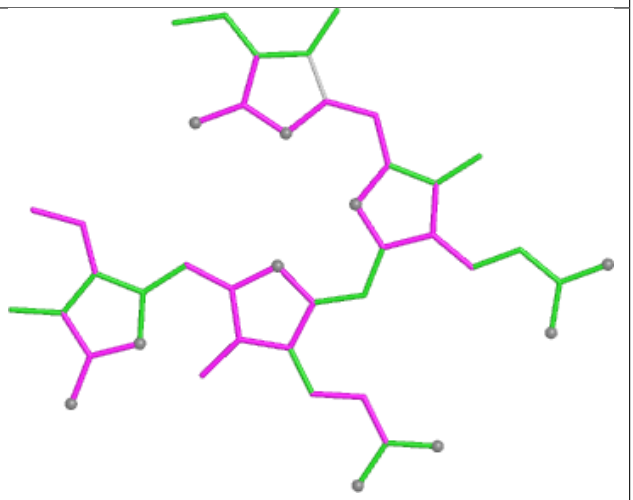


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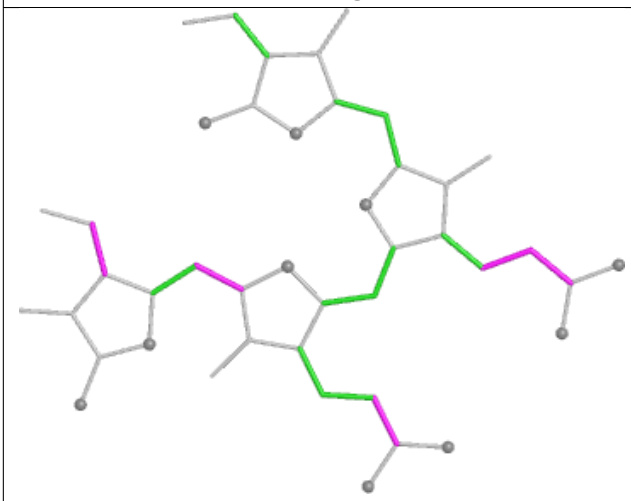
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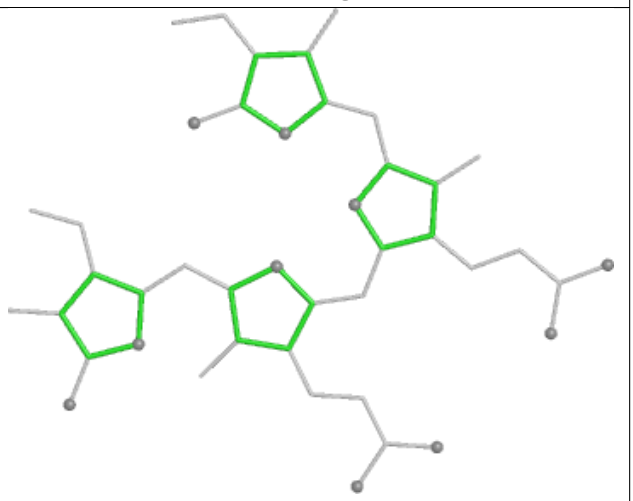
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Bond angles

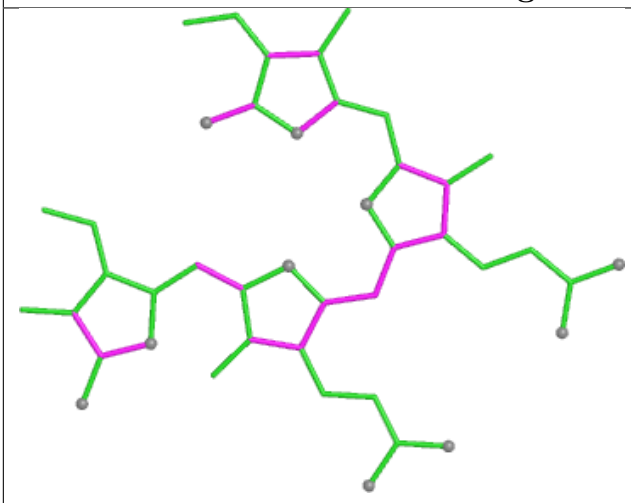


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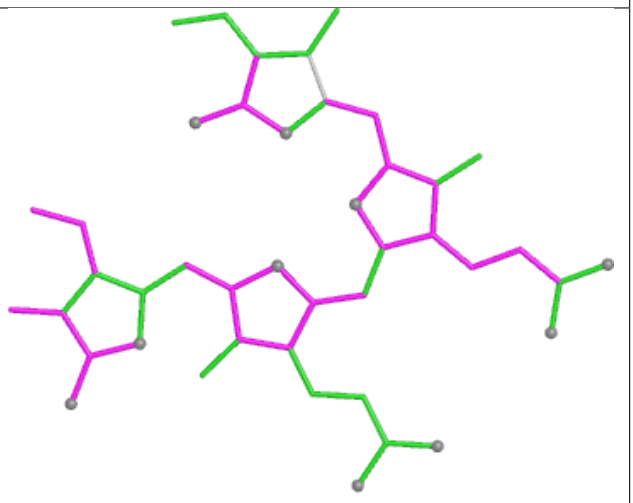


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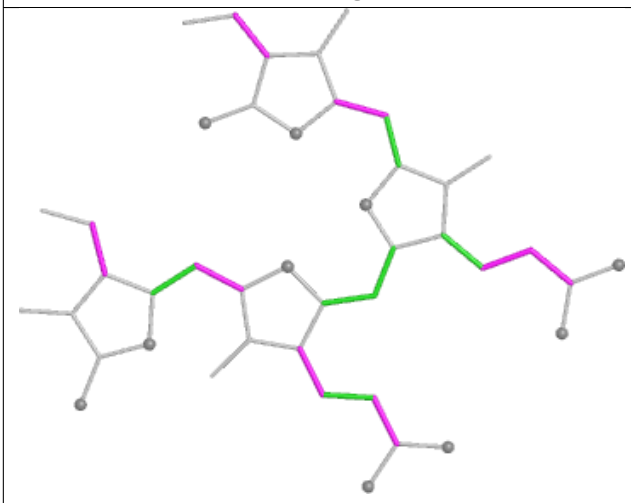
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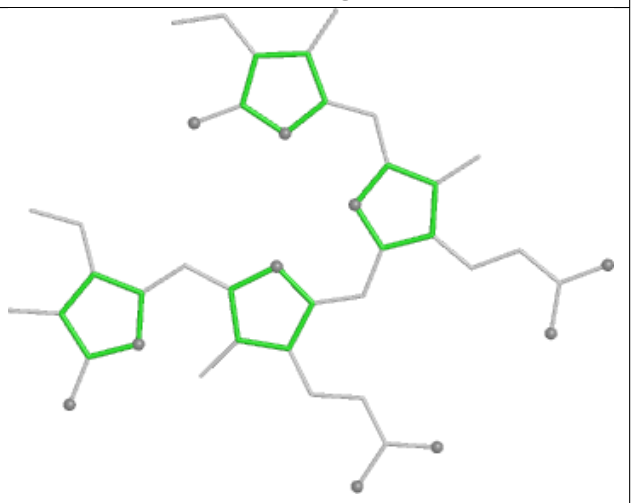
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Bond angles

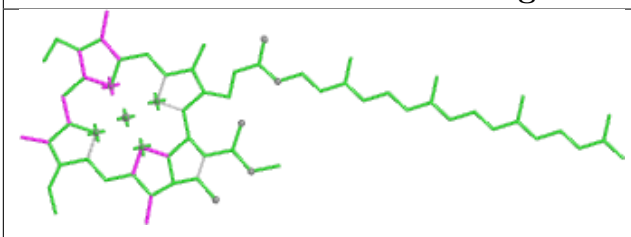


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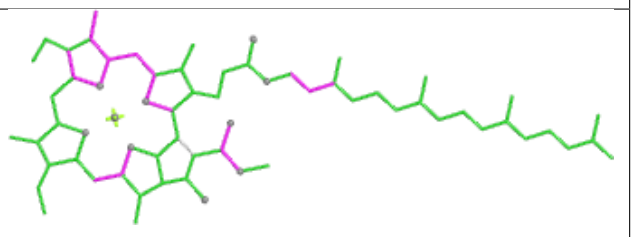


Rings

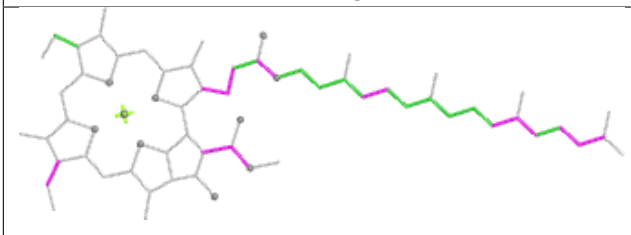
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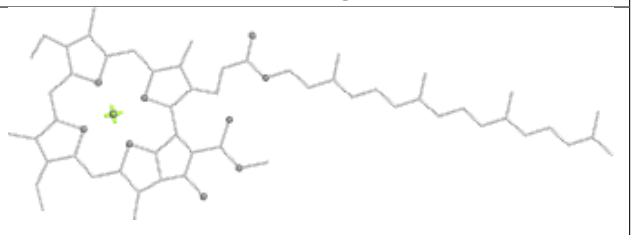
Bond lengths



Bond angles

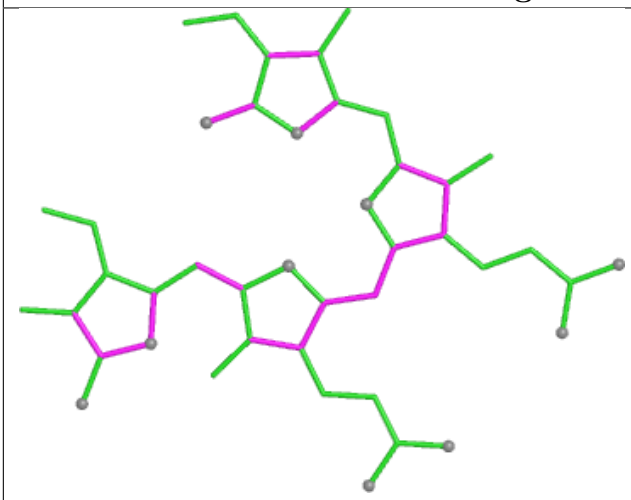


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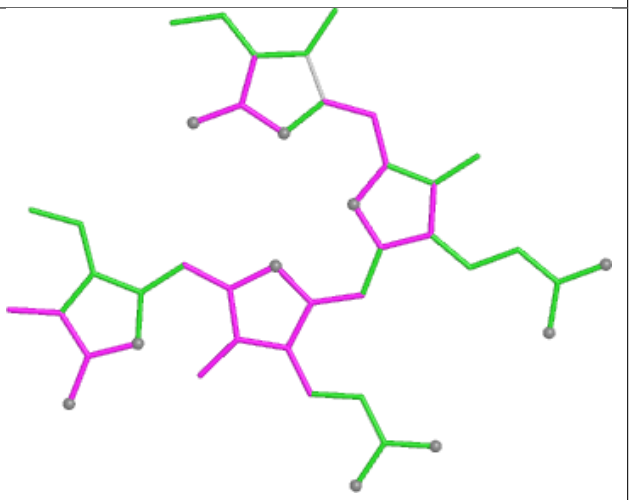


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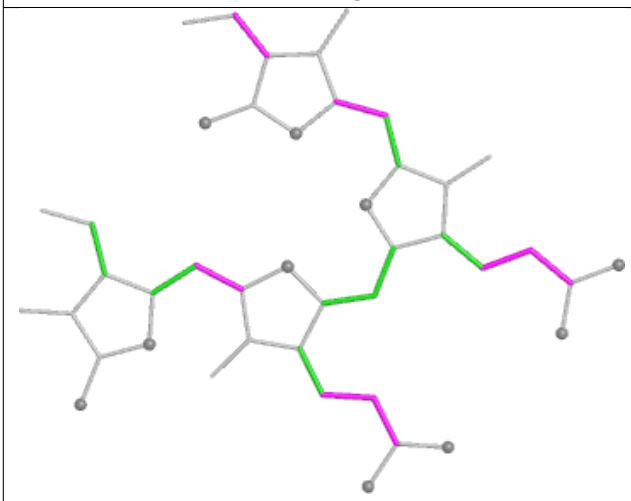
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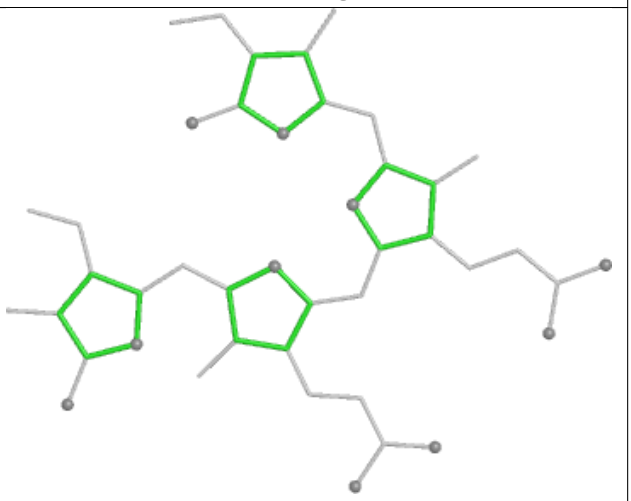
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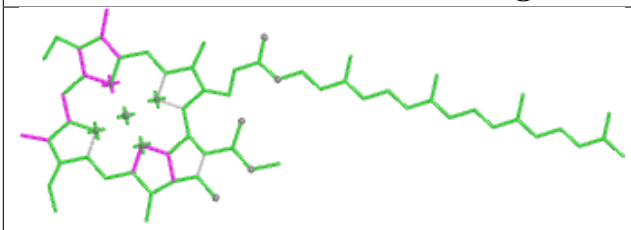


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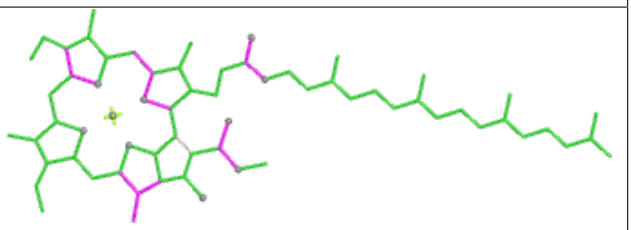


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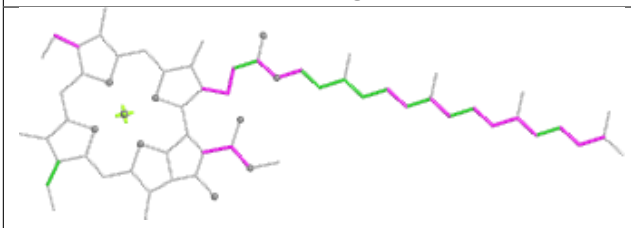
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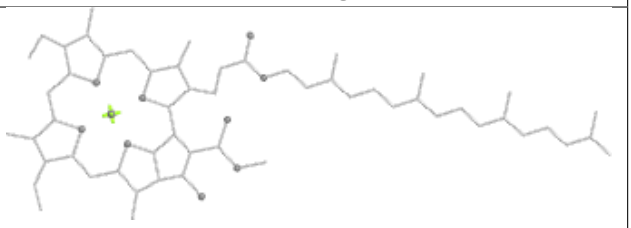
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Bond angles

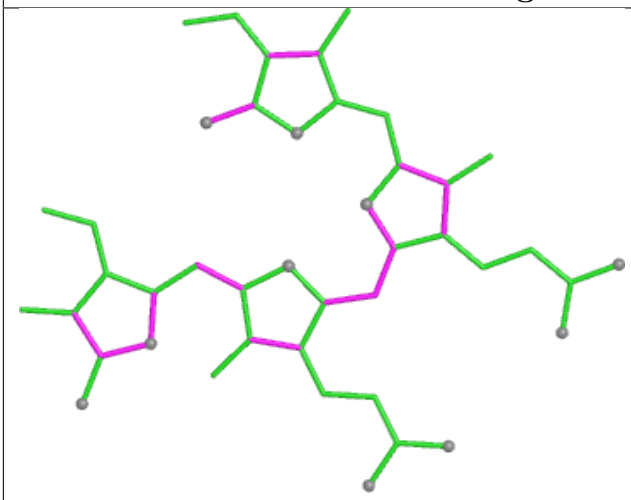


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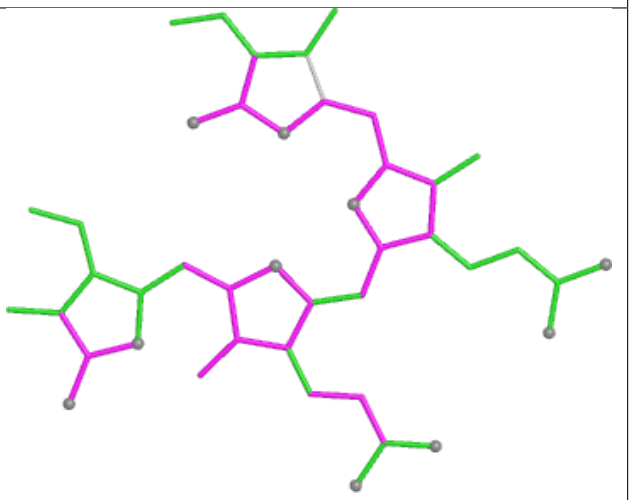


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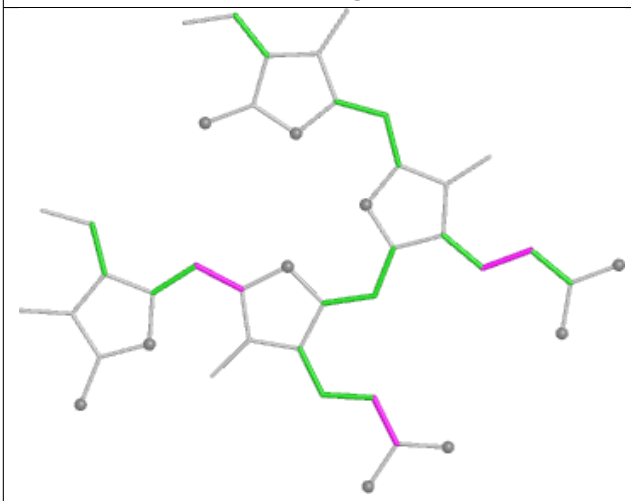
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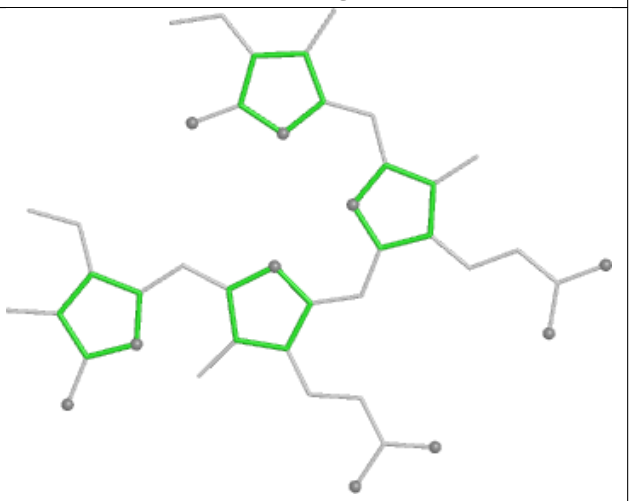
Bond lengths



Bond angles

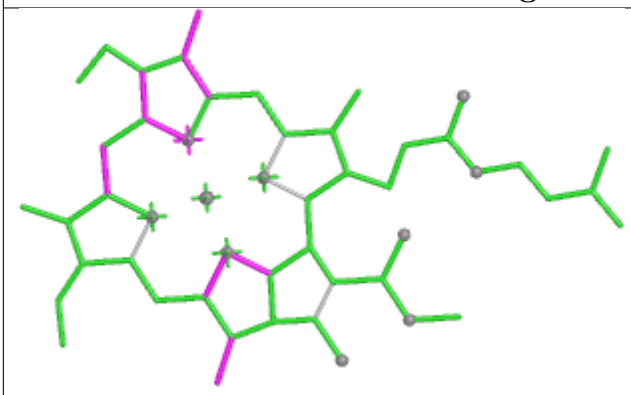


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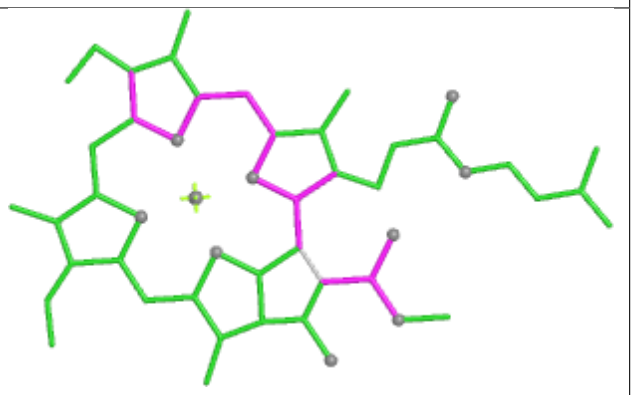


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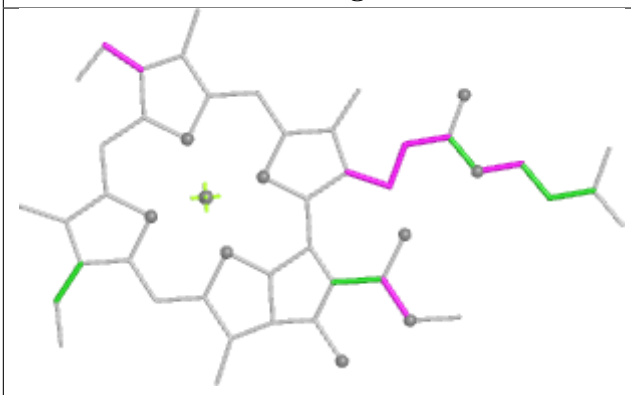
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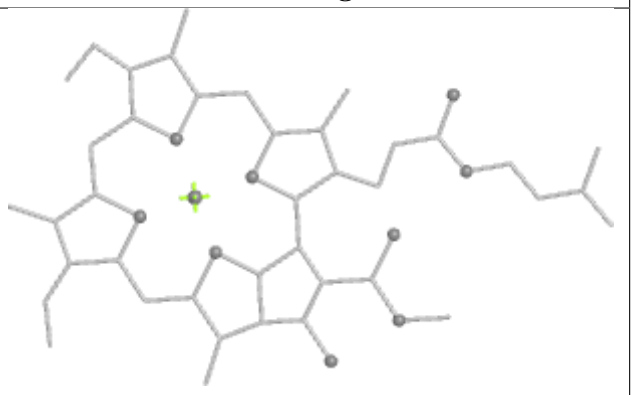
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Bond angles

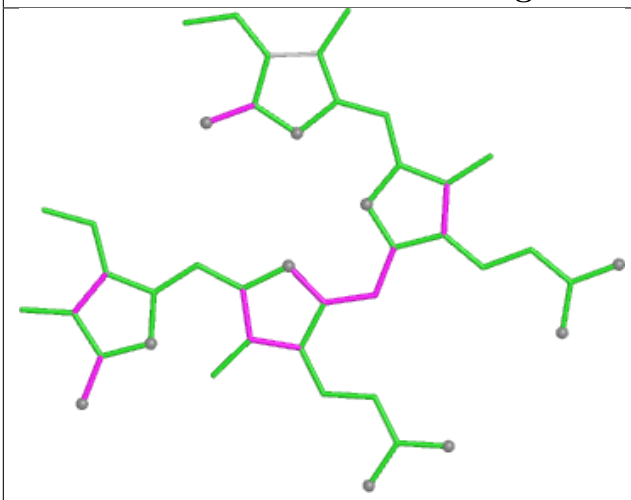


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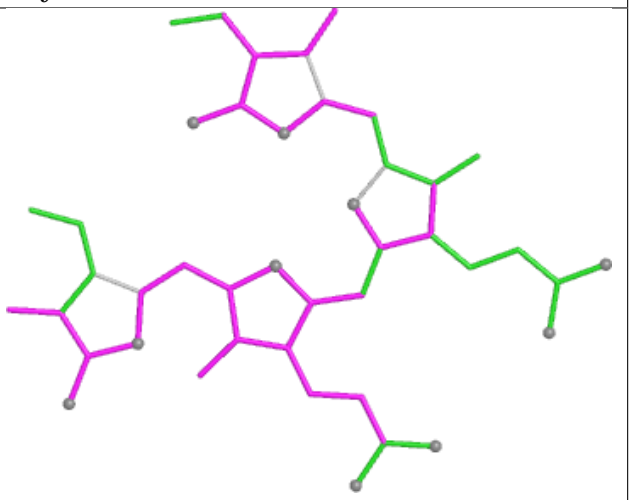


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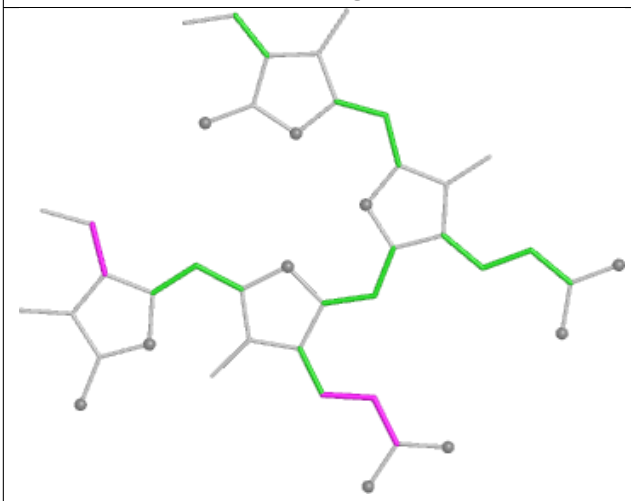
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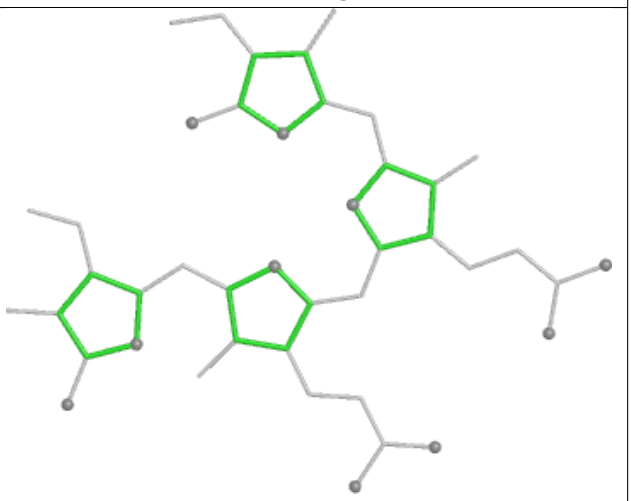
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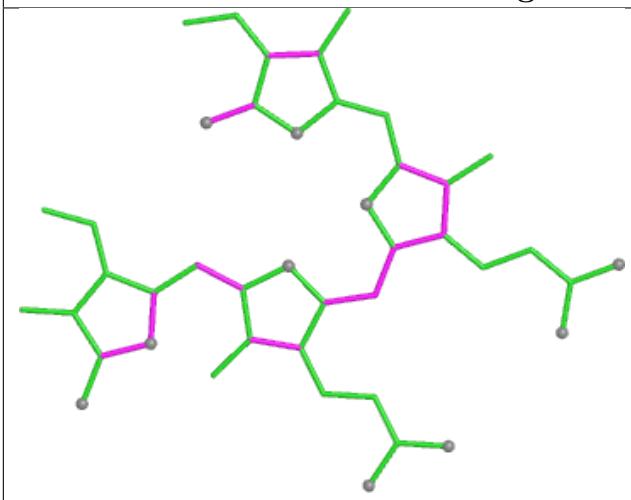


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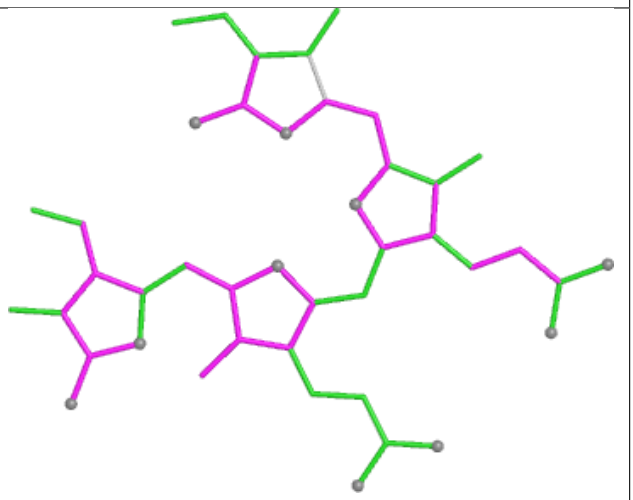


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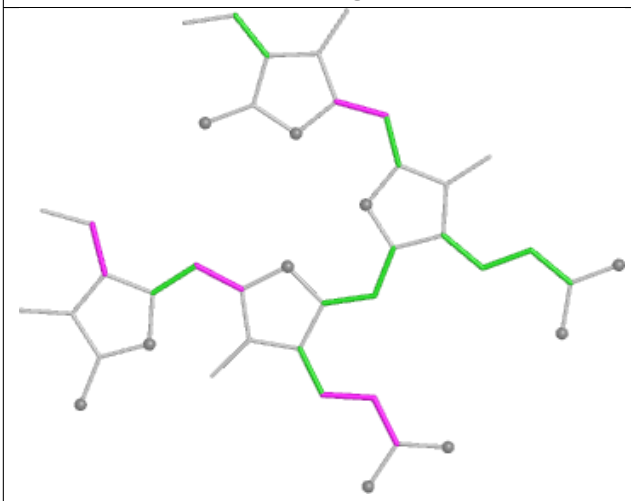
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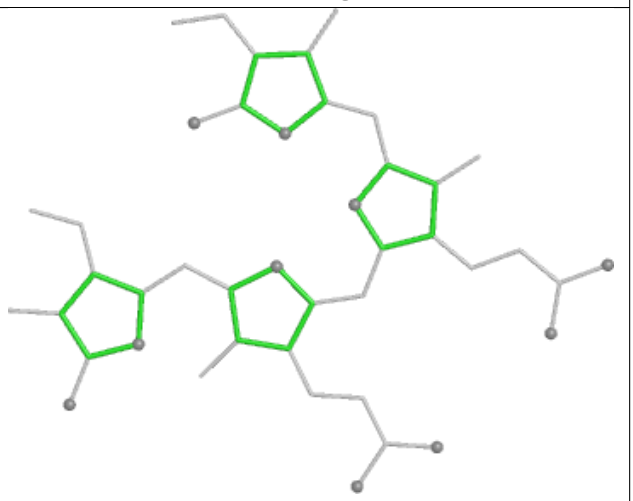
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Bond angles

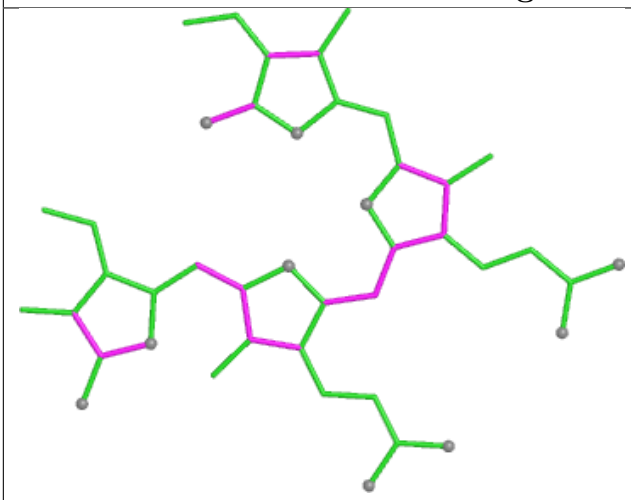


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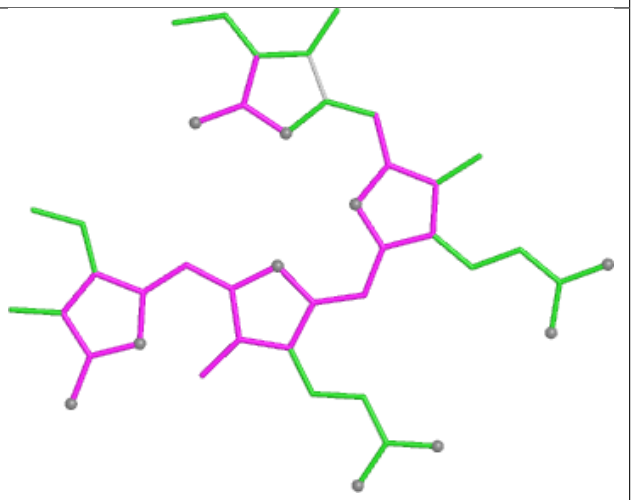


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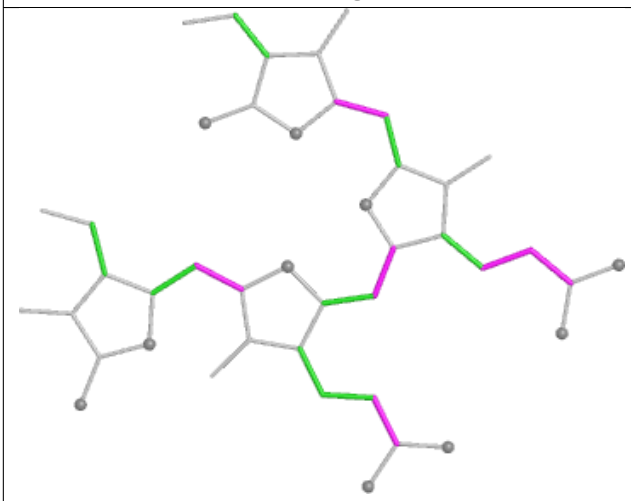
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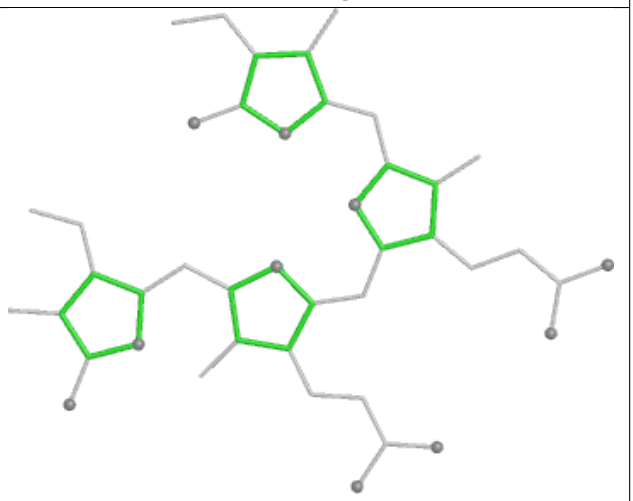
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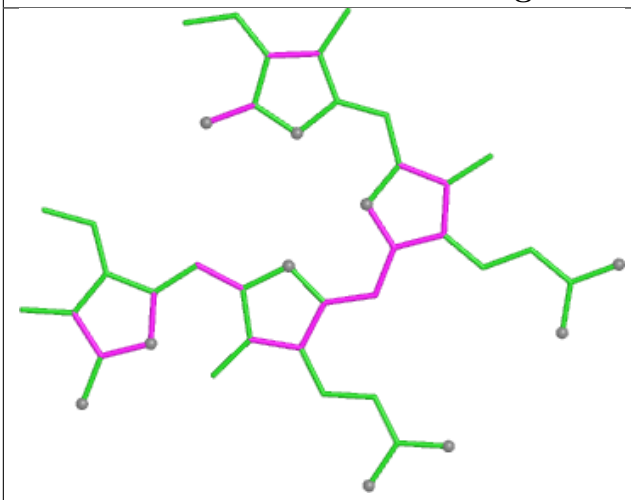


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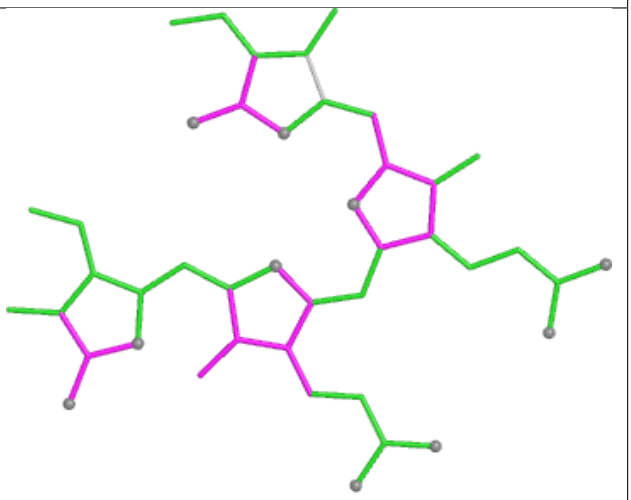


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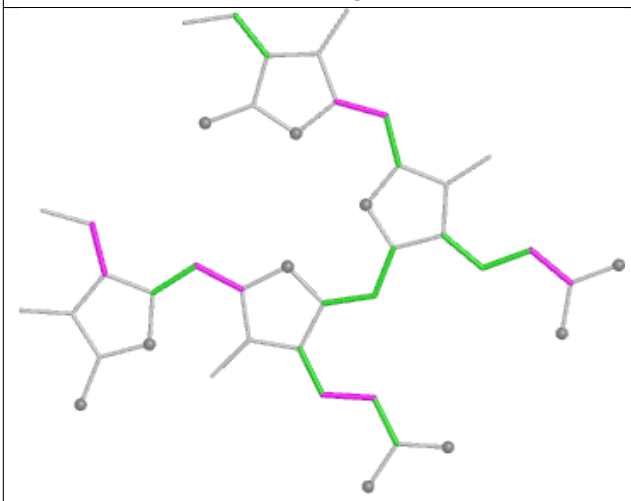
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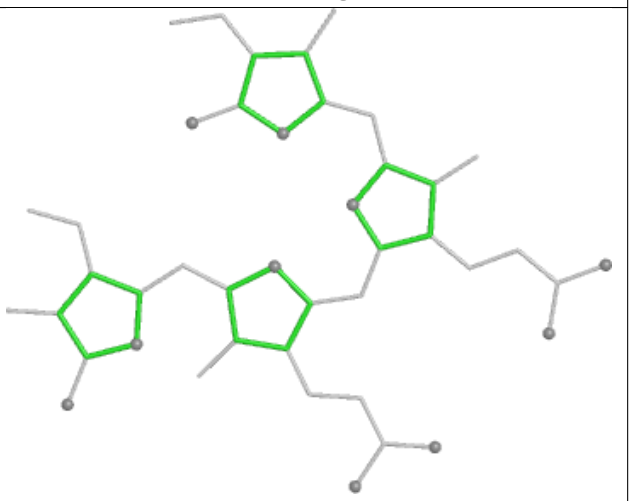
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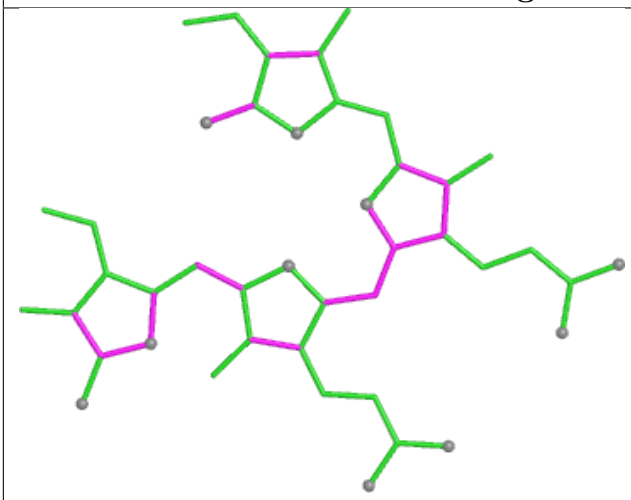


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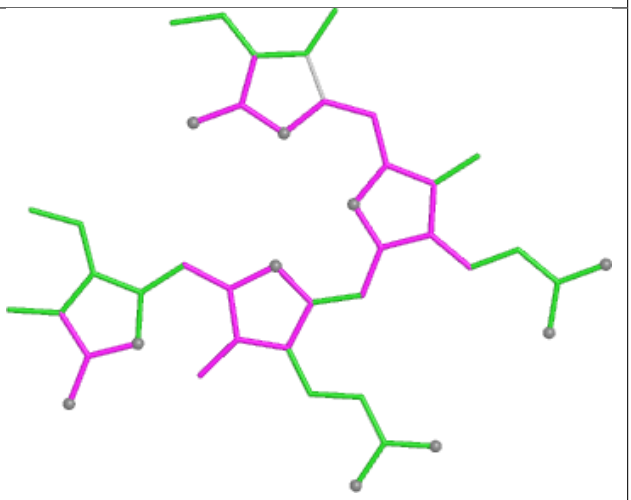


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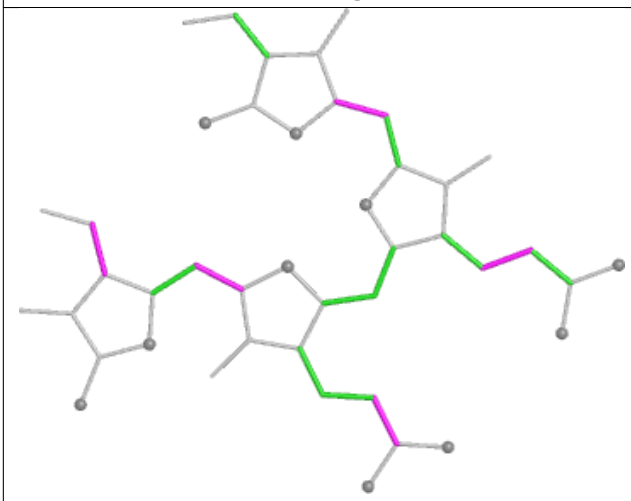
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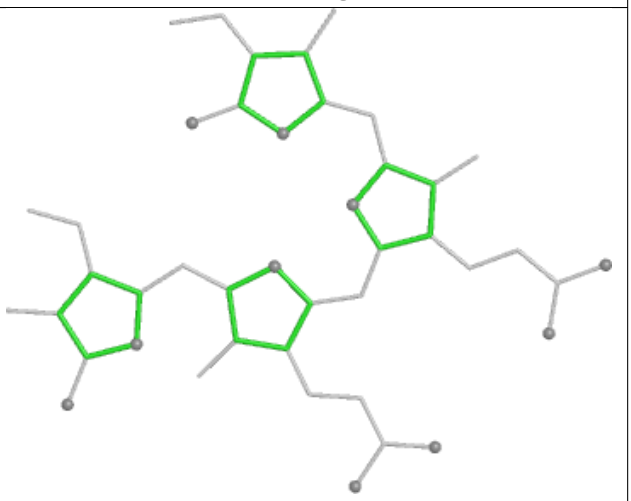
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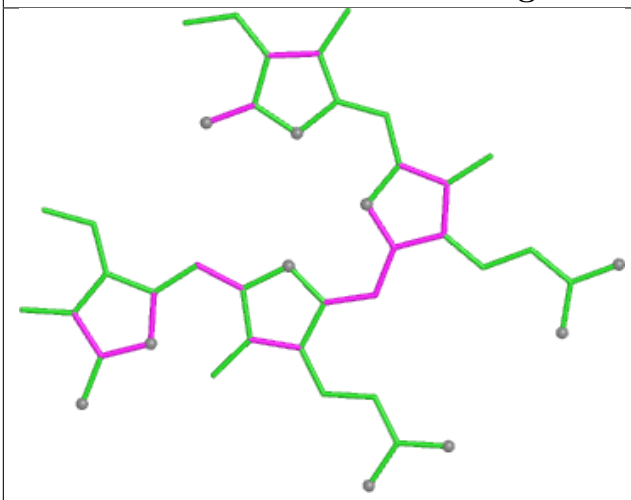


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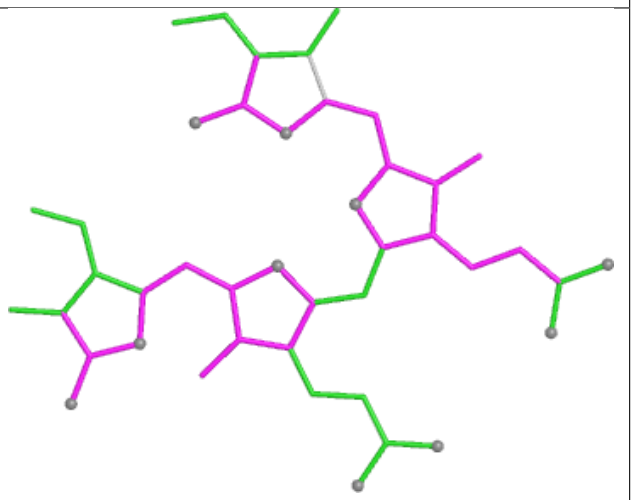


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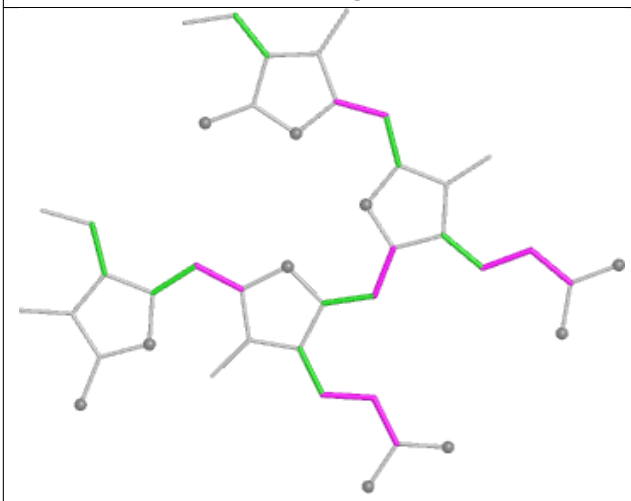
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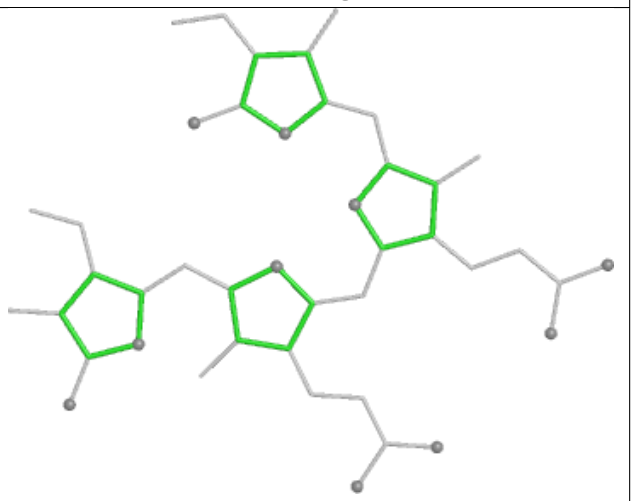
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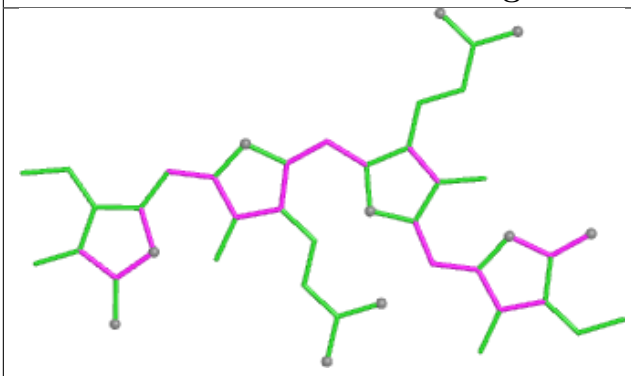


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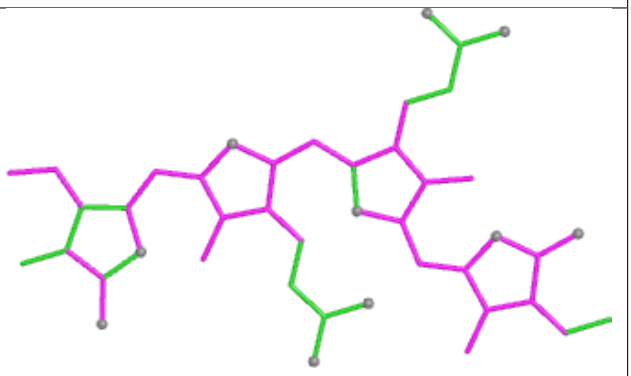


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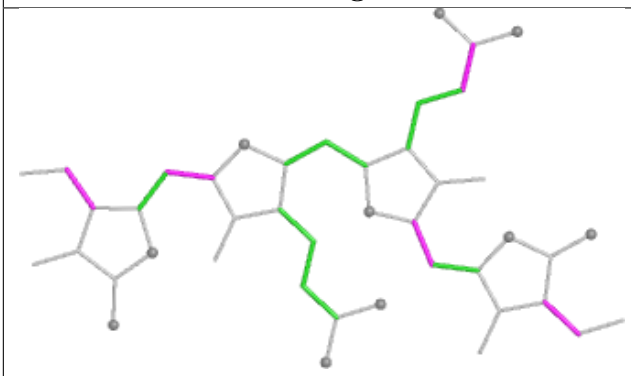
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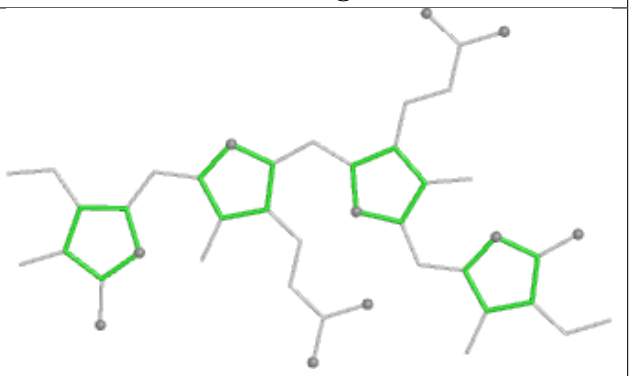
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Bond angles

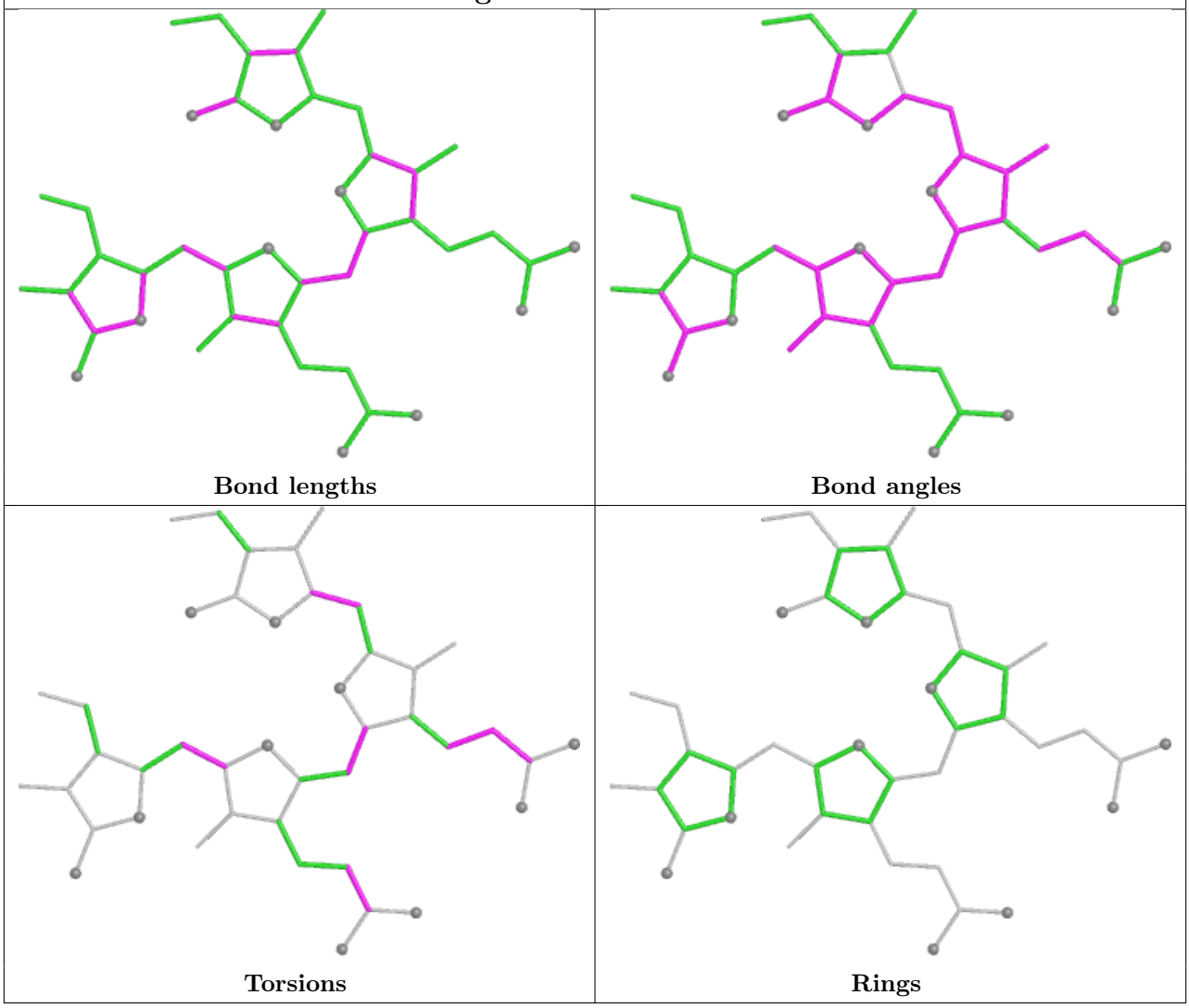


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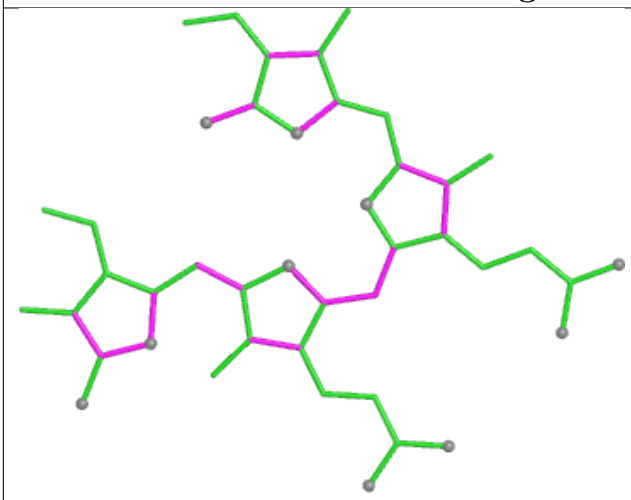
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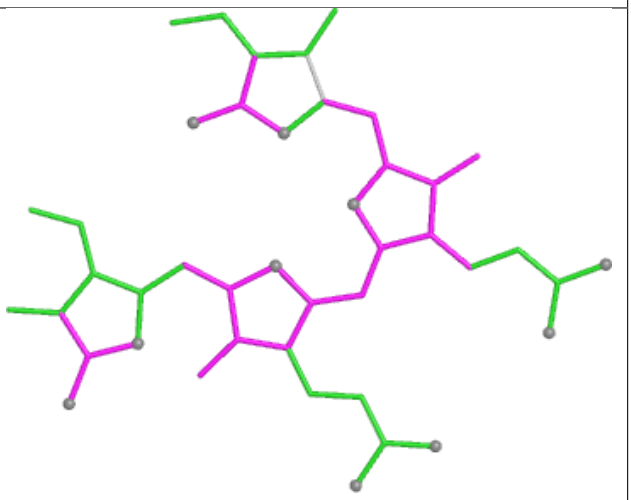
Bond lengths | Bond angles

Torsions | Rings

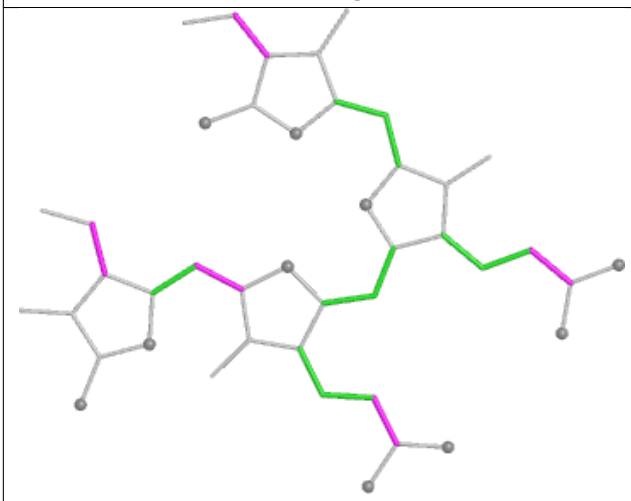
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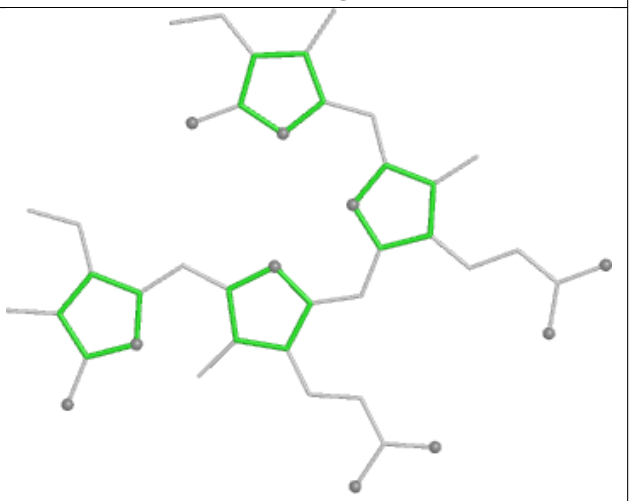
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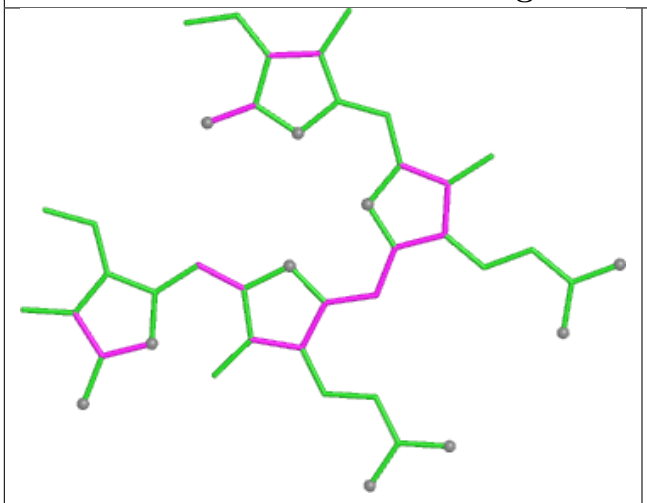


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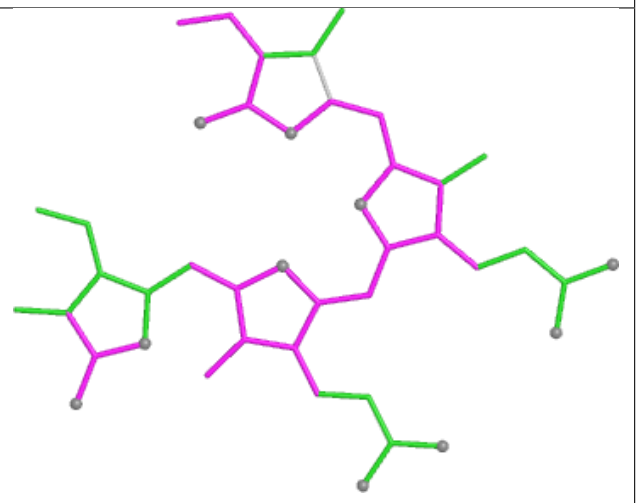


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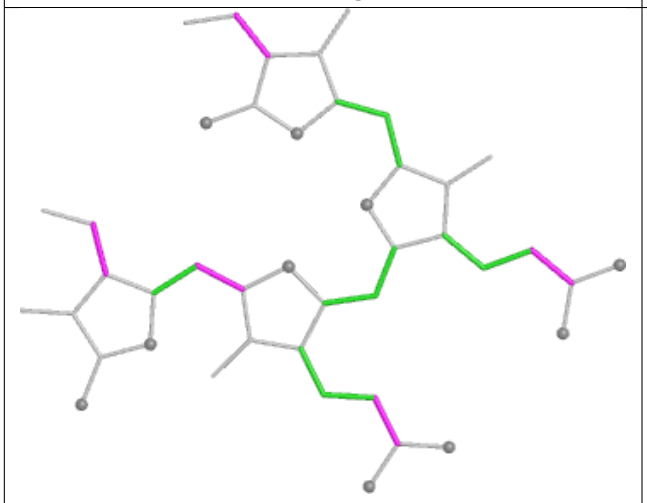
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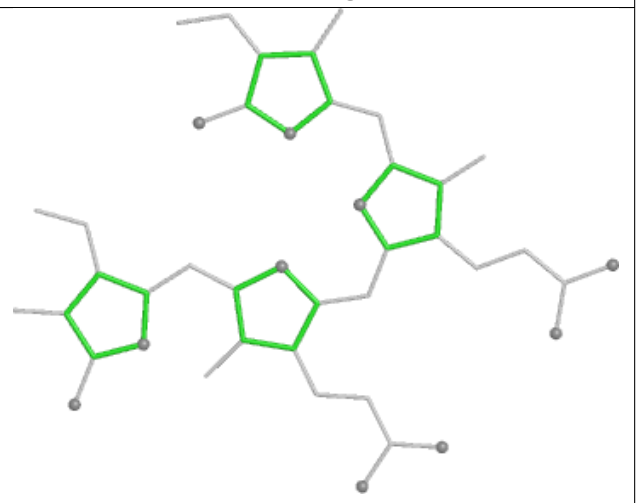
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Bond angles

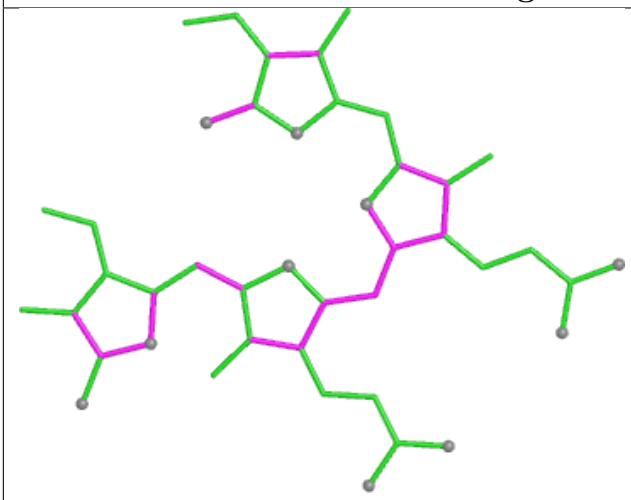


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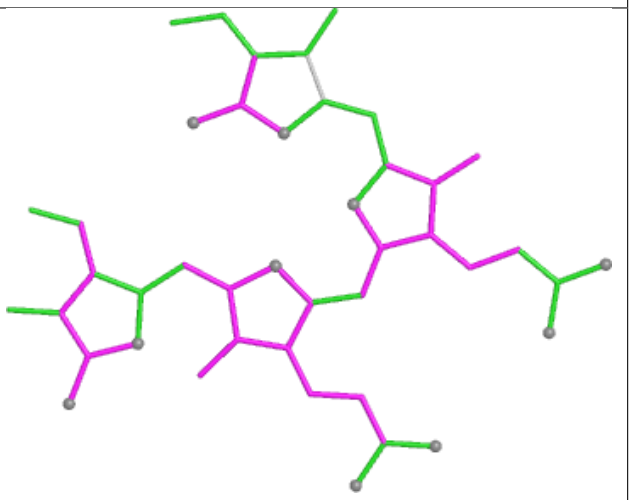


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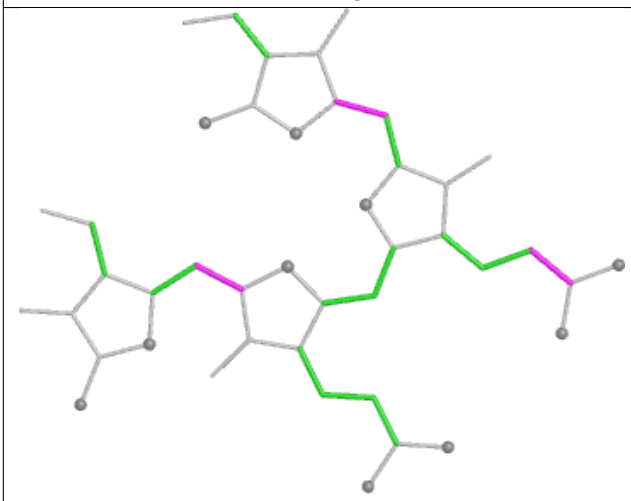
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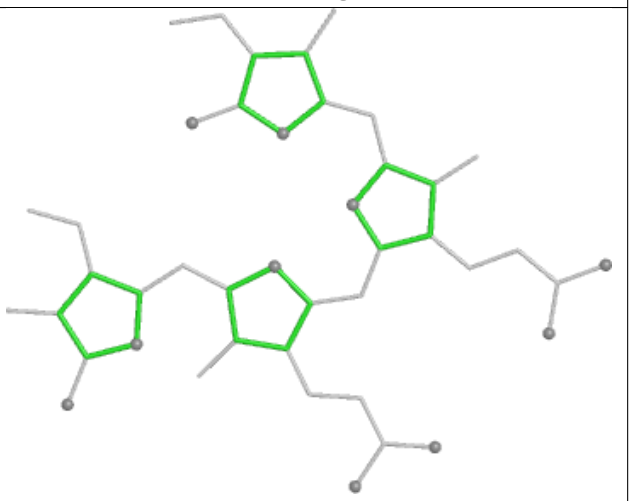
Bond lengths



Bond angles

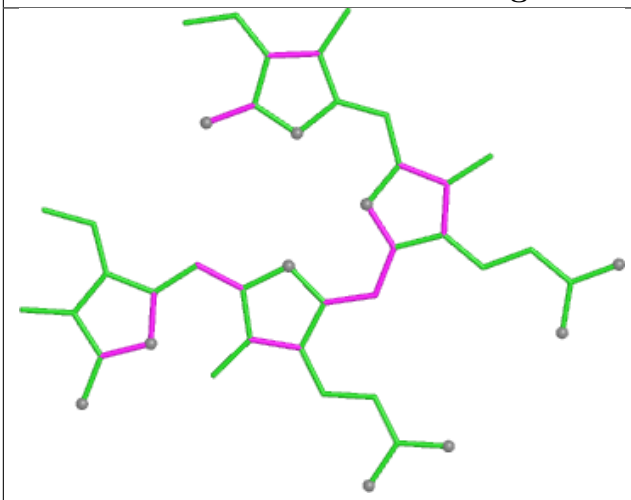


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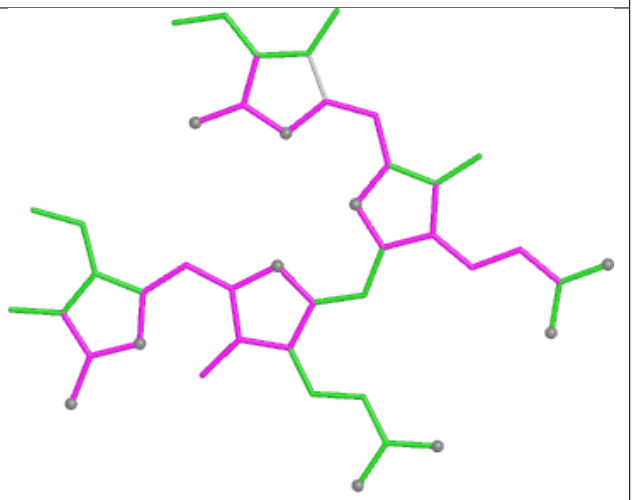


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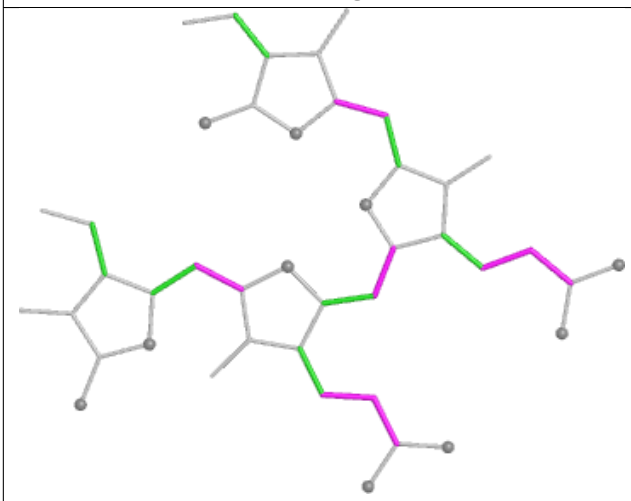
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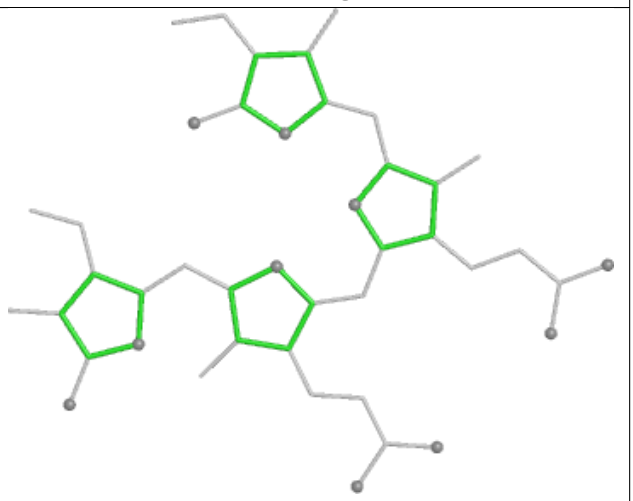
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Bond angles

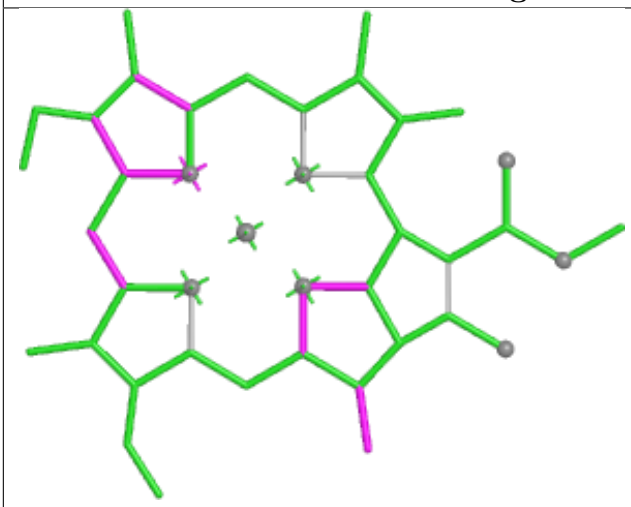


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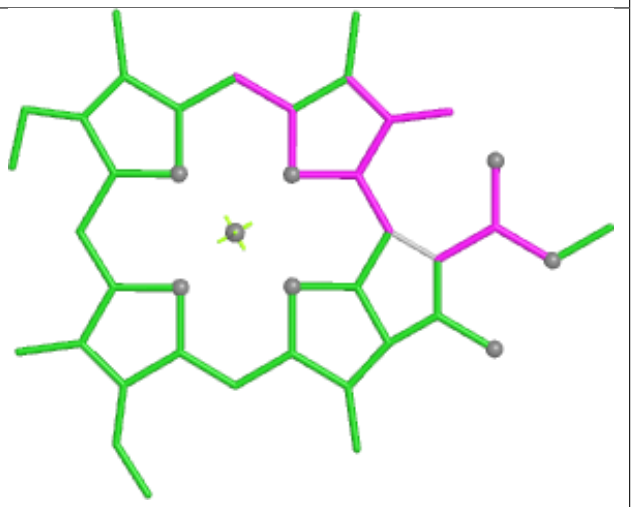


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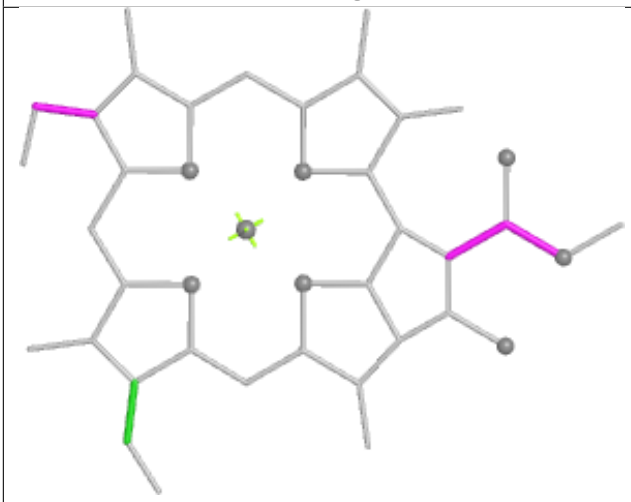
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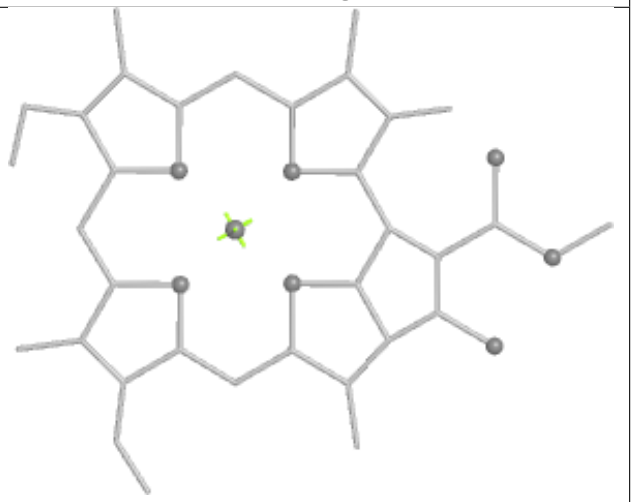
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Bond angles

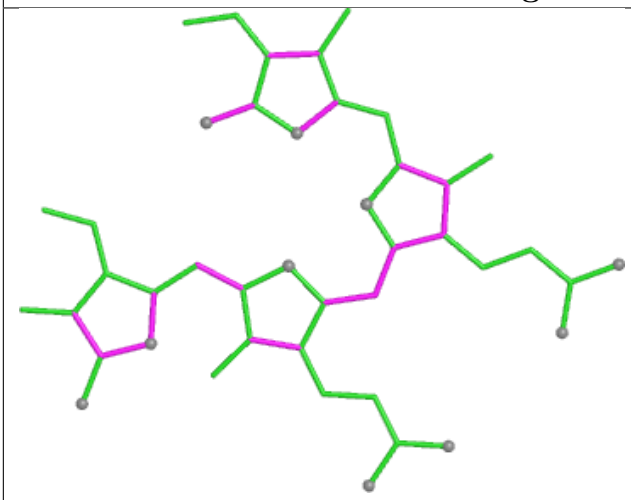


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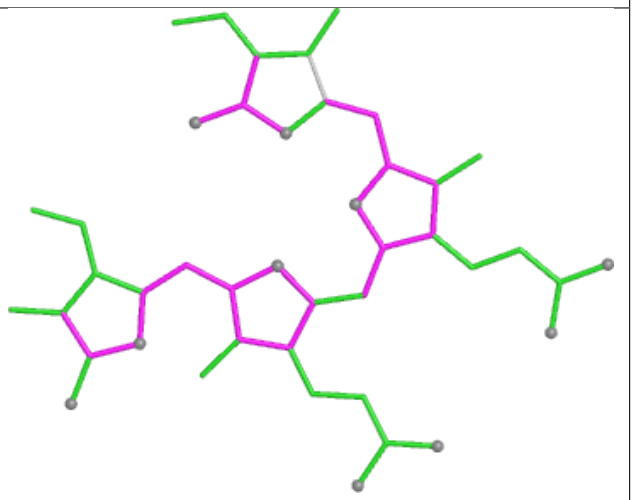


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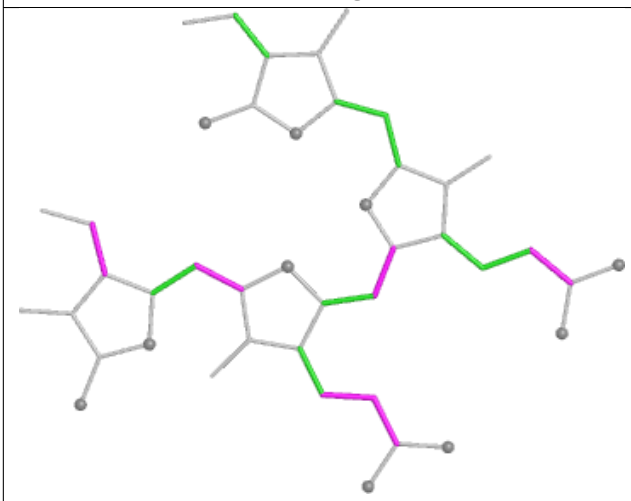
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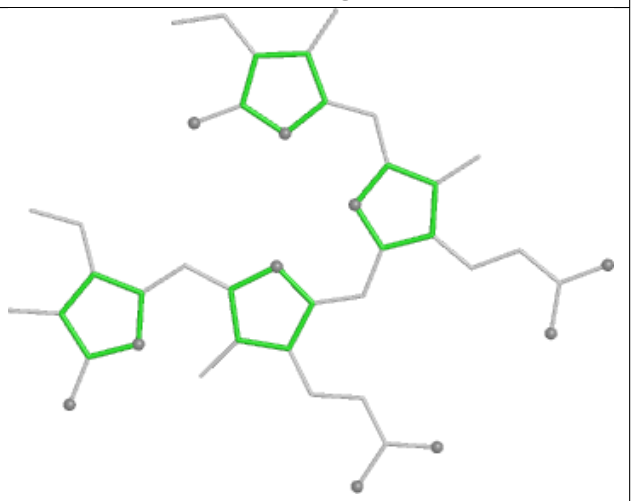
Bond lengths



Bond angles

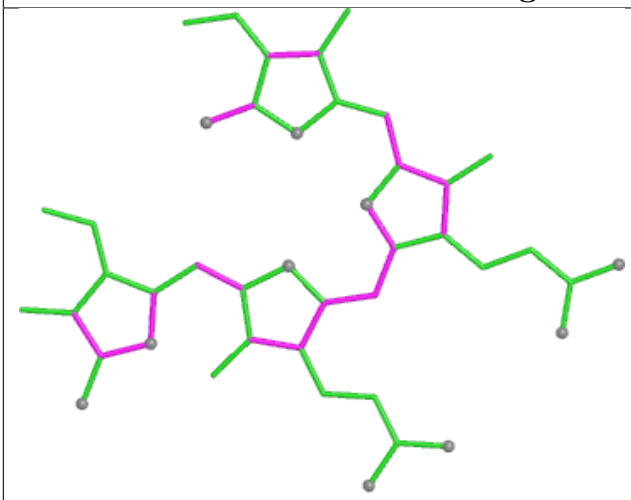


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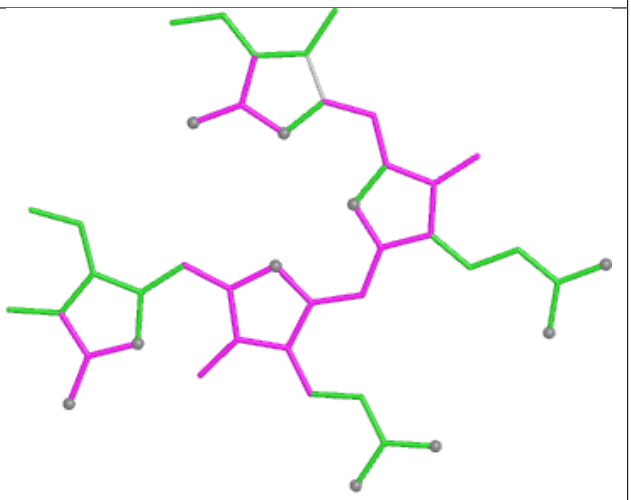


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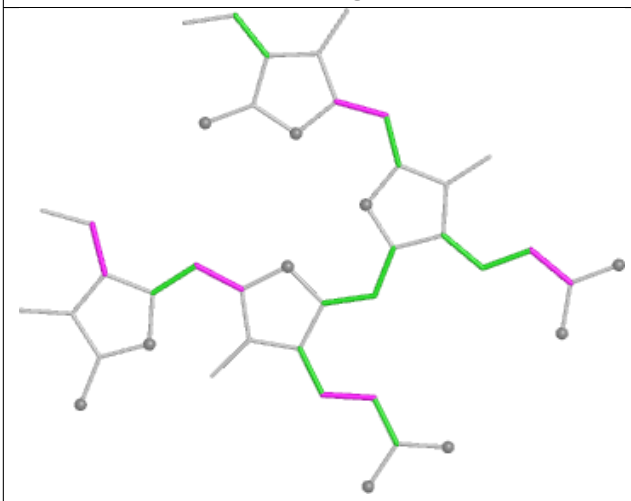
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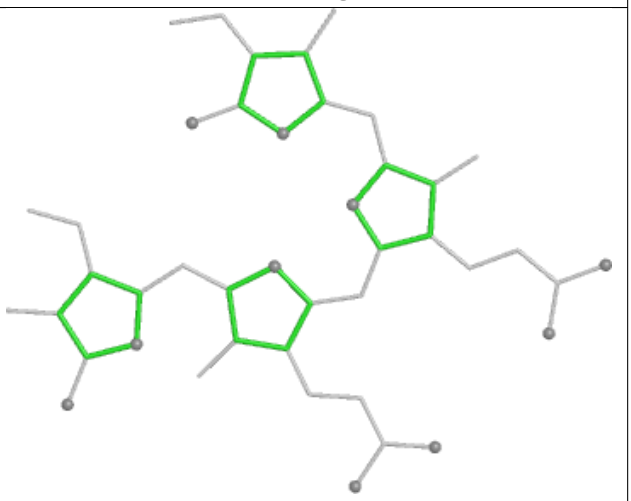
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Bond angles

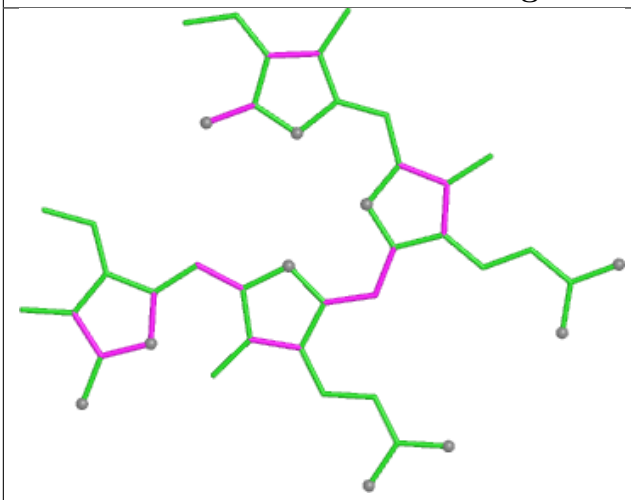


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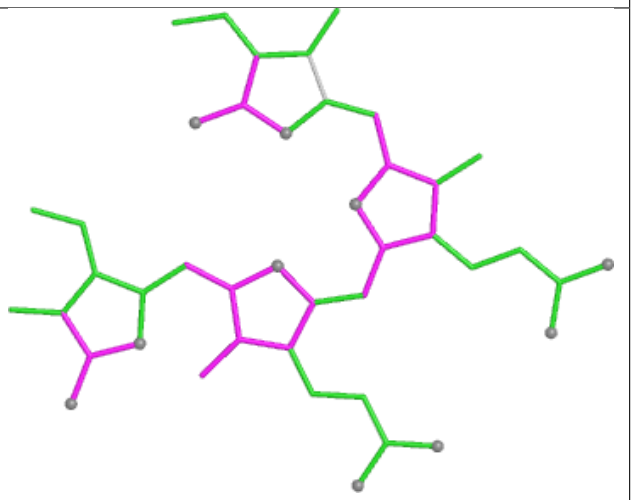


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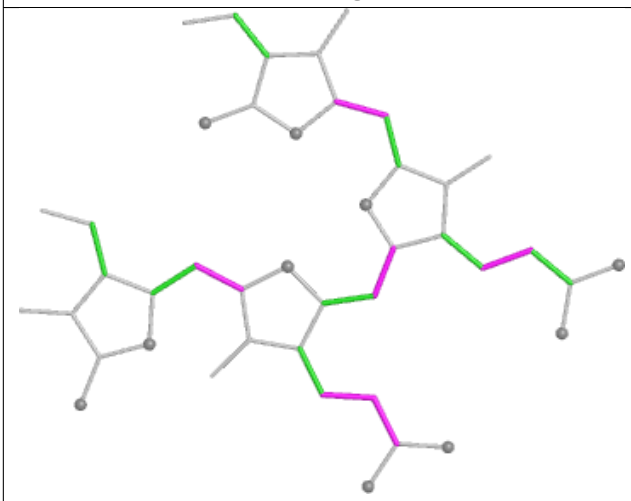
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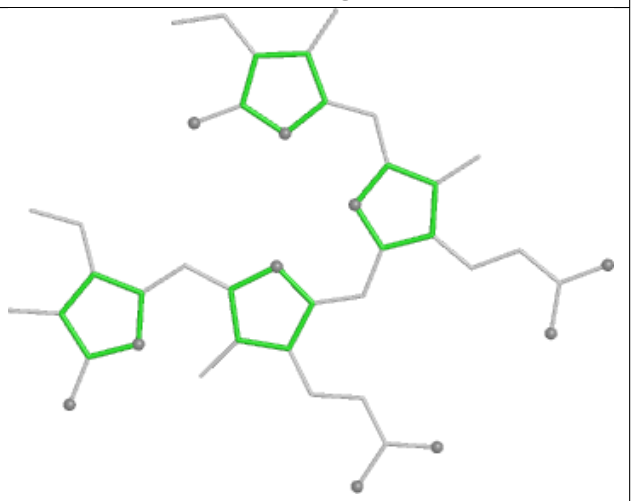
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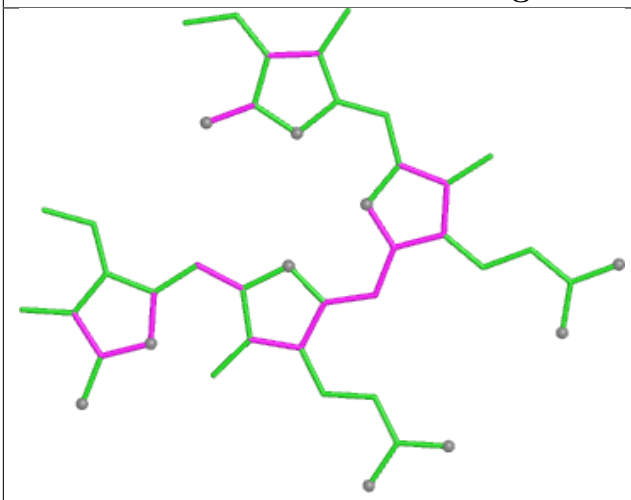


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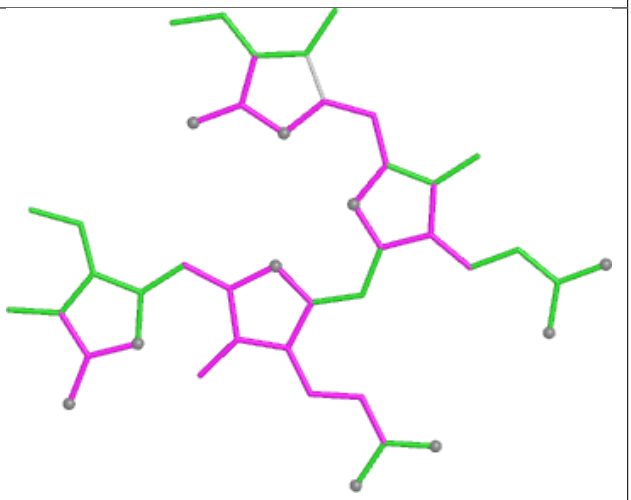


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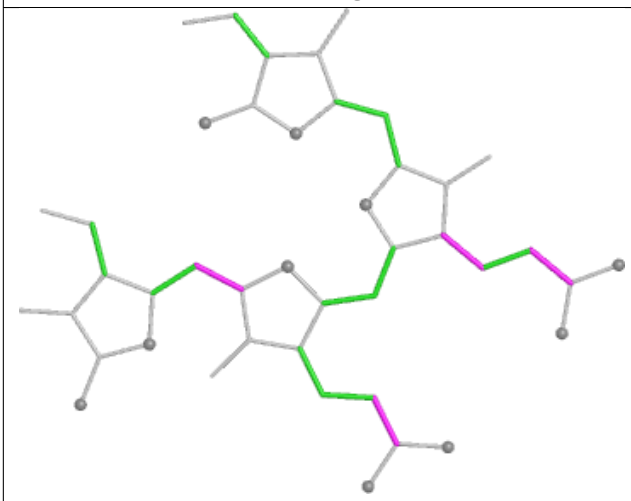
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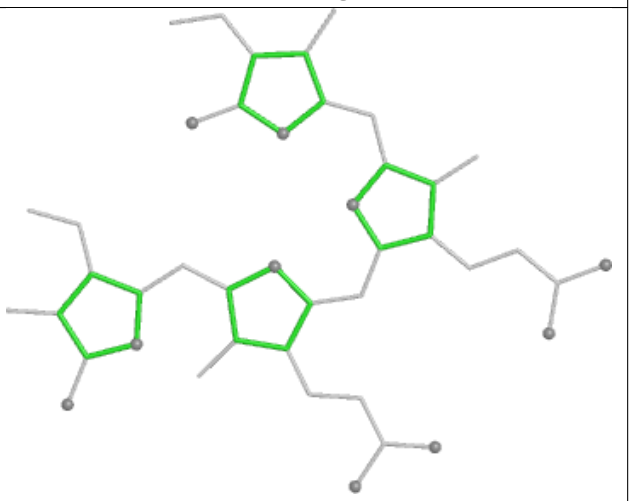
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Bond angles

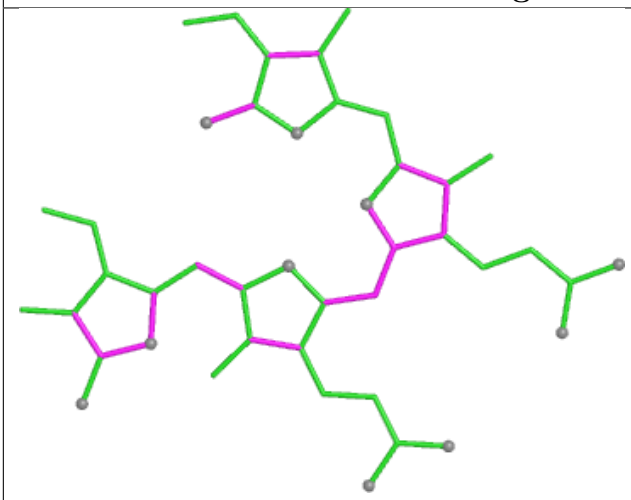


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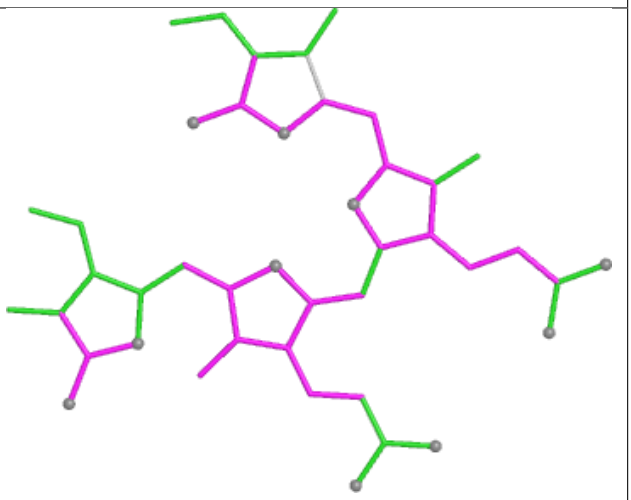


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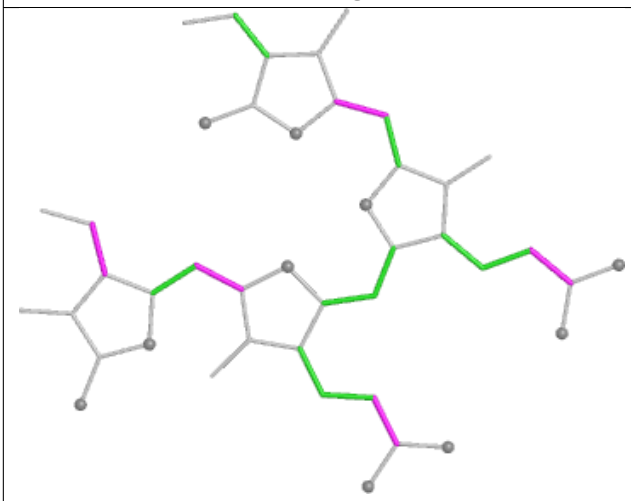
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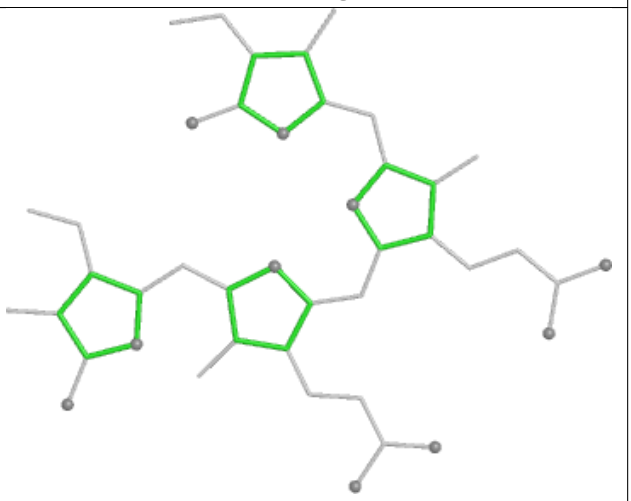
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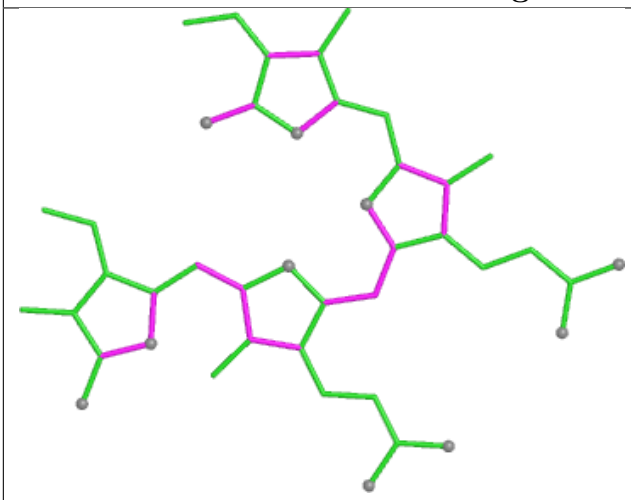


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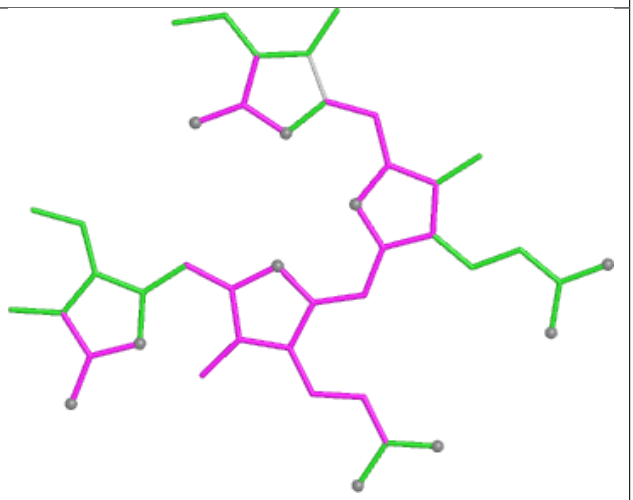


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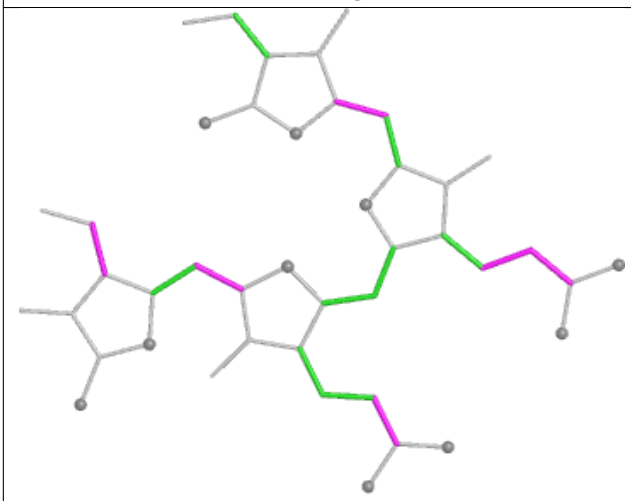
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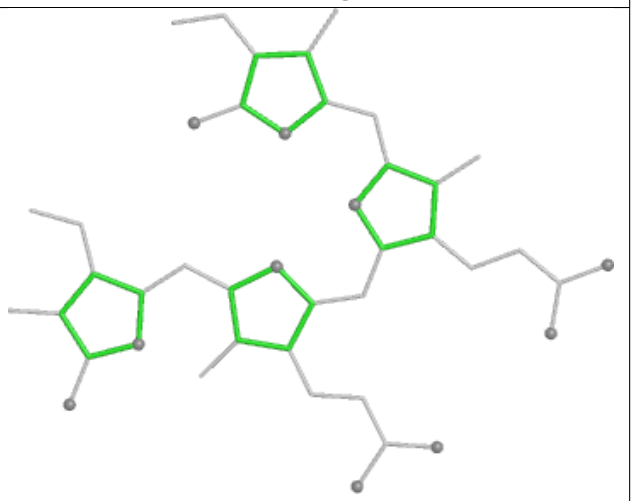
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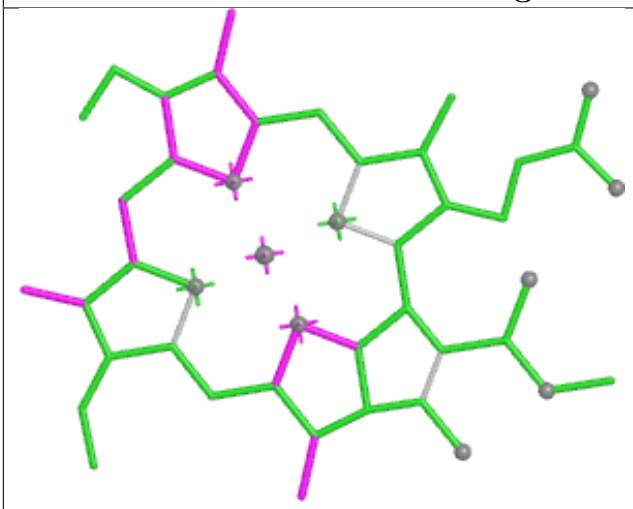


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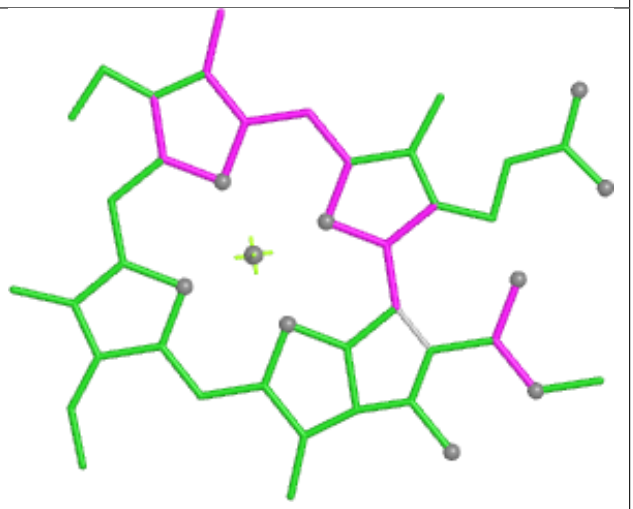


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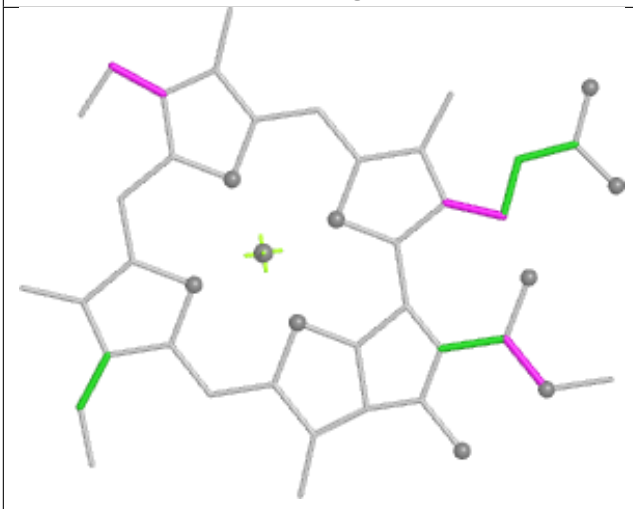
Ligand CLA K2 103



Bond lengths



Bond angles

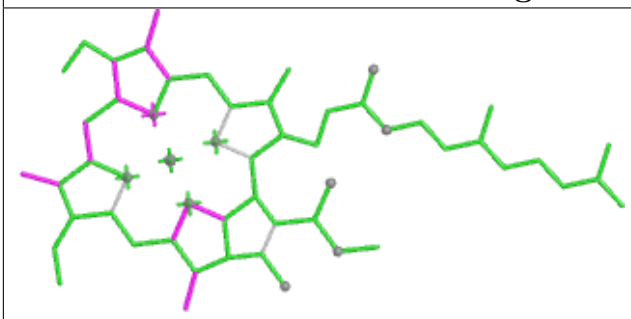


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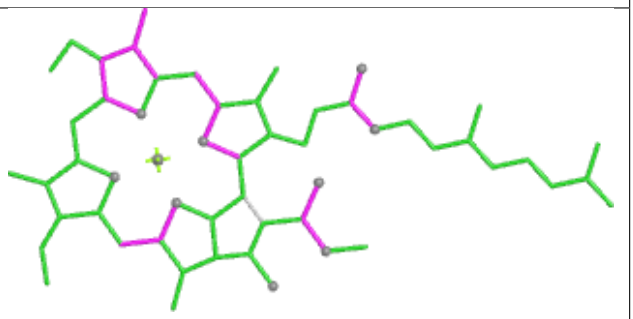


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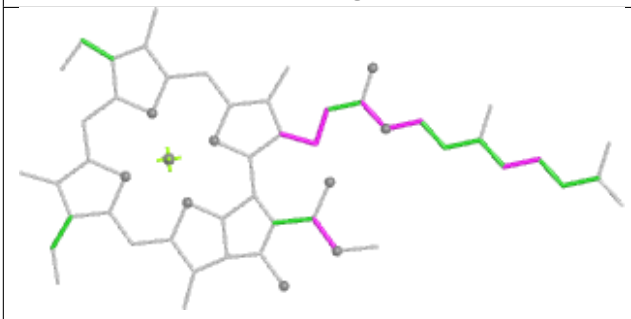
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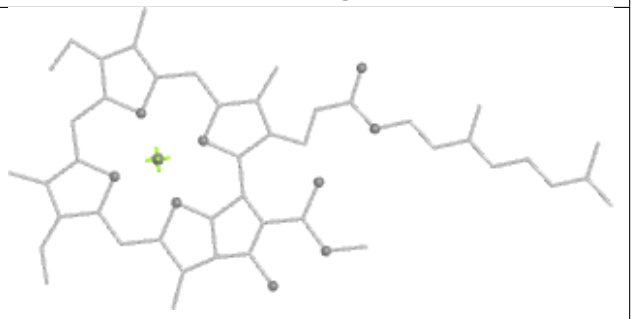
Bond lengths



Bond angles

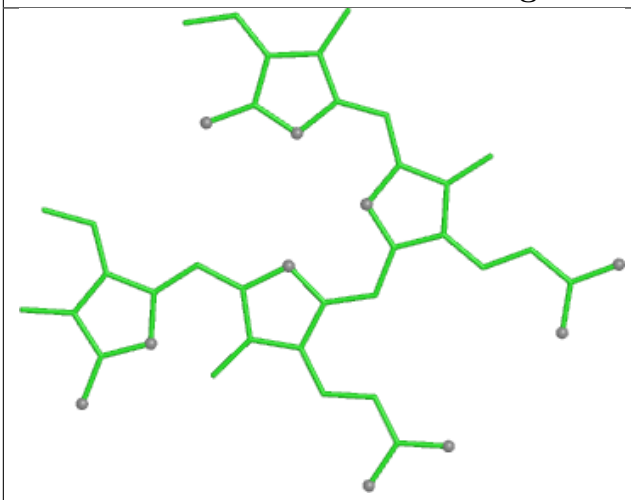


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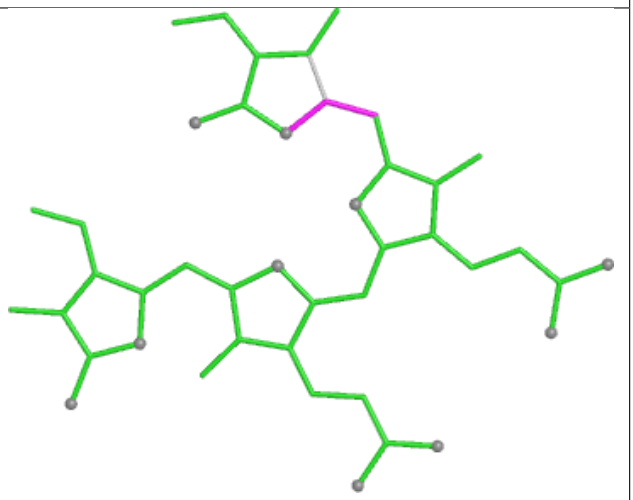


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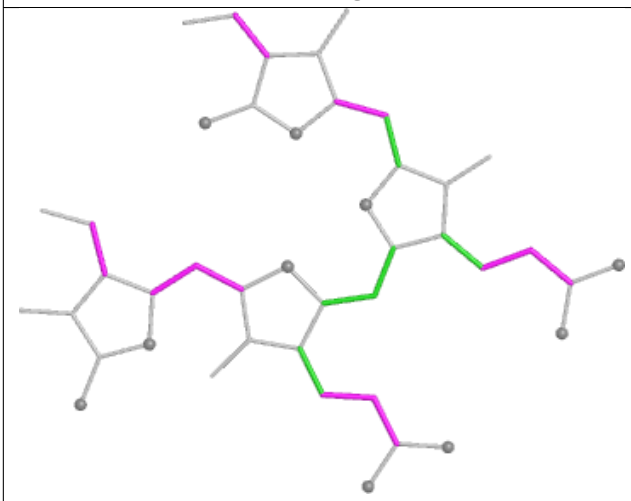
Ligand PEB IF 202



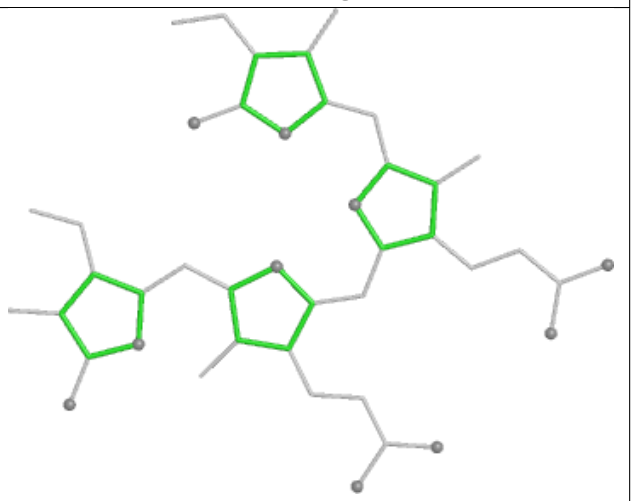
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Bond angles

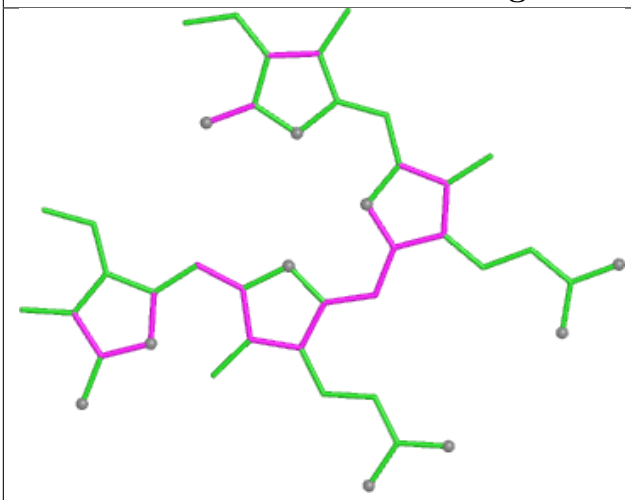


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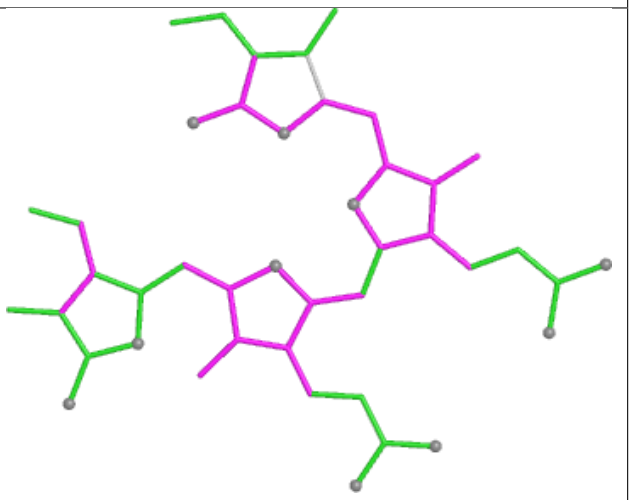


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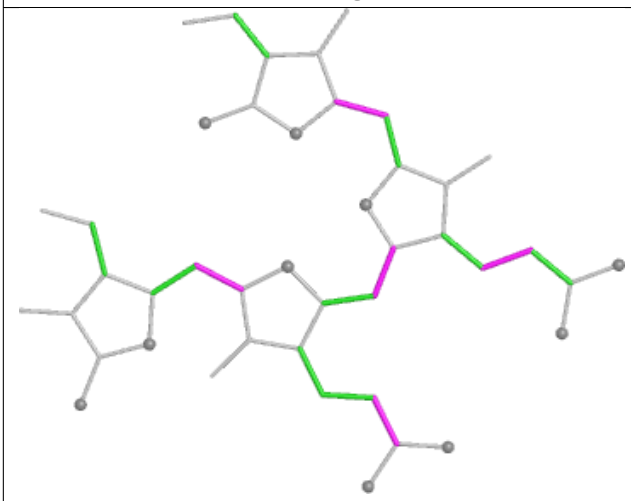
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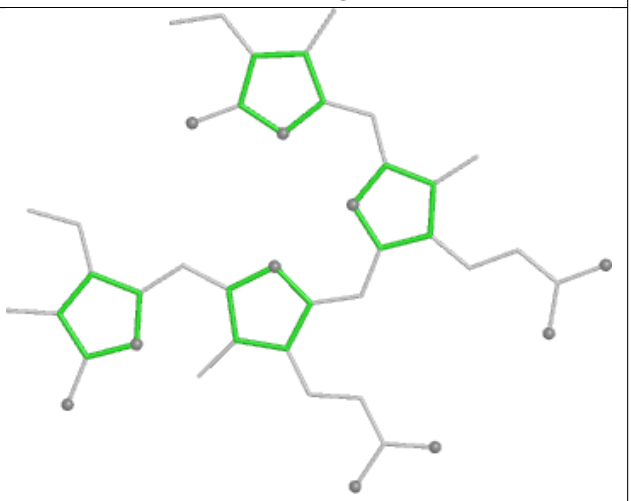
Bond lengths



Bond angles

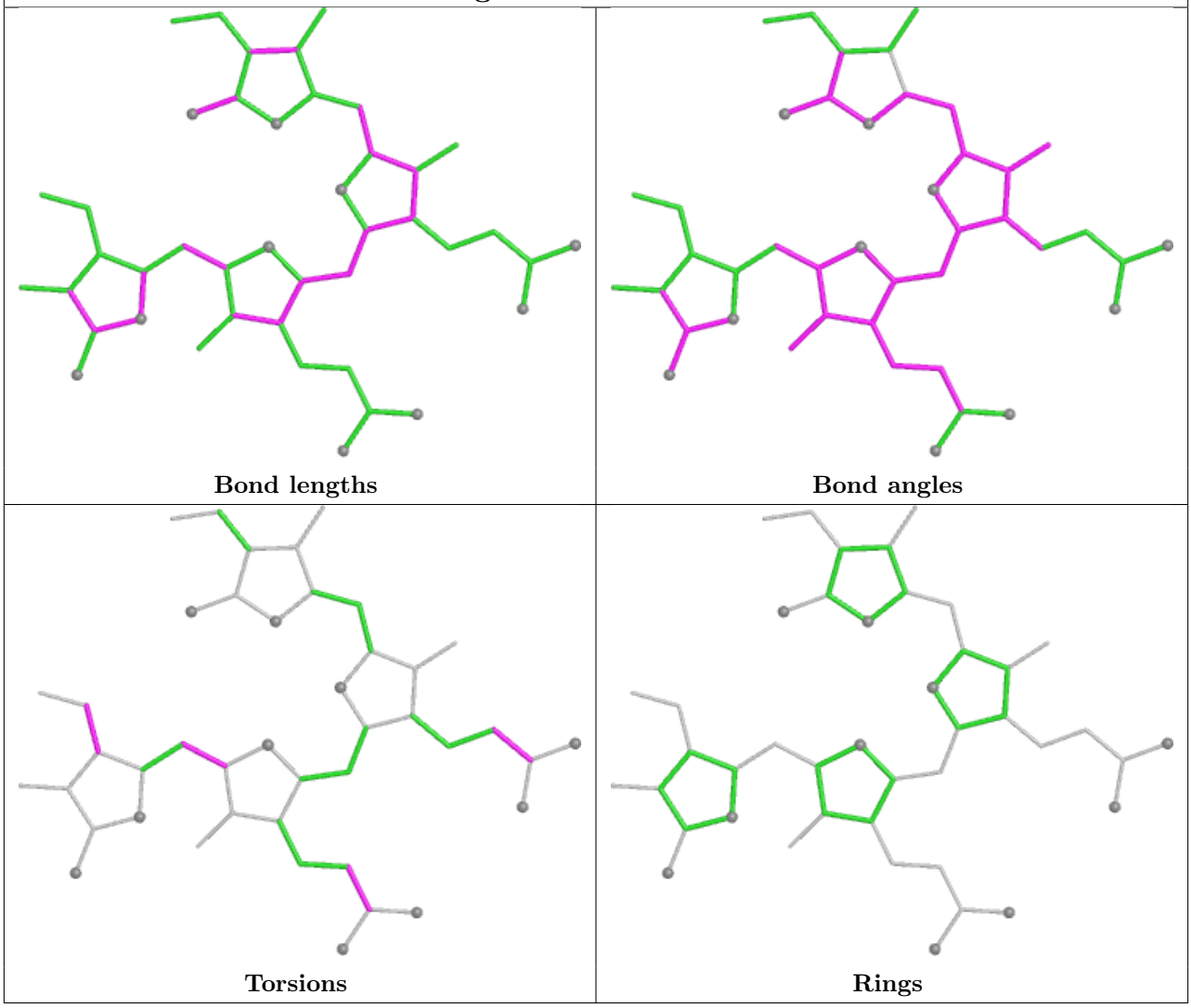


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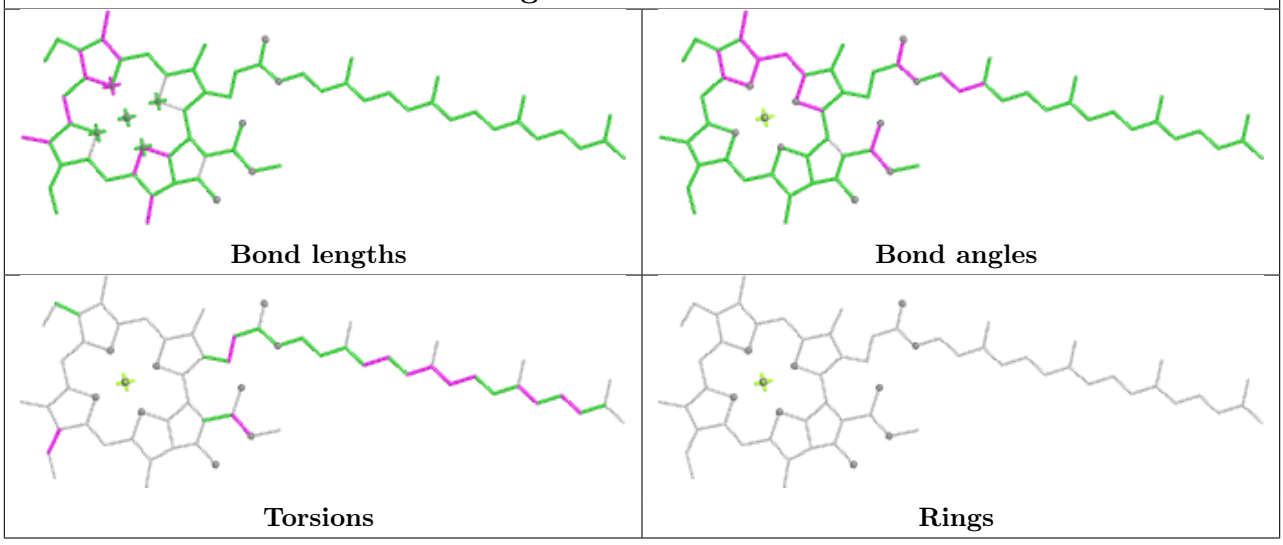


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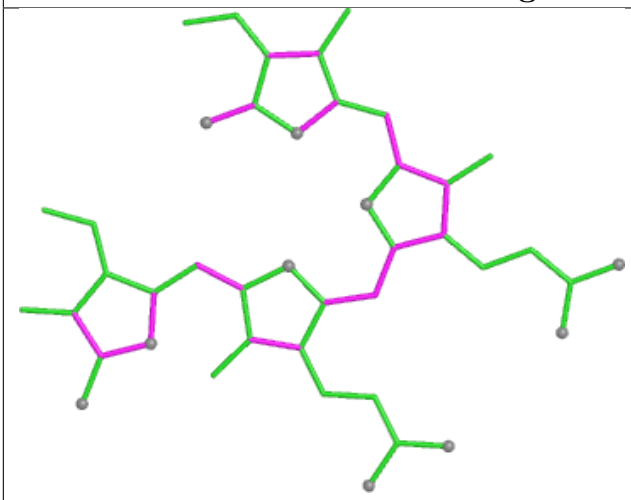
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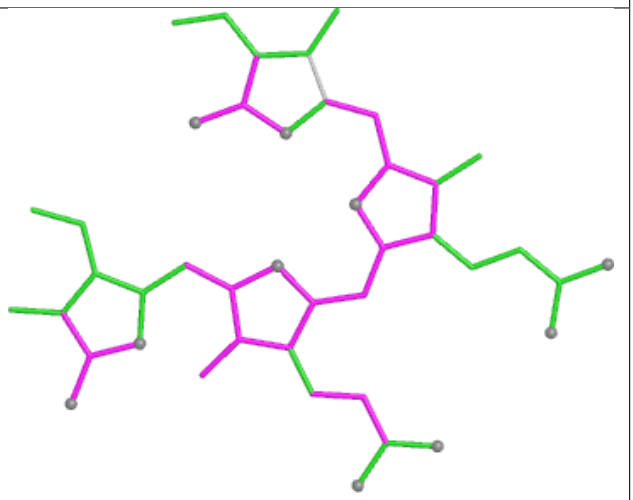
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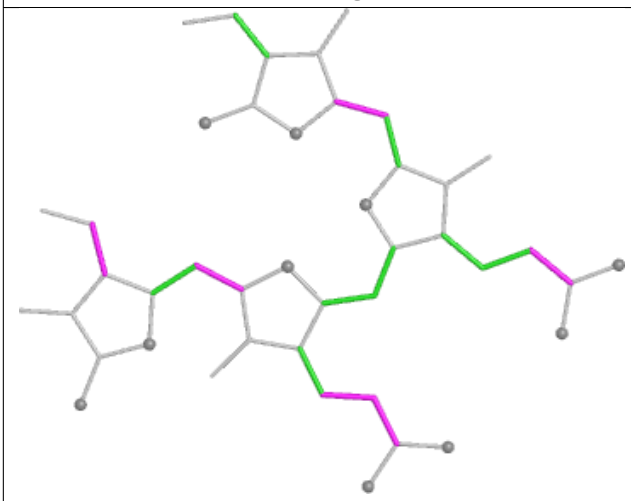
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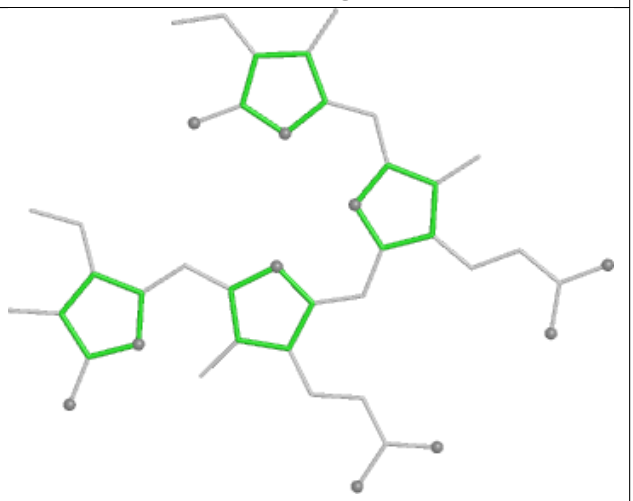
Bond lengths



Bond angles

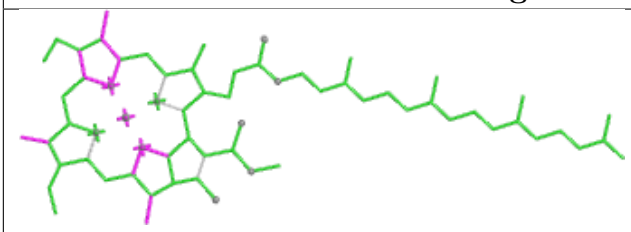


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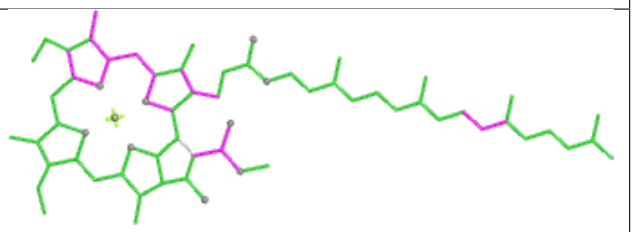


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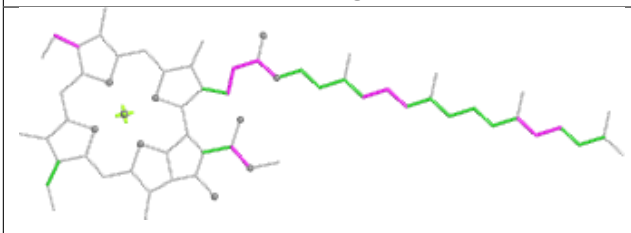
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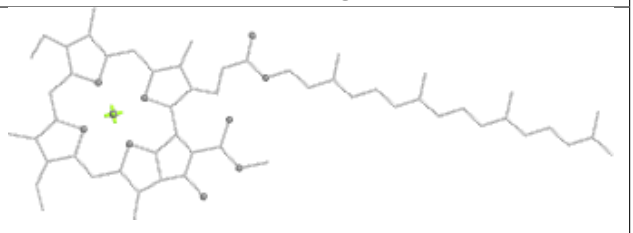
Bond lengths



Bond angles

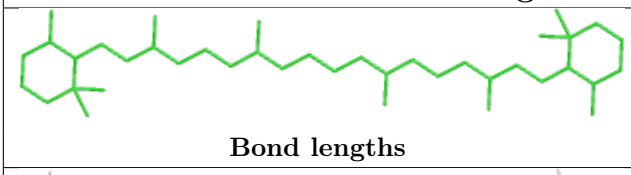


Torsions

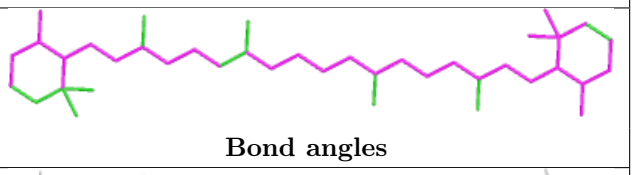


Rings

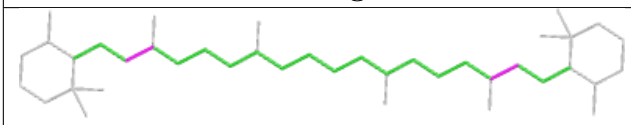
Ligand BCR cL 518



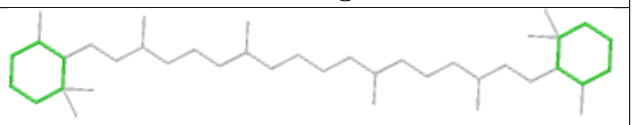
Bond lengths



Bond angles

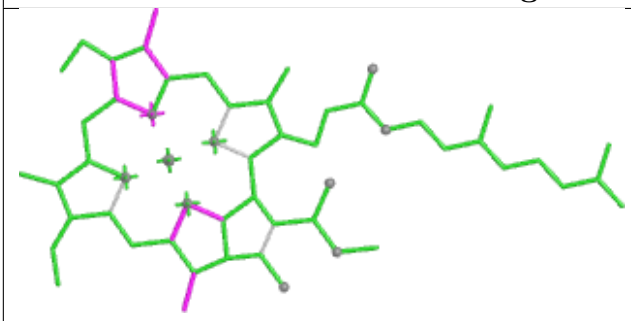


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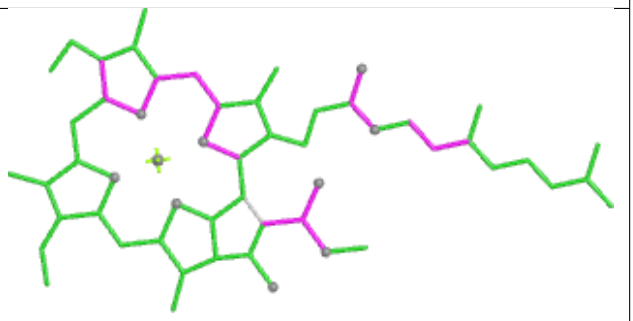


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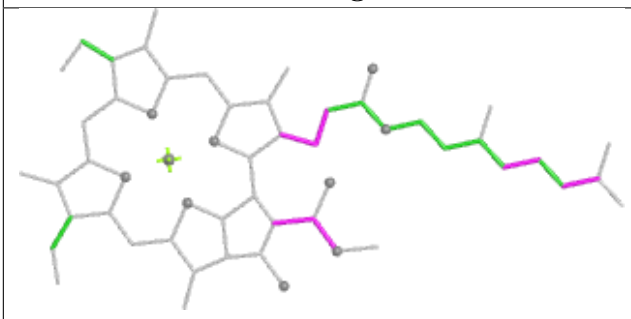
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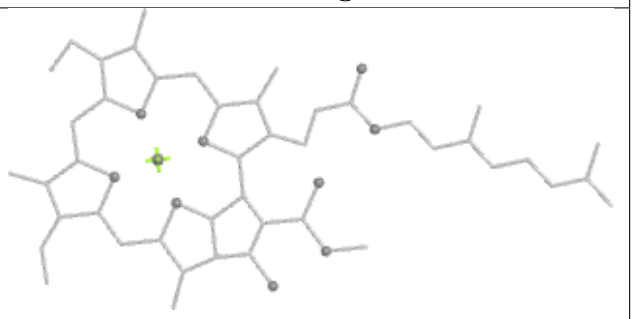
Bond lengths



Bond angles

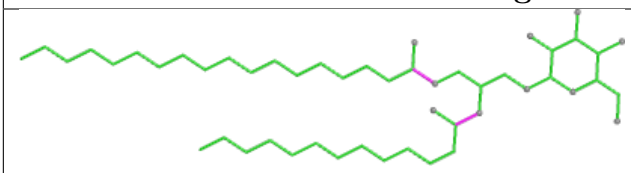


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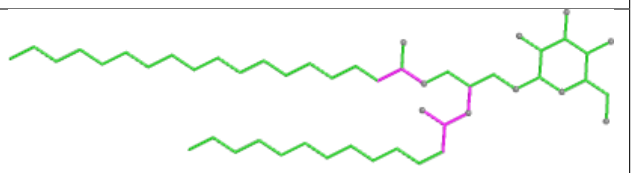


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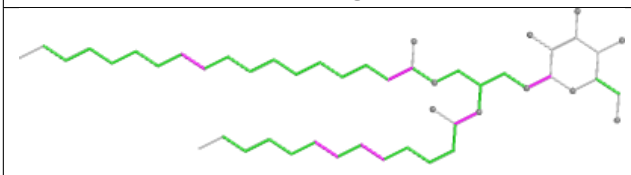
Ligand LMG x6 601



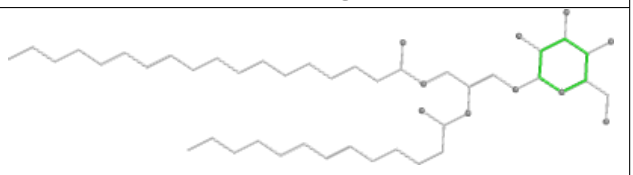
Bond lengths



Bond angles

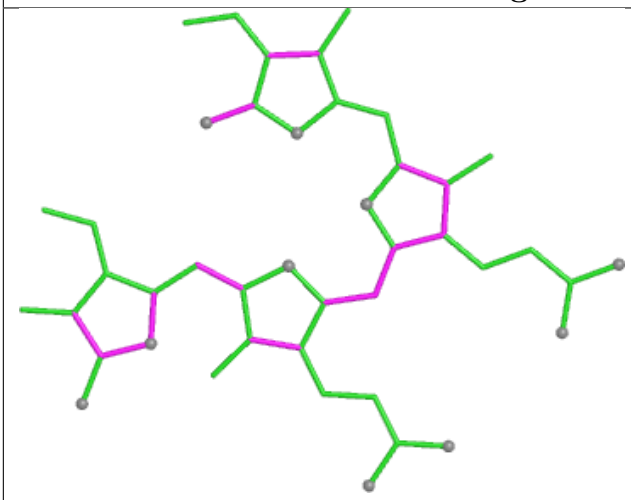


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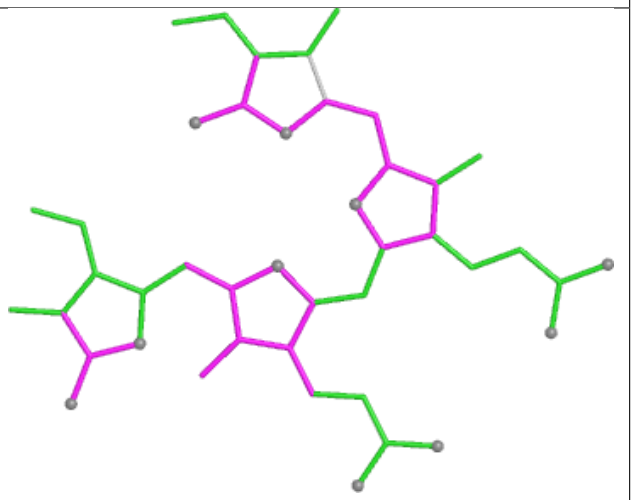


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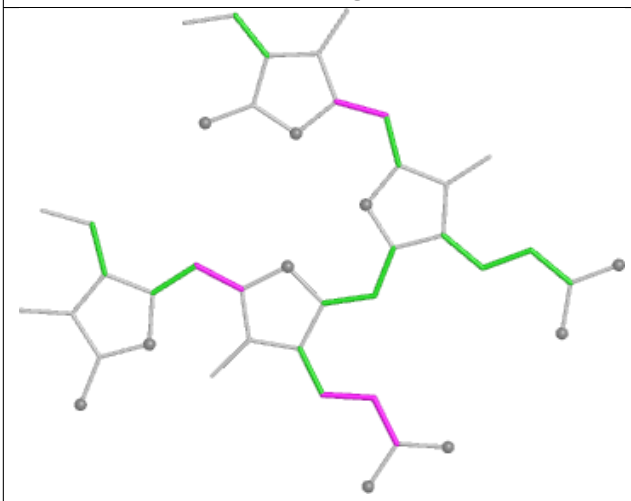
Ligand PEB W9 203



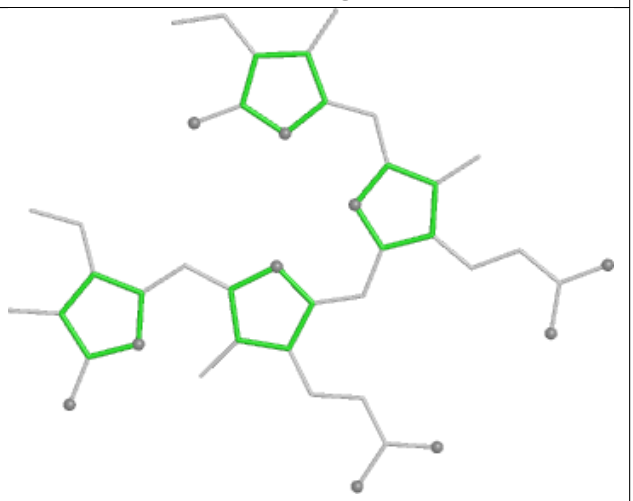
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Bond angles

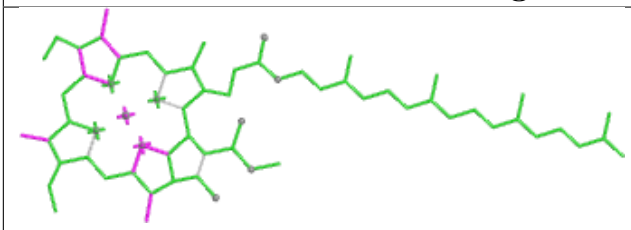


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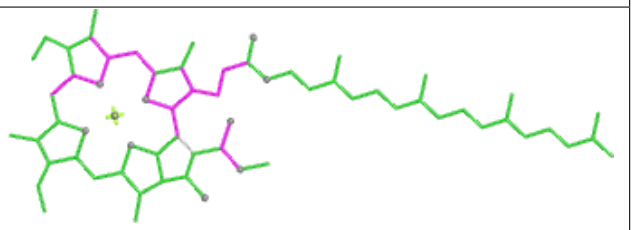


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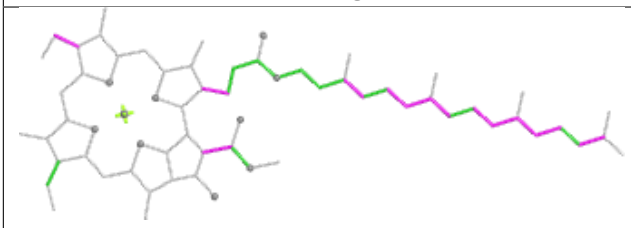
Ligand CLA BN 825



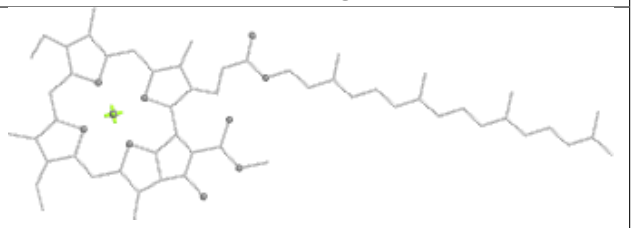
Bond lengths



Bond angles

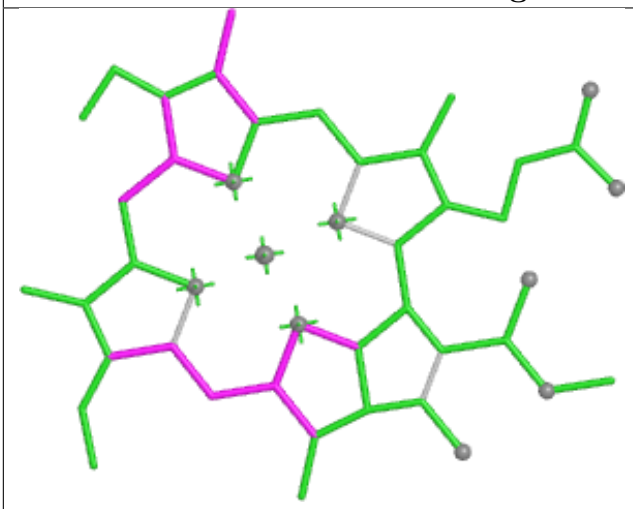


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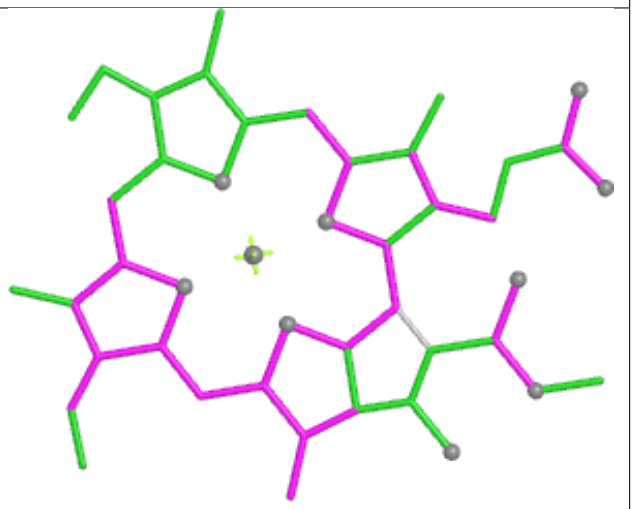


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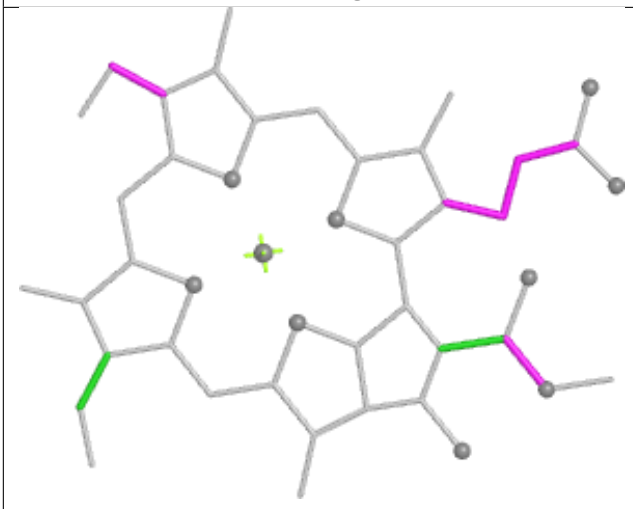
Ligand CLA AN 852



Bond lengths



Bond angles

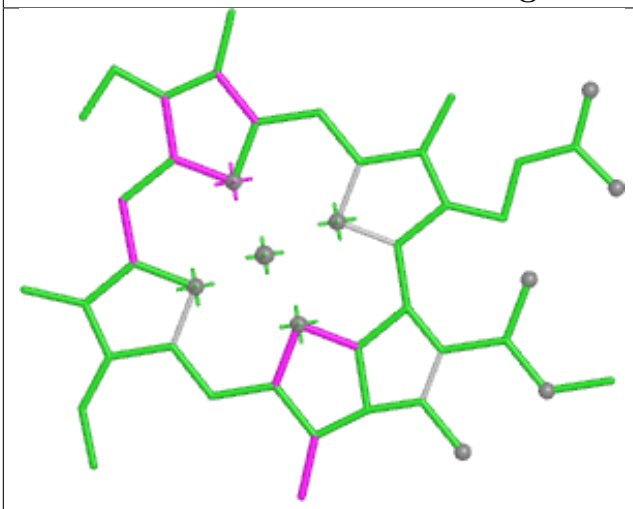


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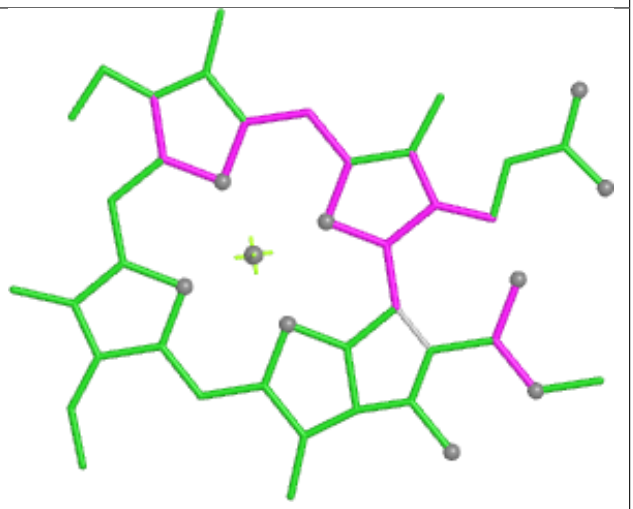


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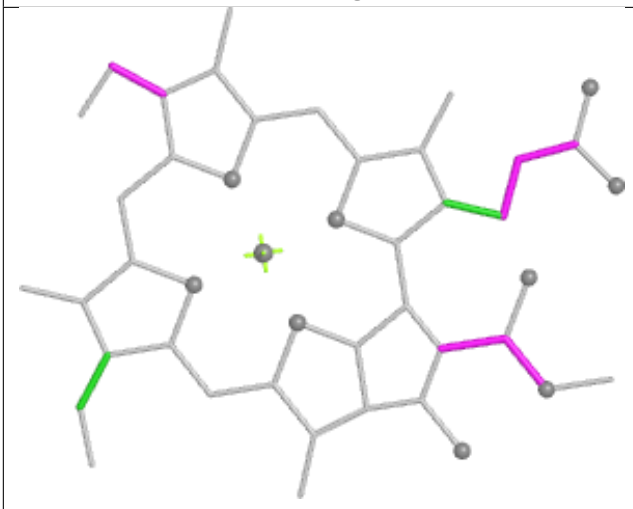
Ligand CLA 62 306



Bond lengths



Bond angles

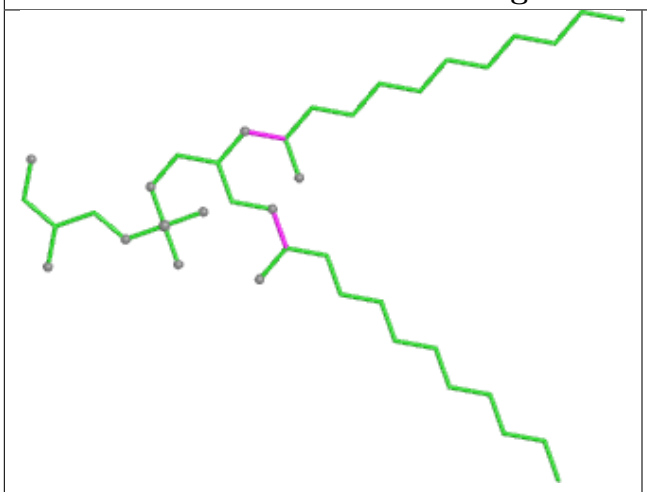


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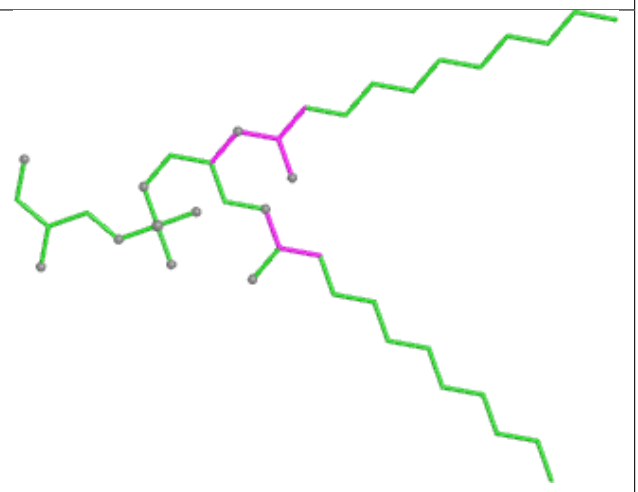


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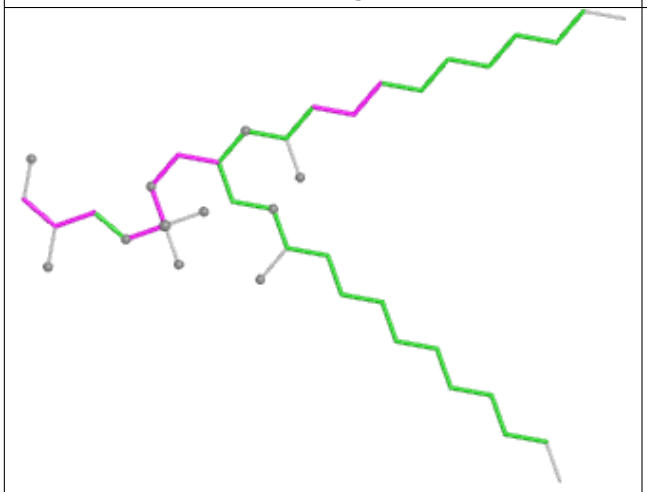
Ligand LHG M6 101



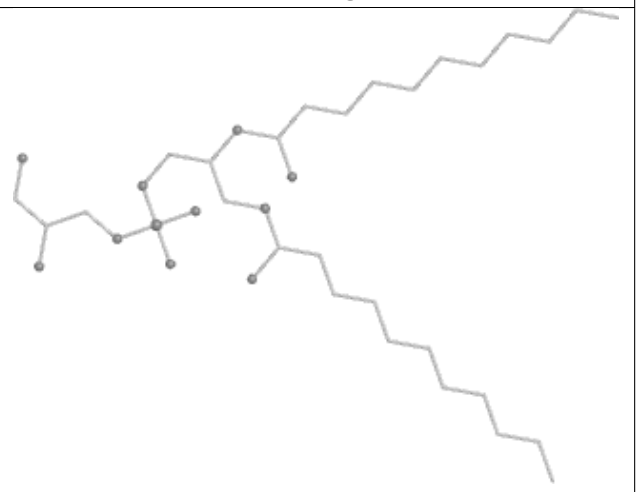
Bond lengths



Bond angles

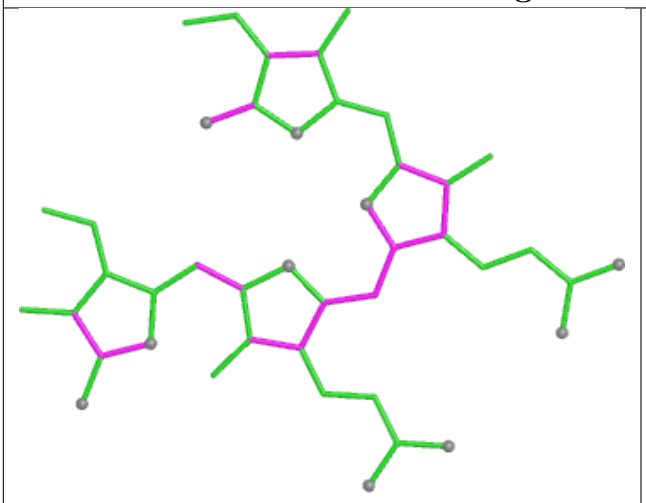


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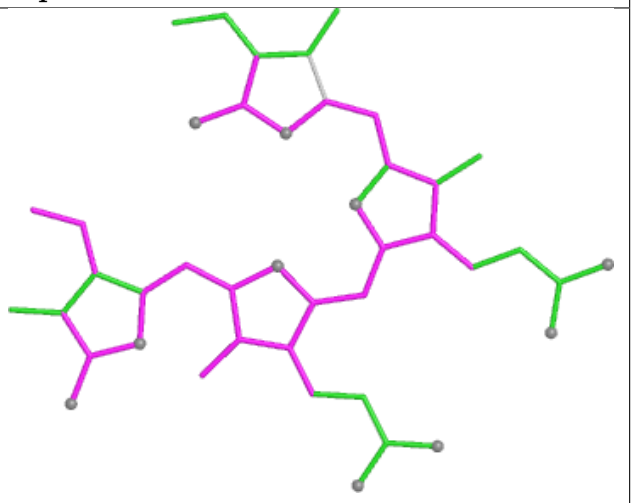


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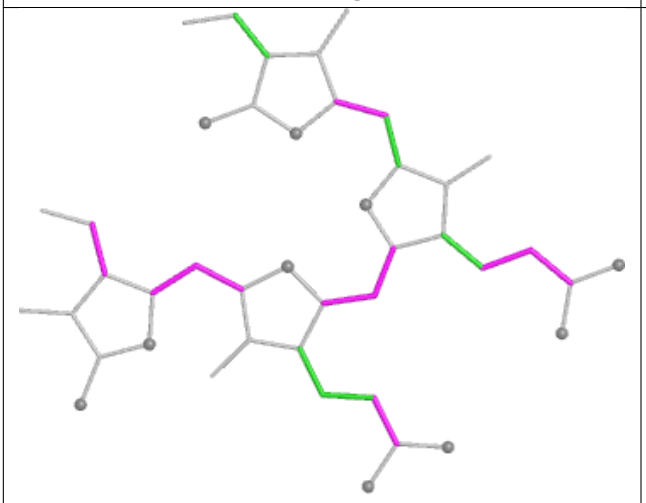
Ligand PEB pC 202



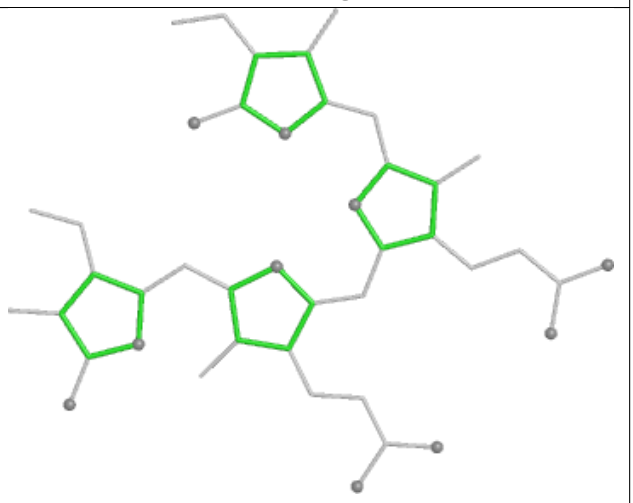
Bond lengths



Bond angles

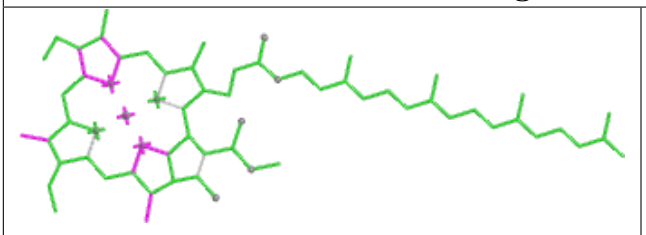


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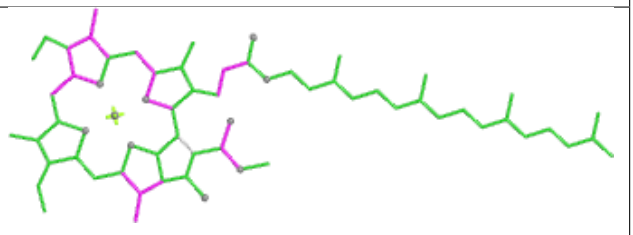


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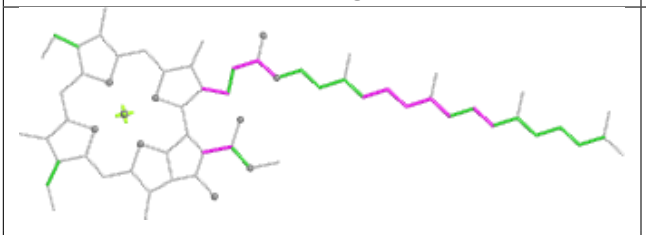
Ligand CLA BL 603



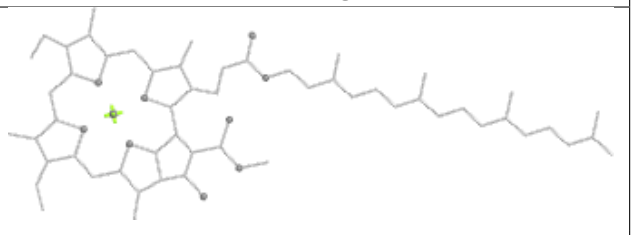
Bond lengths



Bond angles

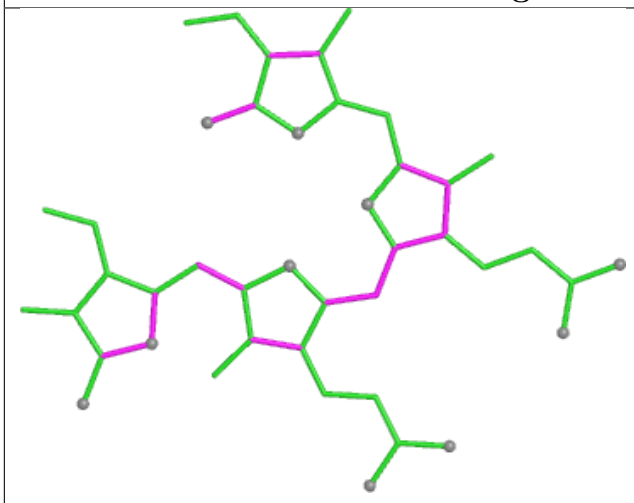


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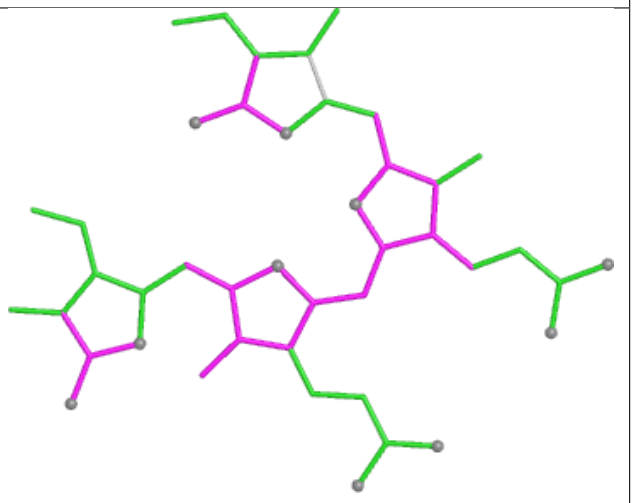


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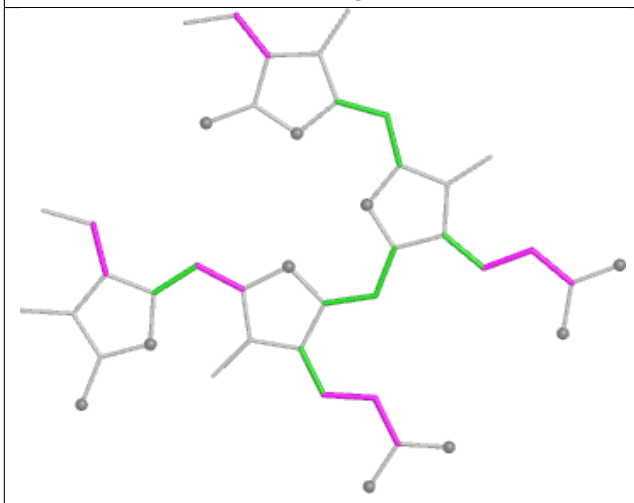
Ligand PEB BD 203



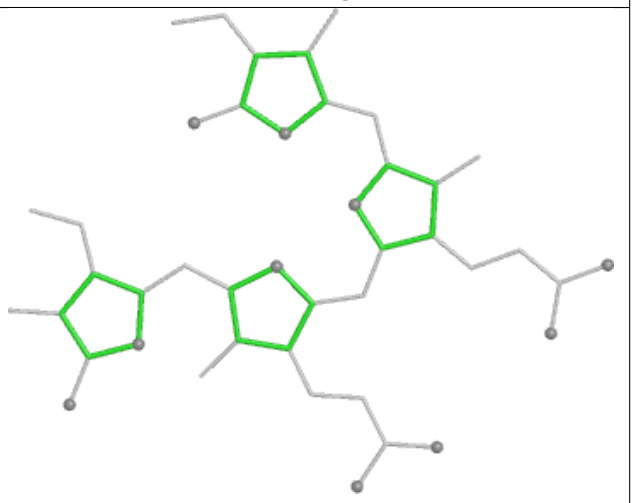
Bond lengths



Bond angles

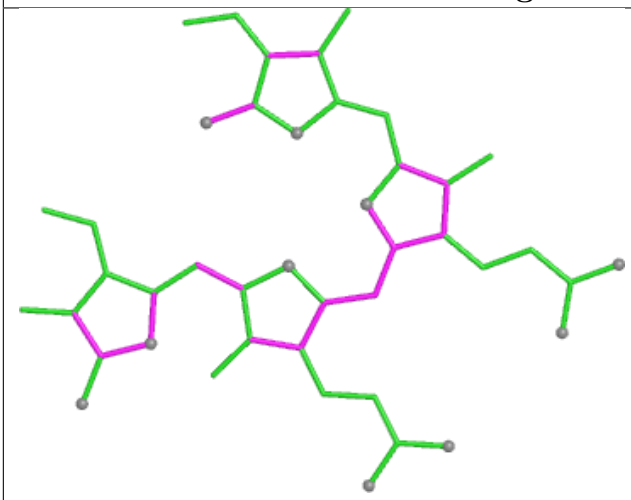


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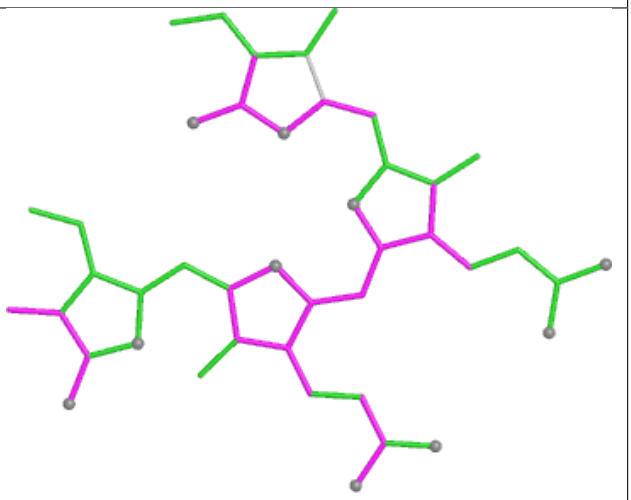


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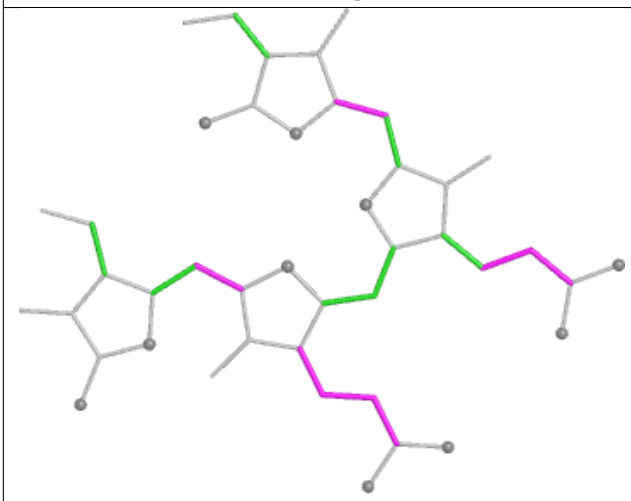
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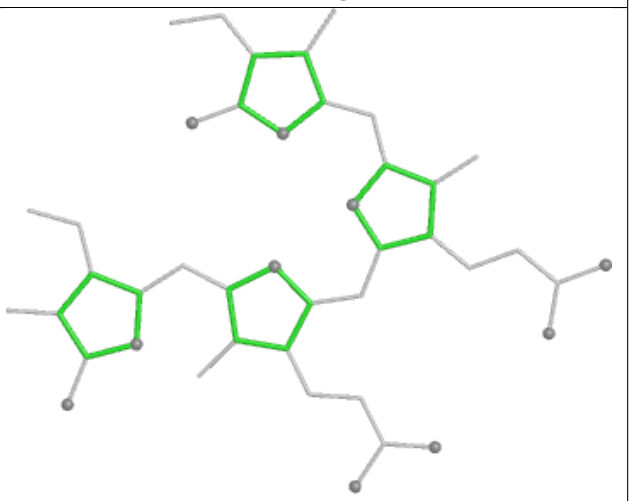
Bond lengths



Bond angles

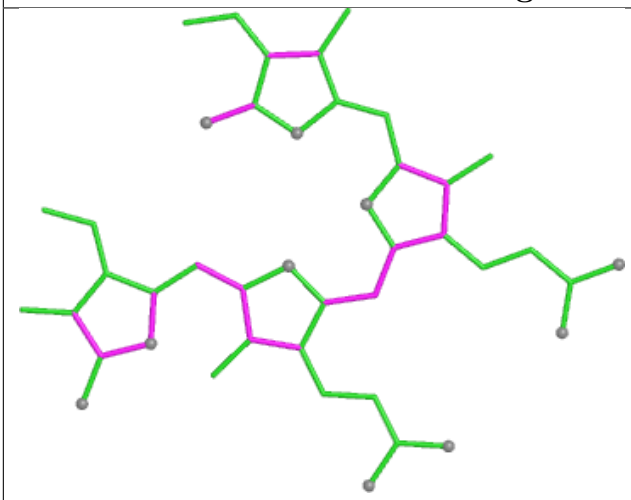


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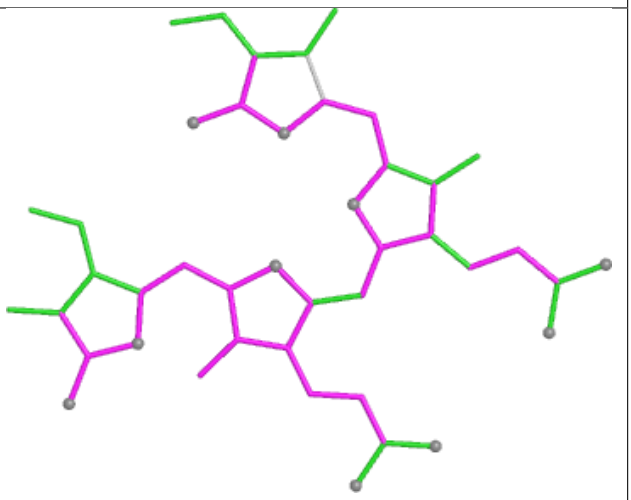


Rings

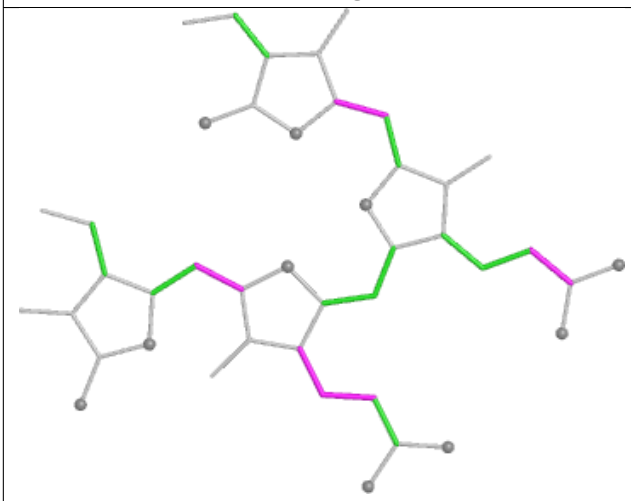
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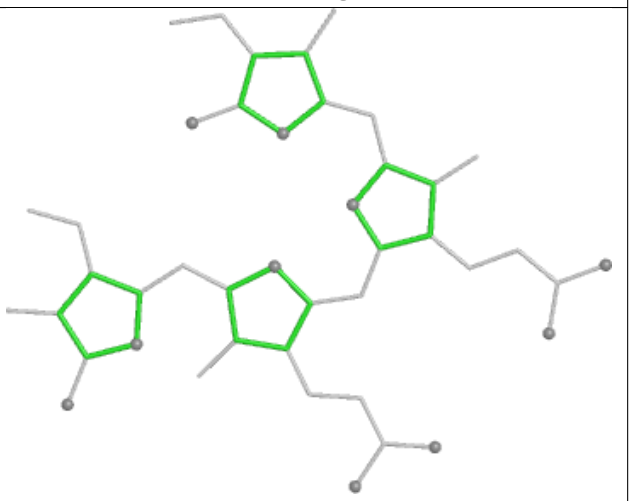
Bond lengths



Bond angles

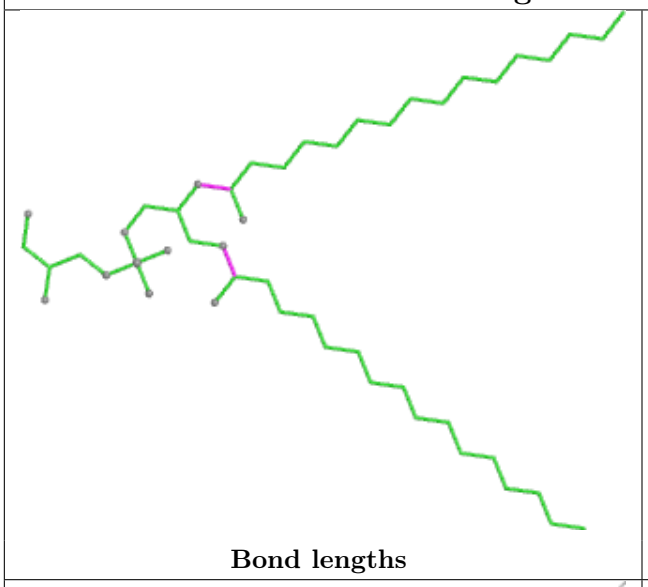


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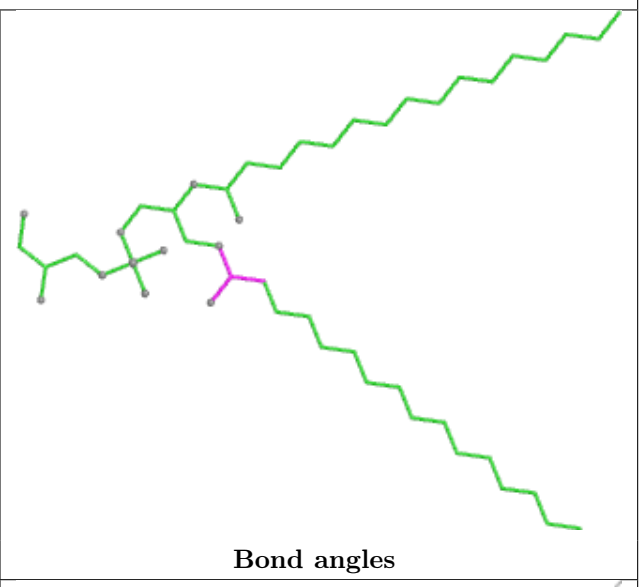


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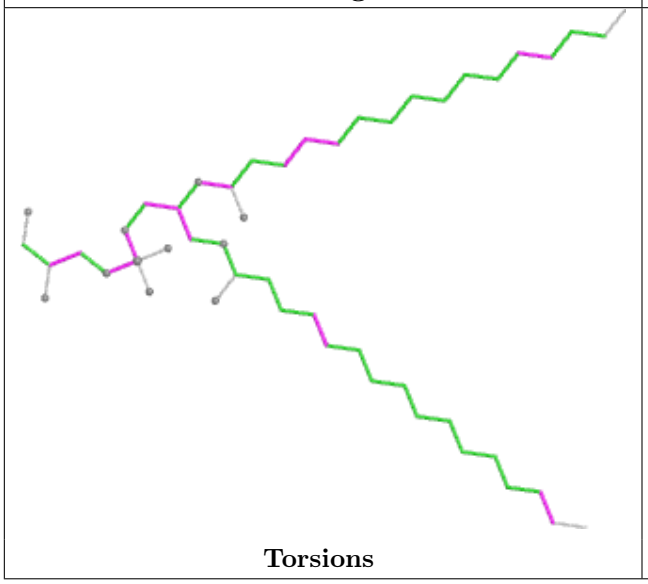
Ligand LHG A2 843



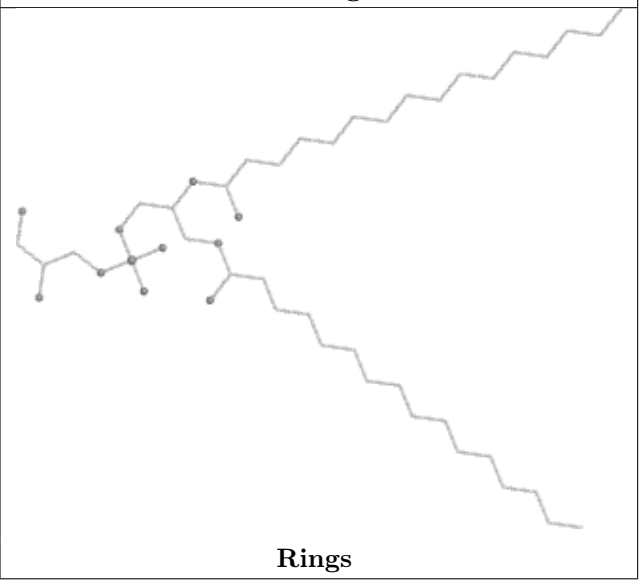
Bond lengths



Bond angles

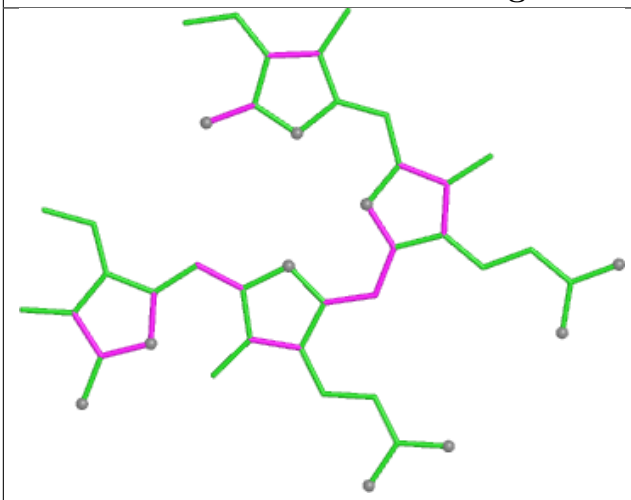


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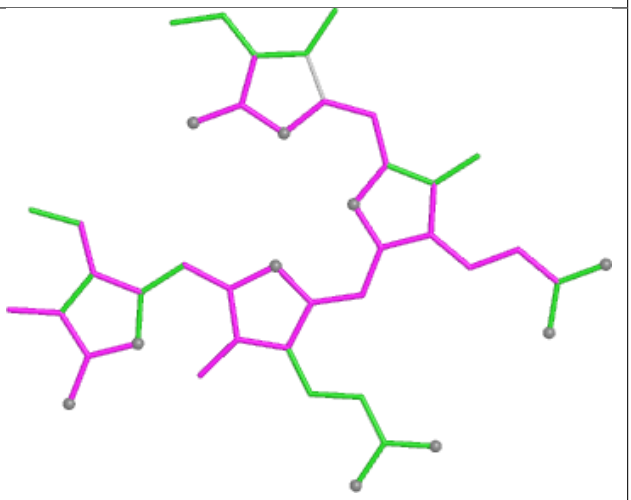


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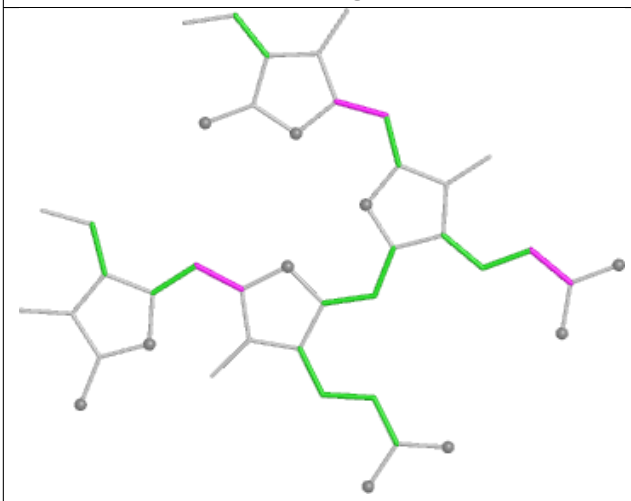
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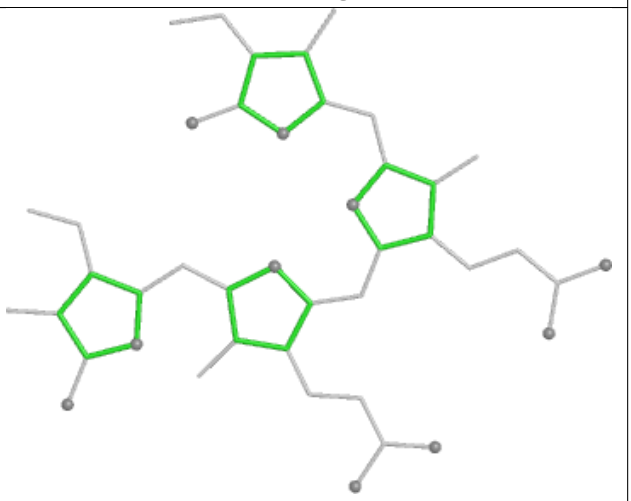
Bond lengths



Bond angles

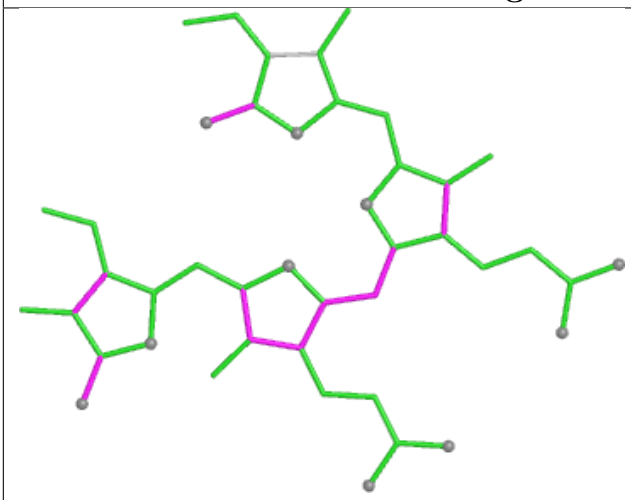


Torsions

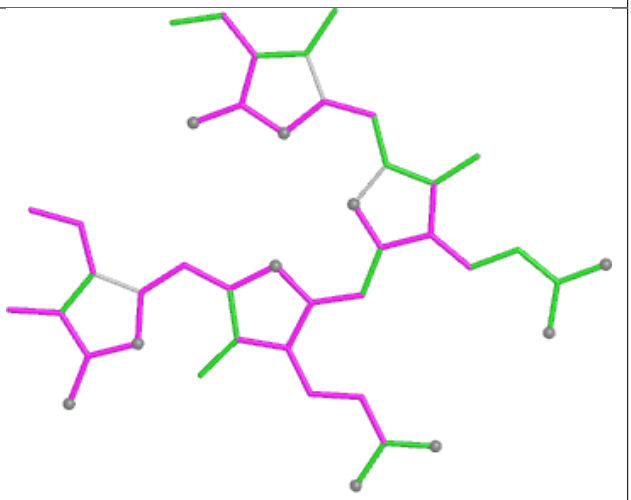


Rings

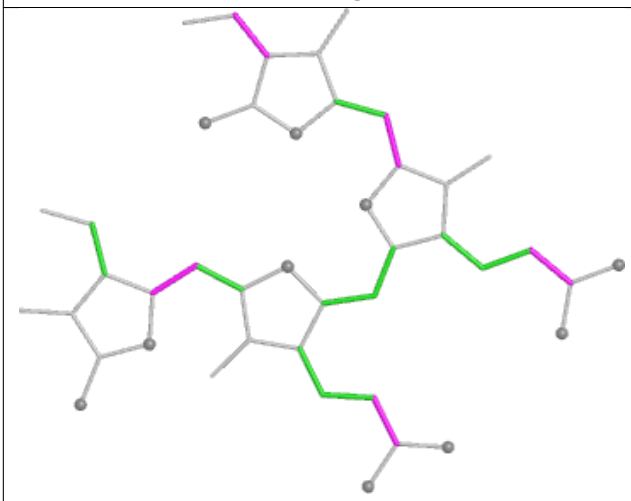
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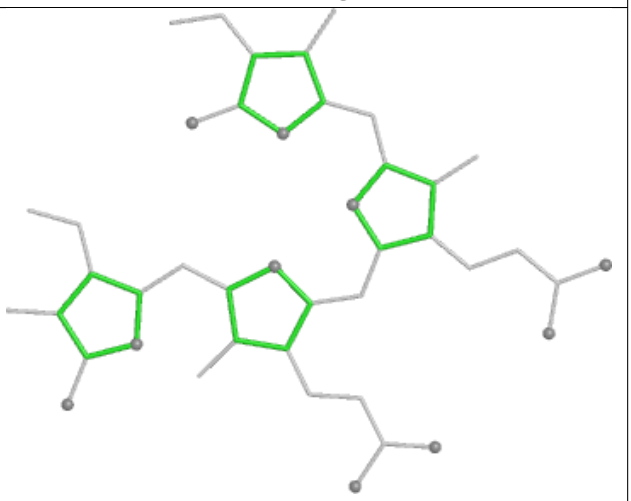
Bond lengths



Bond angles

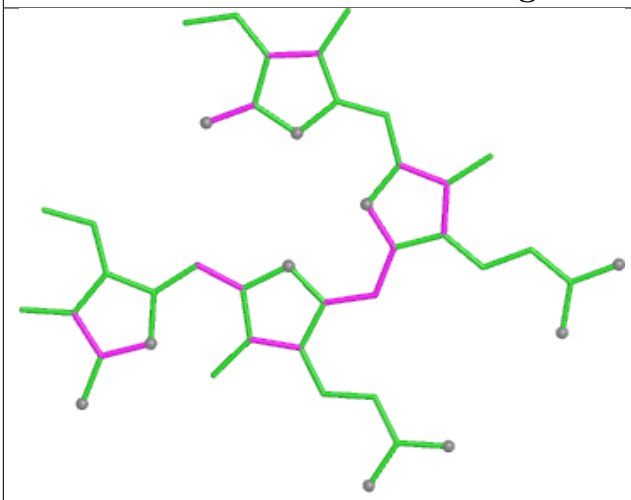


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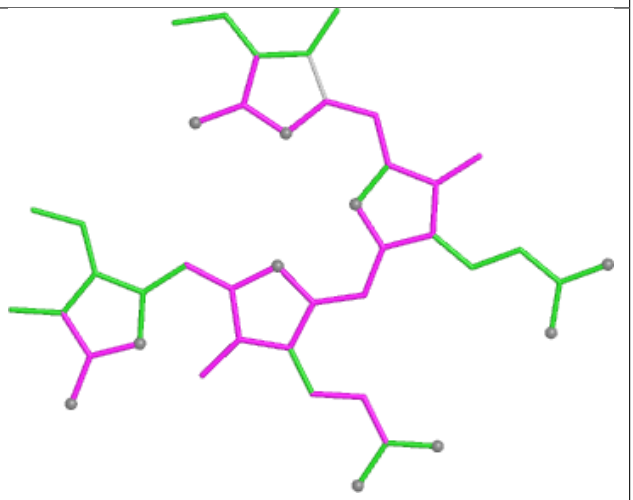


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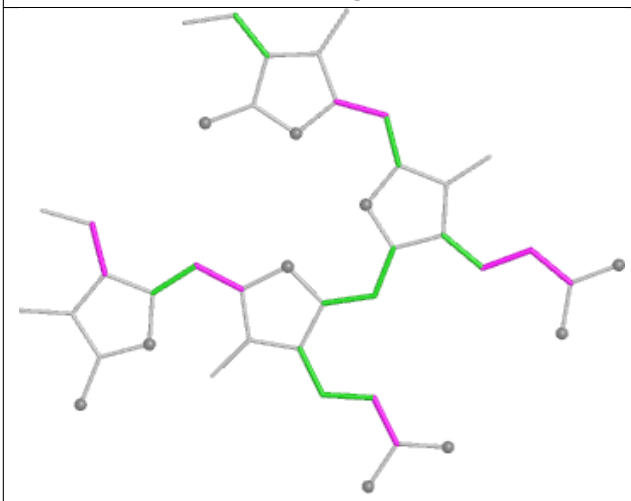
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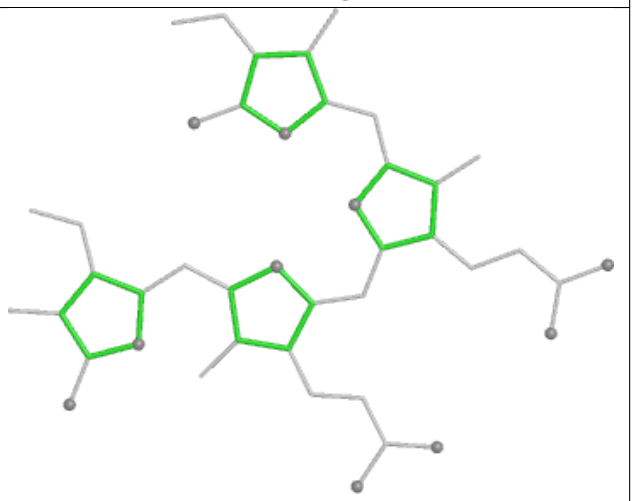
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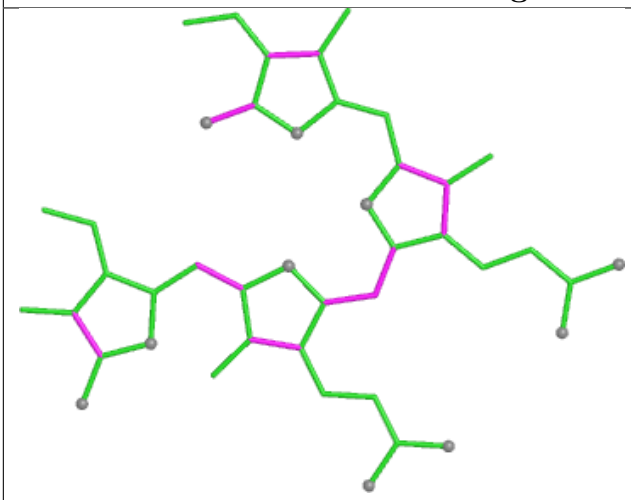


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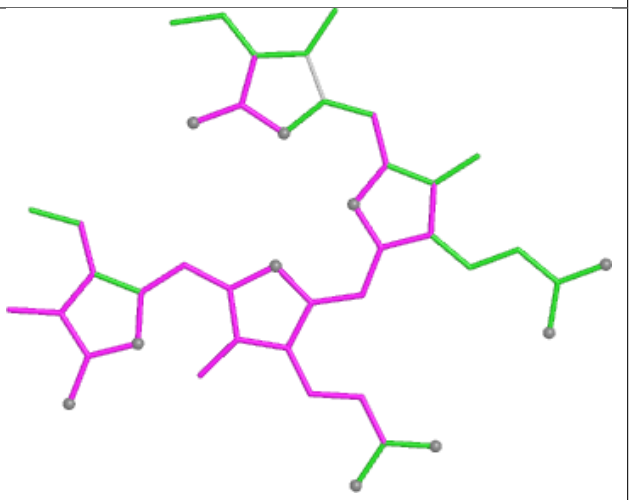


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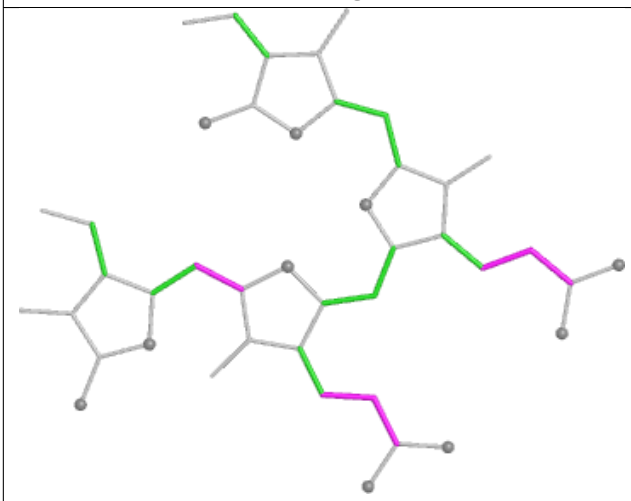
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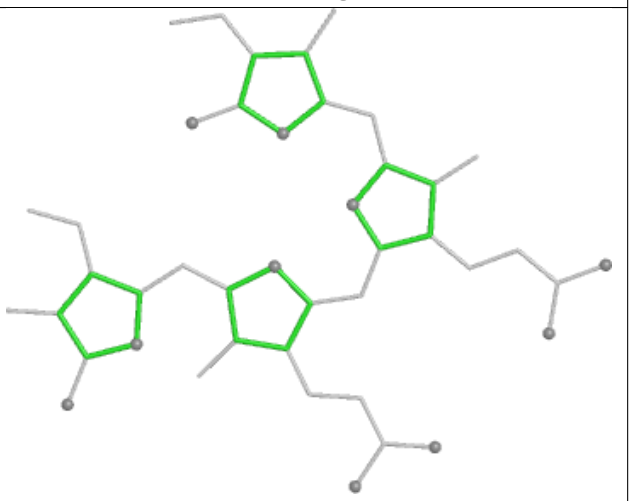
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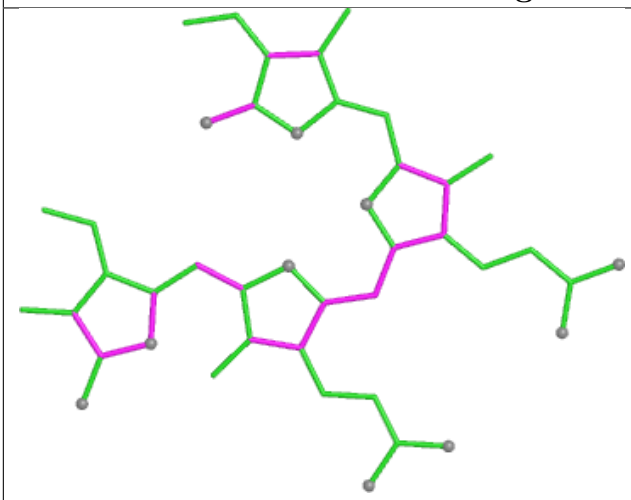


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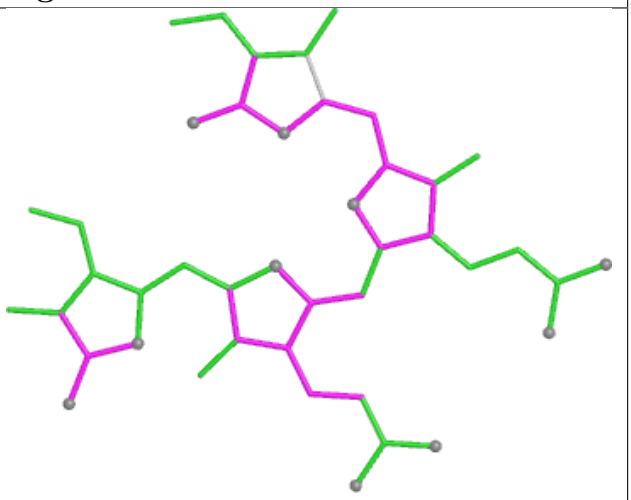


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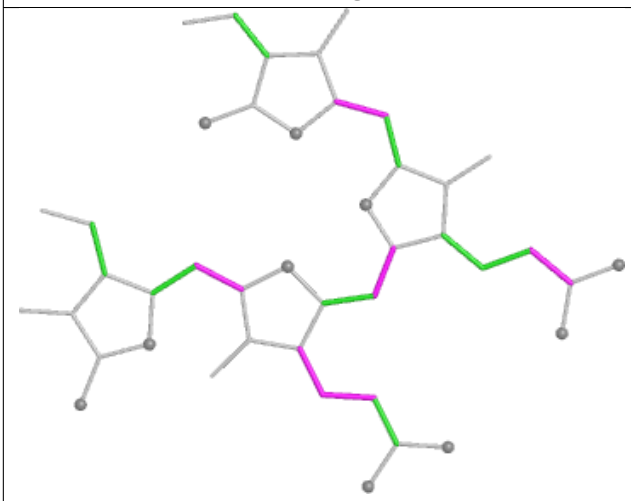
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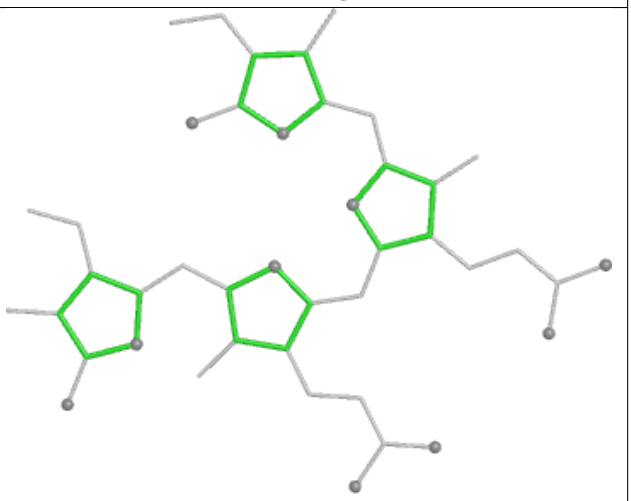
Bond lengths



Bond angles



Torsions

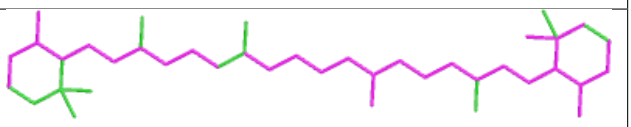


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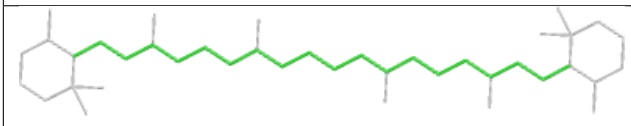
Ligand BCR B6 601



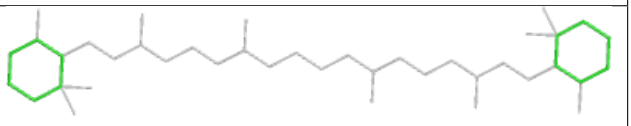
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Bond angles

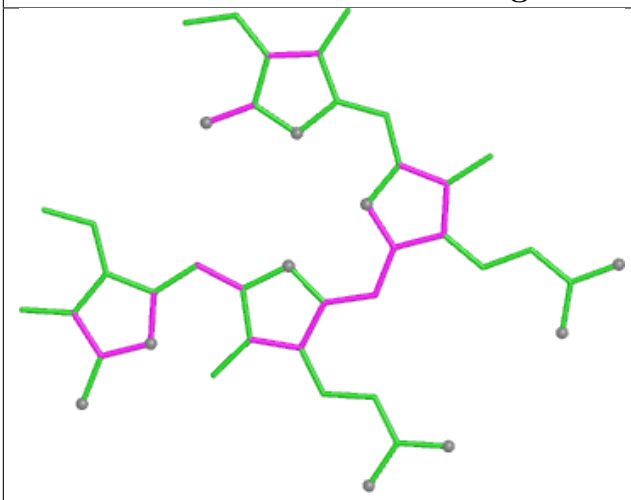


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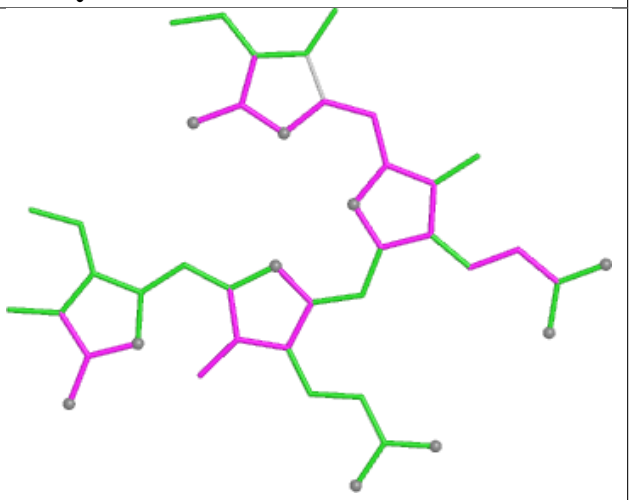


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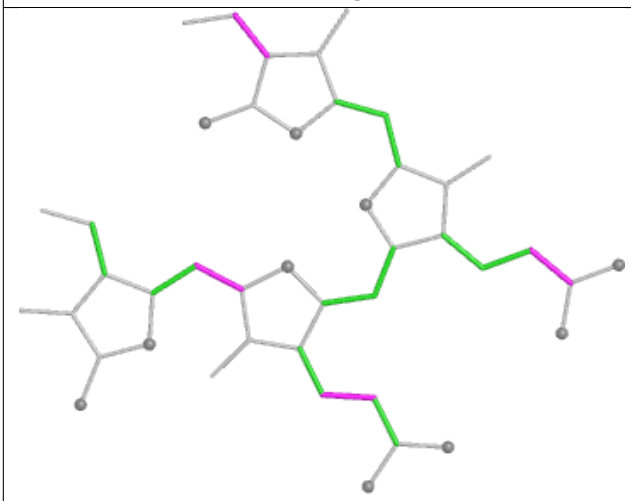
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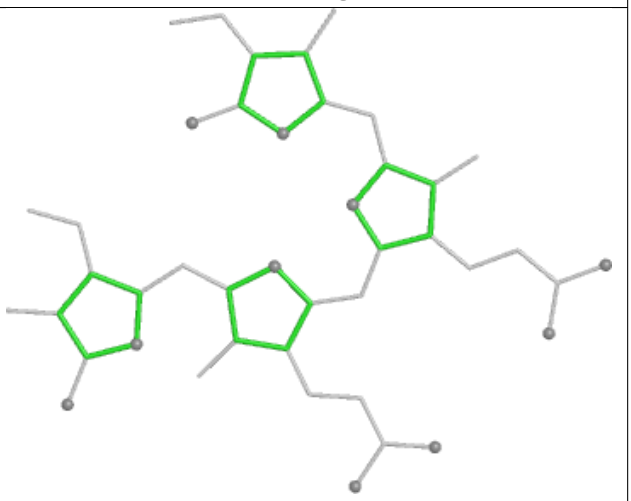
Bond lengths



Bond angles

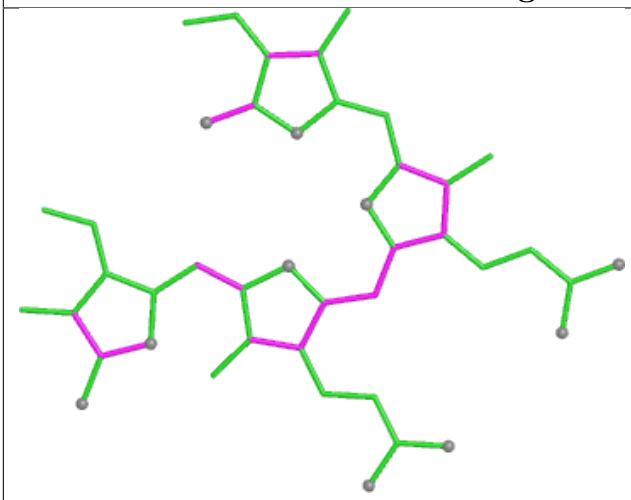


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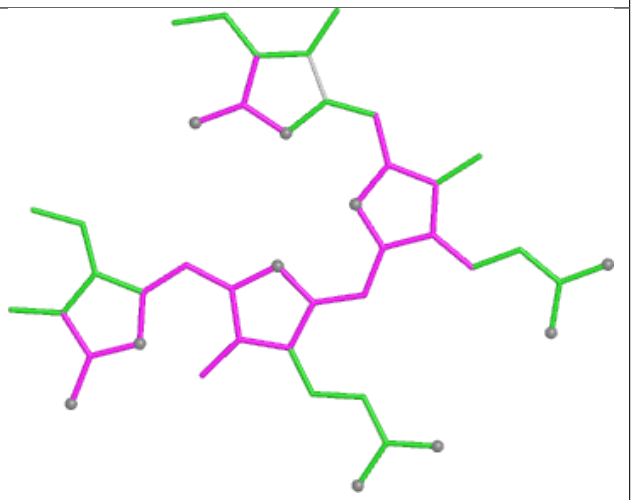


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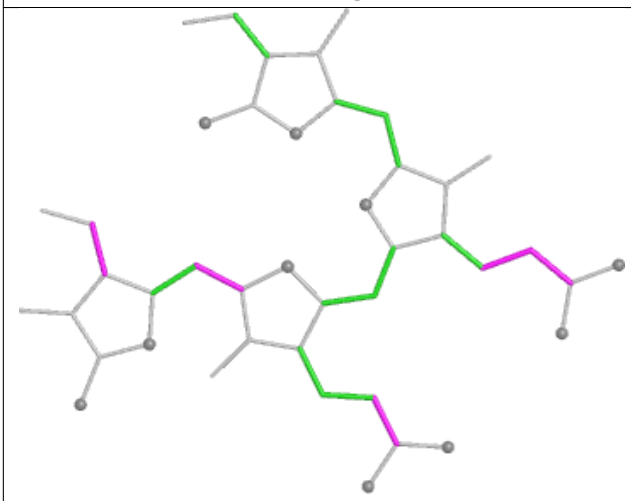
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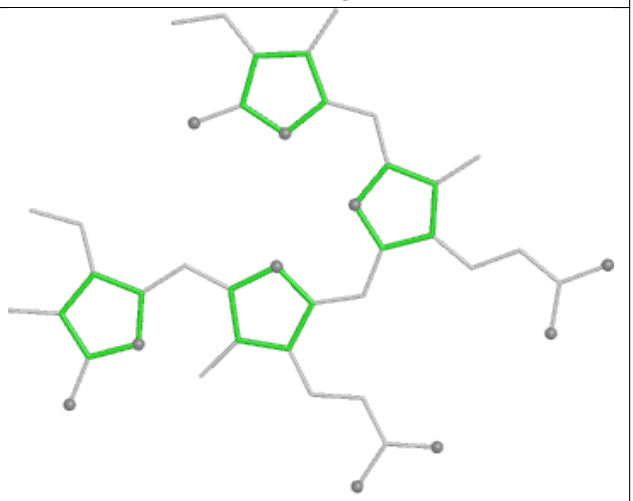
Bond lengths



Bond angles

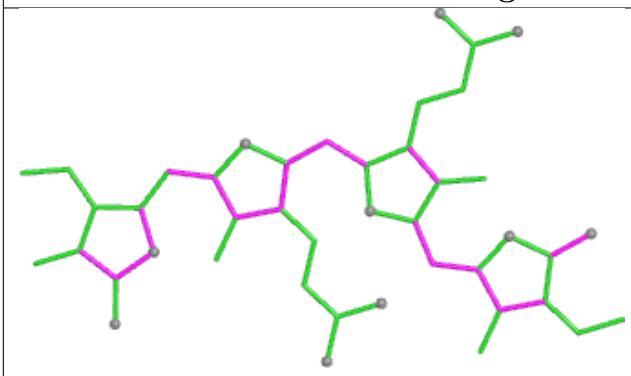


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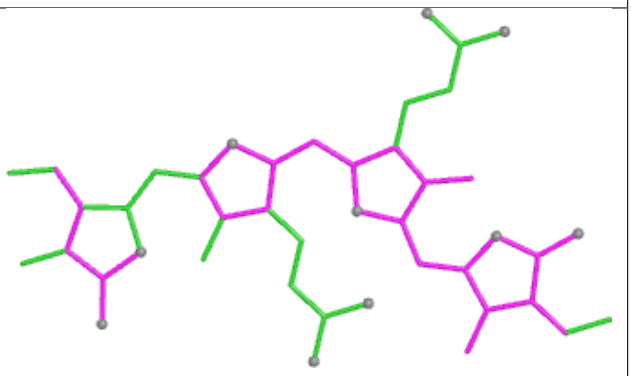


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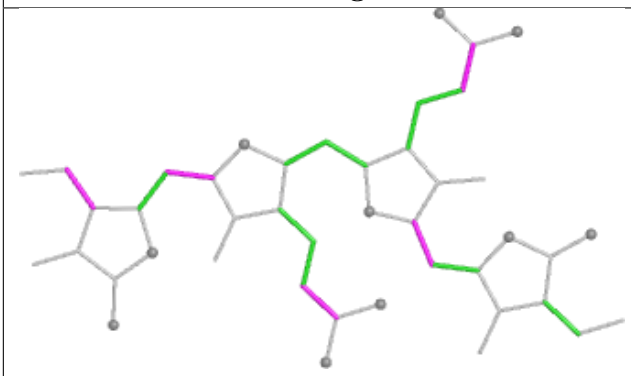
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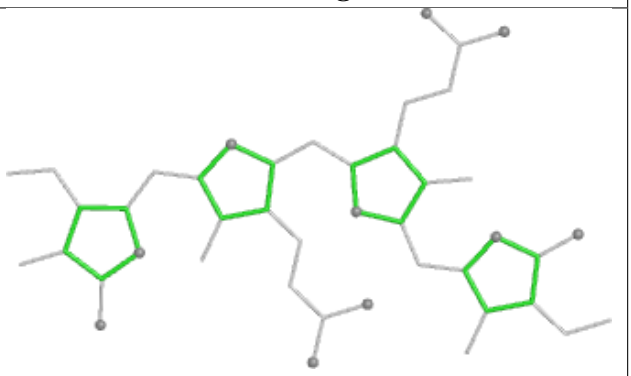
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Bond angles

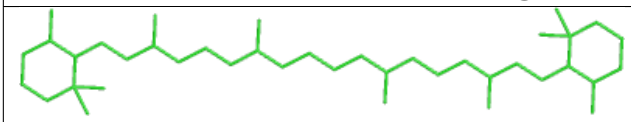


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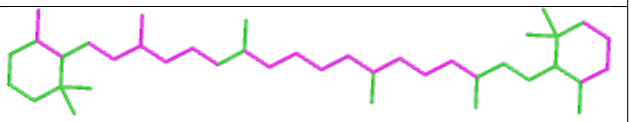


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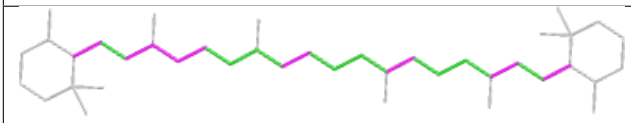
Ligand BCR L2 201



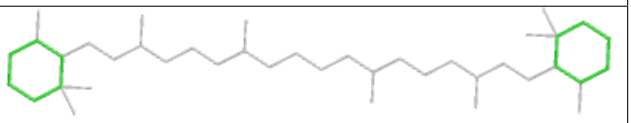
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Bond angles

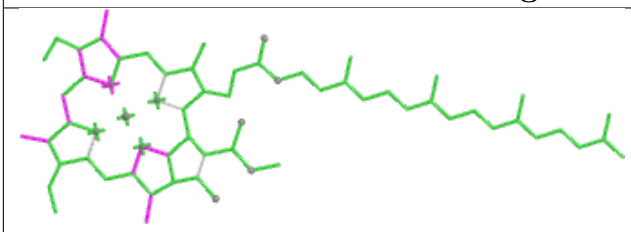


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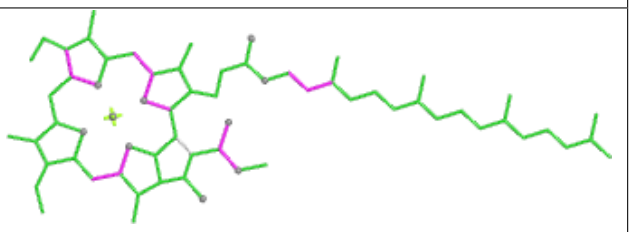


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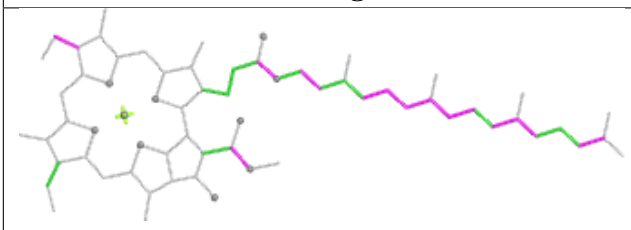
Ligand CLA c6 612



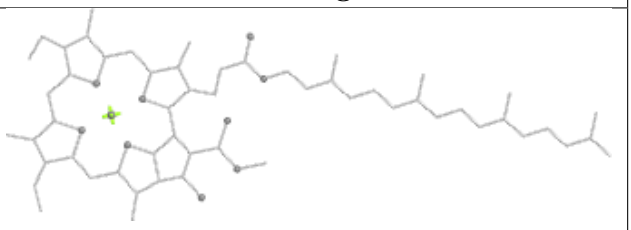
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Bond angles

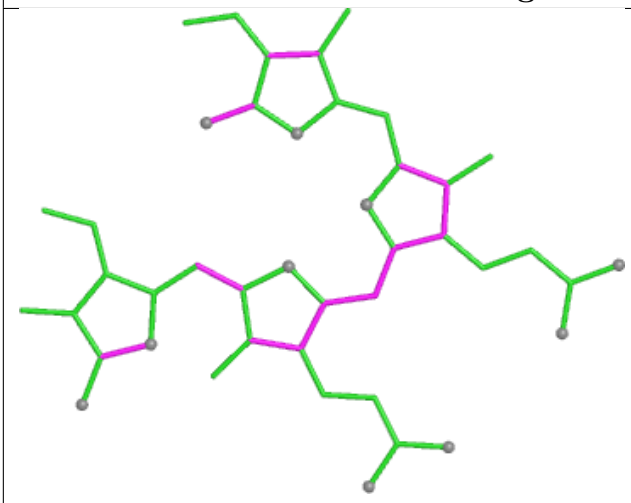


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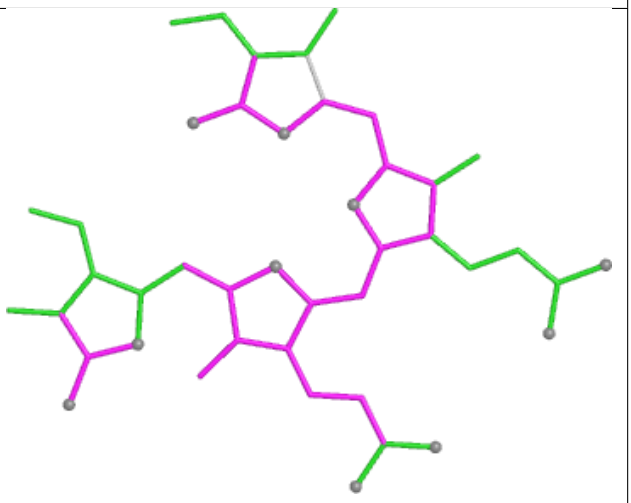


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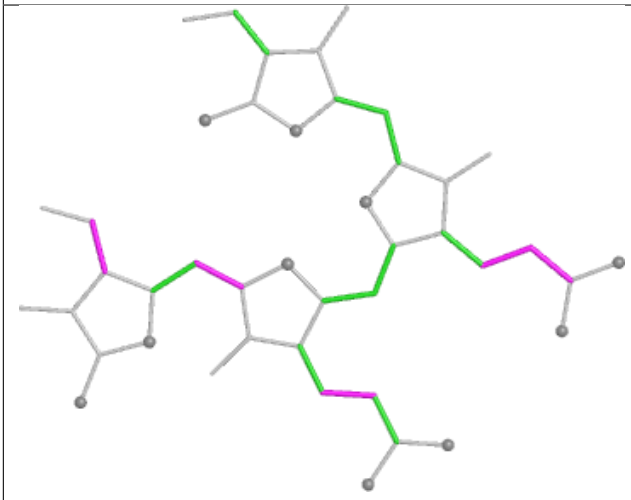
Ligand PEB F9 202



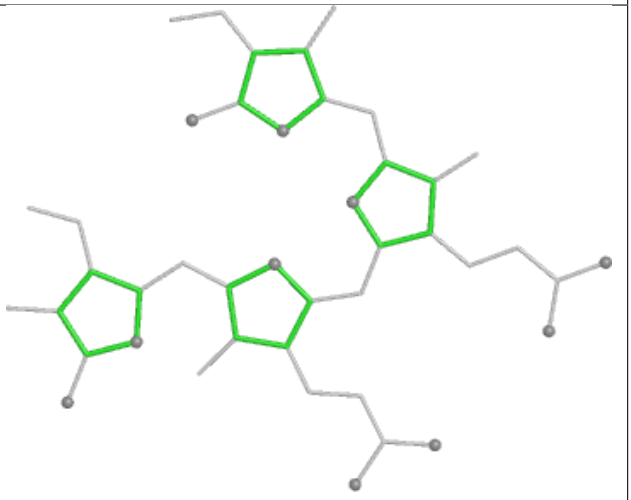
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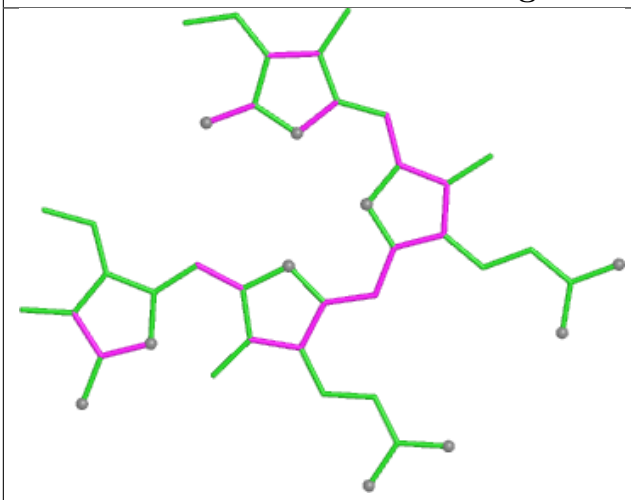


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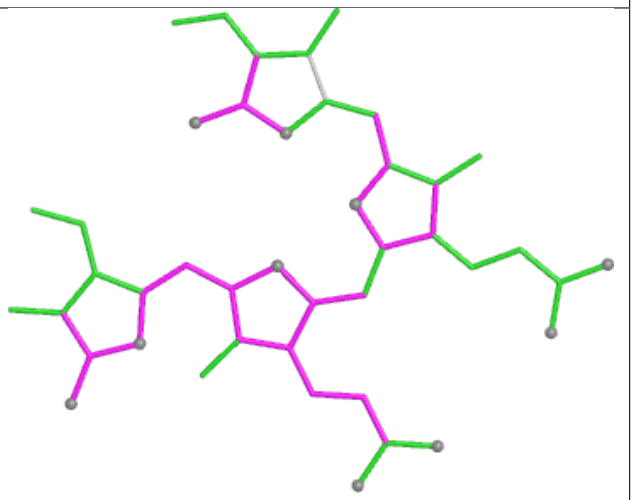


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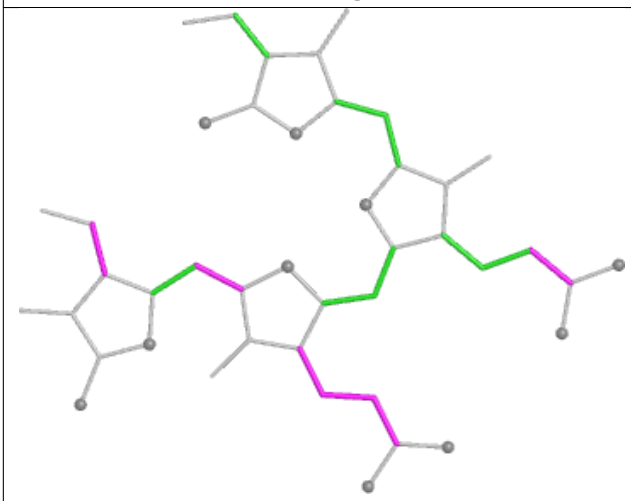
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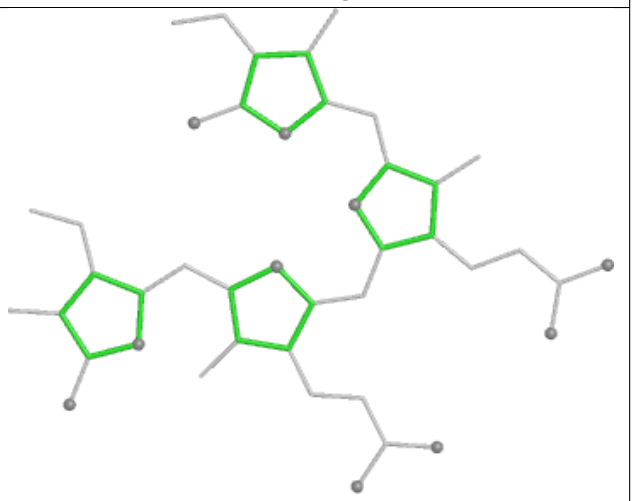
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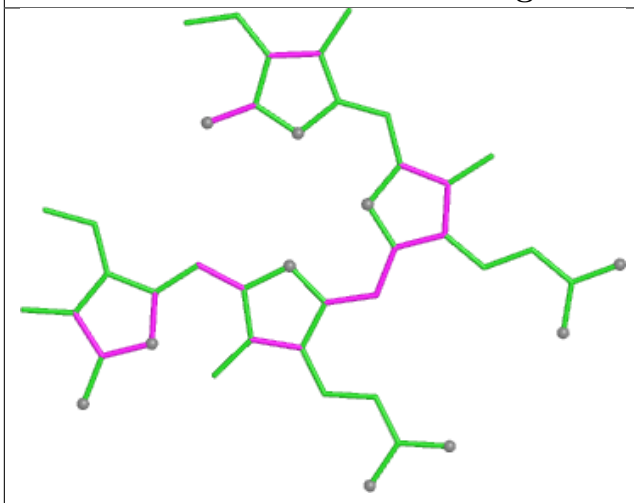


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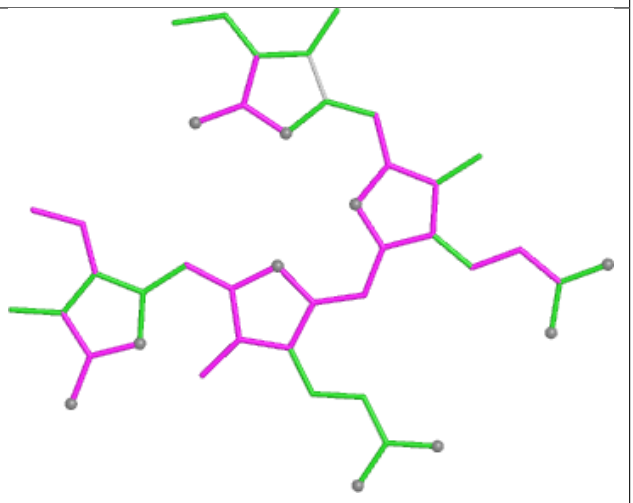


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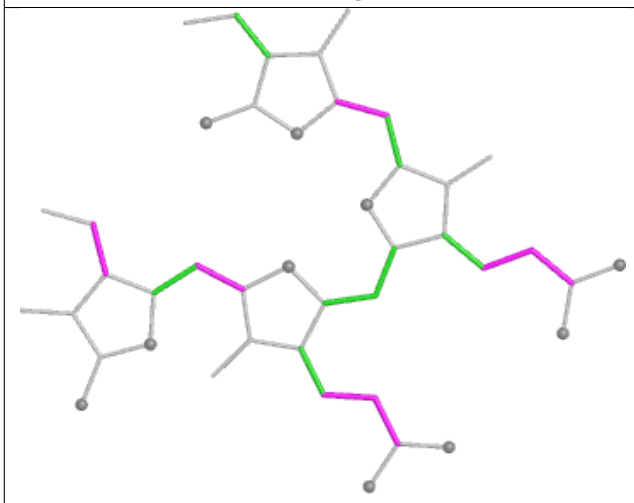
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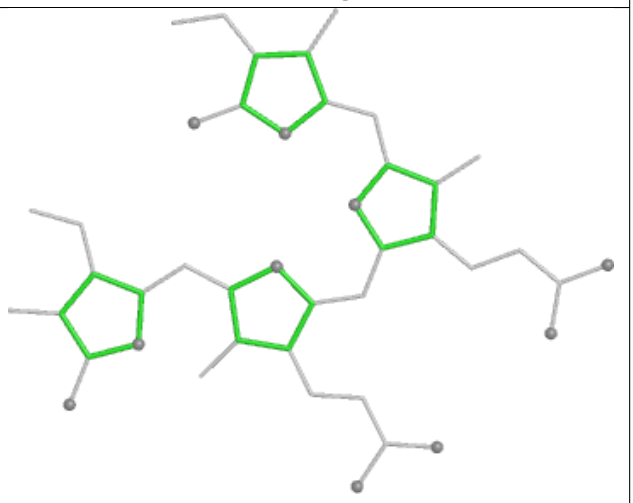
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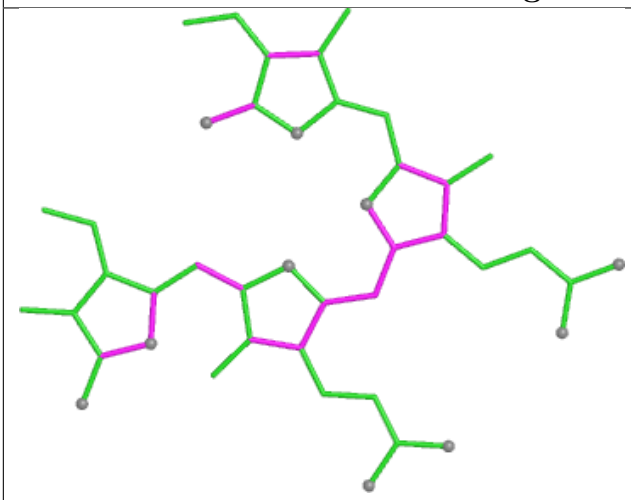


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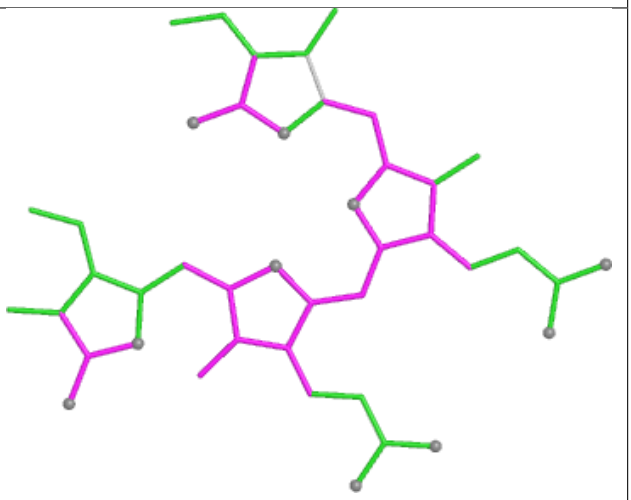


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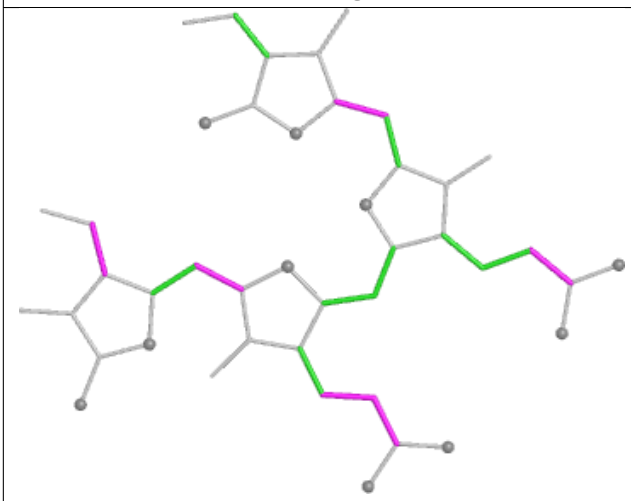
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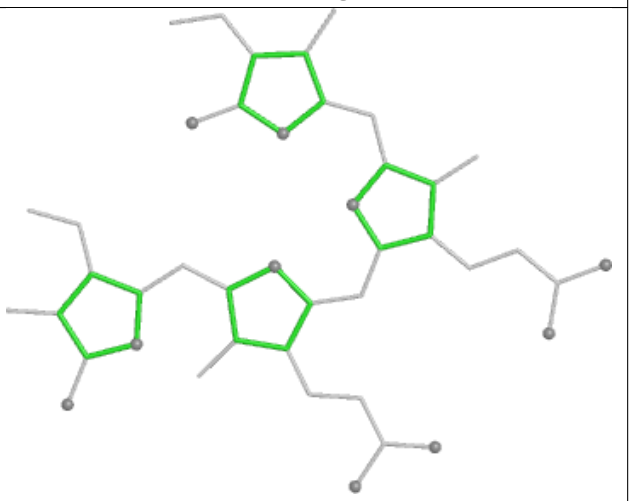
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Bond angles

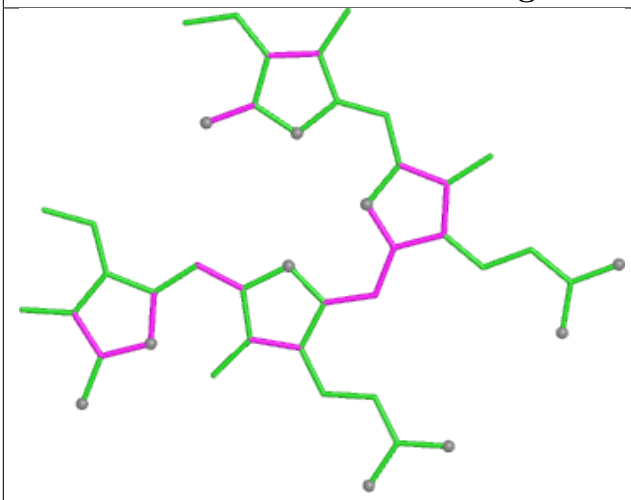


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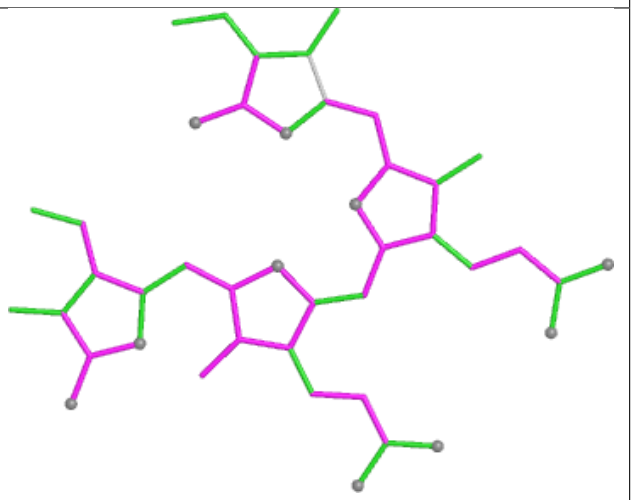


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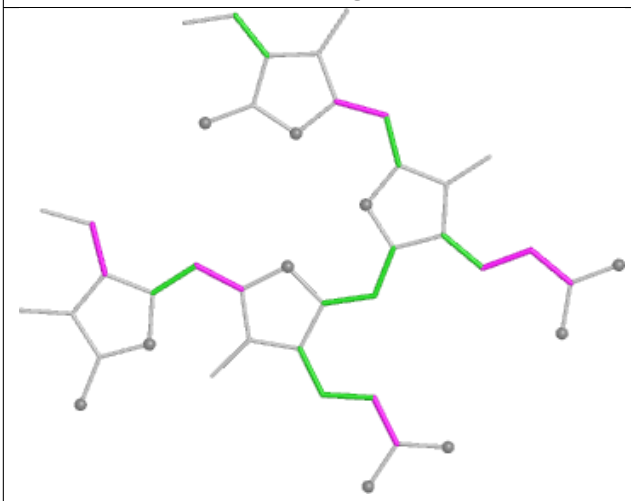
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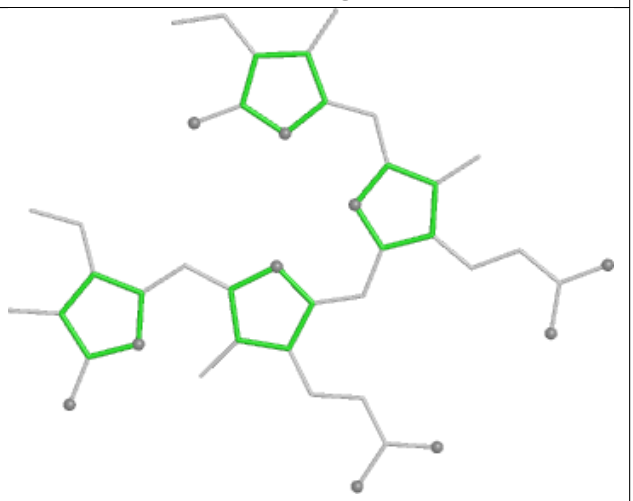
Bond lengths



Bond angles

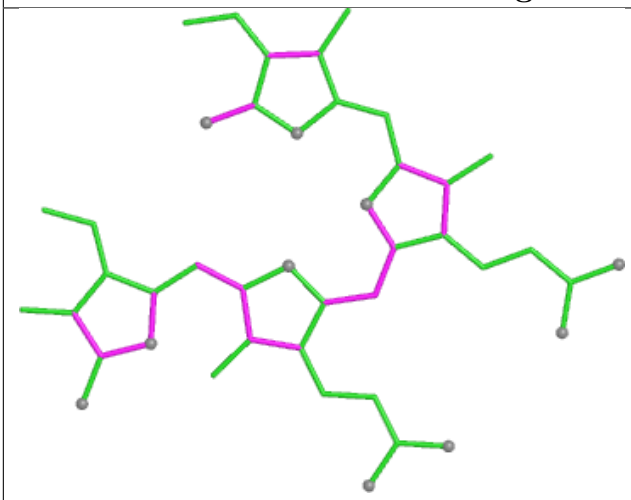


Torsions

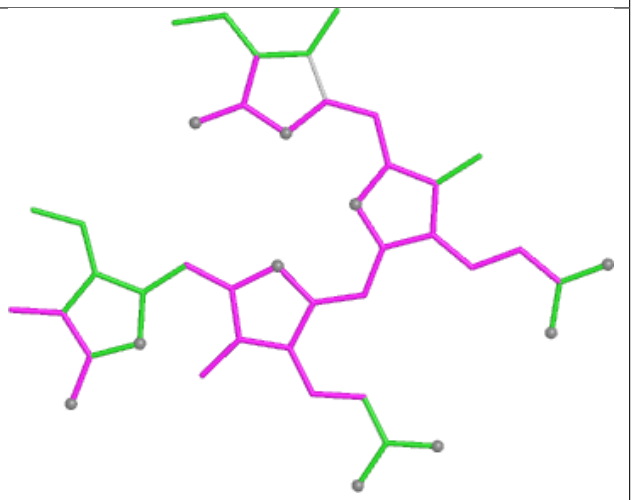


Rings

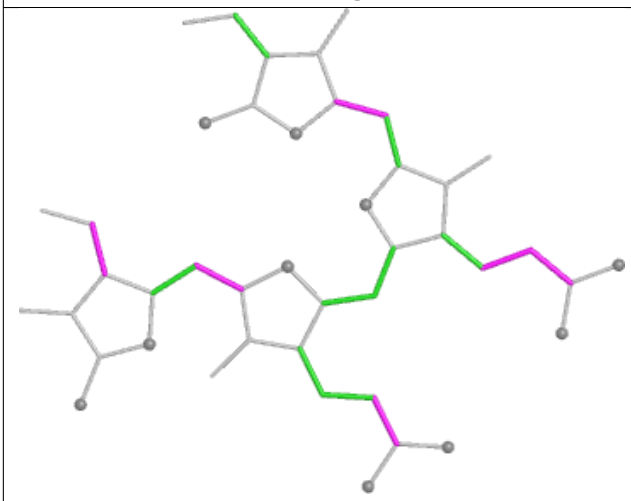
Ligand PEB R5 201



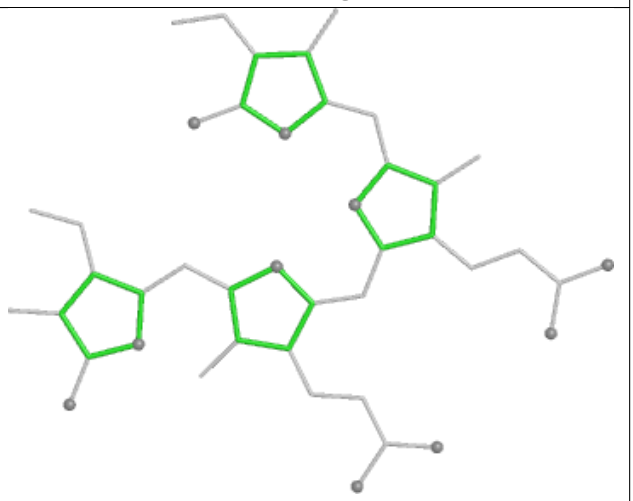
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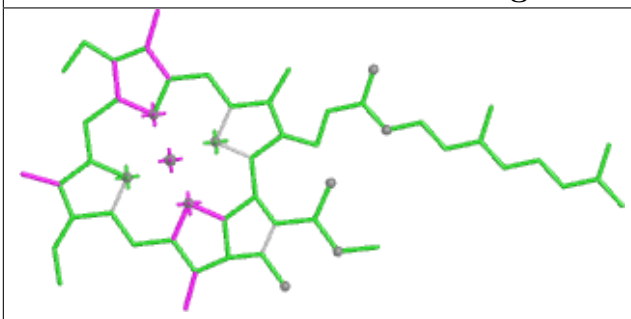
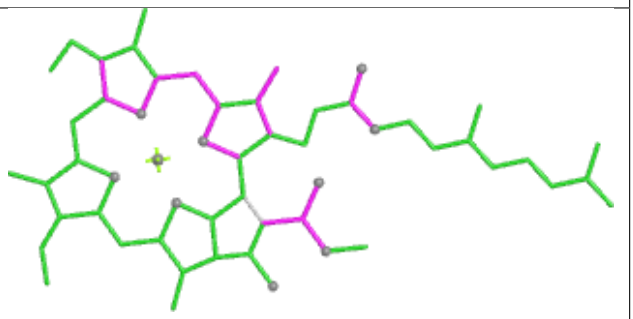
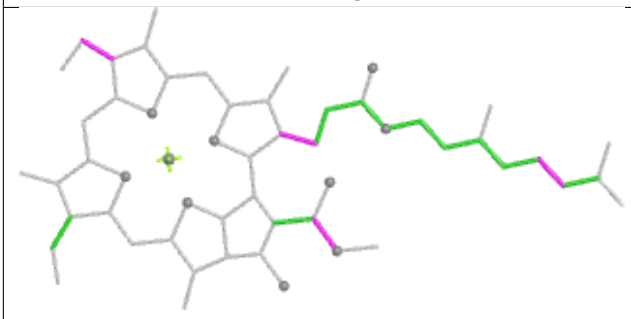
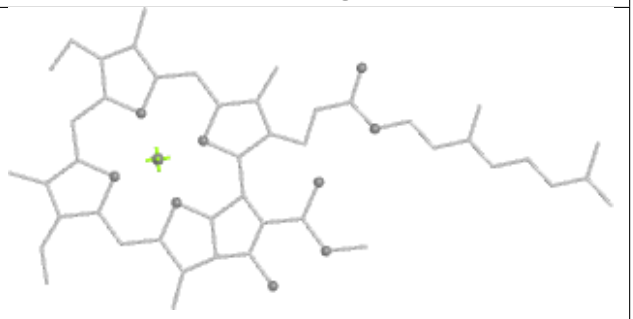
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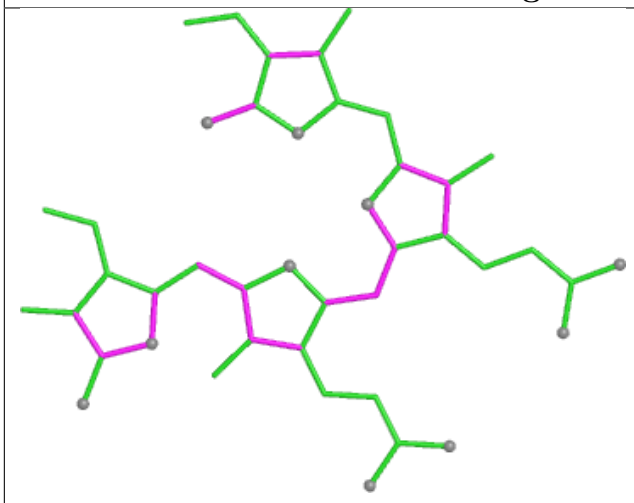
Torsions



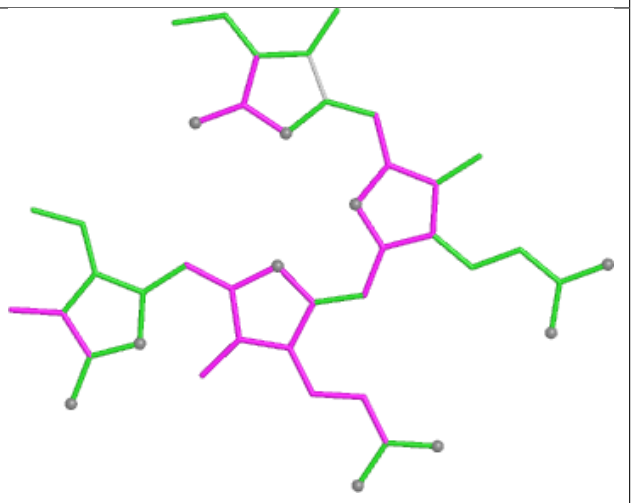
Rings

Ligand CLA BN 812	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

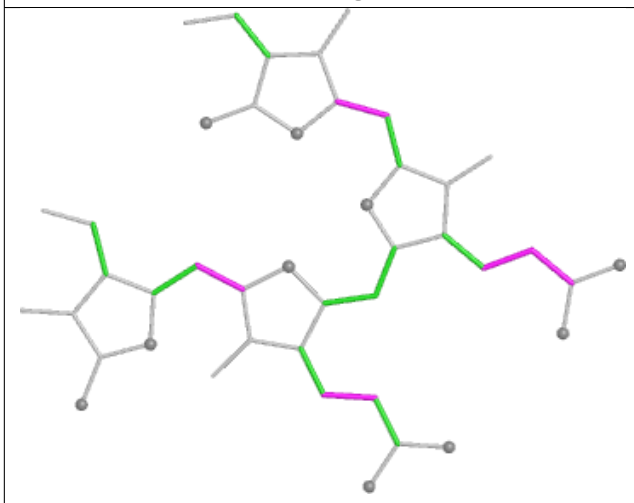
Ligand PEB IJ 202



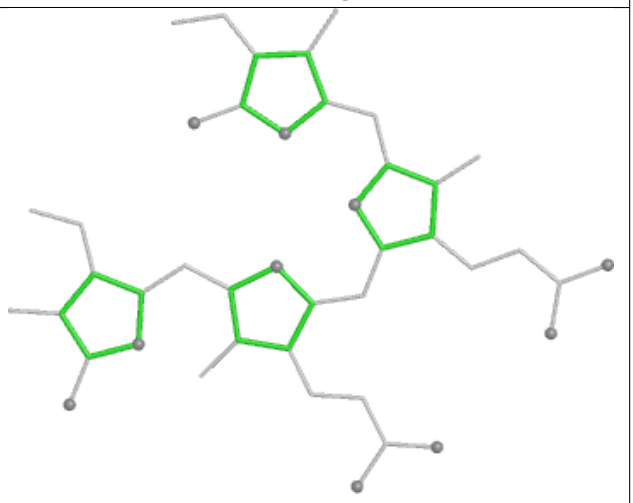
Bond lengths



Bond angles

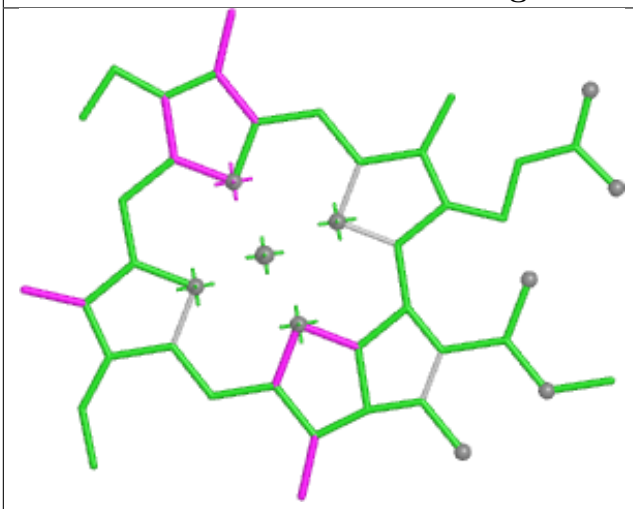


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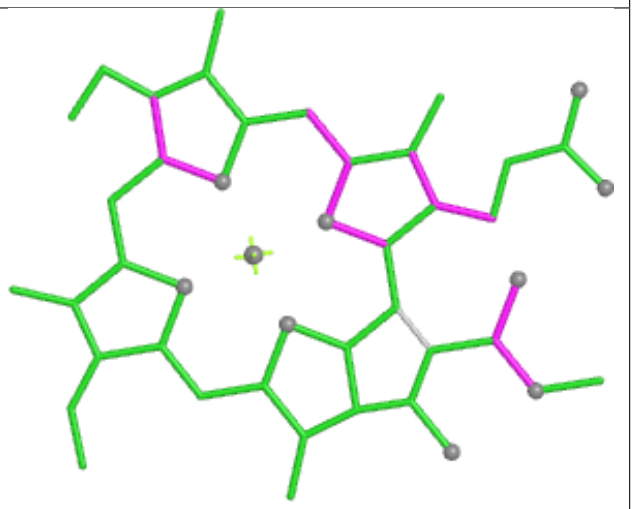


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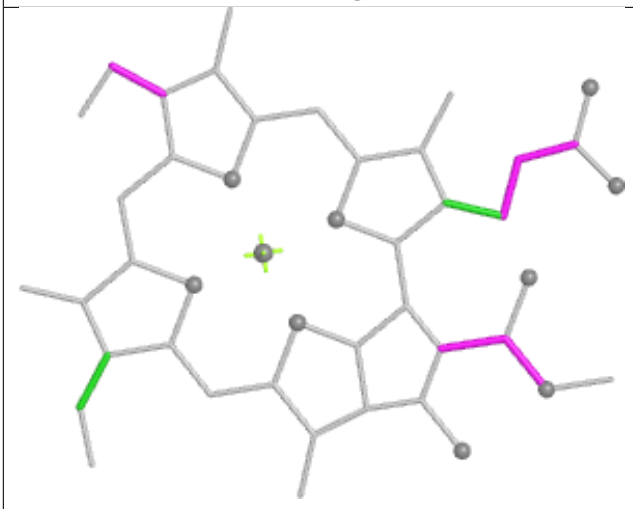
Ligand CLA AN 818



Bond lengths



Bond angles

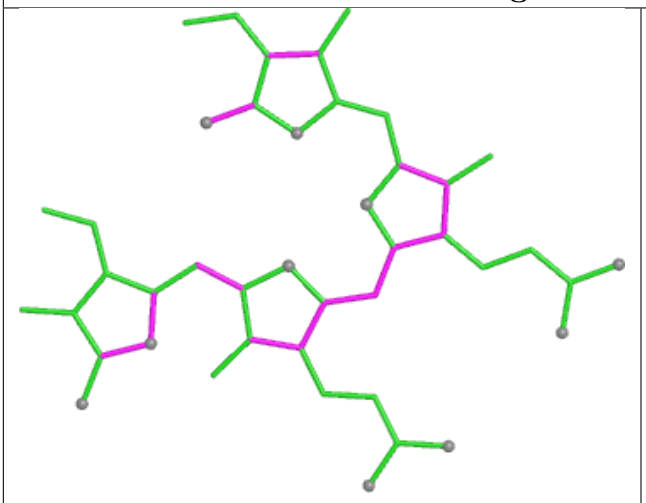


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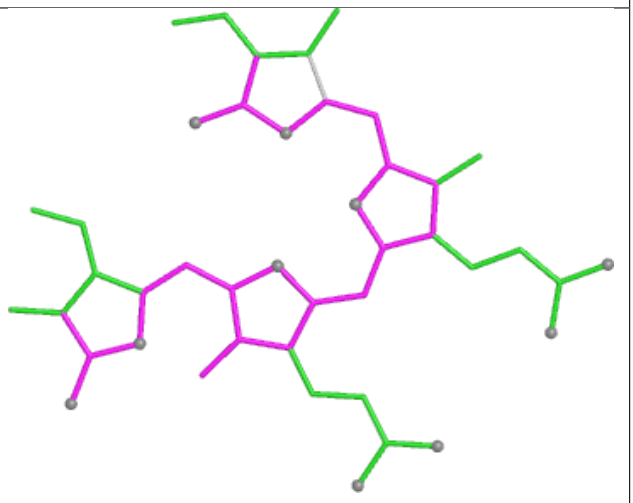


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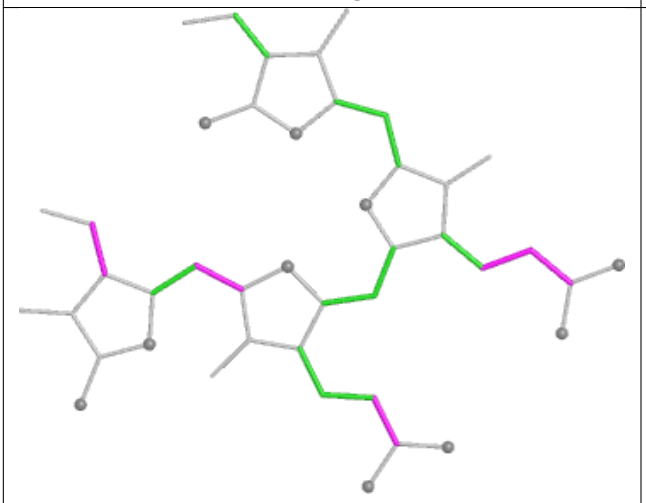
Ligand PEB UH 203



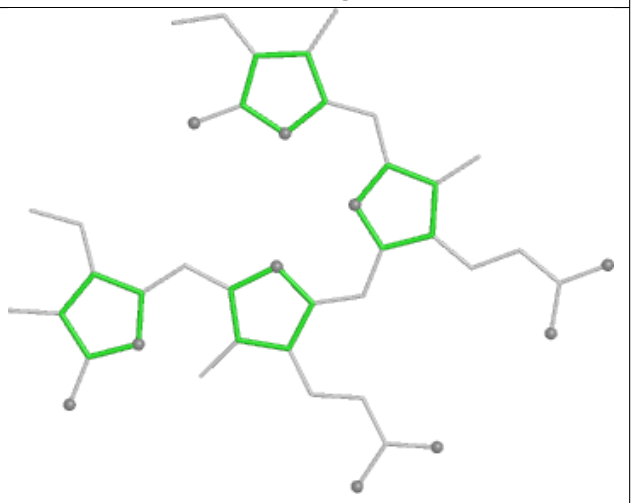
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Bond angles

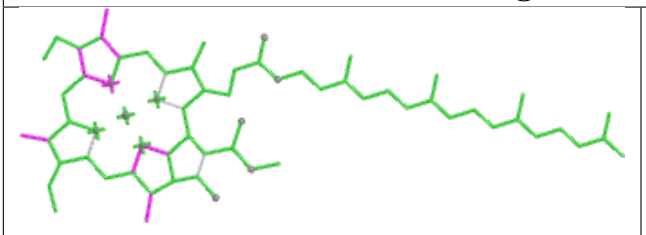


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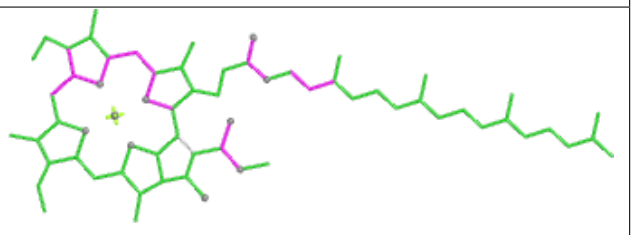


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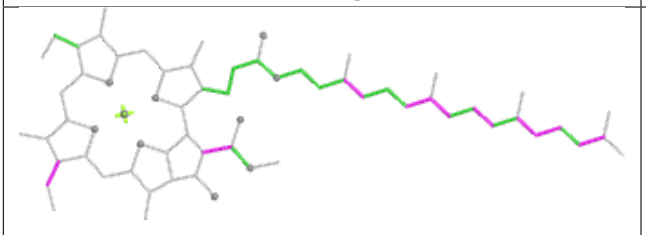
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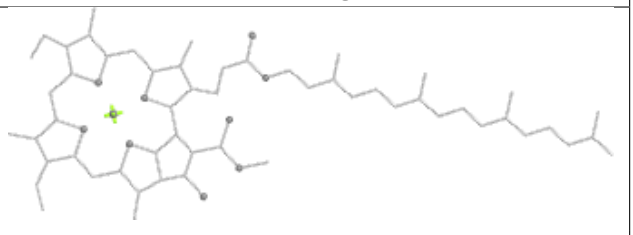
Bond lengths



Bond angles

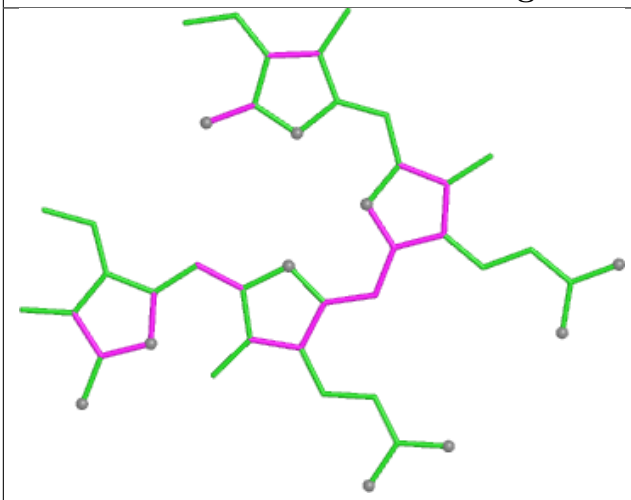


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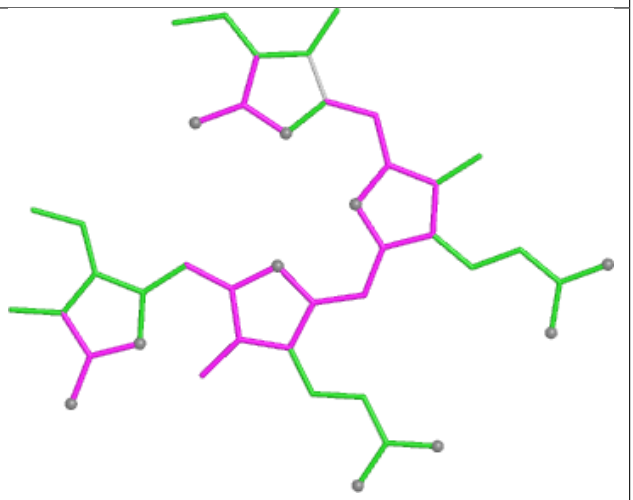


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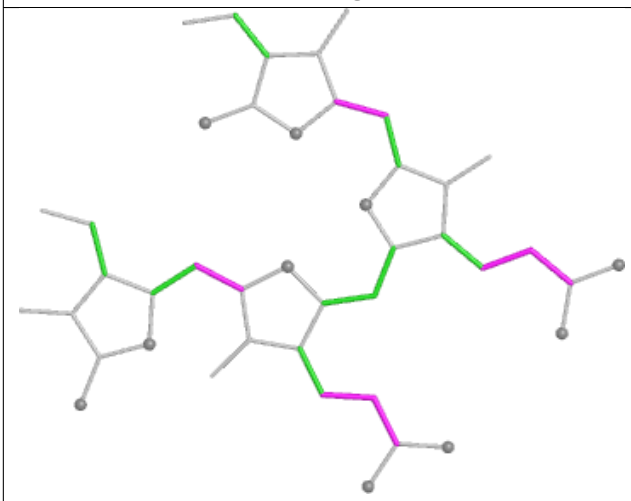
Ligand PEB AI 202



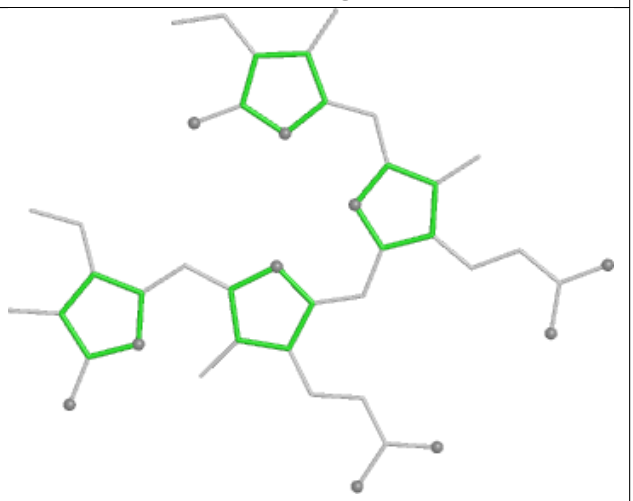
Bond lengths



Bond angles

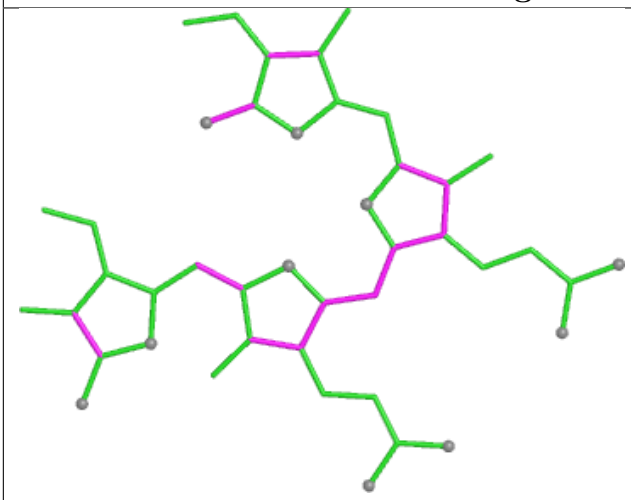


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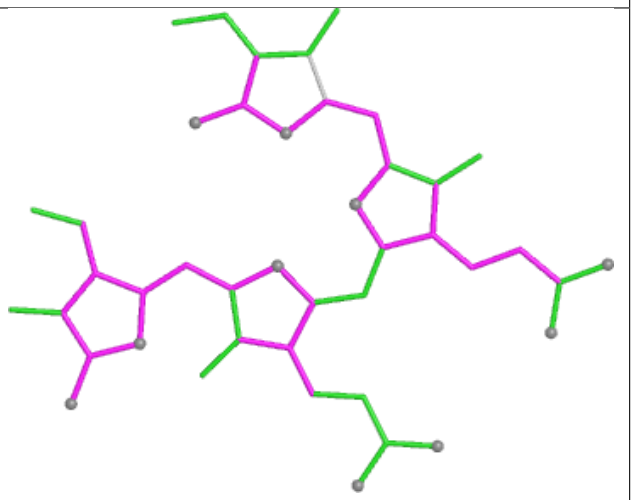


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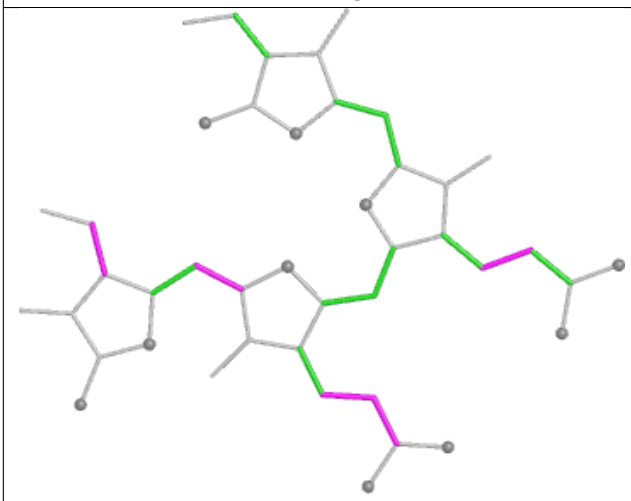
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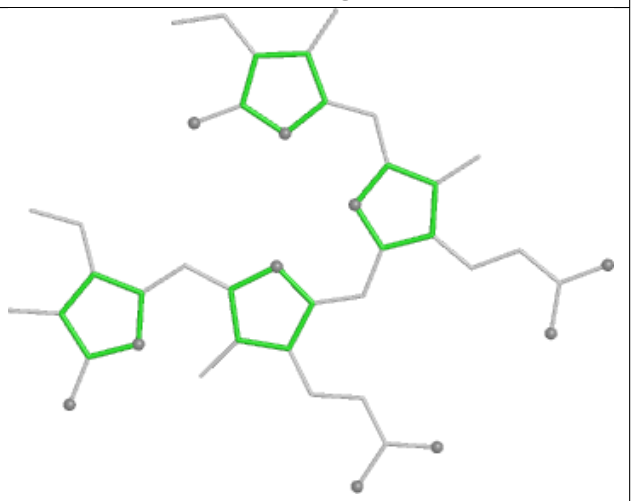
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Bond angles

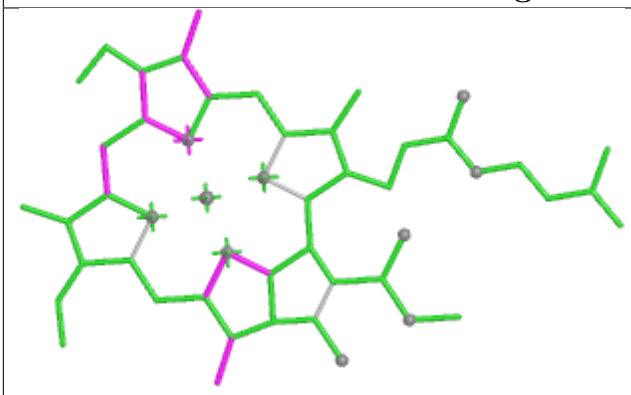


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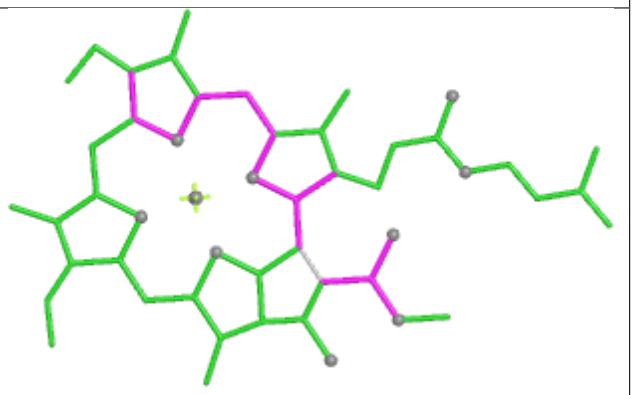


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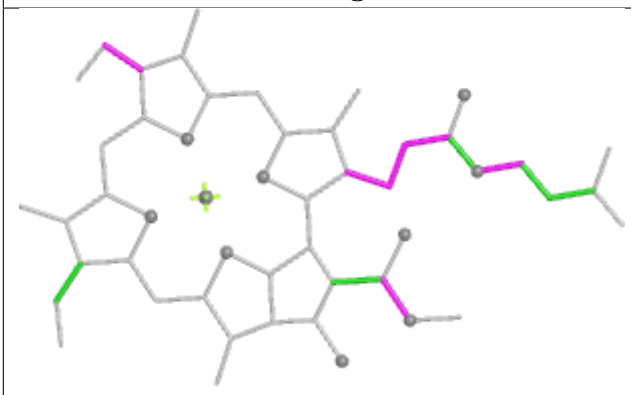
Ligand CLA 7N 607



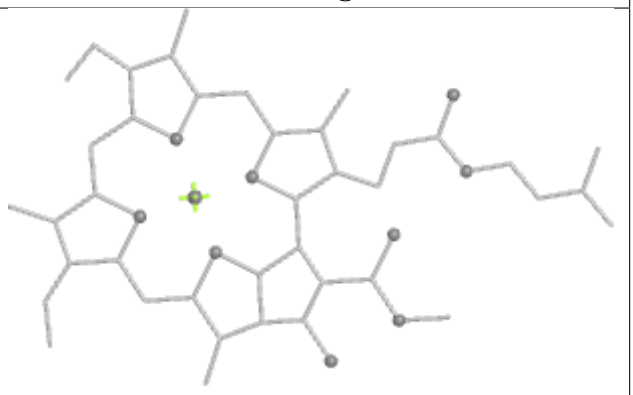
Bond lengths



Bond angles

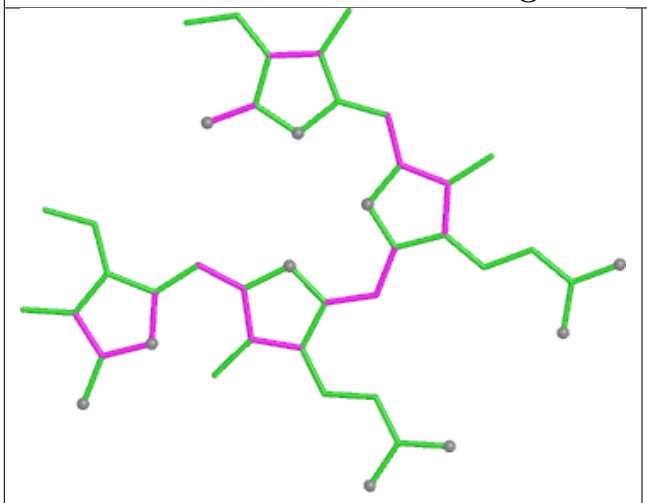


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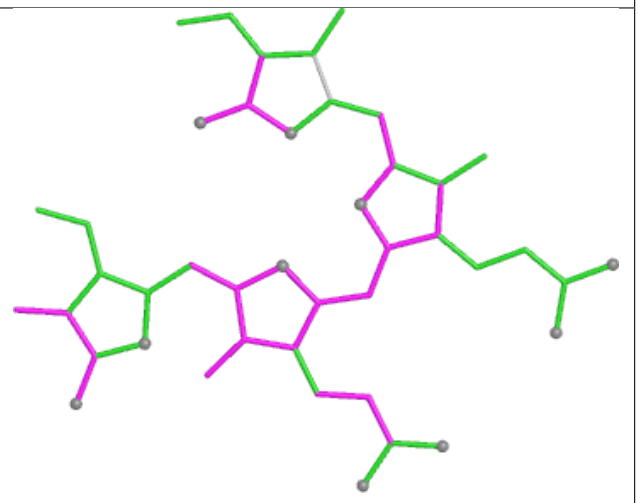


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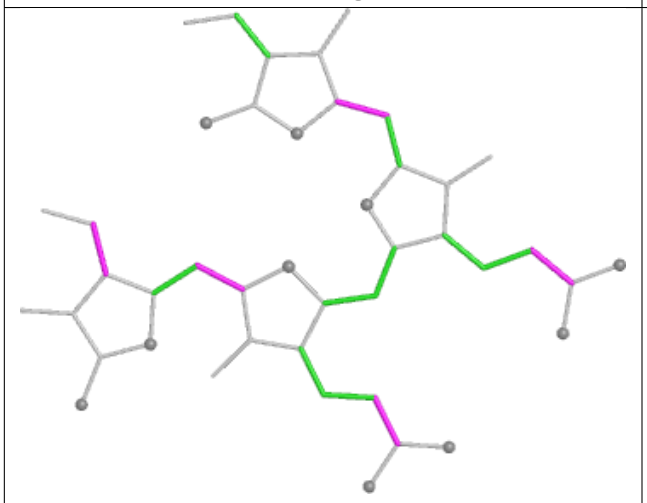
Ligand PEB d1 202



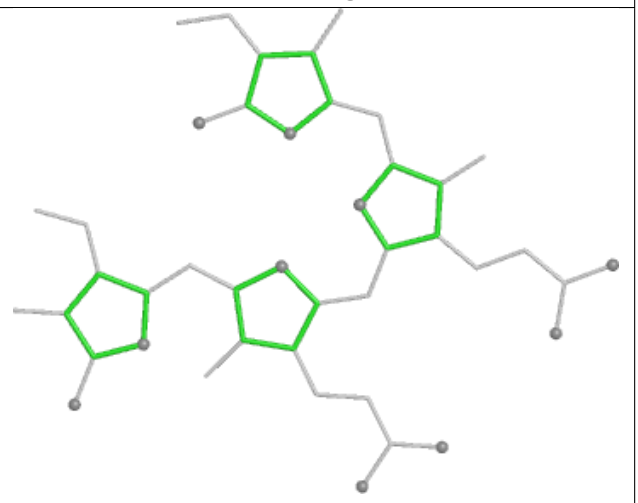
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Bond angles

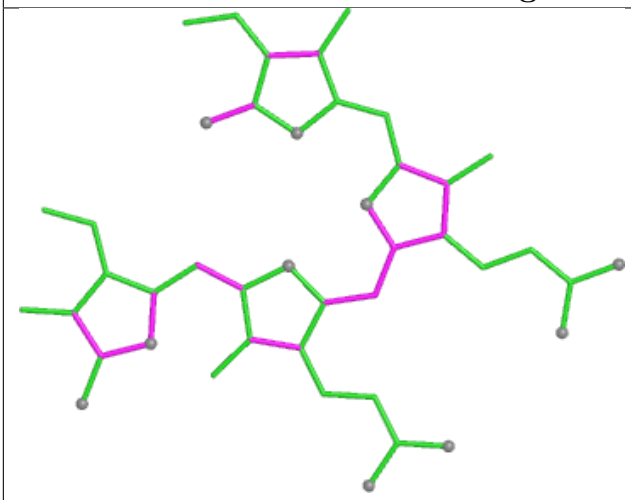


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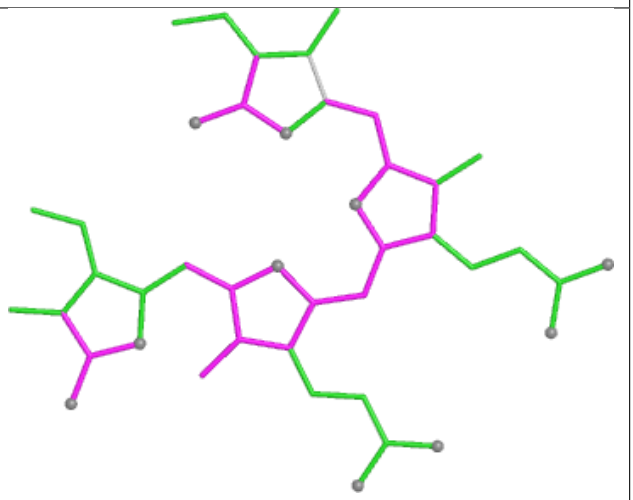


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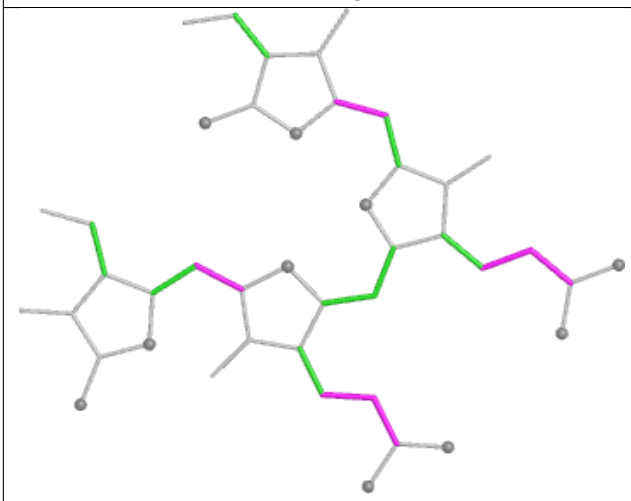
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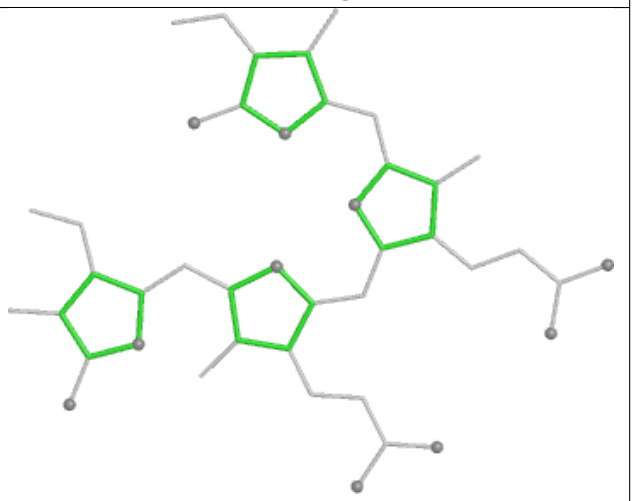
Bond lengths



Bond angles

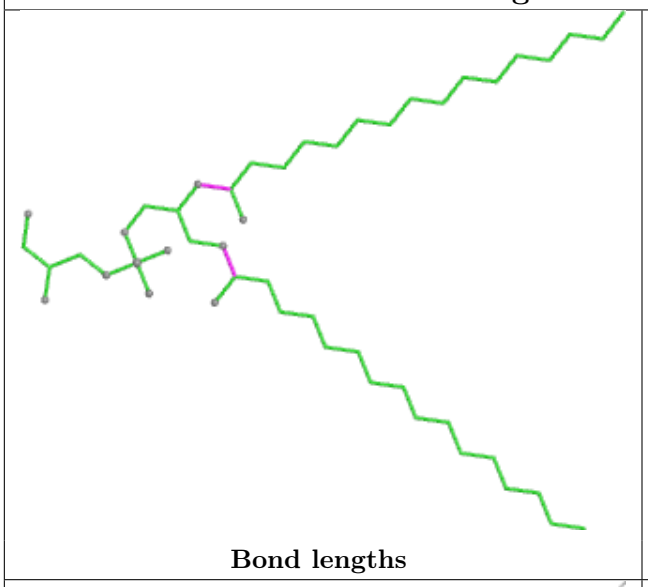


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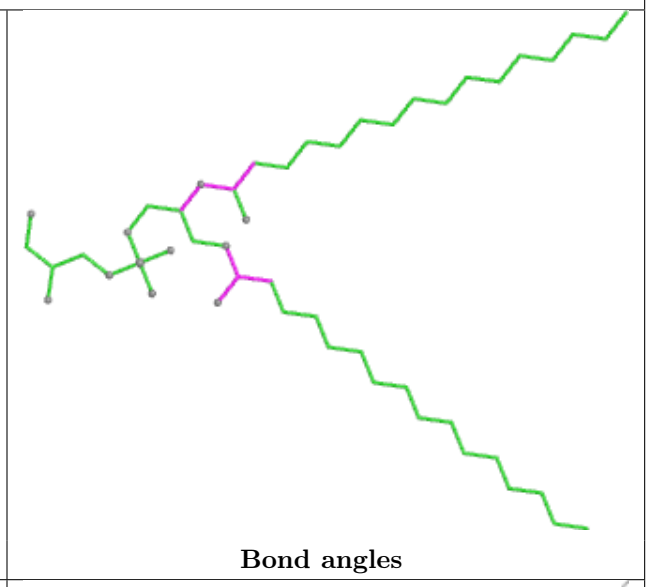


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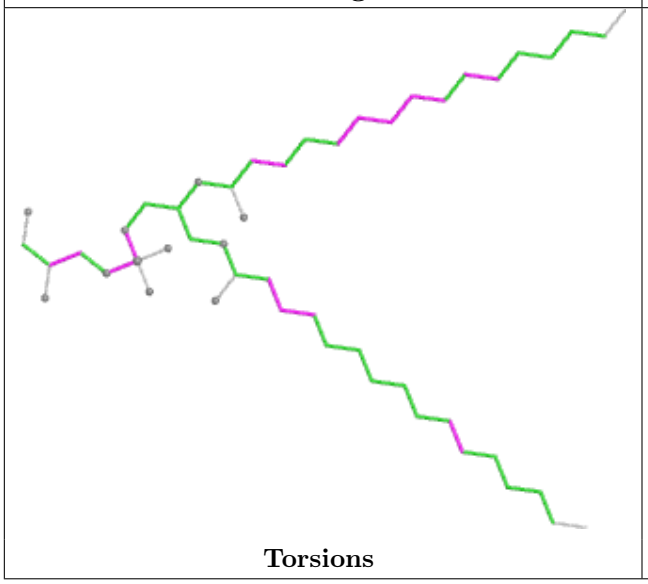
Ligand LHG DL 407



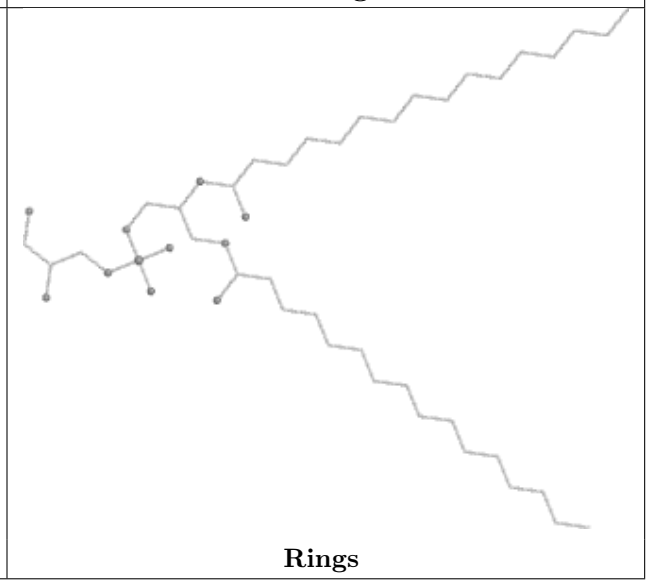
Bond lengths



Bond angles

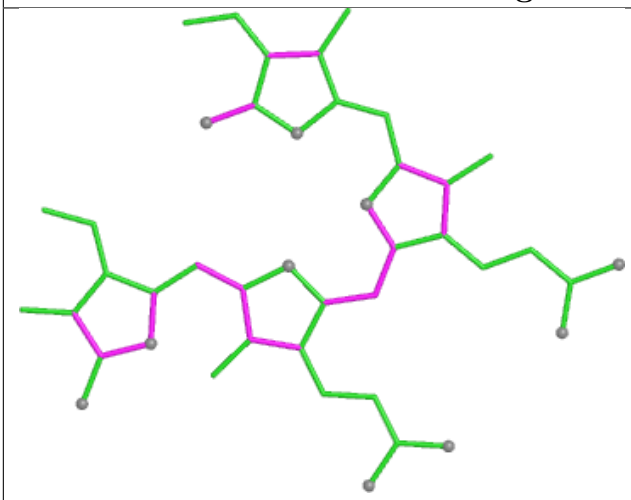


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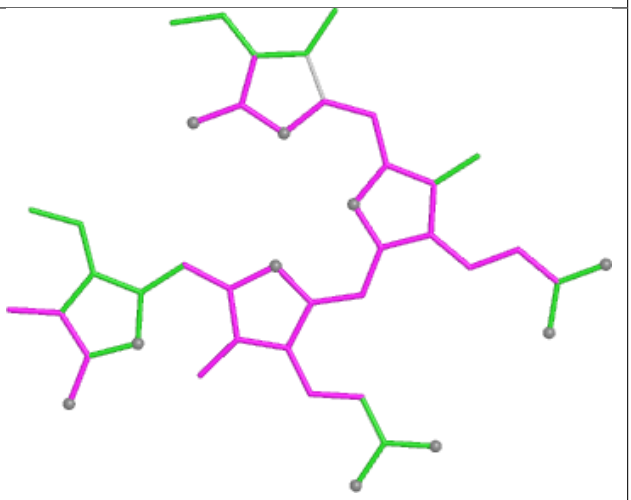


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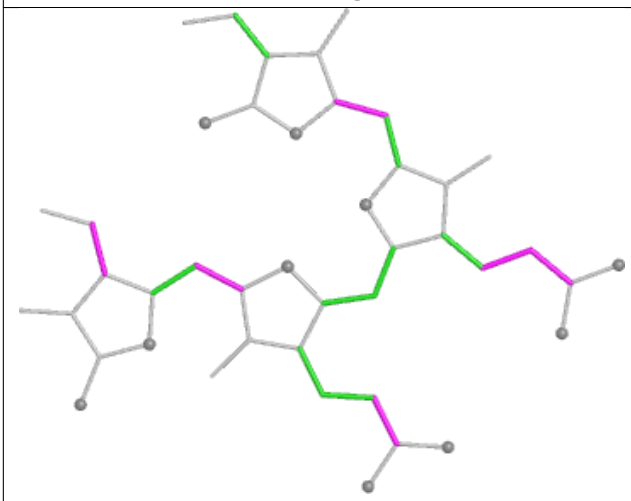
Ligand PEB C5 201



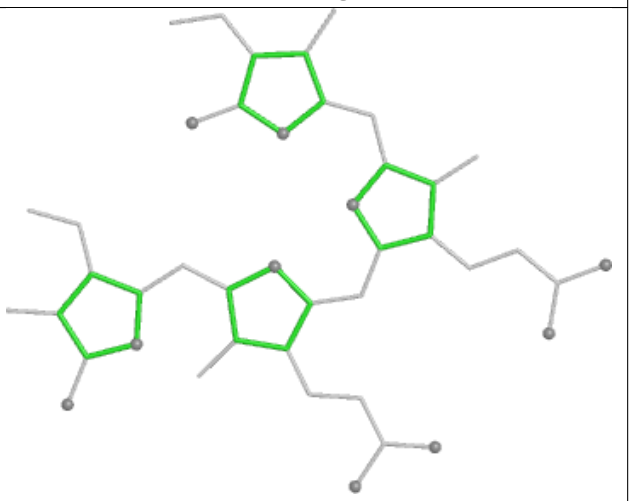
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Bond angles

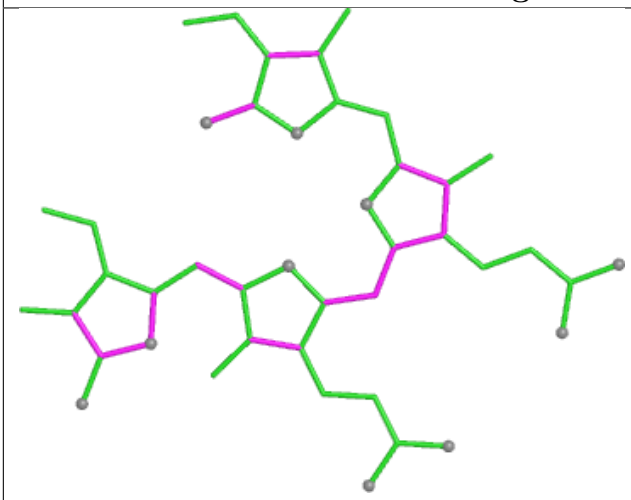


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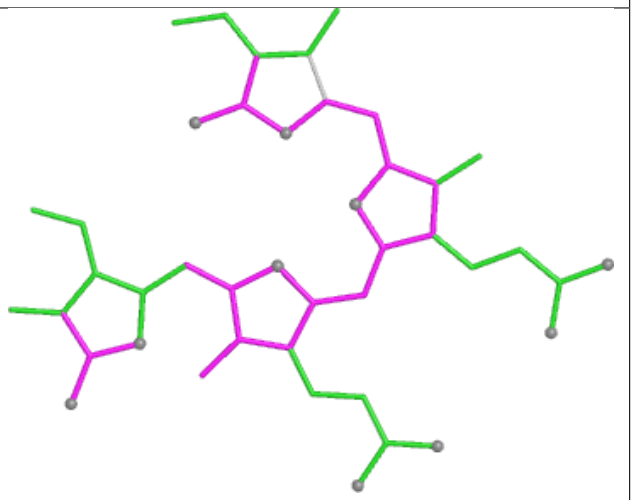


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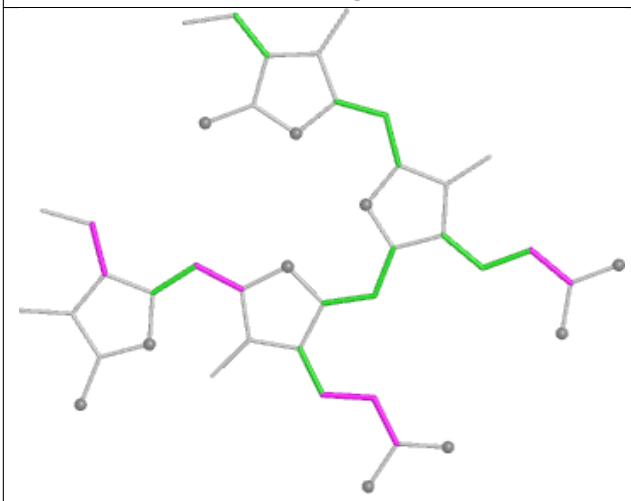
Ligand PEB aM 204



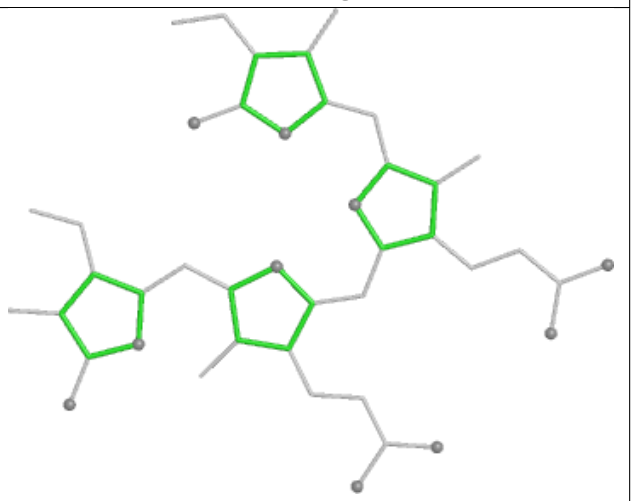
Bond lengths



Bond angles

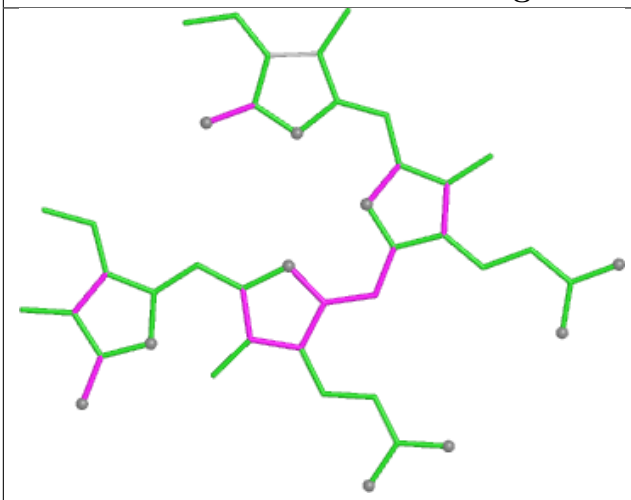


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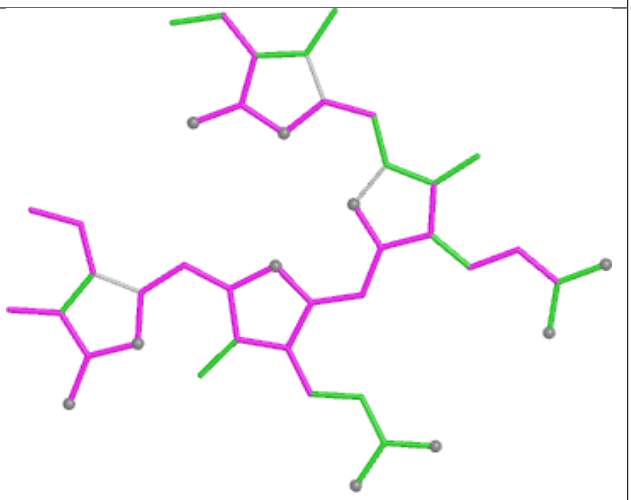


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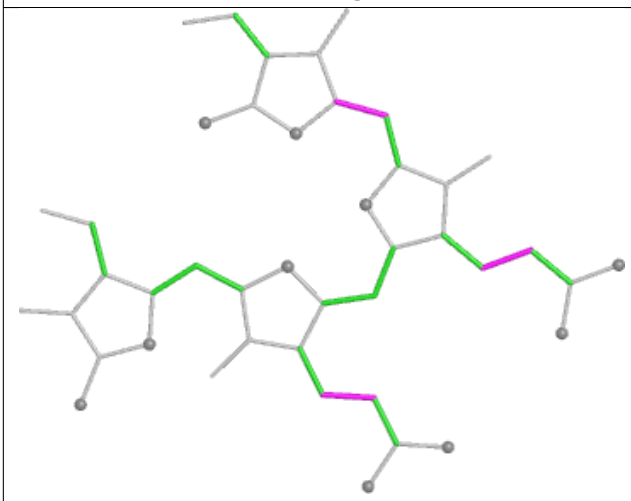
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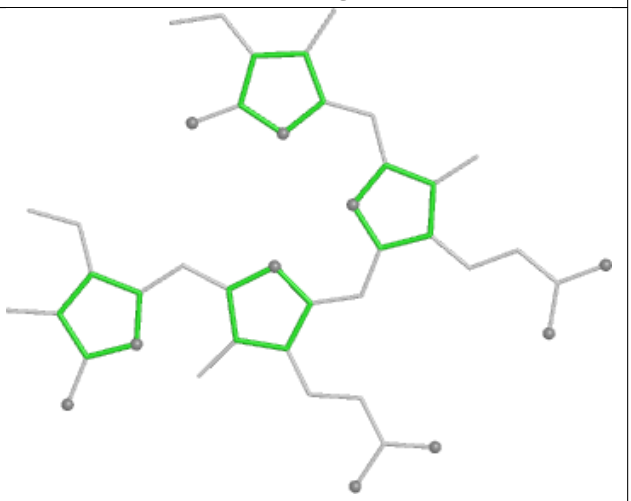
Bond lengths



Bond angles

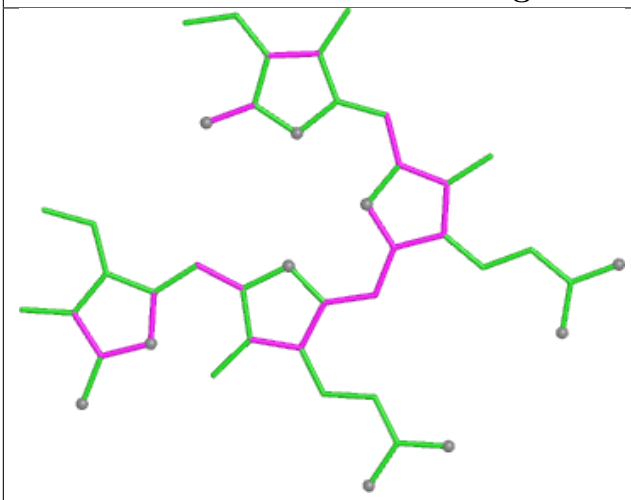


Torsions

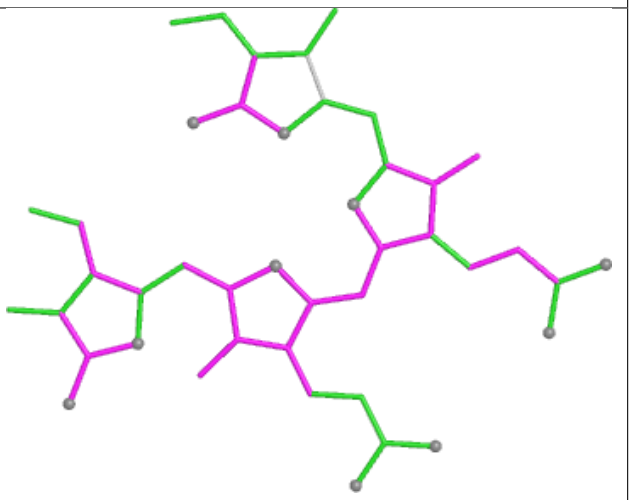


Rings

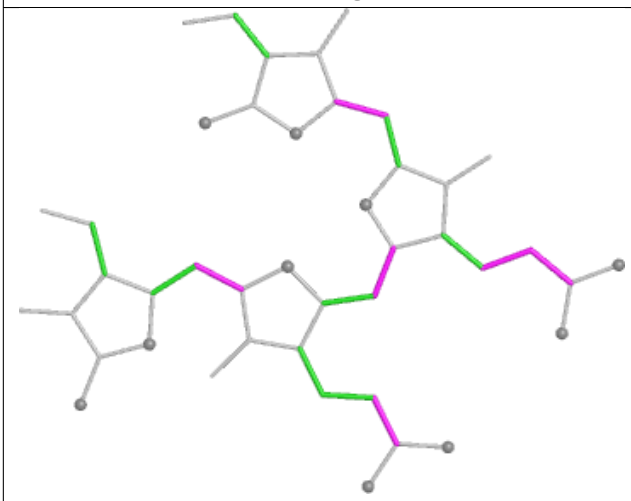
Ligand PEB XF 203



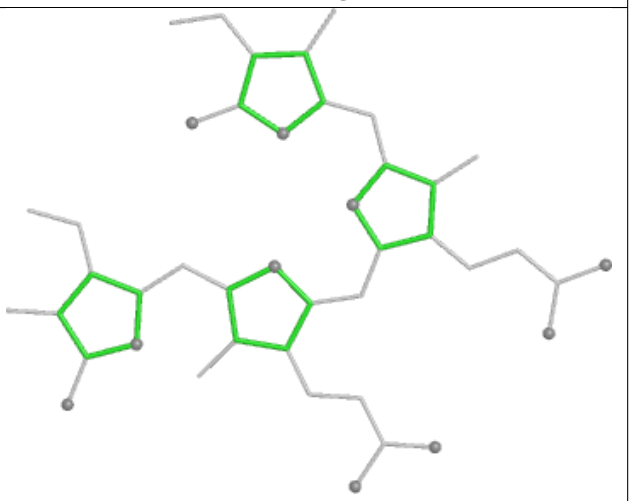
Bond lengths



Bond angles

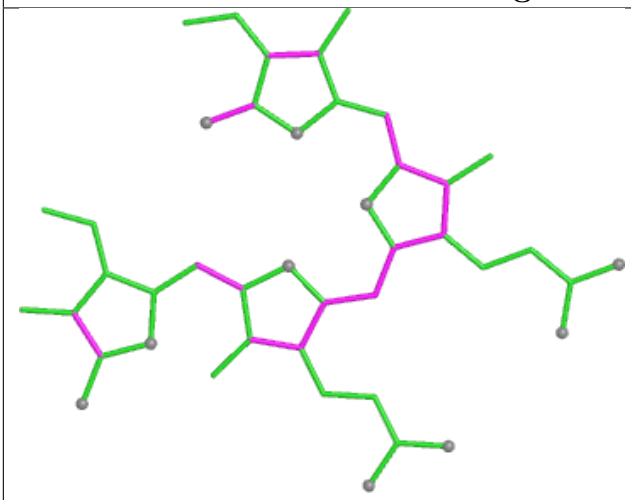


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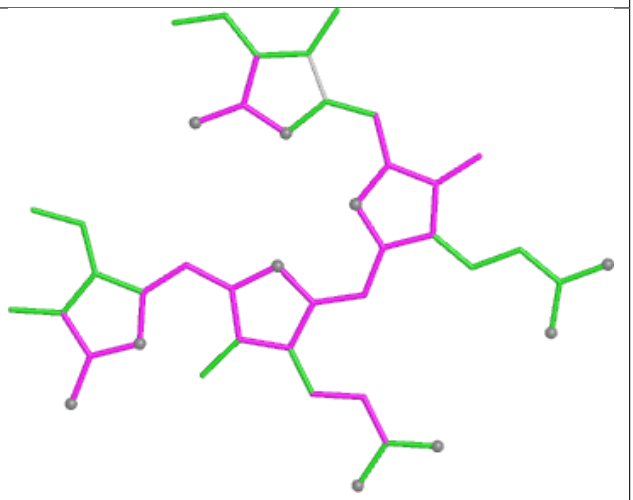


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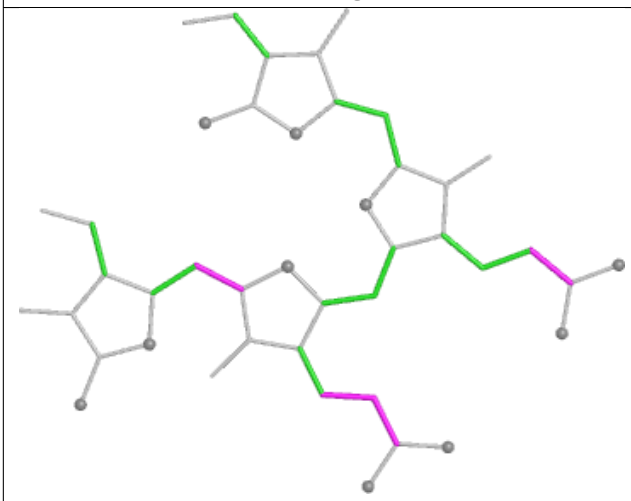
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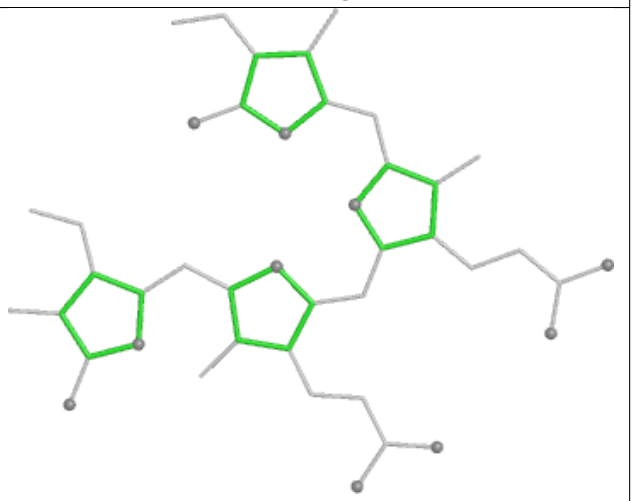
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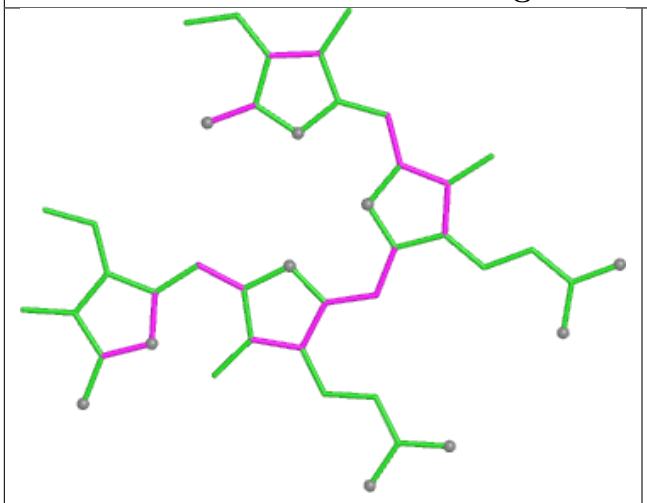


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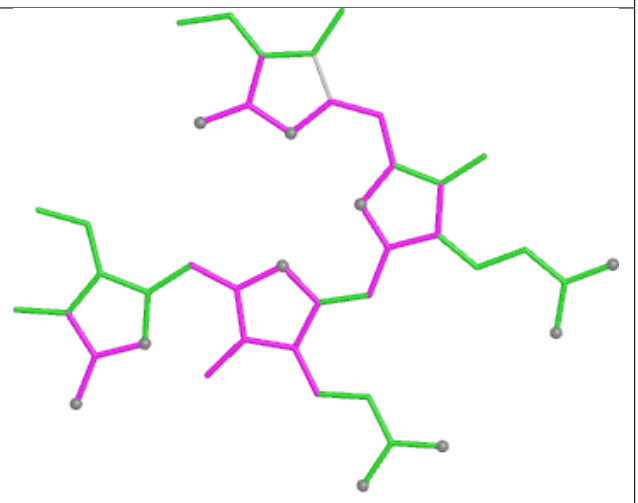


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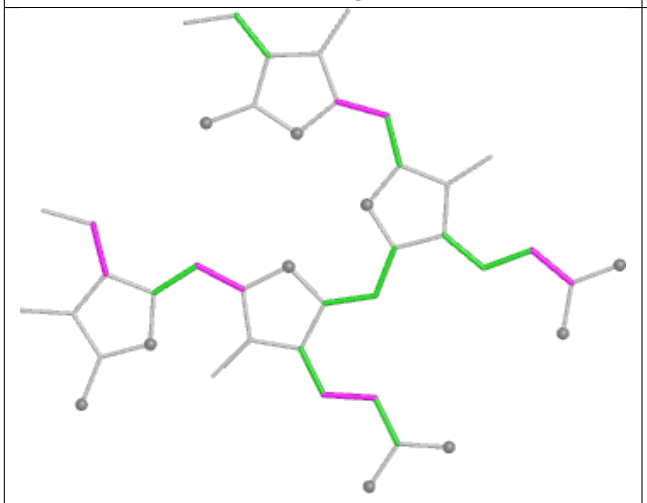
Ligand PEB ZH 202



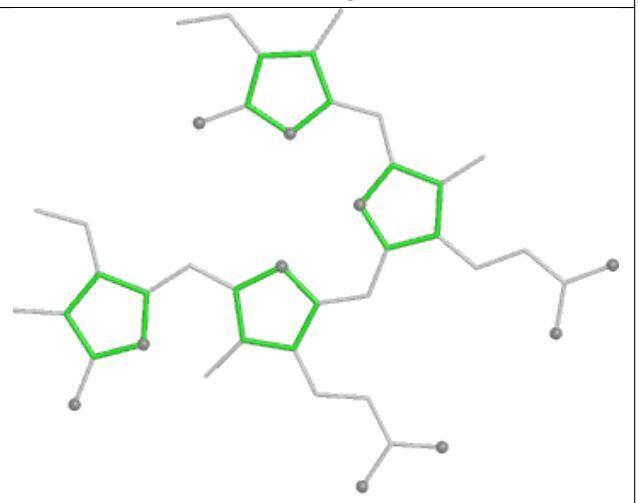
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Bond angles

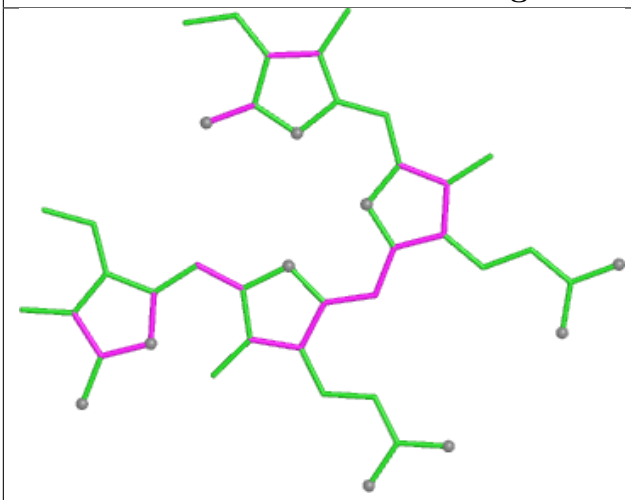


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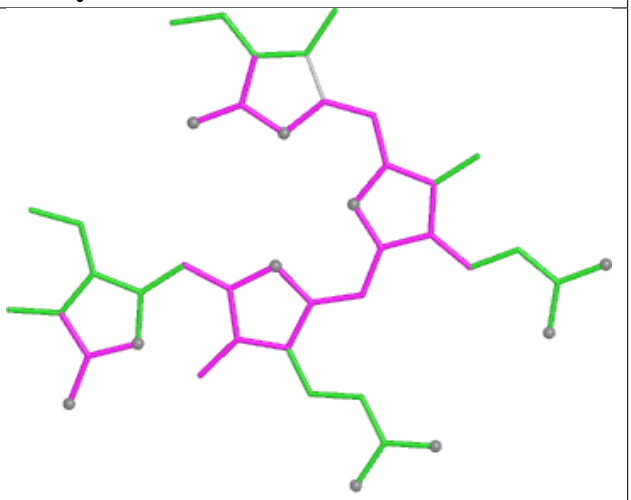


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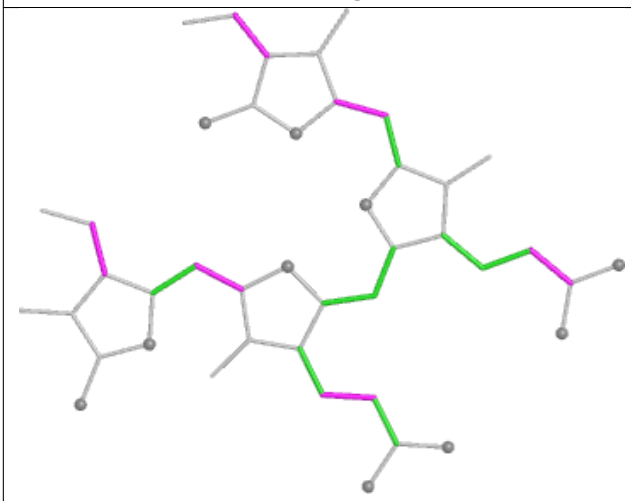
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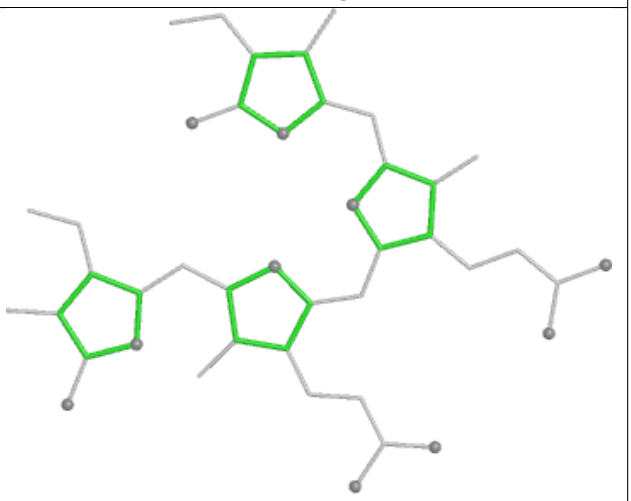
Bond lengths



Bond angles

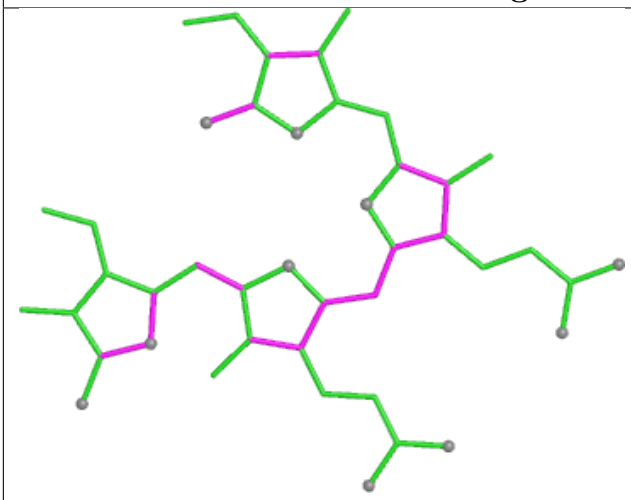


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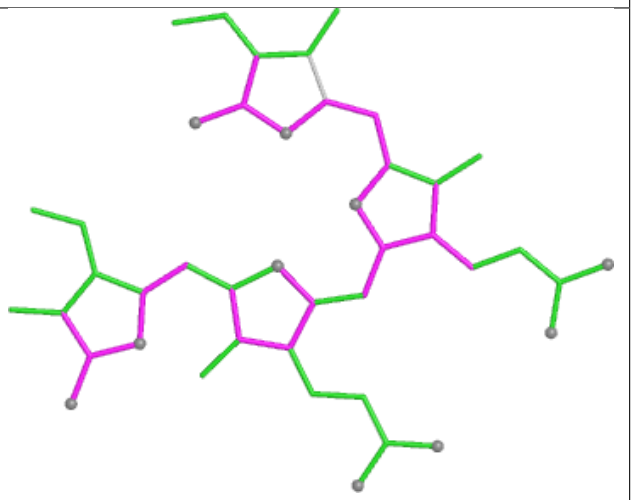


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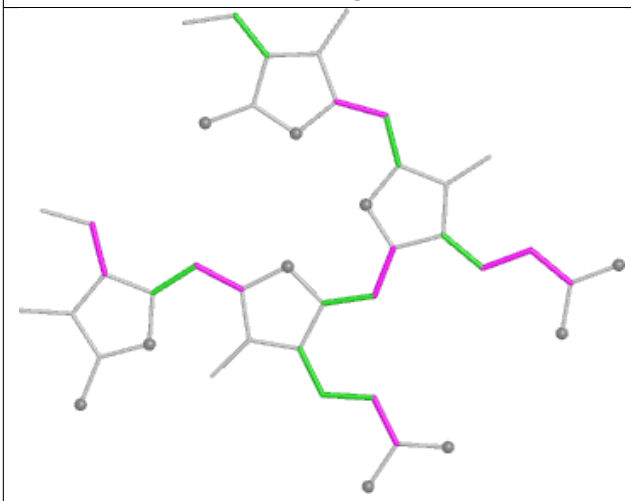
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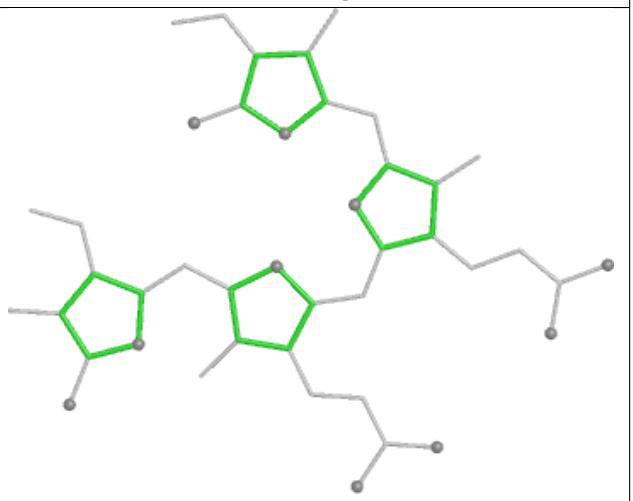
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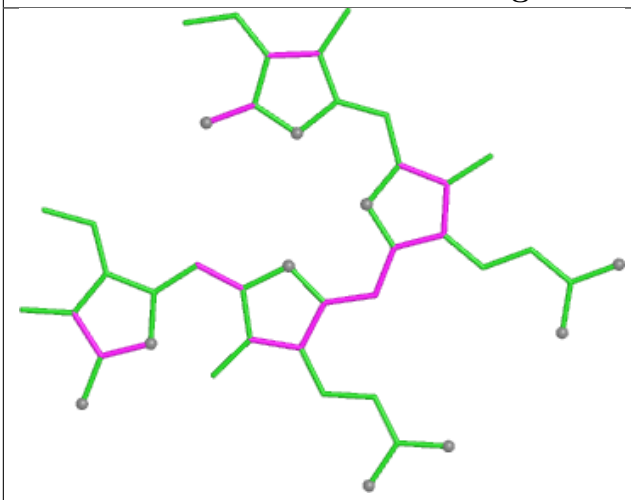


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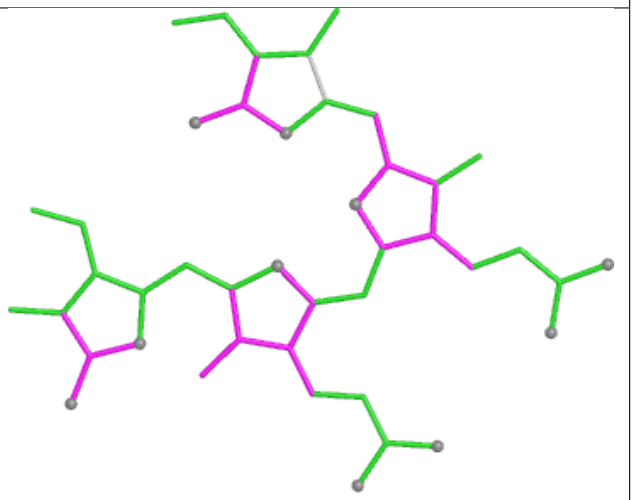


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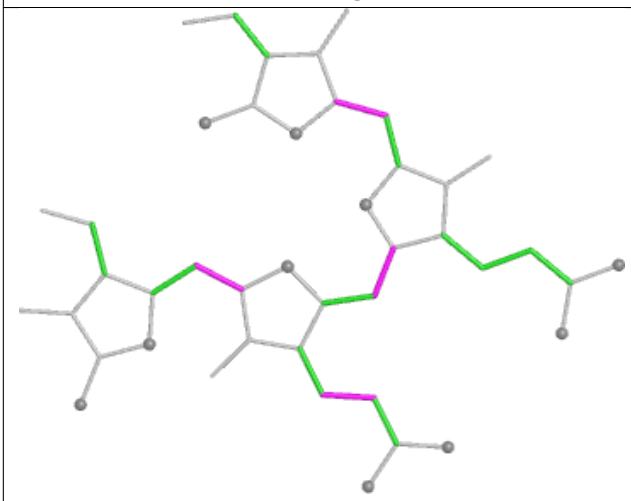
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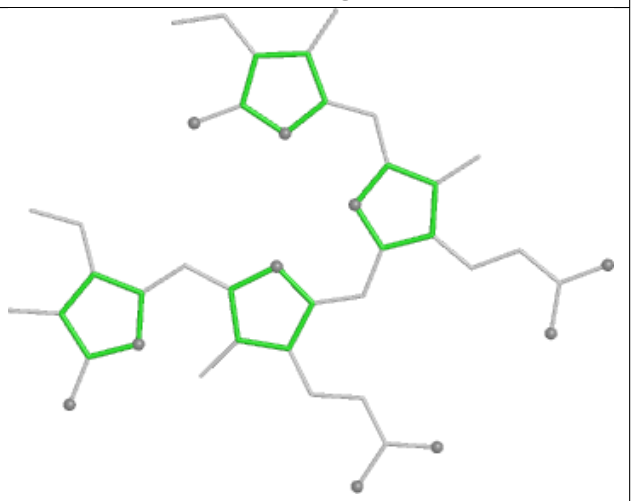
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Bond angles

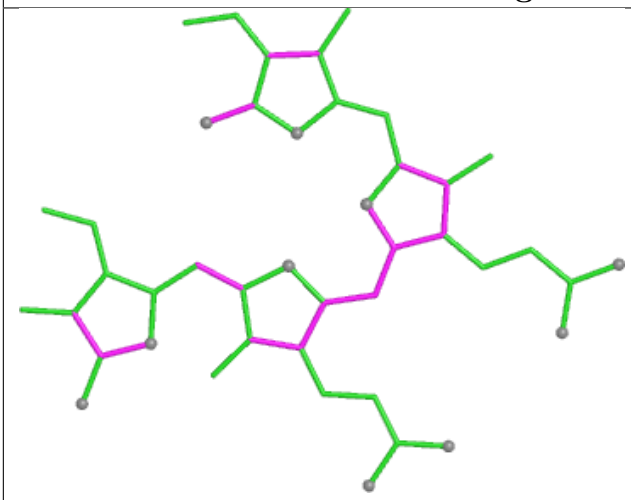


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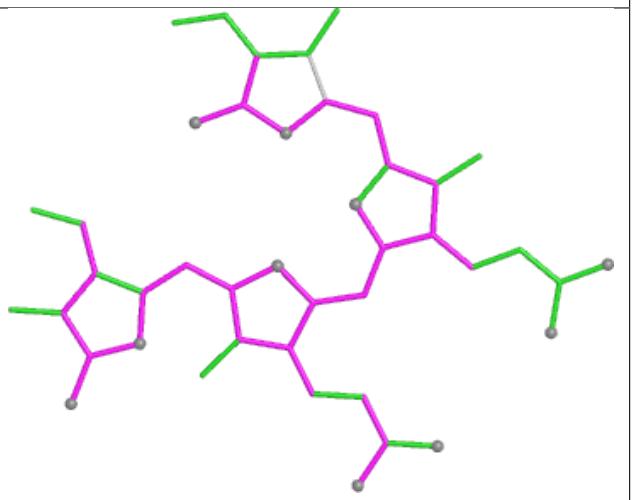


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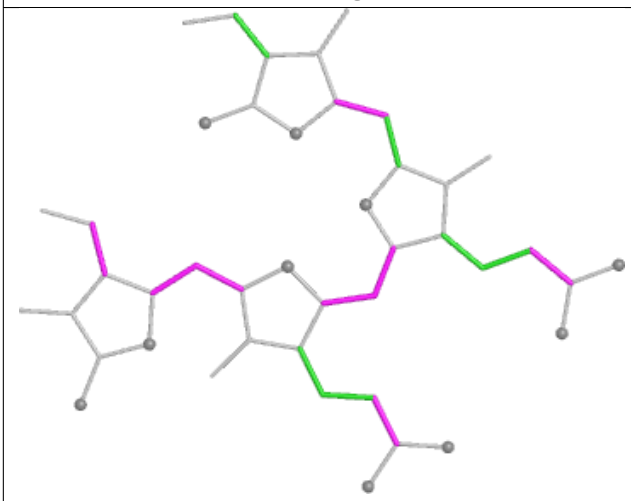
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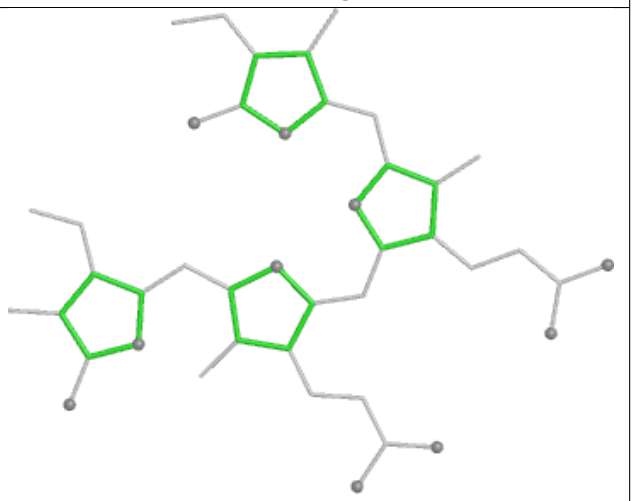
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Bond angles

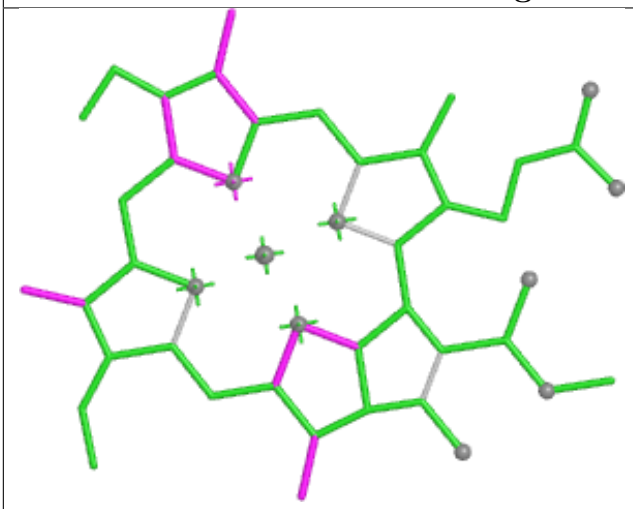


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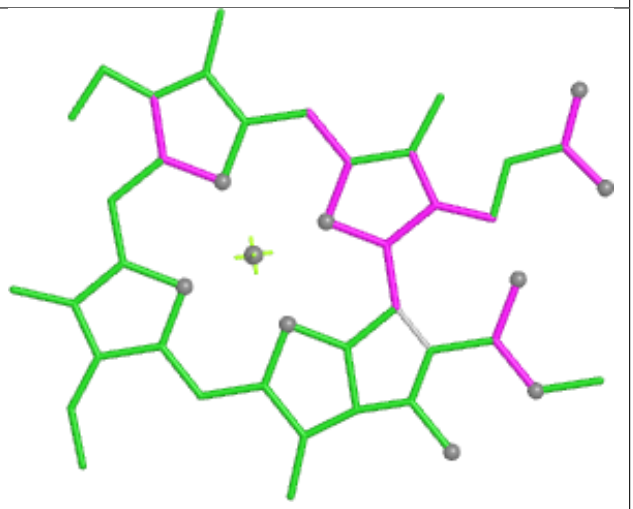


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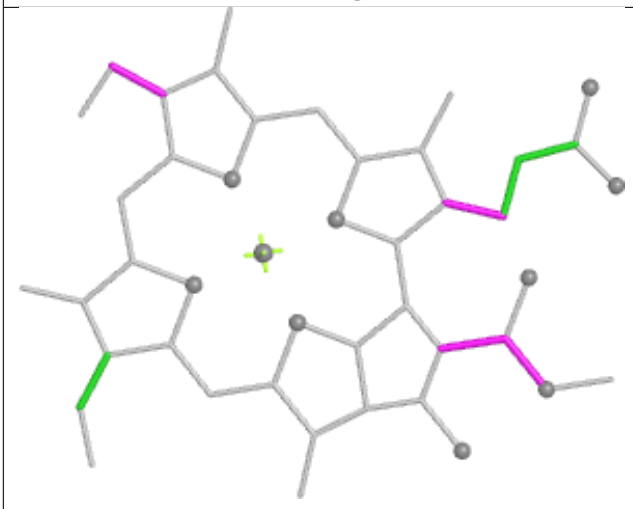
Ligand CLA 3N 313



Bond lengths



Bond angles

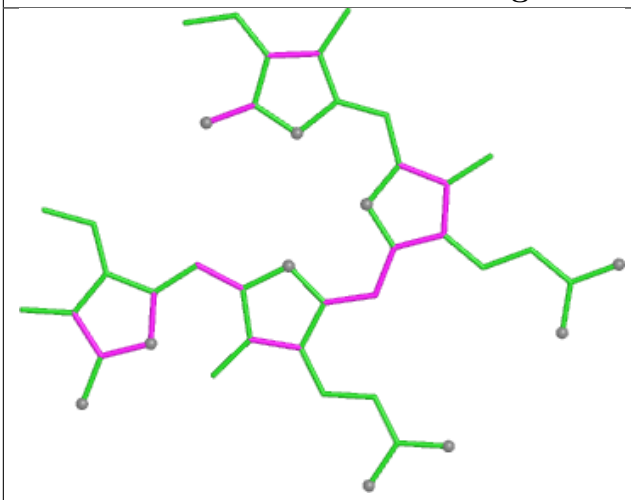


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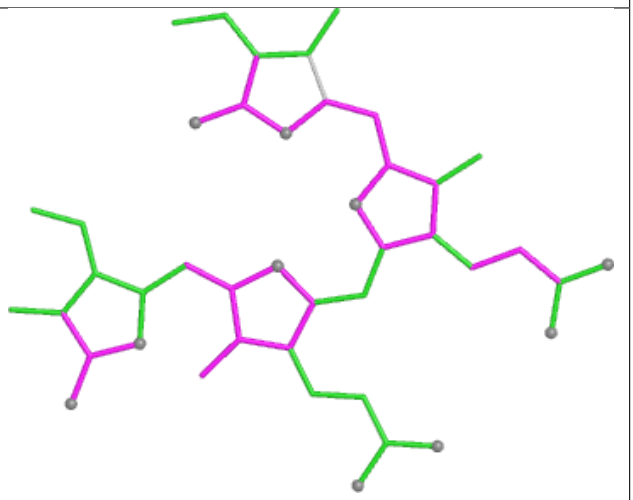


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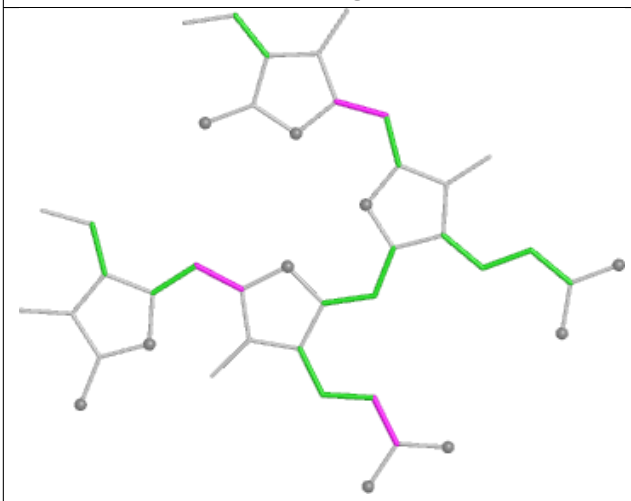
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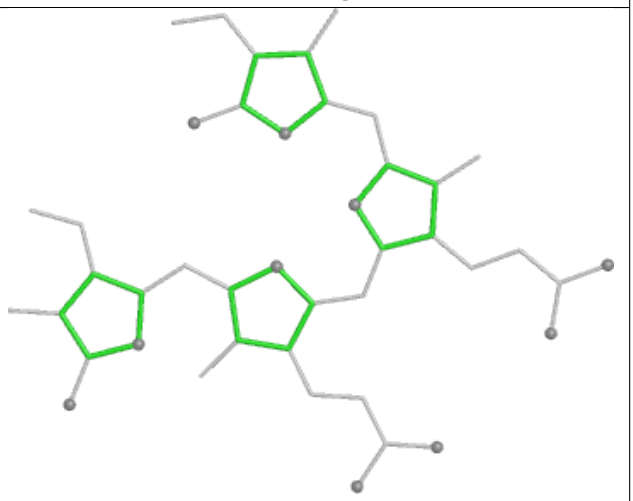
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Bond angles

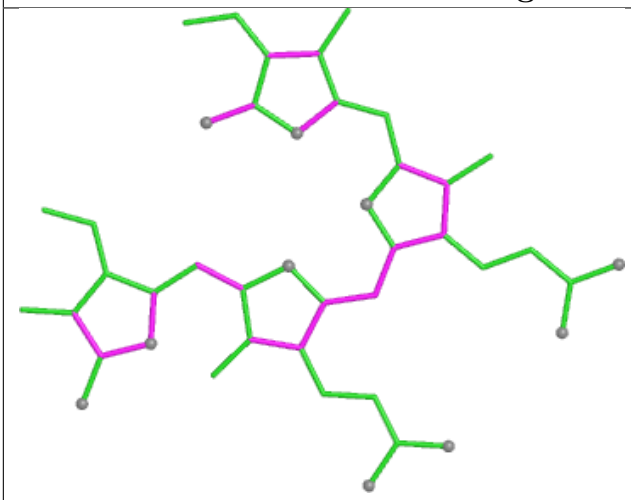


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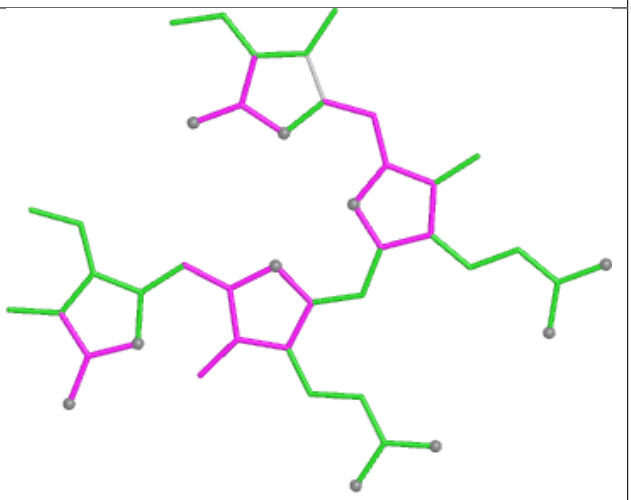


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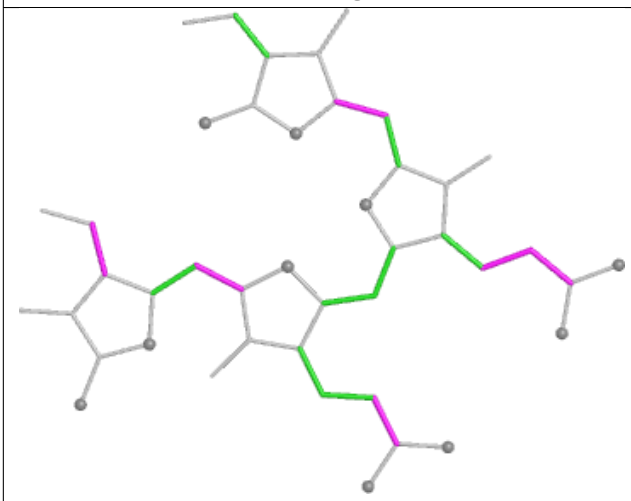
Ligand PEB E7 202



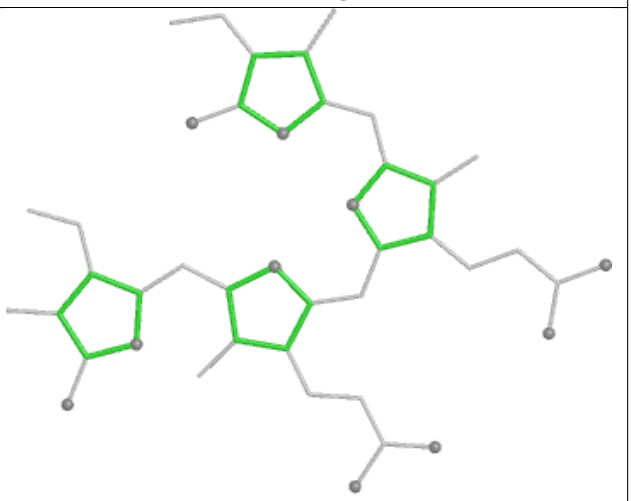
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Bond angles

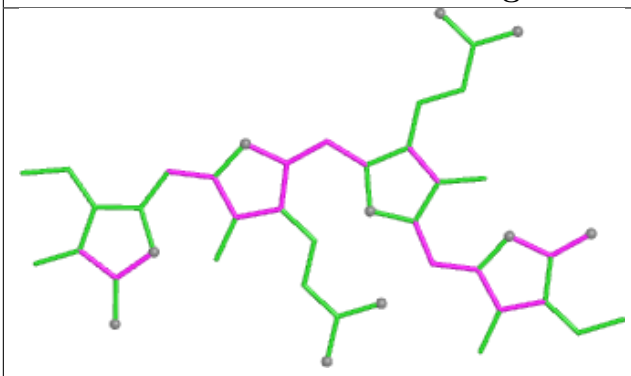


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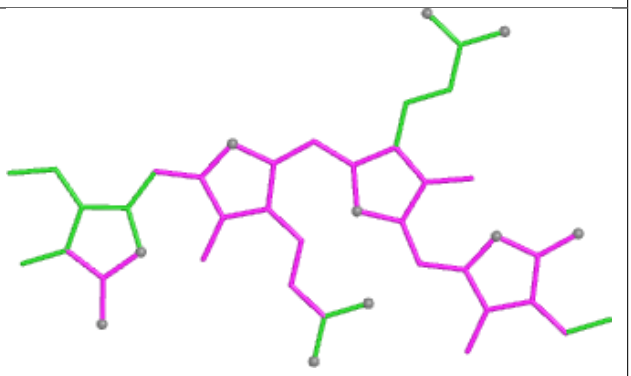


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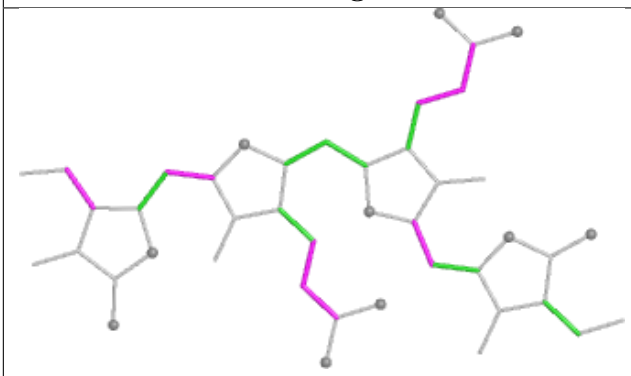
Ligand CYC JH 1003



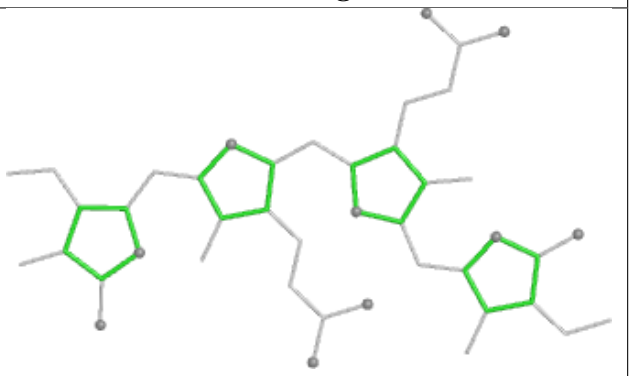
Bond lengths



Bond angles

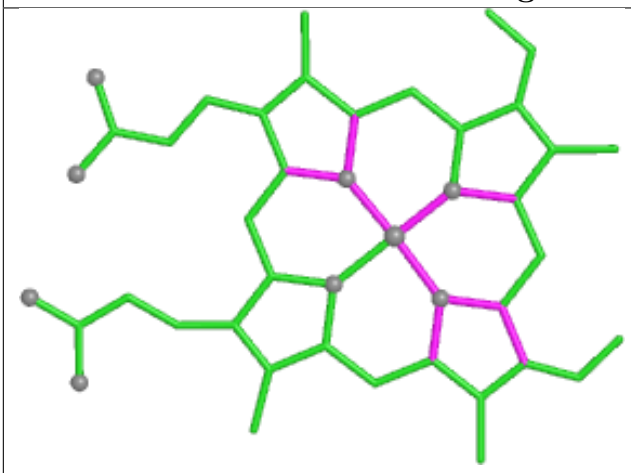


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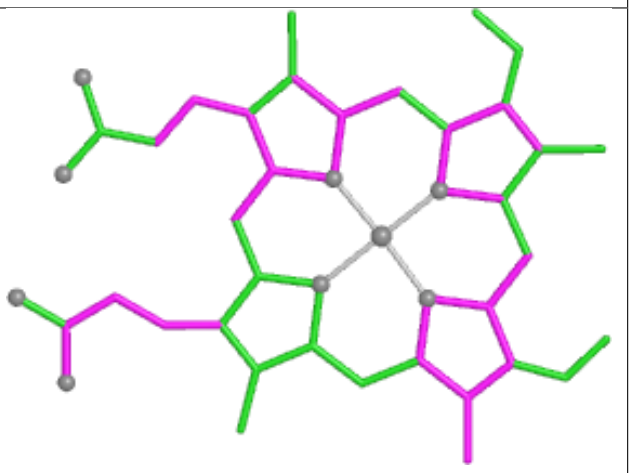


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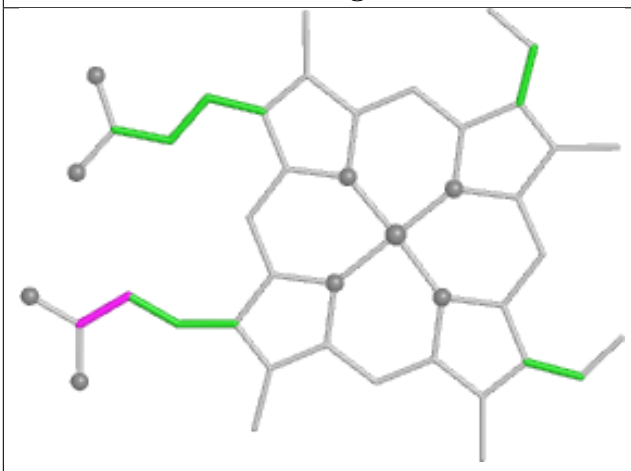
Ligand HEM f6 101



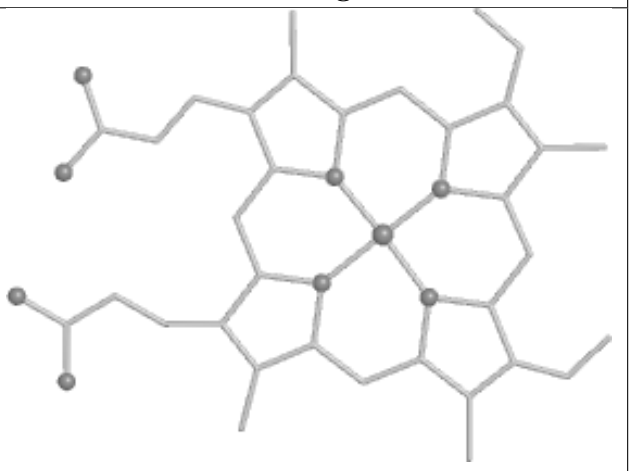
Bond lengths



Bond angles

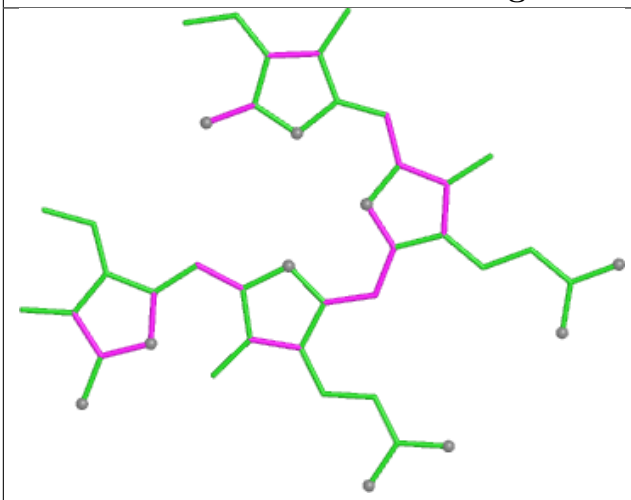


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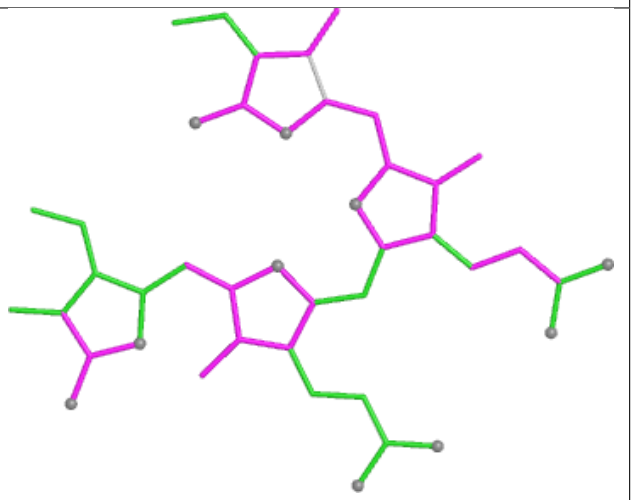


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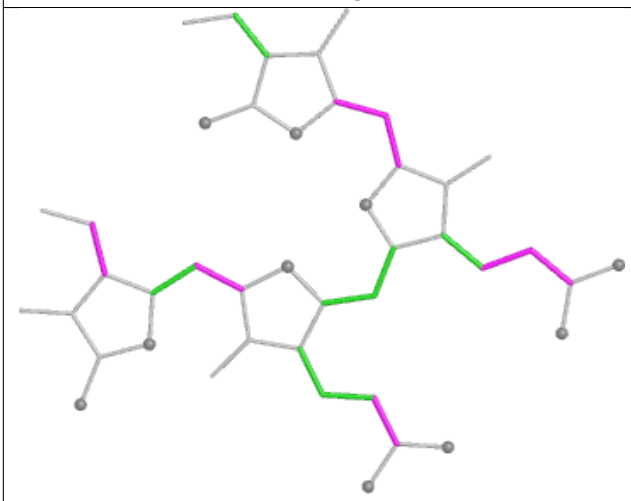
Ligand PEB MP 203



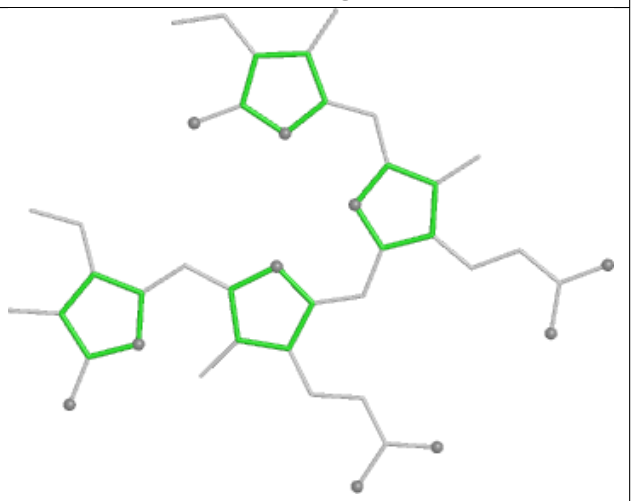
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Bond angles

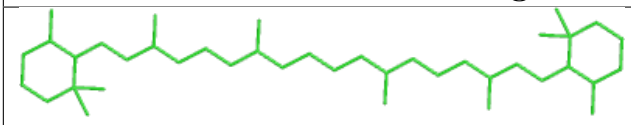


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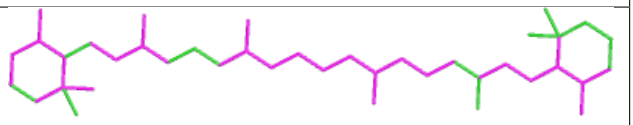


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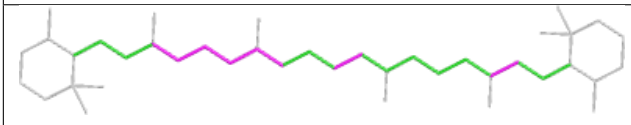
Ligand BCR LN 205



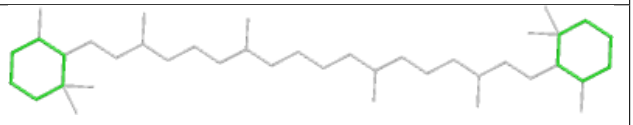
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Bond angles

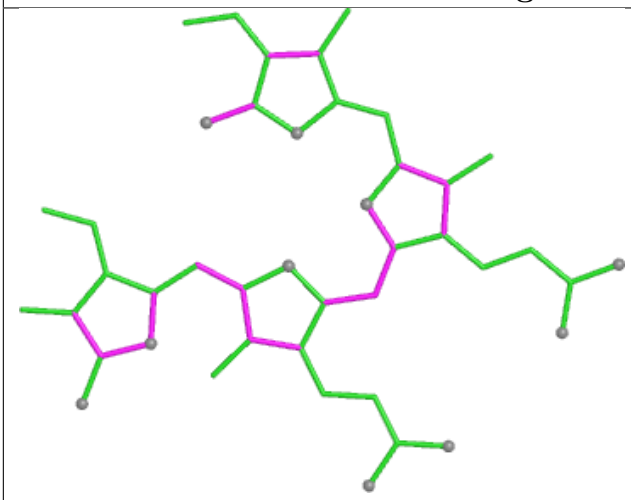


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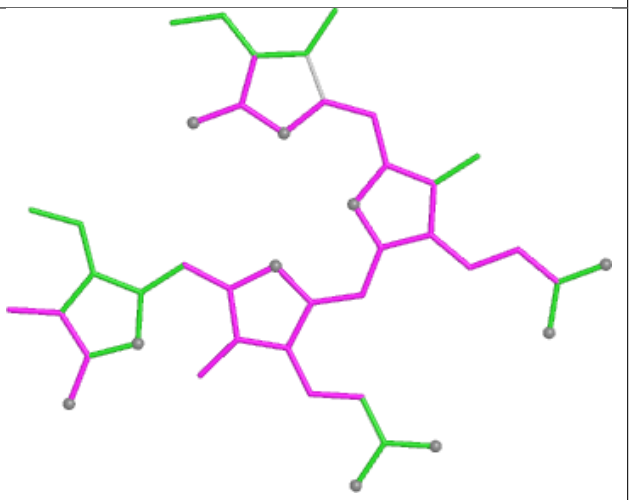


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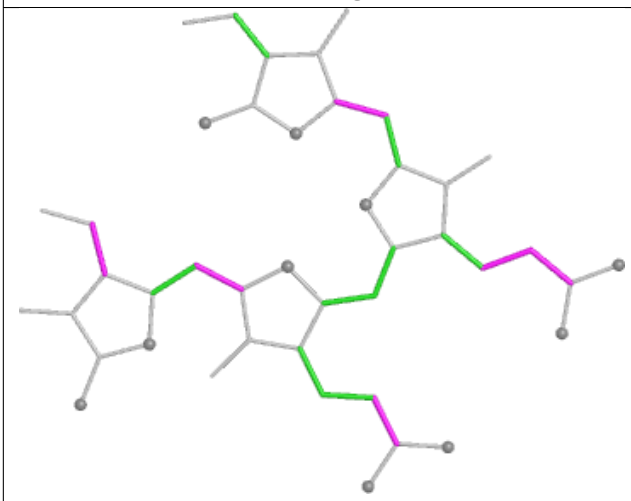
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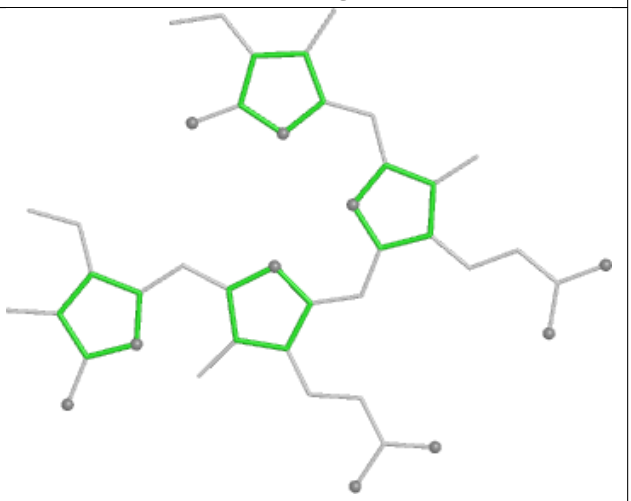
Bond lengths



Bond angles

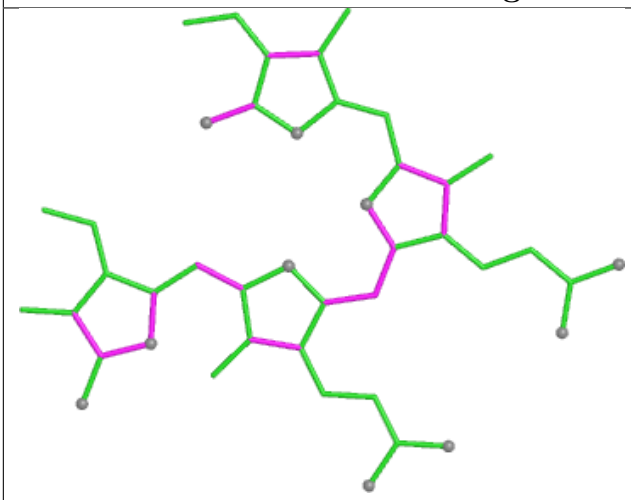


Torsions

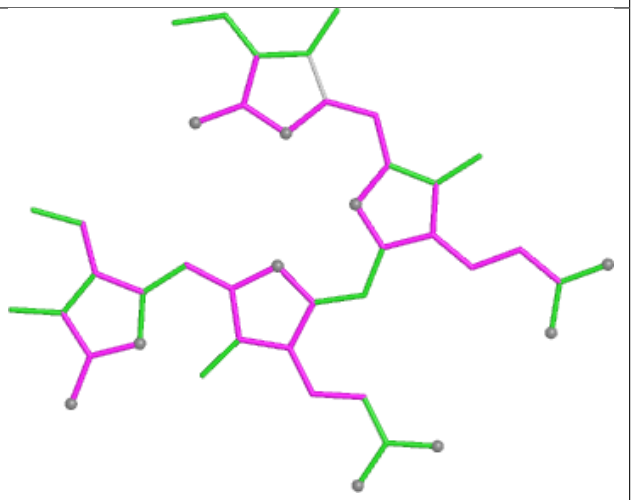


Rings

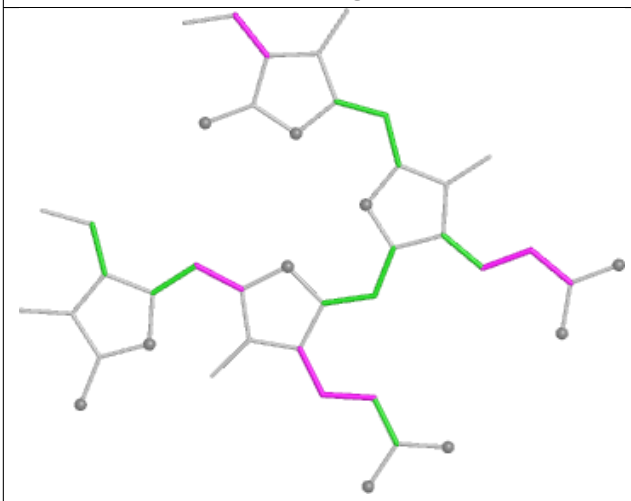
Ligand PEB GE 1002



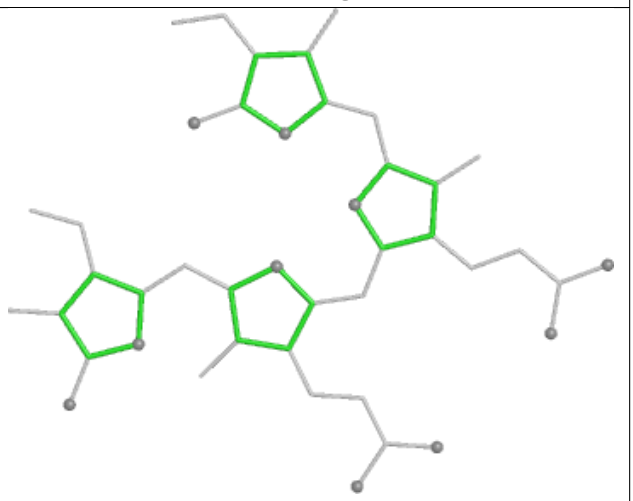
Bond lengths



Bond angles

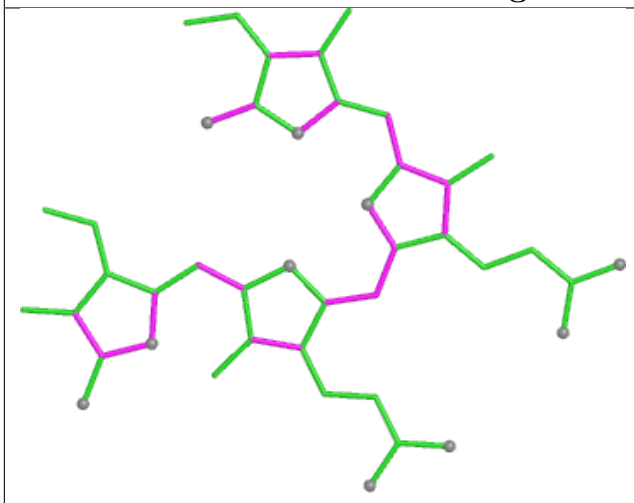


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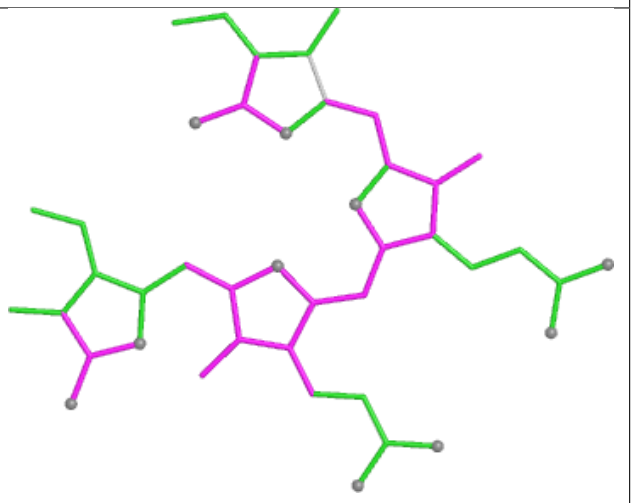


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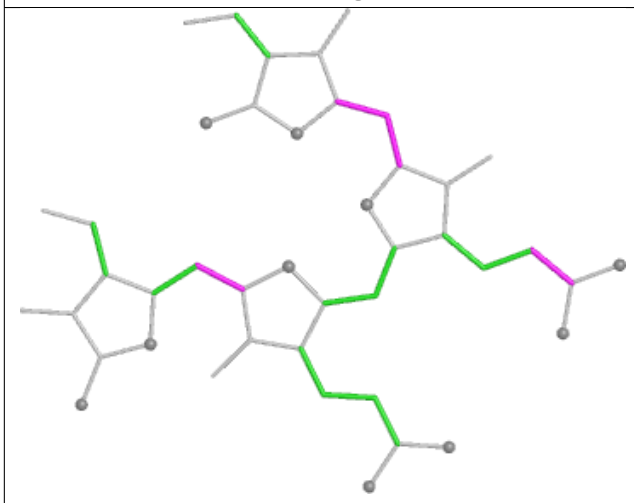
Ligand PEB TM 201



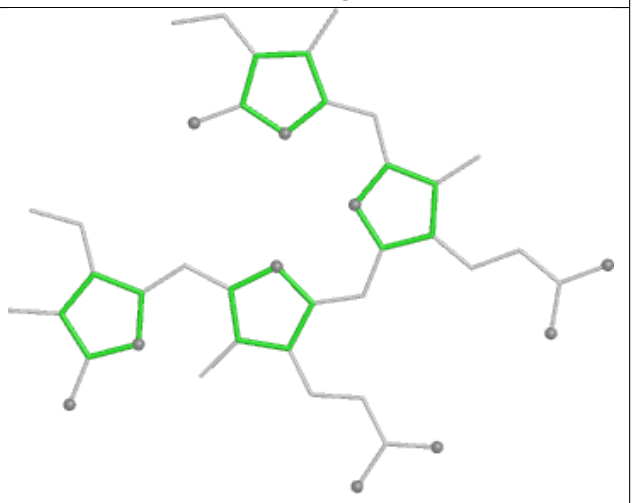
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Bond angles

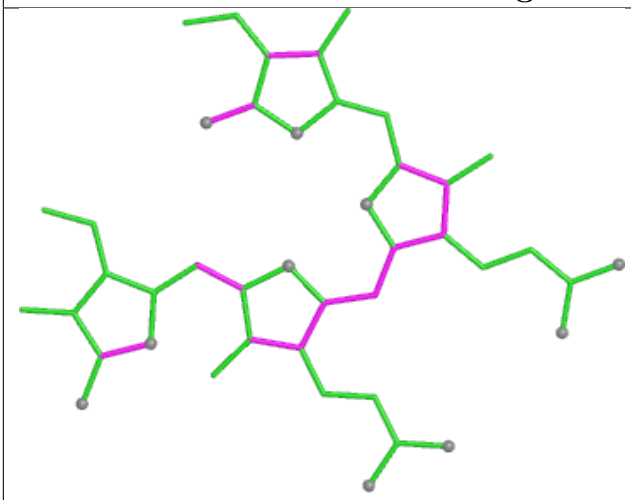


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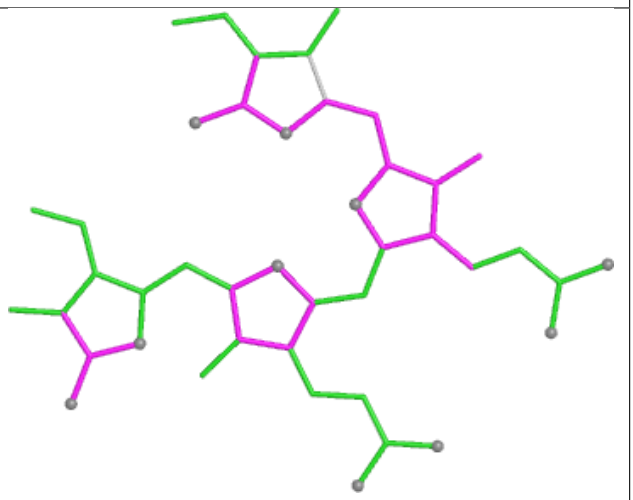


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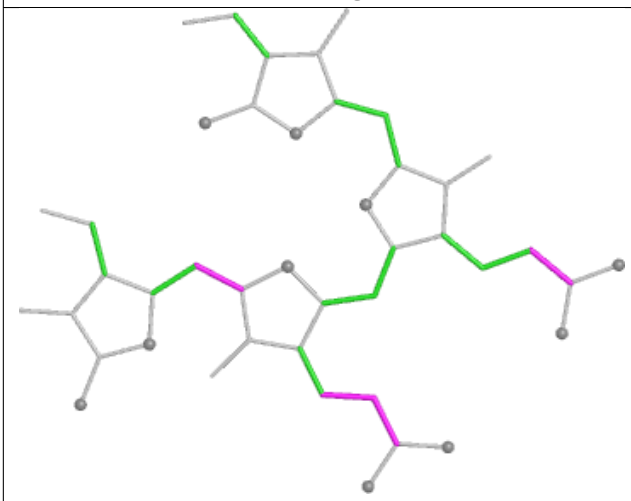
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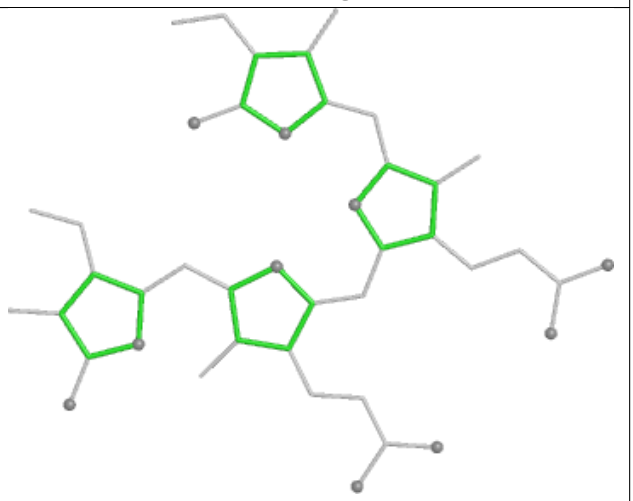
Bond lengths



Bond angles

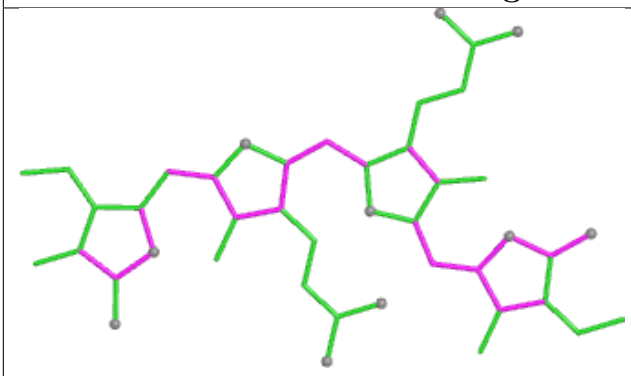


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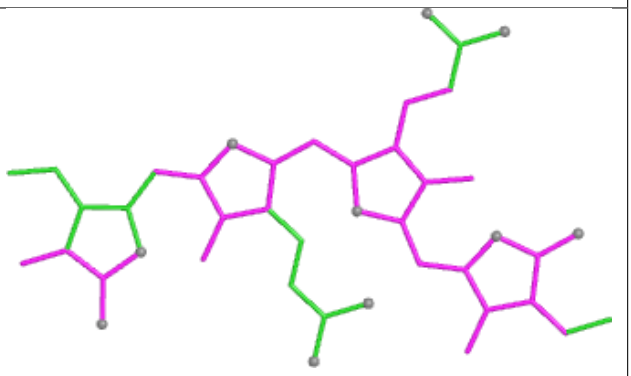


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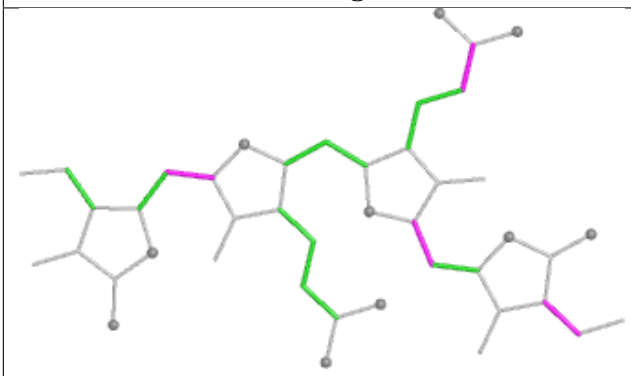
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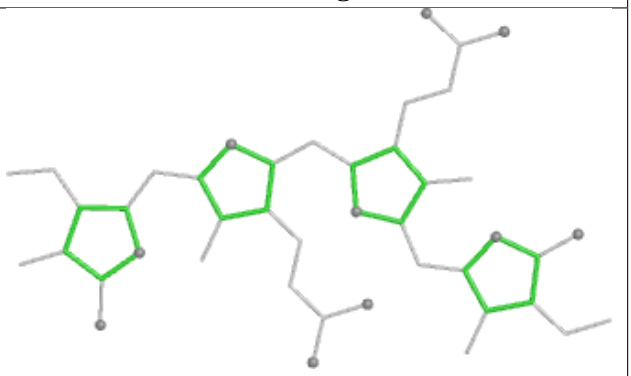
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Bond angles

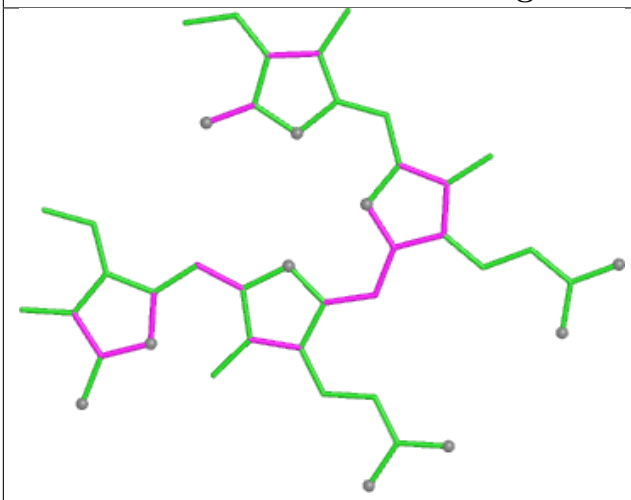


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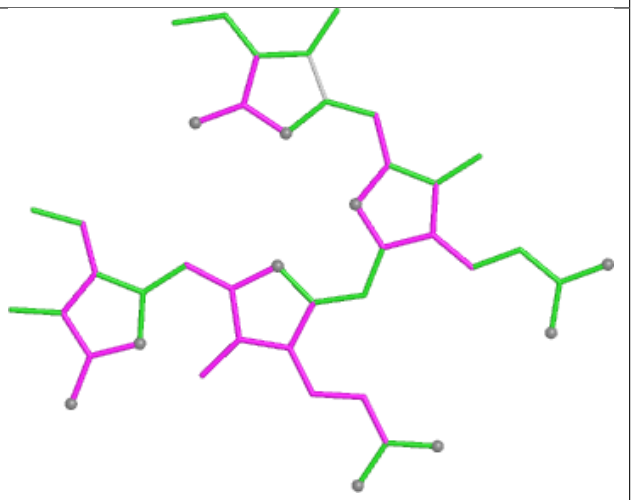


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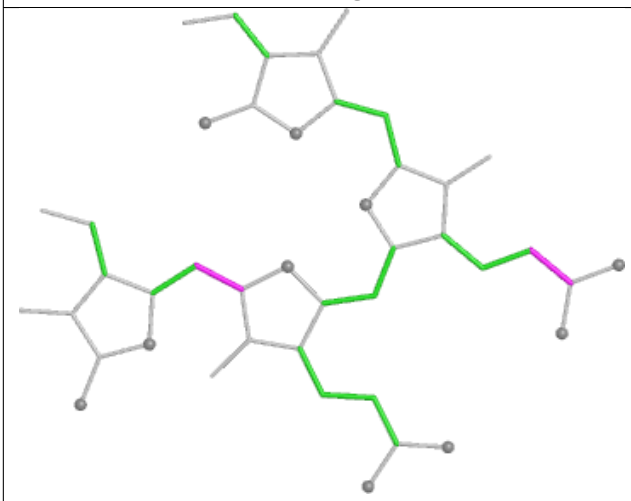
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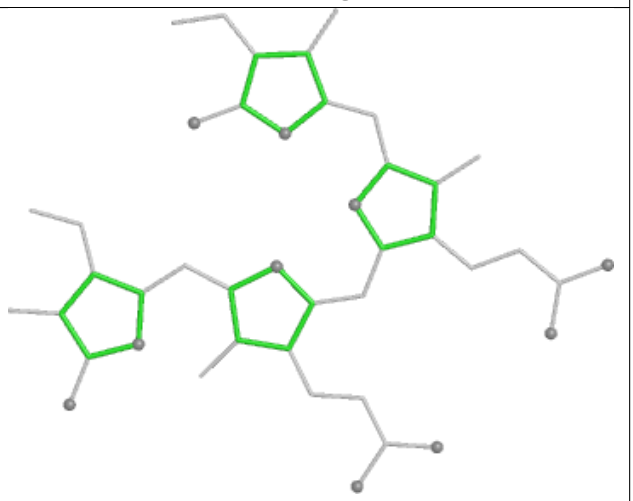
Bond lengths



Bond angles

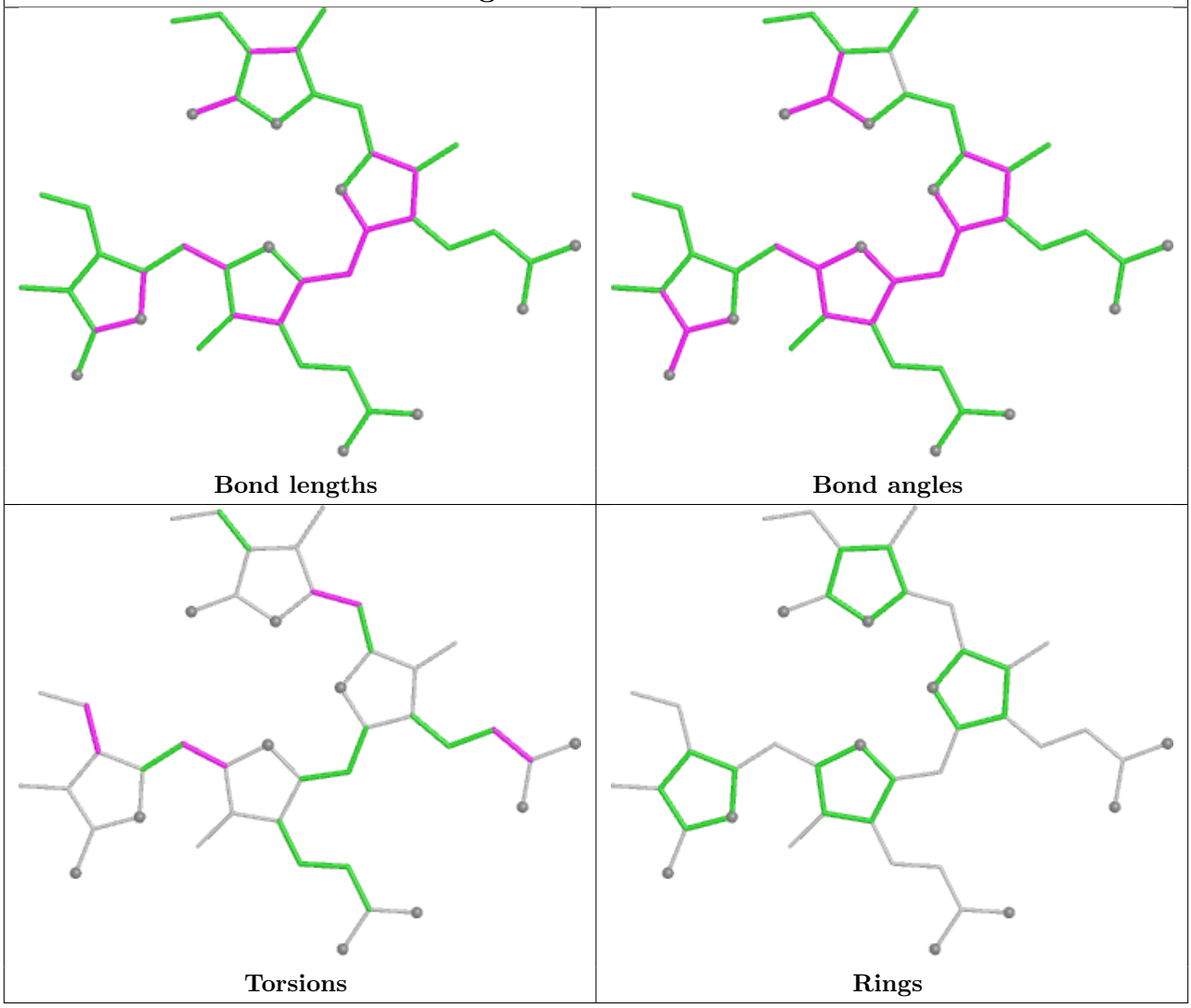


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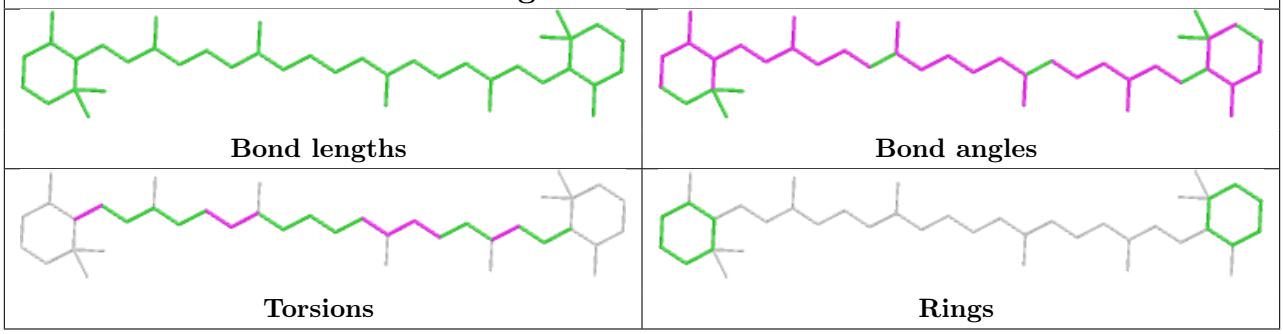


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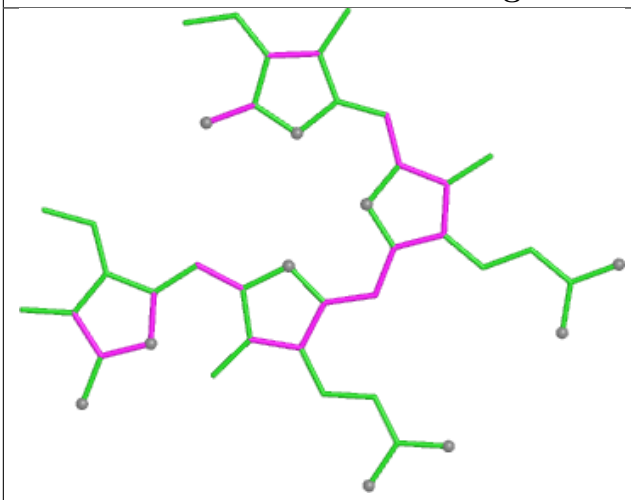
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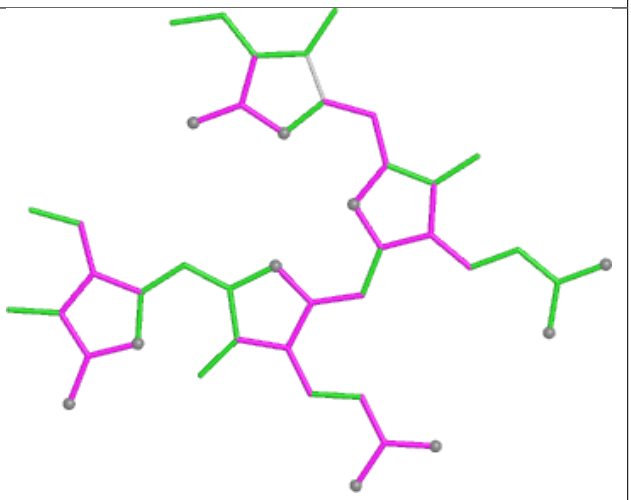
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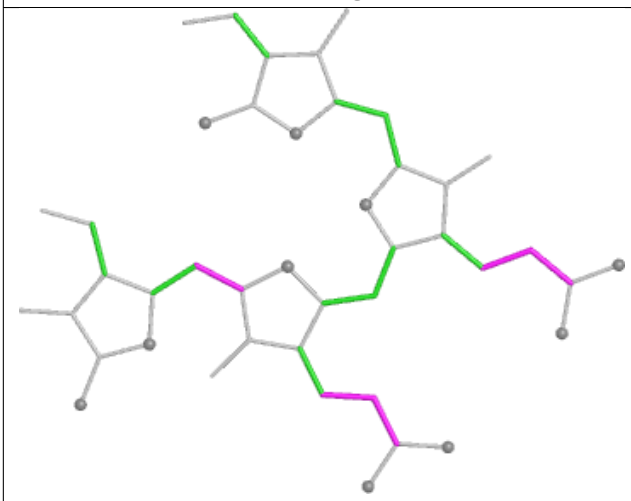
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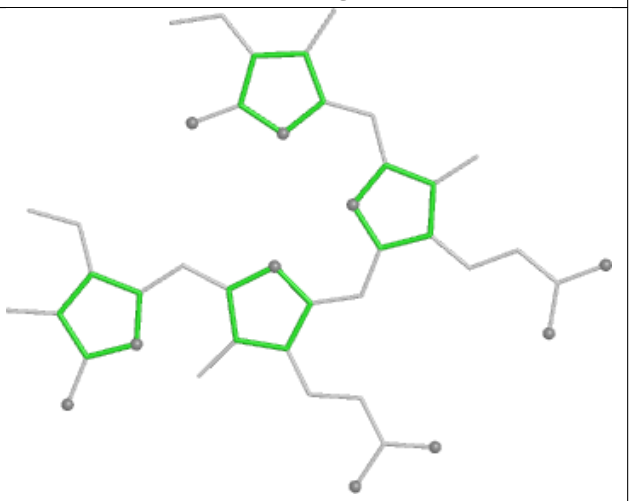
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Bond angles

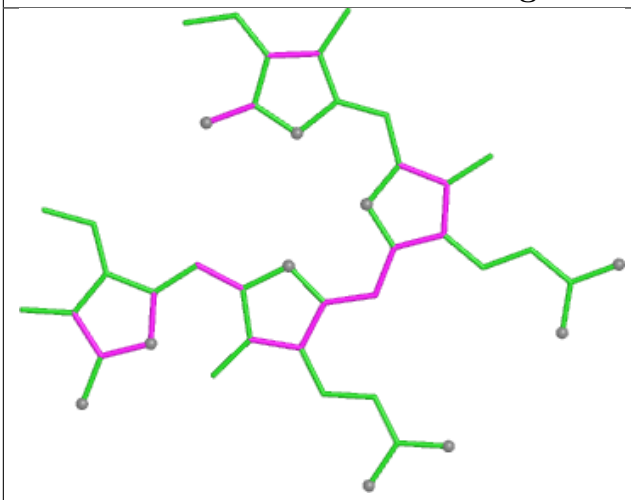


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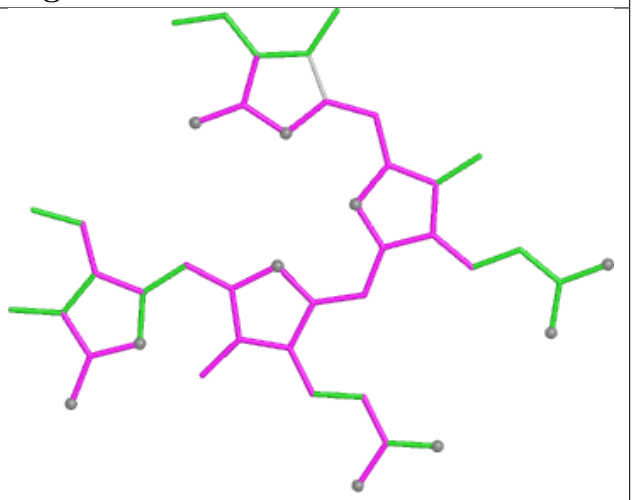


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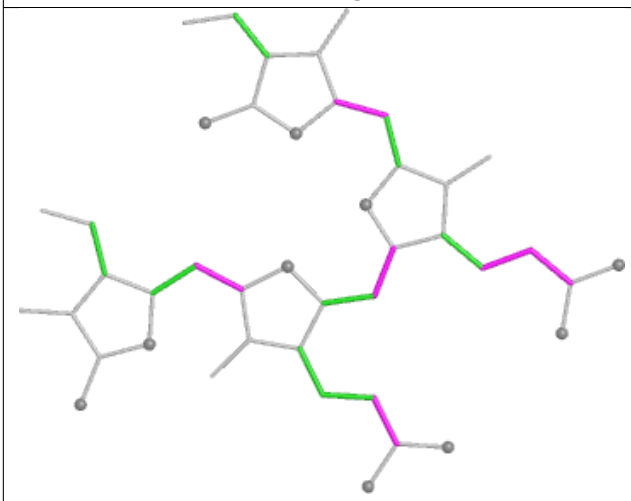
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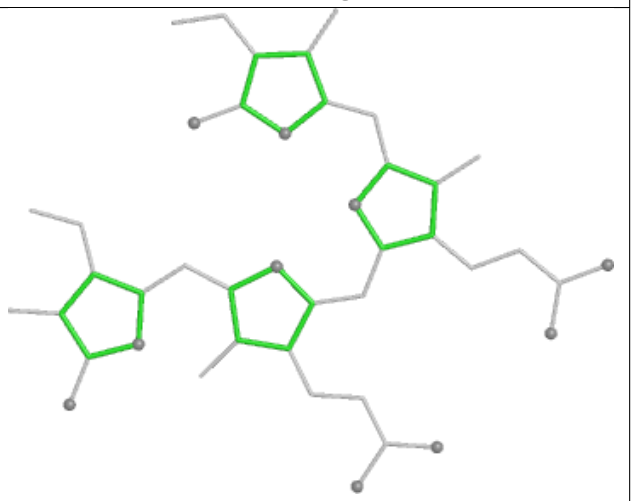
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Bond angles

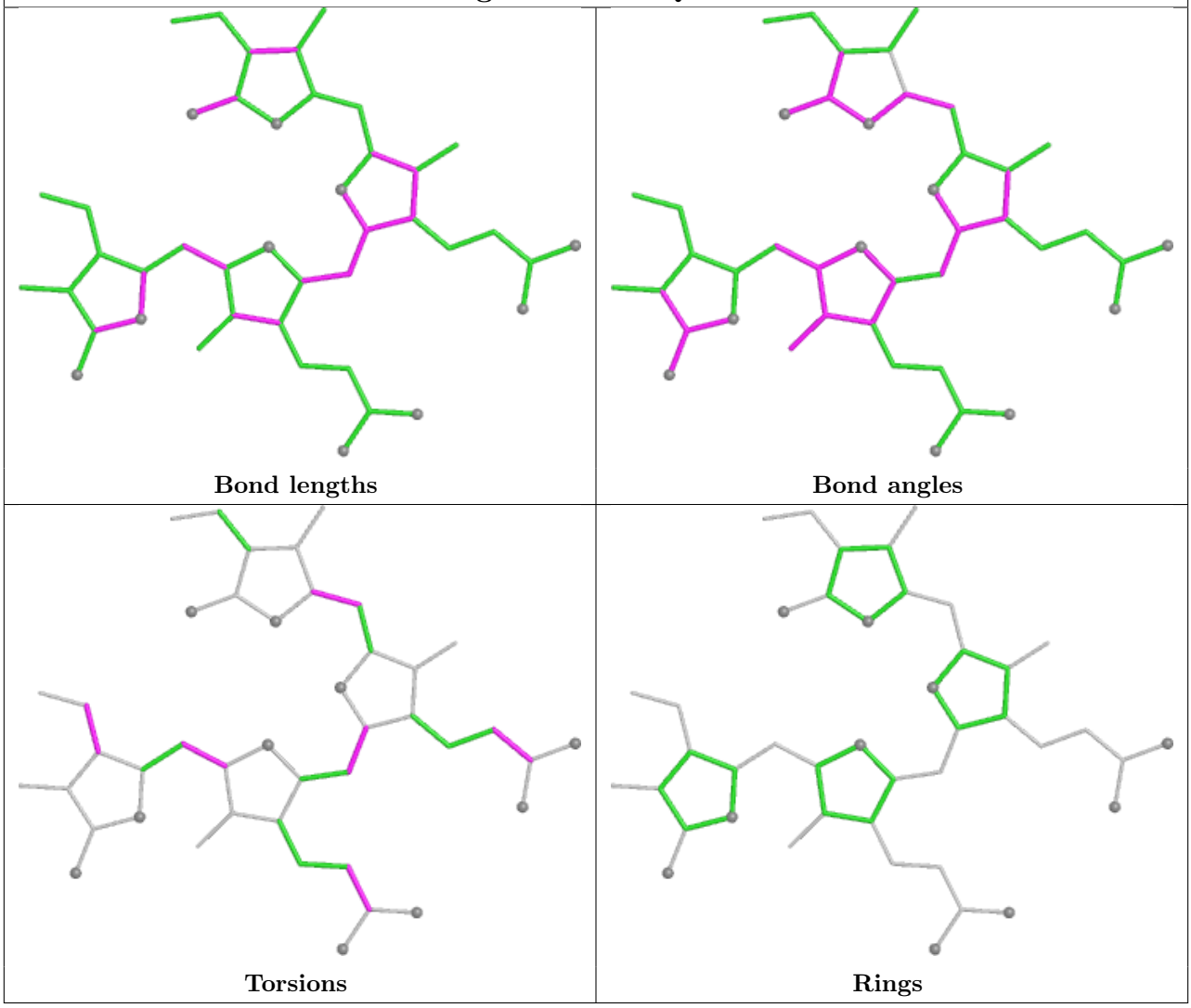


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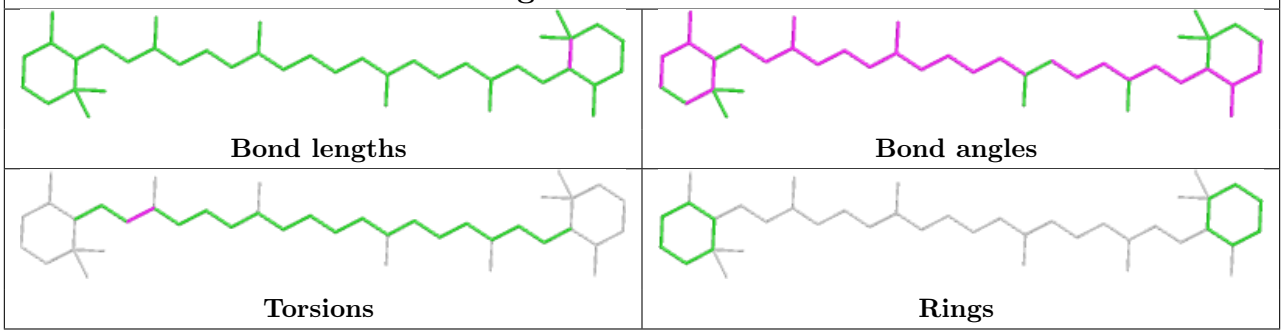


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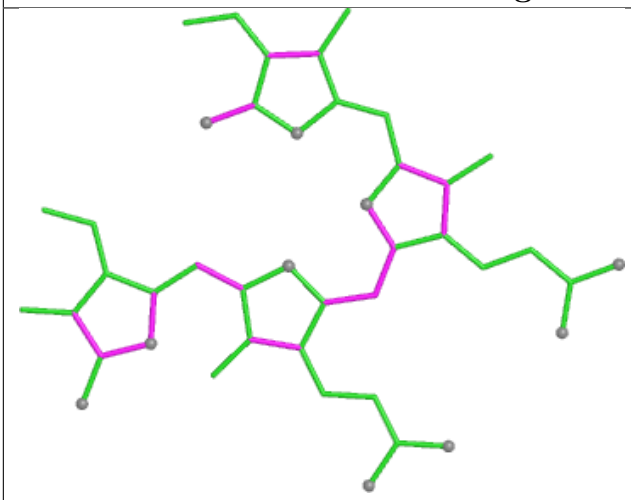
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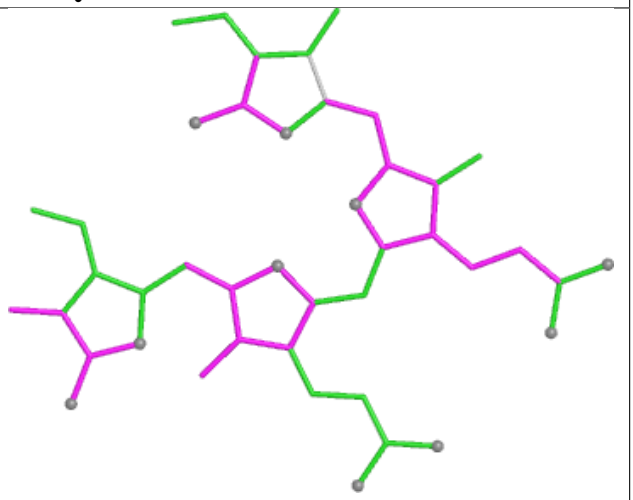
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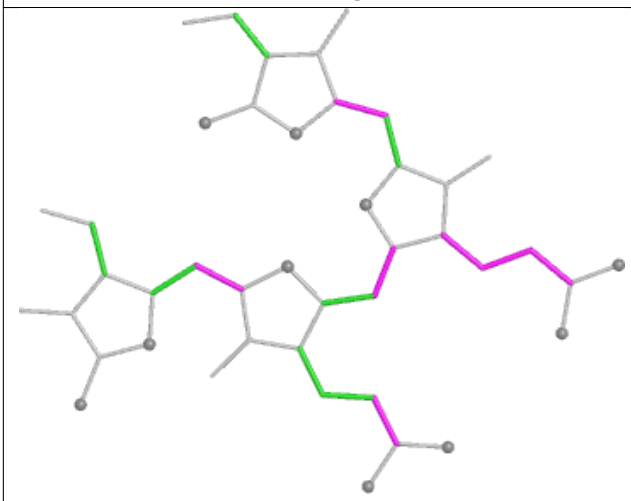
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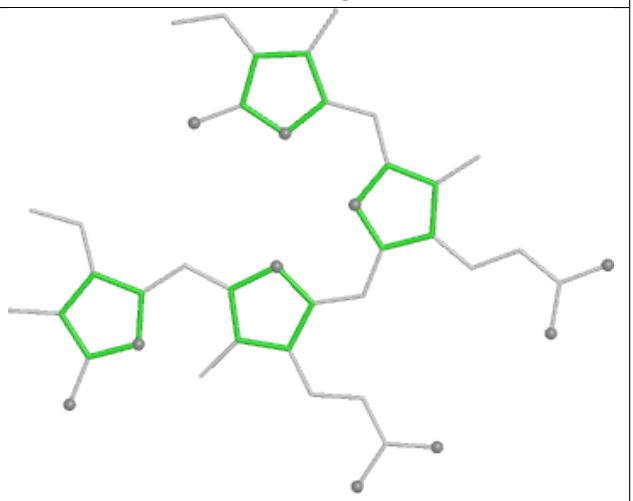
Bond lengths



Bond angles

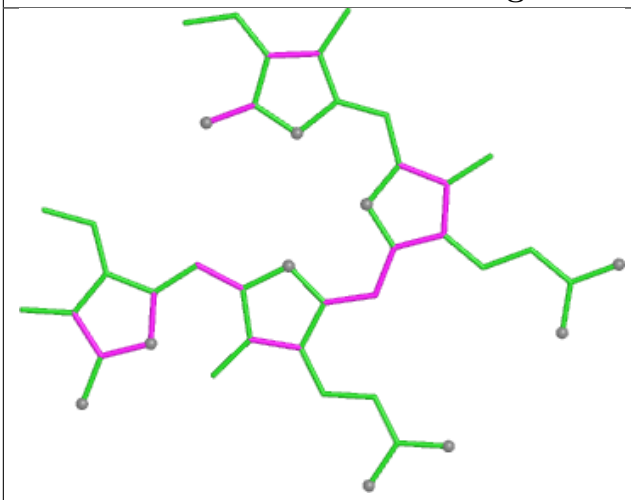


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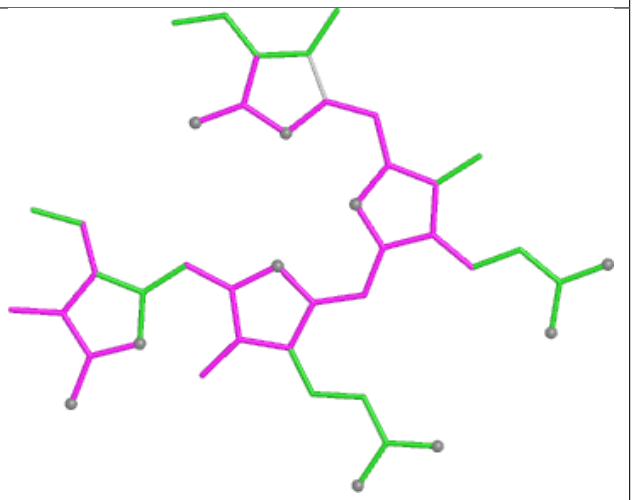


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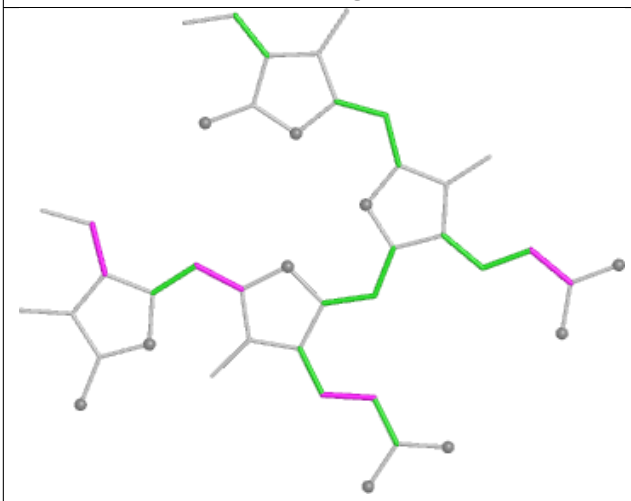
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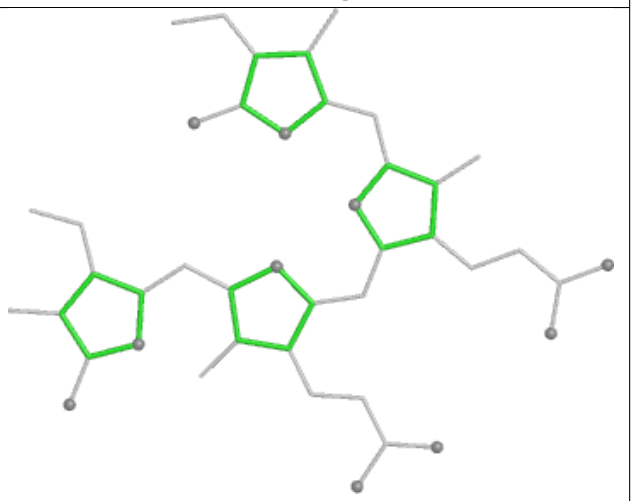
Bond lengths



Bond angles

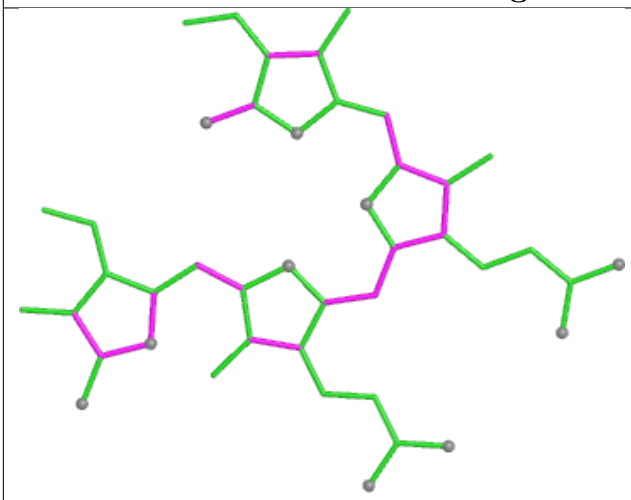


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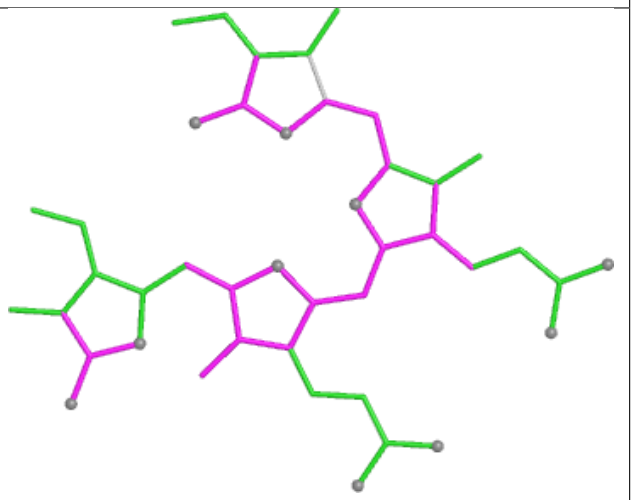


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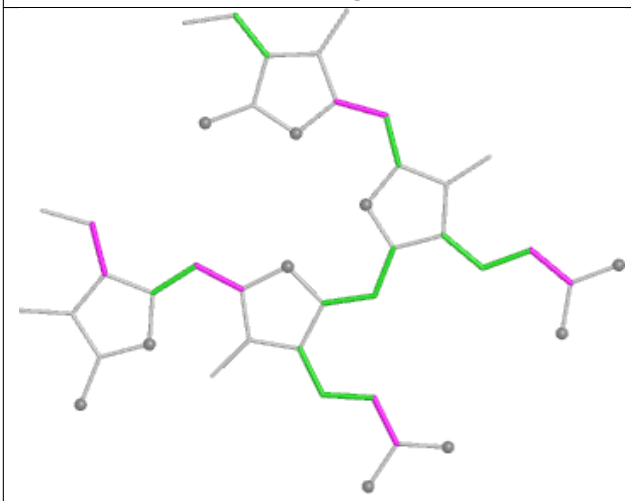
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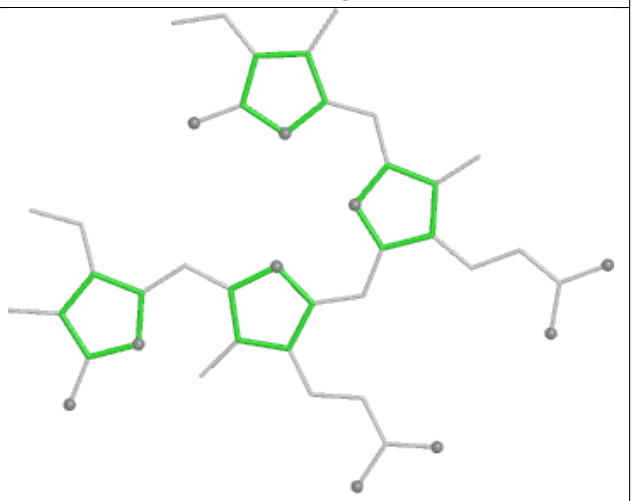
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Bond angles

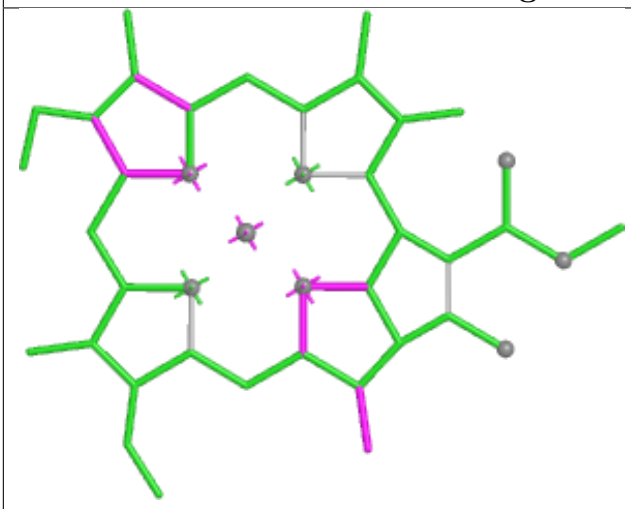


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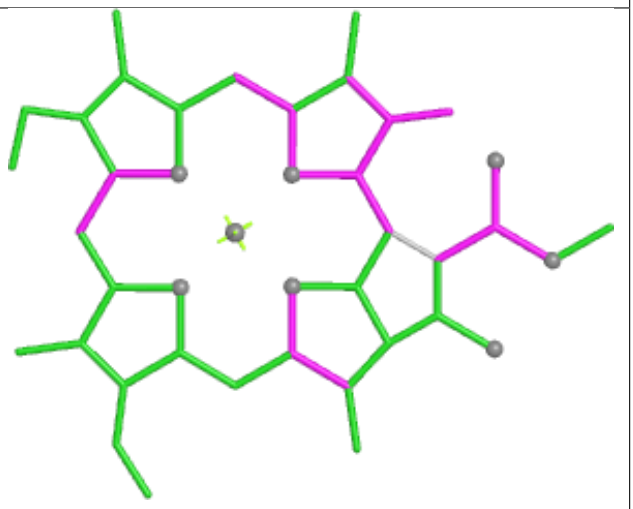


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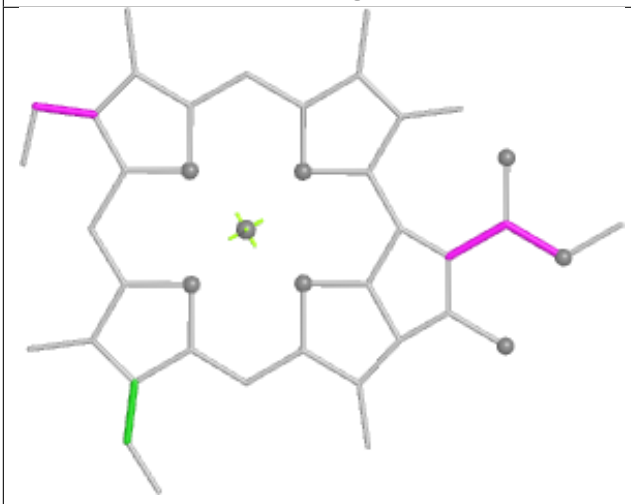
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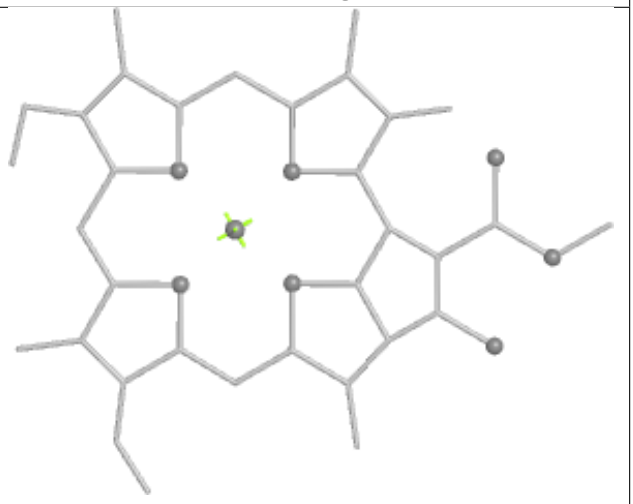
Bond lengths



Bond angles

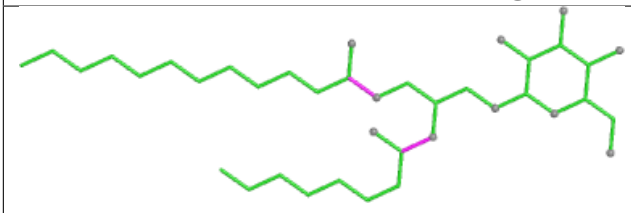


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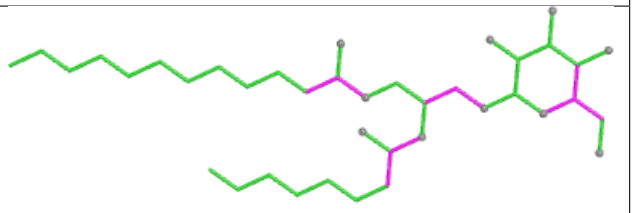


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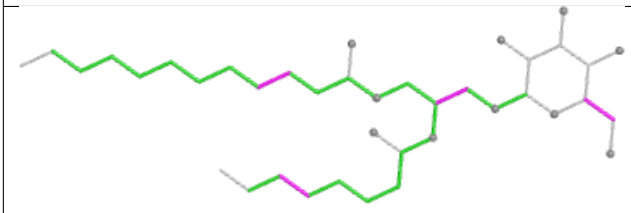
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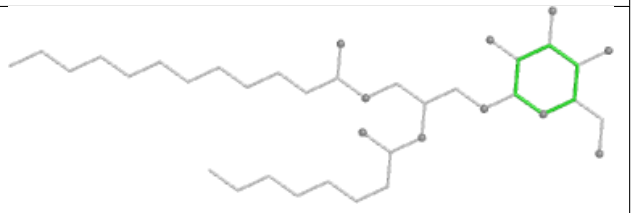
Bond lengths



Bond angles

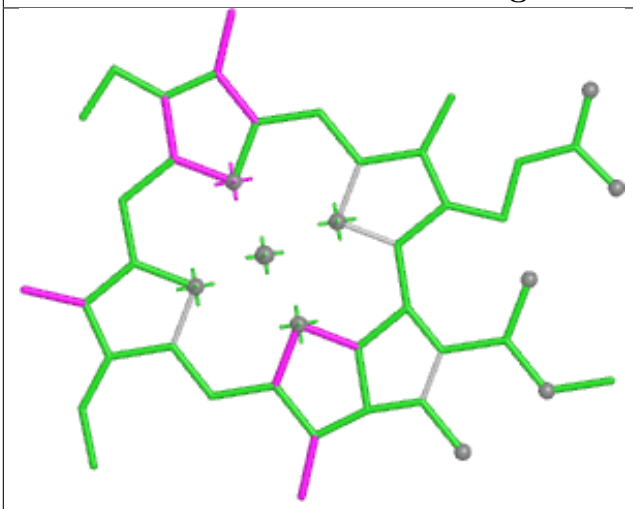


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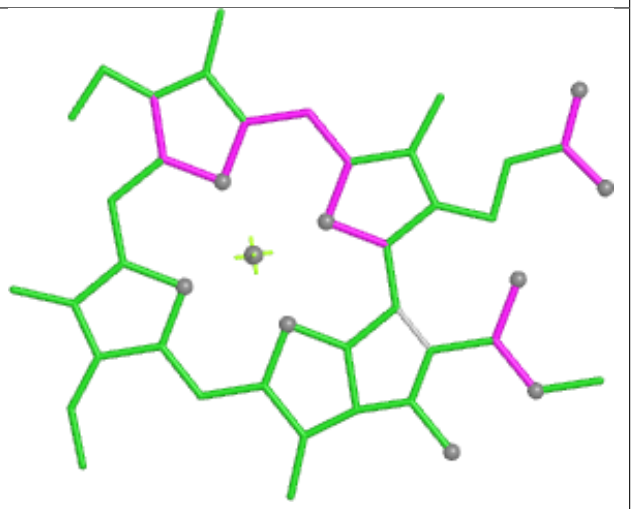


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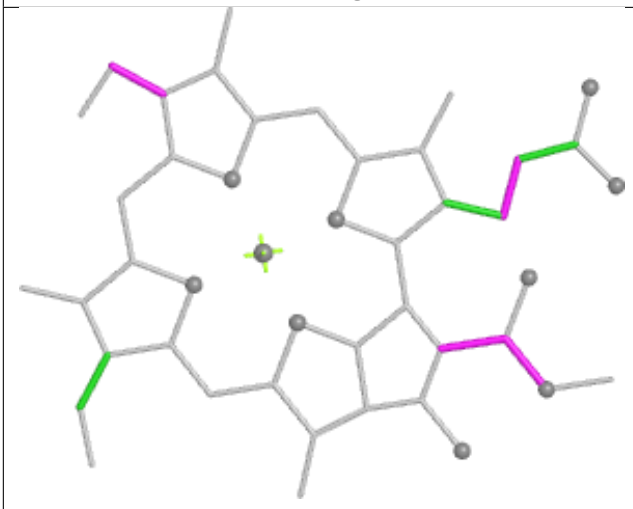
Ligand CLA AN 836



Bond lengths



Bond angles

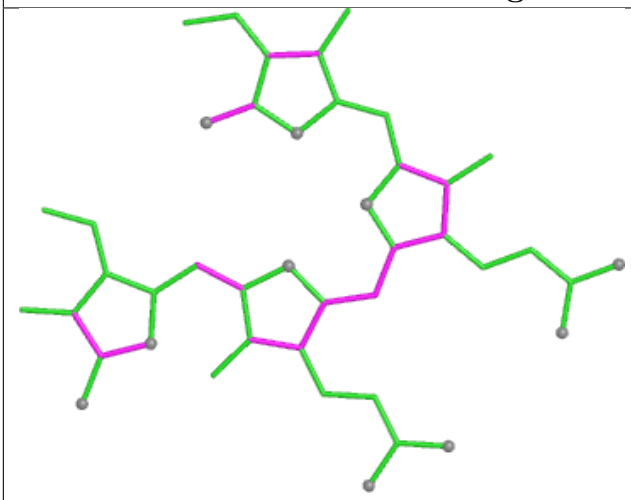


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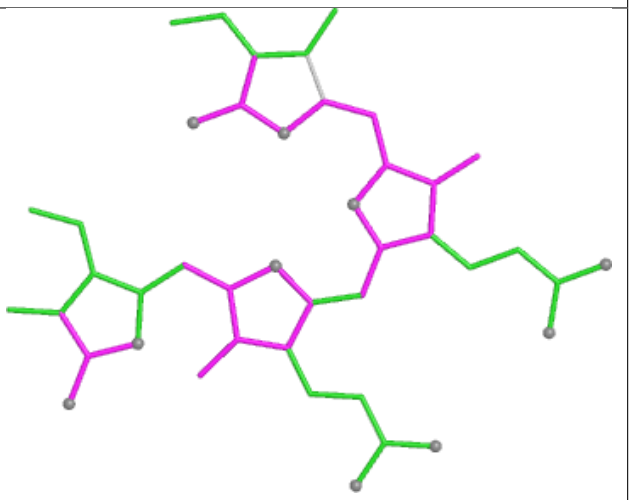


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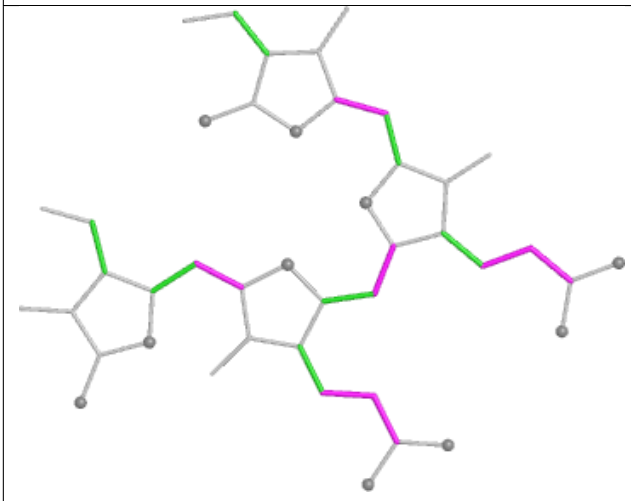
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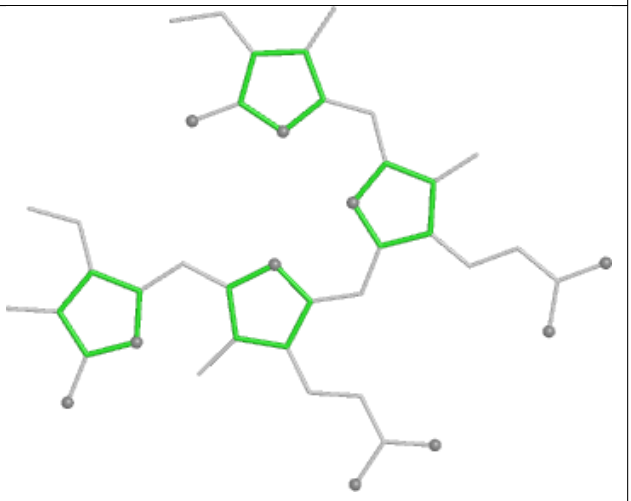
Bond lengths



Bond angles

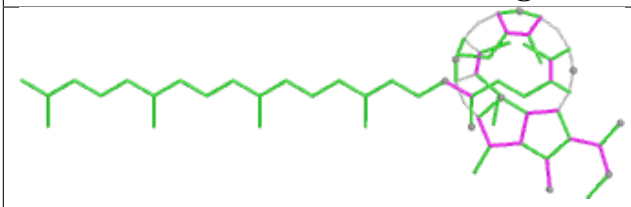


Torsions

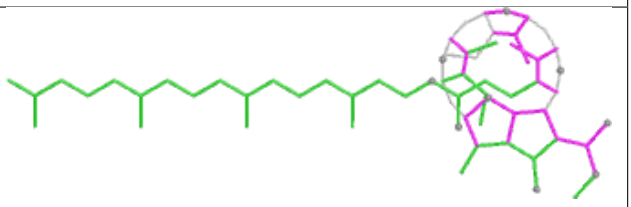


Rings

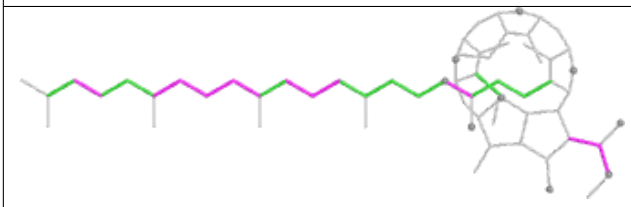
Ligand PHO aL 610



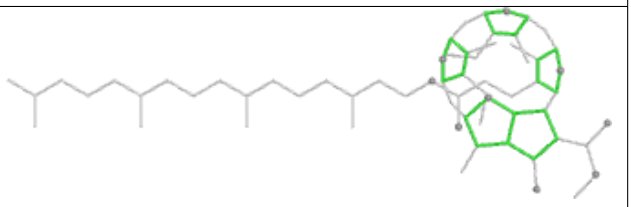
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Bond angles

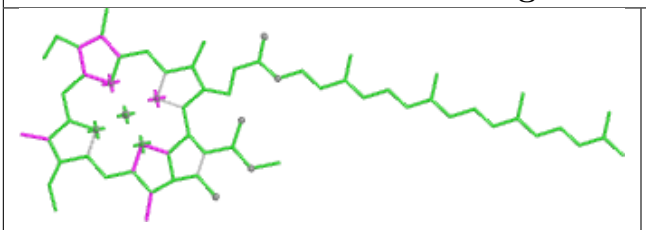


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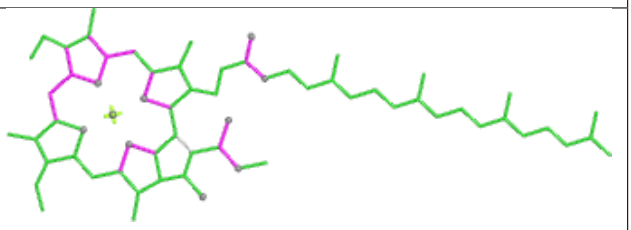


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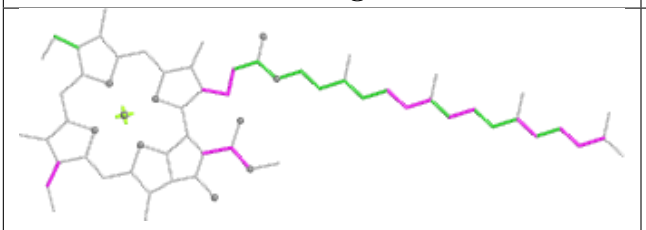
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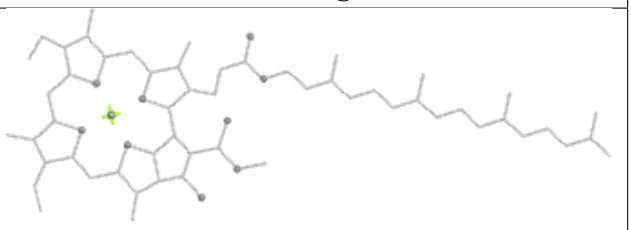
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Bond angles

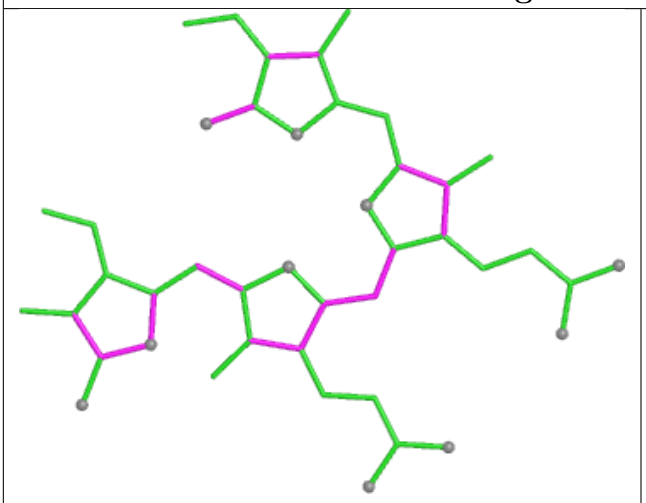


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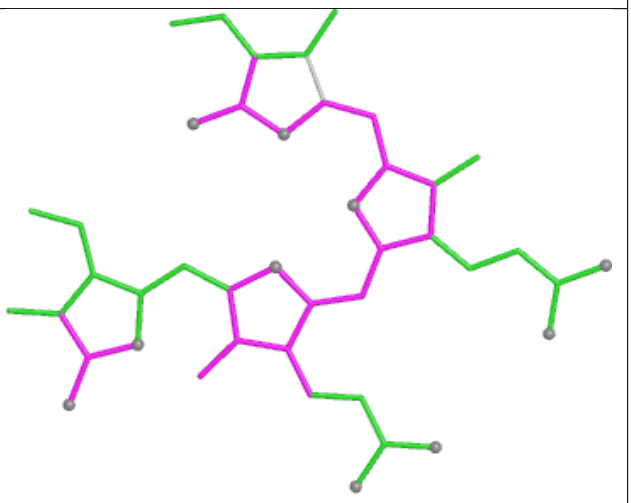


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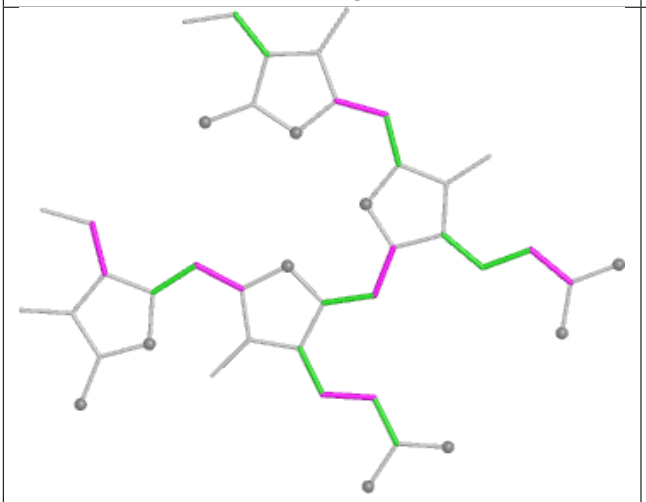
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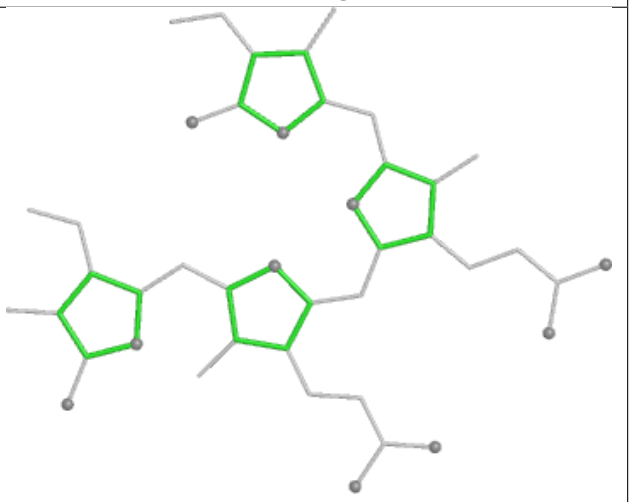
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Bond angles

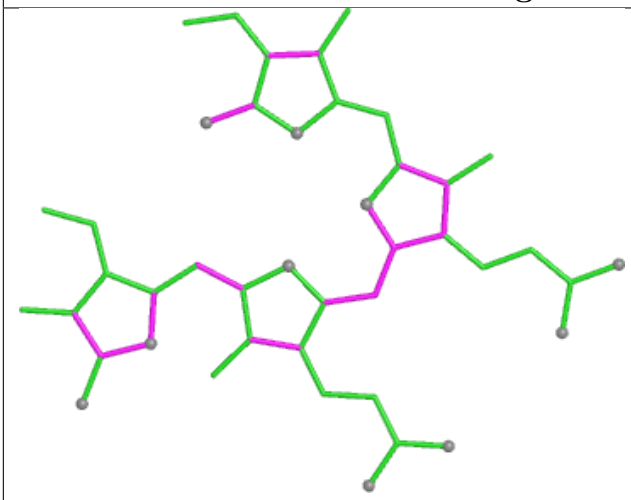


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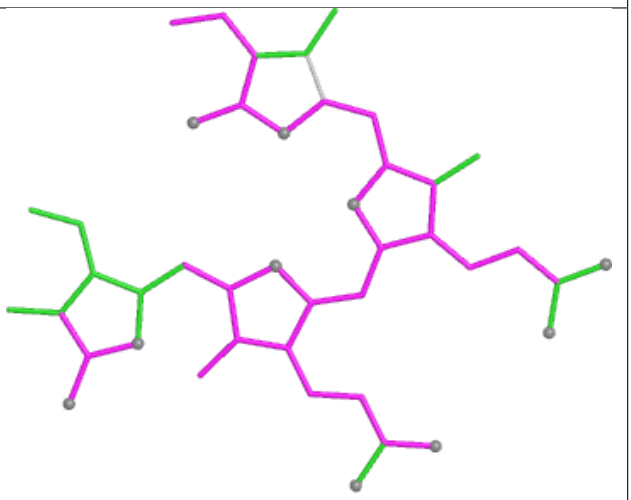


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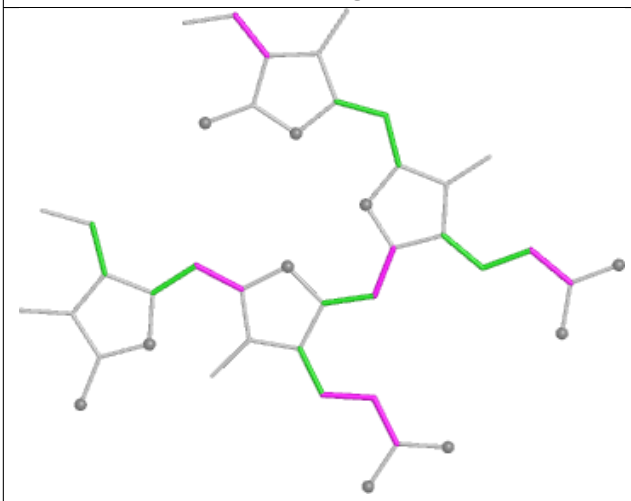
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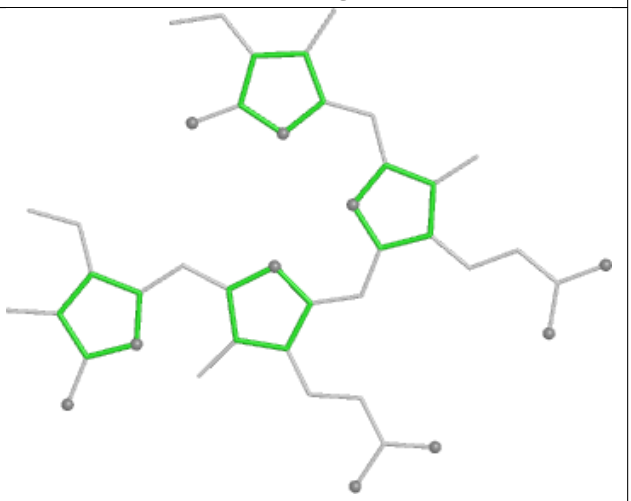
Bond lengths



Bond angles

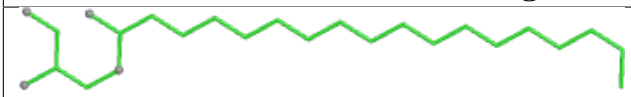


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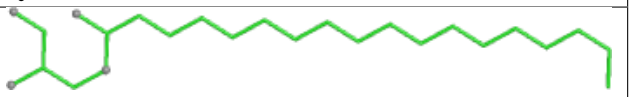


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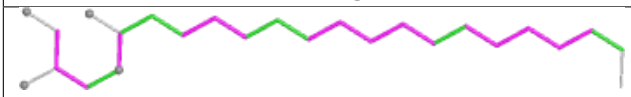
Ligand 3XQ J2 104



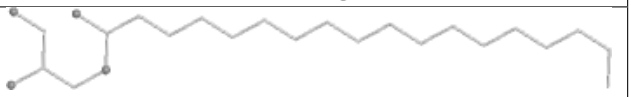
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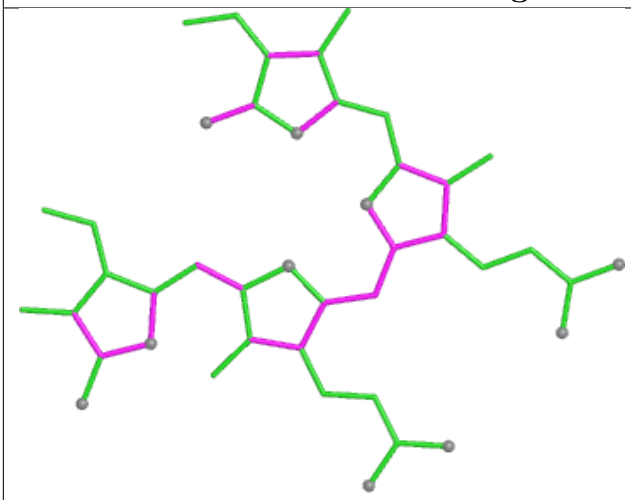


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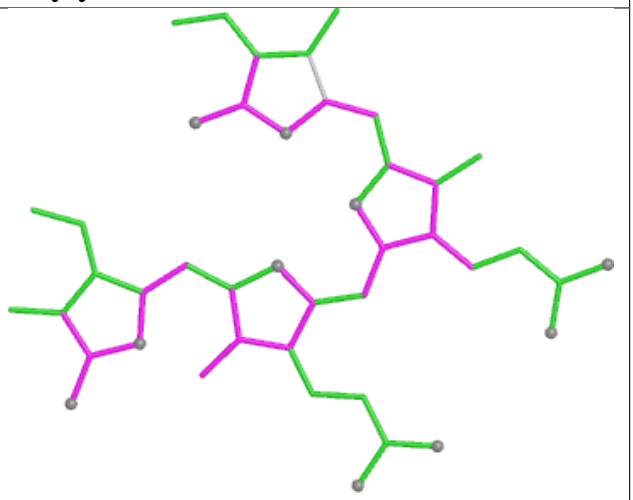


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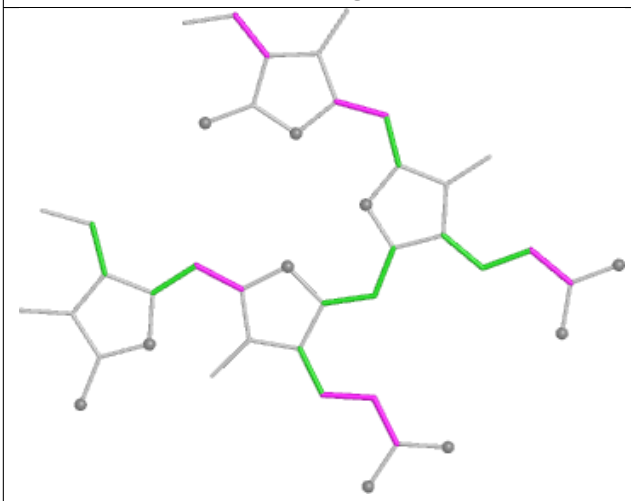
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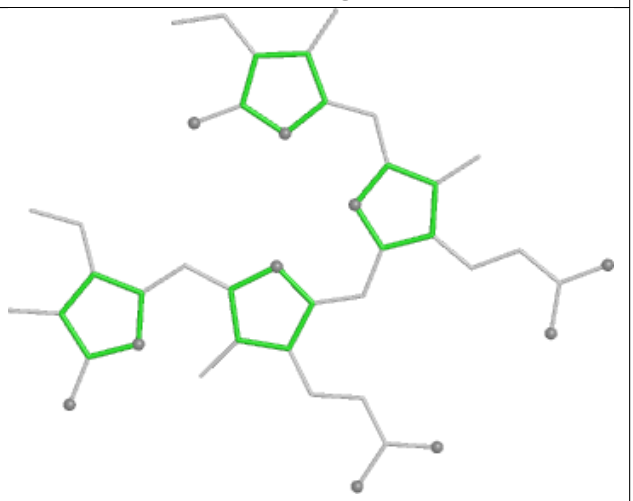
Bond lengths



Bond angles



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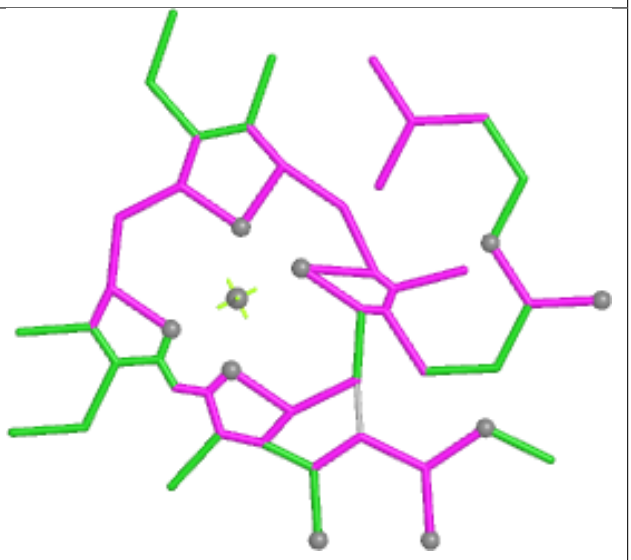


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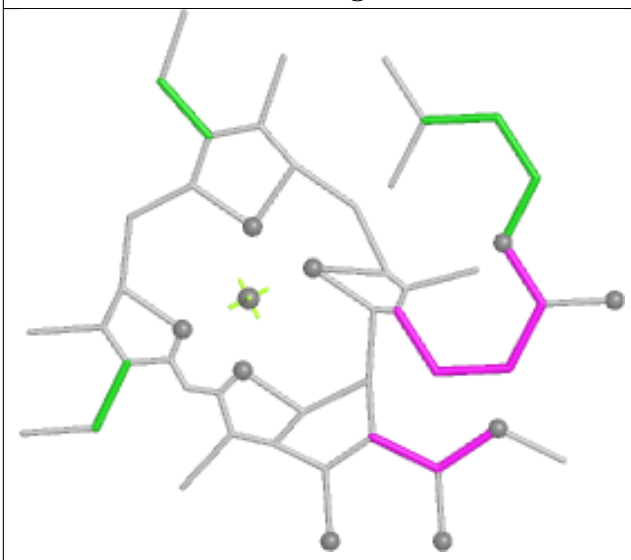
Ligand CLA 62 309



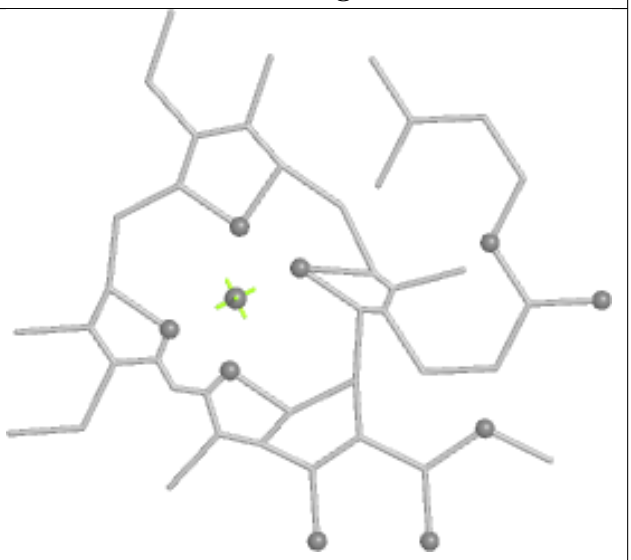
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Bond angles

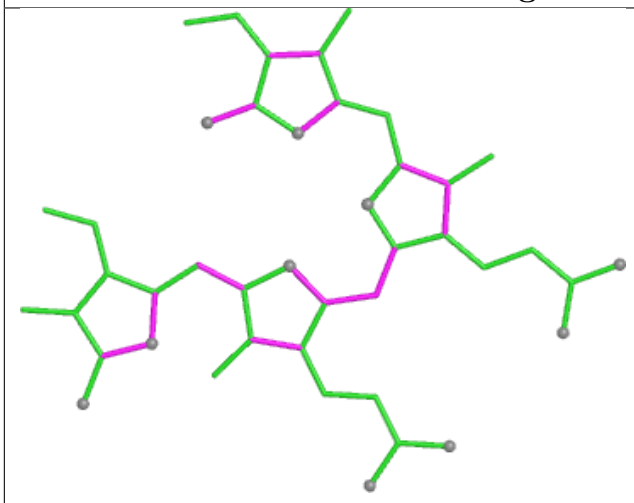


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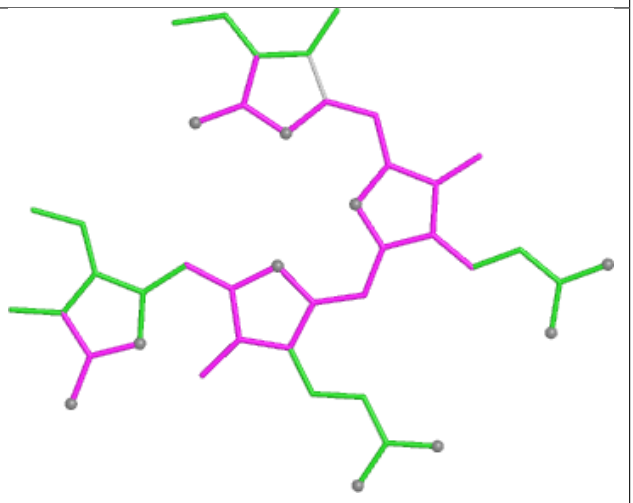


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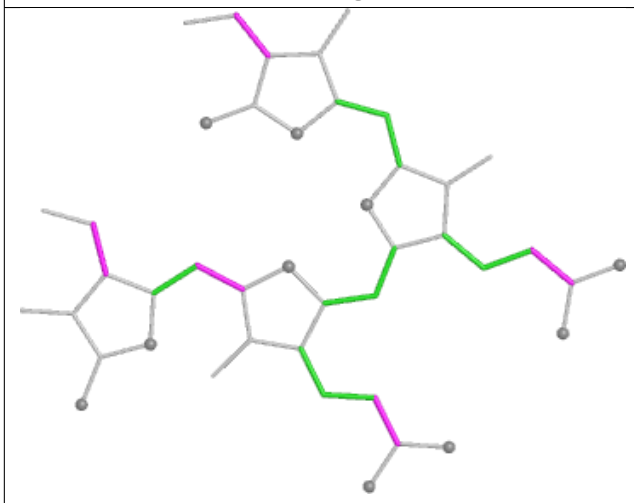
Ligand PEB OI 202



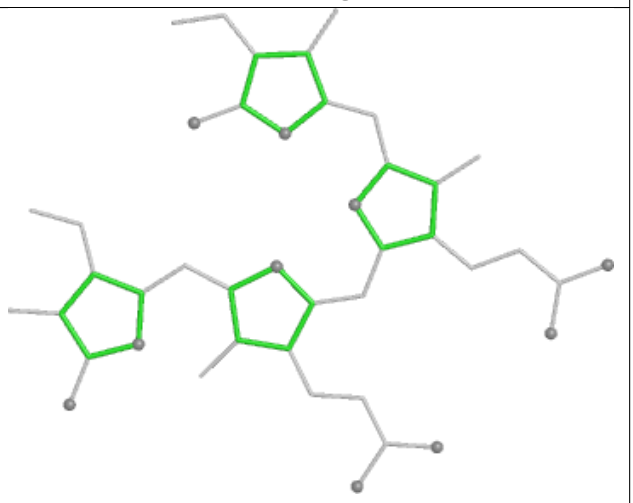
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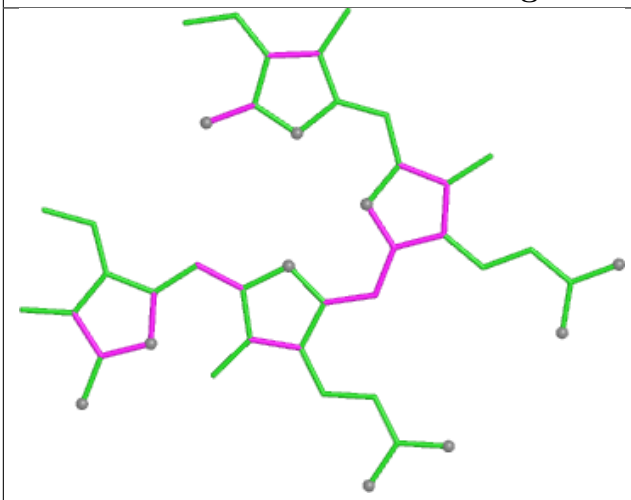


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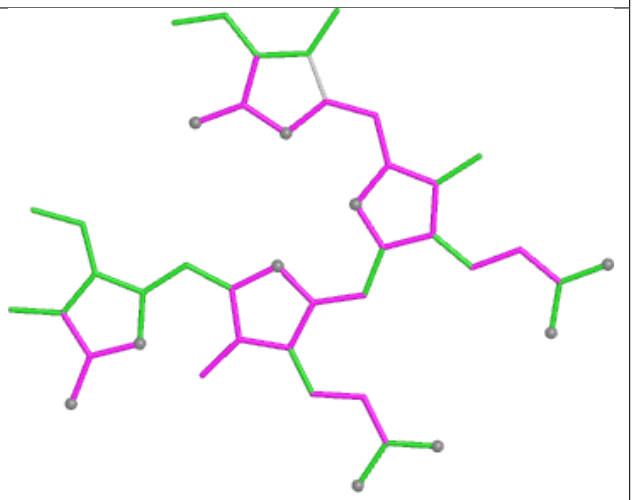


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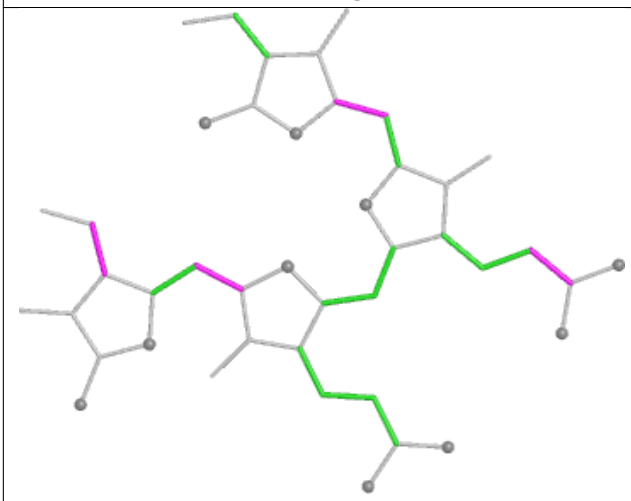
Ligand PEB c1 201



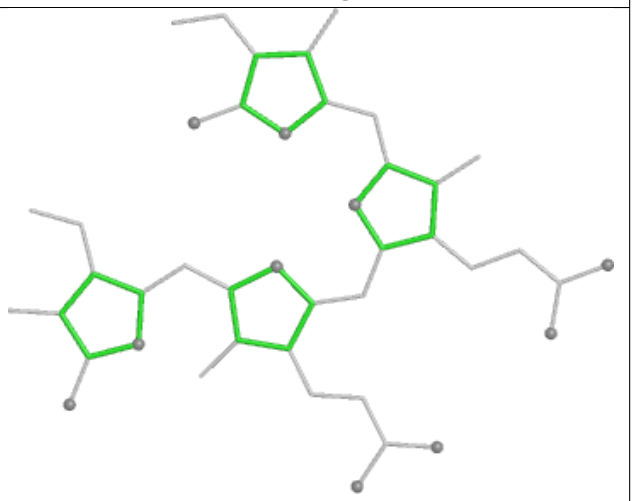
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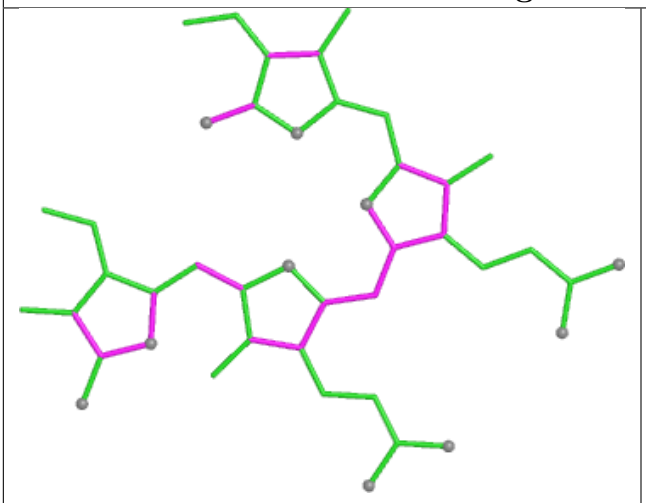


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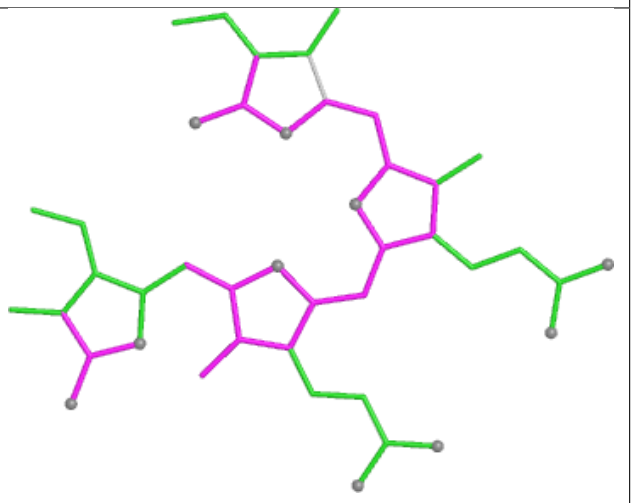


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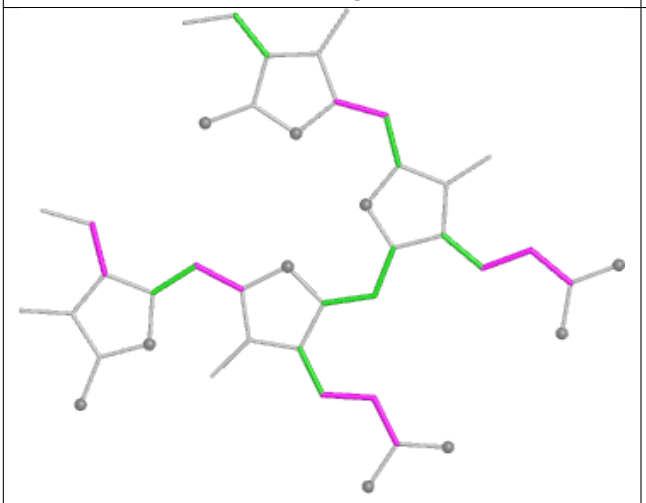
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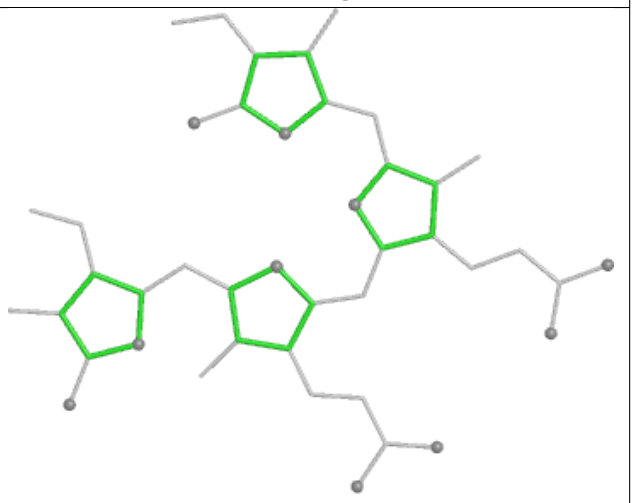
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Bond angles

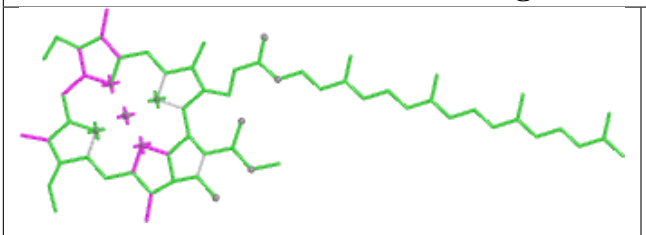


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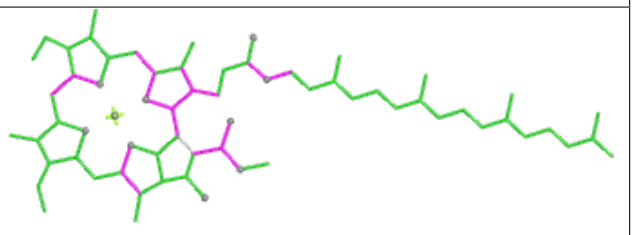


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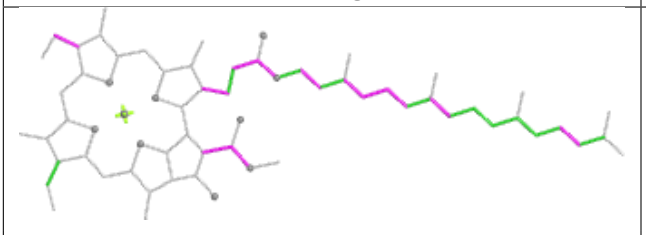
Ligand CLA A2 811



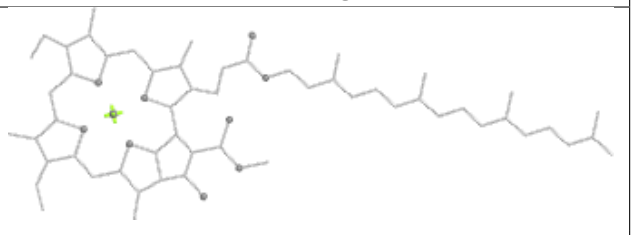
Bond lengths



Bond angles

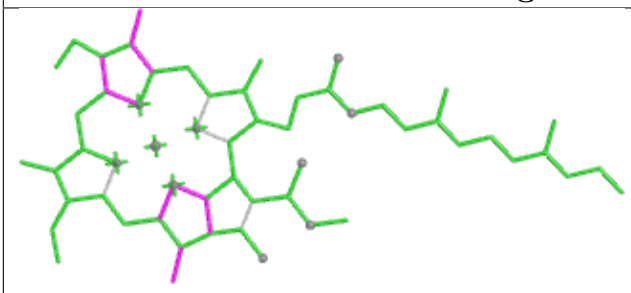


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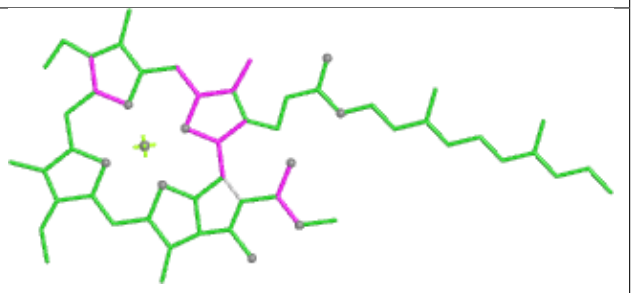


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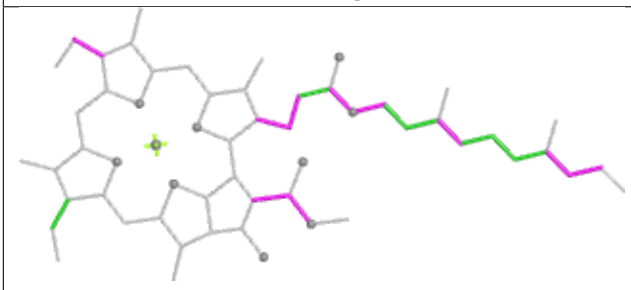
Ligand CLA L2 202



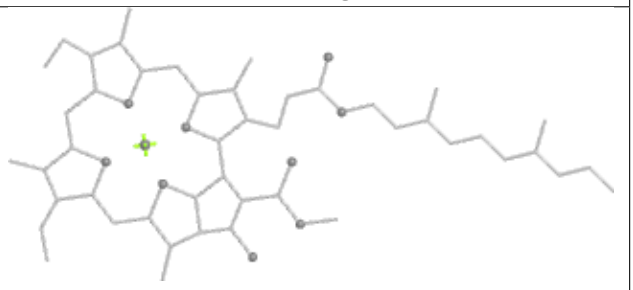
Bond lengths



Bond angles

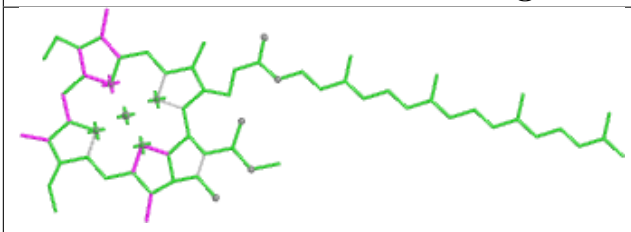


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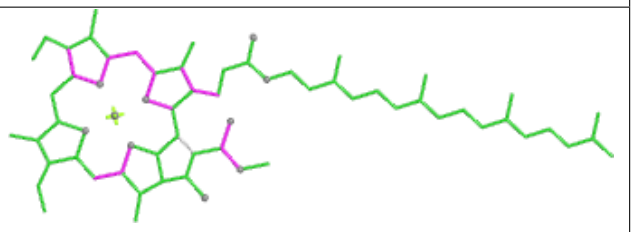


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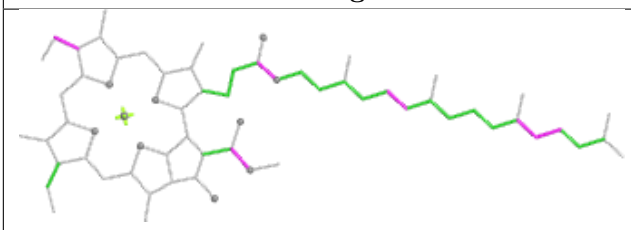
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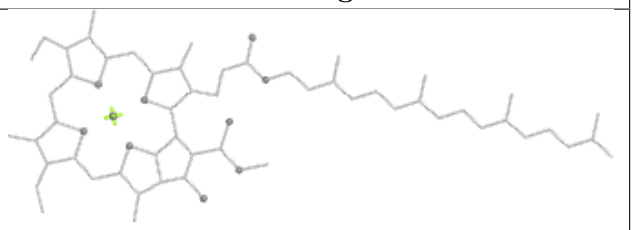
Bond lengths



Bond angles

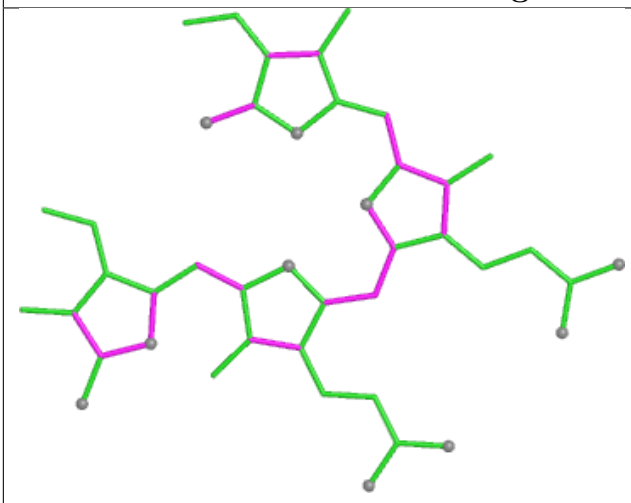


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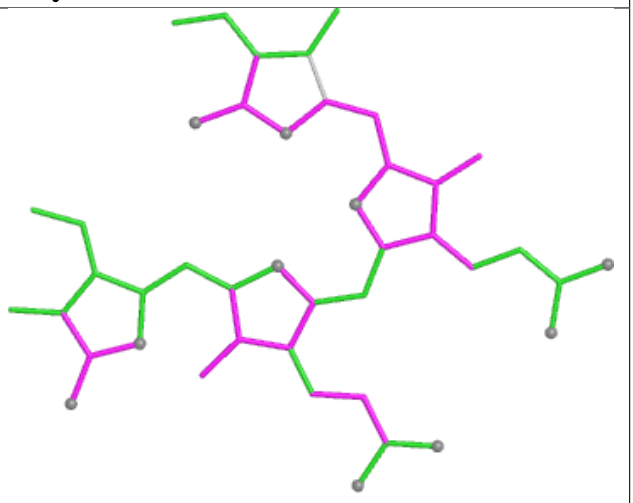


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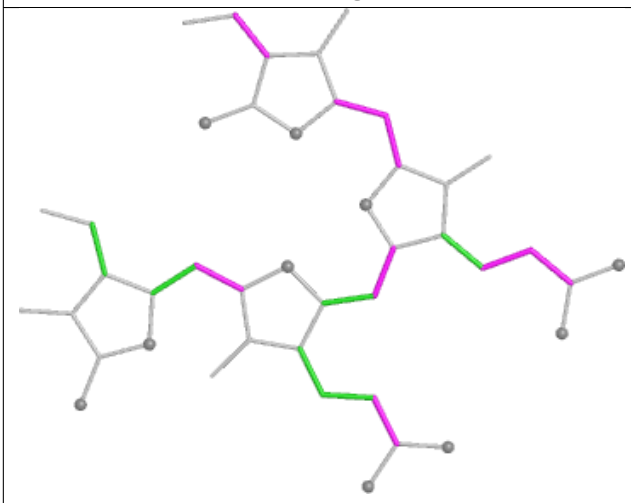
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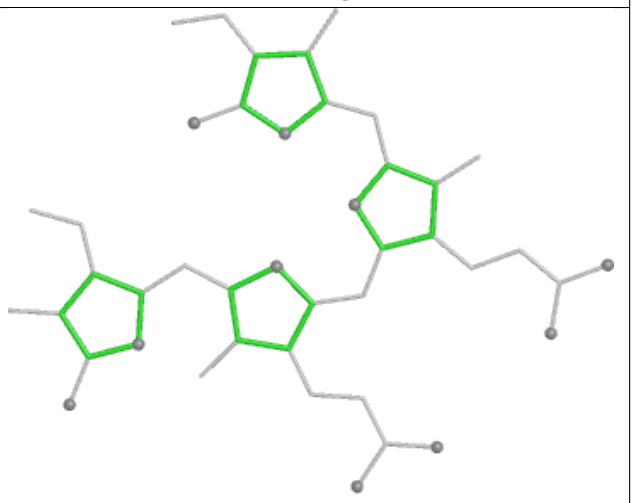
Bond lengths



Bond angles

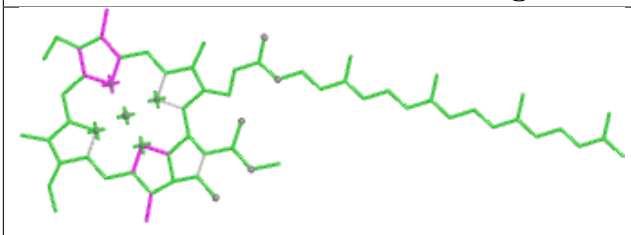


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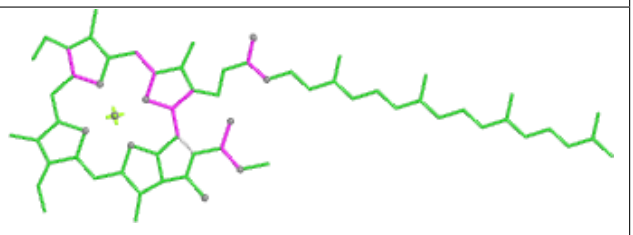


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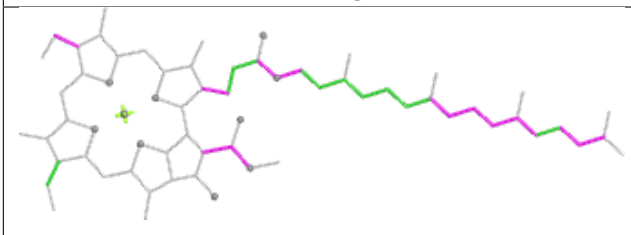
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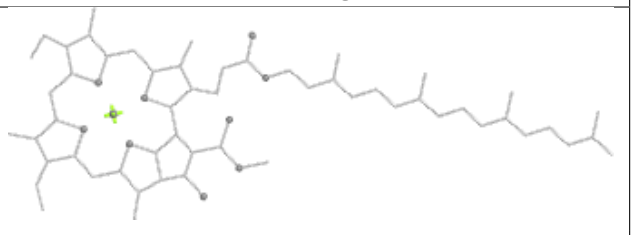
Bond lengths



Bond angles

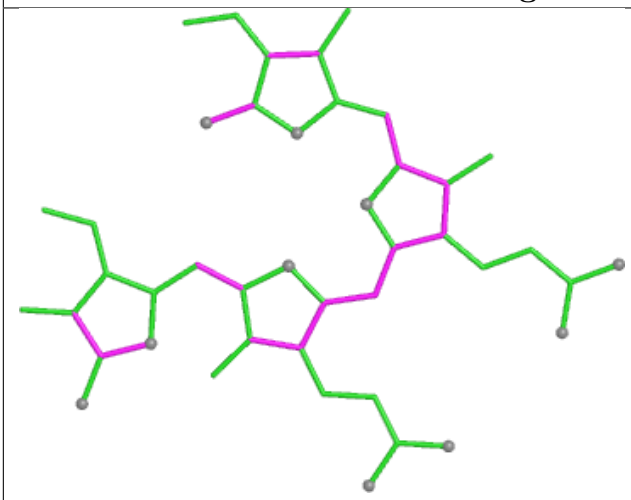


Torsions

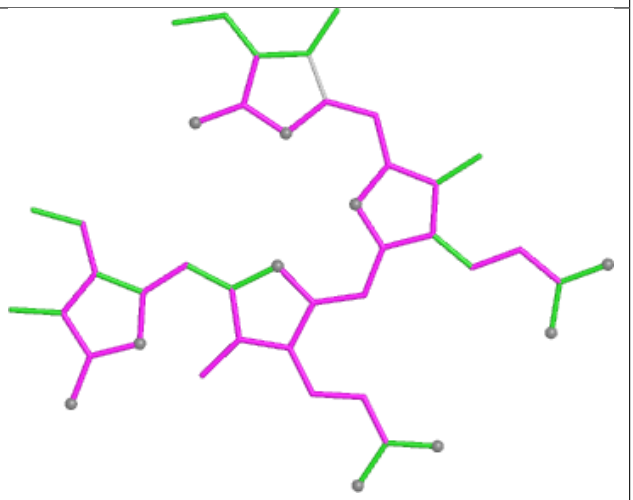


Rings

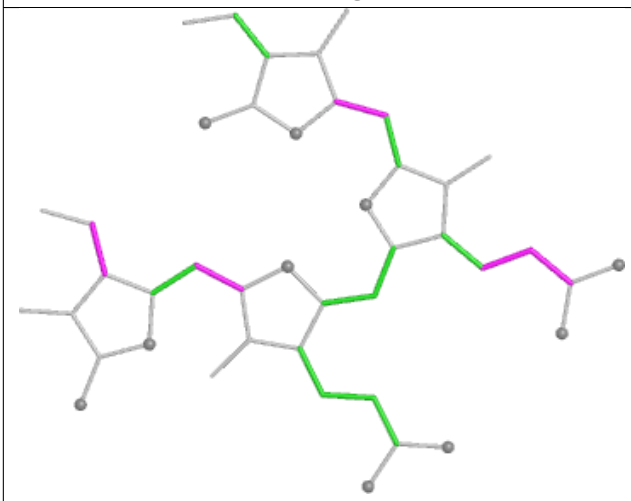
Ligand PEB J9 202



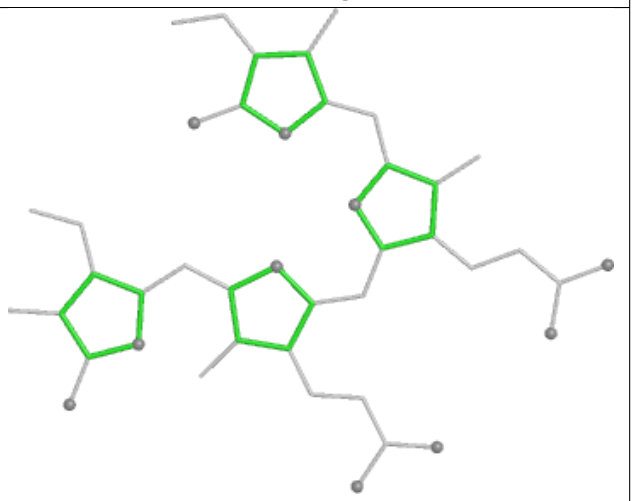
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Bond angles

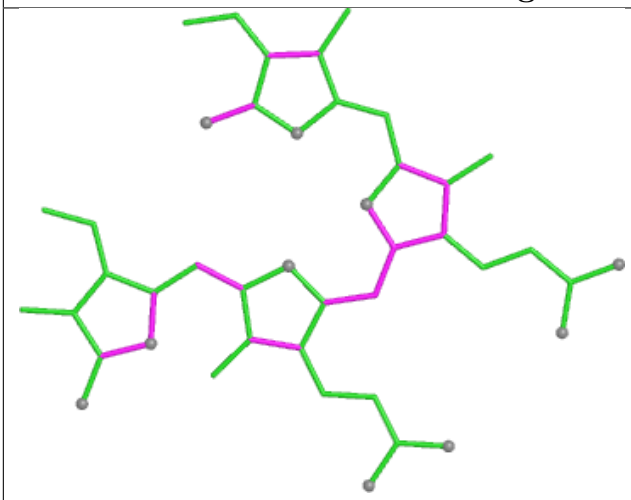


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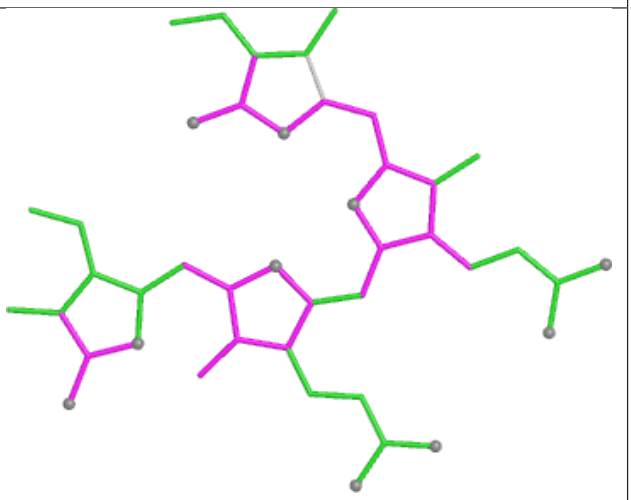


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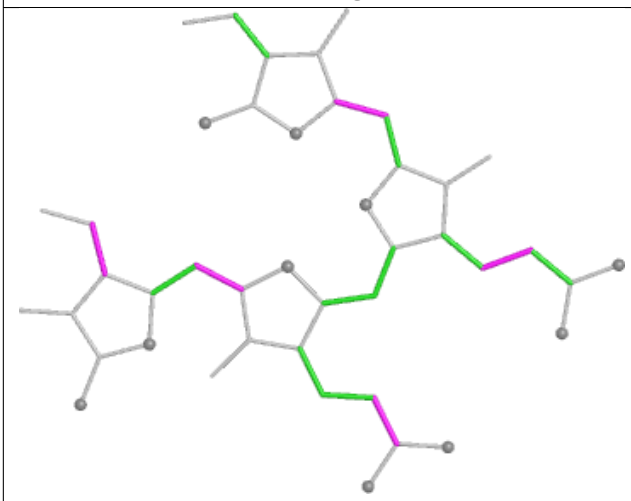
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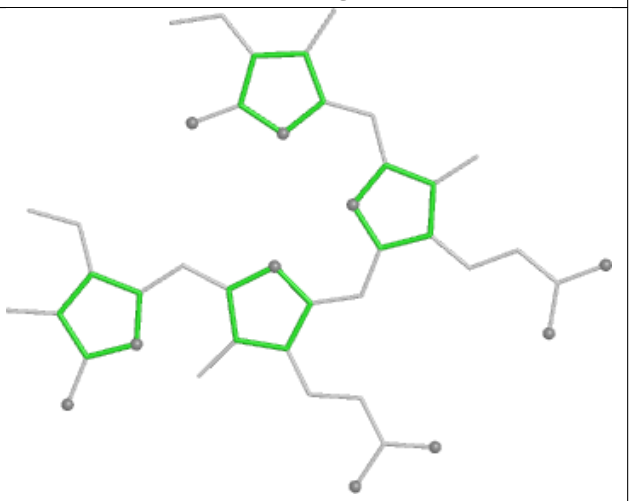
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Bond angles

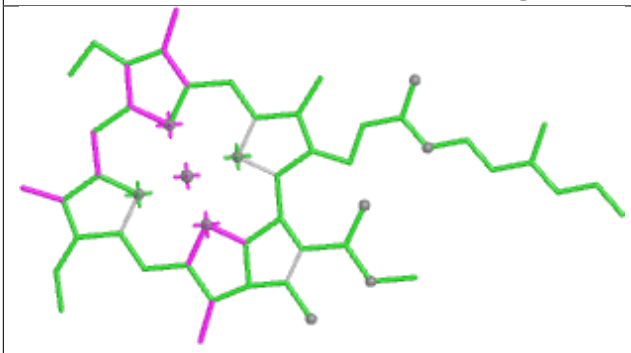


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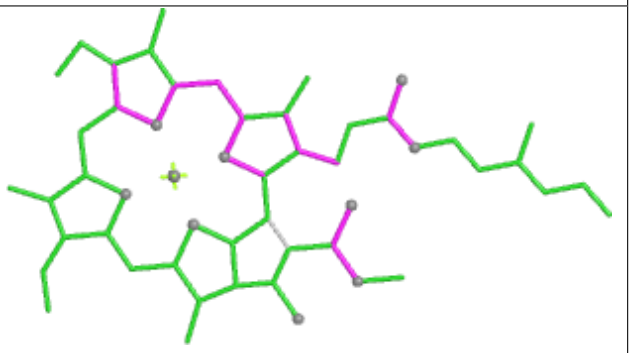


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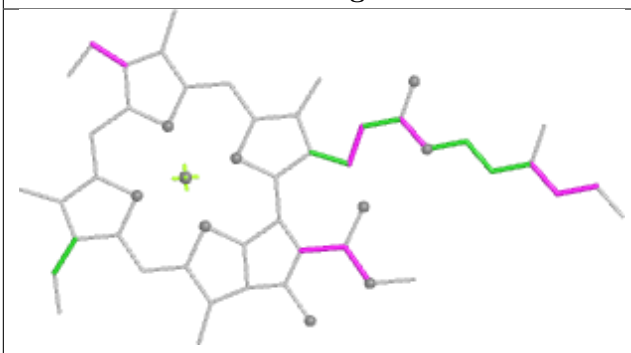
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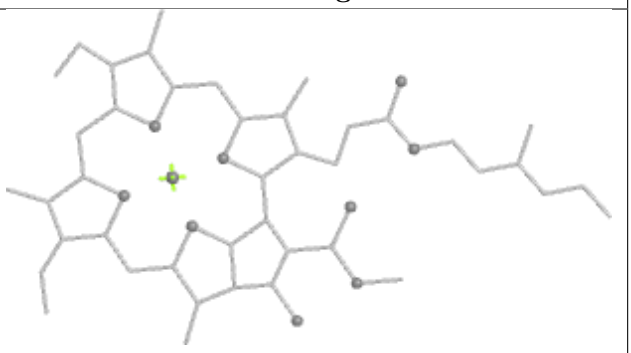
Bond lengths



Bond angles

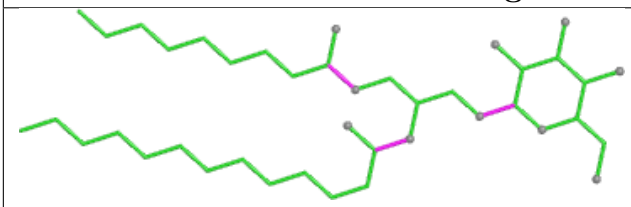


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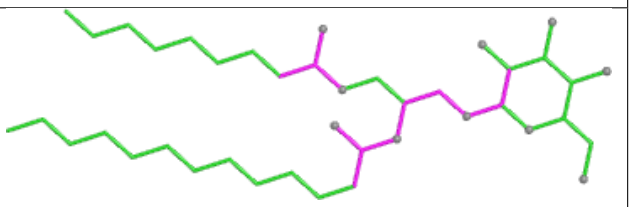


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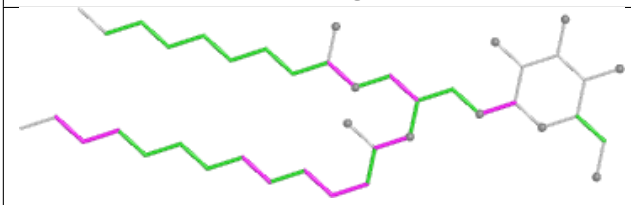
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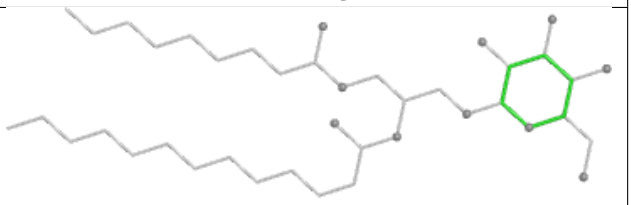
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Bond angles

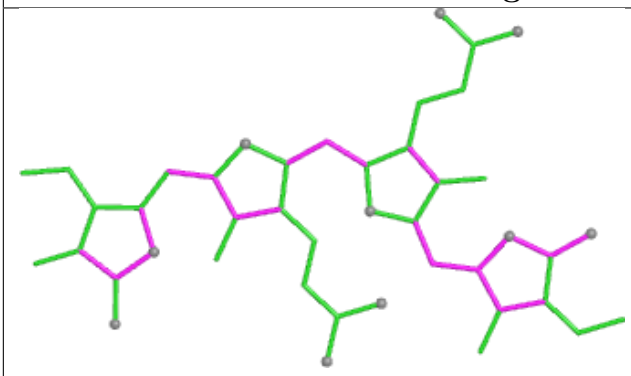


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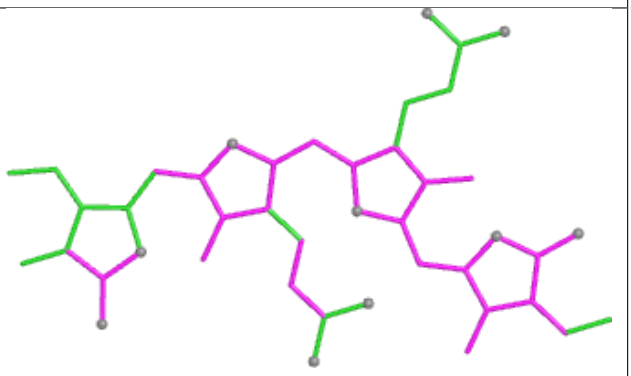


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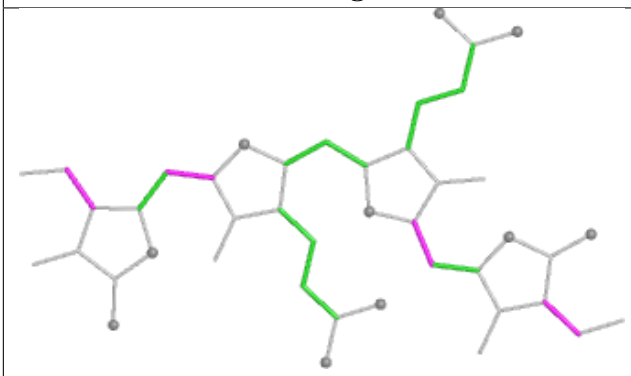
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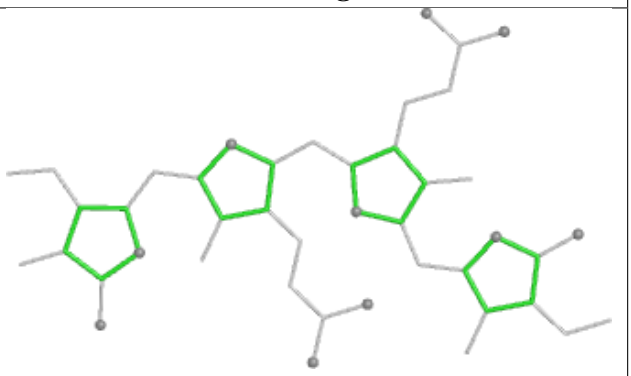
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Bond angles

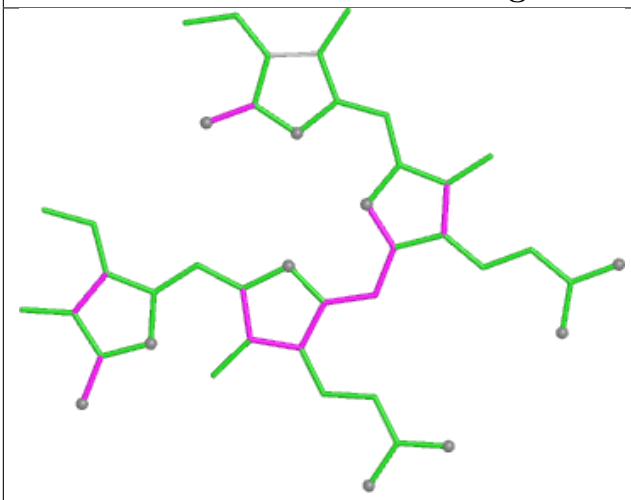


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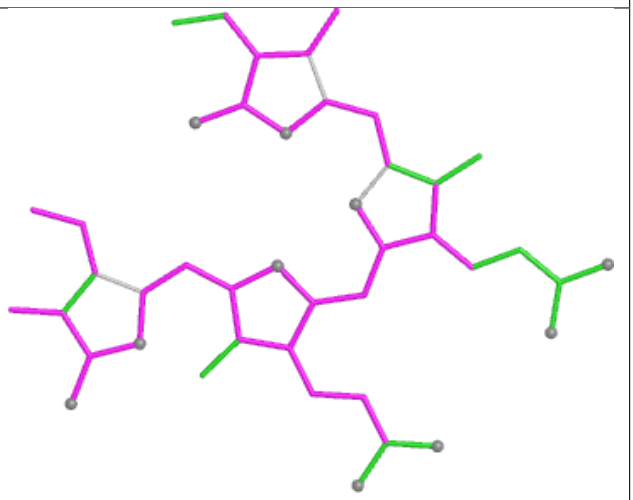


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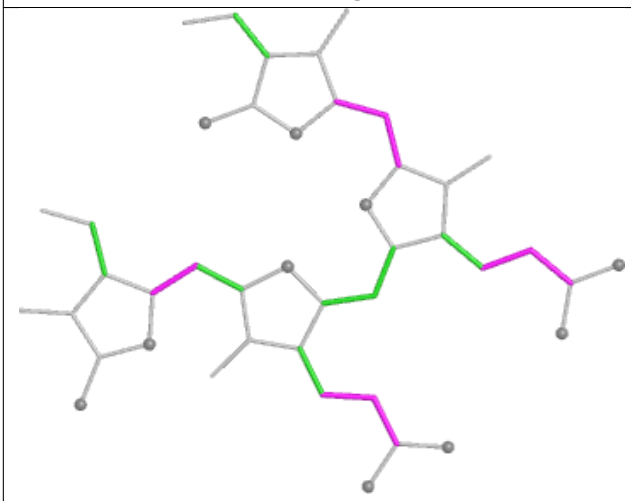
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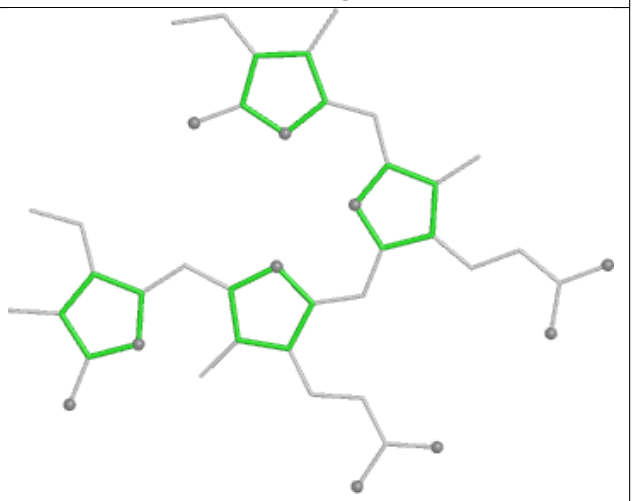
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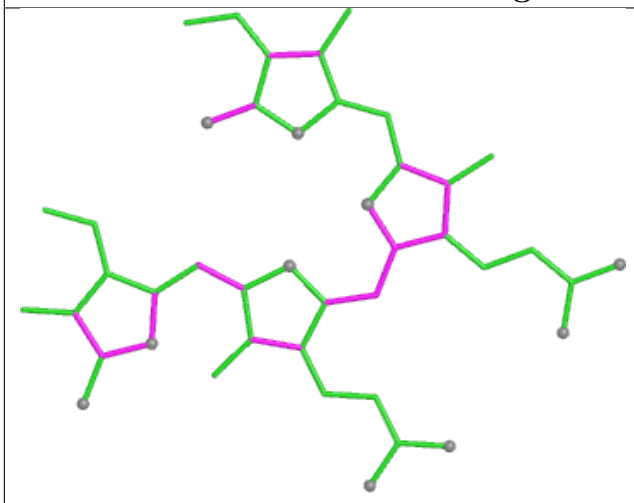


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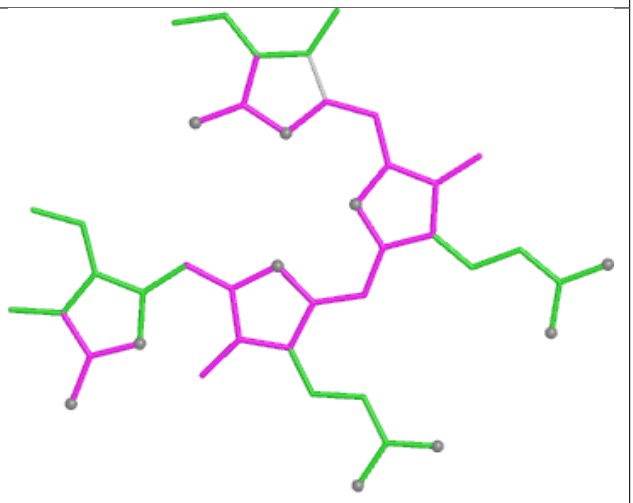


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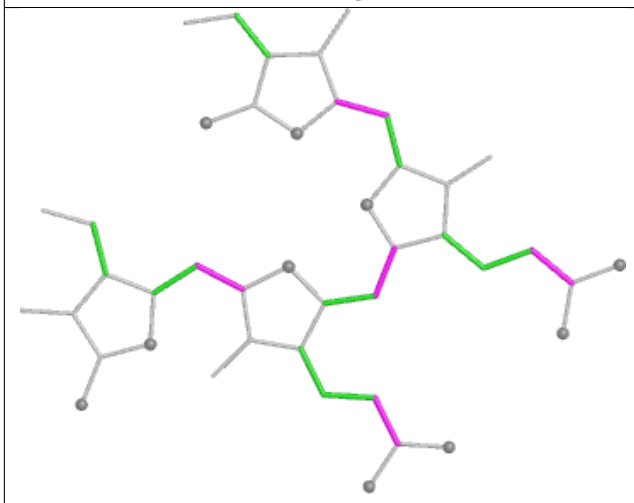
Ligand PEB VE 202



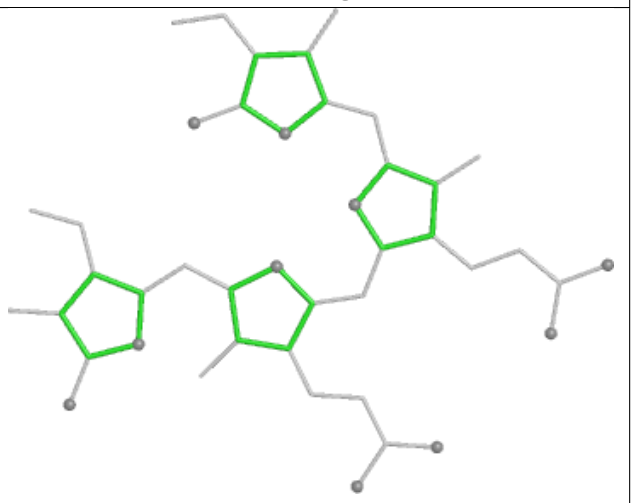
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Bond angles

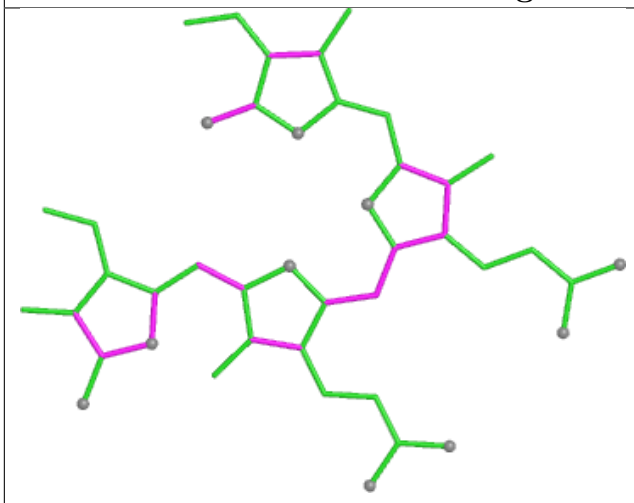


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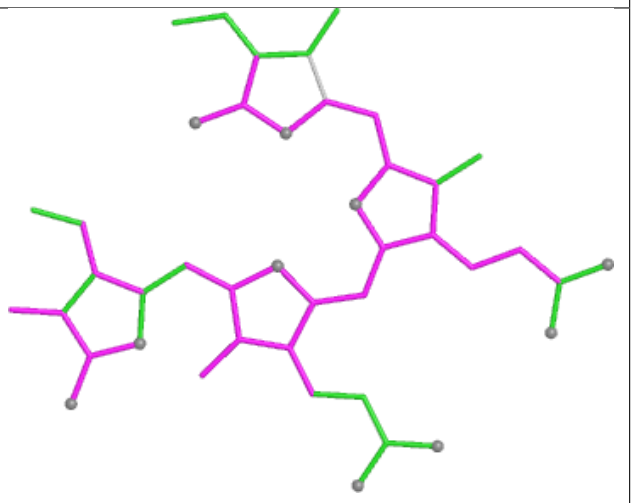


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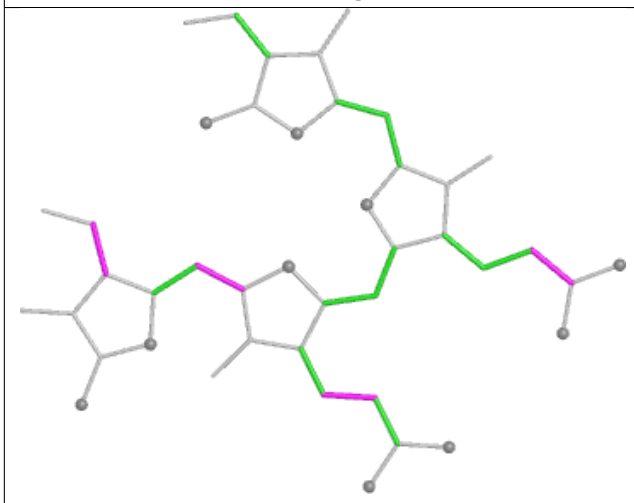
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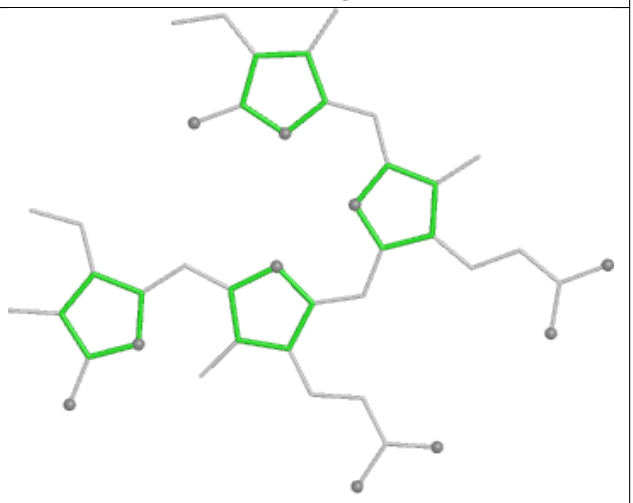
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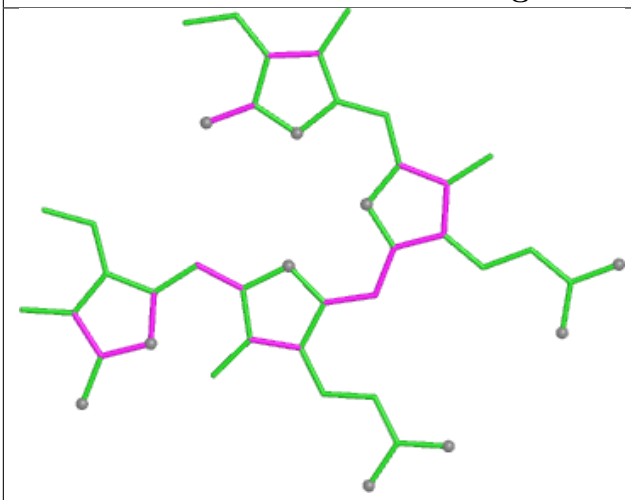


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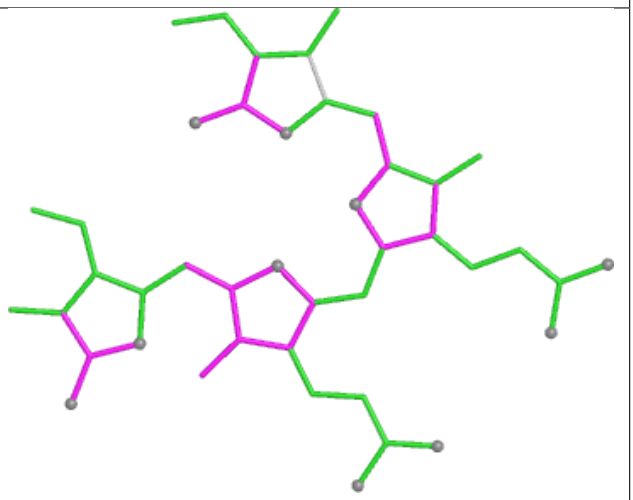


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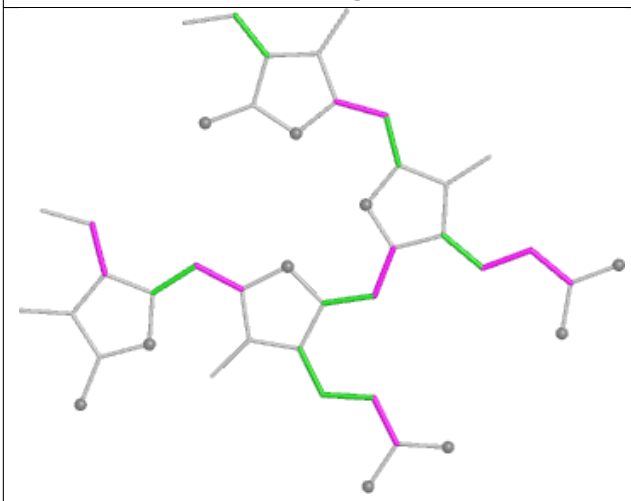
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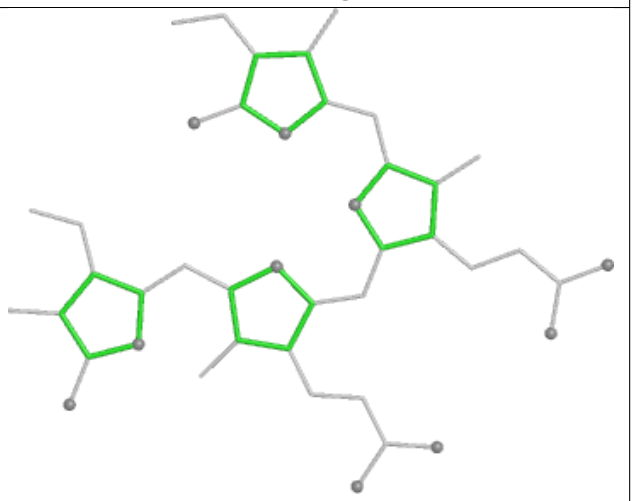
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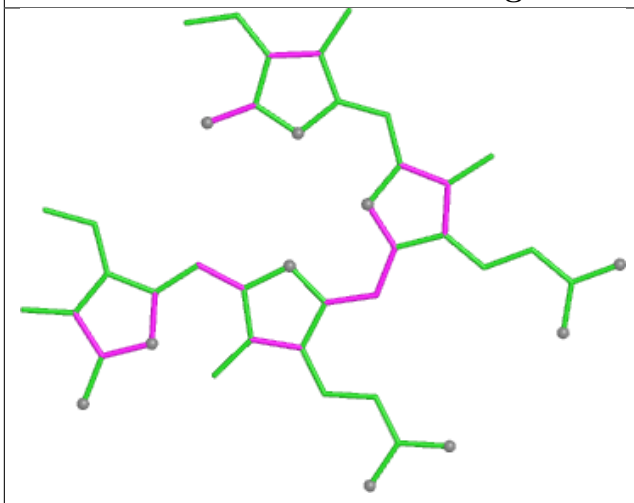


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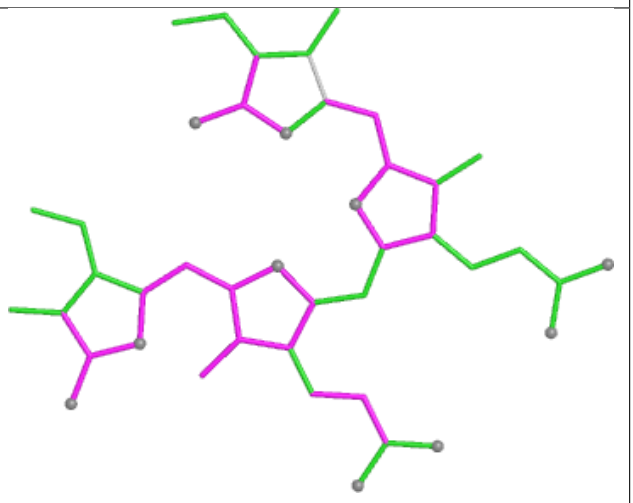


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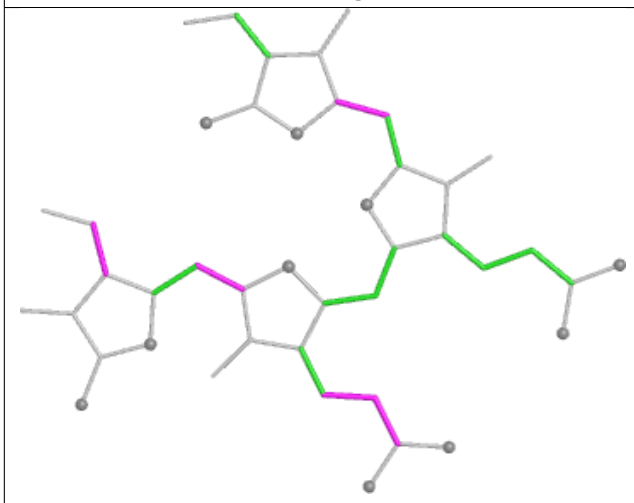
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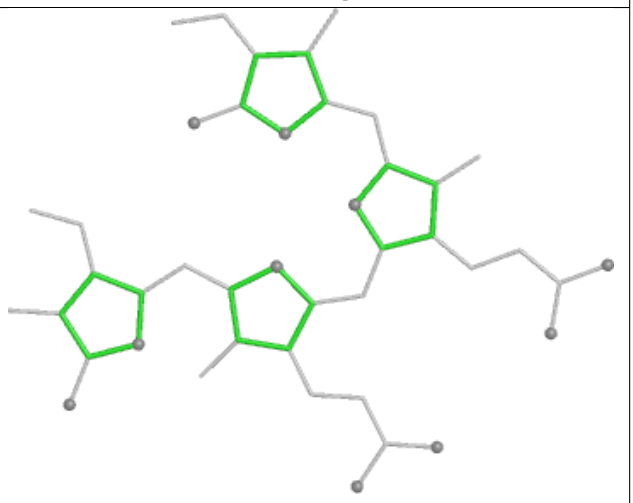
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Bond angles

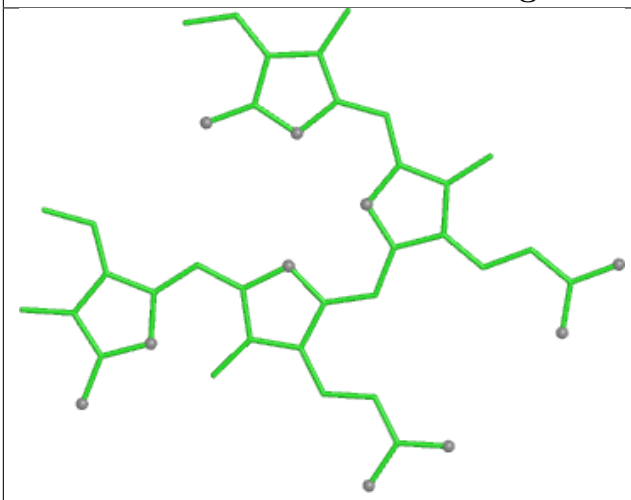


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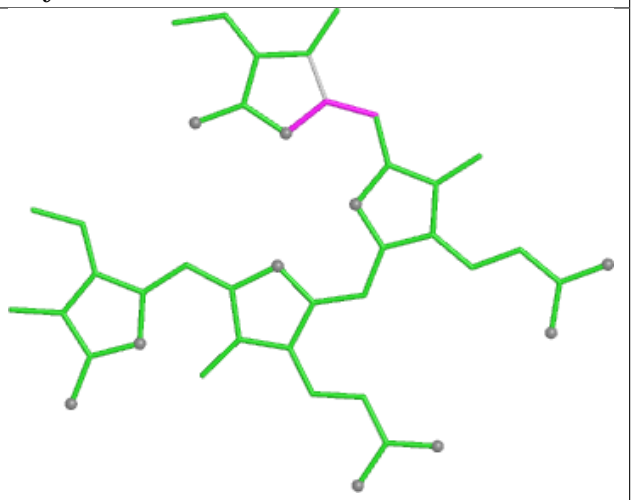


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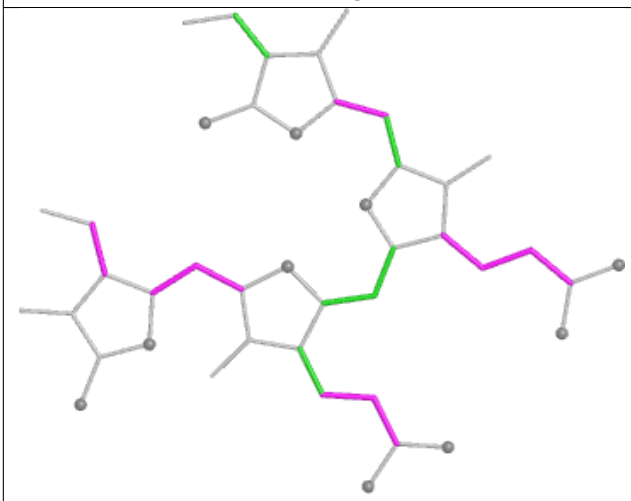
Ligand PEB y8 201



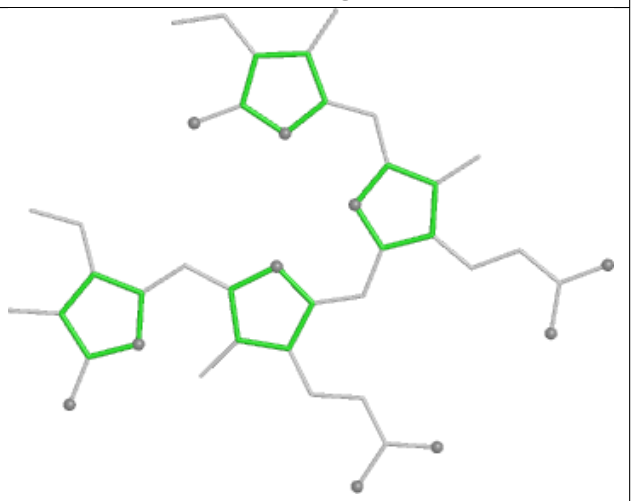
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Bond angles

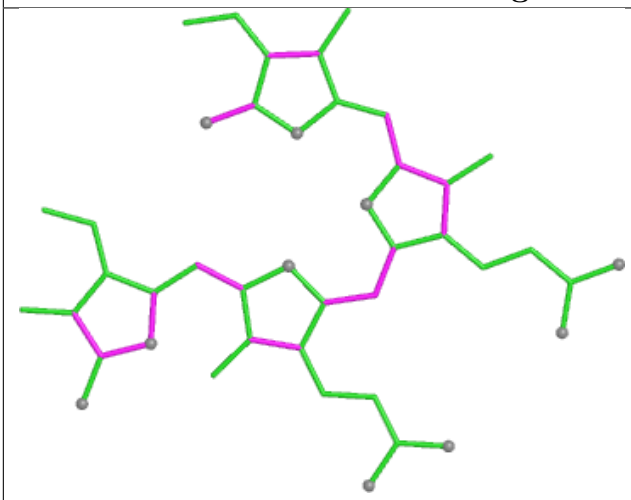


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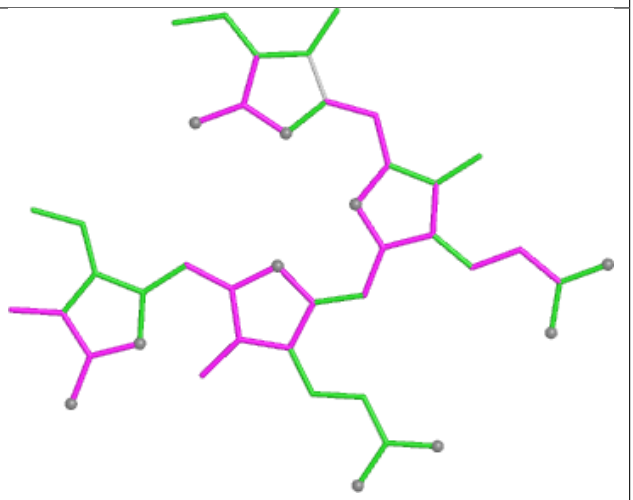


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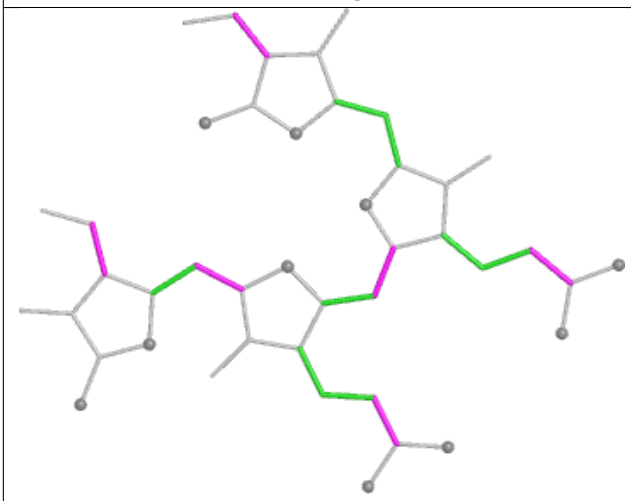
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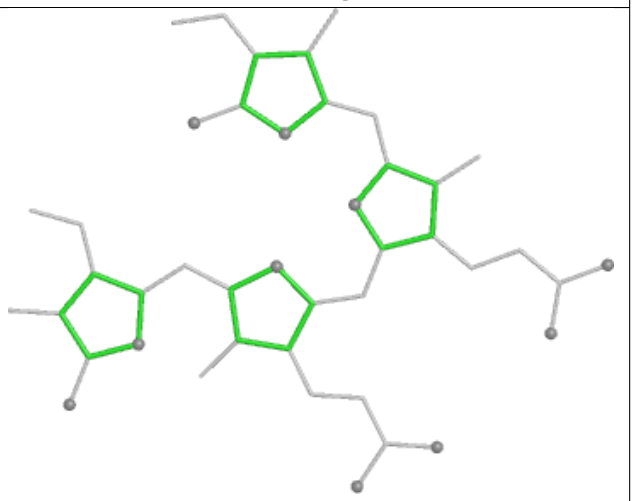
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Bond angles

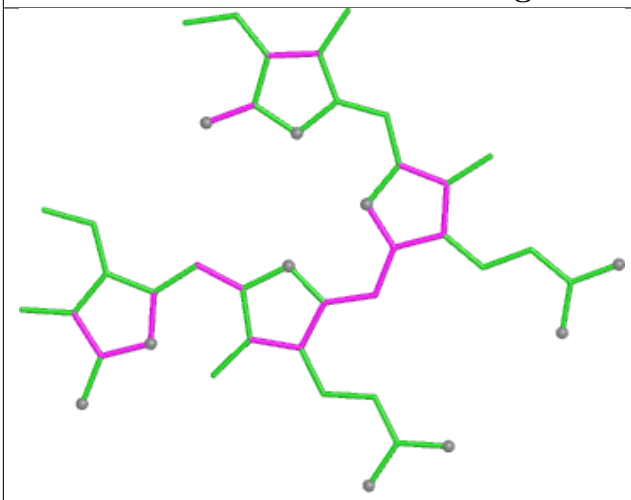


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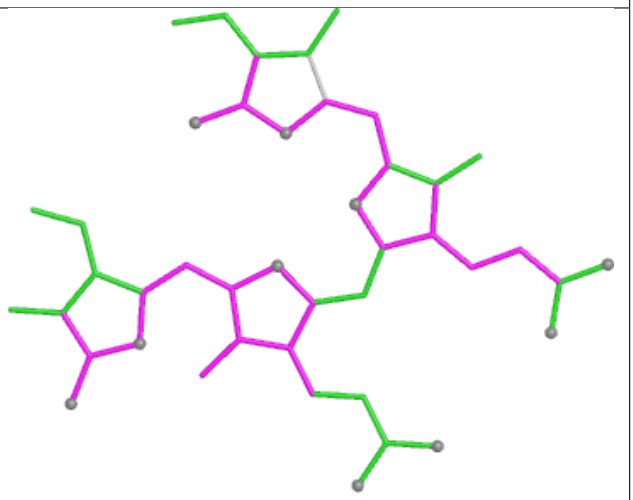


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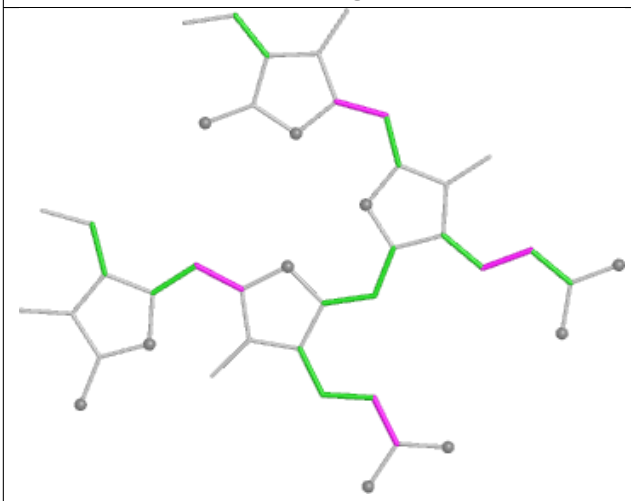
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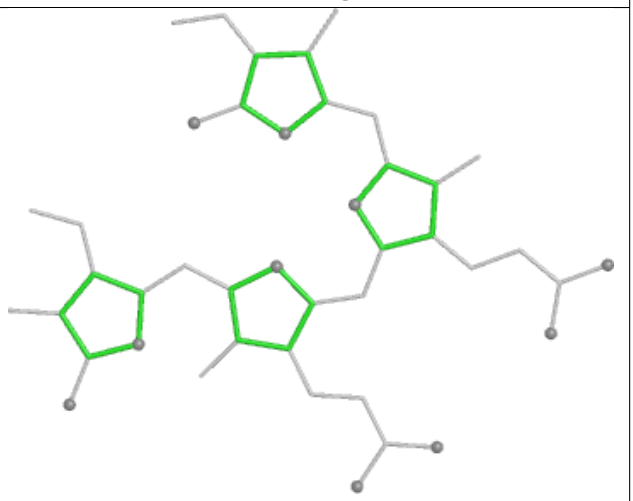
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Bond angles

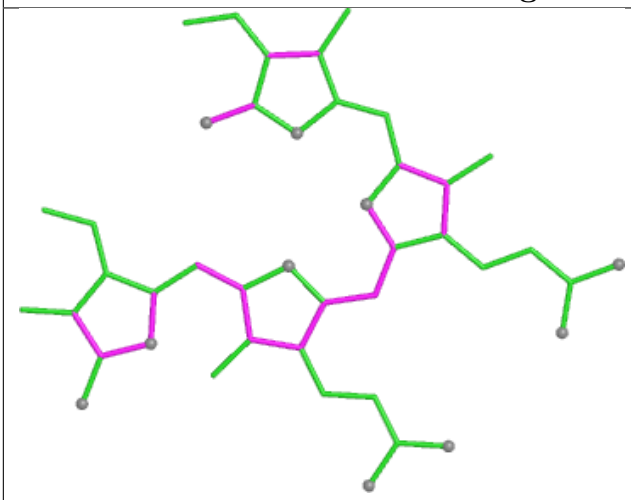


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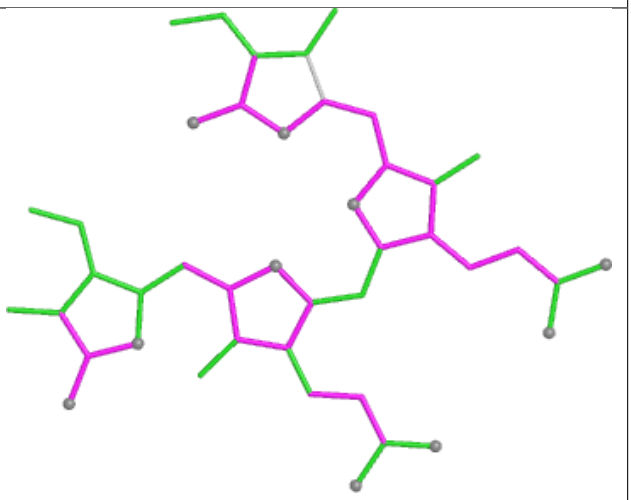


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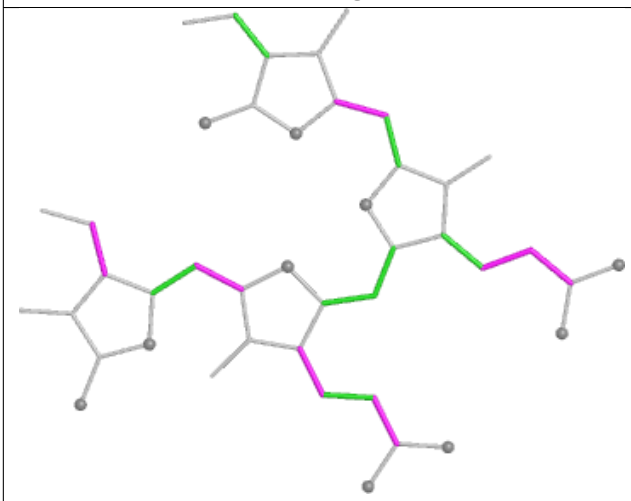
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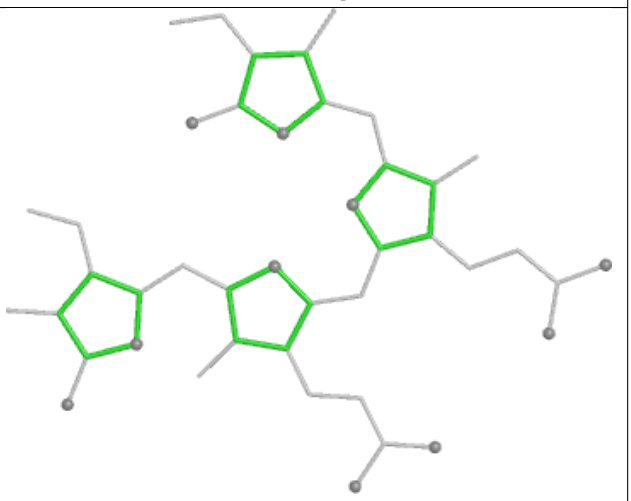
Bond lengths



Bond angles

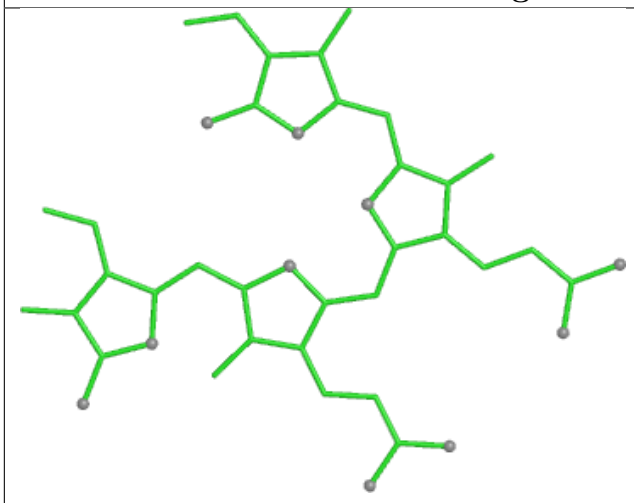


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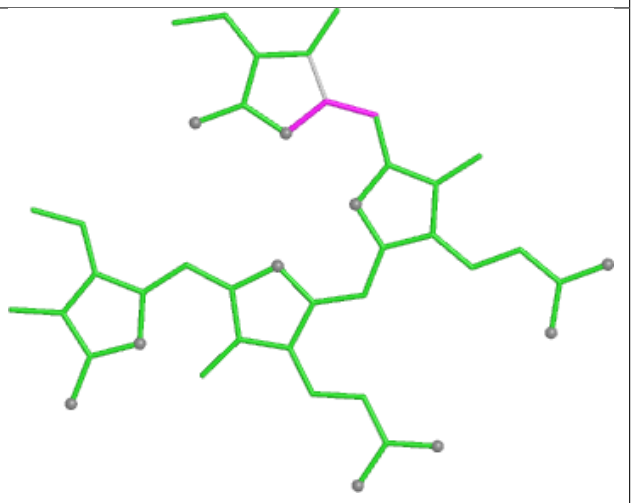


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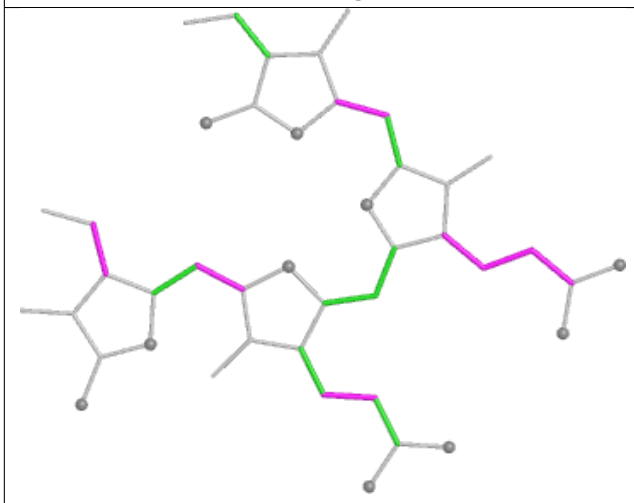
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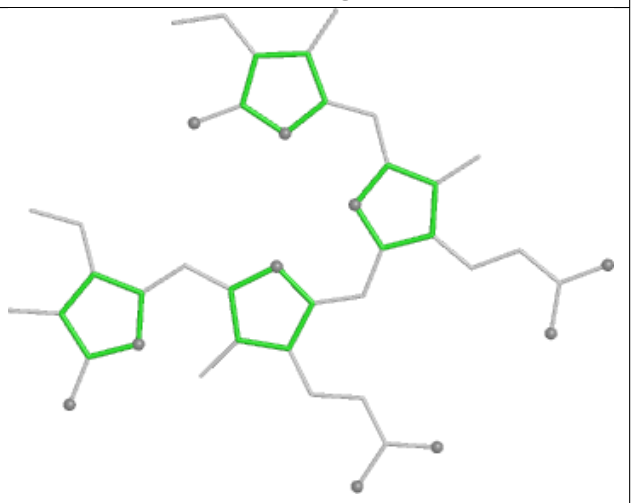
Bond lengths



Bond angles

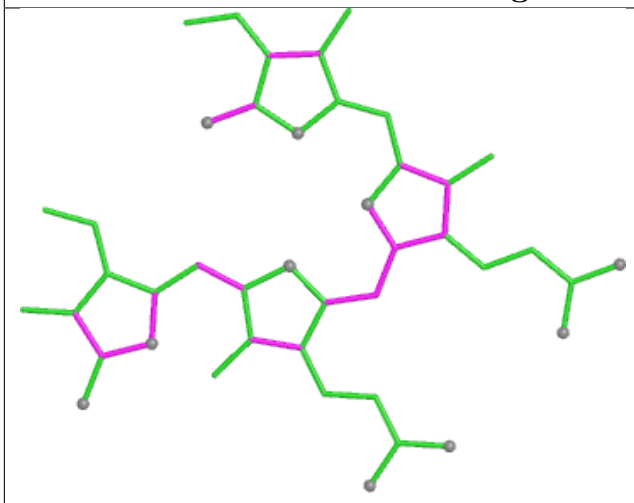


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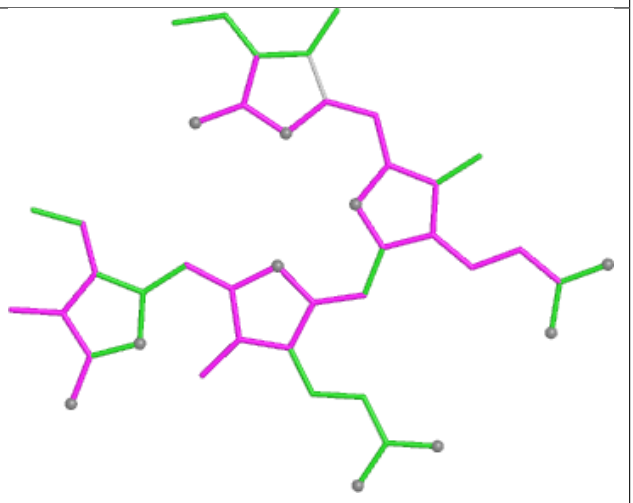


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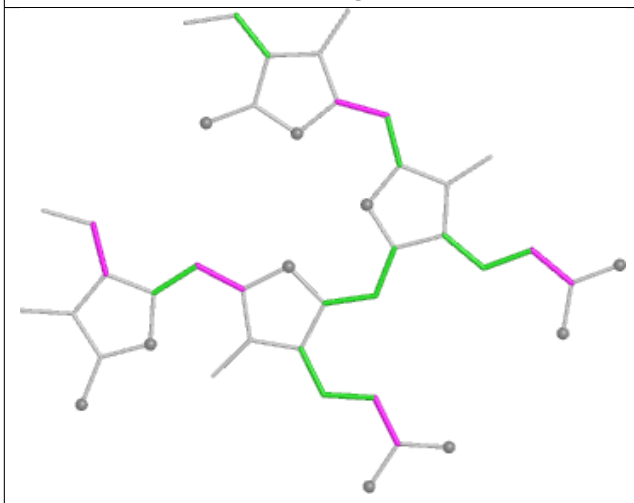
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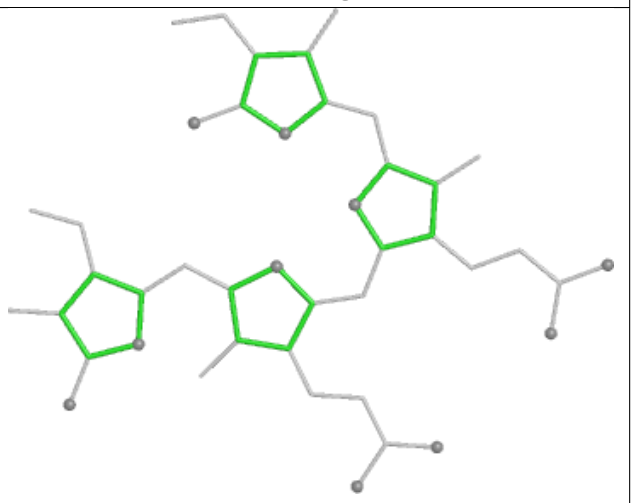
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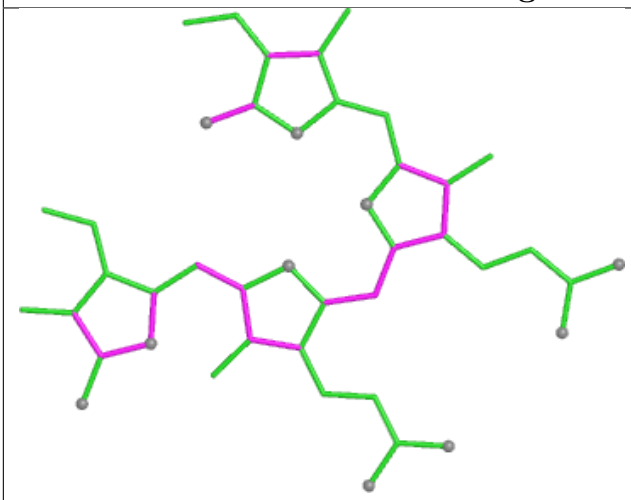


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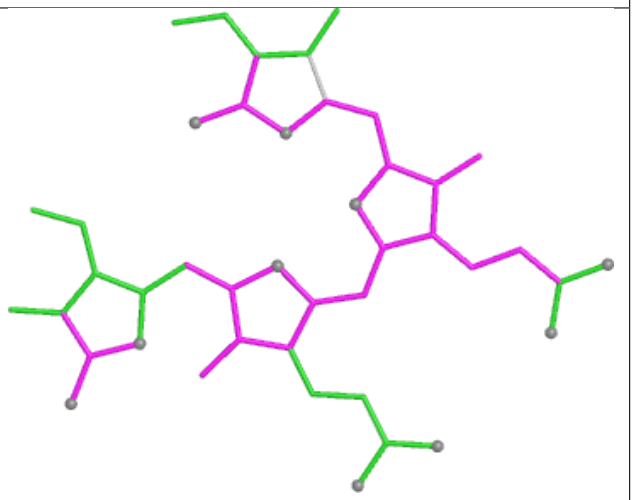


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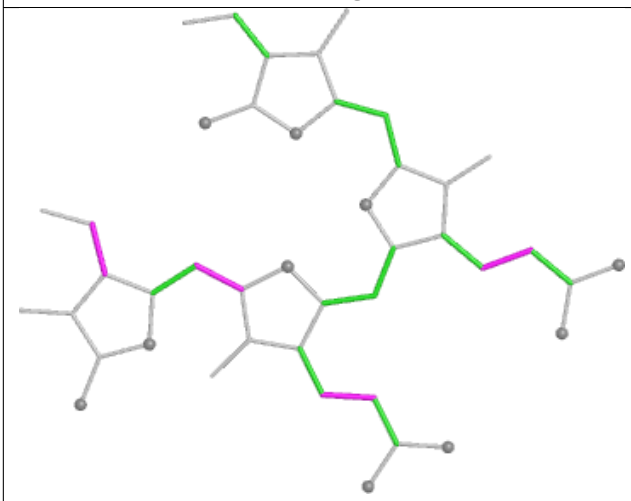
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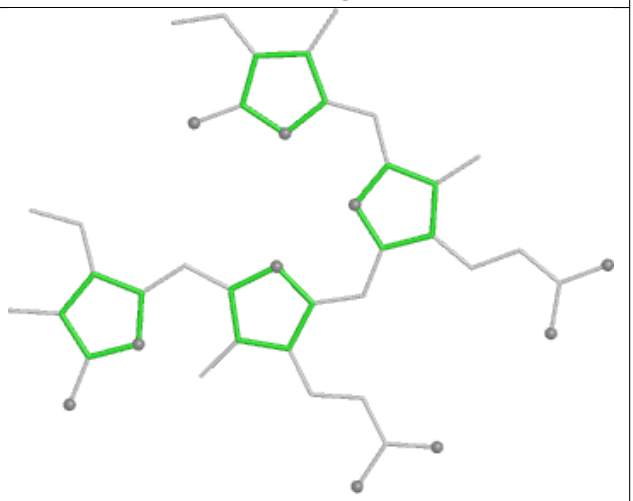
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Bond angles

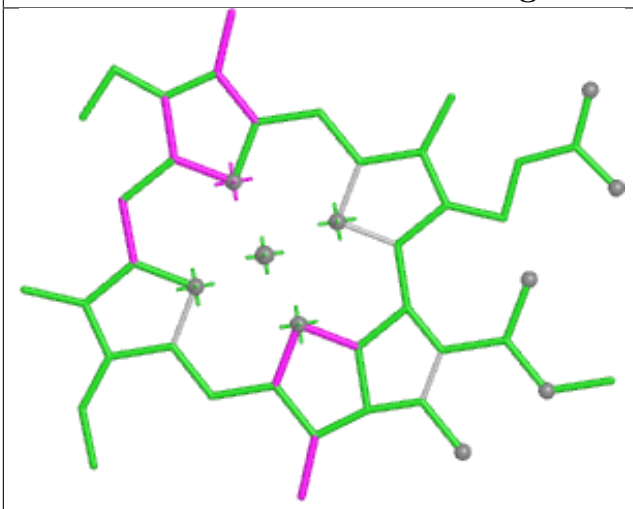


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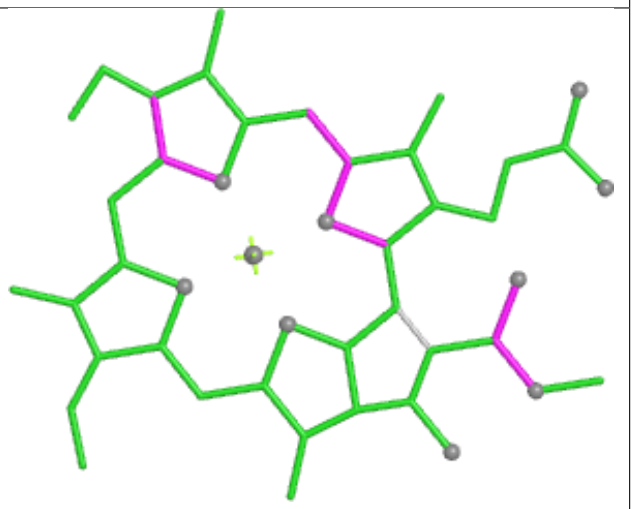


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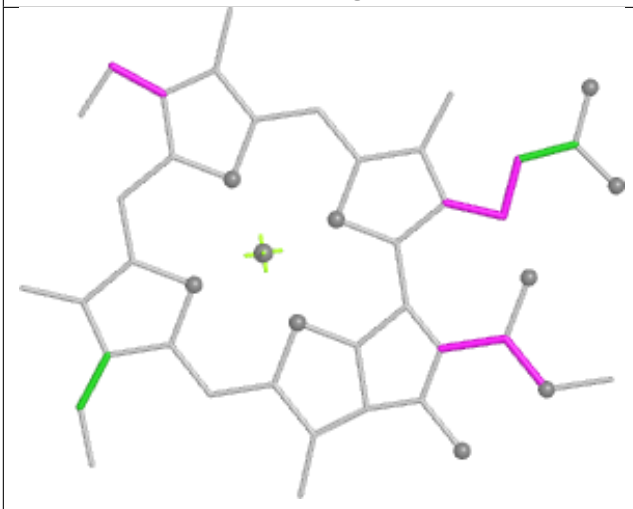
Ligand CLA 62 302



Bond lengths



Bond angles

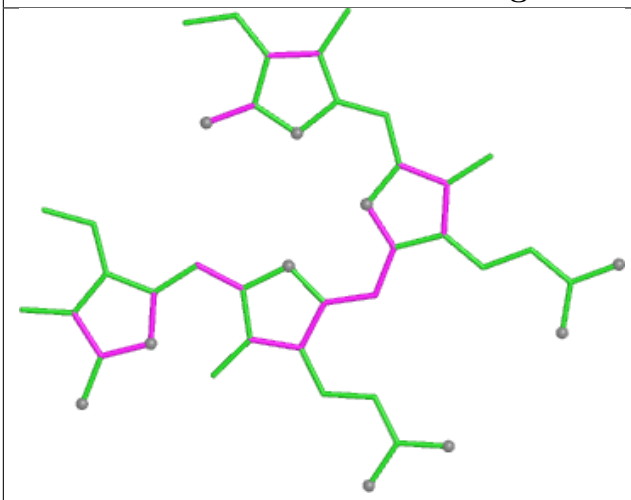


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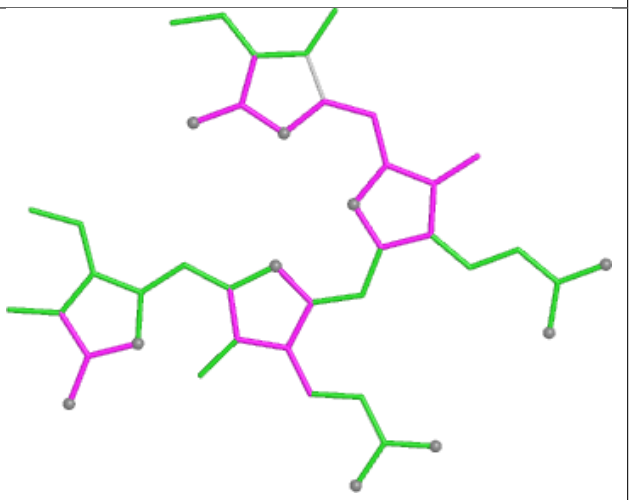


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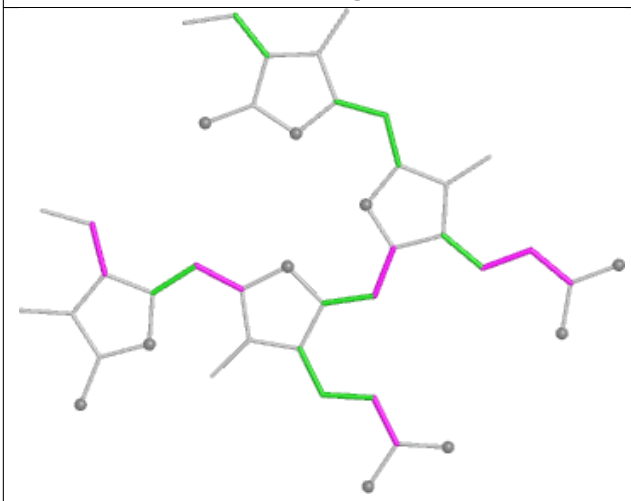
Ligand PEB AK 202



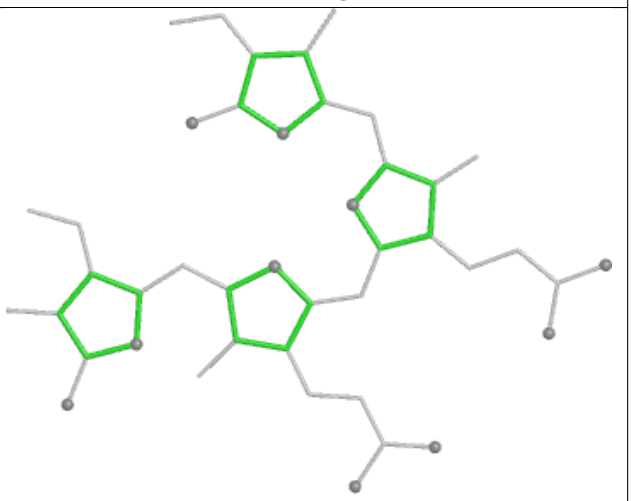
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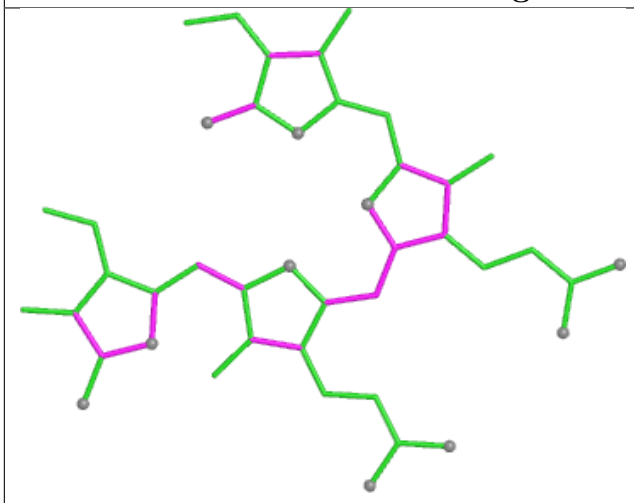


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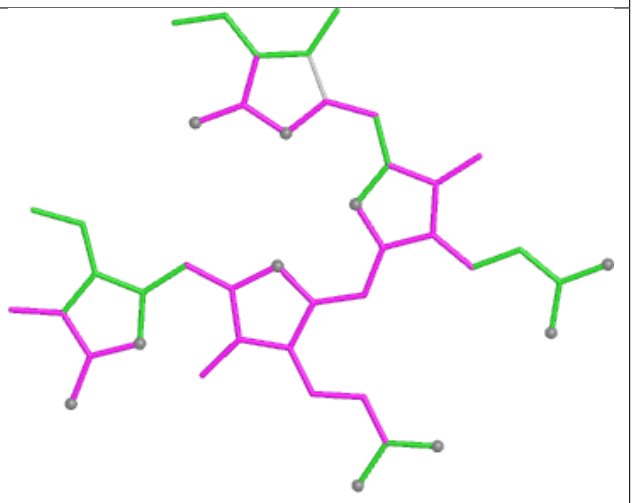


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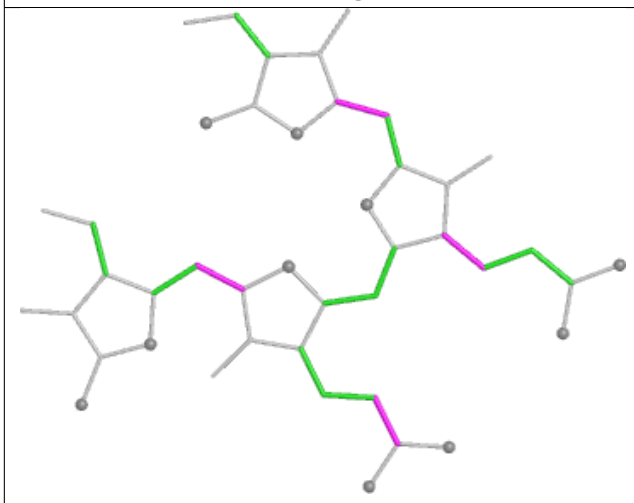
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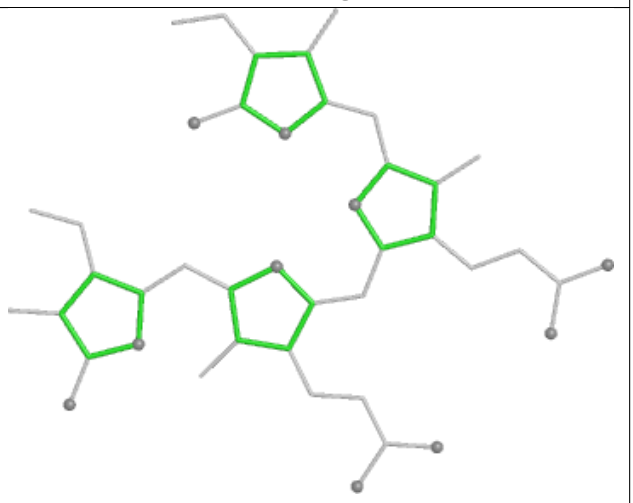
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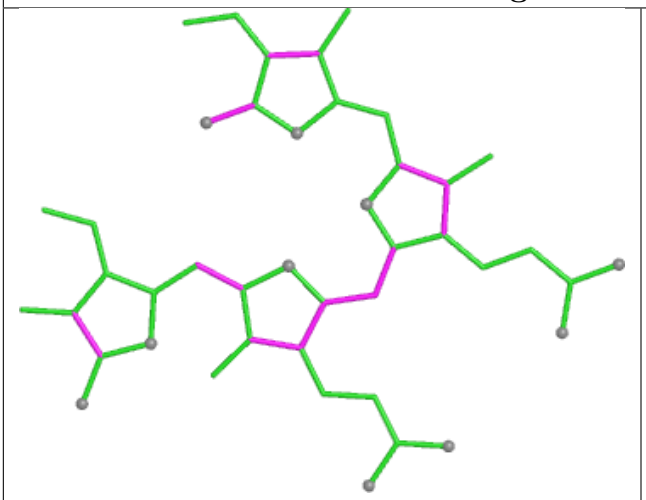


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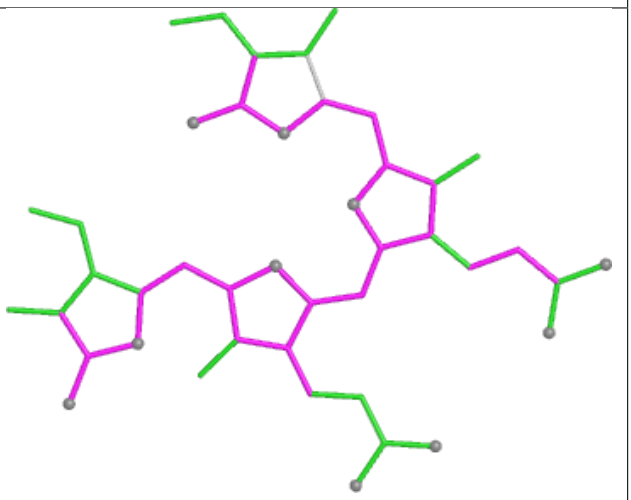


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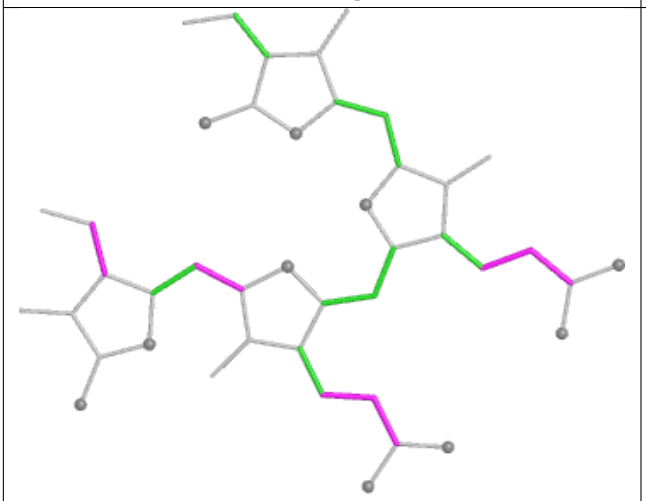
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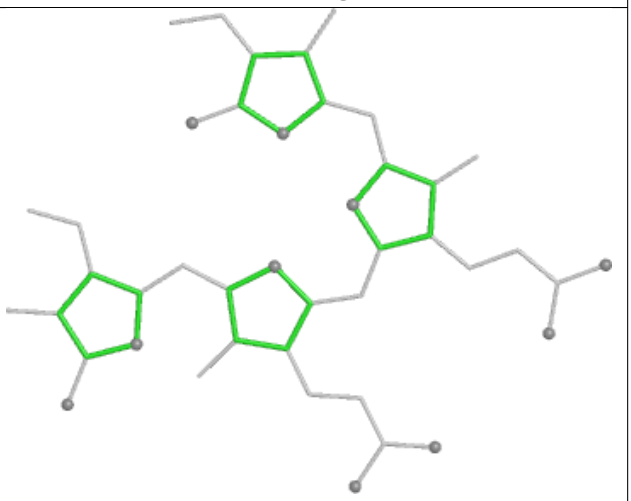
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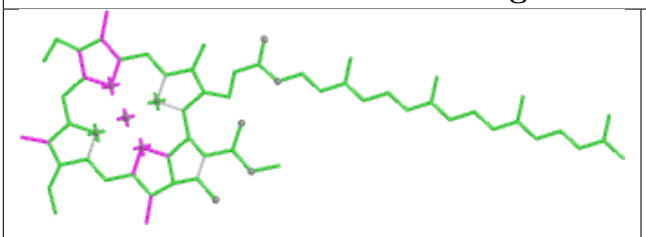


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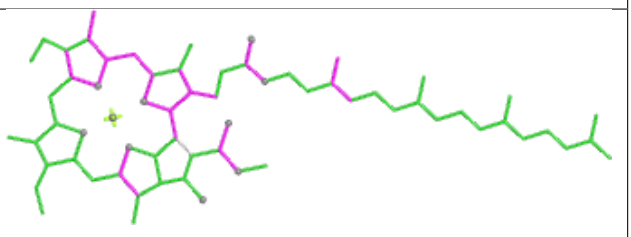


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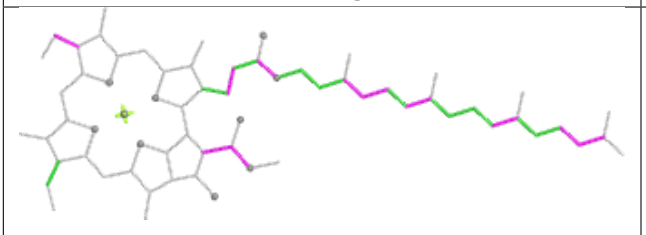
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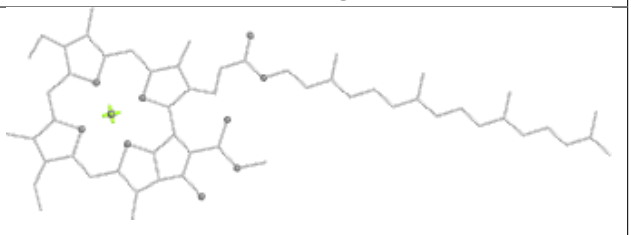
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Bond angles

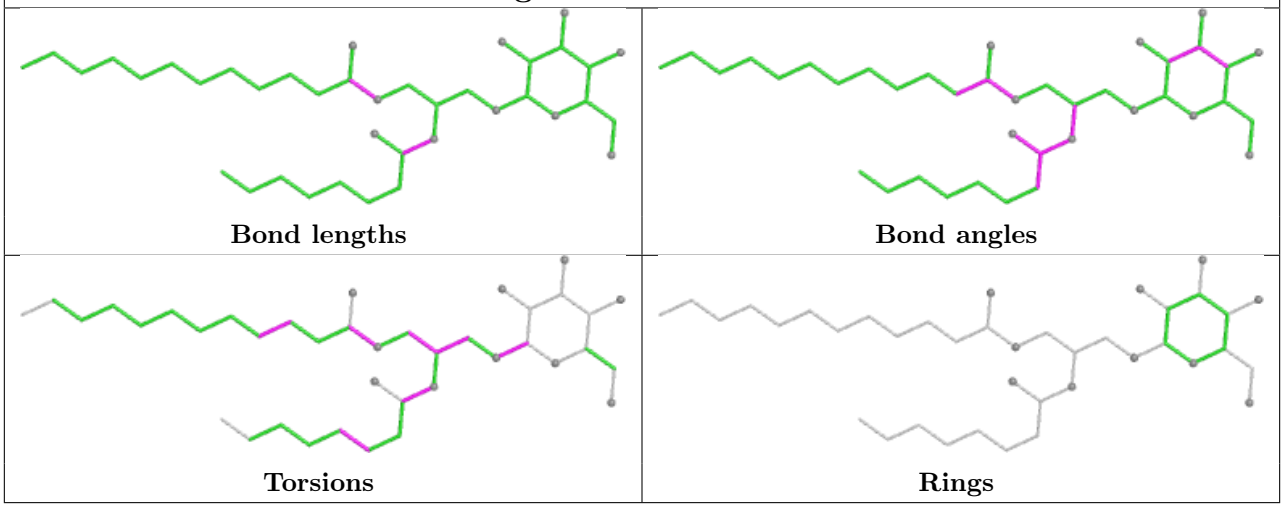


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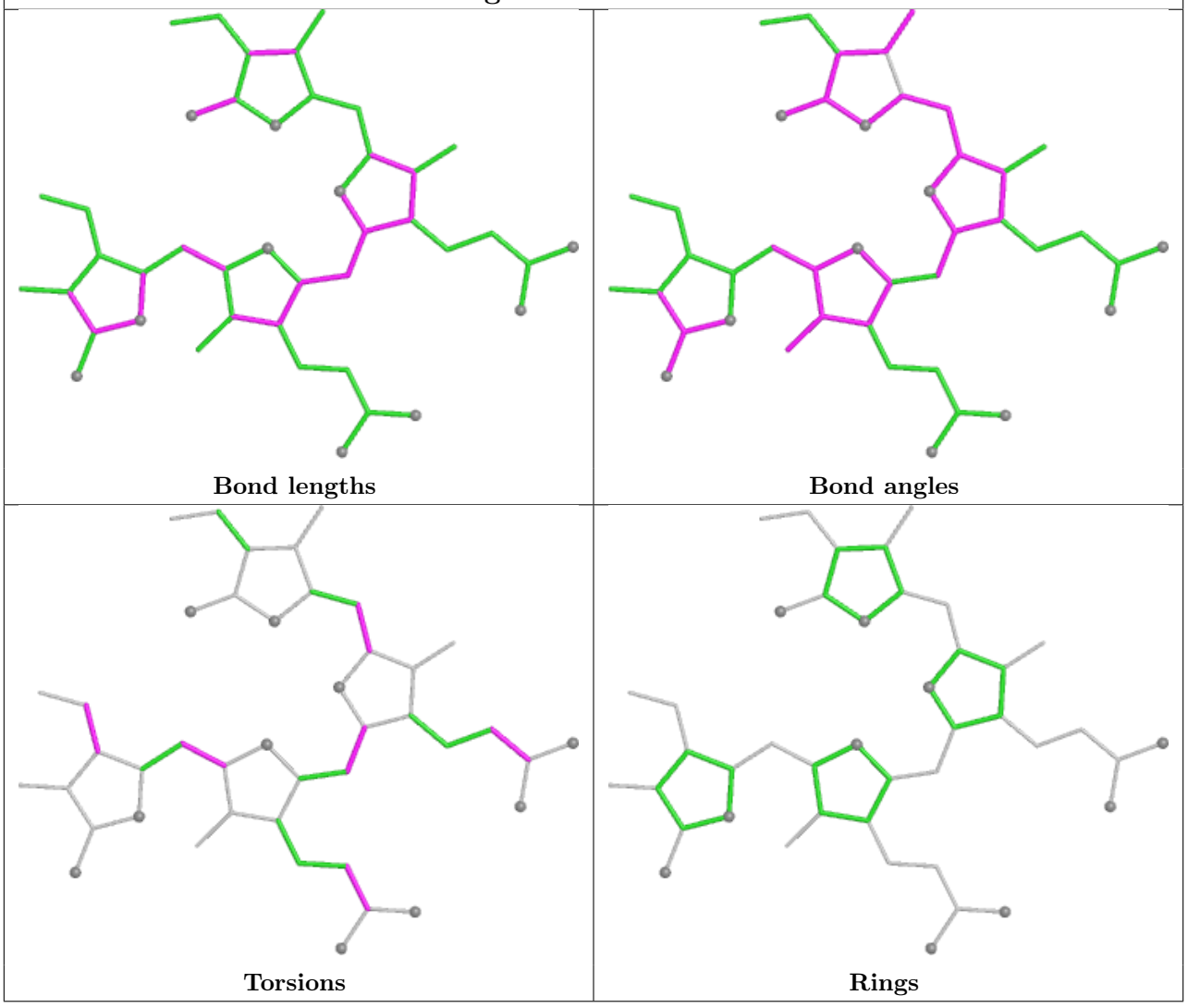


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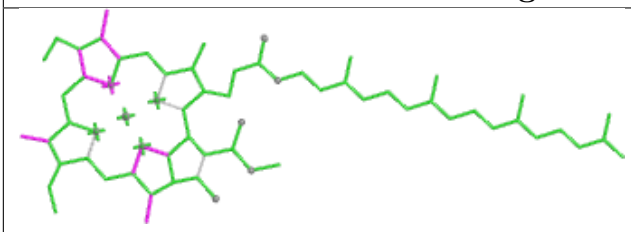
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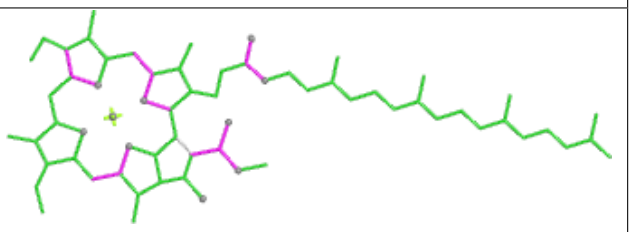
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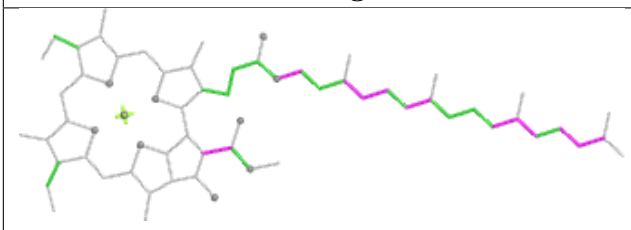
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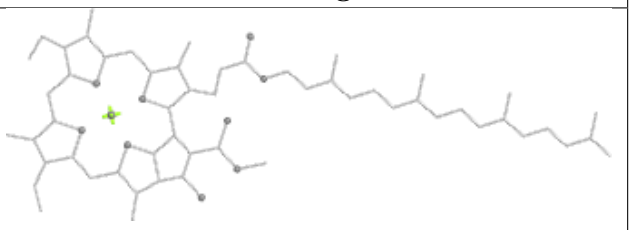
Bond lengths



Bond angles

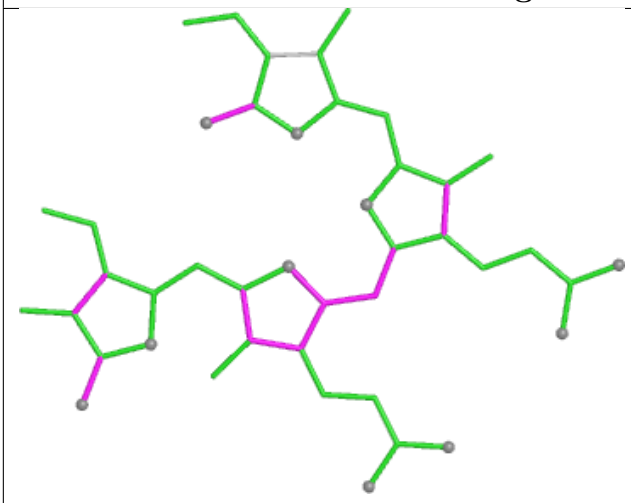


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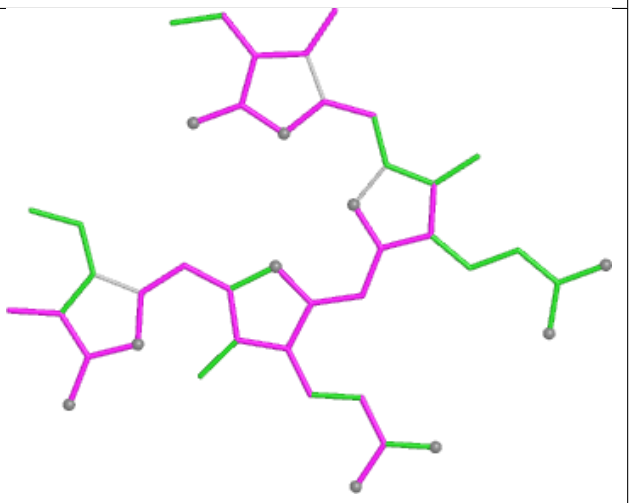


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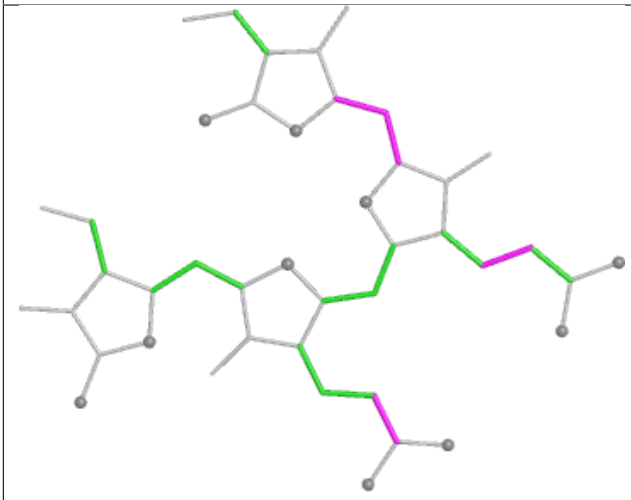
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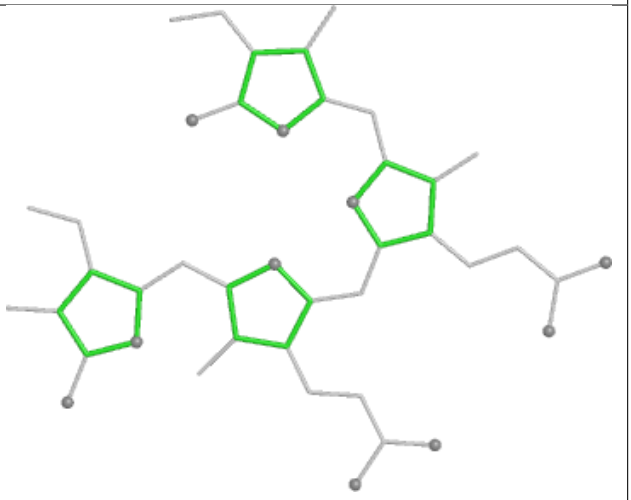
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Bond angles

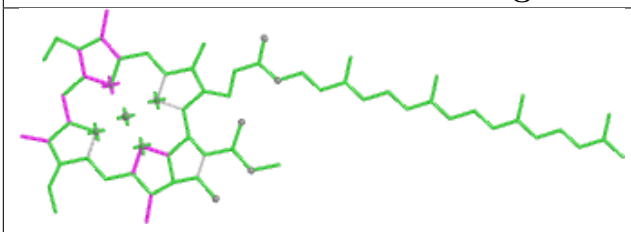


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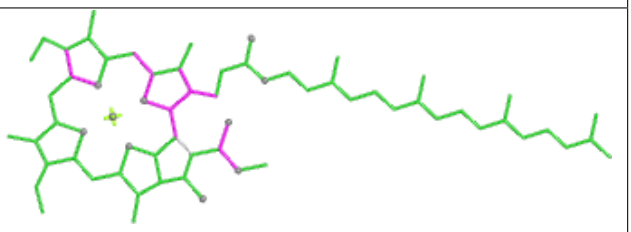


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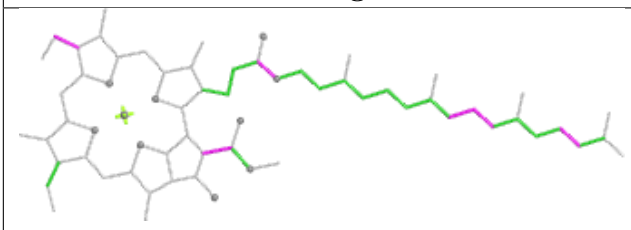
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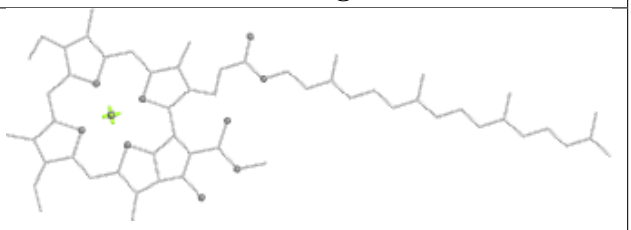
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Bond angles

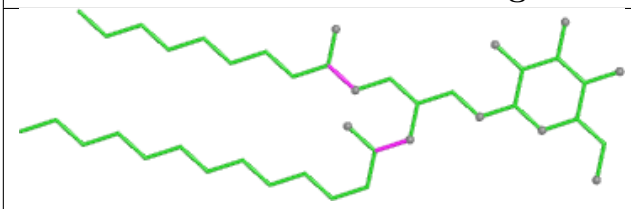


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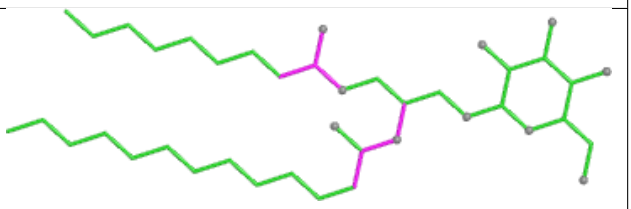


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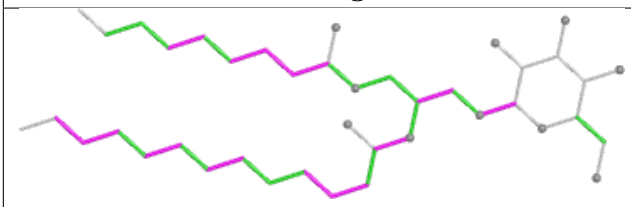
Ligand LMG m6 101



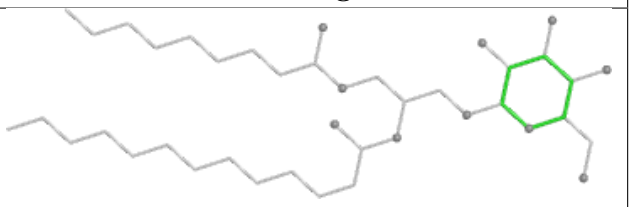
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Bond angles

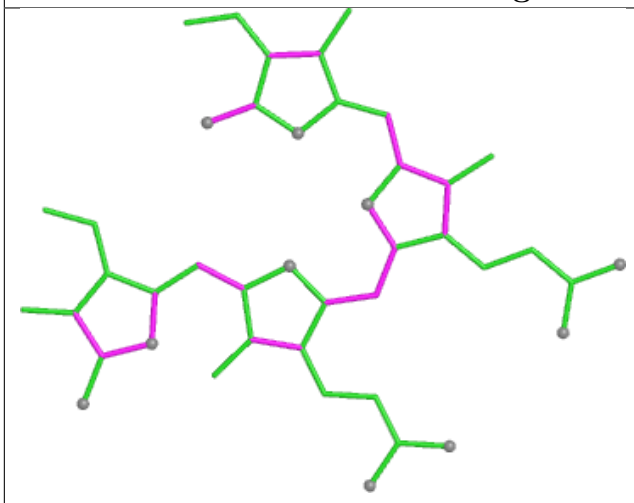


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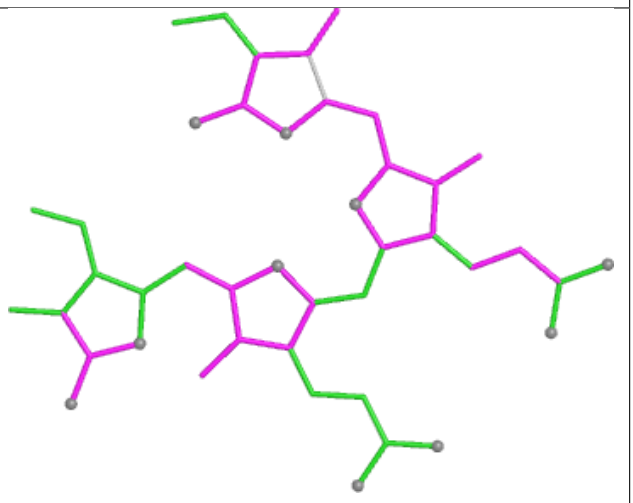


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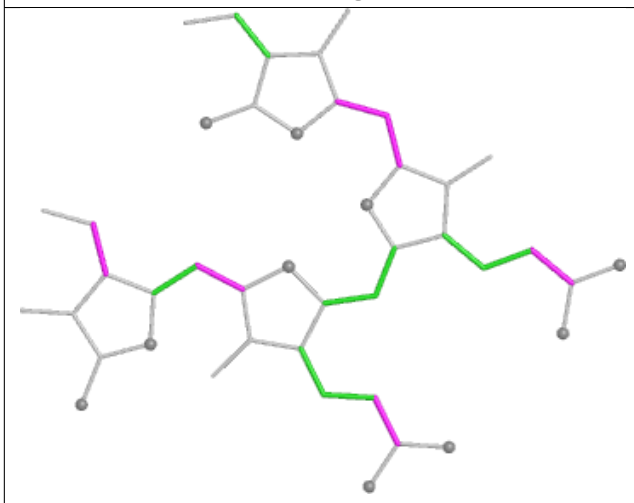
Ligand PEB AP 203



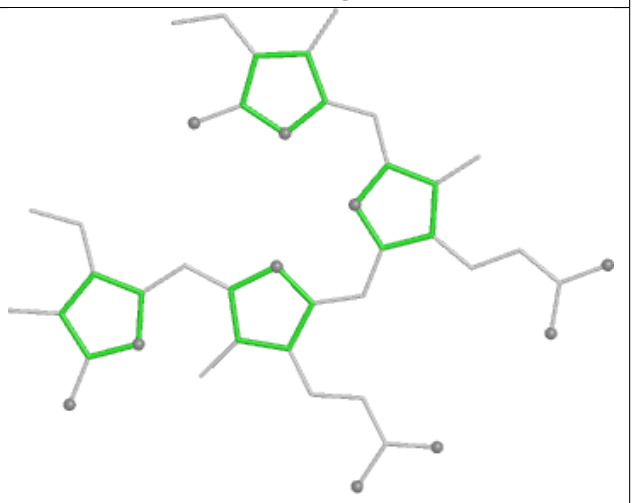
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Bond angles

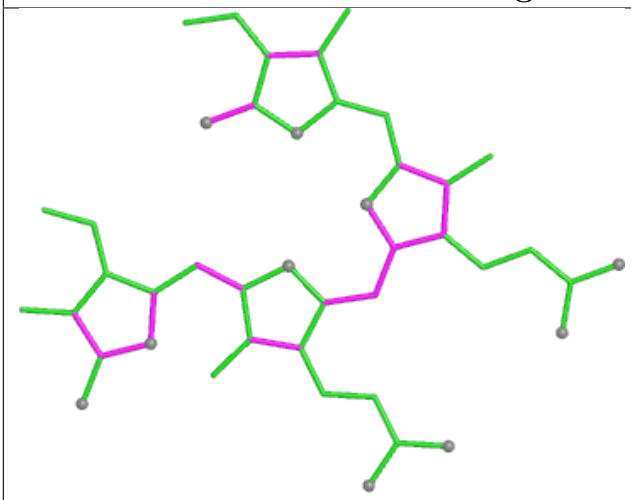


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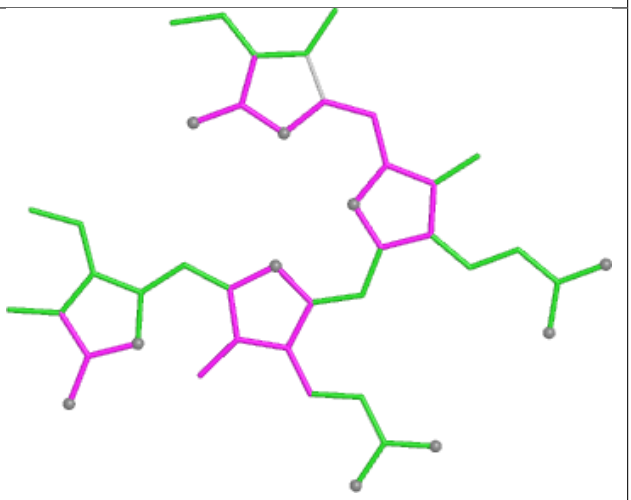


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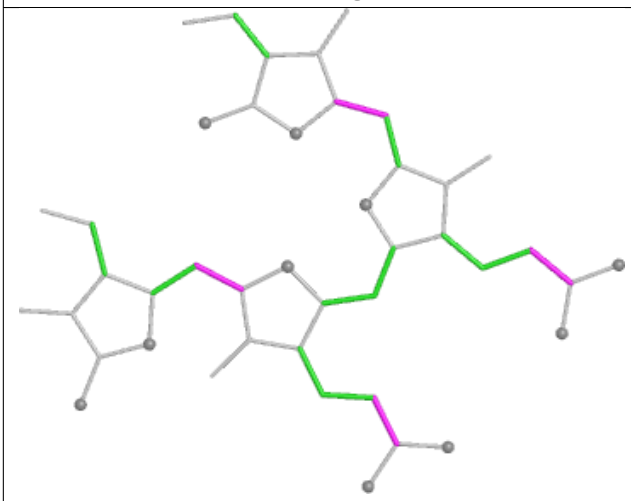
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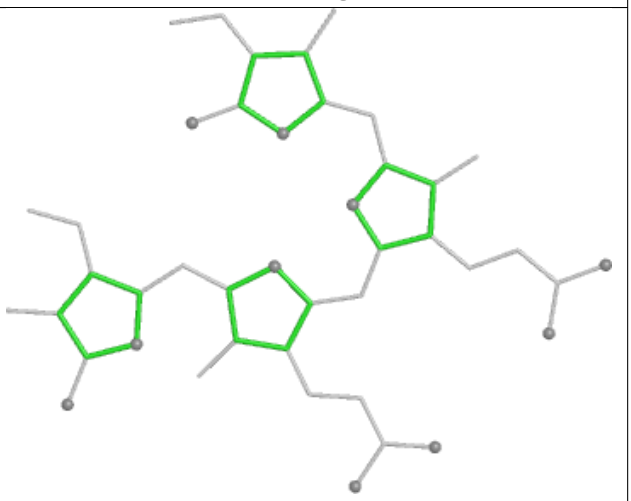
Bond lengths



Bond angles

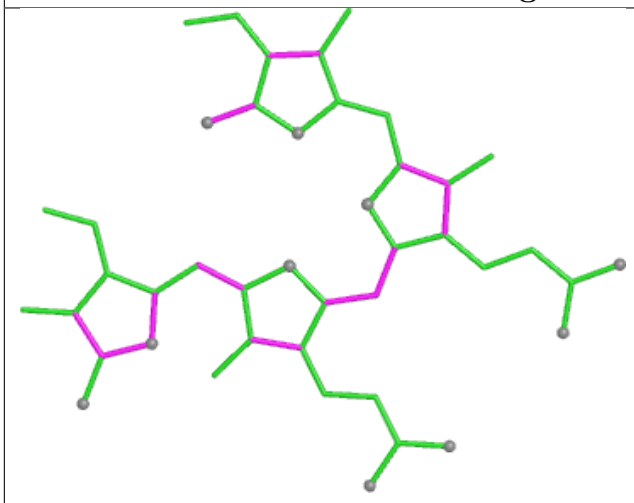


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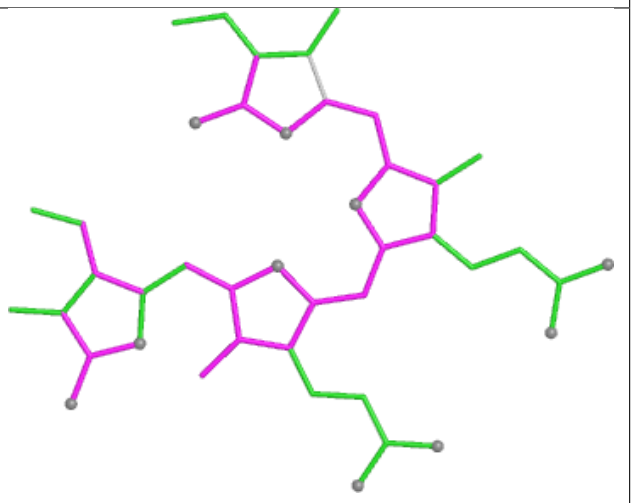


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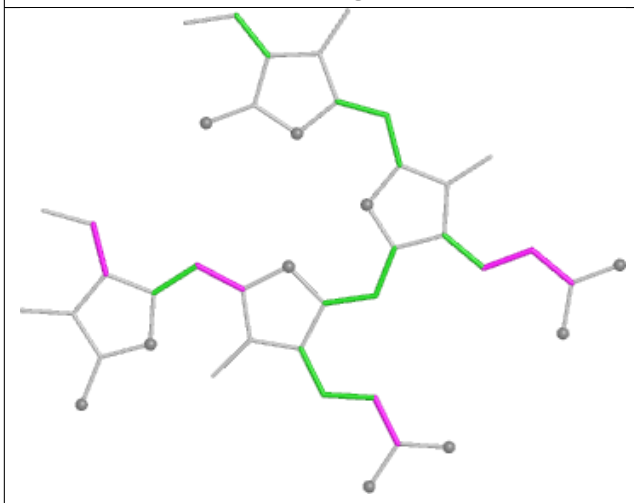
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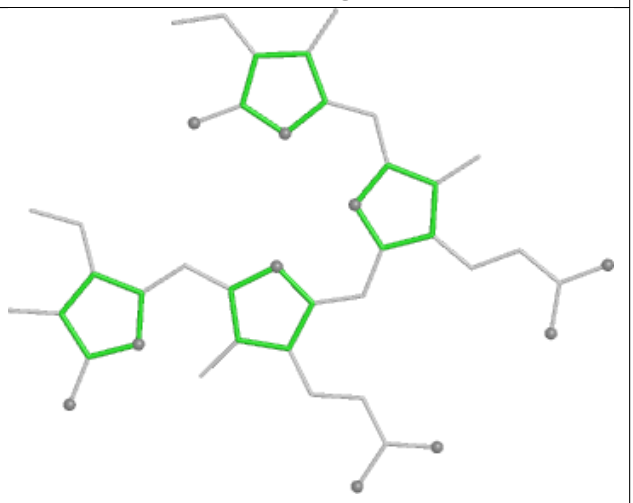
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Bond angles

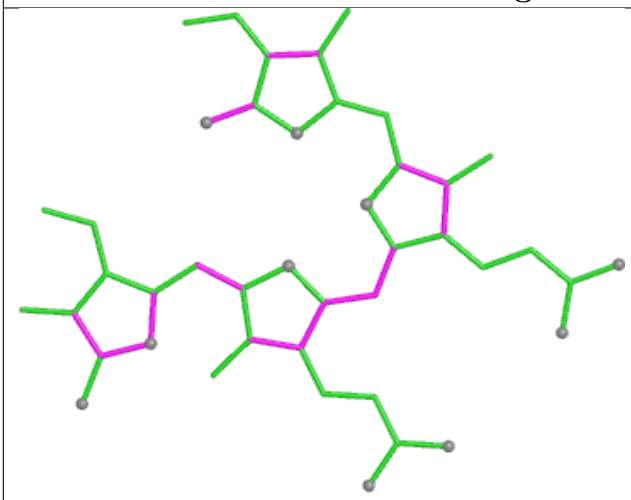


Torsions

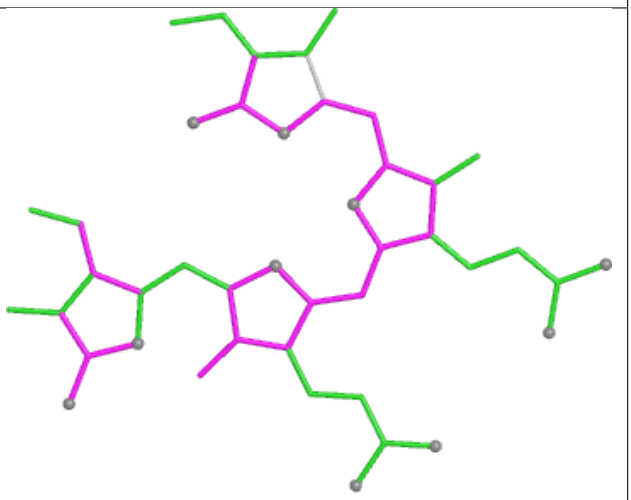


Rings

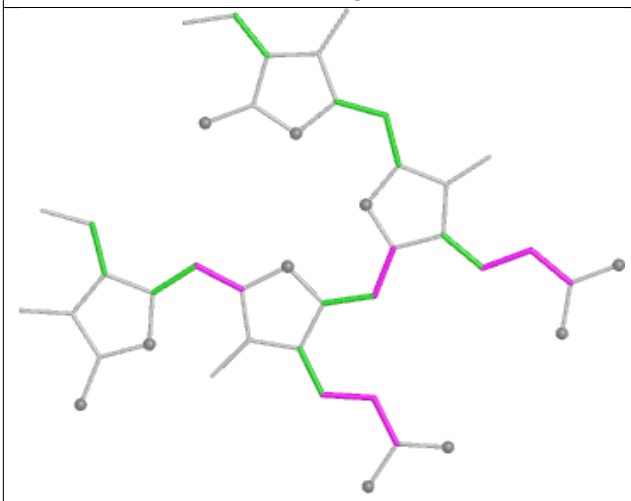
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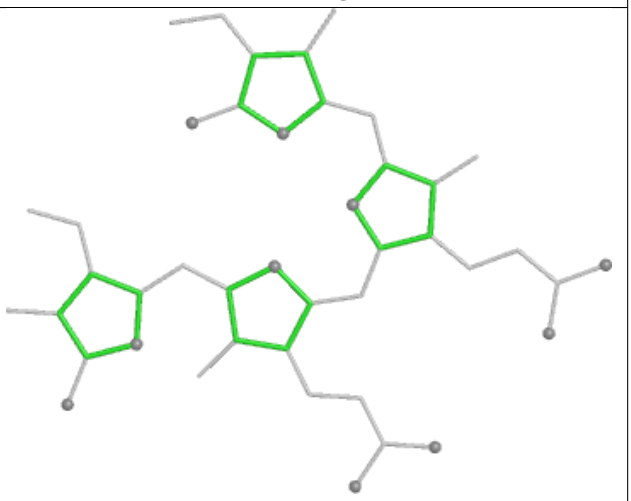
Bond lengths



Bond angles

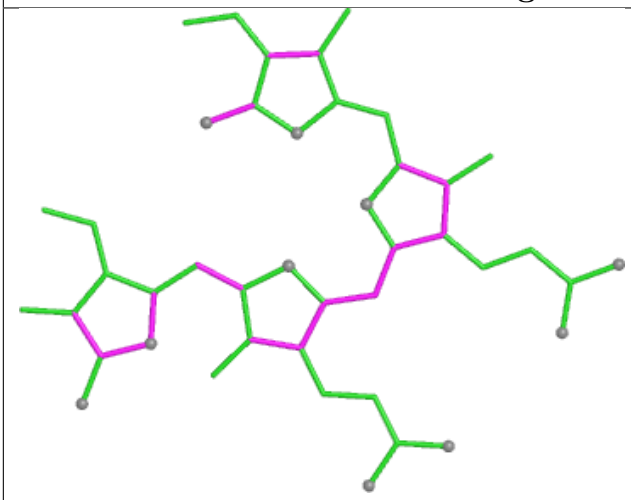


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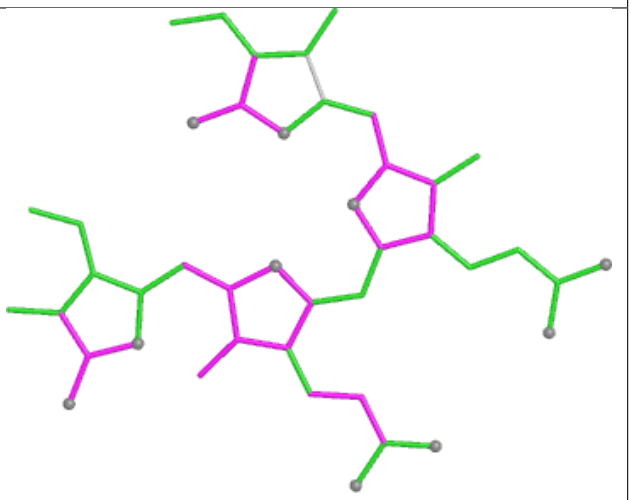


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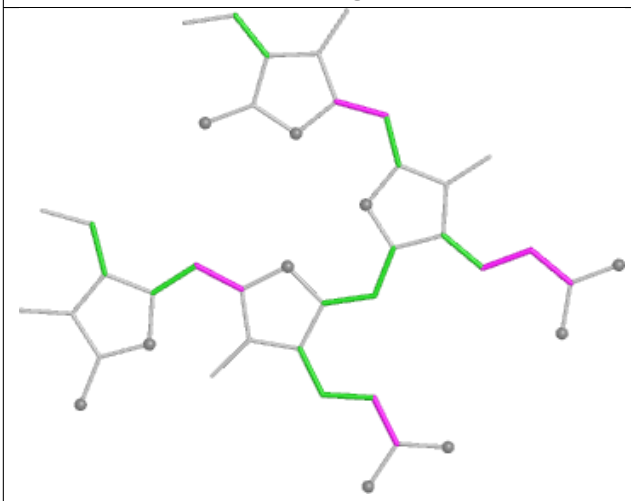
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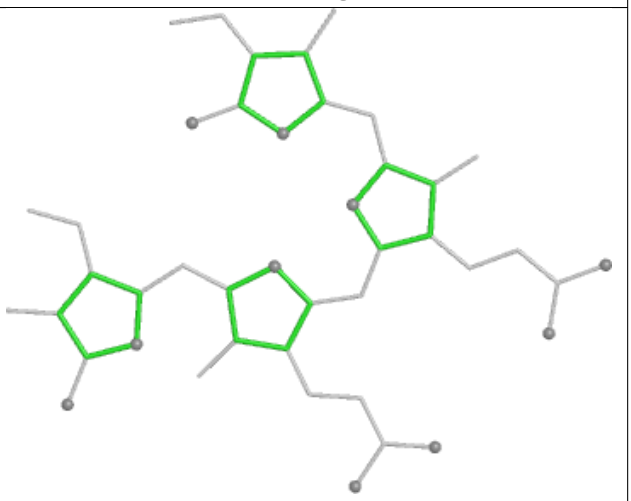
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Bond angles

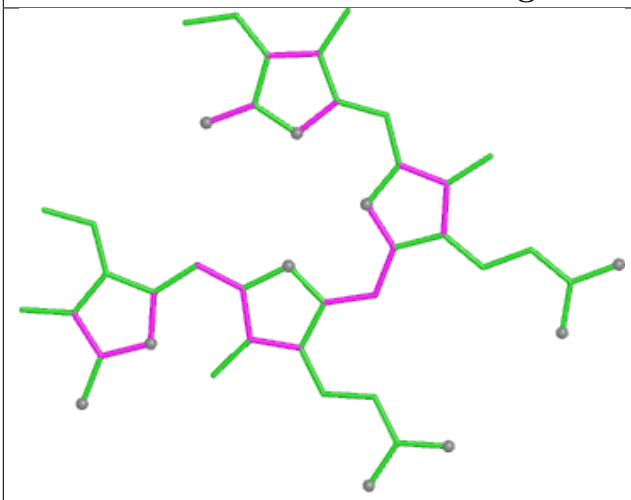


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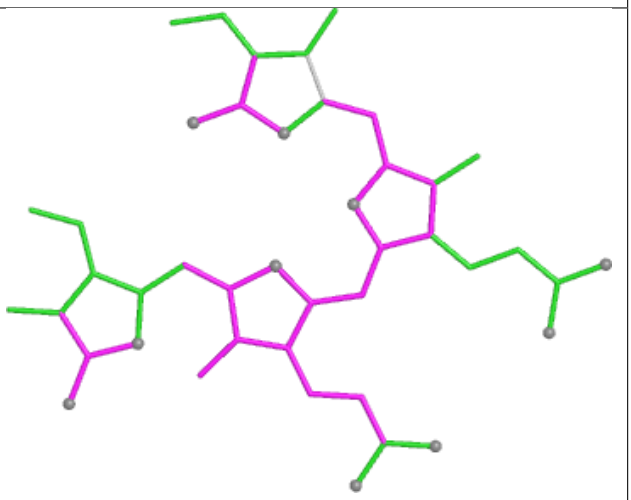


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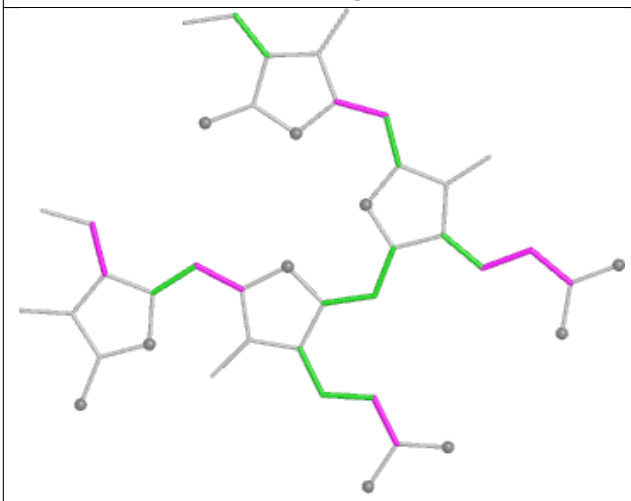
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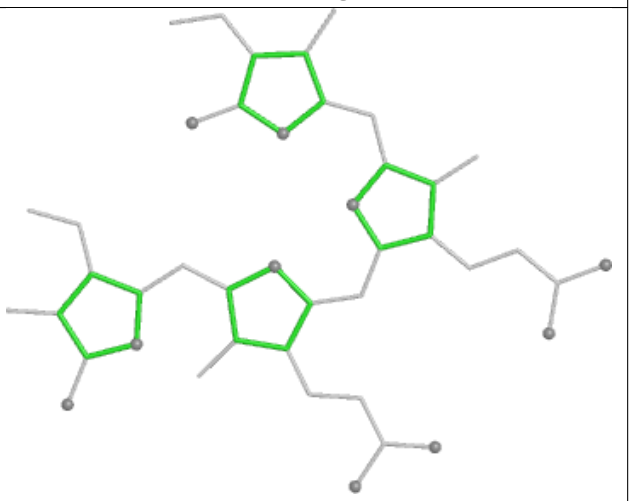
Bond lengths



Bond angles

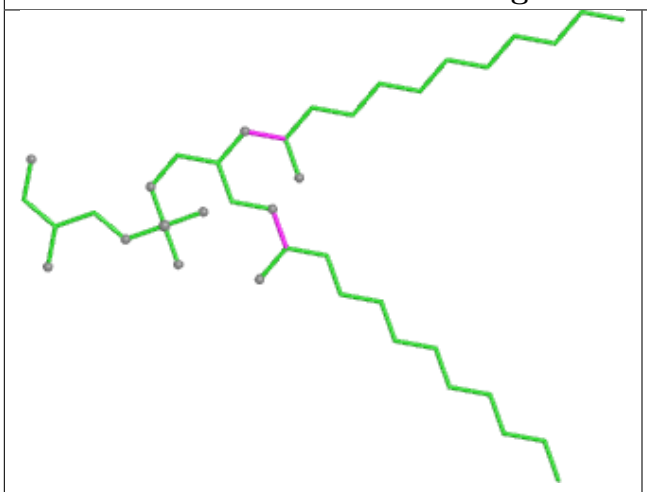


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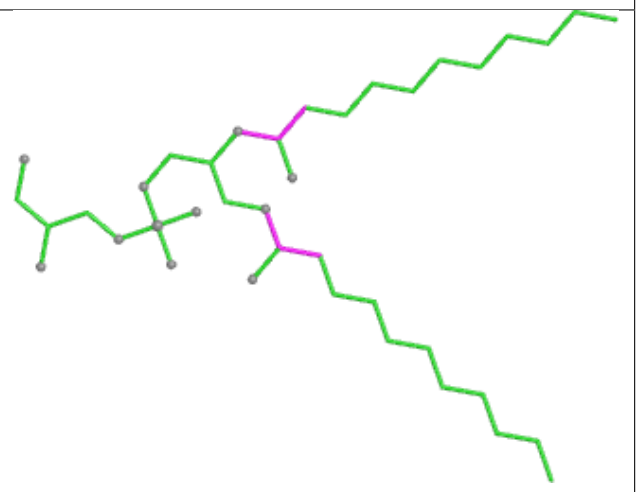


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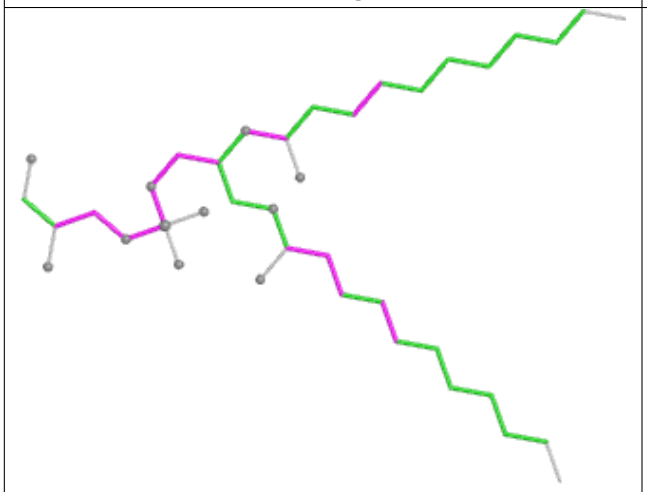
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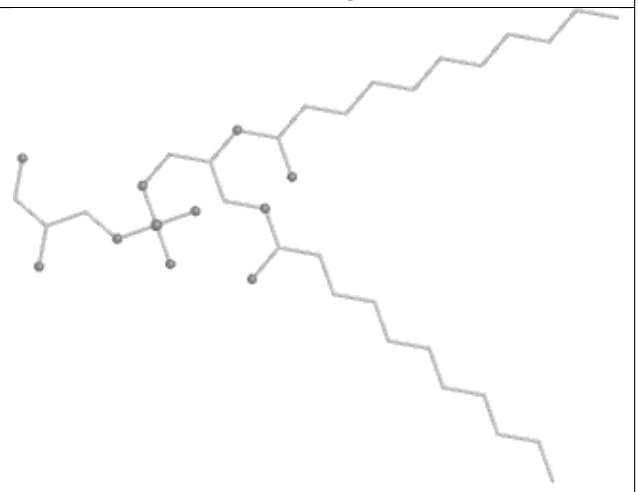
Bond lengths



Bond angles

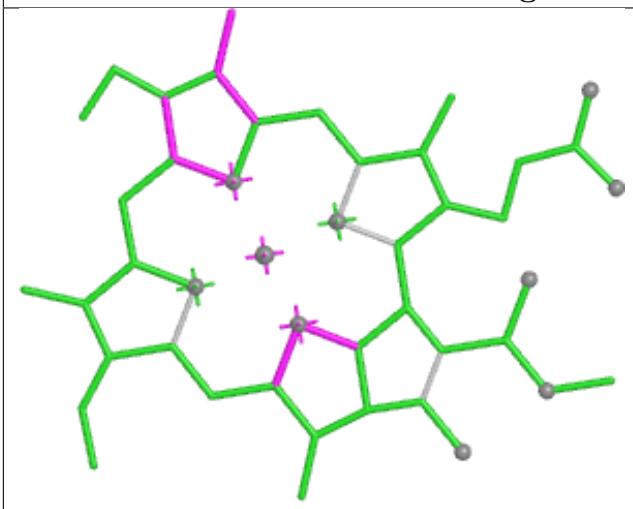


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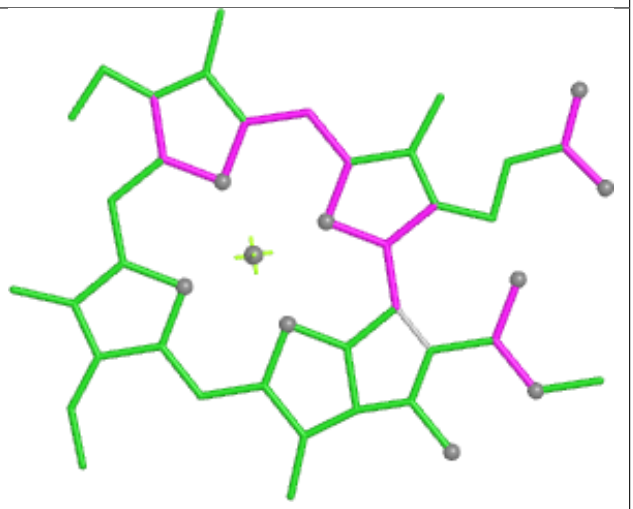


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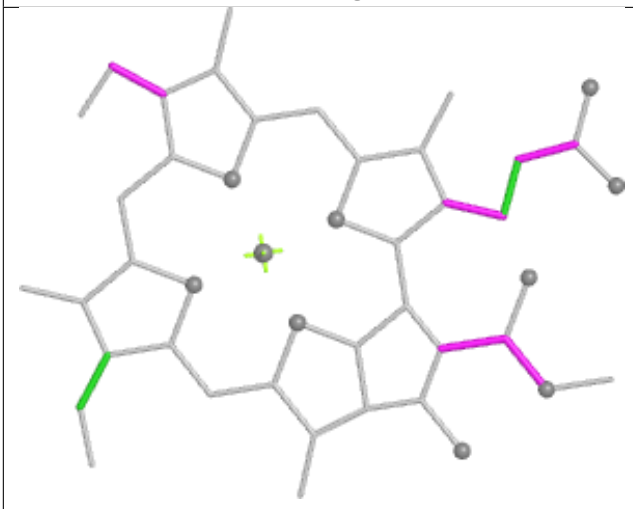
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Bond lengths



Bond angles

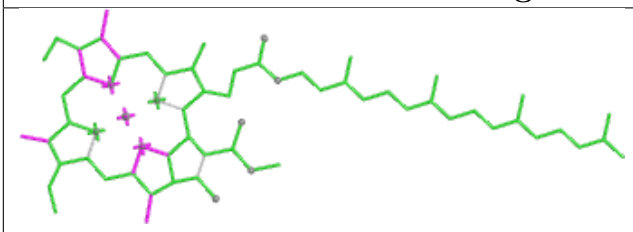


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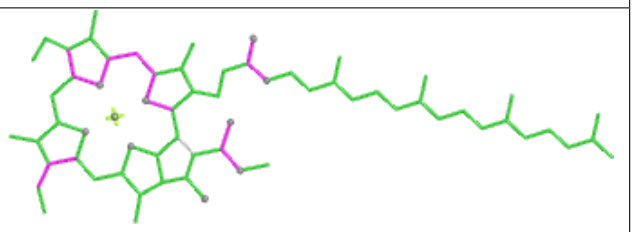


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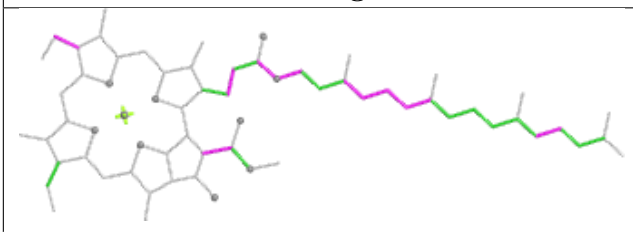
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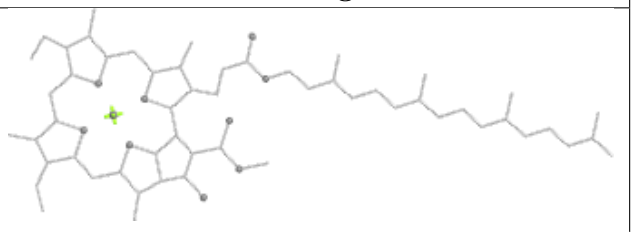
Bond lengths



Bond angles

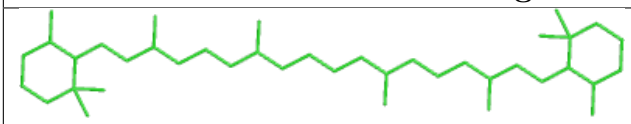


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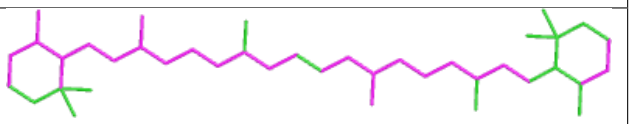


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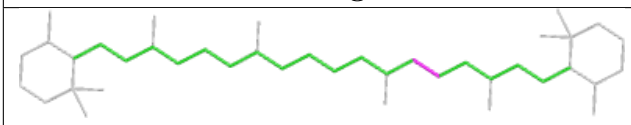
Ligand BCR bL 602



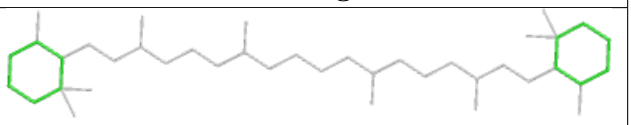
Bond lengths



Bond angles

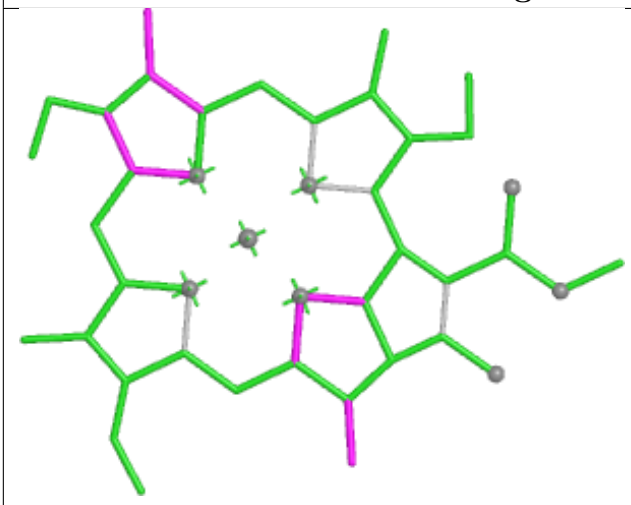


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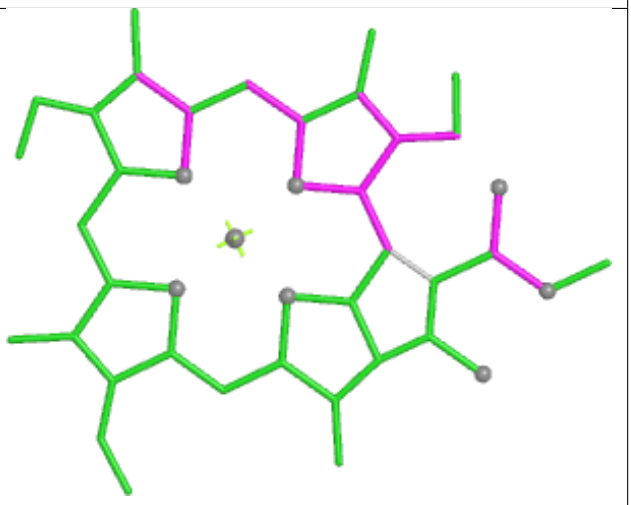


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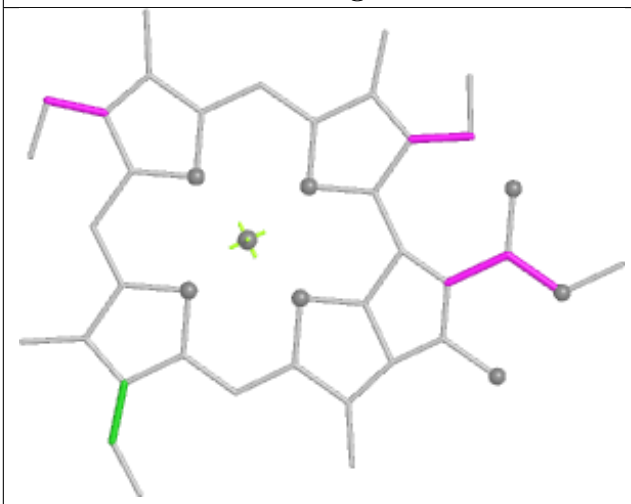
Ligand CLA 4N 610



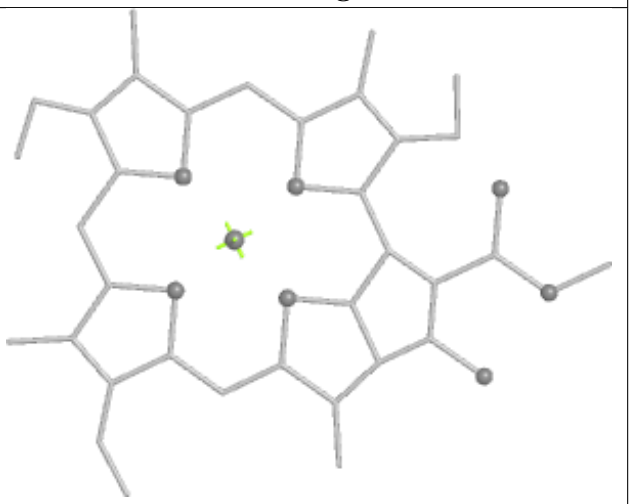
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Bond angles

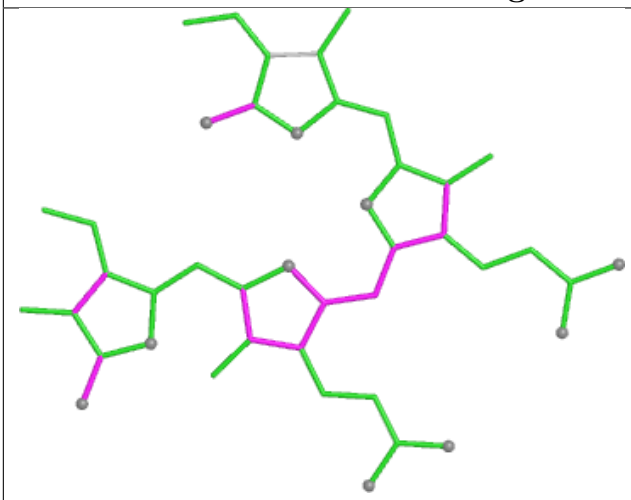


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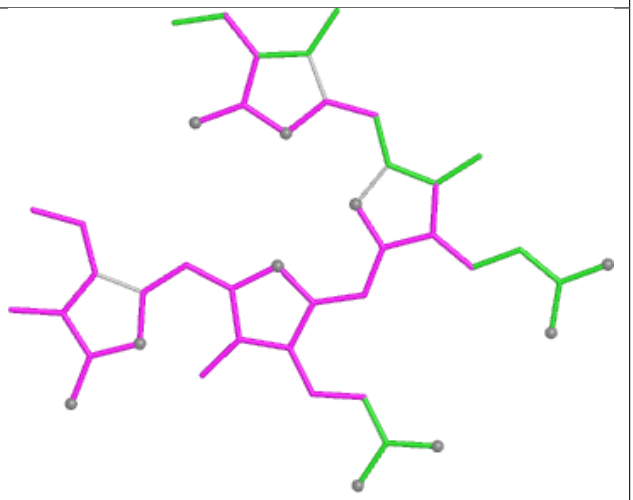


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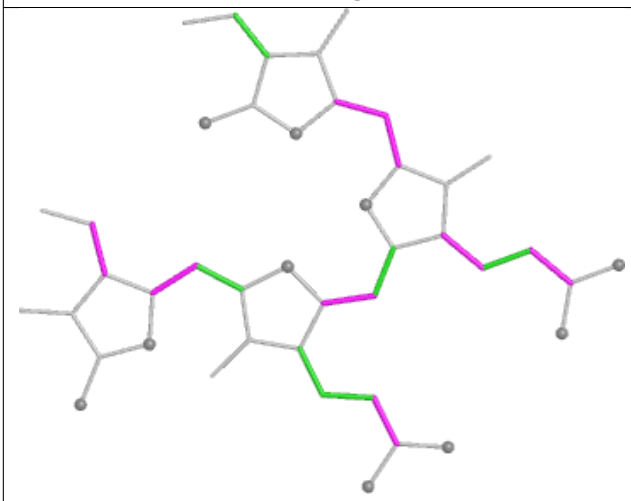
Ligand PUB AH 304



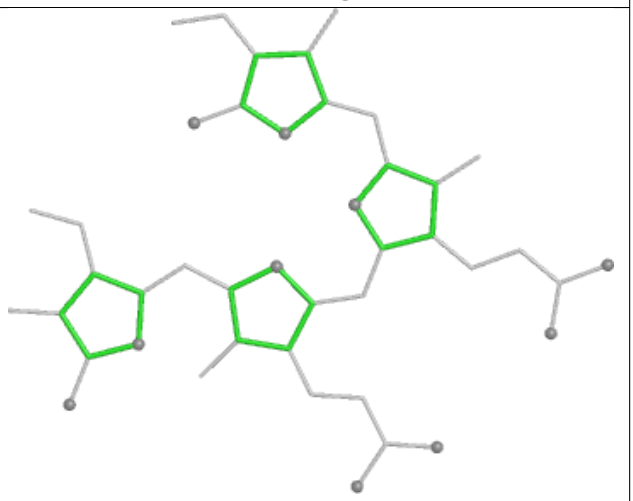
Bond lengths



Bond angles

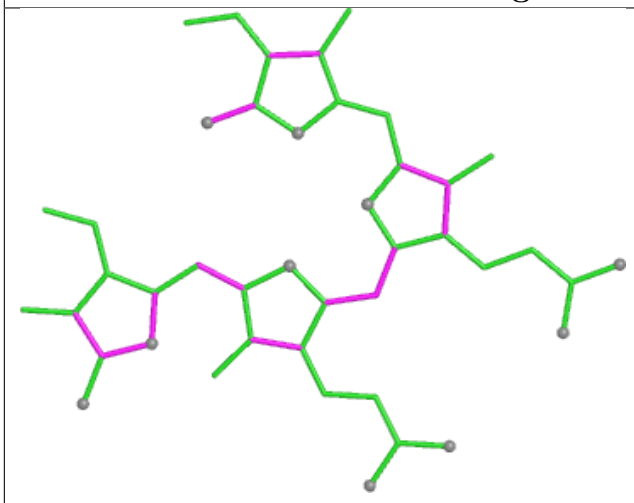


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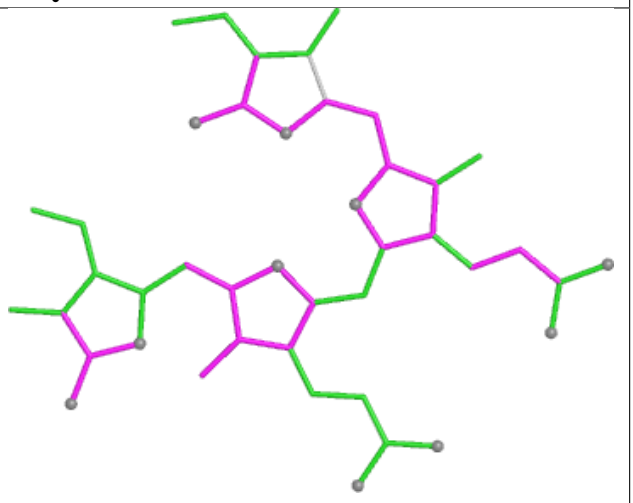


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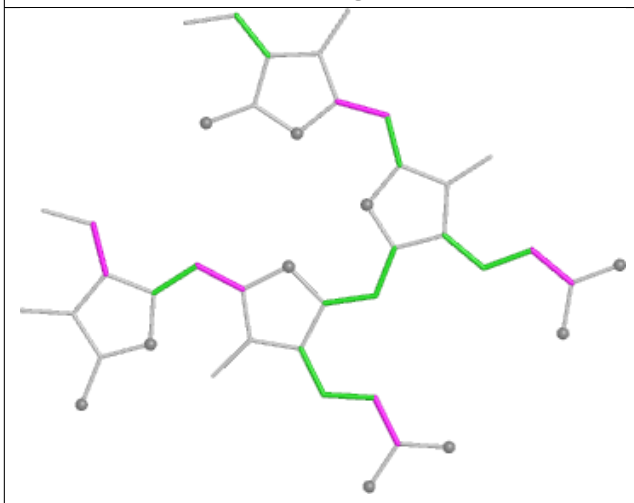
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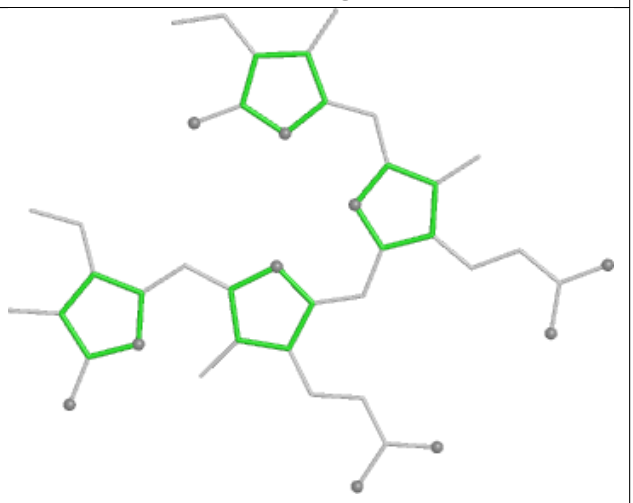
Bond lengths



Bond angles

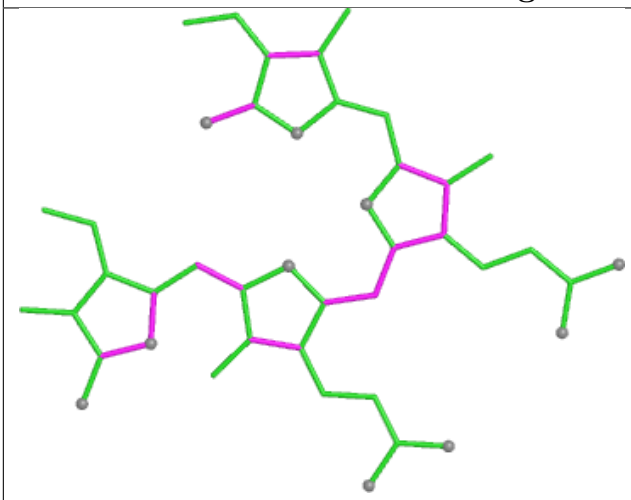


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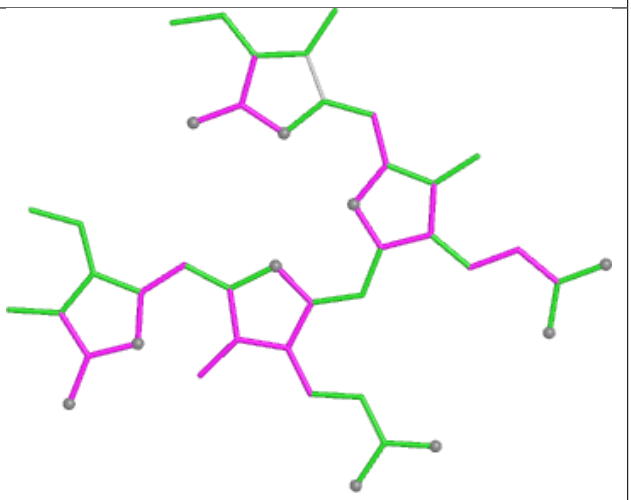


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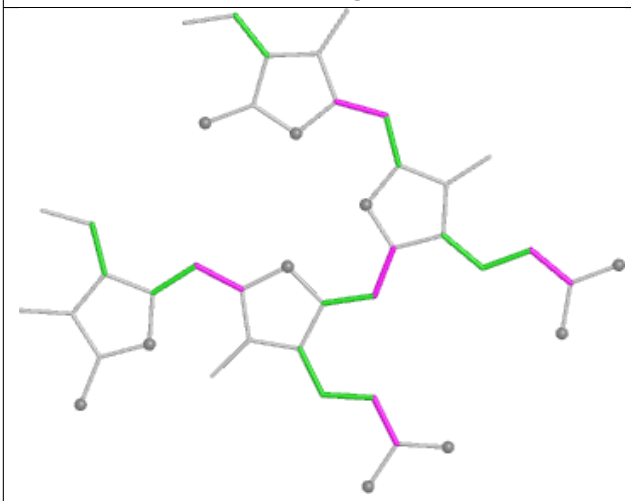
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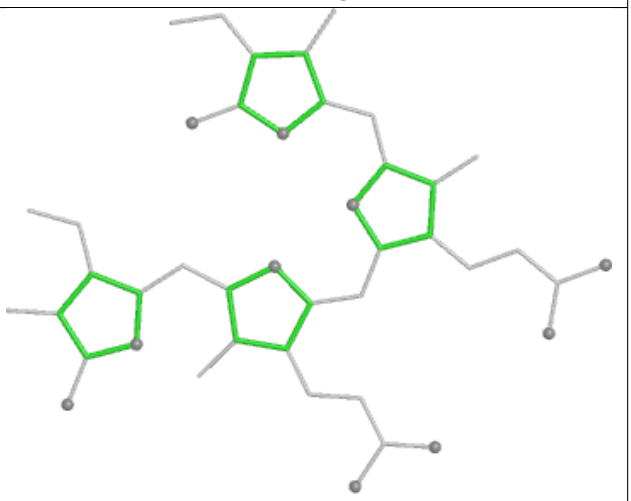
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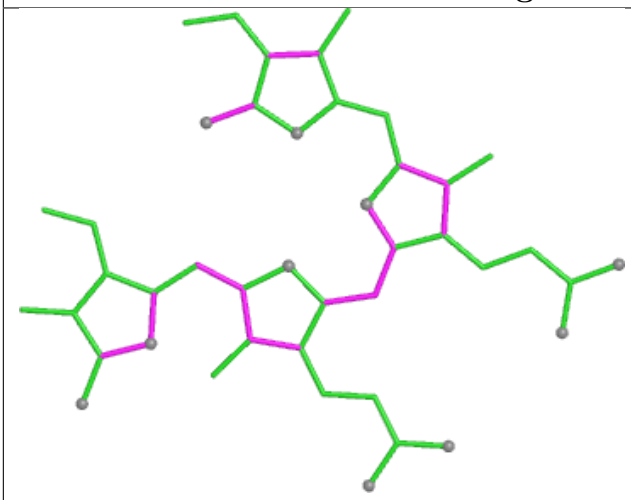


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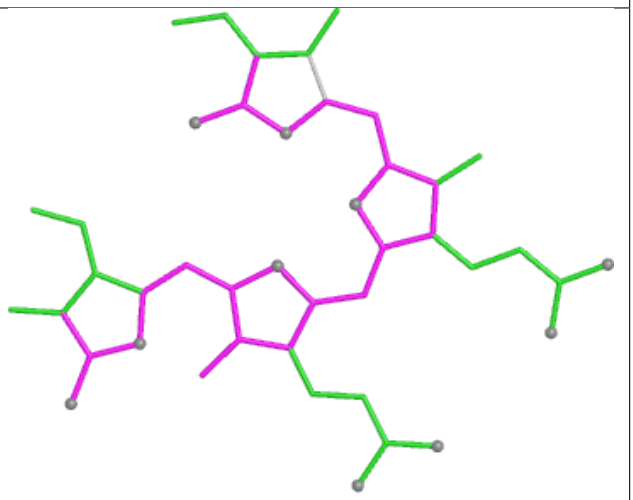


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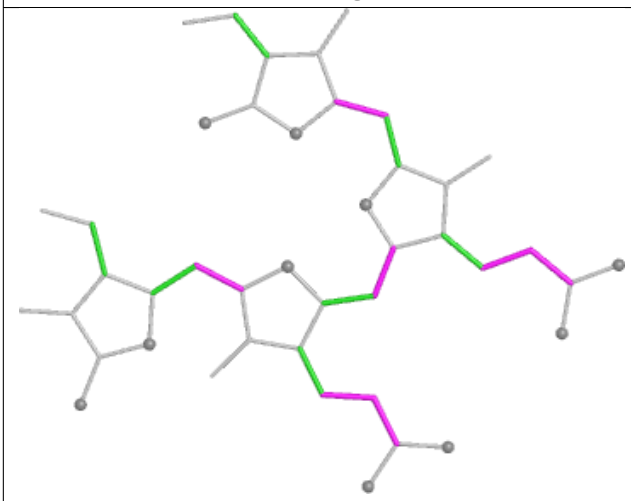
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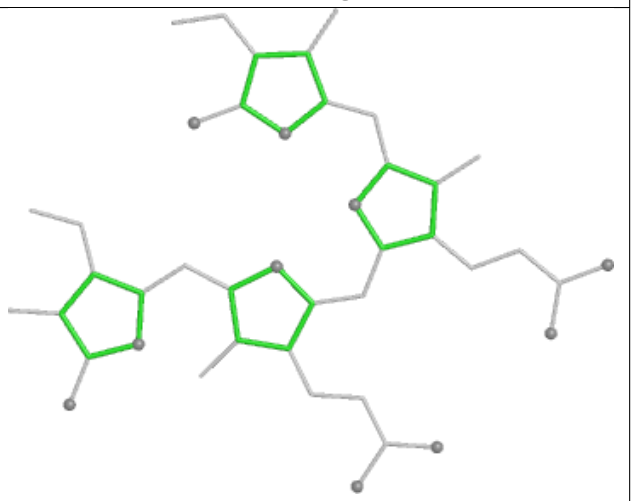
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Bond angles

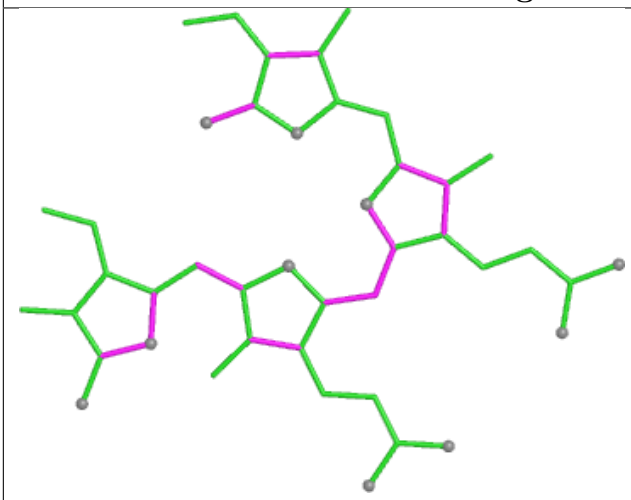


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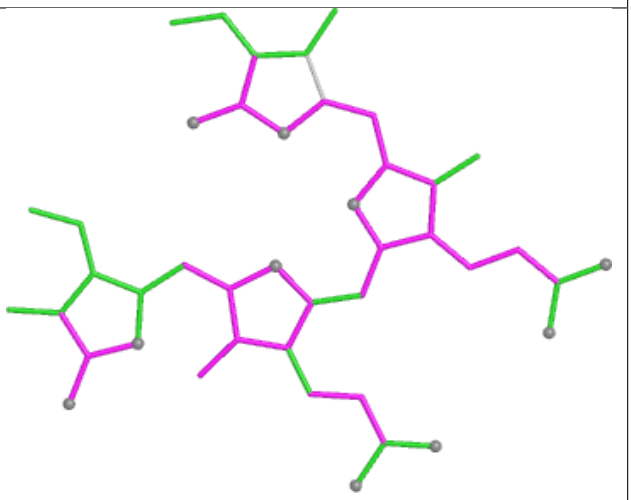


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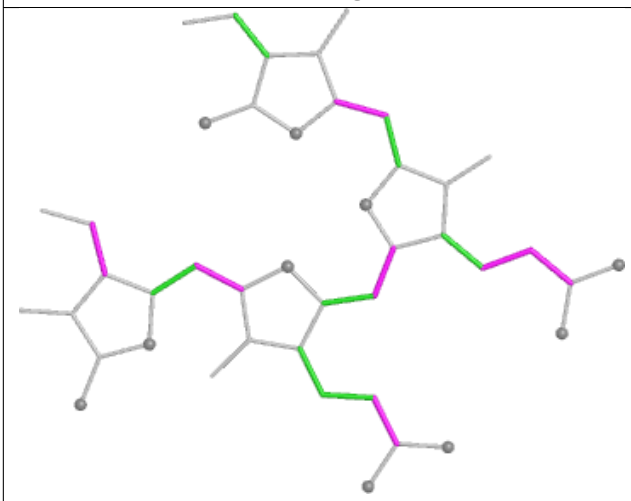
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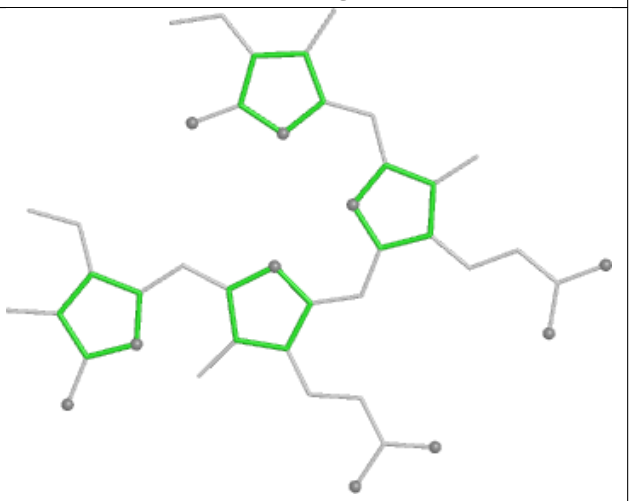
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Bond angles

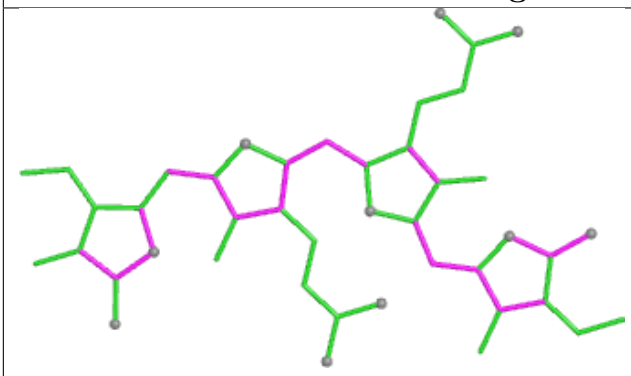


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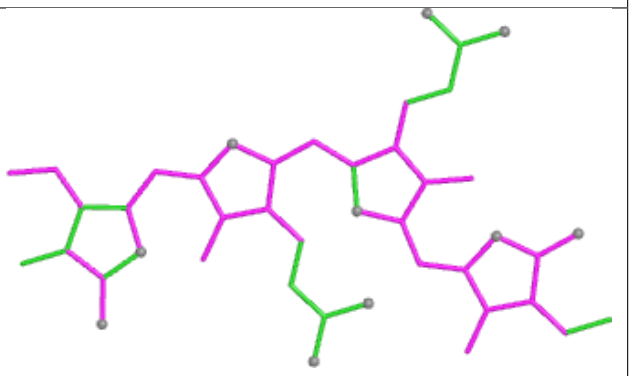


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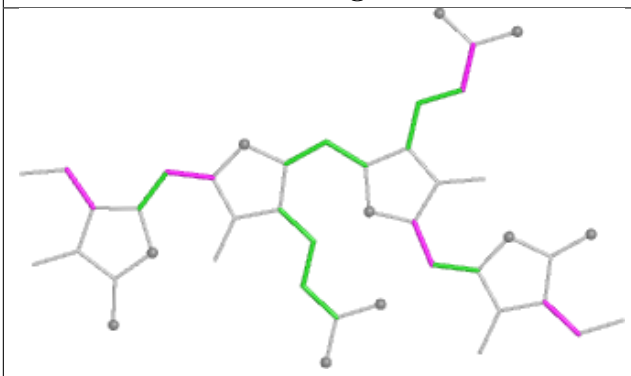
Ligand CYC c3 1001



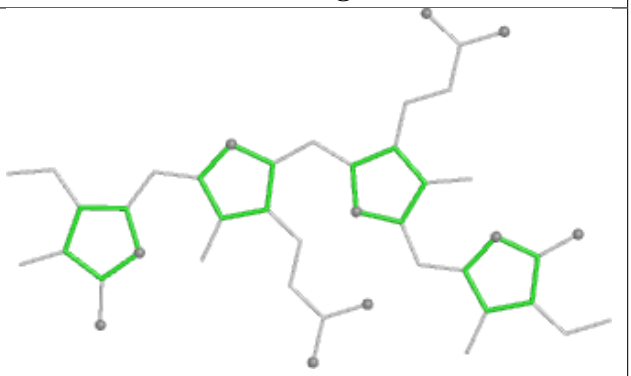
Bond lengths



Bond angles

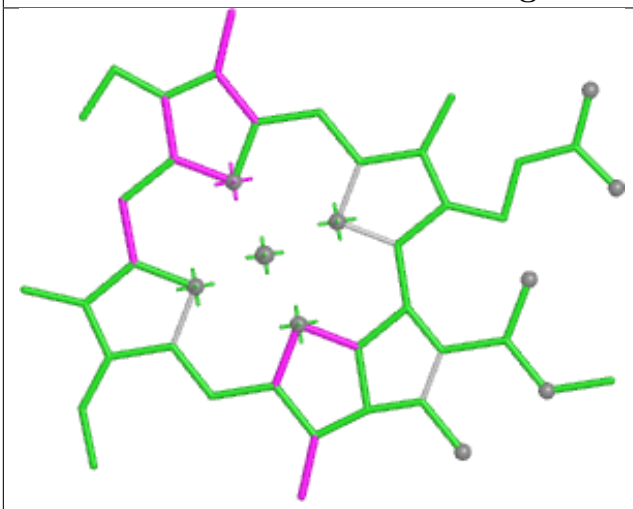


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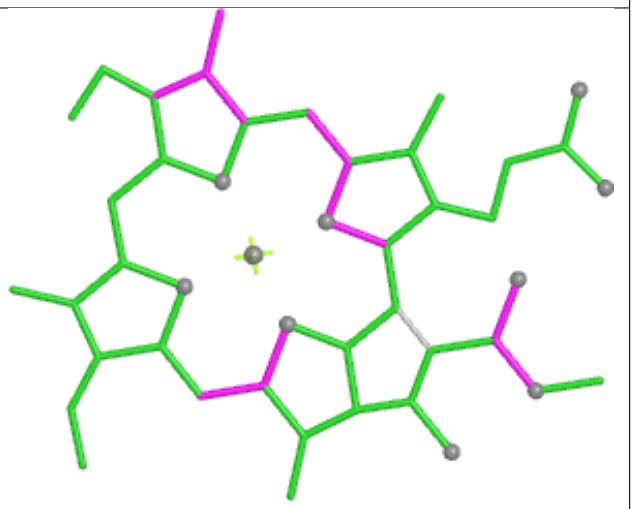


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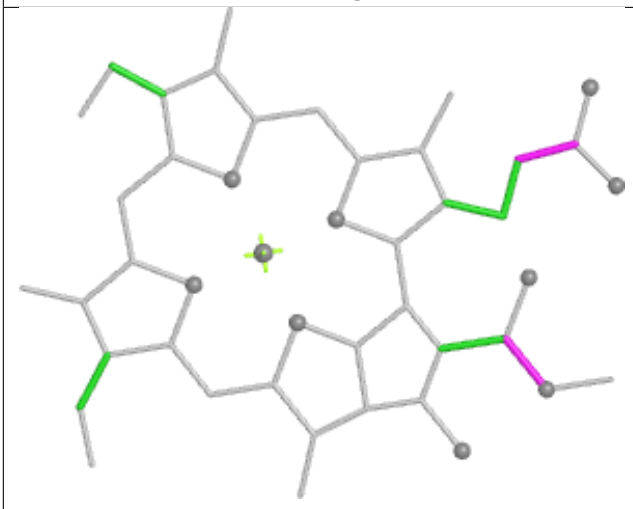
Ligand CLA 12 603



Bond lengths



Bond angles

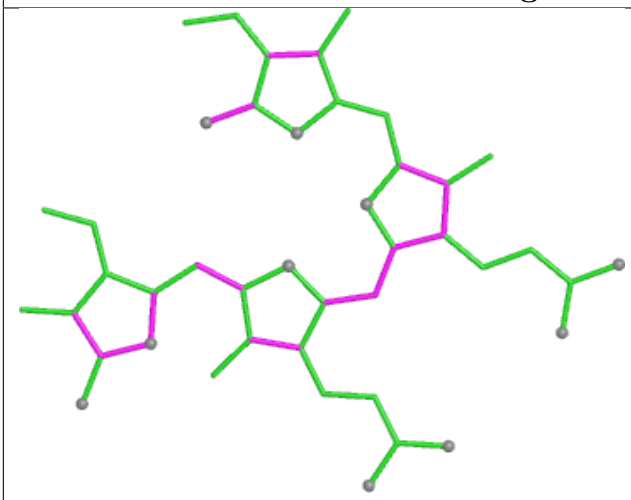


Torsions

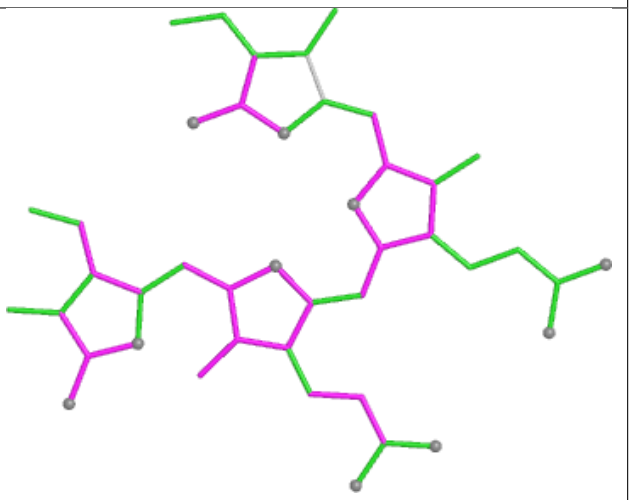


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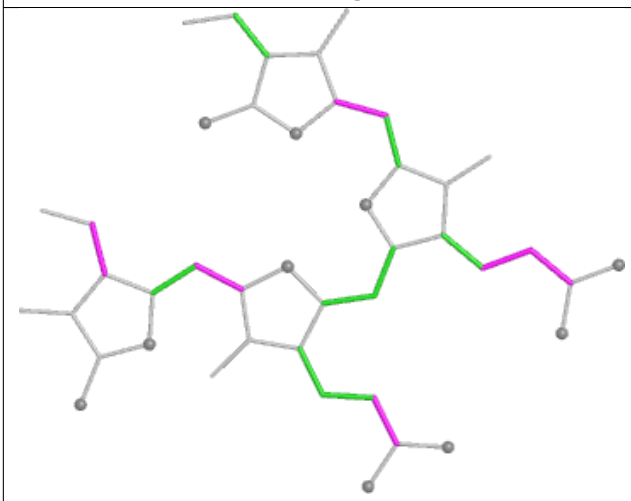
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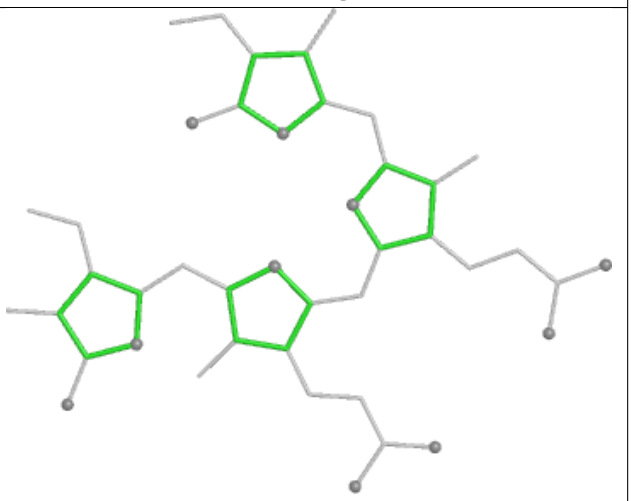
Bond lengths



Bond angles

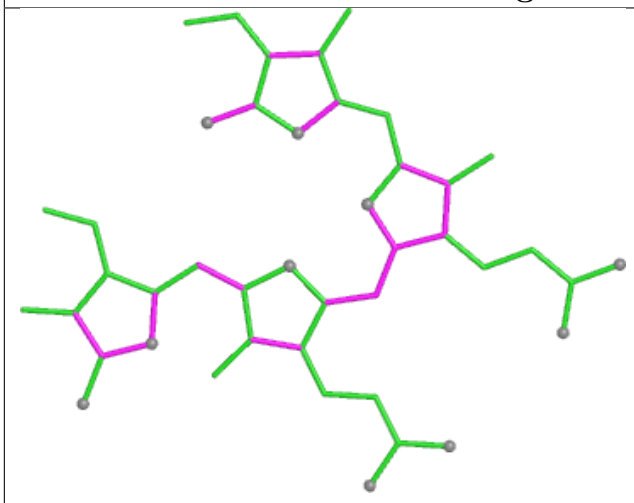


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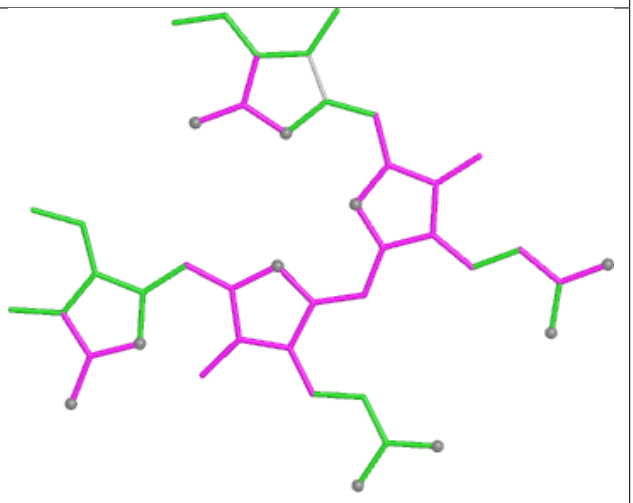


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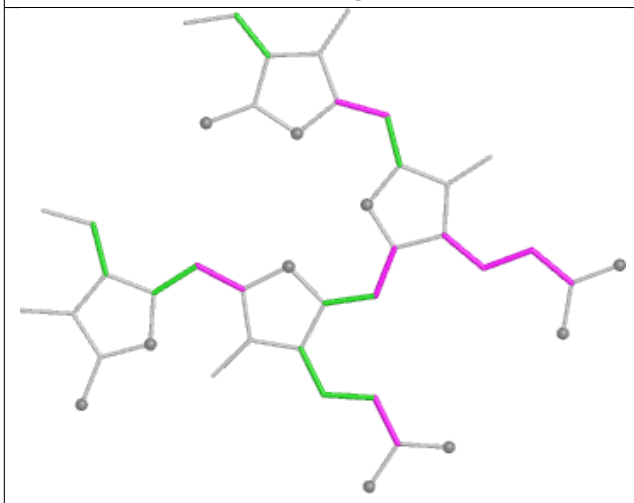
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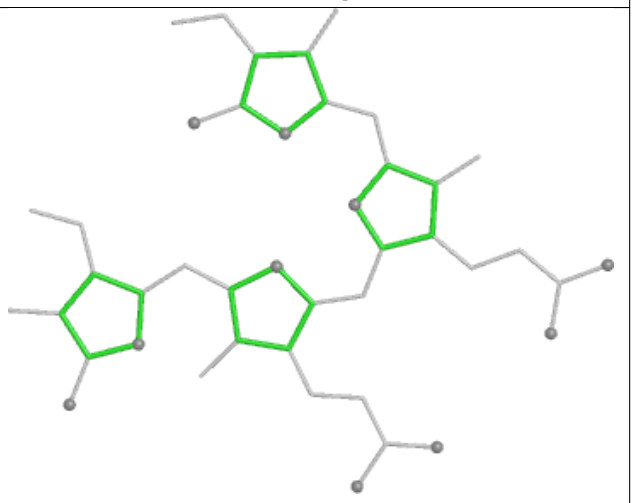
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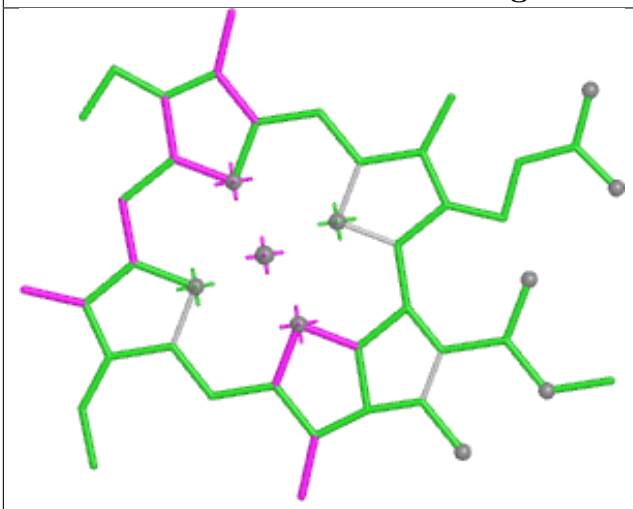


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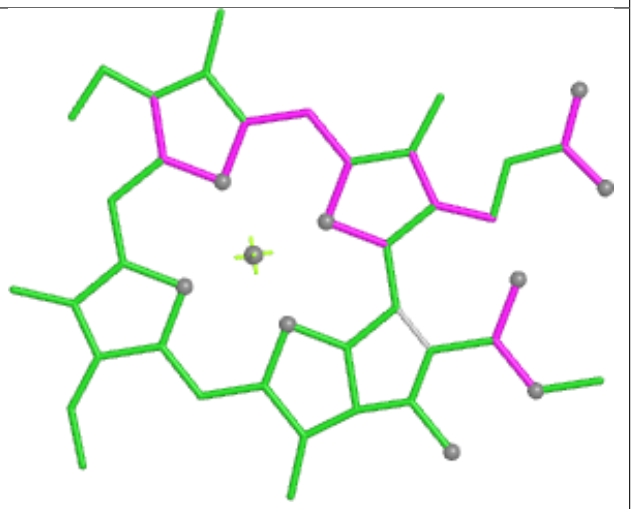


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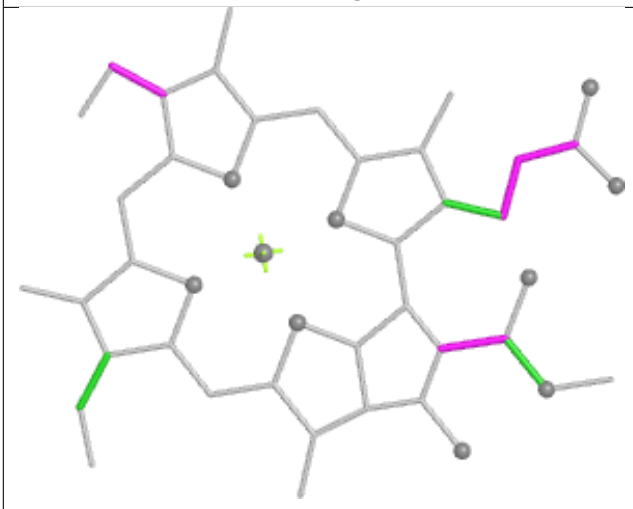
Ligand CLA BN 828



Bond lengths



Bond angles

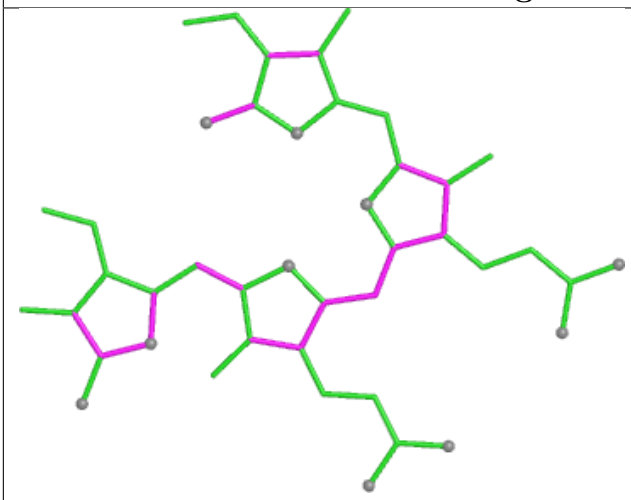


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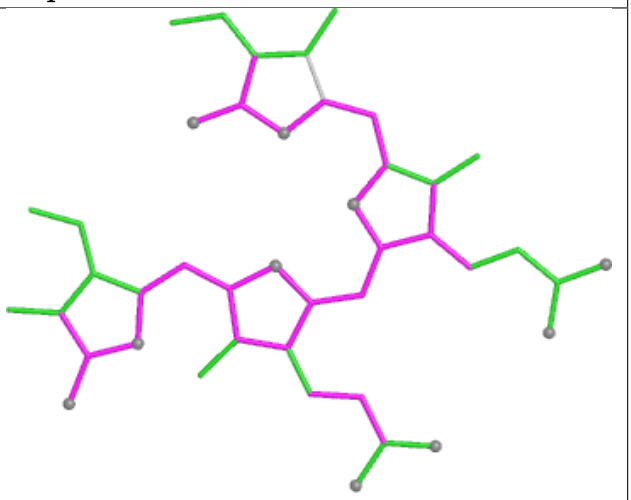


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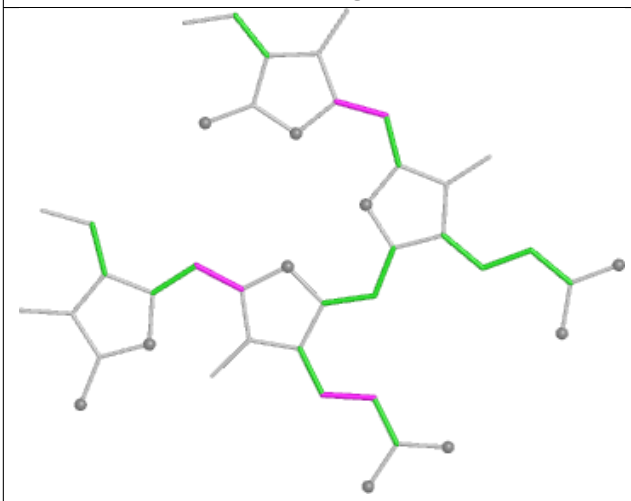
Ligand PEB qC 201



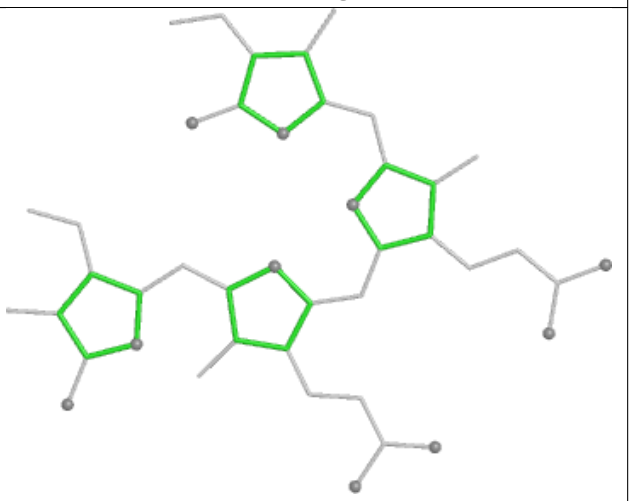
Bond lengths



Bond angles

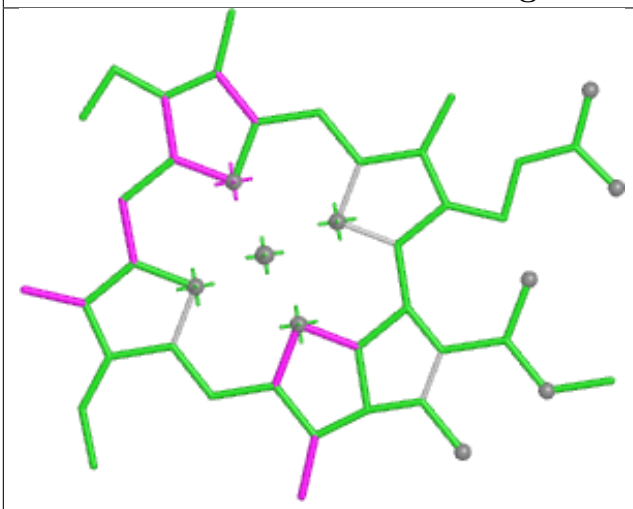


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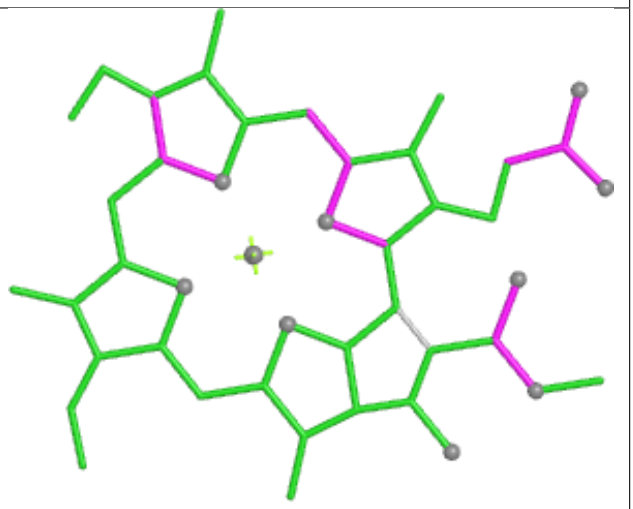


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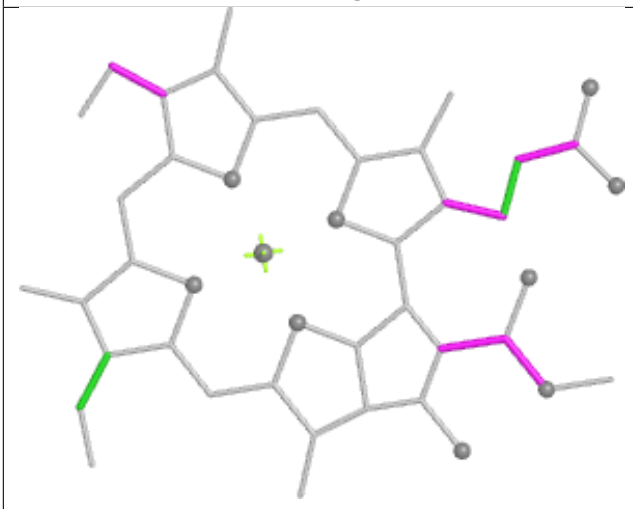
Ligand CLA 12 601



Bond lengths



Bond angles

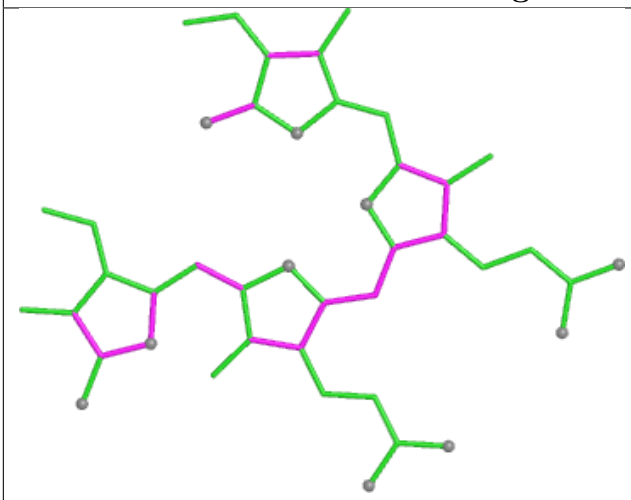


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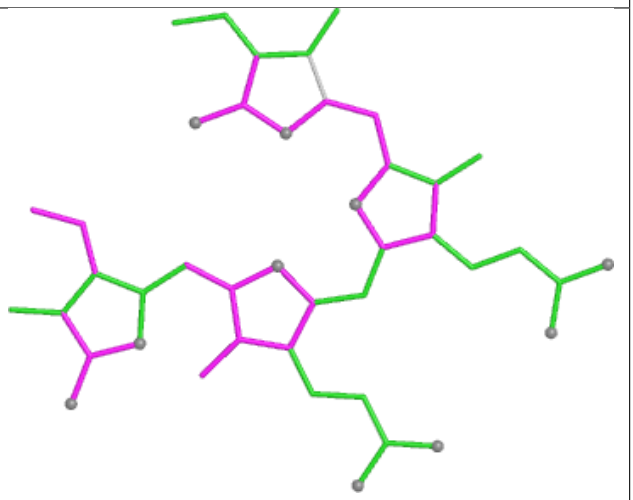


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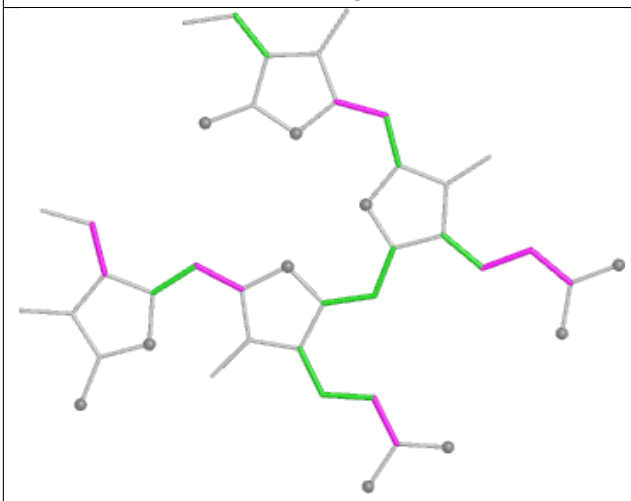
Ligand PEB aM 201



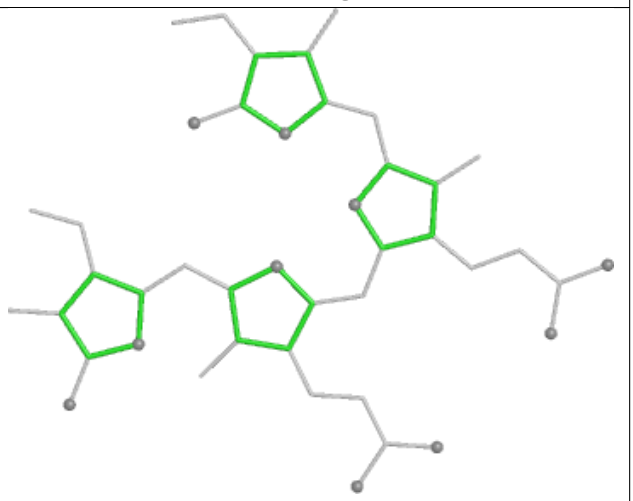
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Bond angles

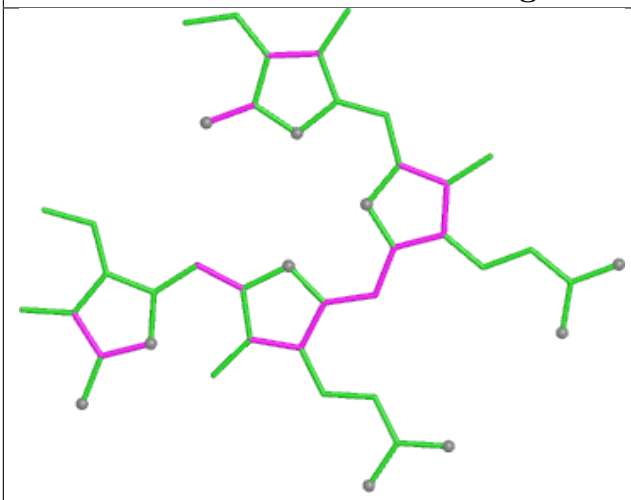


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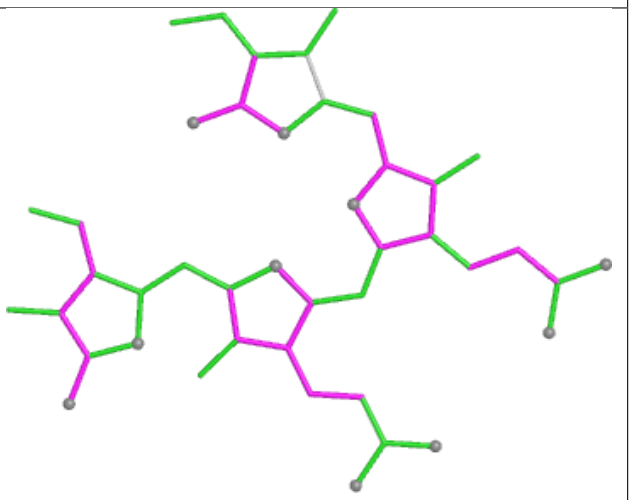


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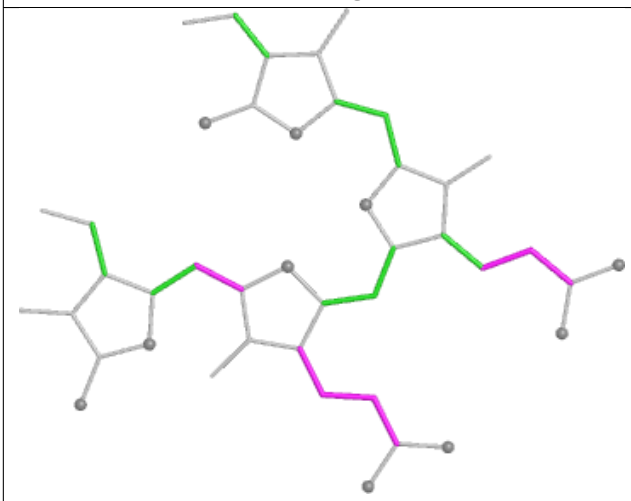
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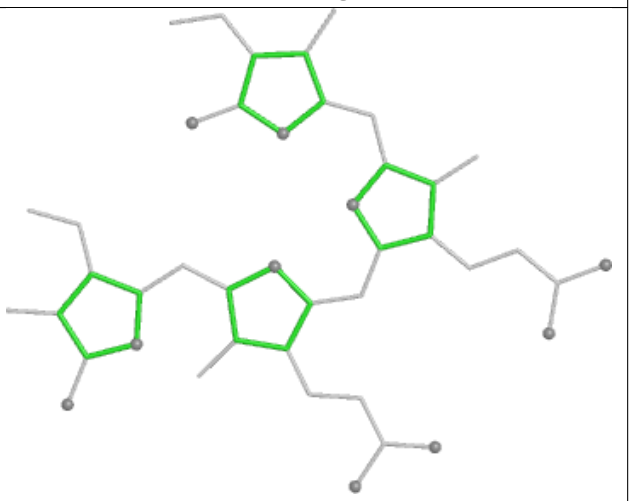
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Bond angles

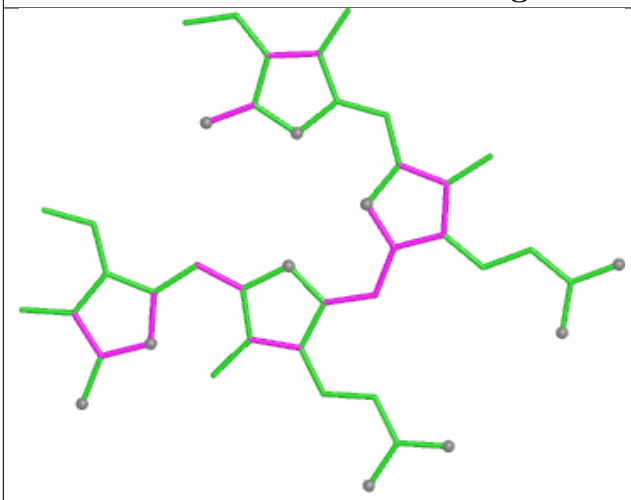


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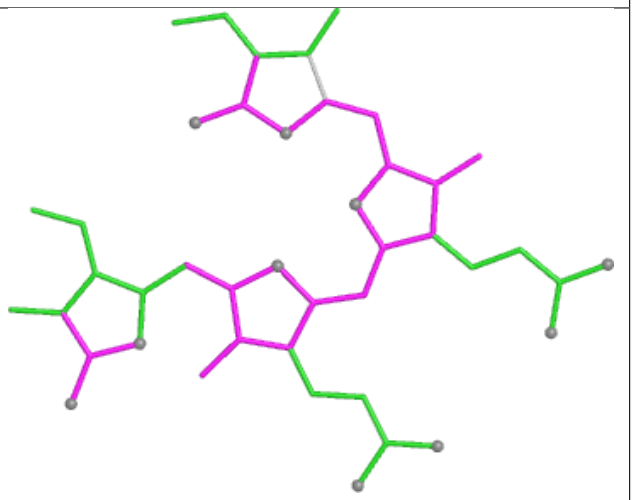


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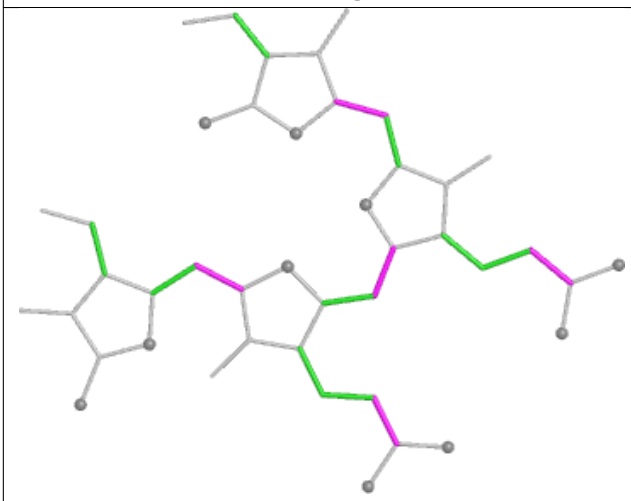
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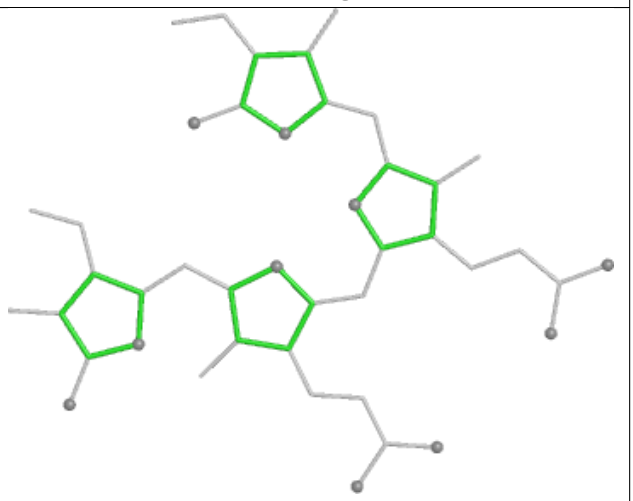
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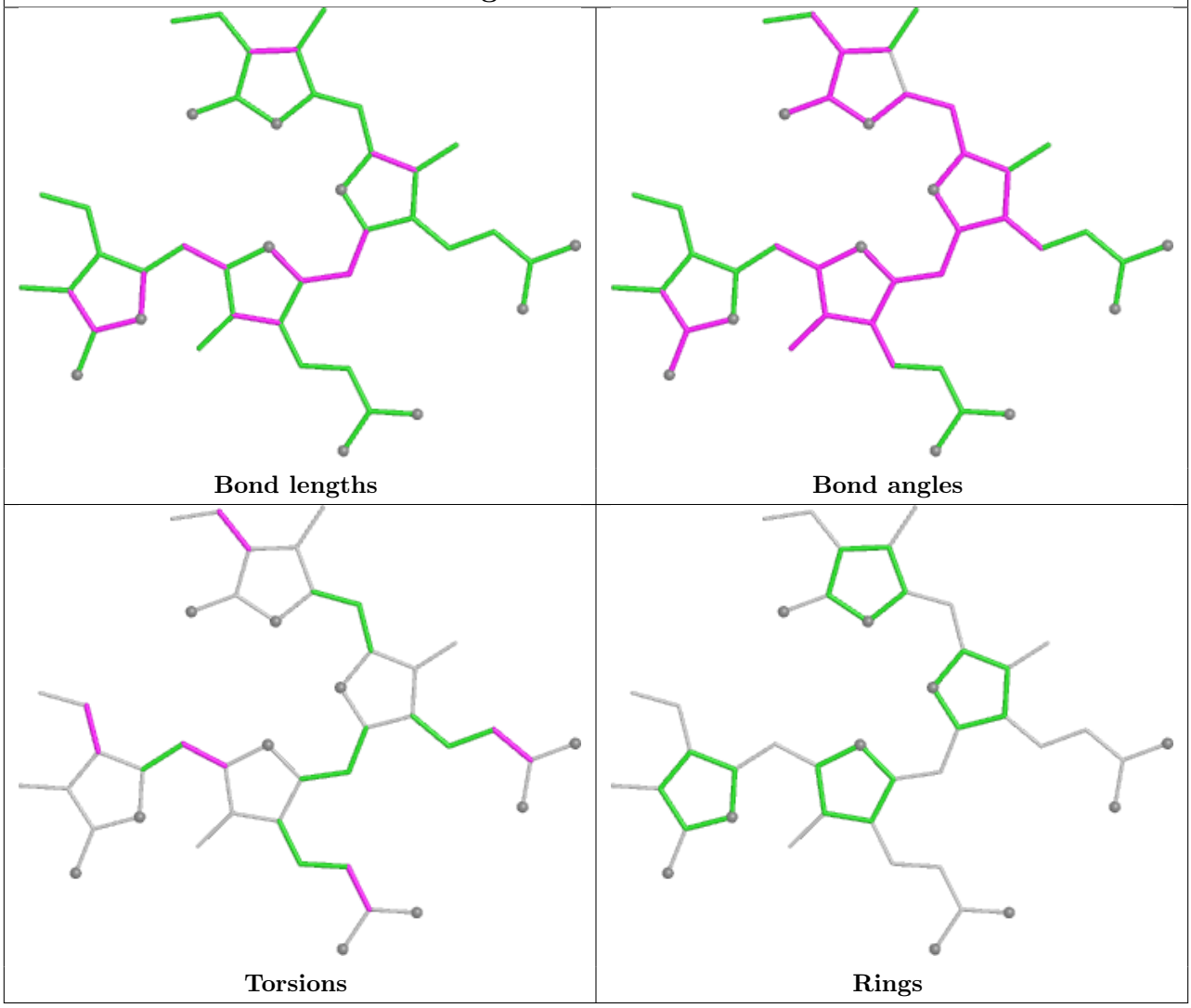


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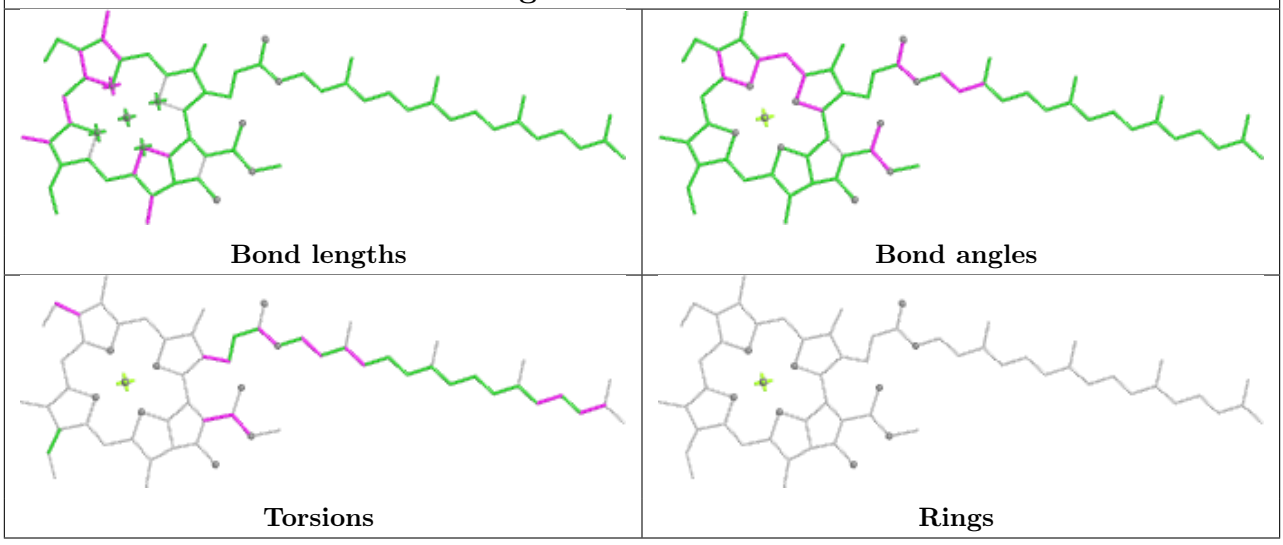


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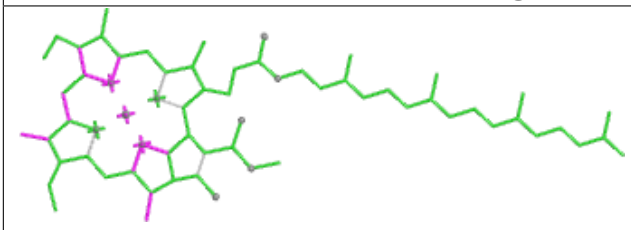
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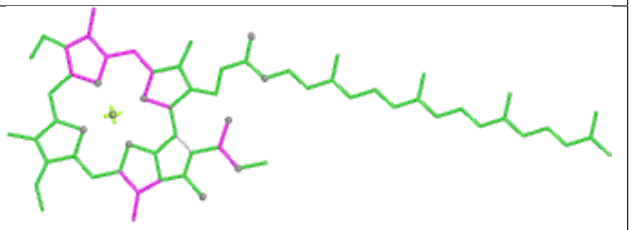
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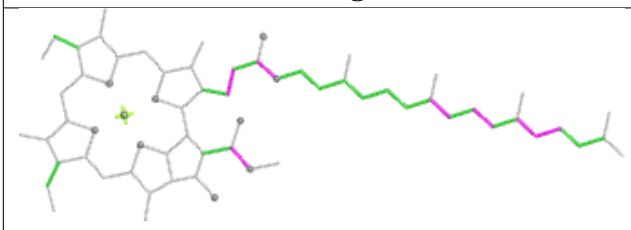
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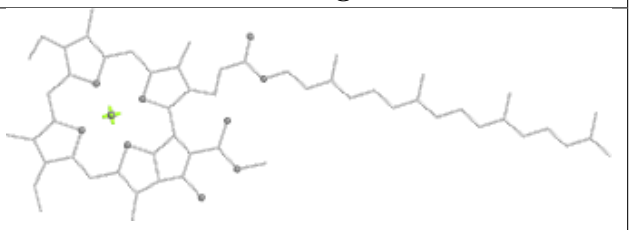
Bond lengths



Bond angles

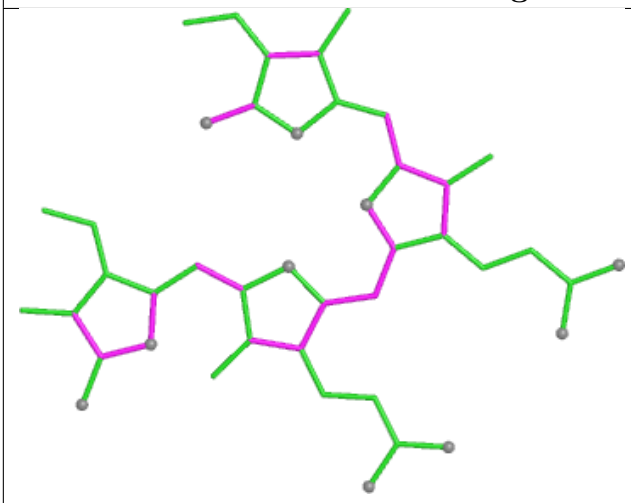


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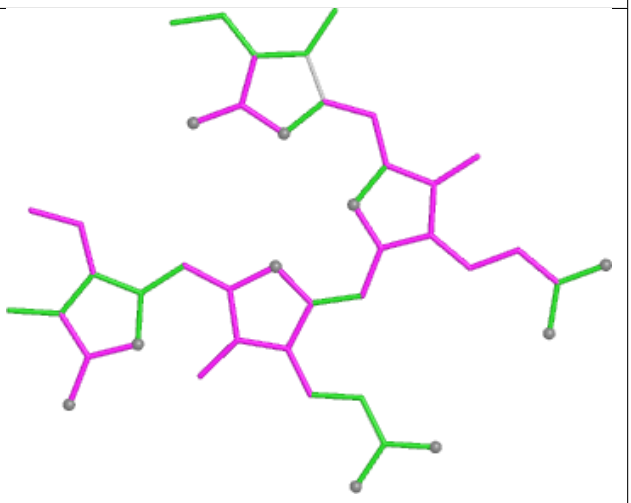


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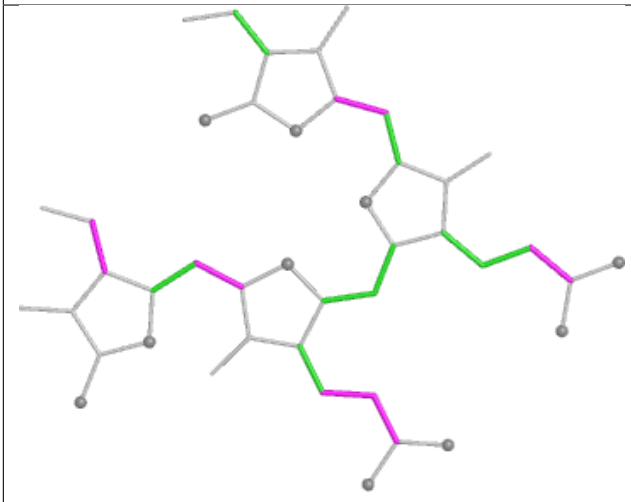
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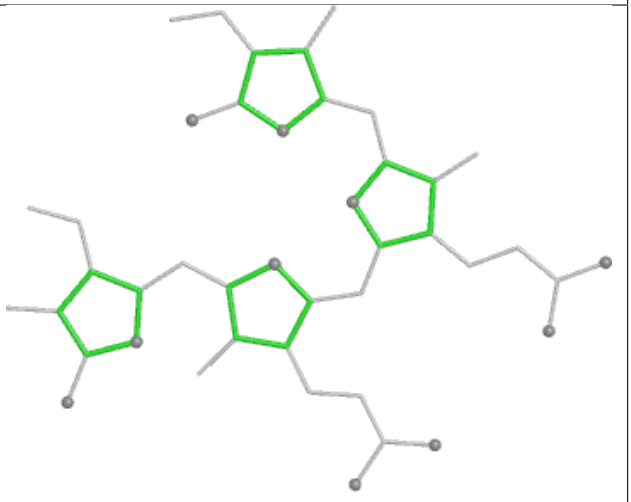
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Bond angles

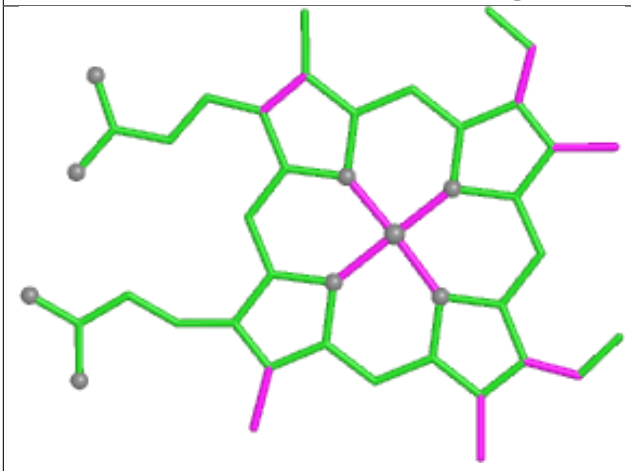


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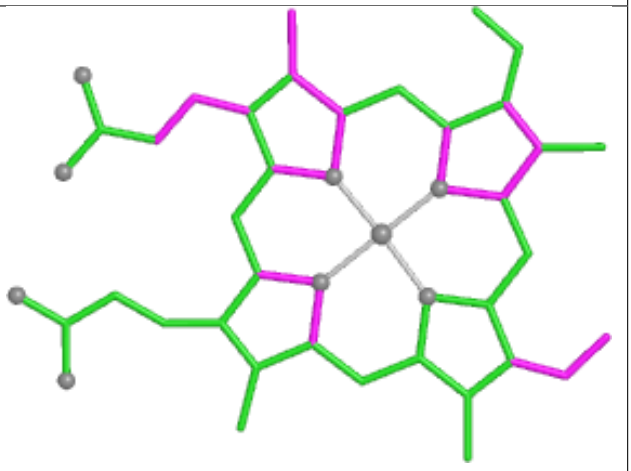


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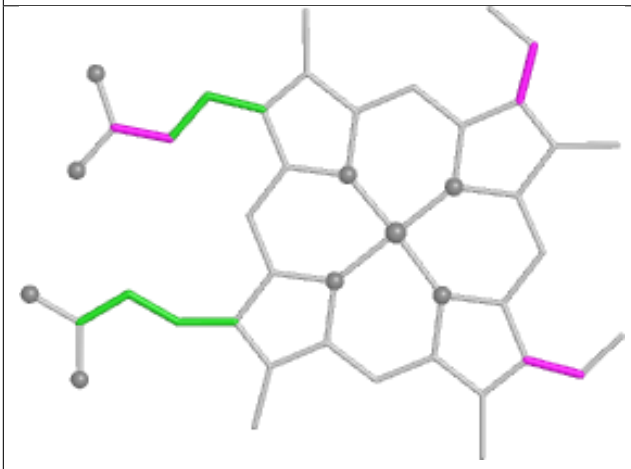
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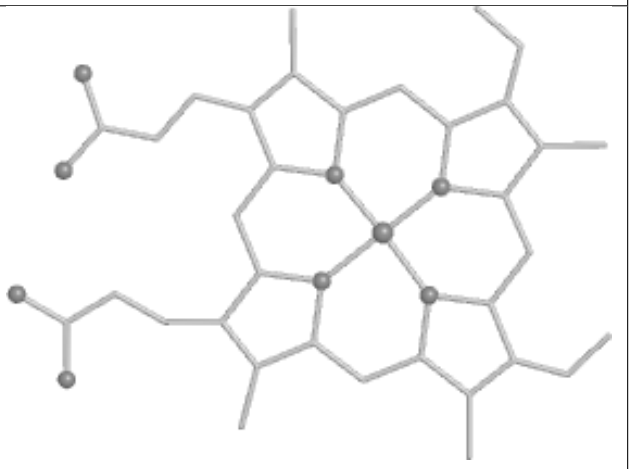
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Bond angles

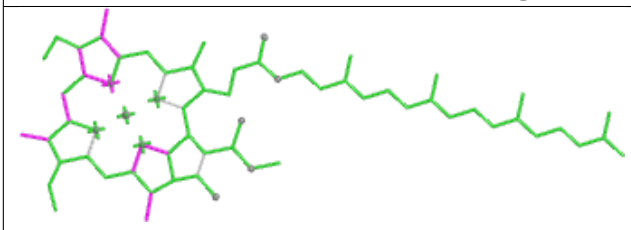


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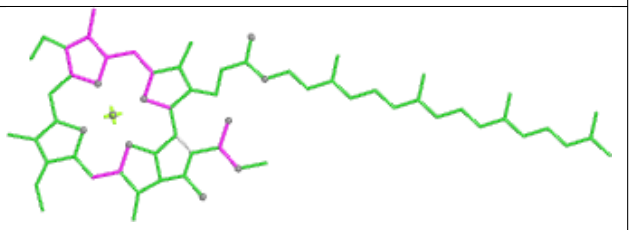


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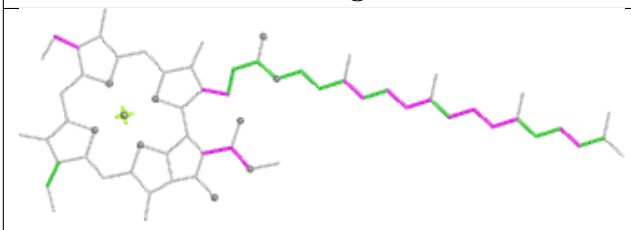
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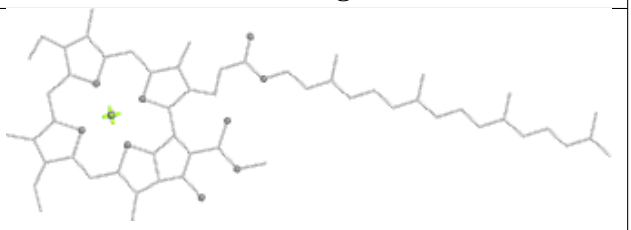
Bond lengths



Bond angles

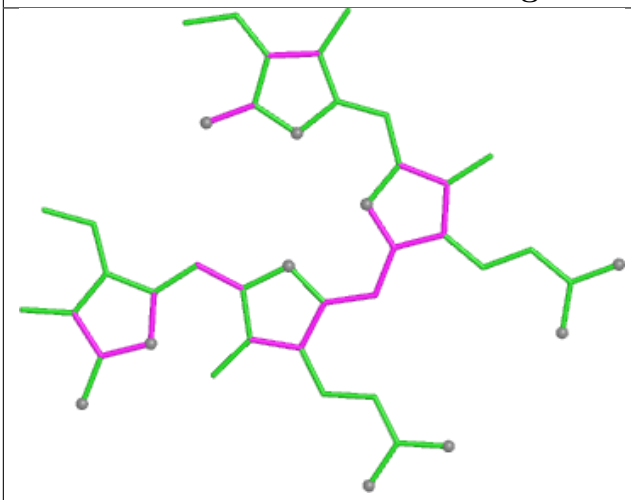


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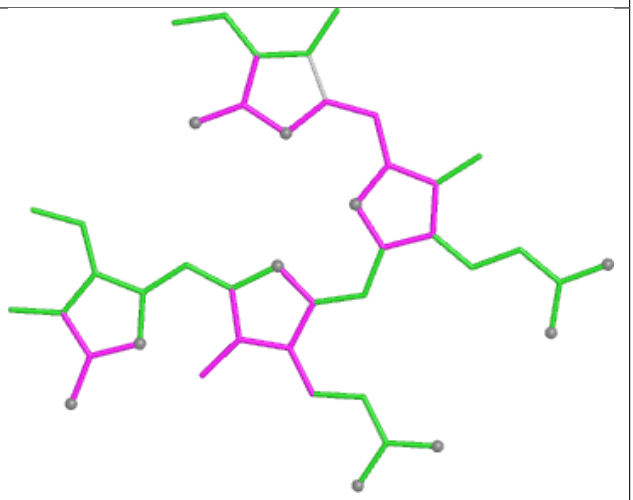


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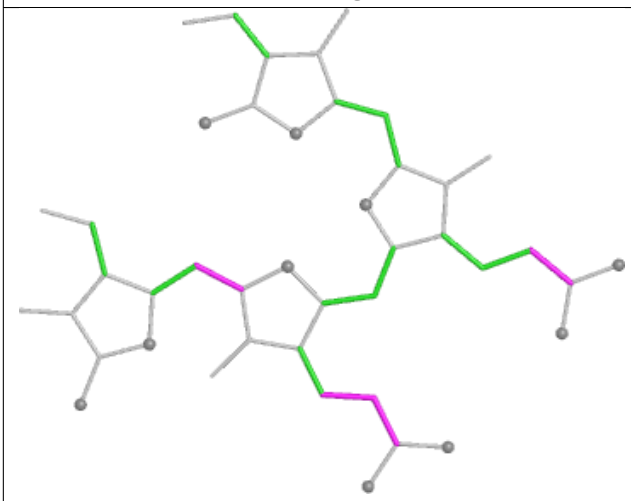
Ligand PEB lE 203



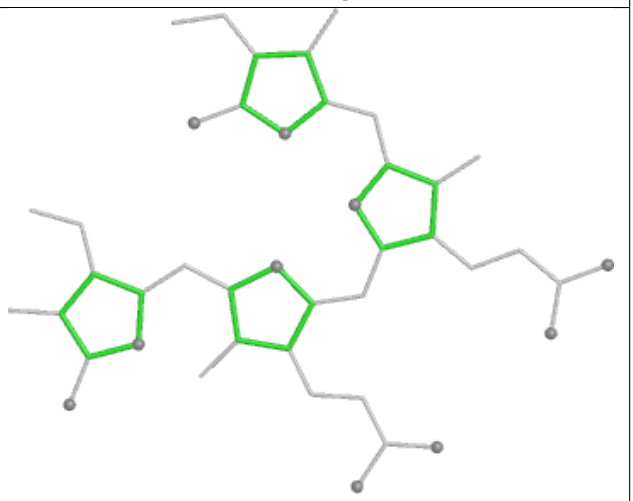
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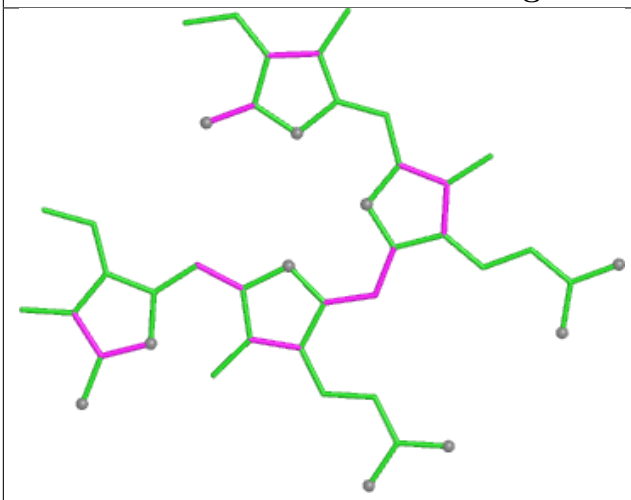


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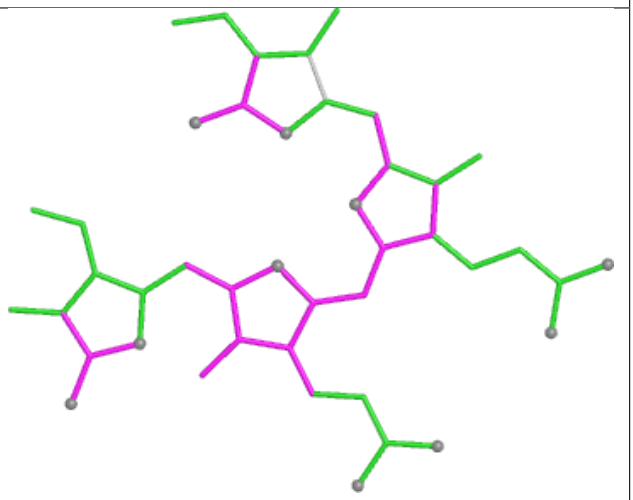


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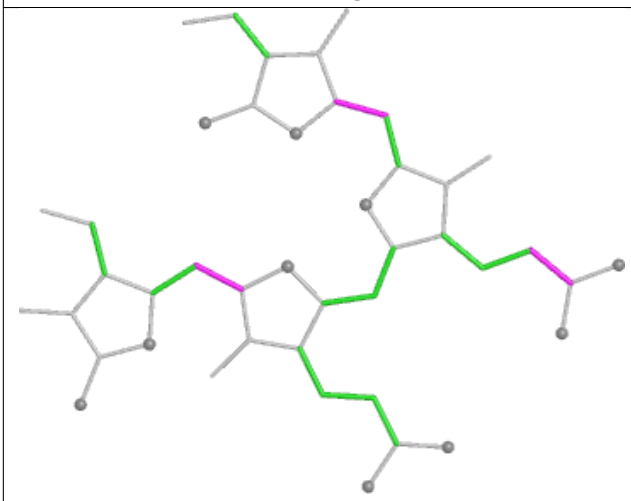
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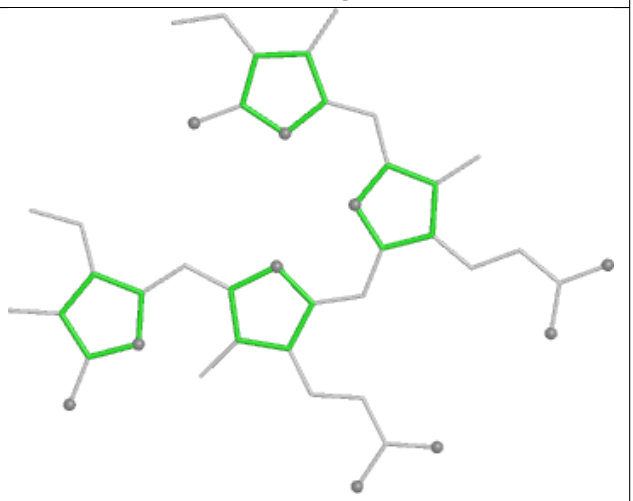
Bond lengths



Bond angles

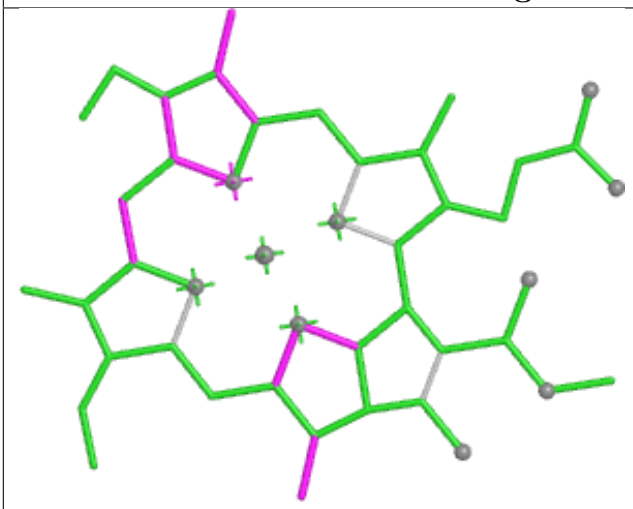


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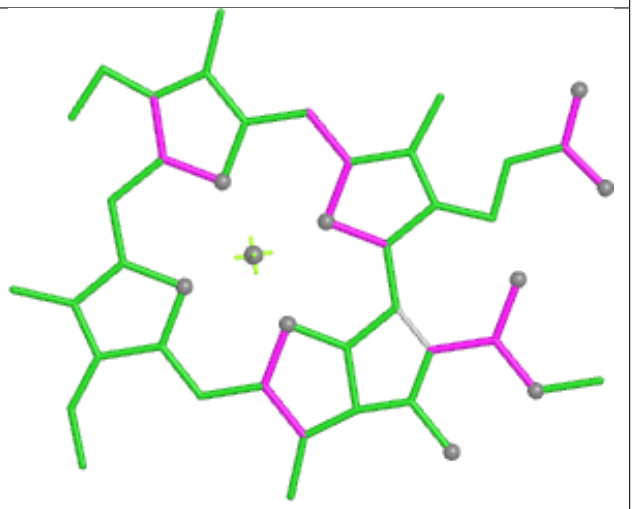


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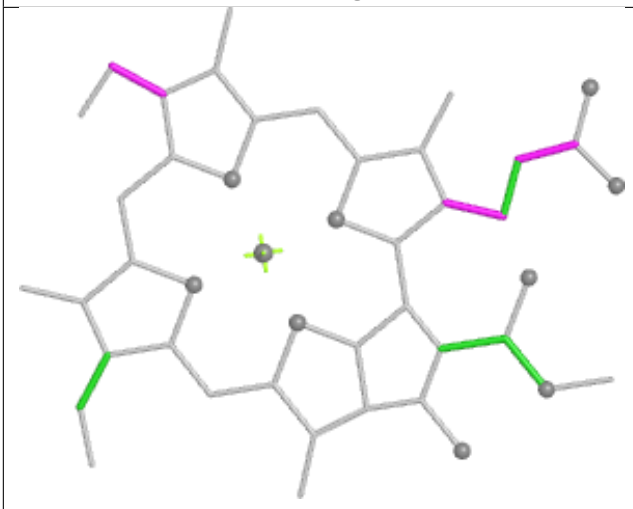
Ligand CLA 6N 607



Bond lengths



Bond angles

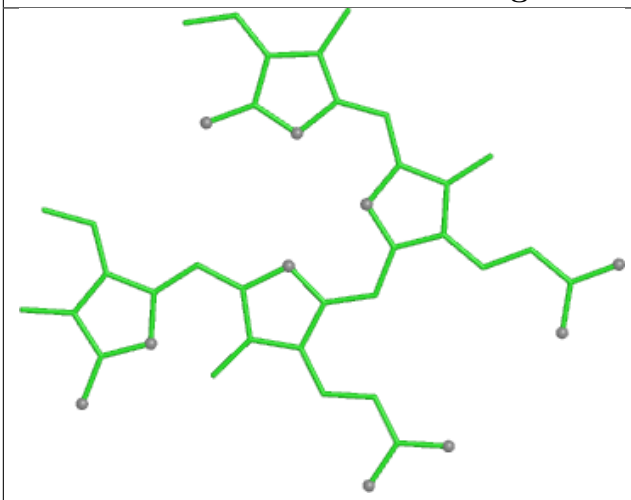


Torsions

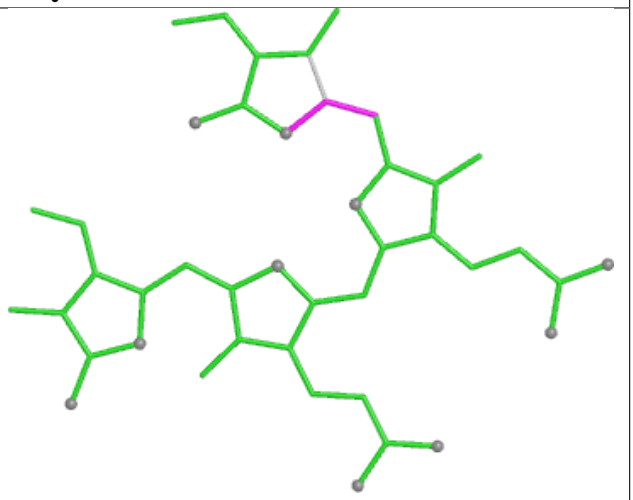


Rings

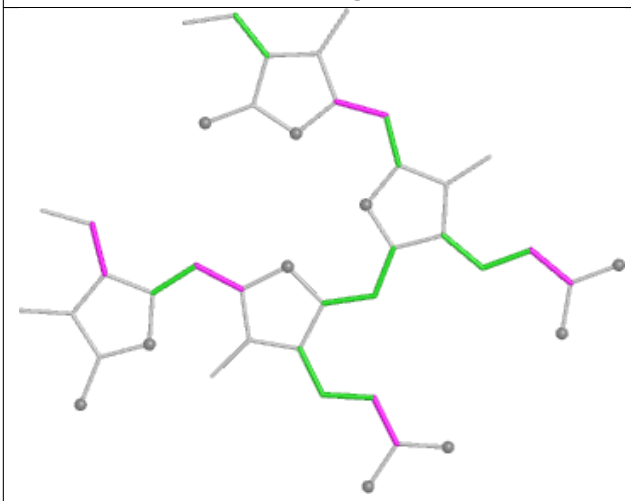
Ligand PEB QO 202



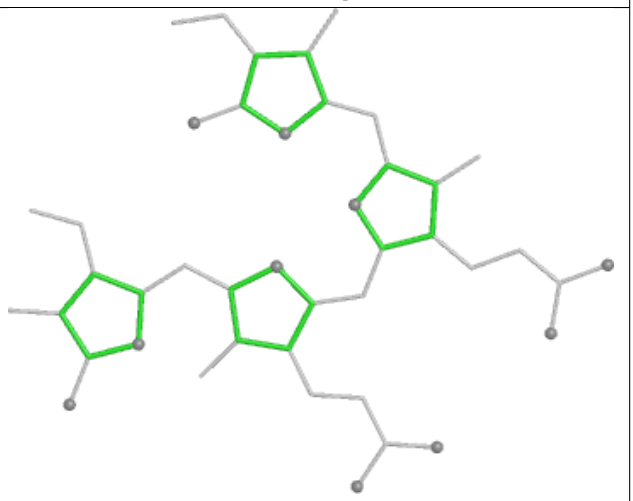
Bond lengths



Bond angles

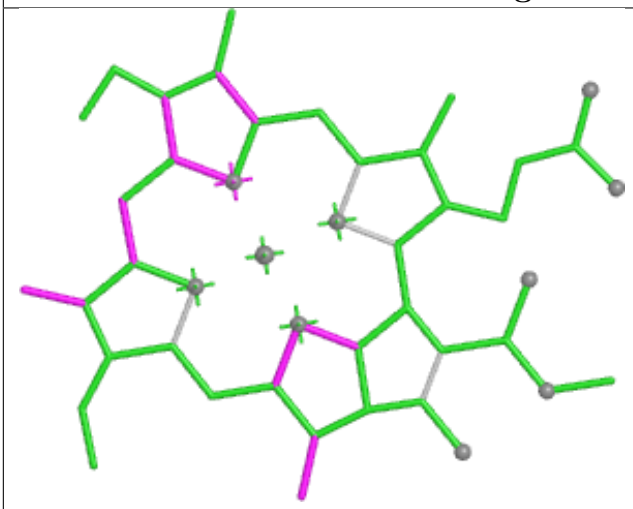


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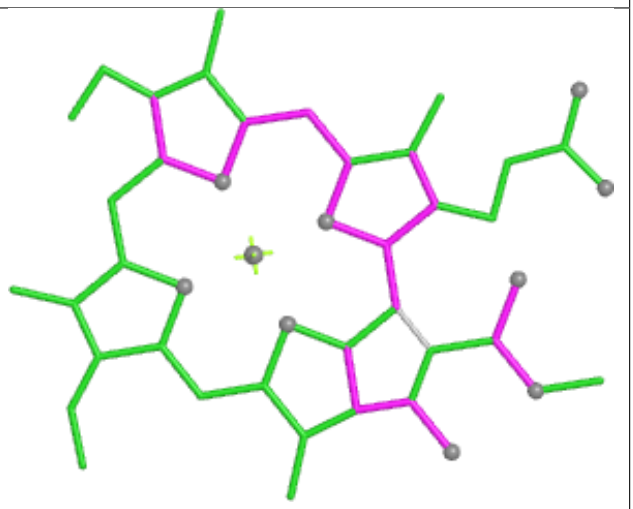


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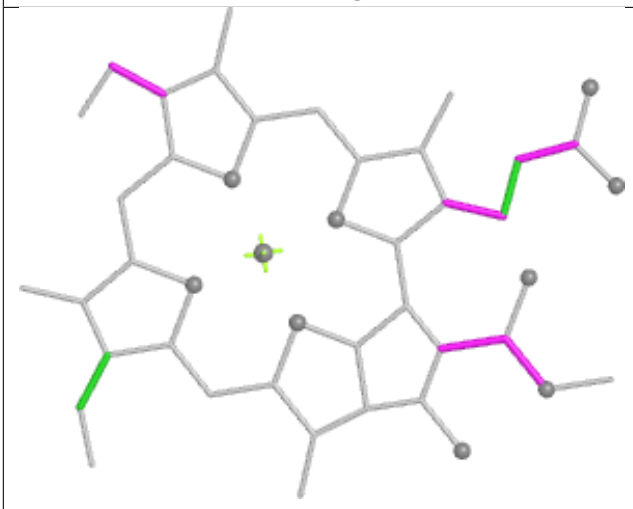
Ligand CLA 4N 607



Bond lengths



Bond angles

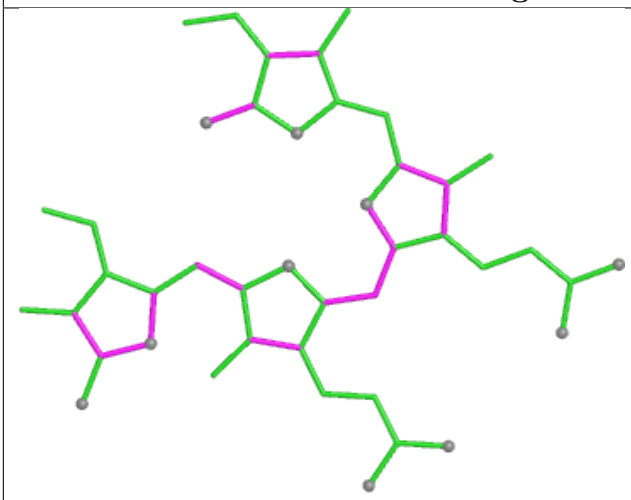


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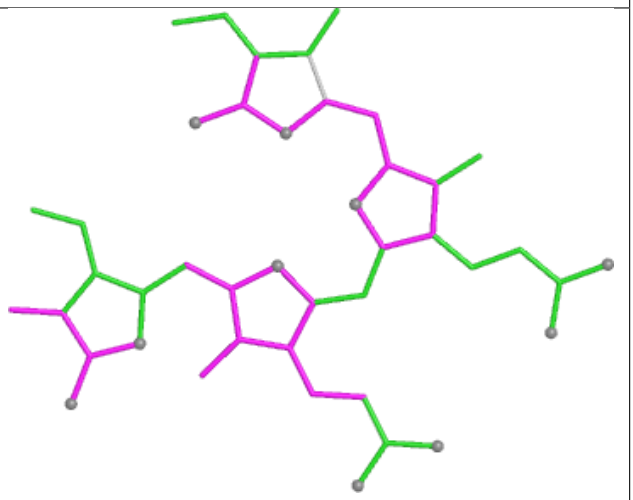


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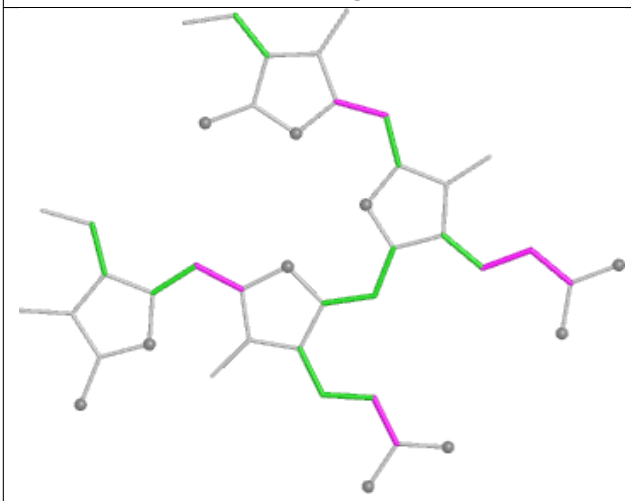
Ligand PEB DB 201



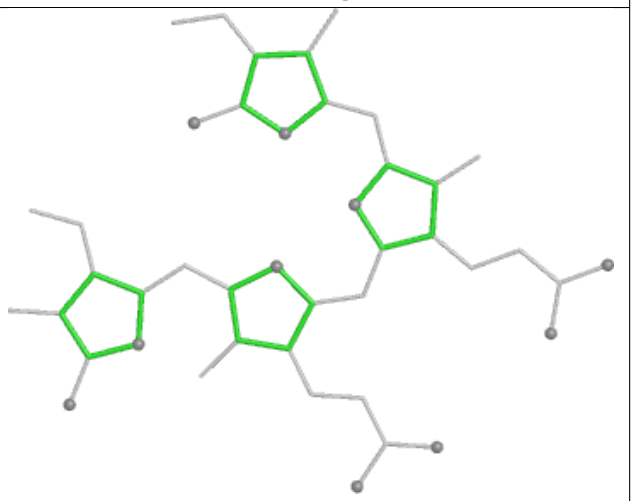
Bond lengths



Bond angles

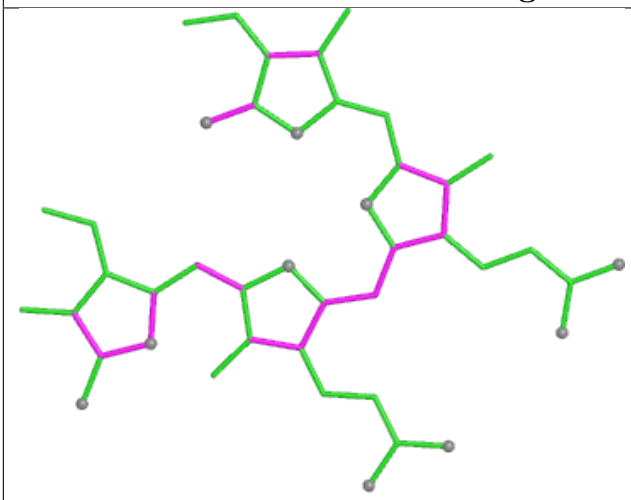


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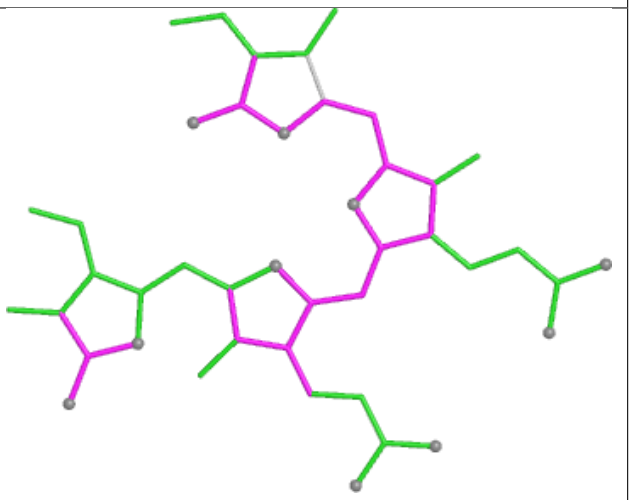


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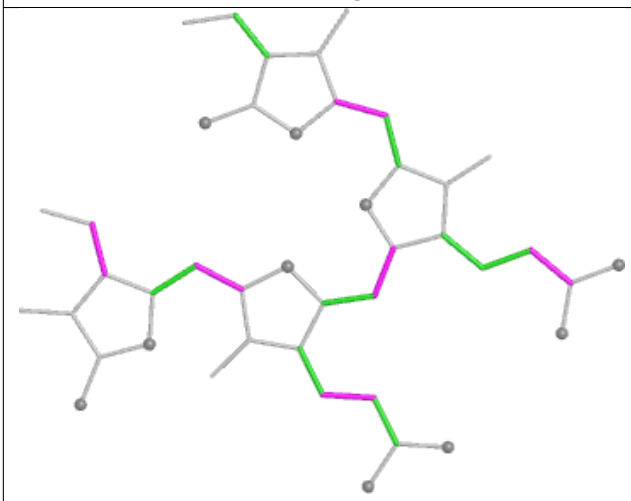
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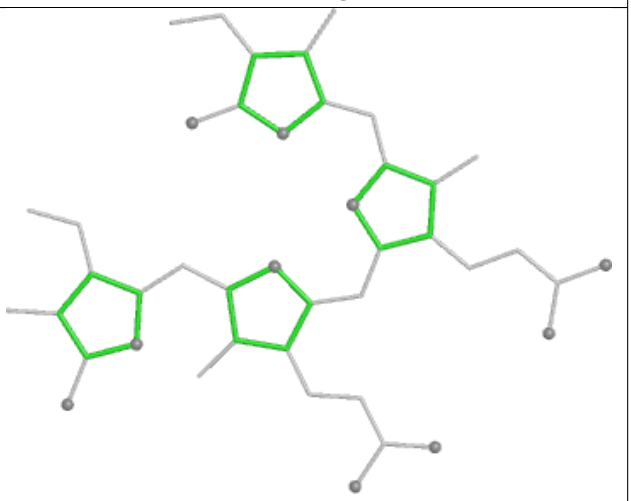
Bond lengths



Bond angles

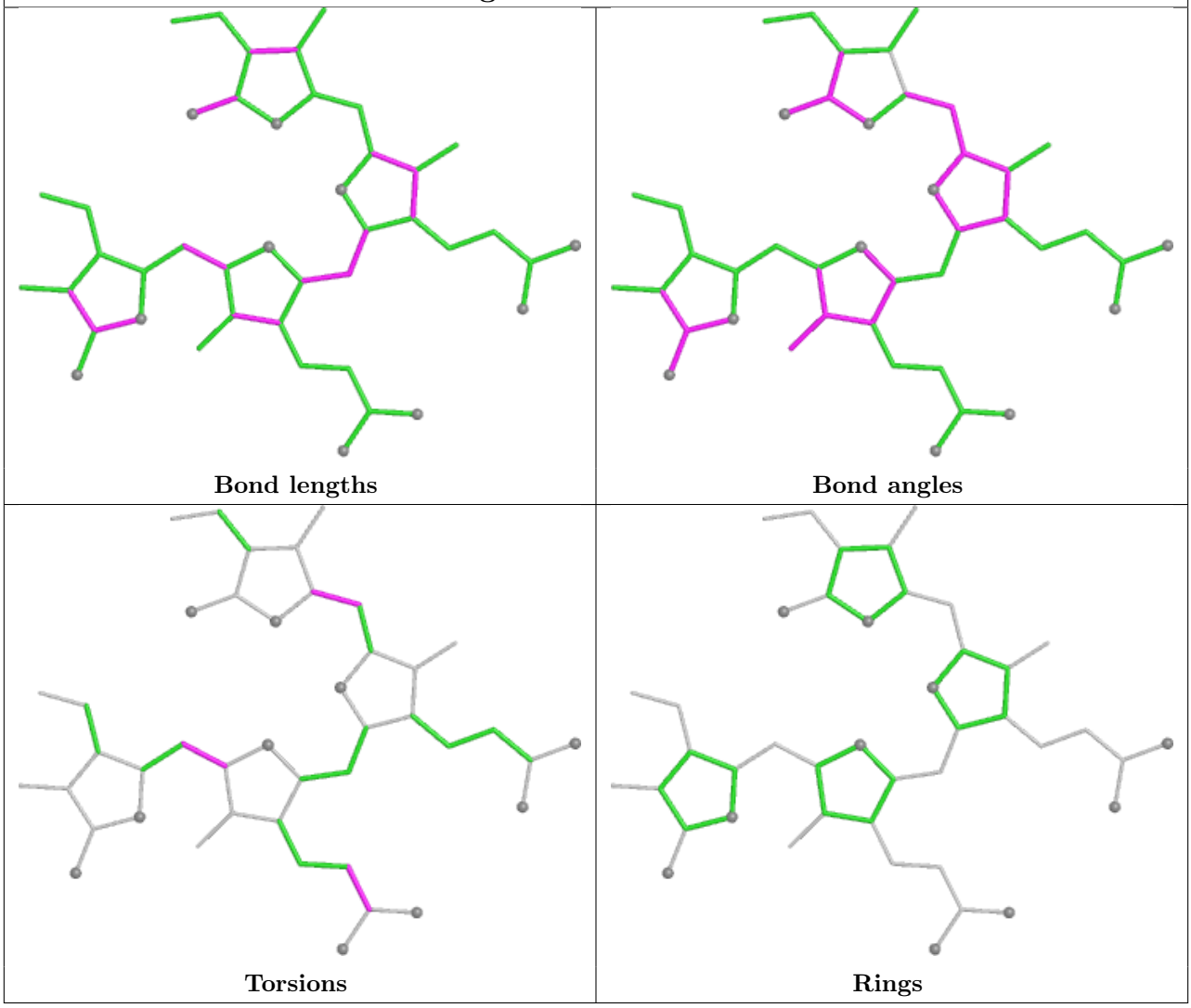


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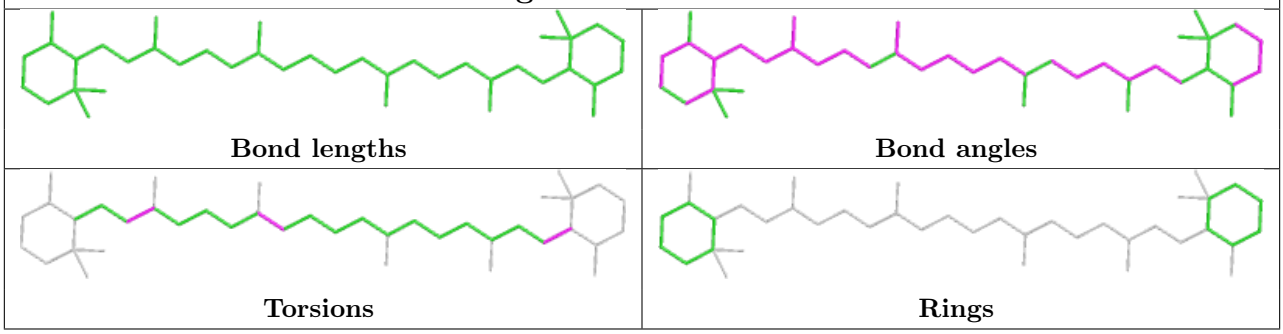


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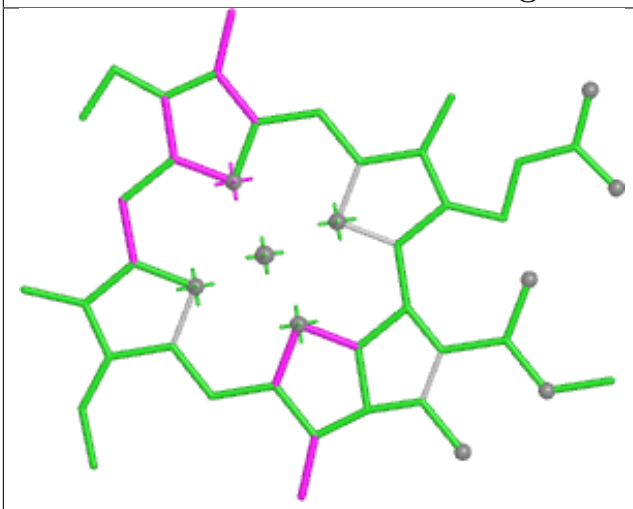
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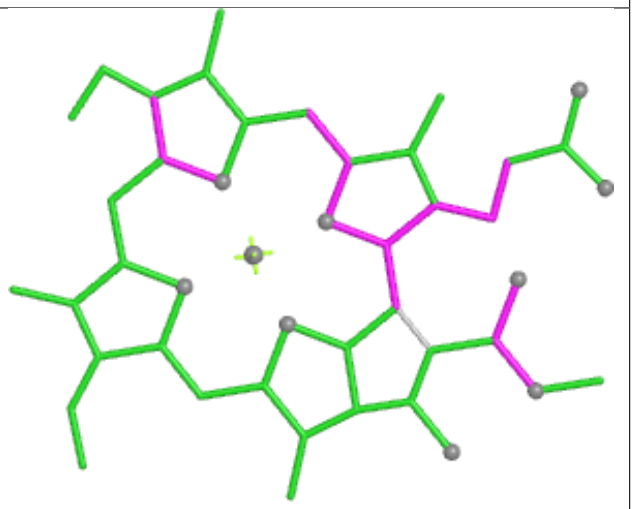
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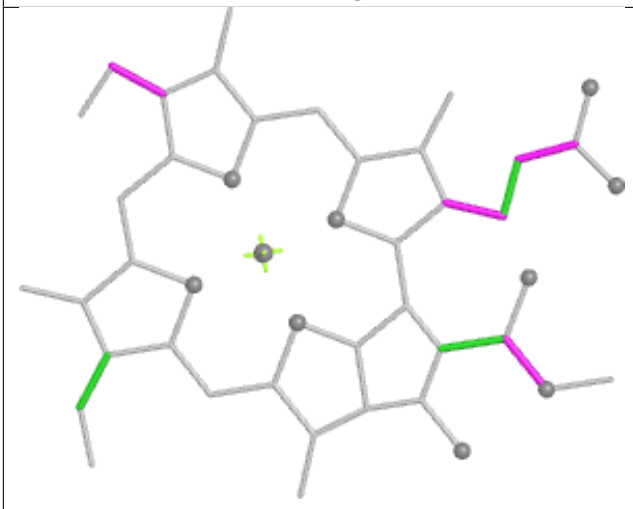
Ligand CLA 72 605



Bond lengths



Bond angles

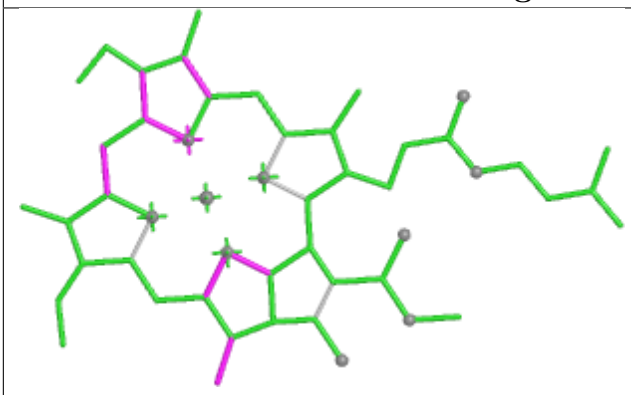


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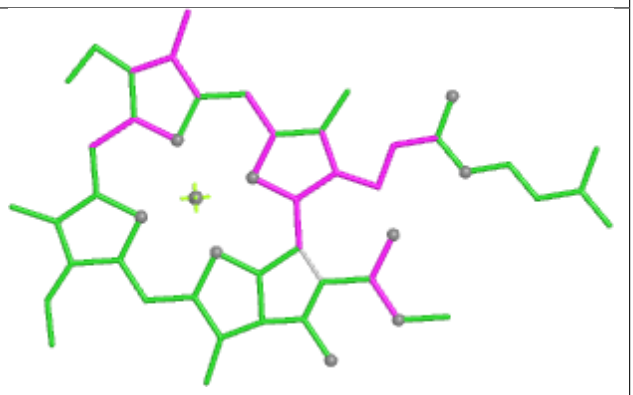


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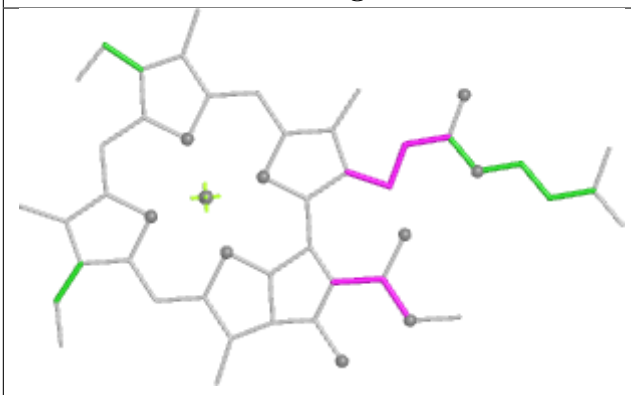
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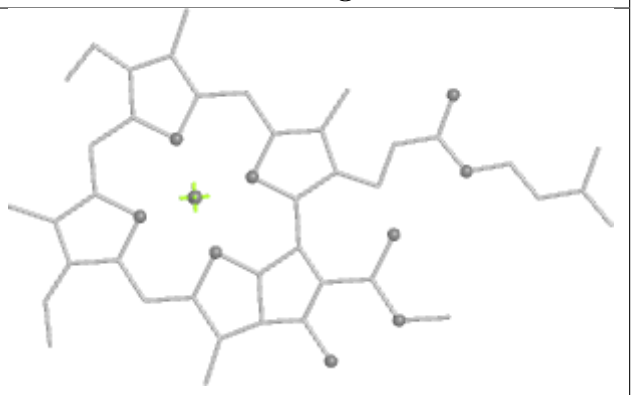
Bond lengths



Bond angles

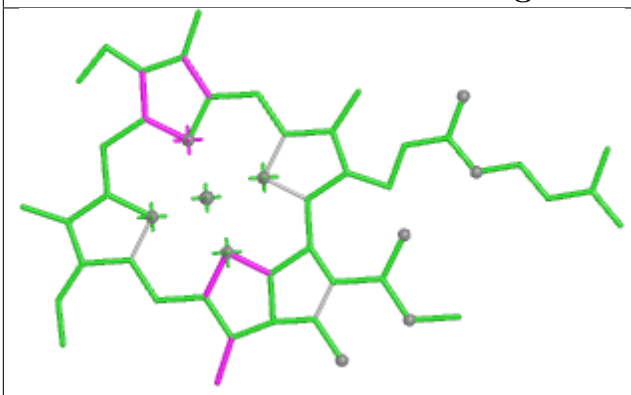


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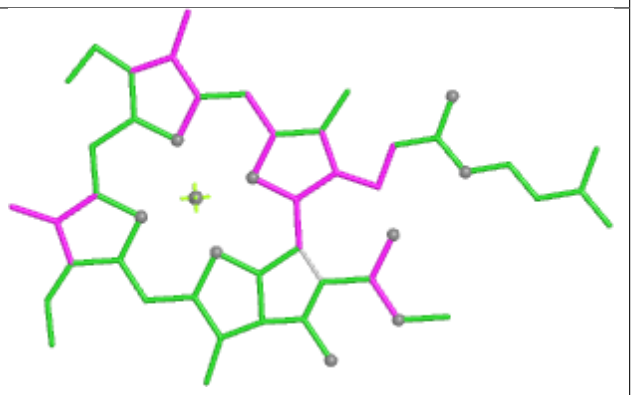


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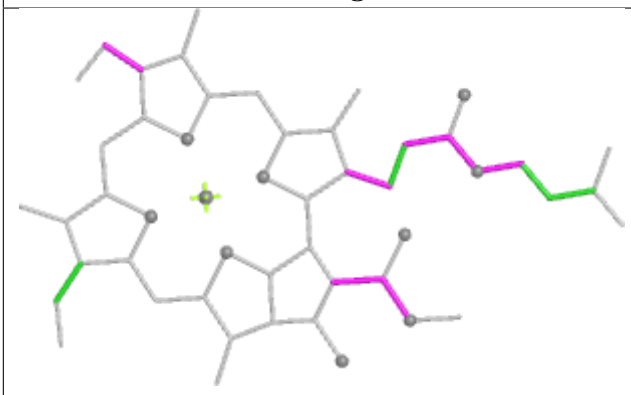
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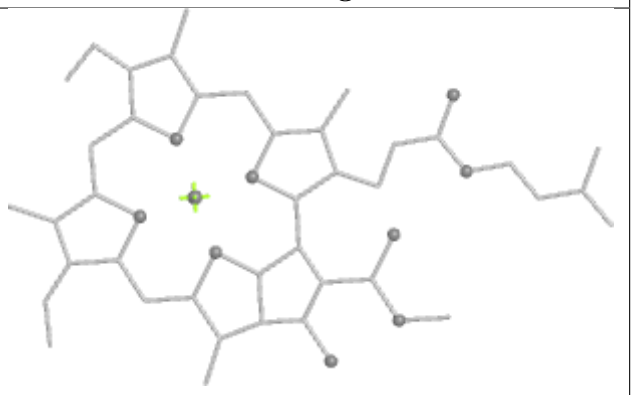
Bond lengths



Bond angles

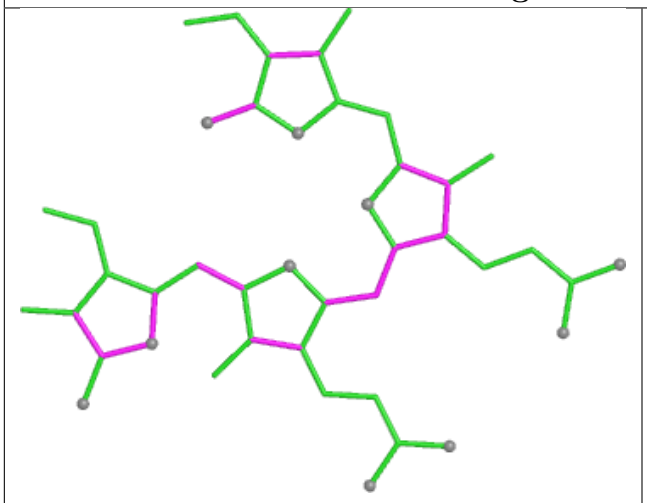


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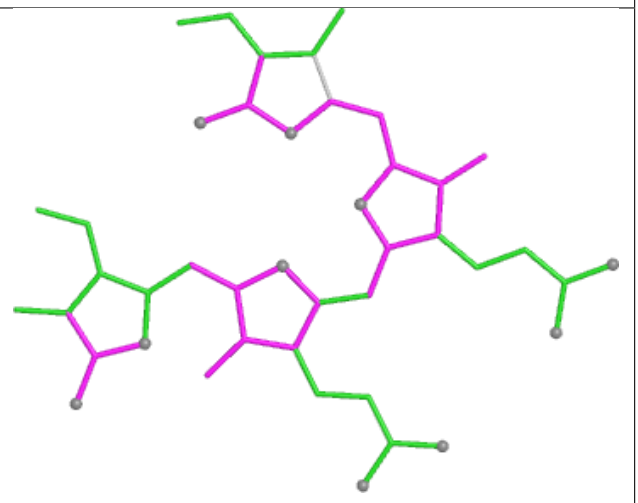


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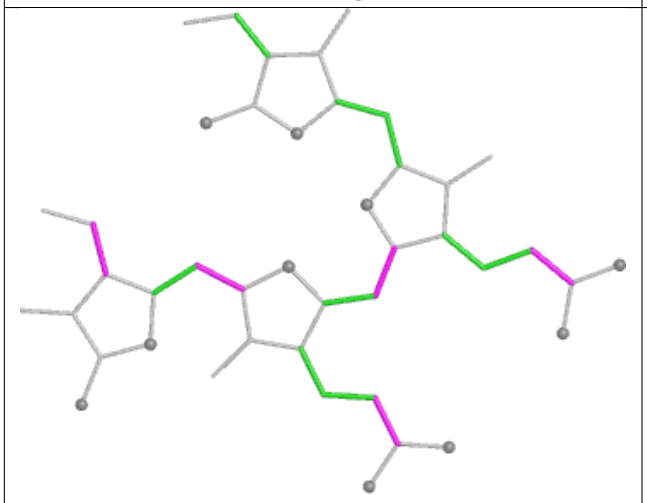
Ligand PEB RD 202



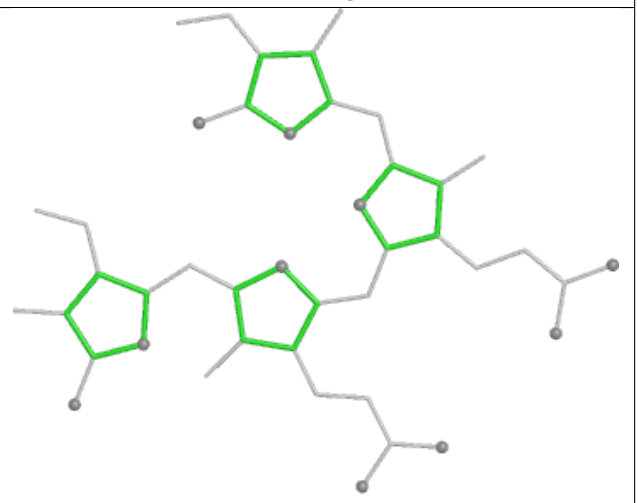
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Bond angles

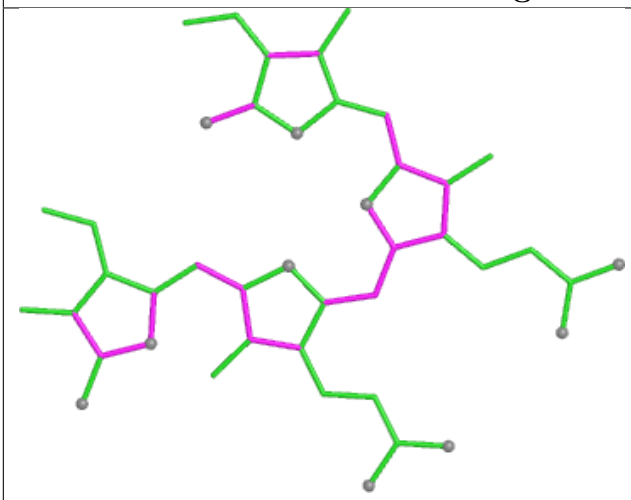


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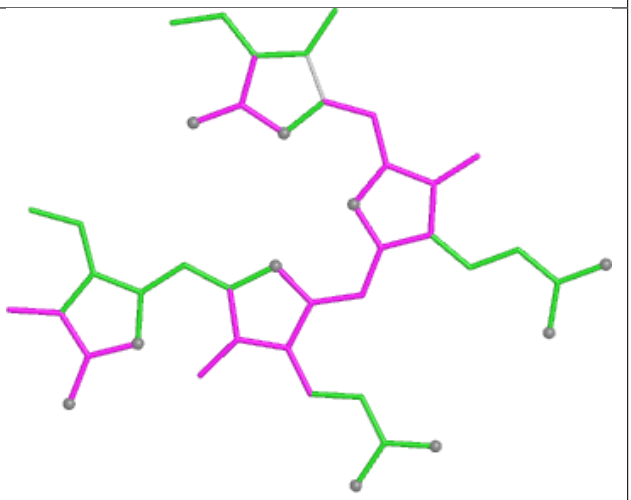


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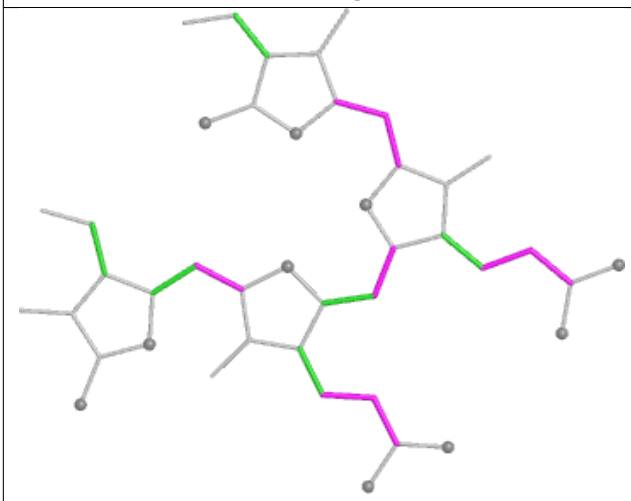
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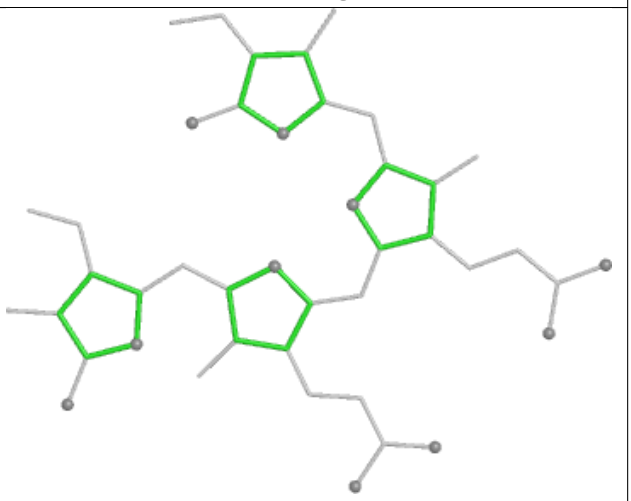
Bond lengths



Bond angles

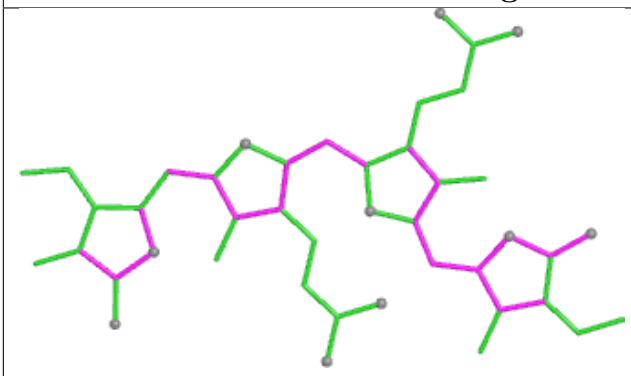


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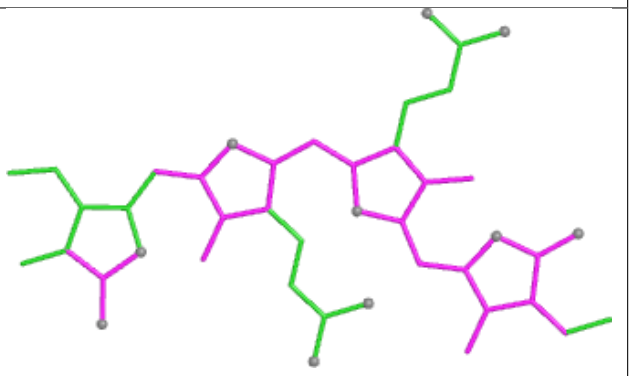


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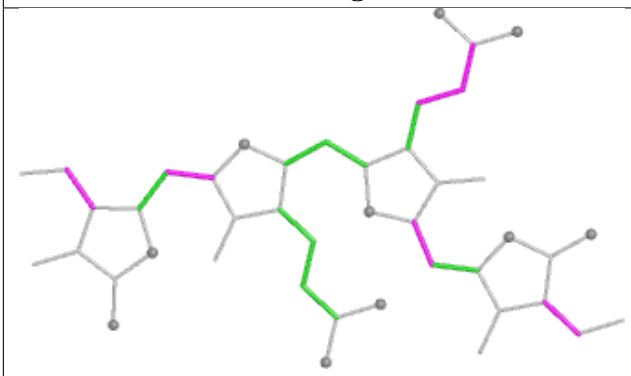
Ligand CYC EO 1001



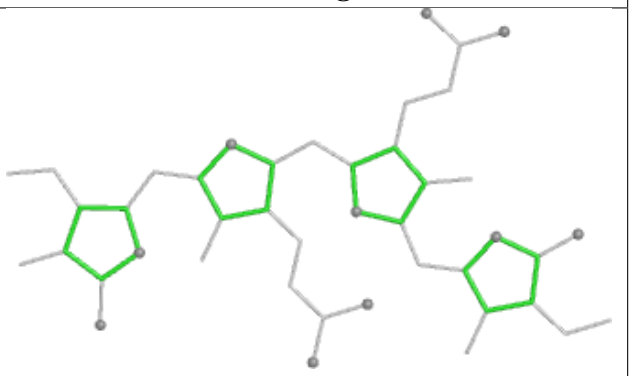
Bond lengths



Bond angles

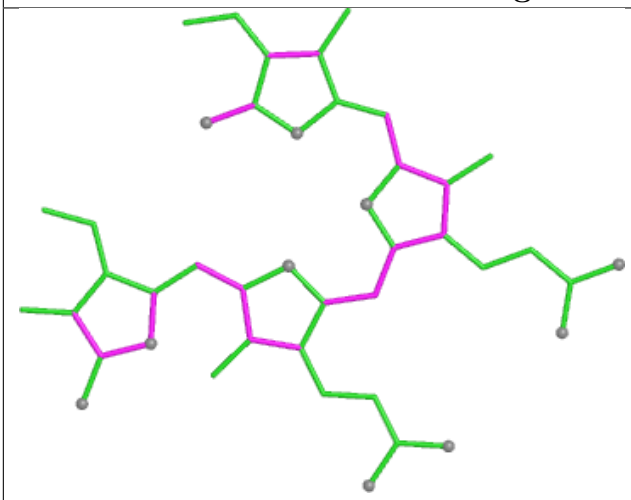


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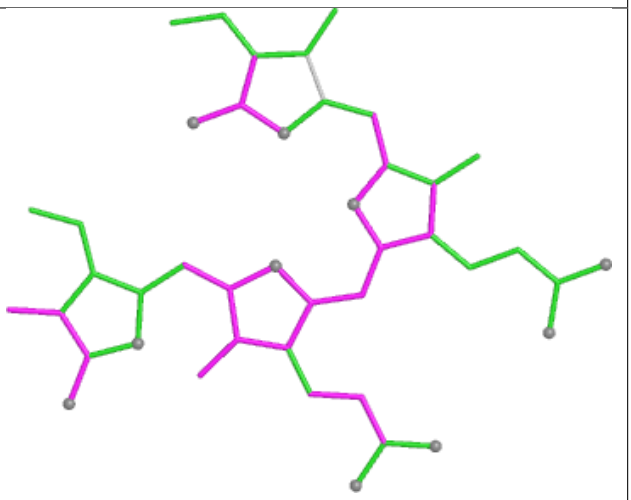


Rings

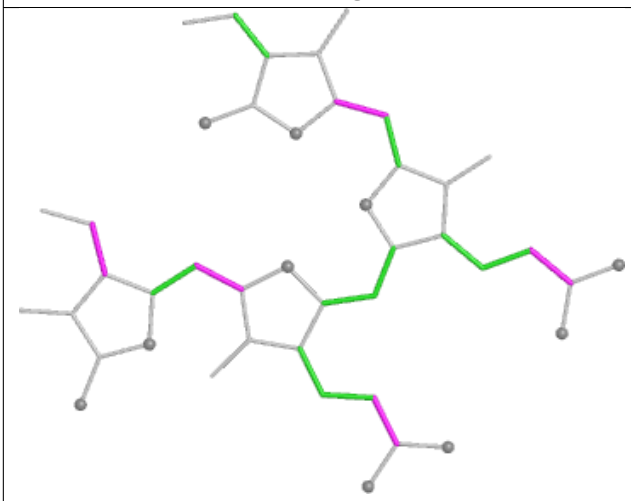
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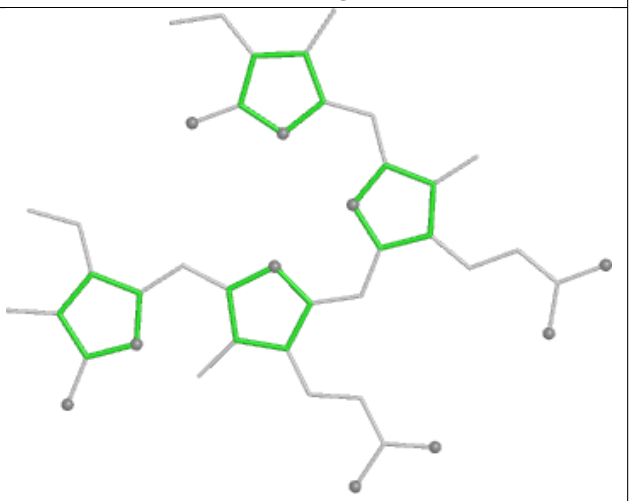
Bond lengths



Bond angles

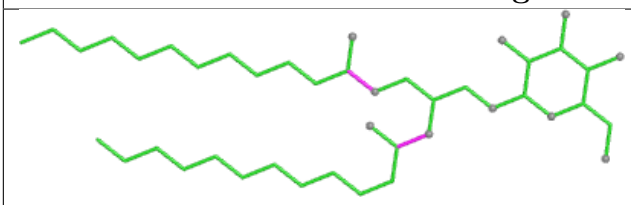


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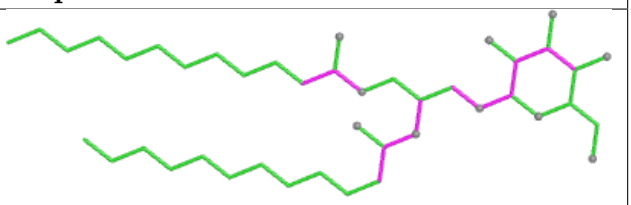


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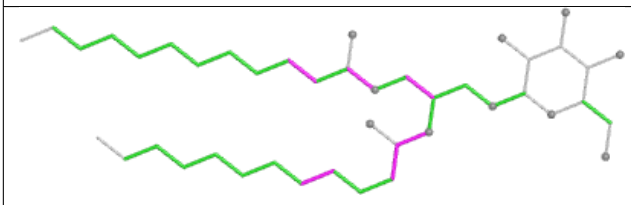
Ligand LMG qL 301



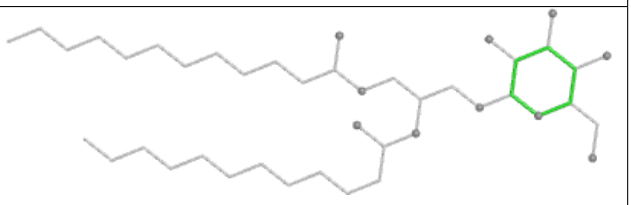
Bond lengths



Bond angles

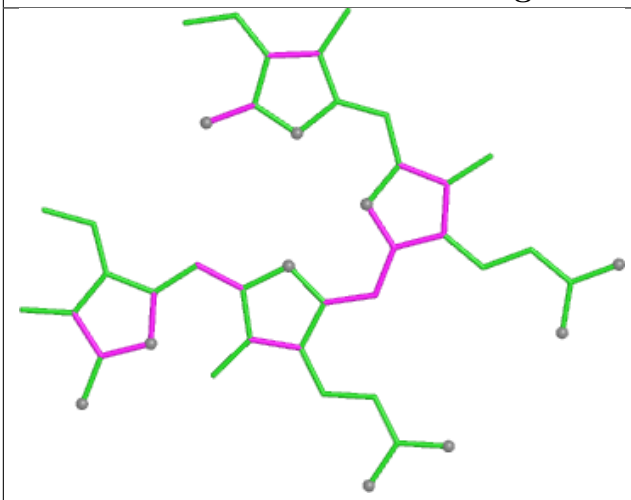


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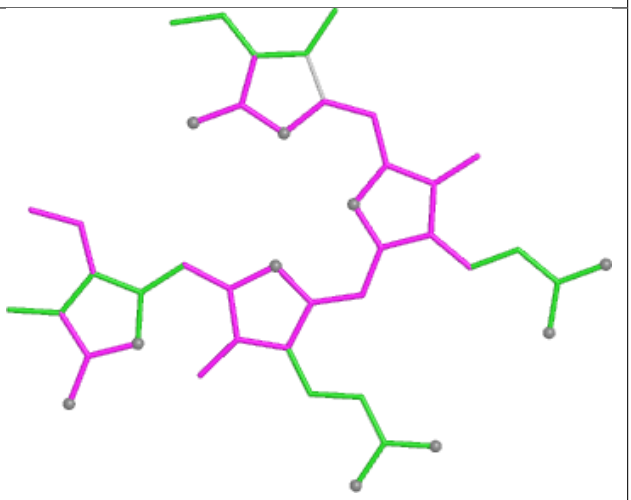


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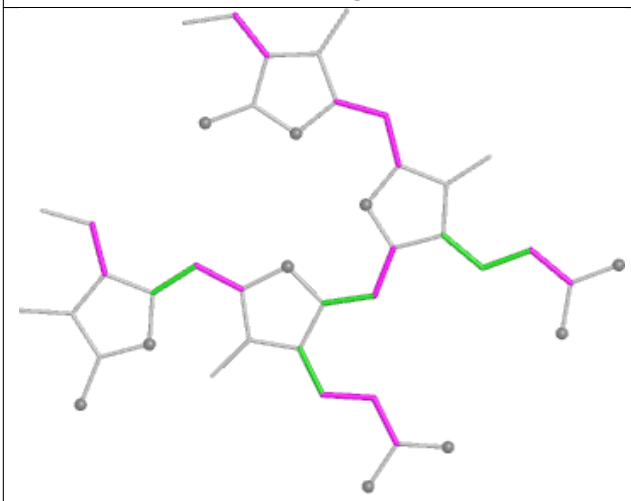
Ligand PEB KJ 202



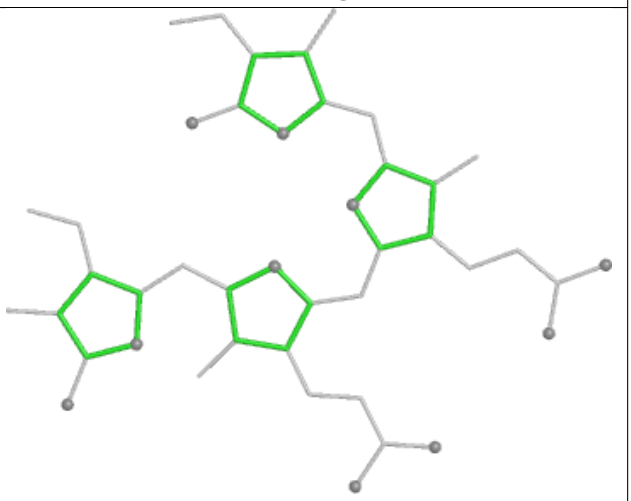
Bond lengths



Bond angles

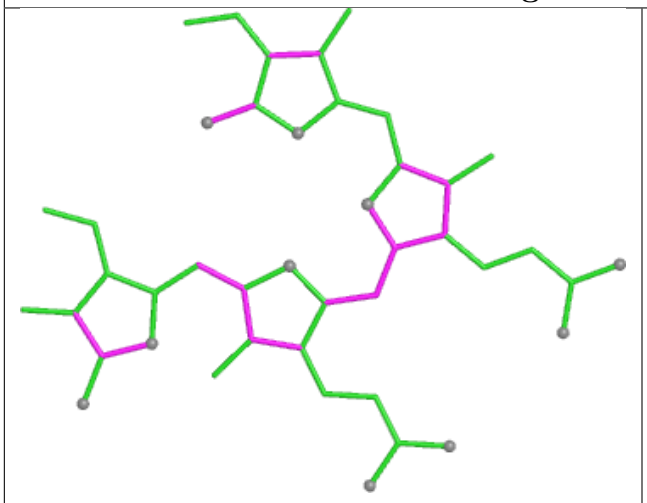


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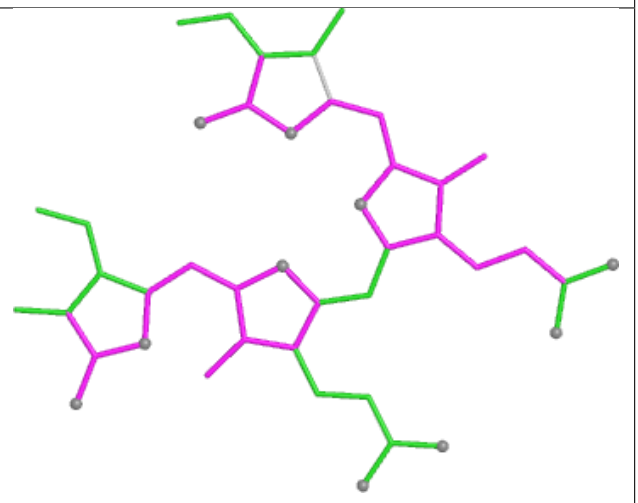


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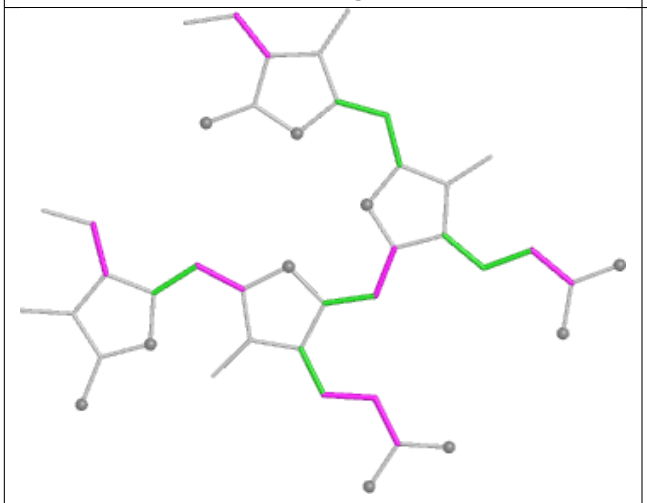
Ligand PEB c1 202



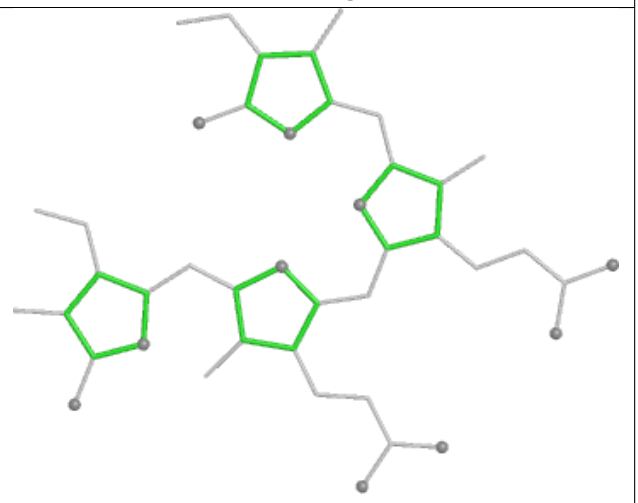
Bond lengths



Bond angles

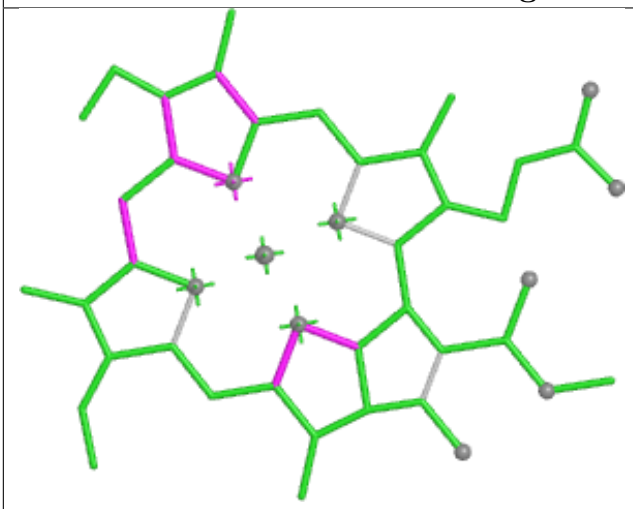


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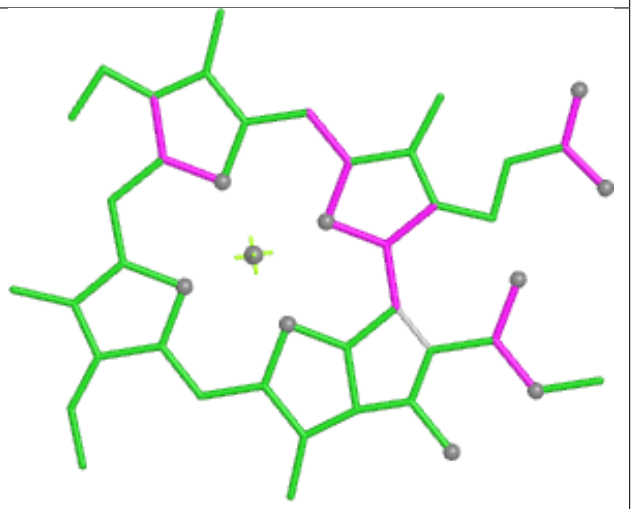


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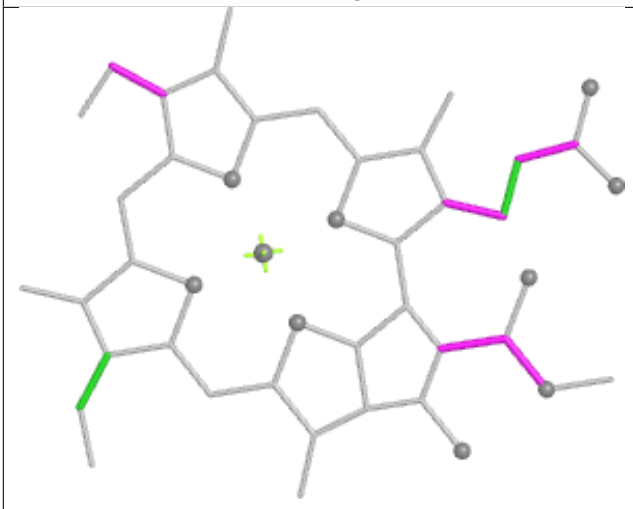
Ligand CLA 72 601



Bond lengths



Bond angles

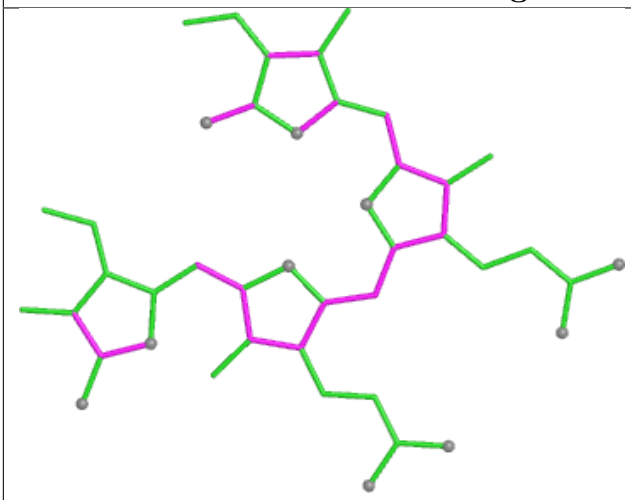


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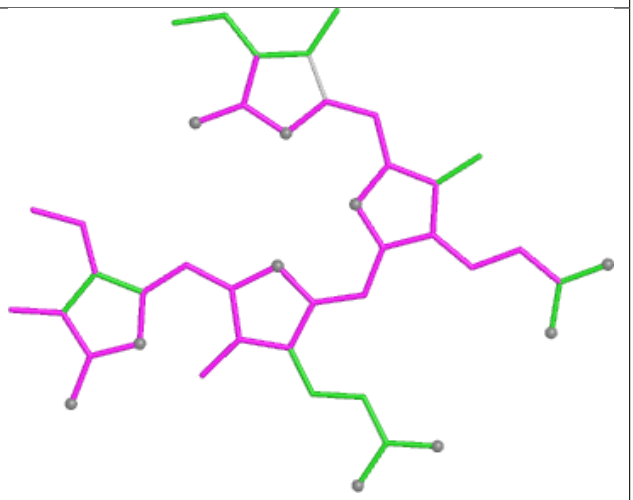


Rings

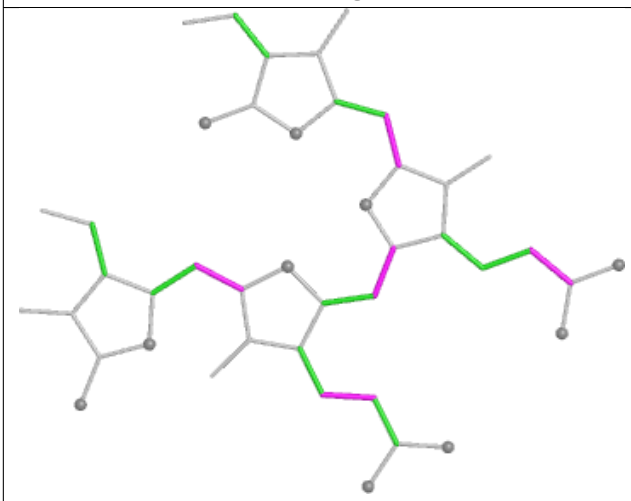
Ligand PEB YK 203



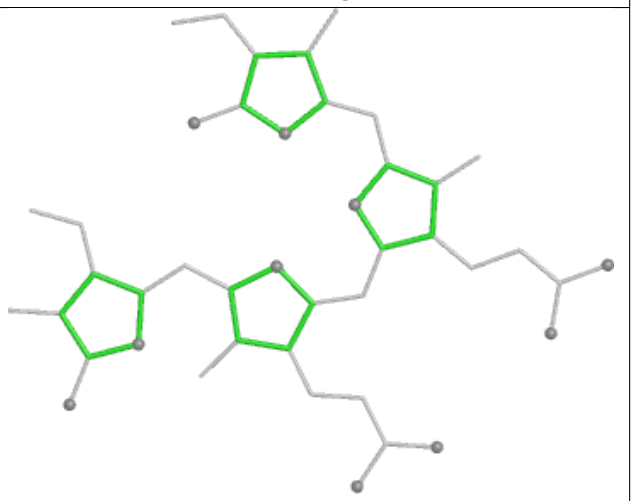
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Bond angles

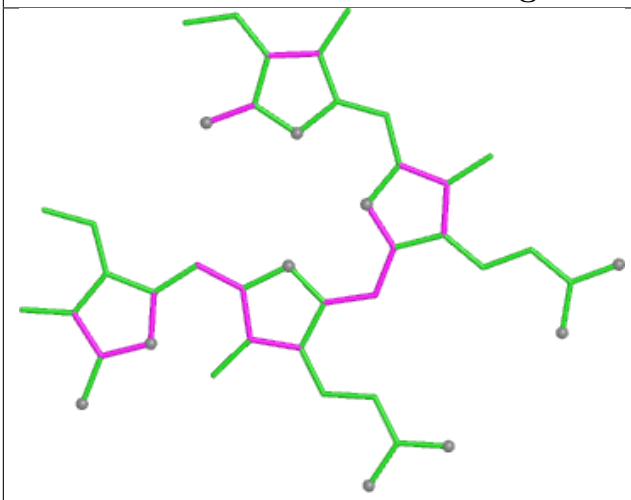


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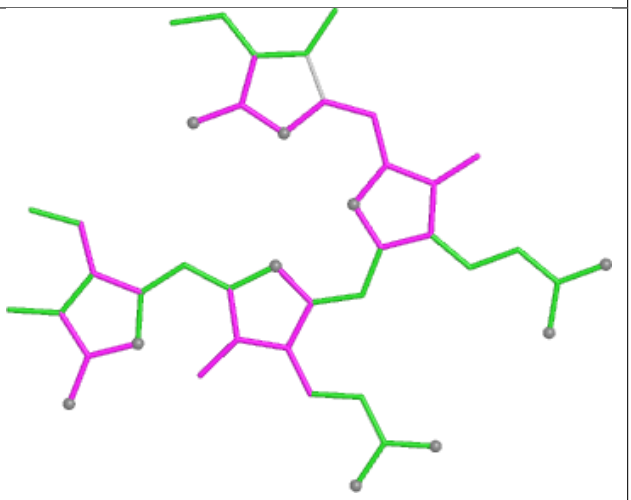


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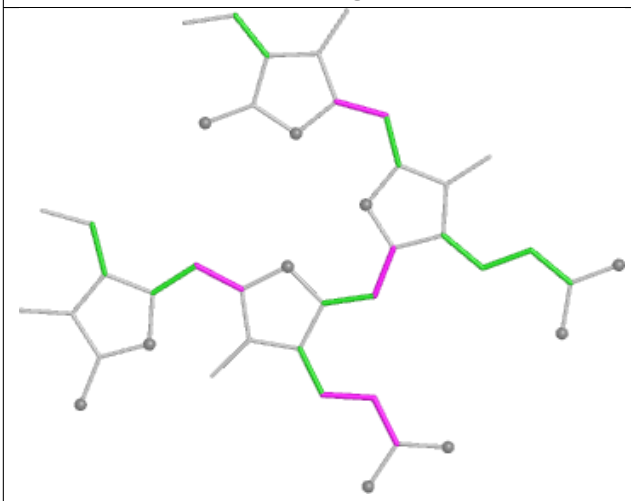
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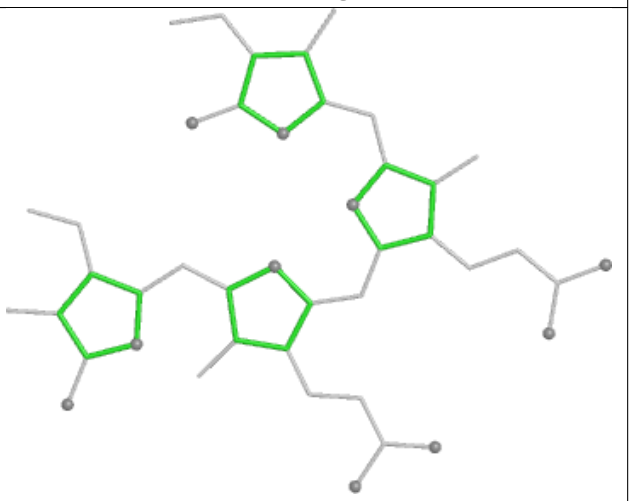
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Bond angles

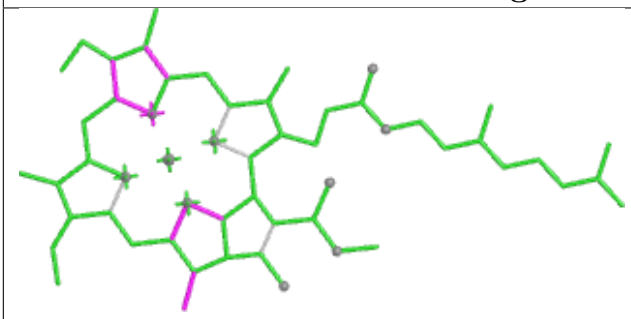


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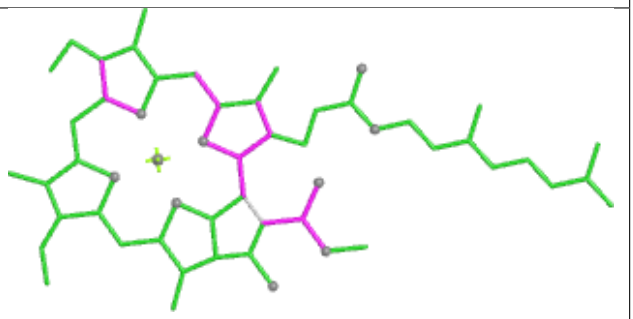


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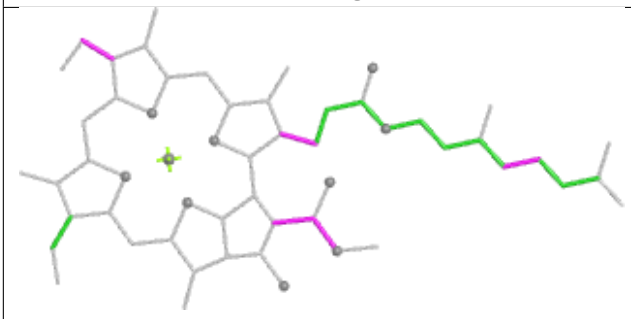
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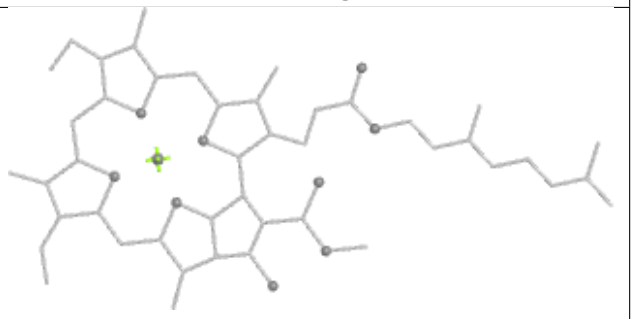
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Bond angles

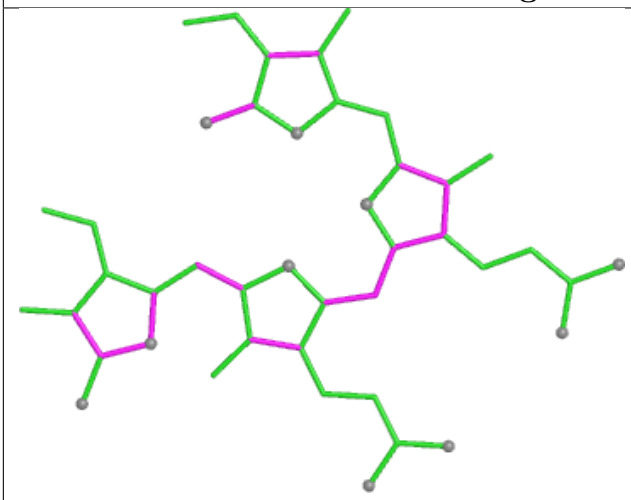


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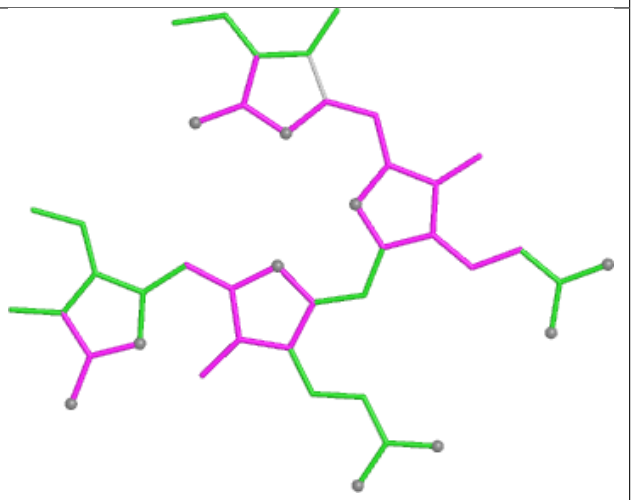


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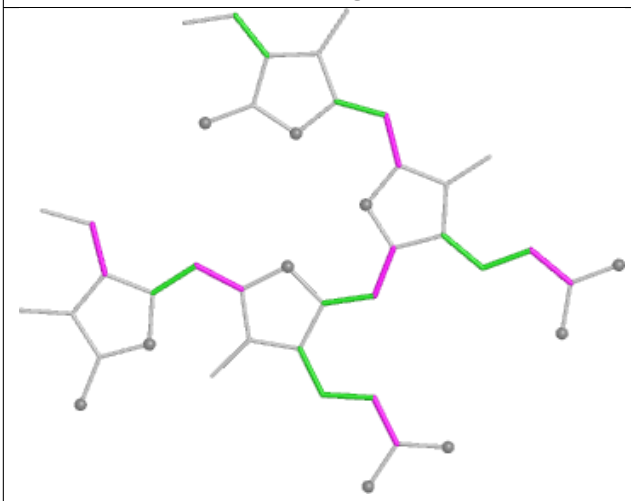
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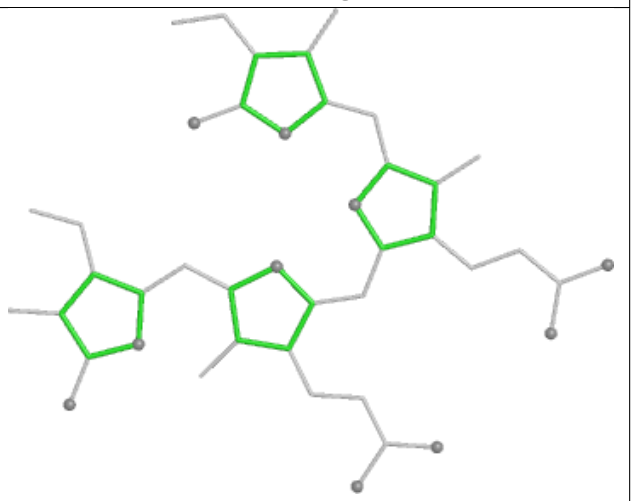
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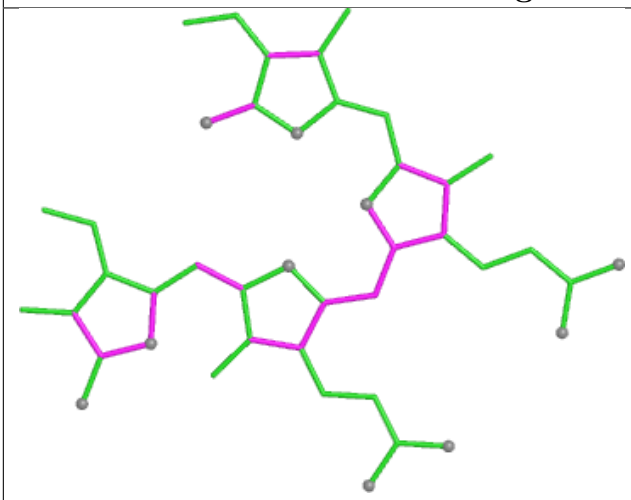


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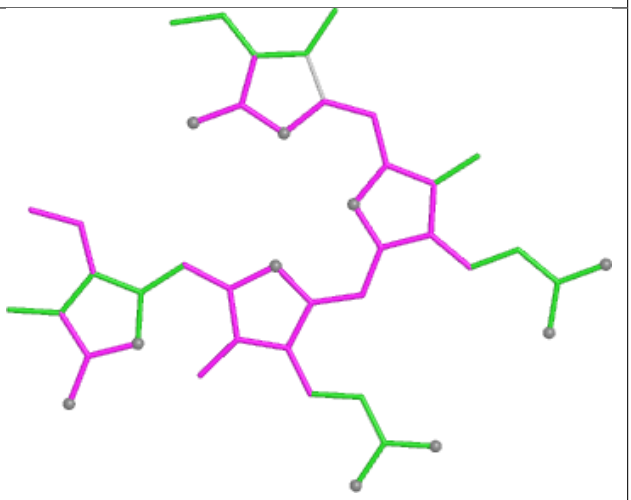


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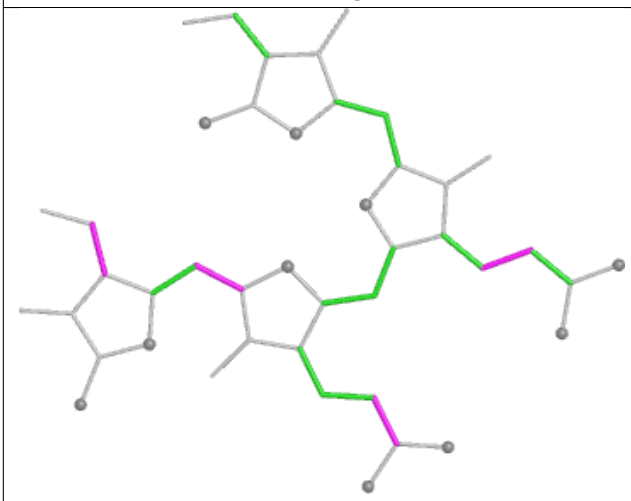
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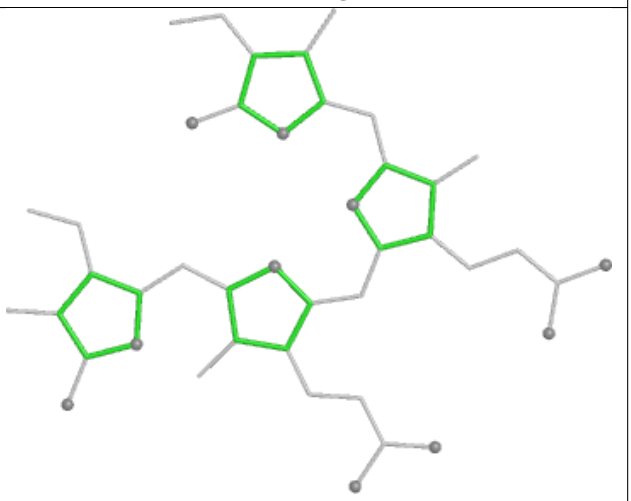
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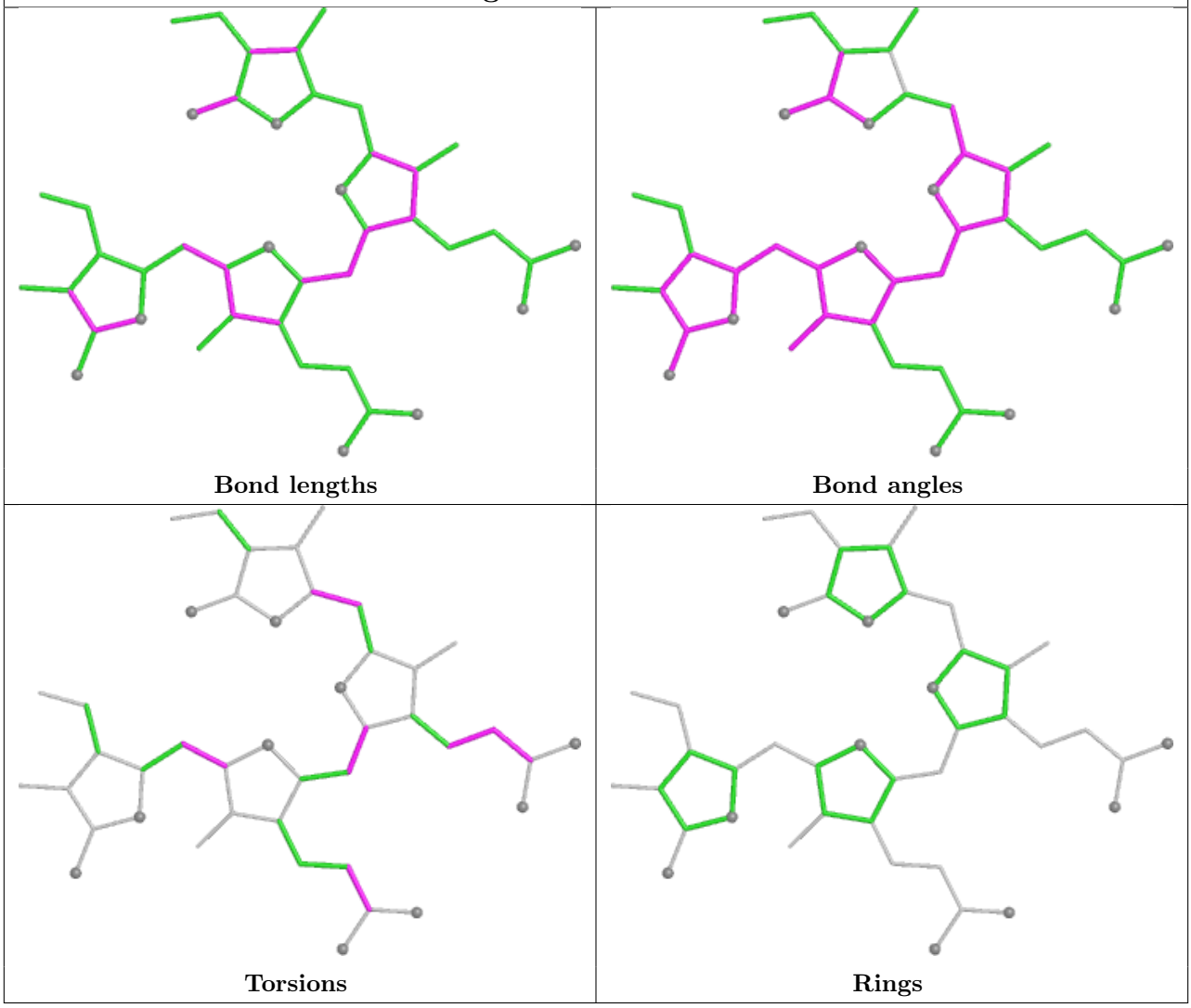


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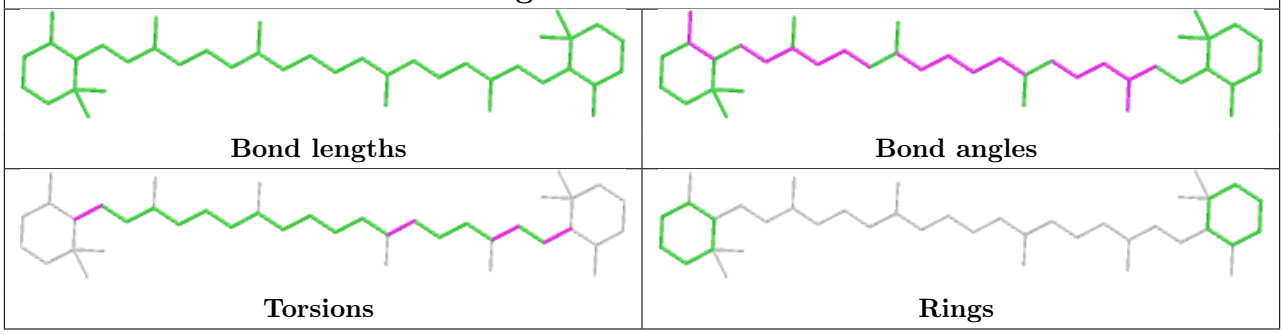


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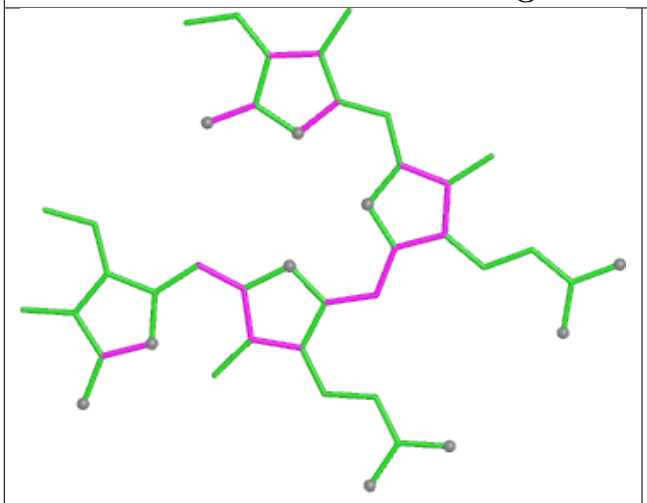
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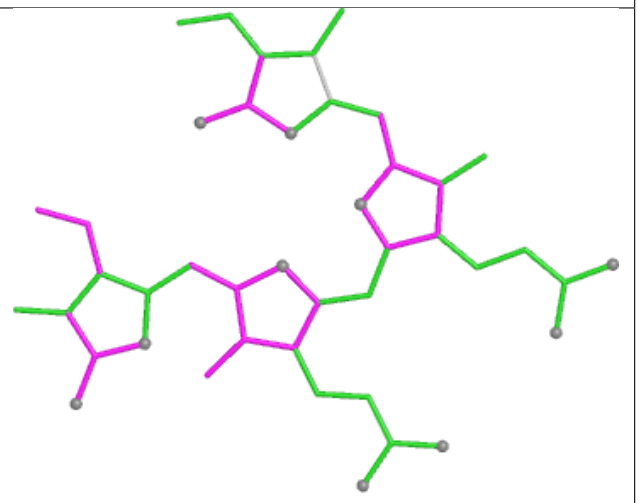
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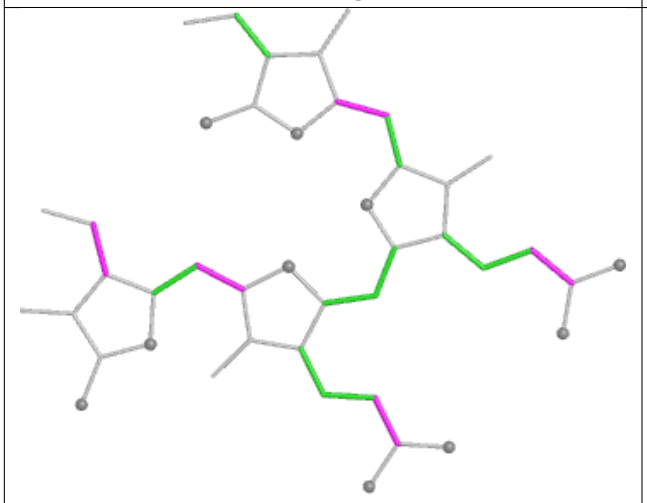
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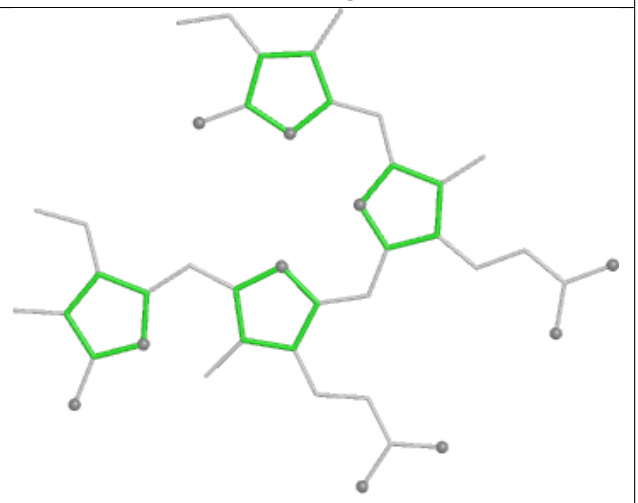
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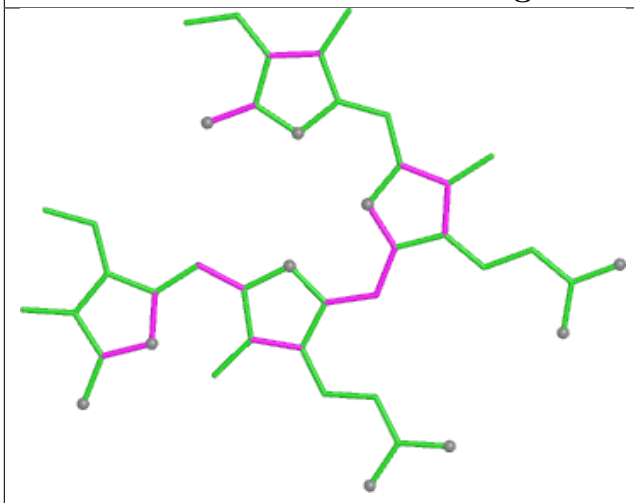


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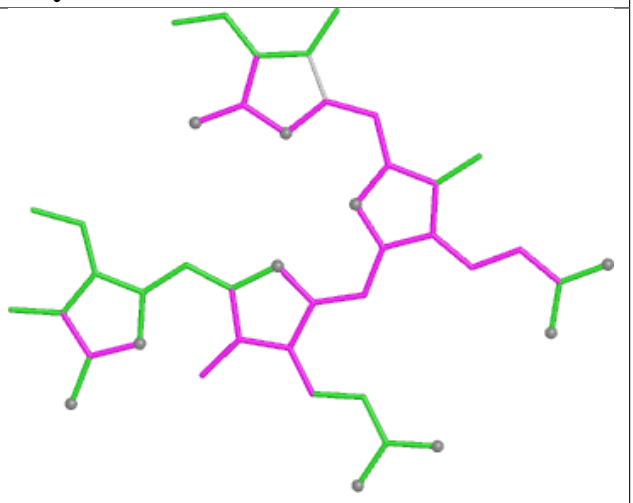


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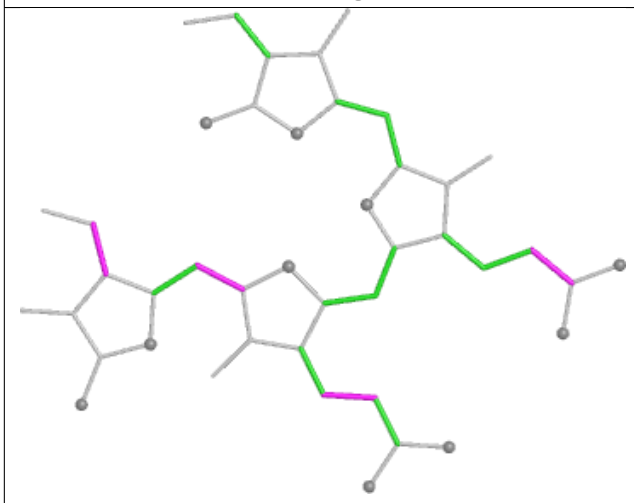
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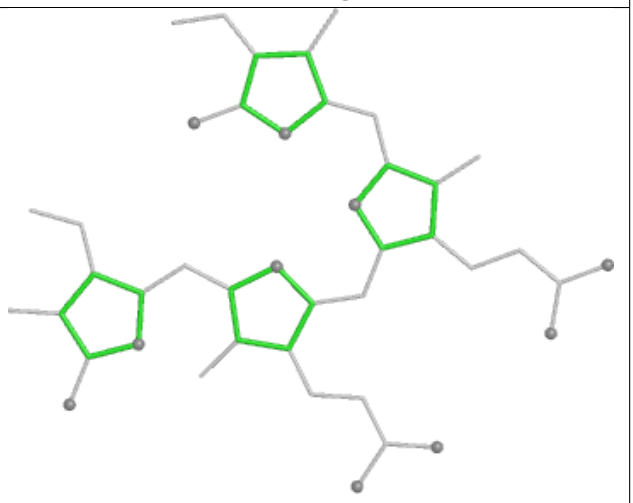
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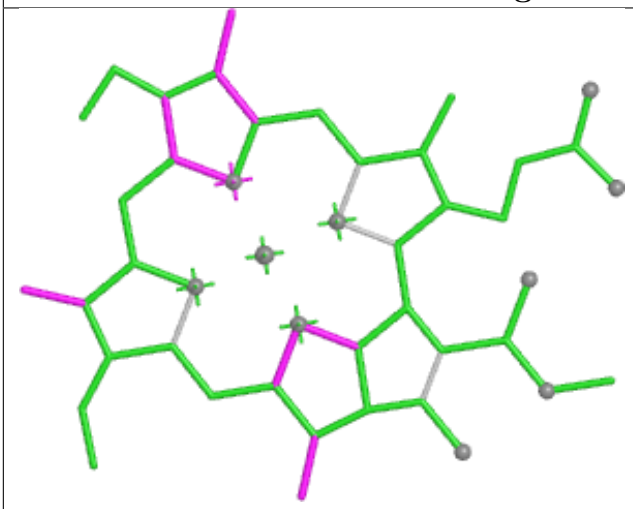


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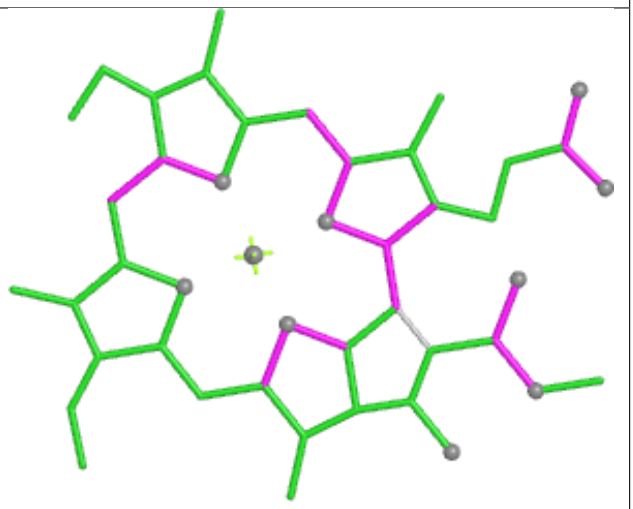


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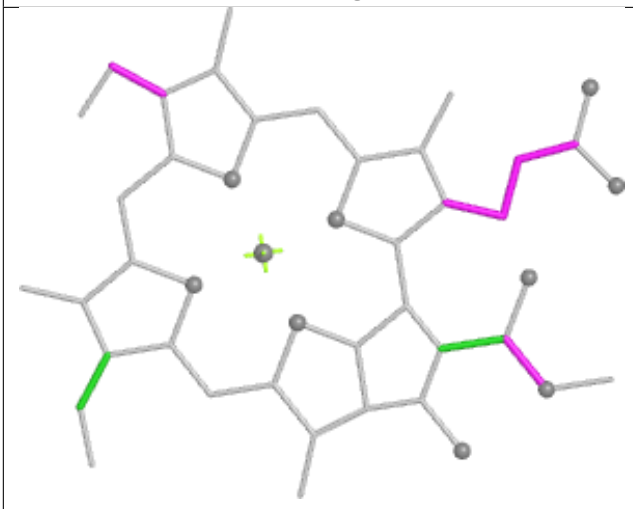
Ligand CLA 4N 601



Bond lengths



Bond angles

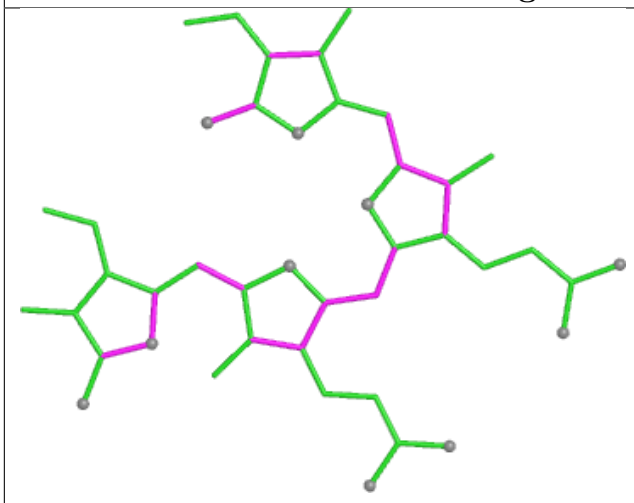


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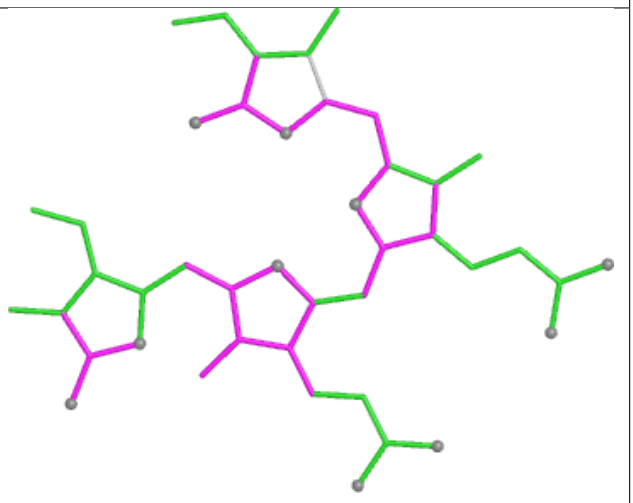


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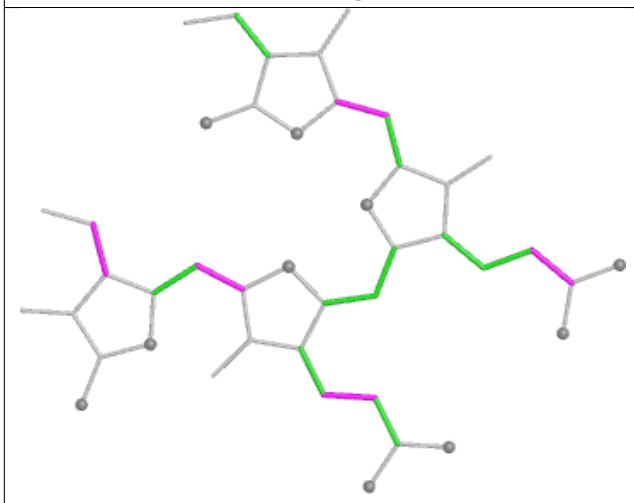
Ligand PEB Z1 202



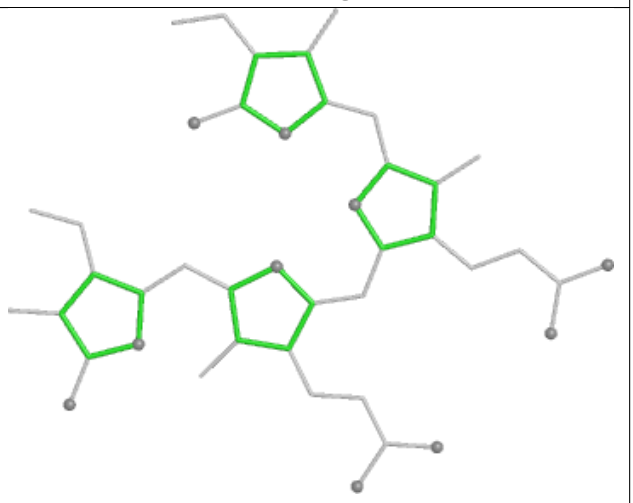
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Bond angles

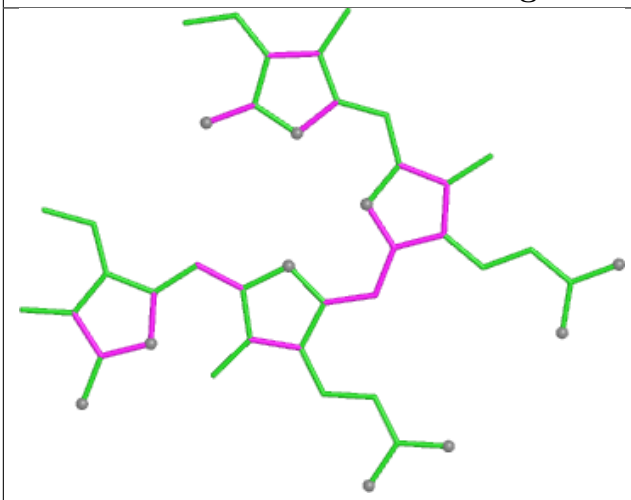


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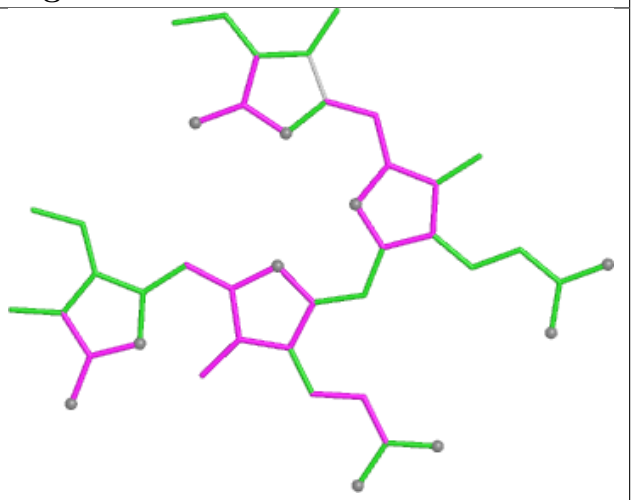


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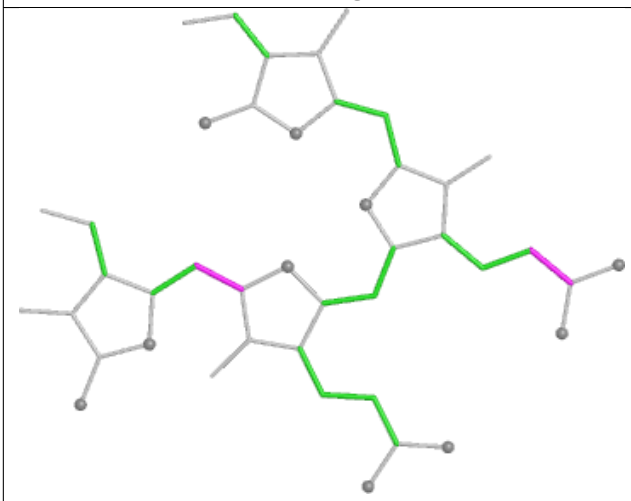
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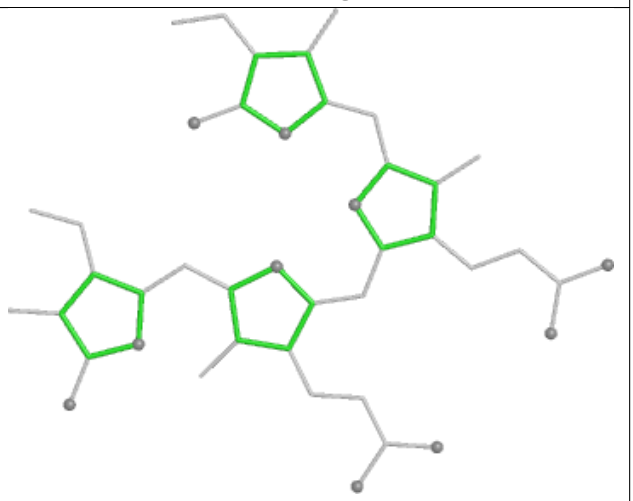
Bond lengths



Bond angles

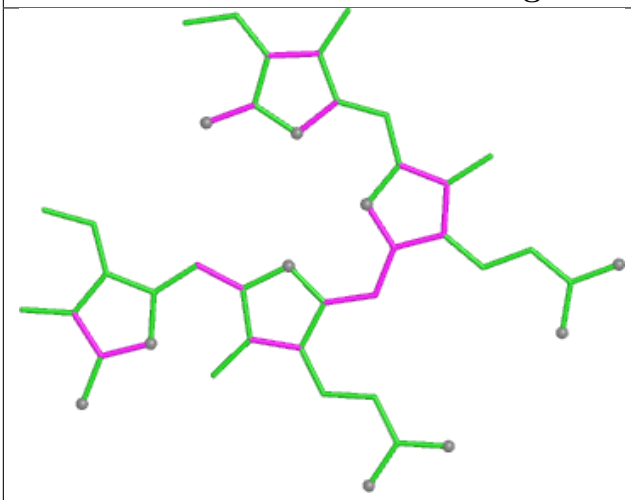


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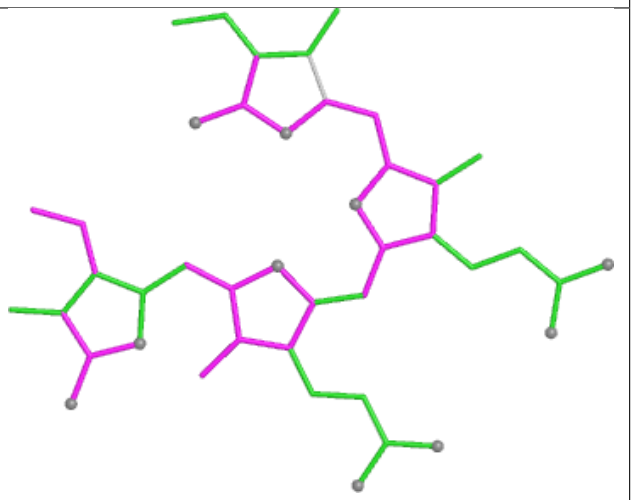


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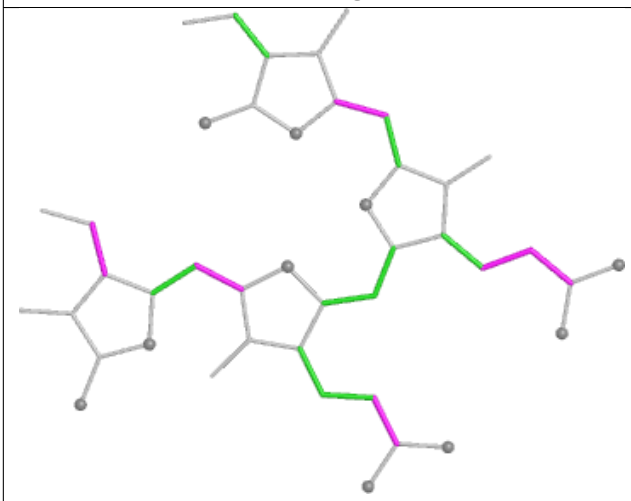
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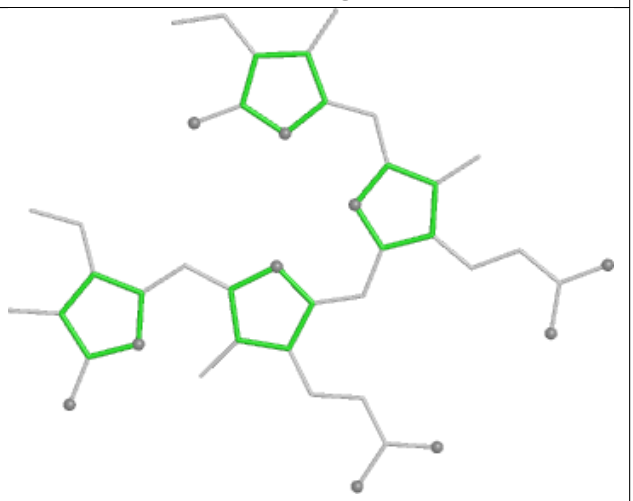
Bond lengths



Bond angles

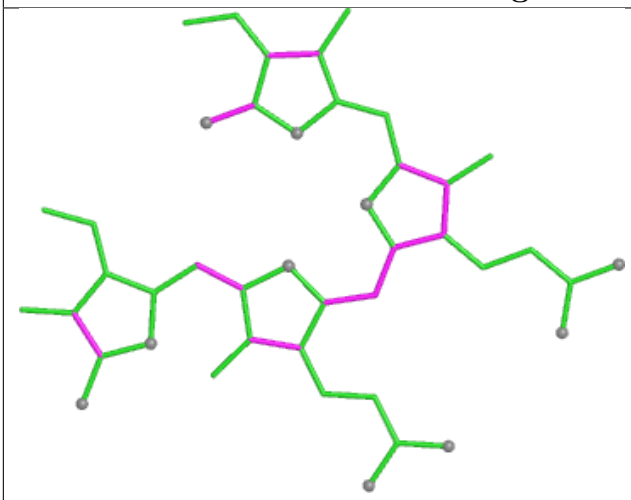


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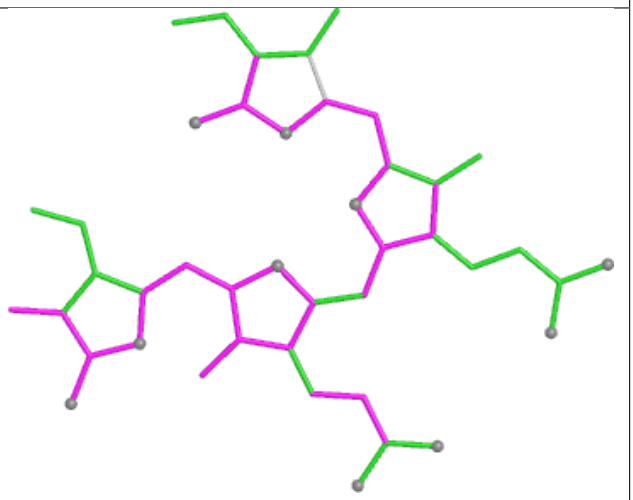


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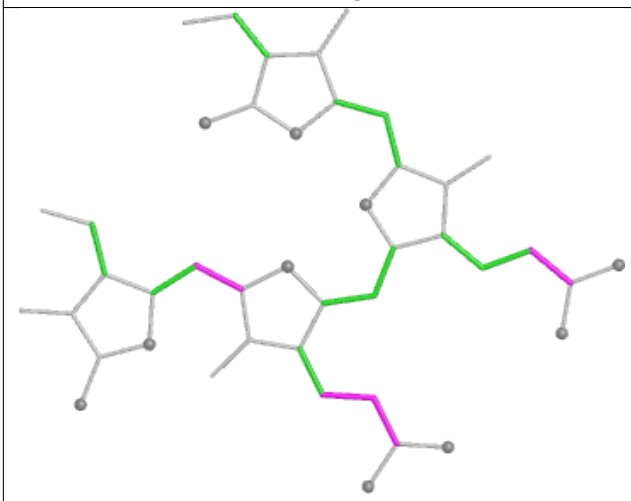
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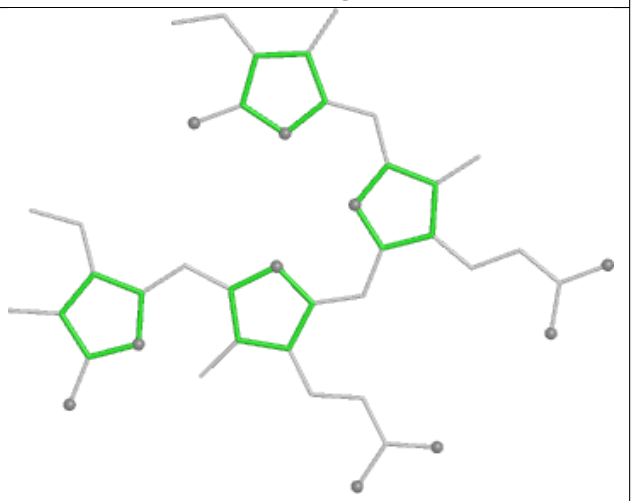
Bond lengths



Bond angles

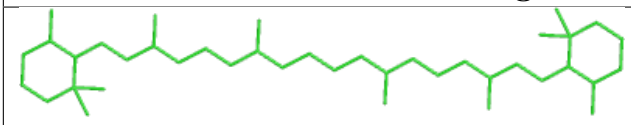


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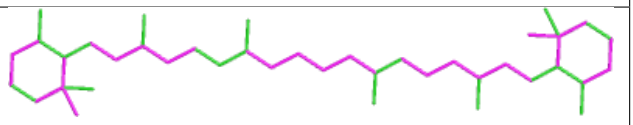


Rings

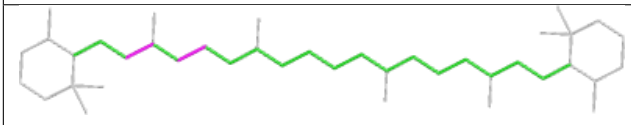
Ligand BCR hL 102



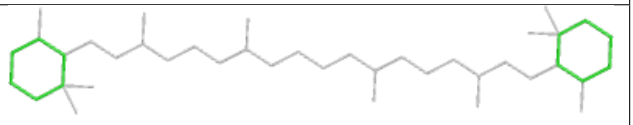
Bond lengths



Bond angles

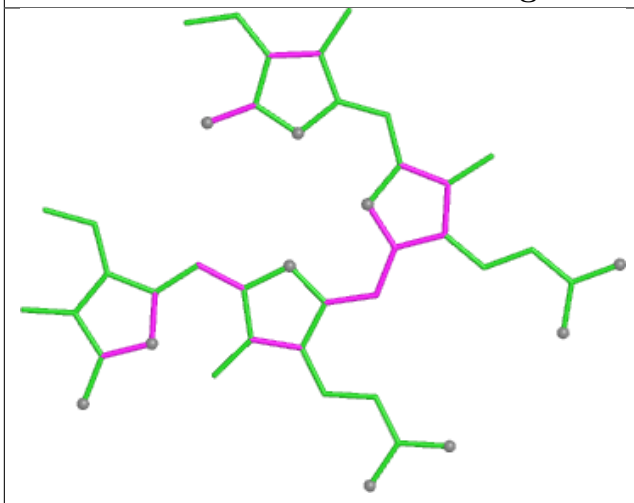


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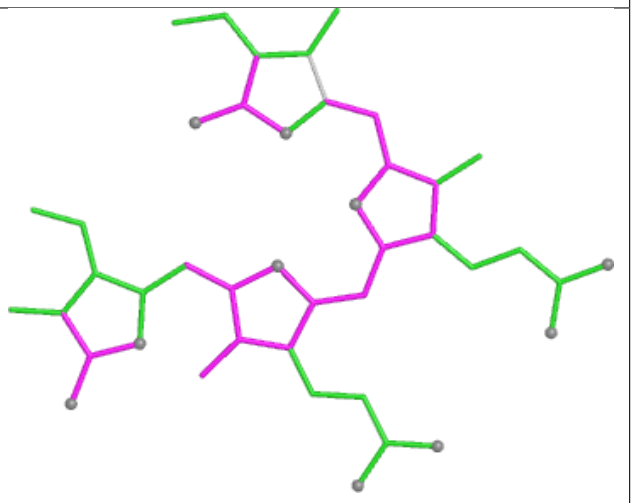


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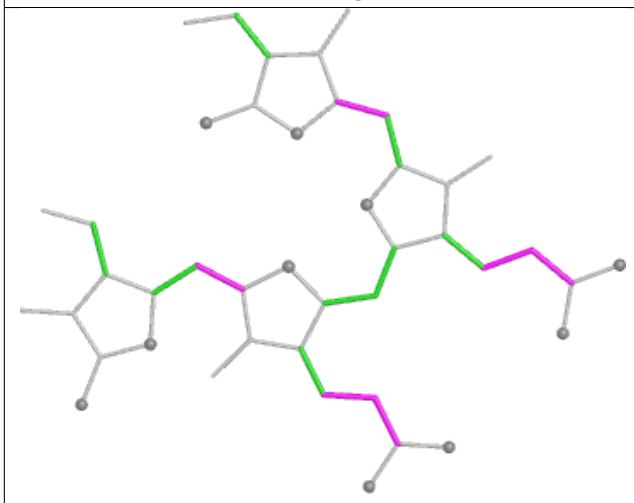
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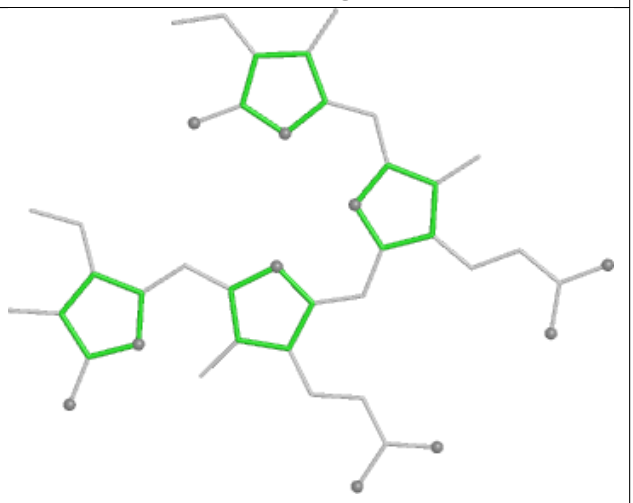
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Bond angles

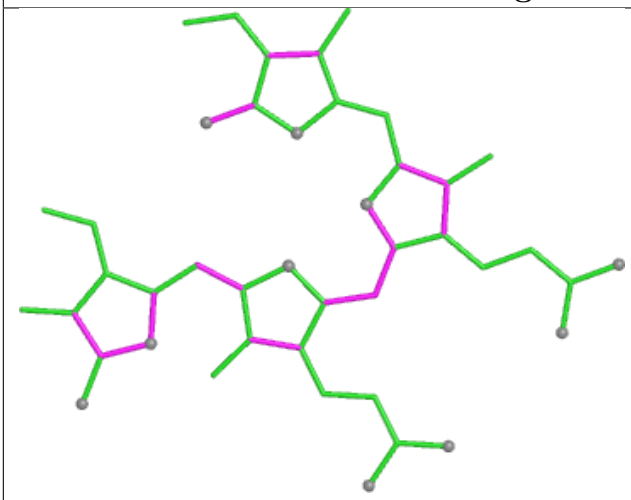


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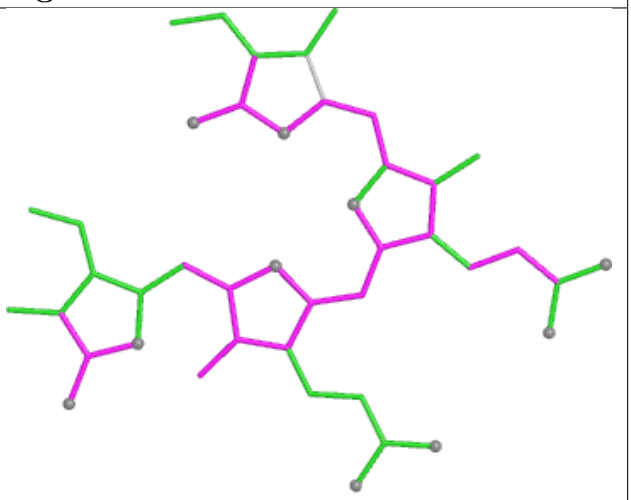


Rings

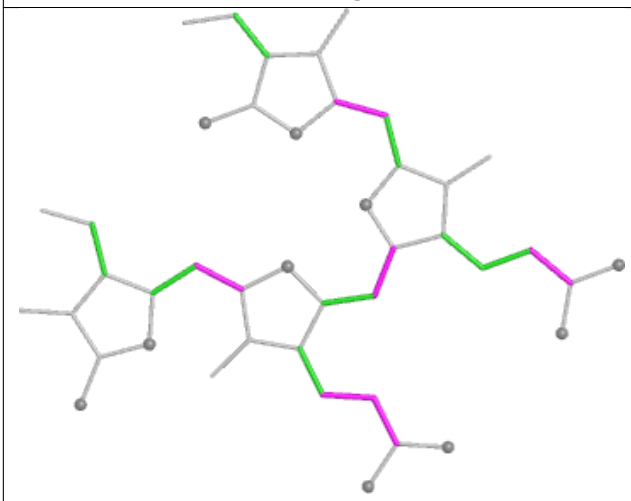
Ligand PEB gG 202



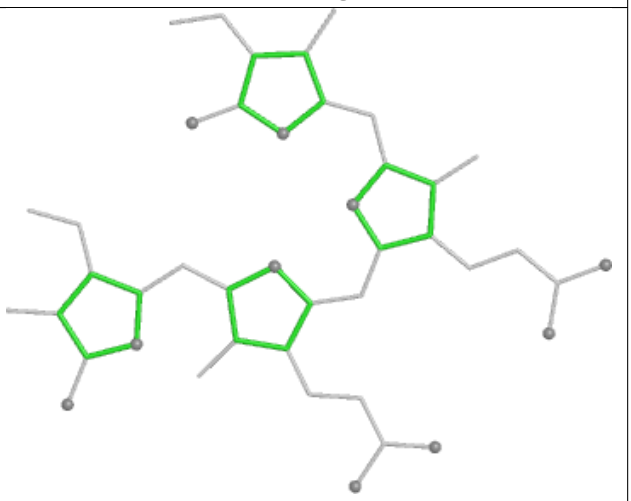
Bond lengths



Bond angles

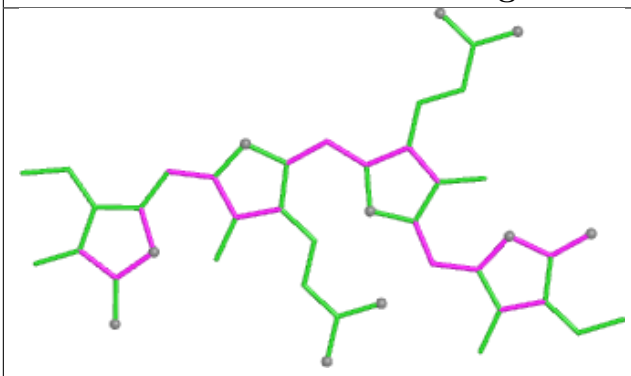


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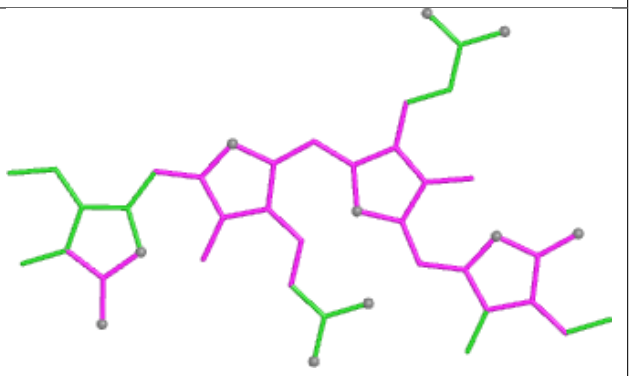


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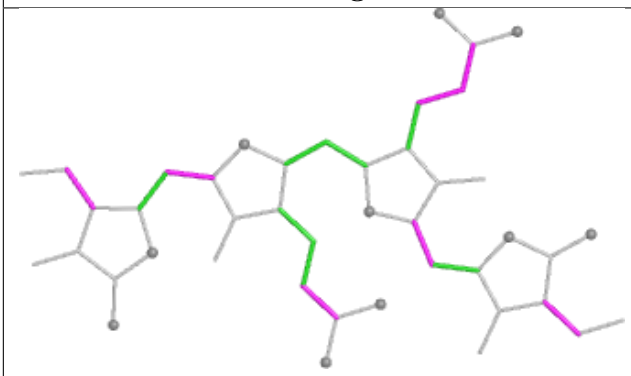
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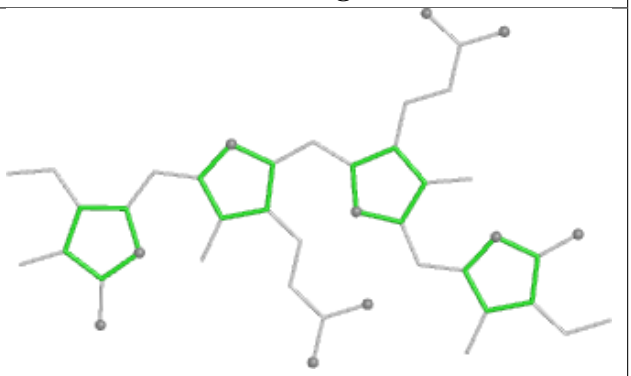
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Bond angles

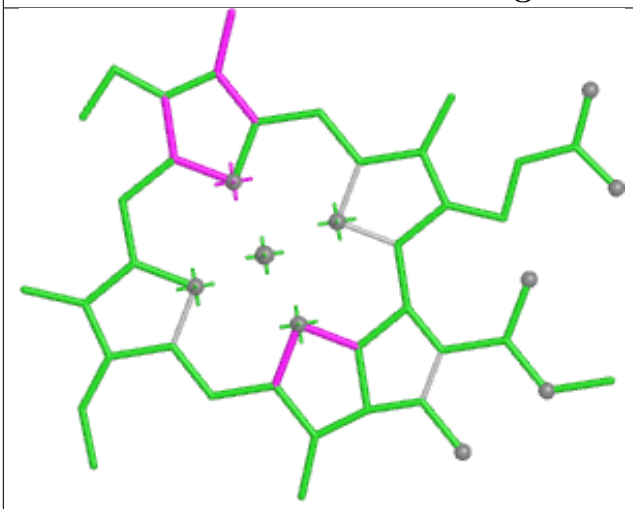


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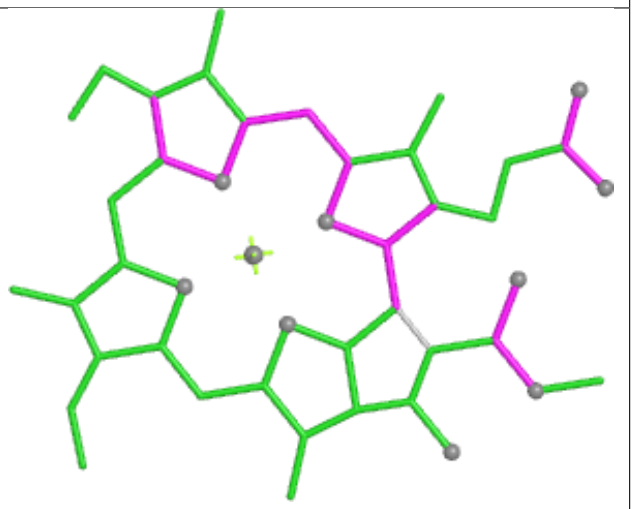


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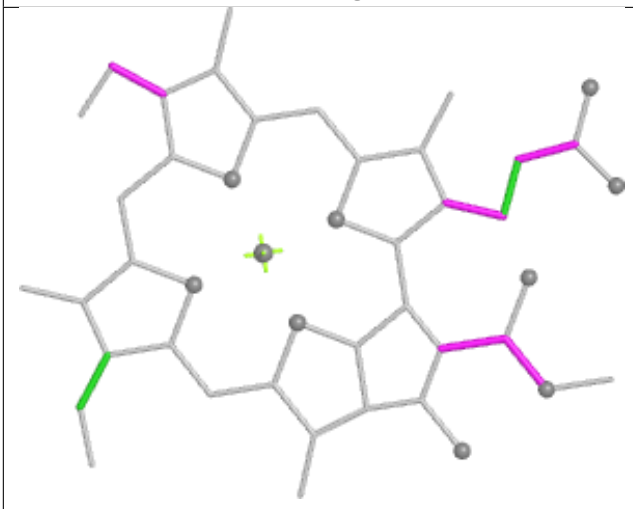
Ligand CLA 5N 601



Bond lengths



Bond angles

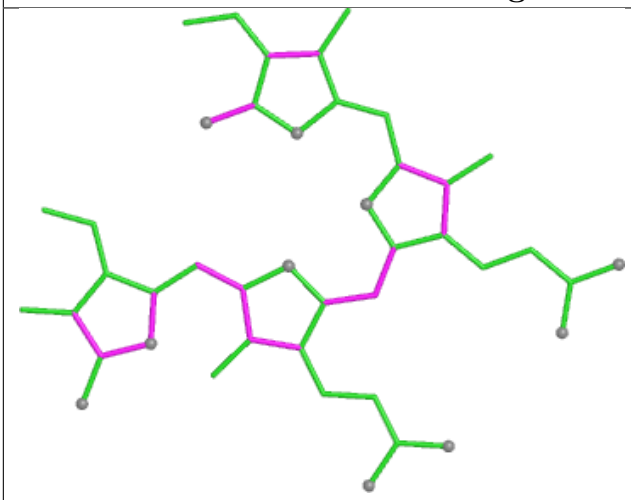


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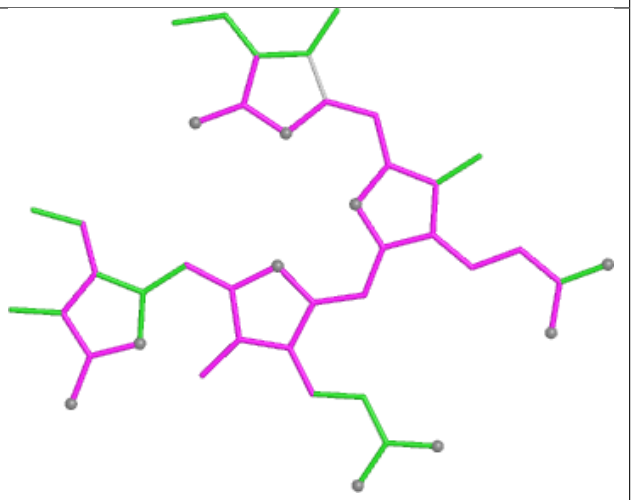


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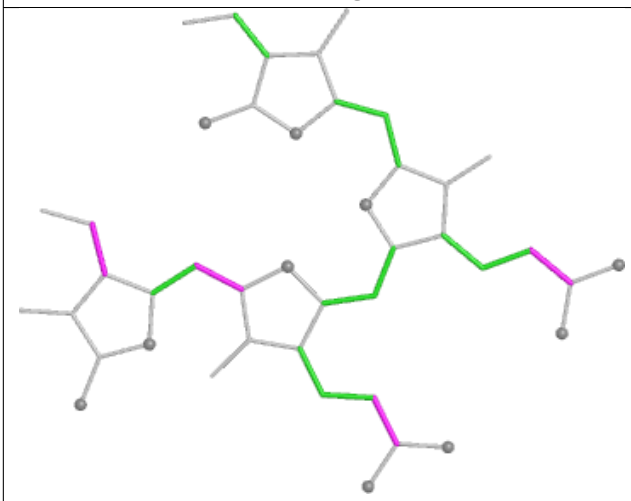
Ligand PEB WF 202



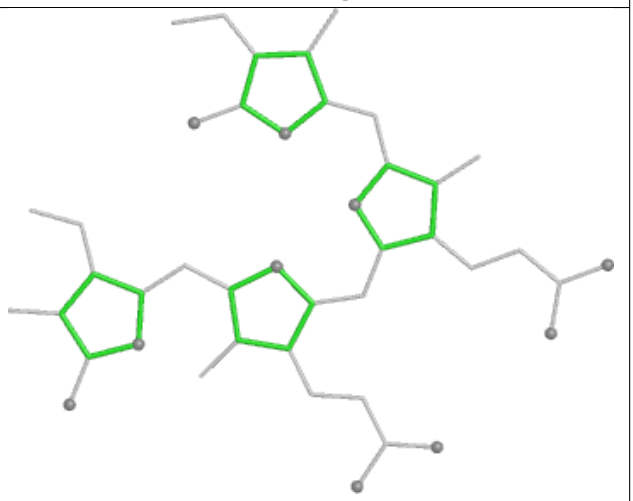
Bond lengths



Bond angles

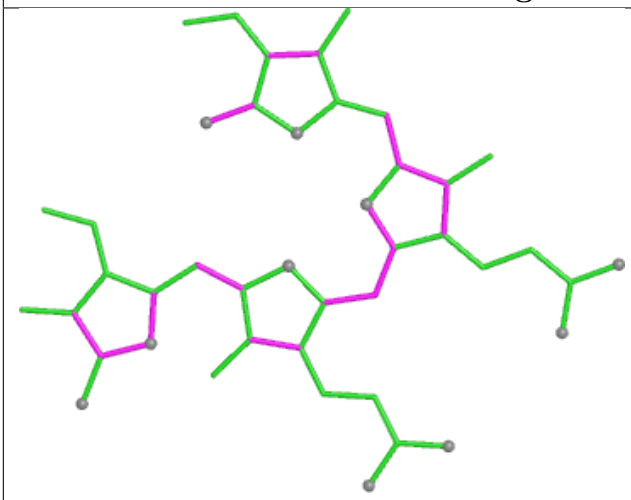


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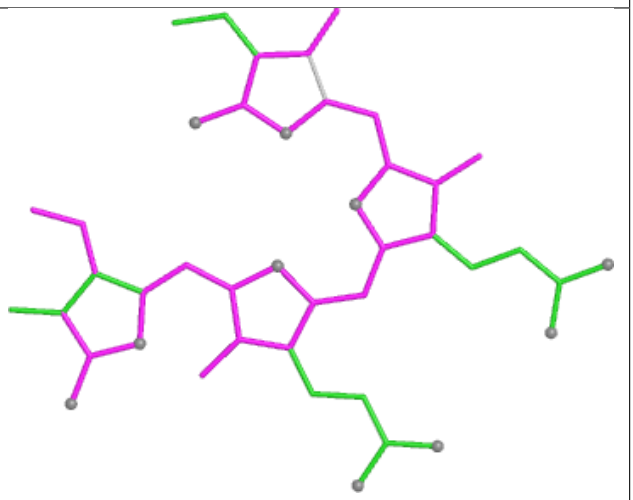


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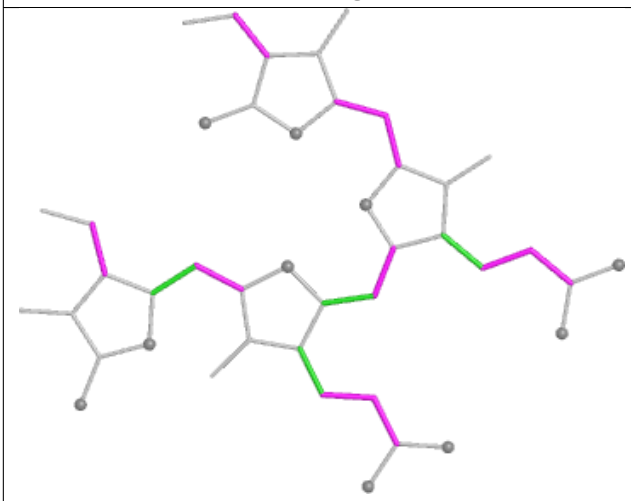
Ligand PEB Y7 301



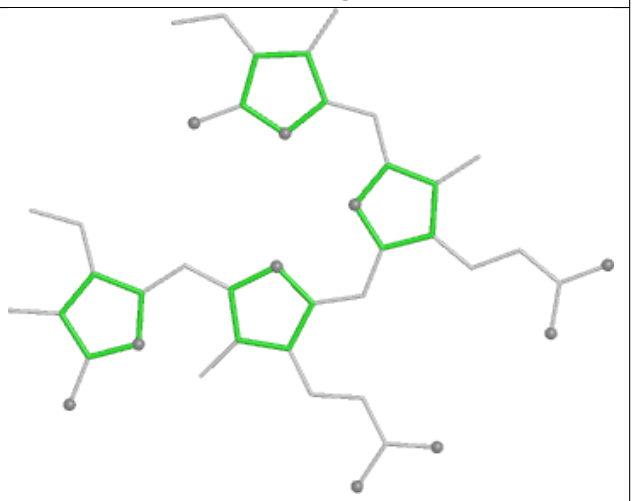
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Bond angles

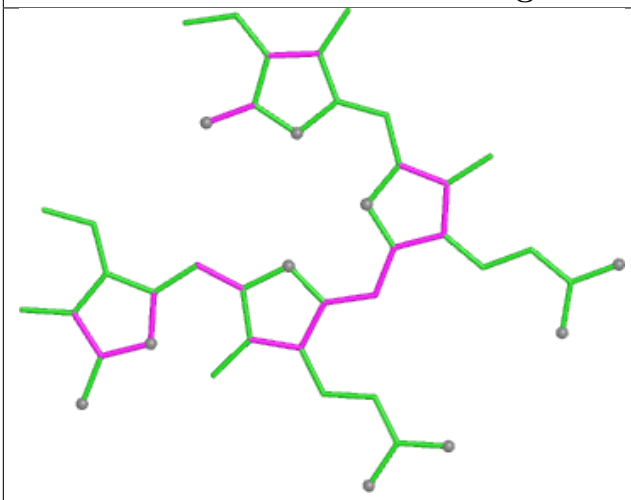


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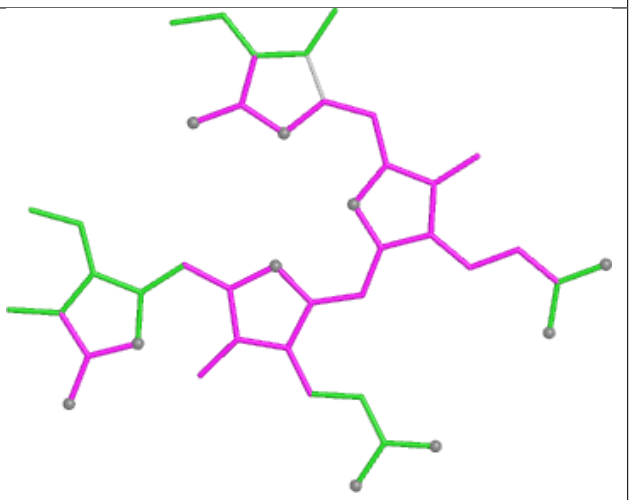


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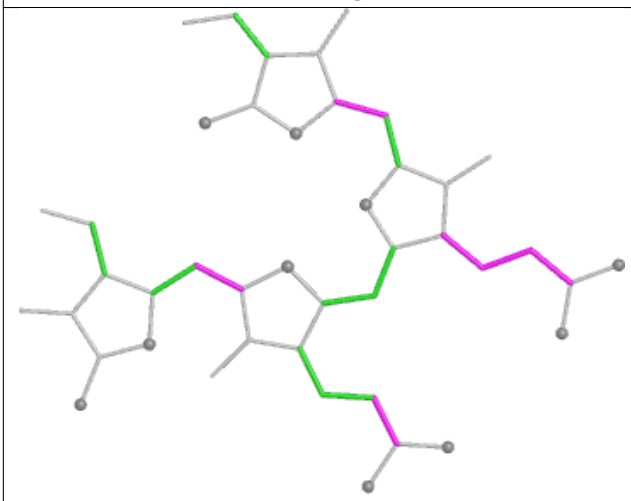
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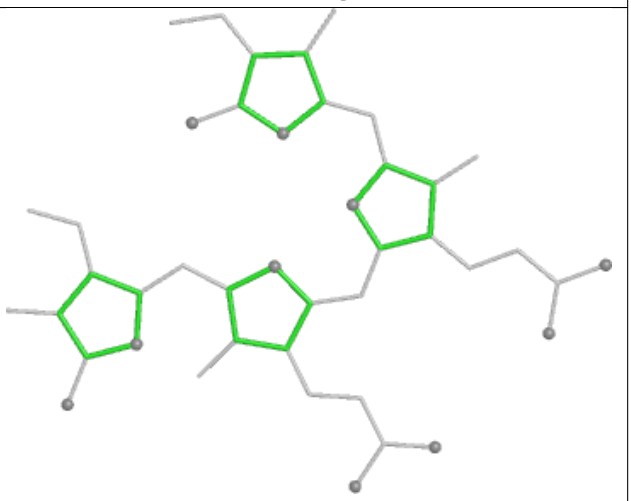
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Bond angles

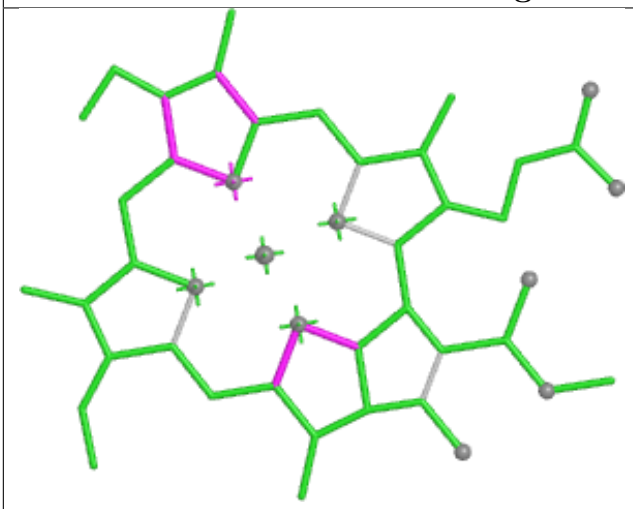


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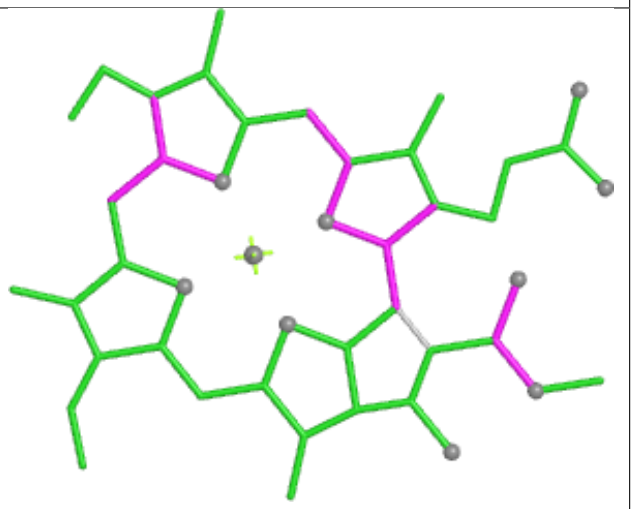


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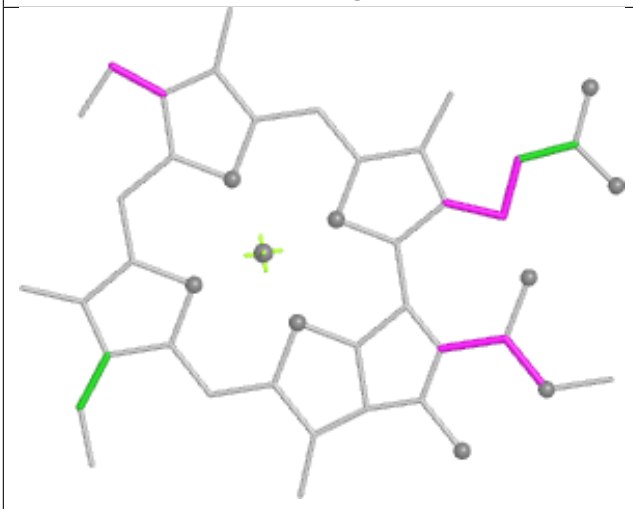
Ligand CLA 2N 302



Bond lengths



Bond angles

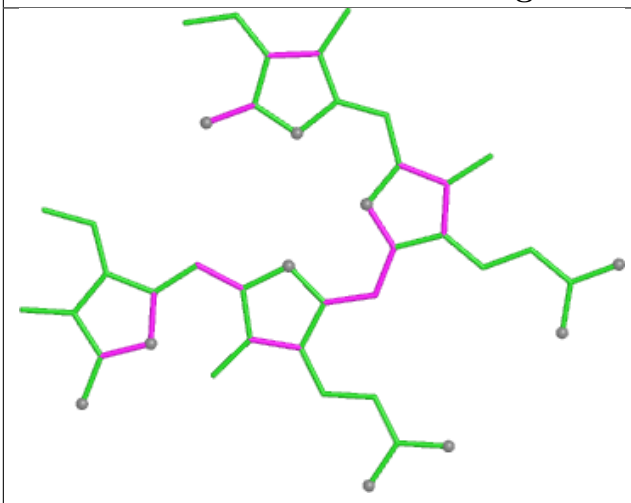


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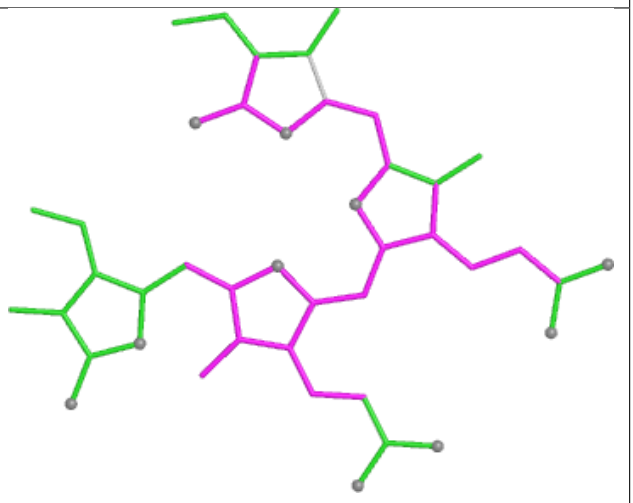


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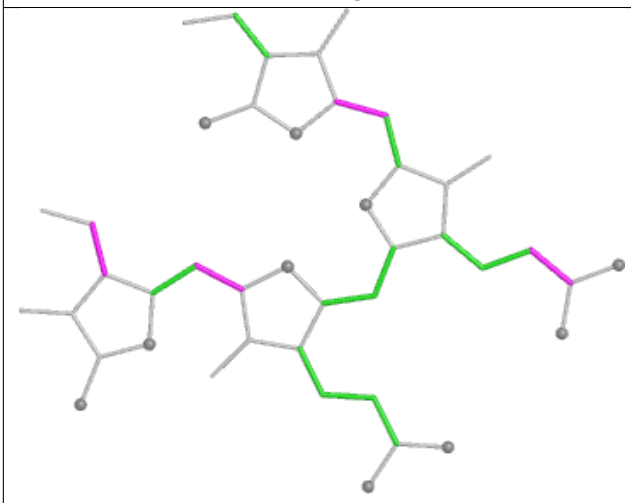
Ligand PEB zK 501



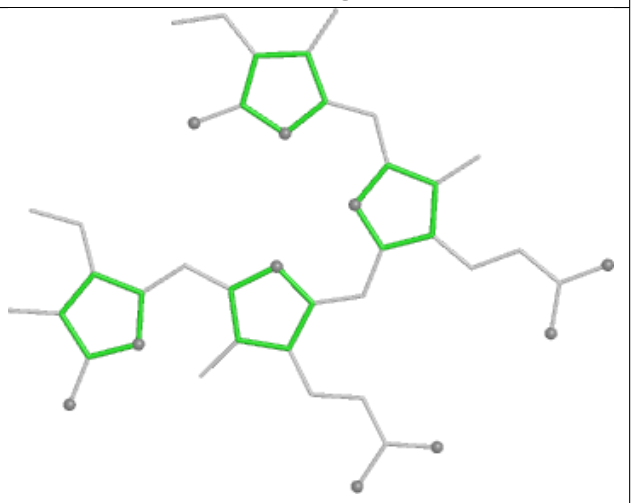
Bond lengths



Bond angles

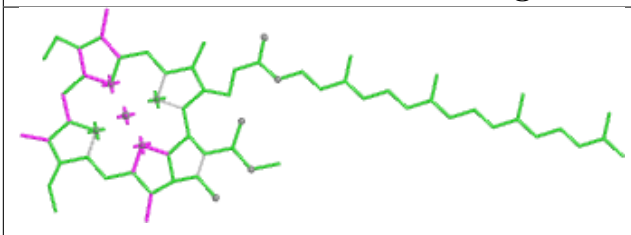


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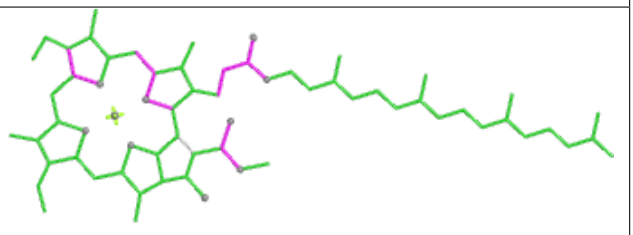


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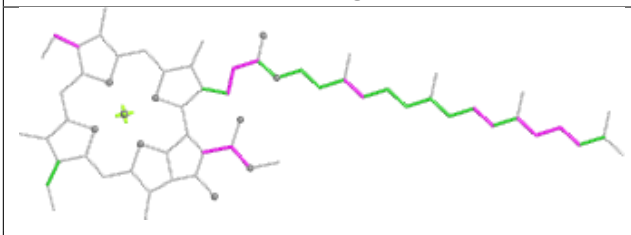
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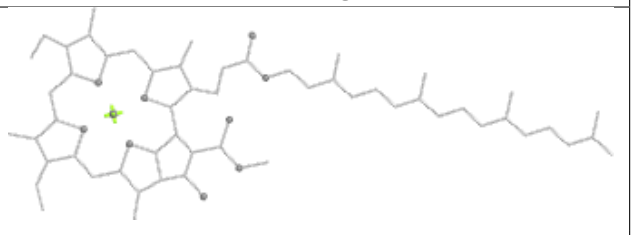
Bond lengths



Bond angles

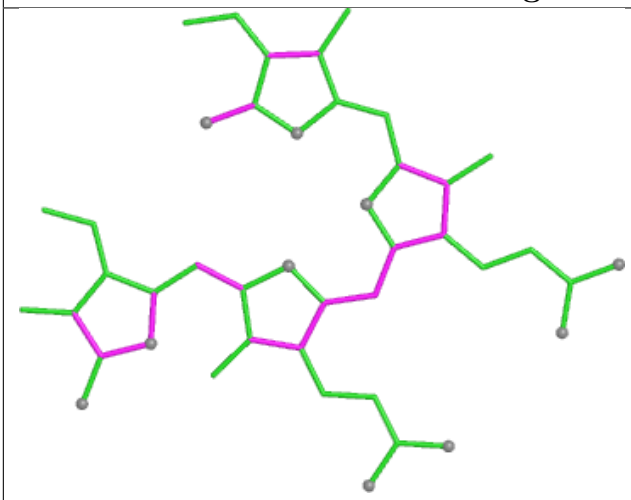


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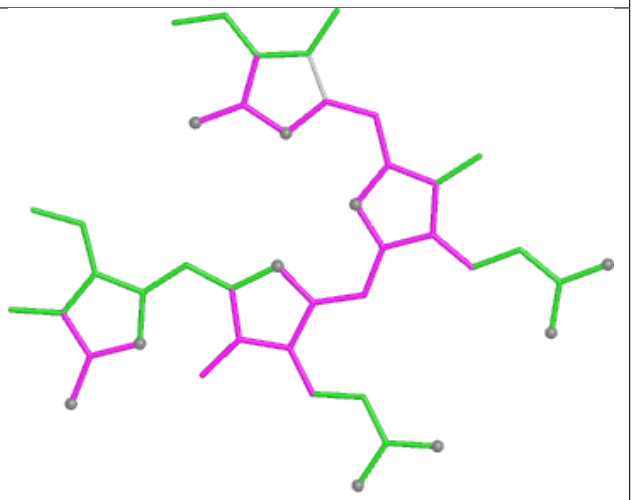


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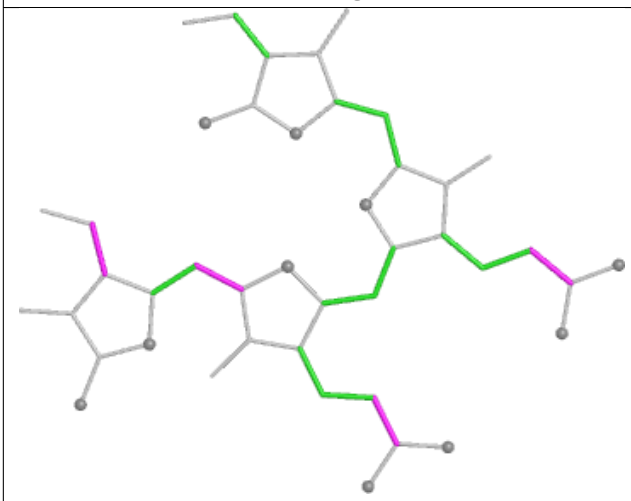
Ligand PEB fJ 203



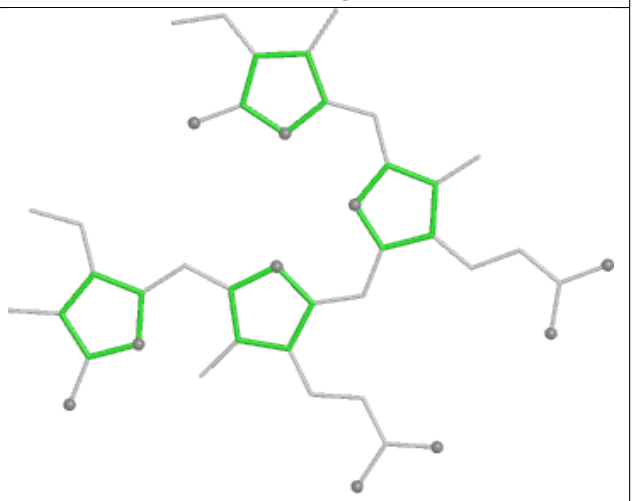
Bond lengths



Bond angles

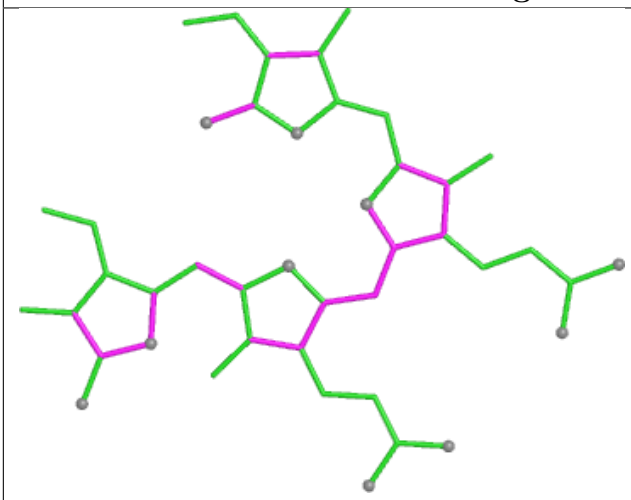


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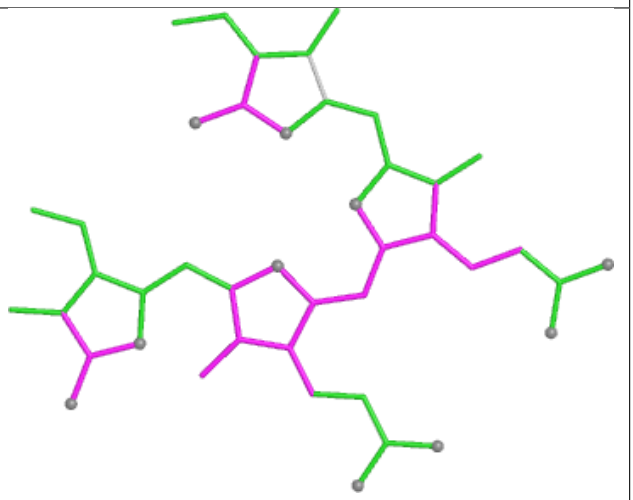


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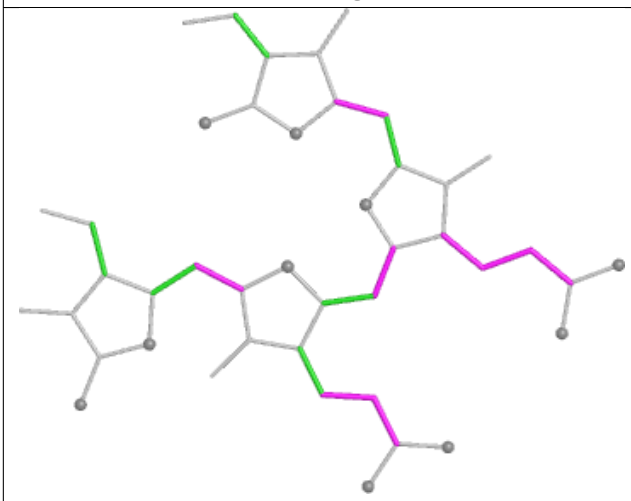
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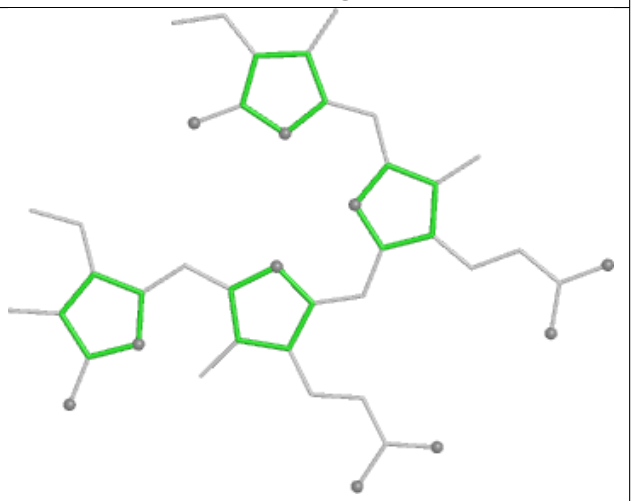
Bond lengths



Bond angles

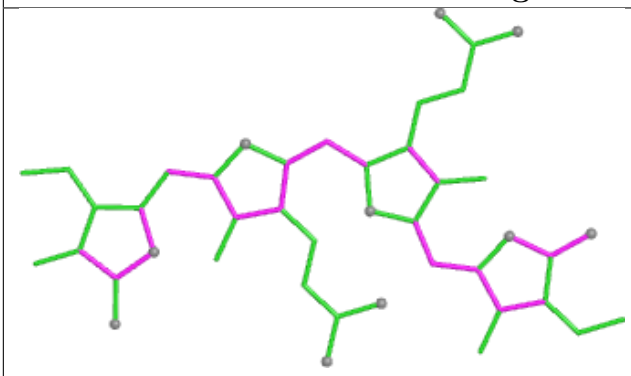


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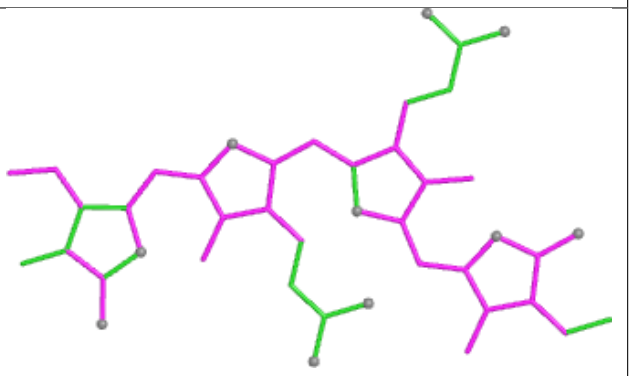


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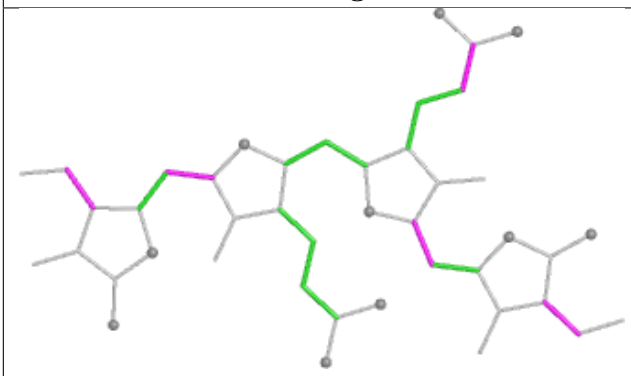
Ligand CYC i3 1001



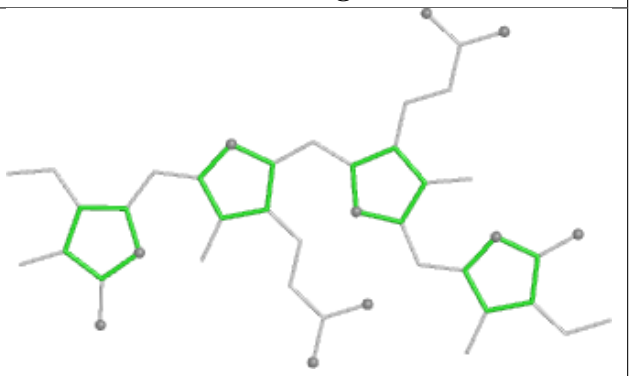
Bond lengths



Bond angles

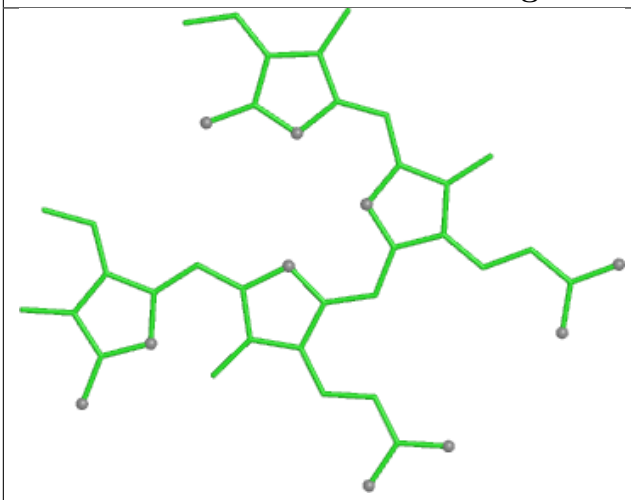


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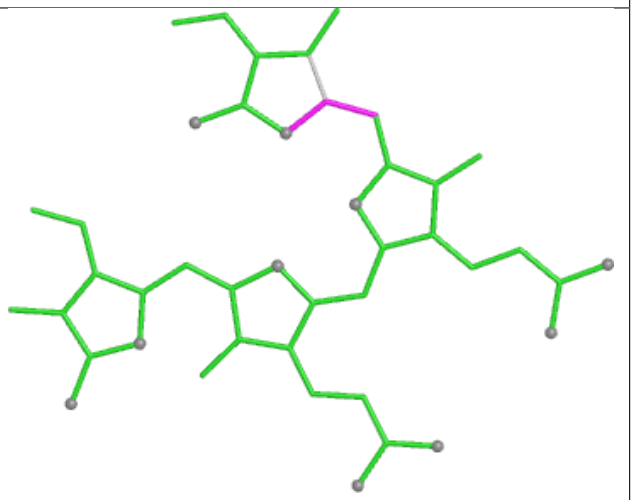


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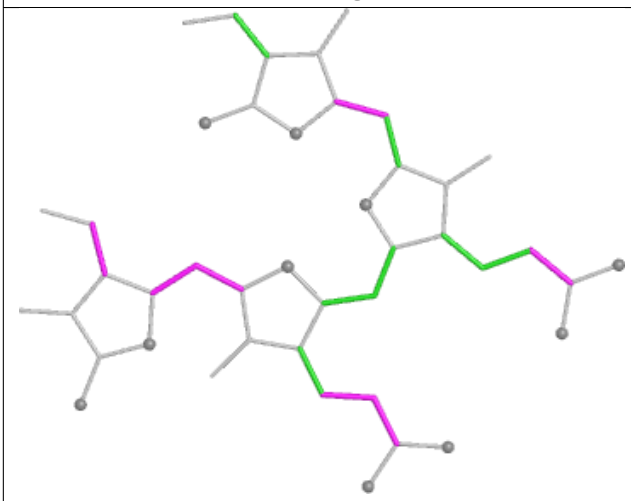
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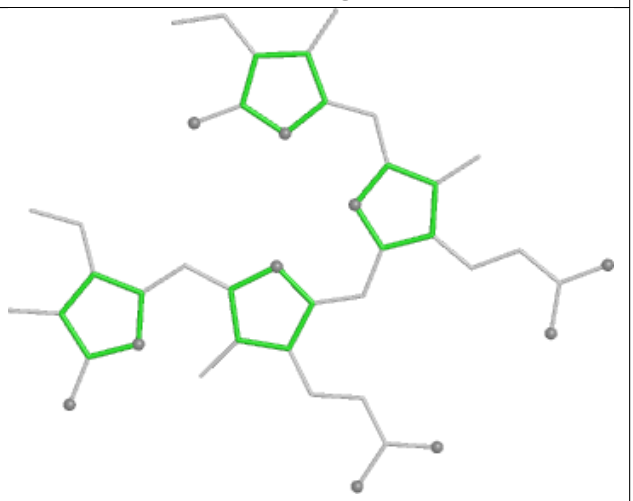
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Bond angles

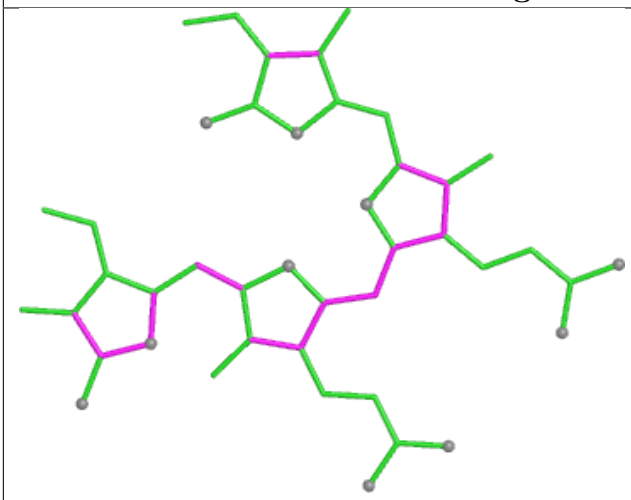


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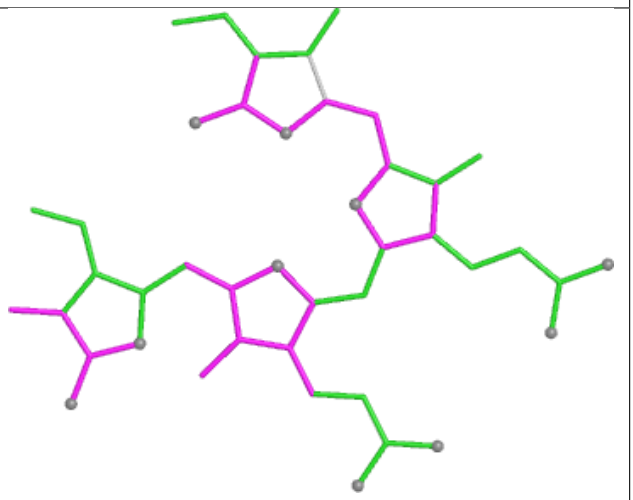


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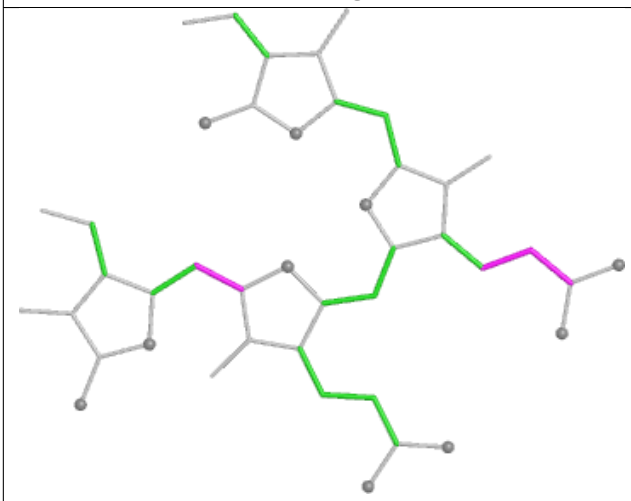
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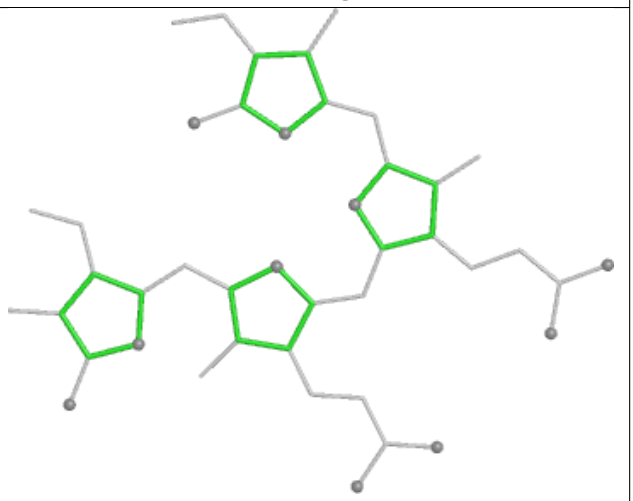
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Bond angles

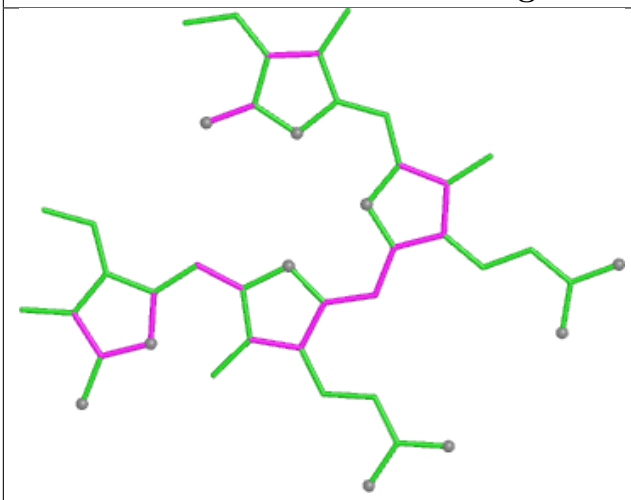


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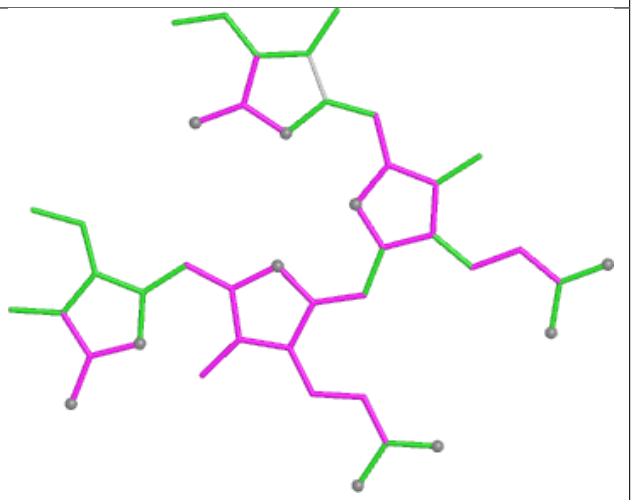


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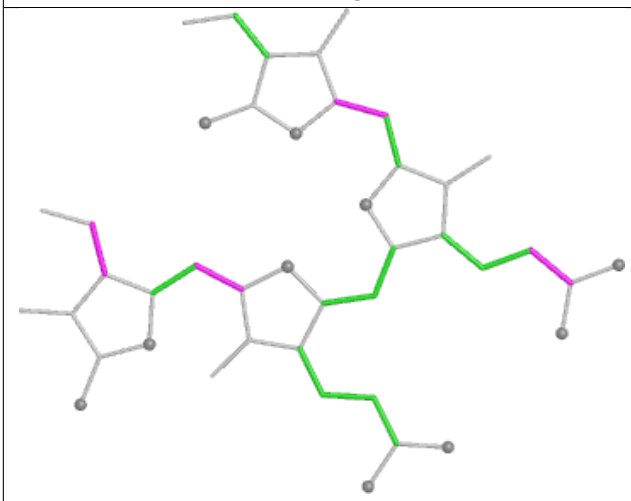
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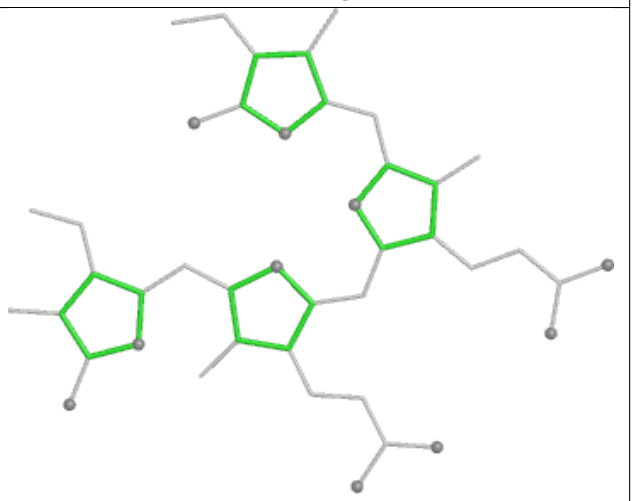
Bond lengths



Bond angles

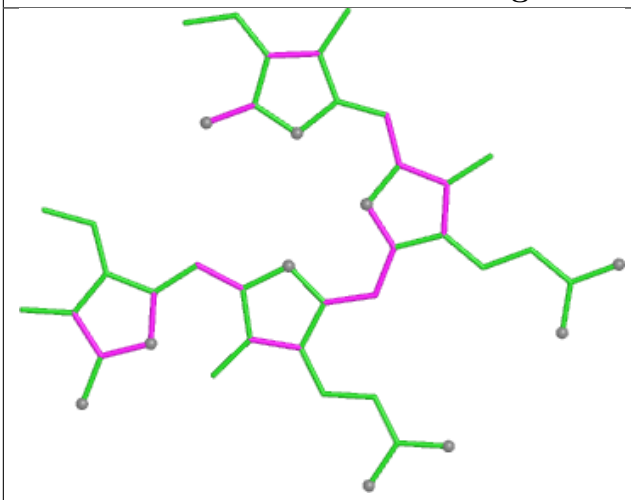


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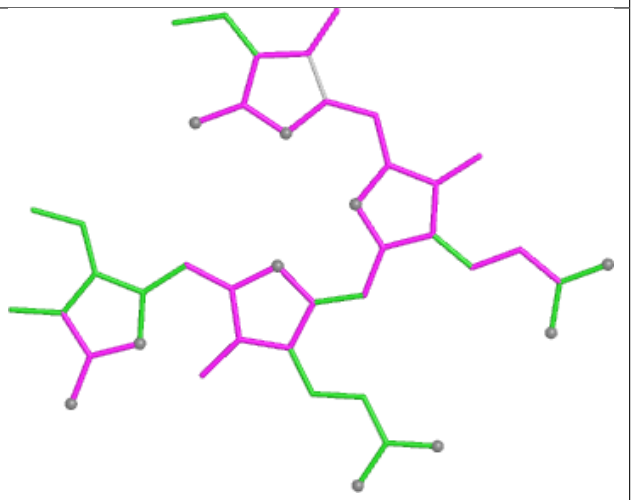


Rings

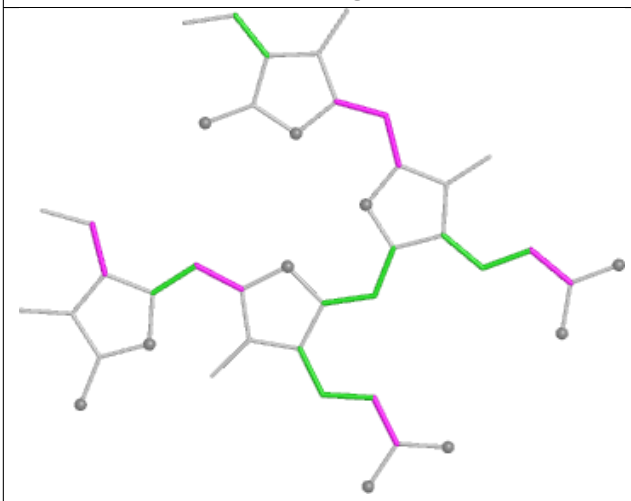
Ligand PEB KP 201



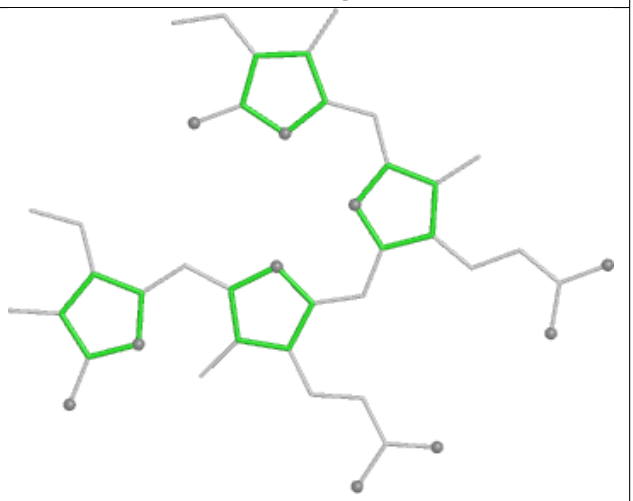
Bond lengths



Bond angles

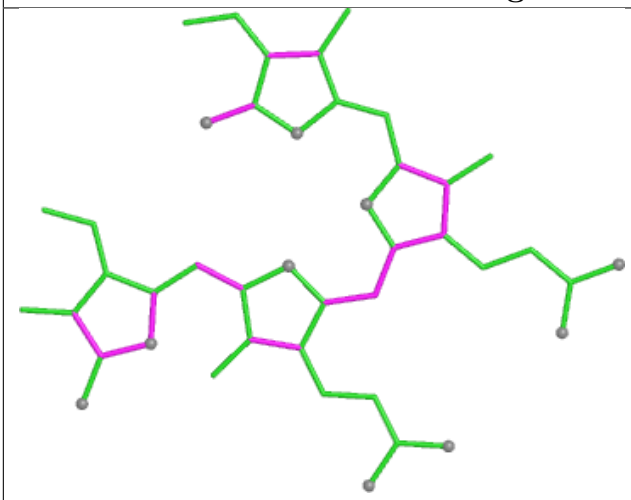


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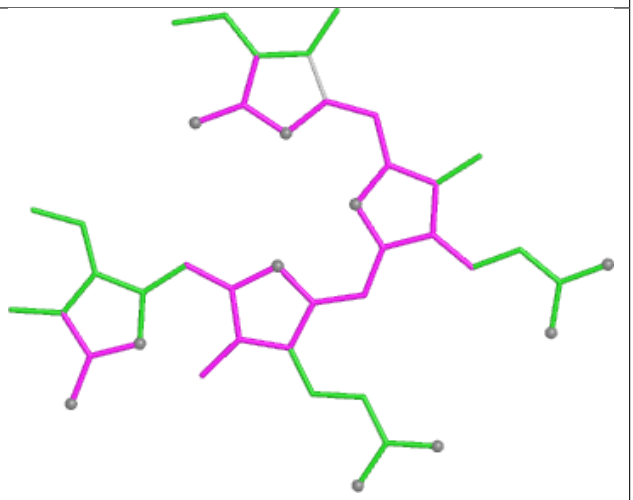


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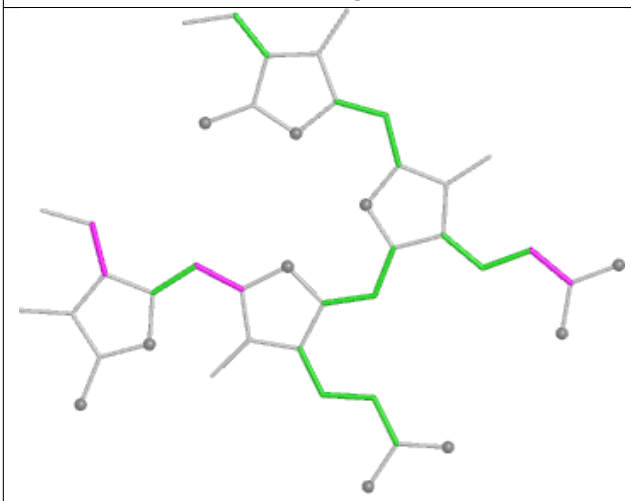
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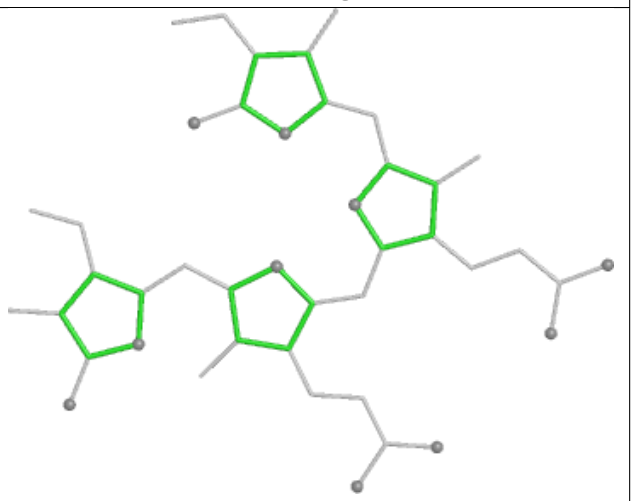
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Bond angles

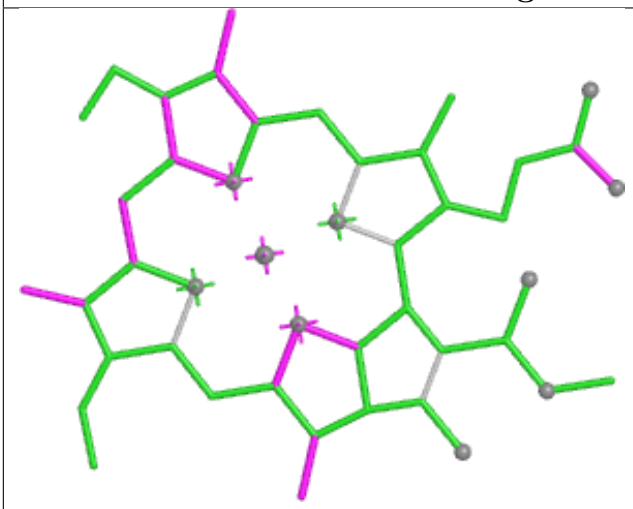


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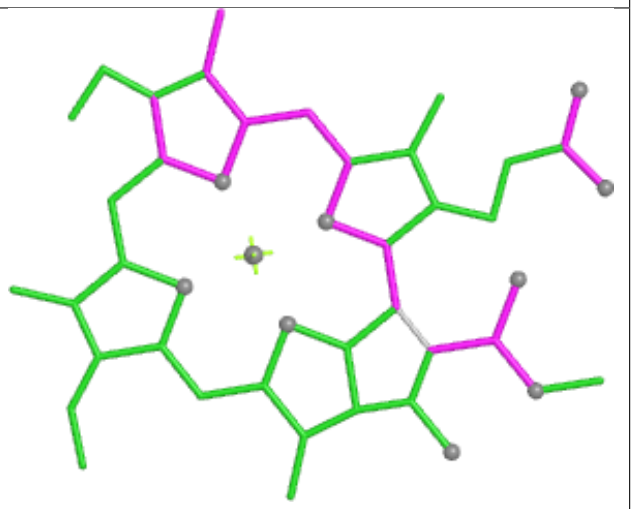


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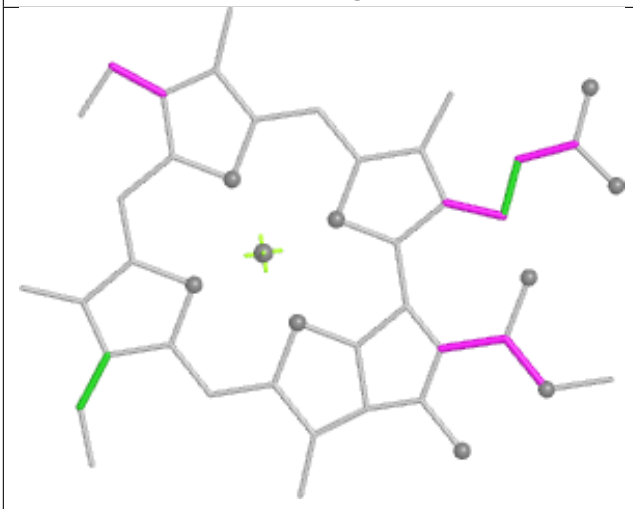
Ligand CLA F2 201



Bond lengths



Bond angles

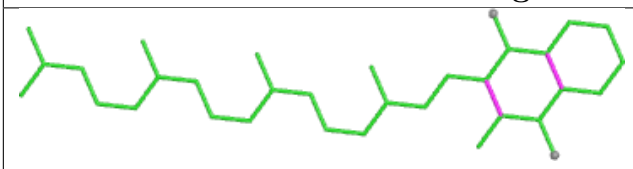


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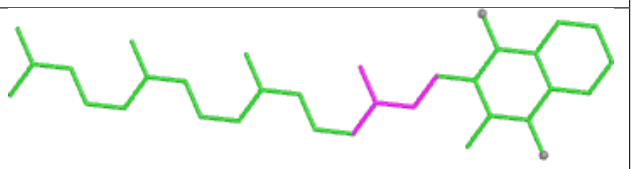


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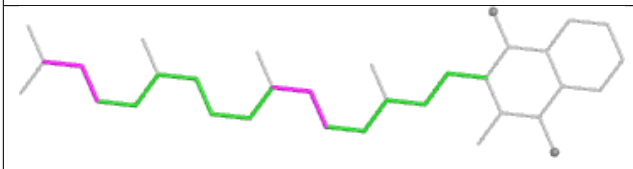
Ligand PQN A2 842



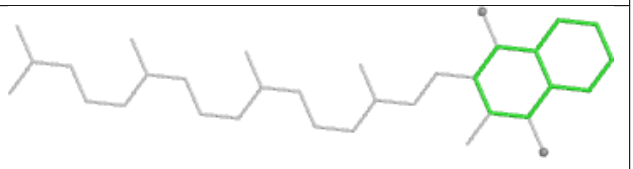
Bond lengths



Bond angles

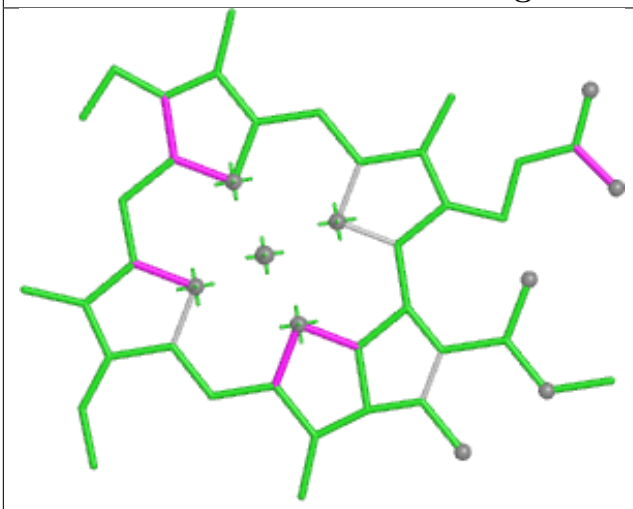


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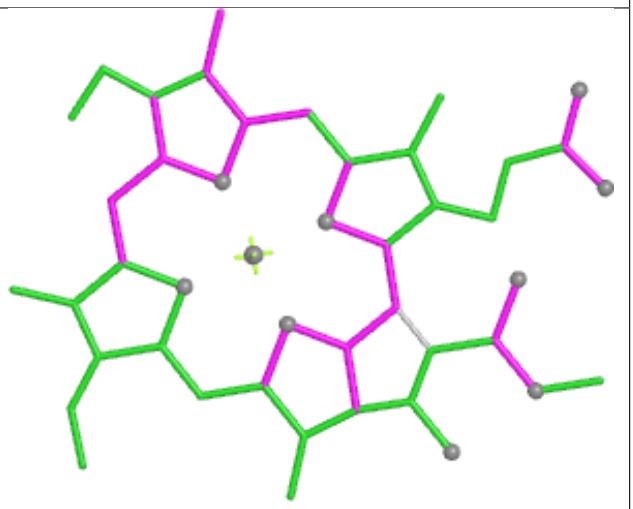


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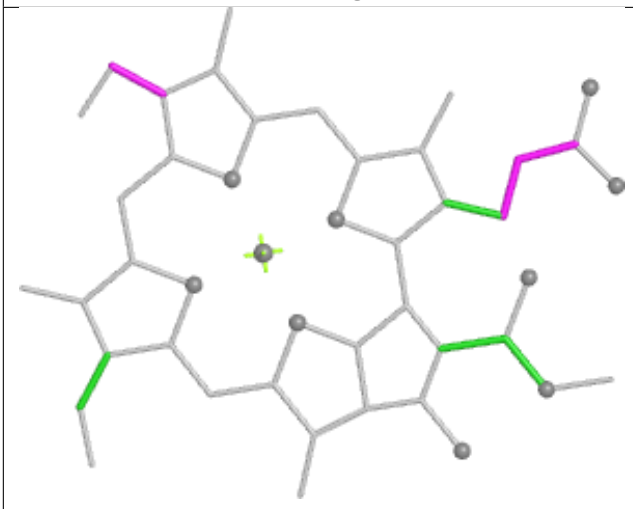
Ligand CLA 3N 308



Bond lengths



Bond angles

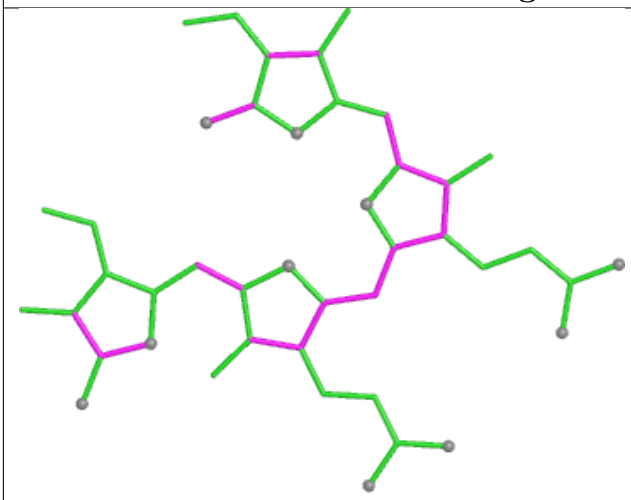


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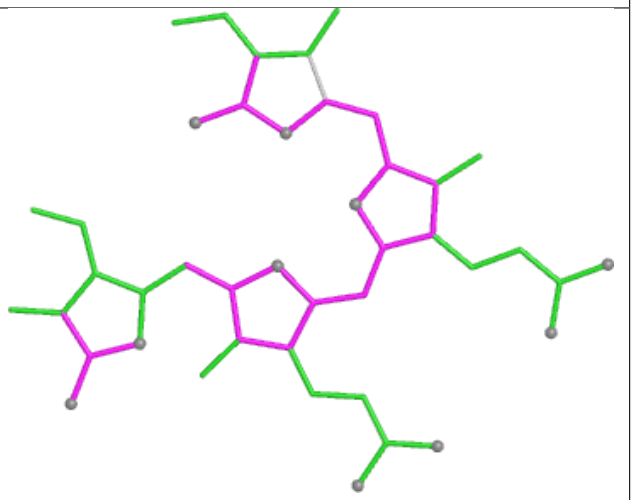


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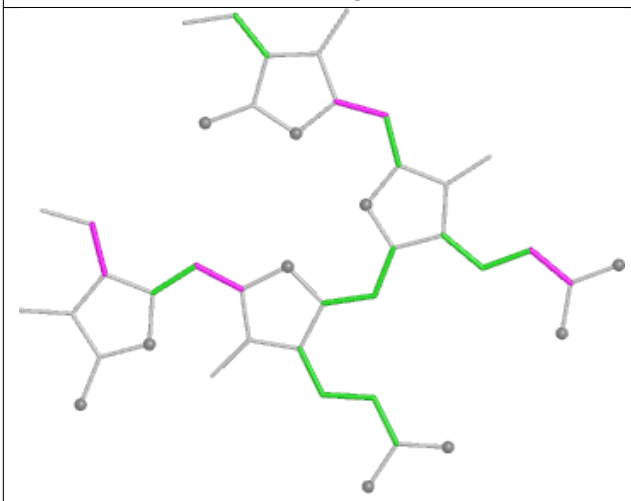
Ligand PEB u8 202



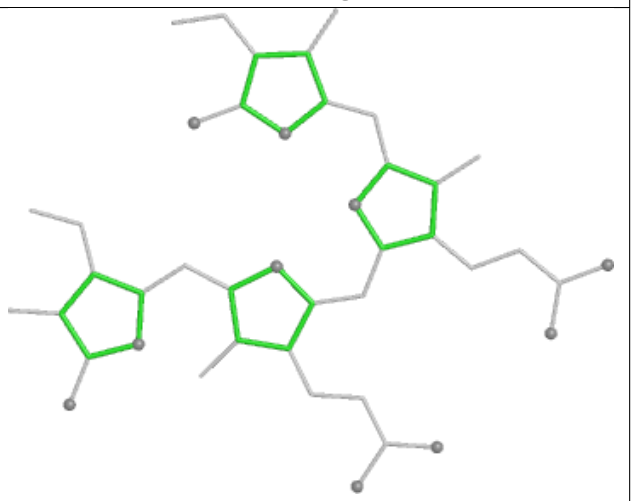
Bond lengths



Bond angles

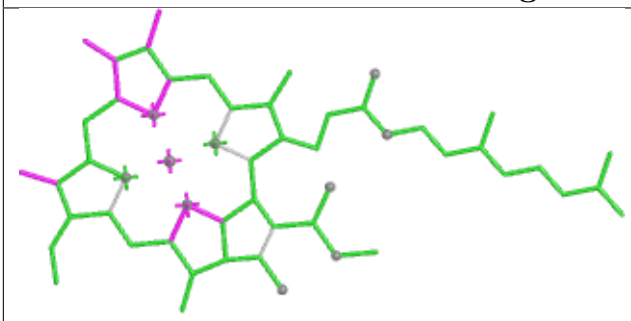


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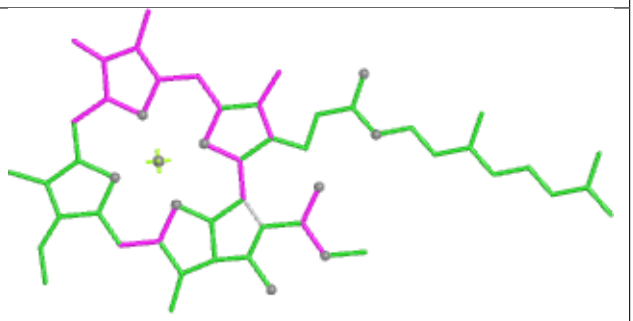


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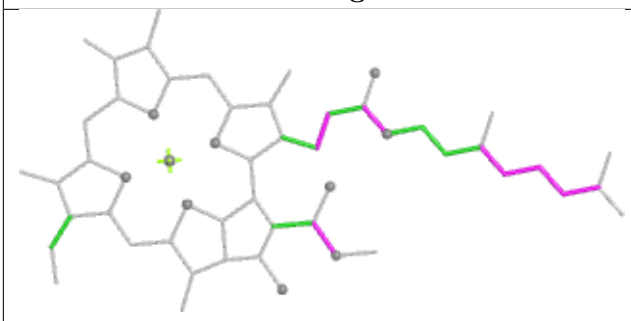
Ligand CLA 22 605



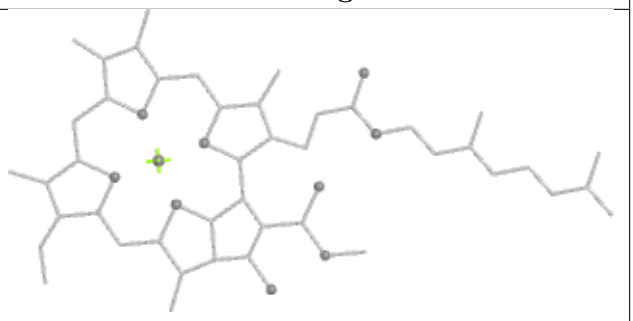
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Bond angles

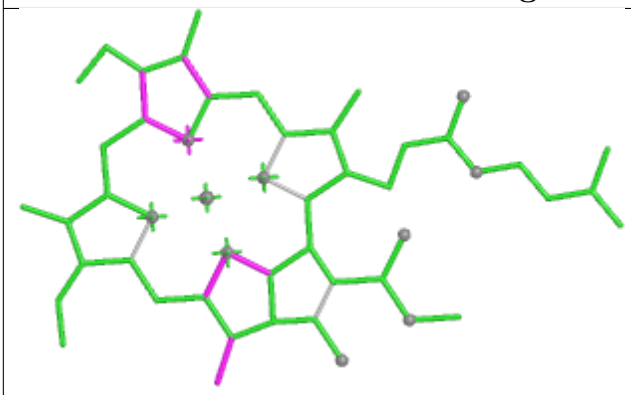


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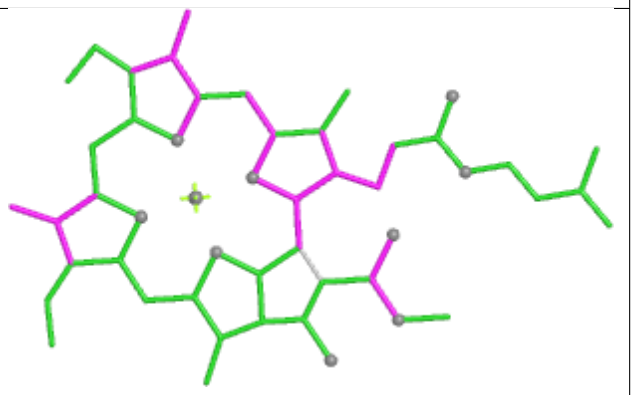


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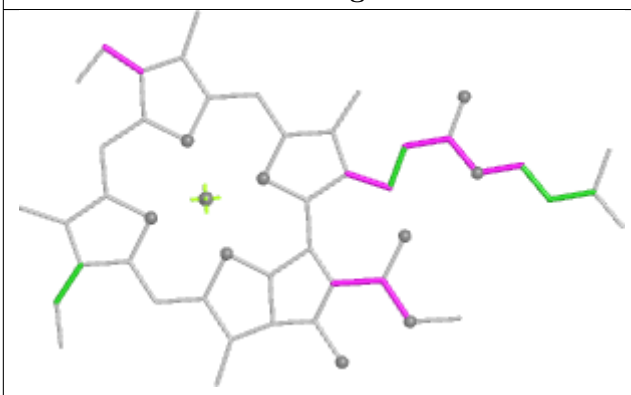
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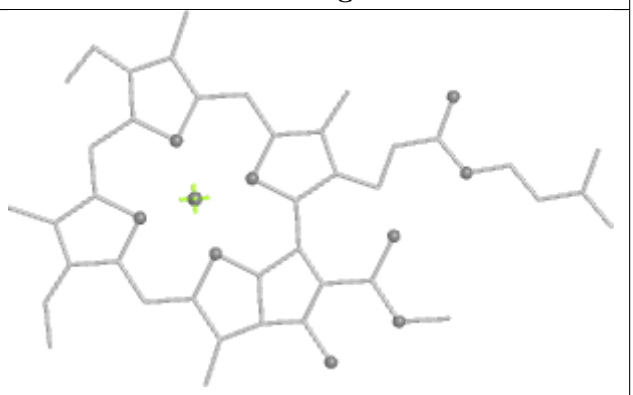
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Bond angles

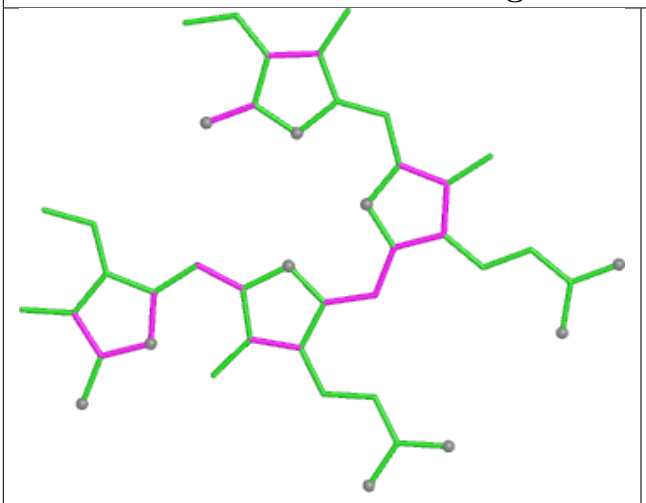


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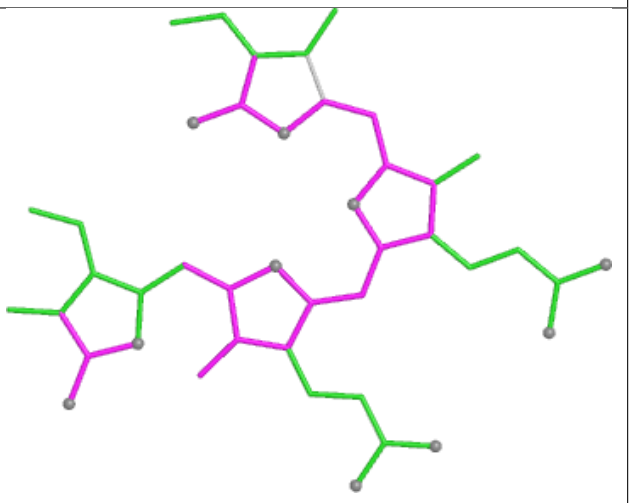


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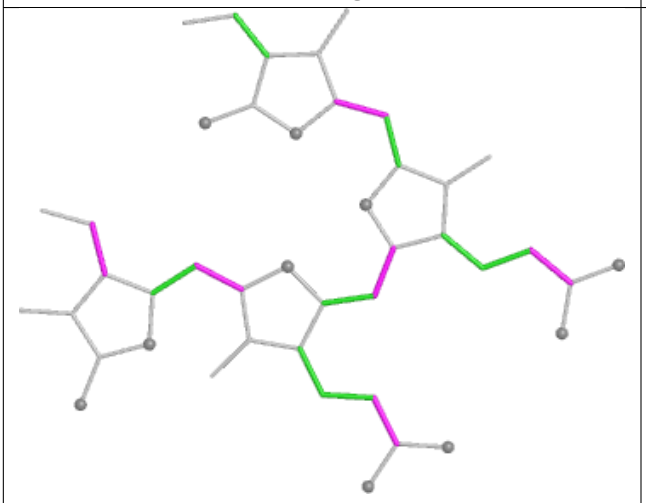
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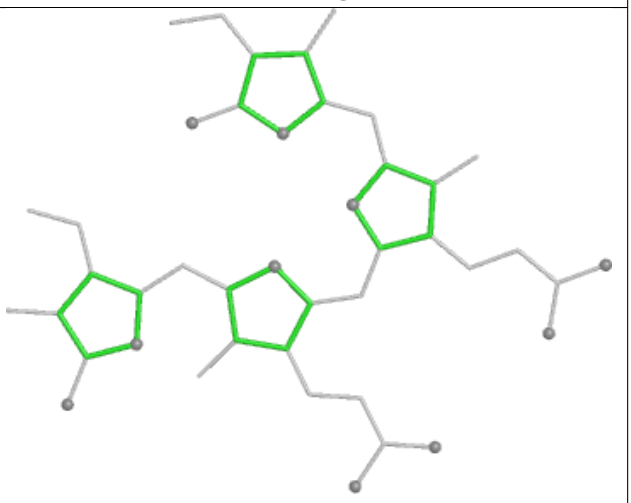
Bond lengths



Bond angles



Torsions

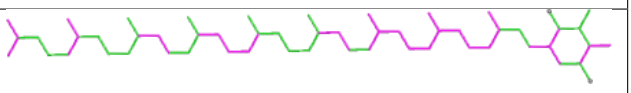


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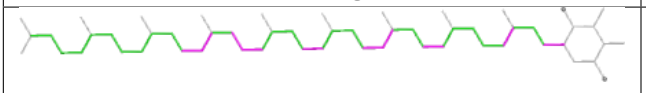
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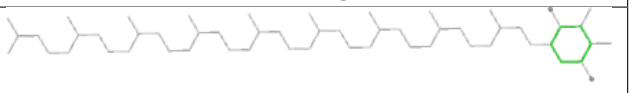
Bond lengths



Bond angles

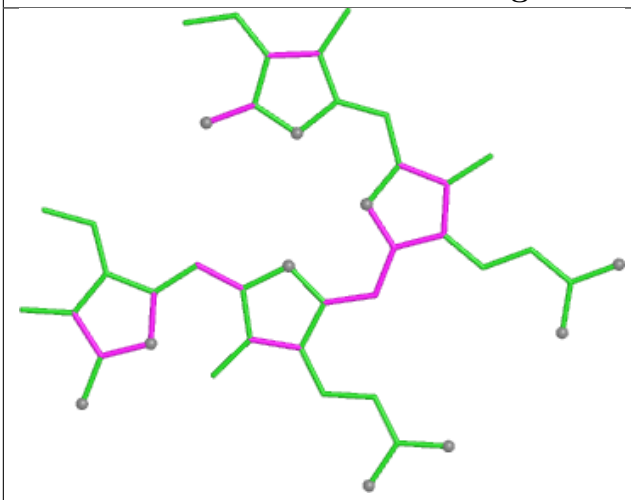


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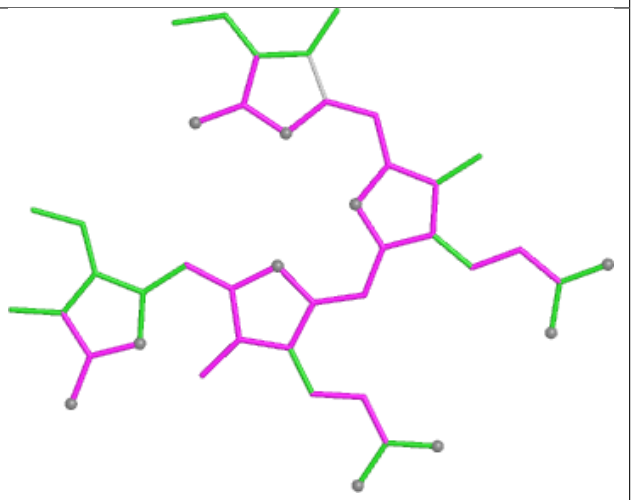


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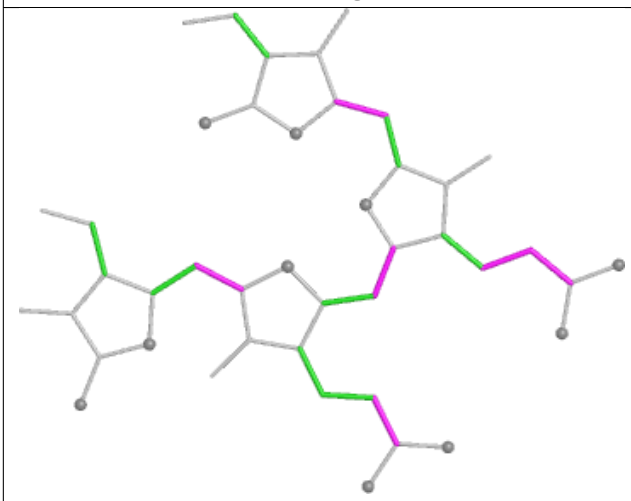
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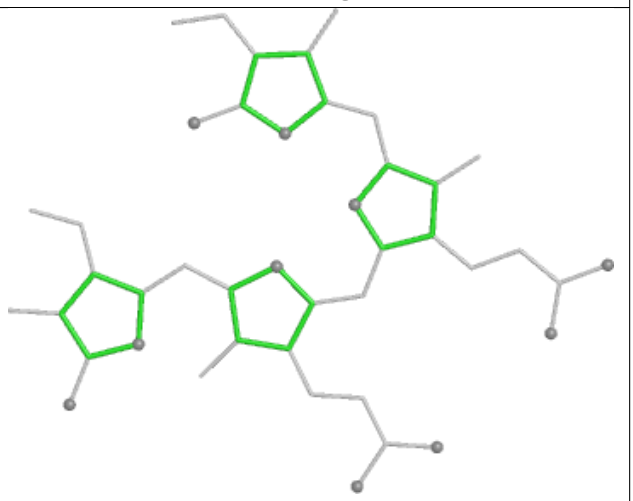
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Bond angles

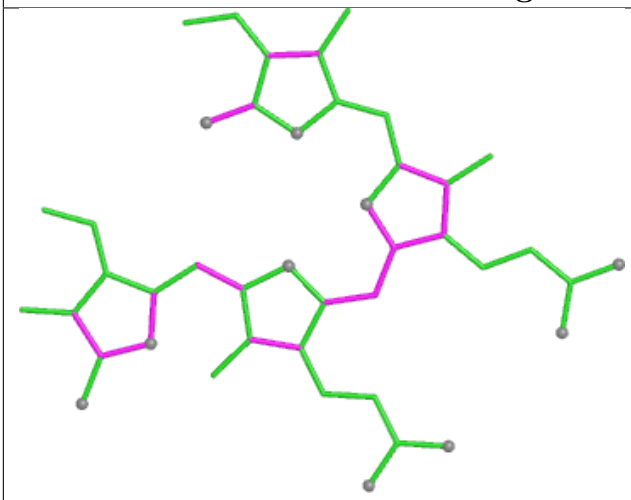


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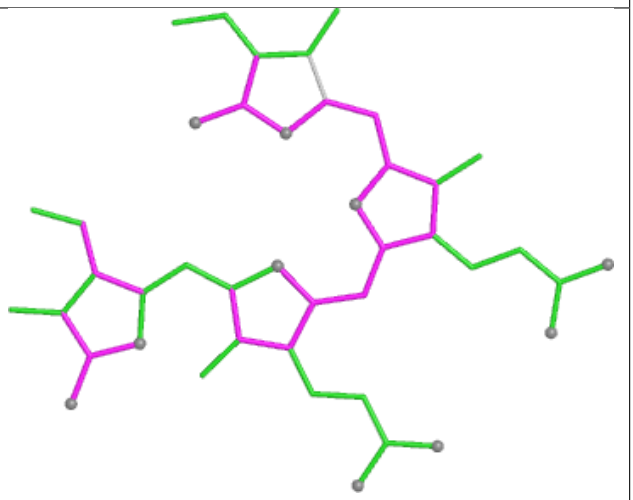


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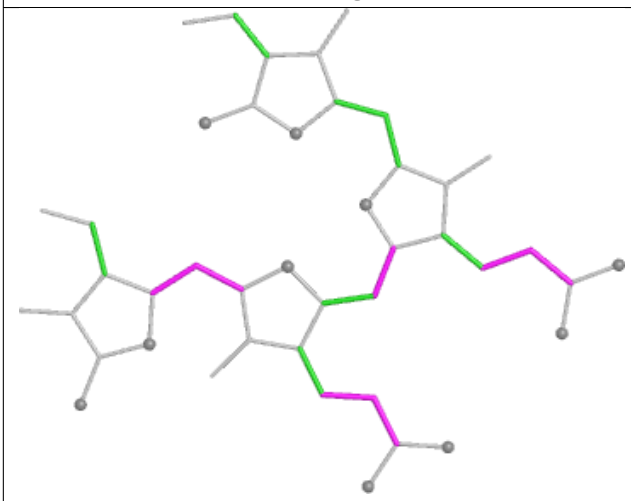
Ligand PEB C5 202



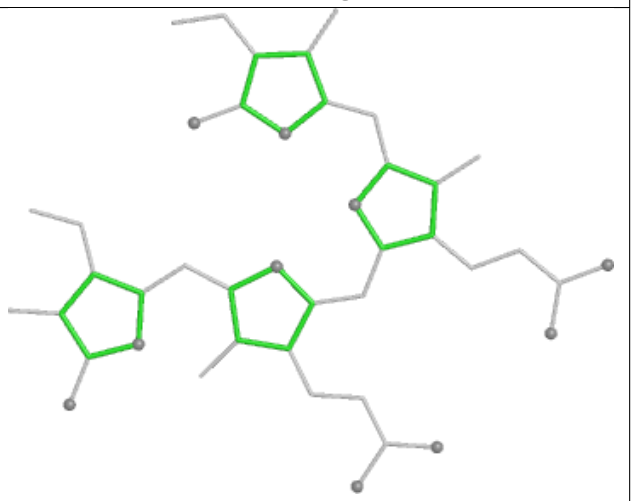
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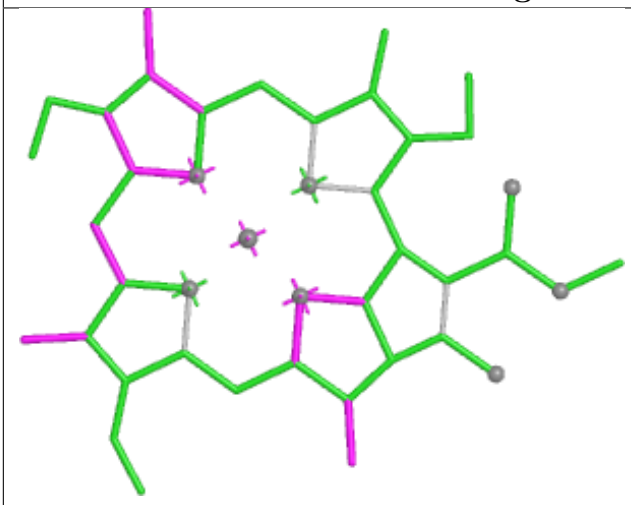


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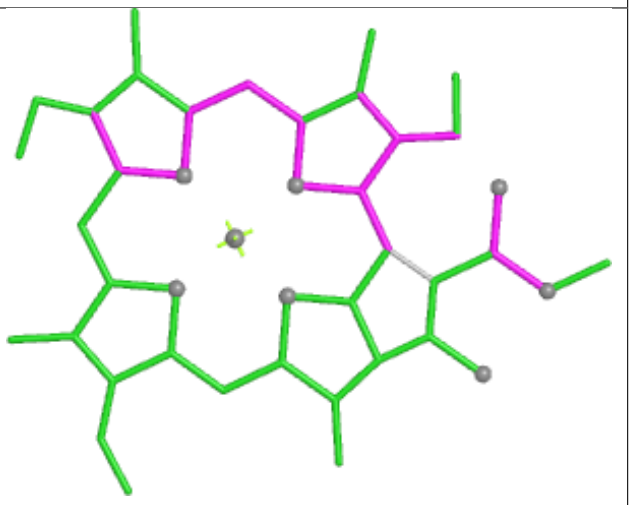


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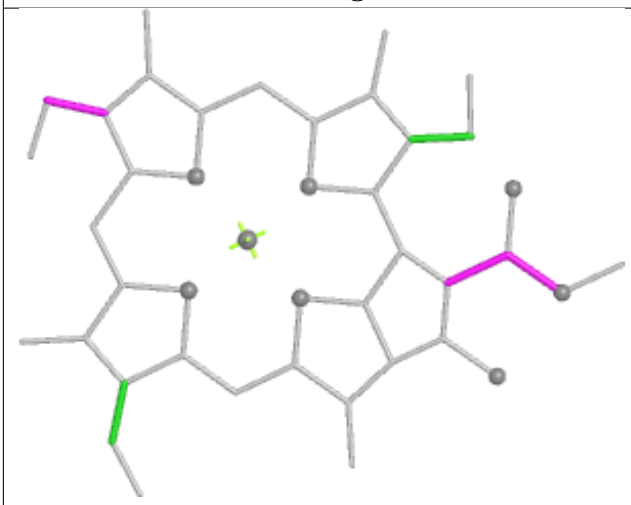
Ligand CLA JN 101



Bond lengths



Bond angles



Torsions

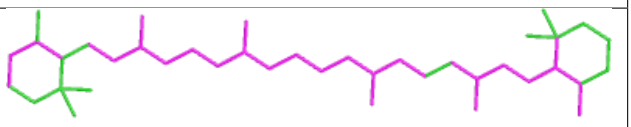


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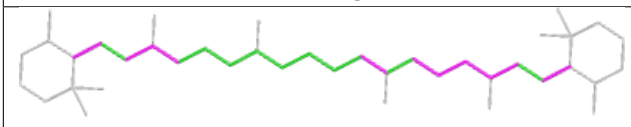
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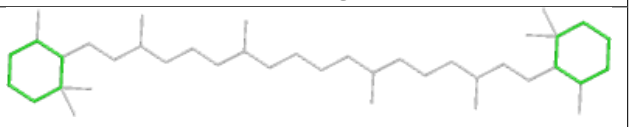
Bond lengths



Bond angles

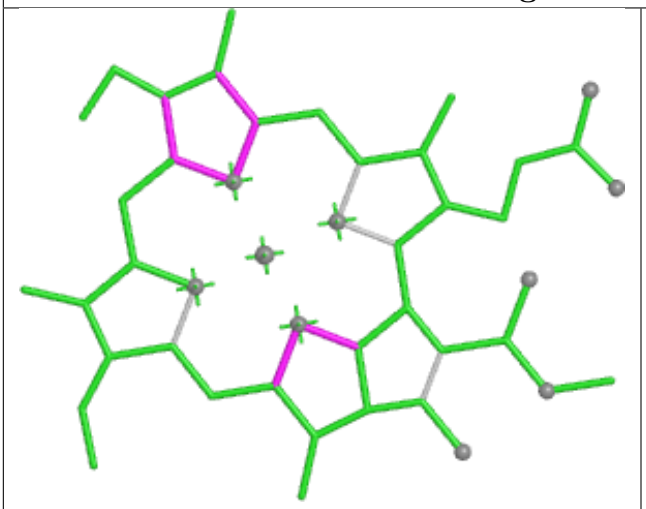


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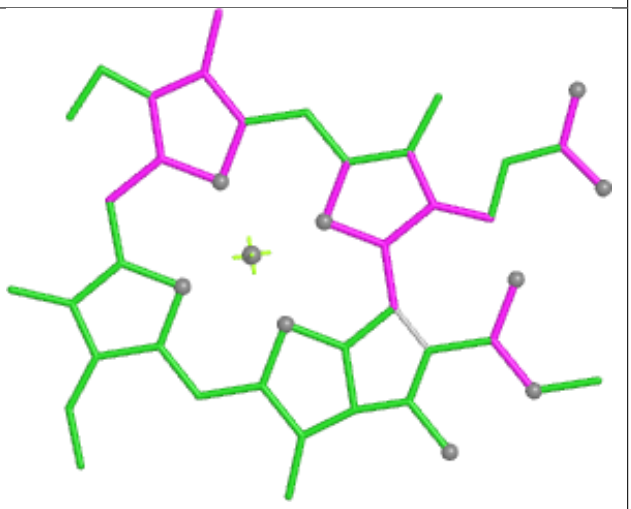


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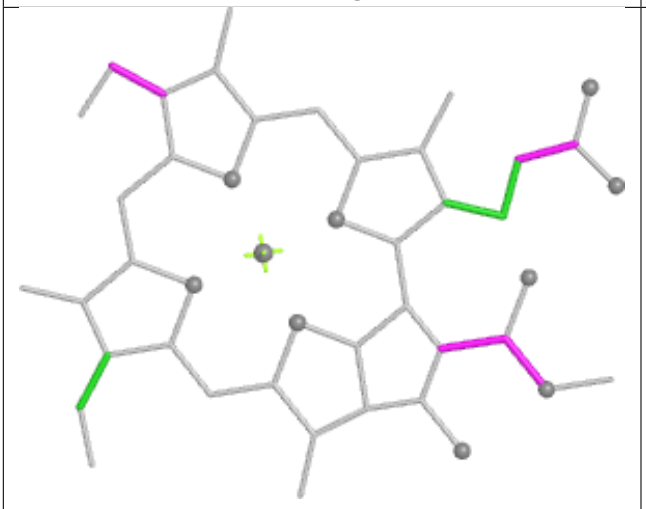
Ligand CLA 32 303



Bond lengths



Bond angles

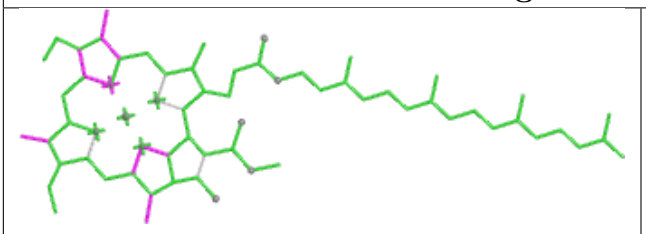


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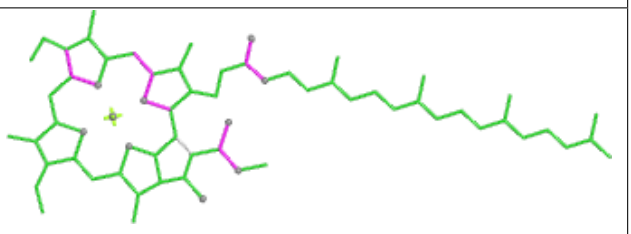


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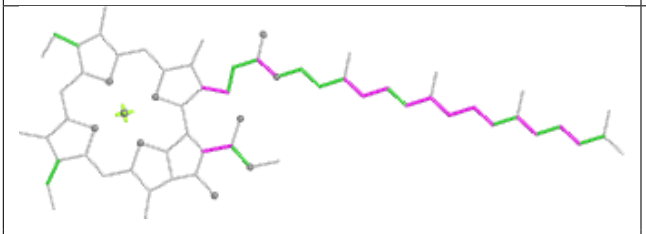
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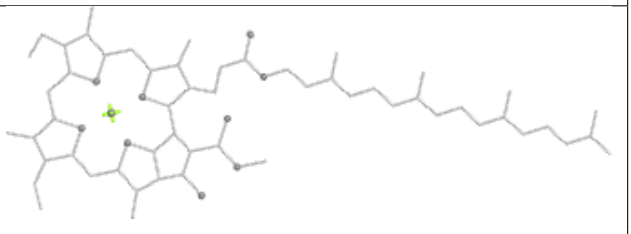
Bond lengths



Bond angles

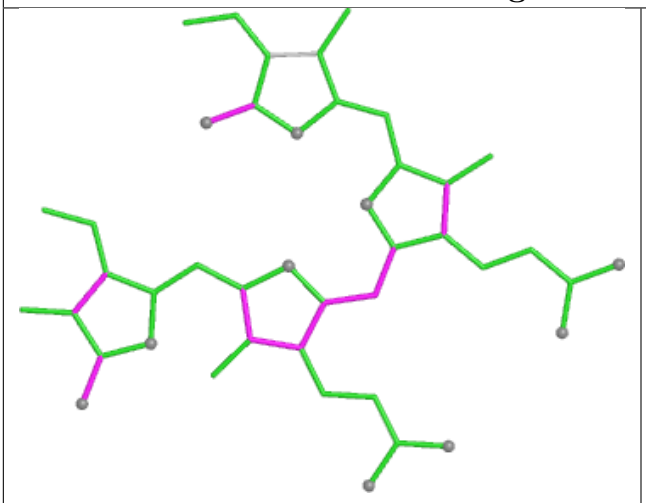


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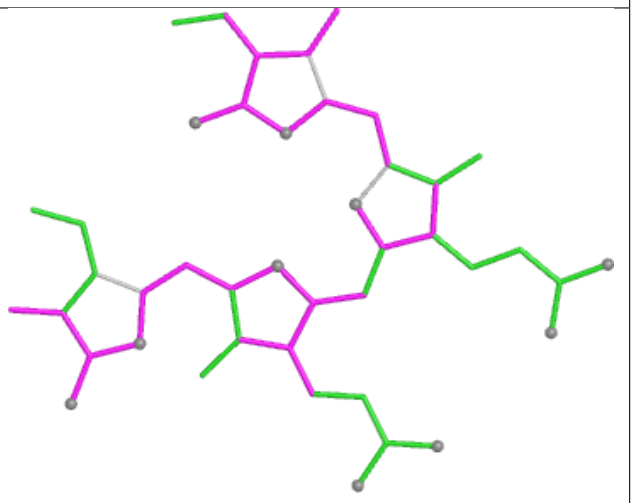


Rings

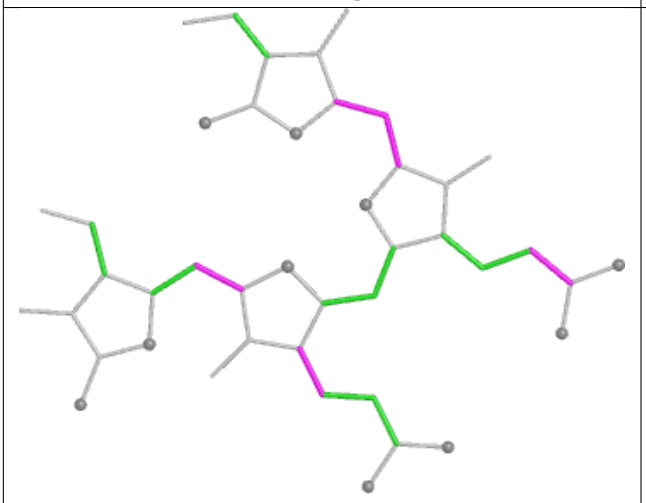
Ligand PUB AD 302



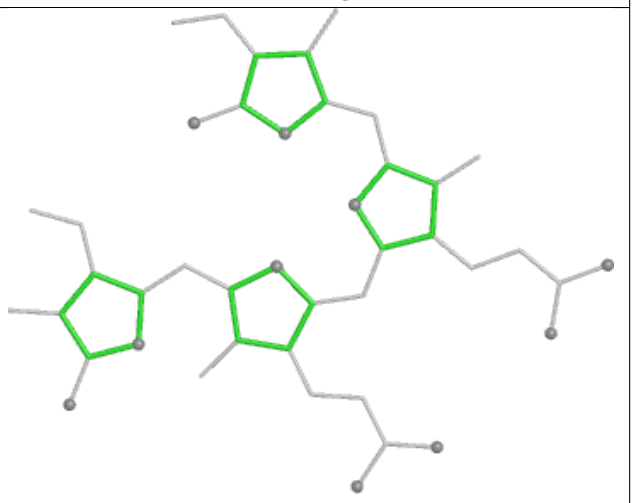
Bond lengths



Bond angles

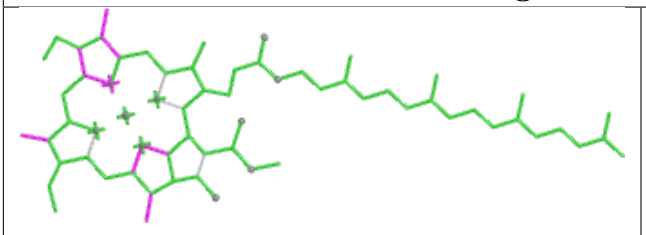


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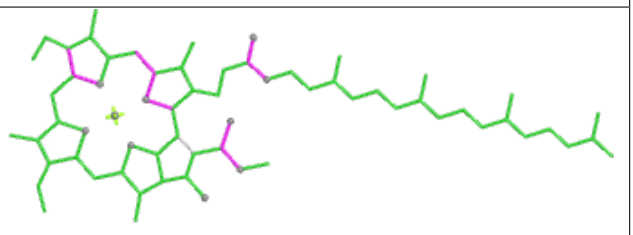


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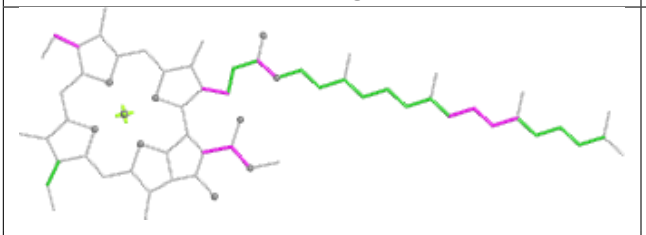
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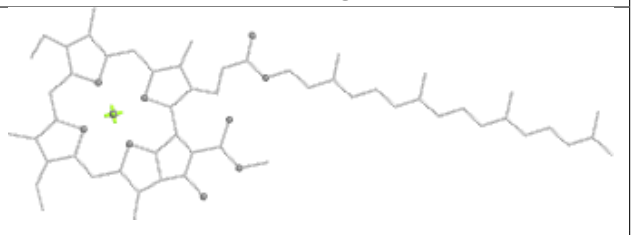
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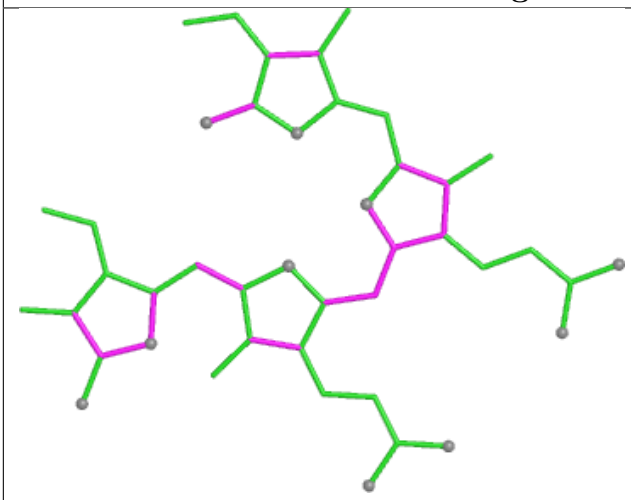


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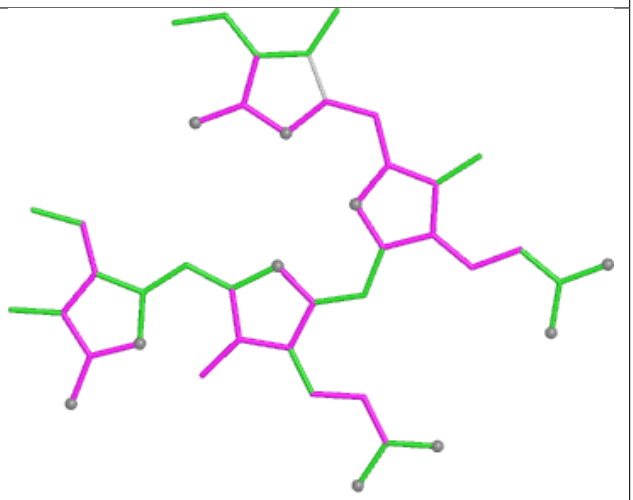


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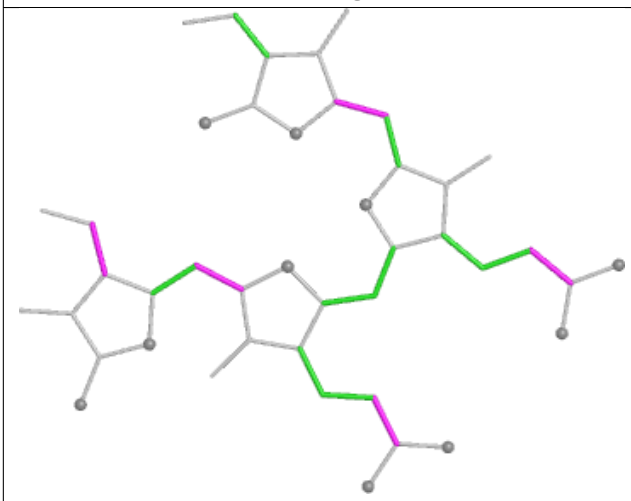
Ligand PEB AB 501



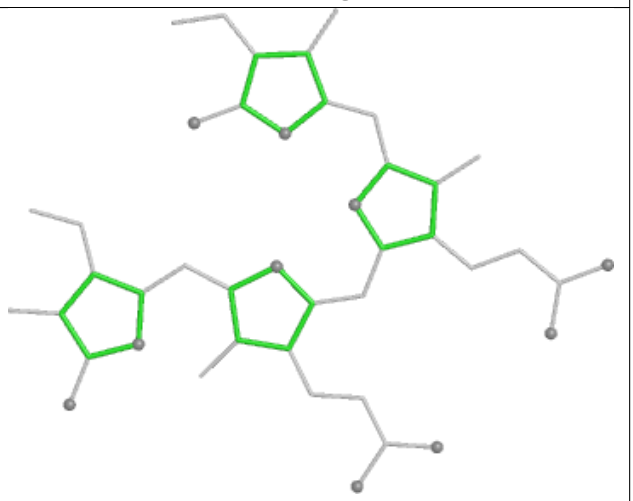
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Bond angles

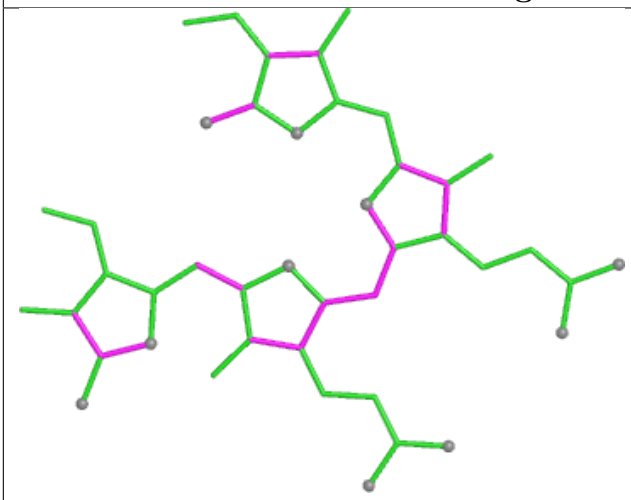


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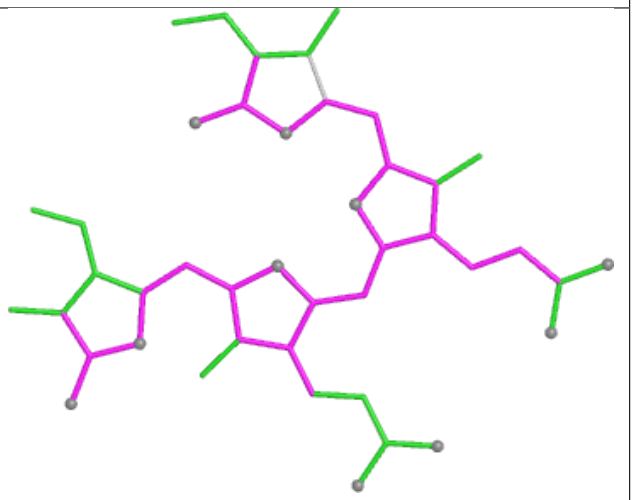


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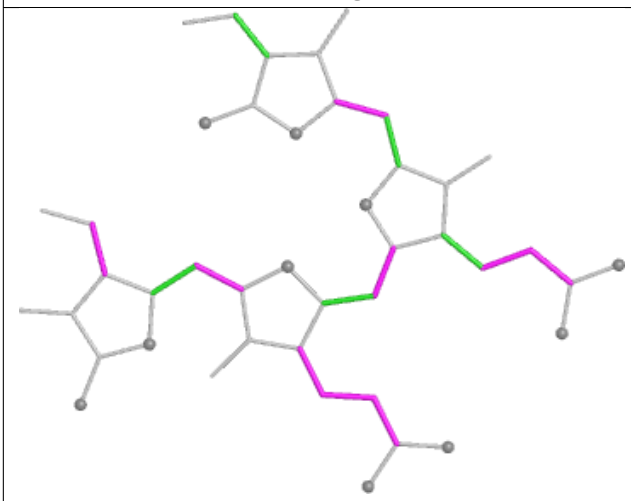
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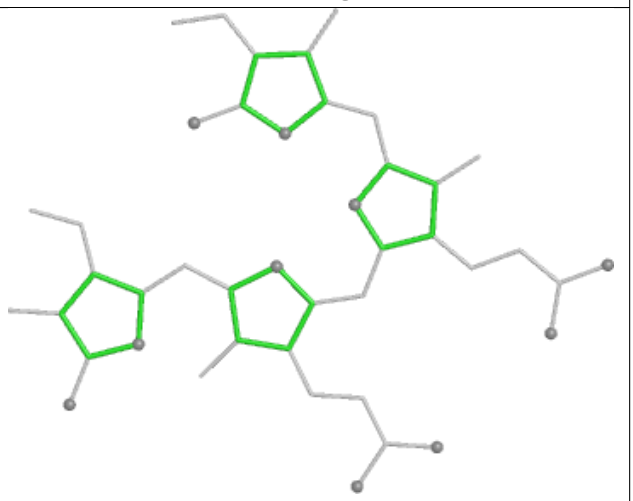
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Bond angles

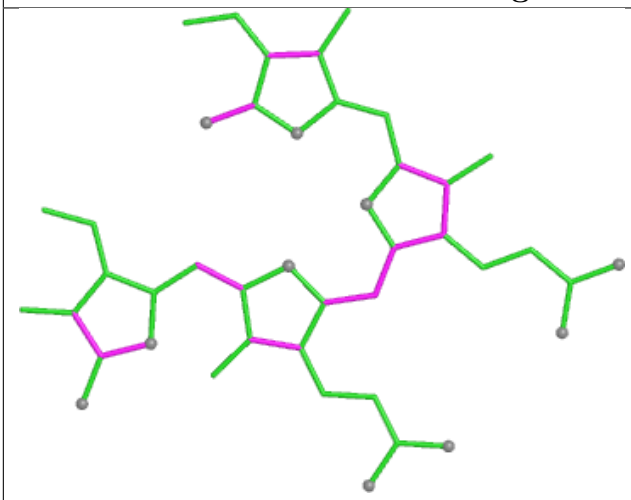


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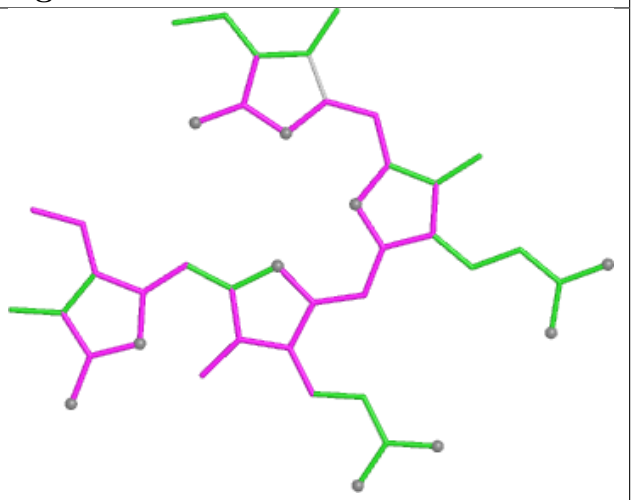


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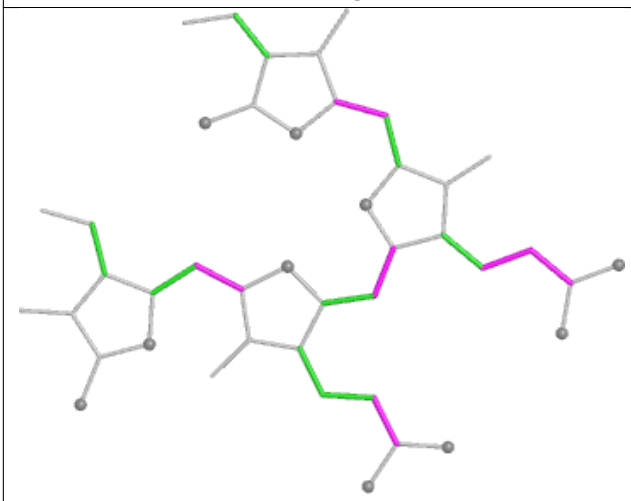
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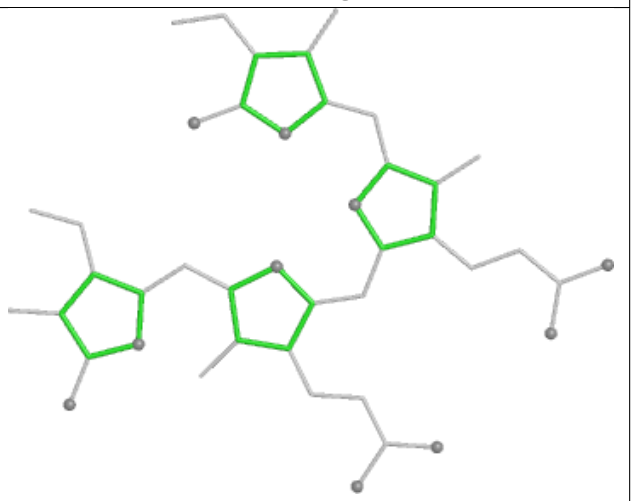
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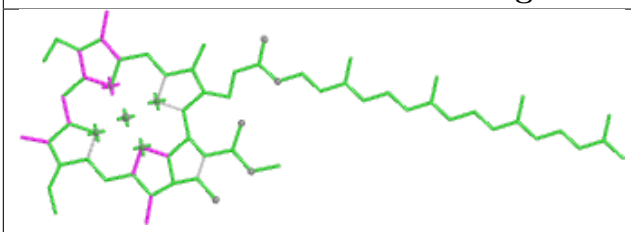


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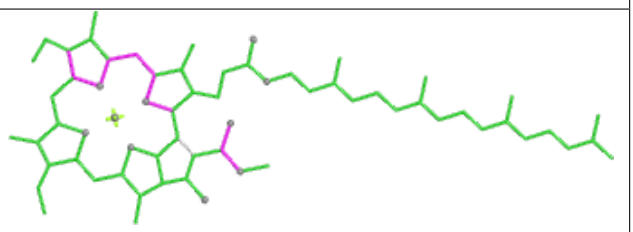


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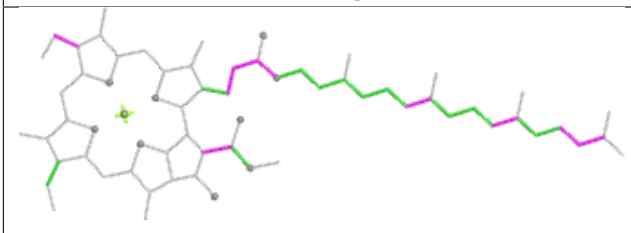
Ligand CLA B6 613



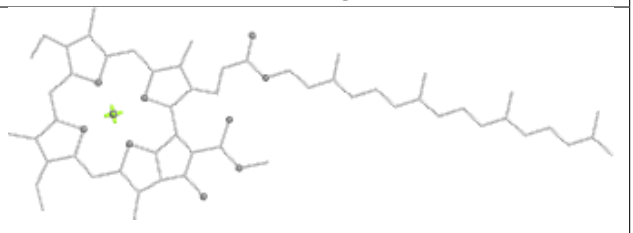
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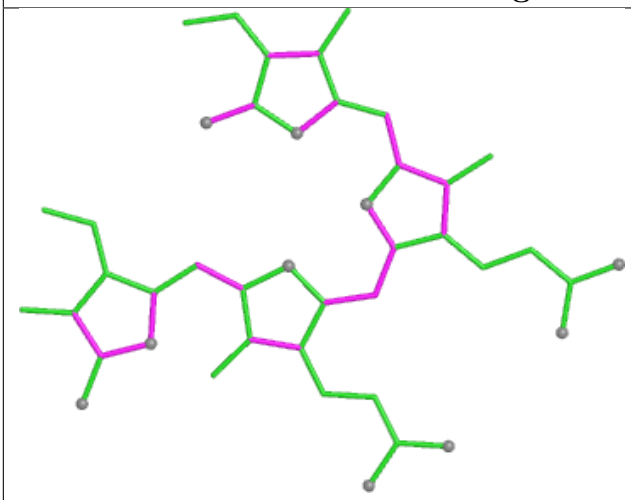


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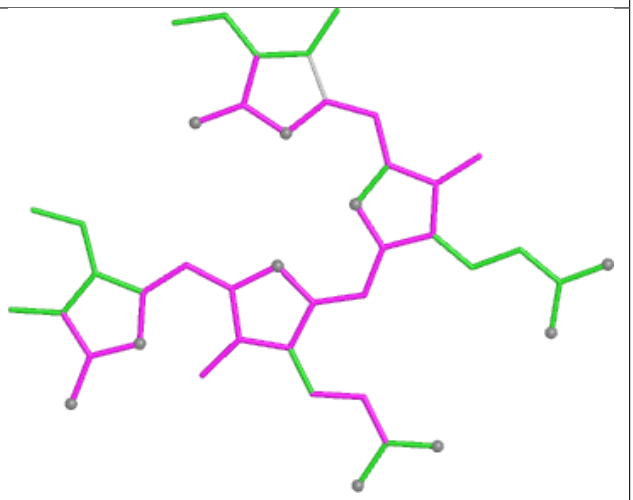


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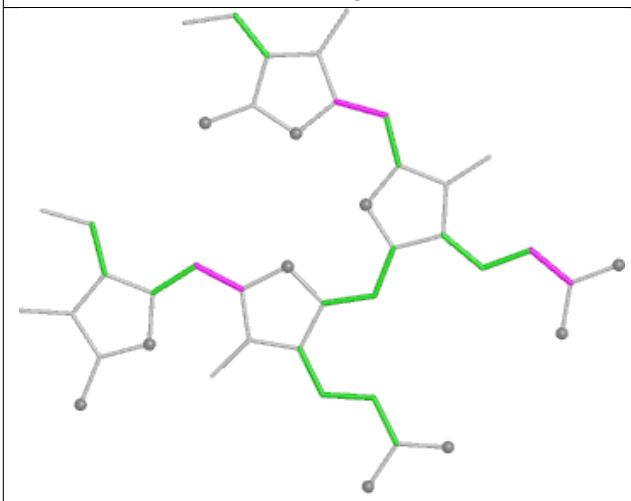
Ligand PEB eM 201



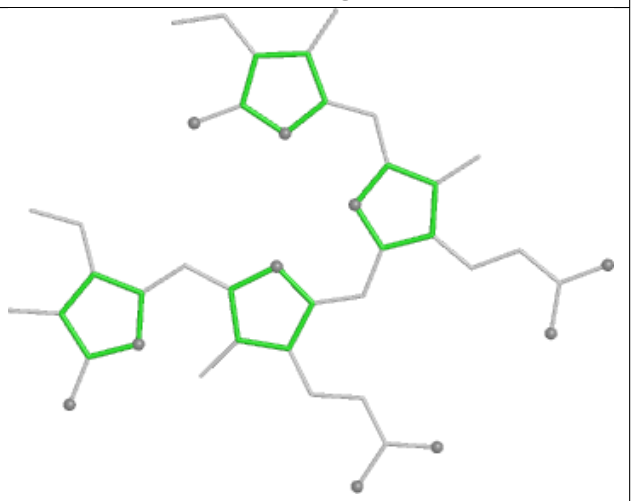
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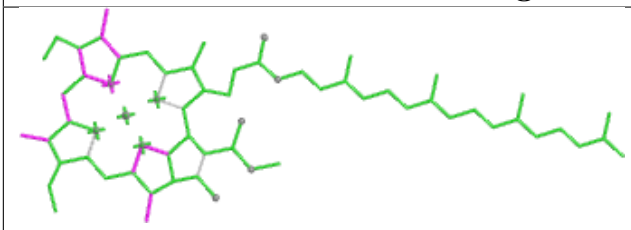


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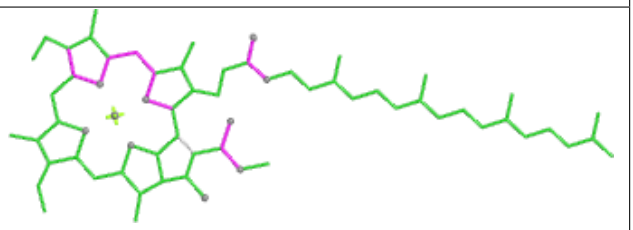


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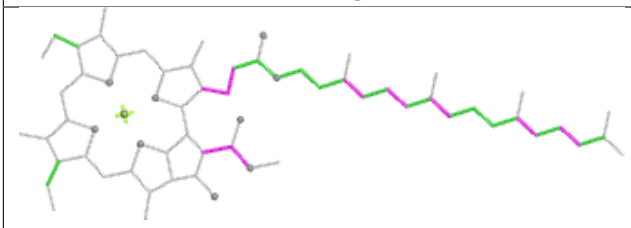
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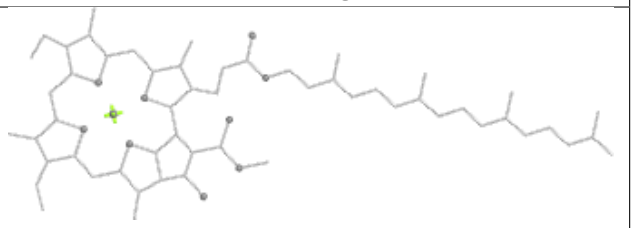
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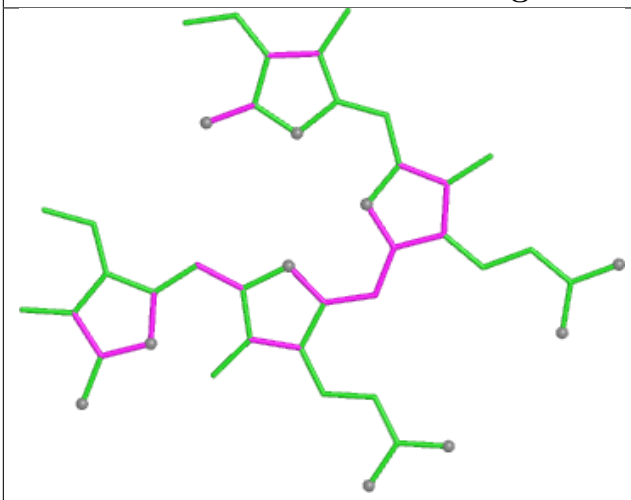


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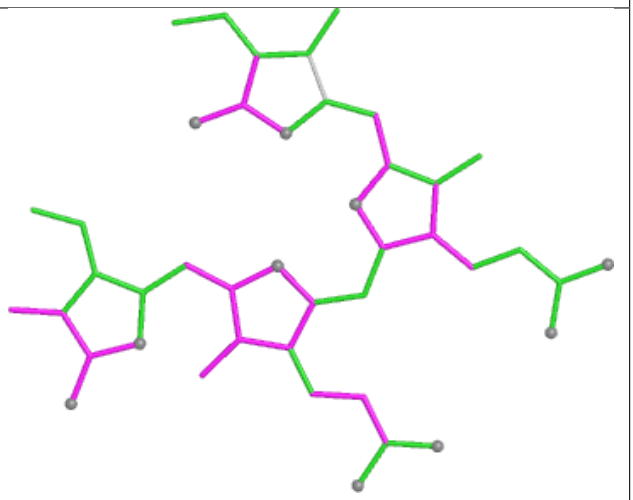


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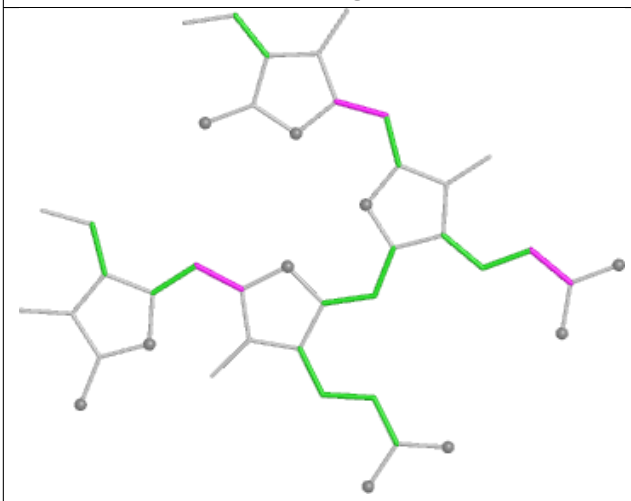
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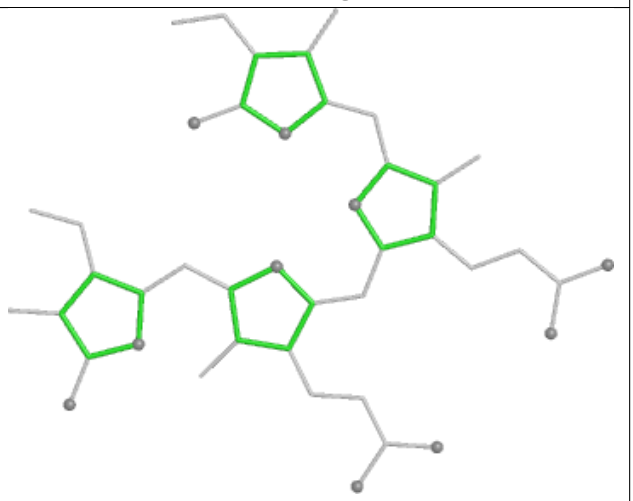
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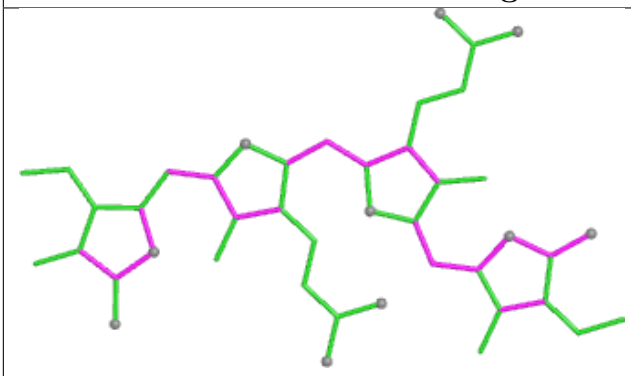


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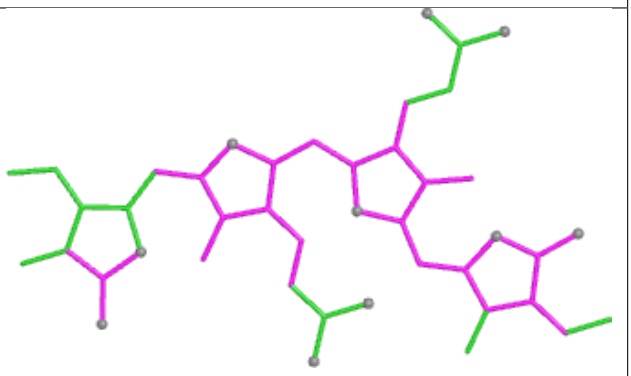


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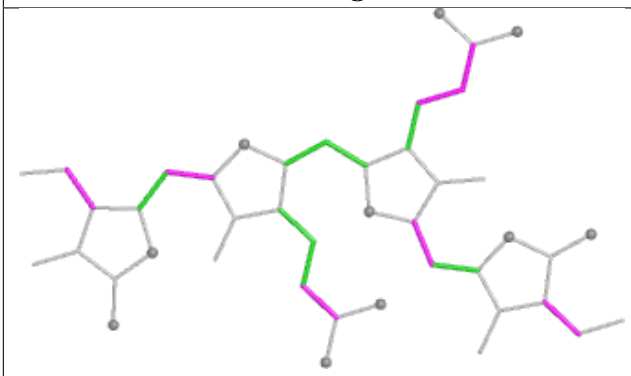
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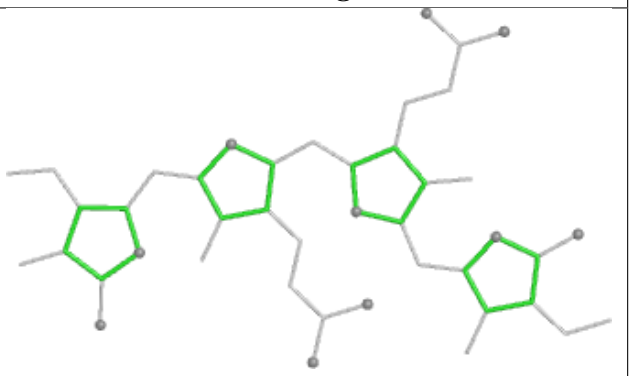
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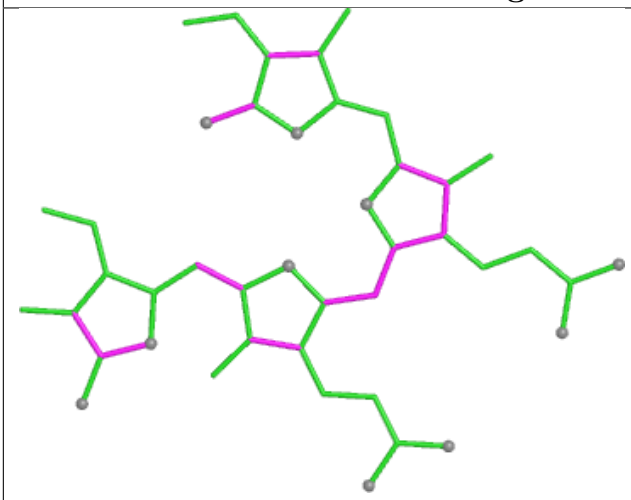


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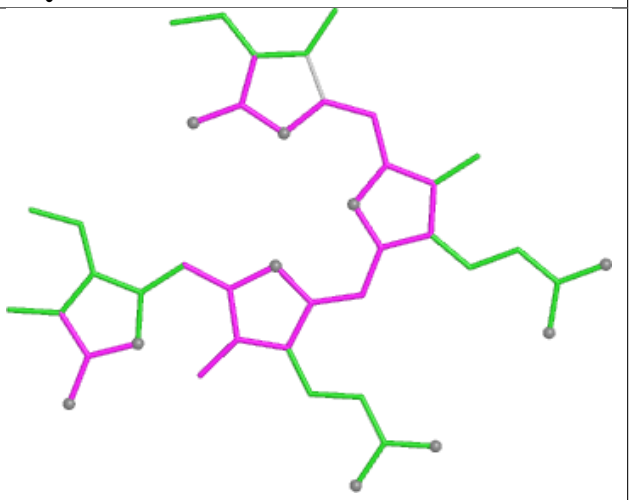


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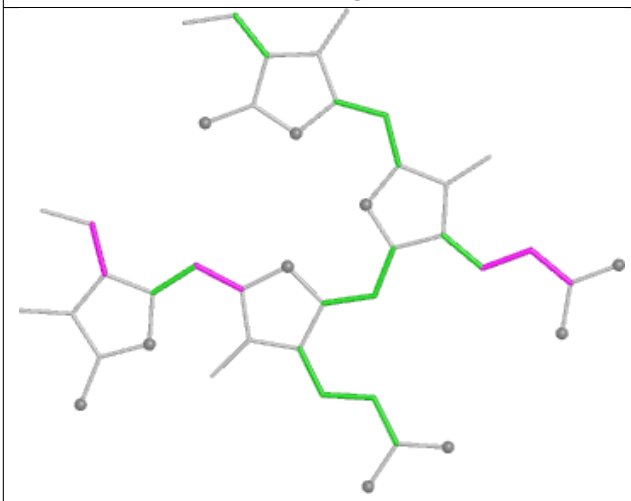
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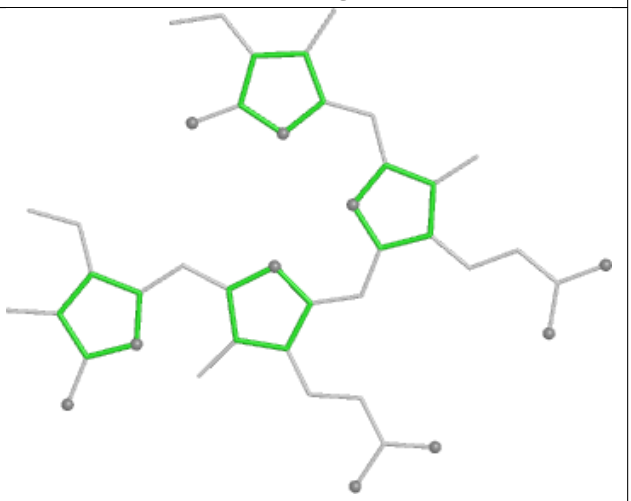
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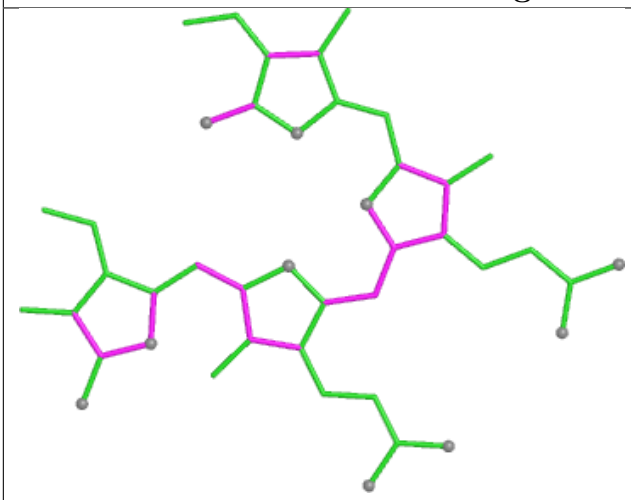


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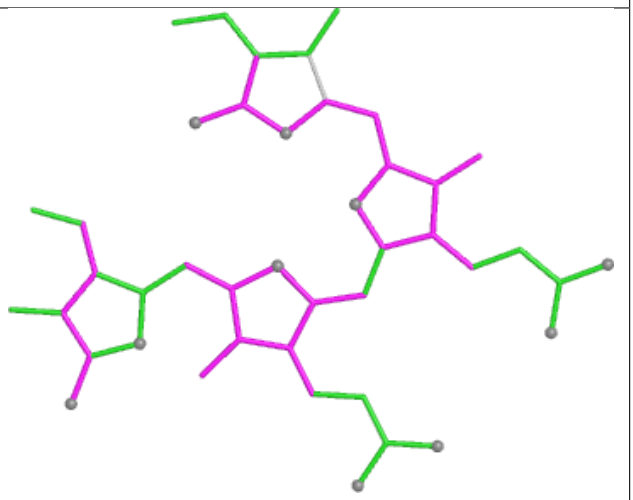


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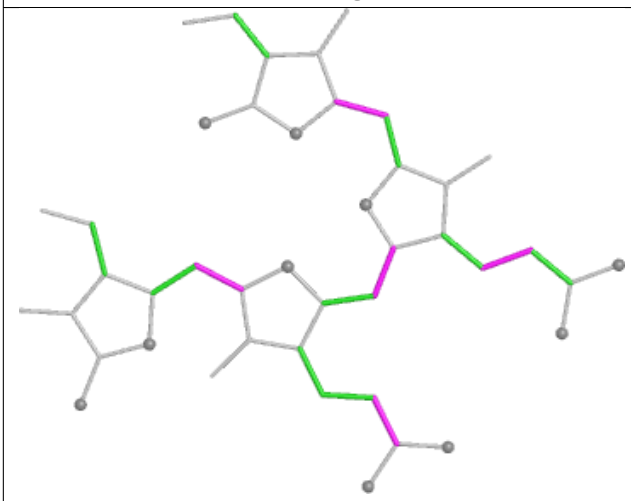
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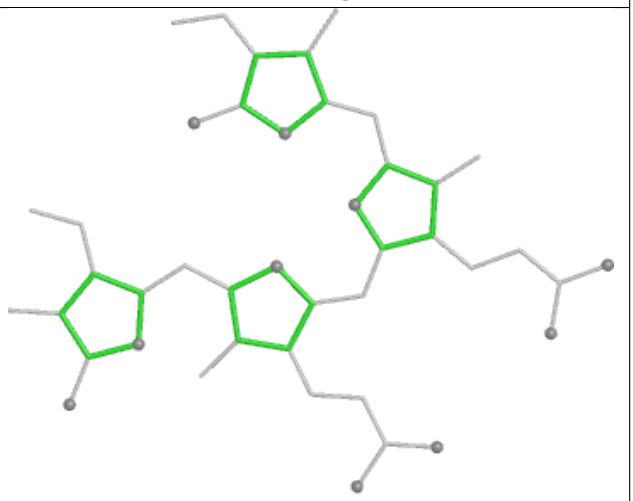
Bond lengths



Bond angles



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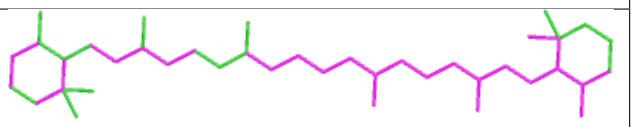


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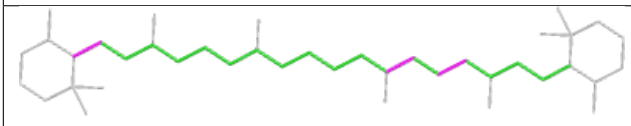
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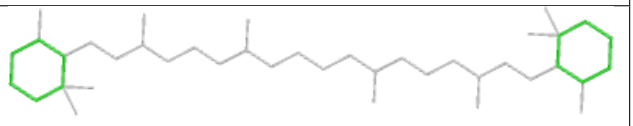
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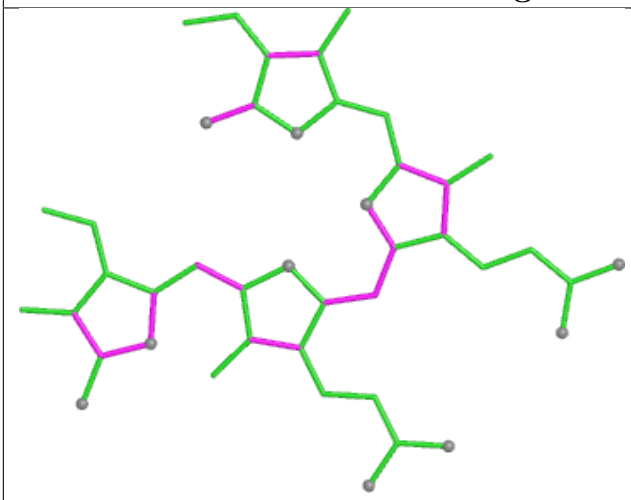


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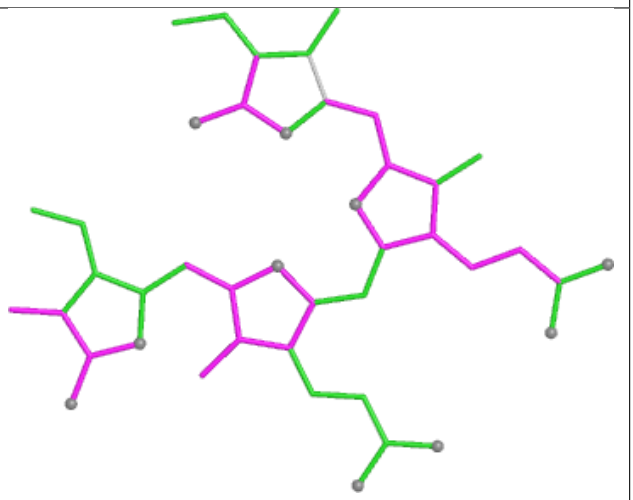


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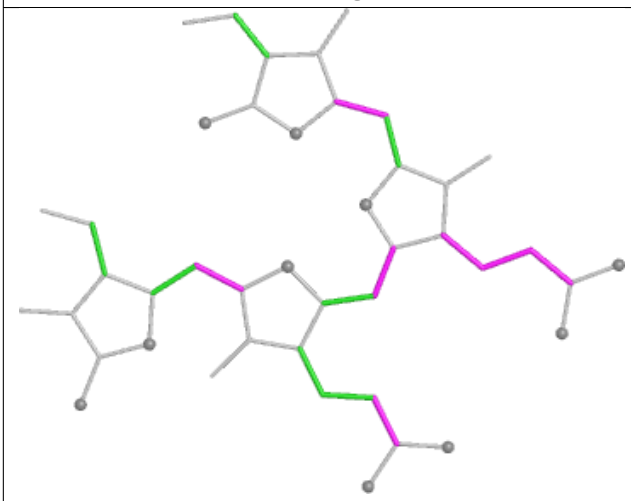
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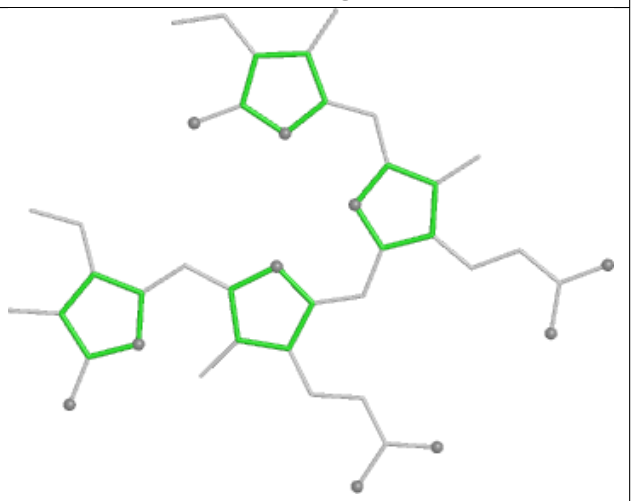
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Bond angles

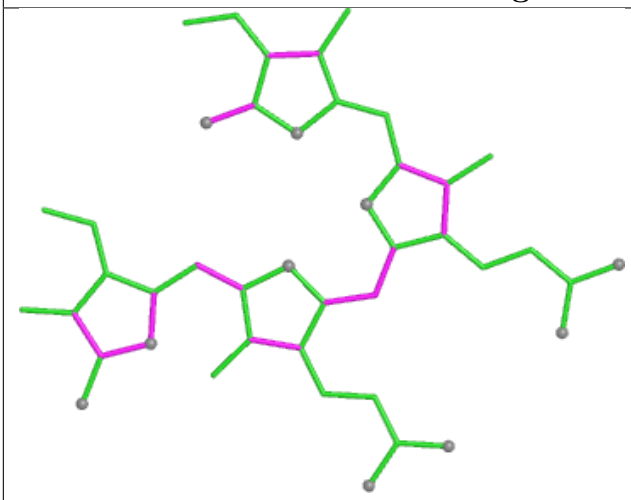


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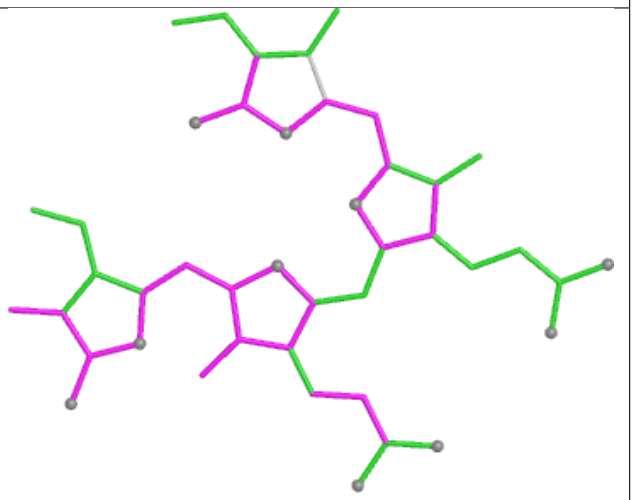


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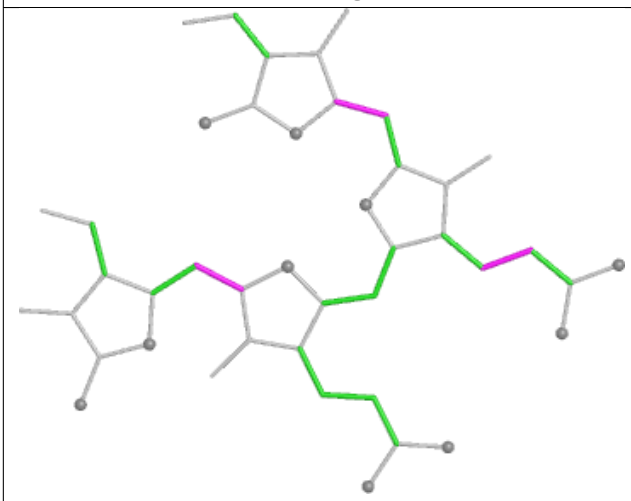
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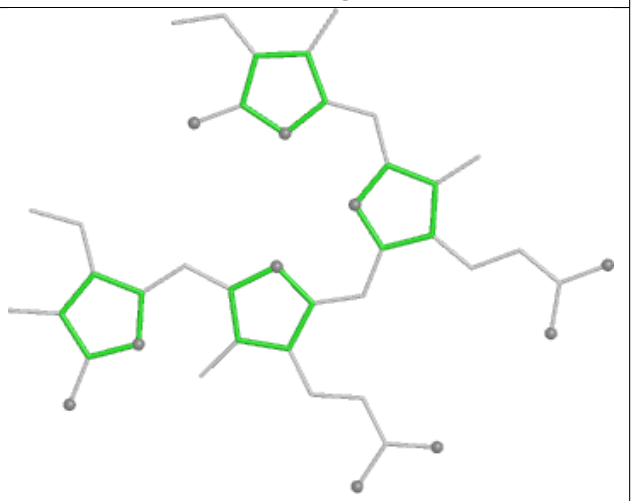
Bond lengths



Bond angles

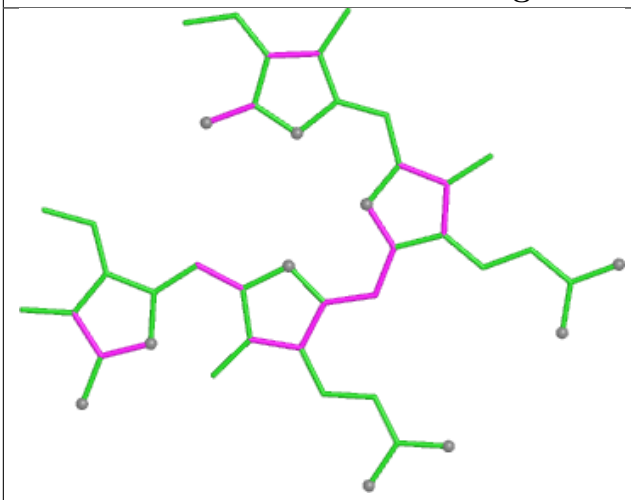


Torsions

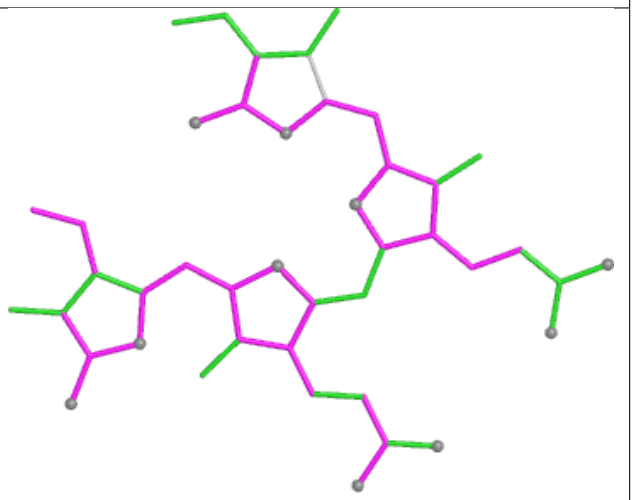


Rings

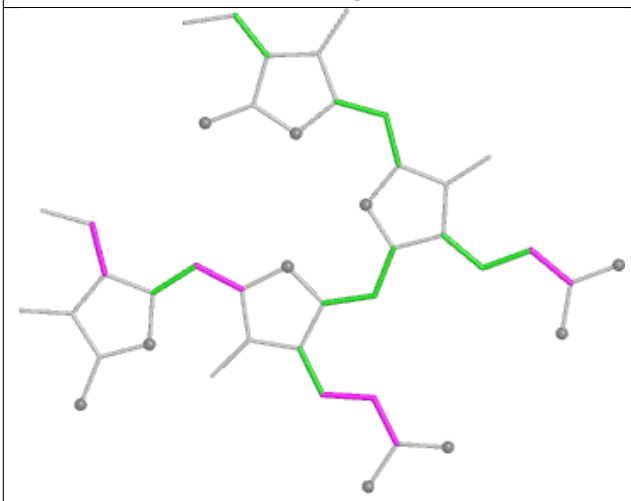
Ligand PEB LK 201



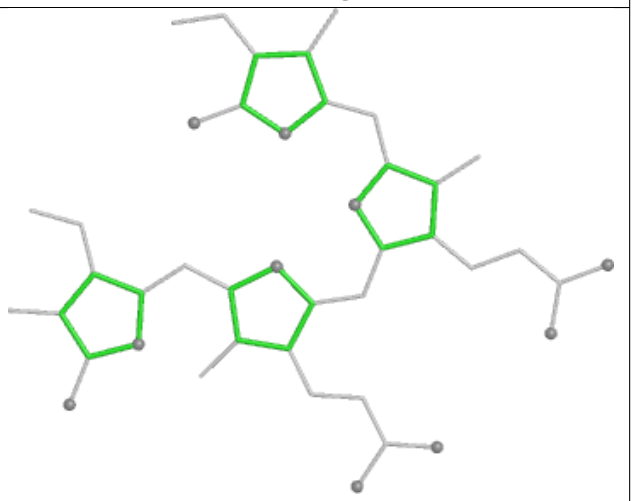
Bond lengths



Bond angles

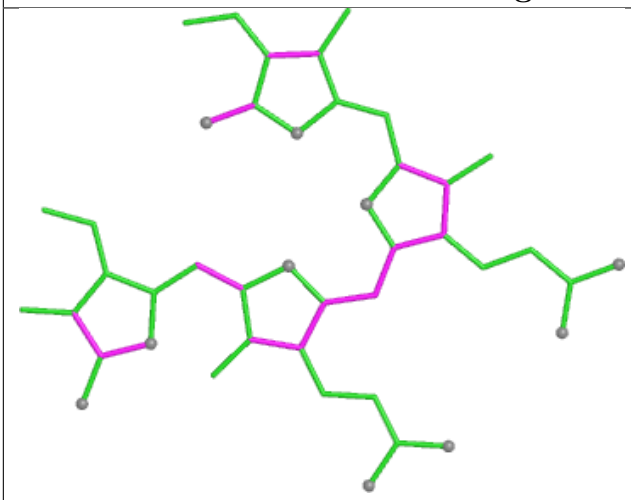


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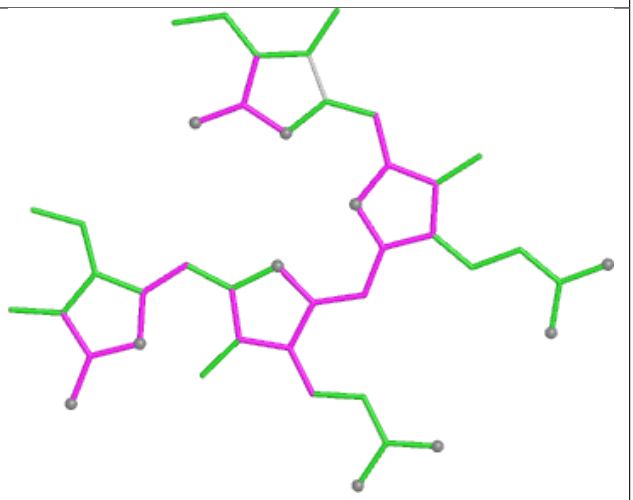


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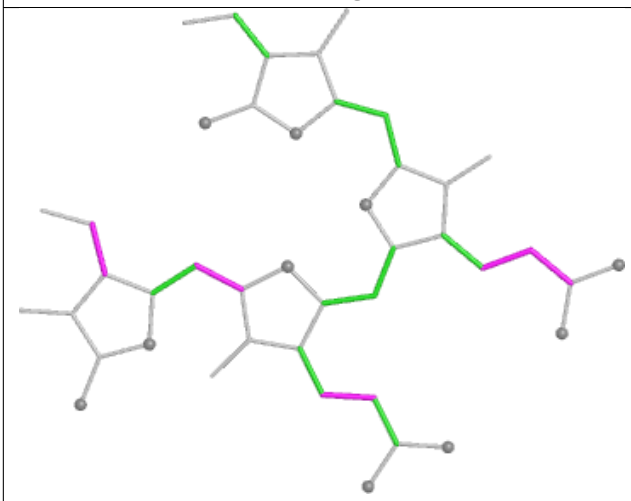
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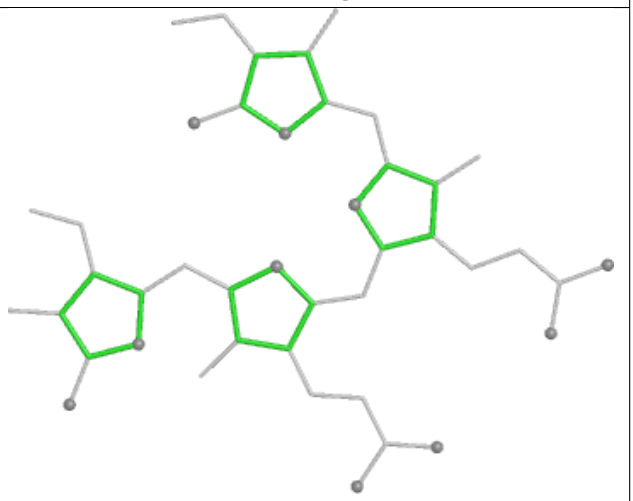
Bond lengths



Bond angles

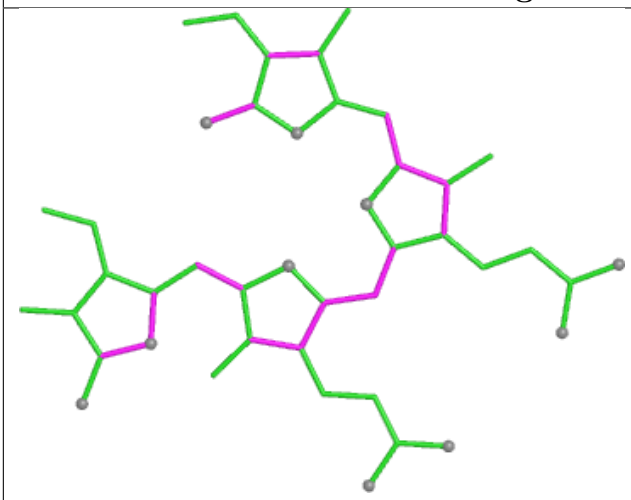


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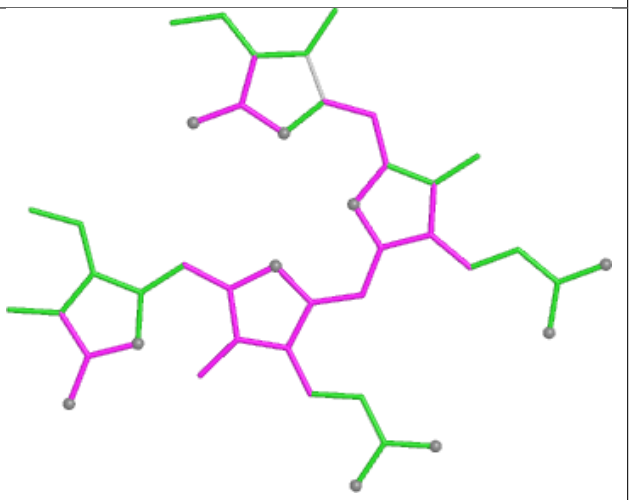


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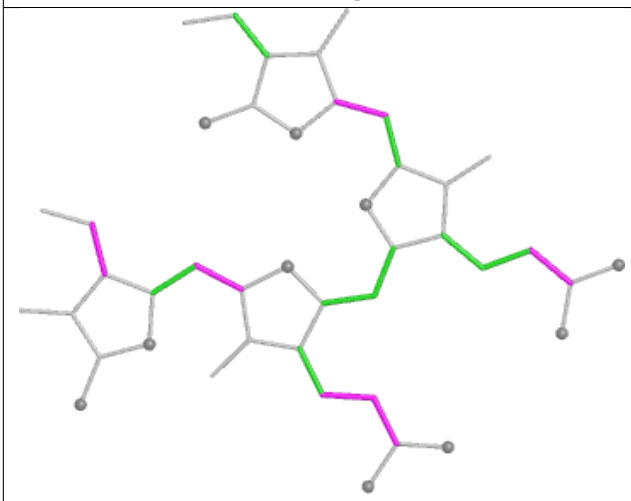
Ligand PEB cK 201



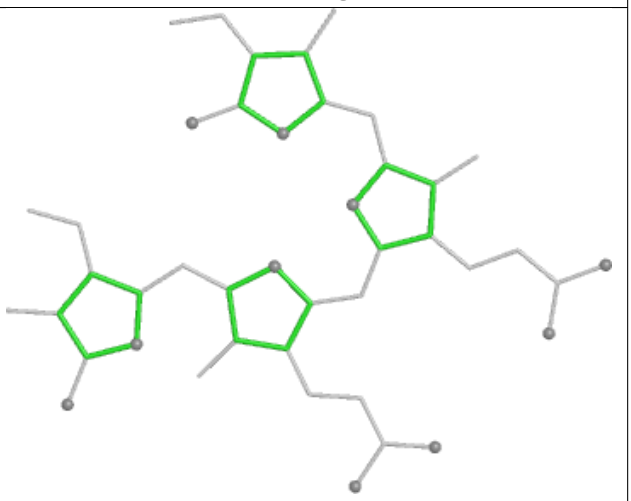
Bond lengths



Bond angles

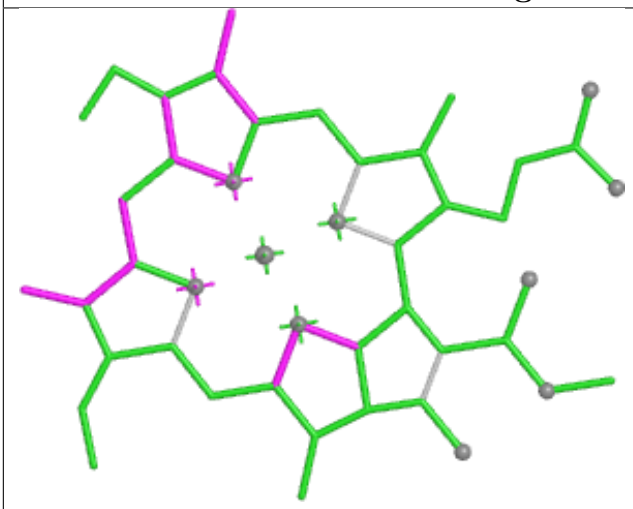


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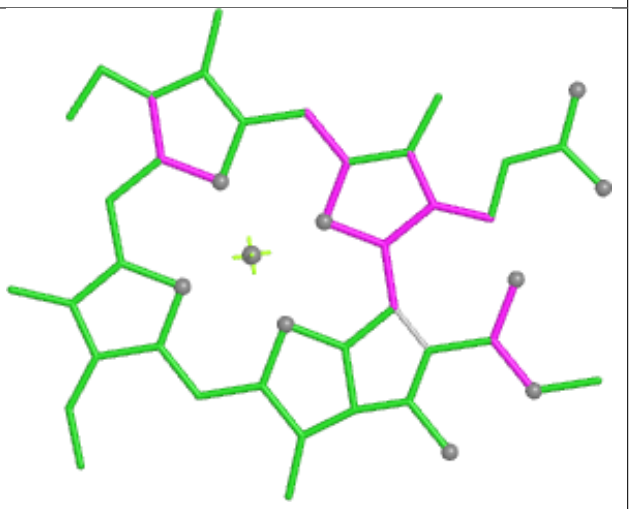


Rings

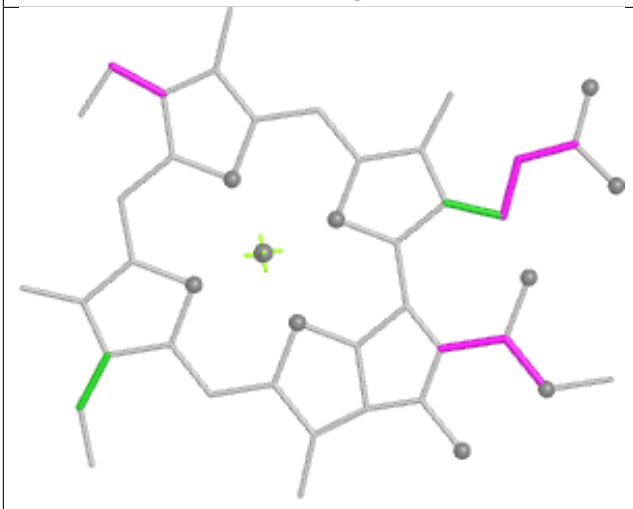
Ligand CLA O2 203



Bond lengths



Bond angles

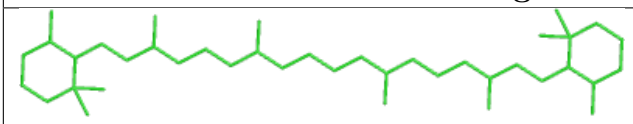


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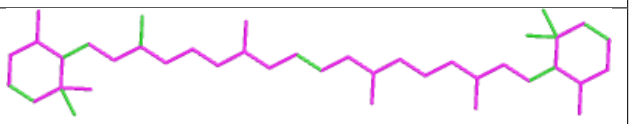


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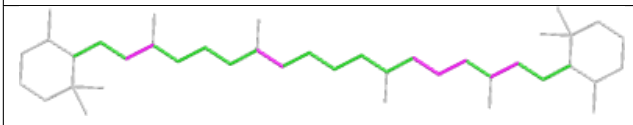
Ligand BCR FL 101



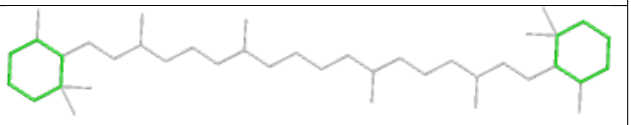
Bond lengths



Bond angles

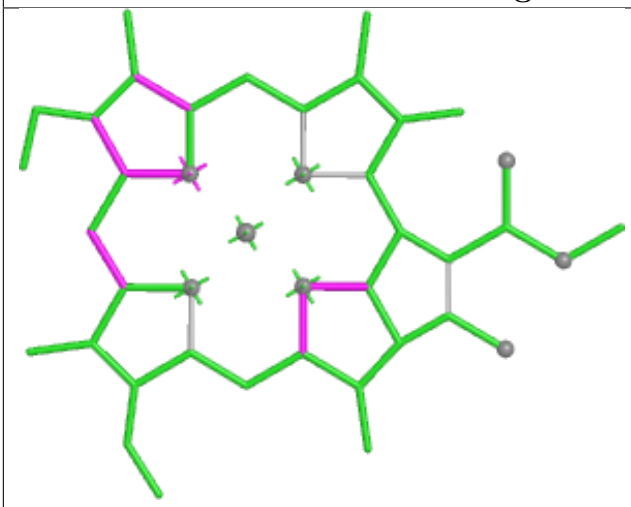


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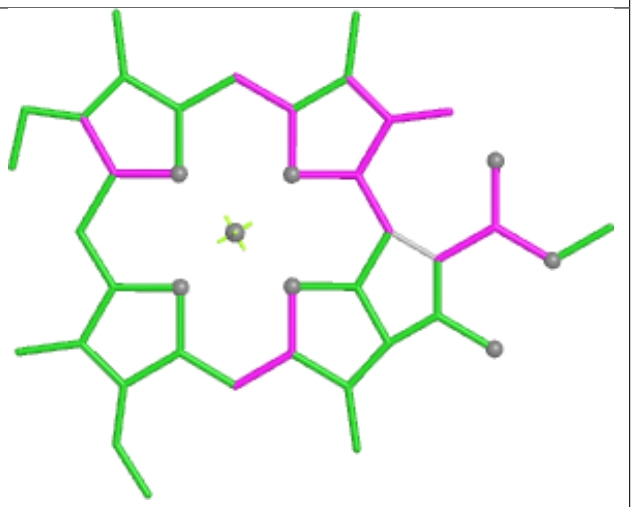


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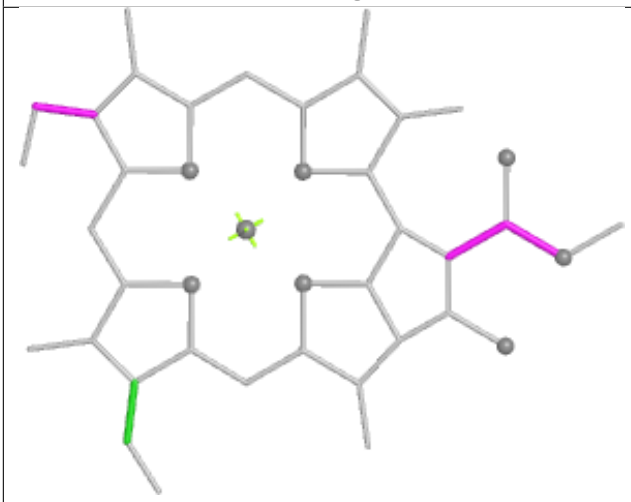
Ligand CLA 7N 608



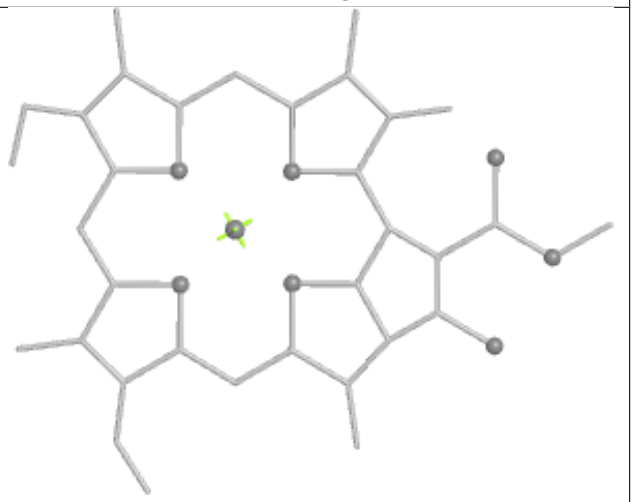
Bond lengths



Bond angles

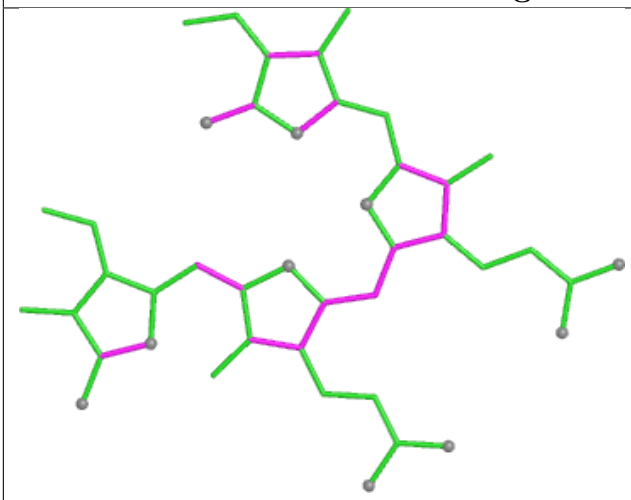


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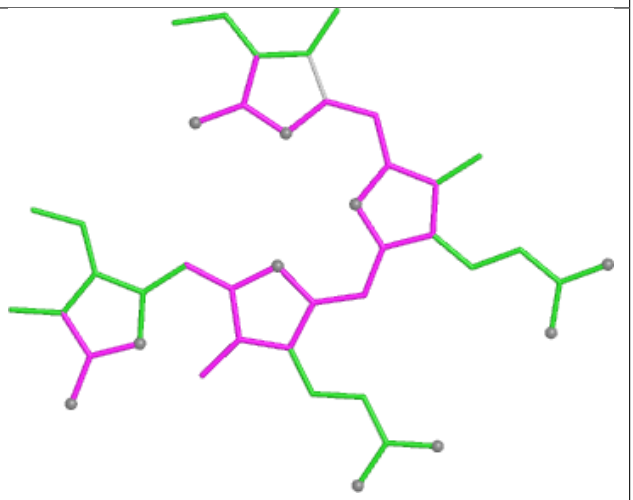


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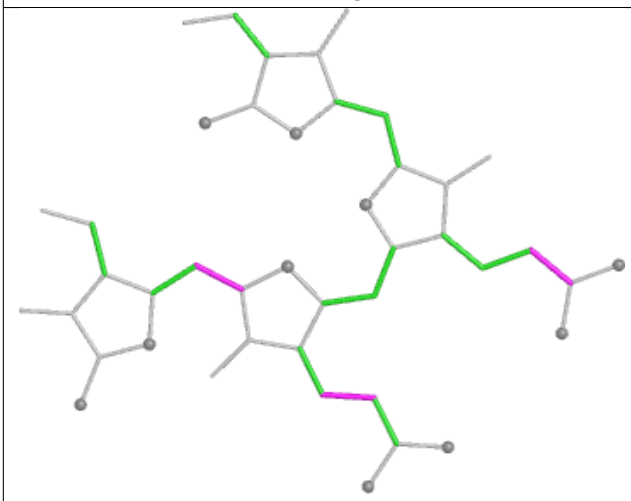
Ligand PEB dH 201



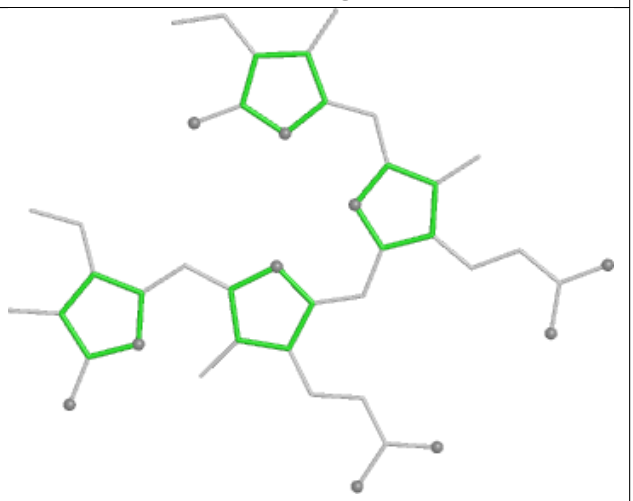
Bond lengths



Bond angles

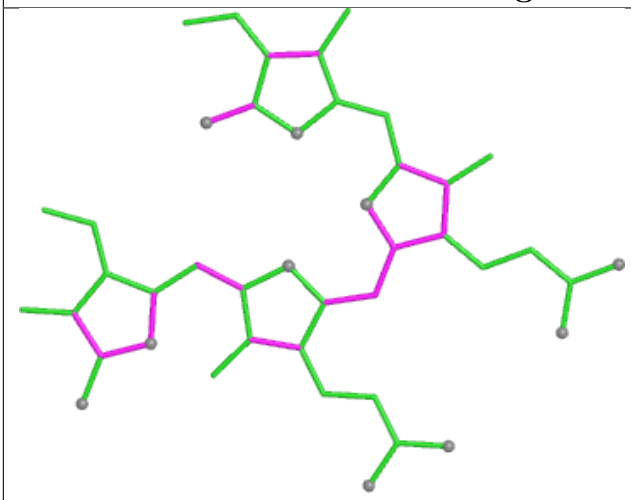


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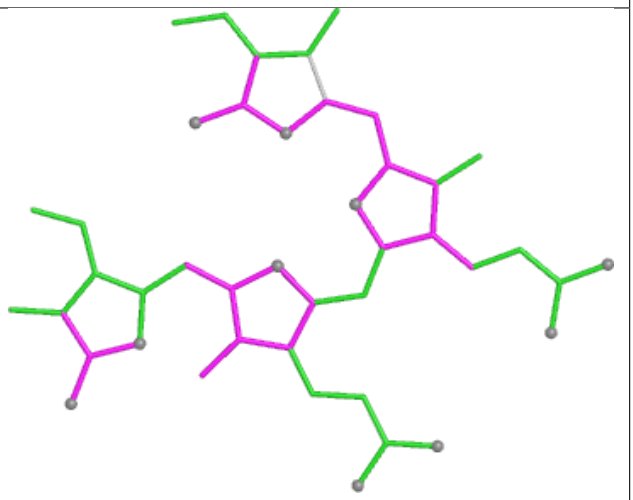


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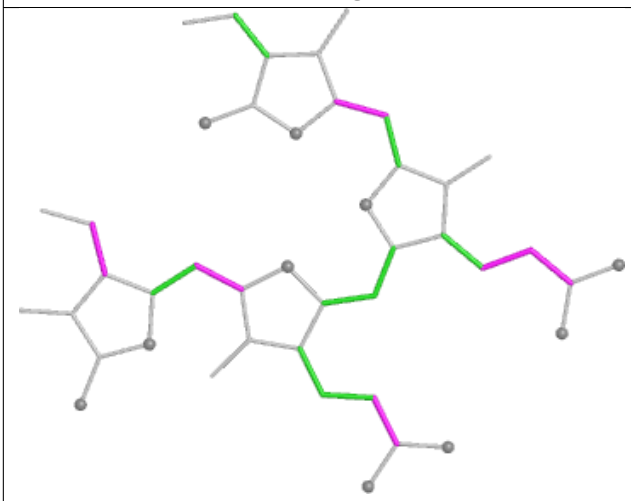
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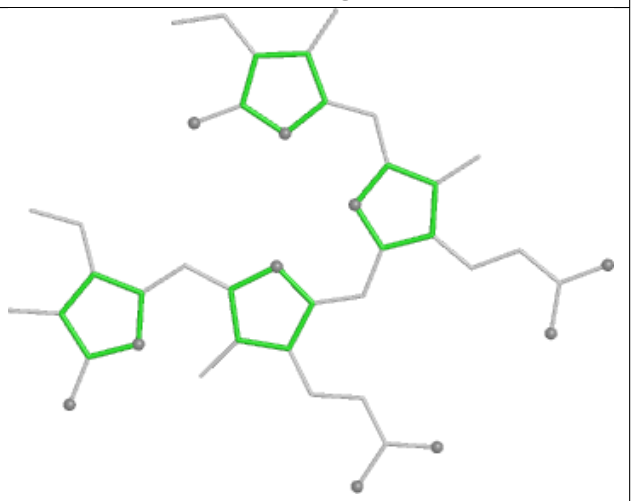
Bond lengths



Bond angles

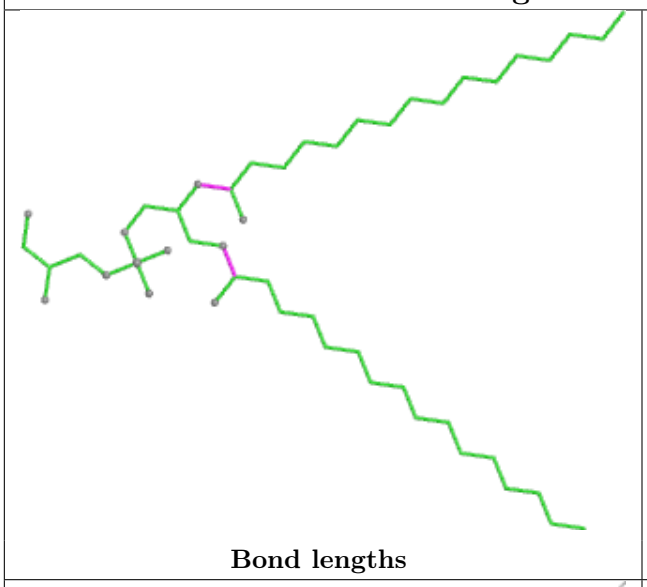


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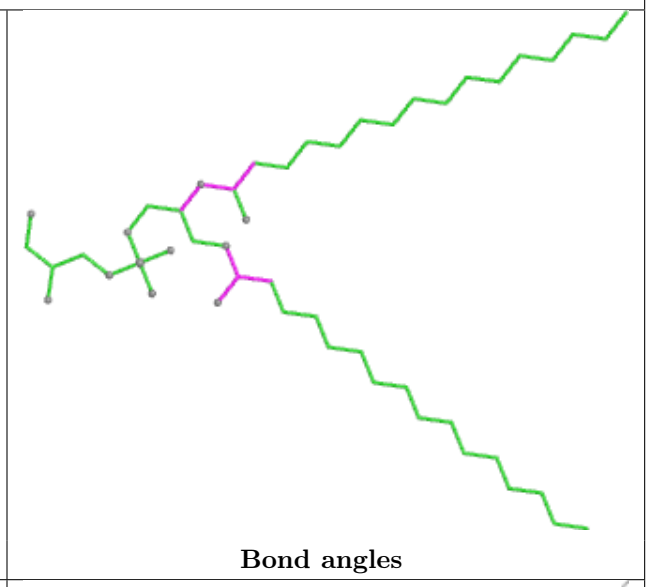


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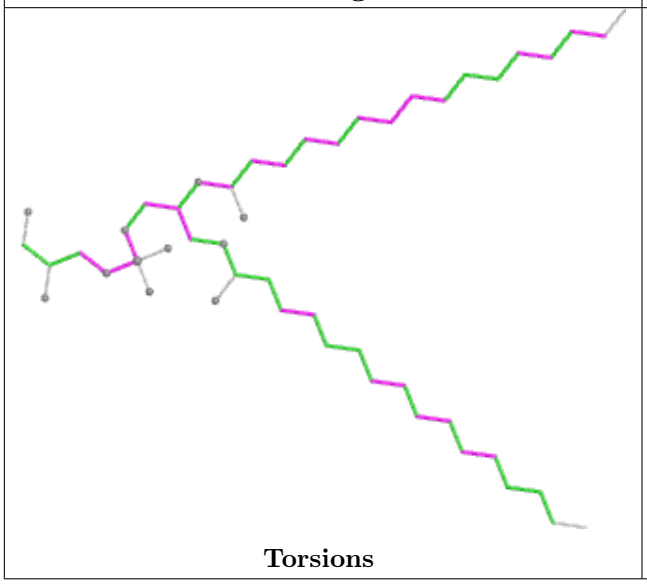
Ligand LHG AL 406



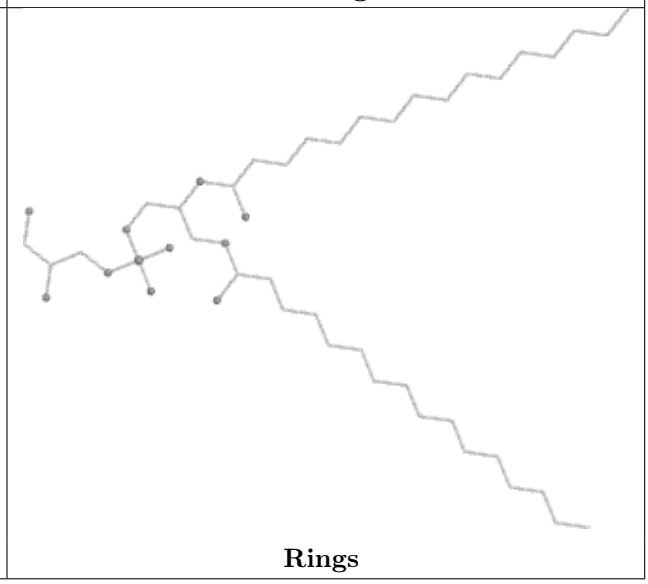
Bond lengths



Bond angles

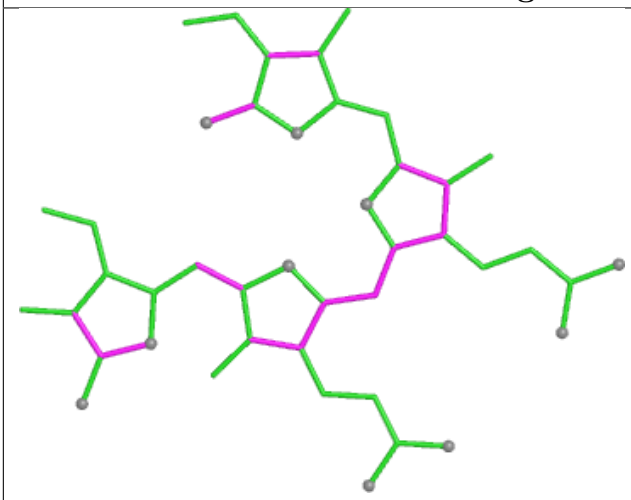


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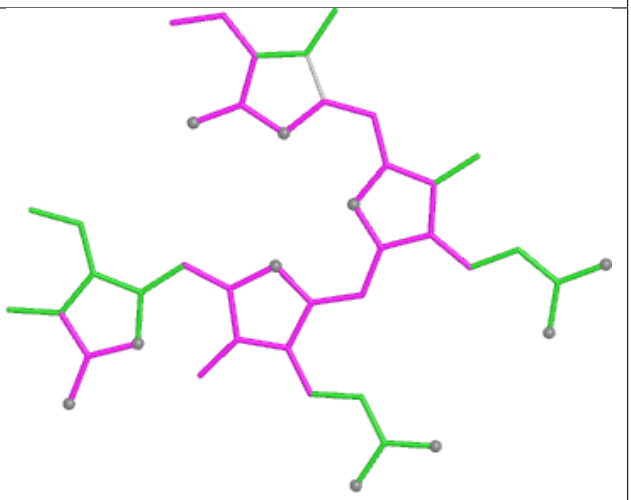


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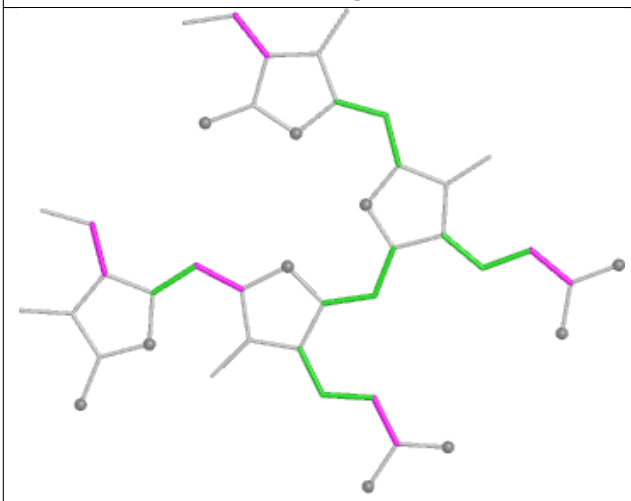
Ligand PEB F7 202



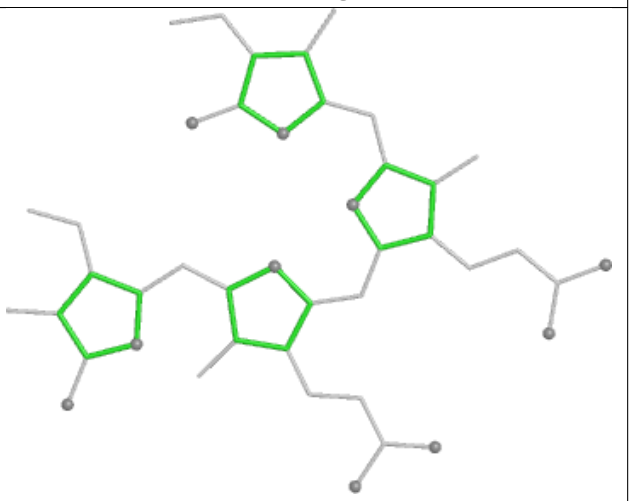
Bond lengths



Bond angles

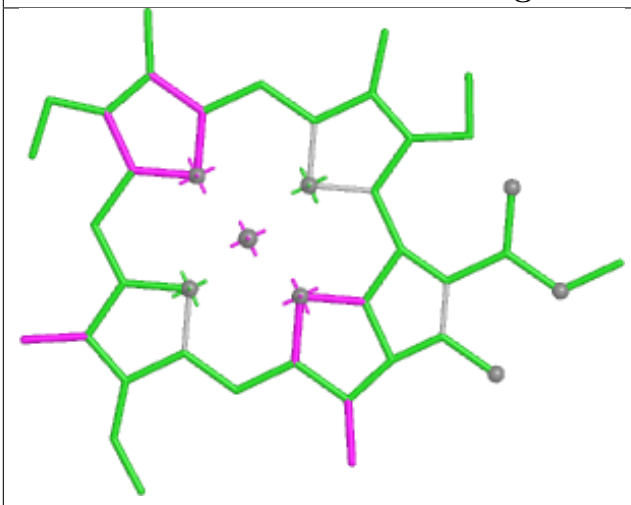


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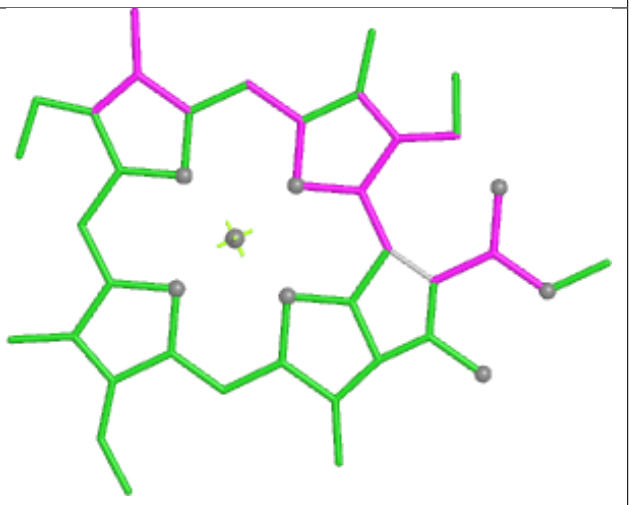


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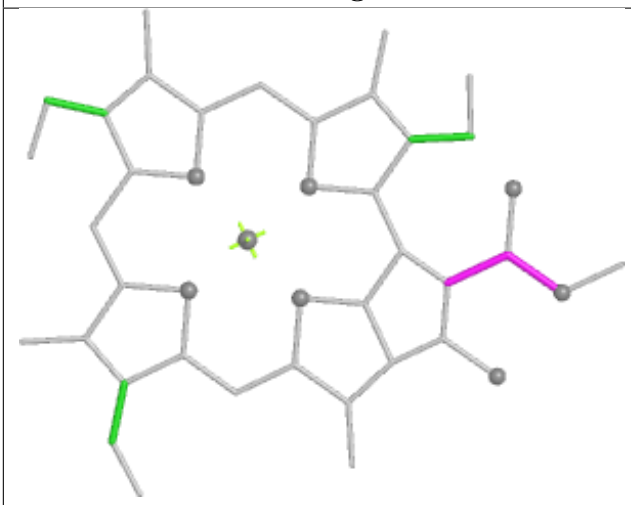
Ligand CLA K2 104



Bond lengths



Bond angles

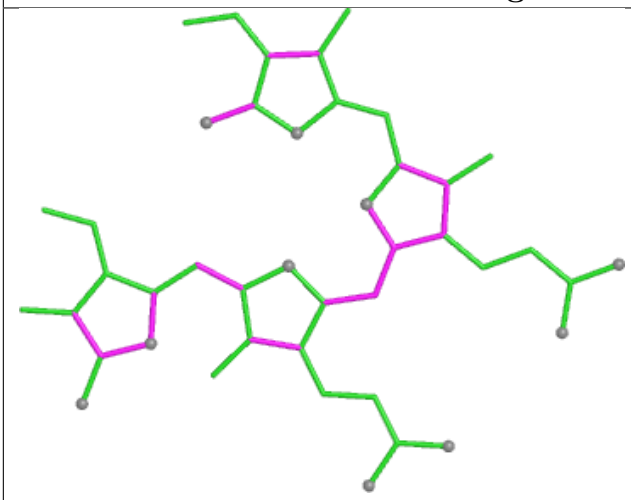


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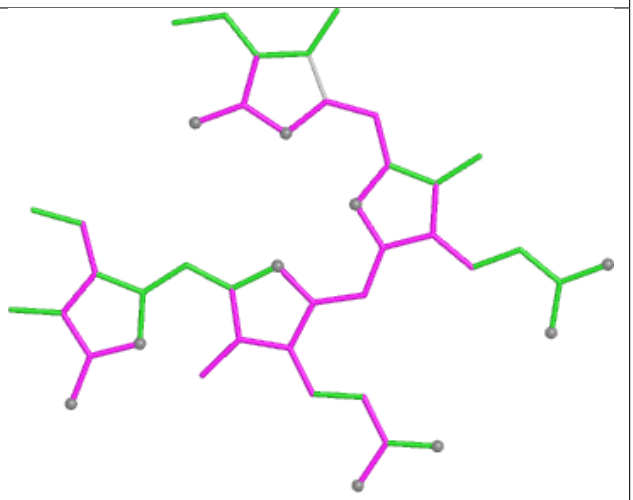


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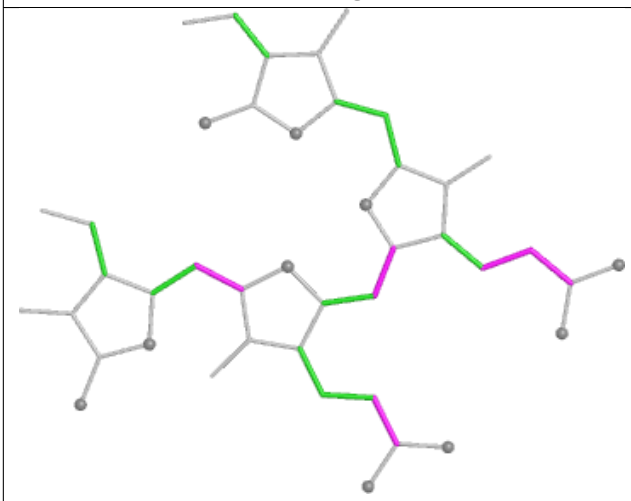
Ligand PEB VM 202



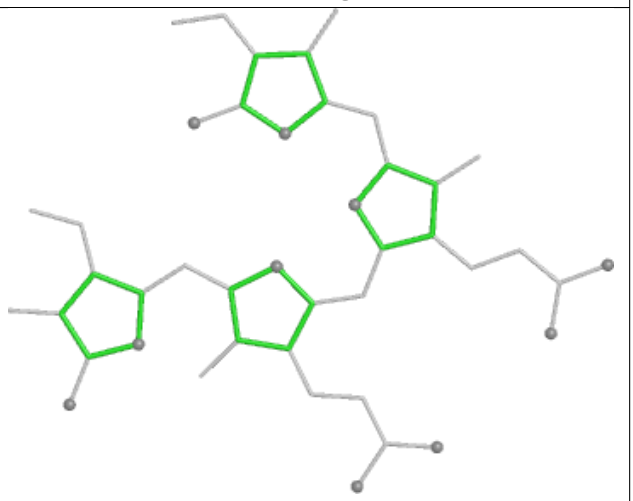
Bond lengths



Bond angles

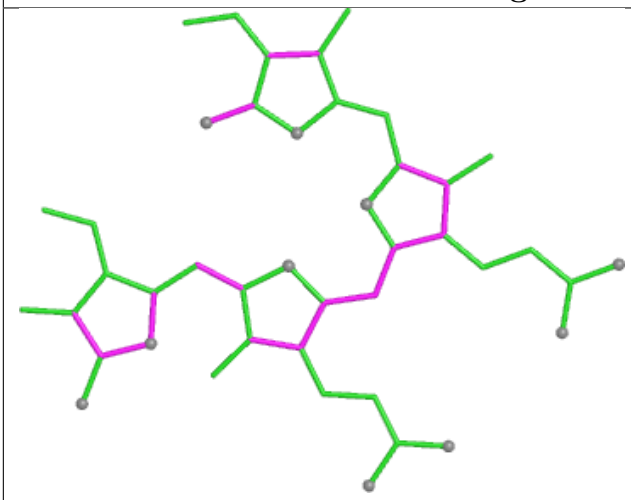


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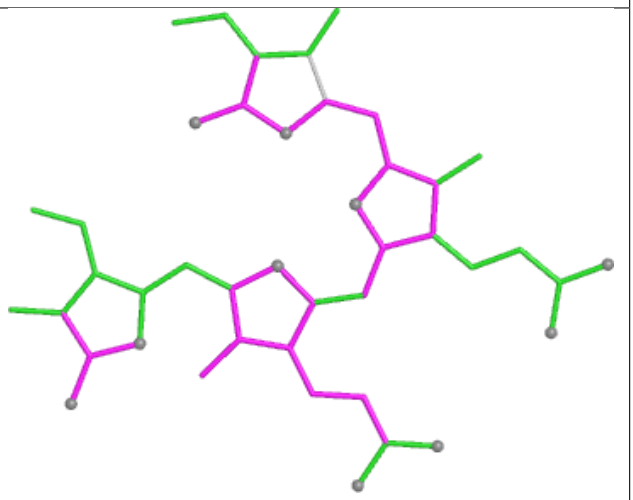


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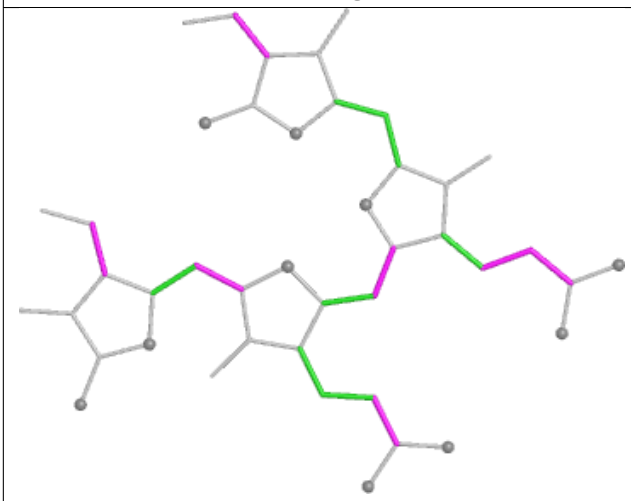
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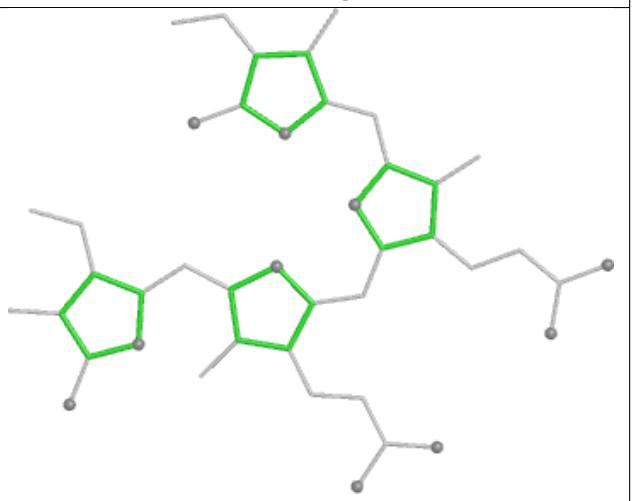
Bond lengths



Bond angles

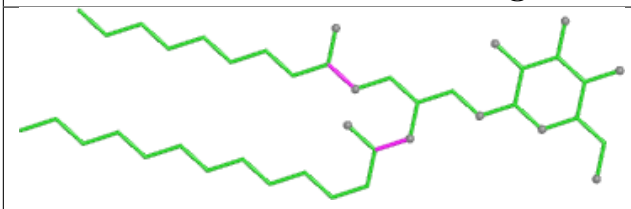


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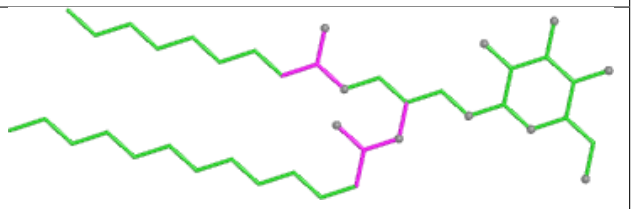


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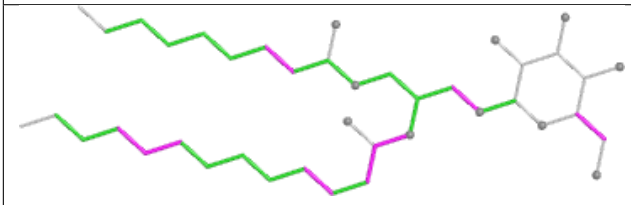
Ligand LMG m6 103



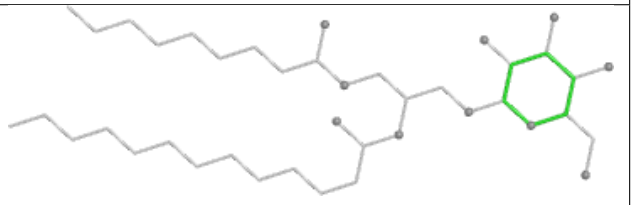
Bond lengths



Bond angles

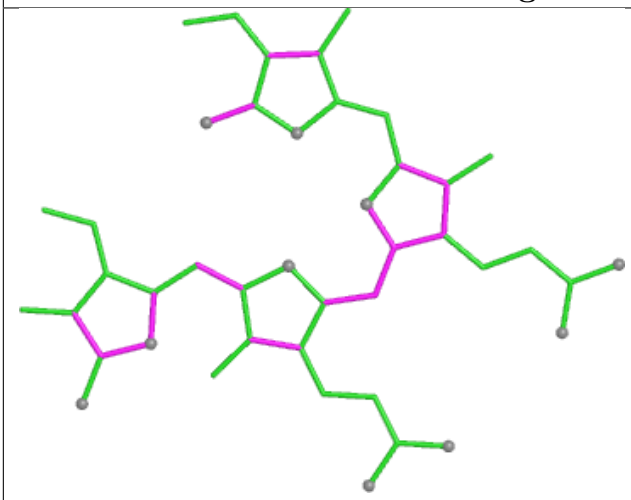


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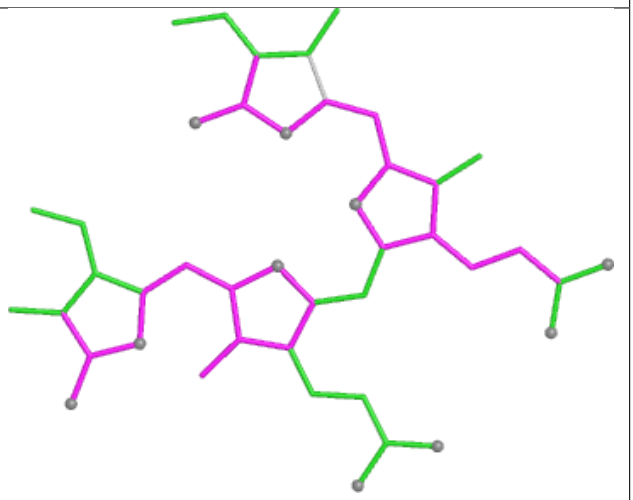


Rings

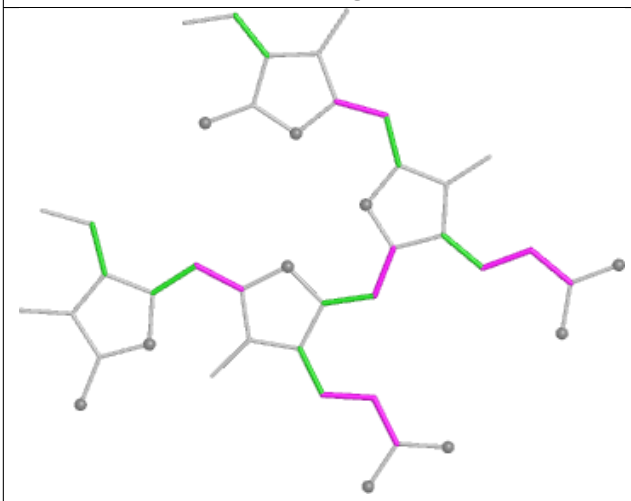
Ligand PEB S5 203



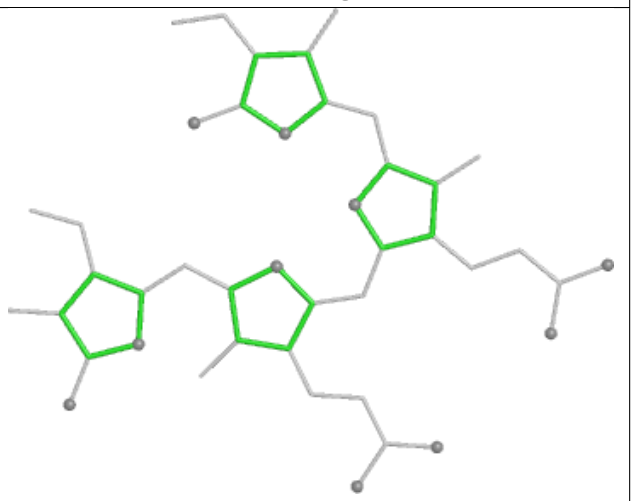
Bond lengths



Bond angles

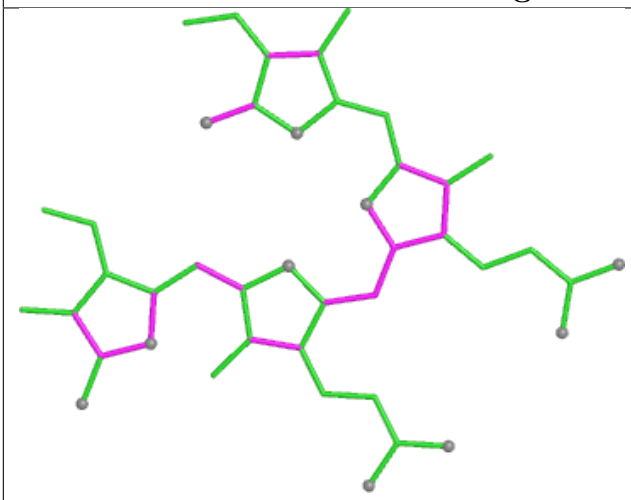


Torsions

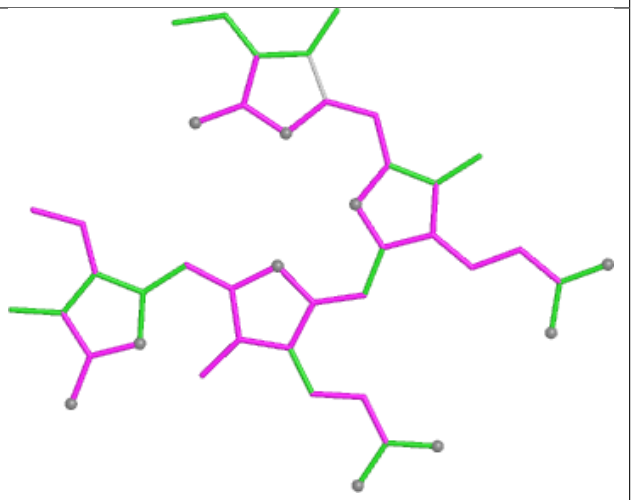


Rings

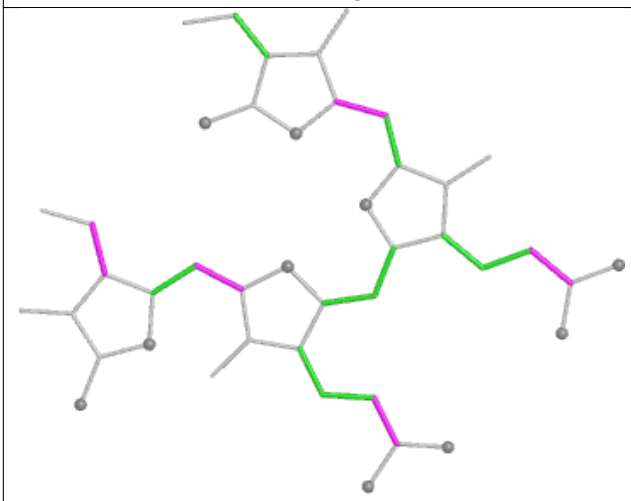
Ligand PEB SG 201



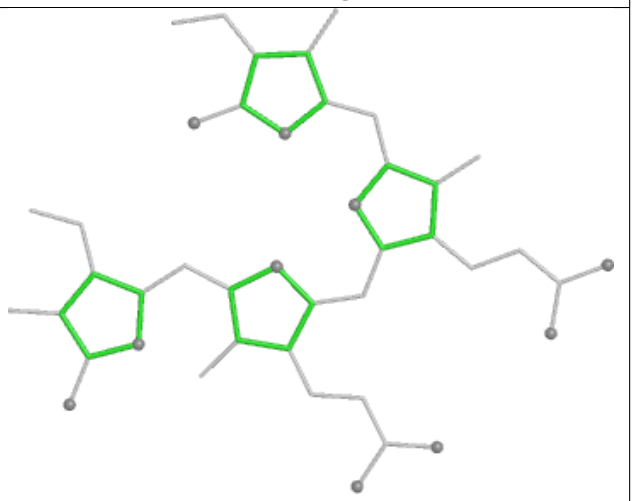
Bond lengths



Bond angles

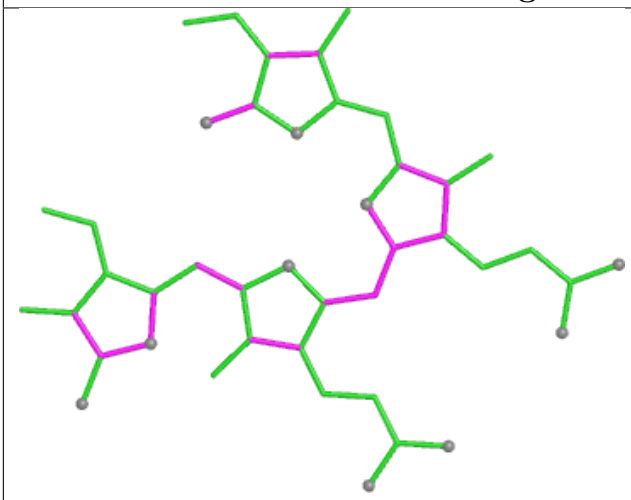


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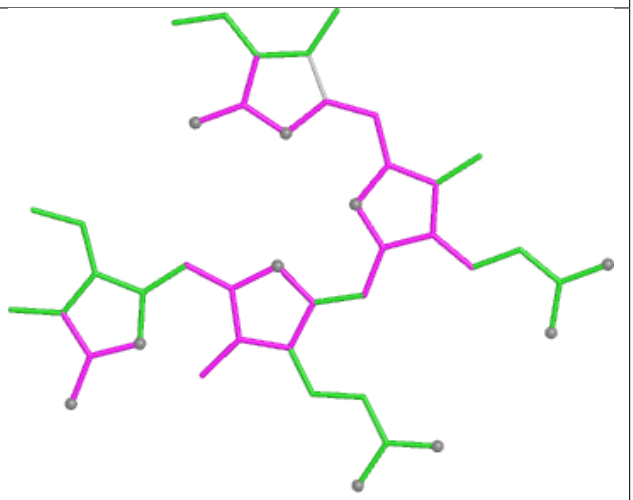


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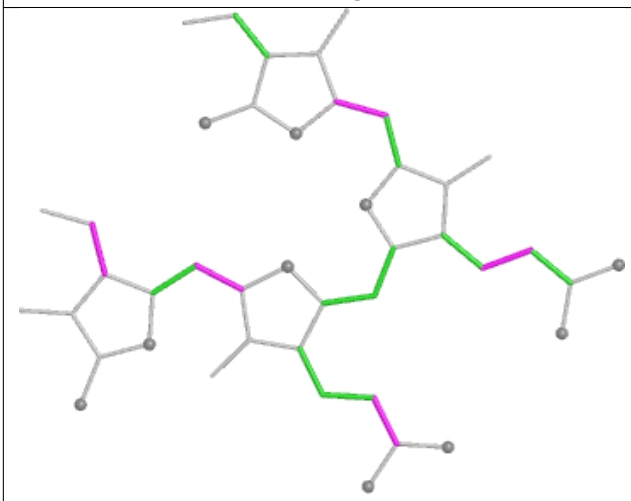
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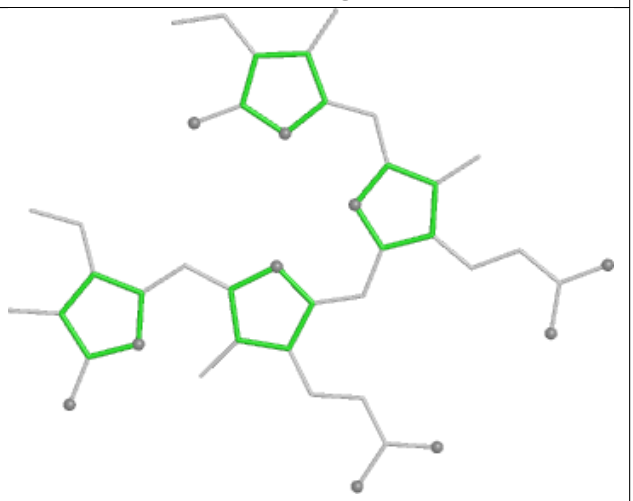
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Bond angles

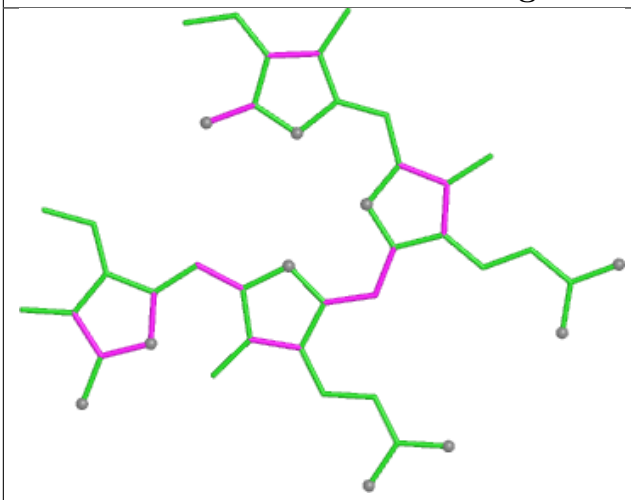


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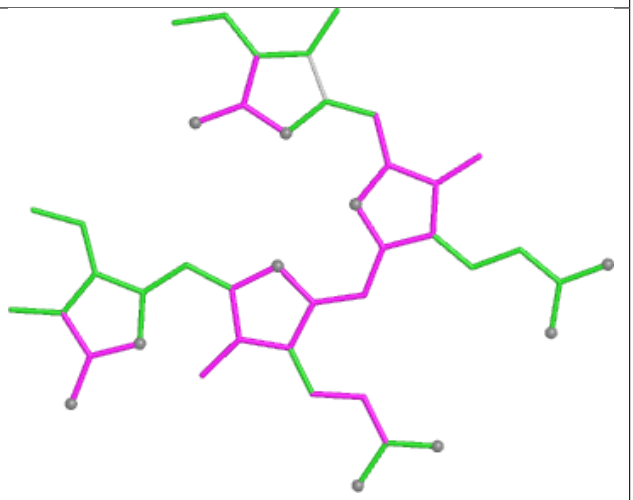


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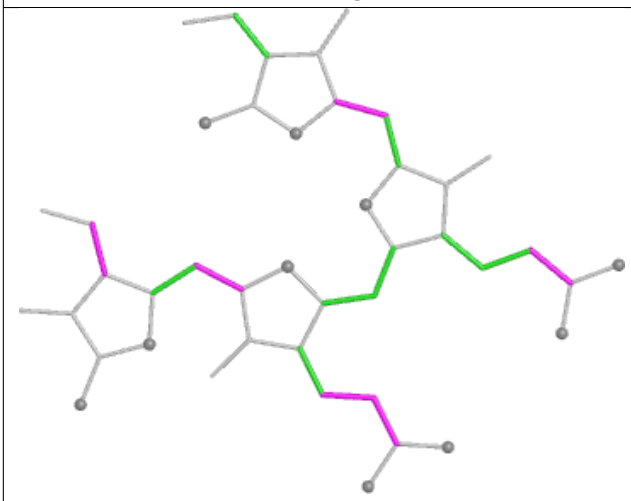
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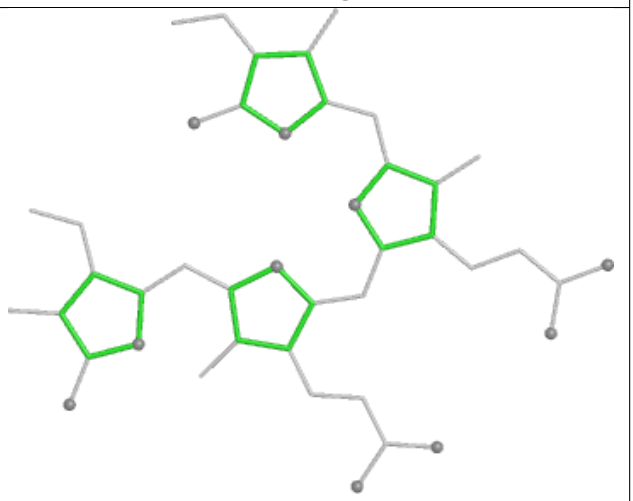
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Bond angles

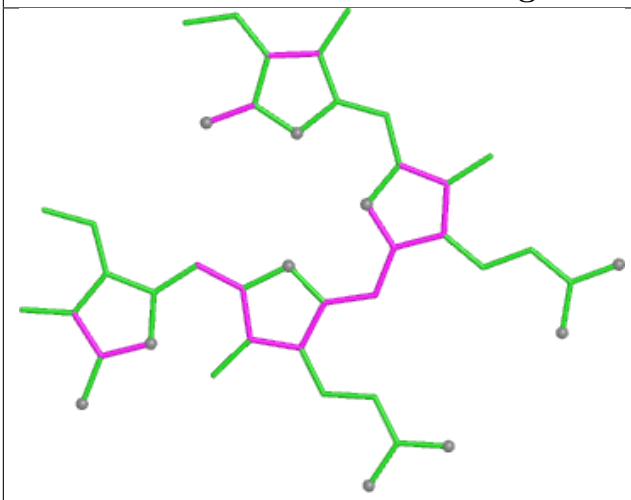


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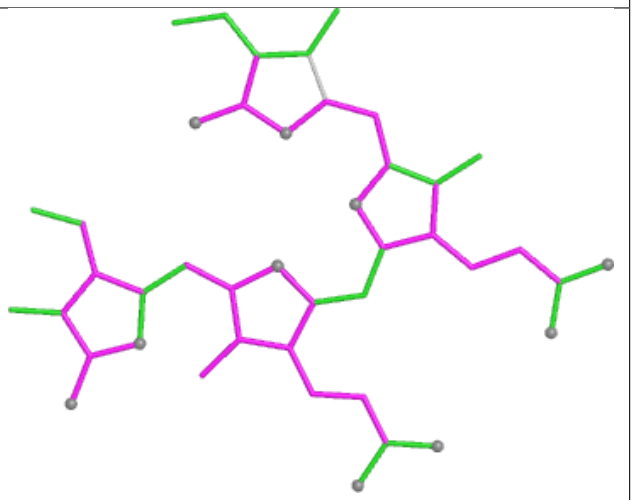


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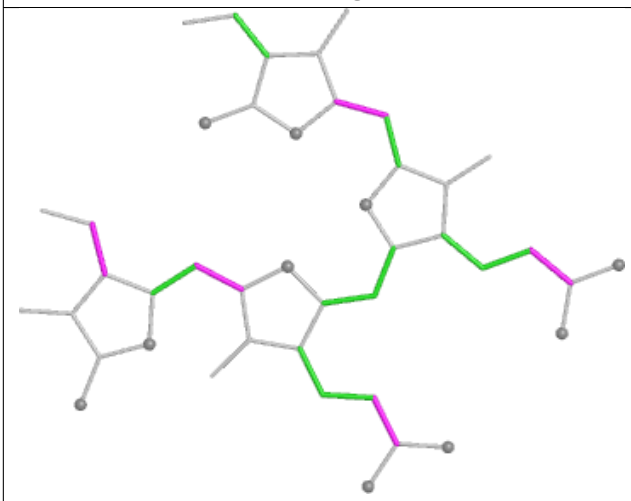
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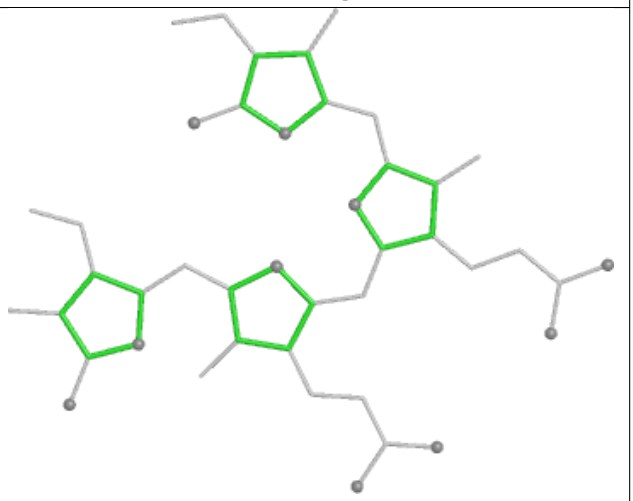
Bond lengths



Bond angles

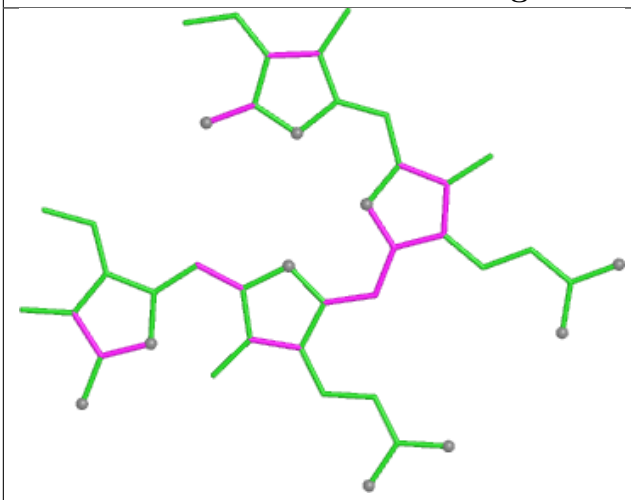


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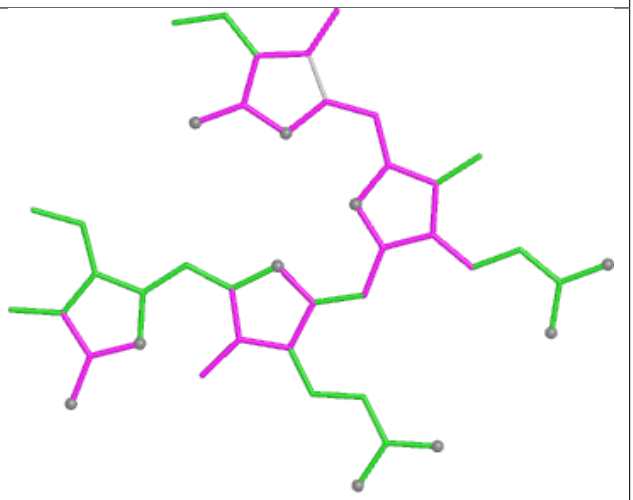


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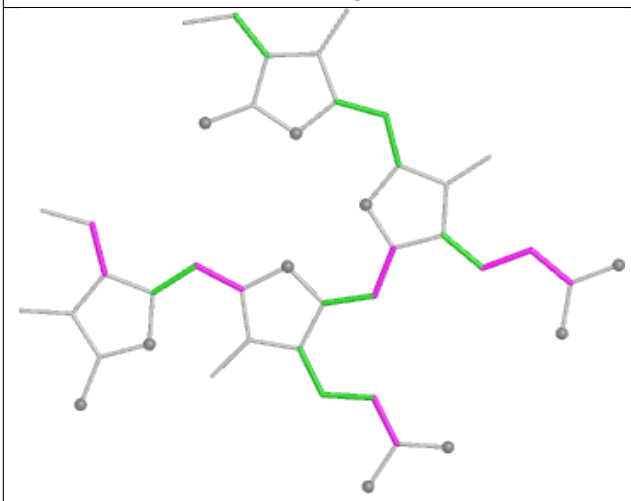
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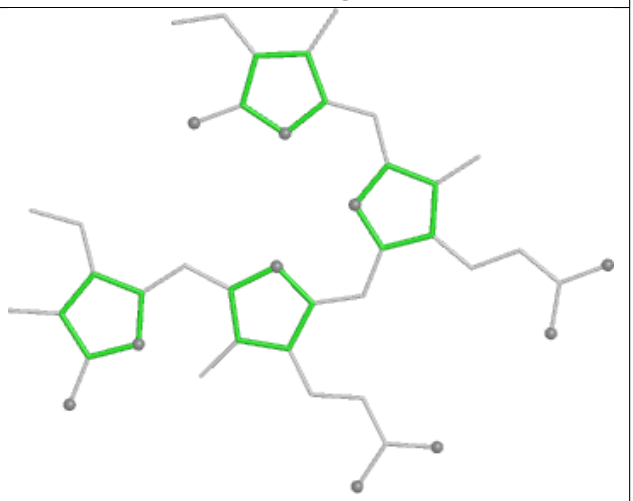
Bond lengths



Bond angles

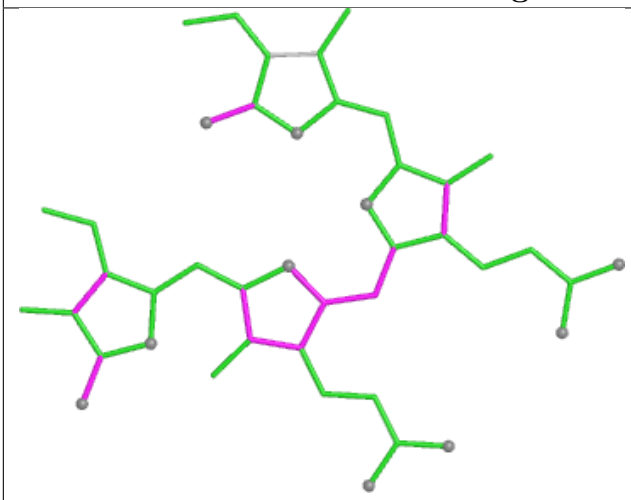


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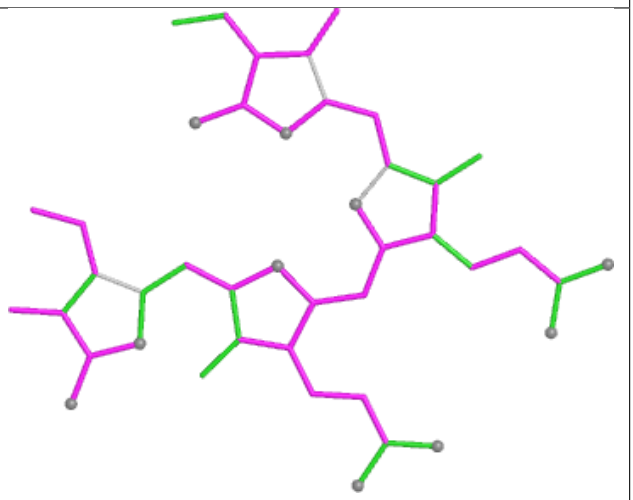


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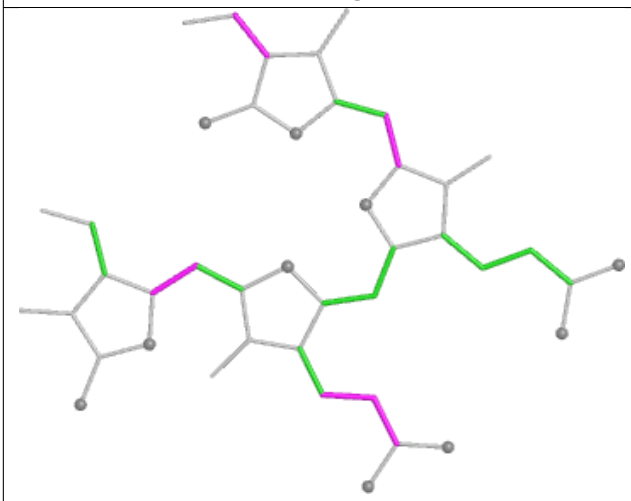
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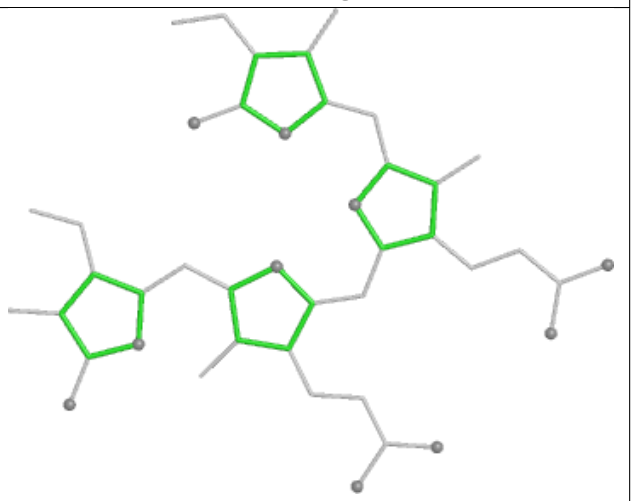
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Bond angles

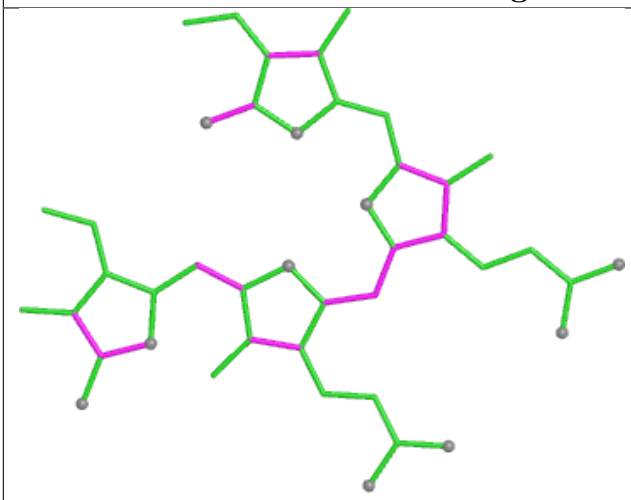


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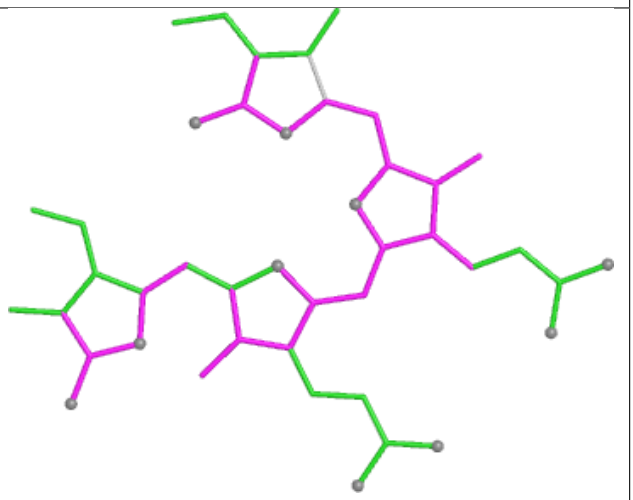


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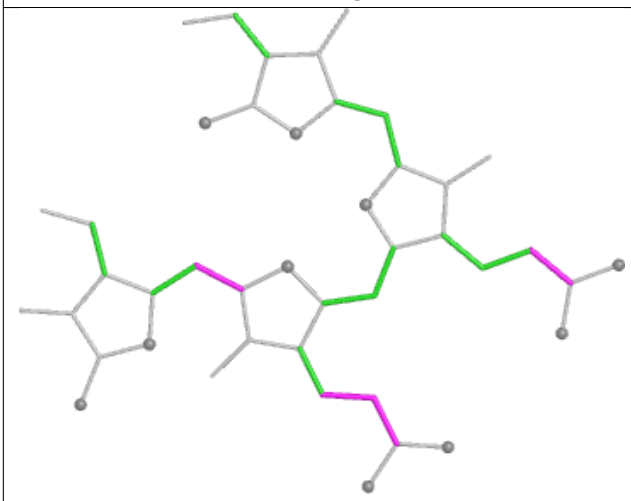
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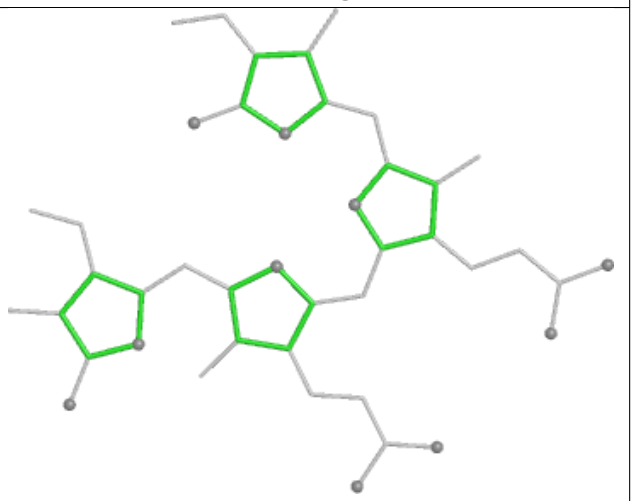
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Bond angles

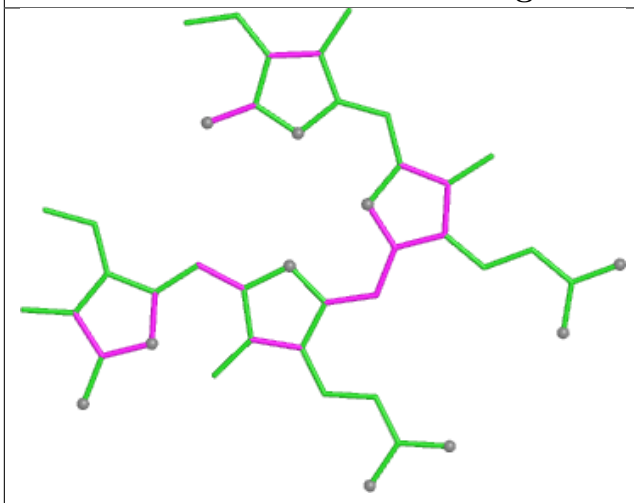


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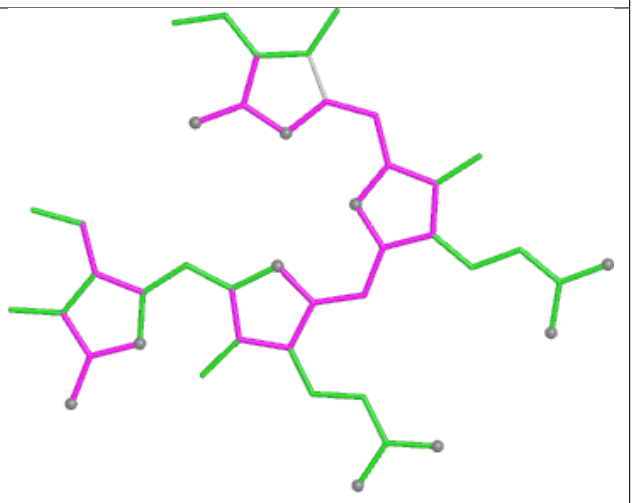


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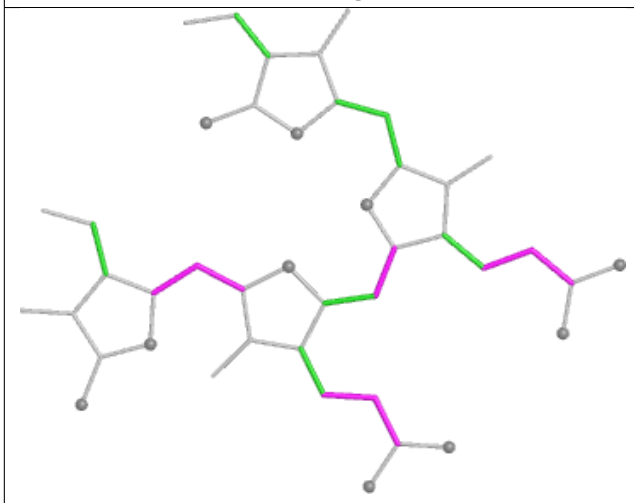
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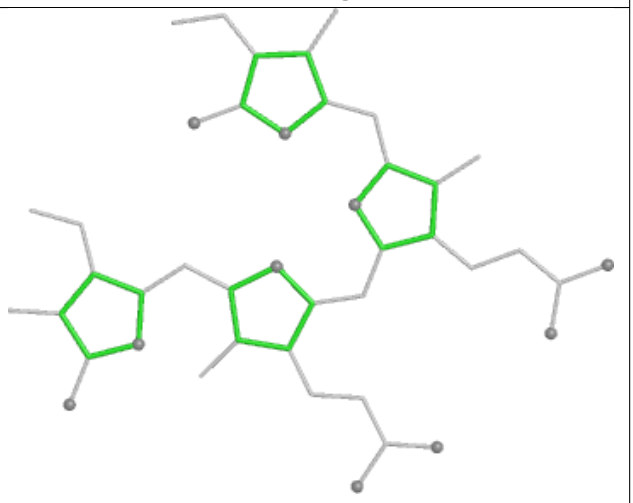
Bond lengths



Bond angles



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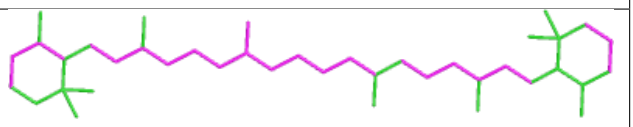


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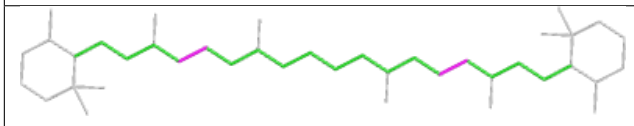
Ligand BCR cL 503



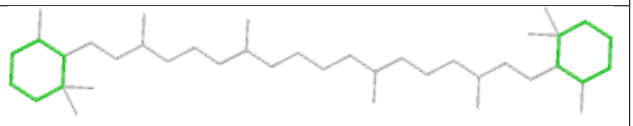
Bond lengths



Bond angles

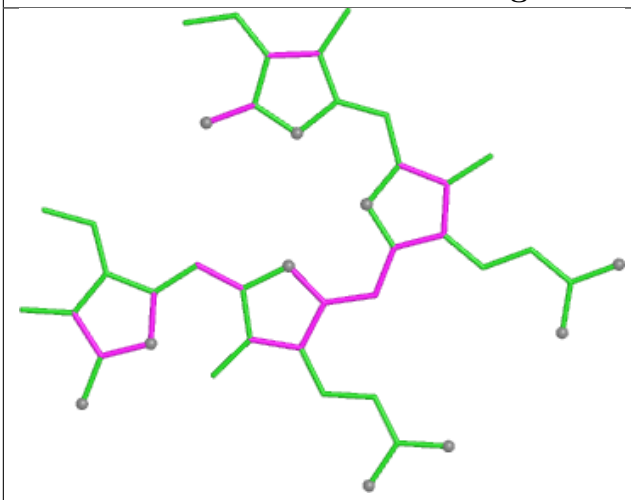


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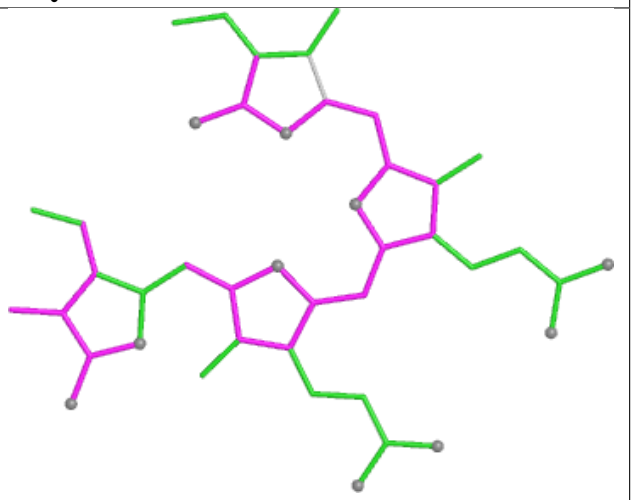


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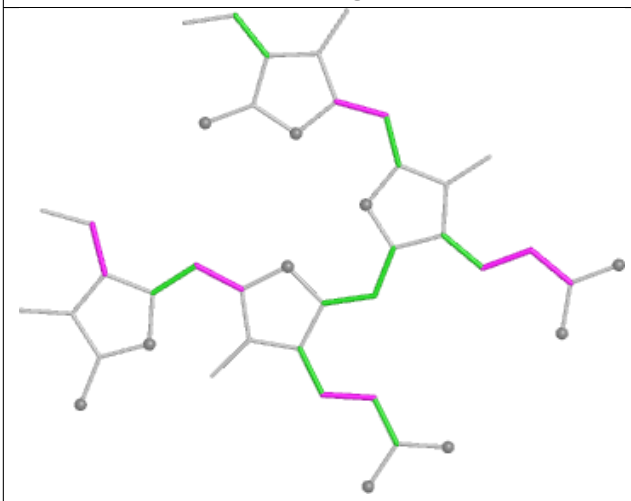
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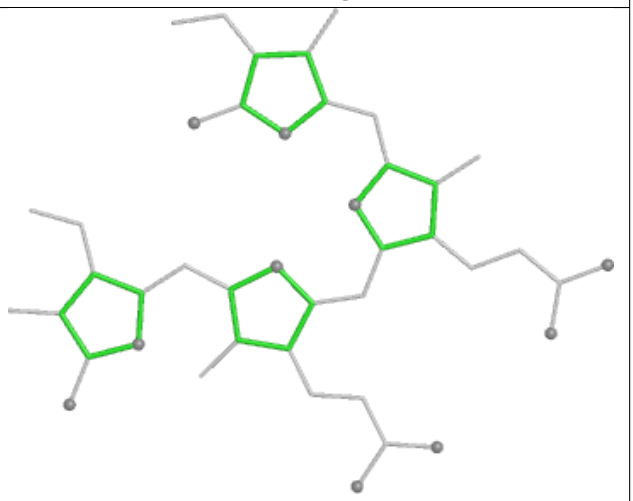
Bond lengths



Bond angles

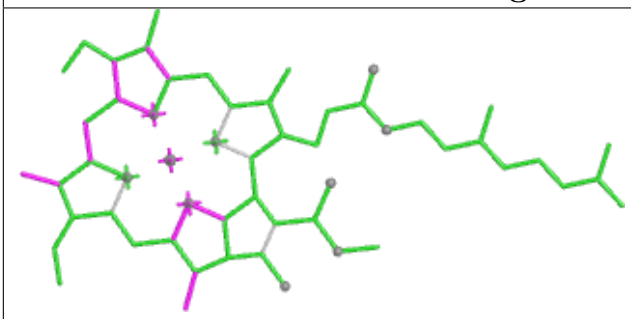


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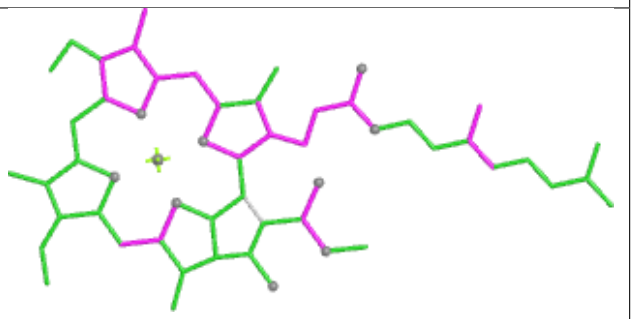


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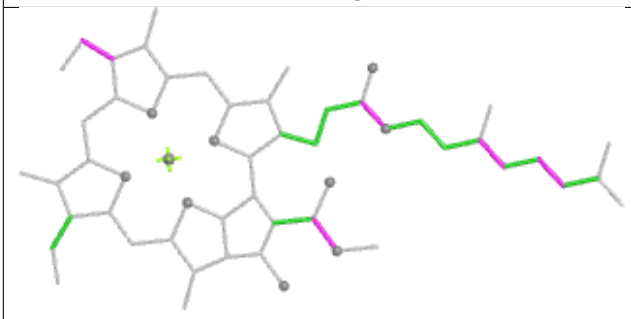
Ligand CLA AN 827



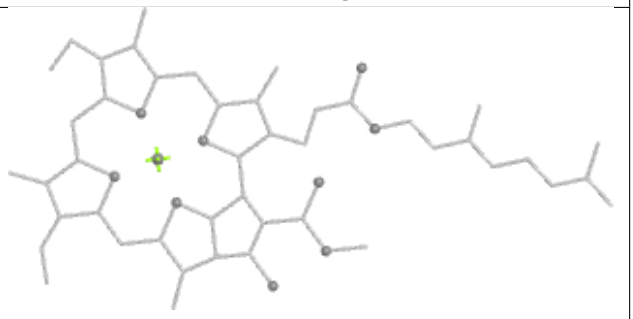
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Bond angles

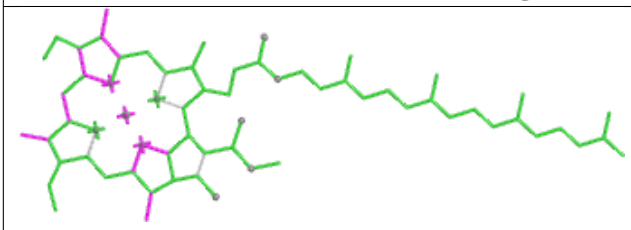


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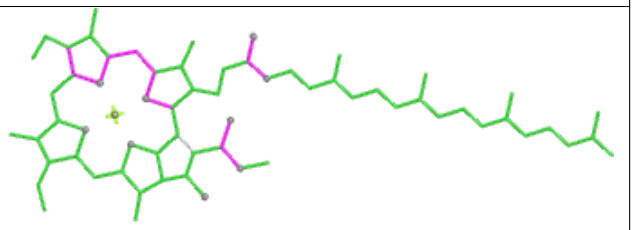


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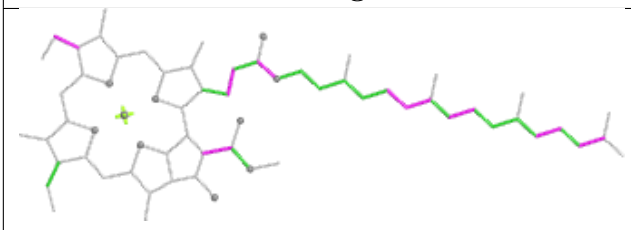
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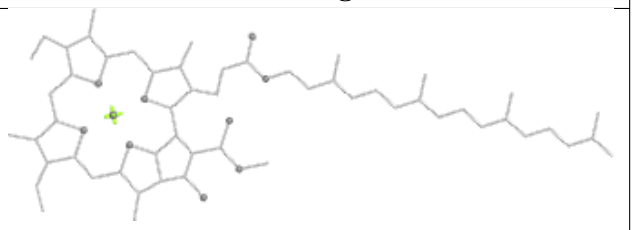
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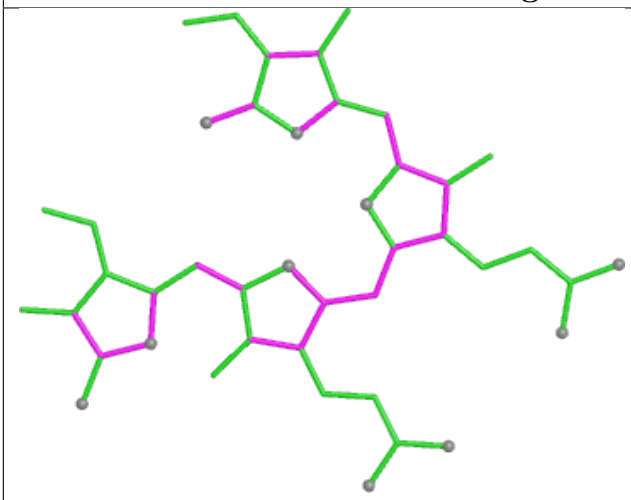


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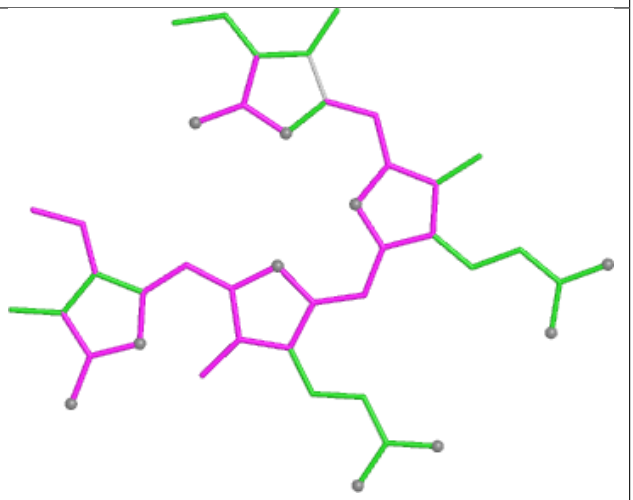


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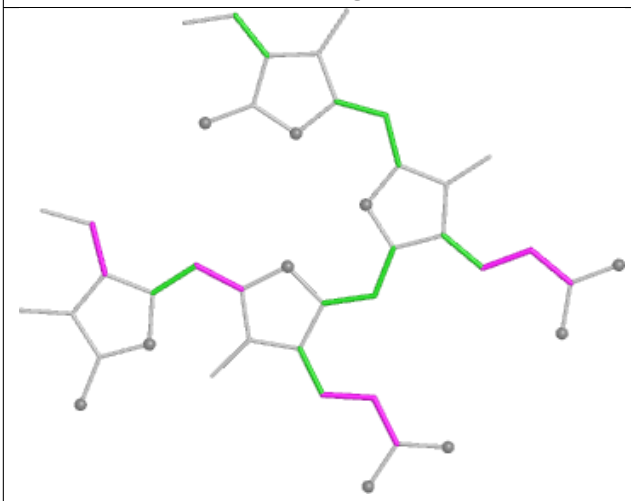
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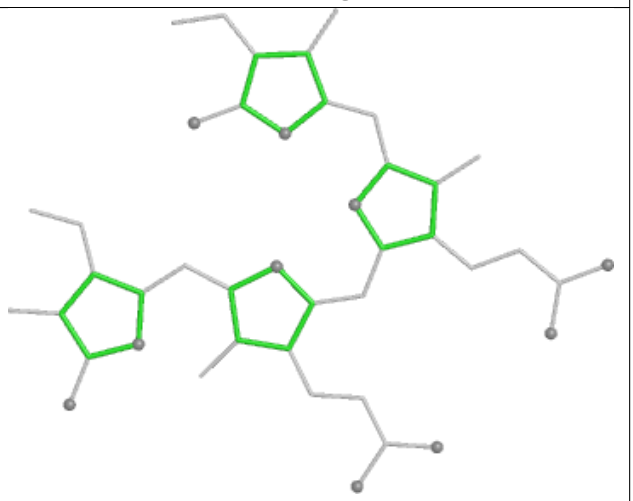
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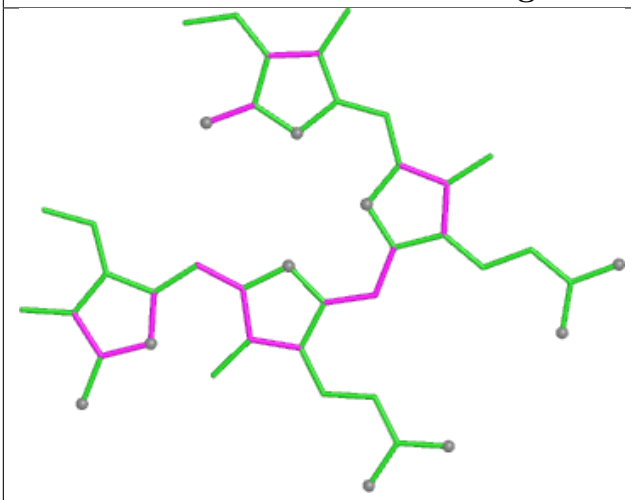


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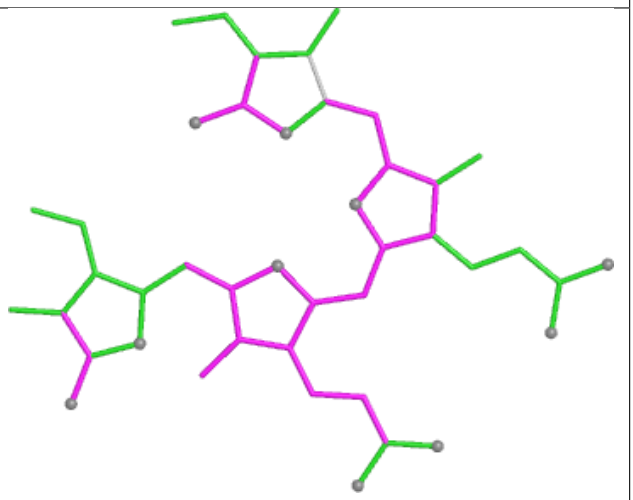


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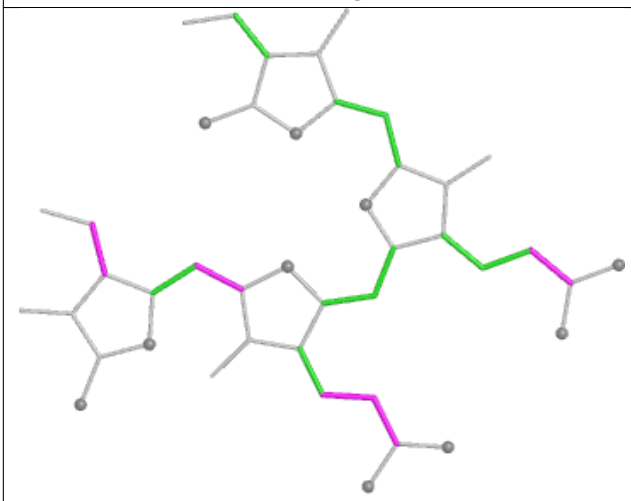
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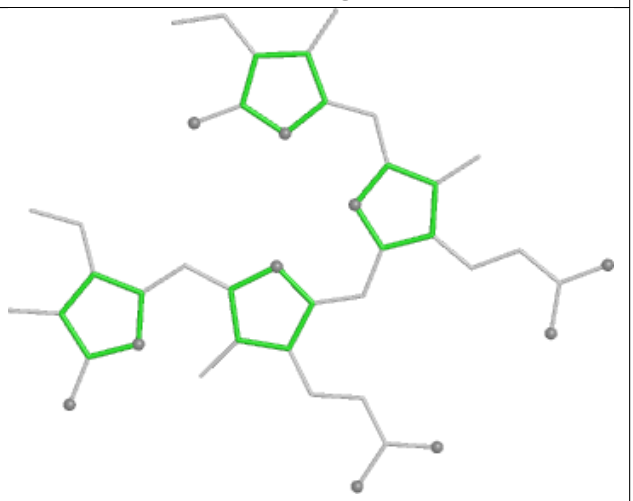
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Bond angles

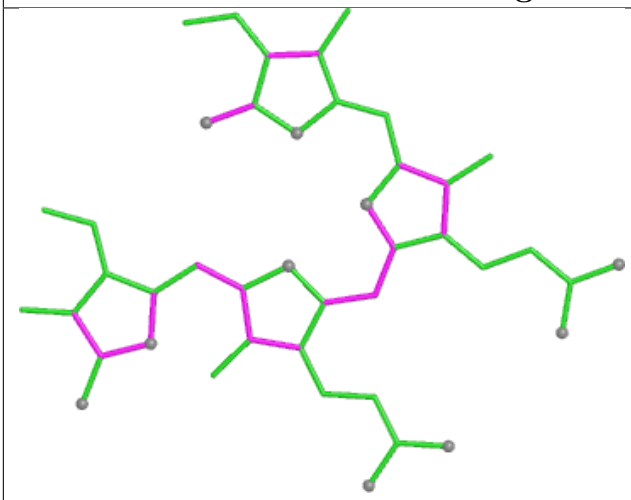


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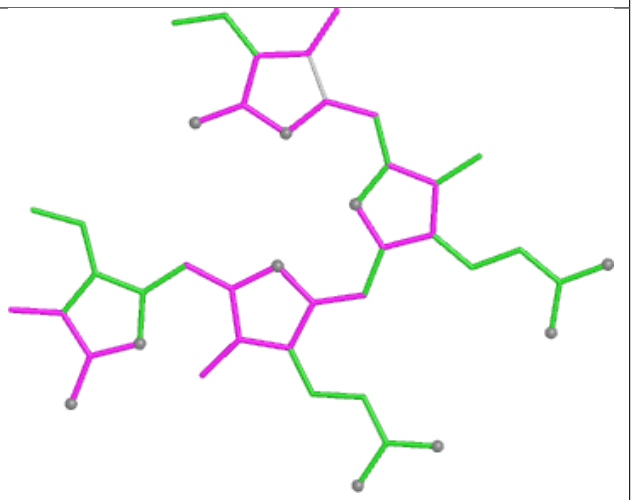


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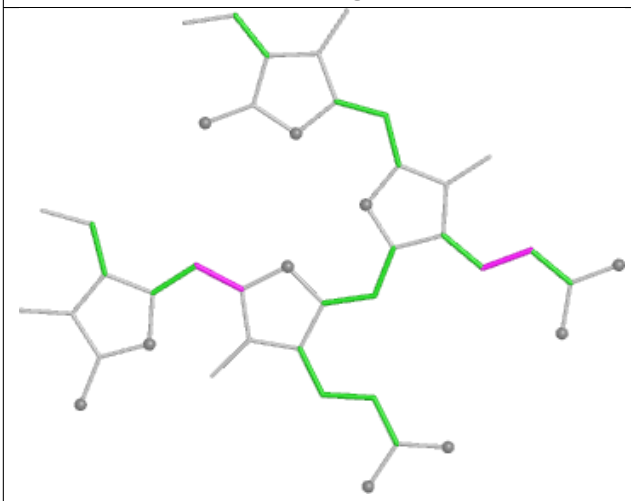
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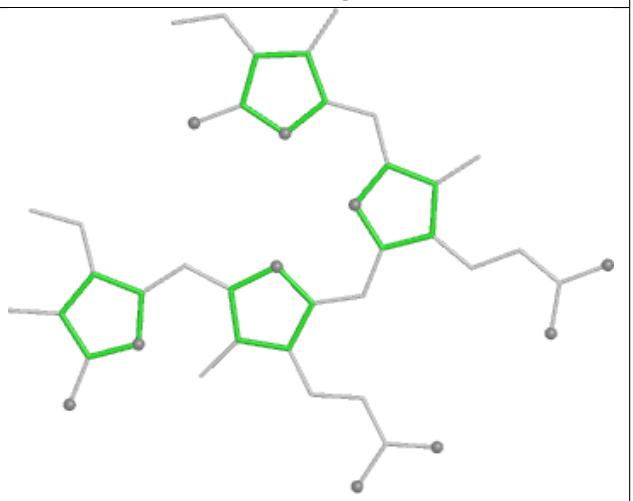
Bond lengths



Bond angles

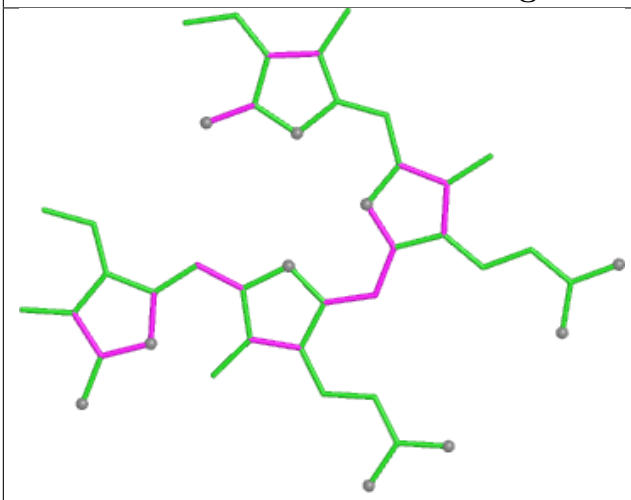


Torsions

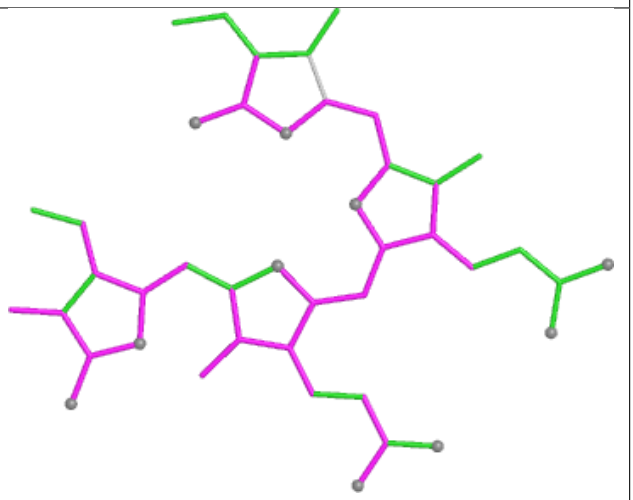


Rings

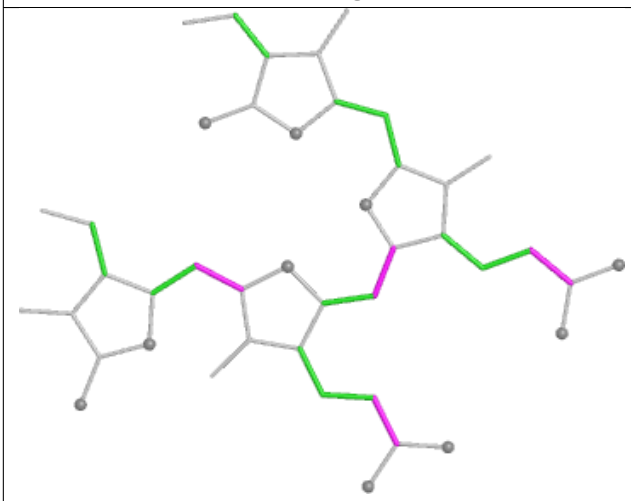
Ligand PEB JJ 202



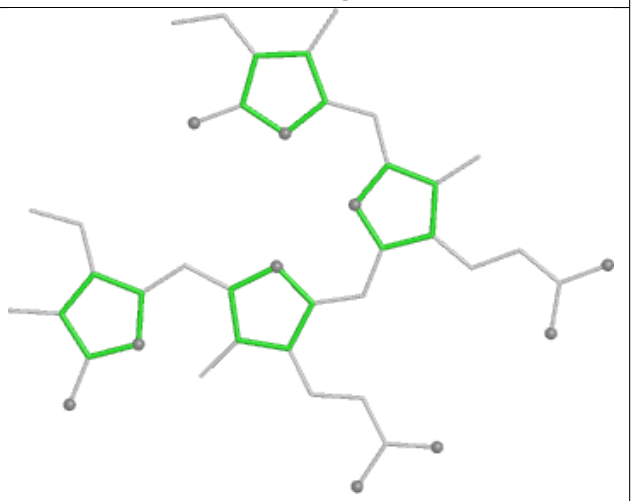
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Bond angles

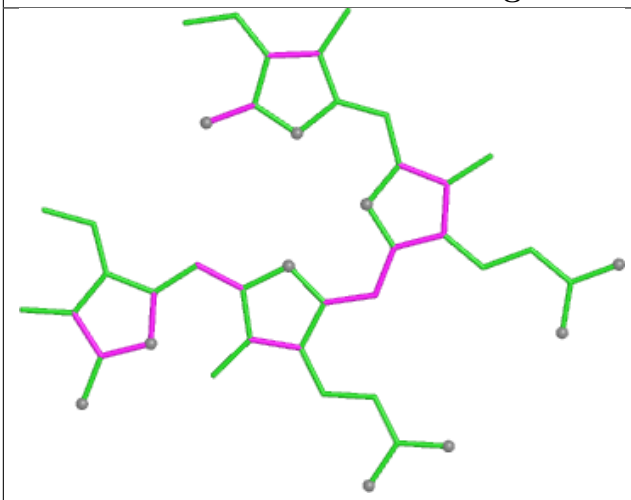


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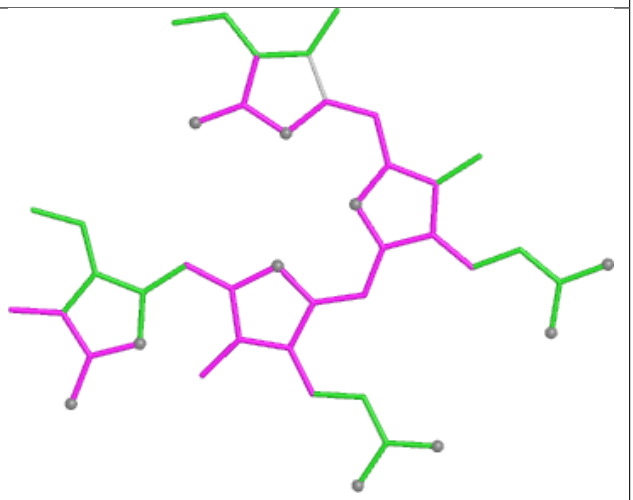


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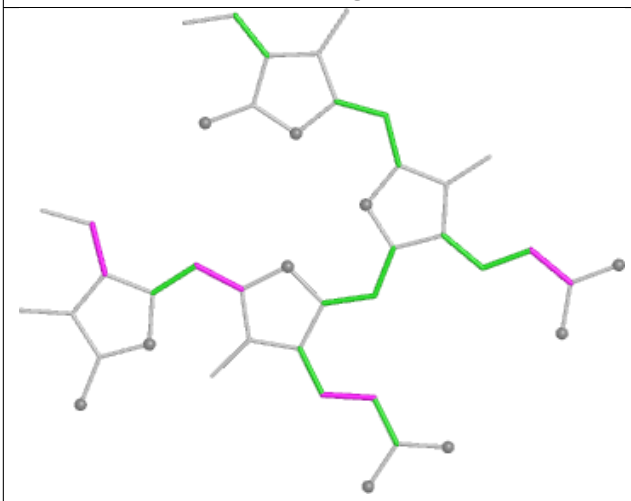
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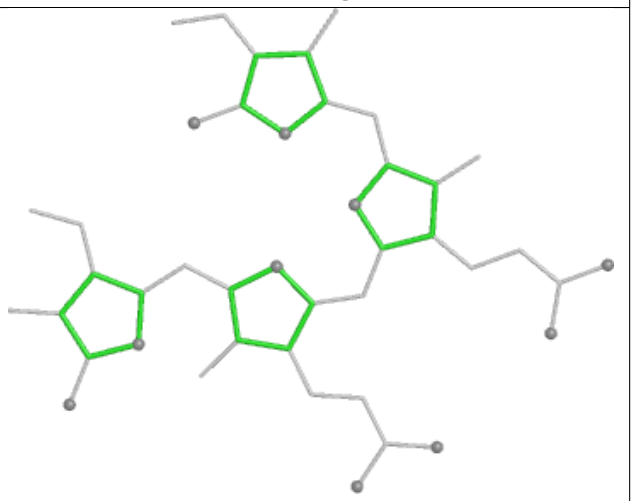
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Bond angles

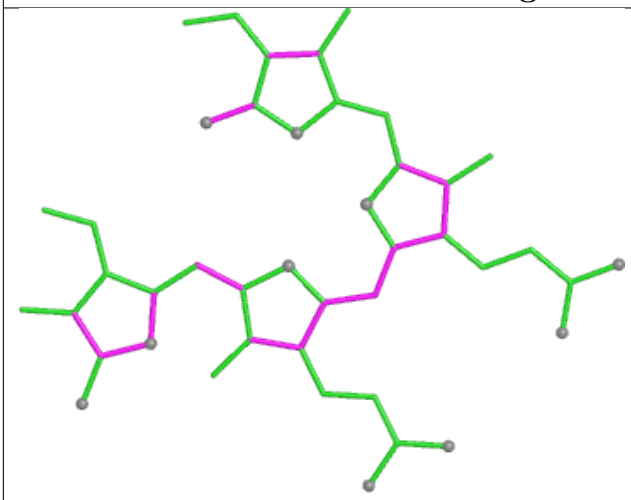


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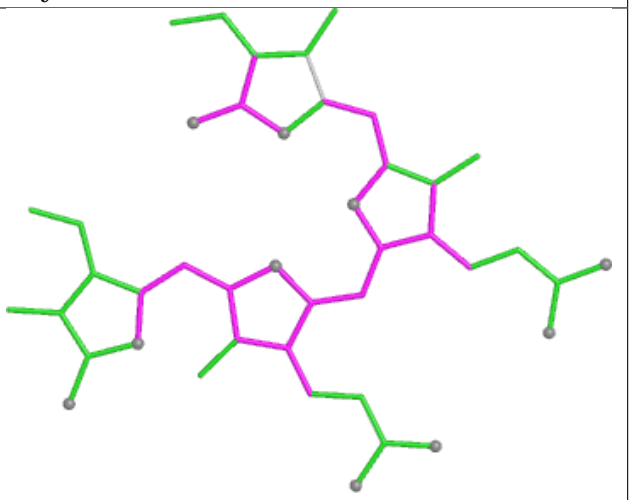


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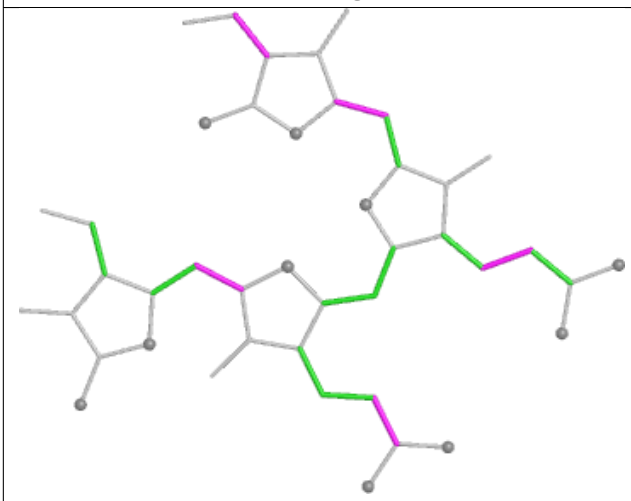
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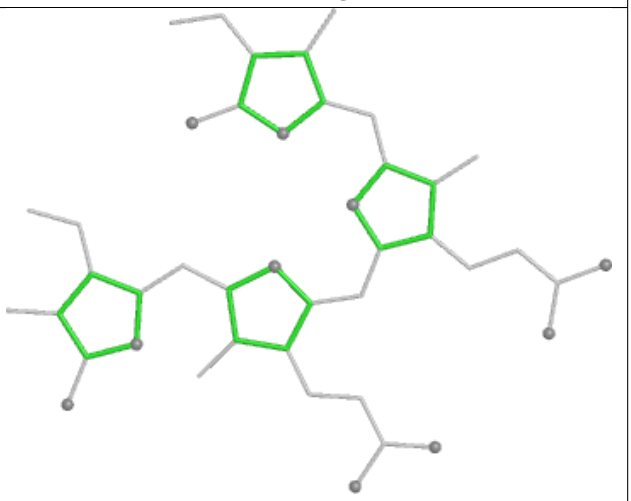
Bond lengths



Bond angles

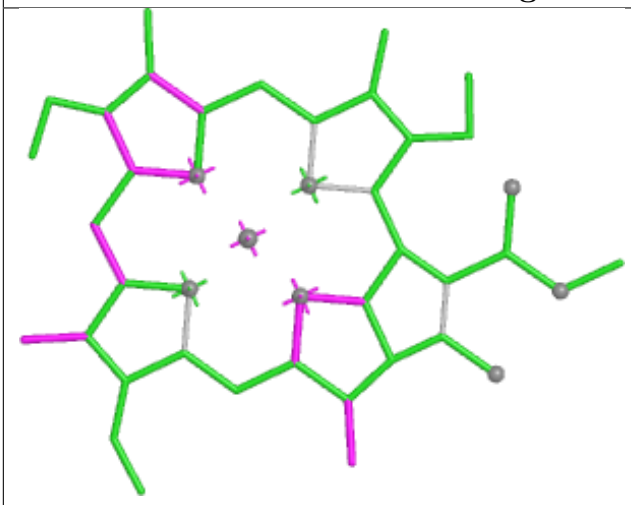


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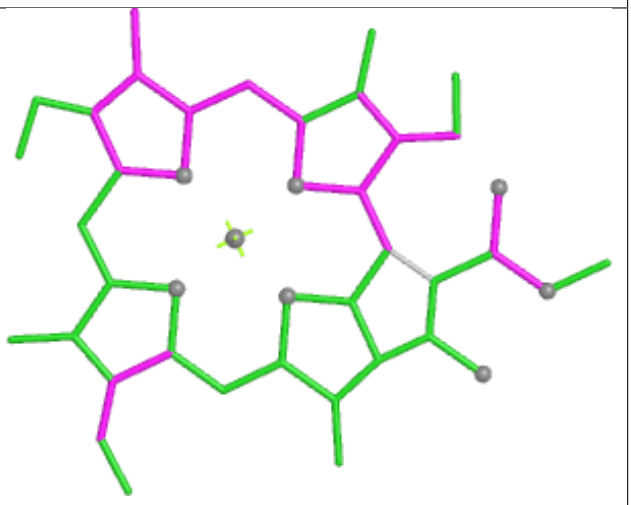


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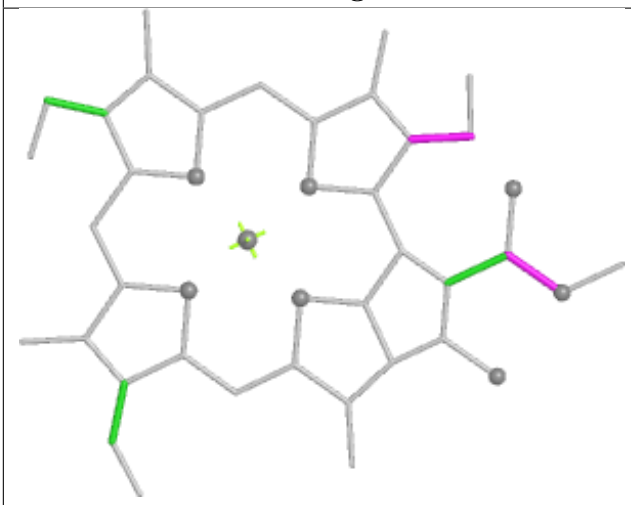
Ligand CLA 22 604



Bond lengths



Bond angles

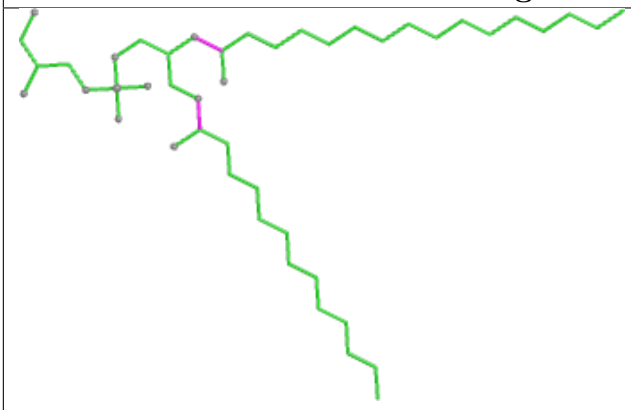


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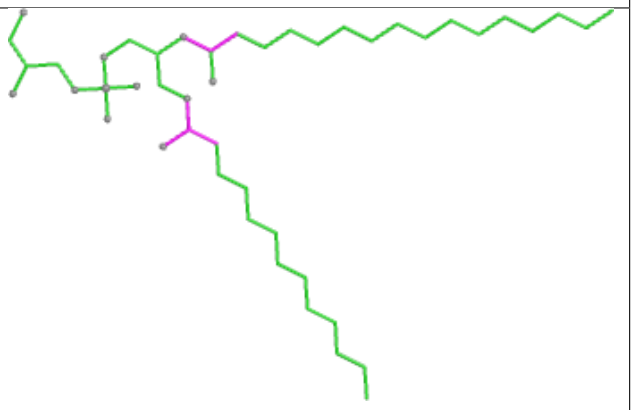


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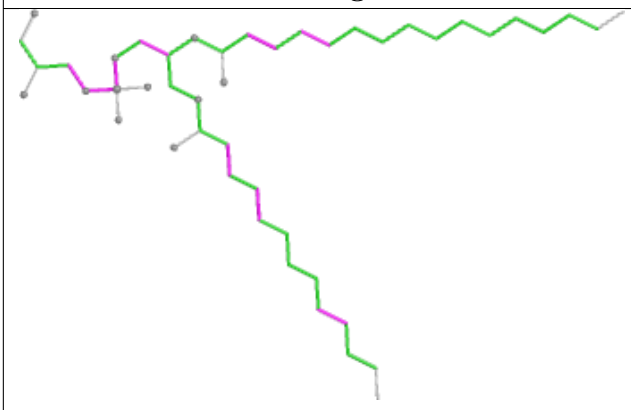
Ligand LHG dL 408



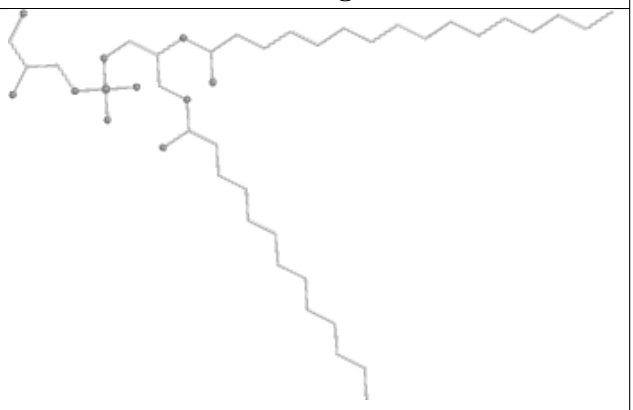
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Bond angles

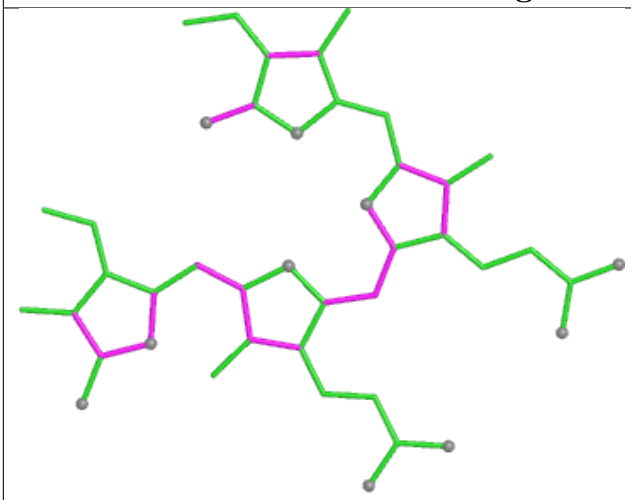


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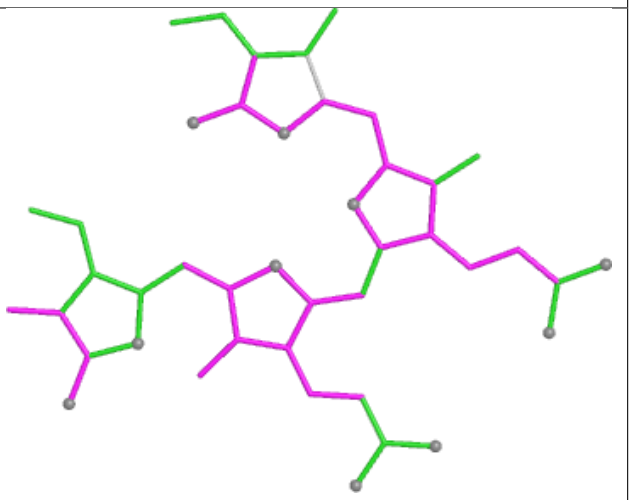


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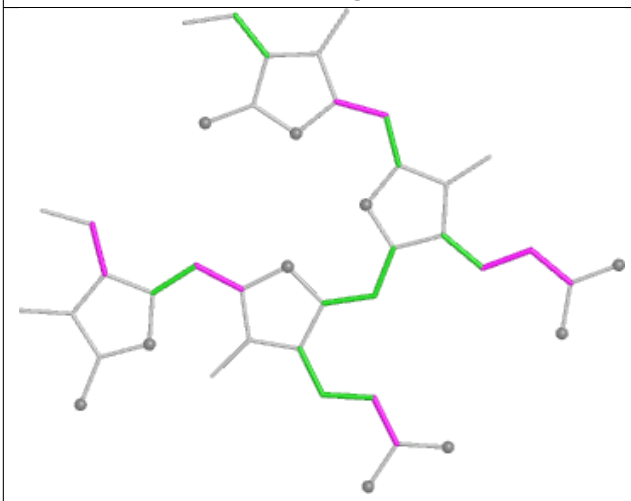
Ligand PEB X5 201



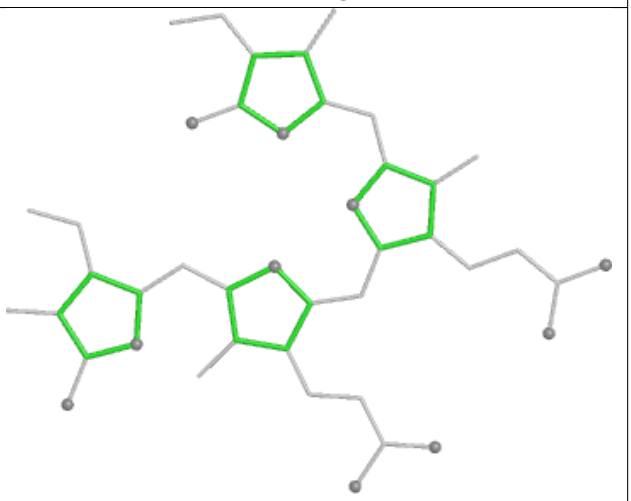
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Bond angles

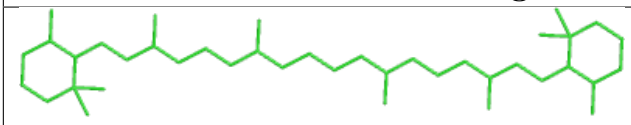


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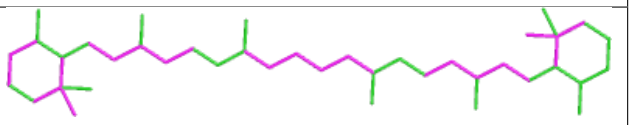


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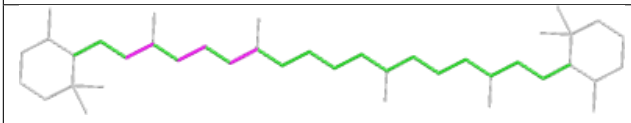
Ligand BCR HL 103



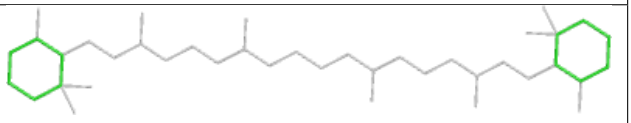
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Bond angles

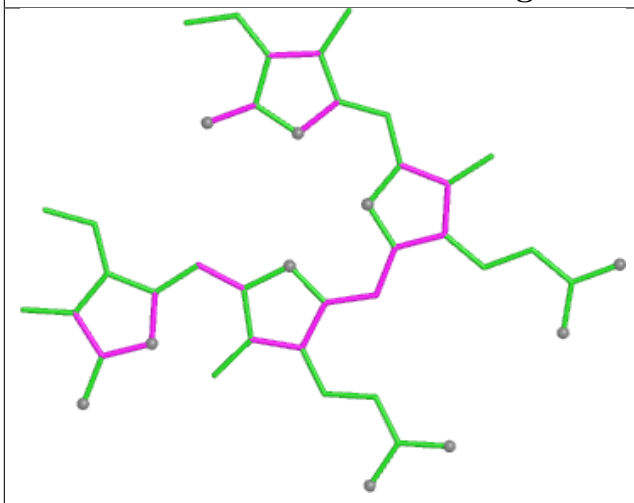


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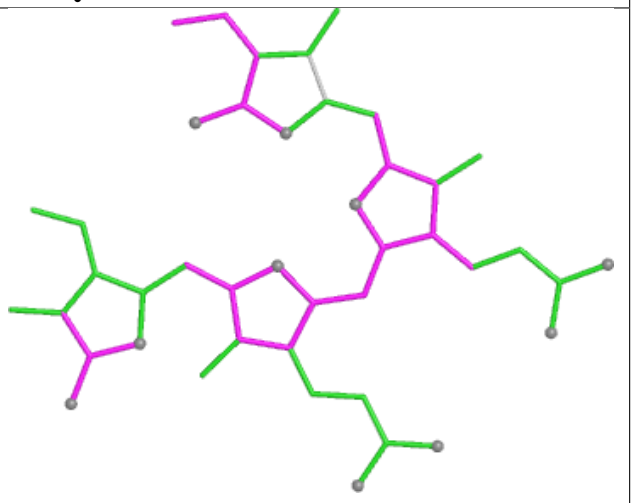


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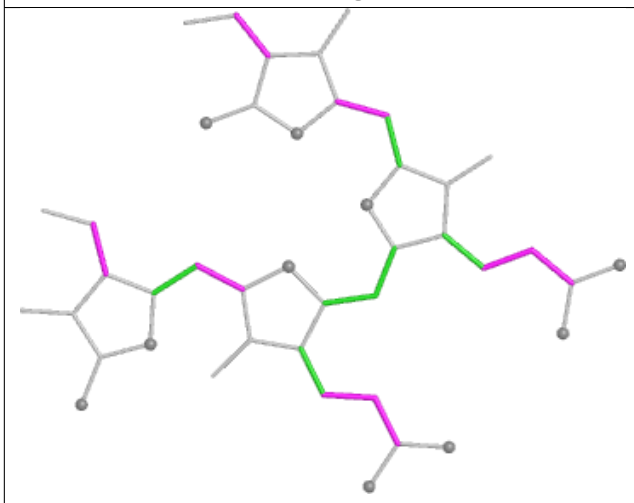
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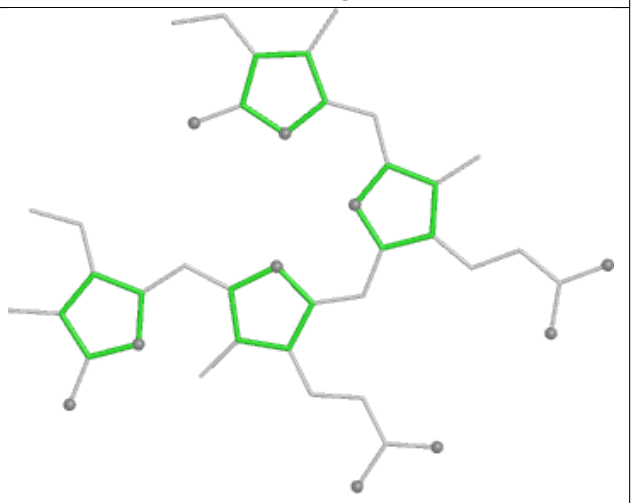
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Bond angles

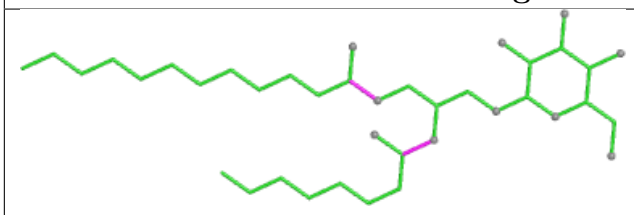


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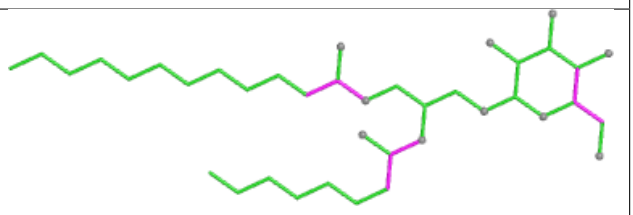


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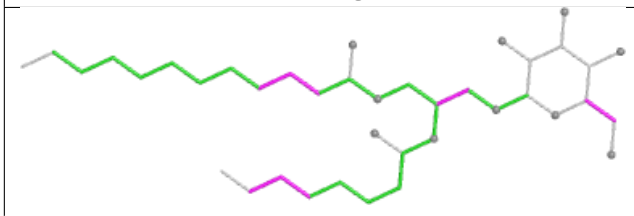
Ligand LMG bL 624



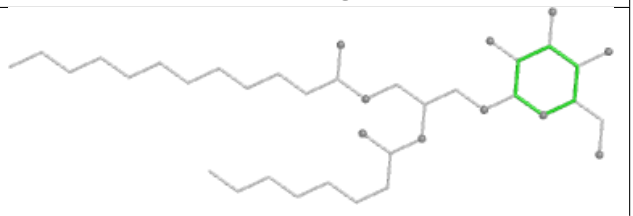
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Bond angles

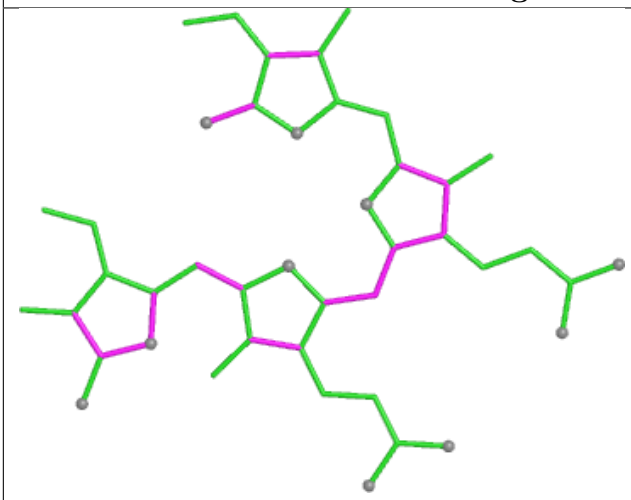


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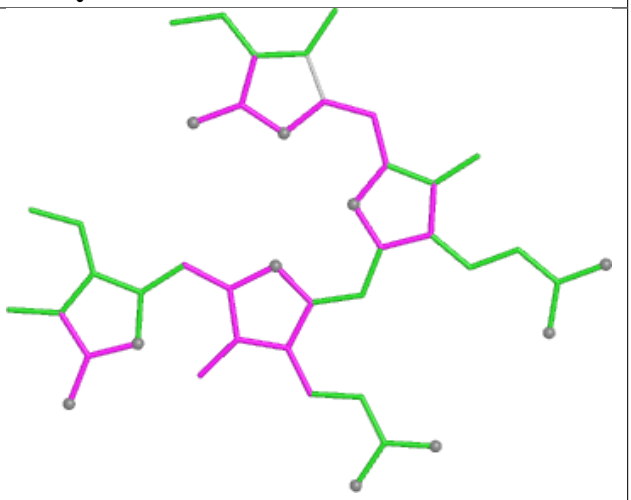


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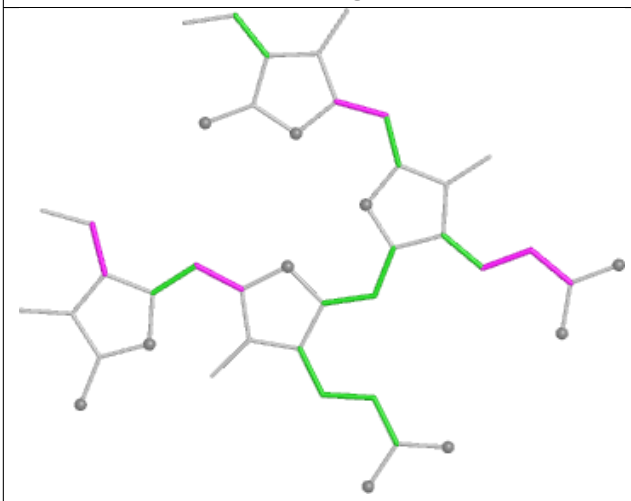
Ligand PEB KQ 201



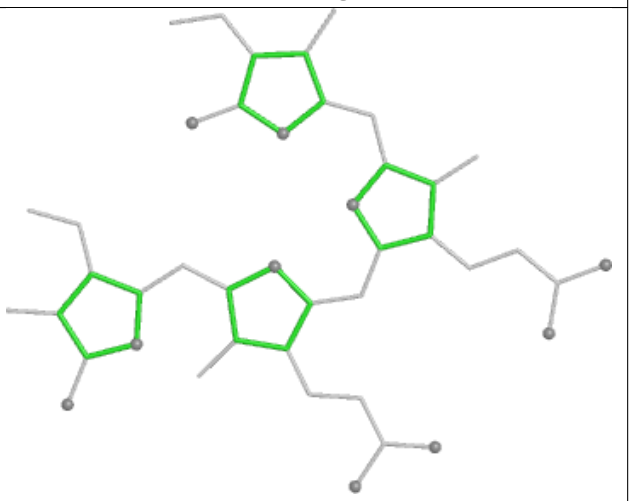
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Bond angles

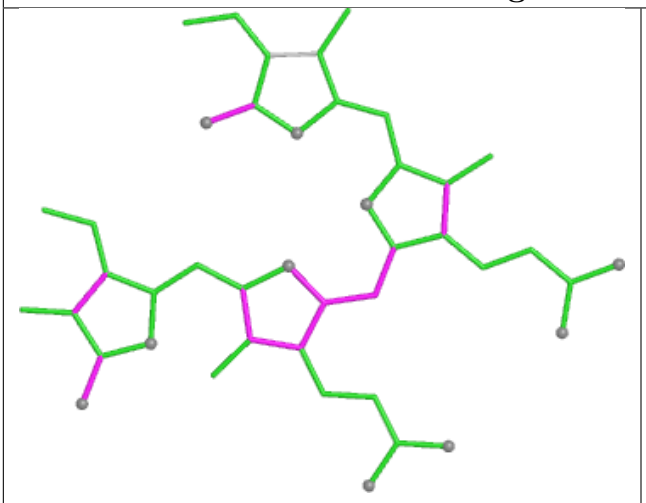


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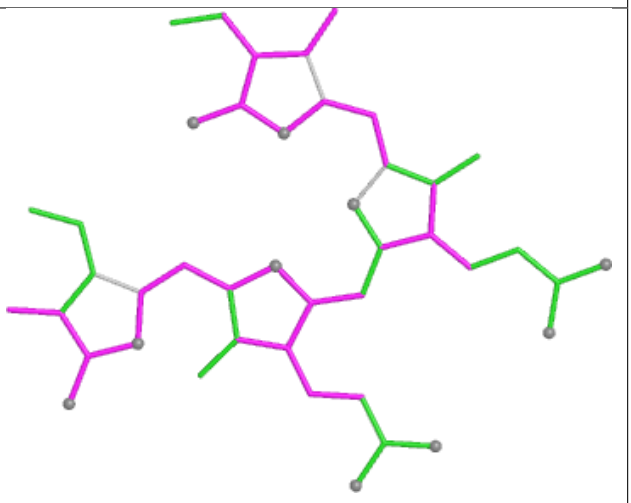


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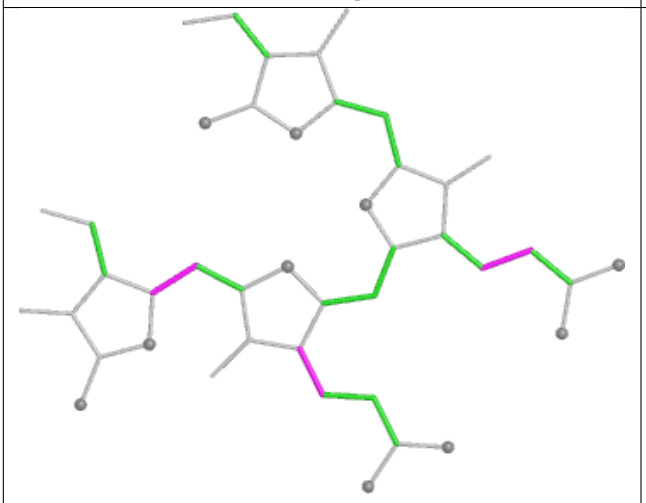
Ligand PUB AH 303



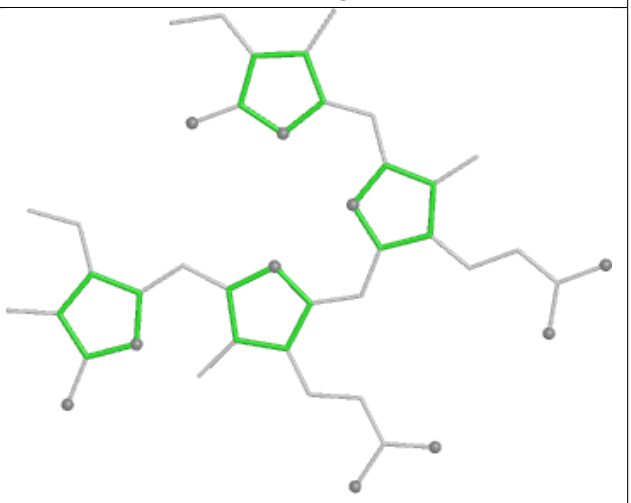
Bond lengths



Bond angles

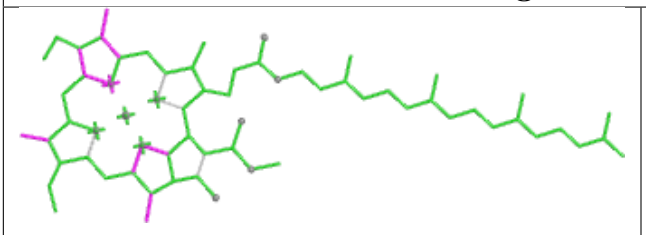


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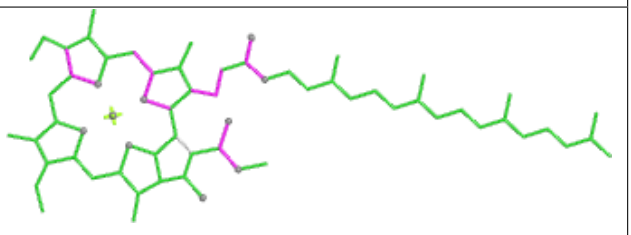


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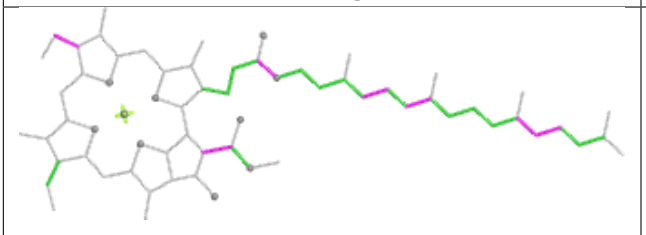
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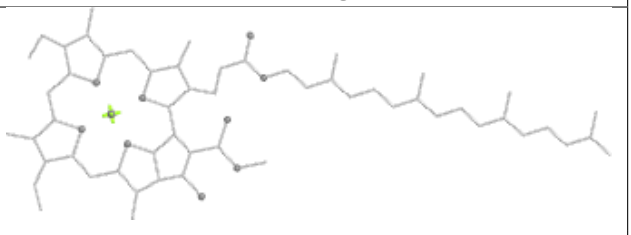
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Bond angles

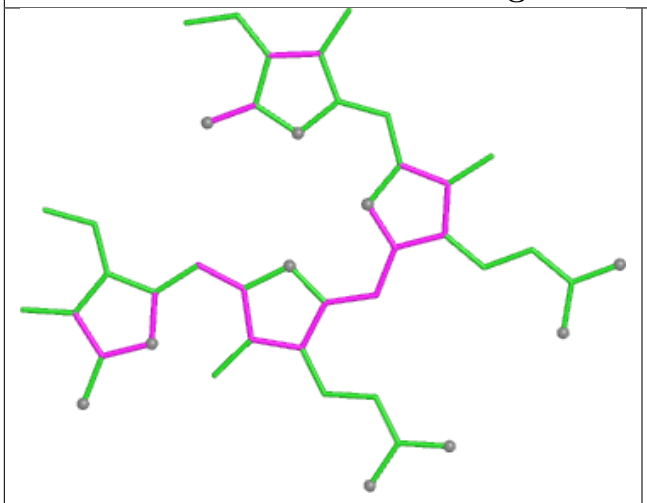


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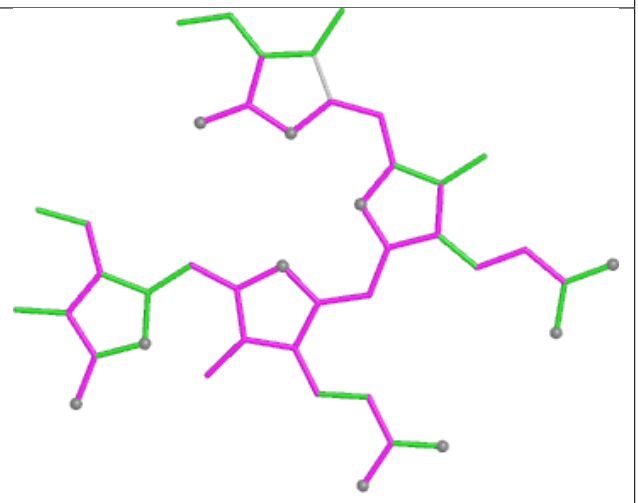


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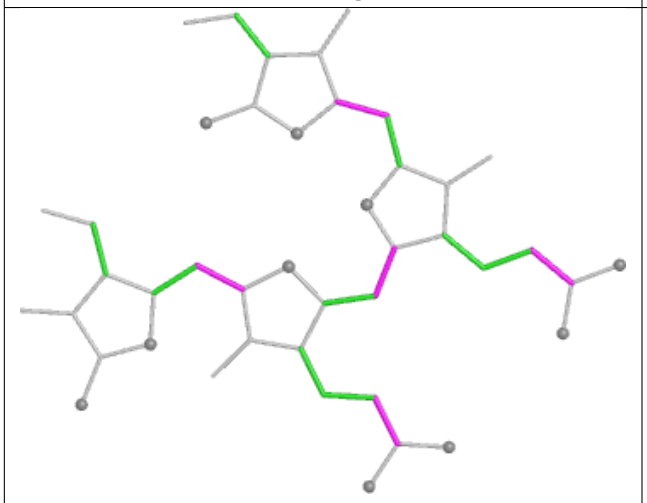
Ligand PEB XM 202



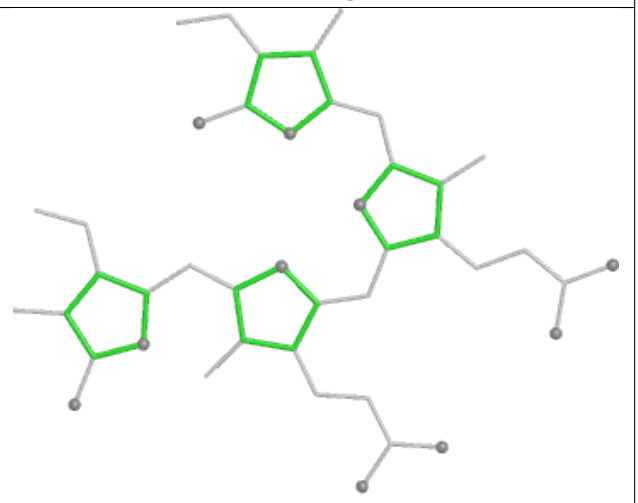
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Bond angles

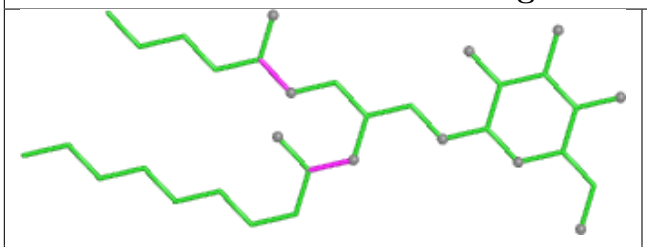


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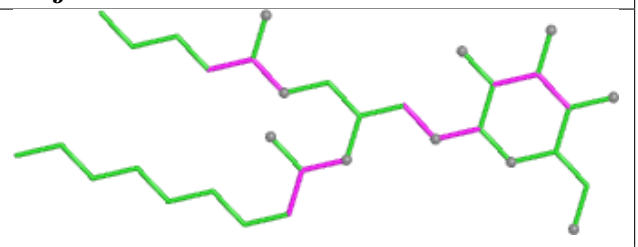


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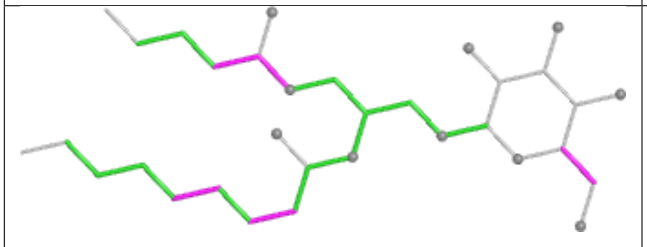
Ligand LMG jL 101



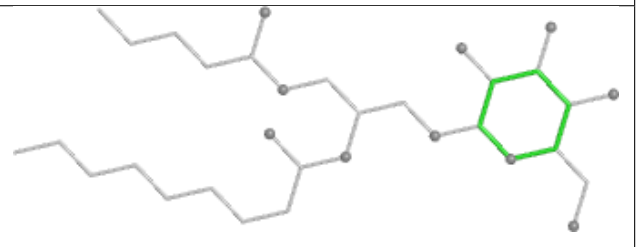
Bond lengths



Bond angles

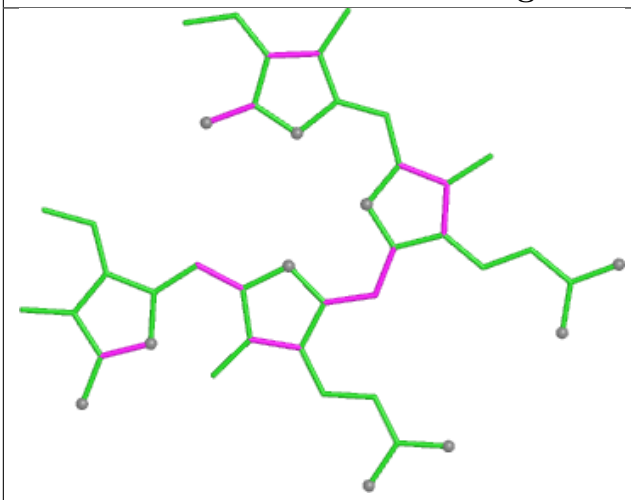


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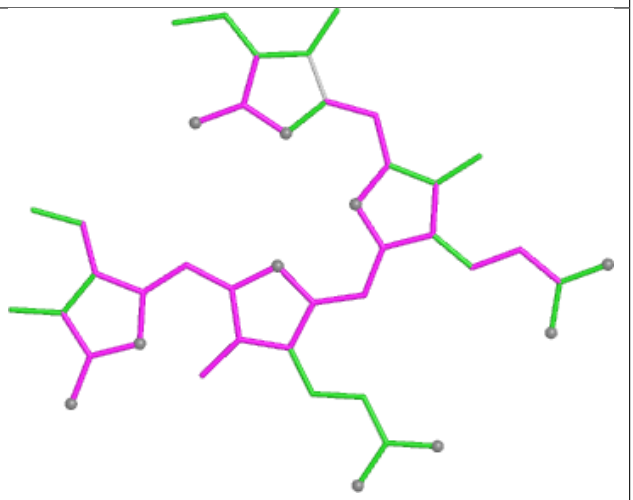


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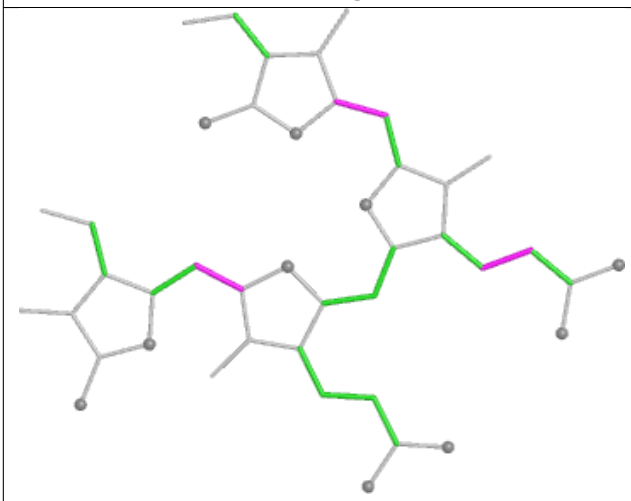
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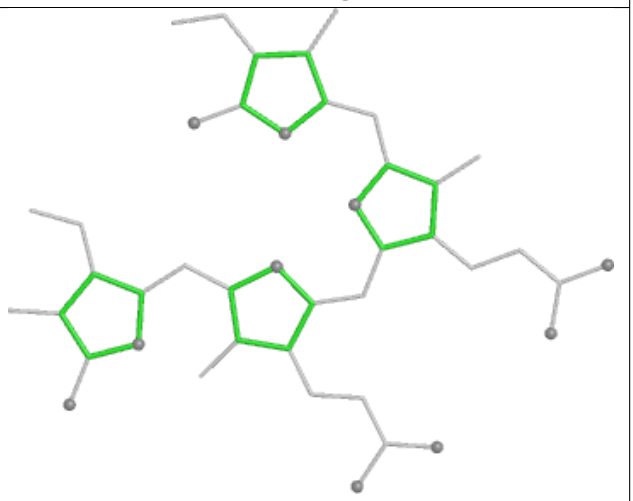
Bond lengths



Bond angles

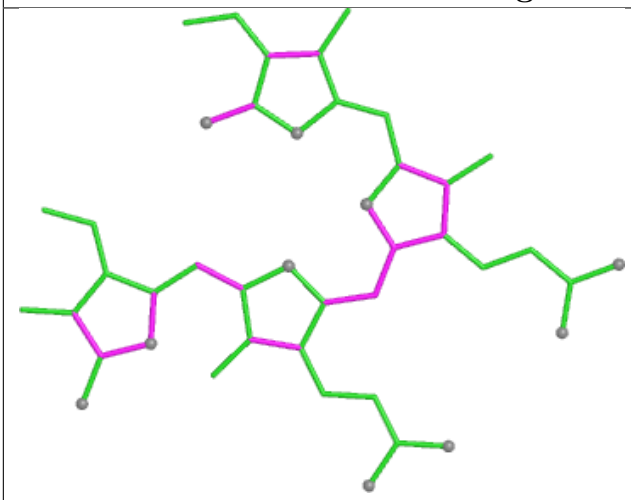


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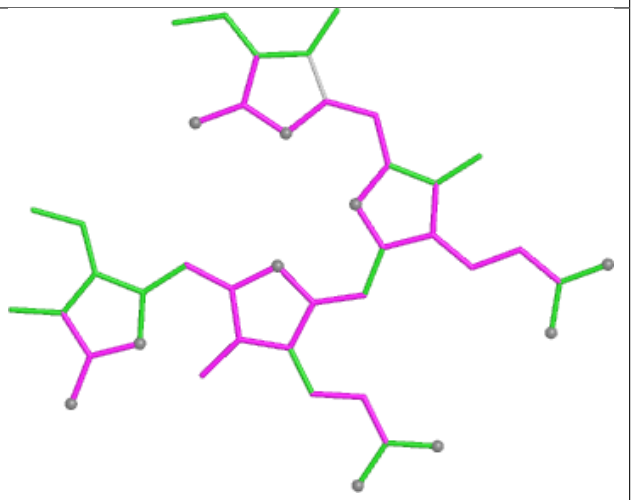


Rings

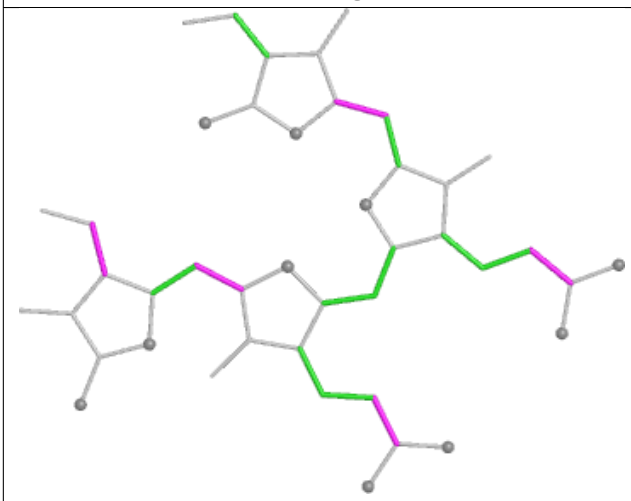
Ligand PEB SE 201



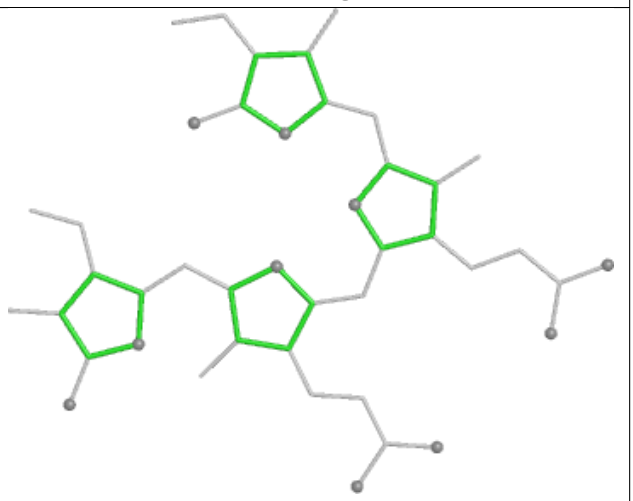
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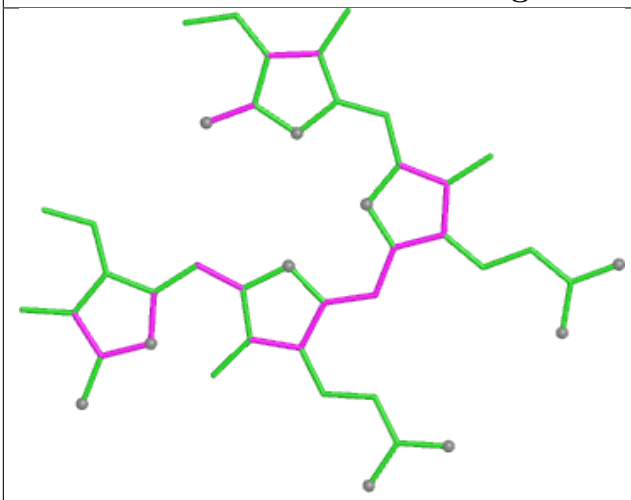


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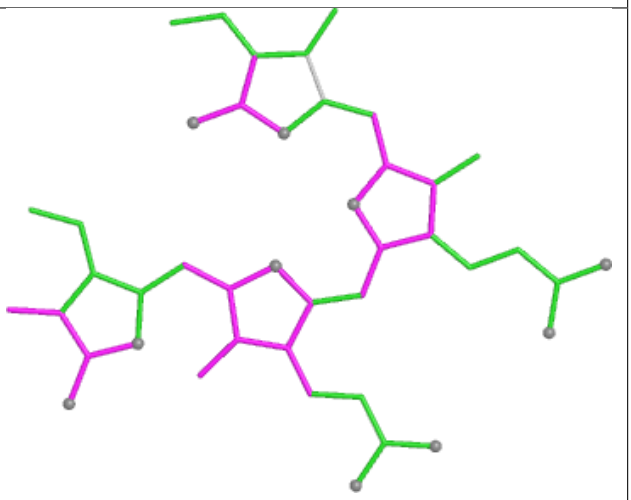


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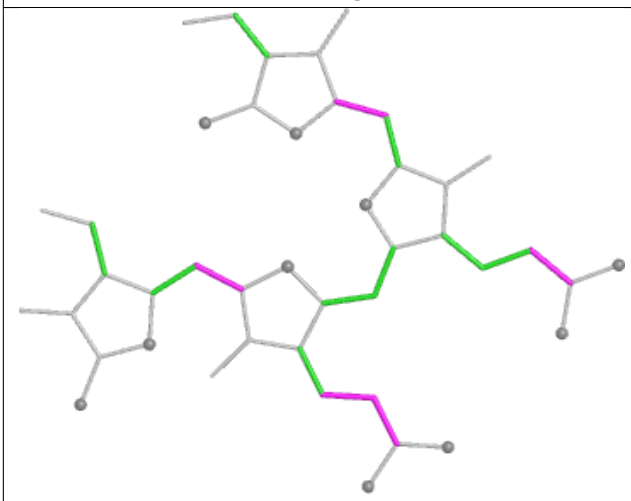
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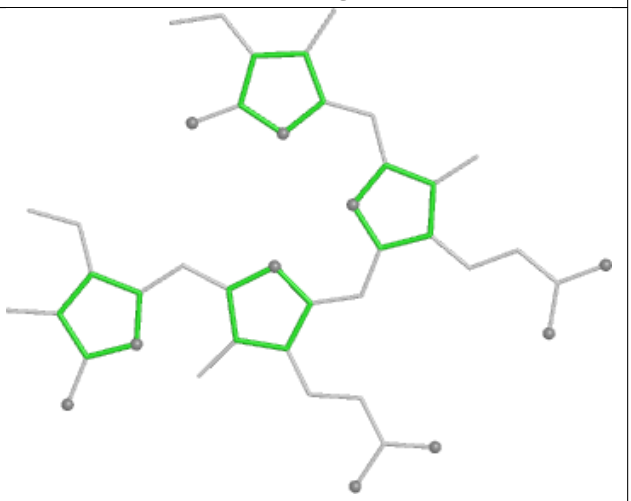
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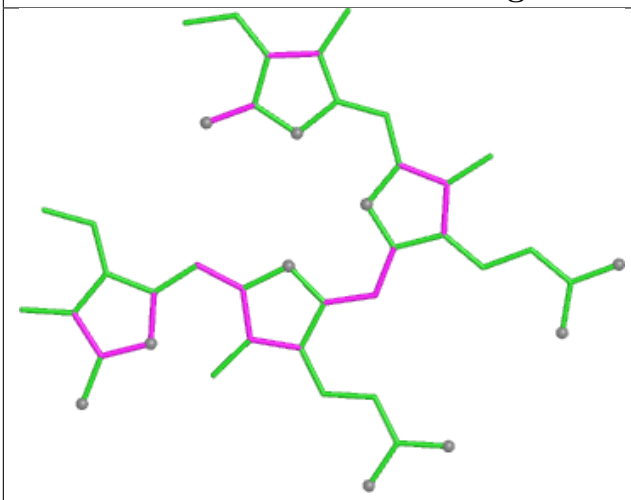


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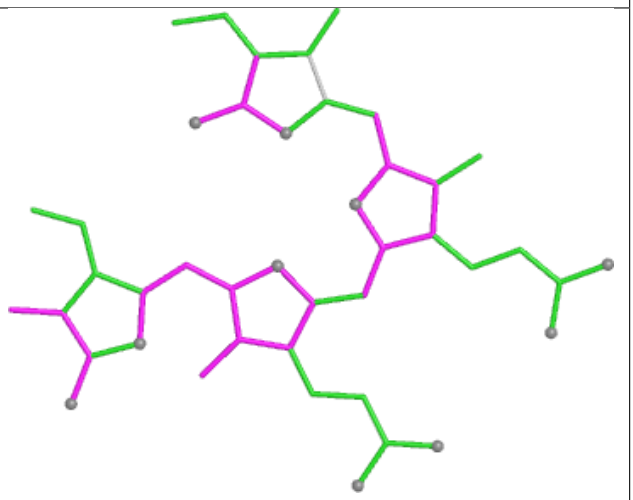


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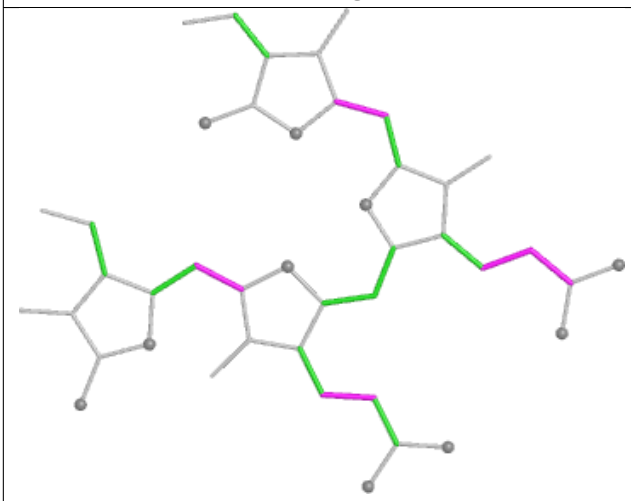
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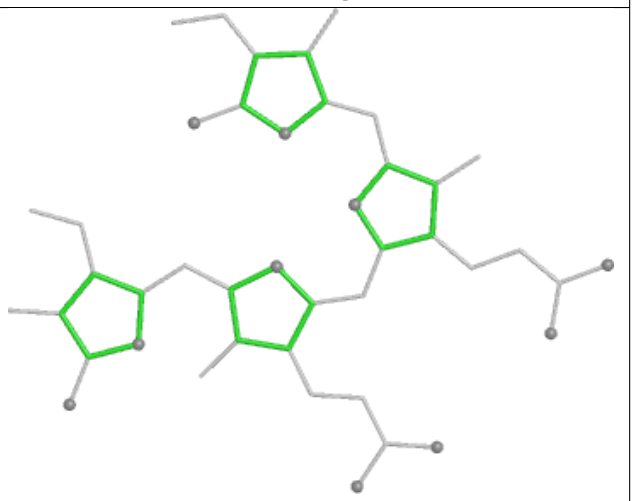
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Bond angles

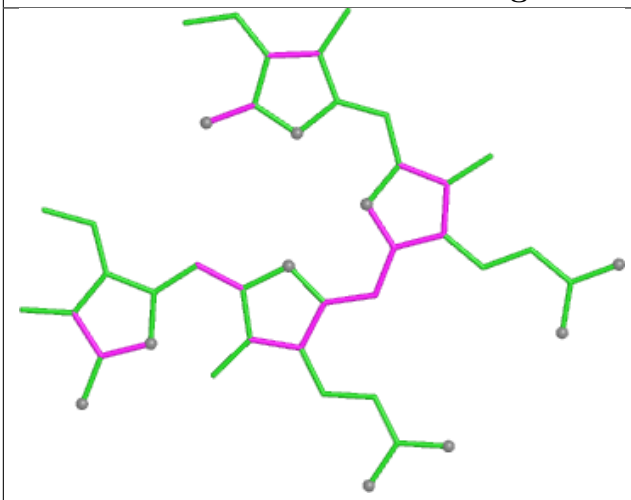


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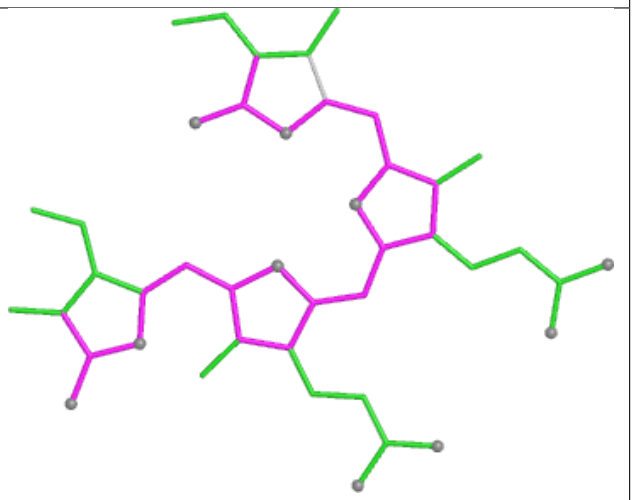


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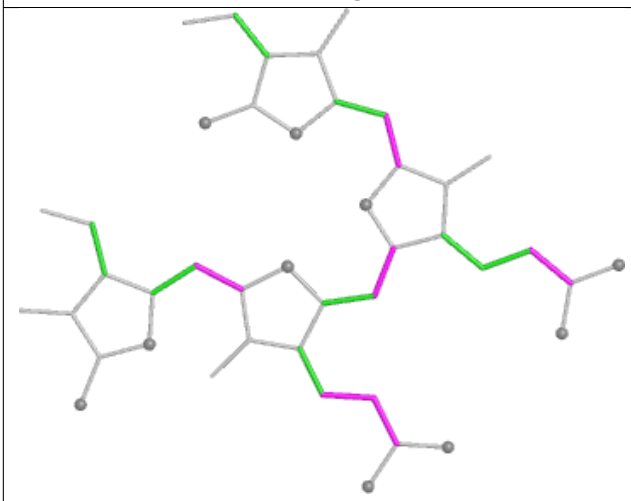
Ligand PEB AD 304



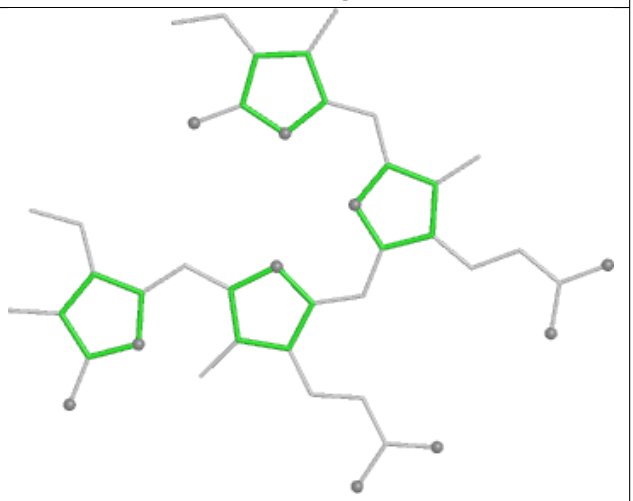
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Bond angles

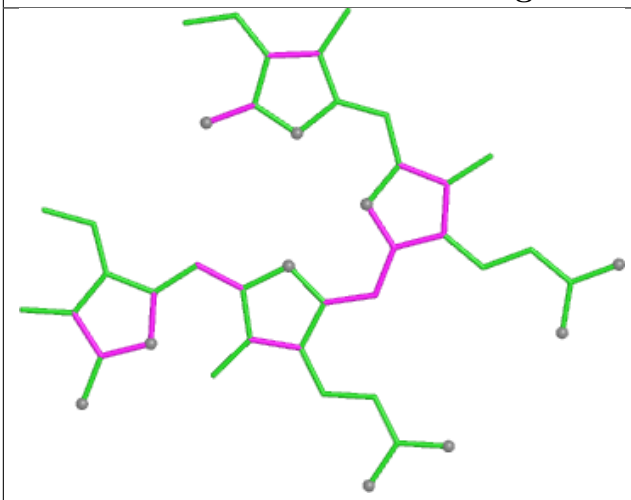


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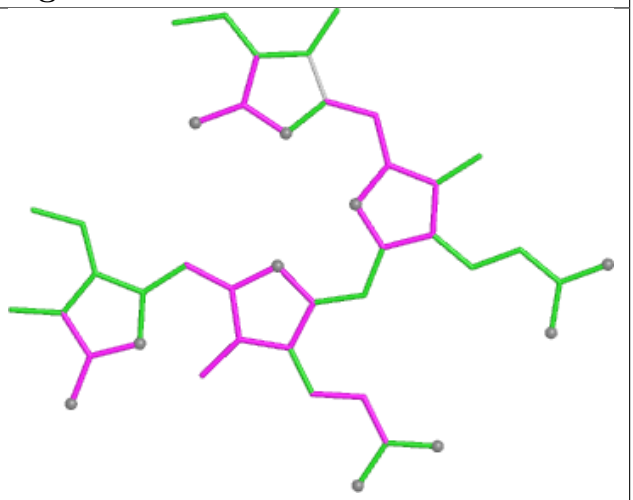


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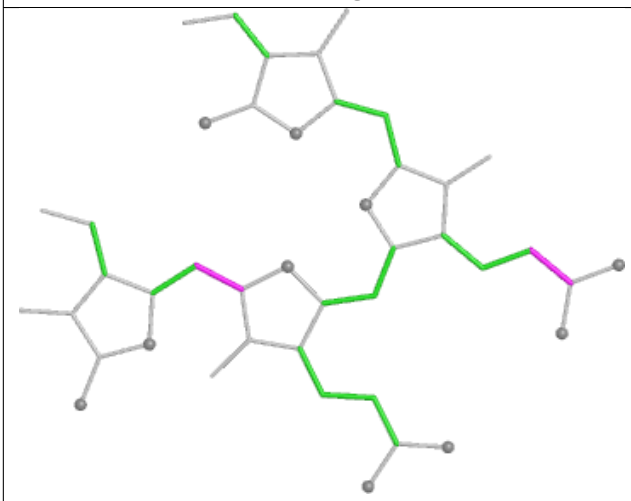
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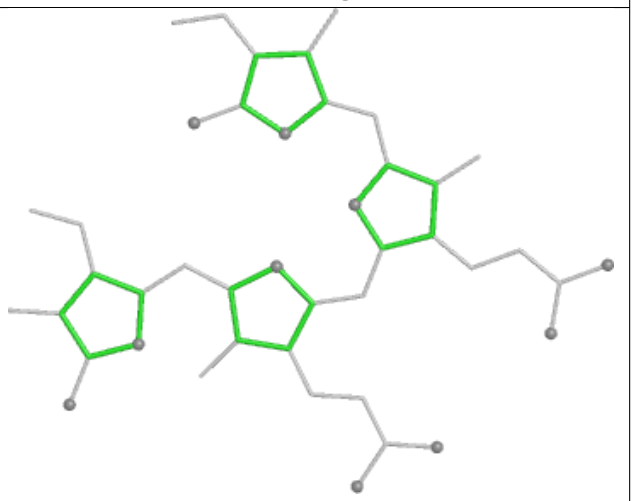
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Bond angles

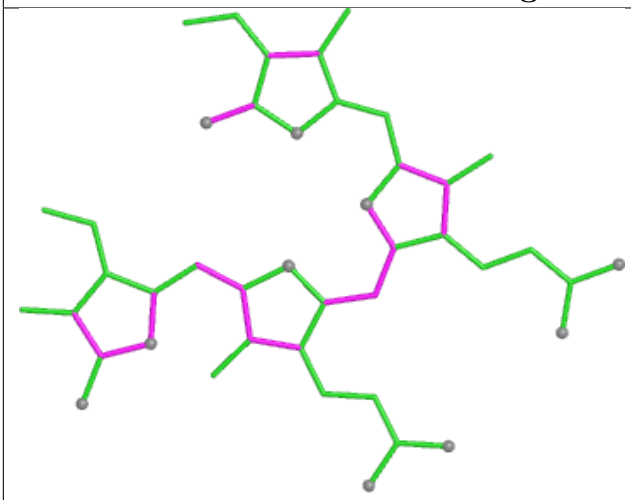


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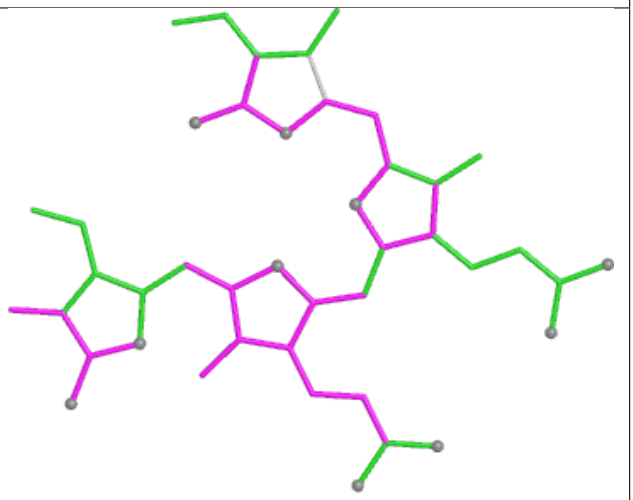


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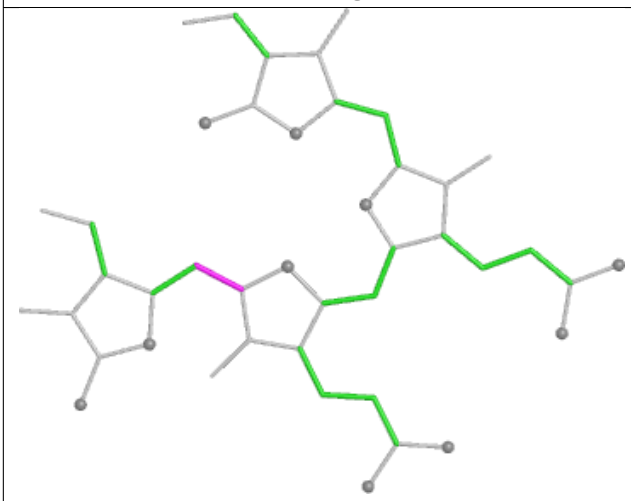
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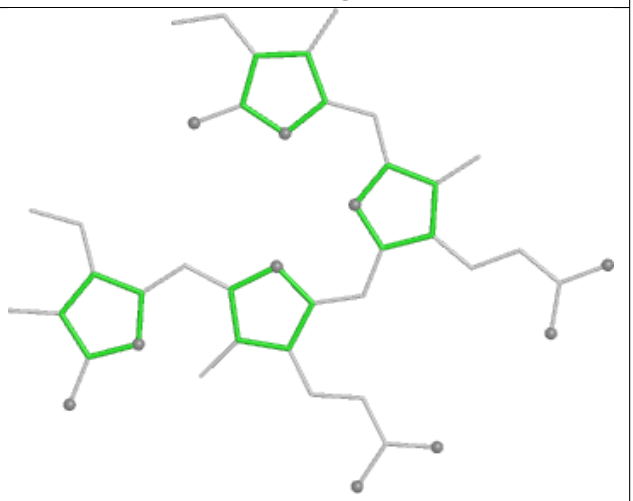
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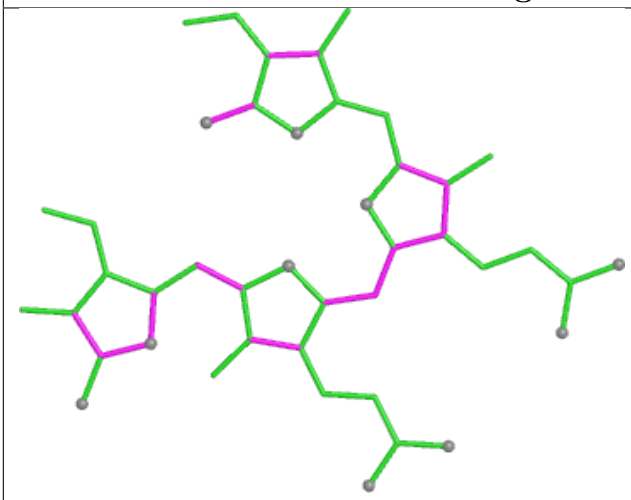


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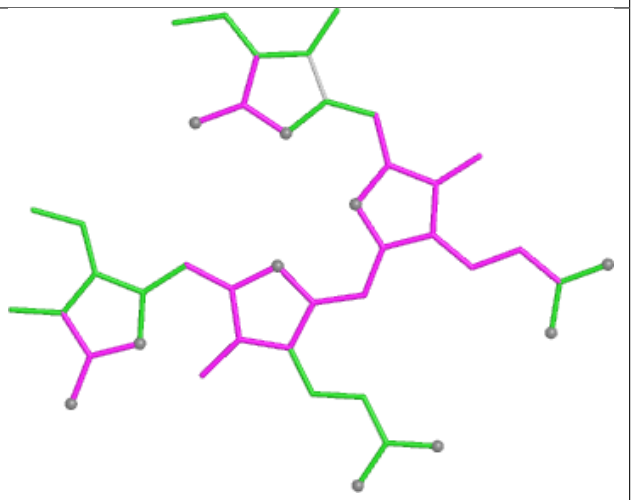


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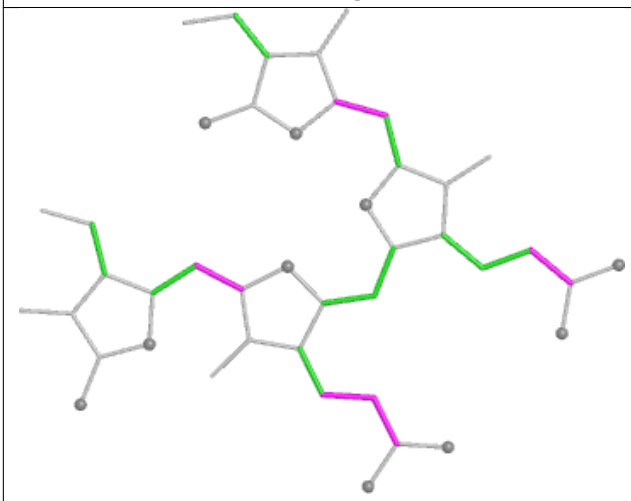
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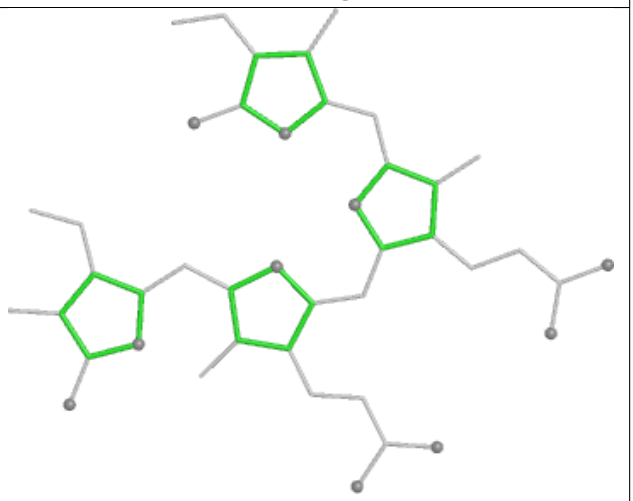
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Bond angles

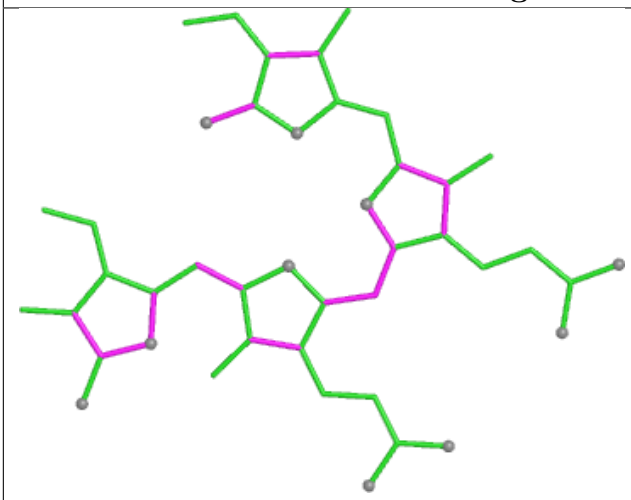


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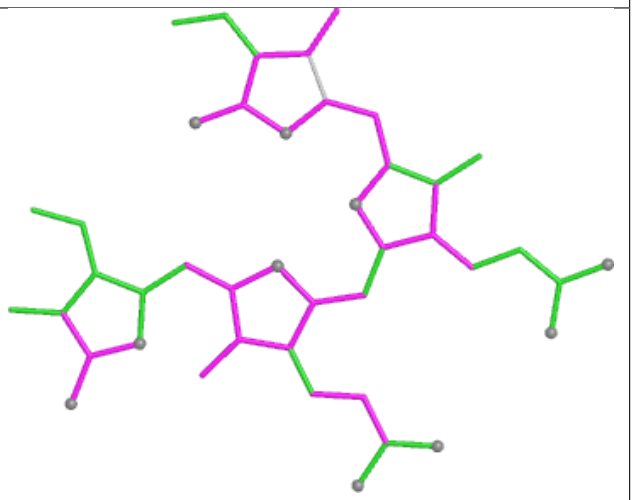


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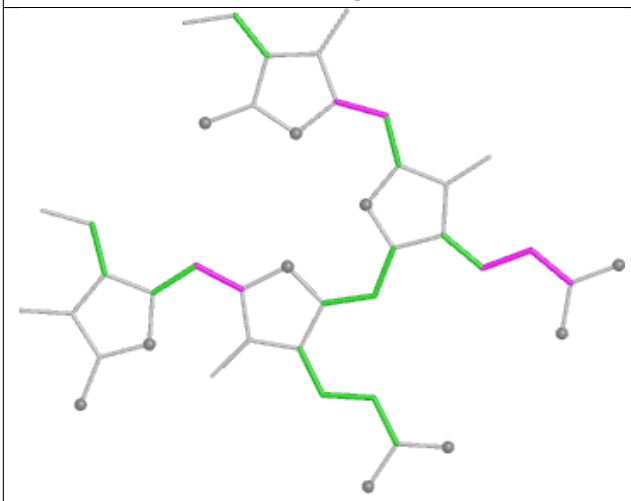
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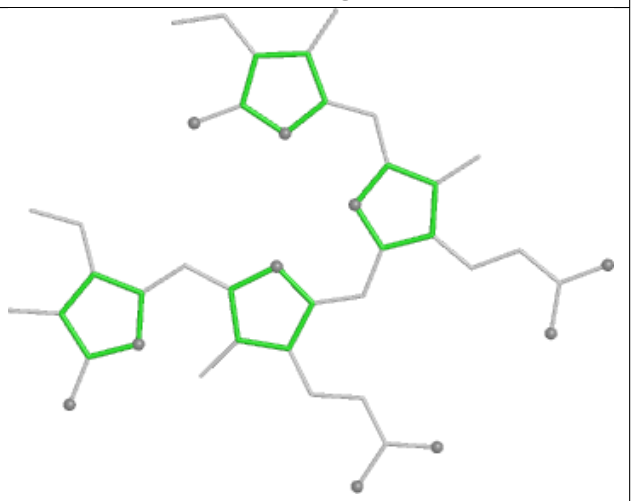
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Bond angles

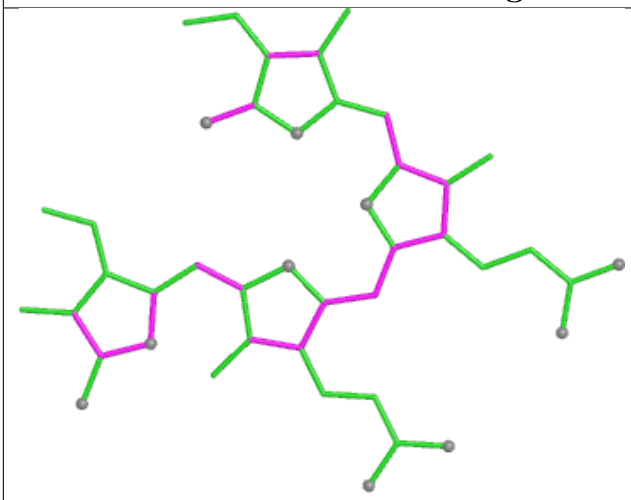


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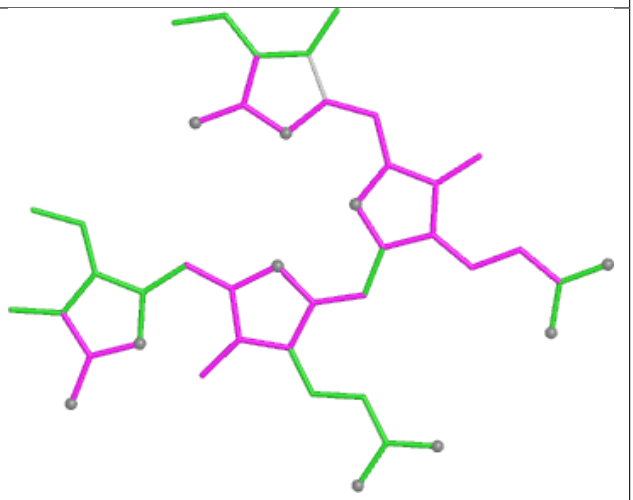


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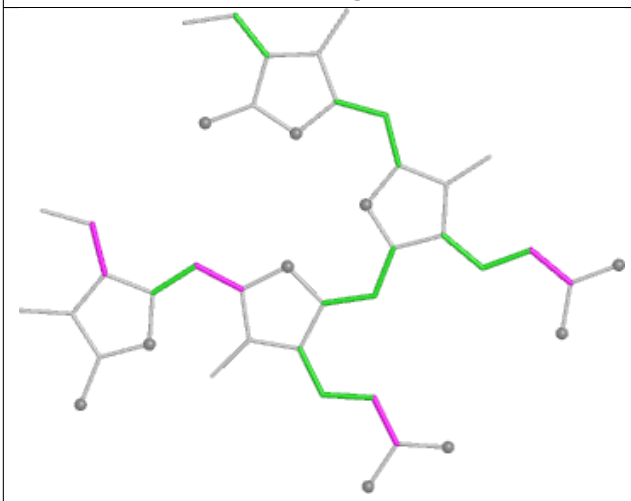
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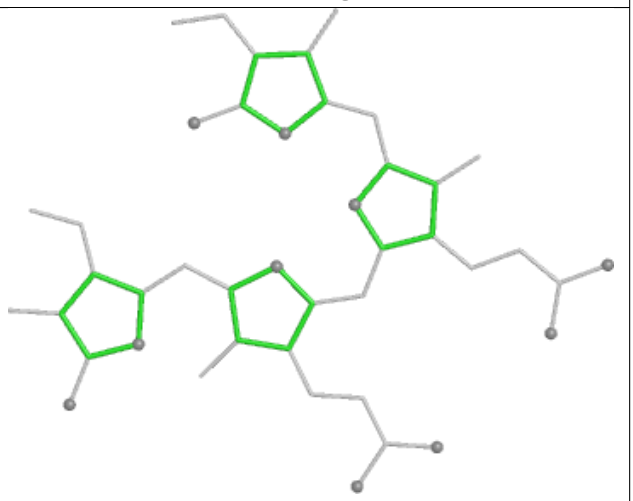
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Bond angles

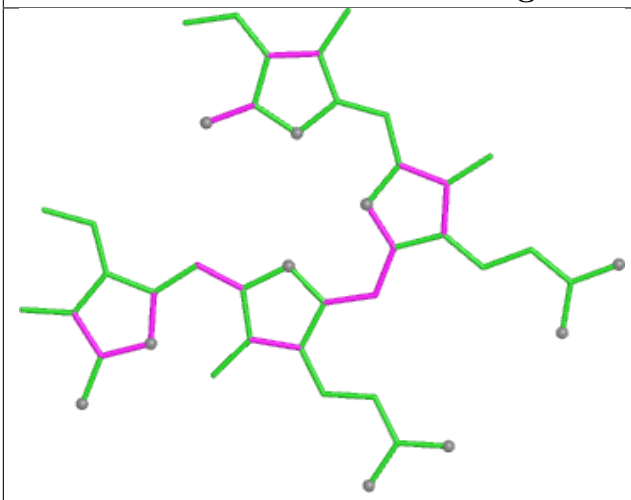


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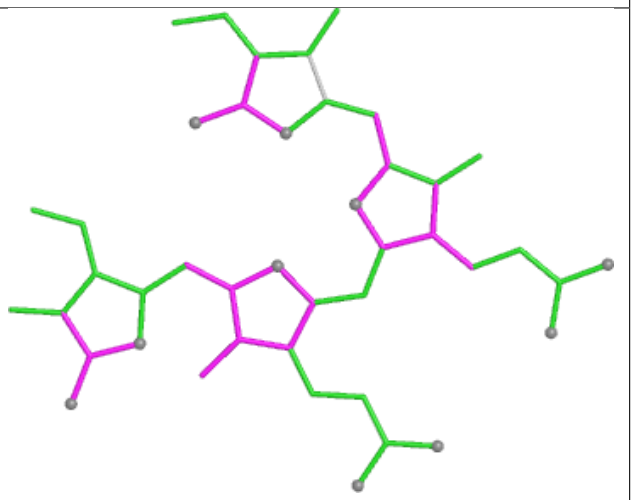


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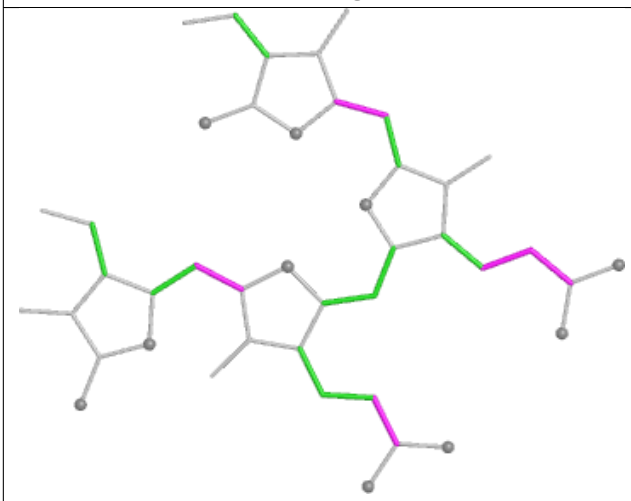
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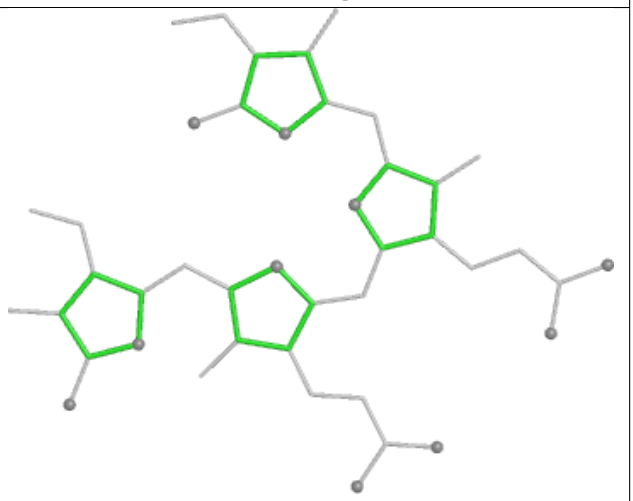
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Bond angles

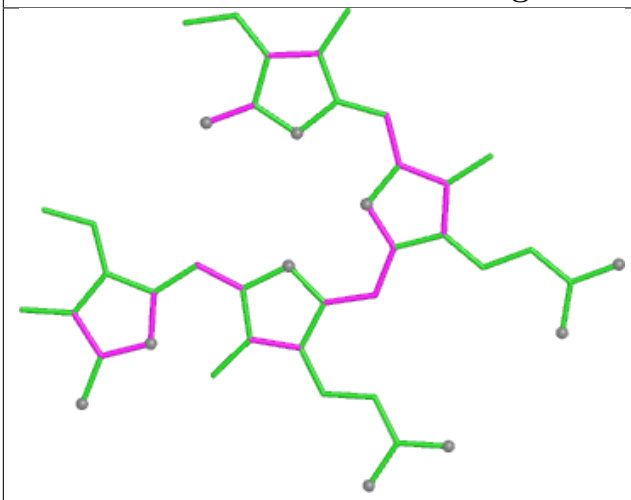


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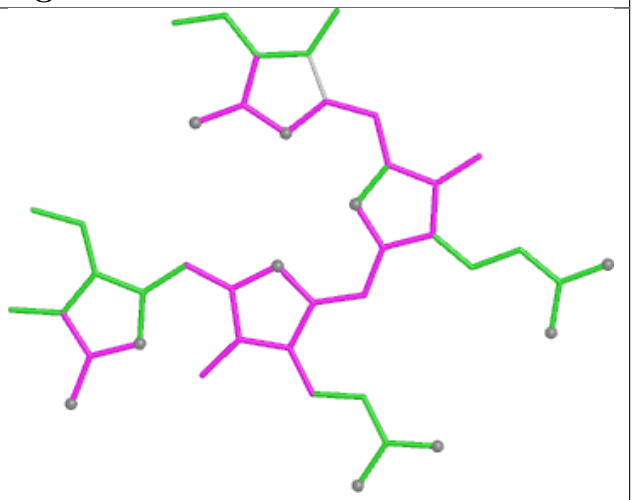


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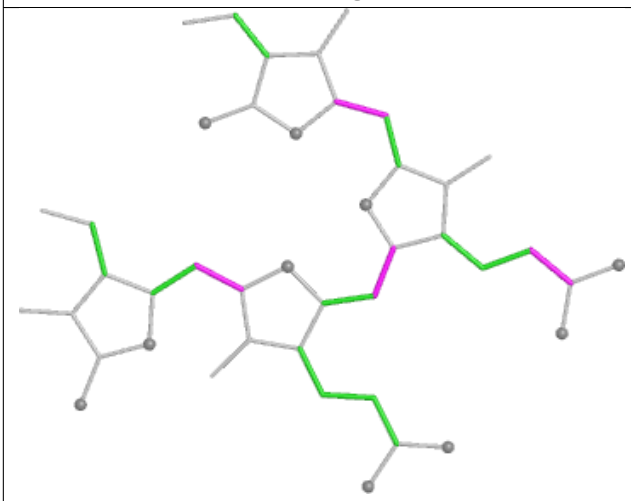
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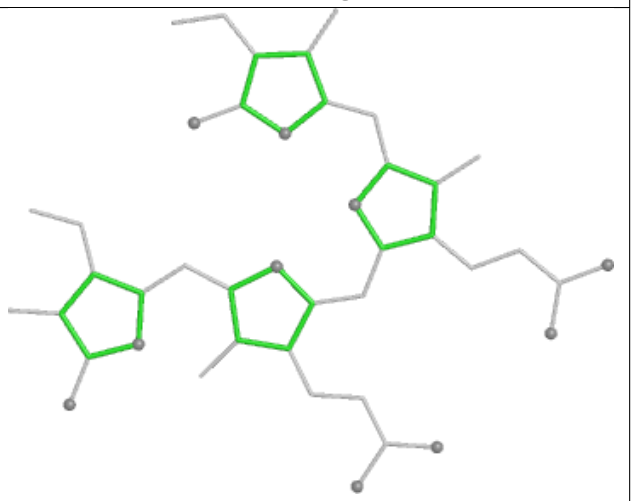
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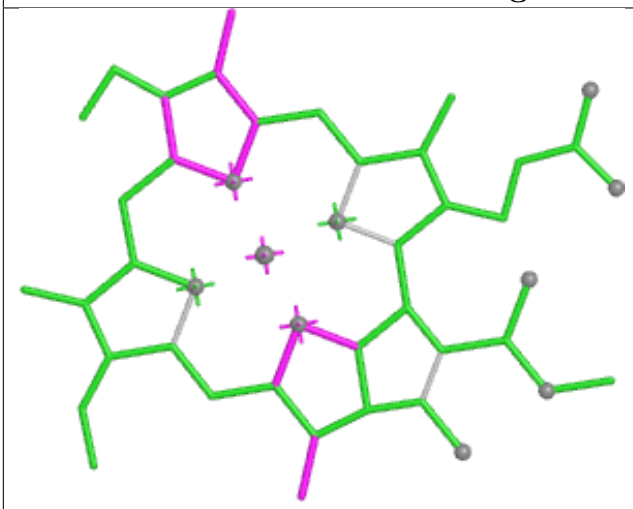


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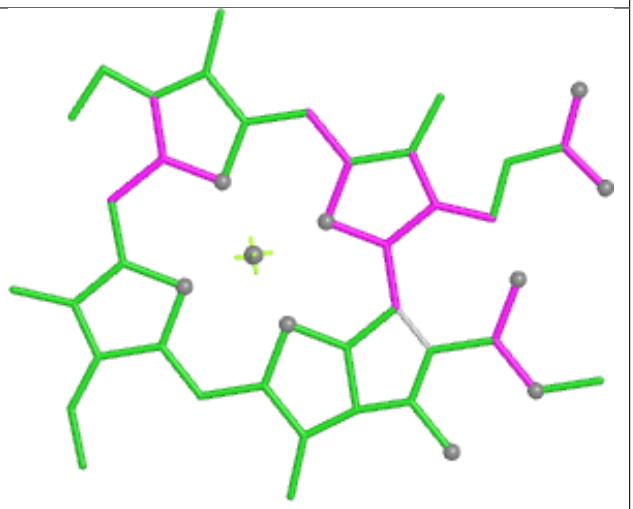


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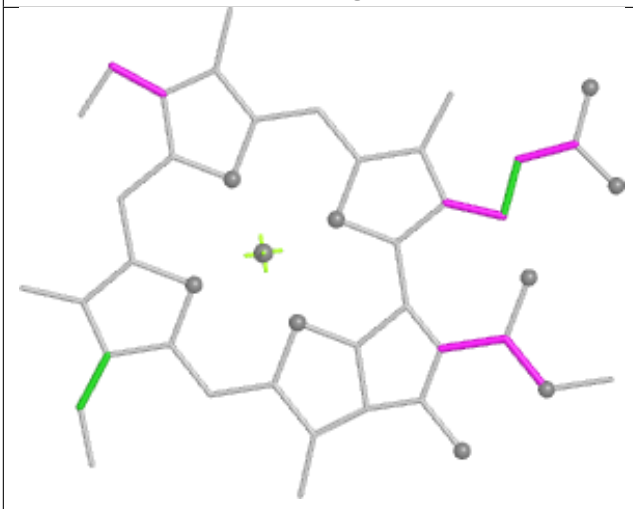
Ligand CLA AN 822



Bond lengths



Bond angles

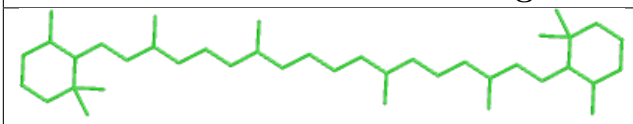


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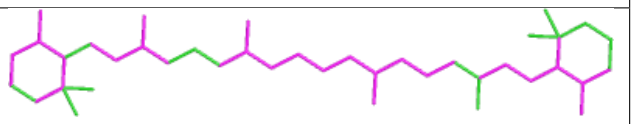


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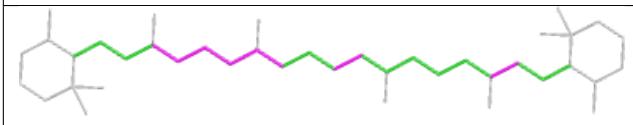
Ligand BCR L2 205



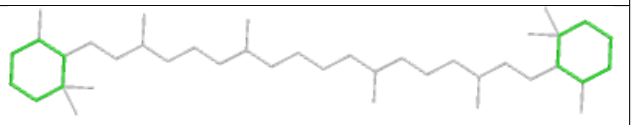
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Bond angles

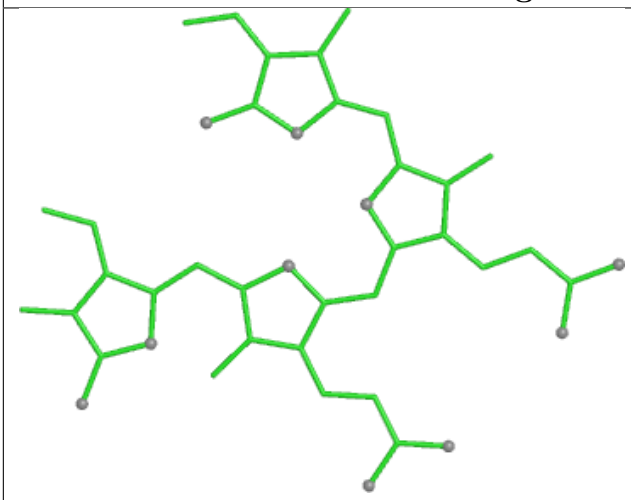


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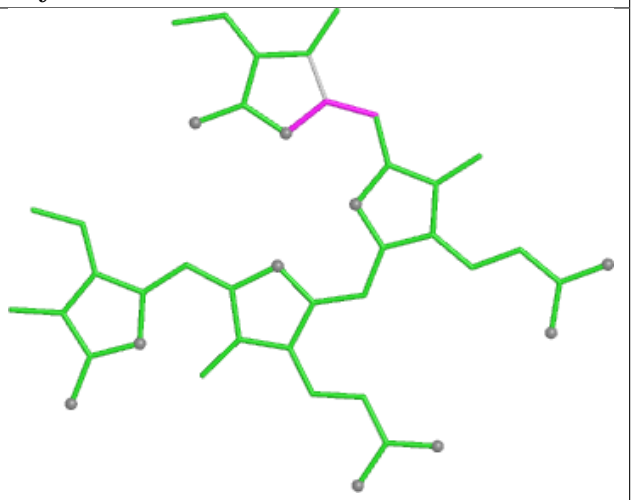


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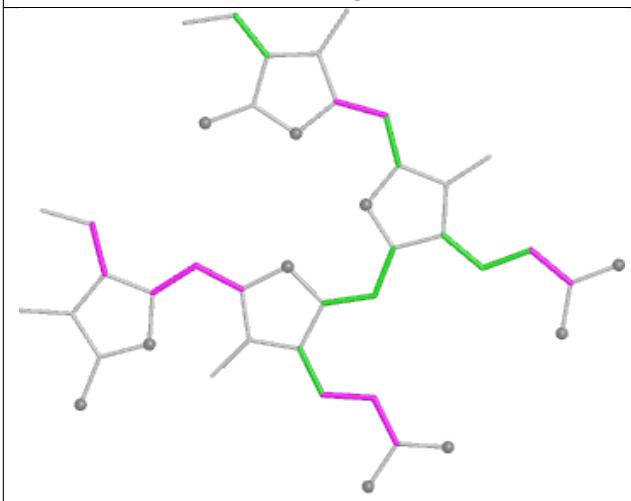
Ligand PEB yC 201



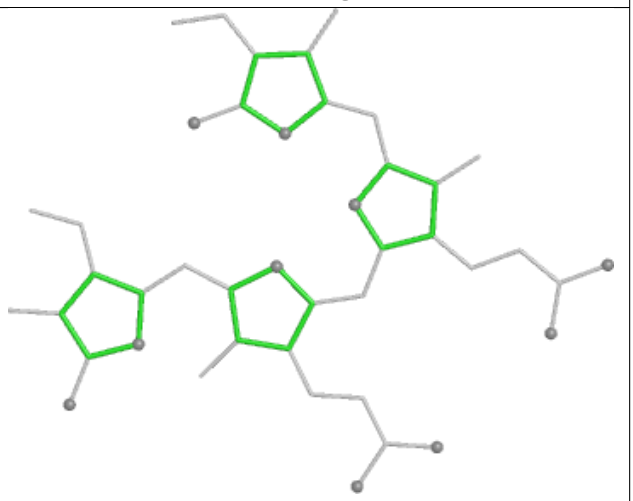
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Bond angles

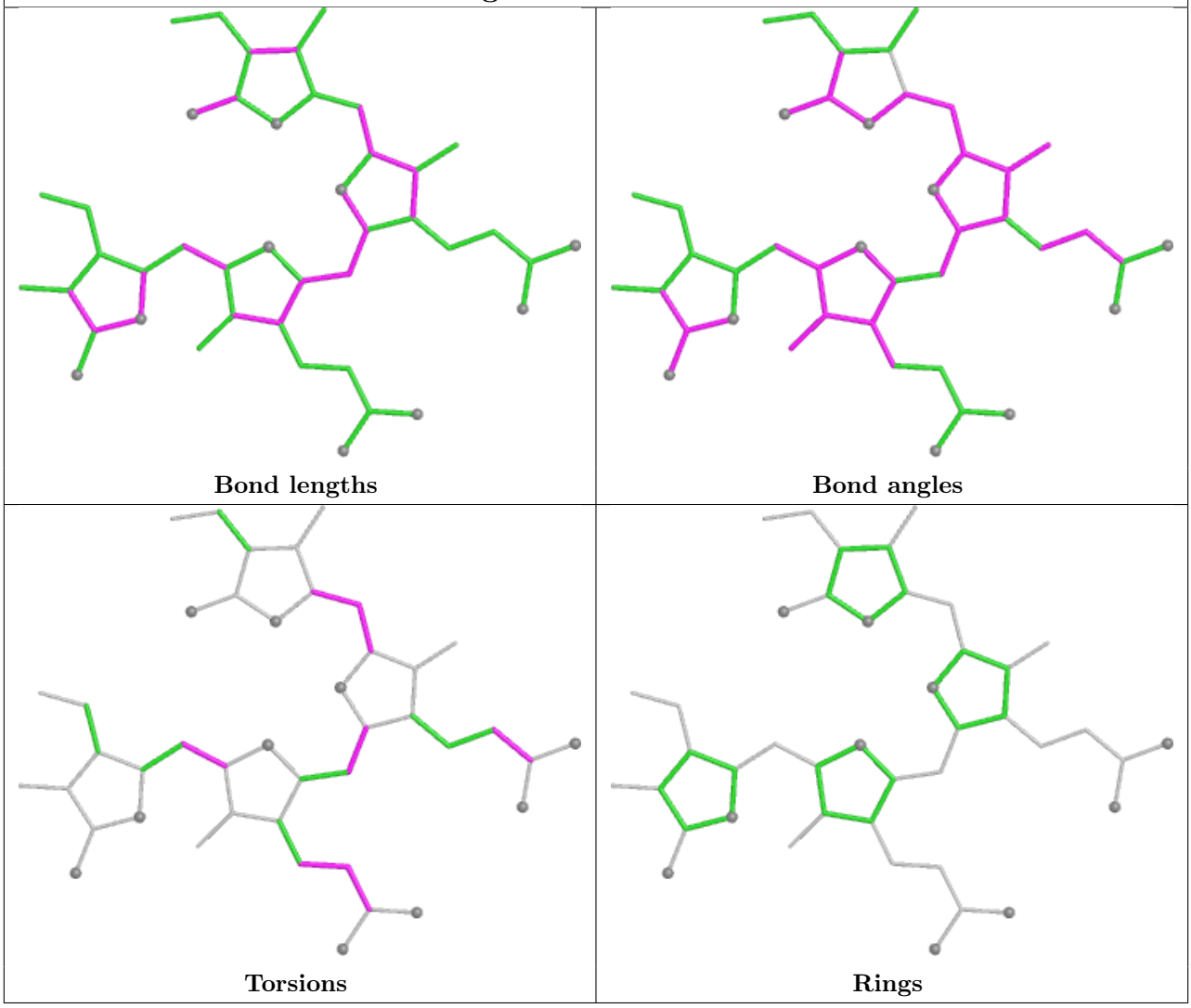


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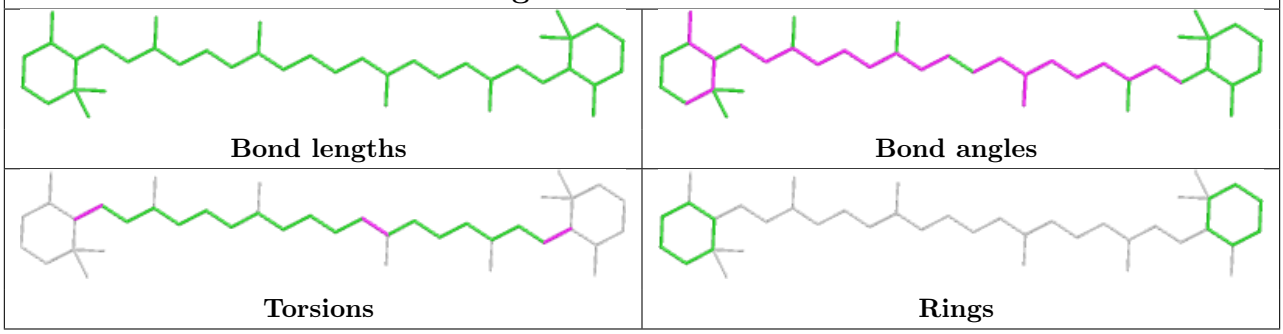


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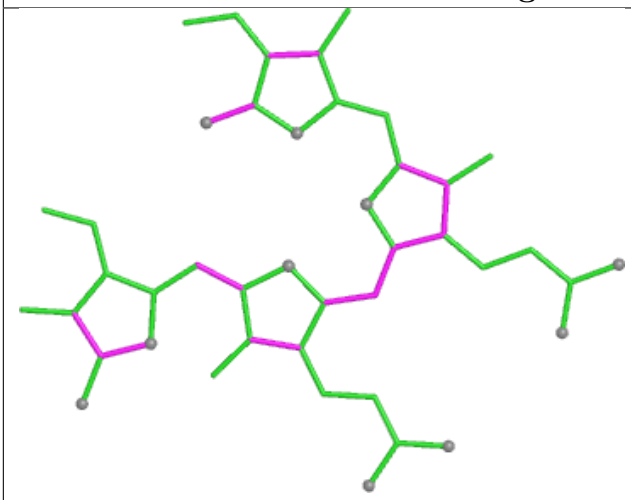
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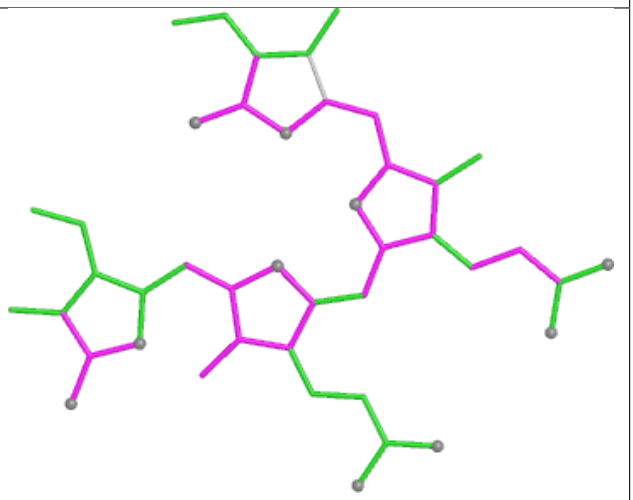
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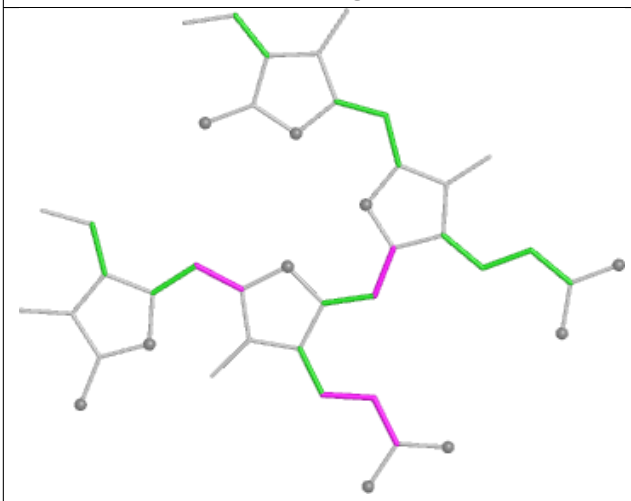
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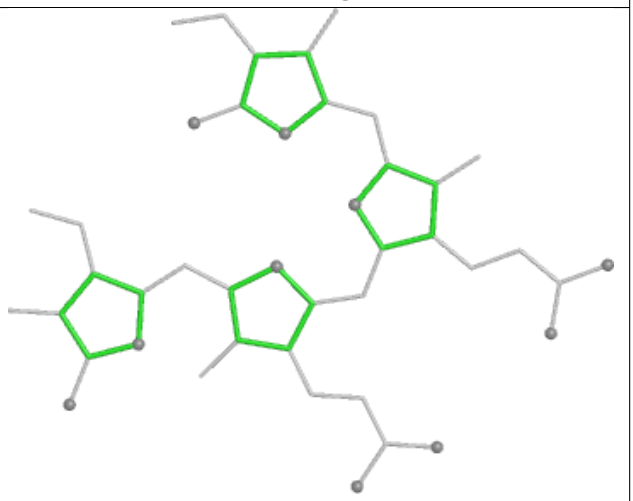
Bond lengths



Bond angles

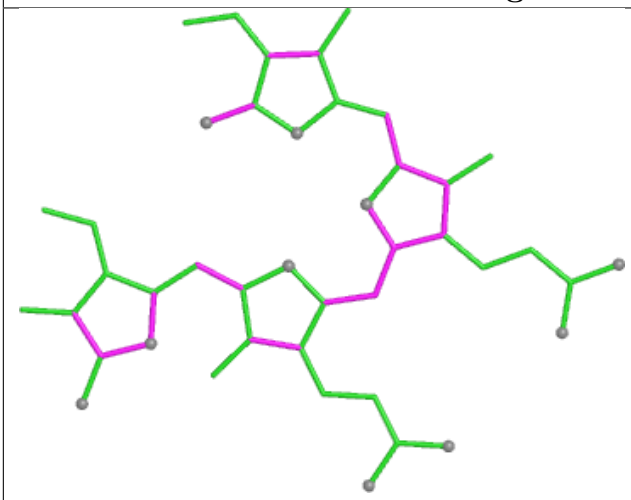


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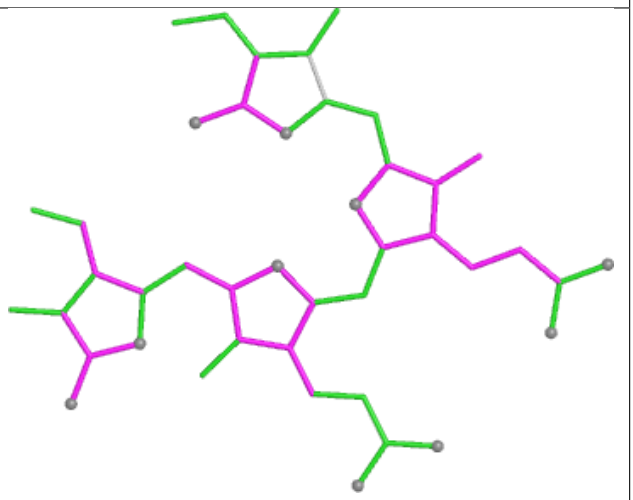


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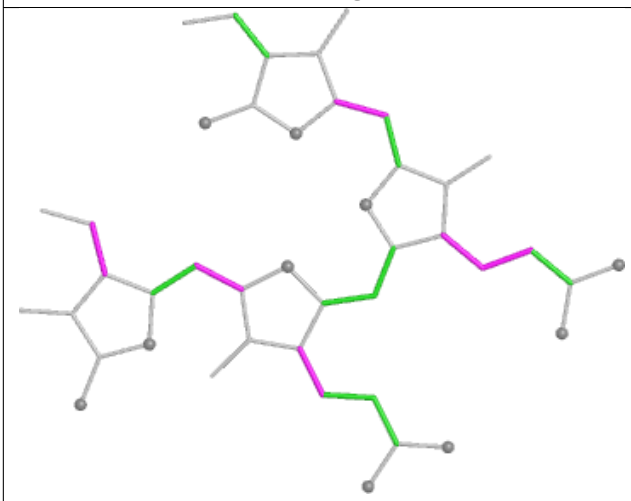
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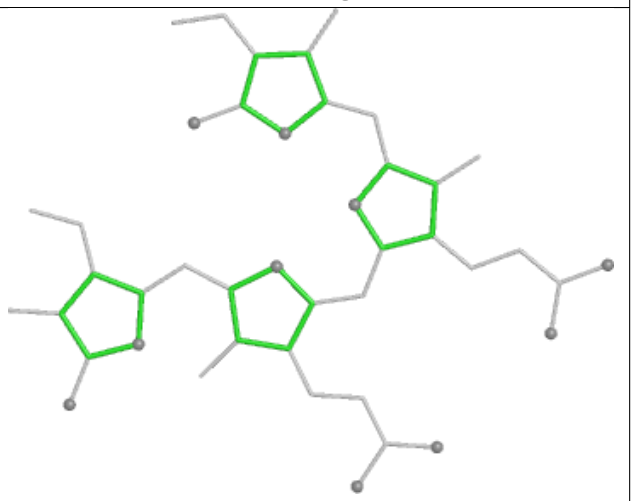
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Bond angles

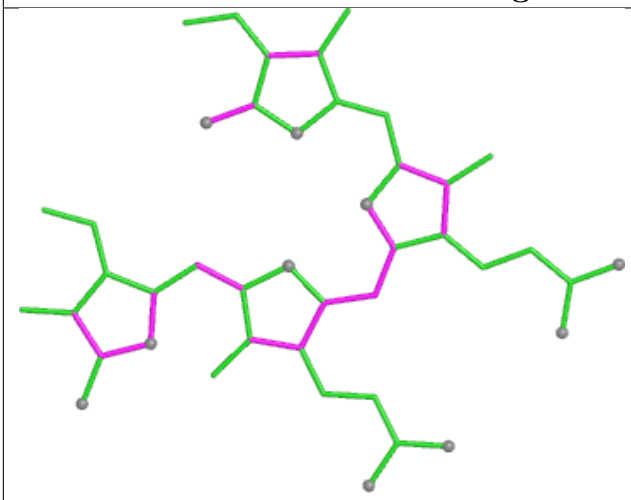


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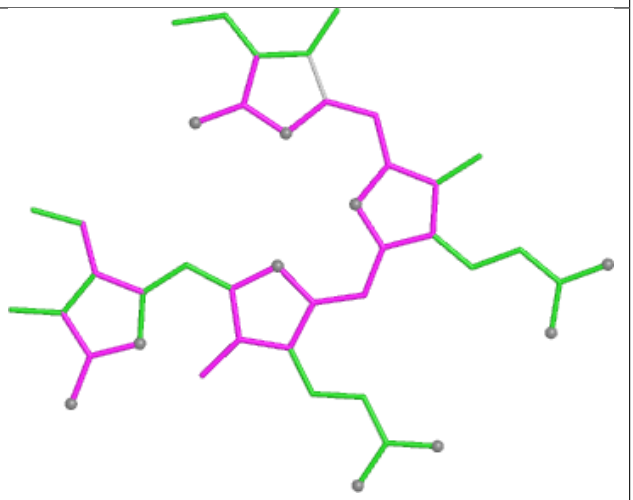


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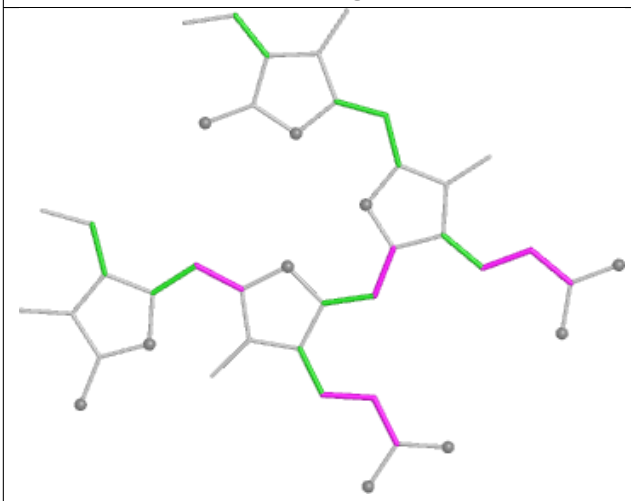
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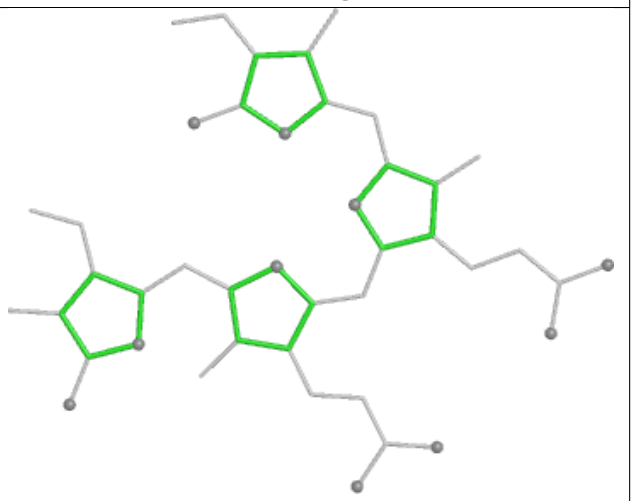
Bond lengths



Bond angles

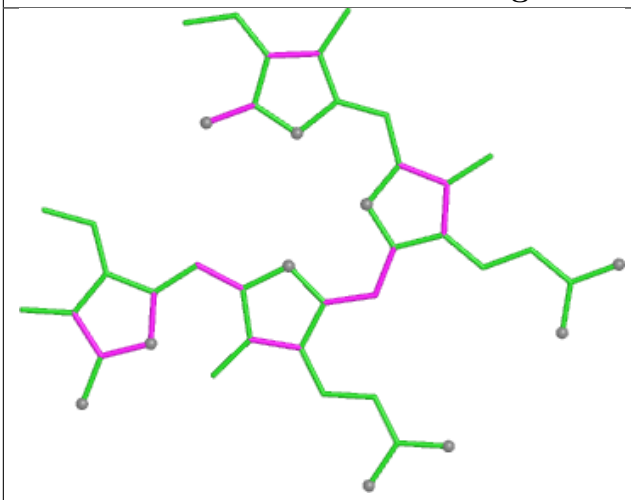


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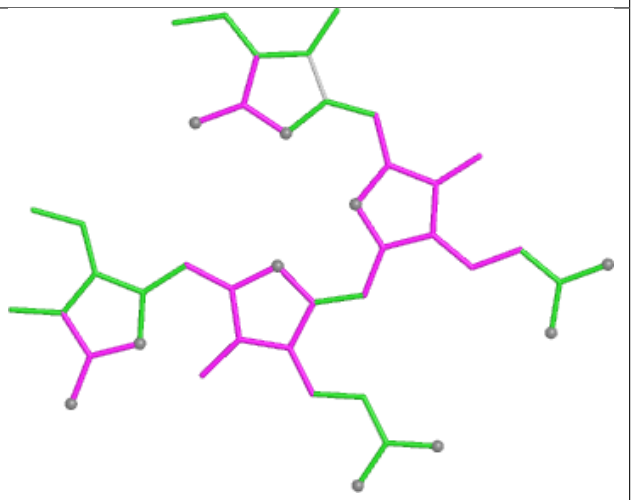


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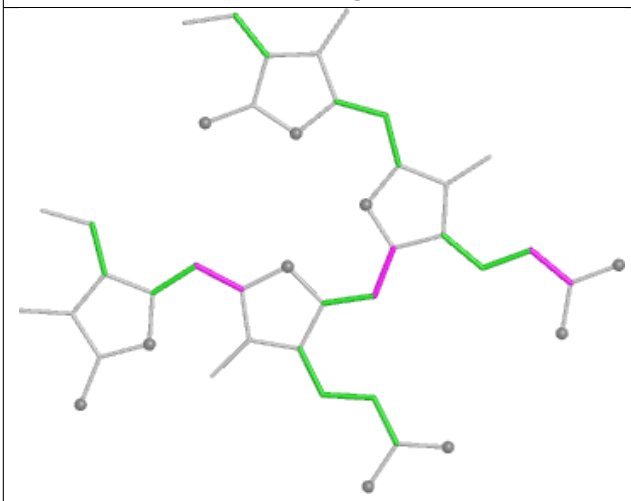
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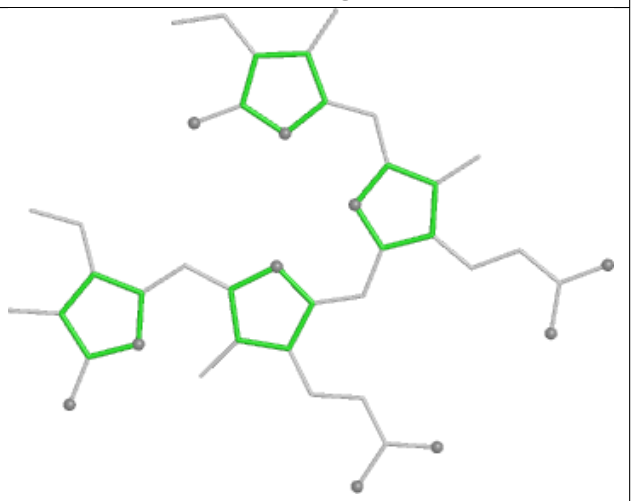
Bond lengths



Bond angles

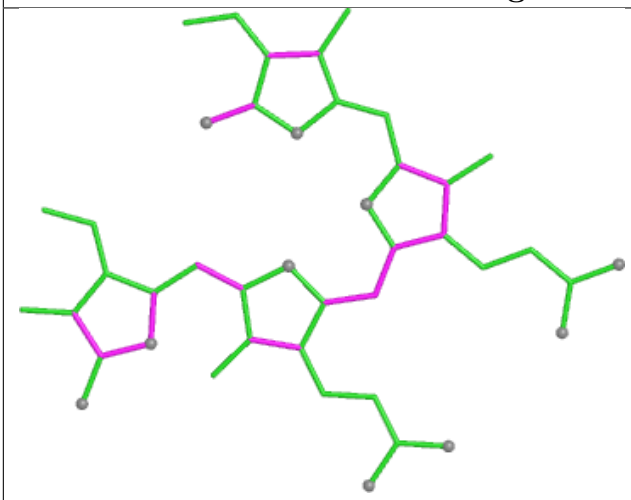


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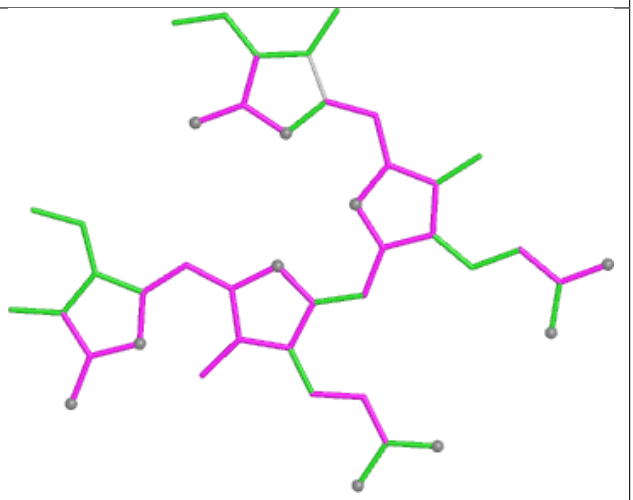


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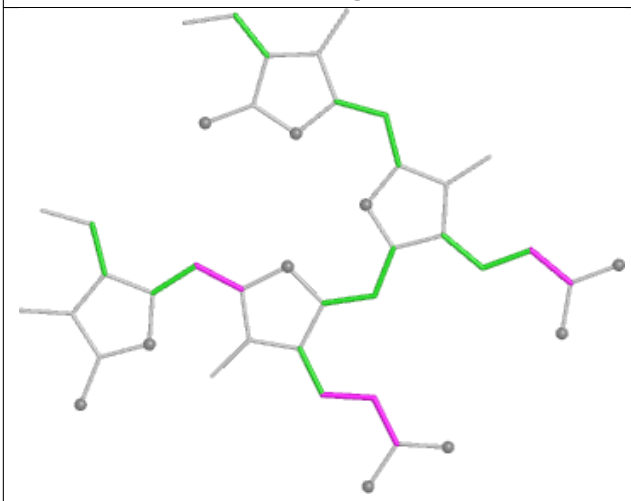
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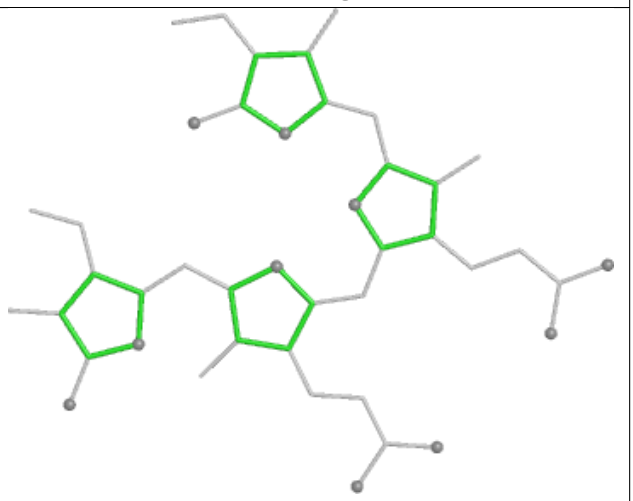
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Bond angles

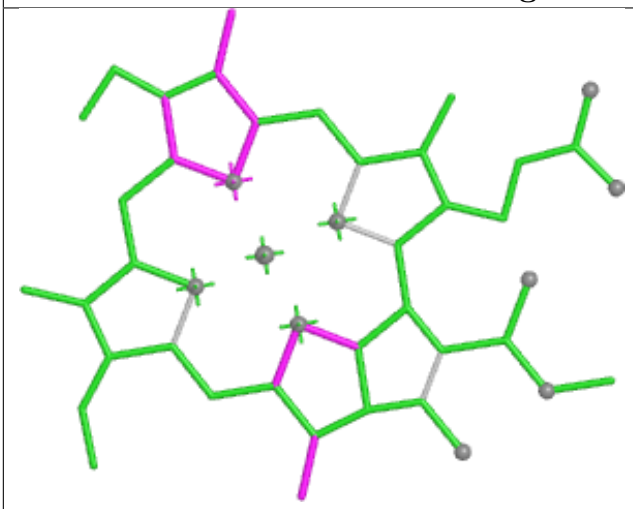


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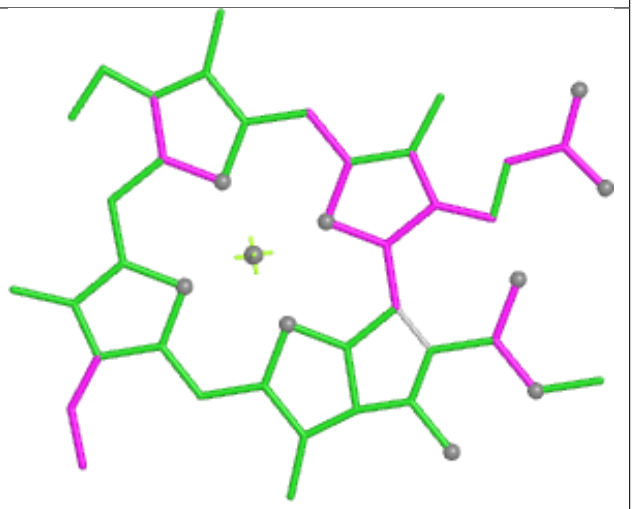


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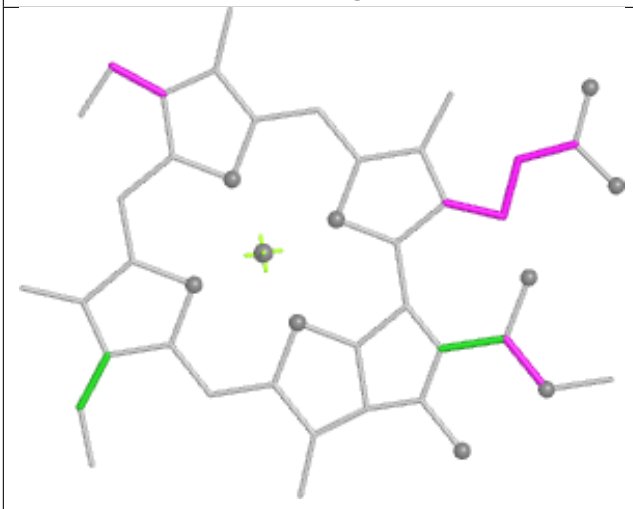
Ligand CLA 42 605



Bond lengths



Bond angles

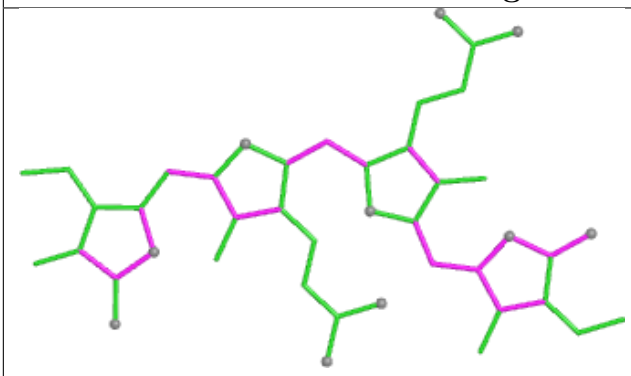


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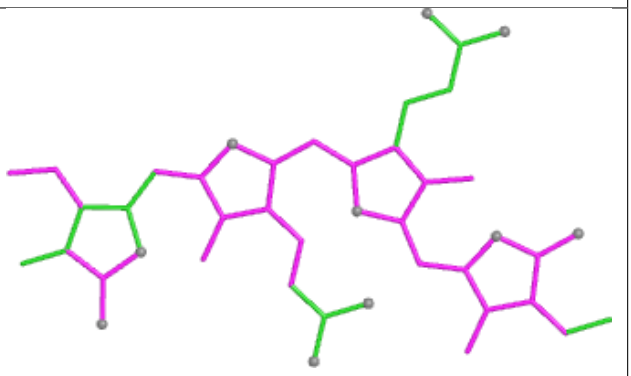


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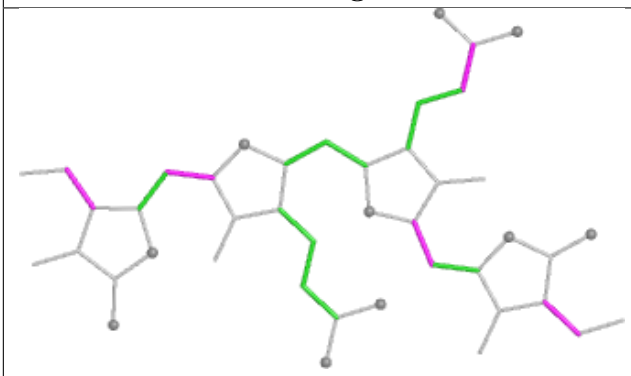
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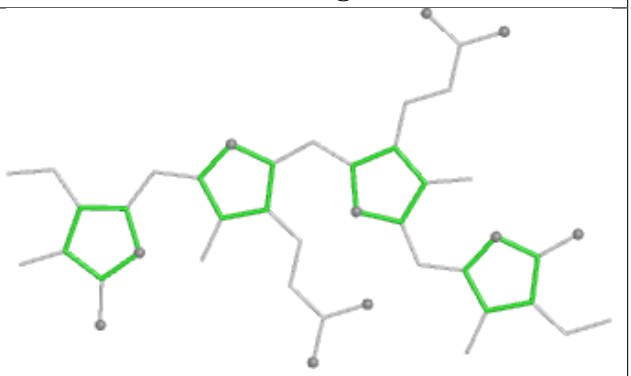
Bond lengths



Bond angles

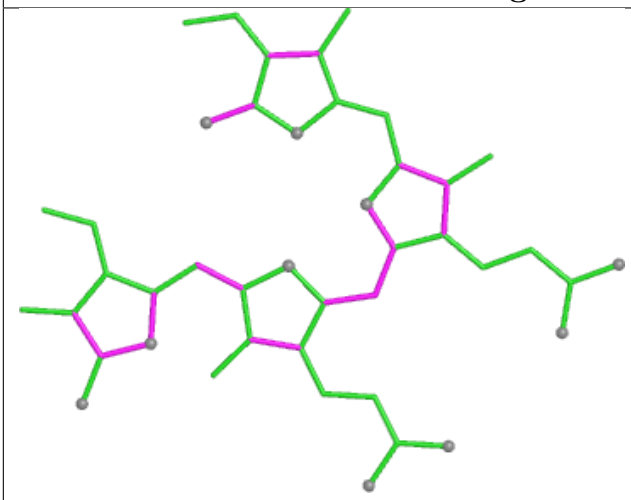


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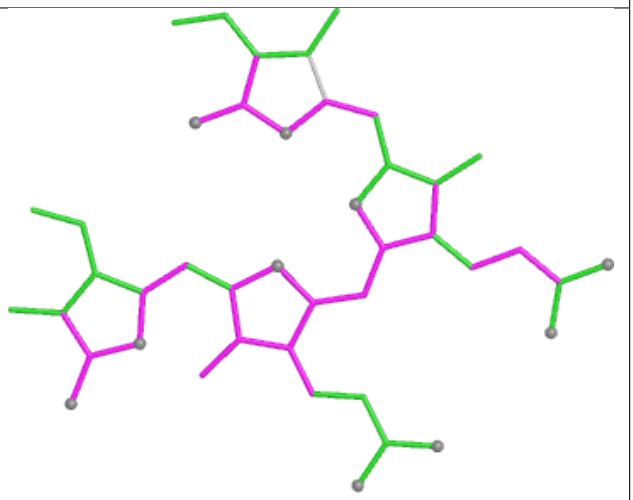


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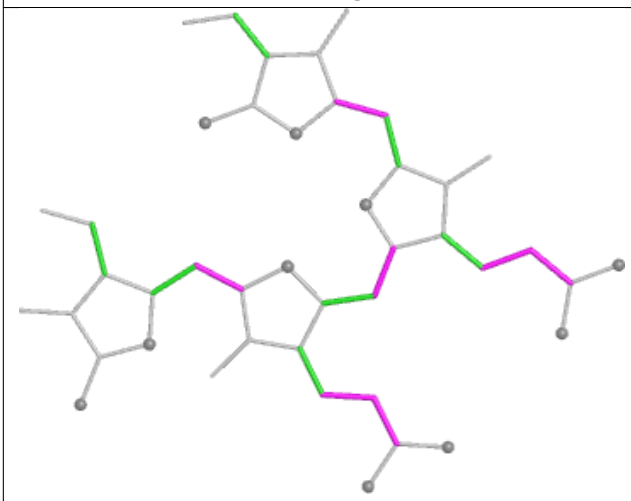
Ligand PEB HK 202



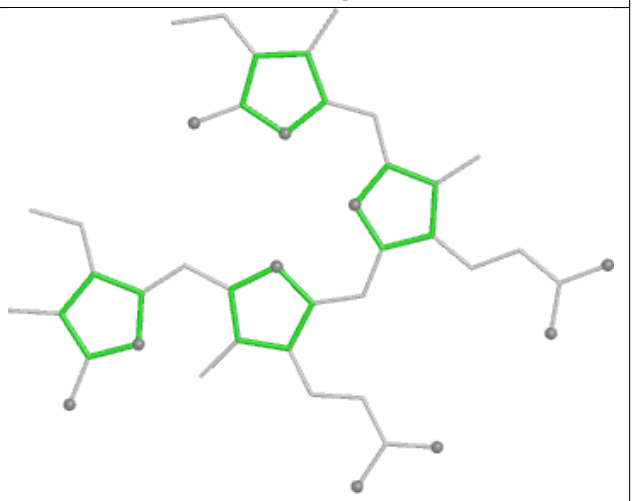
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Bond angles

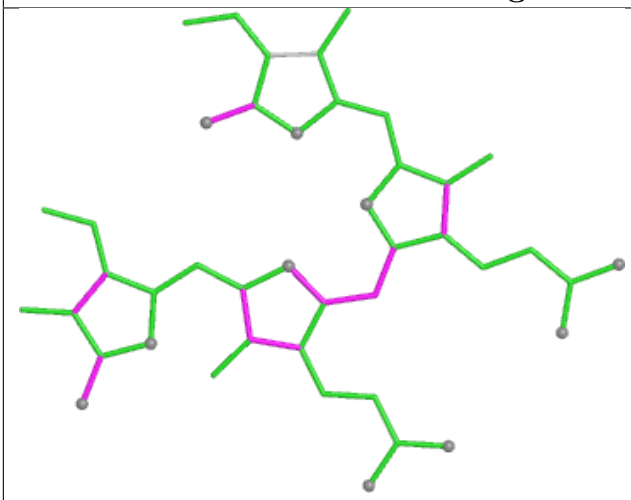


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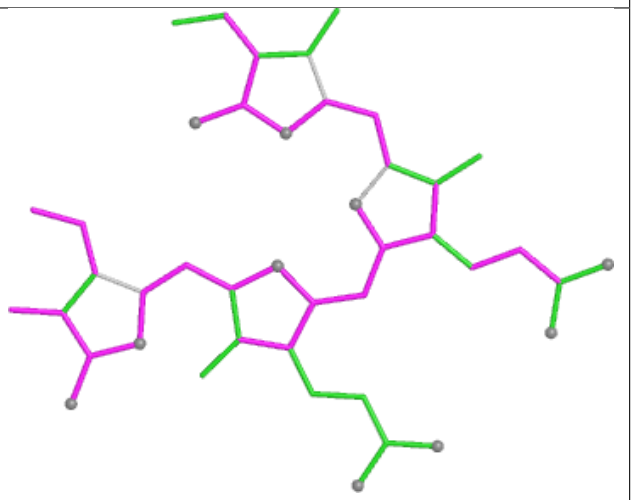


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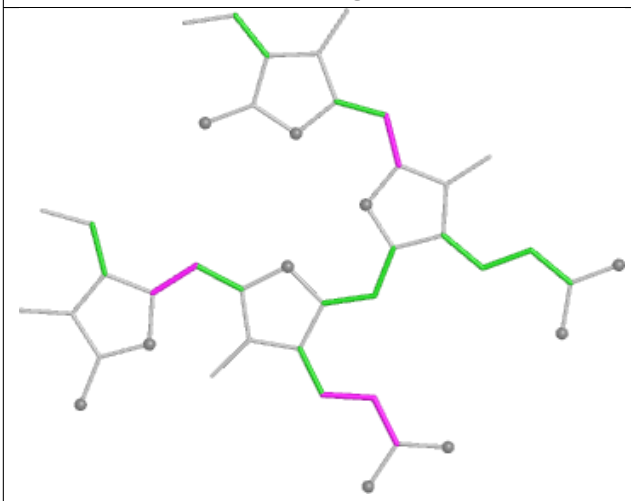
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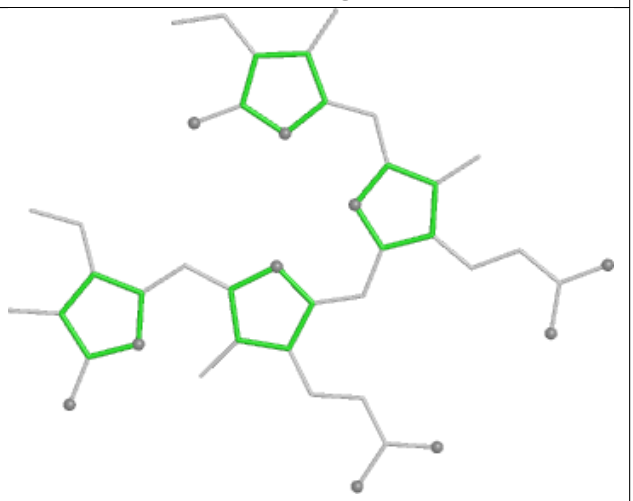
Bond lengths



Bond angles

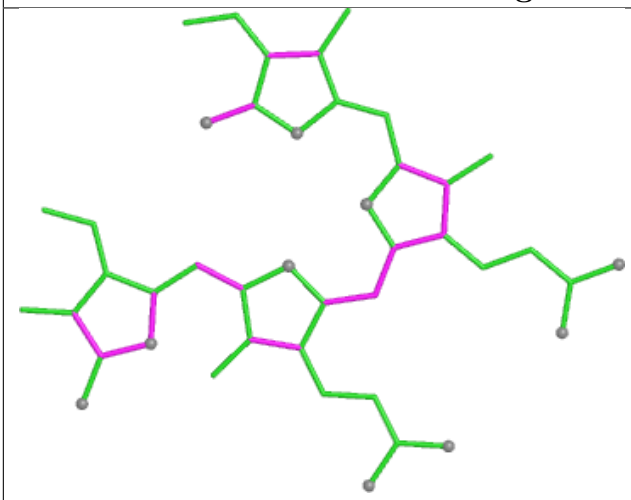


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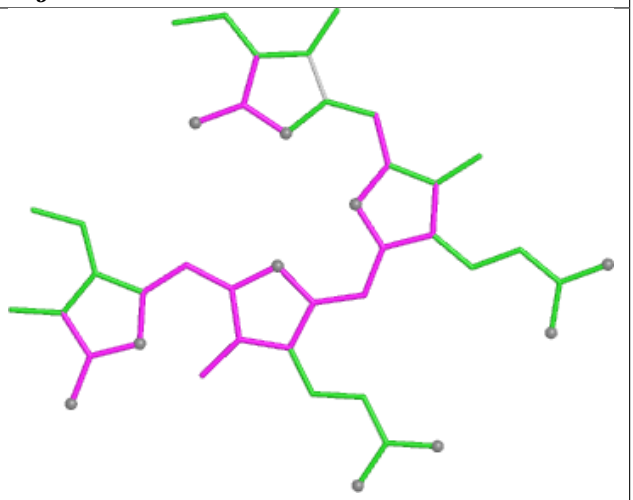


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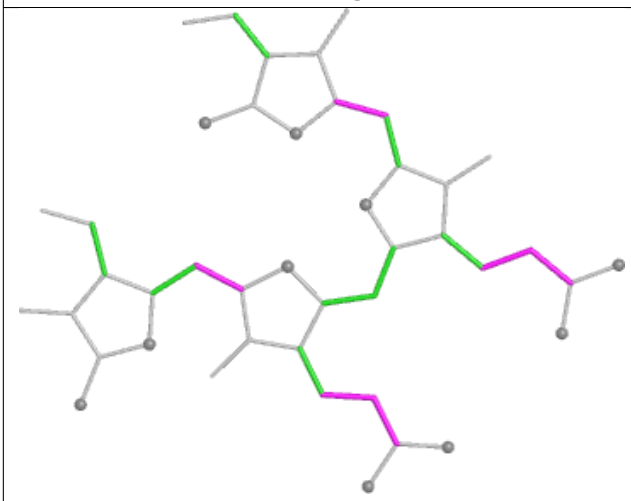
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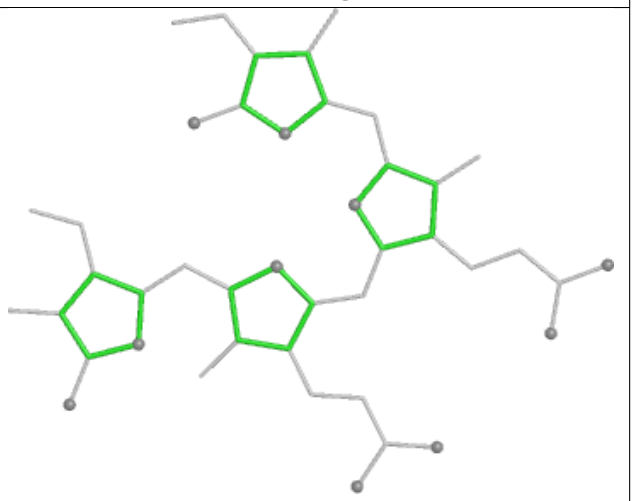
Bond lengths



Bond angles

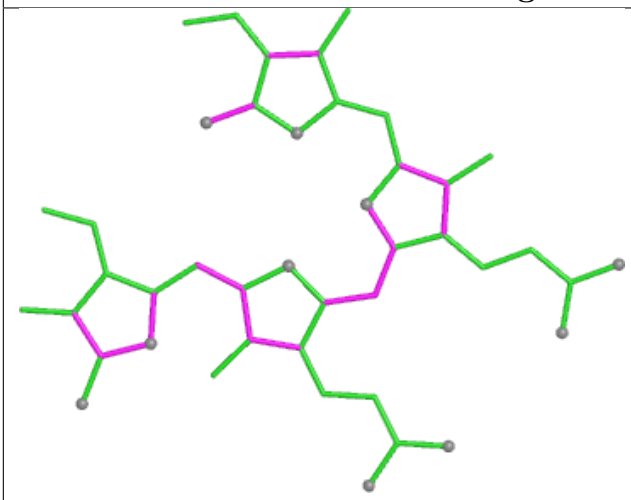


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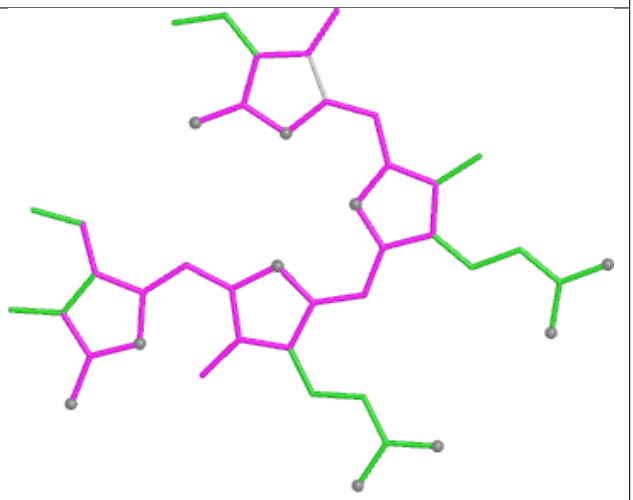


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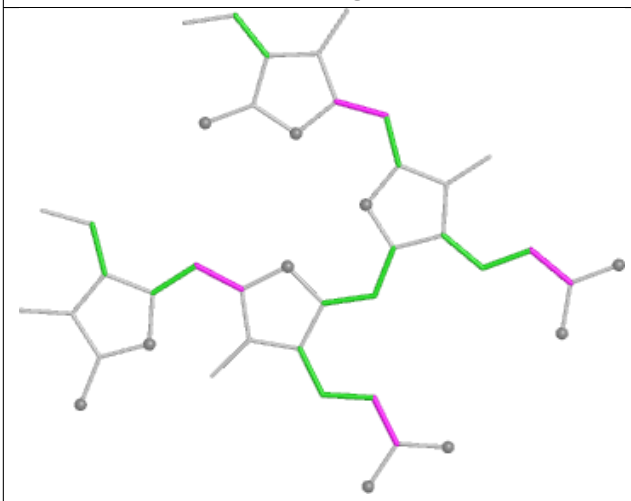
Ligand PEB Z5 304



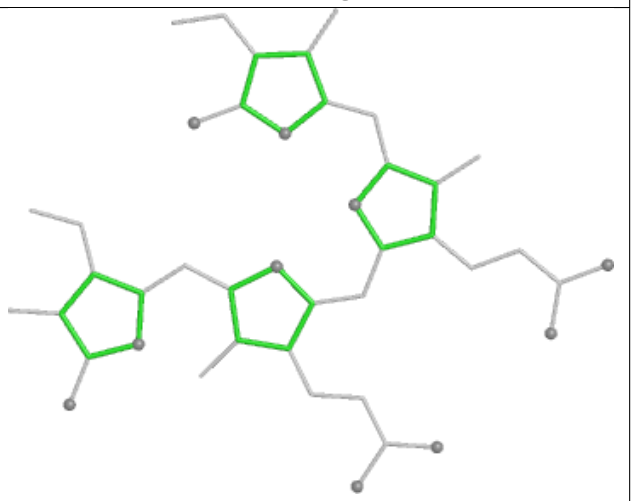
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Bond angles

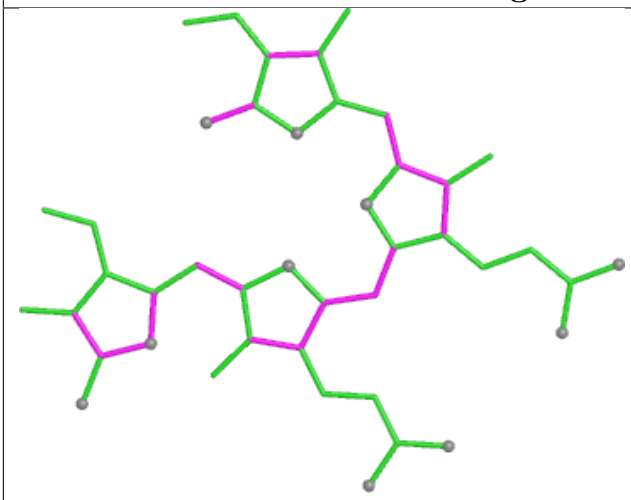


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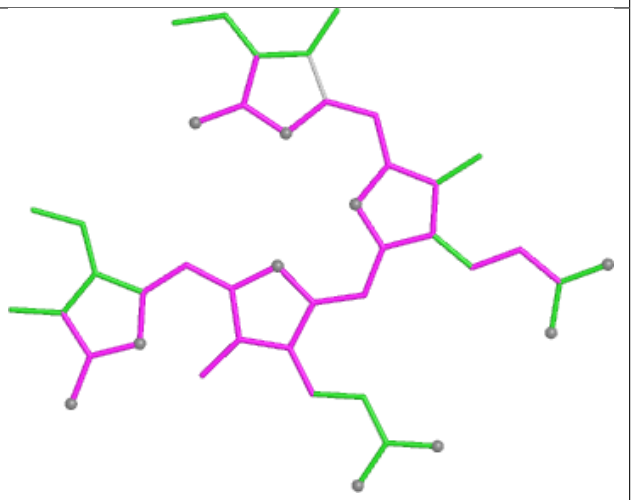


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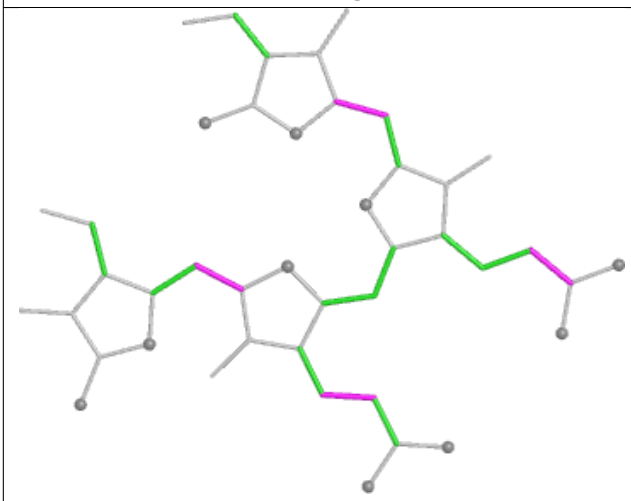
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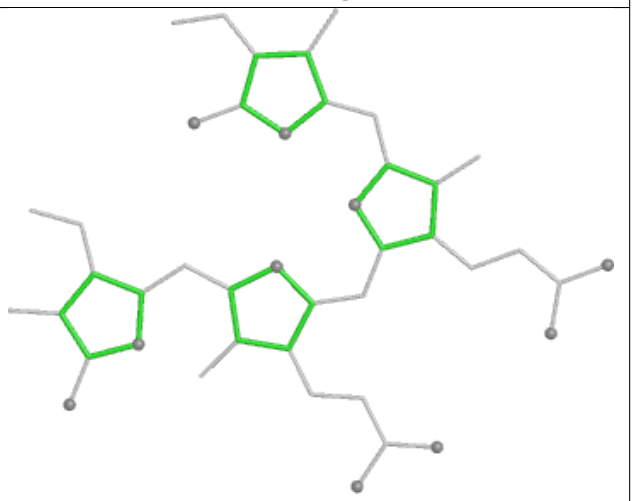
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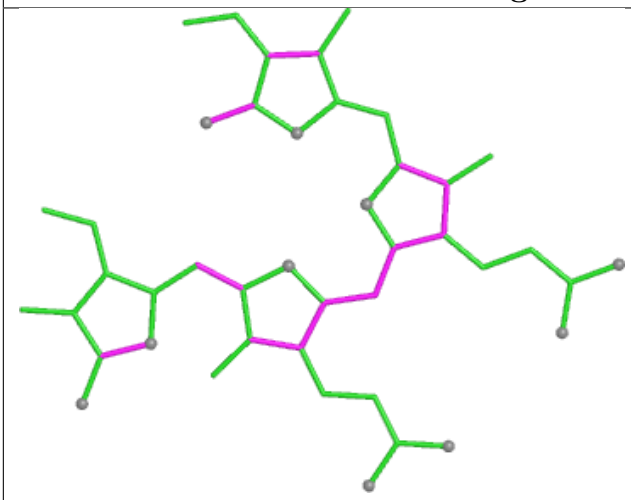


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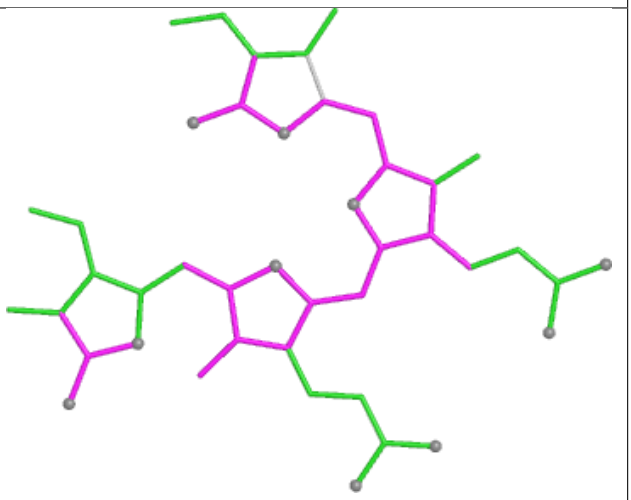


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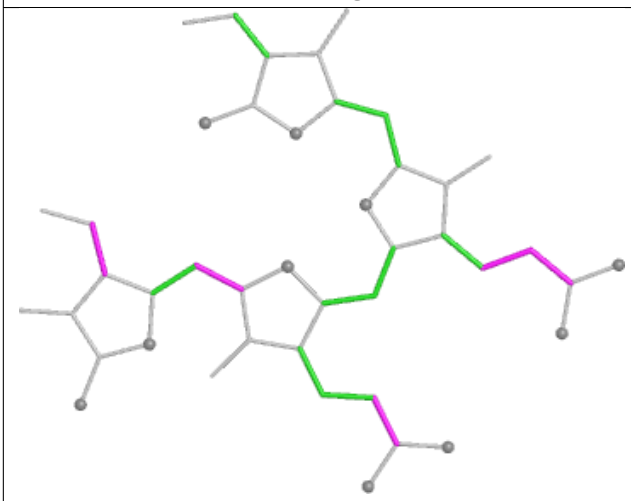
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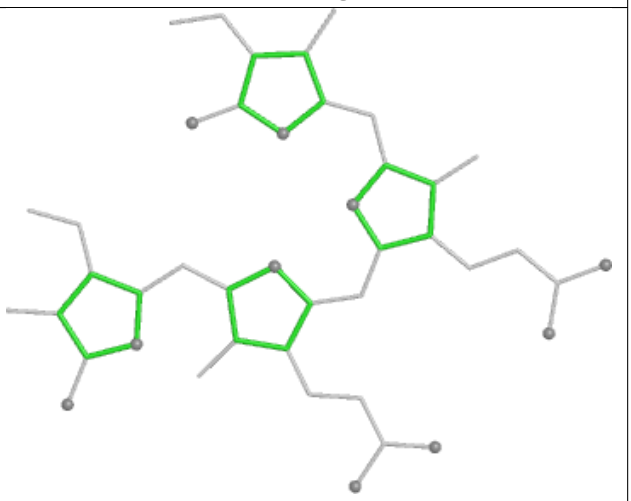
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Bond angles

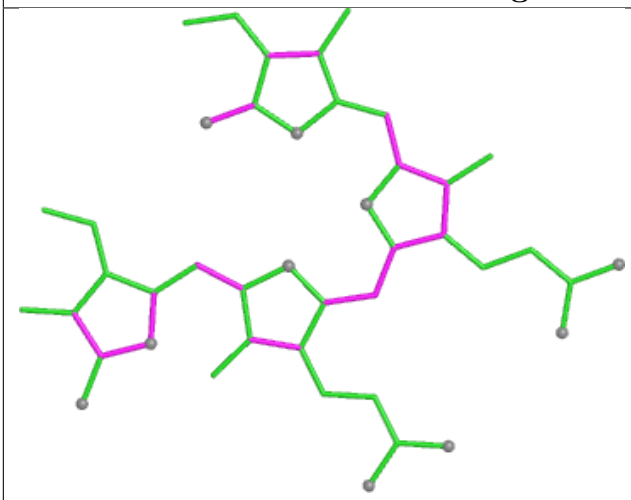


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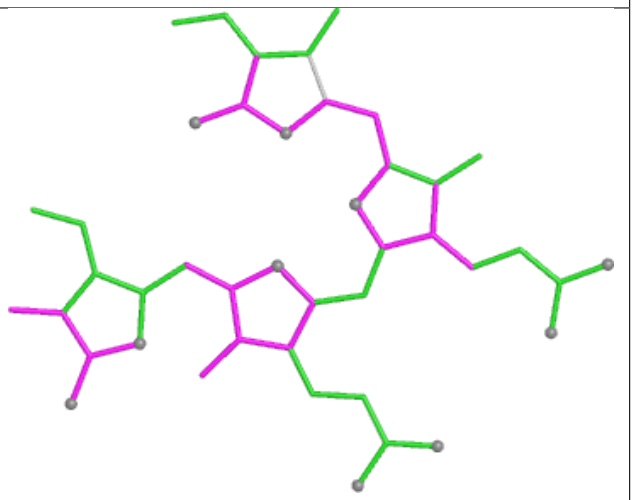


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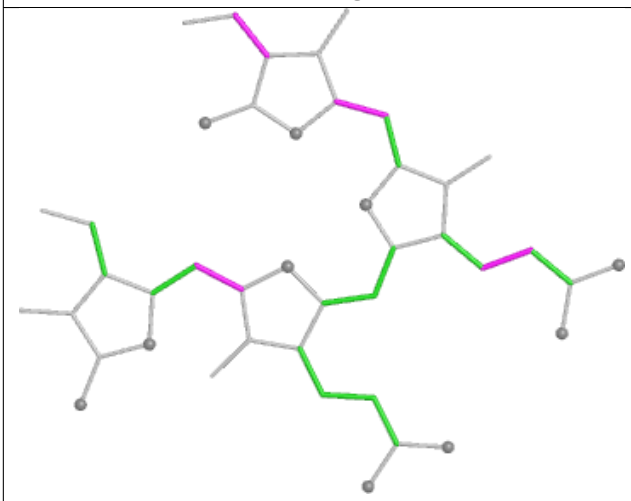
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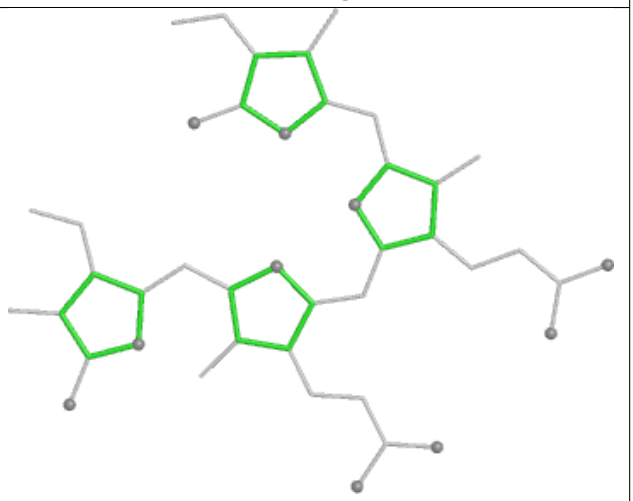
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Bond angles

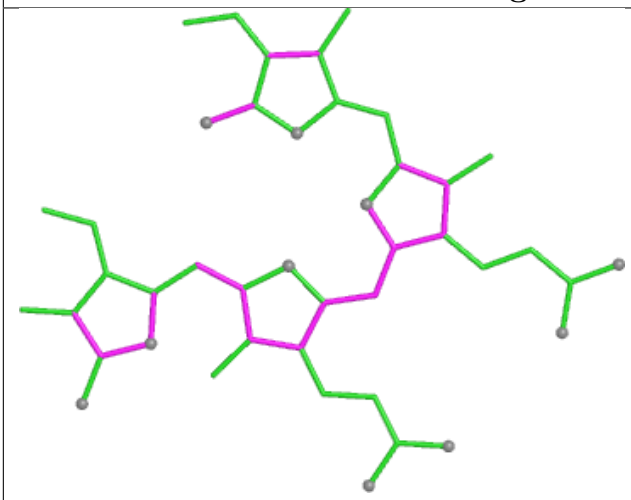


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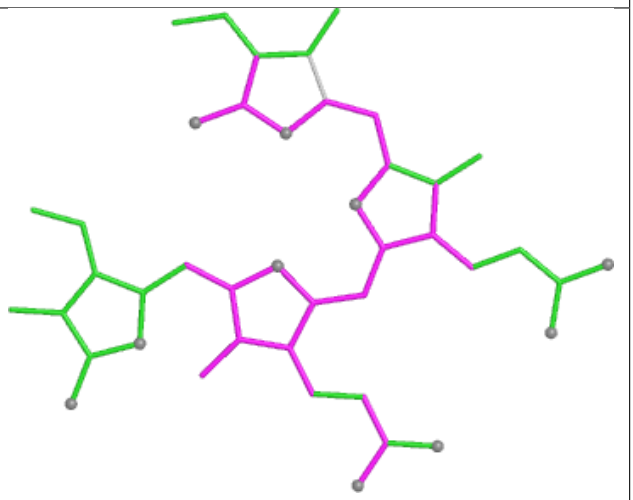


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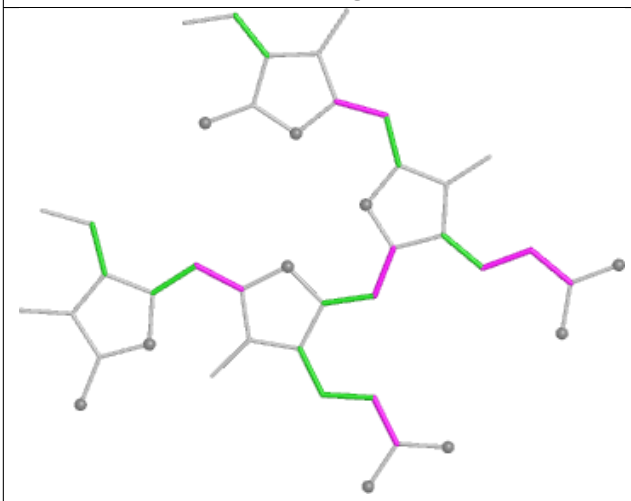
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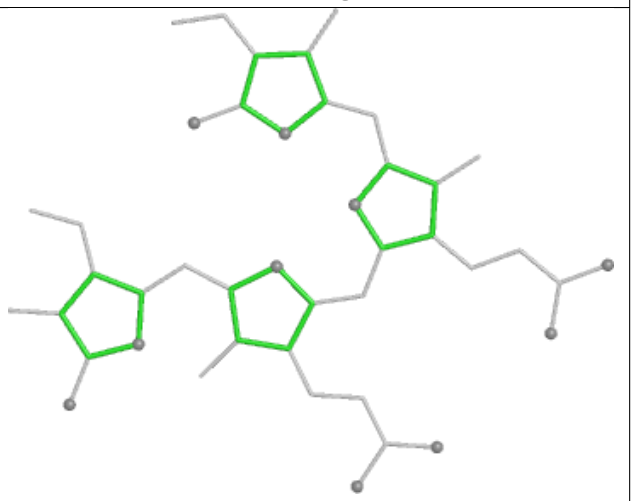
Bond lengths



Bond angles

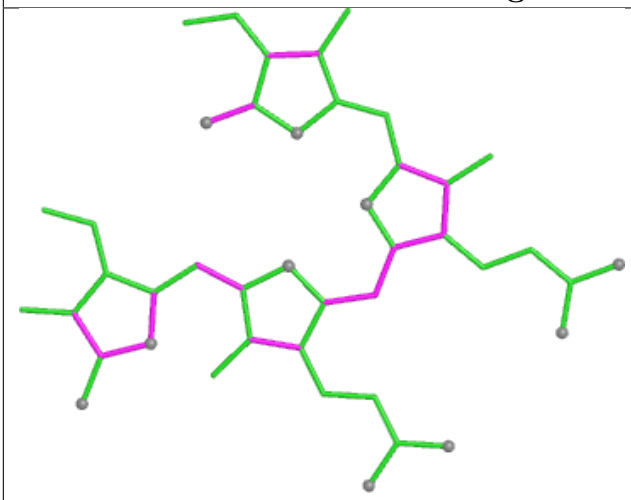


Torsions

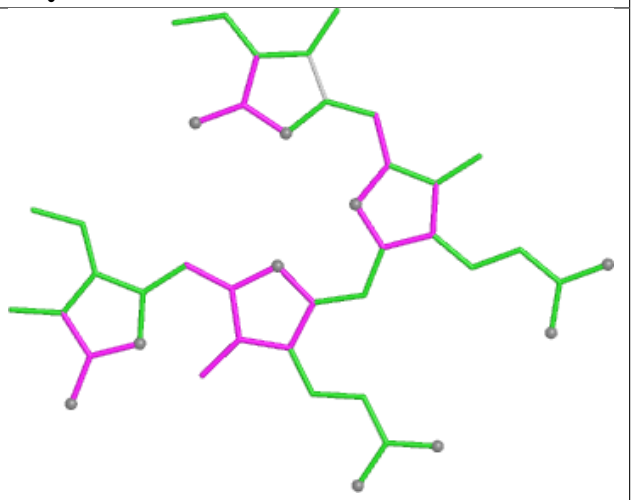


Rings

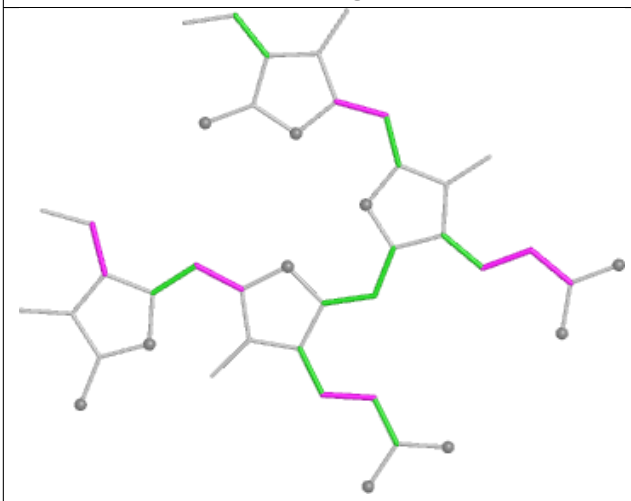
Ligand PEB QM 203



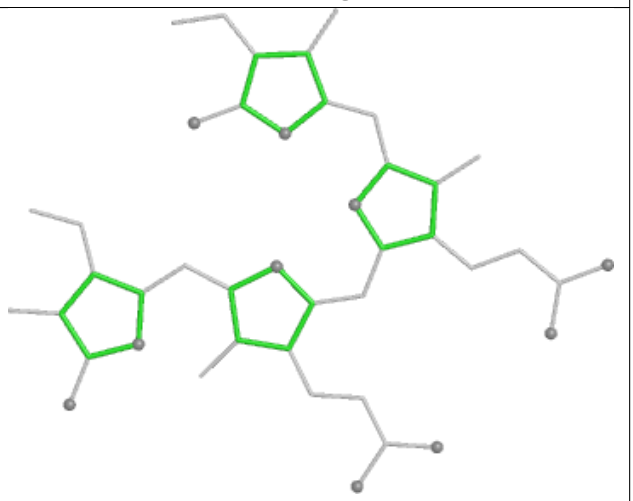
Bond lengths



Bond angles

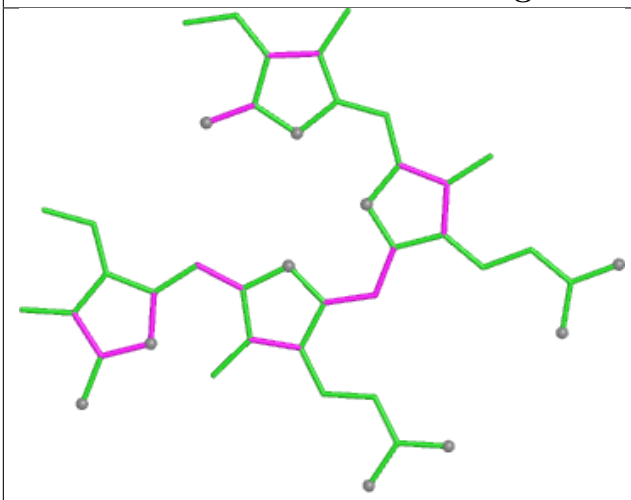


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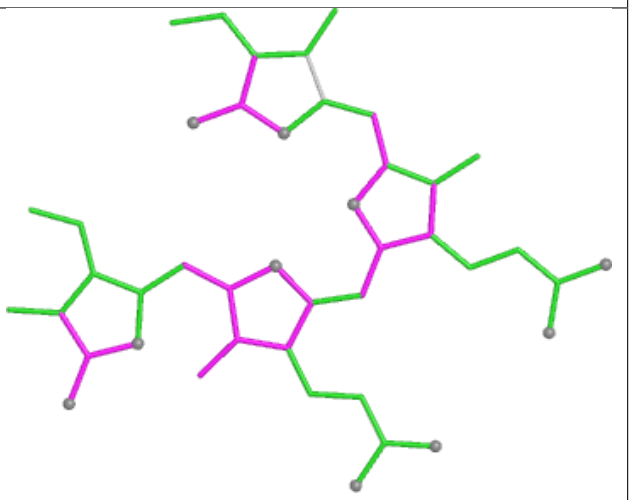


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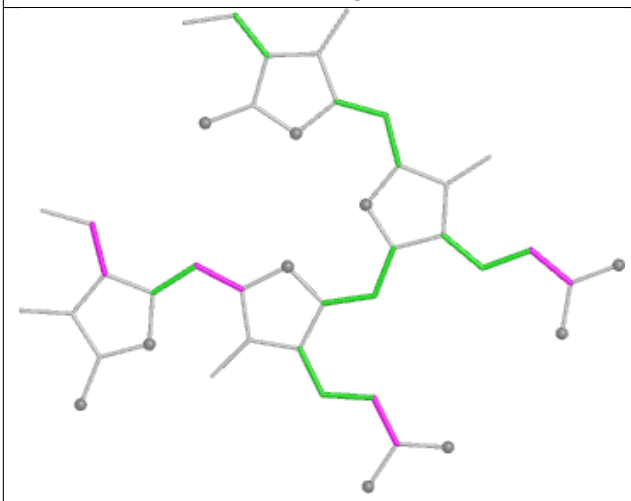
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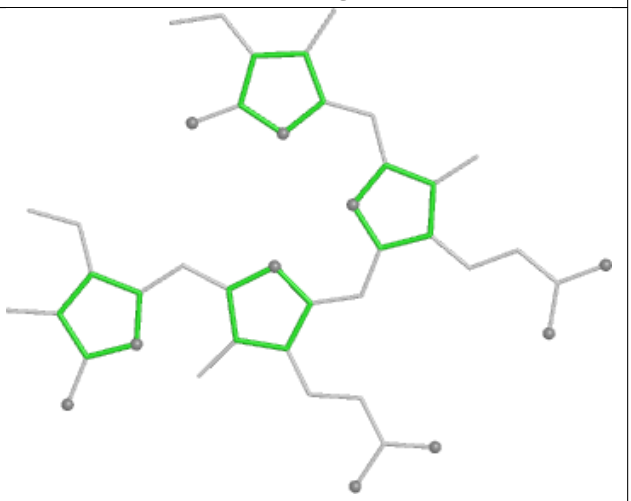
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Bond angles

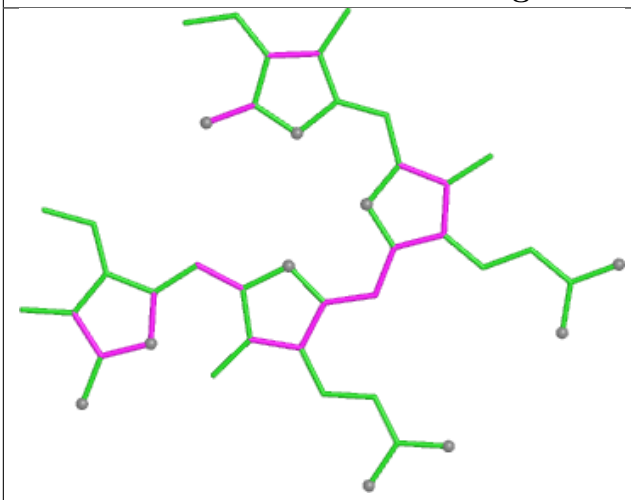


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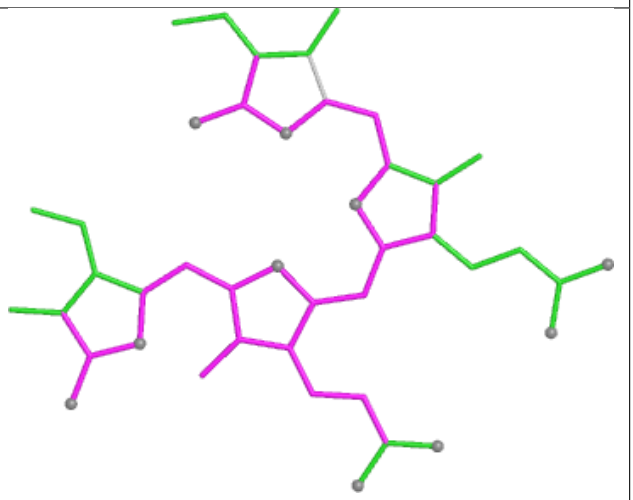


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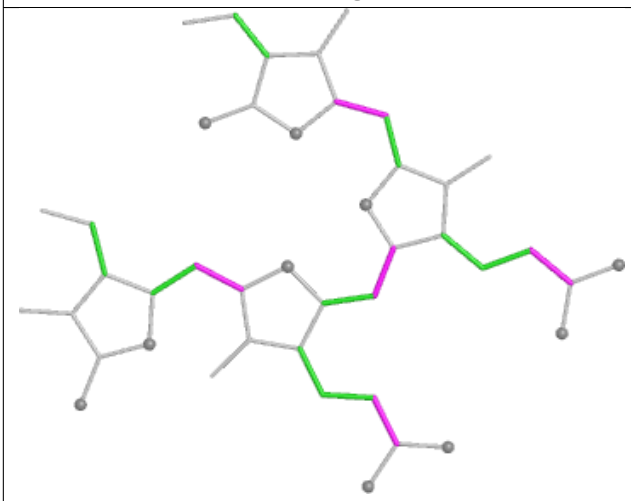
Ligand PEB AE 301



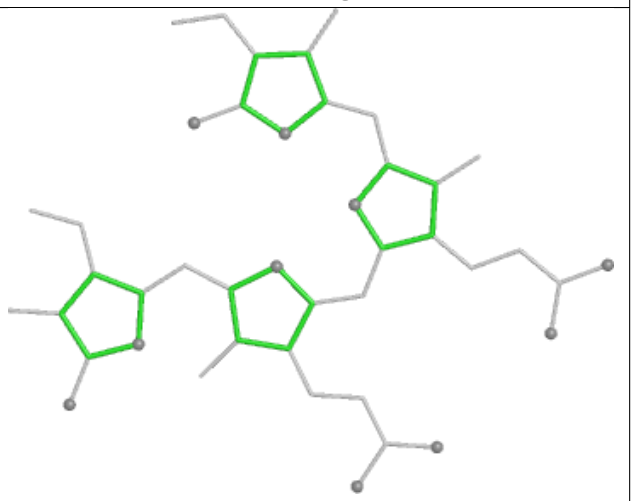
Bond lengths



Bond angles

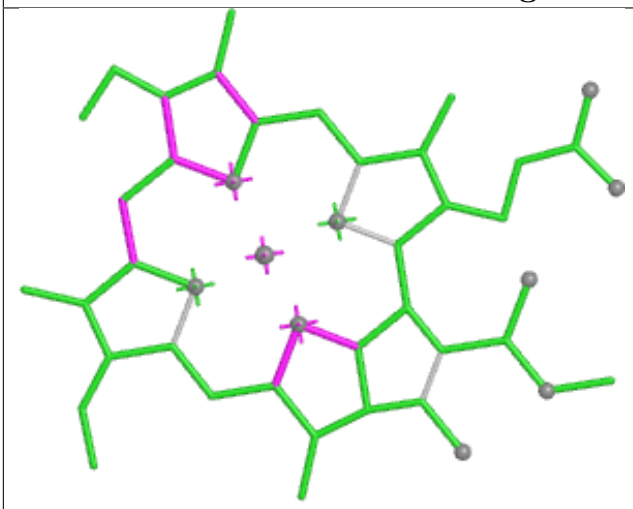


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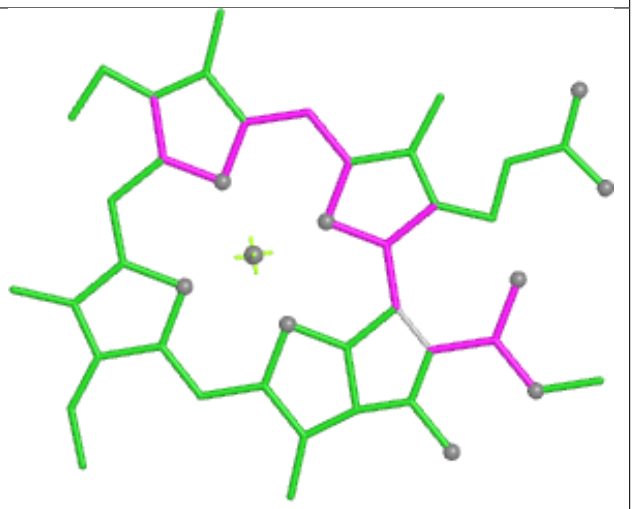


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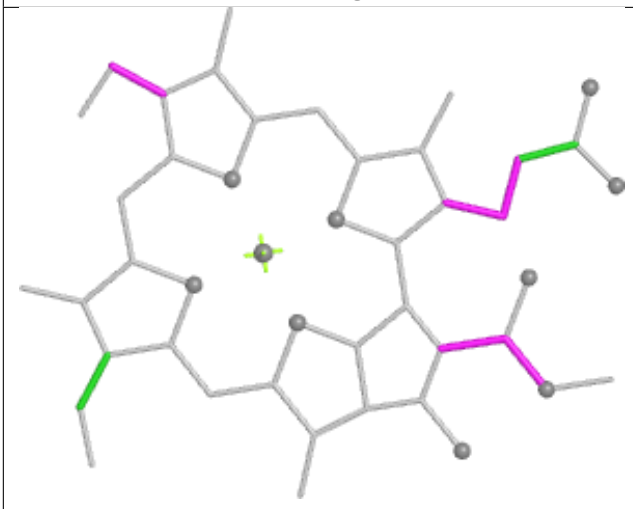
Ligand CLA 12 610



Bond lengths



Bond angles

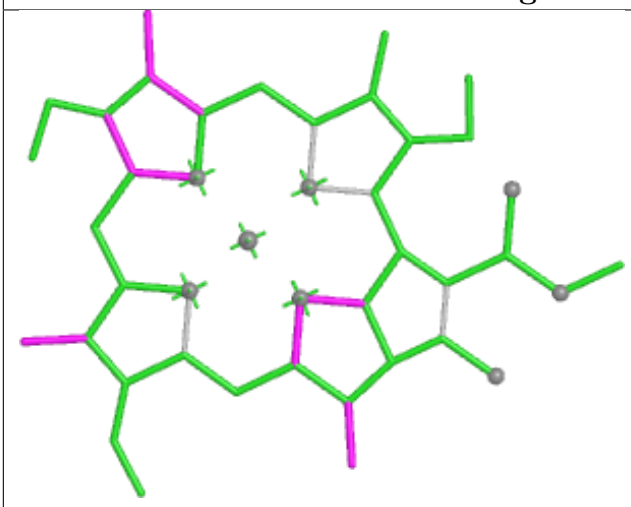


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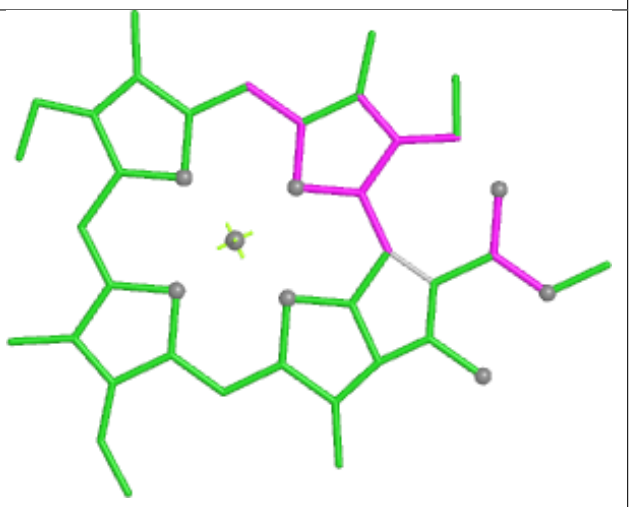


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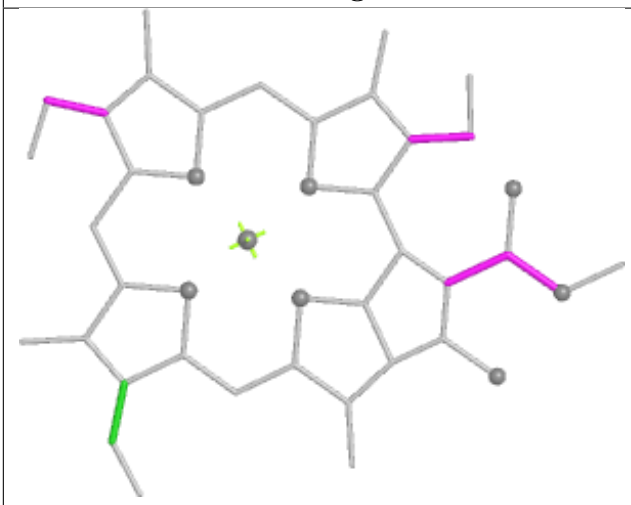
Ligand CLA 52 609



Bond lengths



Bond angles

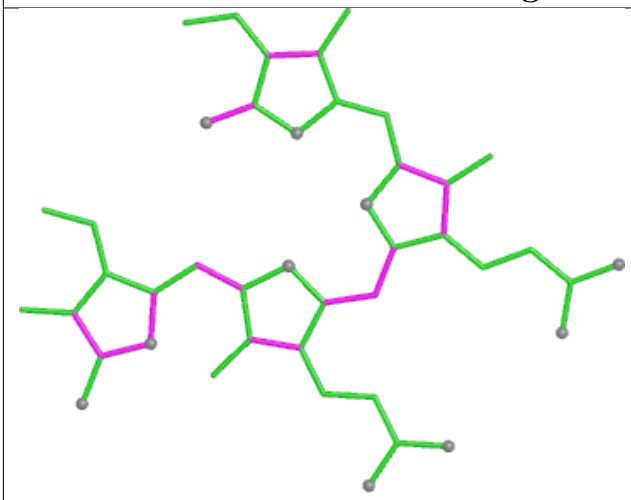


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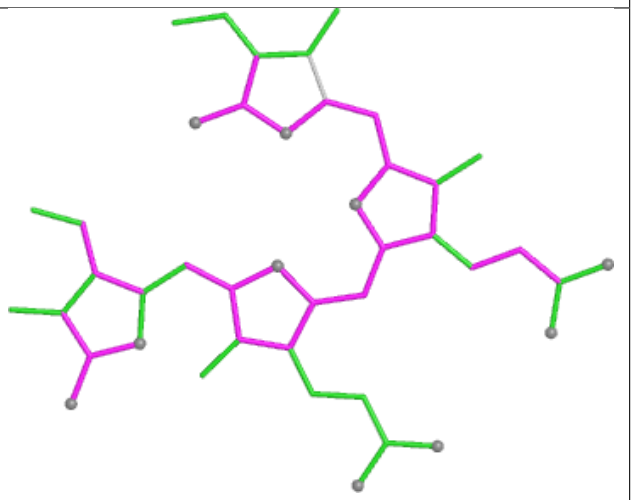


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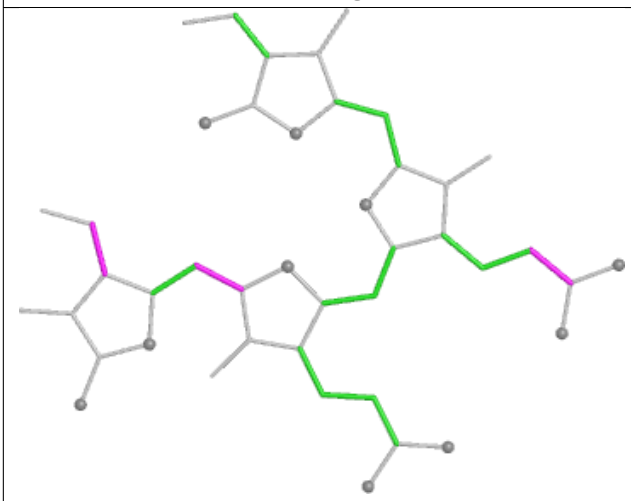
Ligand PEB IJ 201



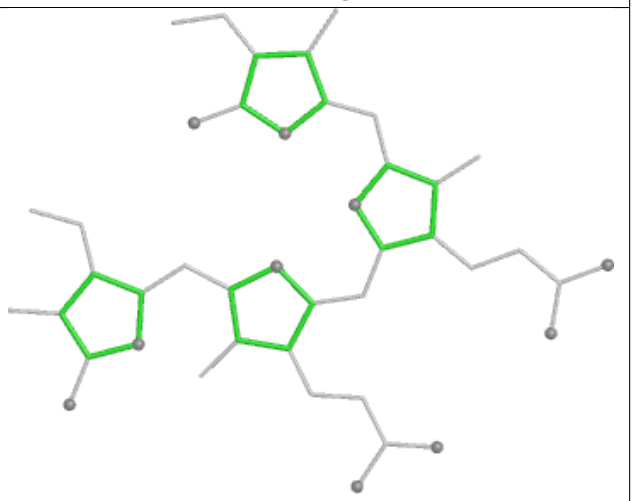
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Bond angles

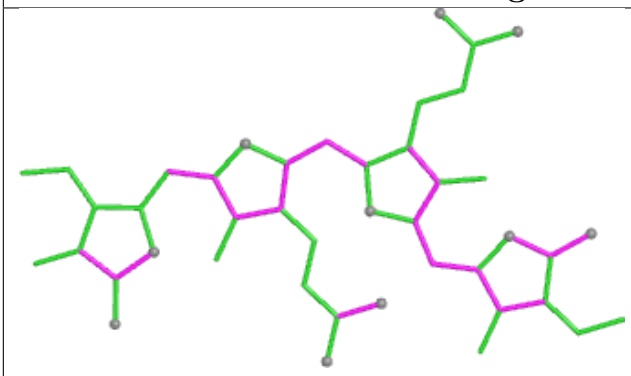


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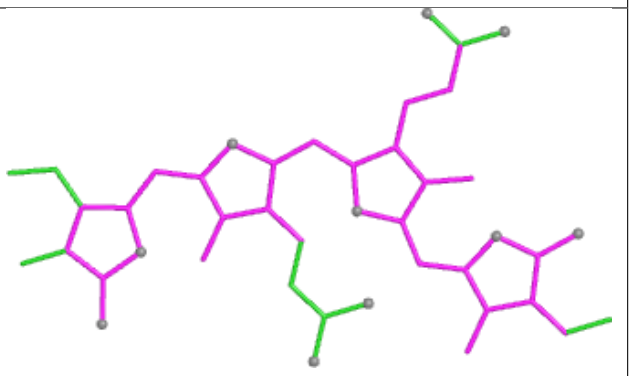


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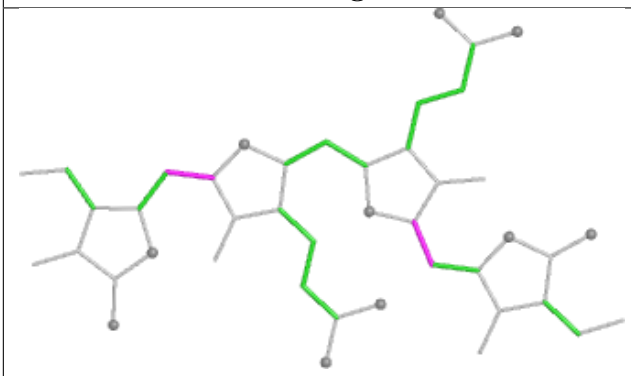
Ligand CYC 73 1001



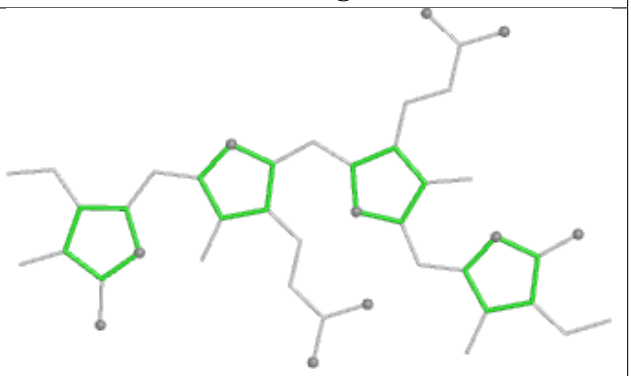
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Bond angles

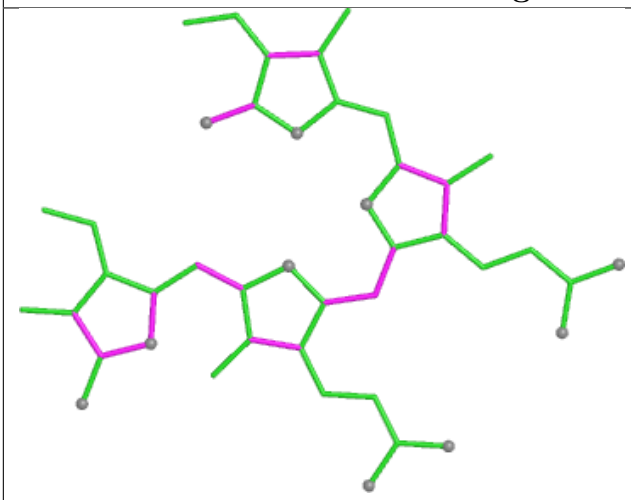


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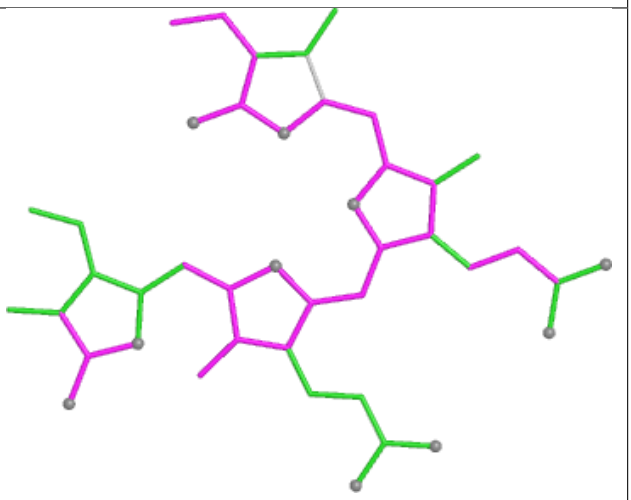


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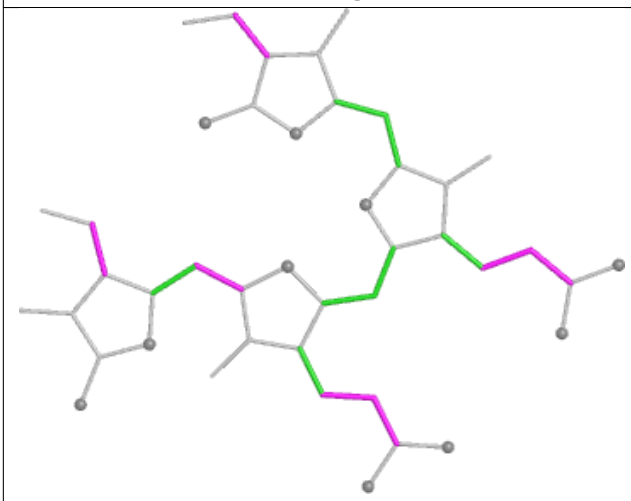
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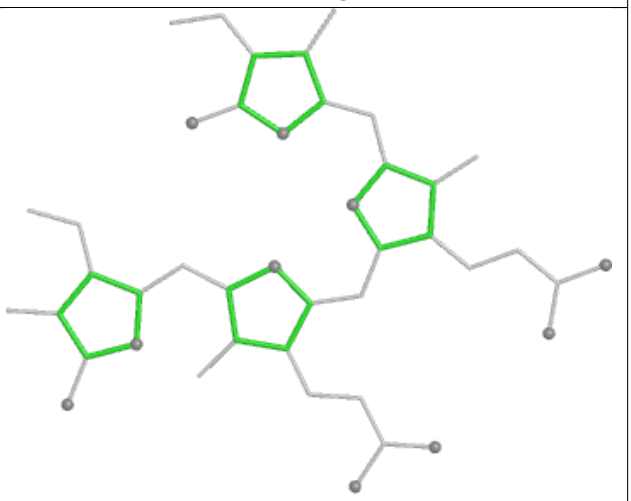
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Bond angles

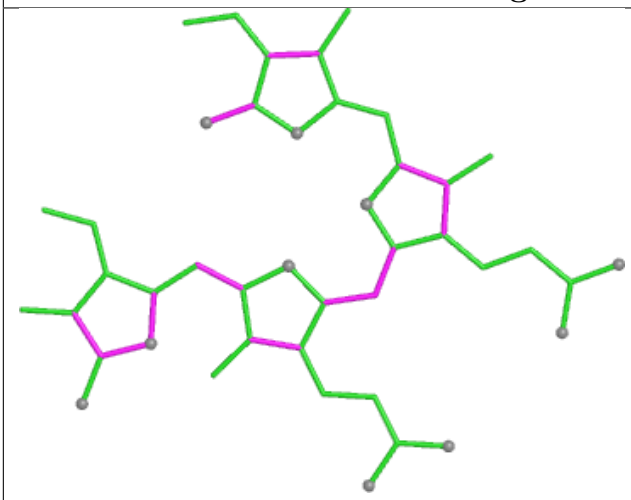


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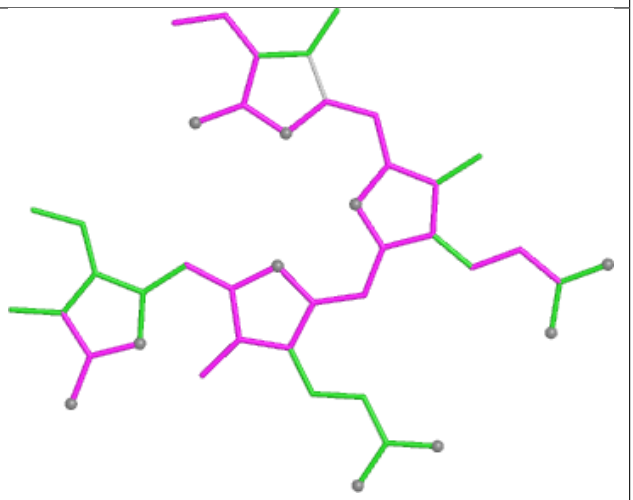


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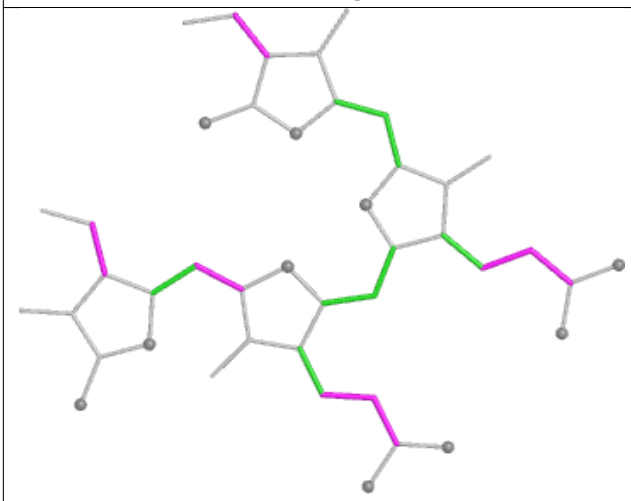
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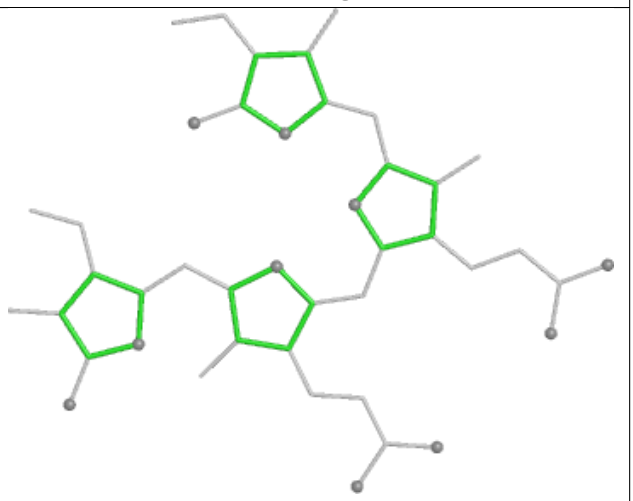
Bond lengths



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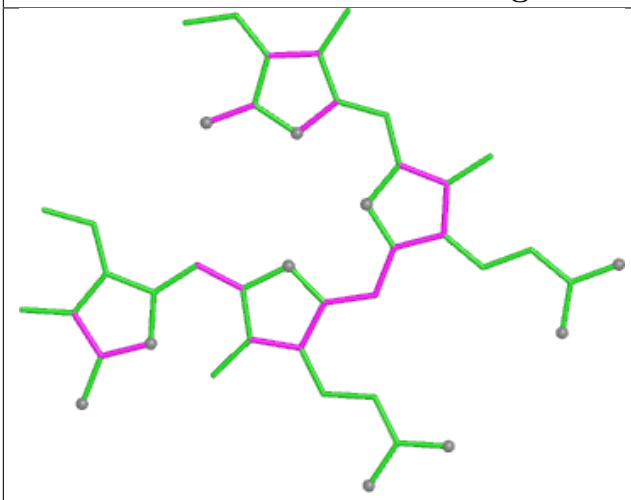


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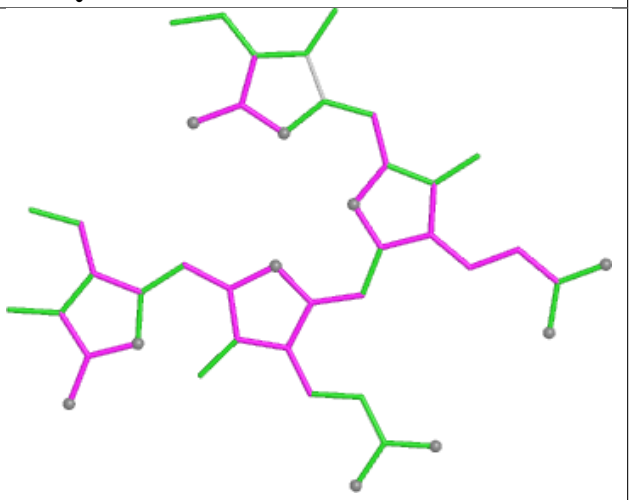


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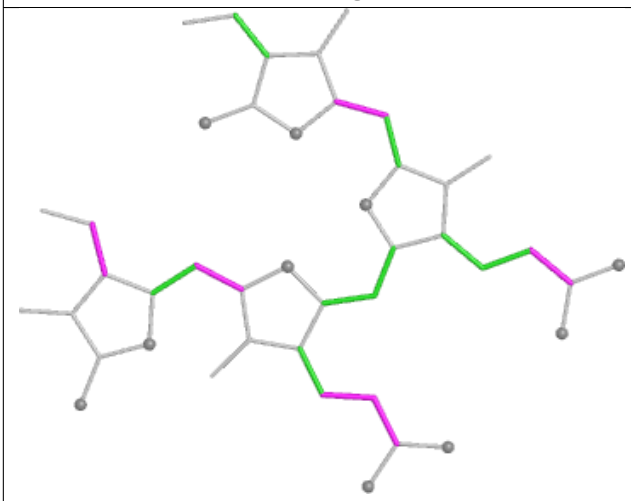
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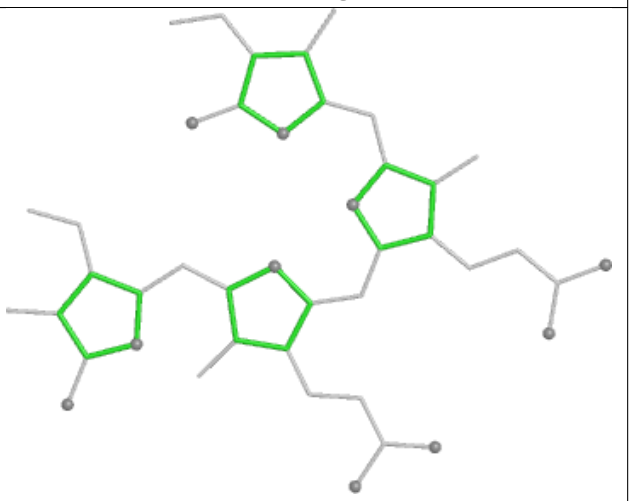
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Bond angles

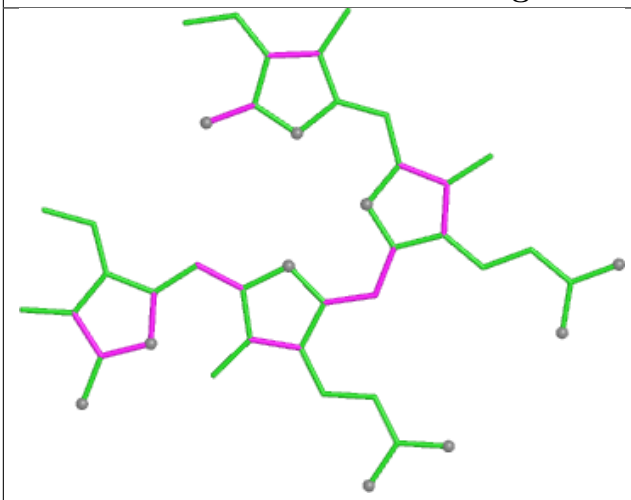


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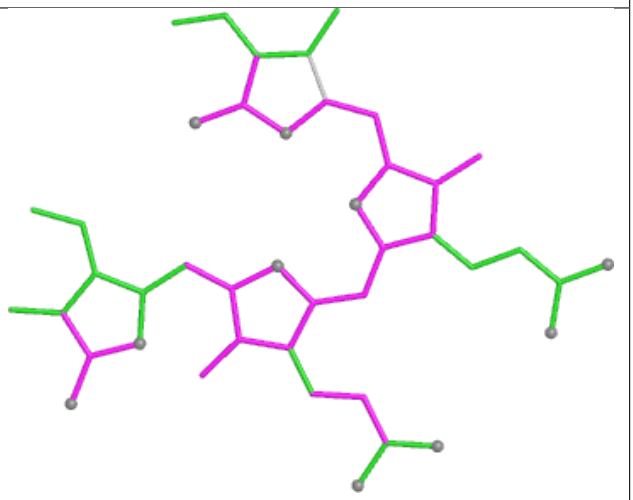


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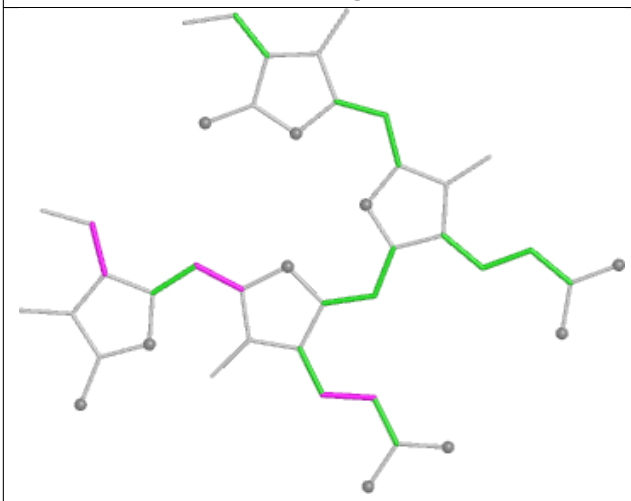
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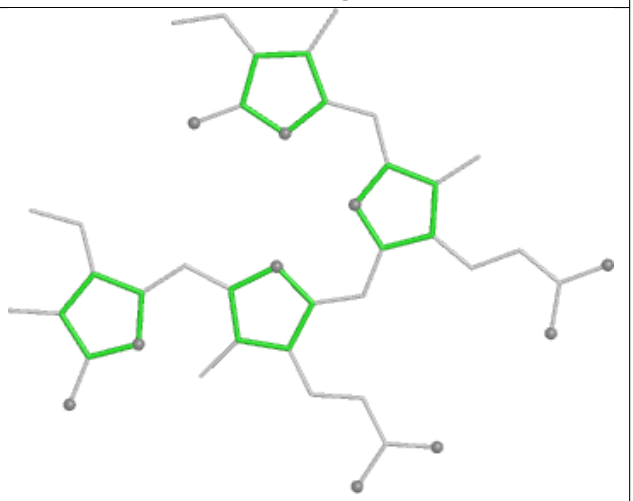
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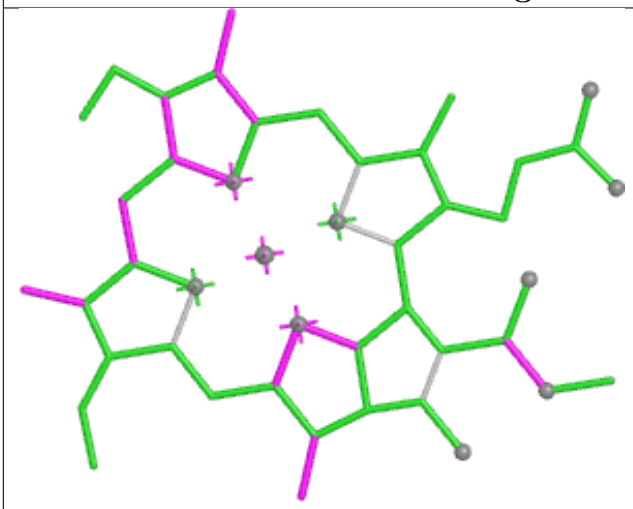


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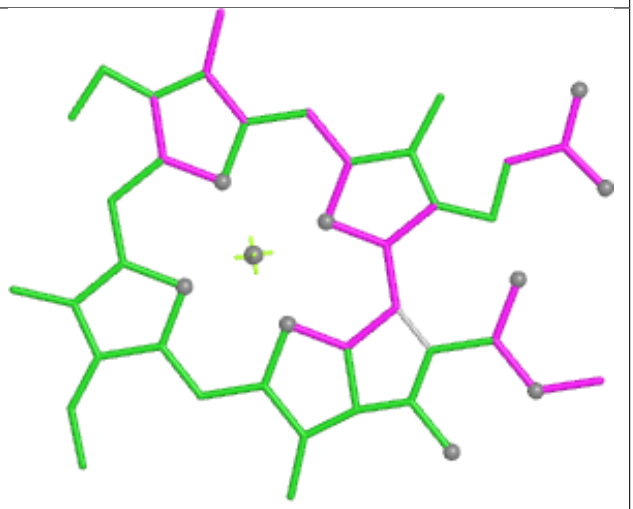


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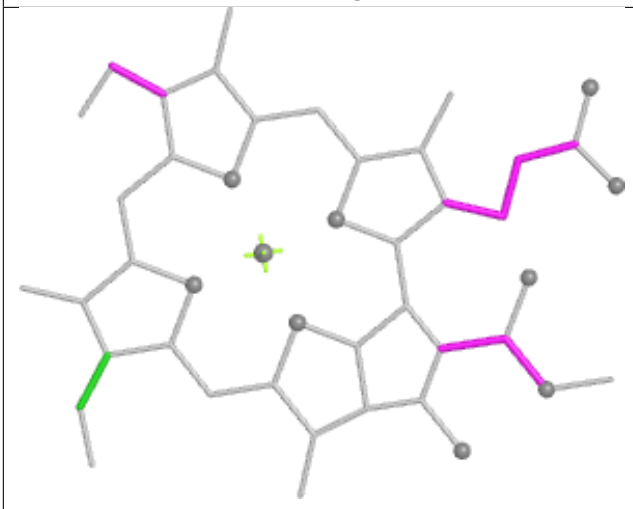
Ligand CLA 8N 306



Bond lengths



Bond angles

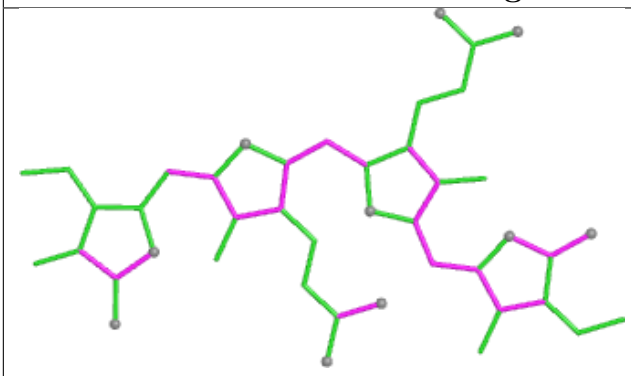


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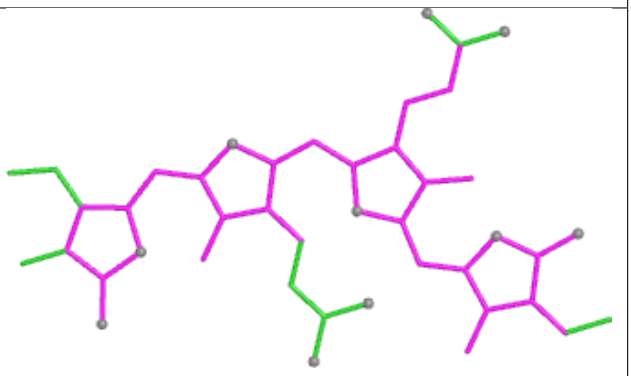


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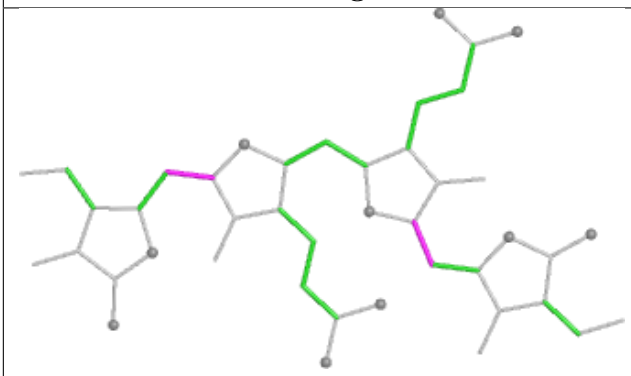
Ligand CYC B3 1001



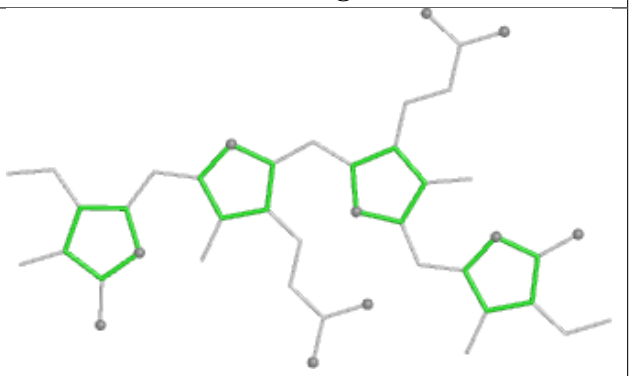
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Bond angles

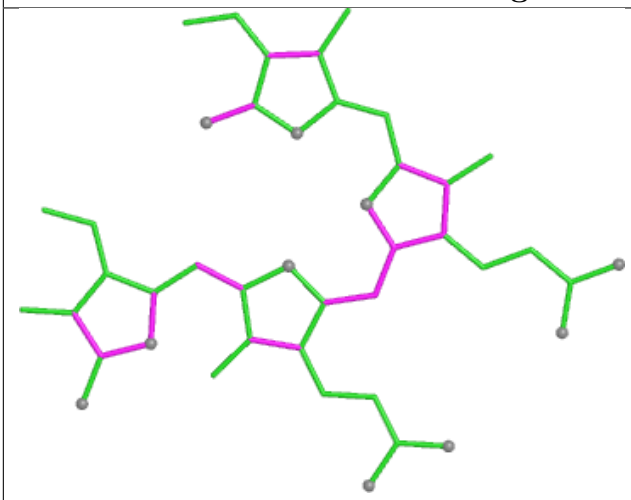


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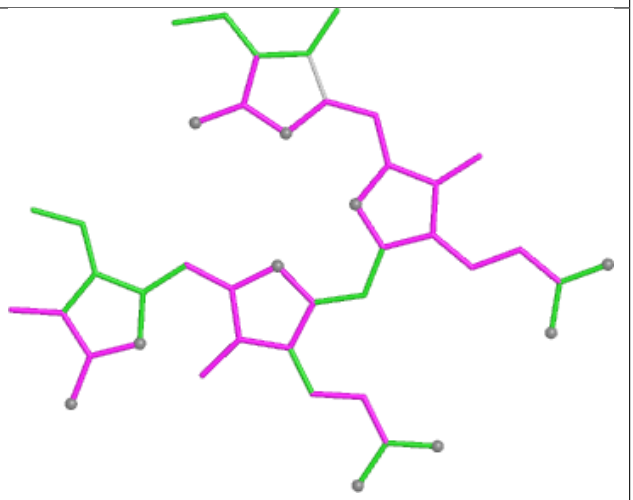


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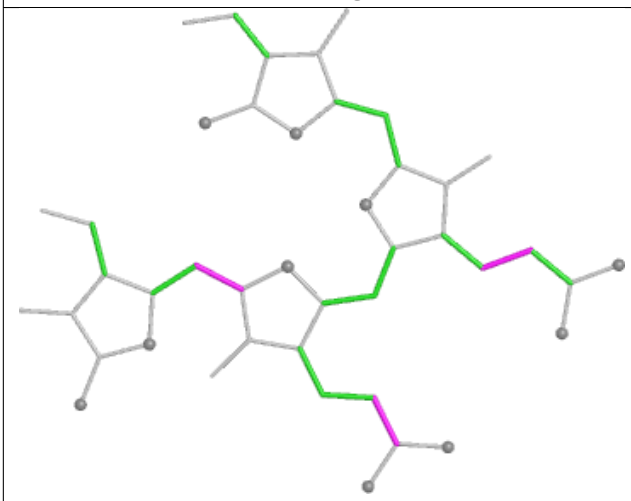
Ligand PEB RA 201



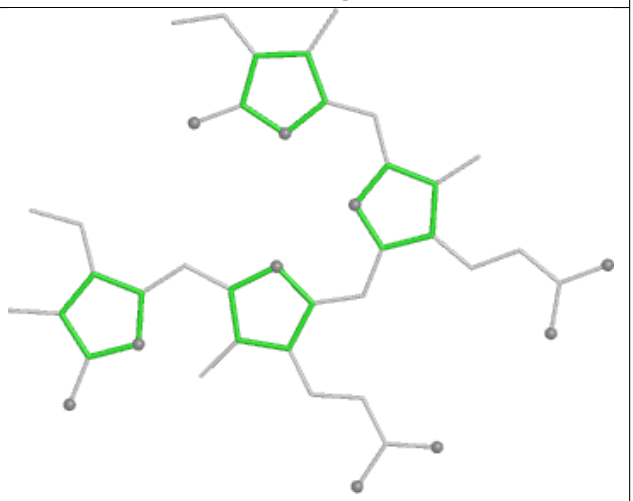
Bond lengths



Bond angles

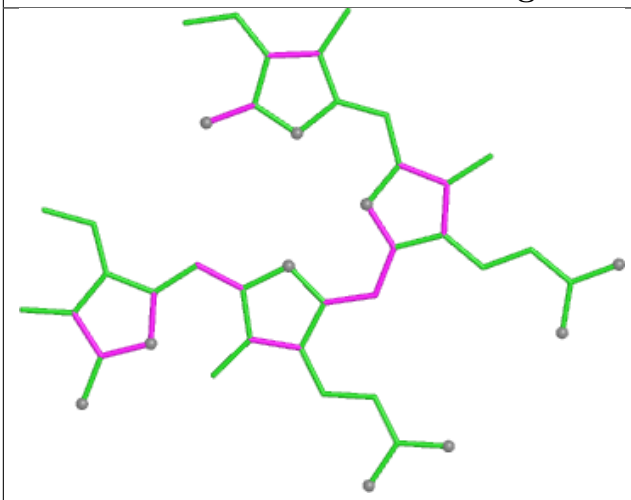


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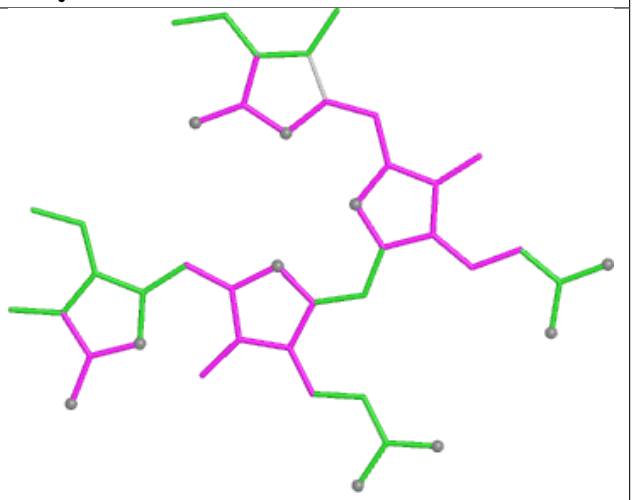


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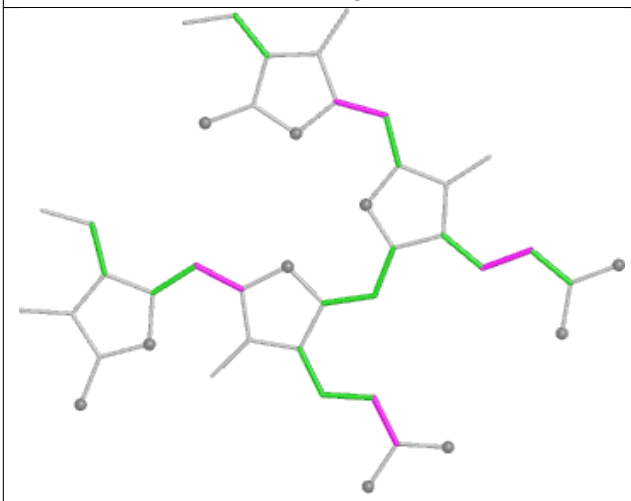
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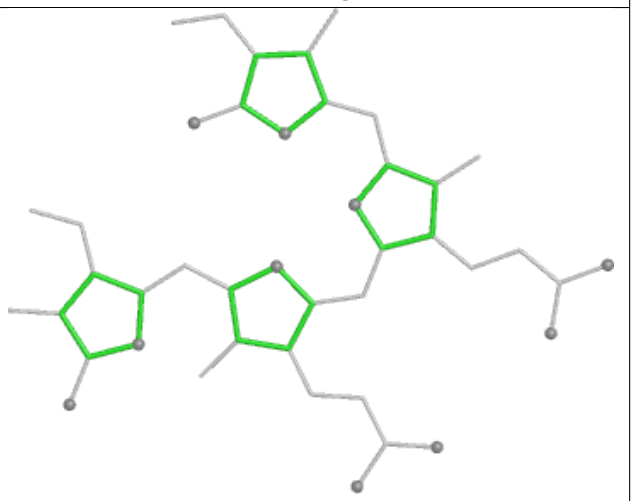
Bond lengths



Bond angles

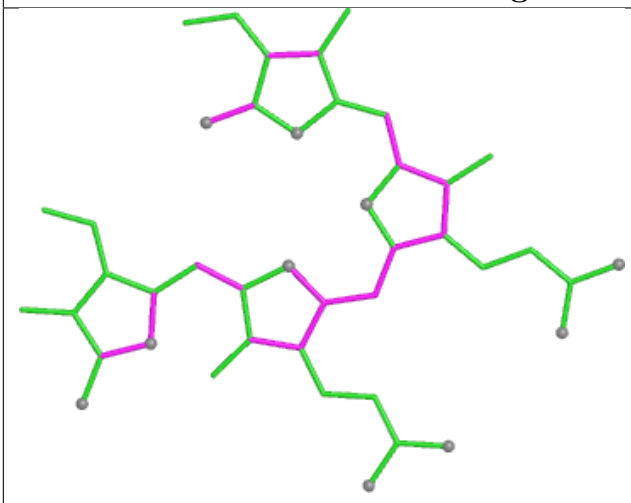


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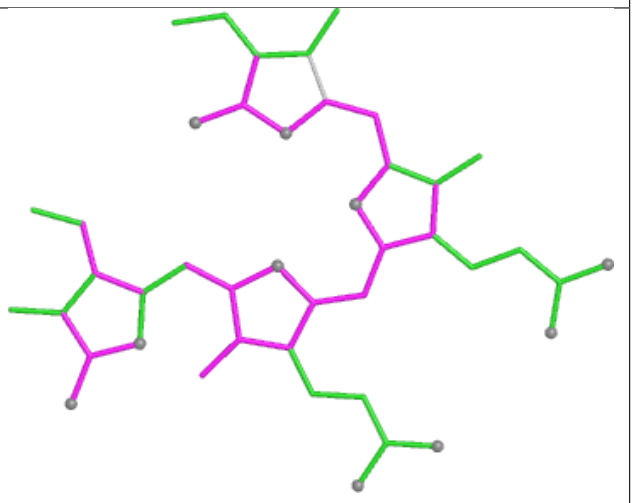


Rings

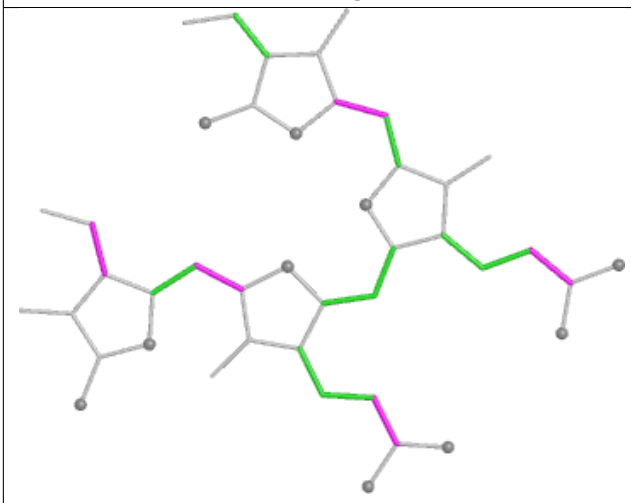
Ligand PEB RD 203



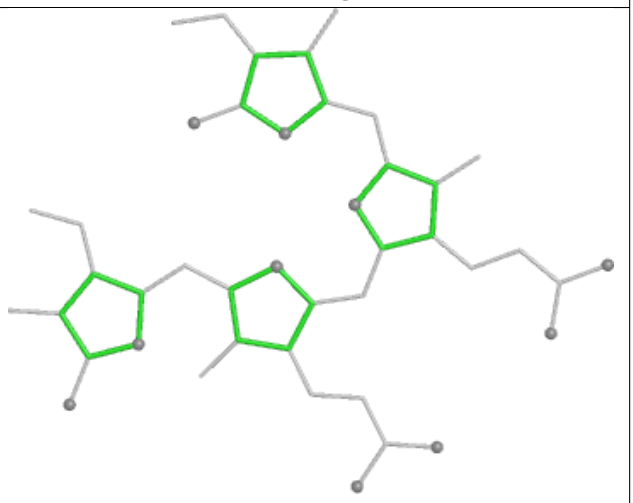
Bond lengths



Bond angles

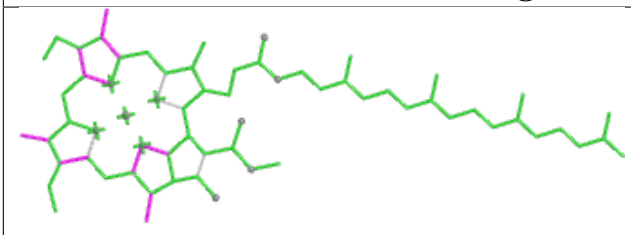


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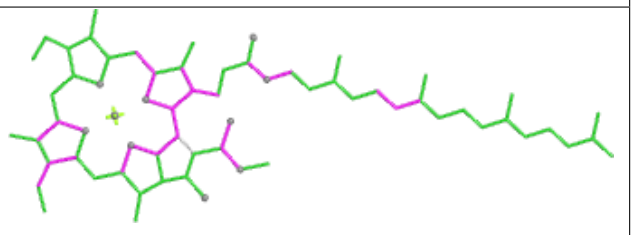


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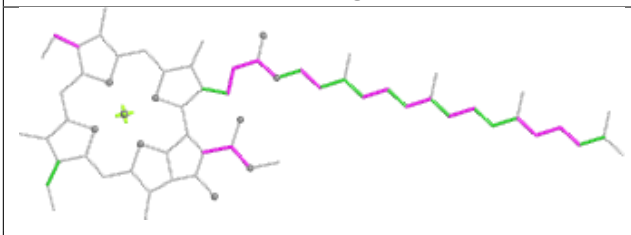
Ligand CLA F2 205



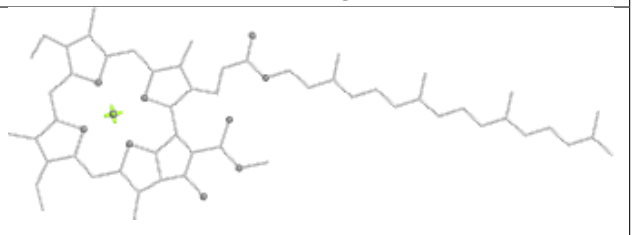
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Bond angles

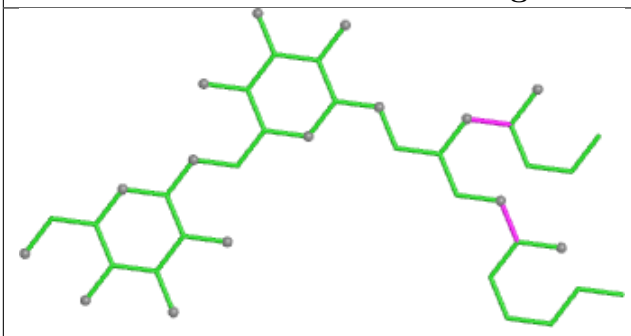


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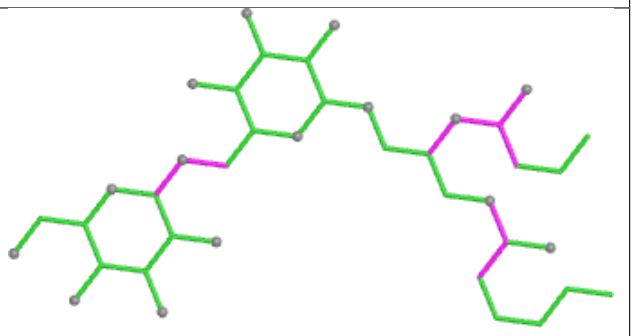


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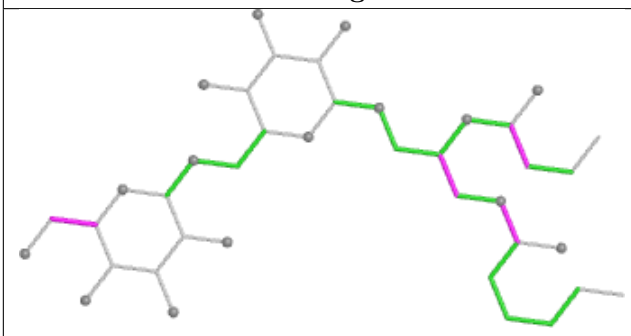
Ligand DGD O6 301



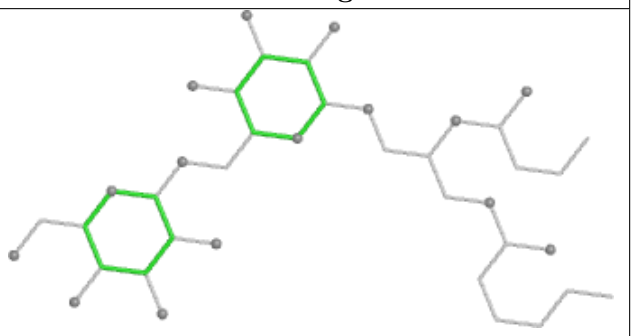
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Bond angles

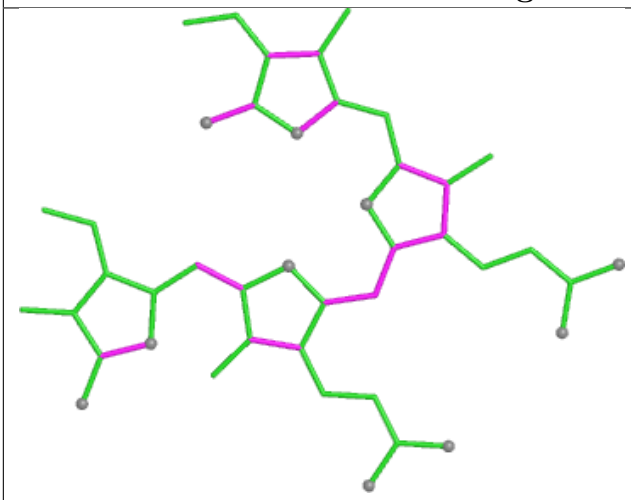


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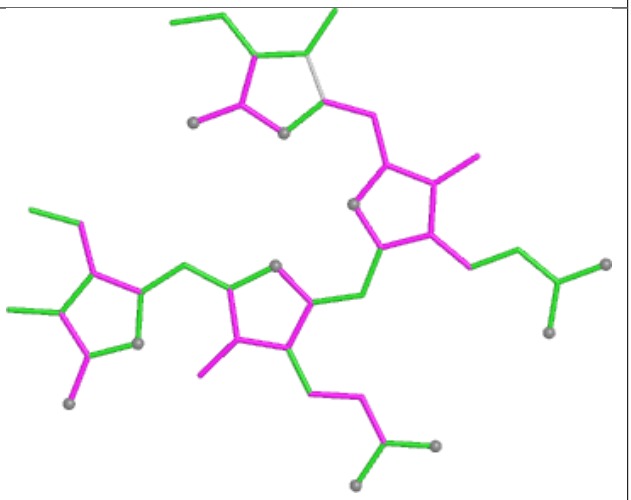


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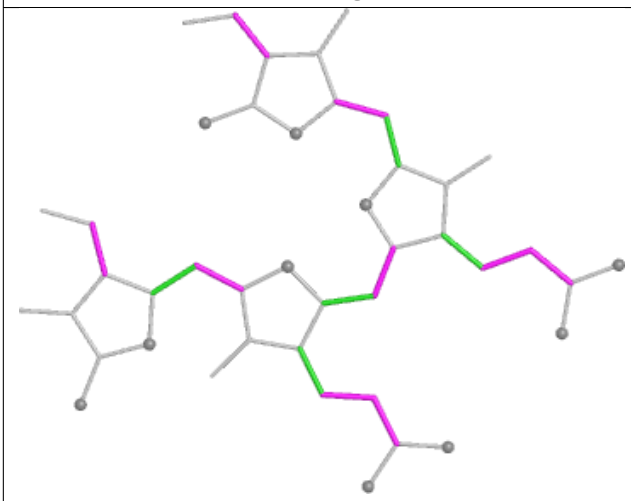
Ligand PEB T1 202



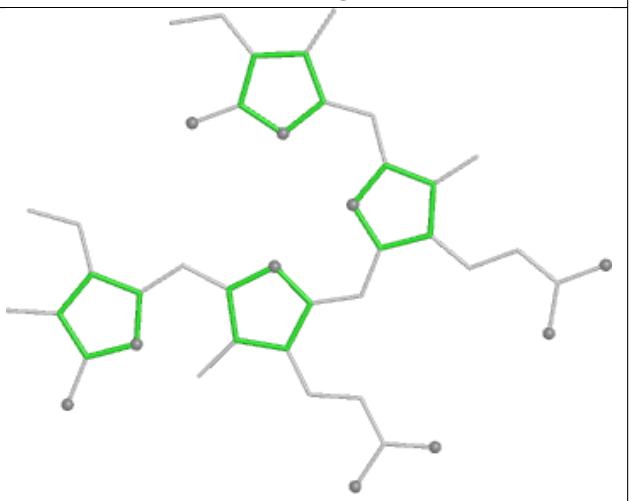
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Bond angles

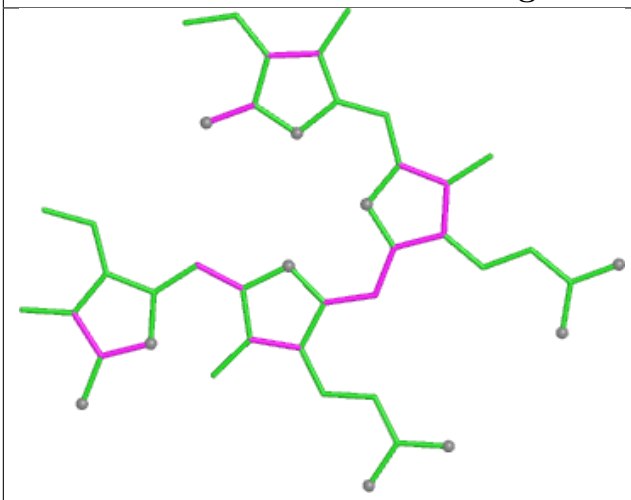


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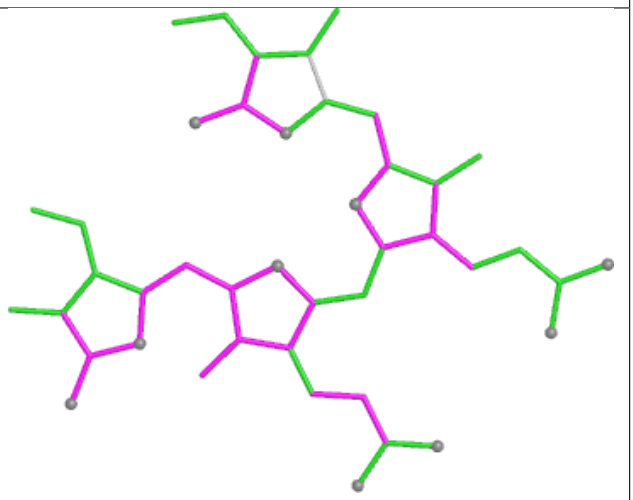


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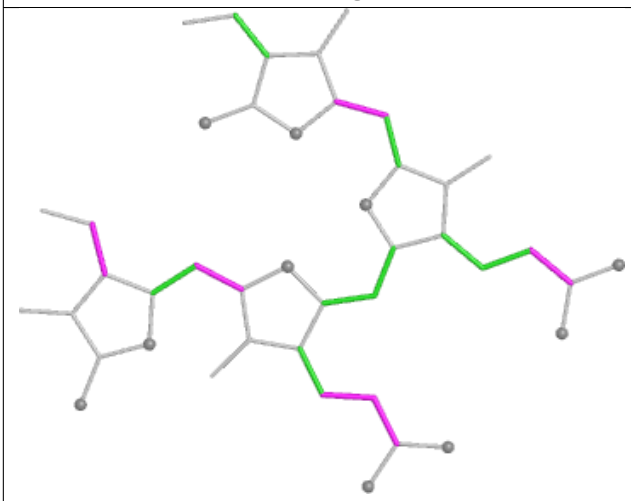
Ligand PEB fK 201



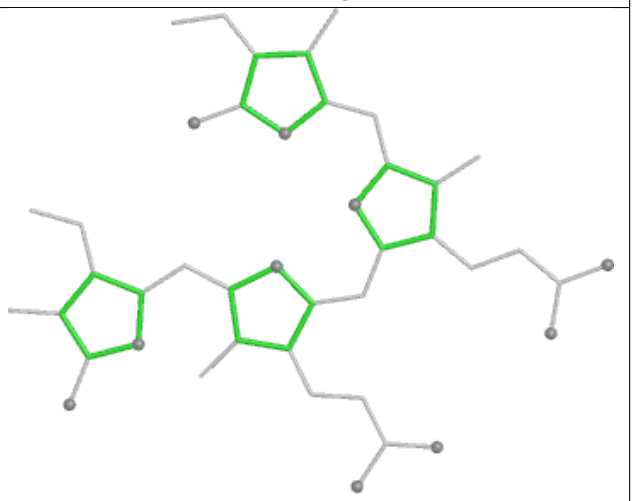
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Bond angles

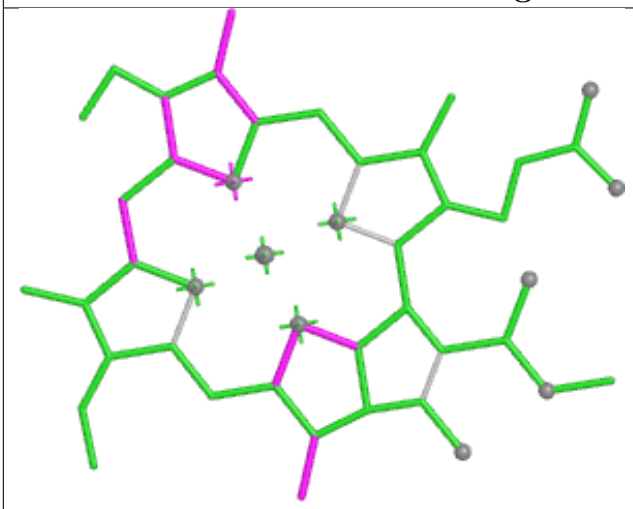


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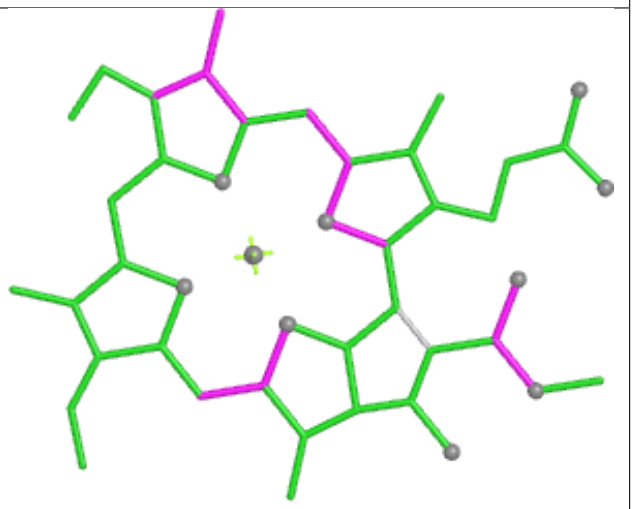


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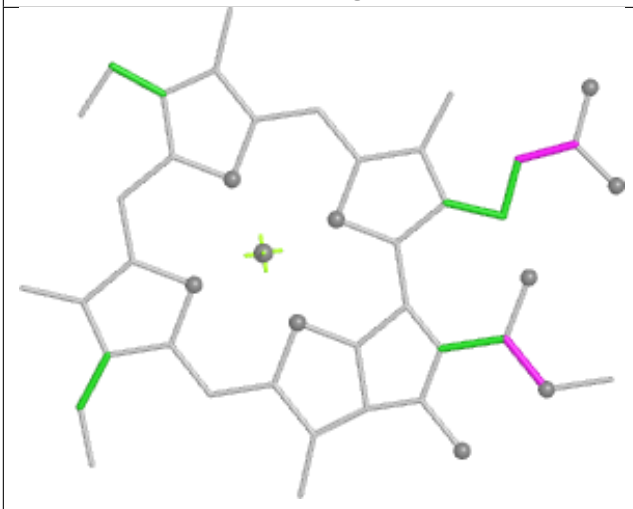
Ligand CLA 1N 603



Bond lengths



Bond angles

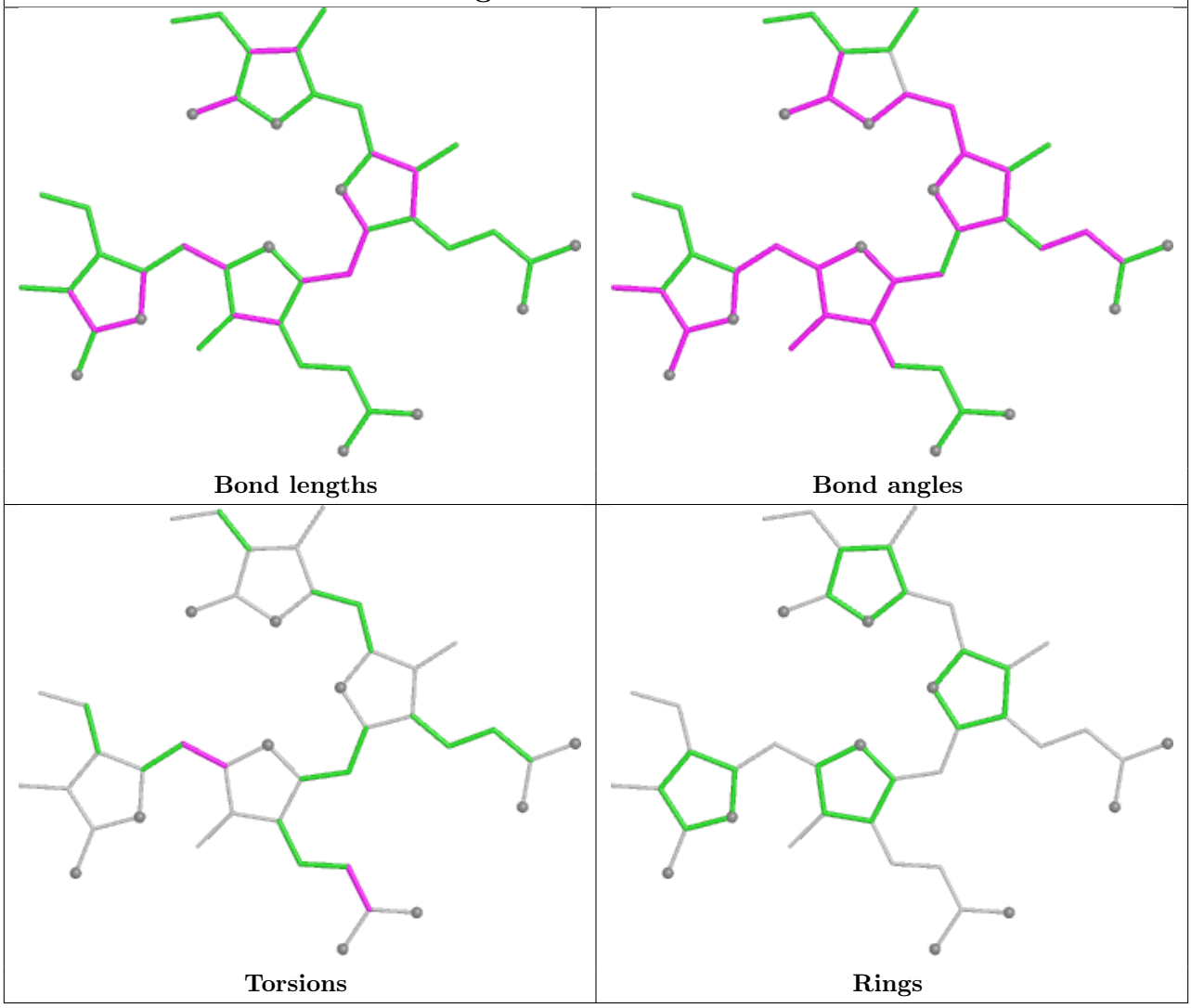


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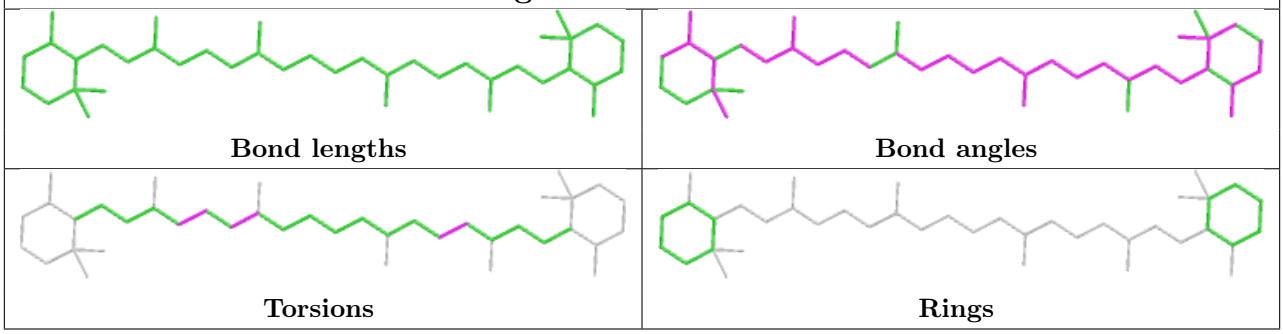


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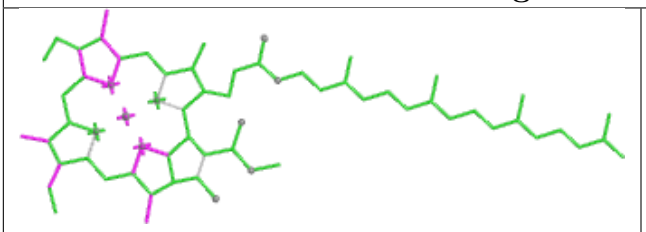
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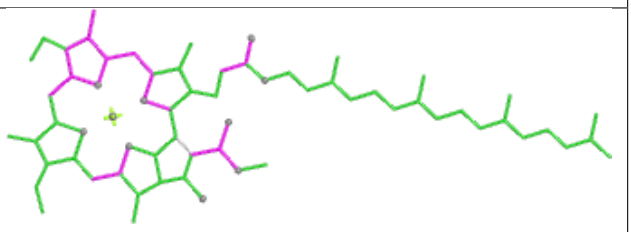
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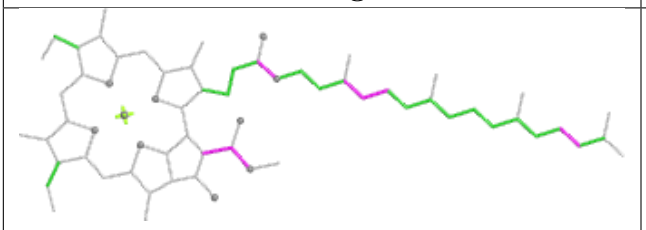
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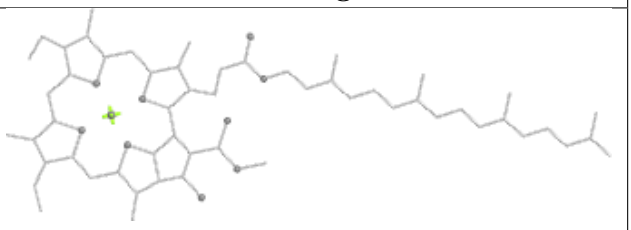
Bond lengths



Bond angles

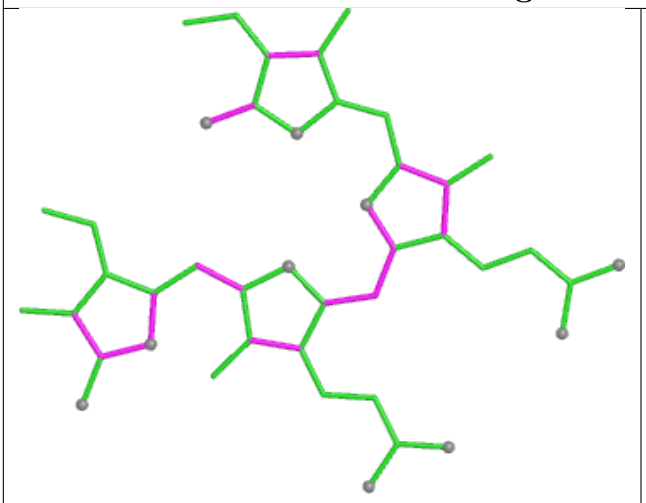


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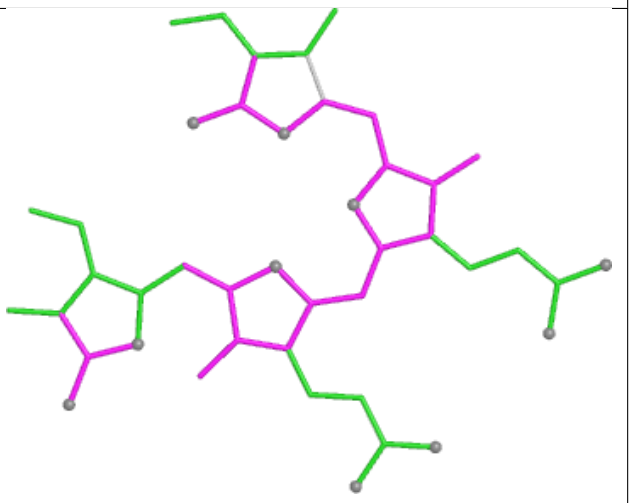


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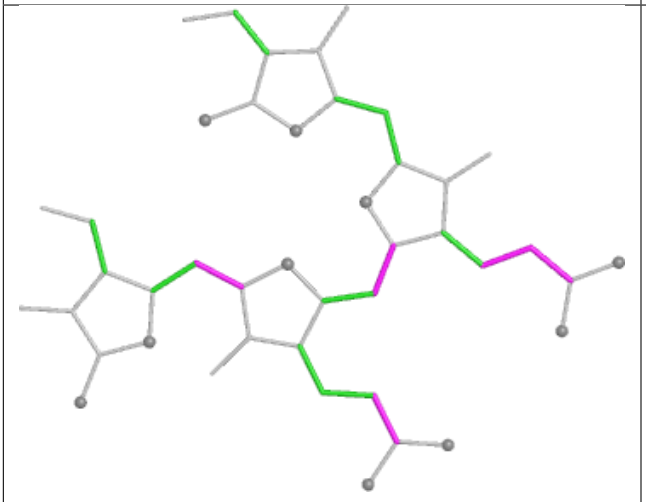
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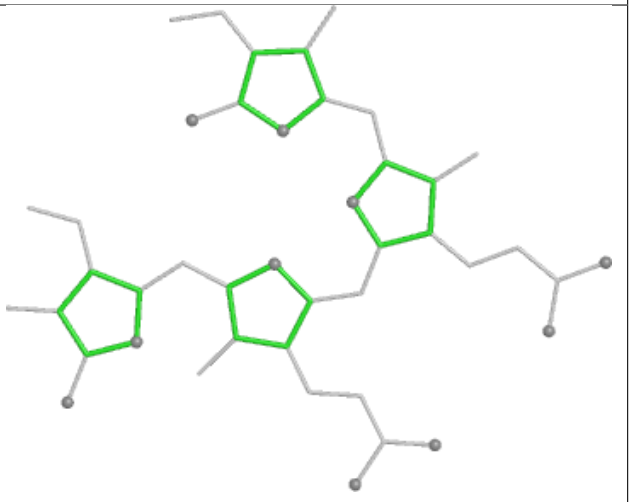
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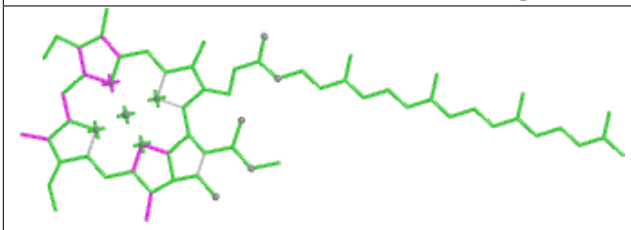


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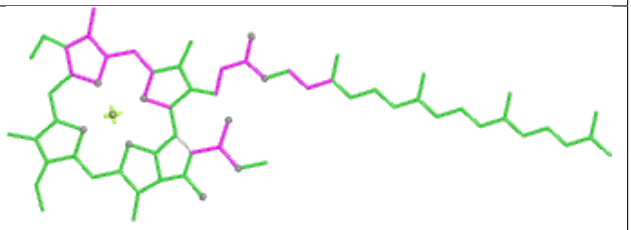


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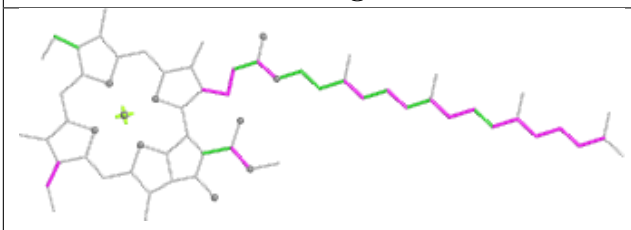
Ligand CLA A6 402



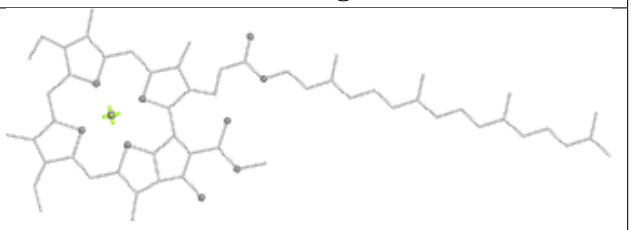
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Bond angles

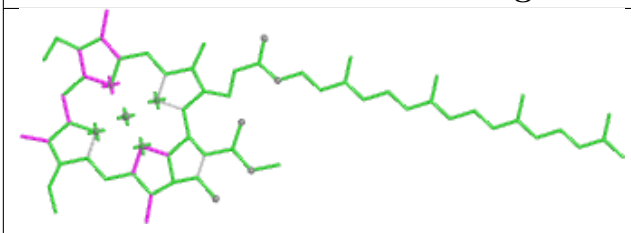


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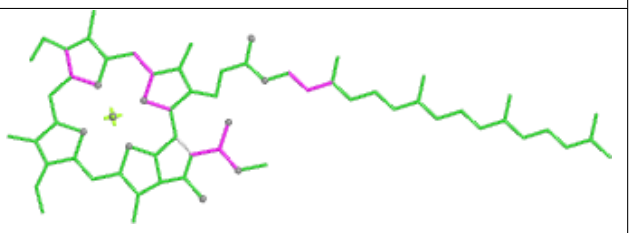


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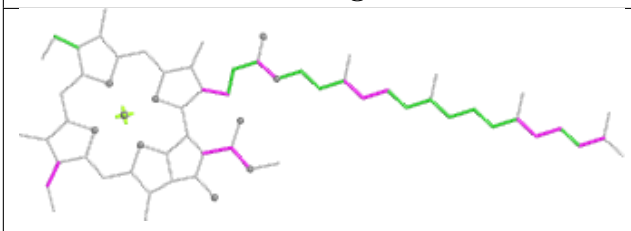
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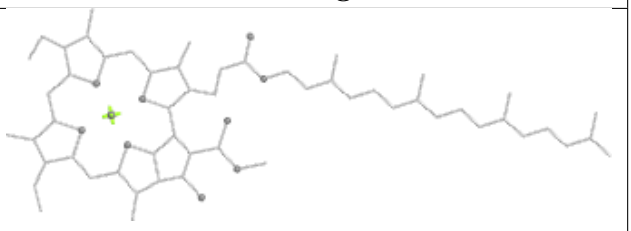
Bond lengths



Bond angles

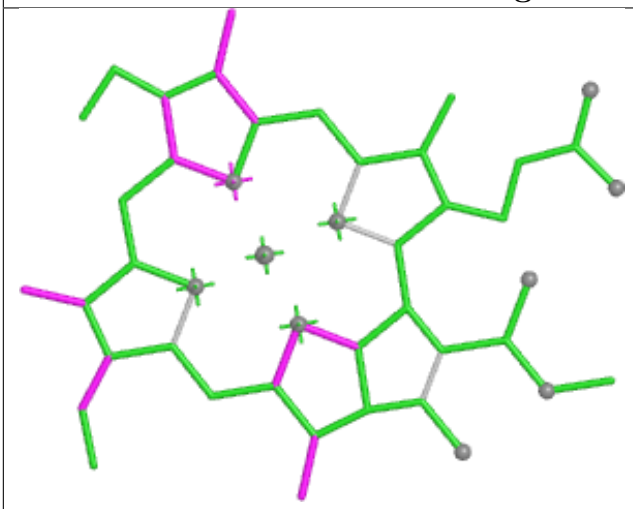


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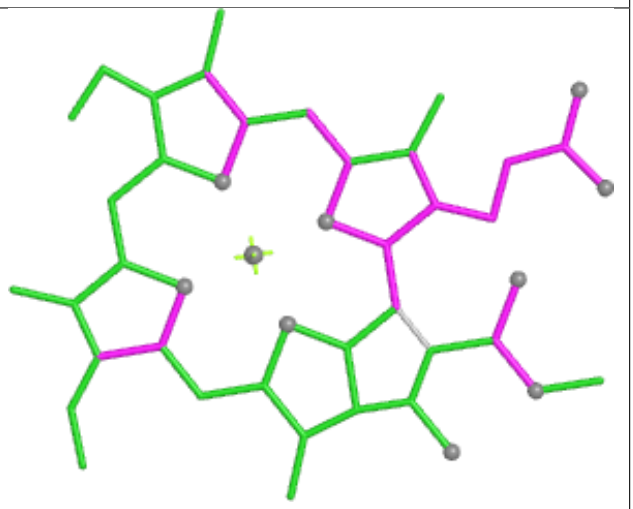


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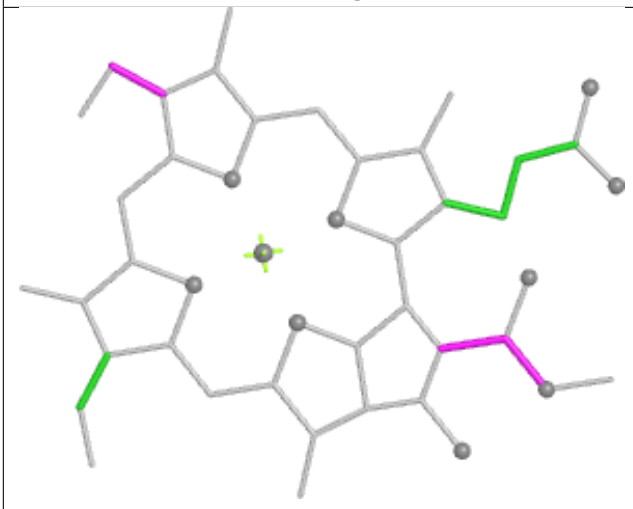
Ligand CLA 8N 304



Bond lengths



Bond angles

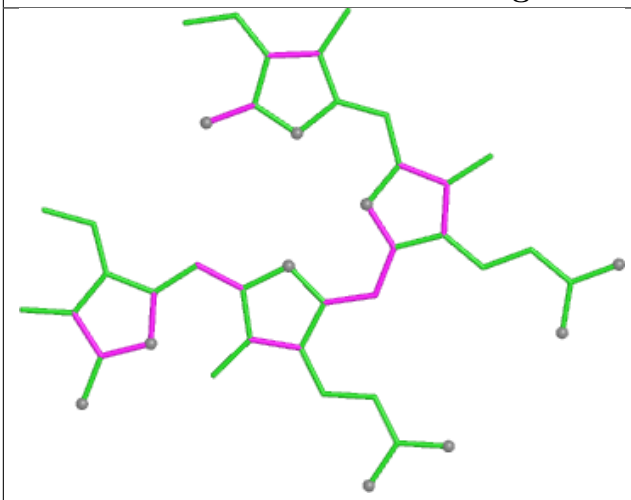


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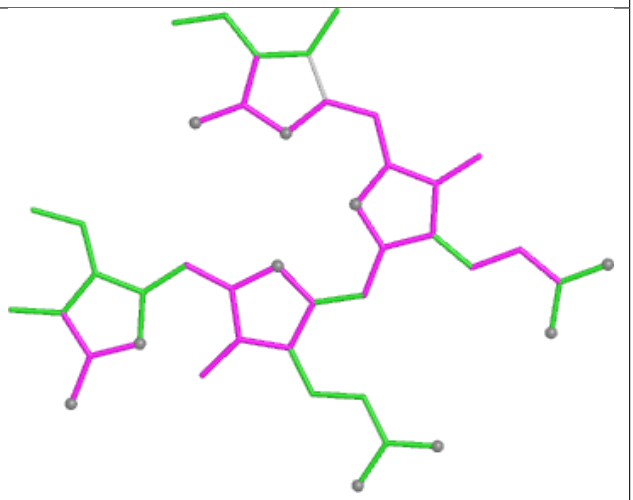


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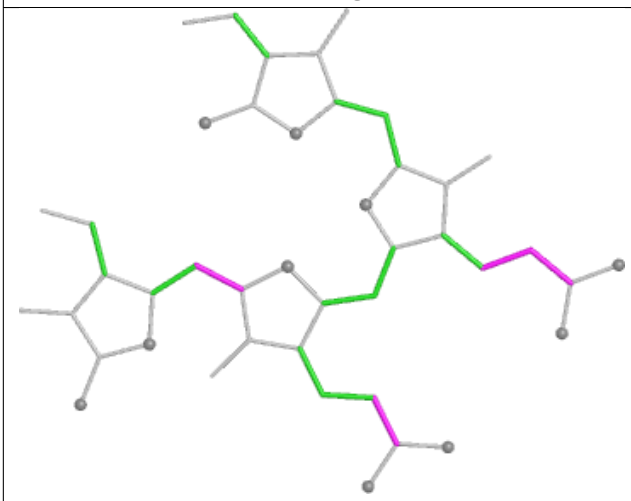
Ligand PEB ED 202



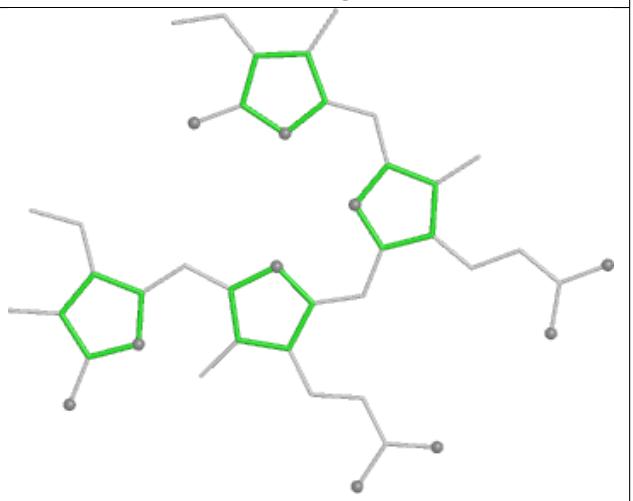
Bond lengths



Bond angles

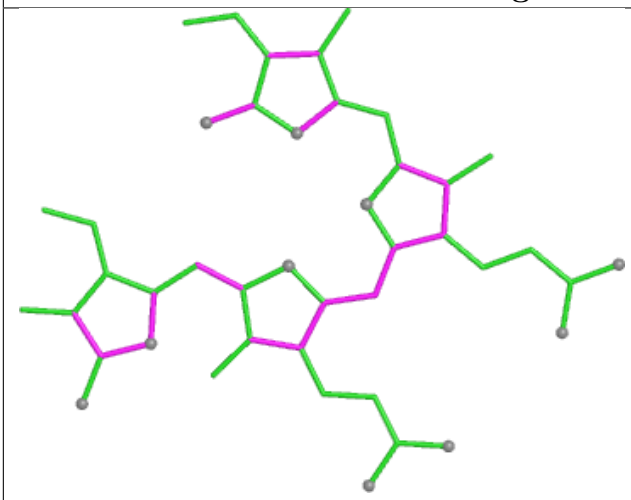


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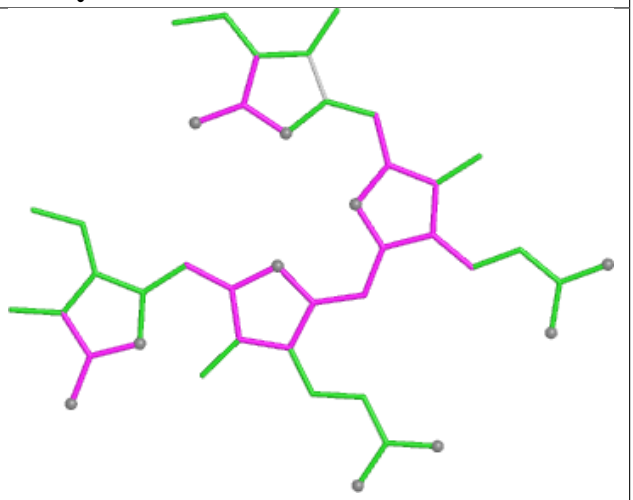


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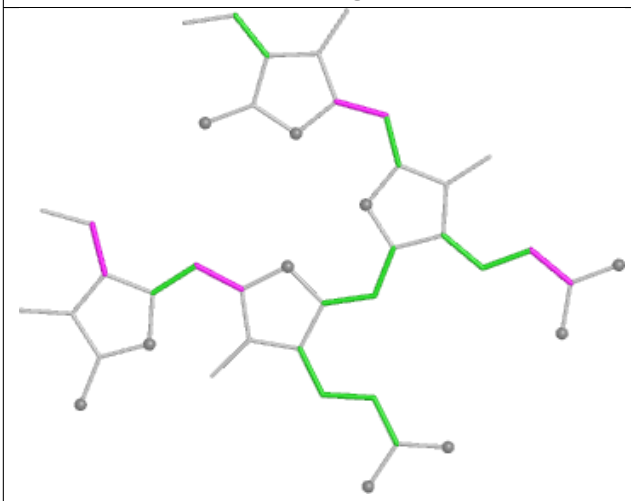
Ligand PEB PQ 201



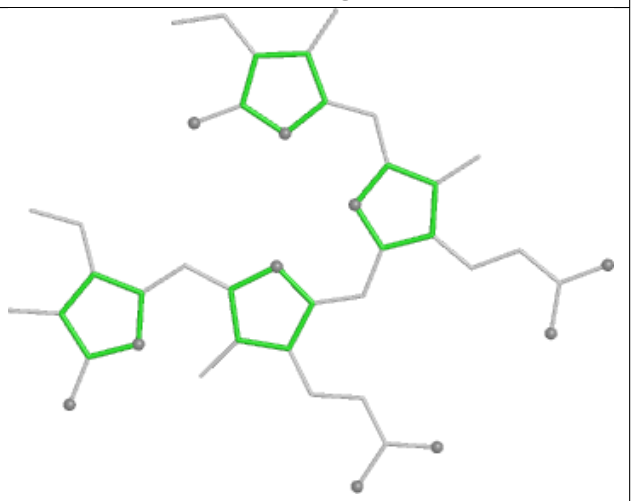
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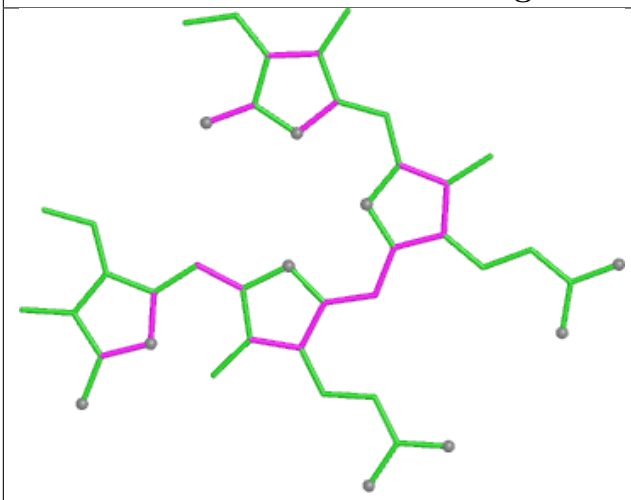


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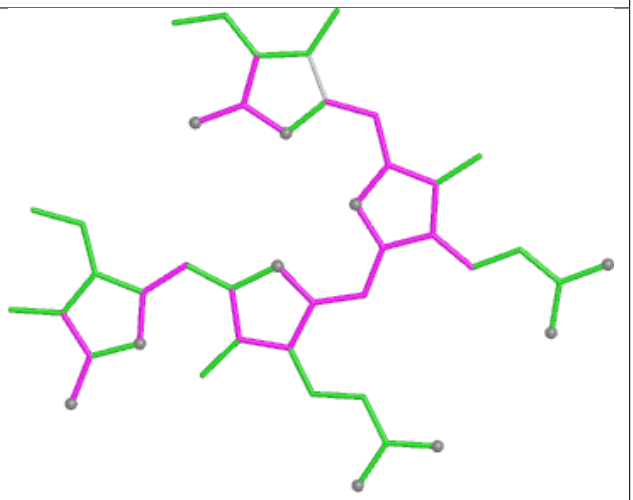


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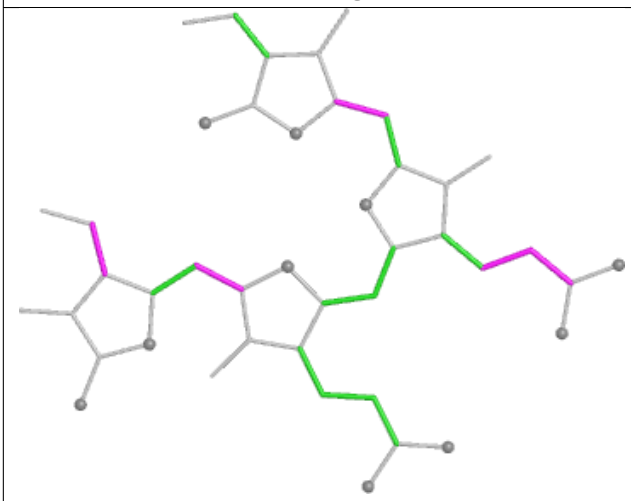
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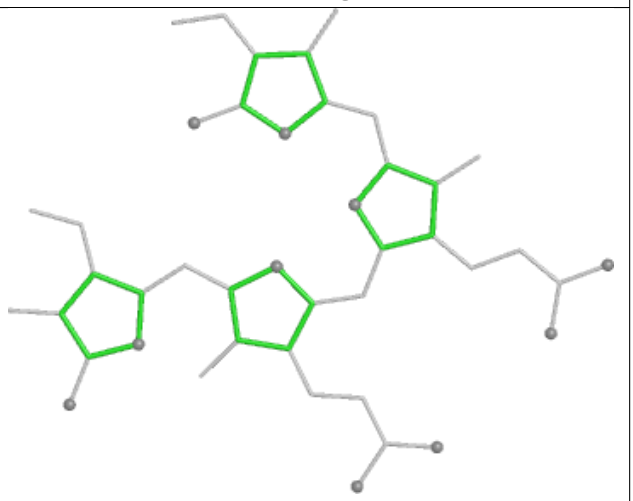
Bond lengths



Bond angles

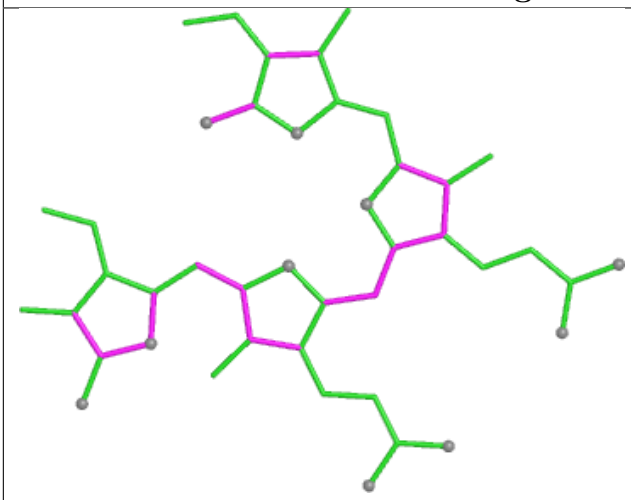


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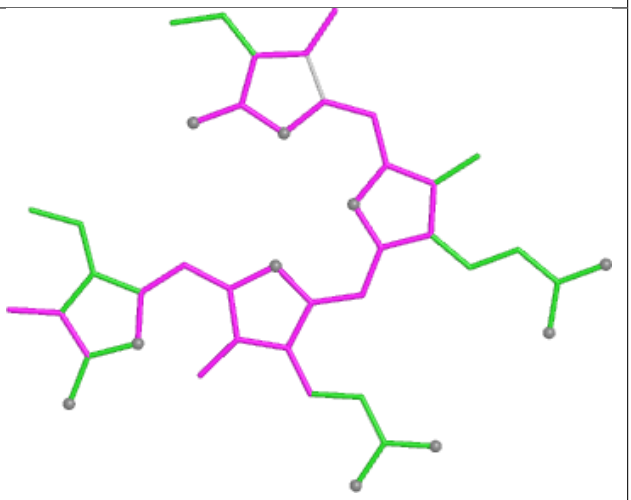


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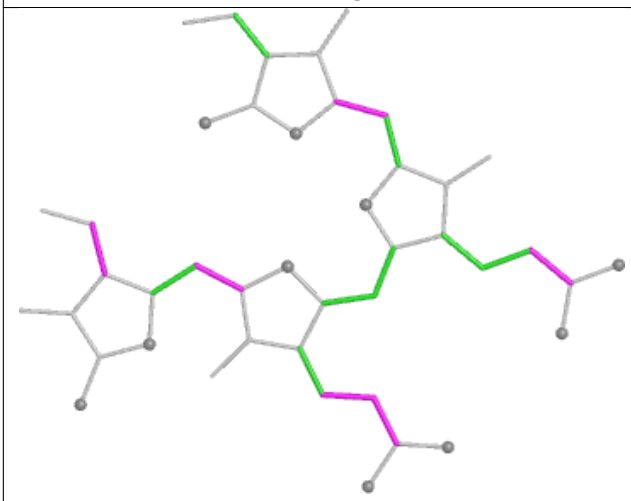
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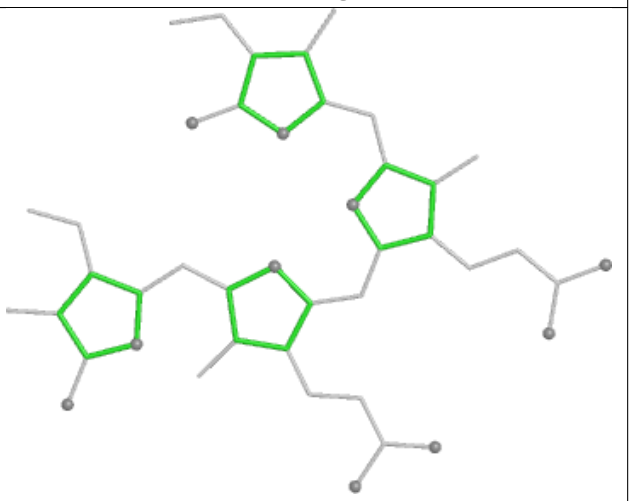
Bond lengths



Bond angles

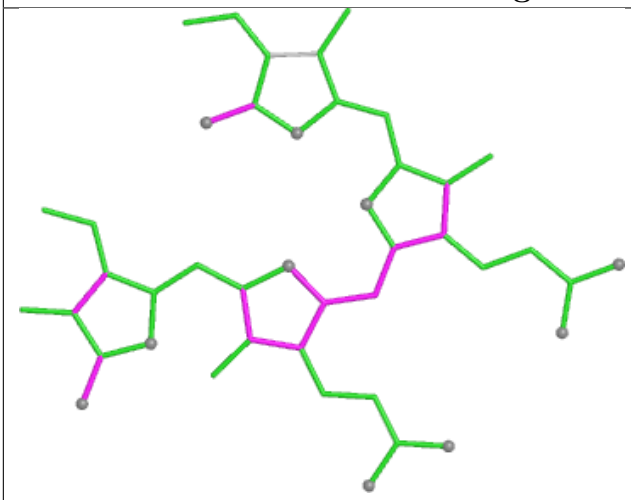


Torsions

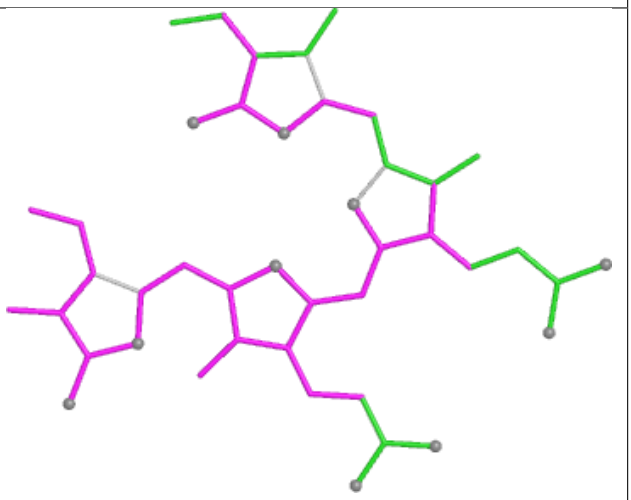


Rings

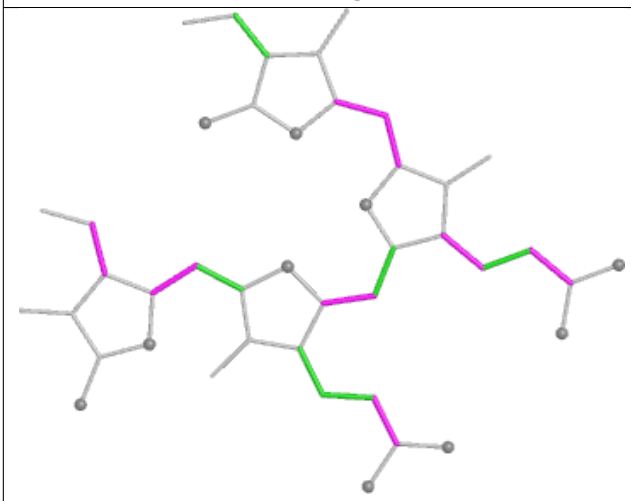
Ligand PUB A1 304



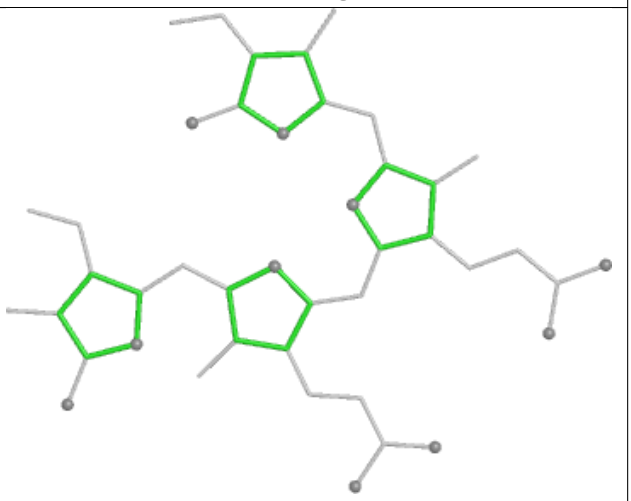
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Bond angles

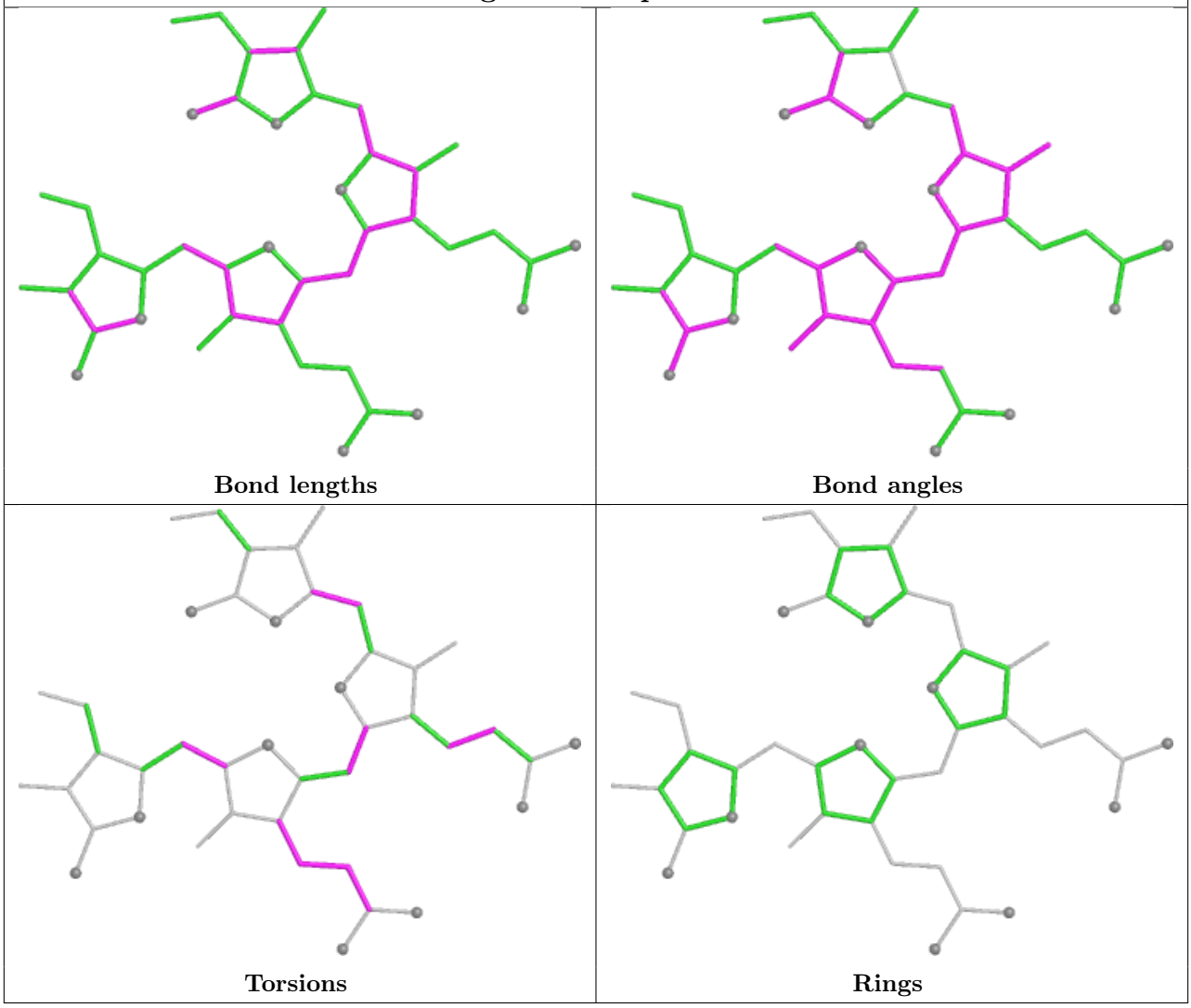


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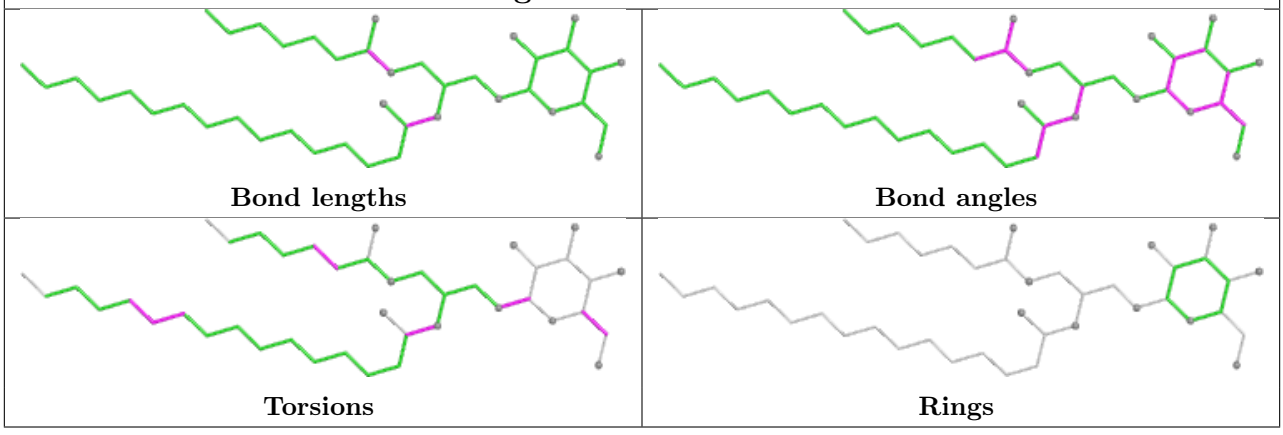


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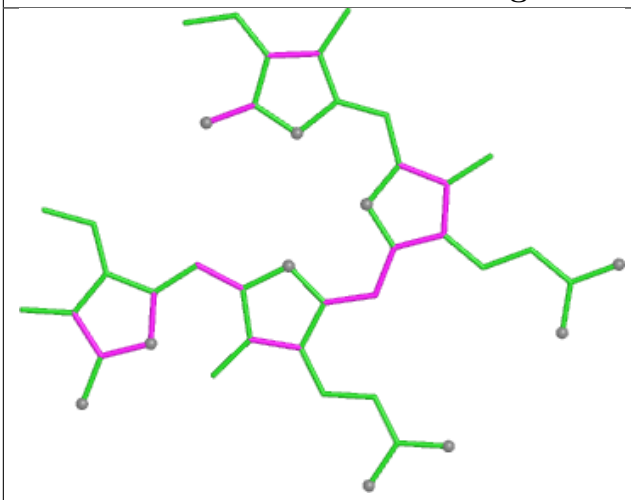
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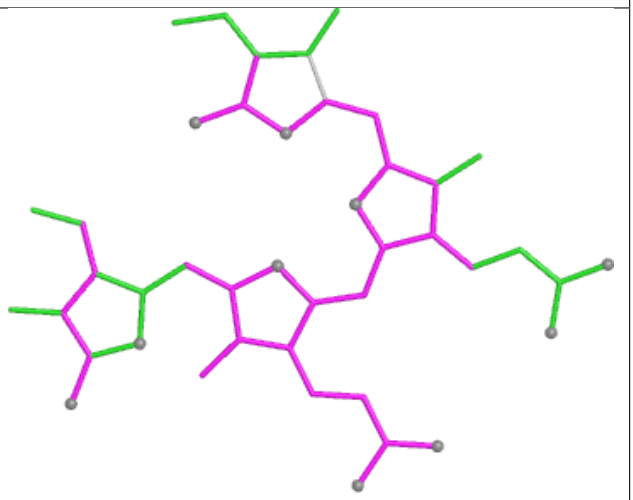
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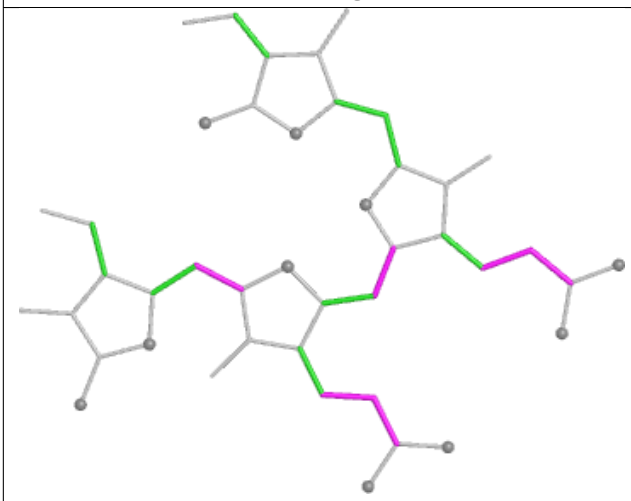
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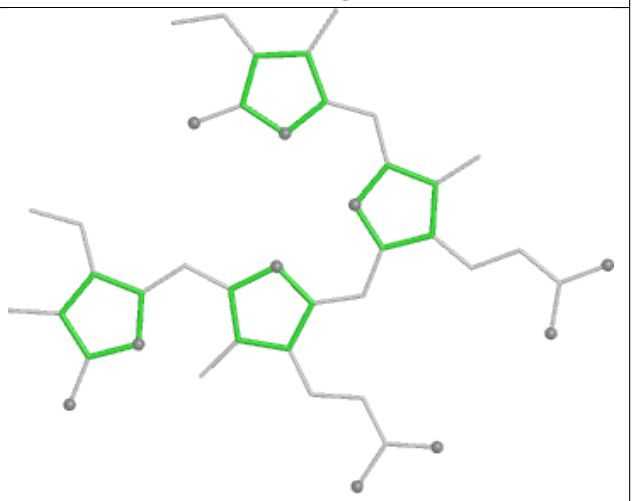
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Bond angles

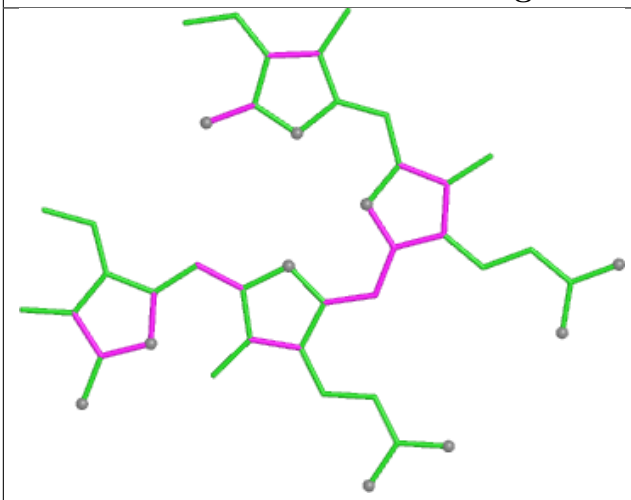


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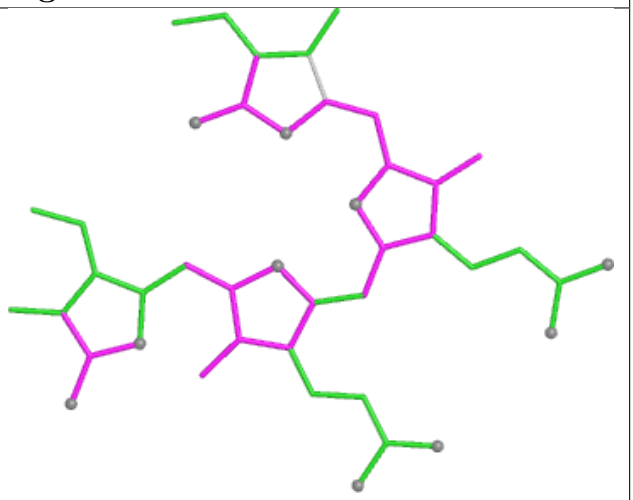


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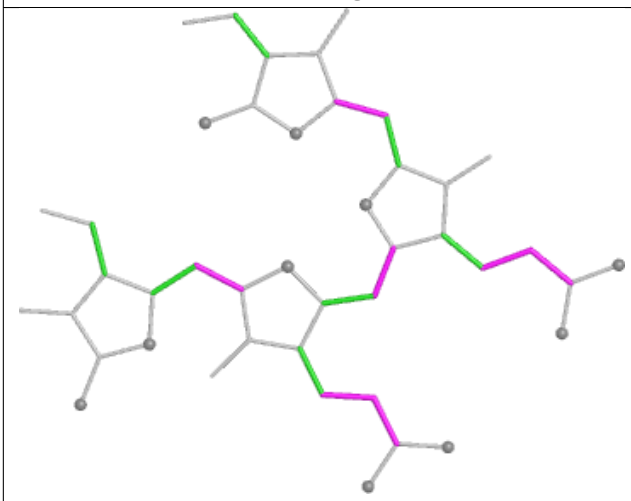
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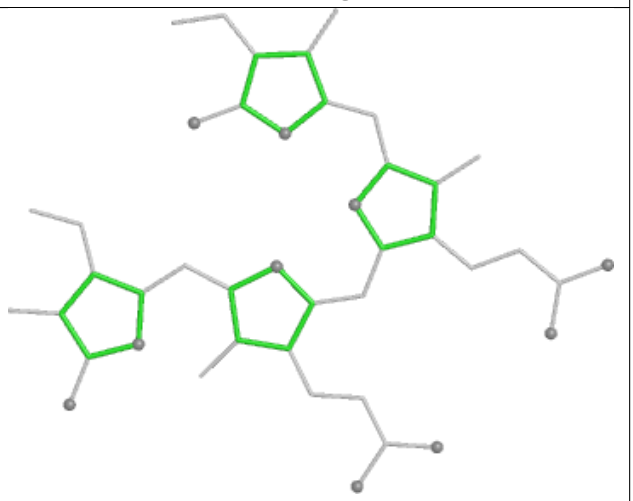
Bond lengths



Bond angles

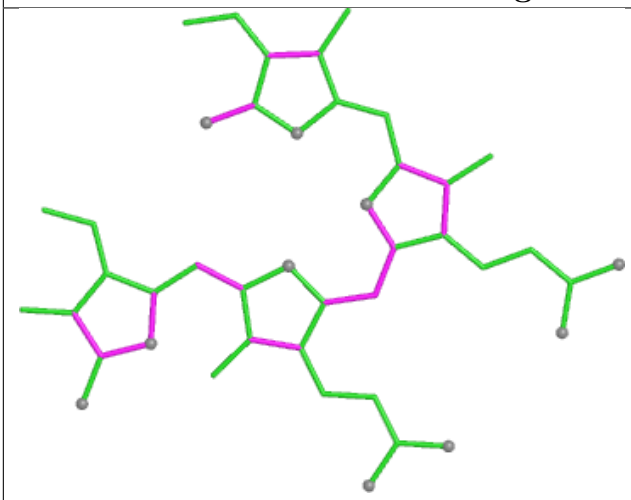


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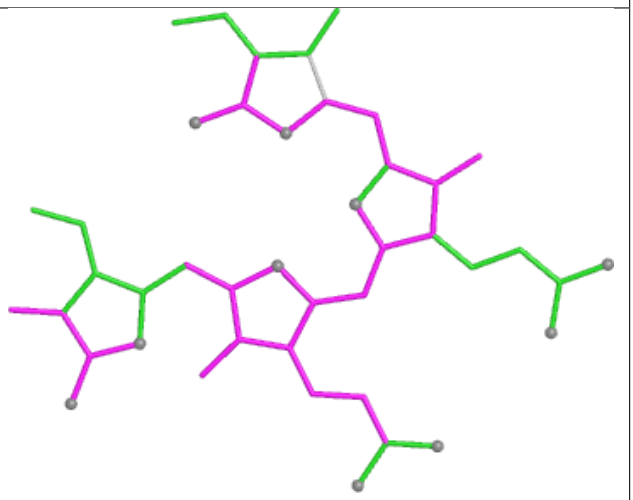


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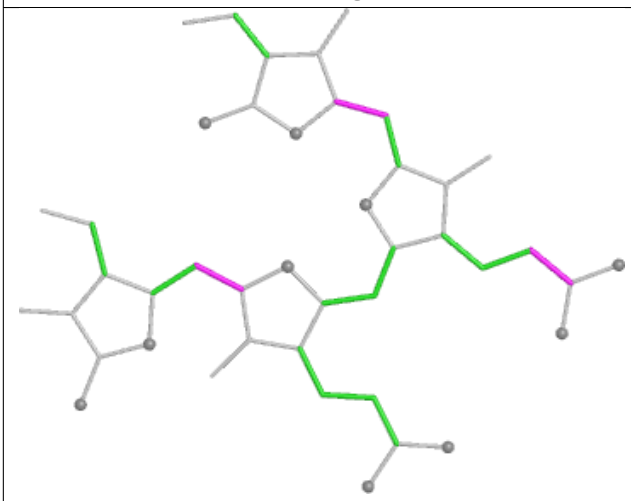
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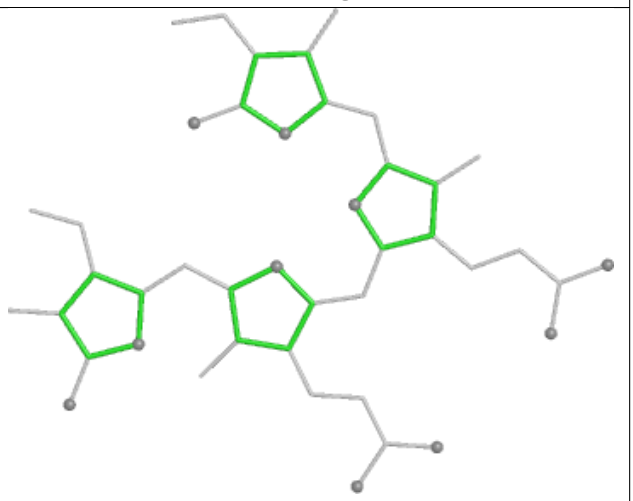
Bond lengths



Bond angles

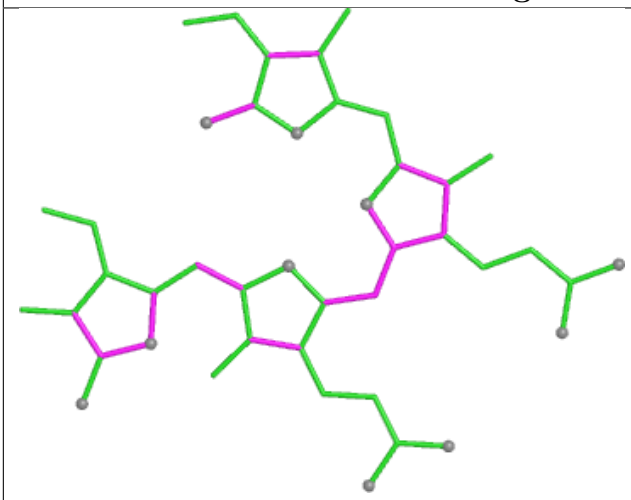


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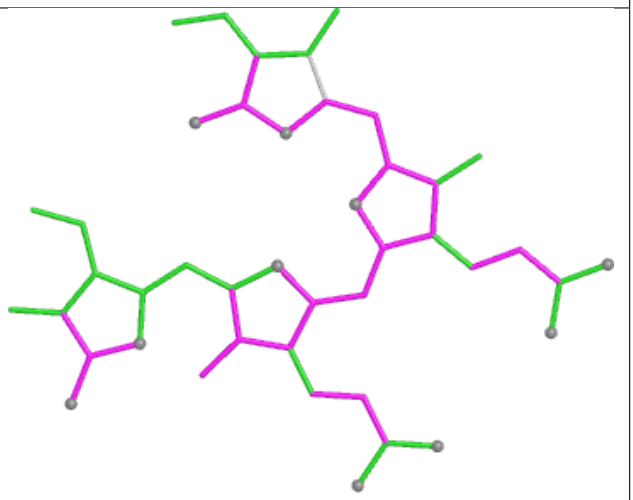


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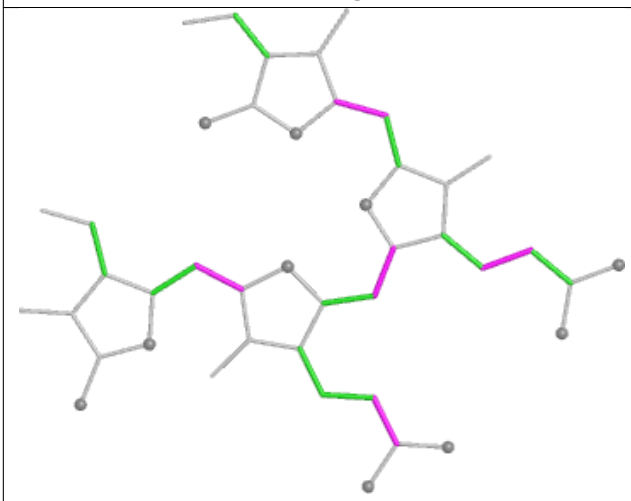
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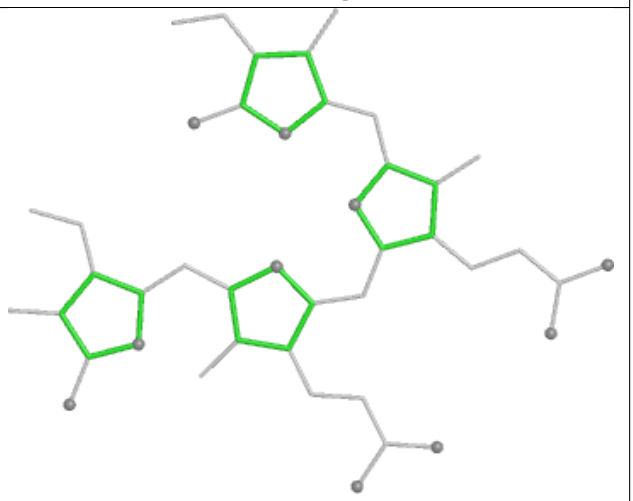
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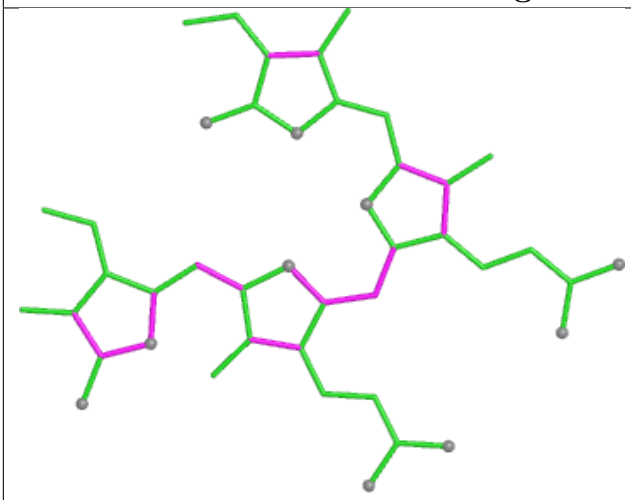


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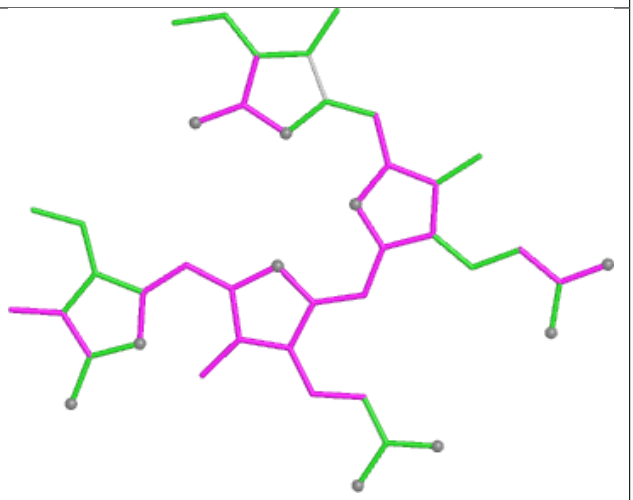


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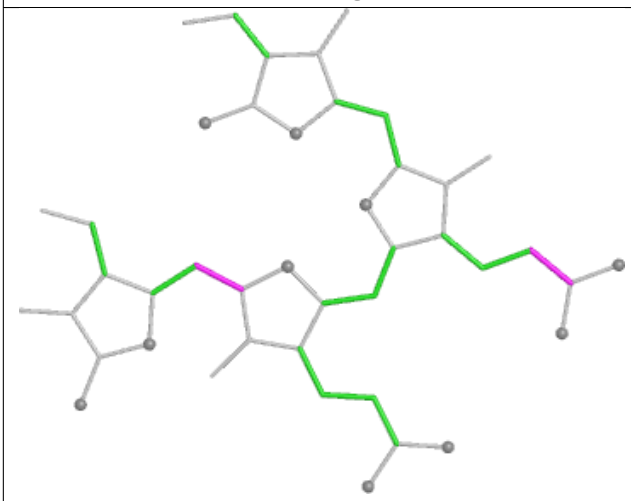
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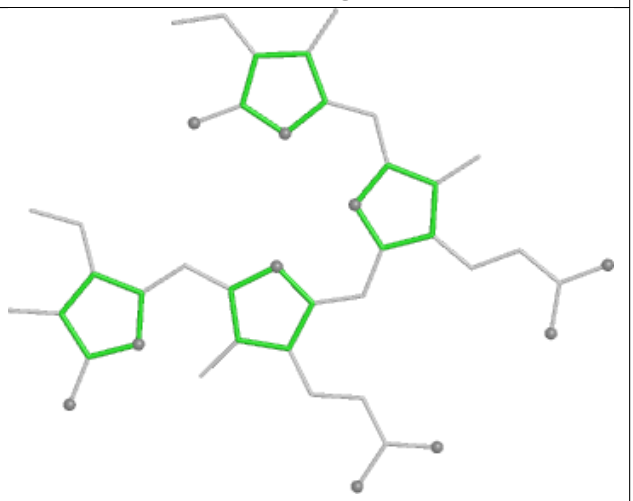
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Bond angles

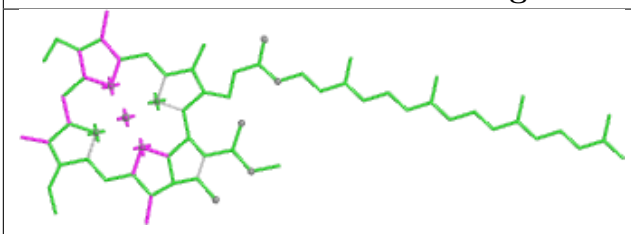


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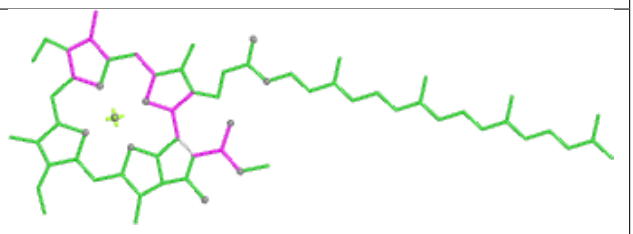


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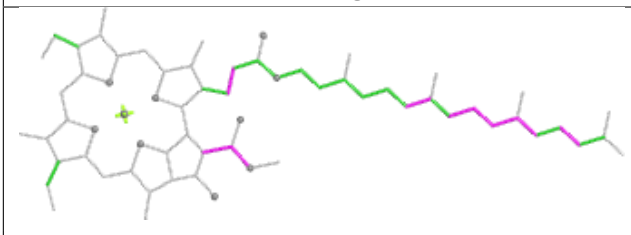
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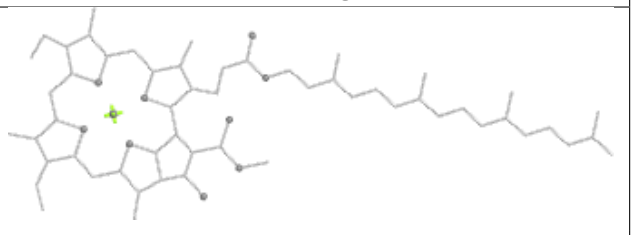
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Bond angles

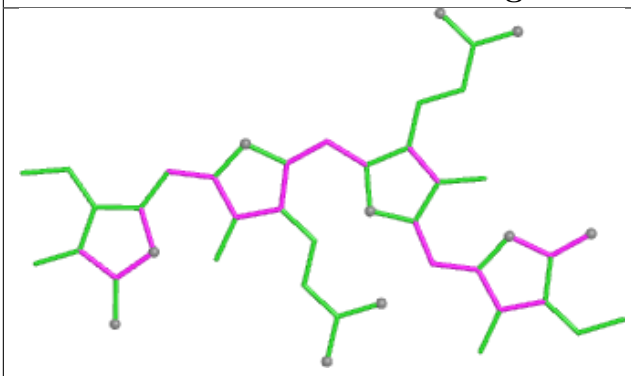


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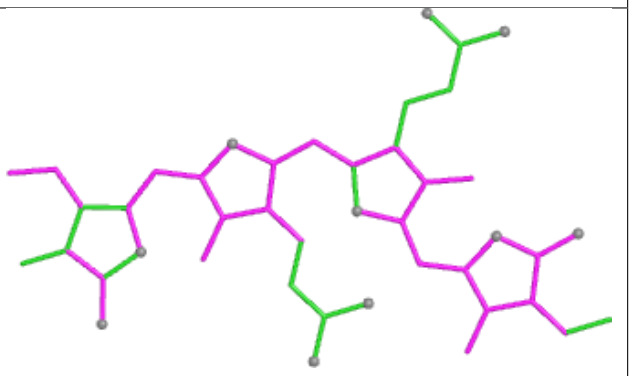


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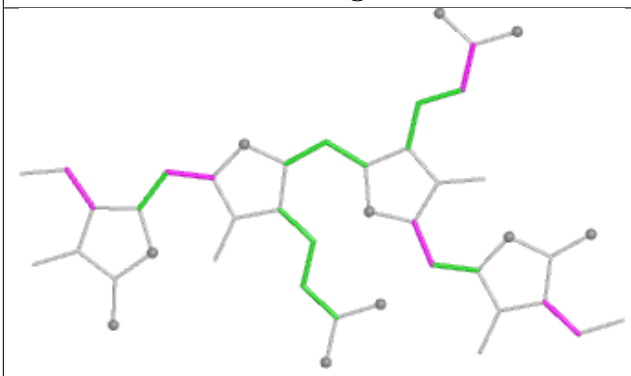
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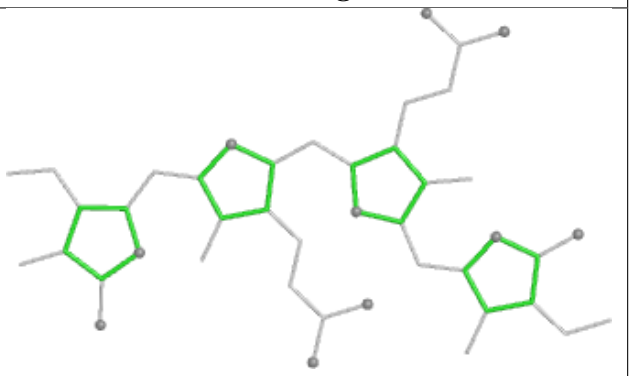
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Bond angles

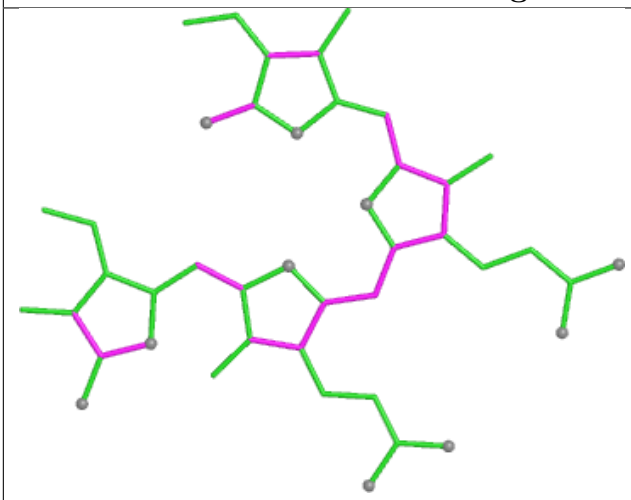


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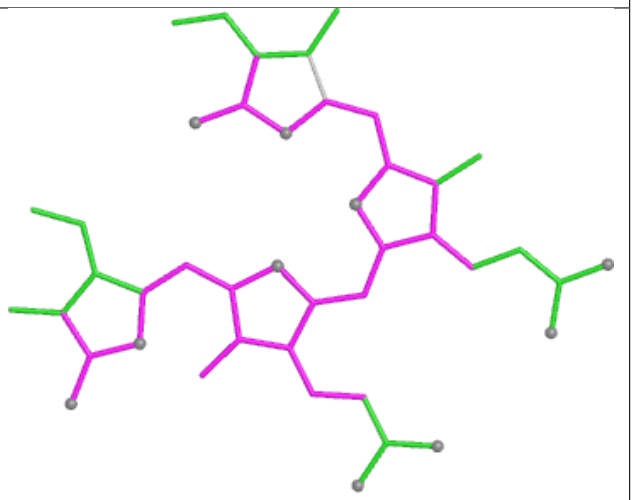


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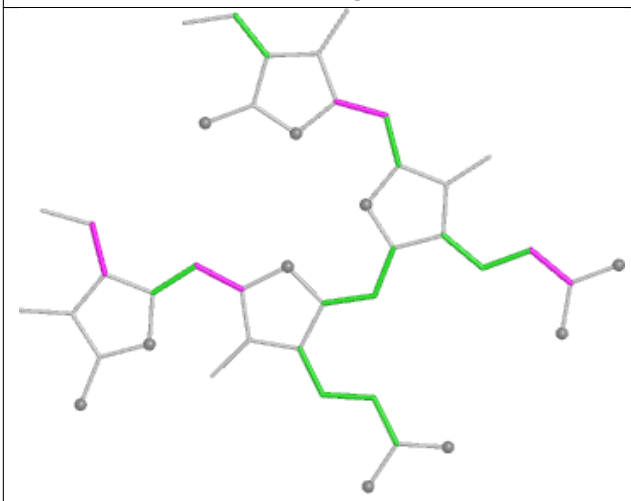
Ligand PEB HA 202



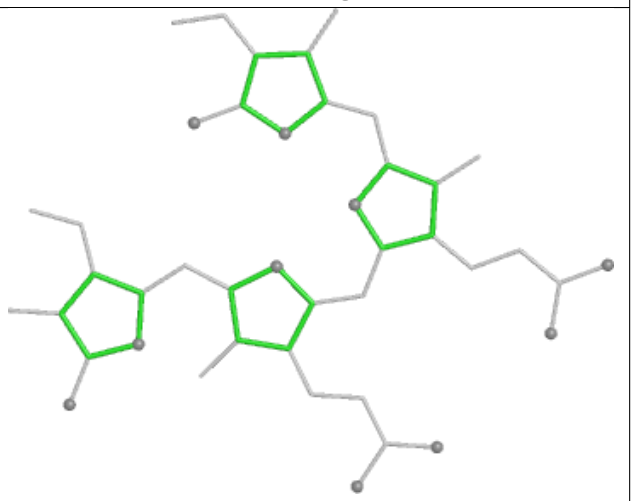
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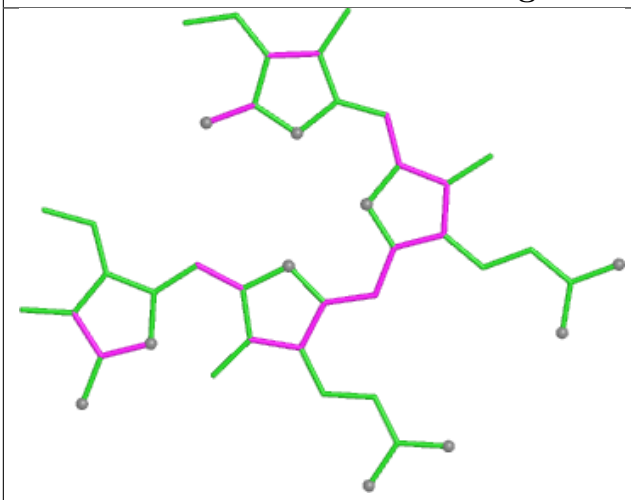


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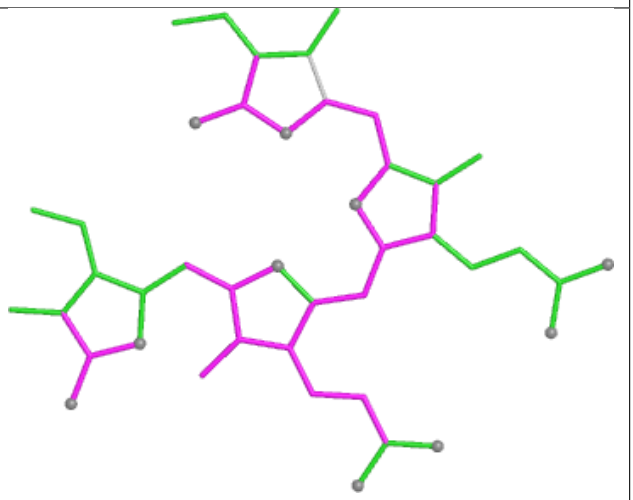


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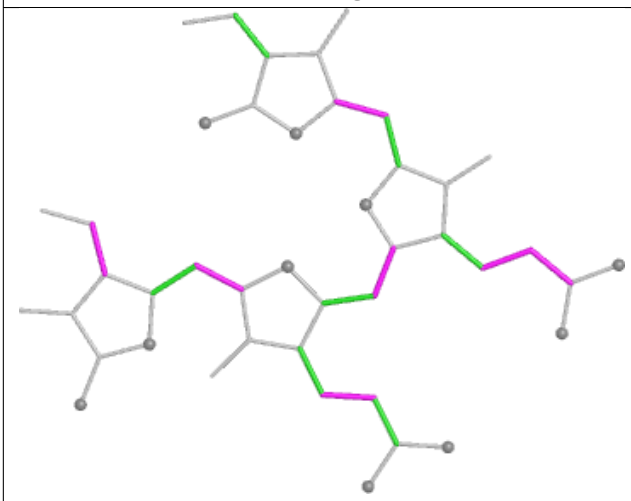
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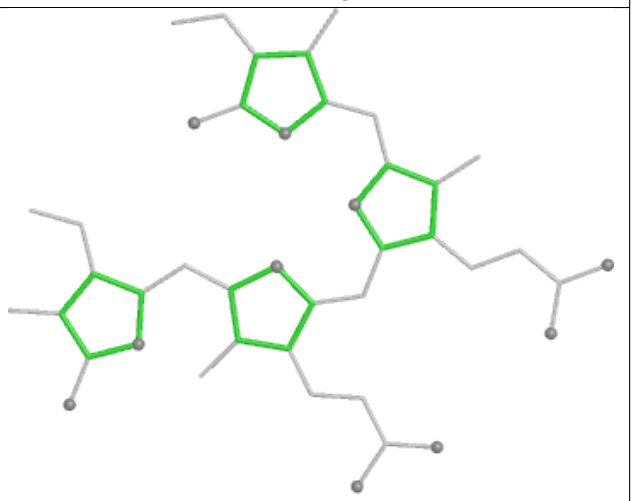
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Bond angles

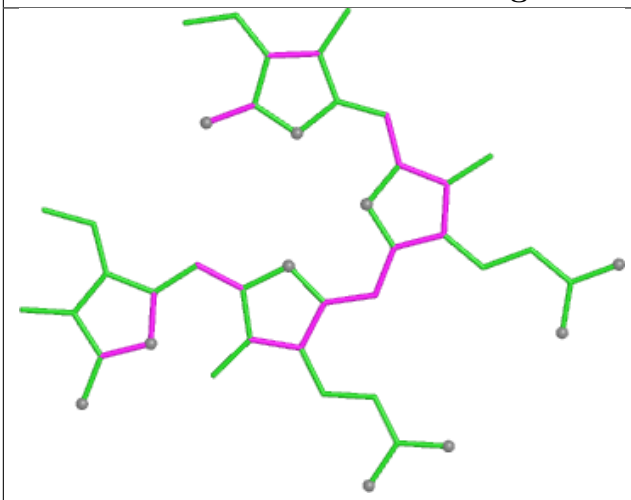


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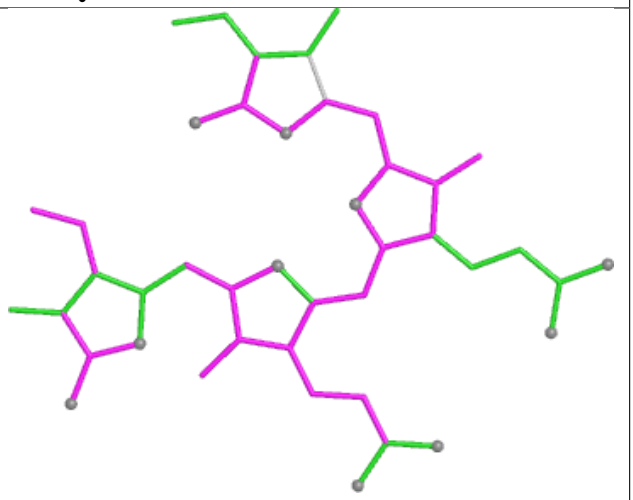


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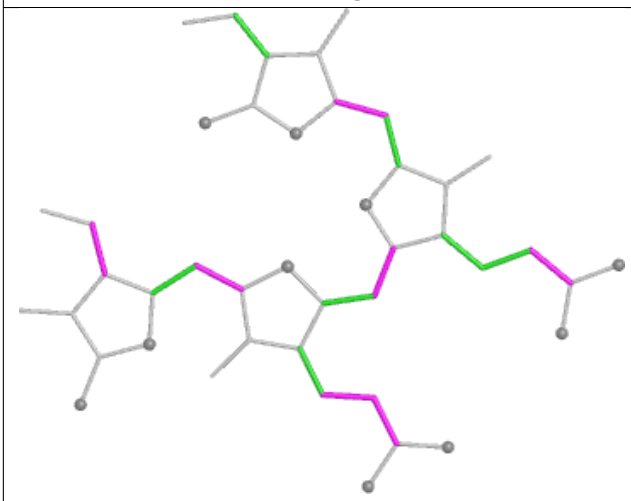
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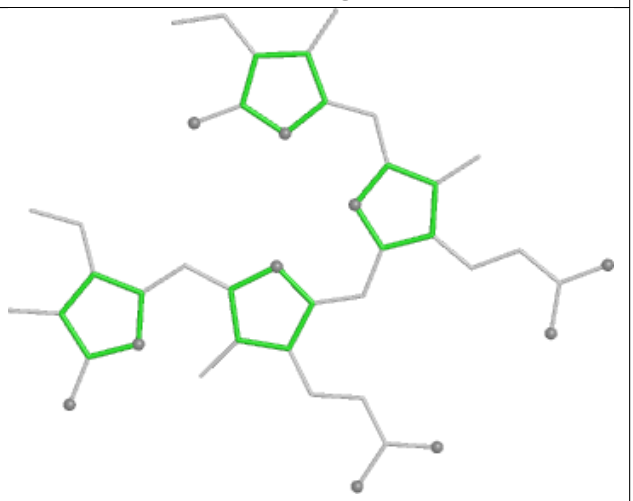
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Bond angles

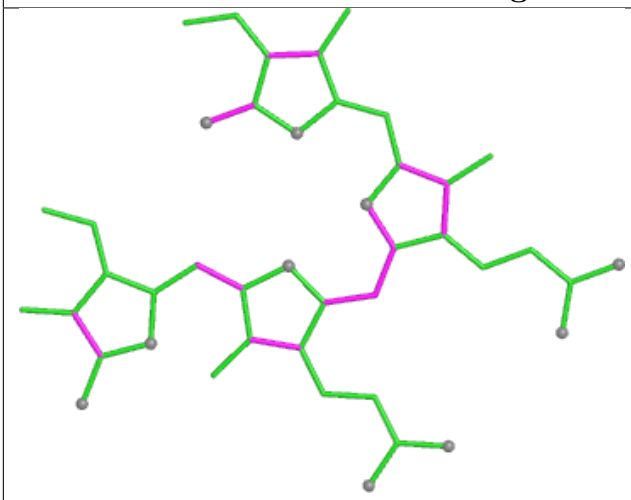


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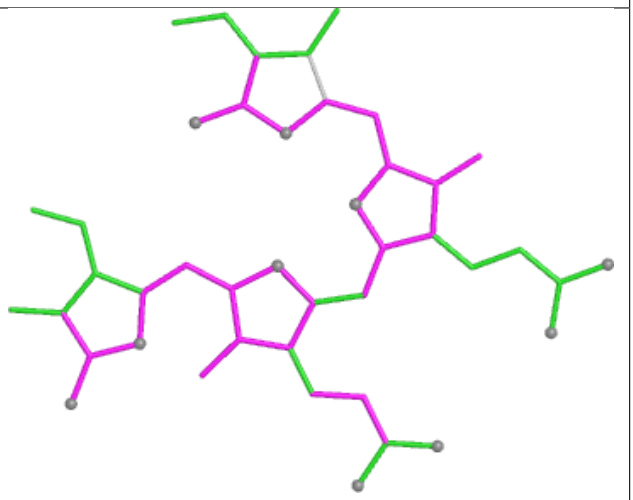


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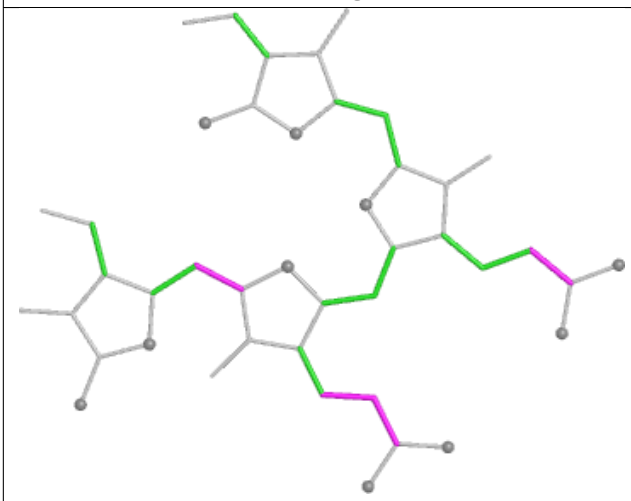
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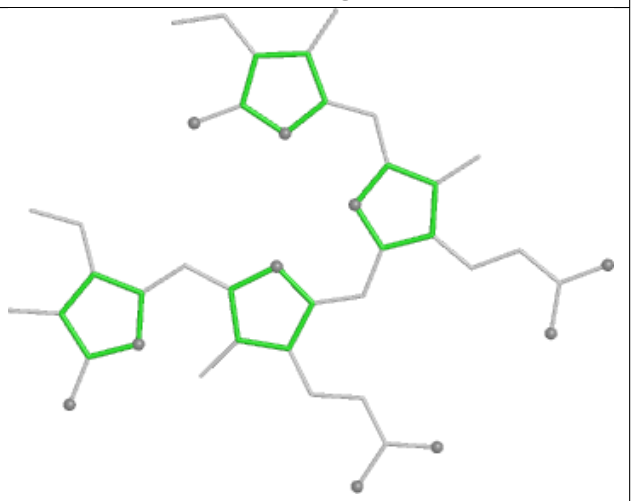
Bond lengths



Bond angles

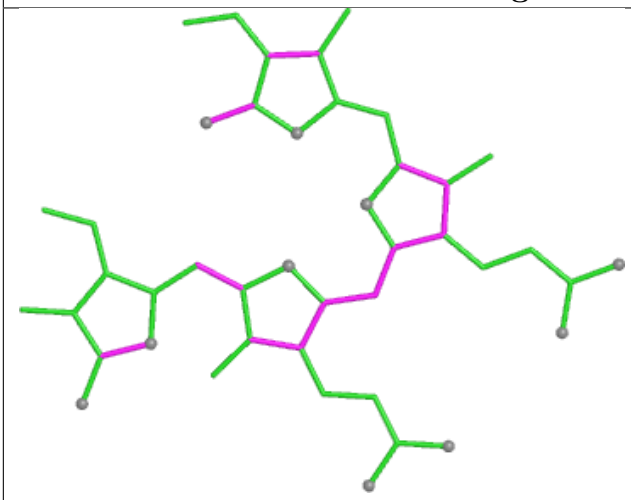


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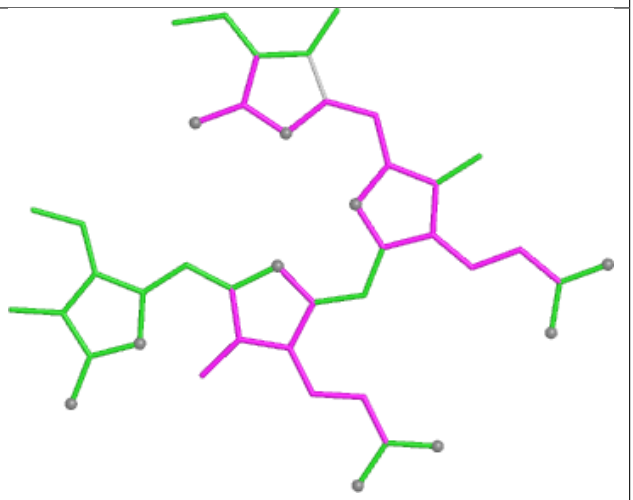


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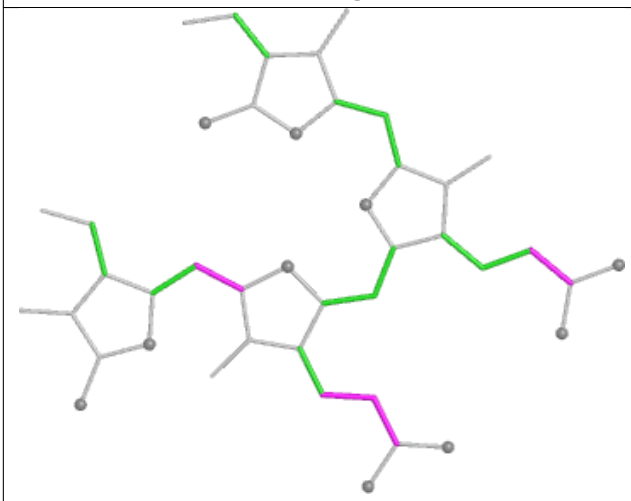
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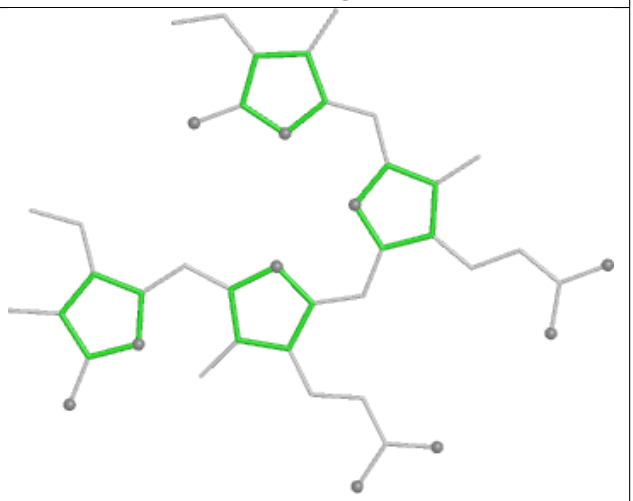
Bond lengths



Bond angles

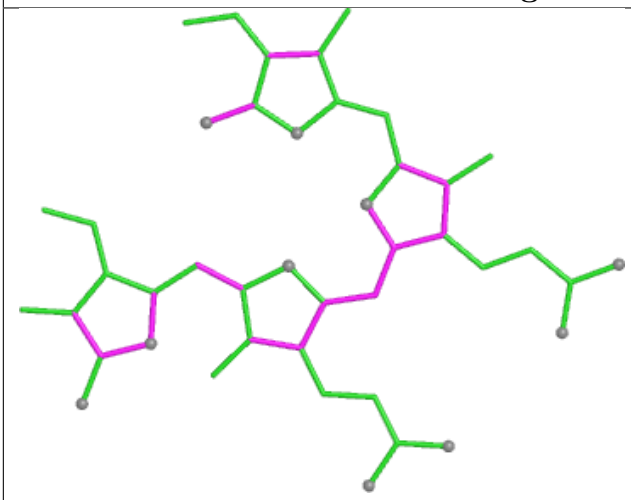


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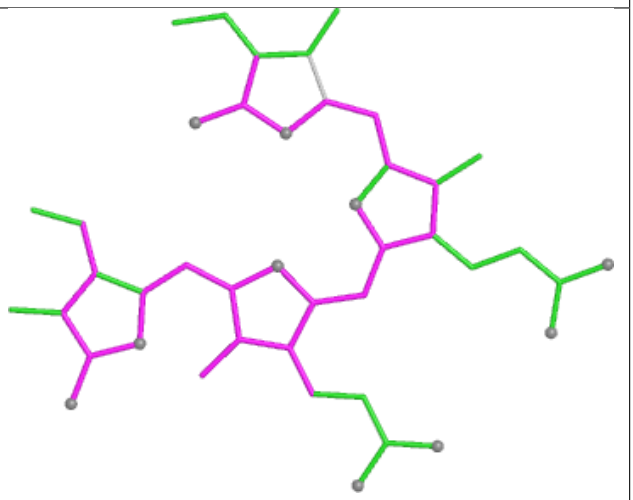


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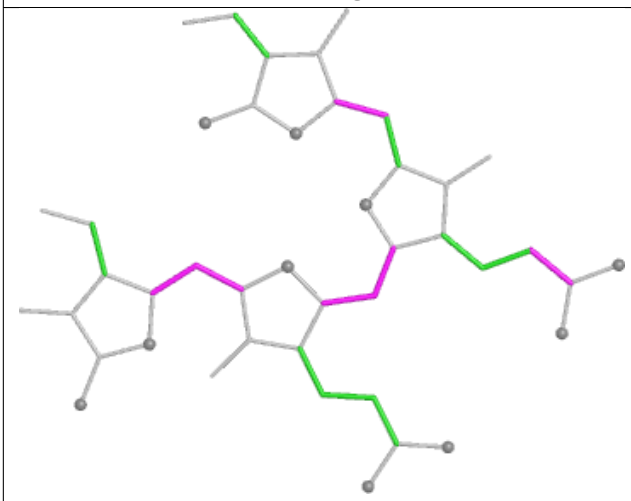
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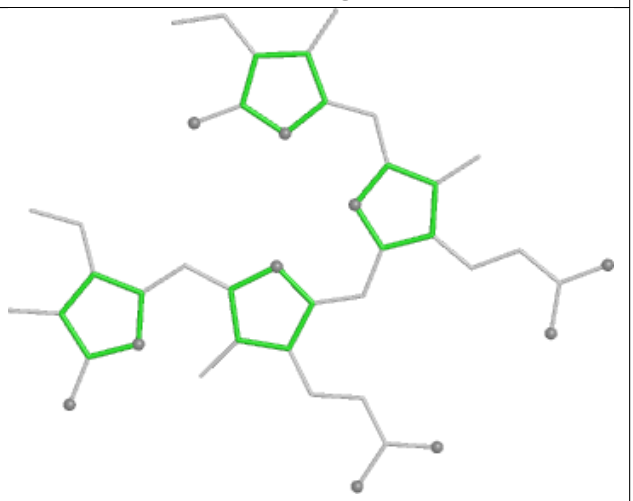
Bond lengths



Bond angles

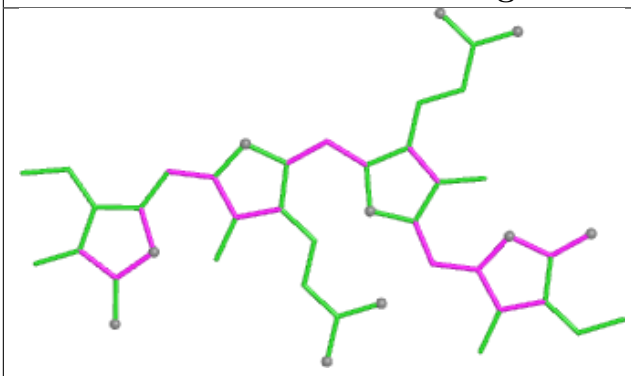


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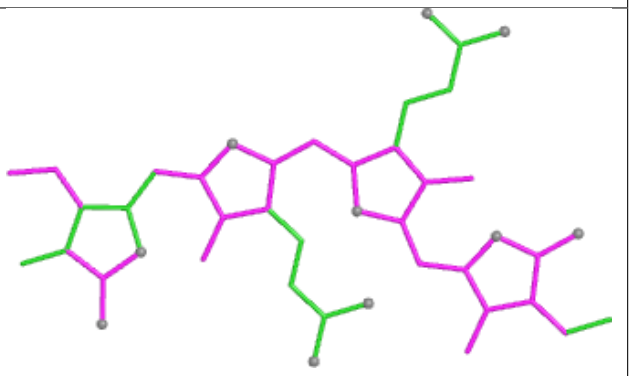


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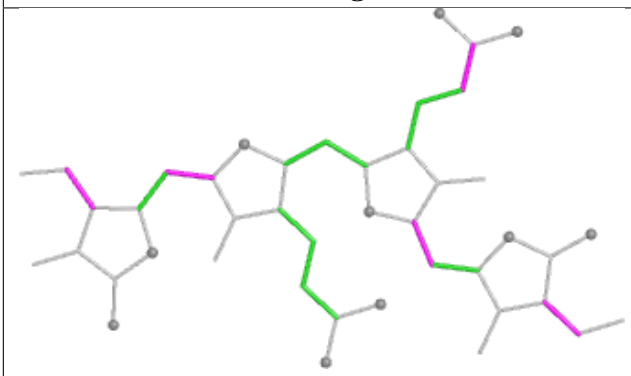
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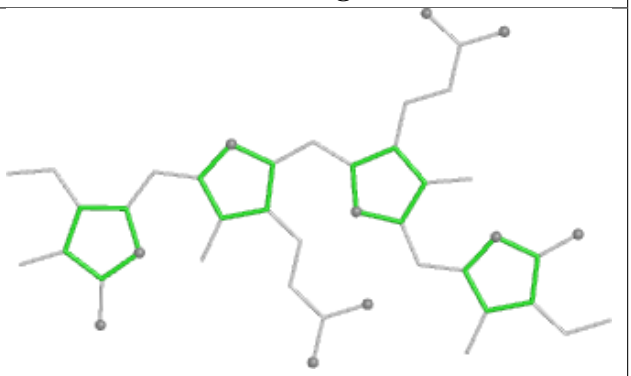
Bond lengths



Bond angles

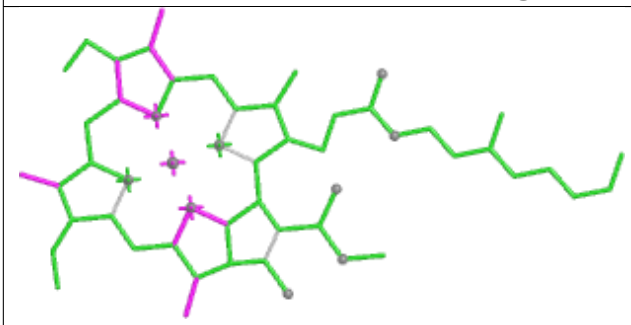


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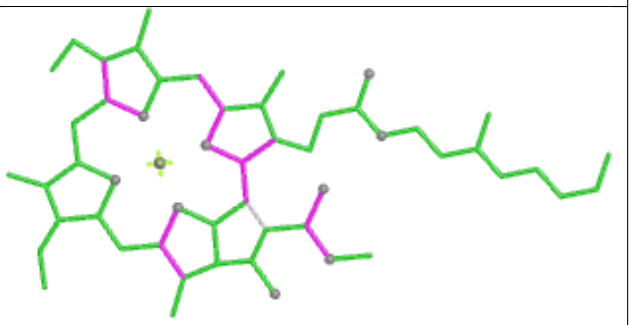


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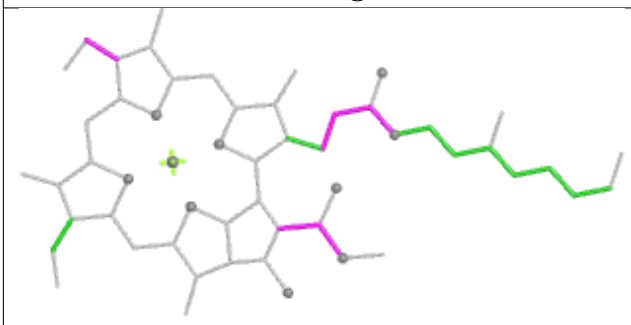
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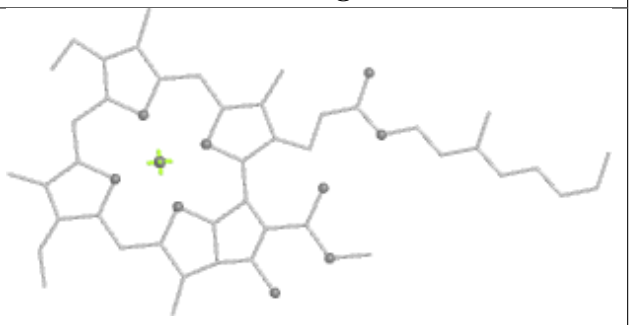
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Bond angles

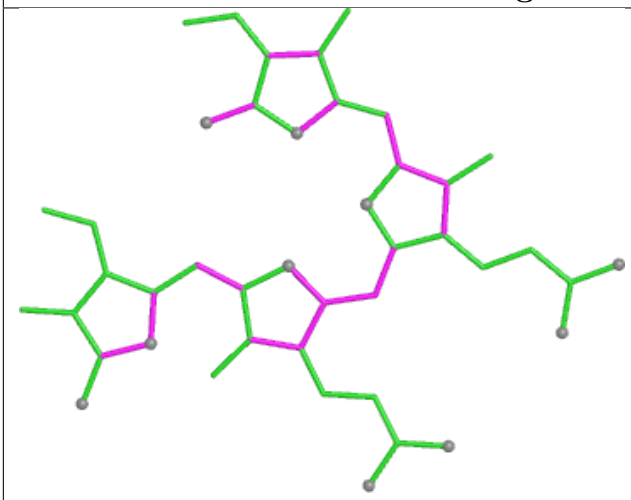


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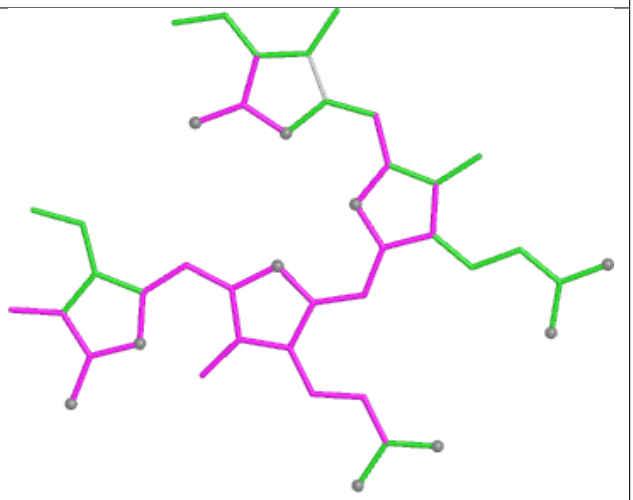


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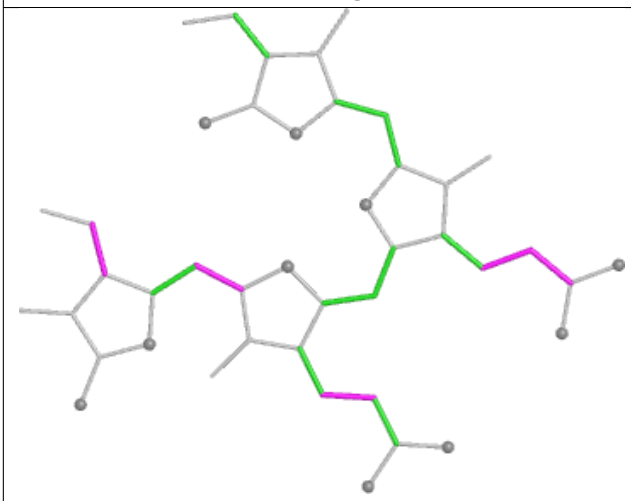
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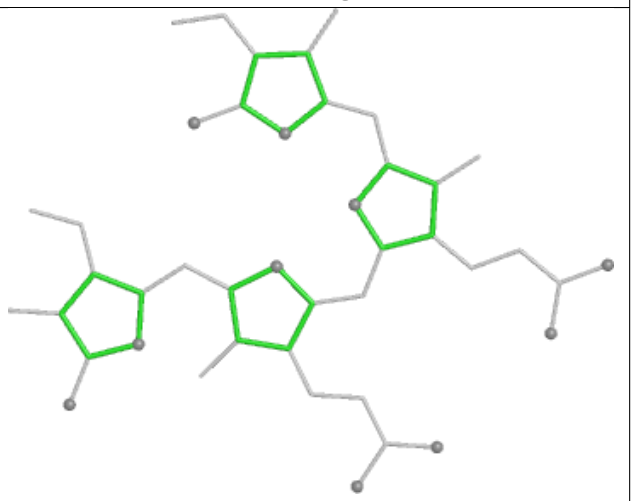
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Bond angles

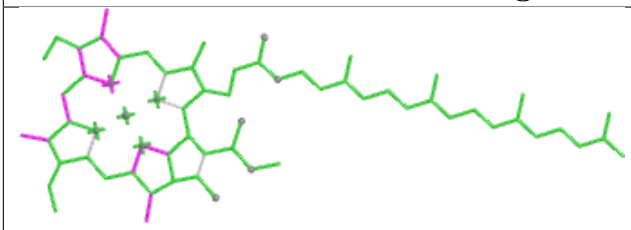


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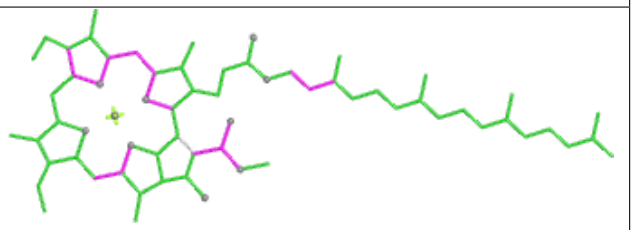


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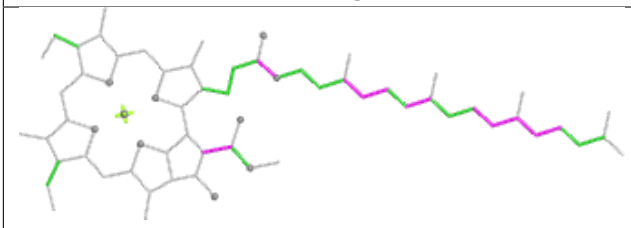
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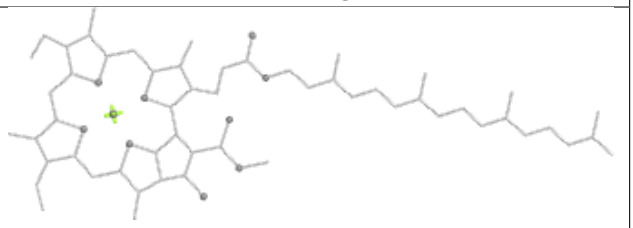
Bond lengths



Bond angles

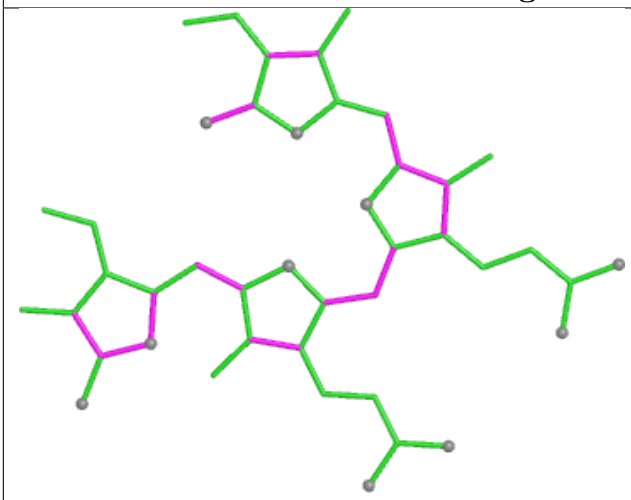


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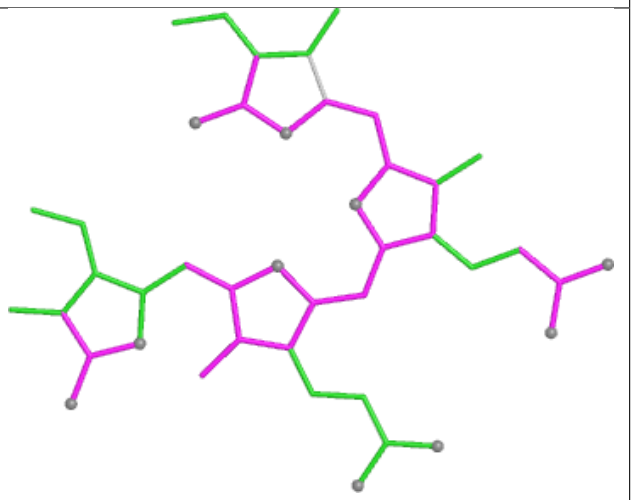


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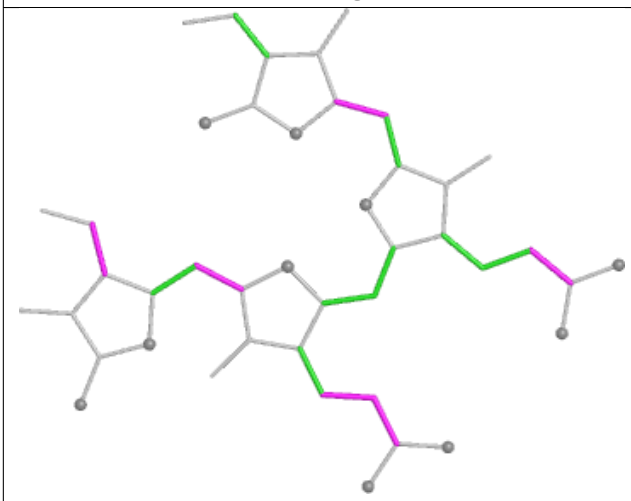
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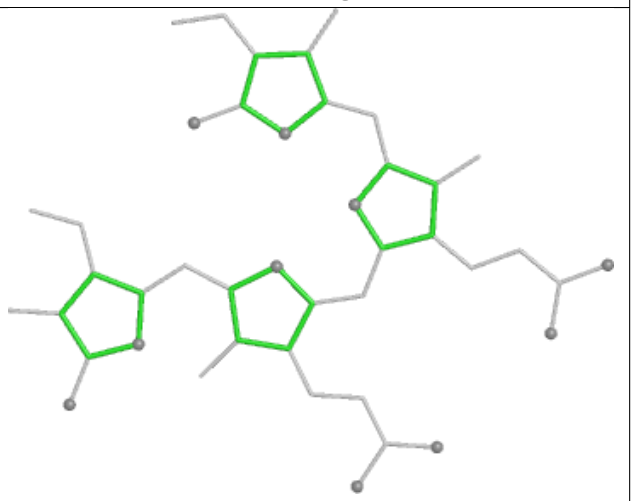
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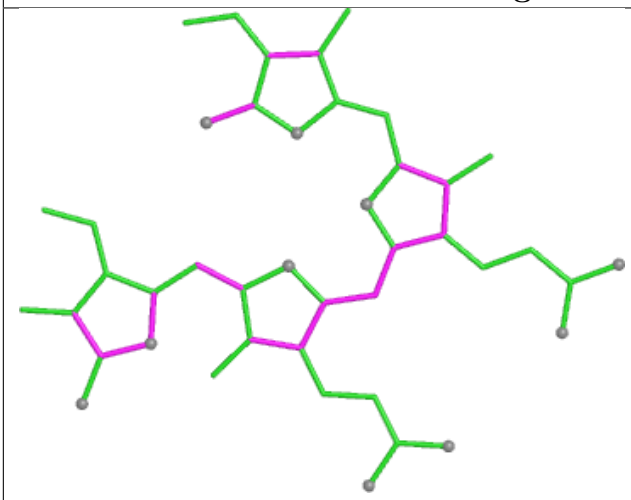


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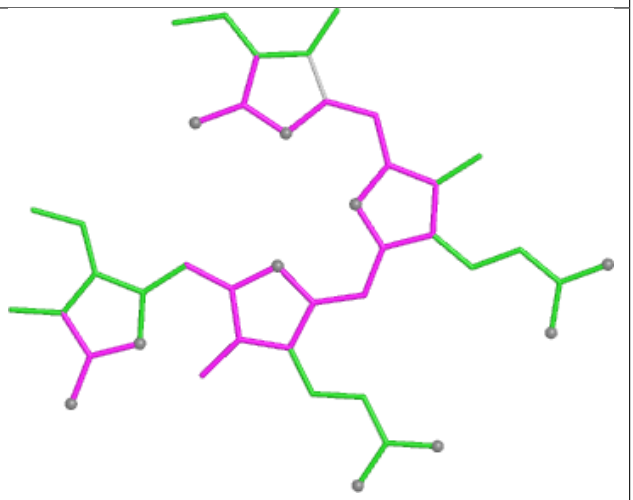


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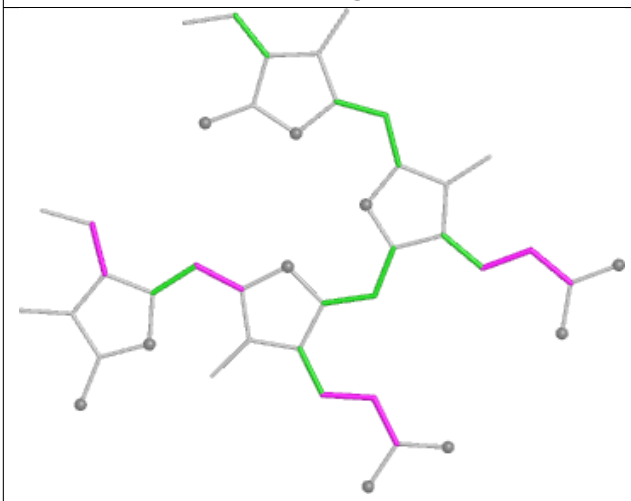
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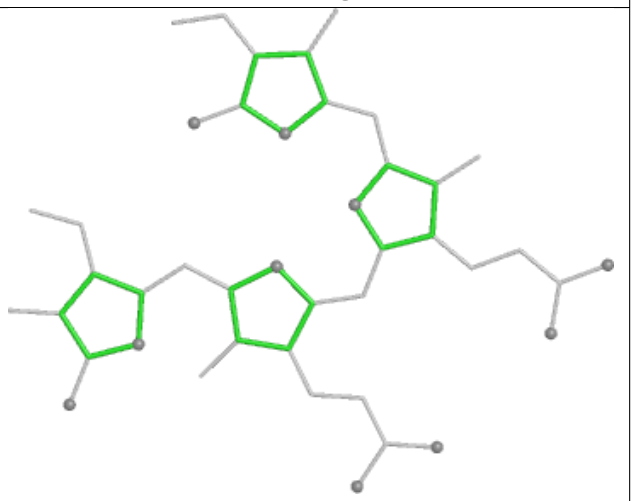
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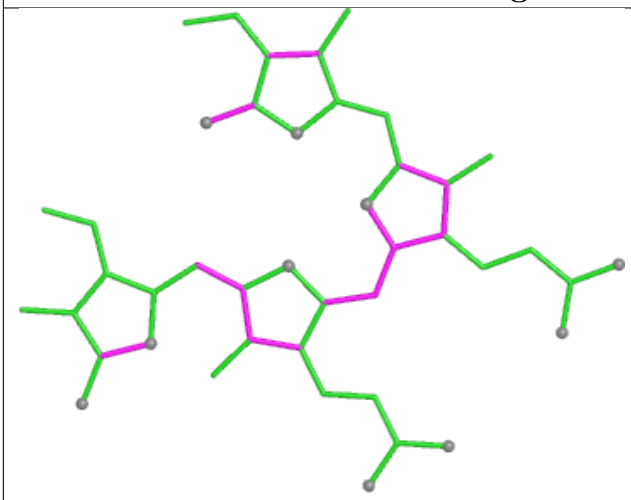


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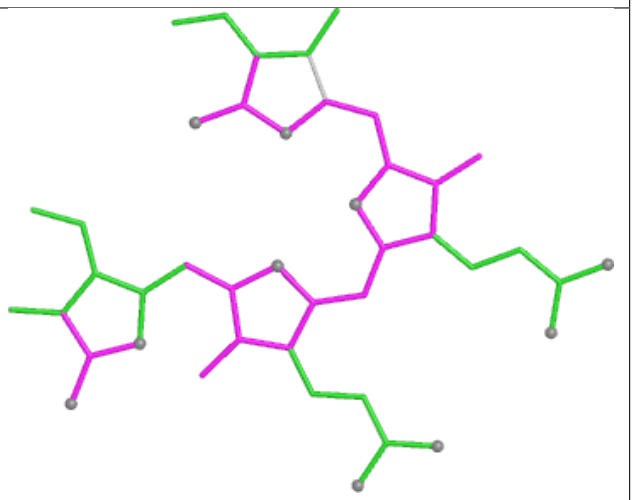


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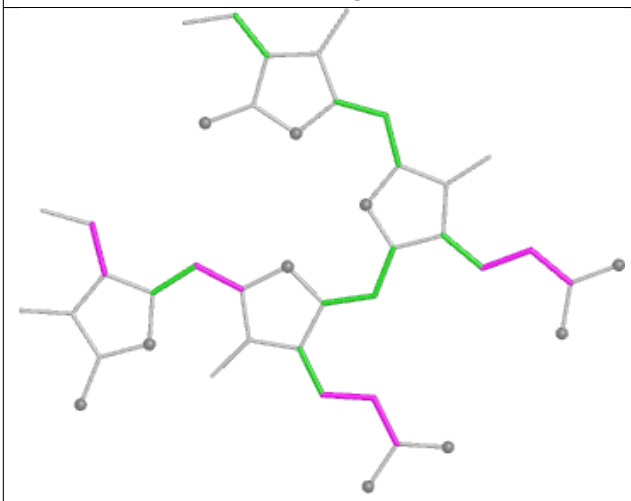
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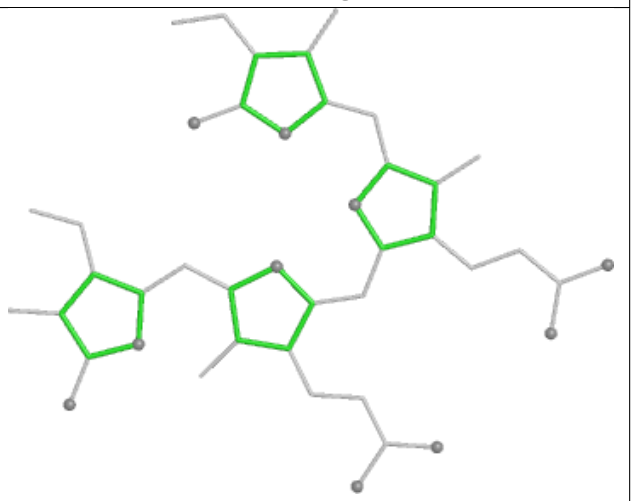
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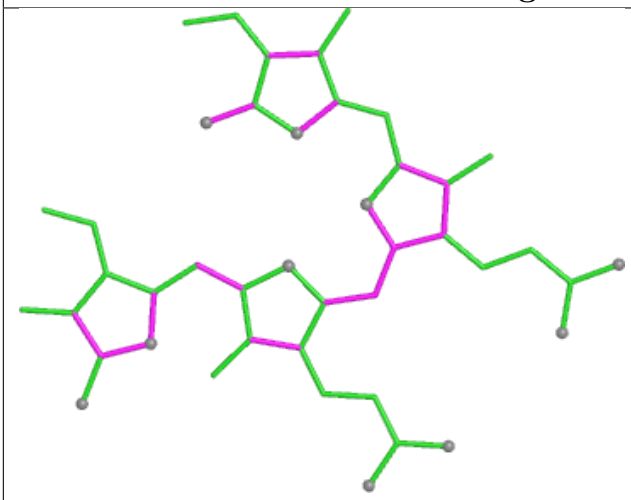


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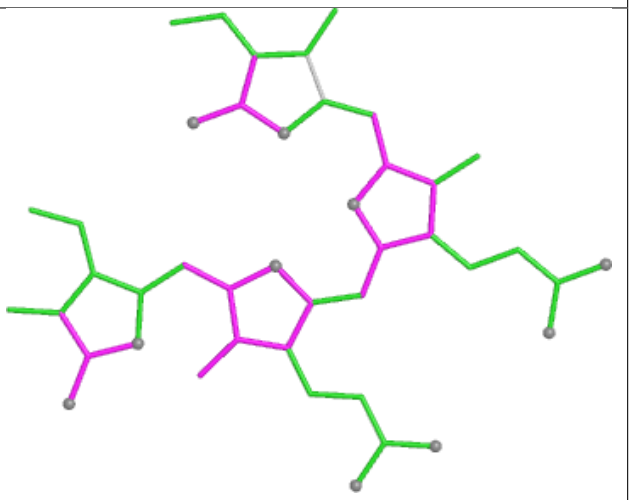


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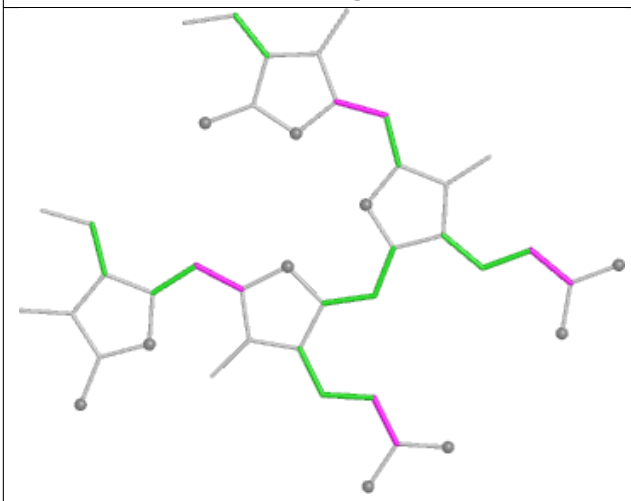
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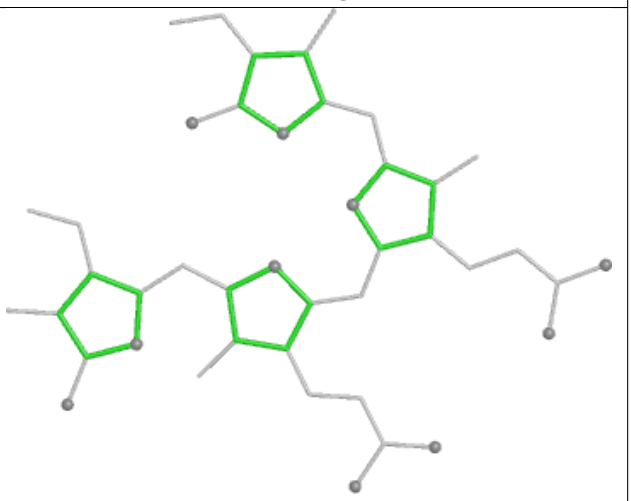
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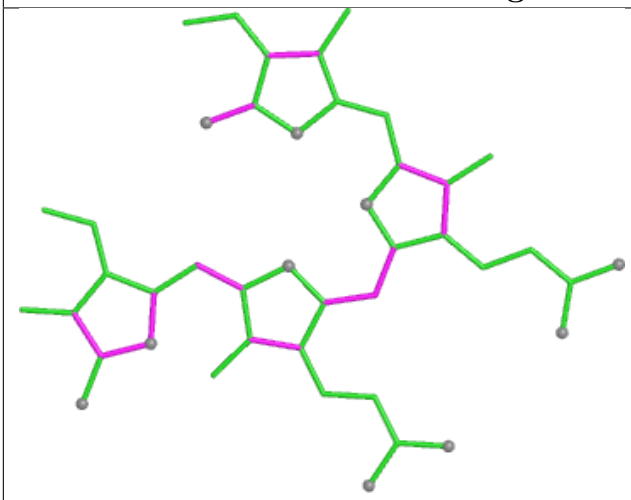


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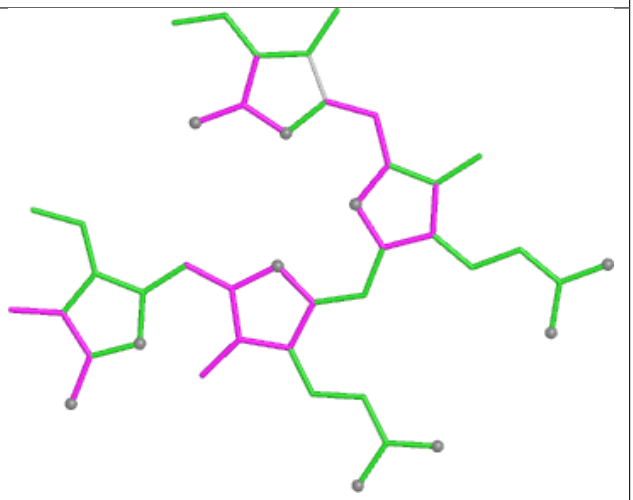


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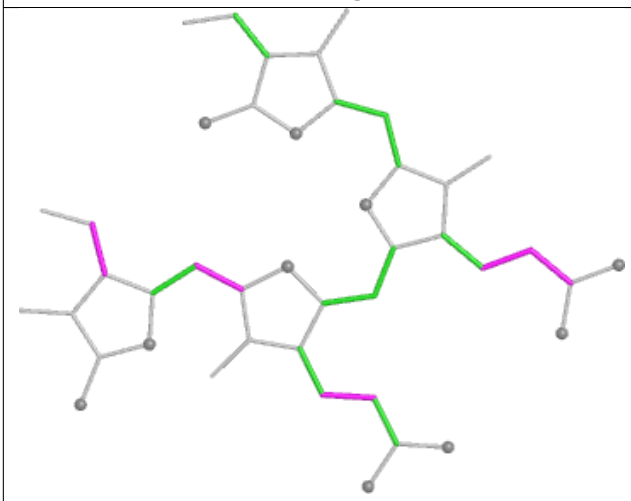
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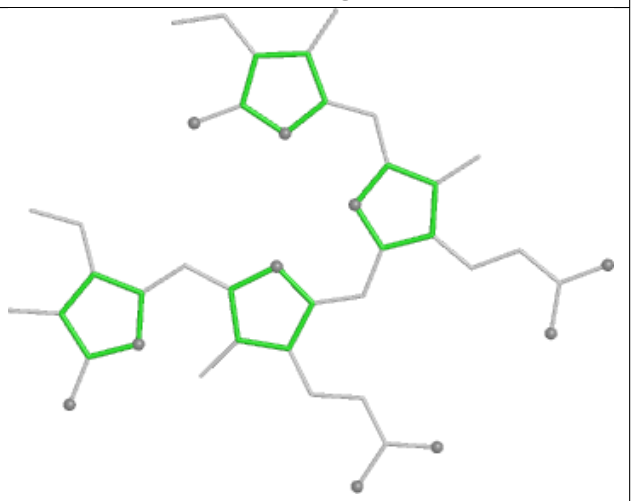
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Bond angles

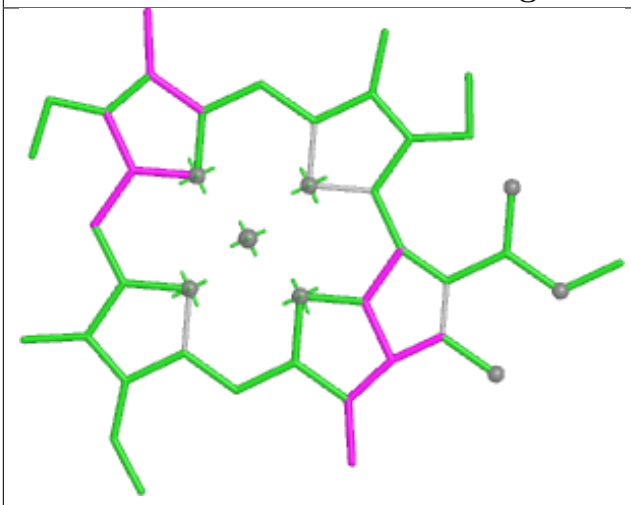


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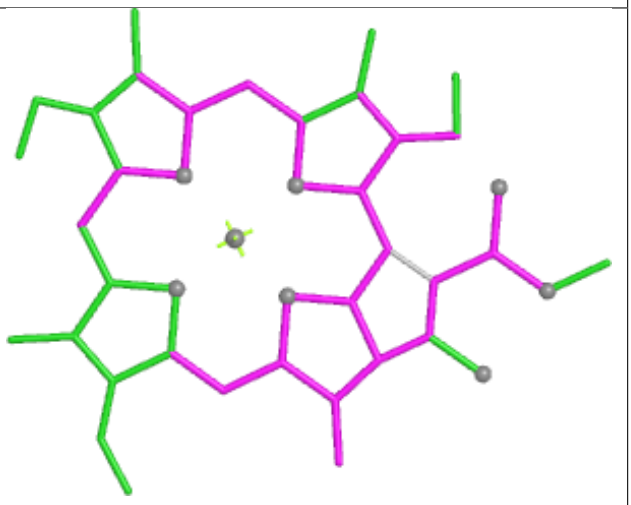


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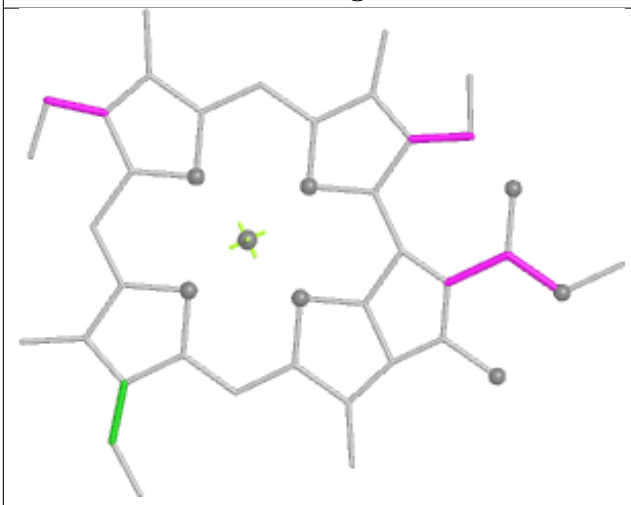
Ligand CLA 42 604



Bond lengths



Bond angles

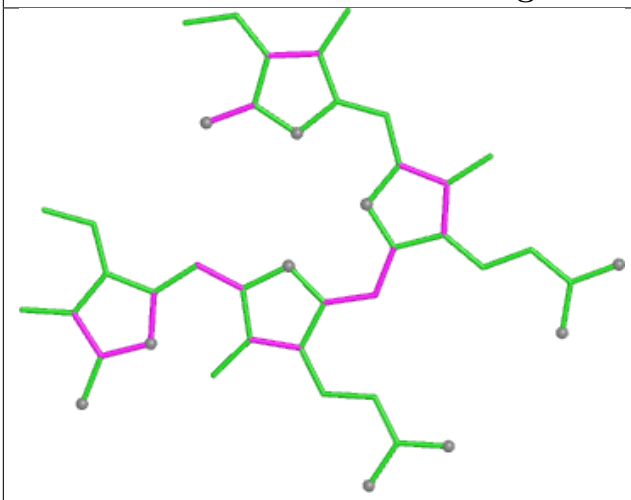


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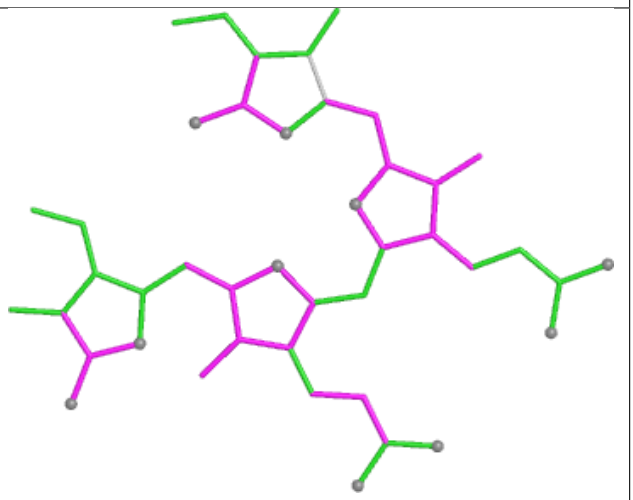


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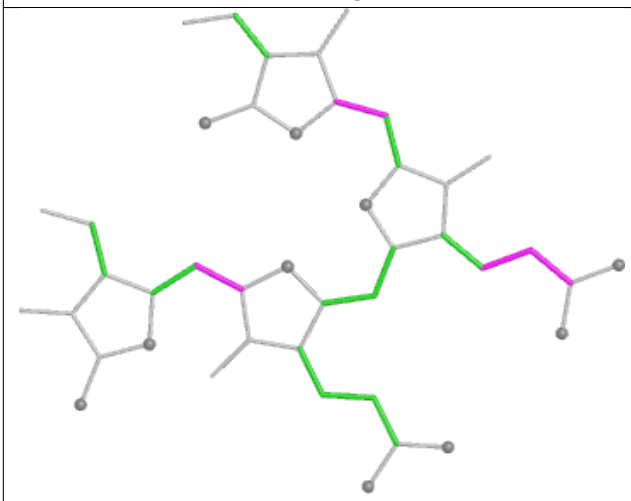
Ligand PEB cB 401



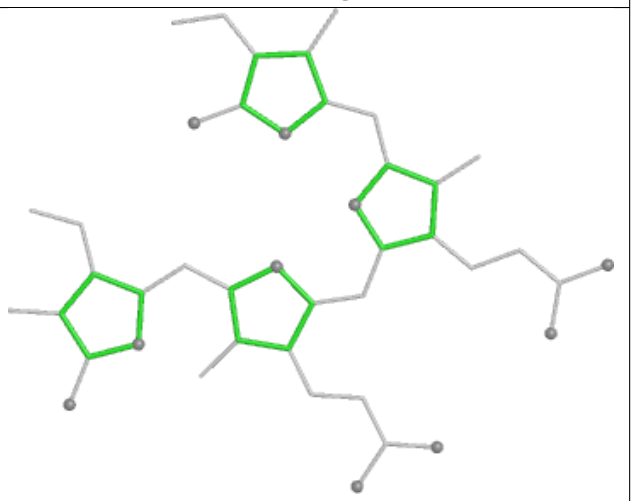
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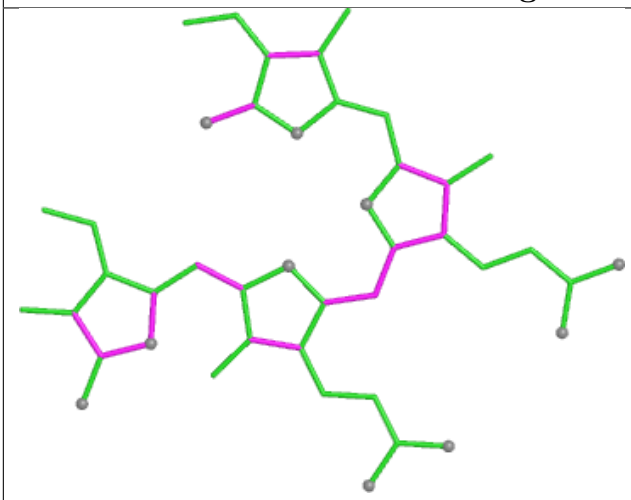


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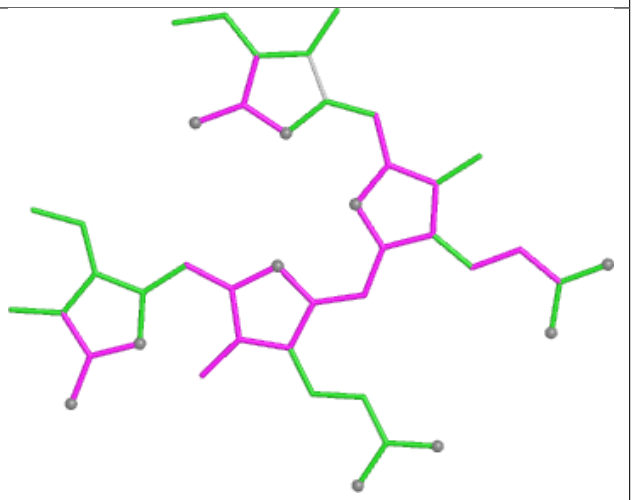


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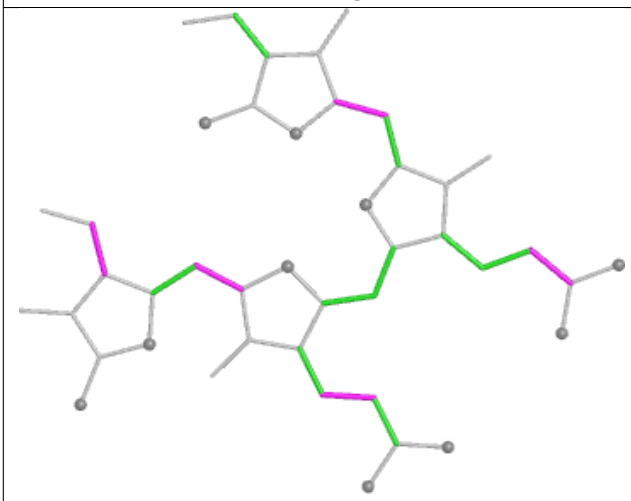
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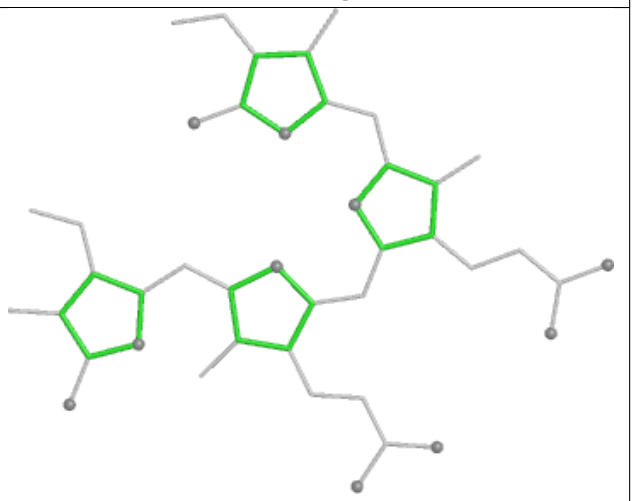
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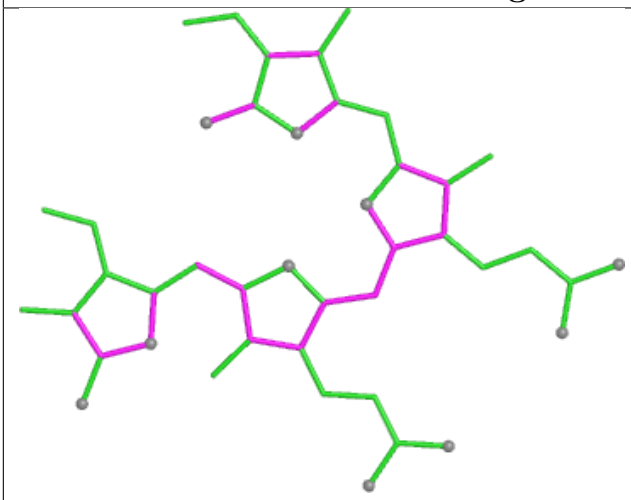


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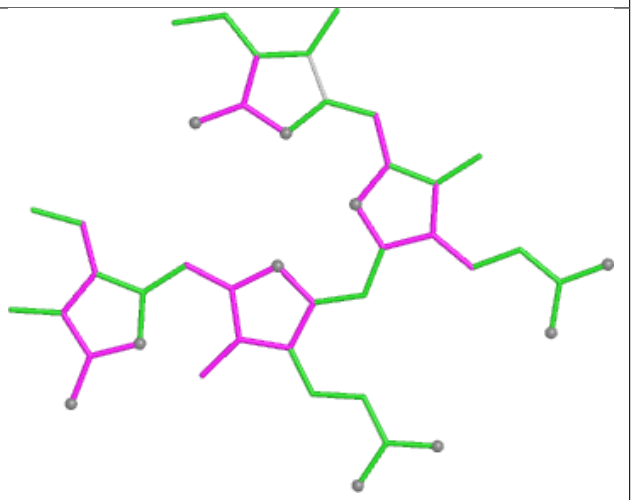


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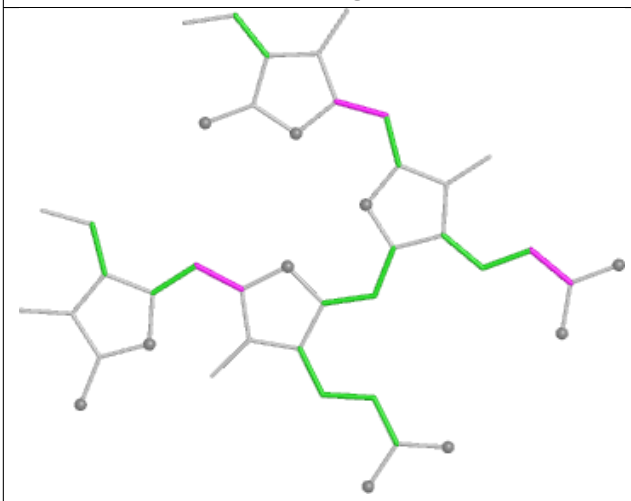
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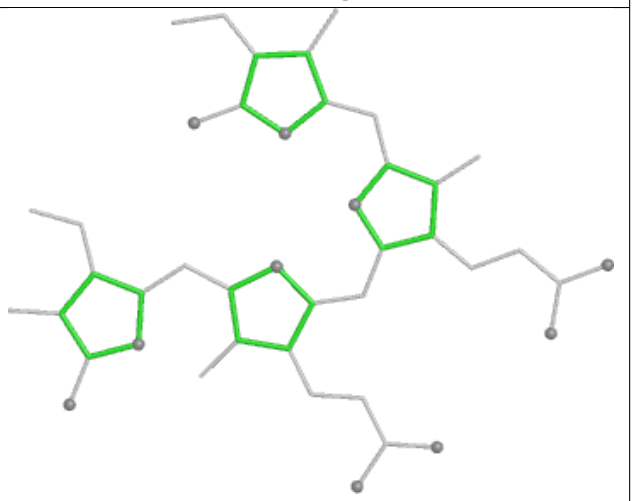
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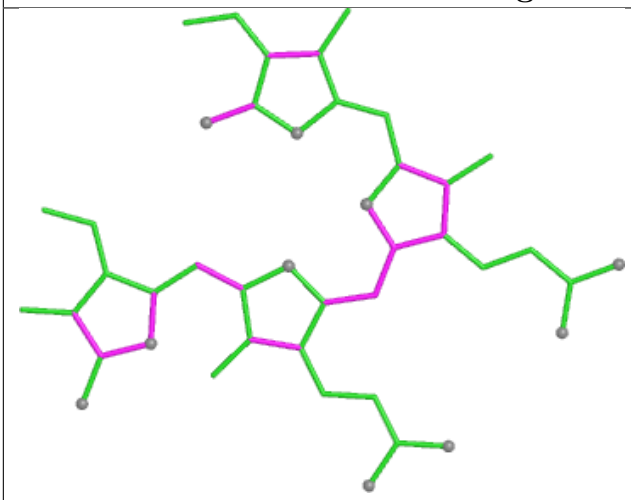


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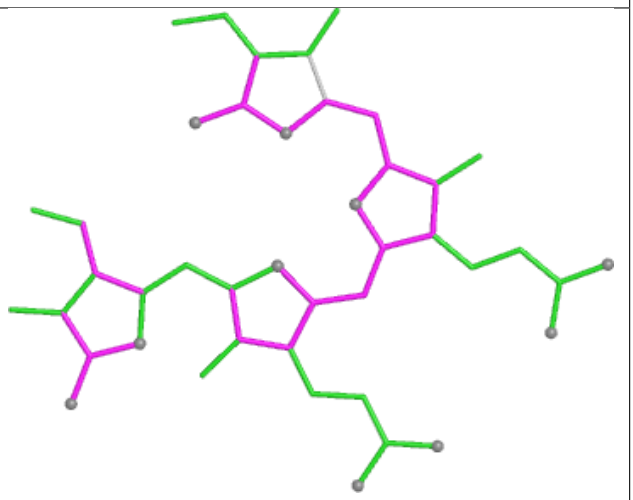


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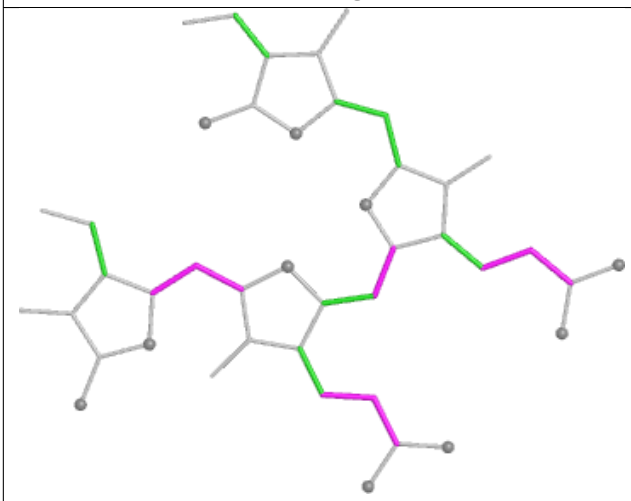
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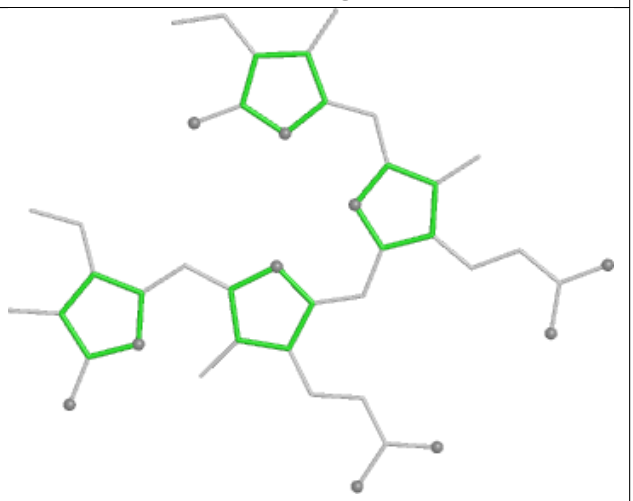
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Bond angles

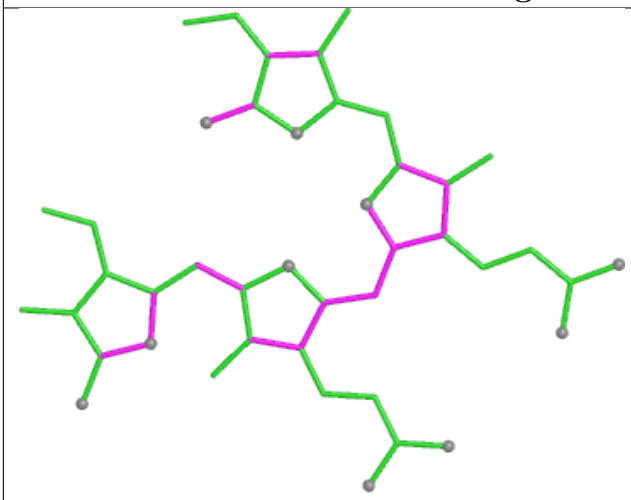


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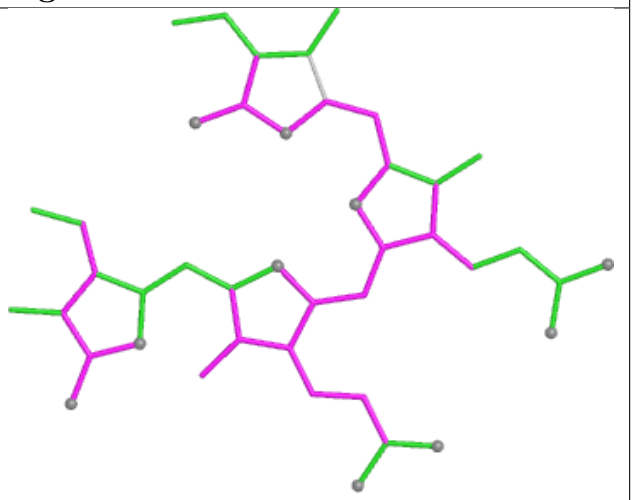


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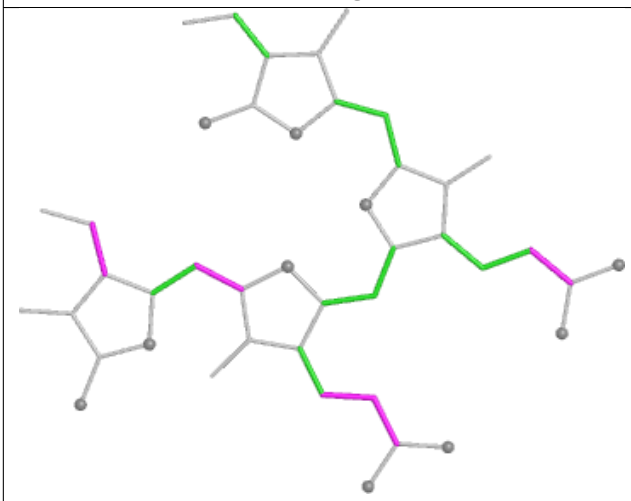
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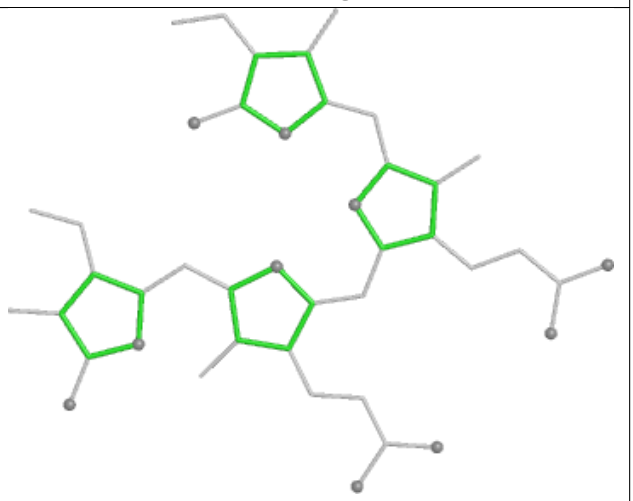
Bond lengths



Bond angles

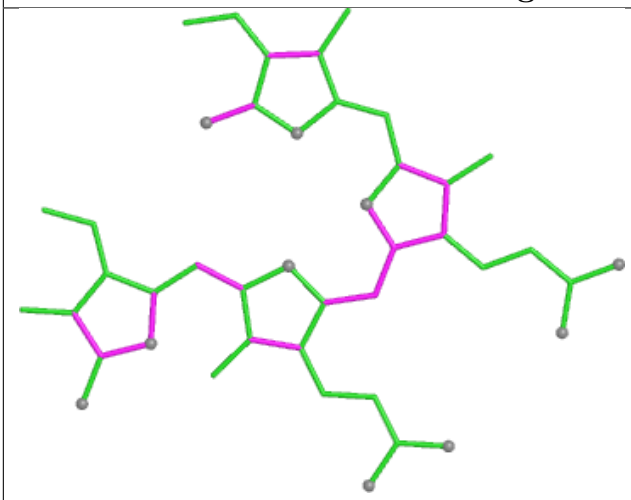


Torsions

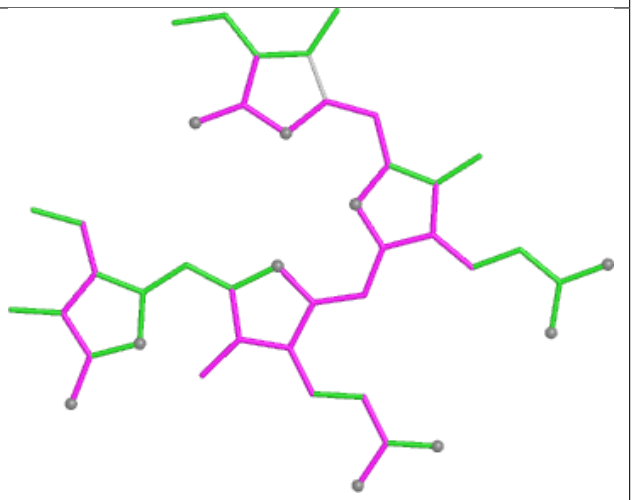


Rings

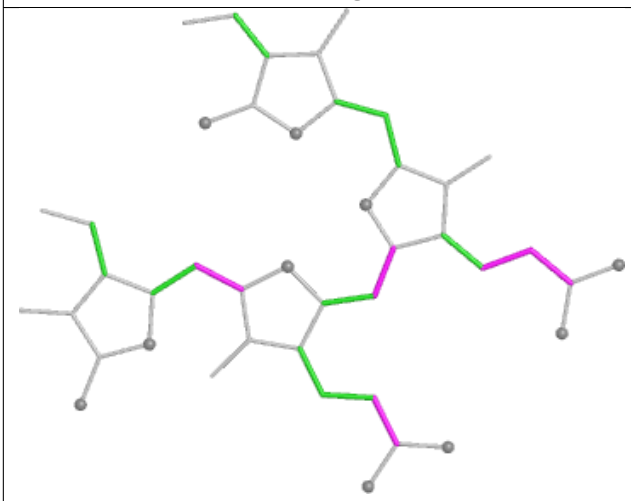
Ligand PEB ZJ 202



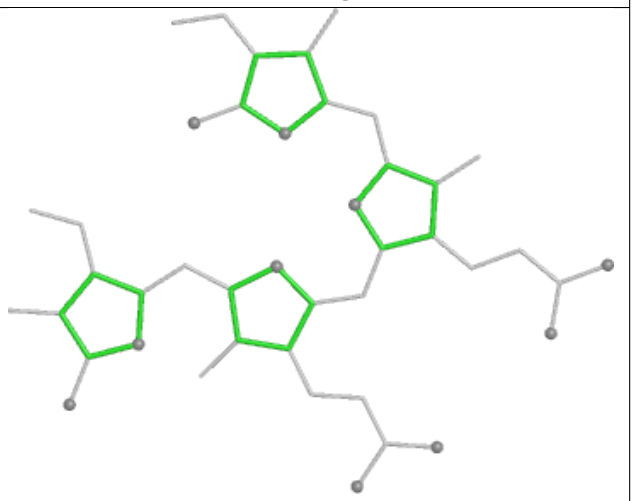
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Bond angles

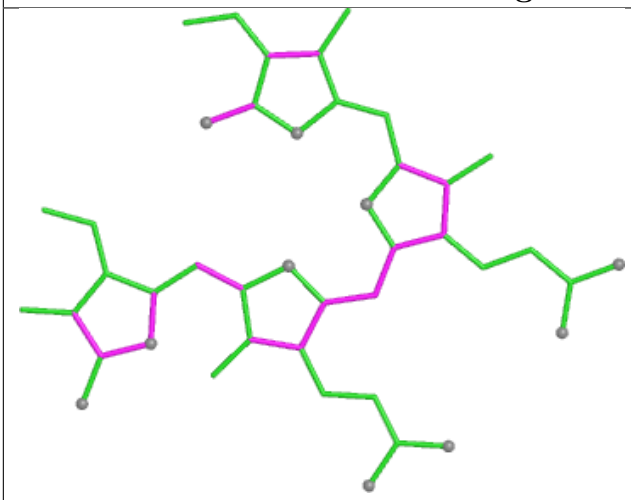


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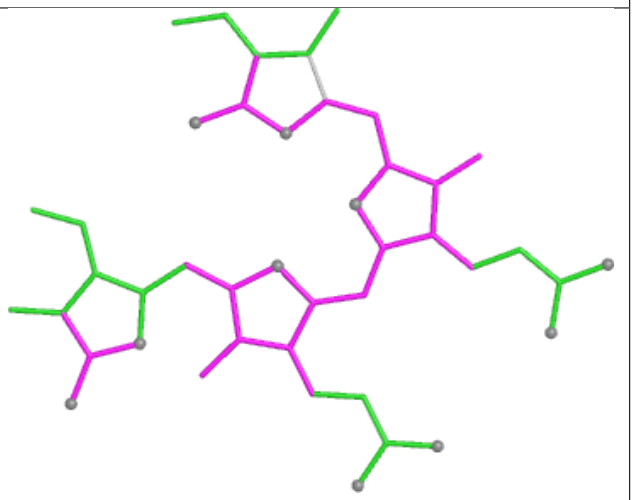


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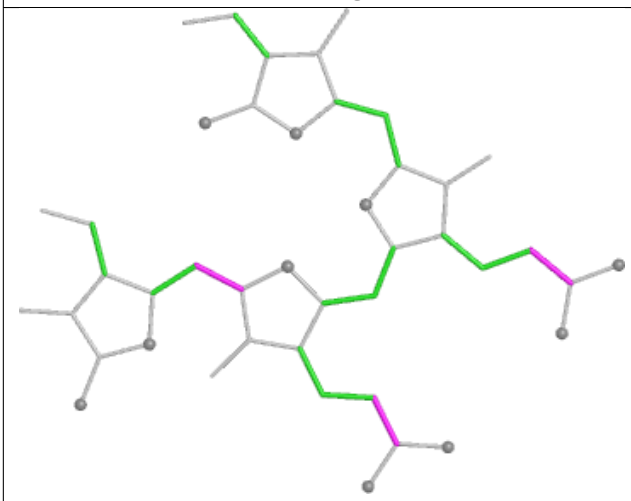
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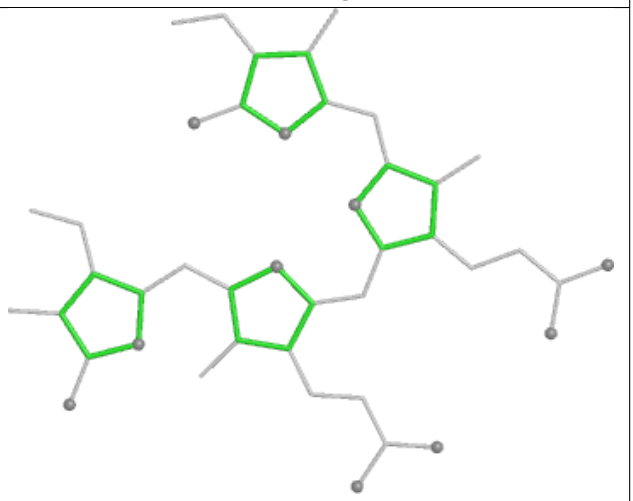
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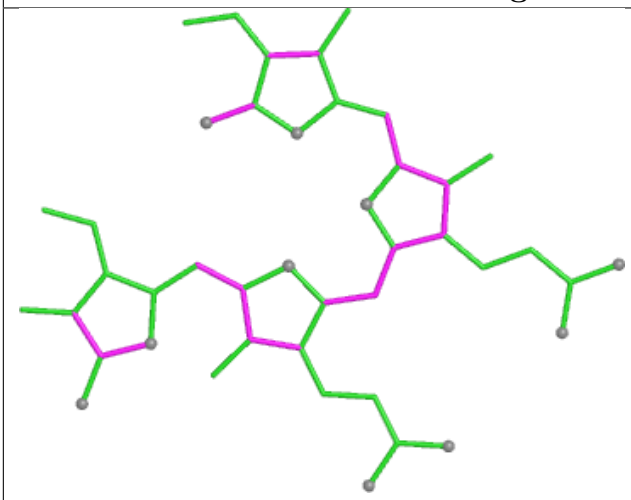


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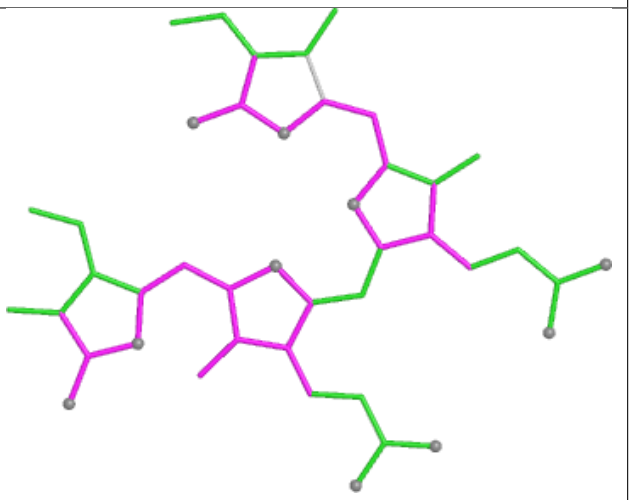


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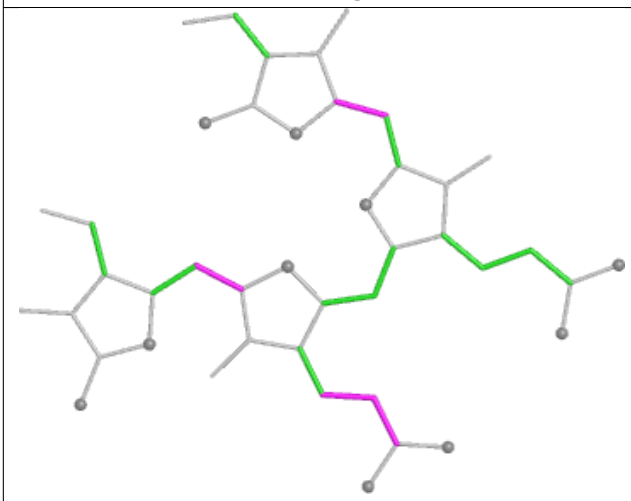
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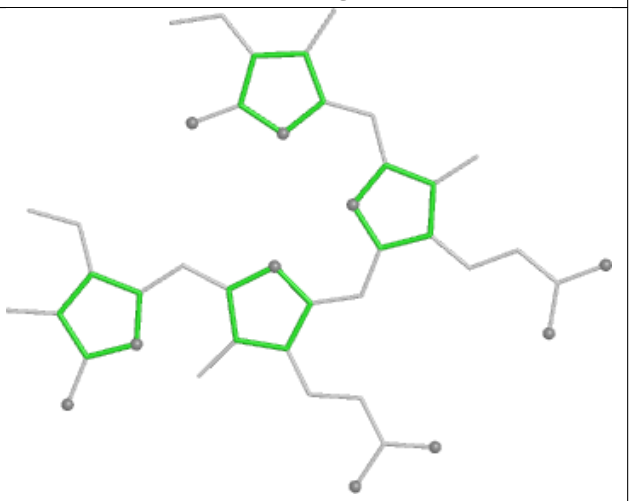
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Bond angles

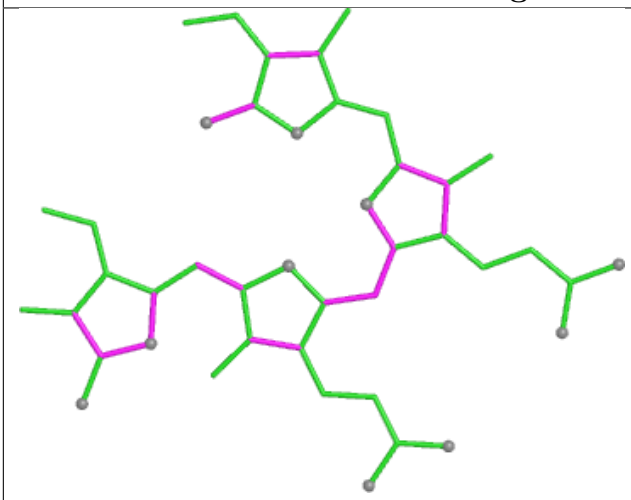


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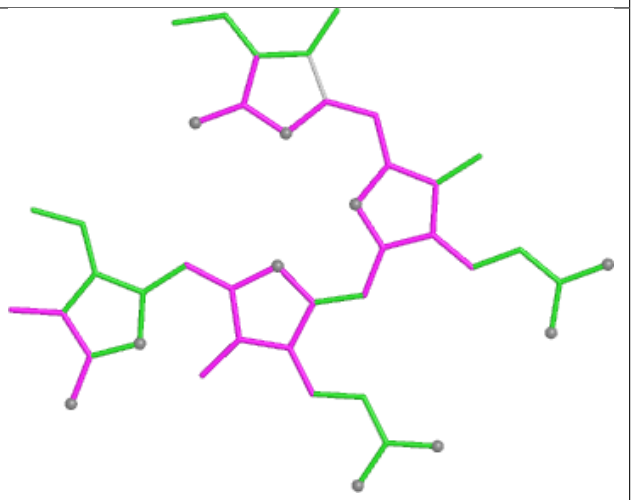


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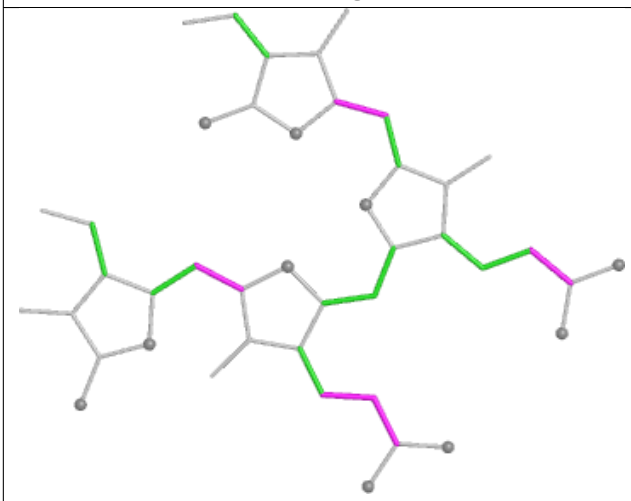
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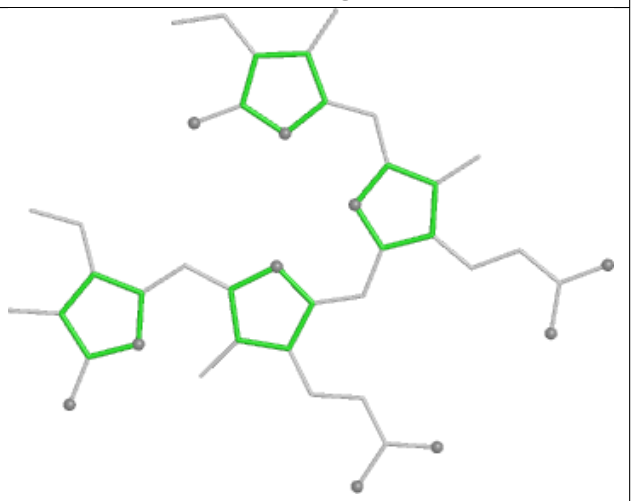
Bond lengths



Bond angles

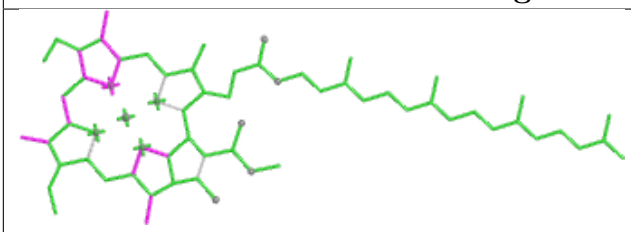


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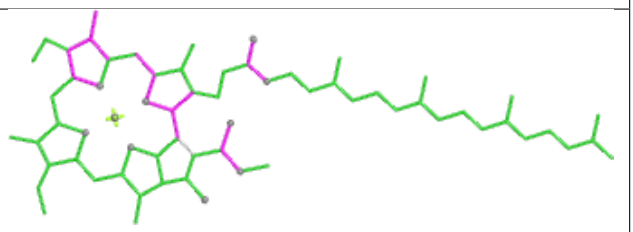


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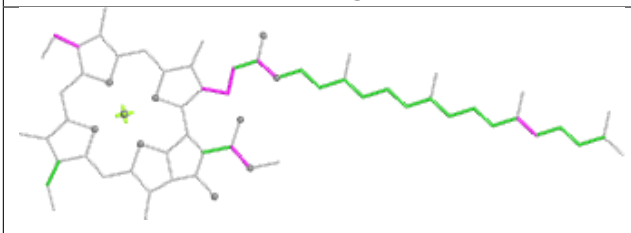
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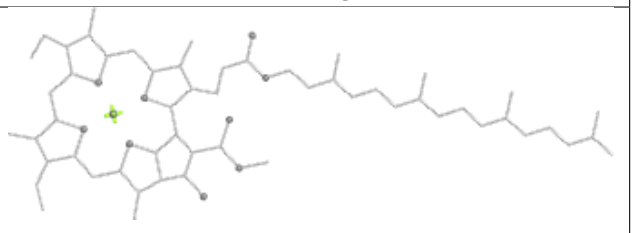
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Bond angles

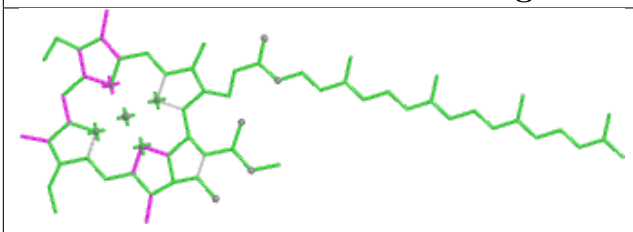


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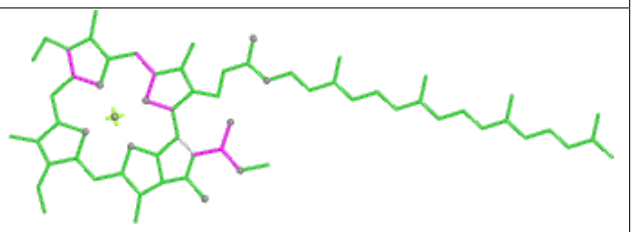


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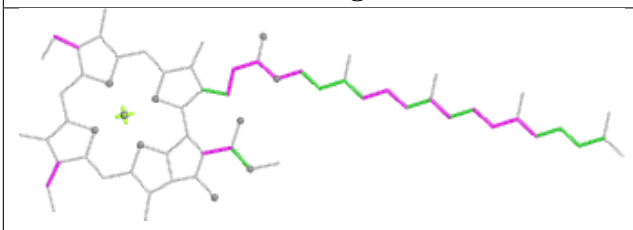
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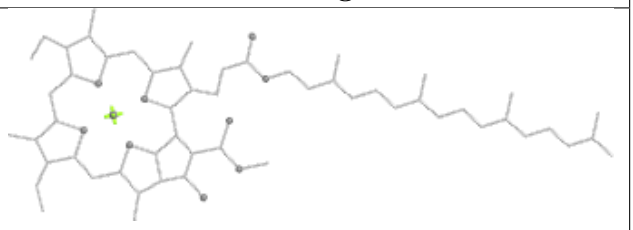
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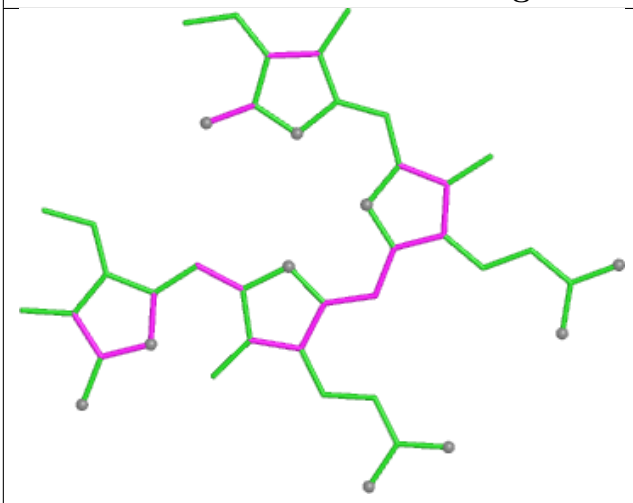


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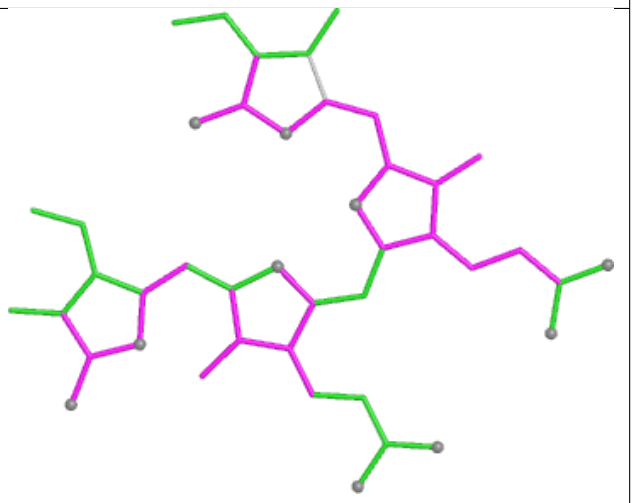


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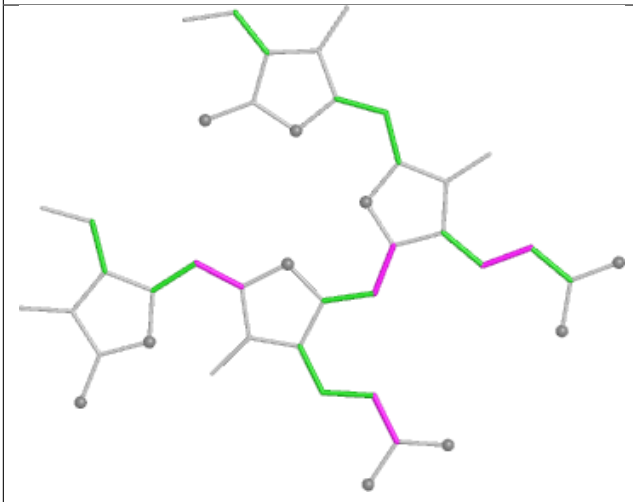
Ligand PEB VA 203



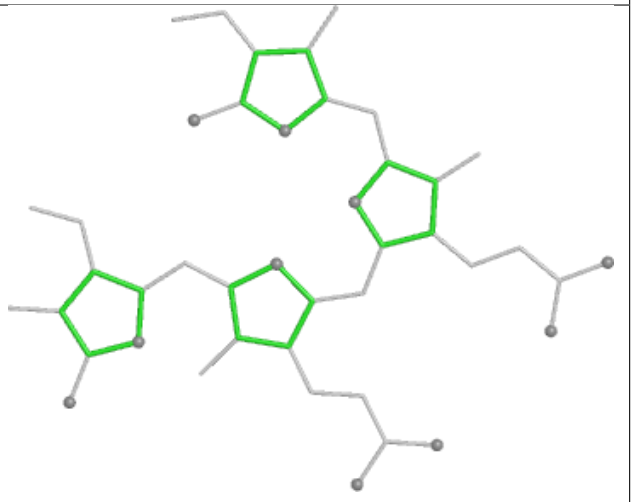
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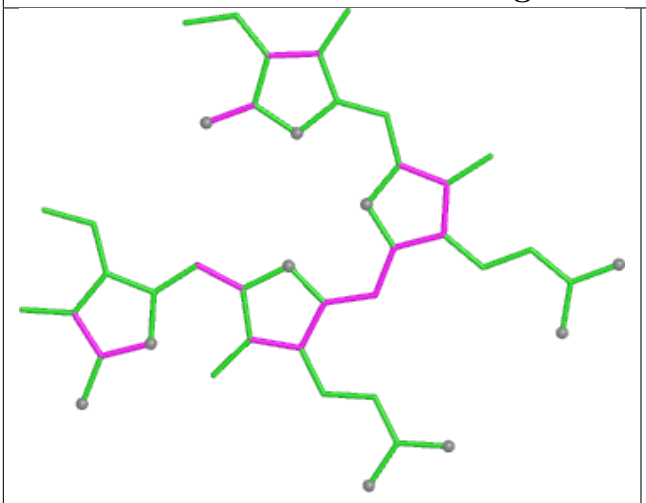


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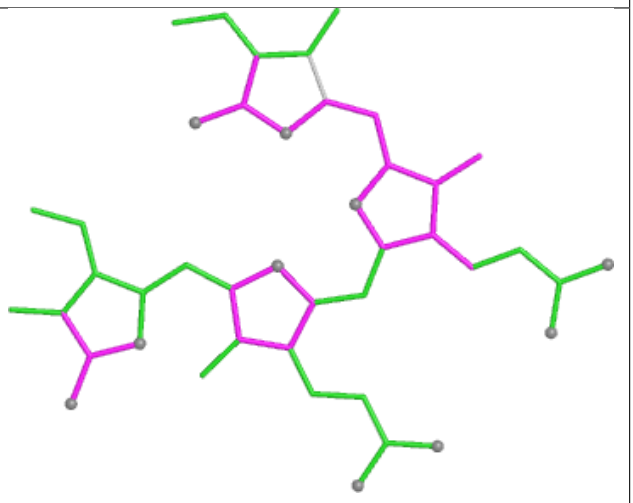


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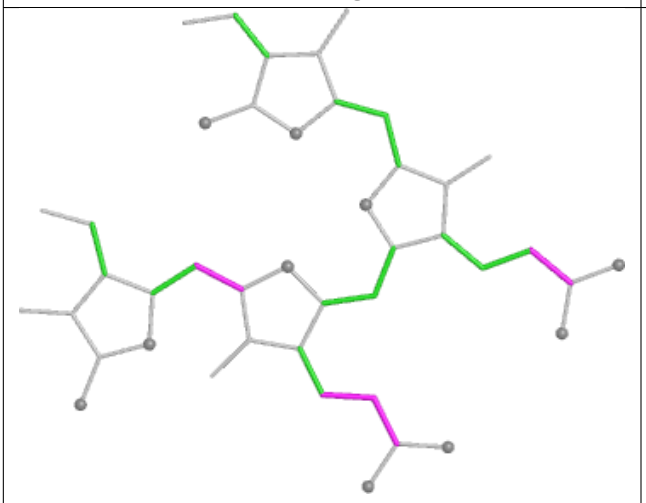
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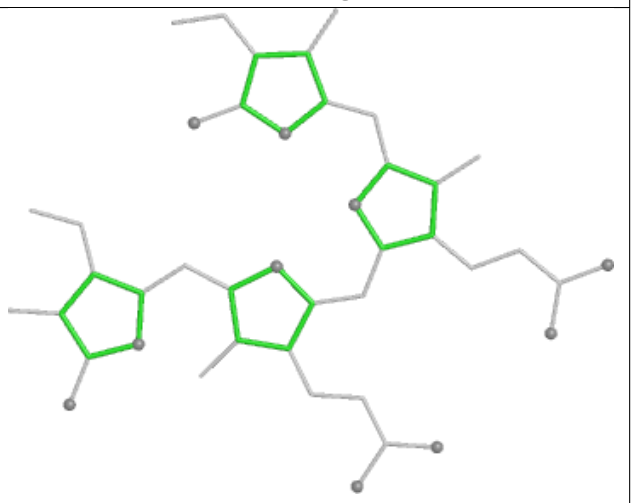
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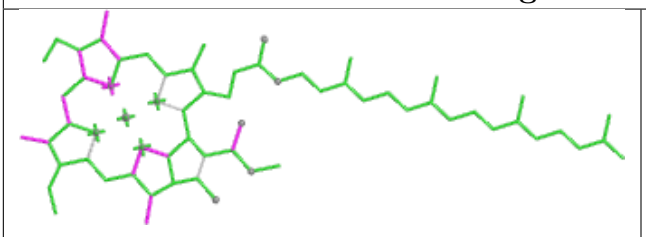


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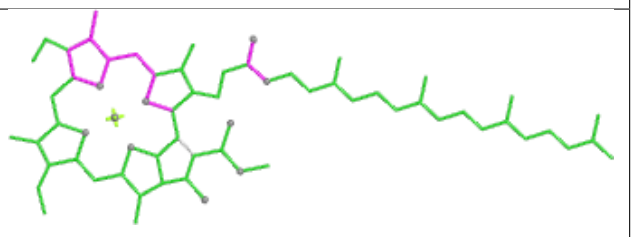


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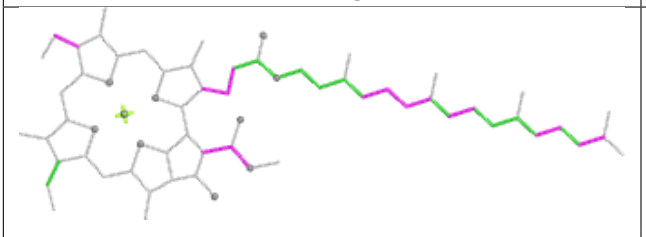
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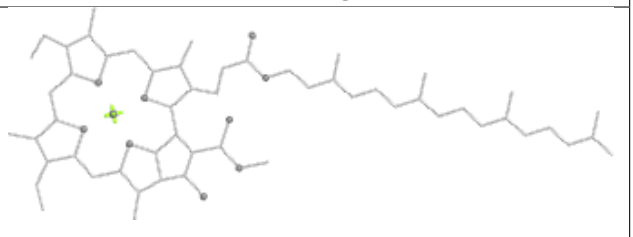
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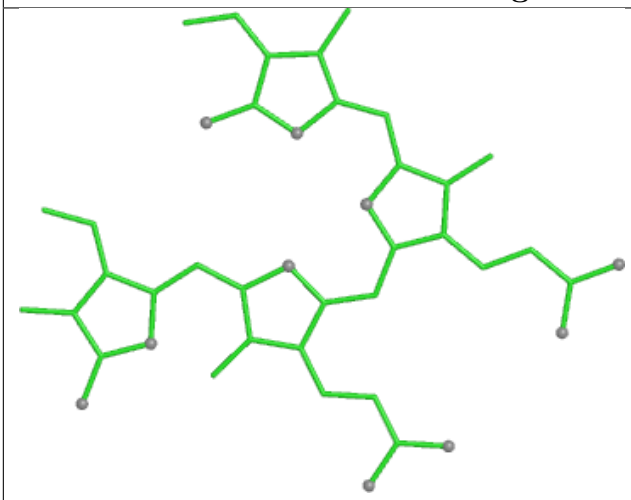


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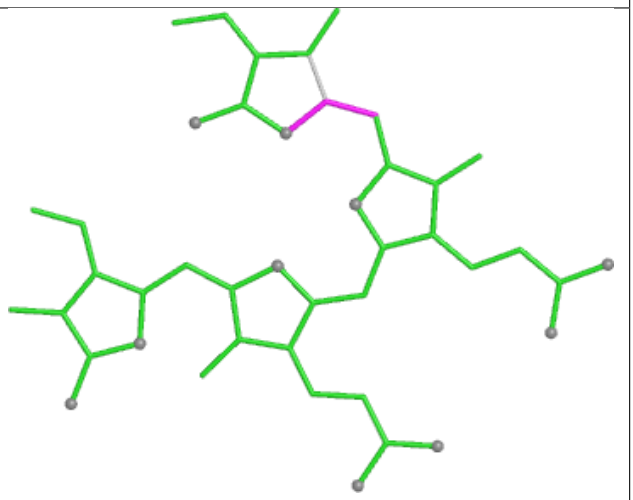


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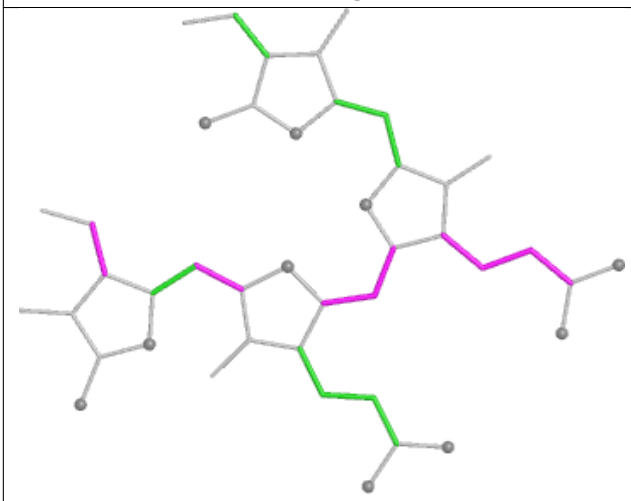
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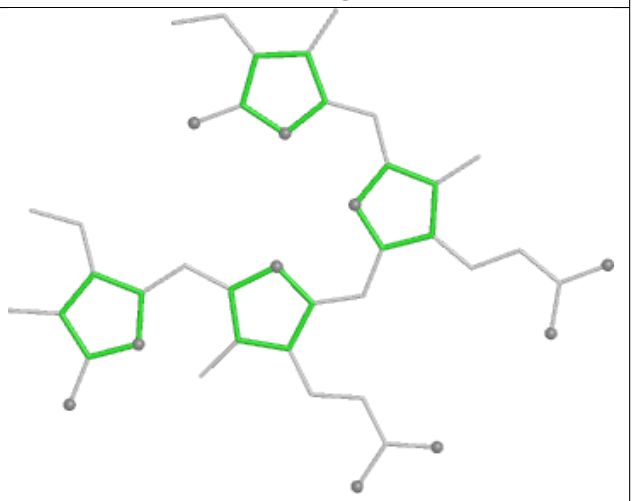
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Bond angles

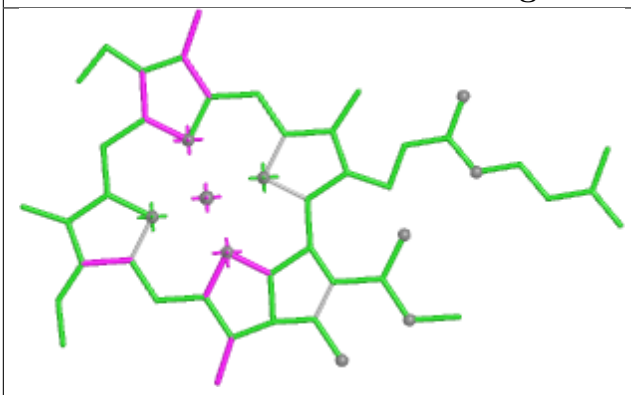


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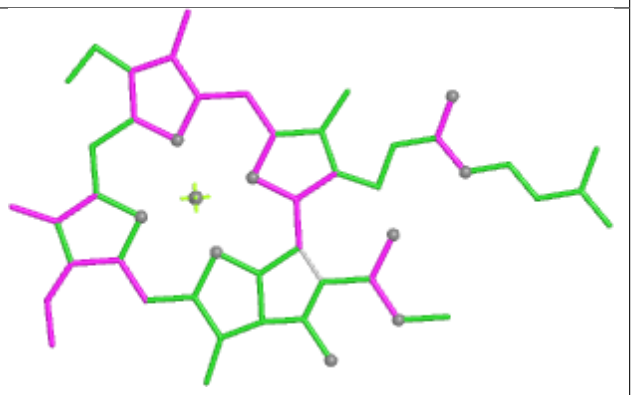


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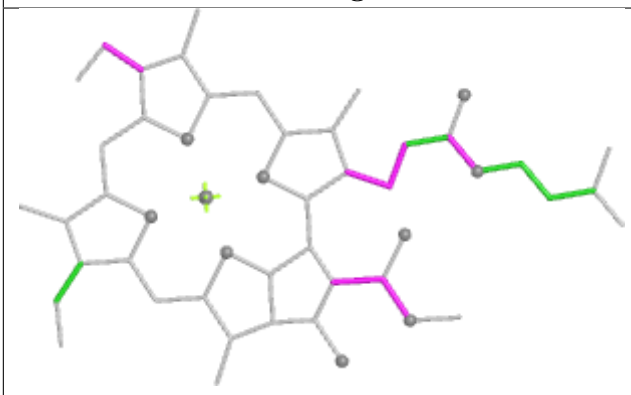
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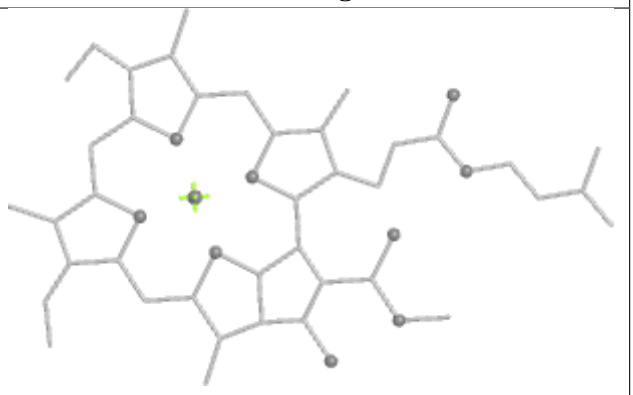
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Bond angles

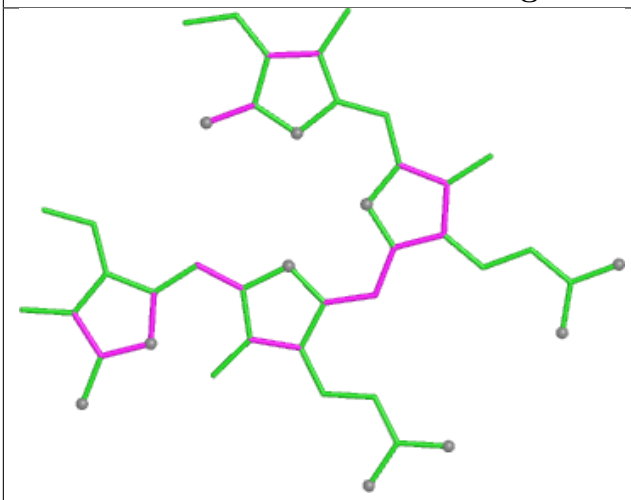


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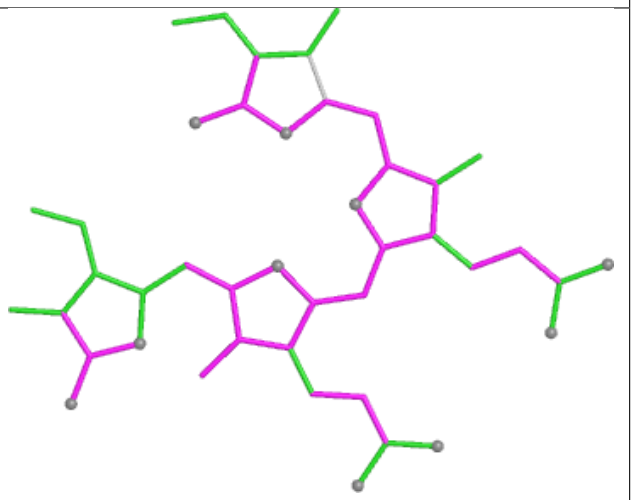


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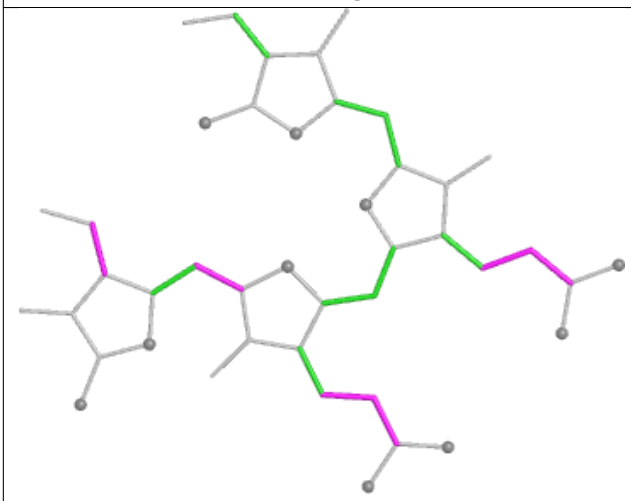
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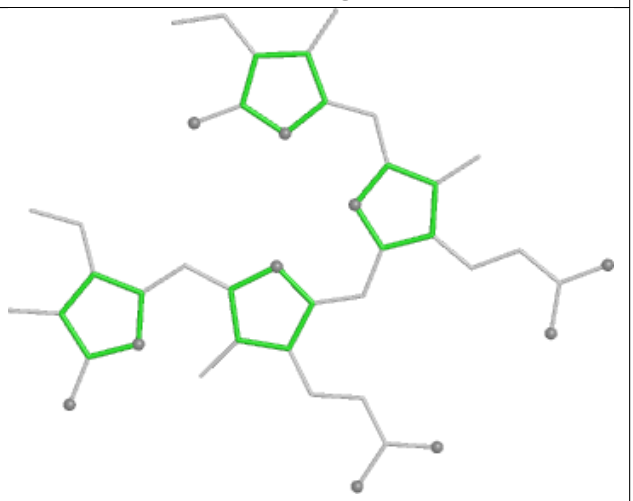
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Bond angles

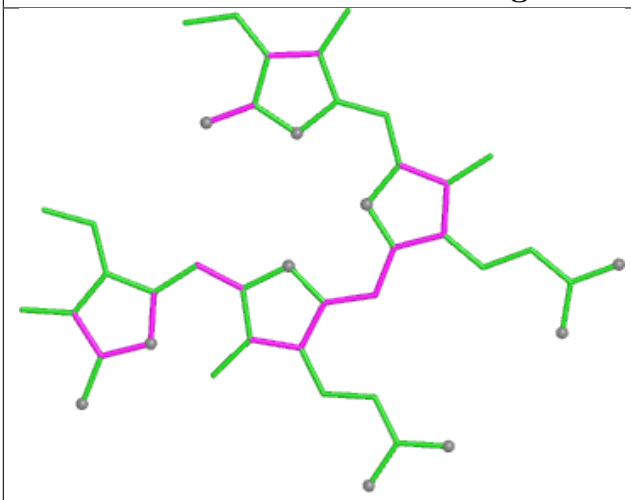


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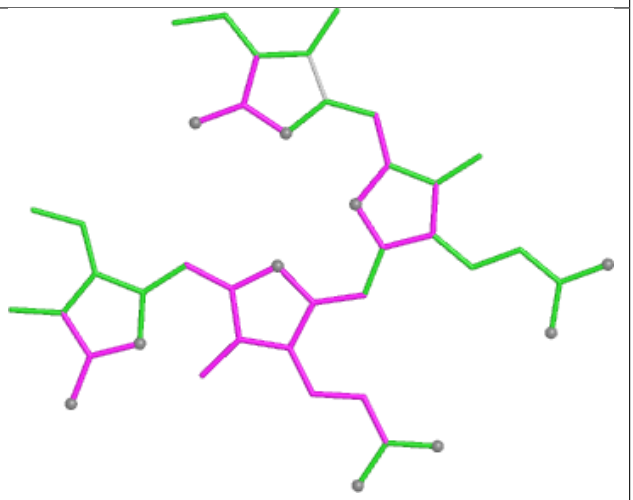


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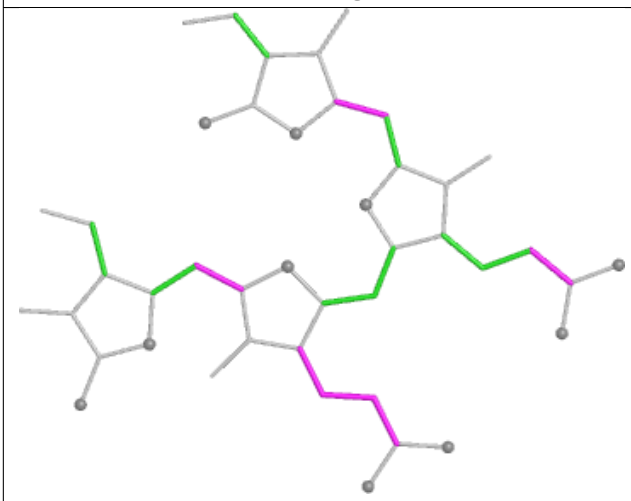
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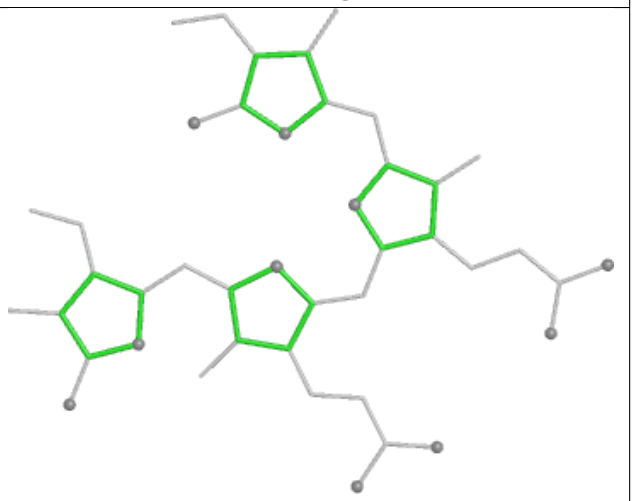
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Bond angles

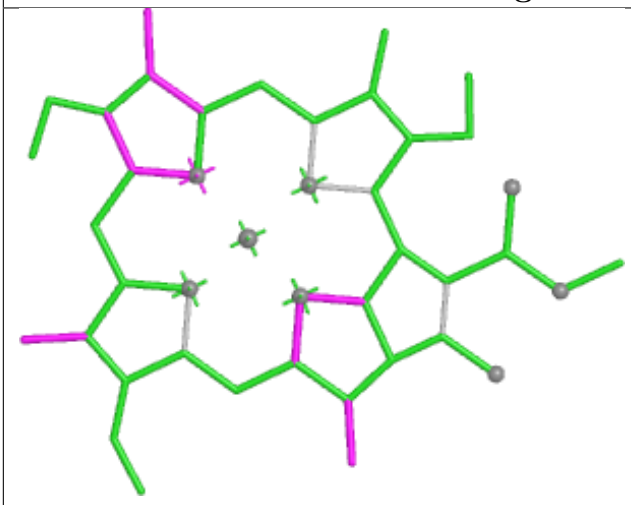


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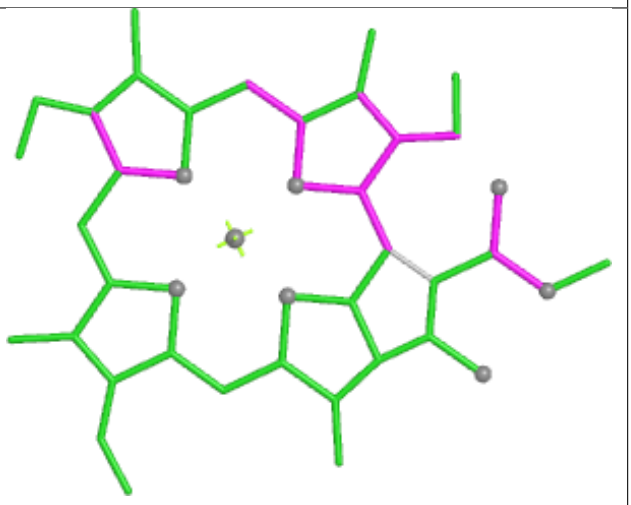


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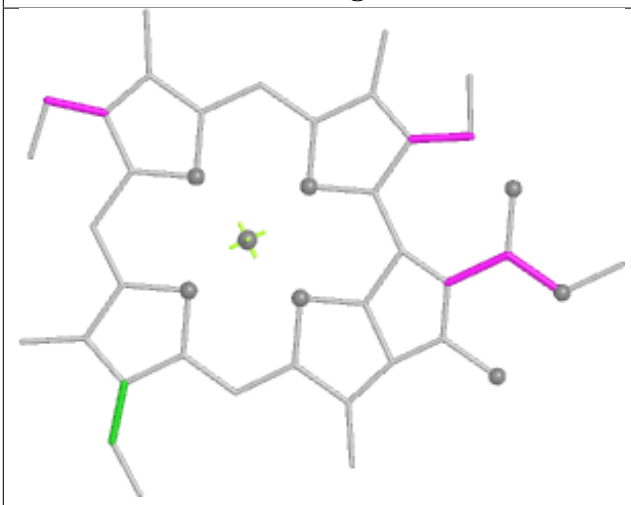
Ligand CLA A2 817



Bond lengths



Bond angles

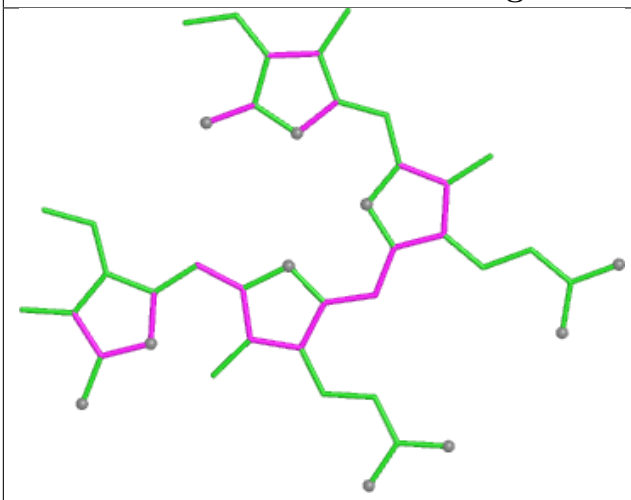


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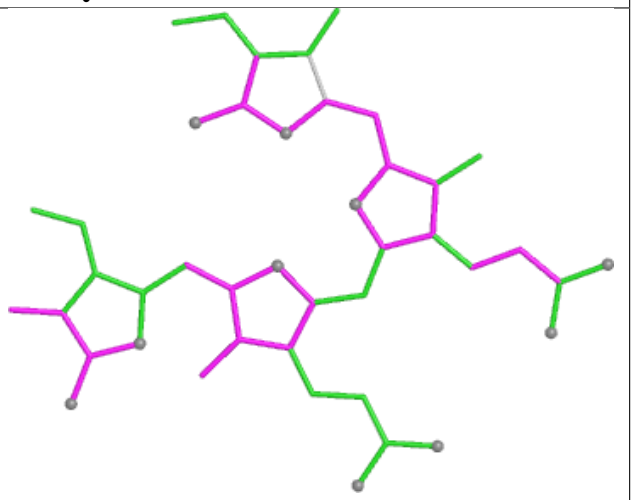


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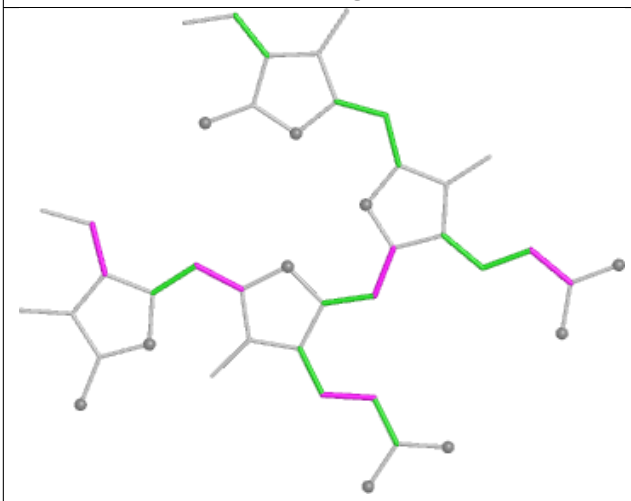
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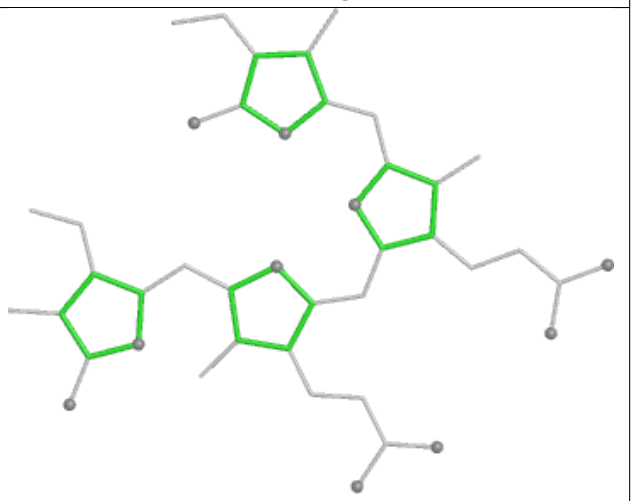
Bond lengths



Bond angles

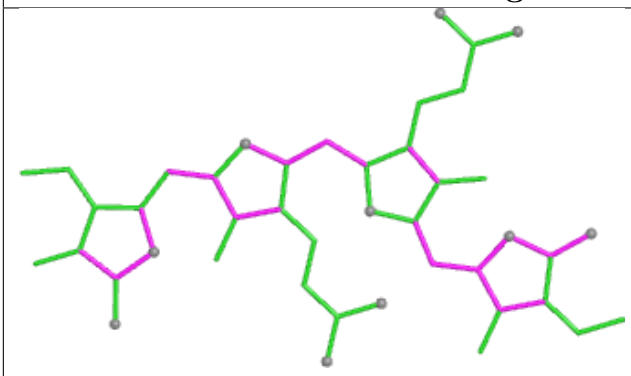


Torsions

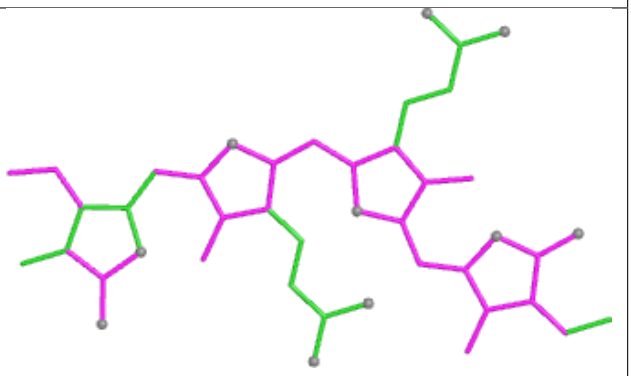


Rings

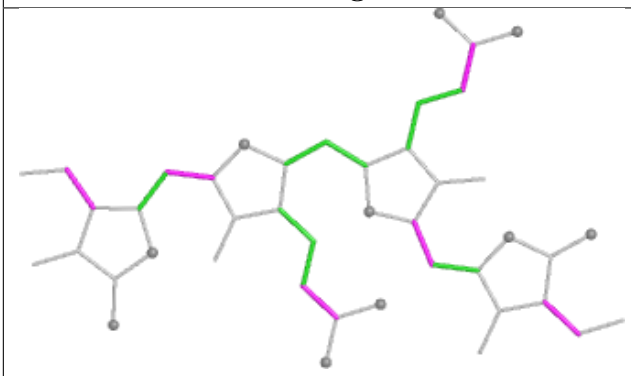
Ligand CYC IO 1001



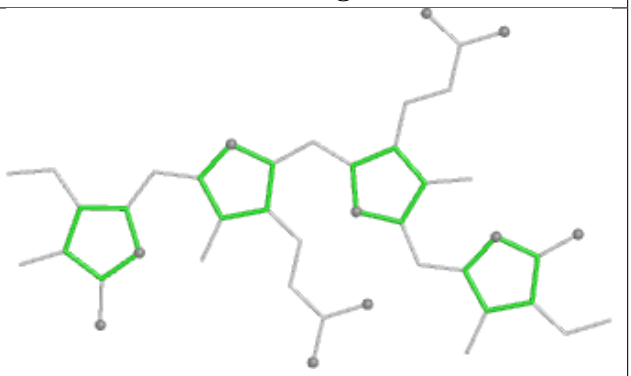
Bond lengths



Bond angles

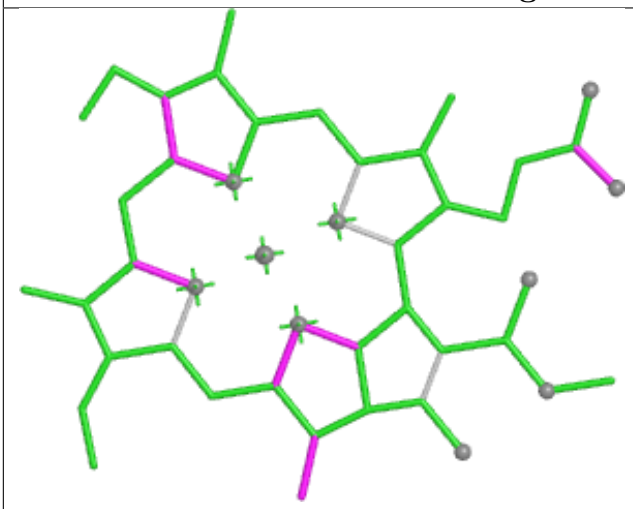


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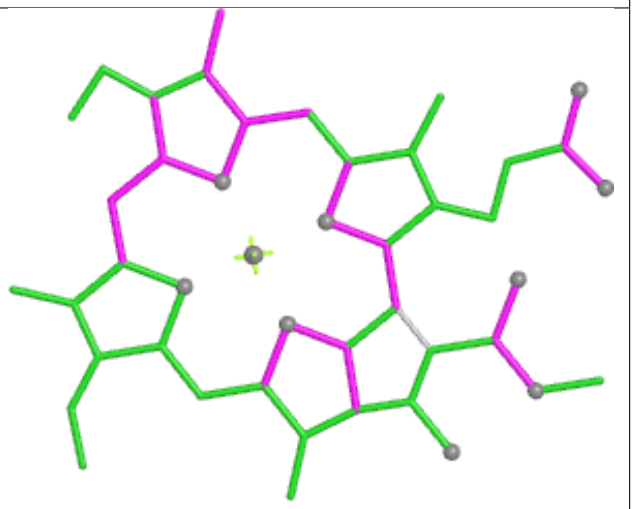


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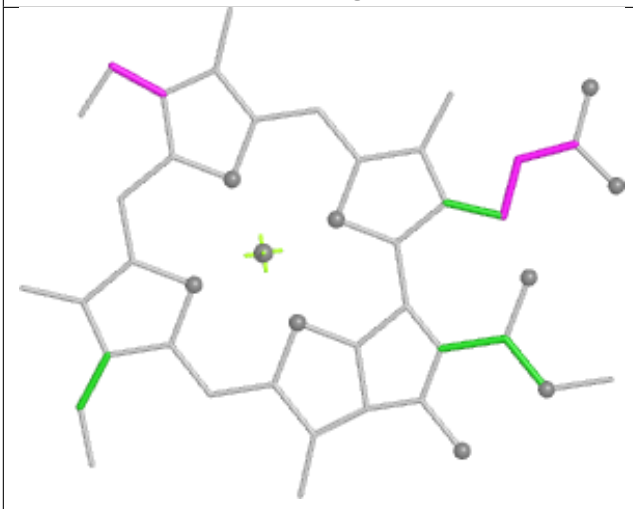
Ligand CLA 32 307



Bond lengths



Bond angles

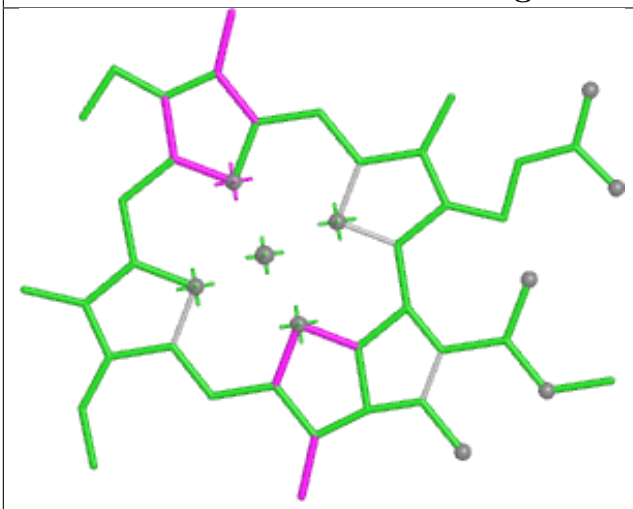


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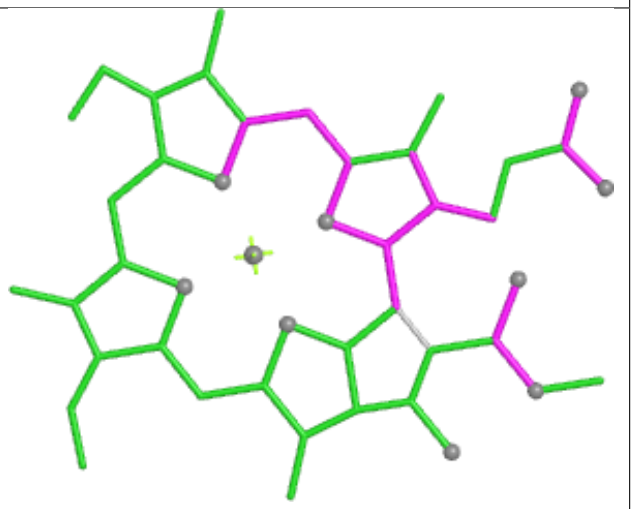


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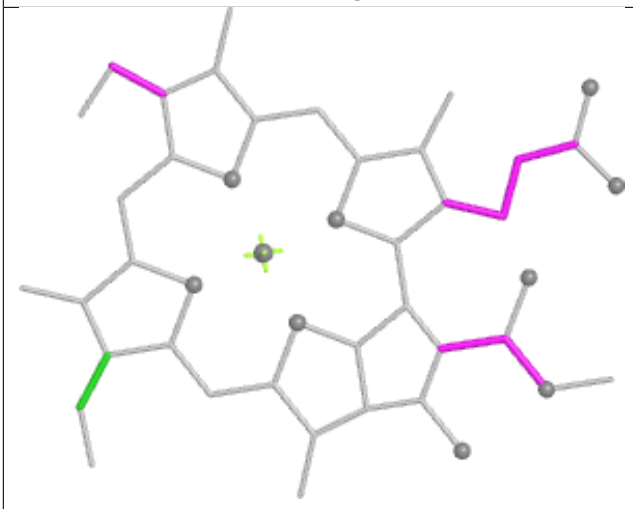
Ligand CLA 5N 611



Bond lengths



Bond angles

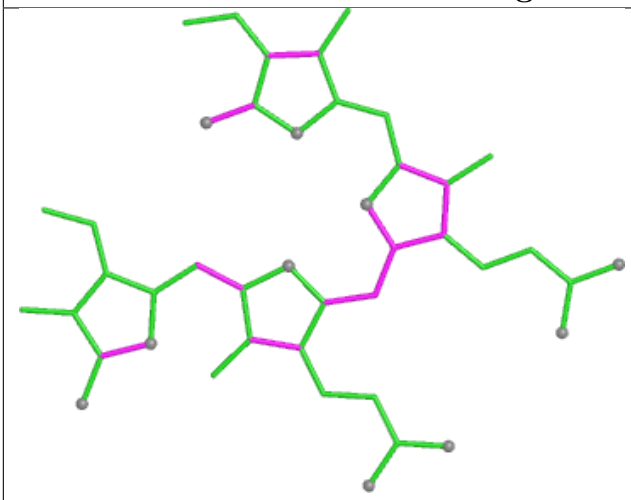


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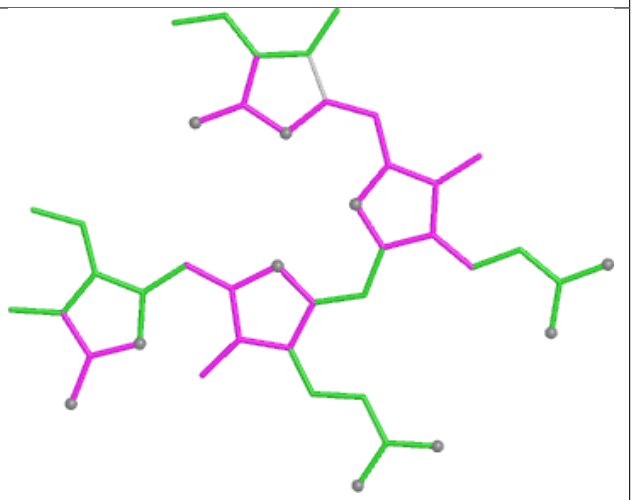


Rings

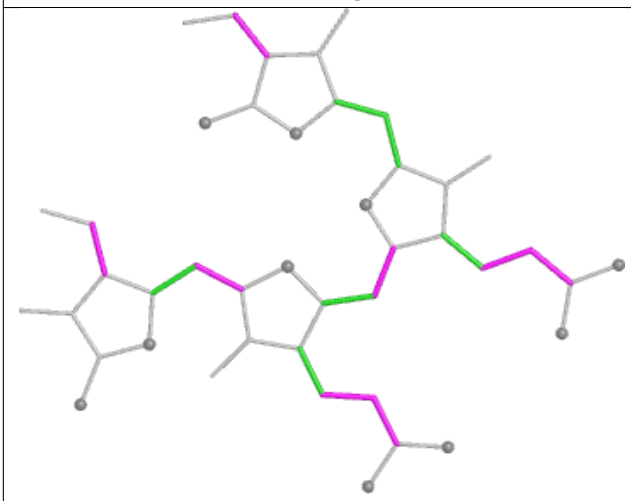
Ligand PEB cK 202



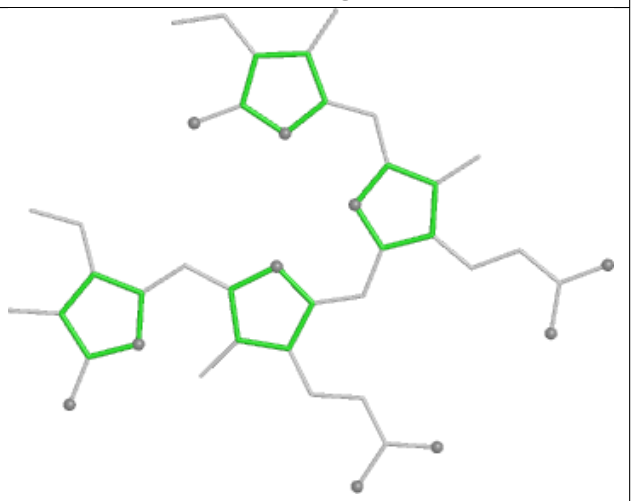
Bond lengths



Bond angles

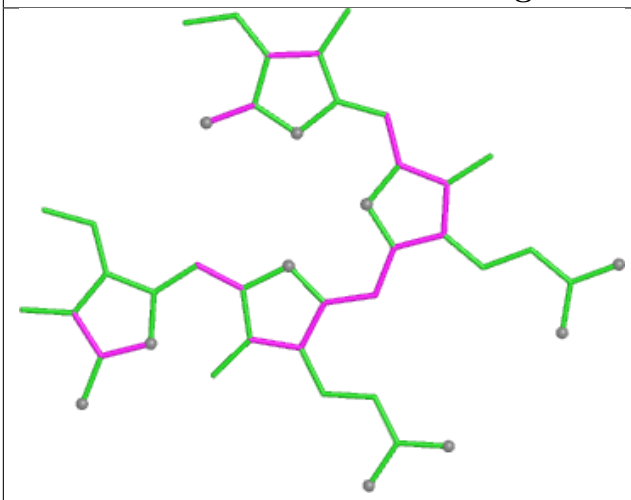


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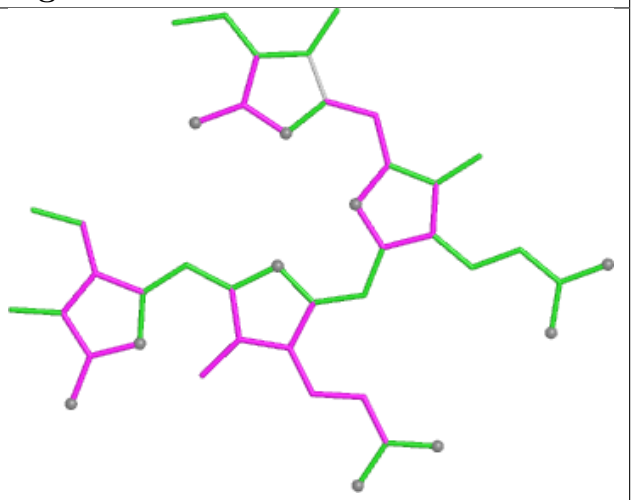


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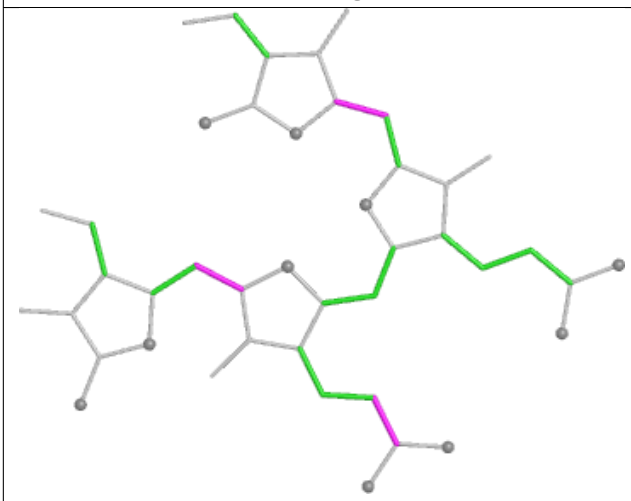
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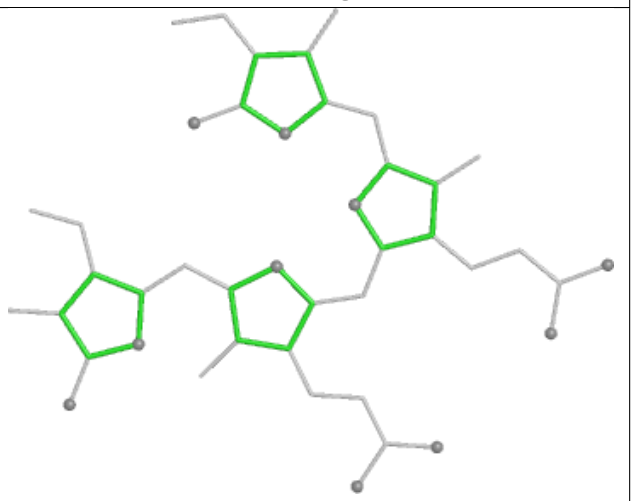
Bond lengths



Bond angles

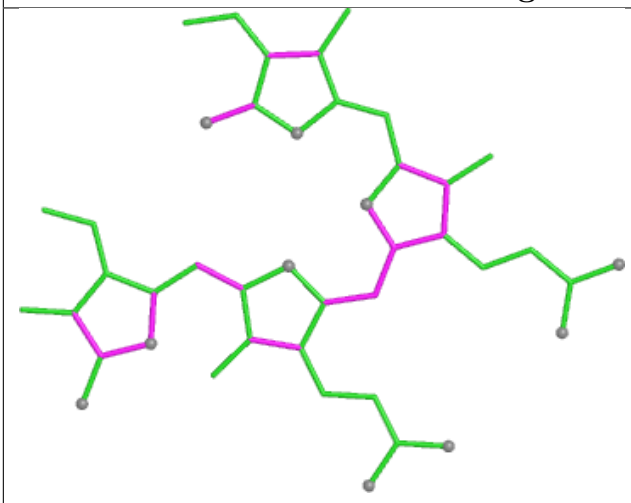


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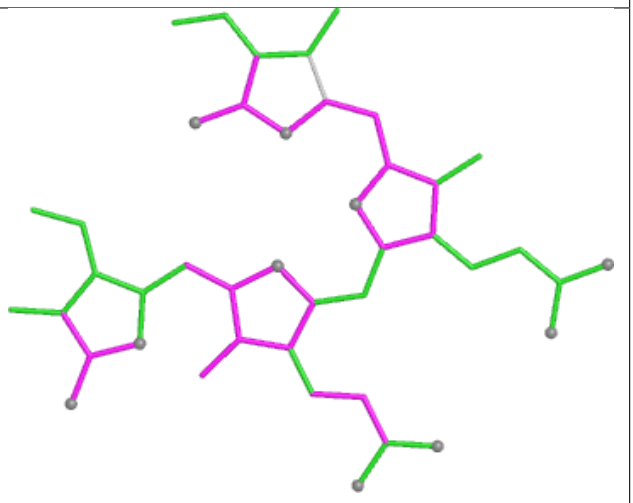


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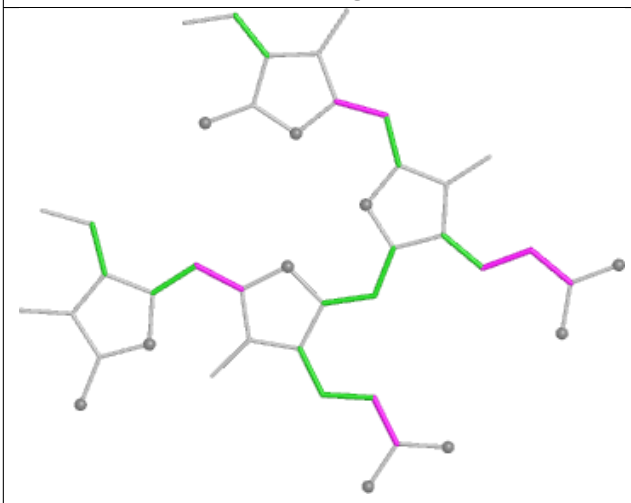
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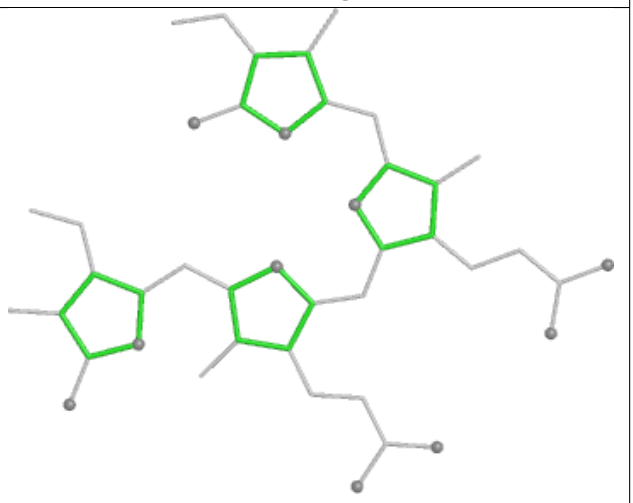
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Bond angles

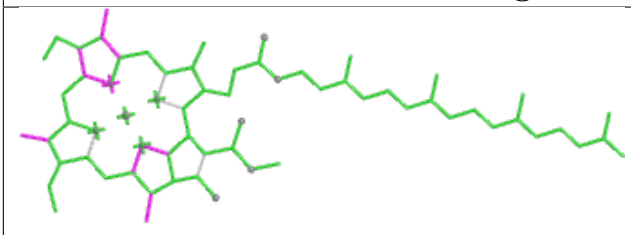


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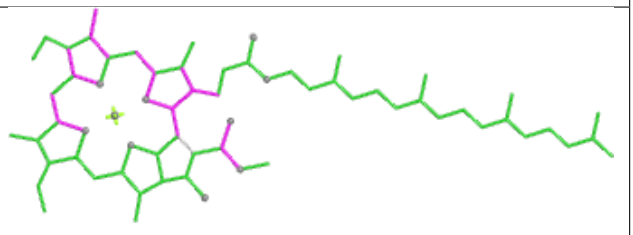


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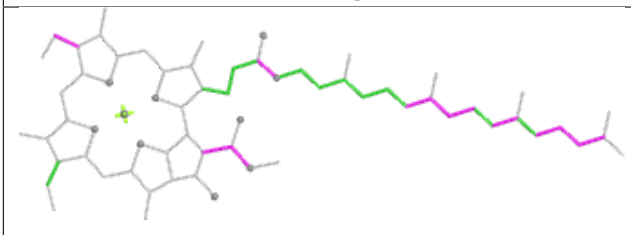
Ligand CLA BL 608



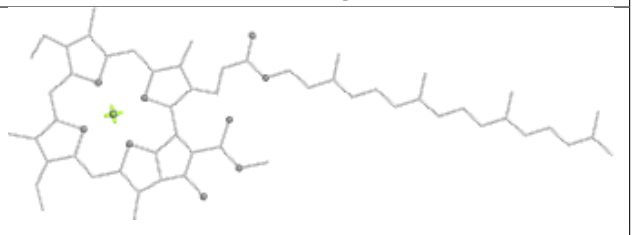
Bond lengths



Bond angles

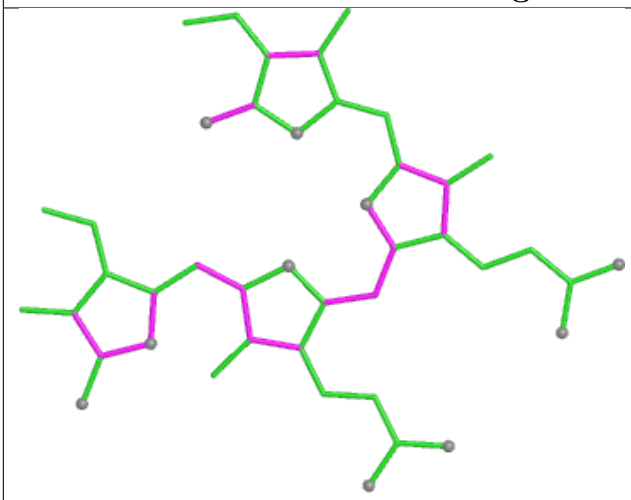


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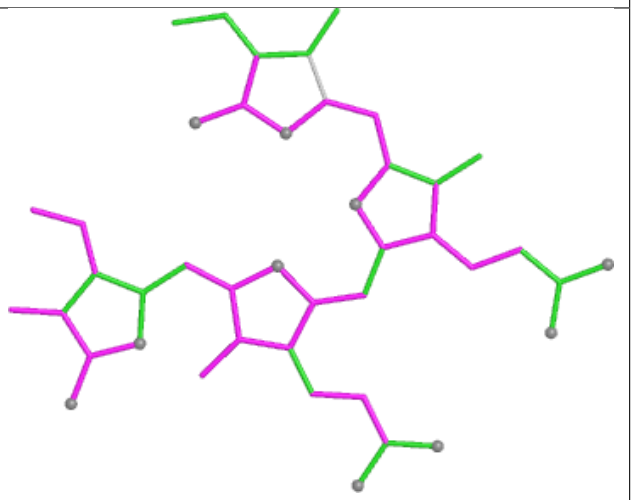


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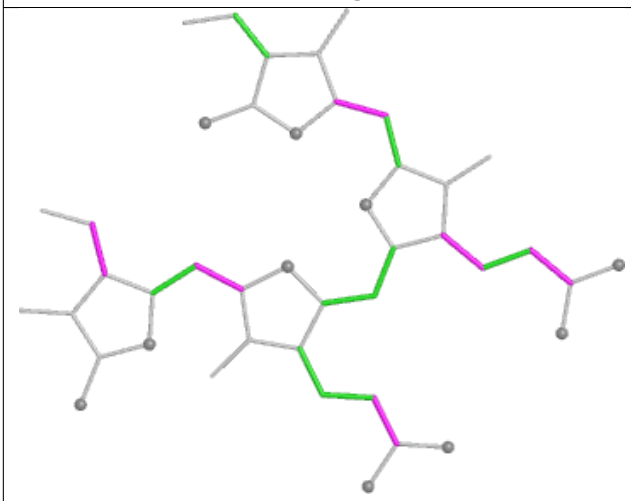
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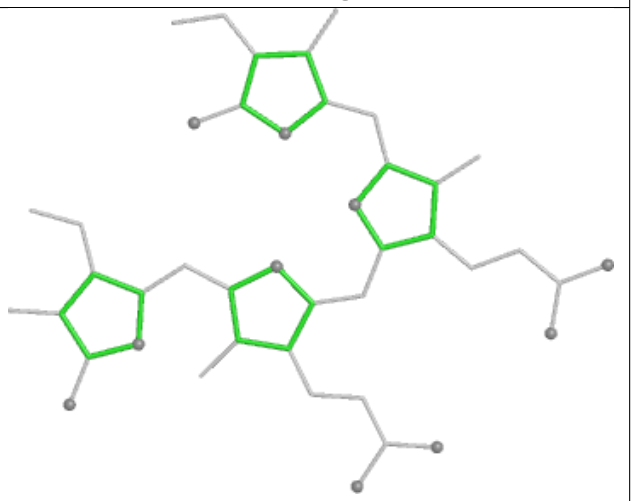
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Bond angles

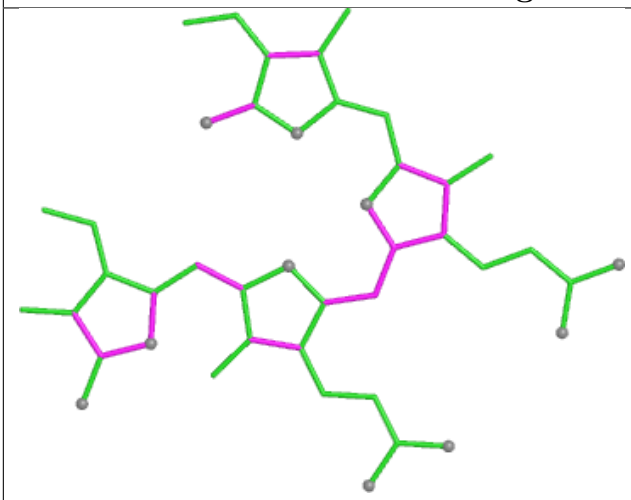


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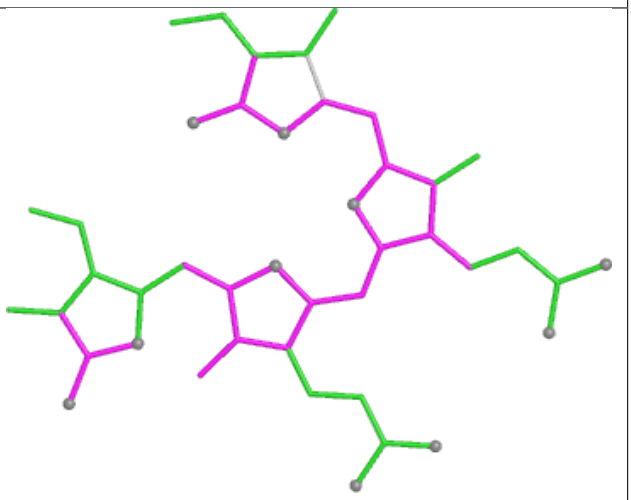


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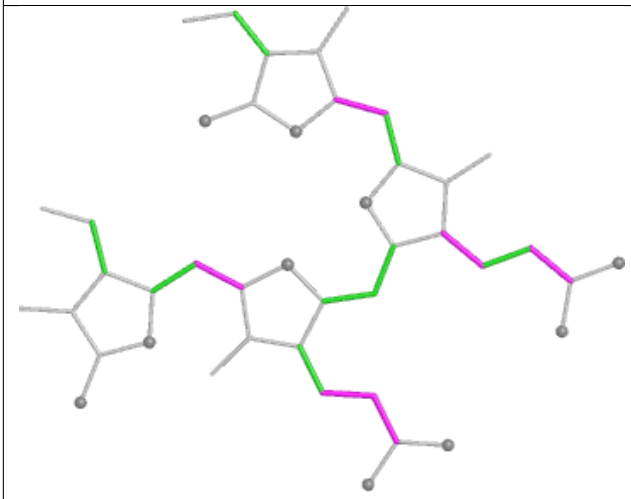
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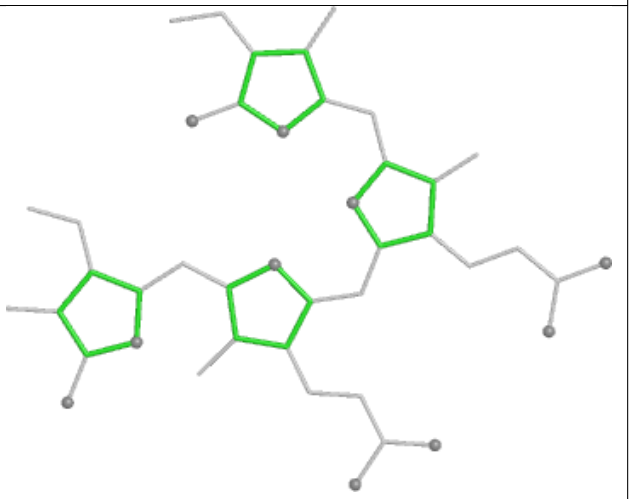
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Bond angles

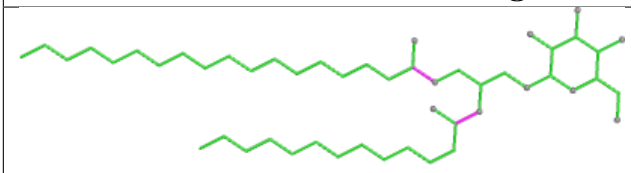


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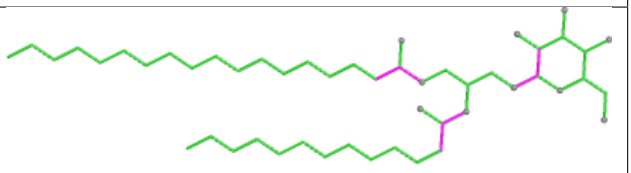


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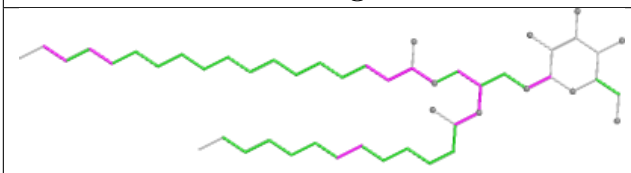
Ligand LMG XL 601



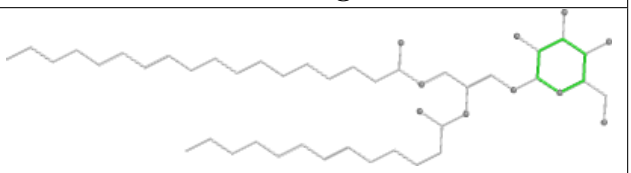
Bond lengths



Bond angles

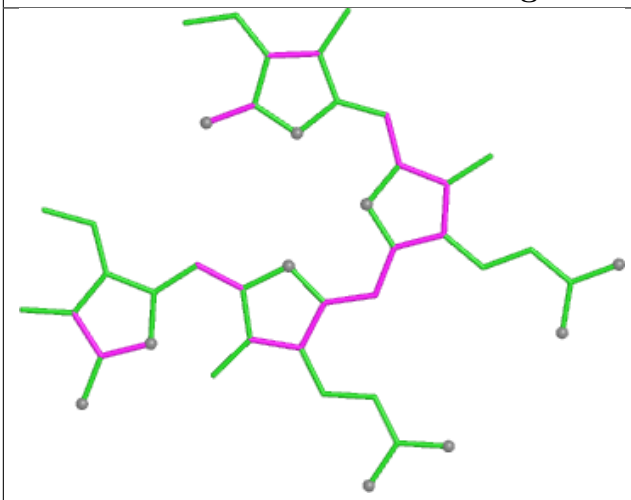


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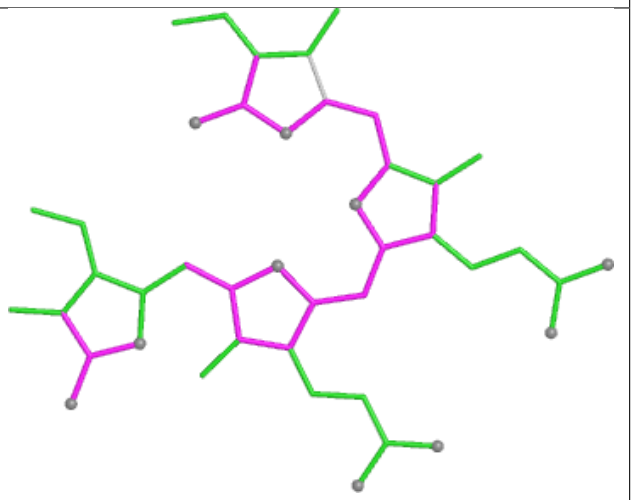


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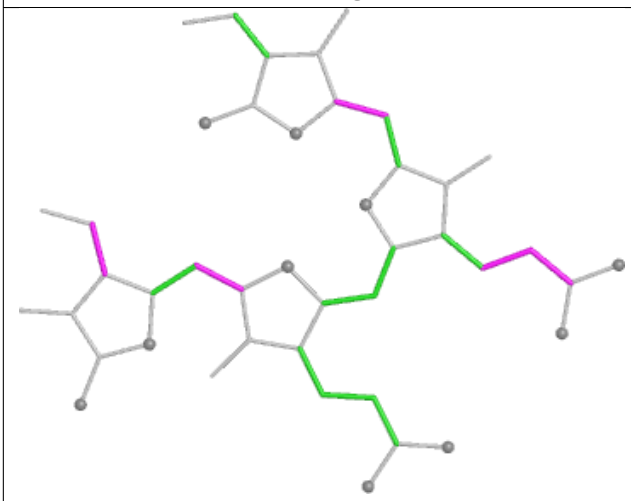
Ligand PEB fE 203



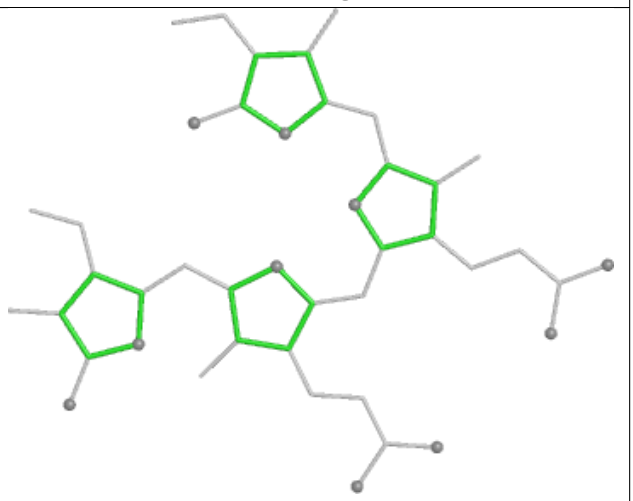
Bond lengths



Bond angles

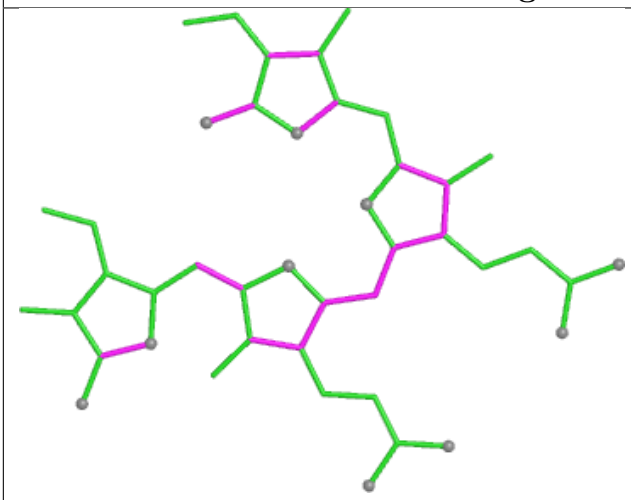


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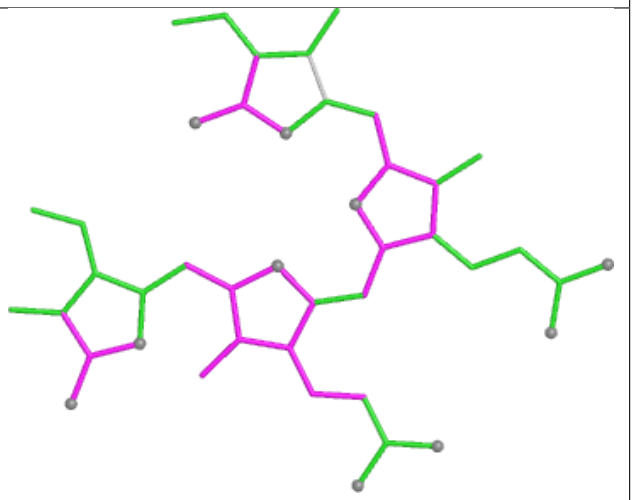


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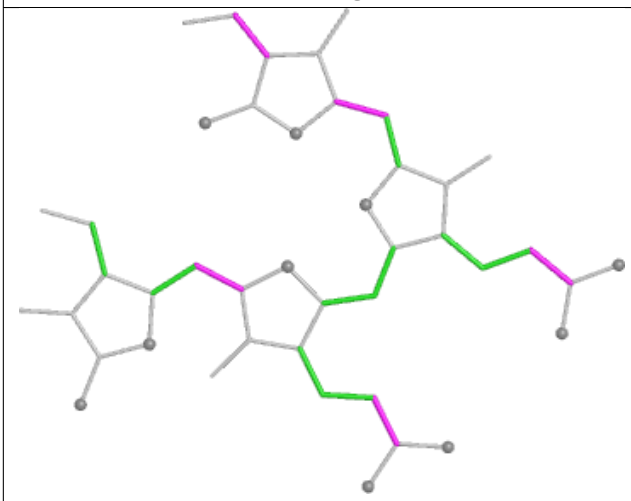
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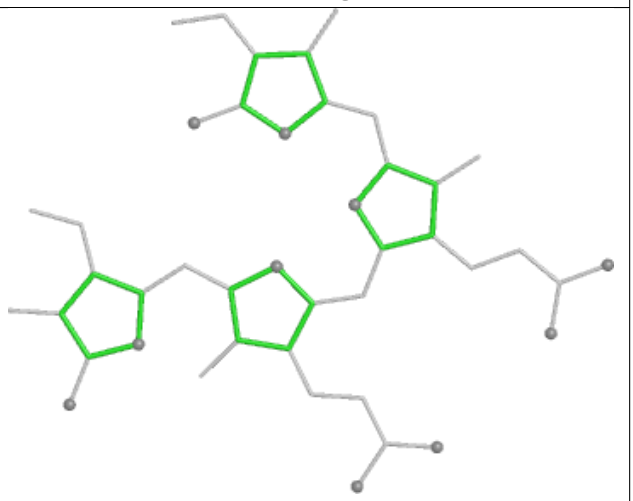
Bond lengths



Bond angles

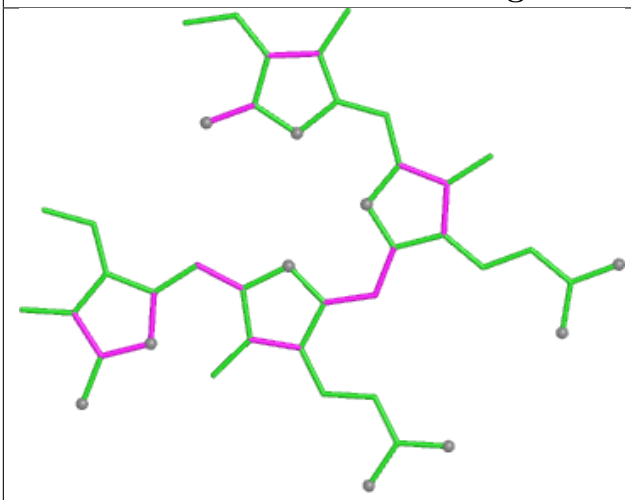


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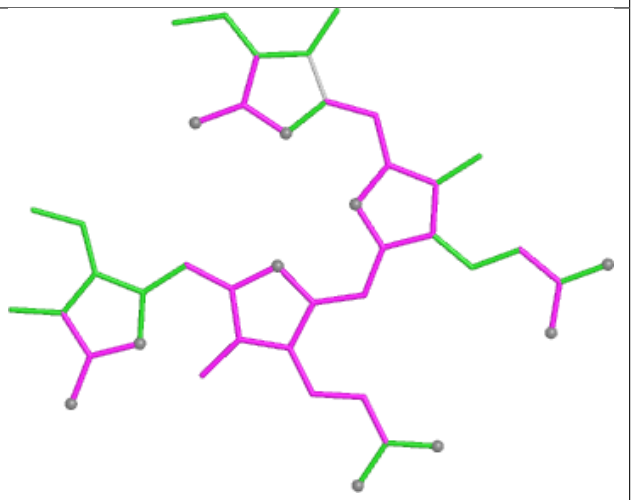


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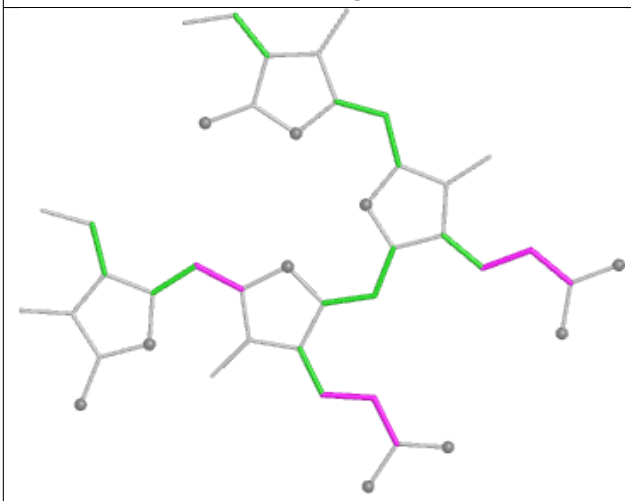
Ligand PEB MA 201



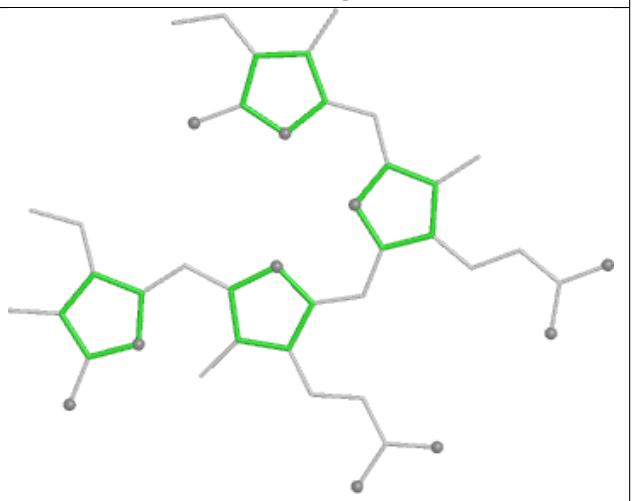
Bond lengths



Bond angles

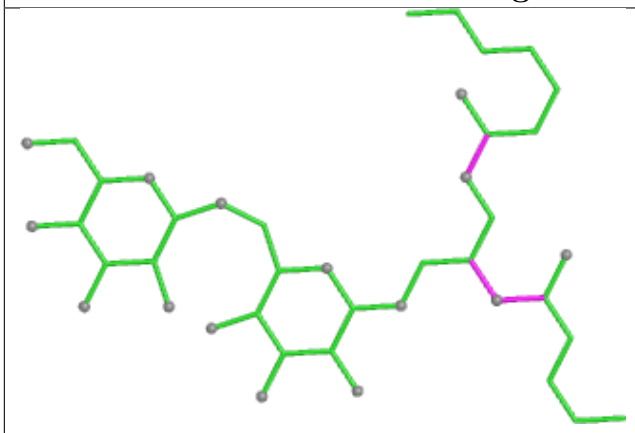


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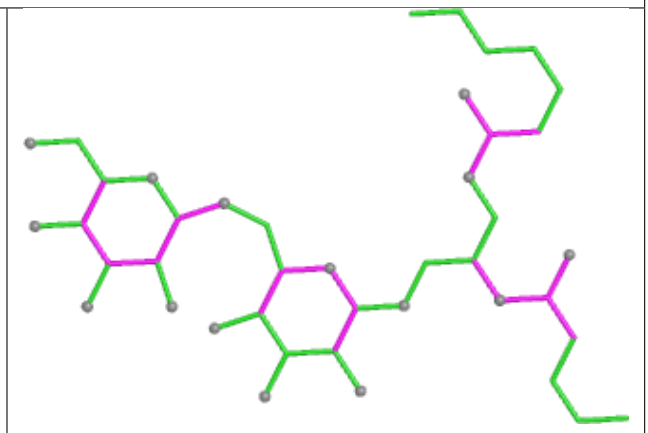


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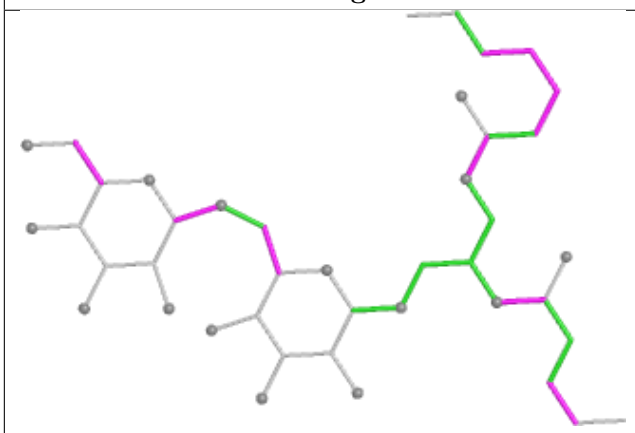
Ligand DGD C6 503



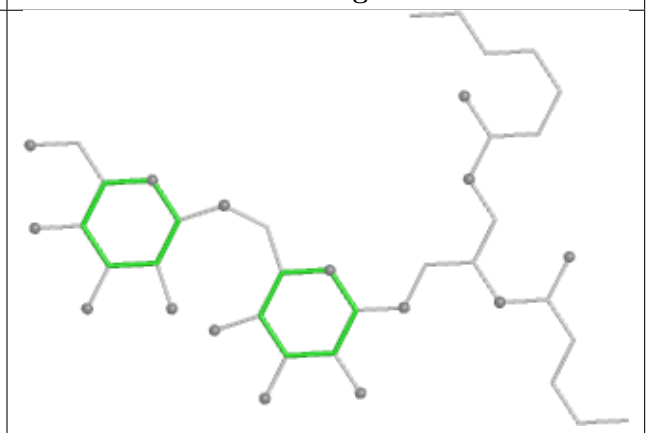
Bond lengths



Bond angles

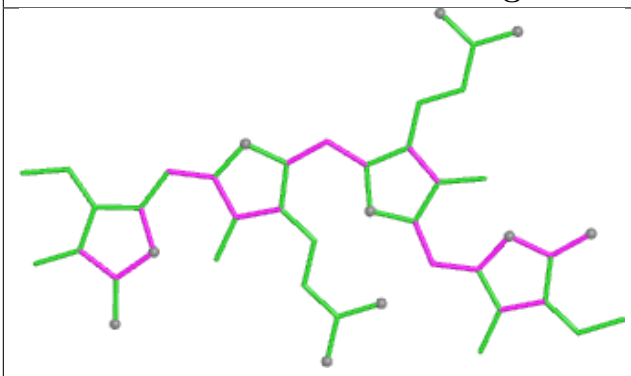


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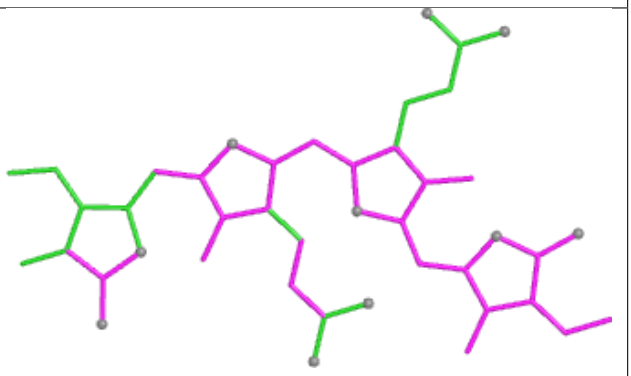


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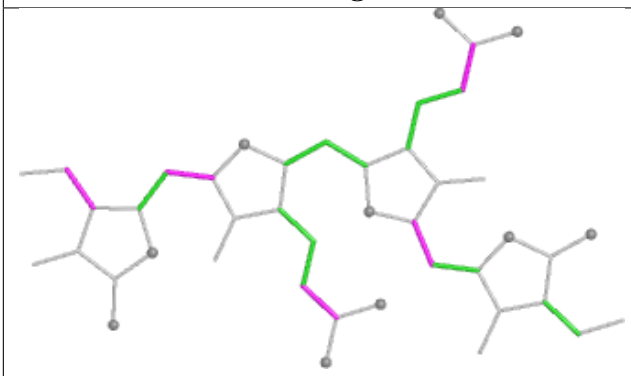
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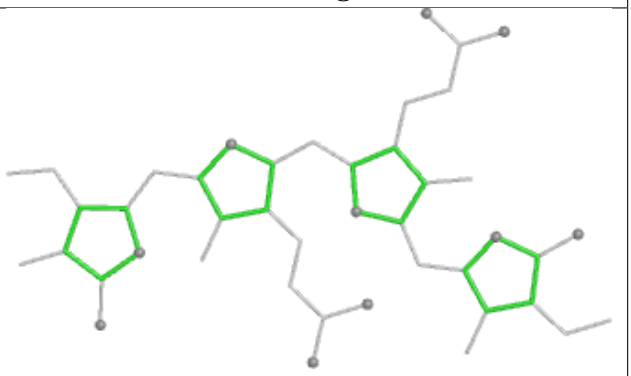
Bond lengths



Bond angles

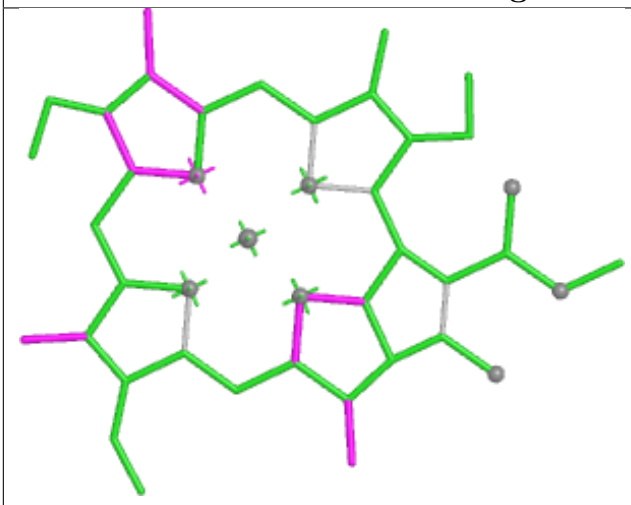


Torsions

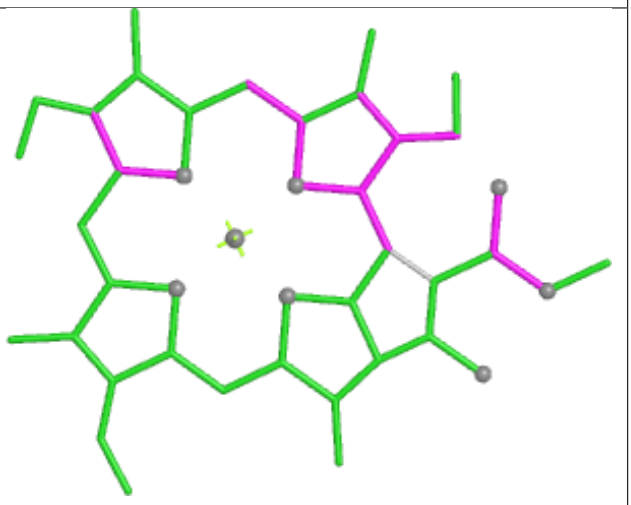


Rings

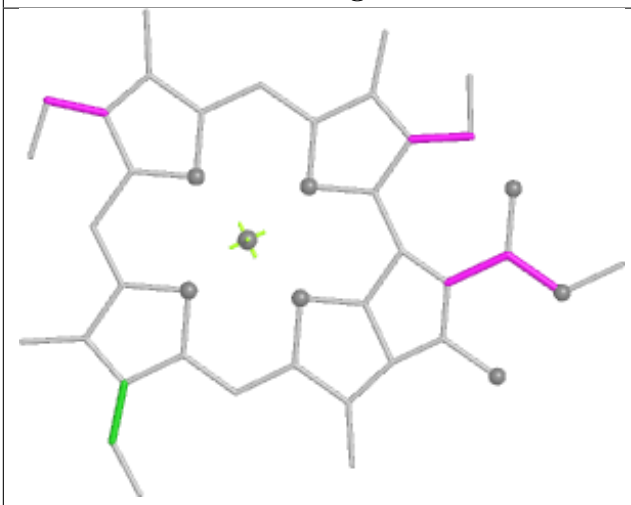
Ligand CLA AN 817



Bond lengths



Bond angles

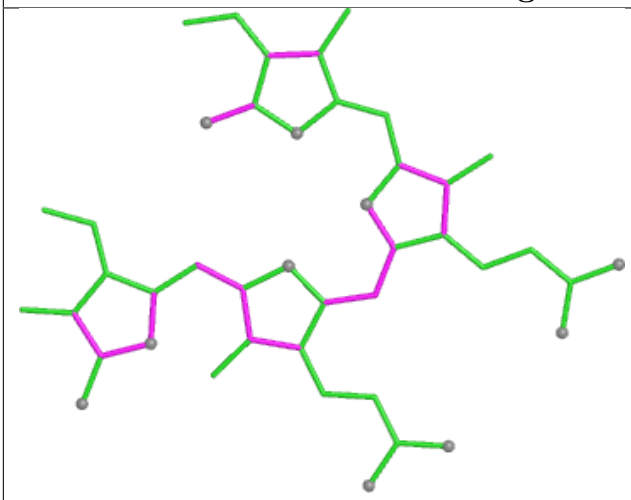


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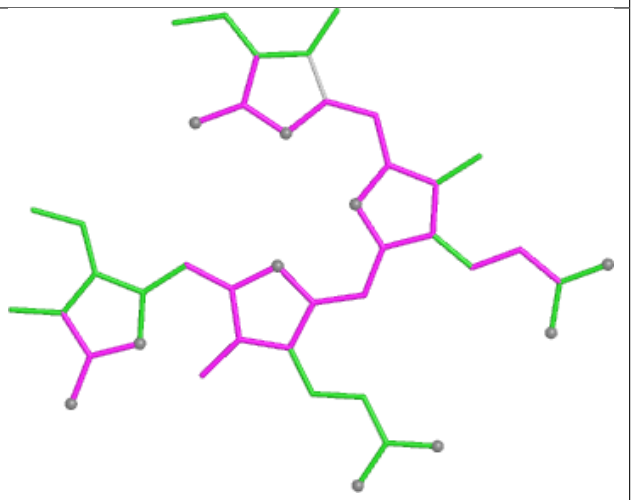


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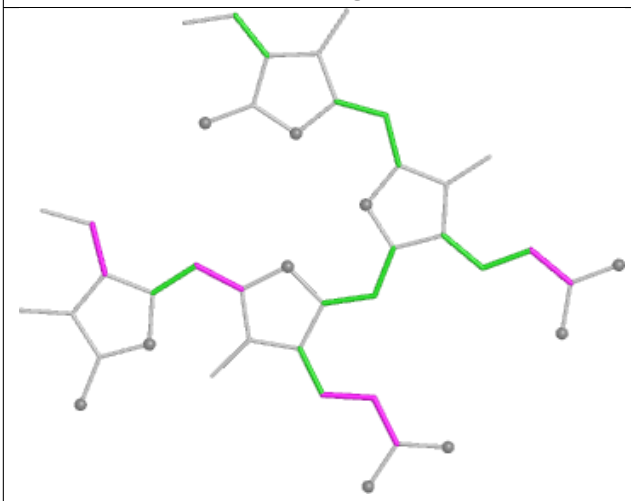
Ligand PEB Z5 301



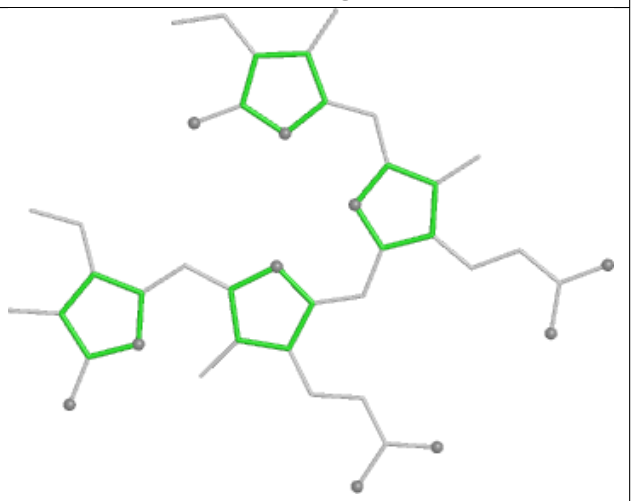
Bond lengths



Bond angles

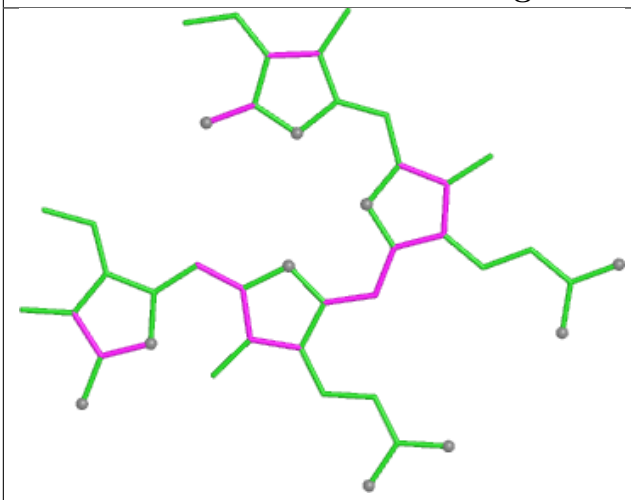


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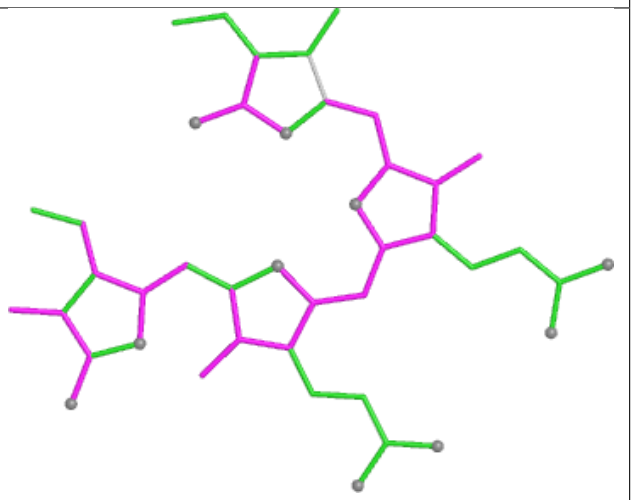


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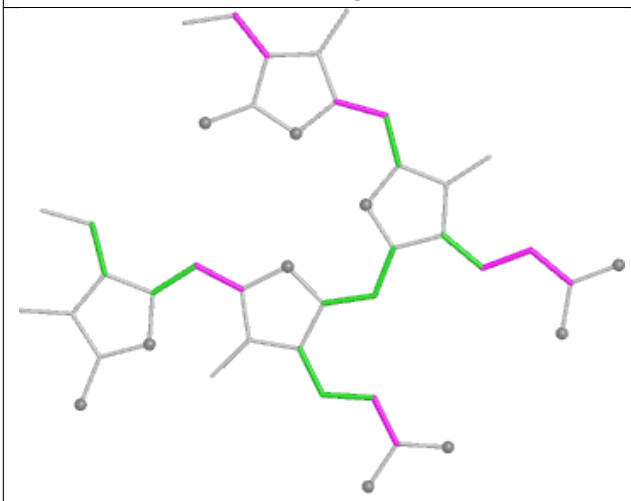
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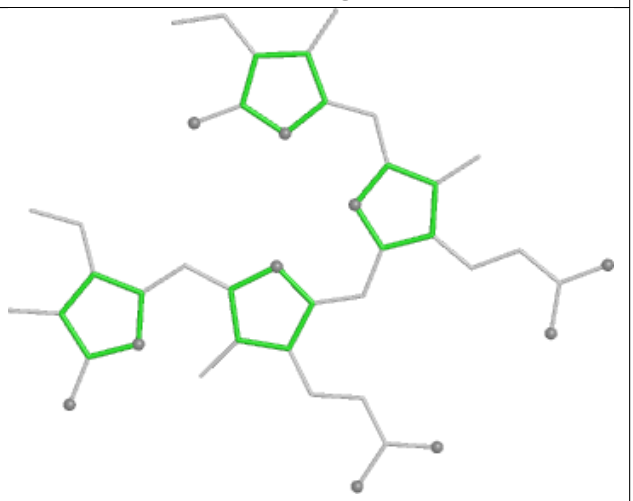
Bond lengths



Bond angles

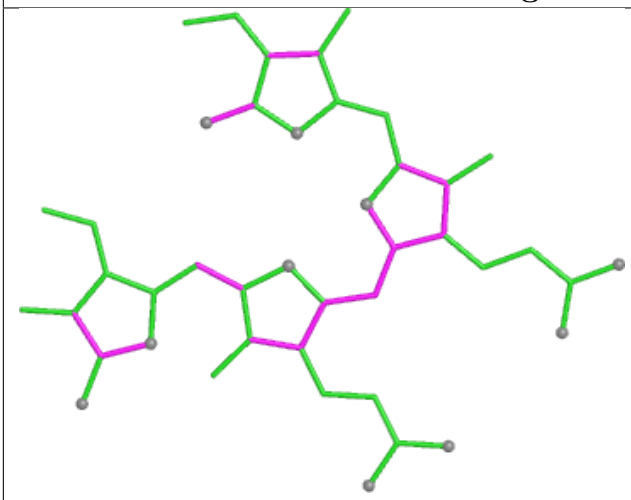


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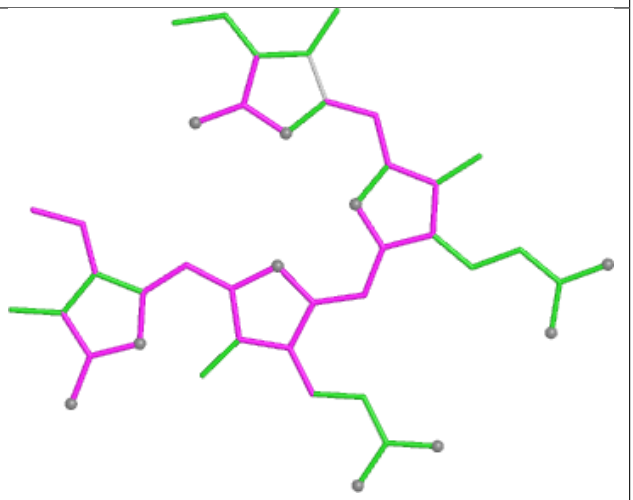


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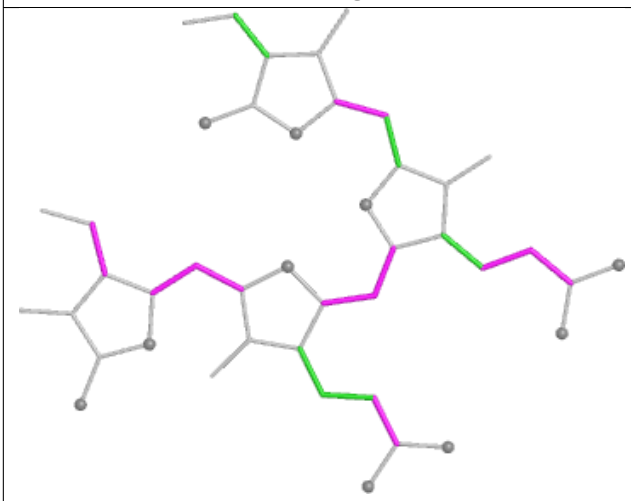
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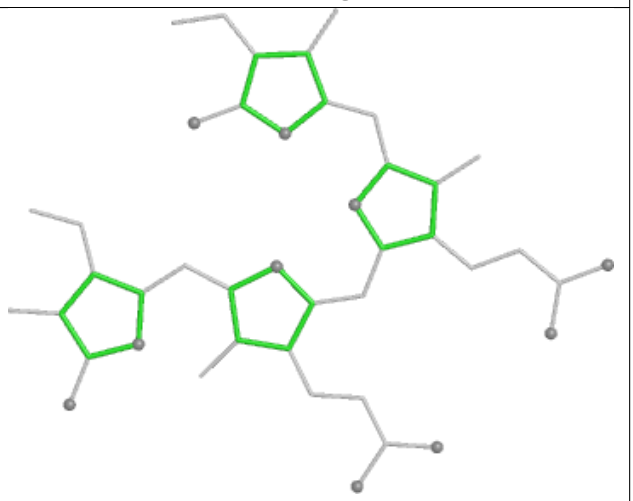
Bond lengths



Bond angles

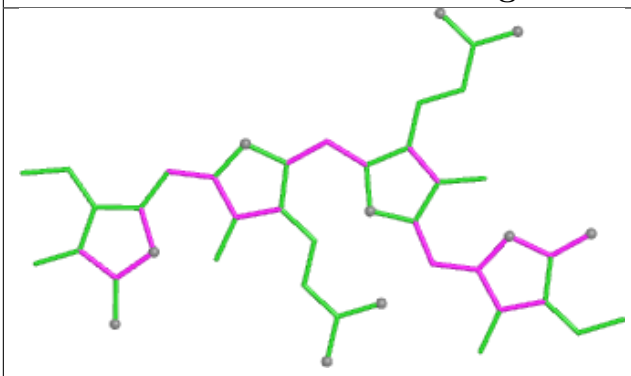


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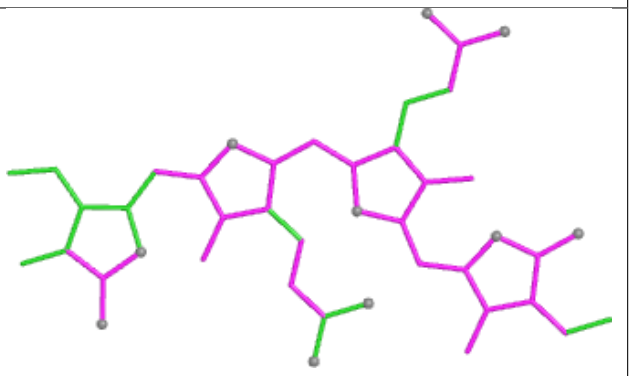


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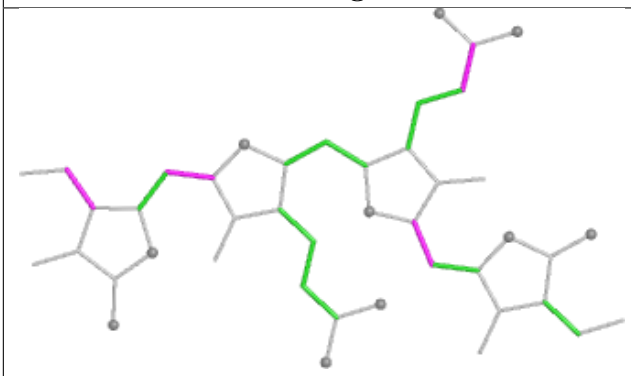
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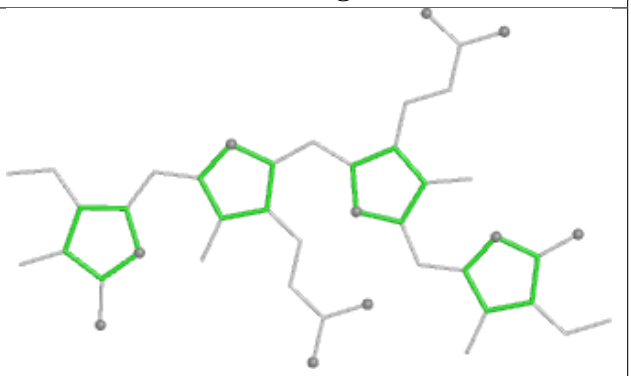
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Bond angles

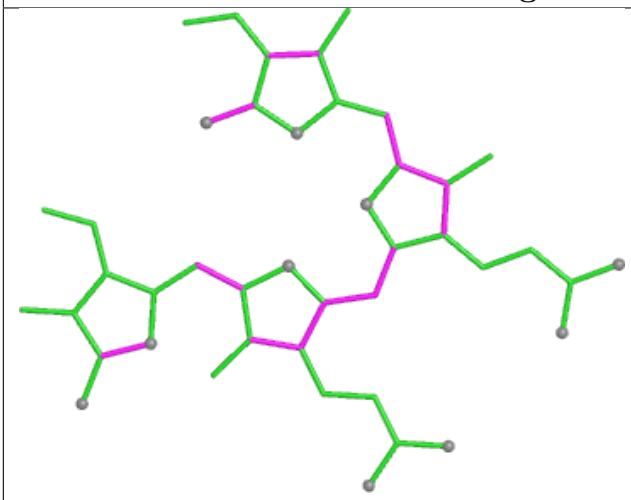


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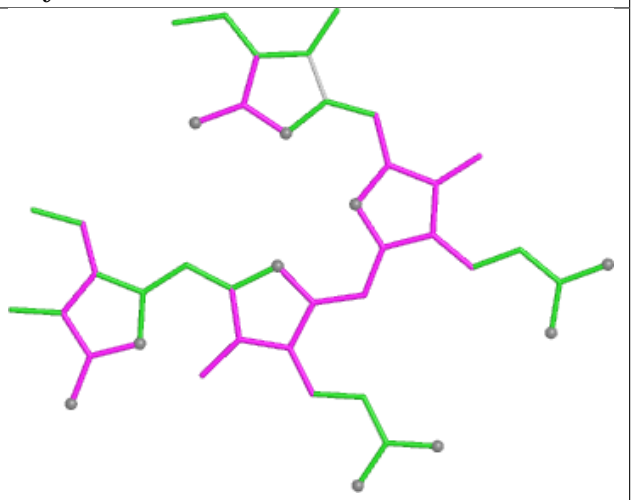


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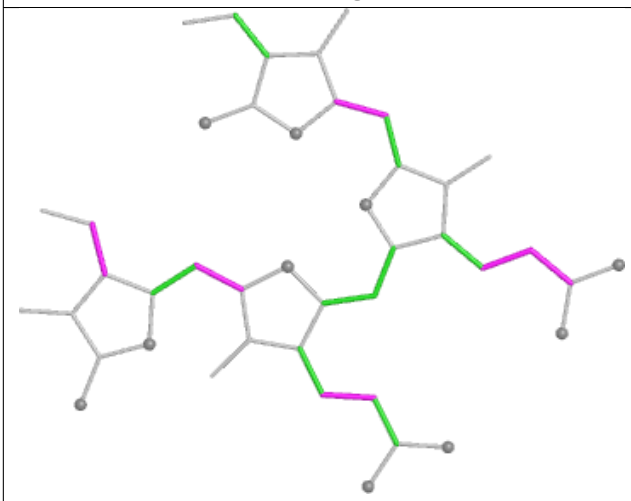
Ligand PEB y8 202



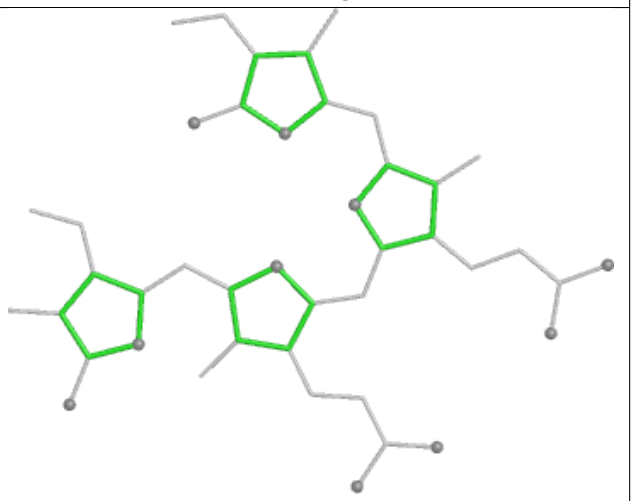
Bond lengths



Bond angles

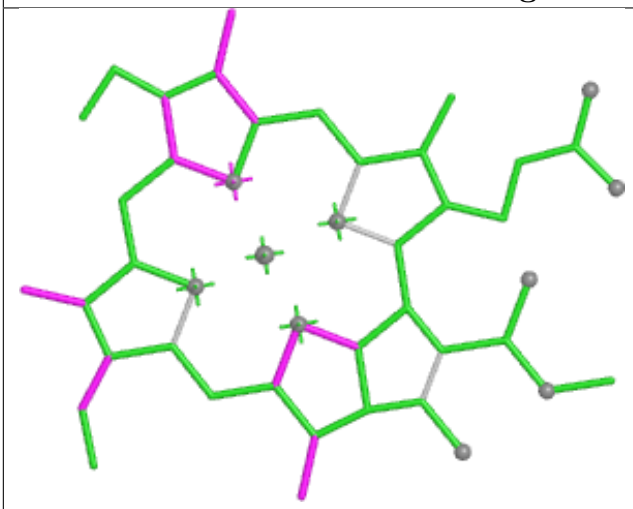


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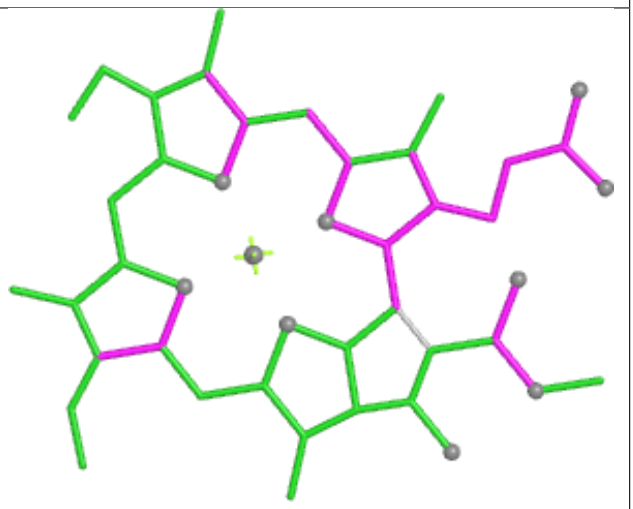


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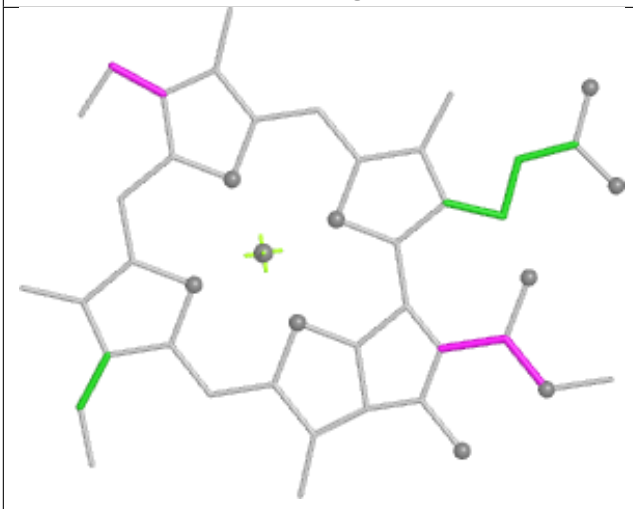
Ligand CLA 82 303



Bond lengths



Bond angles

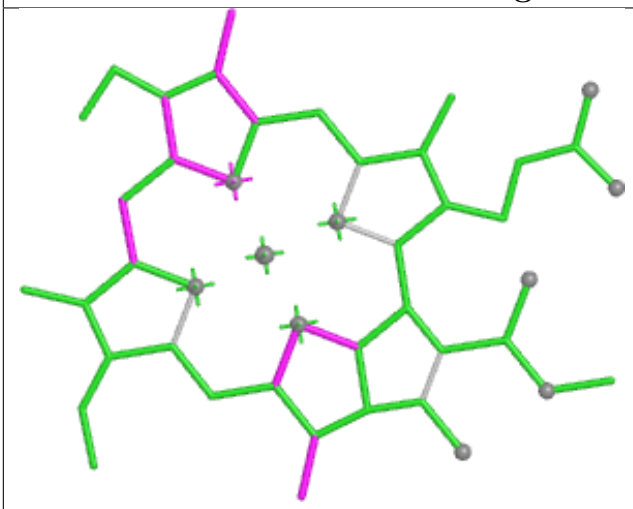


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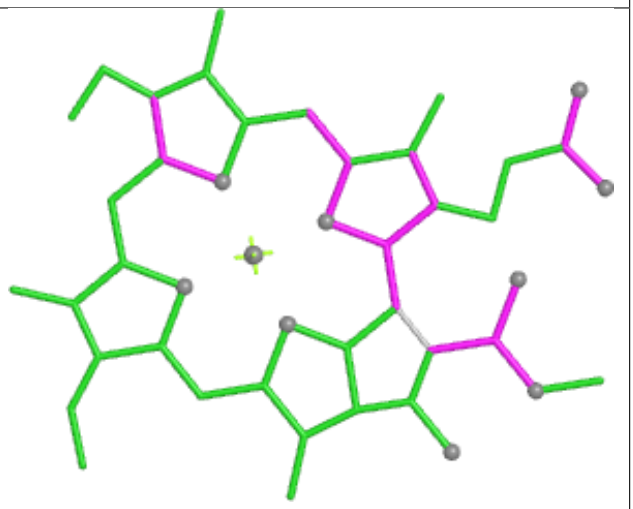


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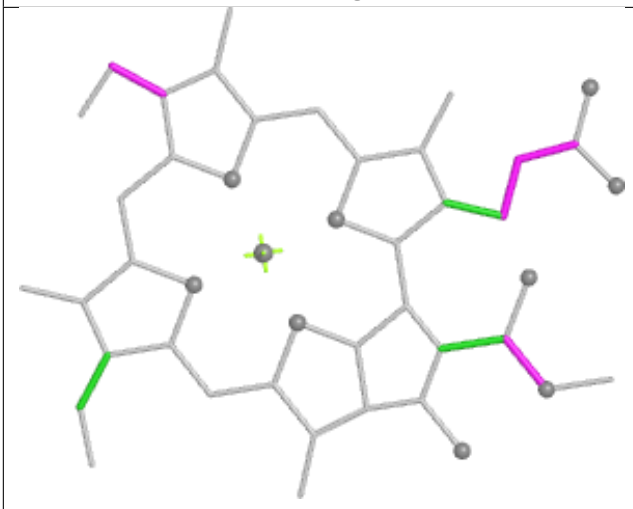
Ligand CLA 7N 603



Bond lengths



Bond angles

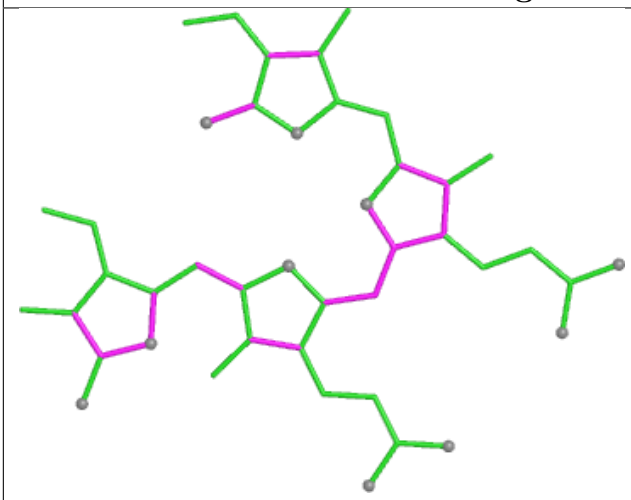


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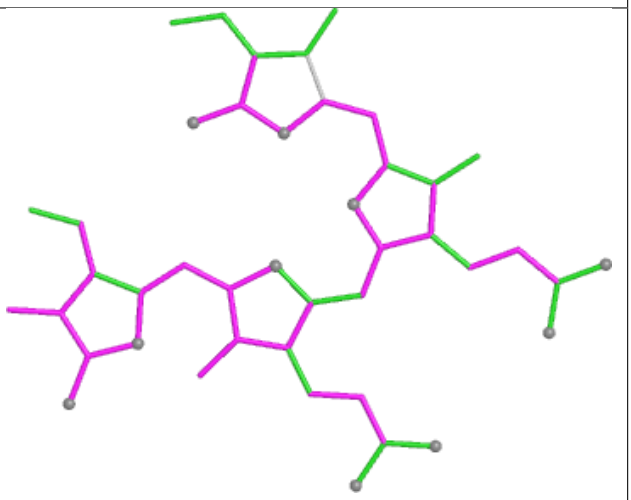


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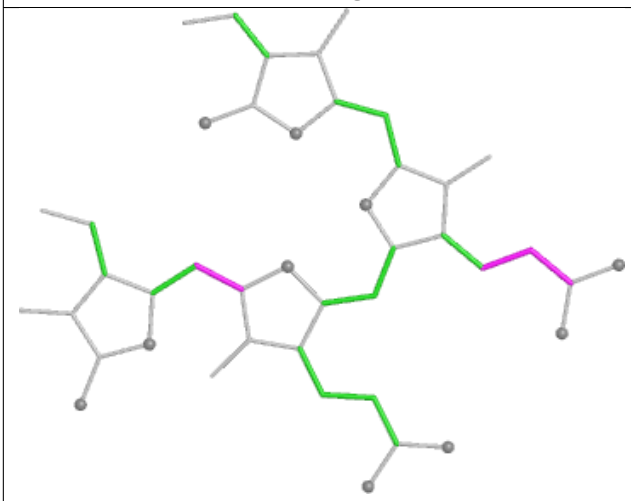
Ligand PEB X7 201



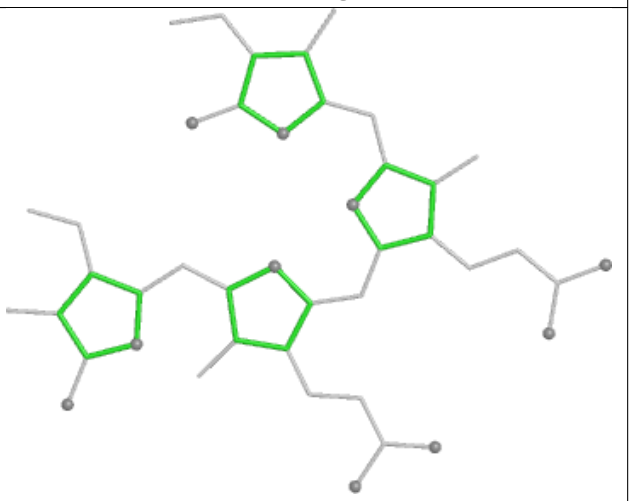
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Bond angles

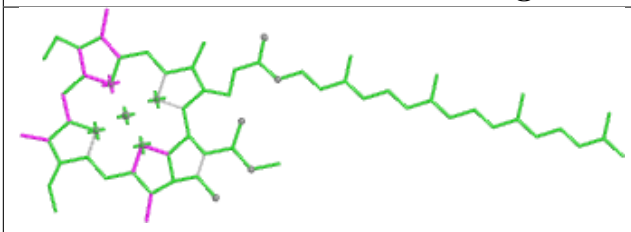


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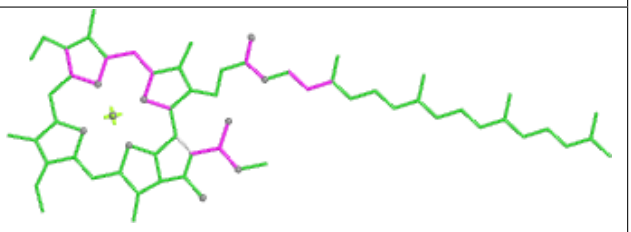


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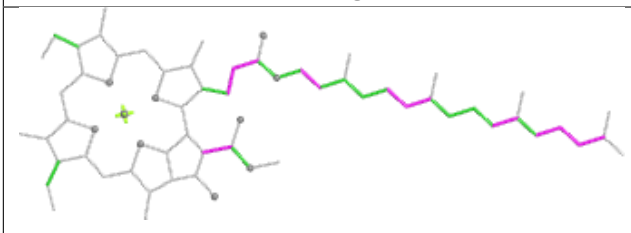
Ligand CLA B6 604



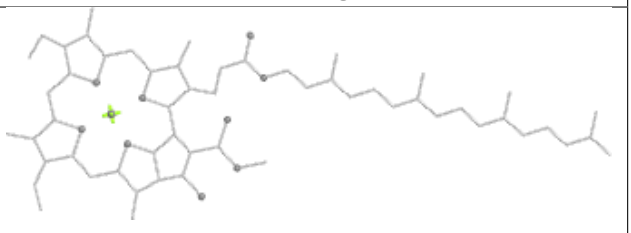
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Bond angles

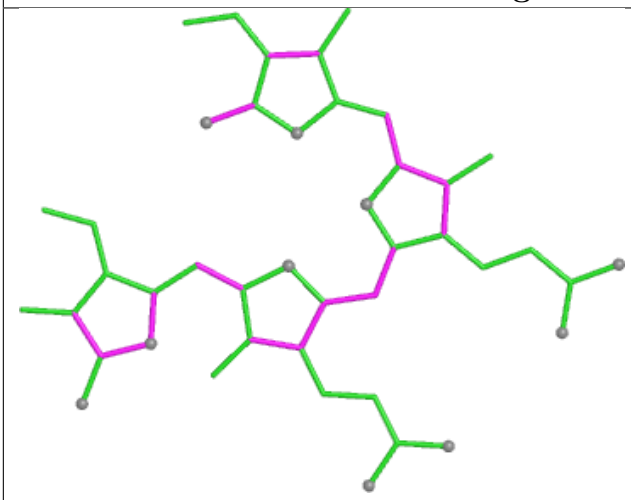


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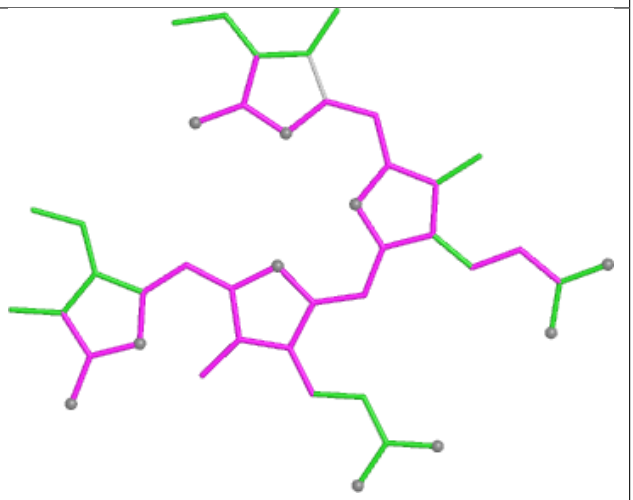


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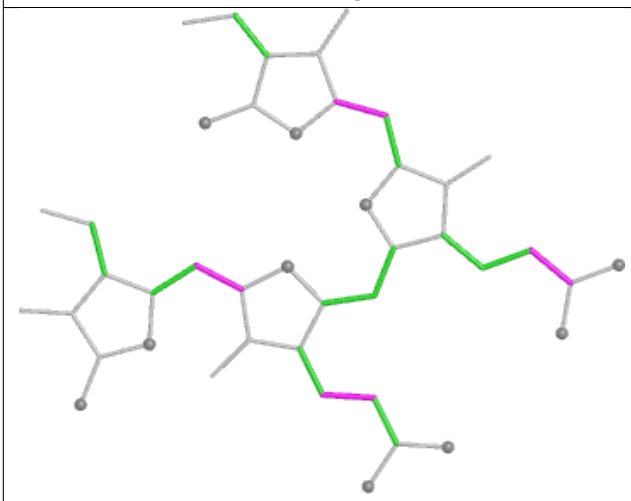
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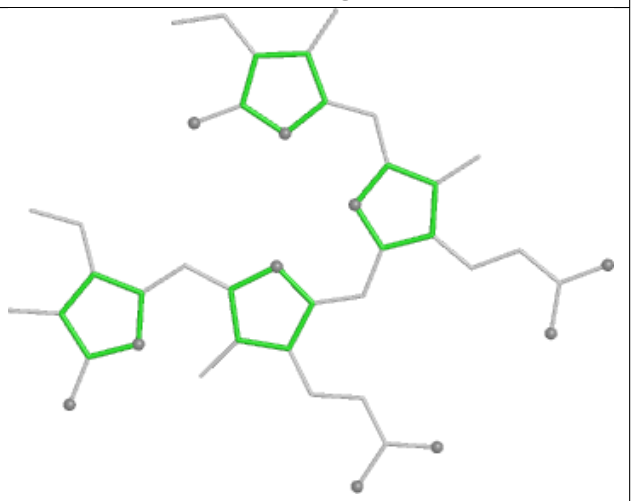
Bond lengths



Bond angles

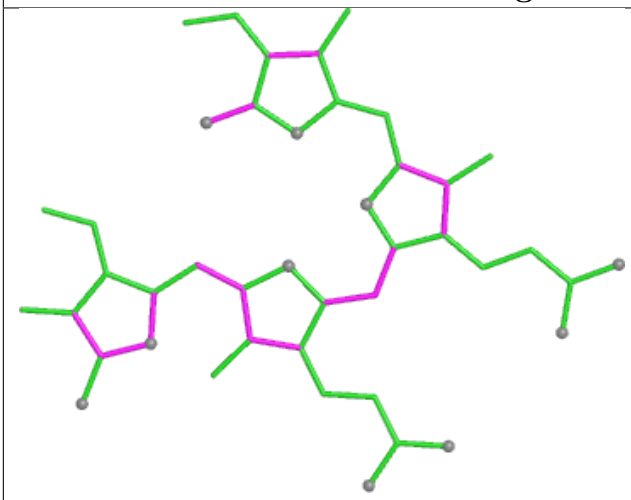


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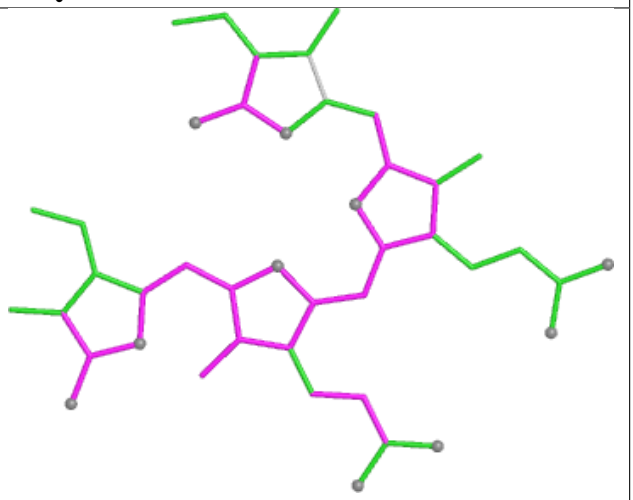


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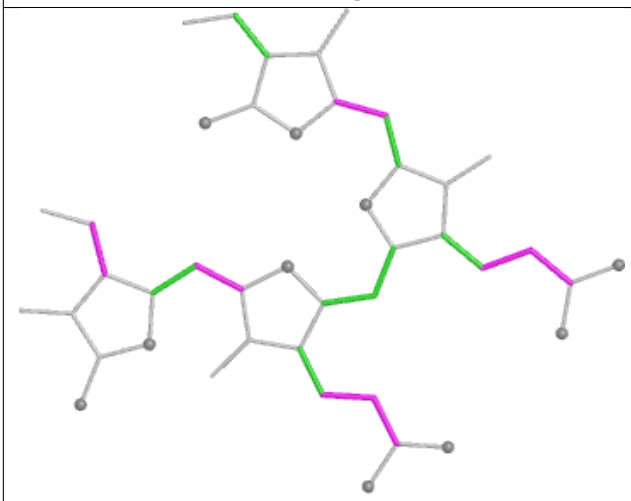
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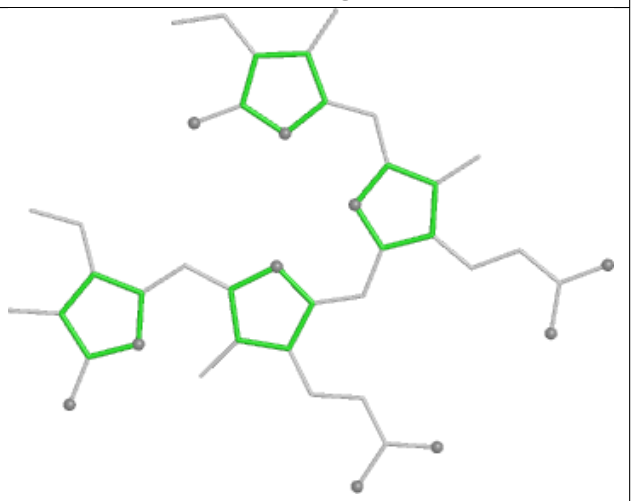
Bond lengths



Bond angles

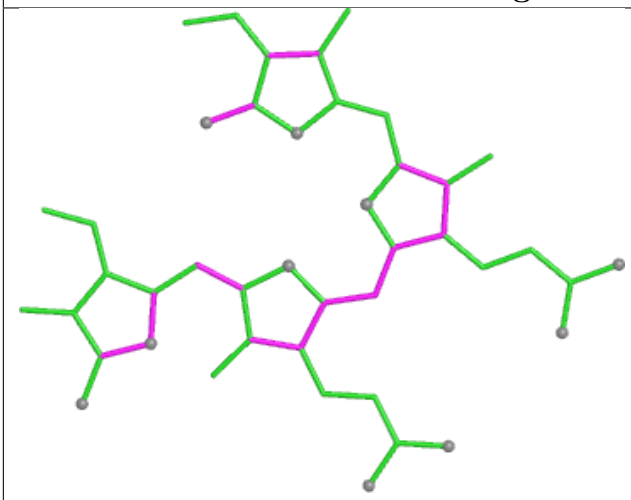


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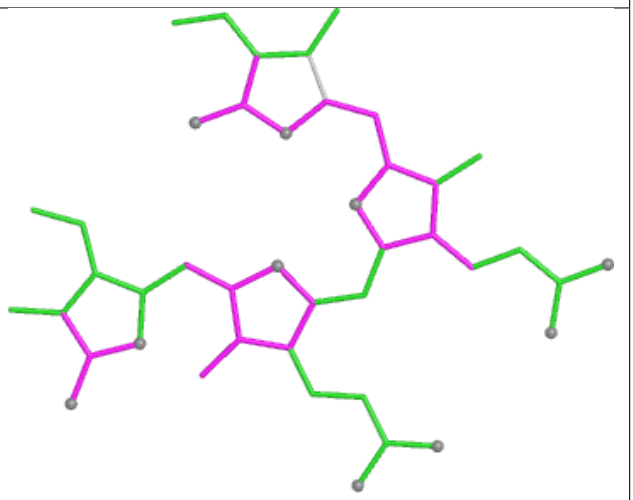


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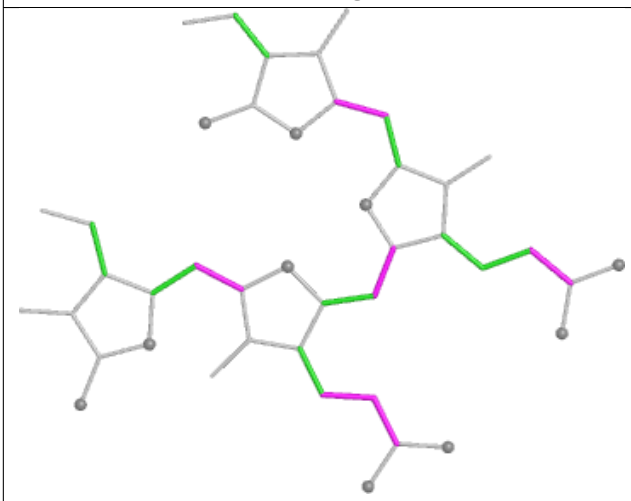
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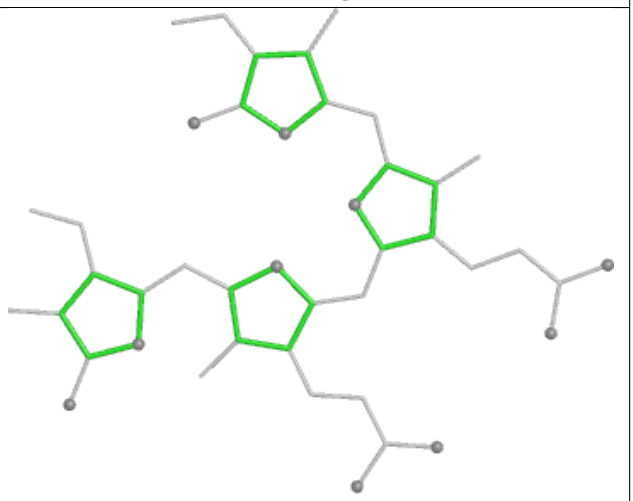
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Bond angles

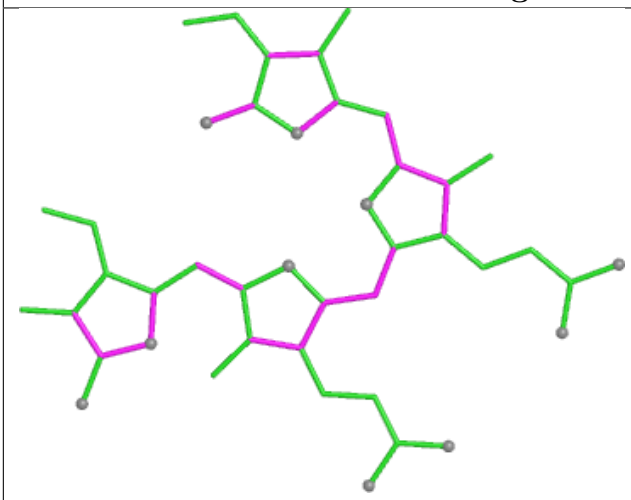


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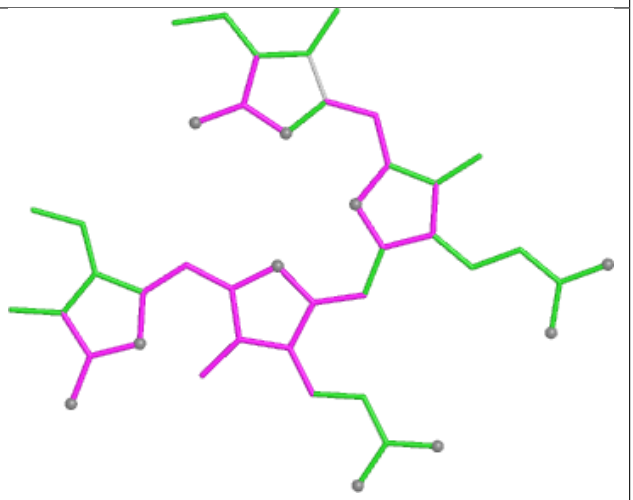


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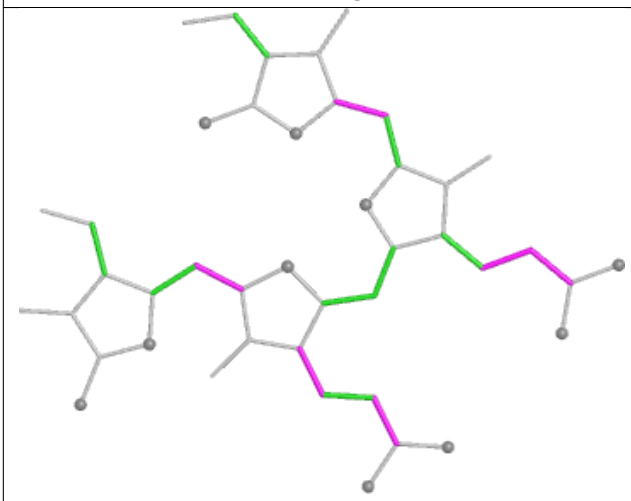
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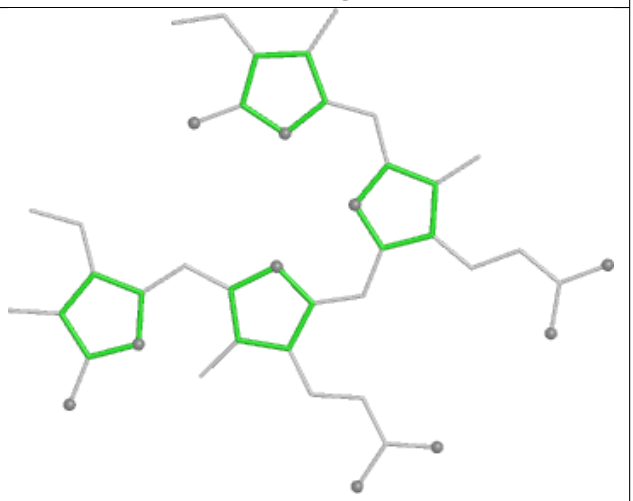
Bond lengths



Bond angles

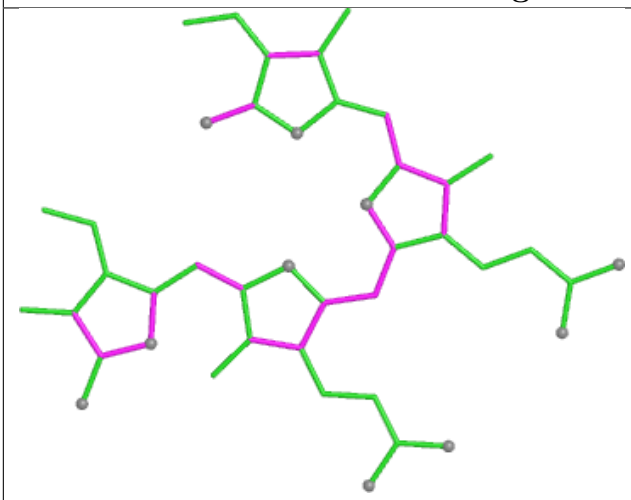


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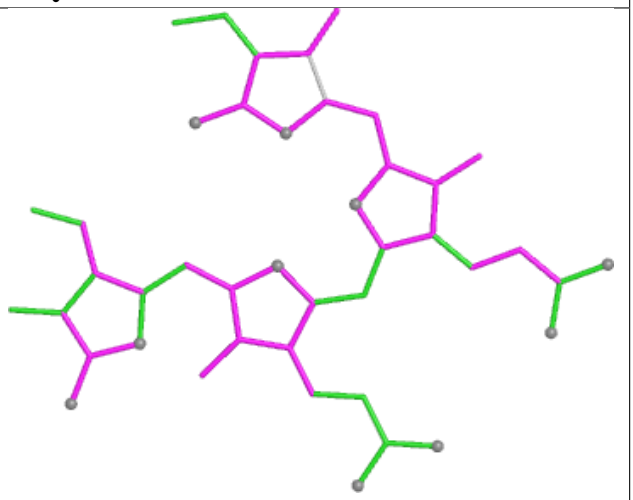


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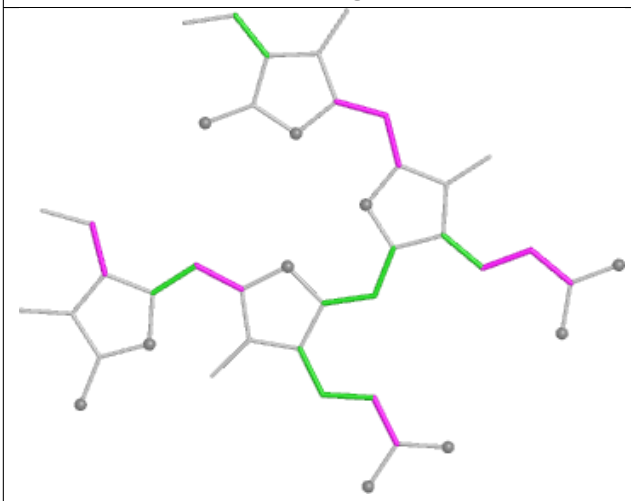
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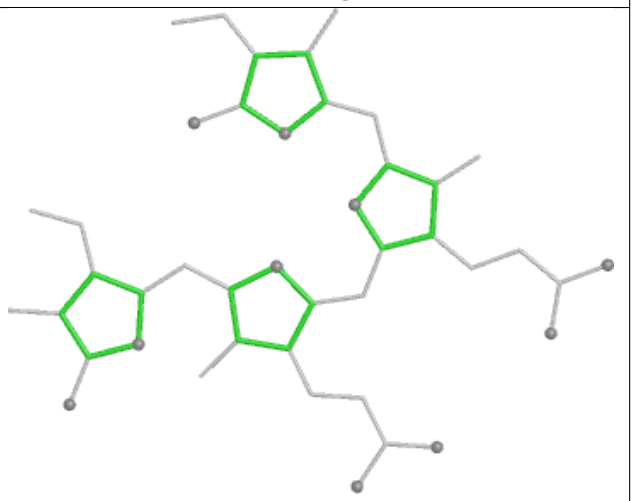
Bond lengths



Bond angles

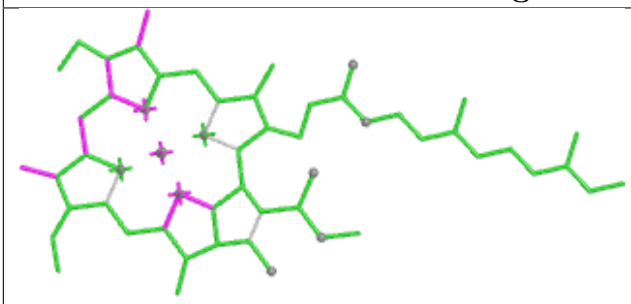


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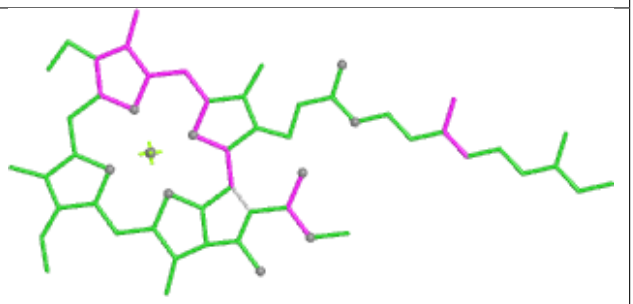


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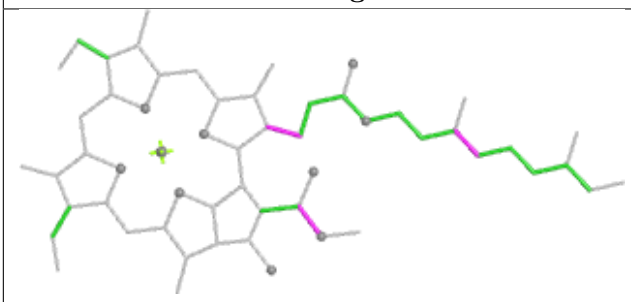
Ligand CLA LN 206



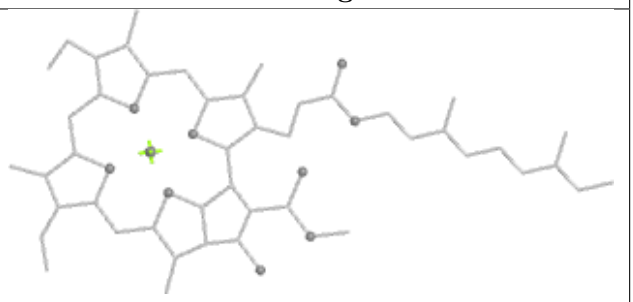
Bond lengths



Bond angles

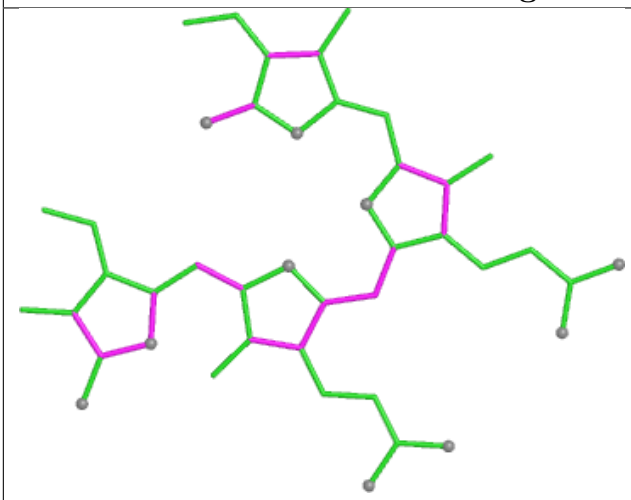


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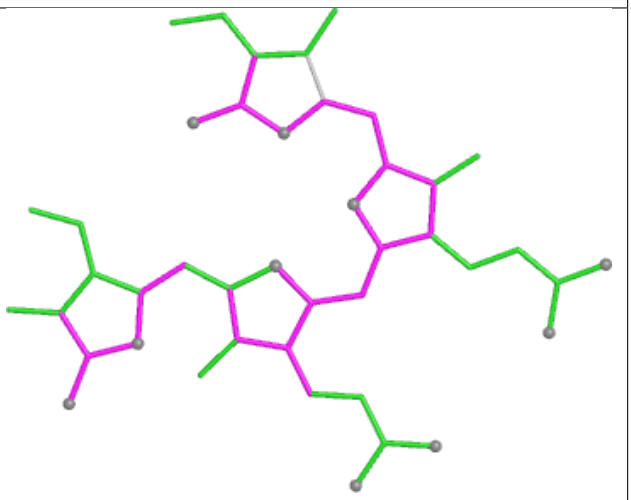


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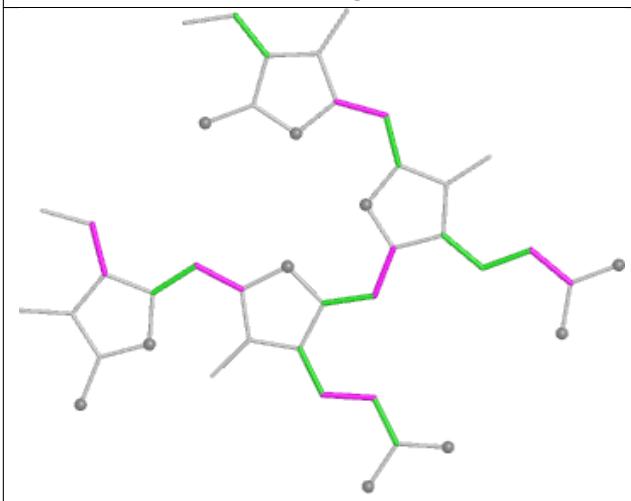
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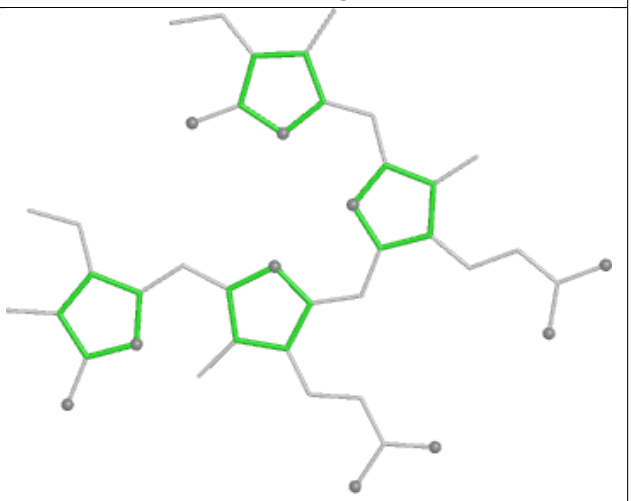
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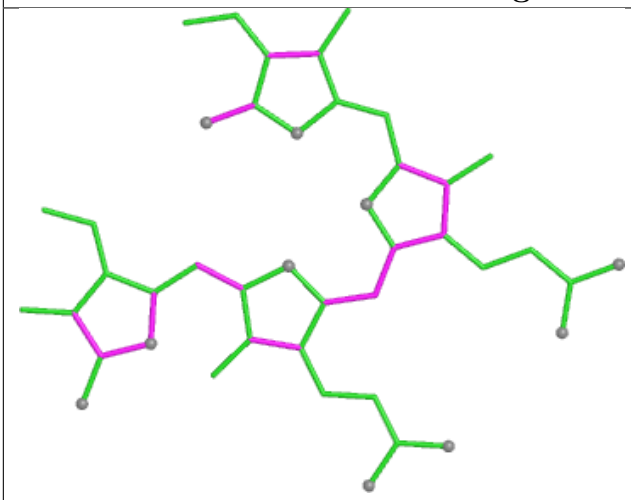


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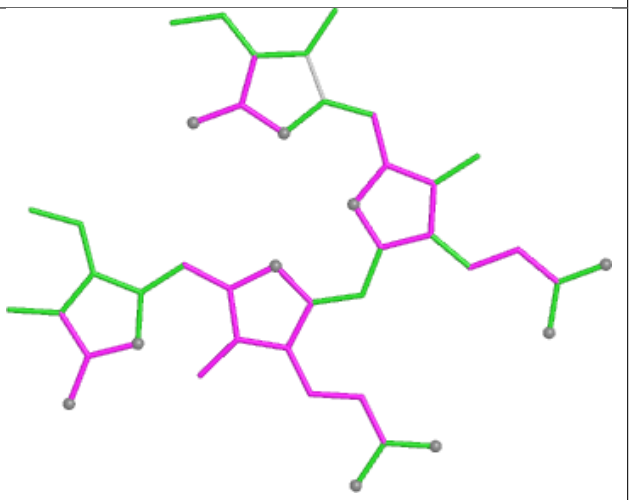


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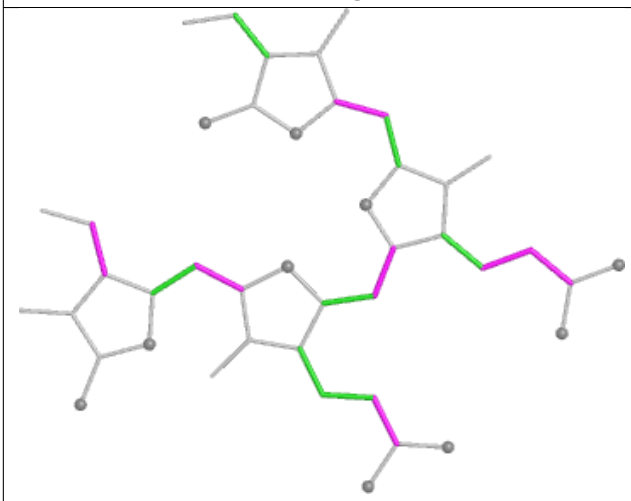
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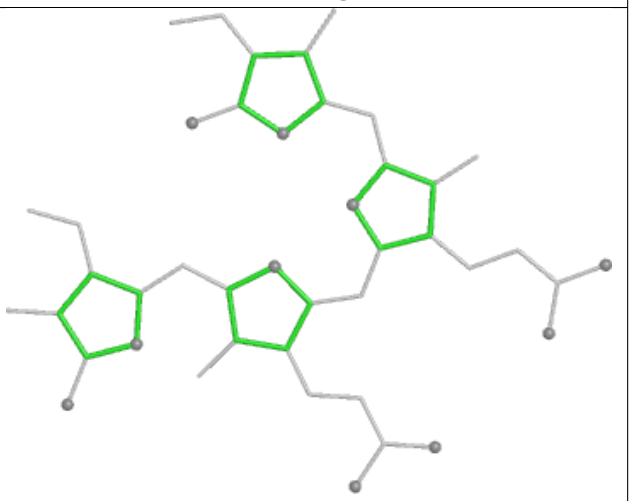
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Bond angles

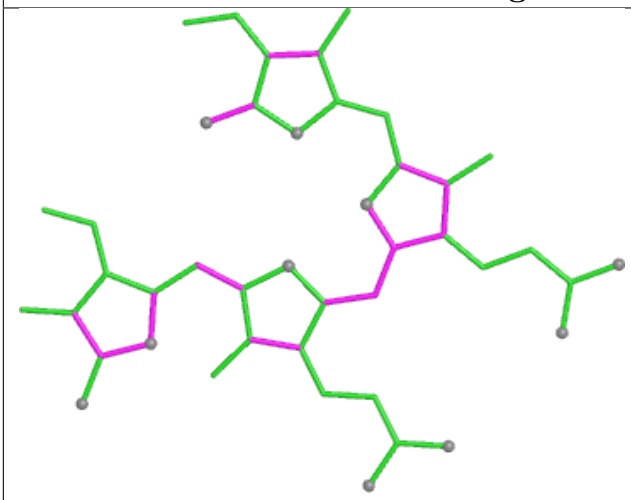


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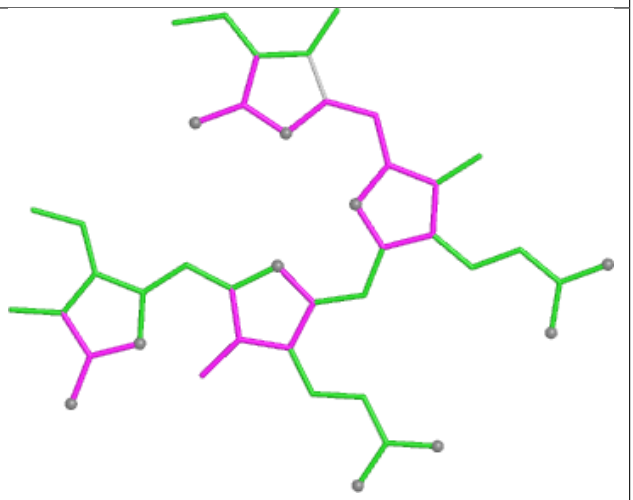


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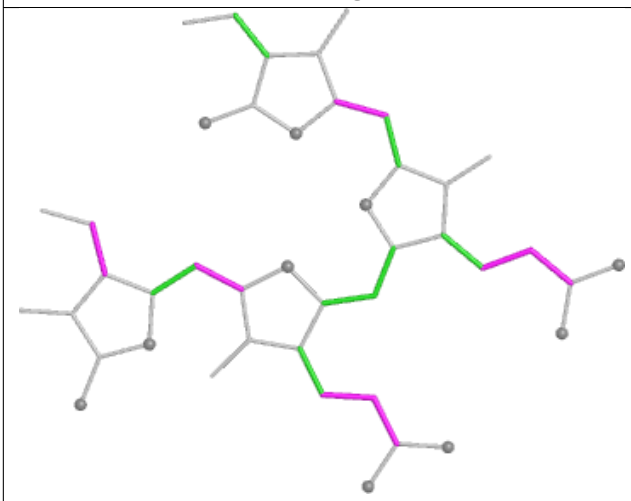
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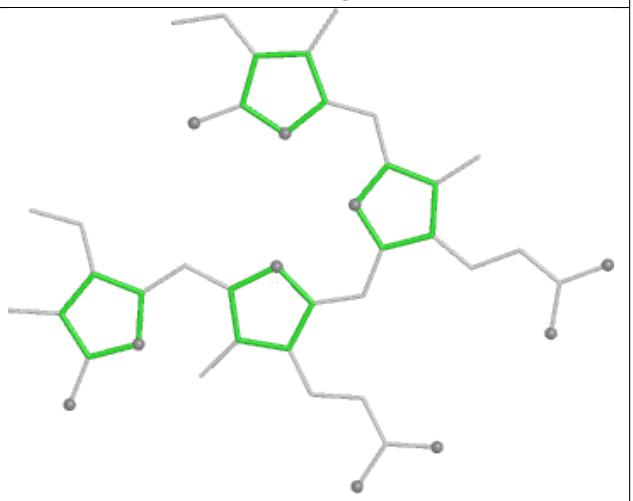
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Bond angles

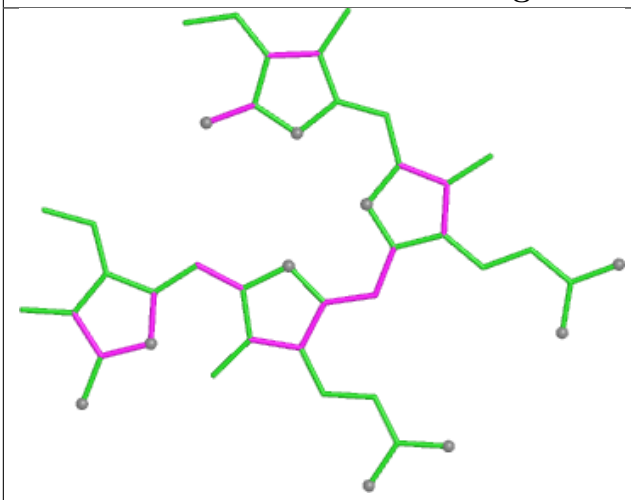


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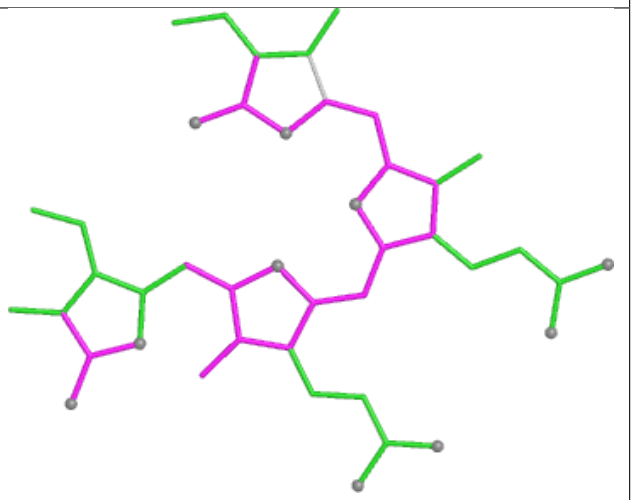


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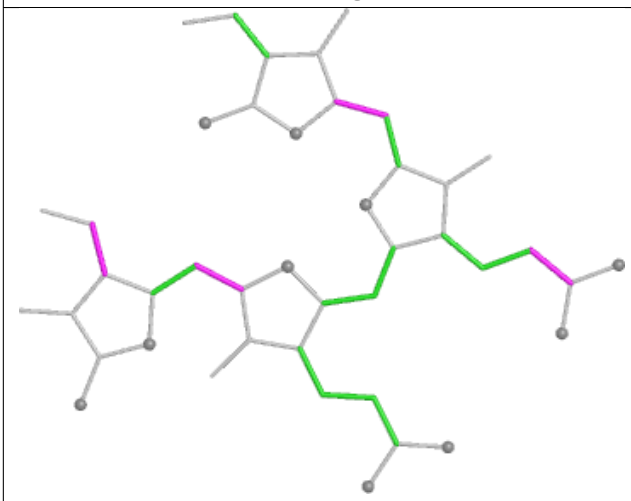
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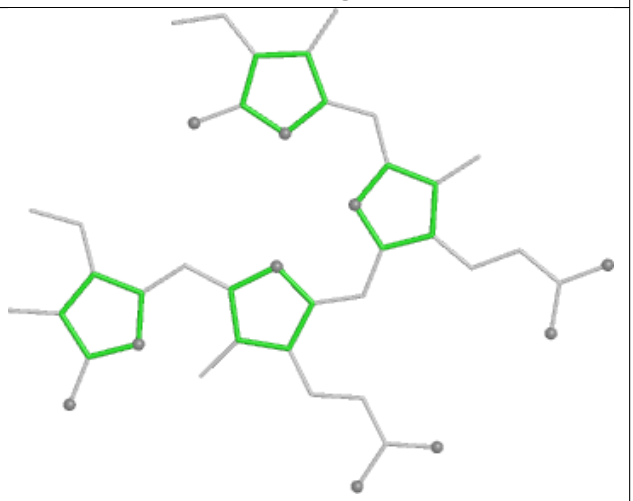
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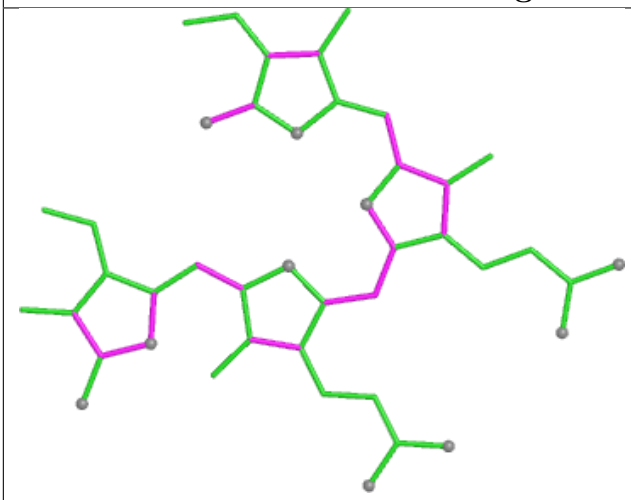


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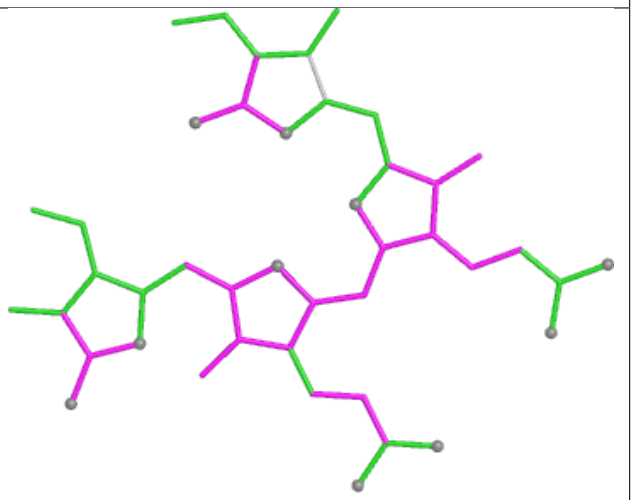


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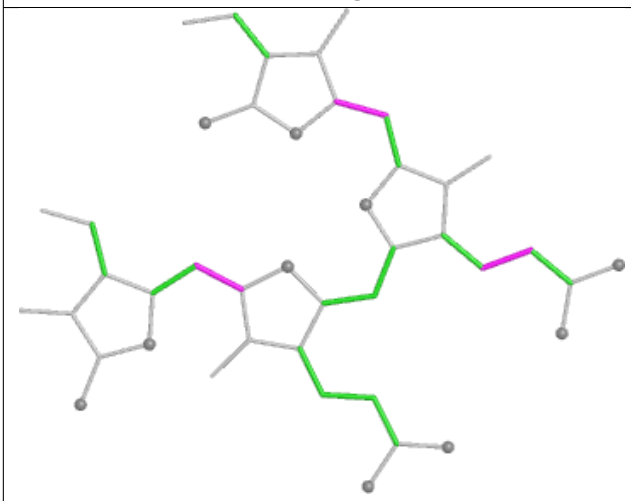
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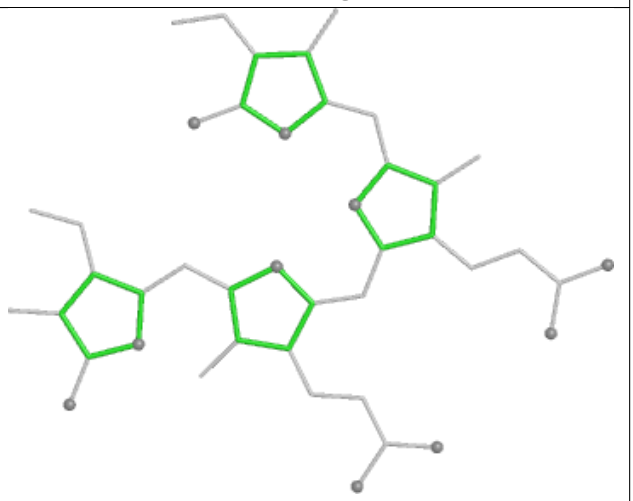
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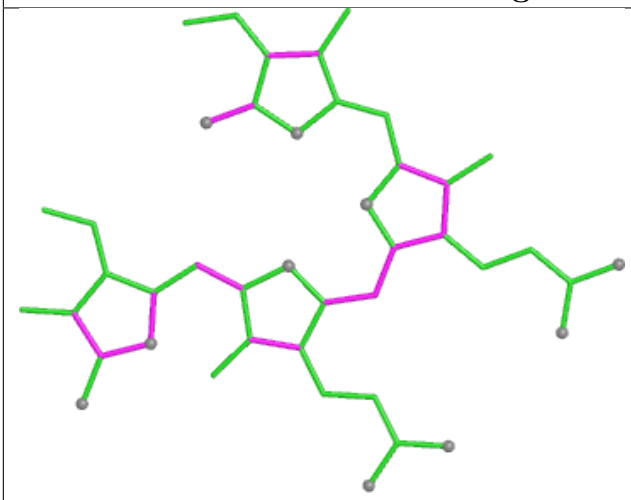


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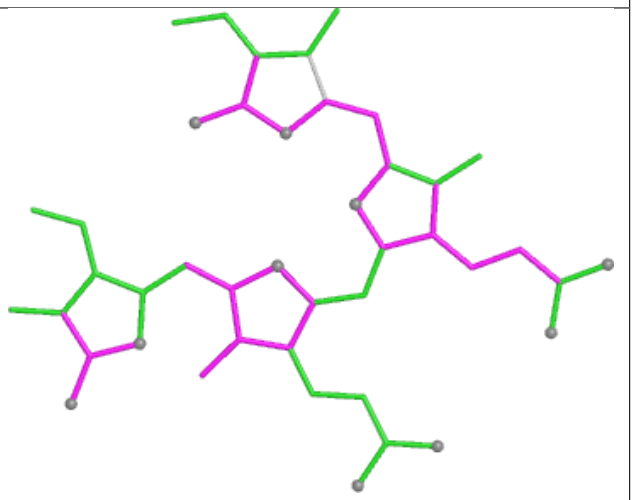


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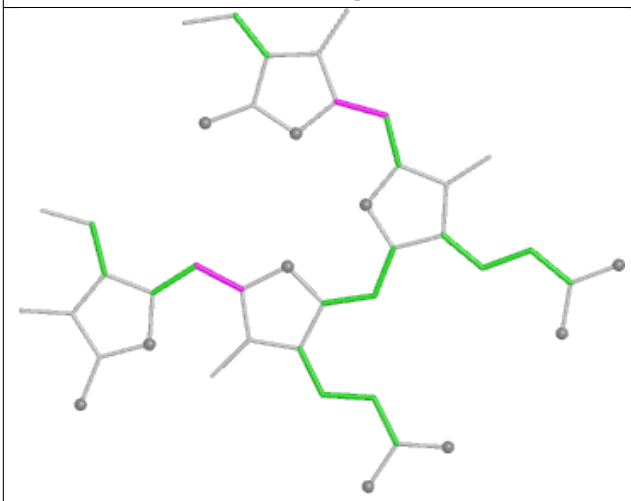
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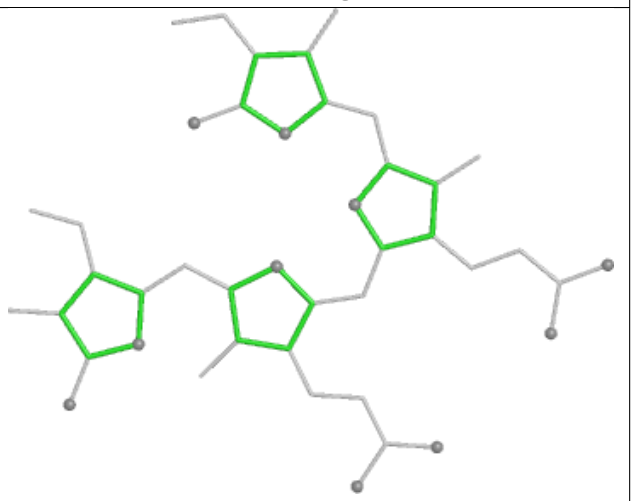
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Bond angles

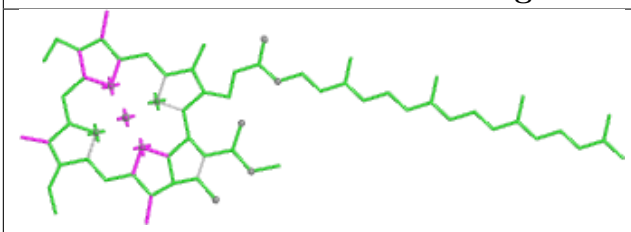


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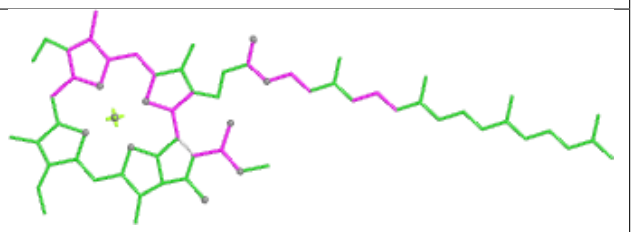


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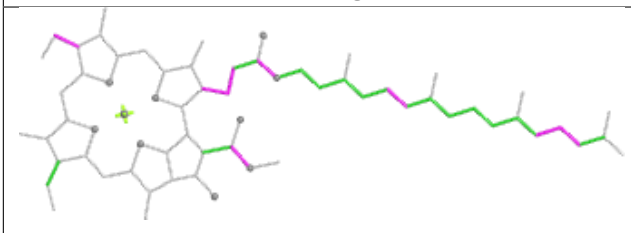
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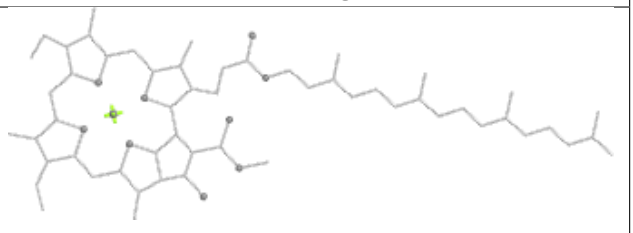
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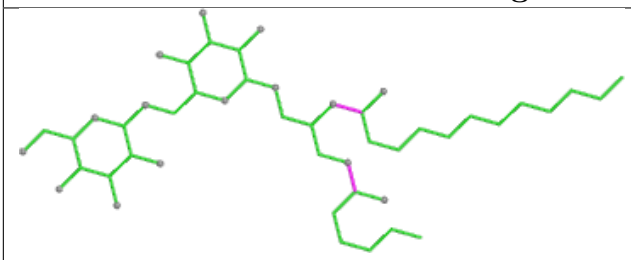


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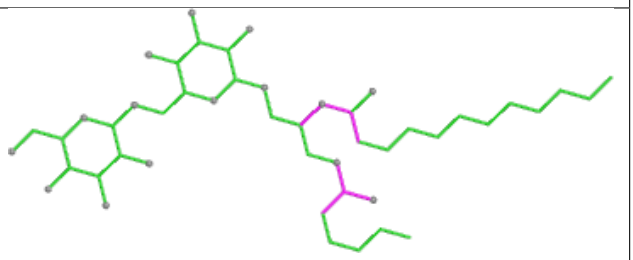


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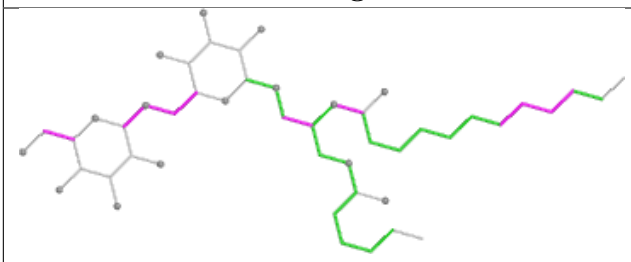
Ligand DGD C6 523



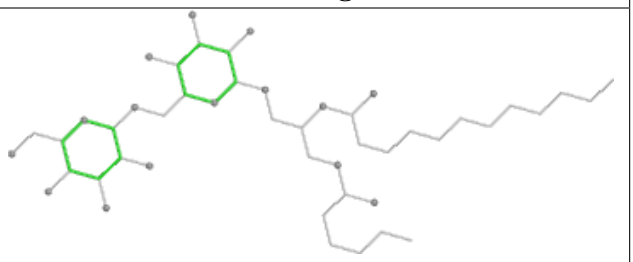
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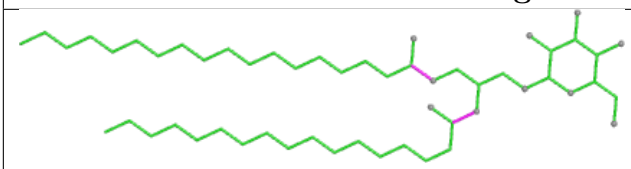


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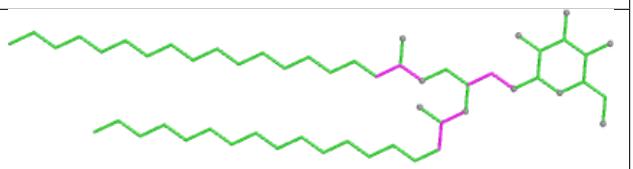


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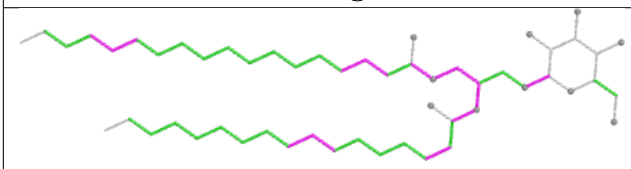
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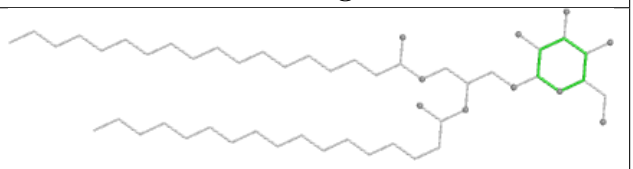
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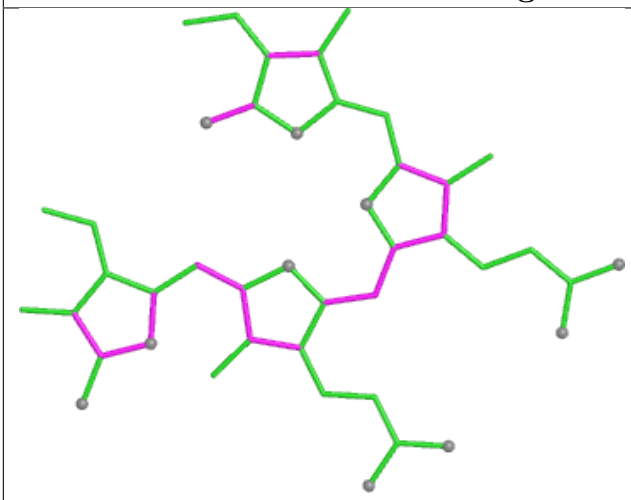


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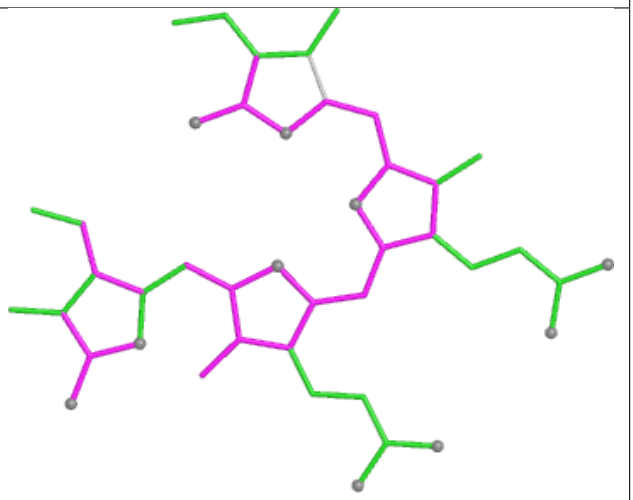


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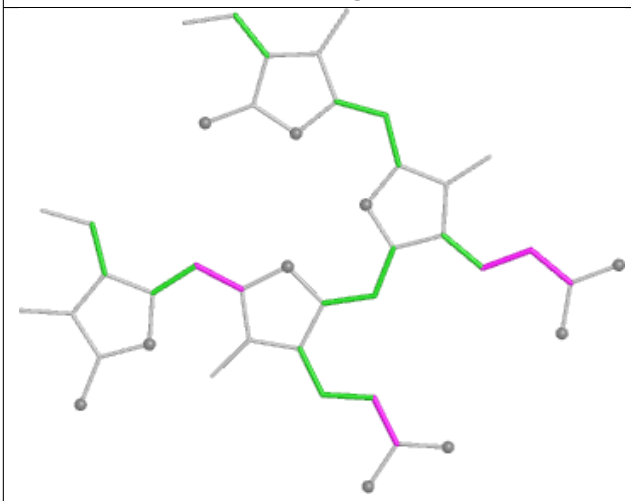
Ligand PEB Z1 203



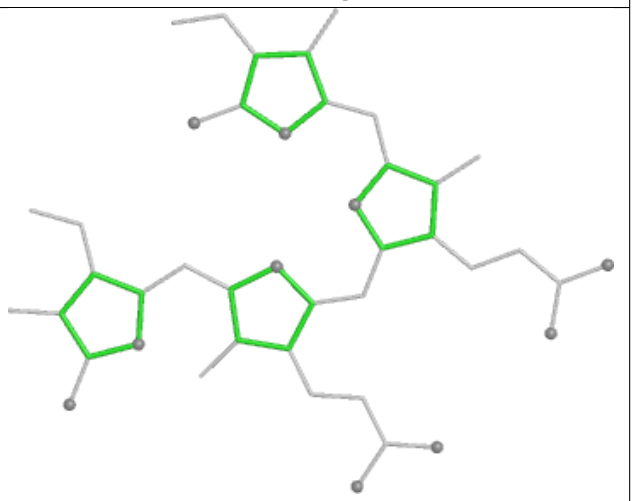
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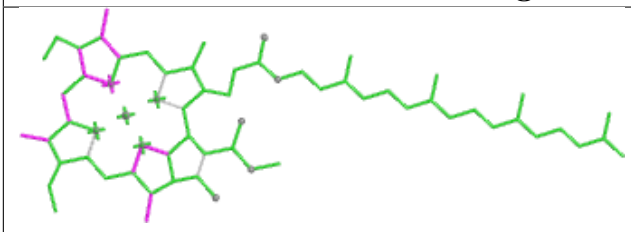


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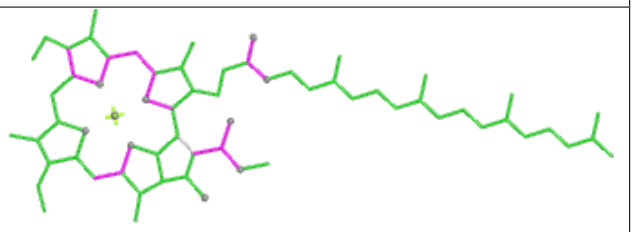


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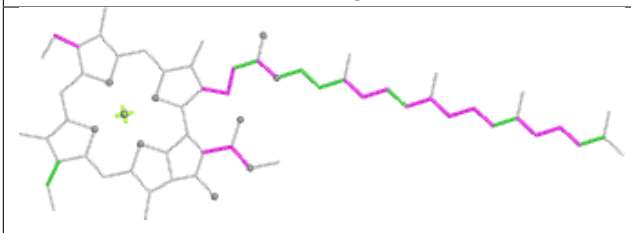
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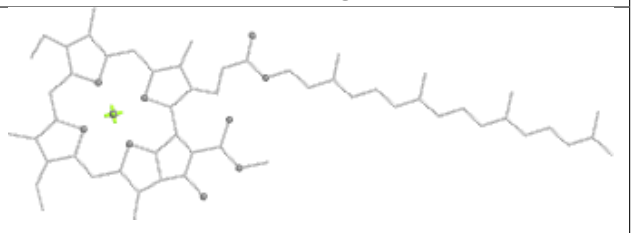
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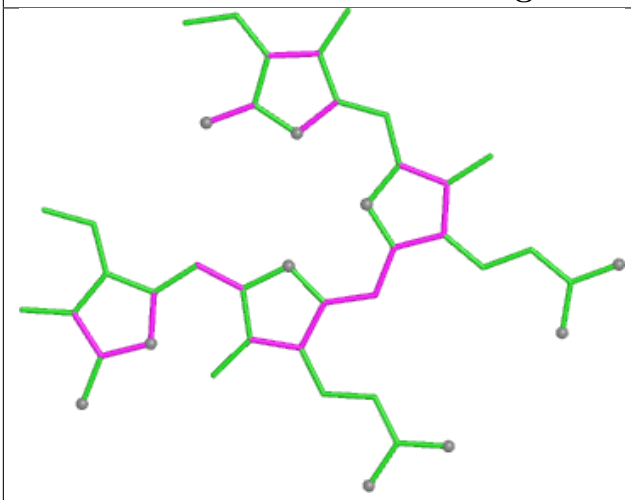


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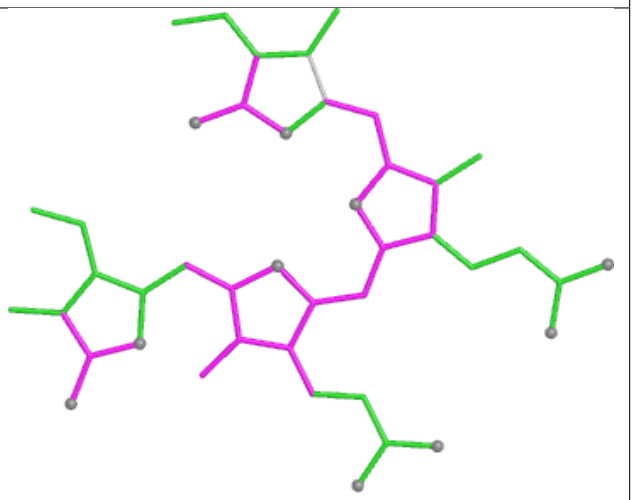


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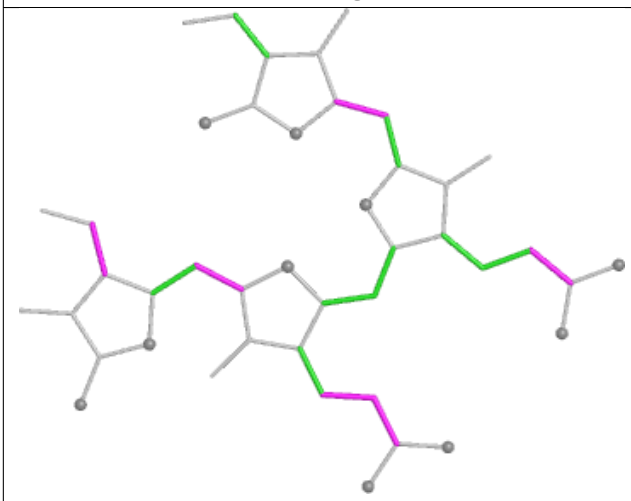
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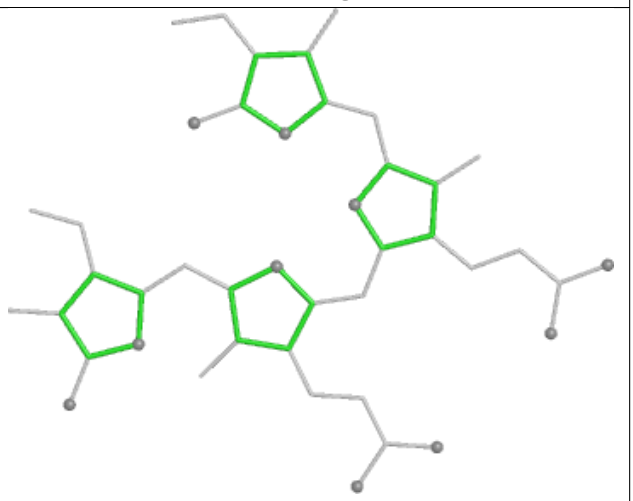
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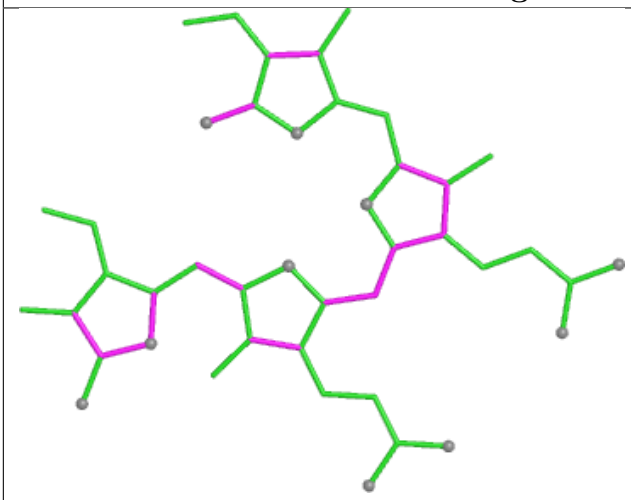


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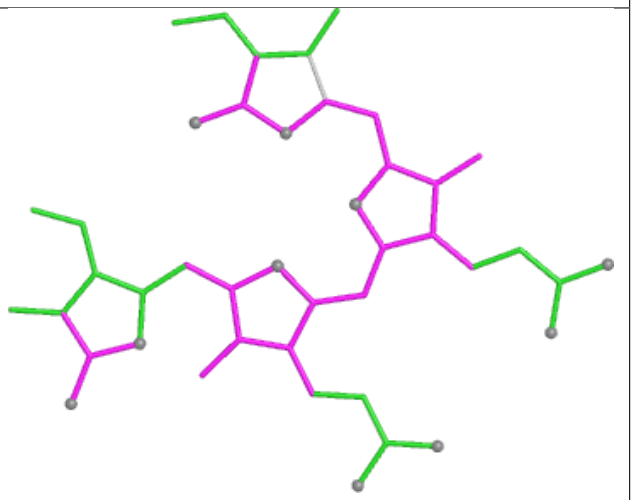


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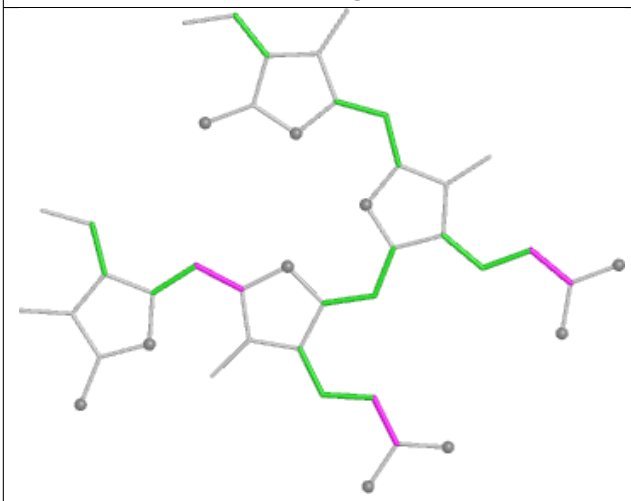
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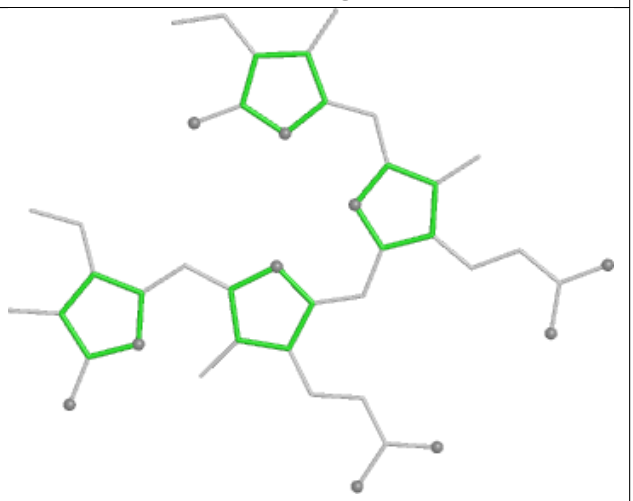
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Bond angles

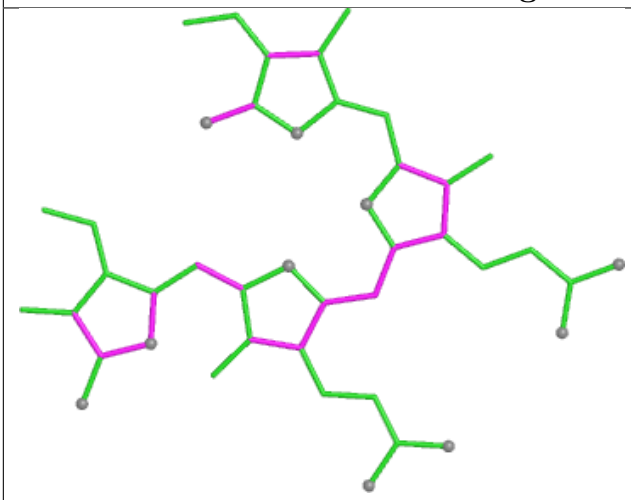


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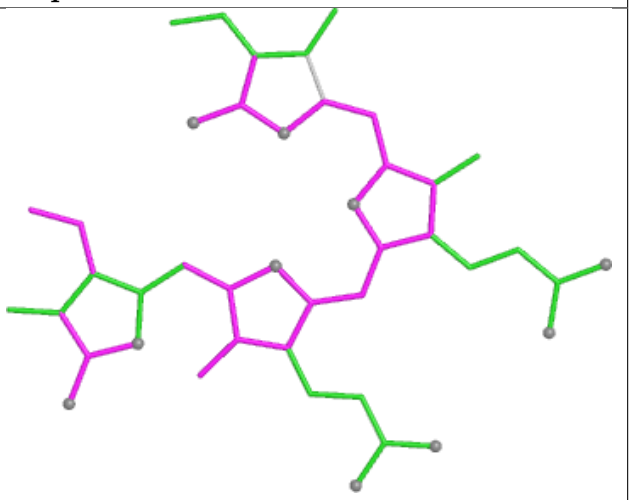


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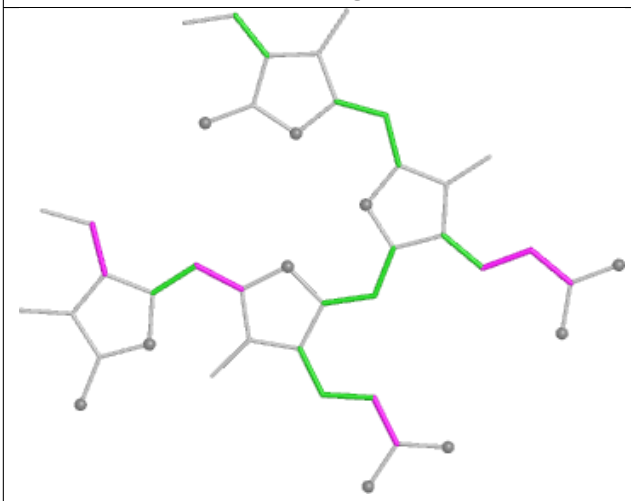
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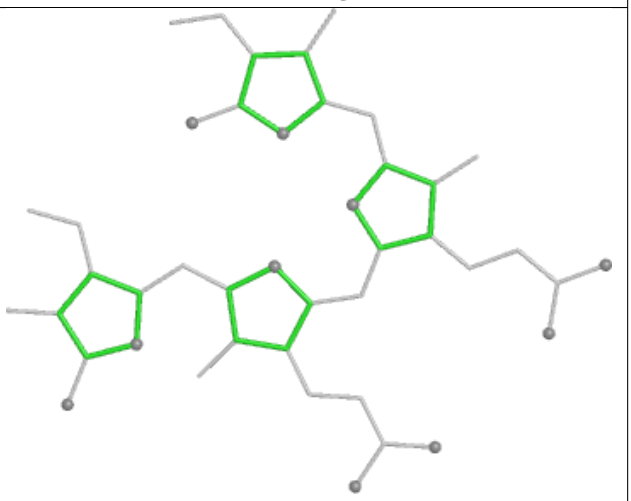
Bond lengths



Bond angles

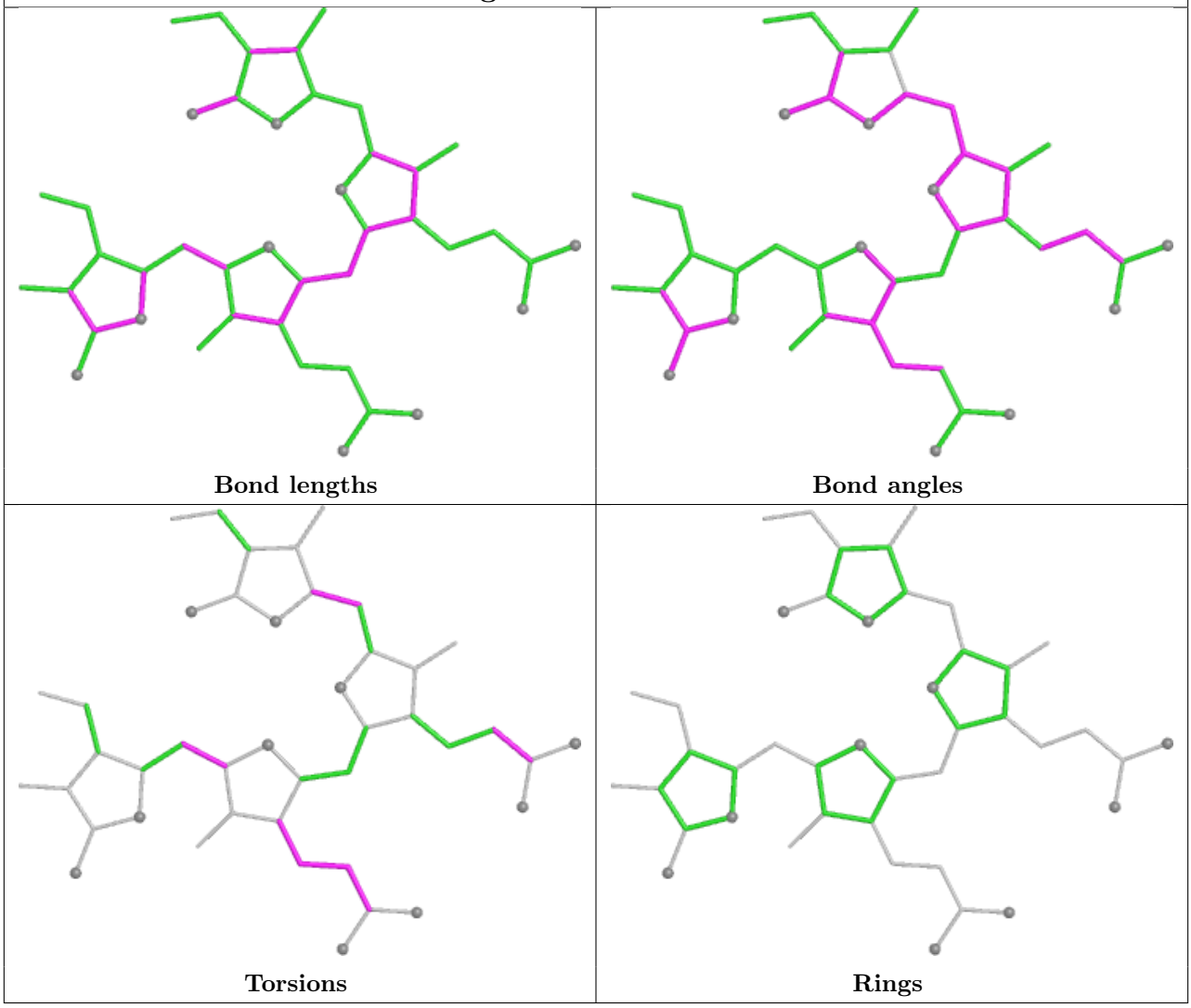


Torsions

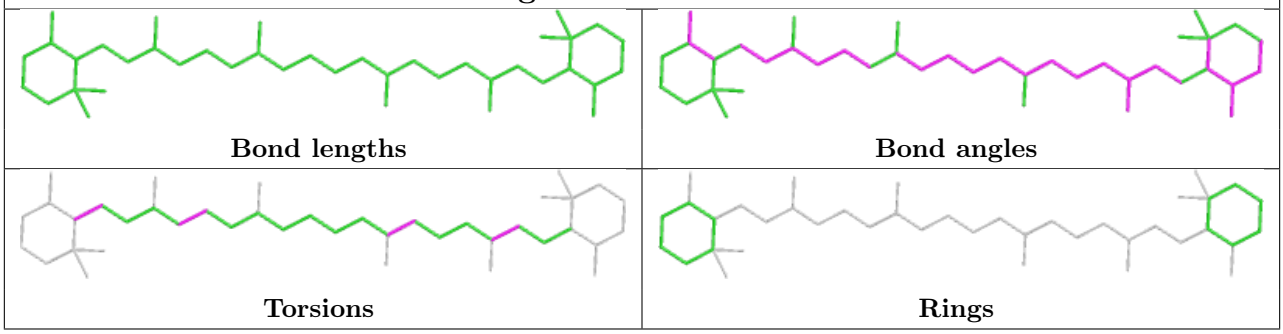


Rings

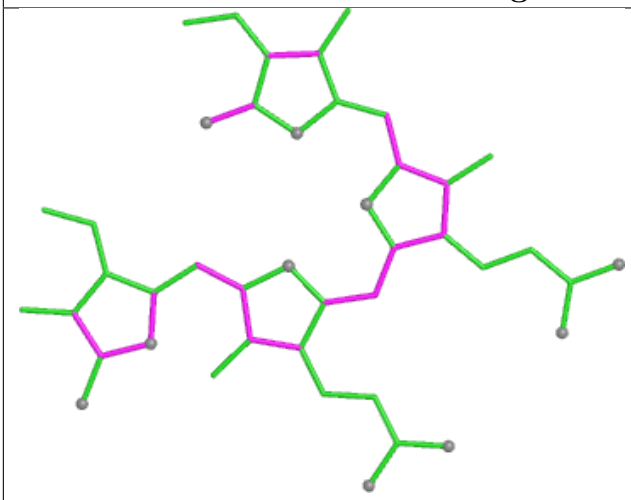
Ligand PEB cO 203



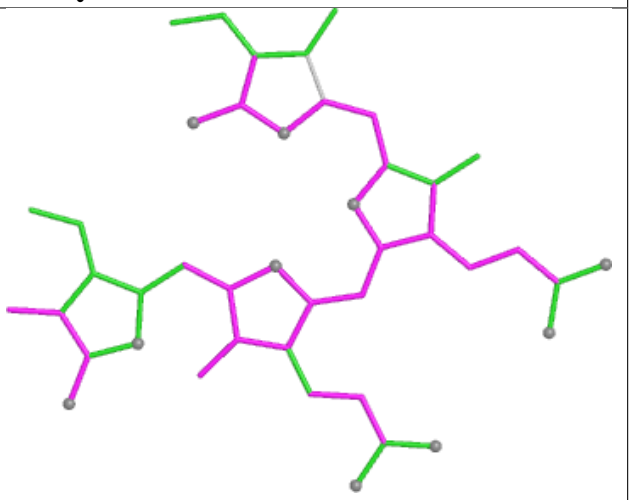
Ligand BCR J2 102



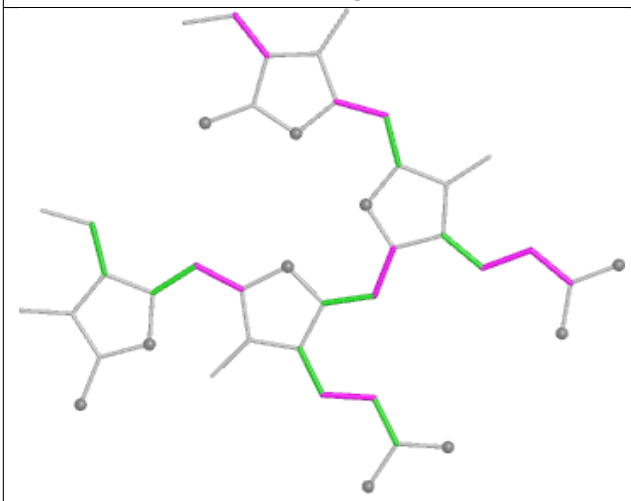
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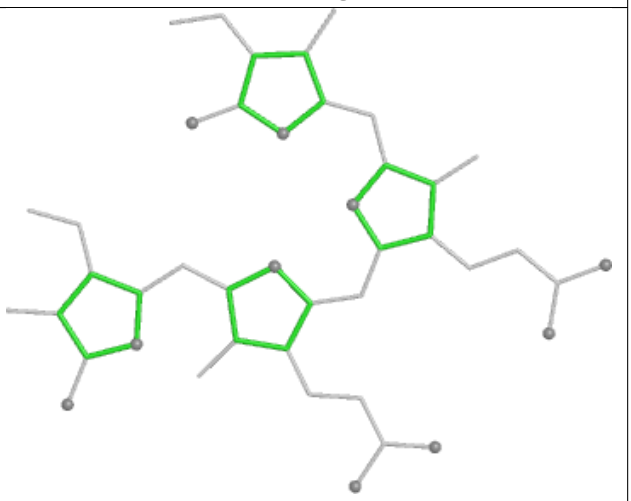
Bond lengths



Bond angles

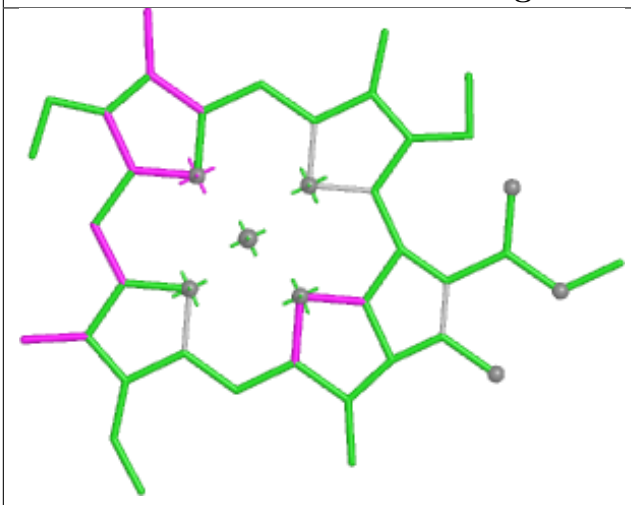


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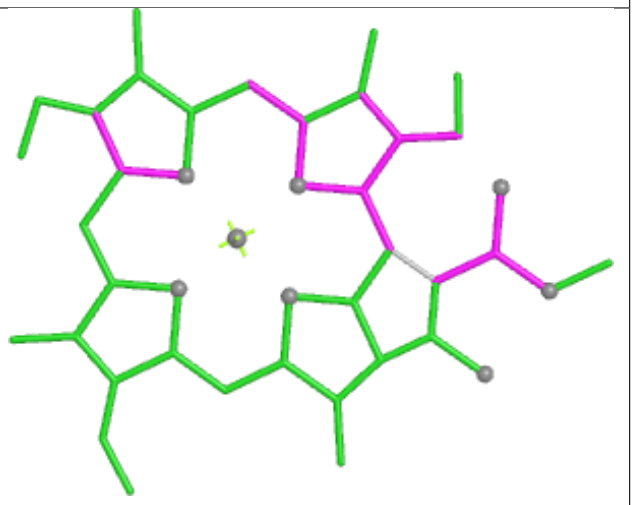


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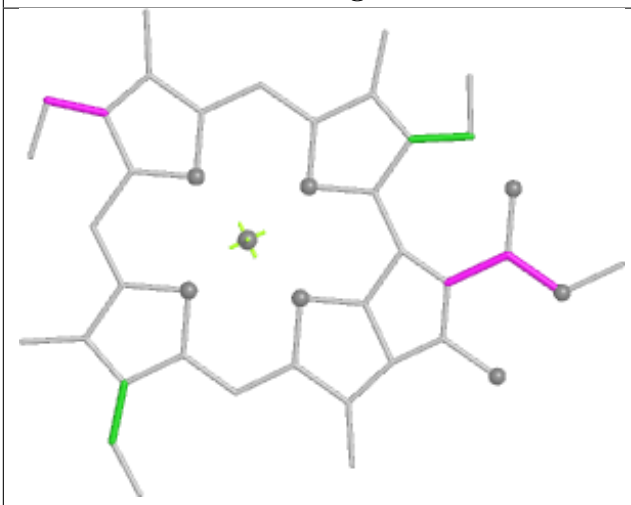
Ligand CLA 6N 610



Bond lengths



Bond angles

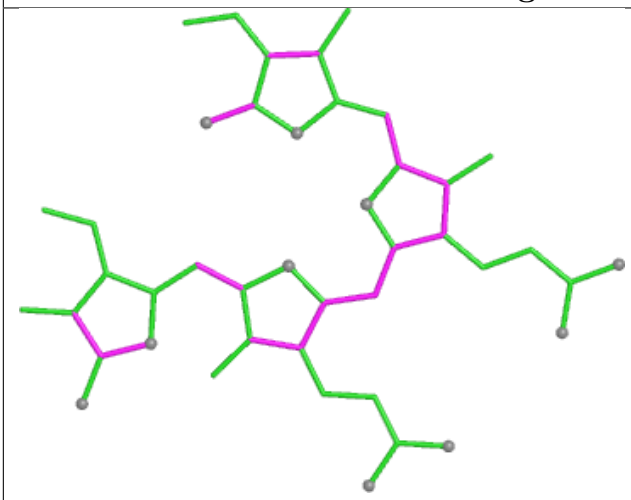


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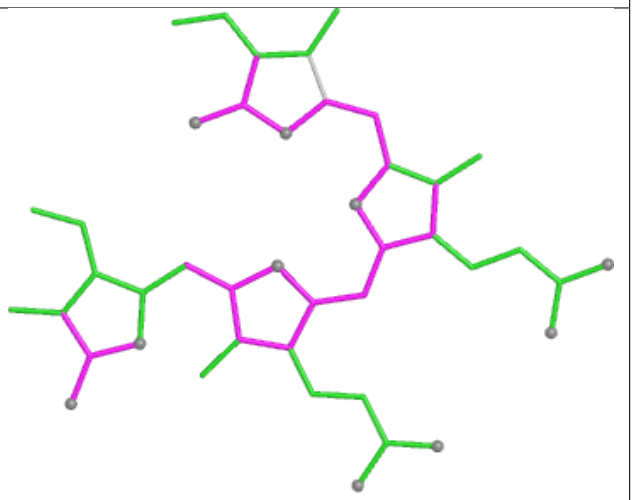


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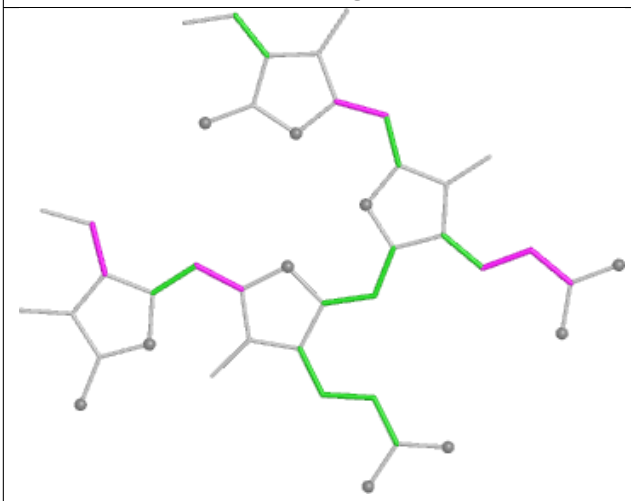
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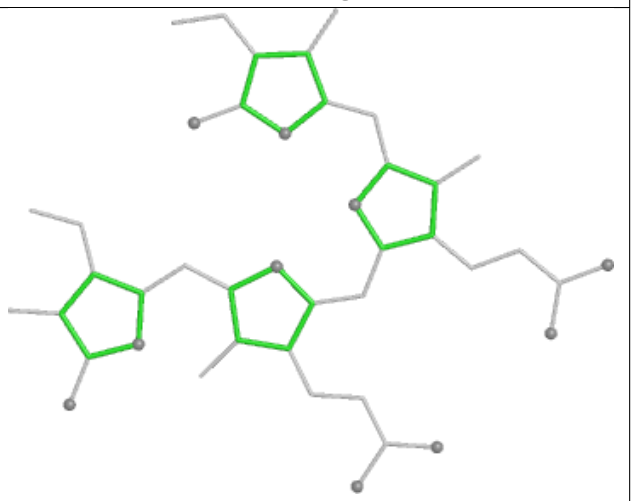
Bond lengths



Bond angles

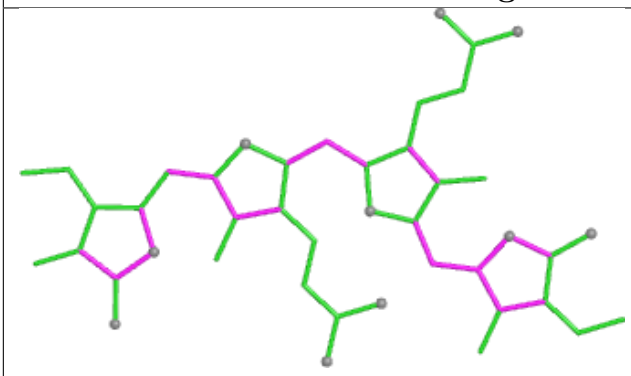


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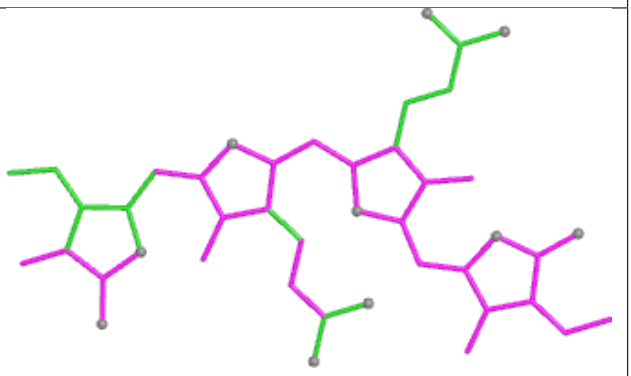


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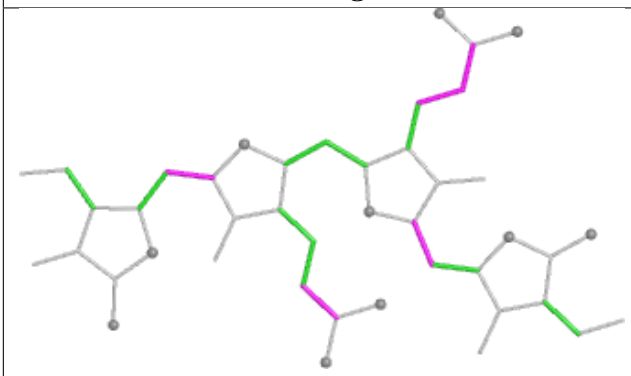
Ligand CYC HG 1001



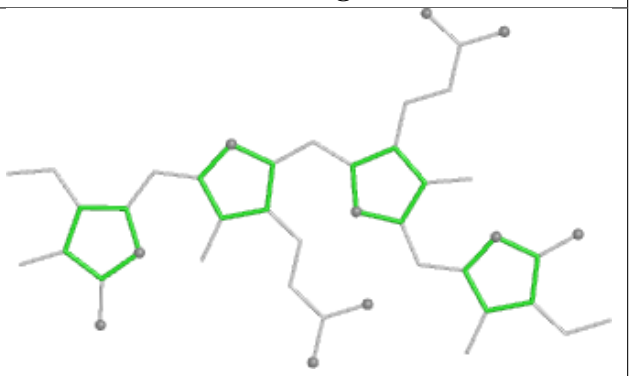
Bond lengths



Bond angles

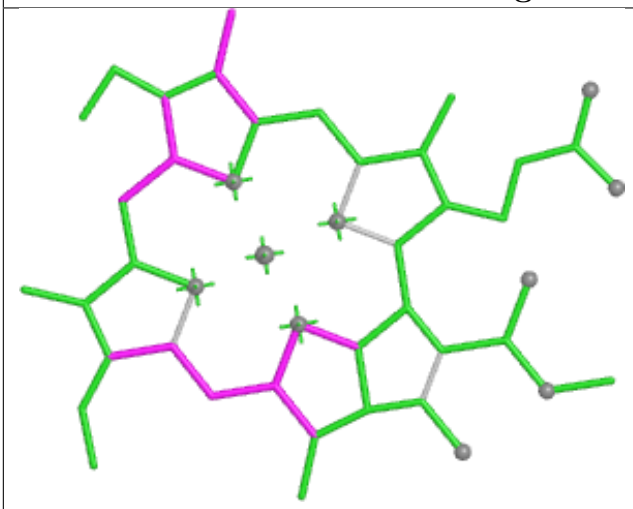


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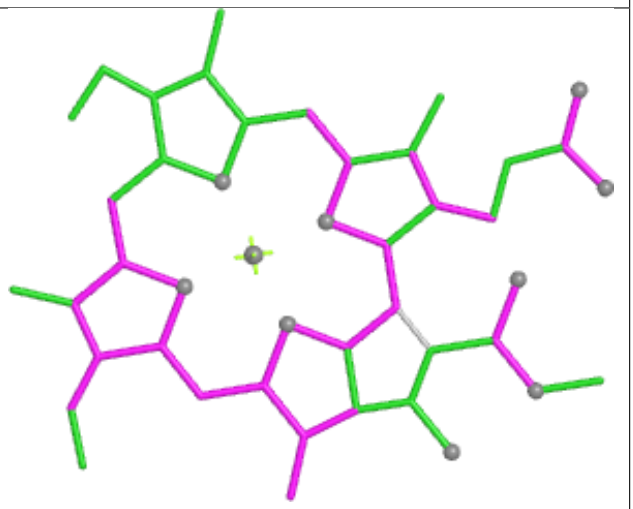


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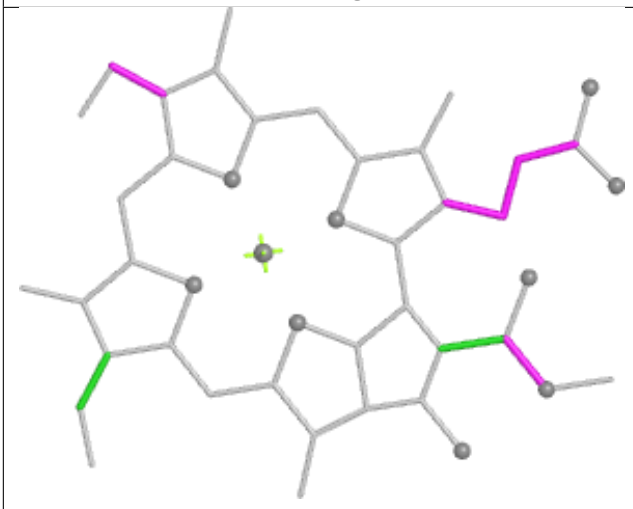
Ligand CLA A2 852



Bond lengths



Bond angles

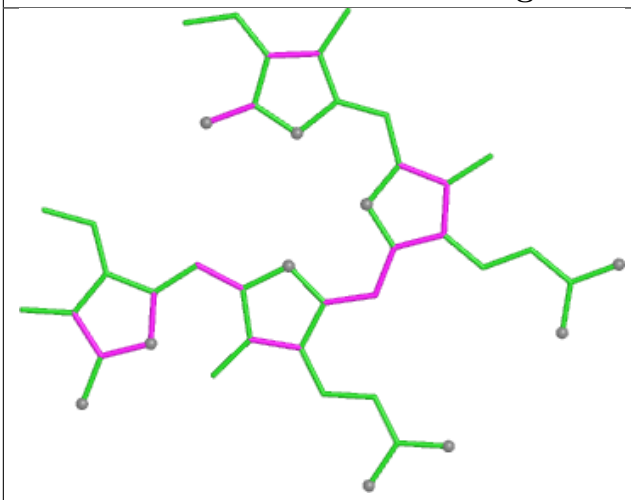


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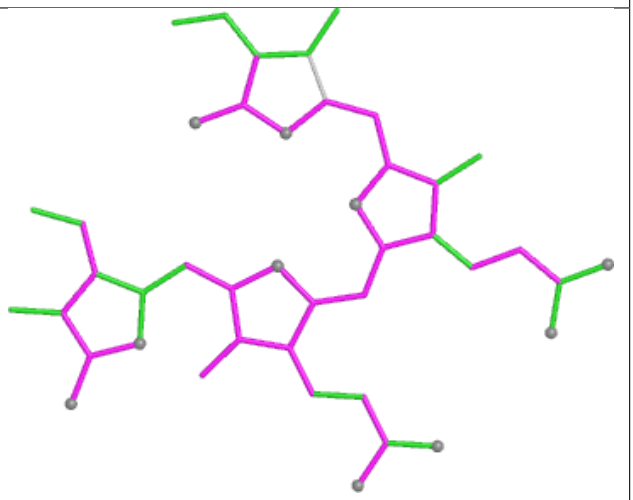


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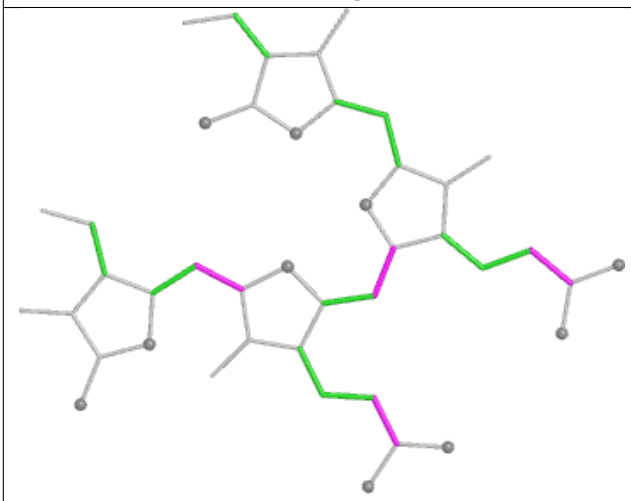
Ligand PEB PJ 202



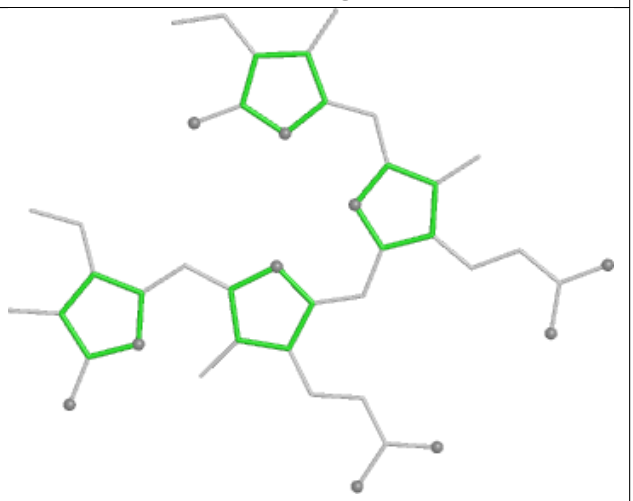
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Bond angles

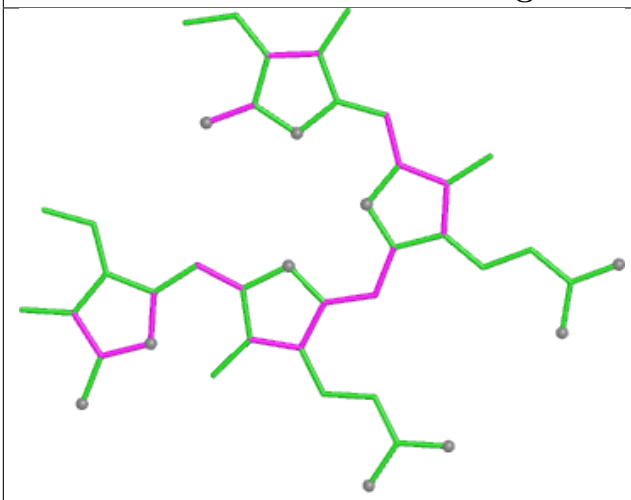


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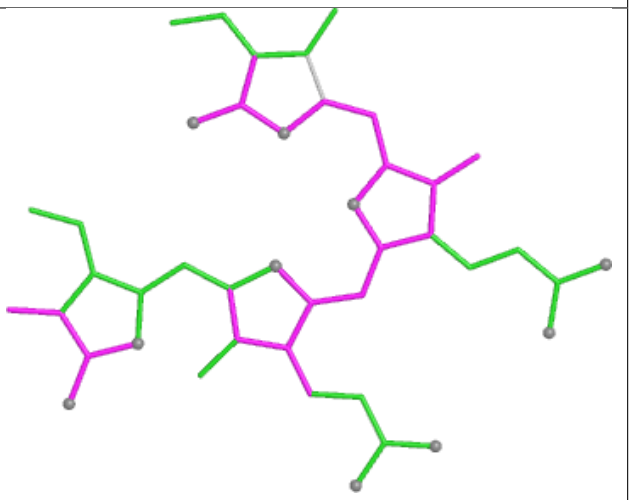


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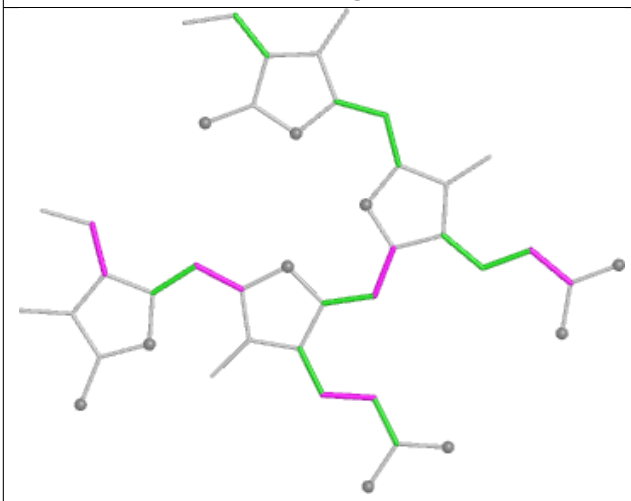
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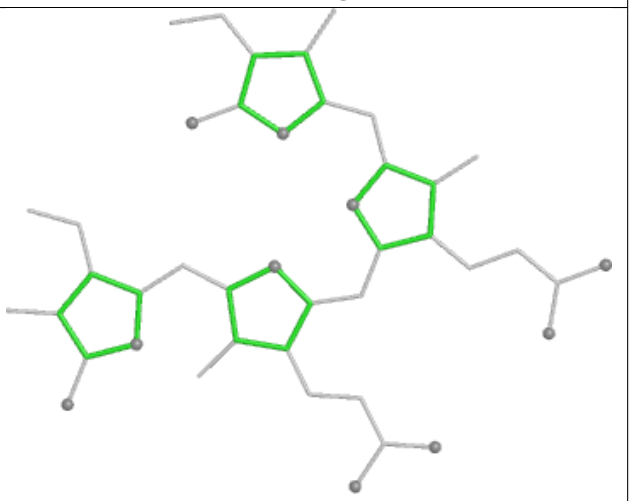
Bond lengths



Bond angles

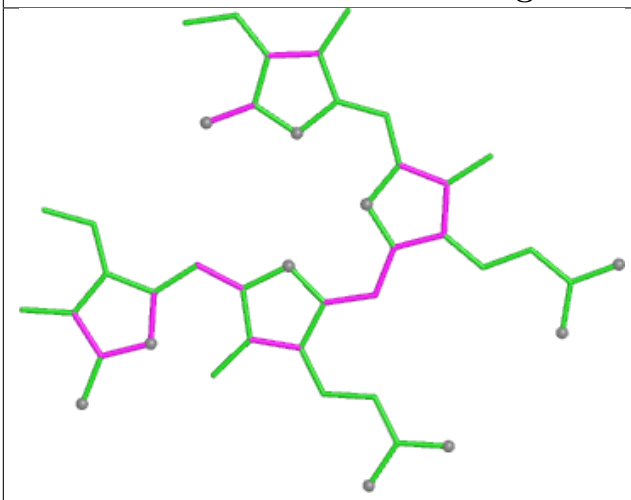


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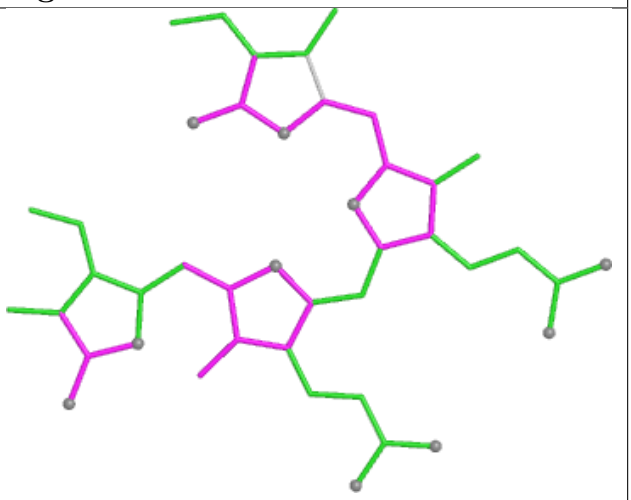


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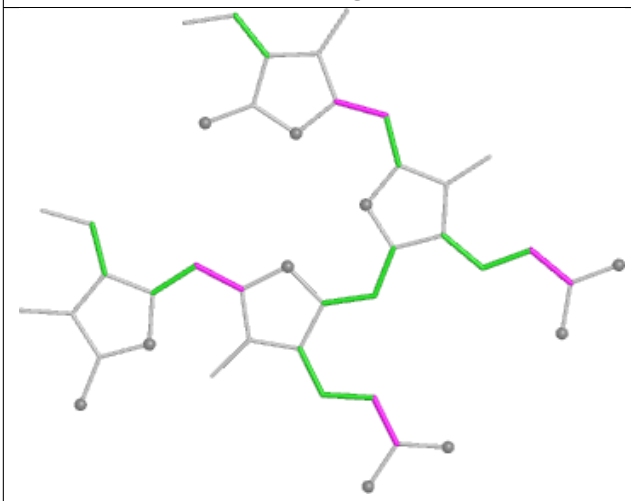
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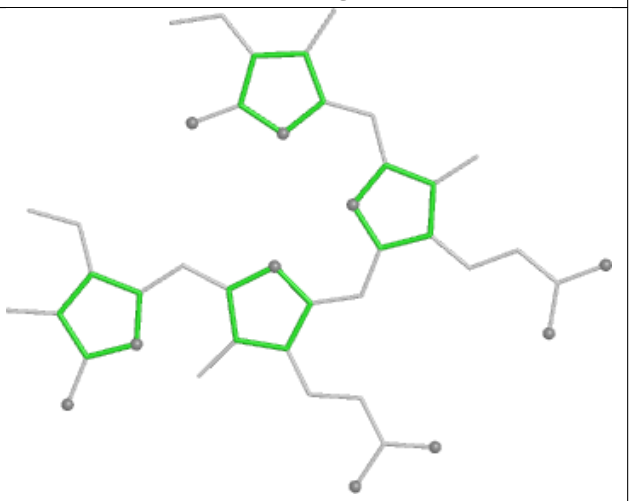
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Bond angles

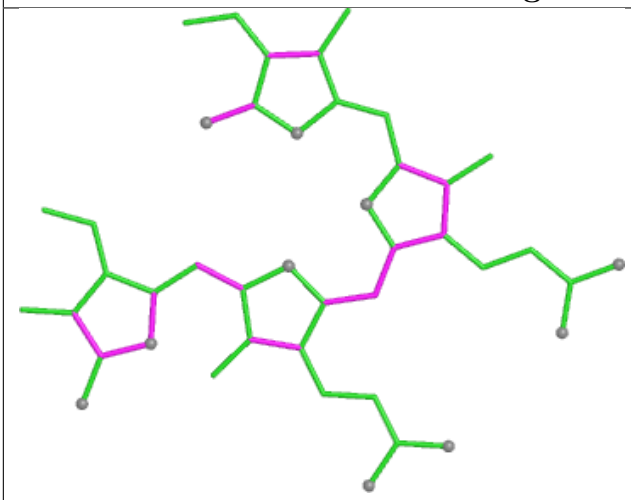


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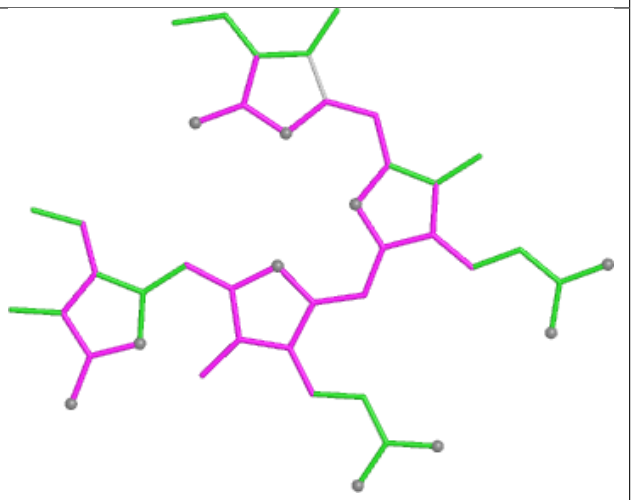


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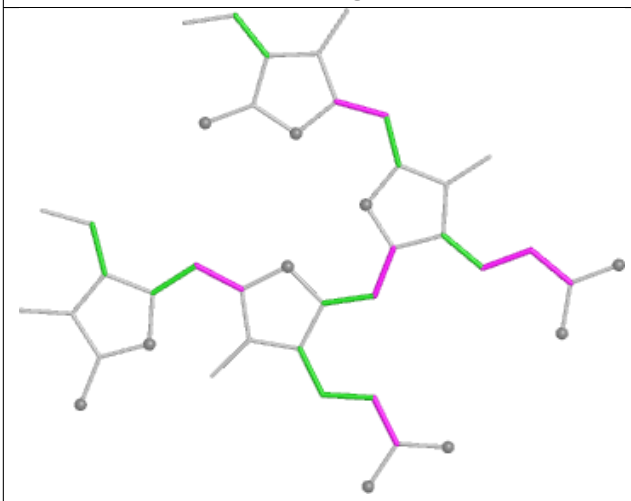
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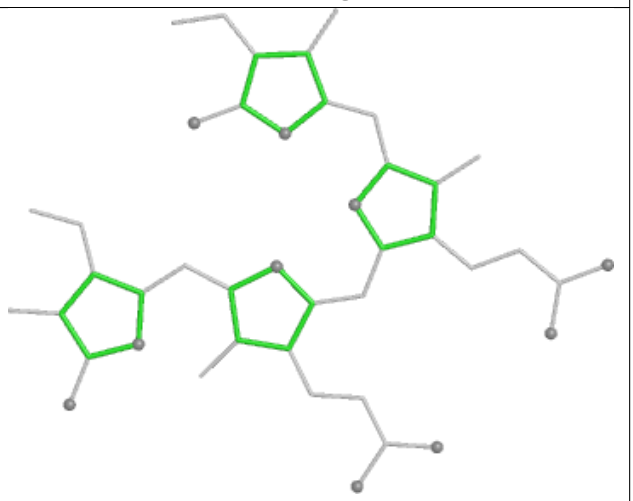
Bond lengths



Bond angles

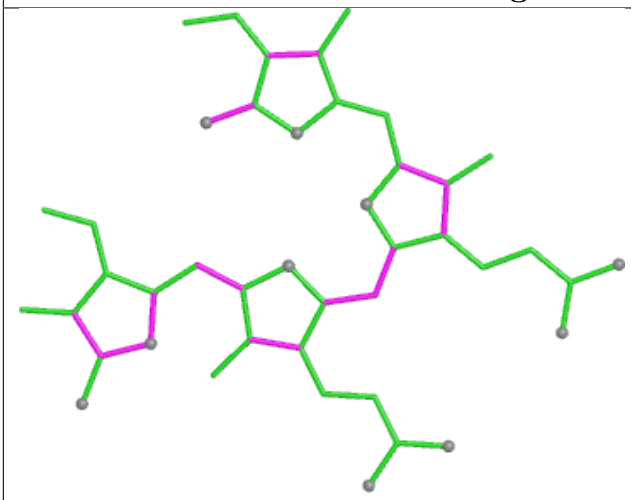


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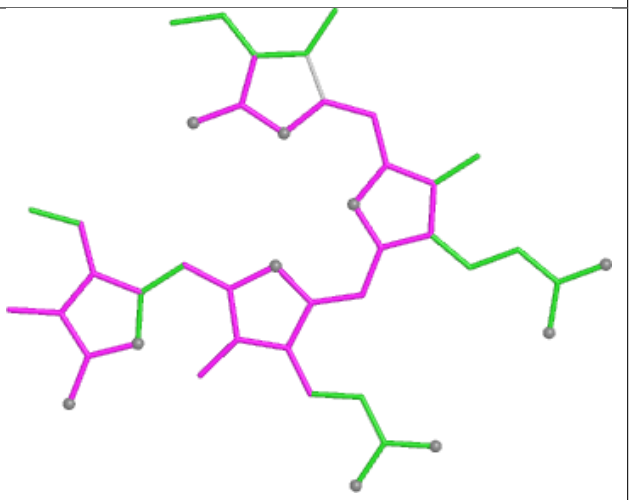


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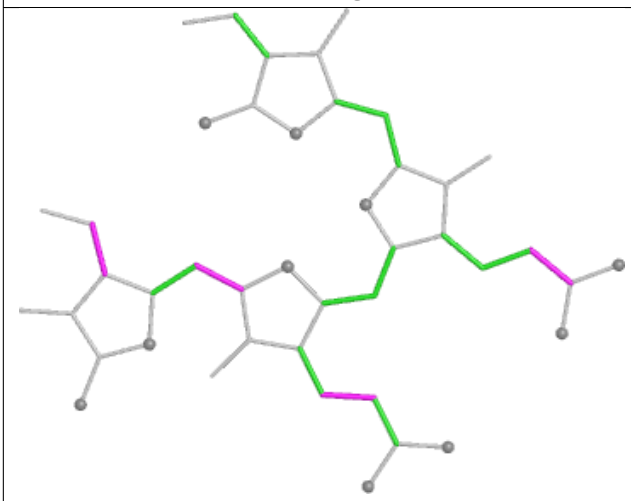
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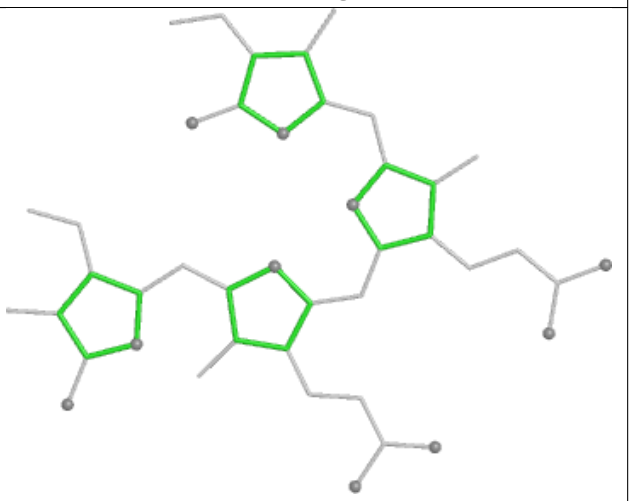
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Bond angles

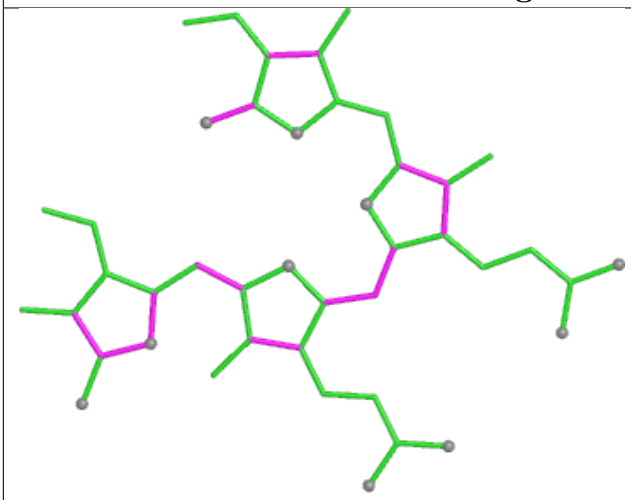


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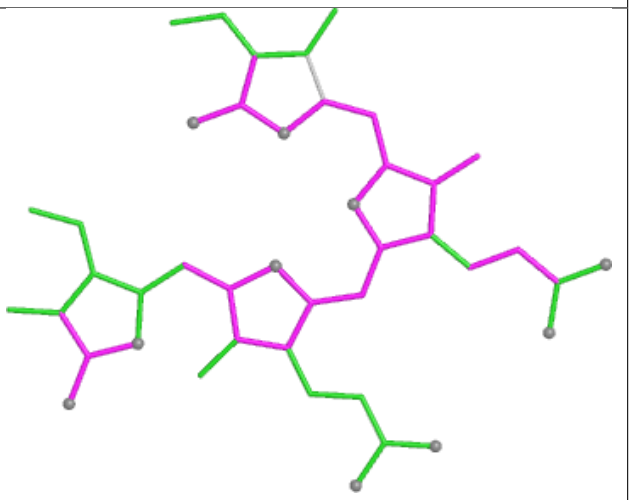


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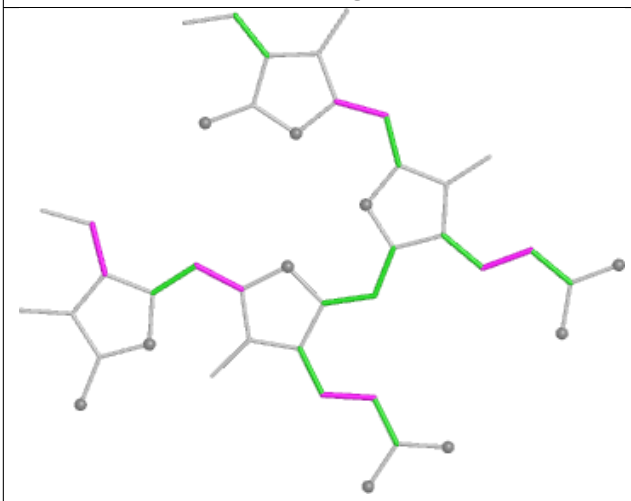
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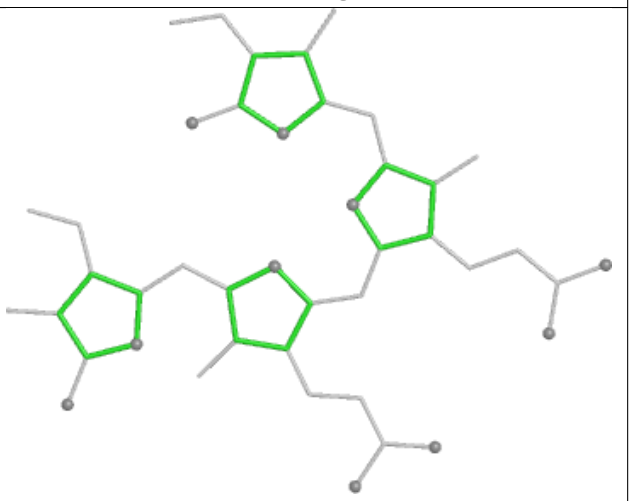
Bond lengths



Bond angles

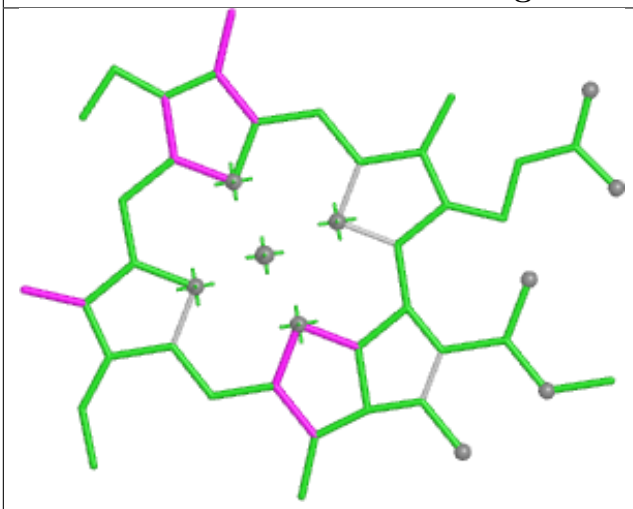


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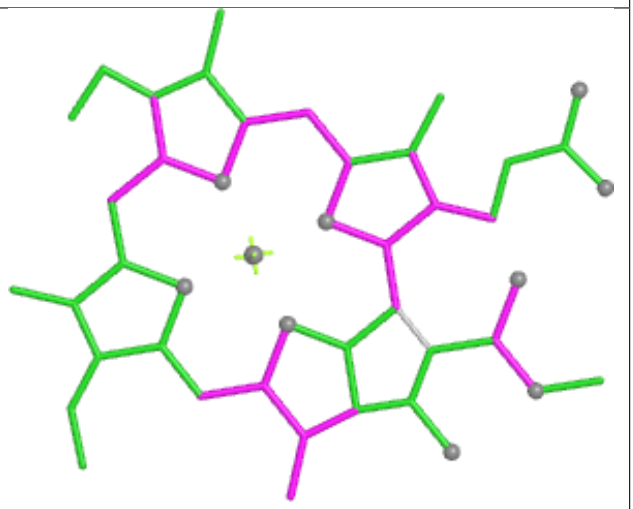


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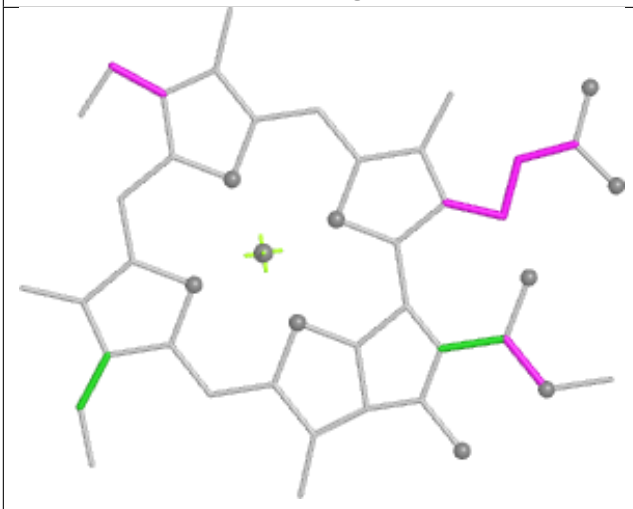
Ligand CLA 3N 303



Bond lengths



Bond angles

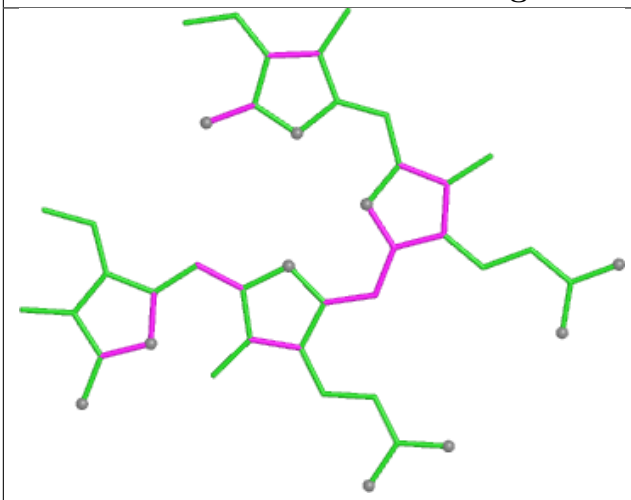


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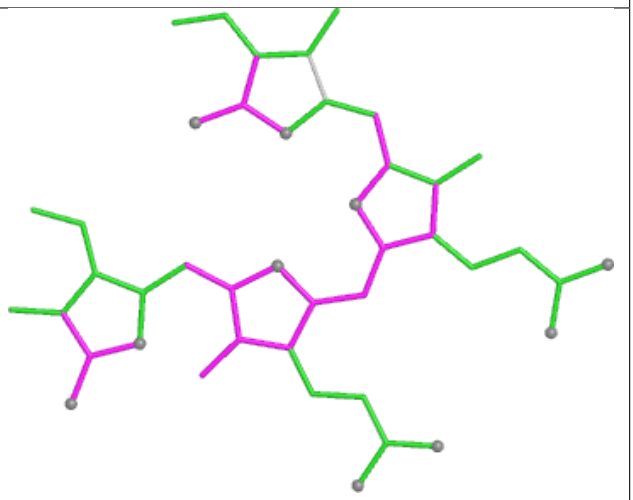


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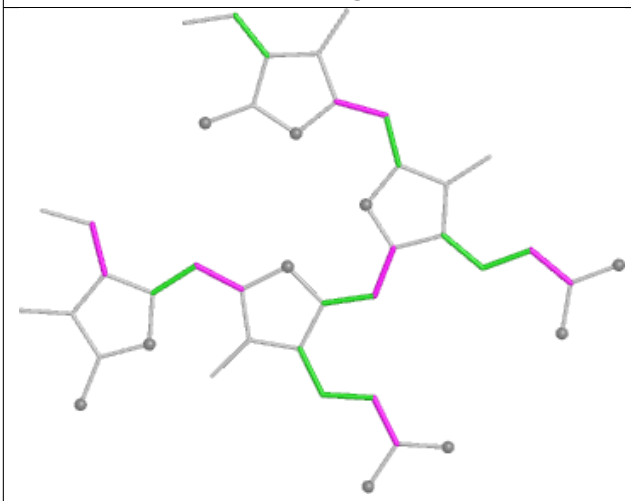
Ligand PEB AH 305



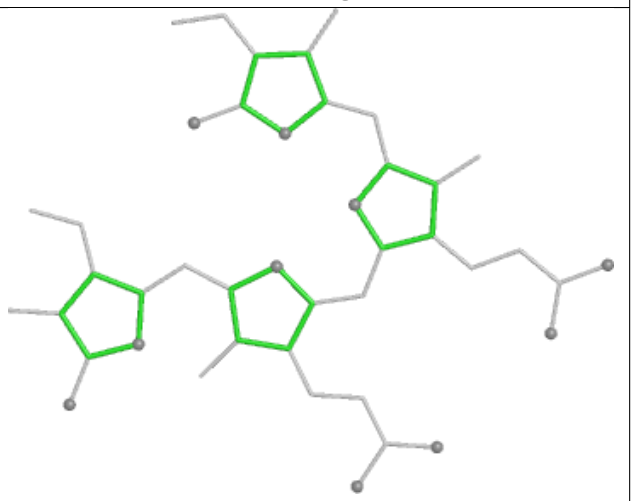
Bond lengths



Bond angles

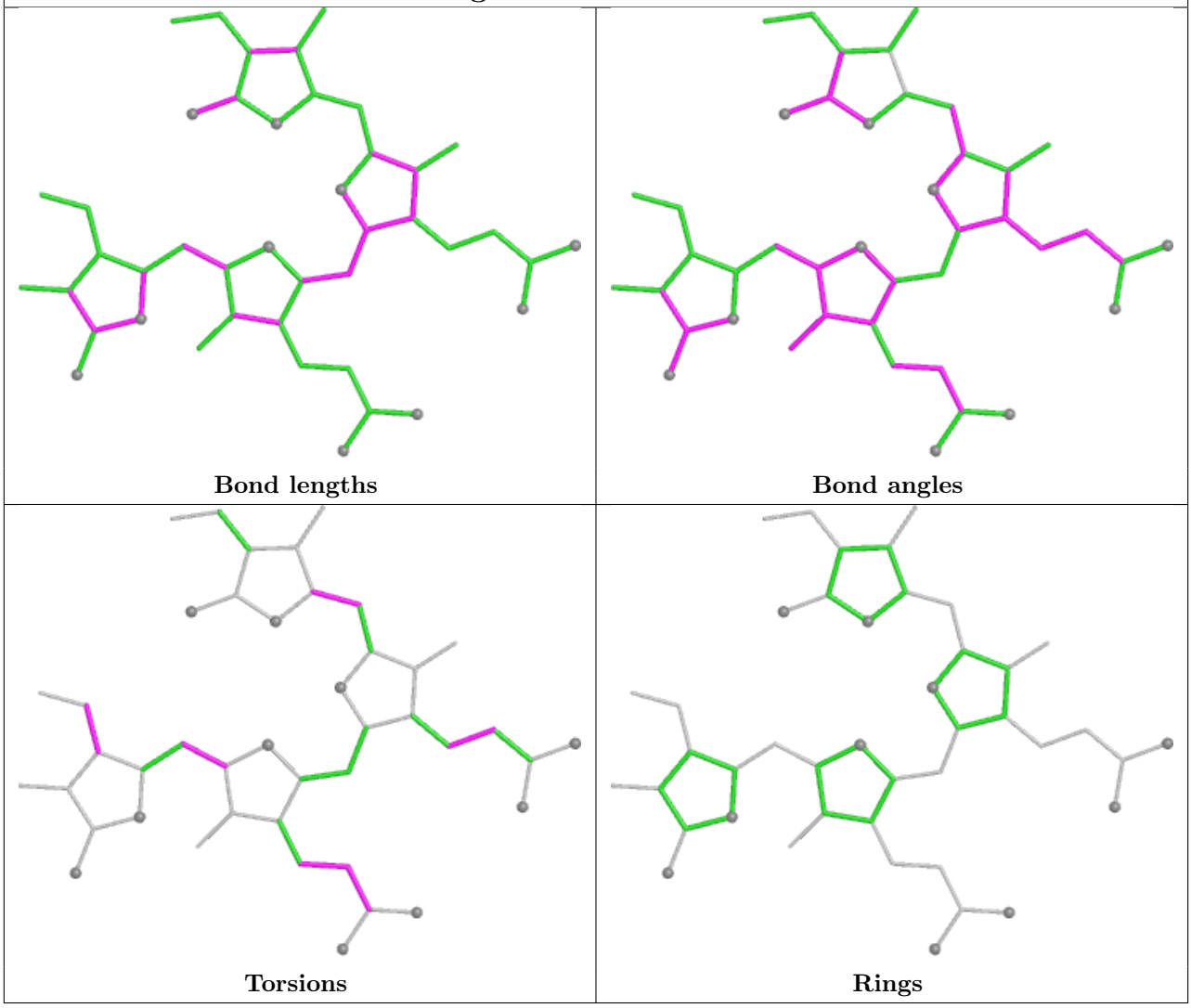


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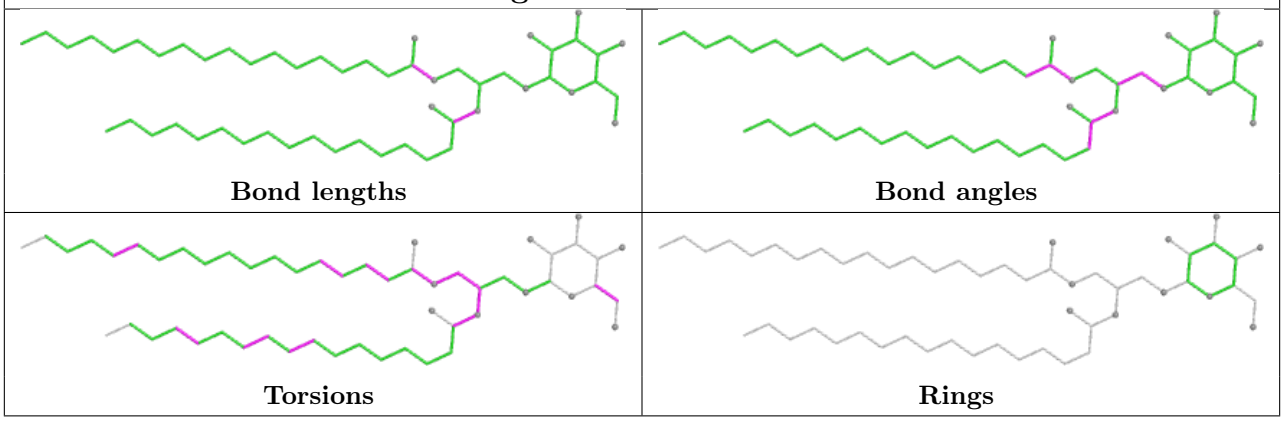


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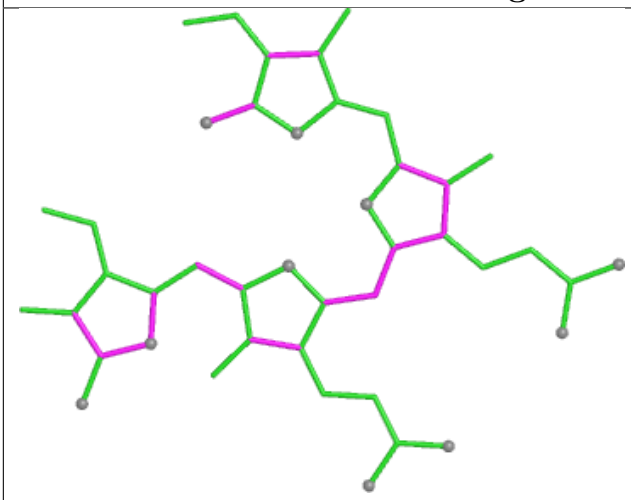
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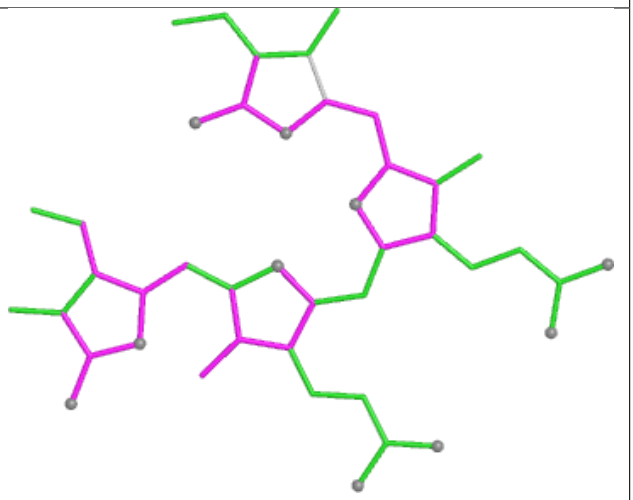
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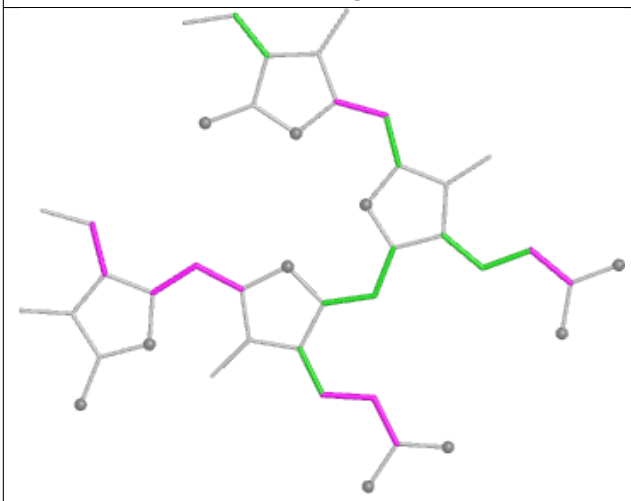
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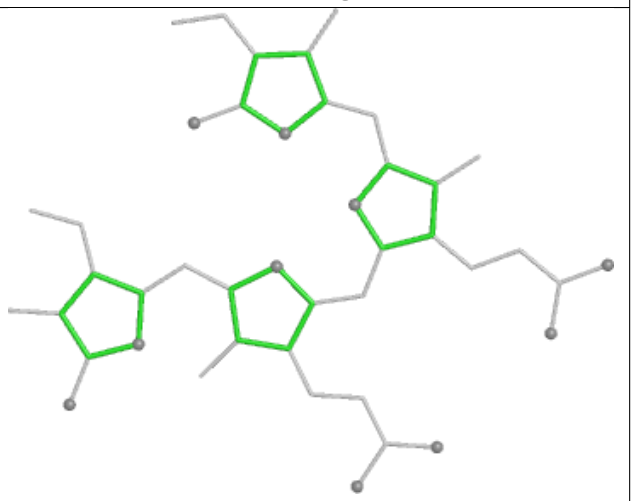
Bond lengths



Bond angles

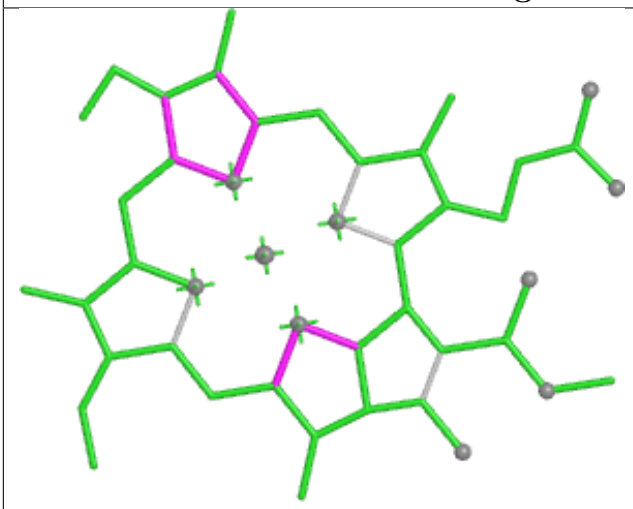


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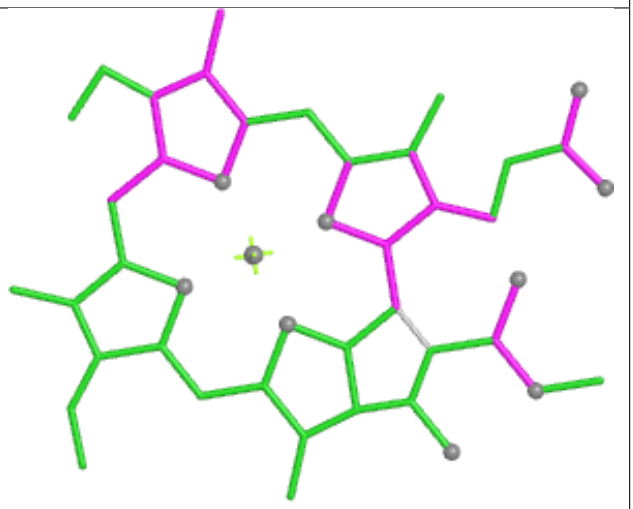


Rings

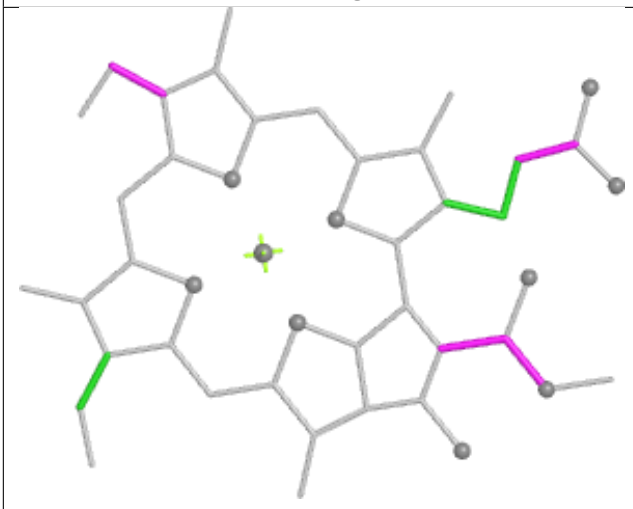
Ligand CLA 3N 304



Bond lengths



Bond angles

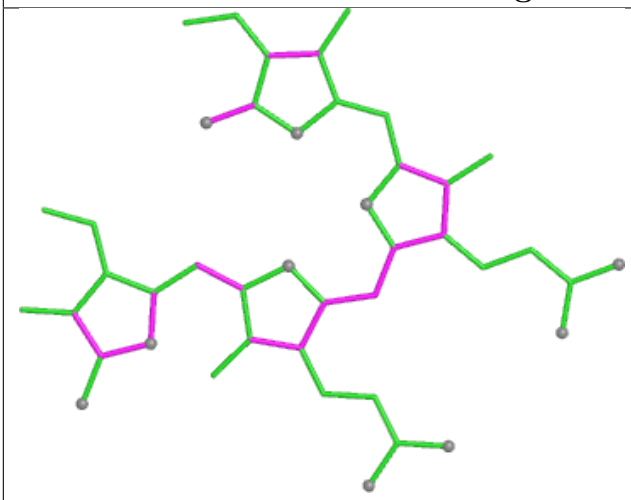


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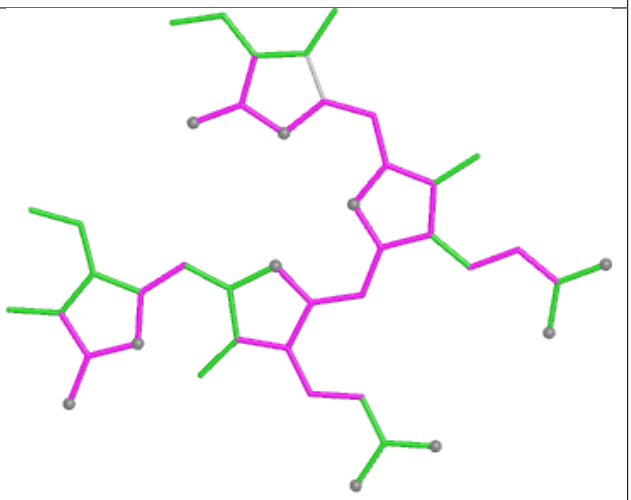


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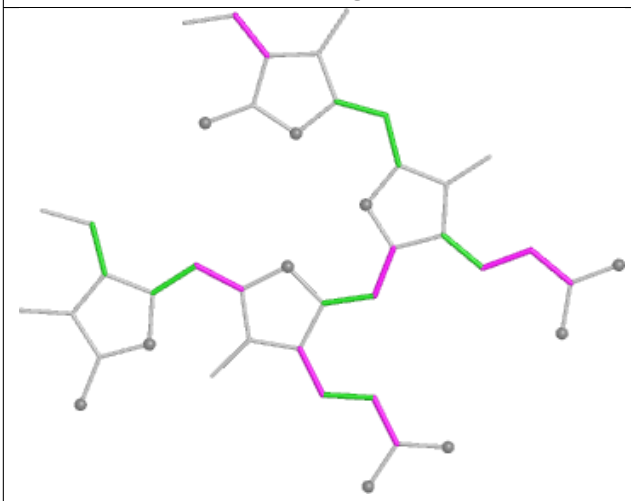
Ligand PEB H7 203



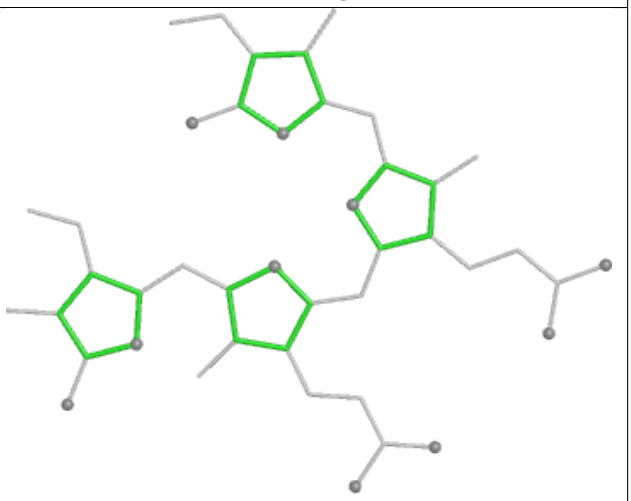
Bond lengths



Bond angles

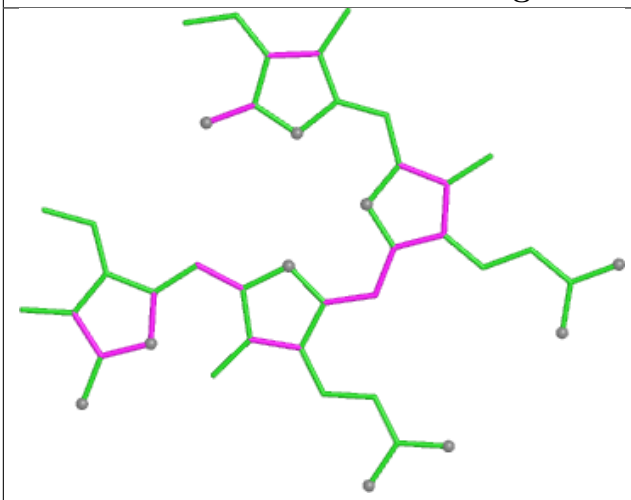


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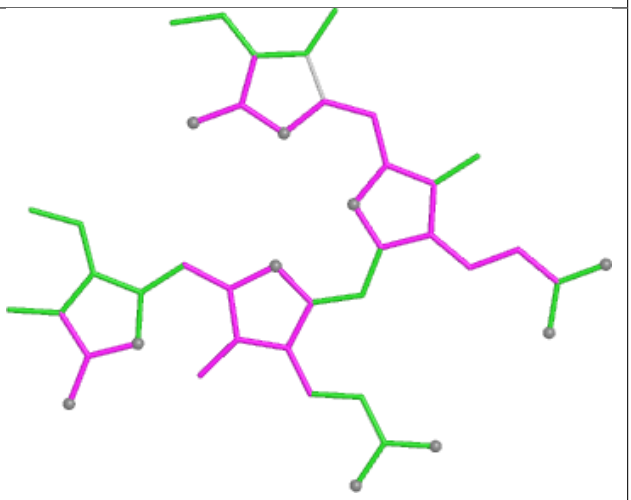


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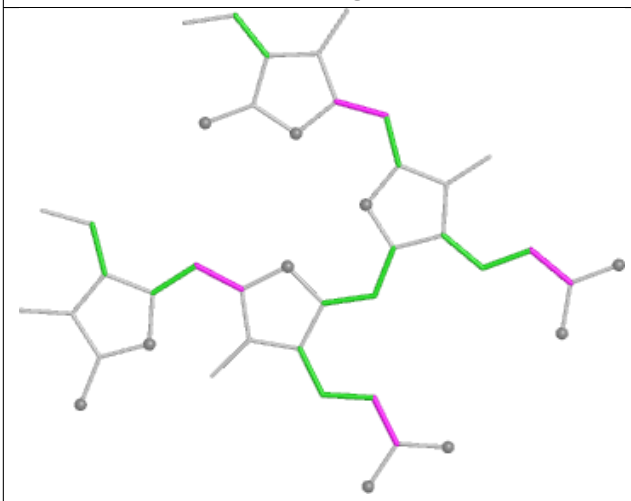
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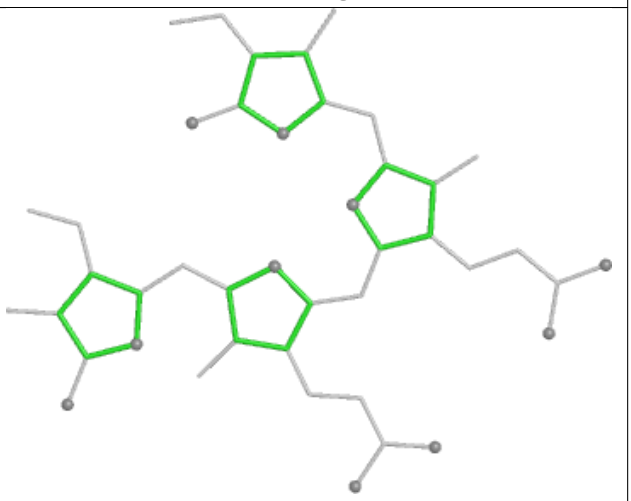
Bond lengths



Bond angles

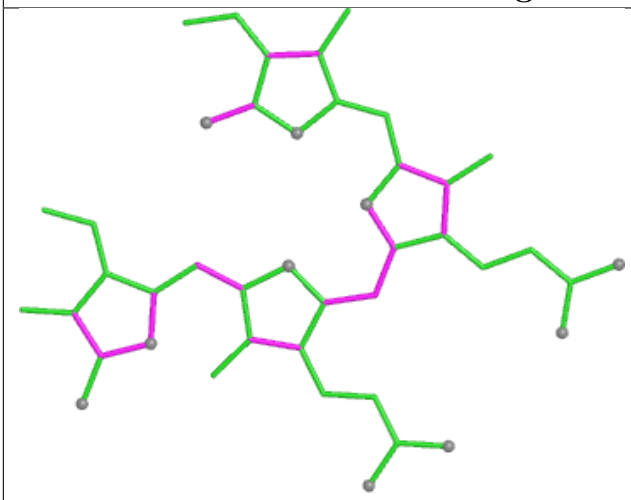


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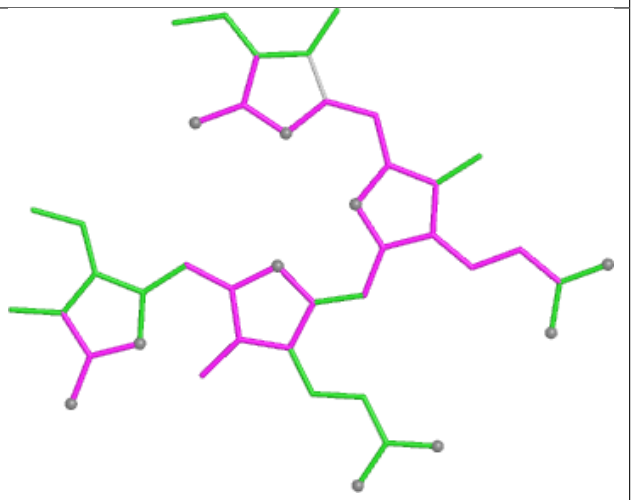


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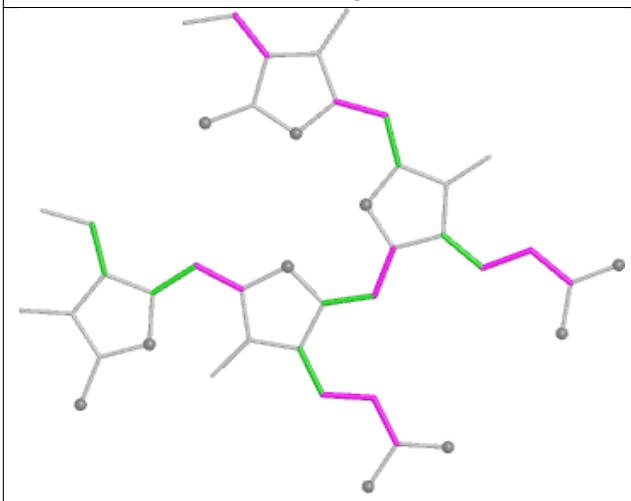
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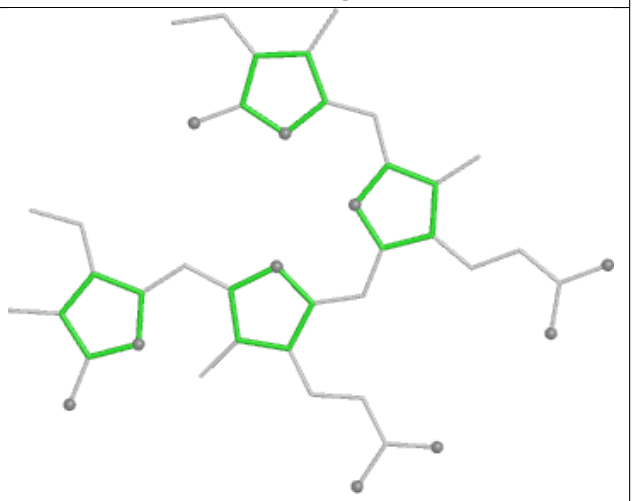
Bond lengths



Bond angles

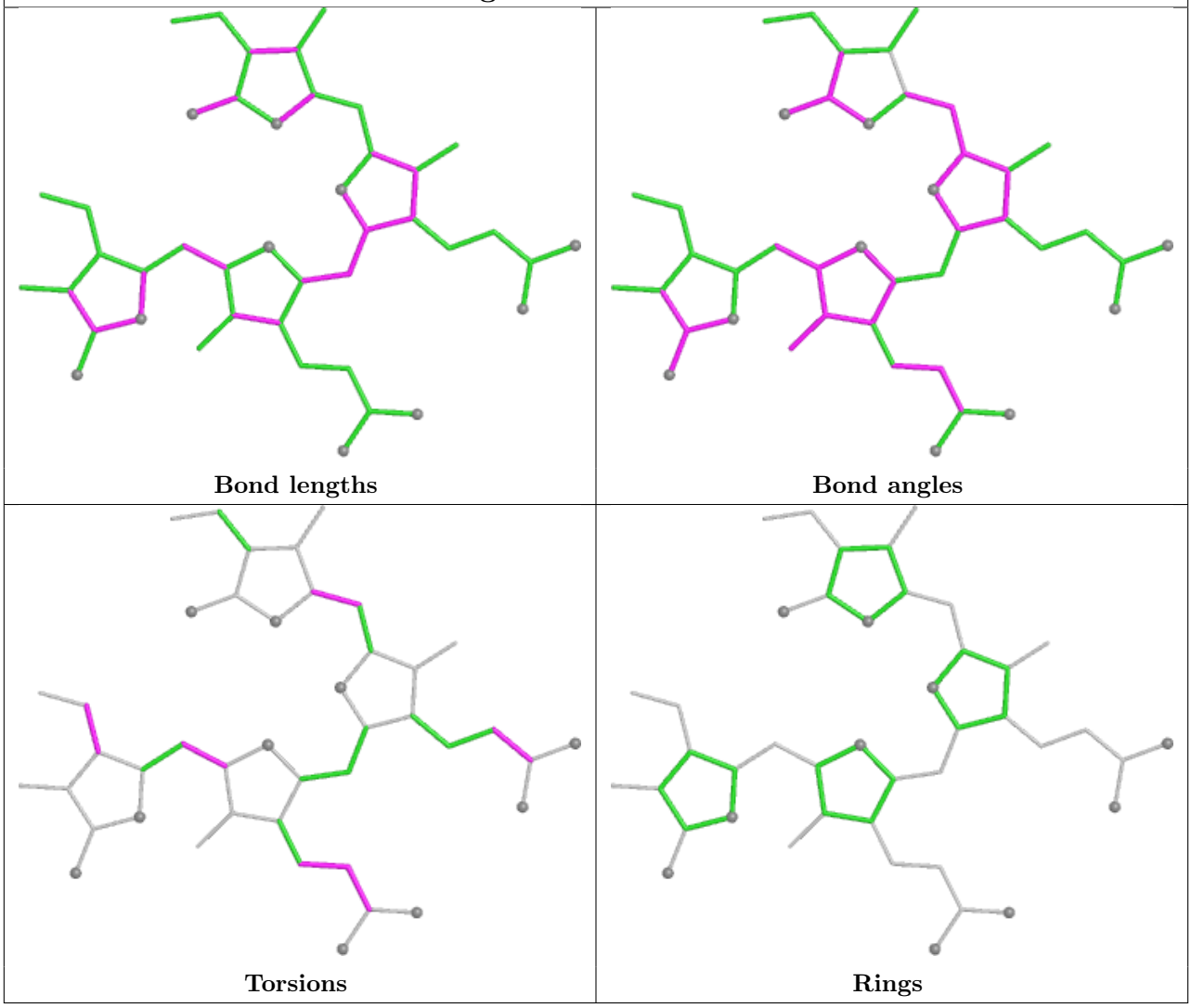


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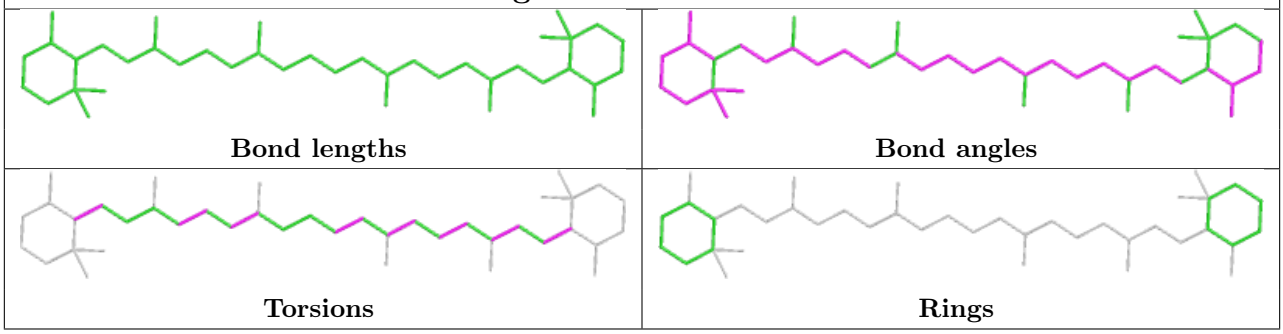


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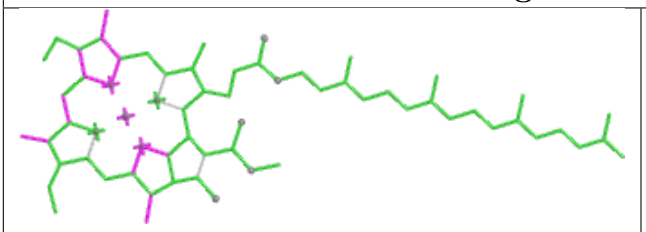
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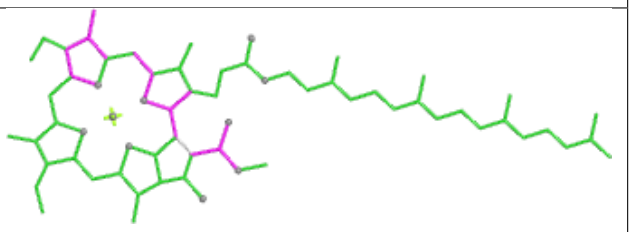
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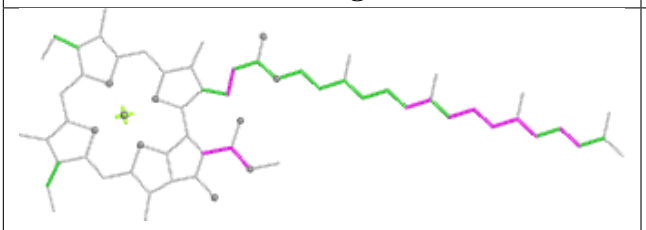
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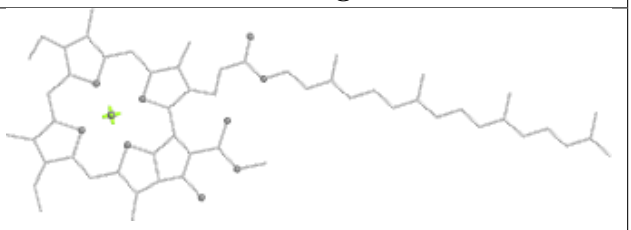
Bond lengths



Bond angles

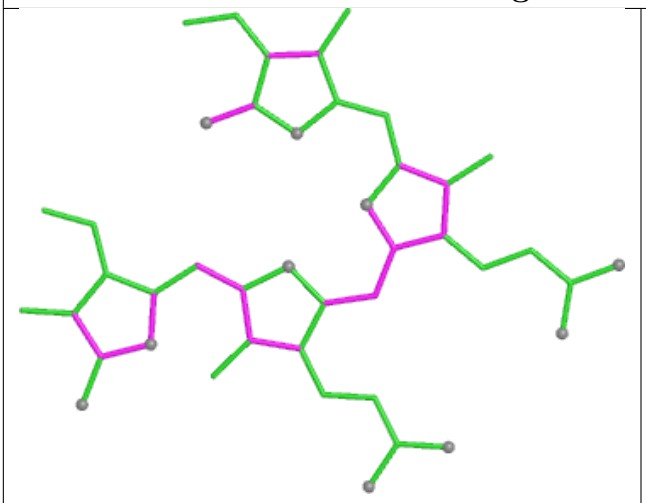


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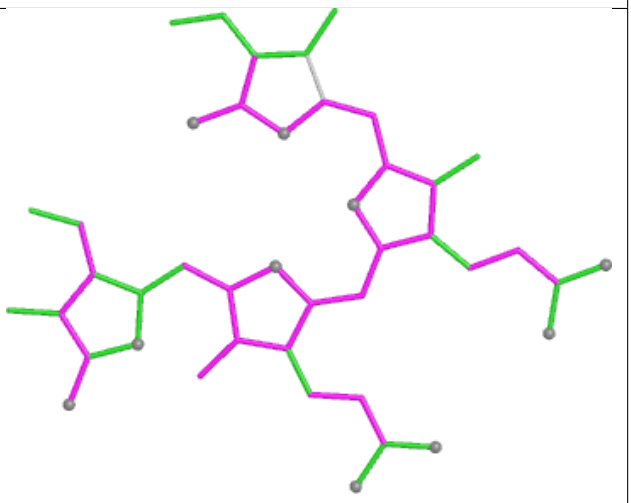


Rings

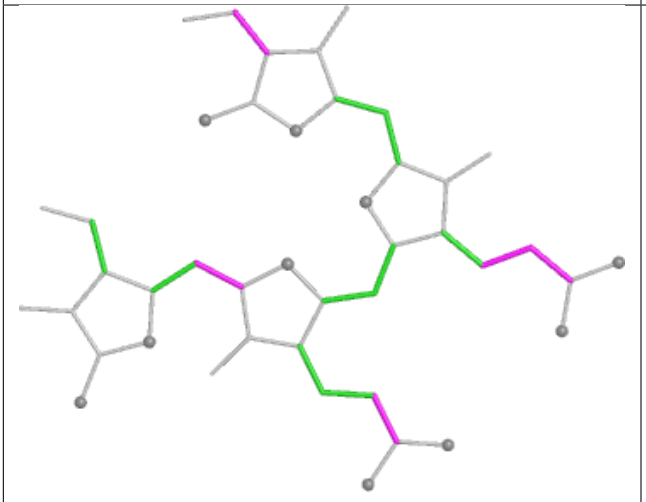
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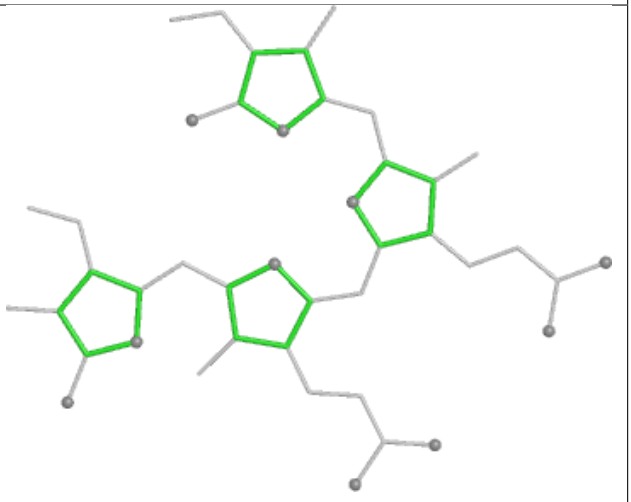
Bond lengths



Bond angles

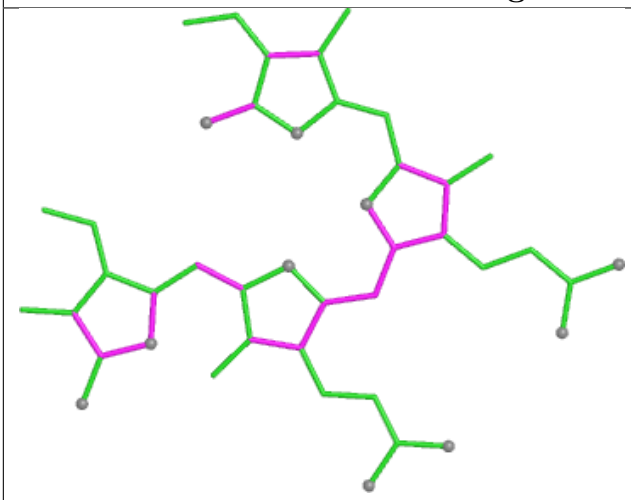


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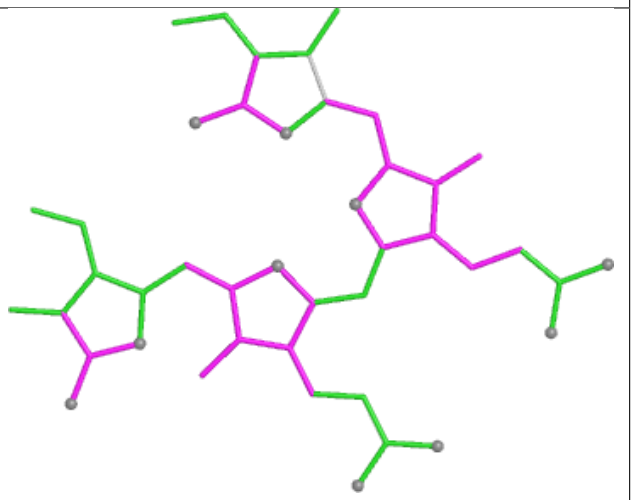


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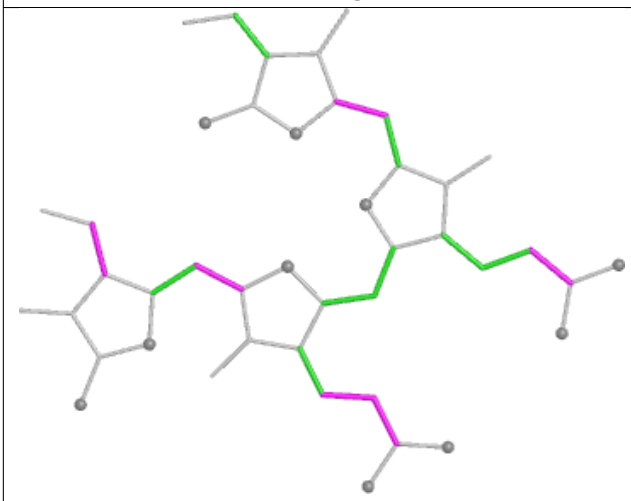
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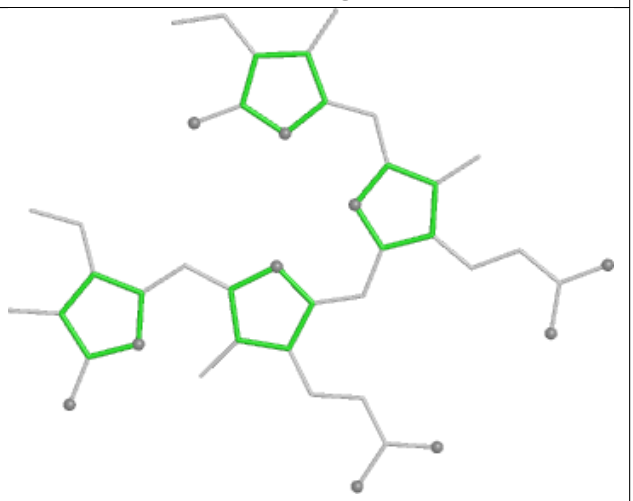
Bond lengths



Bond angles

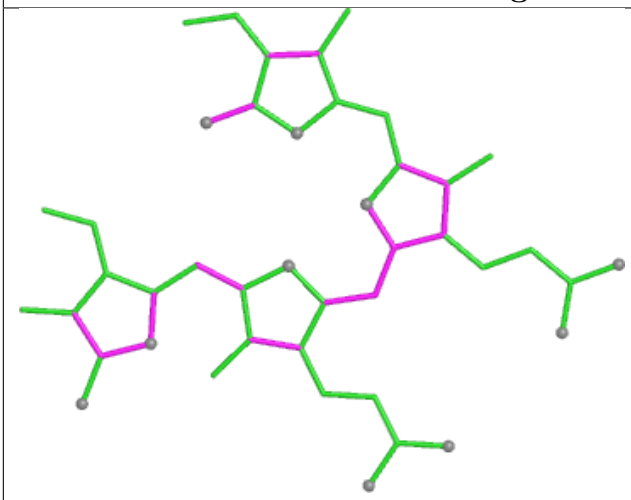


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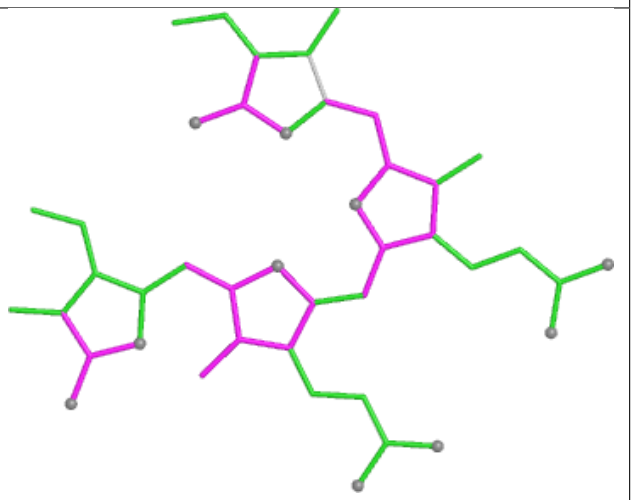


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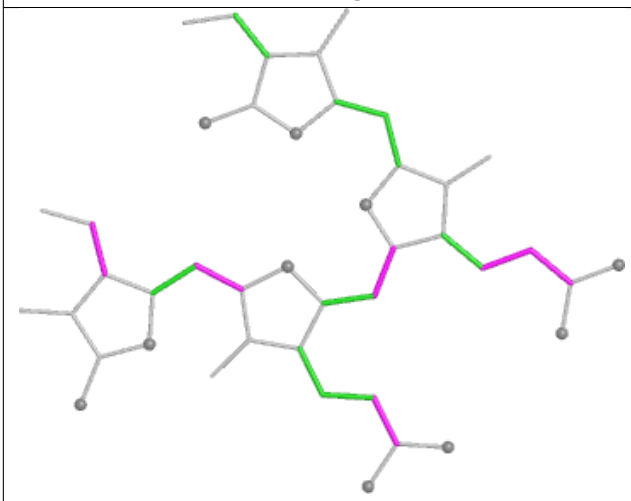
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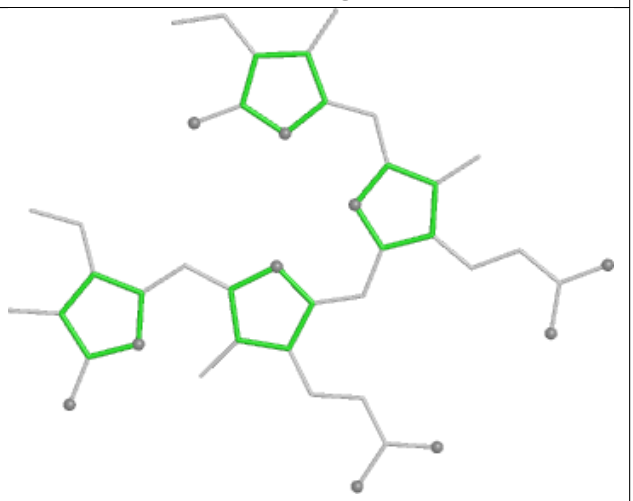
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Bond angles

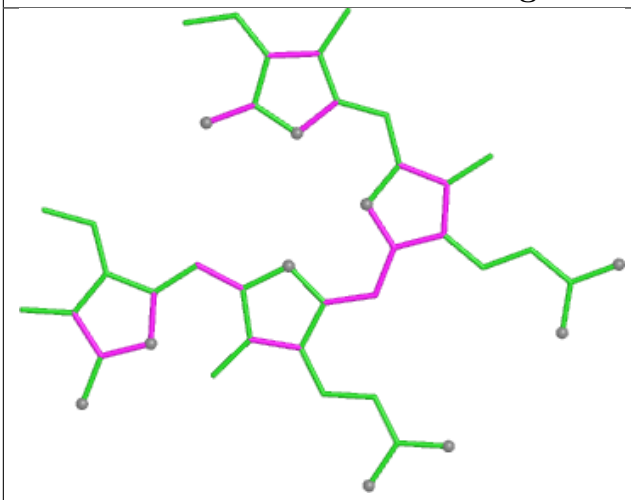


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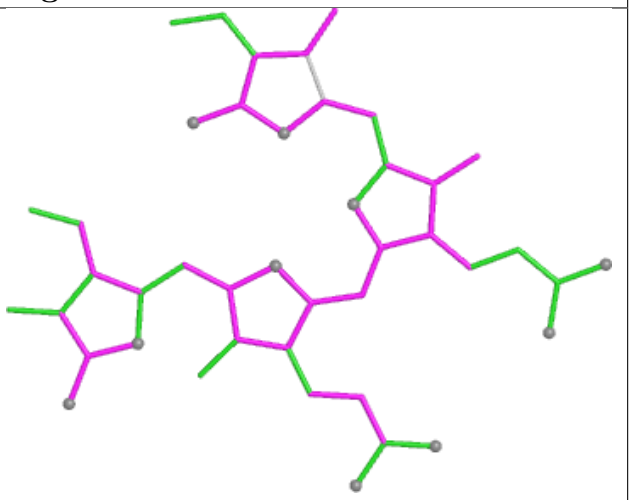


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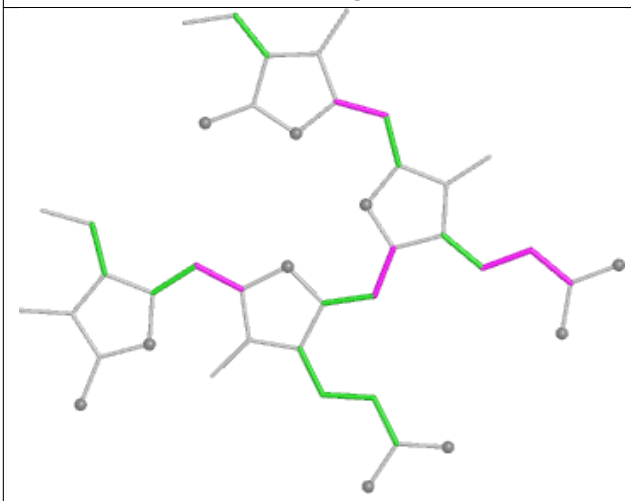
Ligand PEB gJ 201



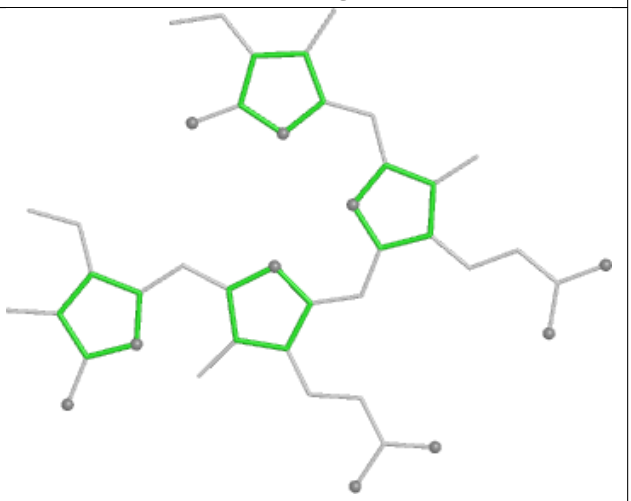
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Bond angles

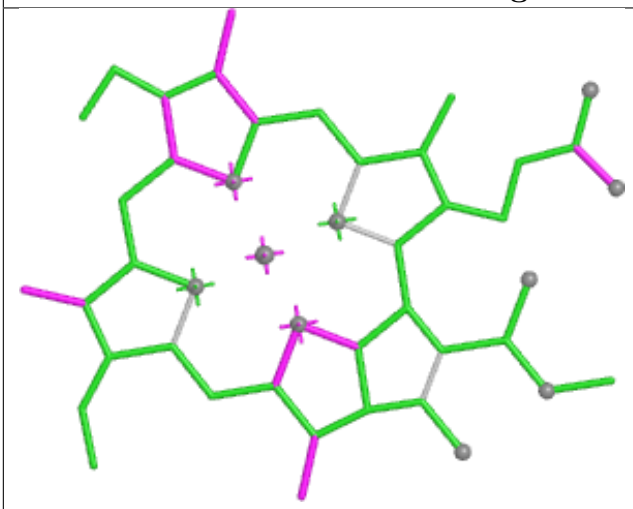


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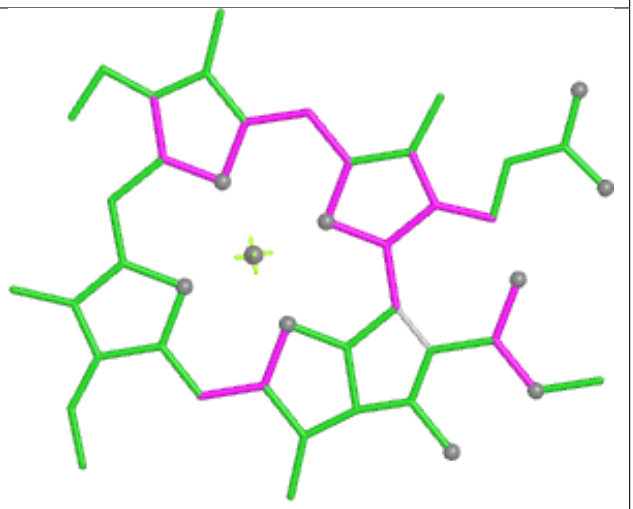


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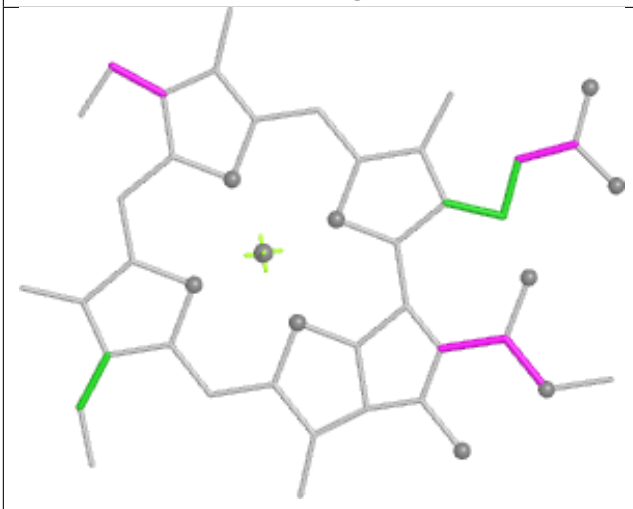
Ligand CLA BN 820



Bond lengths



Bond angles

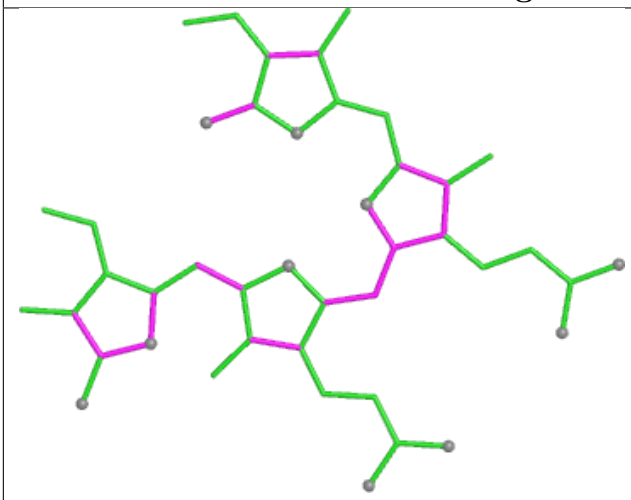


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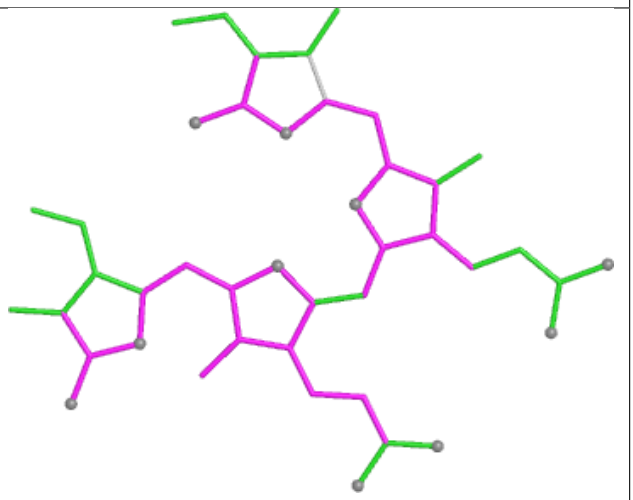


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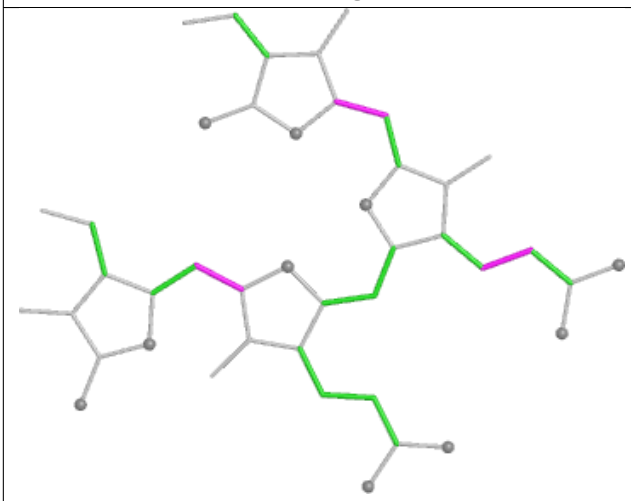
Ligand PEB Y4 201



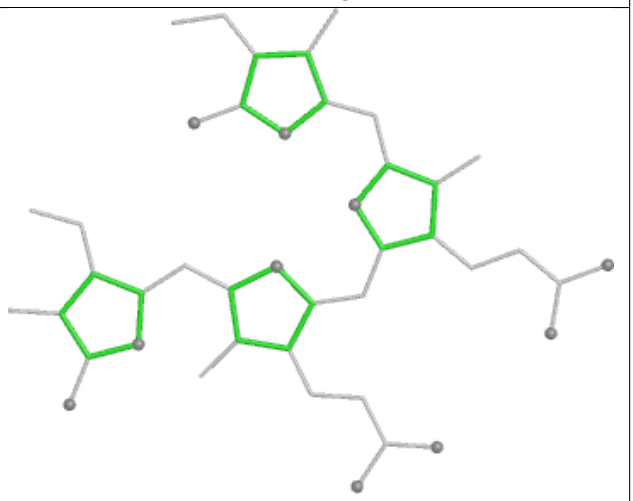
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Bond angles

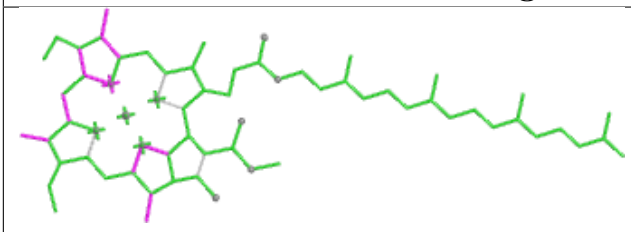


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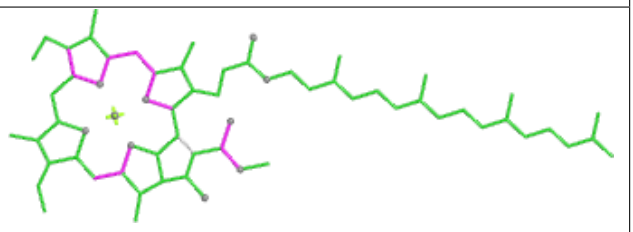


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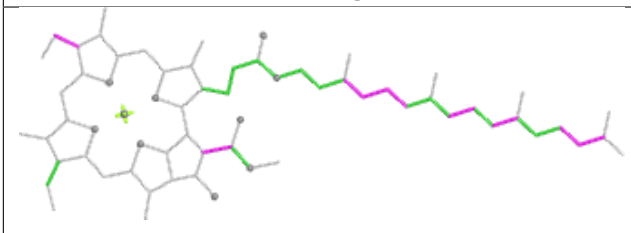
Ligand CLA b6 607



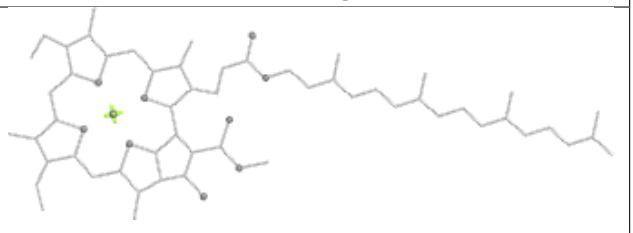
Bond lengths



Bond angles

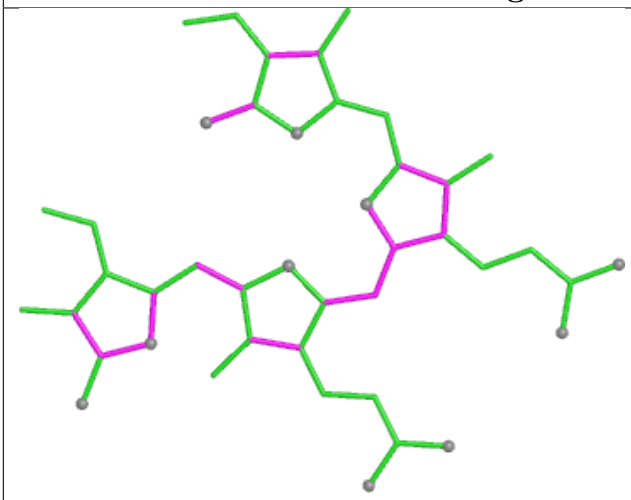


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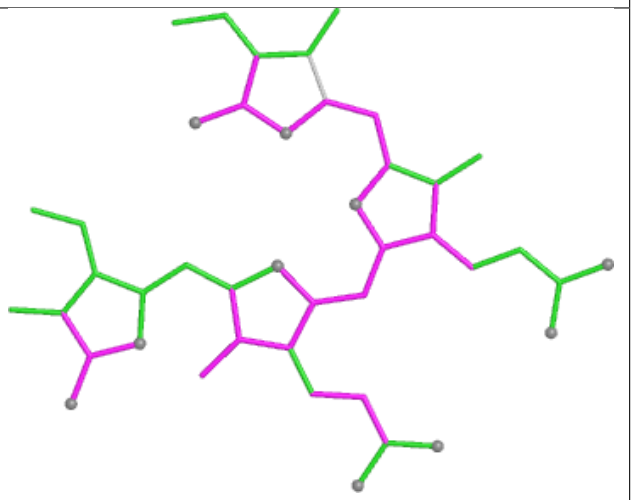


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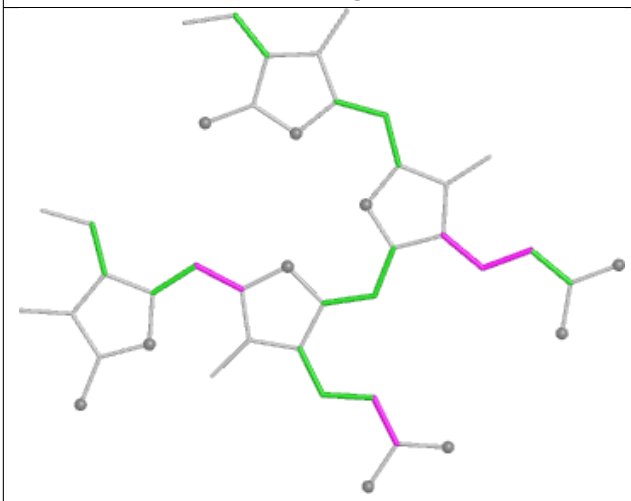
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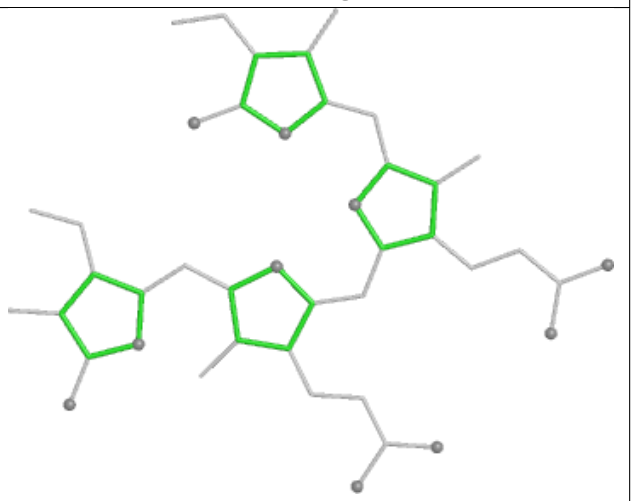
Bond lengths



Bond angles

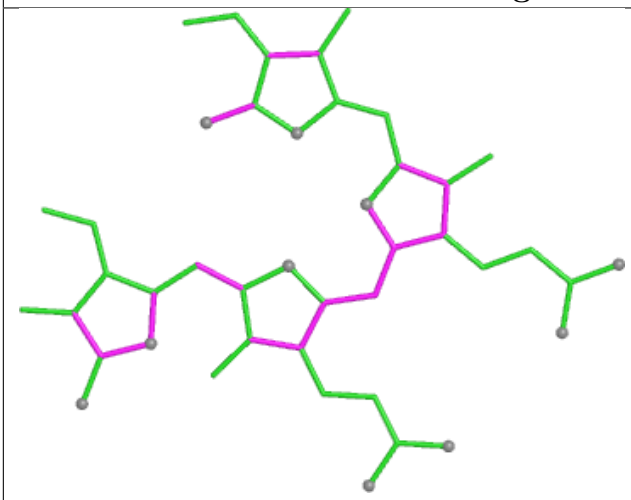


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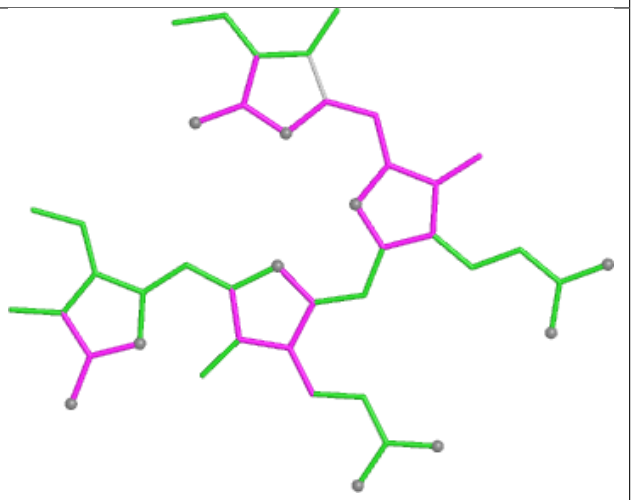


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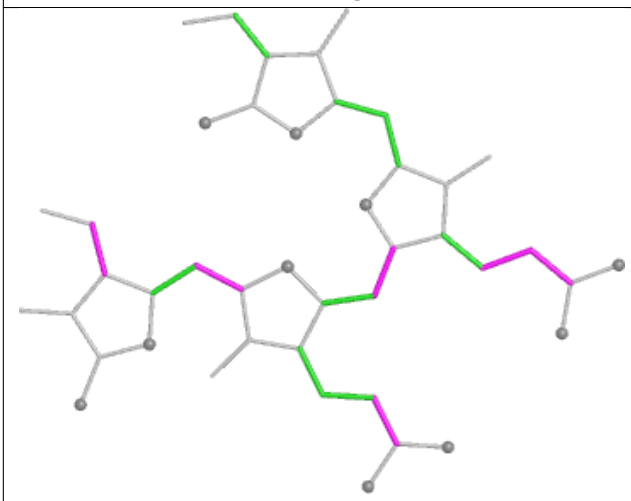
Ligand PEB AF 202



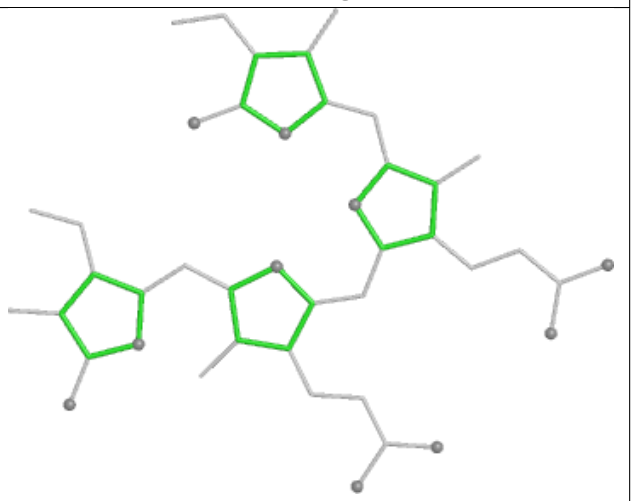
Bond lengths



Bond angles

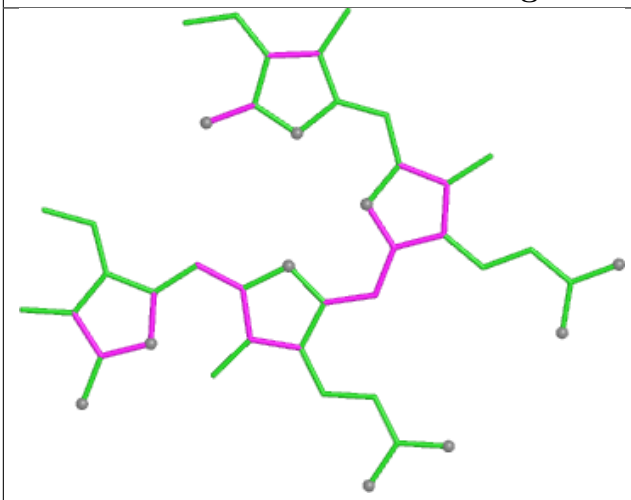


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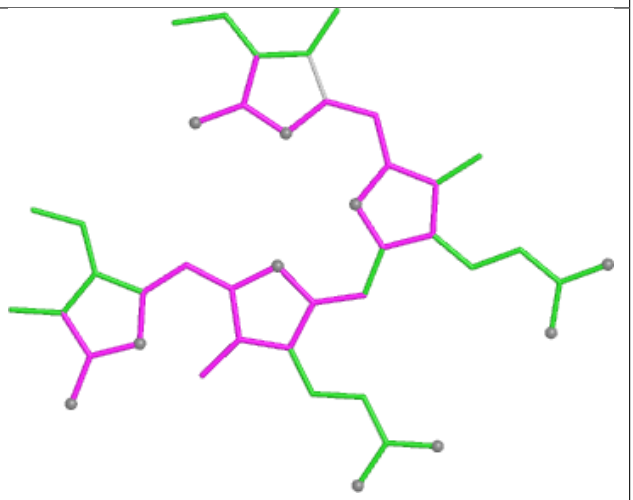


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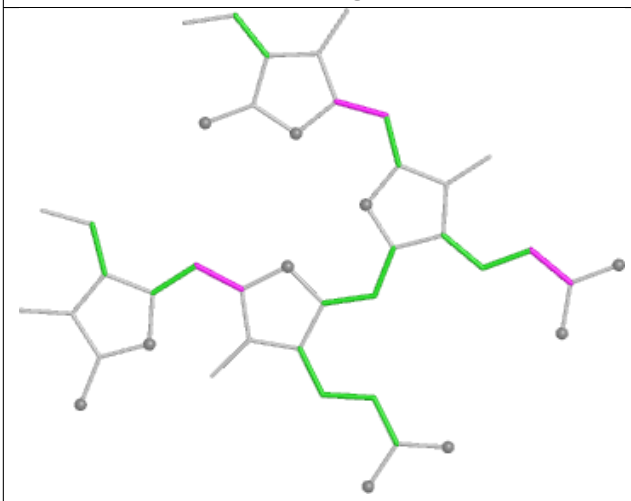
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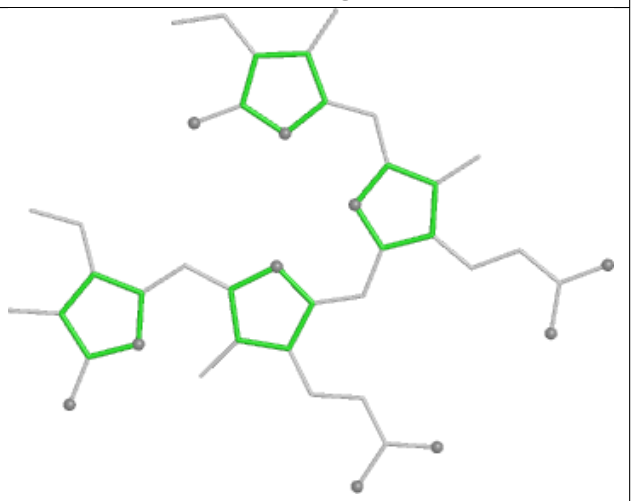
Bond lengths



Bond angles

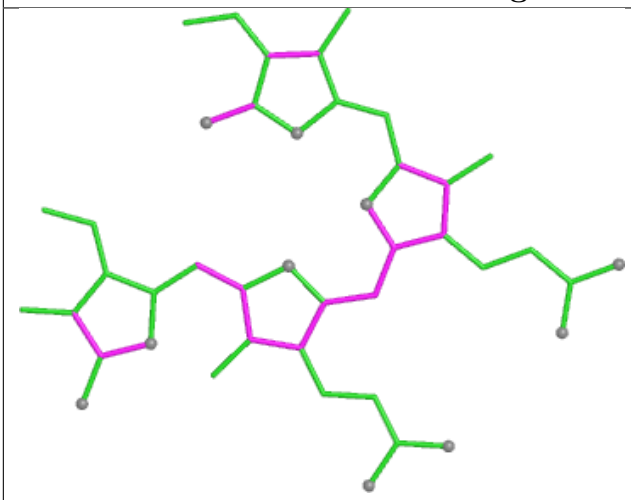


Torsions

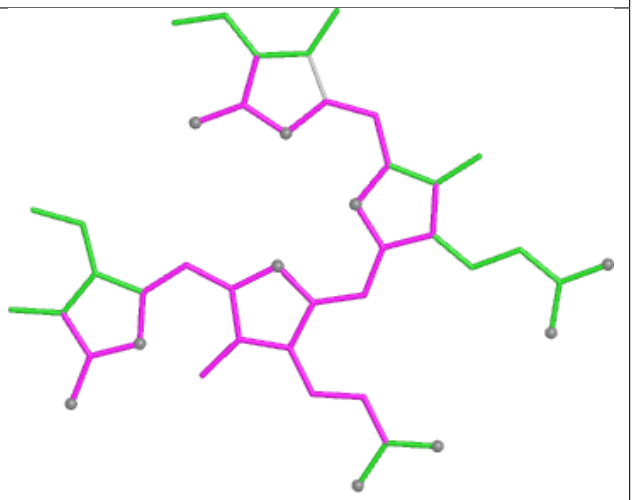


Rings

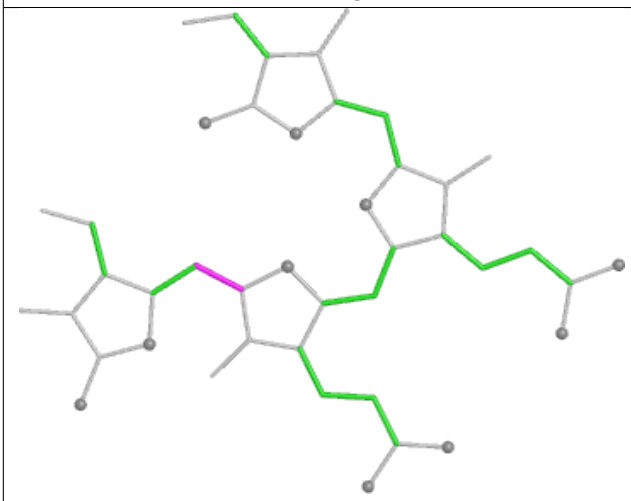
Ligand PEB VH 201



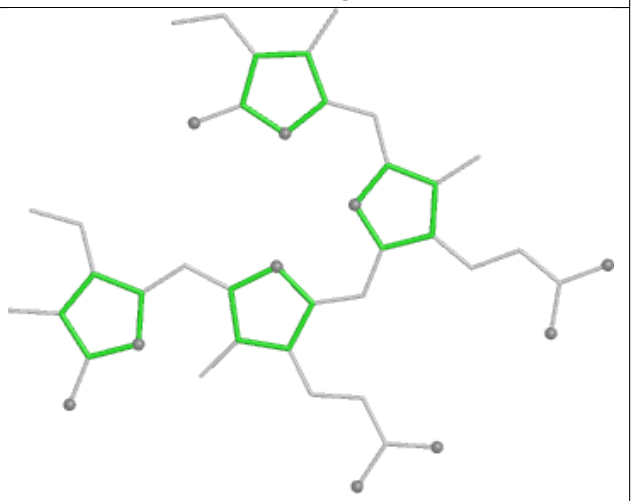
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Bond angles

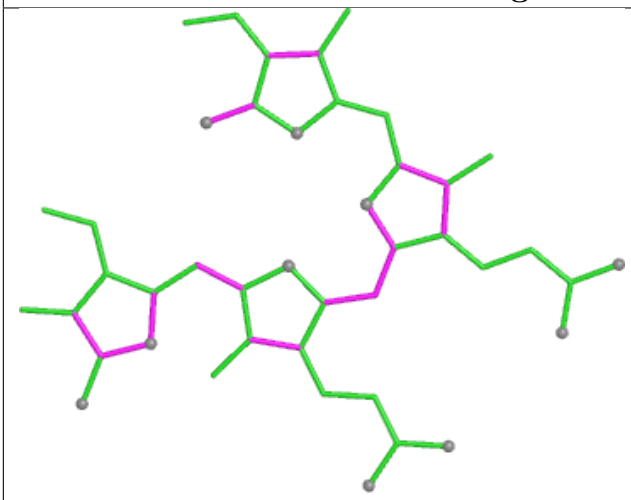


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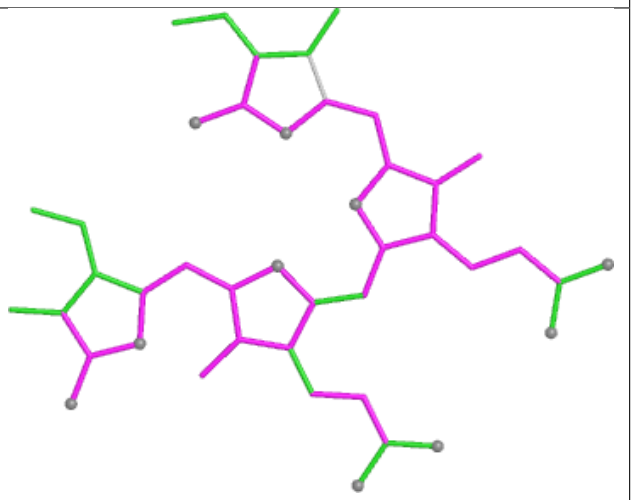


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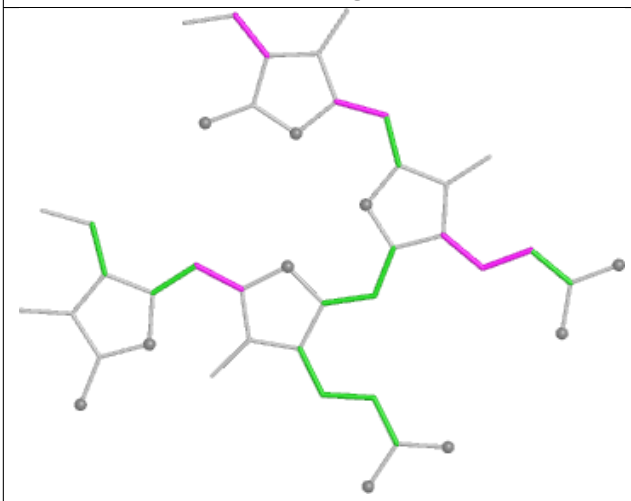
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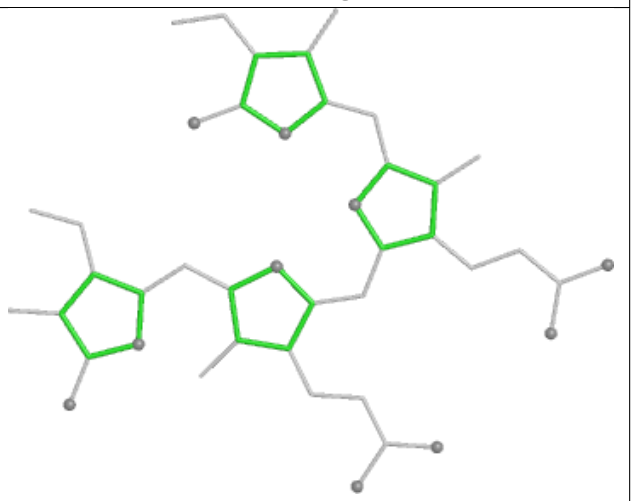
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Bond angles

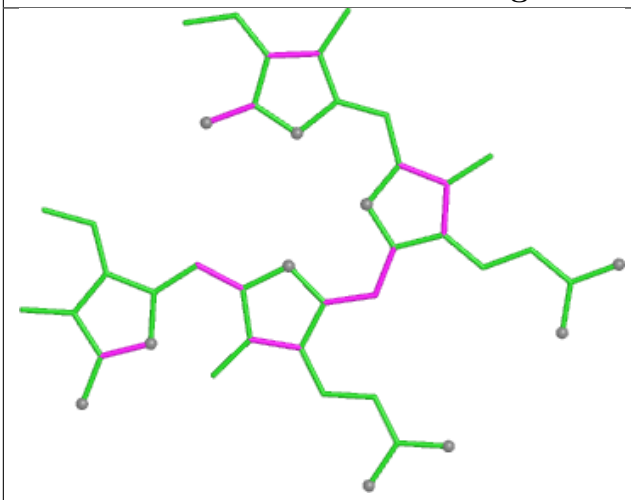


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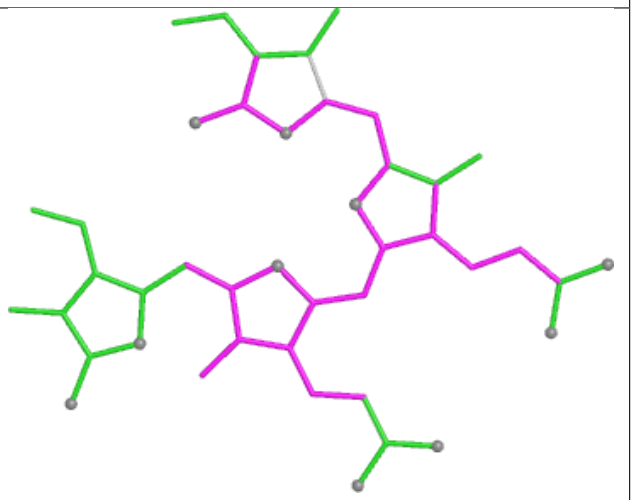


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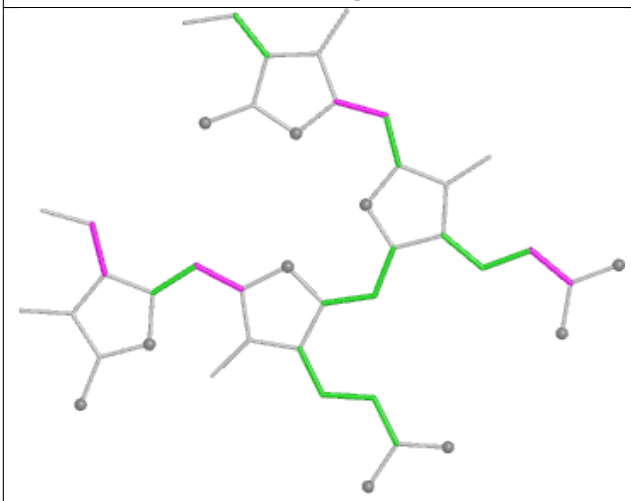
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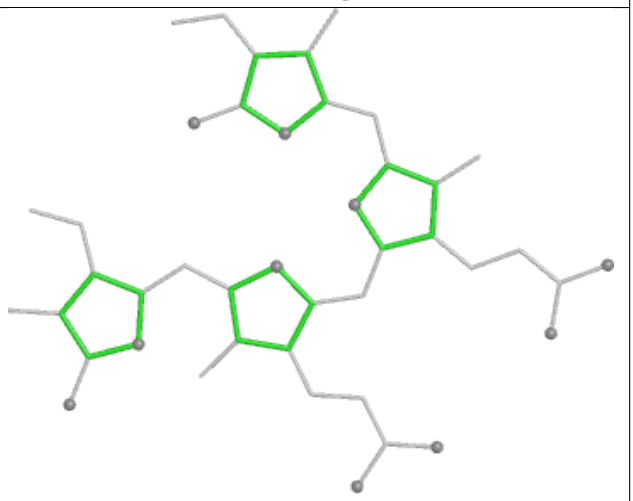
Bond lengths



Bond angles

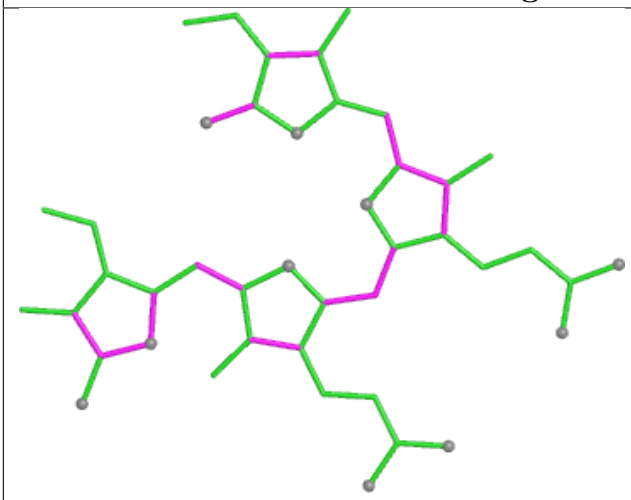


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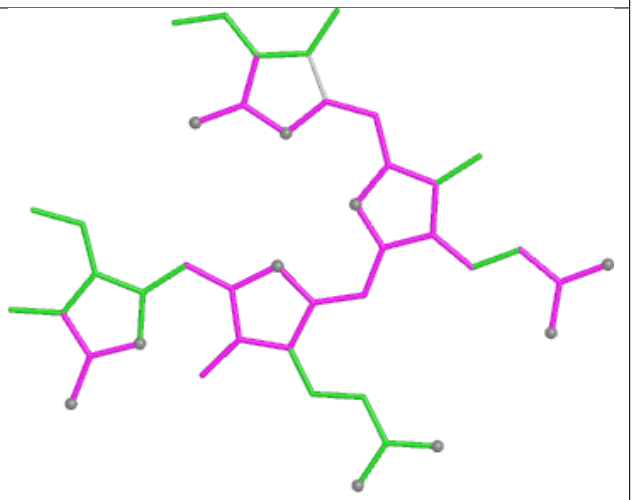


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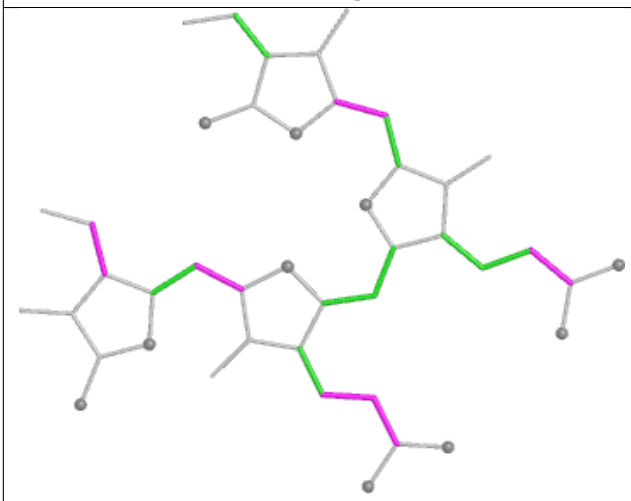
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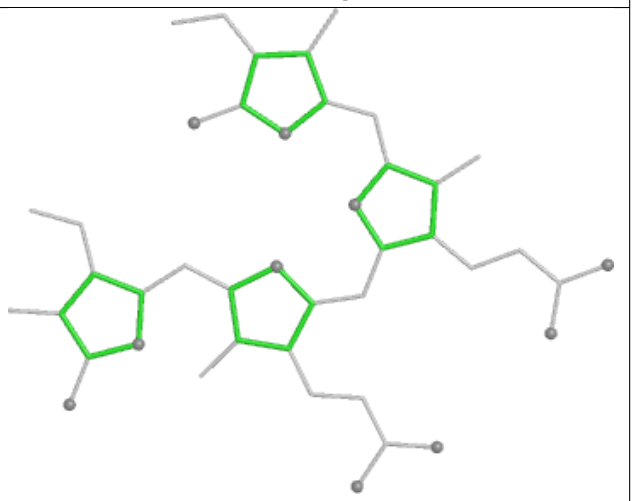
Bond lengths



Bond angles

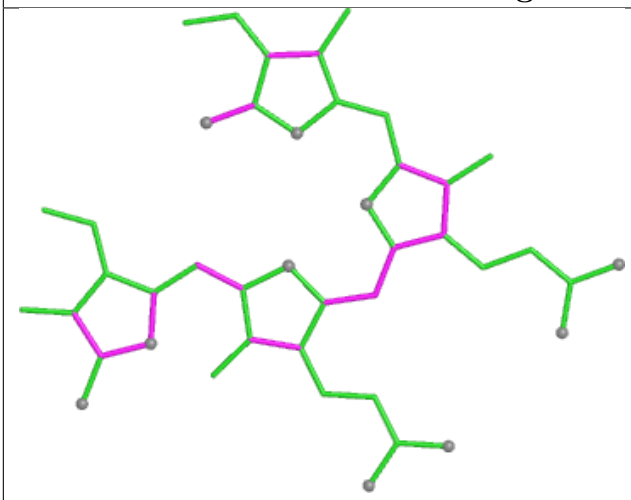


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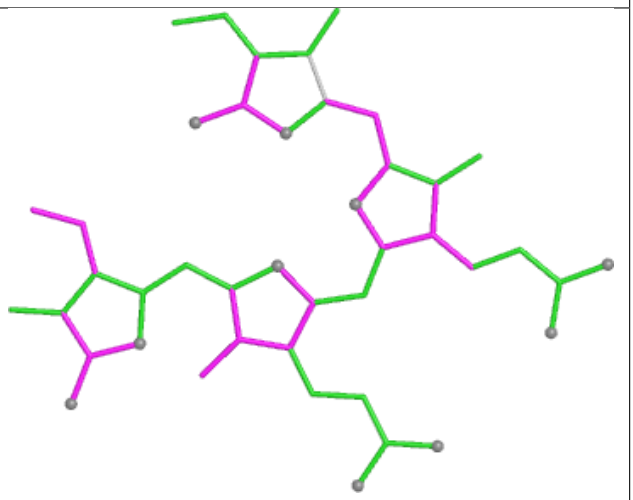


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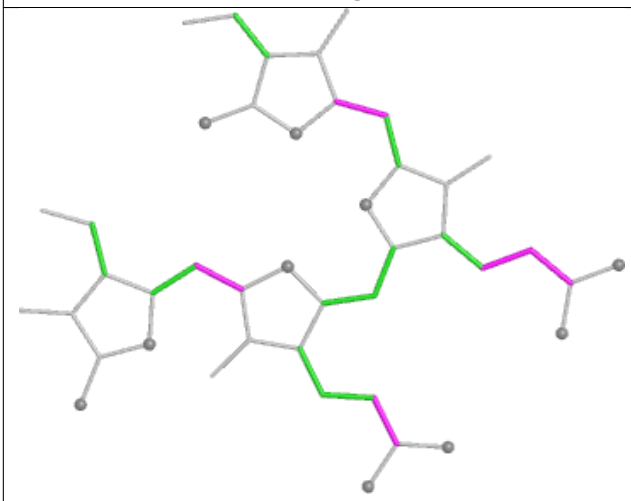
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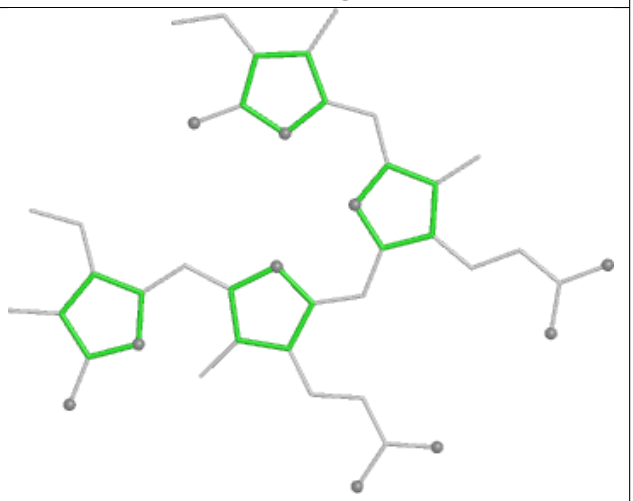
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Bond angles

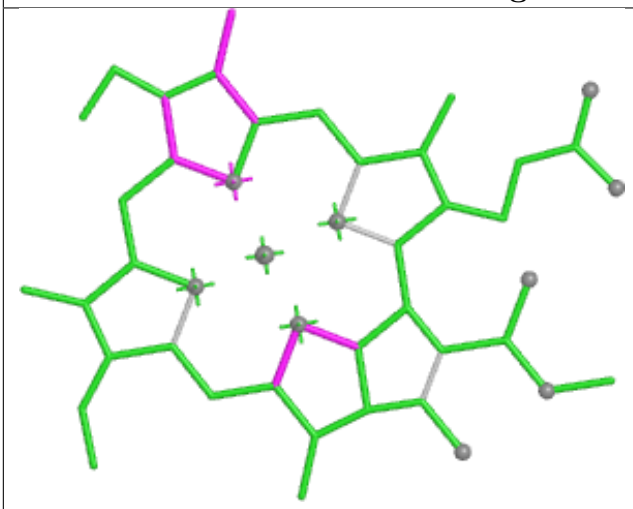


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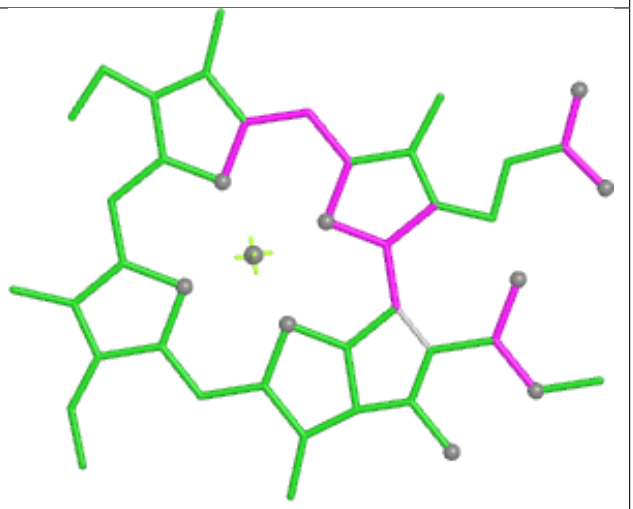


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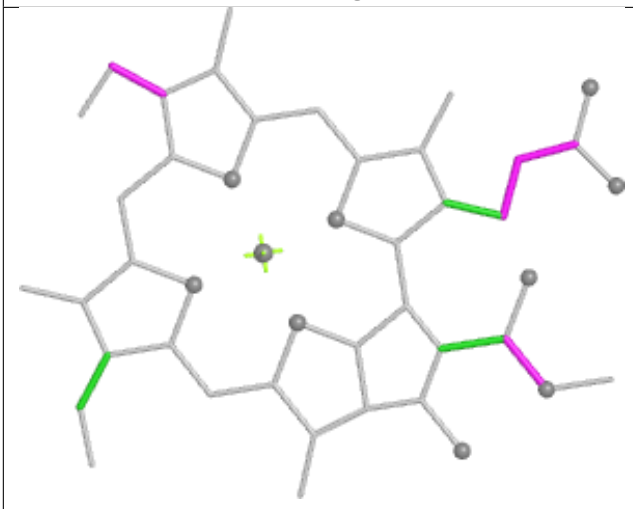
Ligand CLA RN 201



Bond lengths



Bond angles

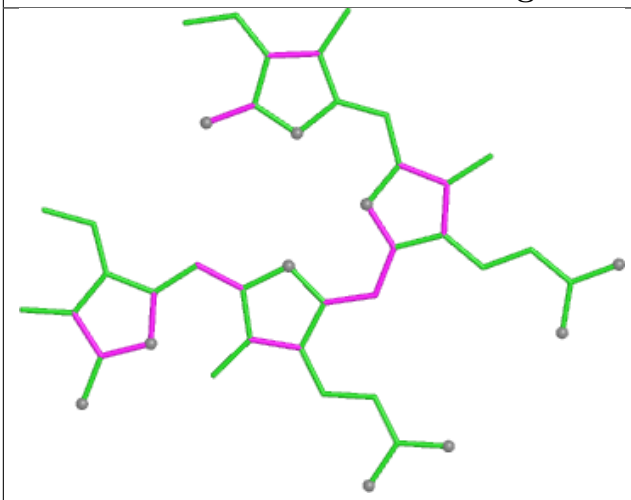


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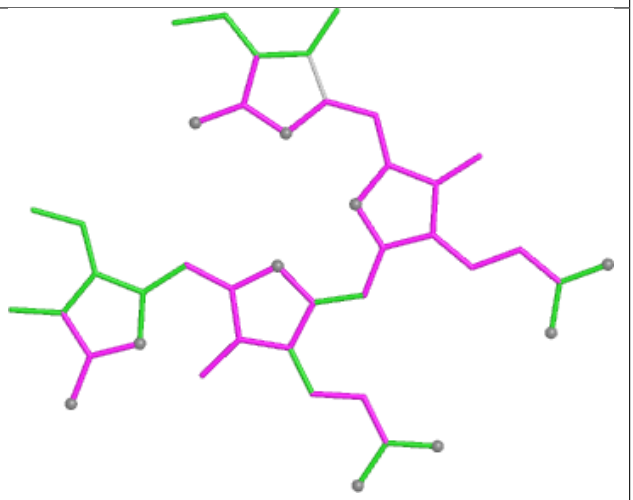


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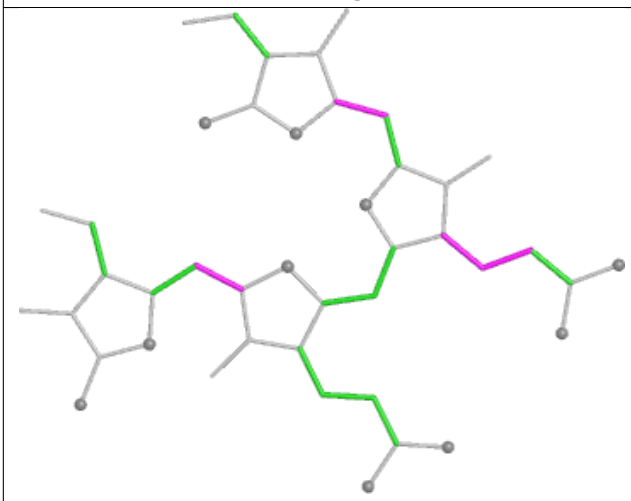
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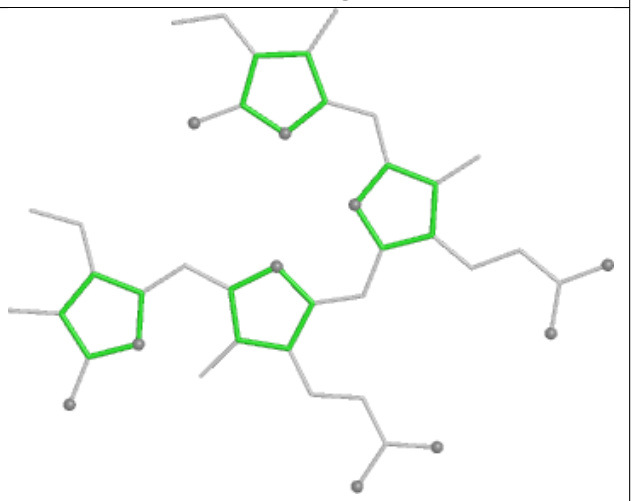
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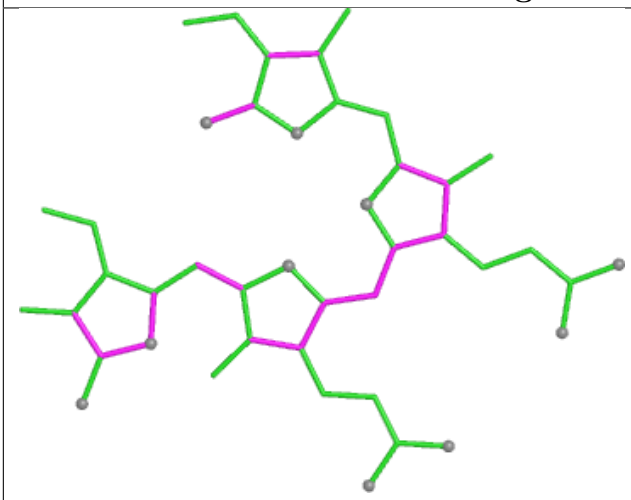


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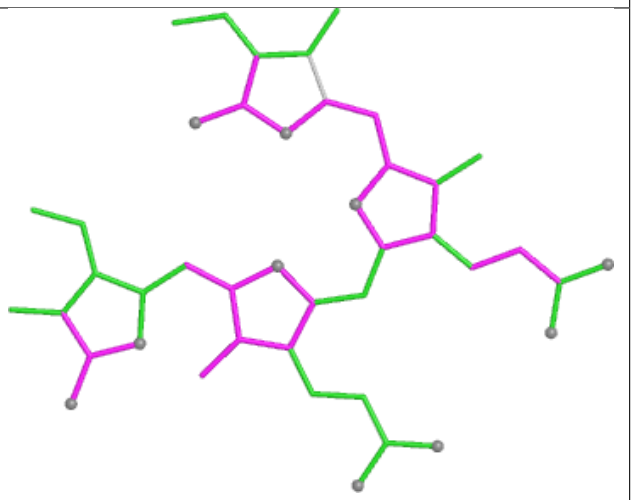


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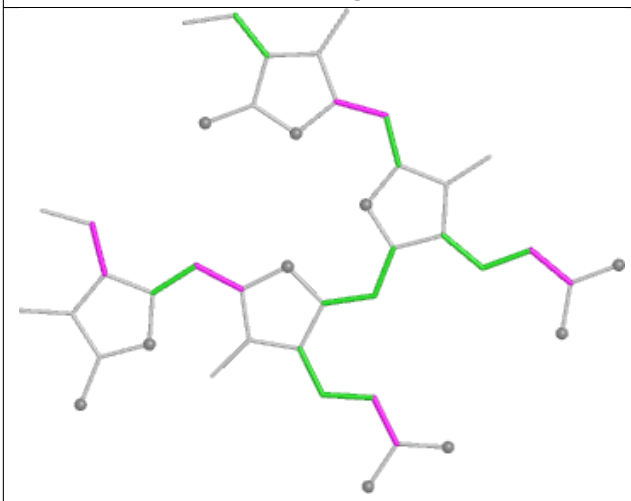
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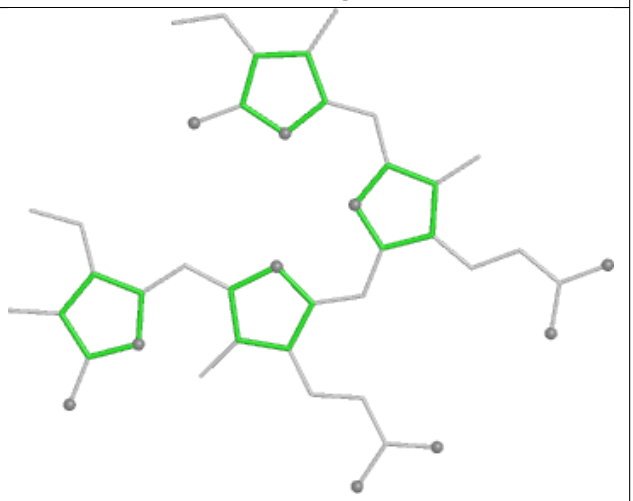
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Bond angles

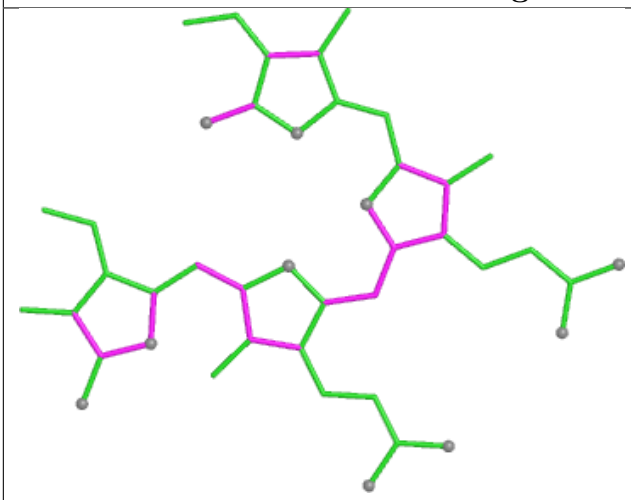


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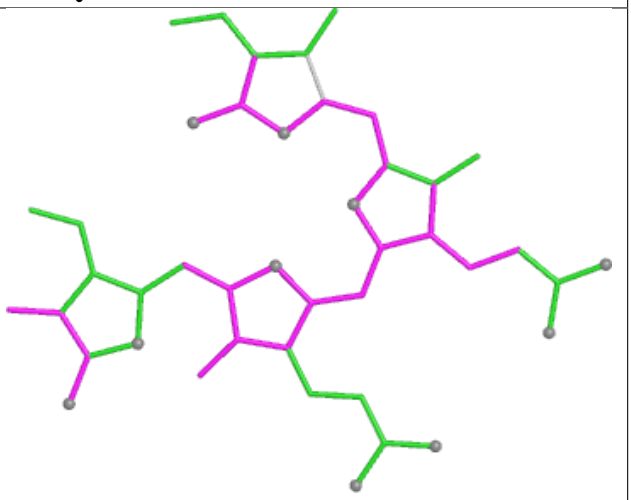


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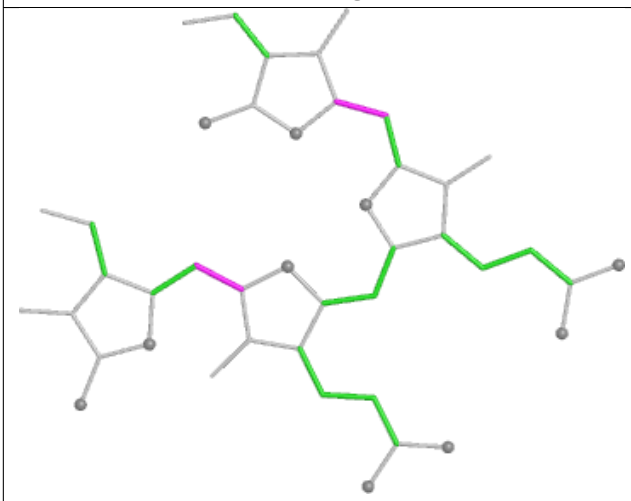
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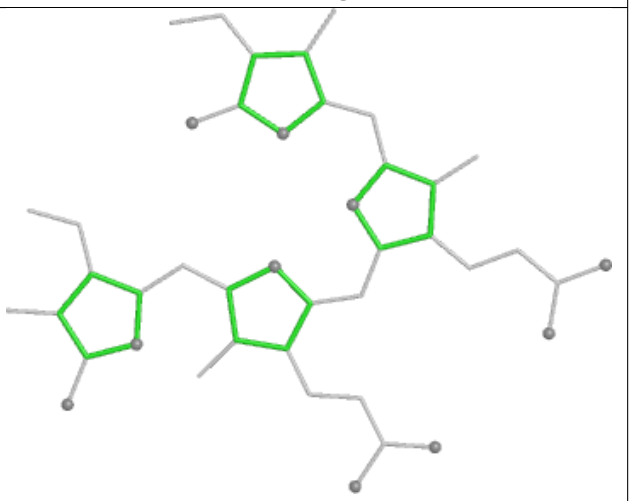
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Bond angles

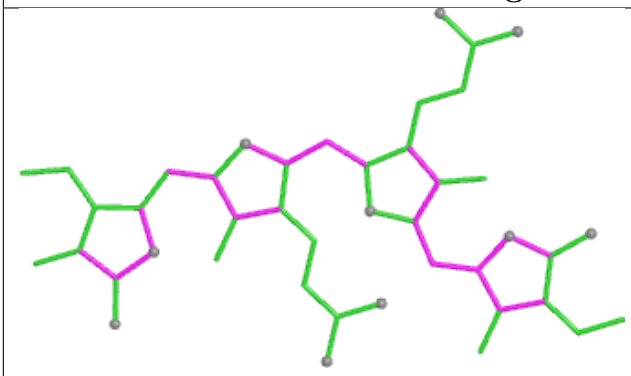


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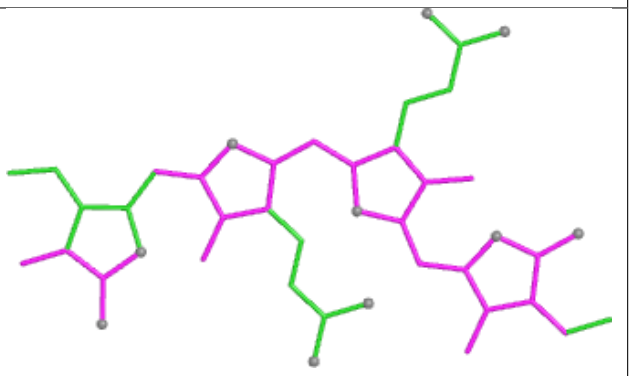


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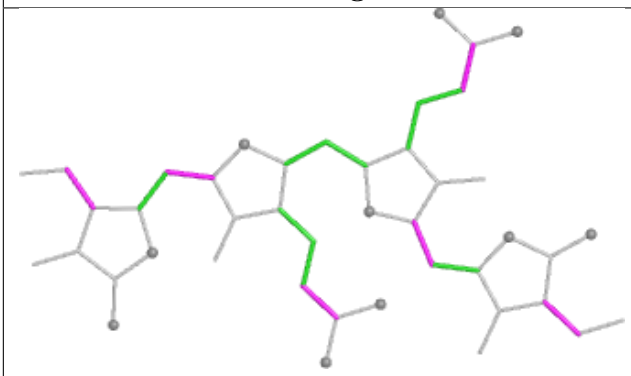
Ligand CYC E1 1001



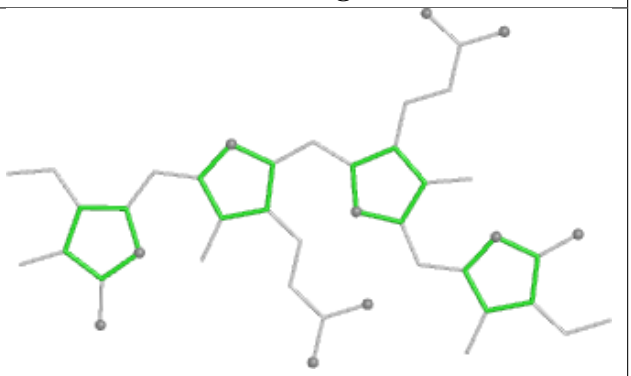
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Bond angles

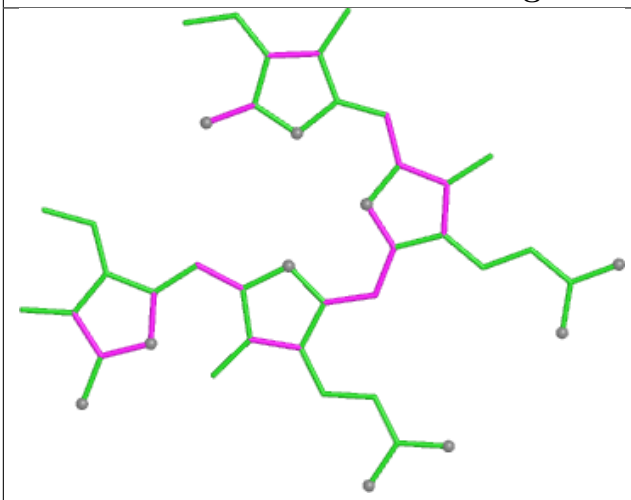


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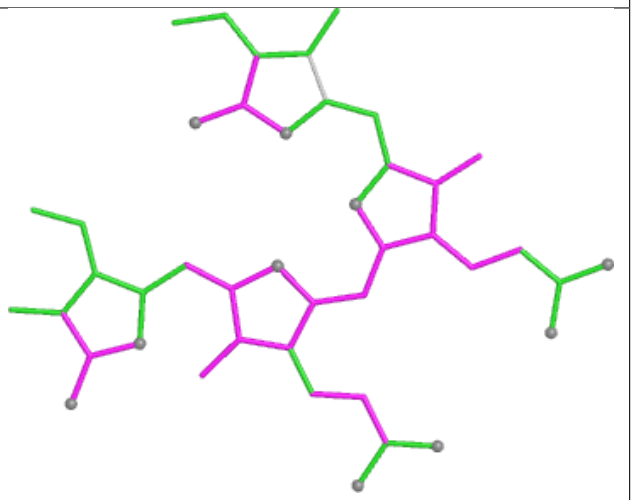


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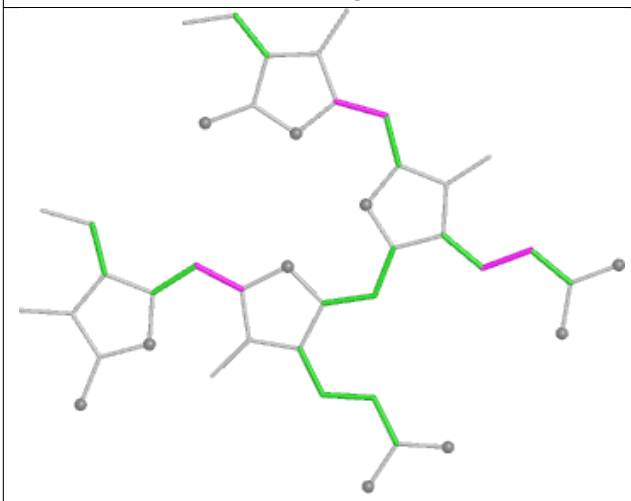
Ligand PEB iJ 201



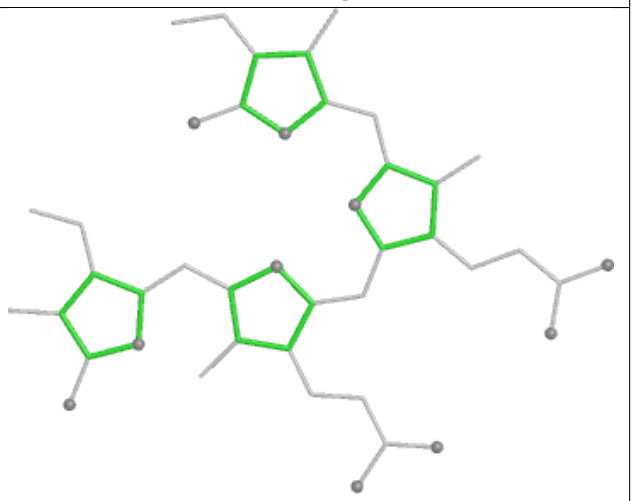
Bond lengths



Bond angles

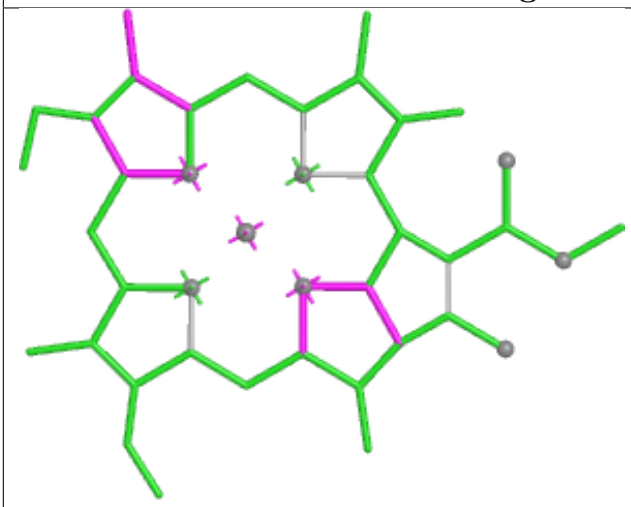


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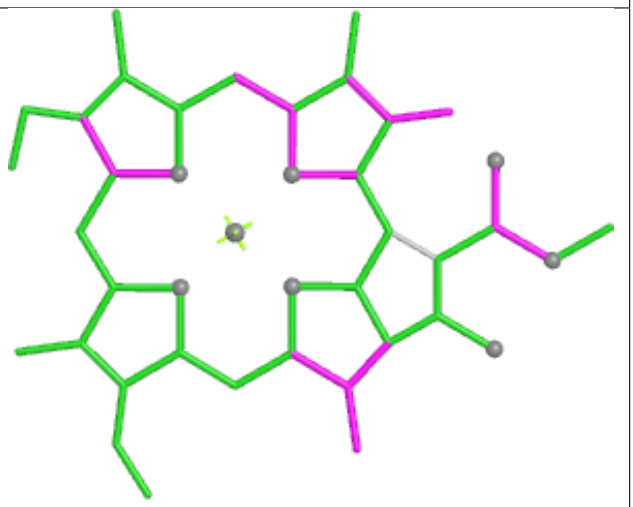


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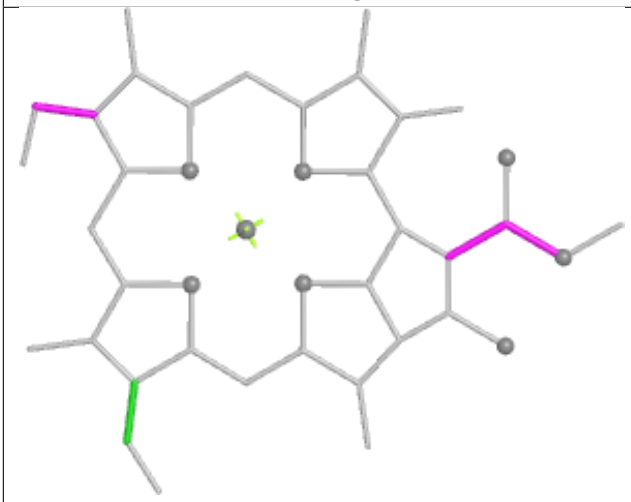
Ligand CLA 22 610



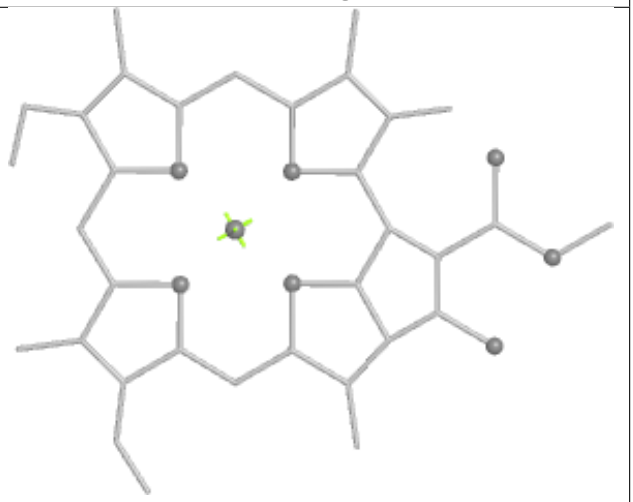
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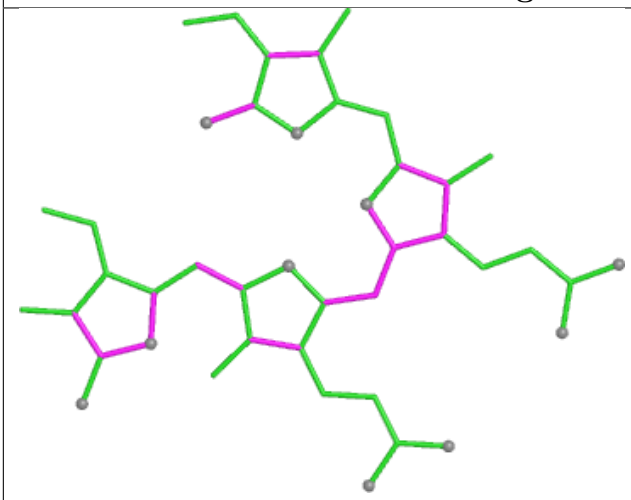


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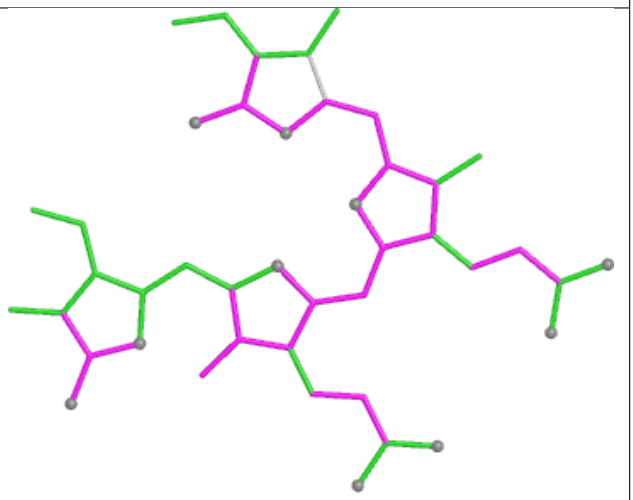


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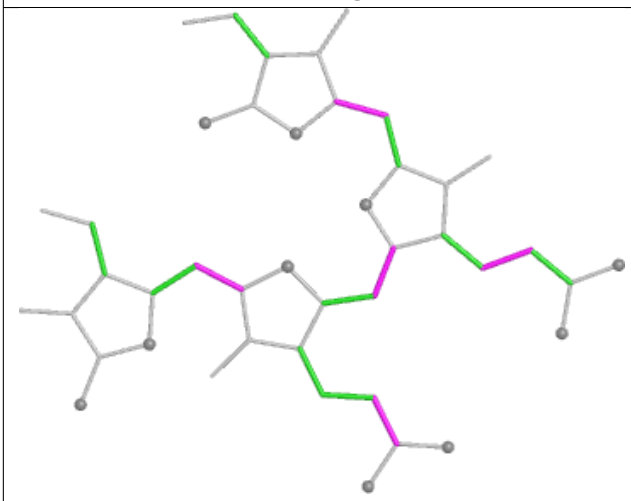
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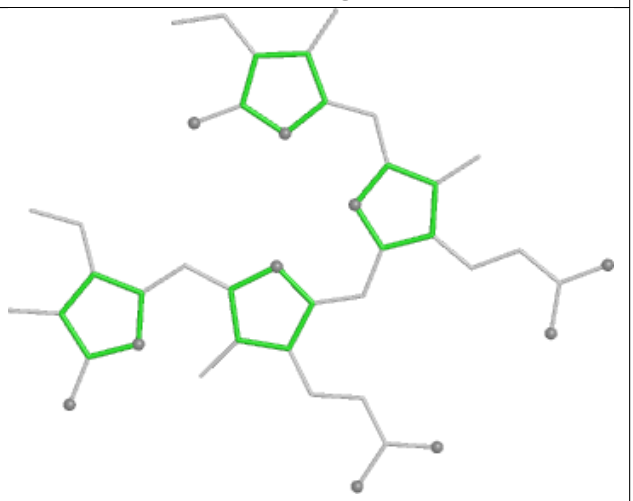
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Bond angles

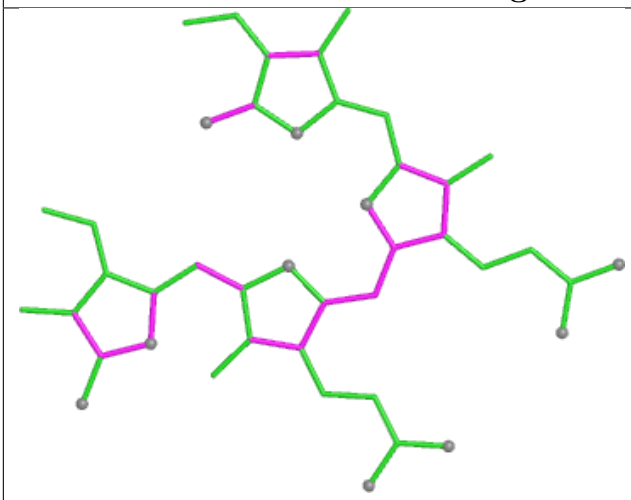


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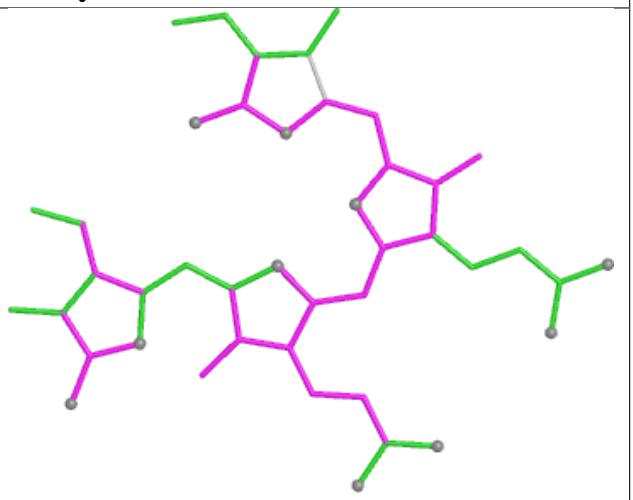


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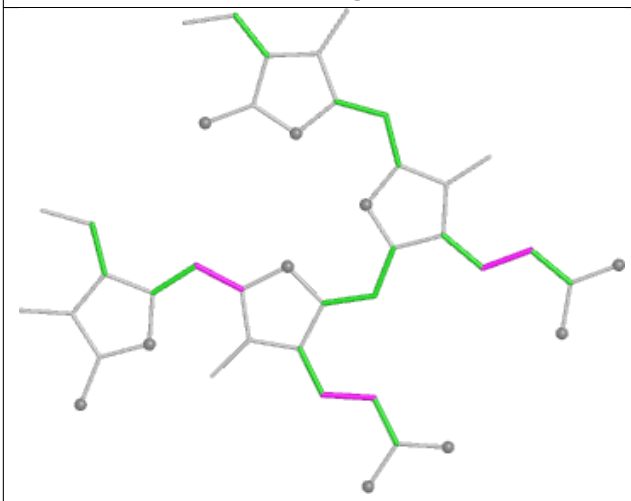
Ligand PEB GQ 201



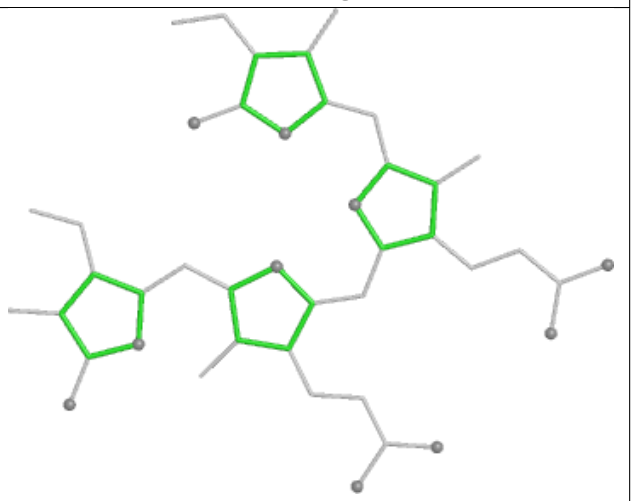
Bond lengths



Bond angles

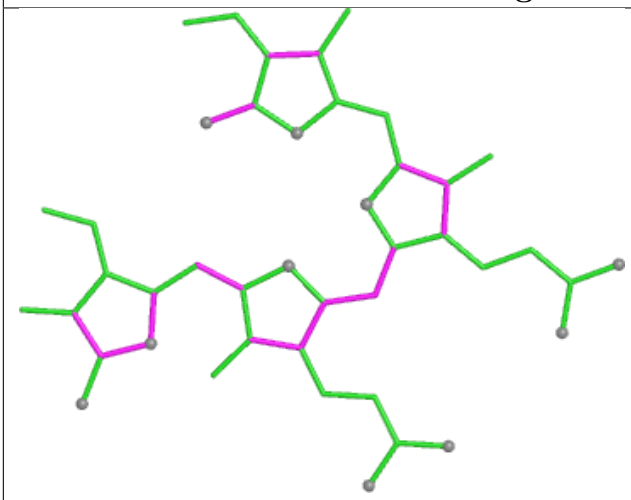


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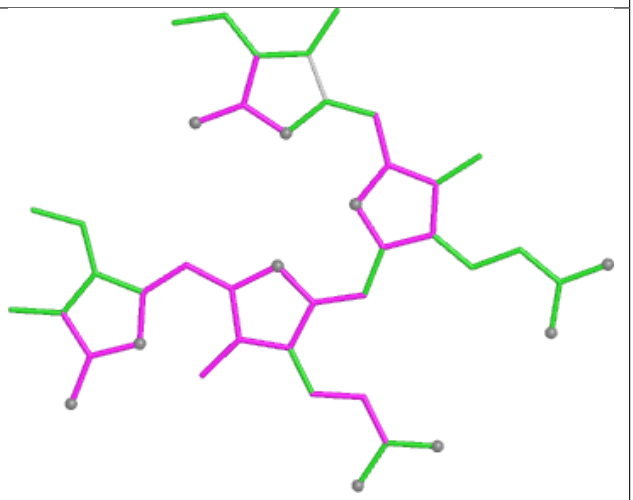


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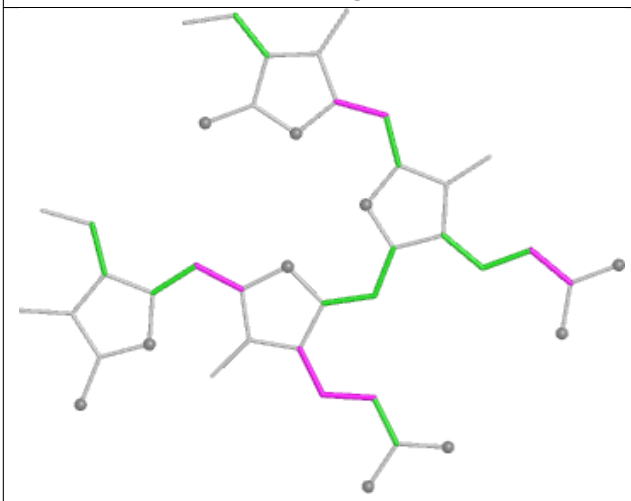
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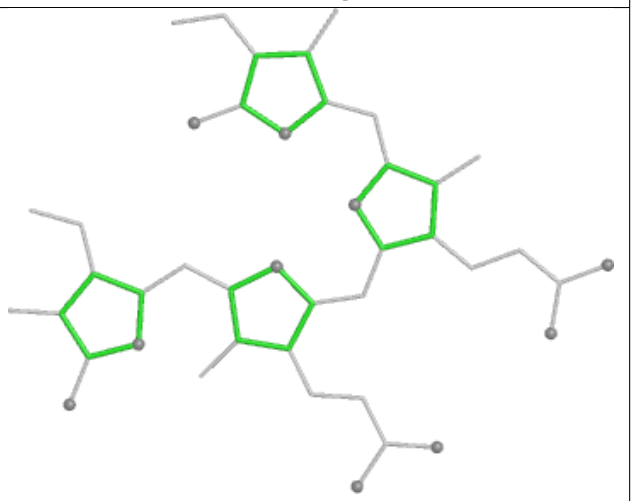
Bond lengths



Bond angles

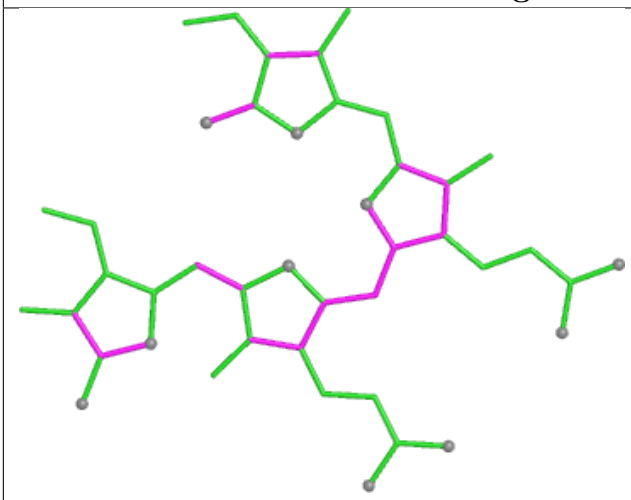


Torsions

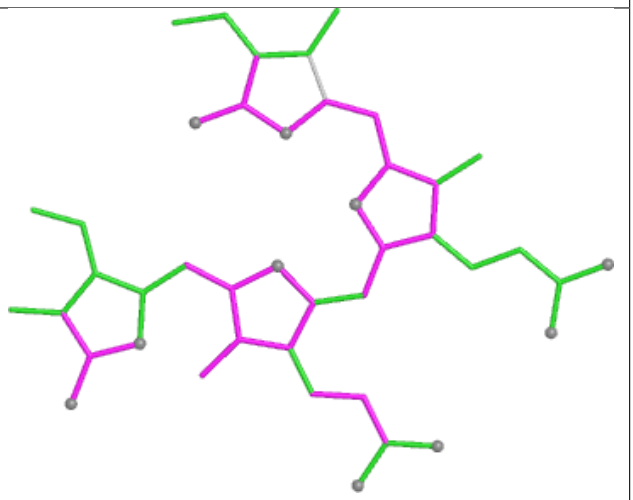


Rings

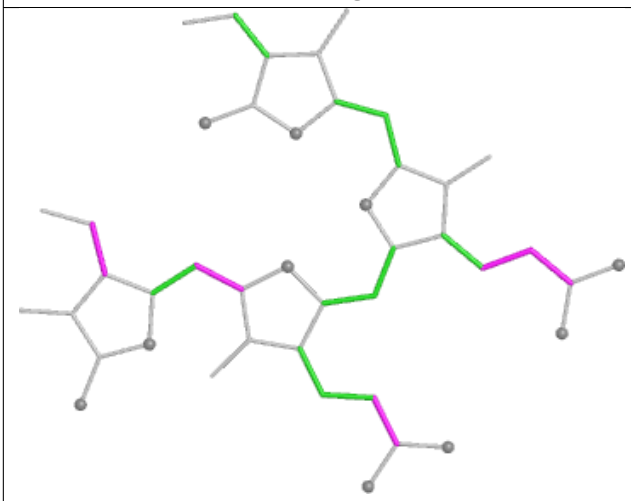
Ligand PEB CP 203



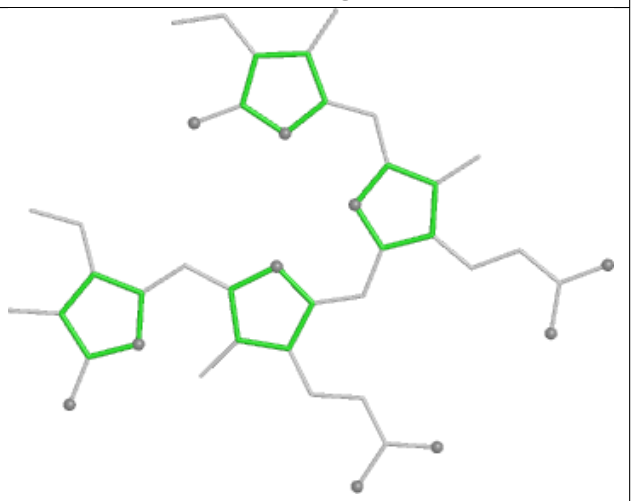
Bond lengths



Bond angles

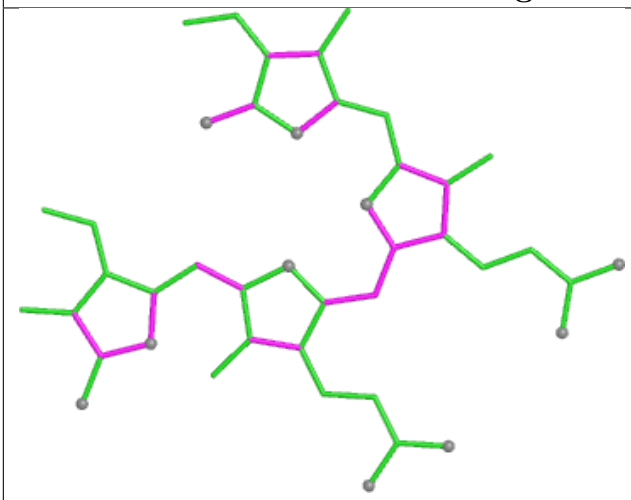


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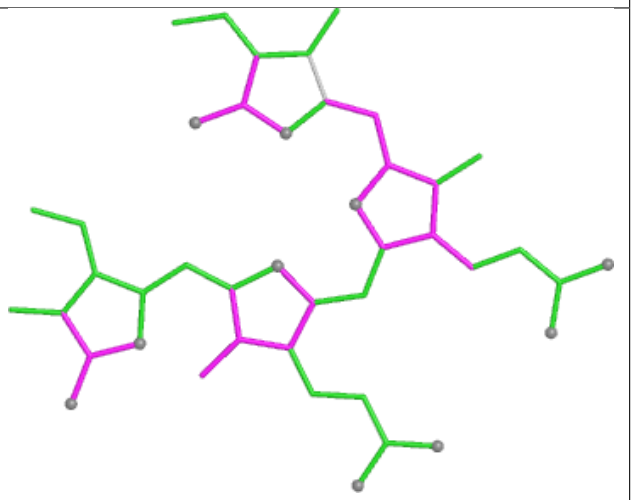


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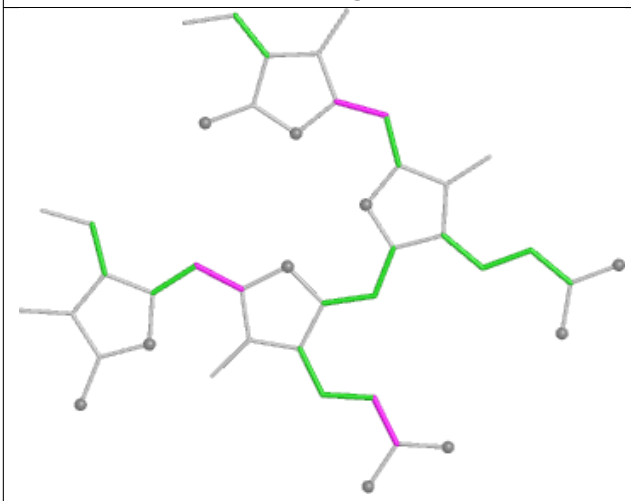
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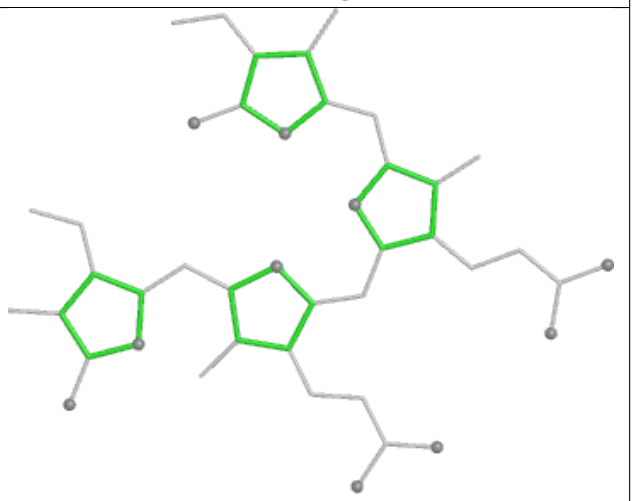
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Bond angles

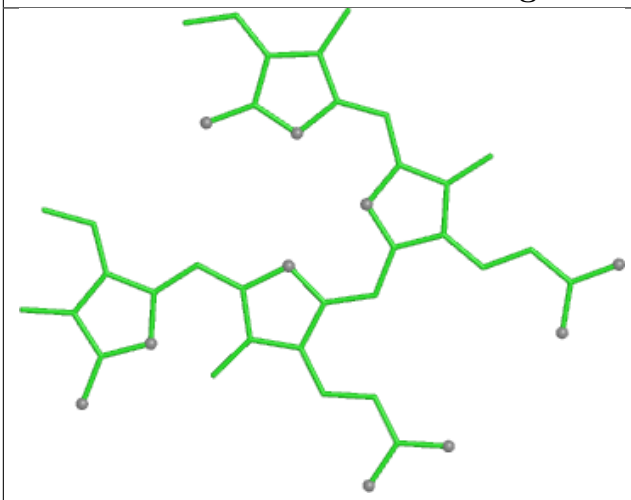


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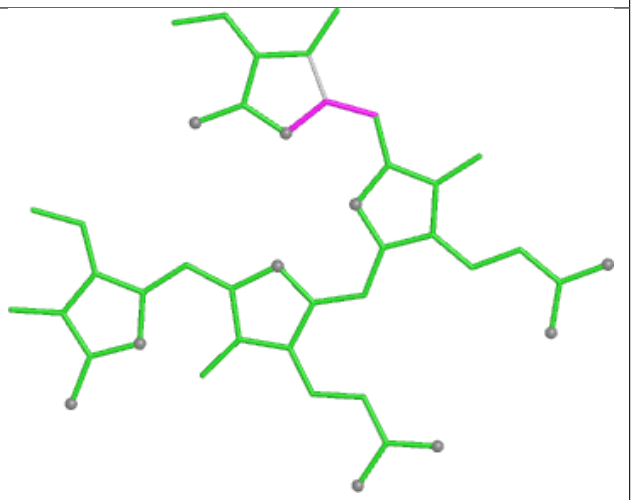


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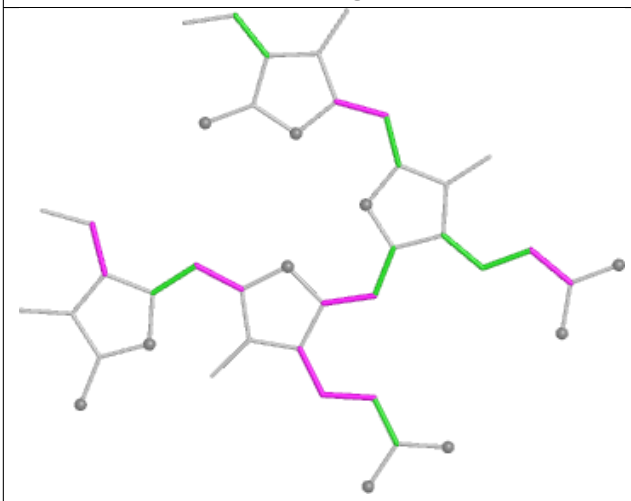
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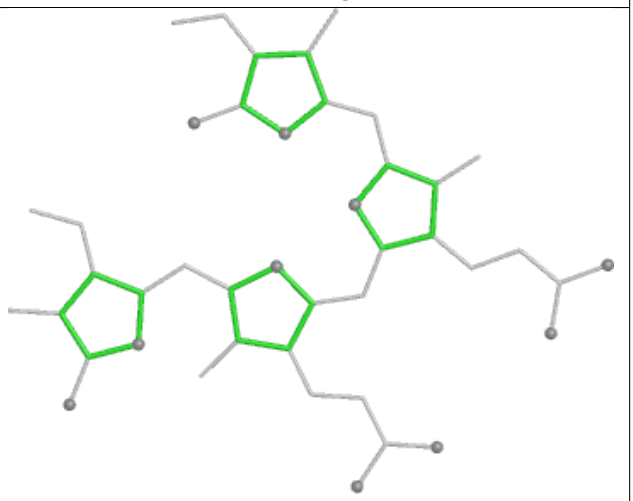
Bond lengths



Bond angles

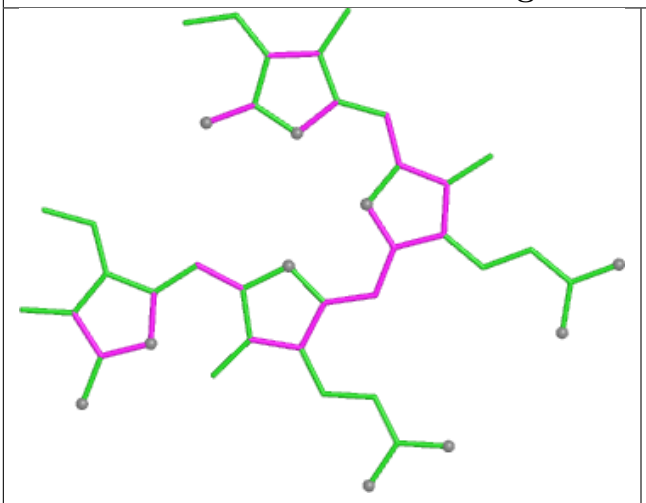


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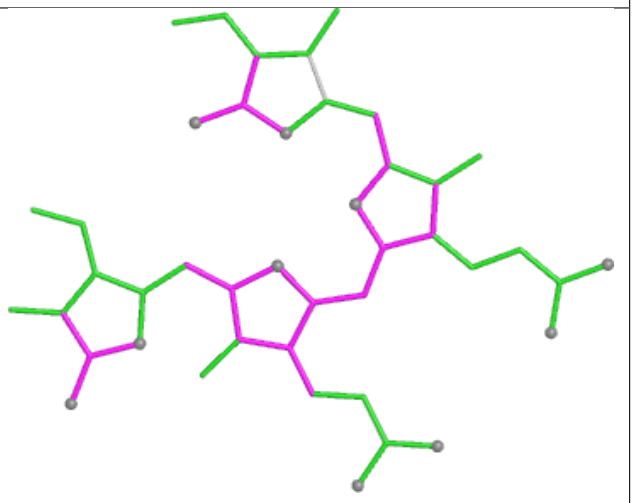


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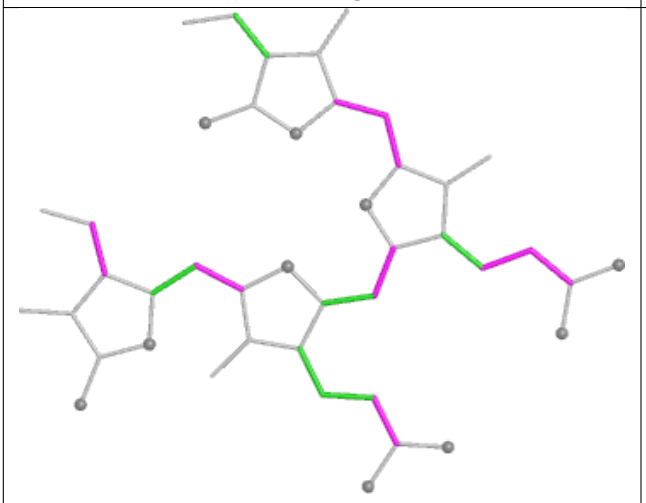
Ligand PEB xF 302



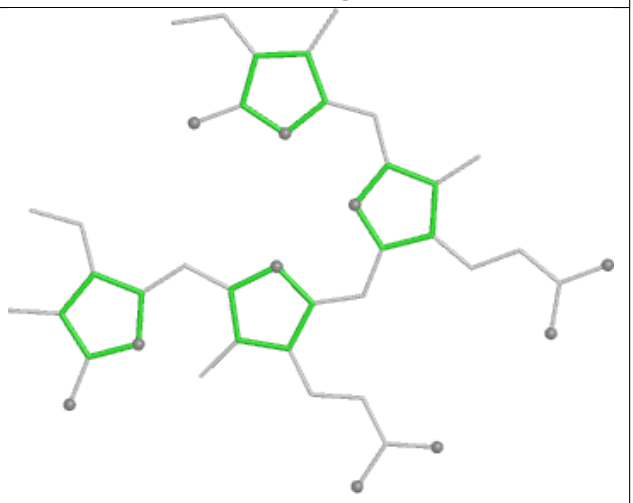
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Bond angles

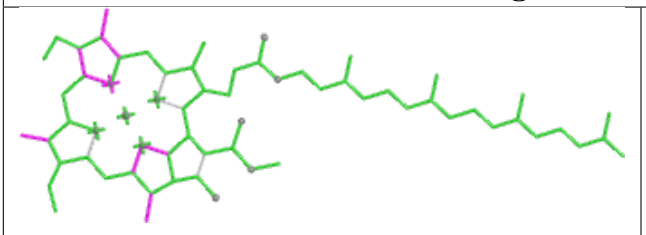


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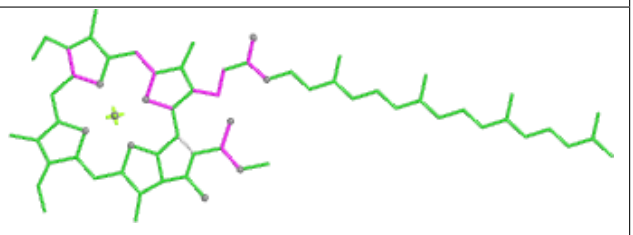


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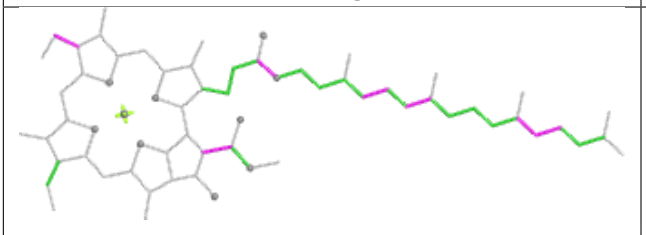
Ligand CLA BN 810



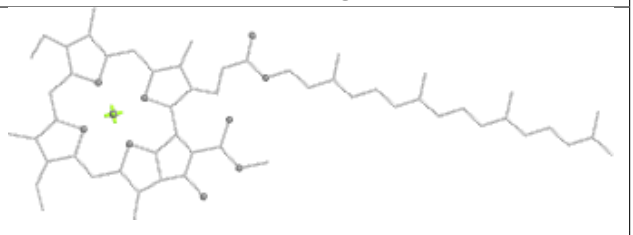
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Bond angles

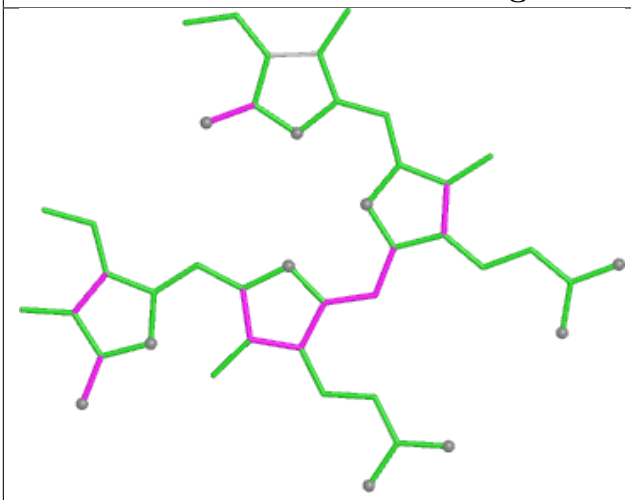


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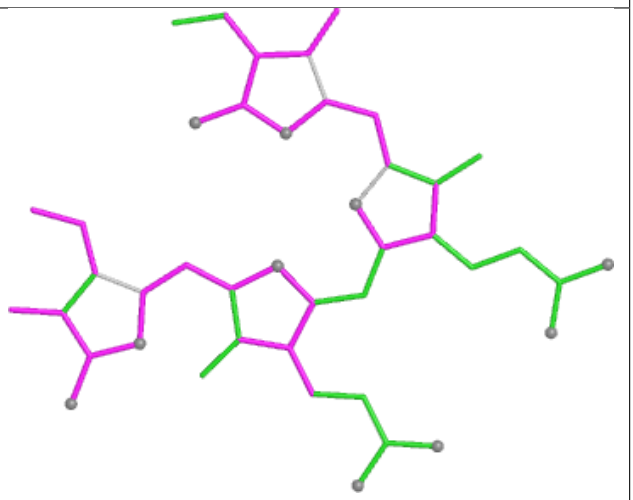


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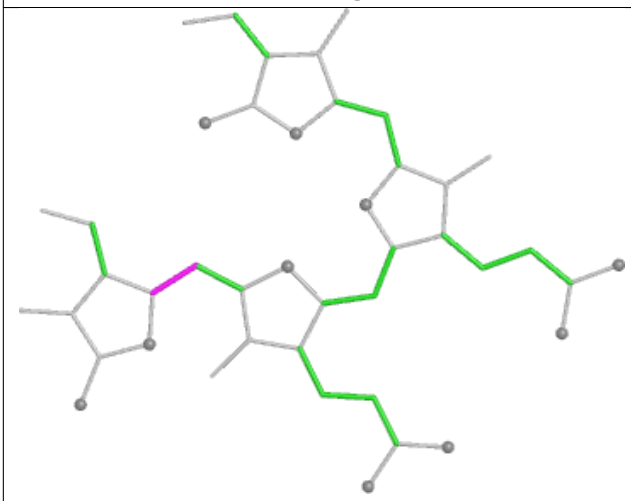
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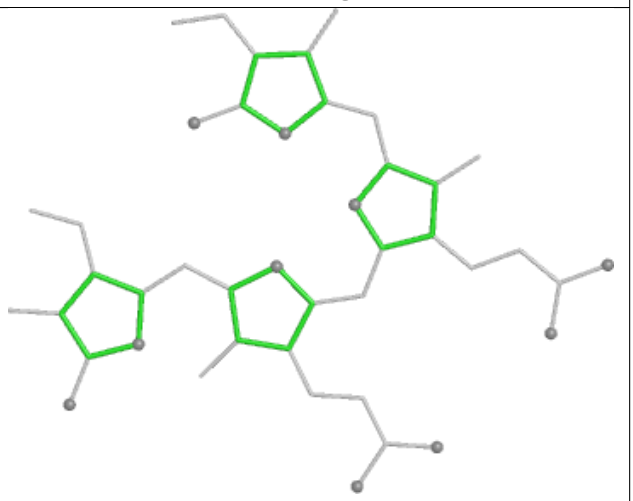
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Bond angles

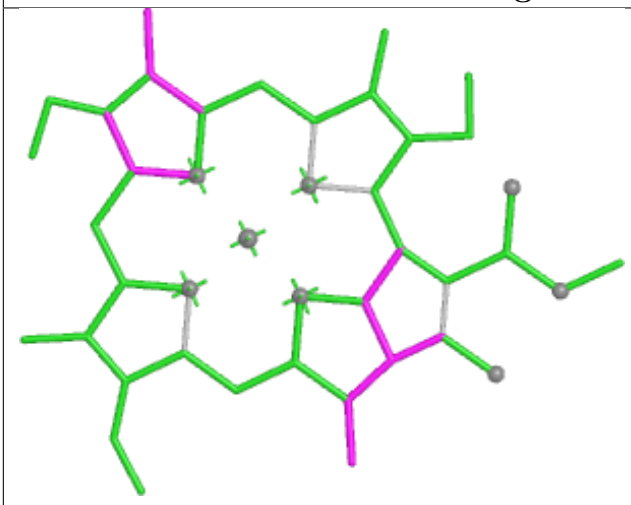


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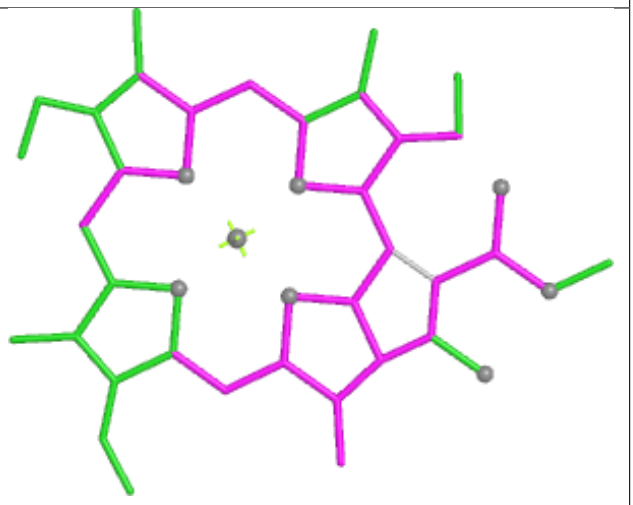


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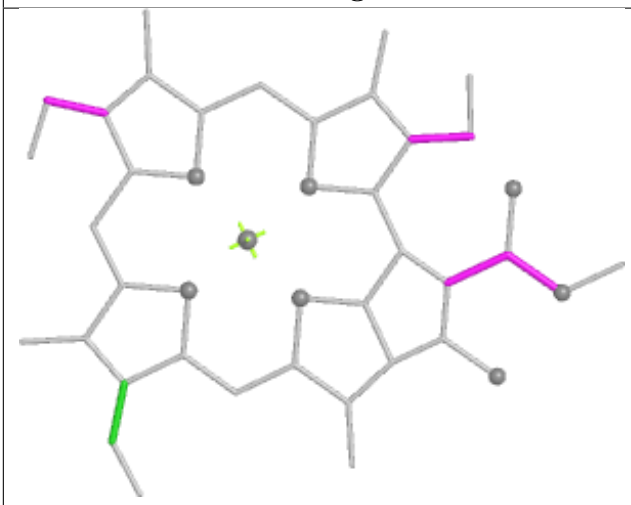
Ligand CLA 4N 604



Bond lengths



Bond angles

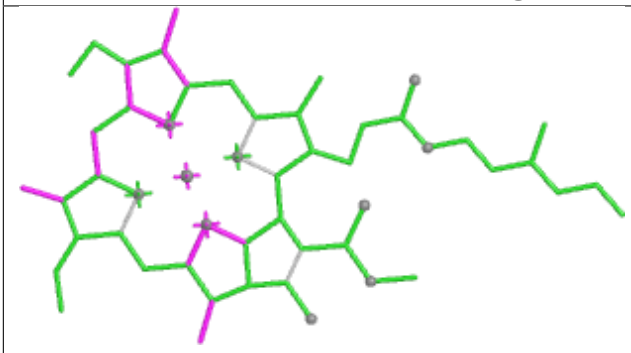


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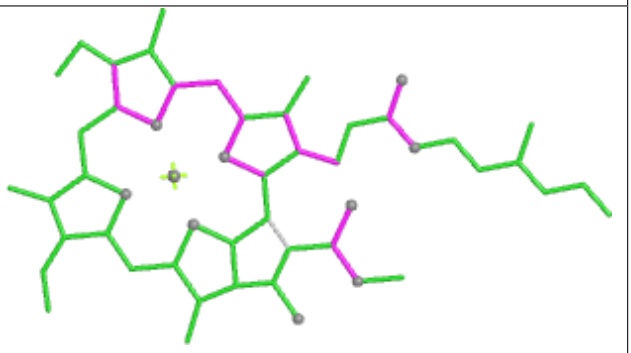


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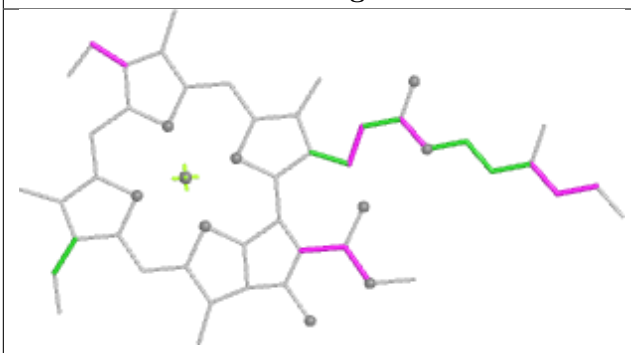
Ligand CLA AN 803



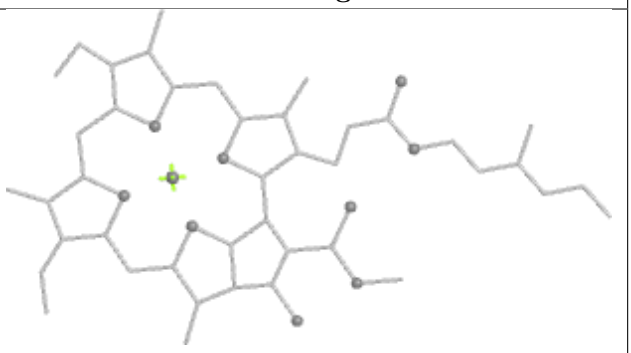
Bond lengths



Bond angles

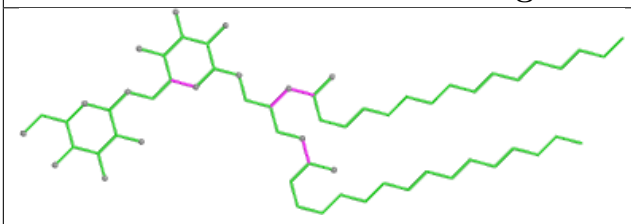


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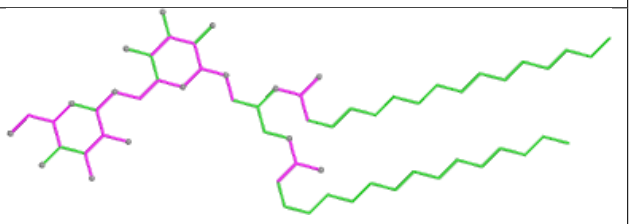


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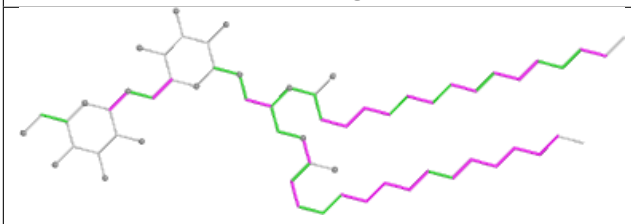
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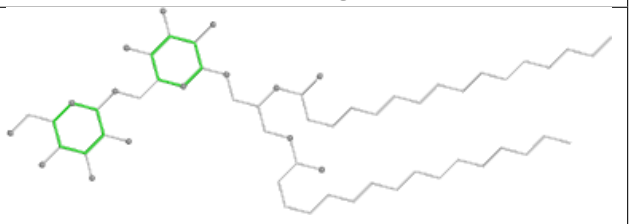
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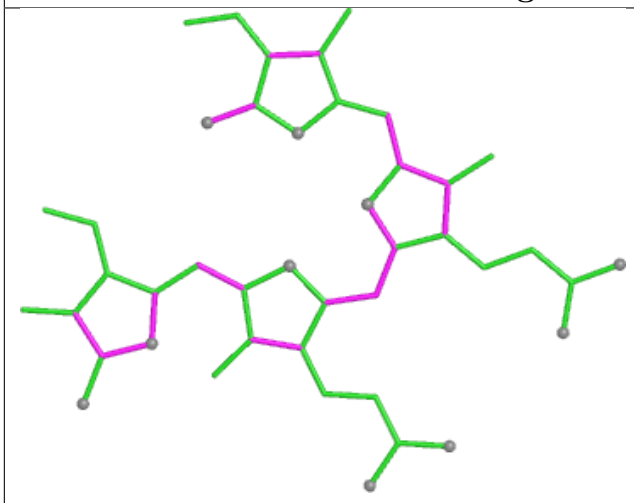


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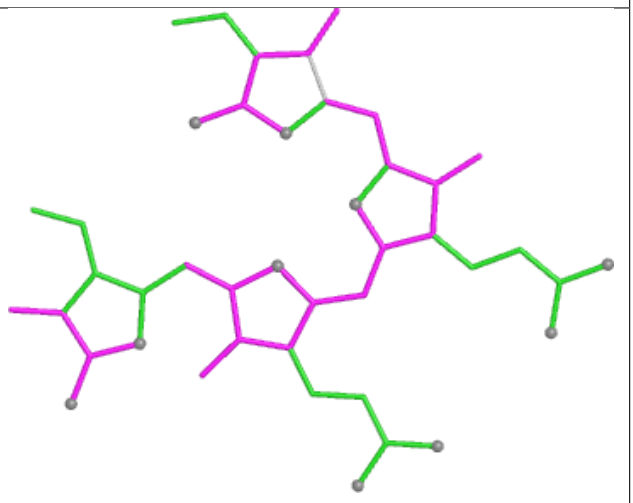


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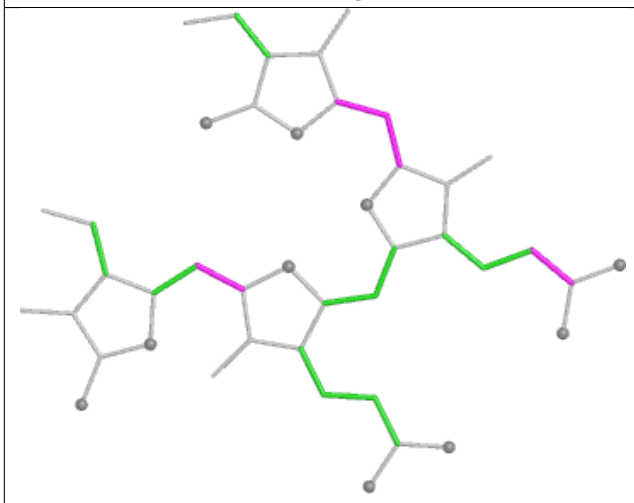
Ligand PEB TJ 201



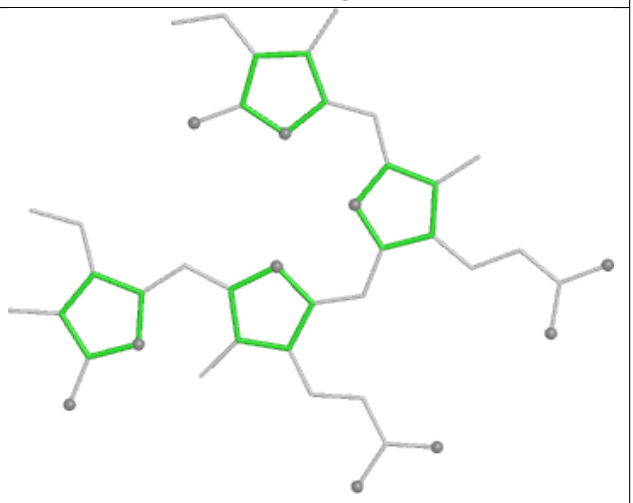
Bond lengths



Bond angles



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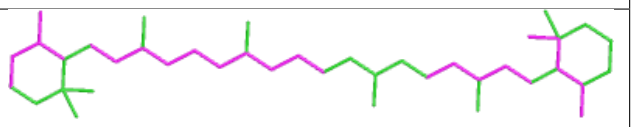


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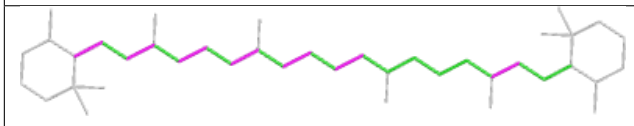
Ligand BCR AN 845



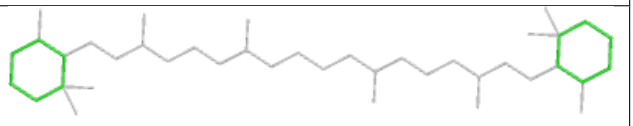
Bond lengths



Bond angles

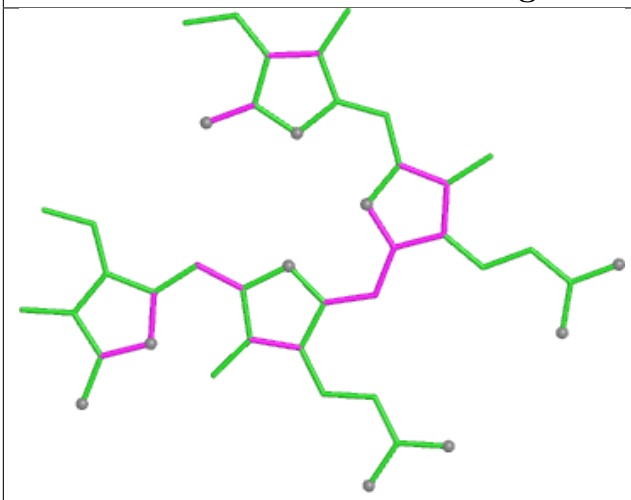


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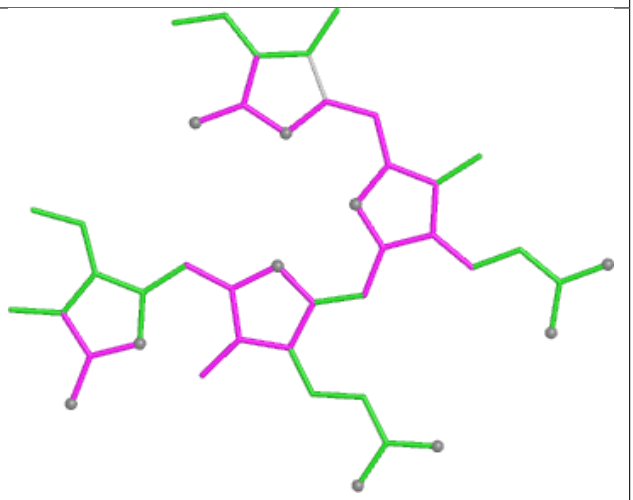


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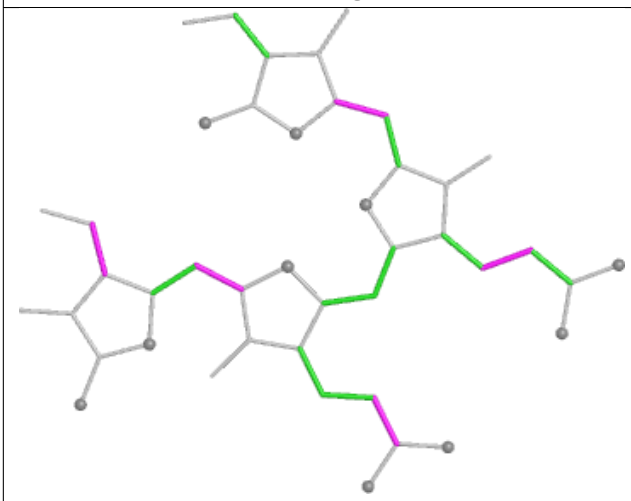
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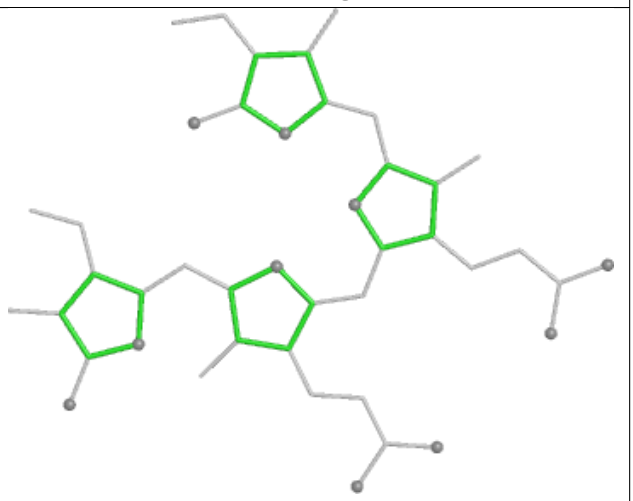
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Bond angles

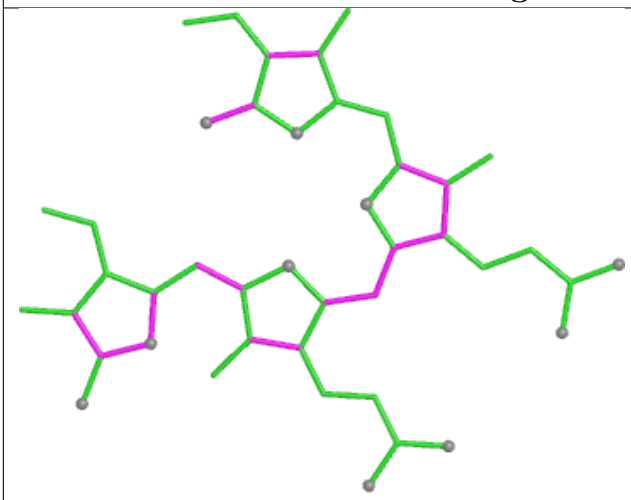


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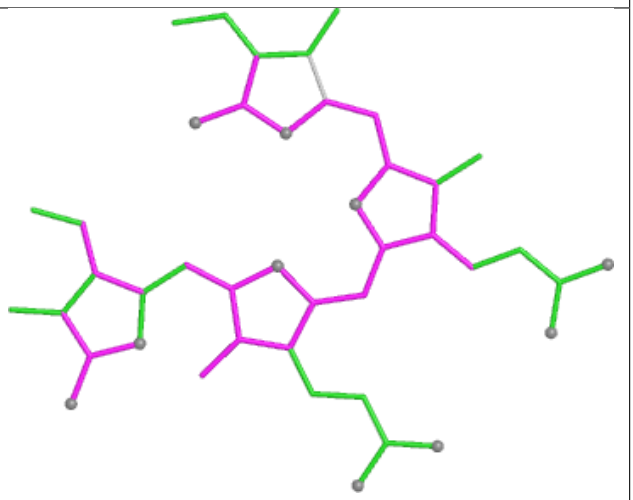


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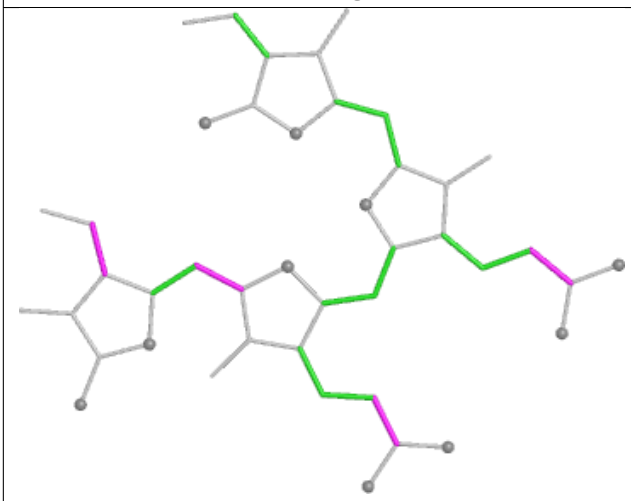
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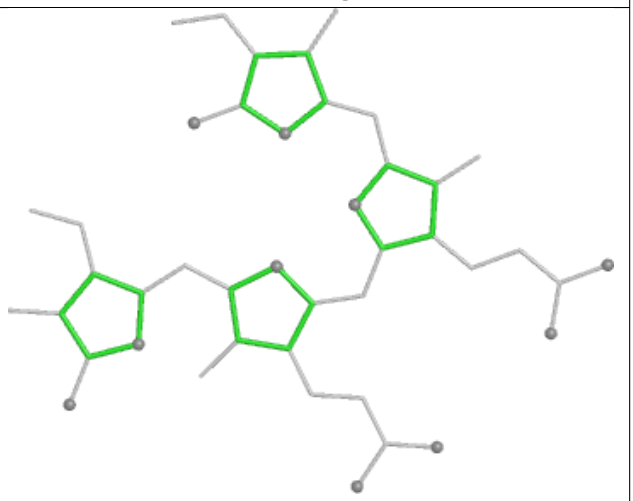
Bond lengths



Bond angles

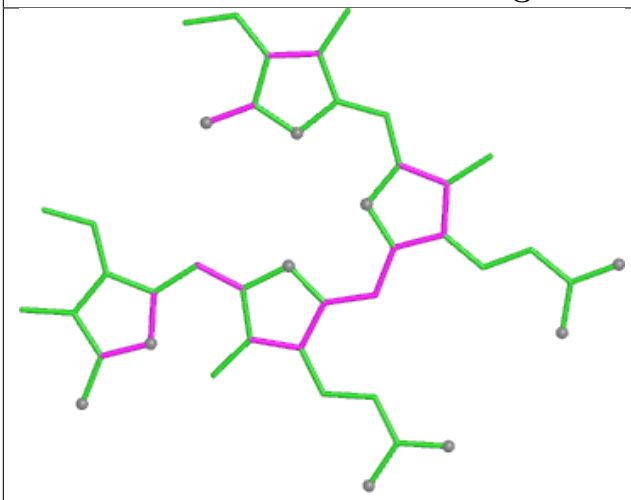


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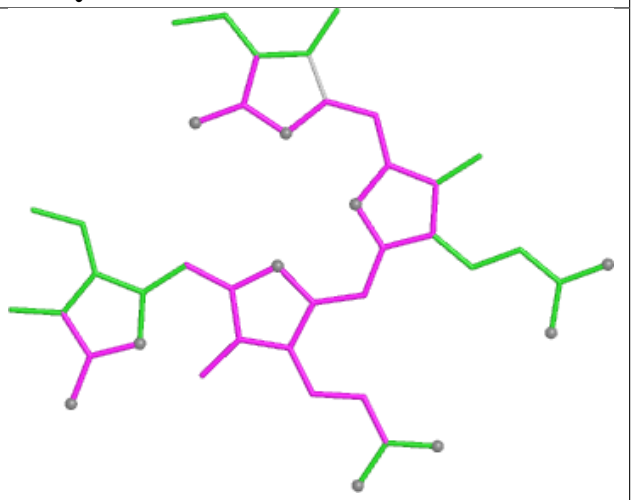


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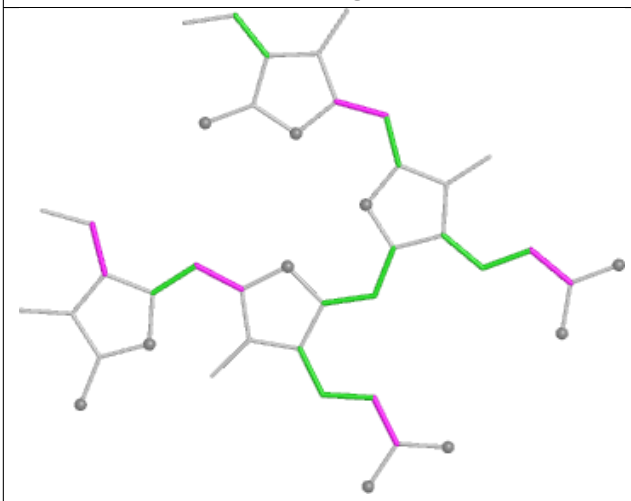
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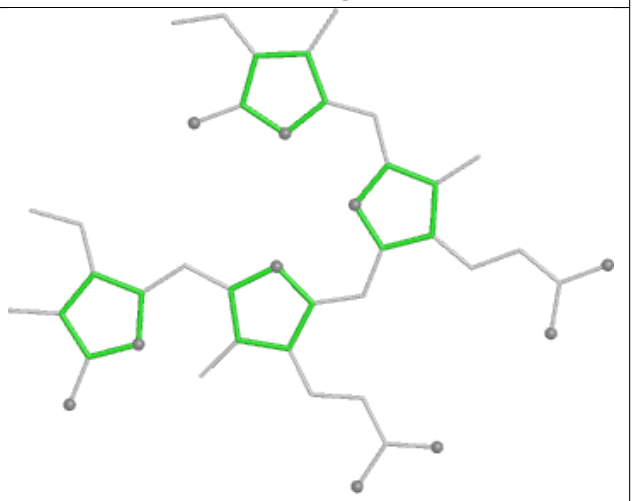
Bond lengths



Bond angles

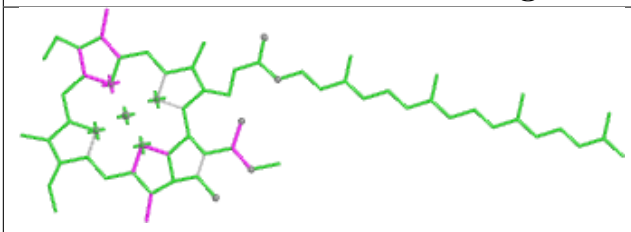


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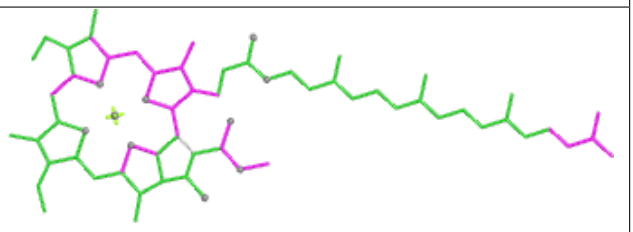


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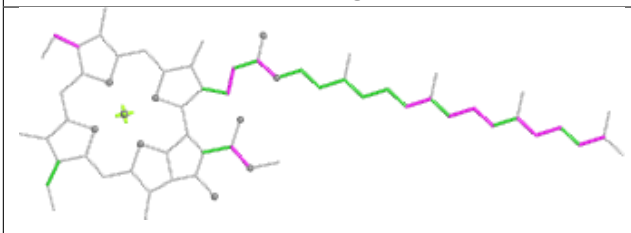
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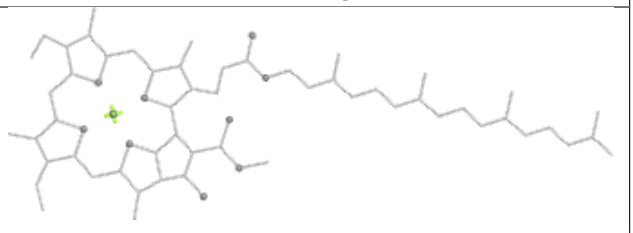
Bond lengths



Bond angles

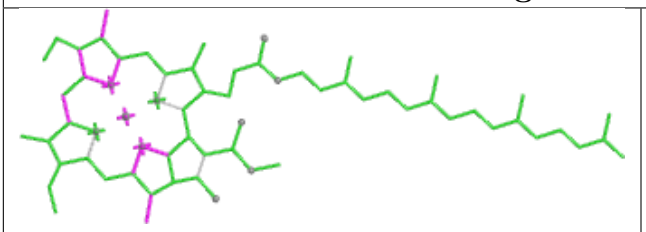


Torsions

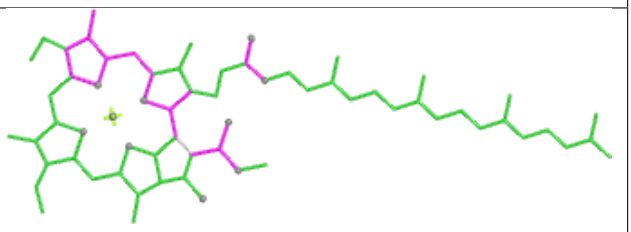


Rings

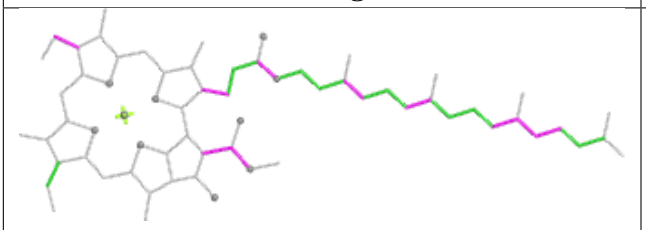
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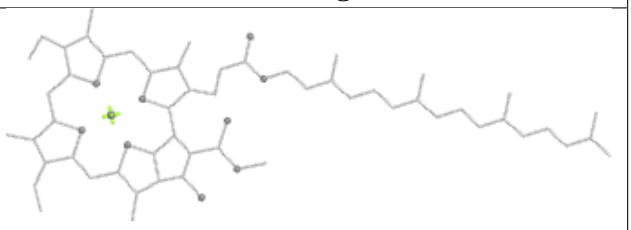
Bond lengths



Bond angles

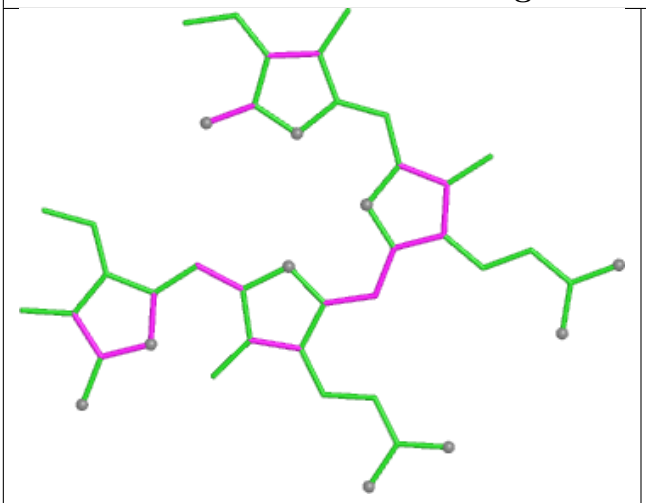


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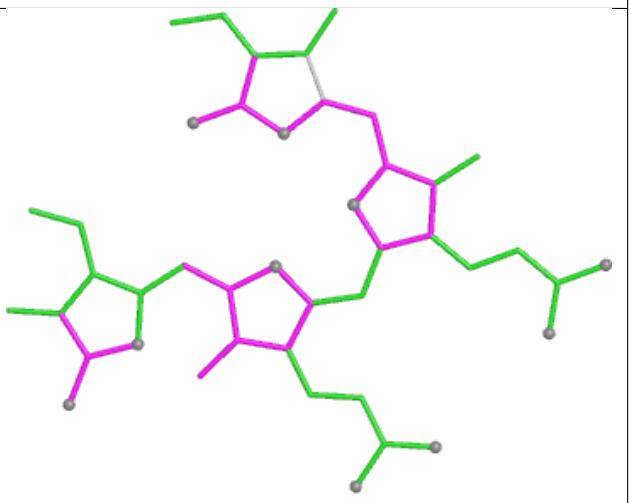


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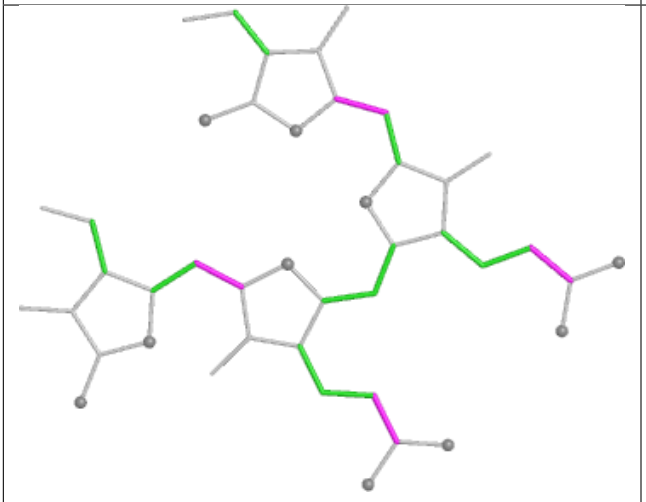
Ligand PEB bO 202



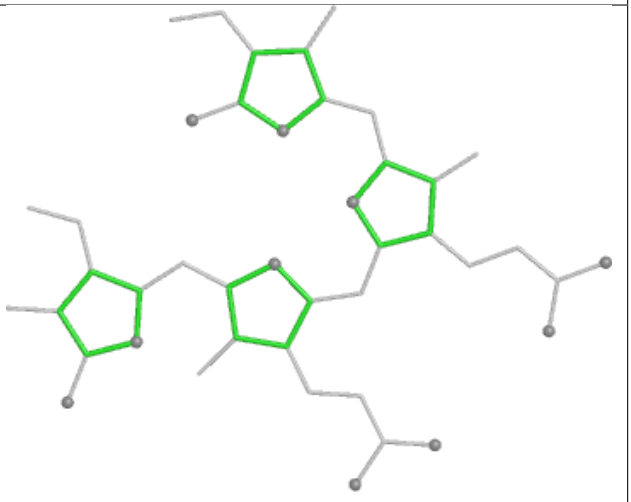
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Bond angles

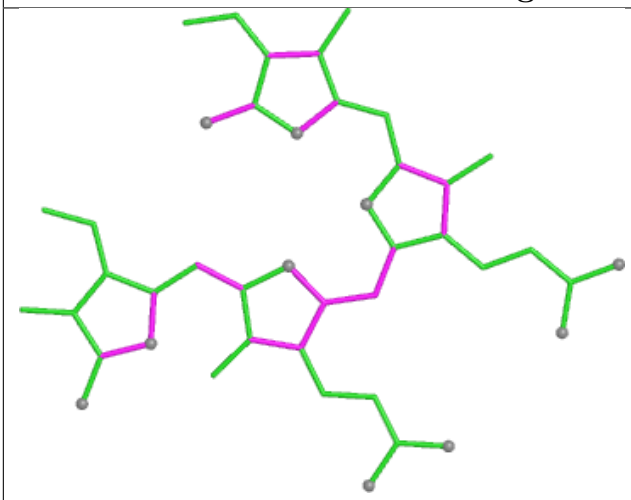


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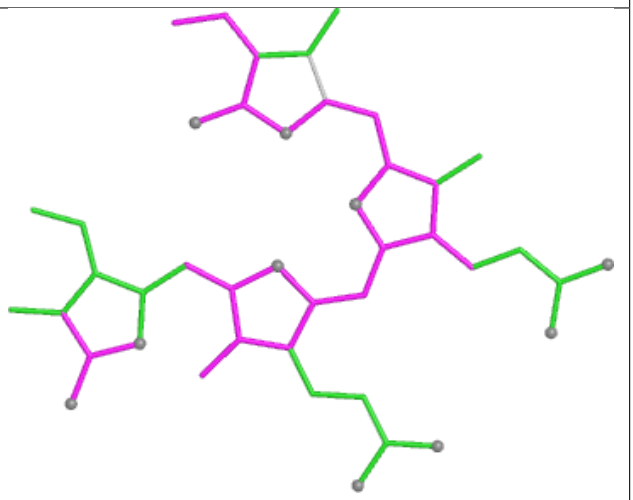


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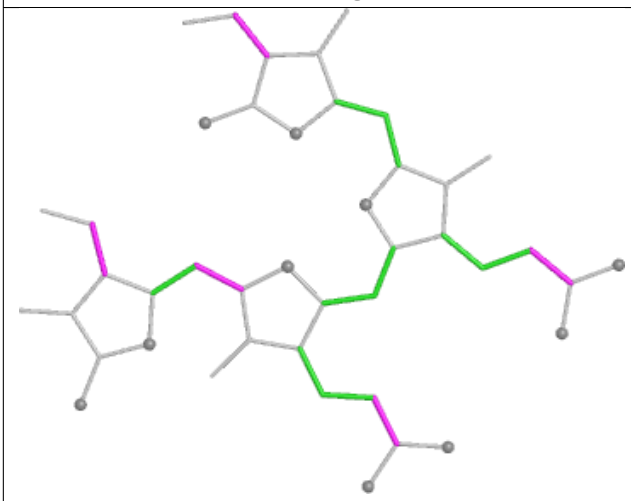
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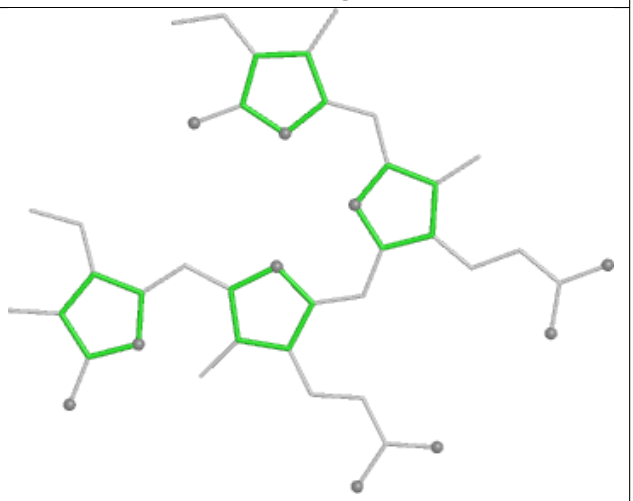
Bond lengths



Bond angles

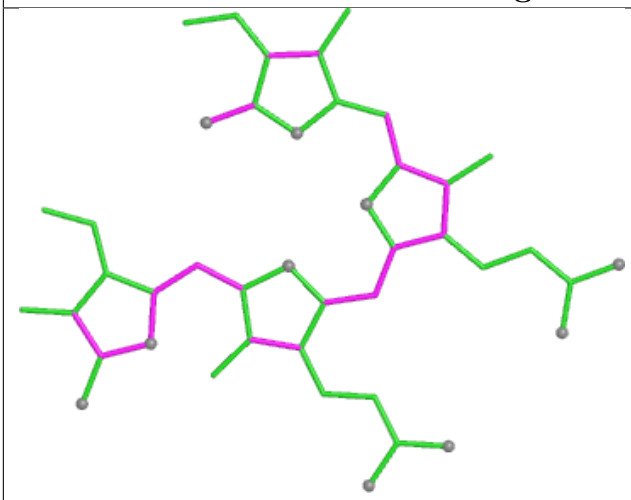


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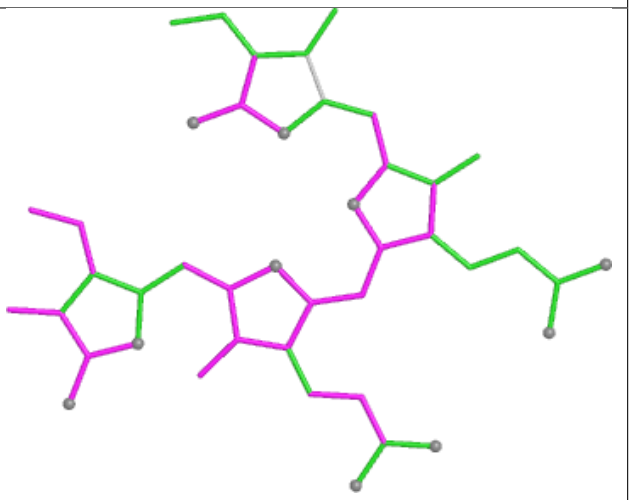


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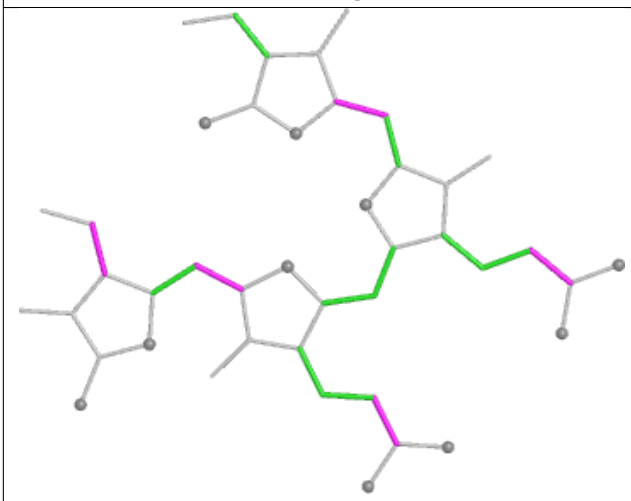
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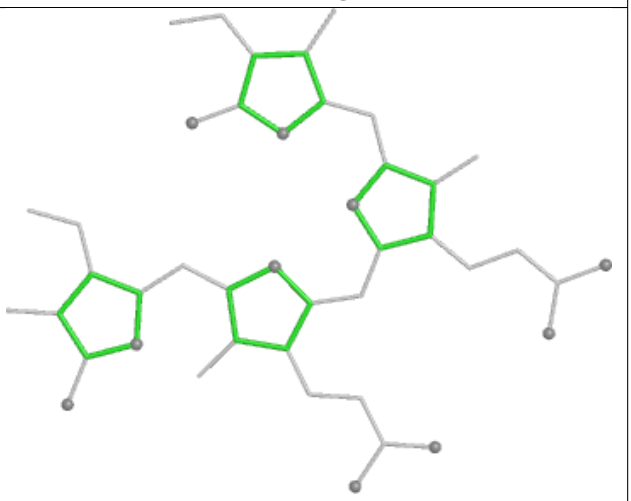
Bond lengths



Bond angles

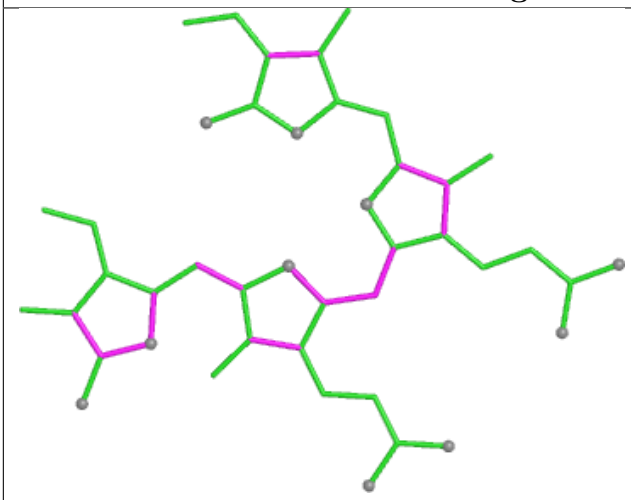


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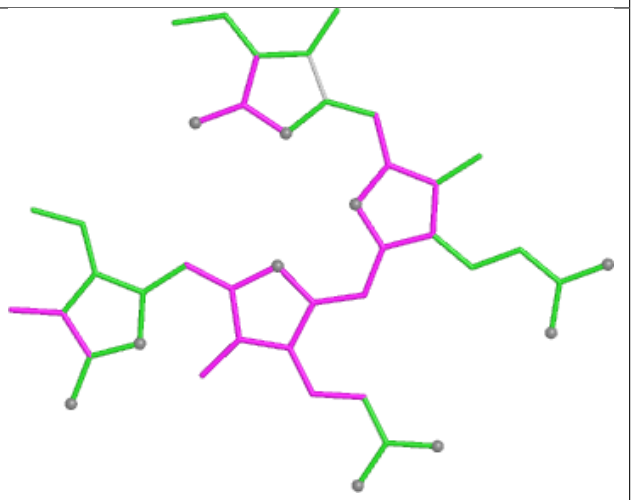


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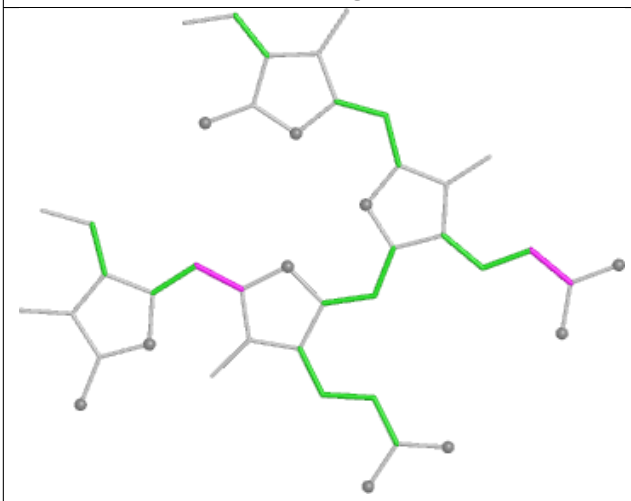
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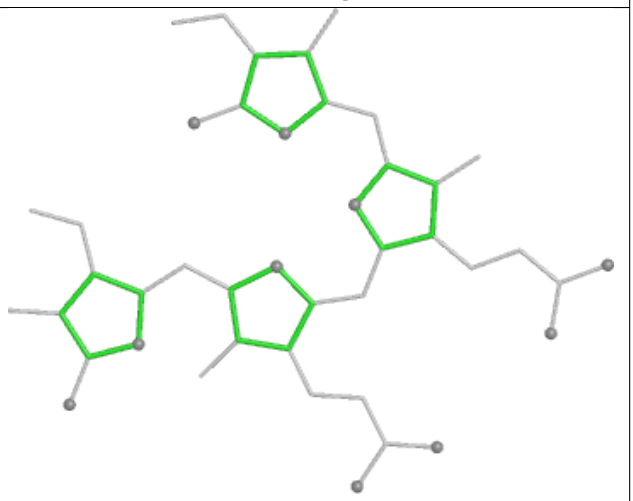
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Bond angles

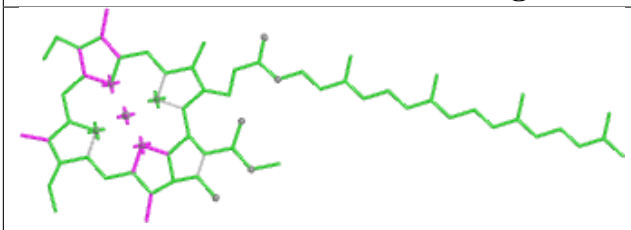


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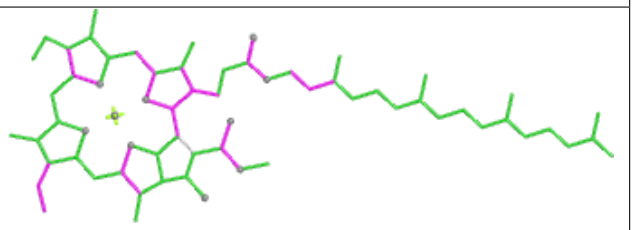


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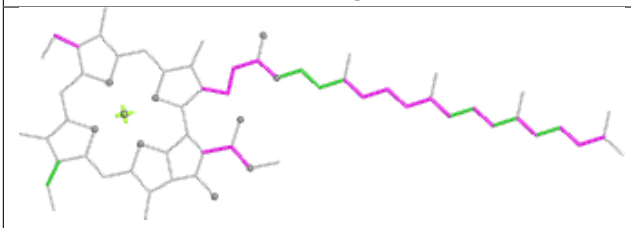
Ligand CLA BN 813



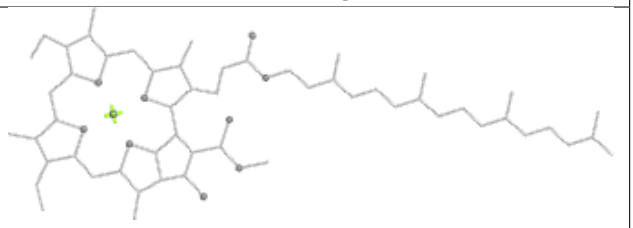
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Bond angles

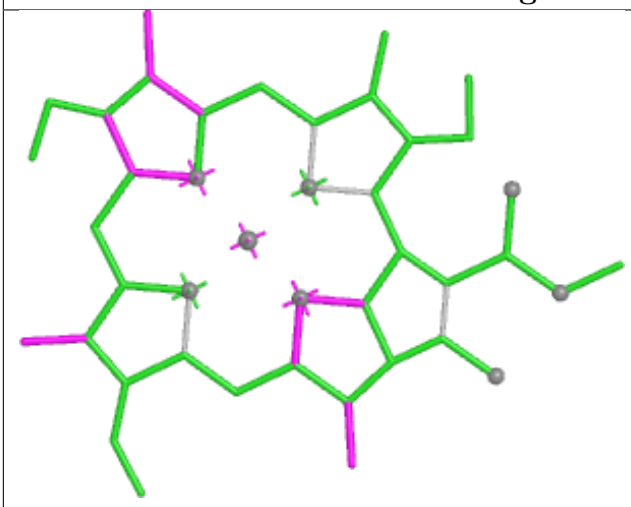


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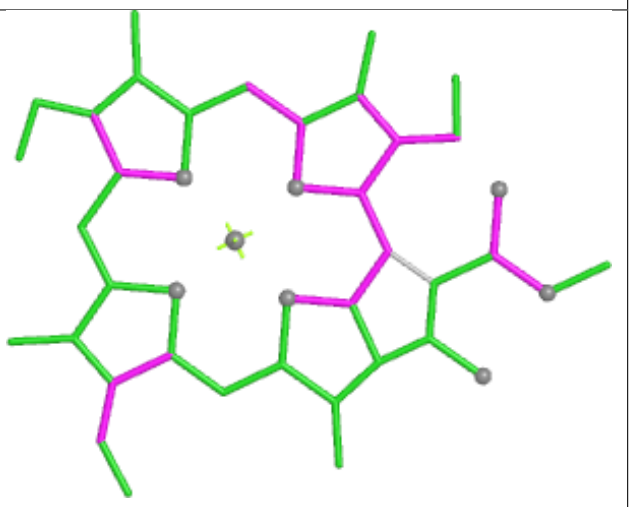


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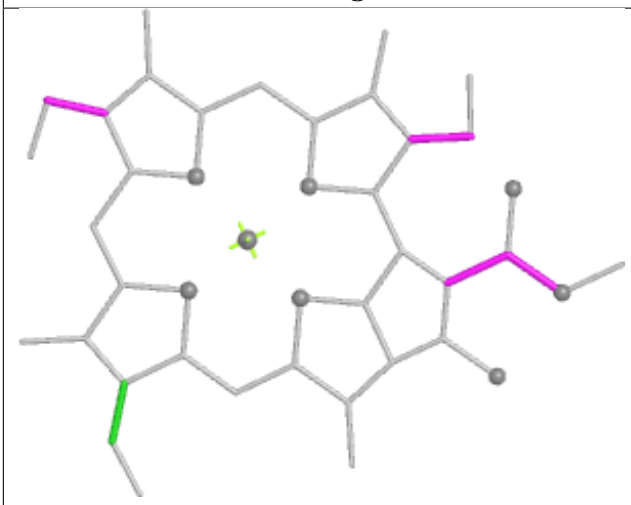
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Bond lengths



Bond angles

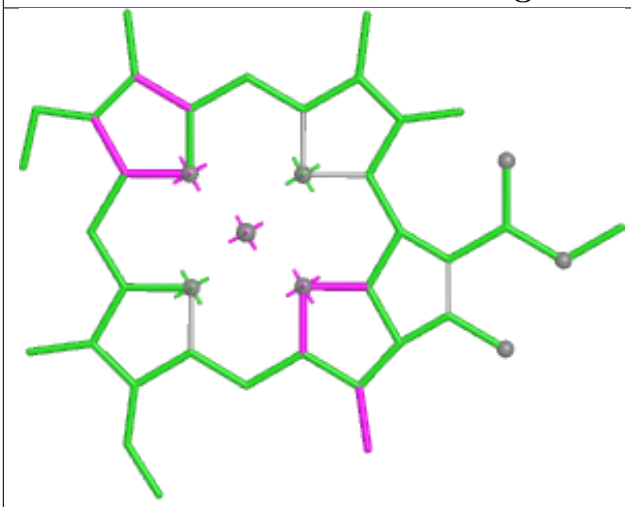


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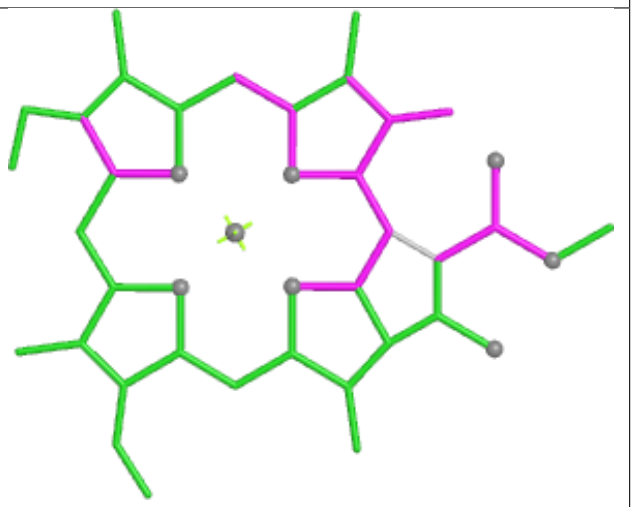


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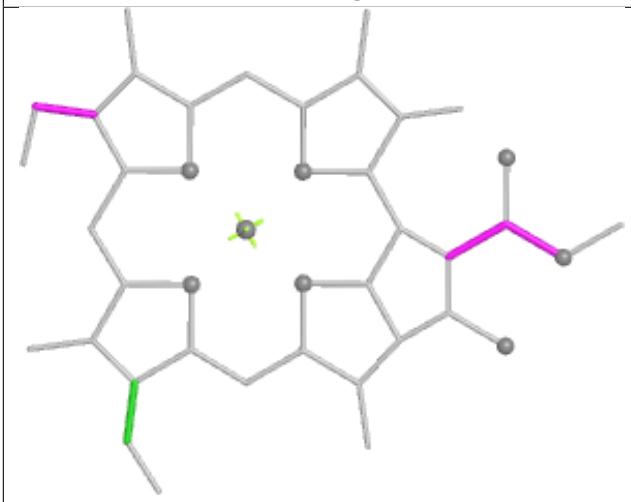
Ligand CLA 3N 310



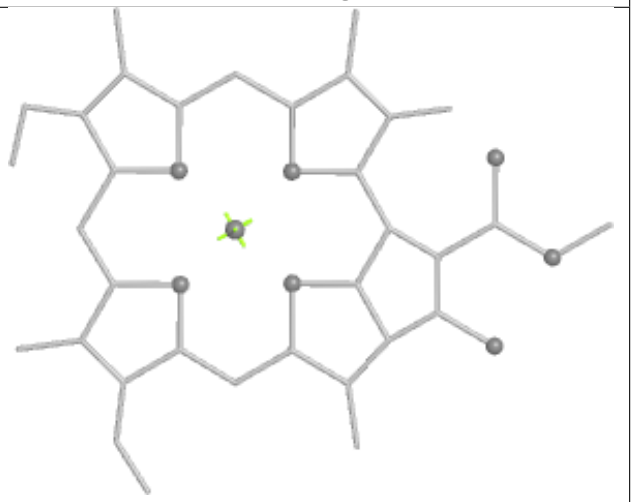
Bond lengths



Bond angles

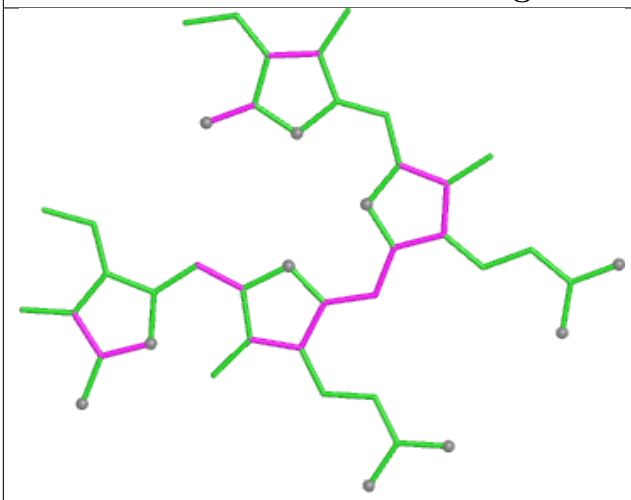


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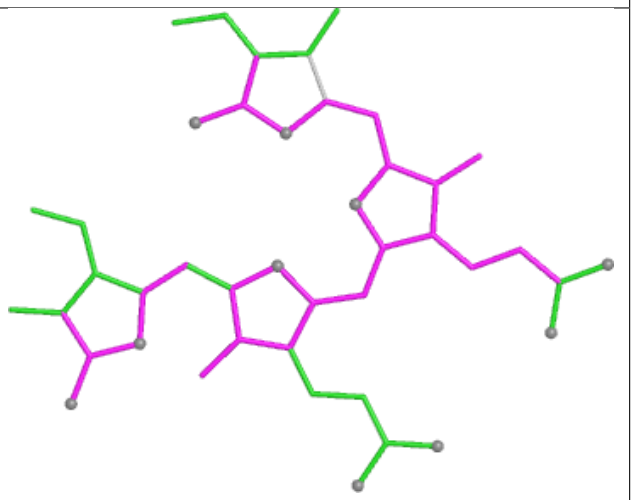


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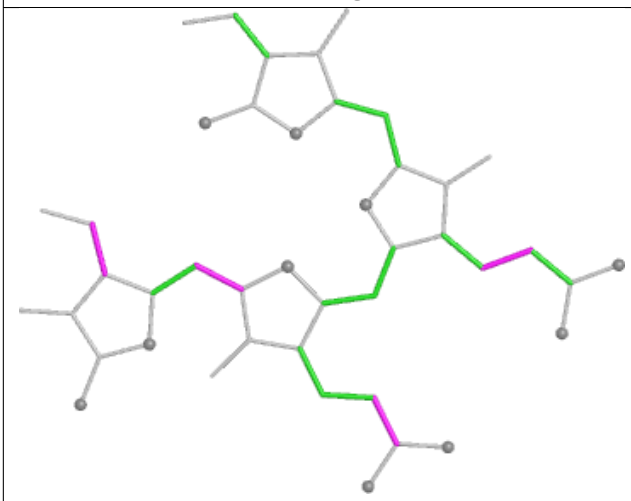
Ligand PEB PA 202



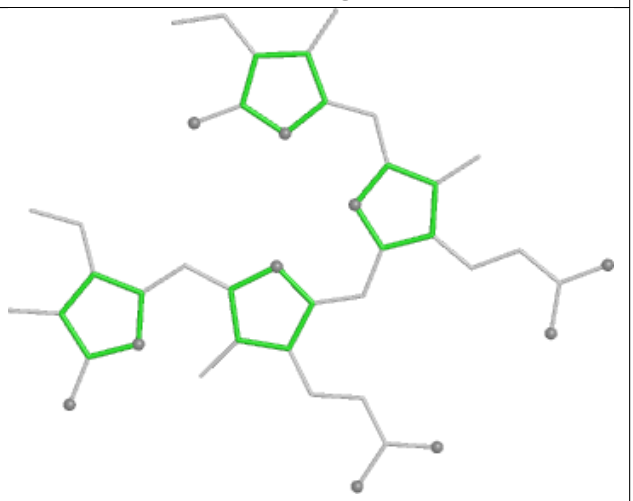
Bond lengths



Bond angles

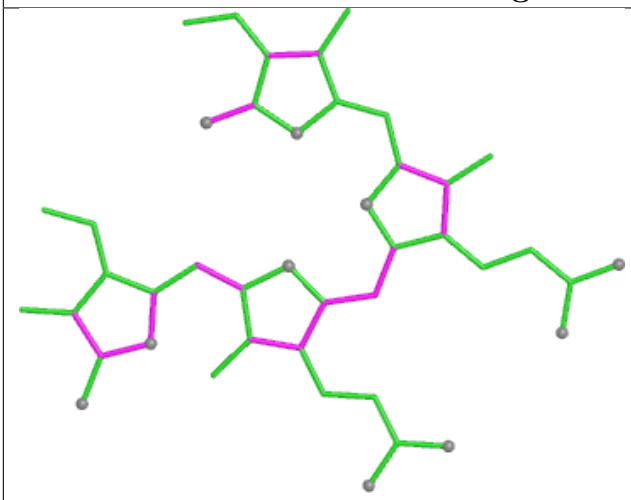


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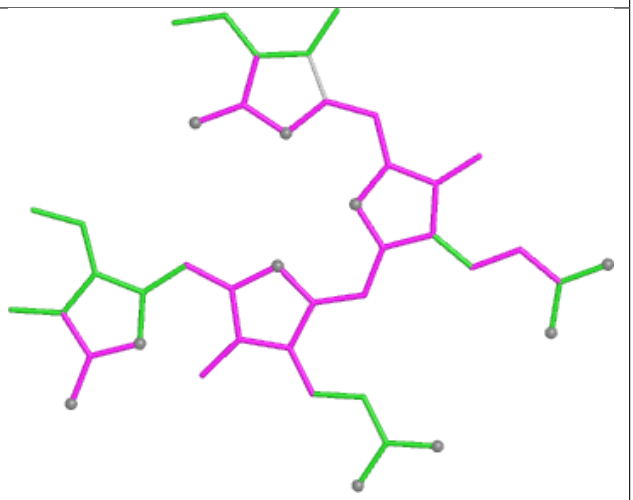


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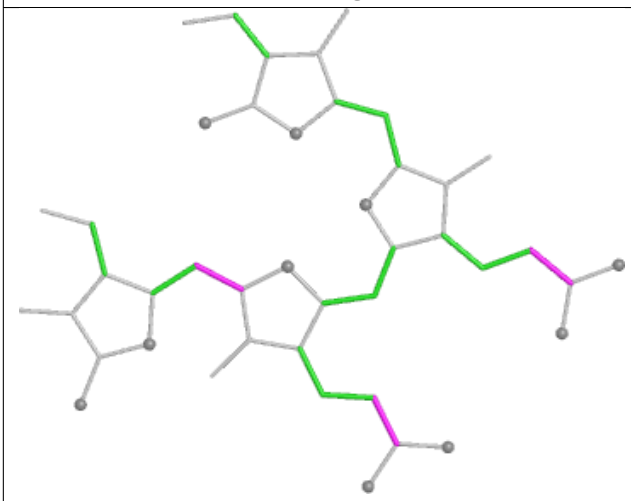
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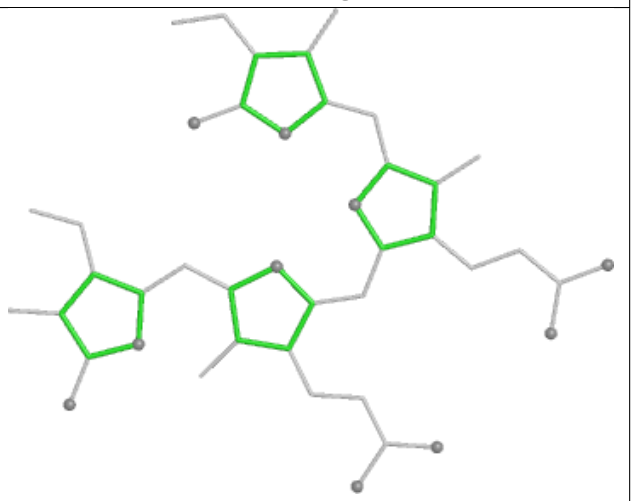
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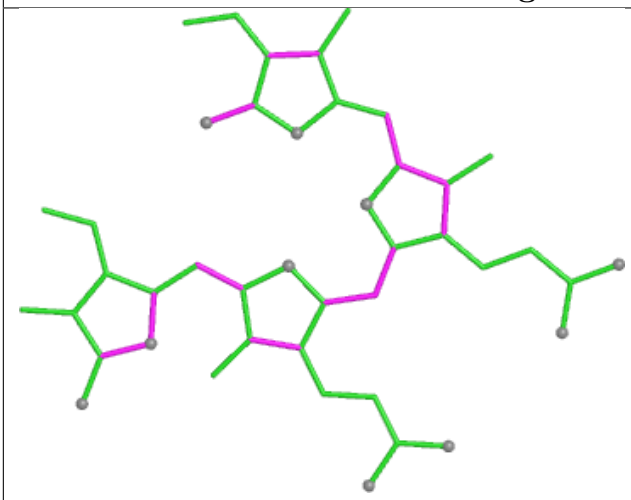


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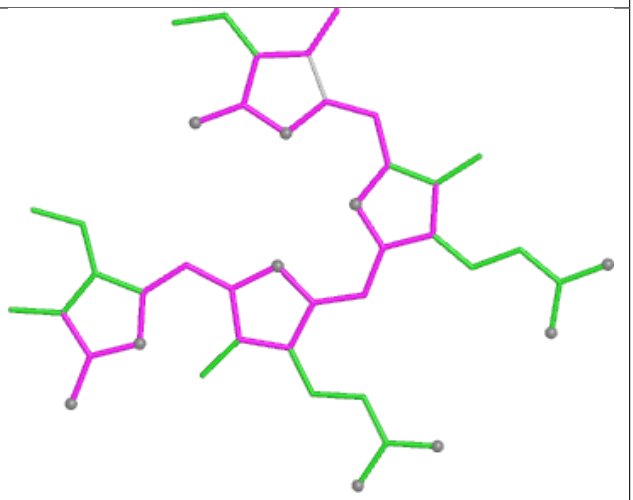


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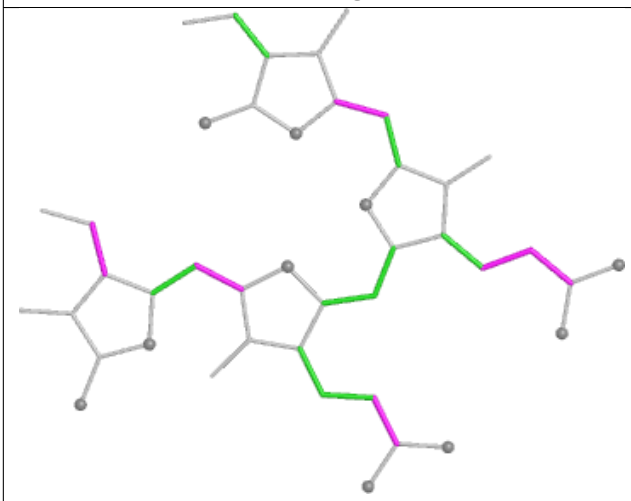
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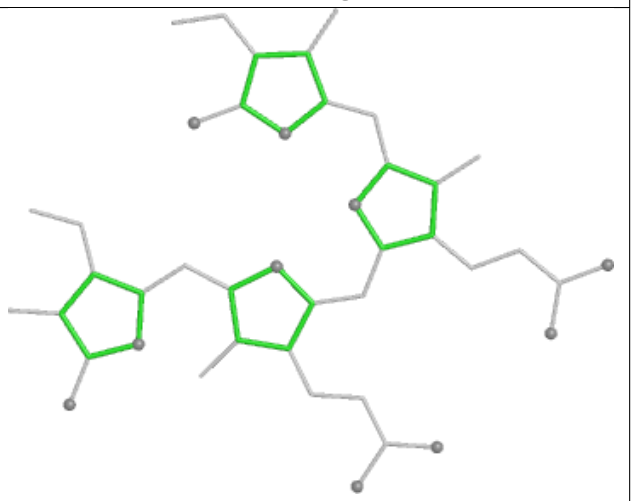
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Bond angles

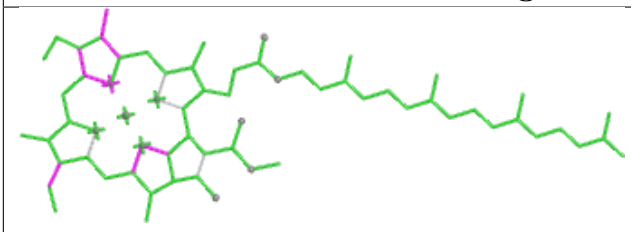


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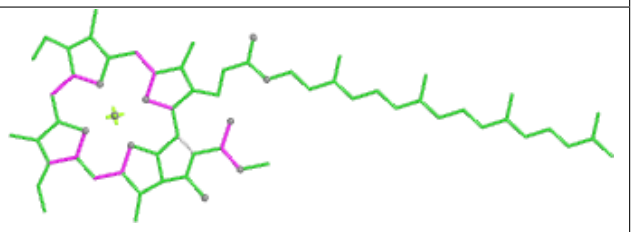


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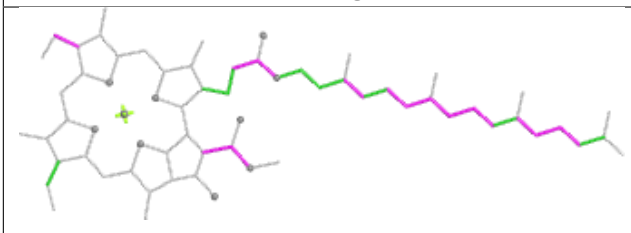
Ligand CLA L2 203



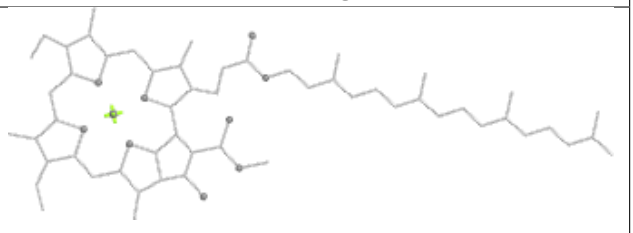
Bond lengths



Bond angles

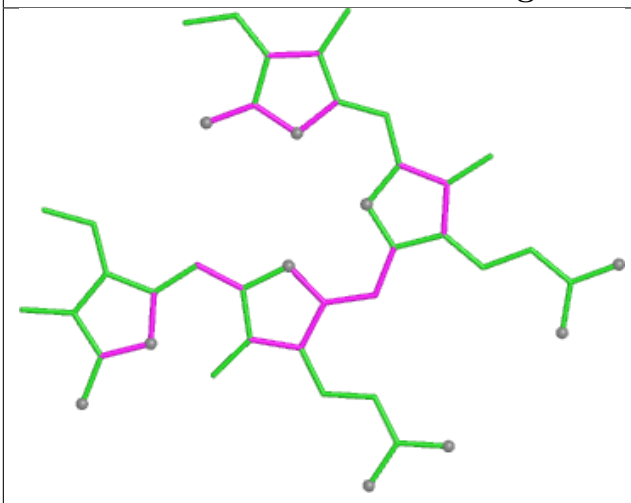


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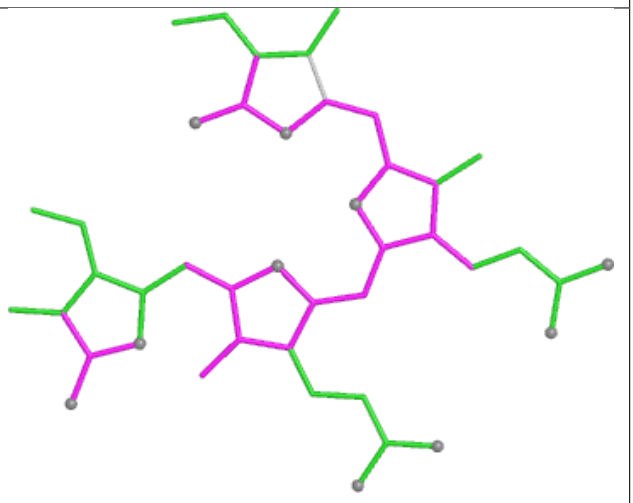


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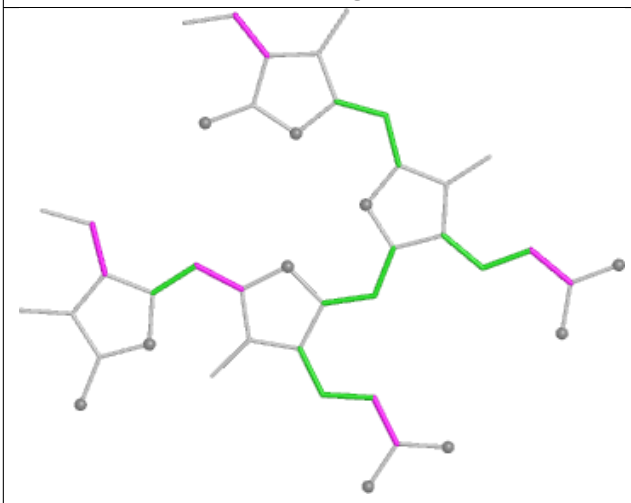
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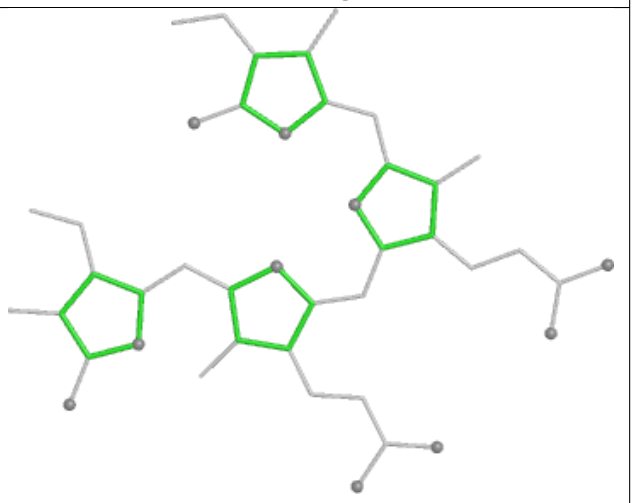
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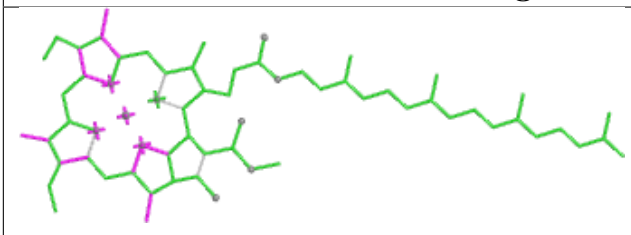


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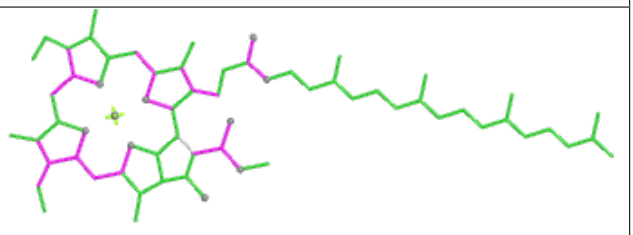


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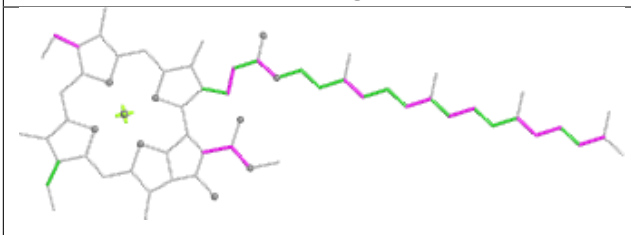
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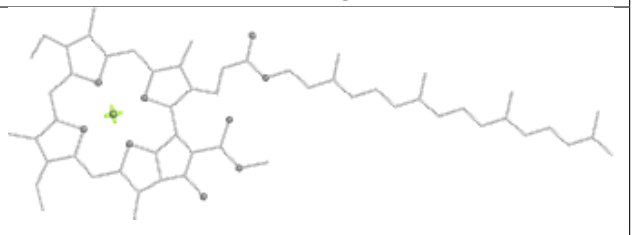
Bond lengths



Bond angles

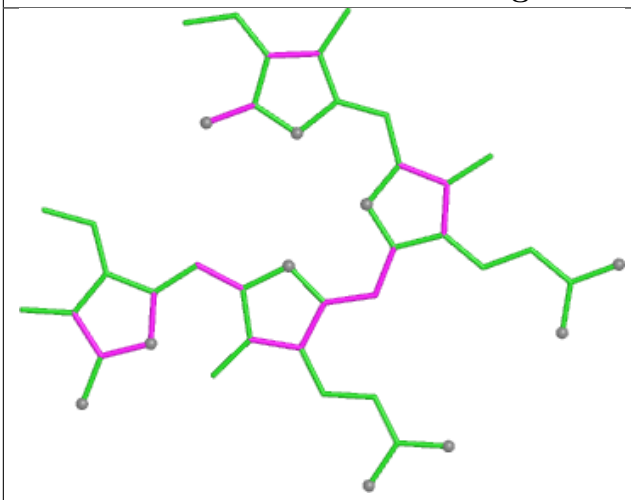


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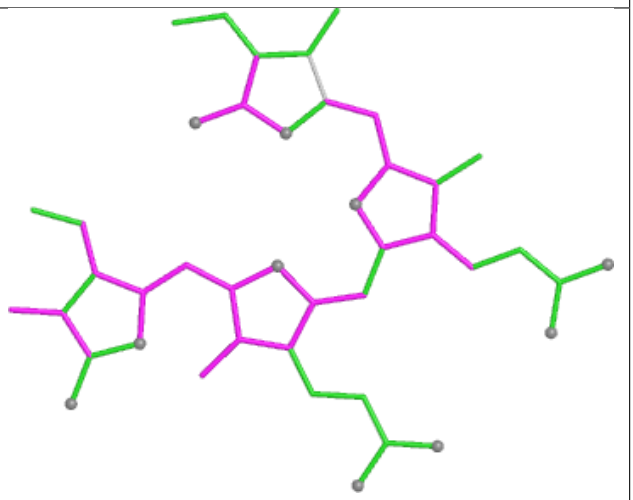


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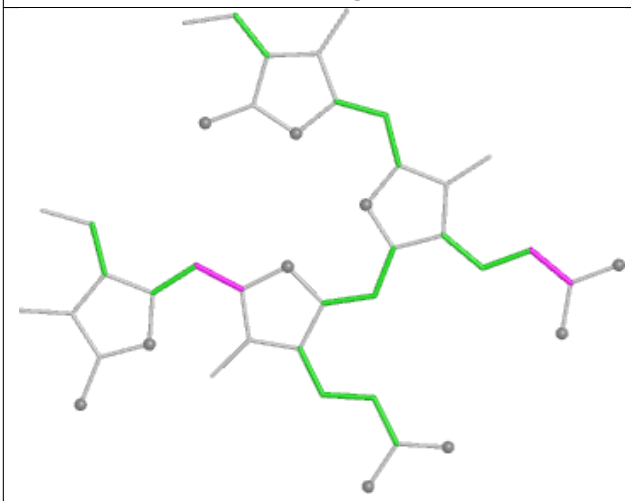
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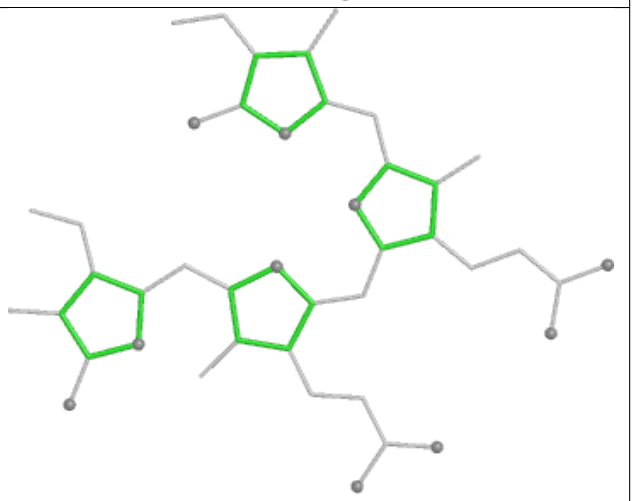
Bond lengths



Bond angles

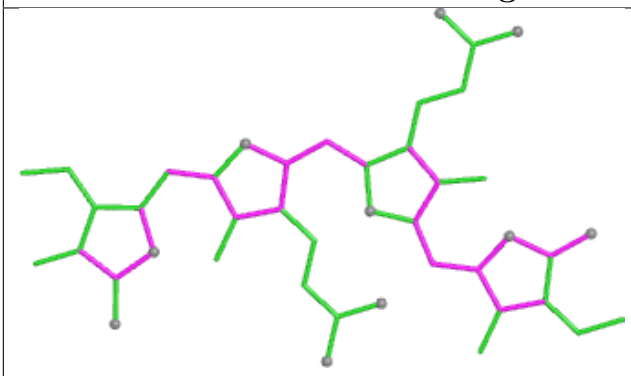


Torsions

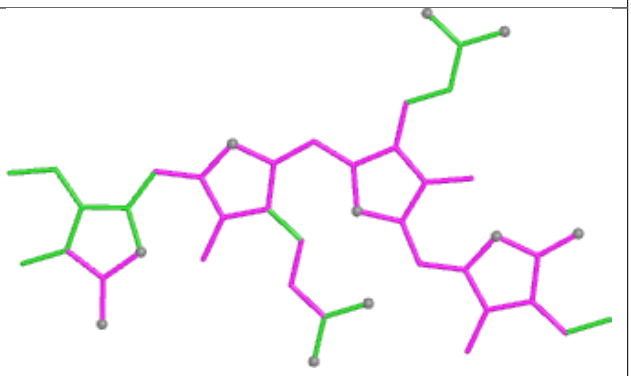


Rings

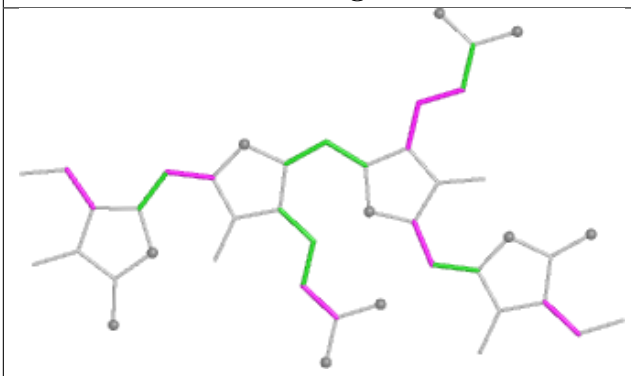
Ligand CYC NO 1001



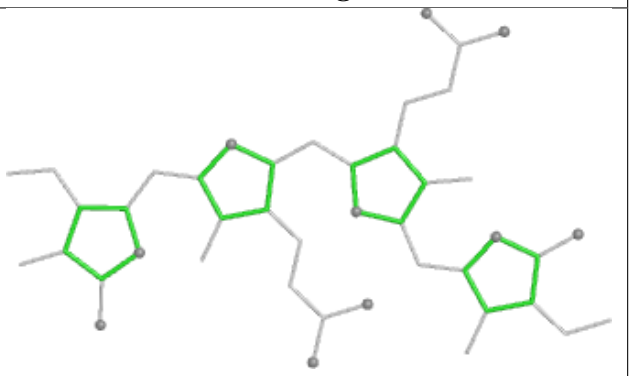
Bond lengths



Bond angles

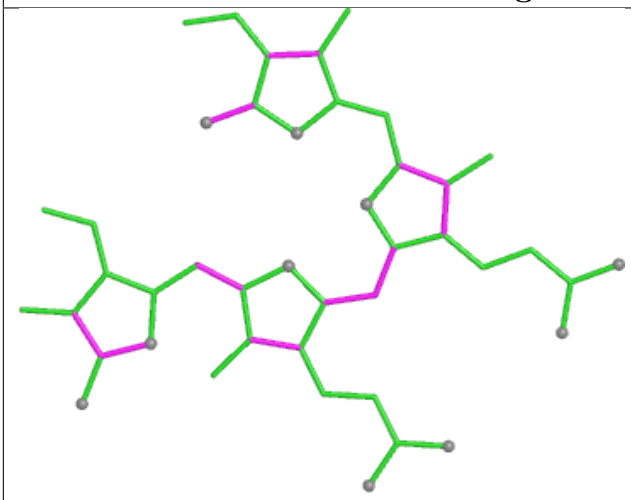


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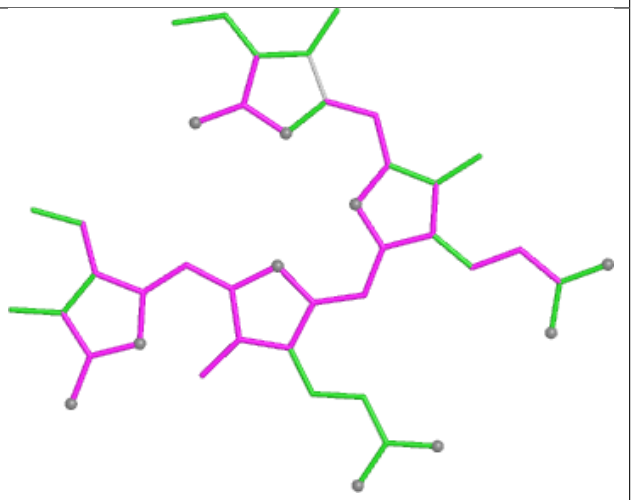


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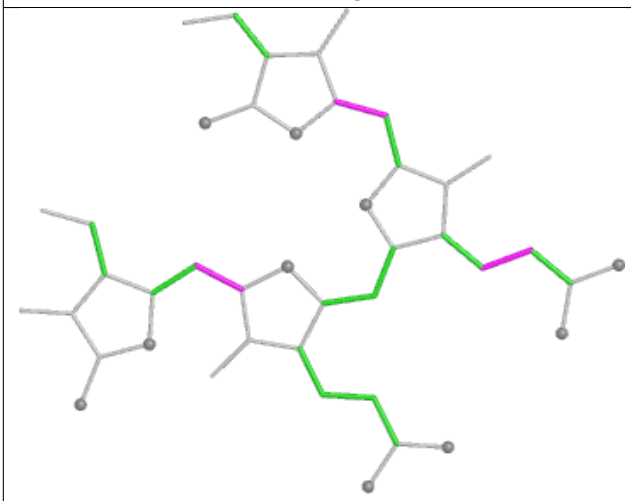
Ligand PEB FA 201



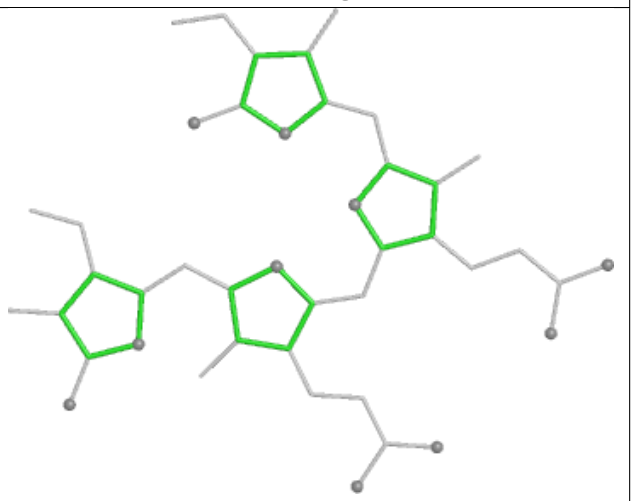
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Bond angles

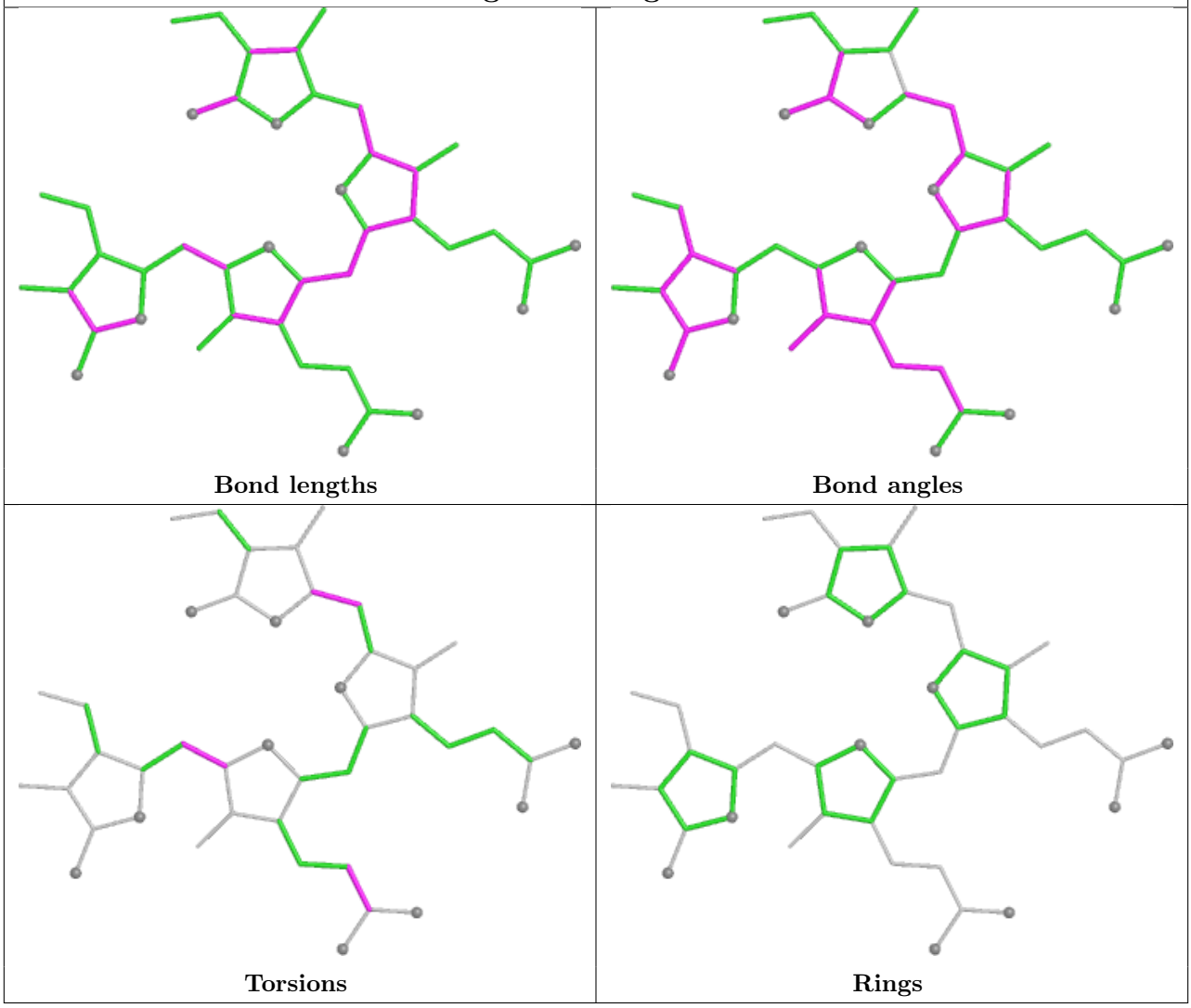


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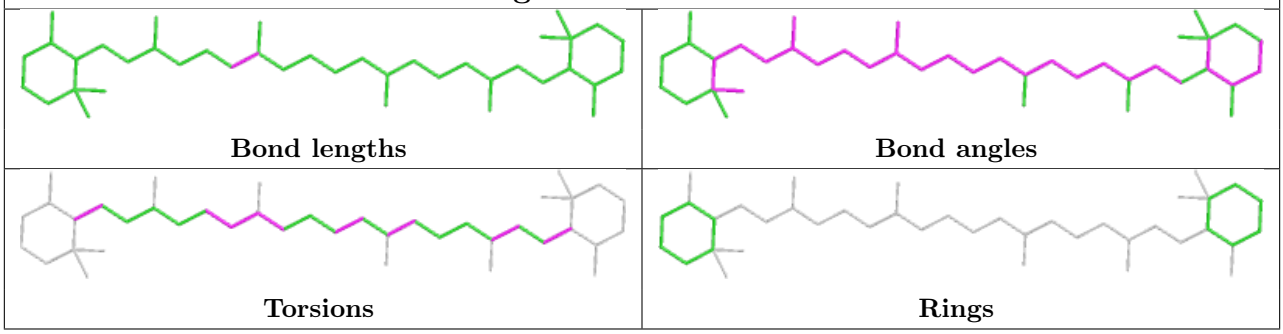


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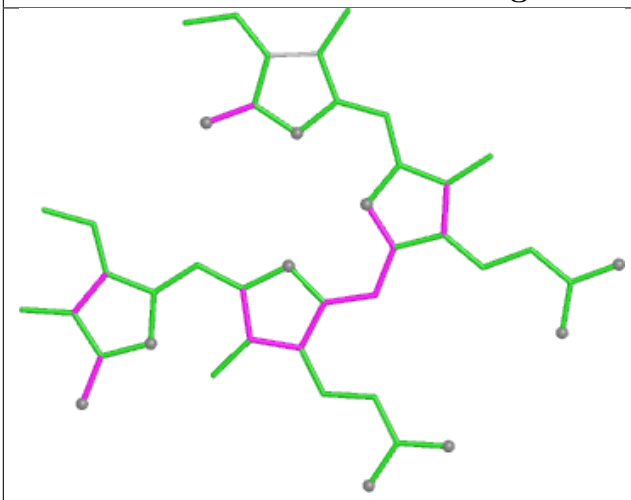
Ligand PEB g1 202



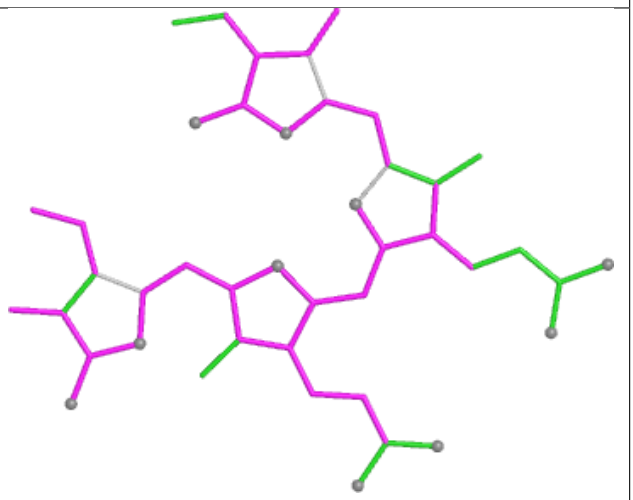
Ligand BCR K2 102



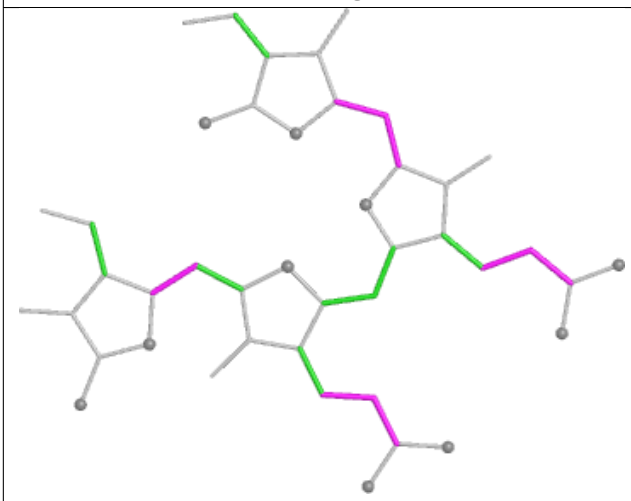
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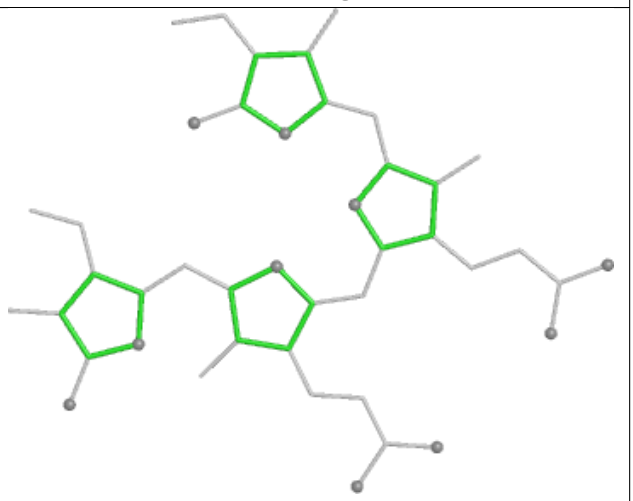
Bond lengths



Bond angles

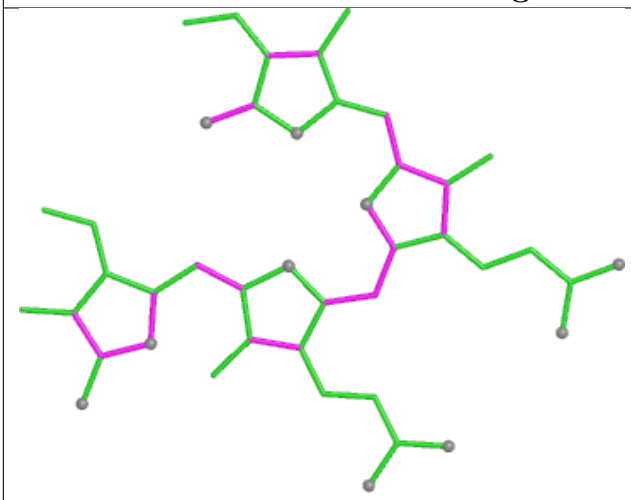


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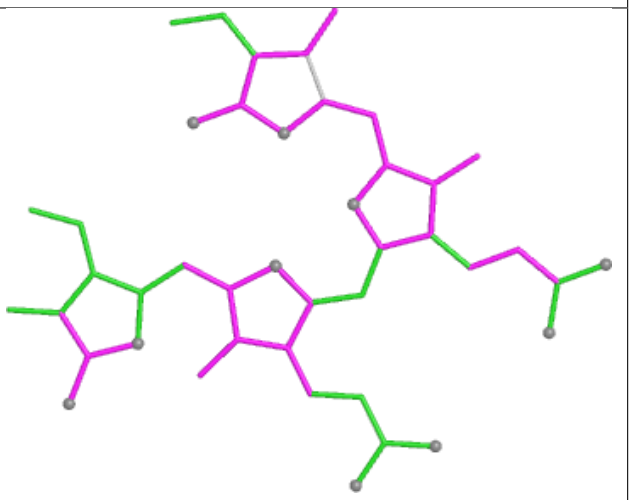


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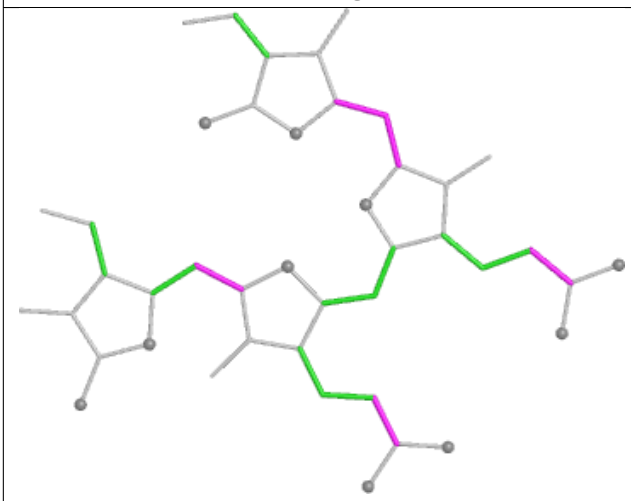
Ligand PEB OP 201



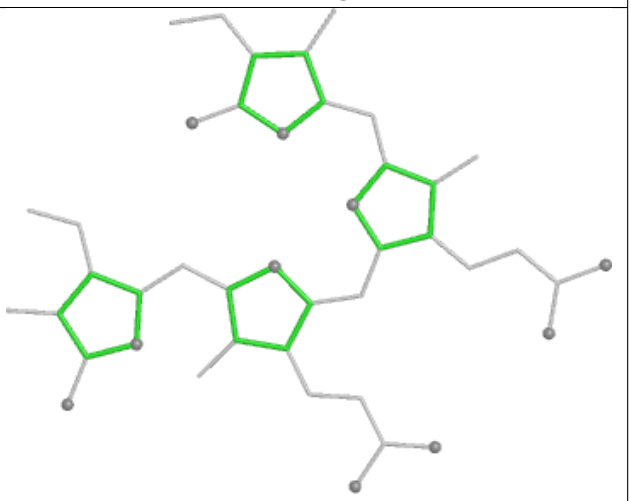
Bond lengths



Bond angles

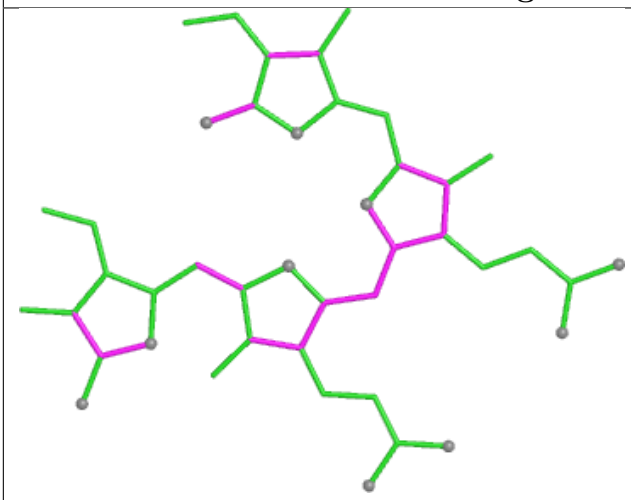


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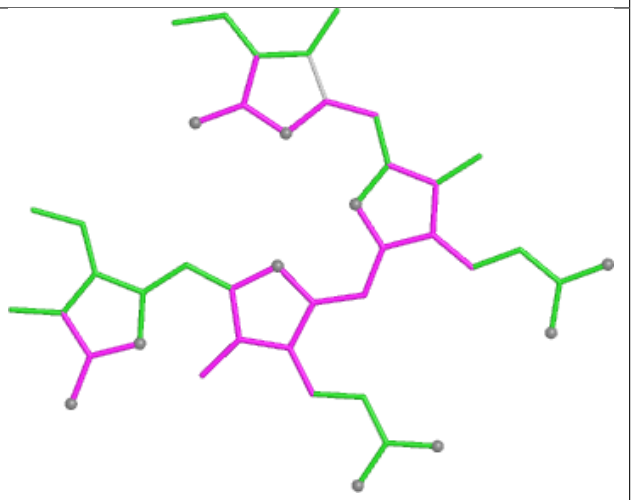


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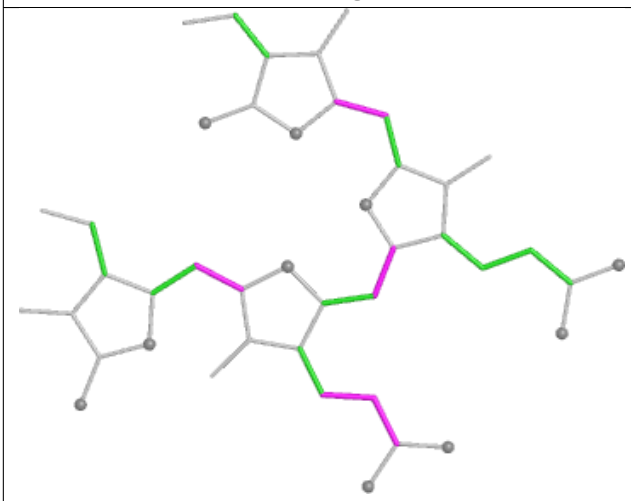
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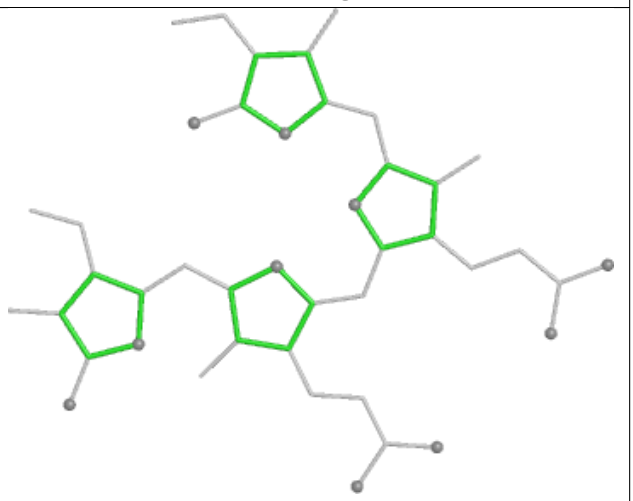
Bond lengths



Bond angles

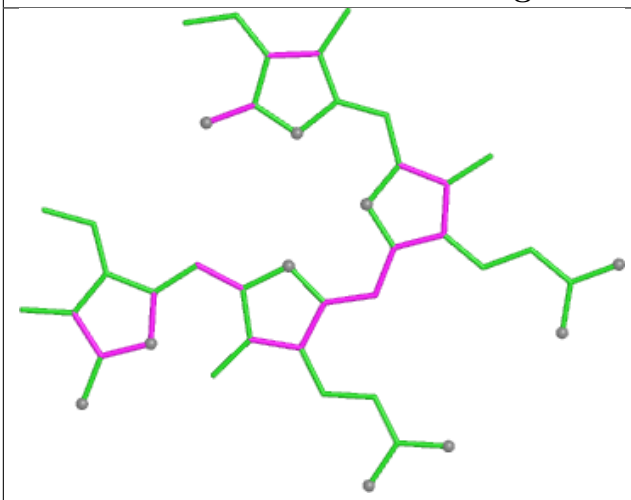


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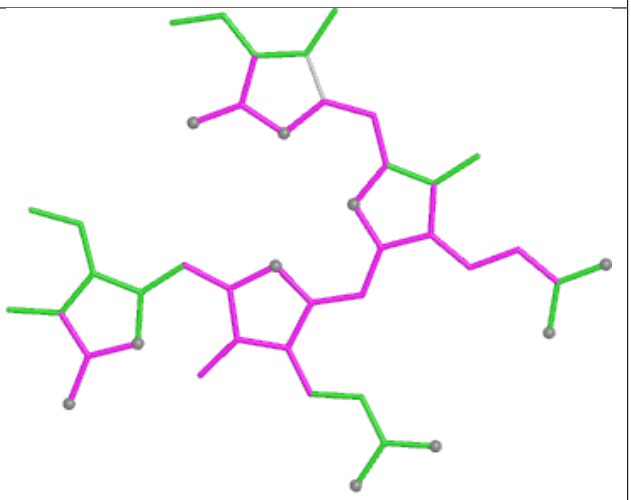


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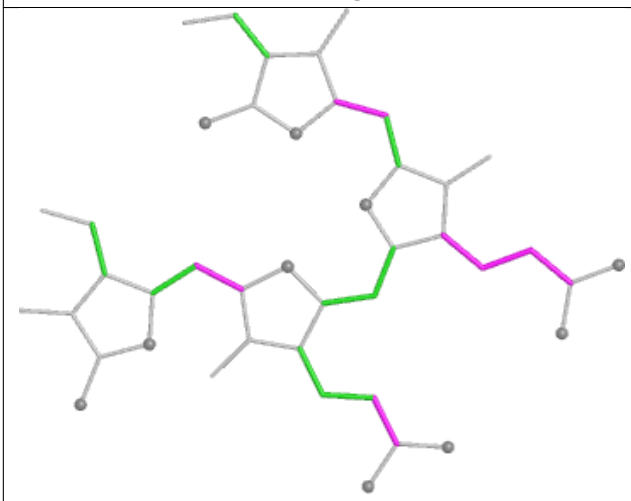
Ligand PEB kG 201



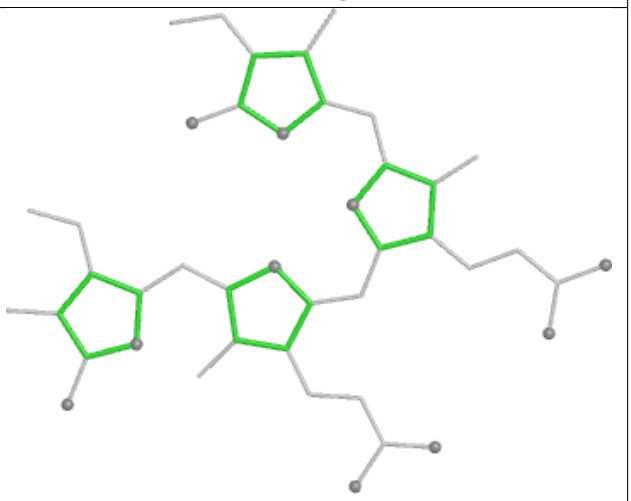
Bond lengths



Bond angles

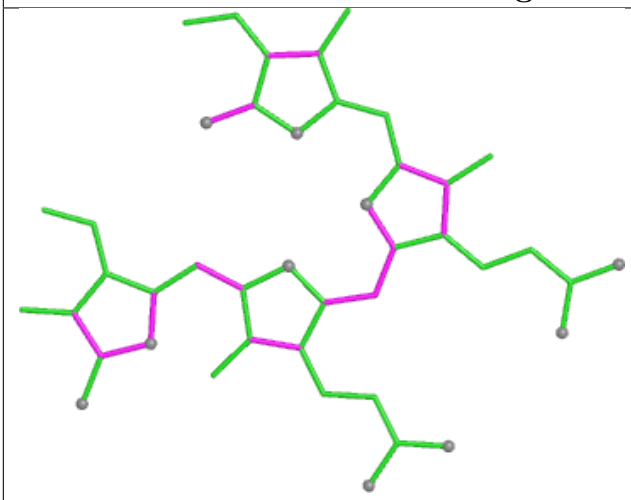


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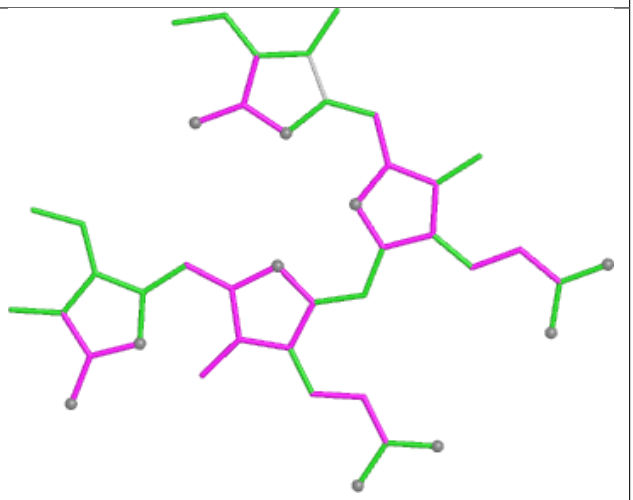


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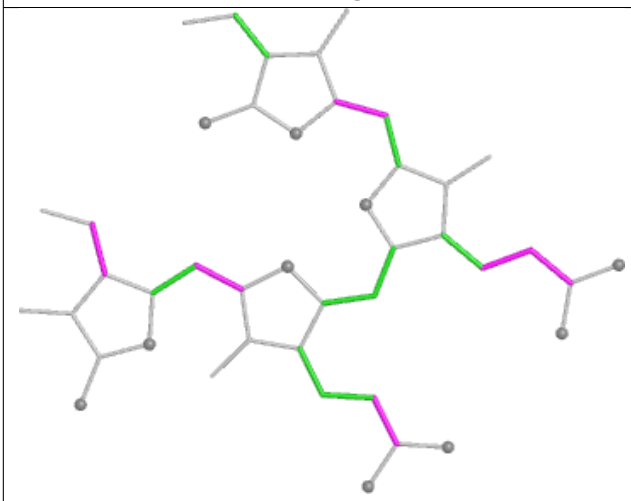
Ligand PEB V7 201



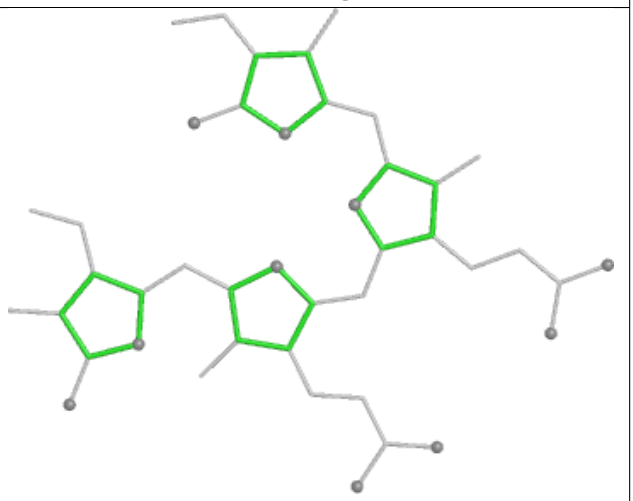
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Bond angles

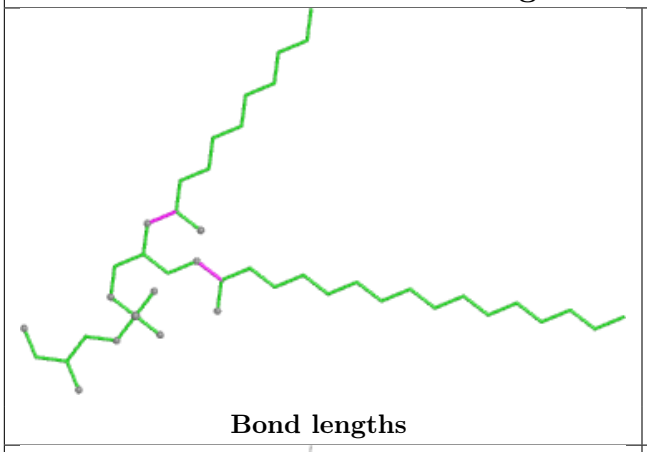


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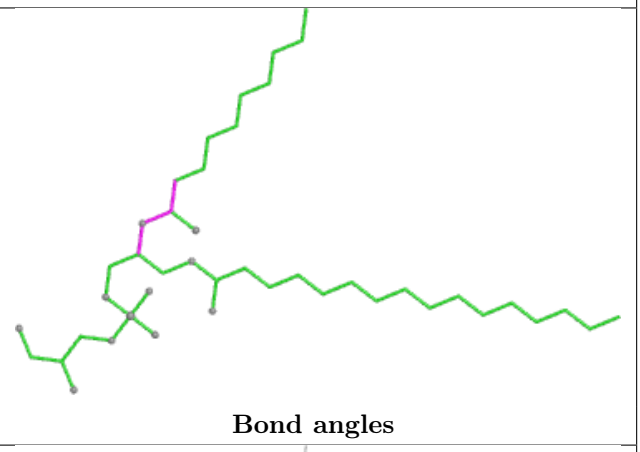


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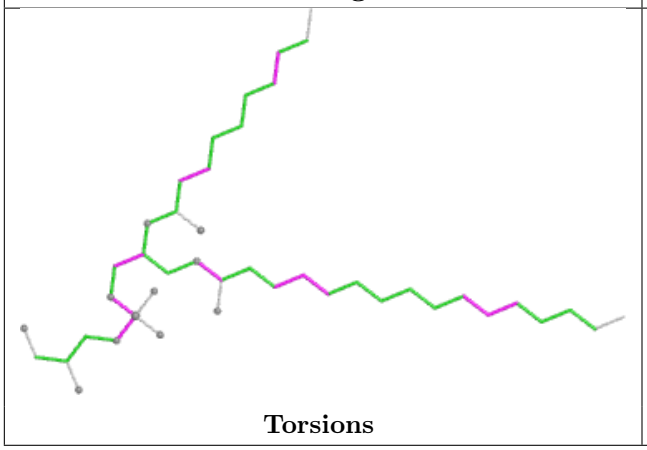
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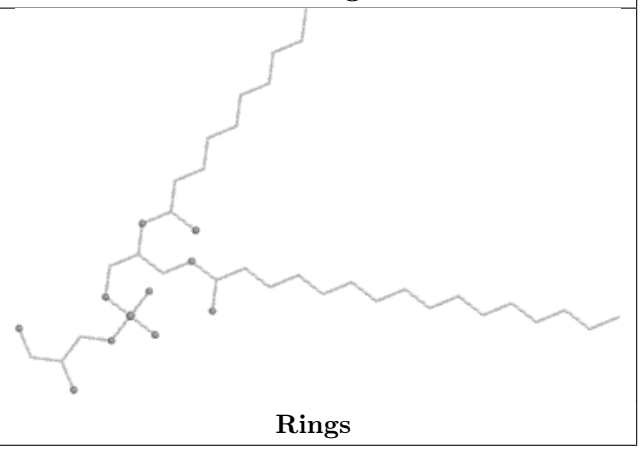
Bond lengths



Bond angles

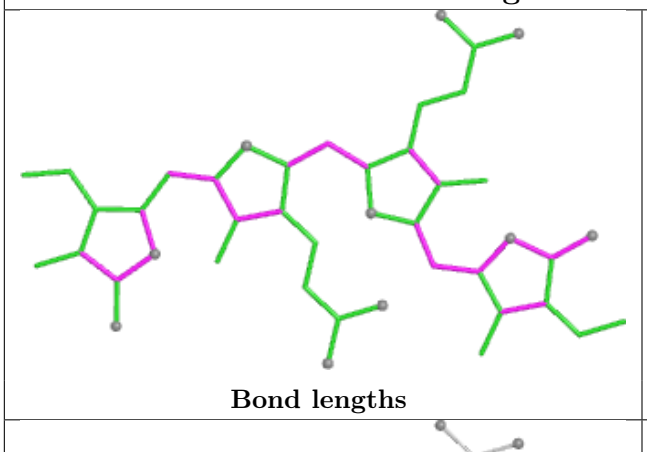


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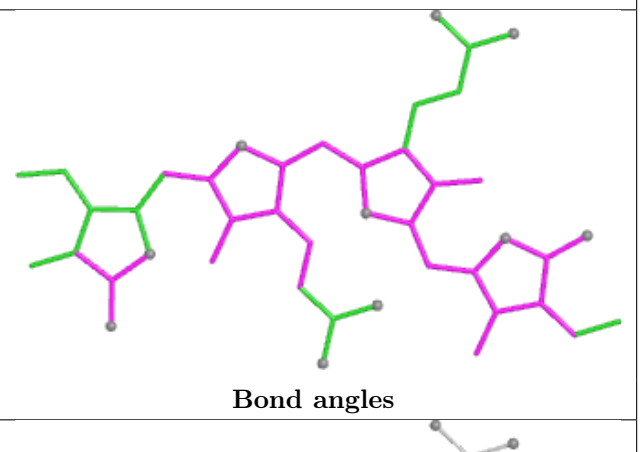


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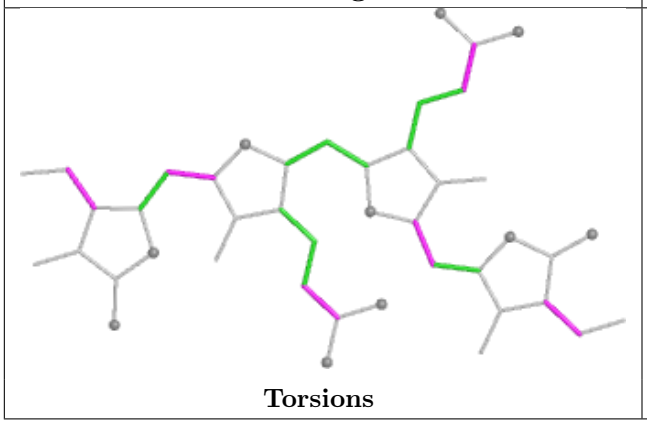
Ligand CYC FO 1001



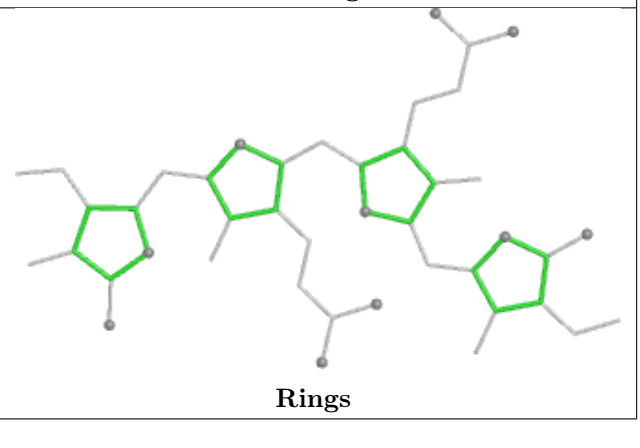
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Bond angles

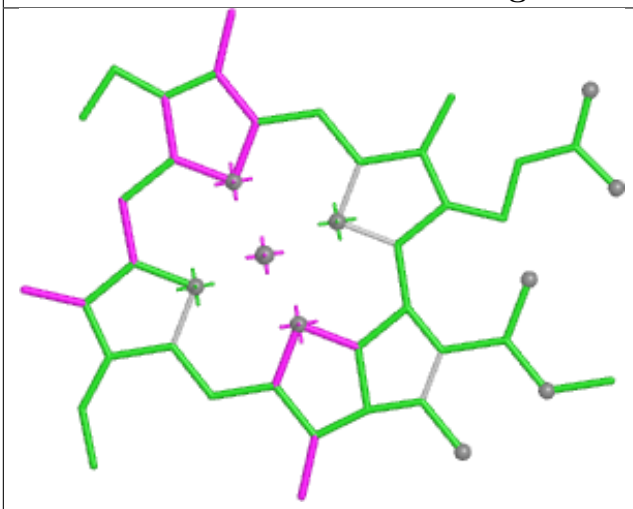


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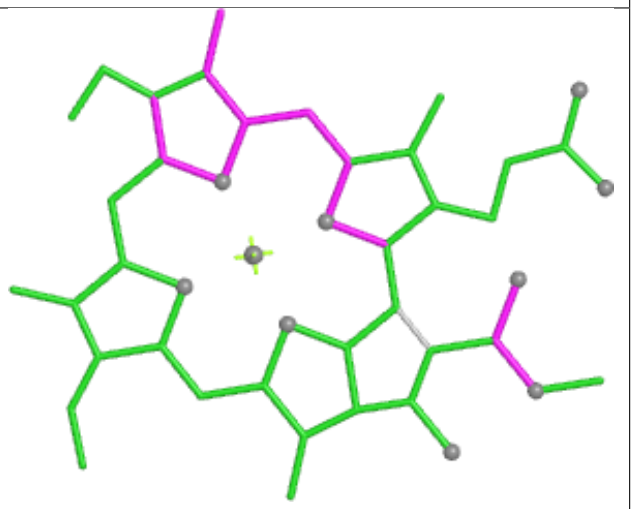


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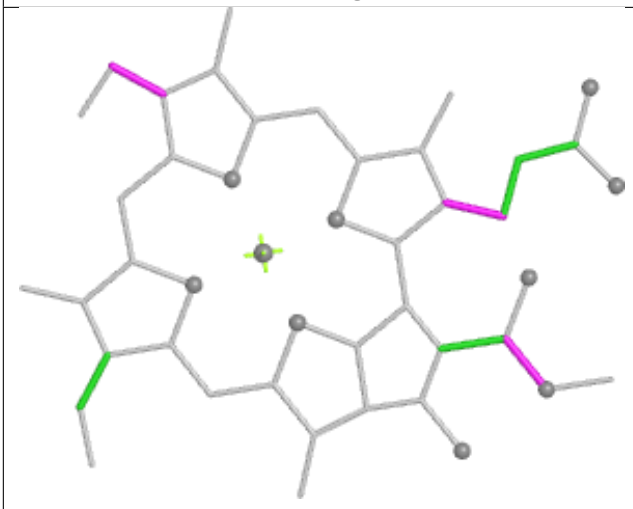
Ligand CLA KN 102



Bond lengths



Bond angles

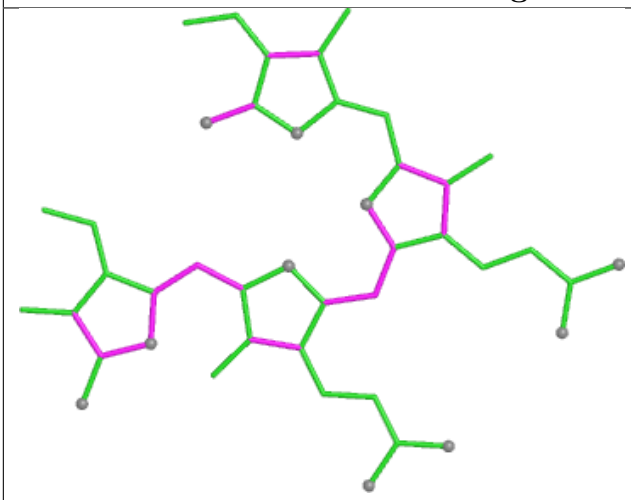


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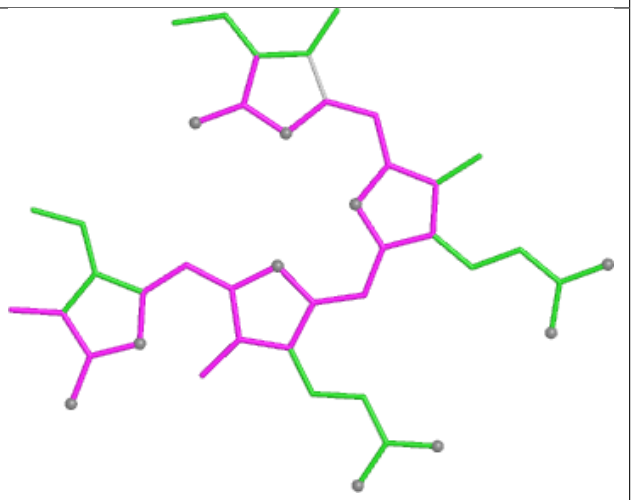


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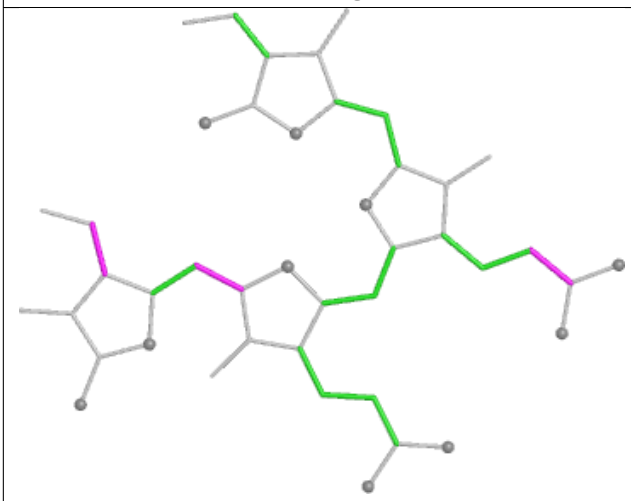
Ligand PEB W4 201



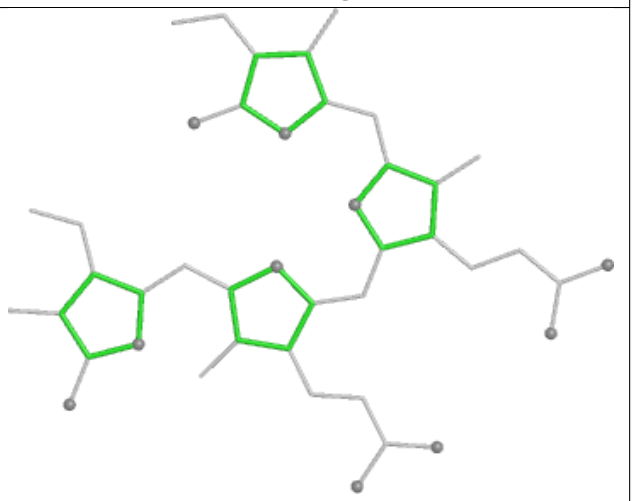
Bond lengths



Bond angles

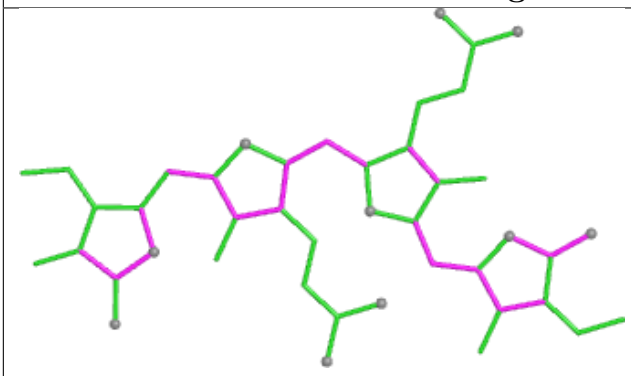


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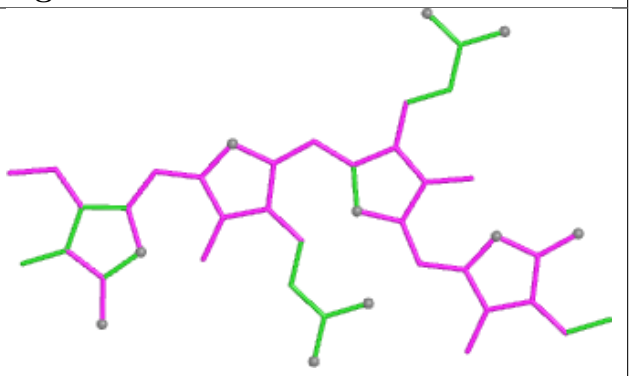


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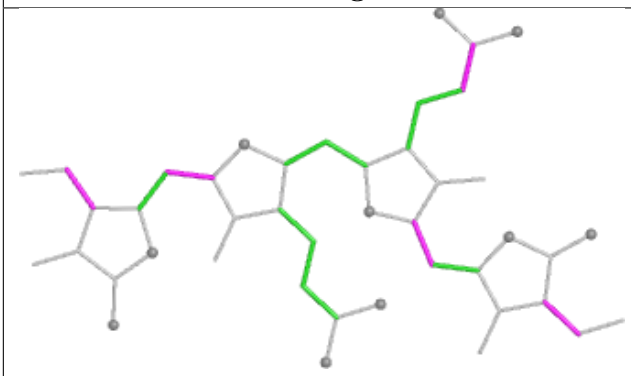
Ligand CYC g3 1001



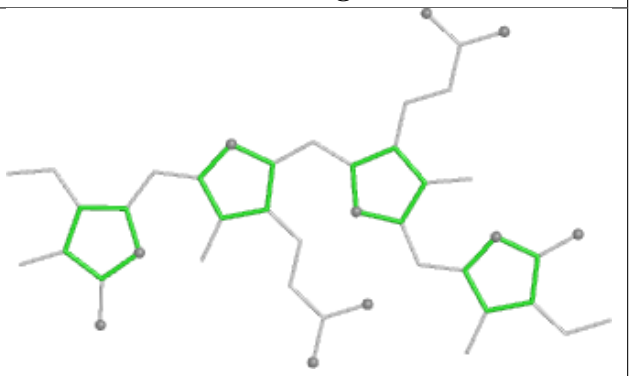
Bond lengths



Bond angles

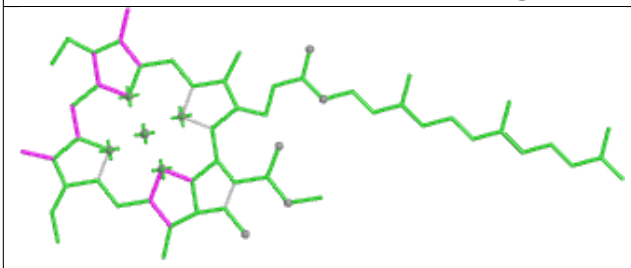


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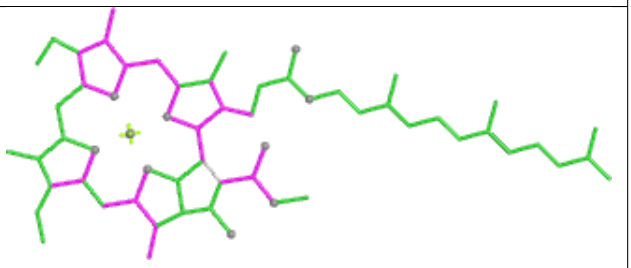


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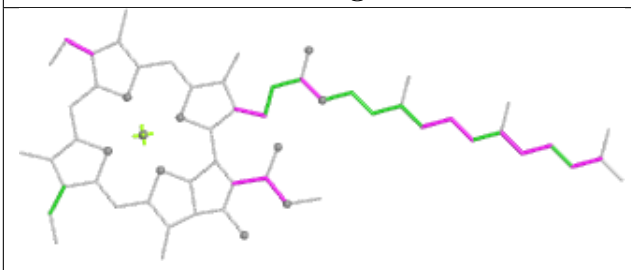
Ligand CLA CL 513



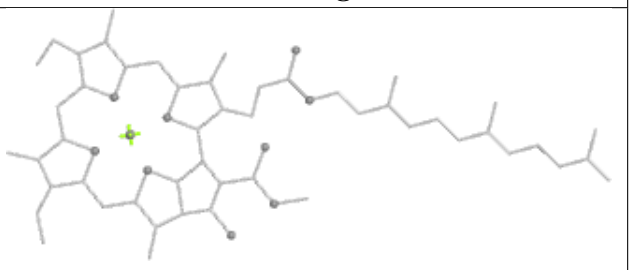
Bond lengths



Bond angles

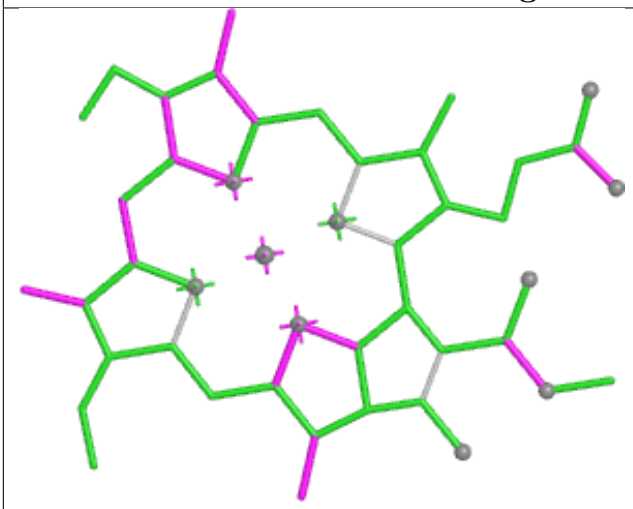


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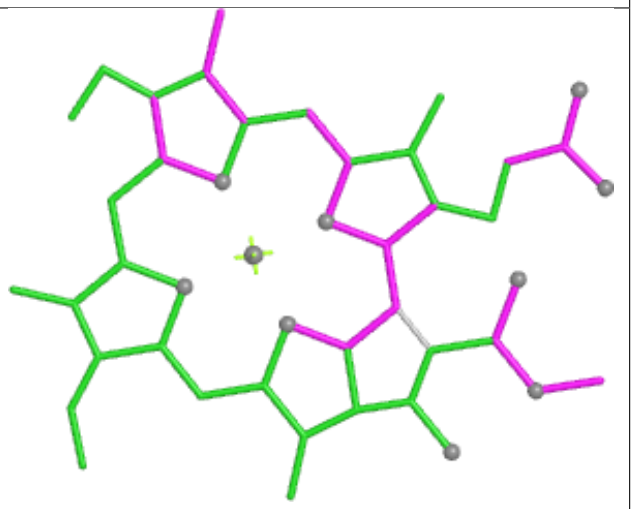


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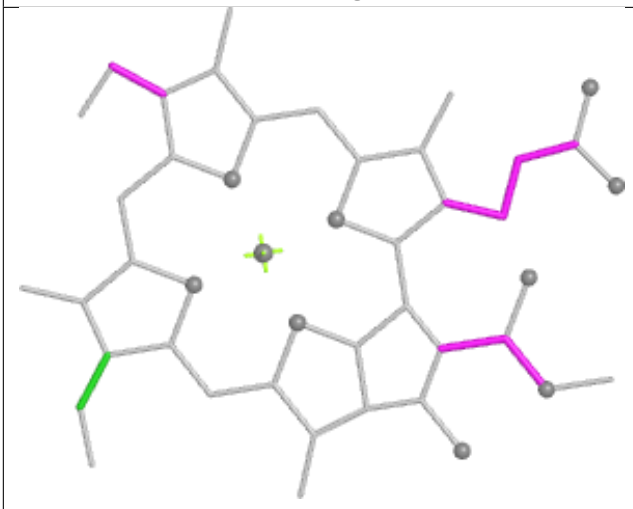
Ligand CLA 82 305



Bond lengths



Bond angles

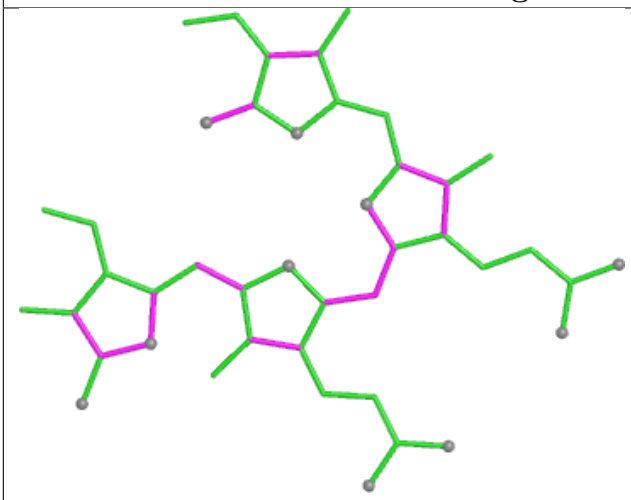


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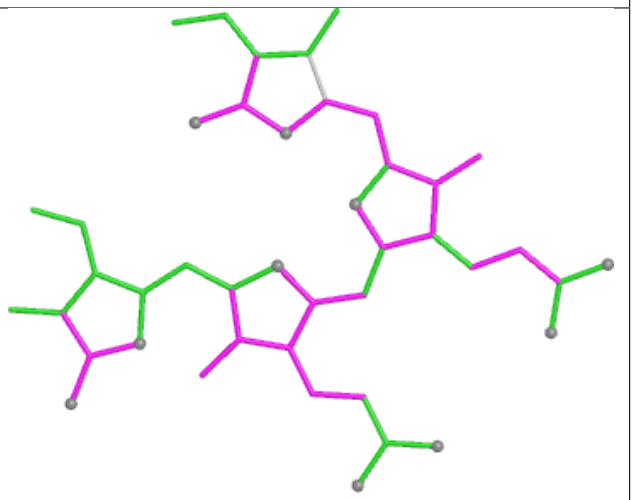


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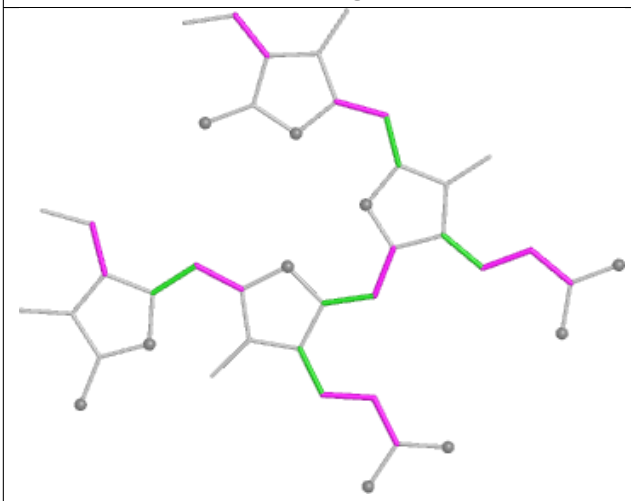
Ligand PEB DB 203



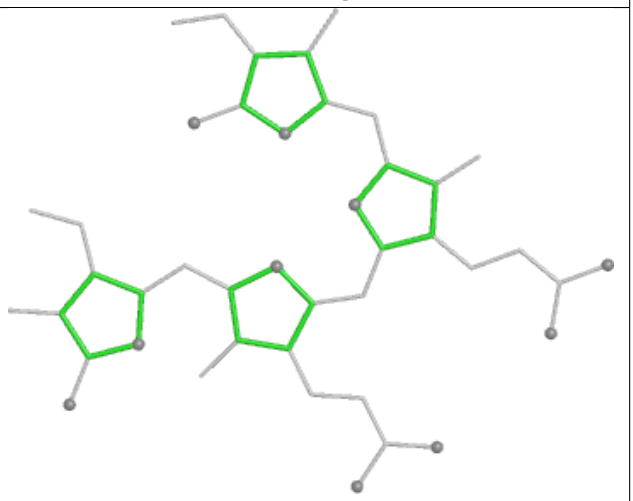
Bond lengths



Bond angles

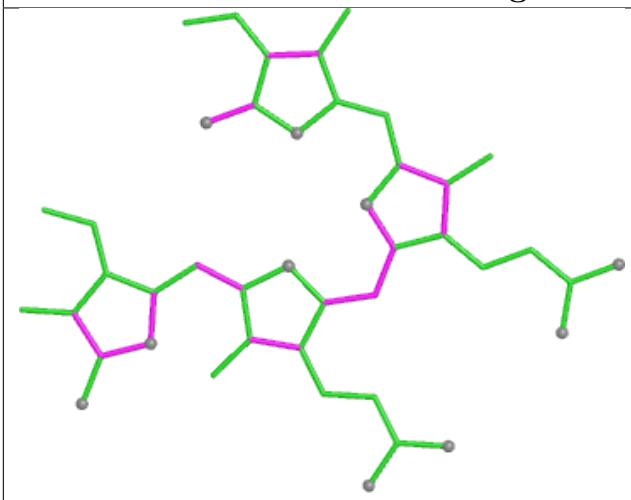


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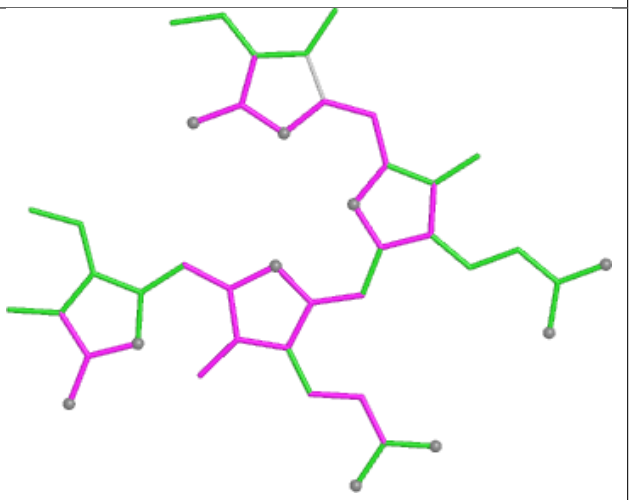


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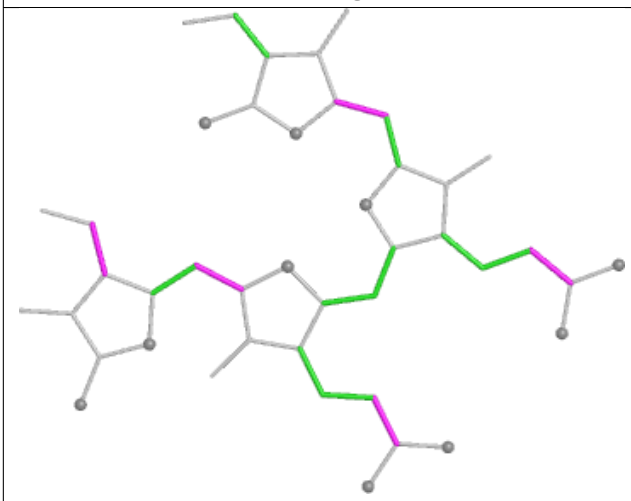
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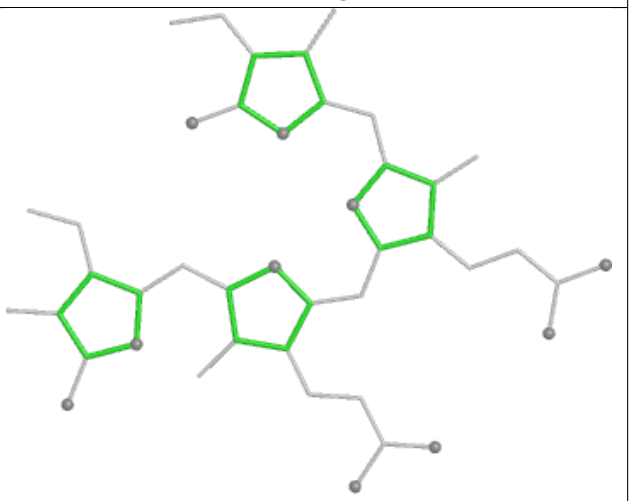
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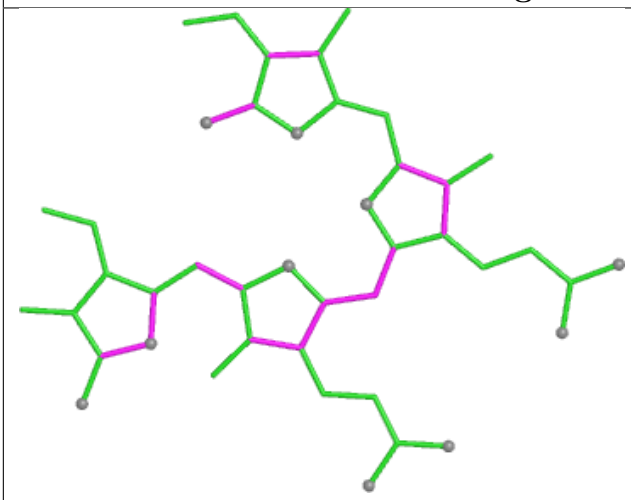


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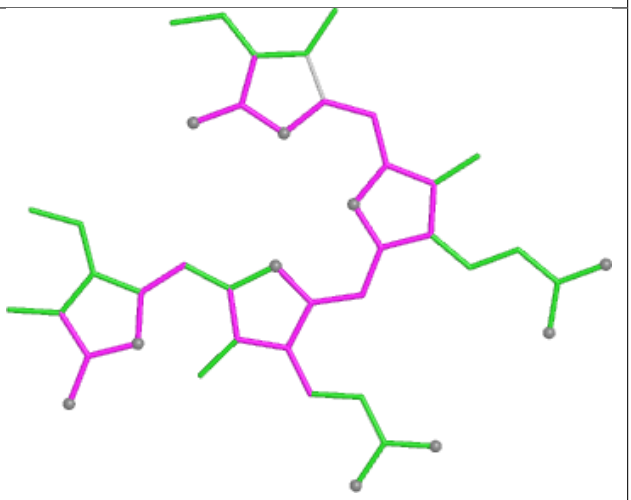


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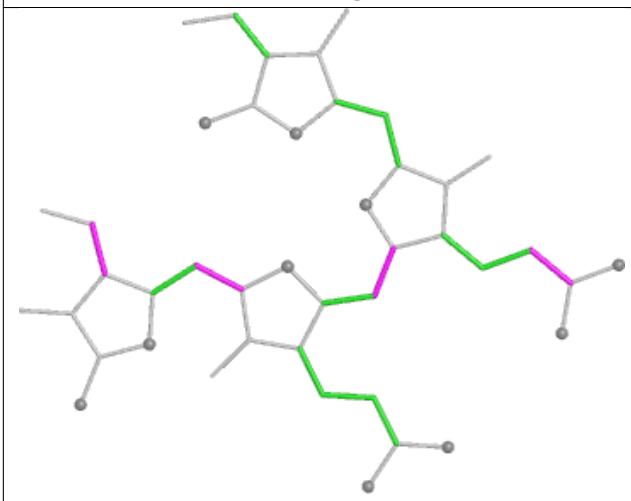
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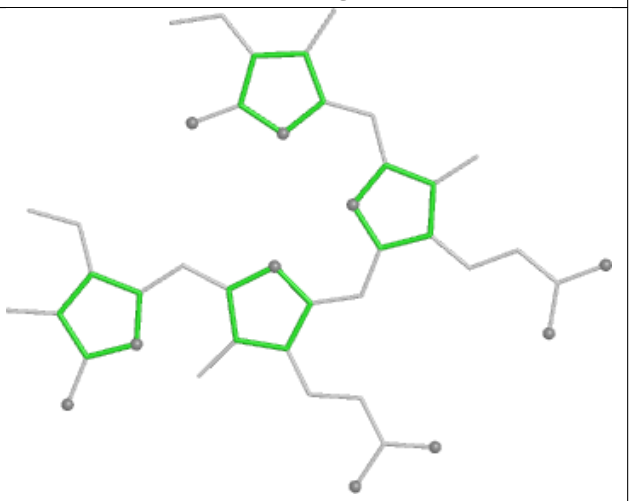
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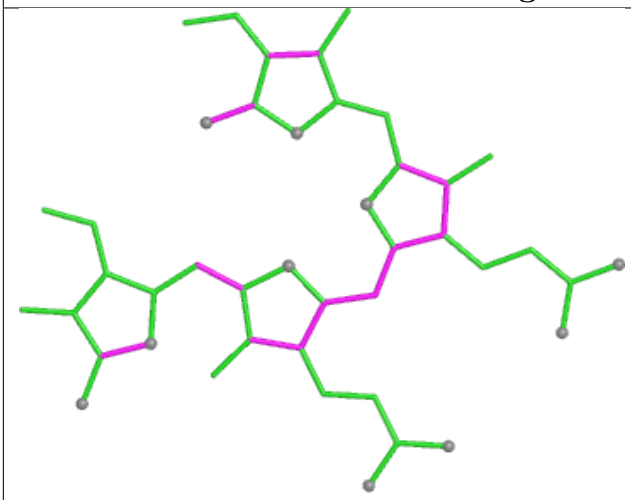


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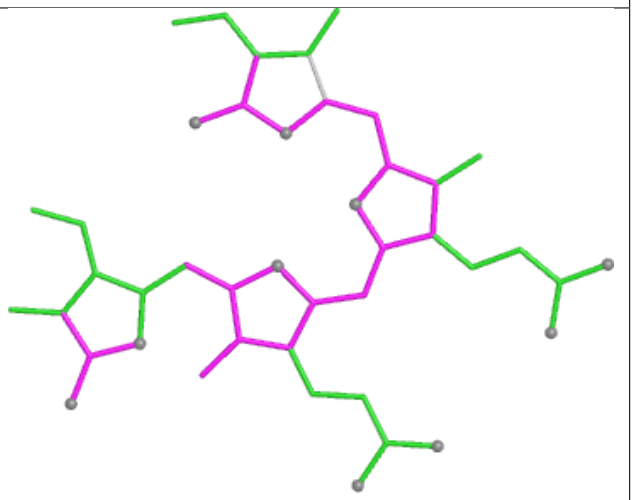


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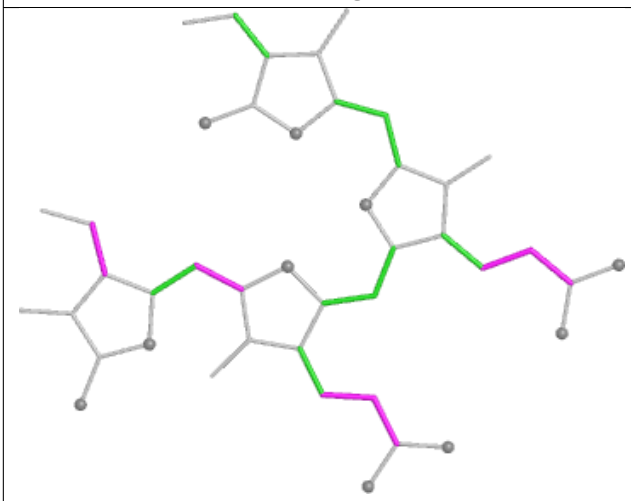
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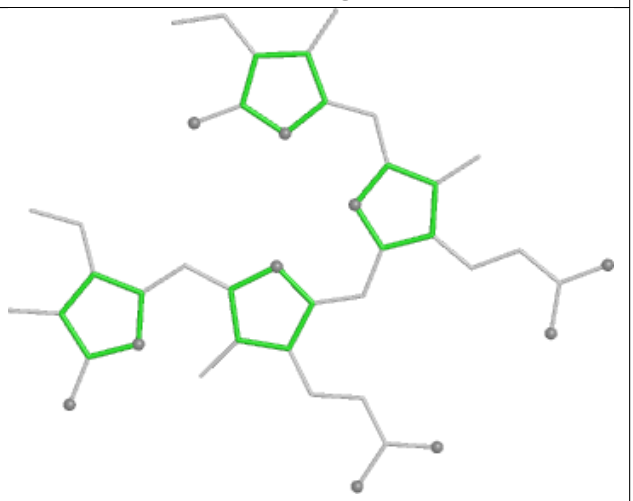
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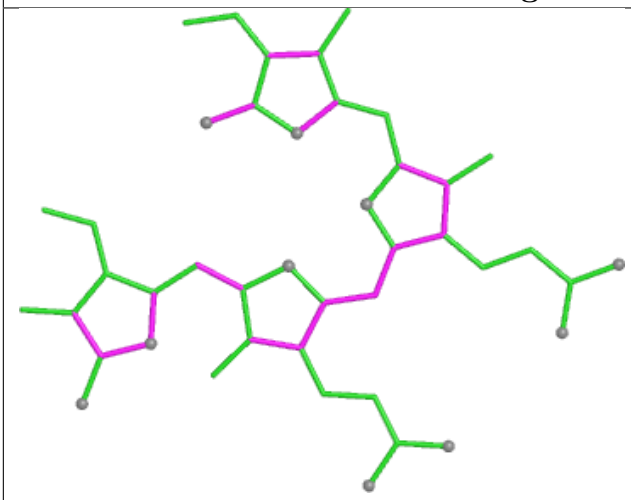


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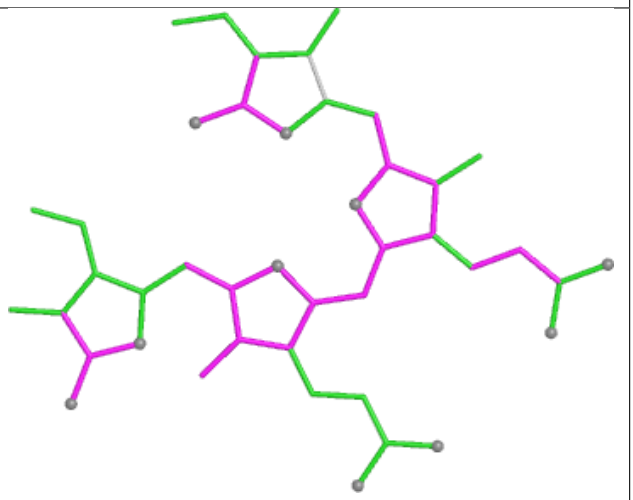


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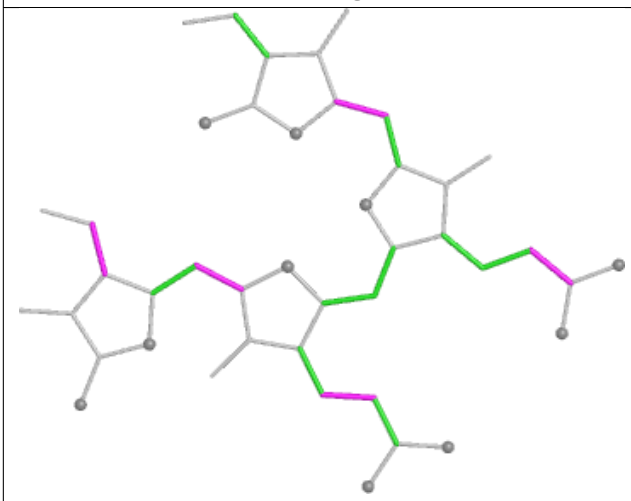
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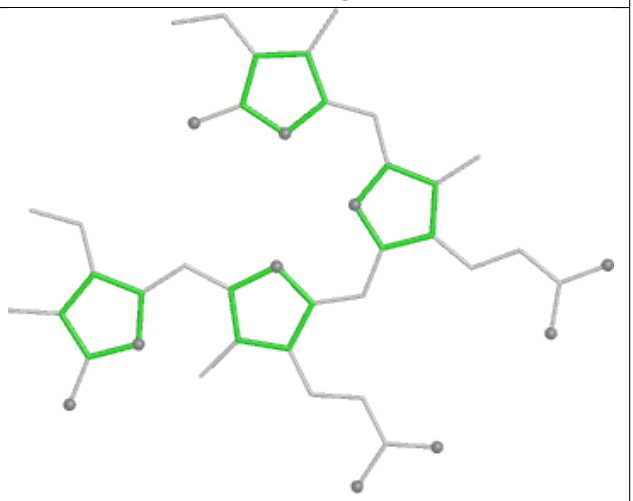
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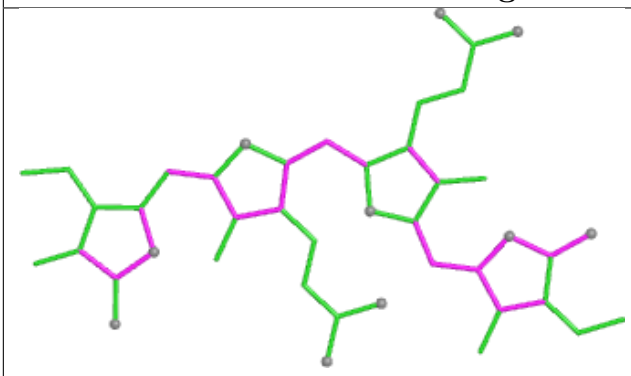


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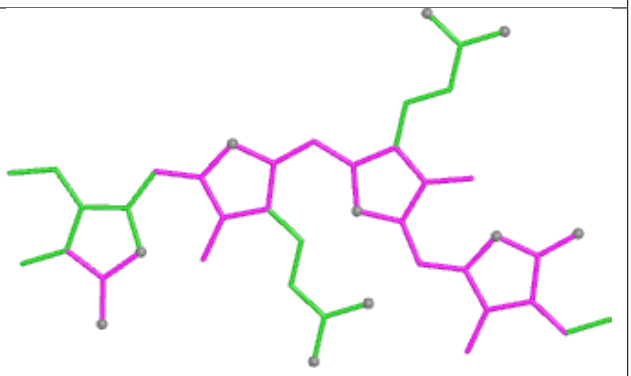


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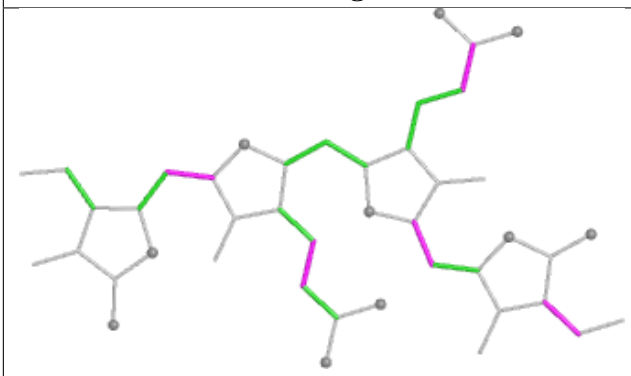
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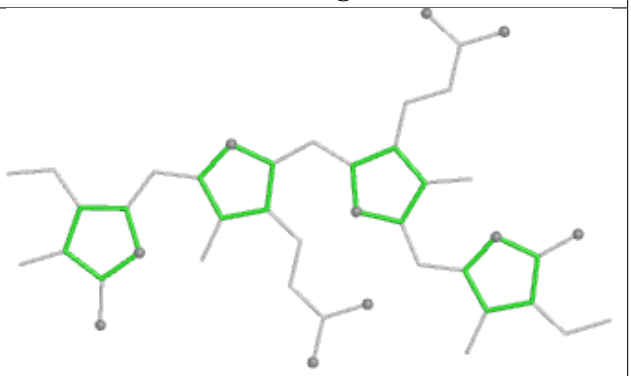
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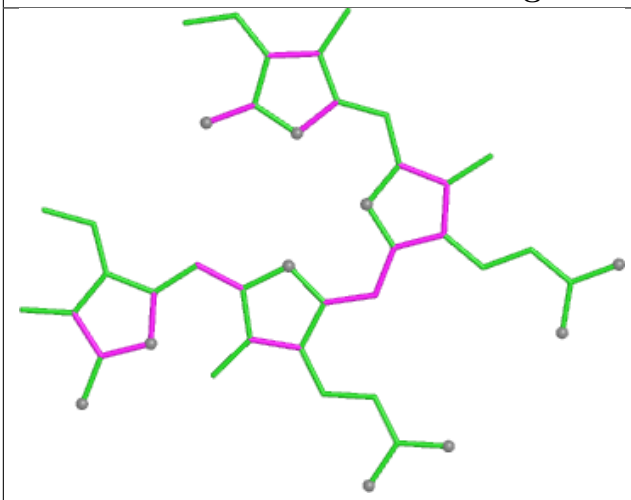


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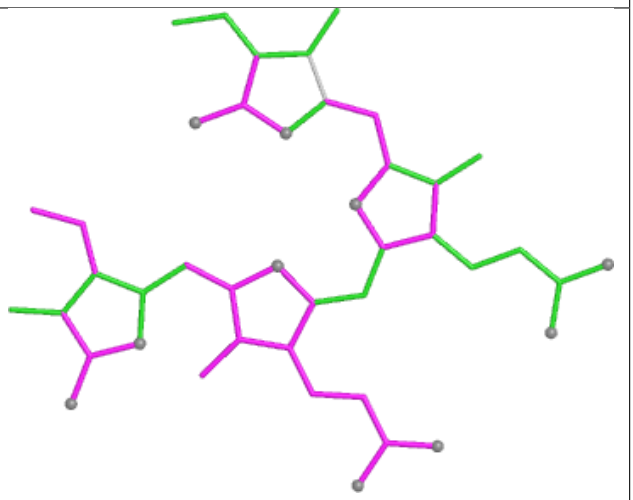


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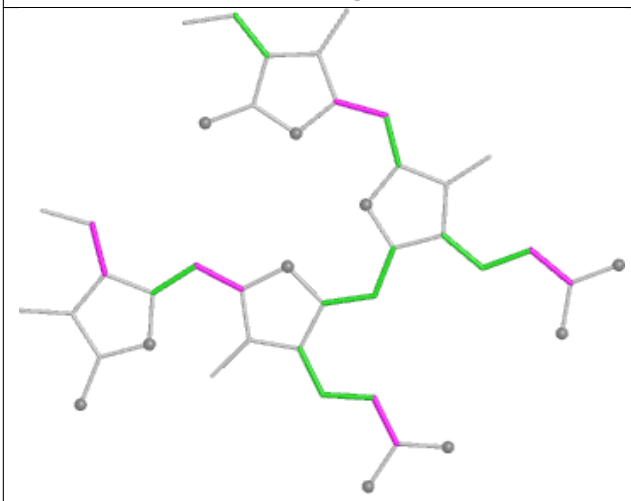
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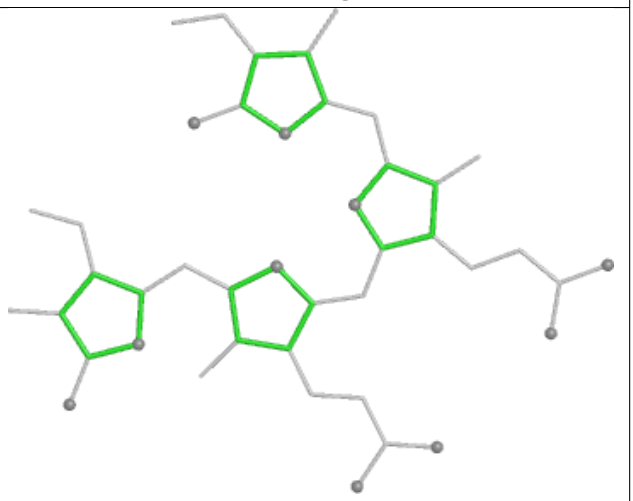
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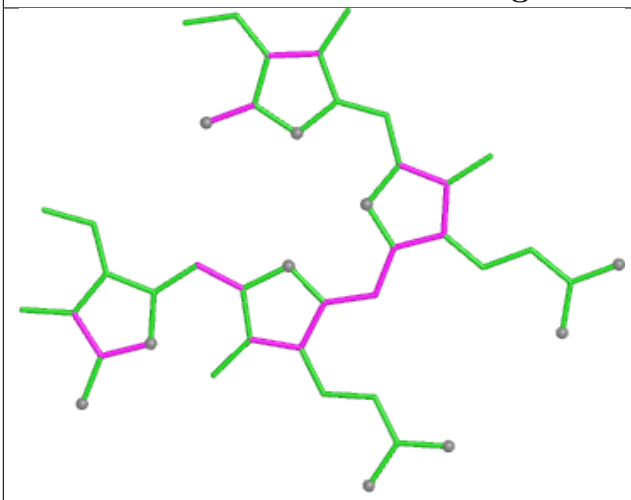


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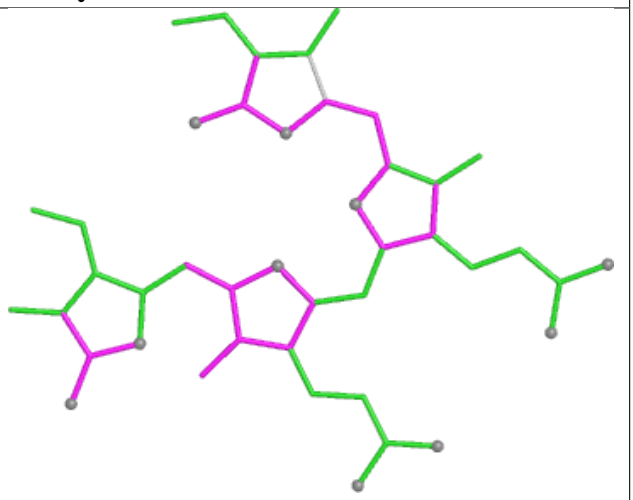


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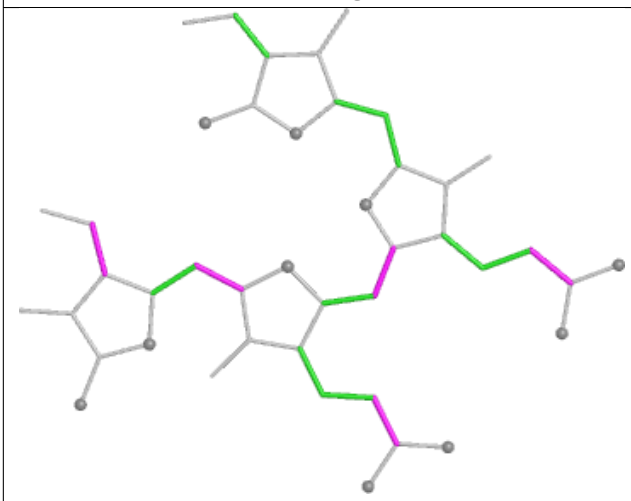
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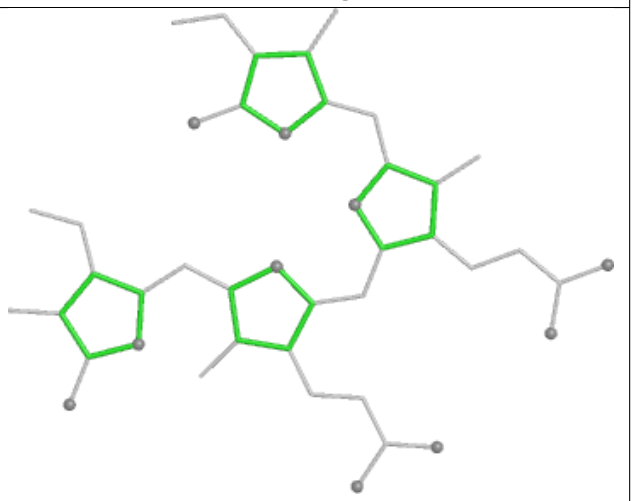
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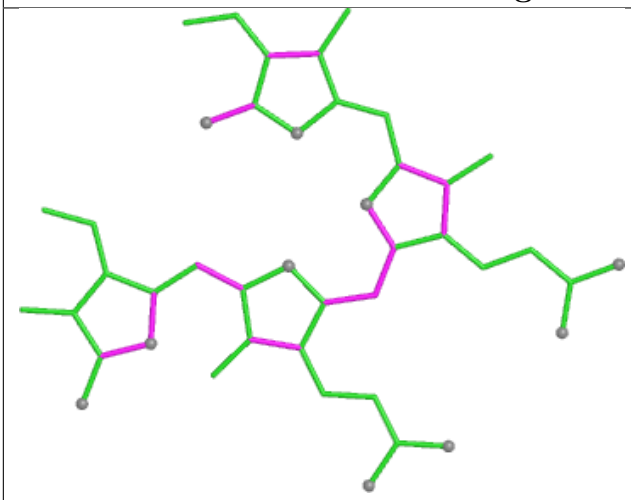


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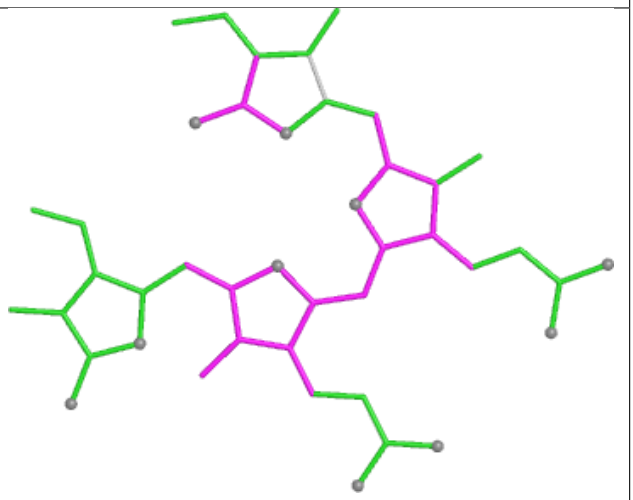


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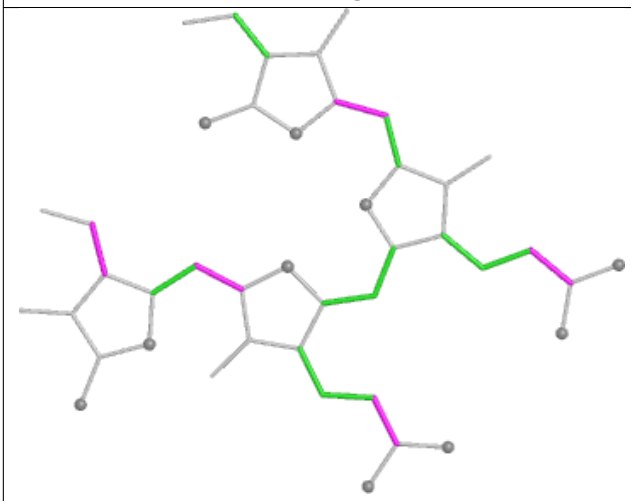
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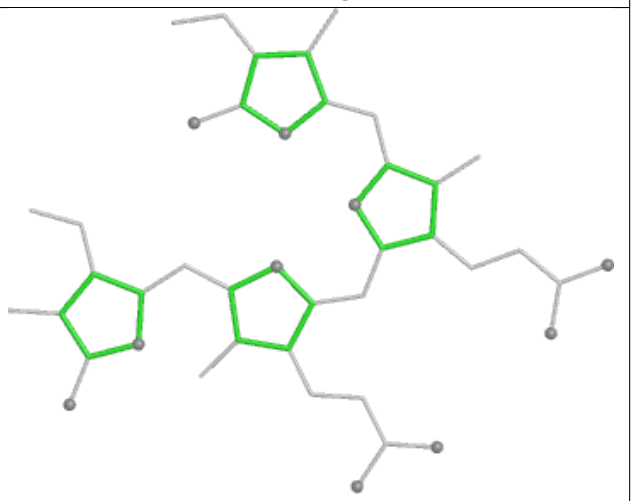
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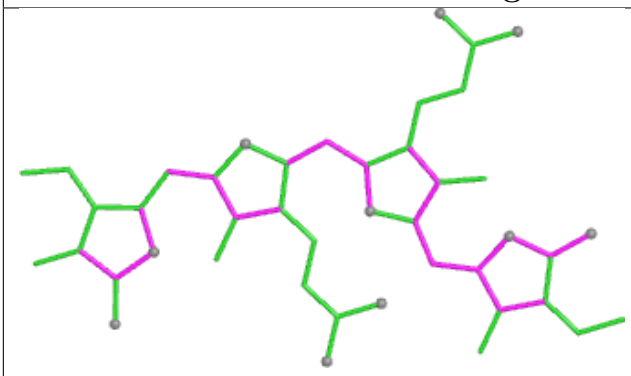


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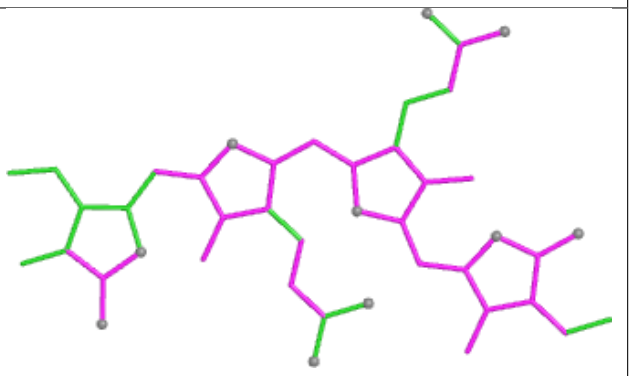


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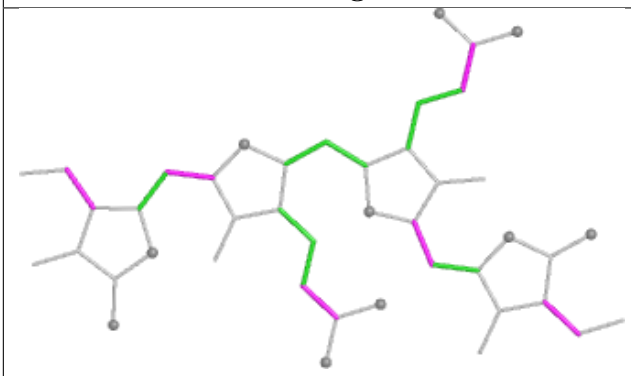
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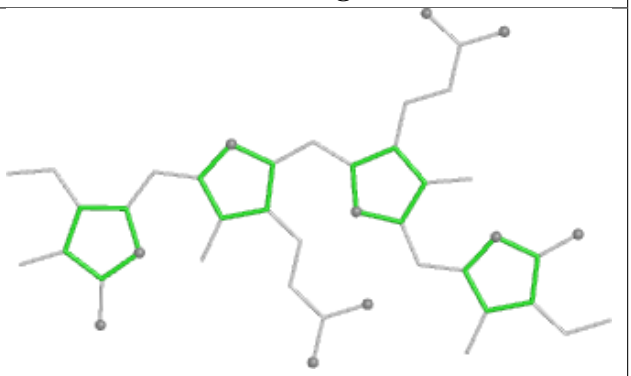
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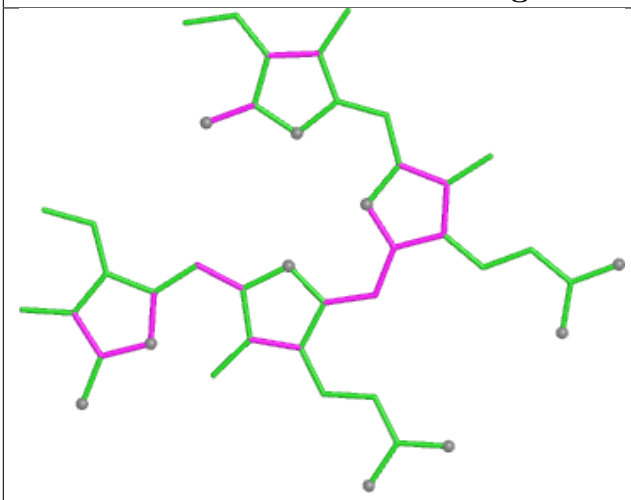


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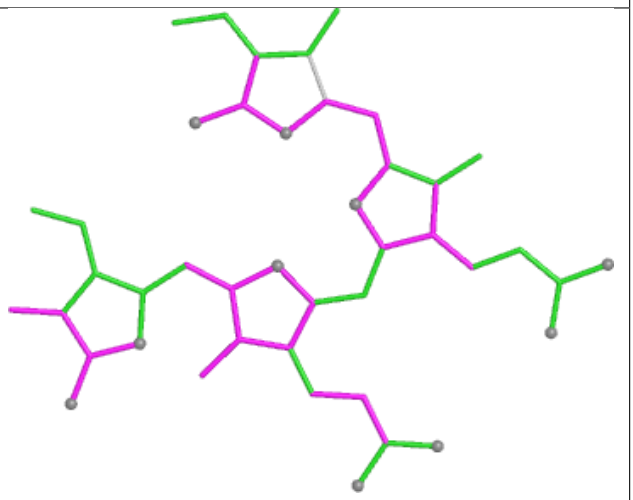


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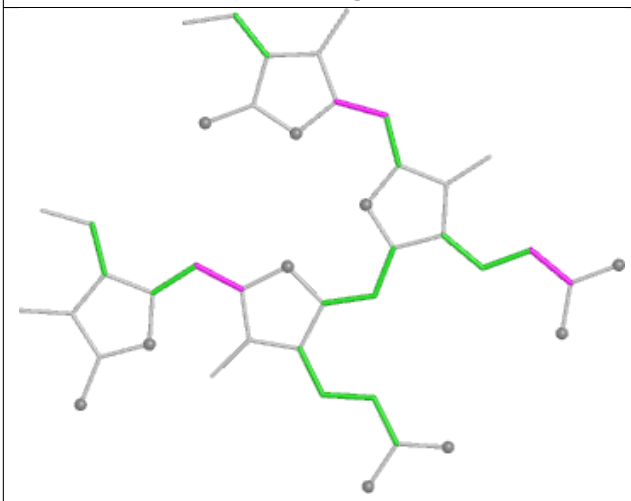
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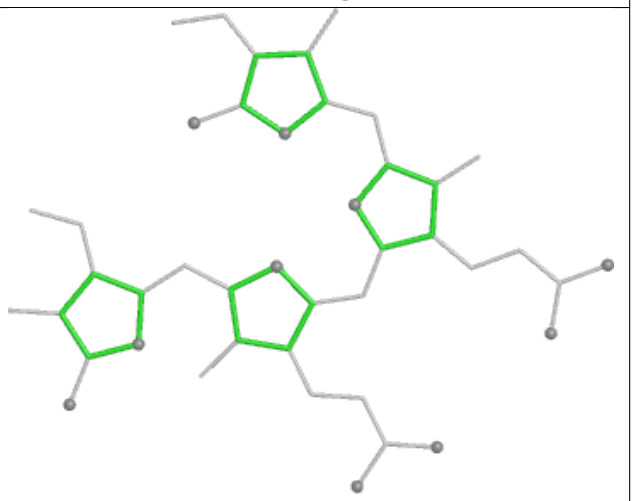
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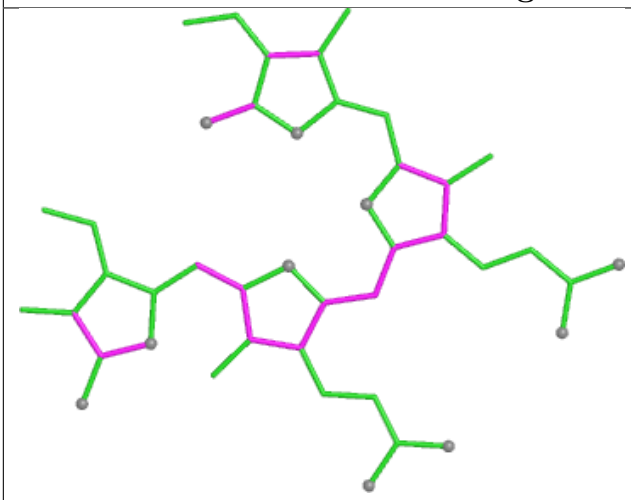


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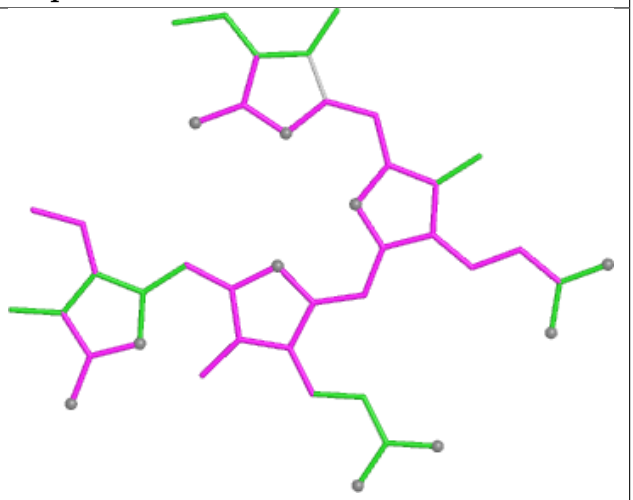


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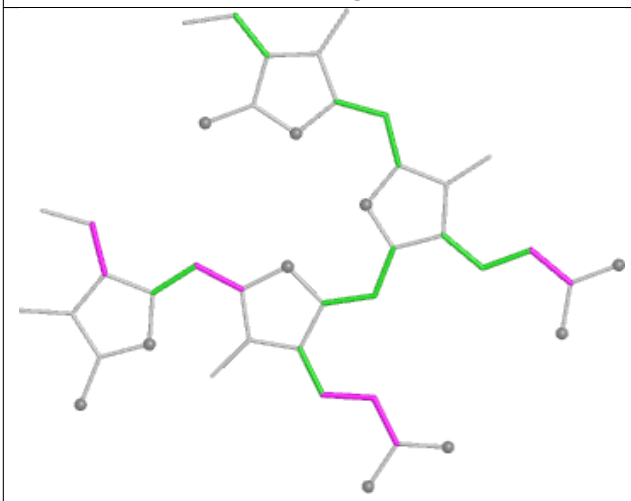
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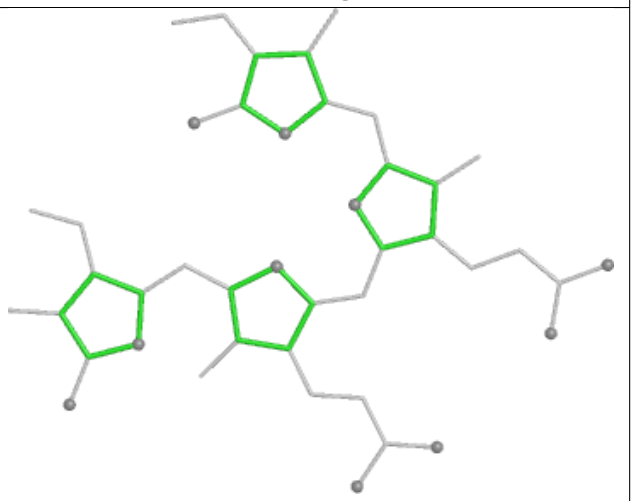
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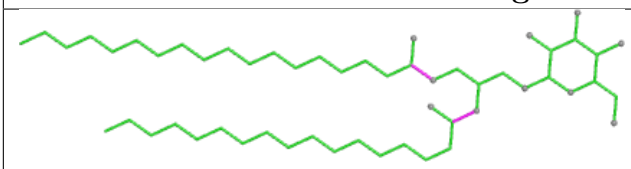


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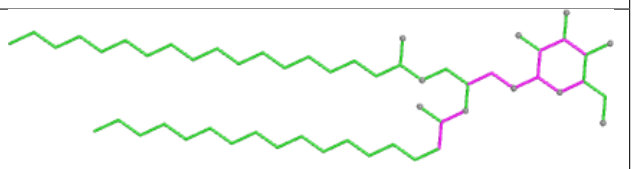


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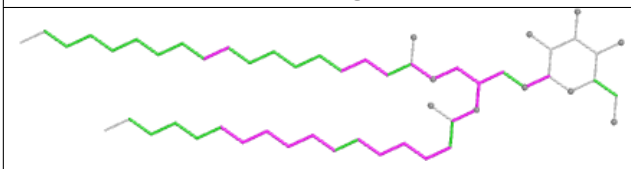
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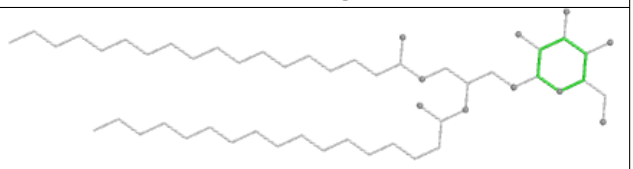
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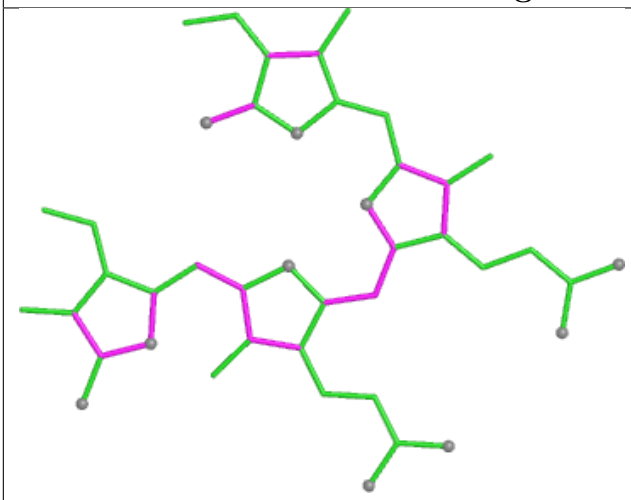


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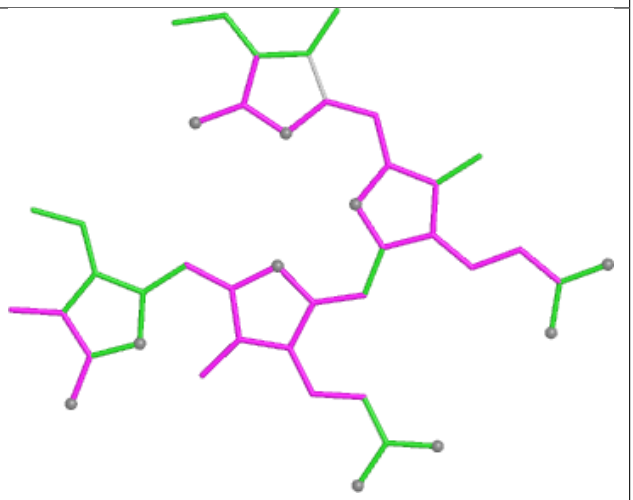


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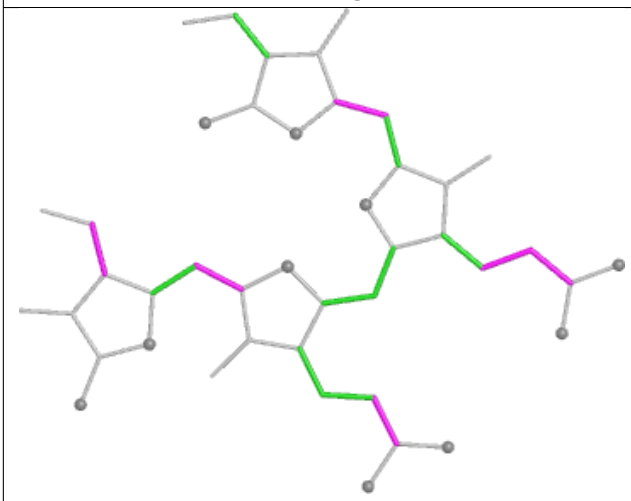
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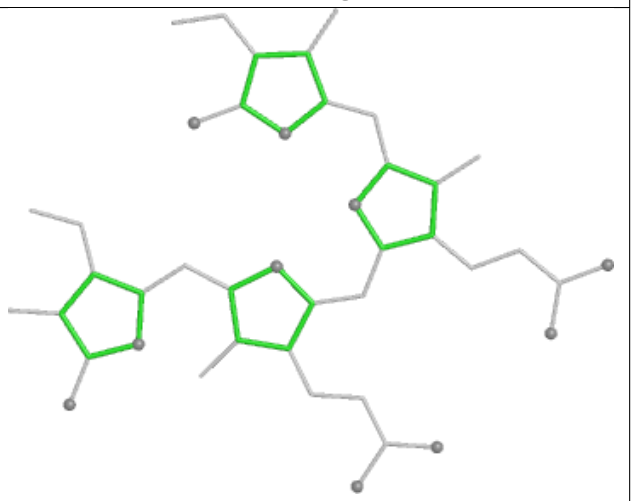
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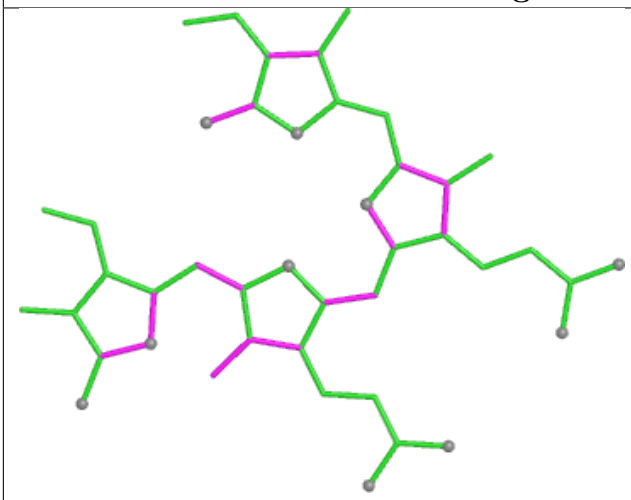


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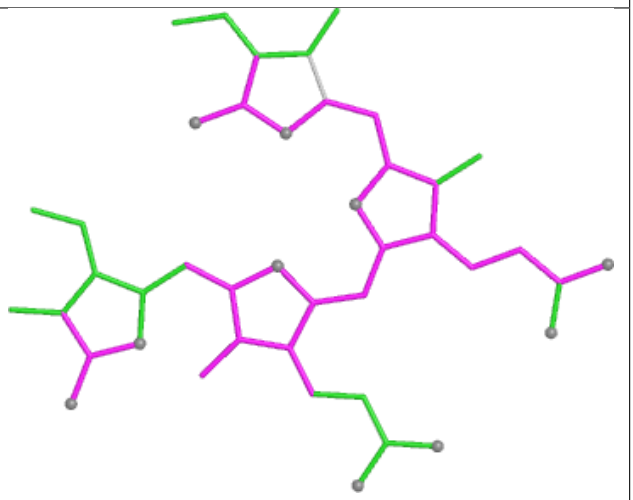


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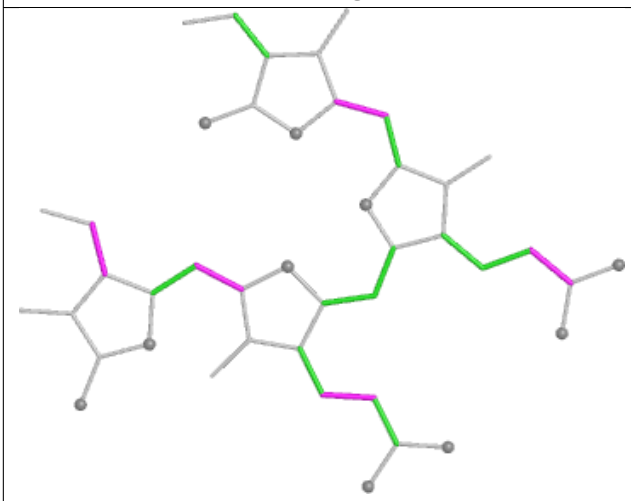
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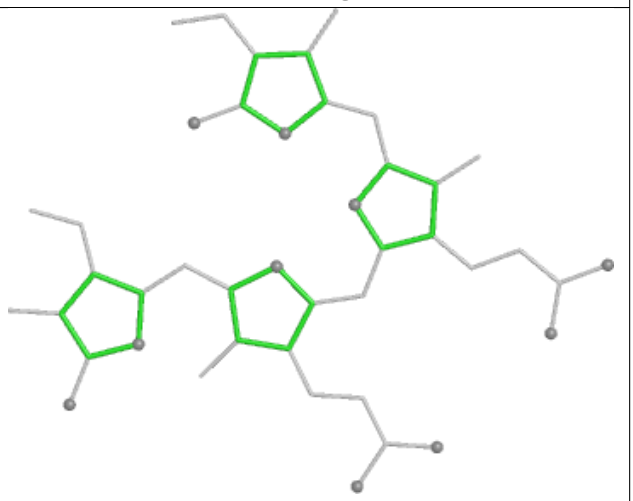
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Bond angles

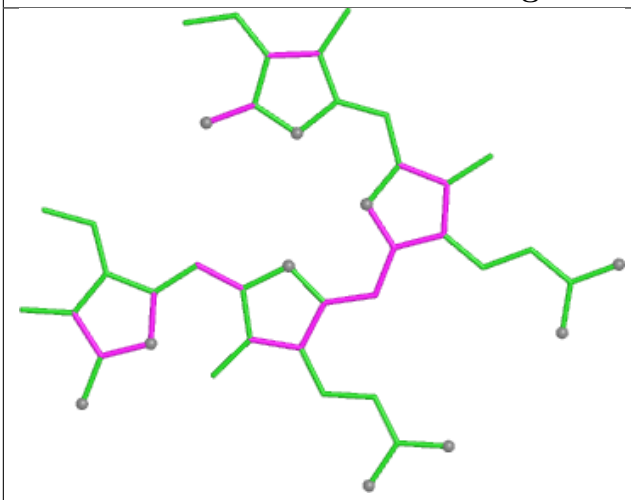


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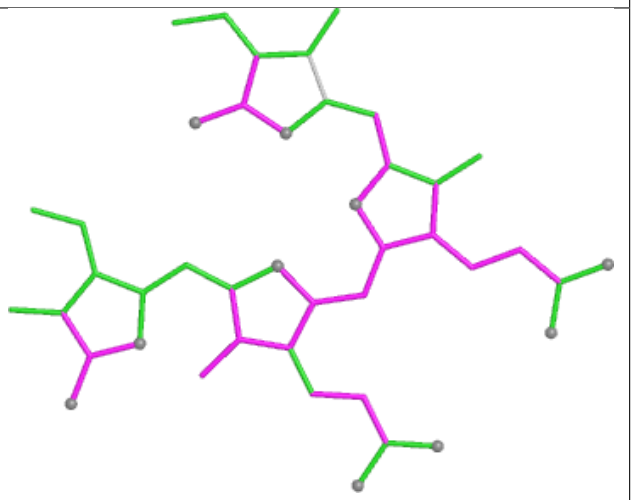


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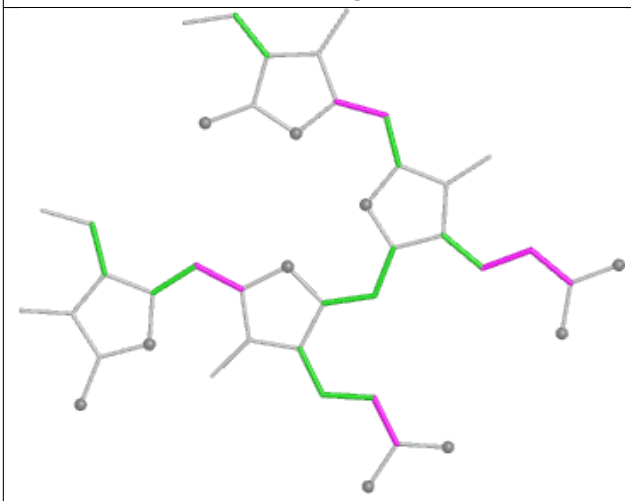
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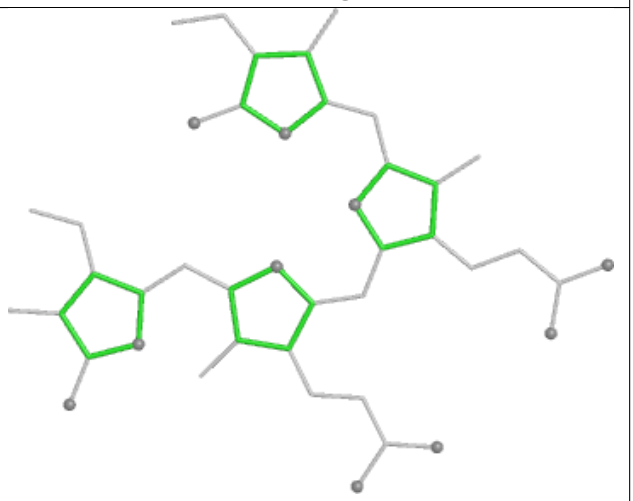
Bond lengths



Bond angles

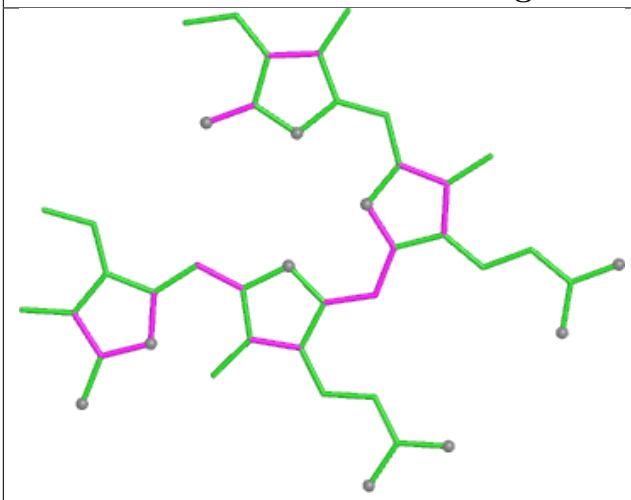


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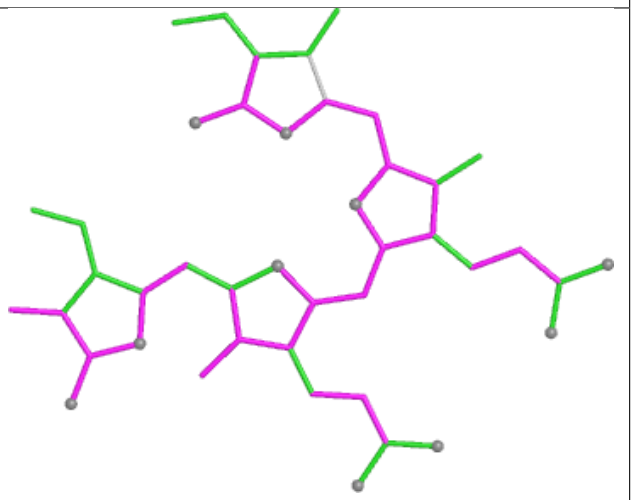


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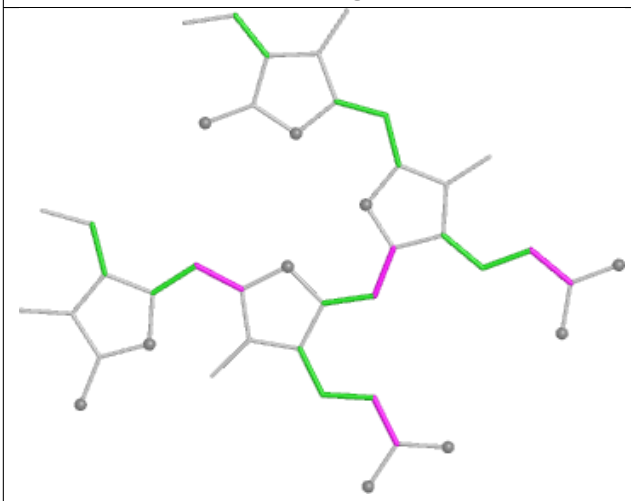
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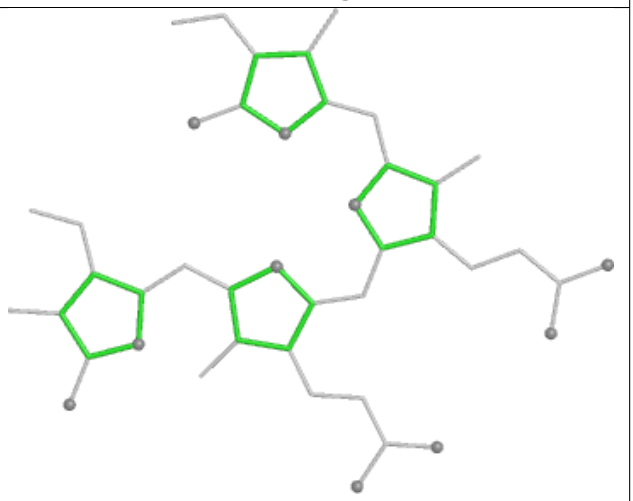
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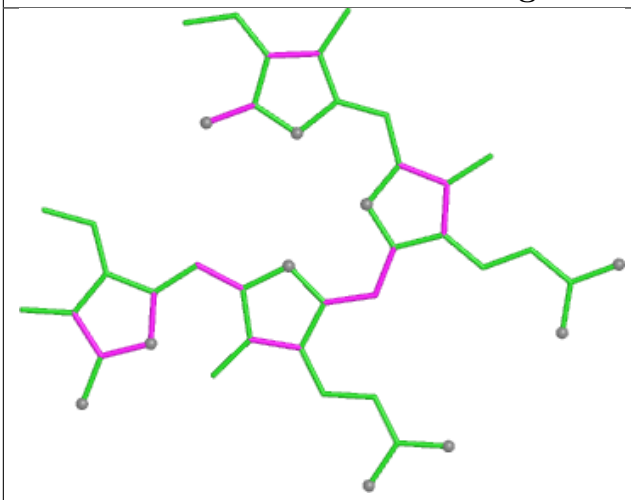


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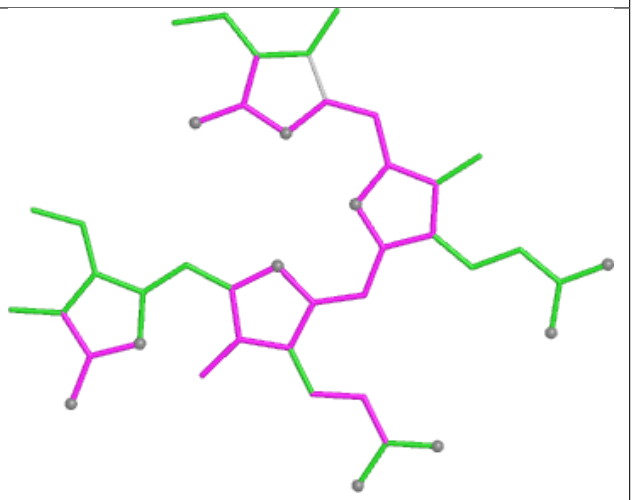


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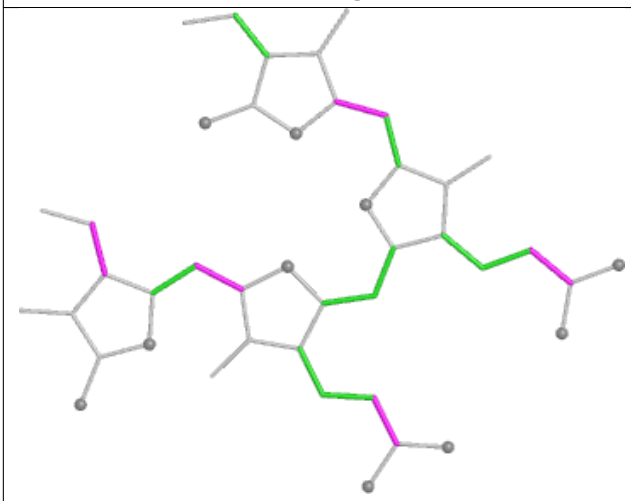
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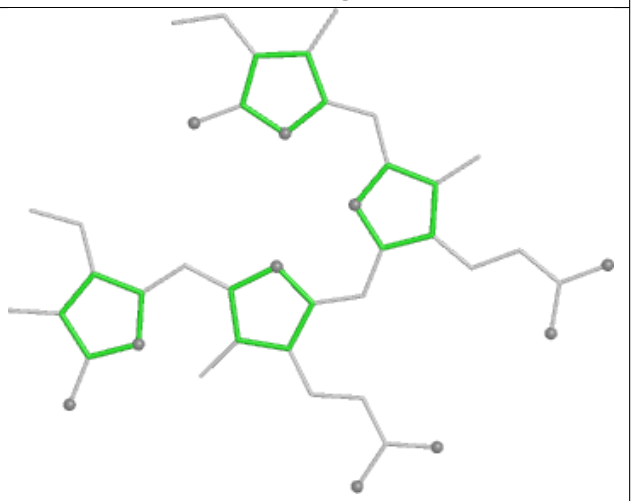
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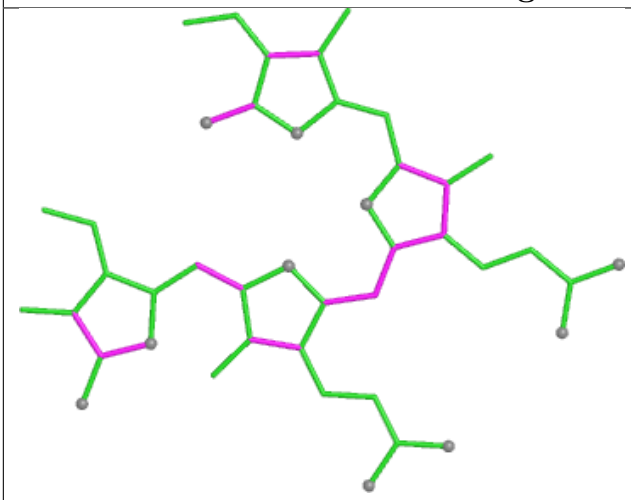


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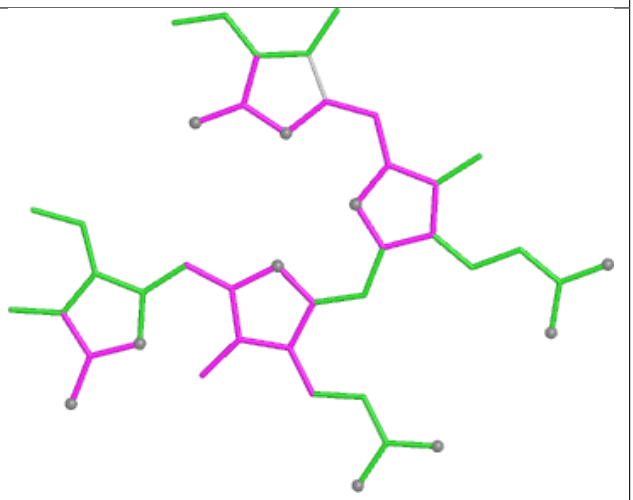


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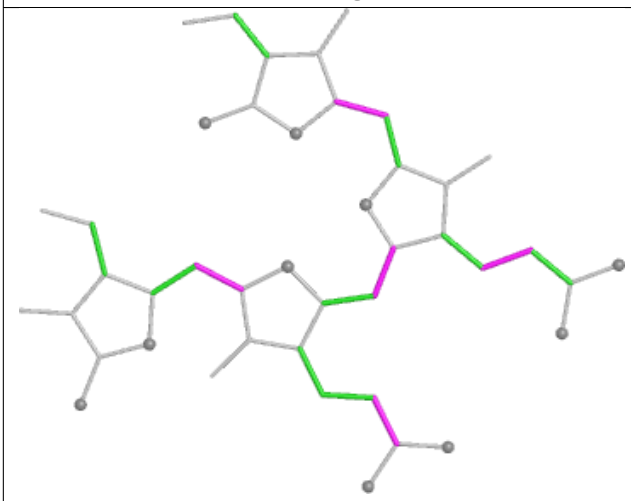
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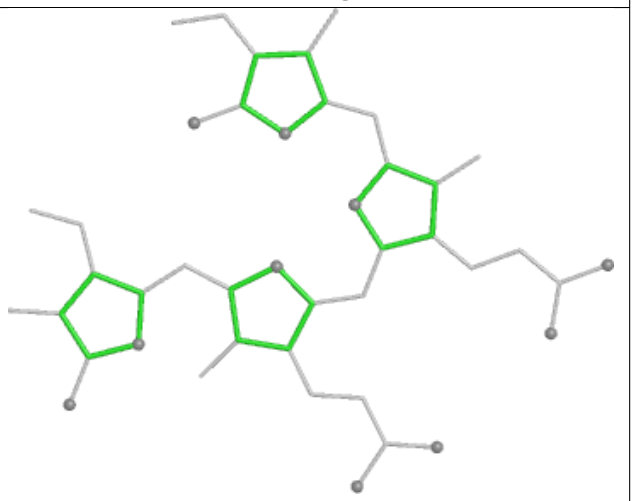
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Bond angles

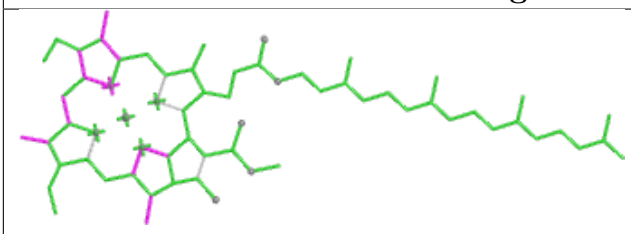


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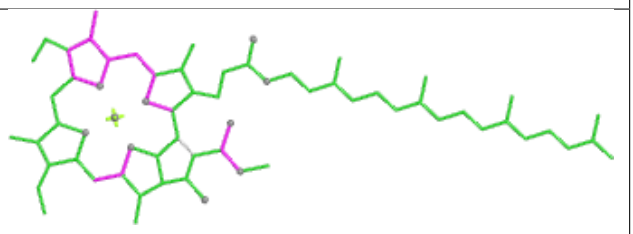


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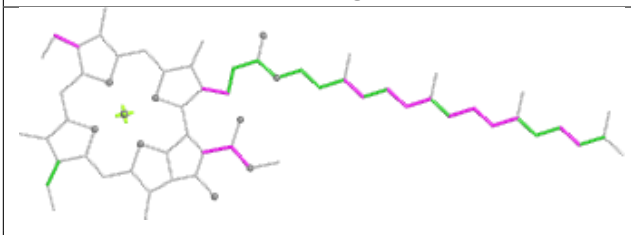
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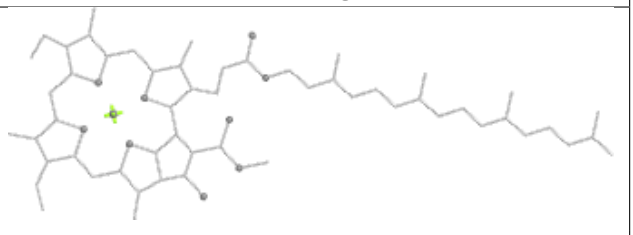
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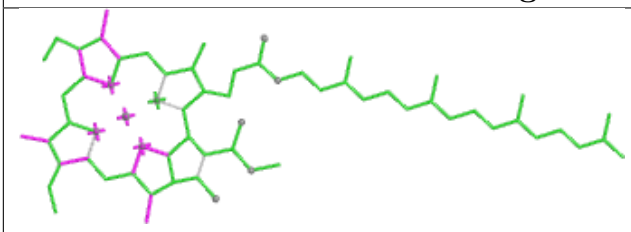


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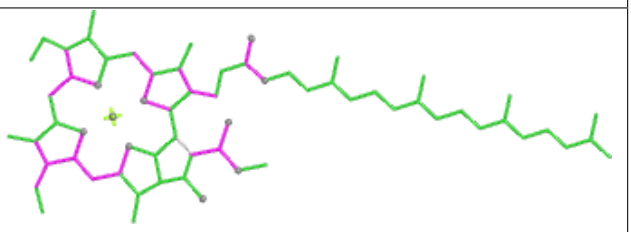


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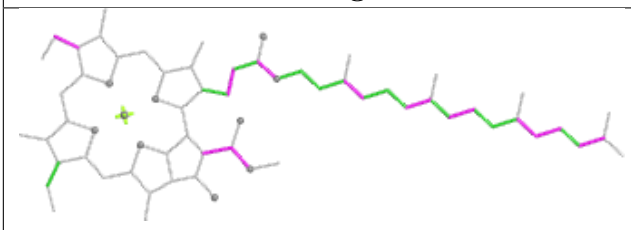
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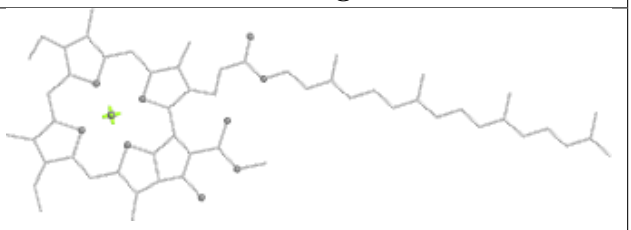
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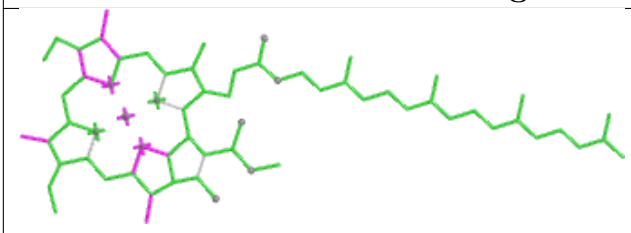


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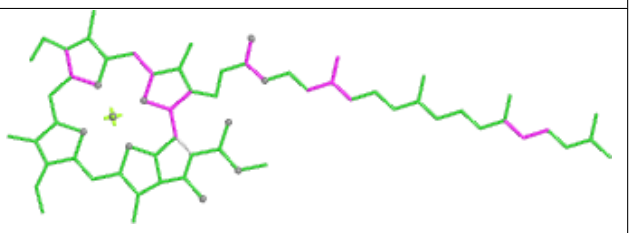


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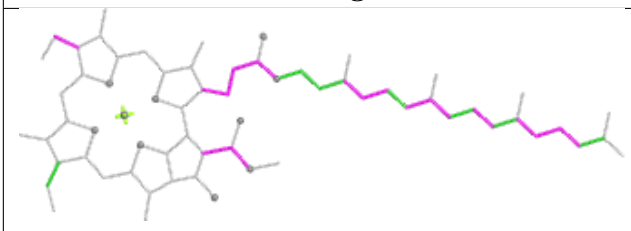
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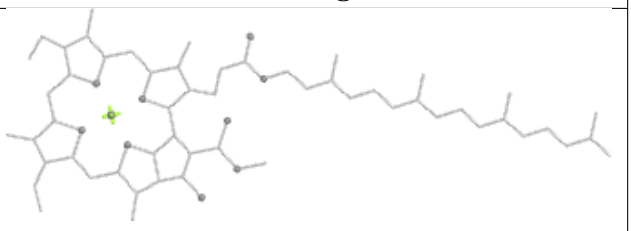
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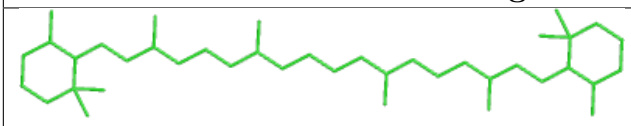


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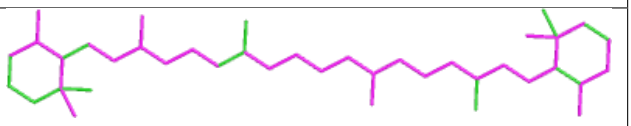


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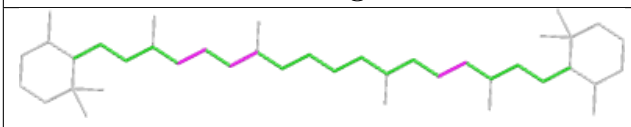
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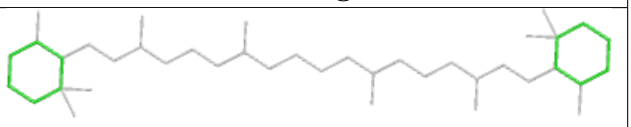
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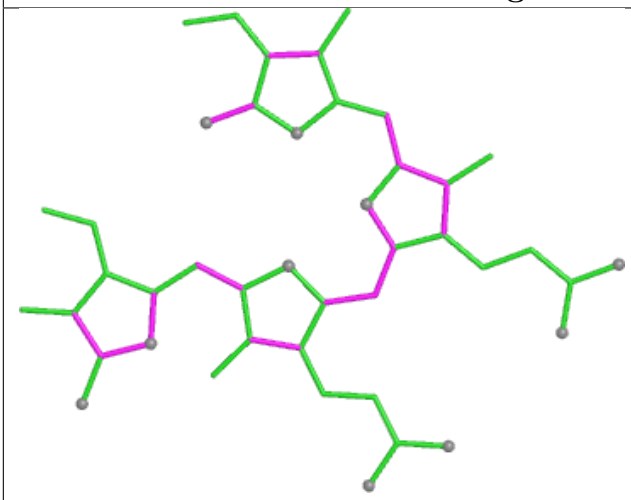


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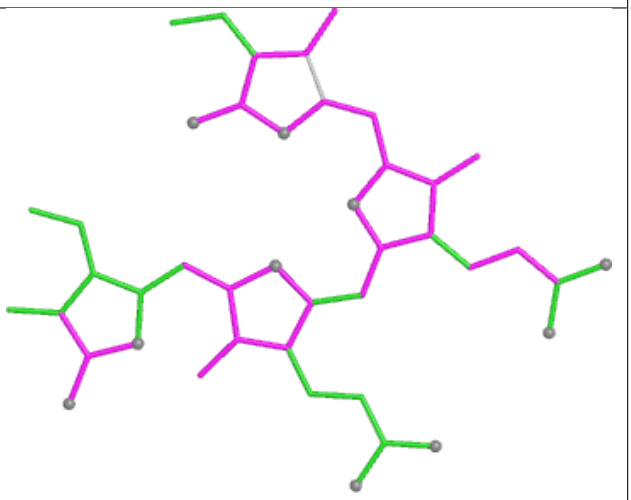


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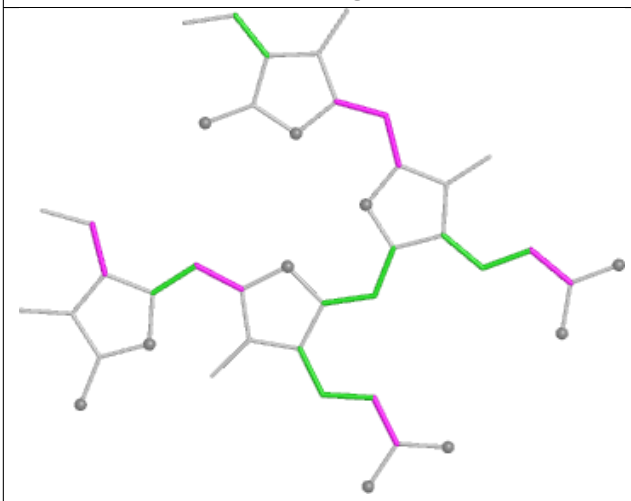
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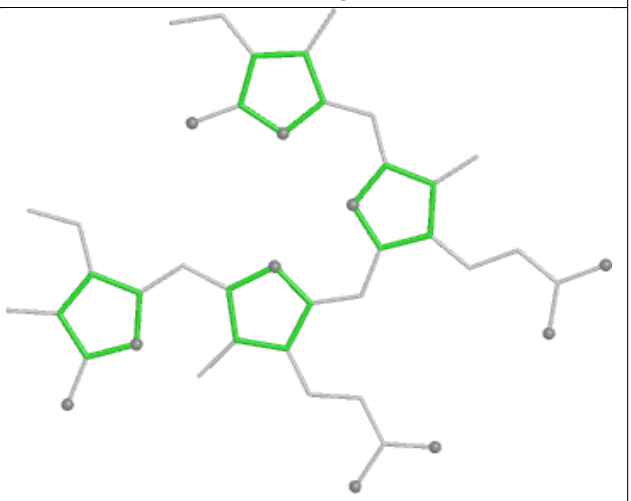
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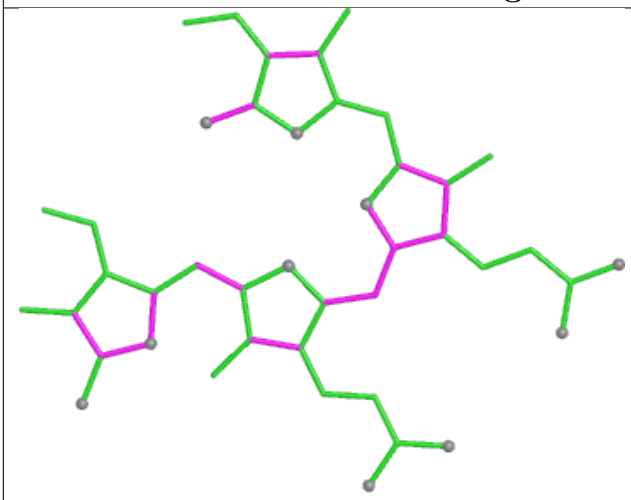


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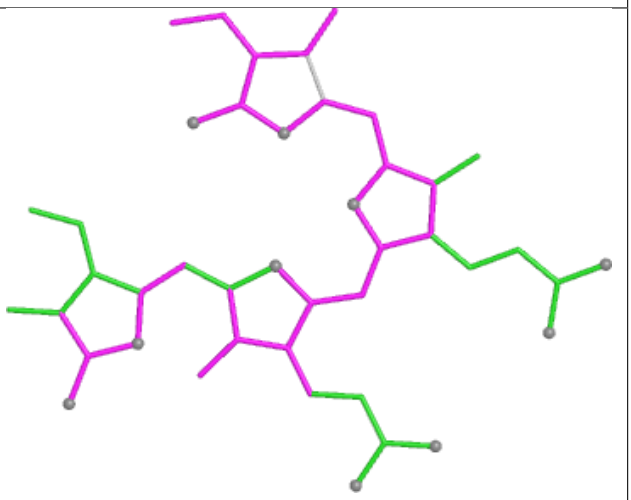


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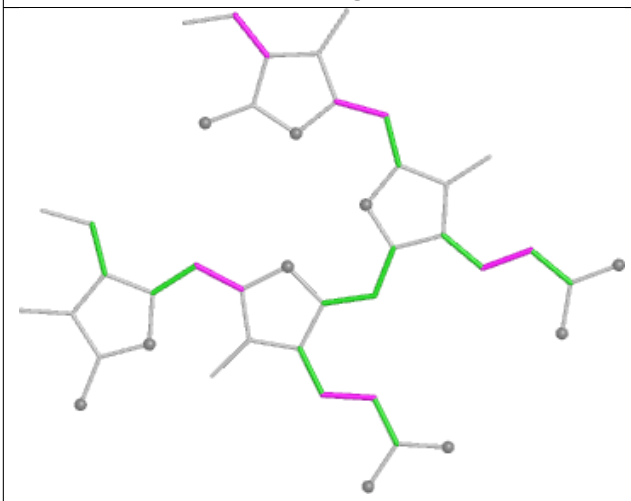
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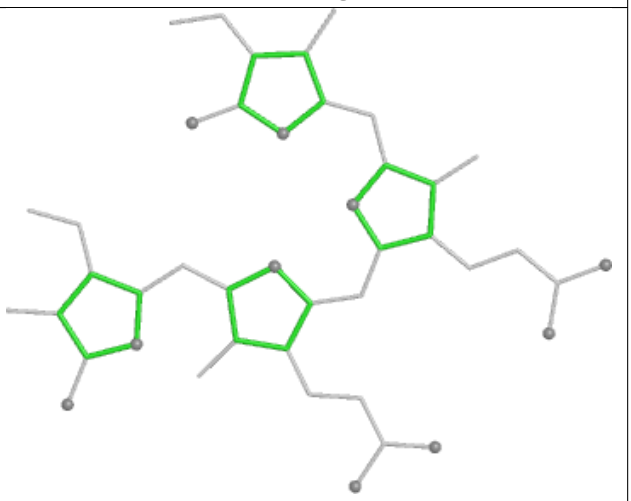
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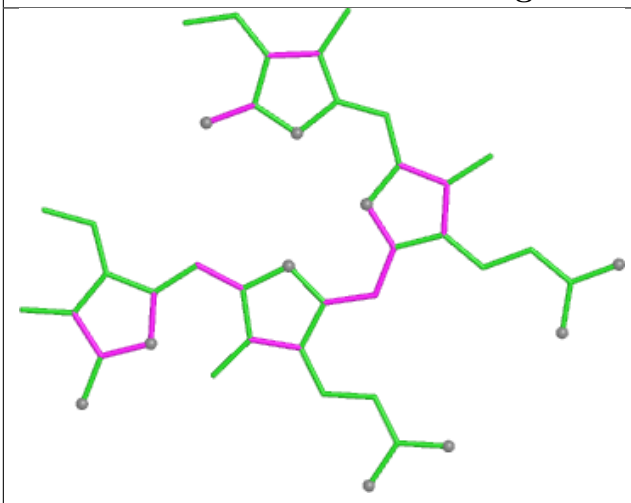


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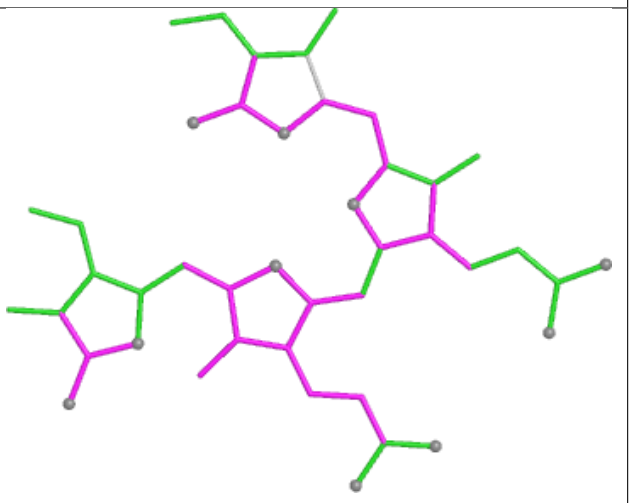


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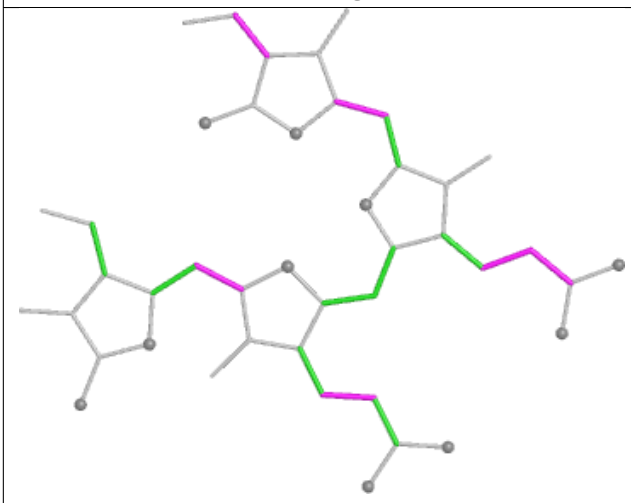
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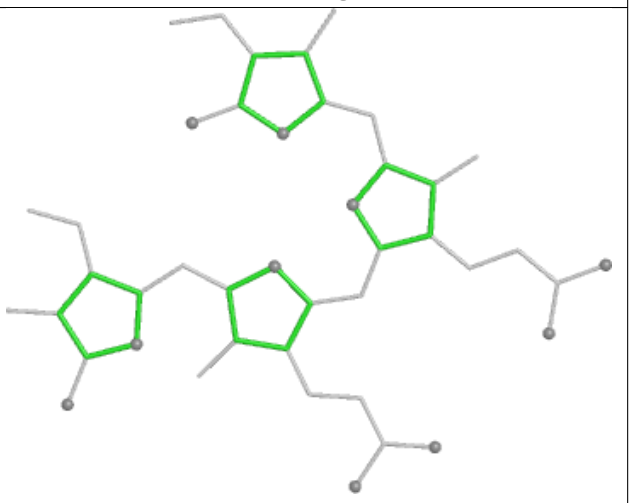
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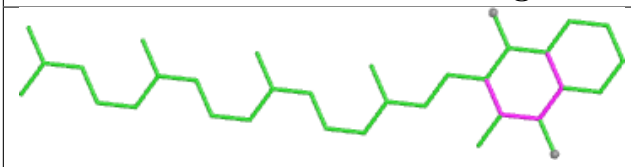


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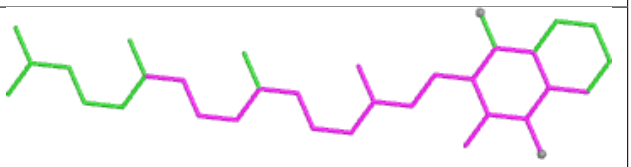


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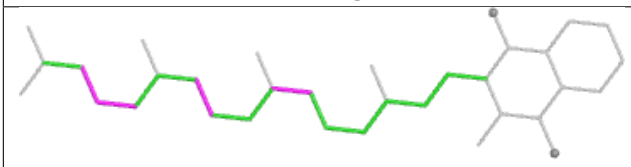
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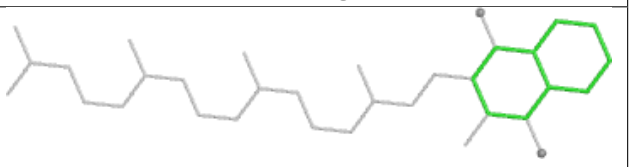
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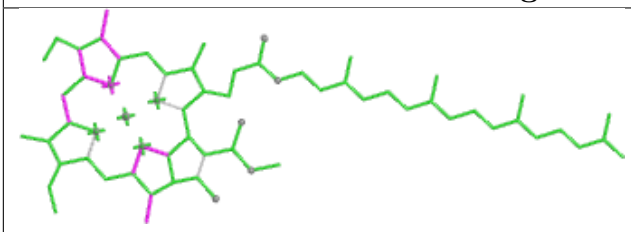


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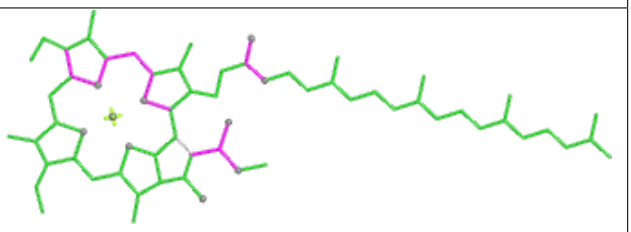


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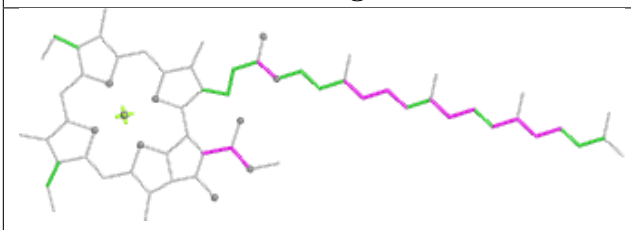
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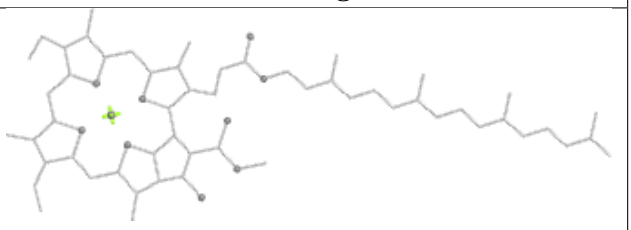
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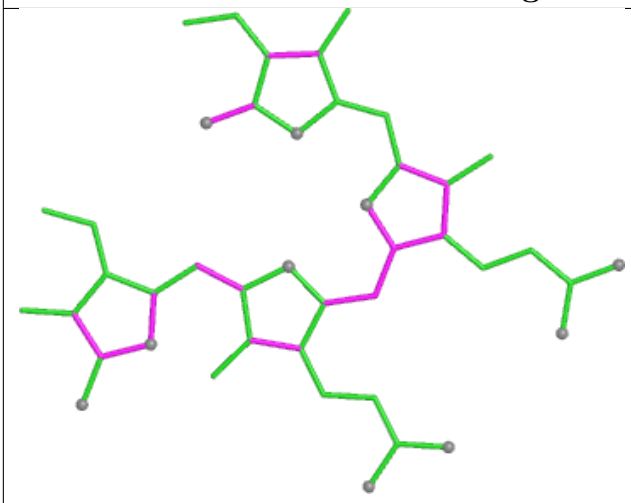


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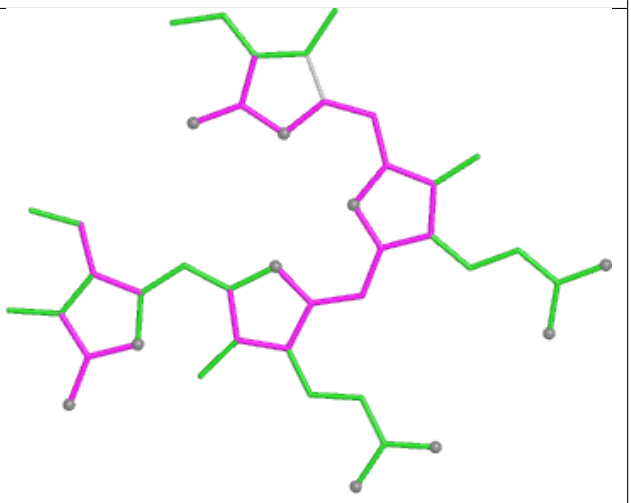


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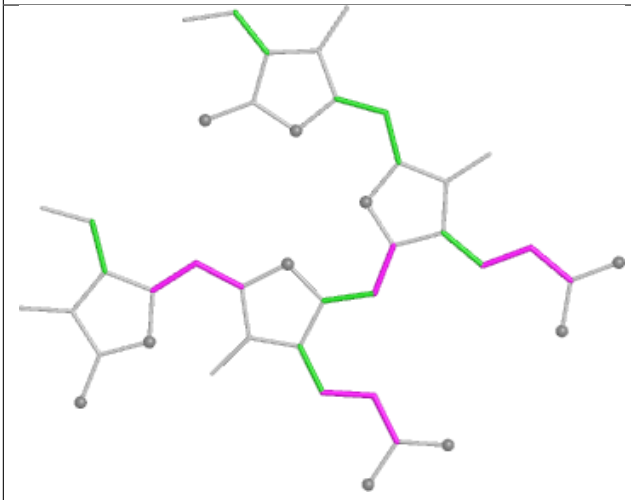
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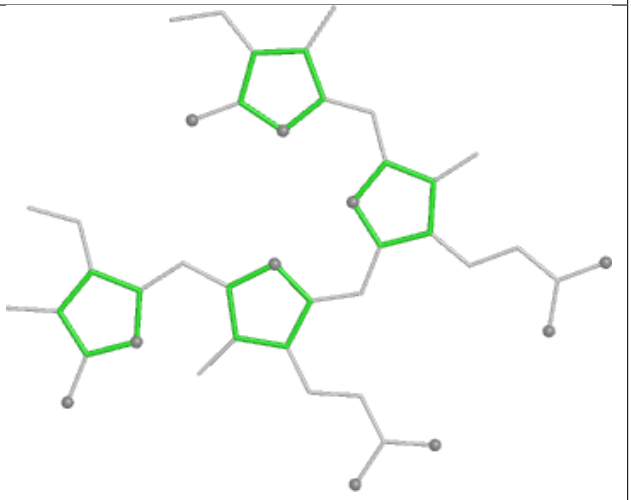
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Bond angles

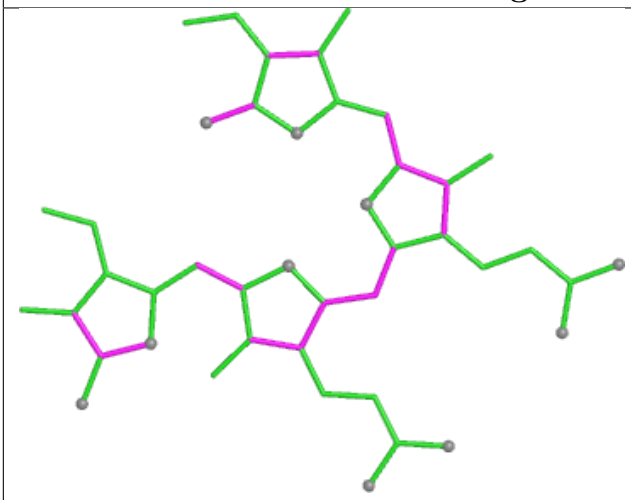


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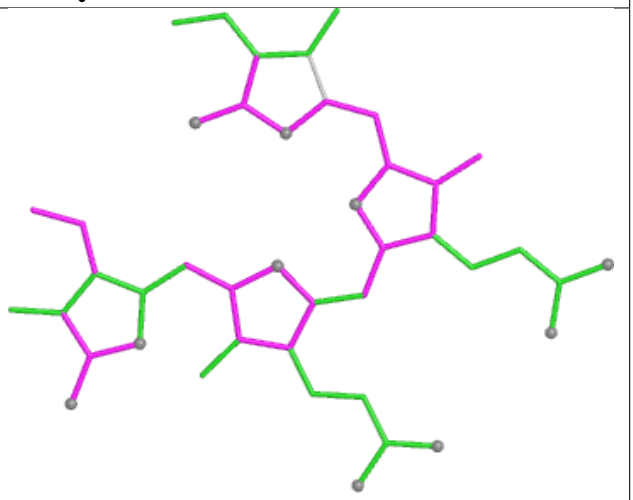


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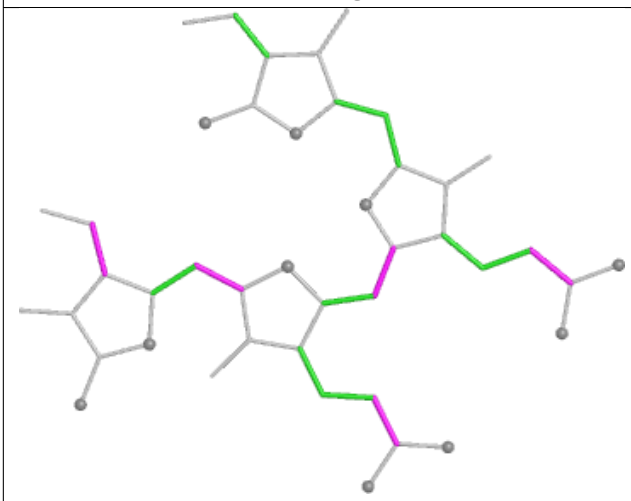
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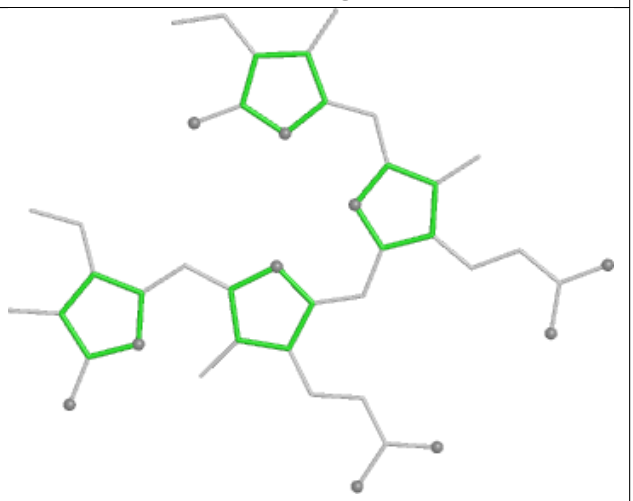
Bond lengths



Bond angles

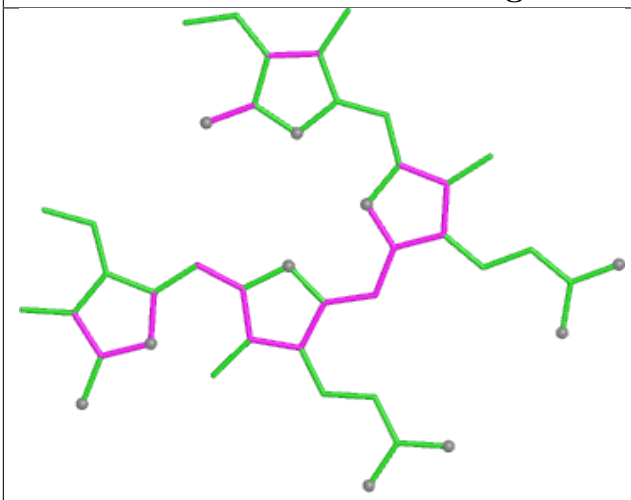


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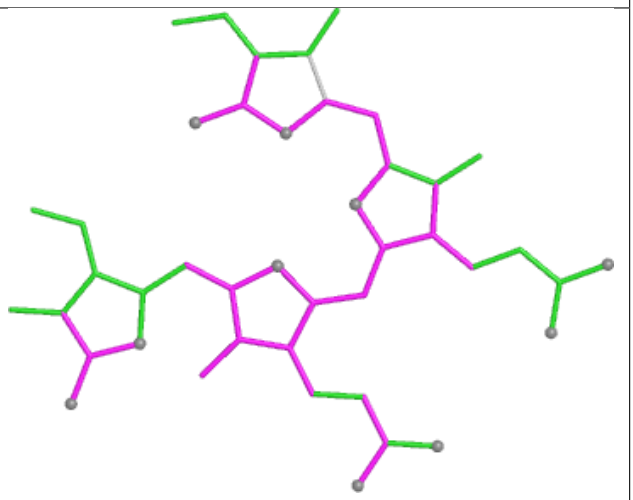


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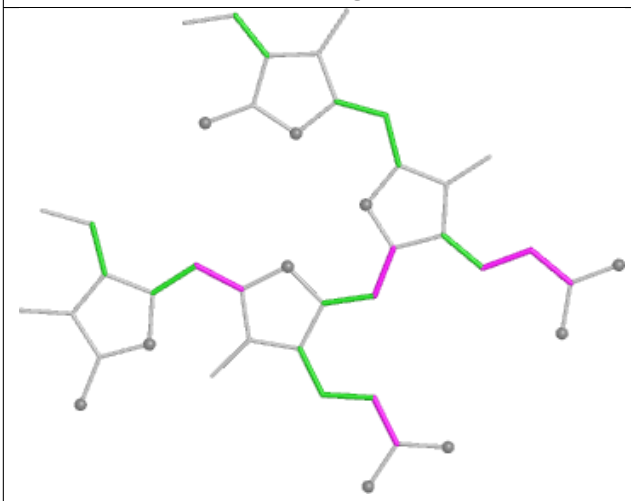
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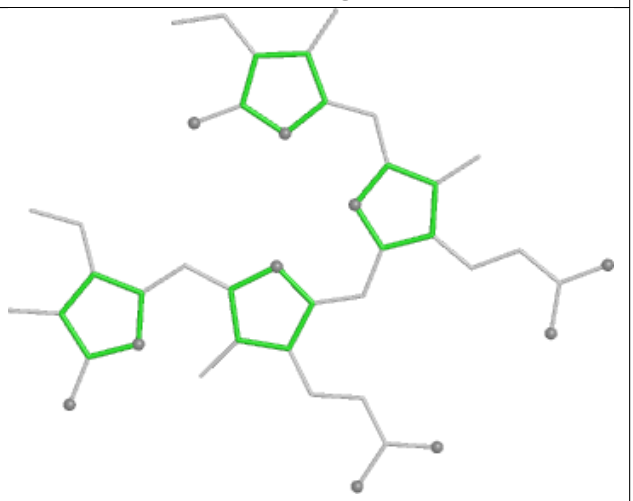
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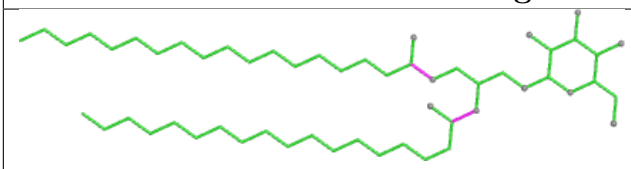


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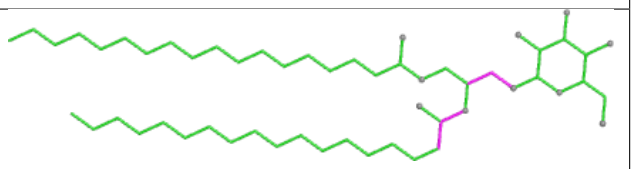


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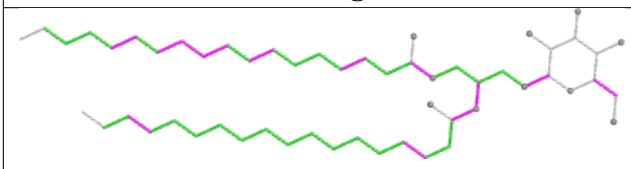
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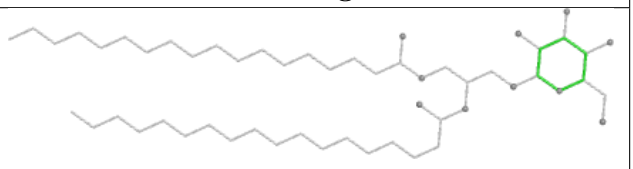
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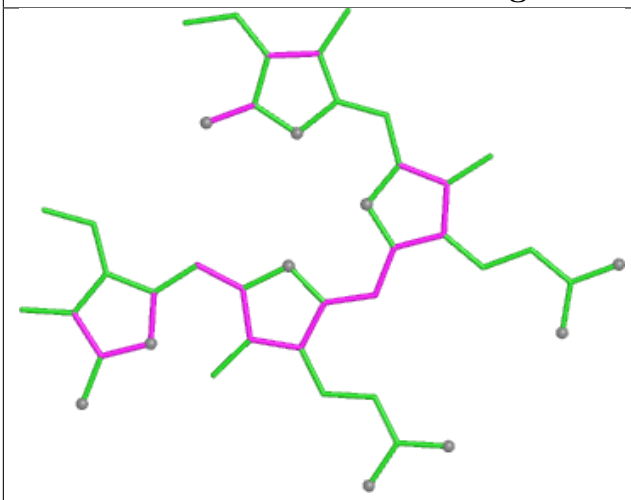


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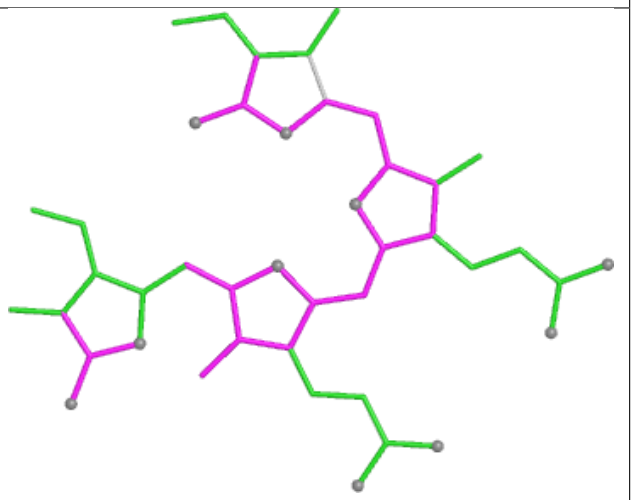


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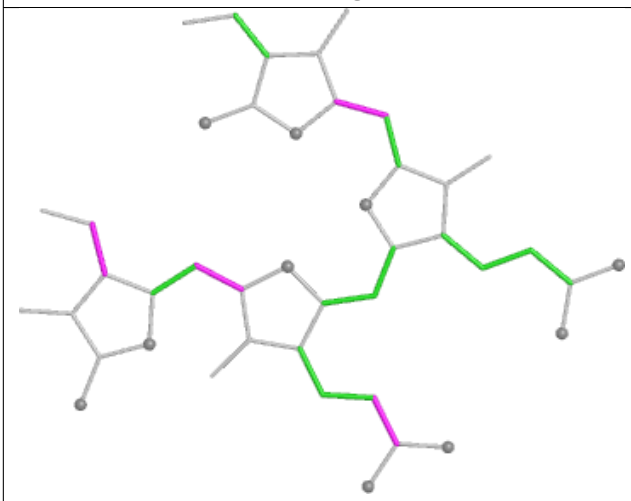
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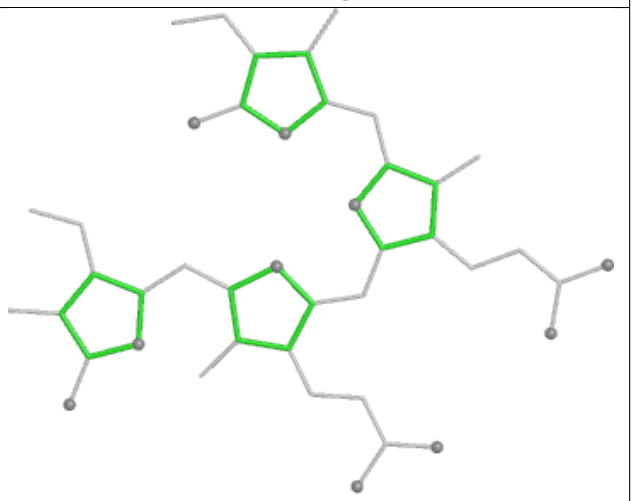
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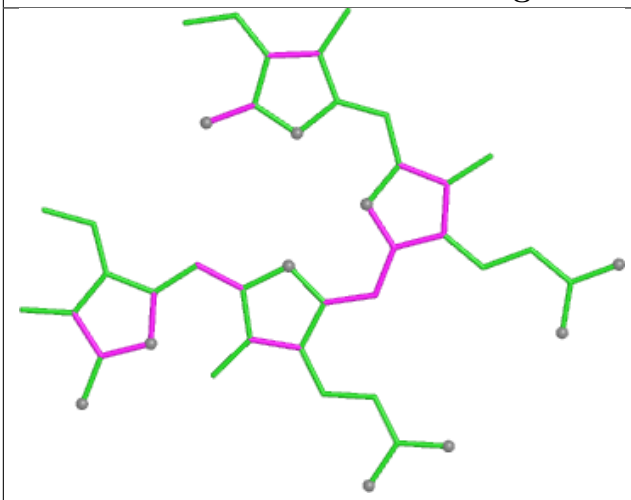


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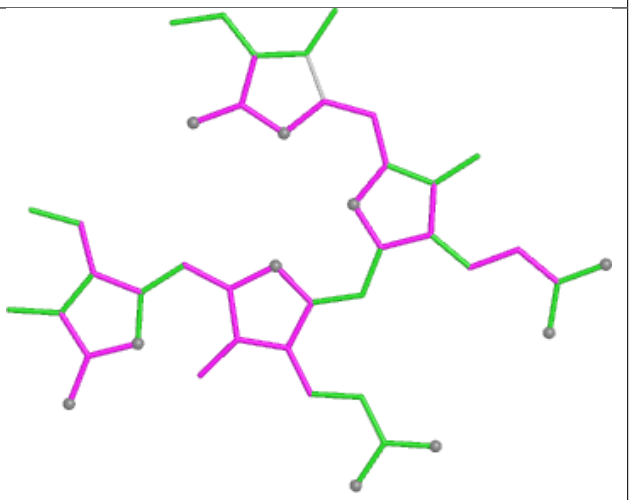


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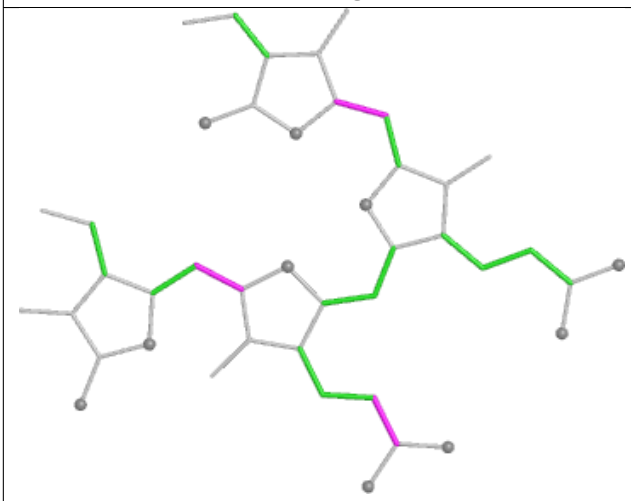
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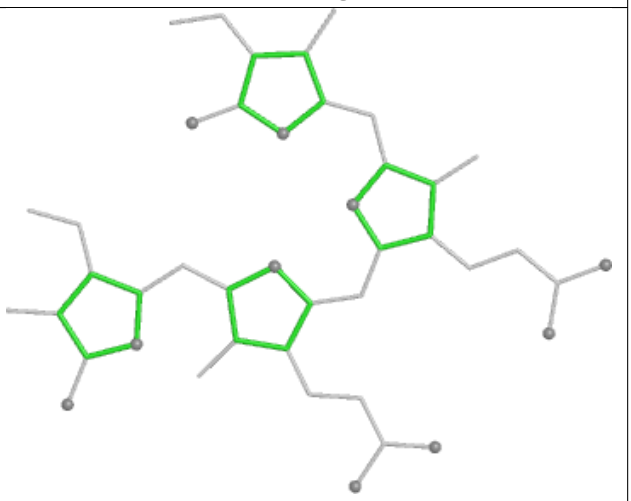
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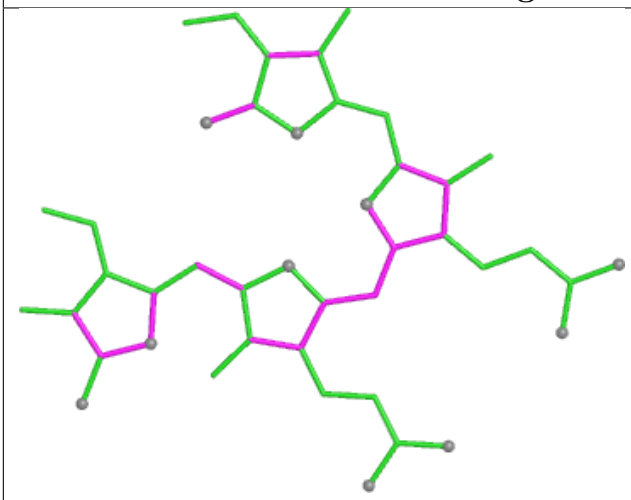


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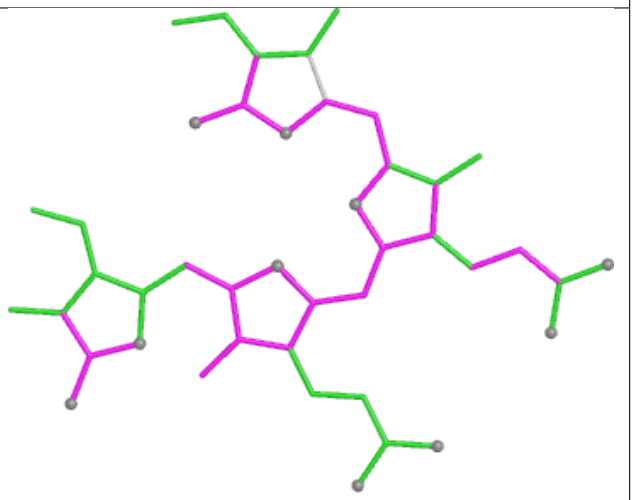


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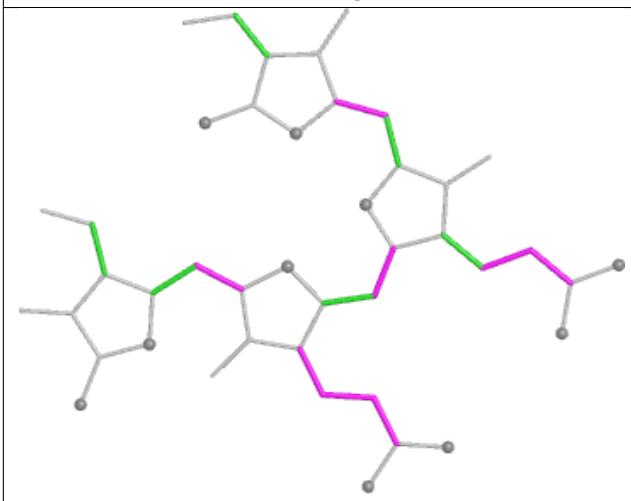
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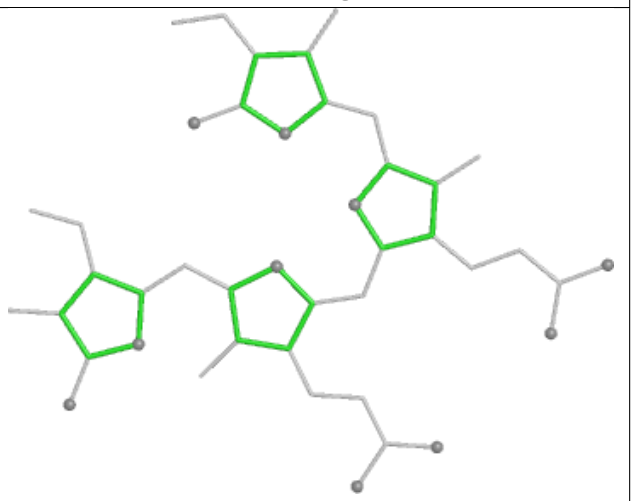
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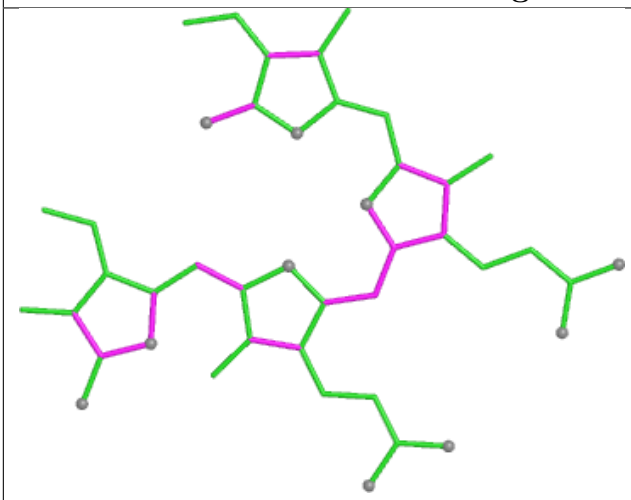


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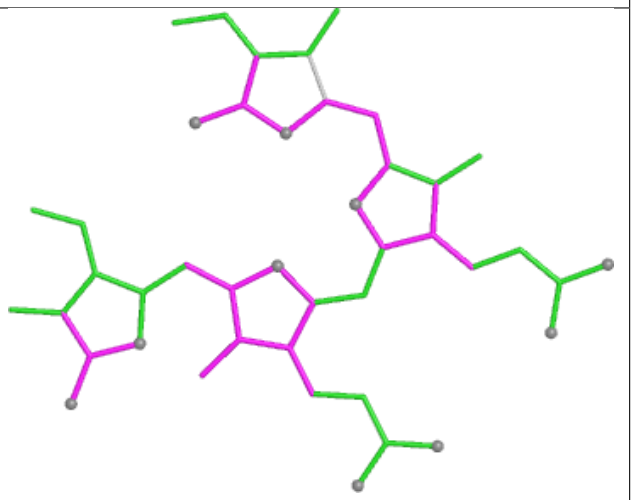


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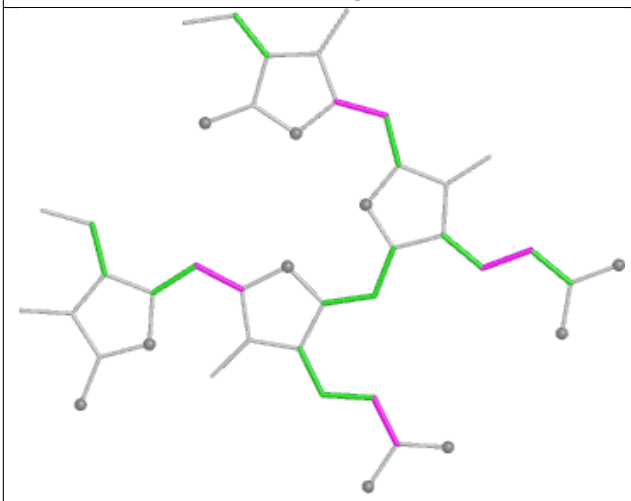
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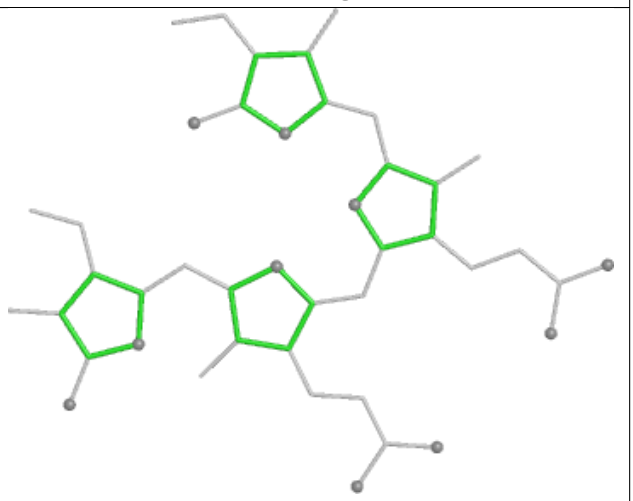
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Bond angles

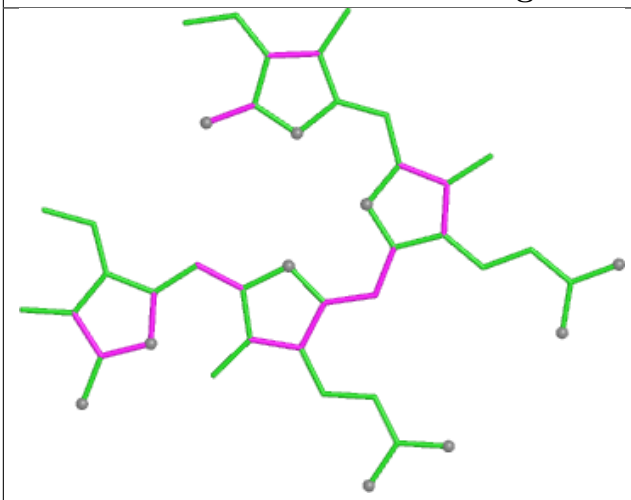


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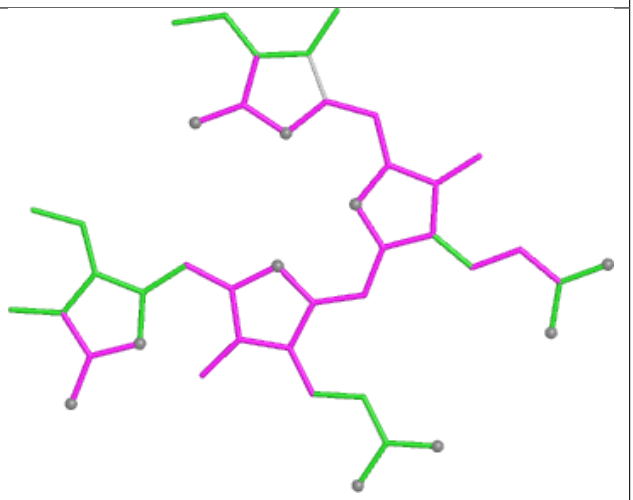


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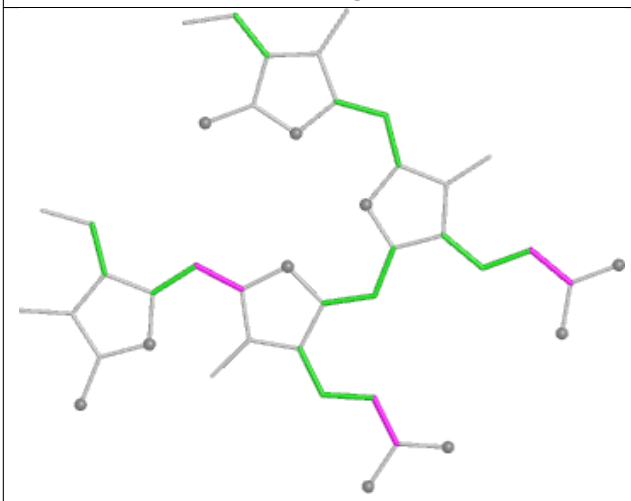
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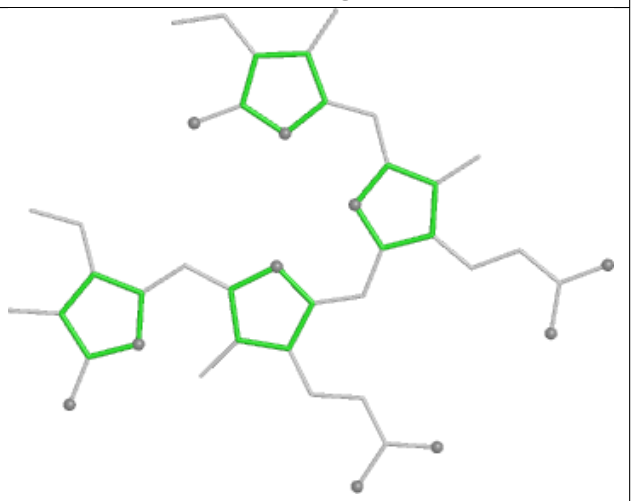
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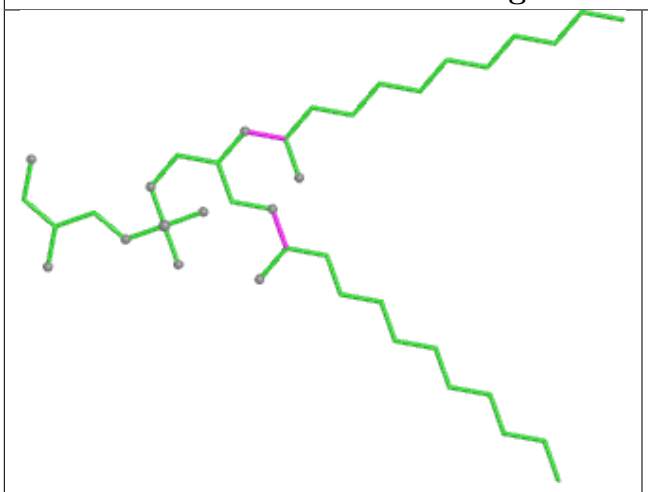


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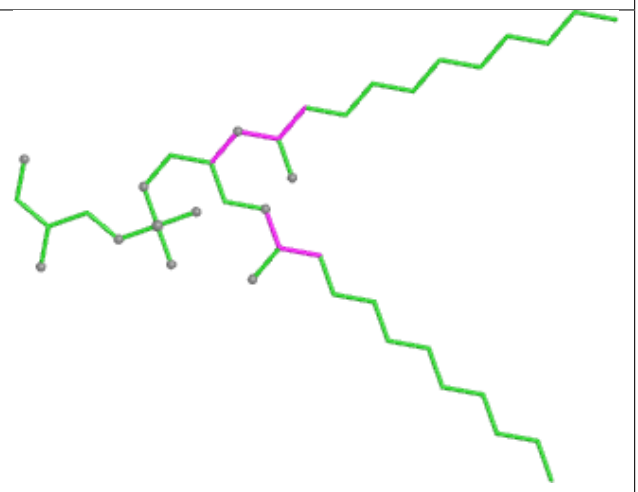


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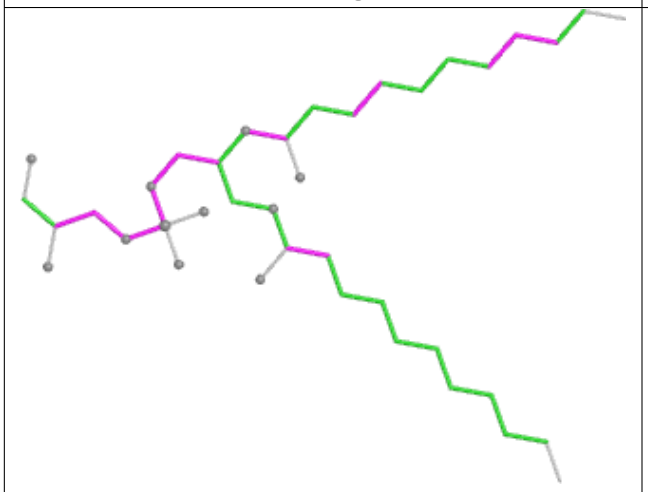
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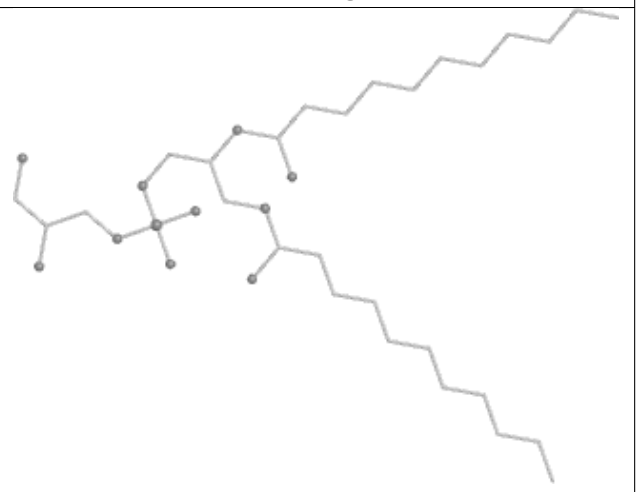
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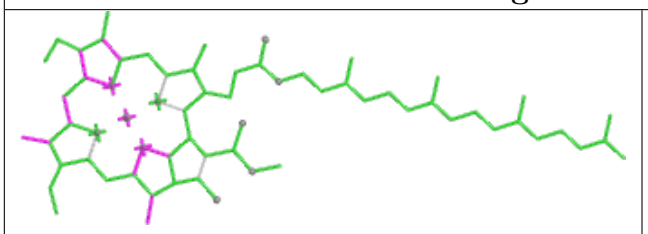


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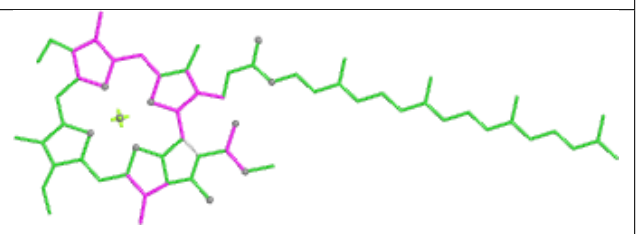


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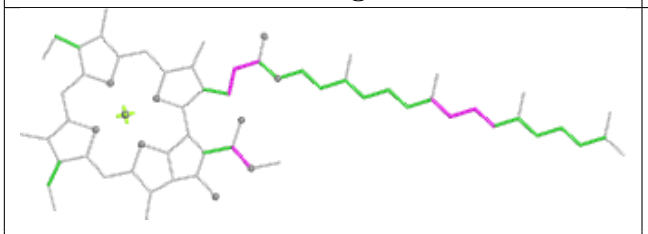
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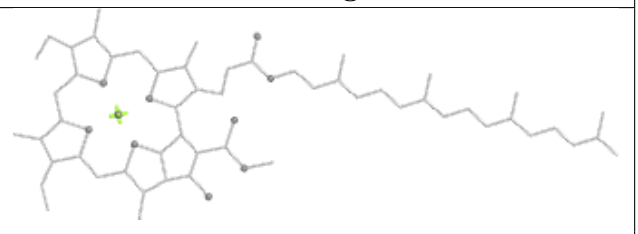
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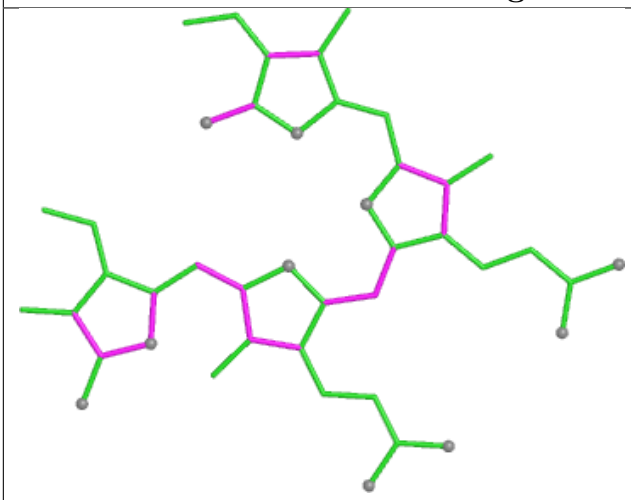


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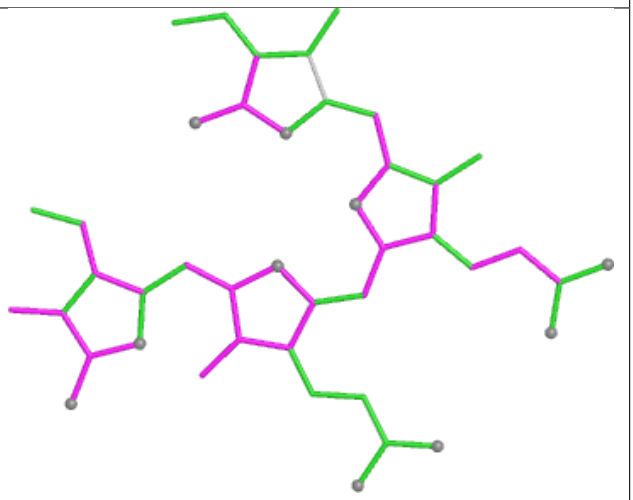


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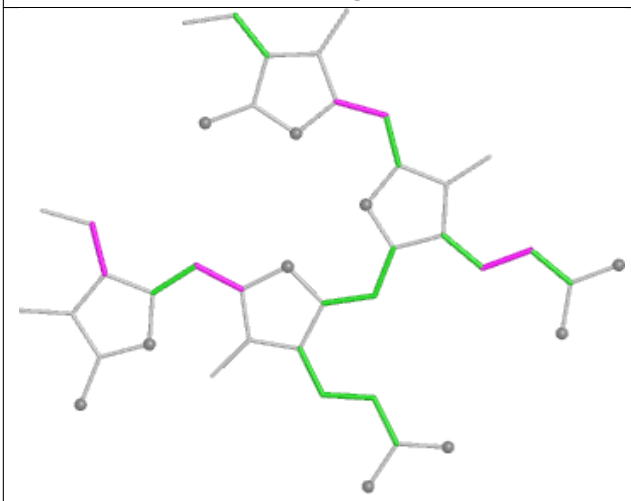
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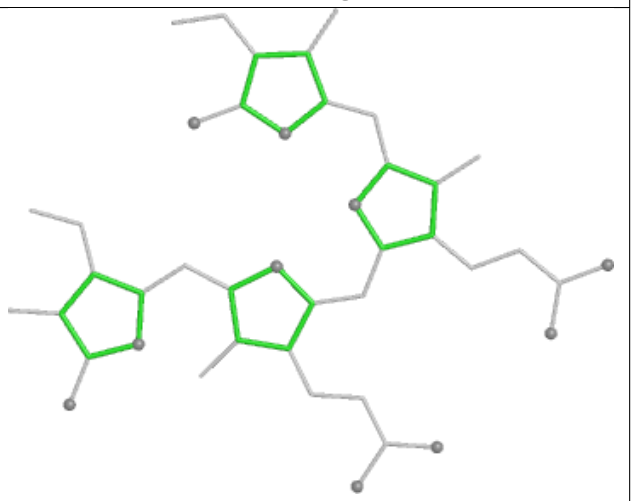
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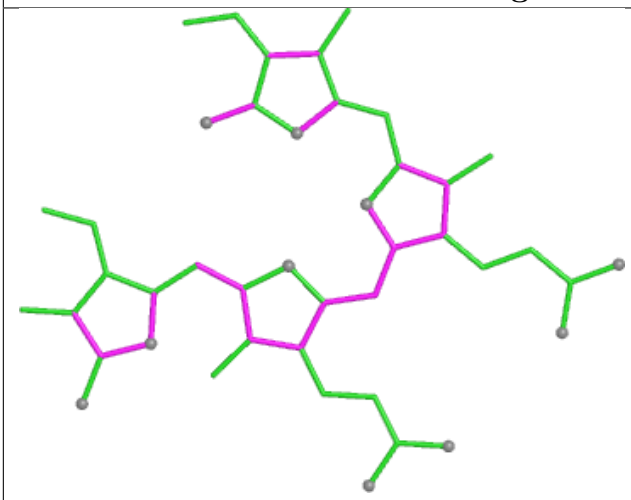


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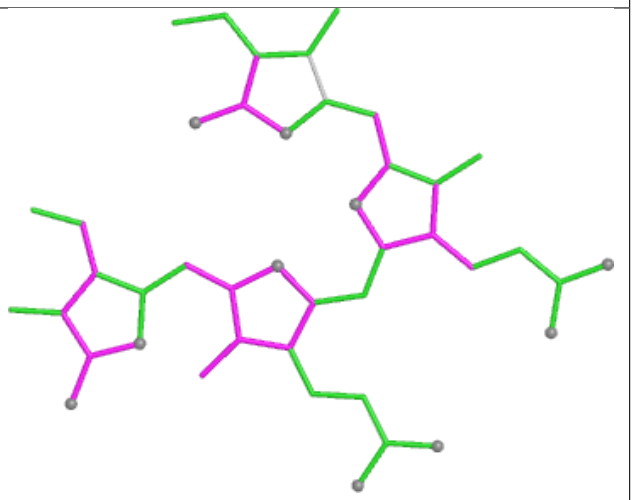


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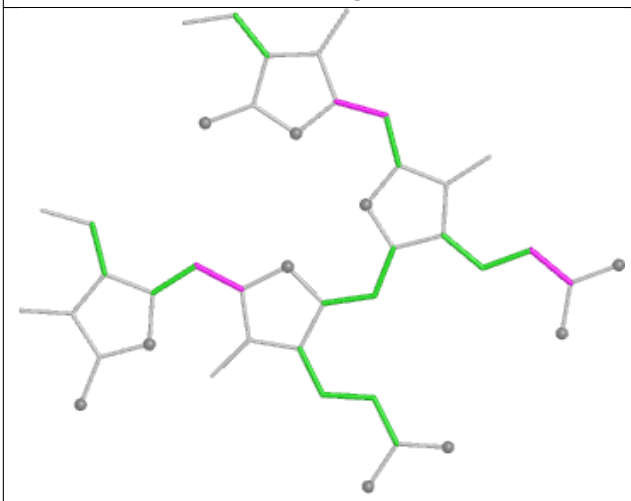
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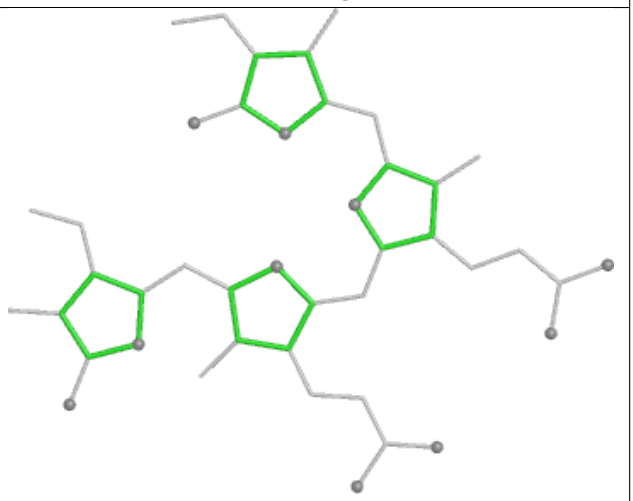
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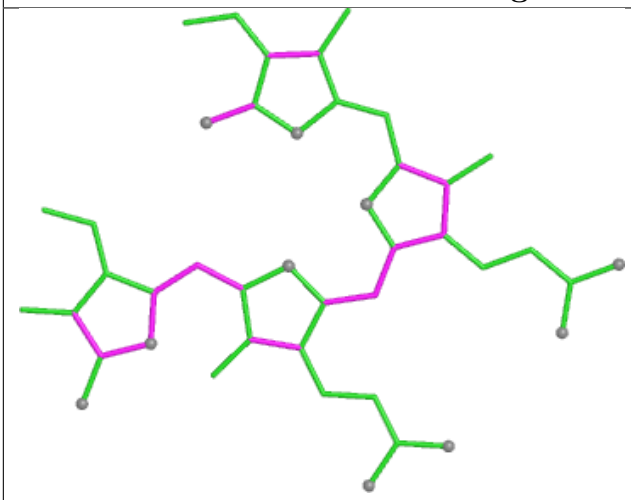


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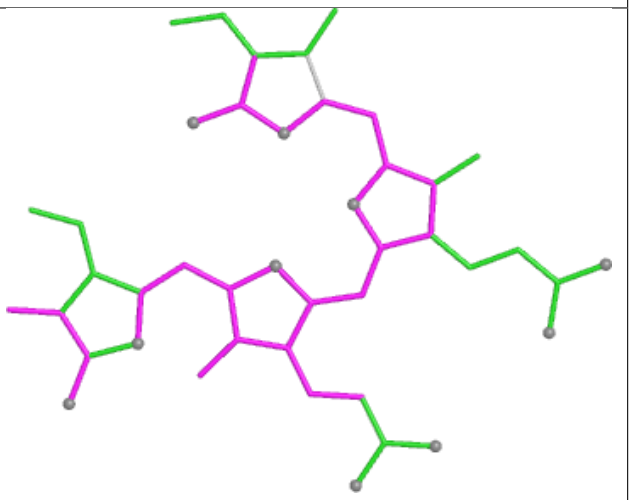


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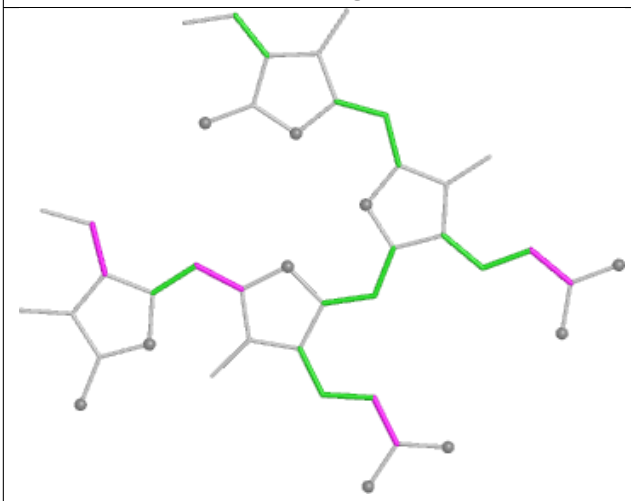
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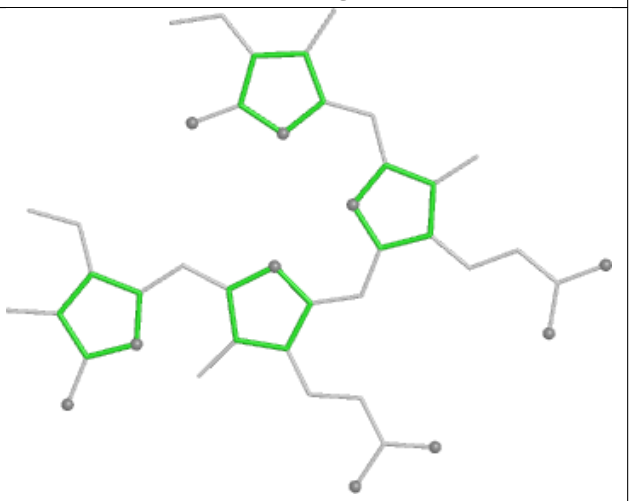
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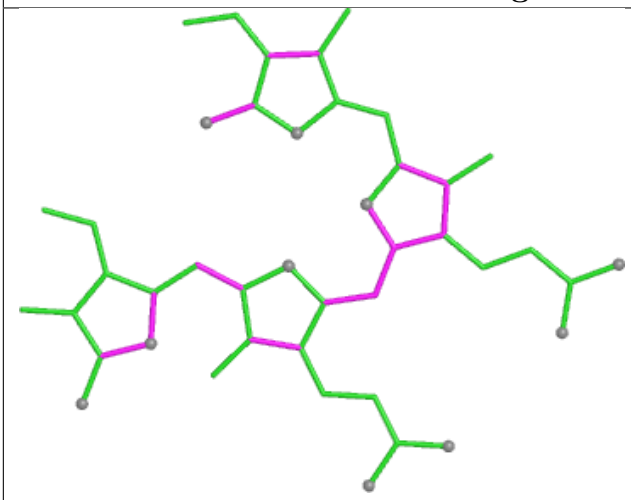


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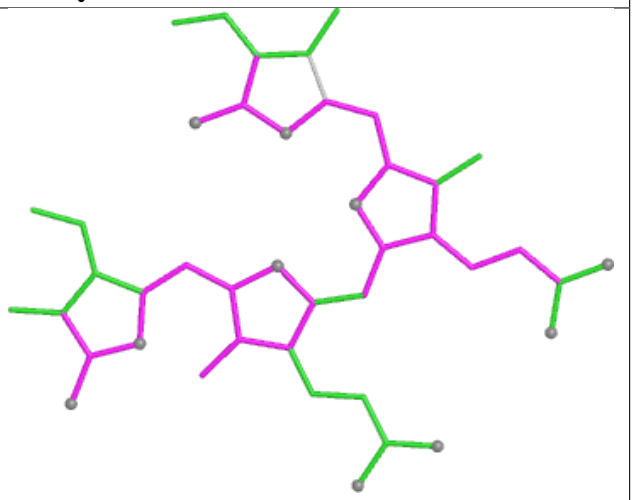


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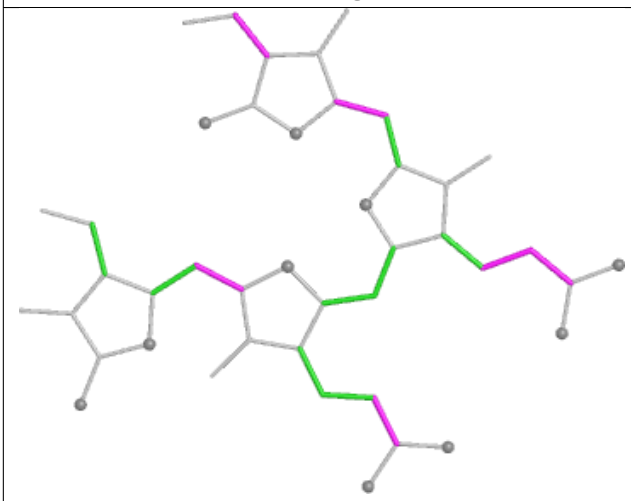
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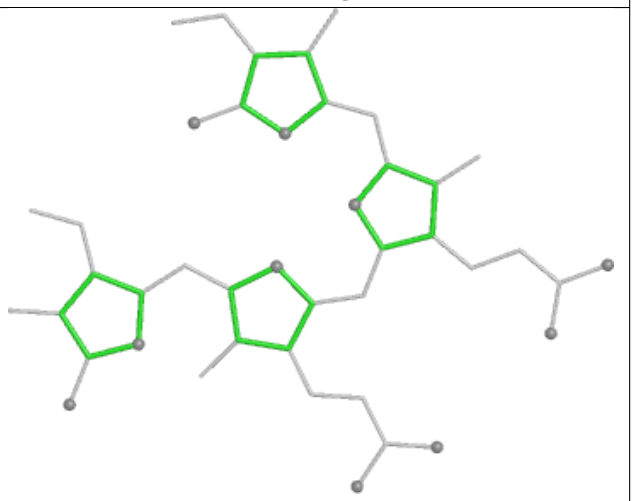
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Bond angles

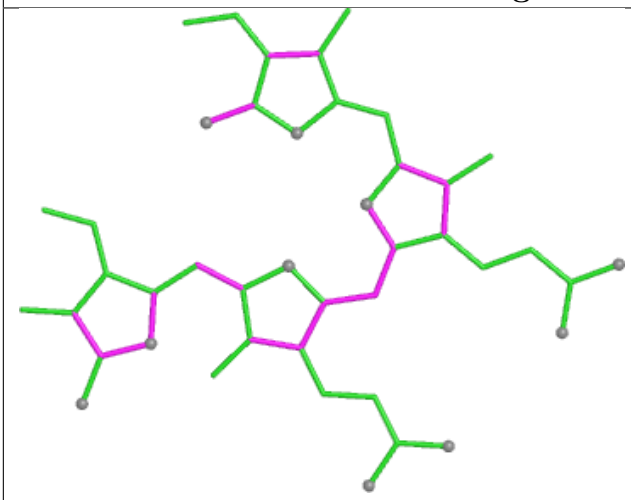


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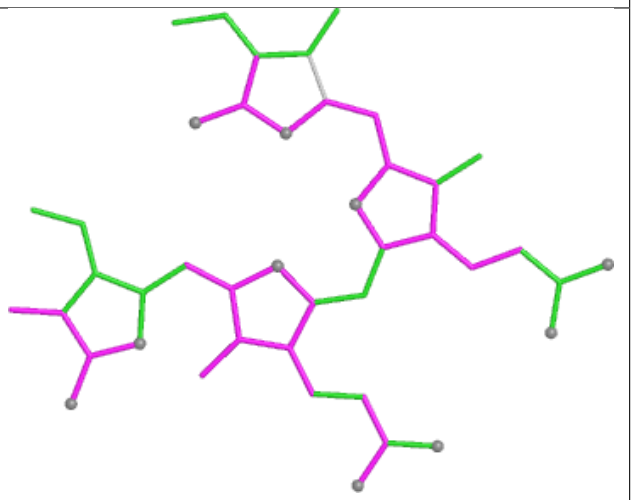


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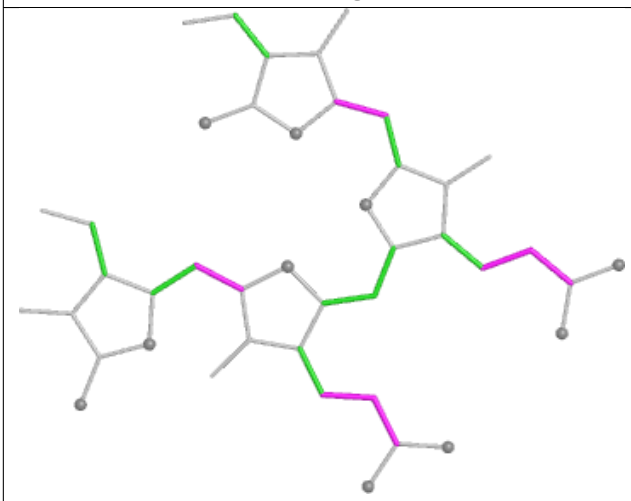
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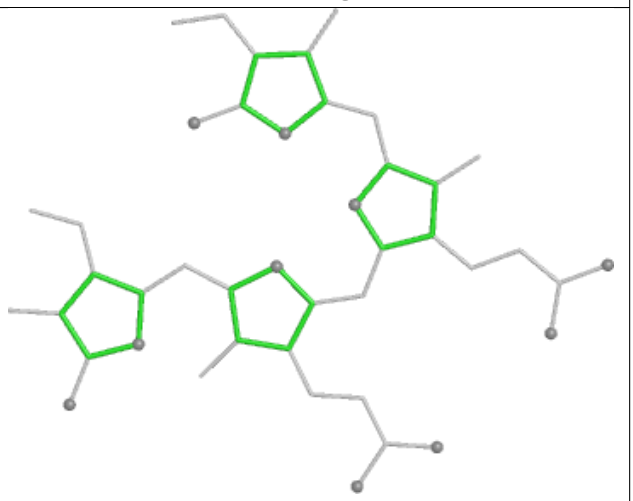
Bond lengths



Bond angles

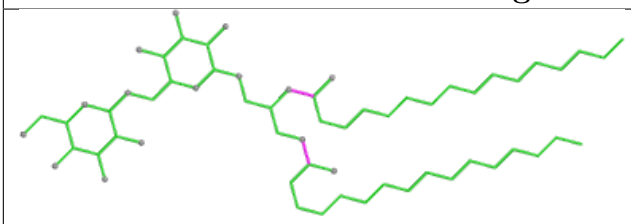


Torsions

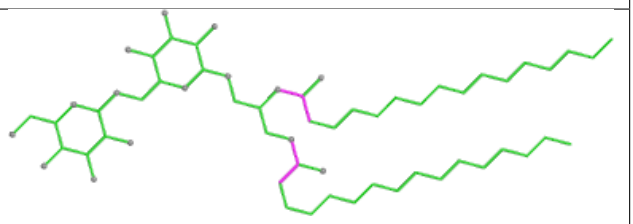


Rings

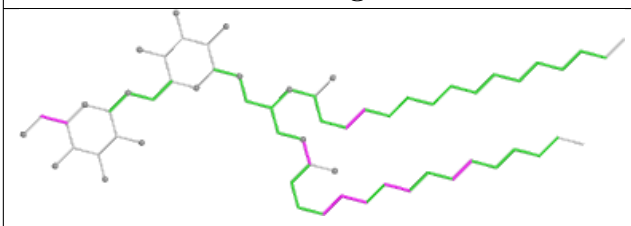
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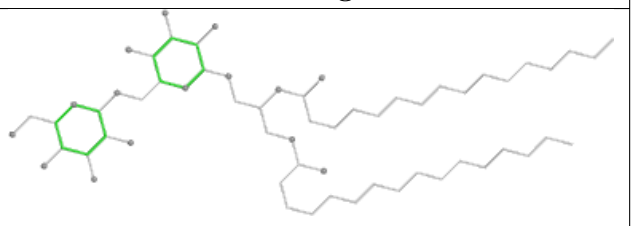
Bond lengths



Bond angles

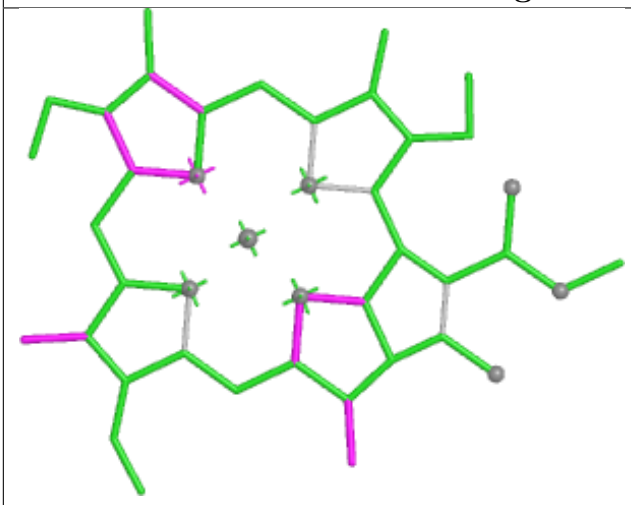


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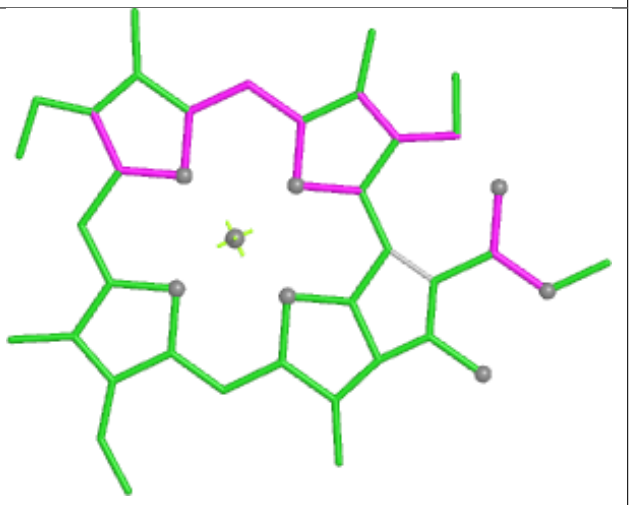


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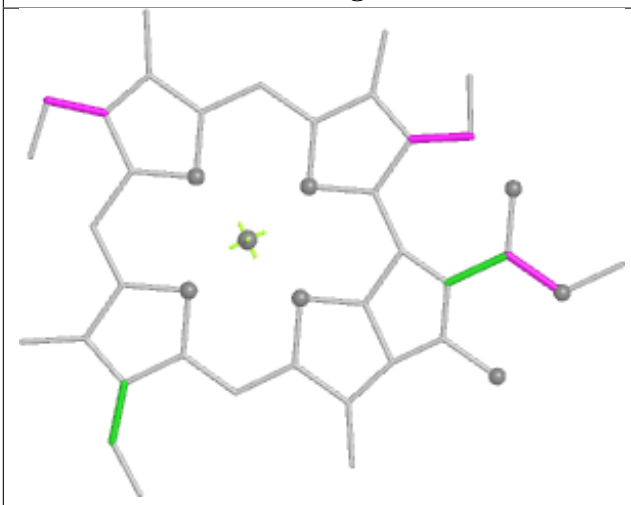
Ligand CLA 8N 307



Bond lengths



Bond angles

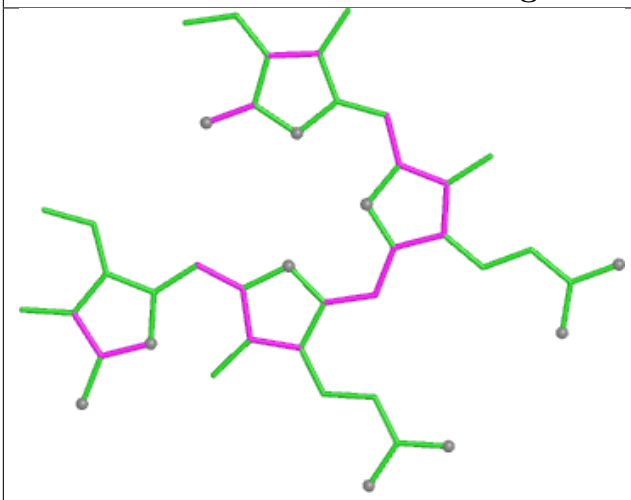


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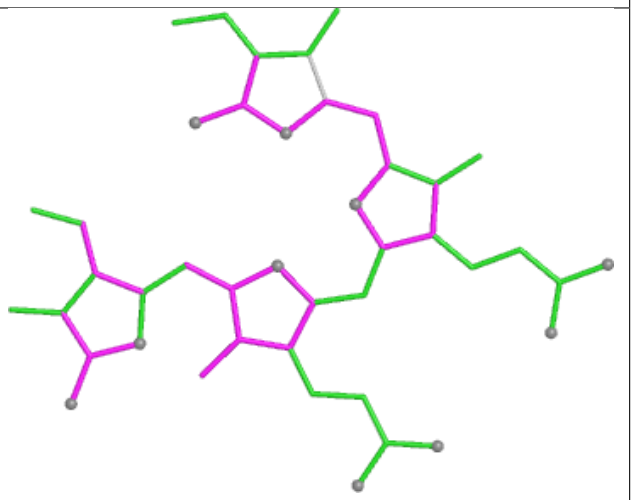


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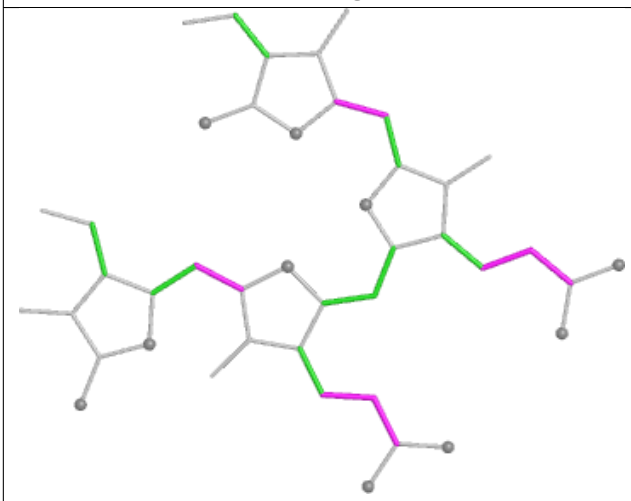
Ligand PEB a1 202



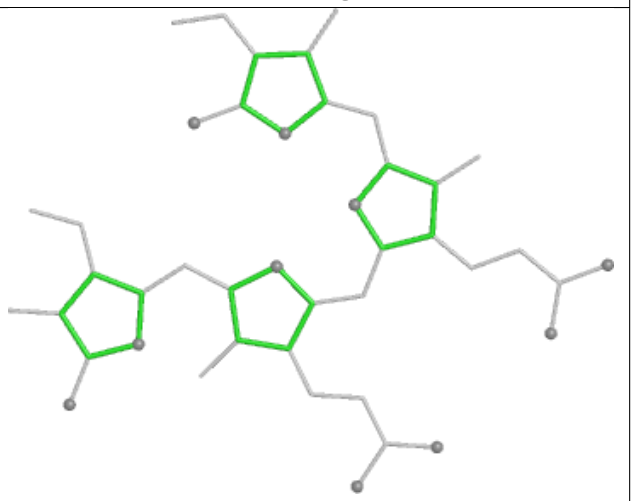
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Bond angles

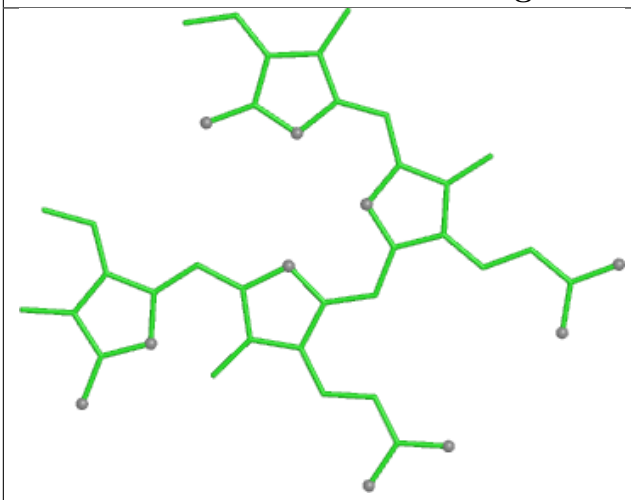


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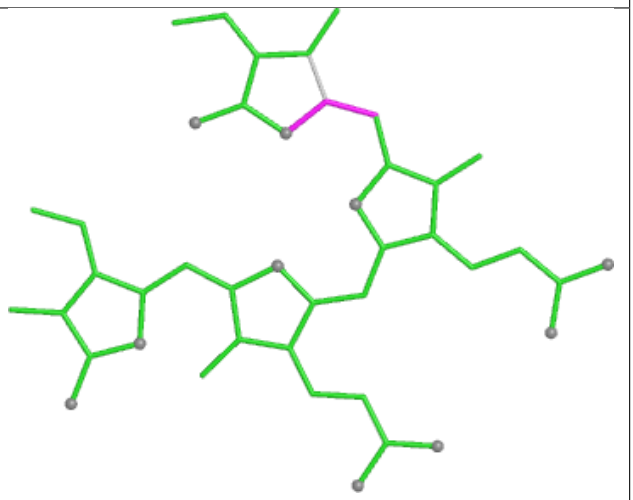


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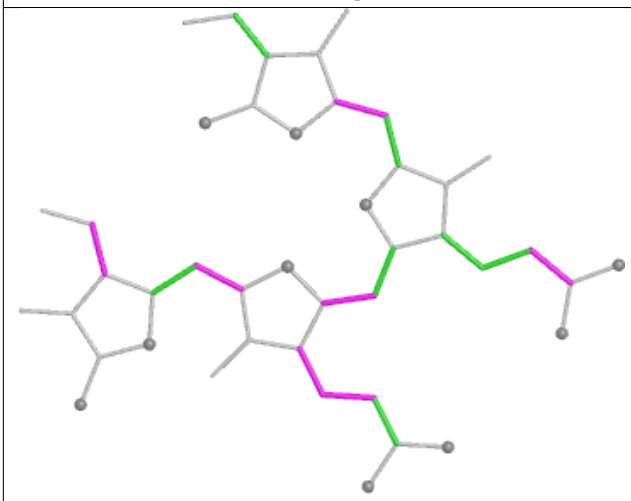
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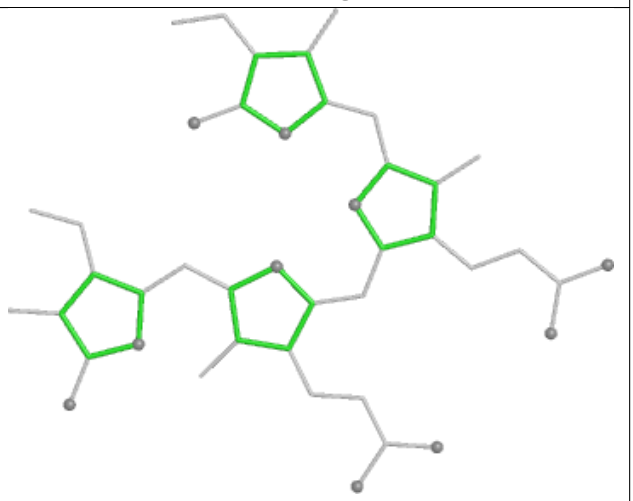
Bond lengths



Bond angles

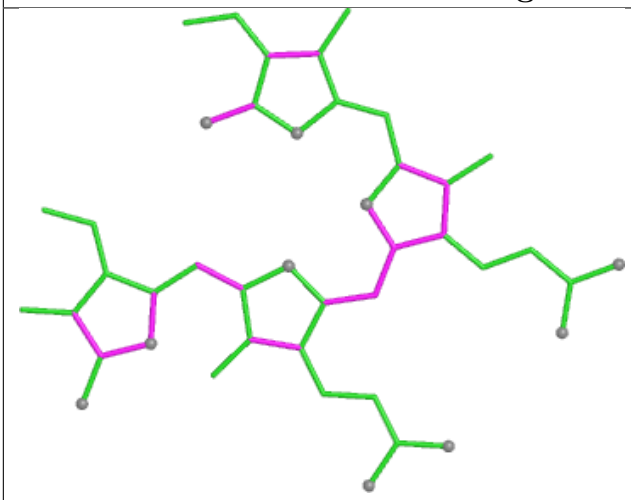


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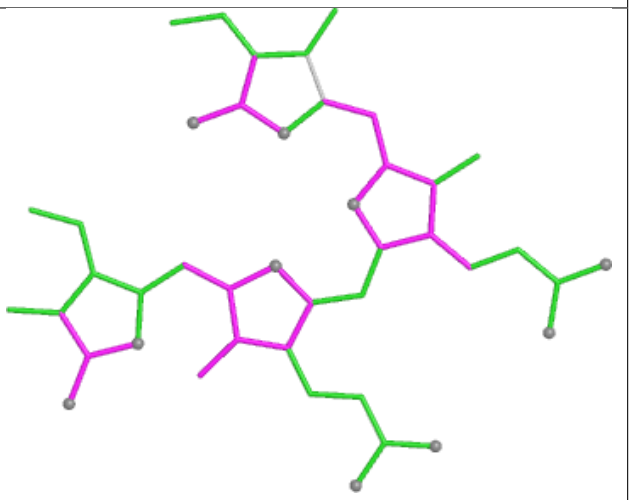


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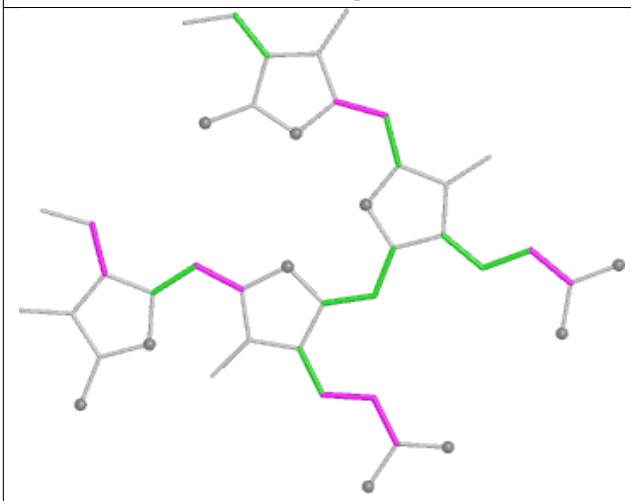
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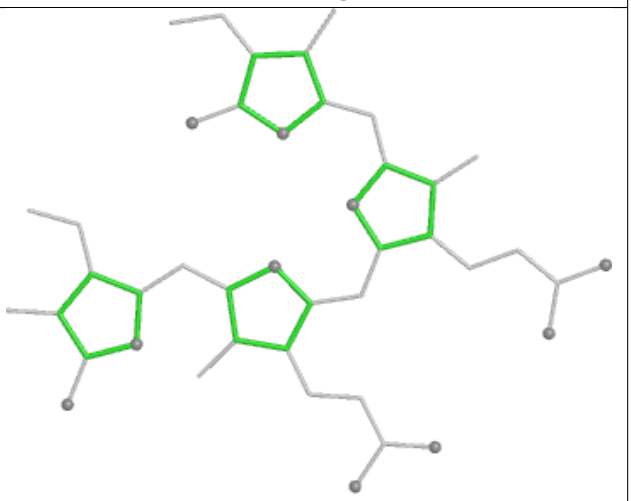
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Bond angles

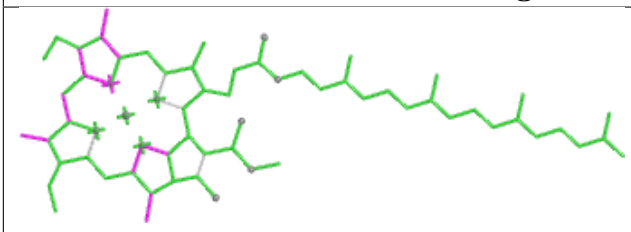


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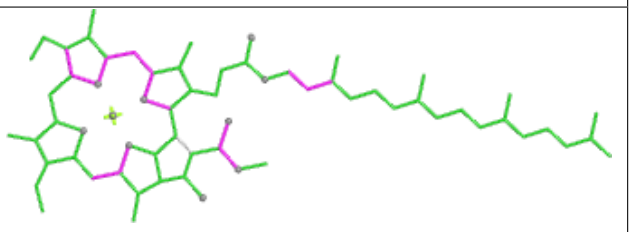


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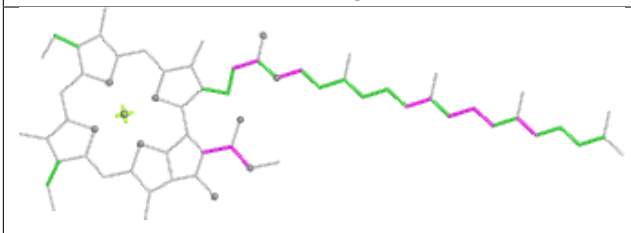
Ligand CLA C6 517



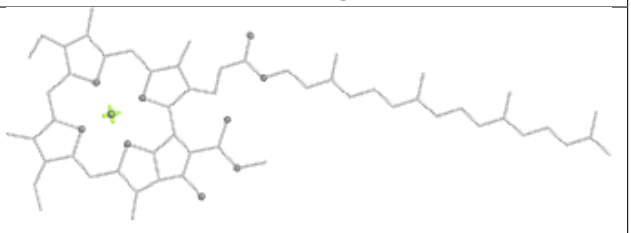
Bond lengths



Bond angles

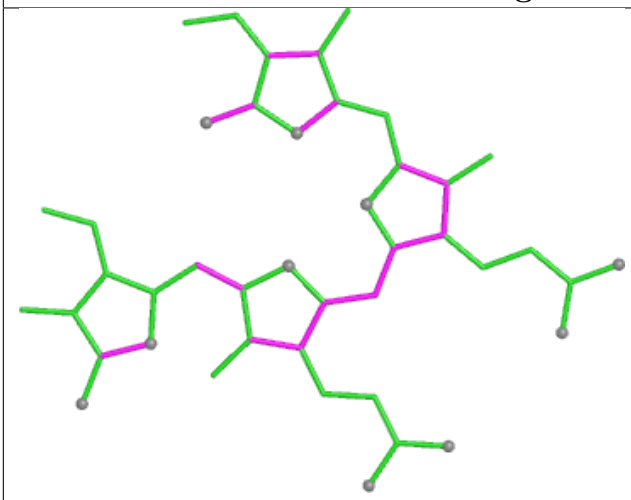


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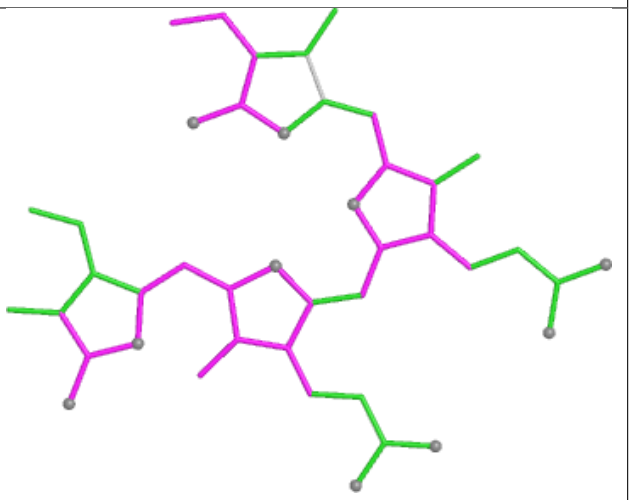


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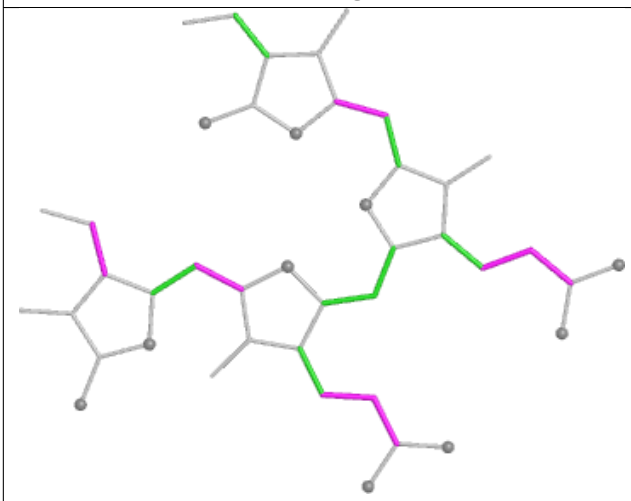
Ligand PEB D7 202



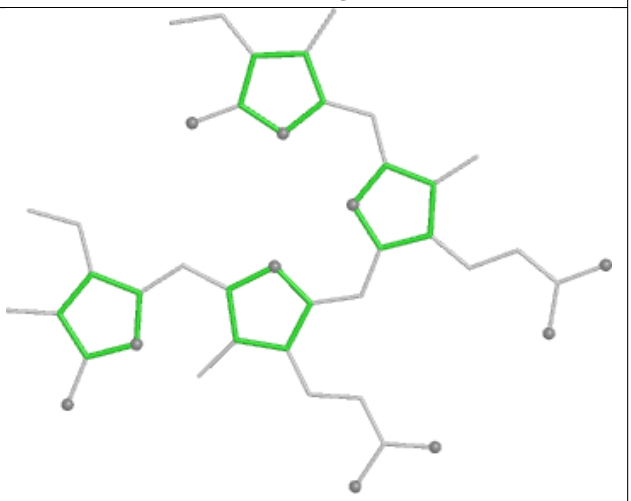
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Bond angles

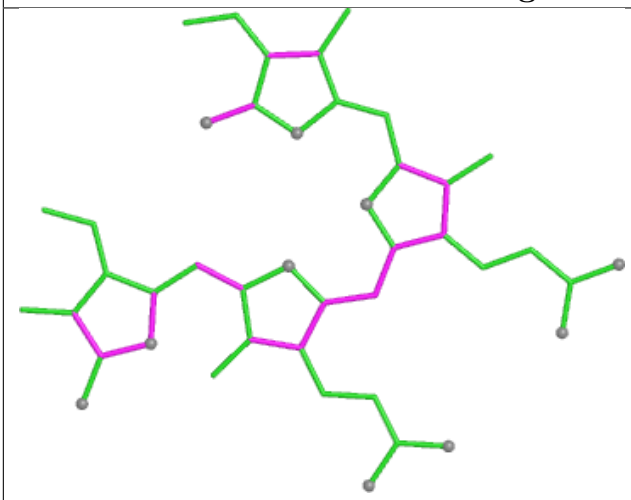


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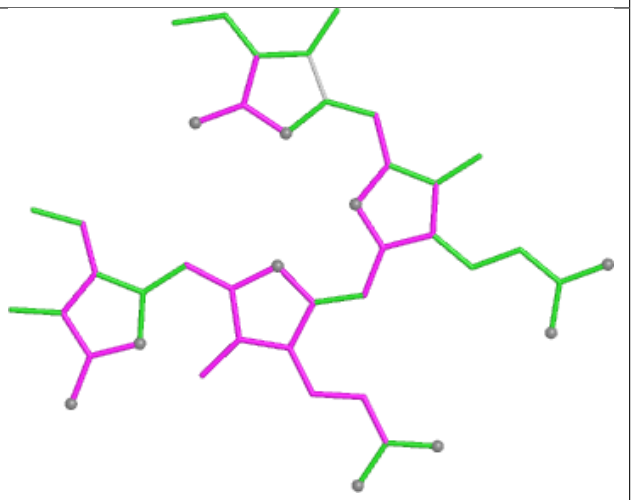


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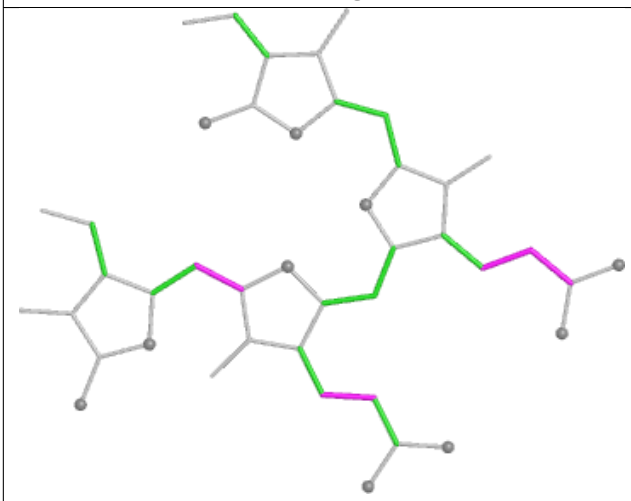
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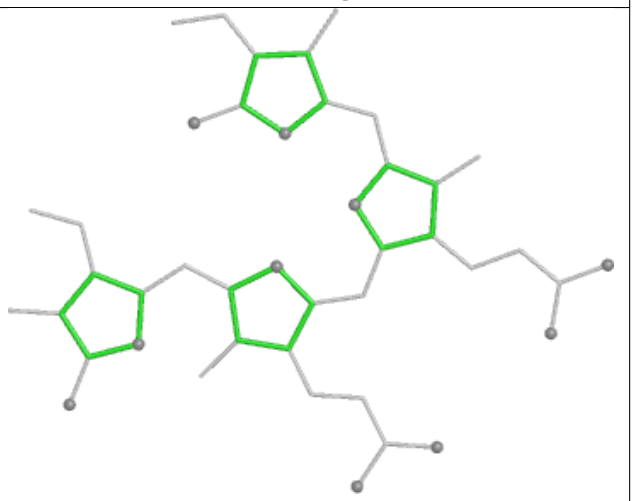
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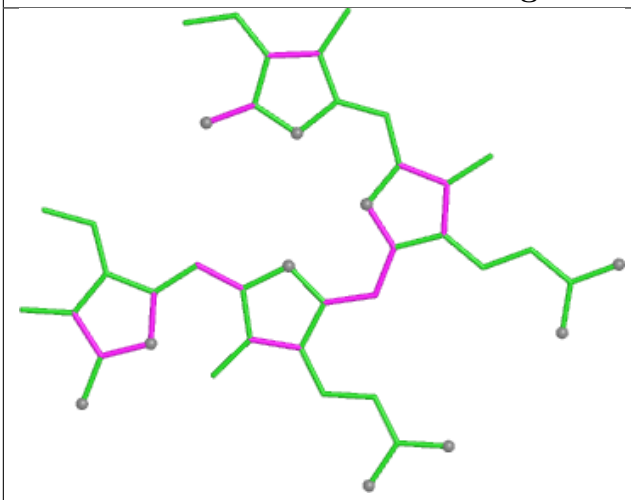


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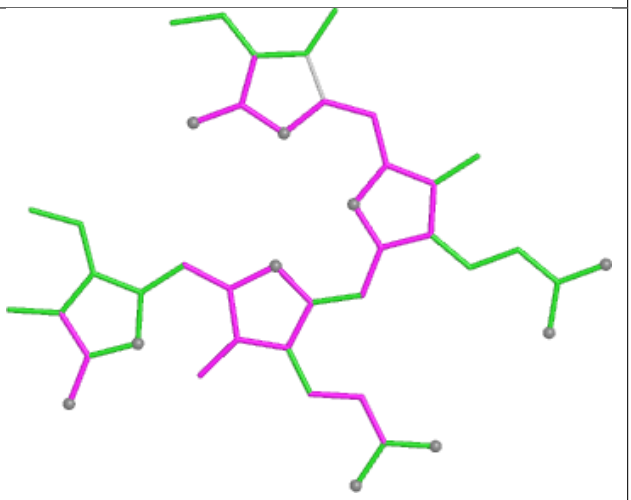


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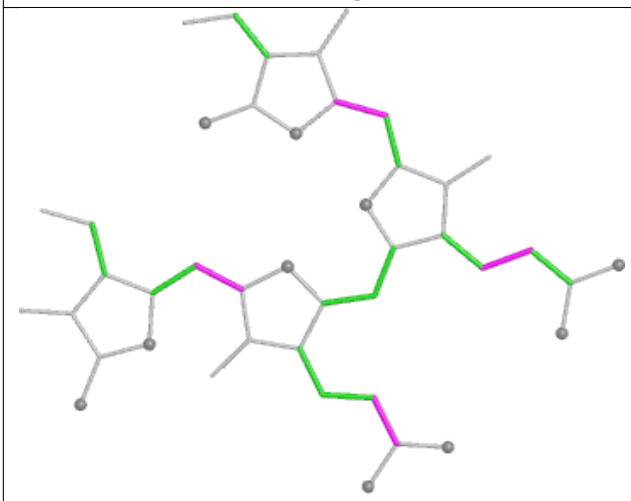
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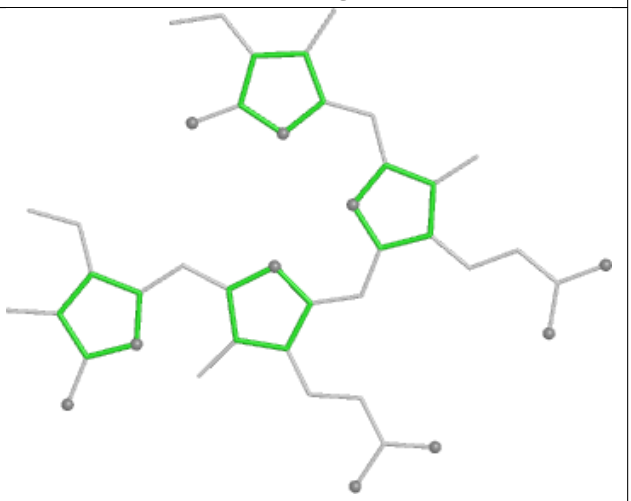
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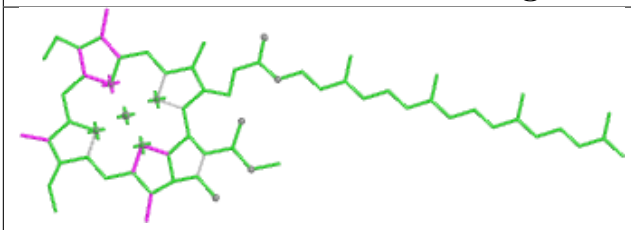


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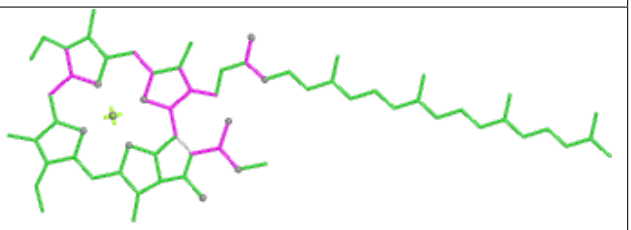


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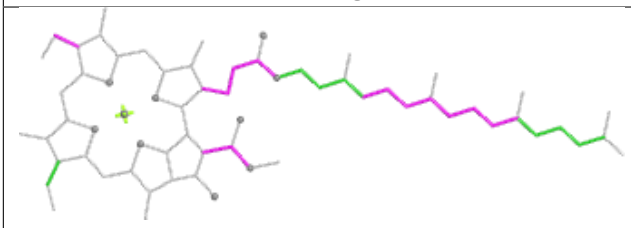
Ligand CLA I2 103



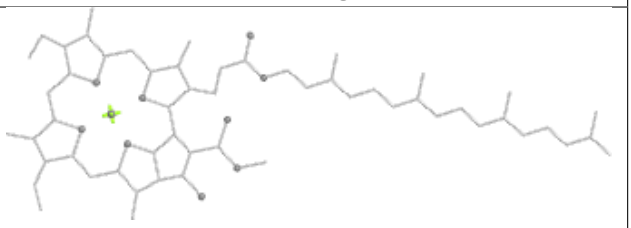
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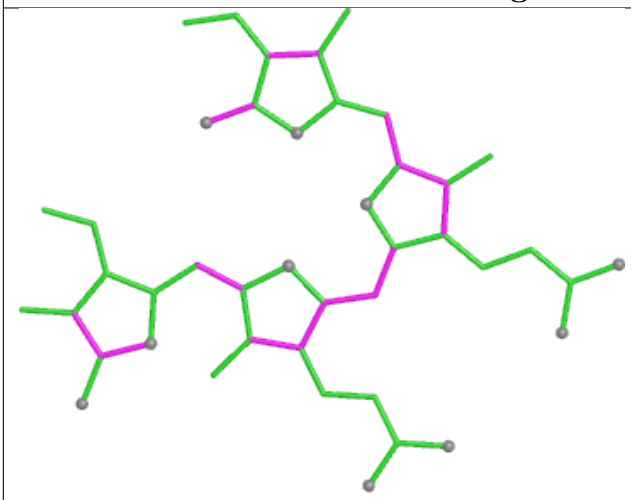


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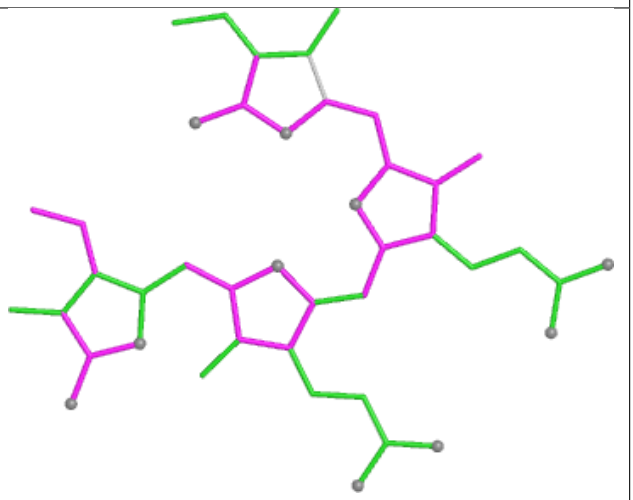


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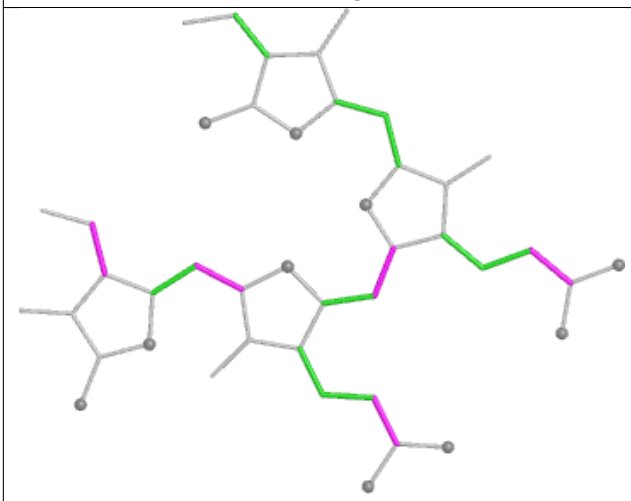
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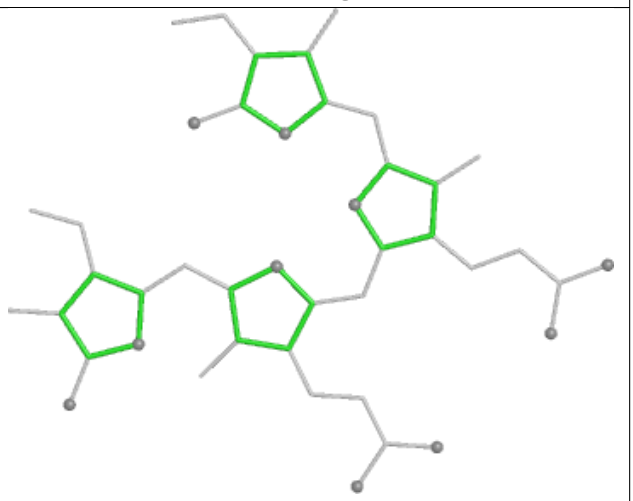
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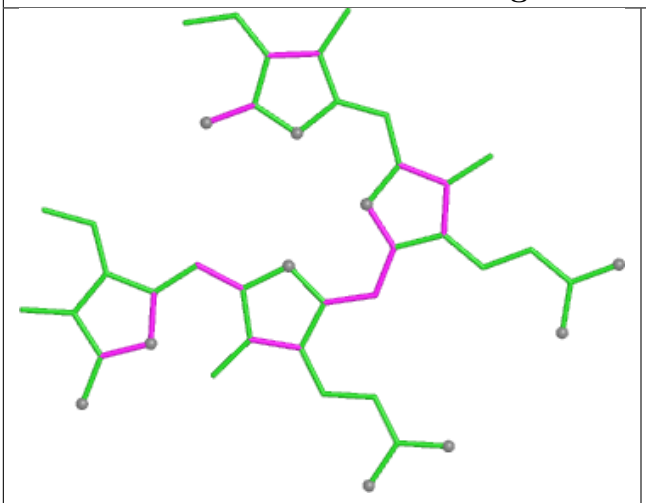


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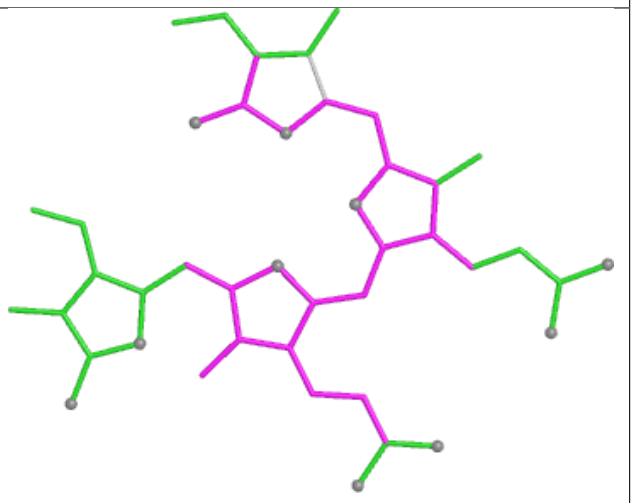


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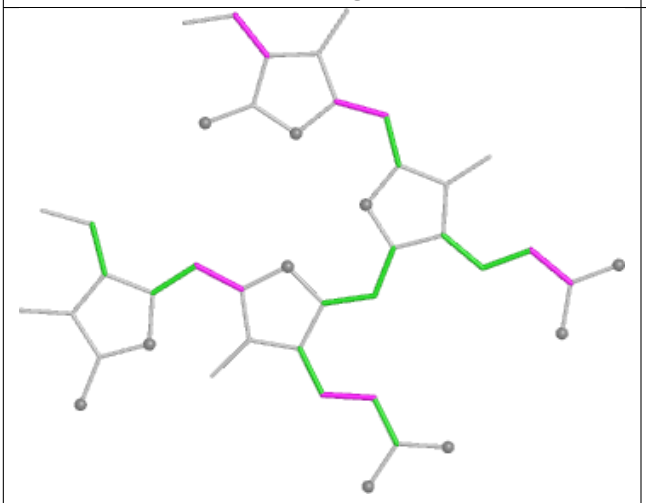
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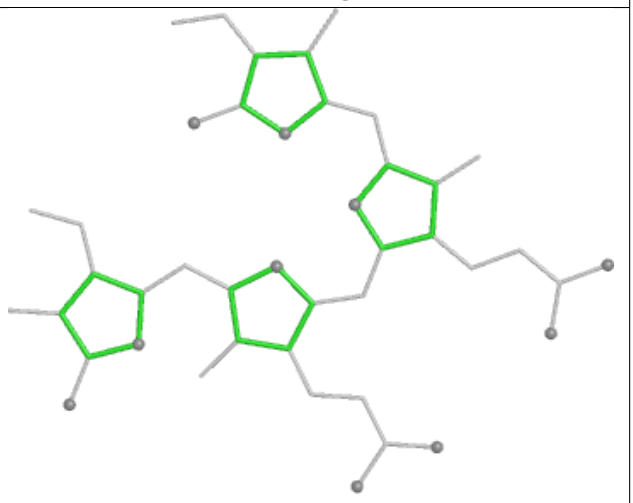
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Bond angles

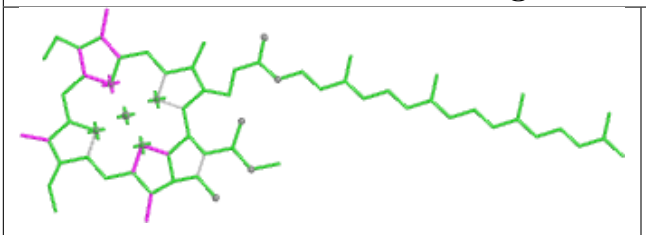


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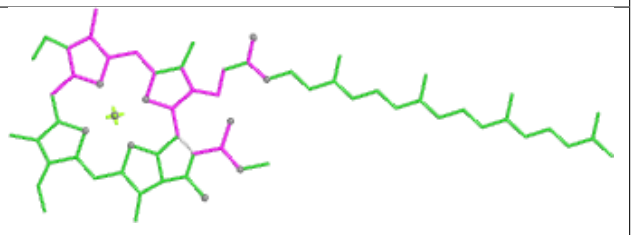


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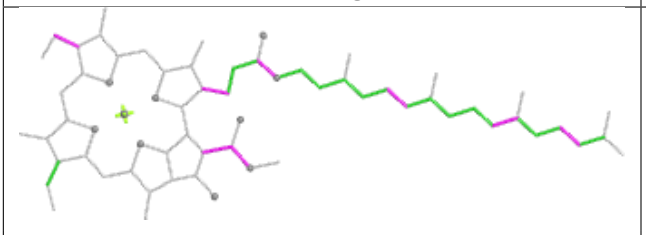
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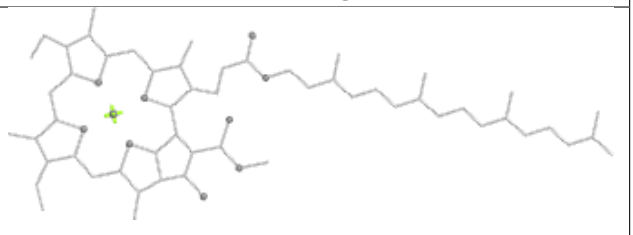
Bond lengths



Bond angles

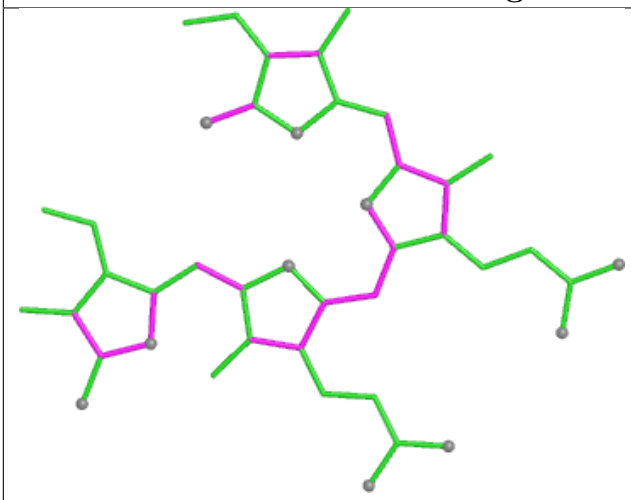


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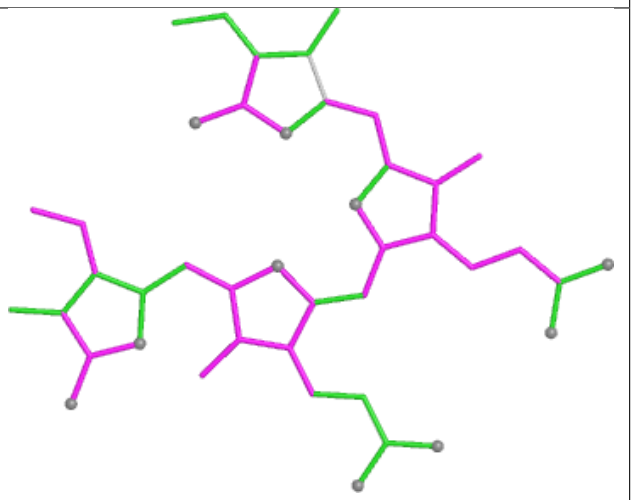


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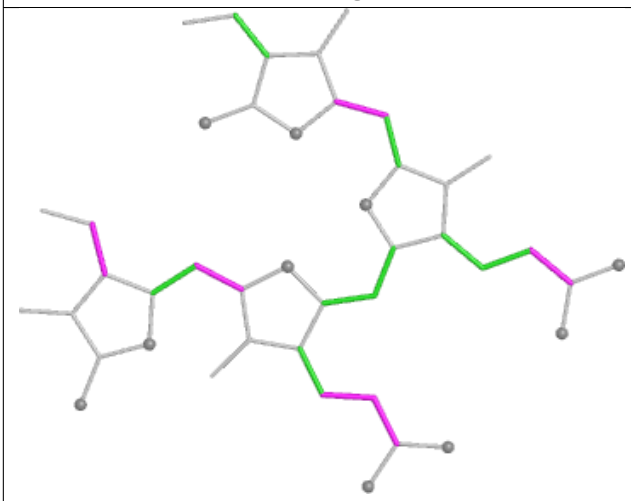
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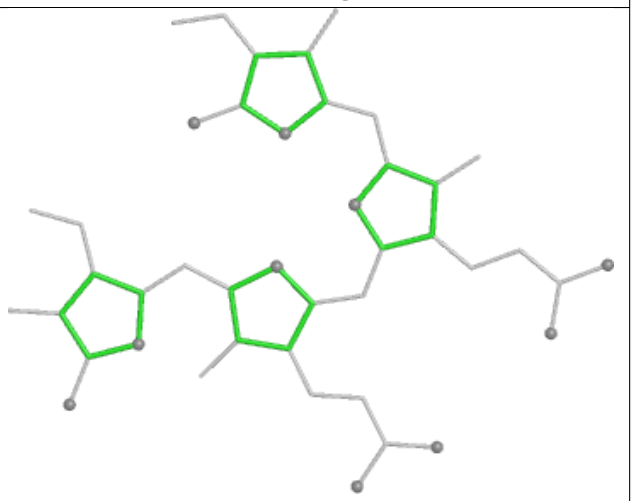
Bond lengths



Bond angles

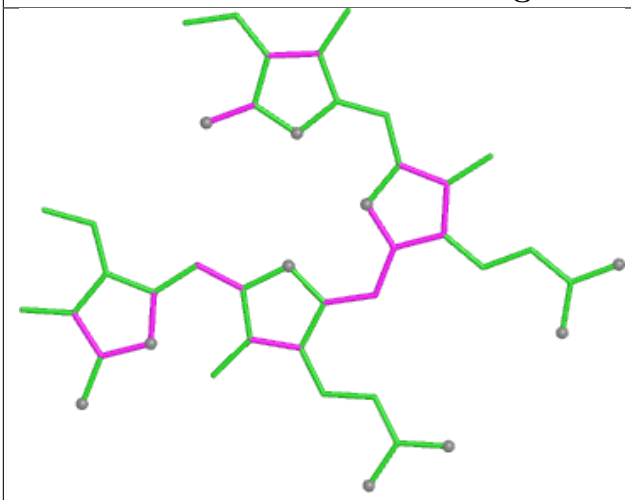


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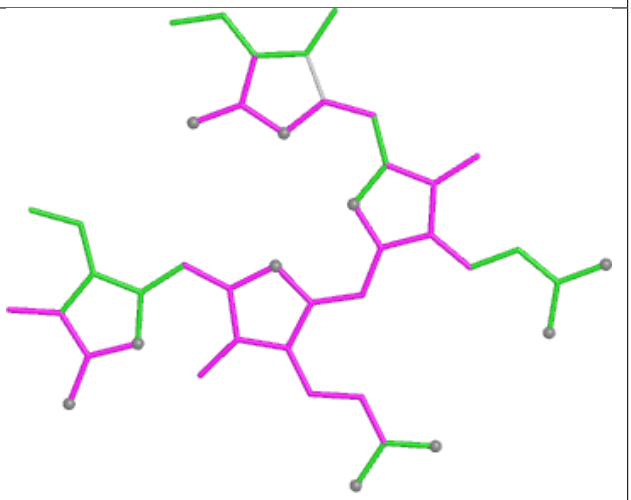


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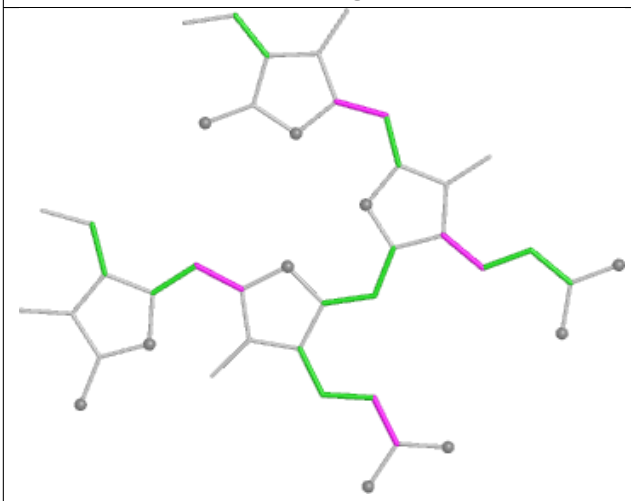
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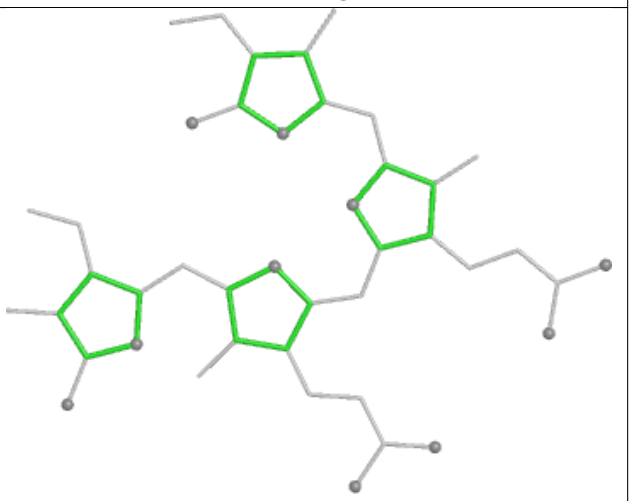
Bond lengths



Bond angles

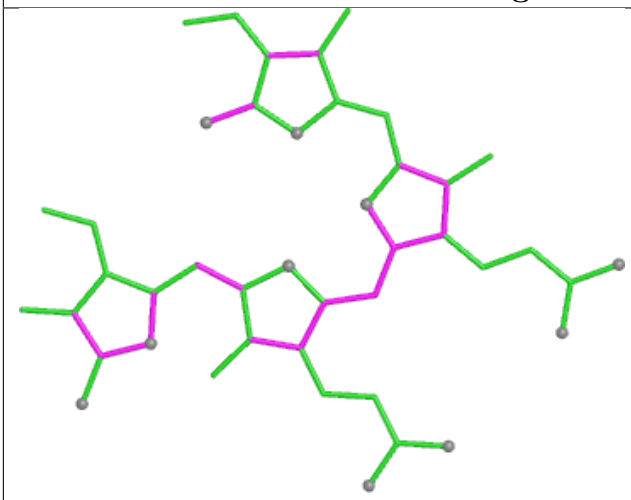


Torsions

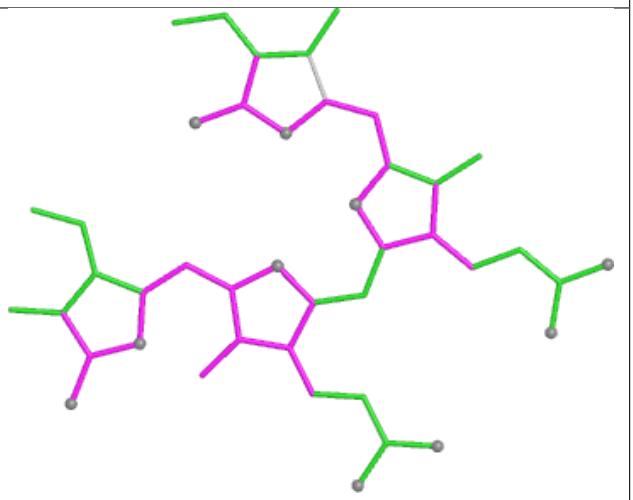


Rings

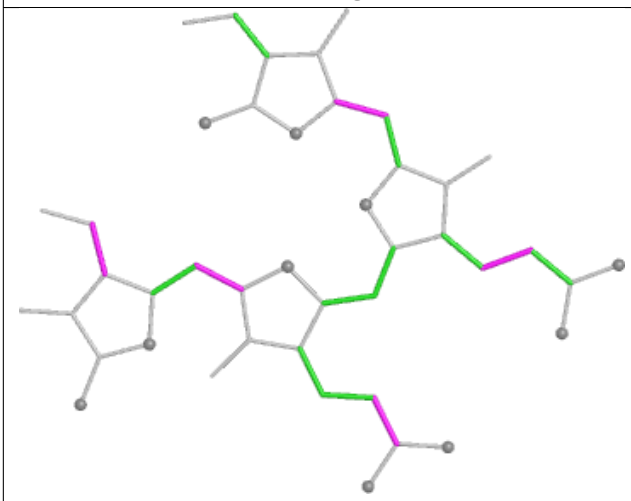
Ligand PEB RP 201



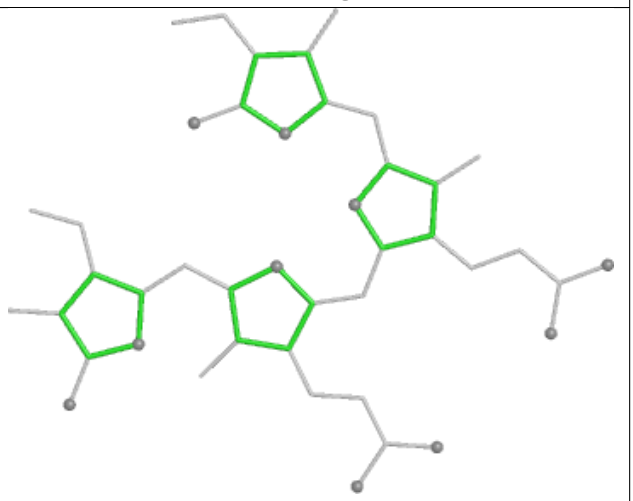
Bond lengths



Bond angles

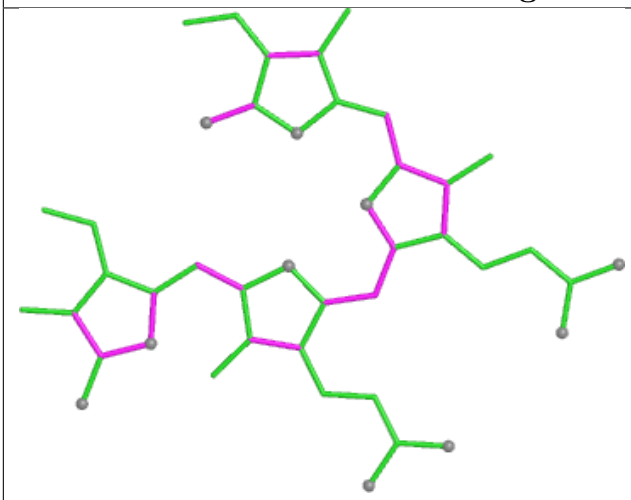


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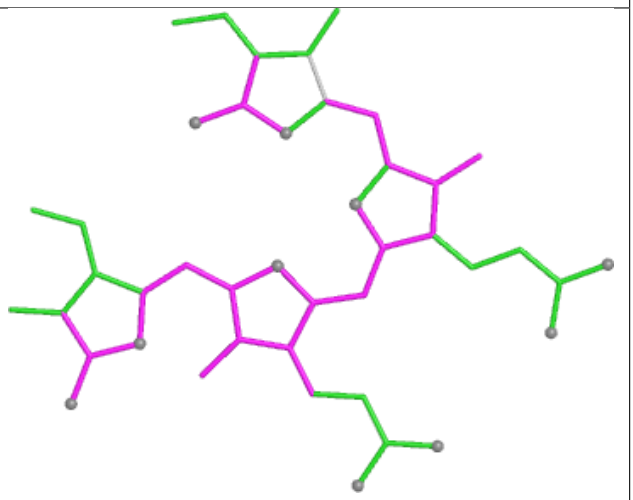


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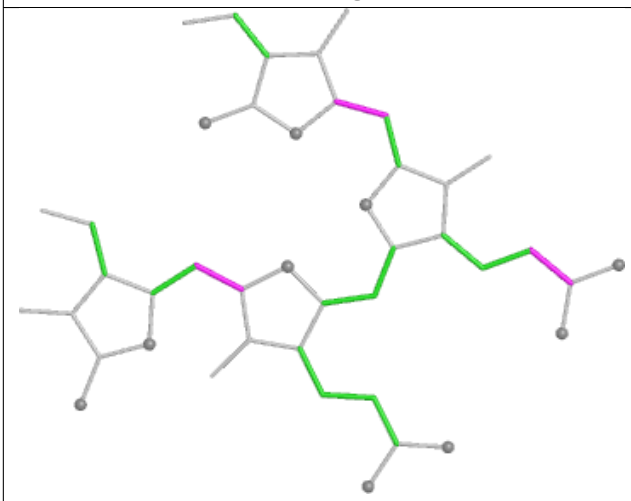
Ligand PEB JJ 201



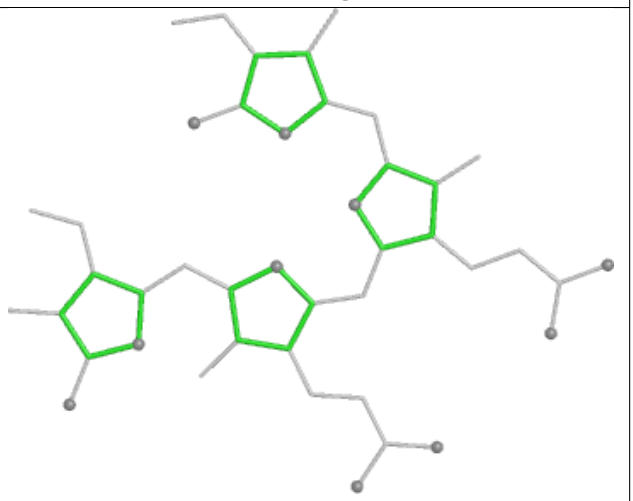
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Bond angles

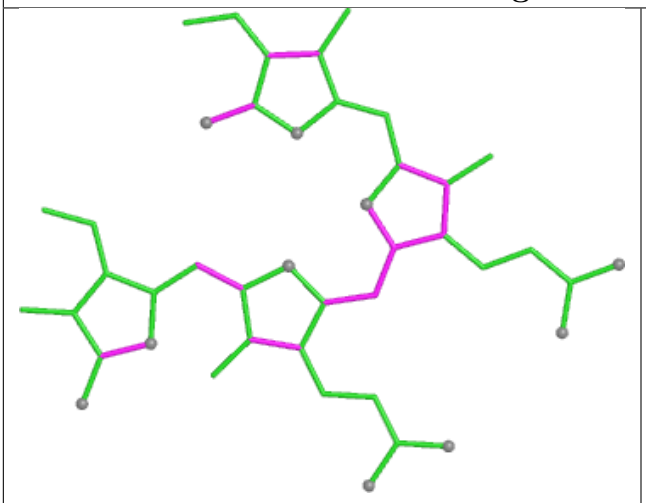


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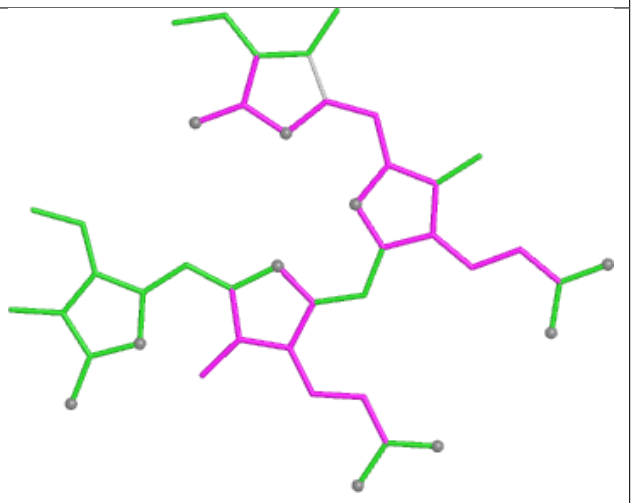


Rings

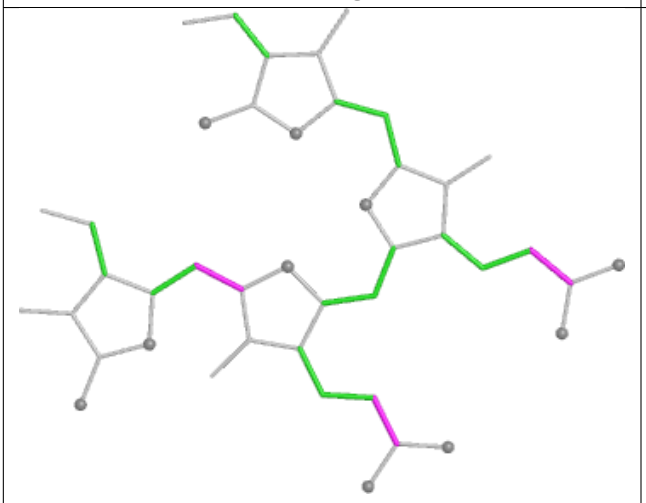
Ligand PEB PO 203



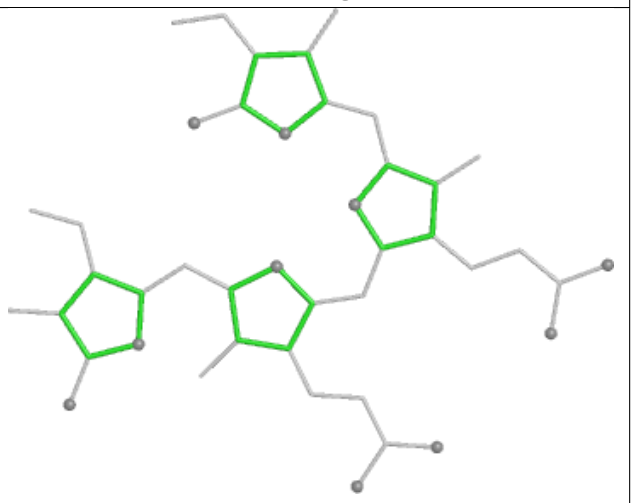
Bond lengths



Bond angles

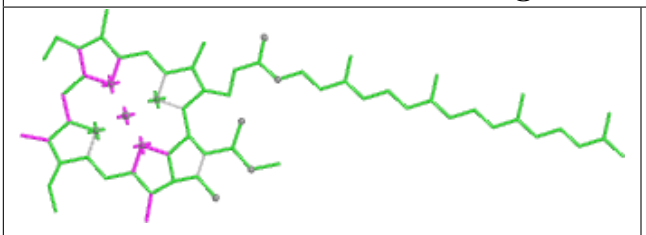


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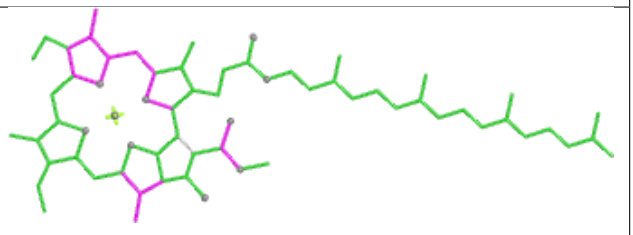


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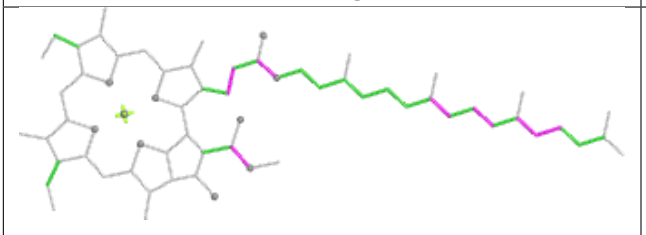
Ligand CLA A2 849



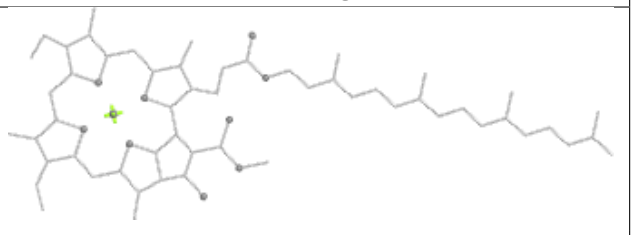
Bond lengths



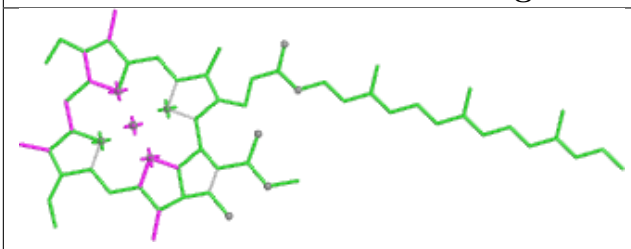
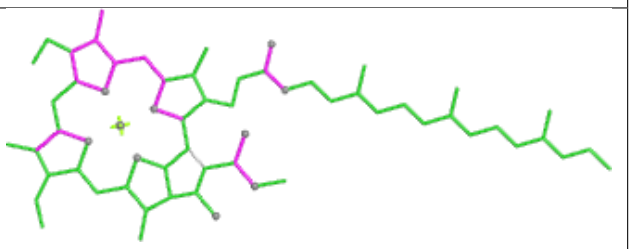
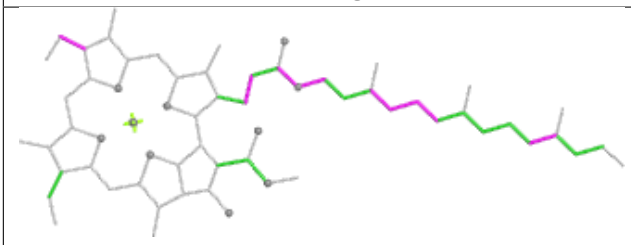
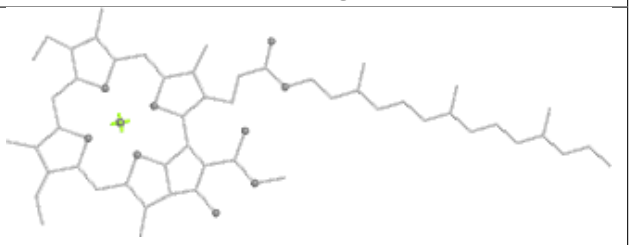
Bond angles

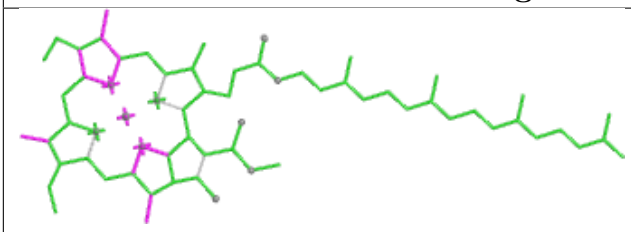
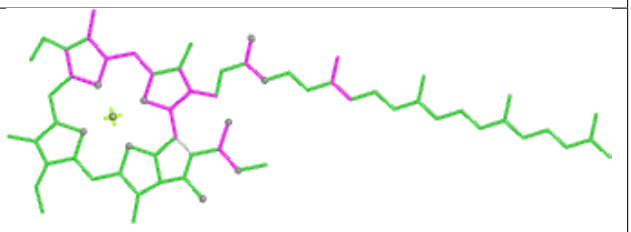
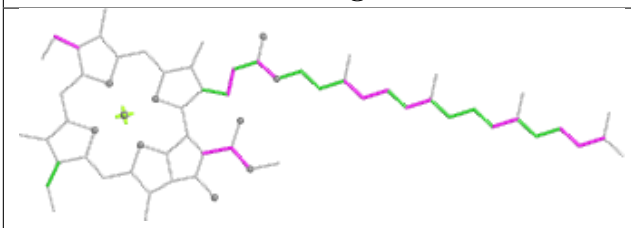
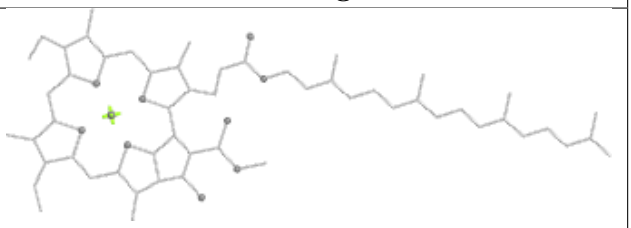


Torsions

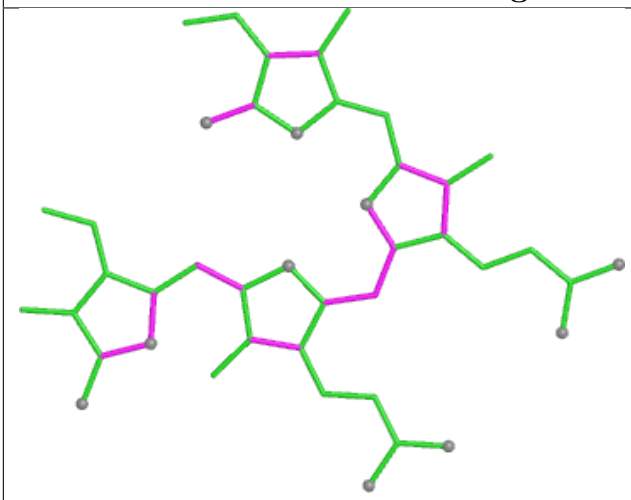


Rings

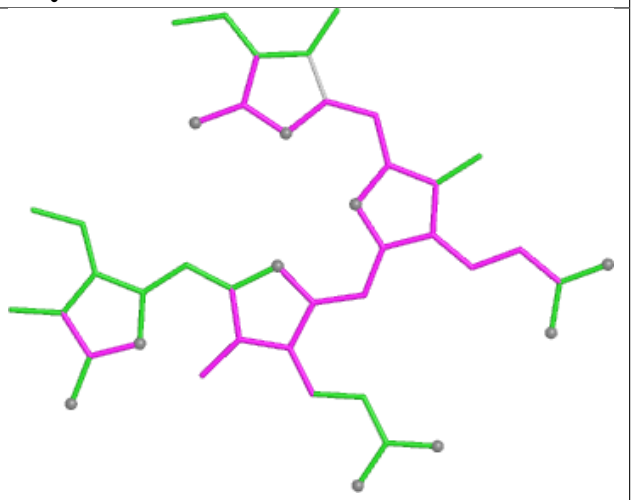
Ligand CLA A2 819	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A2 815	
	
Bond lengths	Bond angles
	
Torsions	Rings

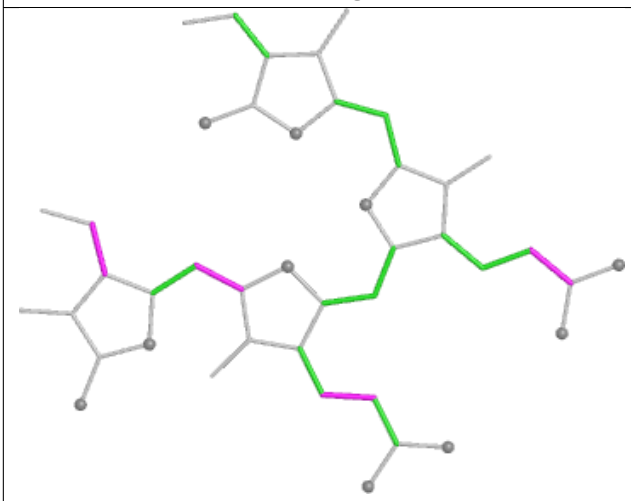
Ligand PEB QK 201



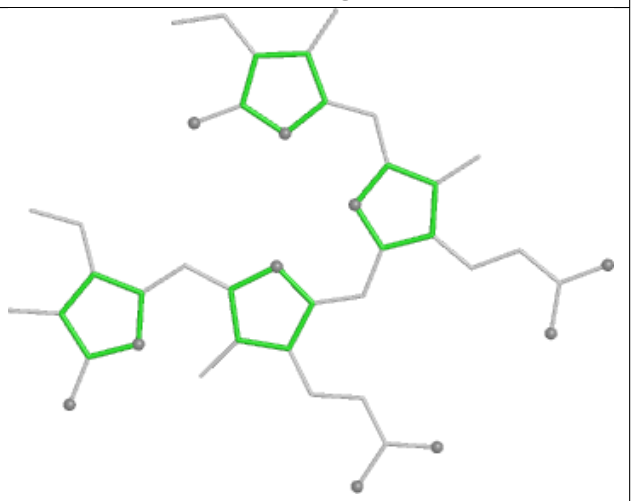
Bond lengths



Bond angles

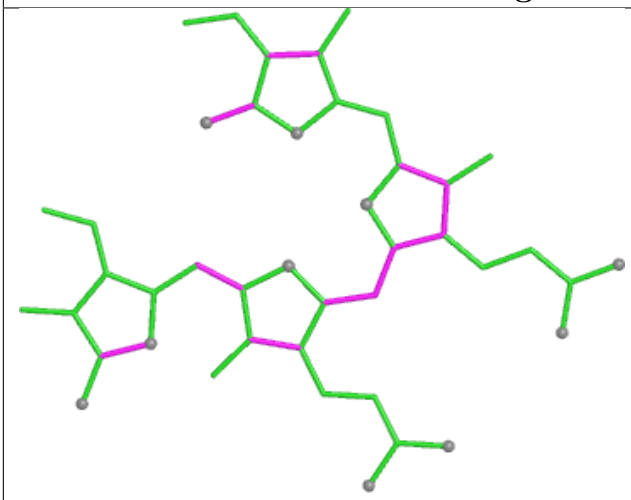


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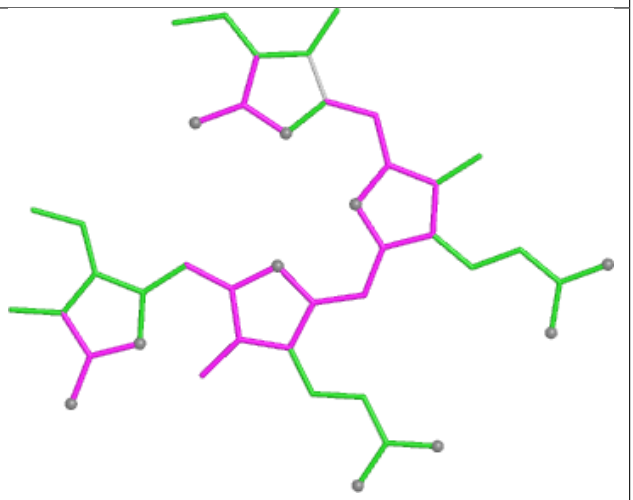


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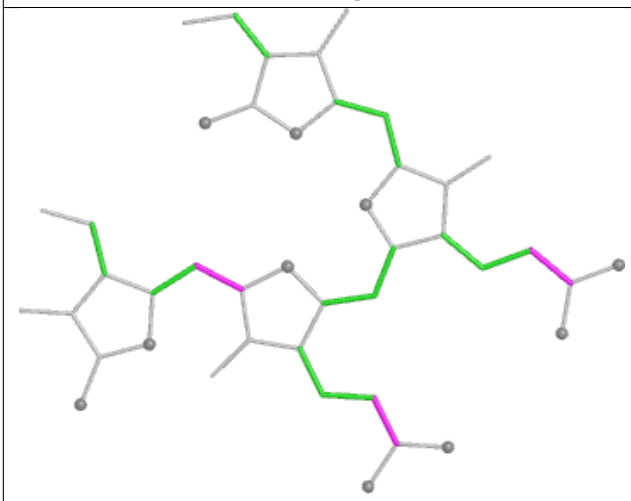
Ligand PEB aH 201



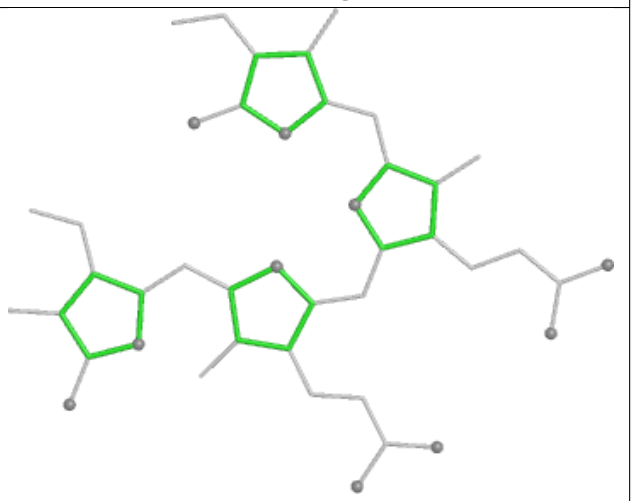
Bond lengths



Bond angles

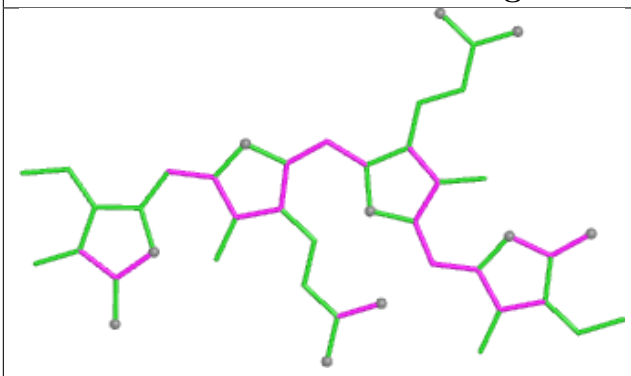


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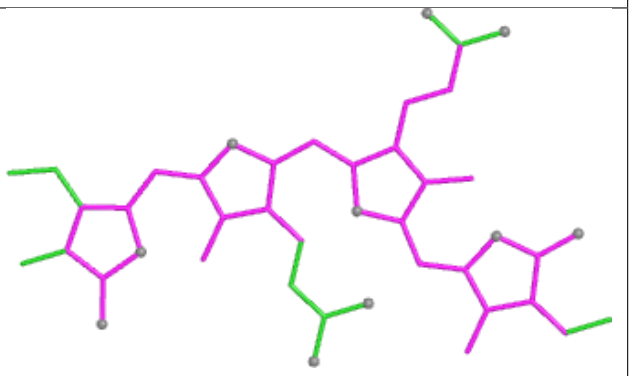


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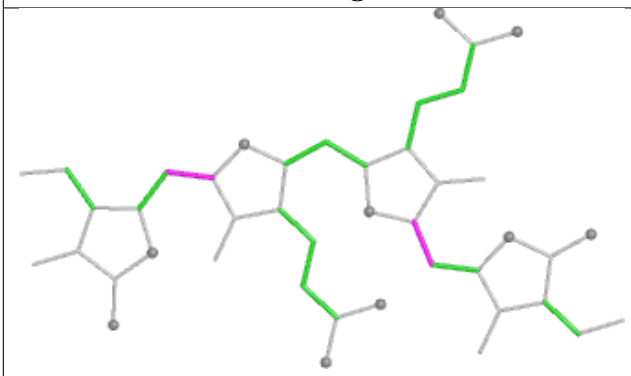
Ligand CYC w3 1001



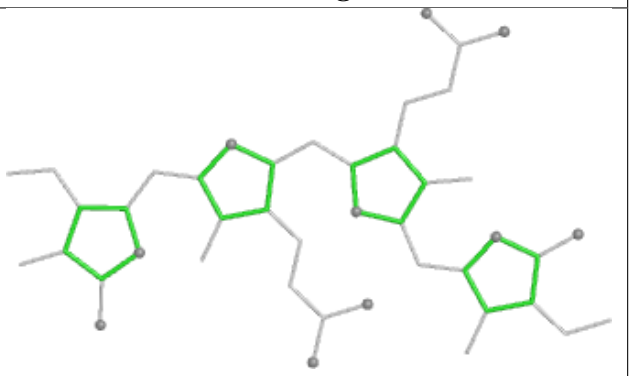
Bond lengths



Bond angles

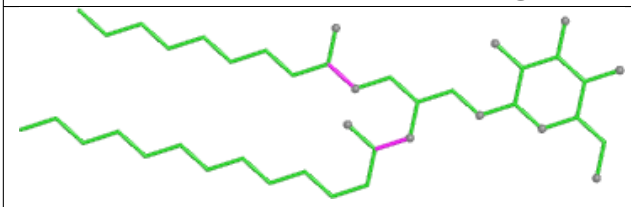


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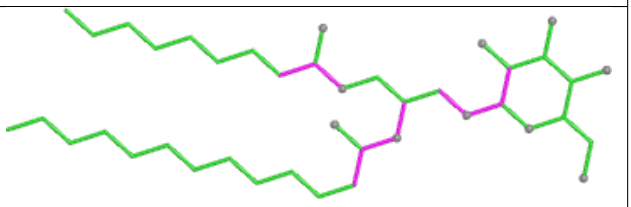


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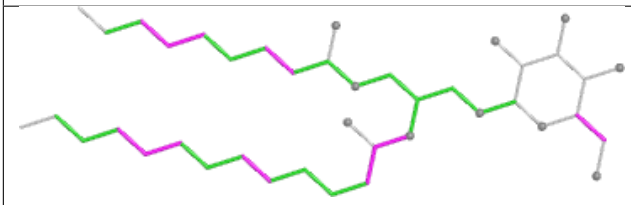
Ligand LMG bL 623



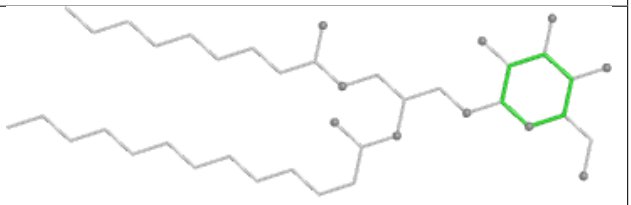
Bond lengths



Bond angles

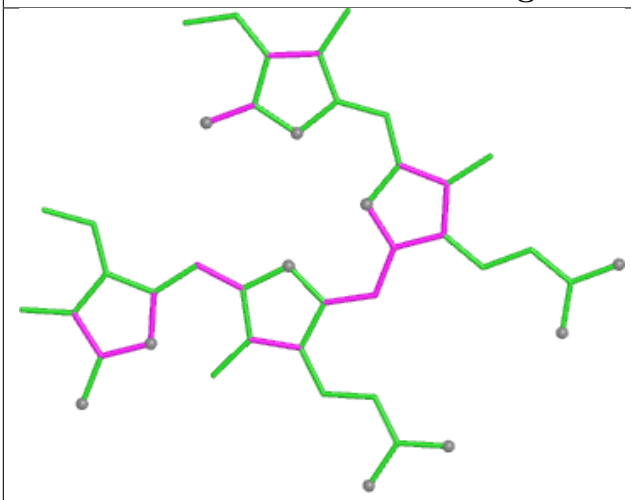


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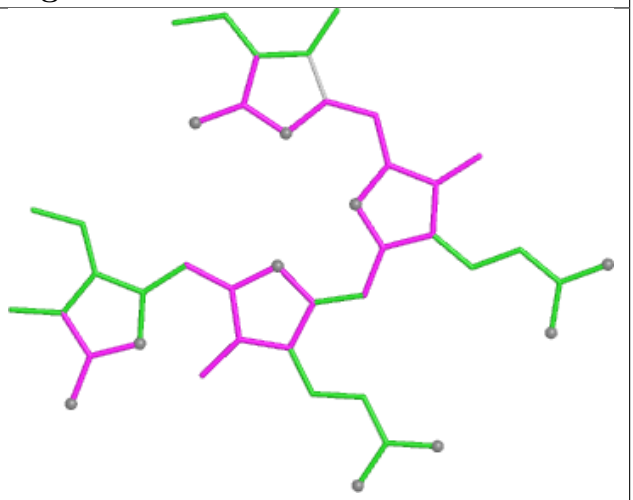


Rings

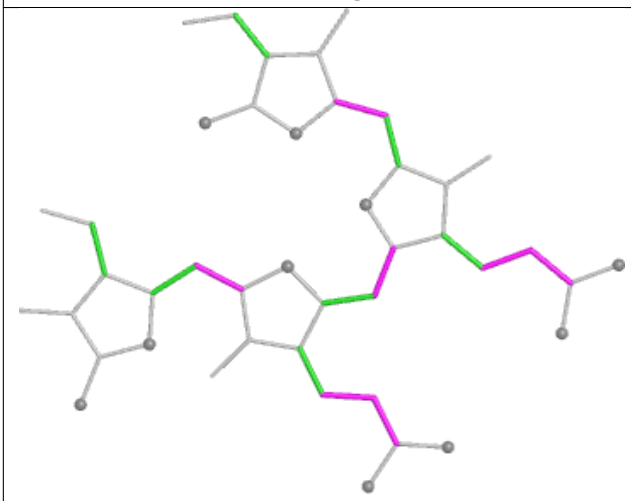
Ligand PEB gF 202



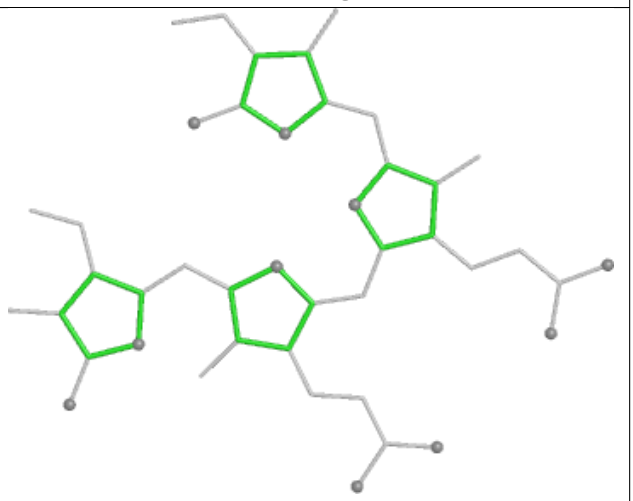
Bond lengths



Bond angles

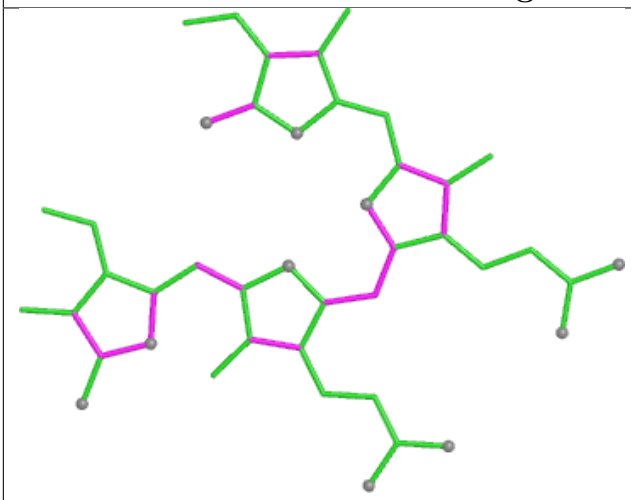


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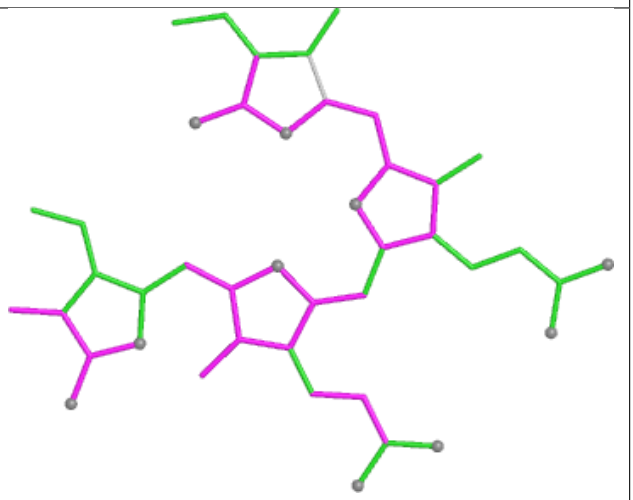


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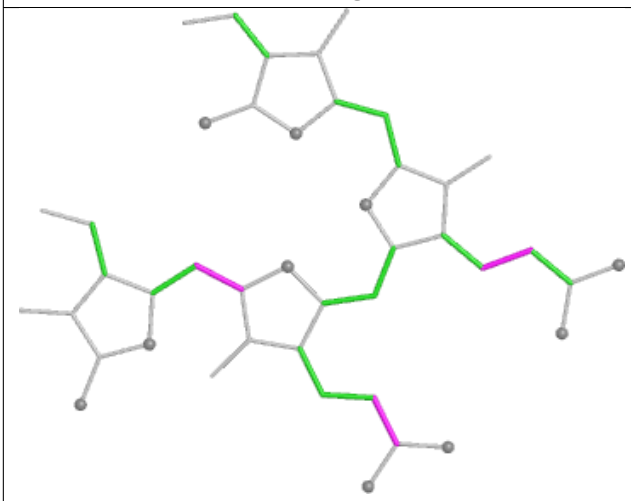
Ligand PEB P4 201



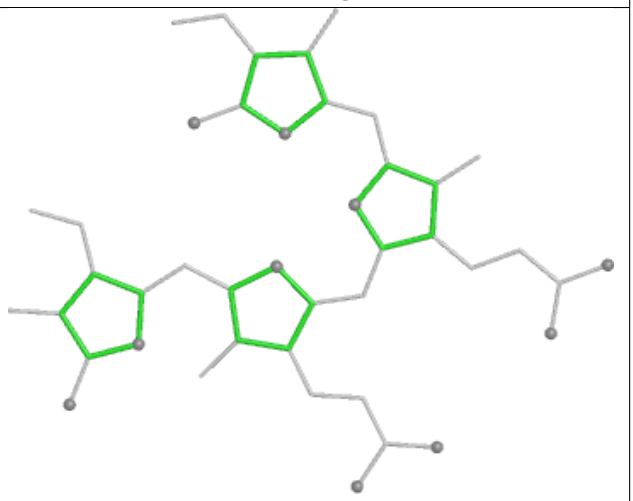
Bond lengths



Bond angles

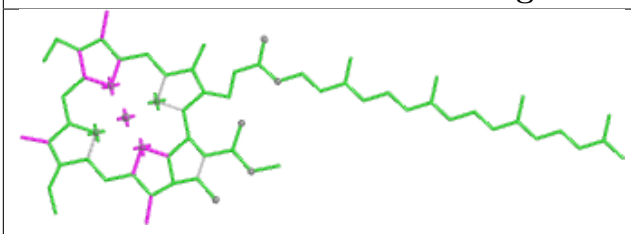


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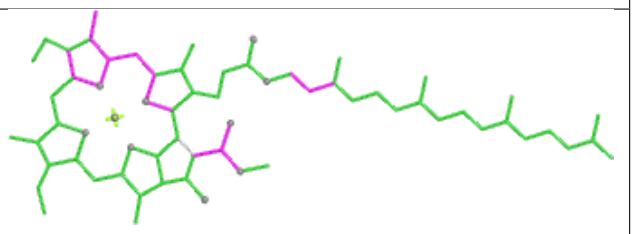


Rings

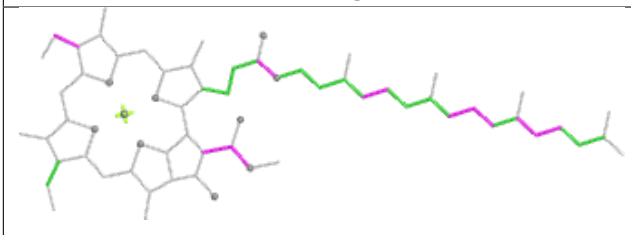
Ligand CLA bL 617



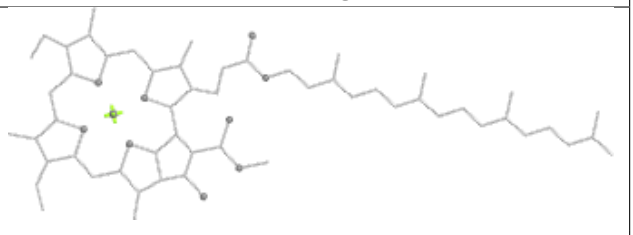
Bond lengths



Bond angles

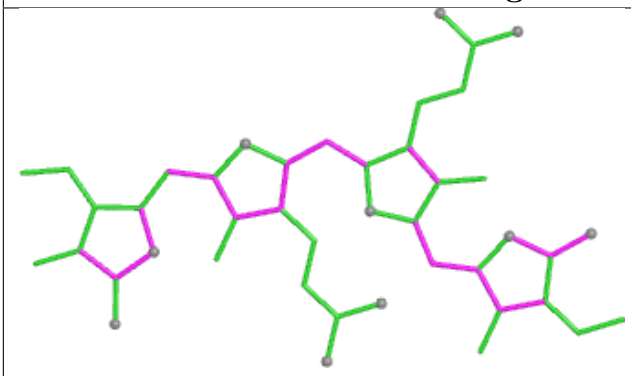


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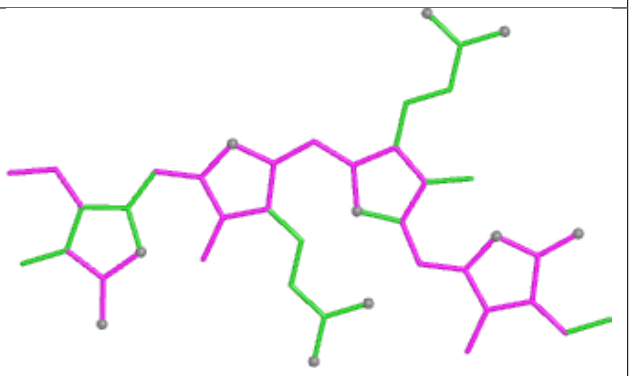


Rings

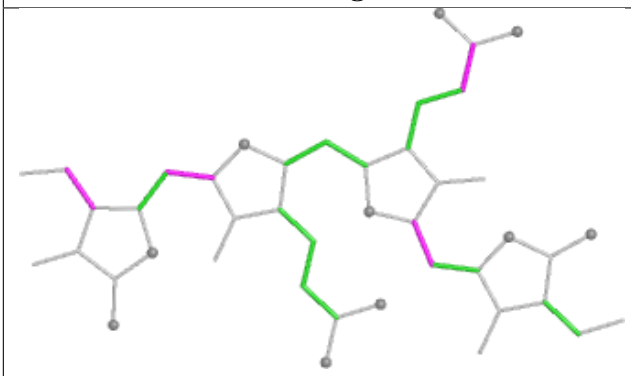
Ligand CYC F1 1001



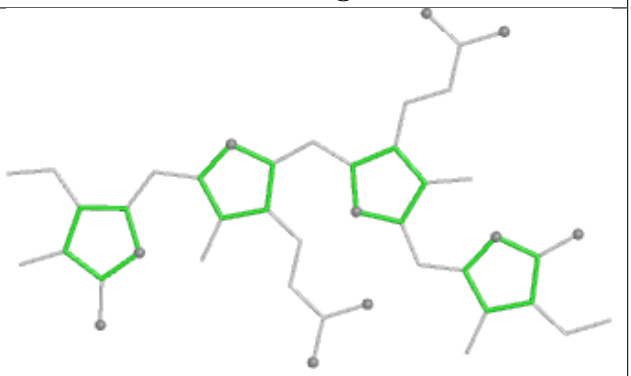
Bond lengths



Bond angles

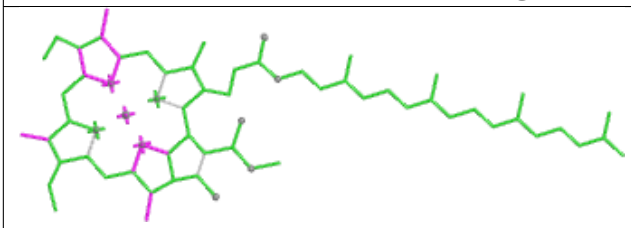


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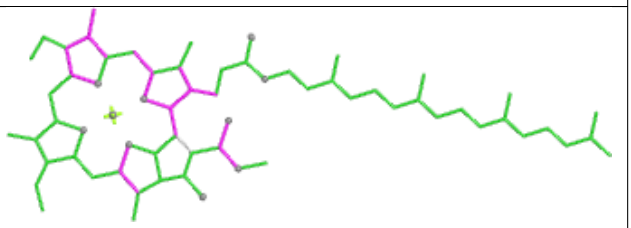


Rings

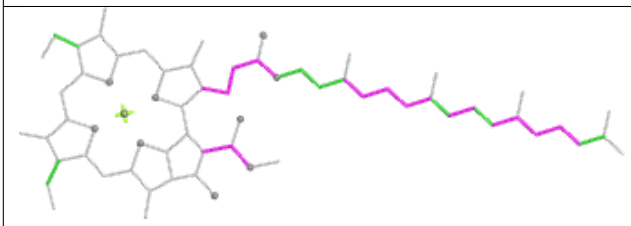
Ligand CLA CL 503



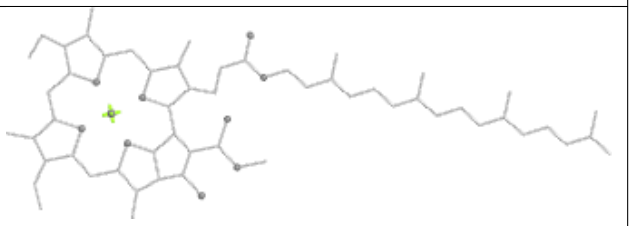
Bond lengths



Bond angles

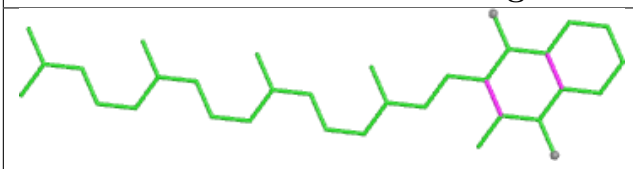


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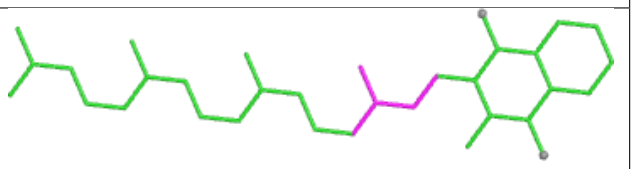


Rings

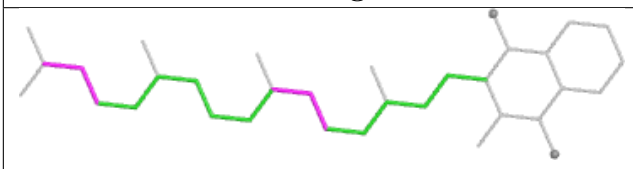
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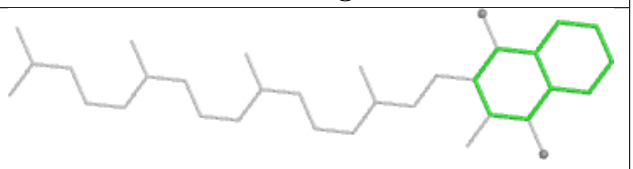
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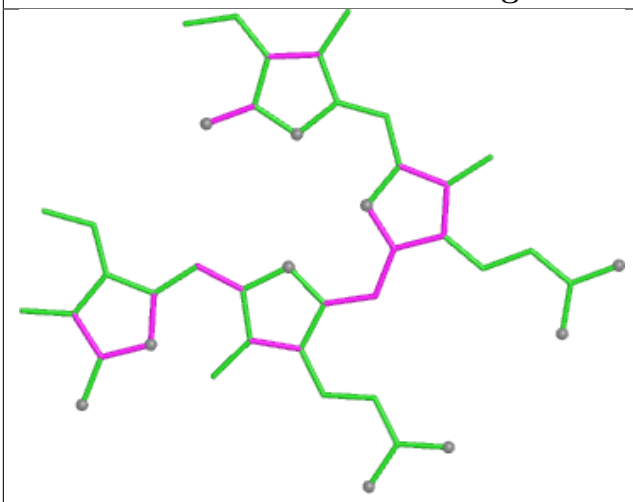


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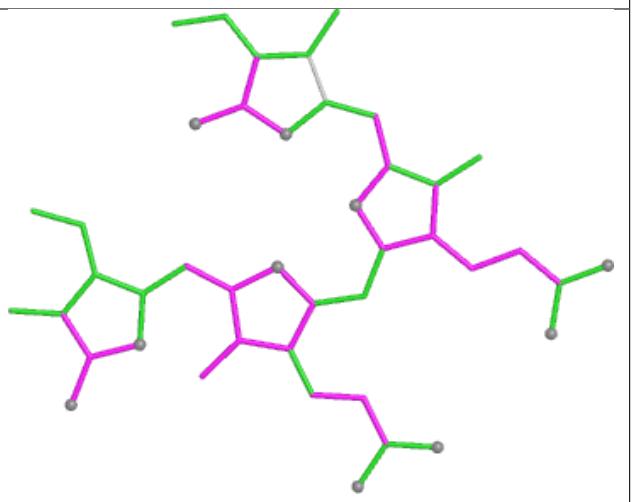


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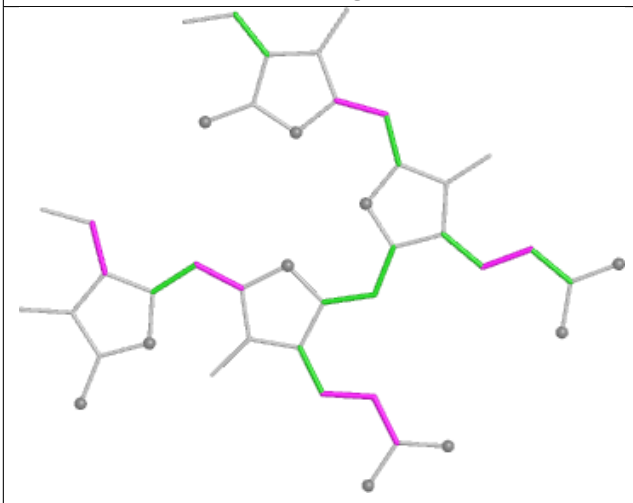
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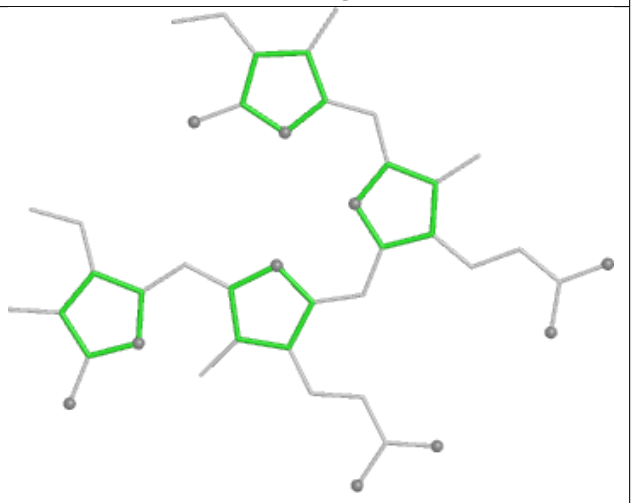
Bond lengths



Bond angles

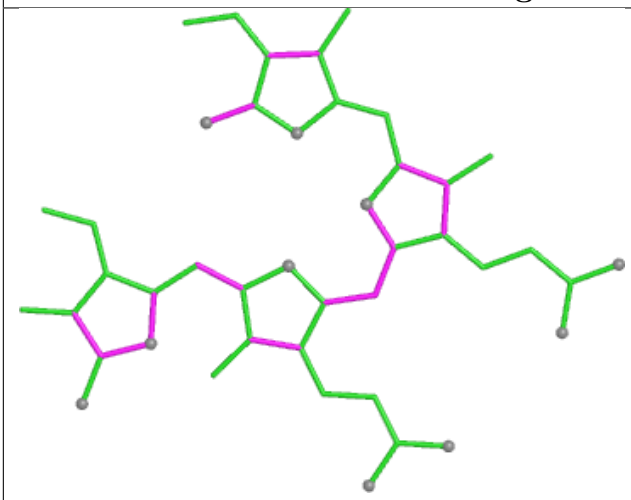


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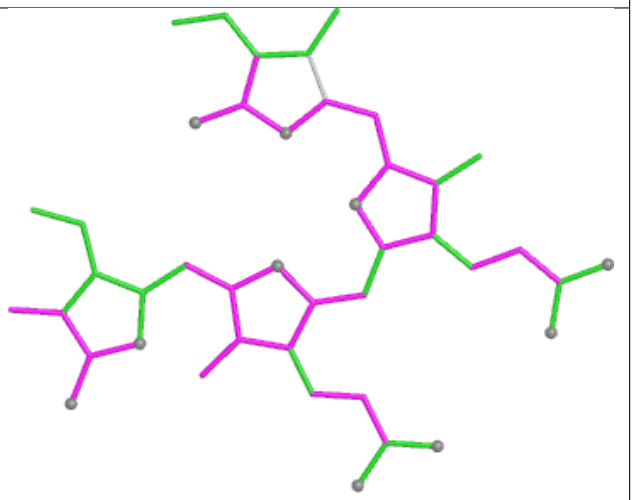


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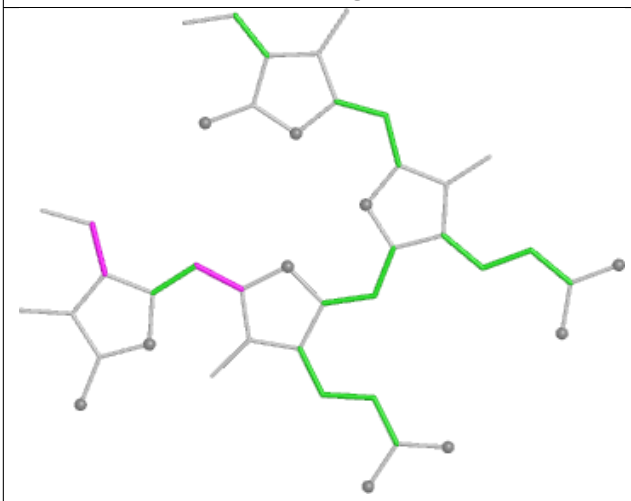
Ligand PEB V4 201



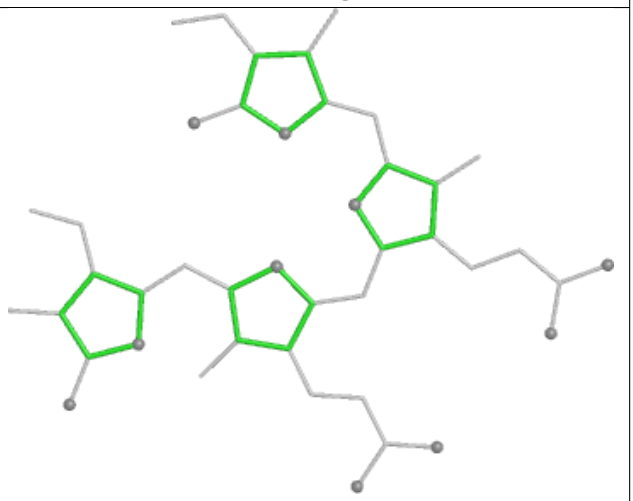
Bond lengths



Bond angles

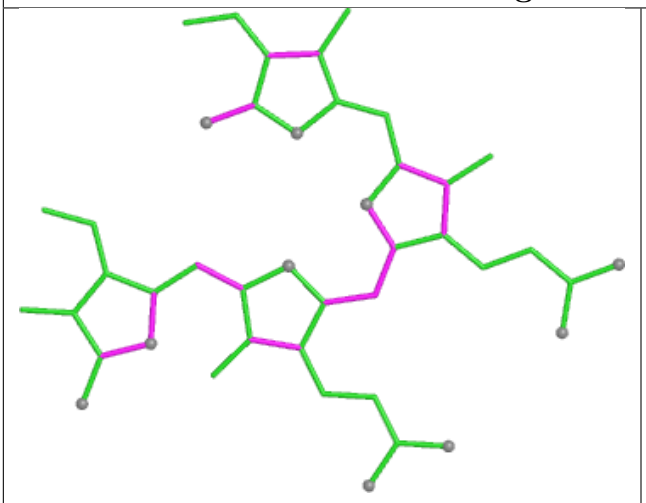


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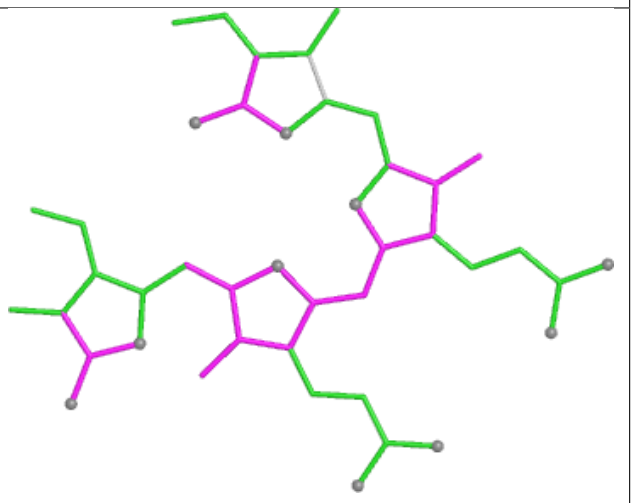


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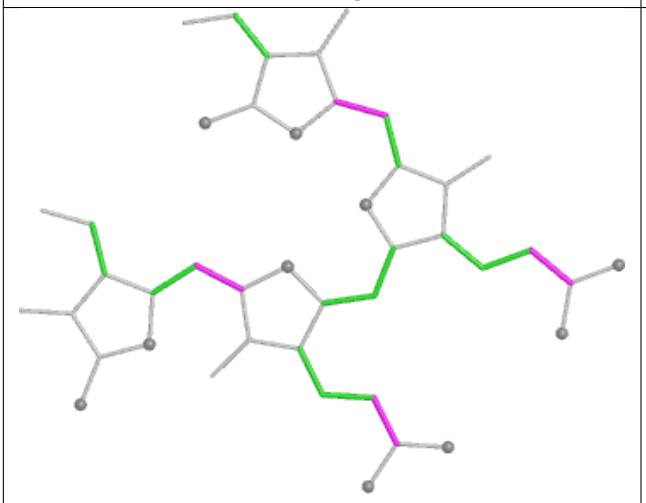
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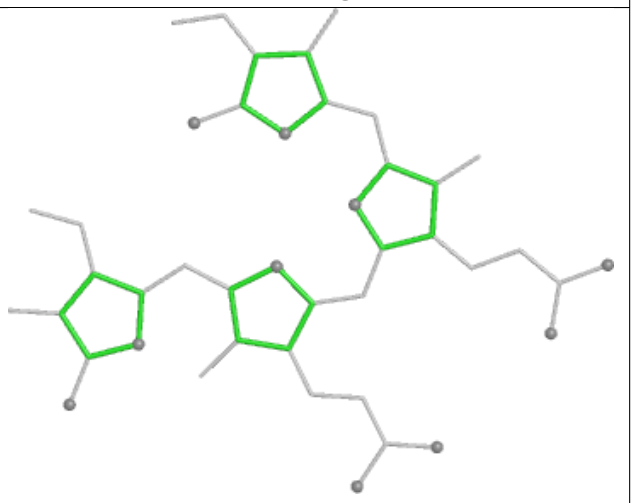
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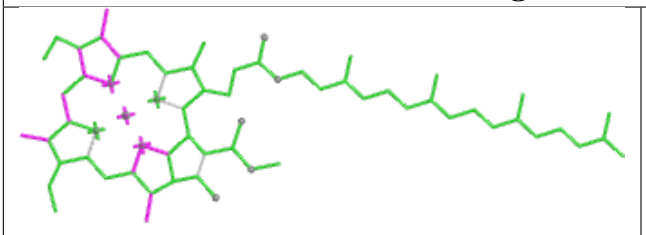


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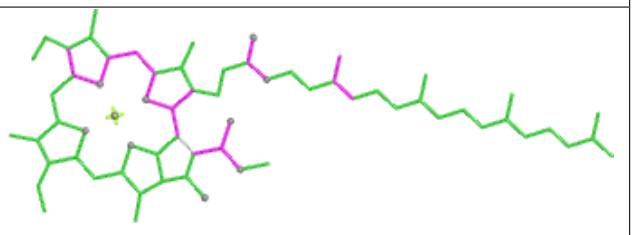


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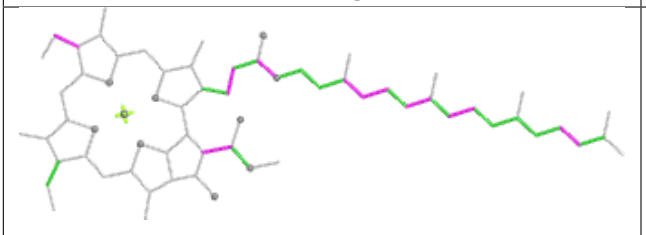
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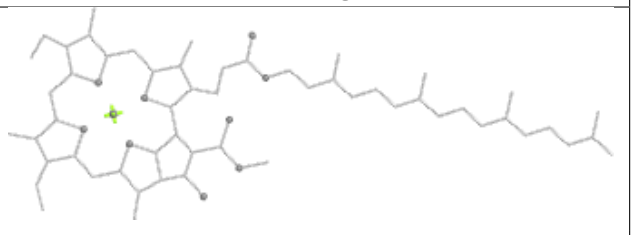
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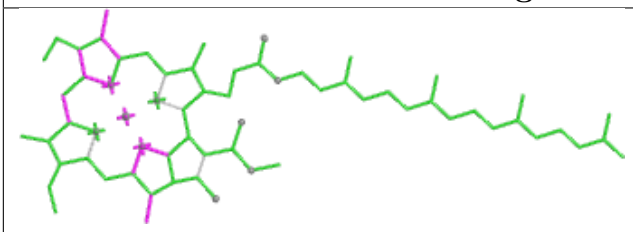


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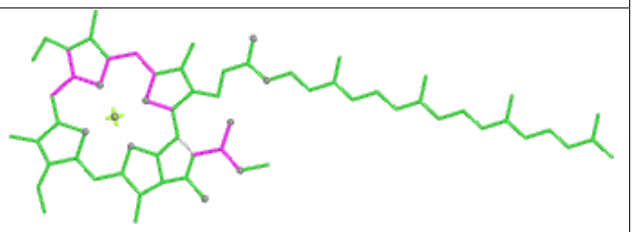


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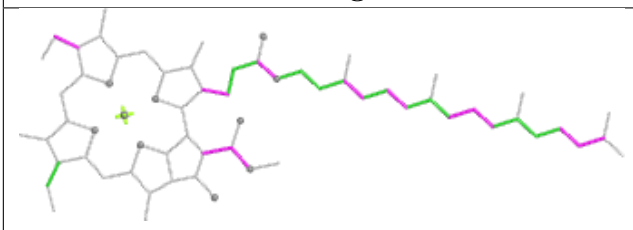
Ligand CLA B2 818



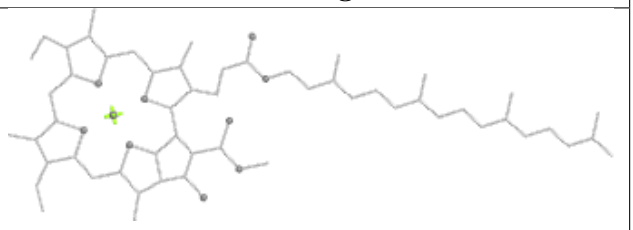
Bond lengths



Bond angles

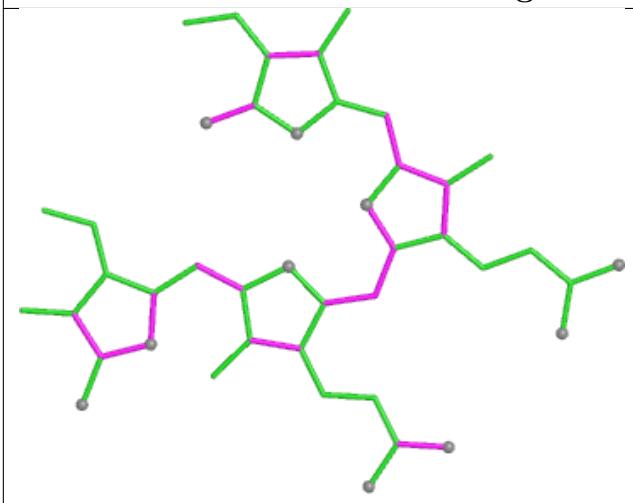


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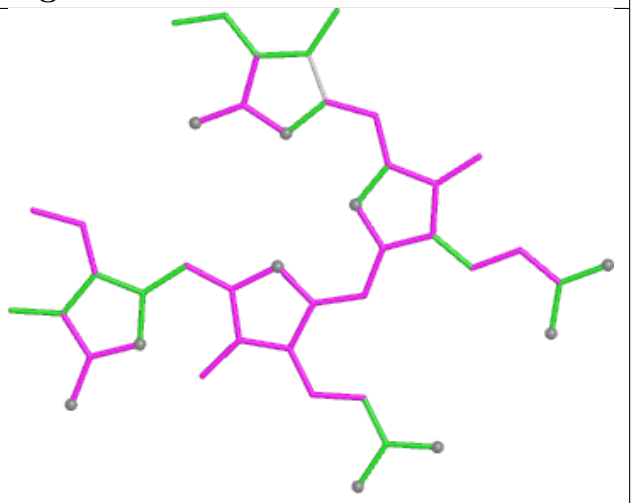


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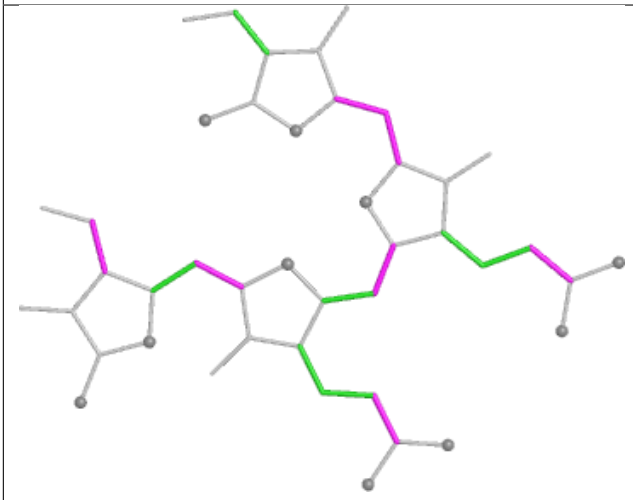
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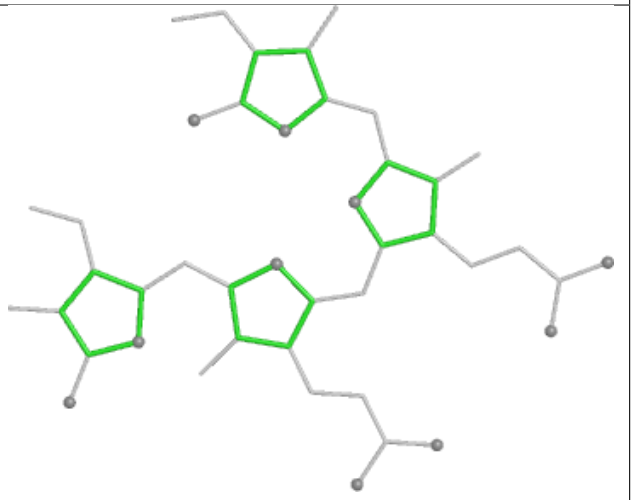
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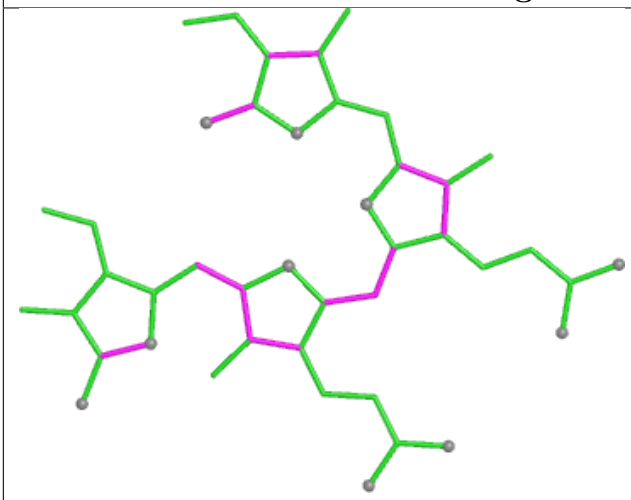


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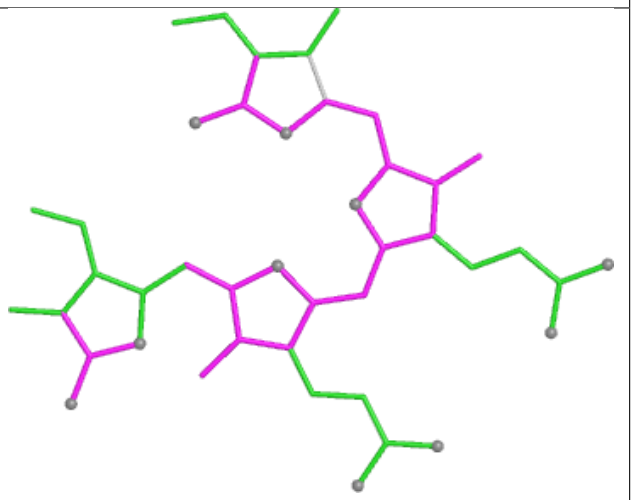


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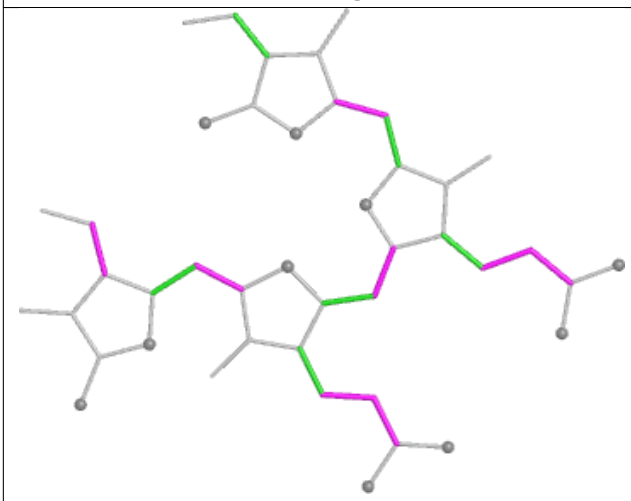
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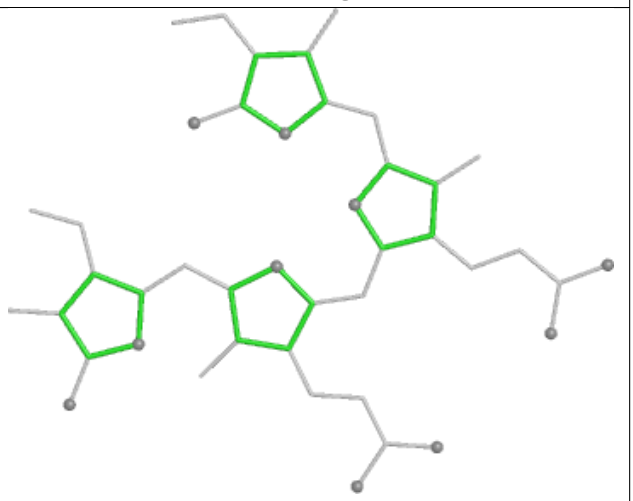
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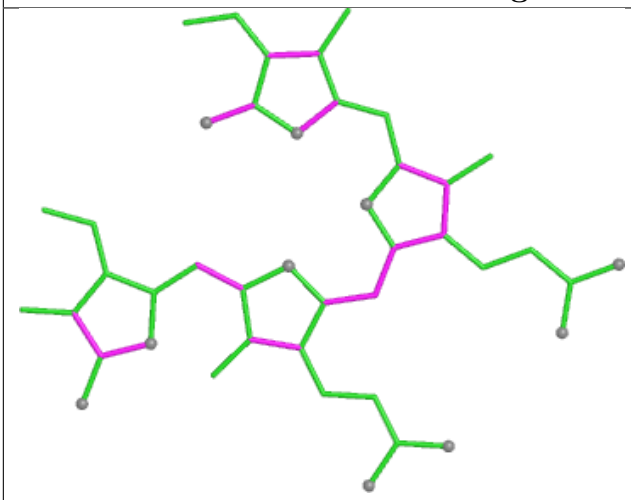


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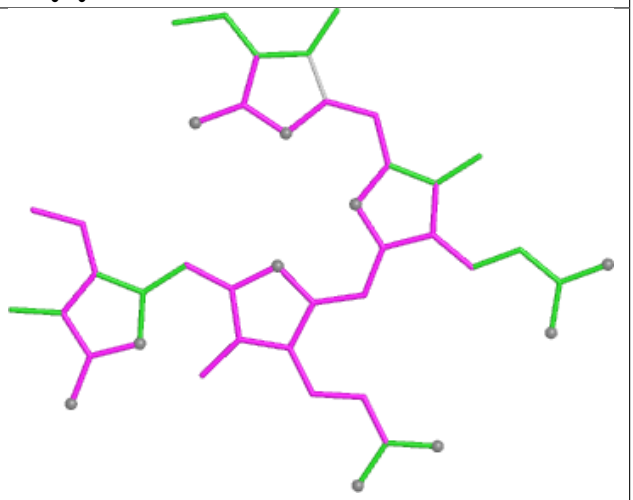


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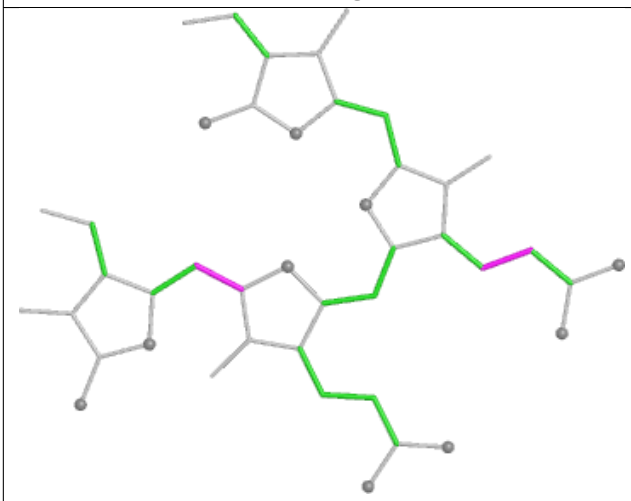
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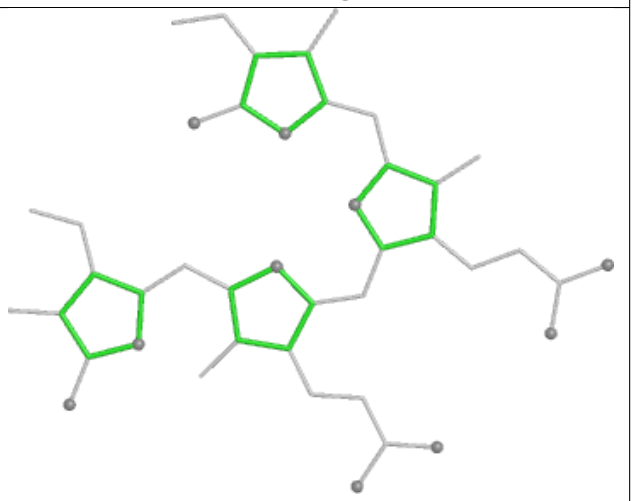
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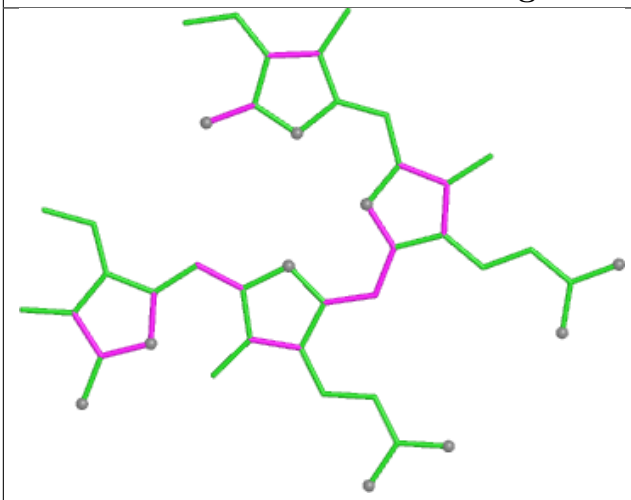


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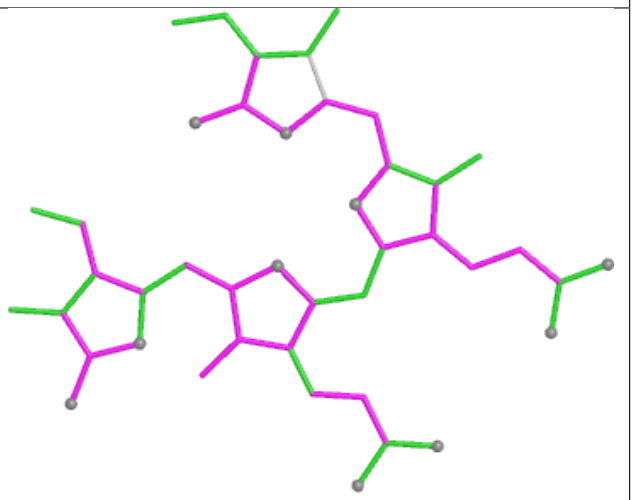


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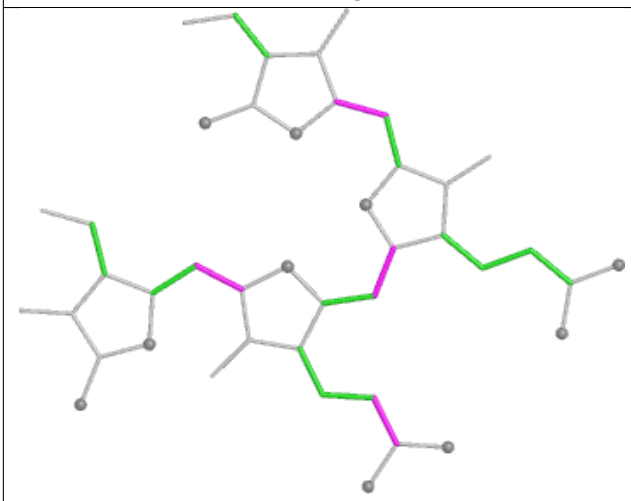
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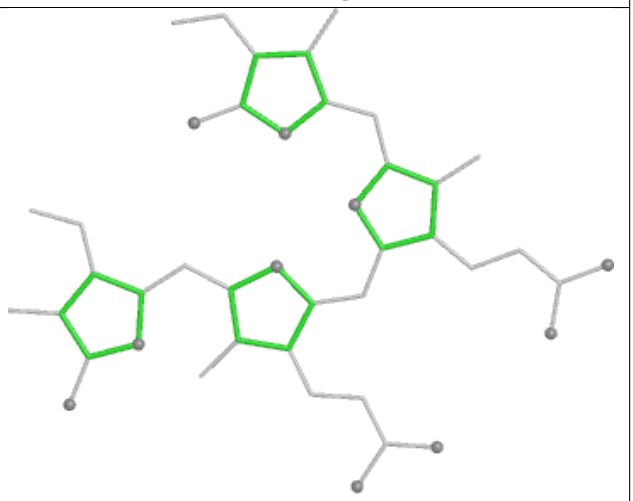
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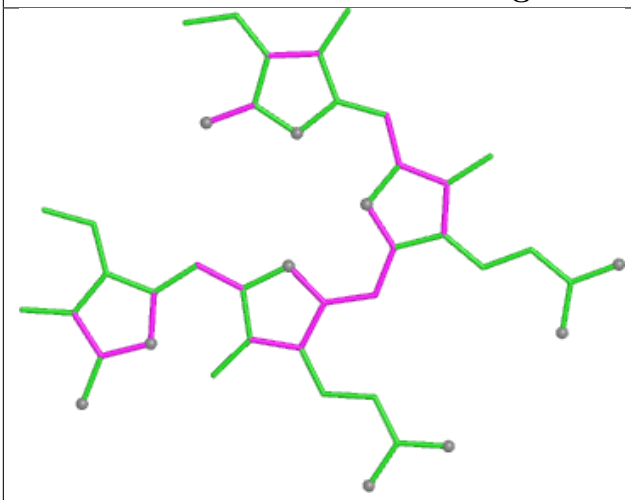


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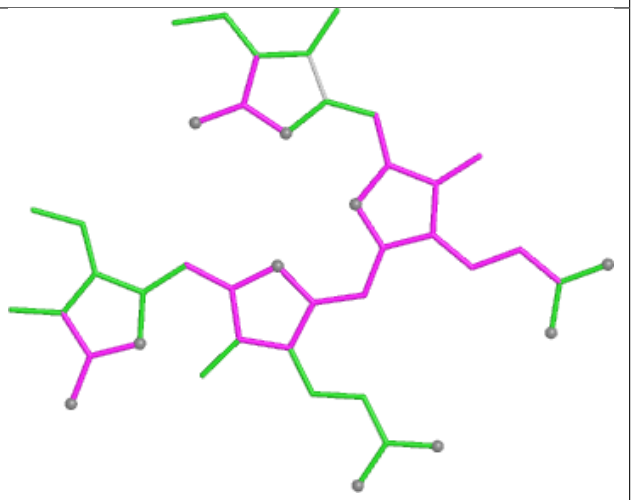


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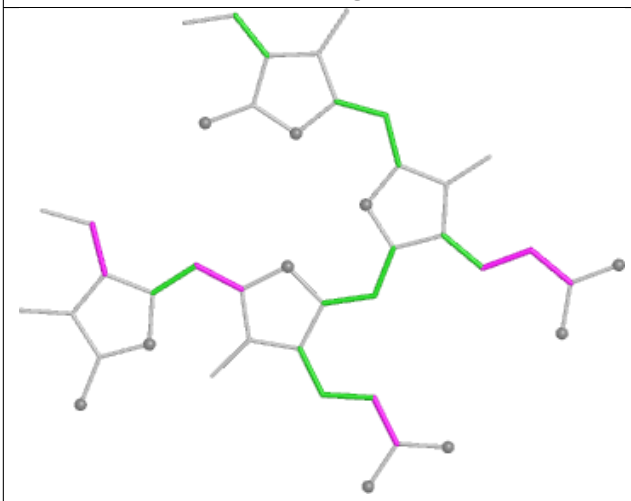
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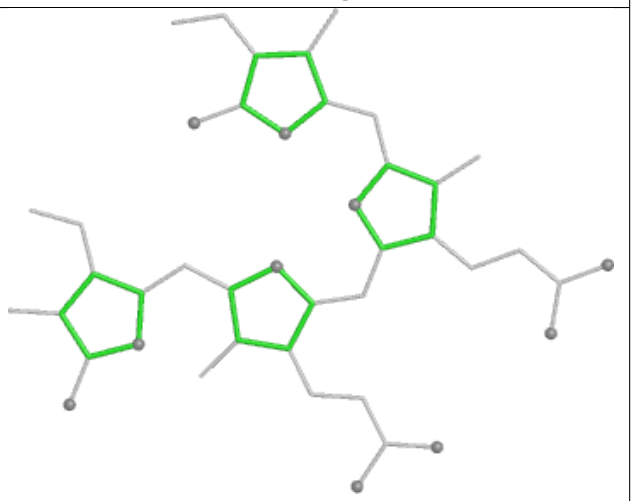
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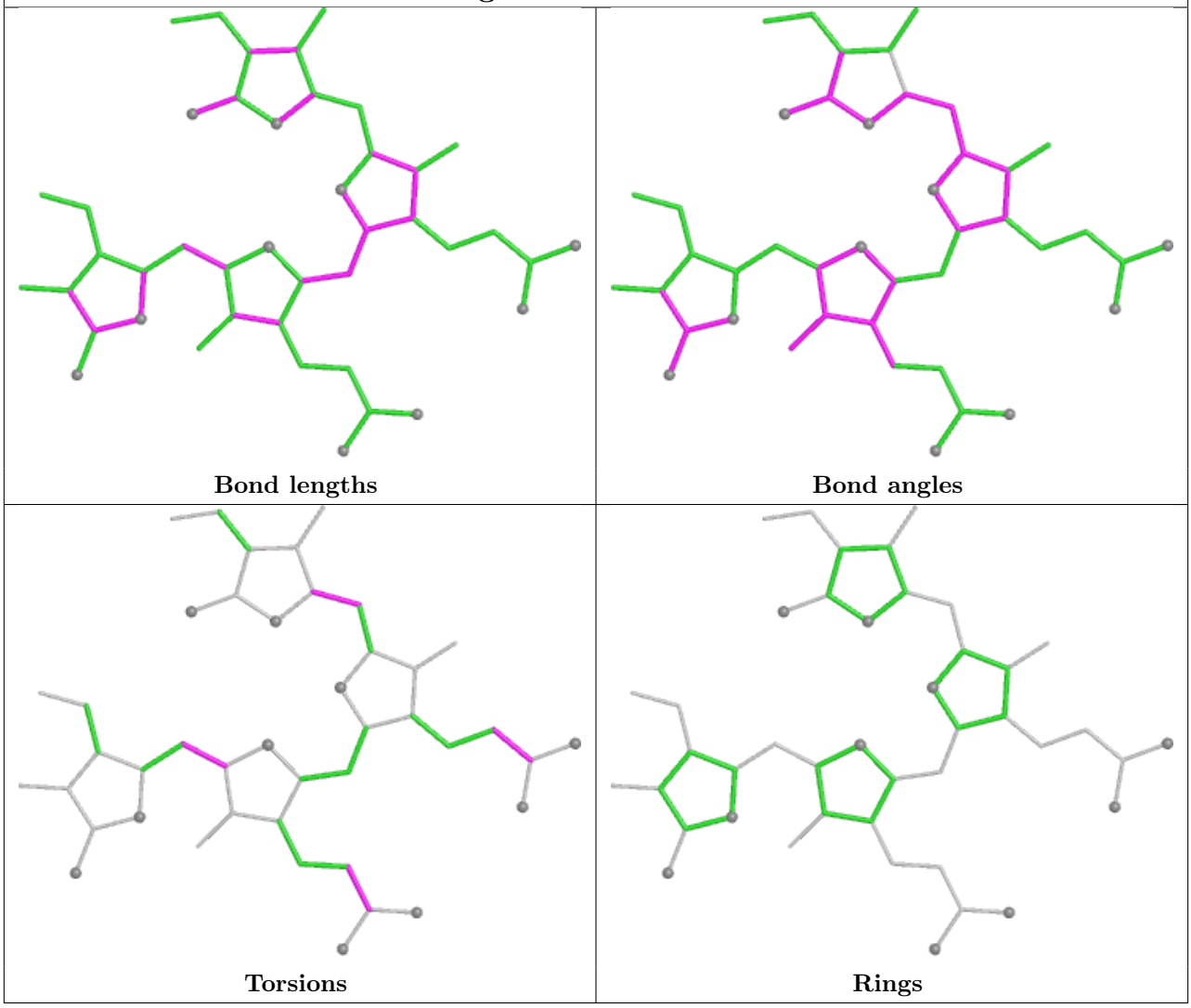


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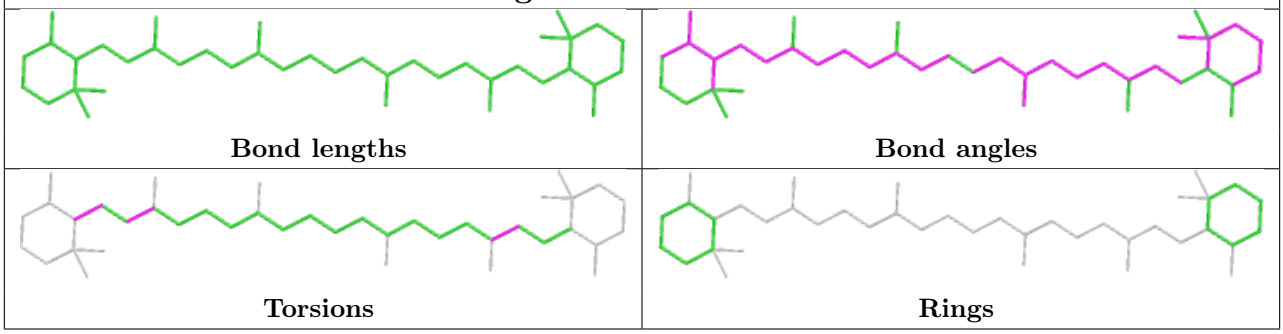


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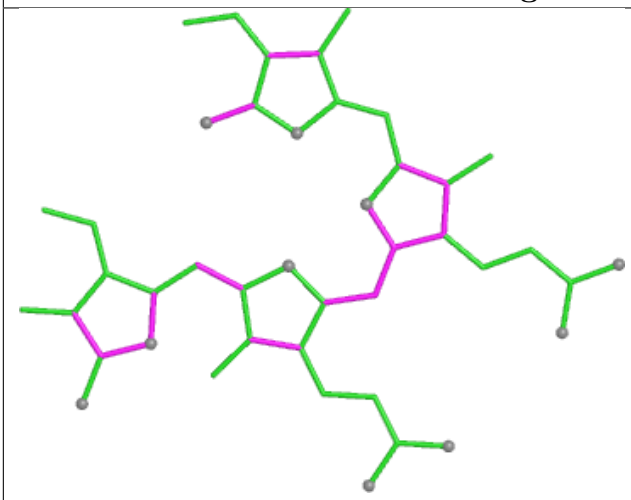
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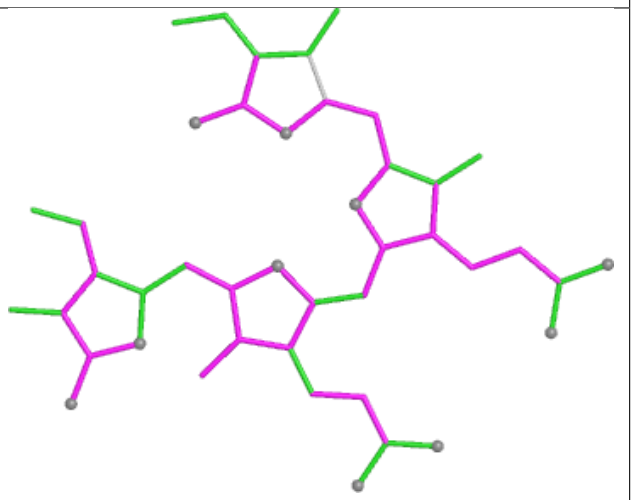
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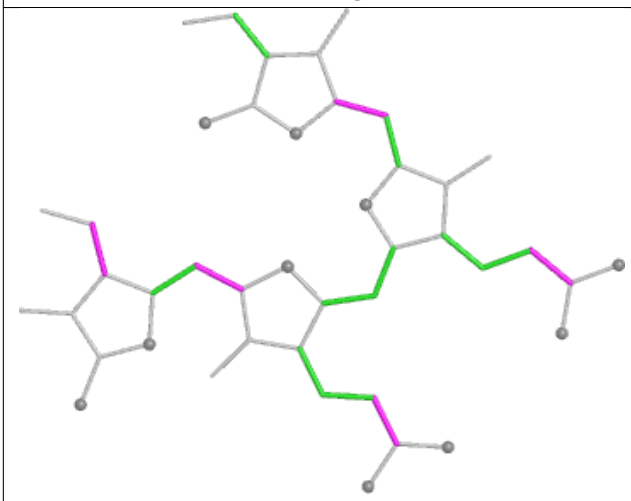
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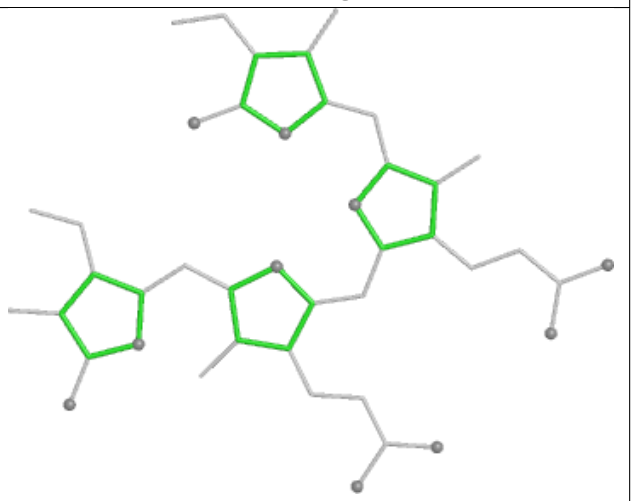
Bond lengths



Bond angles

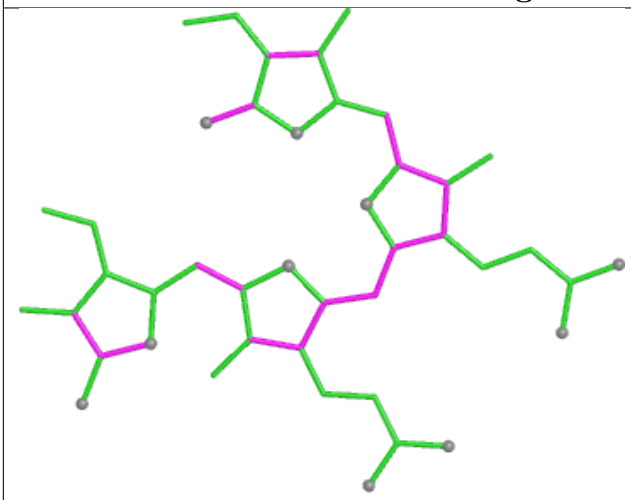


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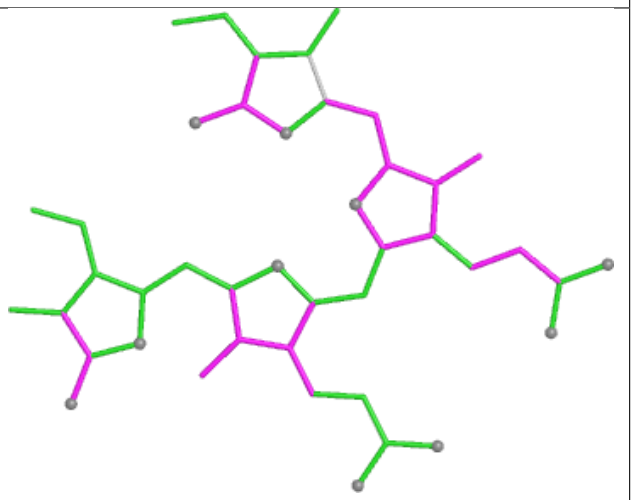


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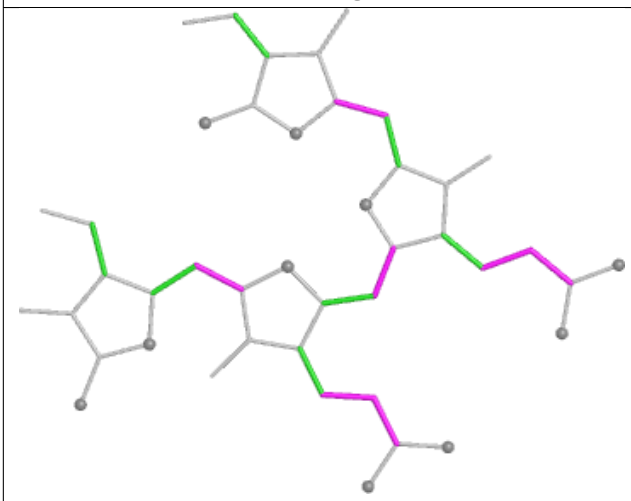
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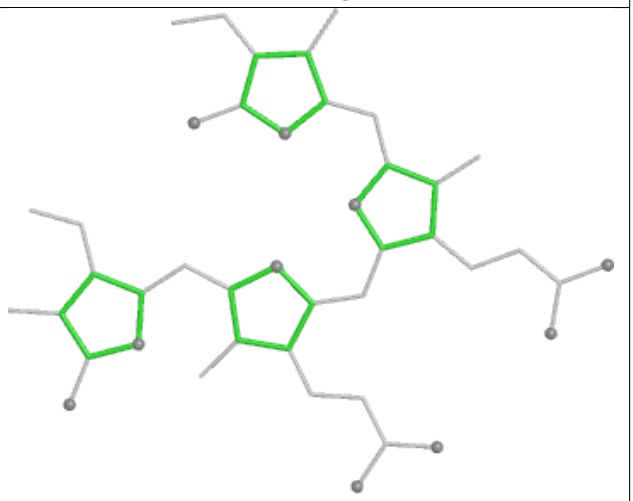
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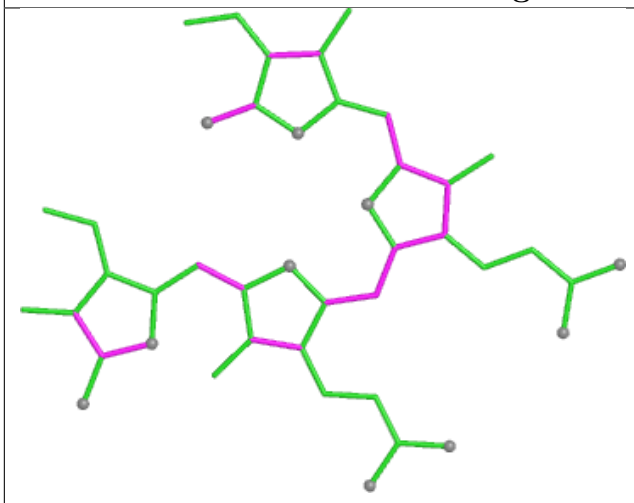


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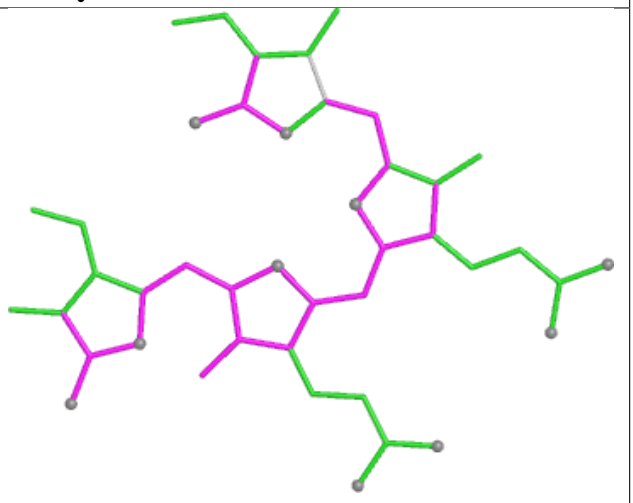


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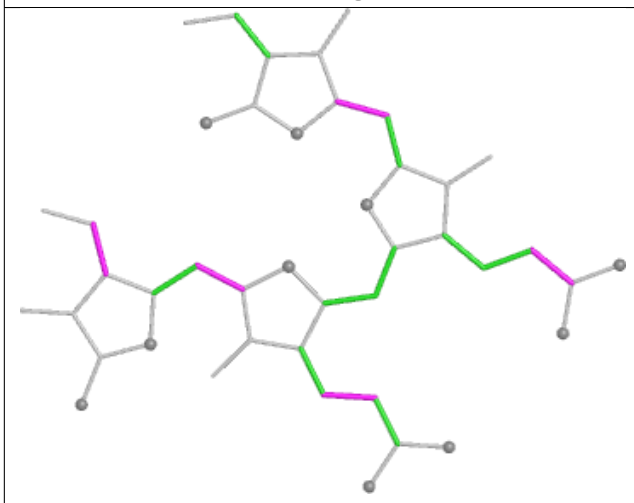
Ligand PEB TQ 202



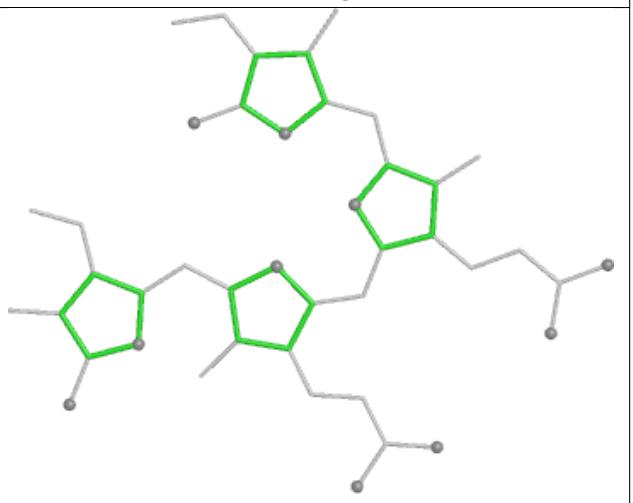
Bond lengths



Bond angles

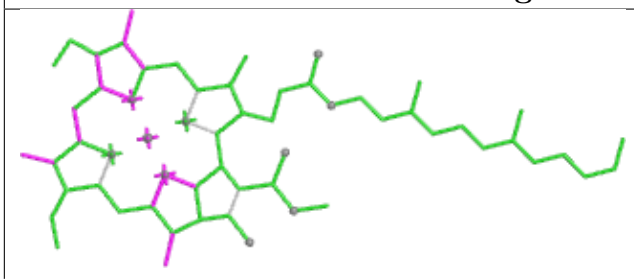


Torsions

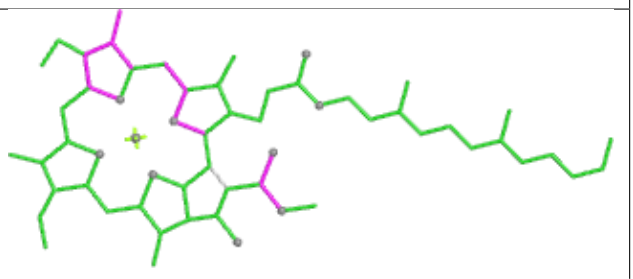


Rings

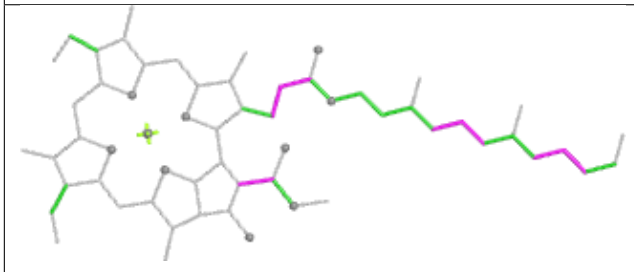
Ligand CLA BL 604



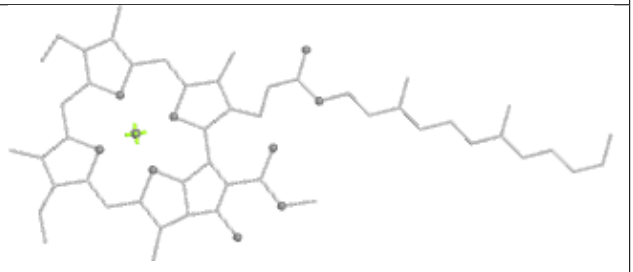
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Bond angles

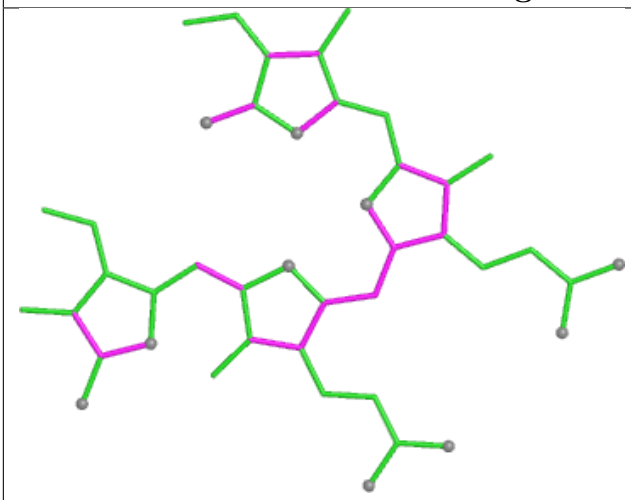


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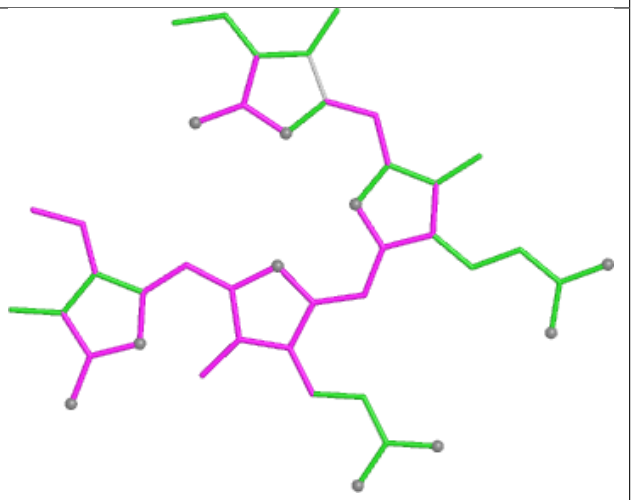


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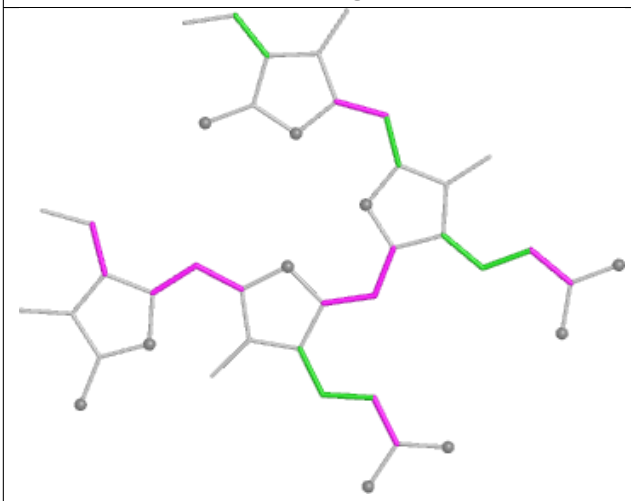
Ligand PEB G9 202



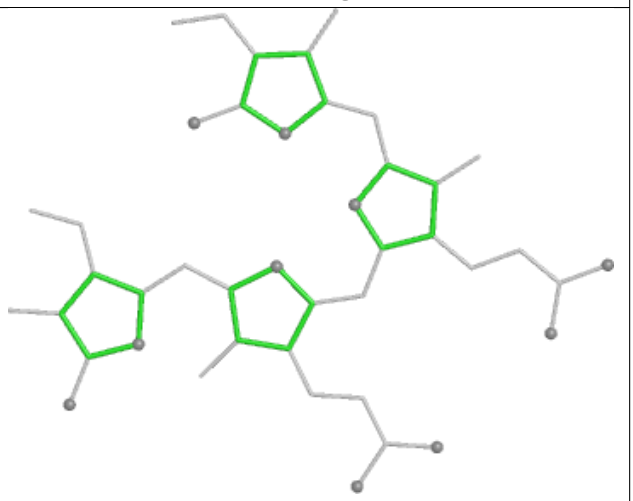
Bond lengths



Bond angles

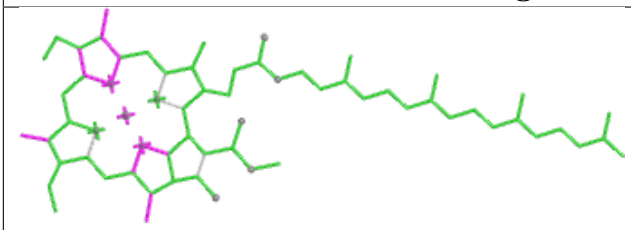


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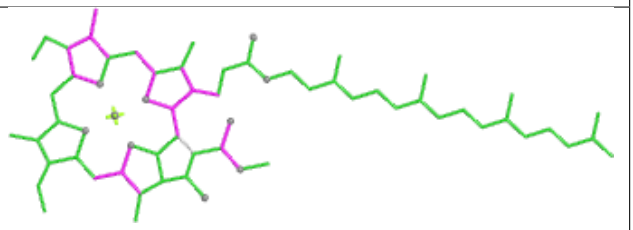


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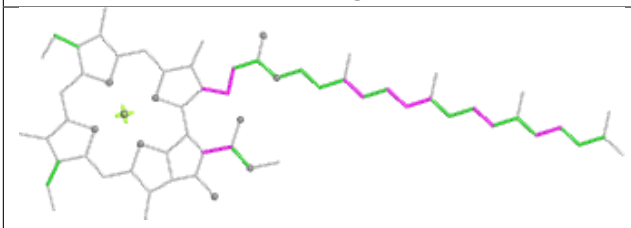
Ligand CLA A2 826



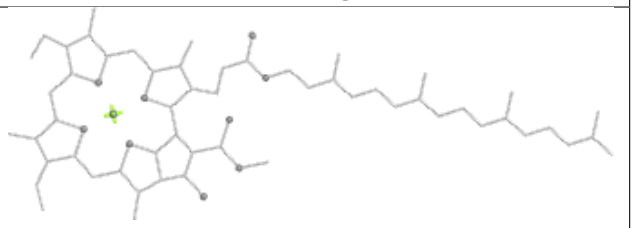
Bond lengths



Bond angles

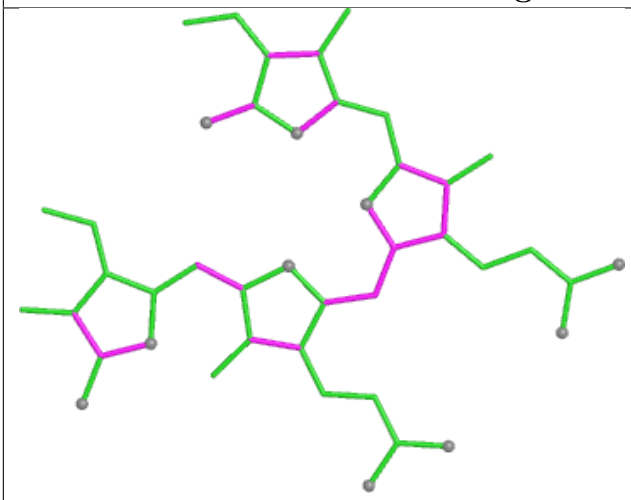


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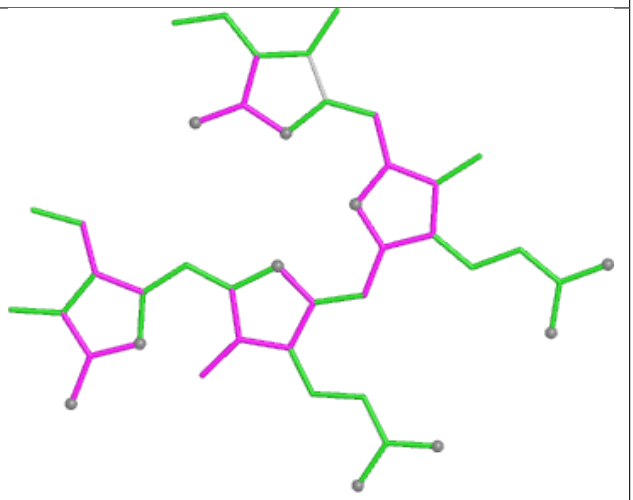


Rings

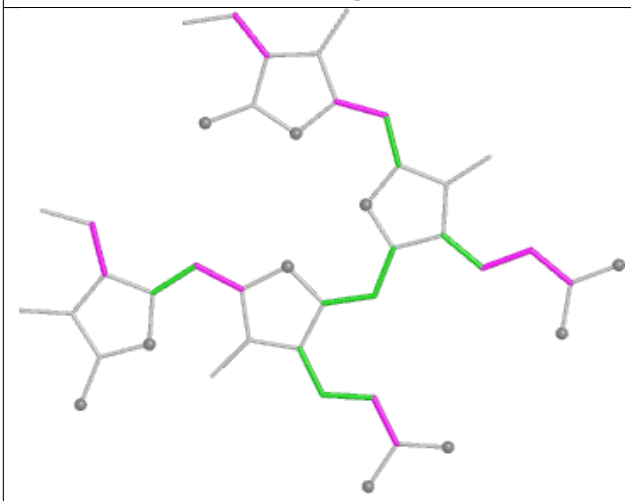
Ligand PEB K7 202



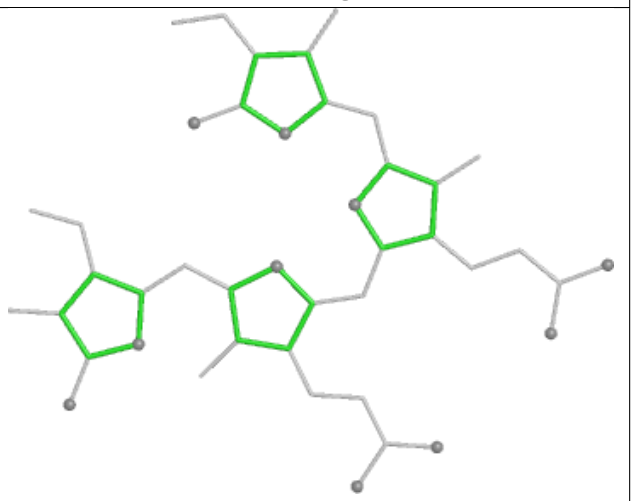
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Bond angles

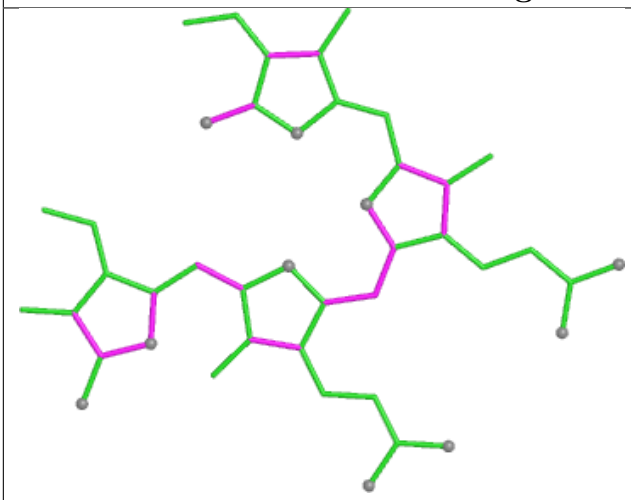


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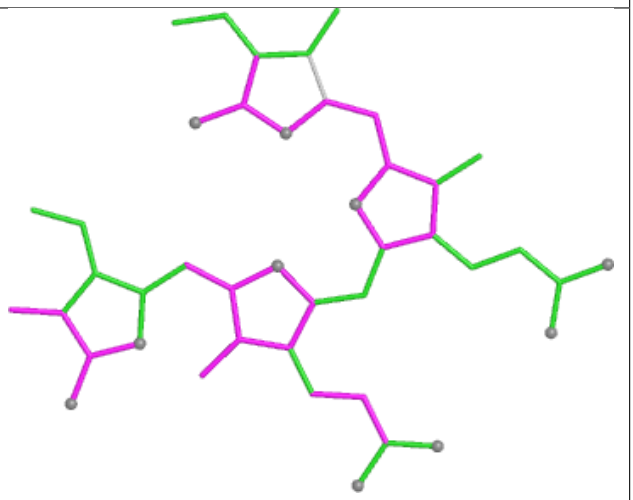


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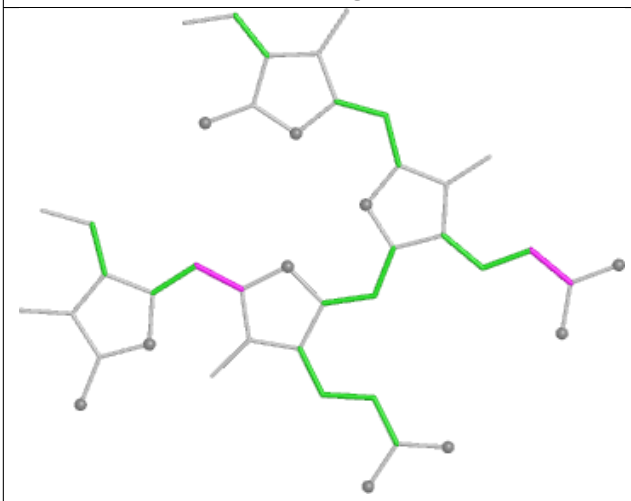
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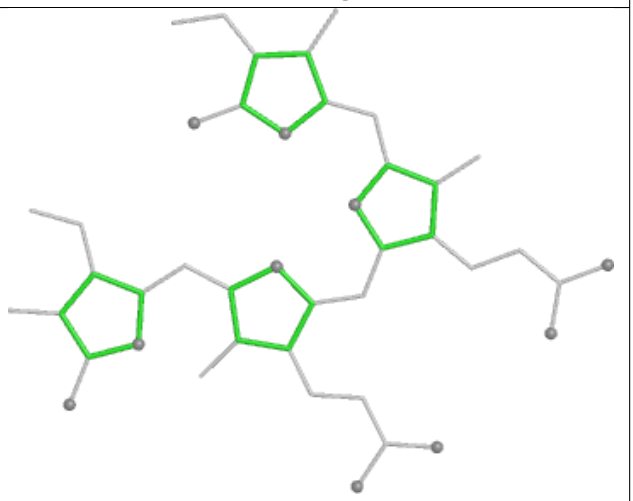
Bond lengths



Bond angles

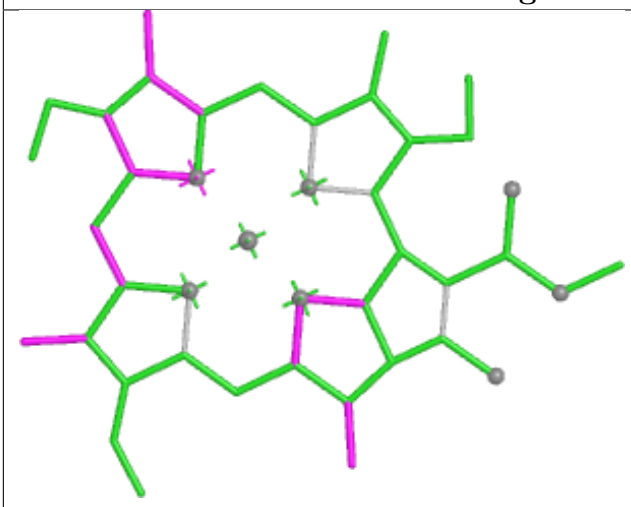


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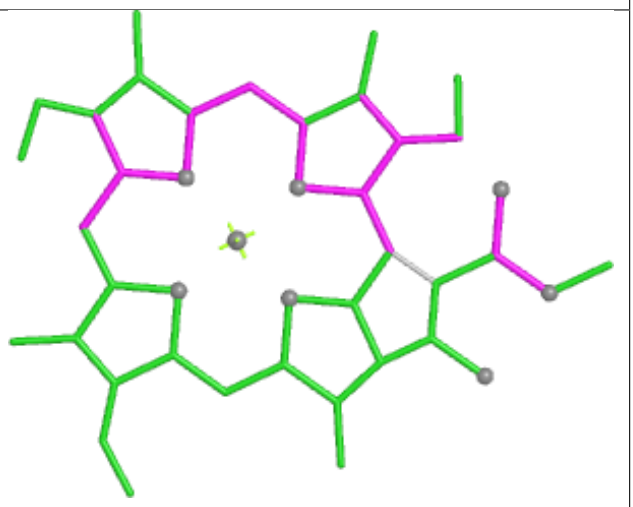


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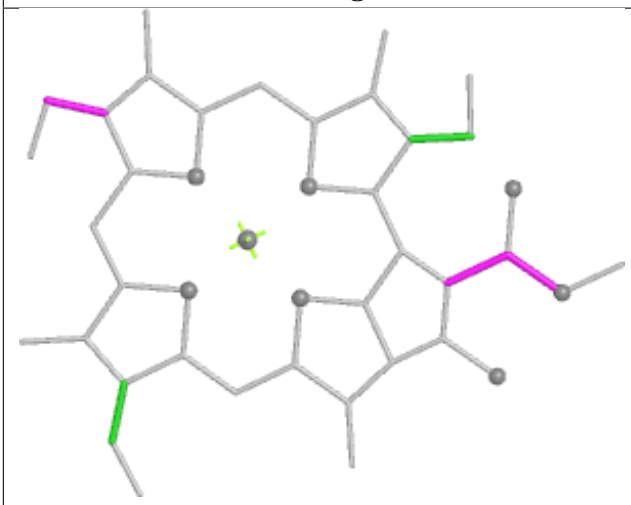
Ligand CLA J2 101



Bond lengths



Bond angles

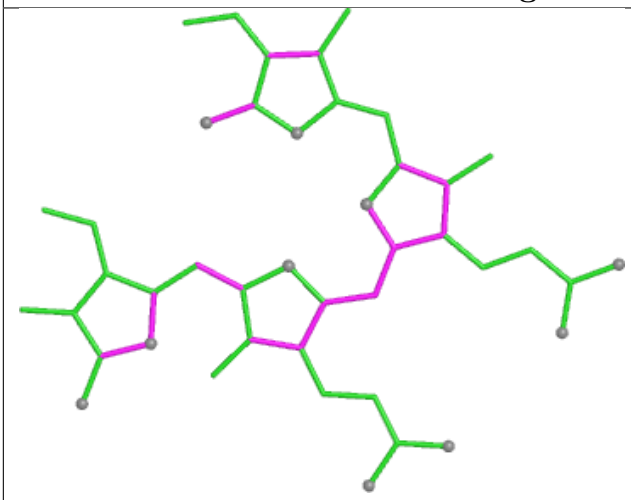


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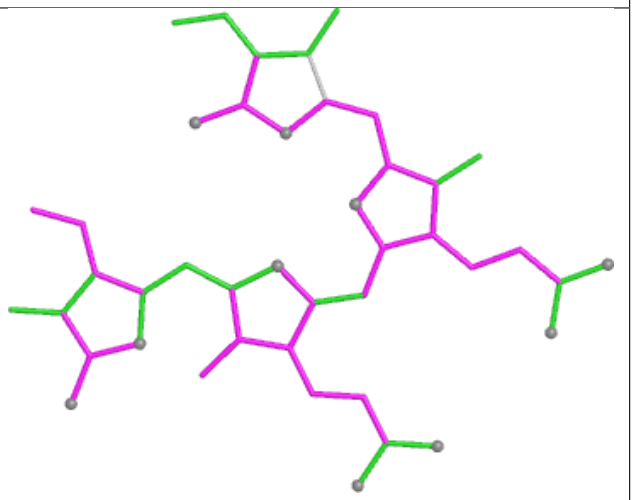


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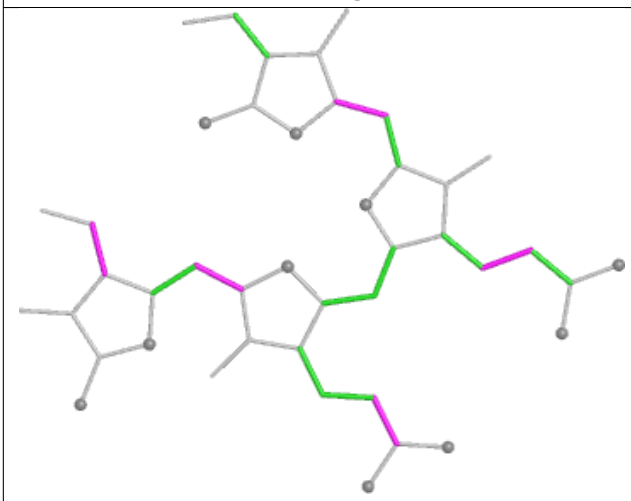
Ligand PEB k1 201



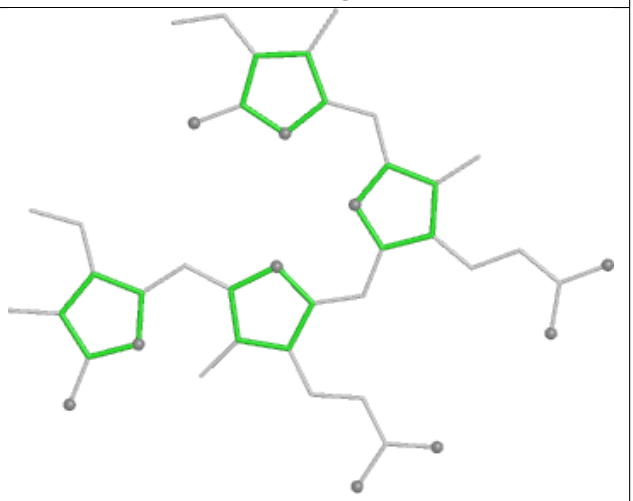
Bond lengths



Bond angles

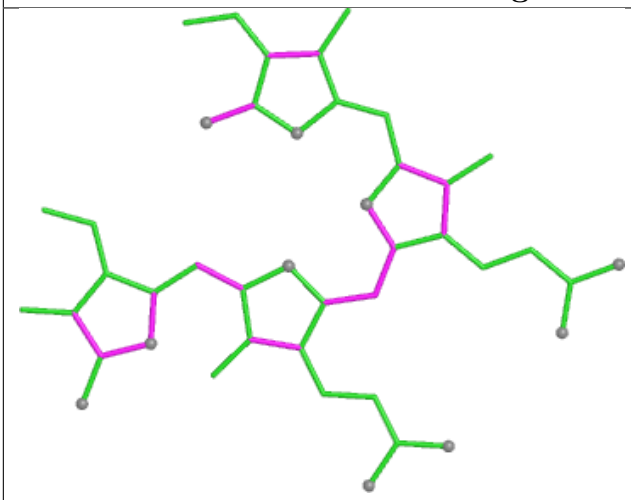


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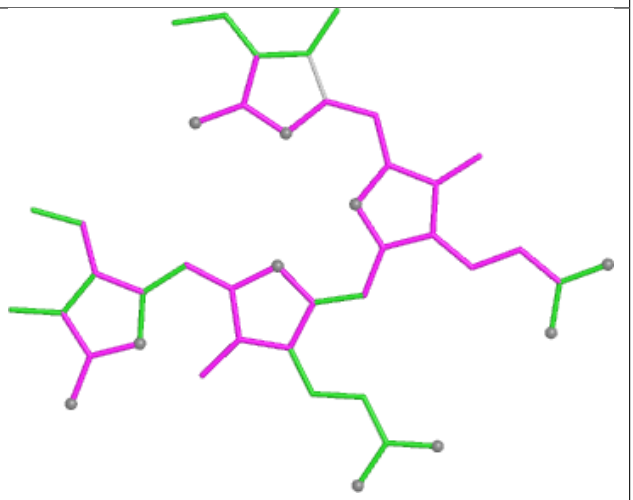


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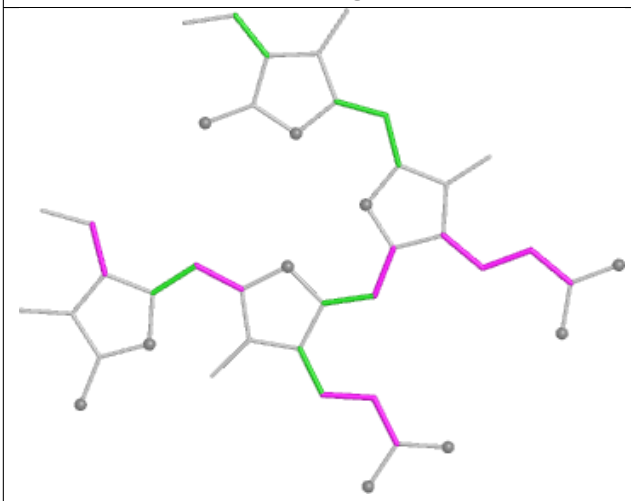
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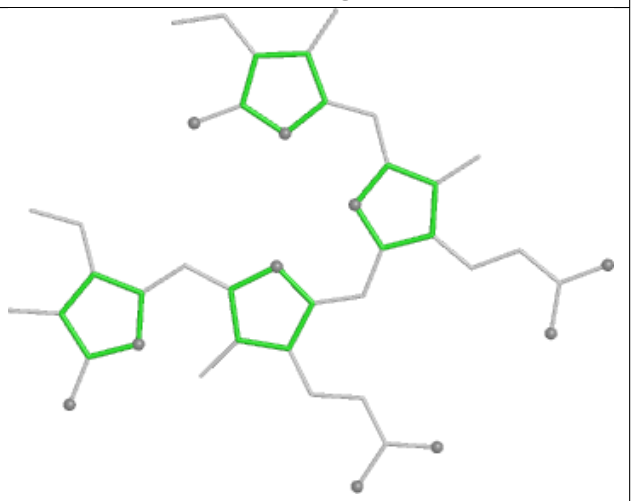
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Bond angles

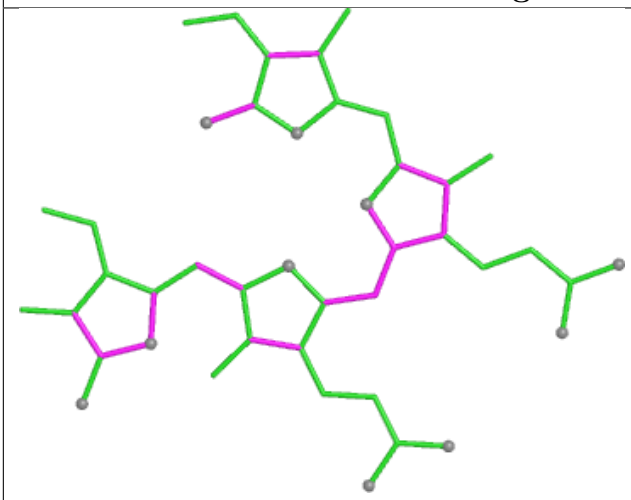


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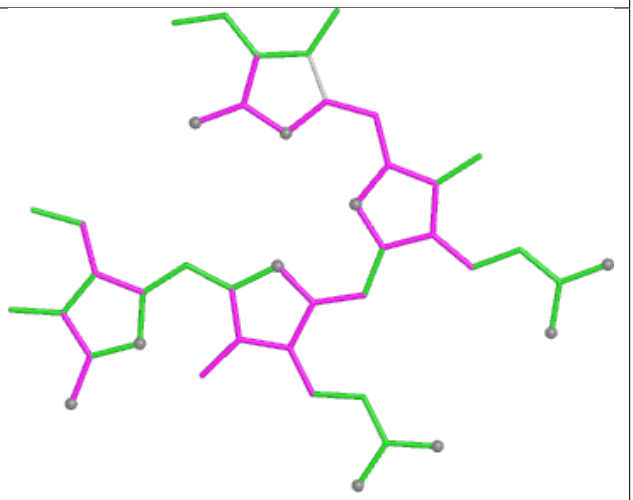


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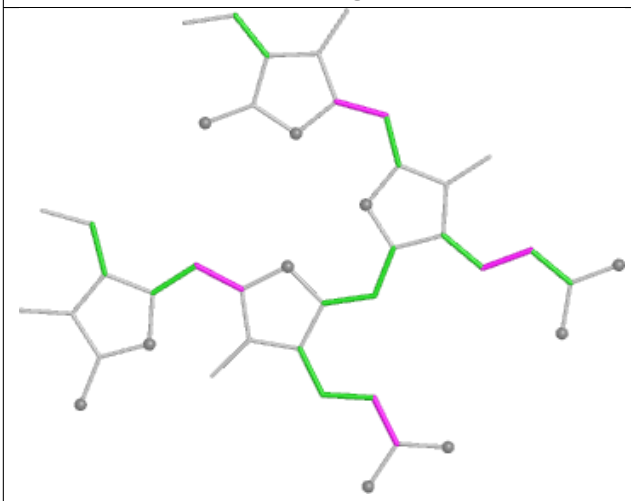
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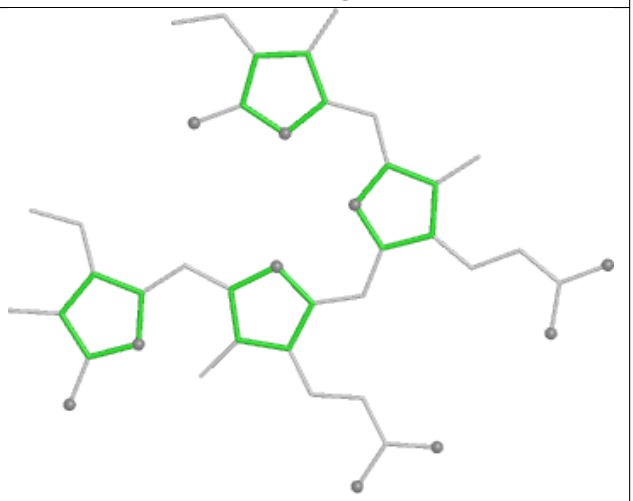
Bond lengths



Bond angles

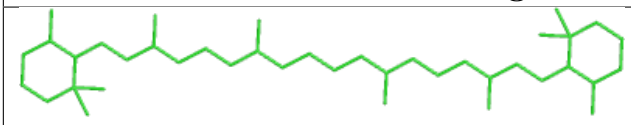


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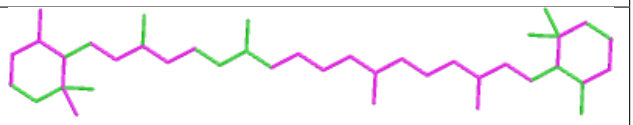


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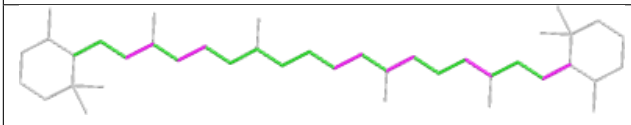
Ligand BCR AN 846



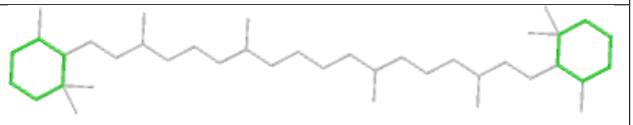
Bond lengths



Bond angles

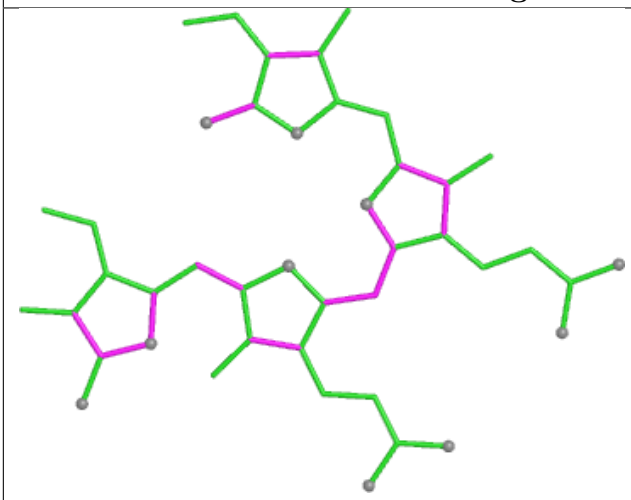


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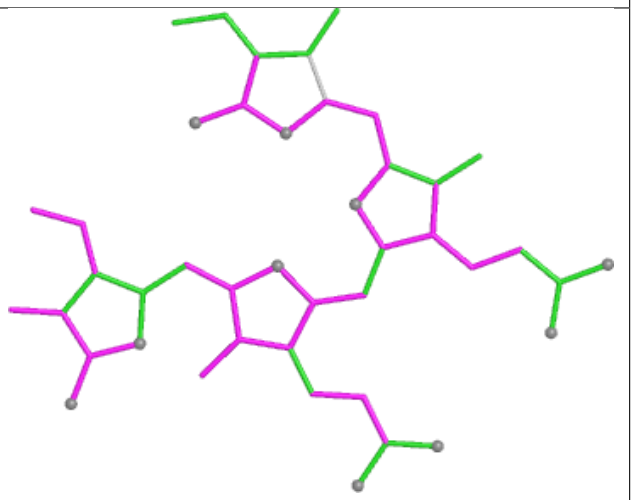


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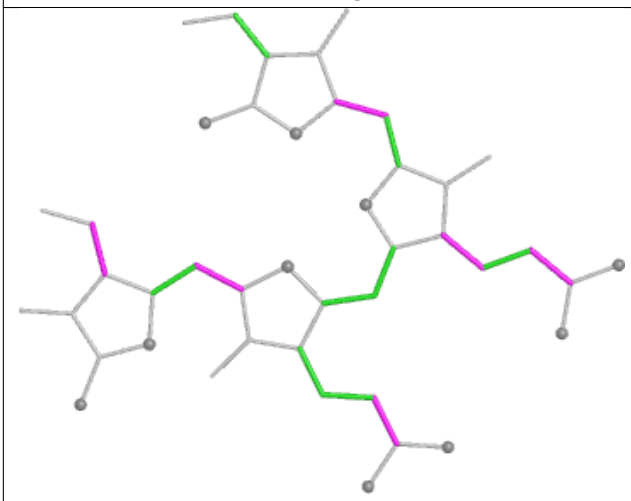
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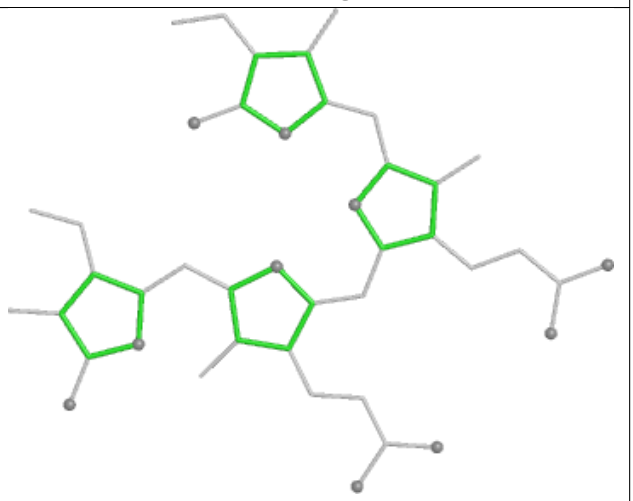
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Bond angles

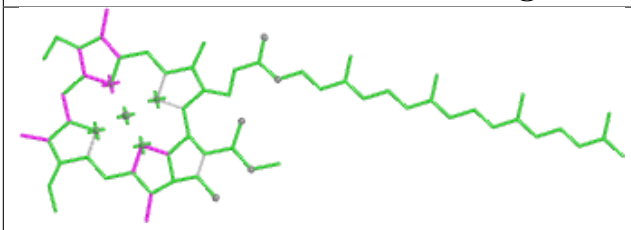


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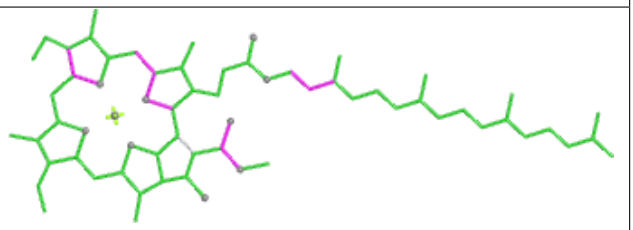


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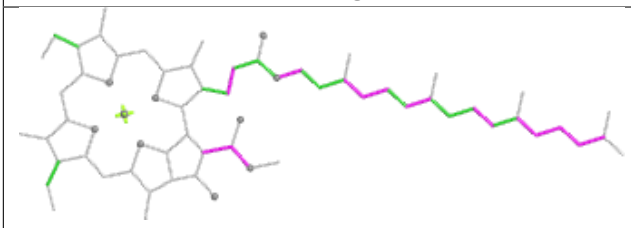
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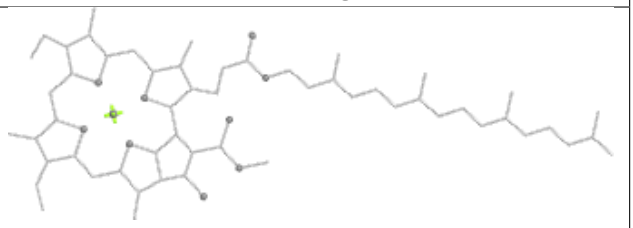
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Bond angles

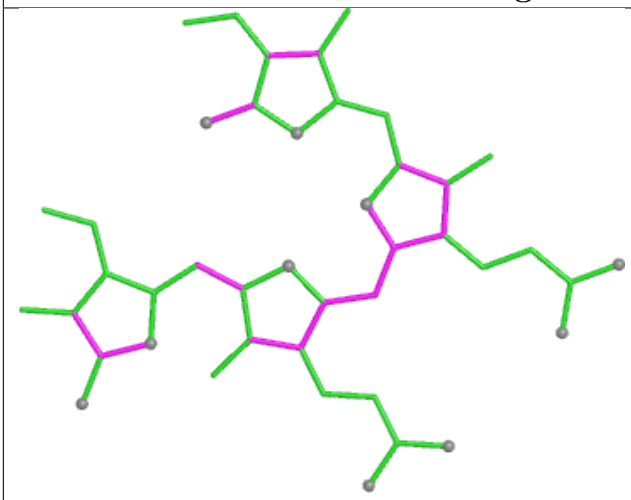


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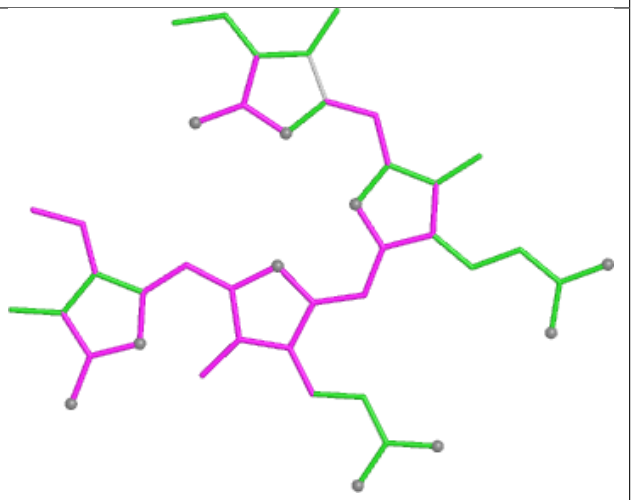


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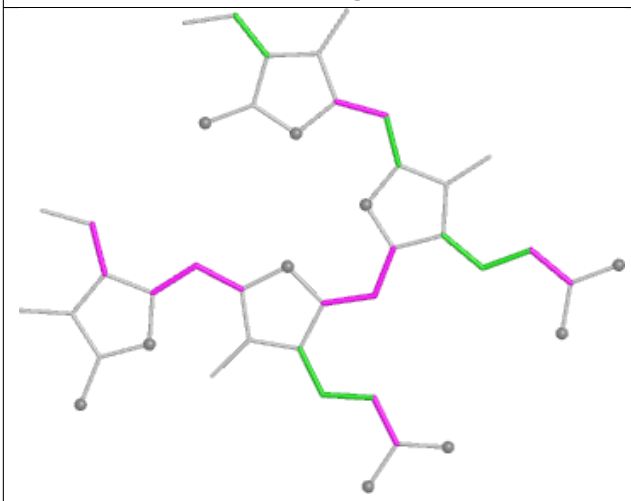
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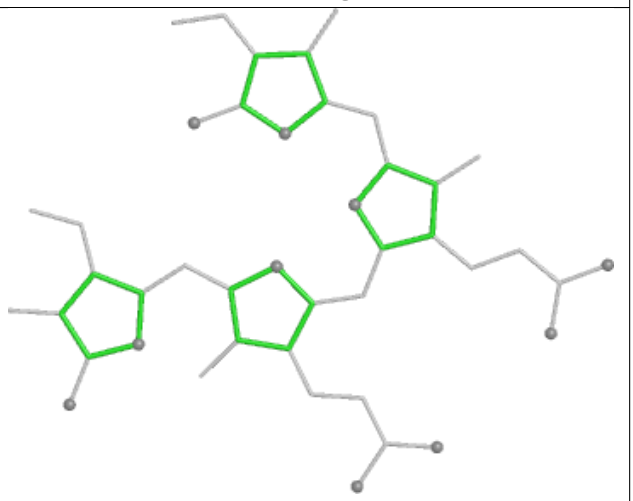
Bond lengths



Bond angles

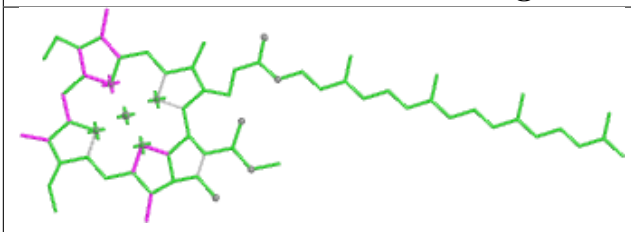


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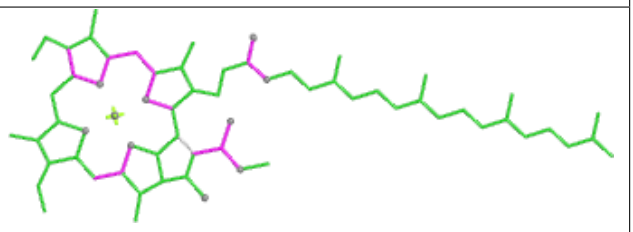


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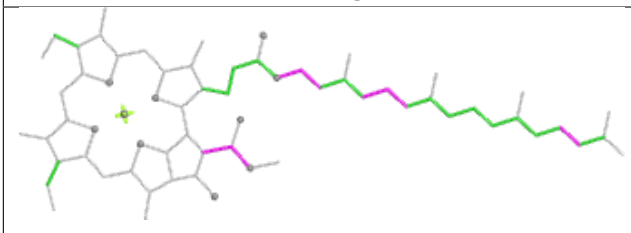
Ligand CLA B6 614



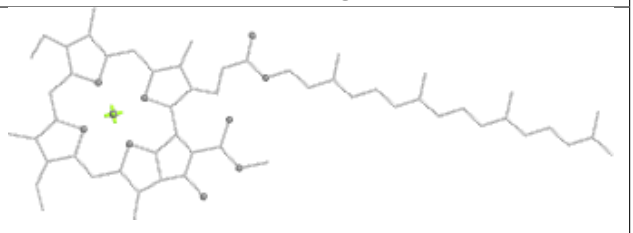
Bond lengths



Bond angles

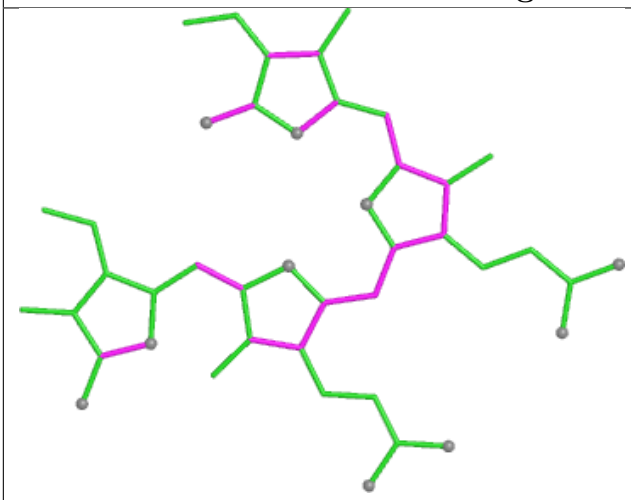


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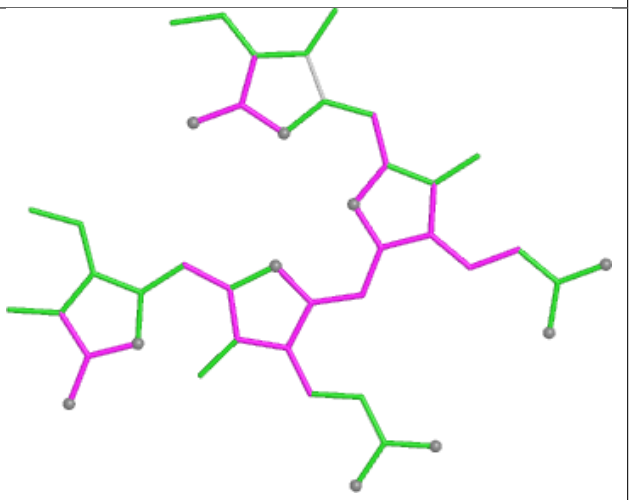


Rings

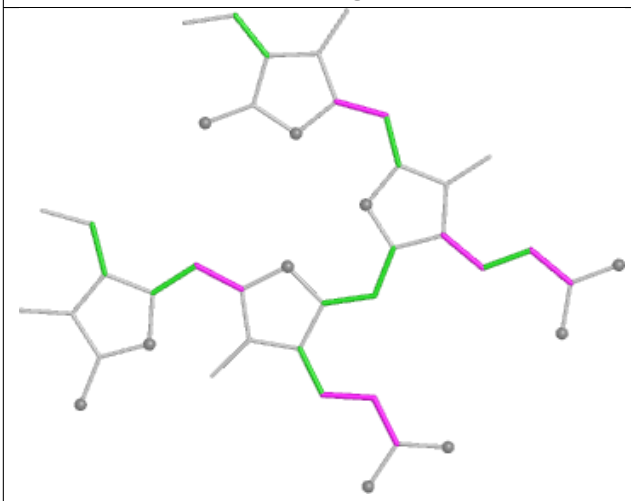
Ligand PEB tK 202



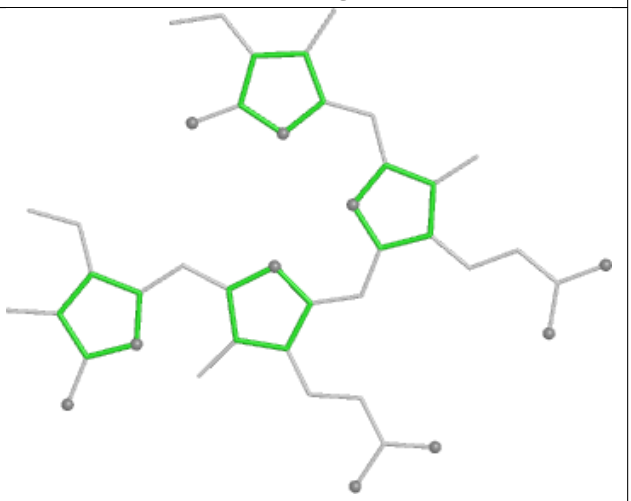
Bond lengths



Bond angles

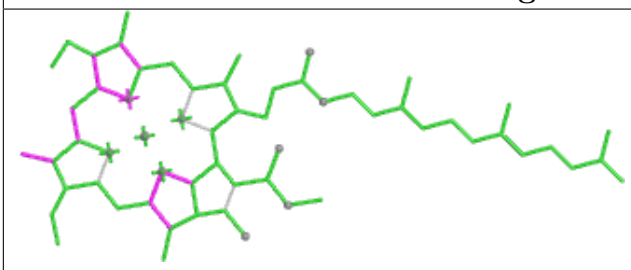


Torsions

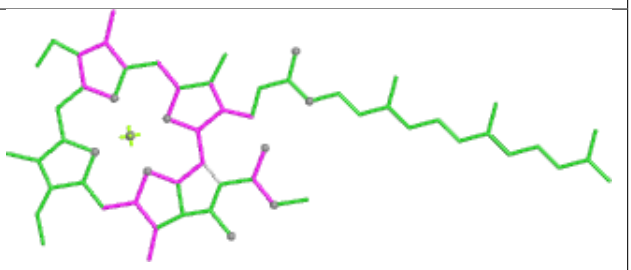


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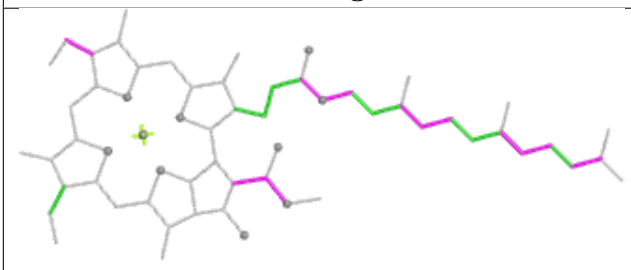
Ligand CLA cL 515



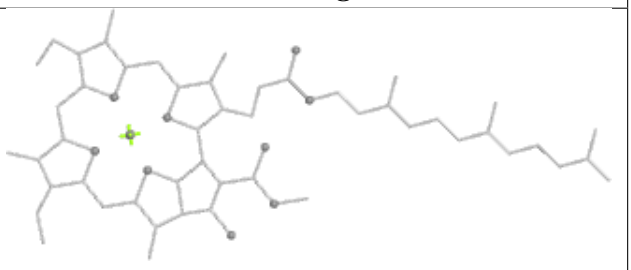
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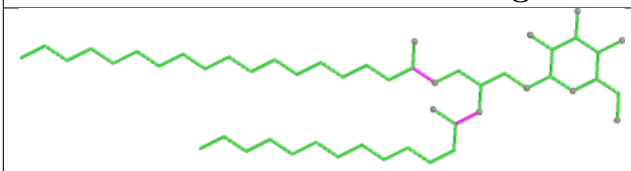
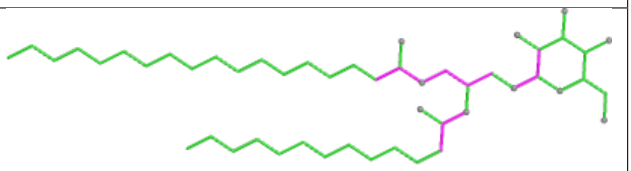
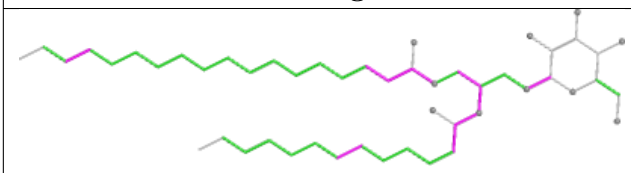
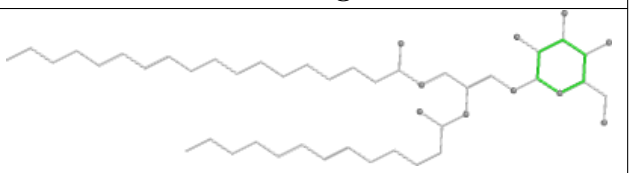
Bond angles

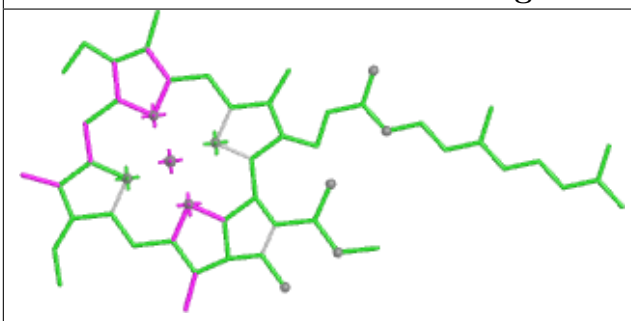
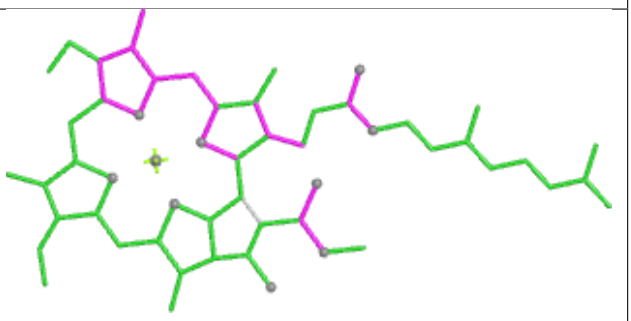
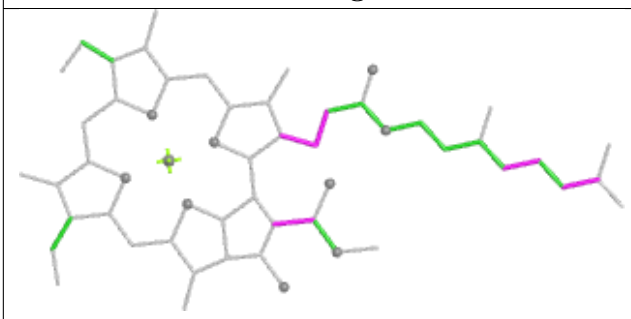
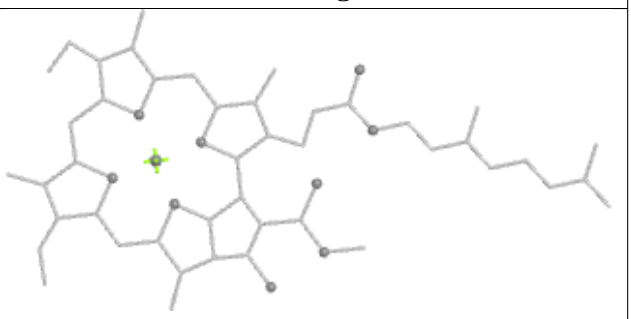


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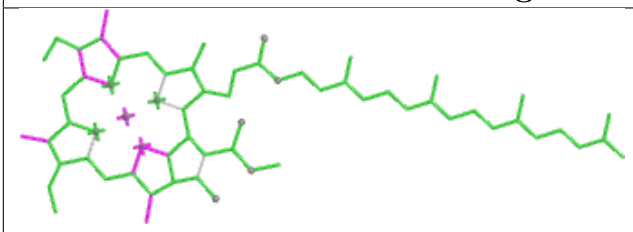


Rings

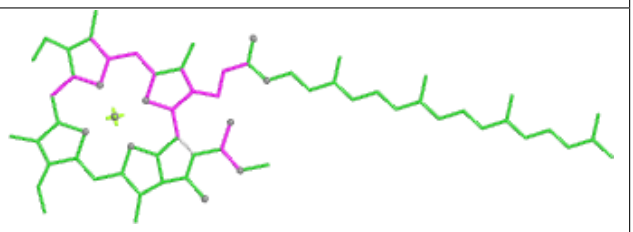
Ligand LMG bL 611	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A2 825	
 Bond lengths	 Bond angles
 Torsions	 Rings

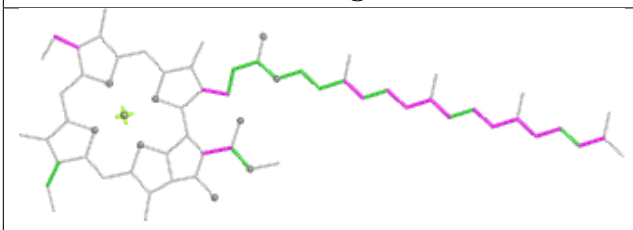
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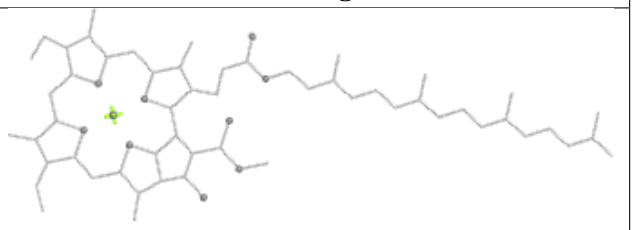
Bond lengths



Bond angles

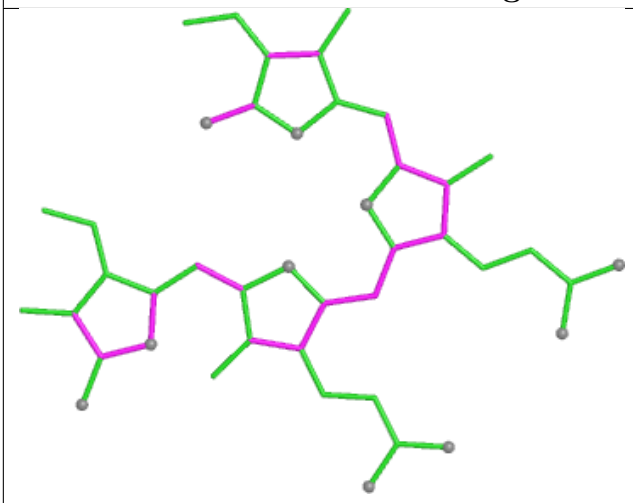


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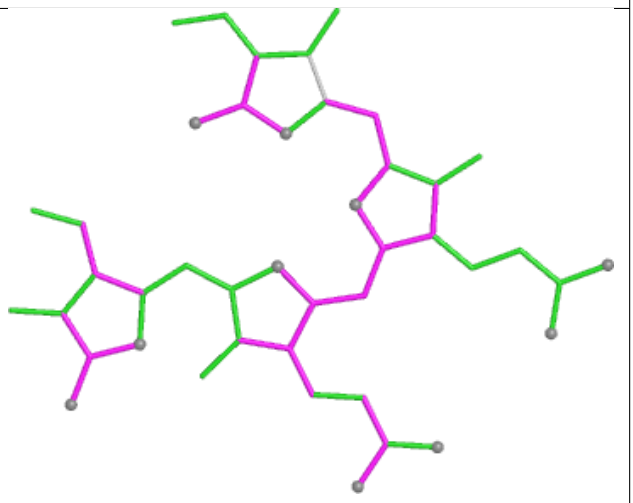


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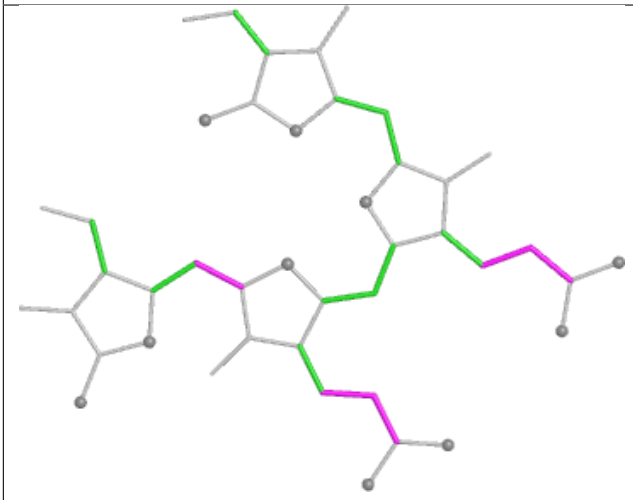
Ligand PEB HE 1002



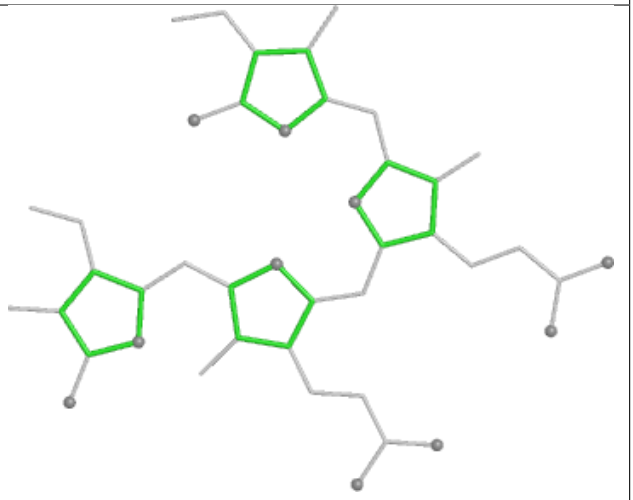
Bond lengths



Bond angles

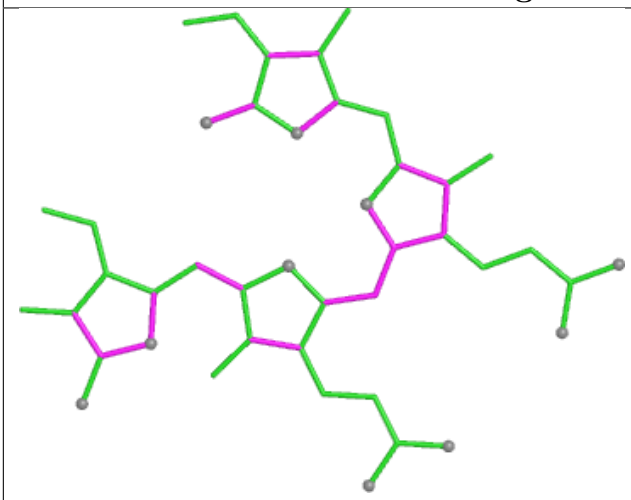


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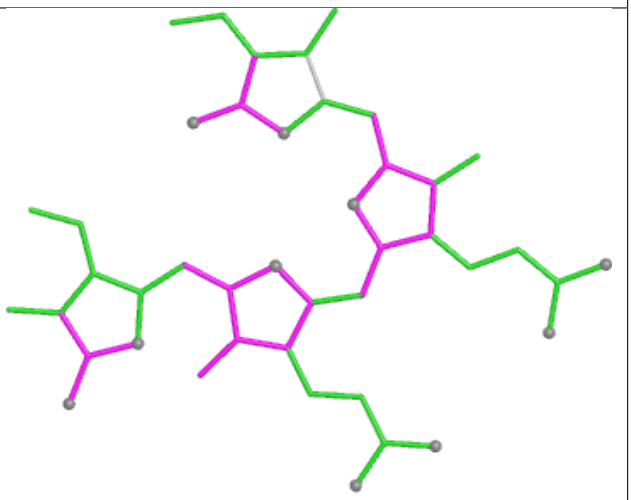


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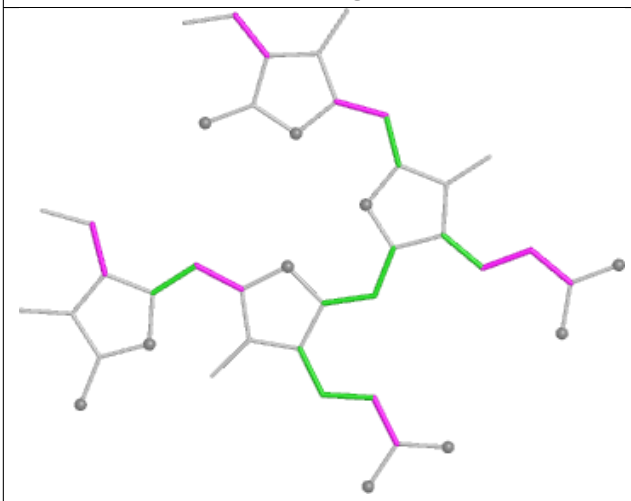
Ligand PEB A7 202



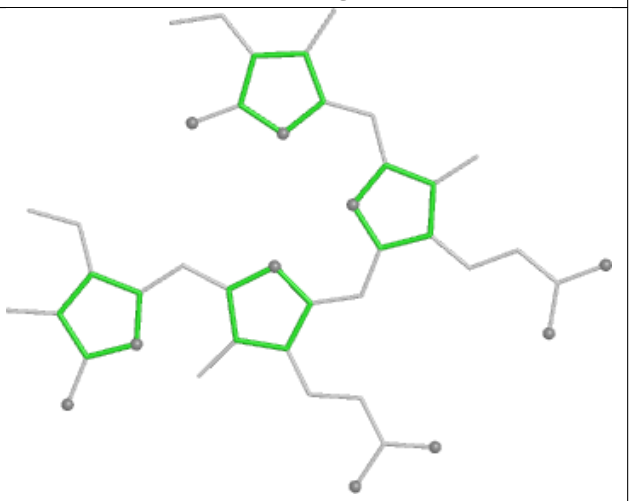
Bond lengths



Bond angles

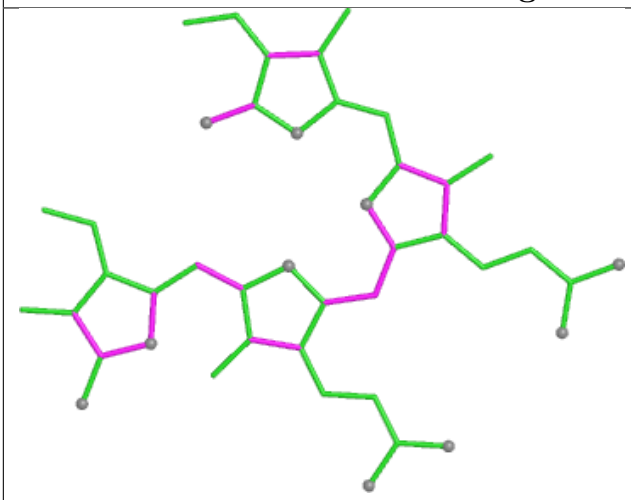


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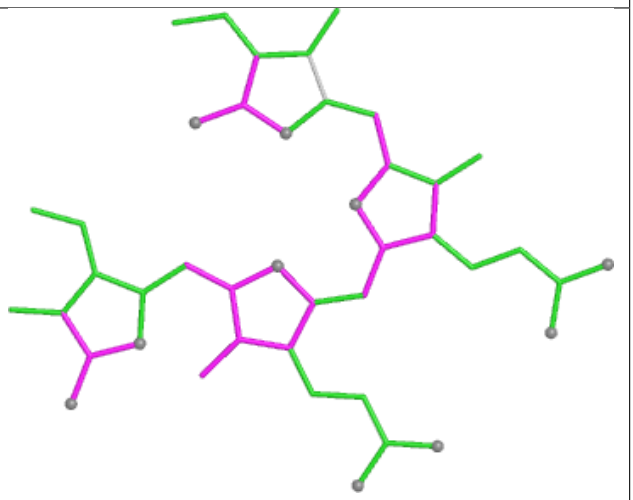


Rings

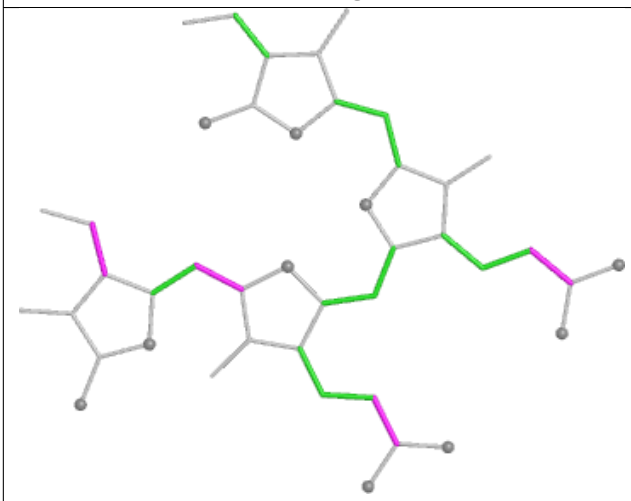
Ligand PEB S7 202



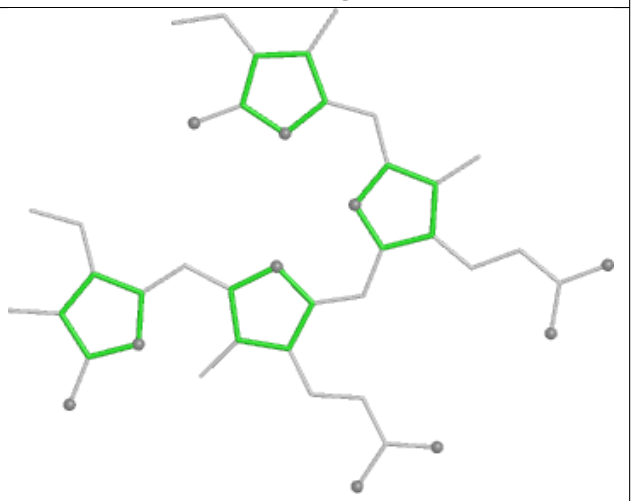
Bond lengths



Bond angles

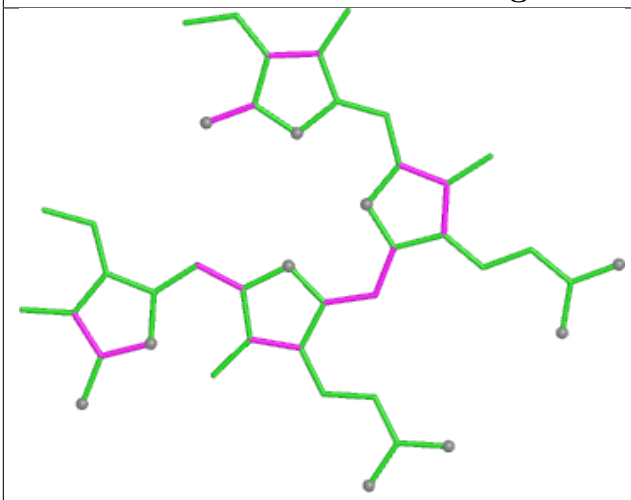


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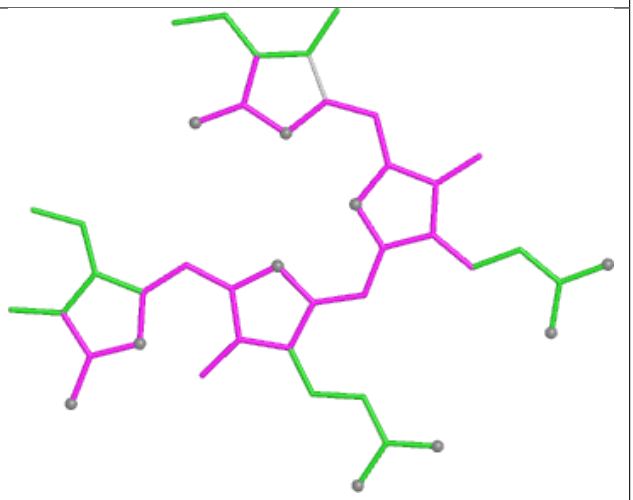


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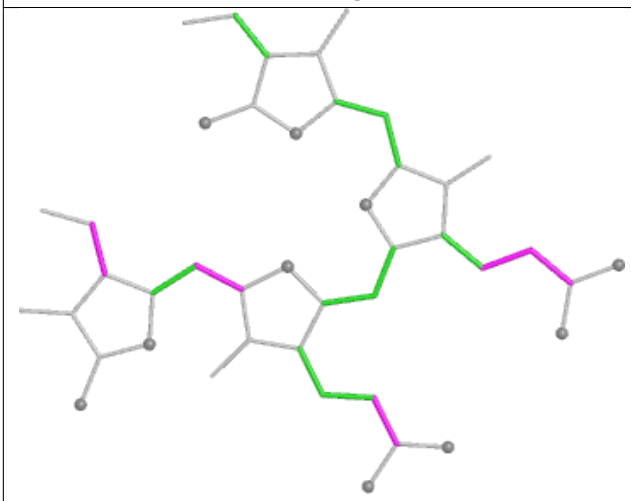
Ligand PEB NA 202



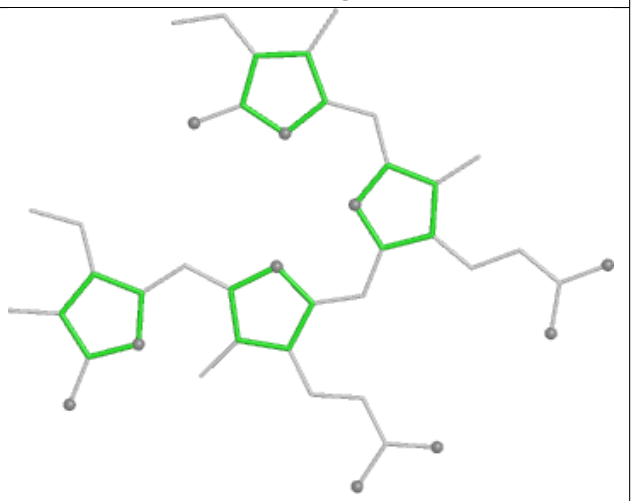
Bond lengths



Bond angles

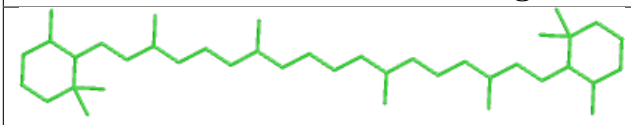


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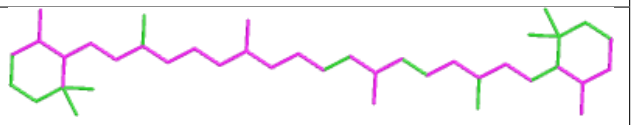


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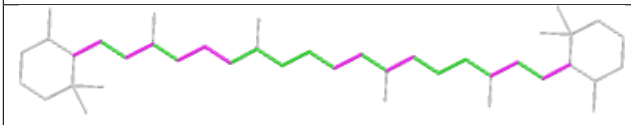
Ligand BCR B2 842



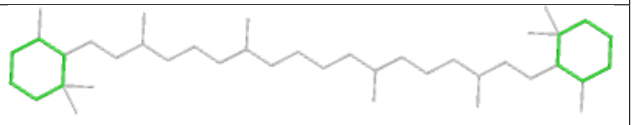
Bond lengths



Bond angles

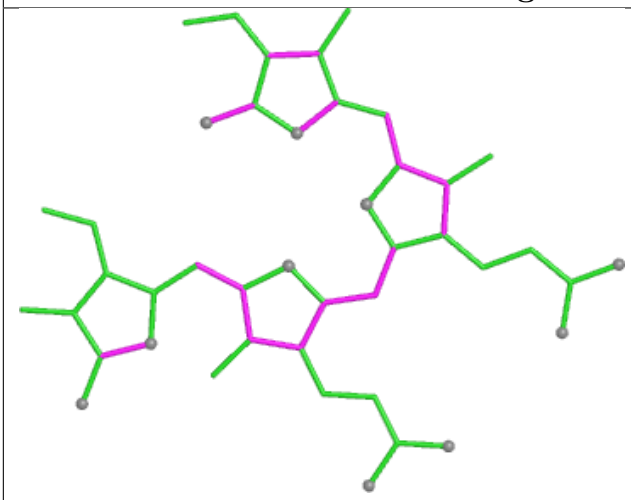


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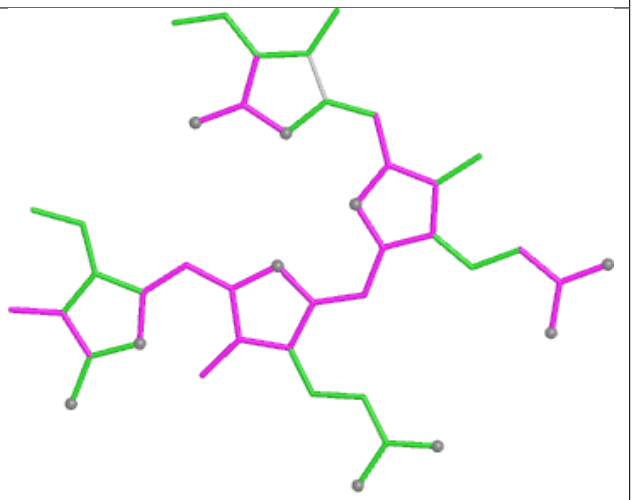


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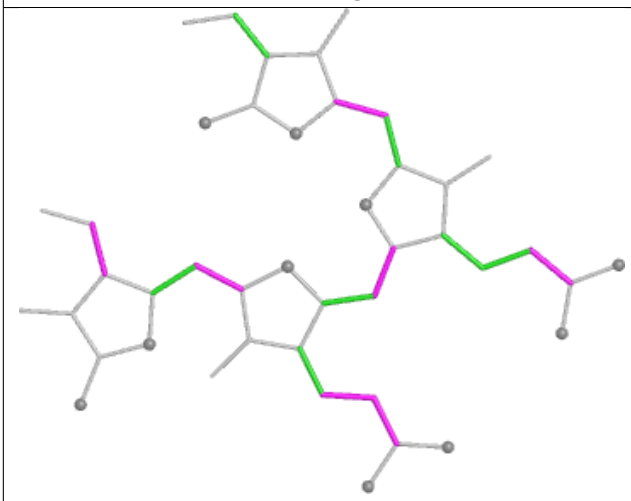
Ligand PEB oF 201



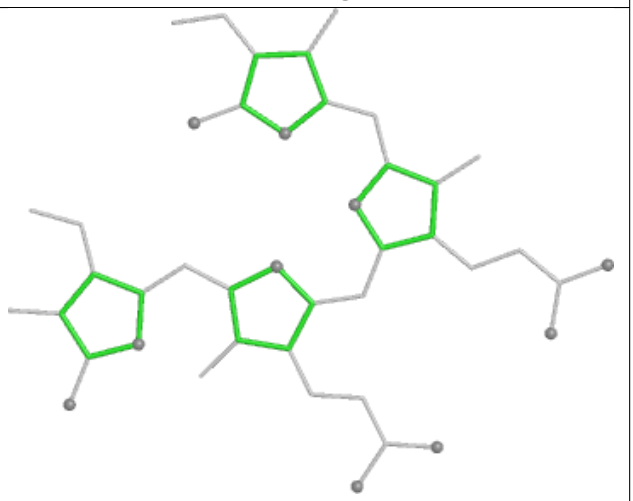
Bond lengths



Bond angles

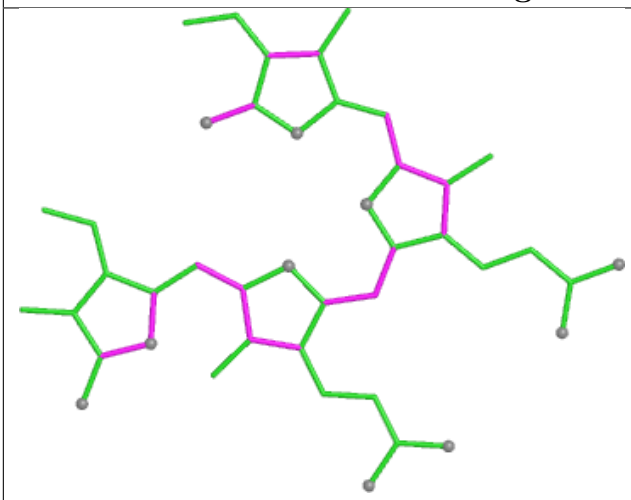


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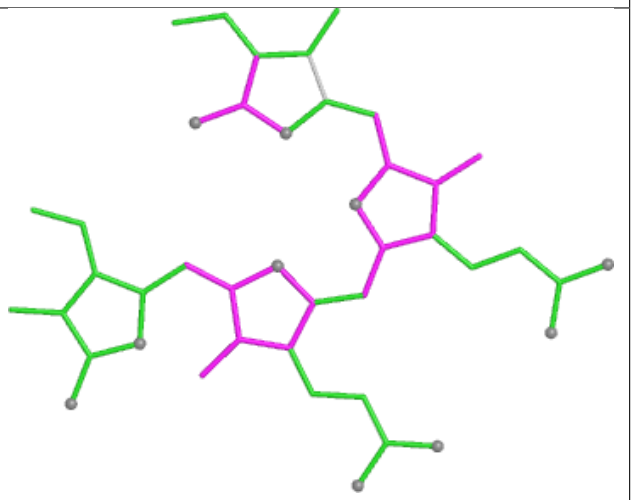


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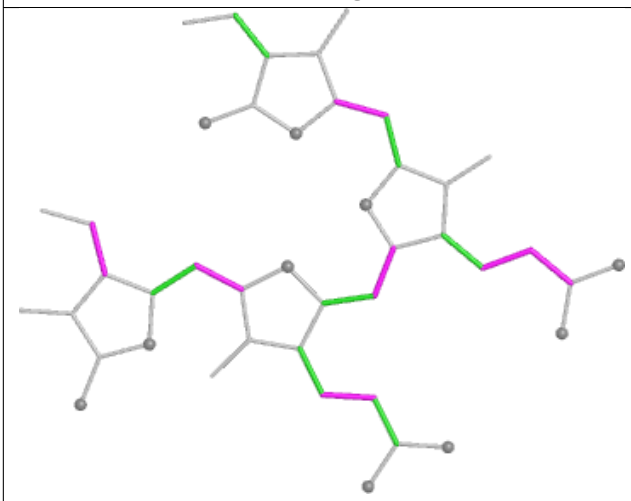
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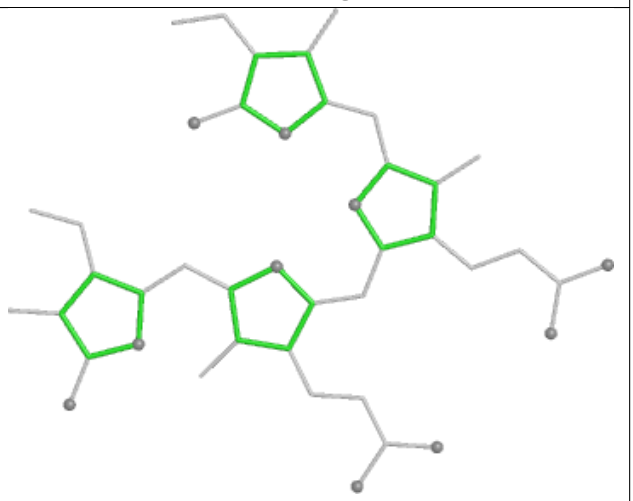
Bond lengths



Bond angles

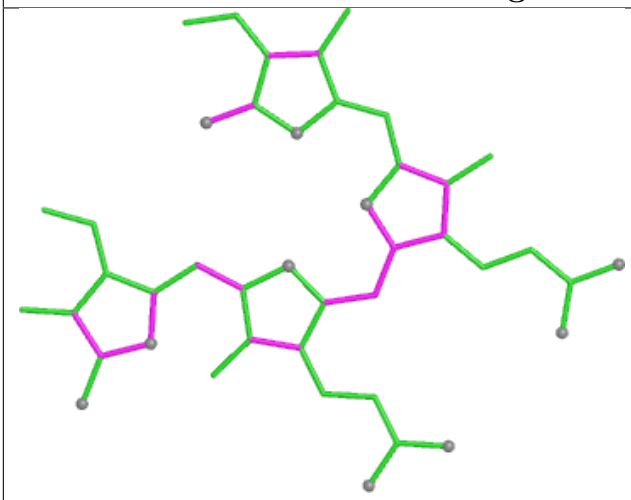


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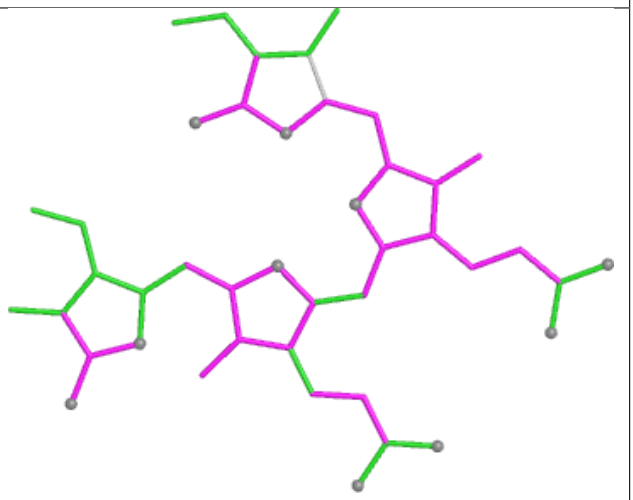


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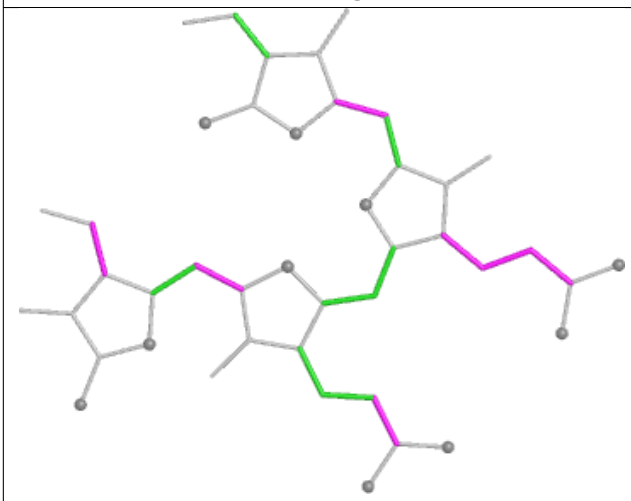
Ligand PEB BM 301



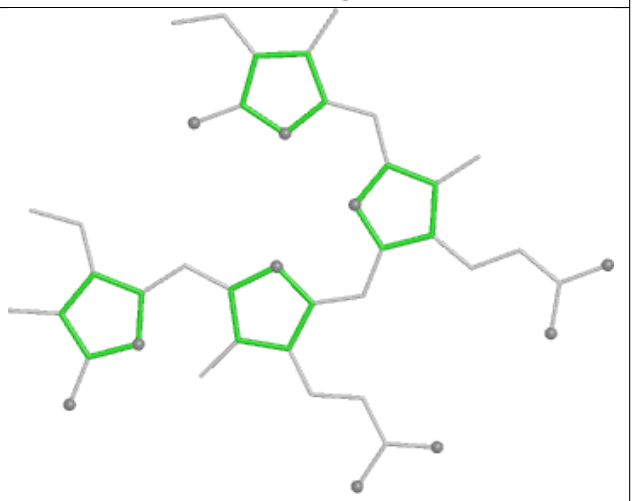
Bond lengths



Bond angles

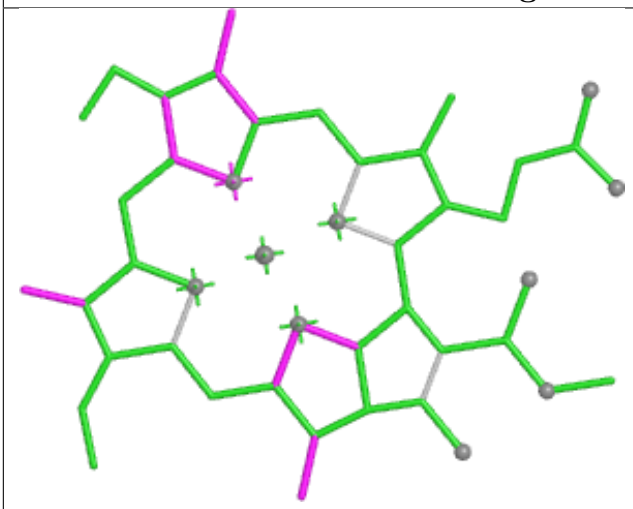


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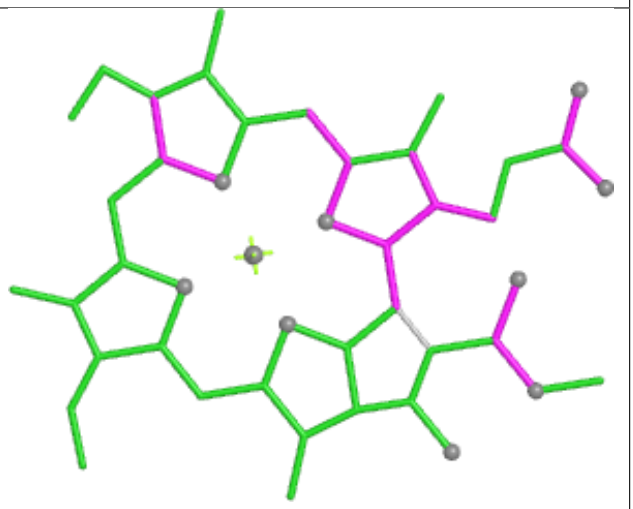


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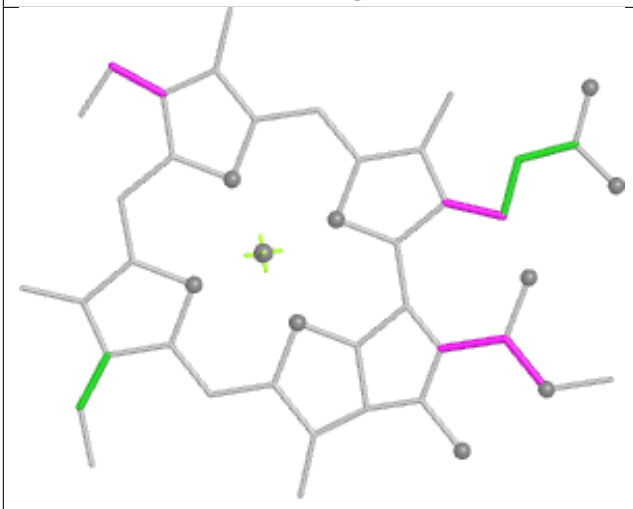
Ligand CLA 32 313



Bond lengths



Bond angles

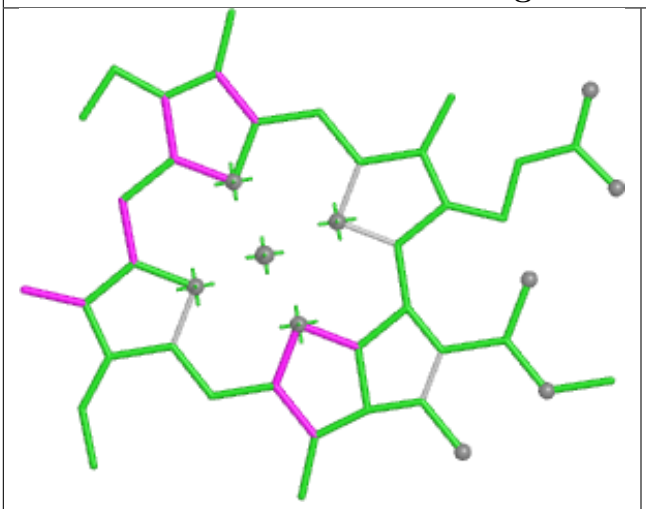


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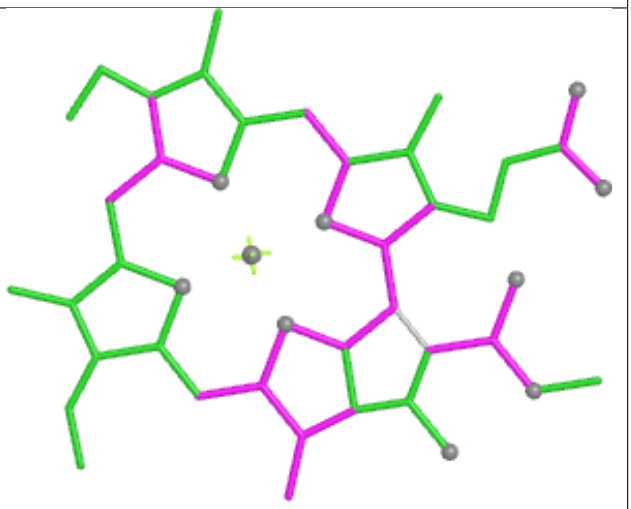


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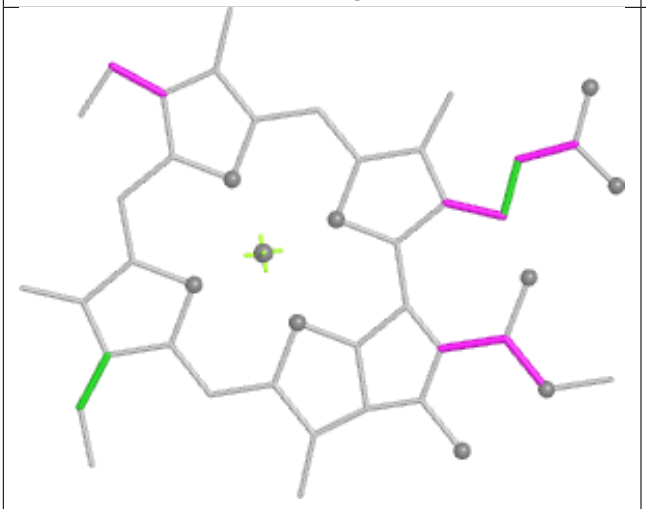
Ligand CLA 6N 612



Bond lengths



Bond angles

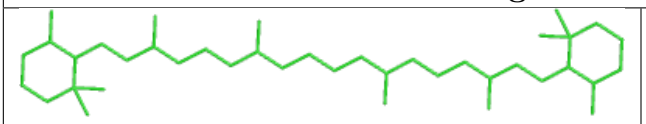


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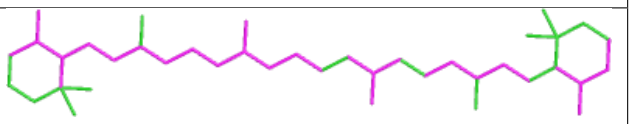


Rings

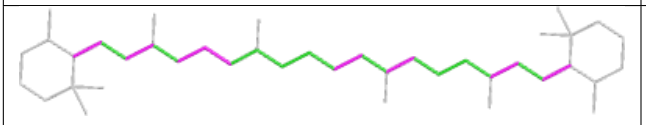
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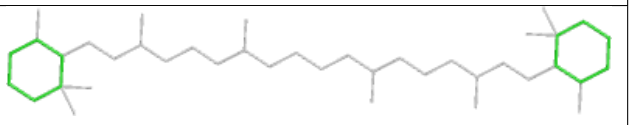
Bond lengths



Bond angles

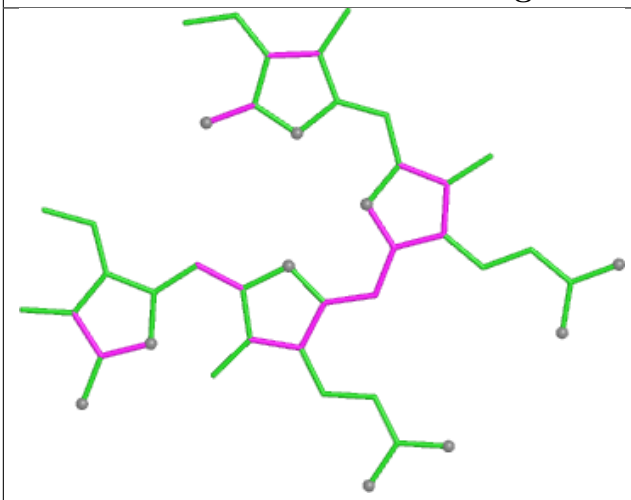


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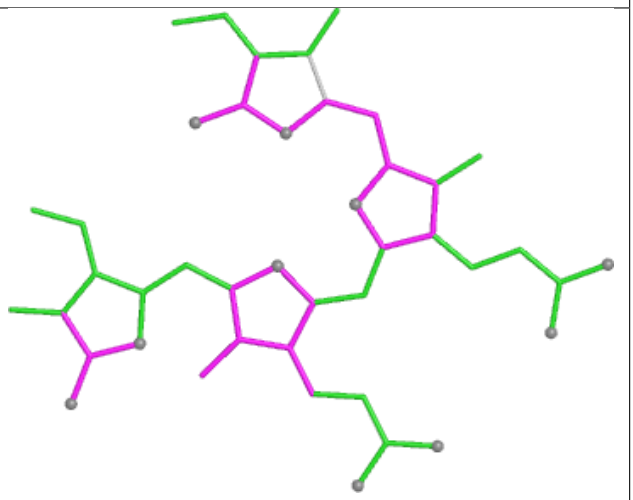


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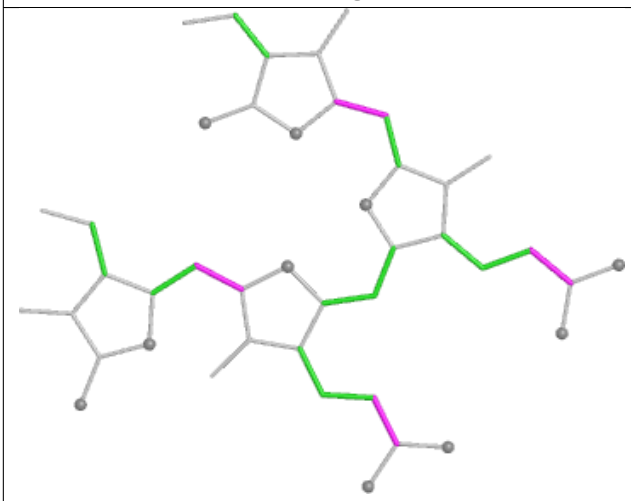
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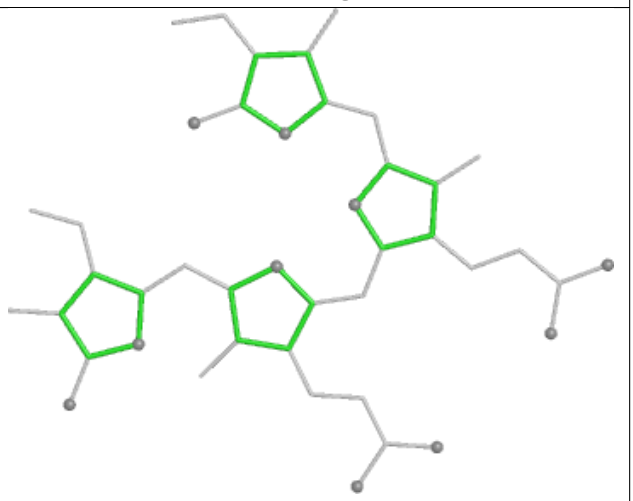
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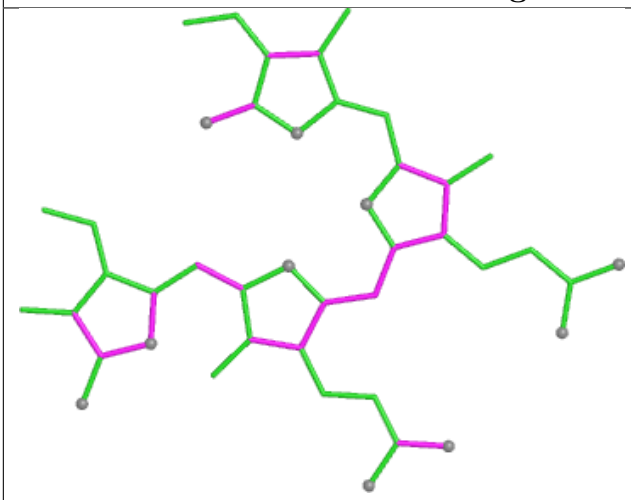


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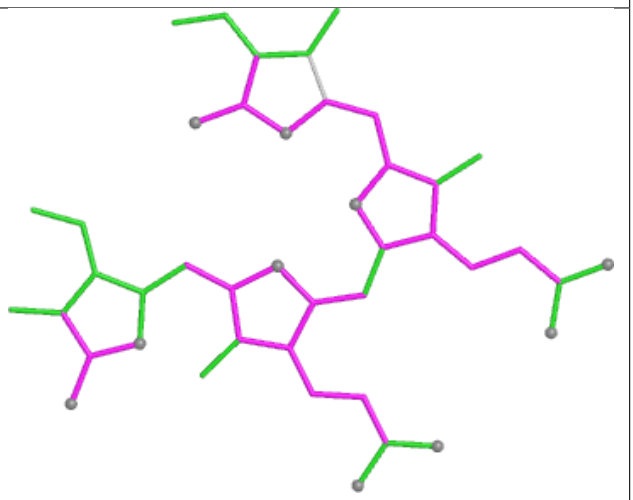


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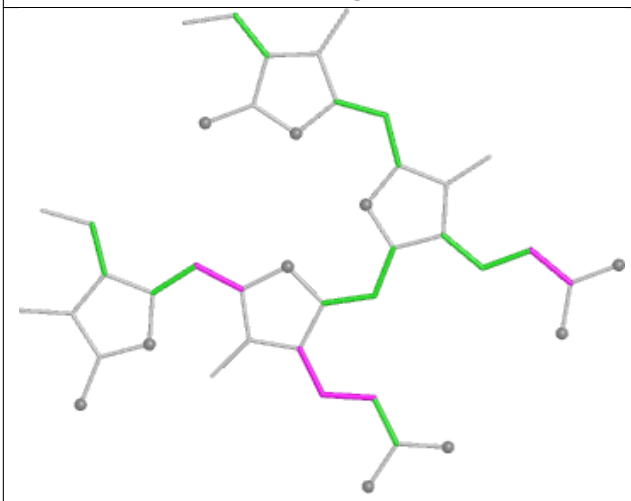
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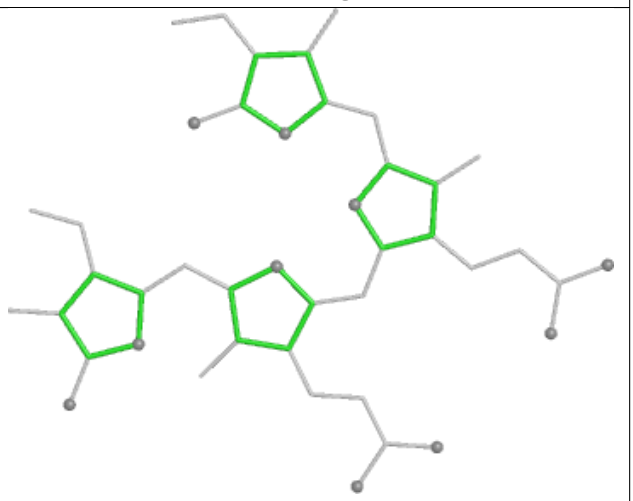
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Bond angles

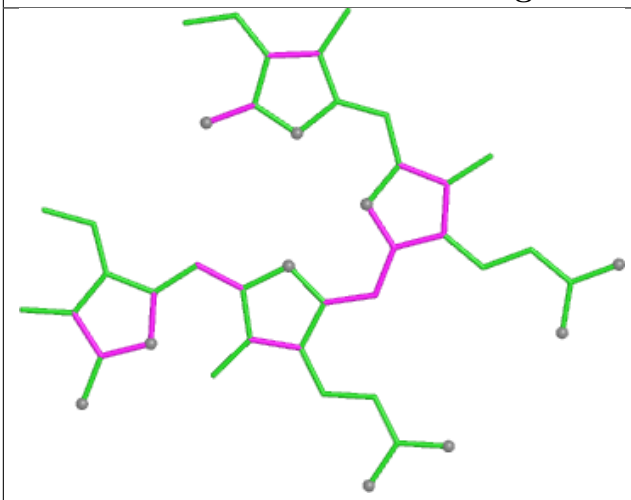


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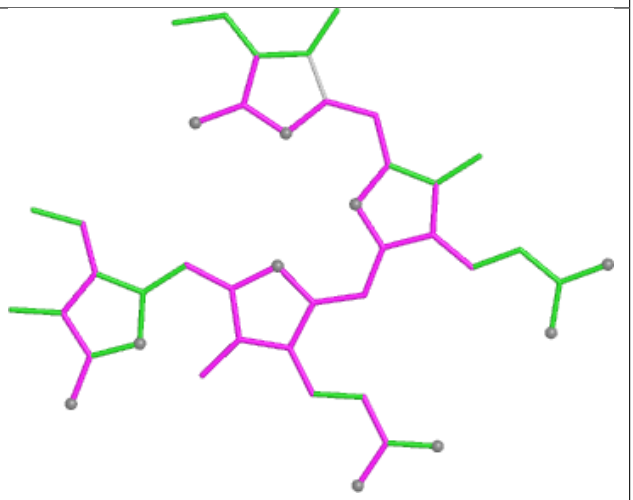


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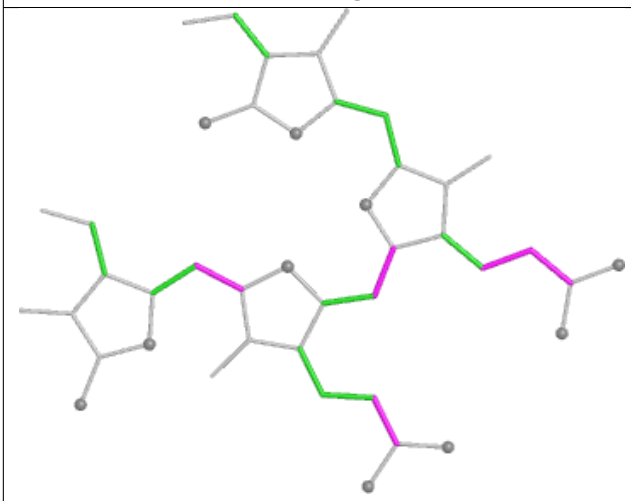
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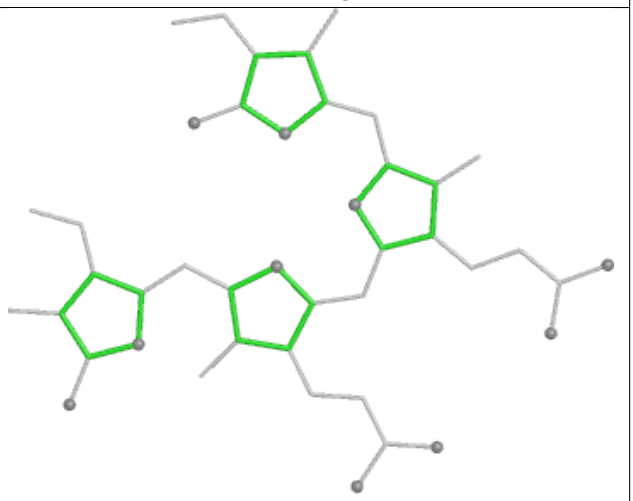
Bond lengths



Bond angles

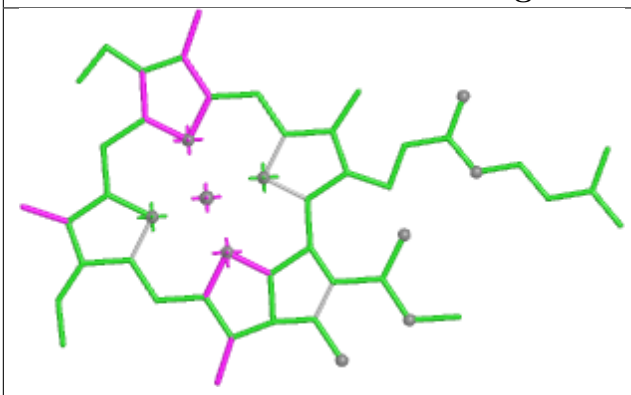


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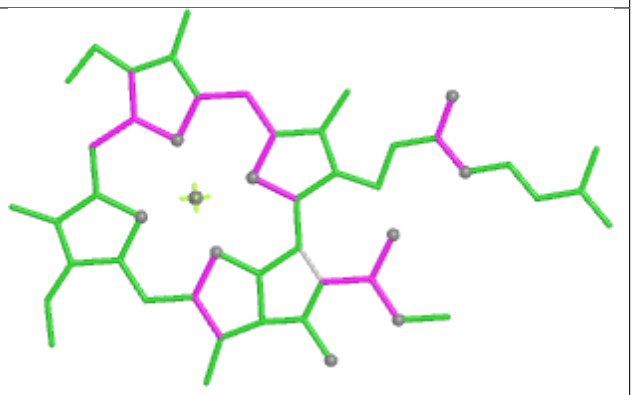


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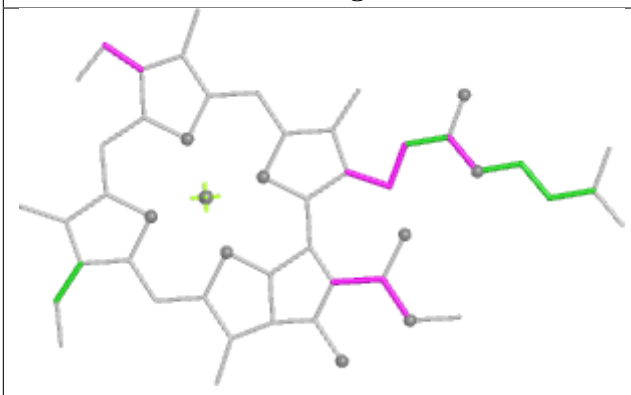
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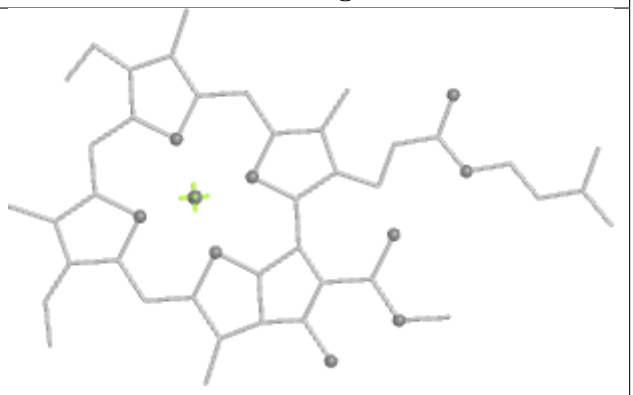
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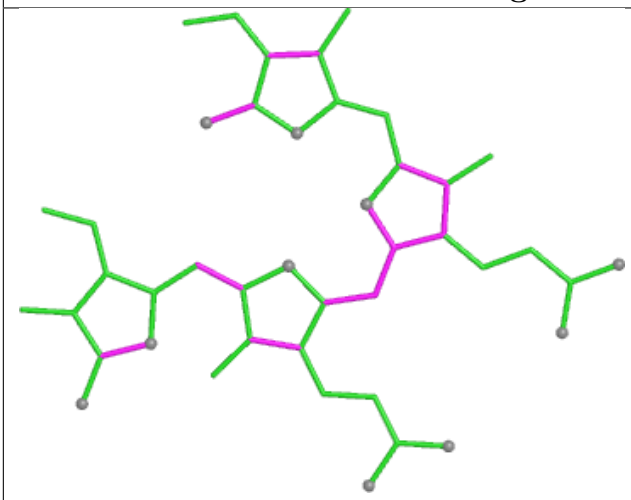


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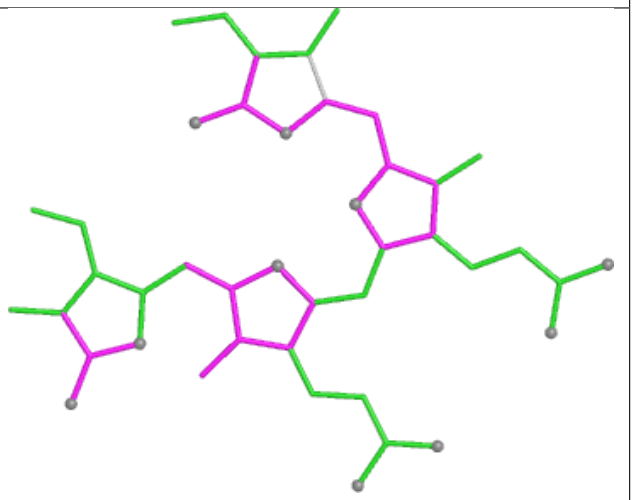


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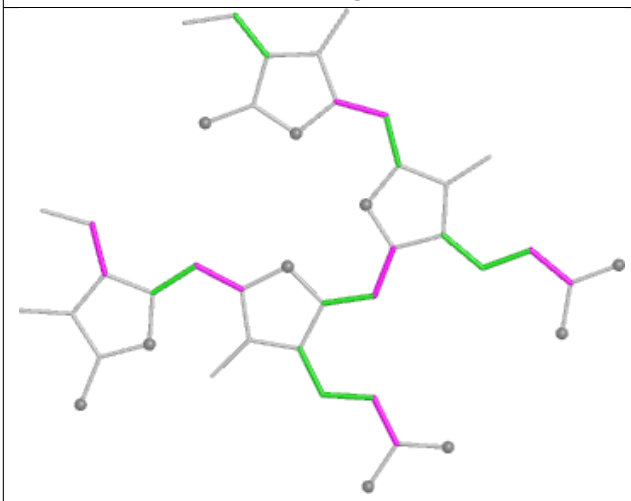
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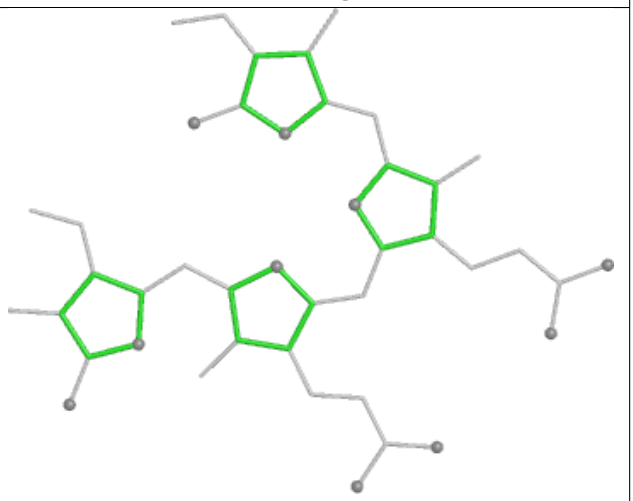
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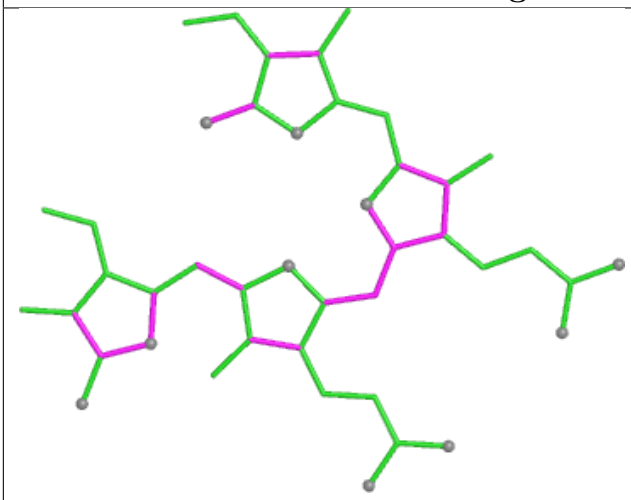


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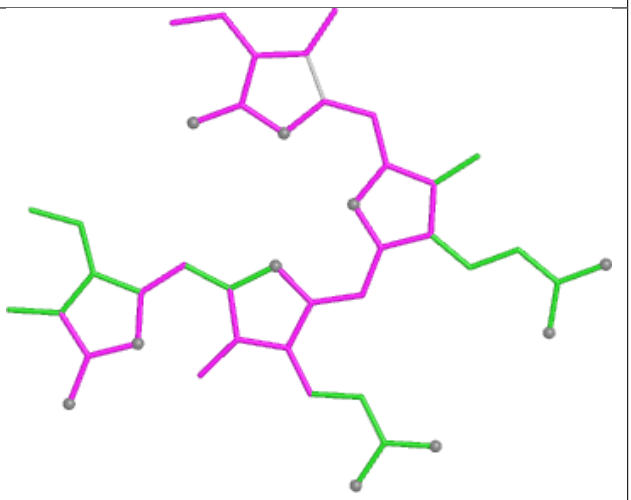


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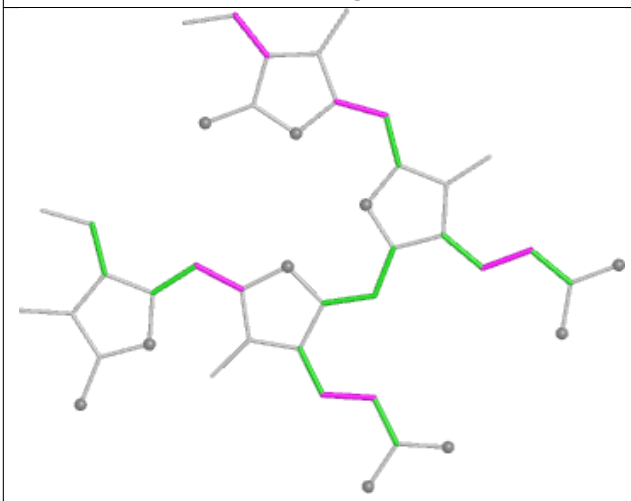
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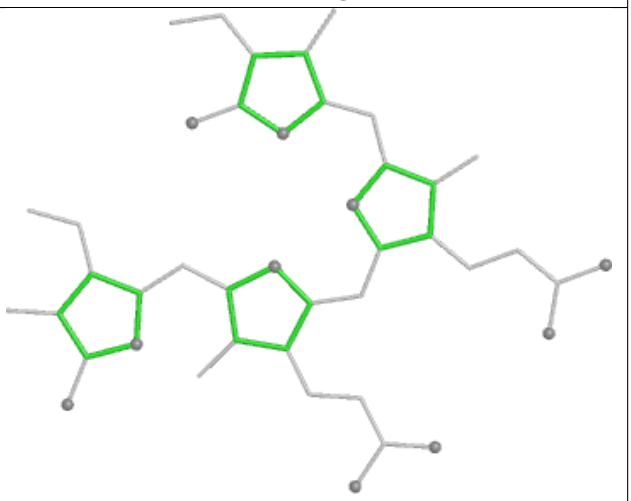
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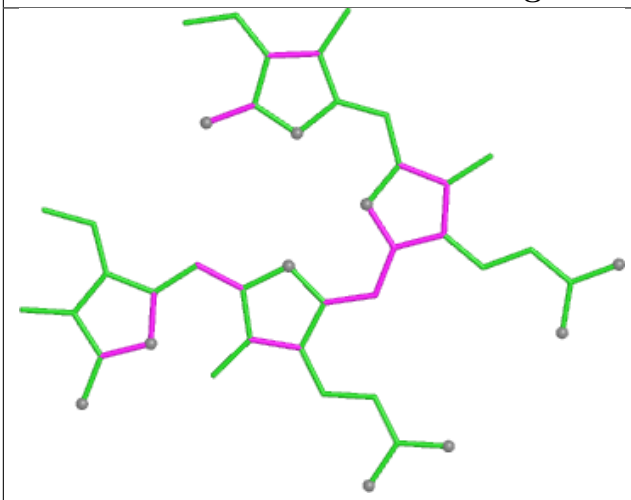


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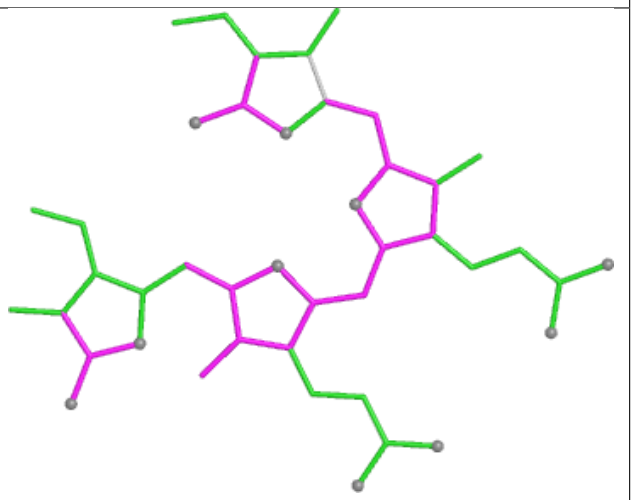


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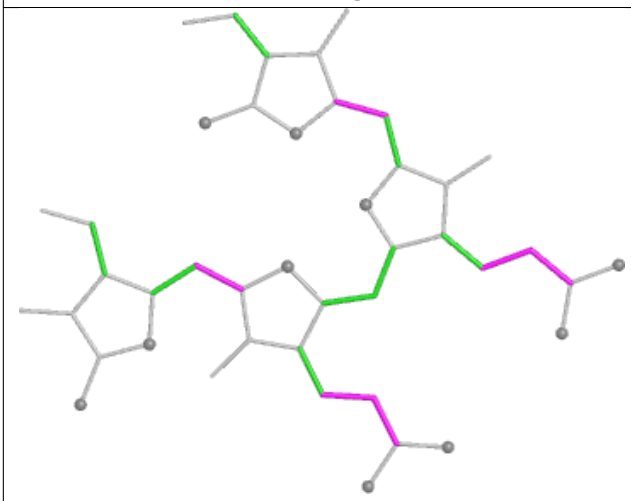
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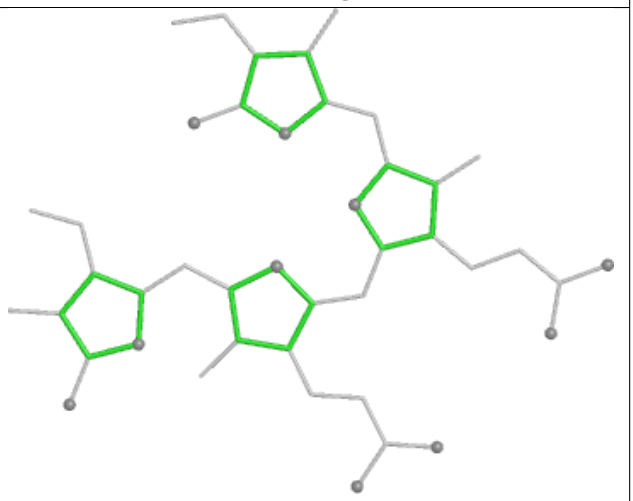
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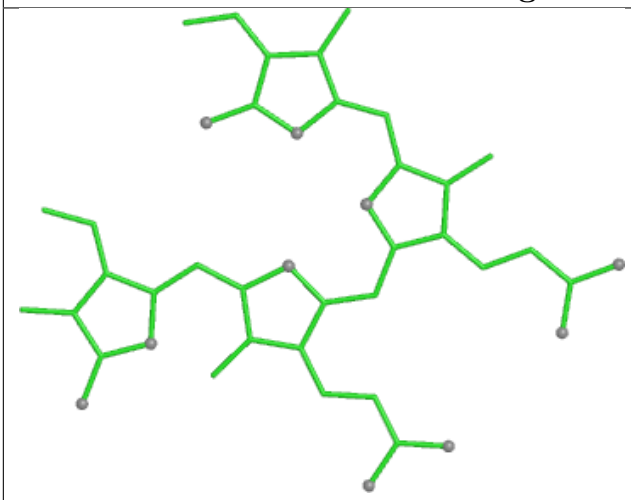


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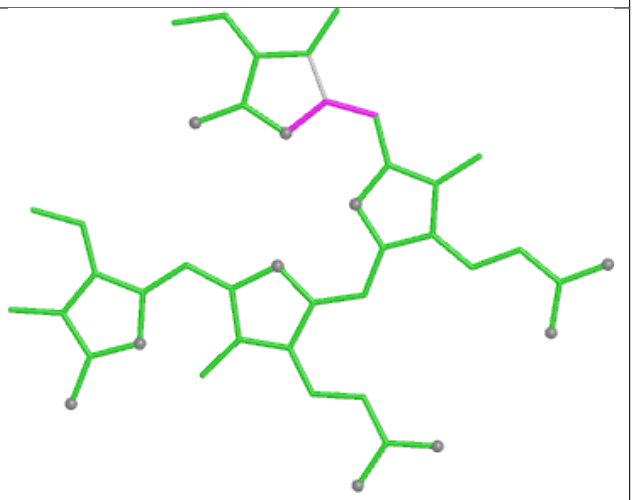


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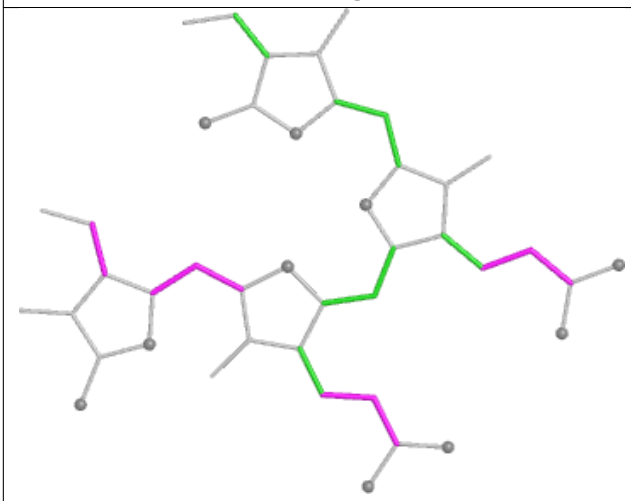
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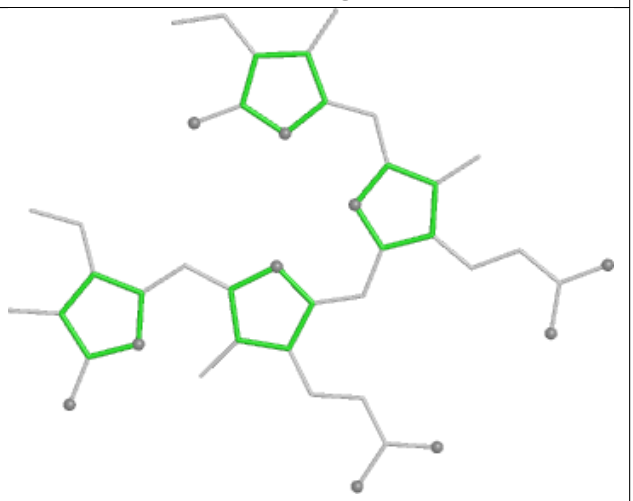
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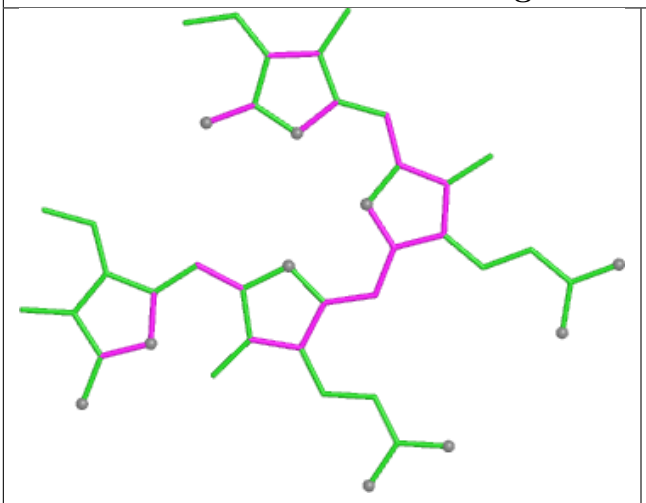


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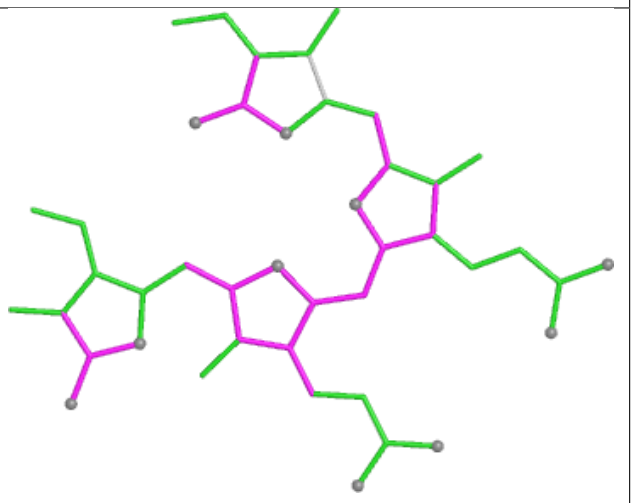


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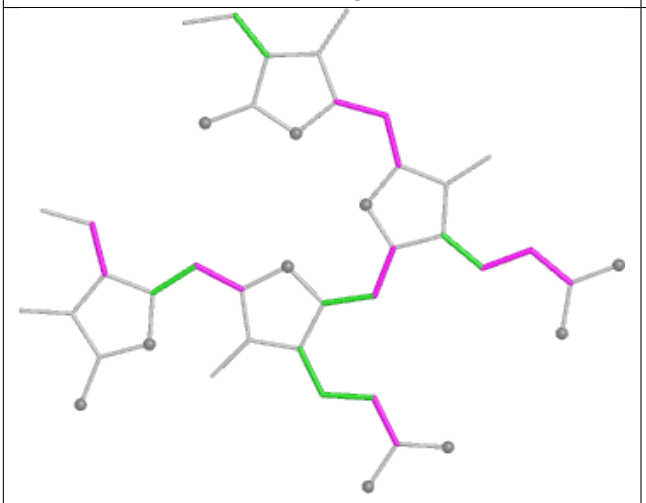
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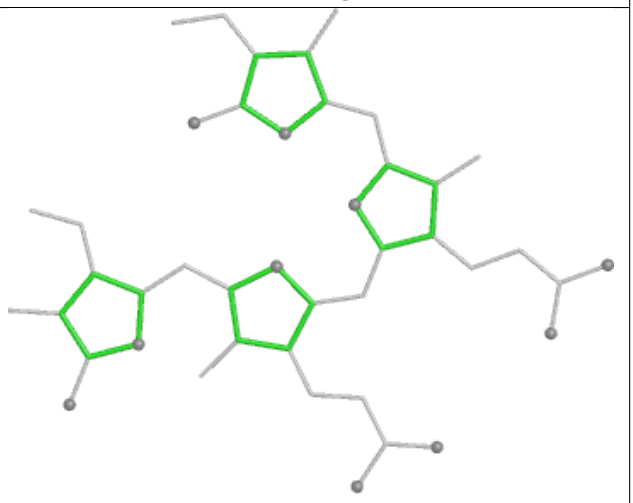
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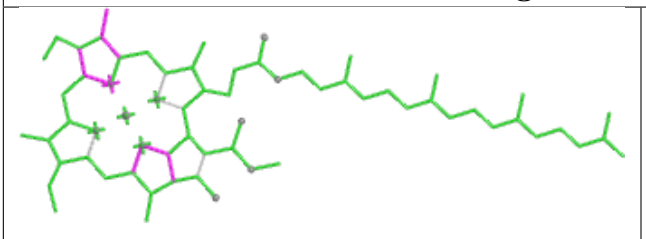


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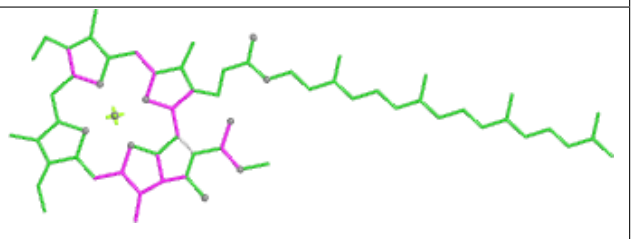


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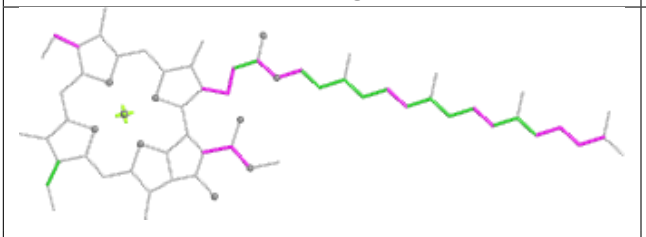
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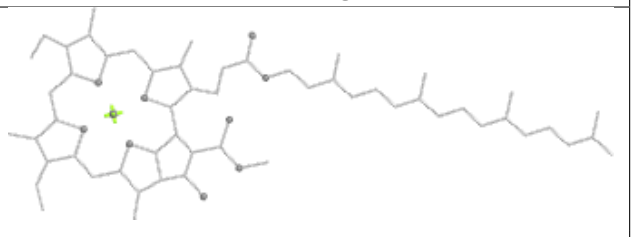
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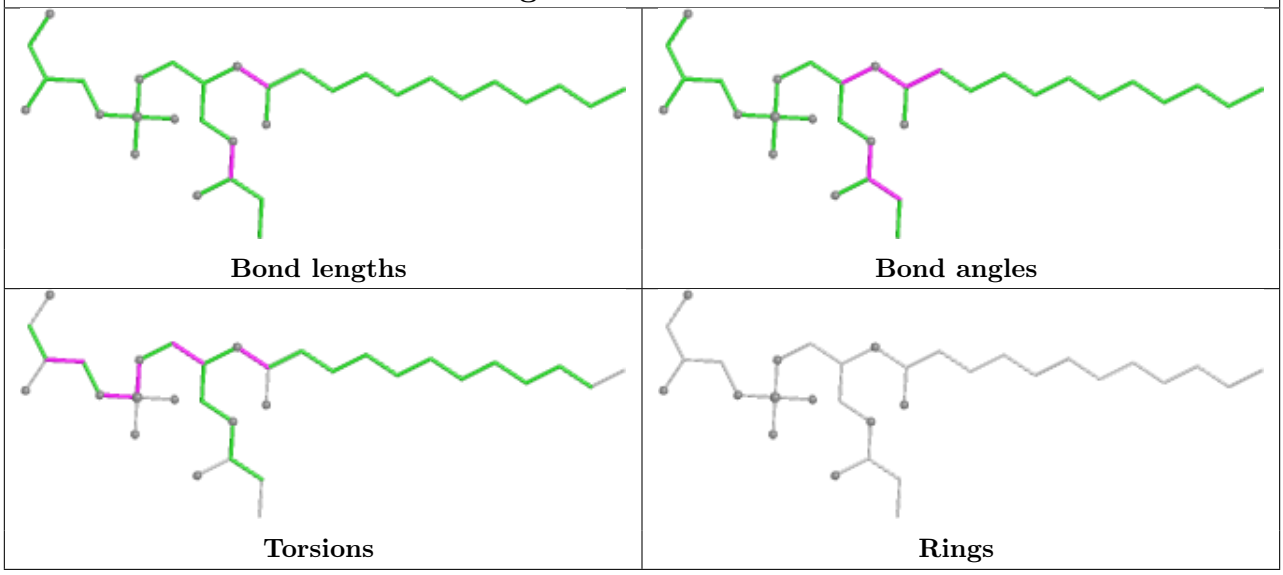


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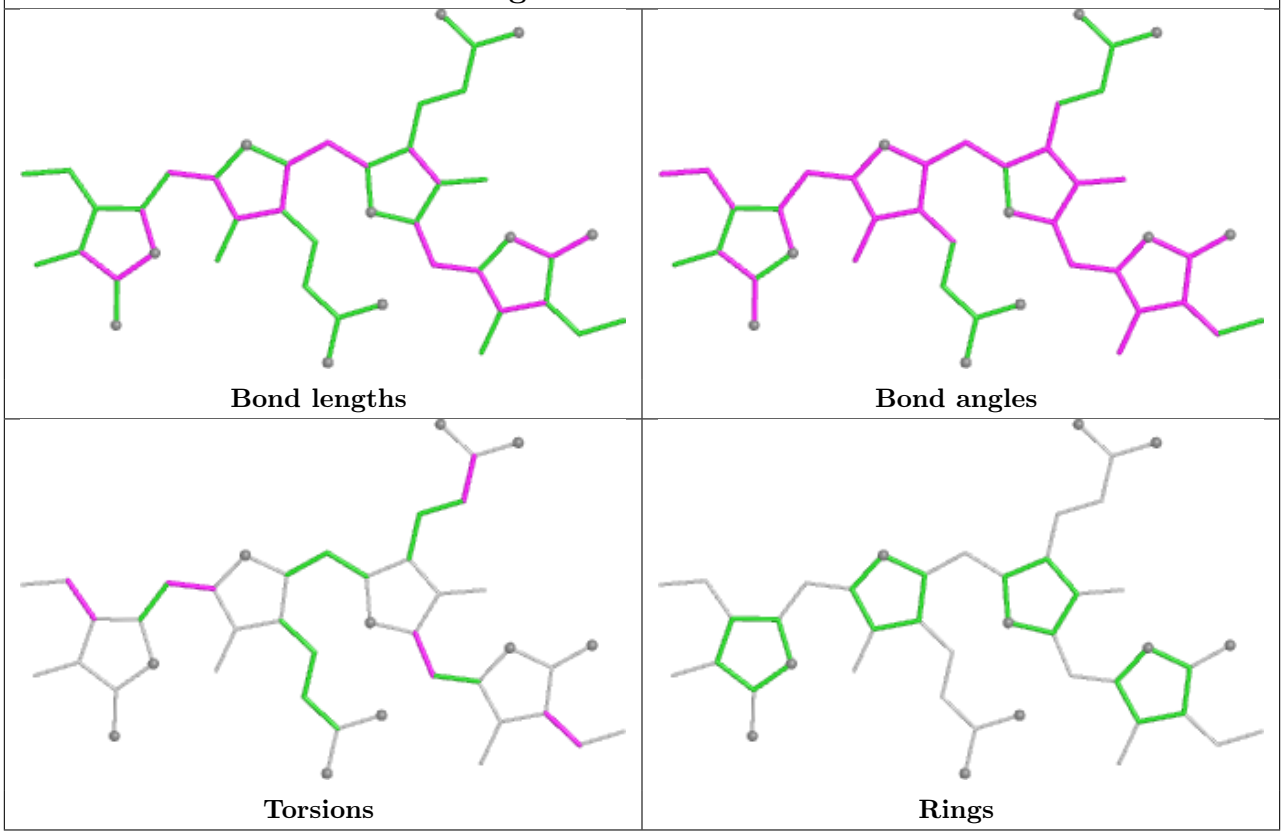


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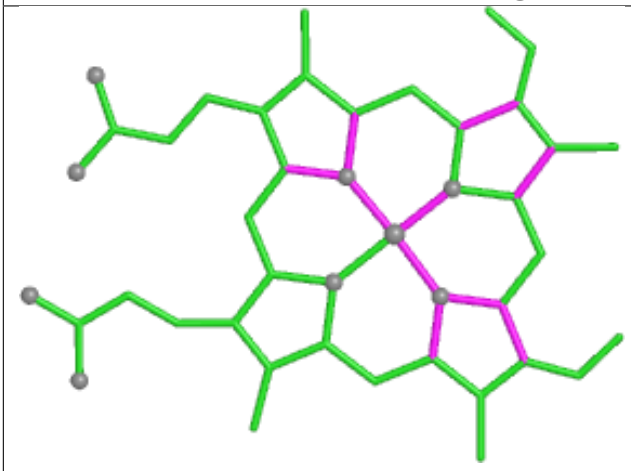
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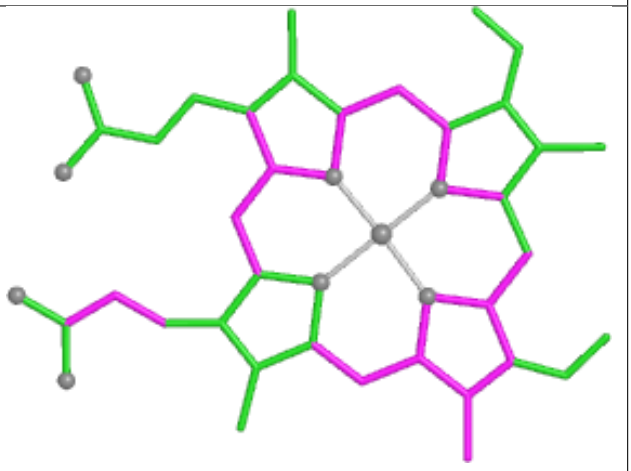
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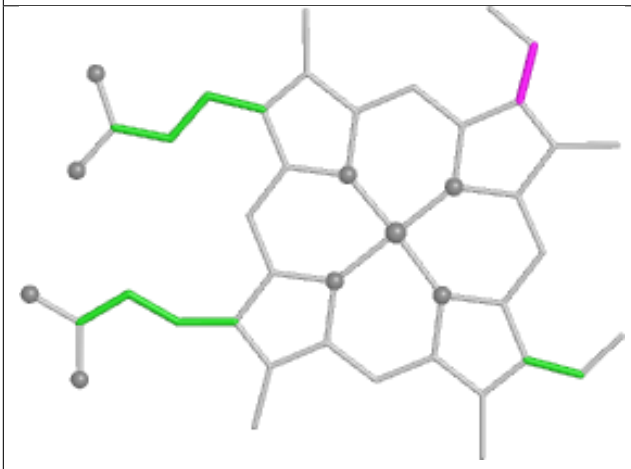
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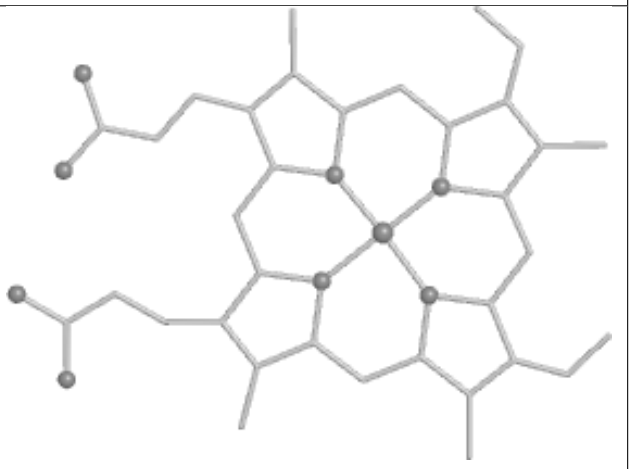
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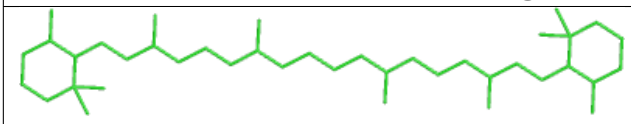


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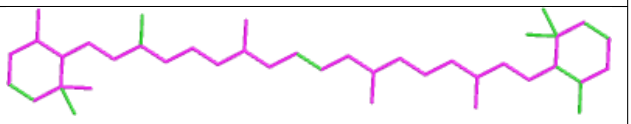


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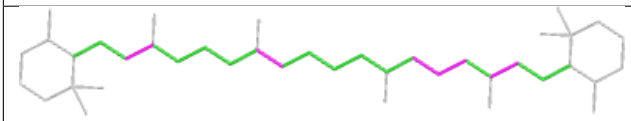
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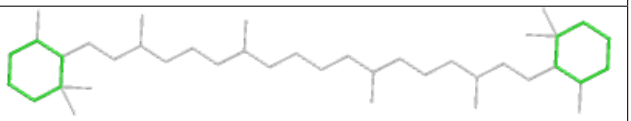
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Bond angles

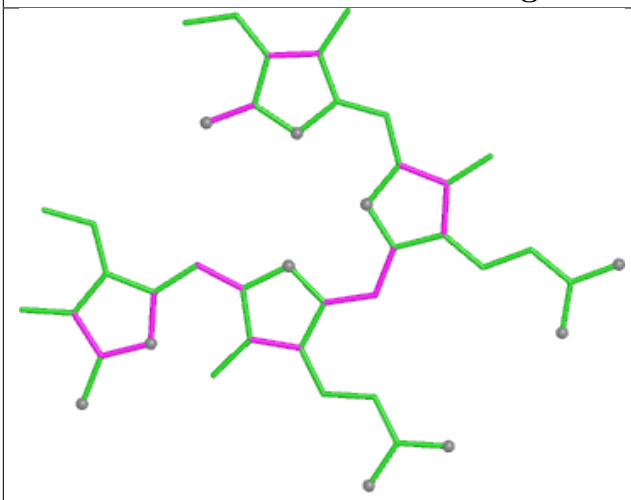


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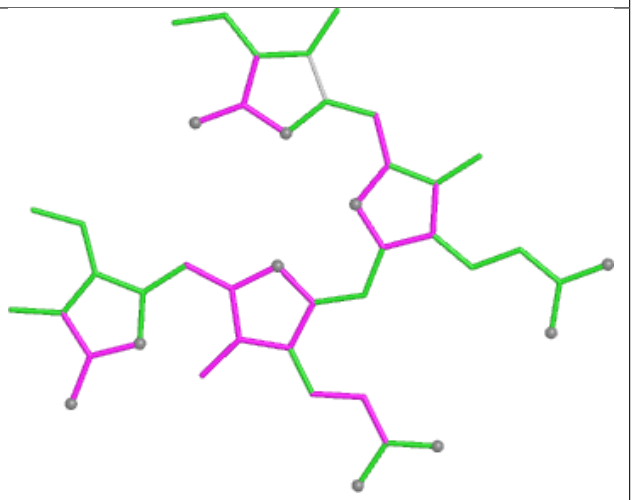


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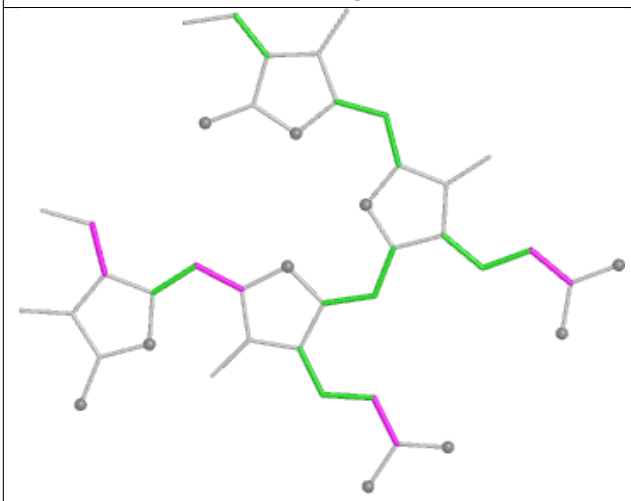
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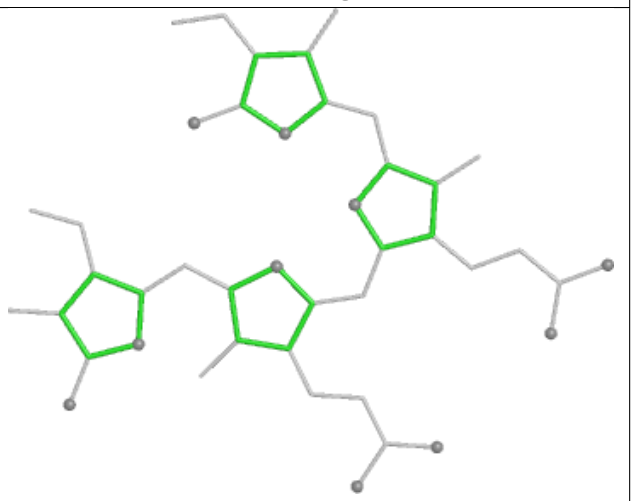
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Bond angles

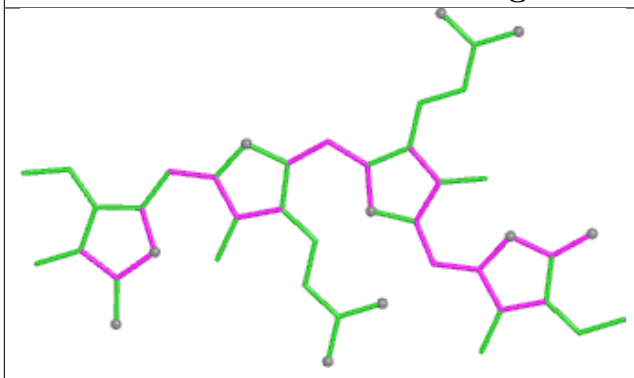


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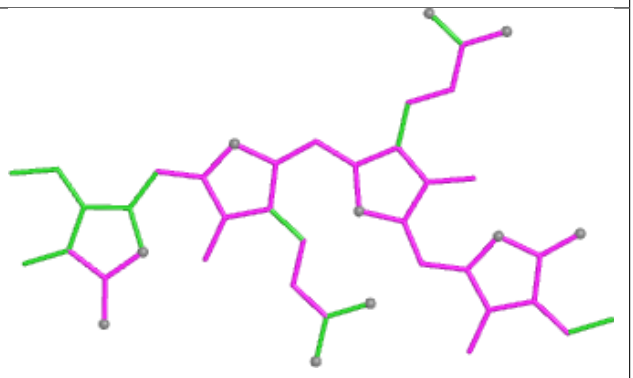


Rings

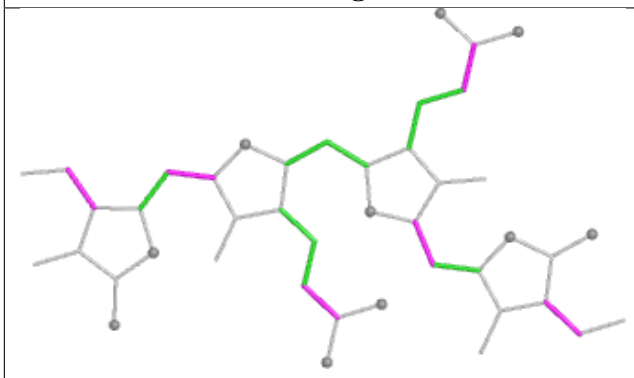
Ligand CYC J4 1001



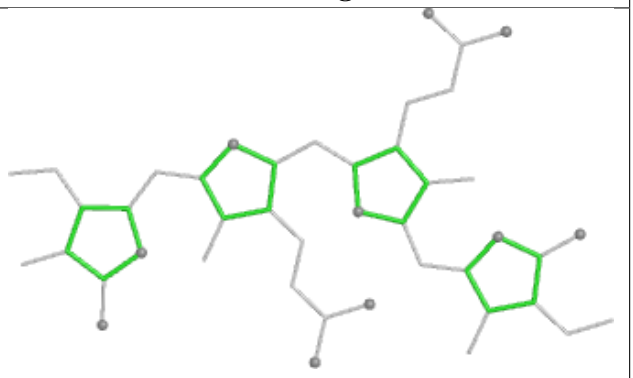
Bond lengths



Bond angles

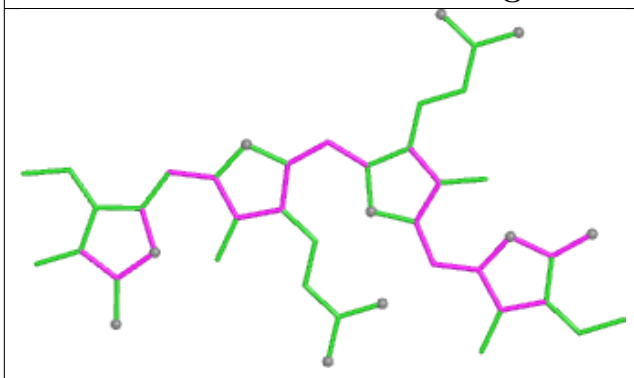


Torsions

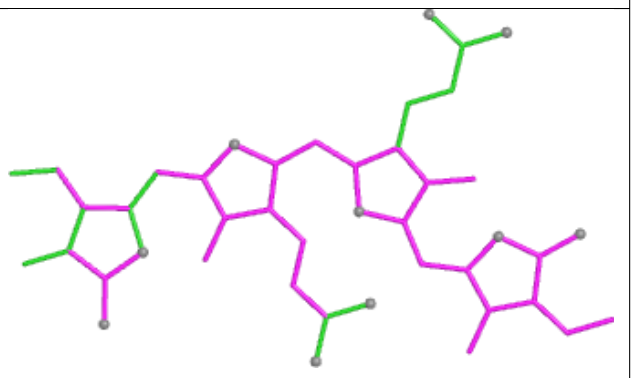


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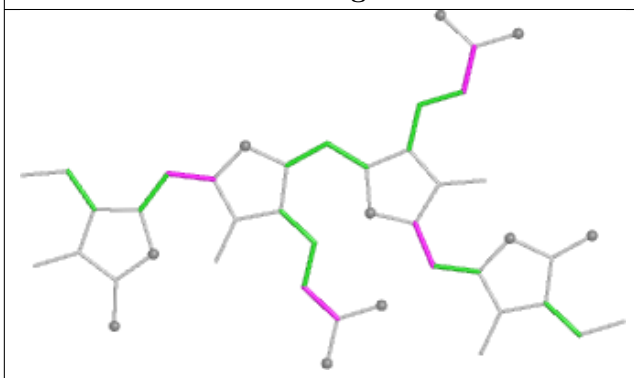
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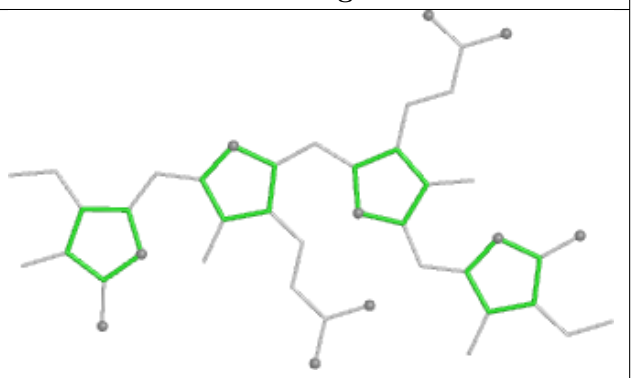
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Bond angles

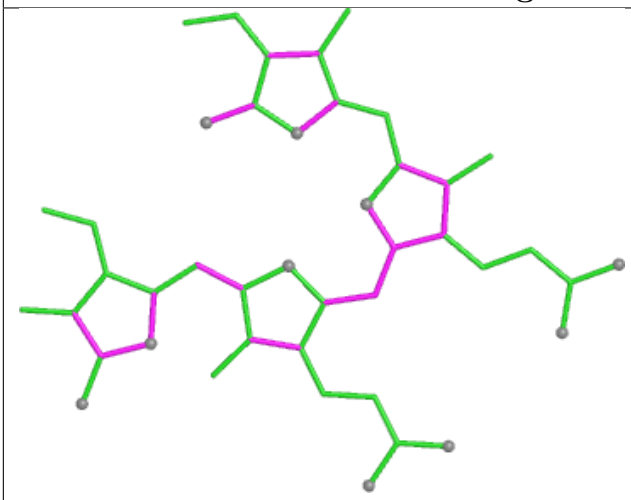


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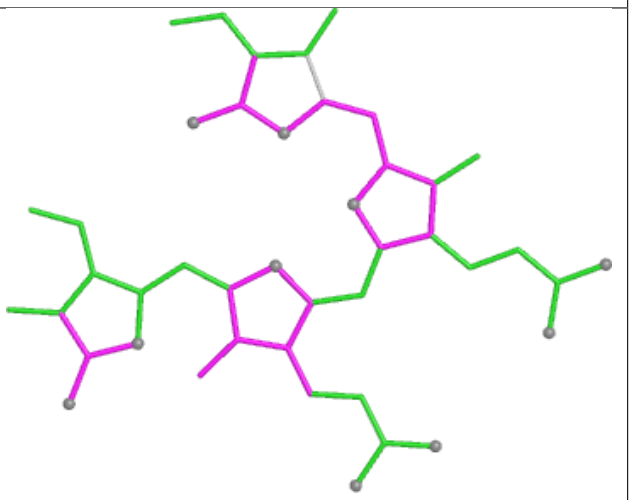


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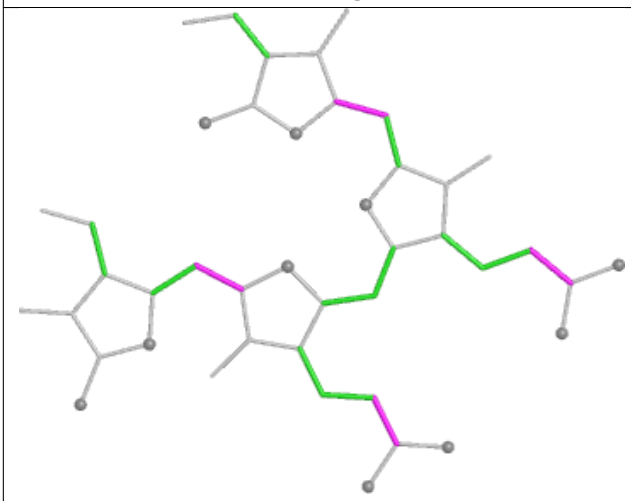
Ligand PEB T9 201



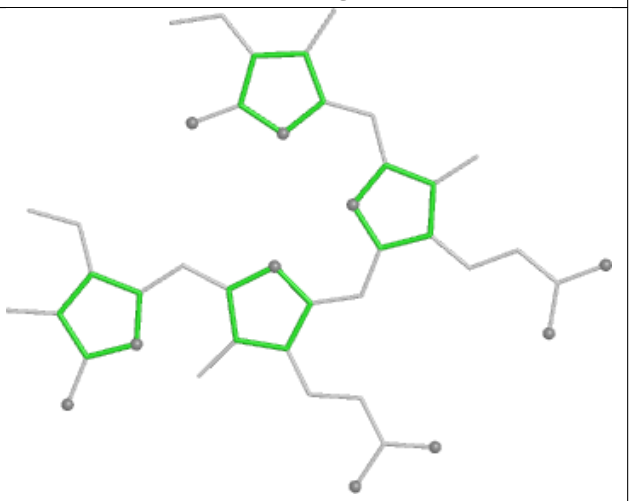
Bond lengths



Bond angles

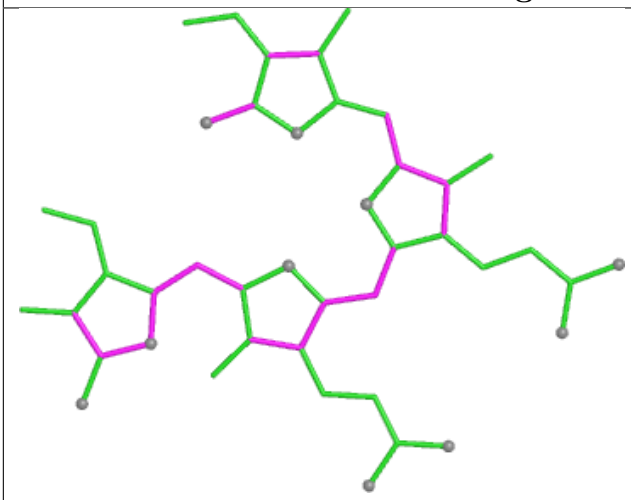


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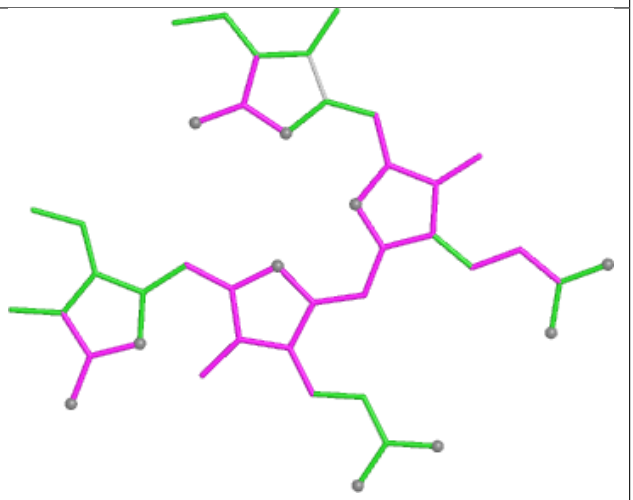


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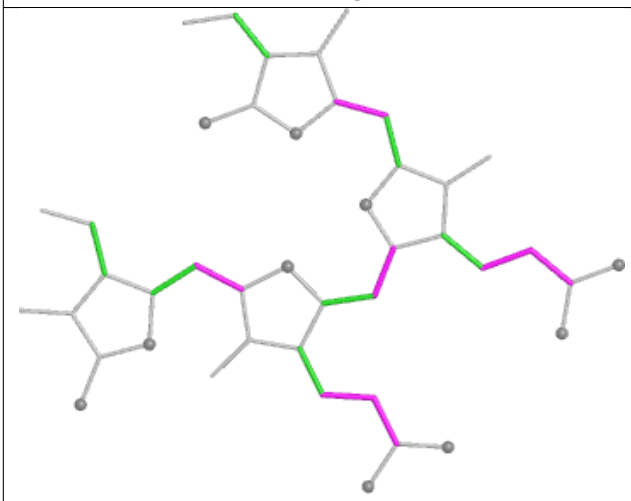
Ligand PEB eK 201



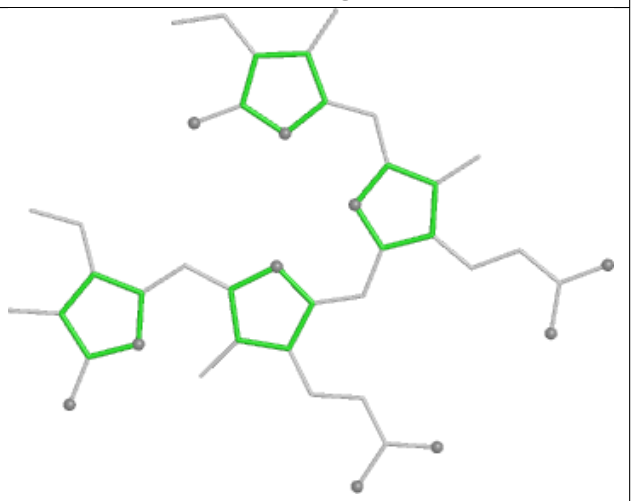
Bond lengths



Bond angles

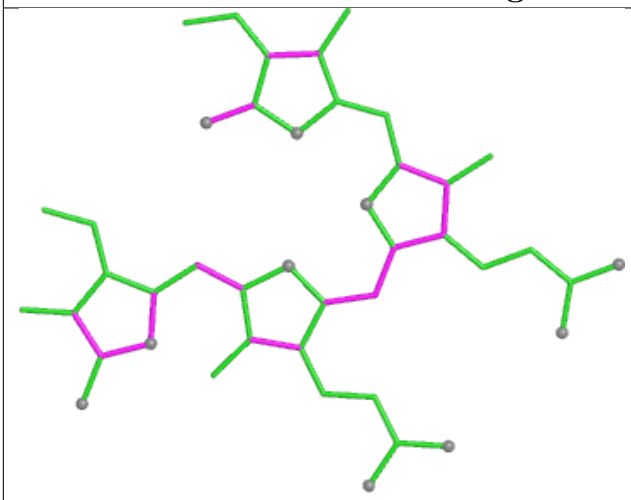


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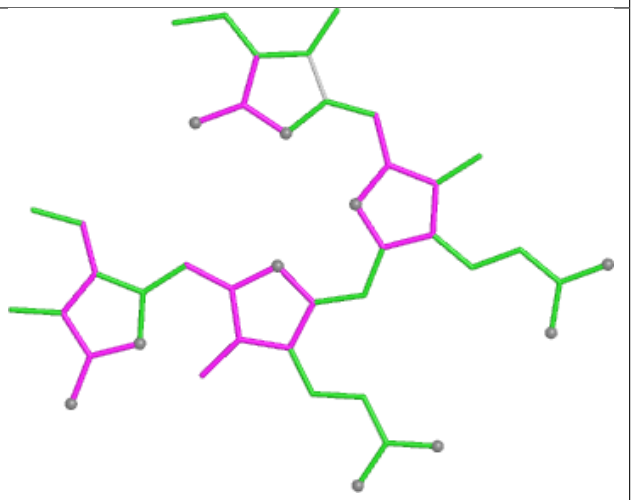


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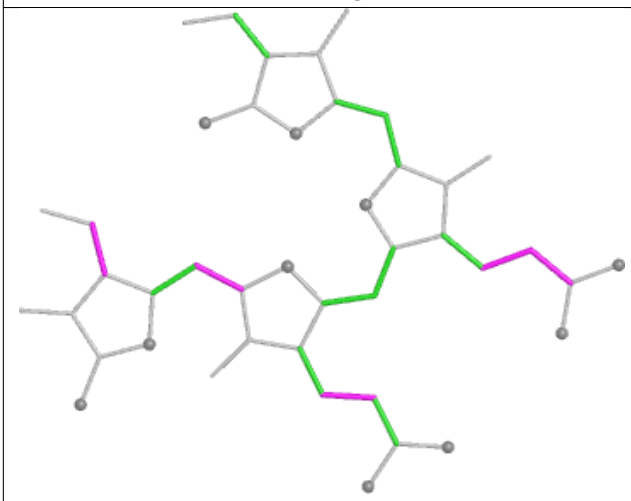
Ligand PEB GM 201



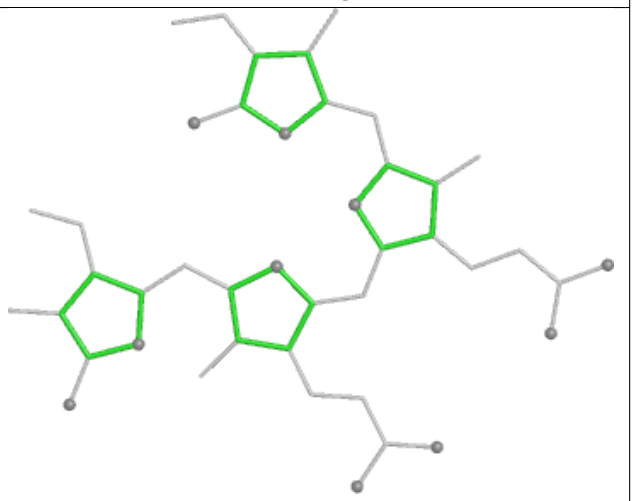
Bond lengths



Bond angles

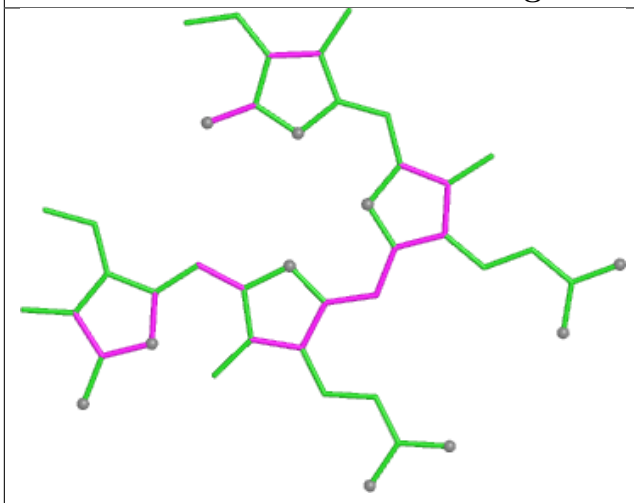


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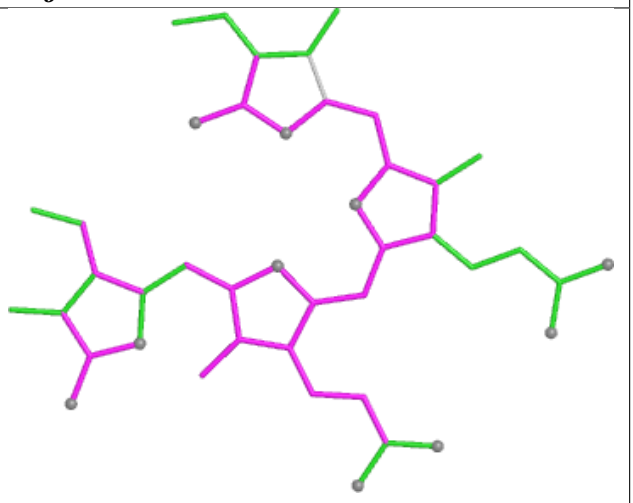


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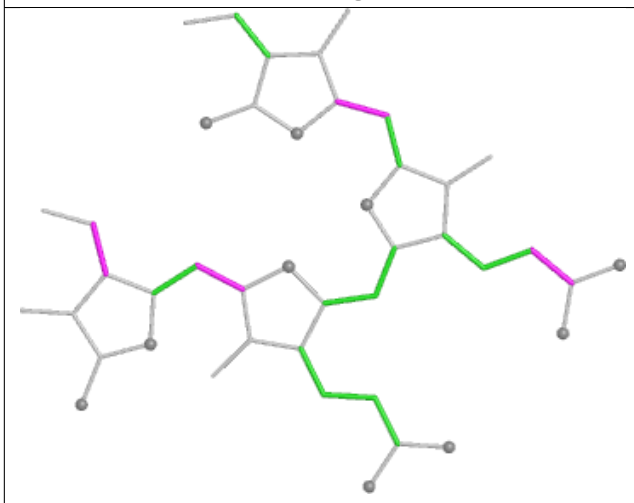
Ligand PEB jJ 203



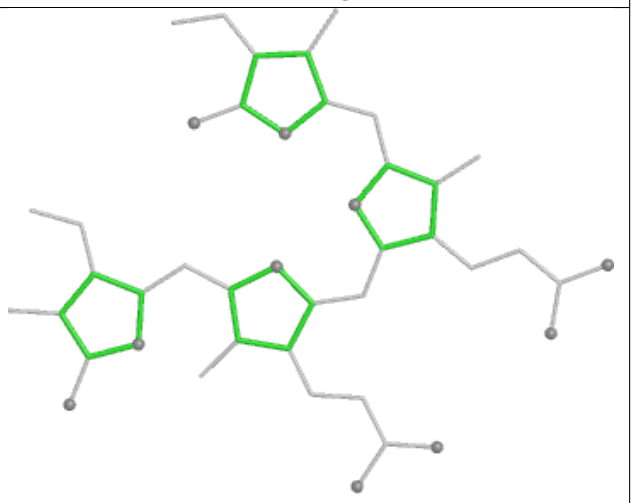
Bond lengths



Bond angles



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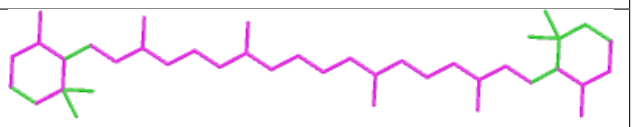


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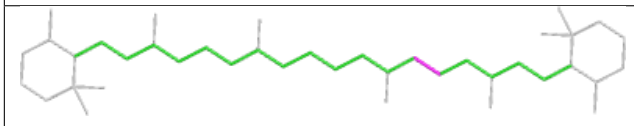
Ligand BCR b6 602



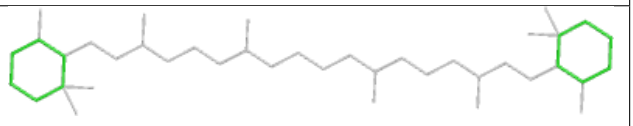
Bond lengths



Bond angles

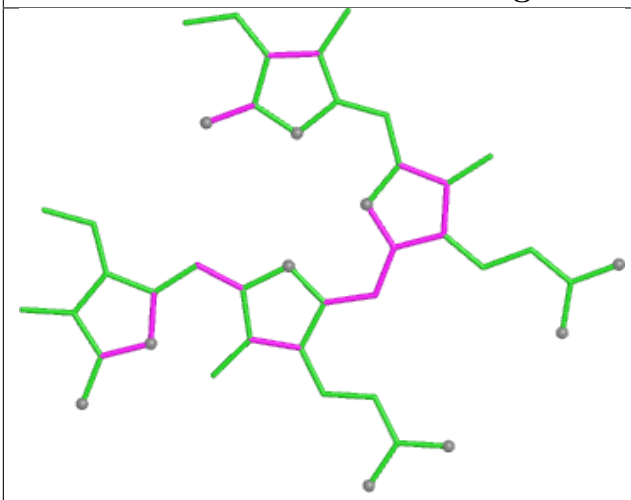


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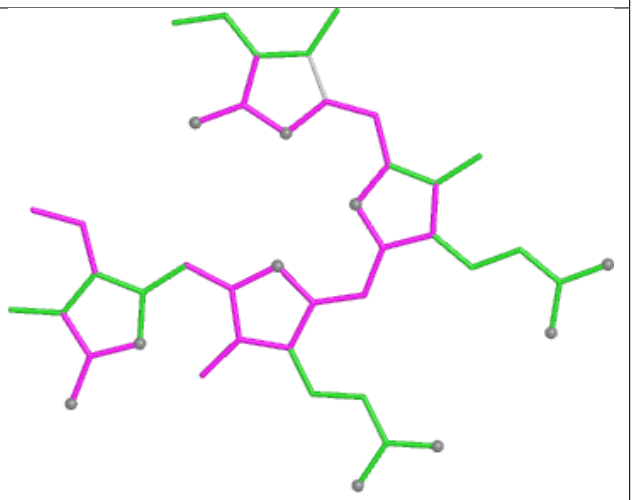


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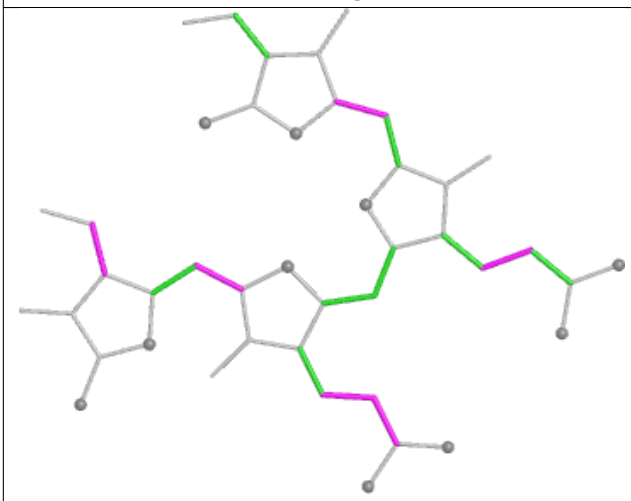
Ligand PEB wF 302



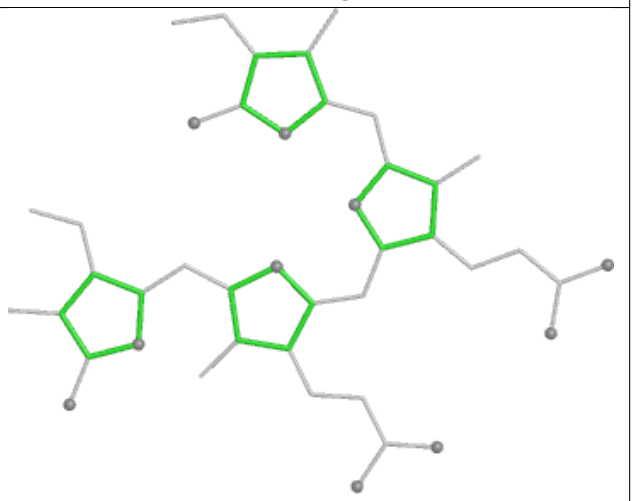
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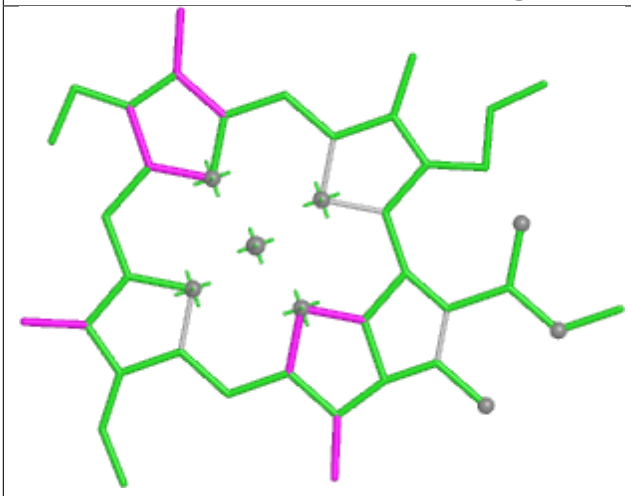
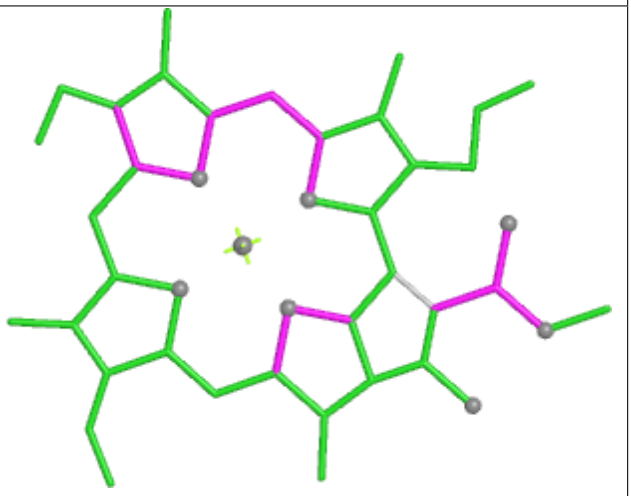
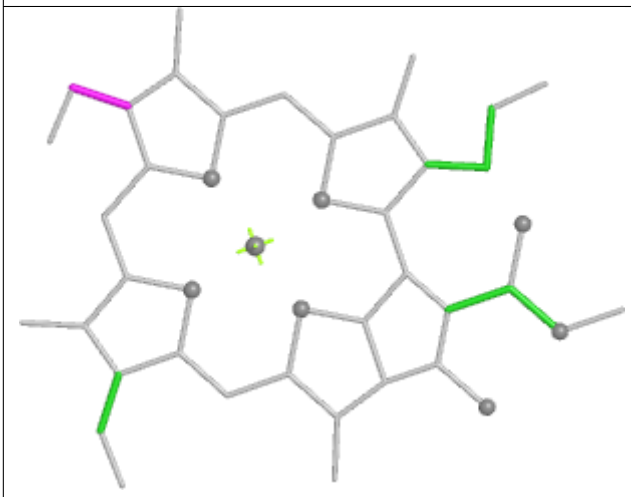
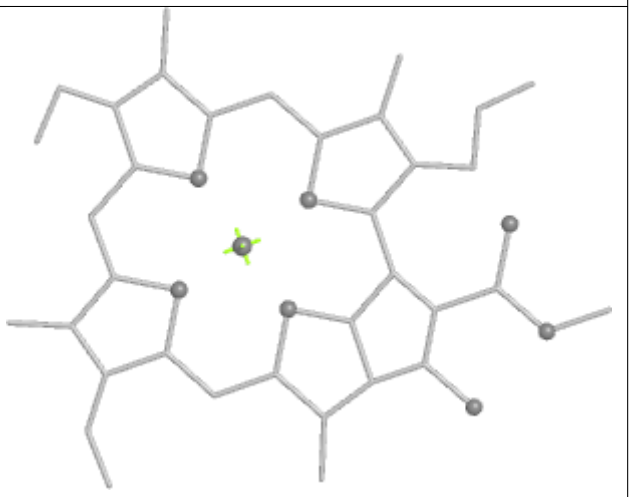
Bond angles



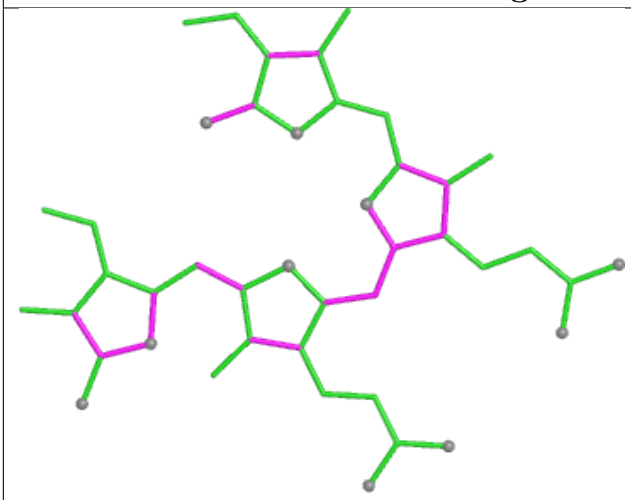
Torsions



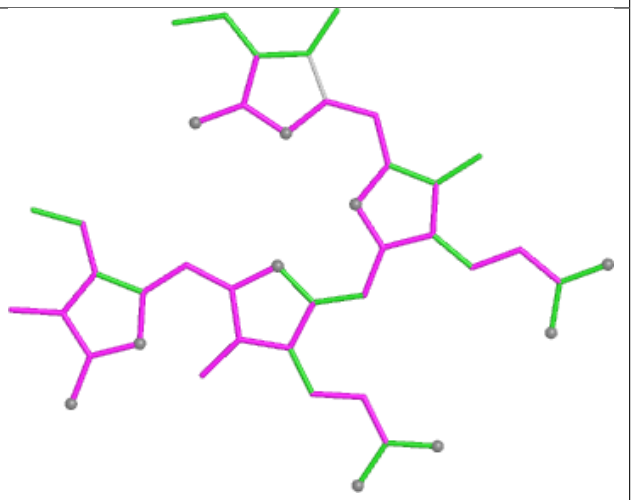
Rings

Ligand CLA BN 821	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

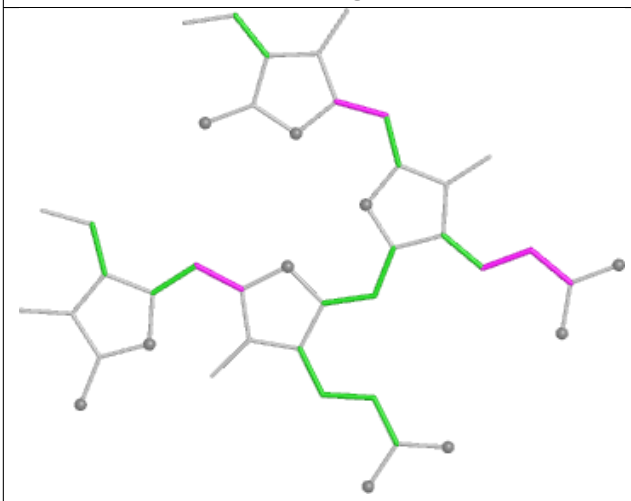
Ligand PEB XA 201



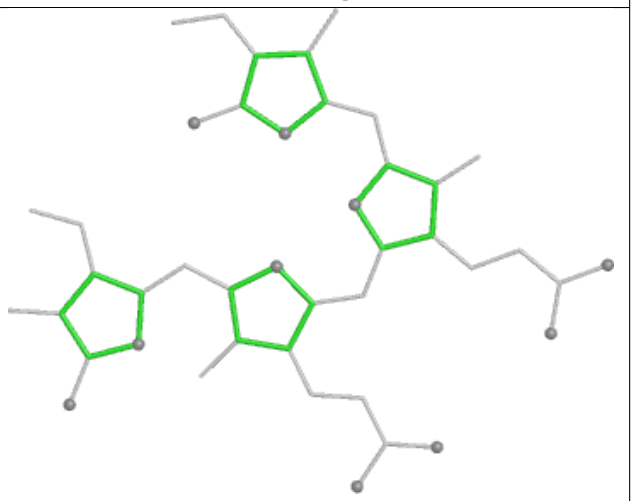
Bond lengths



Bond angles

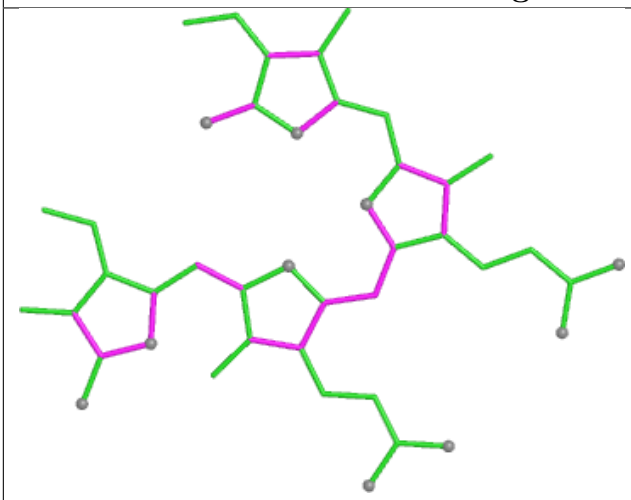


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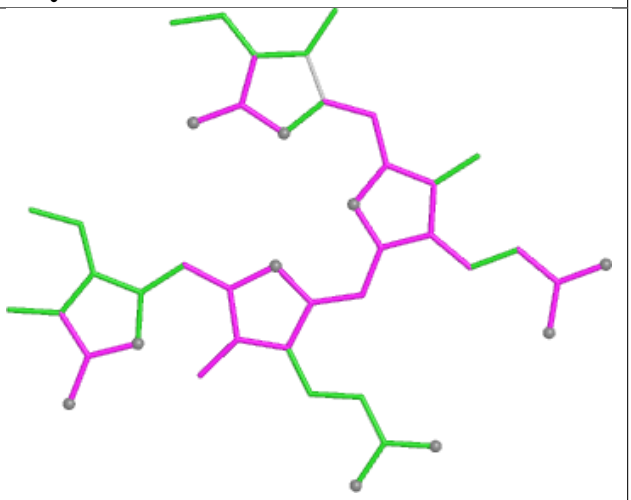


Rings

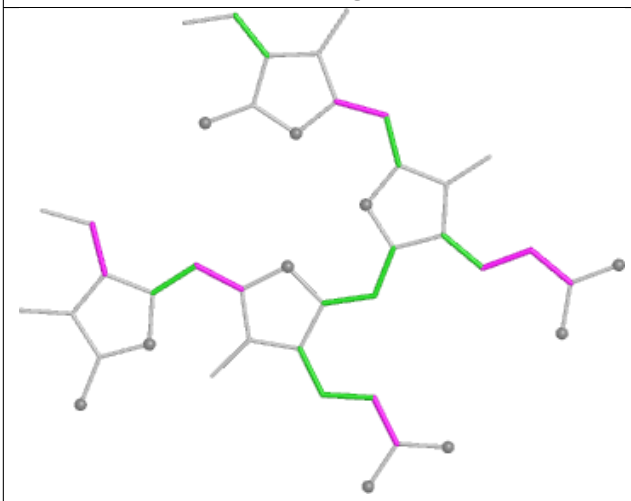
Ligand PEB QP 202



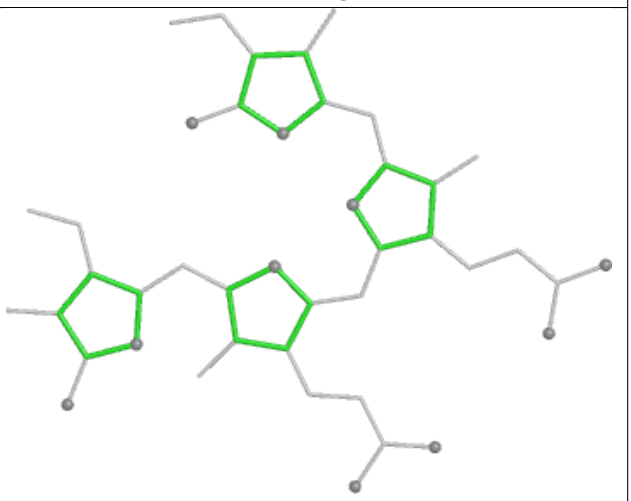
Bond lengths



Bond angles

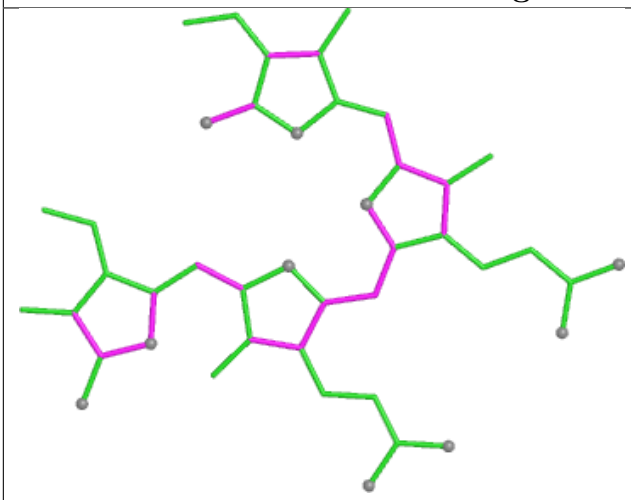


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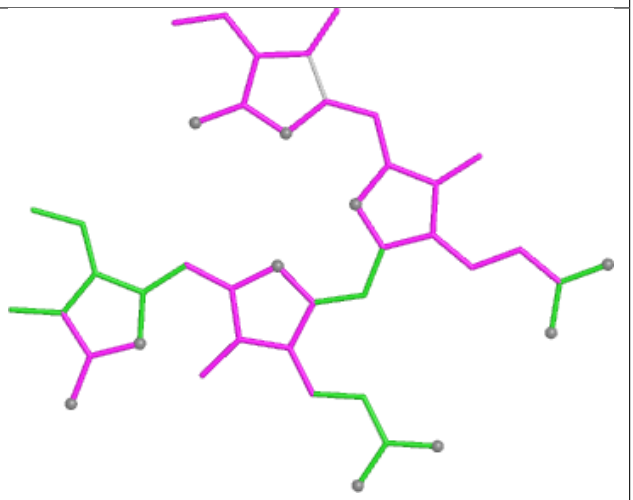


Rings

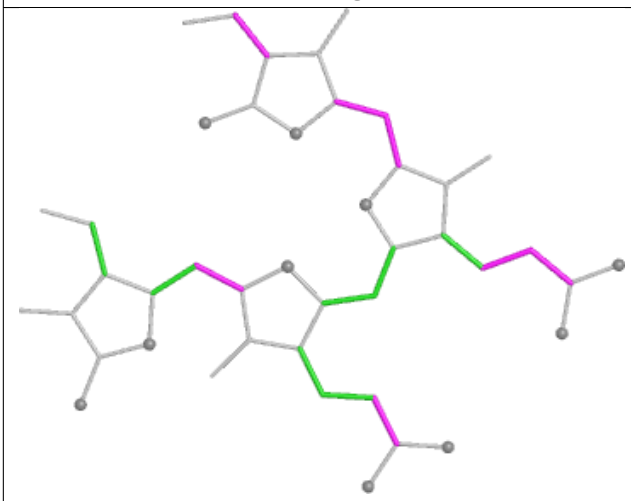
Ligand PEB CP 201



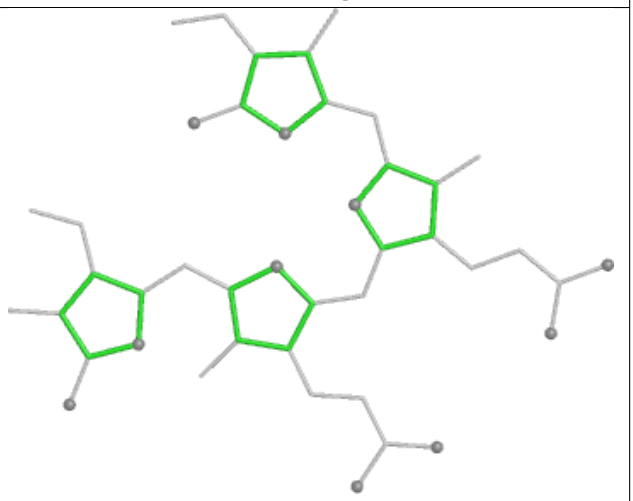
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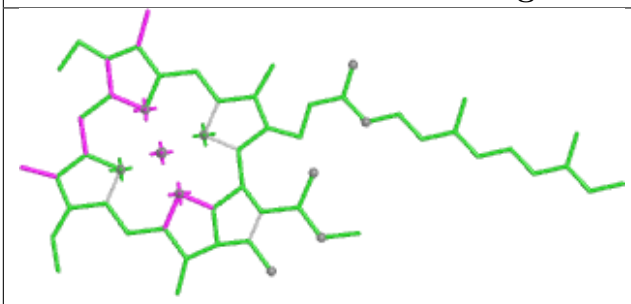
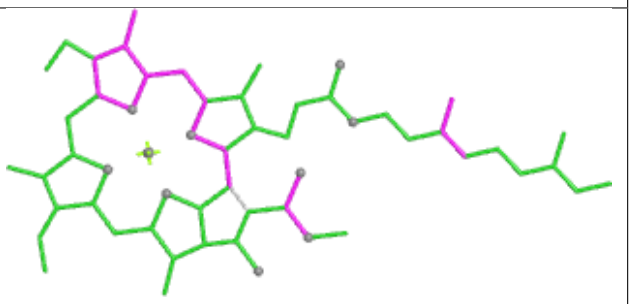
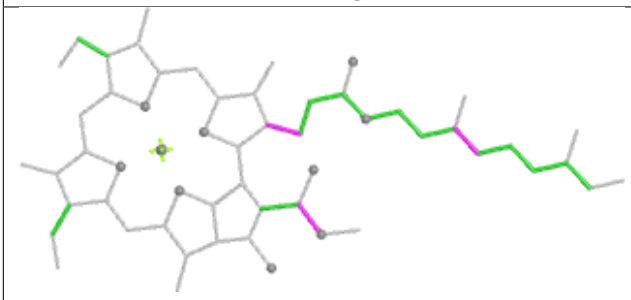
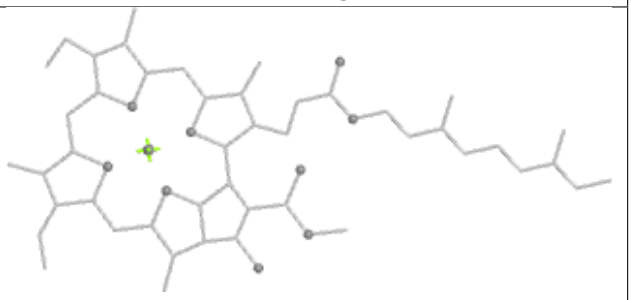
Bond angles

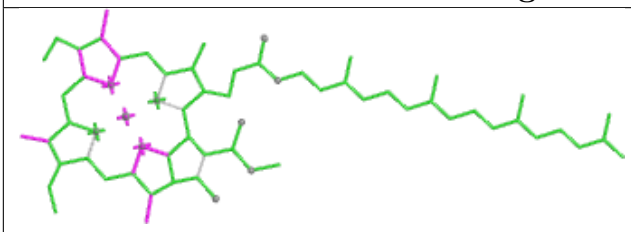
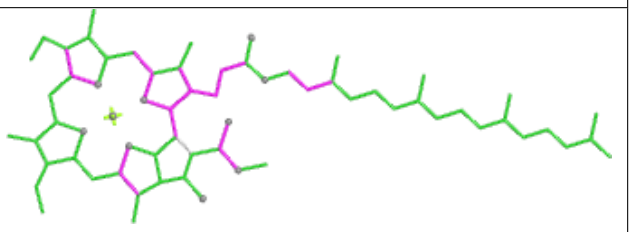
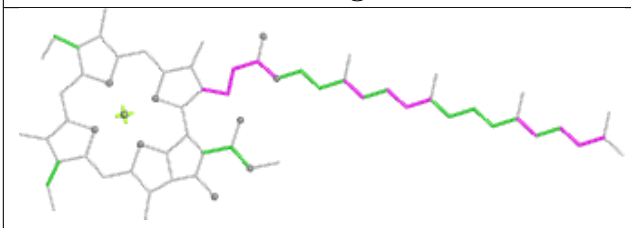
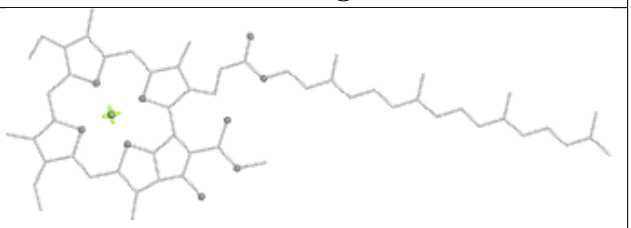


Torsions

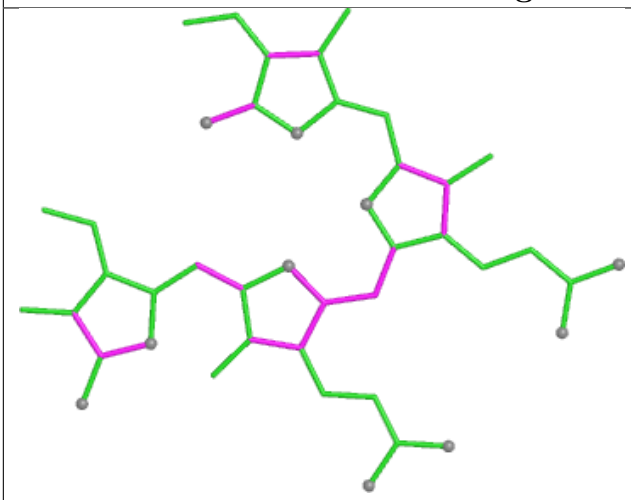


Rings

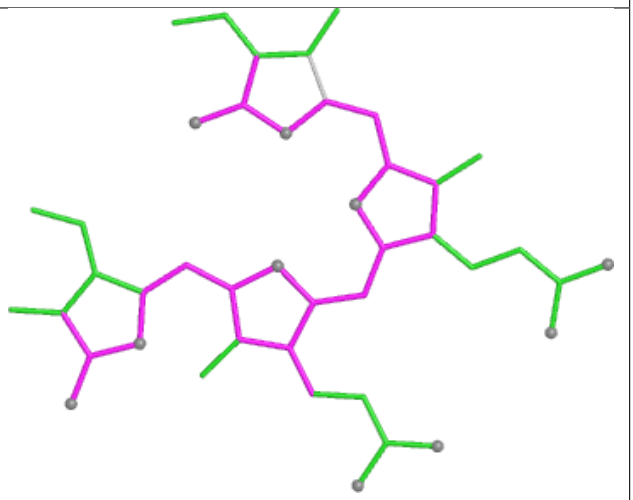
Ligand CLA L2 206	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA b6 608	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

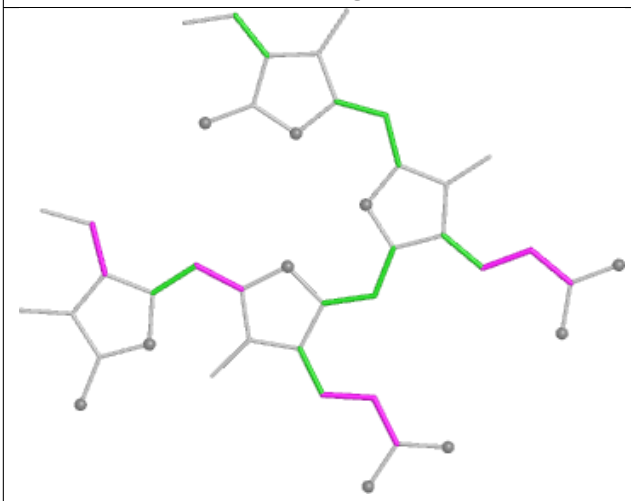
Ligand PEB R7 202



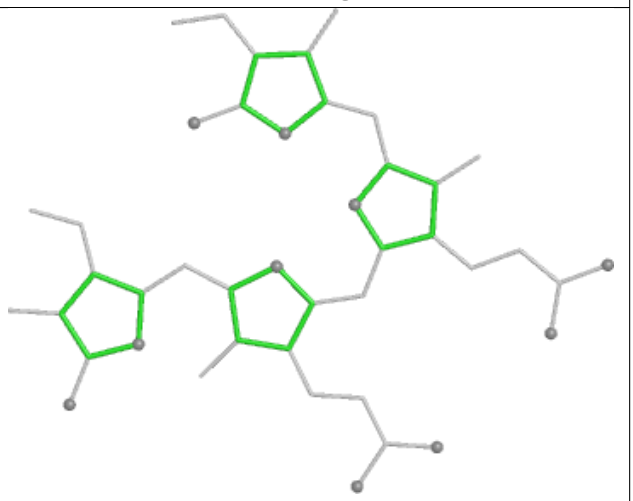
Bond lengths



Bond angles

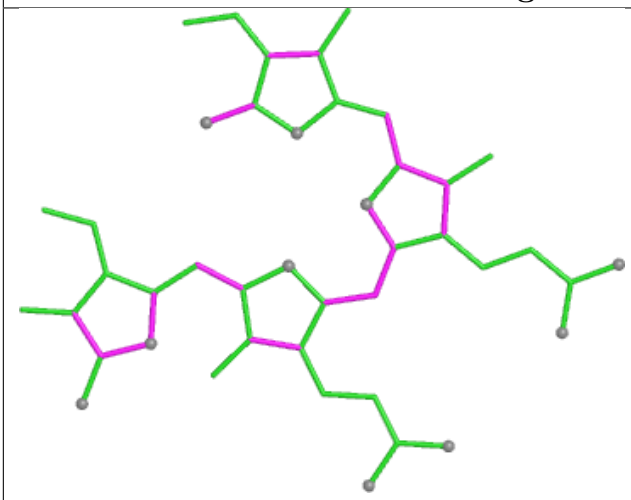


Torsions

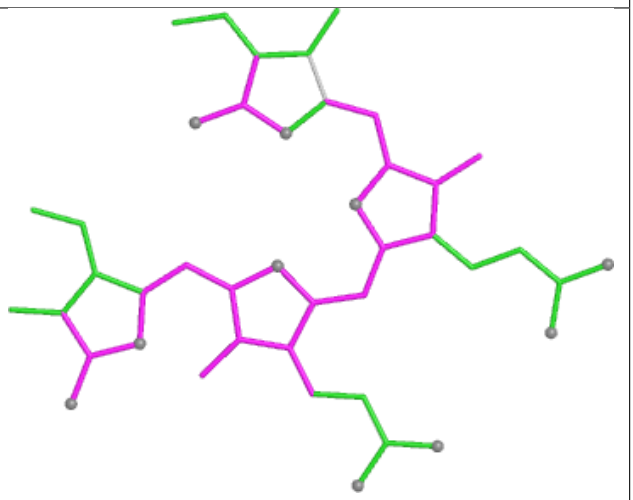


Rings

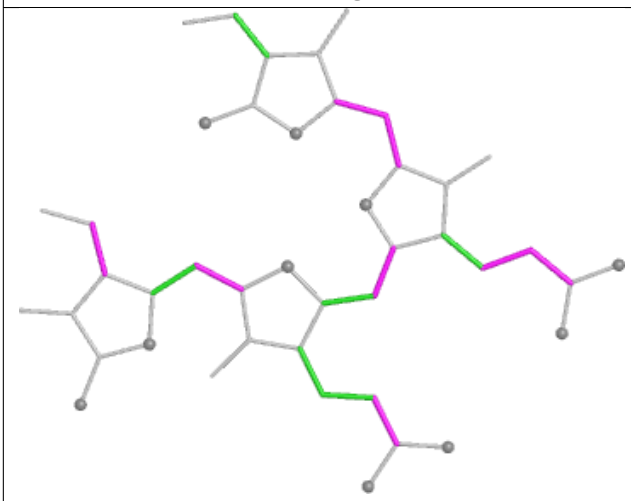
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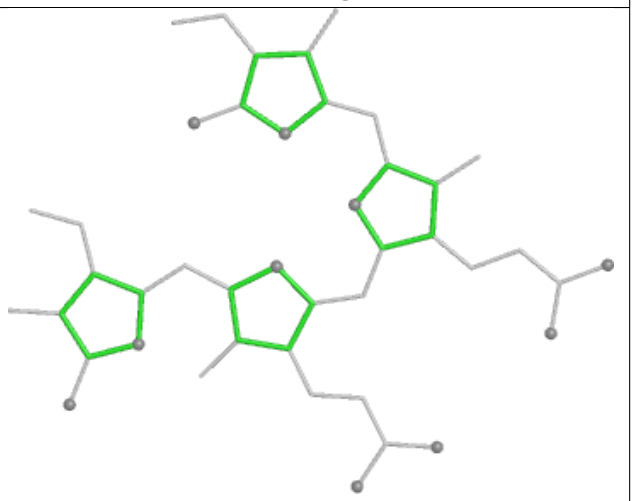
Bond lengths



Bond angles

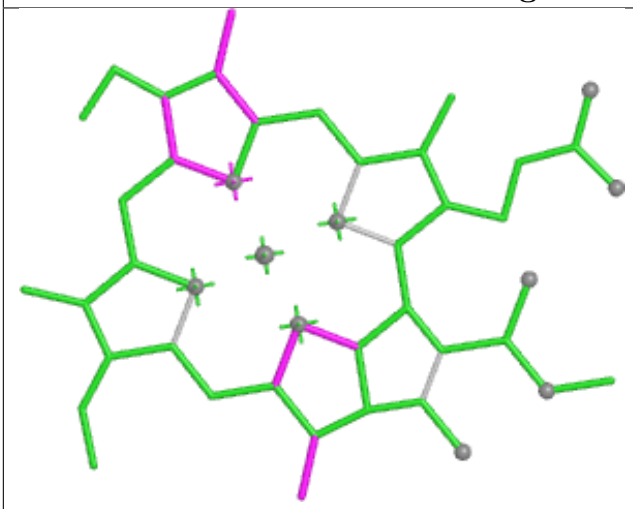


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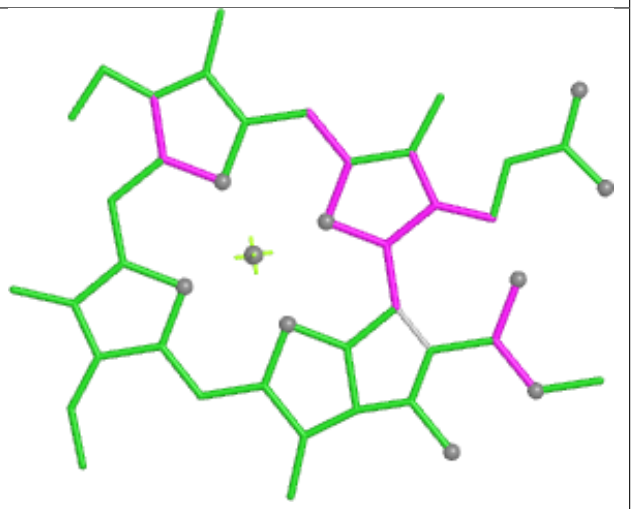


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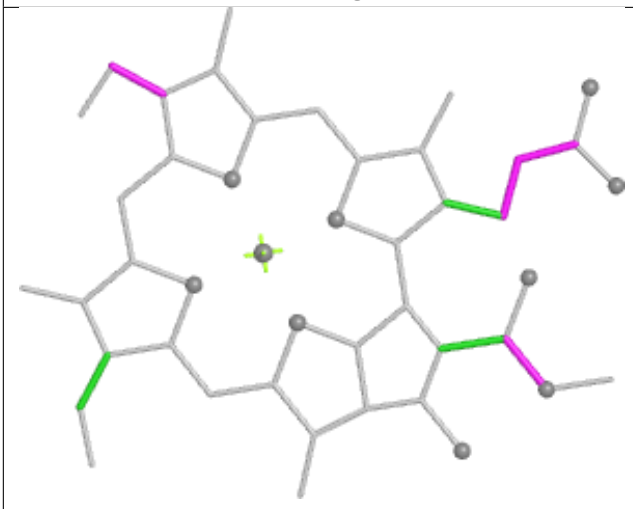
Ligand CLA 82 304



Bond lengths



Bond angles

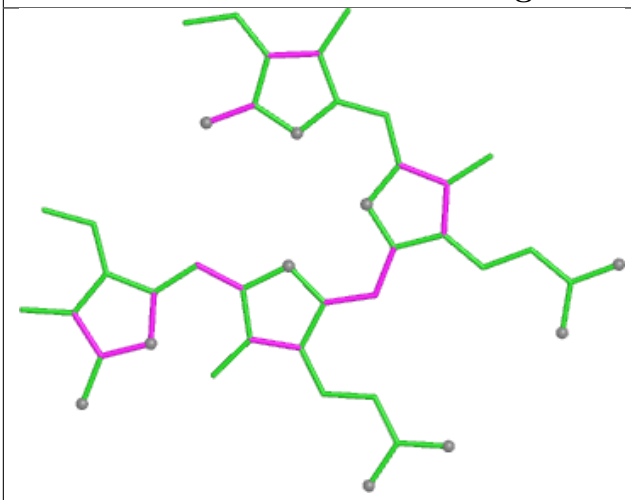


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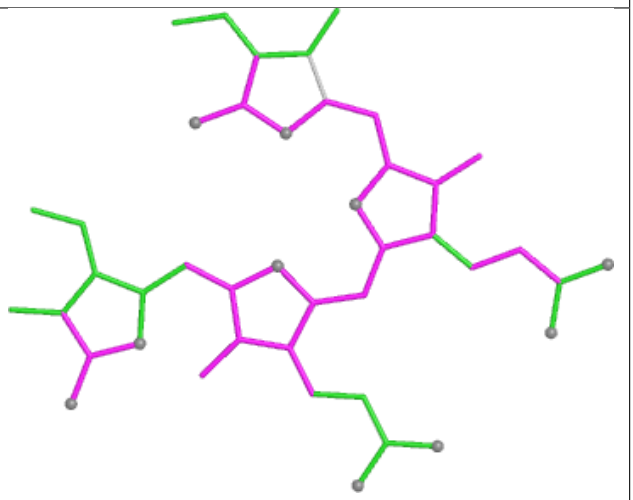


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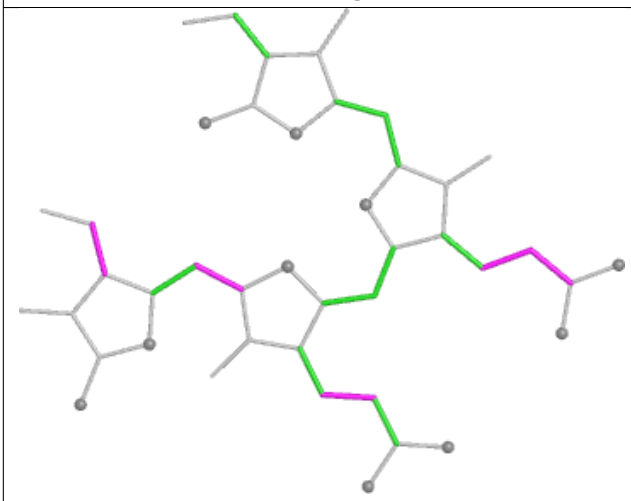
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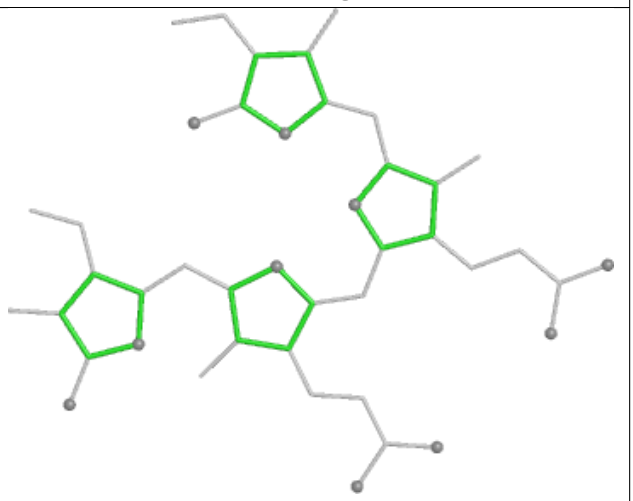
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Bond angles

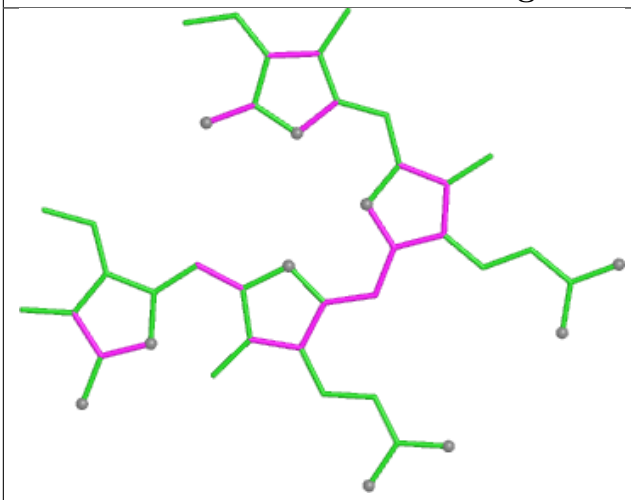


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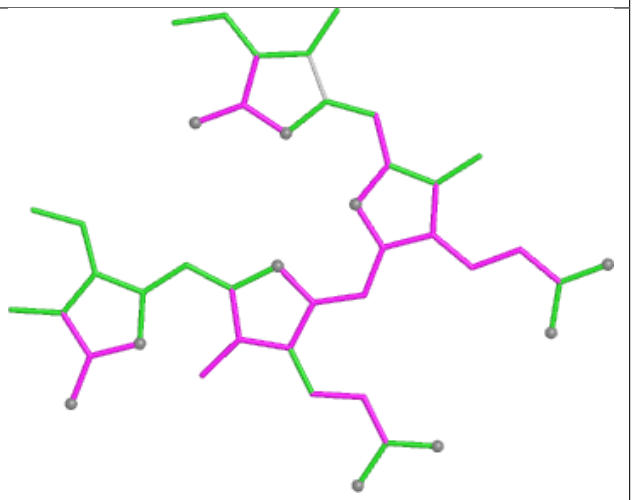


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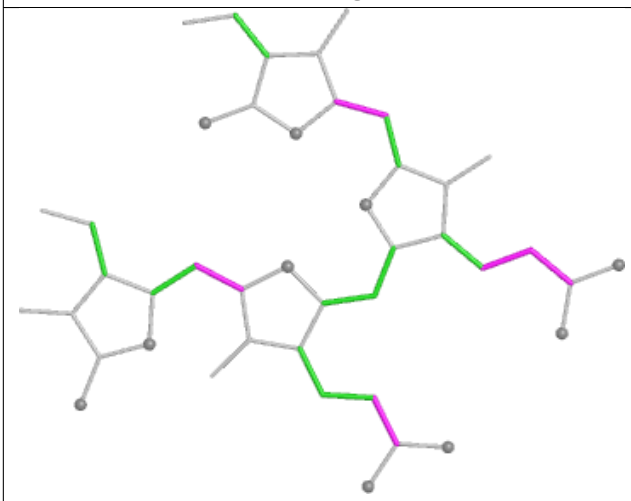
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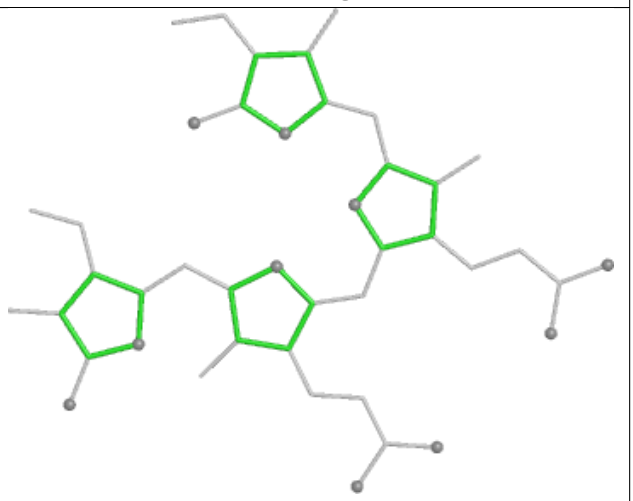
Bond lengths



Bond angles

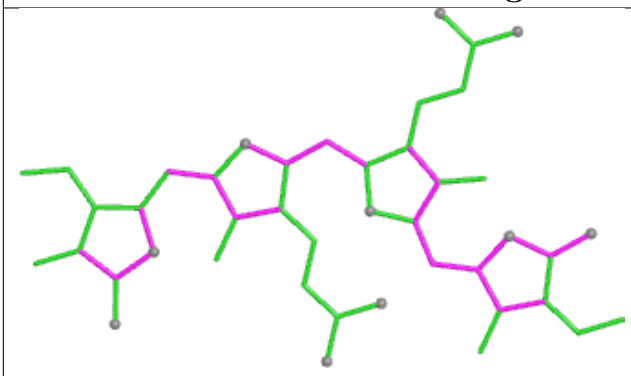


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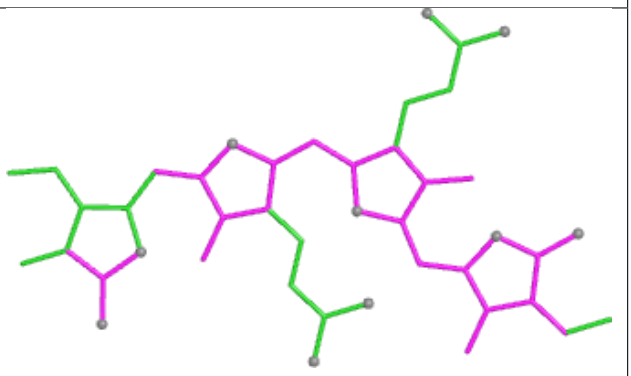


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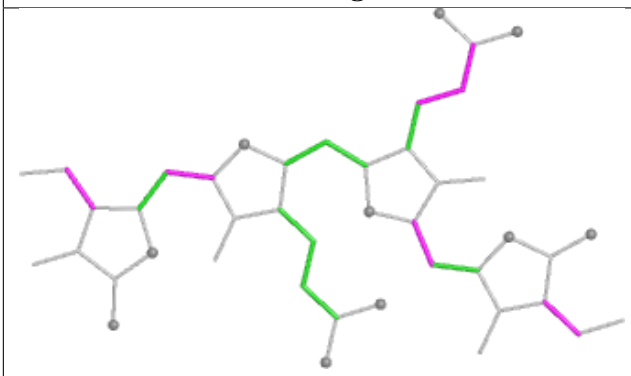
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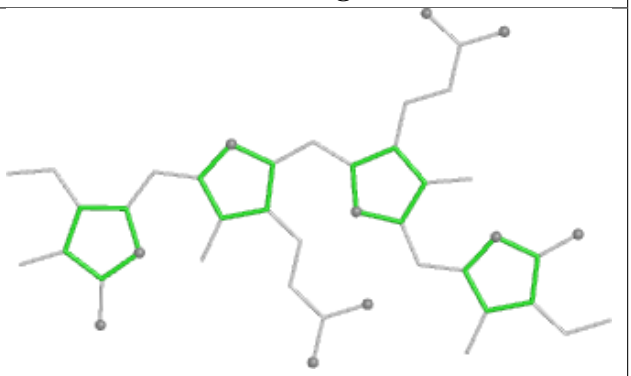
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Bond angles

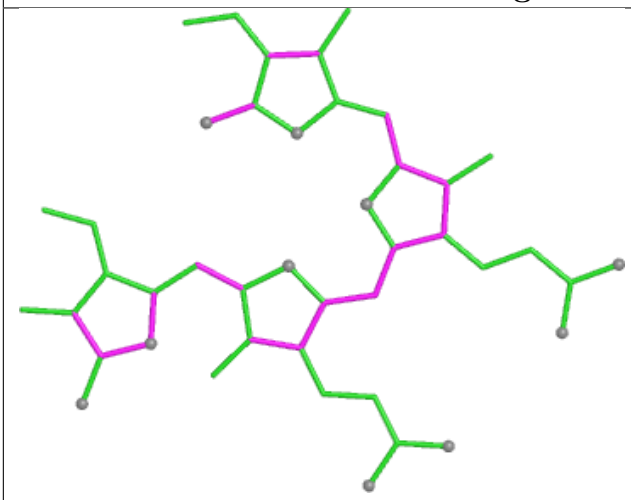


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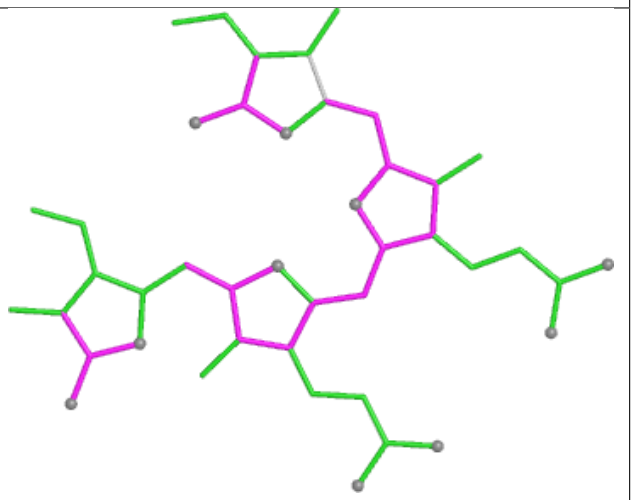


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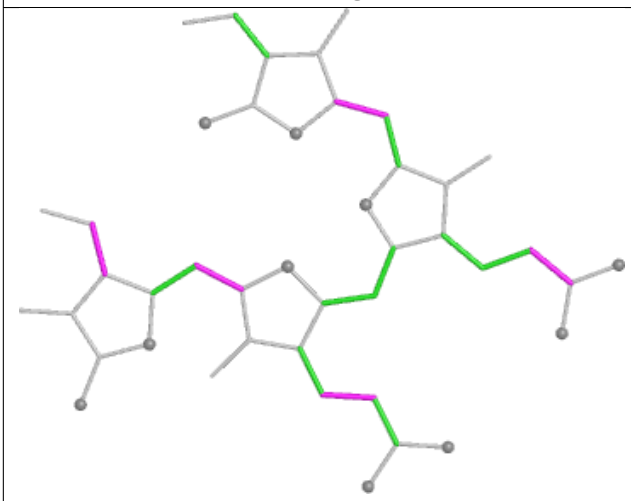
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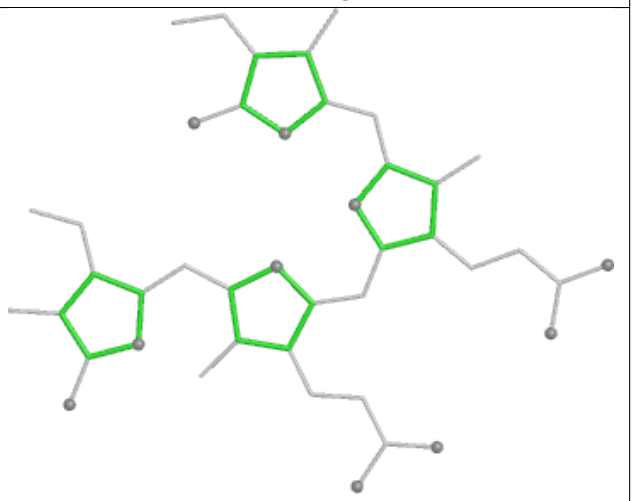
Bond lengths



Bond angles

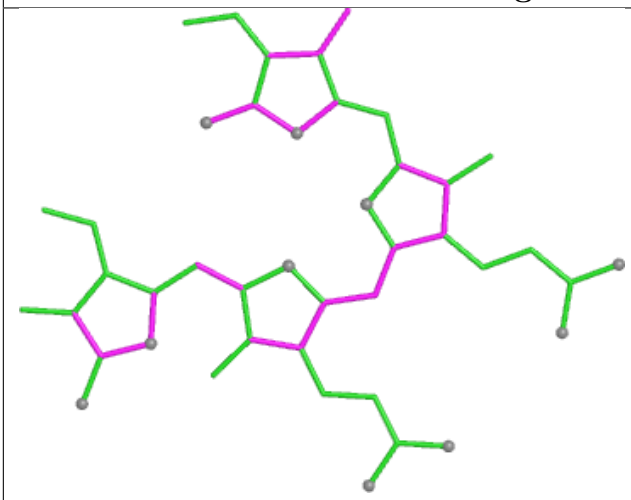


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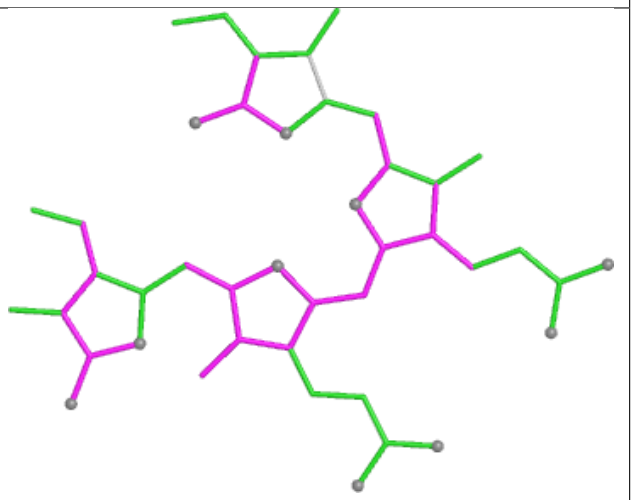


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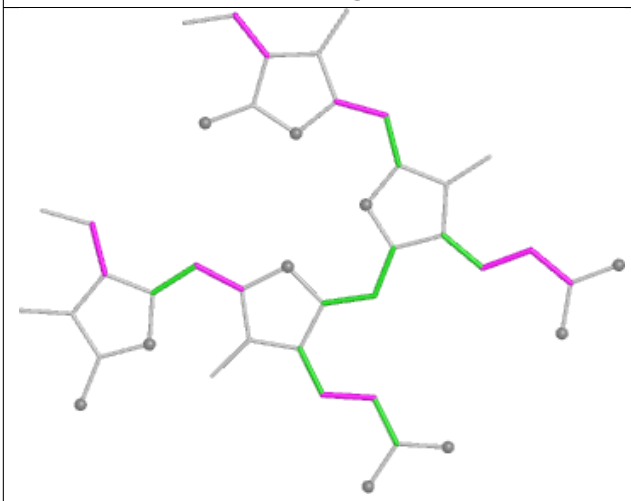
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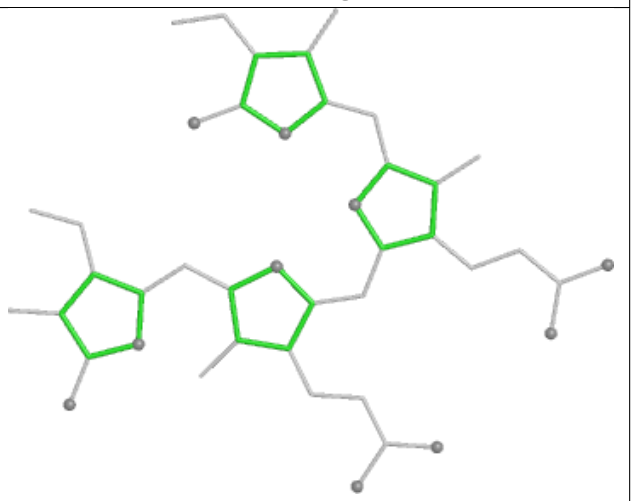
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Bond angles

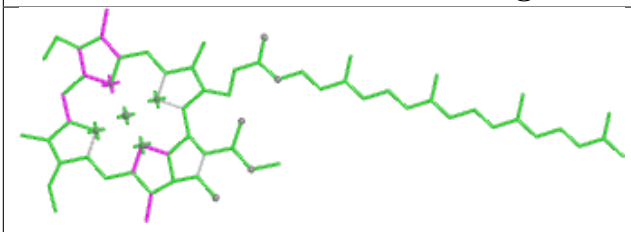


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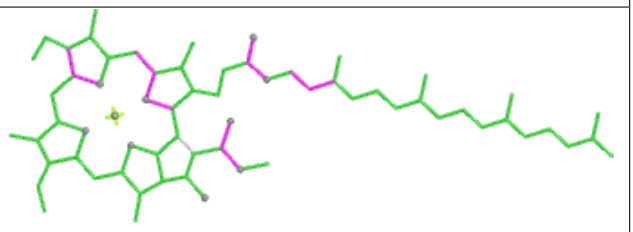


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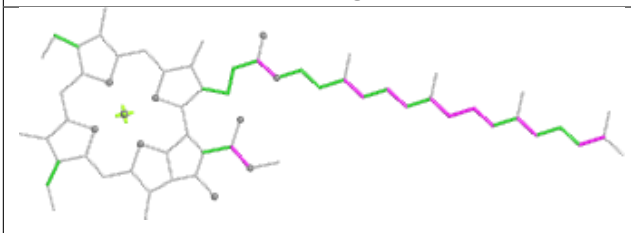
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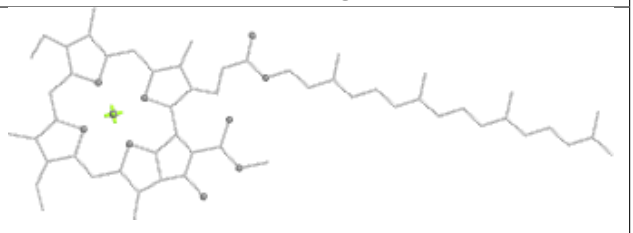
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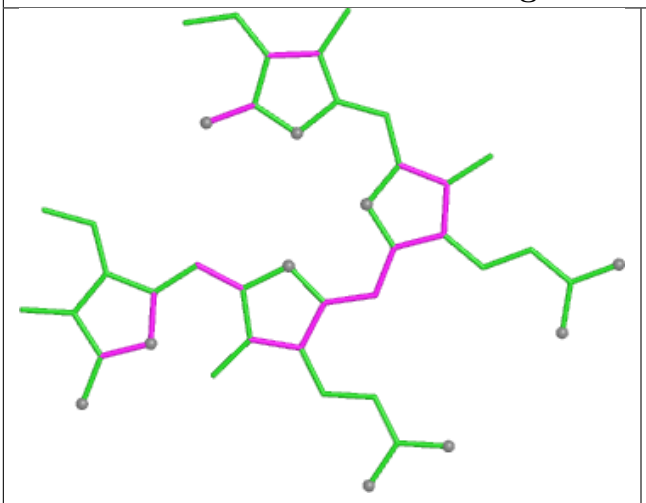


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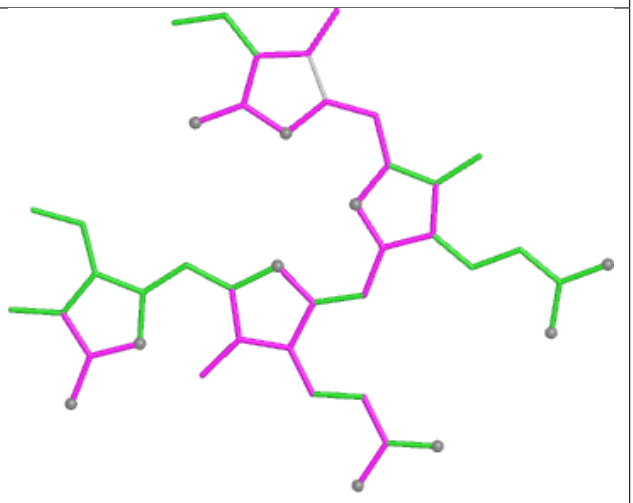


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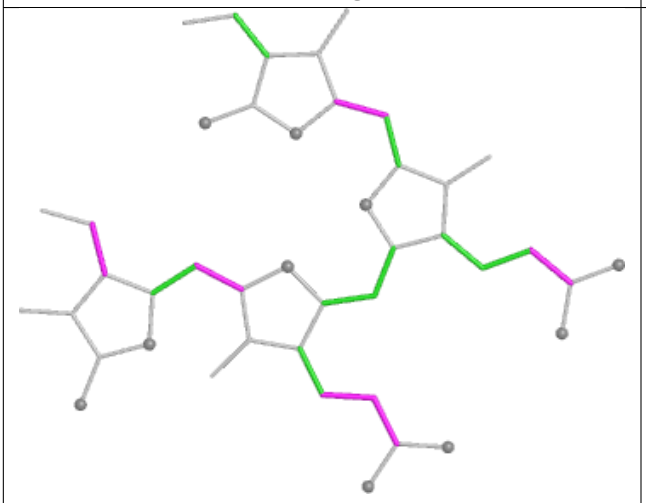
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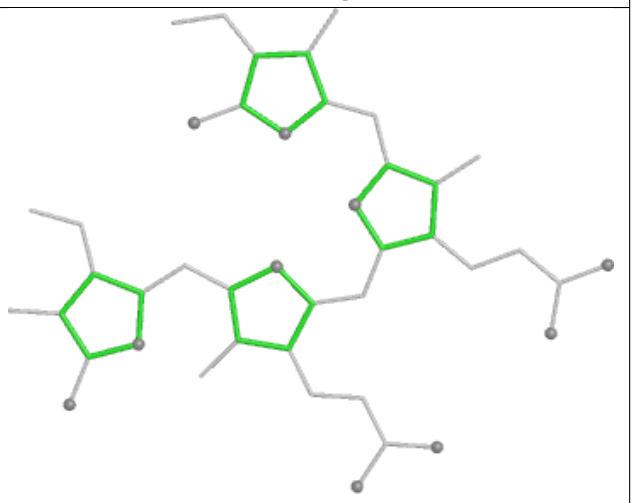
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Bond angles

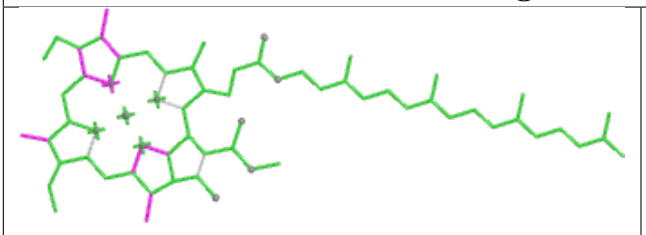


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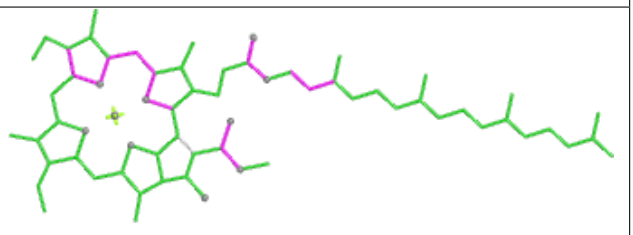


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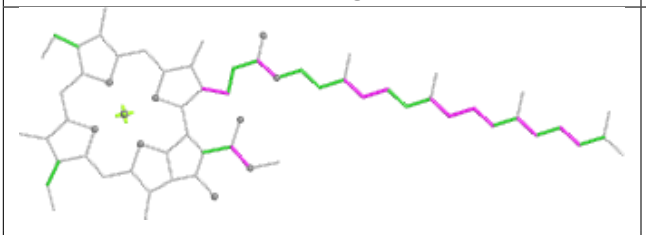
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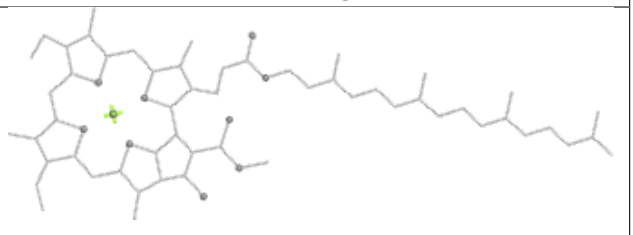
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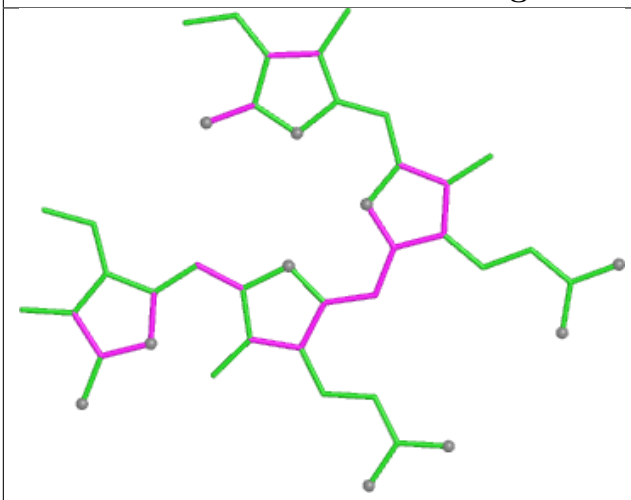


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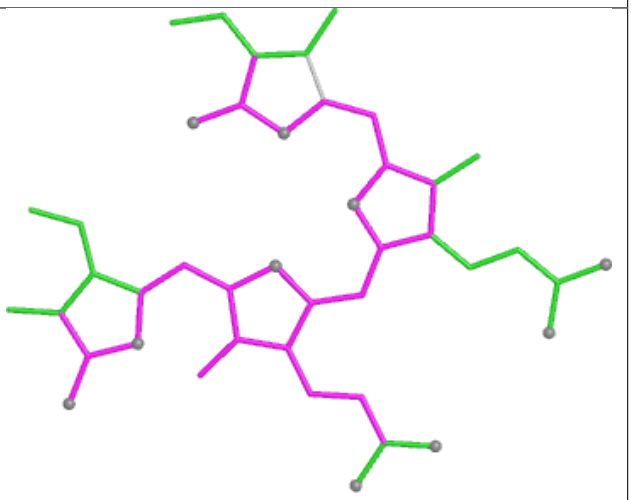


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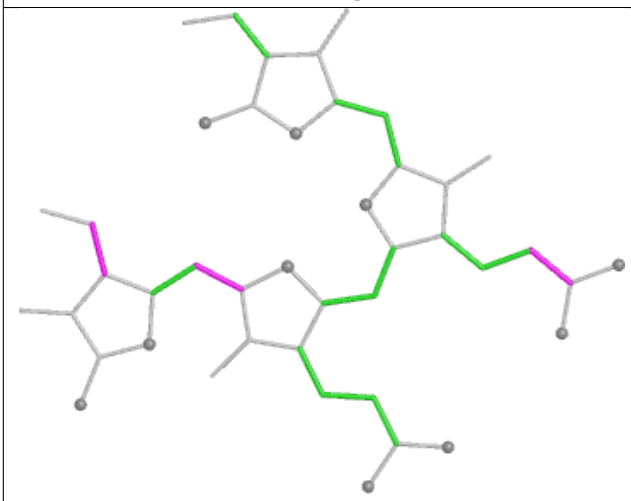
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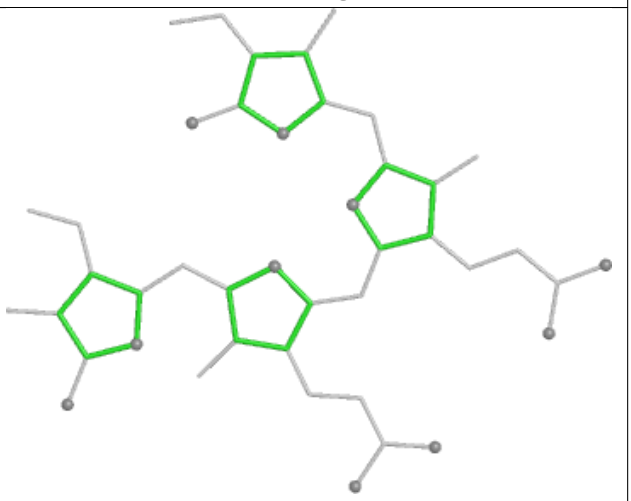
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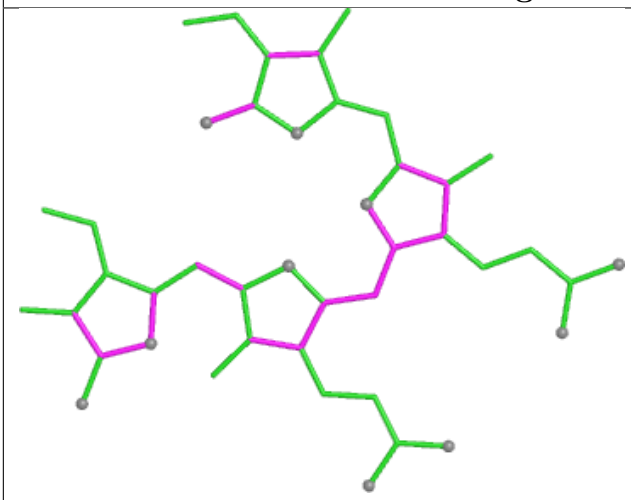


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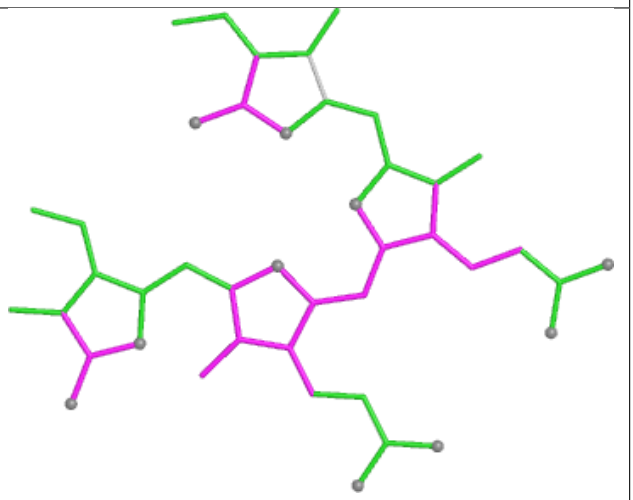


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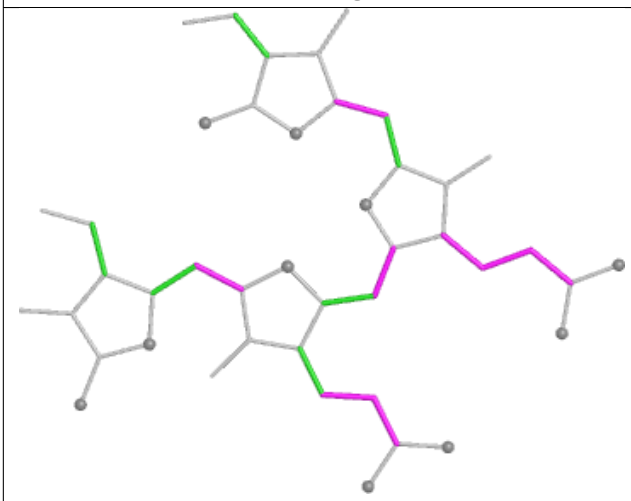
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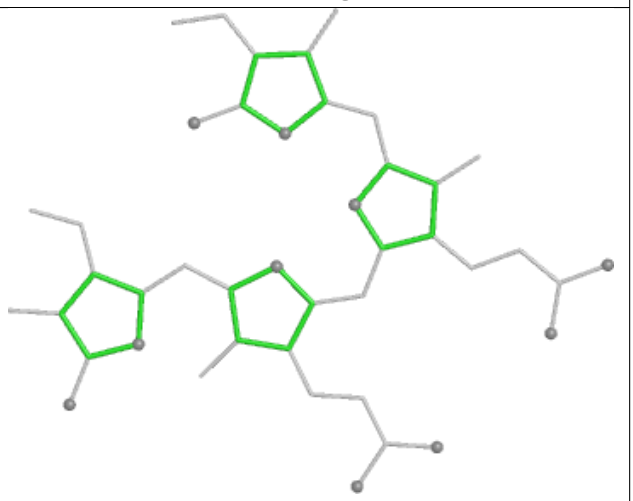
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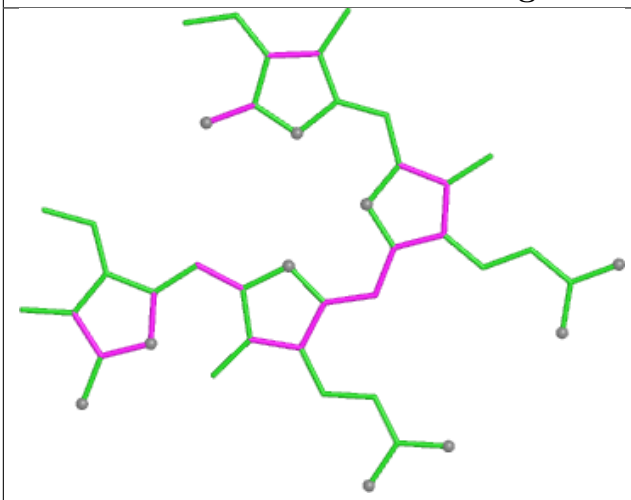


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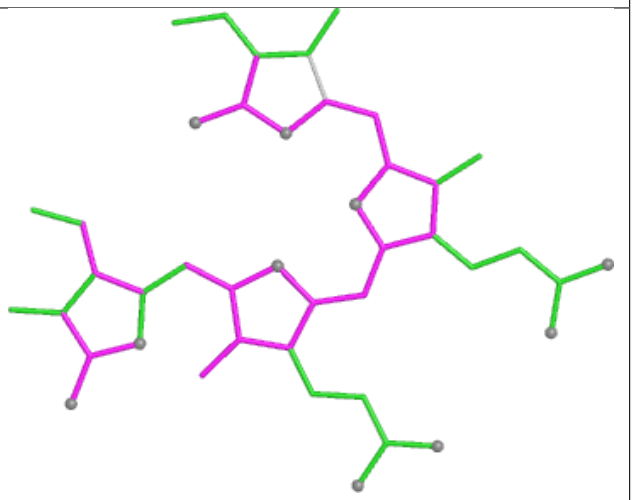


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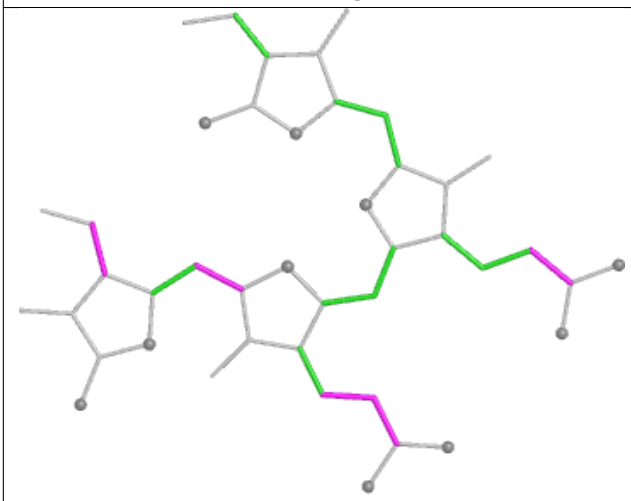
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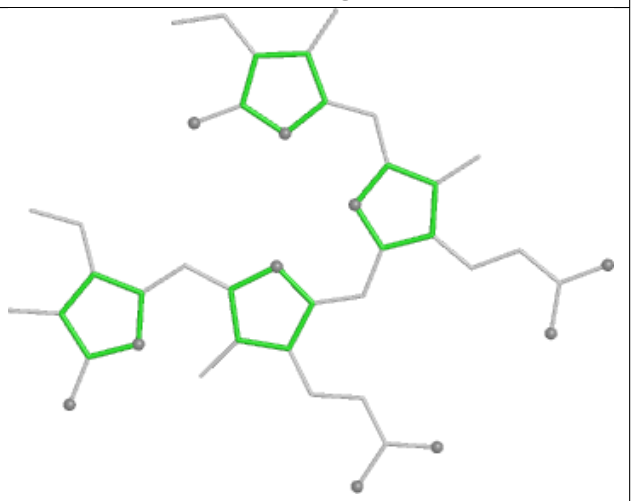
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Bond angles

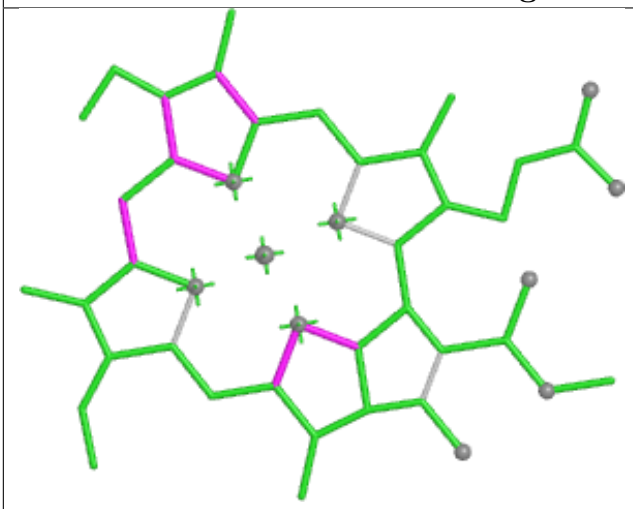


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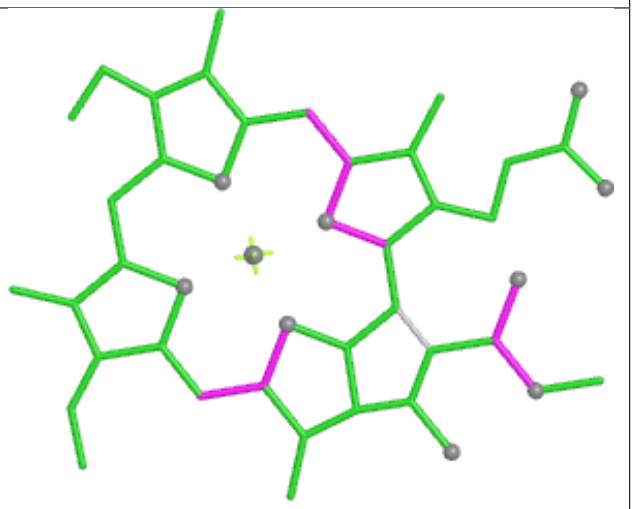


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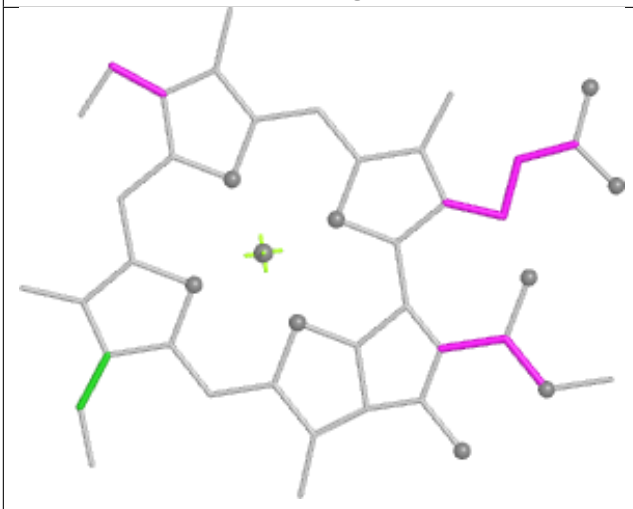
Ligand CLA 62 312



Bond lengths



Bond angles

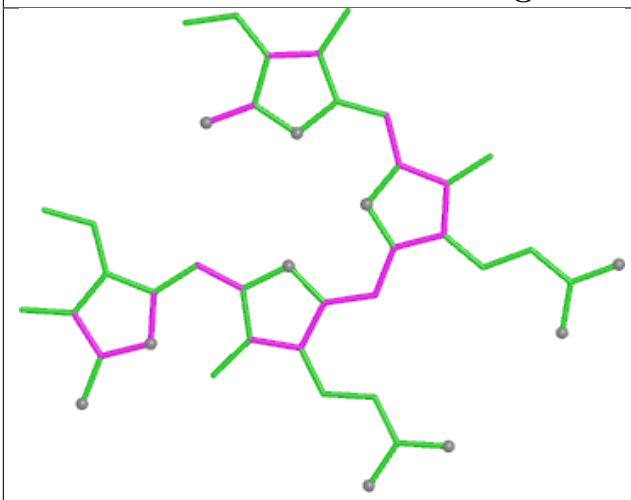


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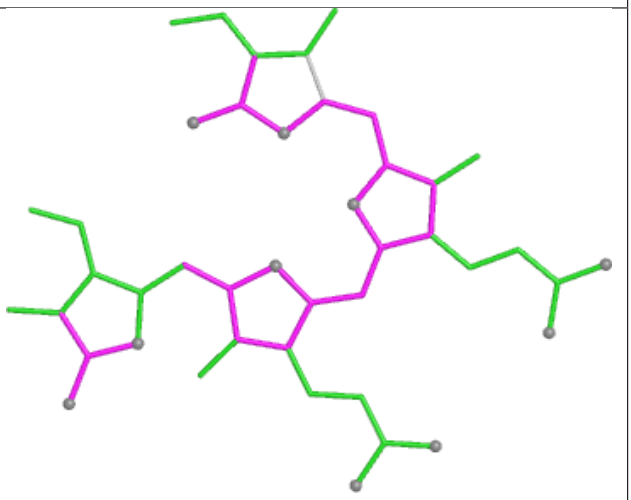


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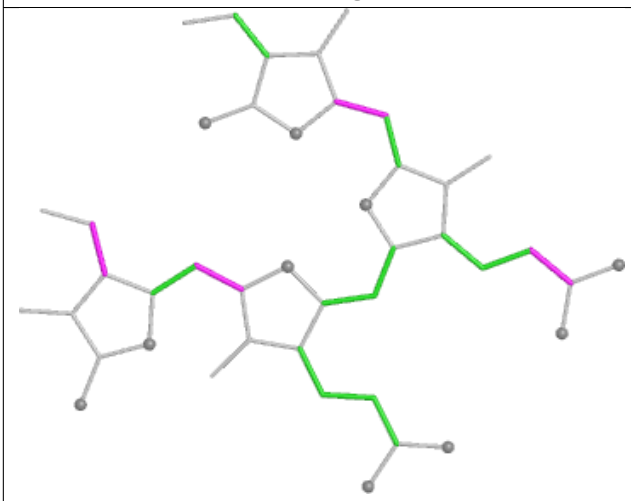
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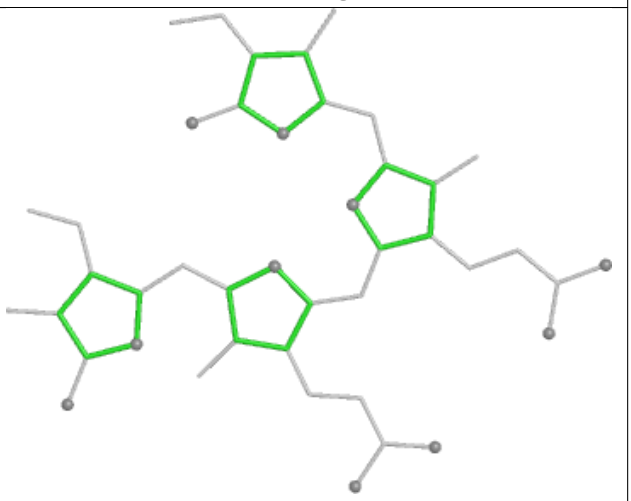
Bond lengths



Bond angles

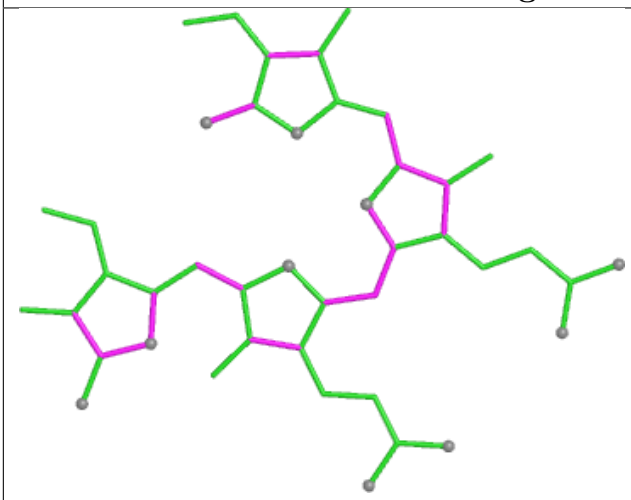


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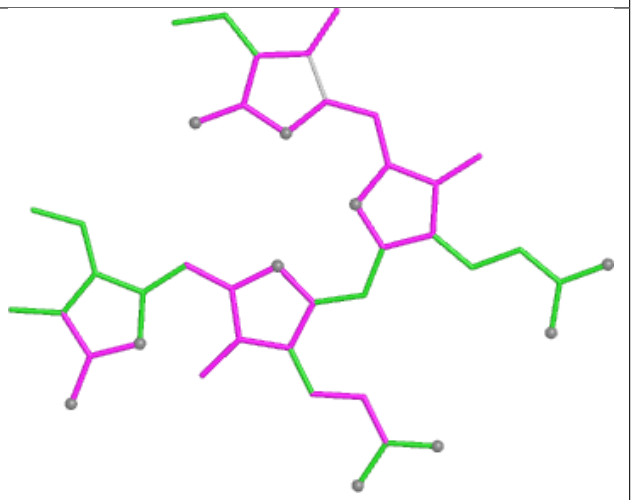


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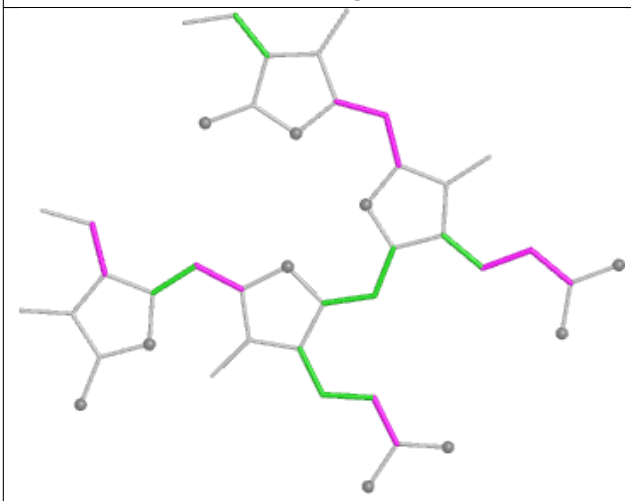
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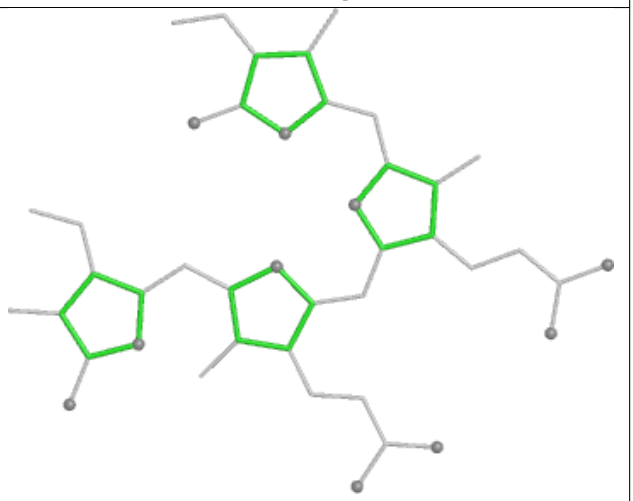
Bond lengths



Bond angles

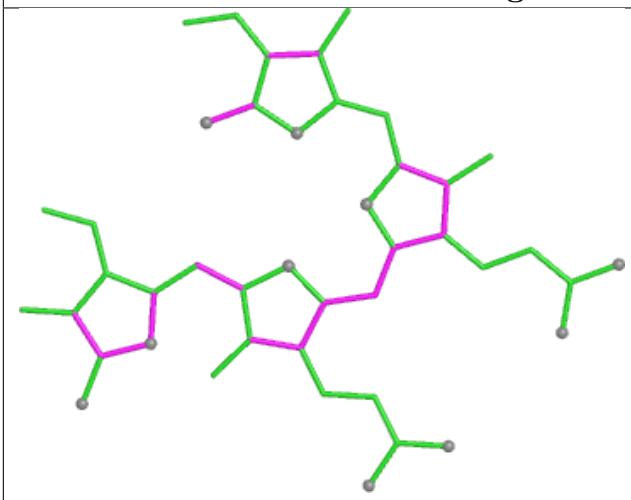


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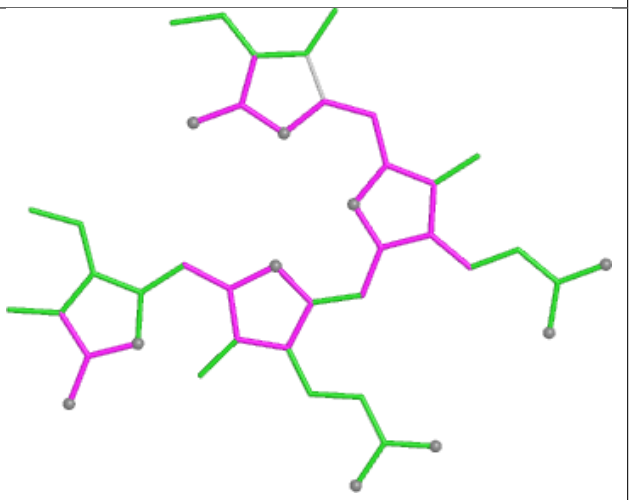


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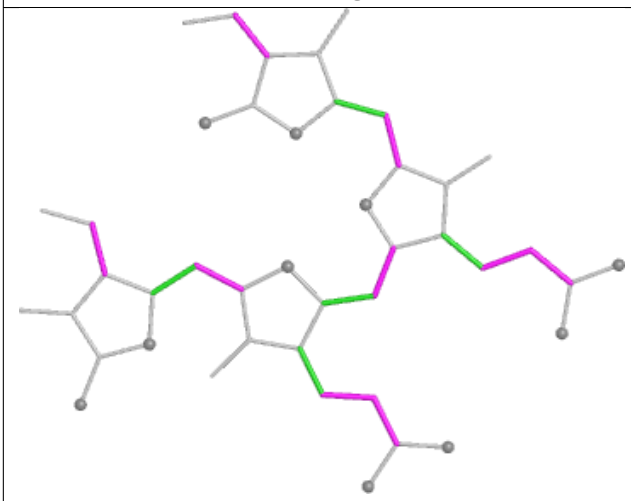
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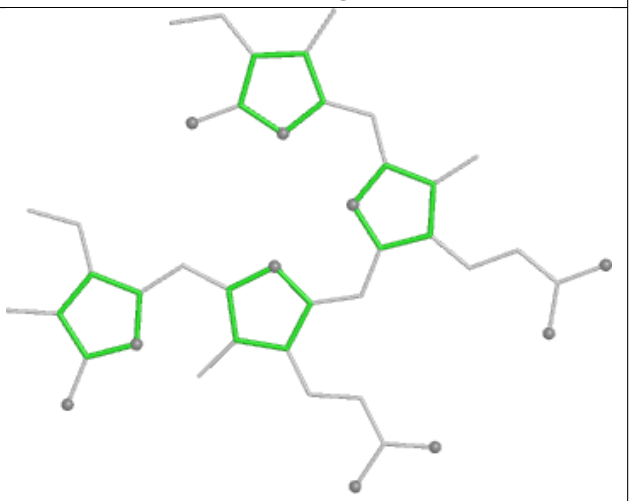
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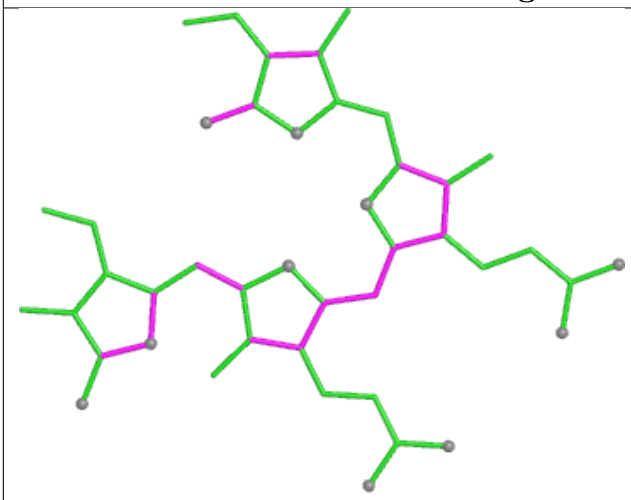


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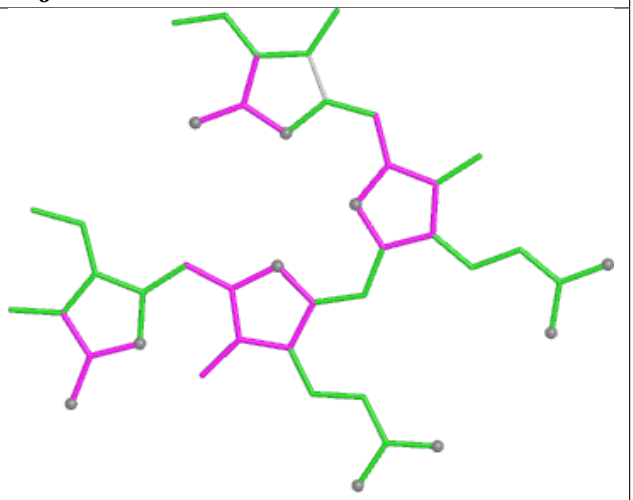


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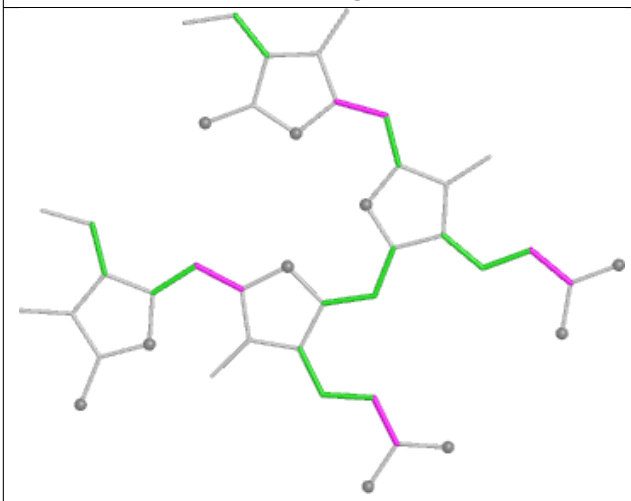
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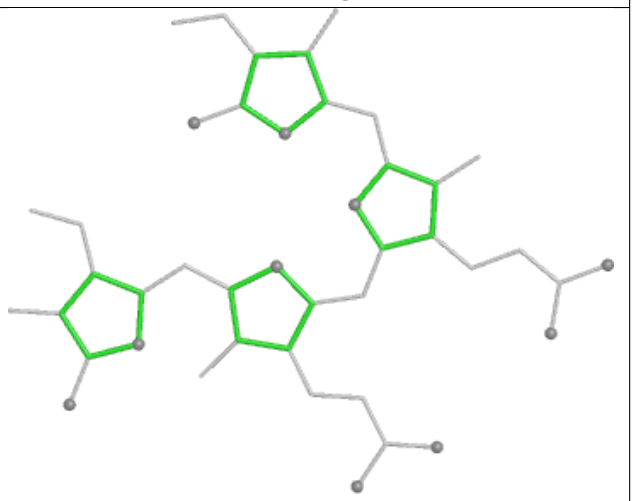
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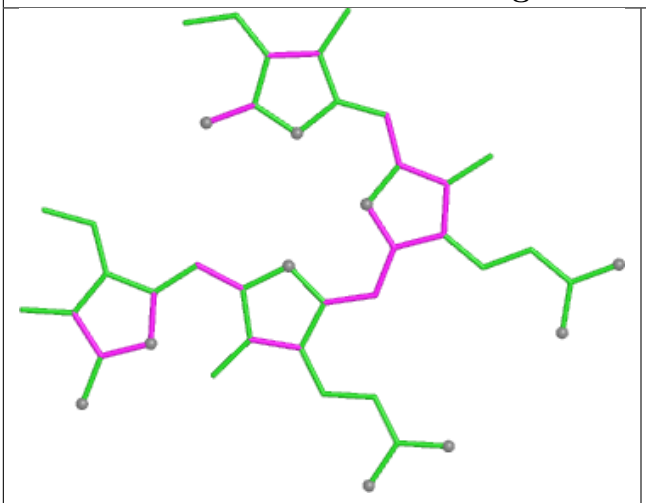


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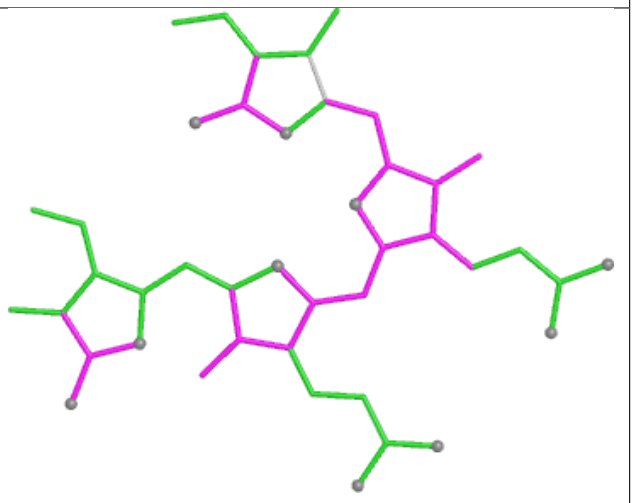


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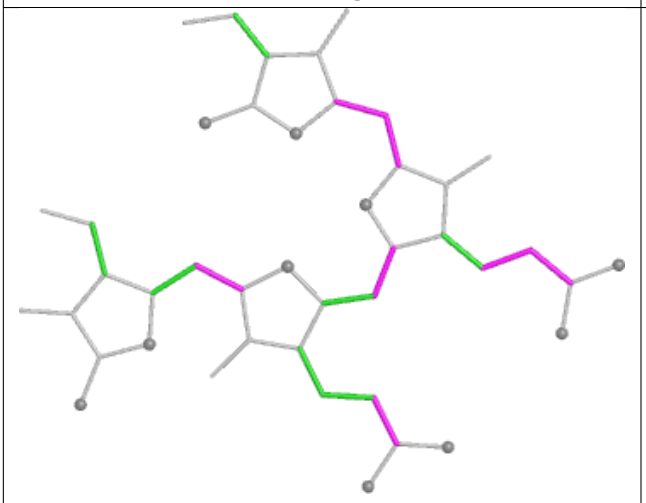
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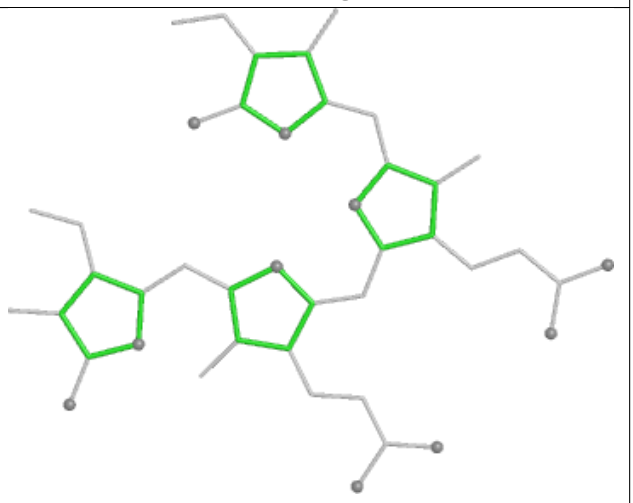
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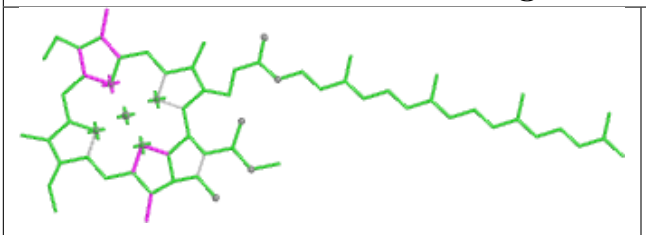


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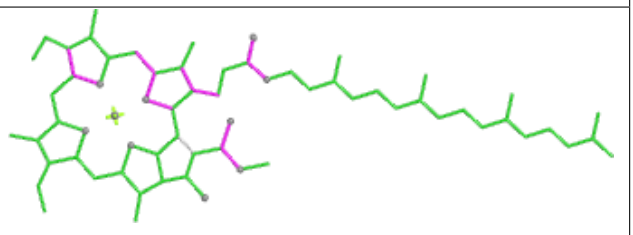


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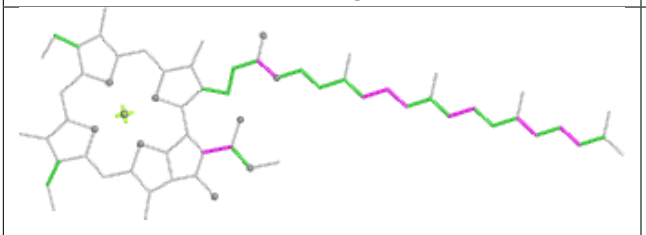
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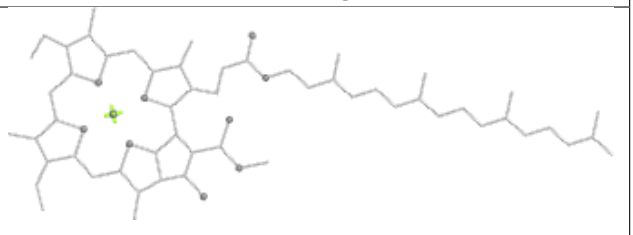
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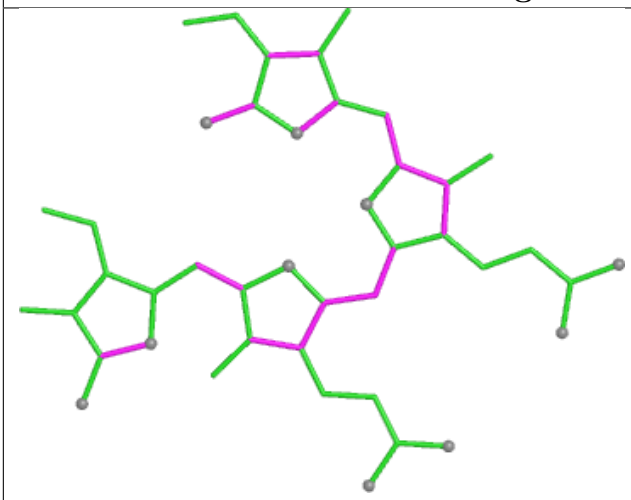


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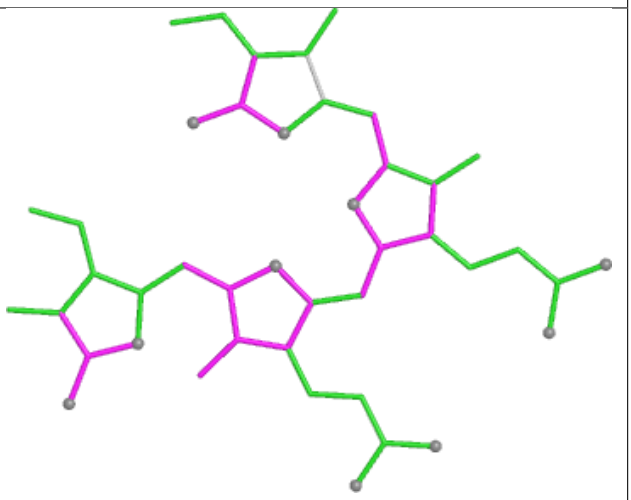


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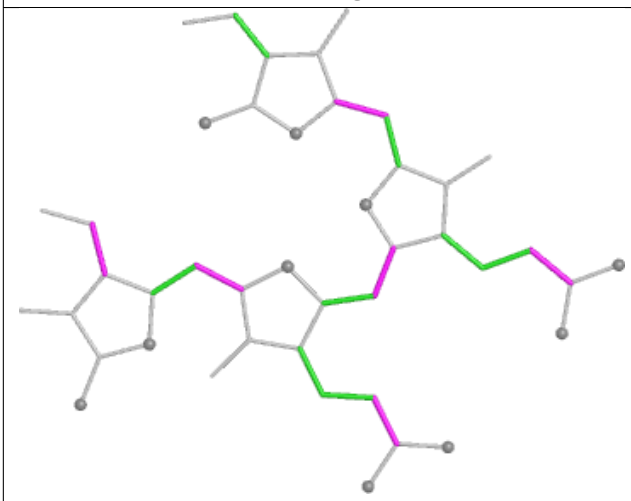
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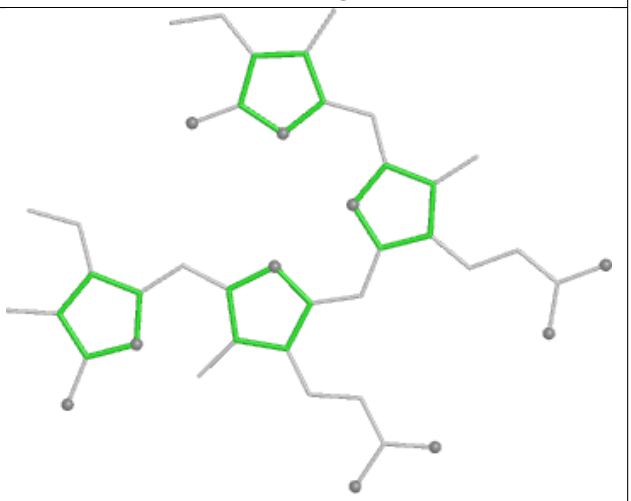
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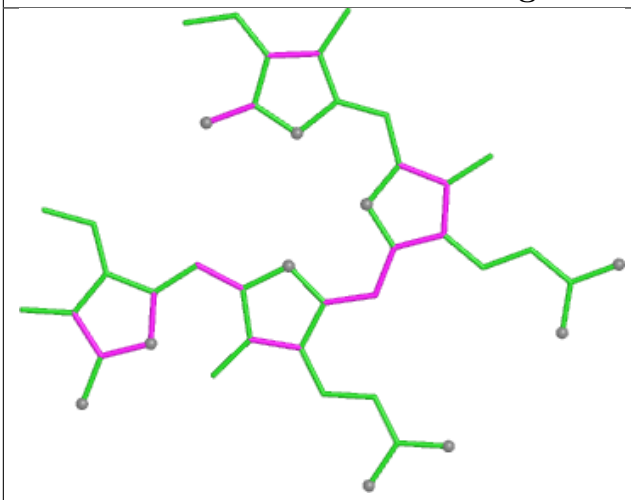


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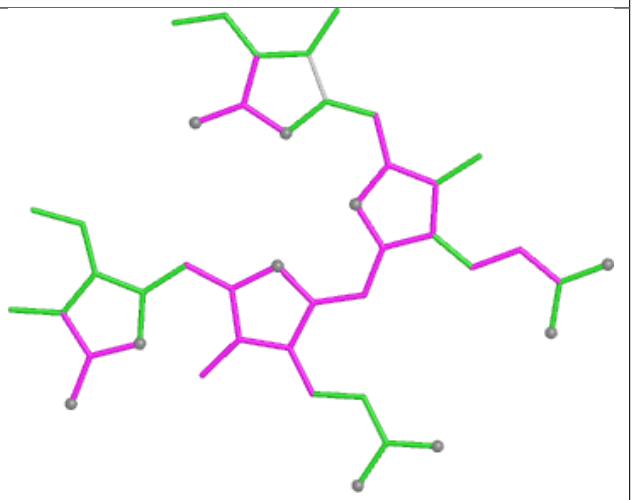


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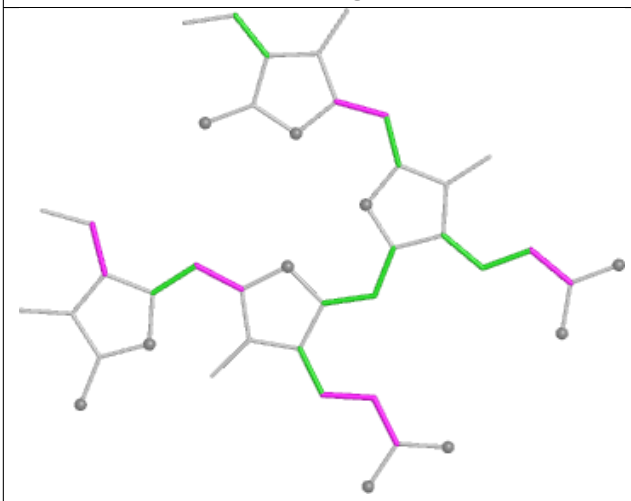
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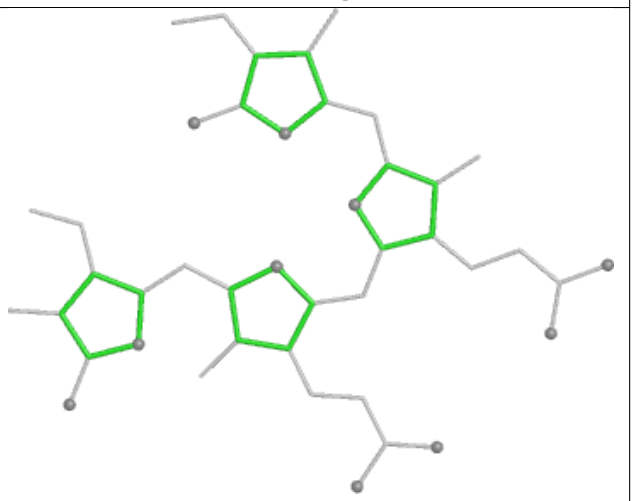
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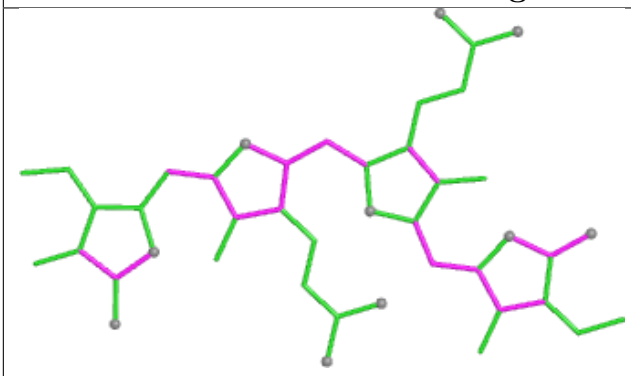


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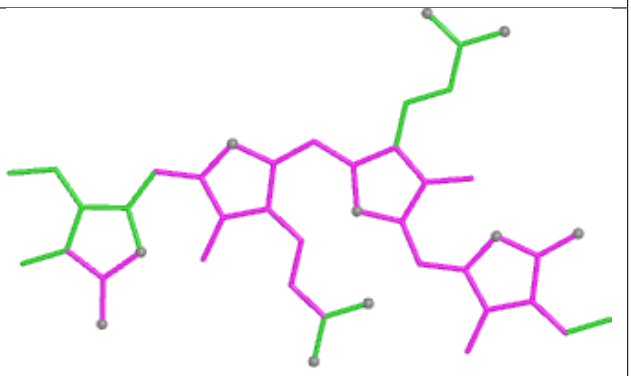


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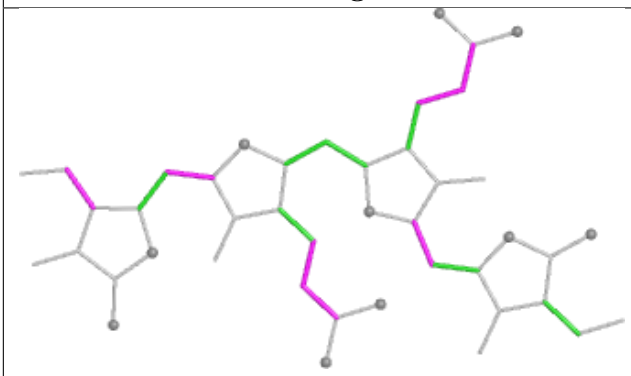
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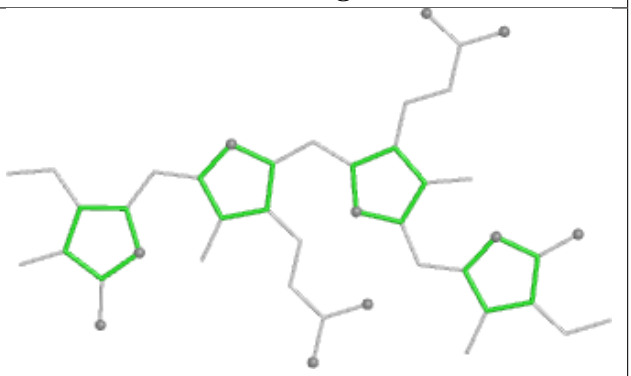
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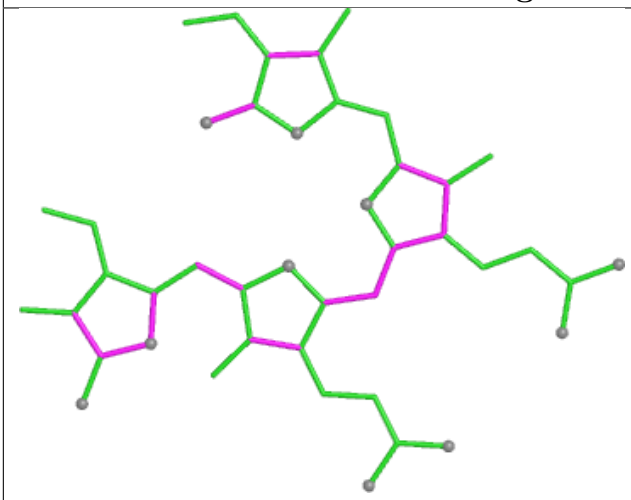


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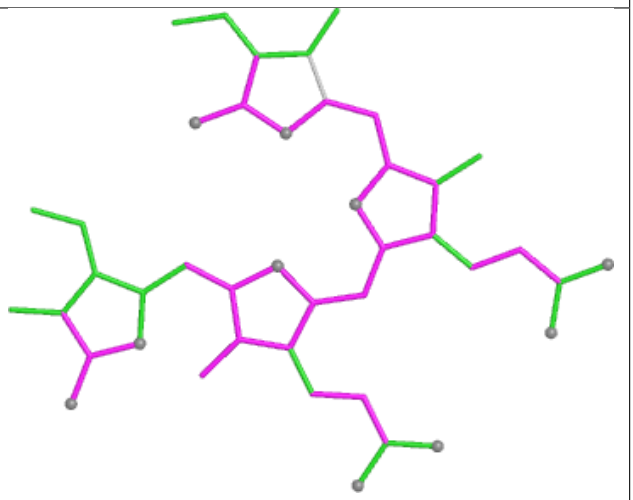


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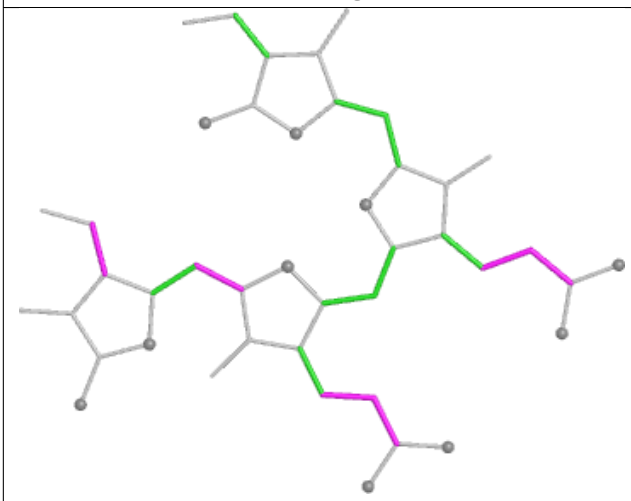
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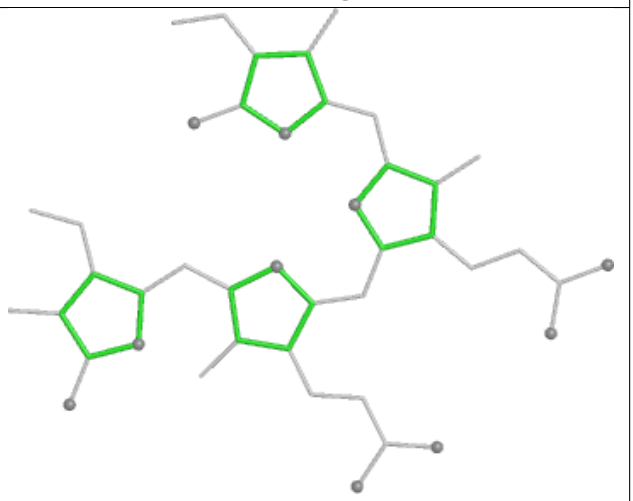
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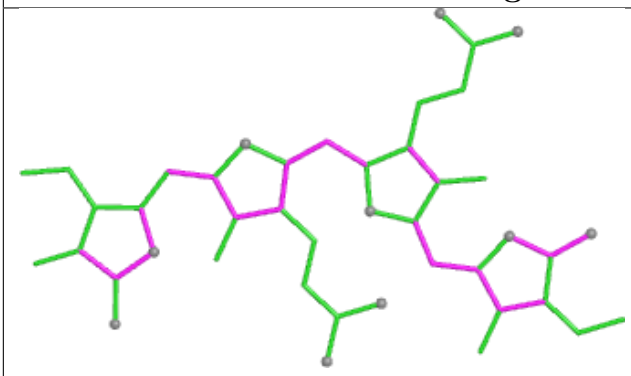


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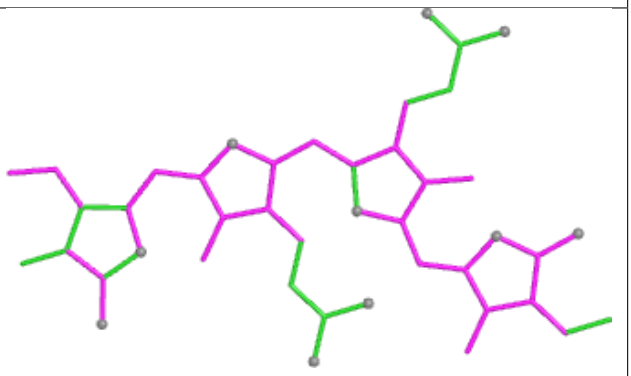


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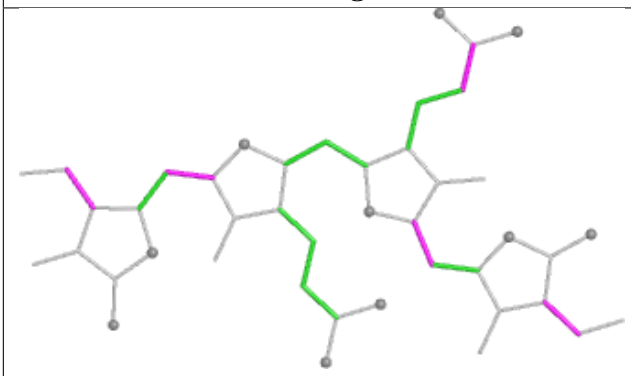
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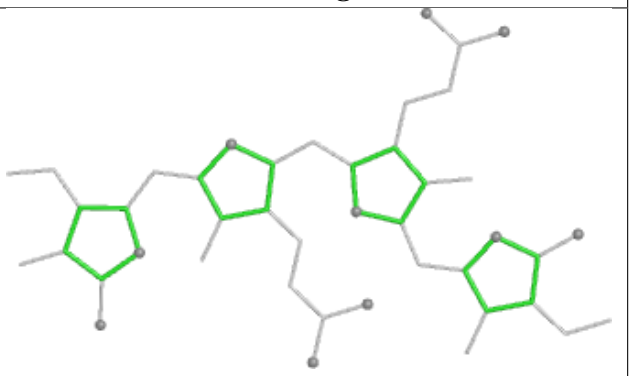
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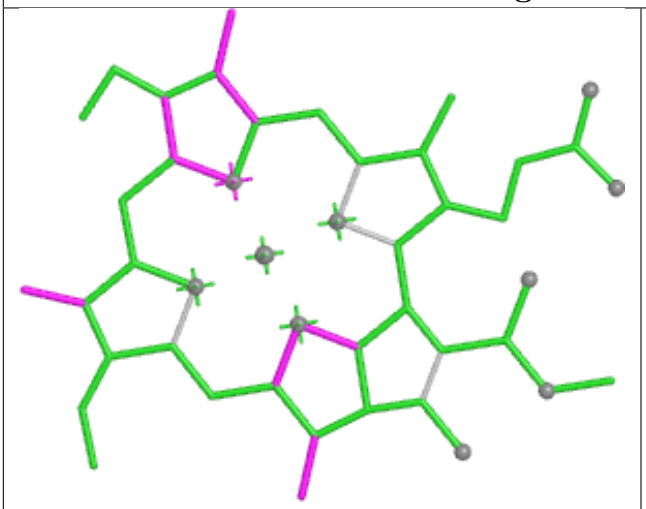


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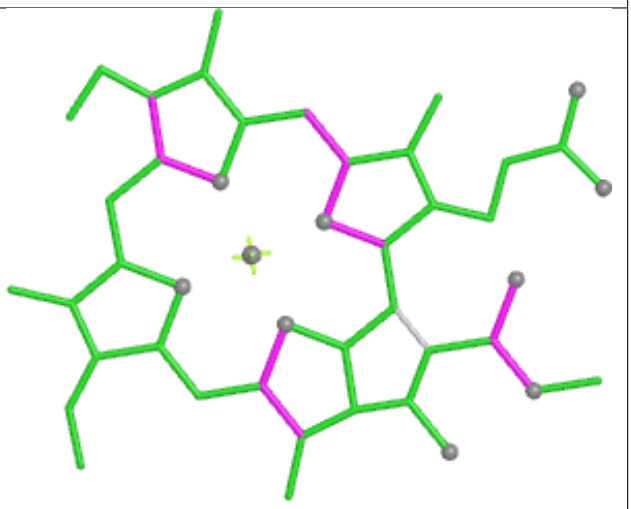


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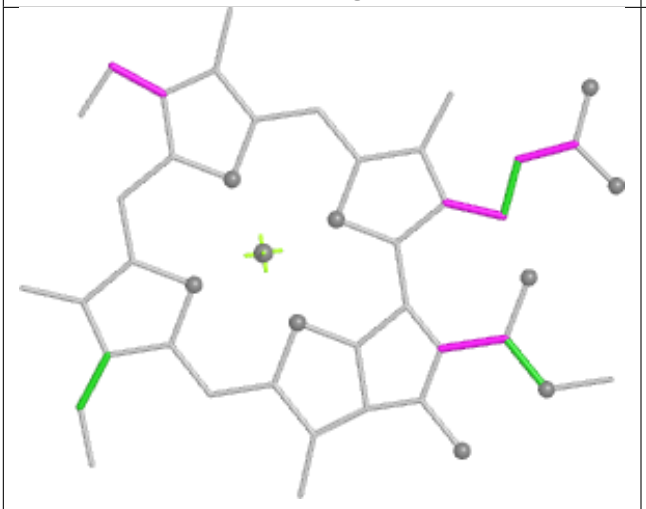
Ligand CLA A2 816



Bond lengths



Bond angles

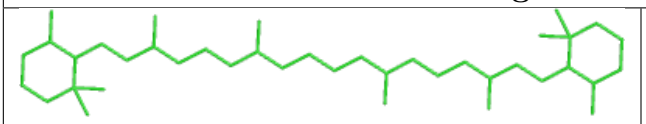


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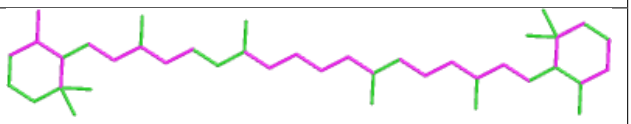


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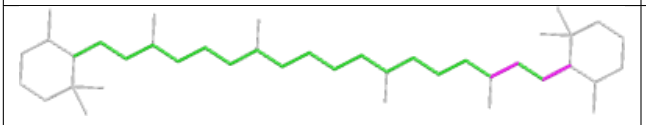
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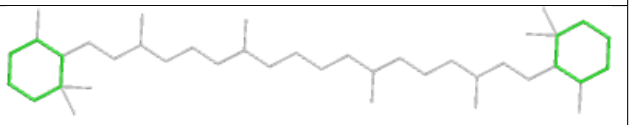
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Bond angles

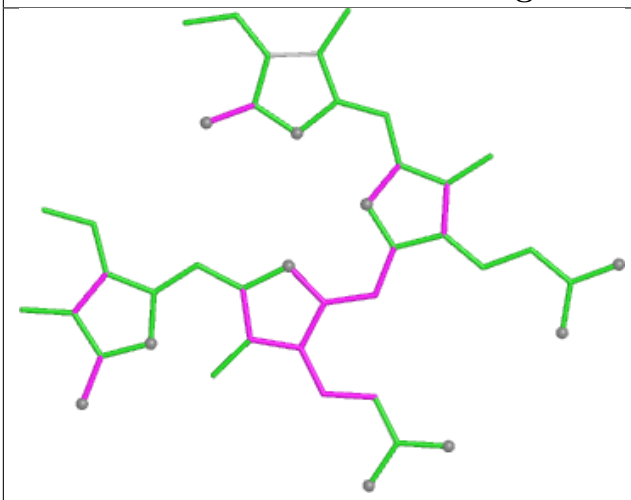


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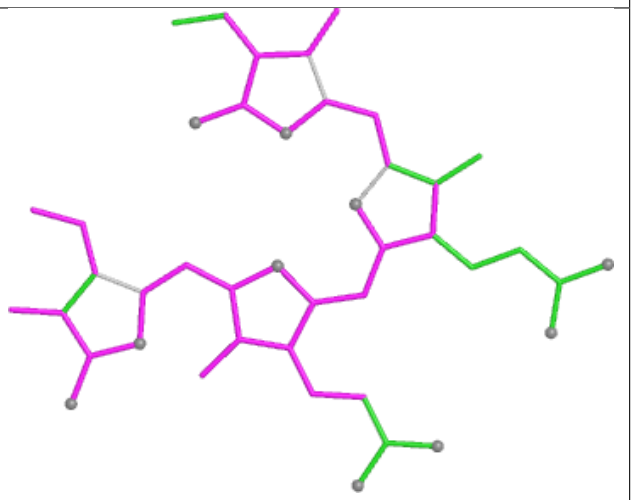


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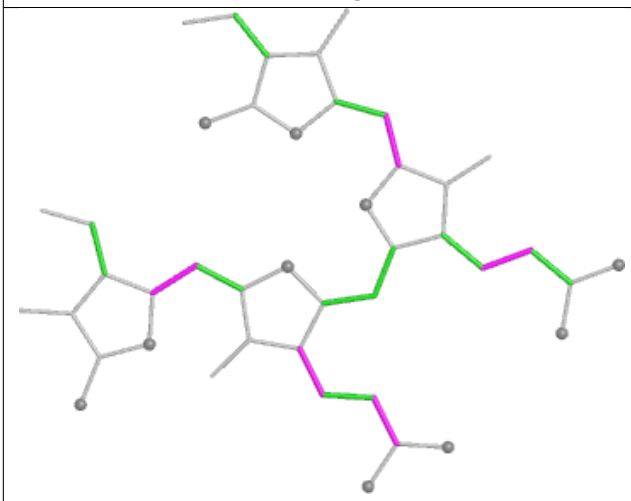
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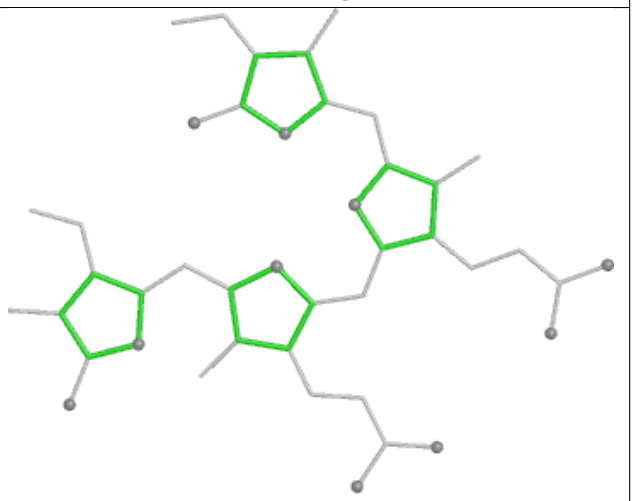
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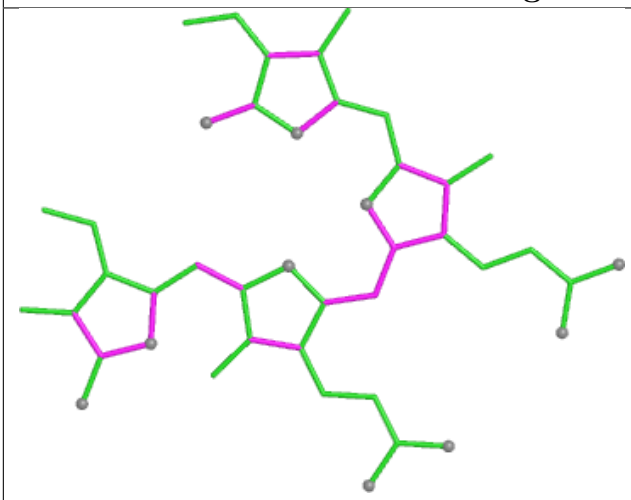


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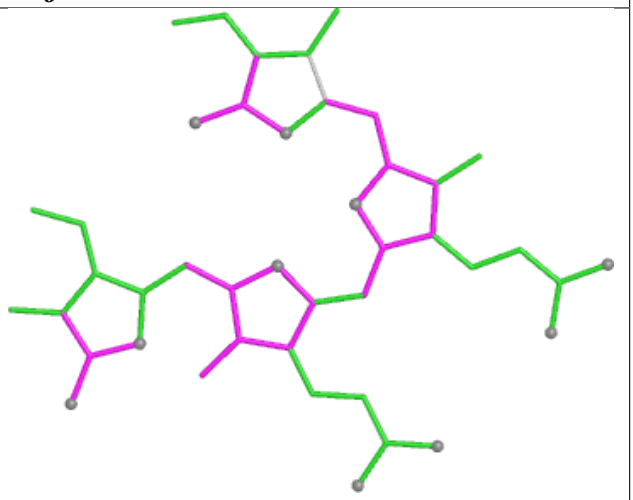


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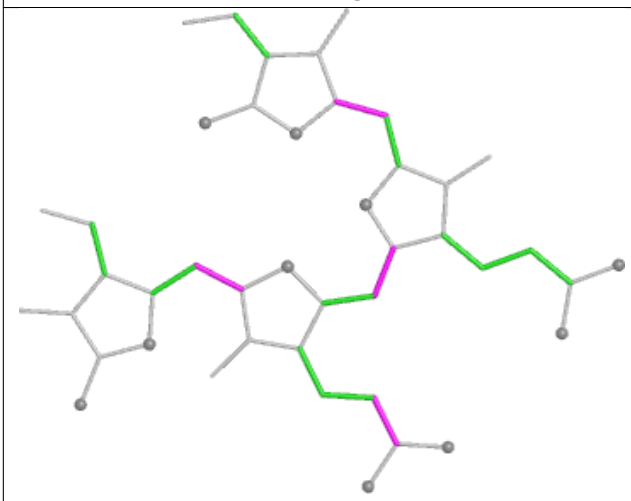
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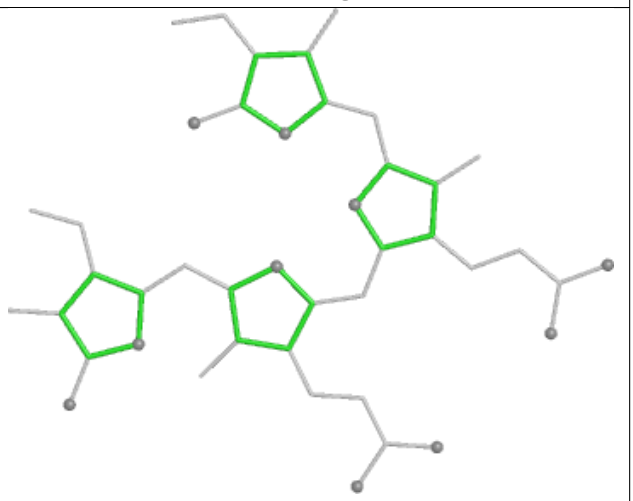
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Bond angles

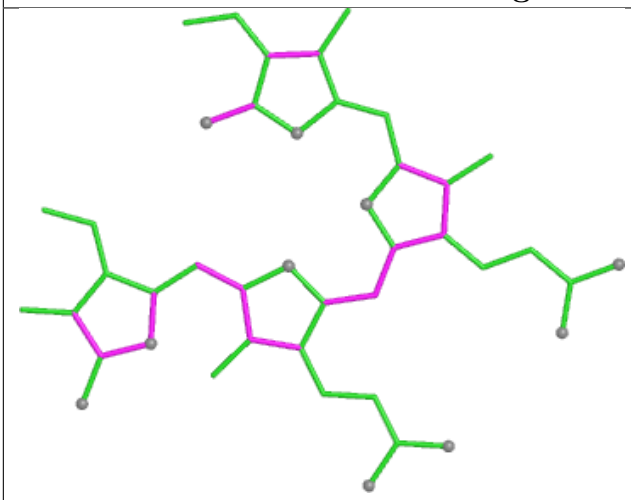


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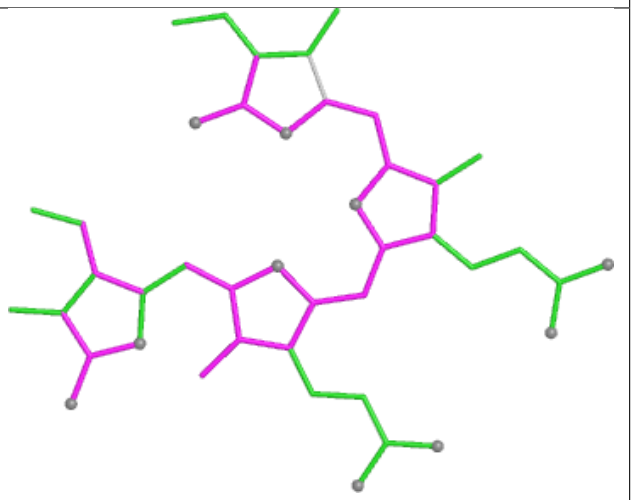


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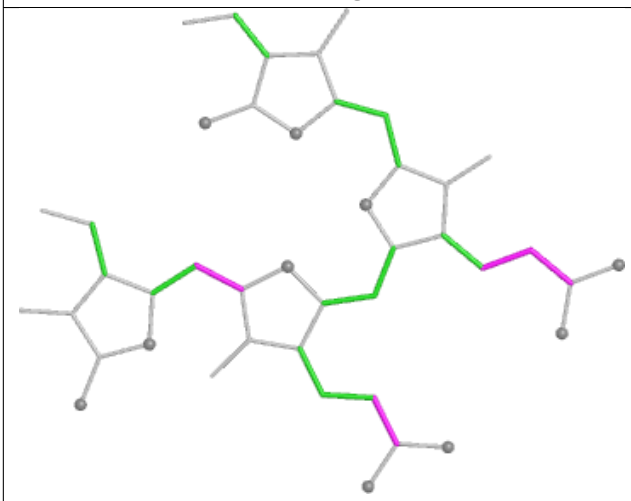
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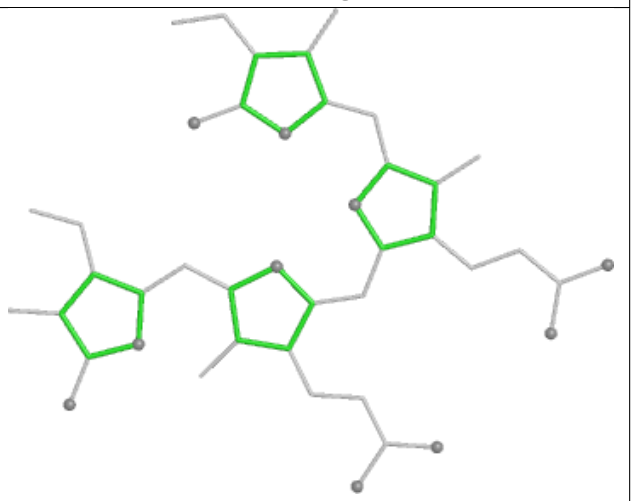
Bond lengths



Bond angles

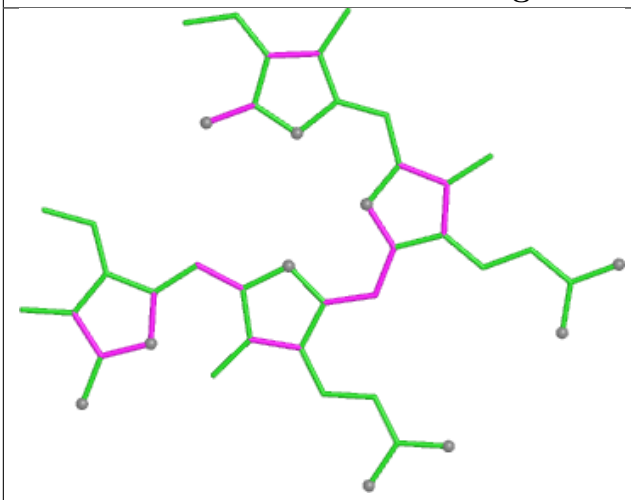


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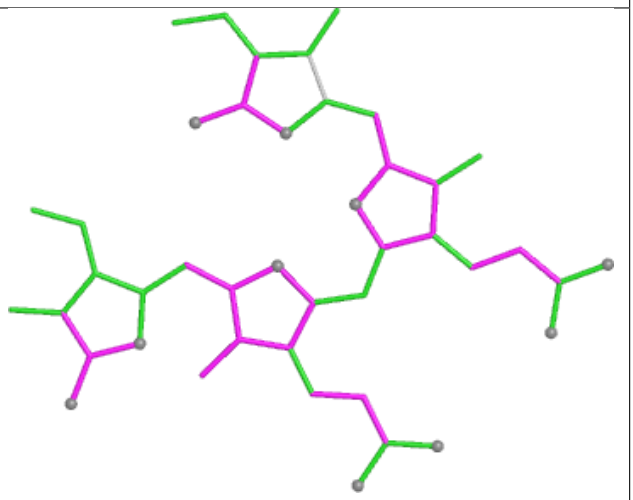


Rings

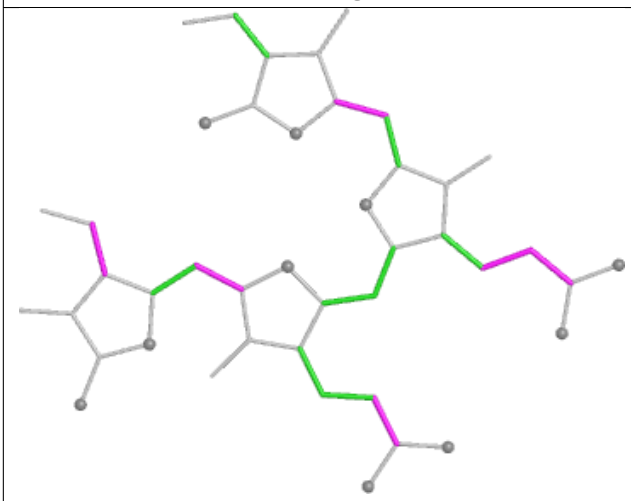
Ligand PEB VA 201



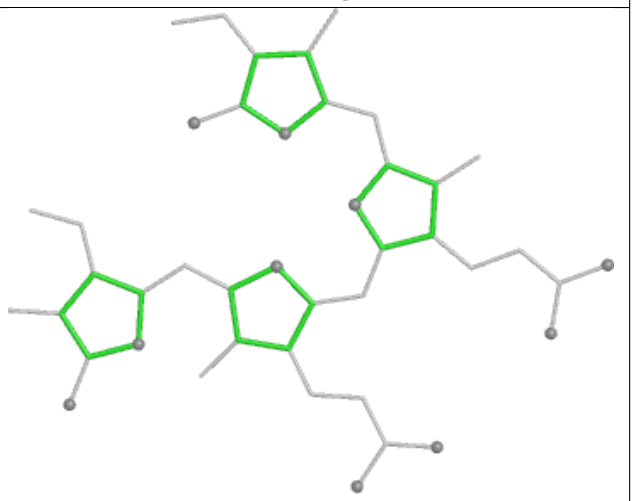
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Bond angles

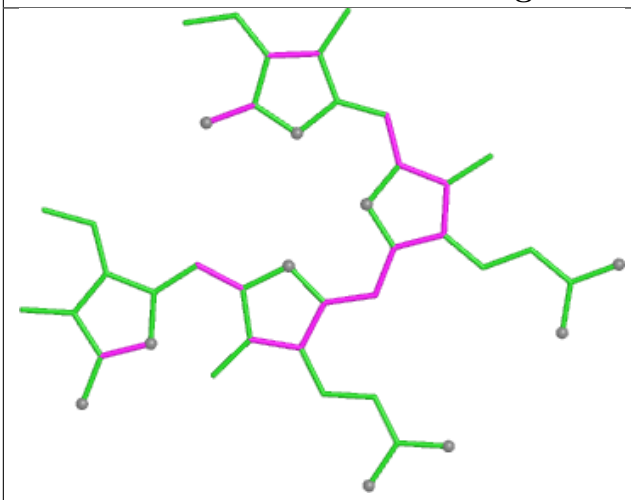


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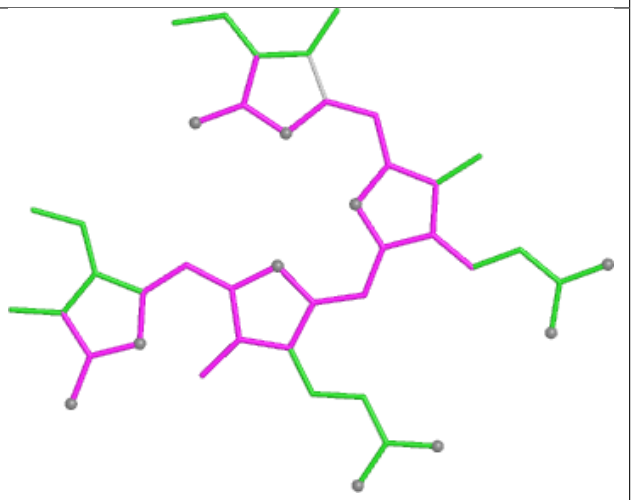


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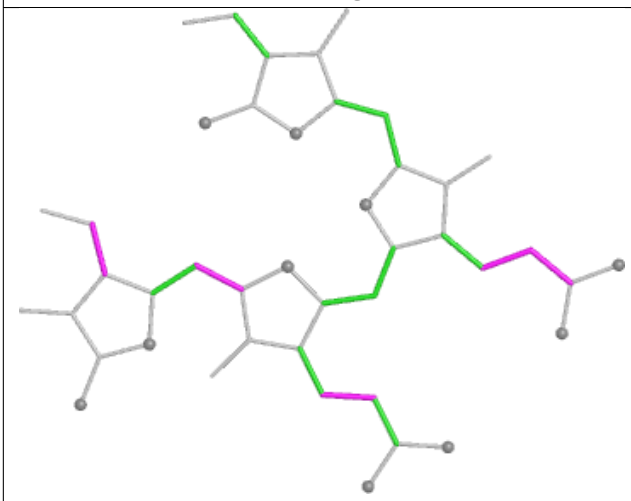
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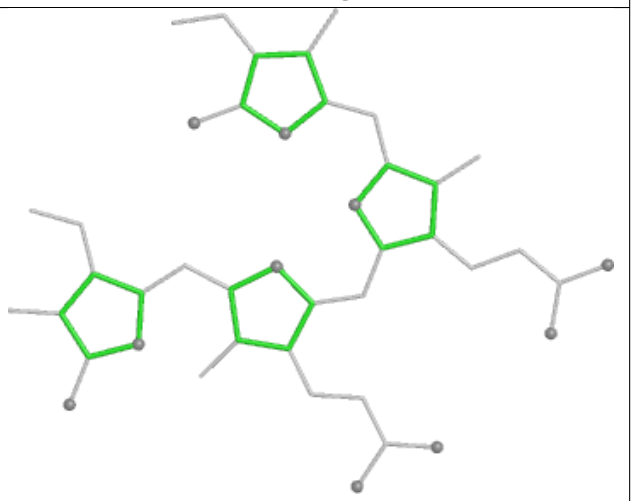
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Bond angles

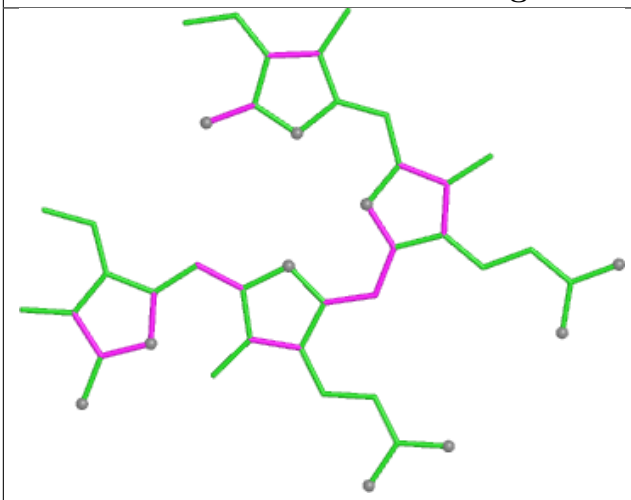


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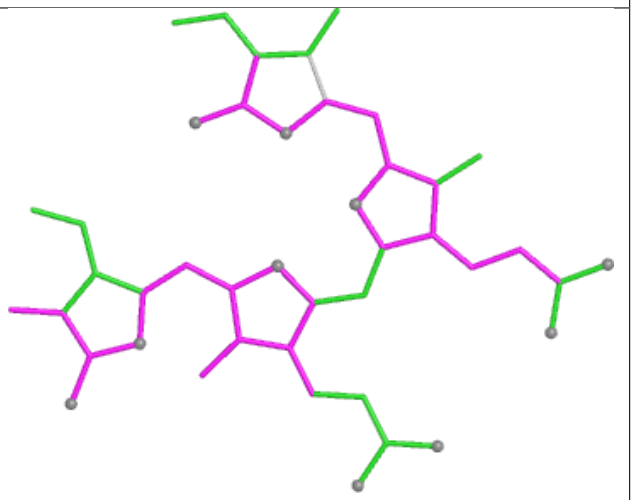


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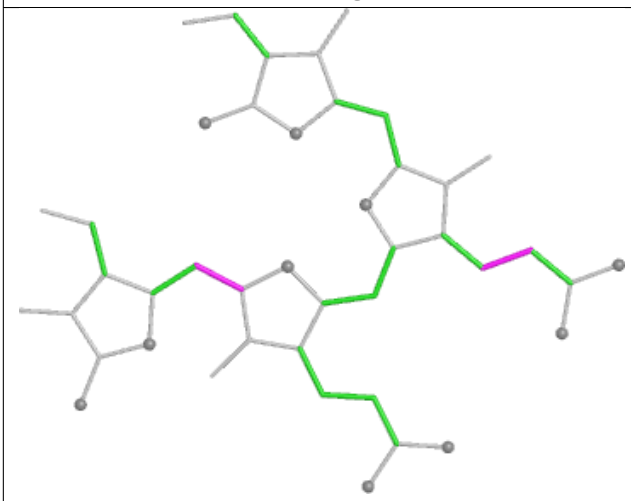
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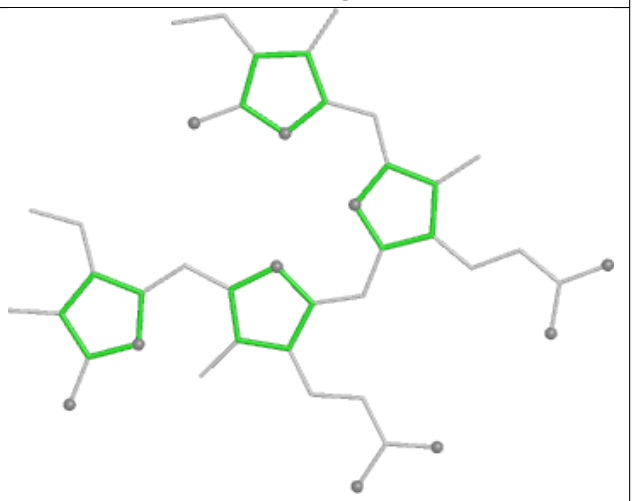
Bond lengths



Bond angles

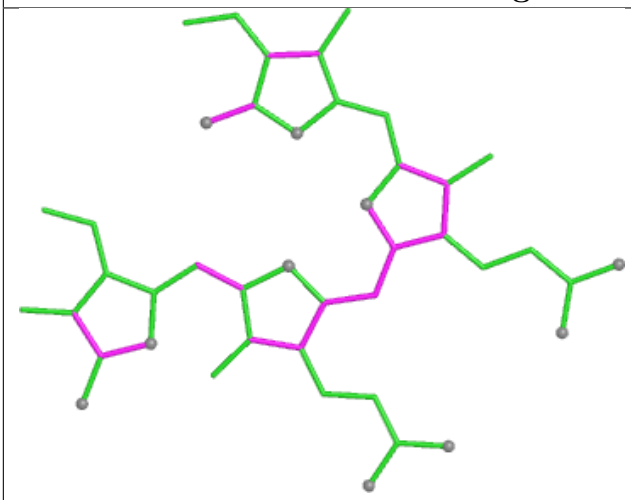


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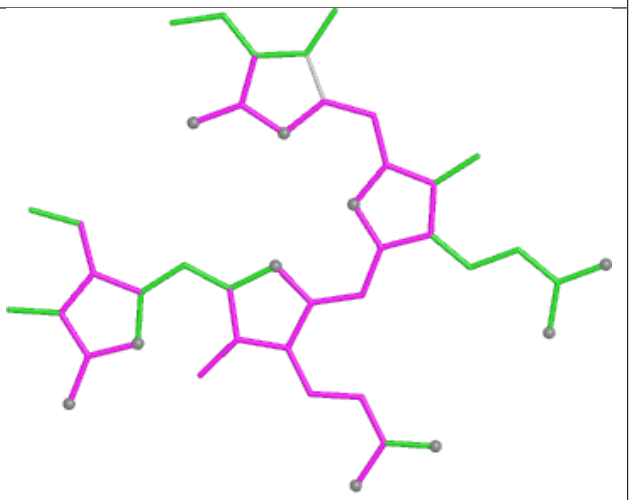


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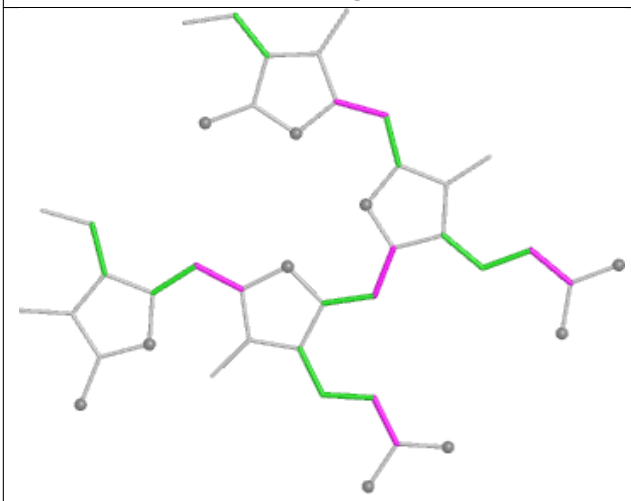
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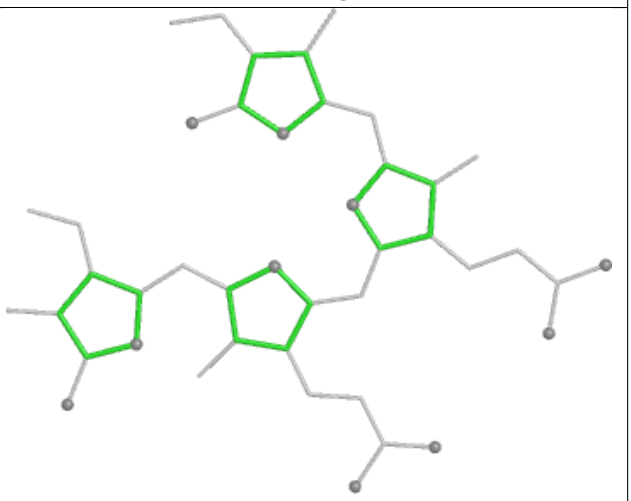
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Bond angles

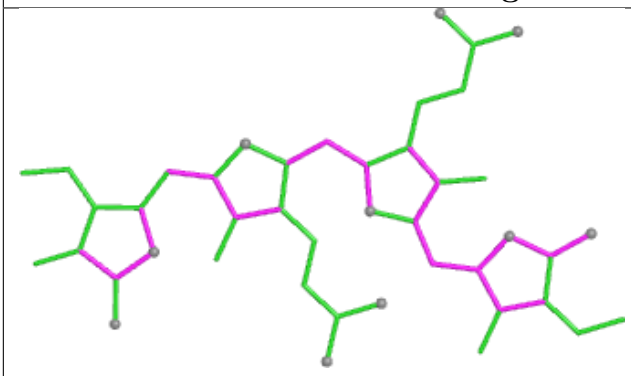


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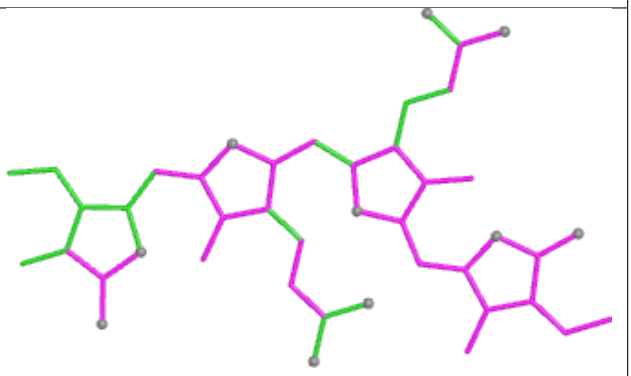


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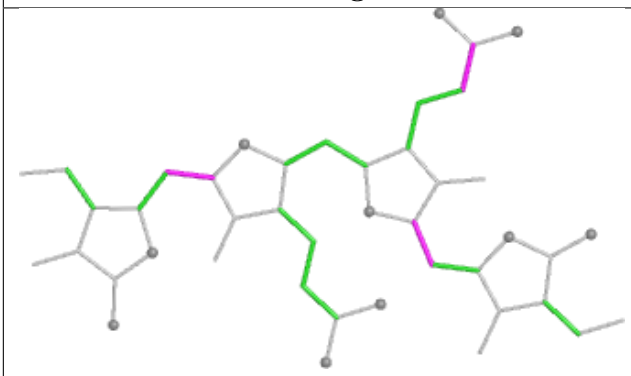
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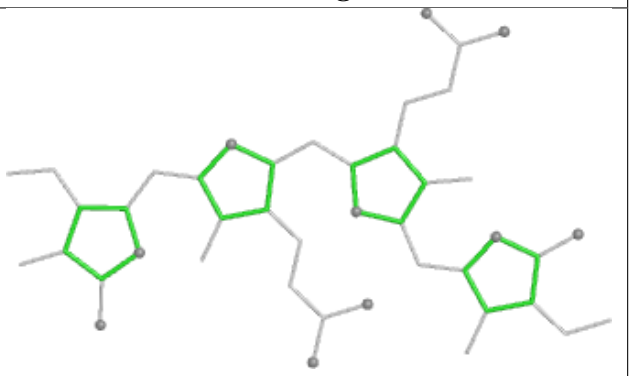
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Bond angles

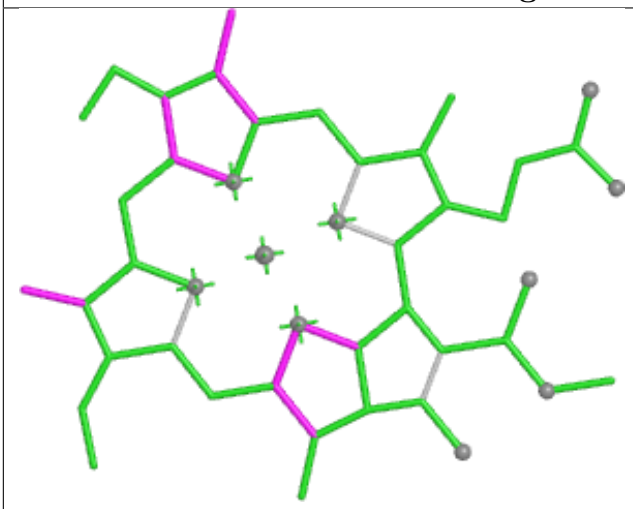


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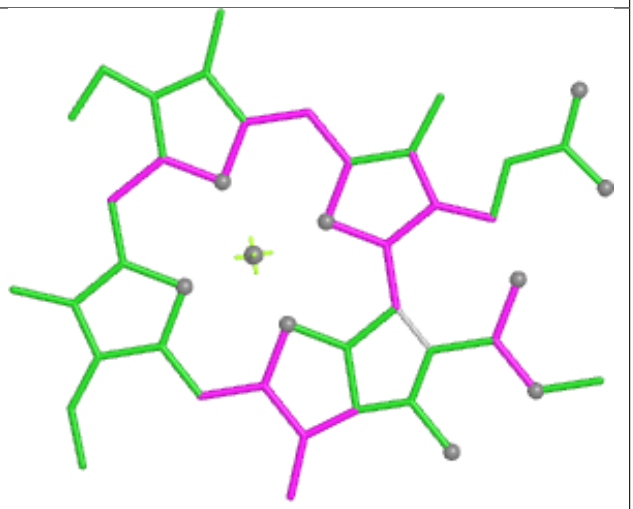


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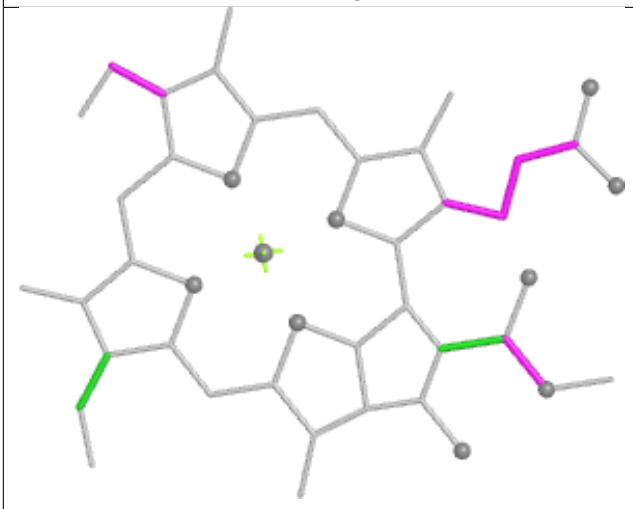
Ligand CLA 32 302



Bond lengths



Bond angles

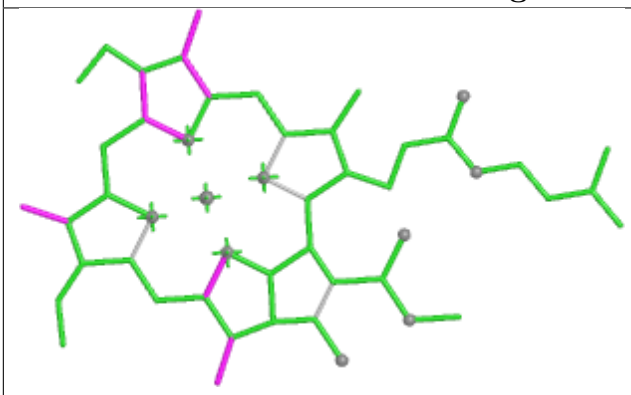


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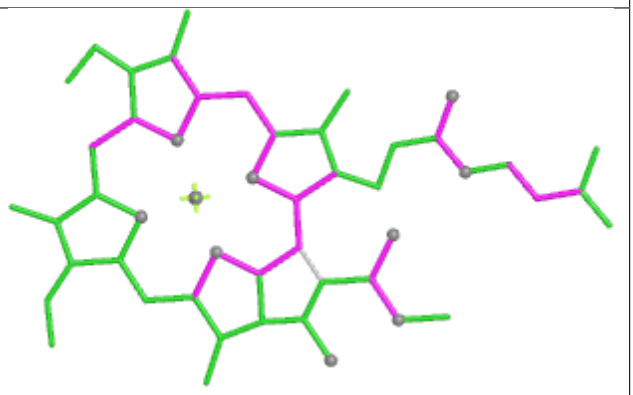


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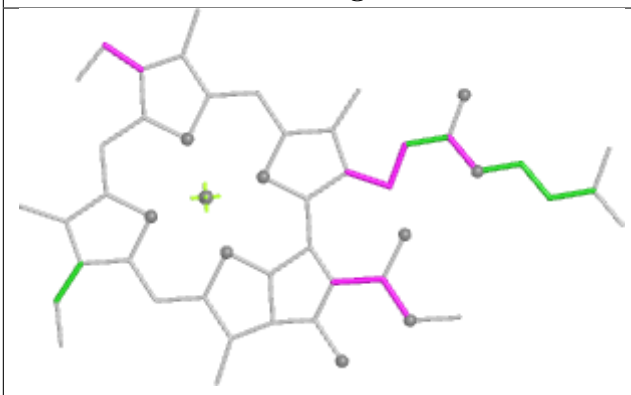
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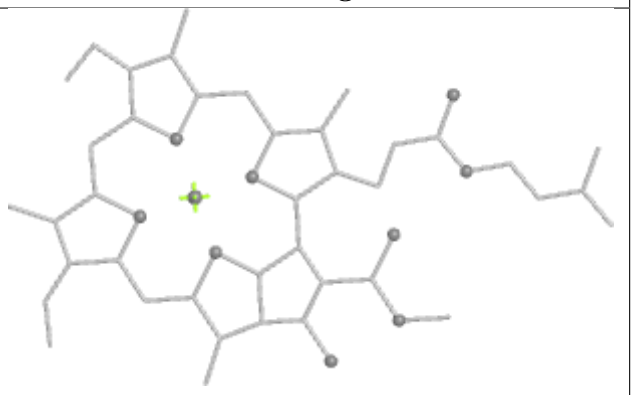
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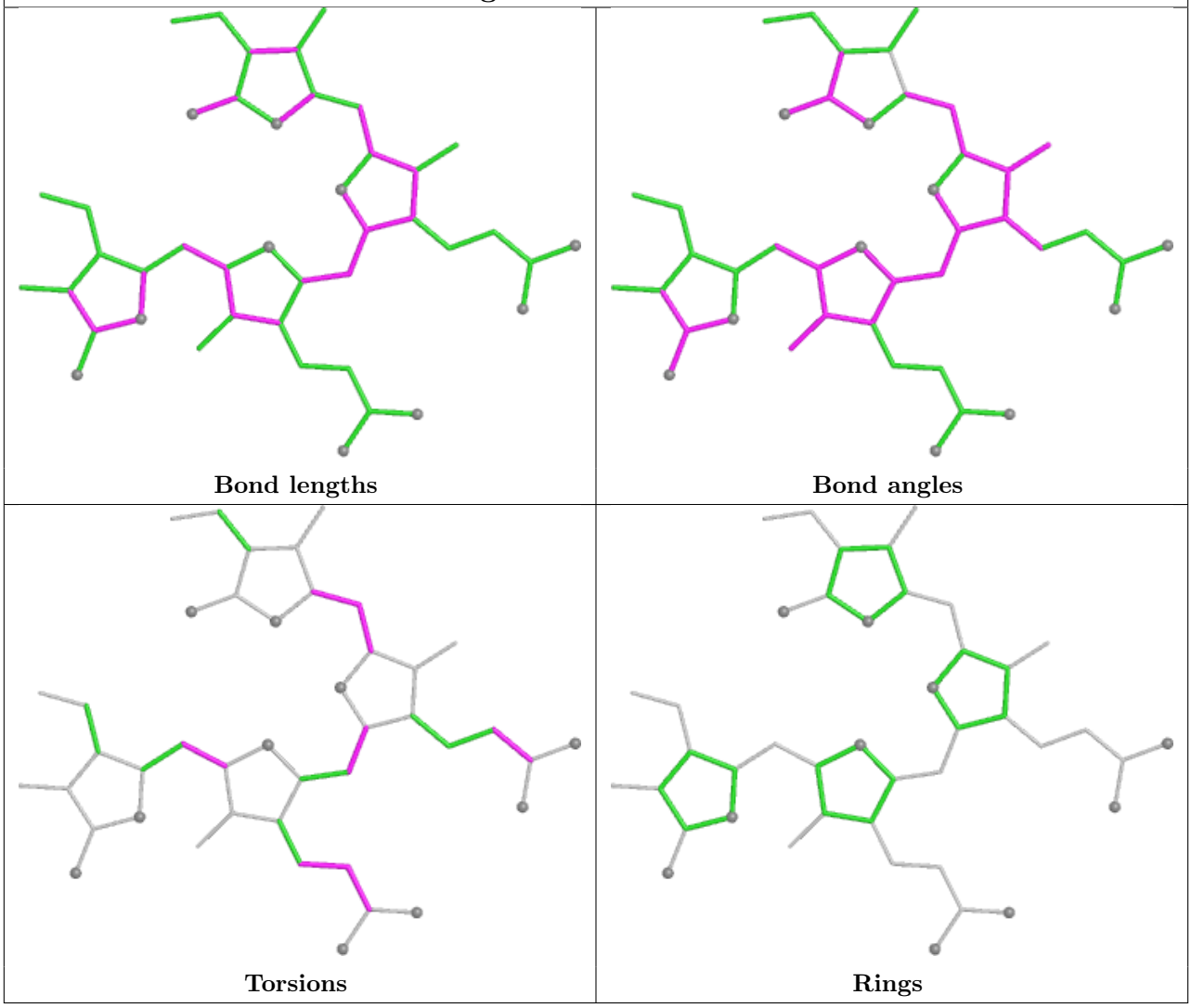


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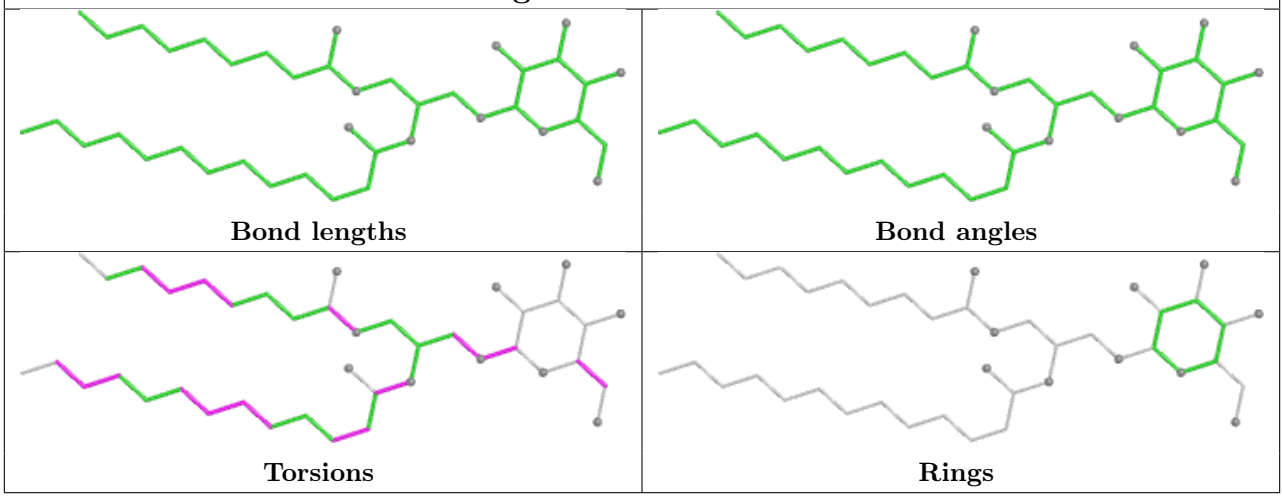


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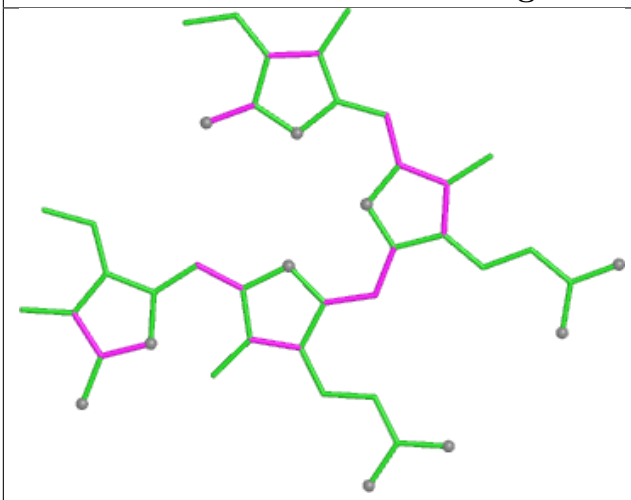
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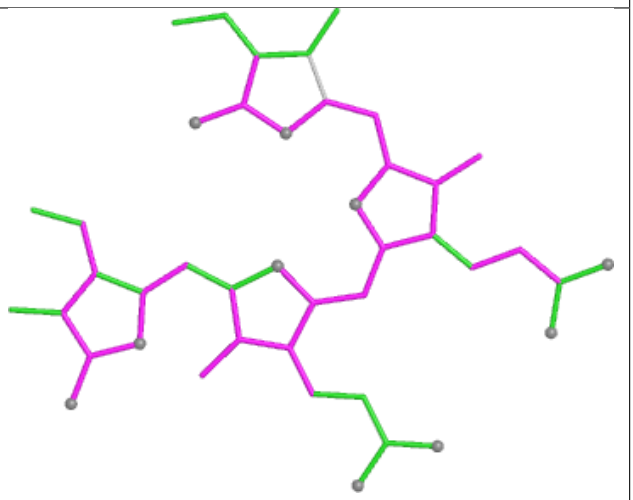
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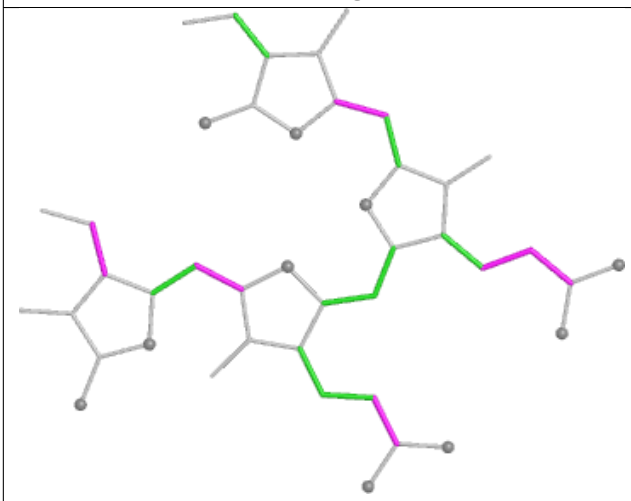
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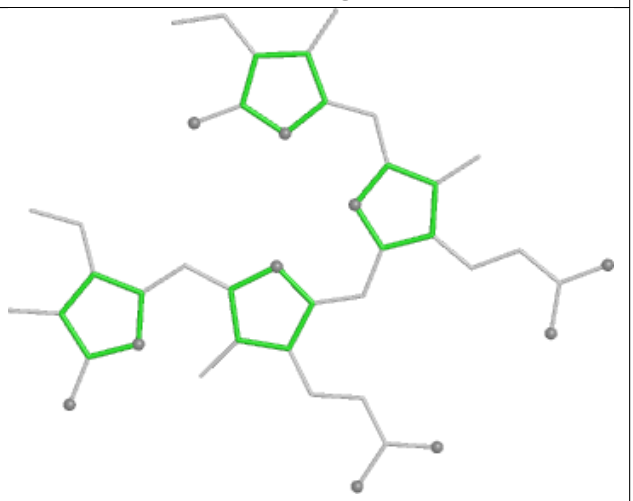
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Bond angles

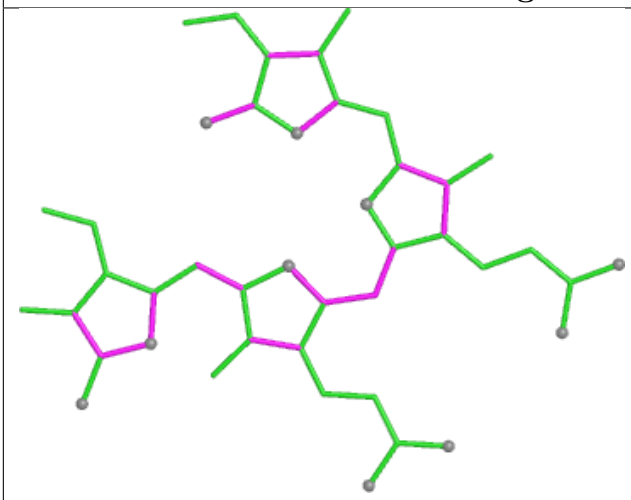


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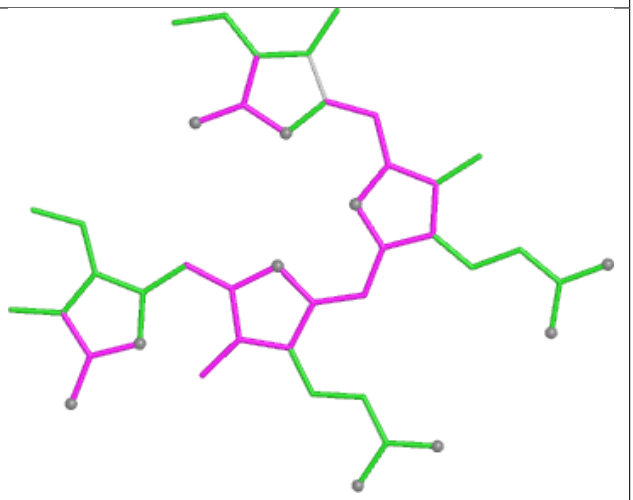


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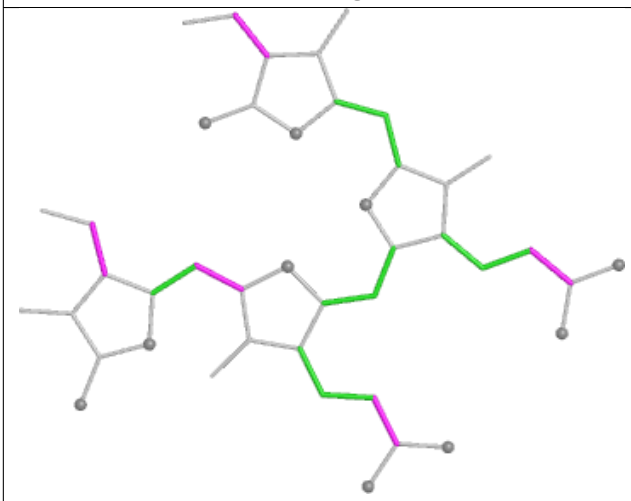
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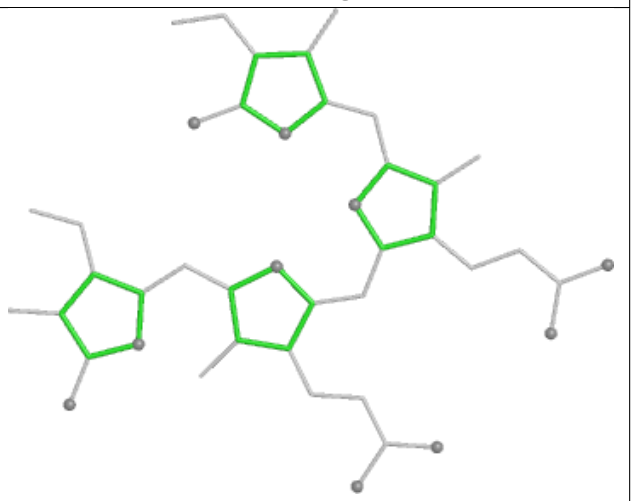
Bond lengths



Bond angles

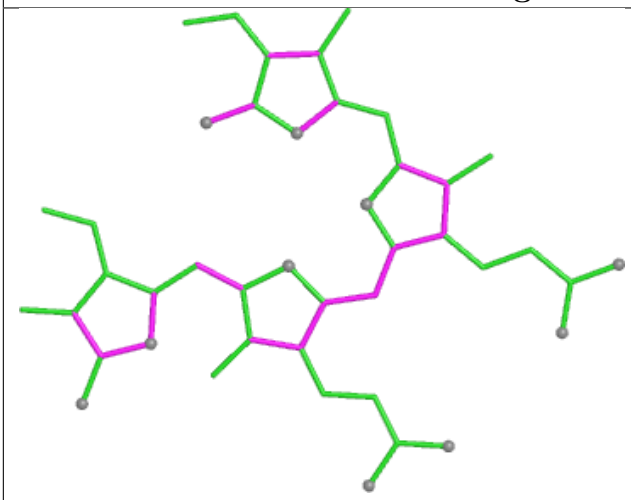


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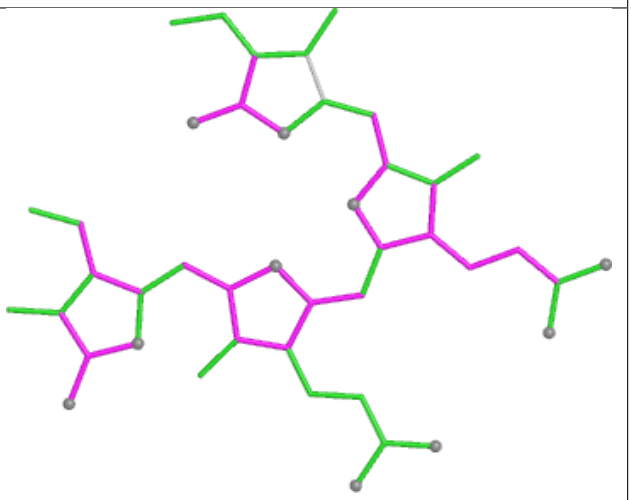


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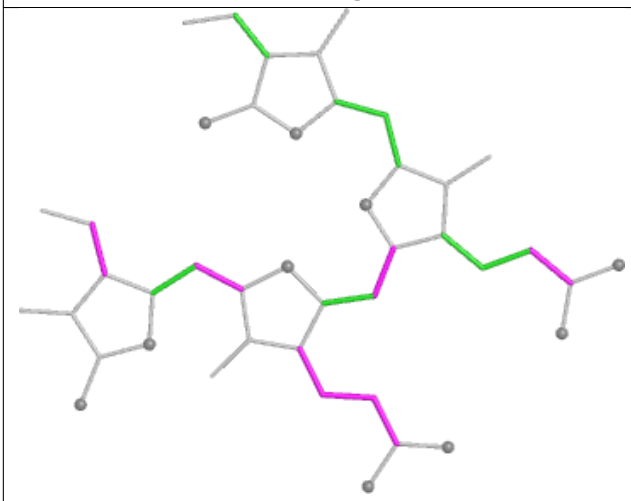
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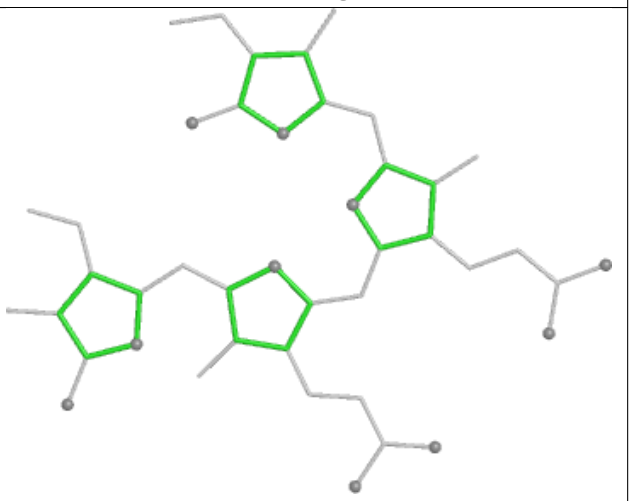
Bond lengths



Bond angles

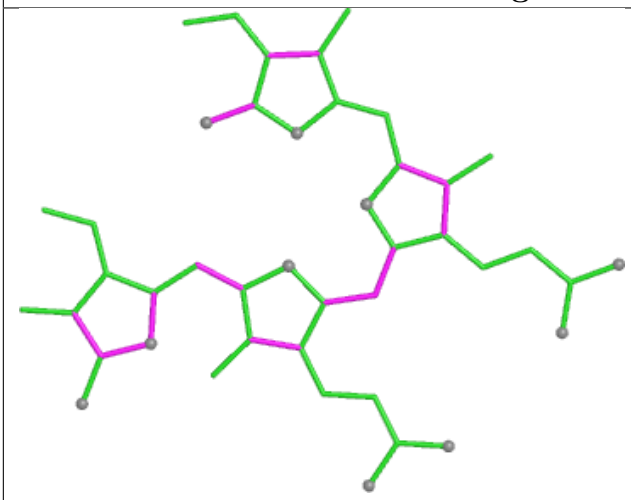


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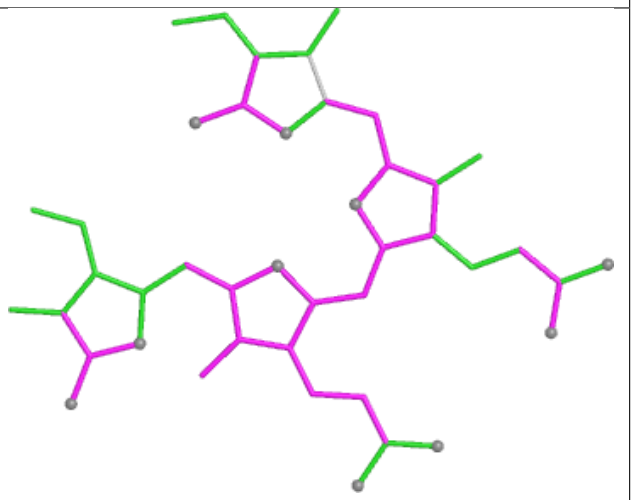


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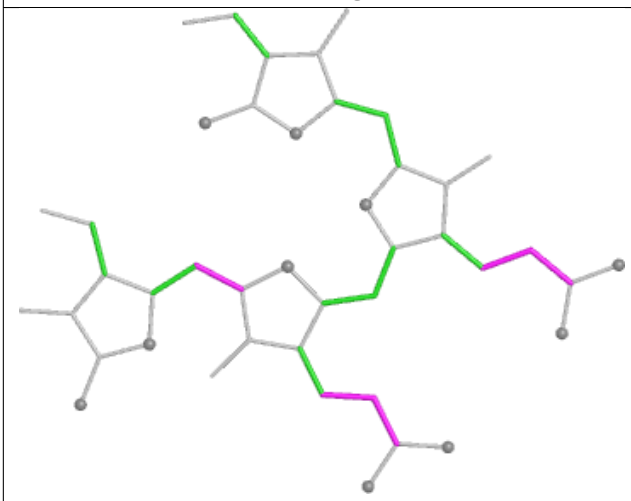
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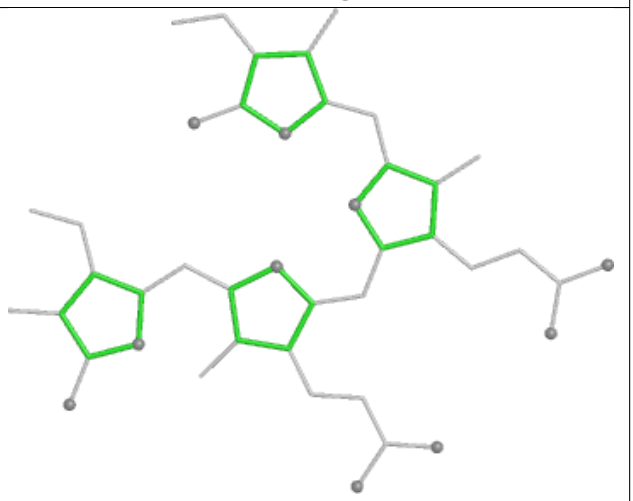
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Bond angles

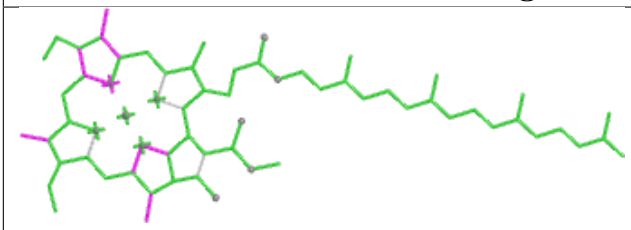


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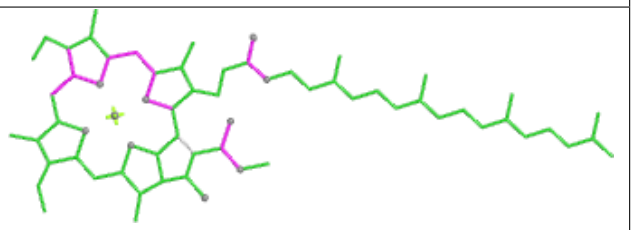


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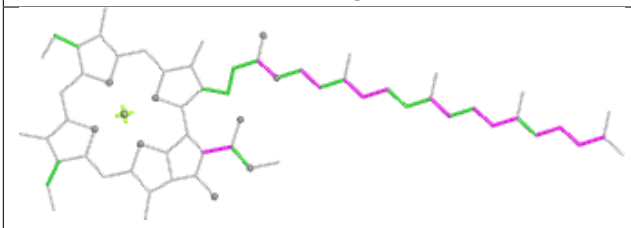
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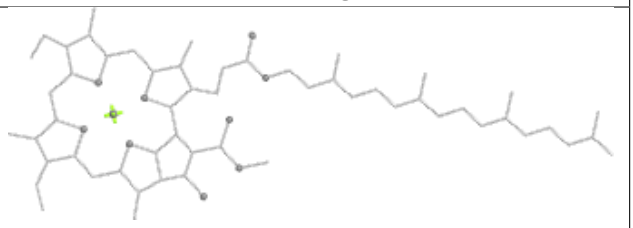
Bond lengths



Bond angles

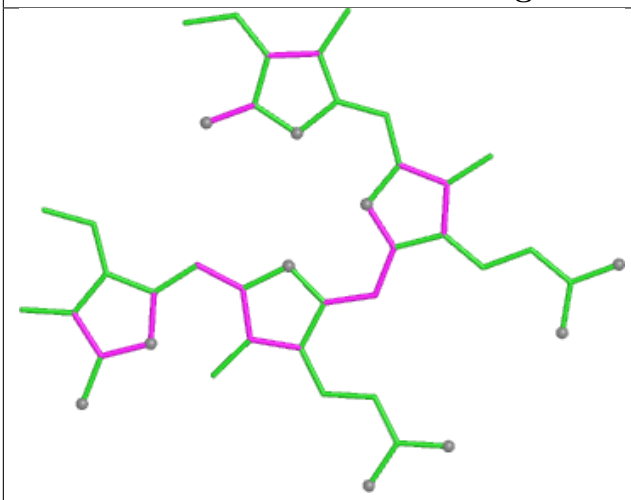


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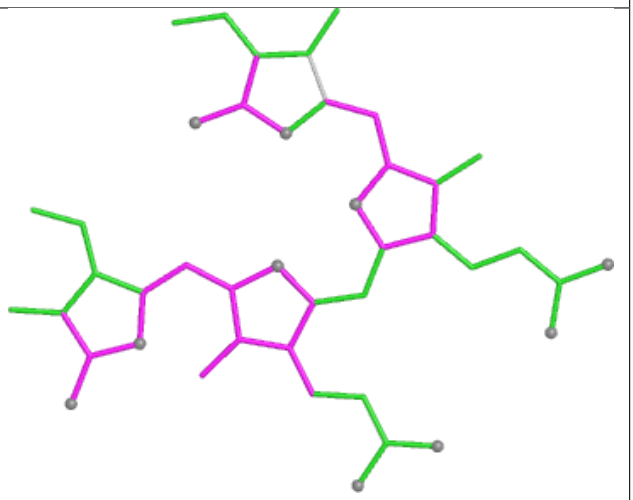


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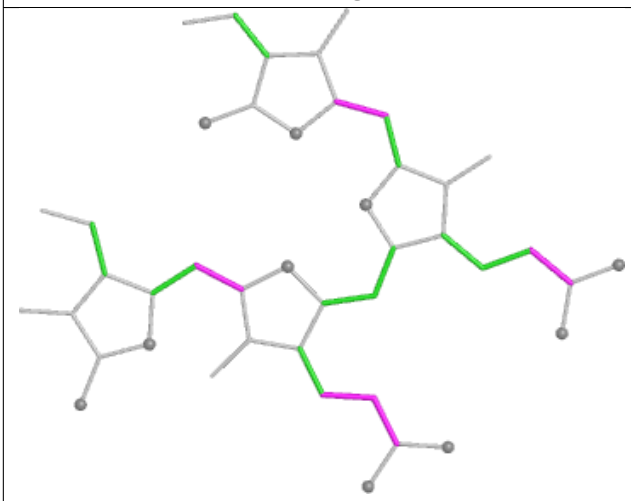
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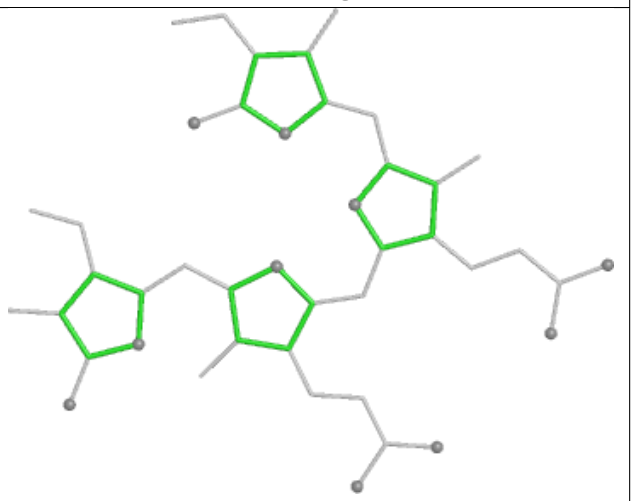
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Bond angles

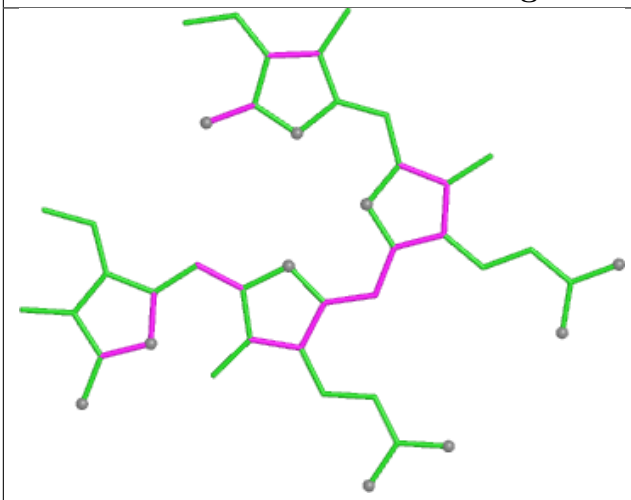


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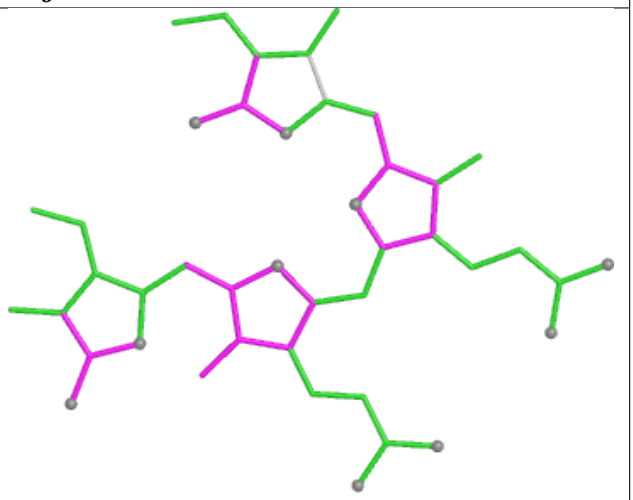


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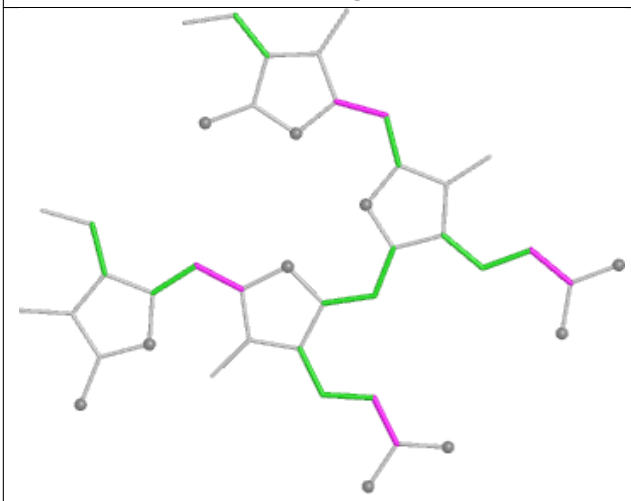
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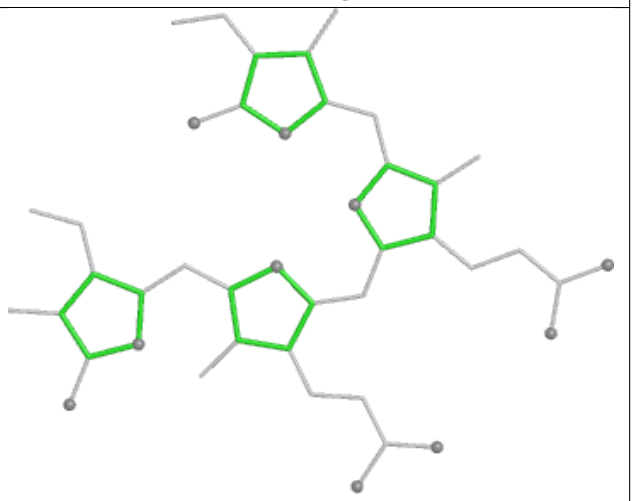
Bond lengths



Bond angles

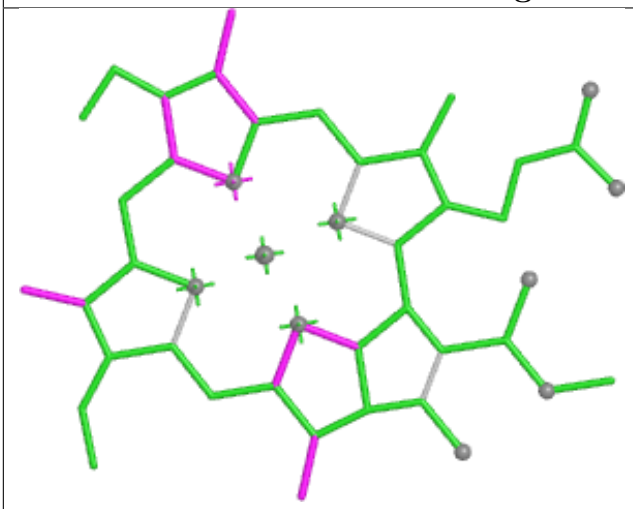


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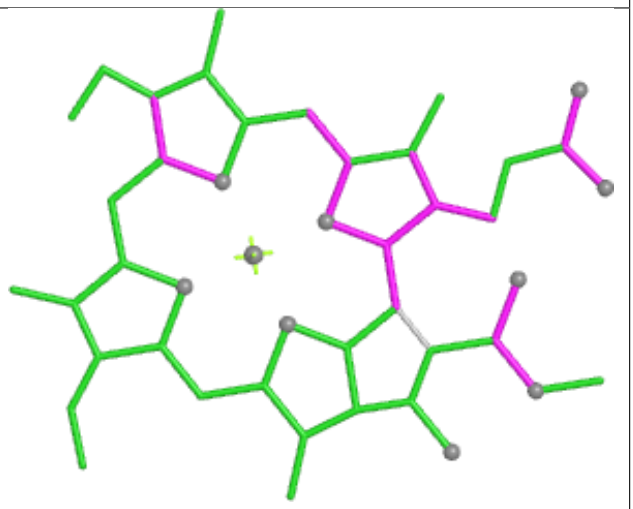


Rings

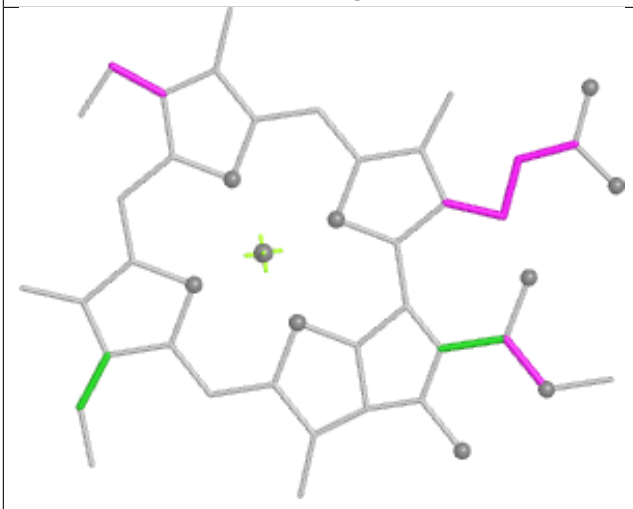
Ligand CLA 1N 611



Bond lengths



Bond angles

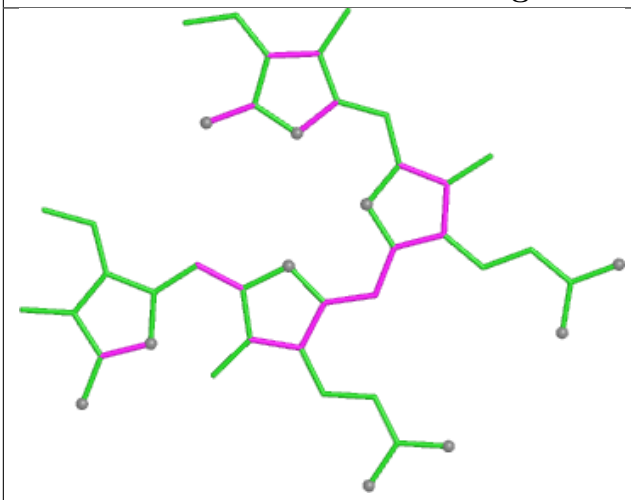


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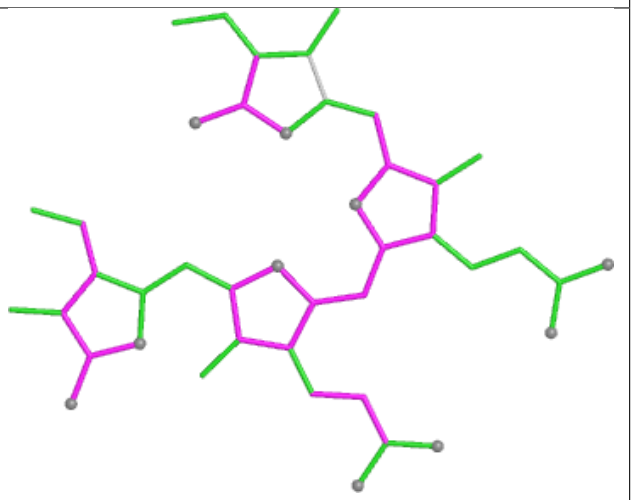


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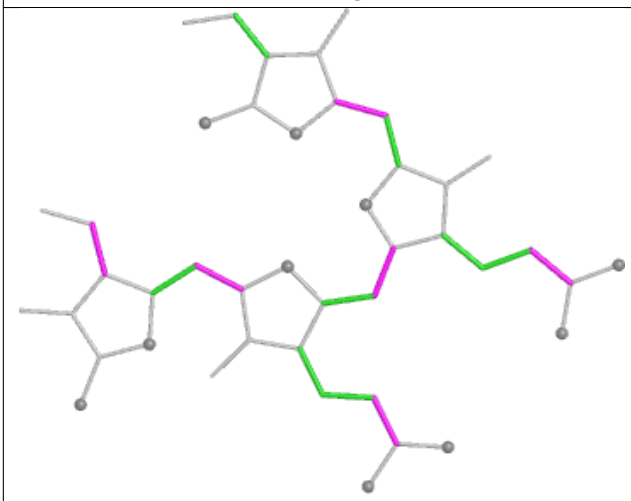
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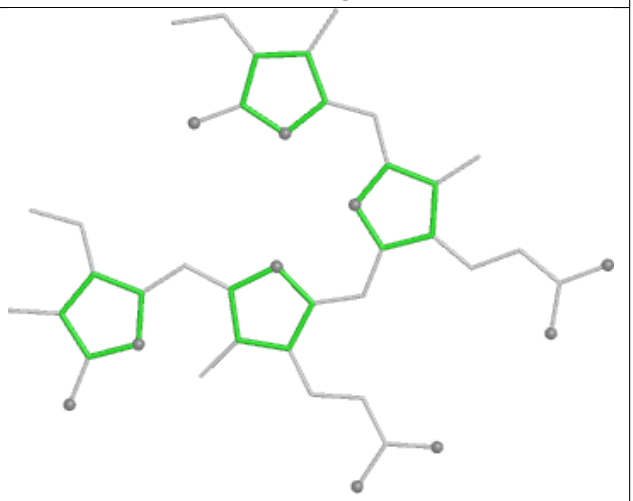
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Bond angles

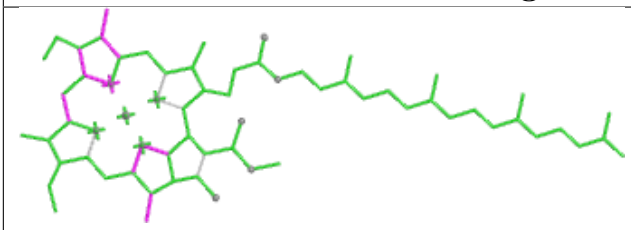


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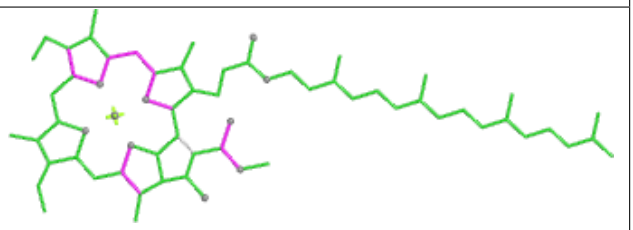


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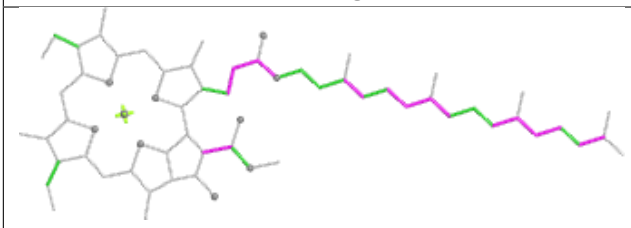
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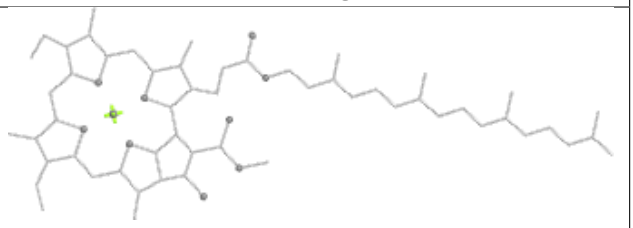
Bond lengths



Bond angles

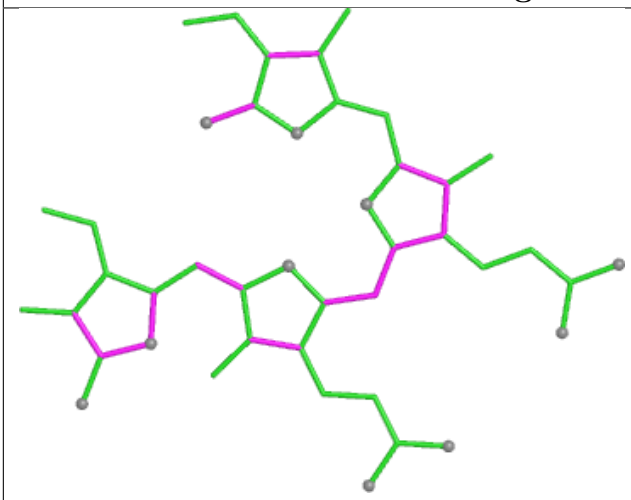


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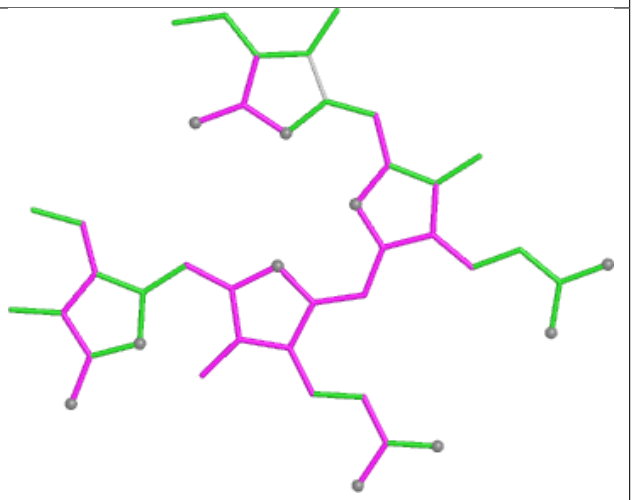


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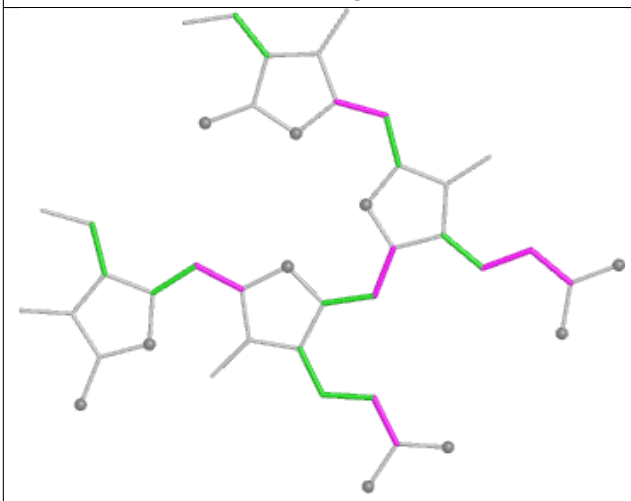
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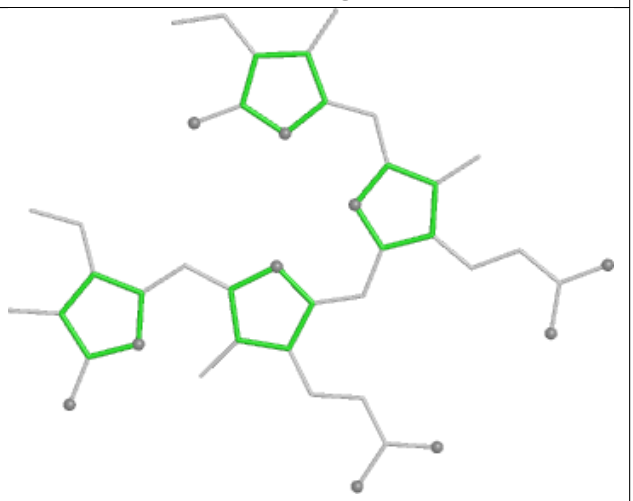
Bond lengths



Bond angles

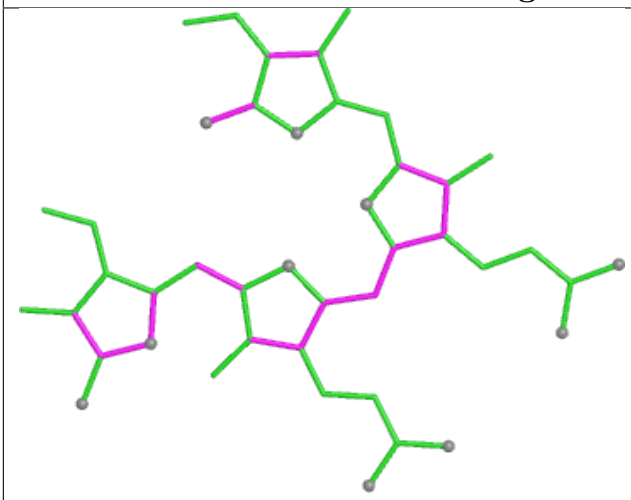


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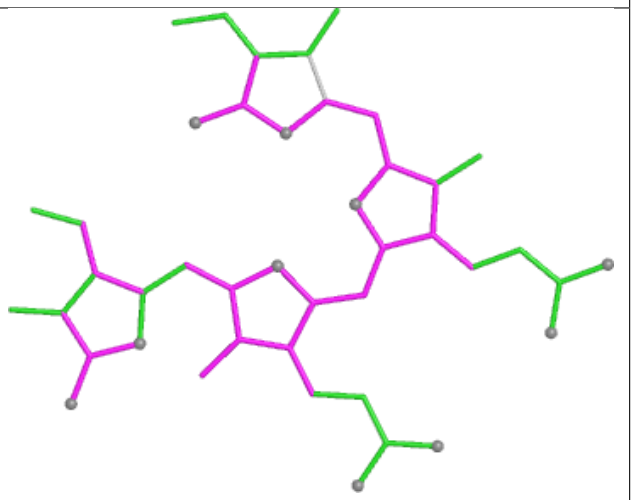


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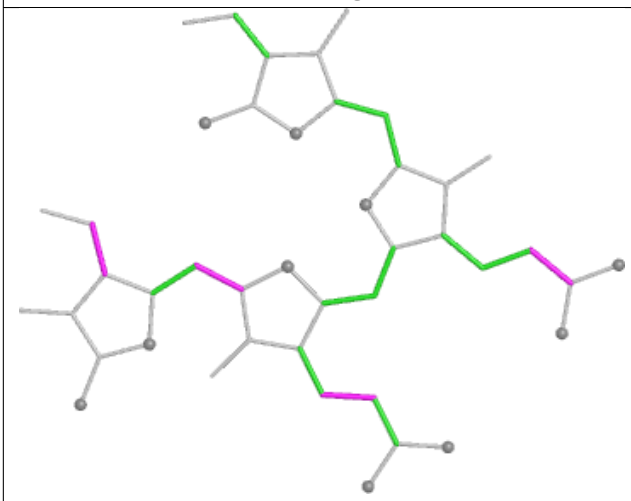
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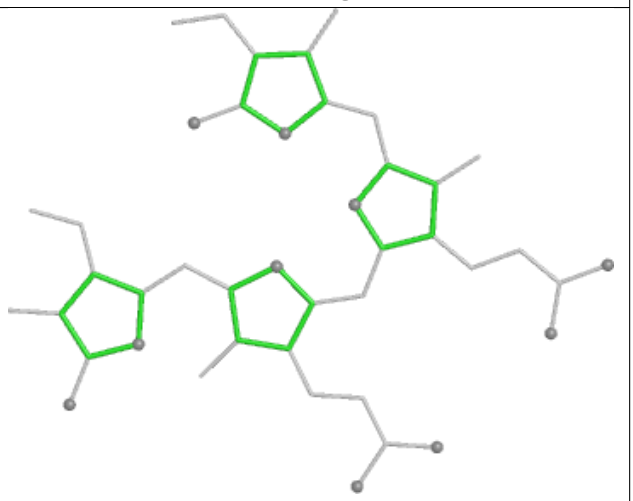
Bond lengths



Bond angles

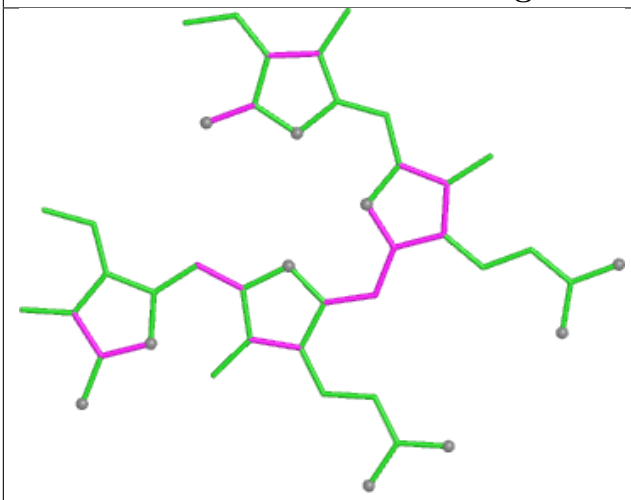


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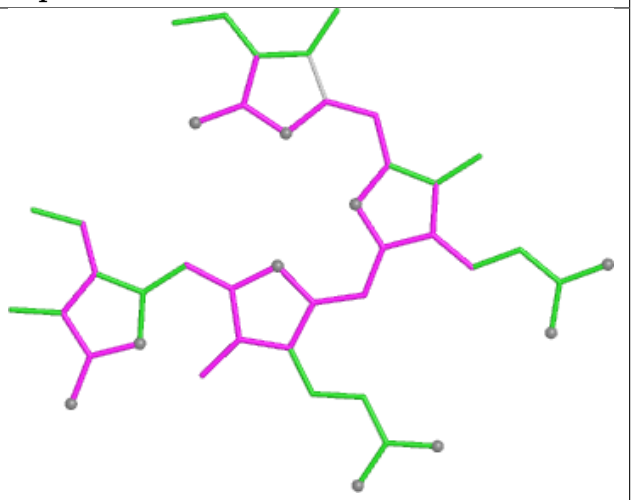


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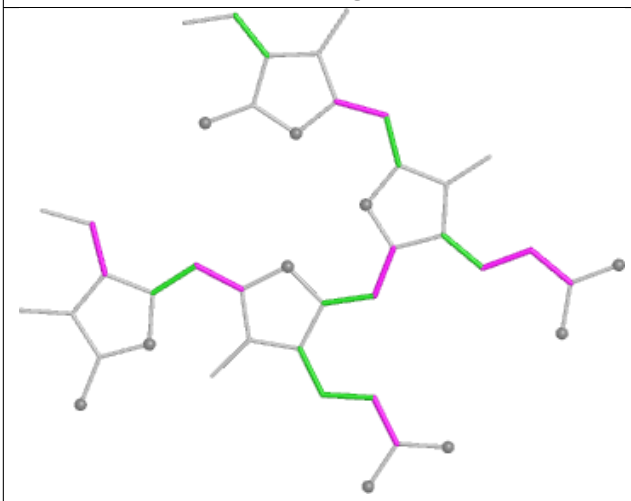
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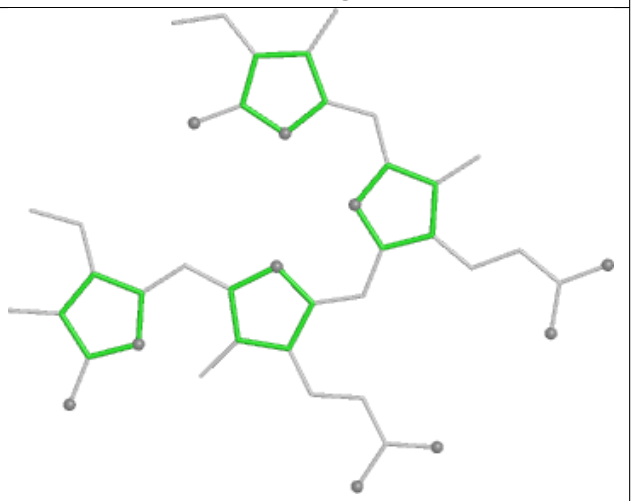
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Bond angles

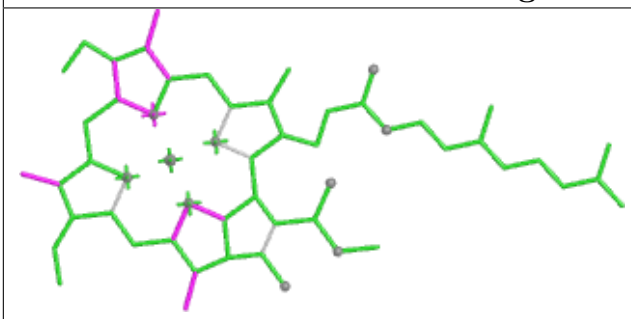


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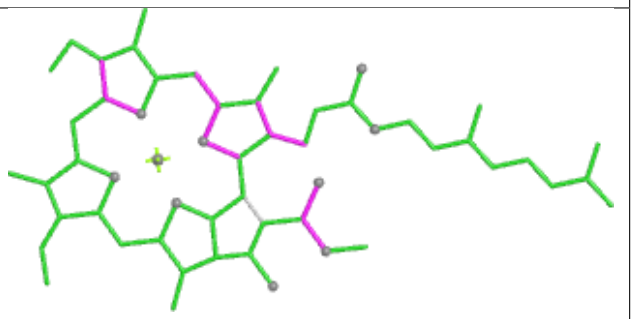


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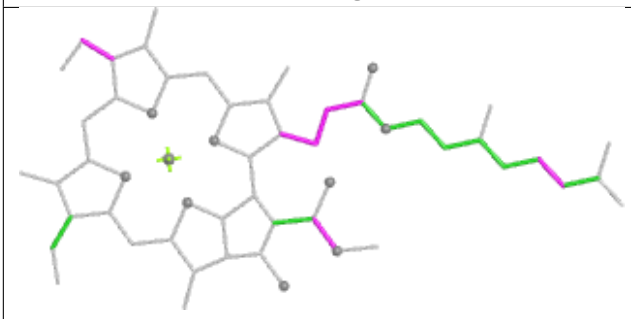
Ligand CLA cL 516



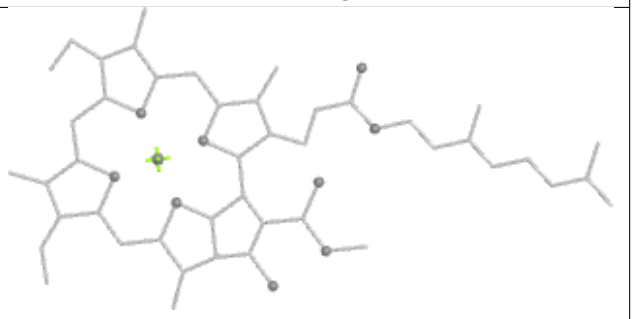
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Bond angles

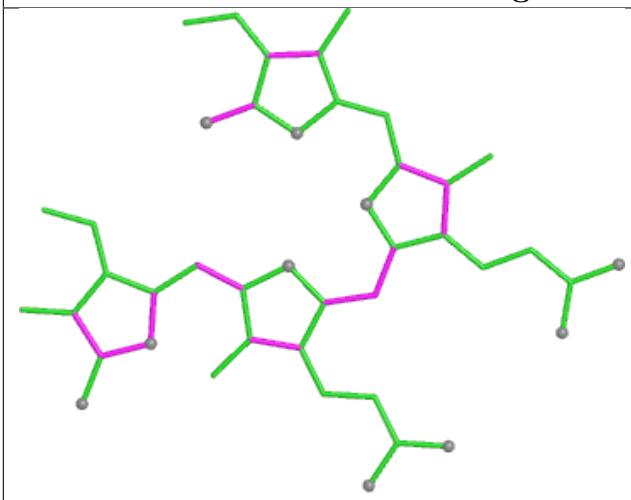


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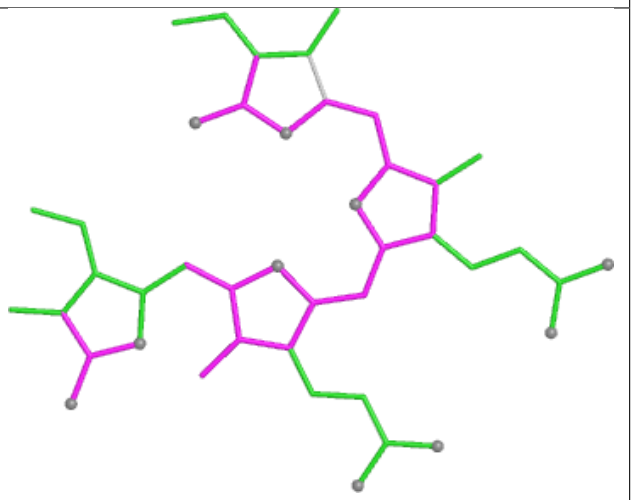


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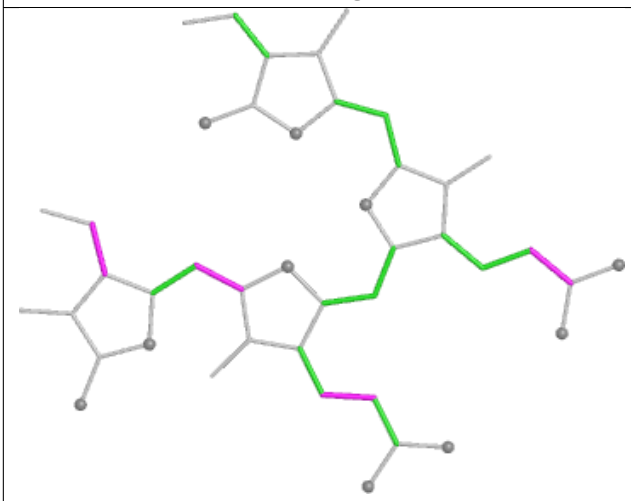
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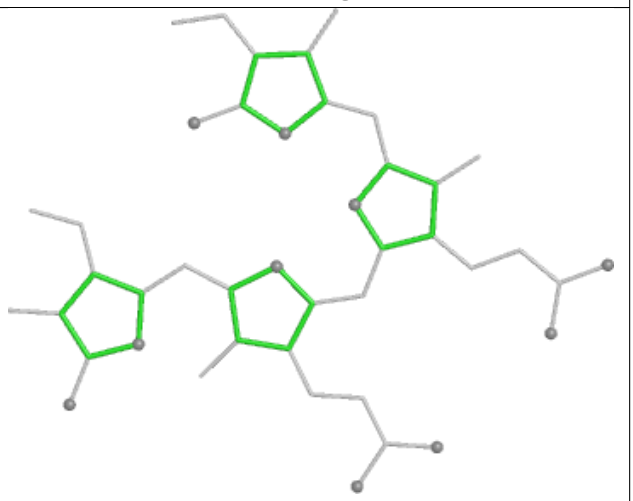
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Bond angles

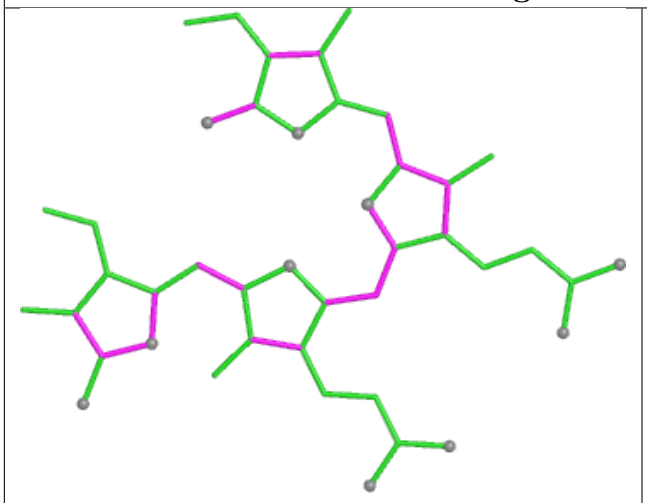


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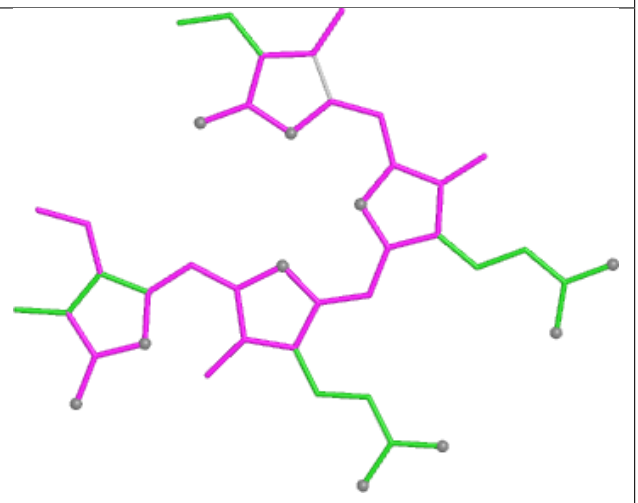


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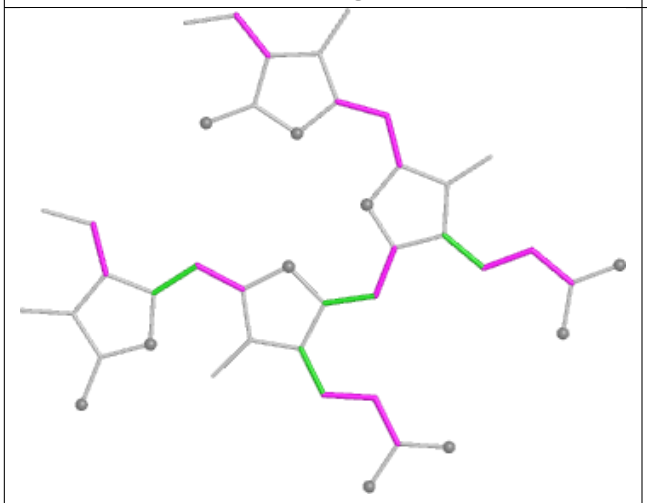
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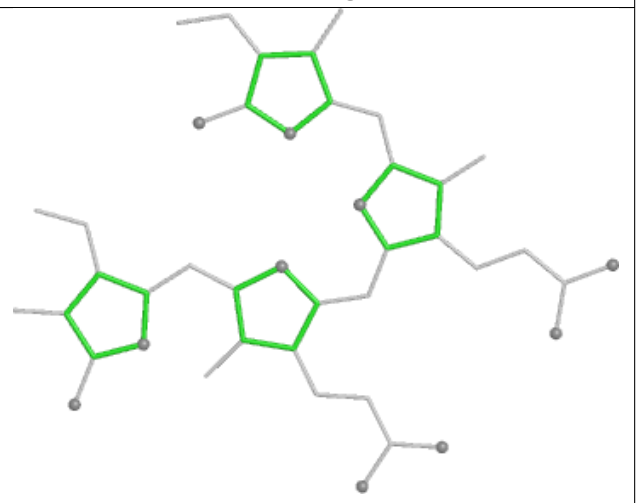
Bond lengths



Bond angles



Torsions

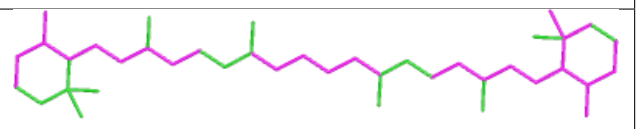


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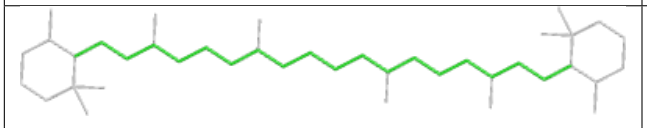
Ligand BCR B6 621



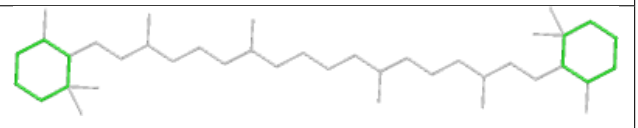
Bond lengths



Bond angles

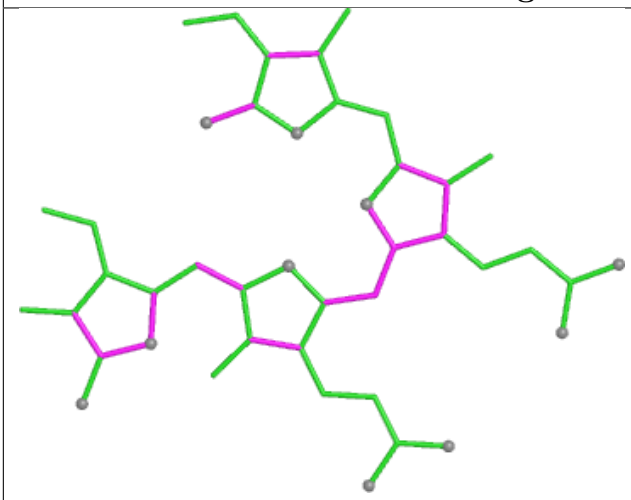


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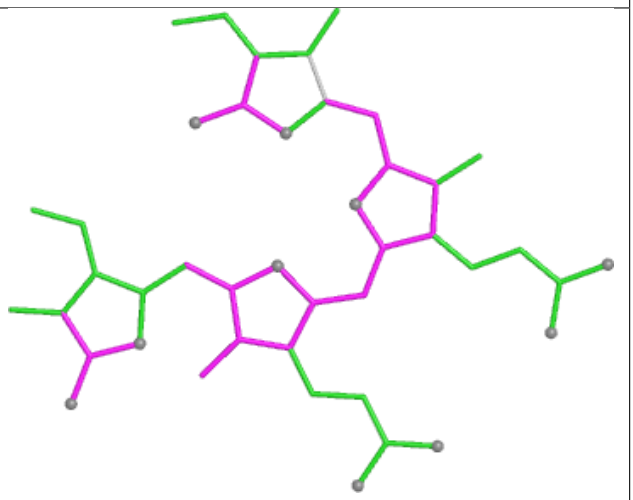


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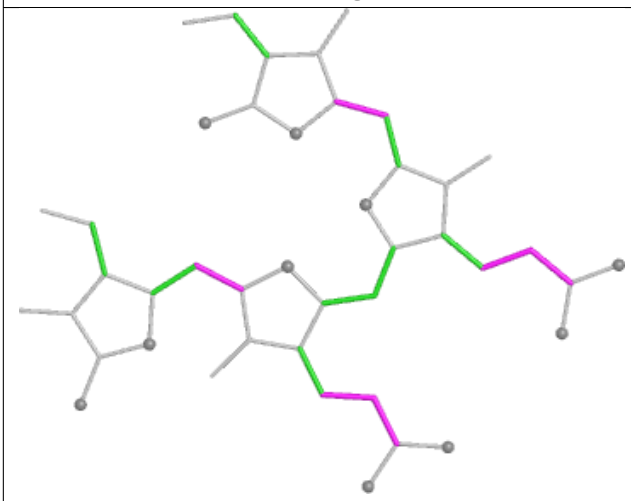
Ligand PEB VI 202



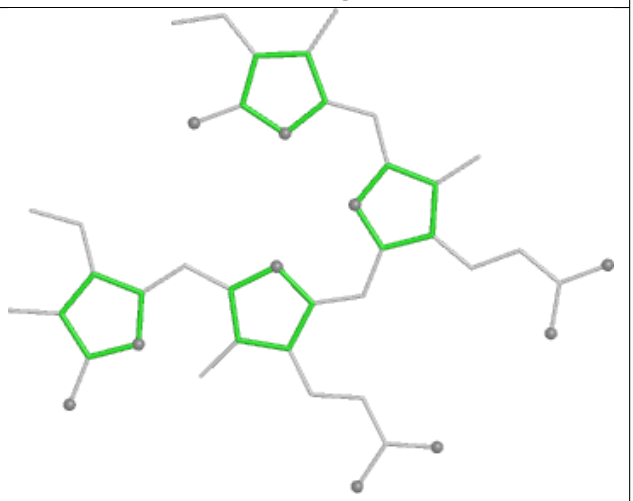
Bond lengths



Bond angles

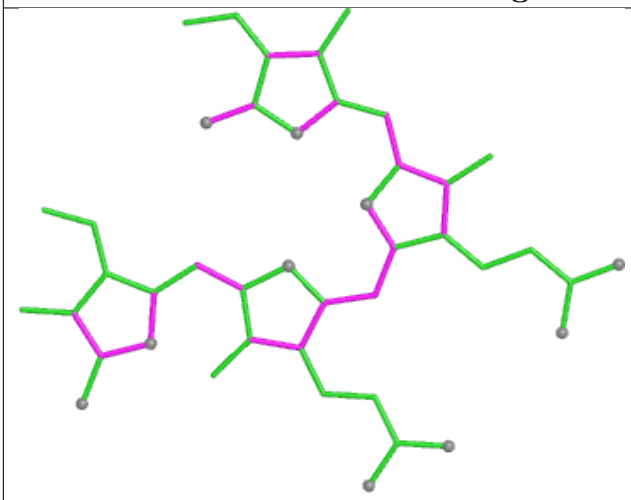


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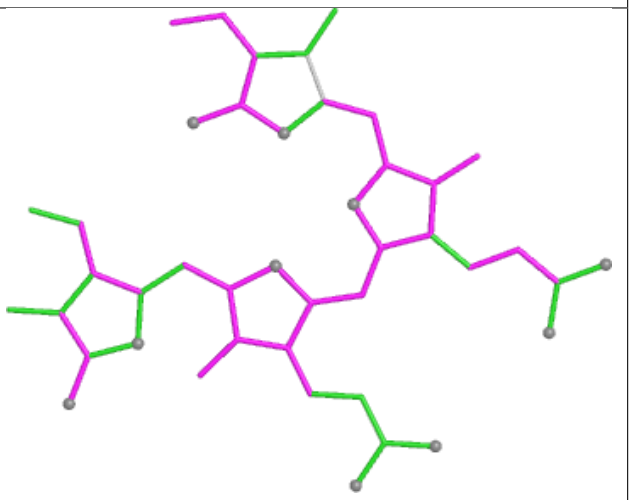


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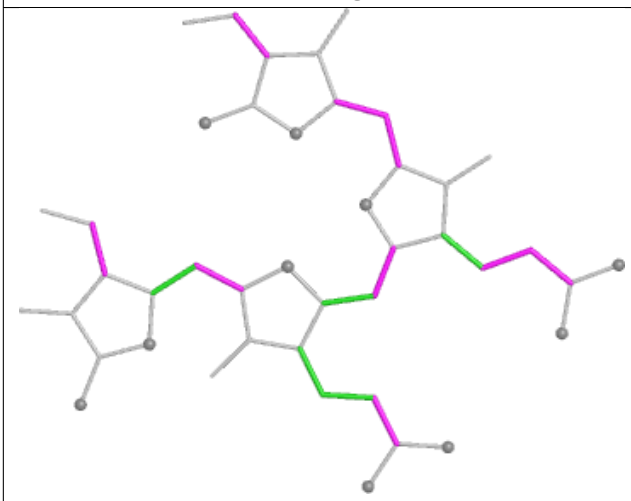
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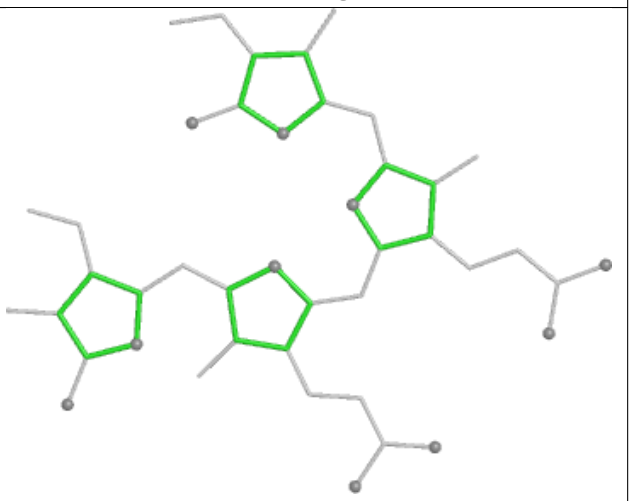
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Bond angles

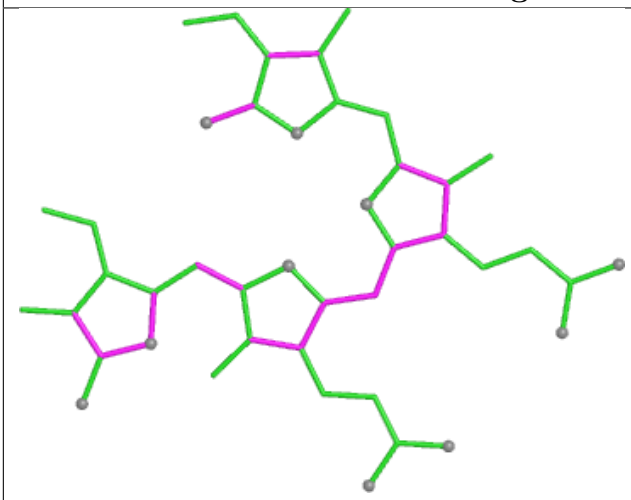


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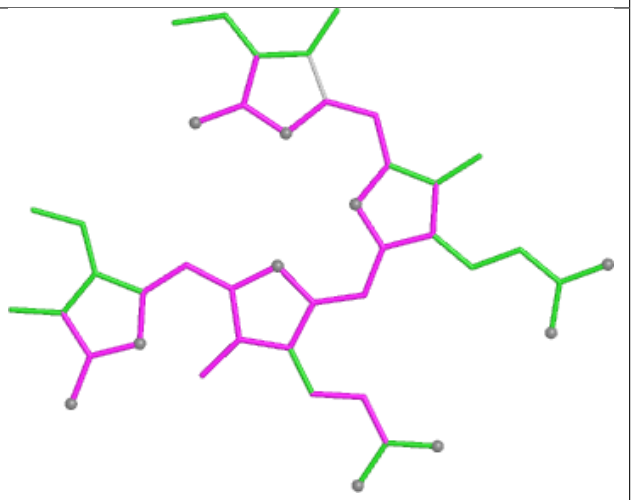


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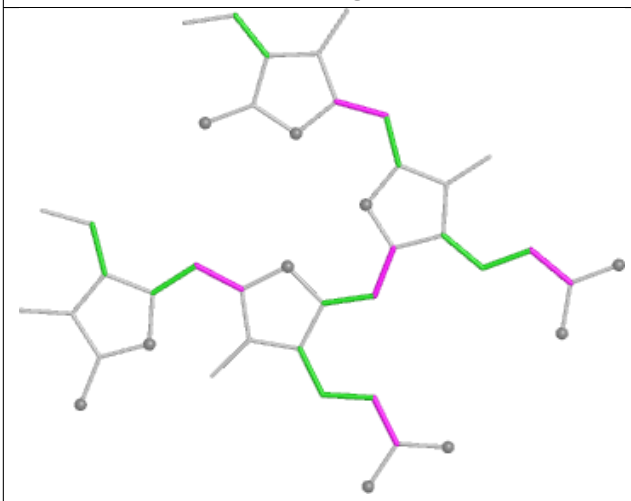
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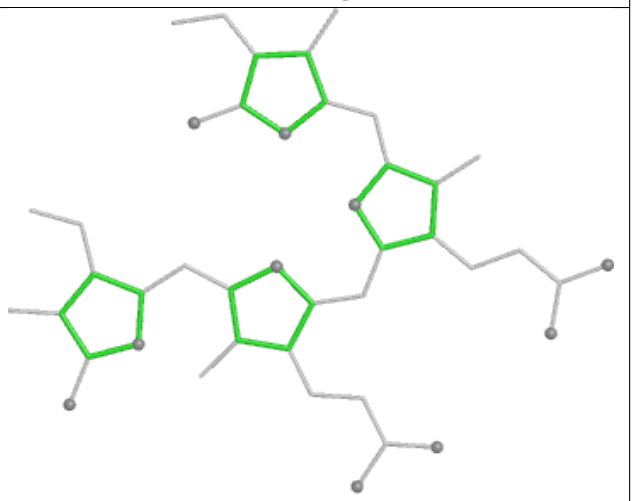
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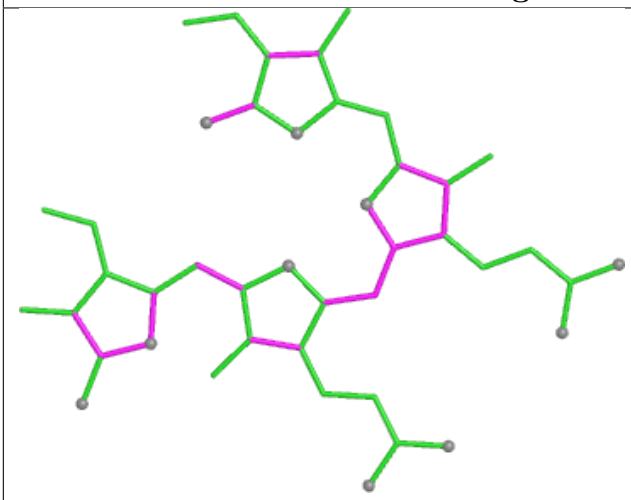


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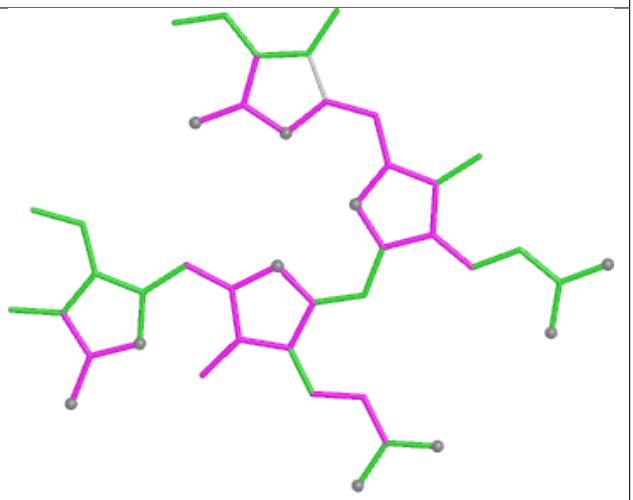


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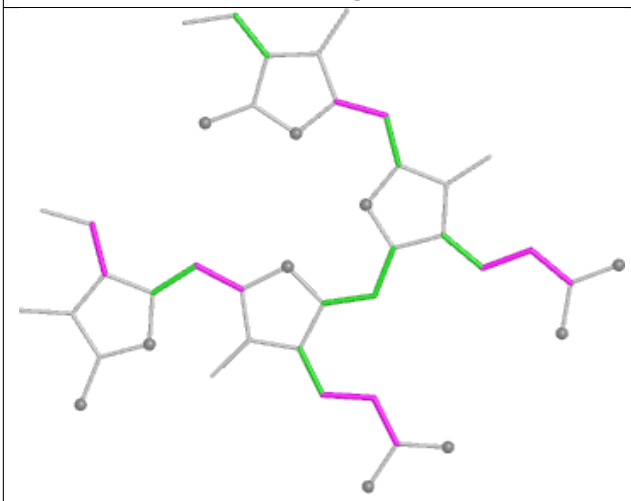
Ligand PEB YP 502



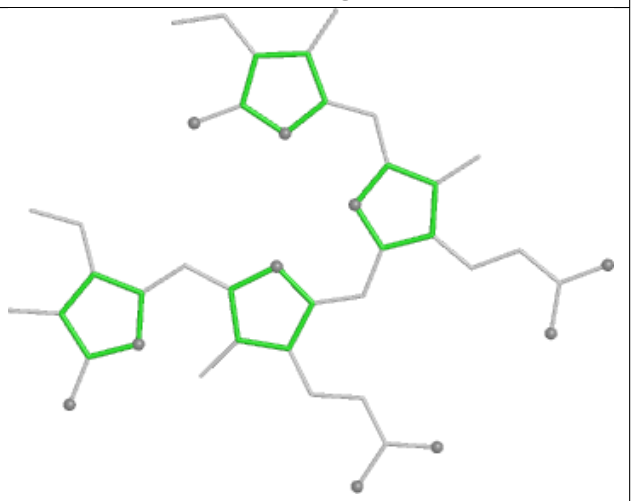
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Bond angles

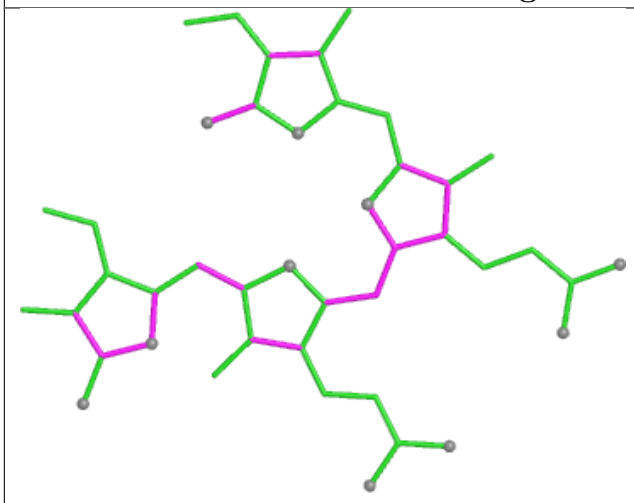


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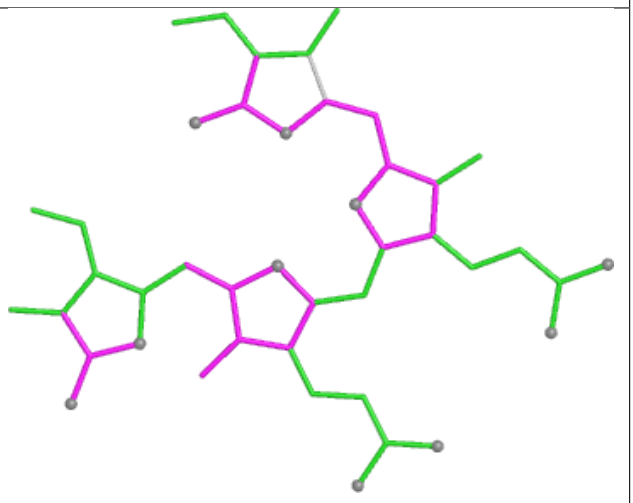


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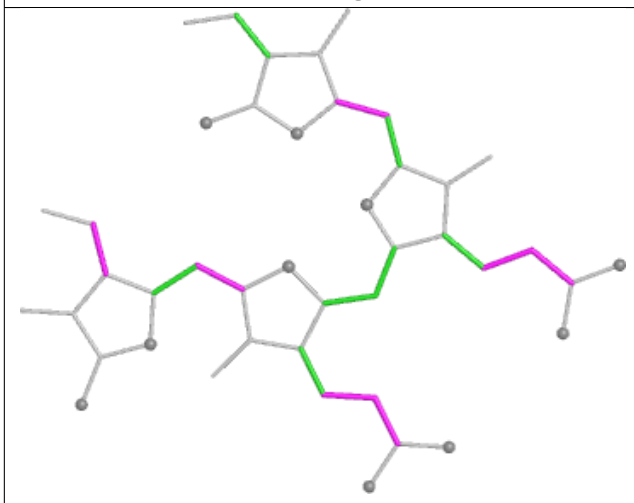
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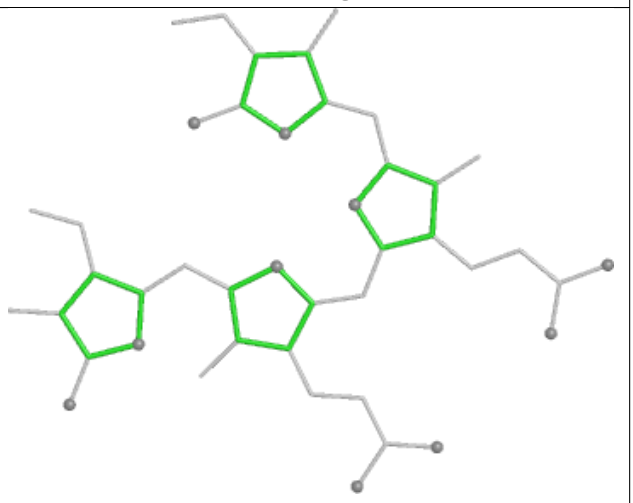
Bond lengths



Bond angles

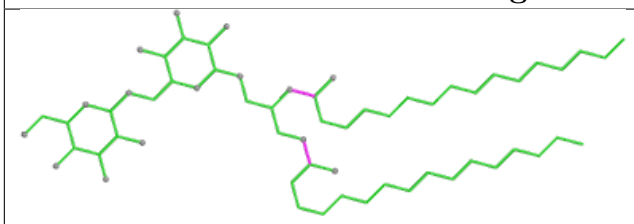


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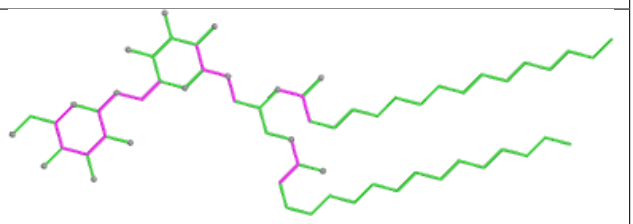


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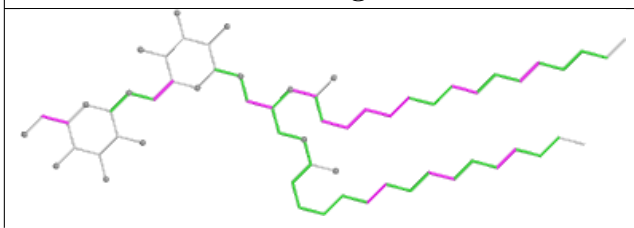
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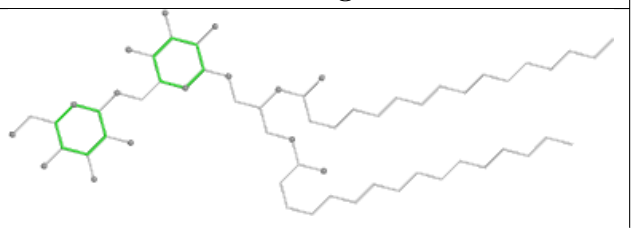
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Bond angles

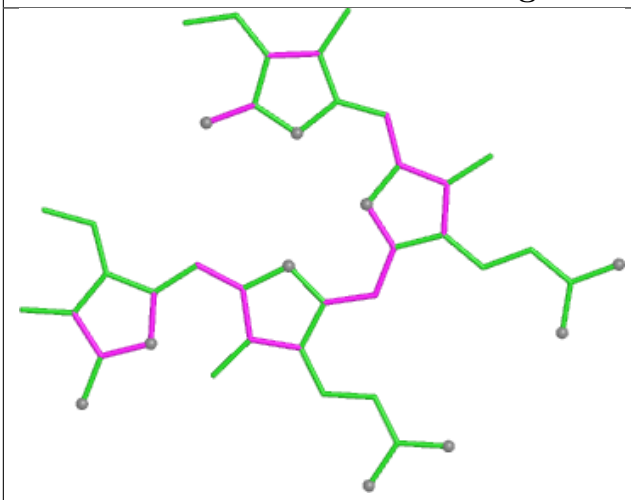


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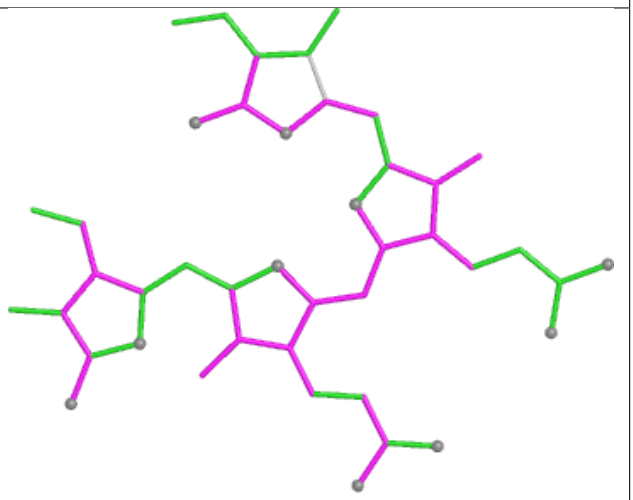


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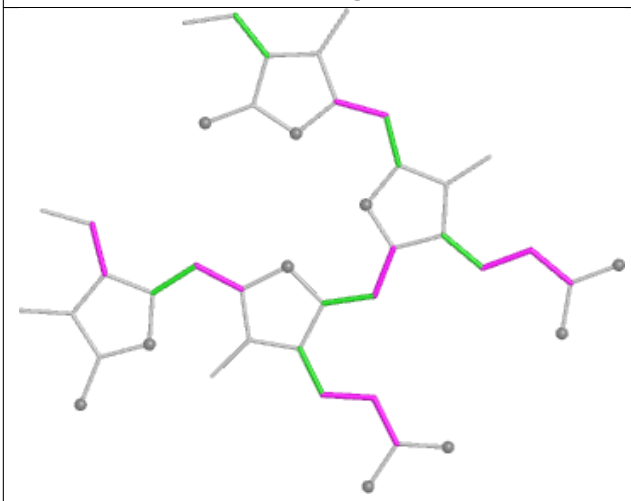
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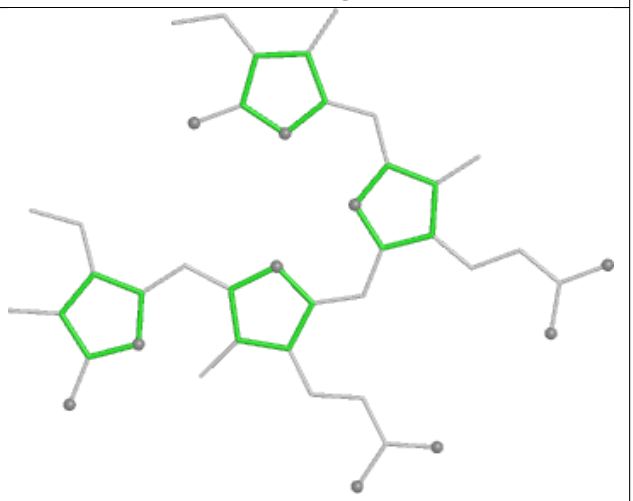
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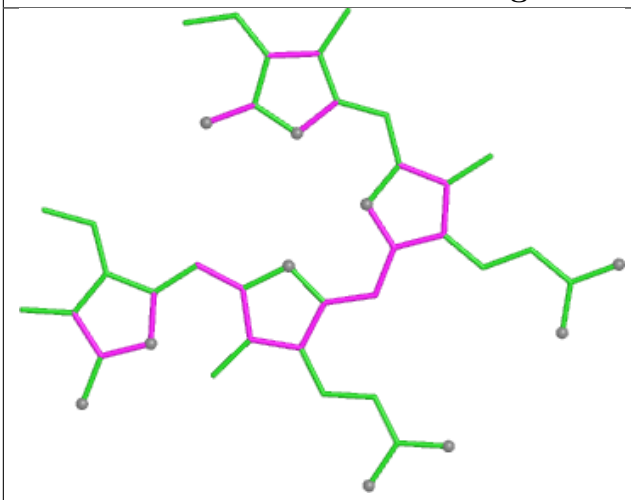


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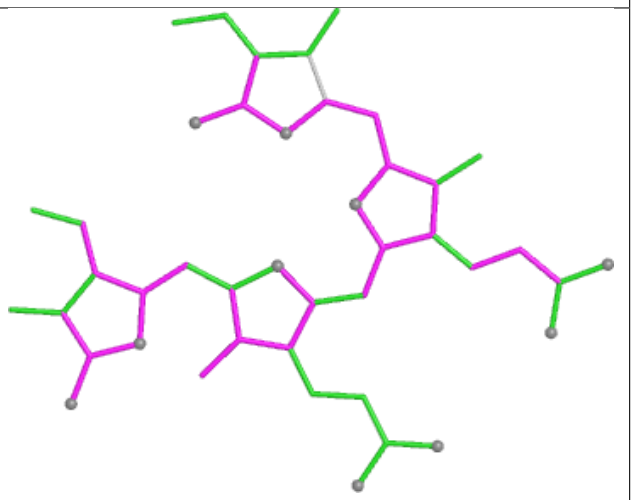


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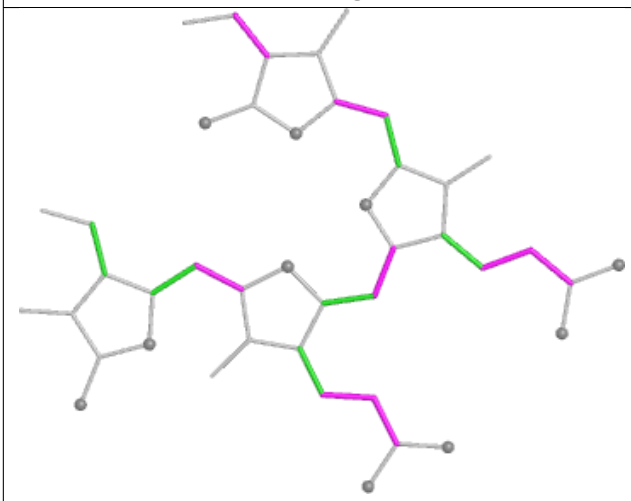
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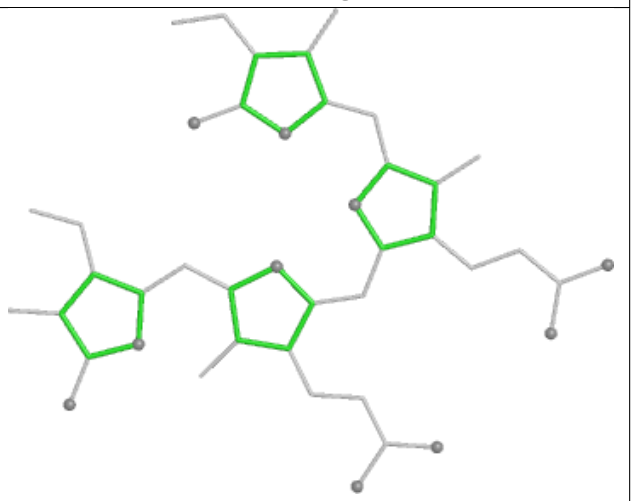
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Bond angles

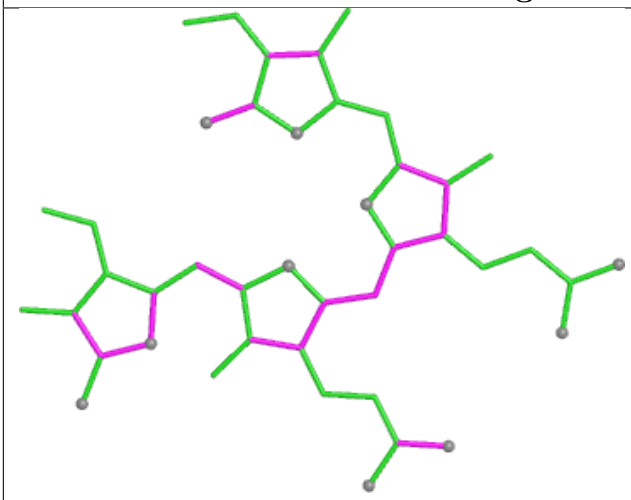


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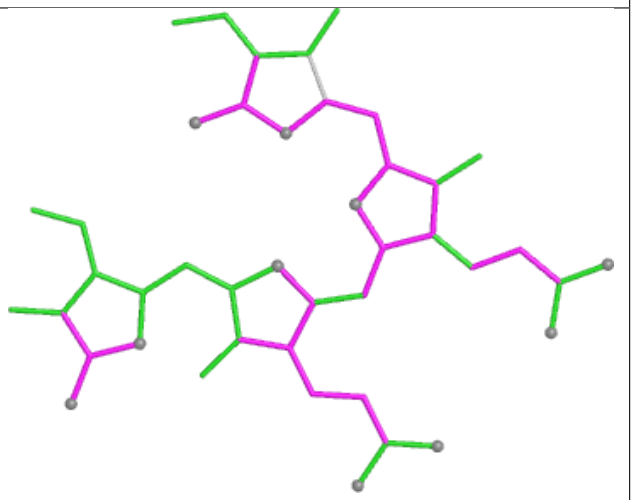


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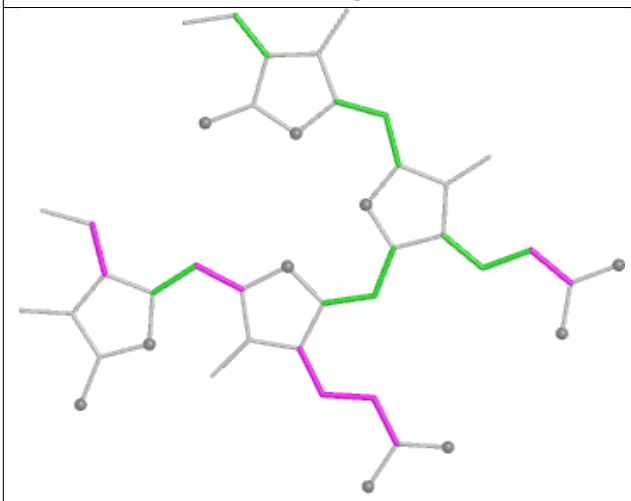
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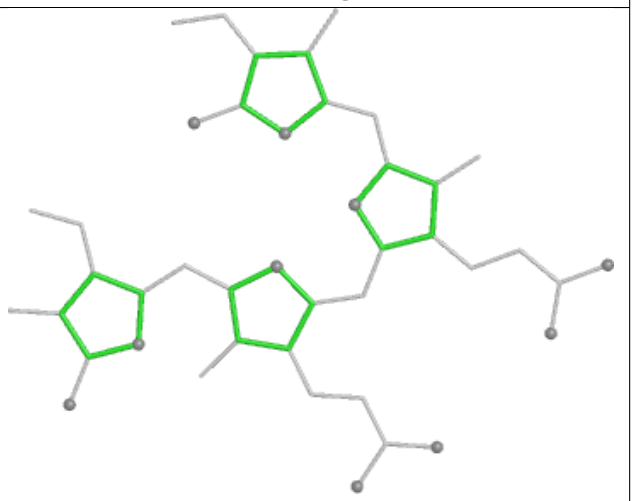
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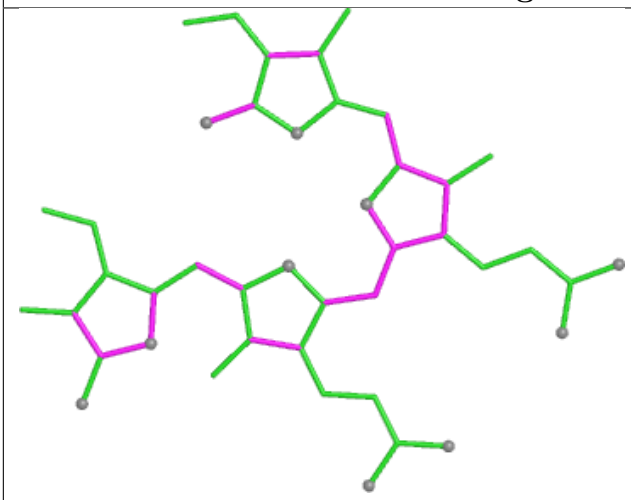


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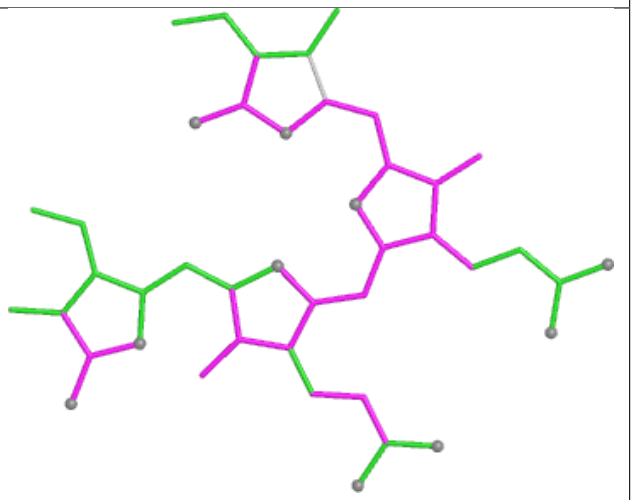


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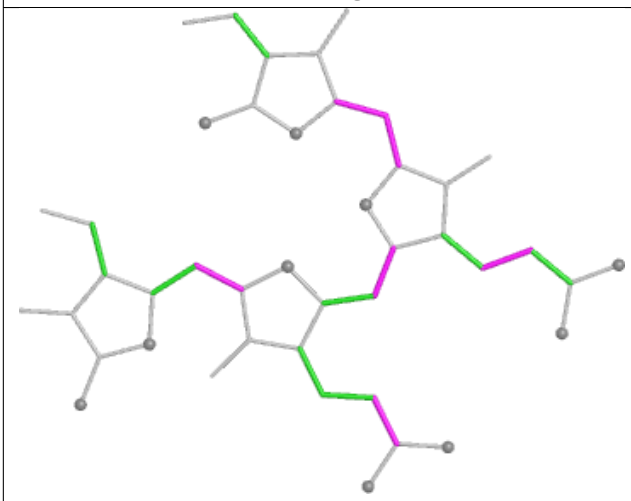
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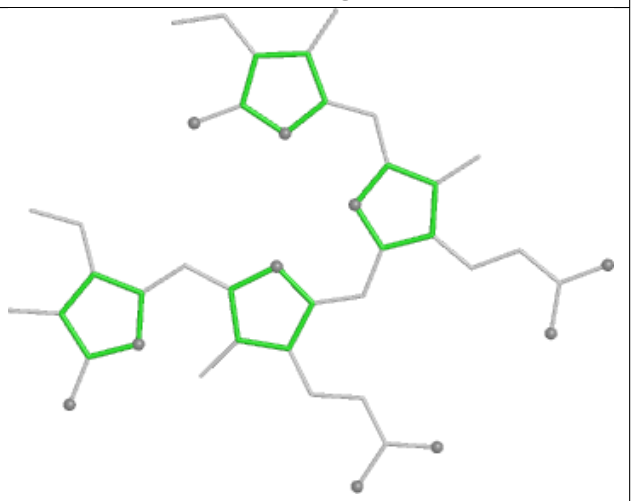
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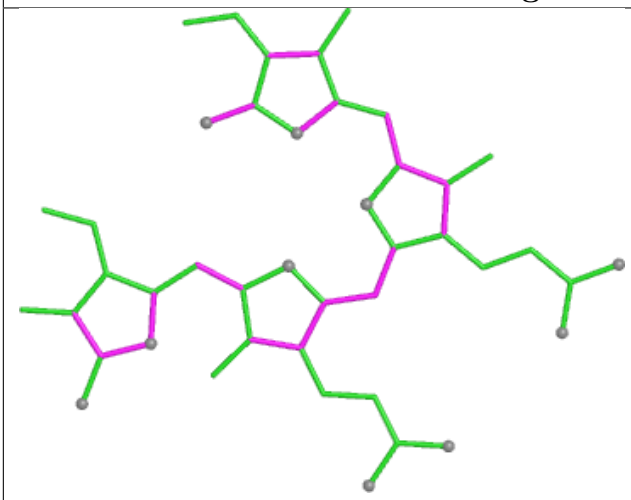


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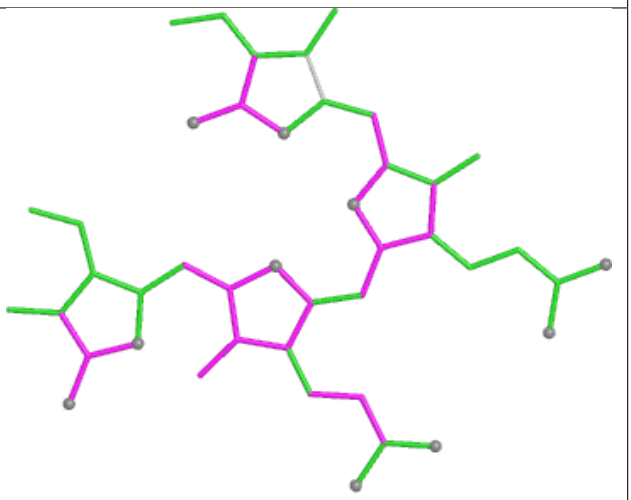


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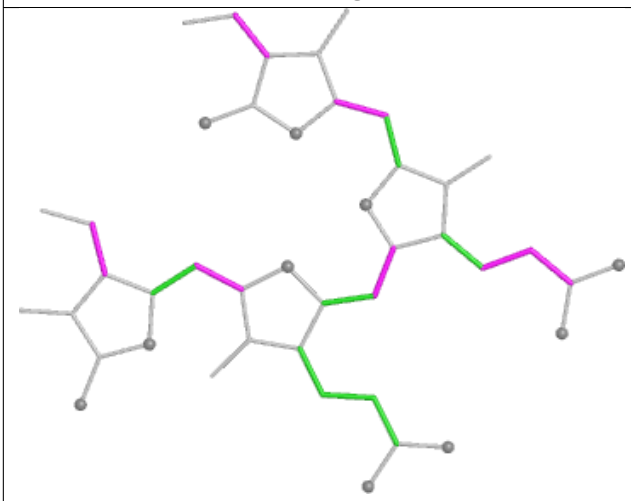
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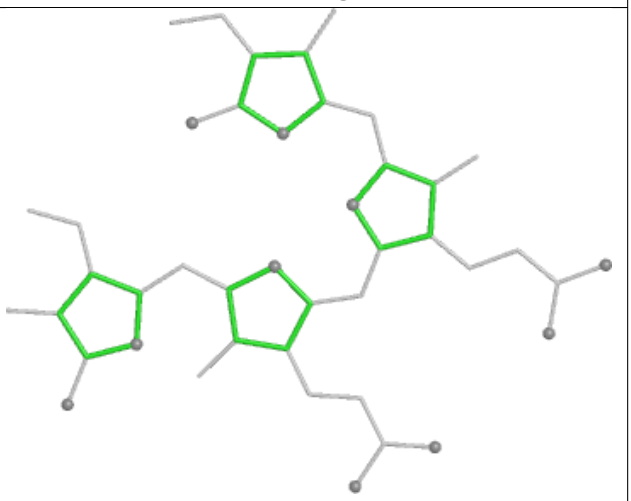
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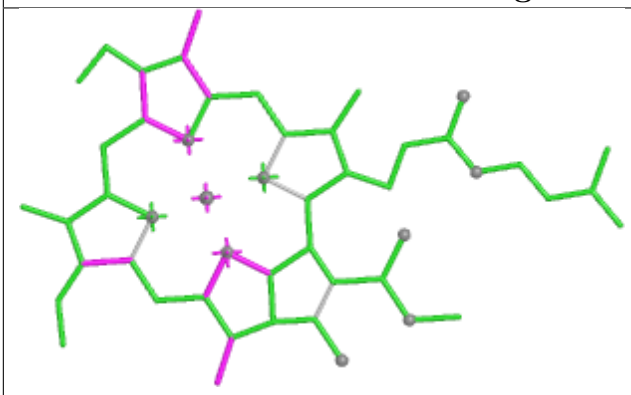


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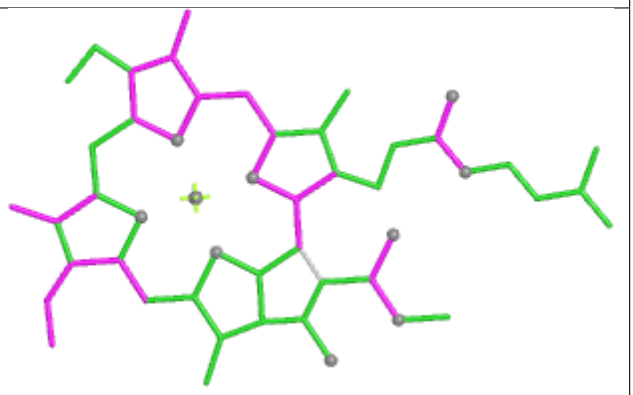


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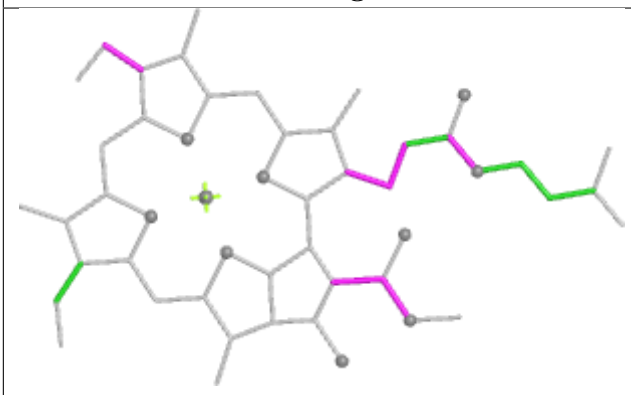
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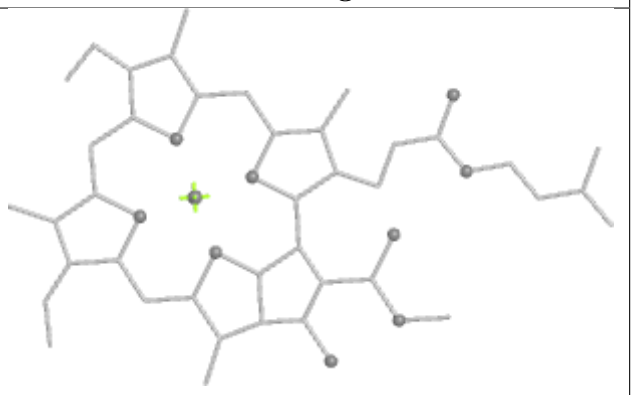
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Bond angles

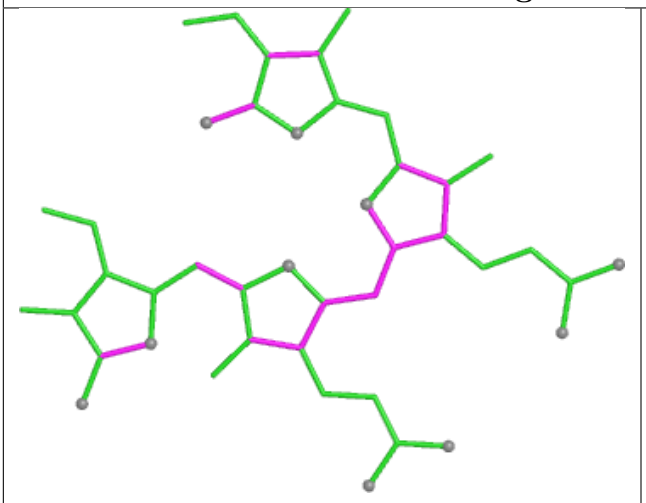


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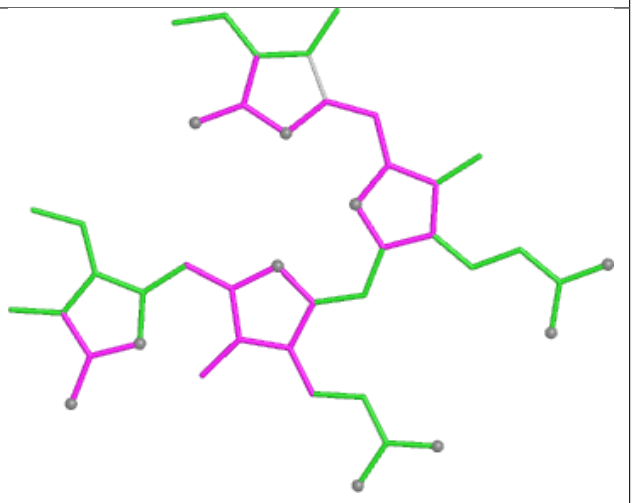


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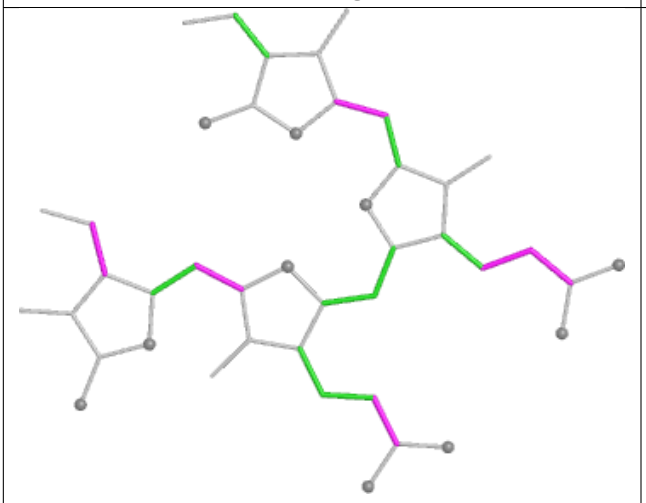
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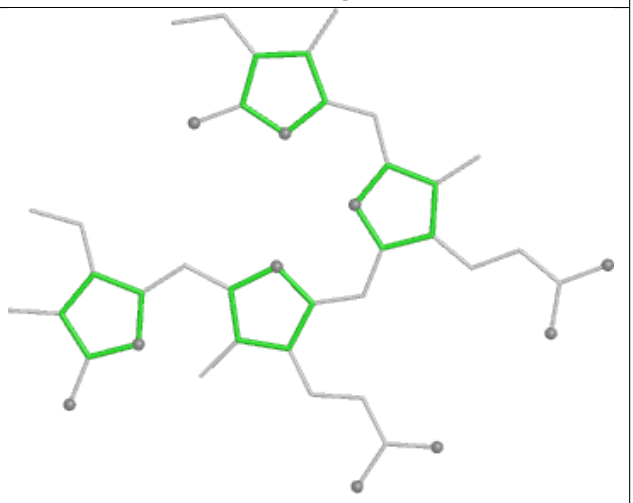
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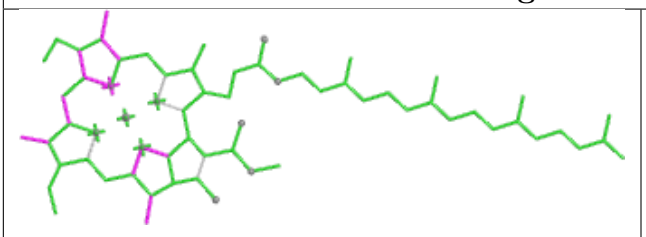


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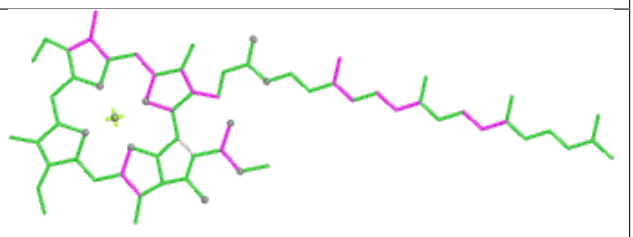


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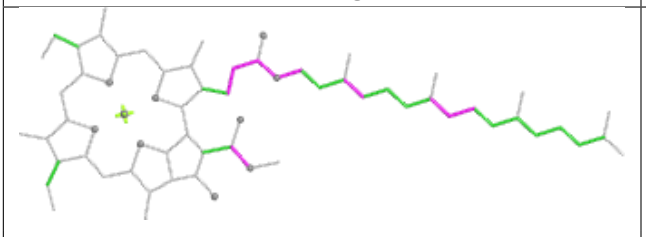
Ligand CLA aL 605



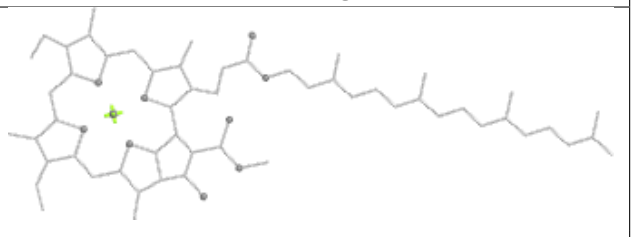
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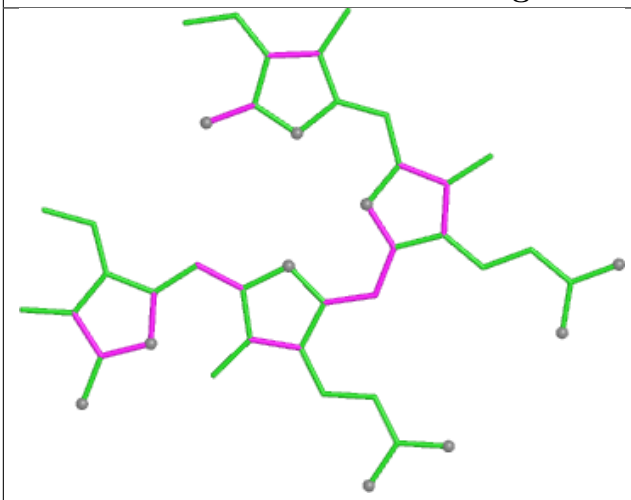


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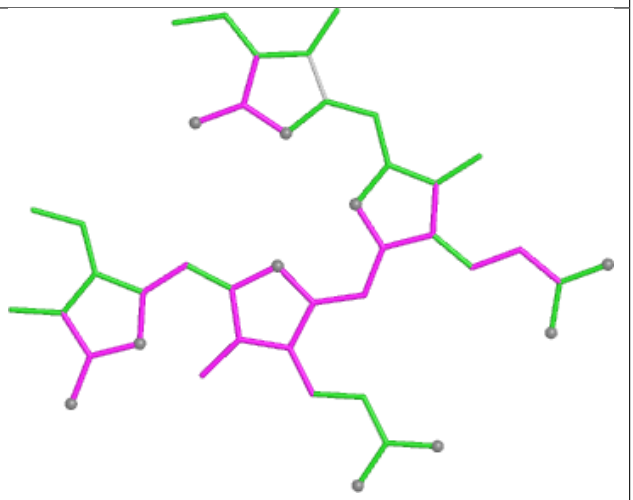


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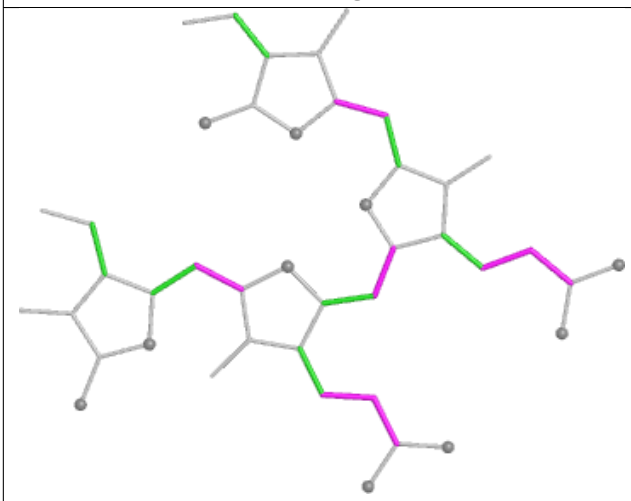
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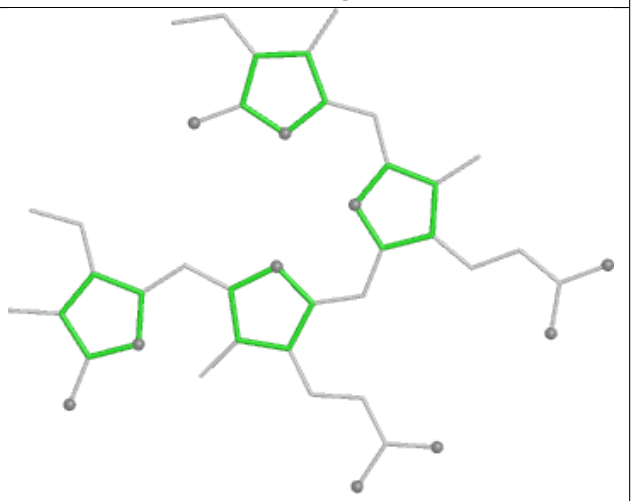
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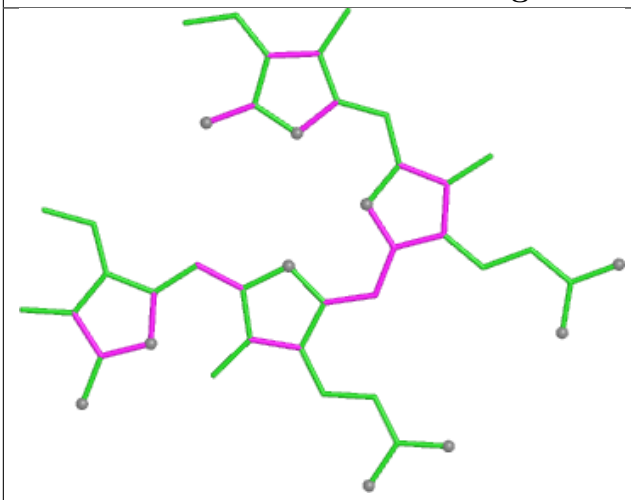


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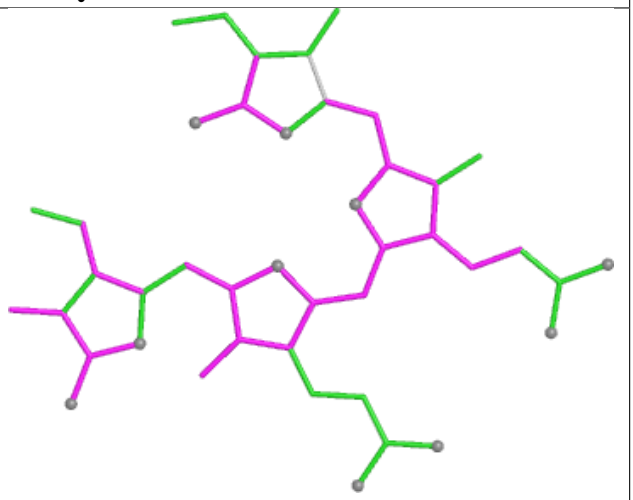


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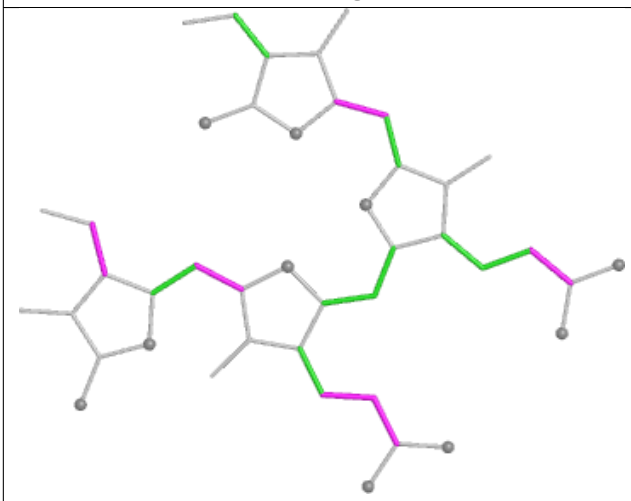
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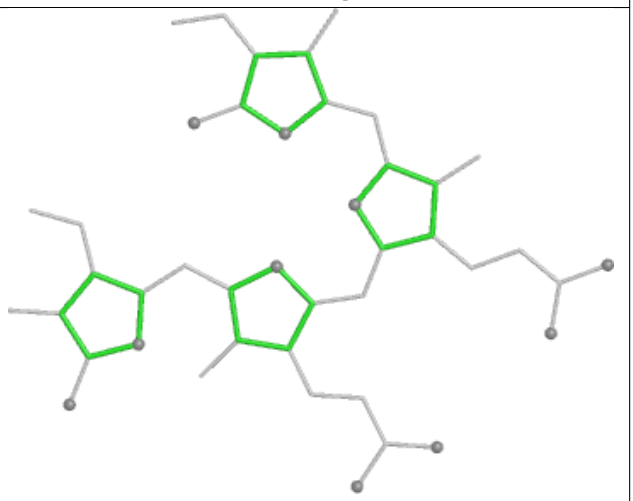
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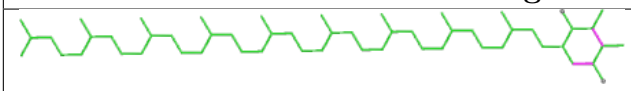


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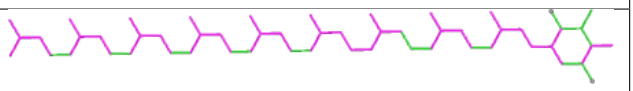


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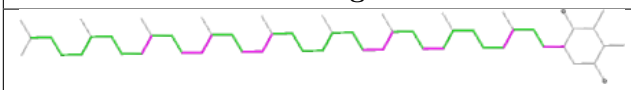
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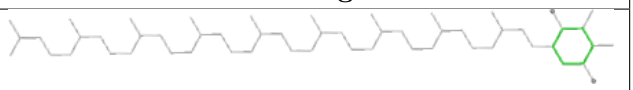
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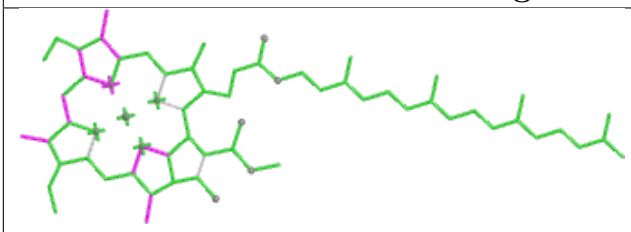


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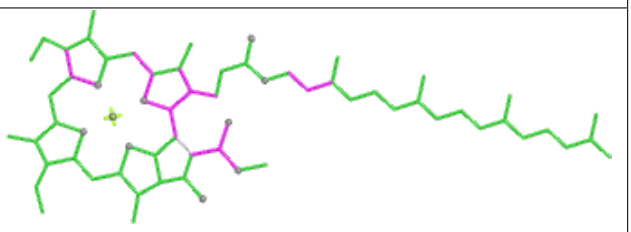


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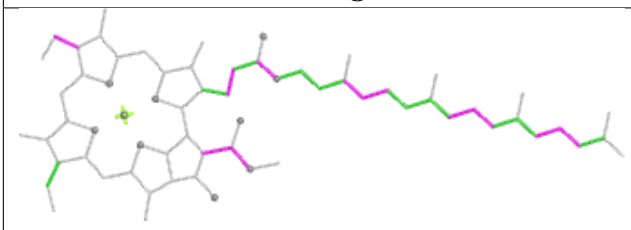
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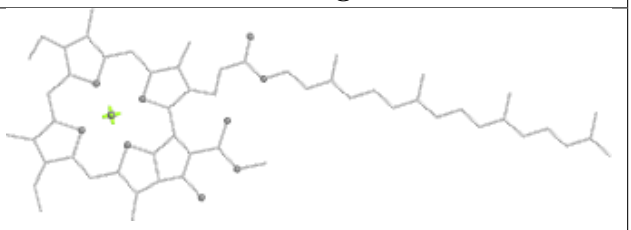
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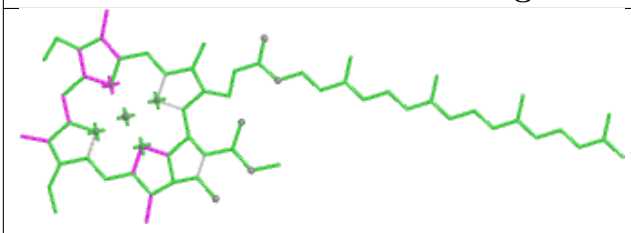


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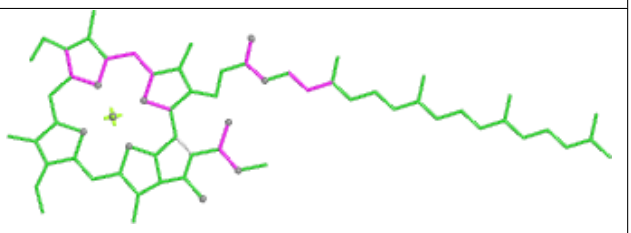


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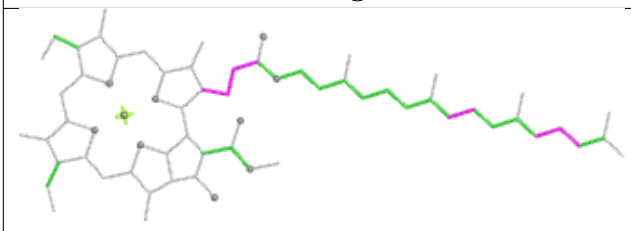
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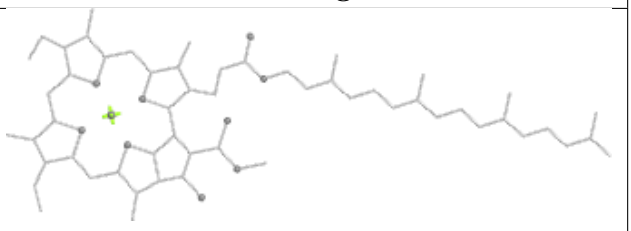
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Bond angles

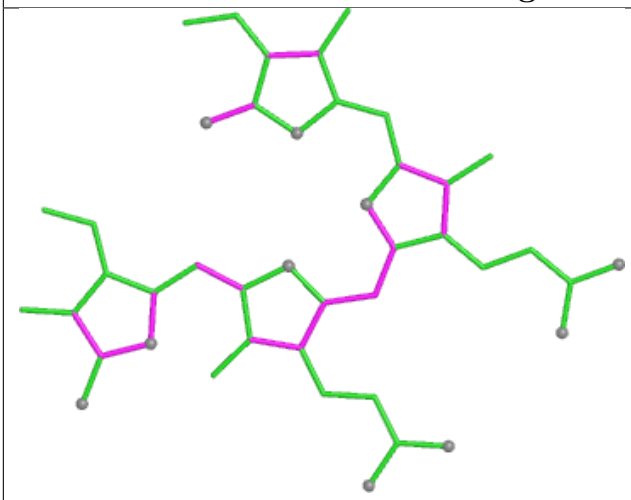


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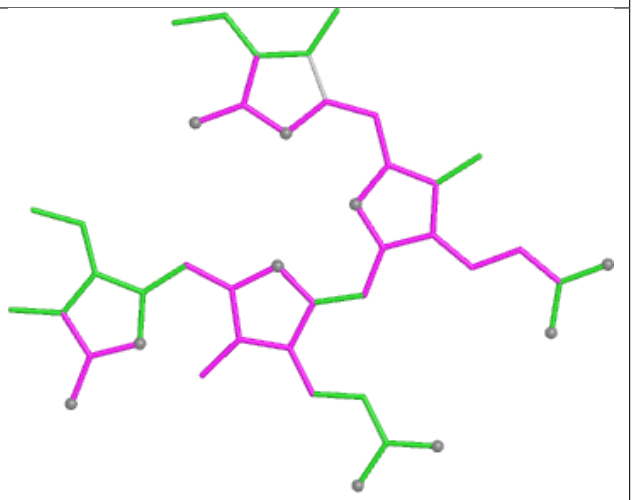


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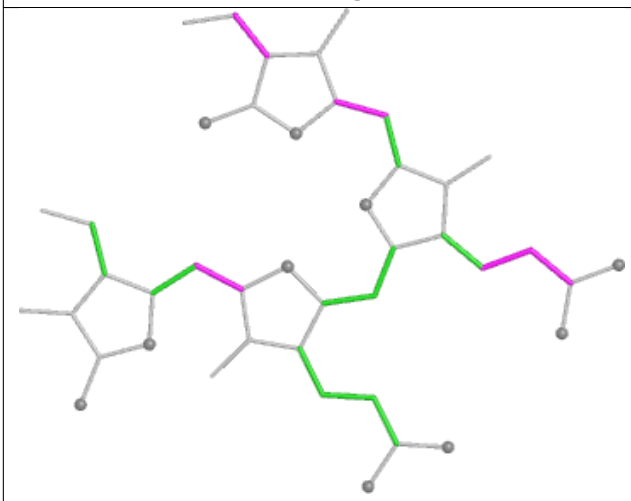
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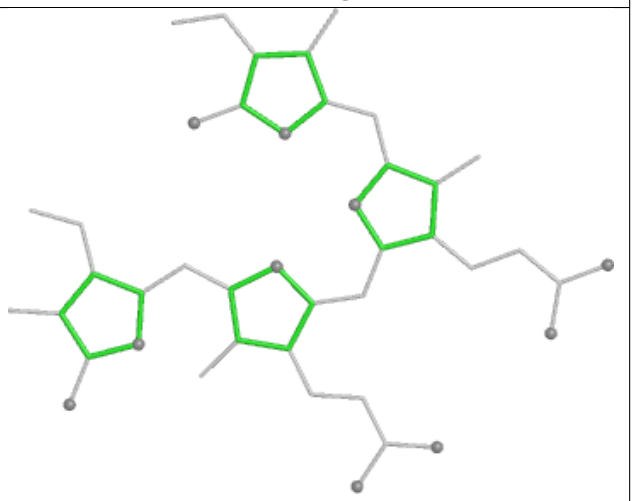
Bond lengths



Bond angles

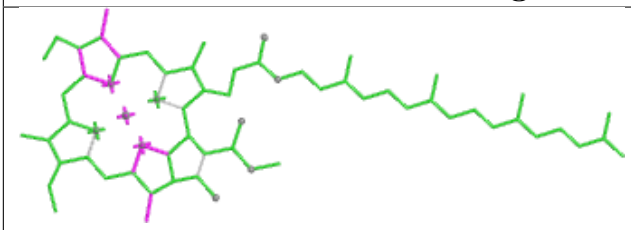


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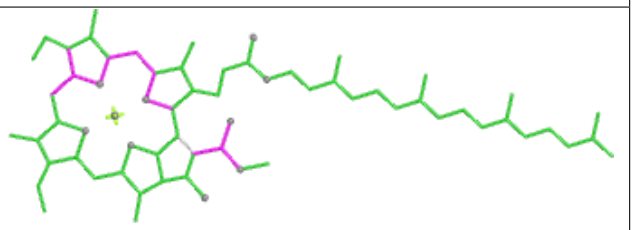


Rings

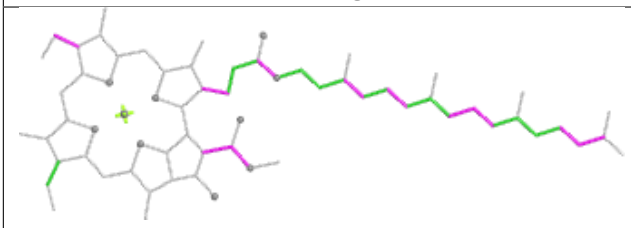
Ligand CLA BN 819



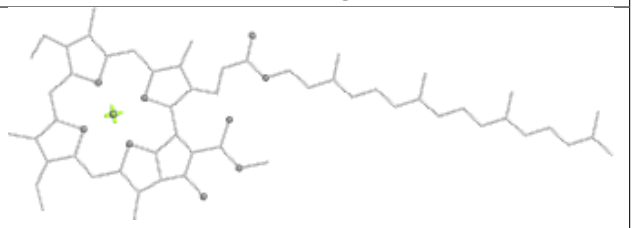
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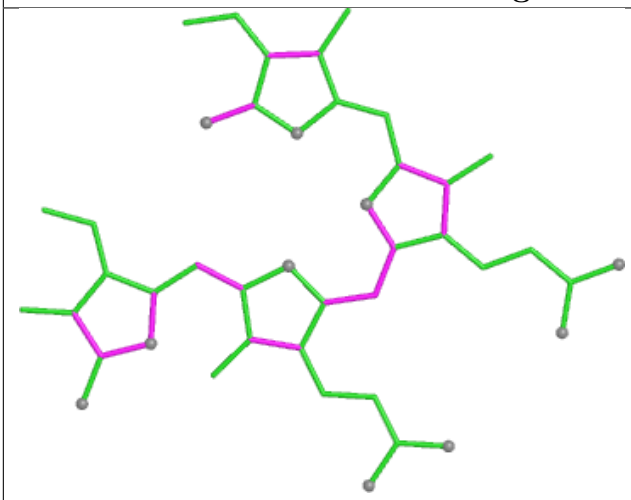


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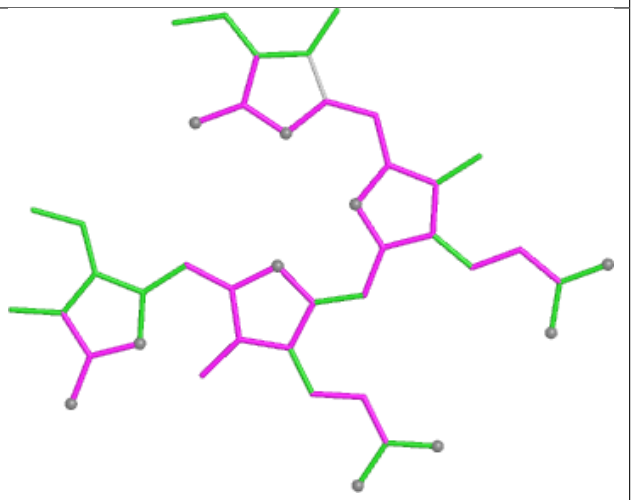


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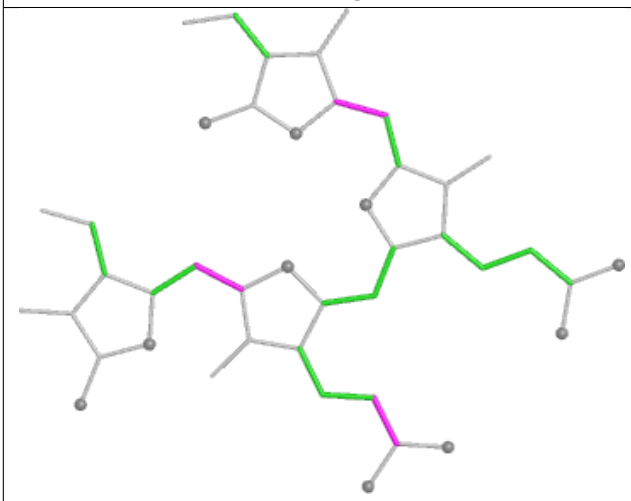
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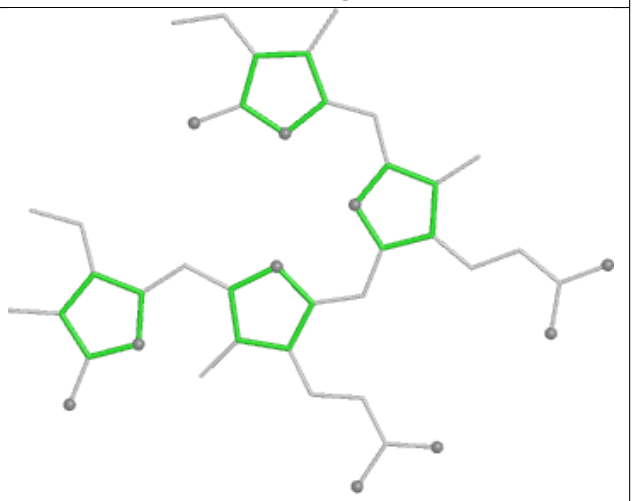
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Bond angles

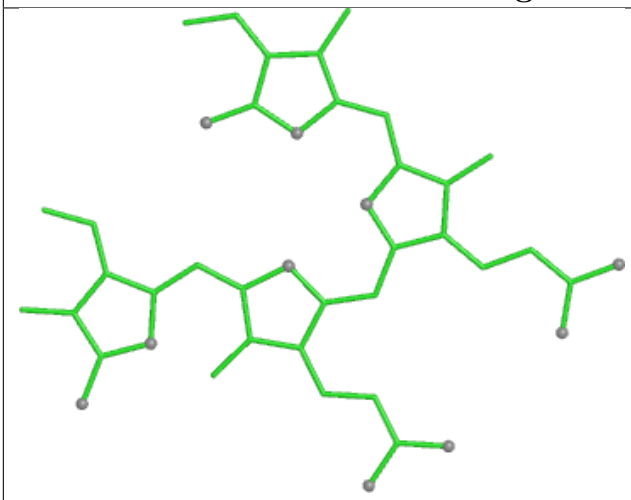


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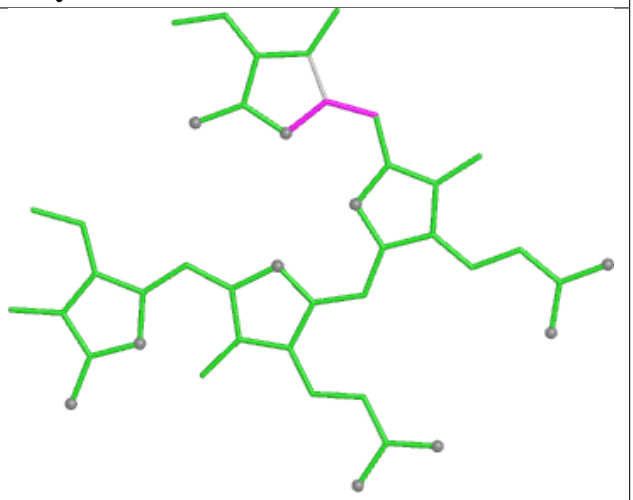


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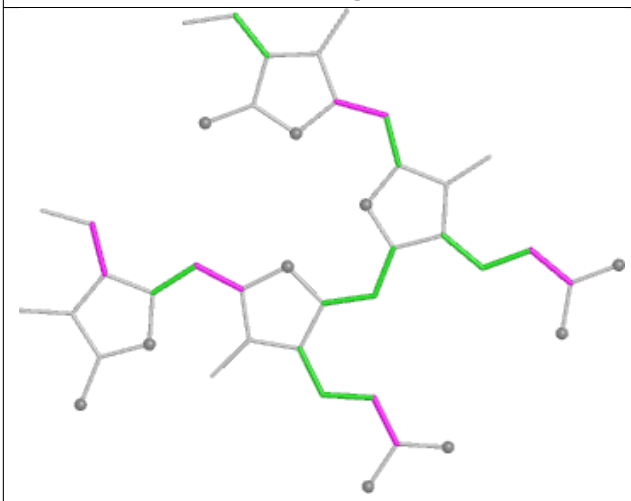
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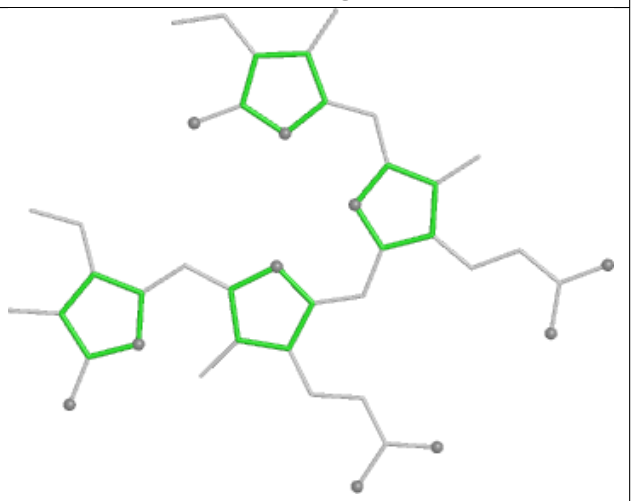
Bond lengths



Bond angles

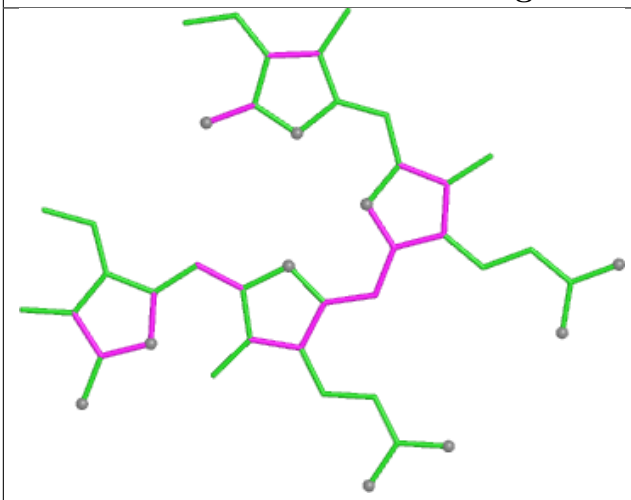


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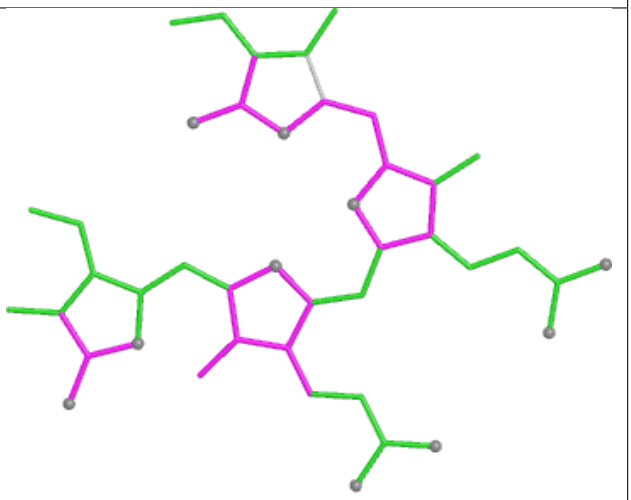


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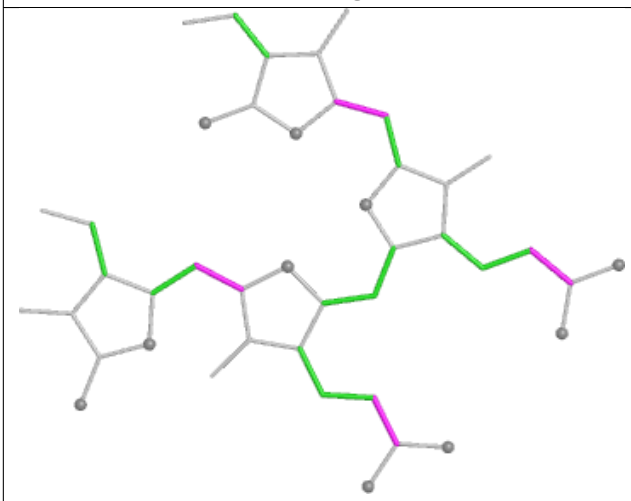
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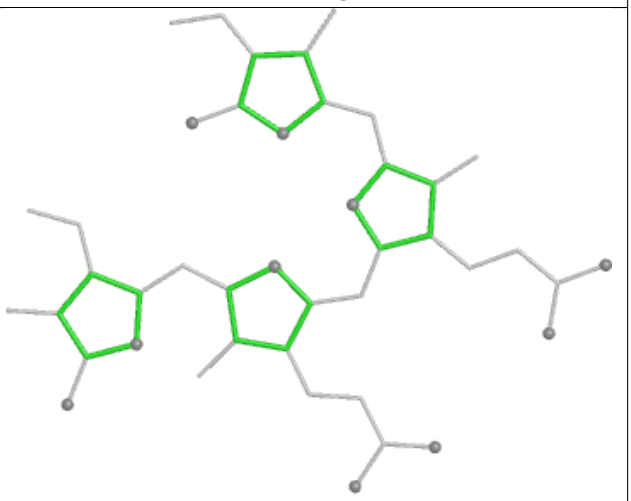
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Bond angles

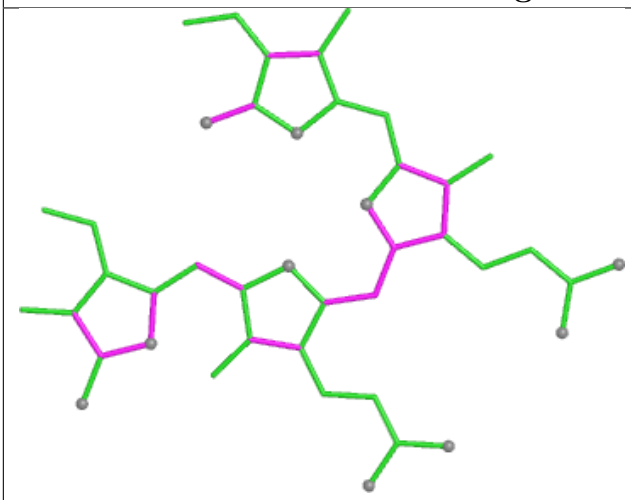


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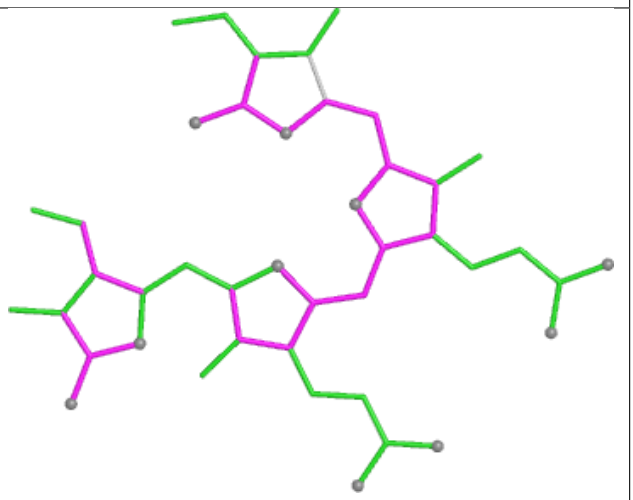


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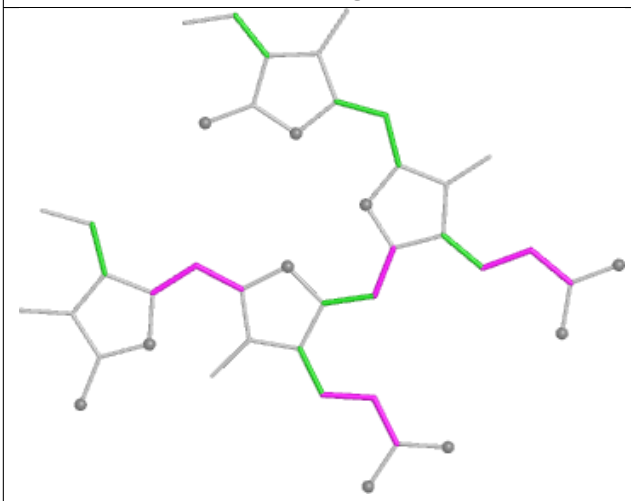
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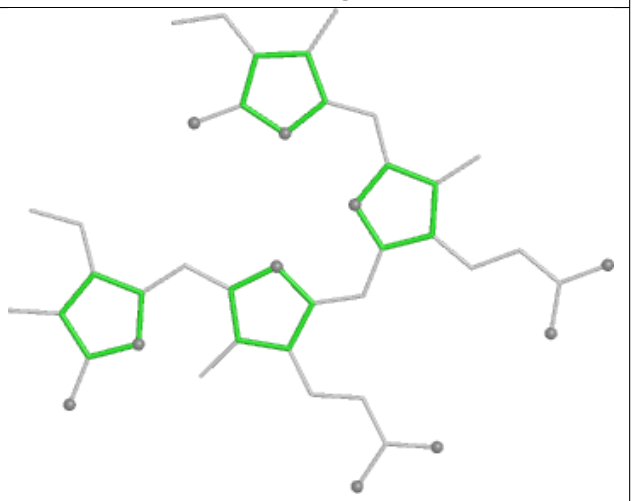
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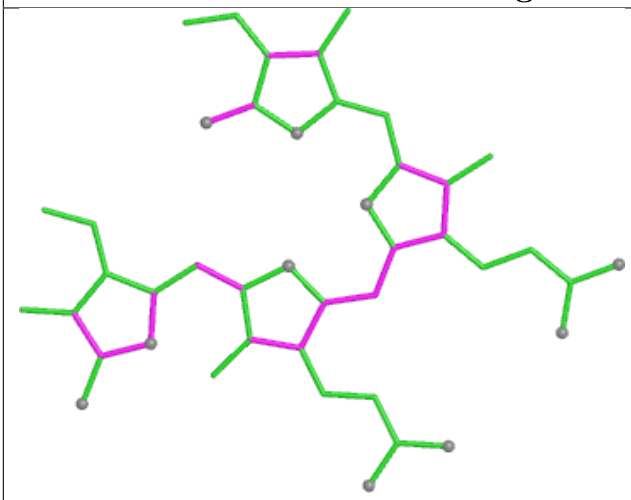


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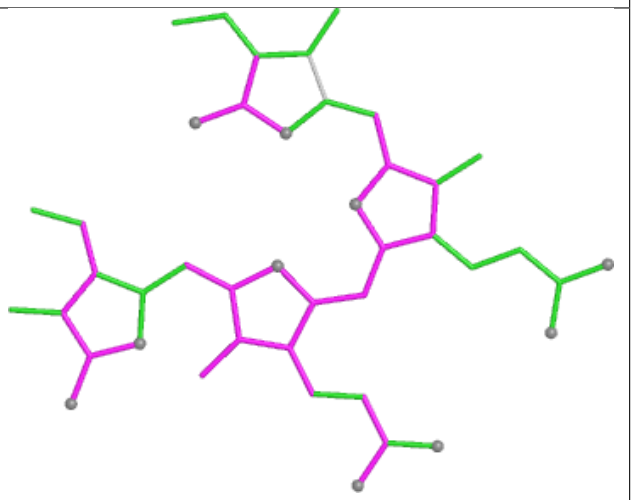


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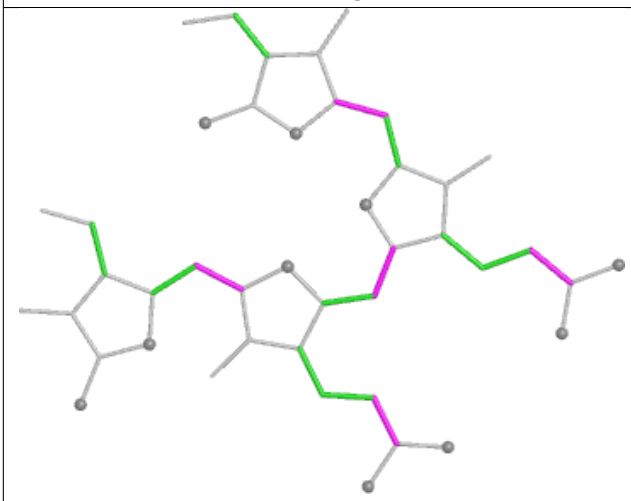
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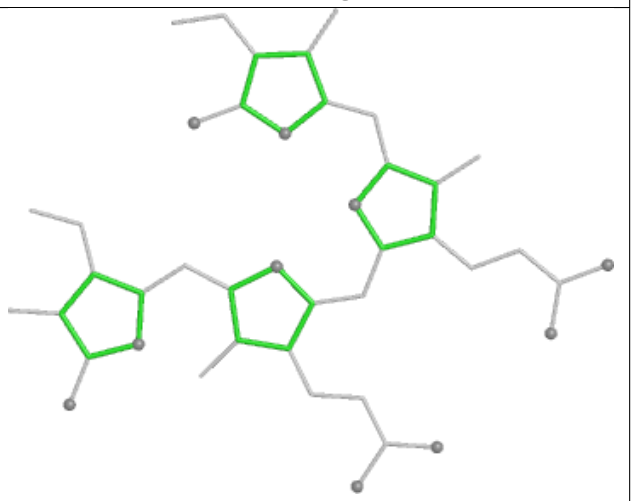
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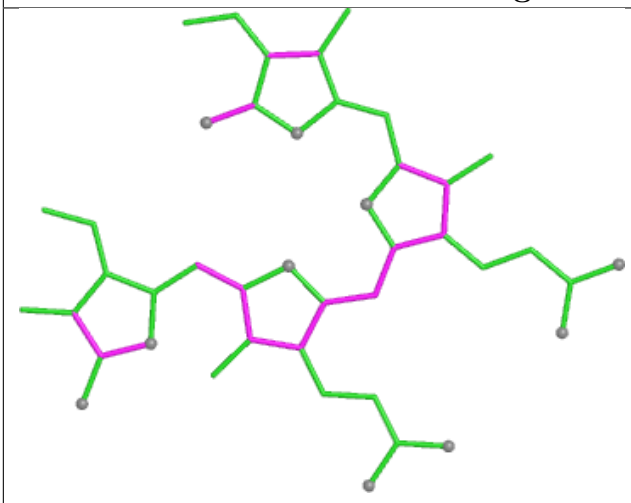


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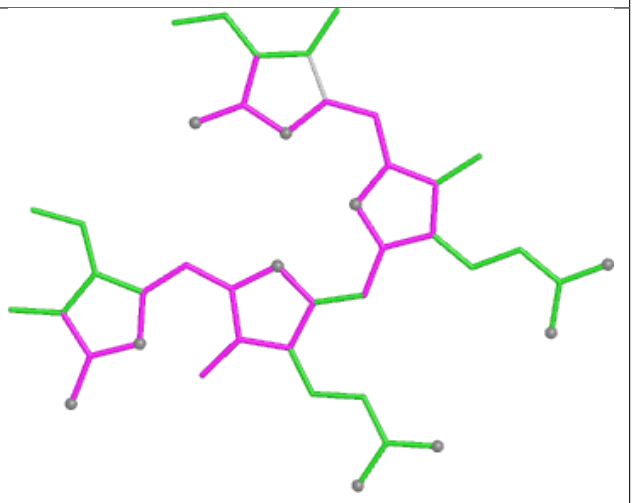


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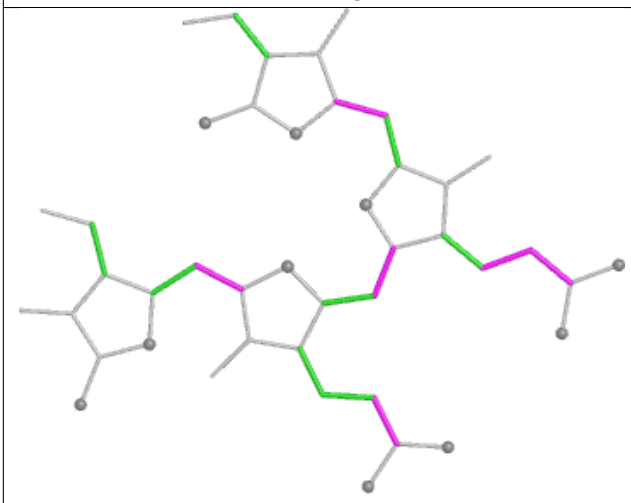
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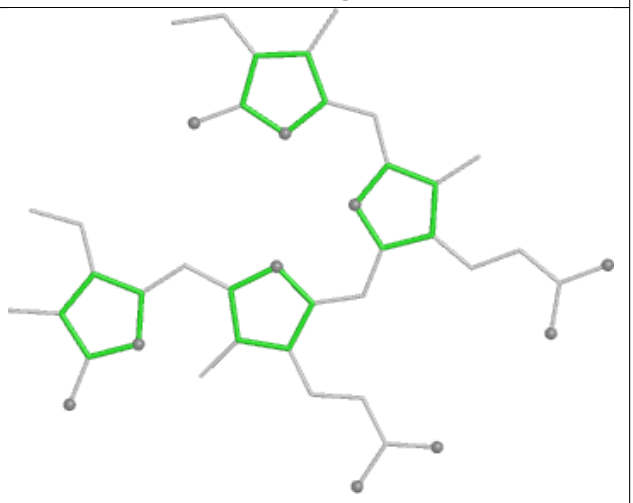
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Bond angles

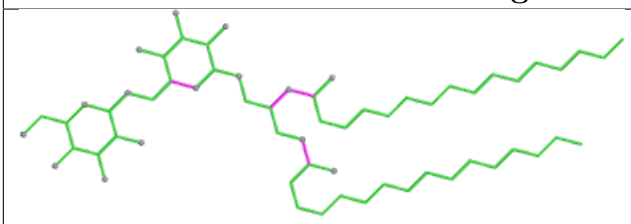


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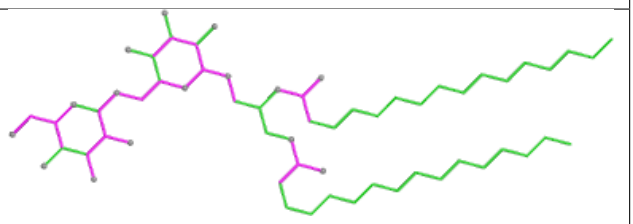


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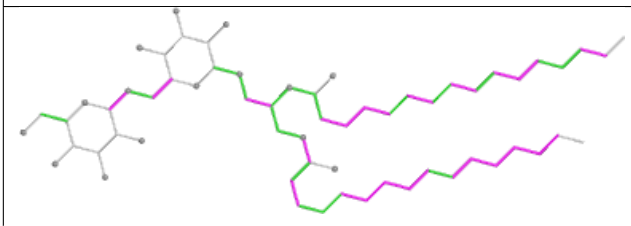
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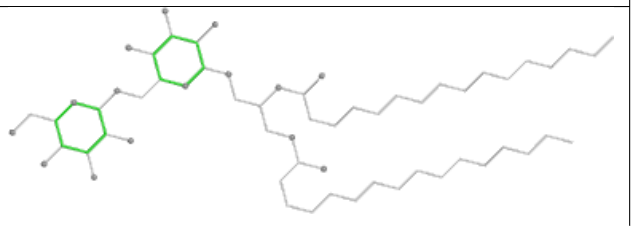
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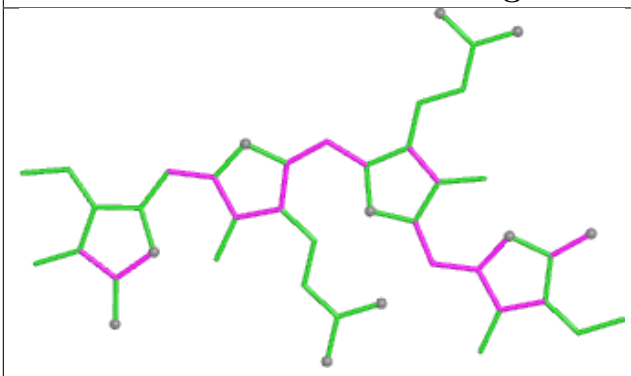


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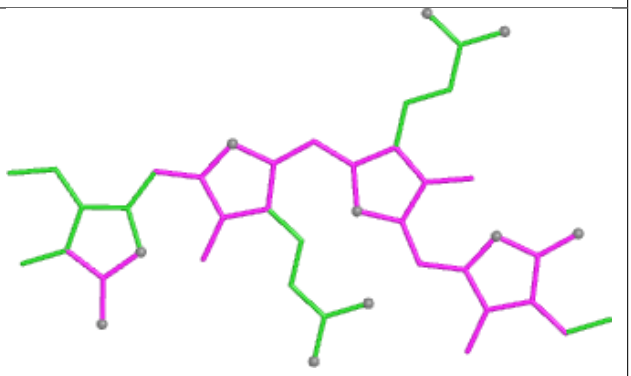


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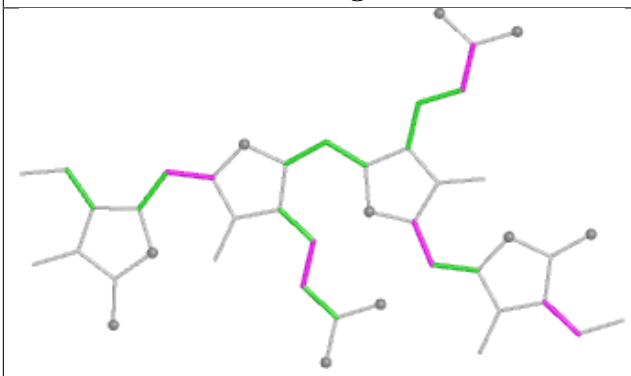
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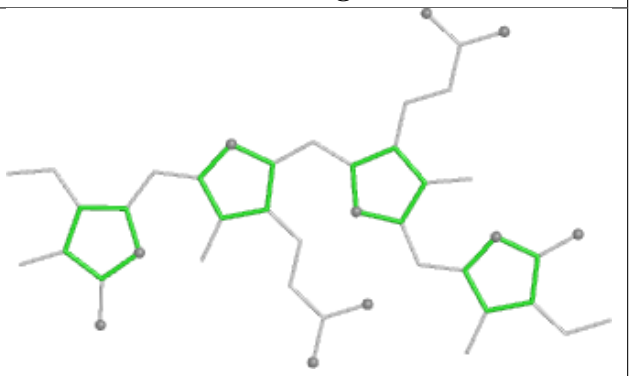
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Bond angles

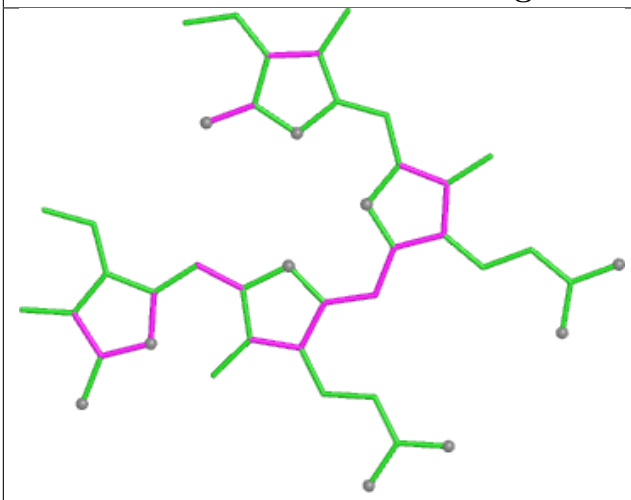


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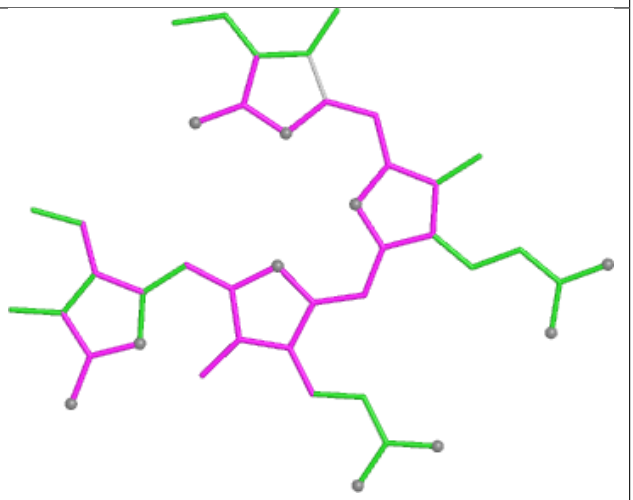


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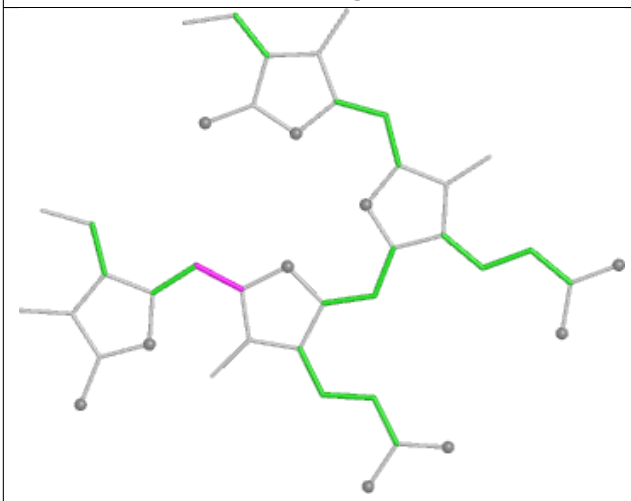
Ligand PEB uC 203



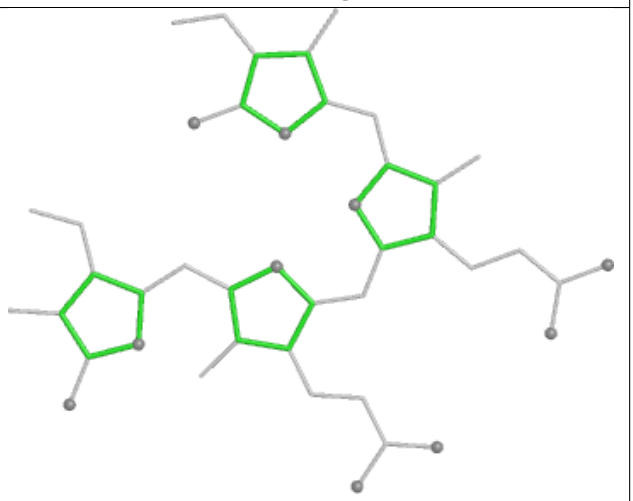
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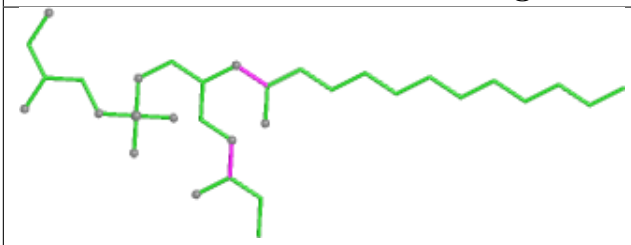


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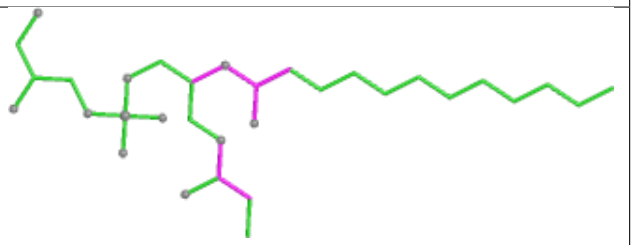


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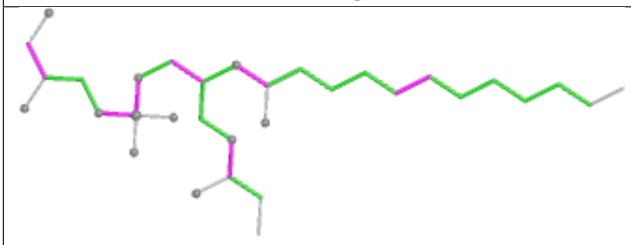
Ligand LHG C6 522



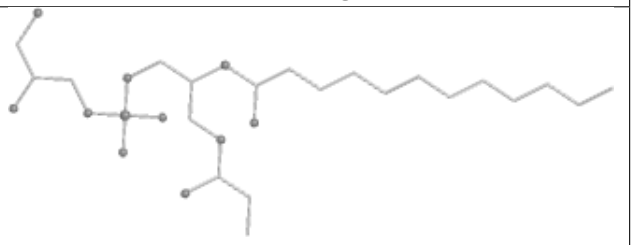
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Bond angles

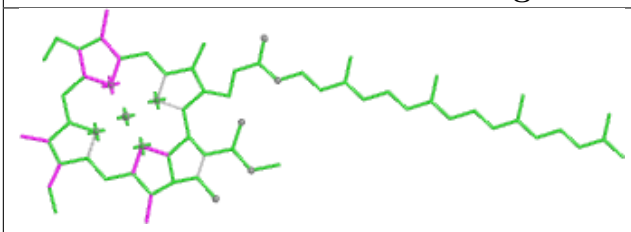


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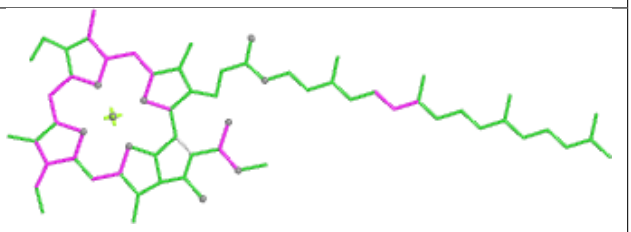


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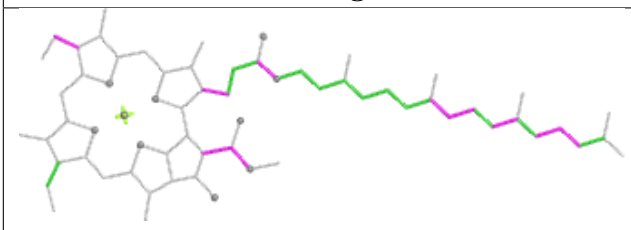
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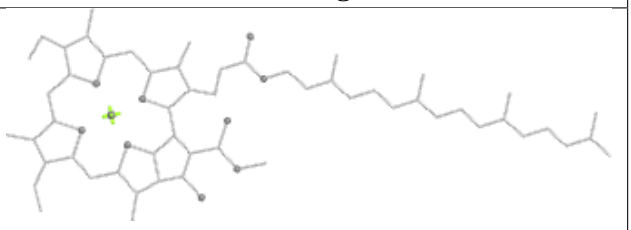
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Bond angles

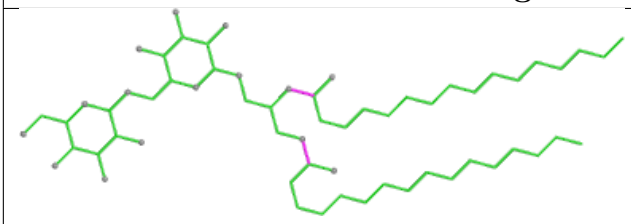


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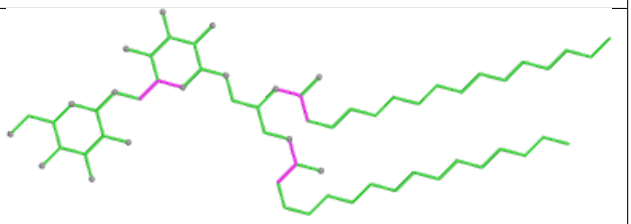


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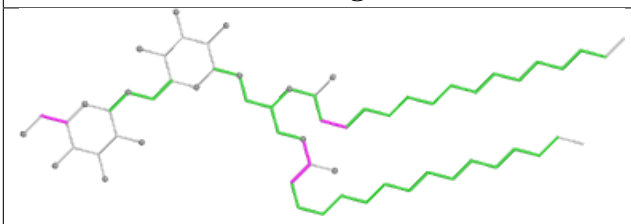
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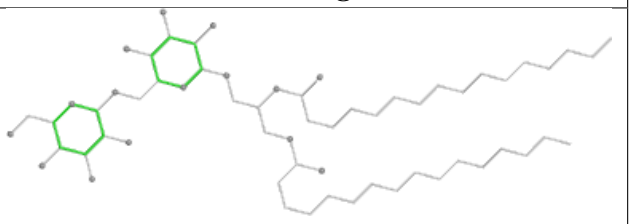
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Bond angles

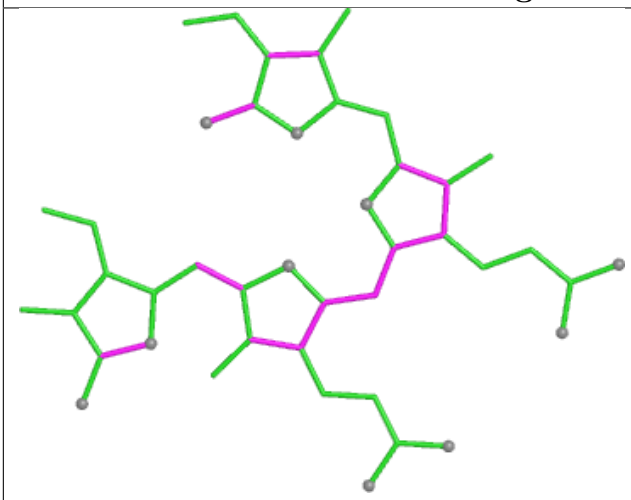


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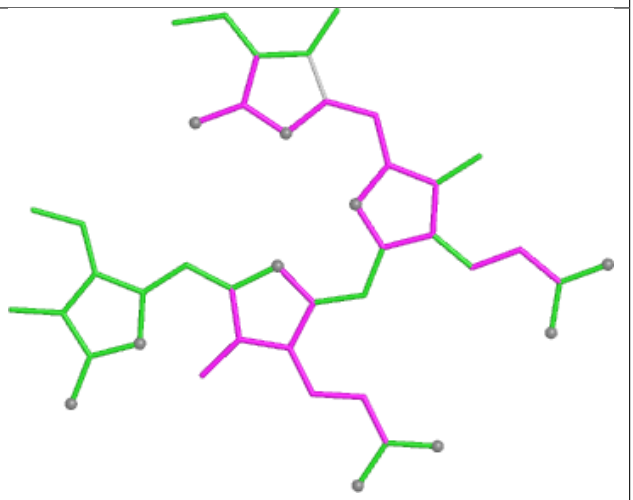


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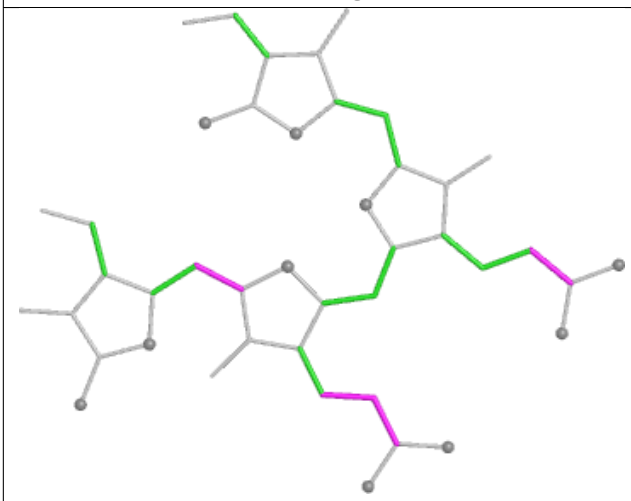
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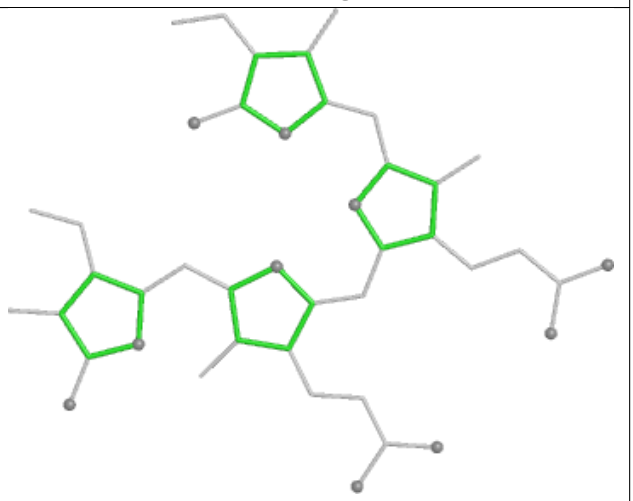
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Bond angles

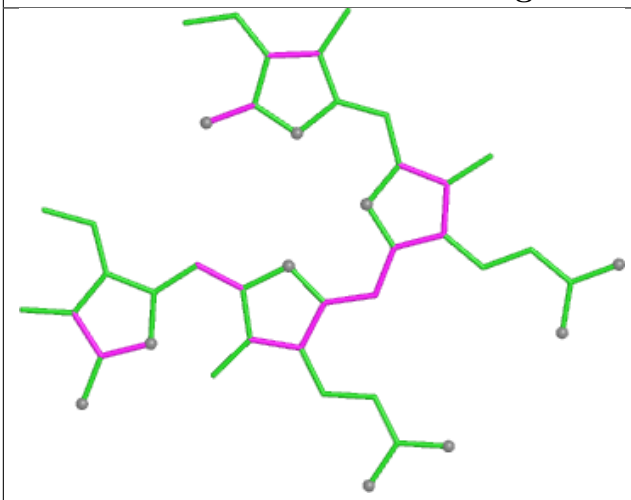


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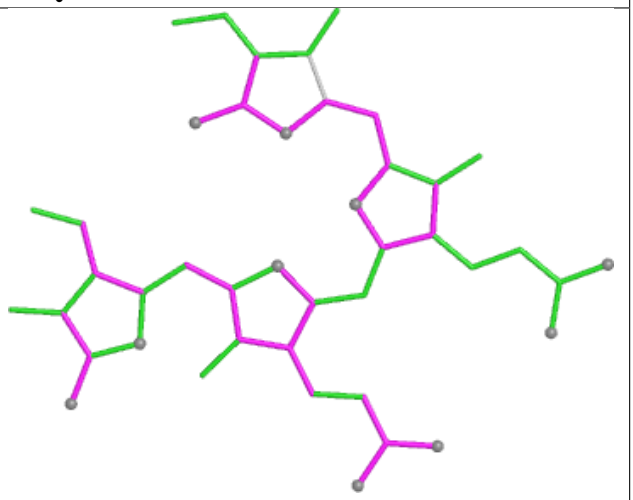


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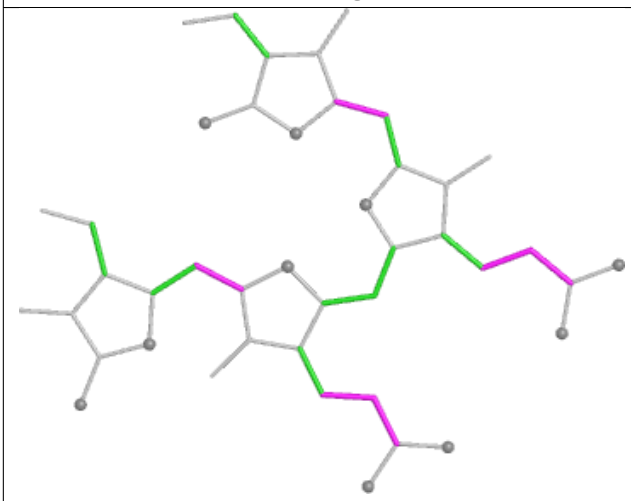
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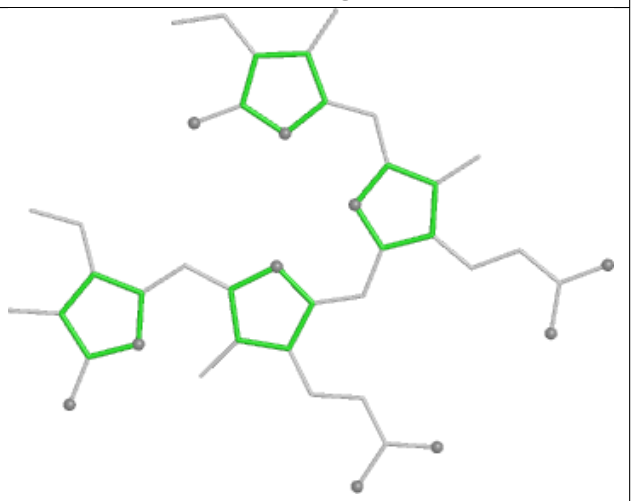
Bond lengths



Bond angles

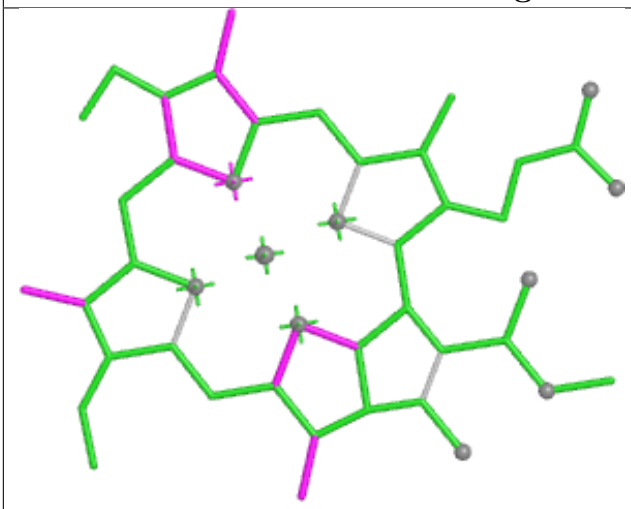


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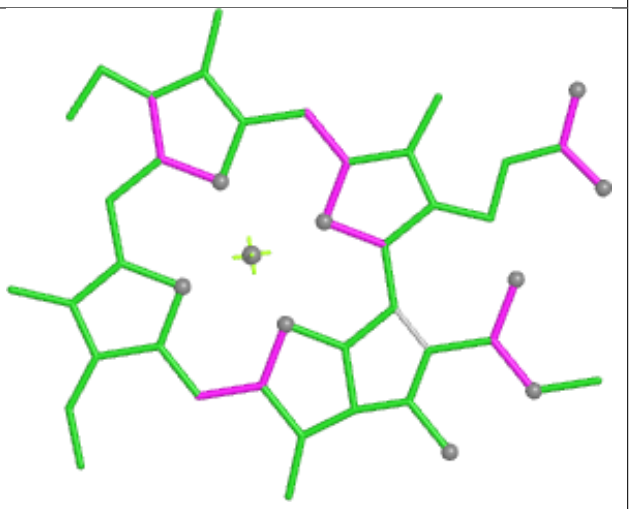


Rings

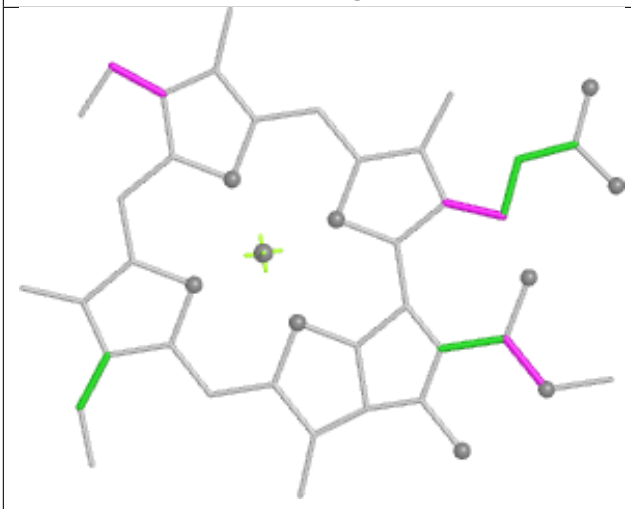
Ligand CLA 5N 610



Bond lengths



Bond angles

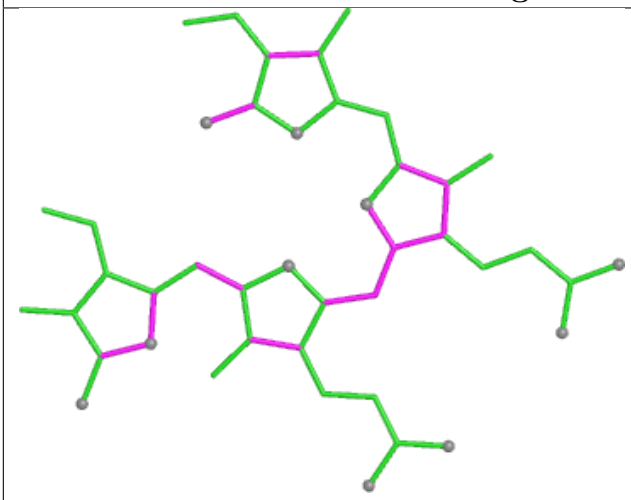


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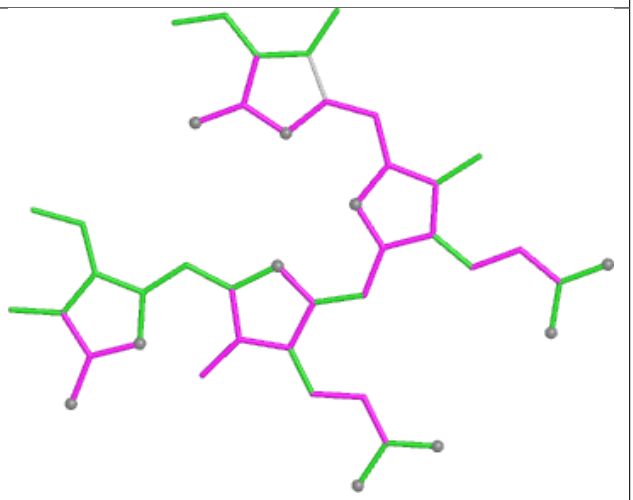


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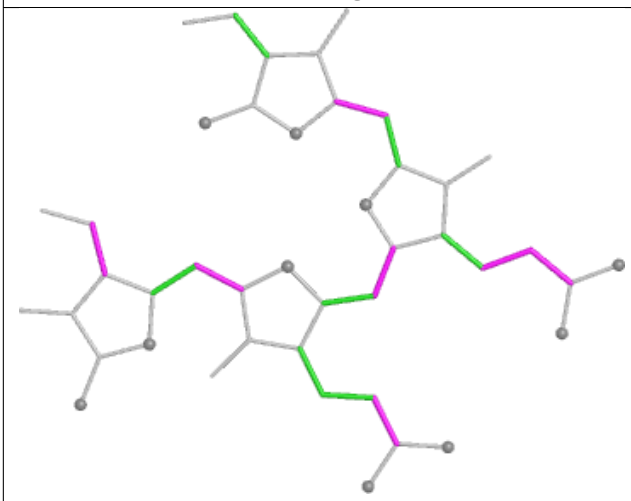
Ligand PEB BA 203



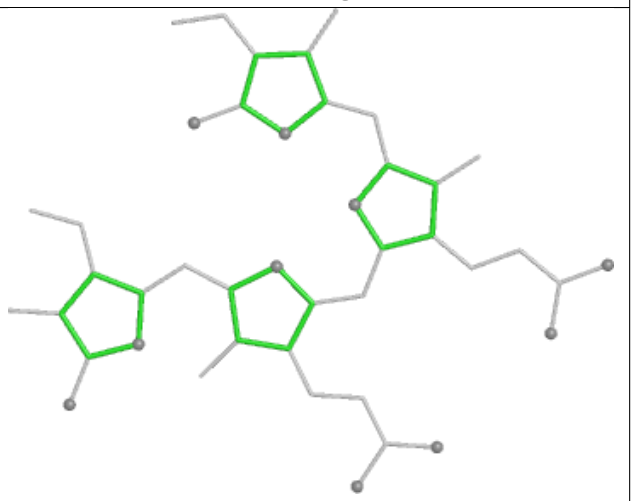
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Bond angles

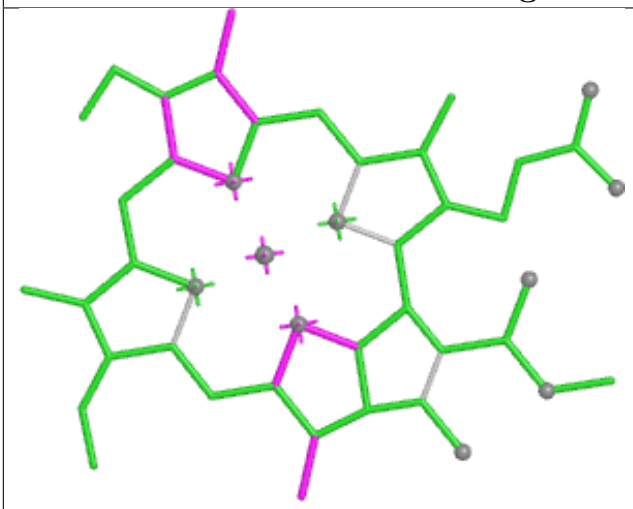


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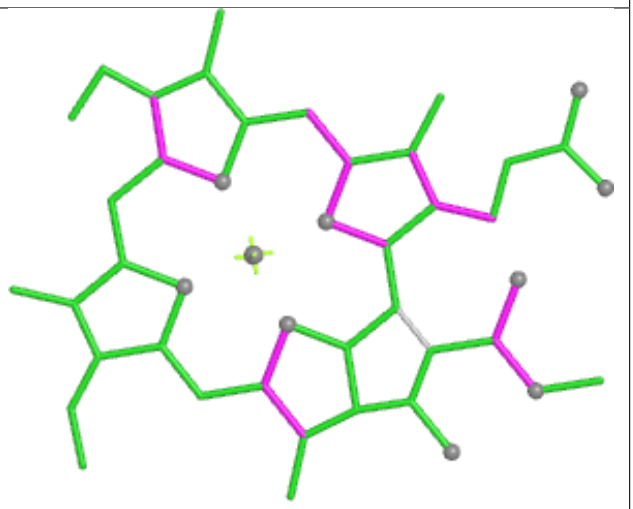


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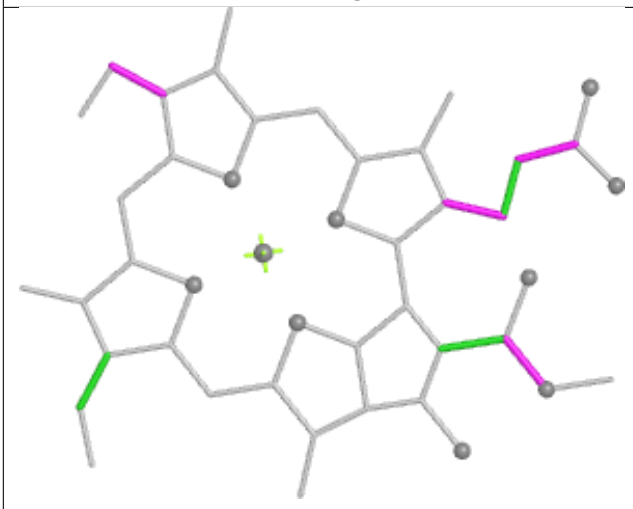
Ligand CLA 42 606



Bond lengths



Bond angles

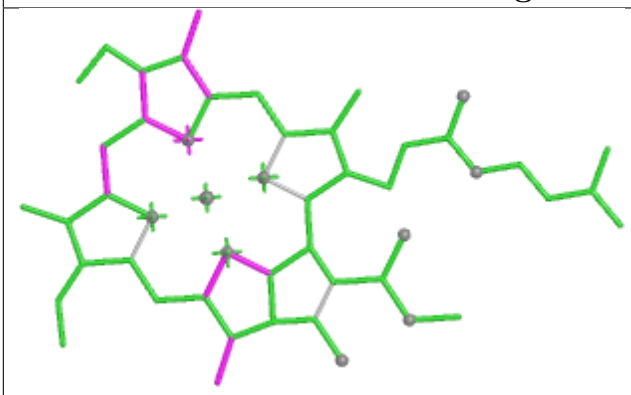


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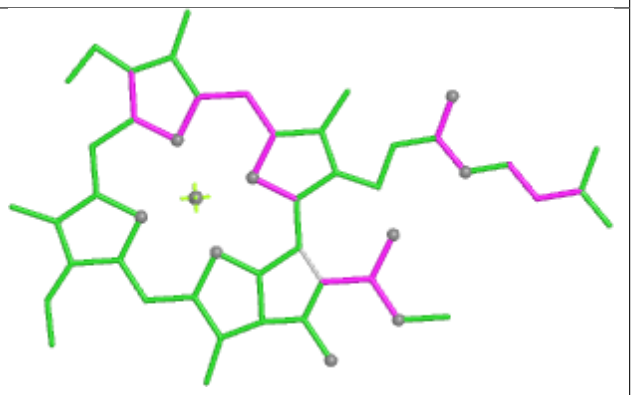


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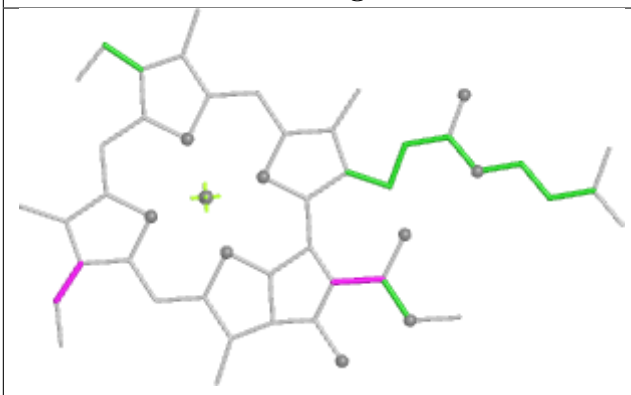
Ligand CLA A6 404



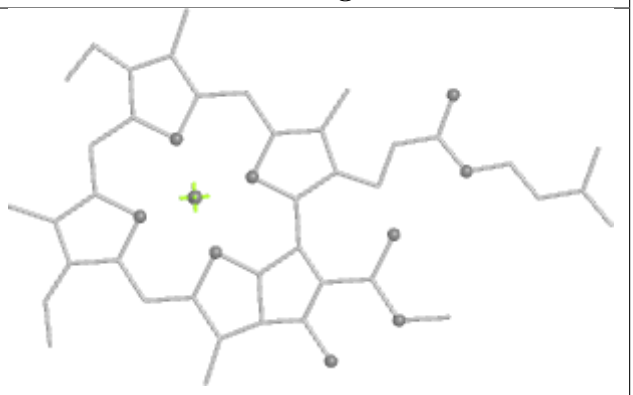
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Bond angles



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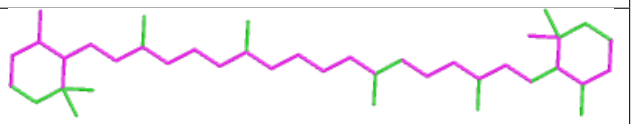


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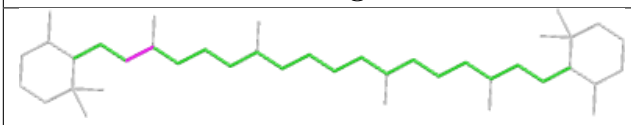
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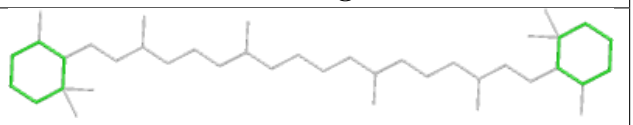
Bond lengths



Bond angles

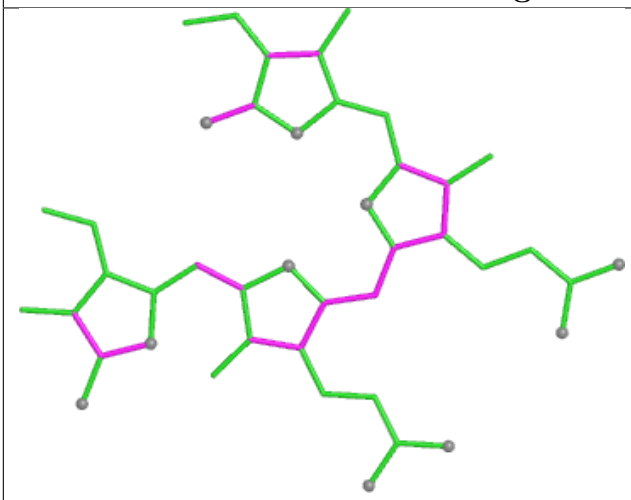


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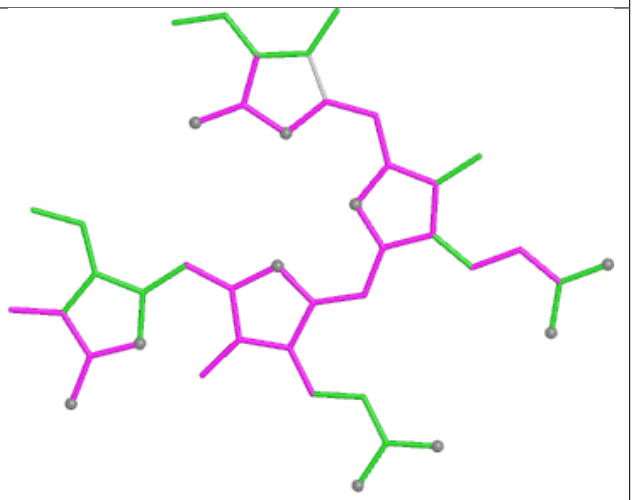


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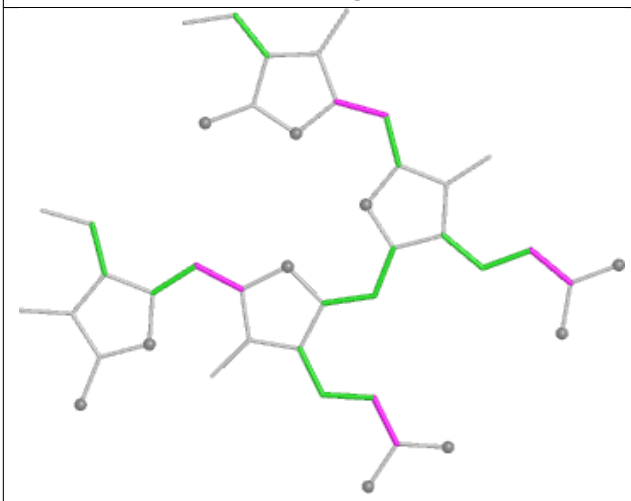
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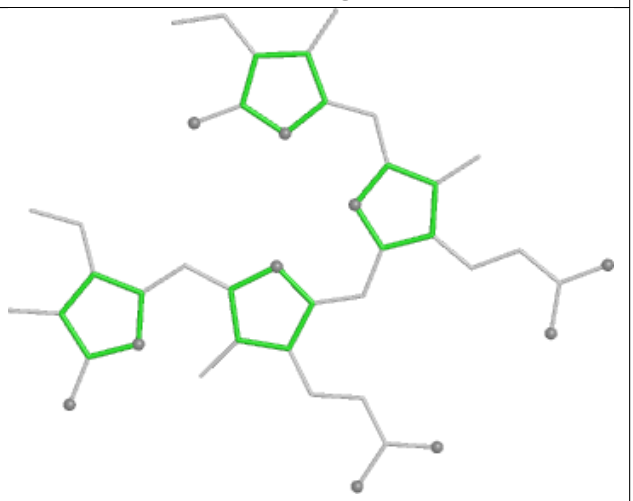
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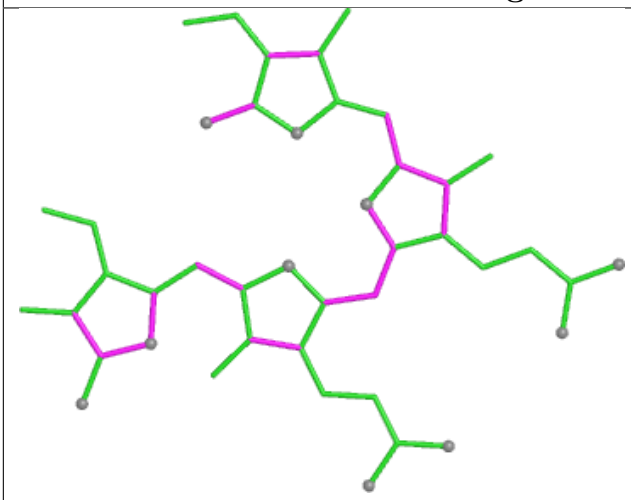


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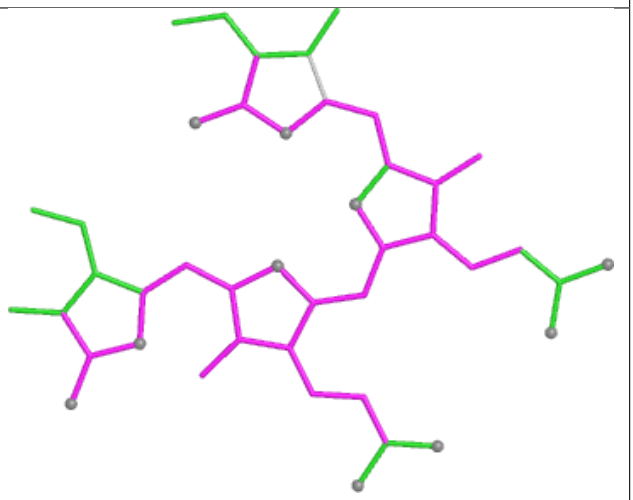


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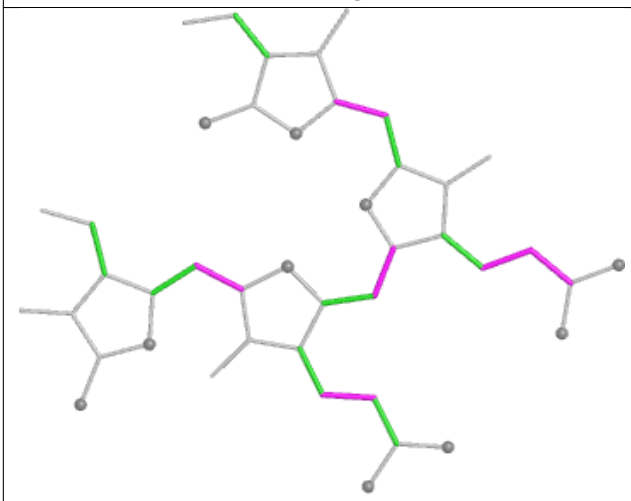
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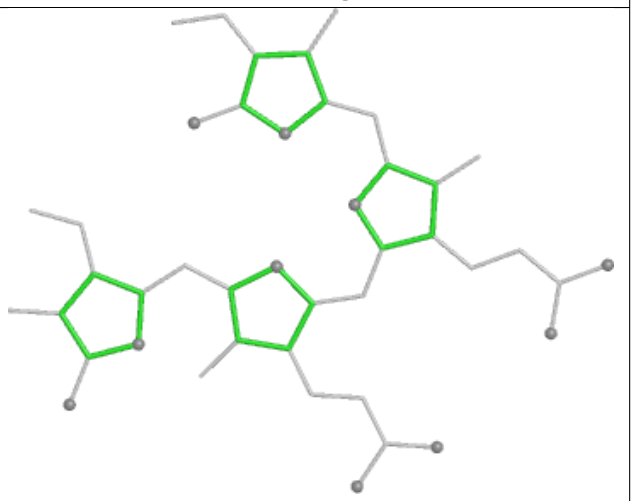
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Bond angles

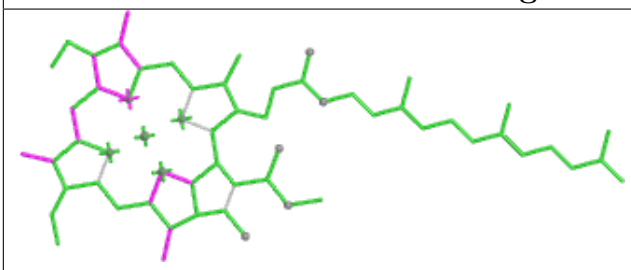


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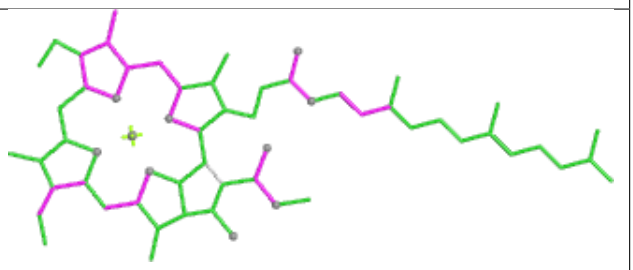


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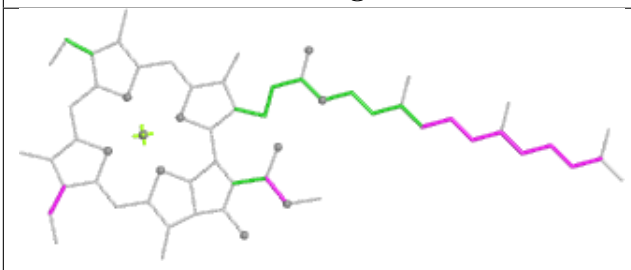
Ligand CLA a6 608



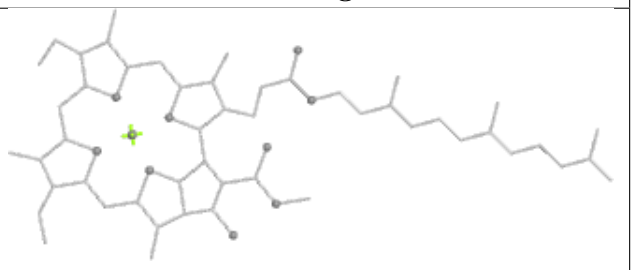
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Bond angles

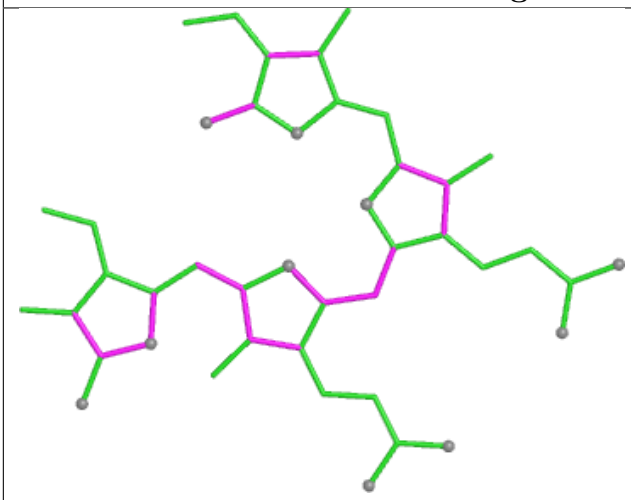


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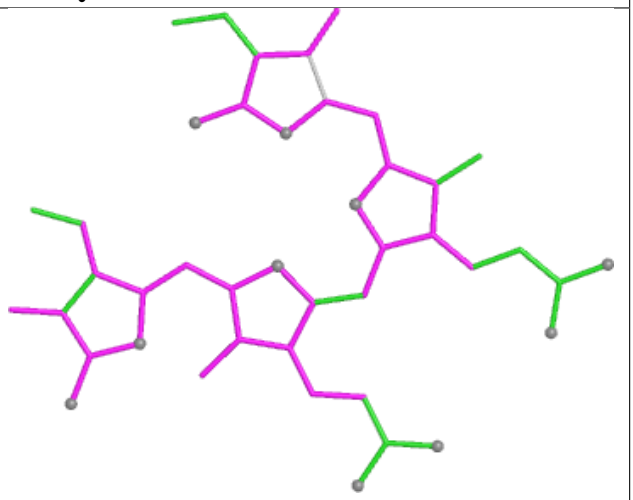


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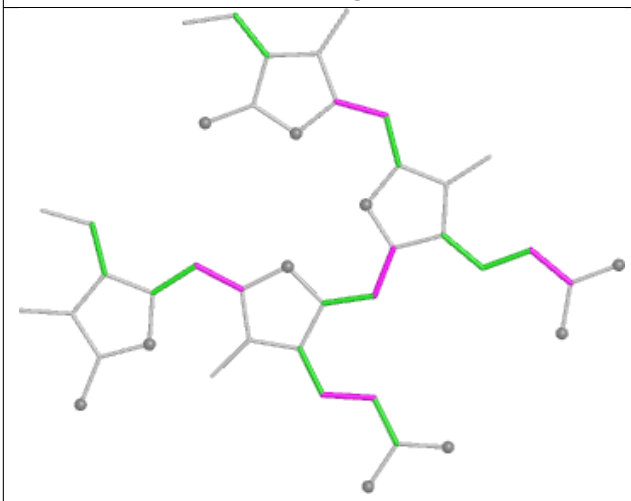
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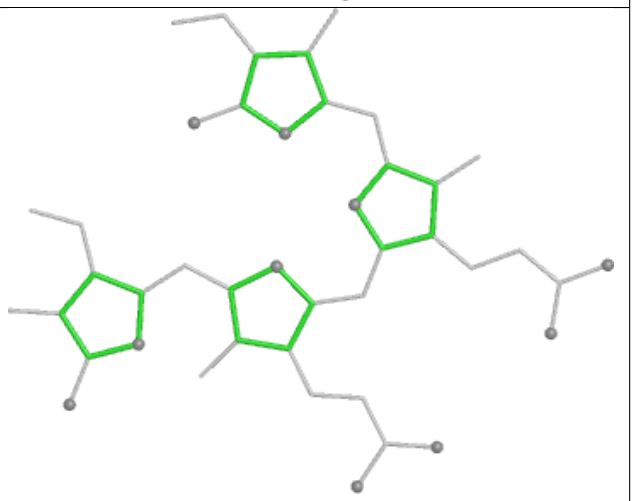
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Bond angles

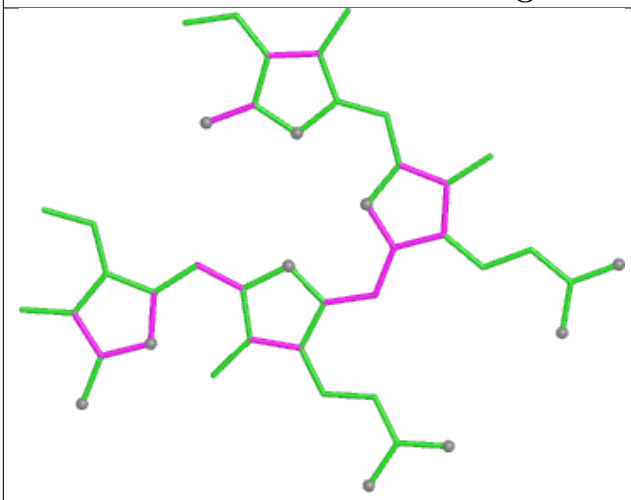


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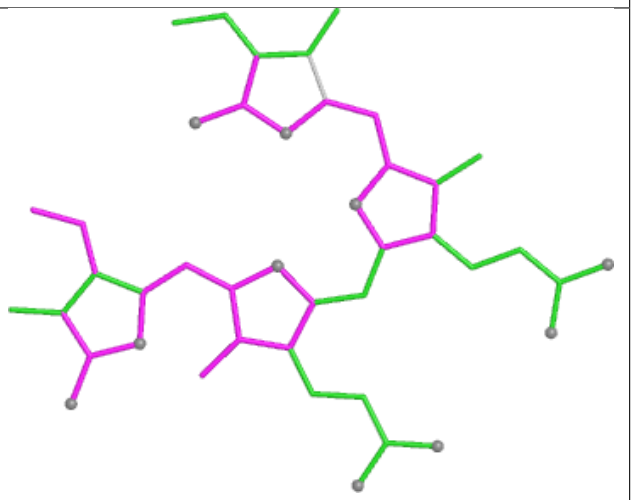


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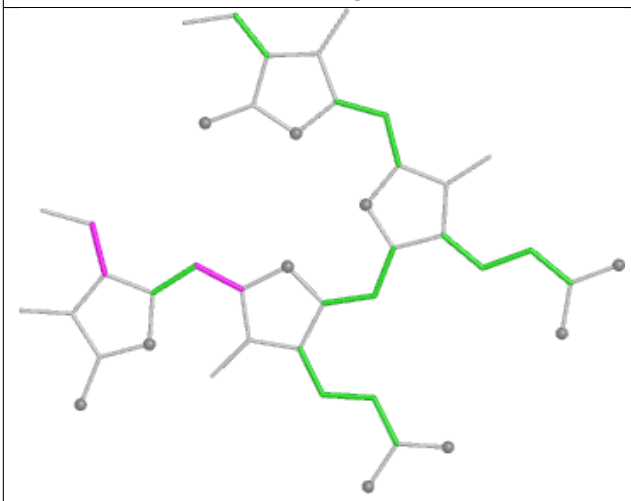
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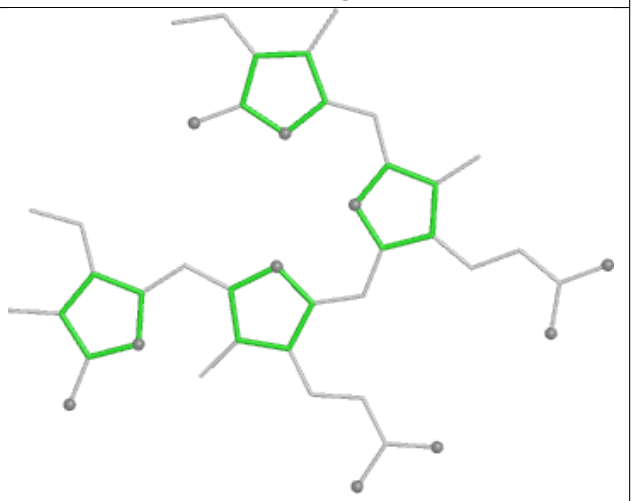
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Bond angles

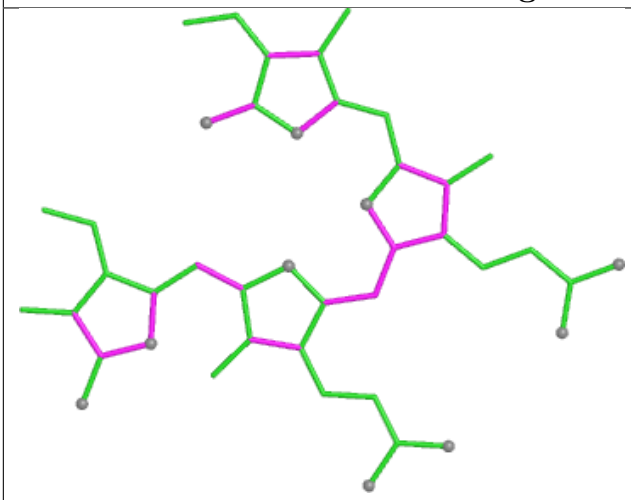


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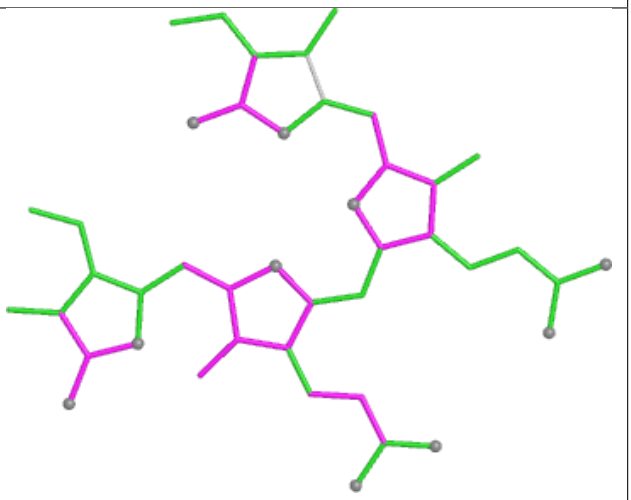


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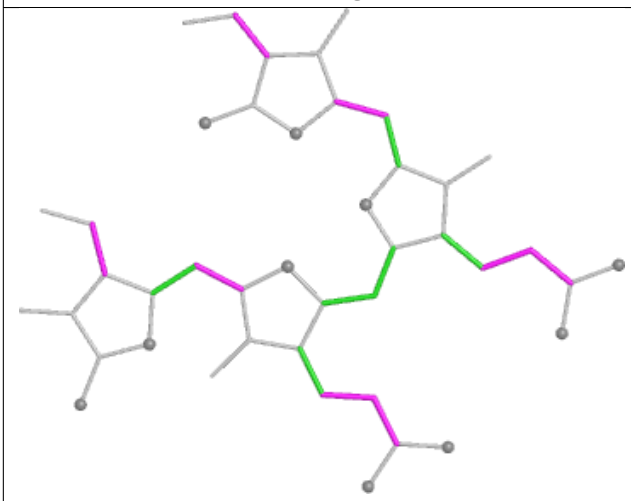
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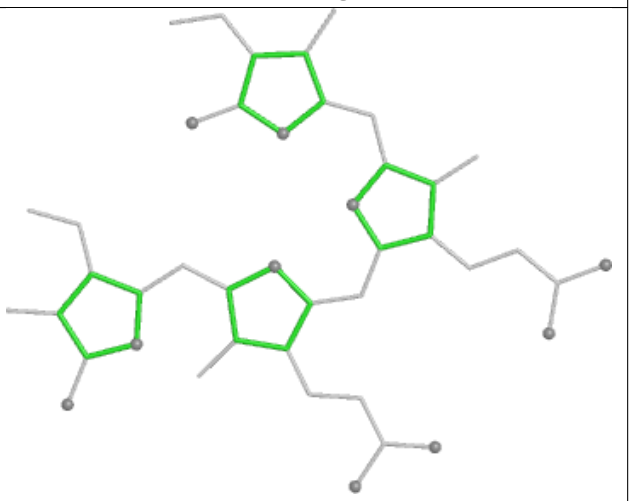
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Bond angles

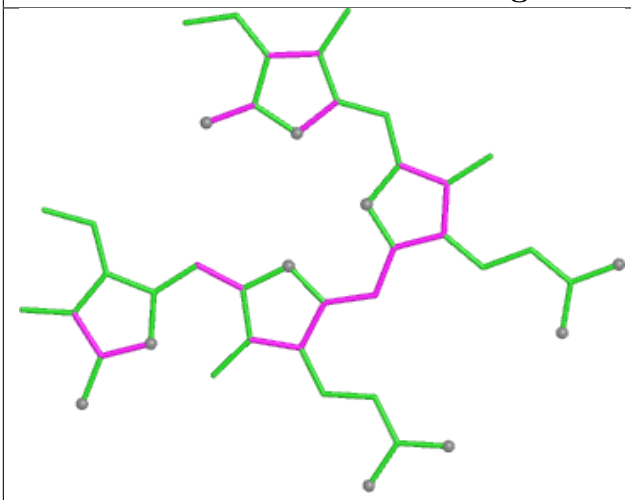


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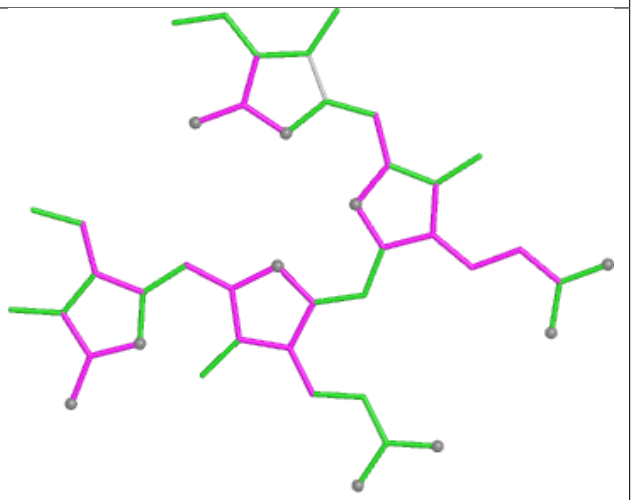


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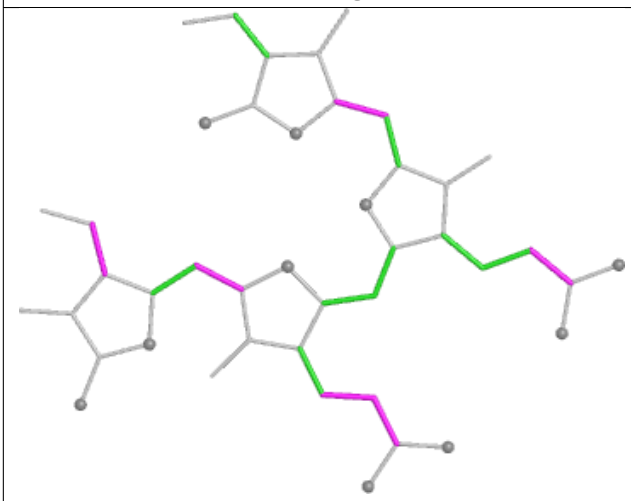
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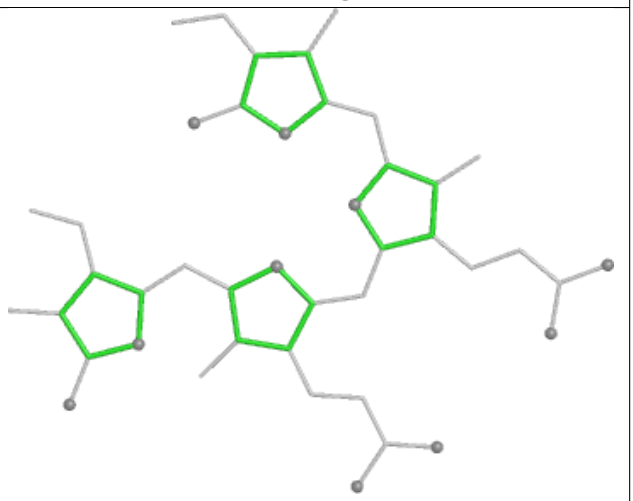
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Bond angles

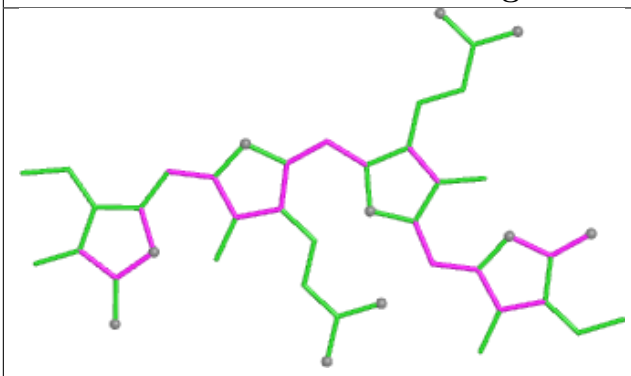


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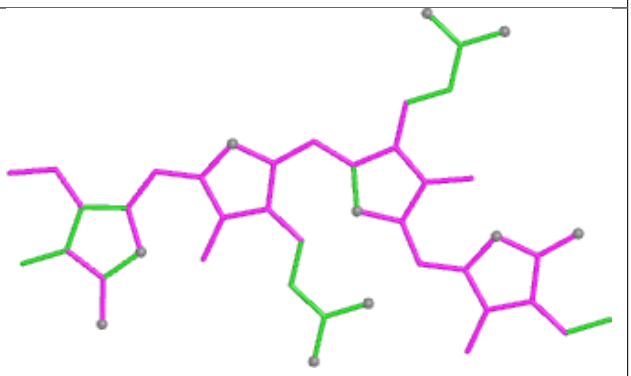


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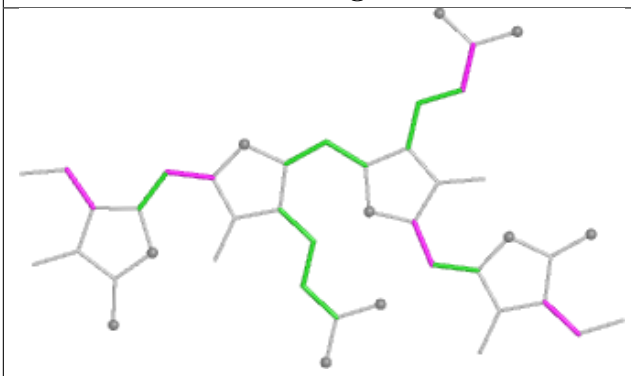
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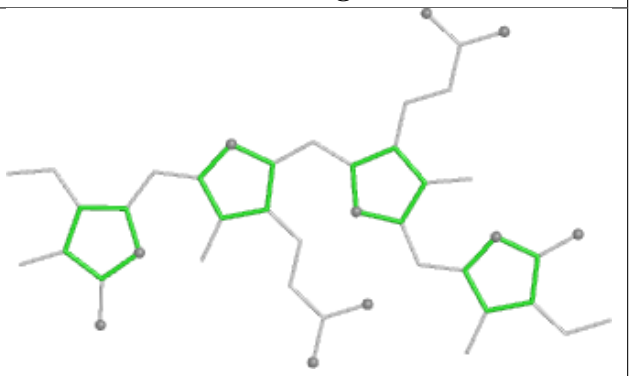
Bond lengths



Bond angles

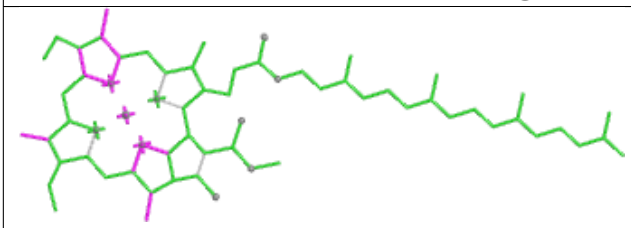


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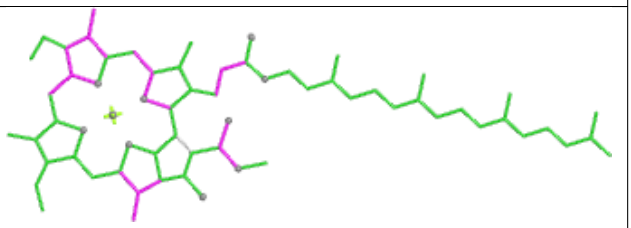


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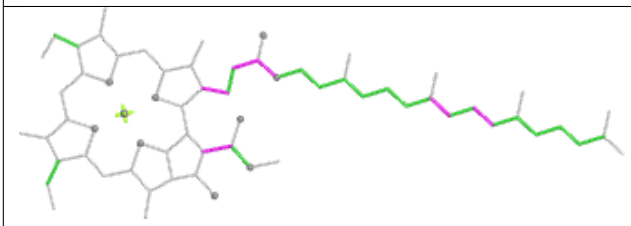
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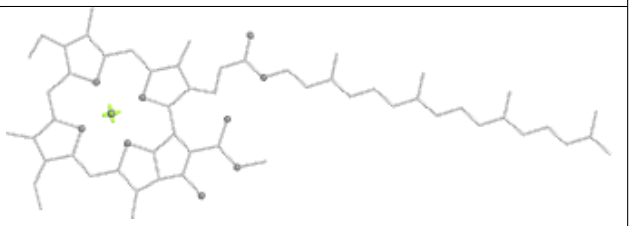
Bond lengths



Bond angles

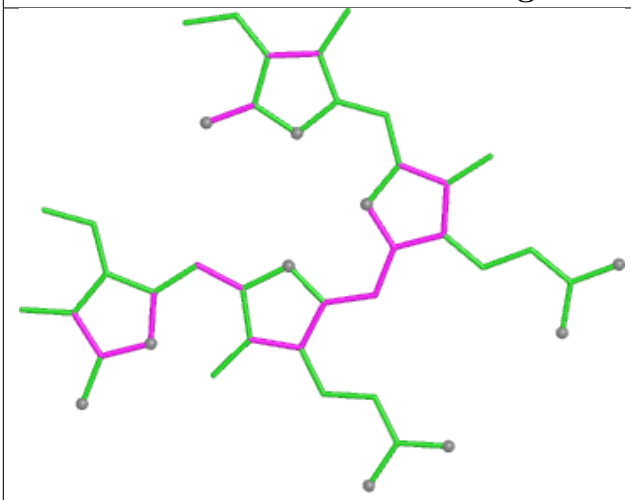


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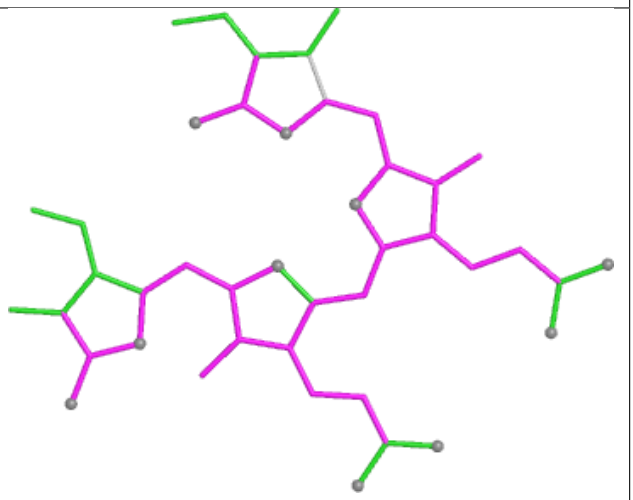


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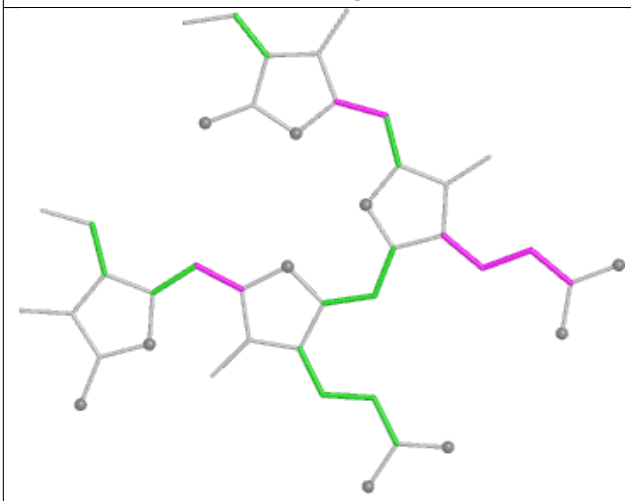
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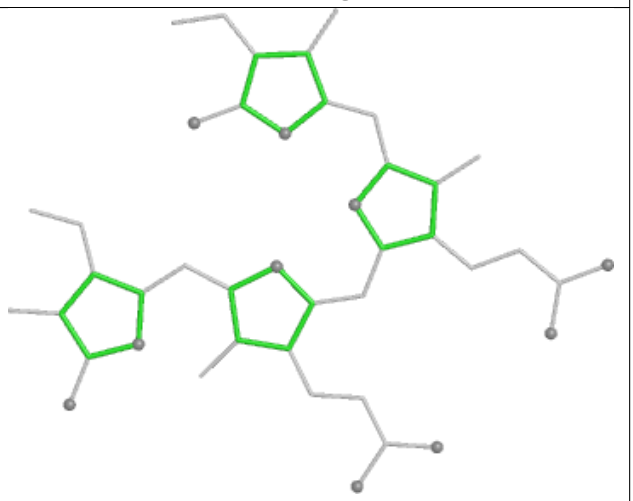
Bond lengths



Bond angles

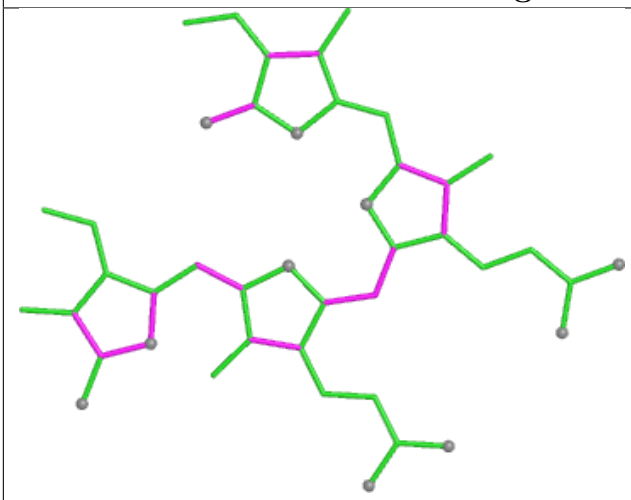


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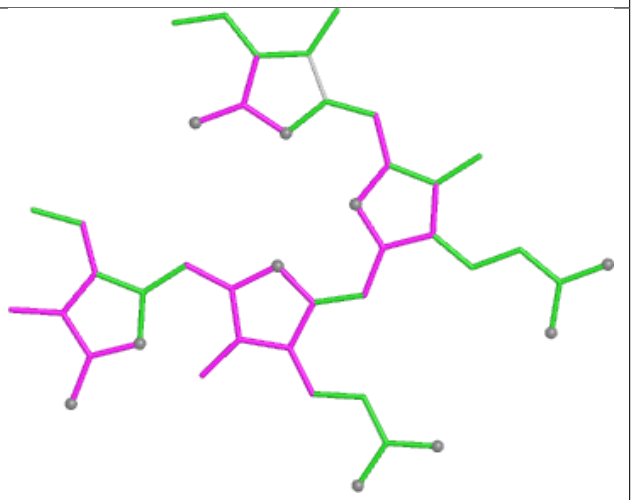


Rings

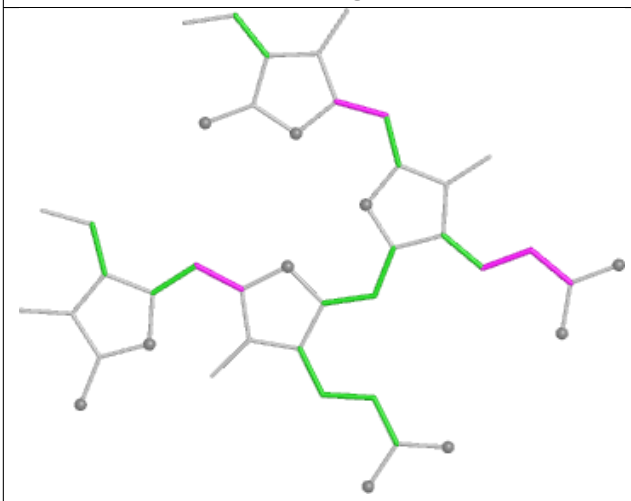
Ligand PEB KJ 201



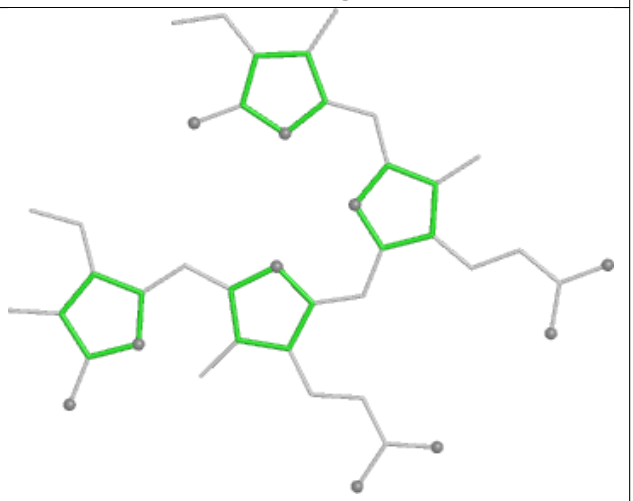
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Bond angles

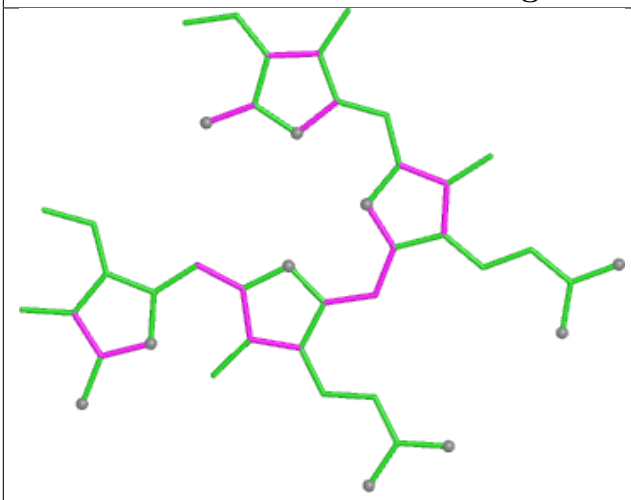


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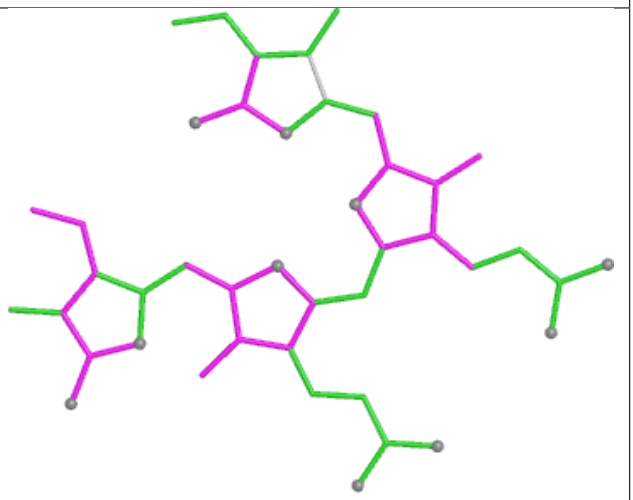


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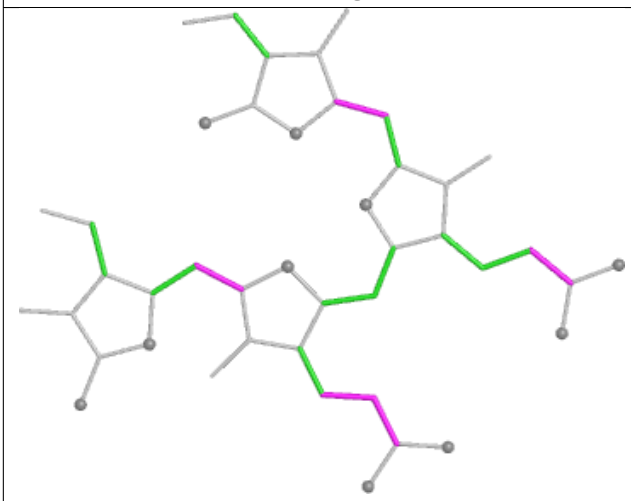
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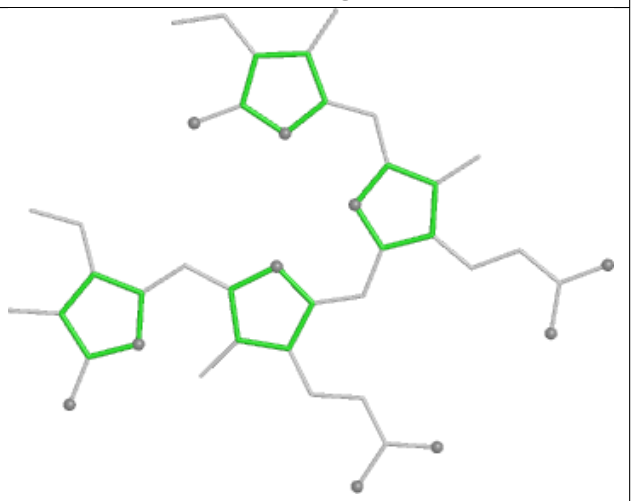
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Bond angles

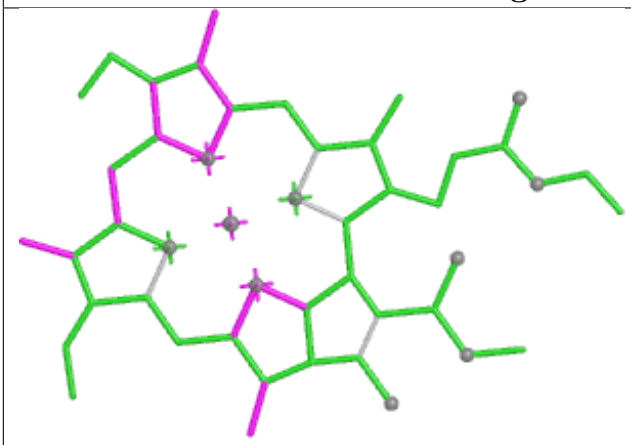


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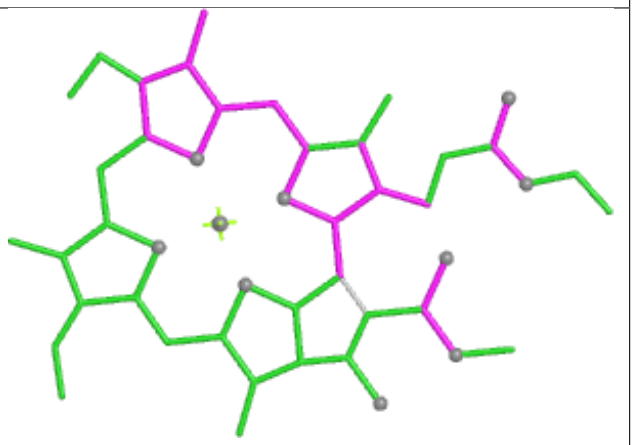


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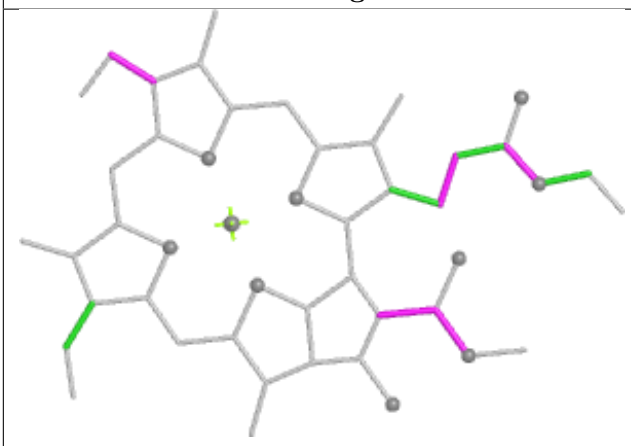
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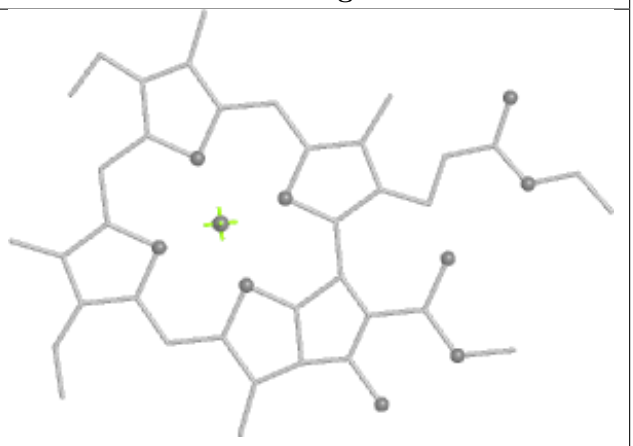
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Bond angles

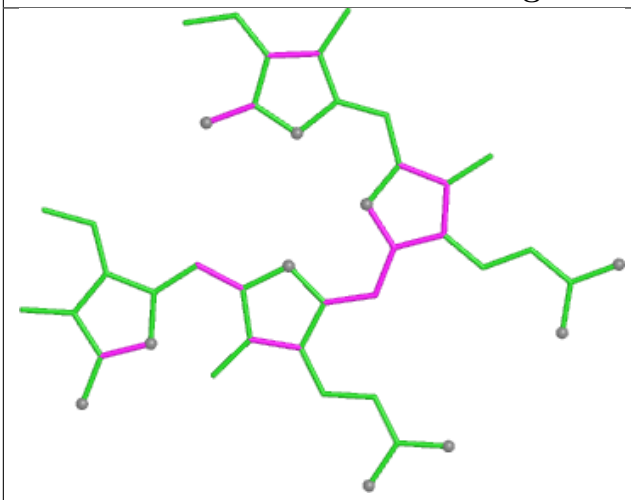


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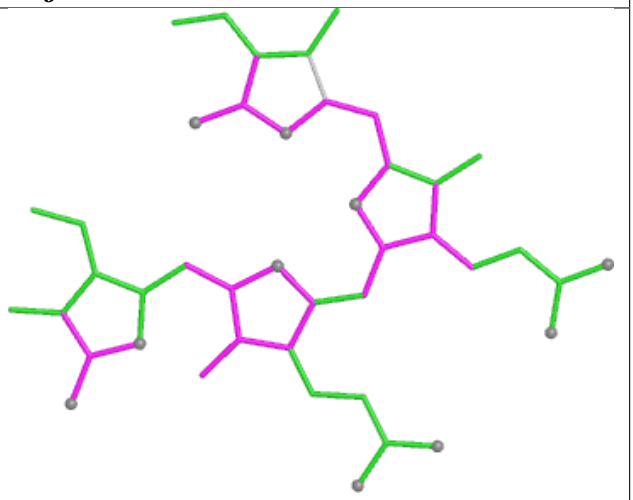


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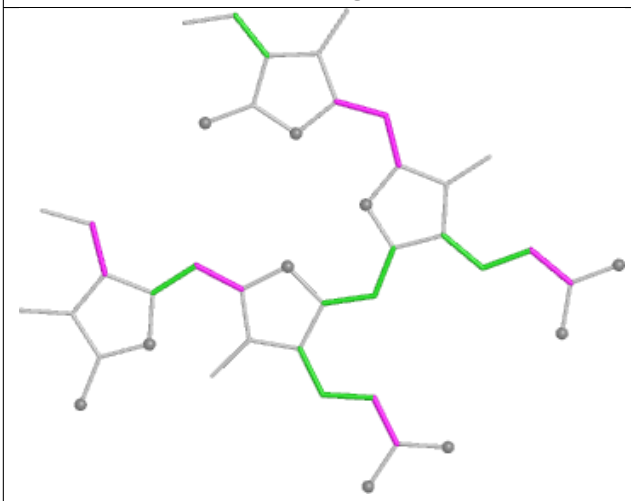
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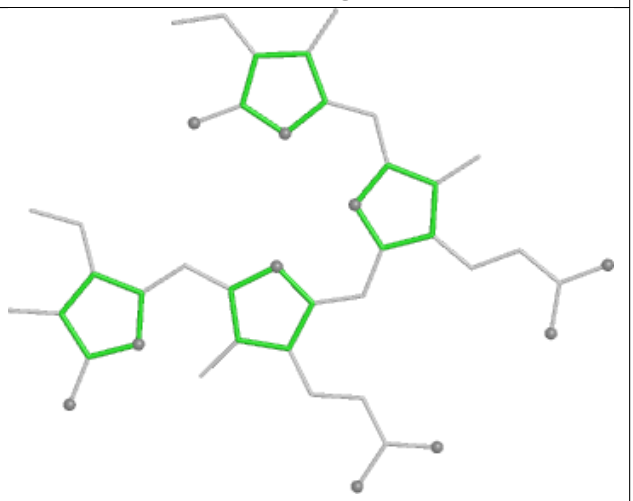
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Bond angles

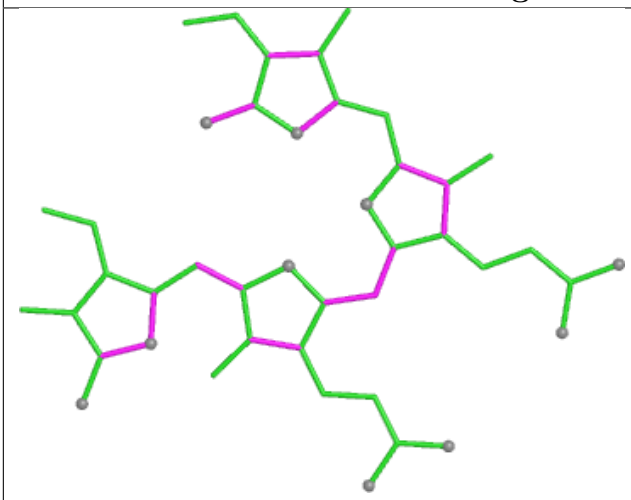


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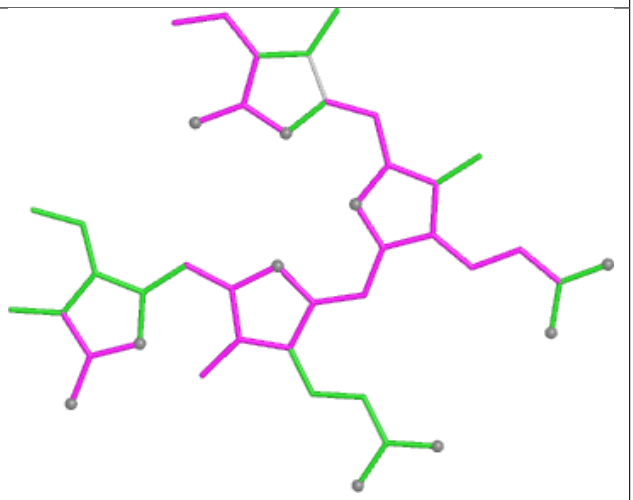


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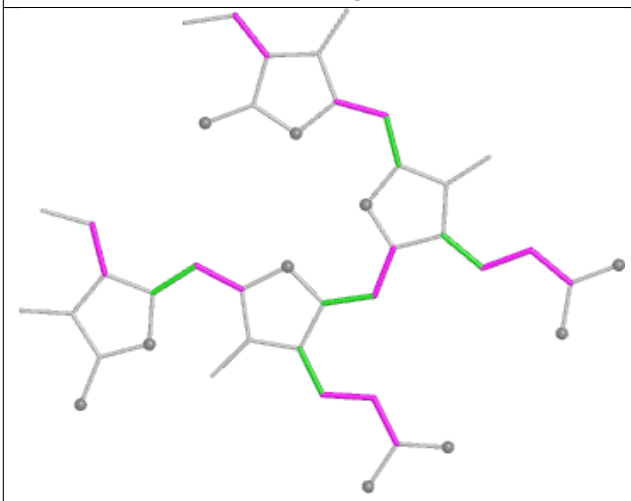
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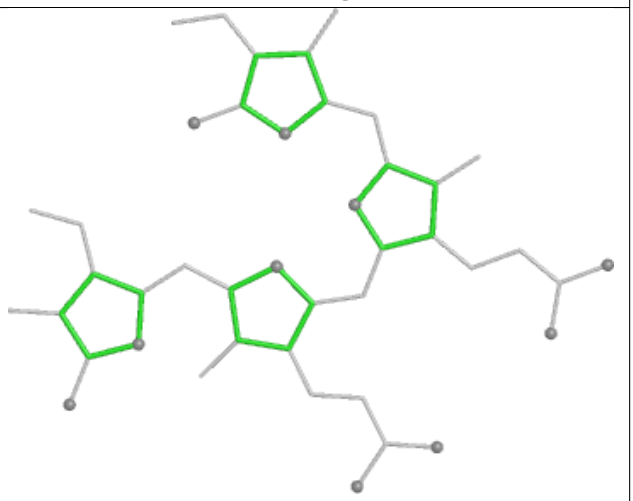
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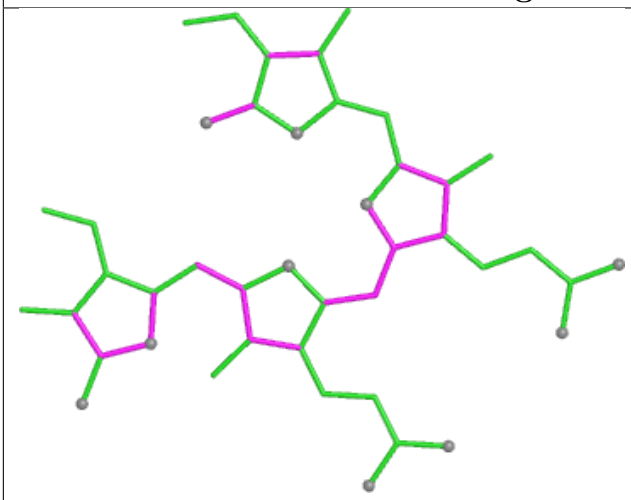


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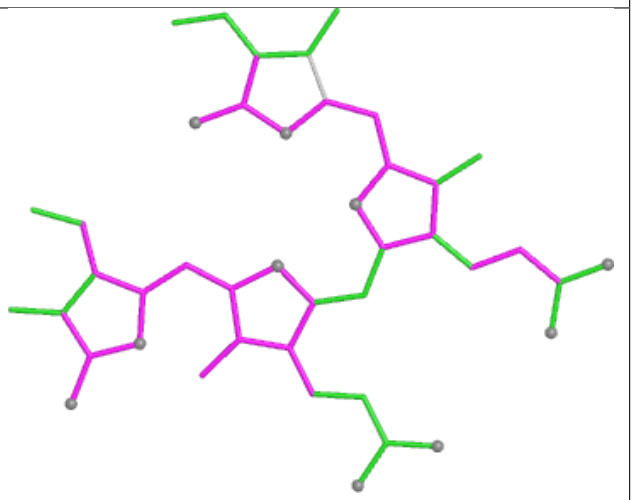


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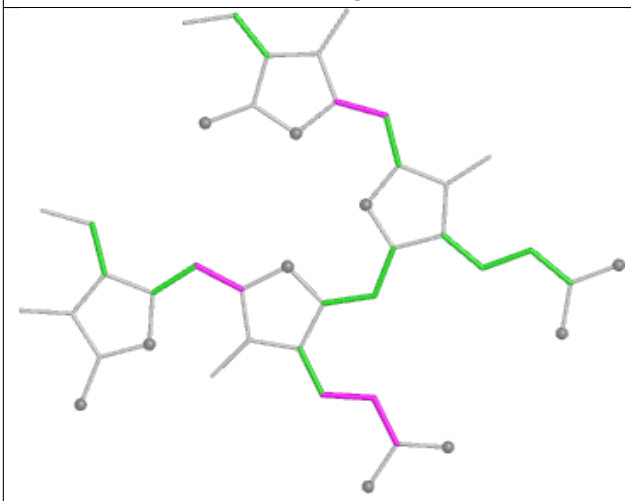
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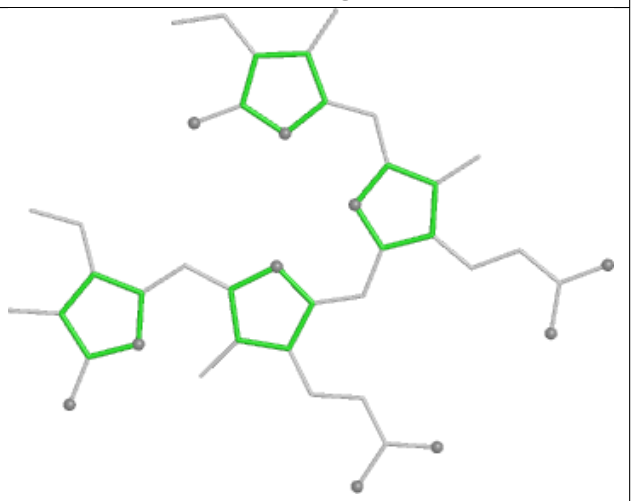
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Bond angles

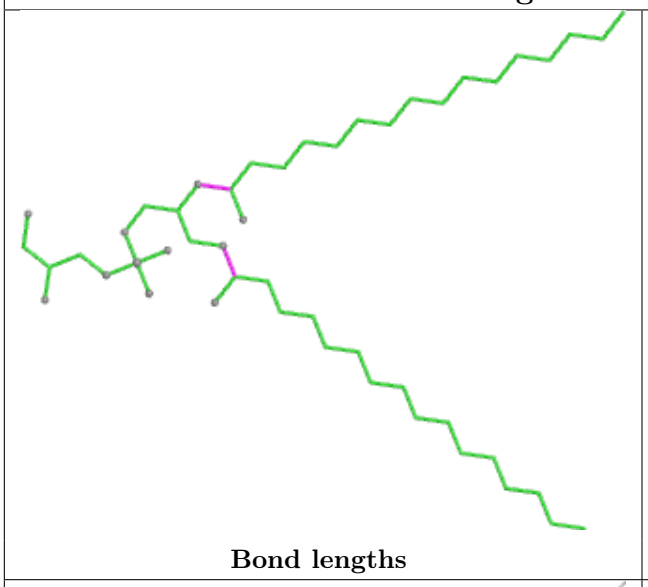


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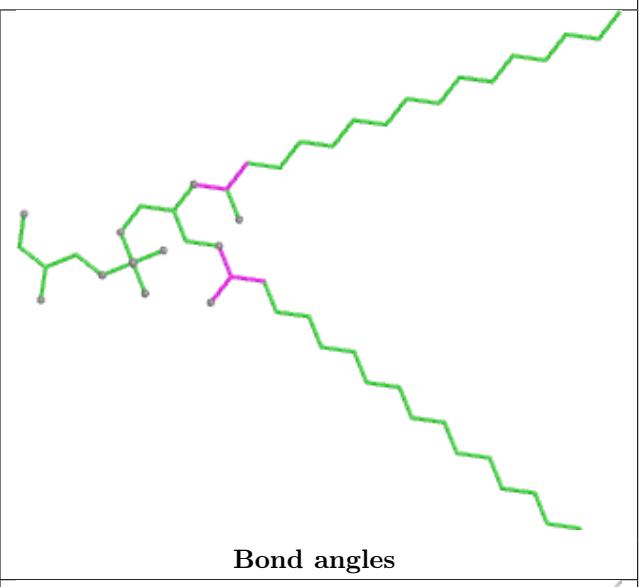


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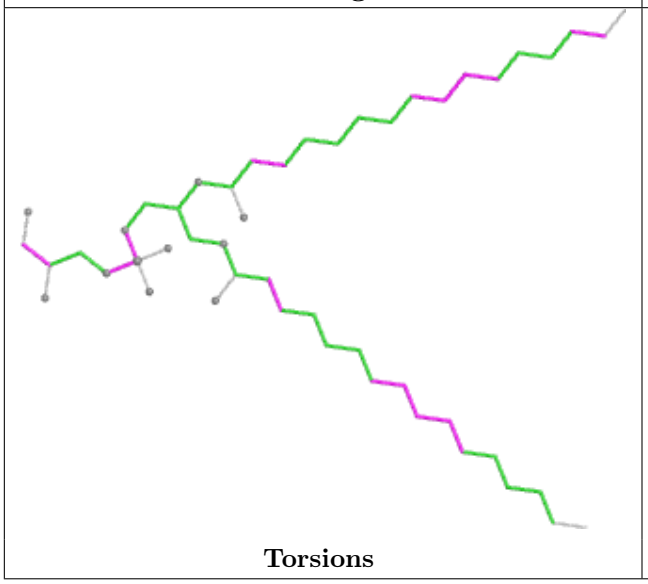
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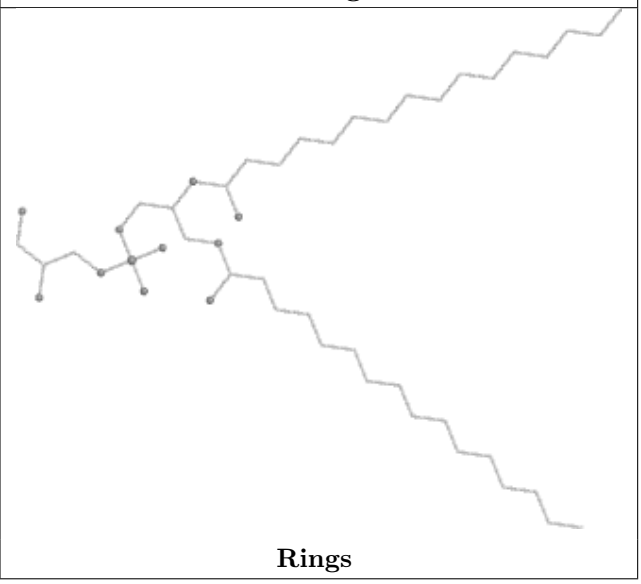
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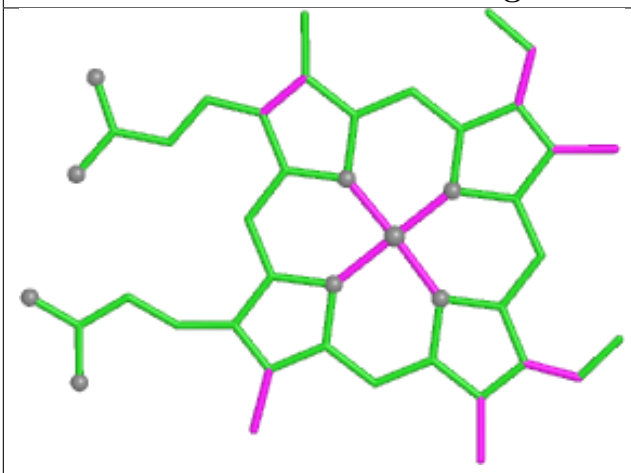


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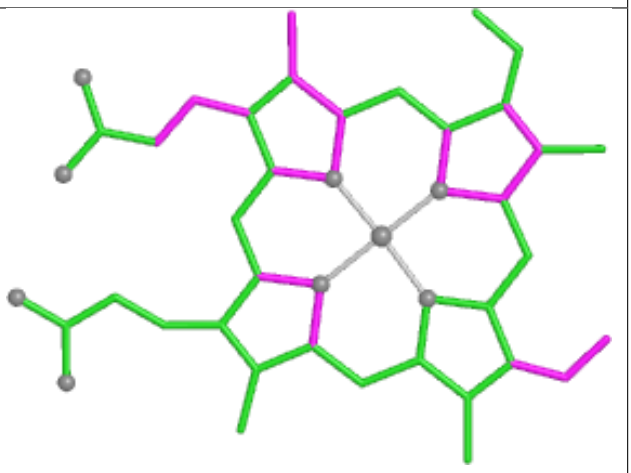


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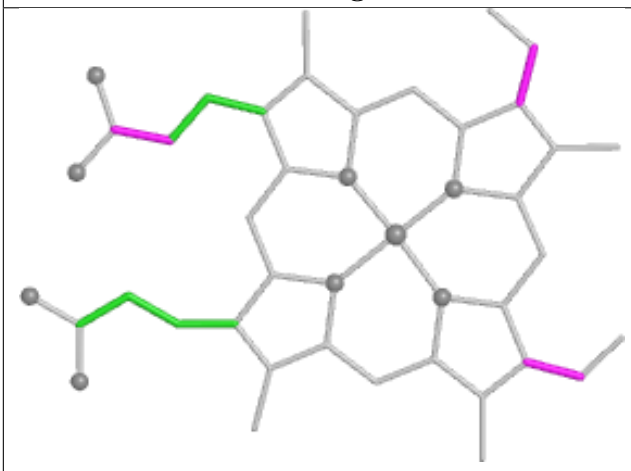
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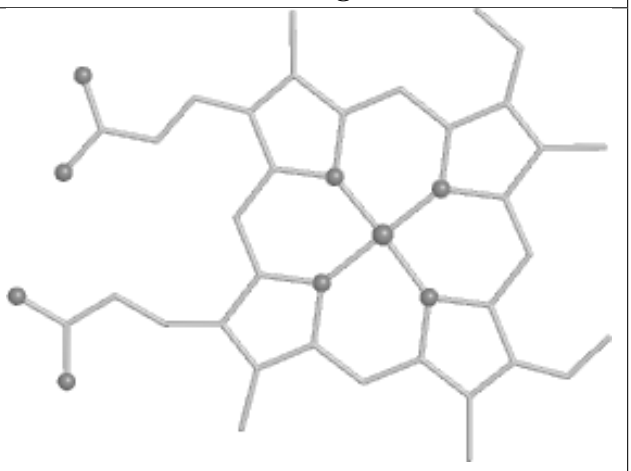
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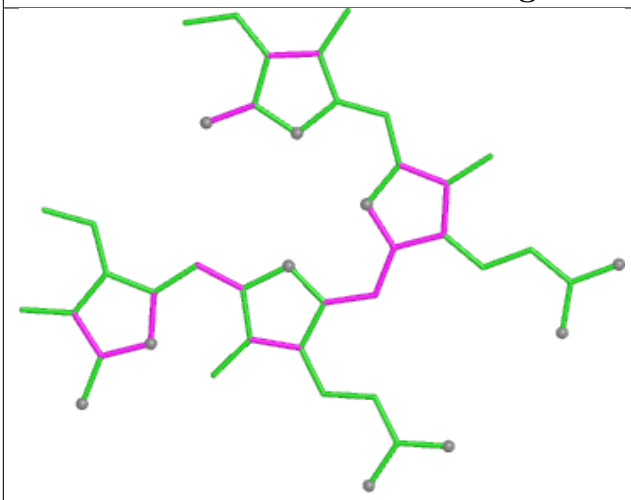


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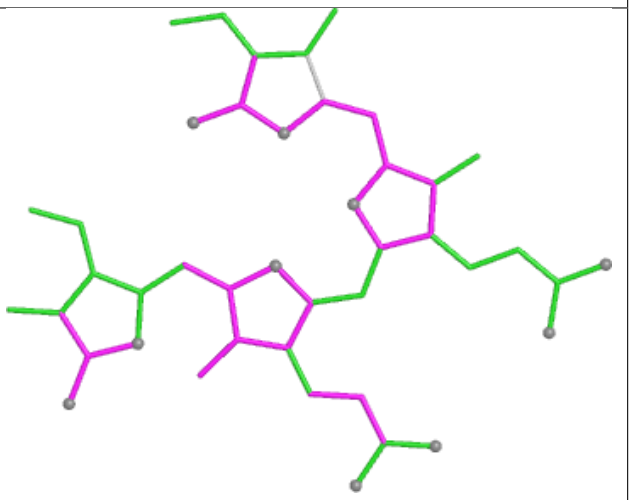


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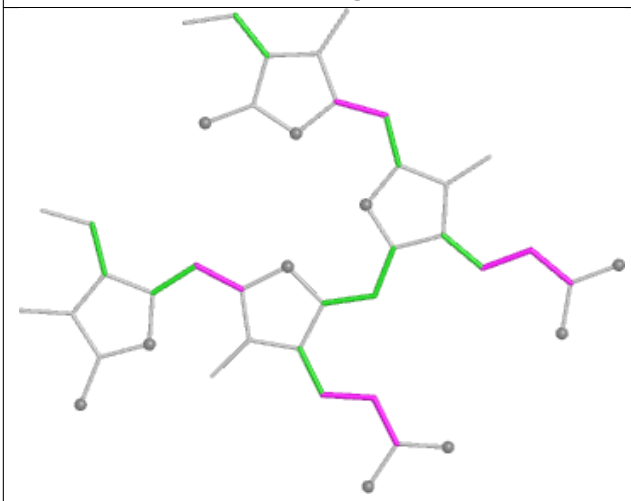
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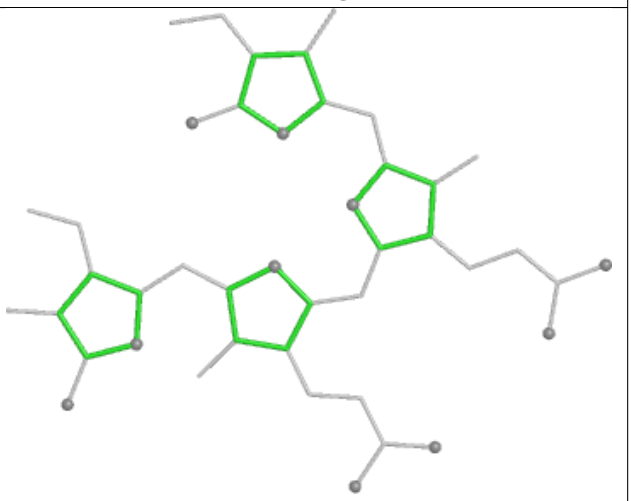
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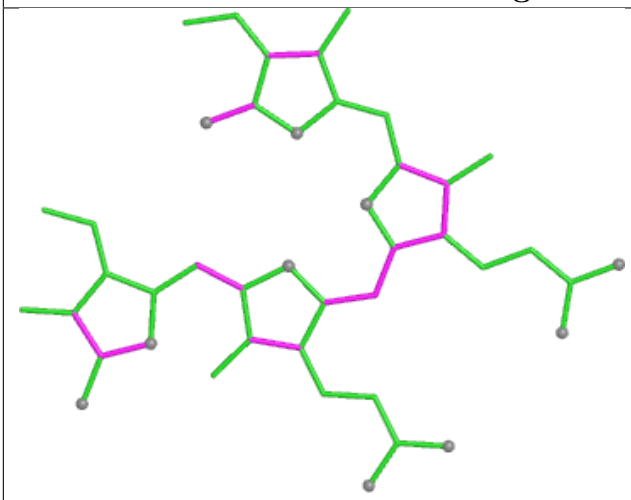


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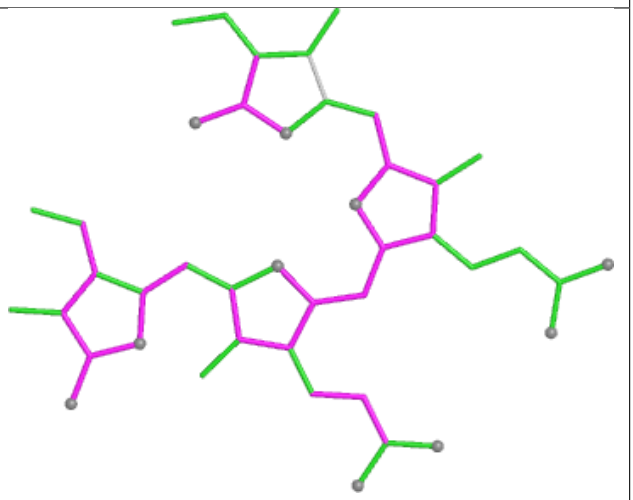


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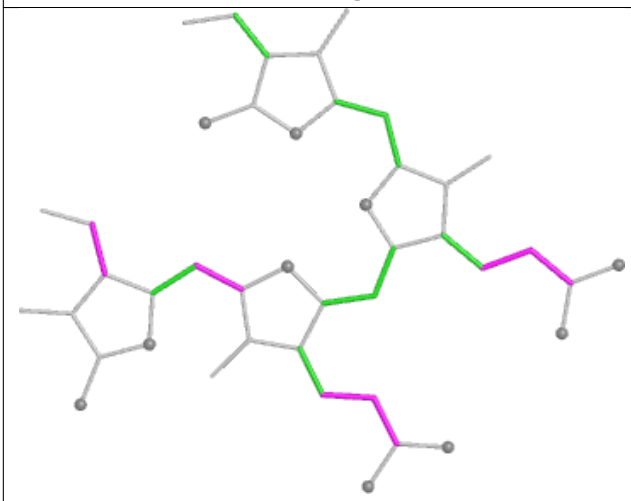
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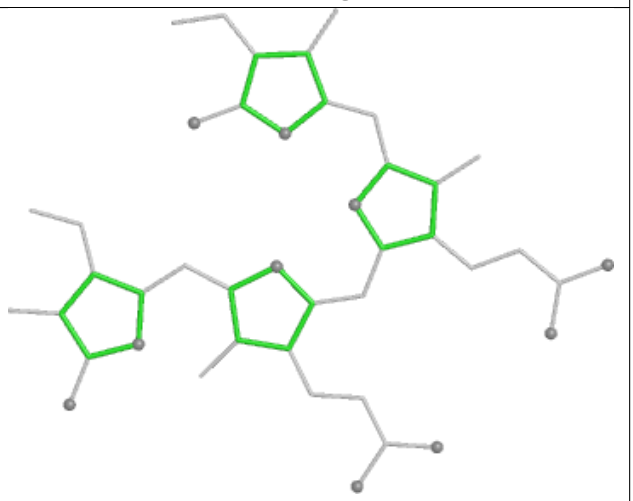
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Bond angles

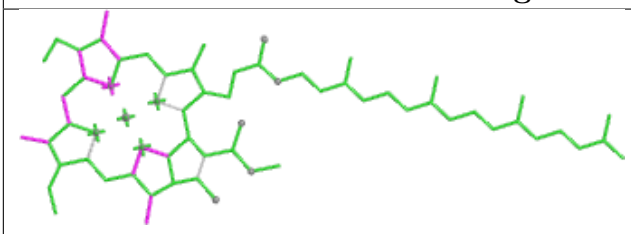


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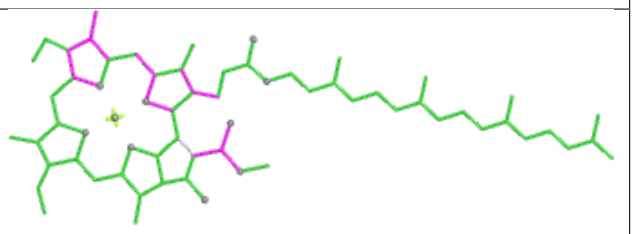


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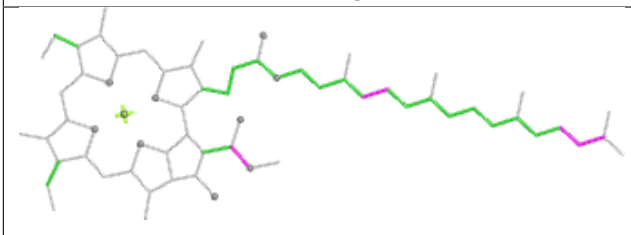
Ligand CLA BL 619



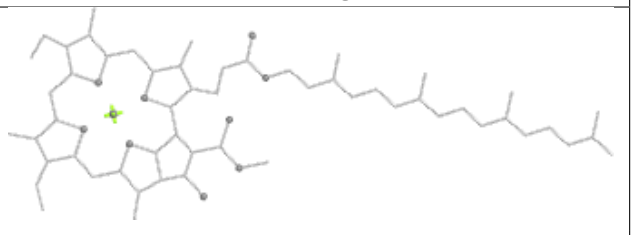
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Bond angles

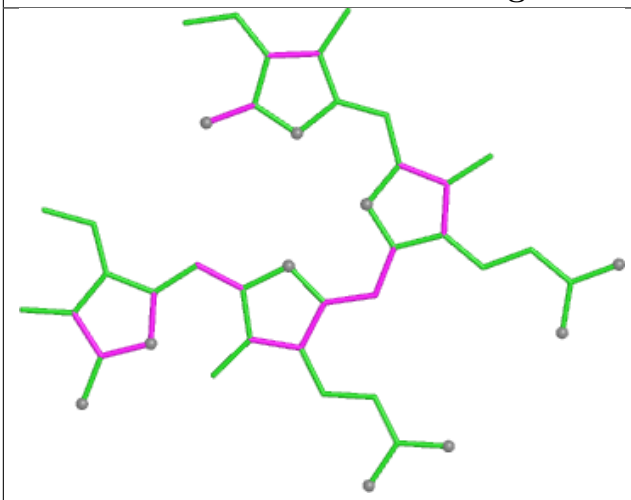


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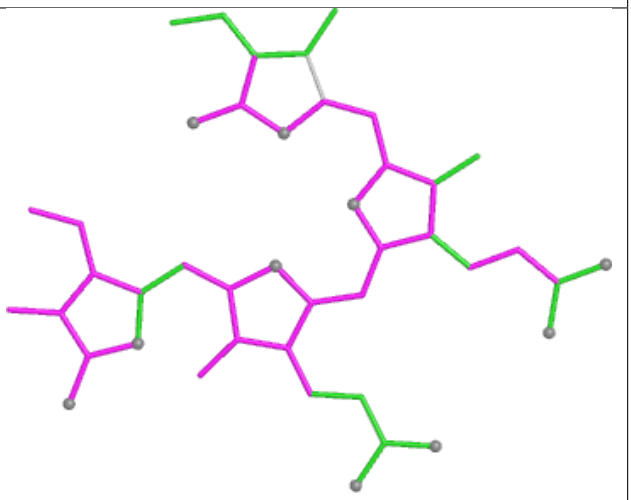


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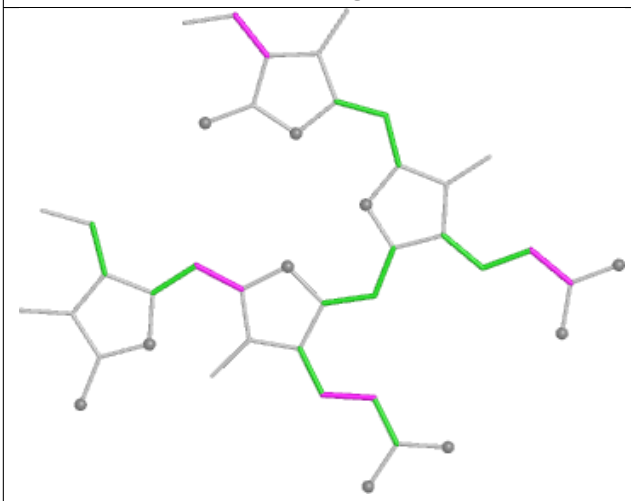
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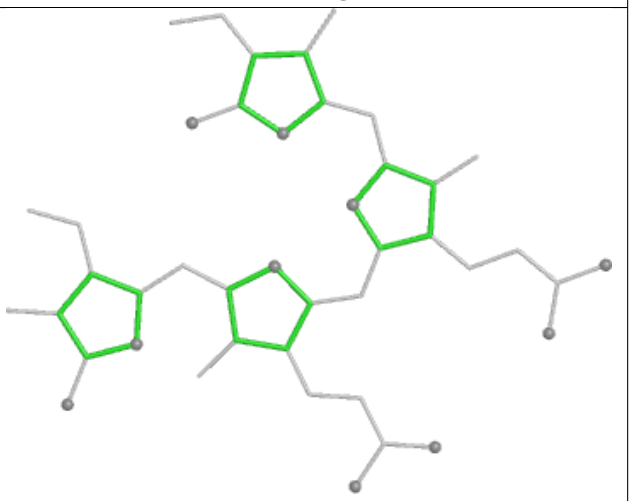
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Bond angles

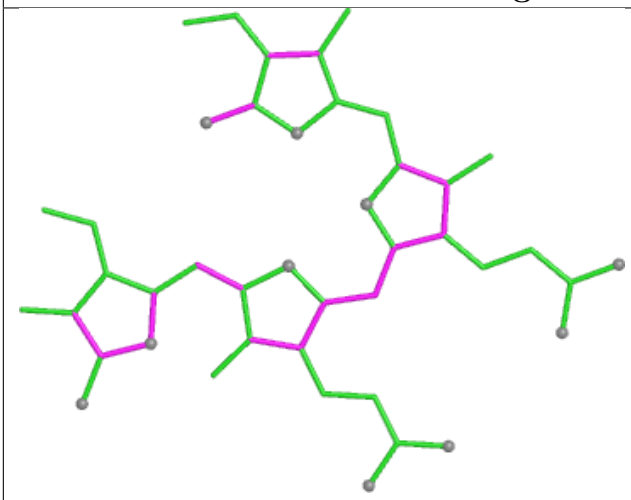


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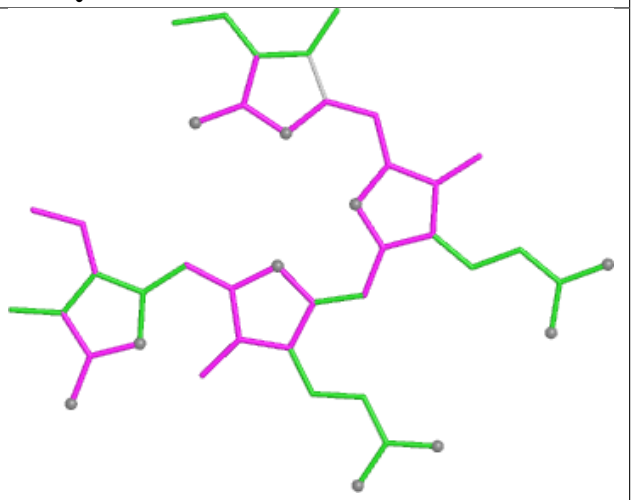


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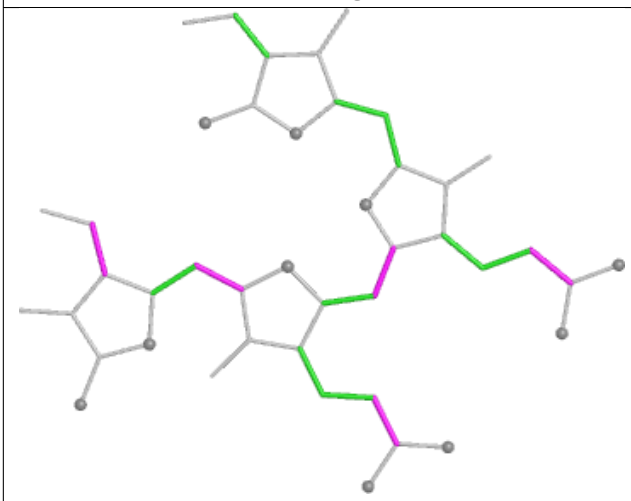
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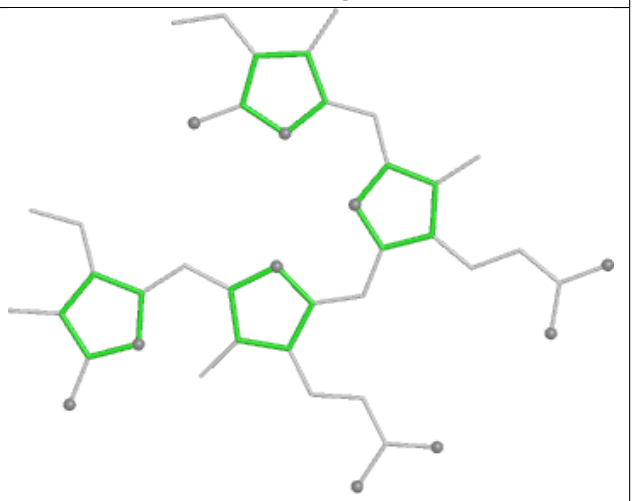
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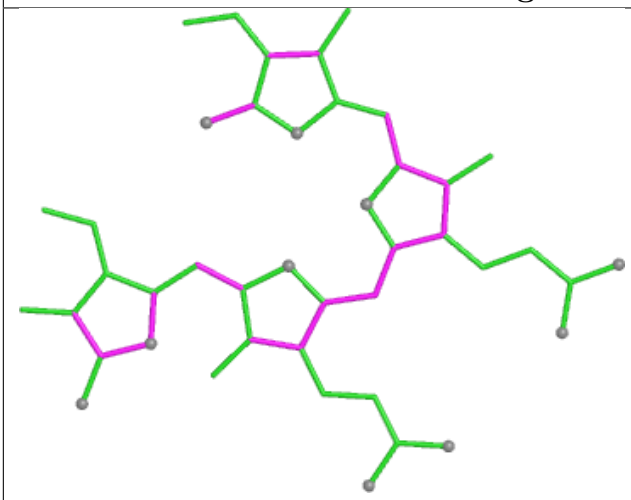


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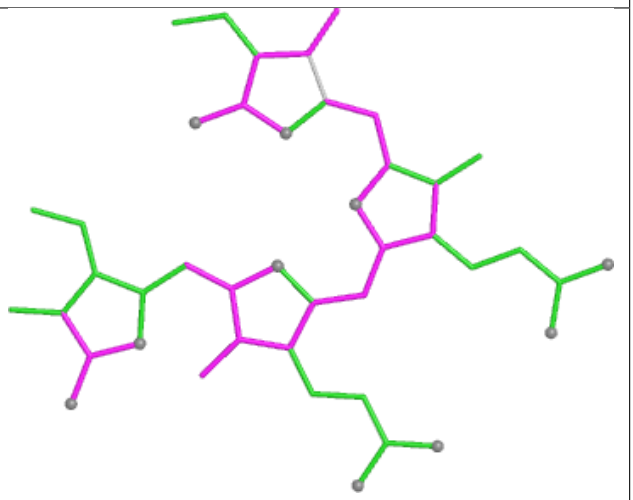


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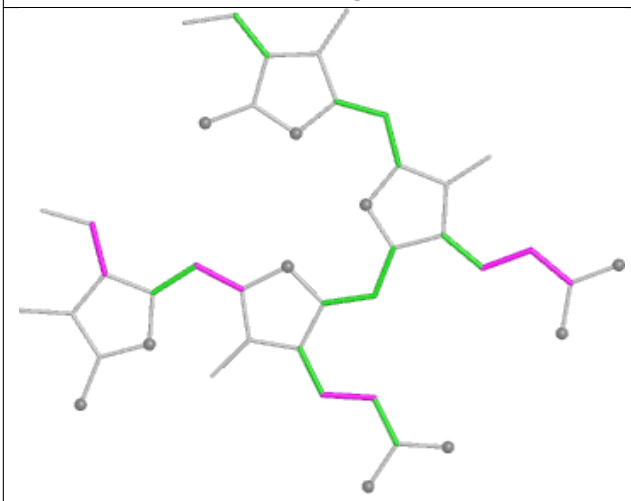
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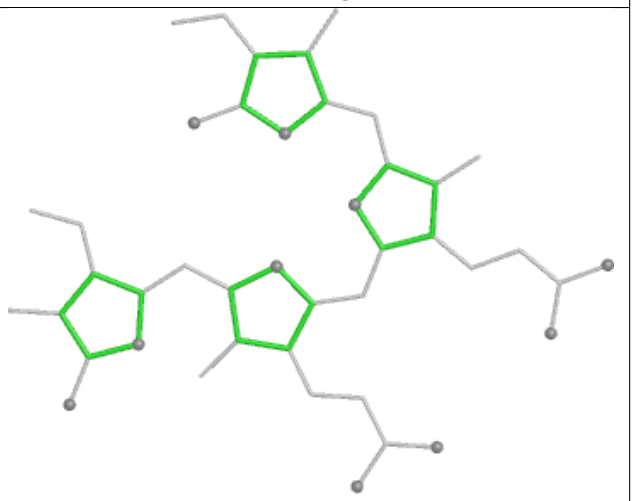
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Bond angles

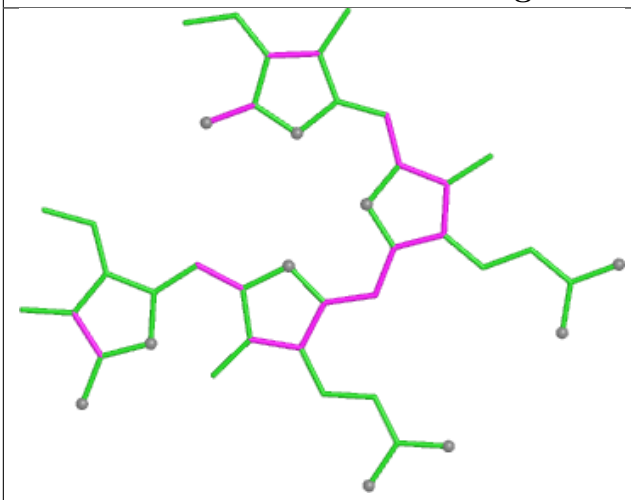


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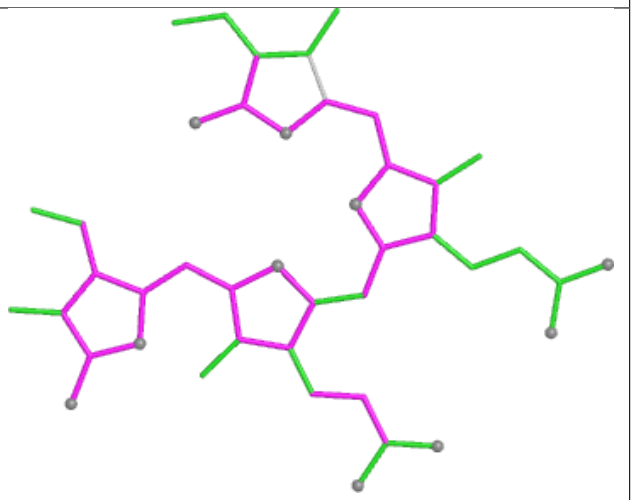


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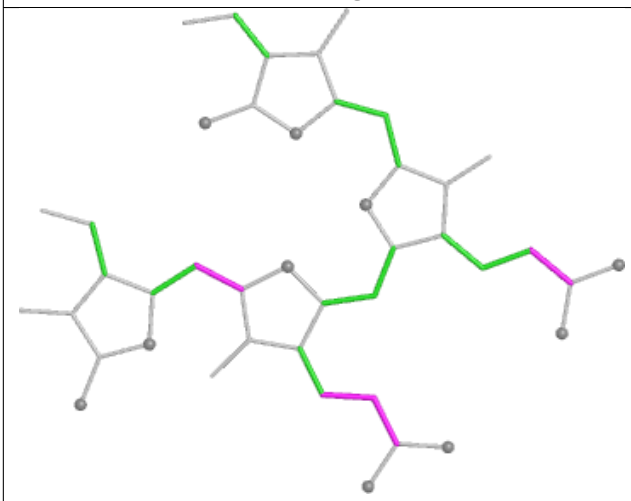
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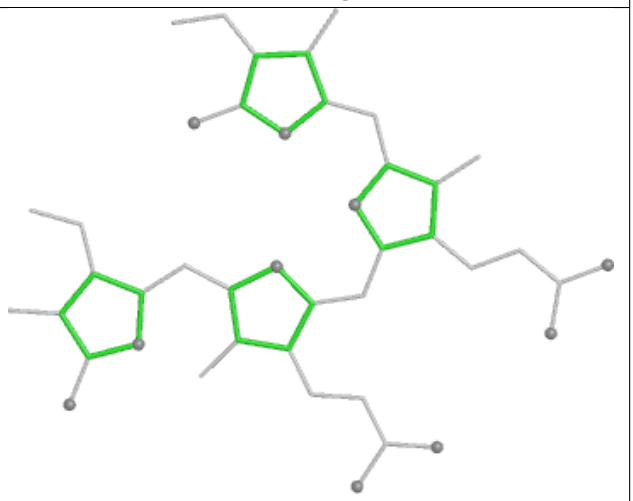
Bond lengths



Bond angles

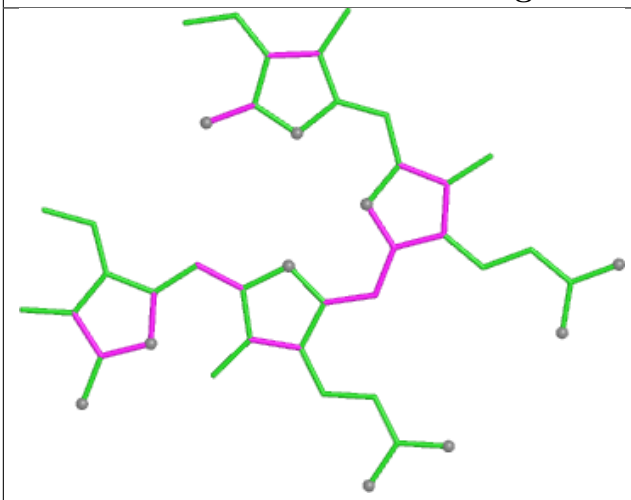


Torsions

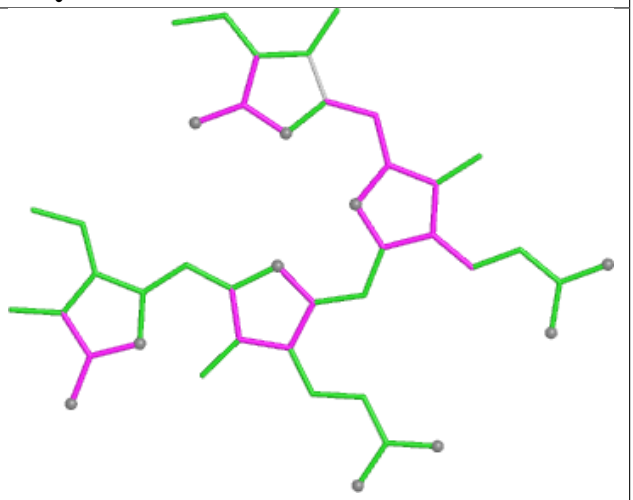


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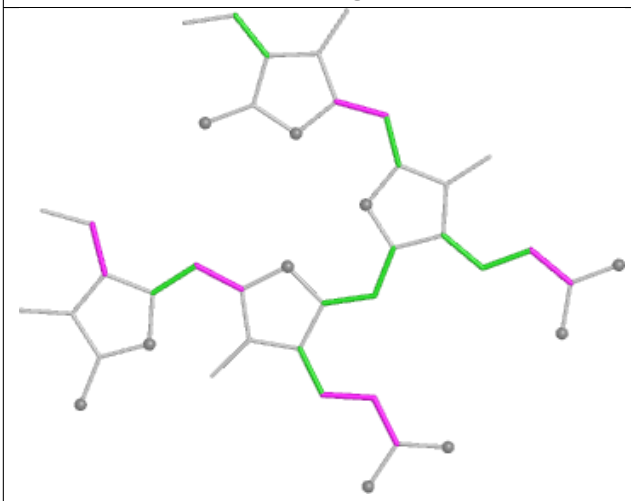
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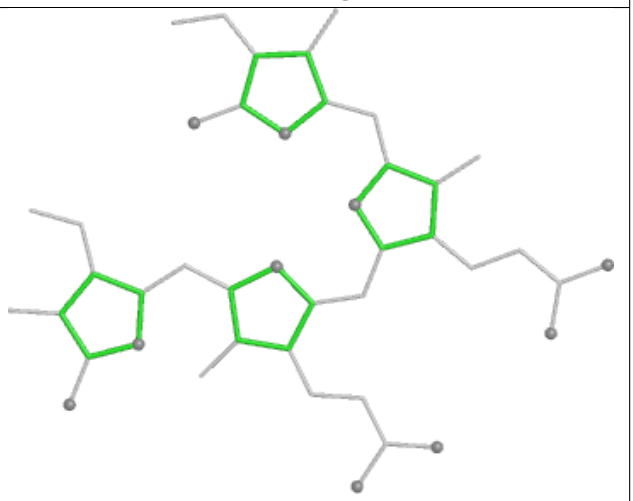
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Bond angles

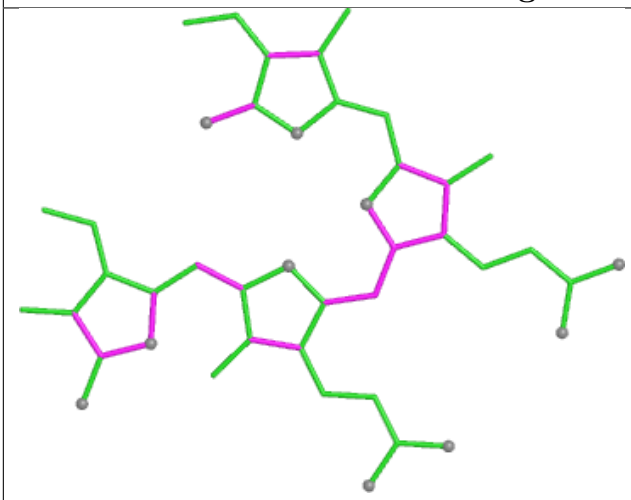


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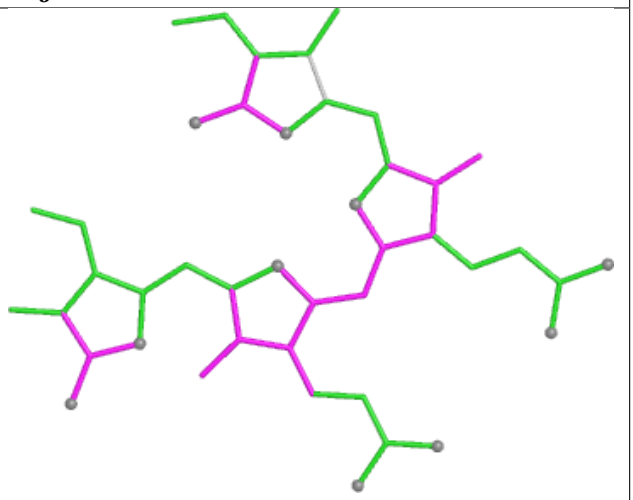


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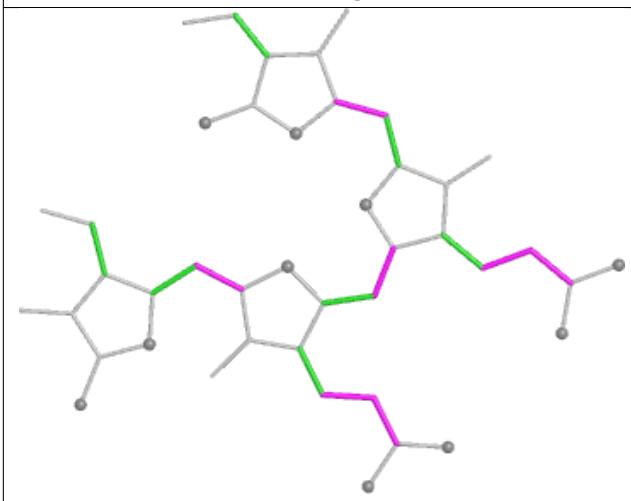
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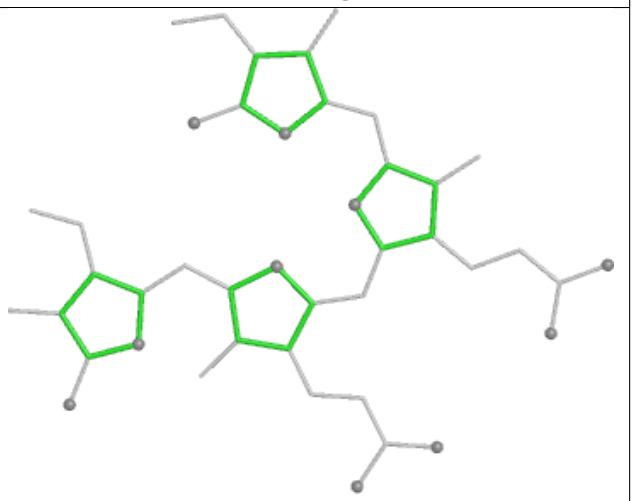
Bond lengths



Bond angles

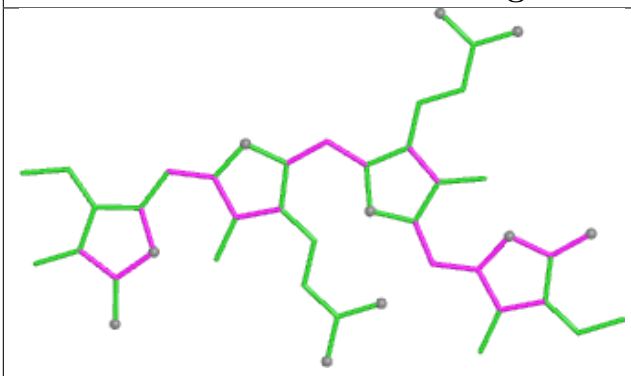


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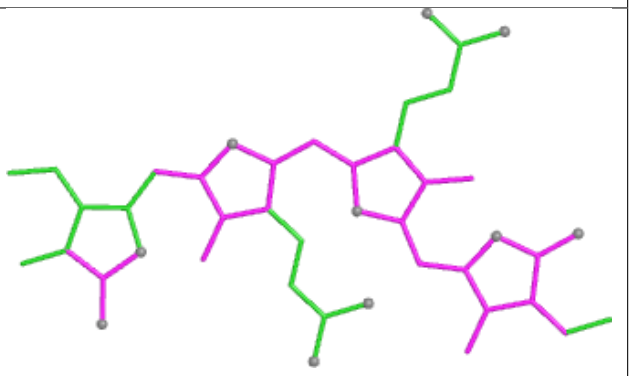


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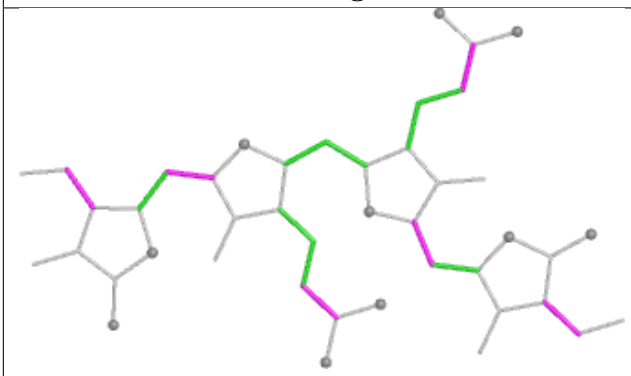
Ligand CYC KG 202



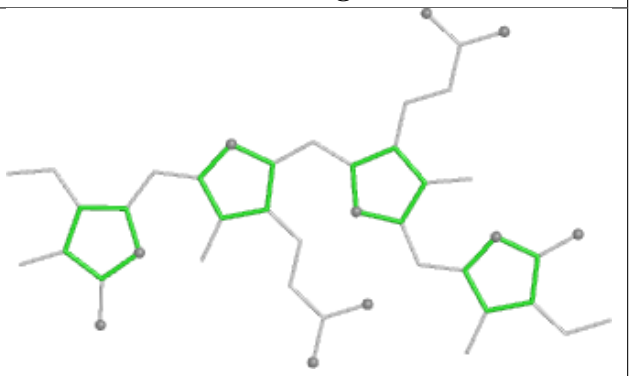
Bond lengths



Bond angles

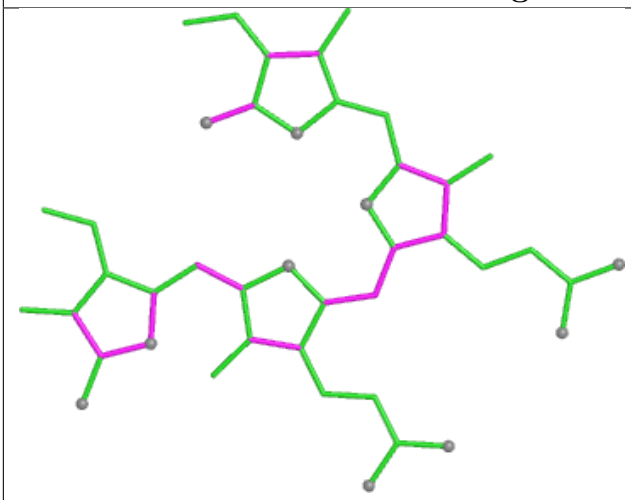


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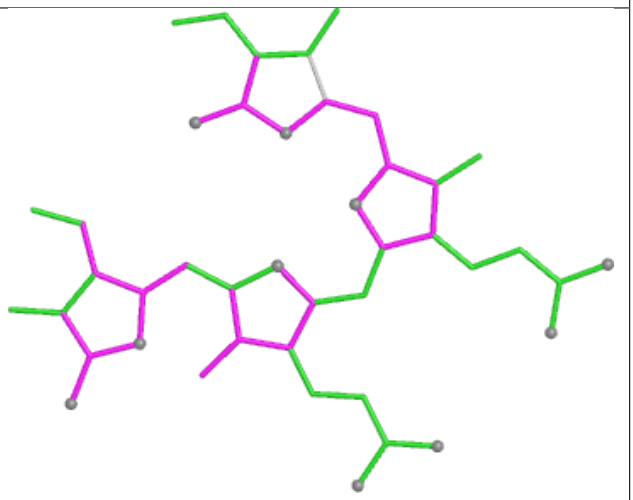


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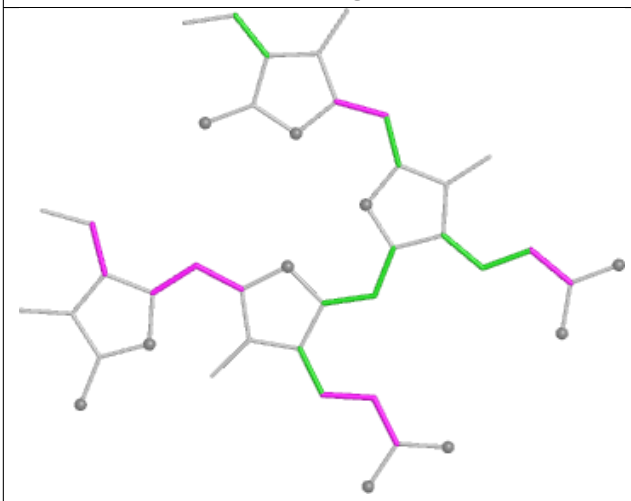
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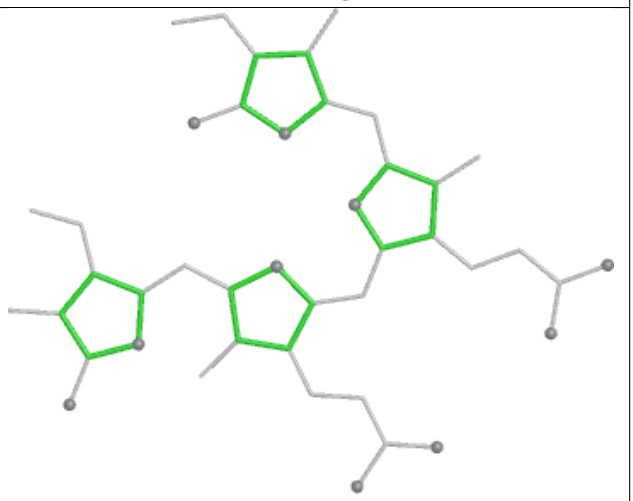
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Bond angles

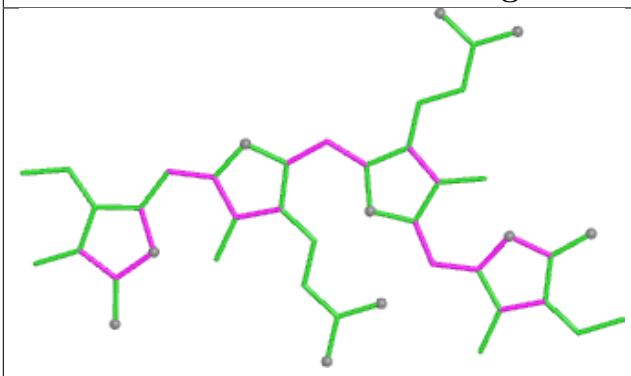


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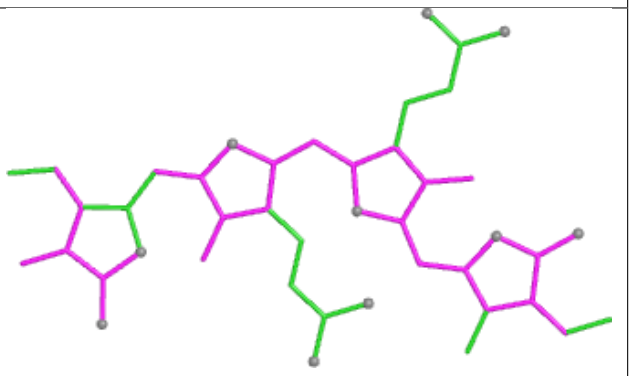


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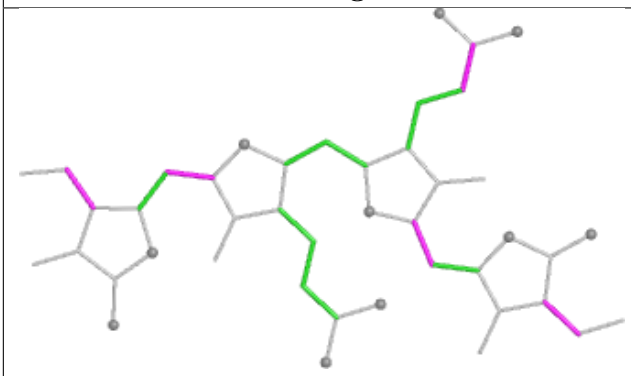
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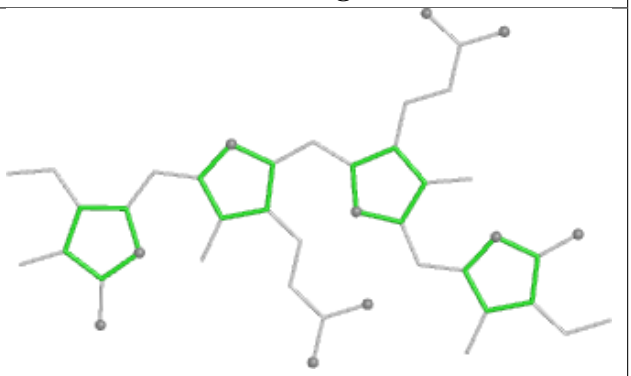
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Bond angles

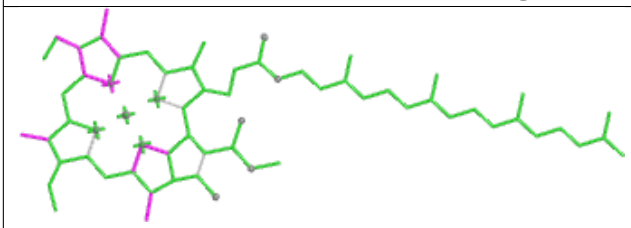


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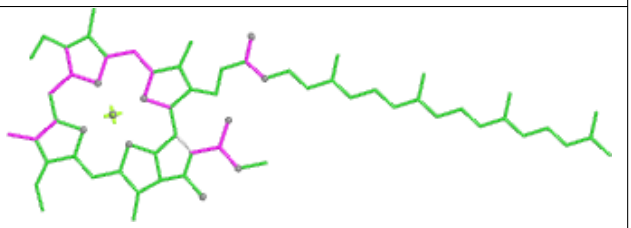


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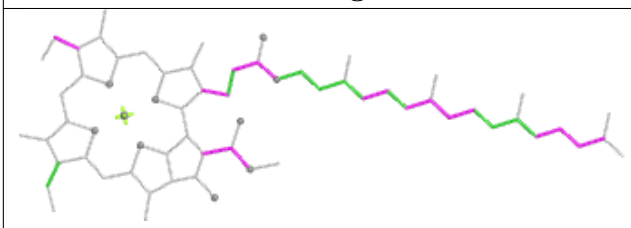
Ligand CLA A2 834



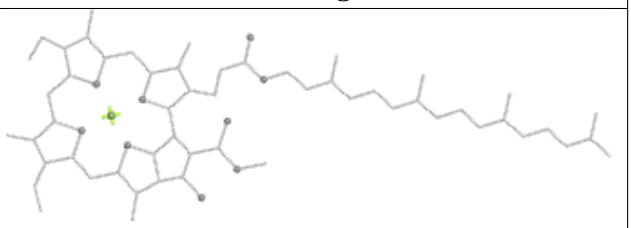
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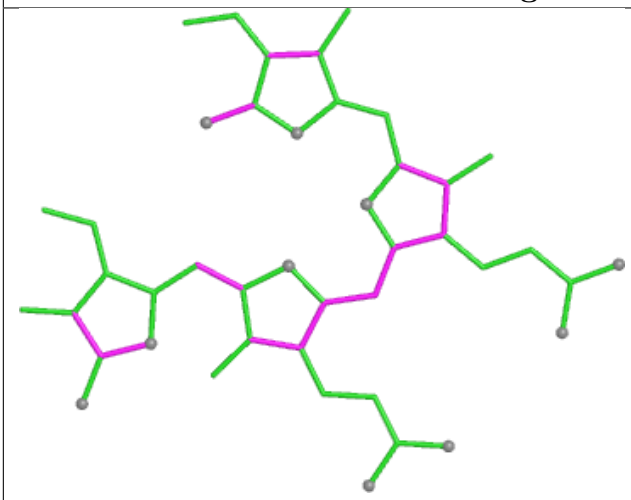


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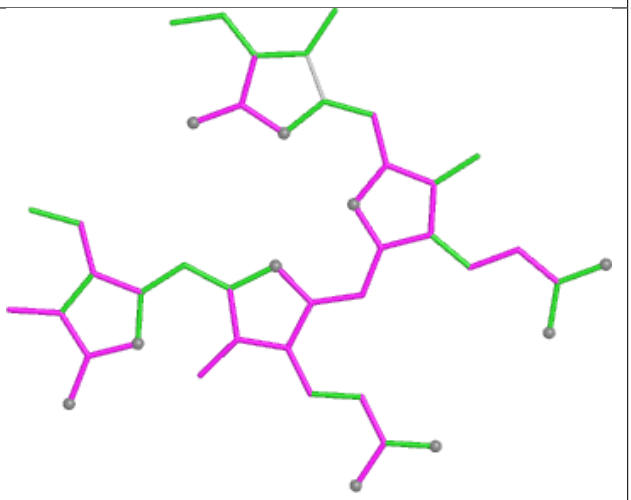


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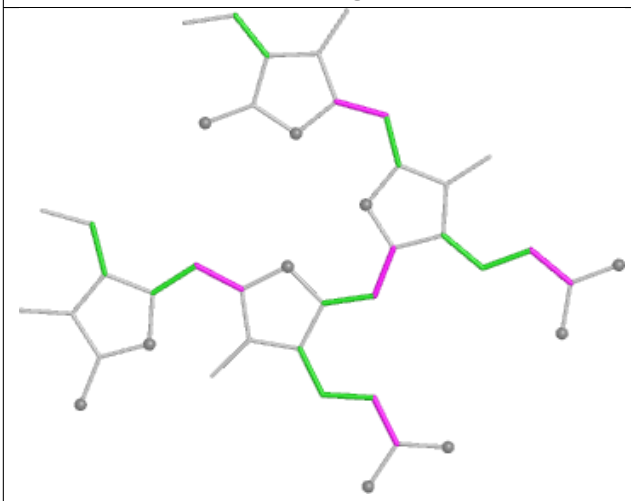
Ligand PEB cJ 202



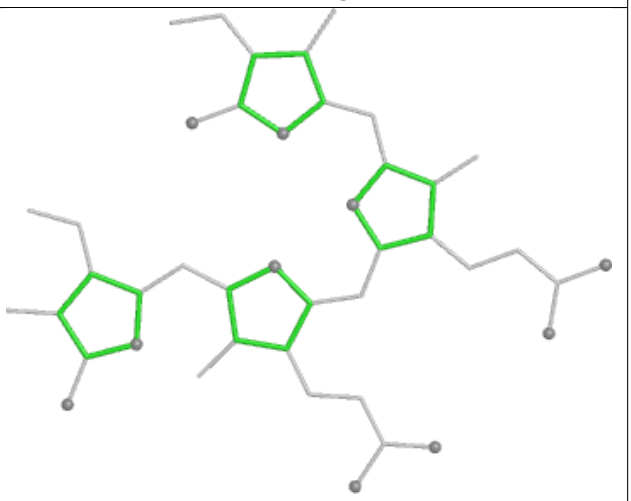
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Bond angles

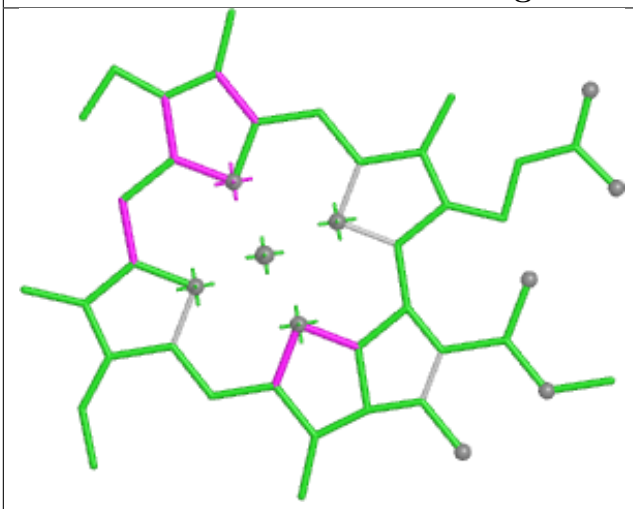


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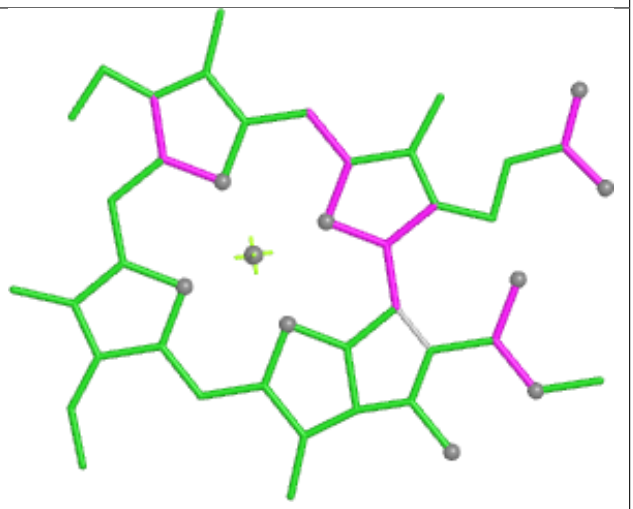


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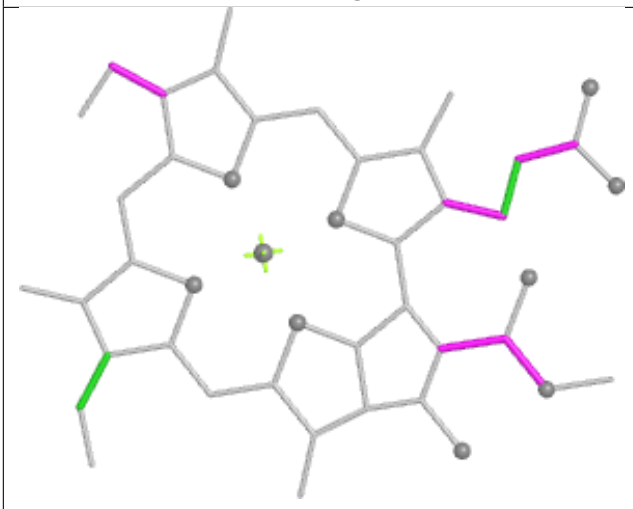
Ligand CLA 7N 601



Bond lengths



Bond angles

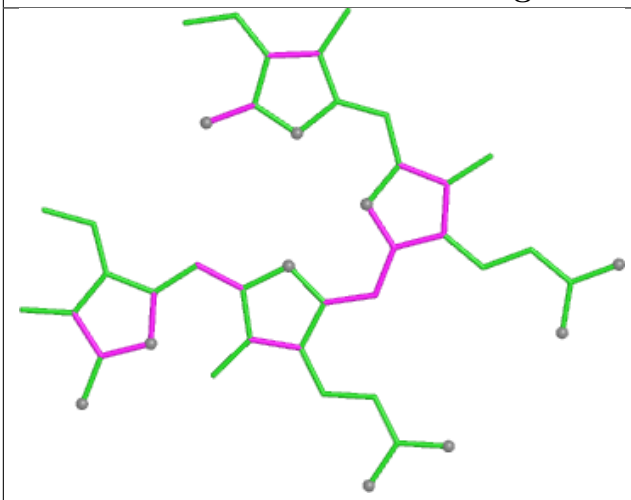


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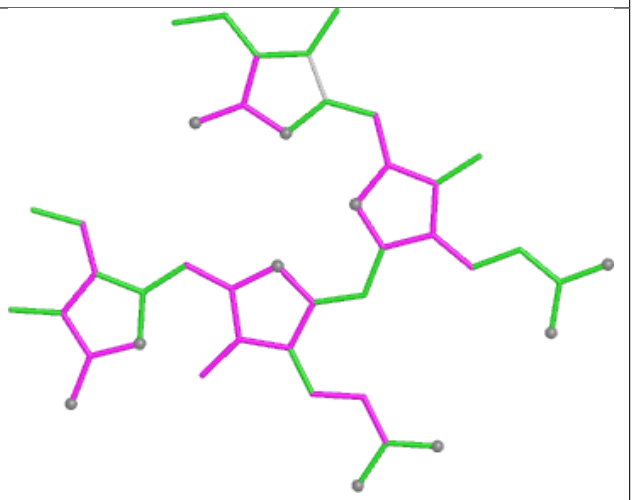


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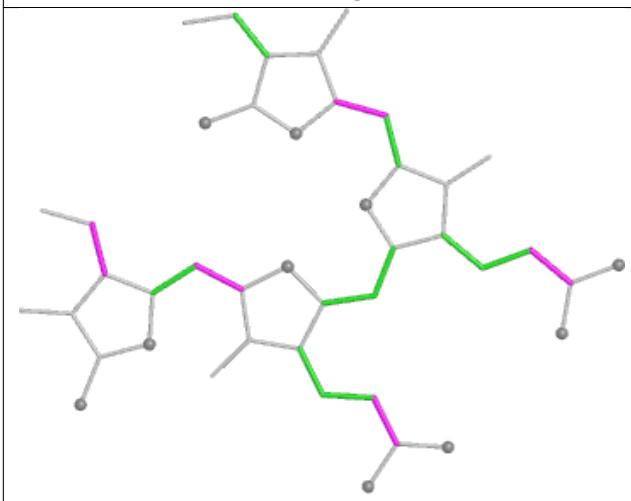
Ligand PEB ZB 201



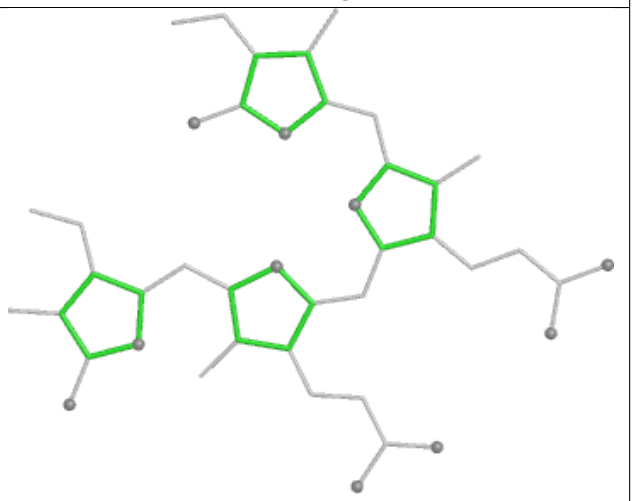
Bond lengths



Bond angles

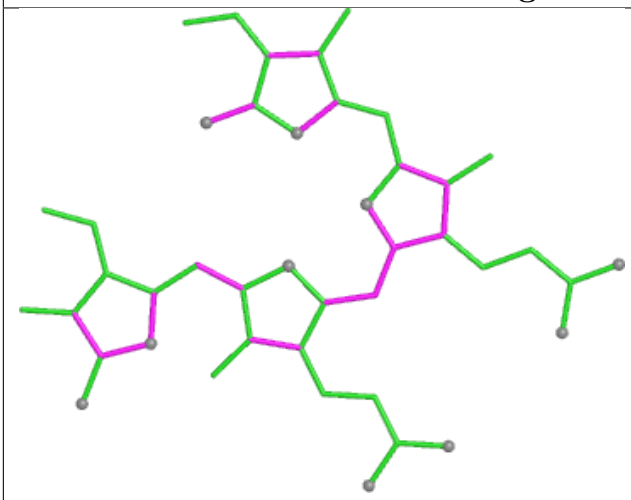


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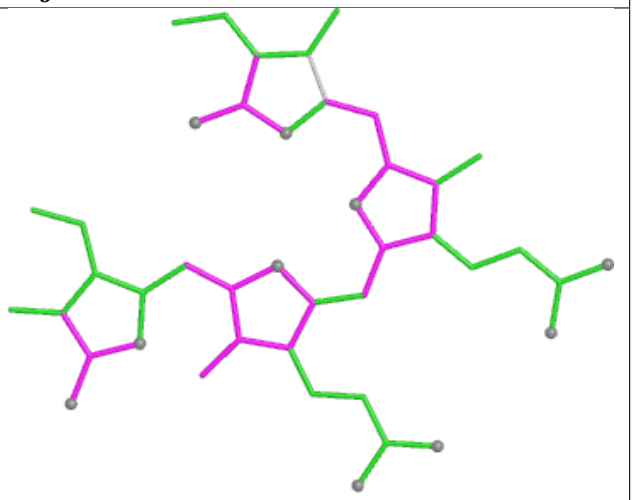


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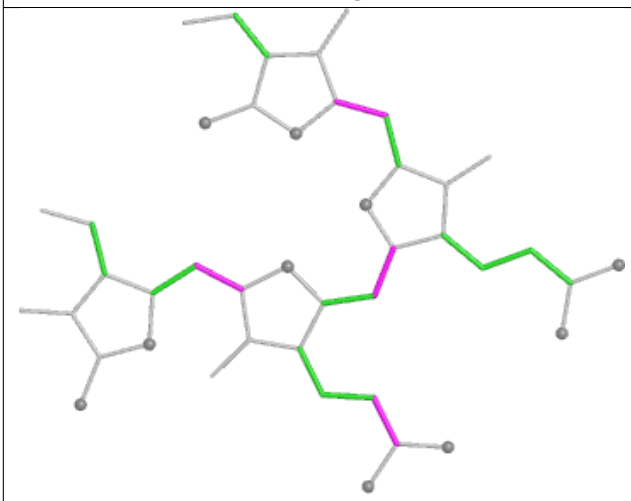
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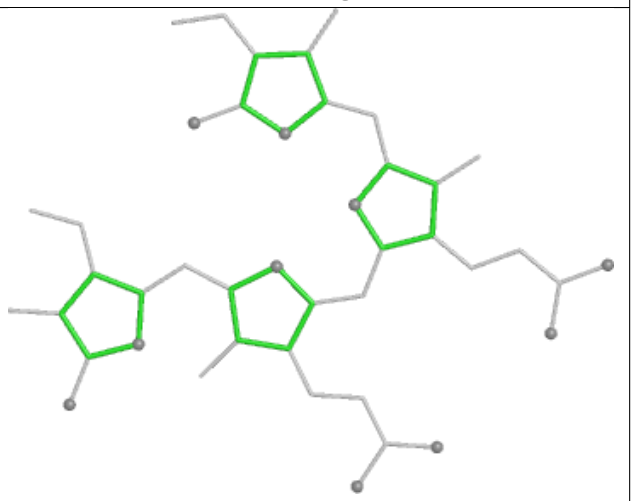
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Bond angles

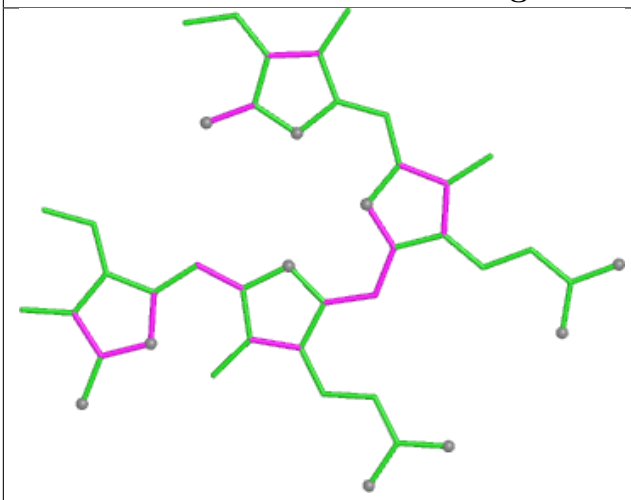


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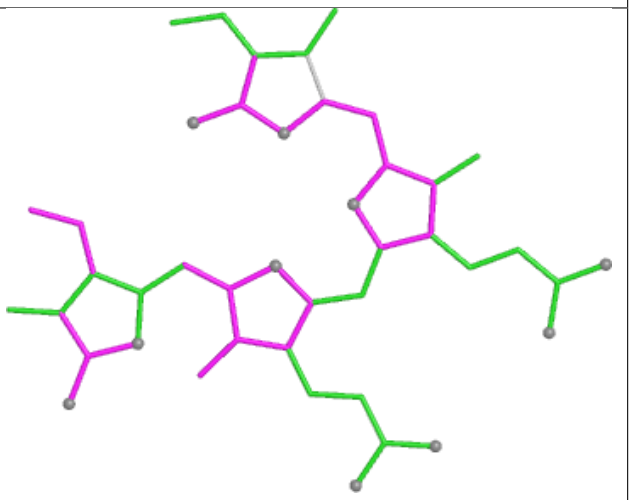


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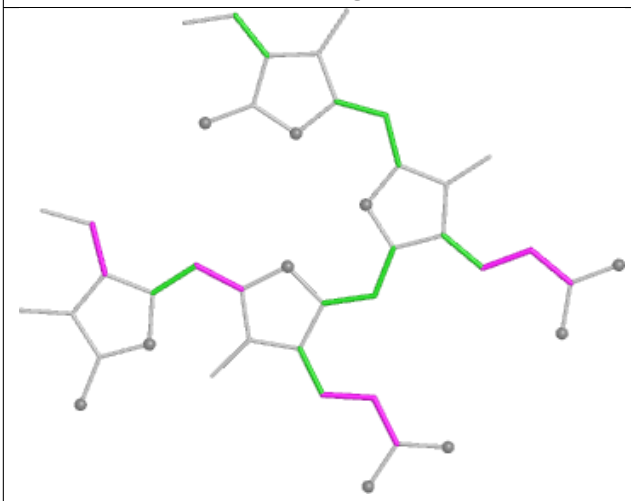
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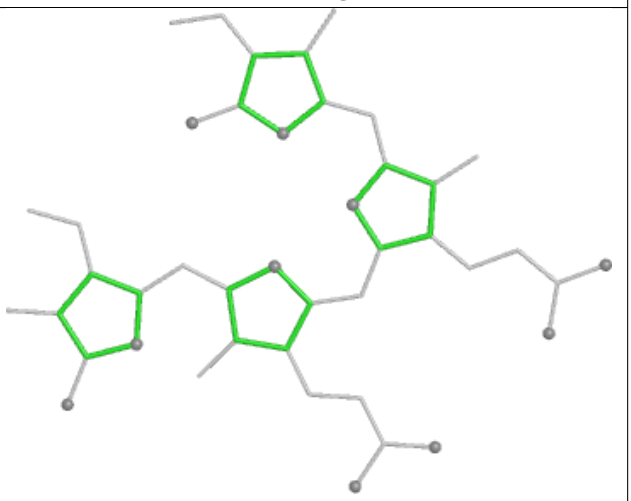
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Bond angles

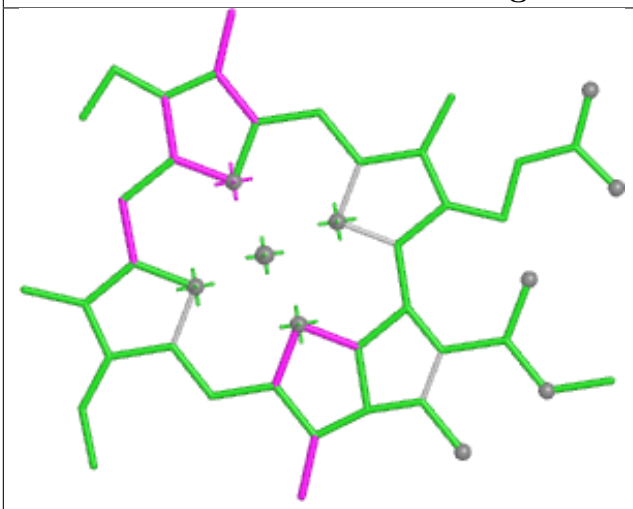


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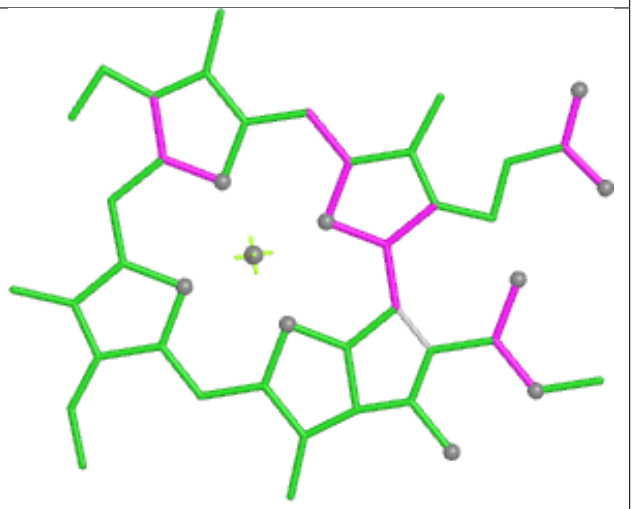


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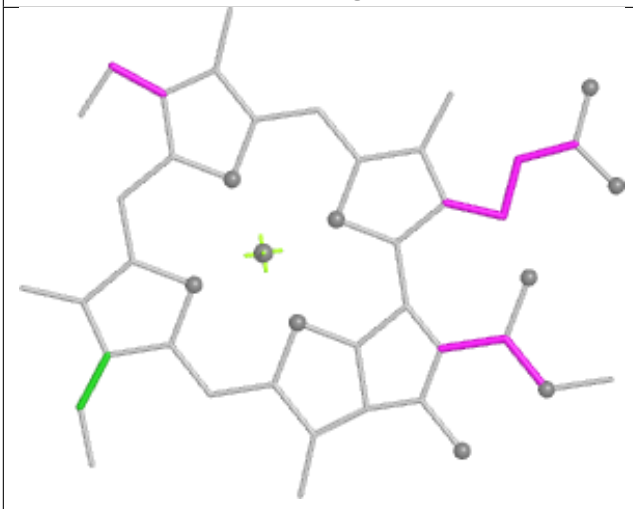
Ligand CLA RN 204



Bond lengths



Bond angles

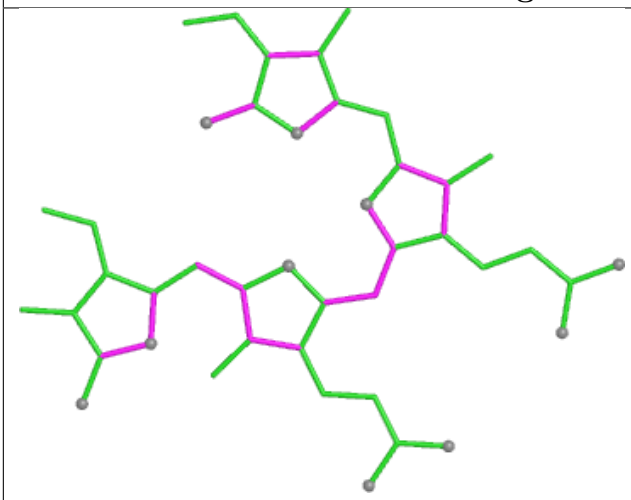


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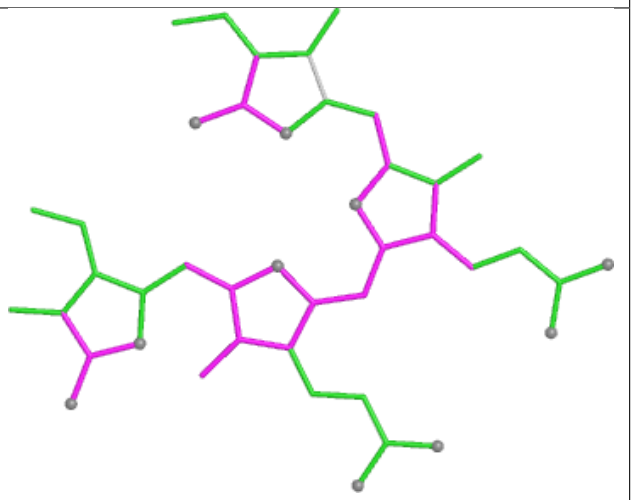


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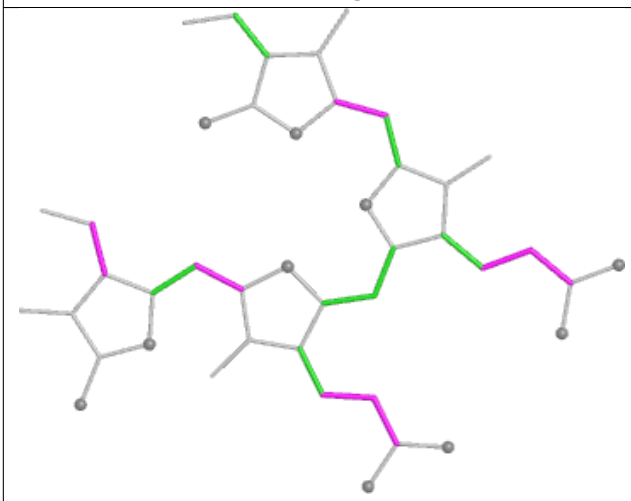
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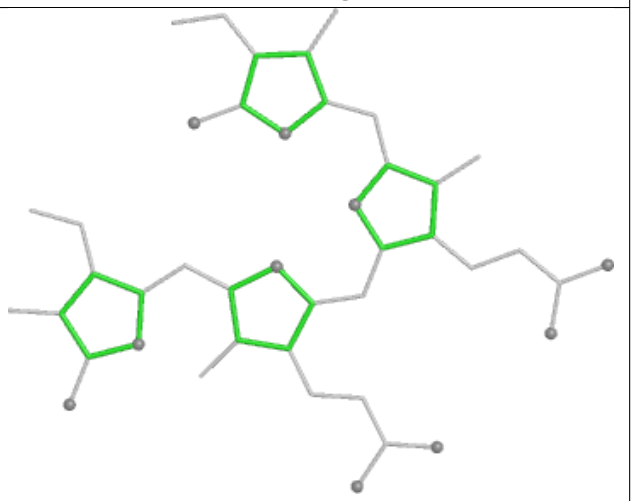
Bond lengths



Bond angles

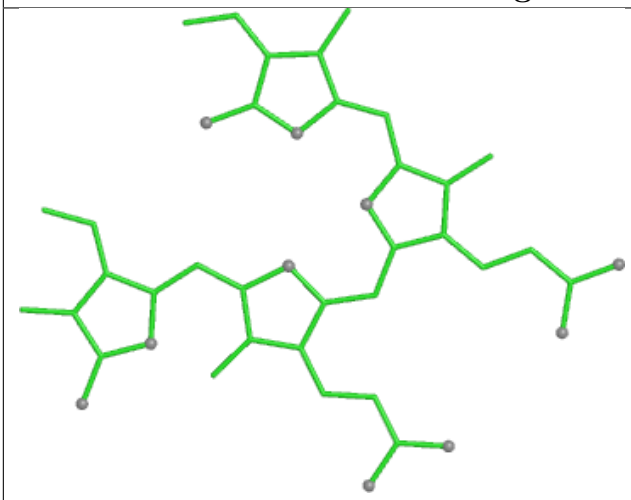


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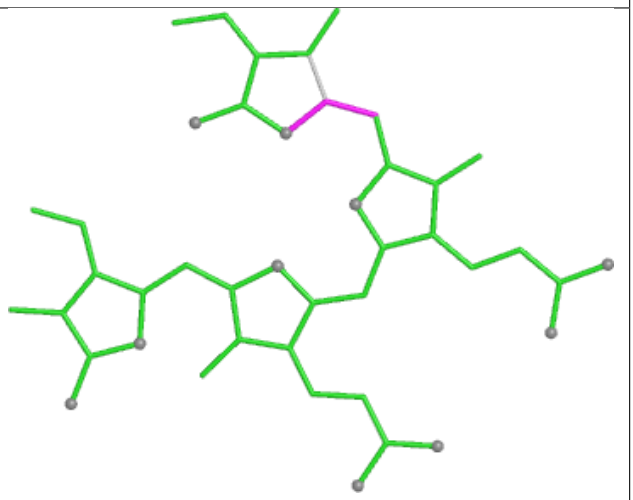


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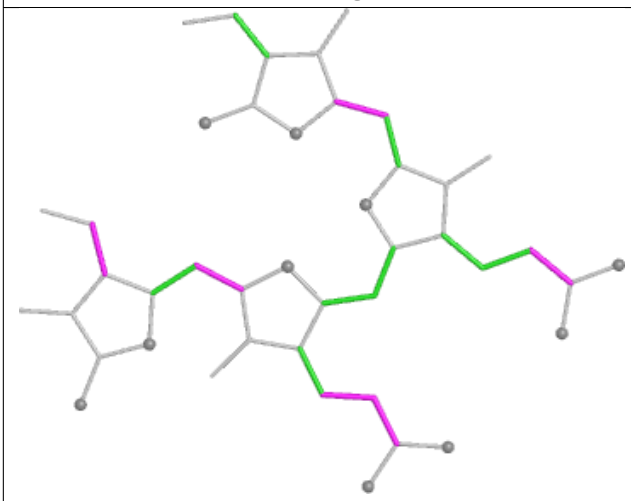
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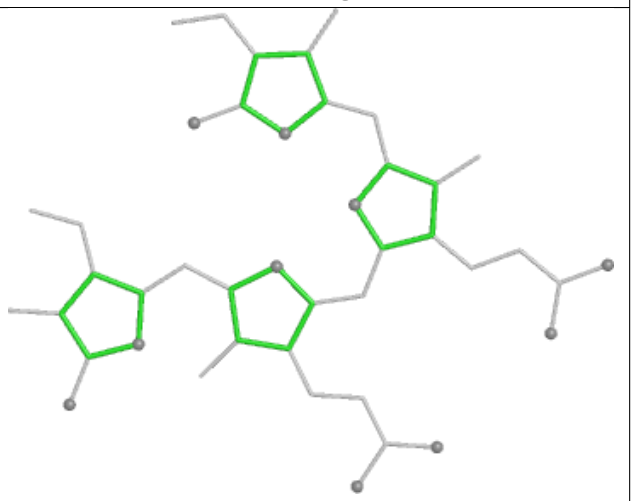
Bond lengths



Bond angles

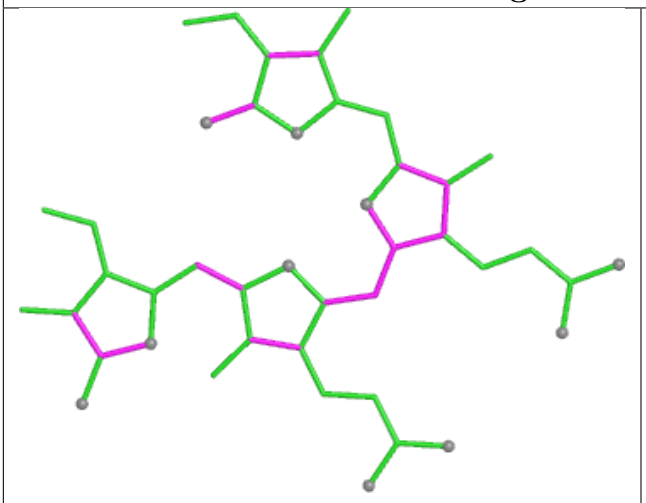


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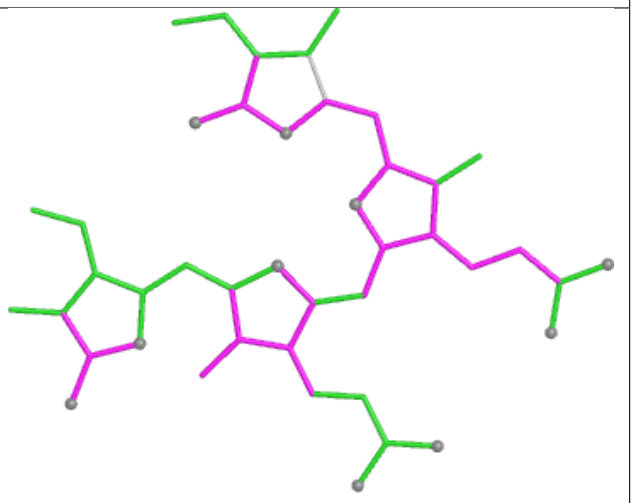


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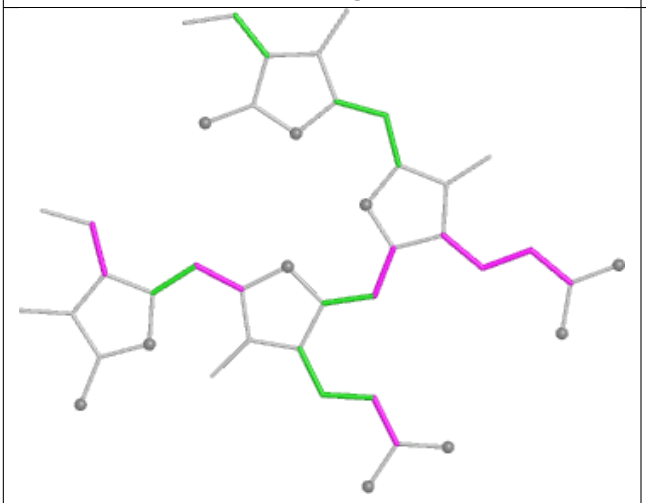
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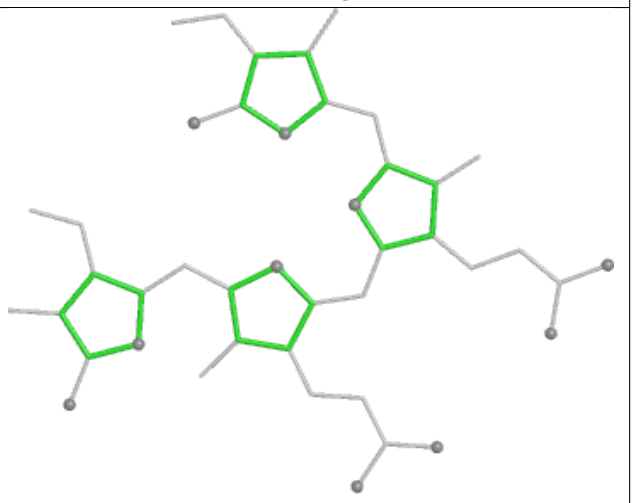
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Bond angles

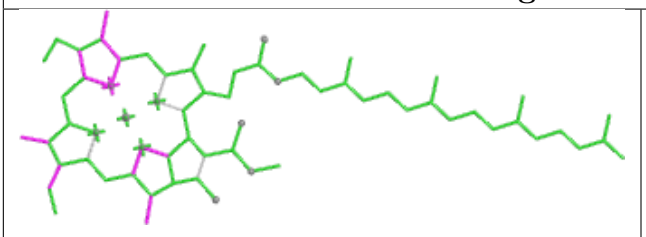


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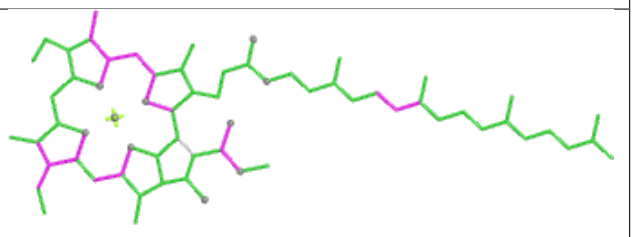


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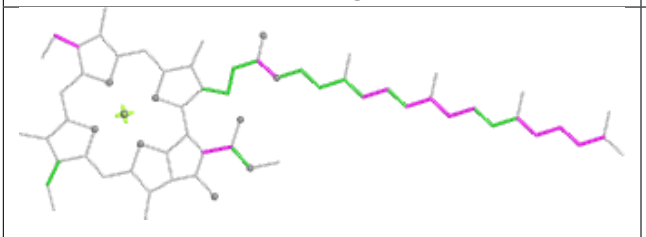
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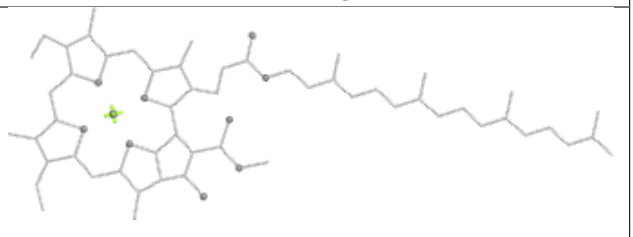
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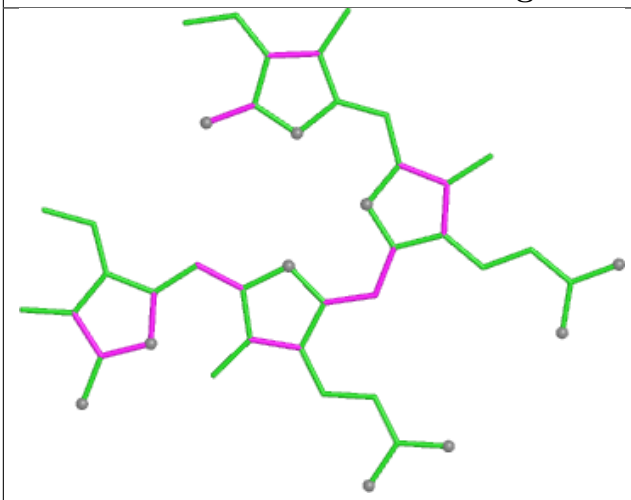


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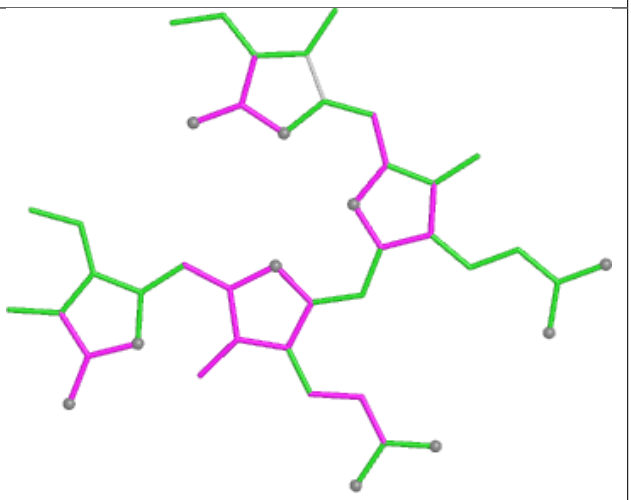


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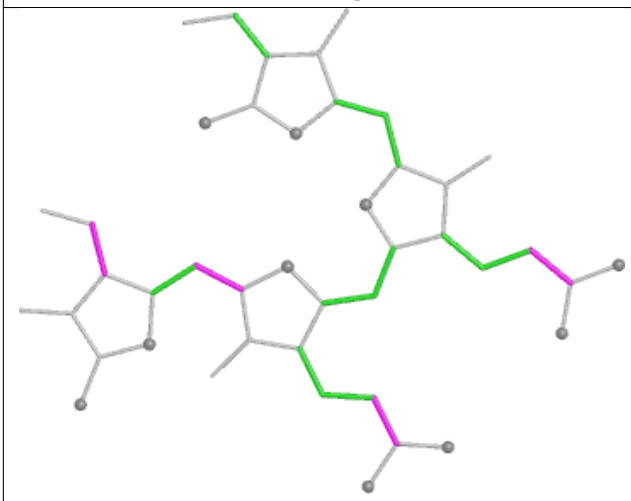
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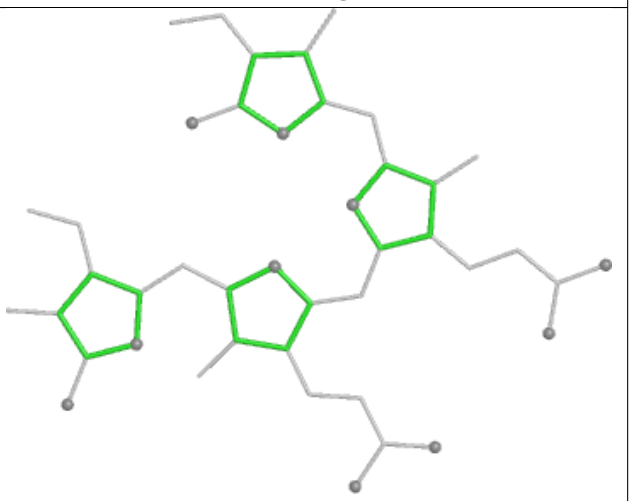
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Bond angles

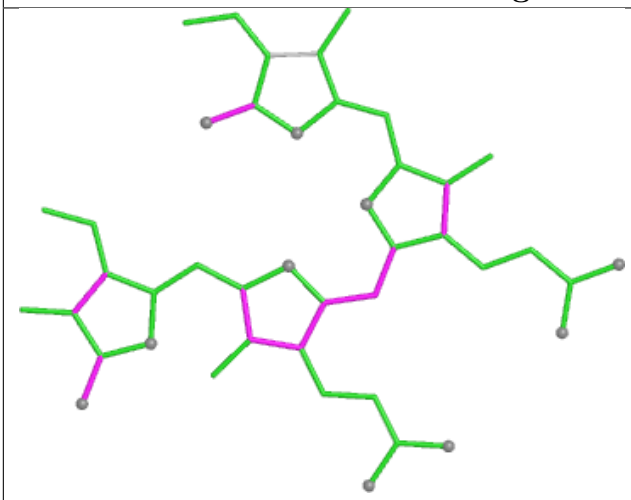


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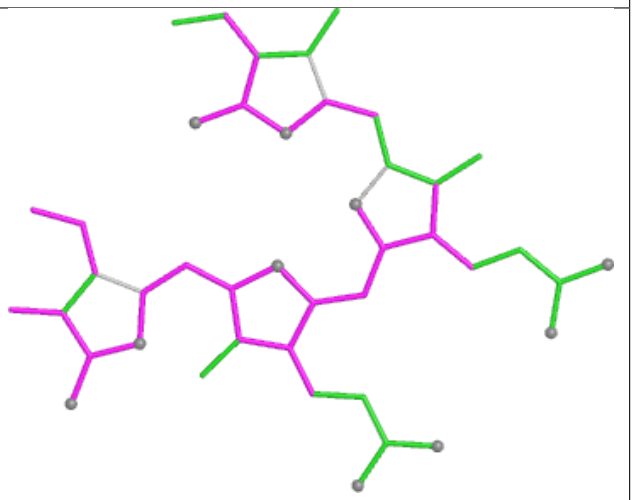


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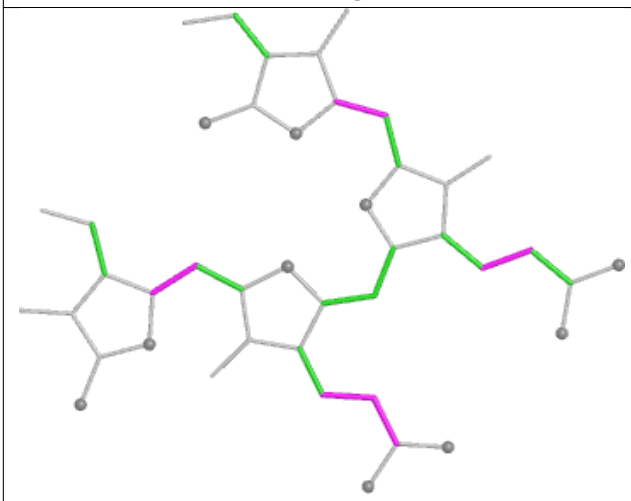
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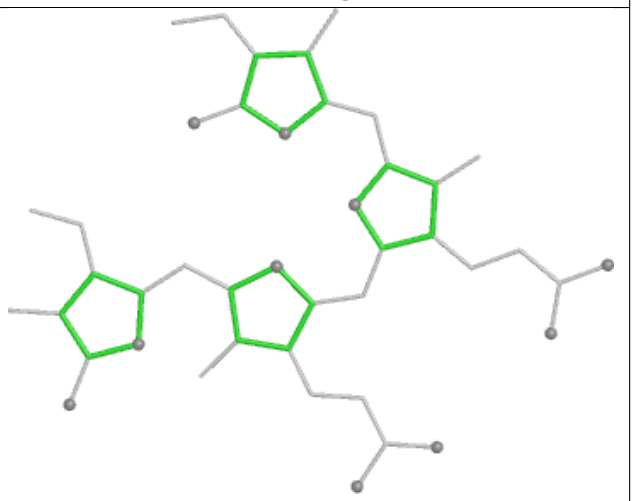
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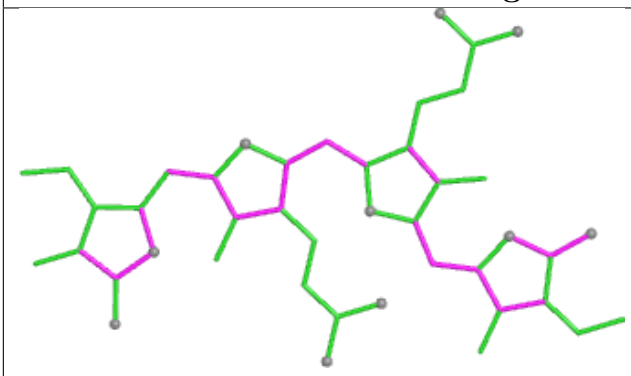


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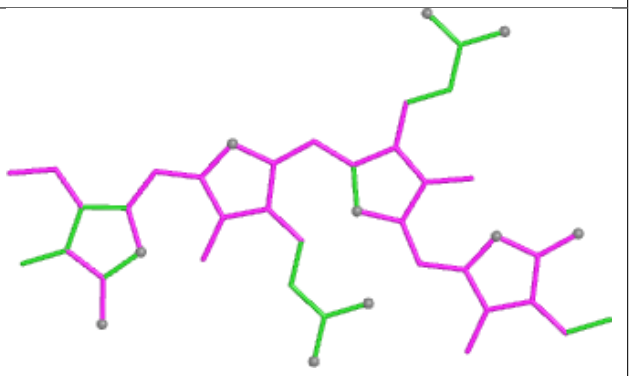


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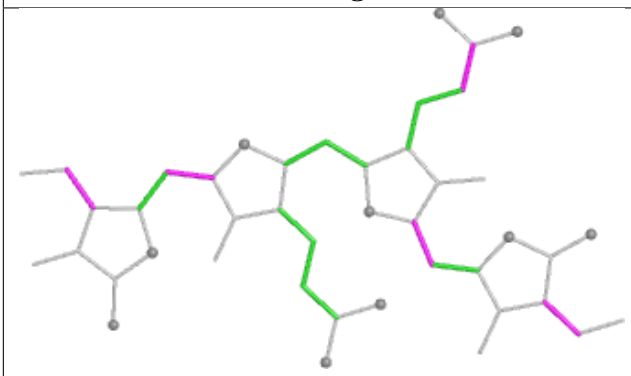
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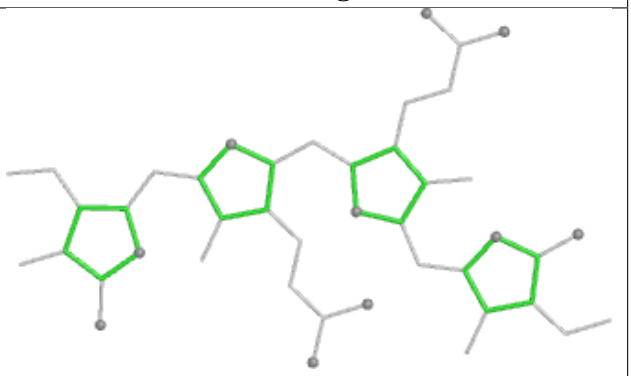
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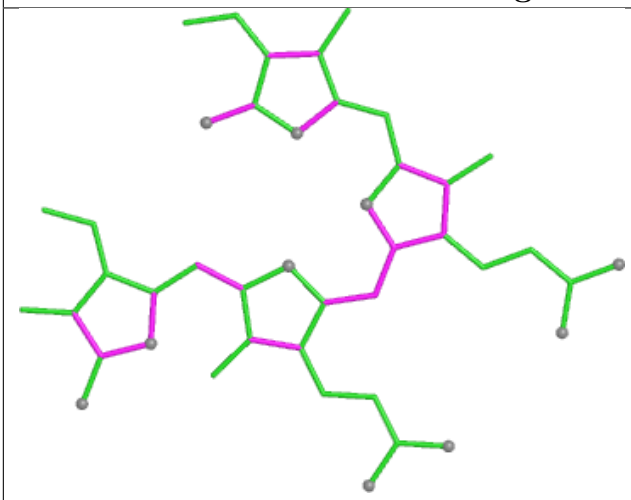


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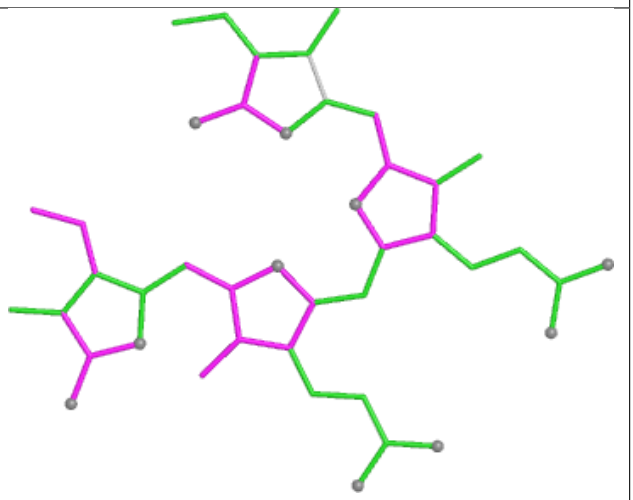


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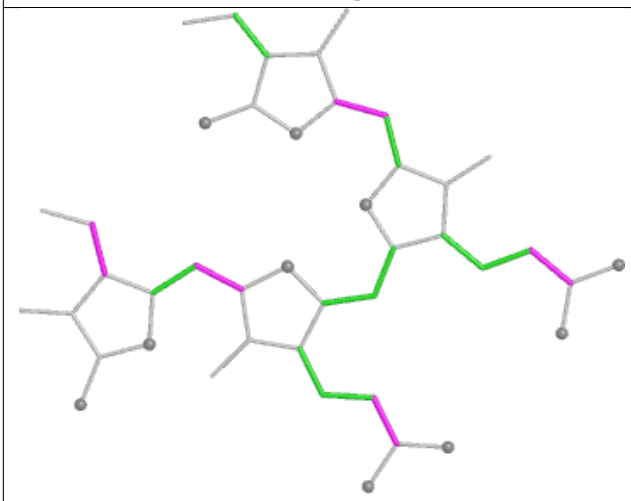
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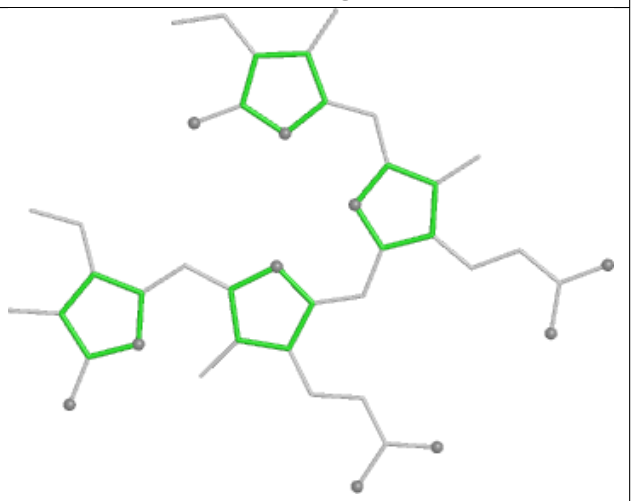
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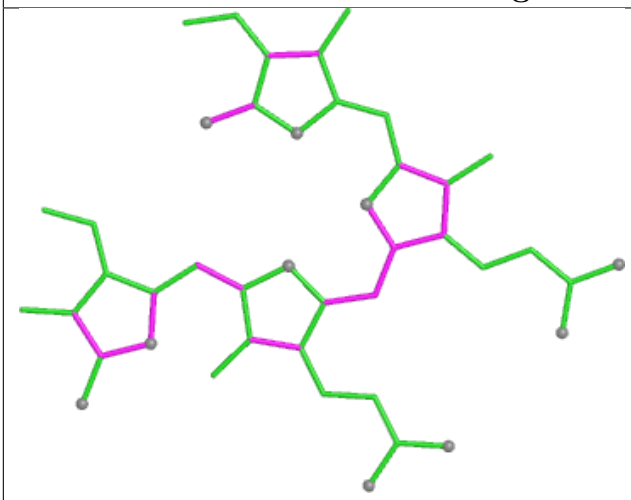


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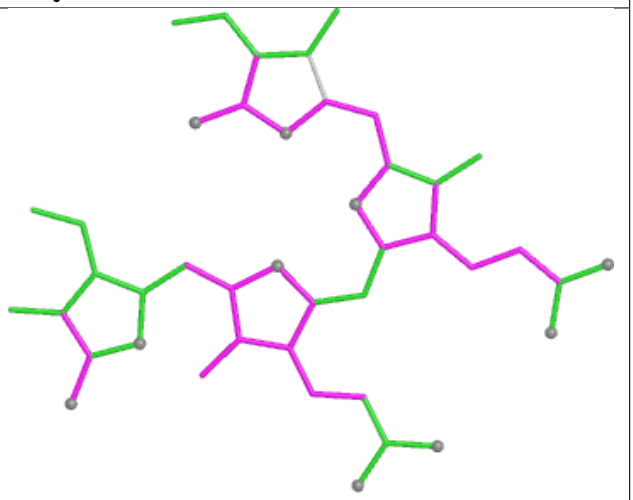


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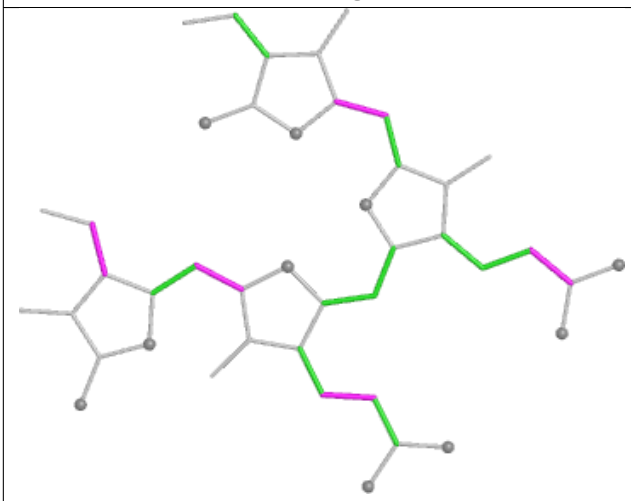
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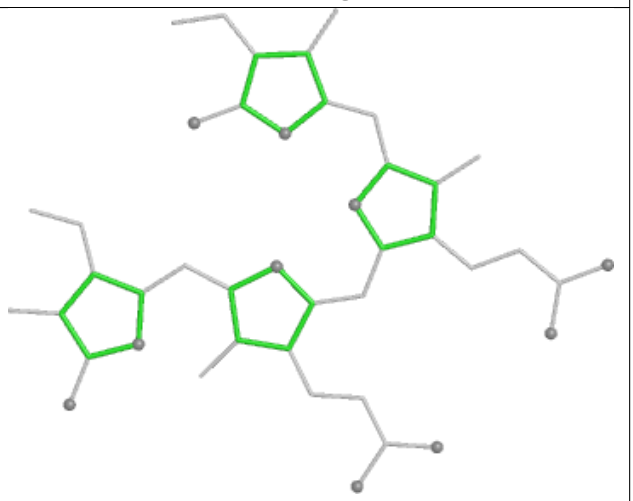
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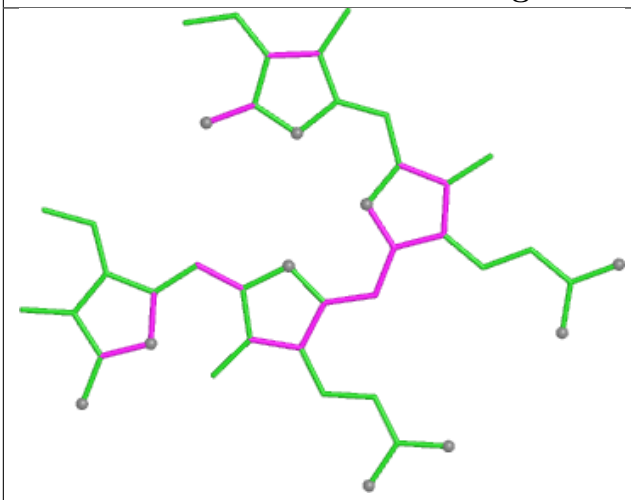


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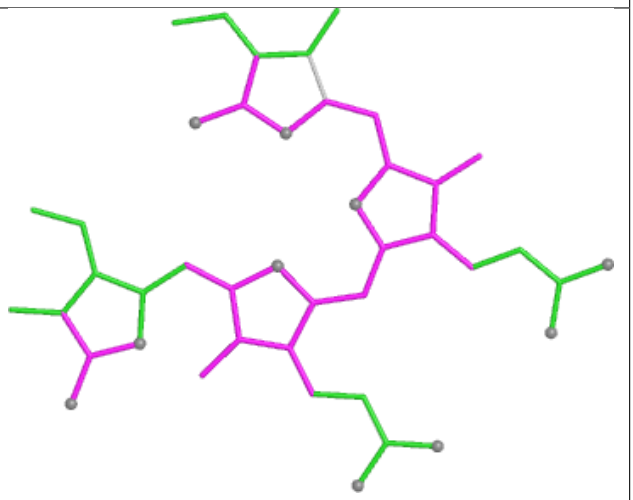


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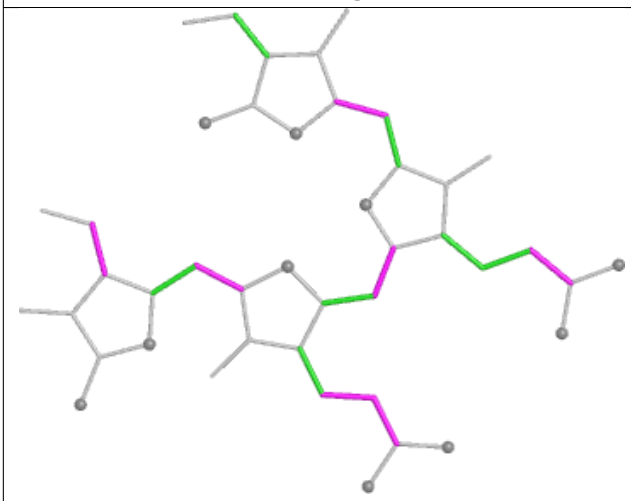
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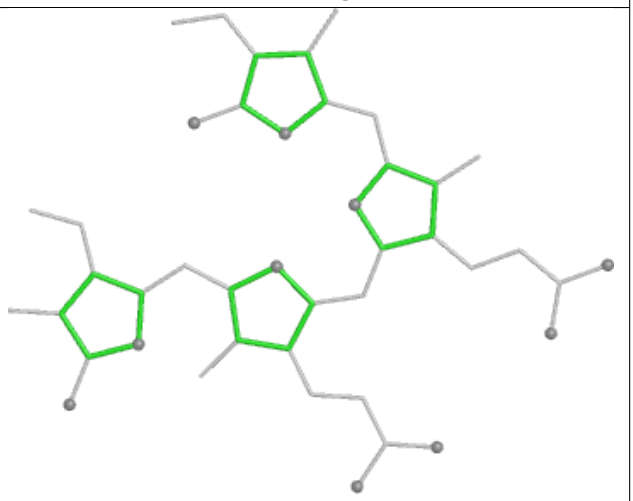
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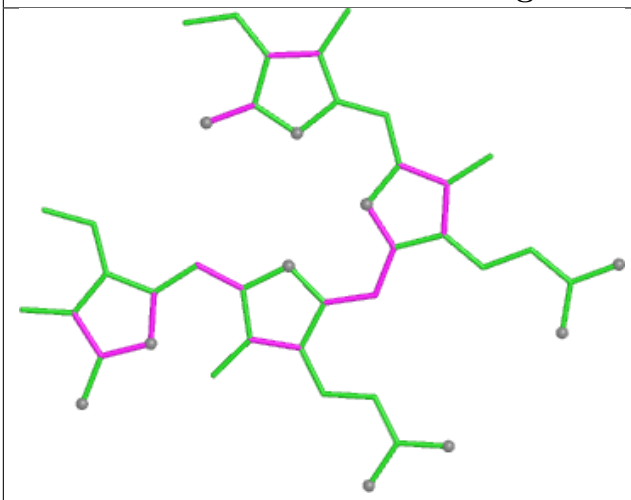


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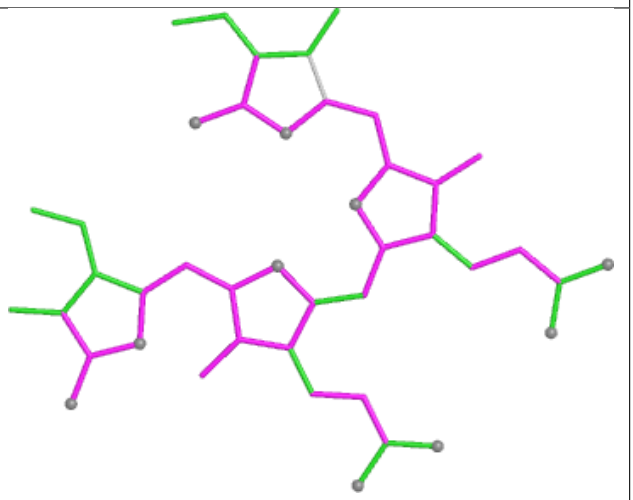


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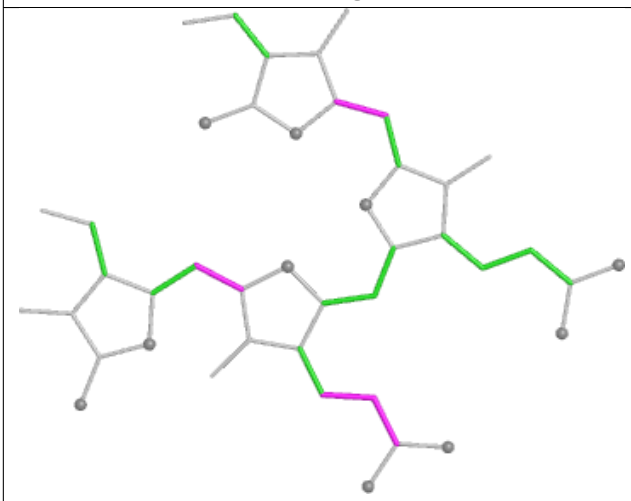
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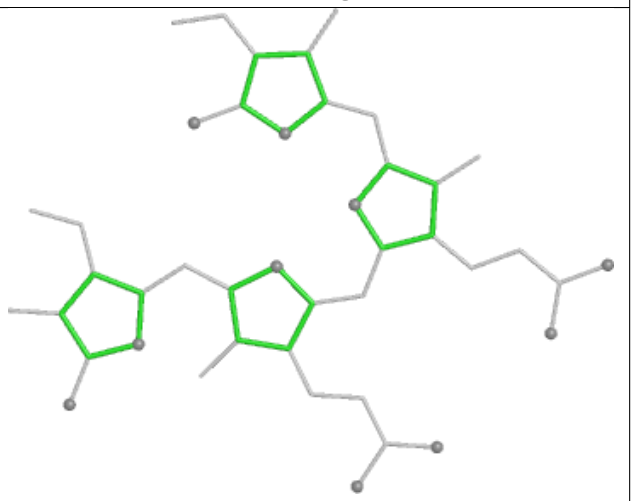
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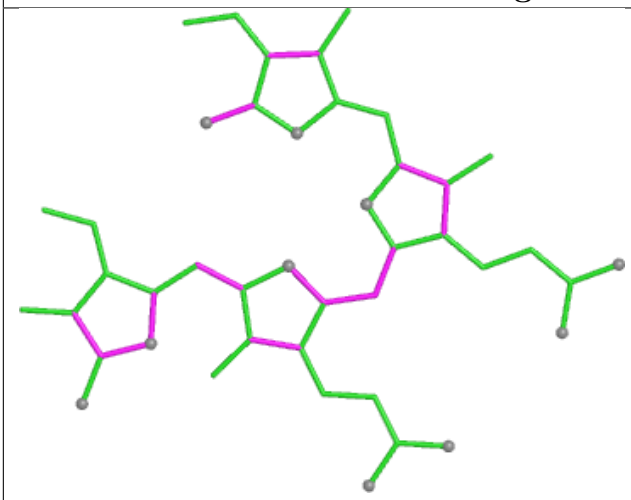


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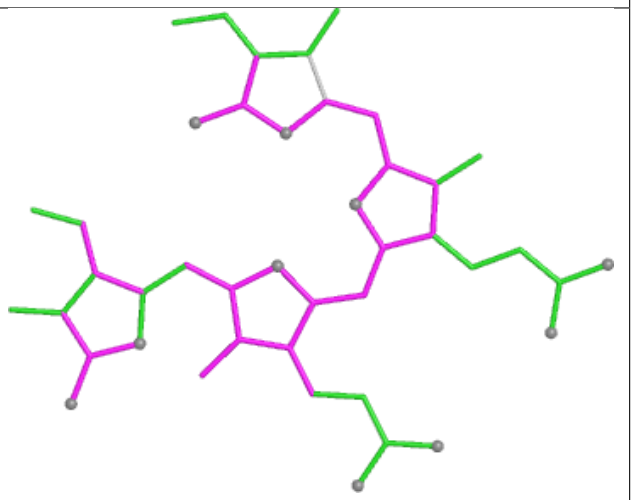


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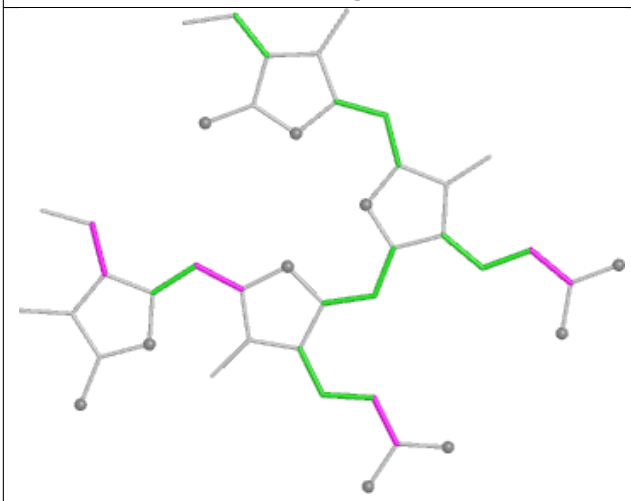
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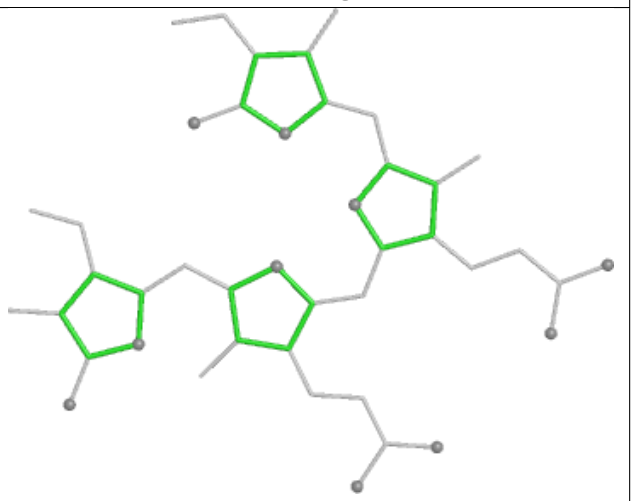
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Bond angles

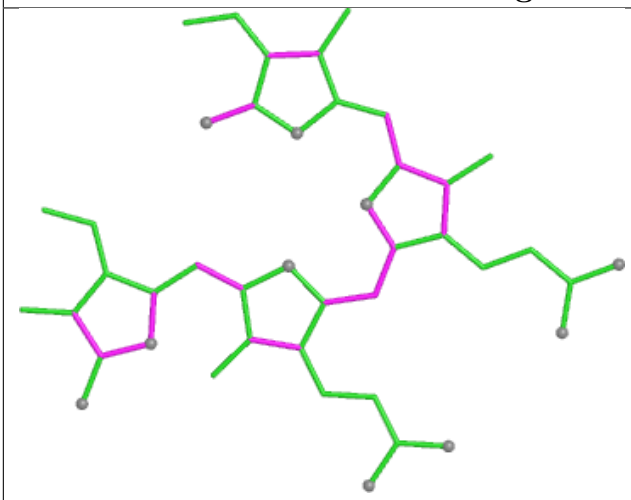


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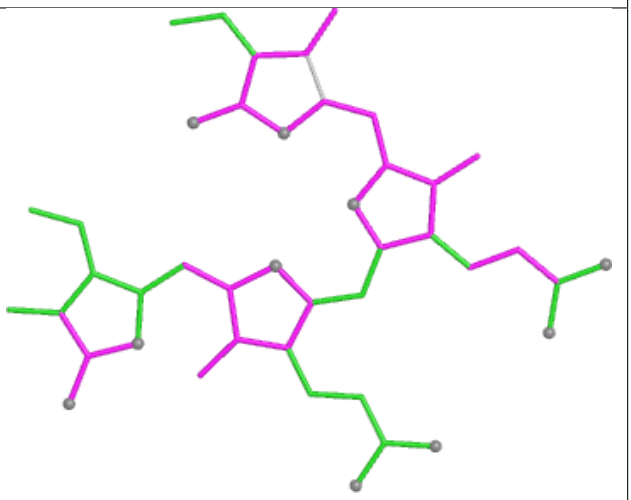


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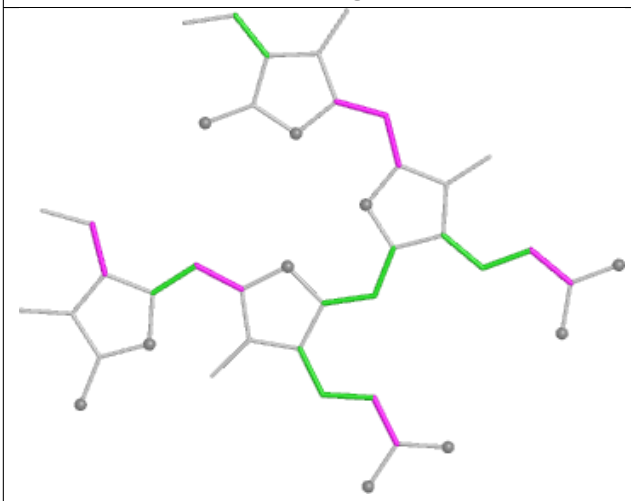
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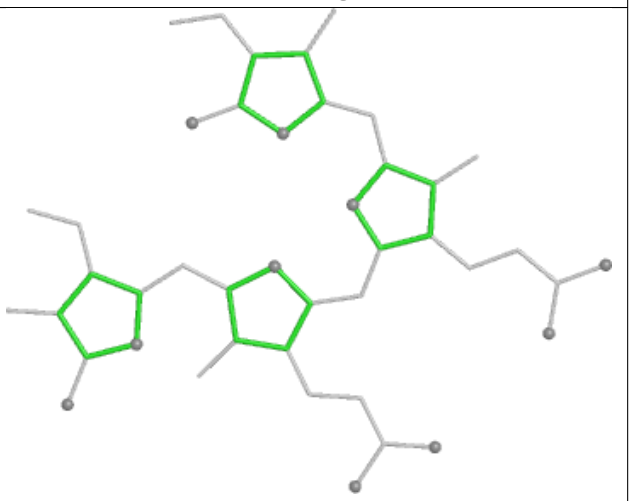
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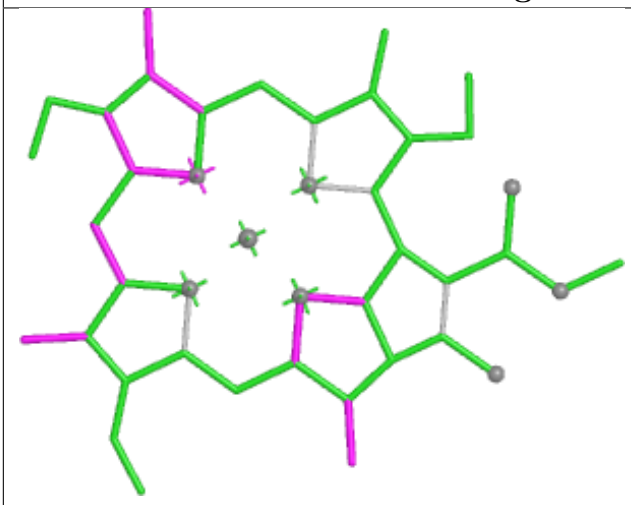


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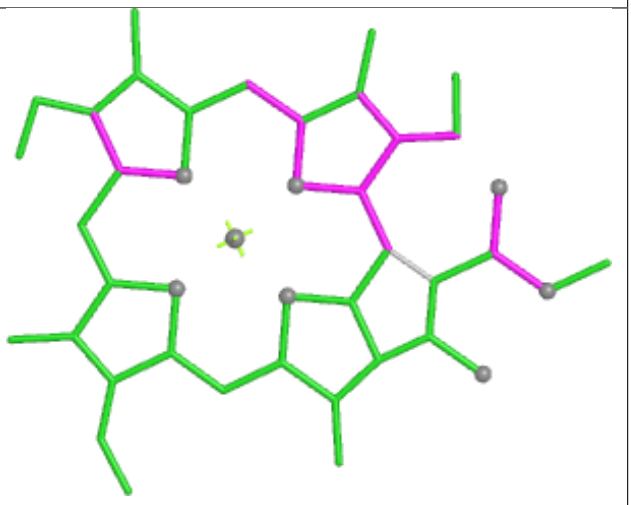


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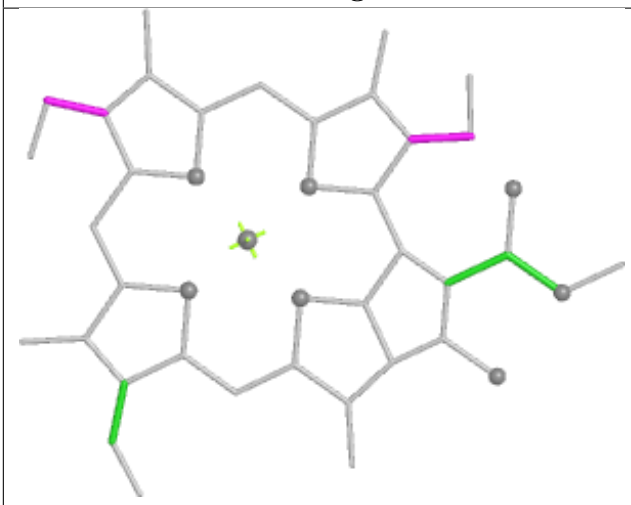
Ligand CLA 1N 604



Bond lengths



Bond angles

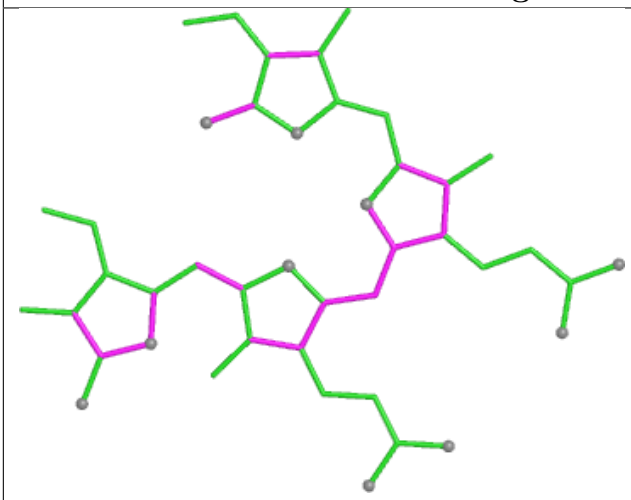


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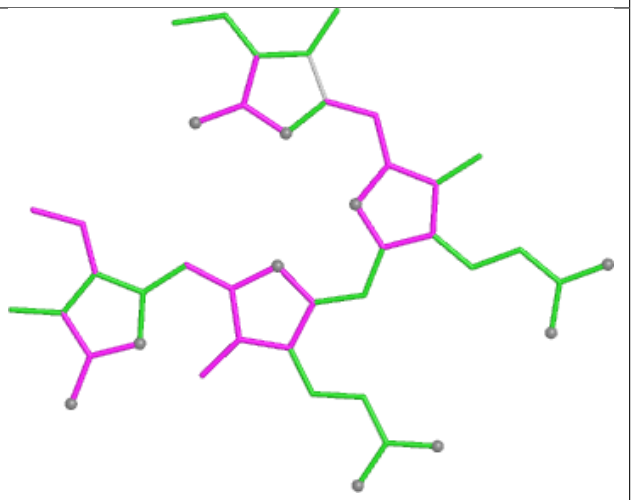


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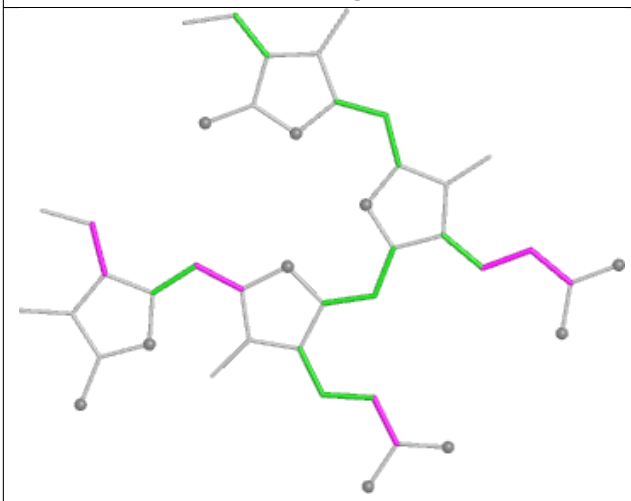
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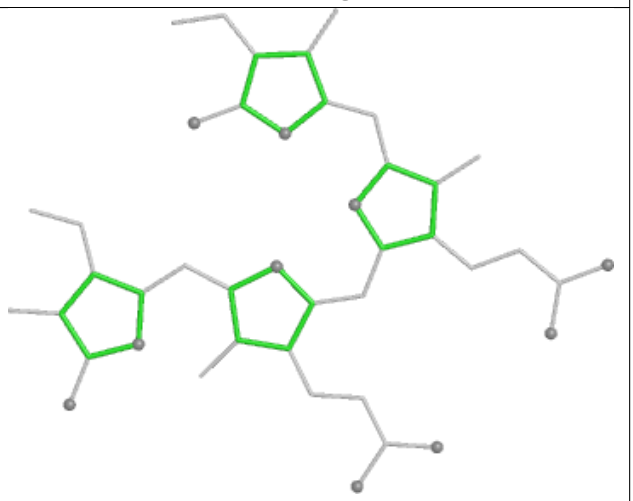
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Bond angles

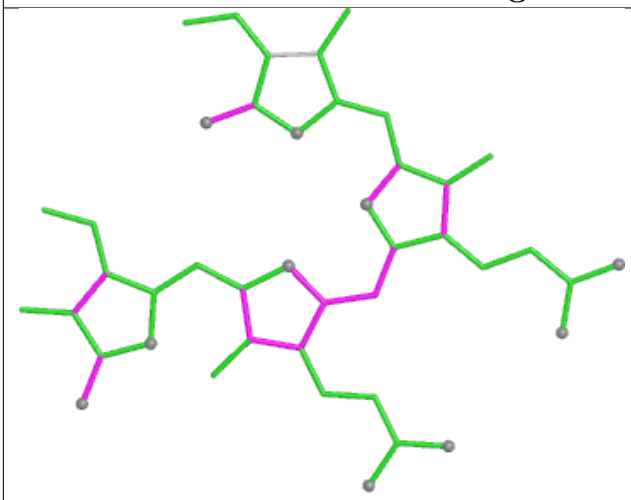


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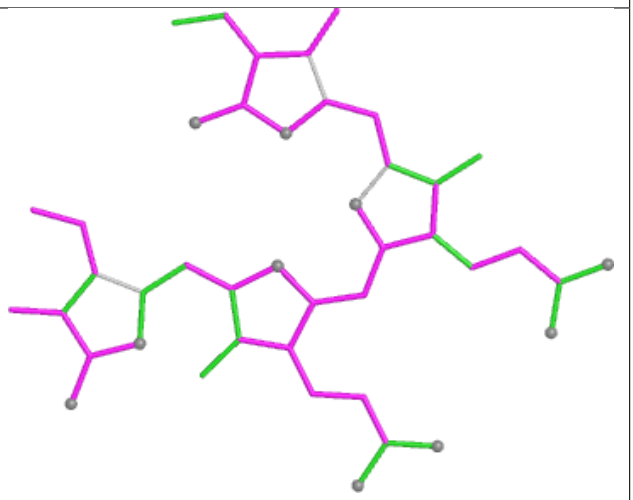


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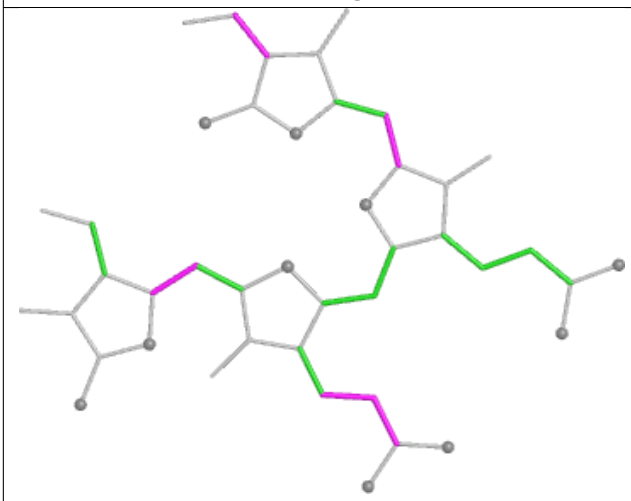
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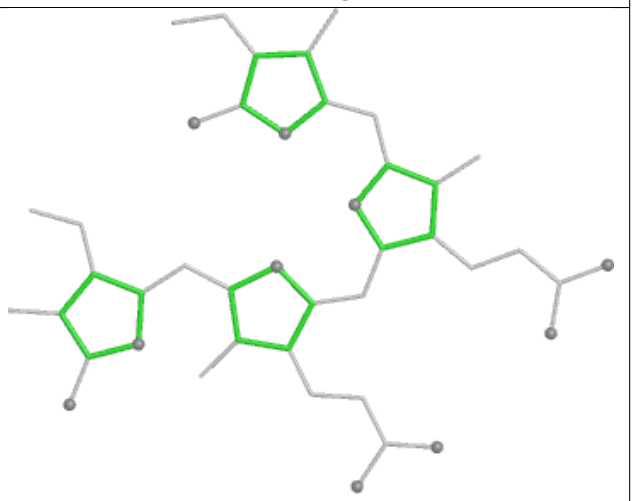
Bond lengths



Bond angles

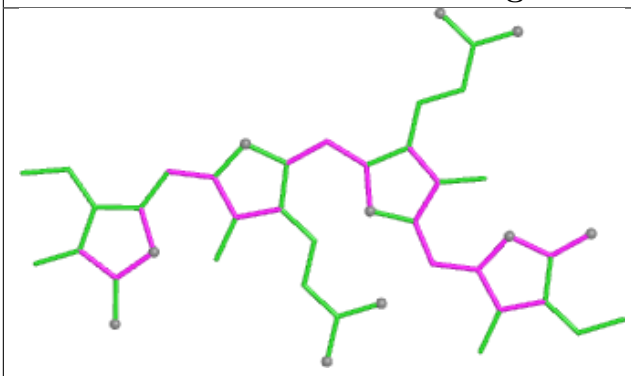


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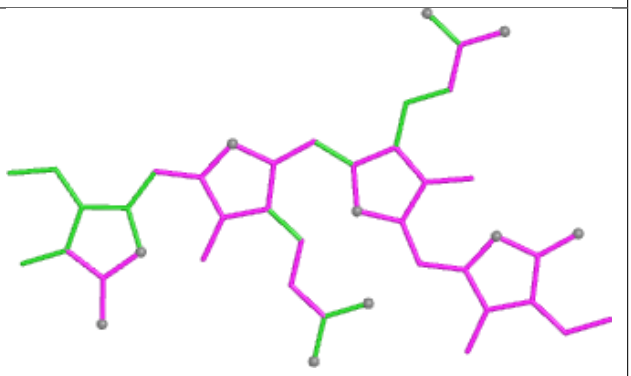


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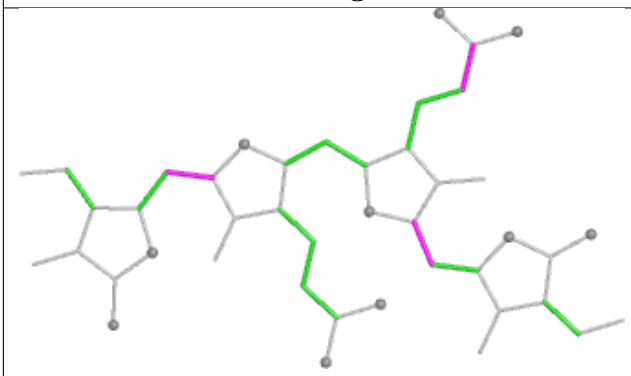
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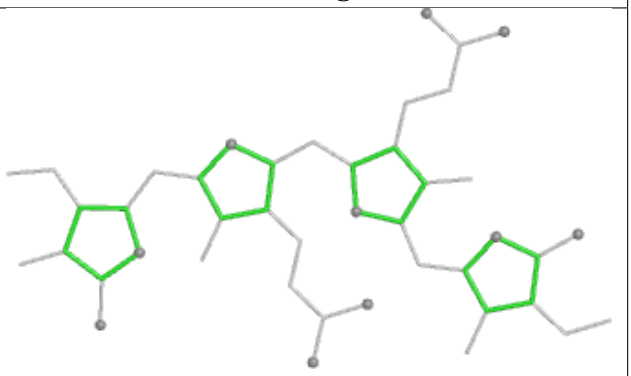
Bond lengths



Bond angles

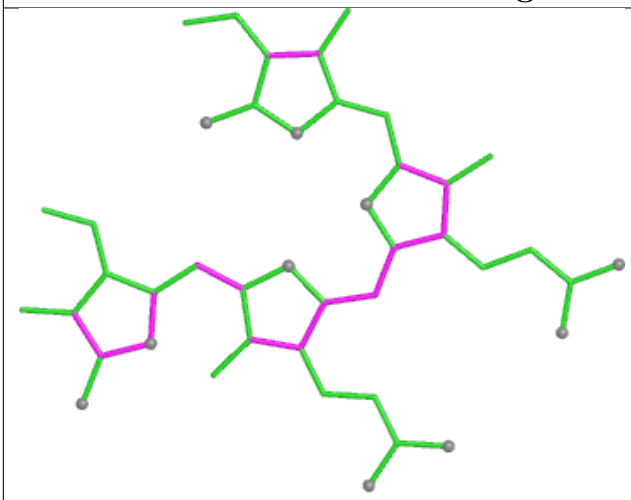


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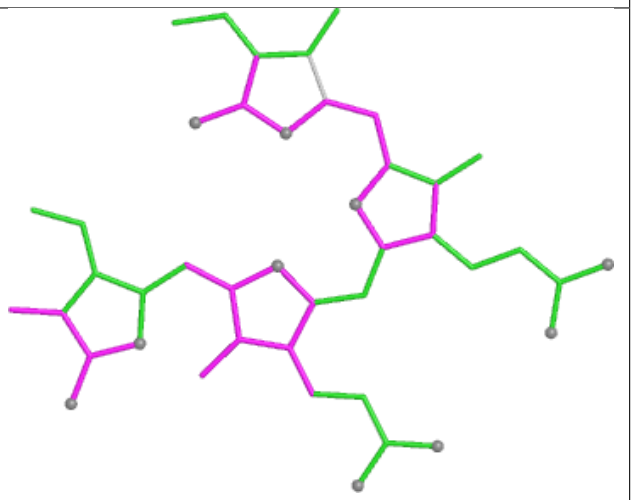


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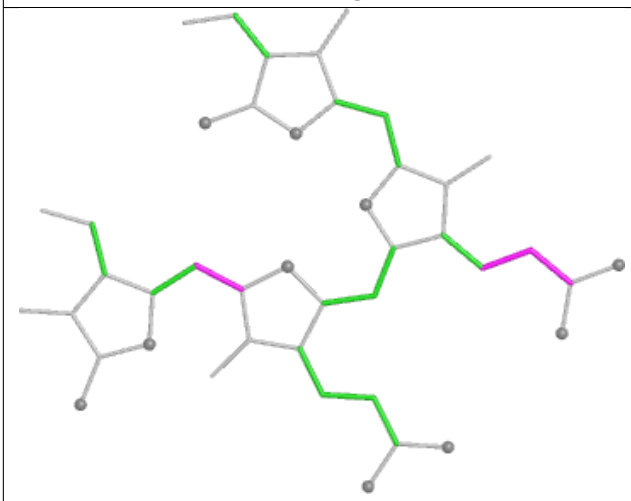
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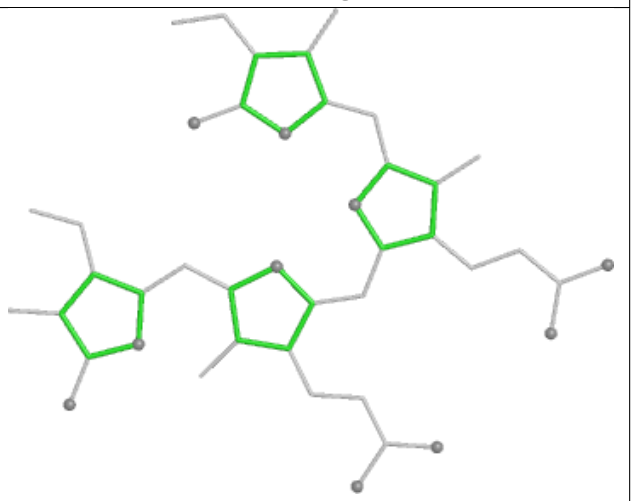
Bond lengths



Bond angles

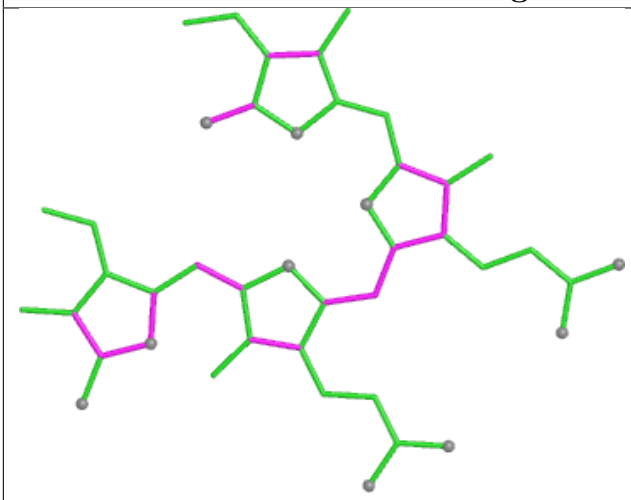


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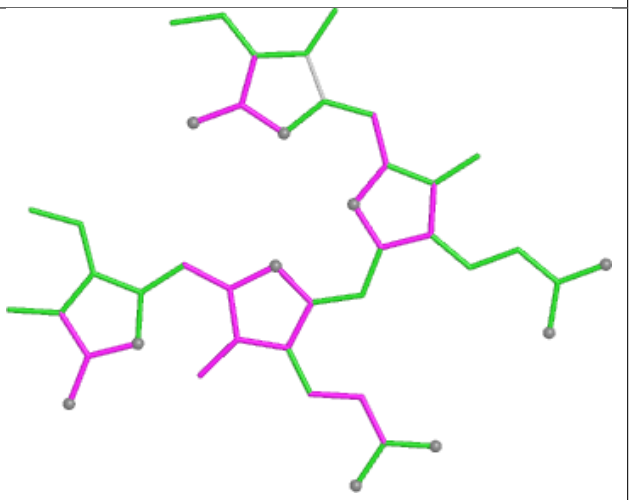


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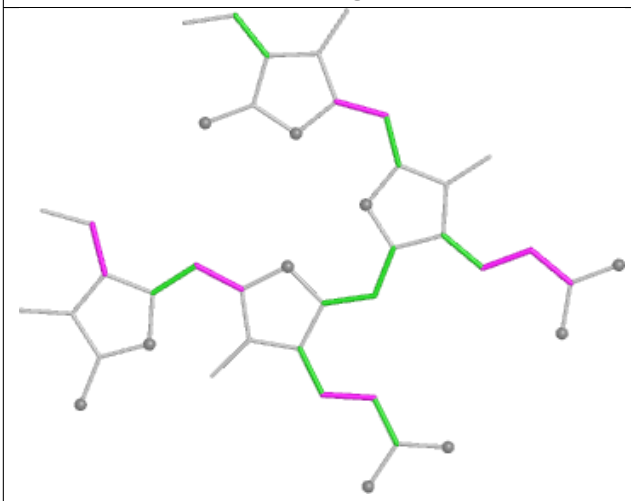
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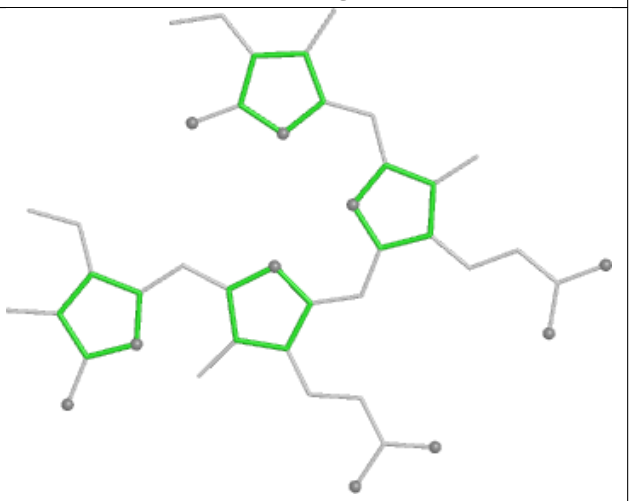
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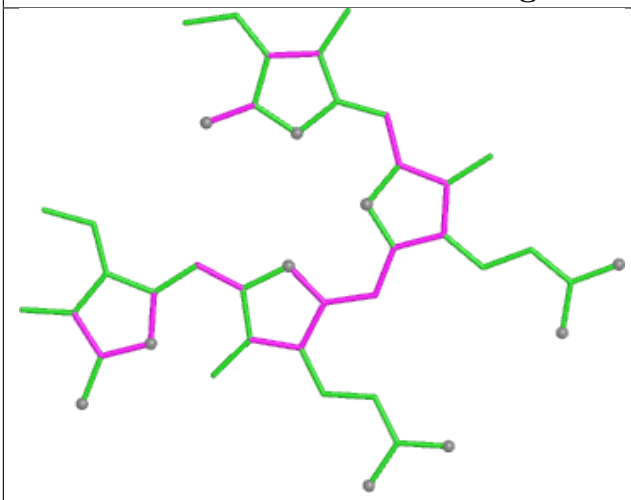


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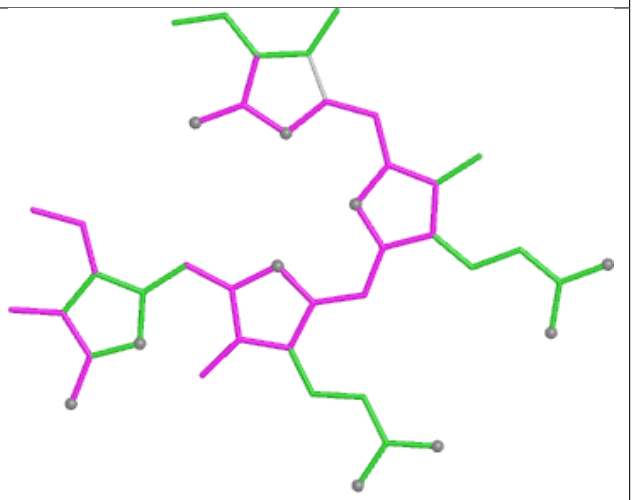


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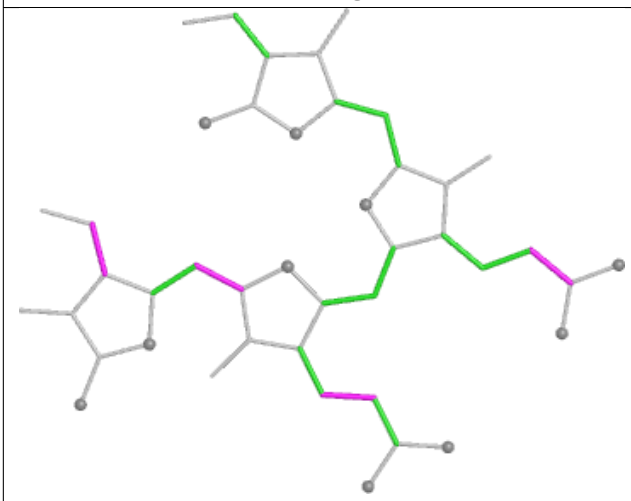
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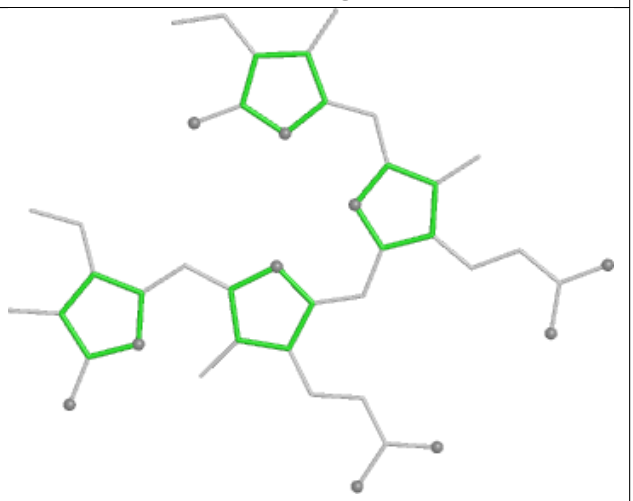
Bond lengths



Bond angles

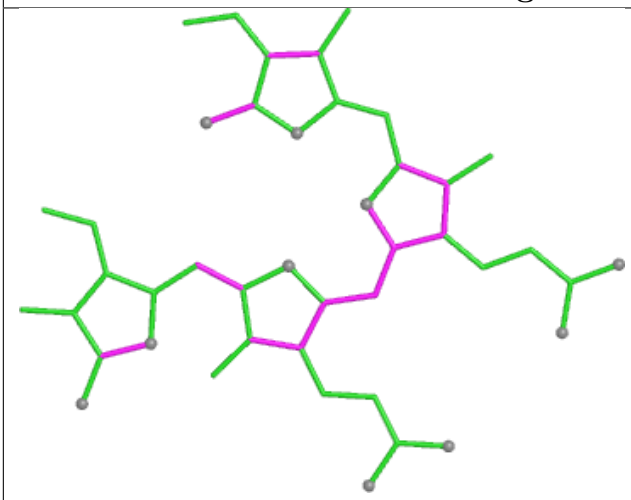


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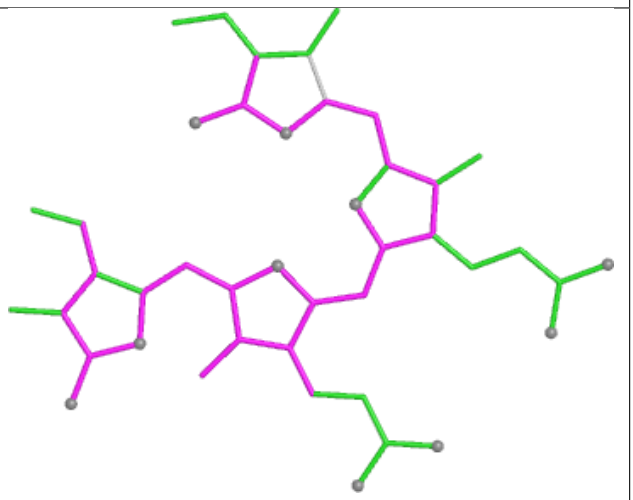


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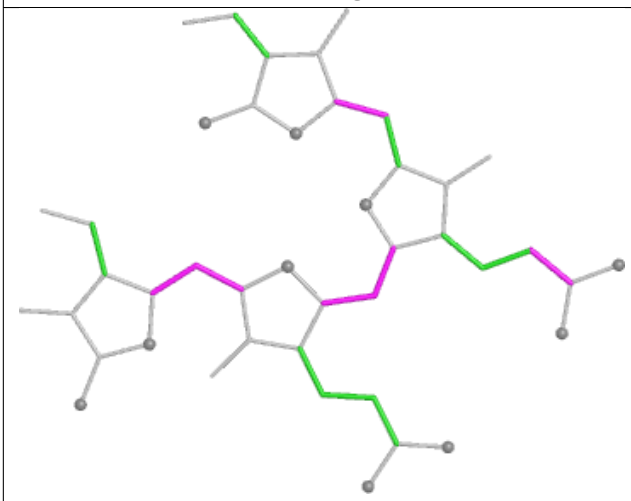
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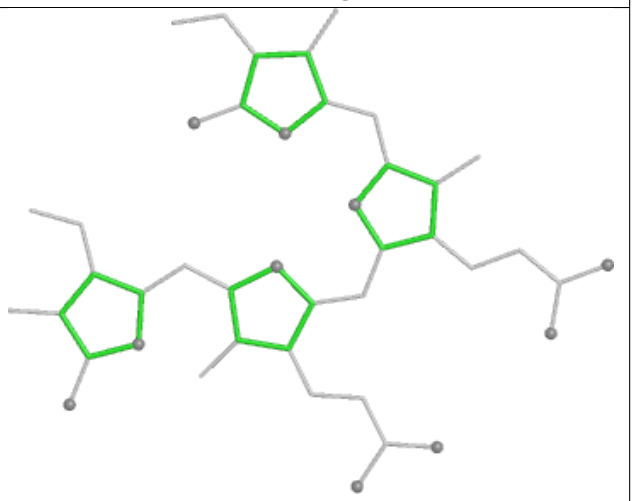
Bond lengths



Bond angles

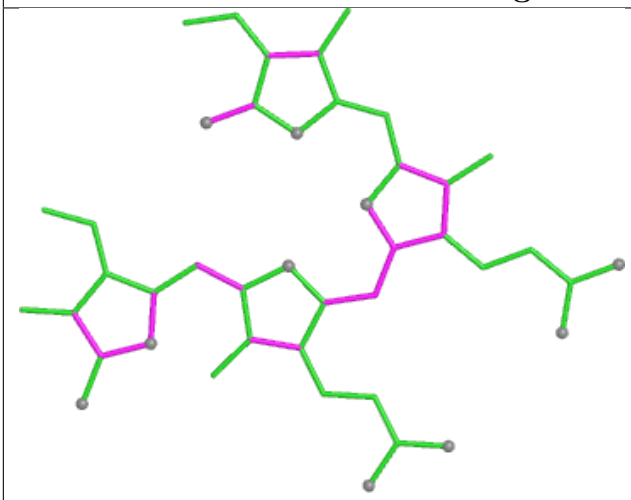


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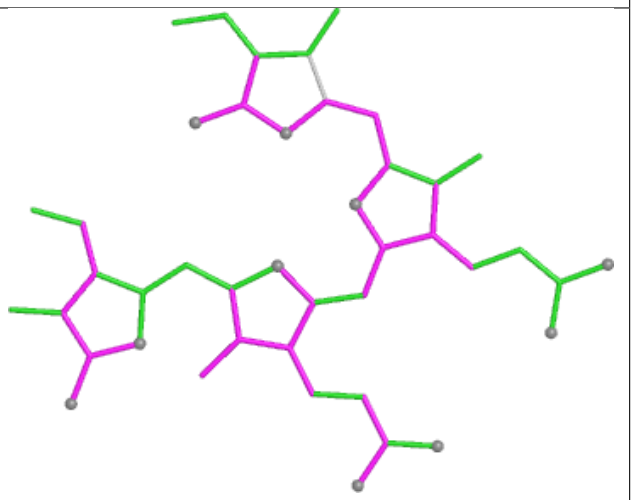


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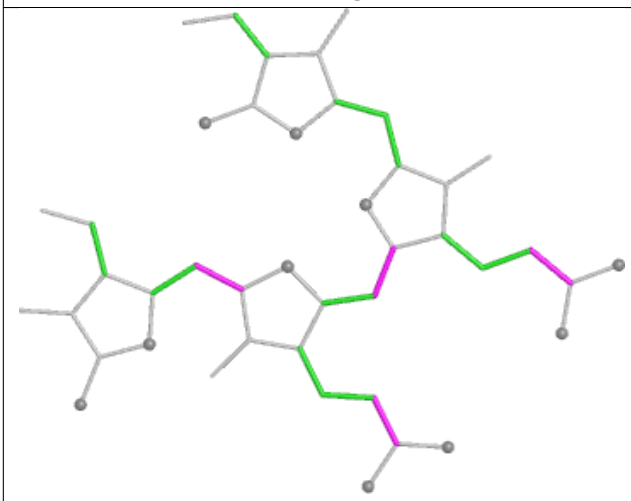
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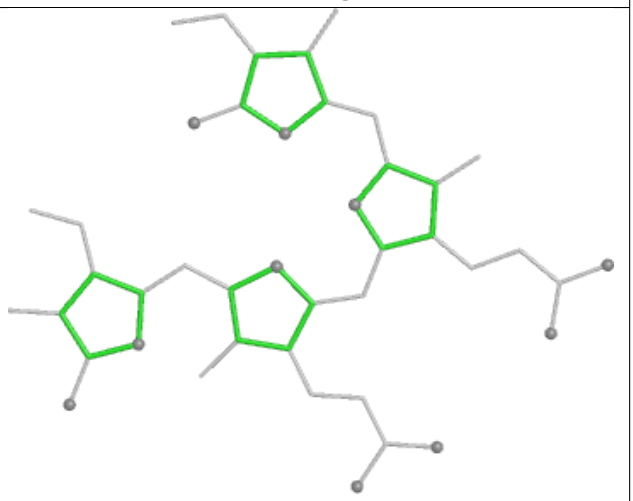
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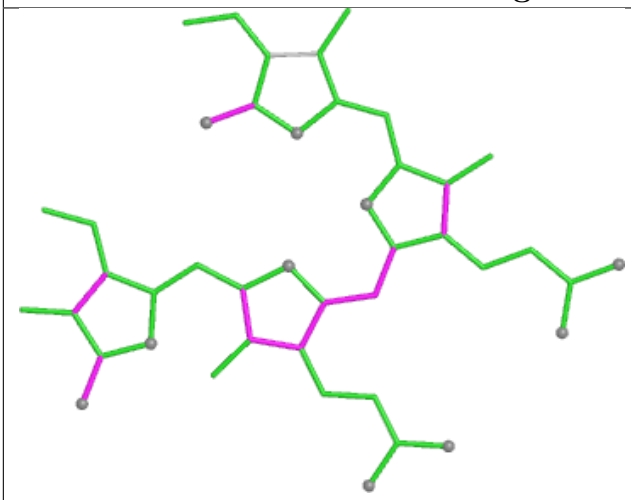


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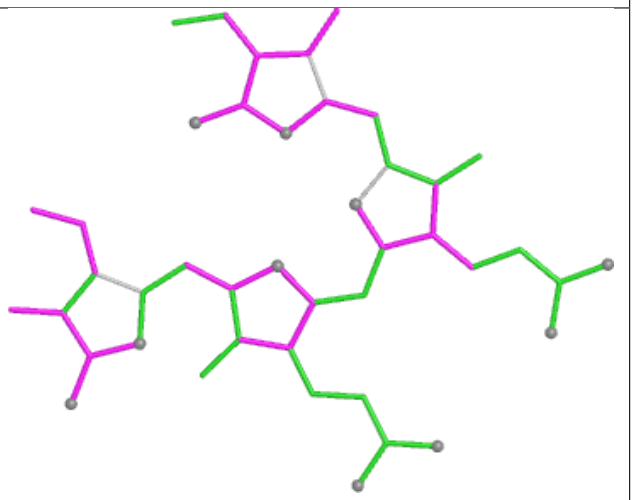


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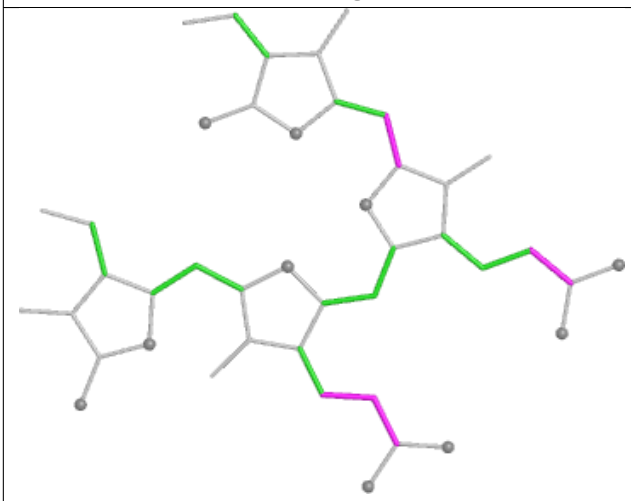
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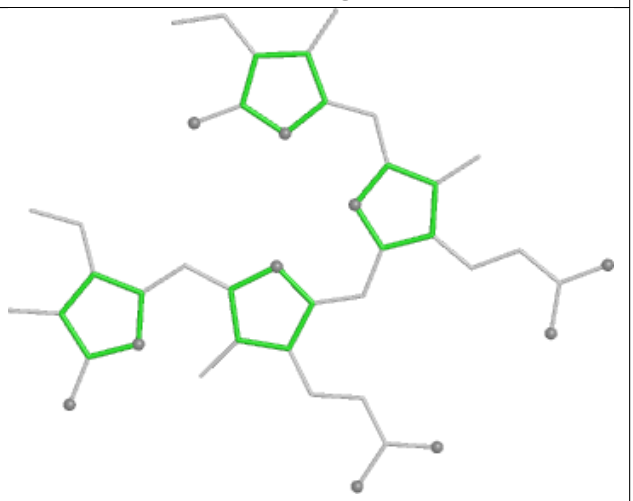
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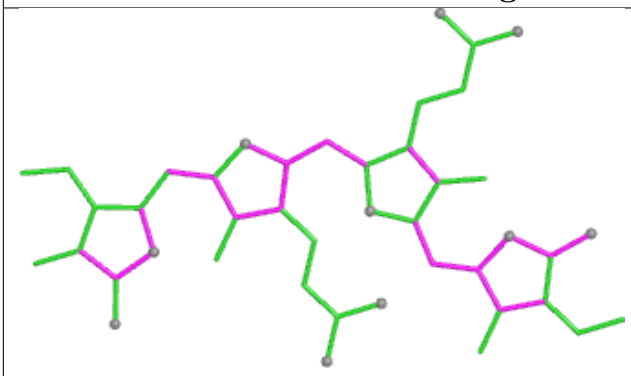


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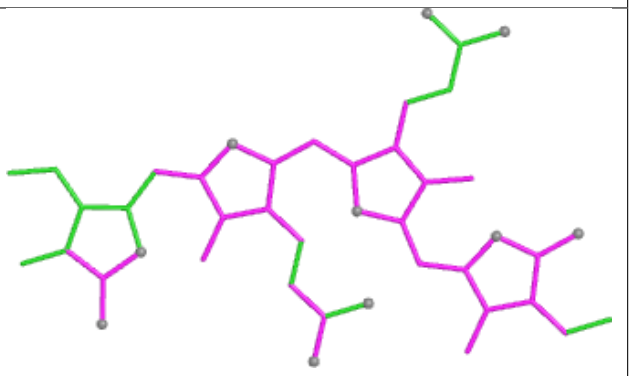


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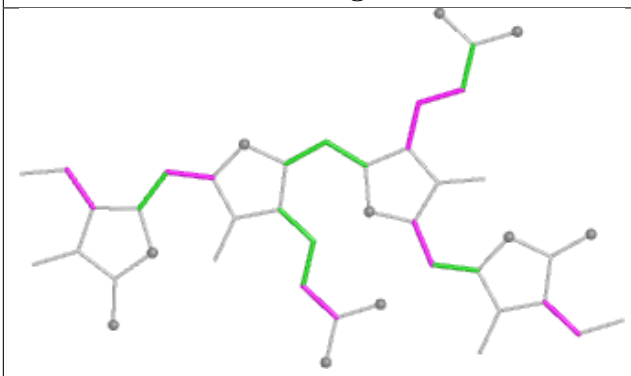
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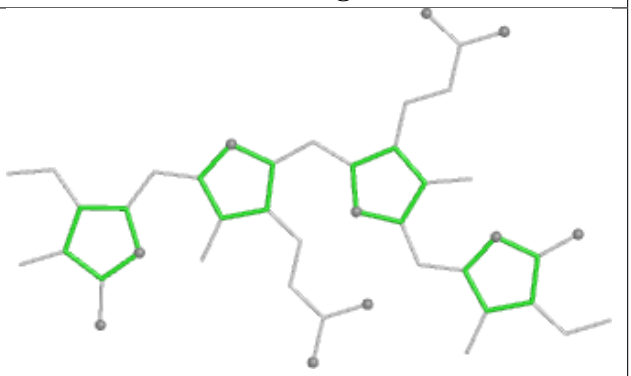
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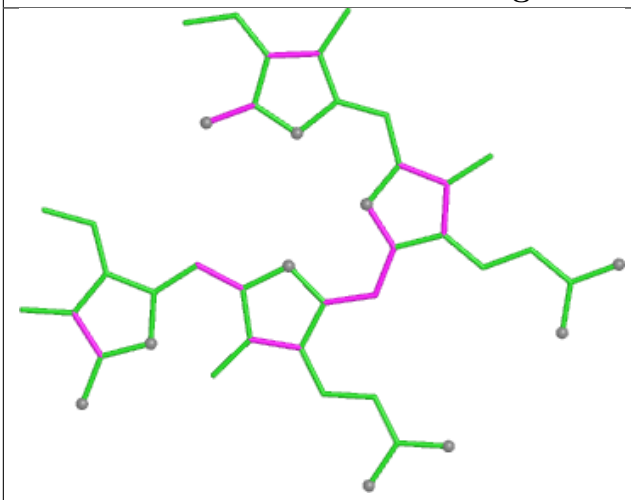


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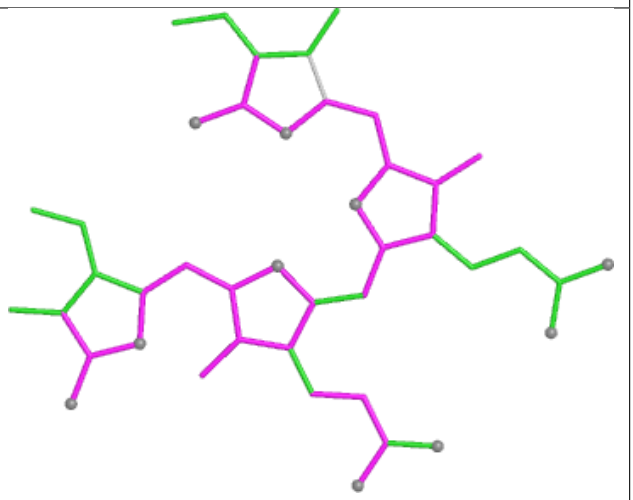


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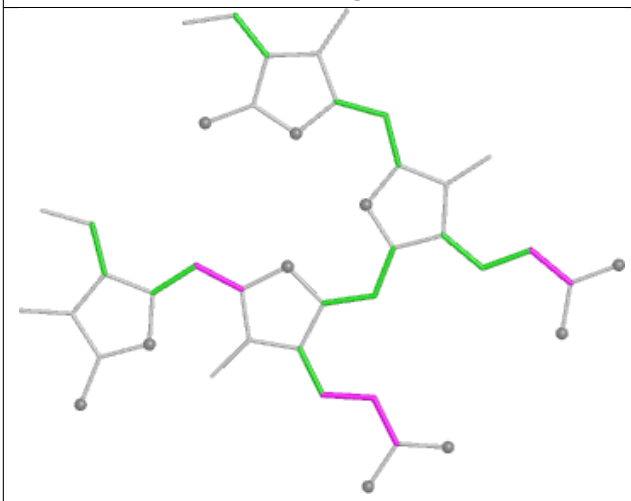
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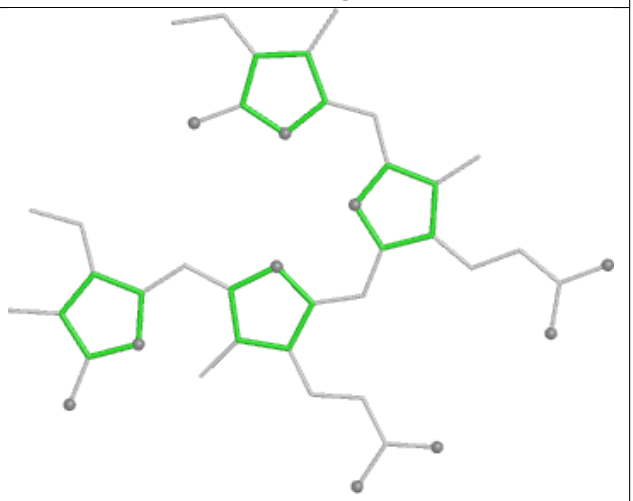
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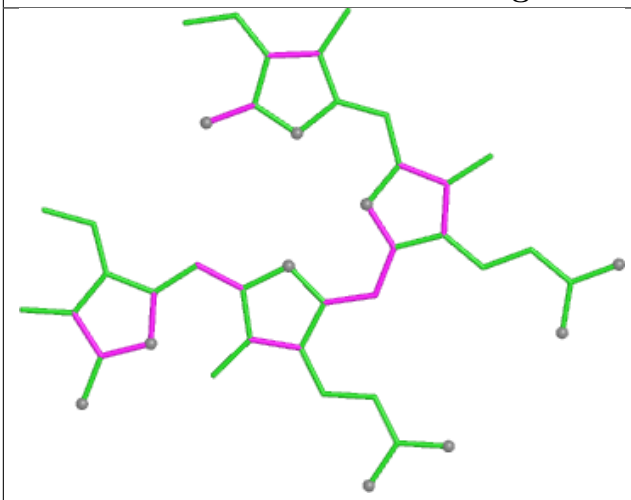


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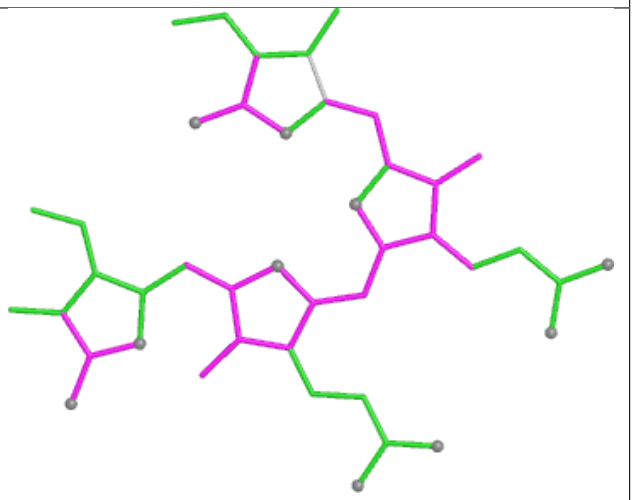


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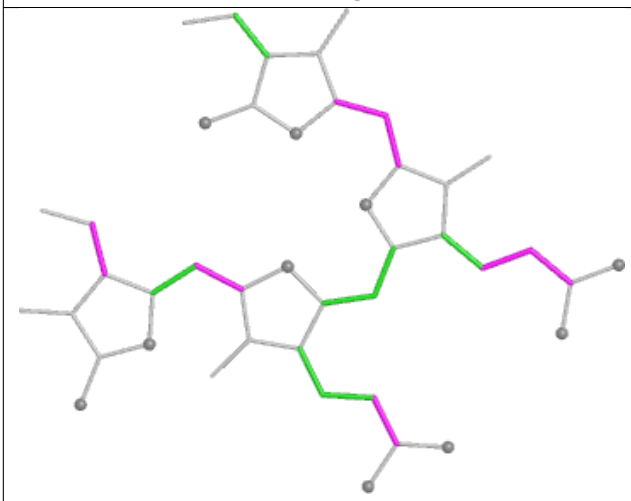
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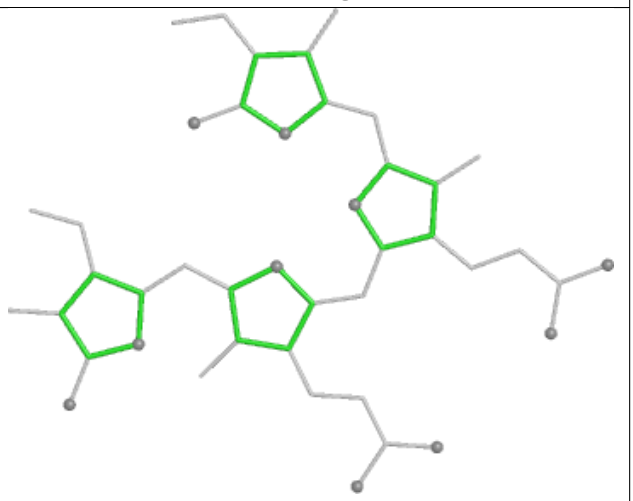
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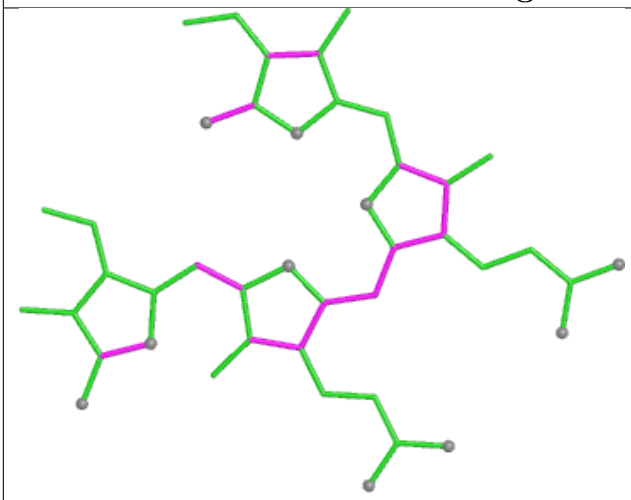


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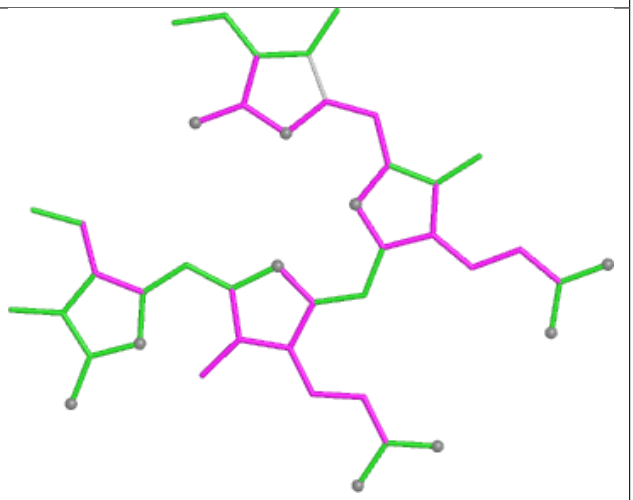


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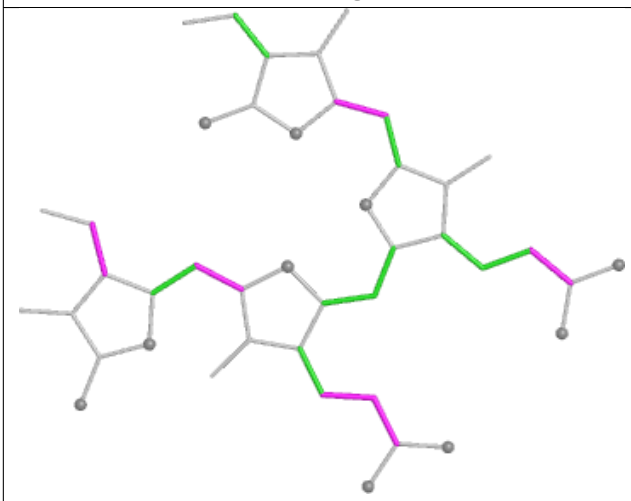
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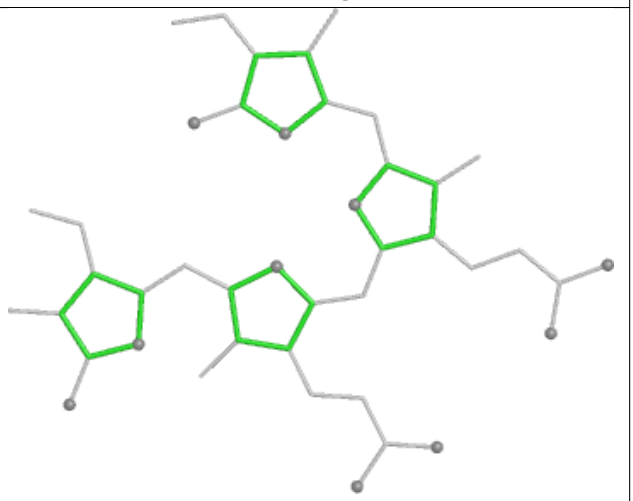
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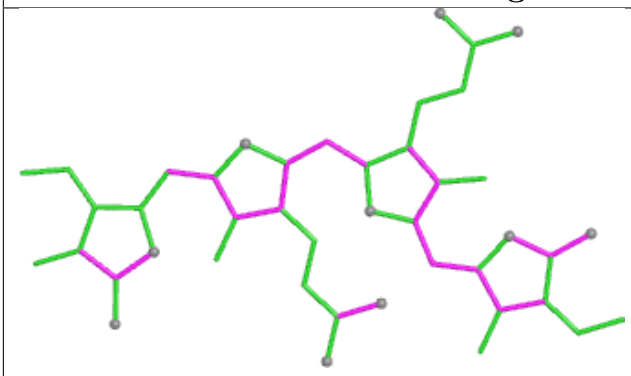


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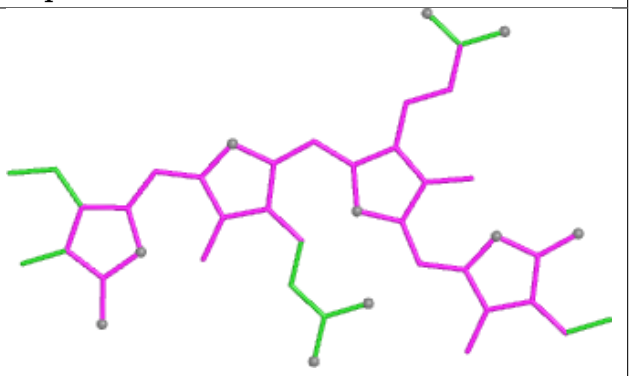


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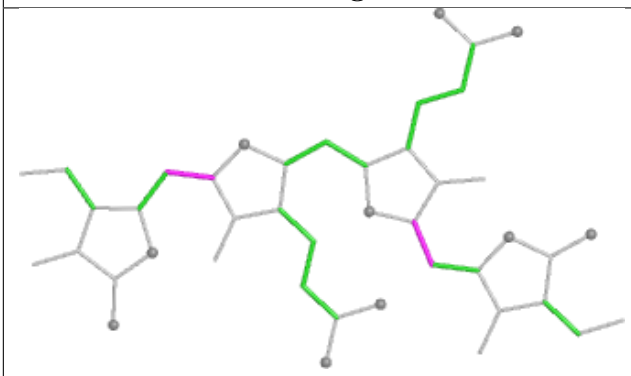
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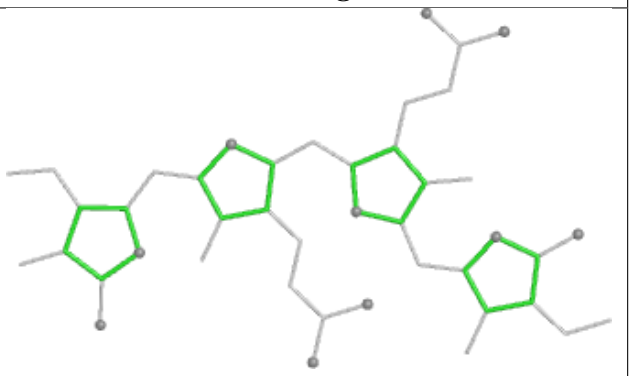
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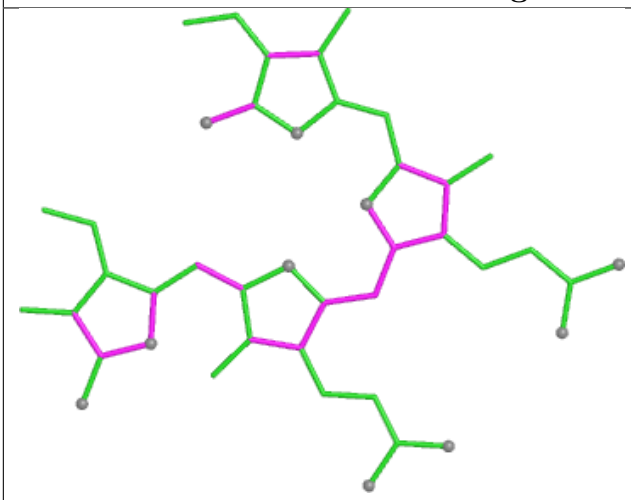


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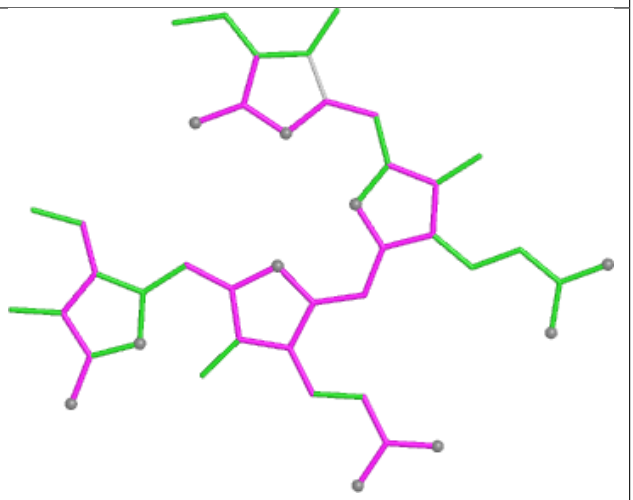


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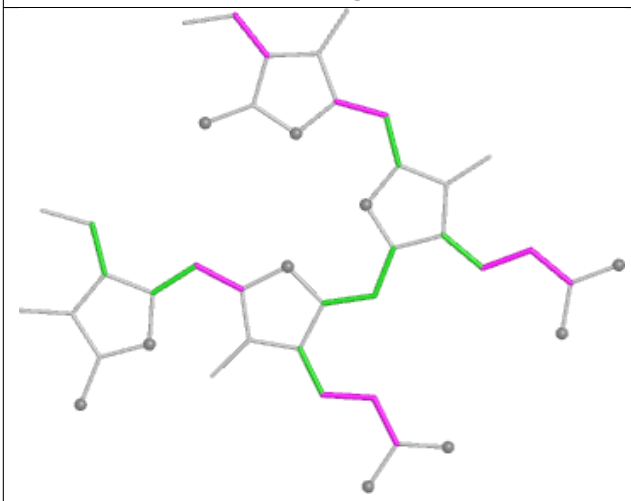
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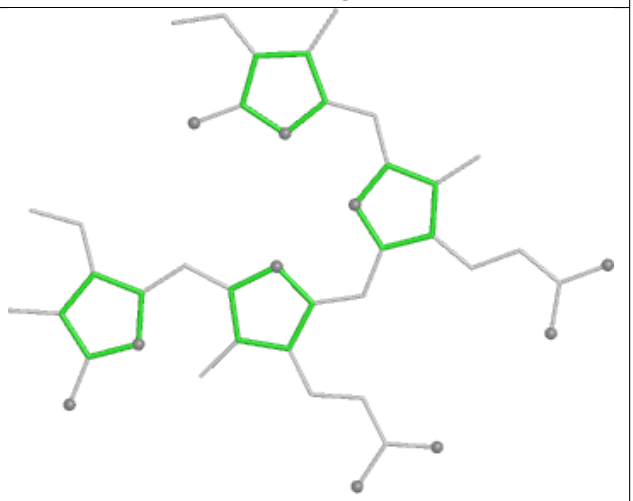
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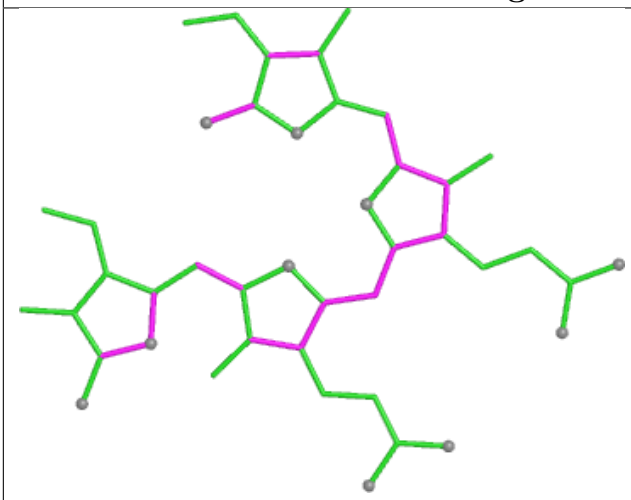


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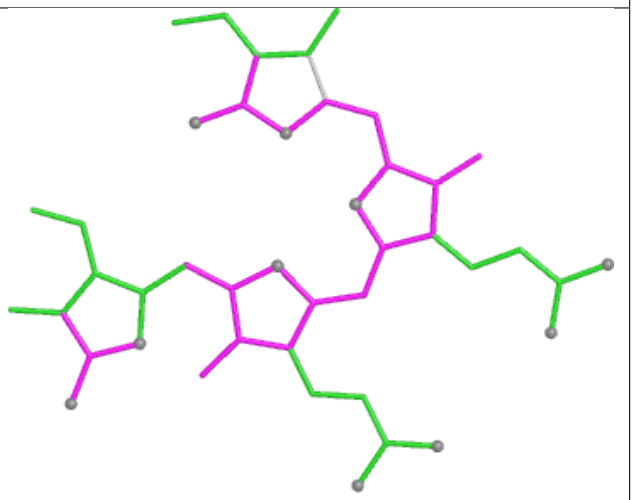


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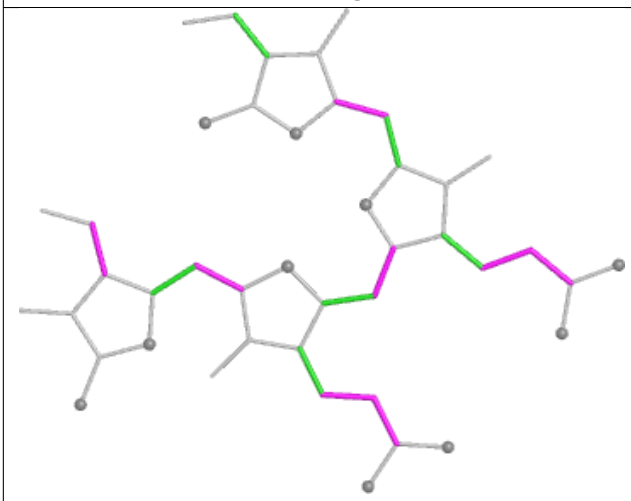
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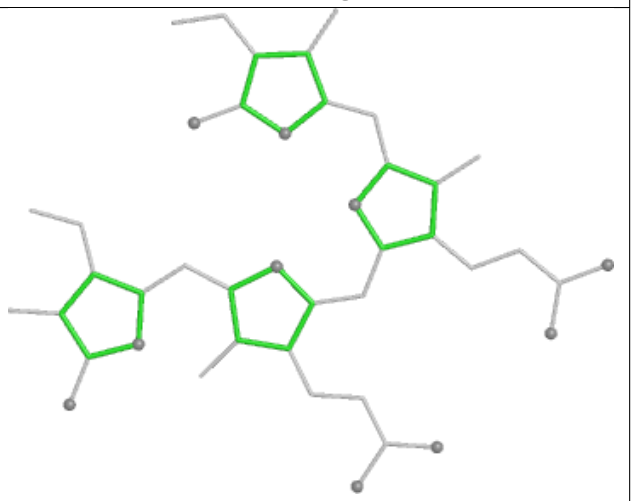
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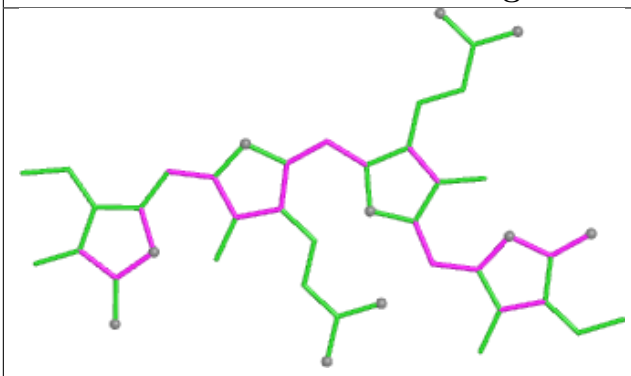


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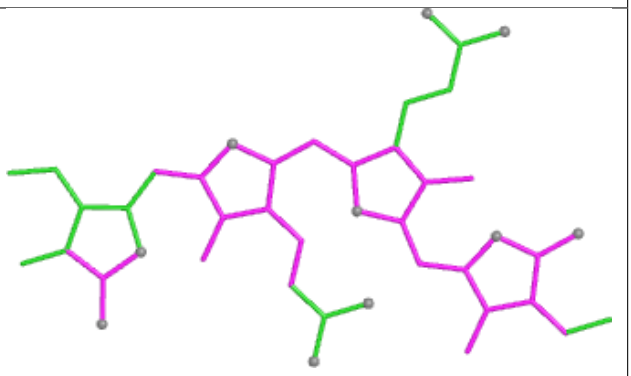


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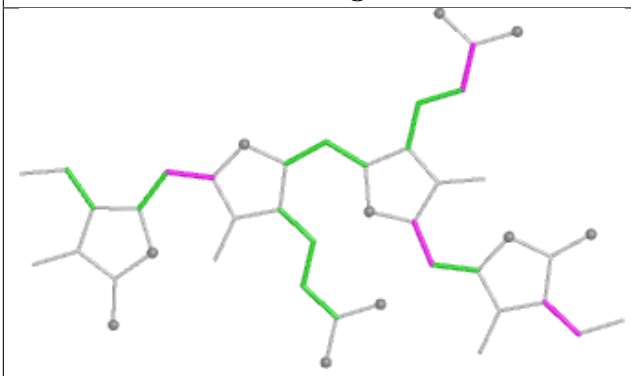
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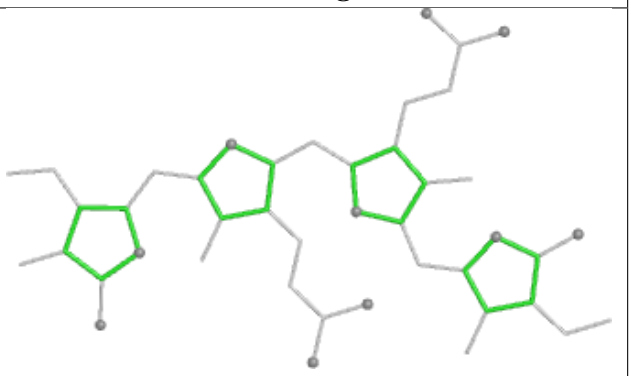
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Bond angles

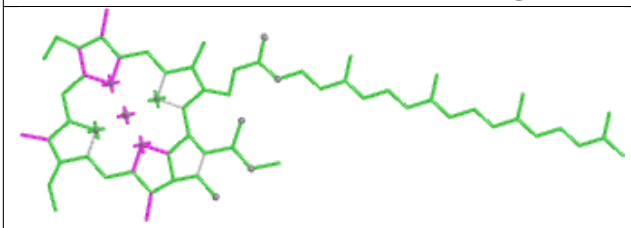


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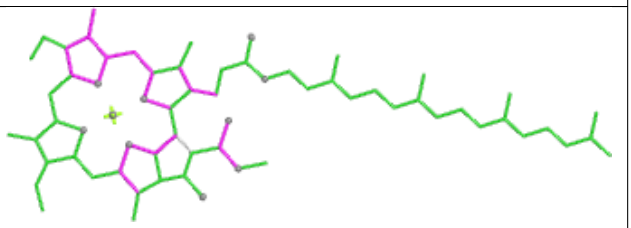


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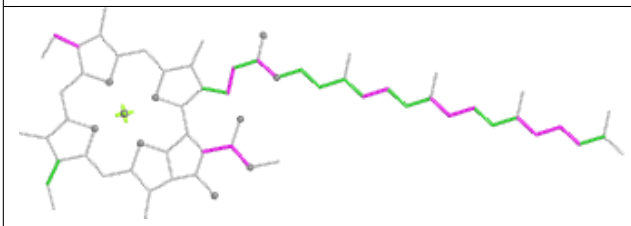
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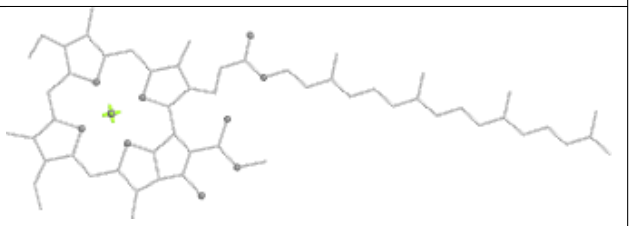
Bond lengths



Bond angles

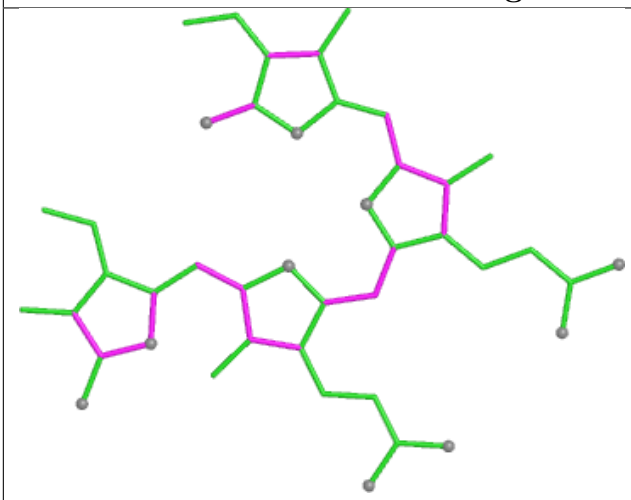


Torsions

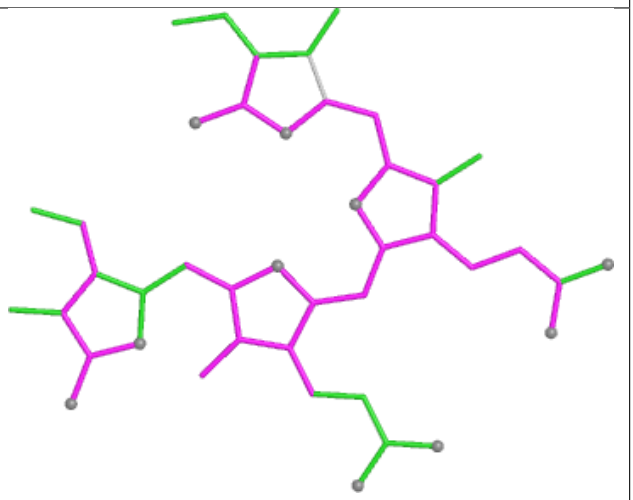


Rings

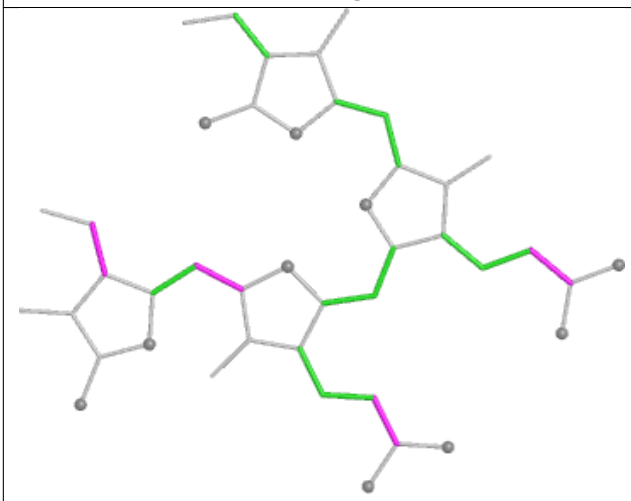
Ligand PEB WK 202



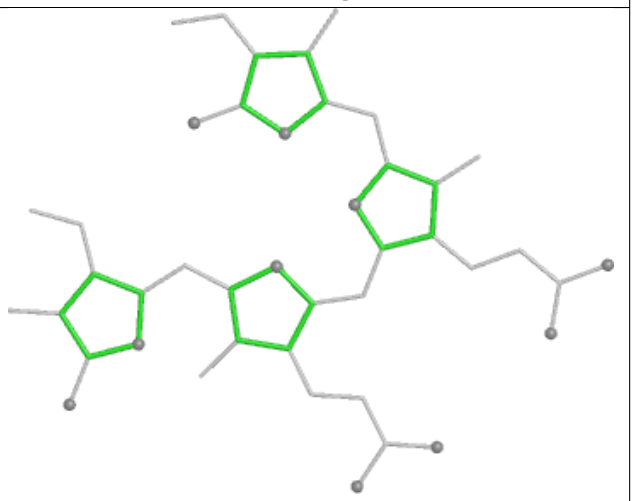
Bond lengths



Bond angles

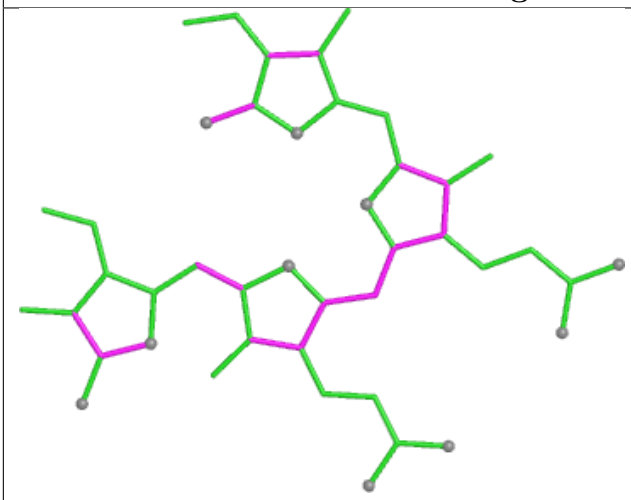


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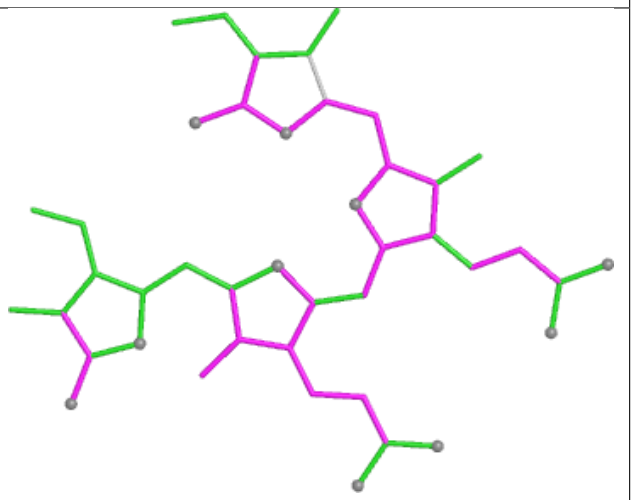


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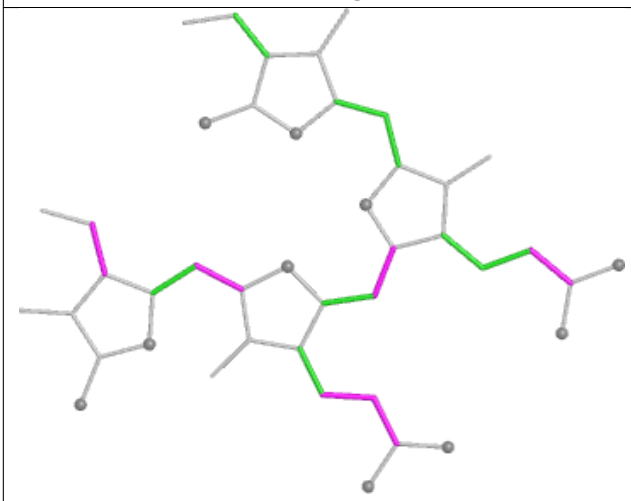
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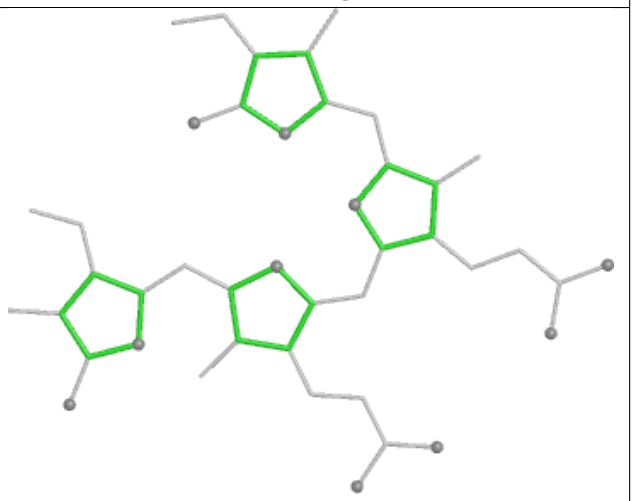
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Bond angles

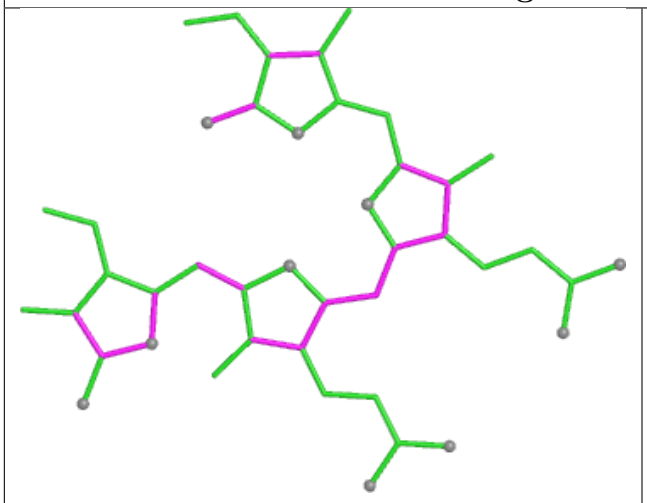


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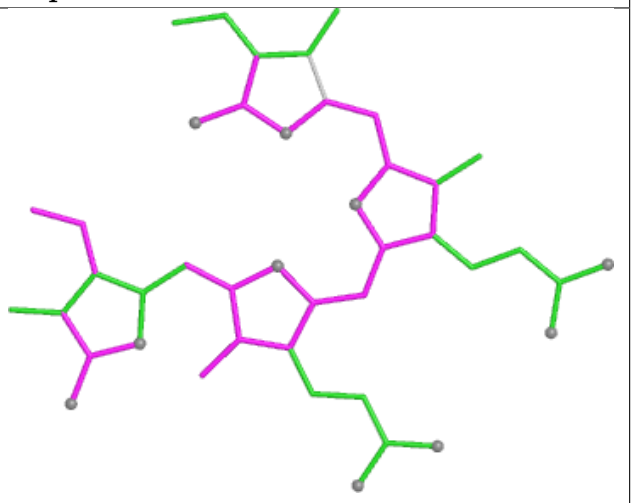


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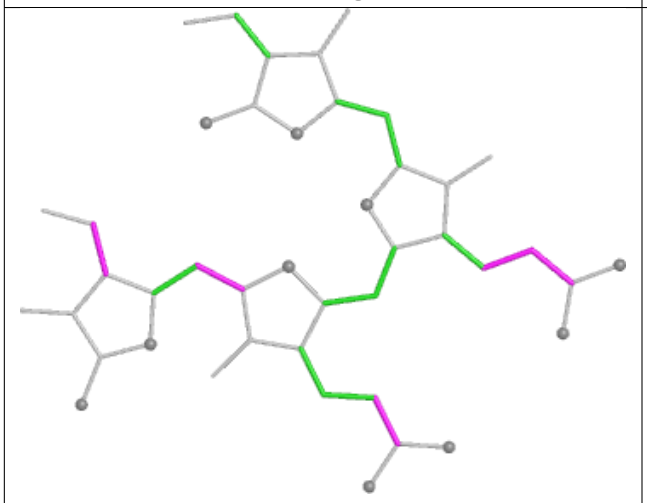
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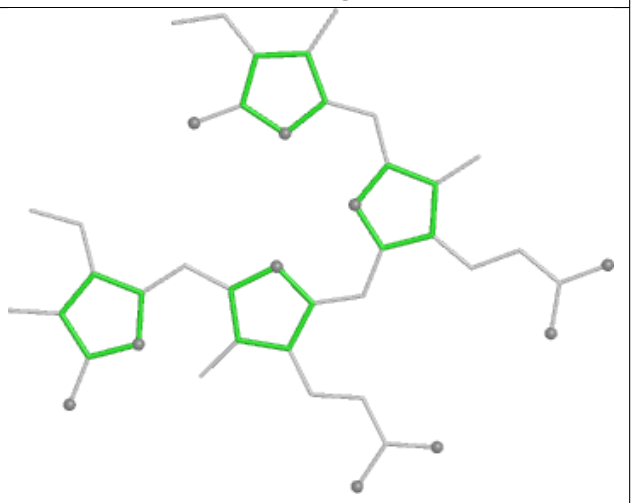
Bond lengths



Bond angles



Torsions

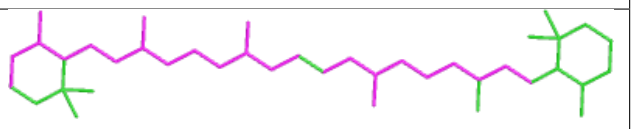


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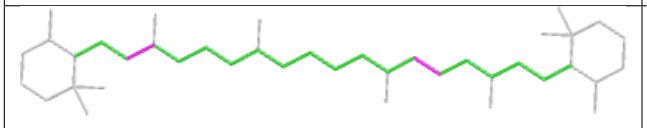
Ligand BCR BL 617



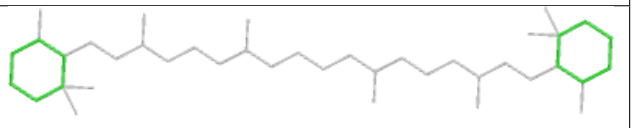
Bond lengths



Bond angles

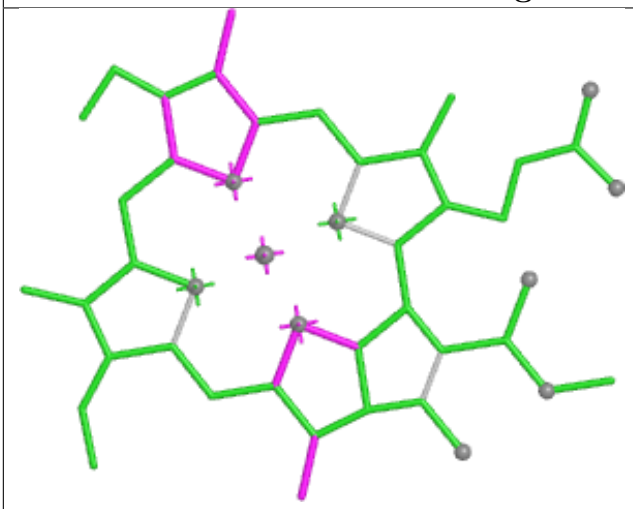


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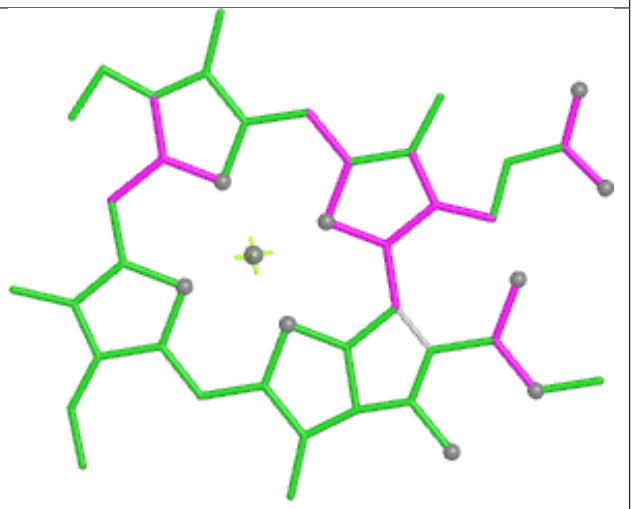


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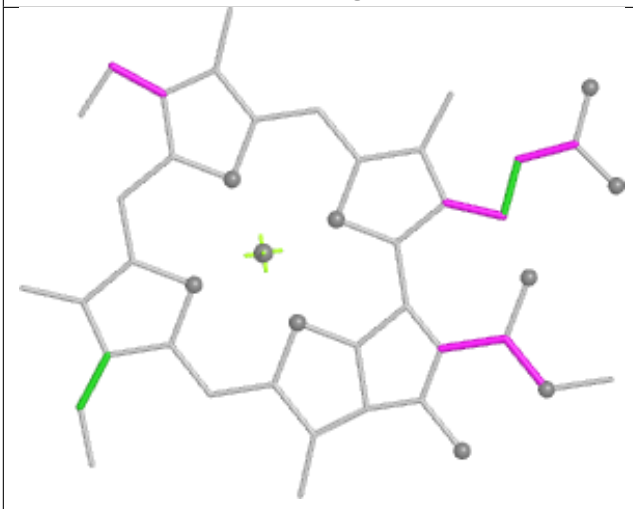
Ligand CLA A2 822



Bond lengths



Bond angles

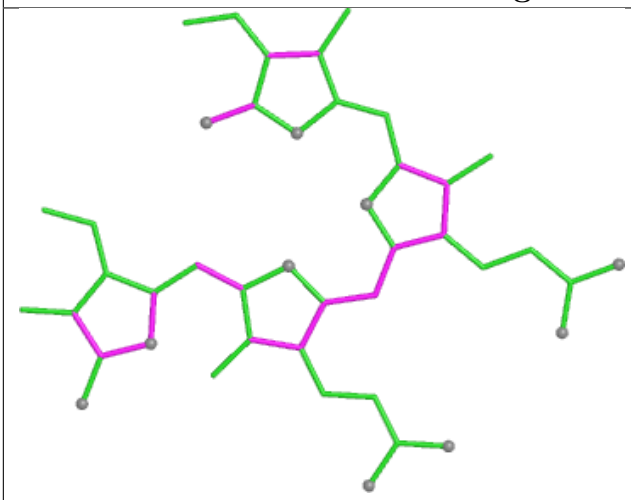


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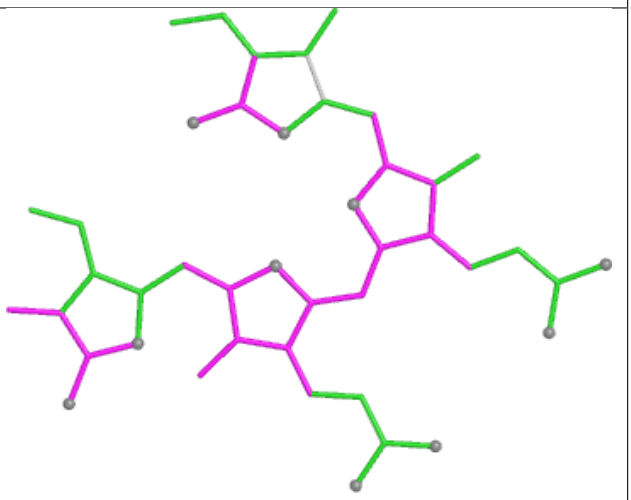


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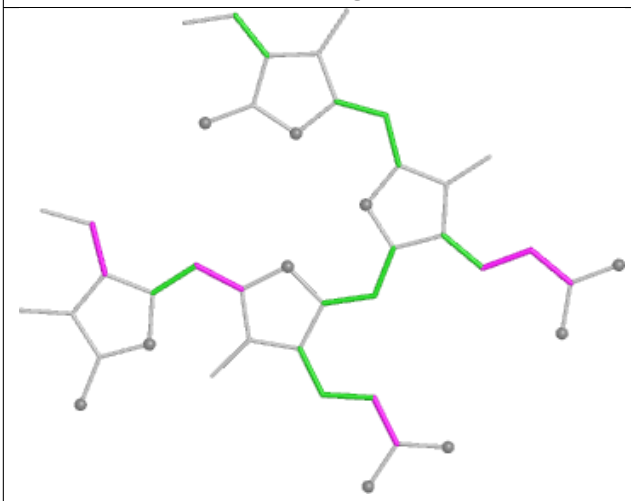
Ligand PEB m4 202



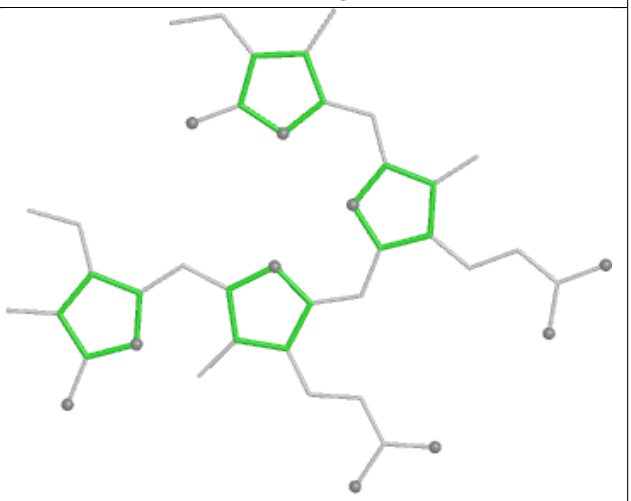
Bond lengths



Bond angles

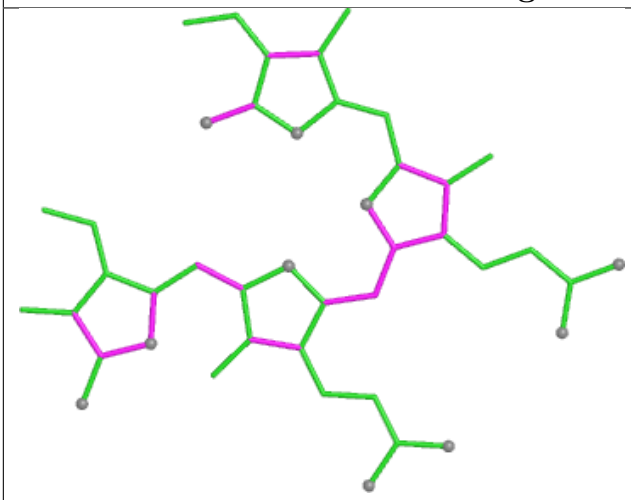


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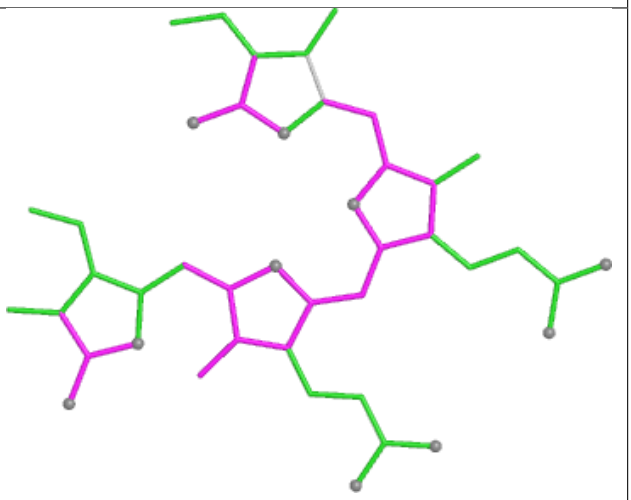


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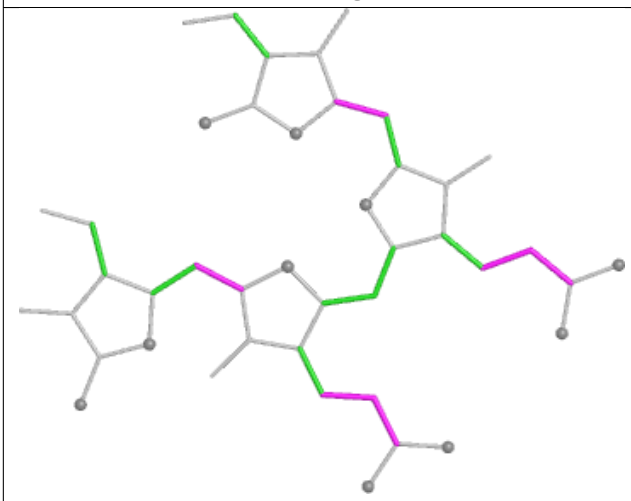
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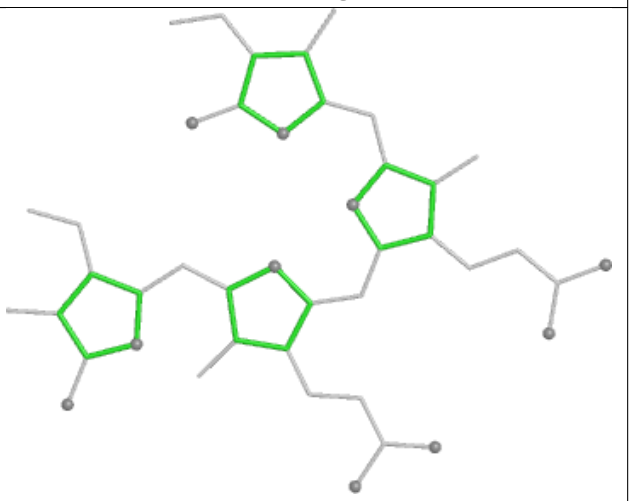
Bond lengths



Bond angles

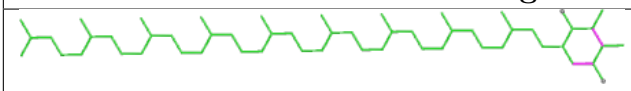


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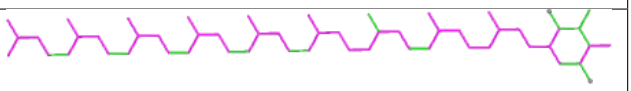


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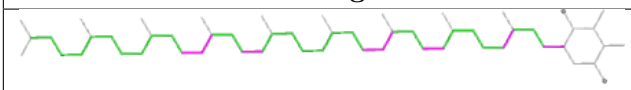
Ligand PL9 D6 408



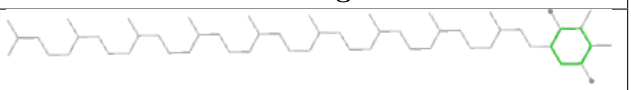
Bond lengths



Bond angles

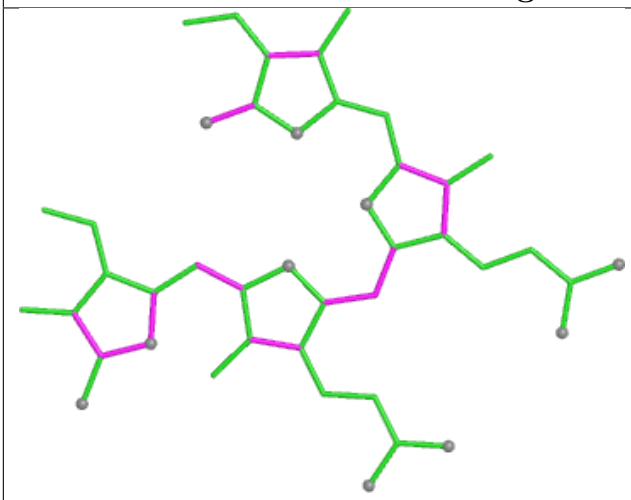


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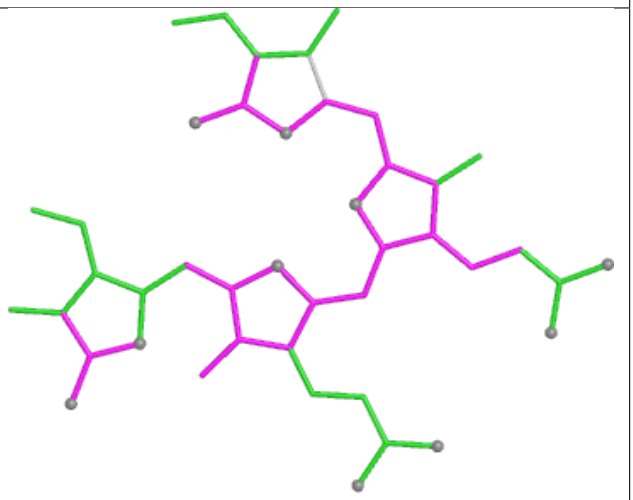


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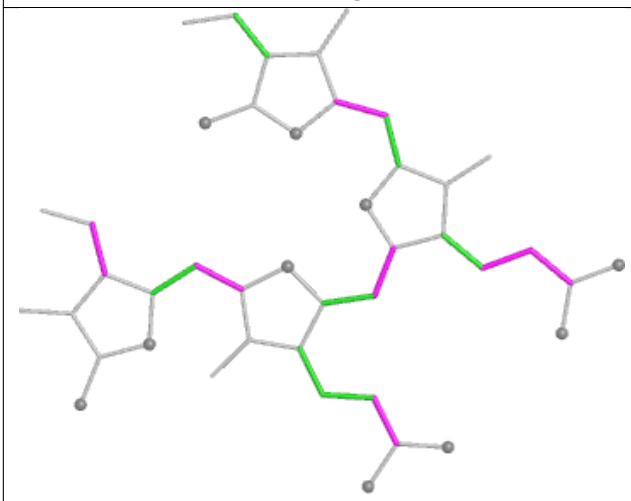
Ligand PEB cB 402



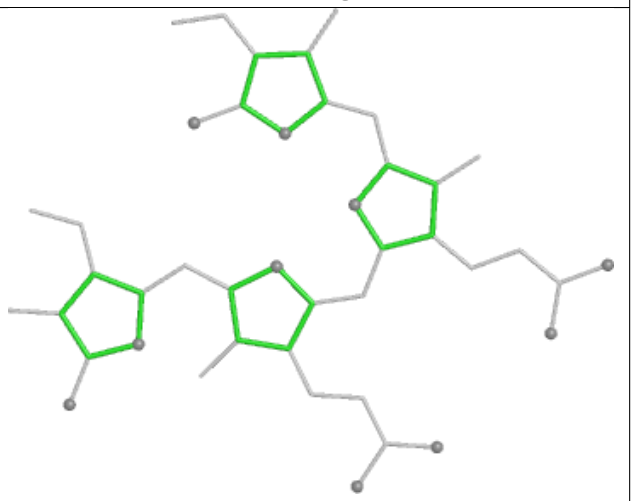
Bond lengths



Bond angles

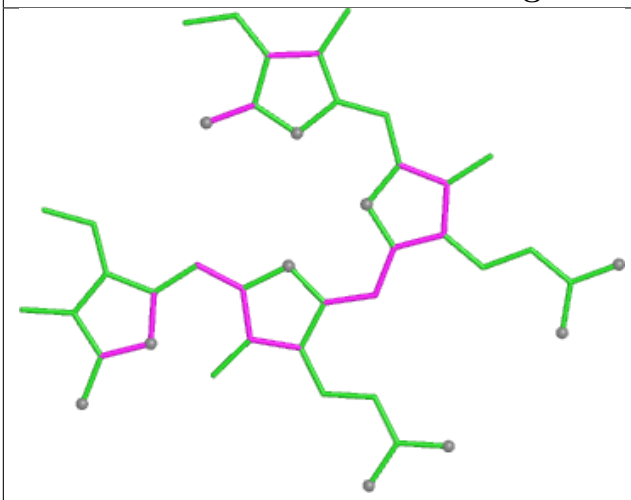


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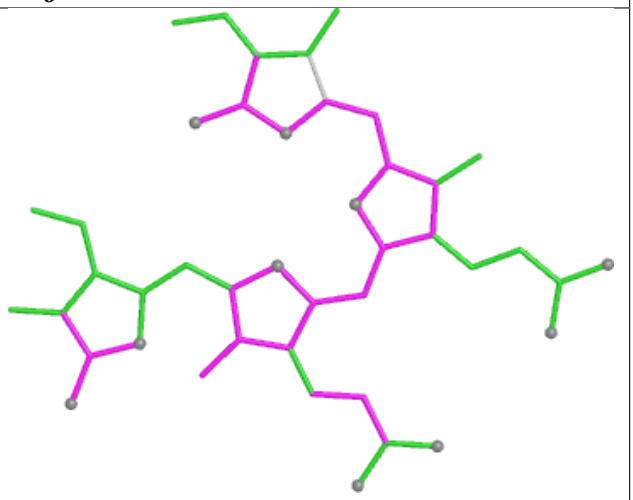


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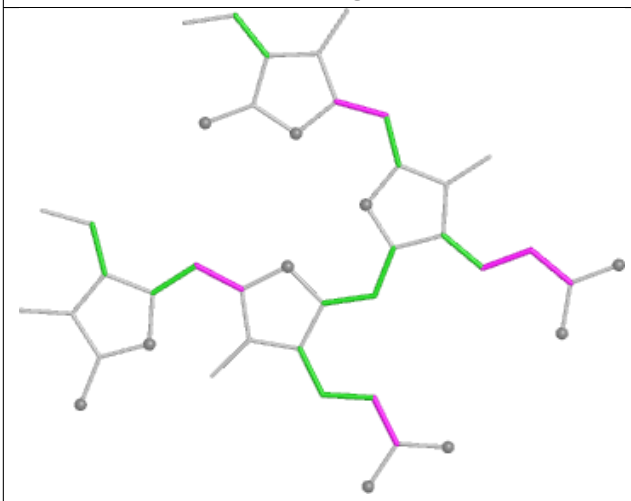
Ligand PEB j1 201



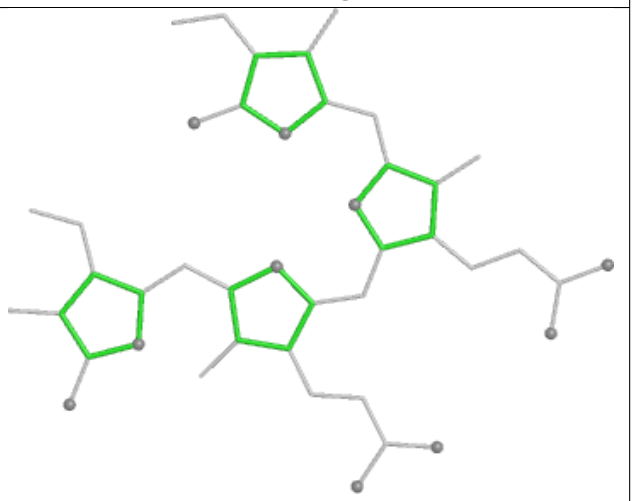
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Bond angles

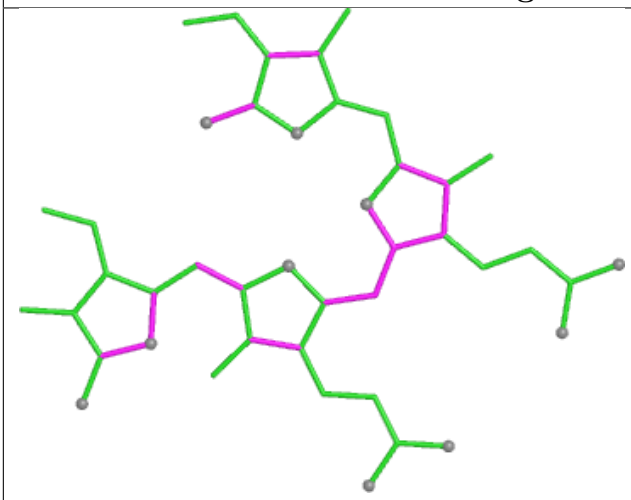


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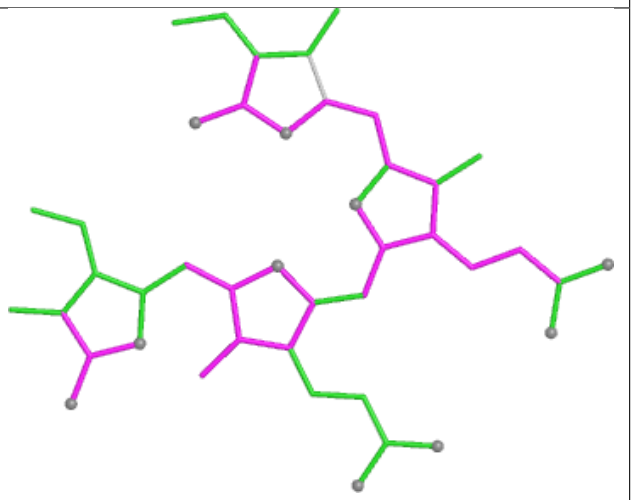


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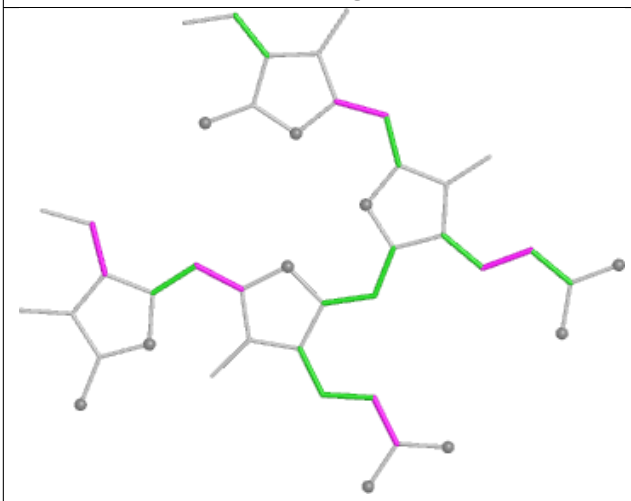
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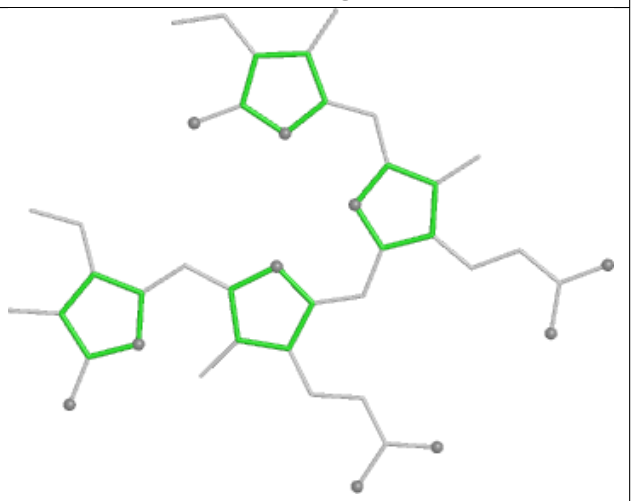
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Bond angles

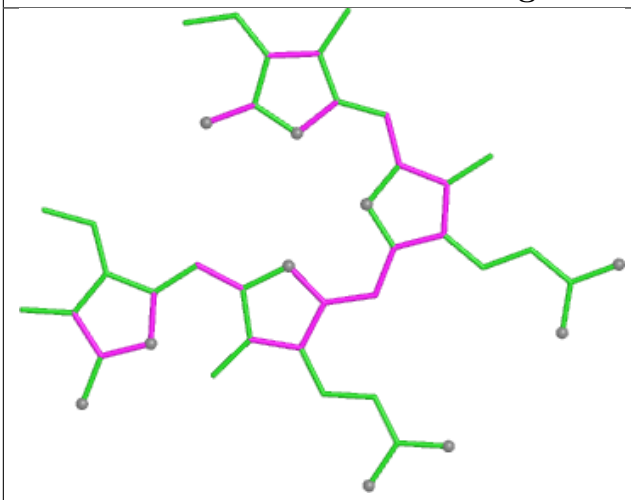


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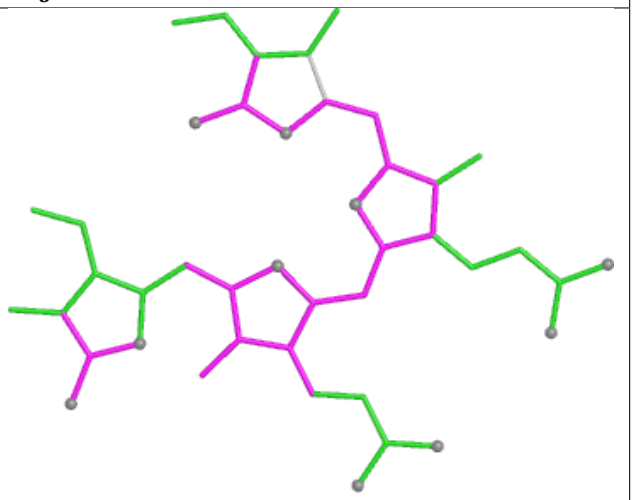


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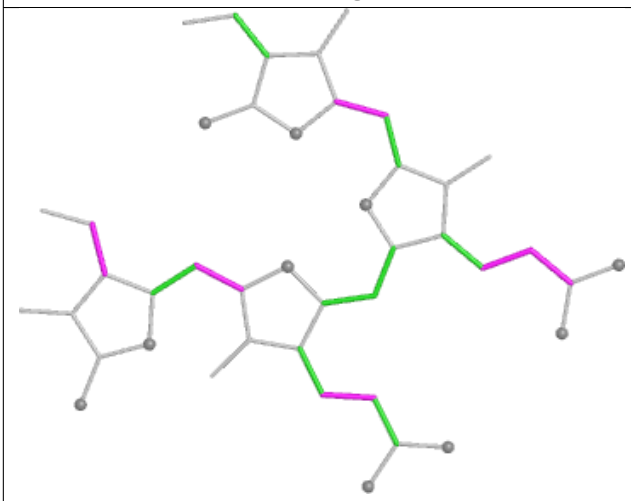
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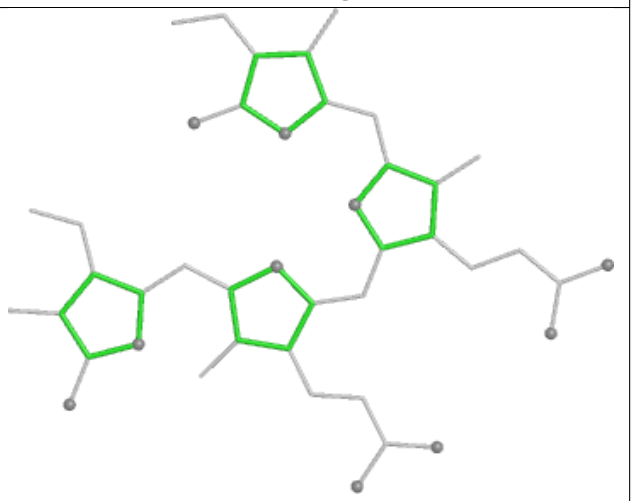
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Bond angles

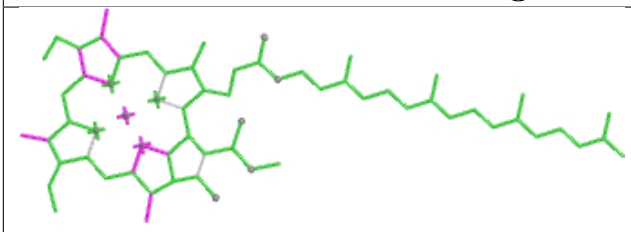


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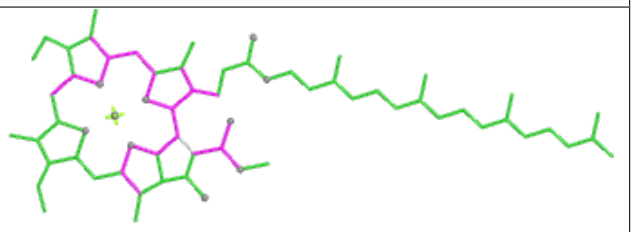


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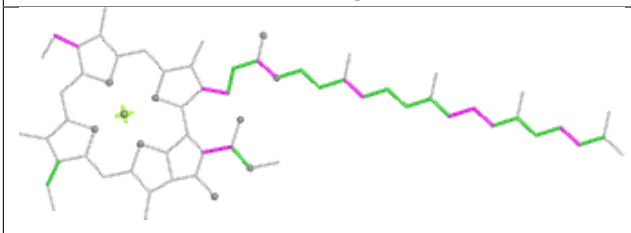
Ligand CLA AN 828



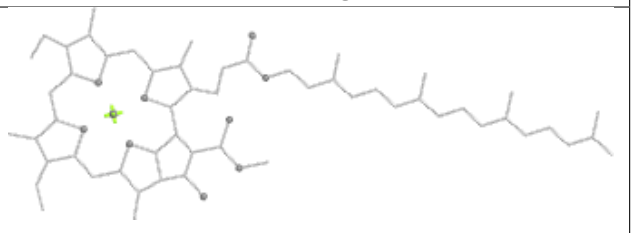
Bond lengths



Bond angles

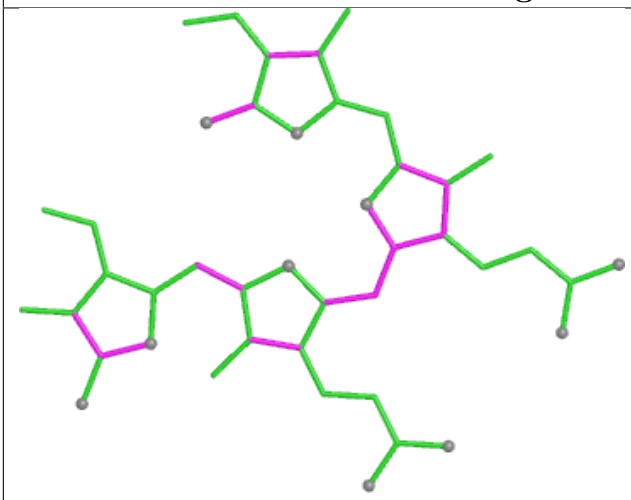


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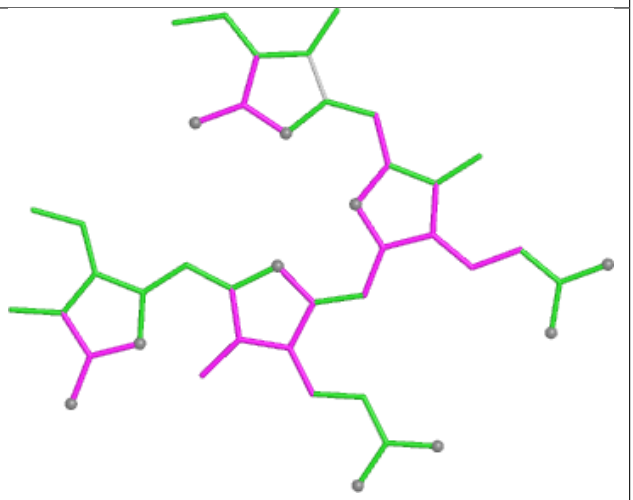


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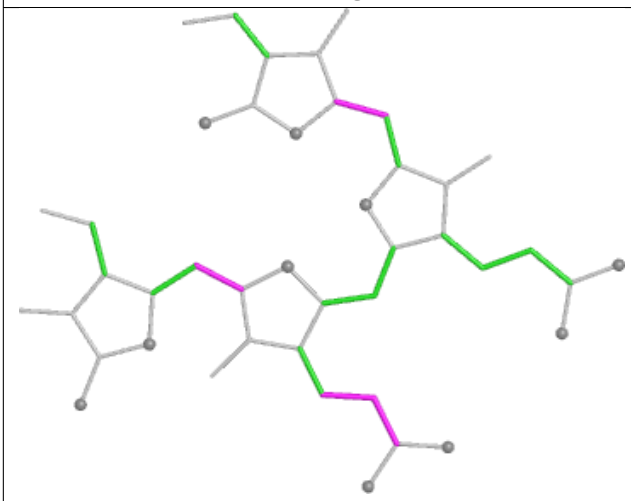
Ligand PEB Y9 203



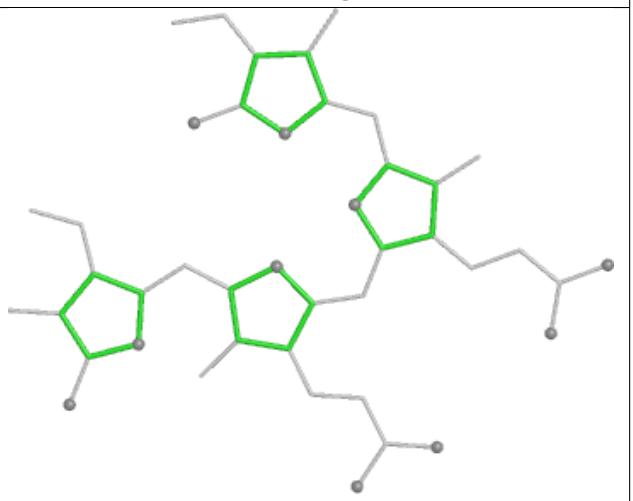
Bond lengths



Bond angles

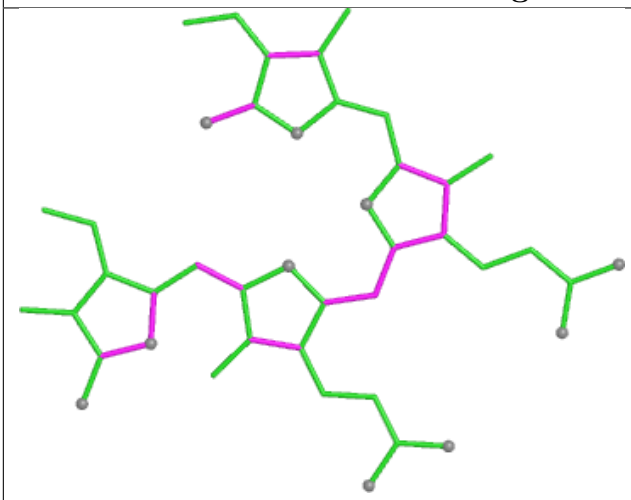


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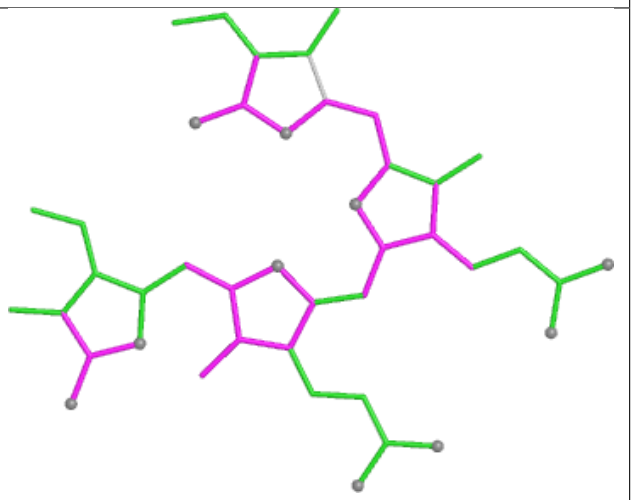


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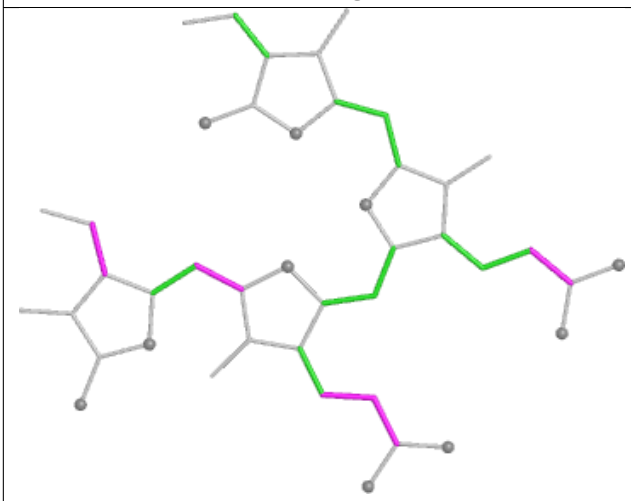
Ligand PEB AO 304



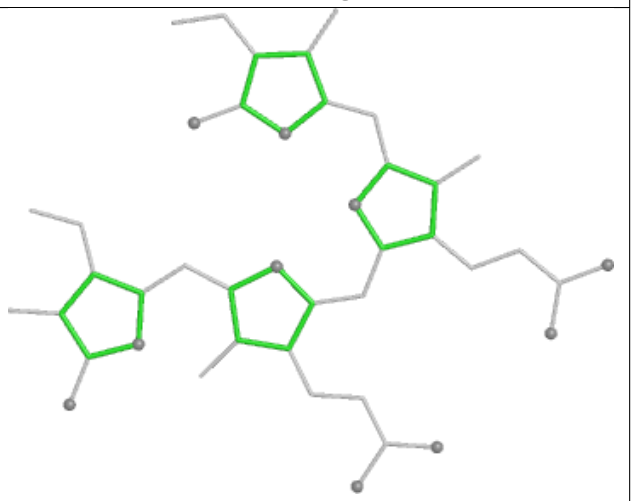
Bond lengths



Bond angles

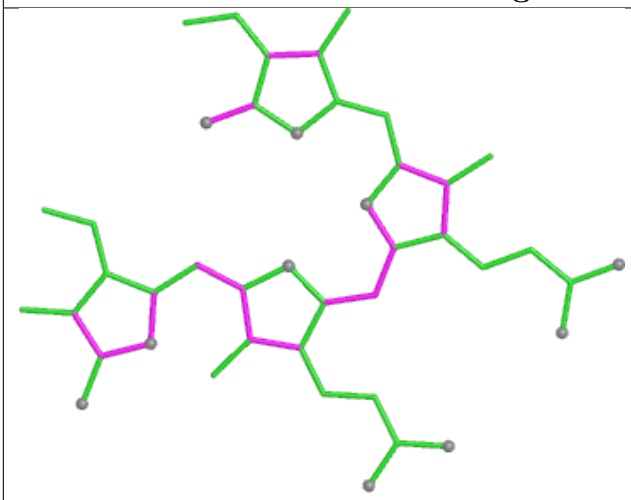


Torsions

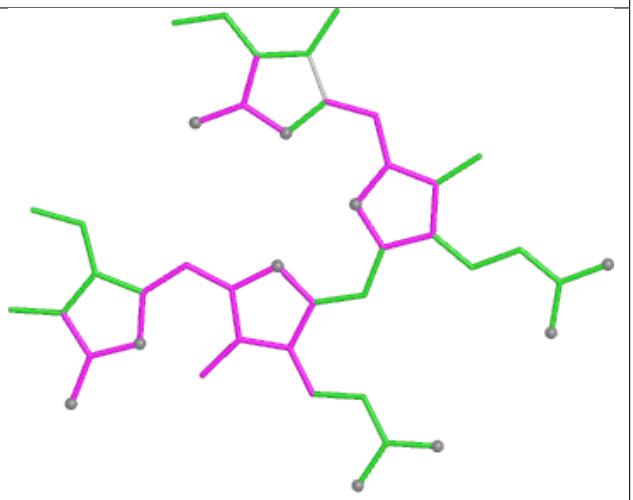


Rings

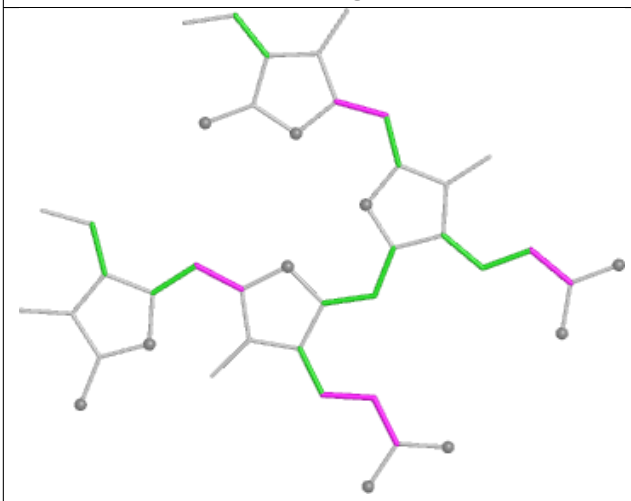
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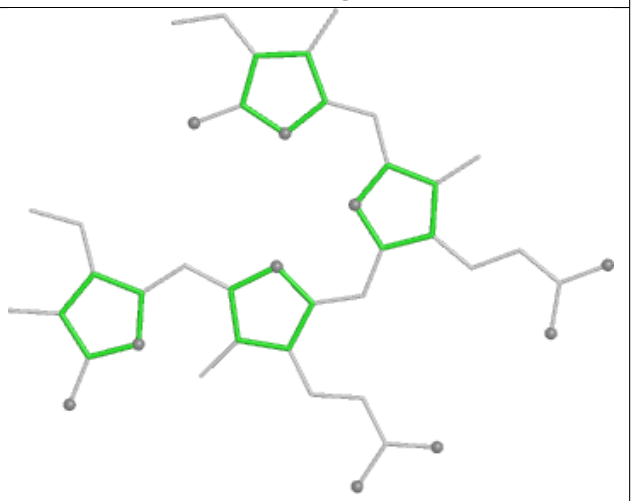
Bond lengths



Bond angles

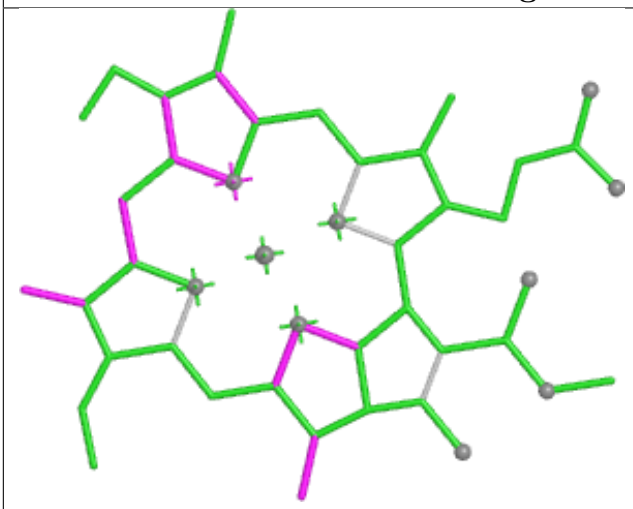


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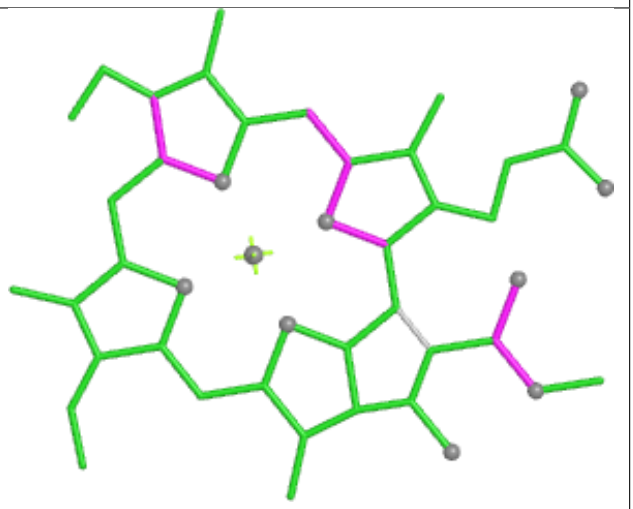


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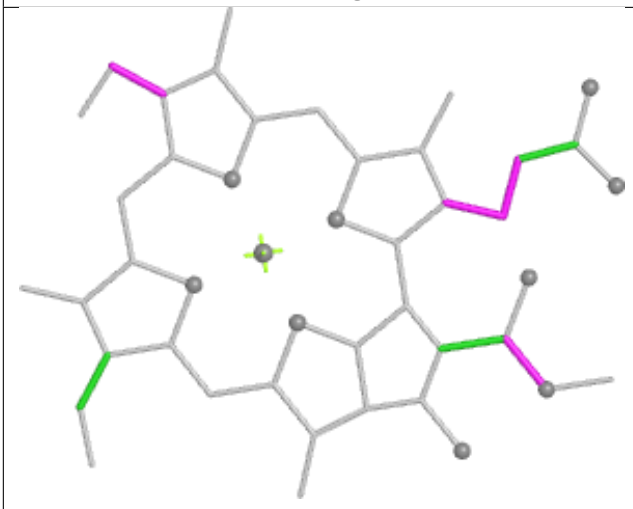
Ligand CLA 42 611



Bond lengths



Bond angles

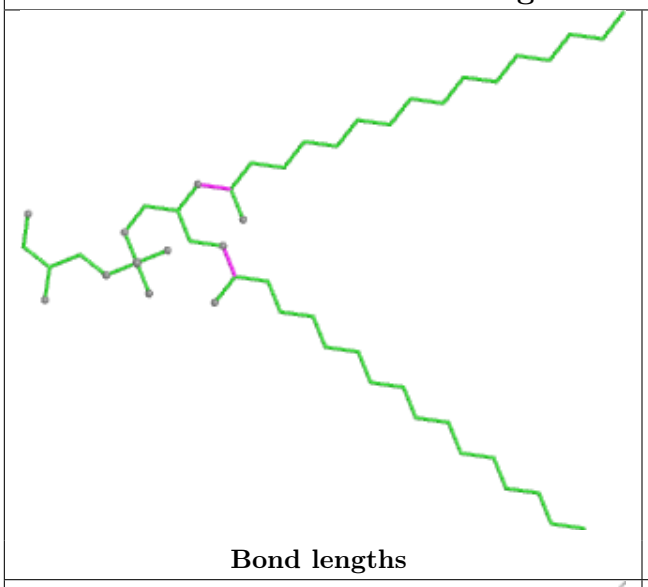


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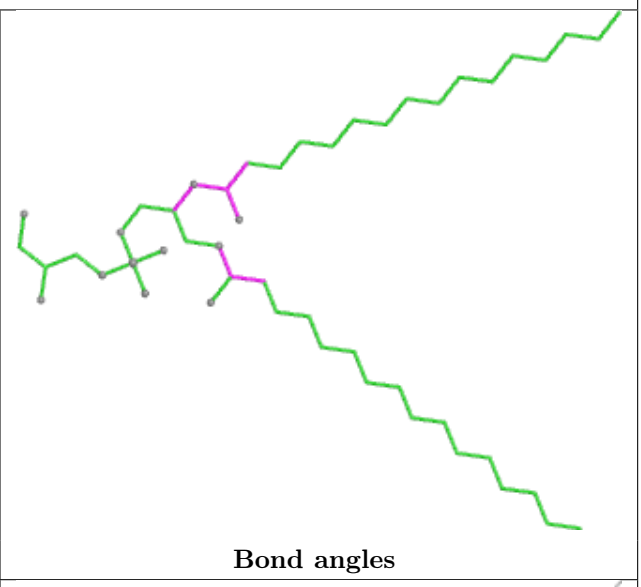


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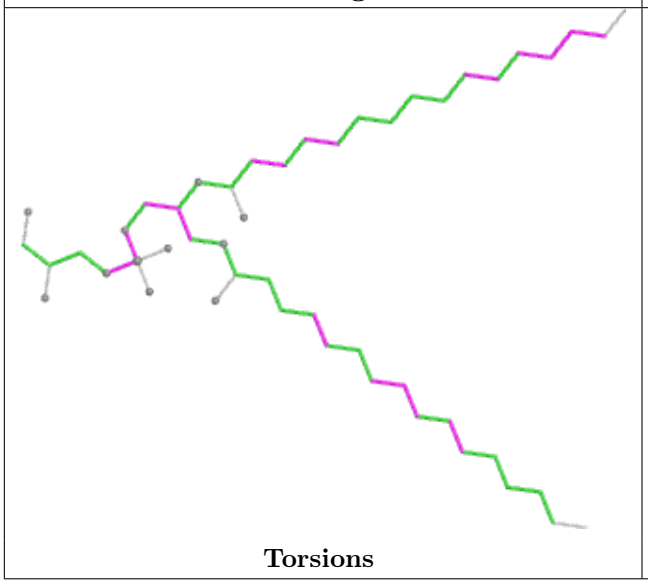
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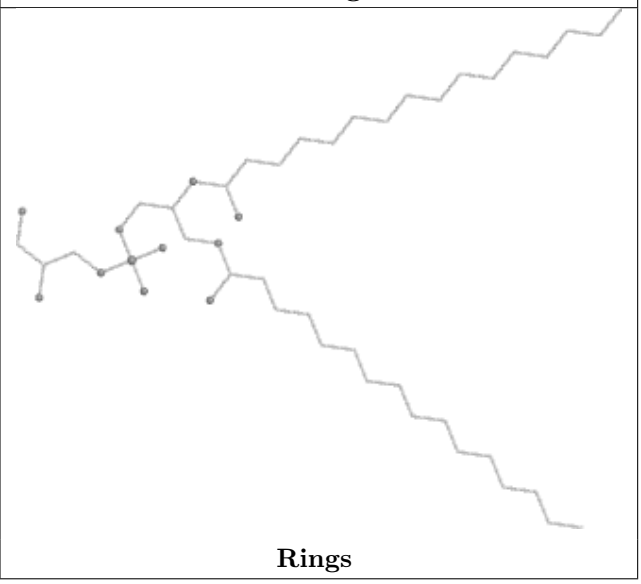
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Bond angles

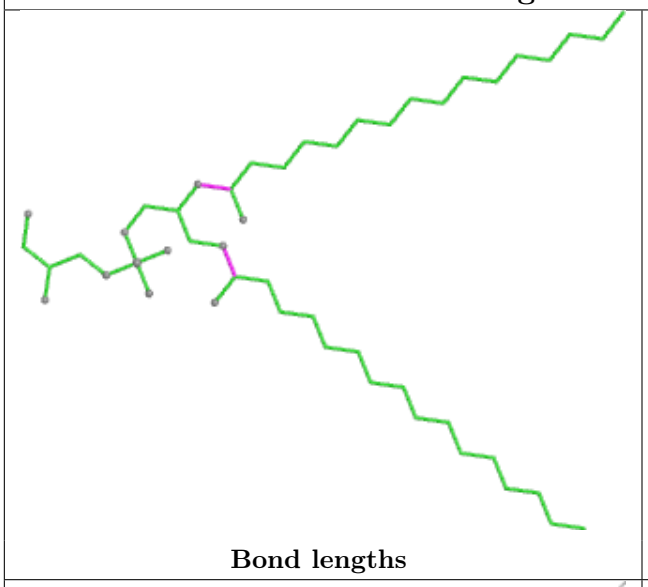


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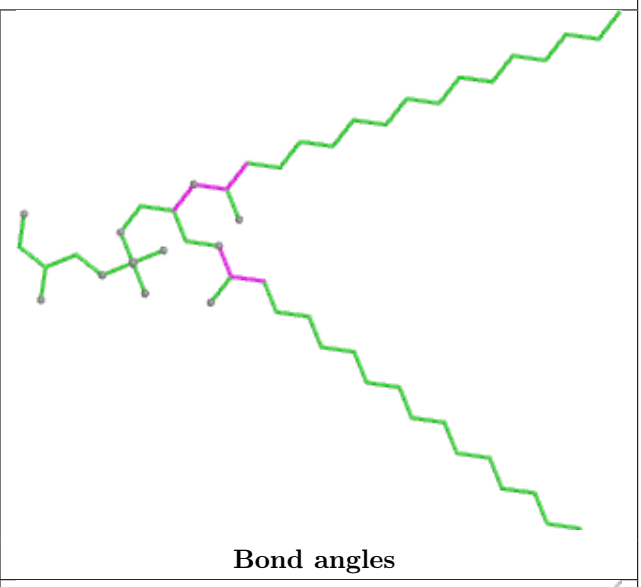


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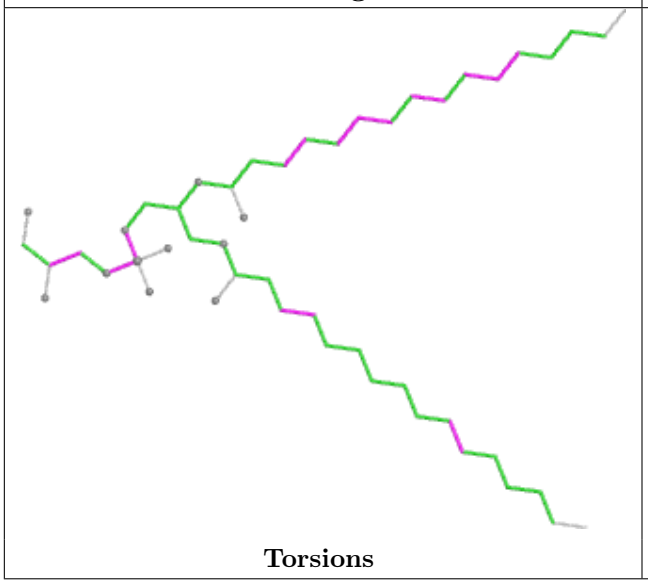
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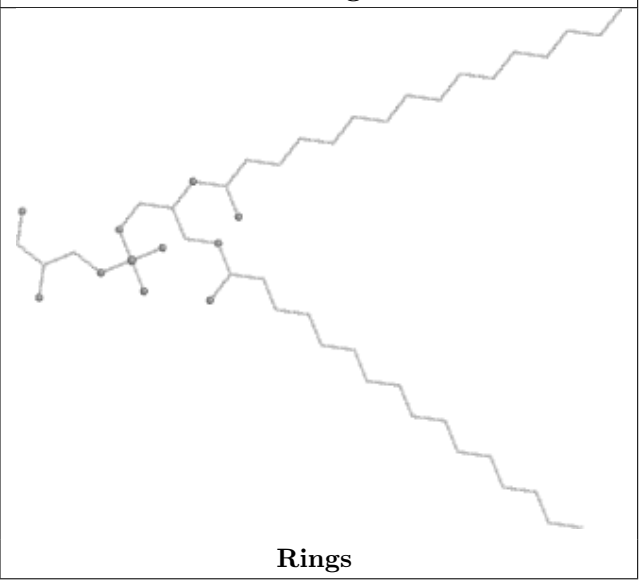
Bond lengths



Bond angles

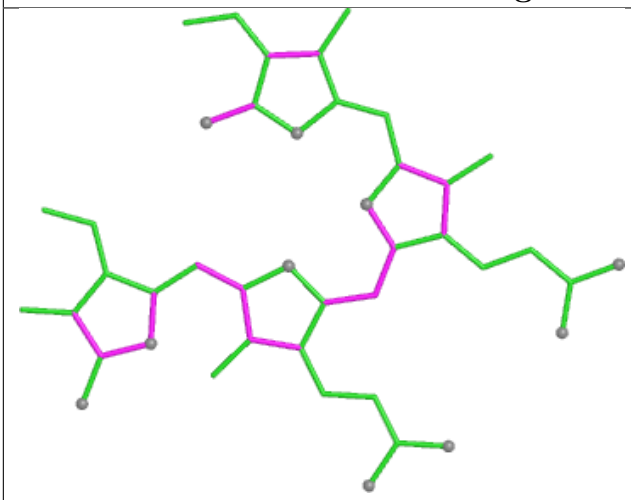


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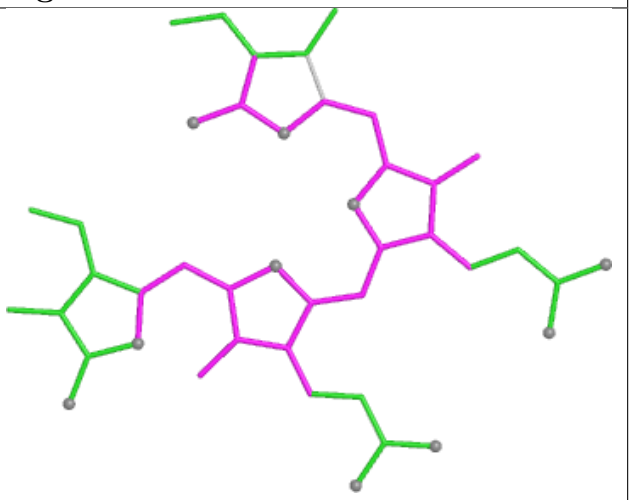


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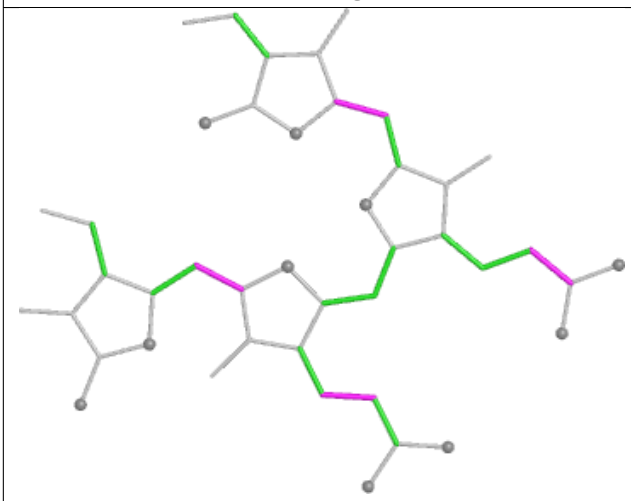
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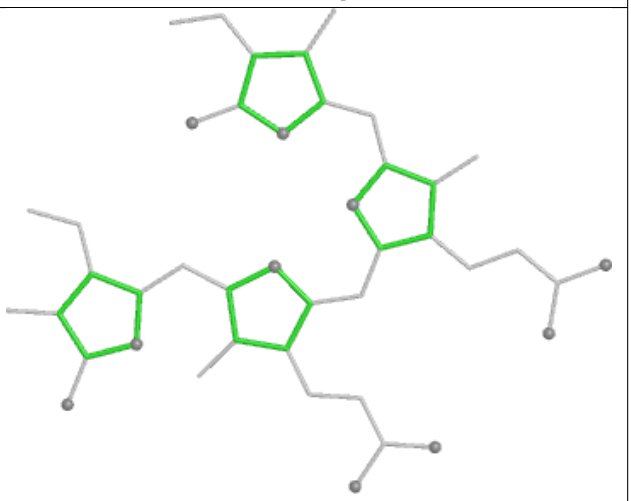
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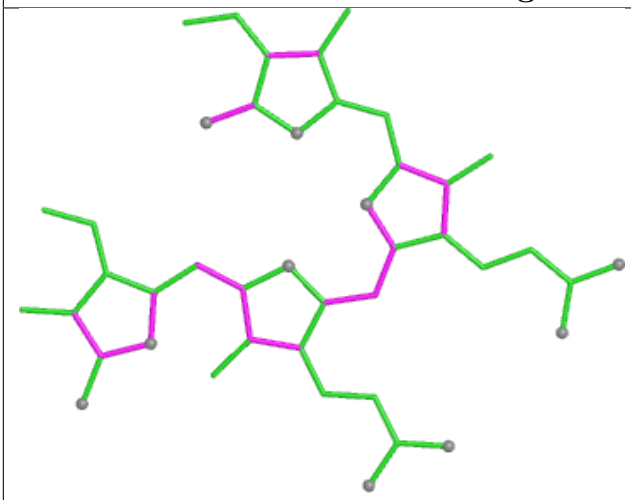


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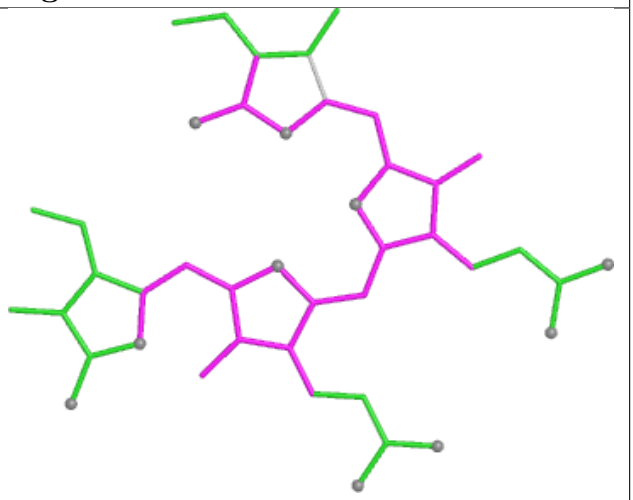


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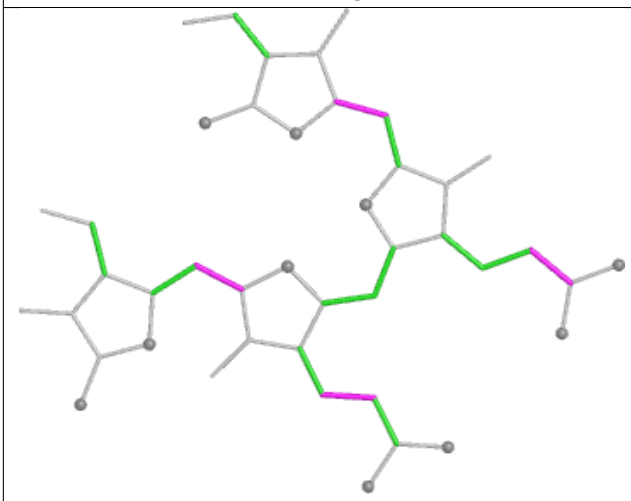
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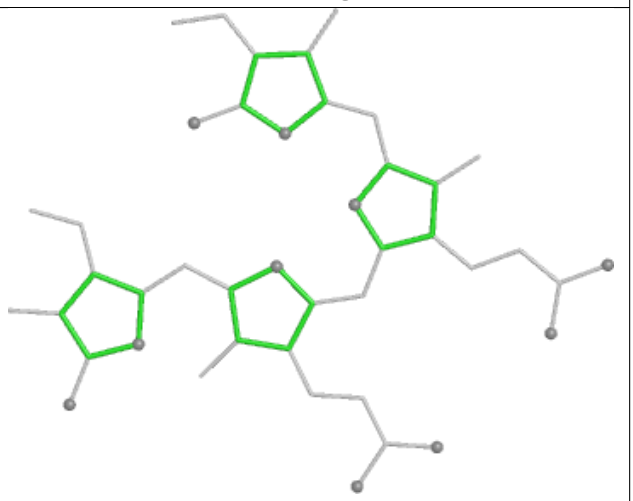
Bond lengths



Bond angles

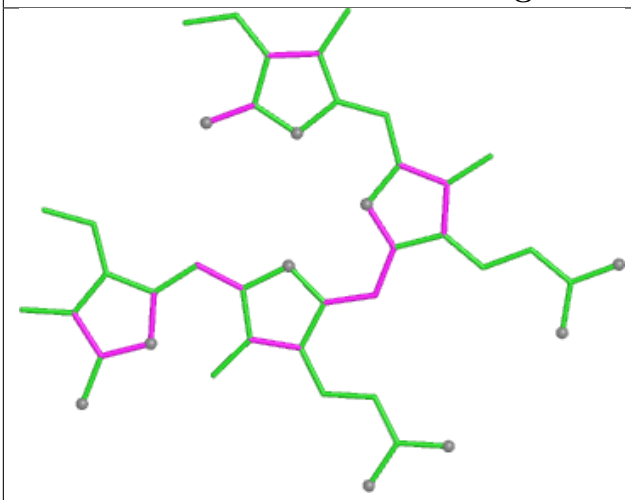


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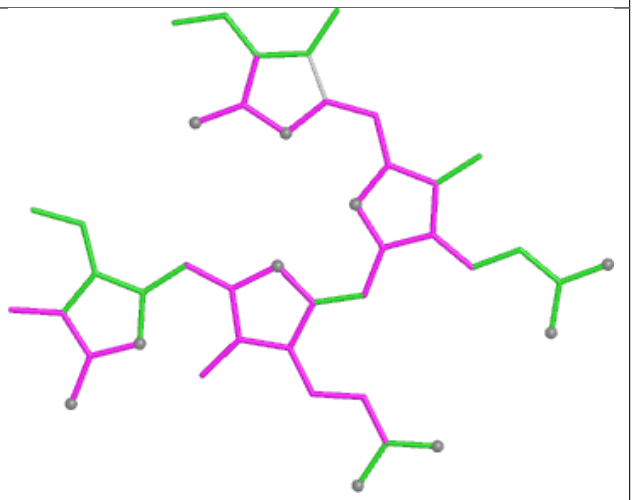


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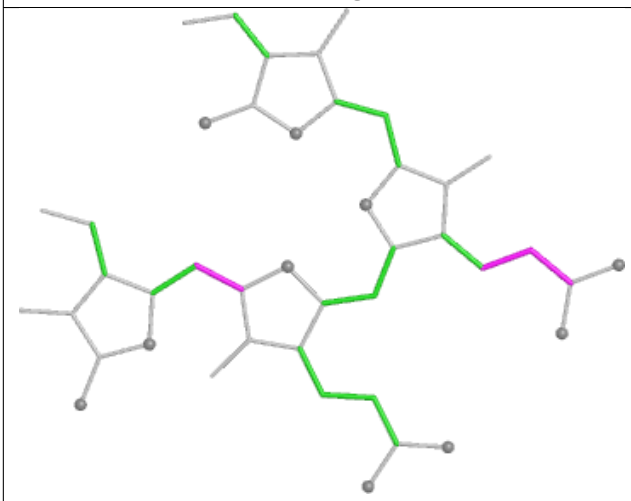
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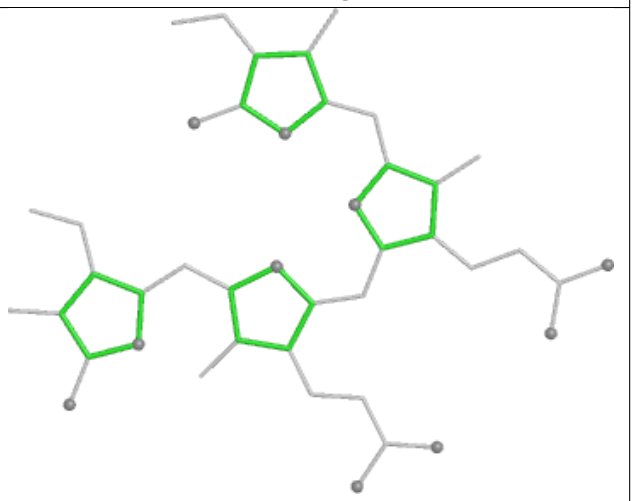
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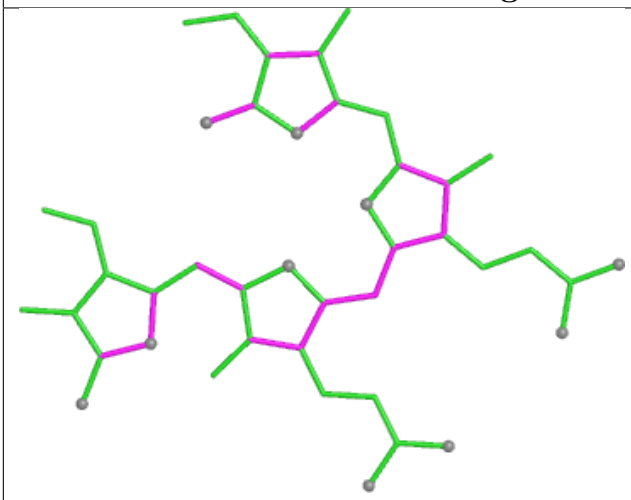


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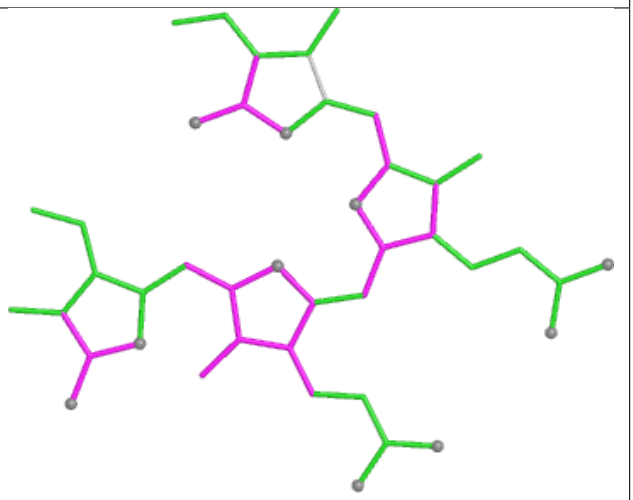


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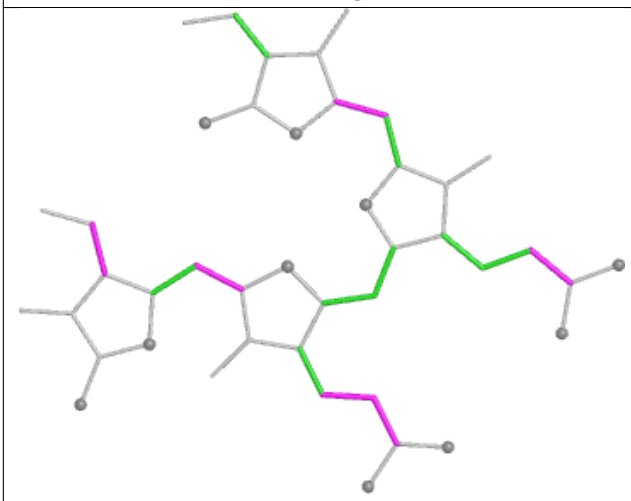
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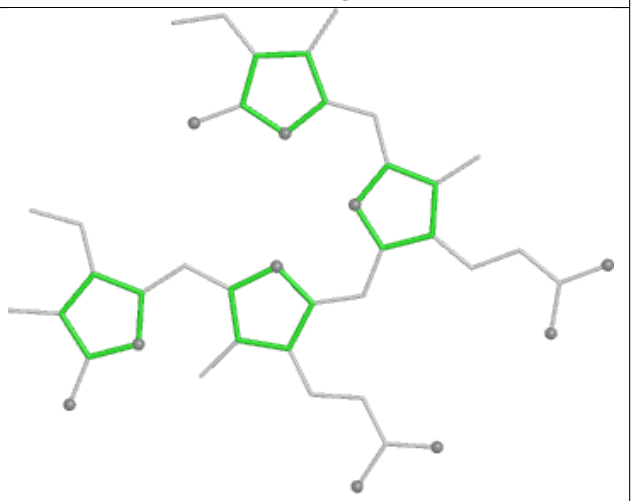
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Bond angles

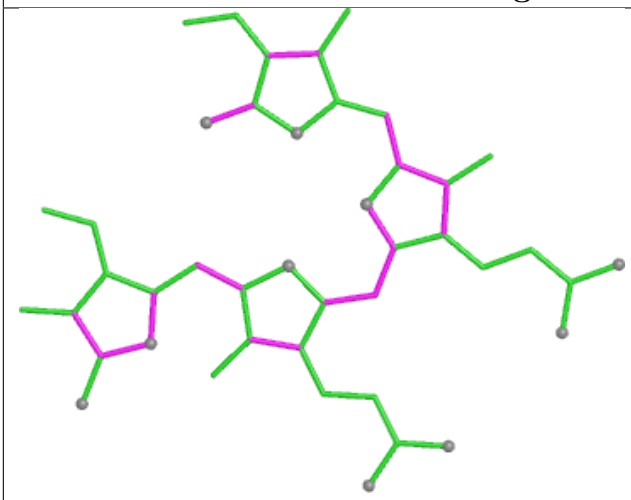


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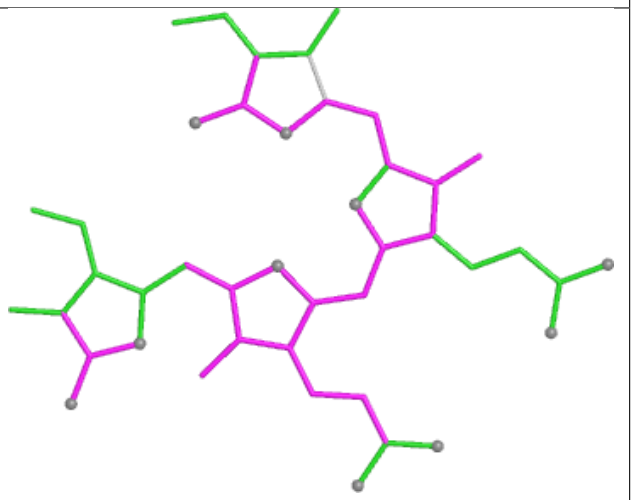


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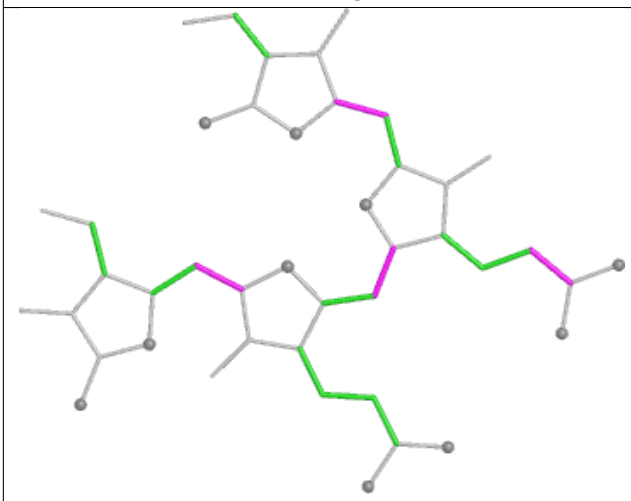
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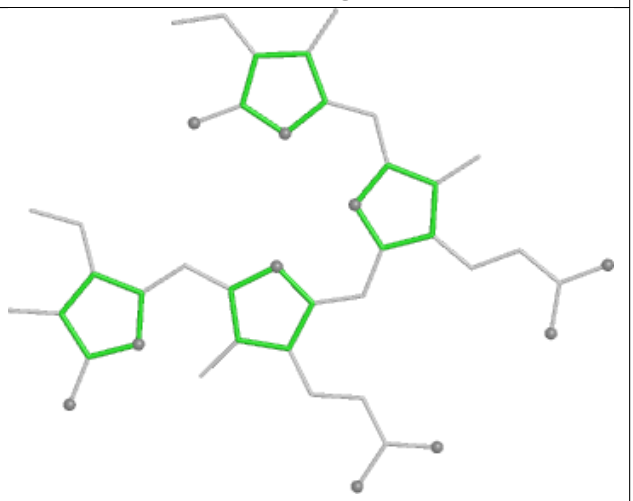
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Bond angles

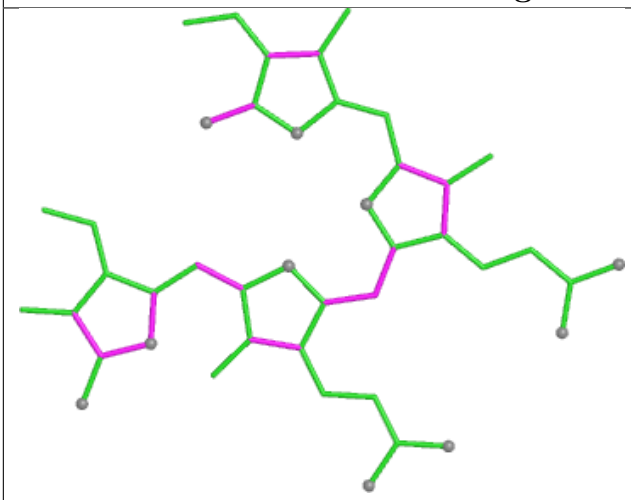


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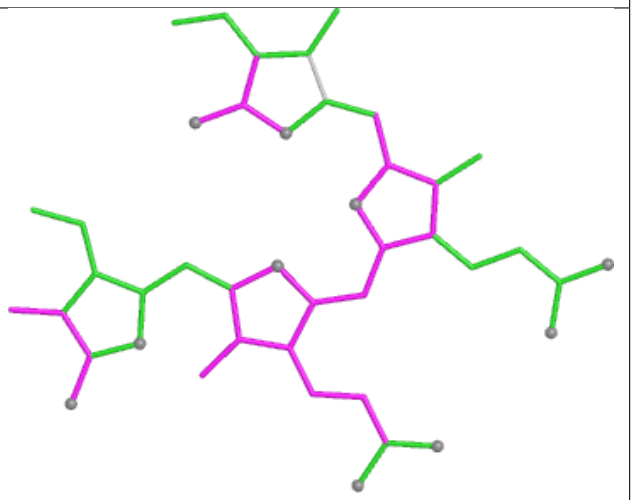


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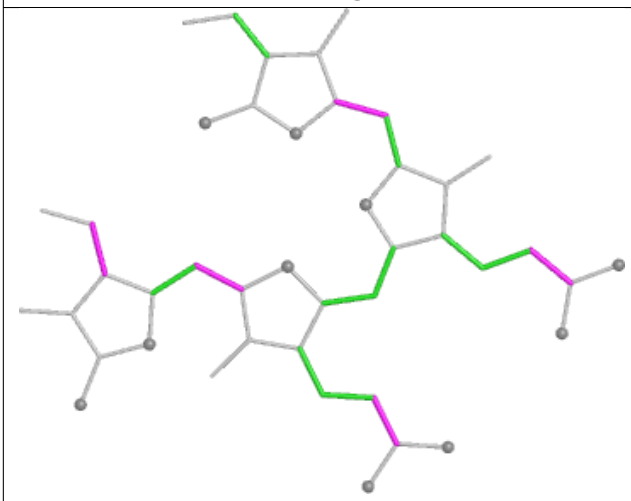
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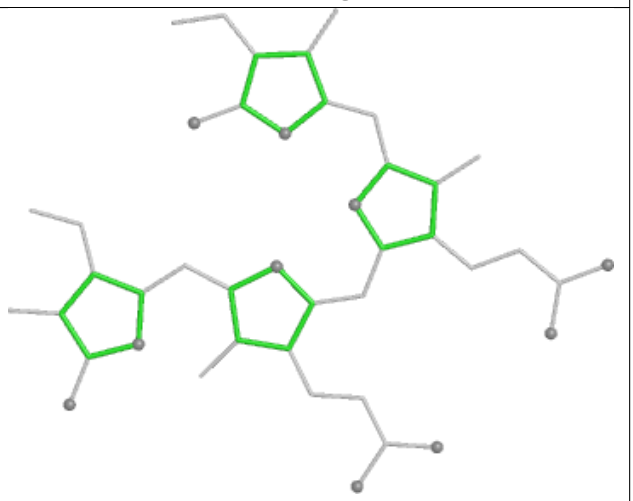
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Bond angles

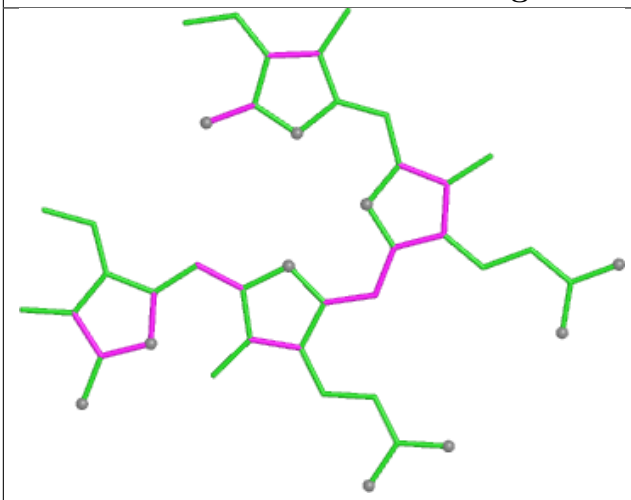


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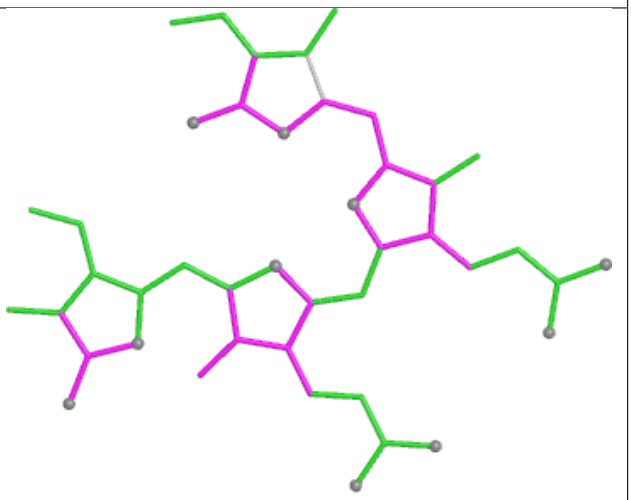


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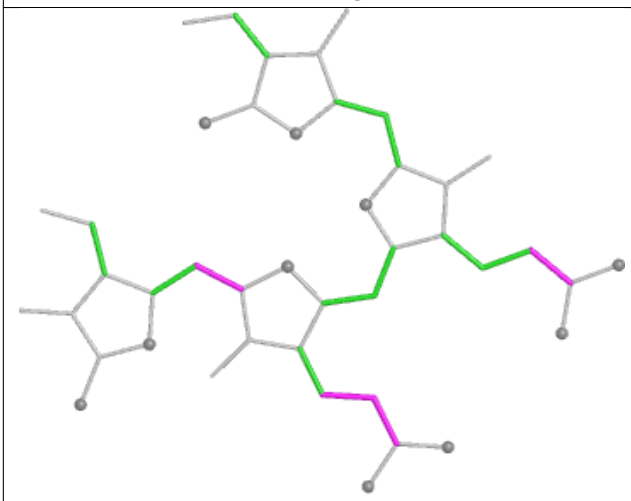
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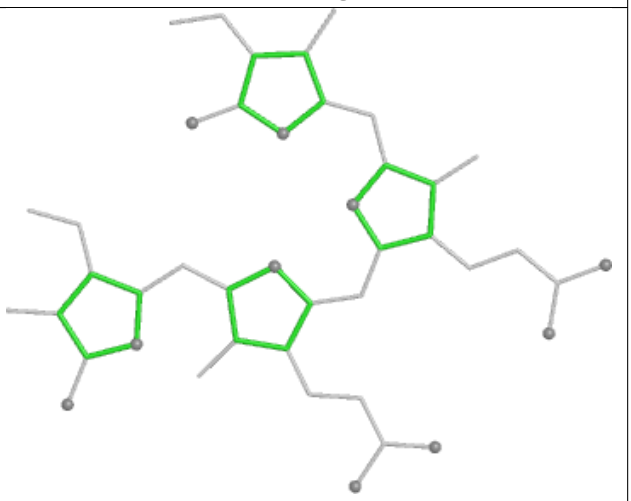
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Bond angles

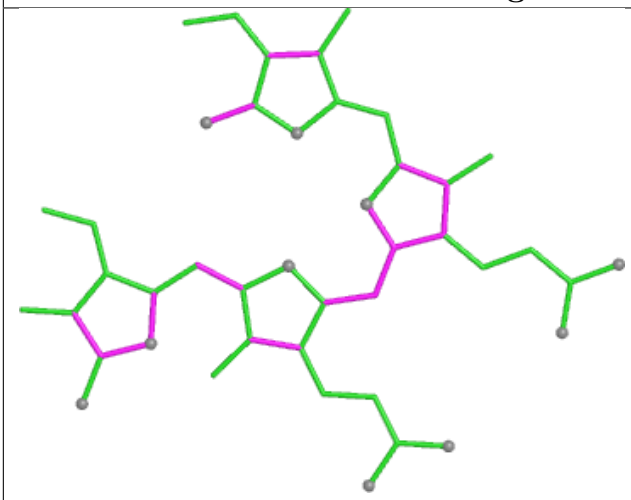


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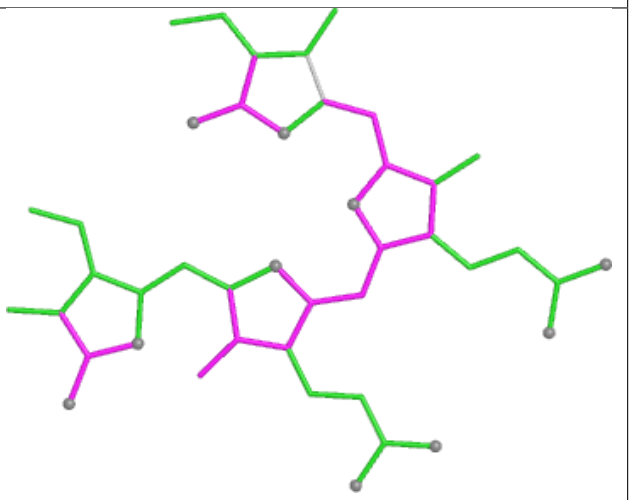


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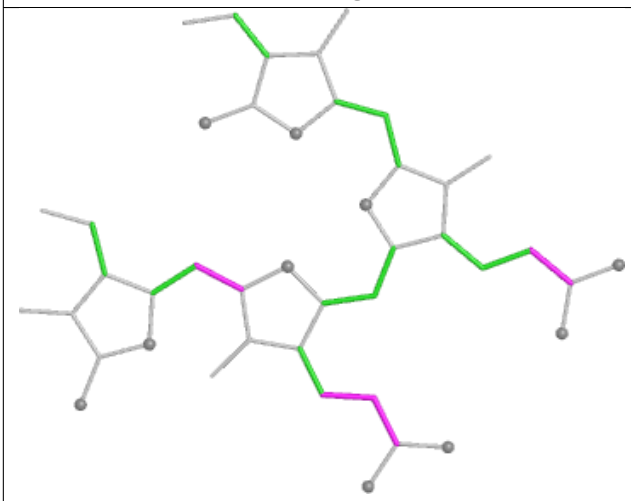
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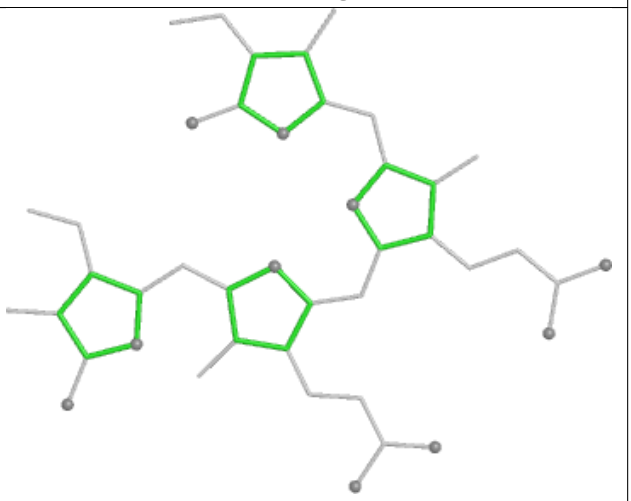
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Bond angles

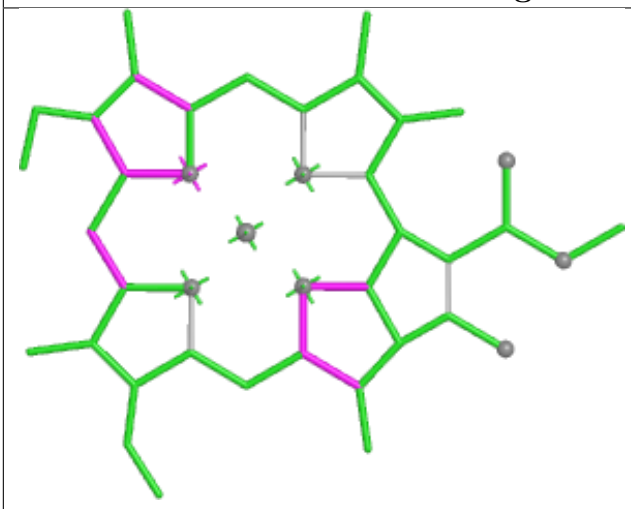


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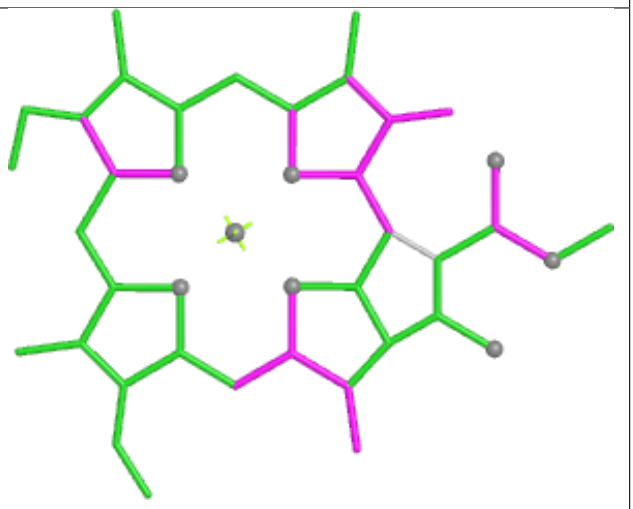


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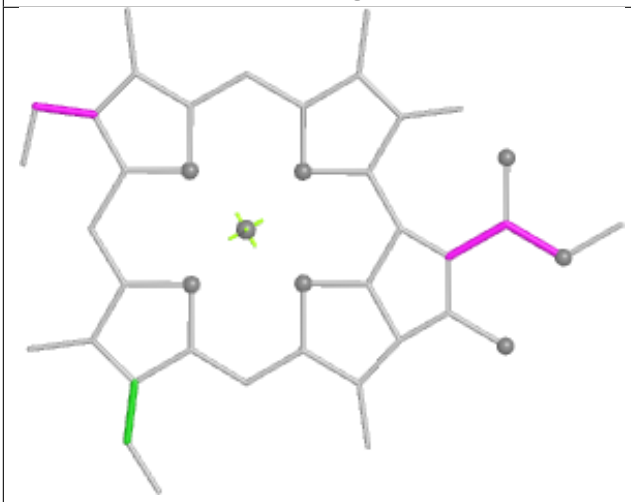
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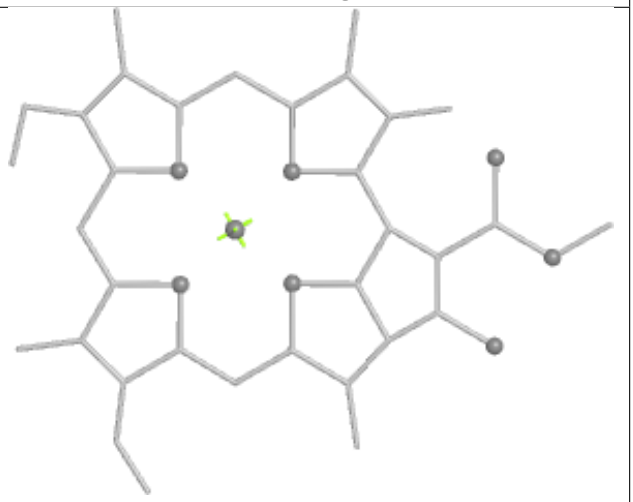
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Bond angles

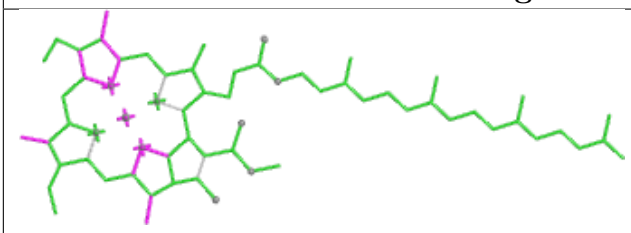


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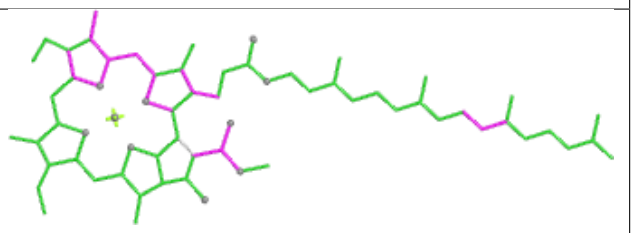


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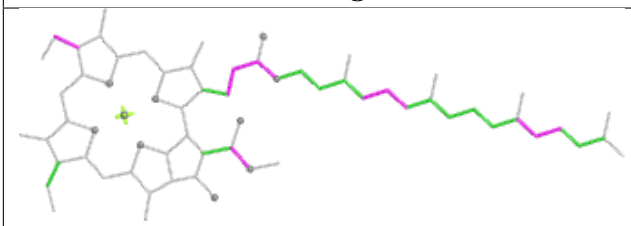
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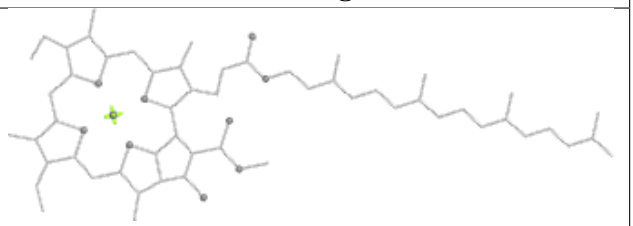
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Bond angles

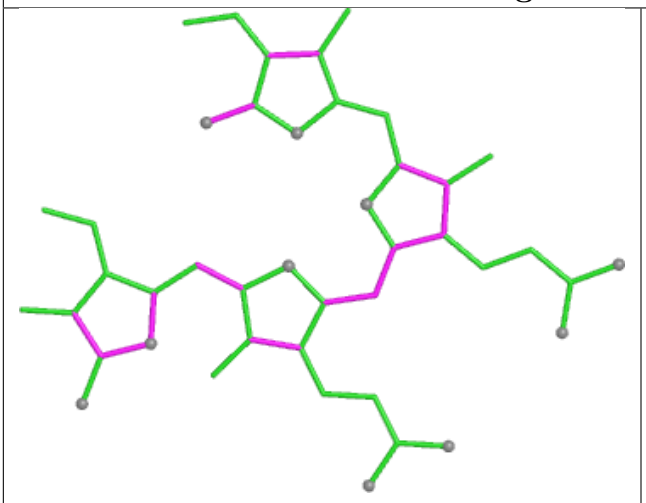


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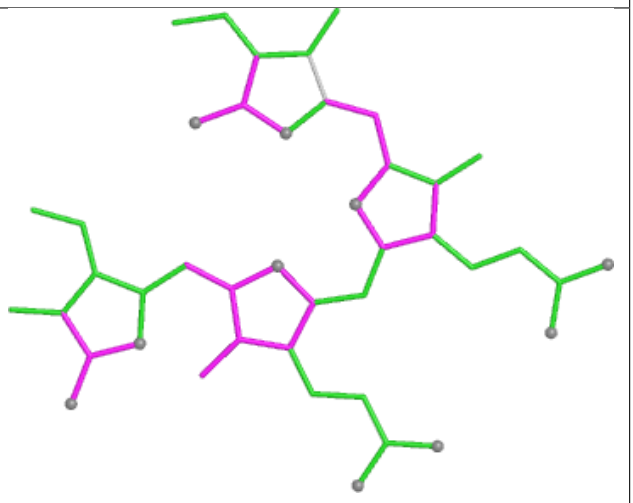


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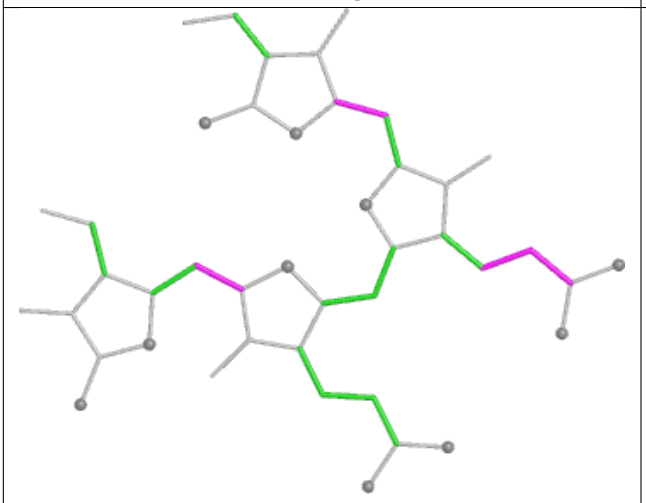
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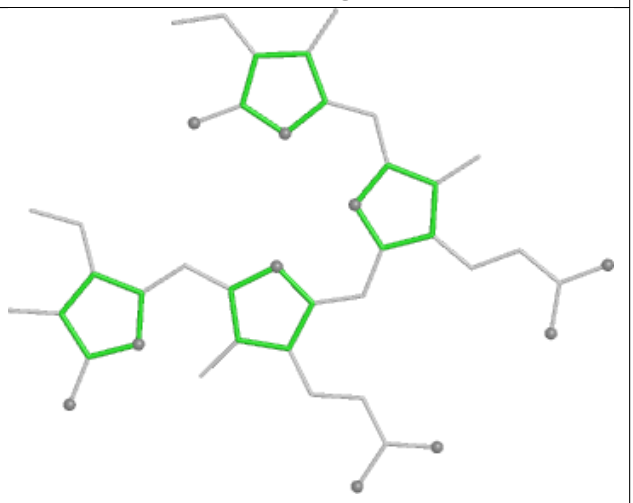
Bond lengths



Bond angles

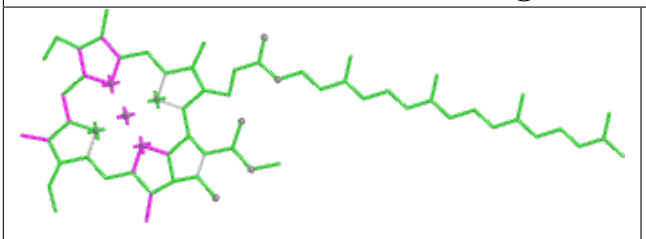


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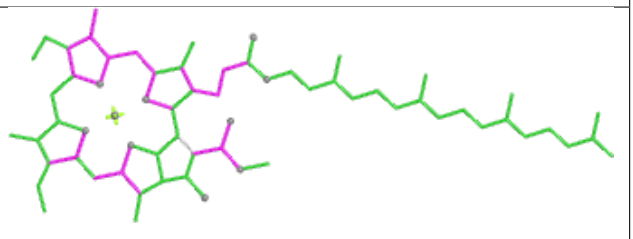


Rings

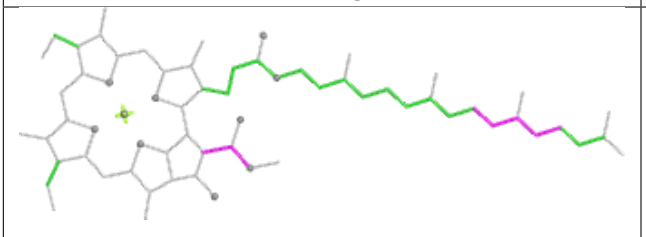
Ligand CLA B2 823



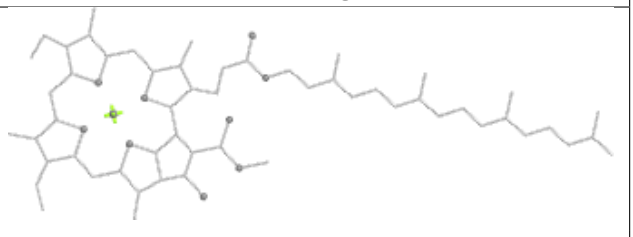
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Bond angles

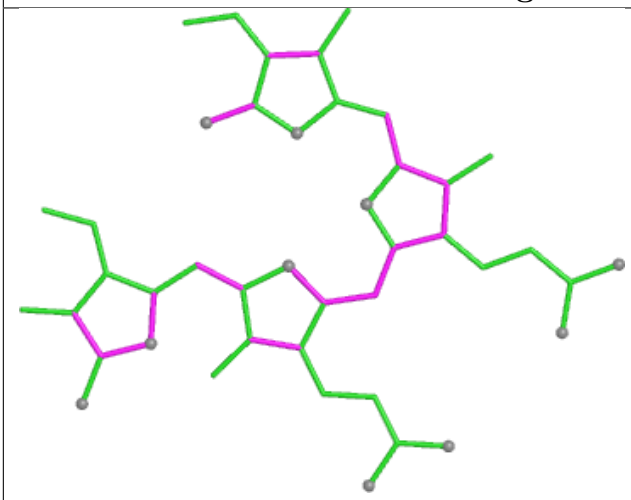


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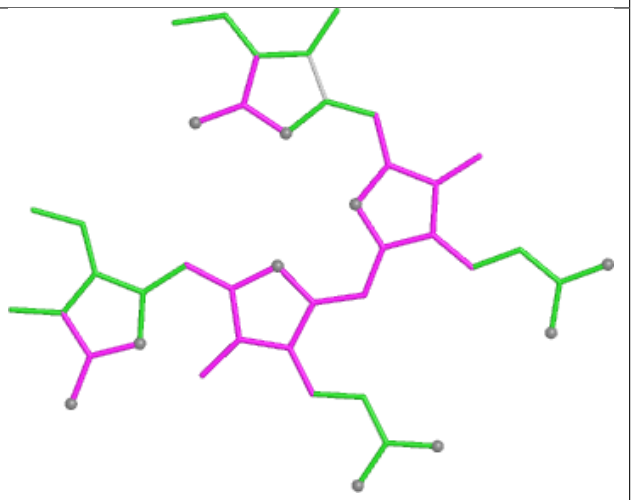


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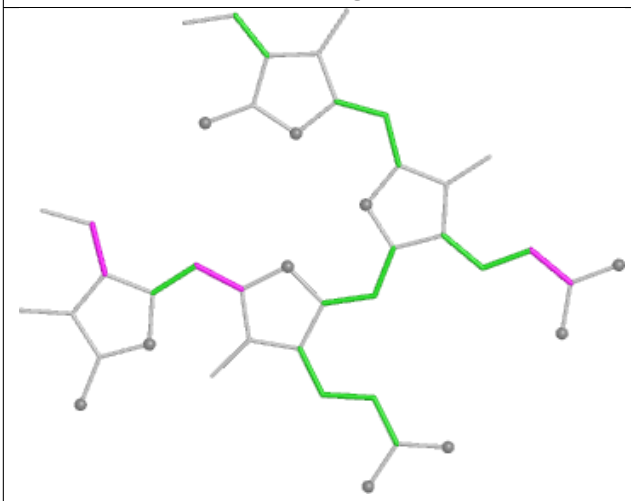
Ligand PEB T4 202



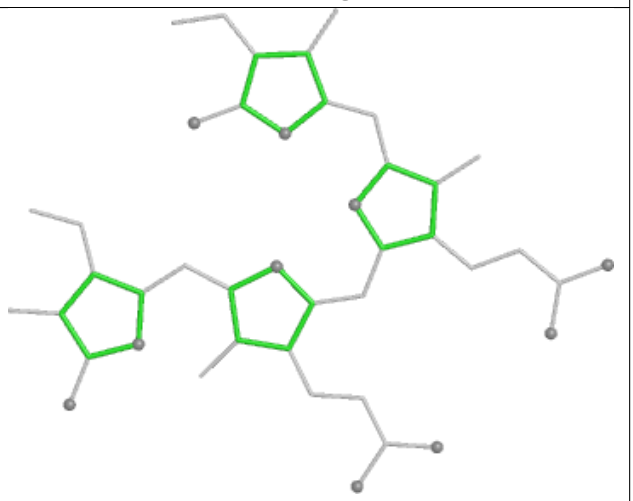
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Bond angles

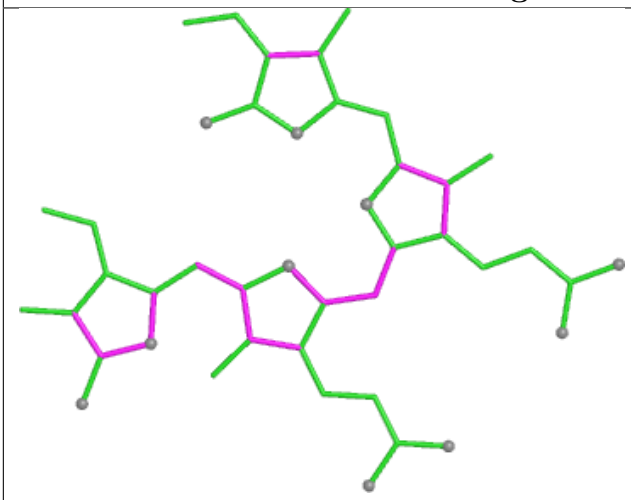


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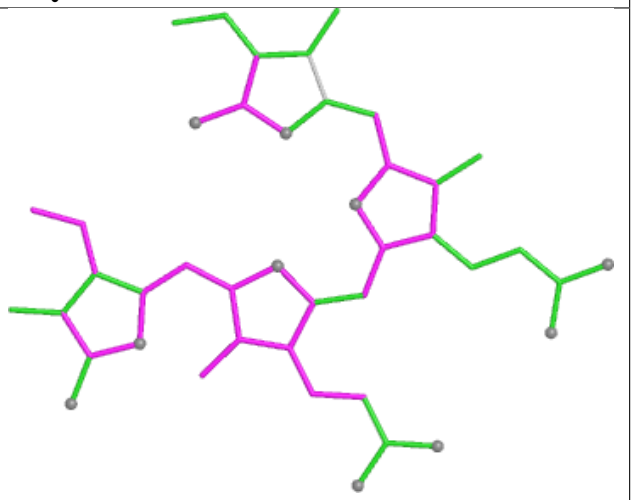


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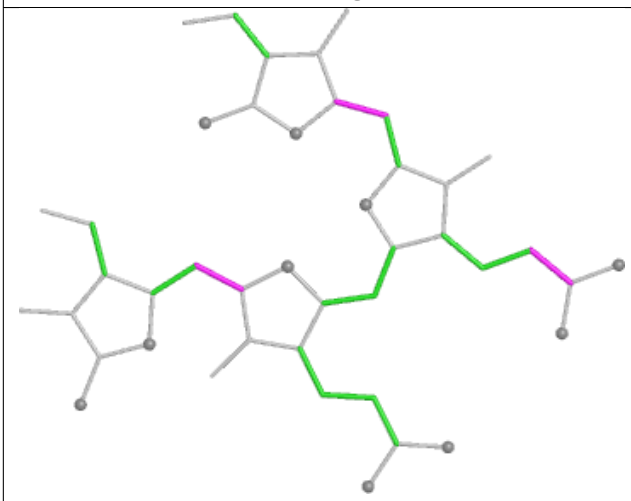
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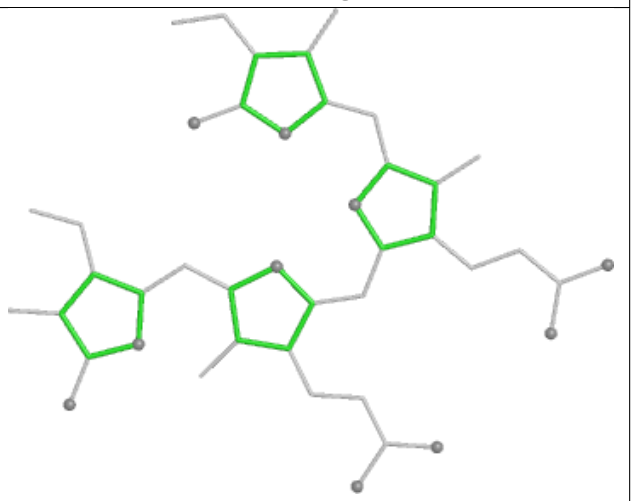
Bond lengths



Bond angles

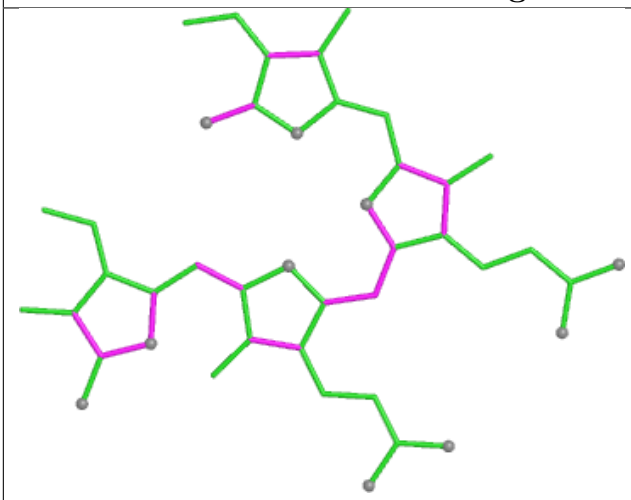


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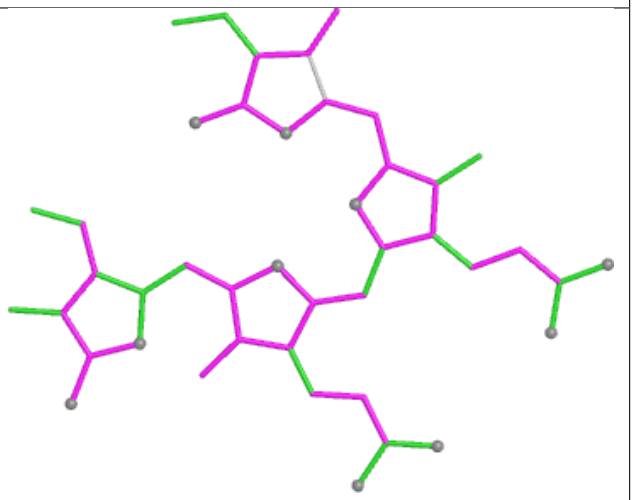


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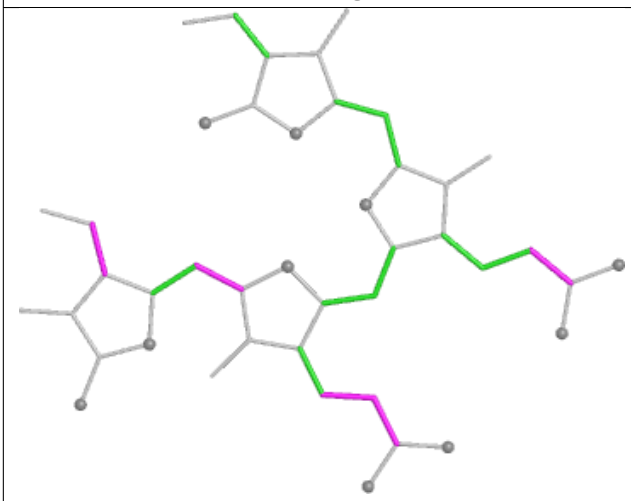
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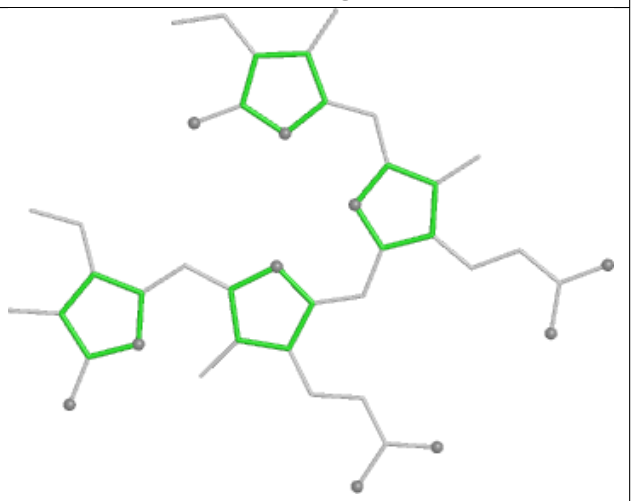
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Bond angles

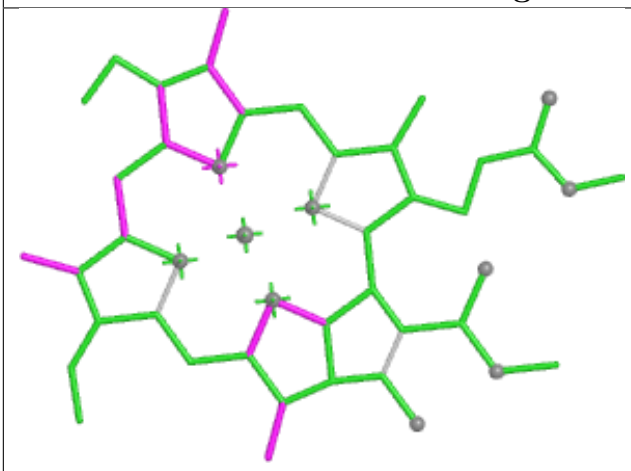


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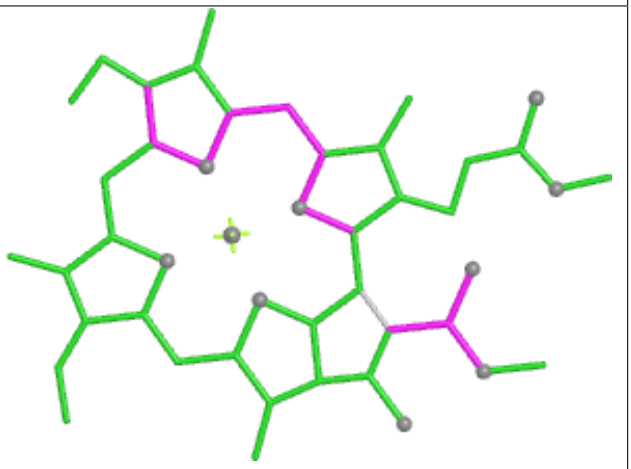


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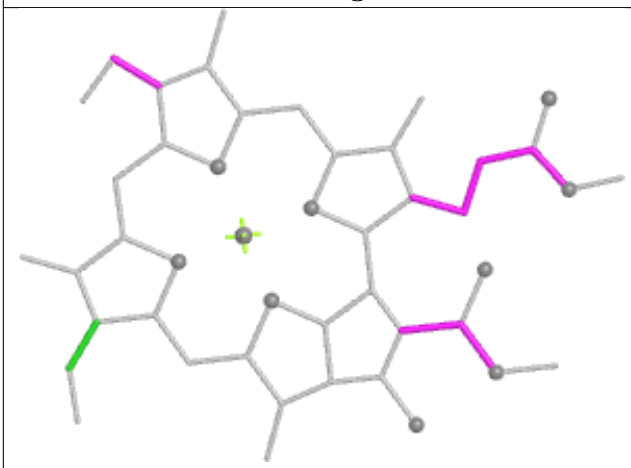
Ligand CLA CL 518



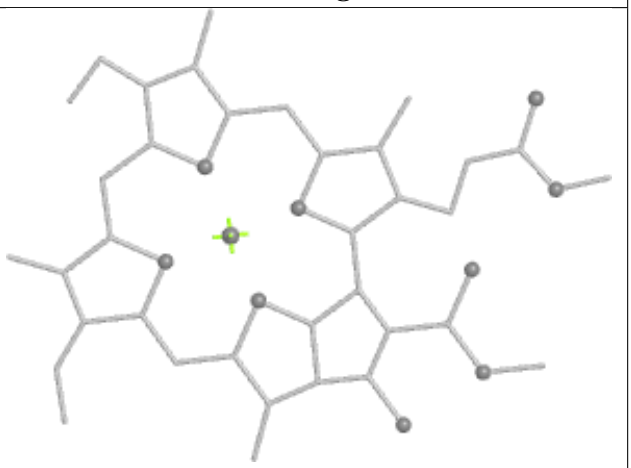
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Bond angles

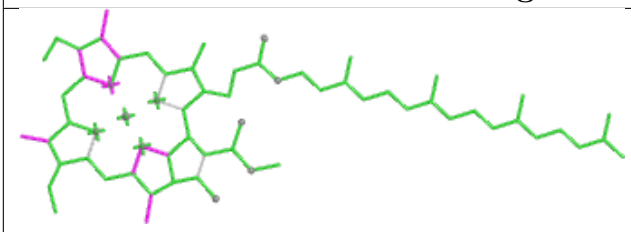


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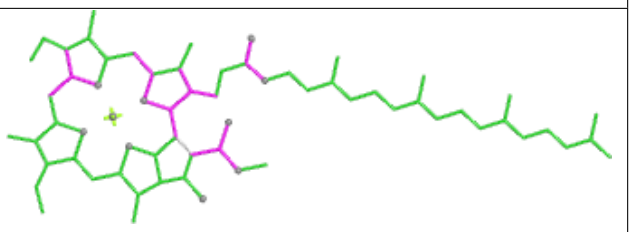


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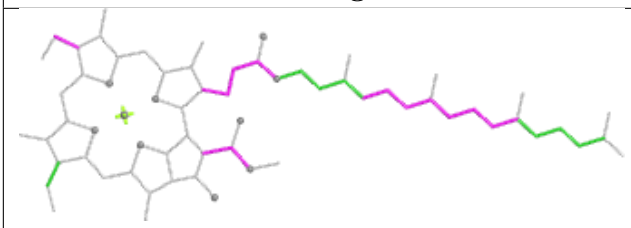
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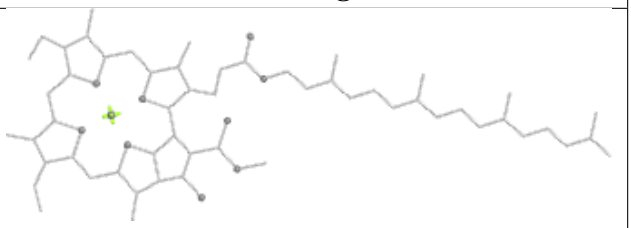
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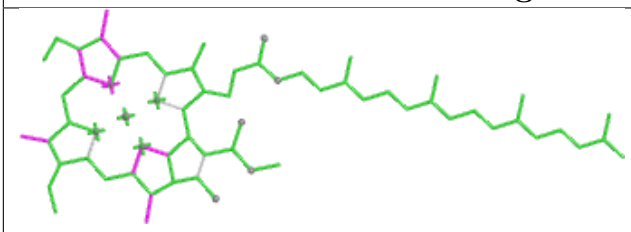


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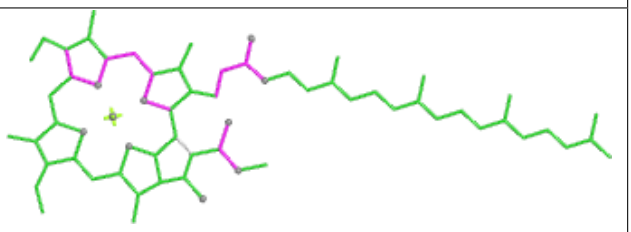


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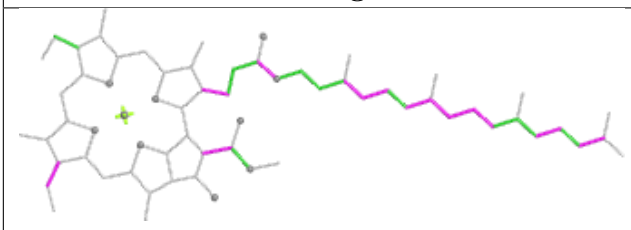
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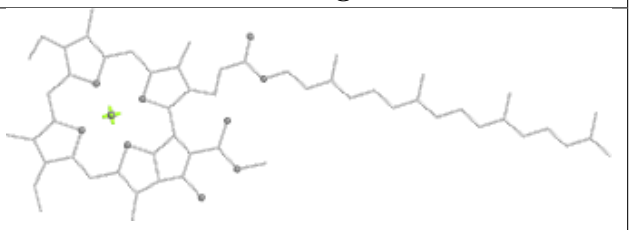
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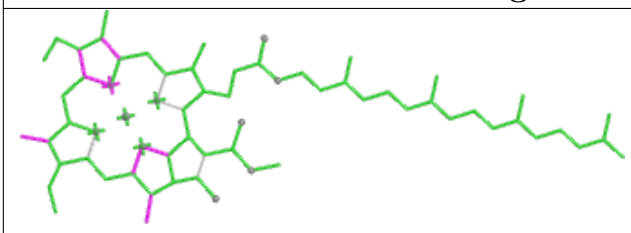


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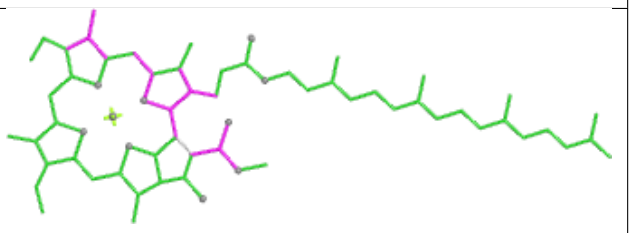


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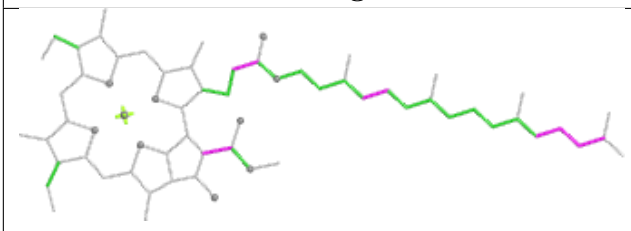
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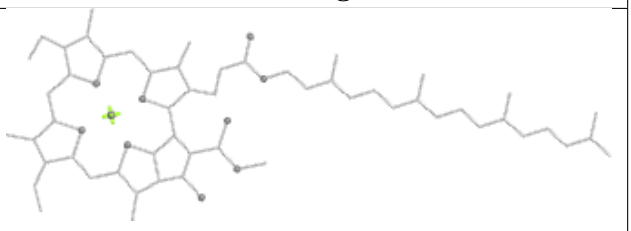
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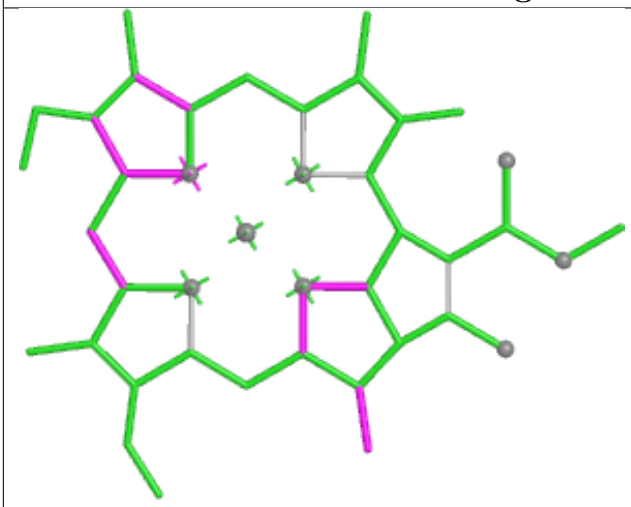


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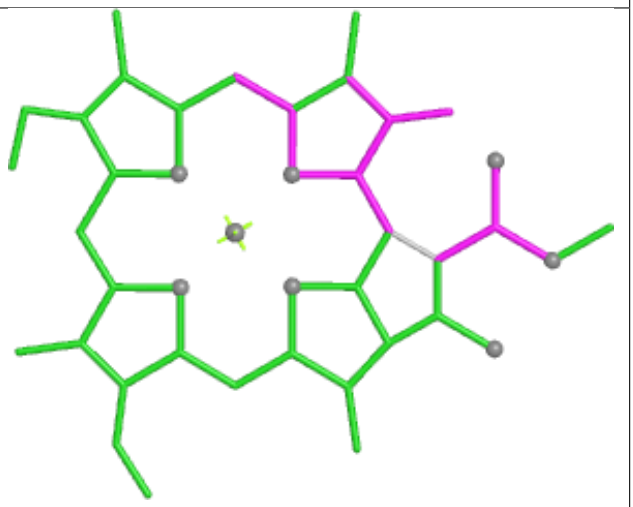


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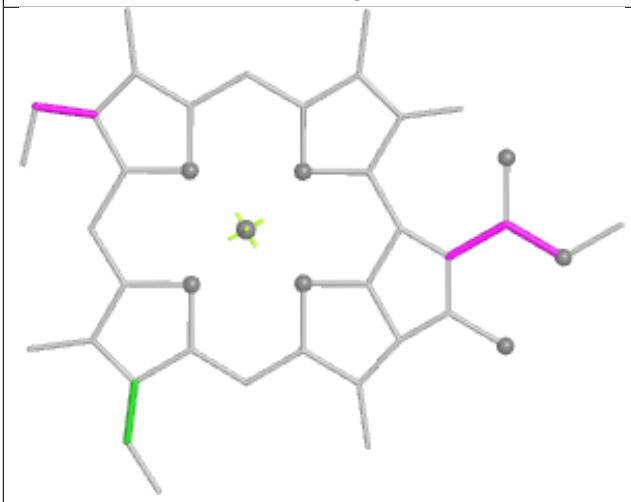
Ligand CLA O2 201



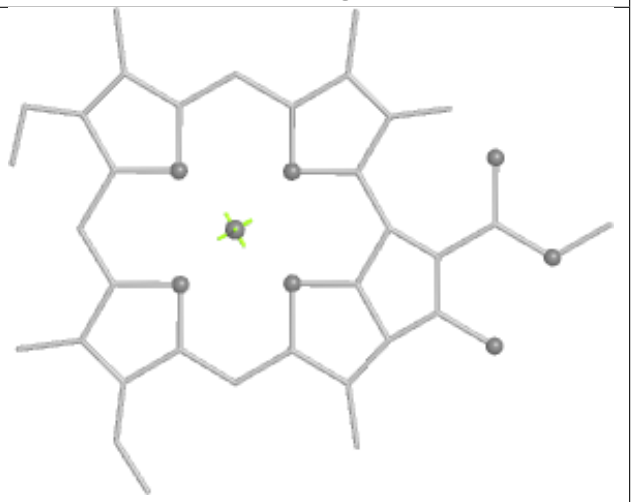
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Bond angles

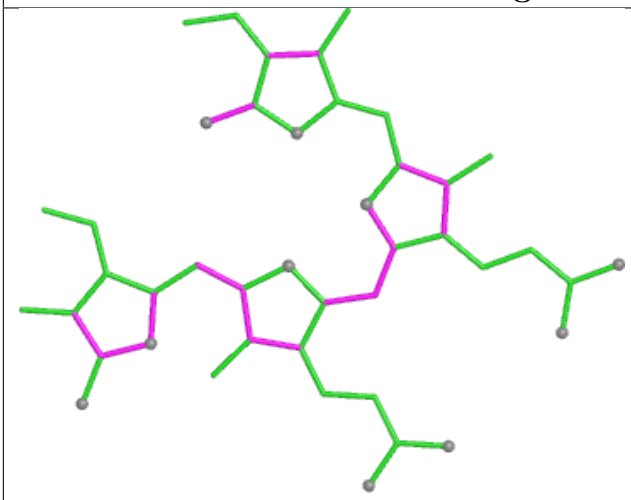


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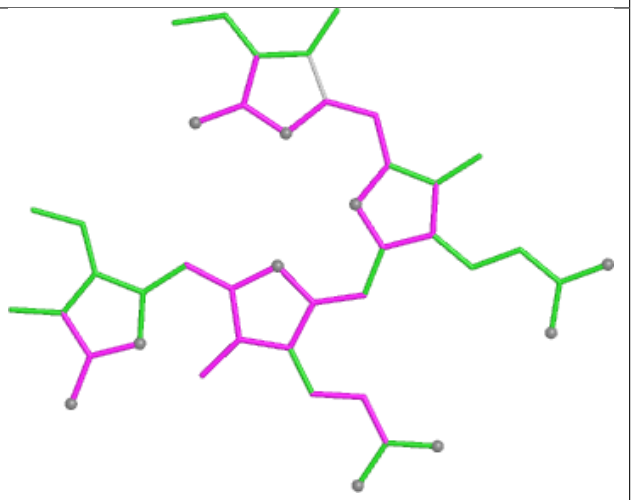


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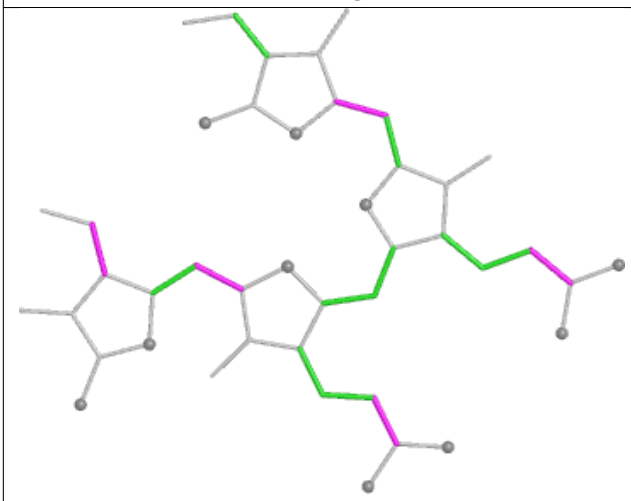
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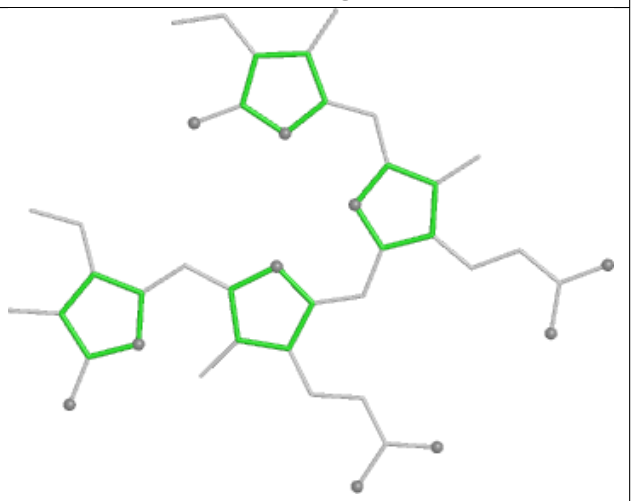
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Bond angles

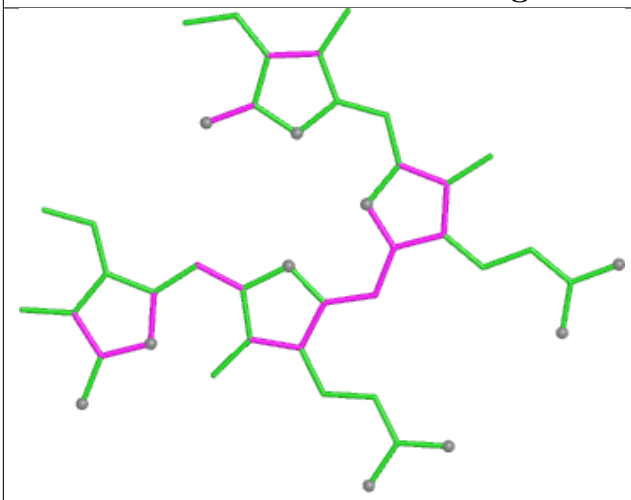


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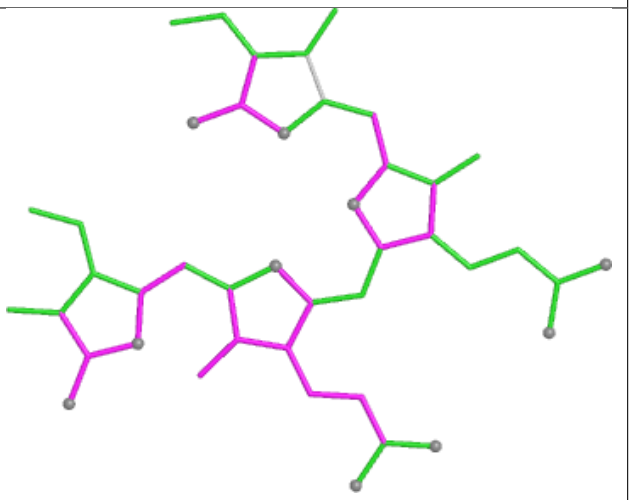


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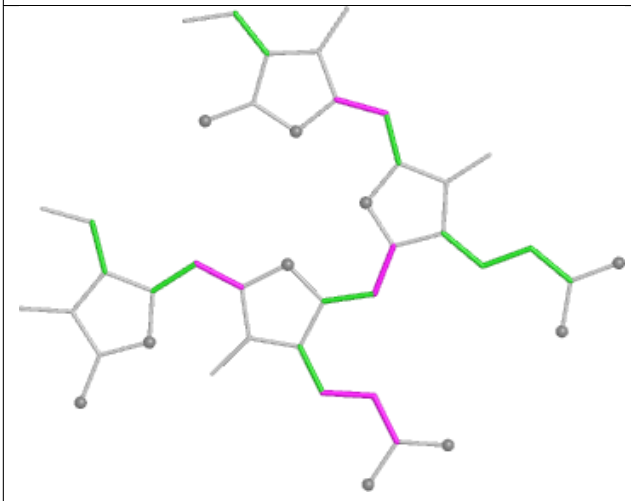
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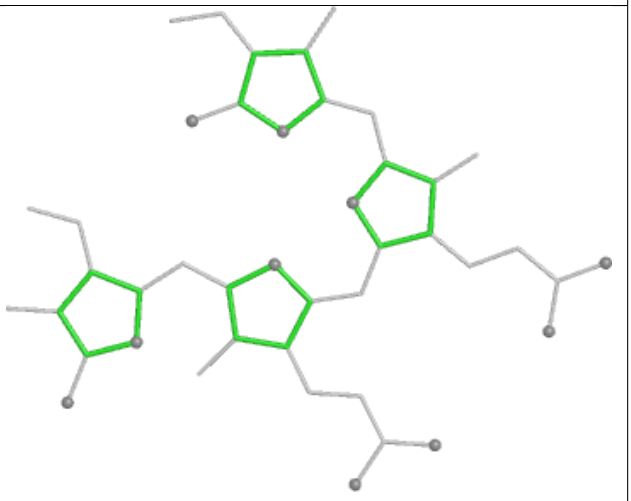
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Bond angles

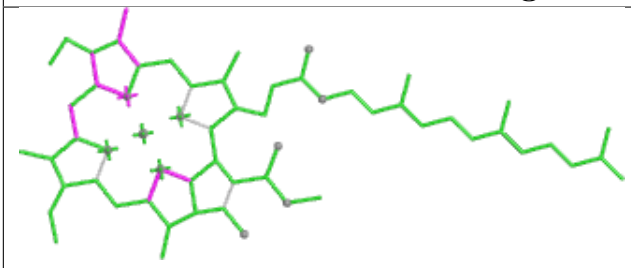


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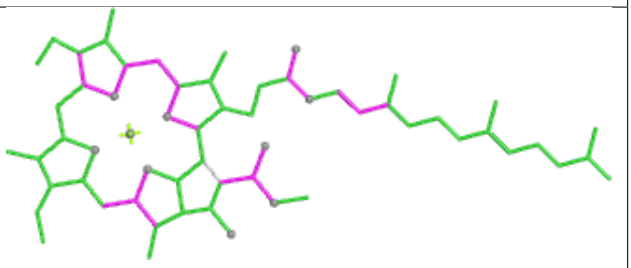


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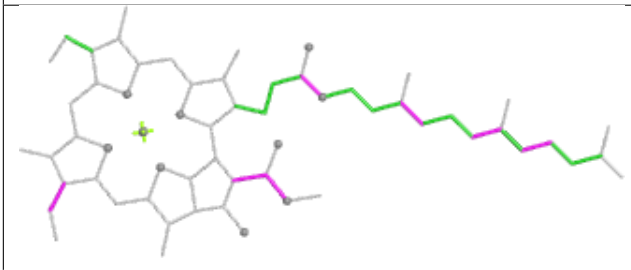
Ligand CLA c6 614



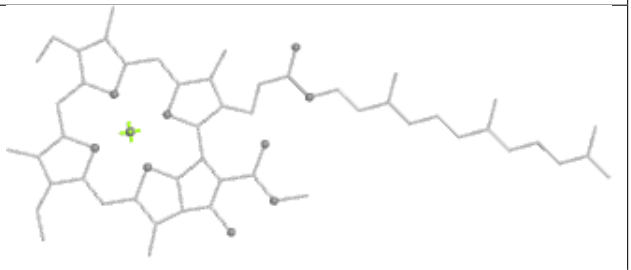
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Bond angles

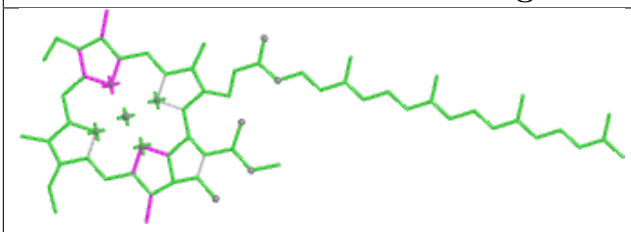


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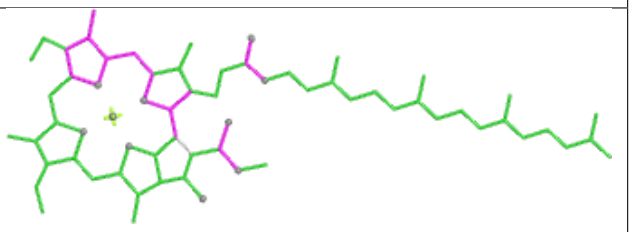


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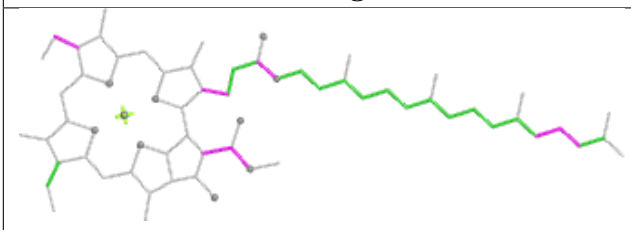
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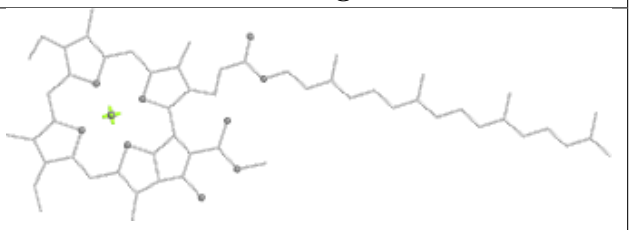
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Bond angles

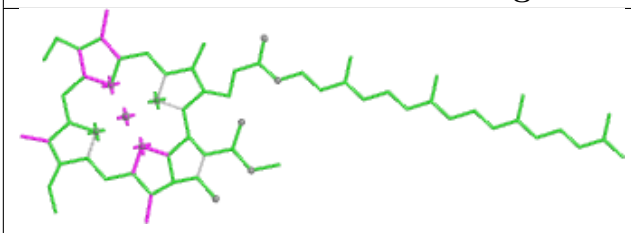


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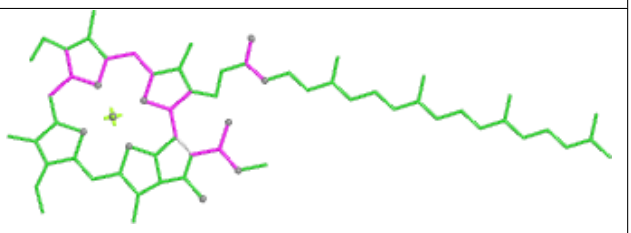


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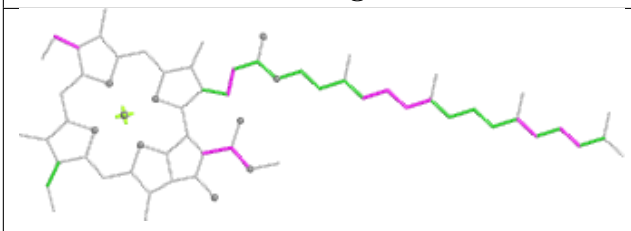
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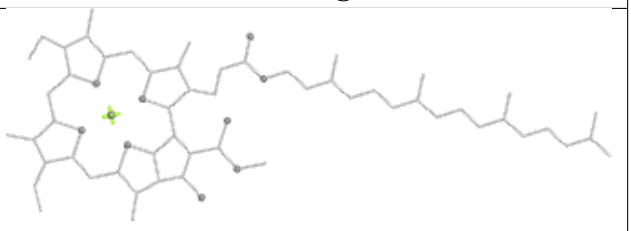
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Bond angles

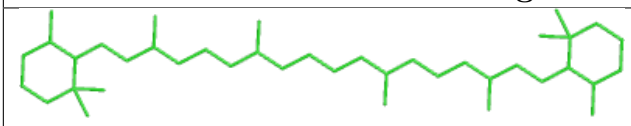


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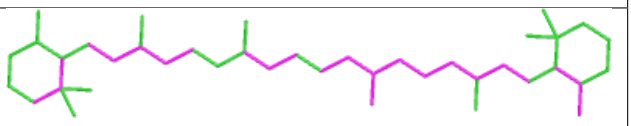


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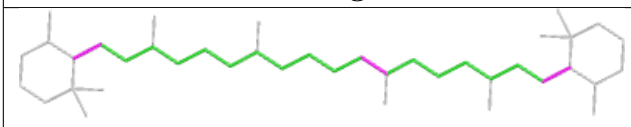
Ligand BCR aL 604



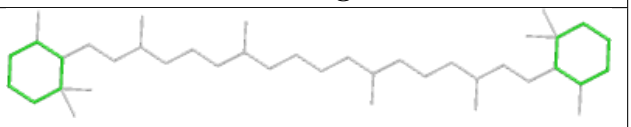
Bond lengths



Bond angles

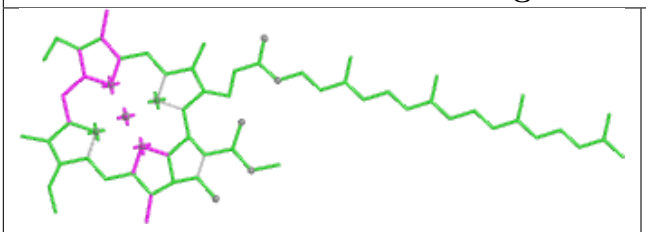


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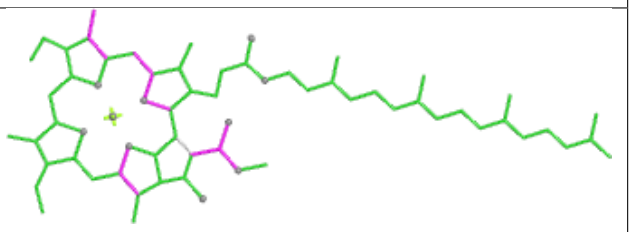


Rings

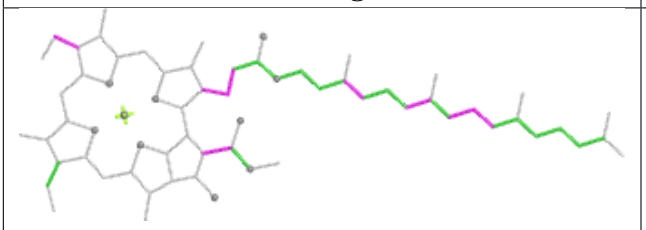
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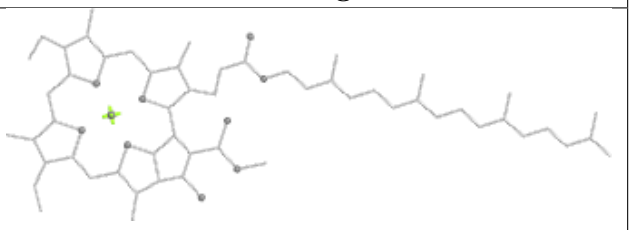
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Bond angles

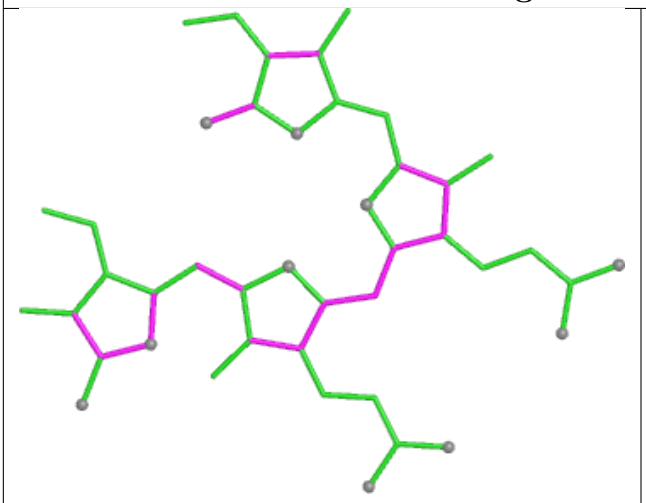


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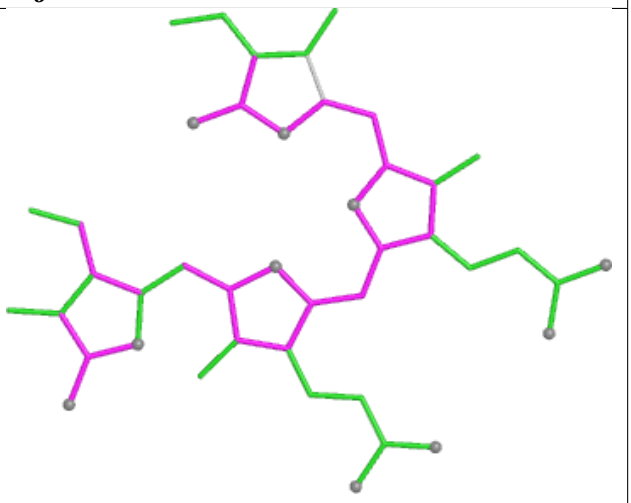


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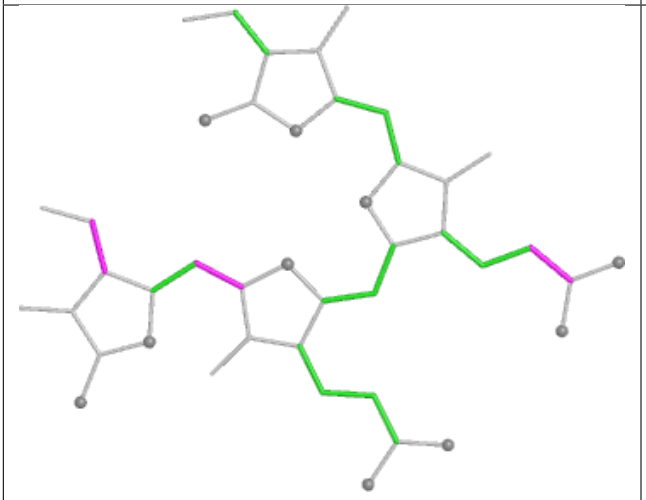
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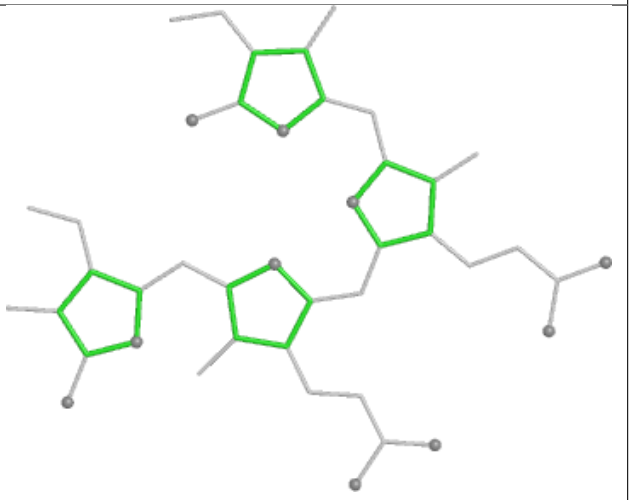
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Bond angles

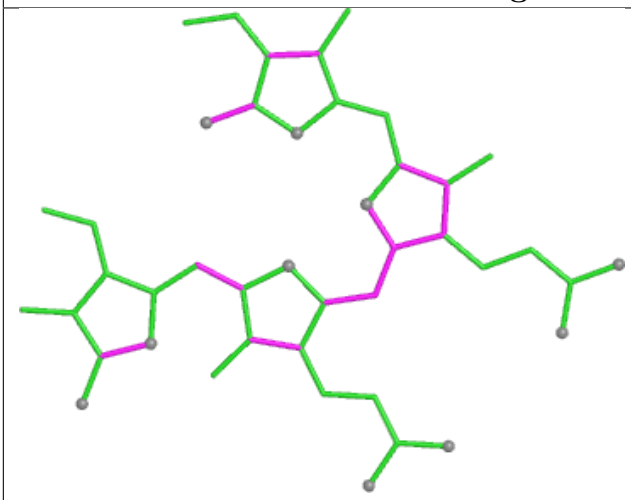


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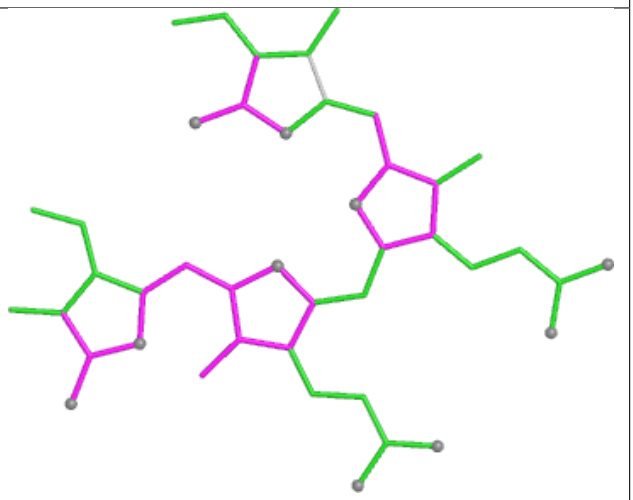


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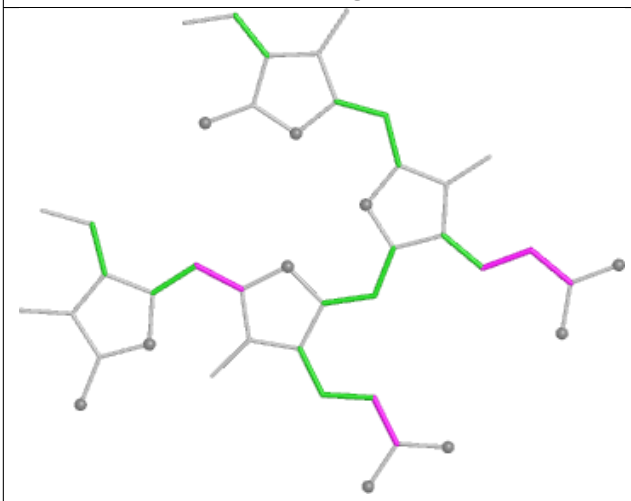
Ligand PEB AH 301



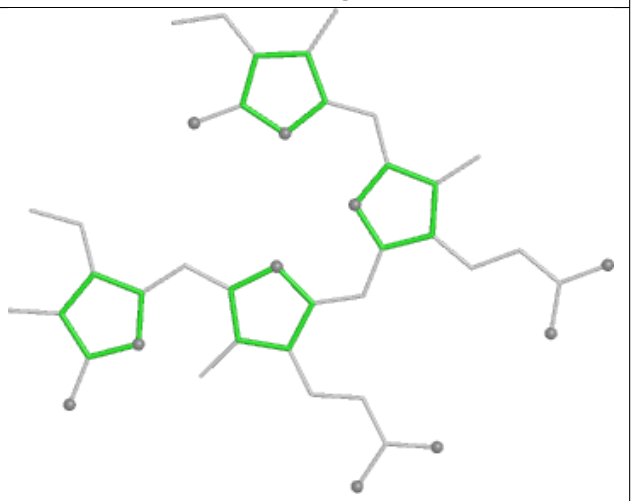
Bond lengths



Bond angles

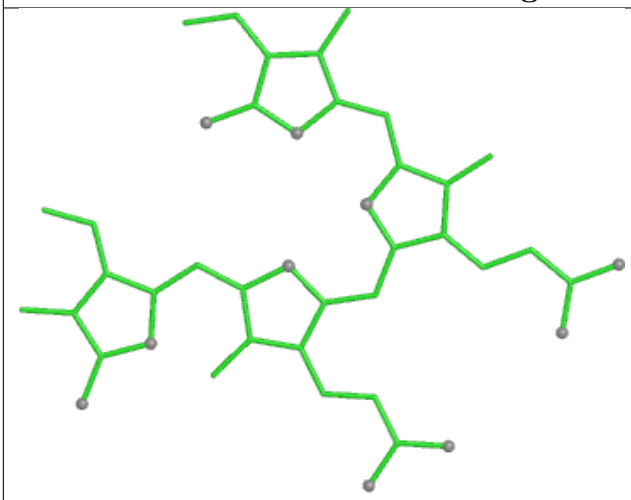


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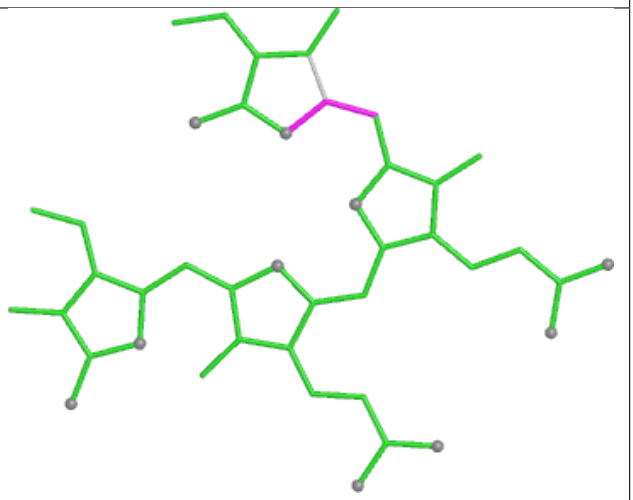


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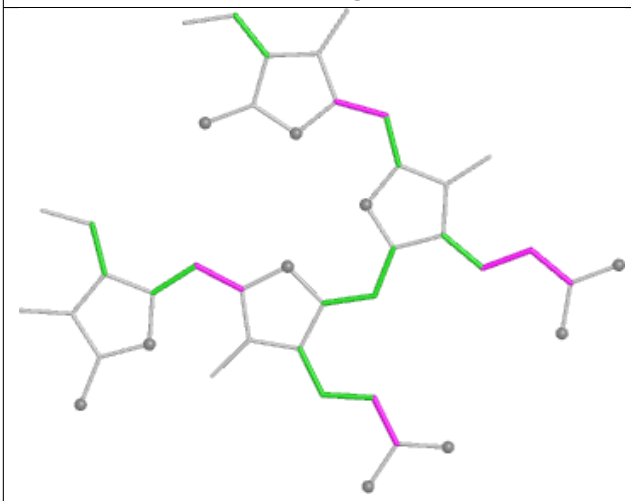
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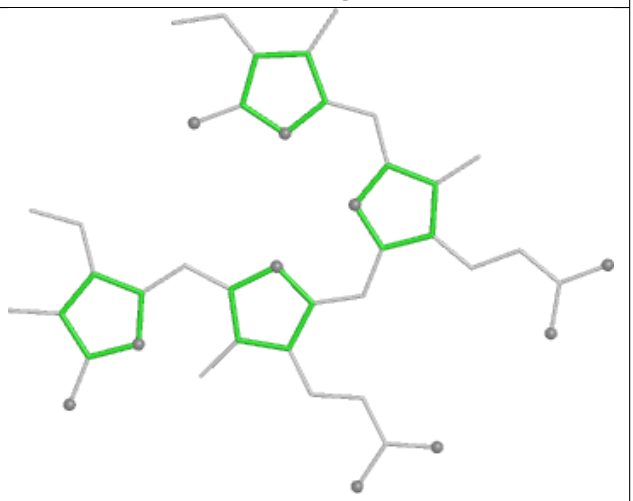
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Bond angles

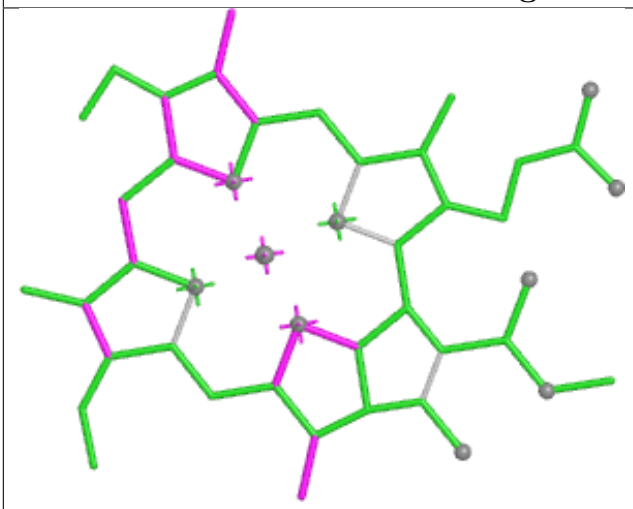


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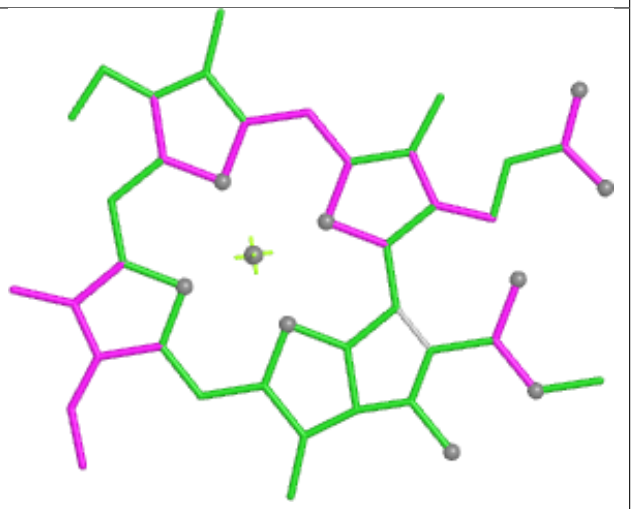


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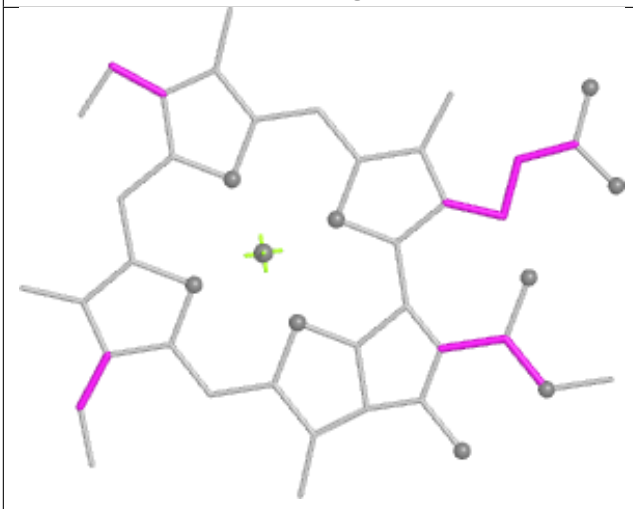
Ligand CLA 82 308



Bond lengths



Bond angles

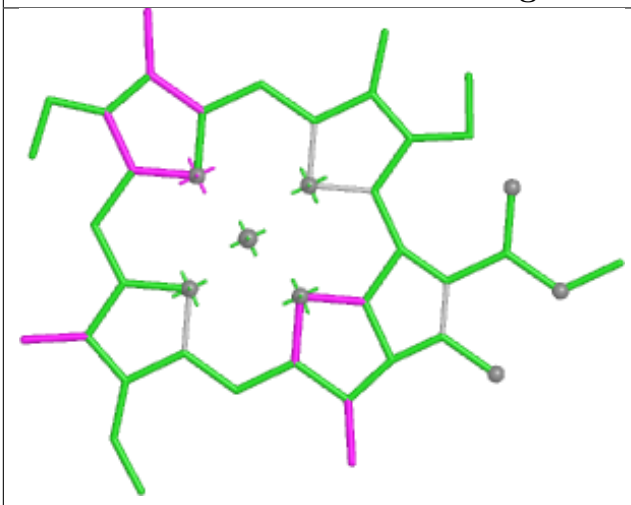


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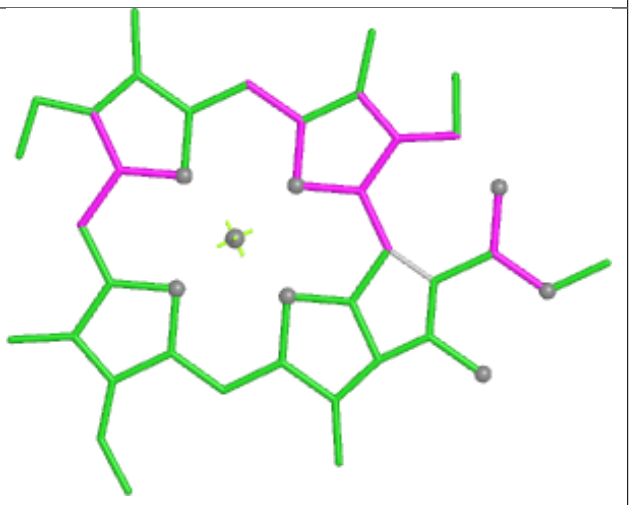


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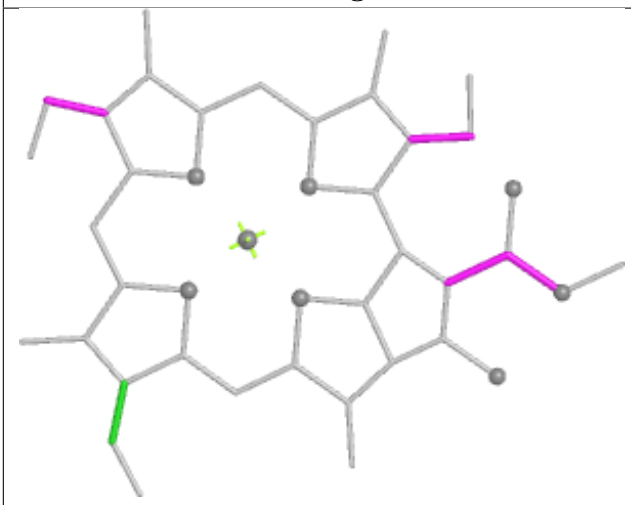
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Bond lengths



Bond angles

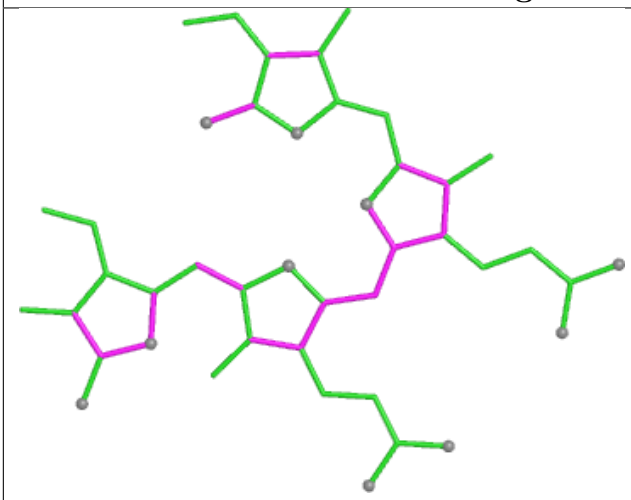


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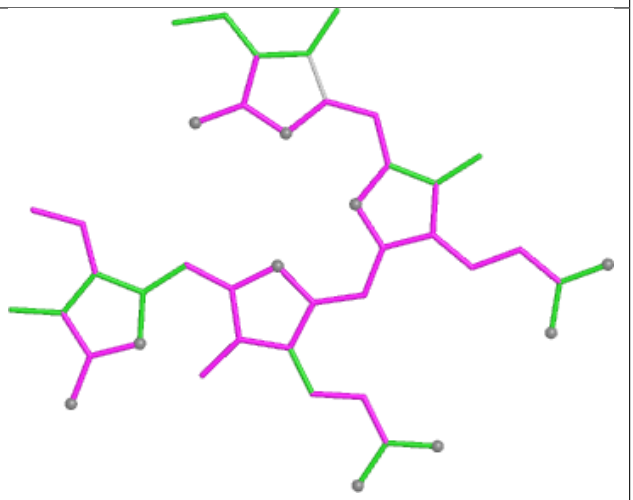


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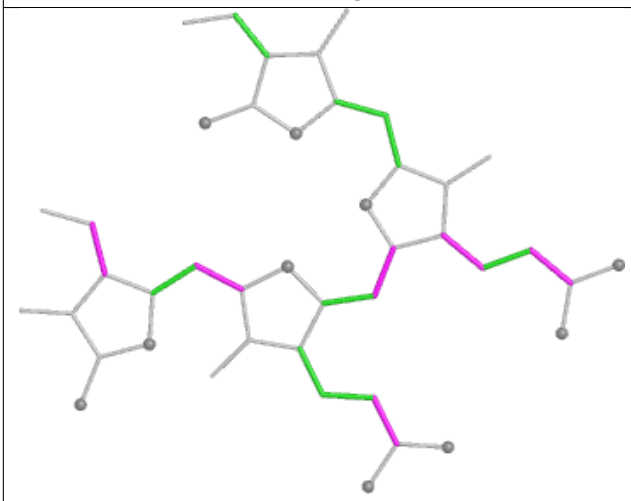
Ligand PEB X7 203



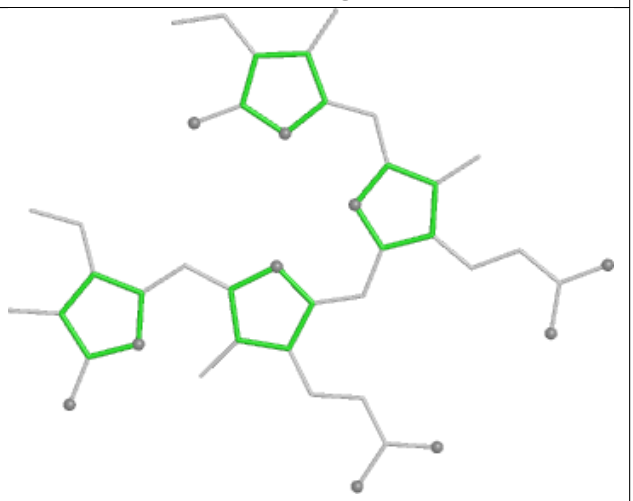
Bond lengths



Bond angles

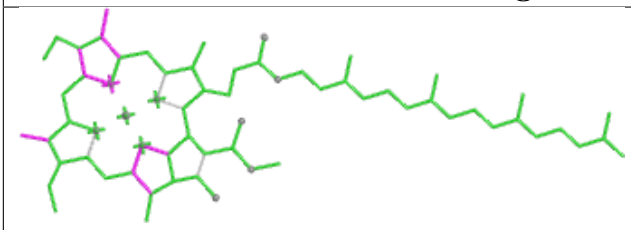


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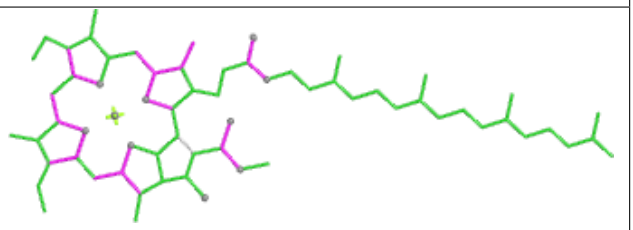


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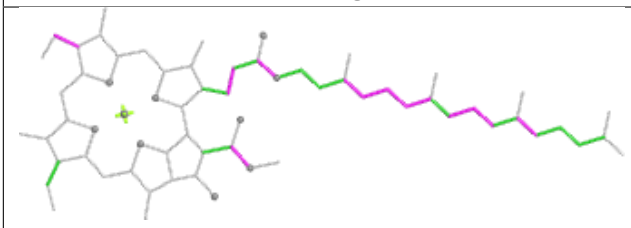
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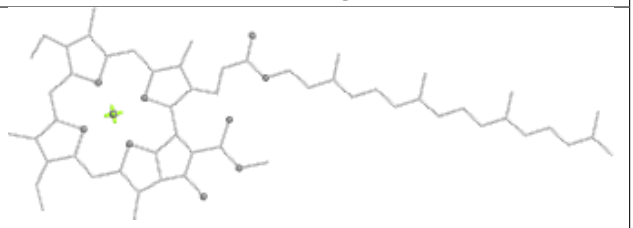
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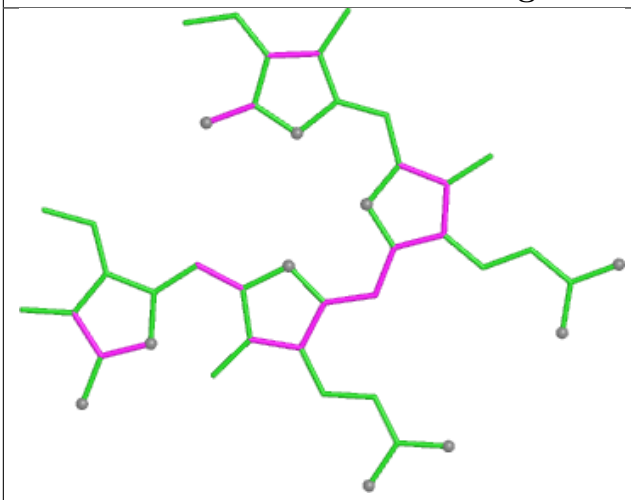


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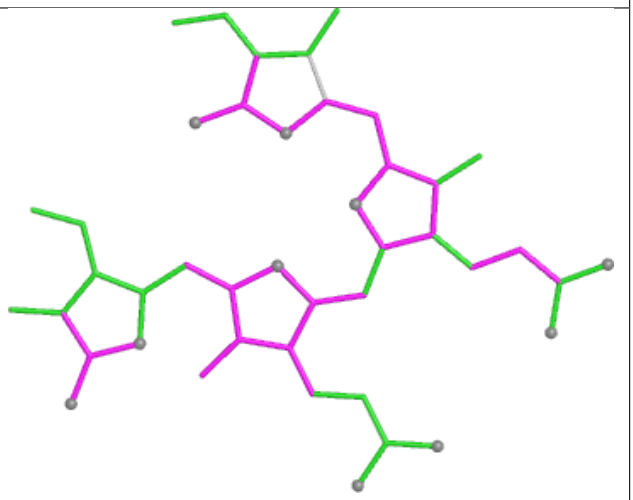


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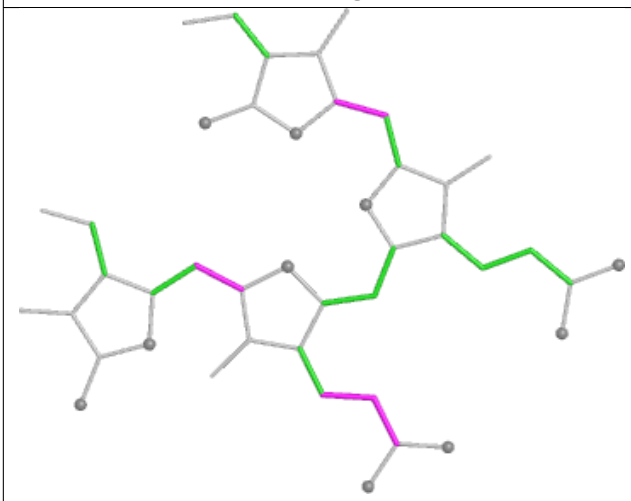
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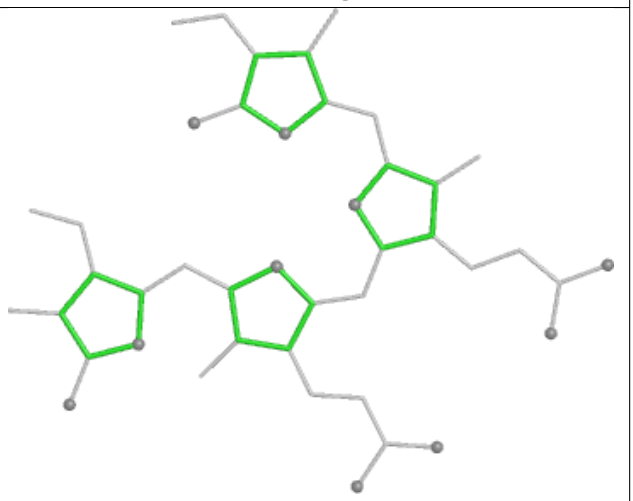
Bond lengths



Bond angles

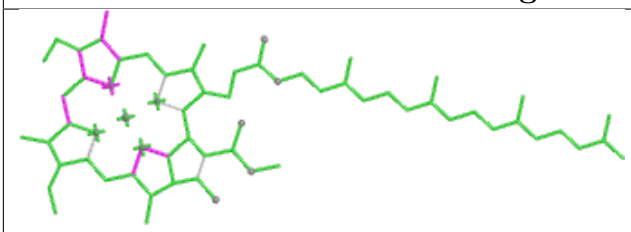


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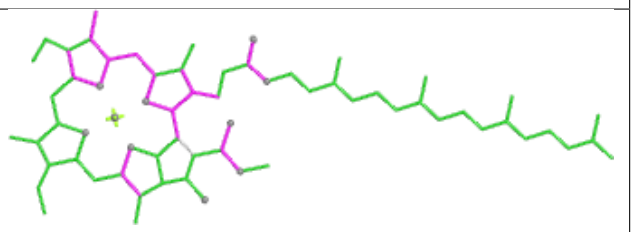


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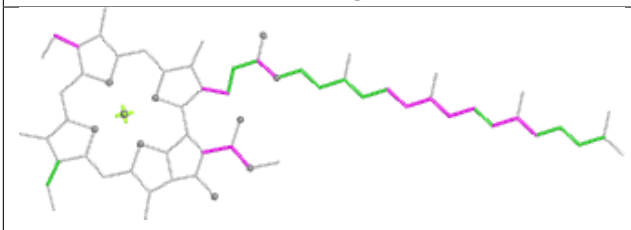
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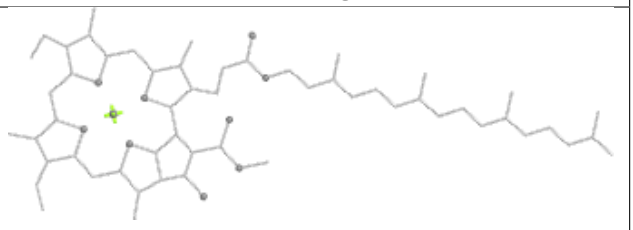
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Bond angles

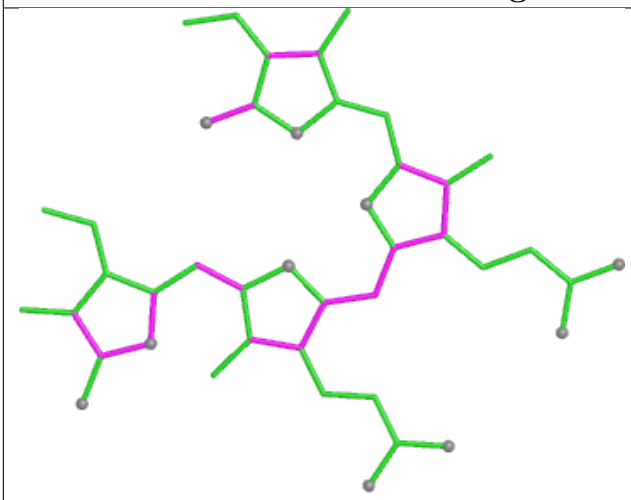


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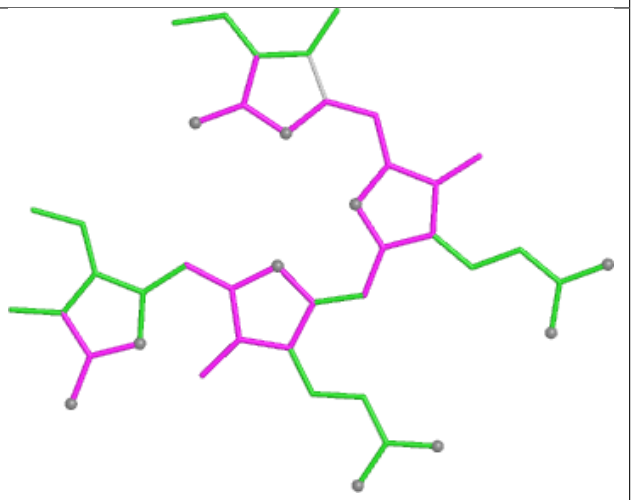


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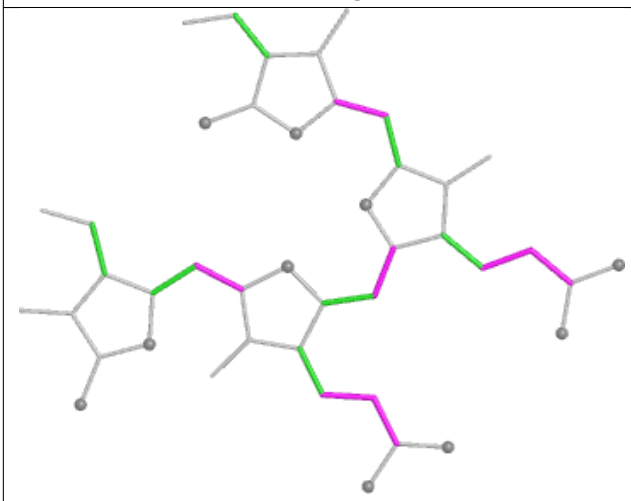
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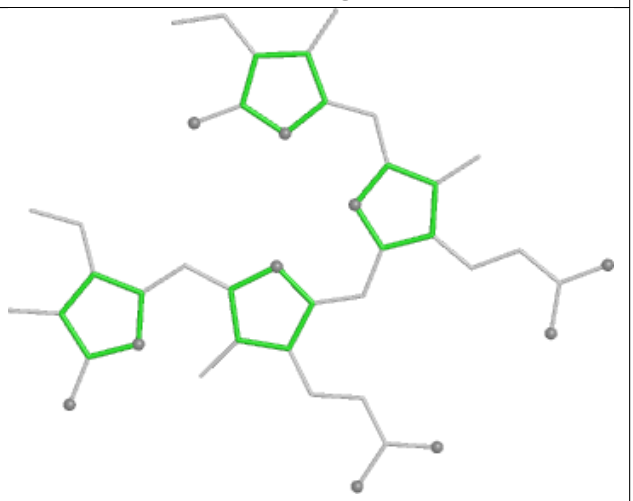
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Bond angles

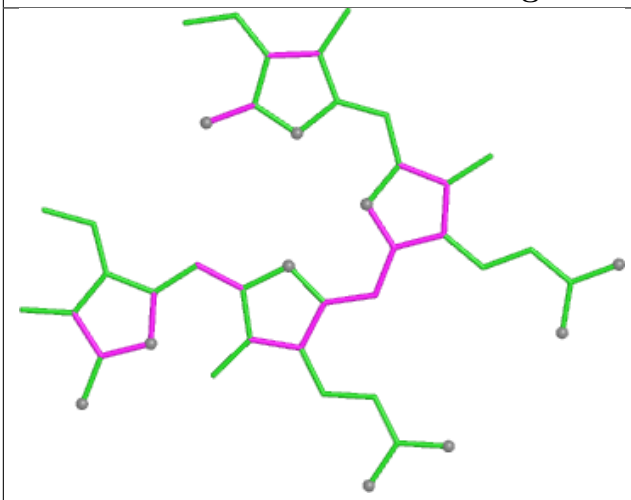


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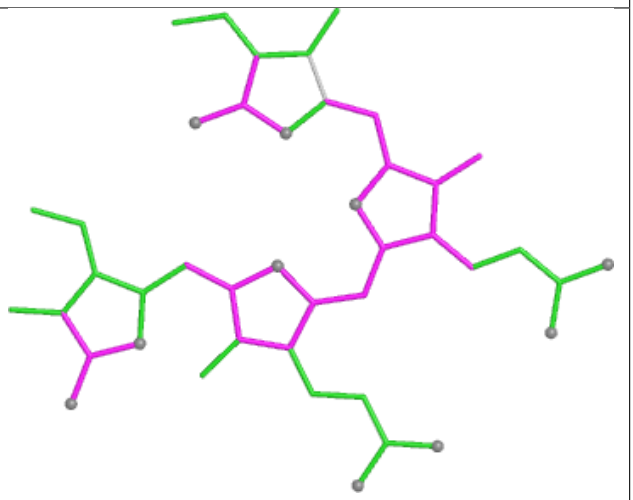


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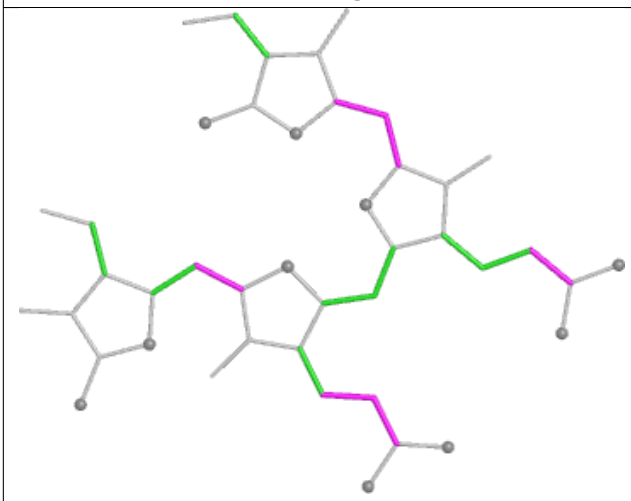
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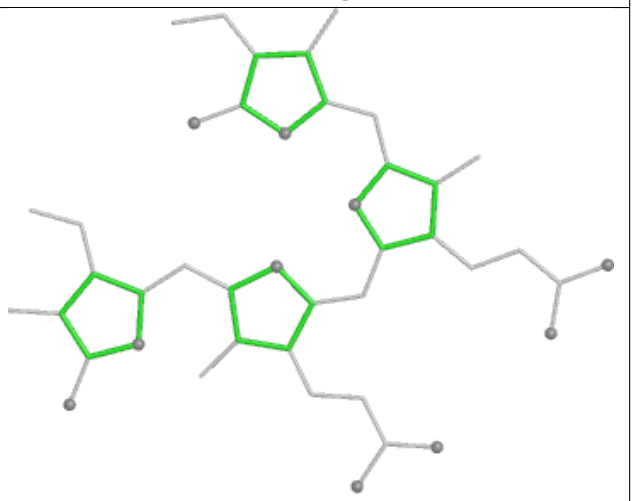
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Bond angles

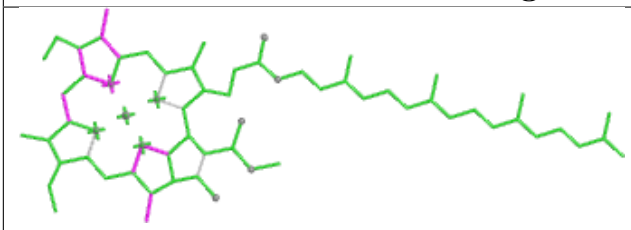


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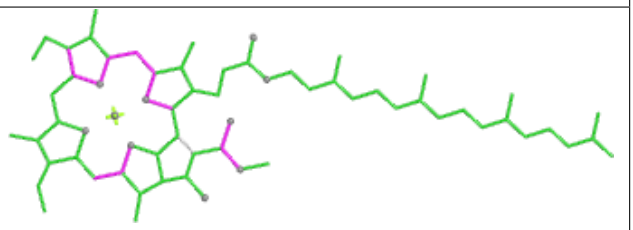


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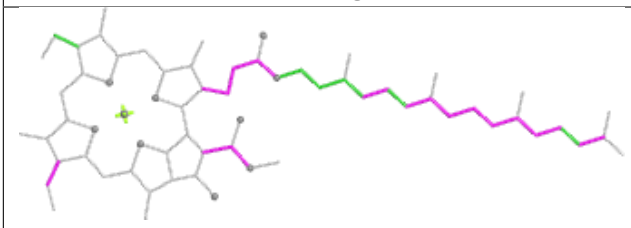
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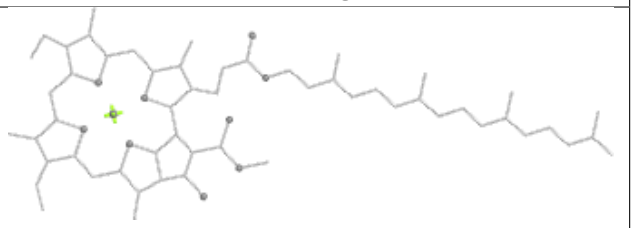
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Bond angles

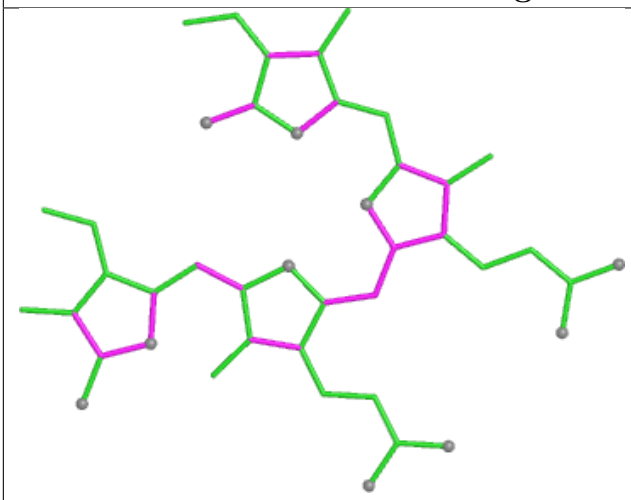


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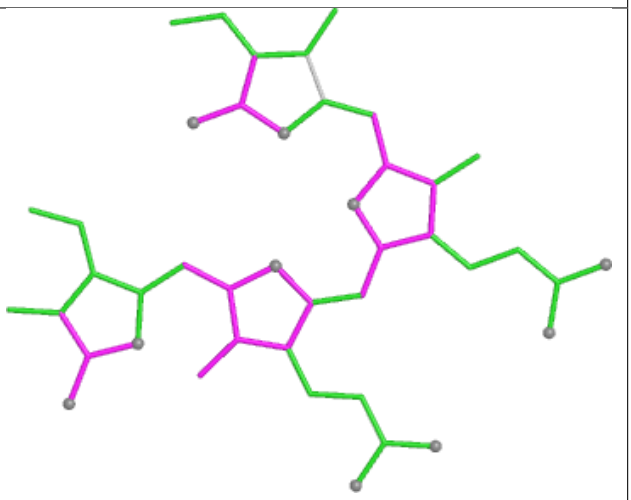


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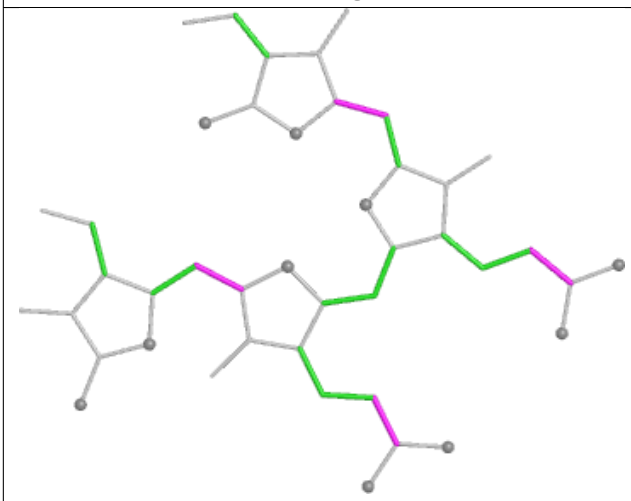
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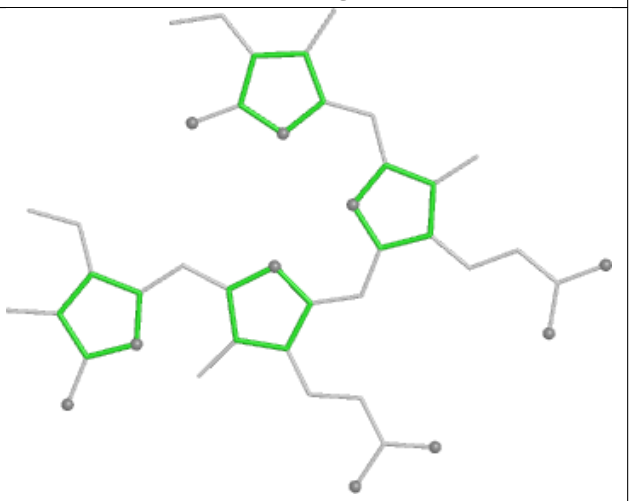
Bond lengths



Bond angles

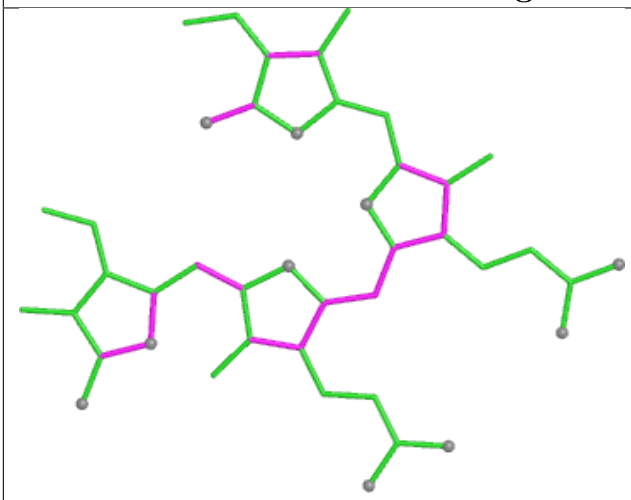


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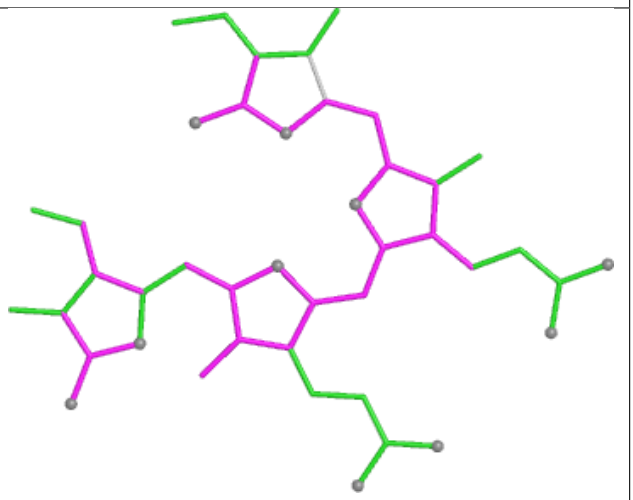


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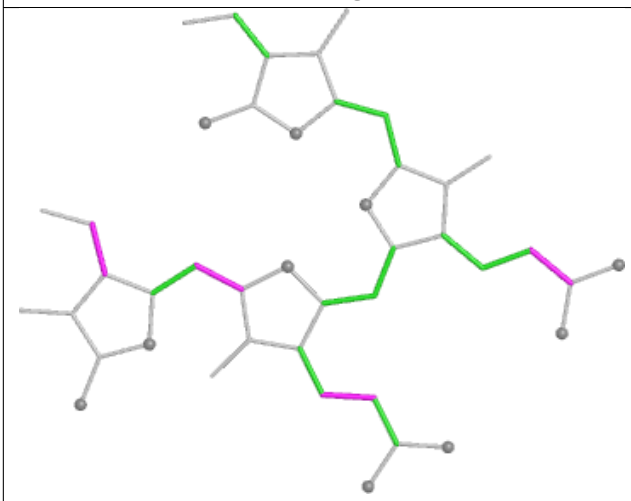
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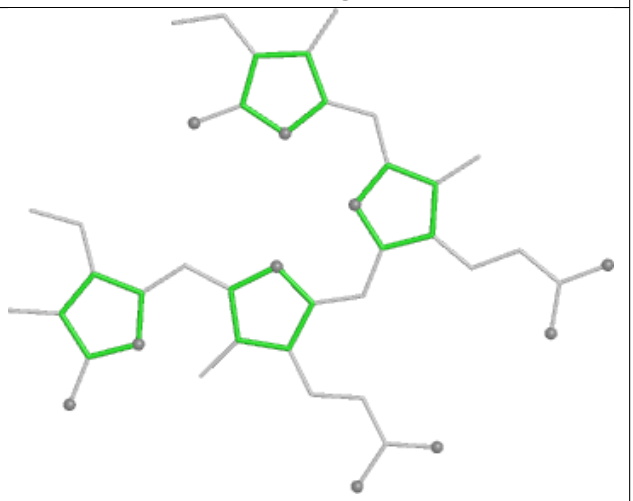
Bond lengths



Bond angles

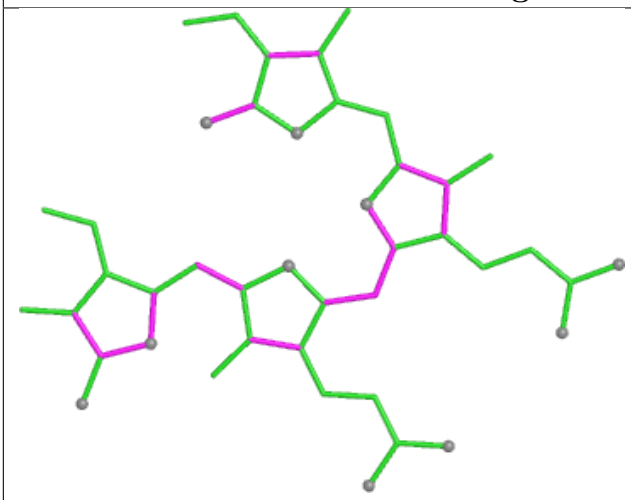


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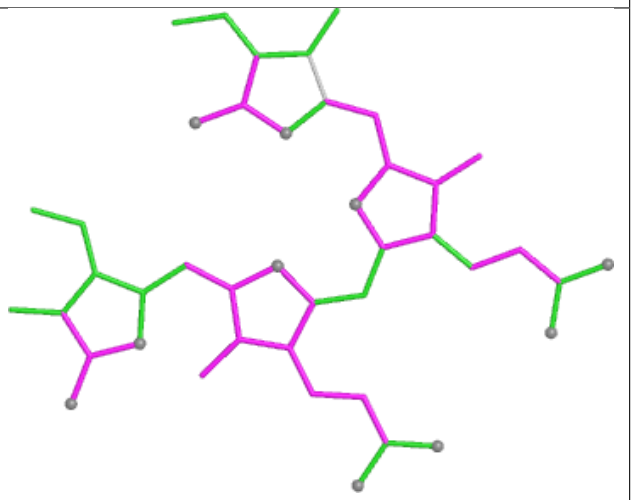


Rings

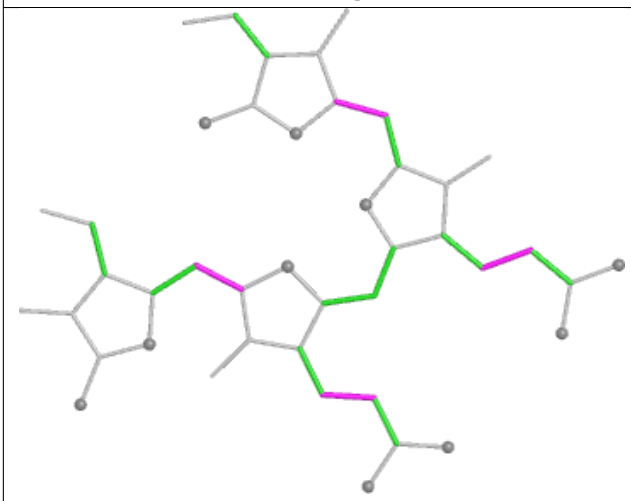
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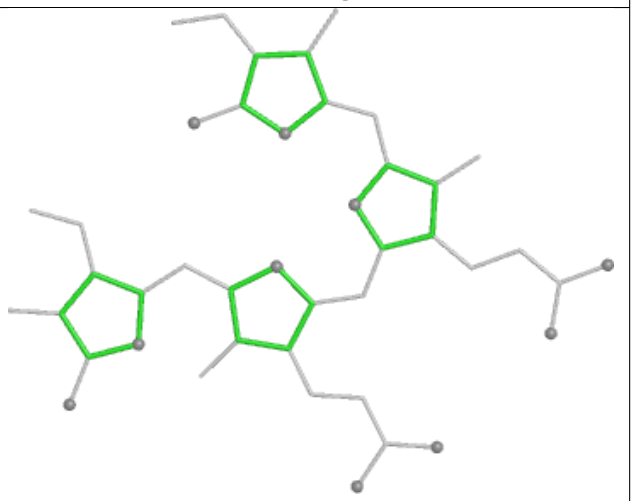
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Bond angles

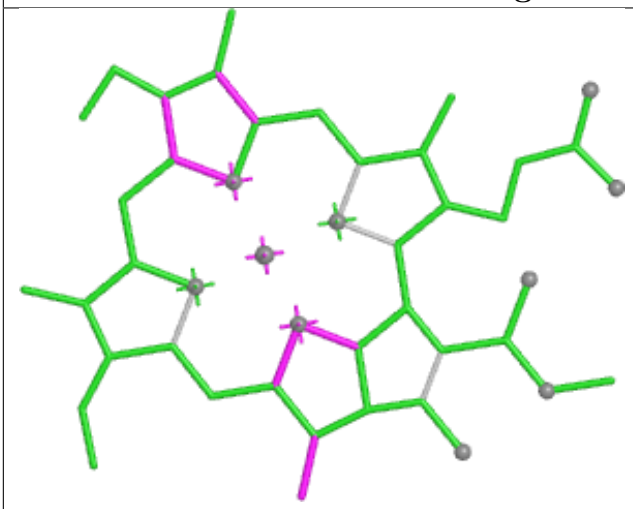


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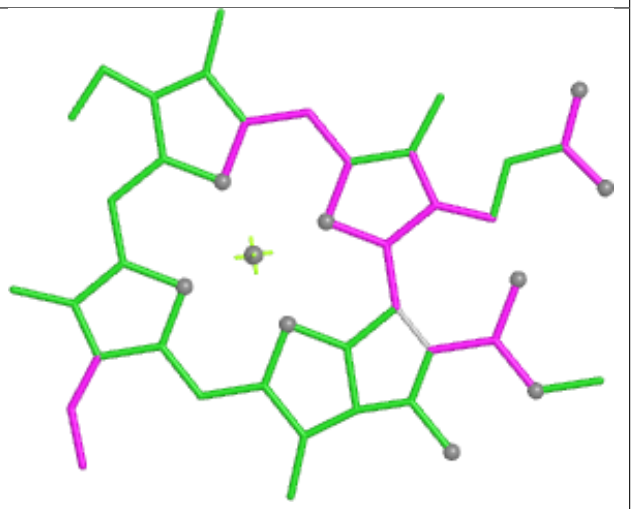


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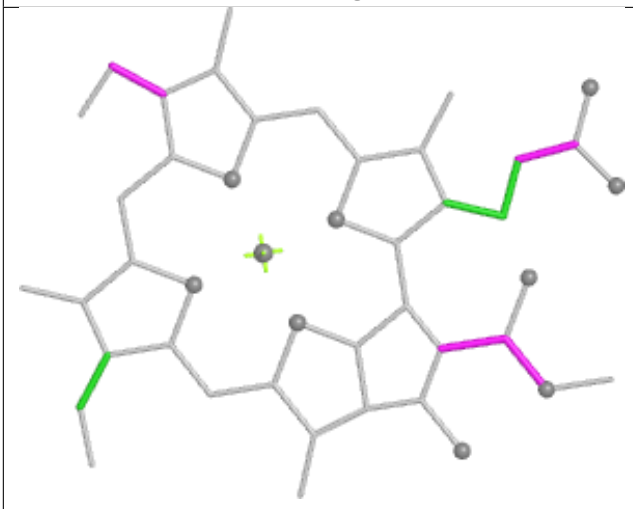
Ligand CLA 2N 307



Bond lengths



Bond angles

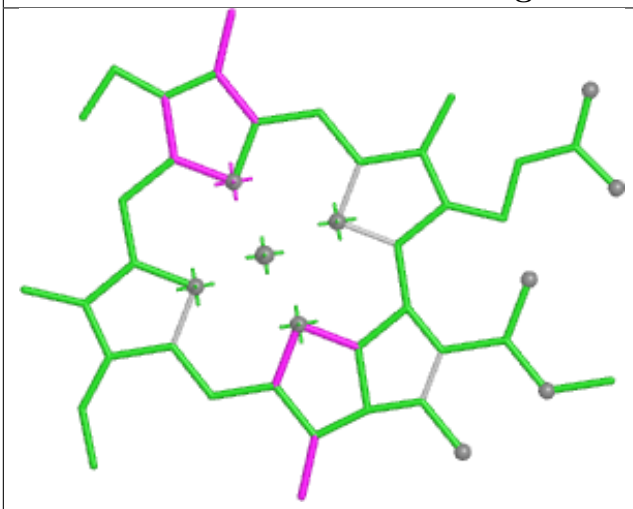


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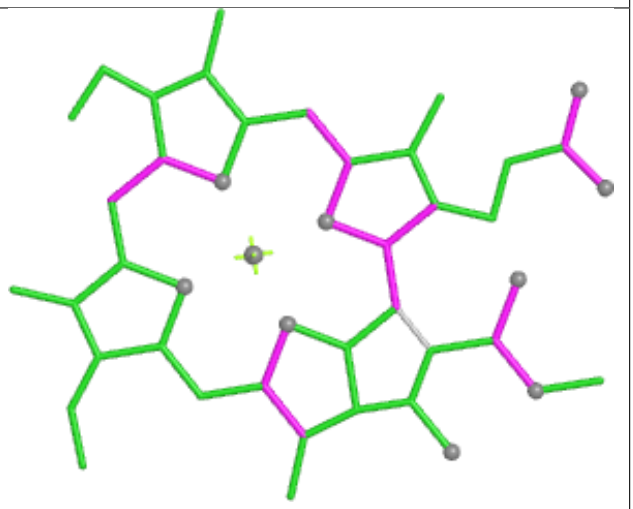


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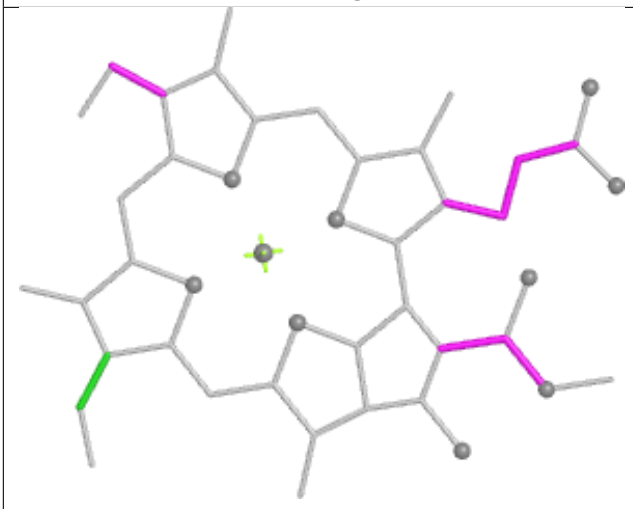
Ligand CLA R2 202



Bond lengths



Bond angles

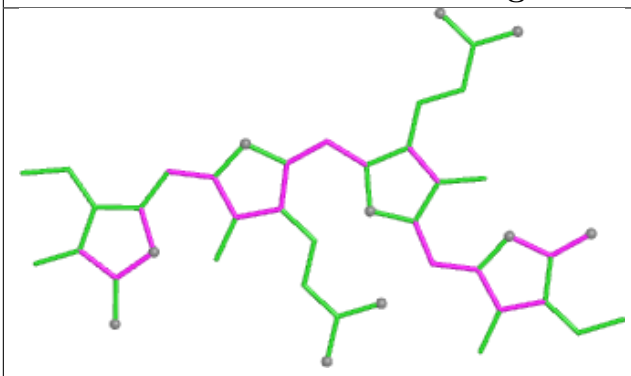


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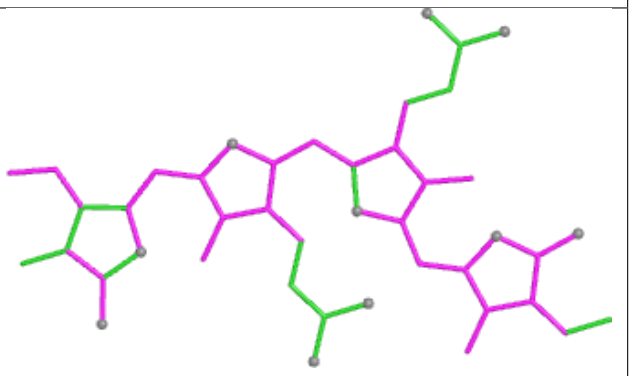


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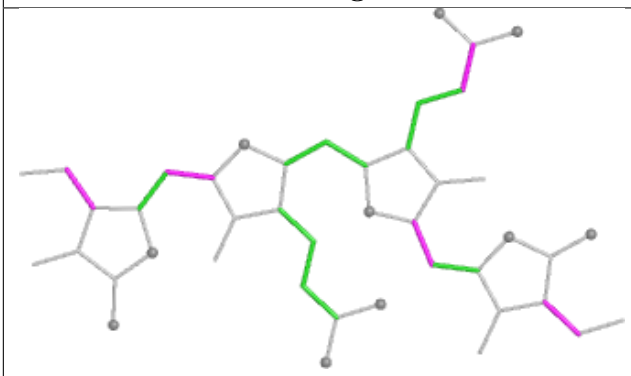
Ligand CYC v3 1001



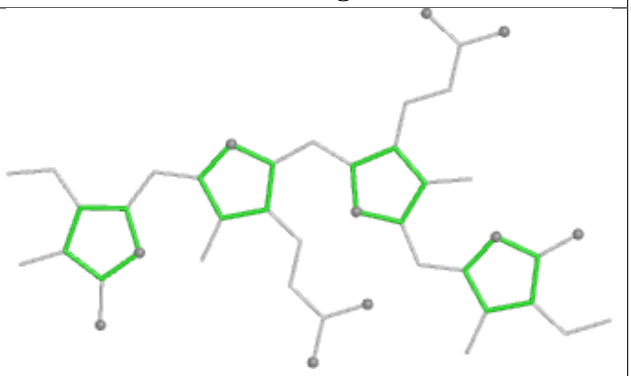
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Bond angles

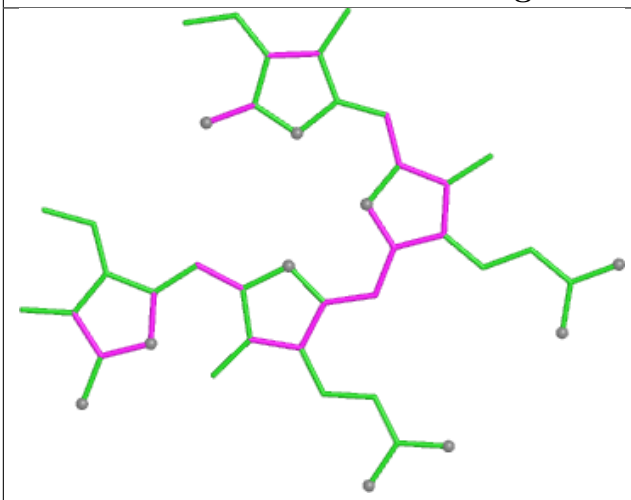


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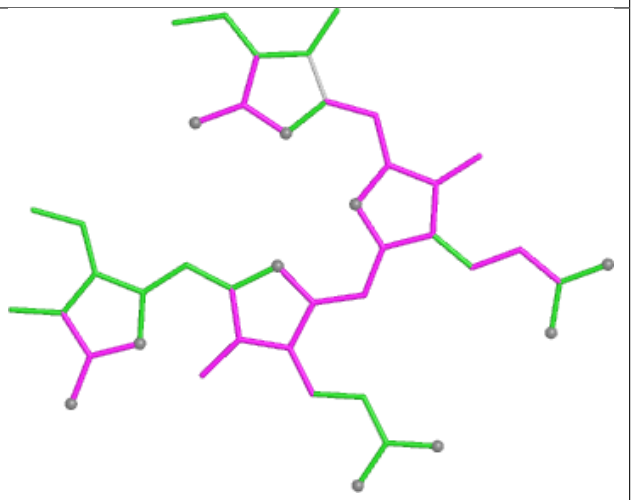


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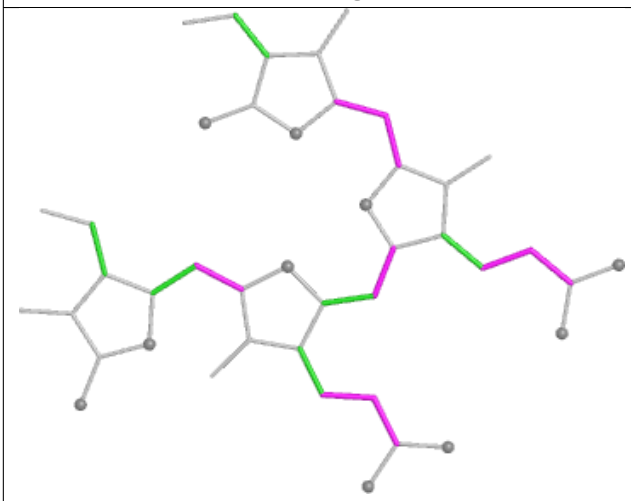
Ligand PEB PF 202



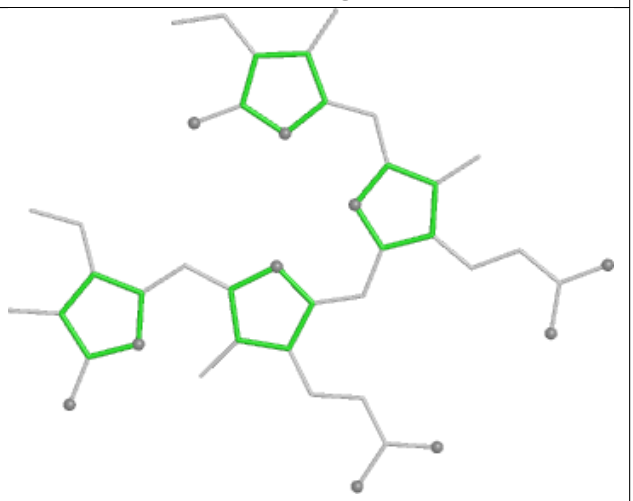
Bond lengths



Bond angles

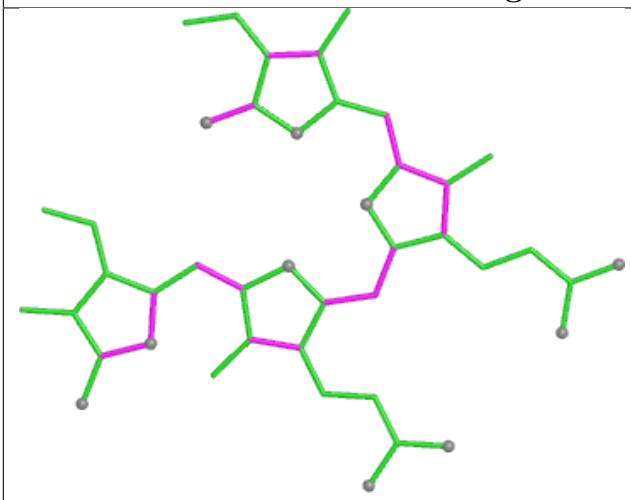


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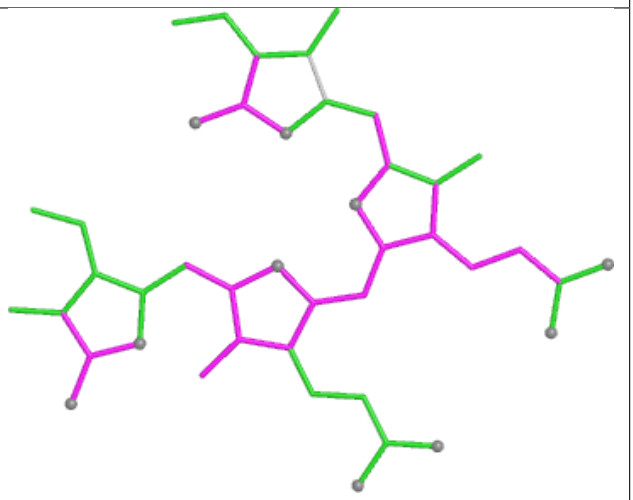


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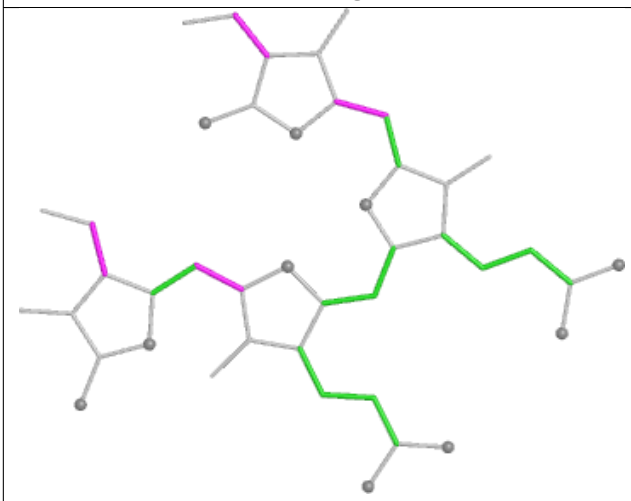
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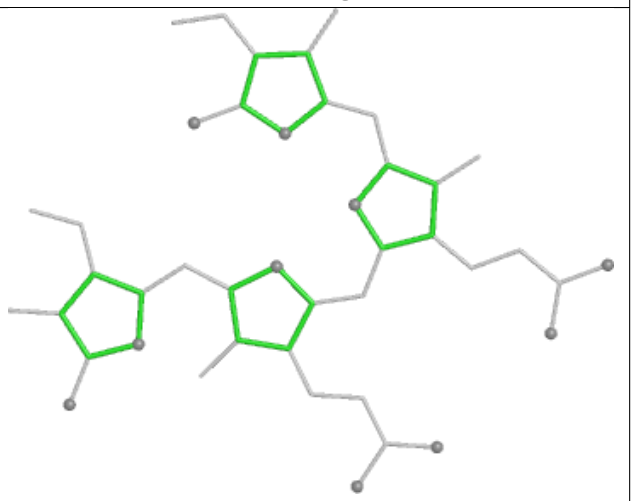
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Bond angles

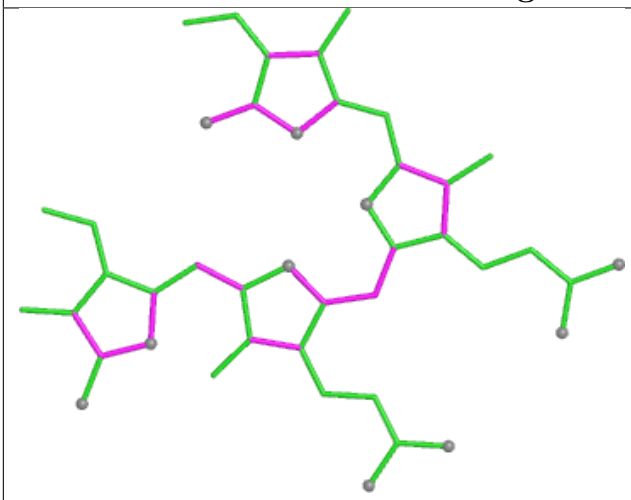


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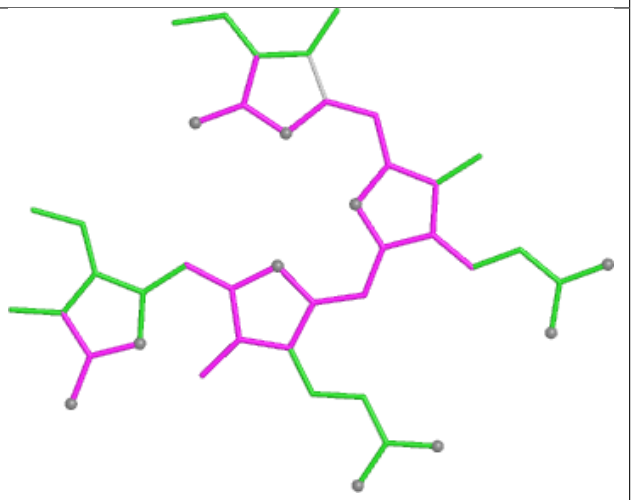


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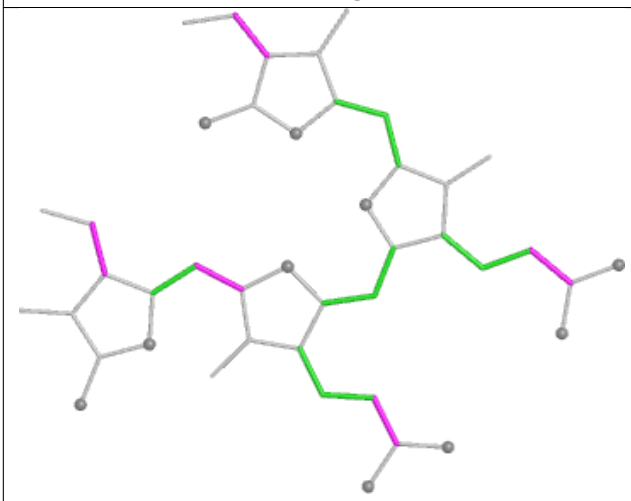
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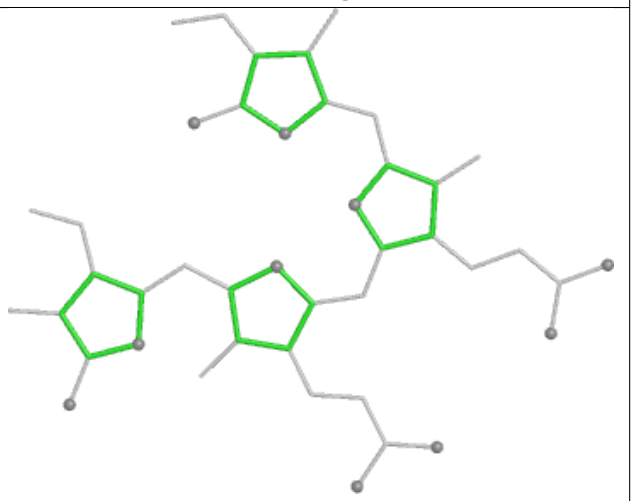
Bond lengths



Bond angles

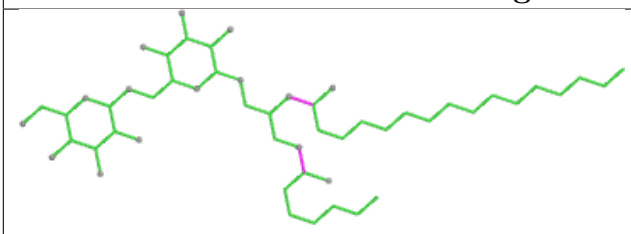


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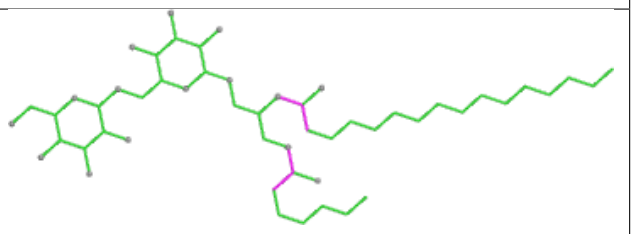


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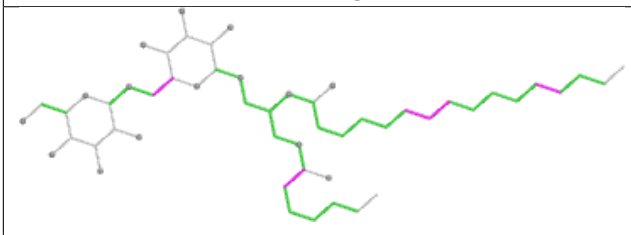
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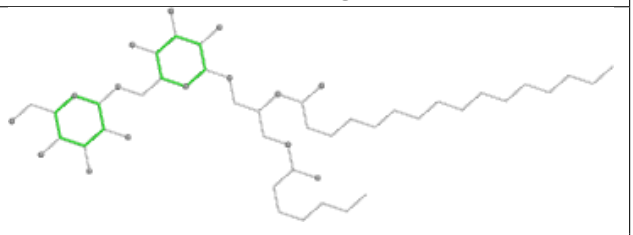
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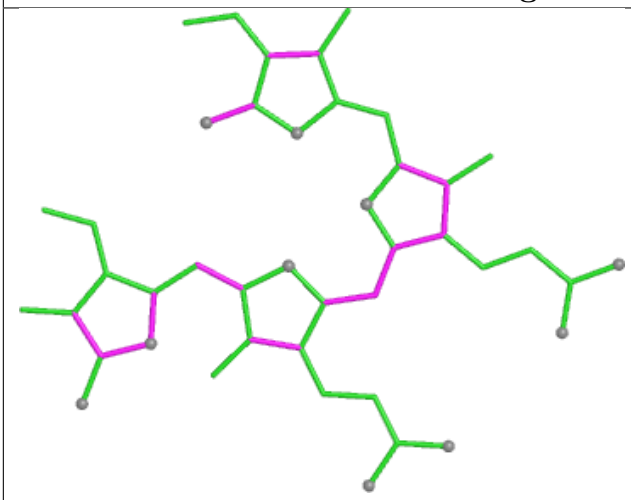


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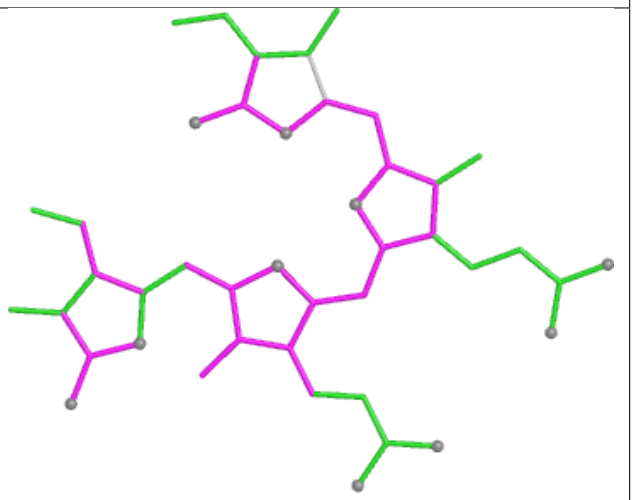


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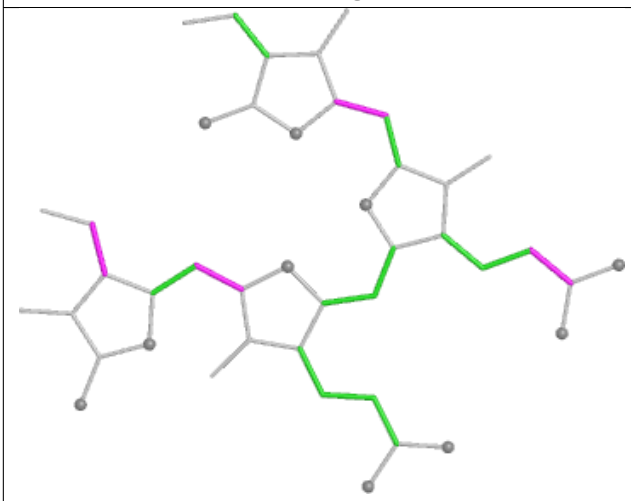
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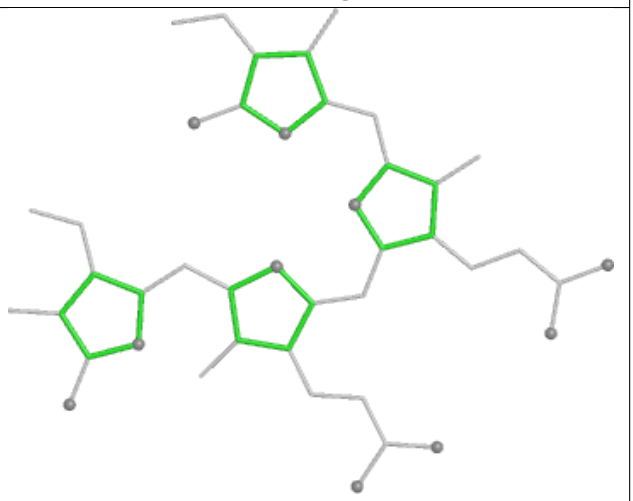
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Bond angles

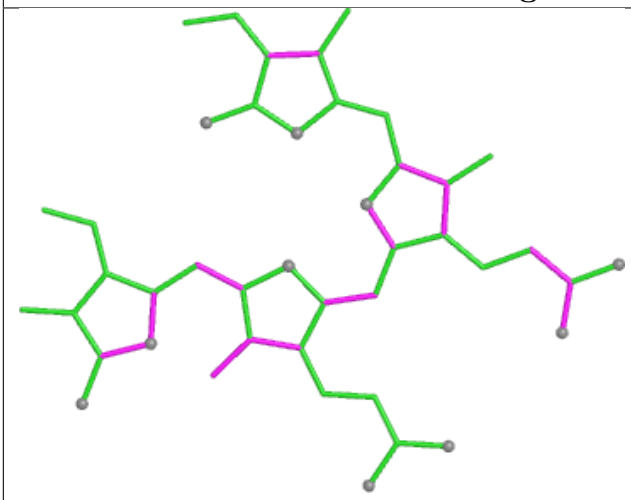


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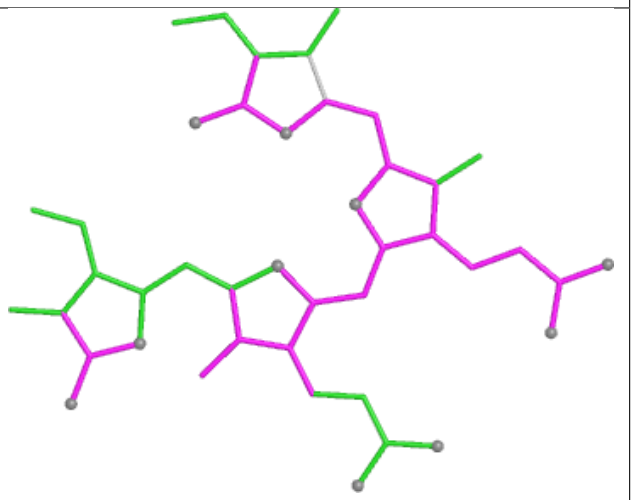


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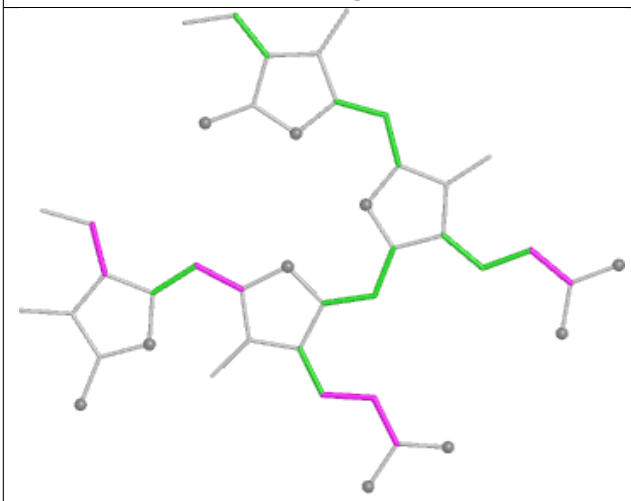
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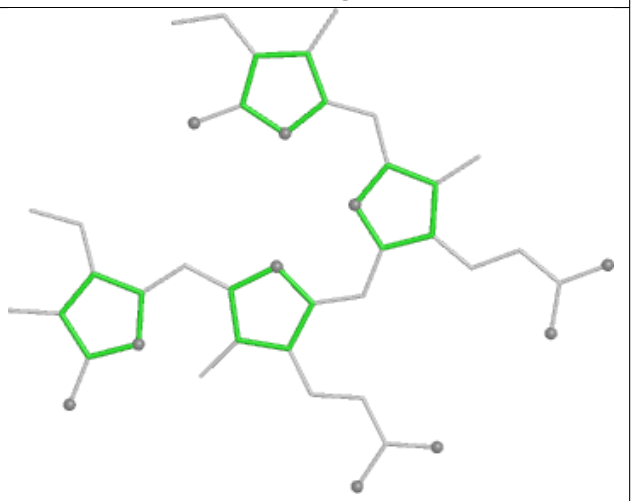
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Bond angles

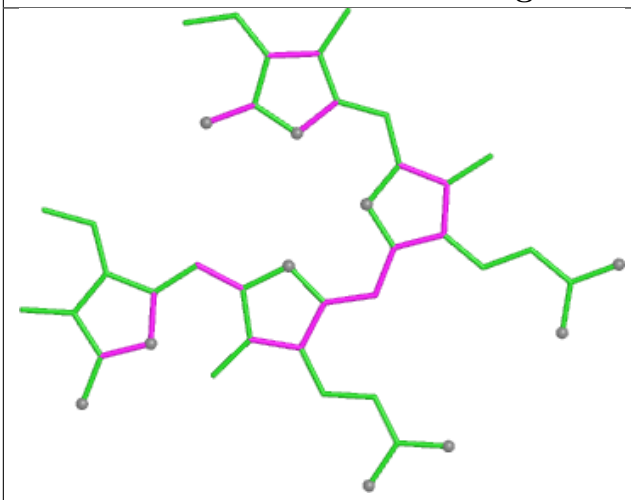


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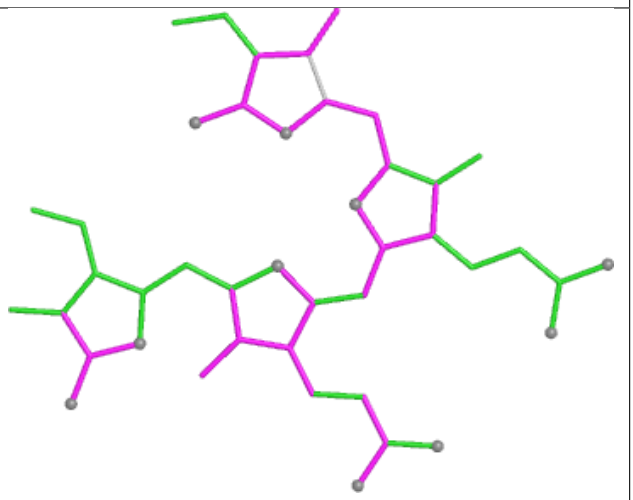


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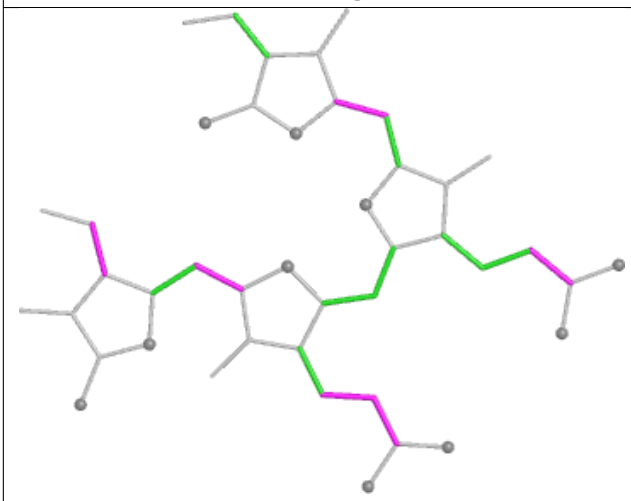
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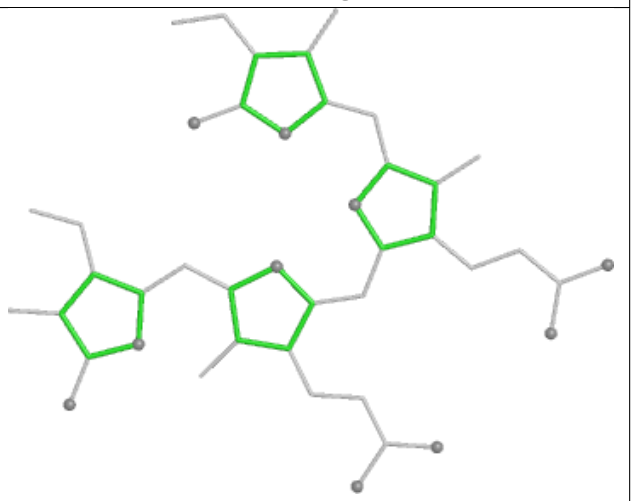
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Bond angles

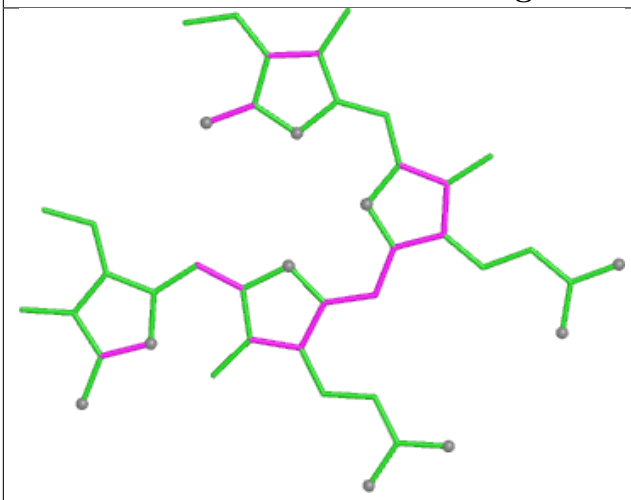


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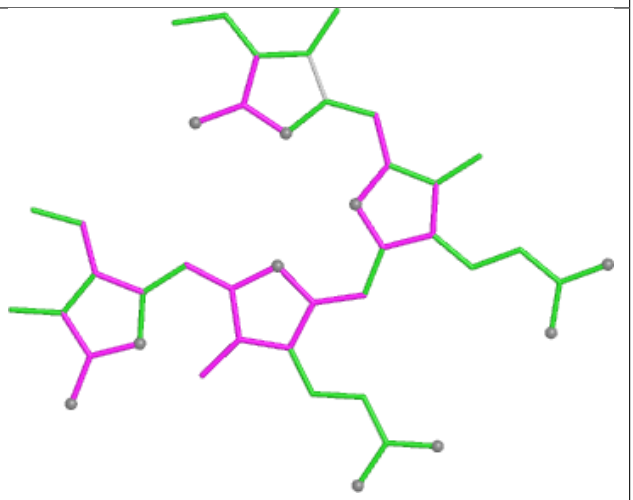


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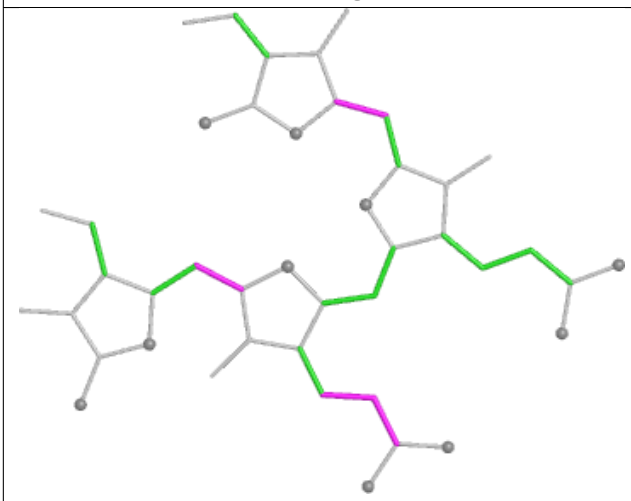
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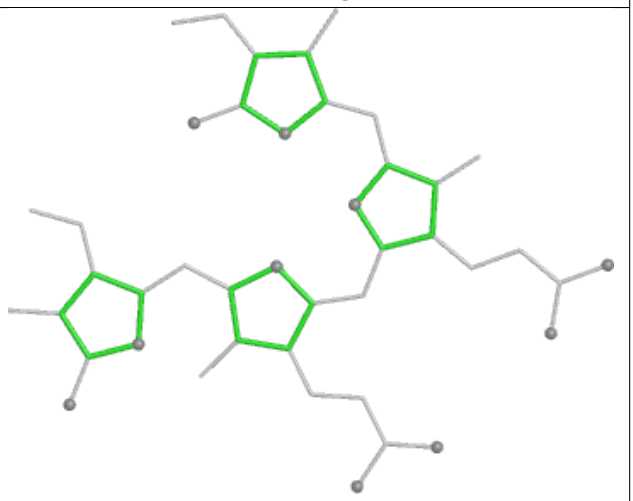
Bond lengths



Bond angles

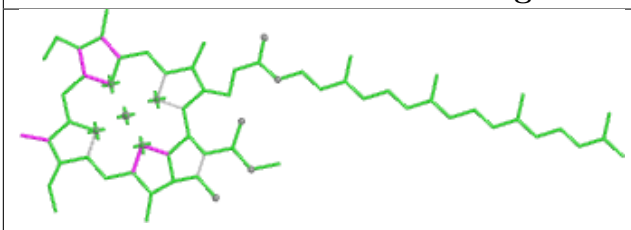


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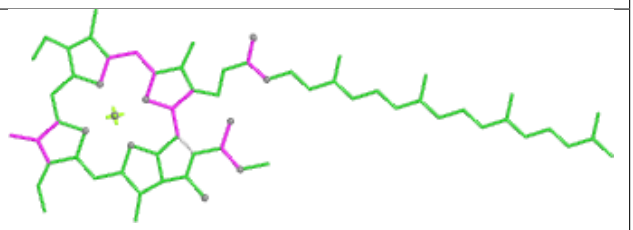


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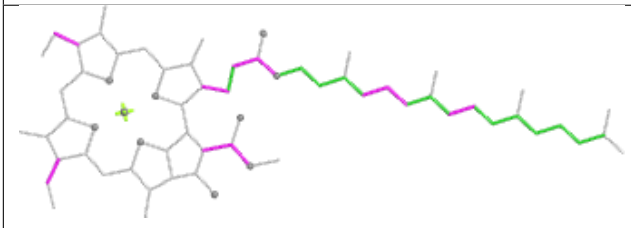
Ligand CLA 1N 602



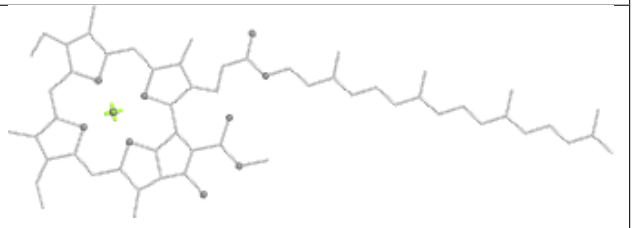
Bond lengths



Bond angles

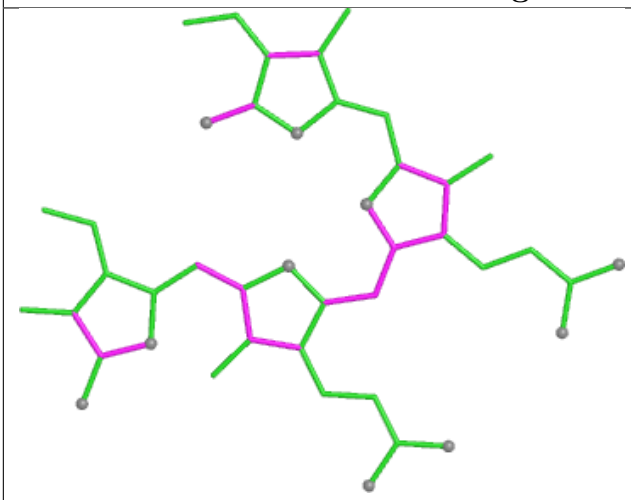


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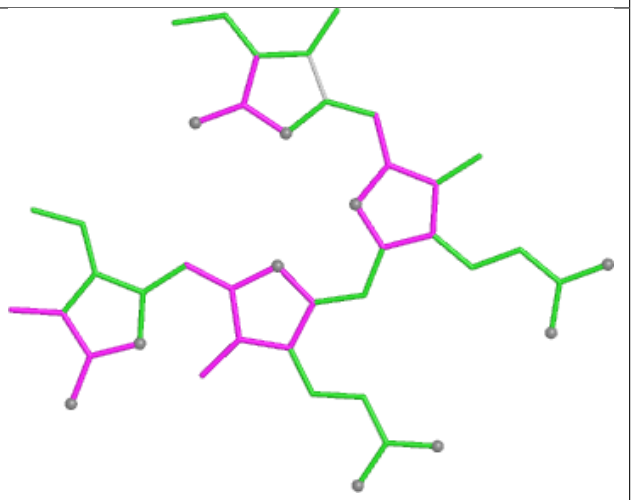


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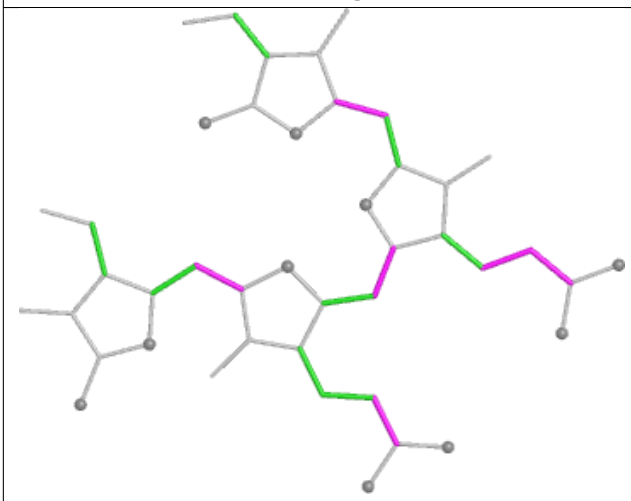
Ligand PEB M9 304



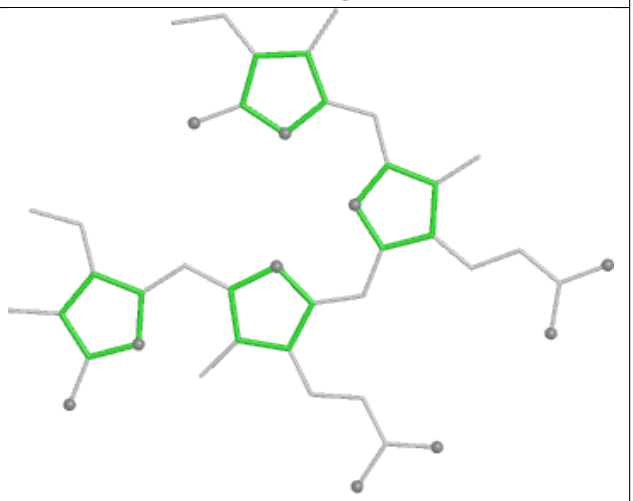
Bond lengths



Bond angles

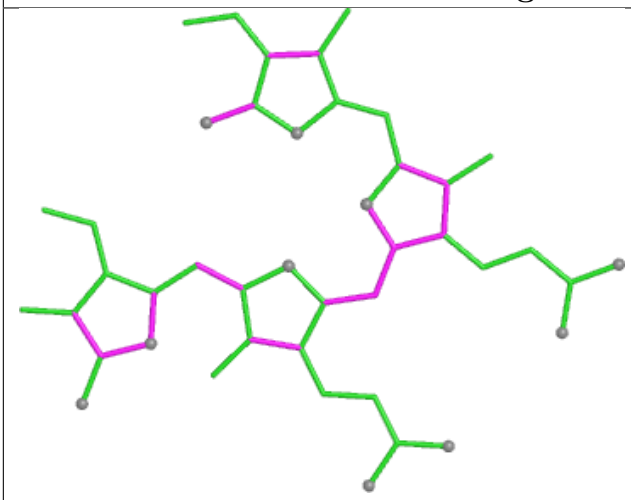


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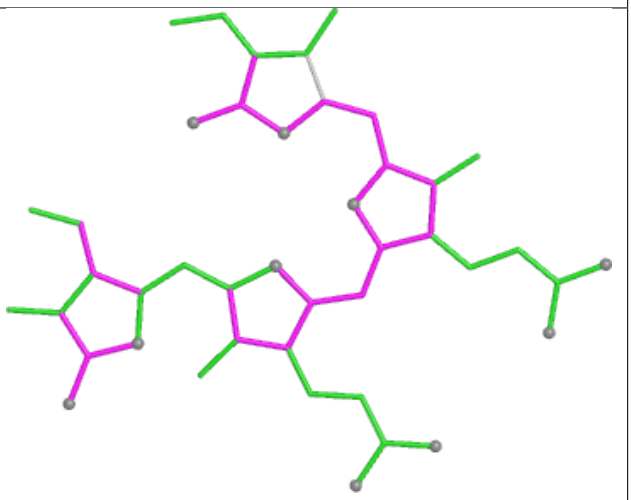


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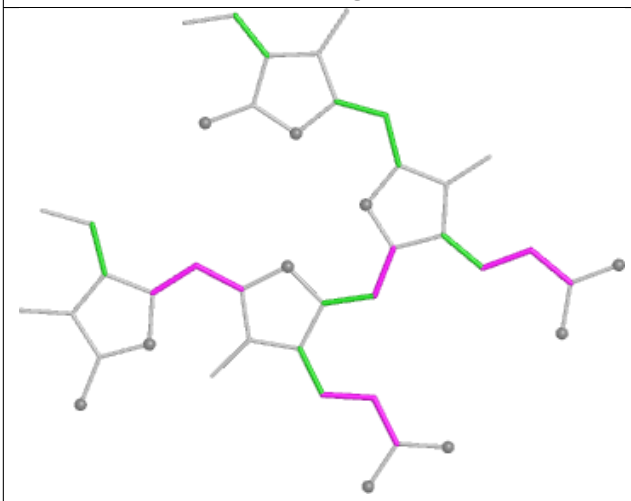
Ligand PEB E5 202



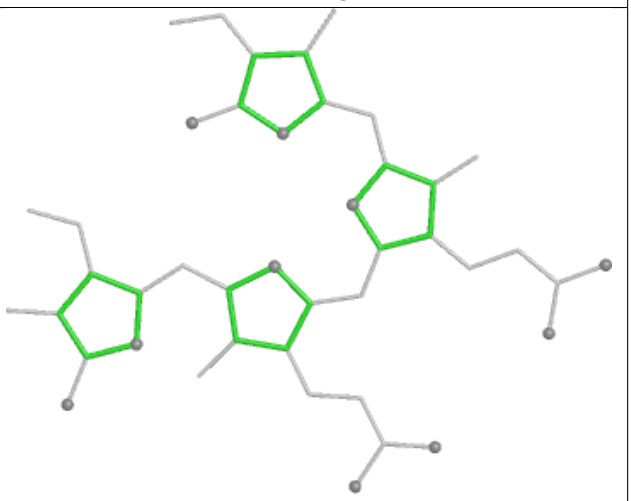
Bond lengths



Bond angles

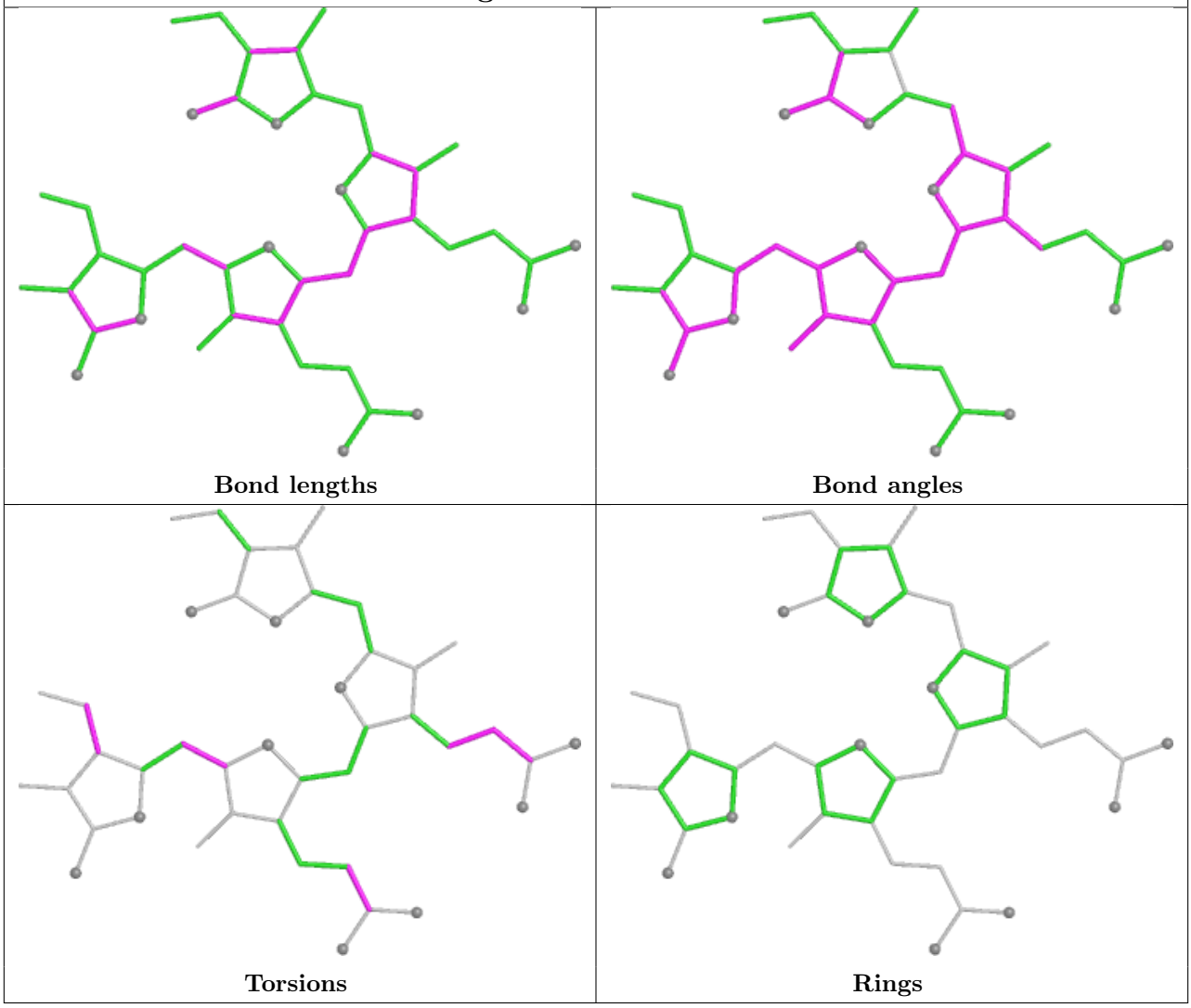


Torsions

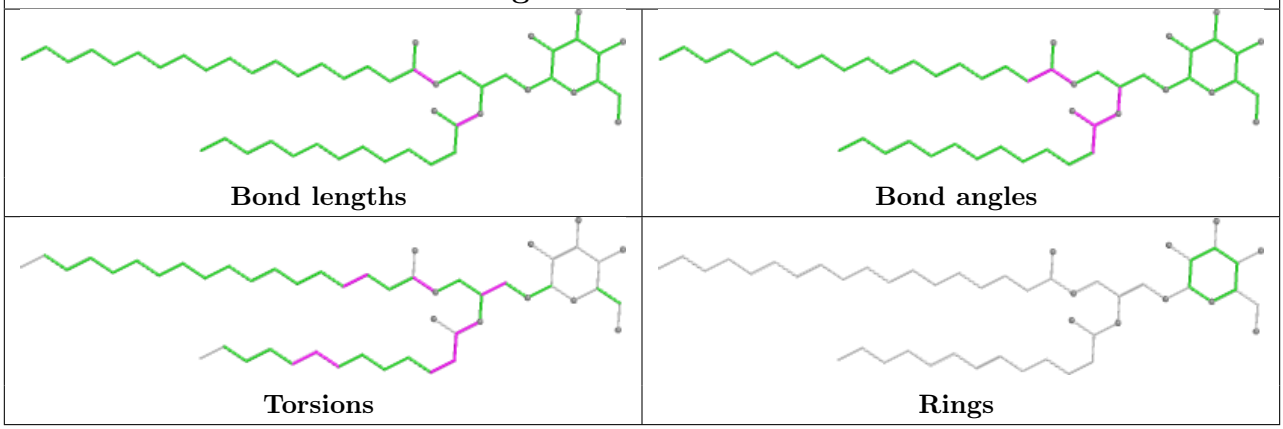


Rings

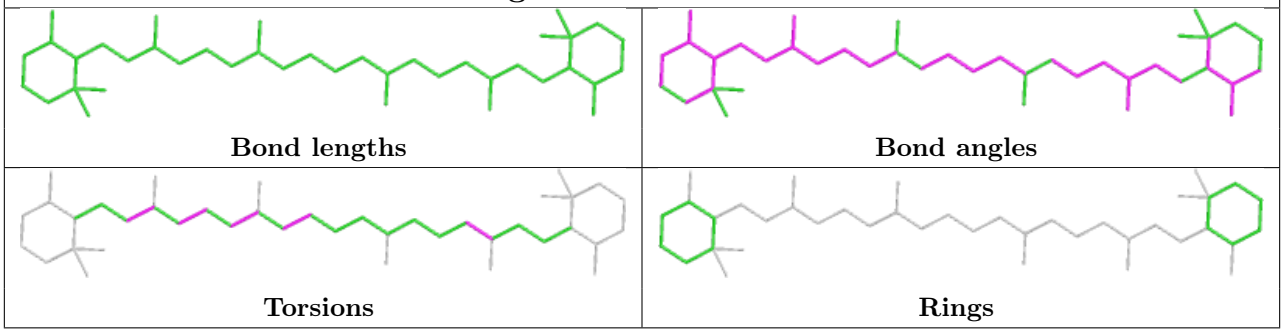
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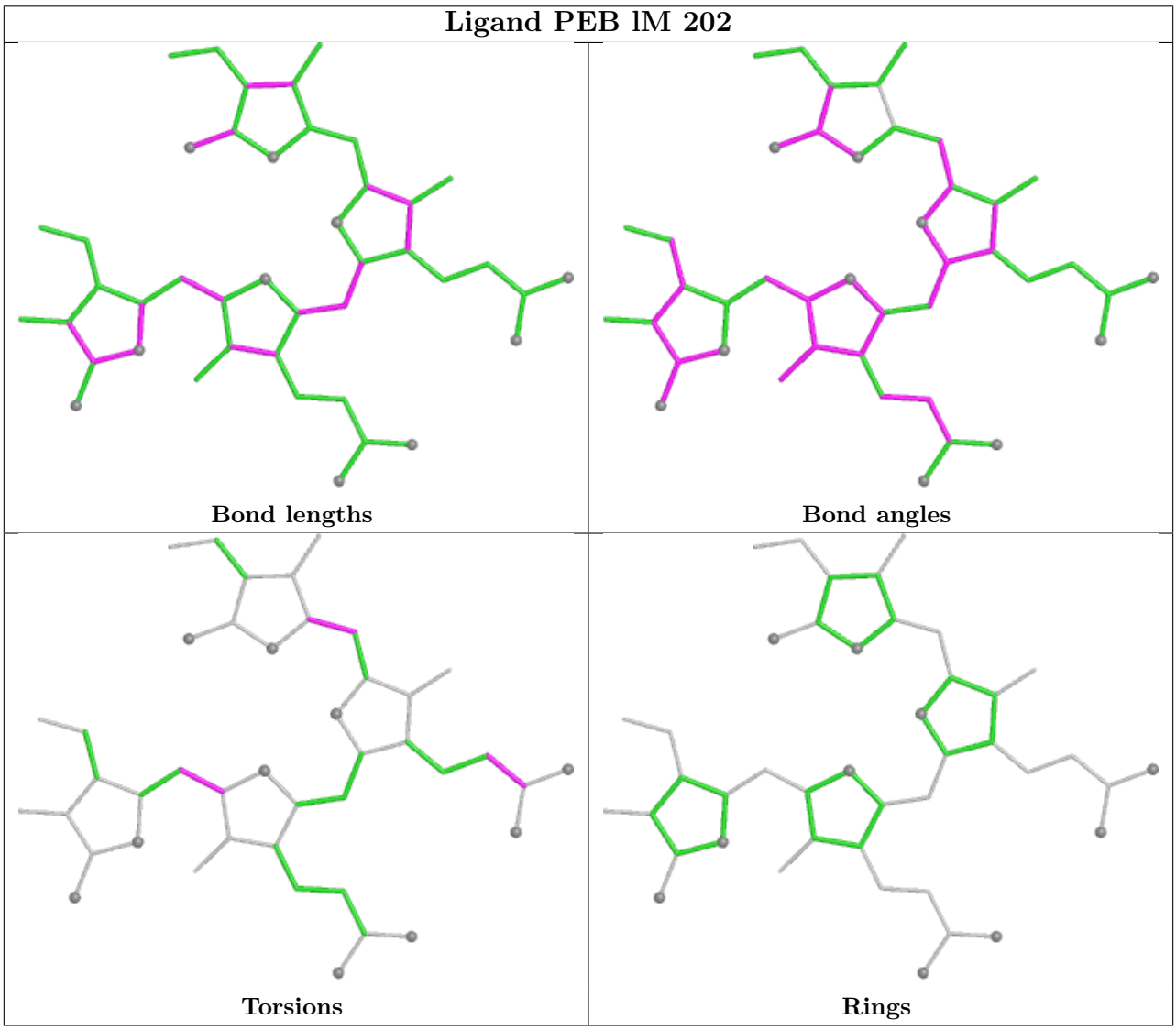
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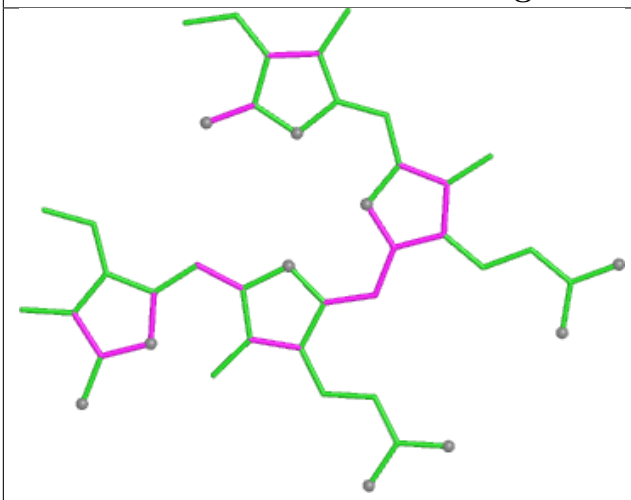
Ligand BCR KN 104



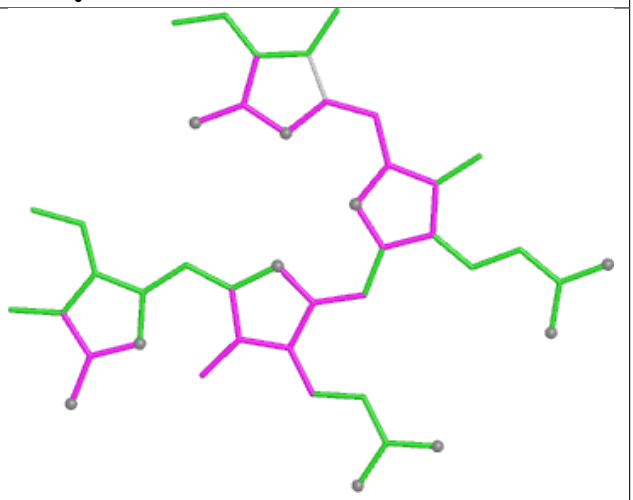
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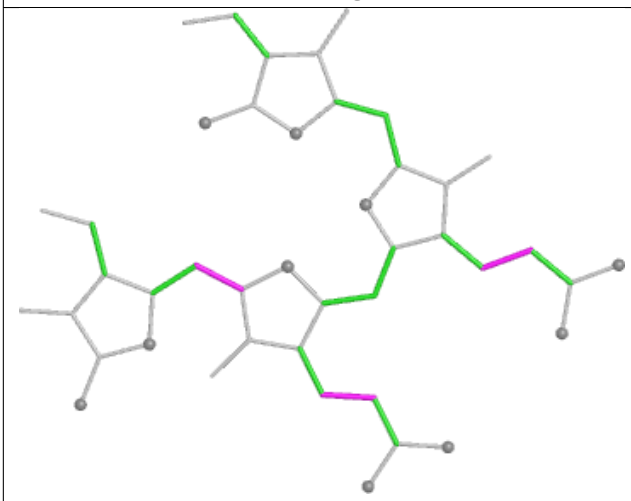
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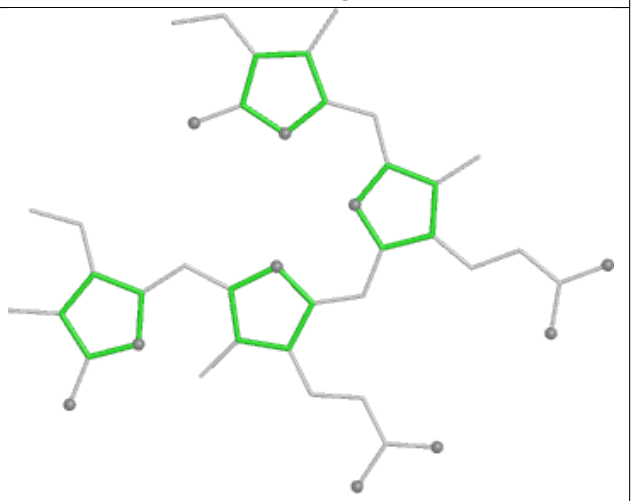
Bond lengths



Bond angles

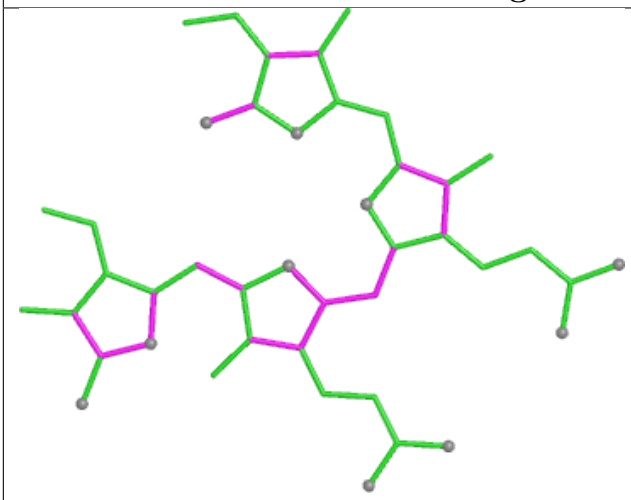


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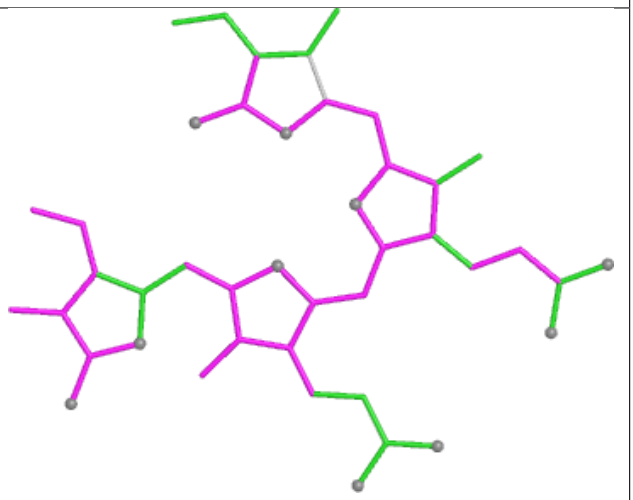


Rings

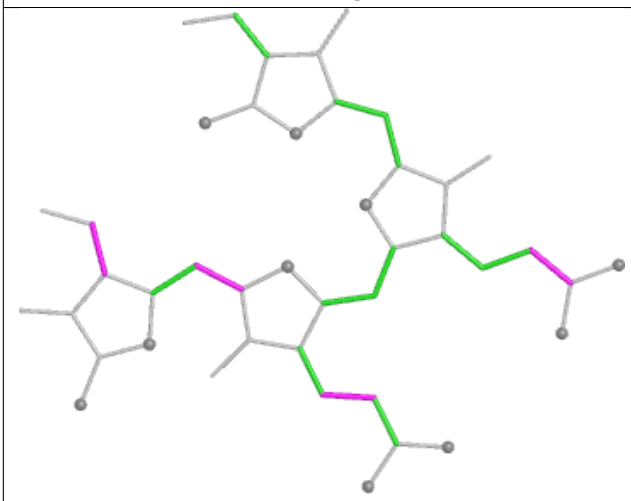
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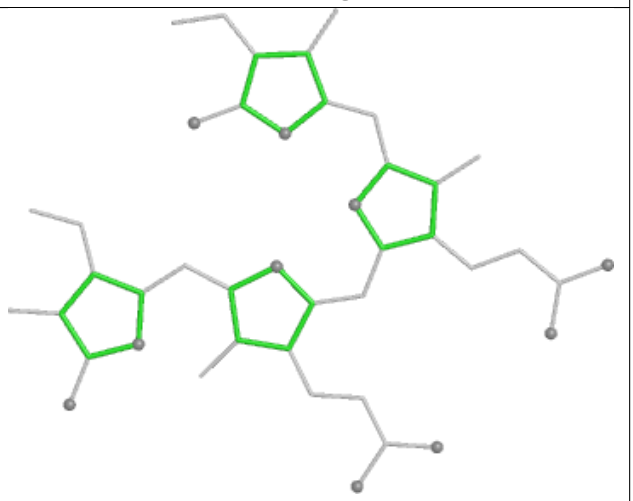
Bond lengths



Bond angles

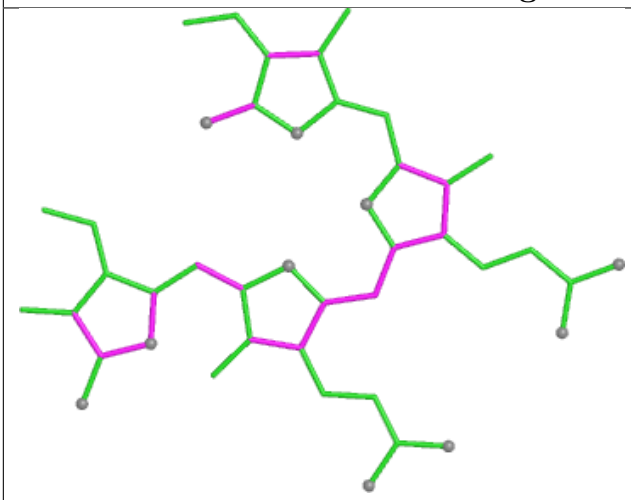


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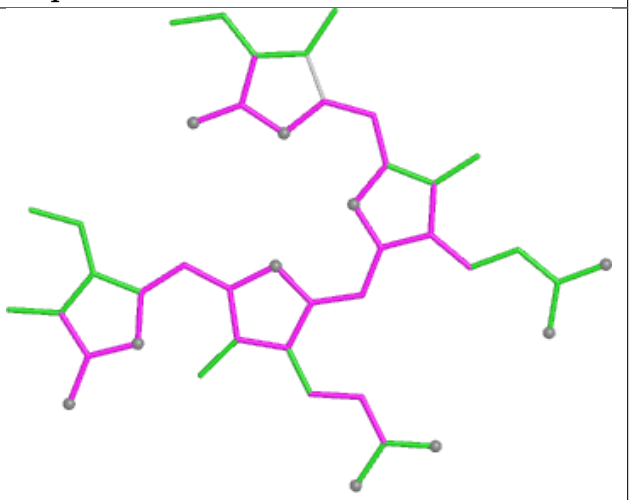


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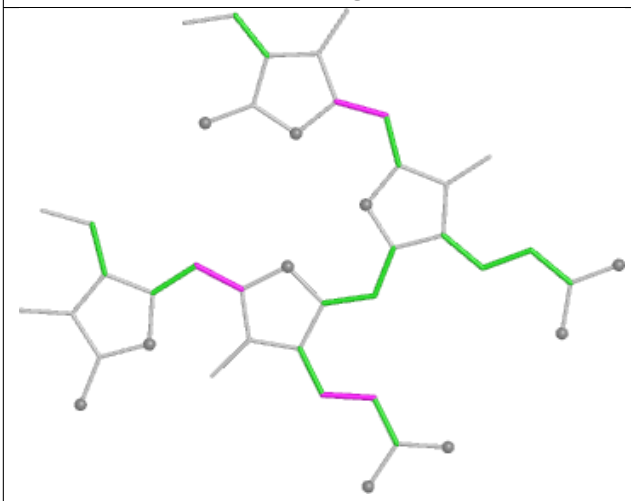
Ligand PEB q8 201



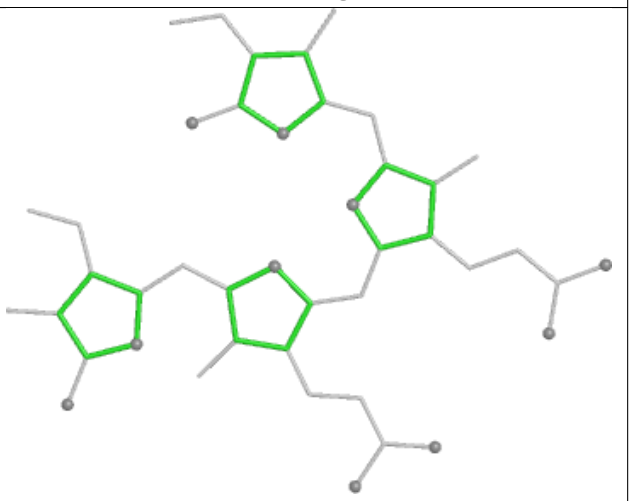
Bond lengths



Bond angles

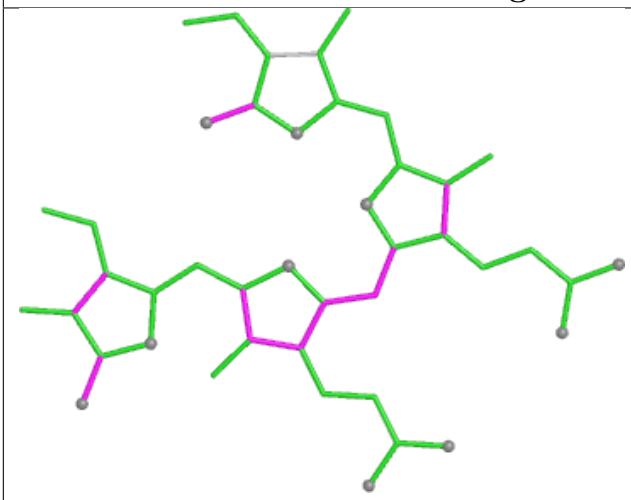


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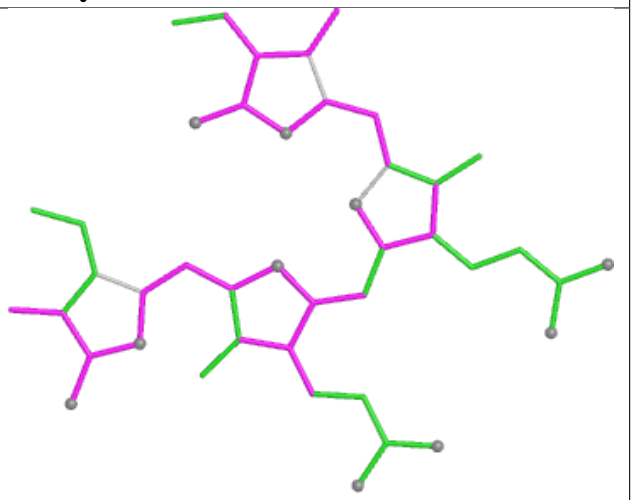


Rings

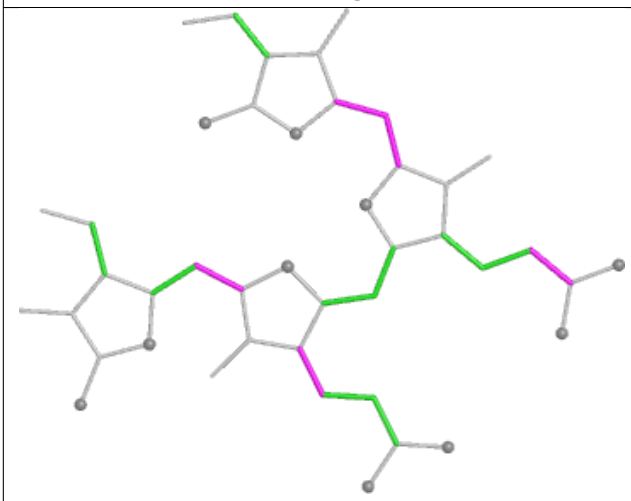
Ligand PUB AQ 302



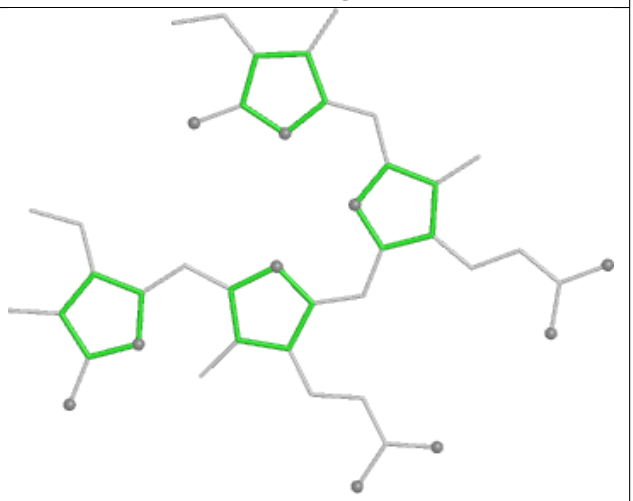
Bond lengths



Bond angles

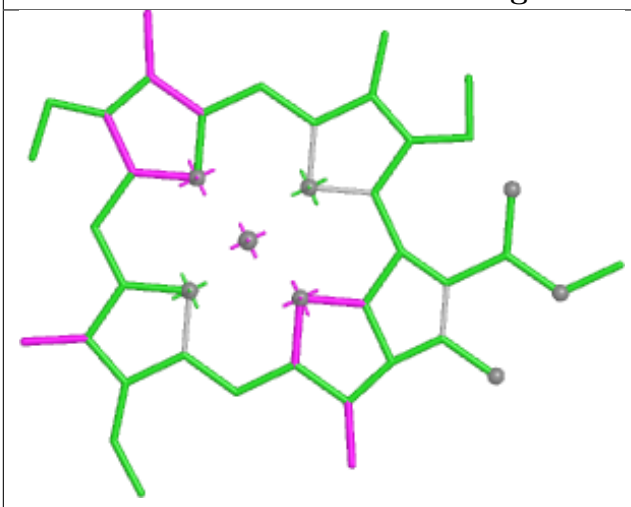


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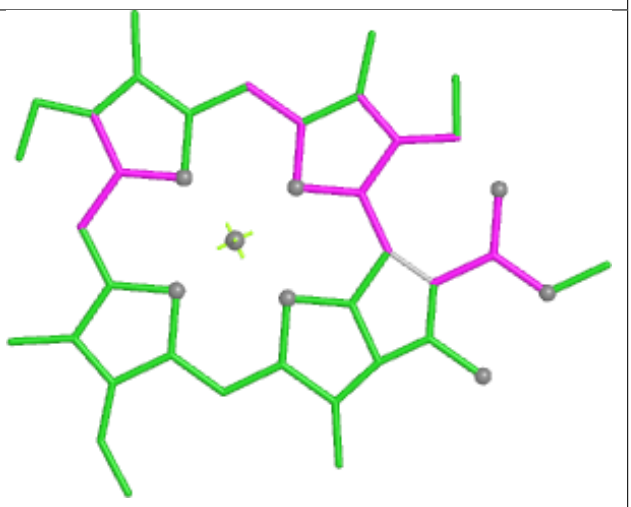


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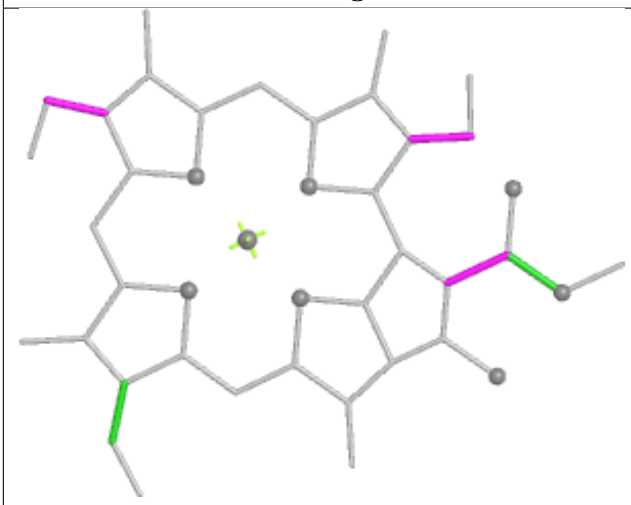
Ligand CLA BN 815



Bond lengths



Bond angles

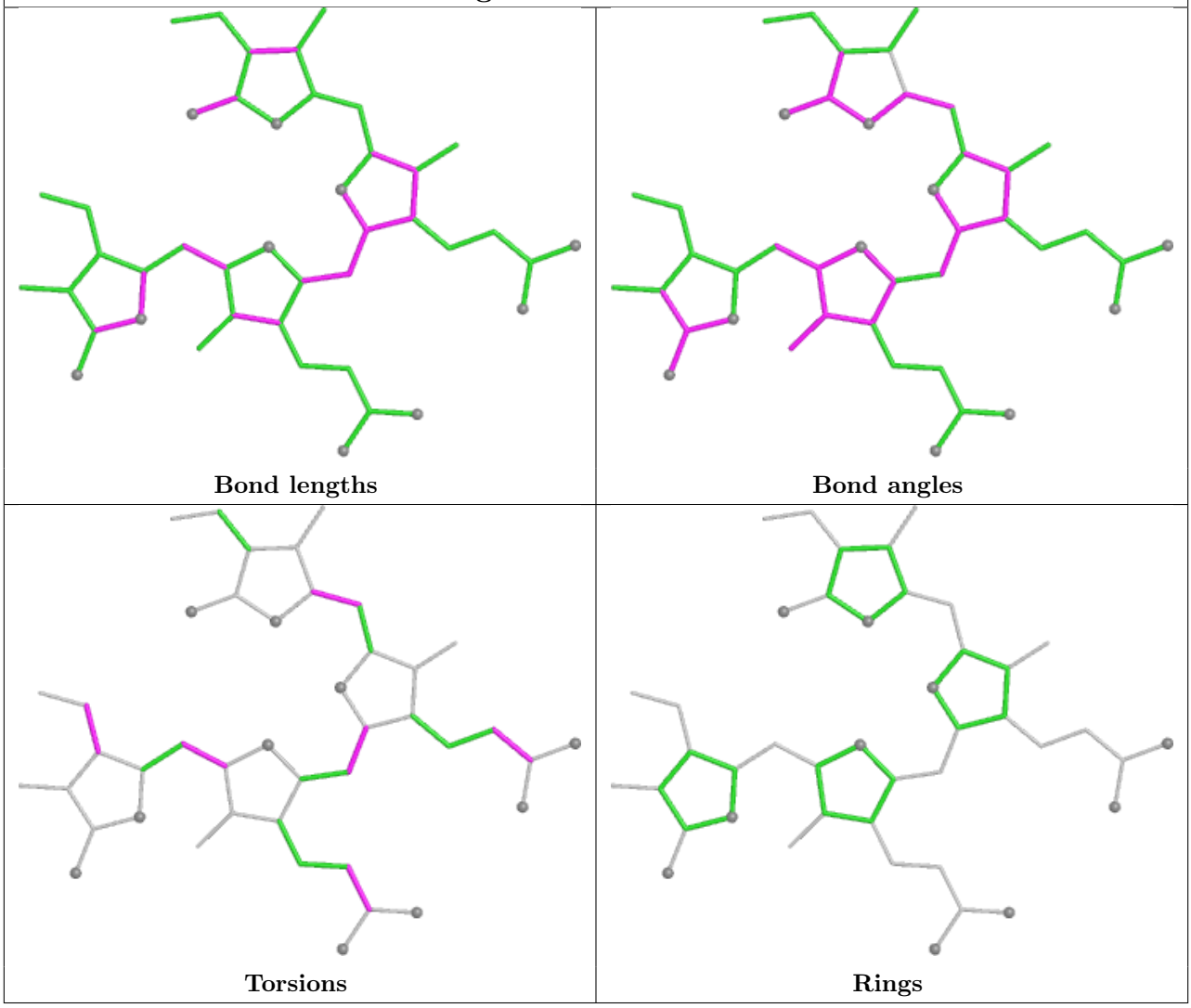


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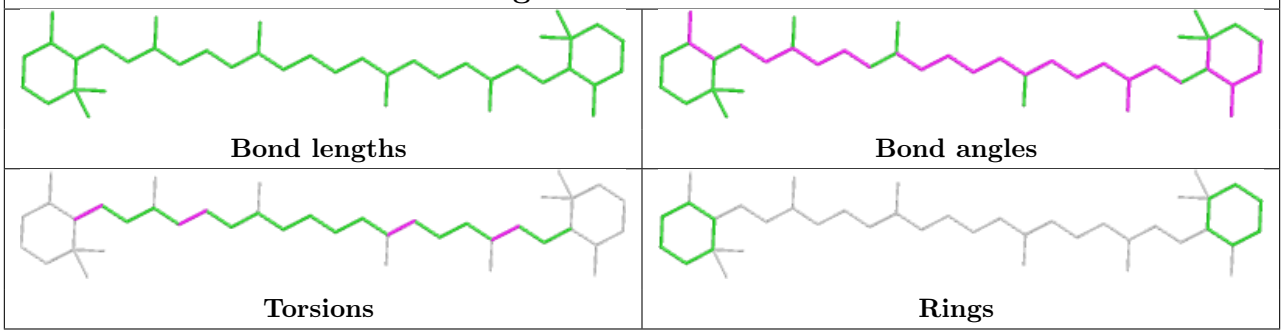


Rings

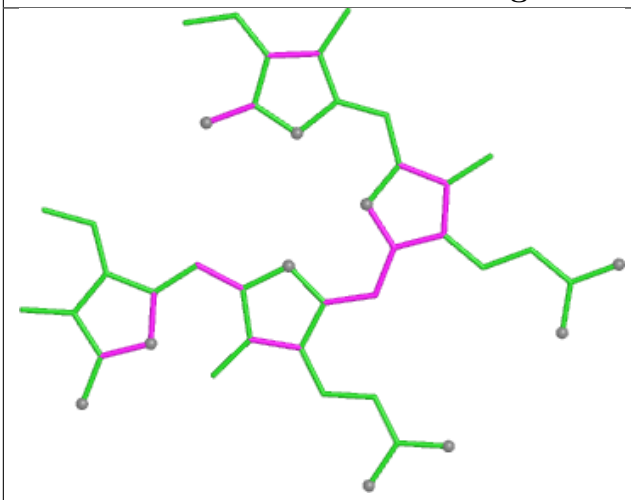
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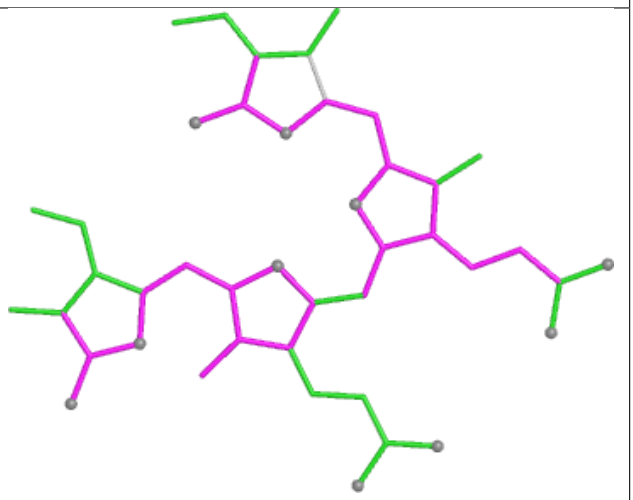
Ligand BCR JN 102



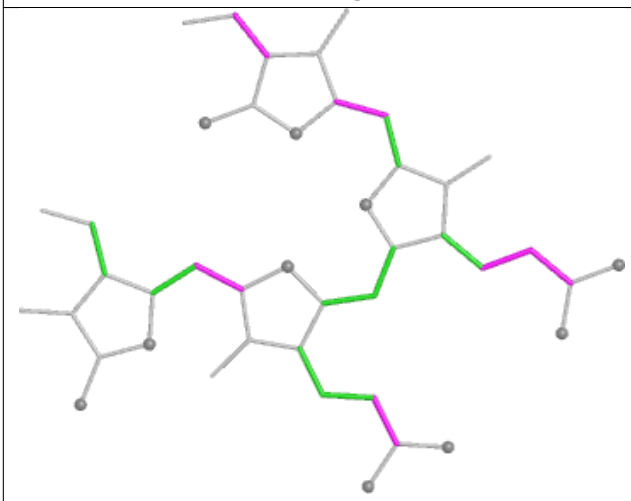
Ligand PEB AD 301



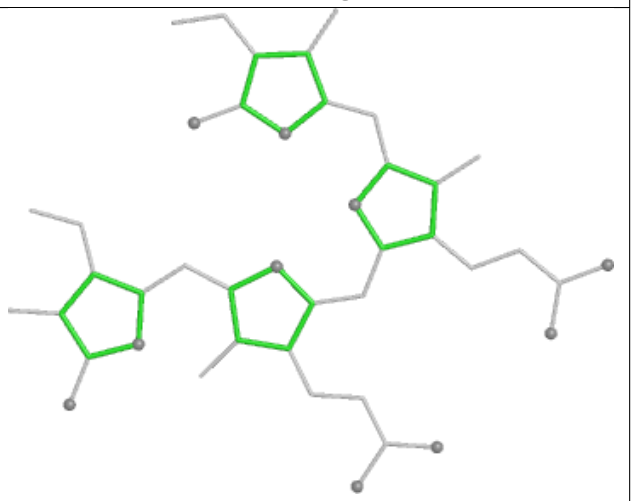
Bond lengths



Bond angles

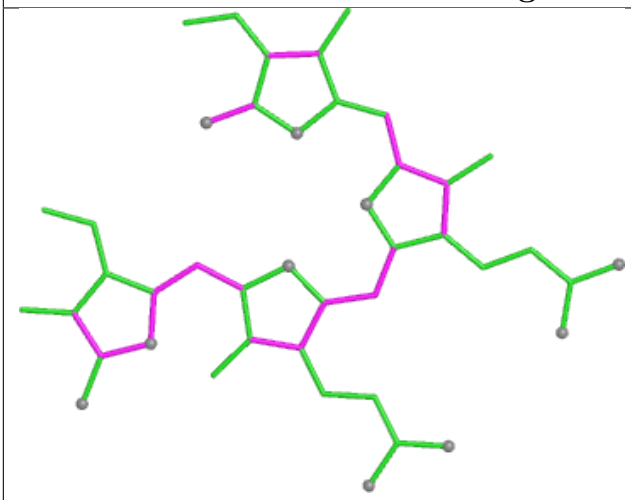


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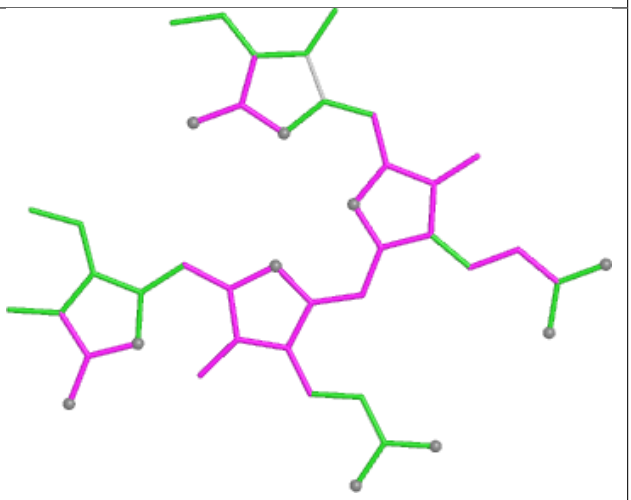


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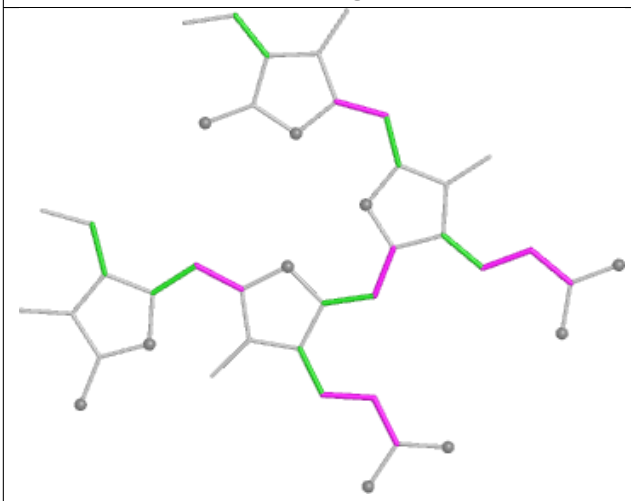
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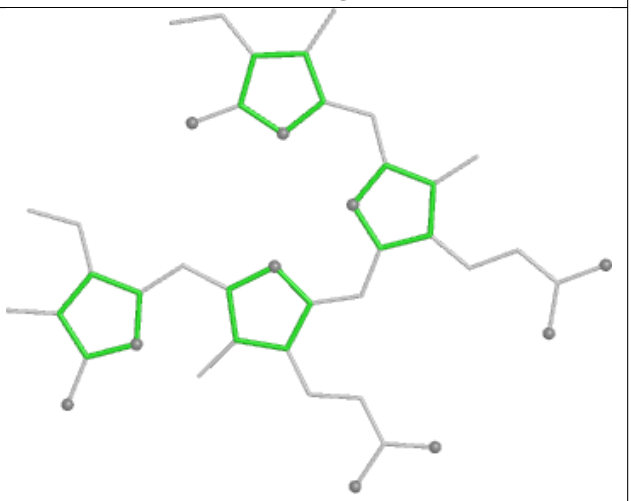
Bond lengths



Bond angles

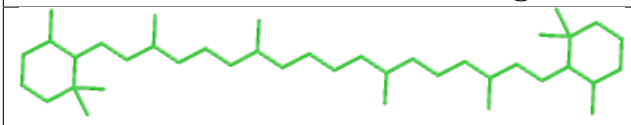


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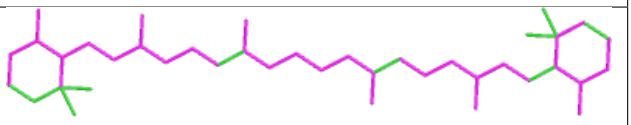


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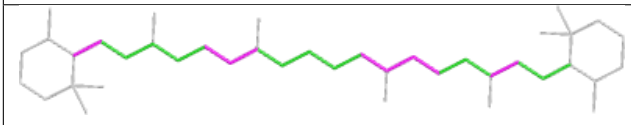
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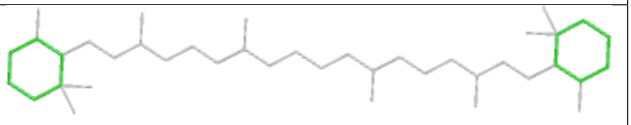
Bond lengths



Bond angles

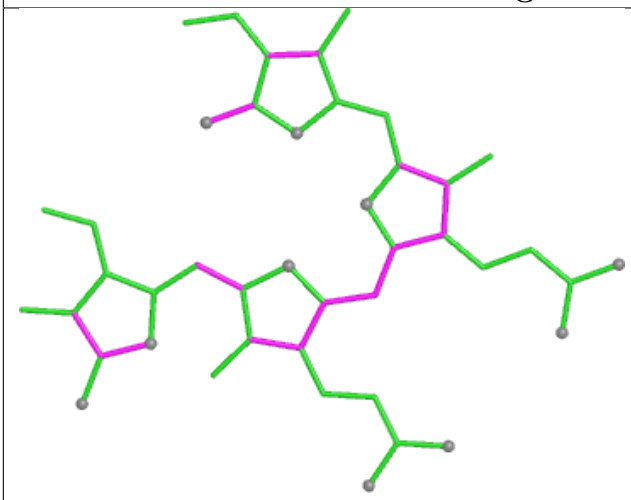


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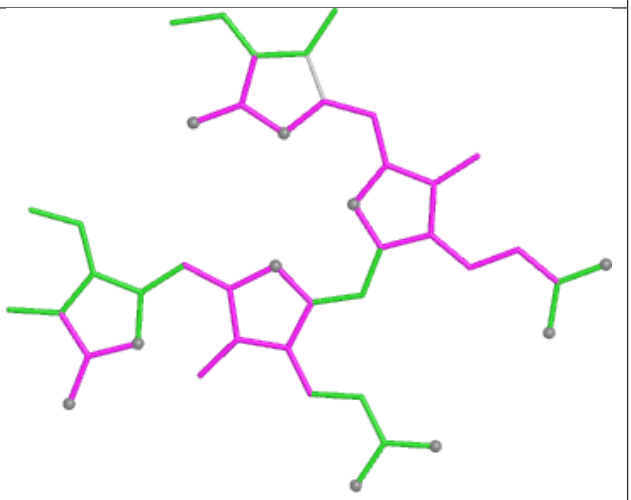


Rings

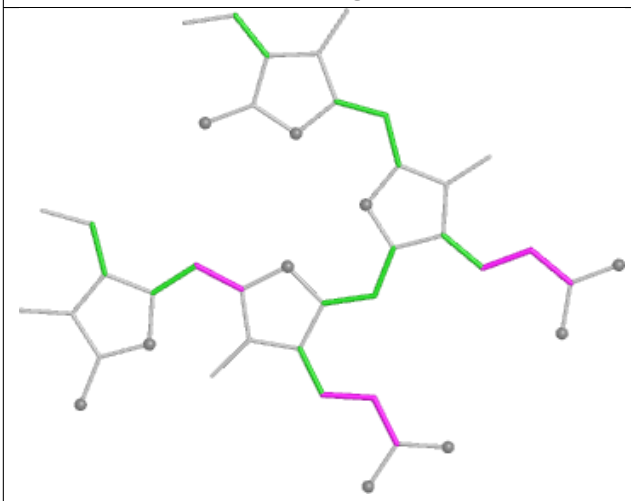
Ligand PEB P1 202



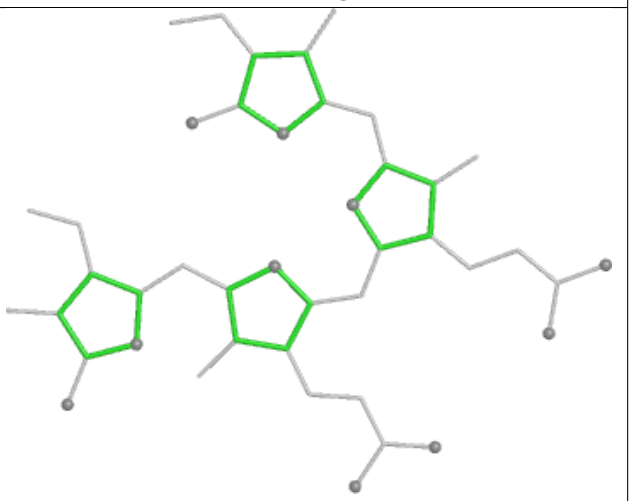
Bond lengths



Bond angles

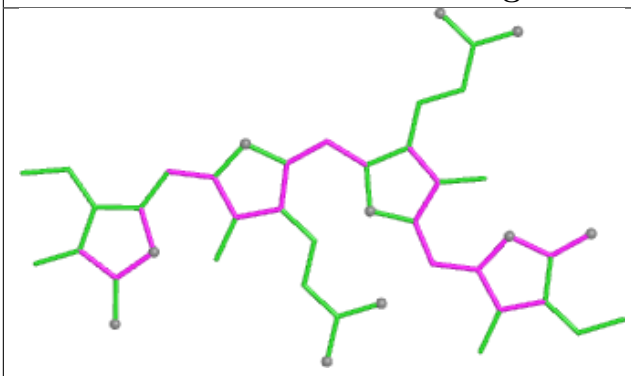


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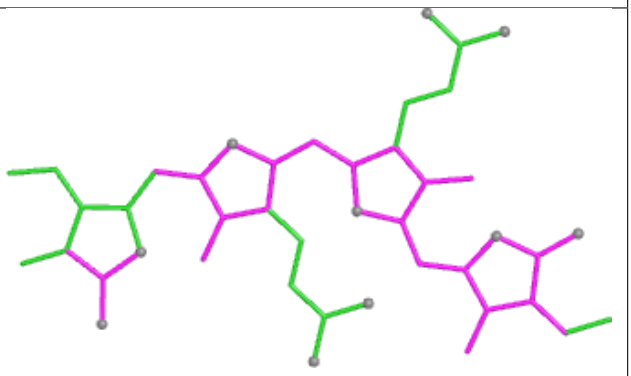


Rings

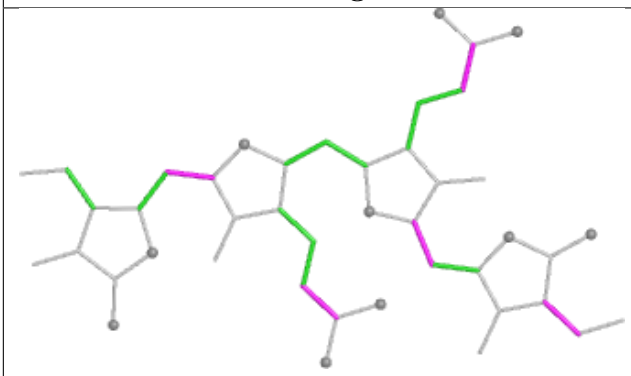
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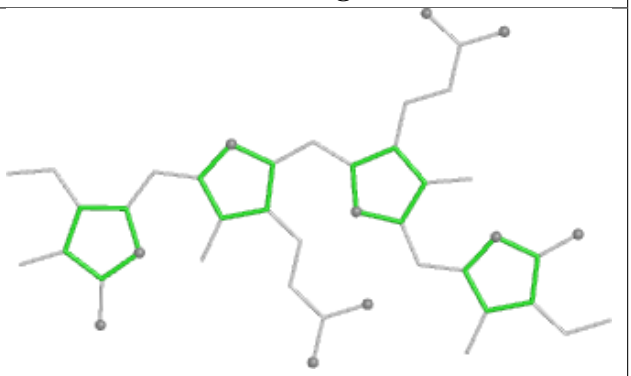
Bond lengths



Bond angles

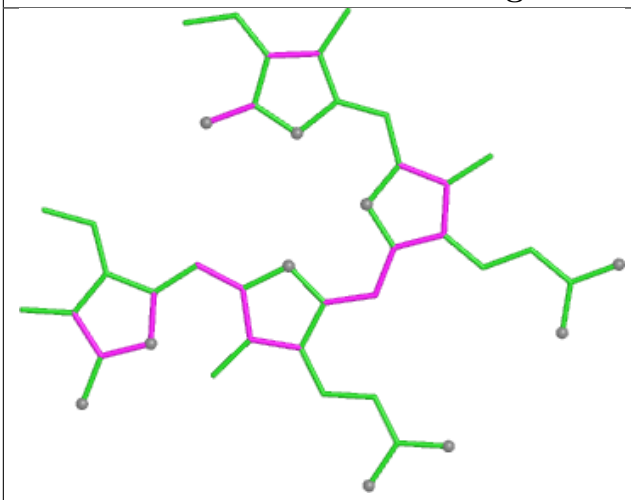


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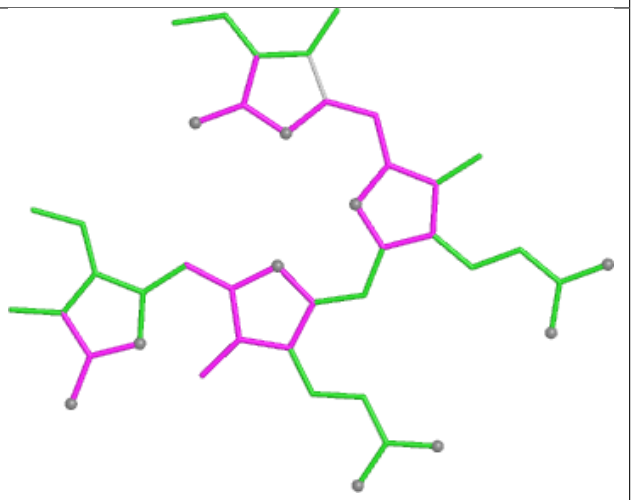


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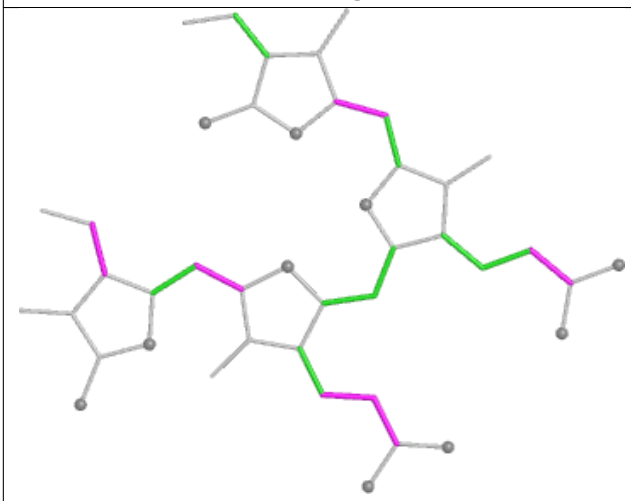
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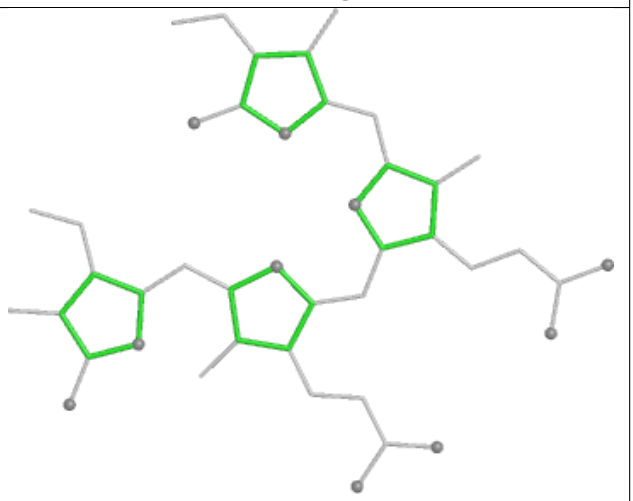
Bond lengths



Bond angles

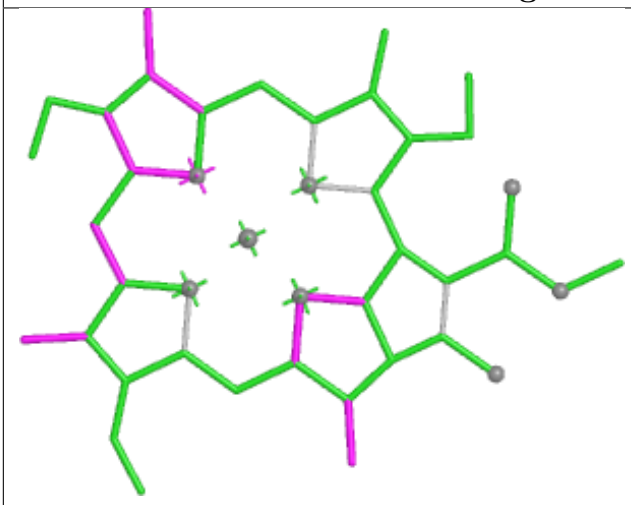


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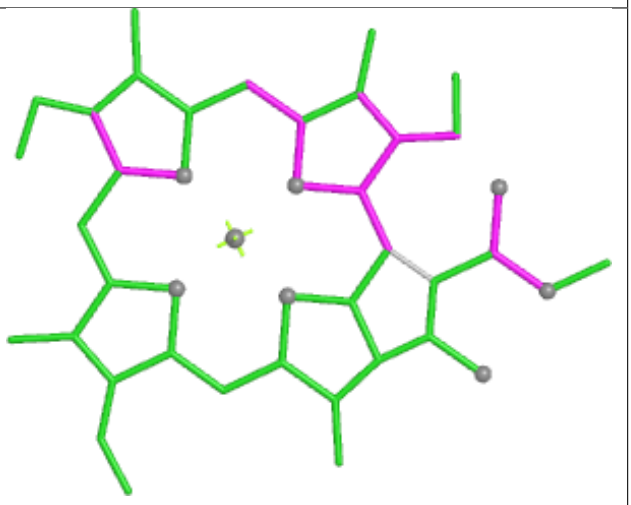


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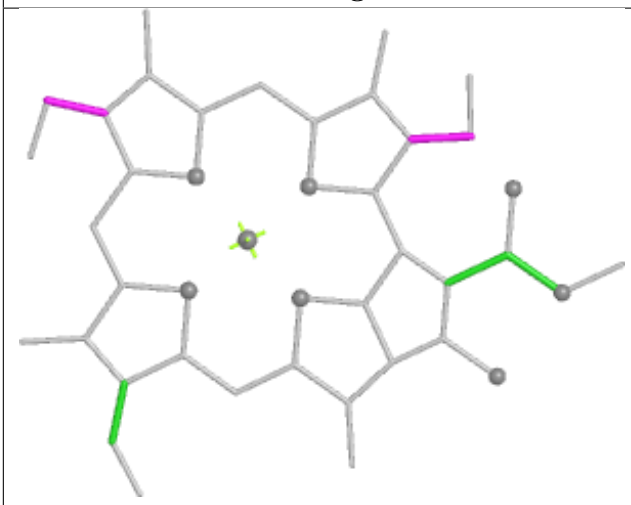
Ligand CLA 12 604



Bond lengths



Bond angles

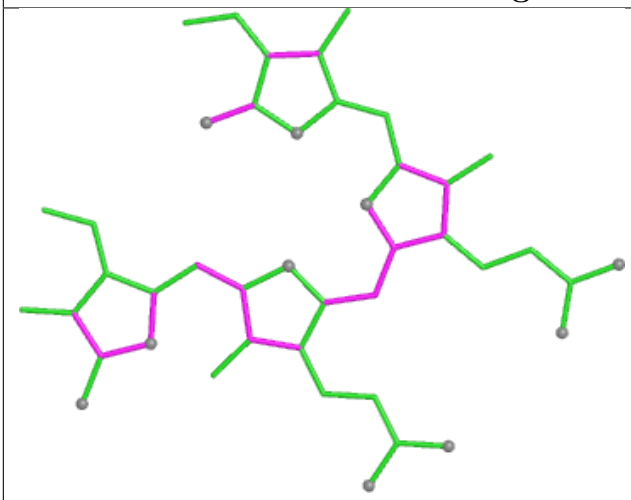


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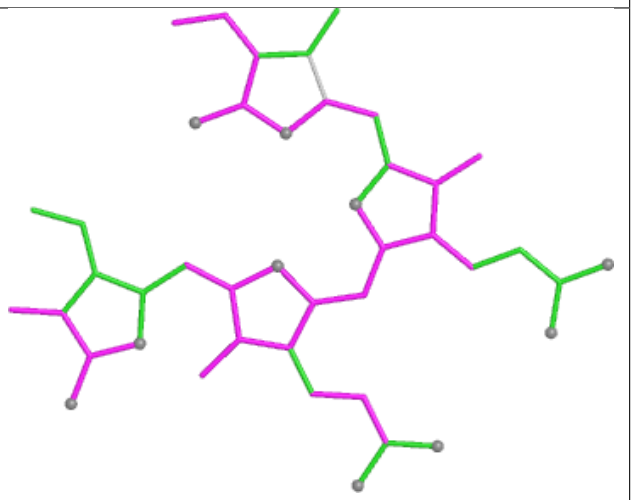


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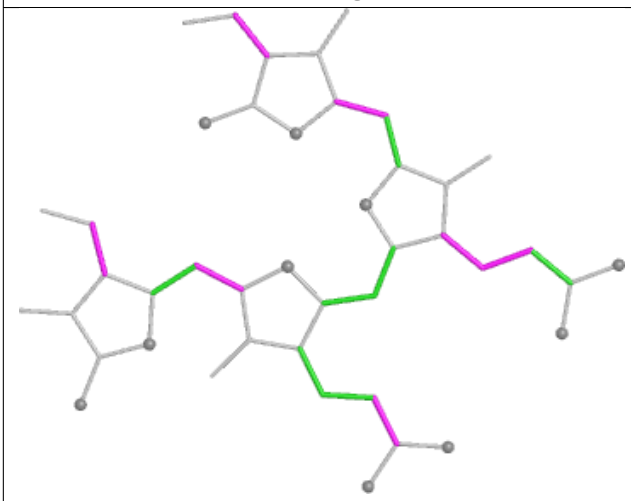
Ligand PEB ED 201



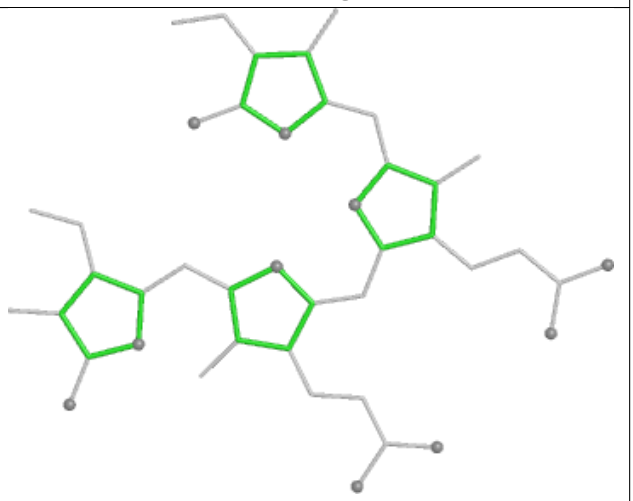
Bond lengths



Bond angles

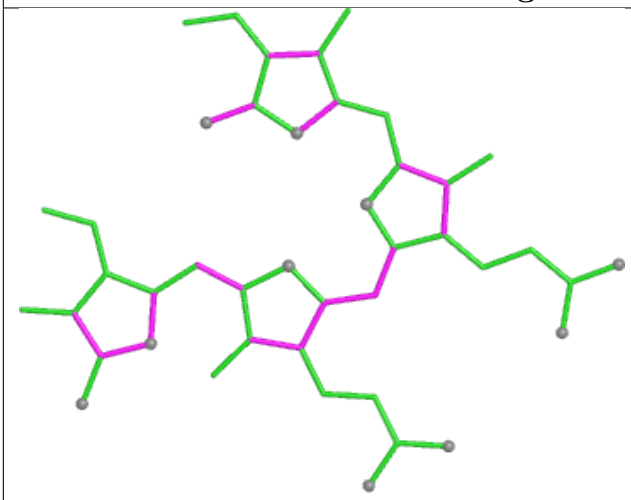


Torsions

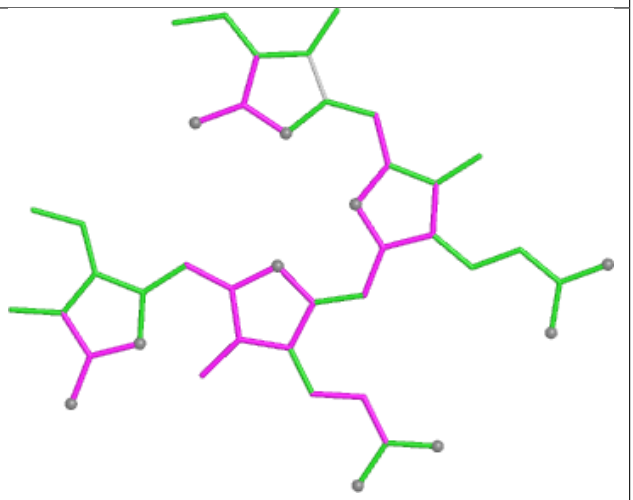


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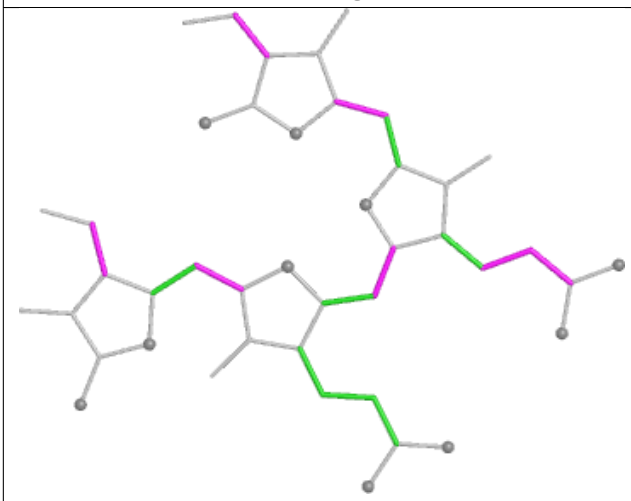
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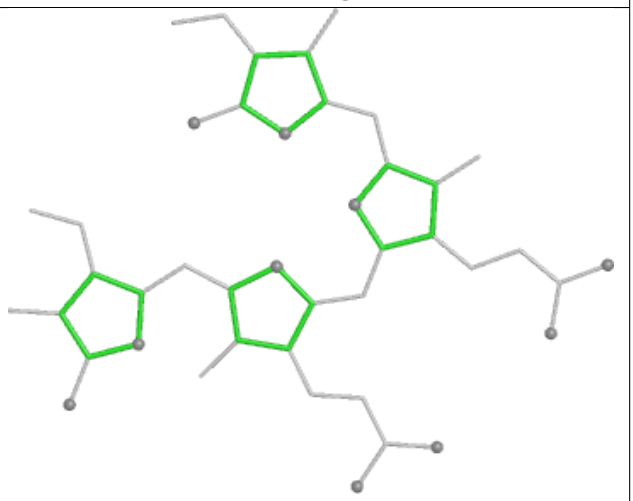
Bond lengths



Bond angles

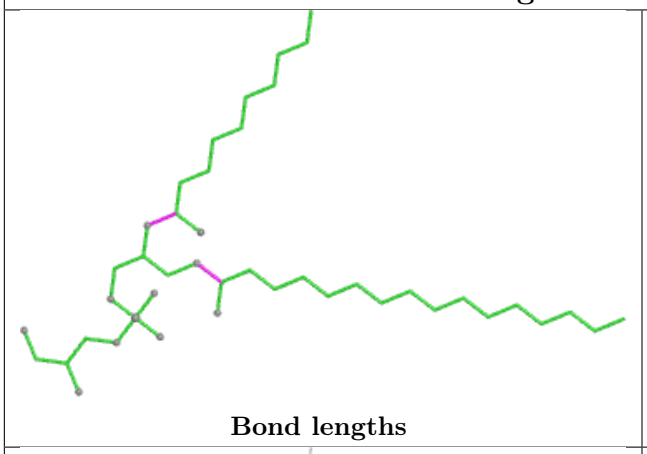


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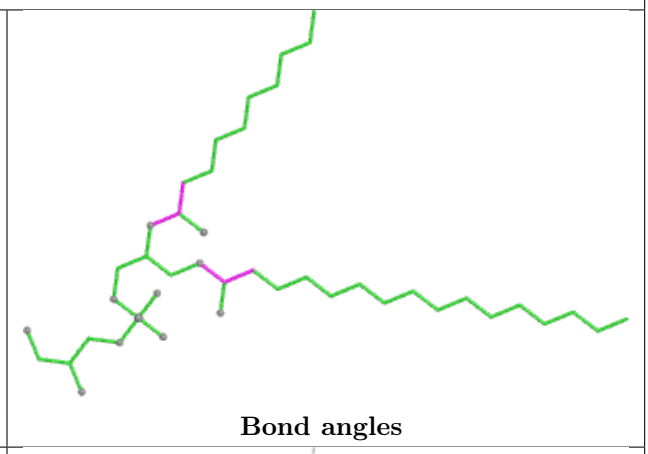


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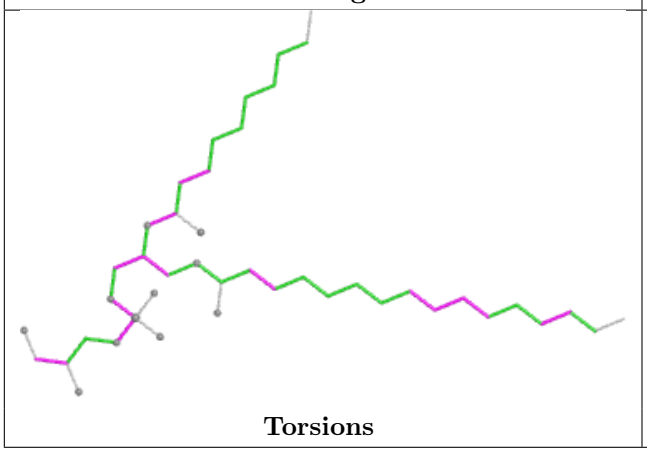
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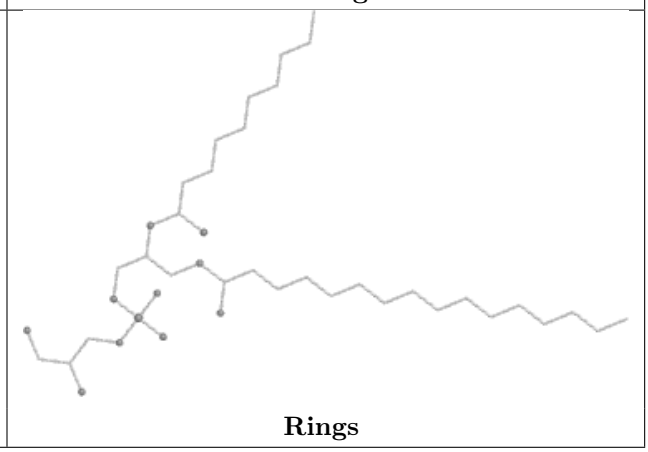
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Bond angles

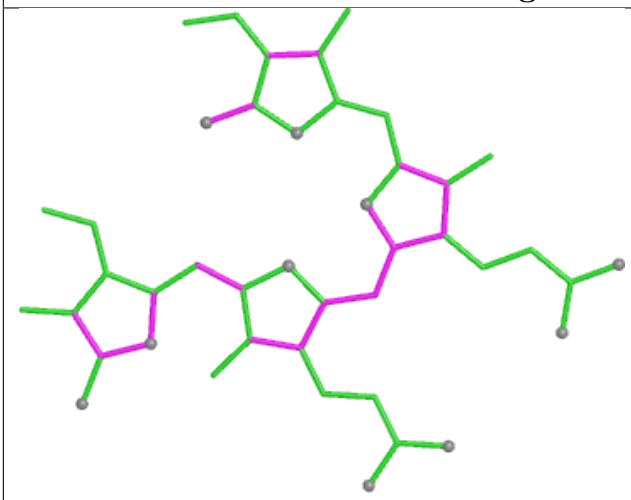


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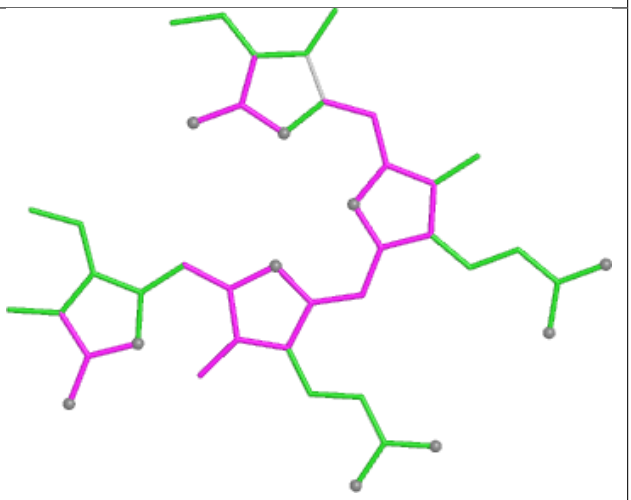


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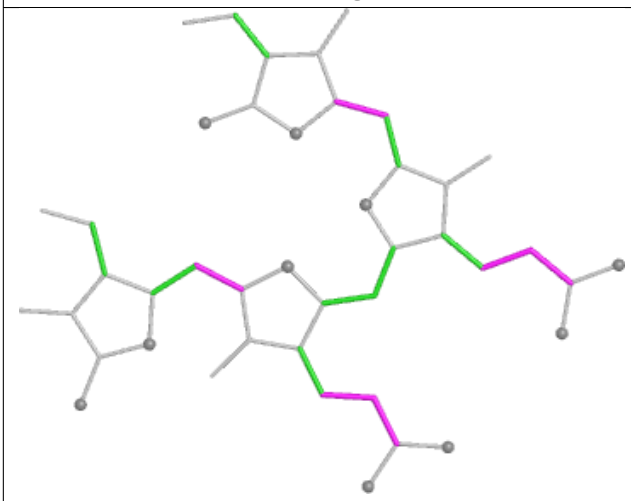
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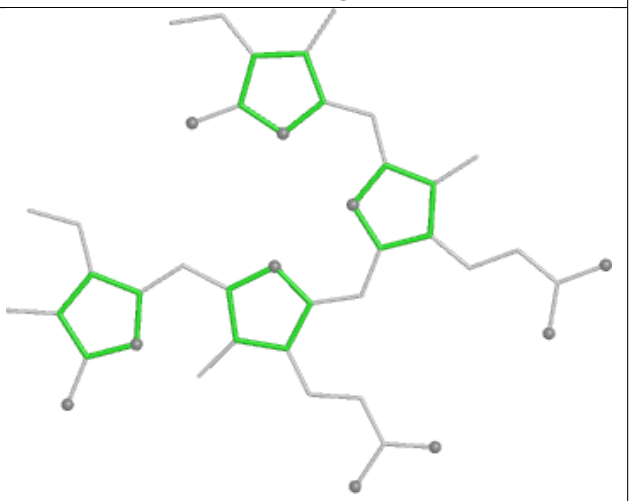
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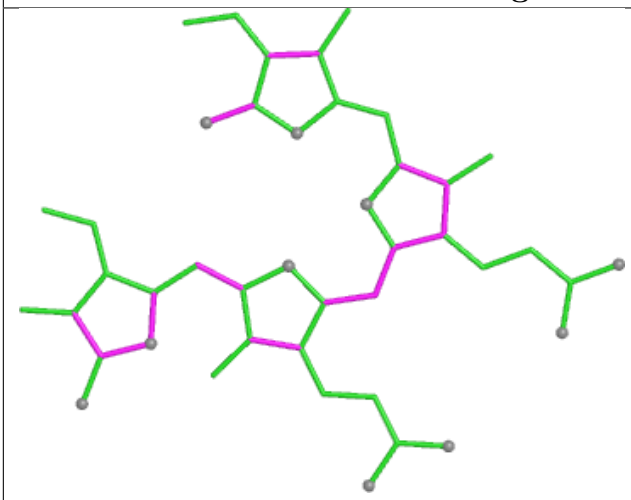


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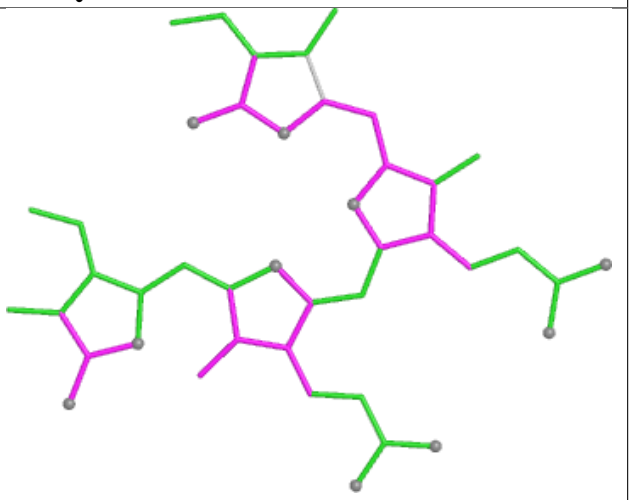


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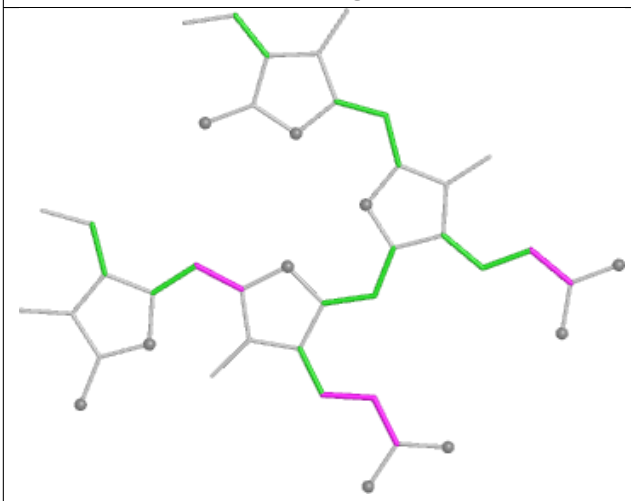
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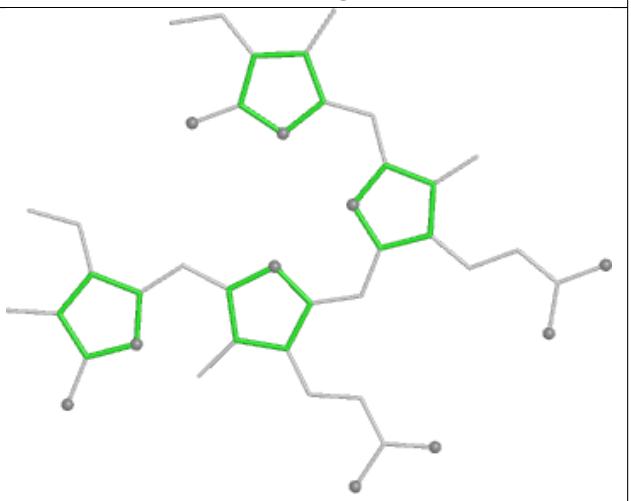
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Bond angles

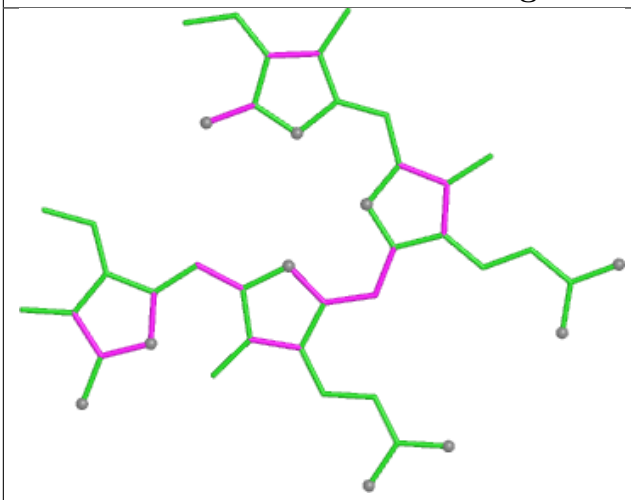


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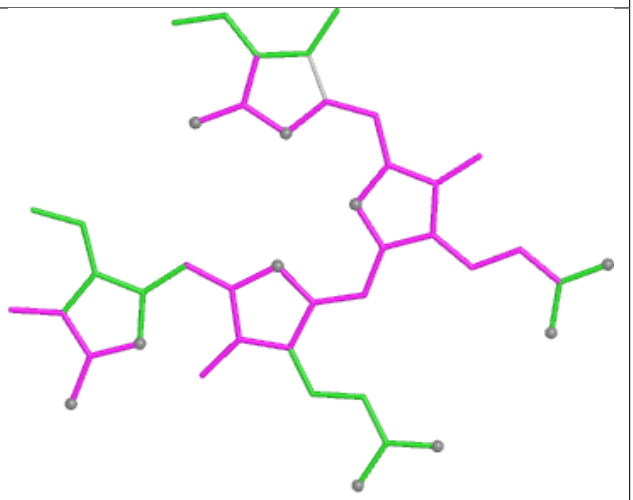


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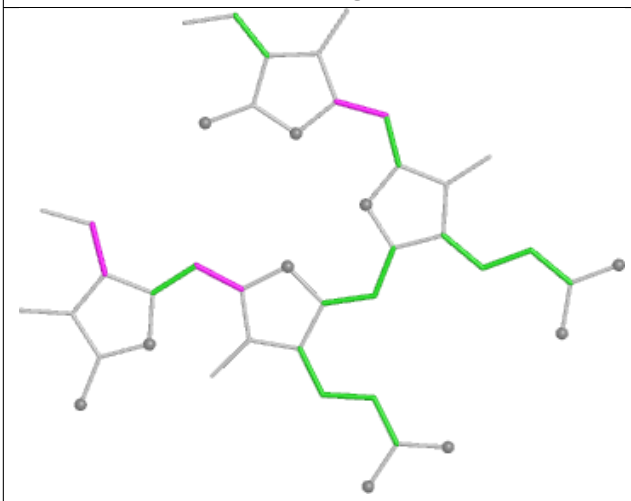
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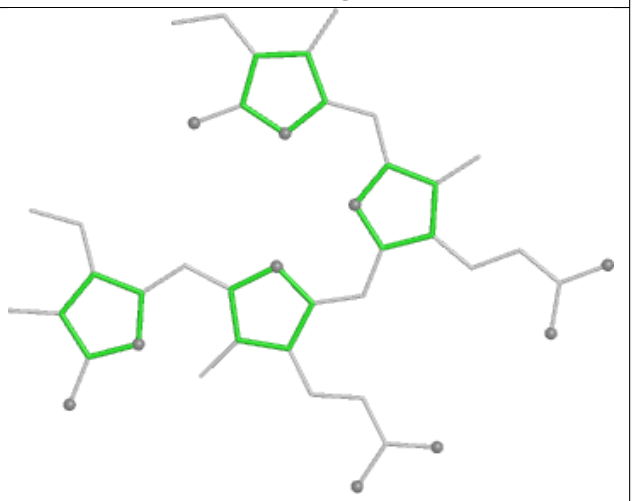
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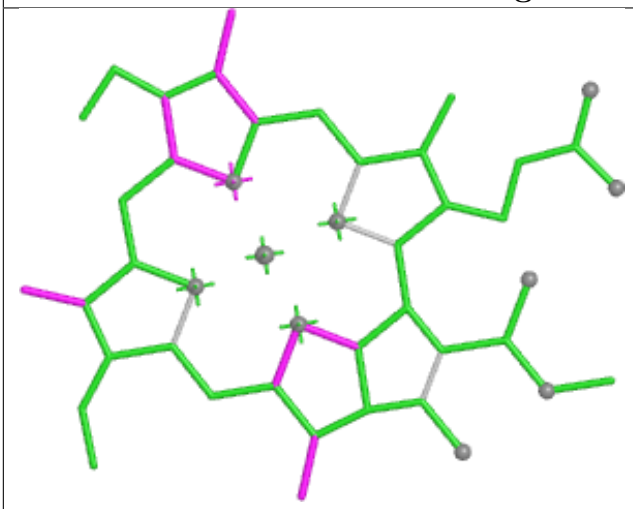


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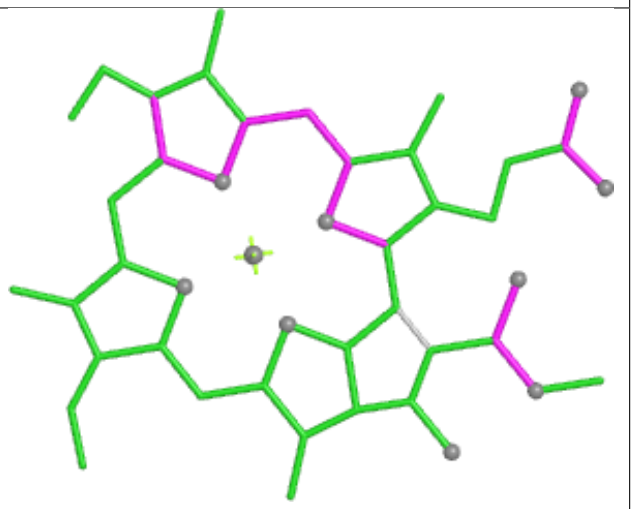


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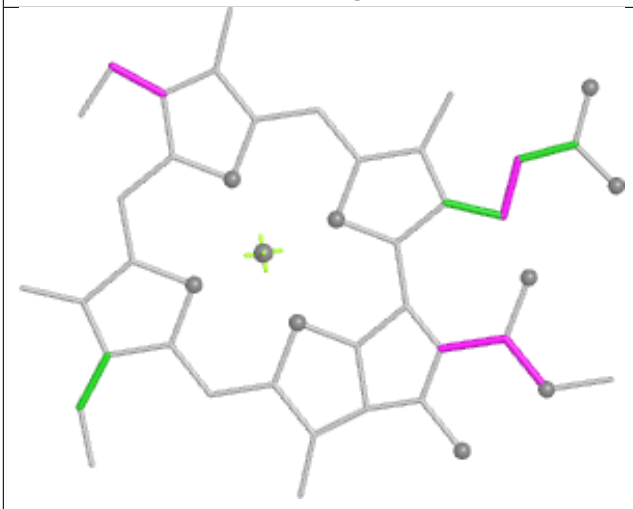
Ligand CLA A2 836



Bond lengths



Bond angles

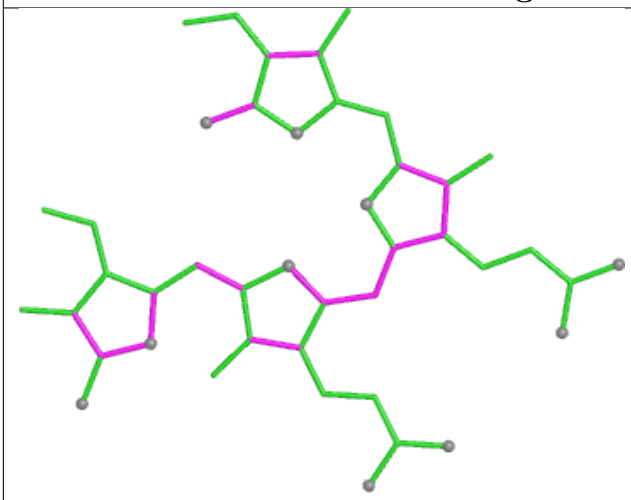


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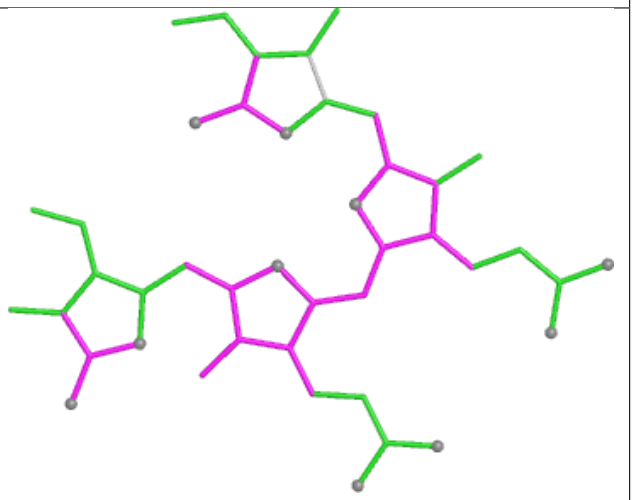


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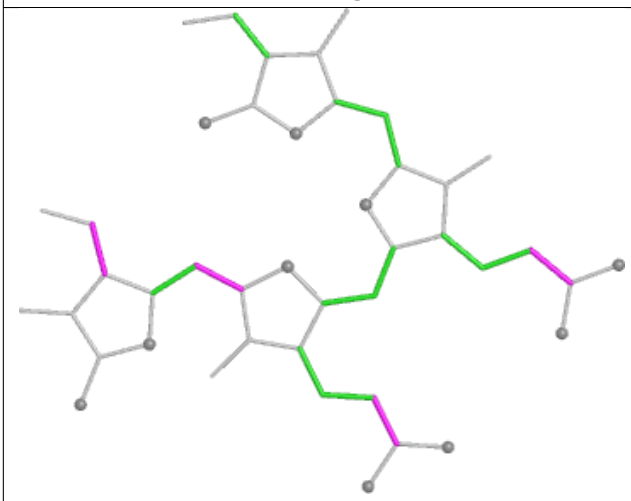
Ligand PEB aO 202



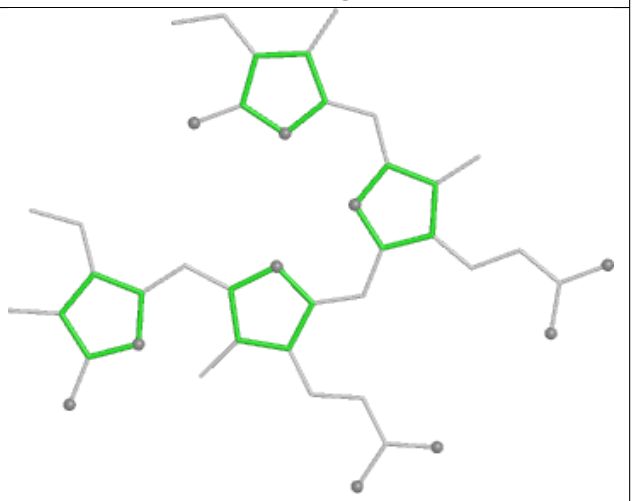
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Bond angles

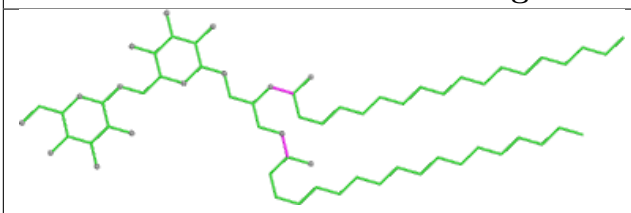


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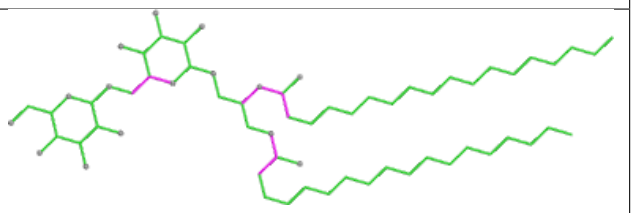


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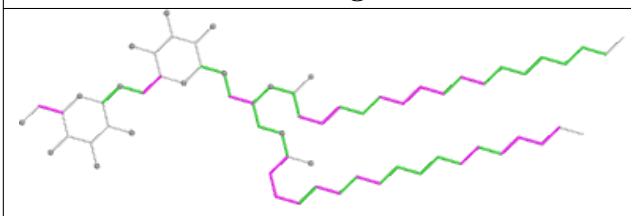
Ligand DGD B2 844



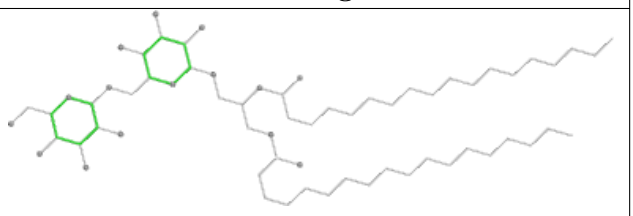
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Bond angles

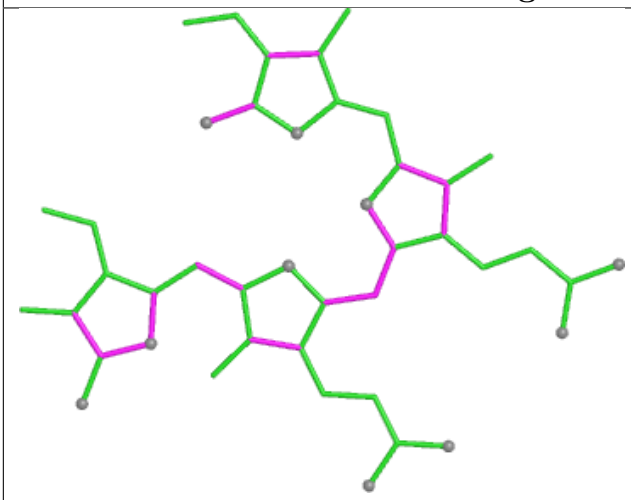


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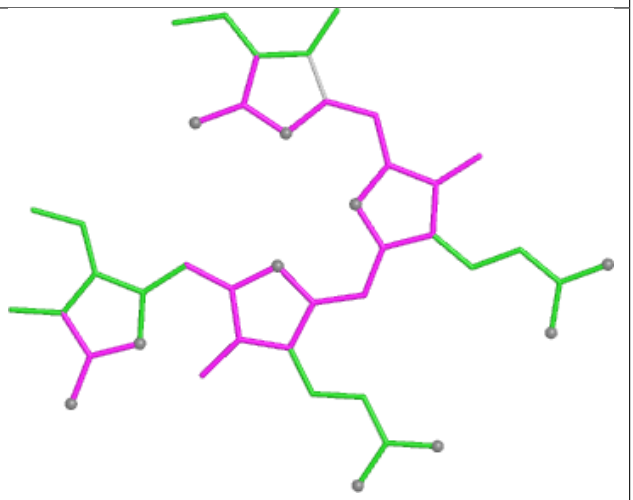


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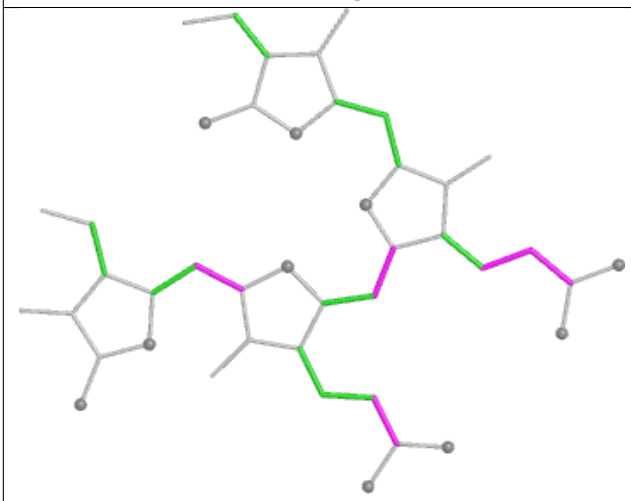
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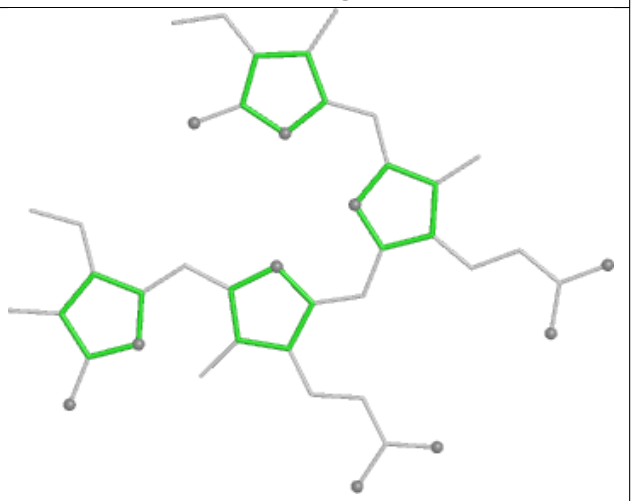
Bond lengths



Bond angles

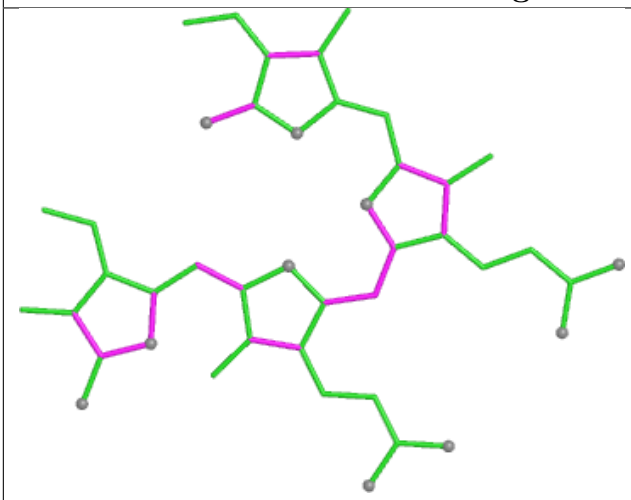


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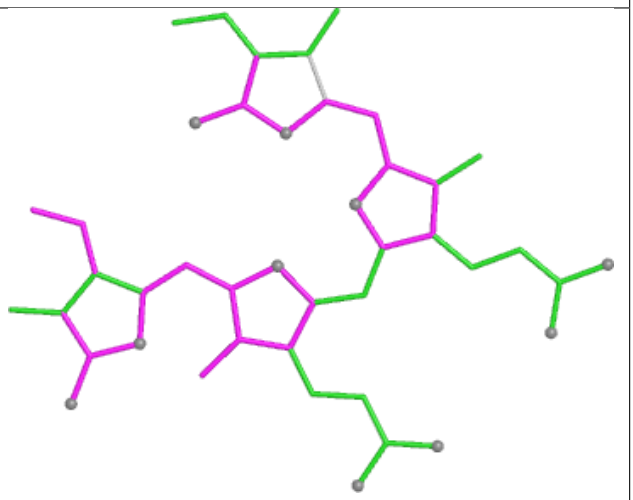


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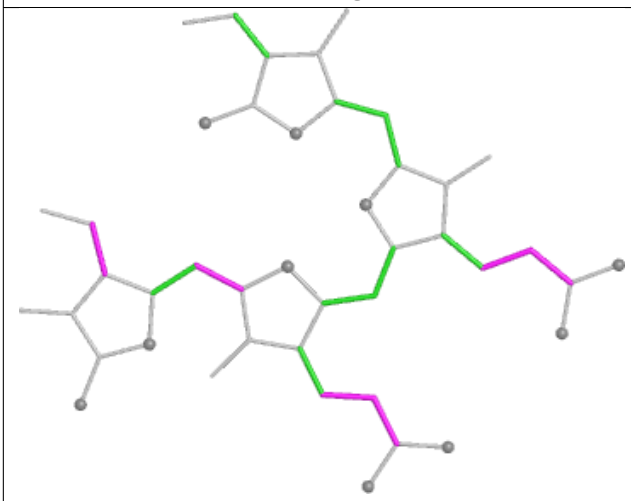
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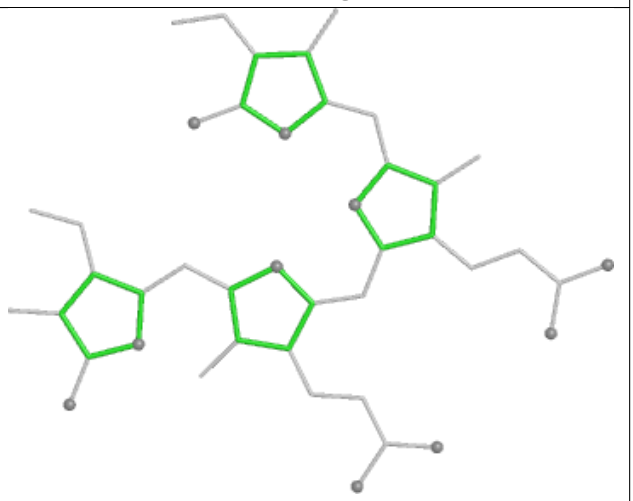
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Bond angles

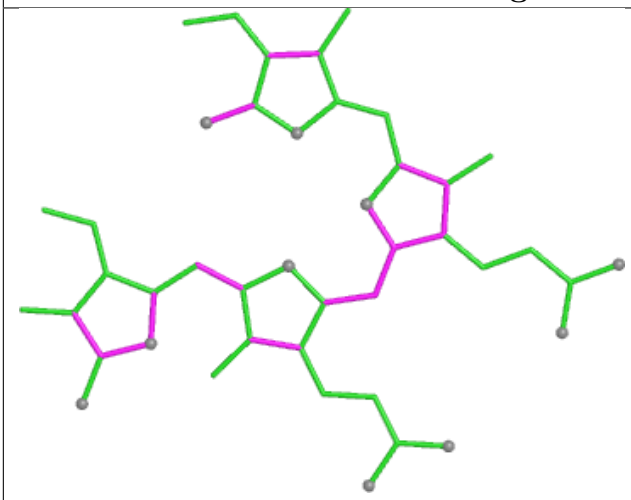


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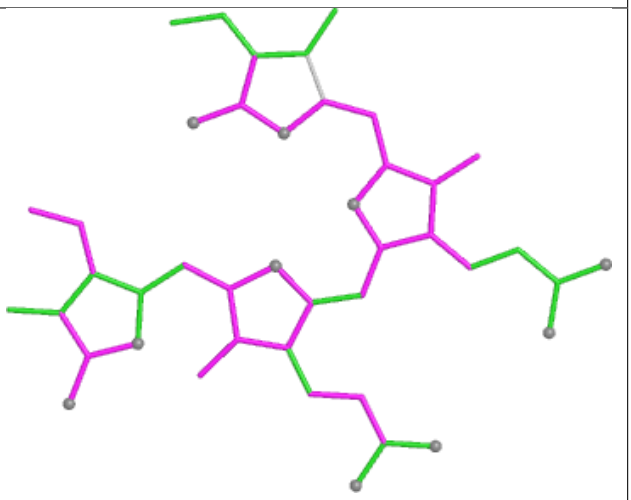


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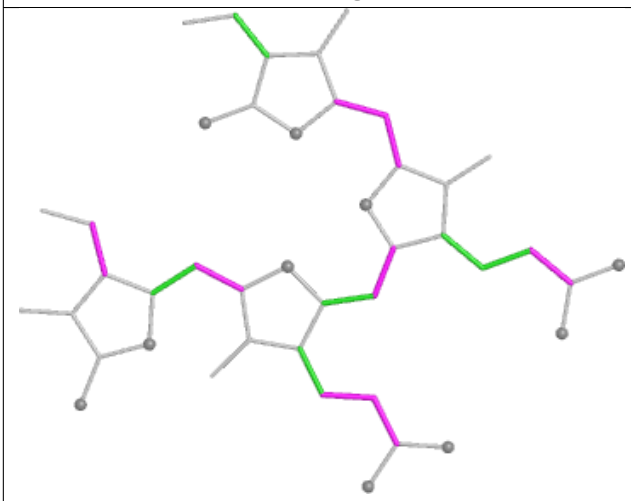
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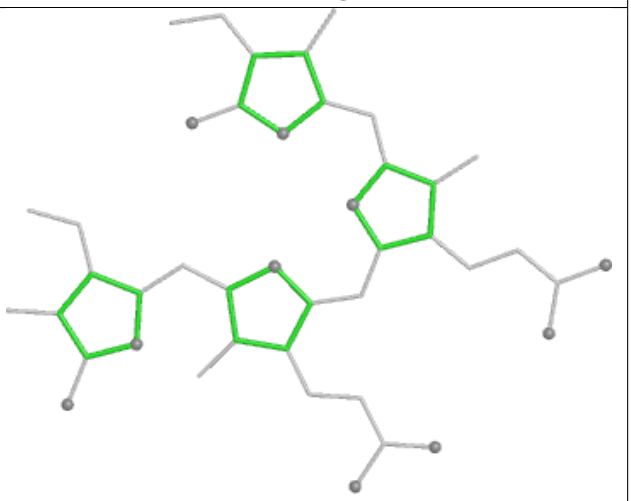
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Bond angles

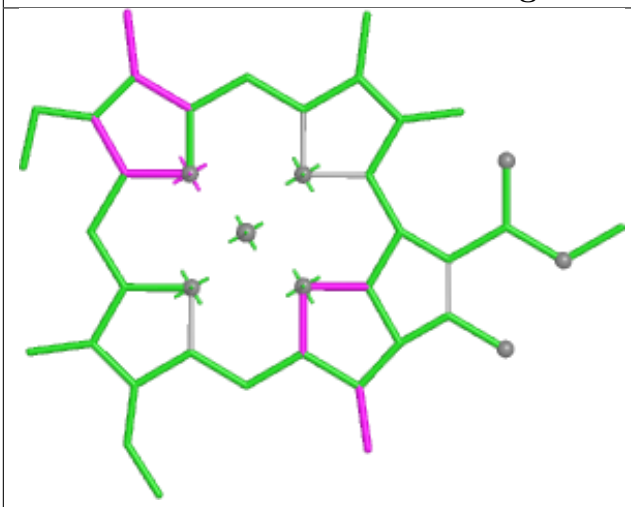


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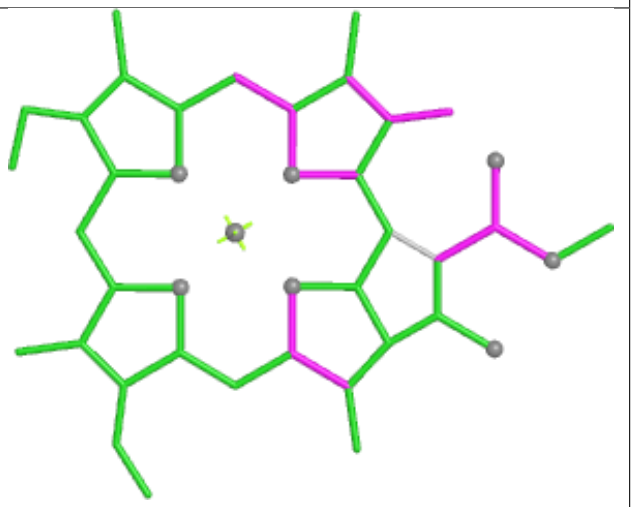


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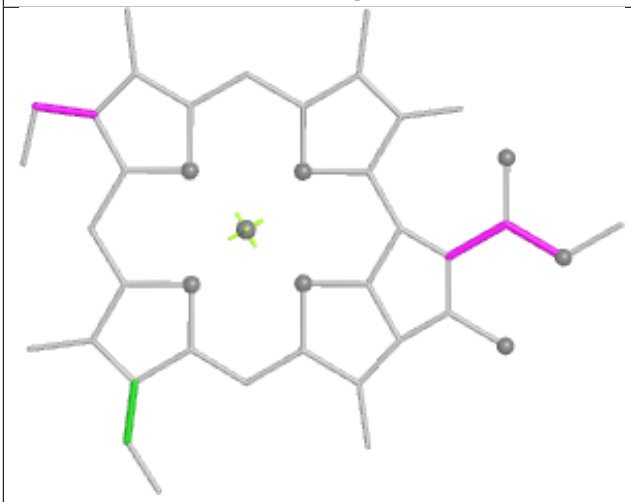
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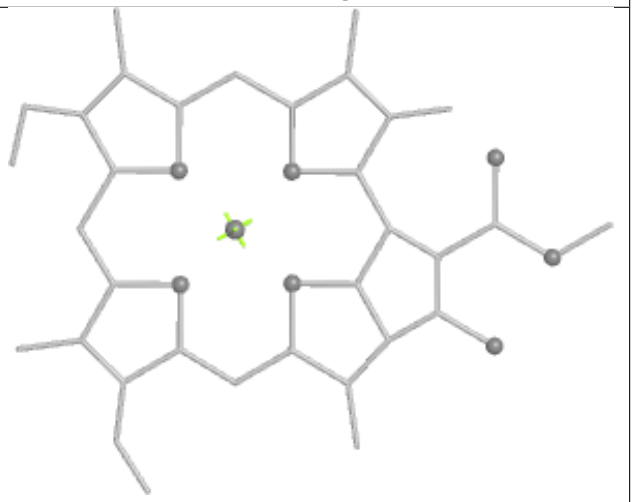
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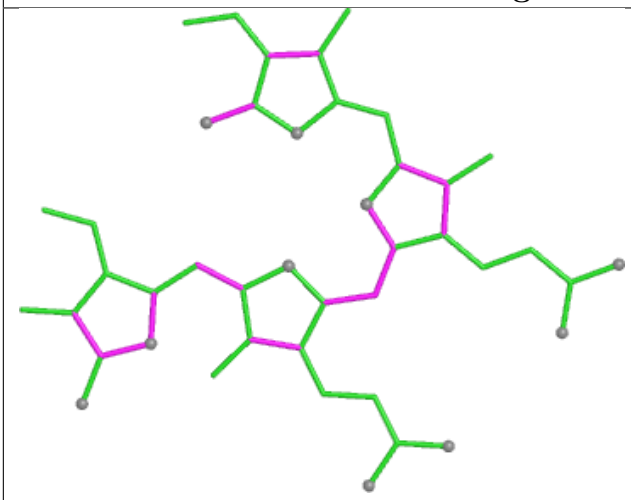


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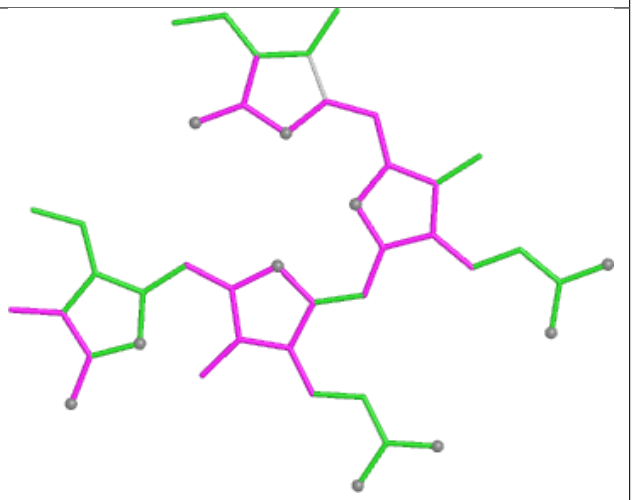


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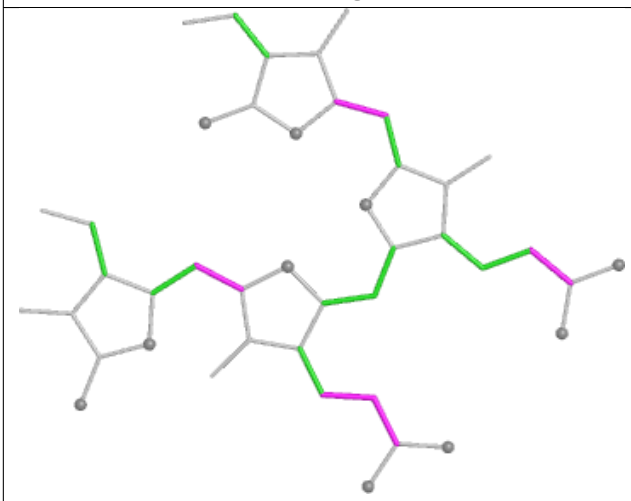
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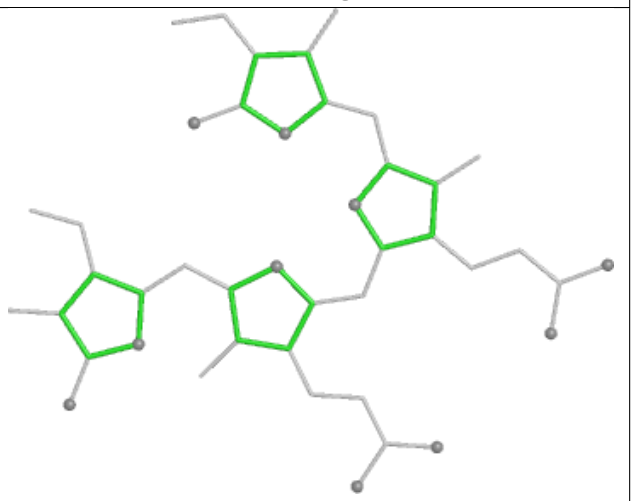
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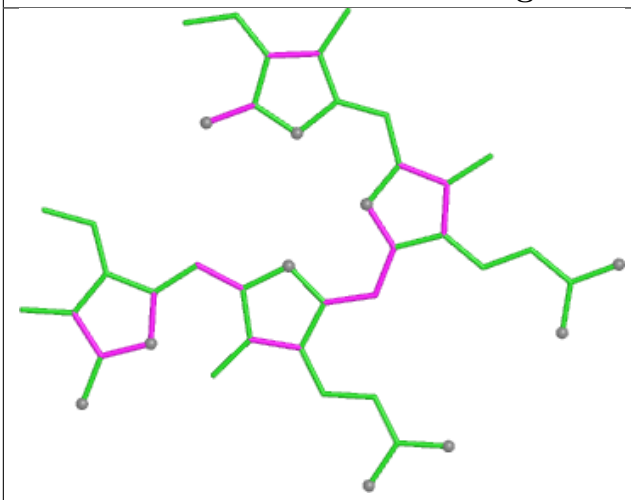


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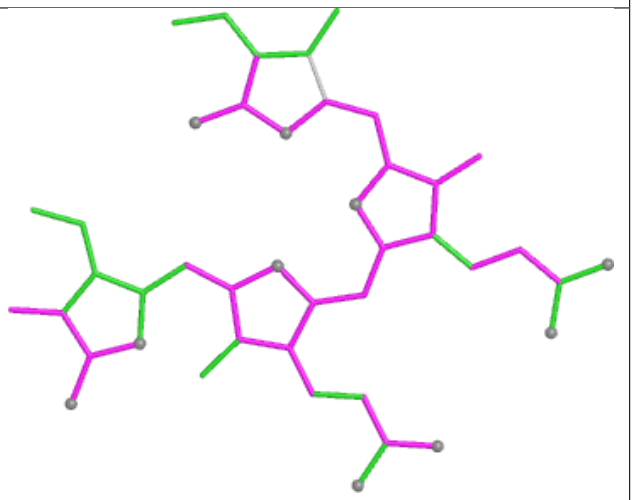


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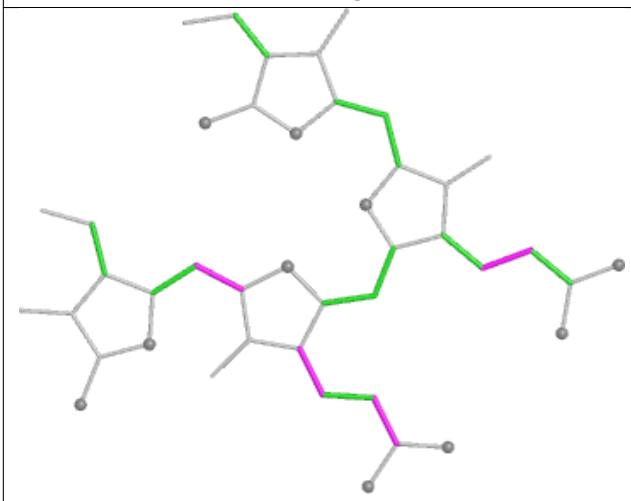
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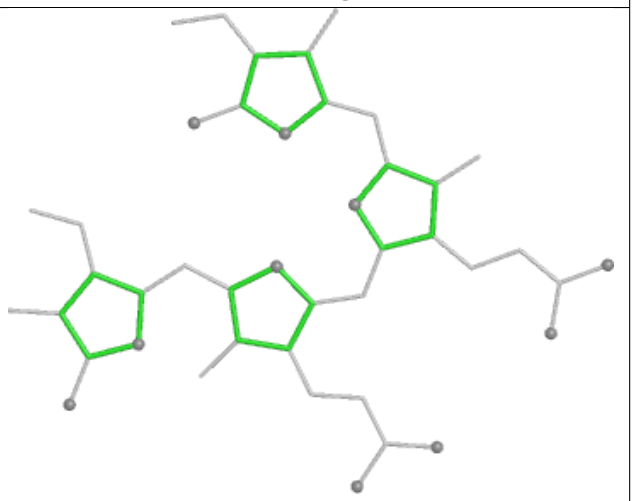
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Bond angles

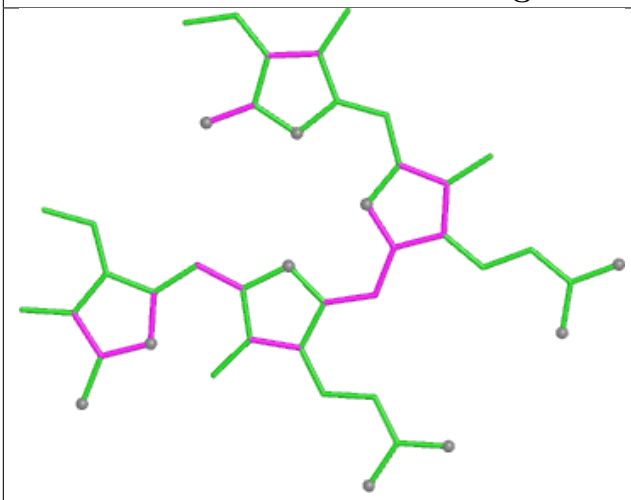


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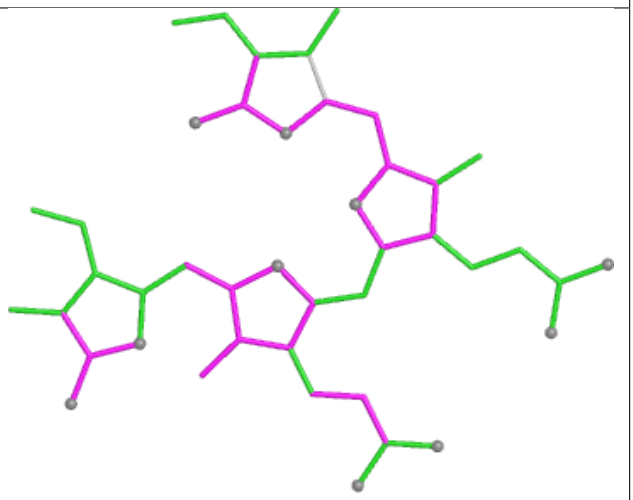


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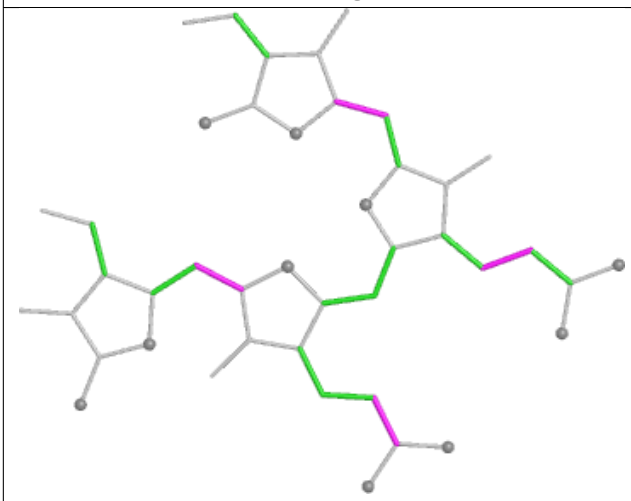
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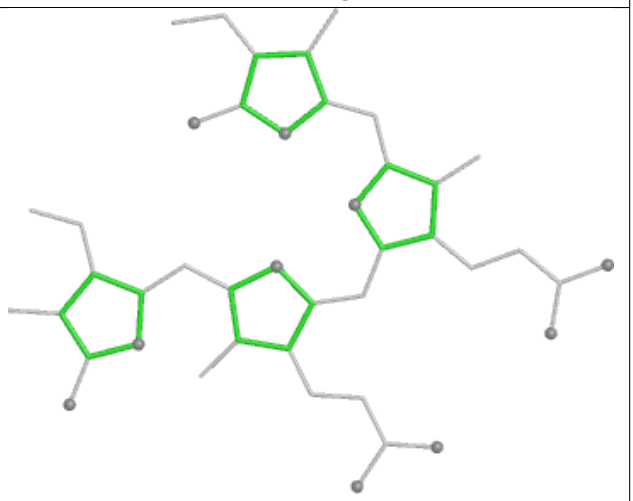
Bond lengths



Bond angles

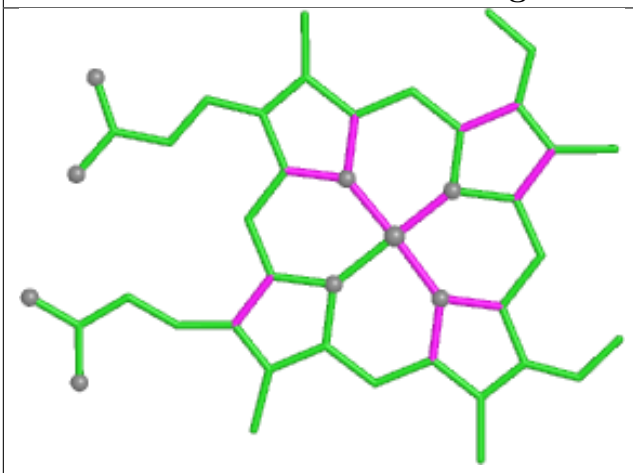


Torsions

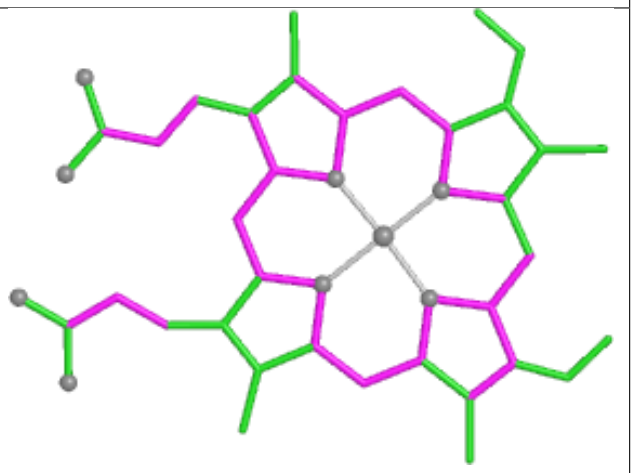


Rings

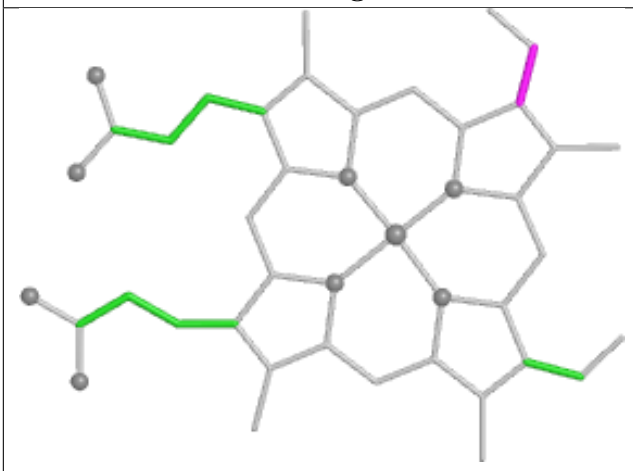
Ligand HEM V6 201



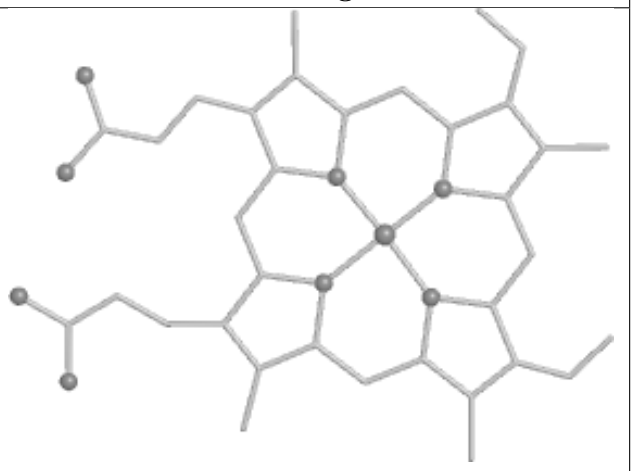
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Bond angles

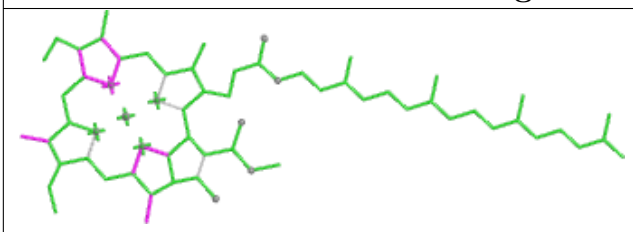


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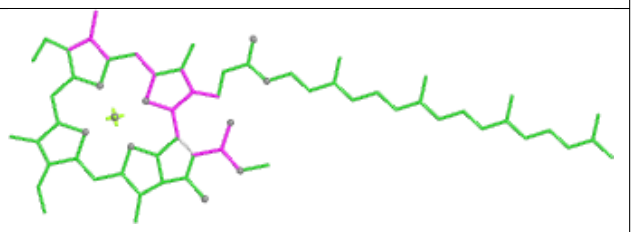


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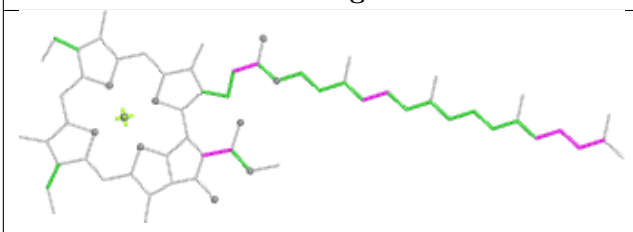
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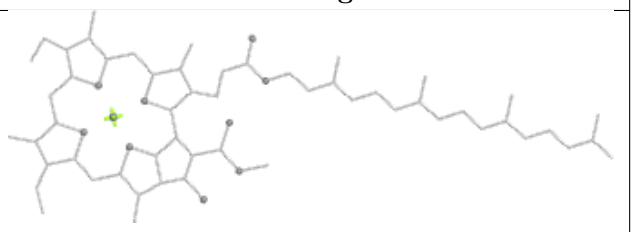
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Bond angles

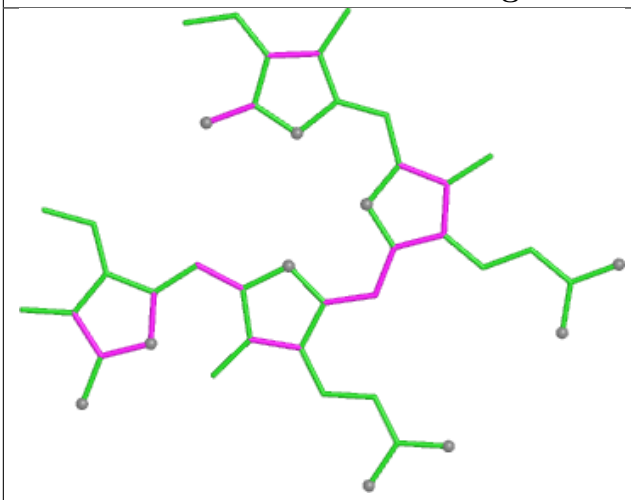


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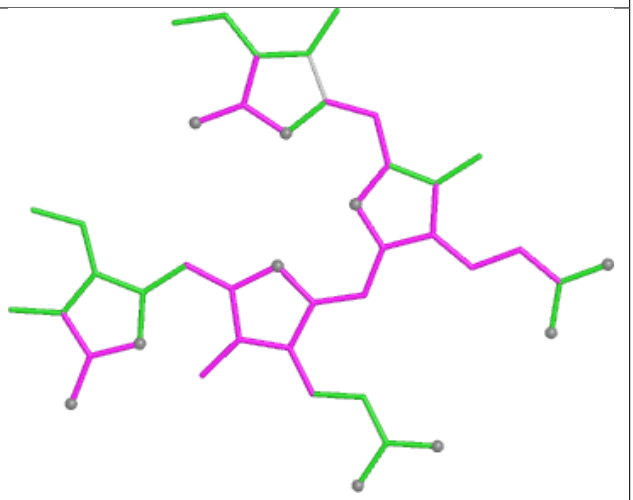


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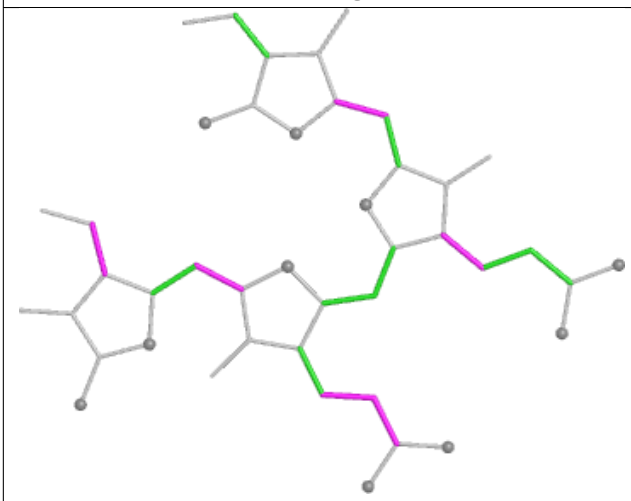
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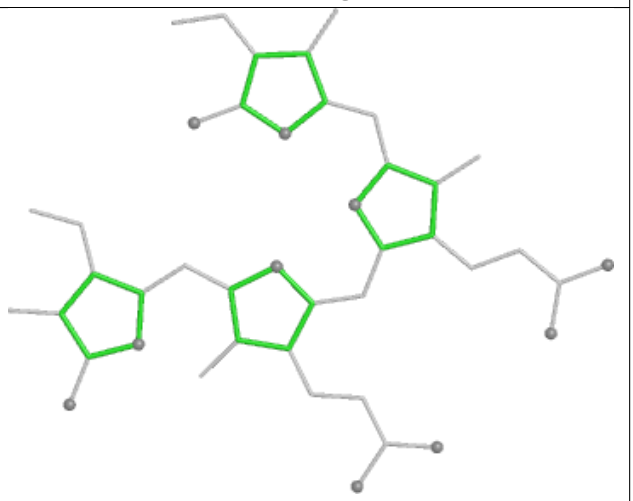
Bond lengths



Bond angles

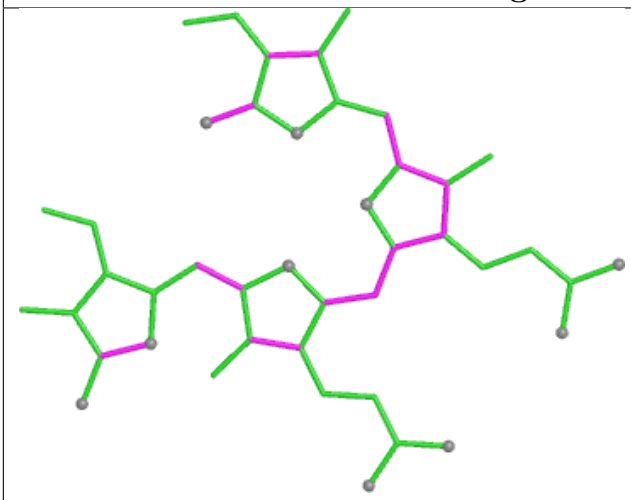


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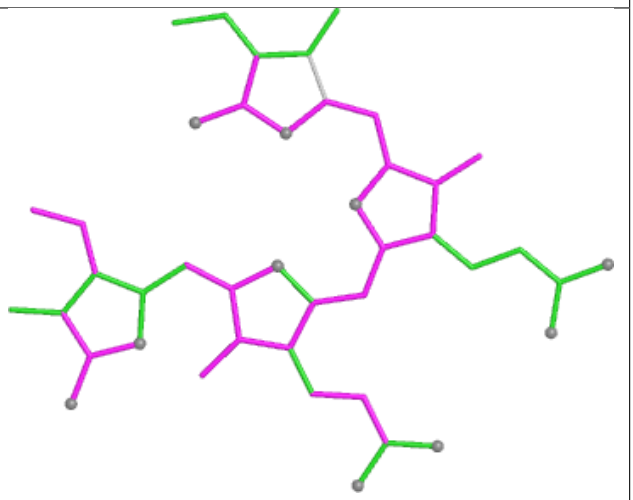


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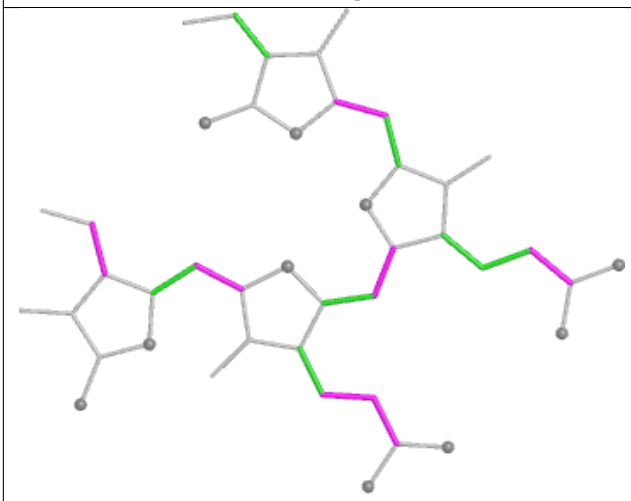
Ligand PEB ND 204



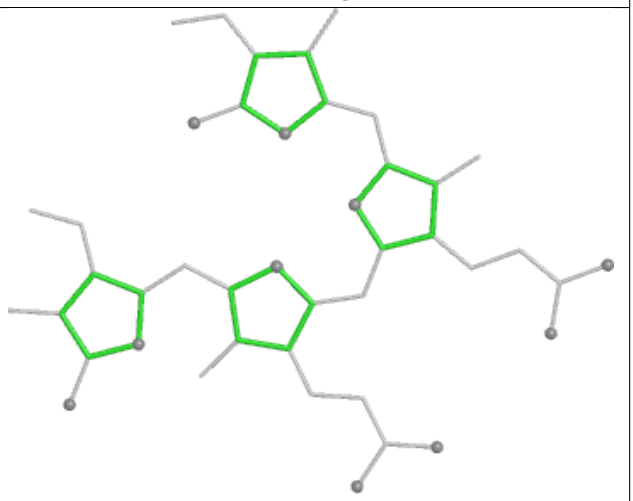
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Bond angles

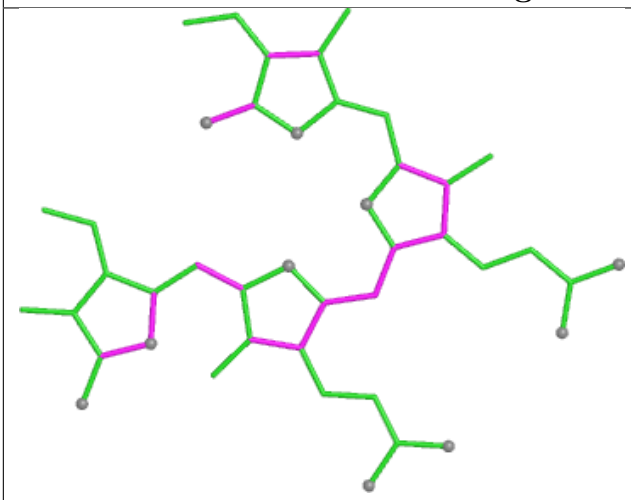


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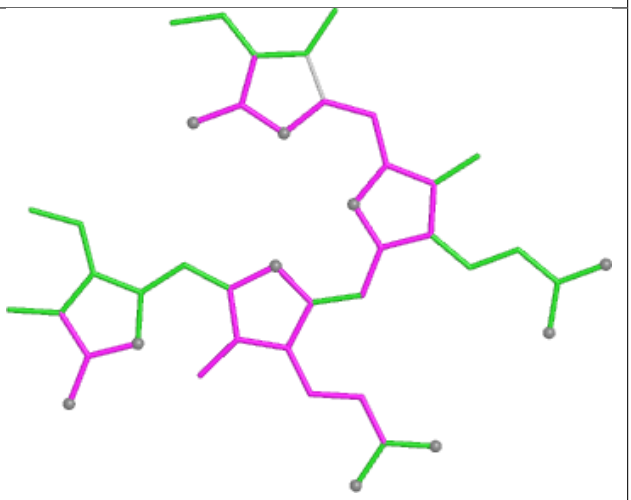


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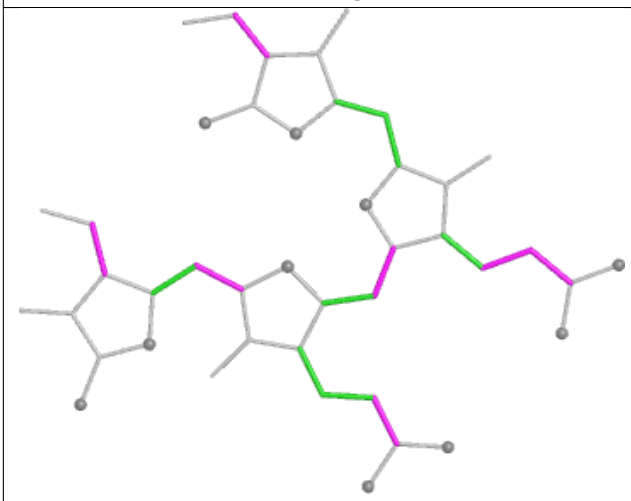
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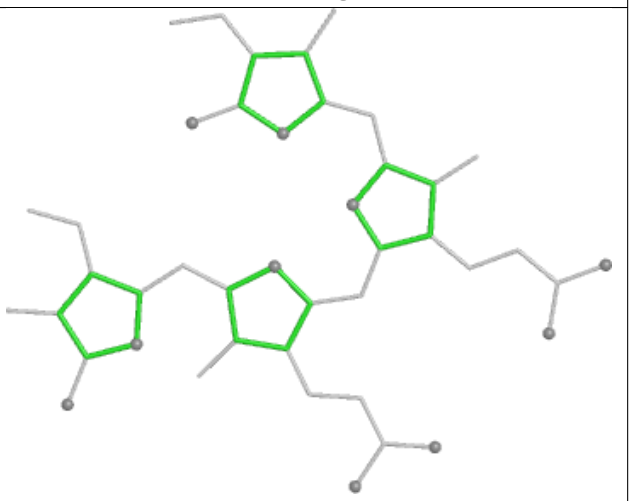
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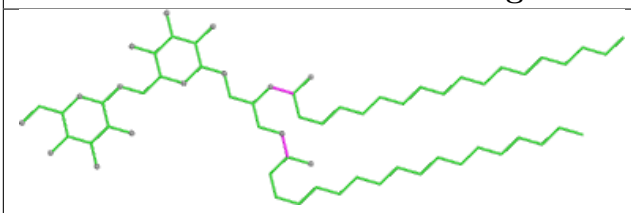


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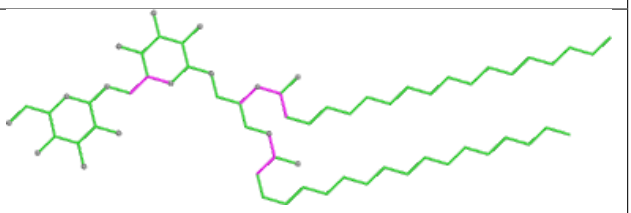


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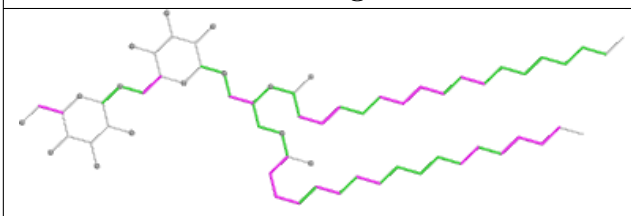
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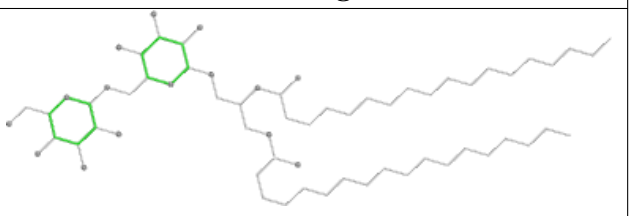
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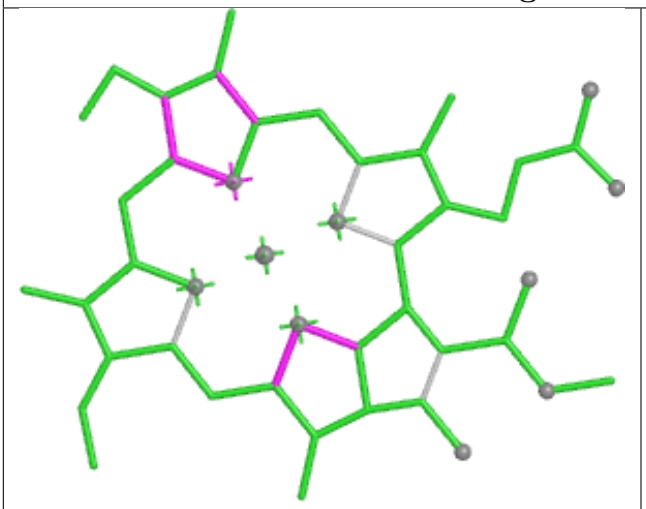


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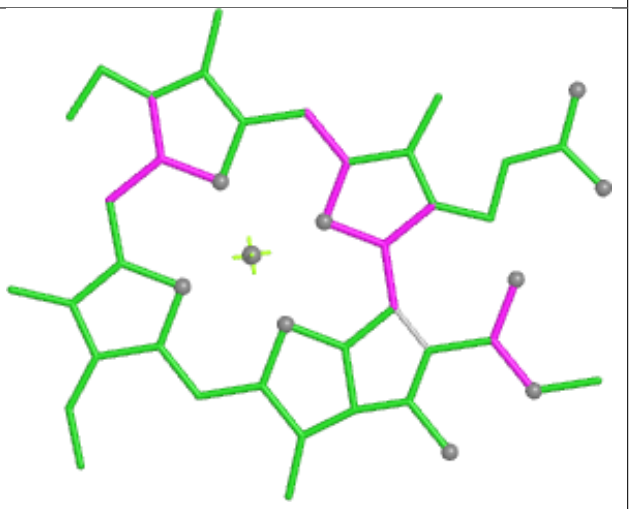


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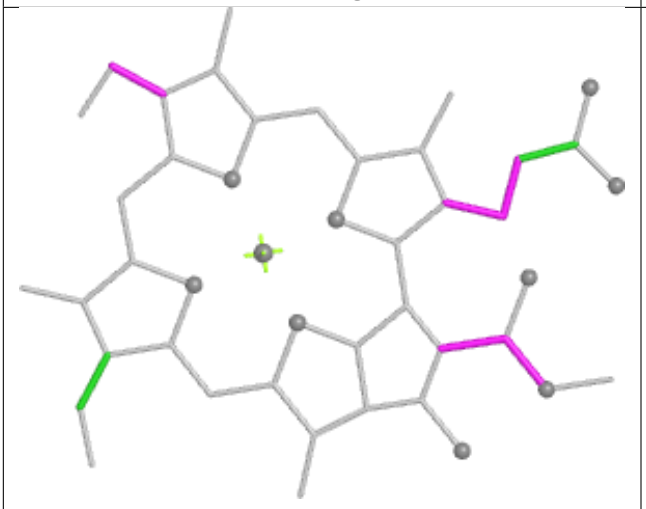
Ligand CLA 22 601



Bond lengths



Bond angles

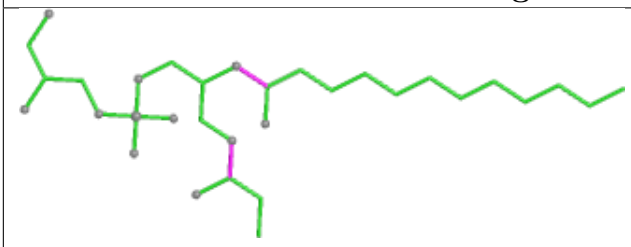


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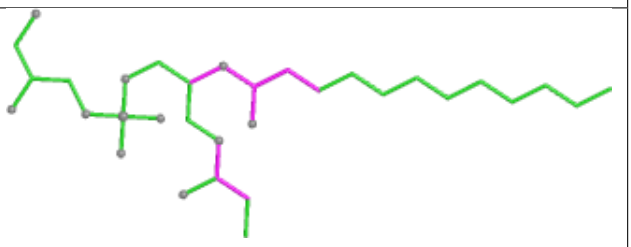


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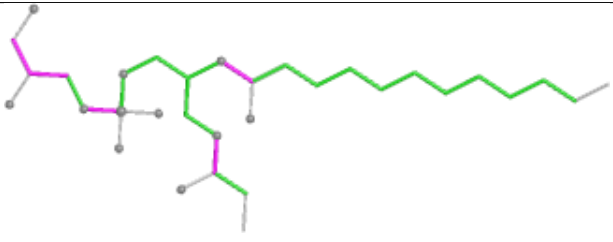
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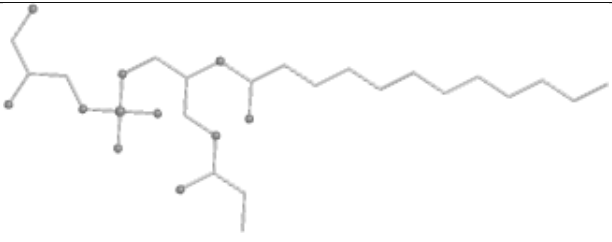
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Bond angles

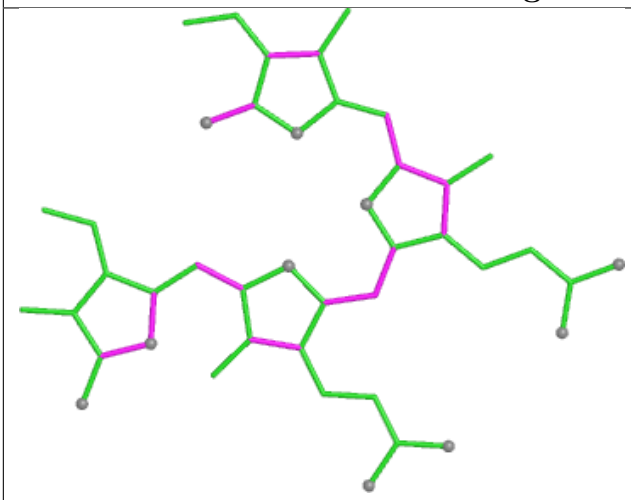


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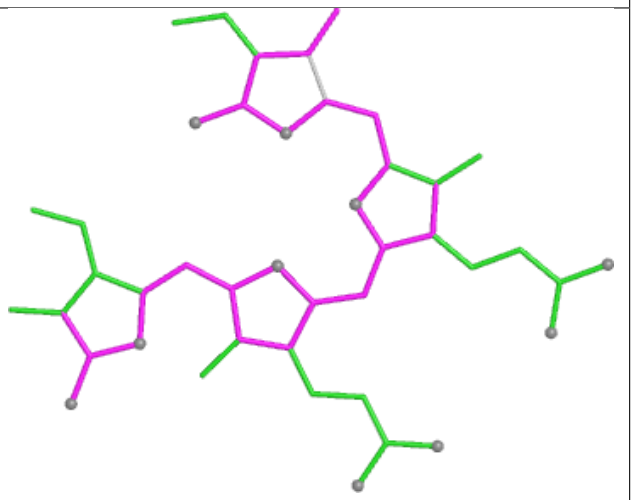


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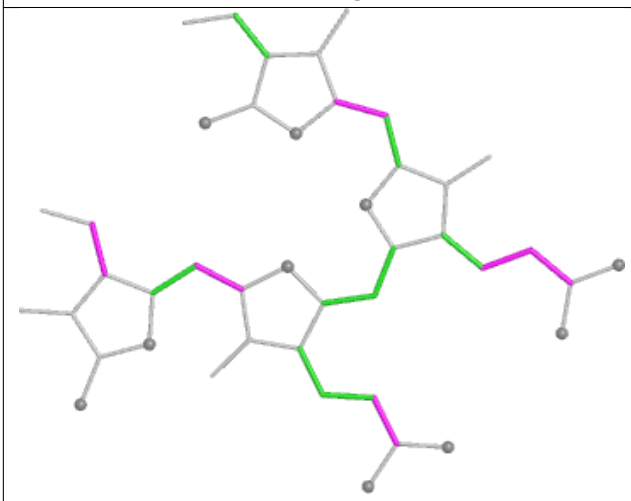
Ligand PEB f1 202



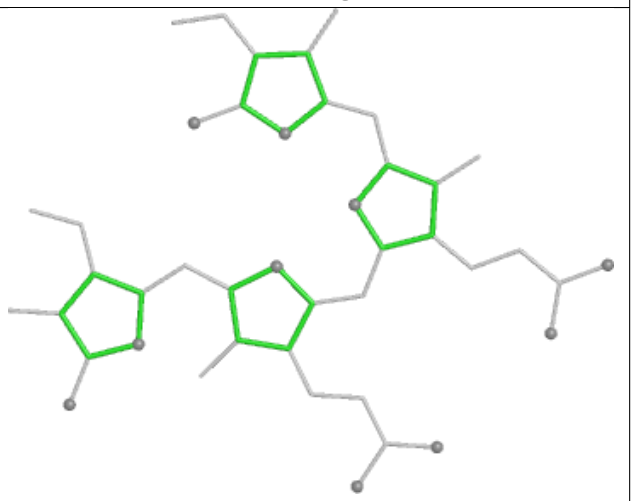
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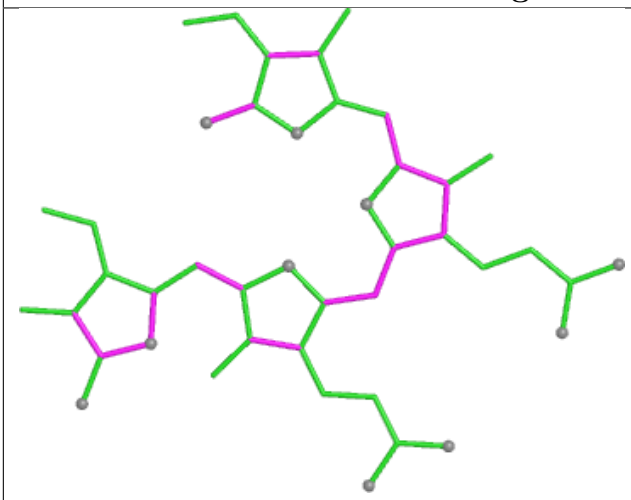


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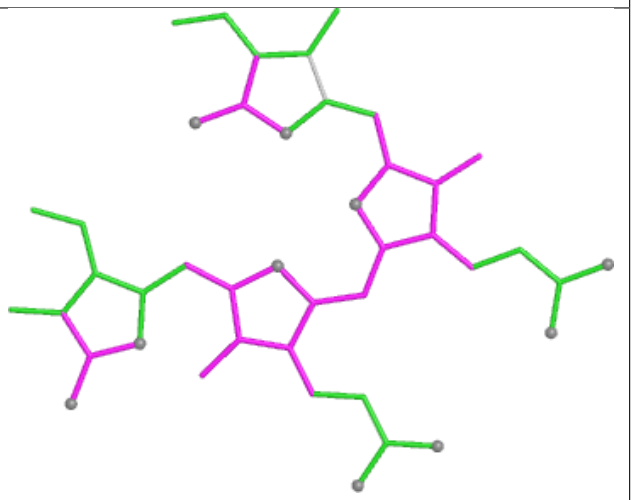


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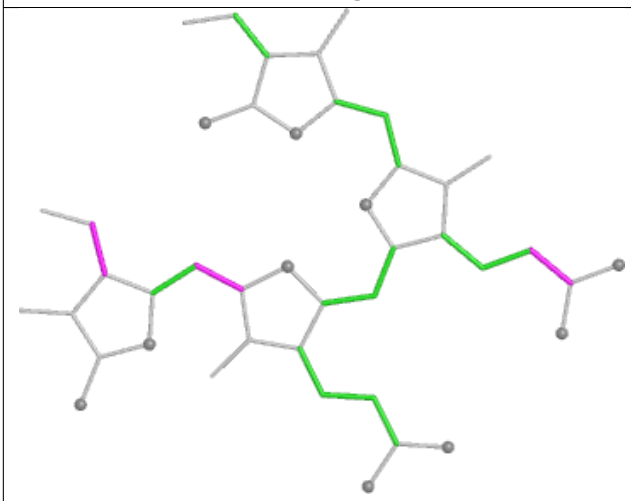
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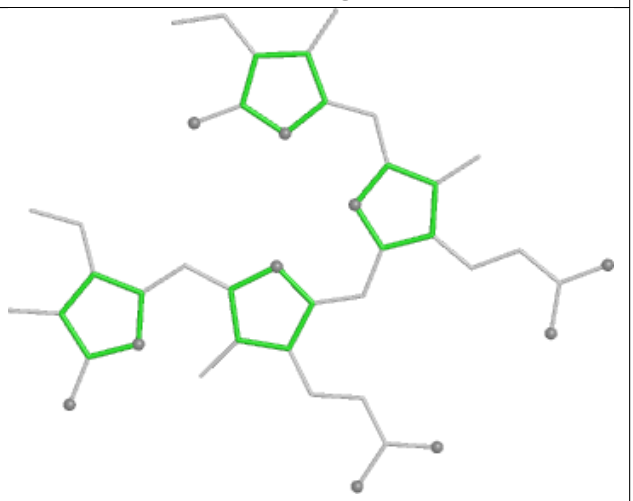
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Bond angles

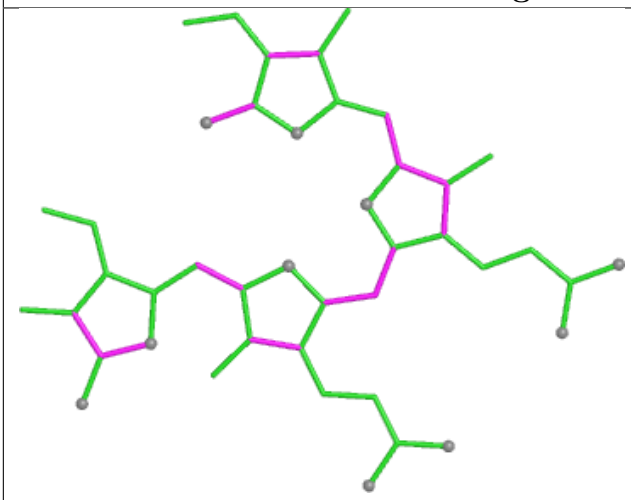


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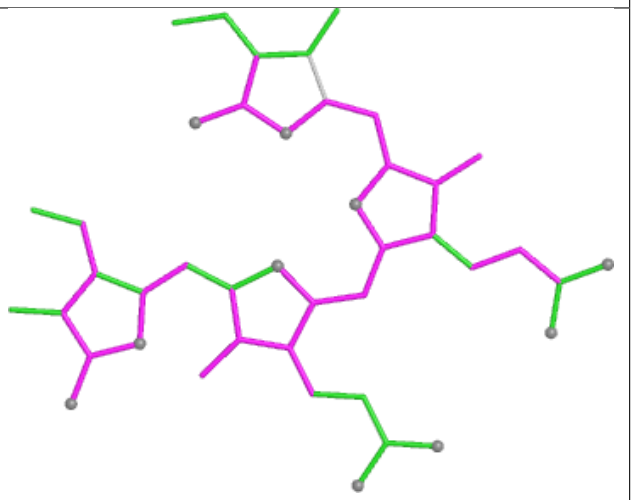


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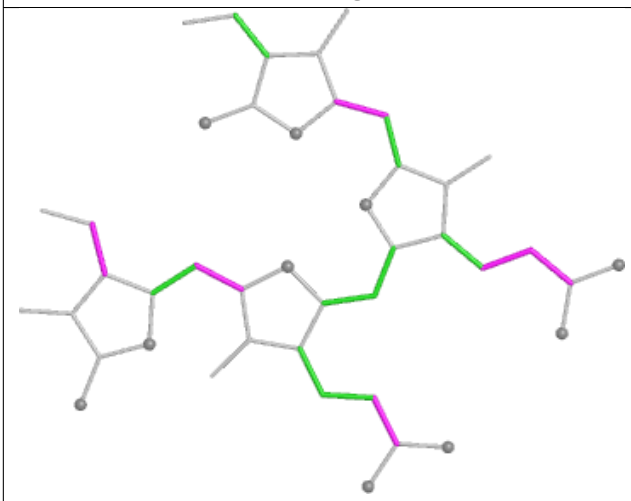
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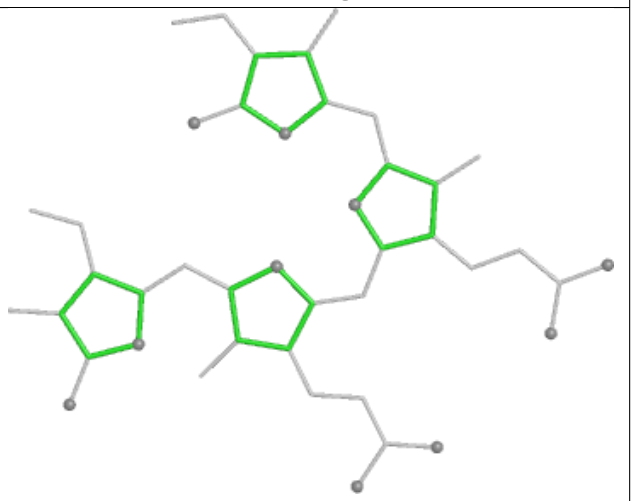
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Bond angles

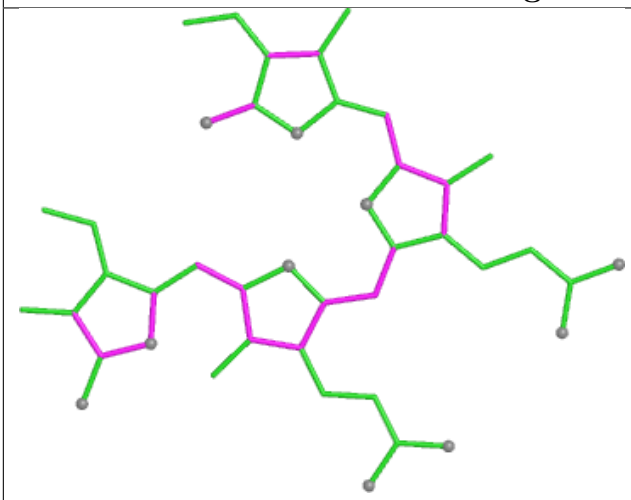


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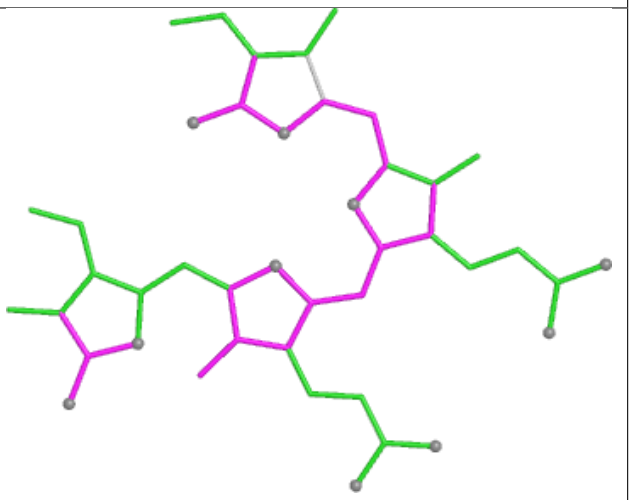


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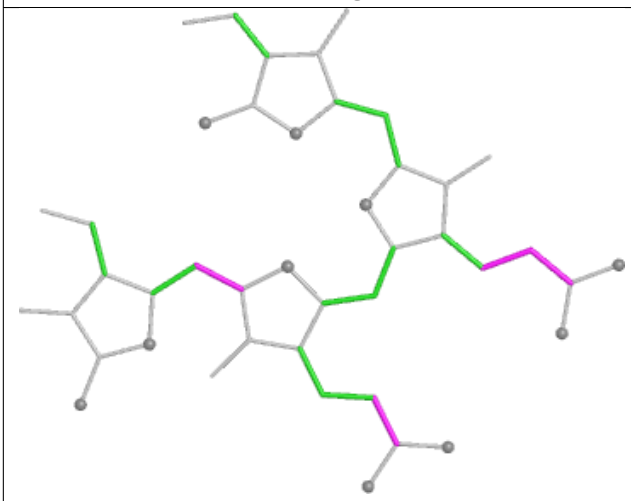
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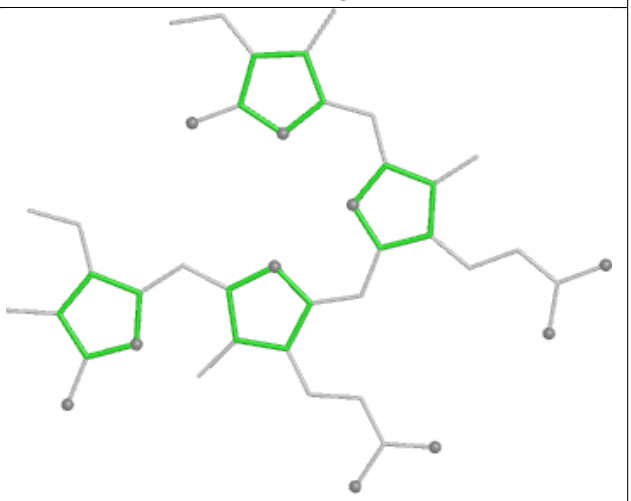
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Bond angles

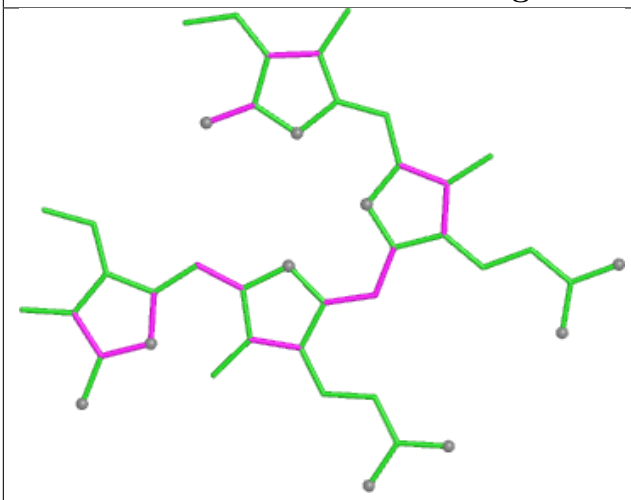


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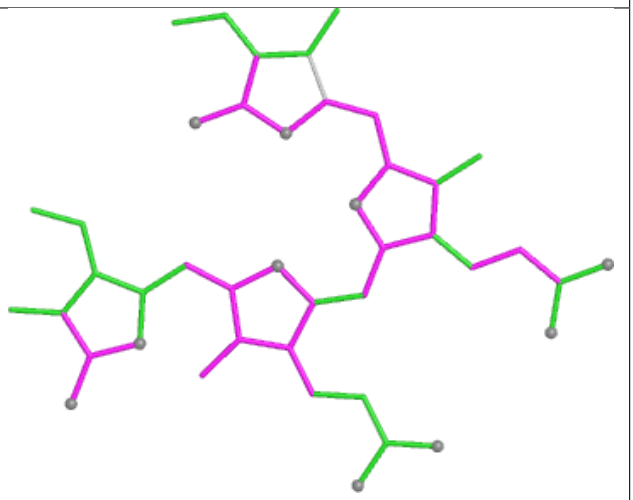


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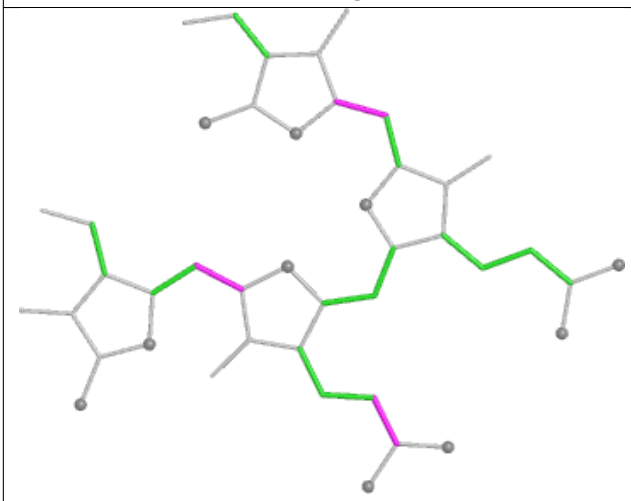
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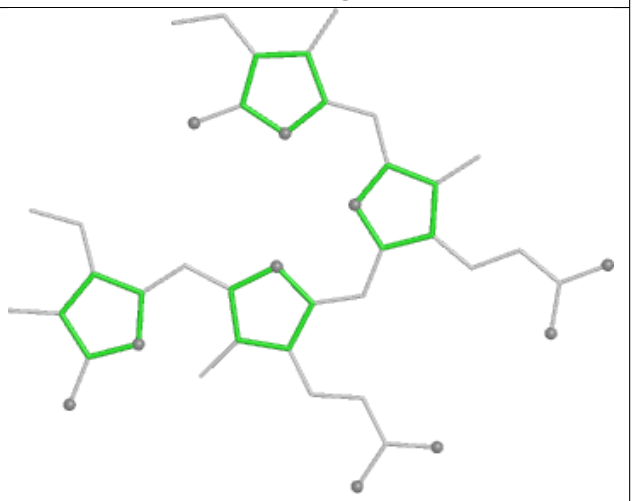
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Bond angles

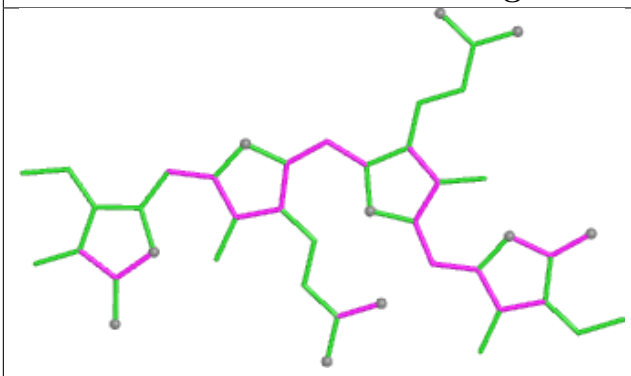


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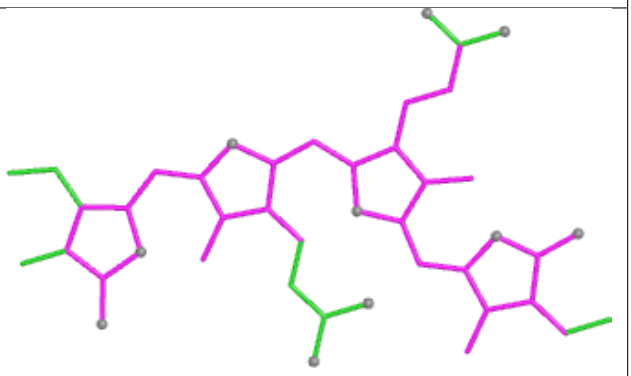


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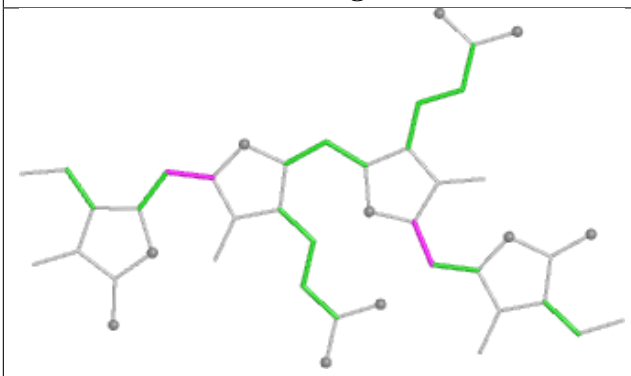
Ligand CYC O3 1001



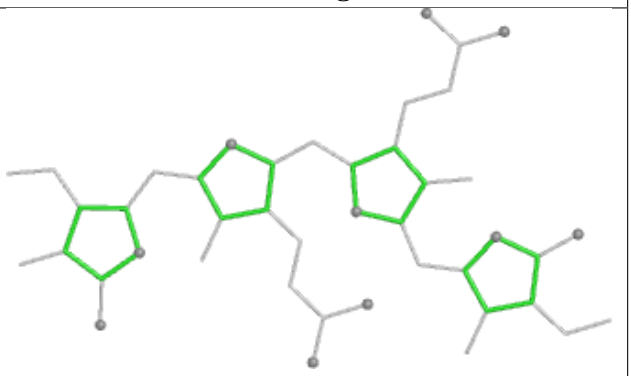
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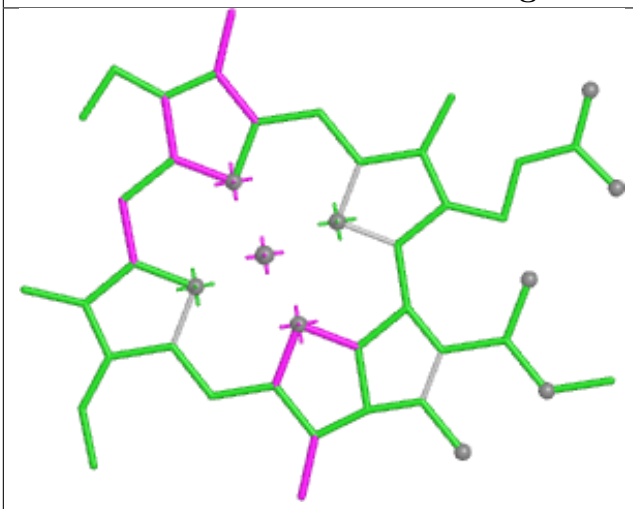


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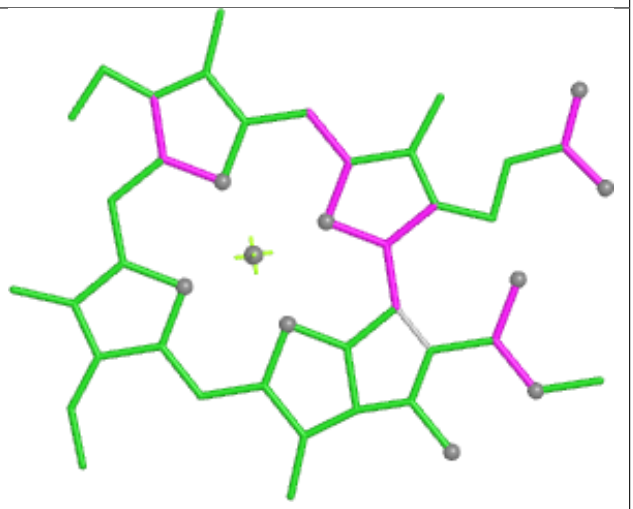


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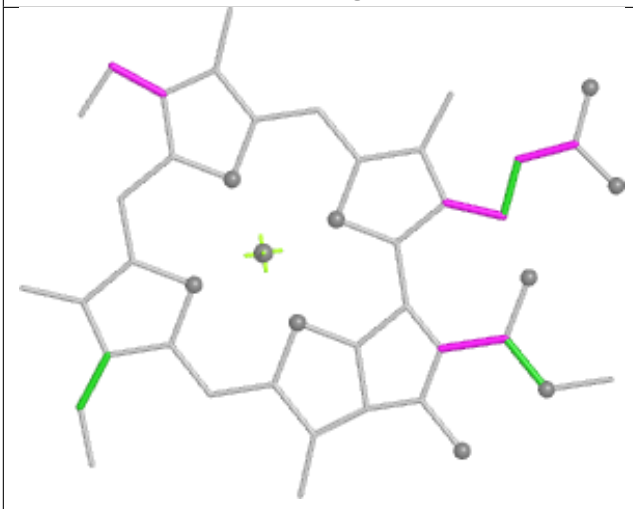
Ligand CLA 72 606



Bond lengths



Bond angles

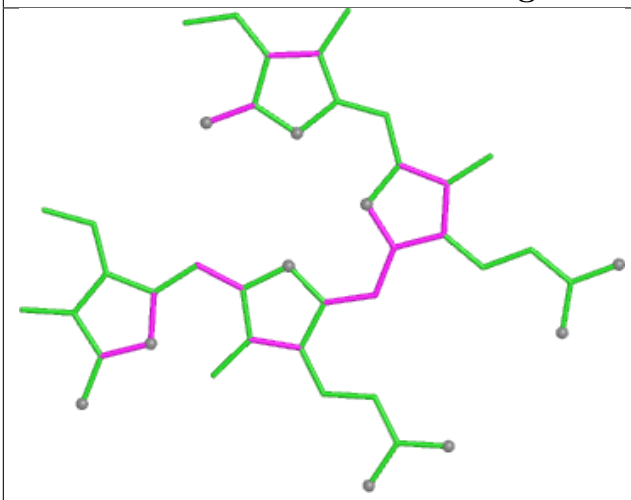


Torsions

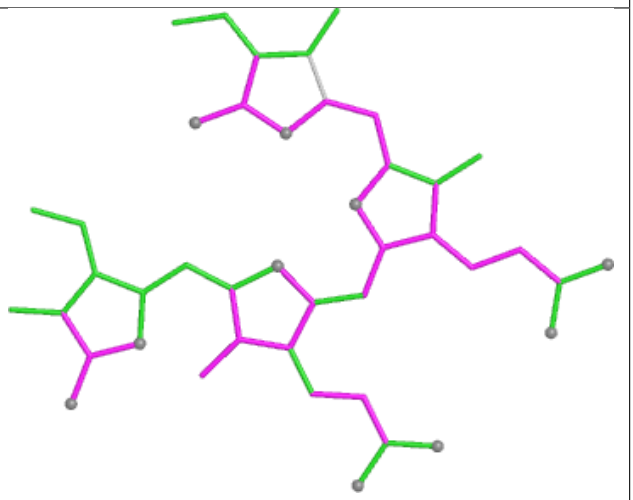


Rings

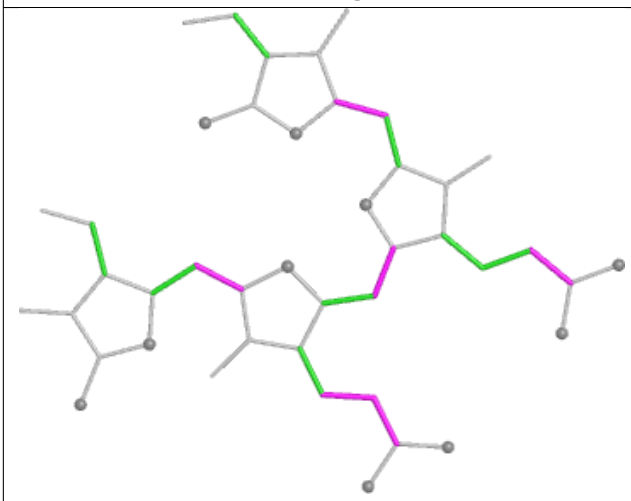
Ligand PEB L7 203



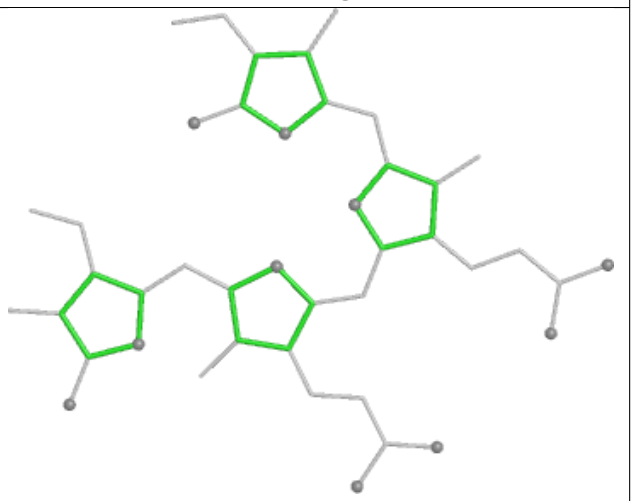
Bond lengths



Bond angles

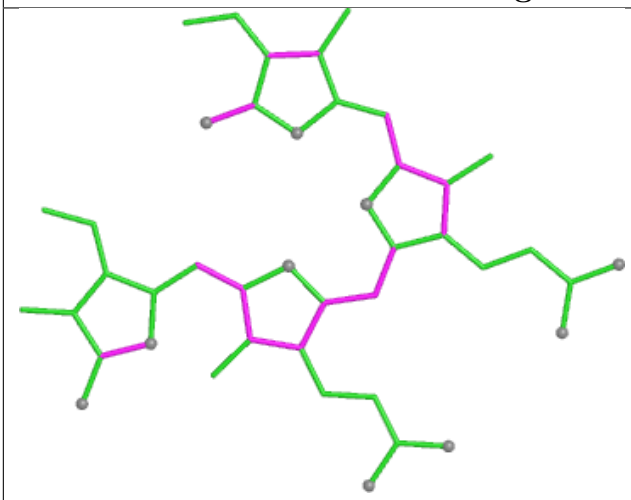


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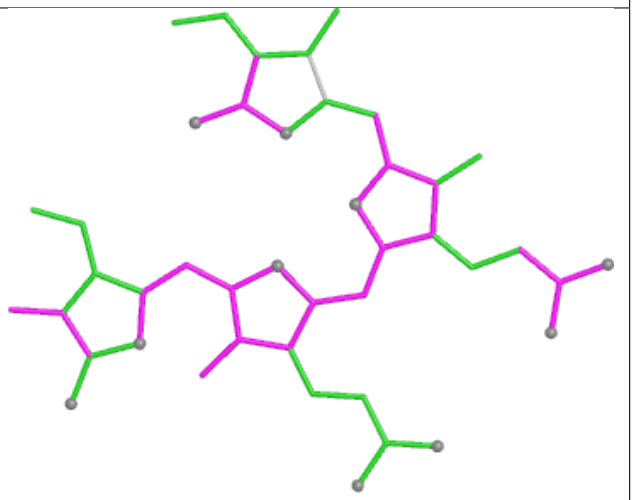


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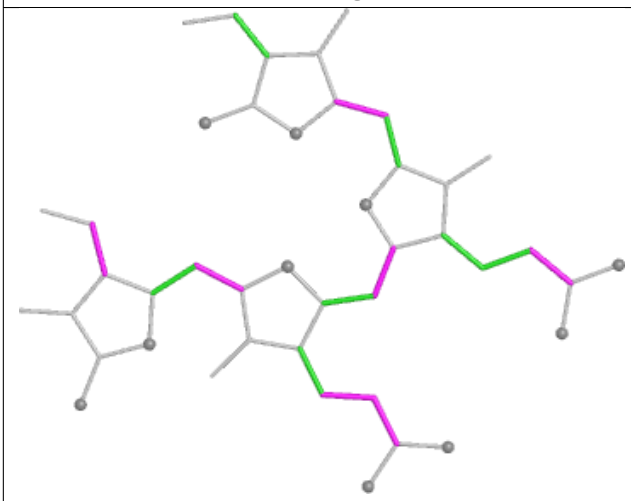
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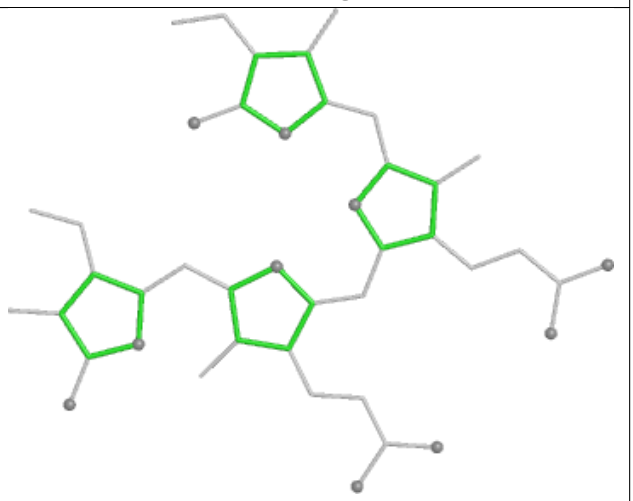
Bond lengths



Bond angles

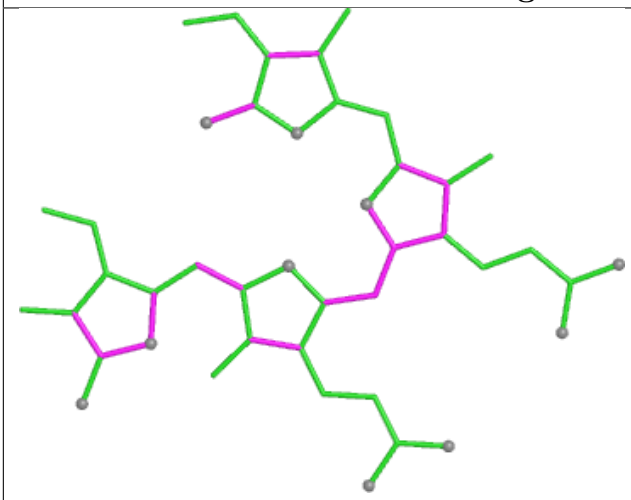


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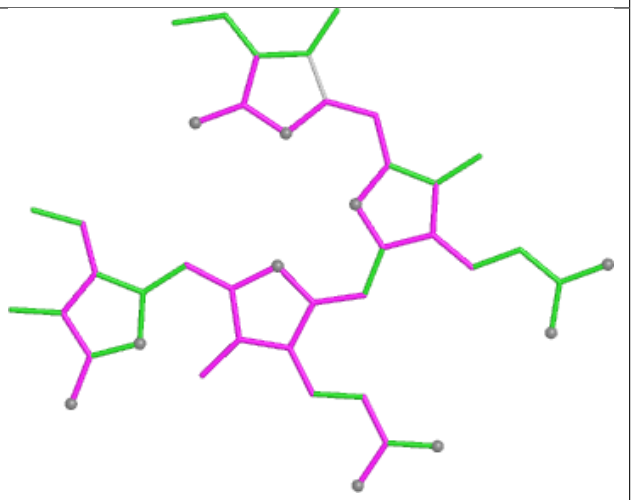


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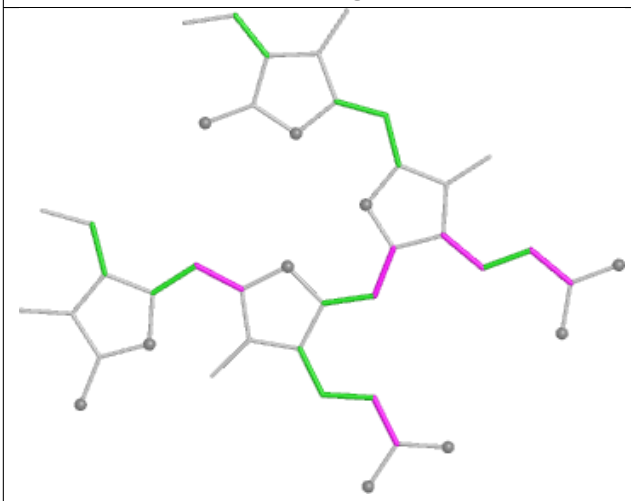
Ligand PEB LJ 202



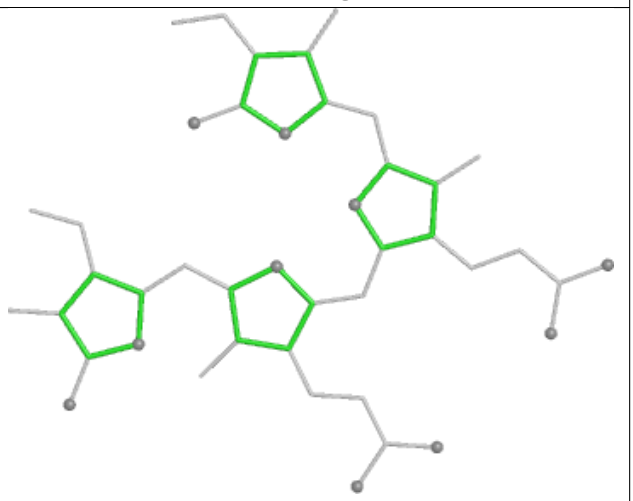
Bond lengths



Bond angles

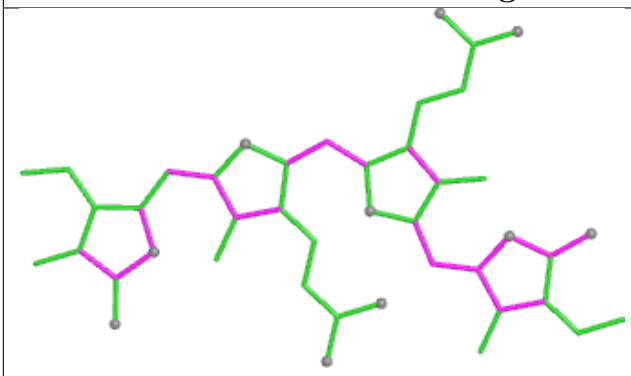


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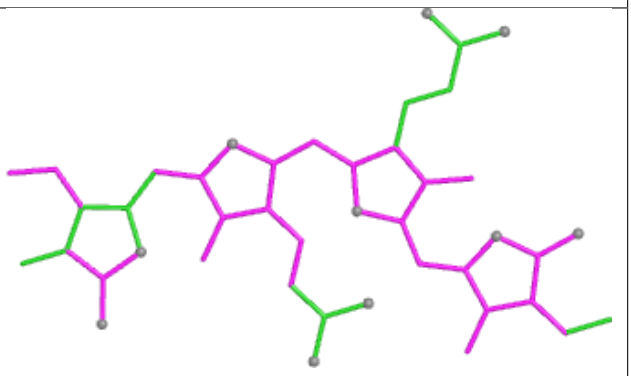


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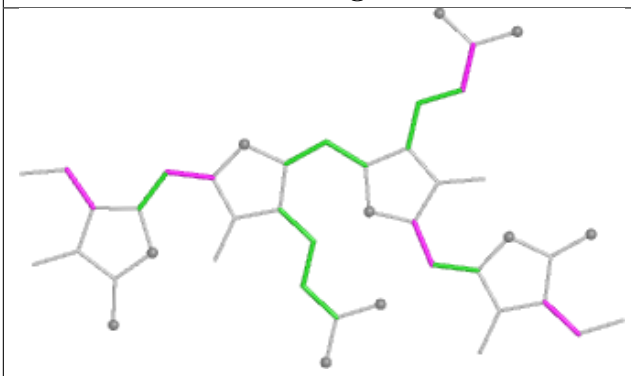
Ligand CYC KO 1001



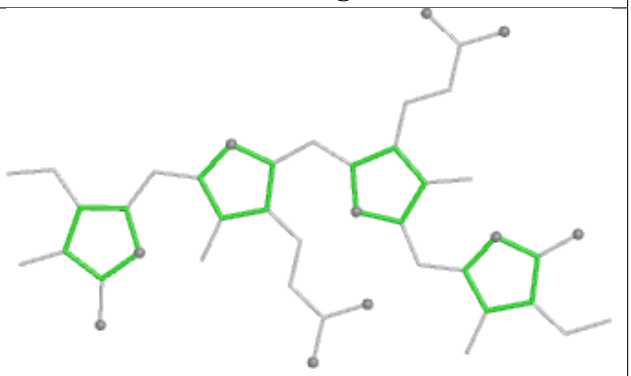
Bond lengths



Bond angles

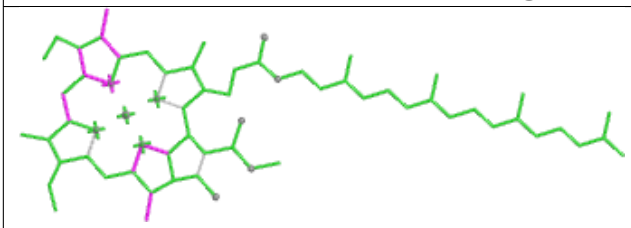


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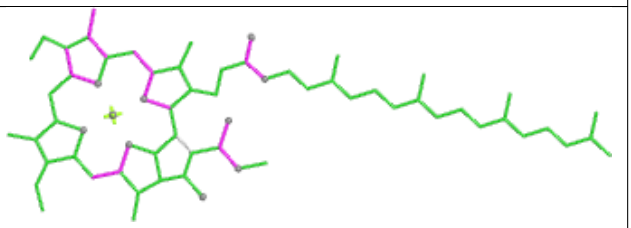


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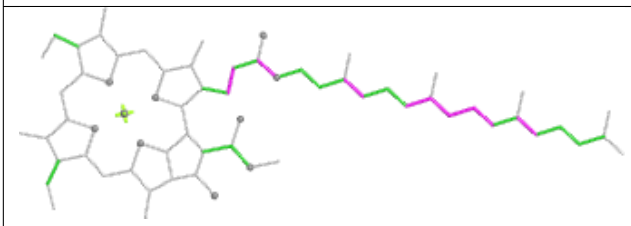
Ligand CLA c6 616



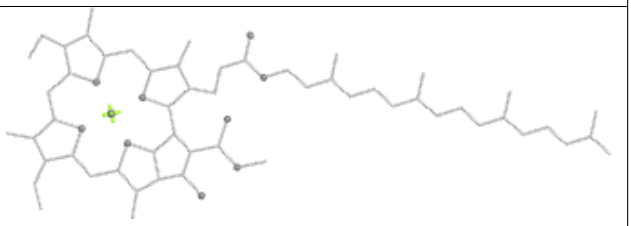
Bond lengths



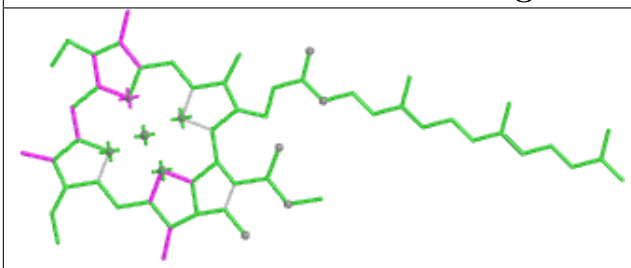
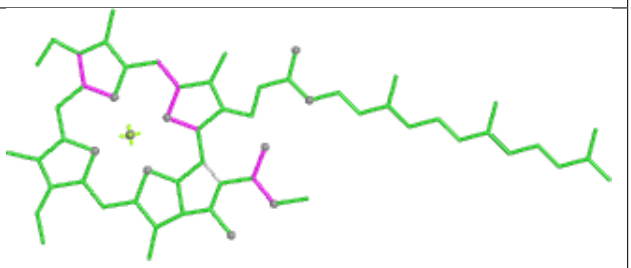
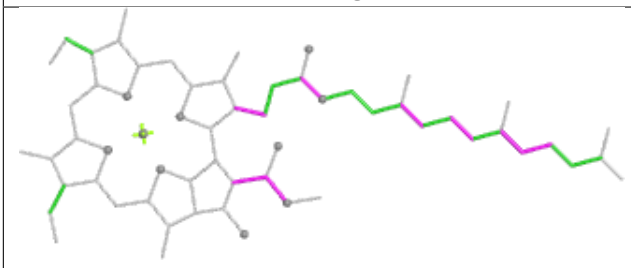
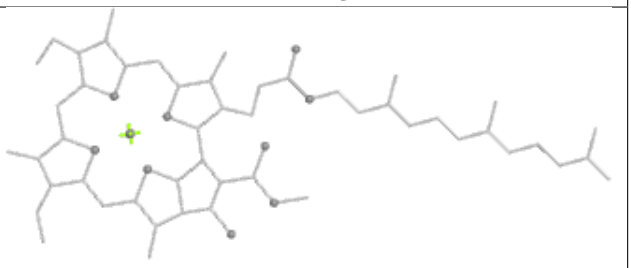
Bond angles

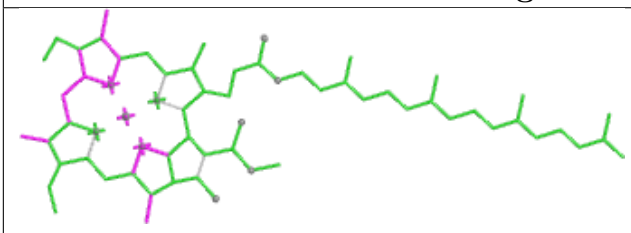
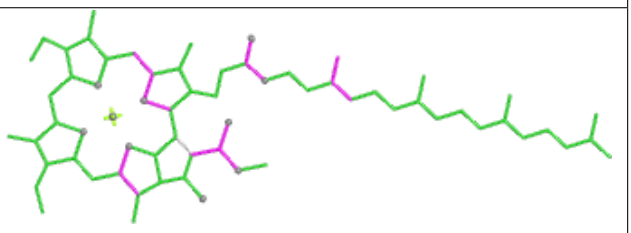
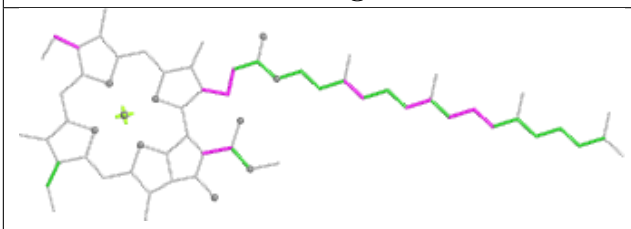
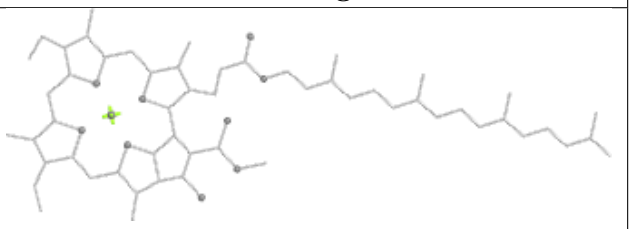


Torsions

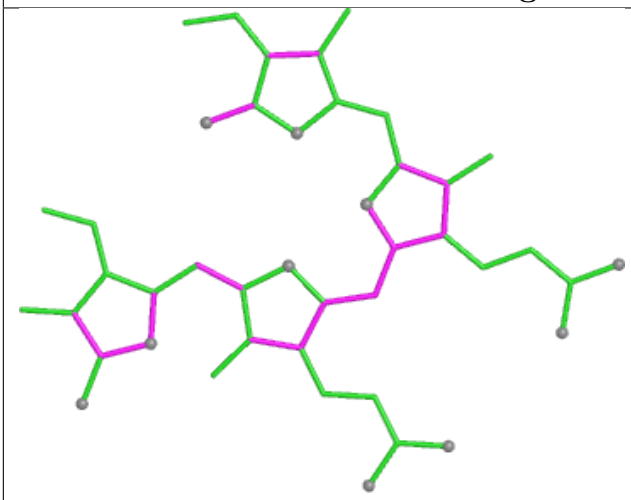


Rings

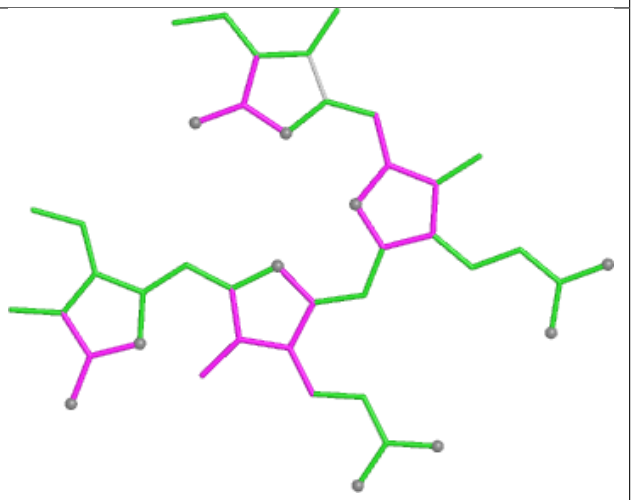
Ligand CLA C6 518	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA bL 606	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

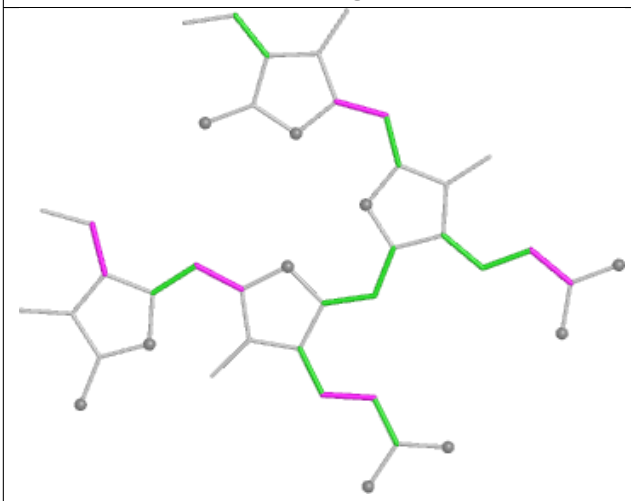
Ligand PEB k4 201



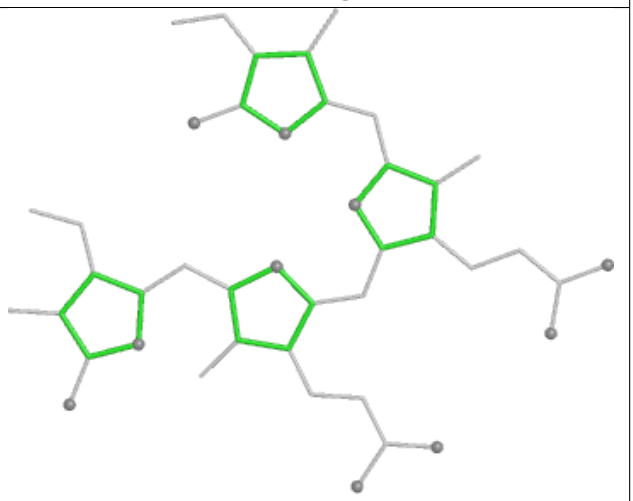
Bond lengths



Bond angles

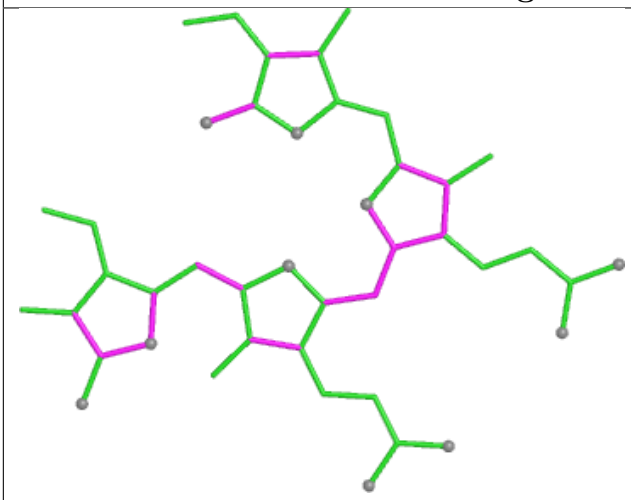


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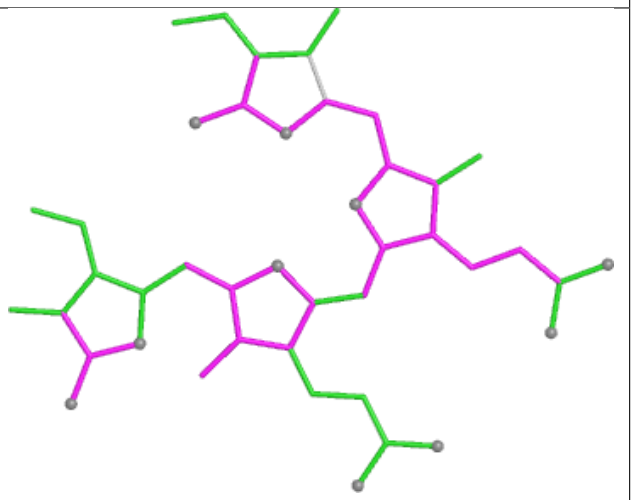


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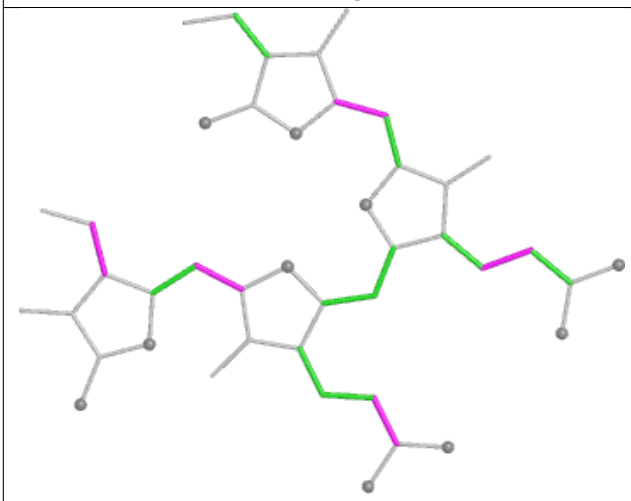
Ligand PEB NI 201



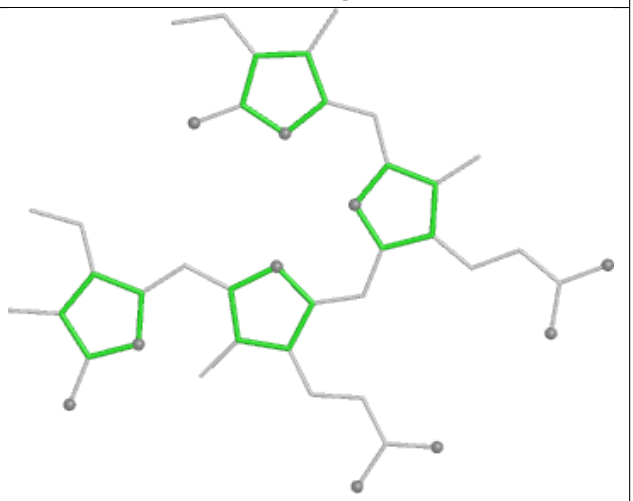
Bond lengths



Bond angles

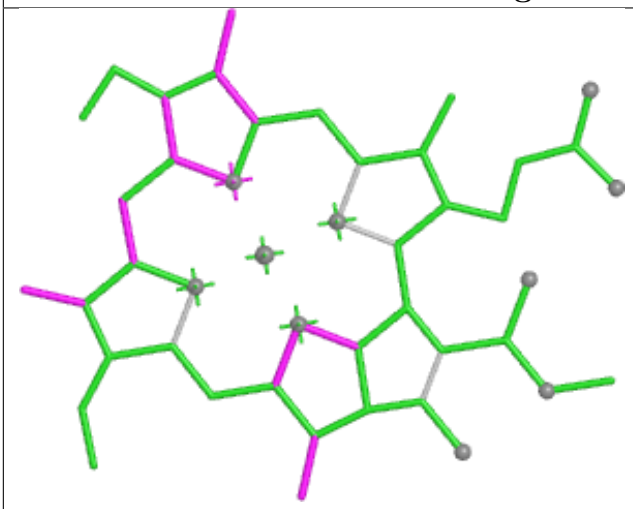


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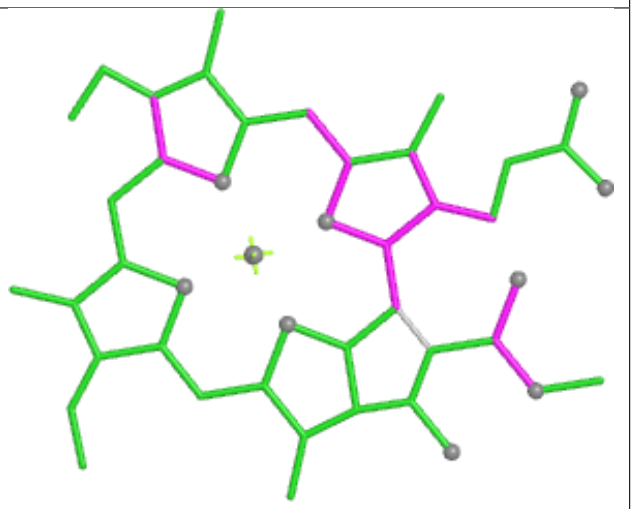


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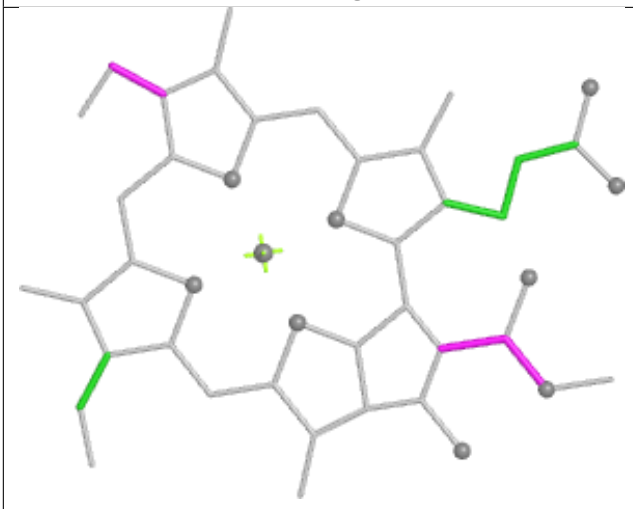
Ligand CLA 7N 610



Bond lengths



Bond angles

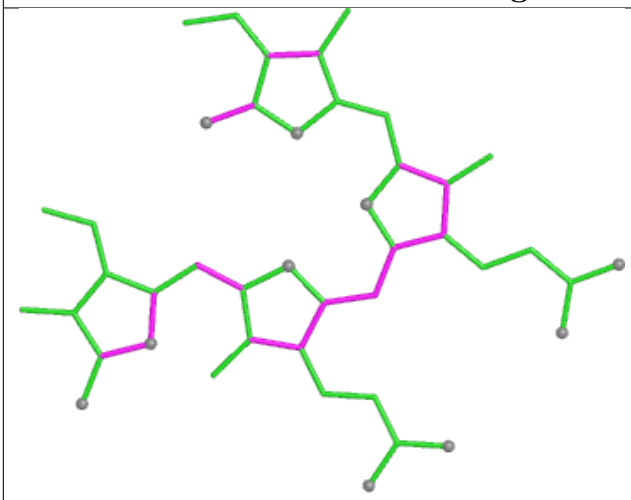


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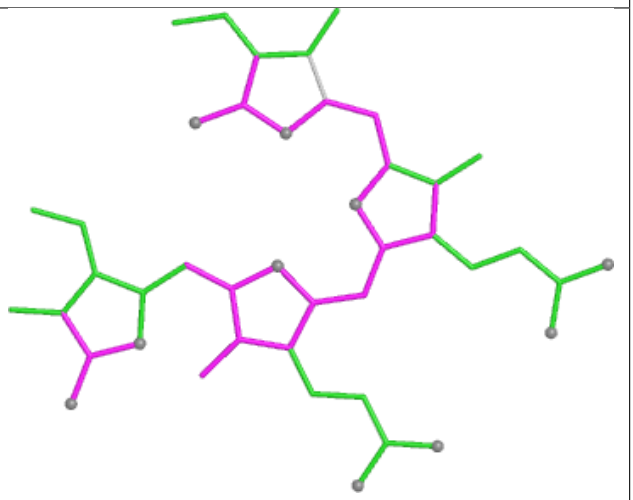


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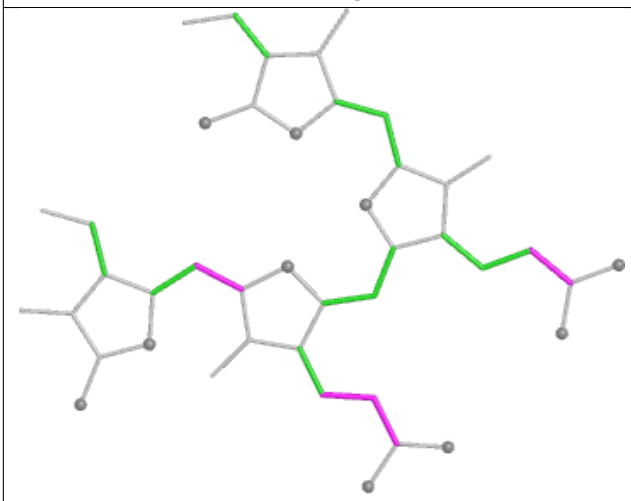
Ligand PEB OH 202



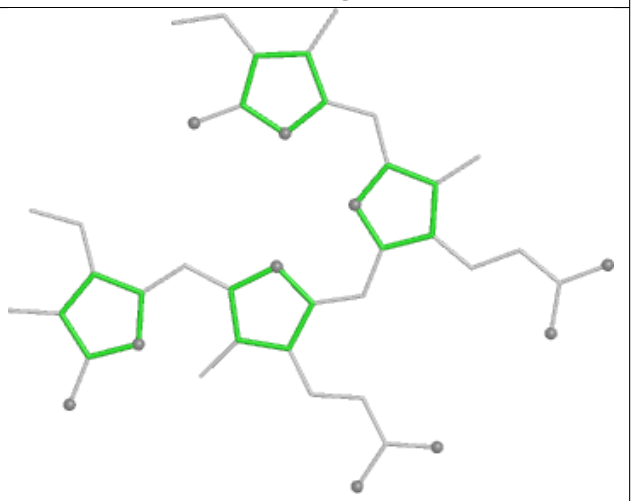
Bond lengths



Bond angles

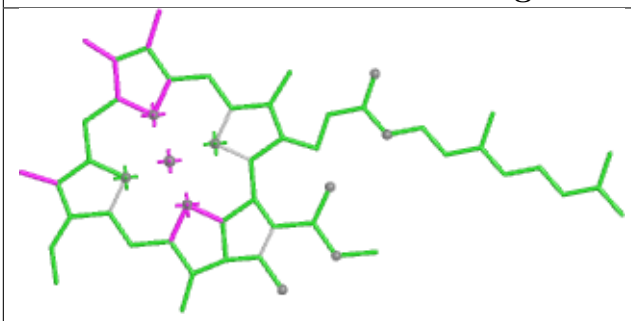


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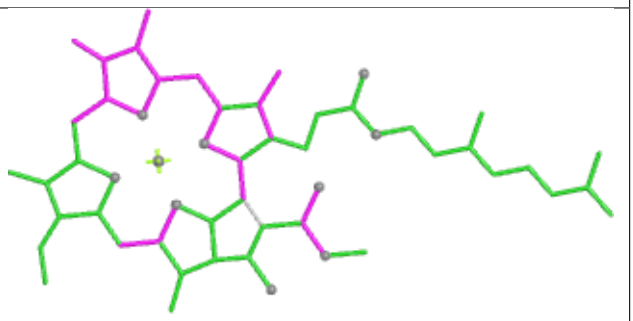


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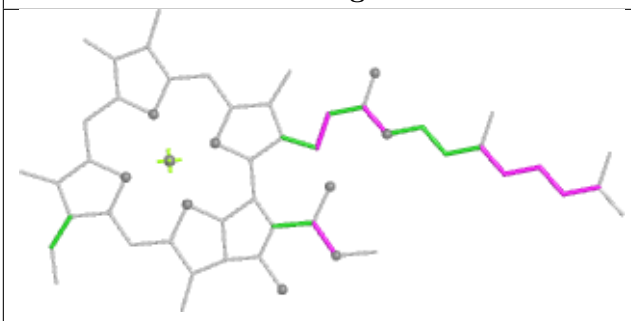
Ligand CLA 2N 301



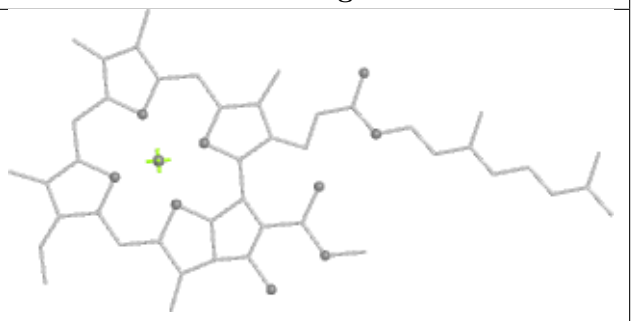
Bond lengths



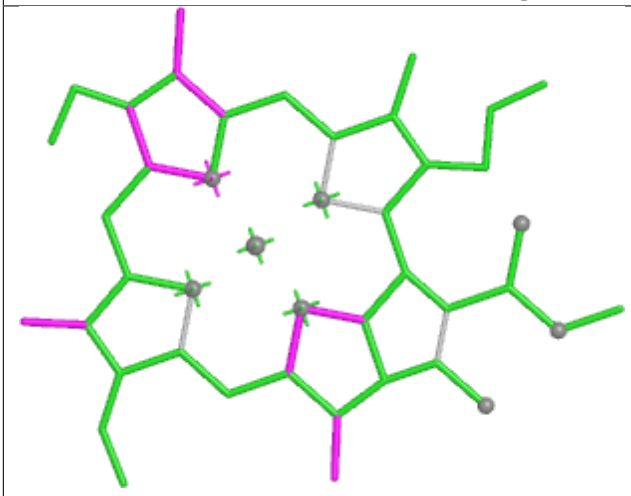
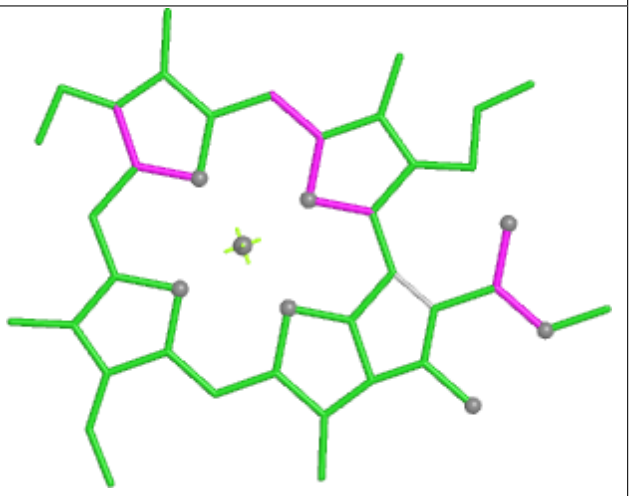
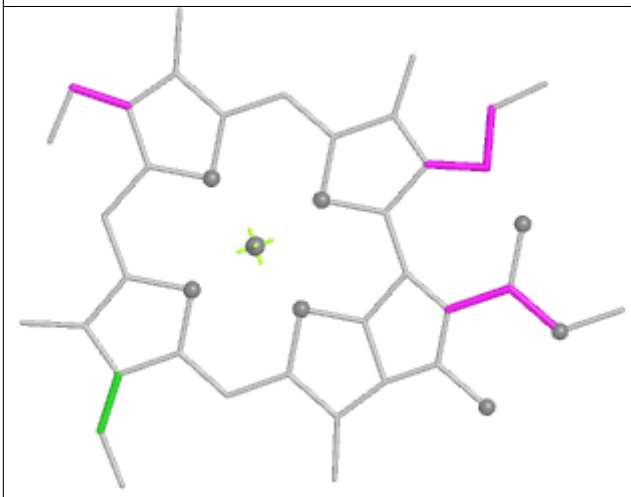
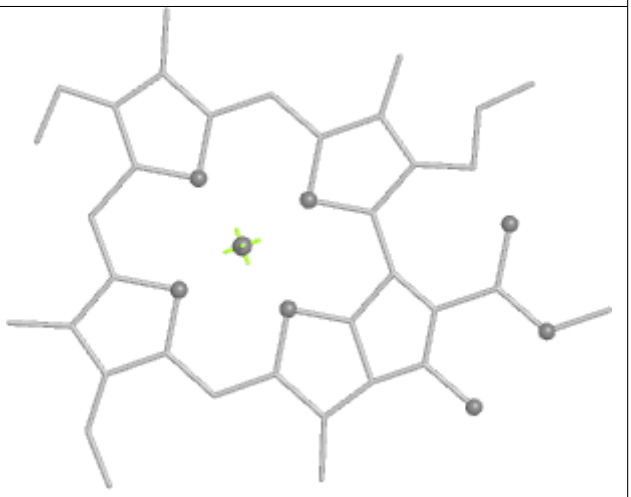
Bond angles



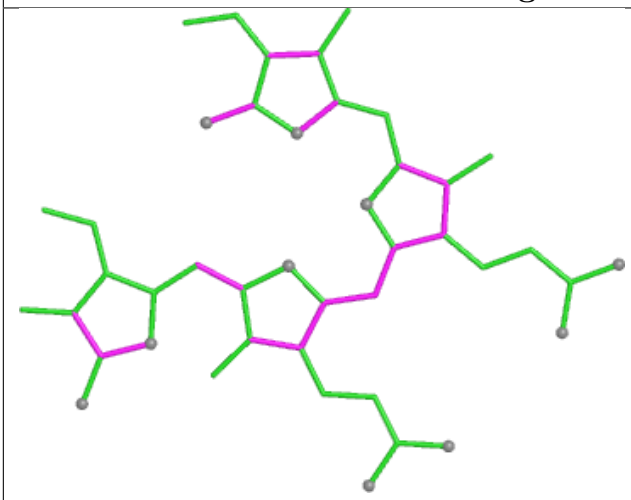
Torsions



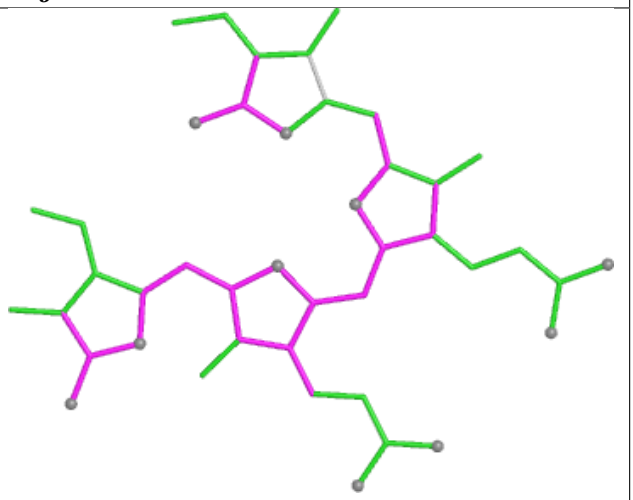
Rings

Ligand CLA B2 829	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

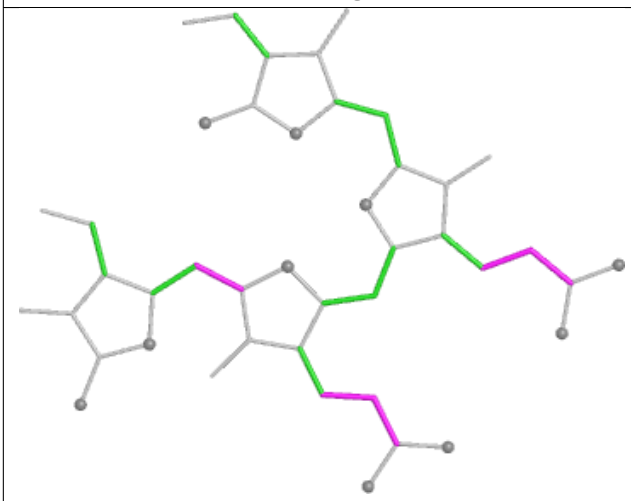
Ligand PEB jH 202



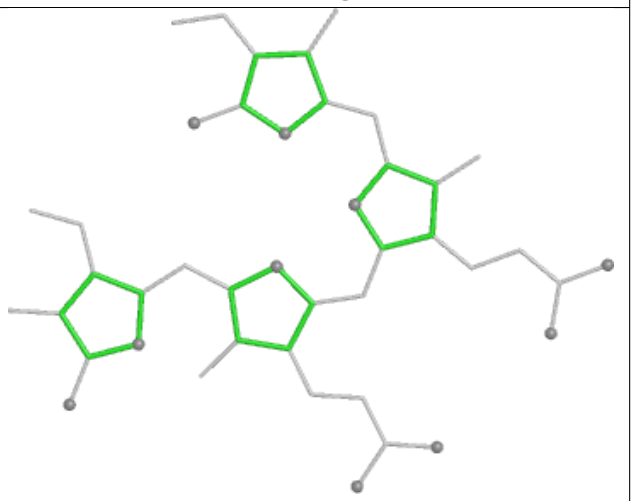
Bond lengths



Bond angles

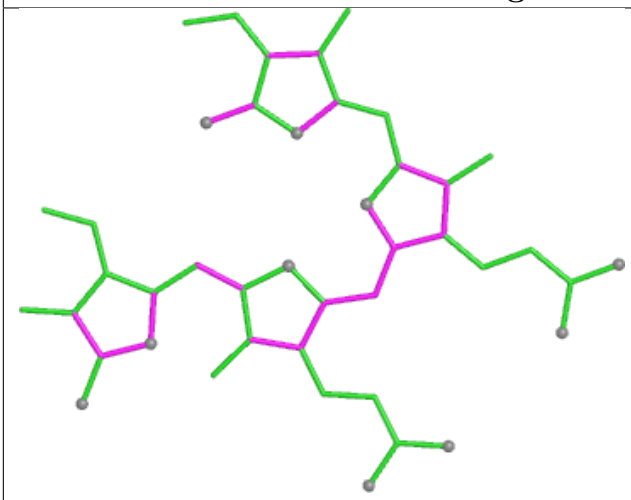


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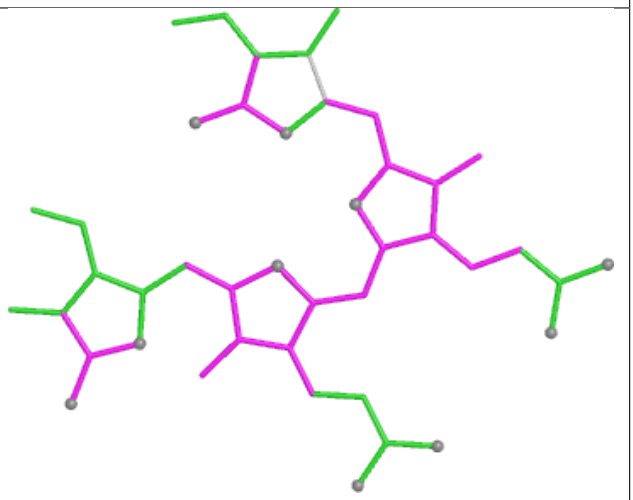


Rings

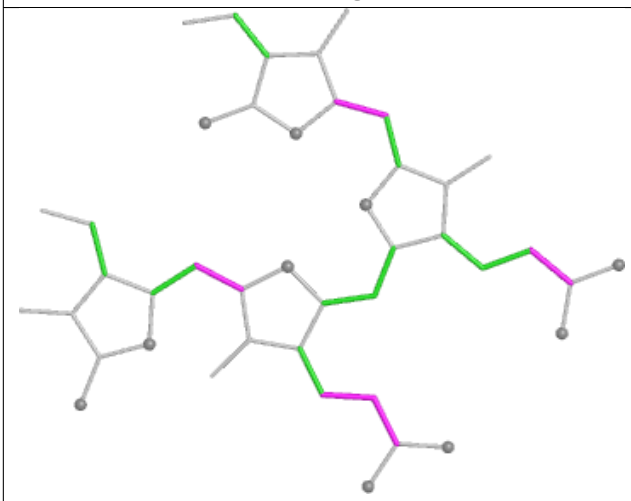
Ligand PEB OM 202



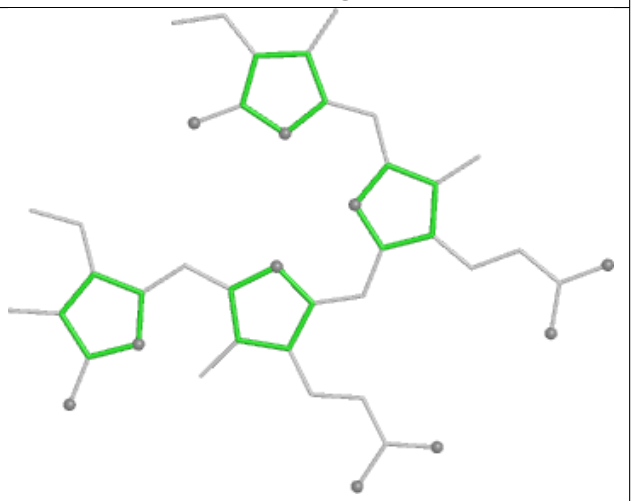
Bond lengths



Bond angles

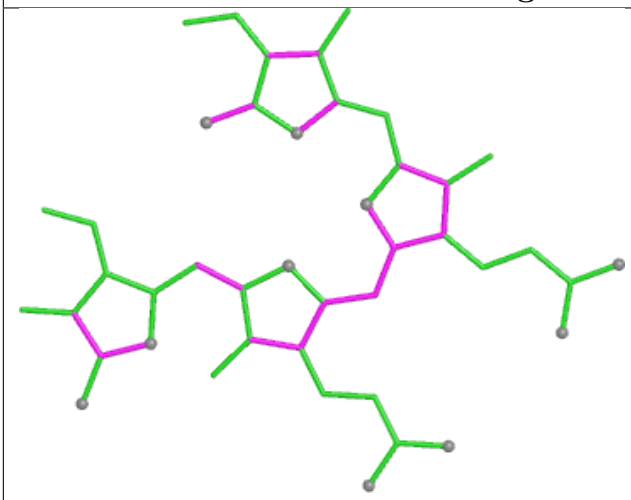


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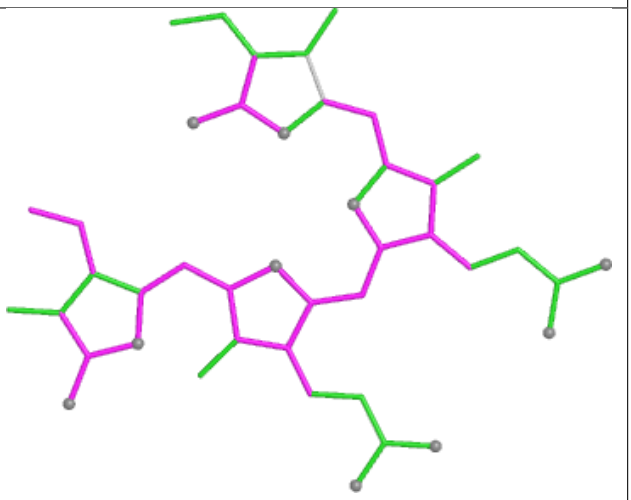


Rings

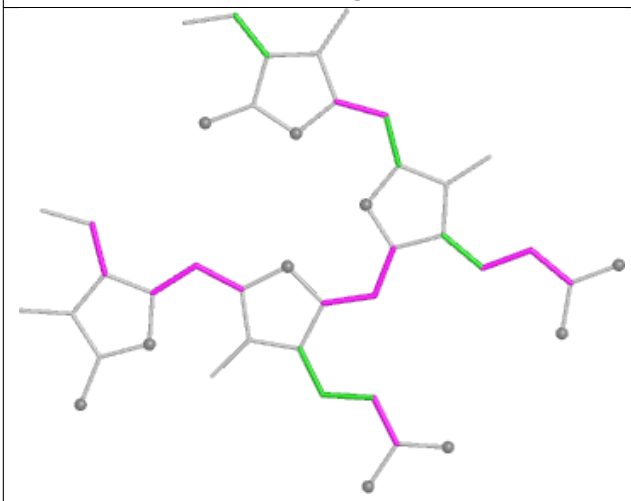
Ligand PEB rC 202



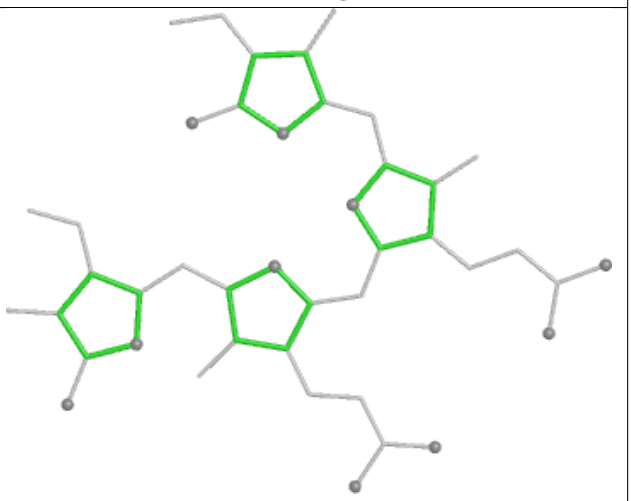
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Bond angles

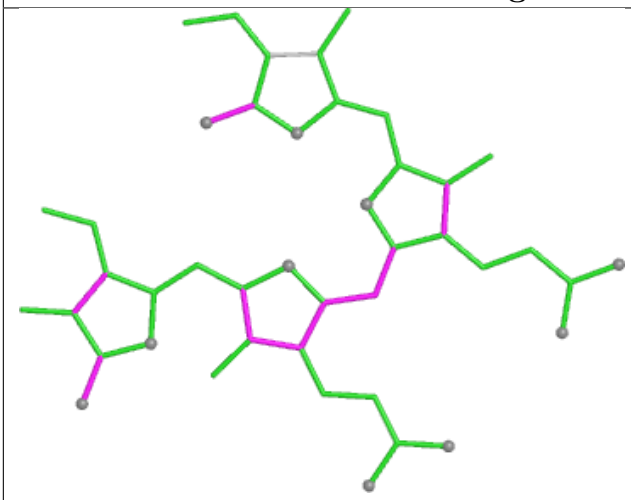


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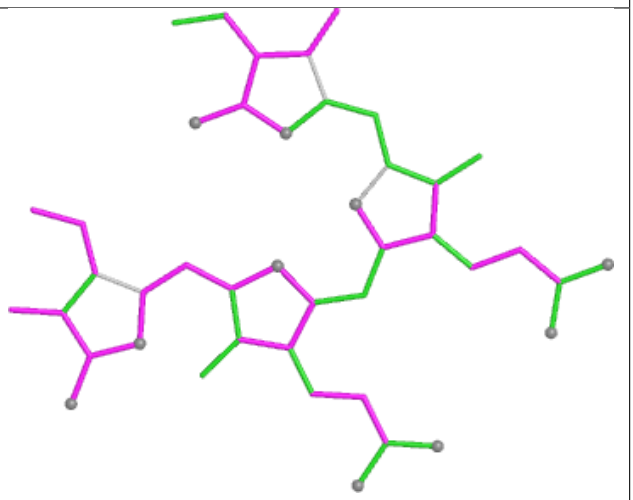


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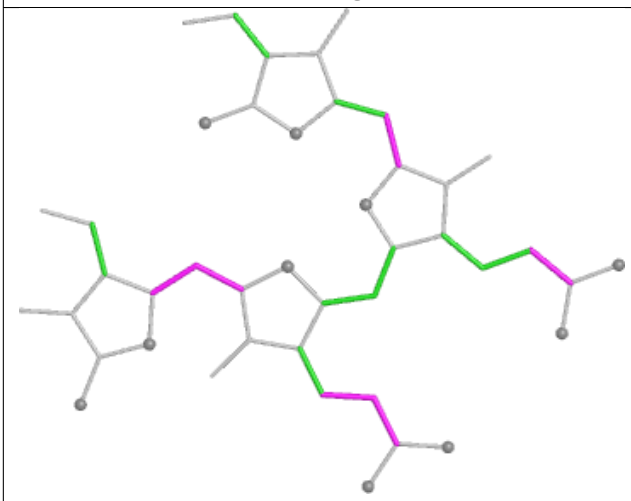
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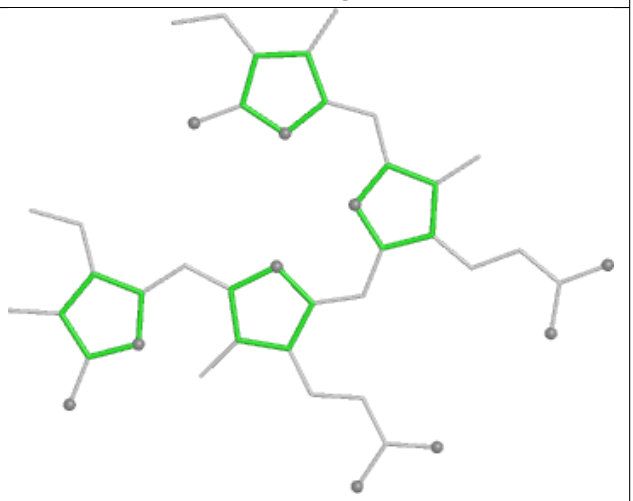
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Bond angles

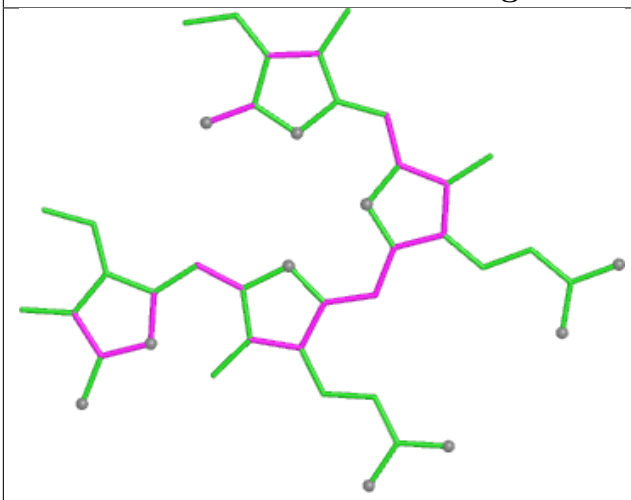


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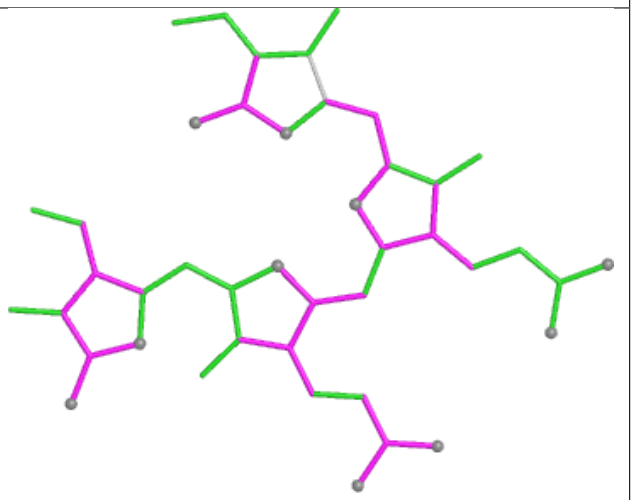


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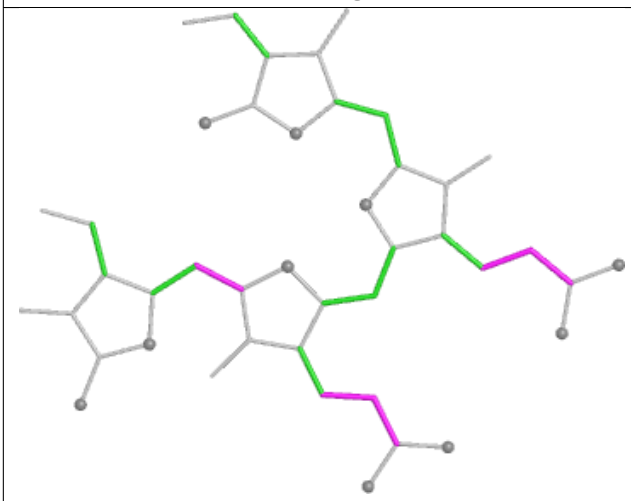
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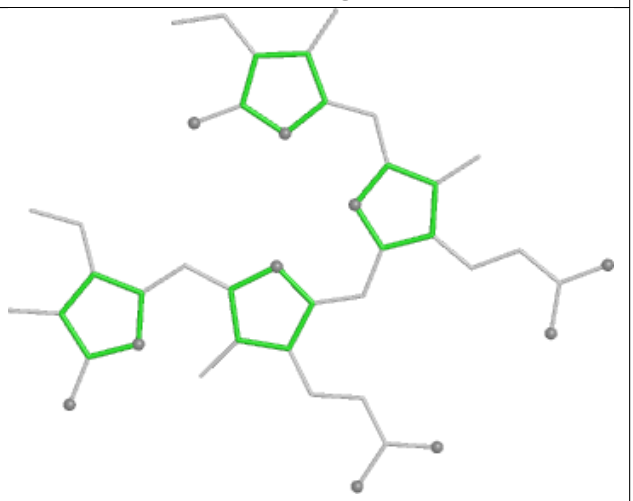
Bond lengths



Bond angles

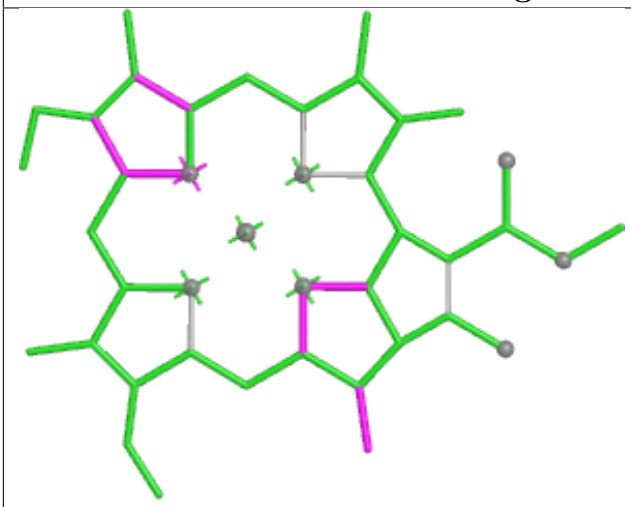


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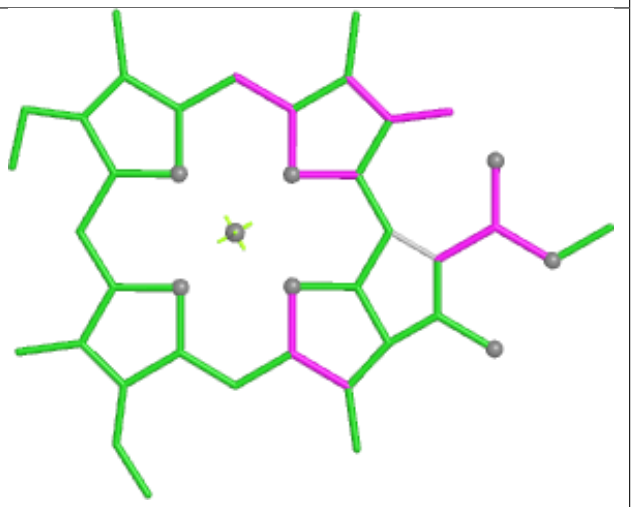


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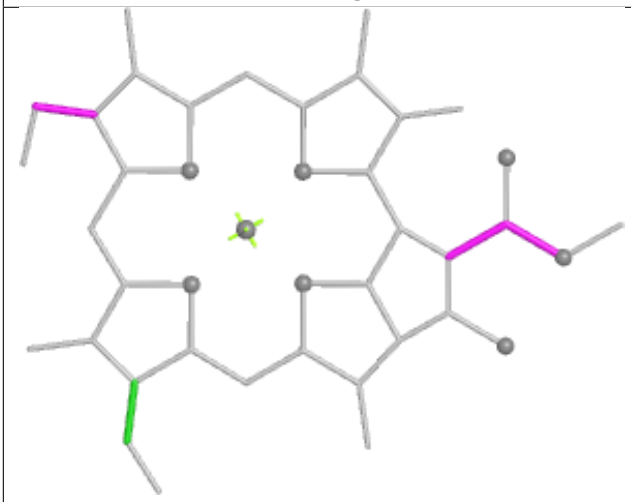
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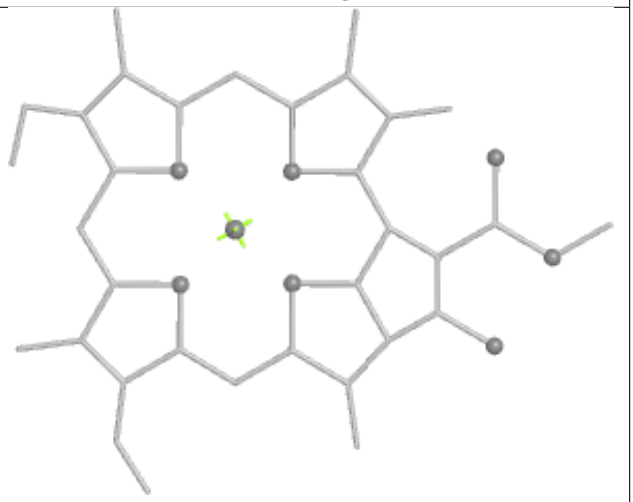
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Bond angles

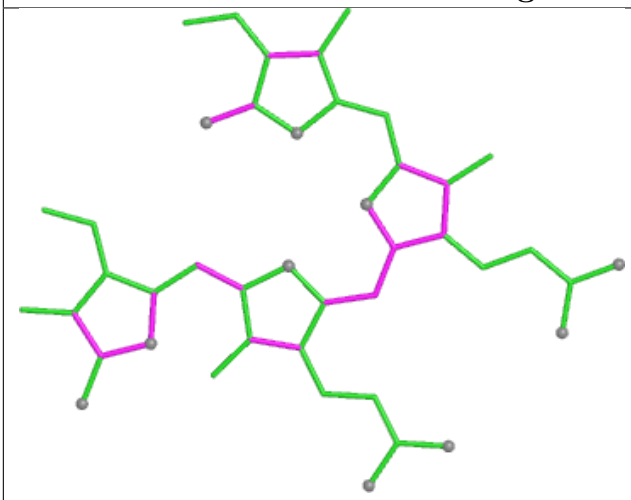


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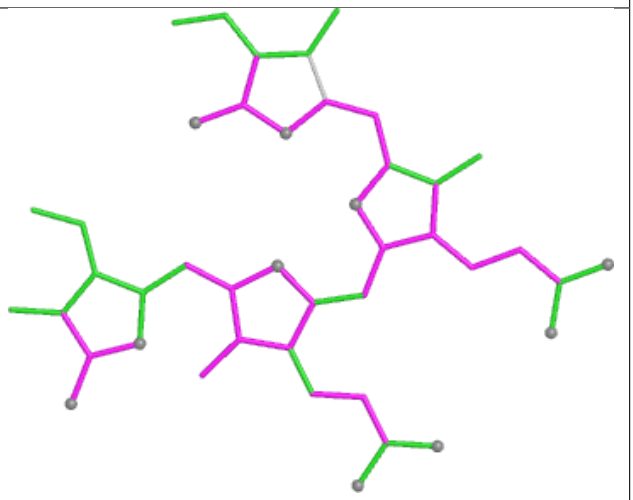


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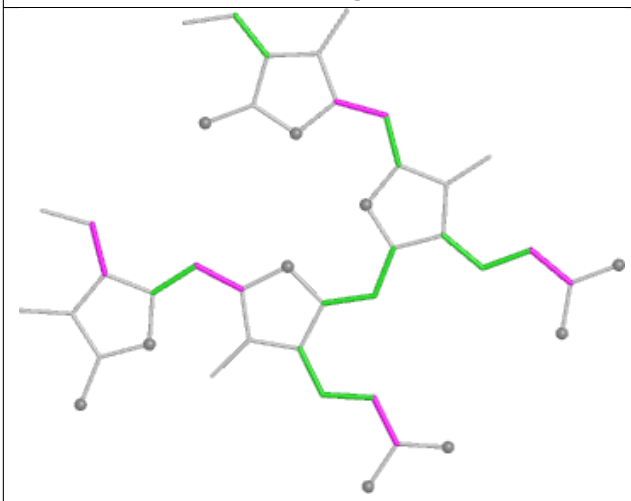
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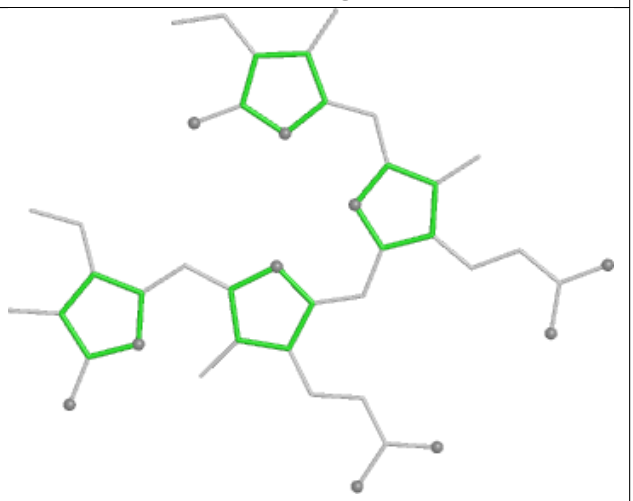
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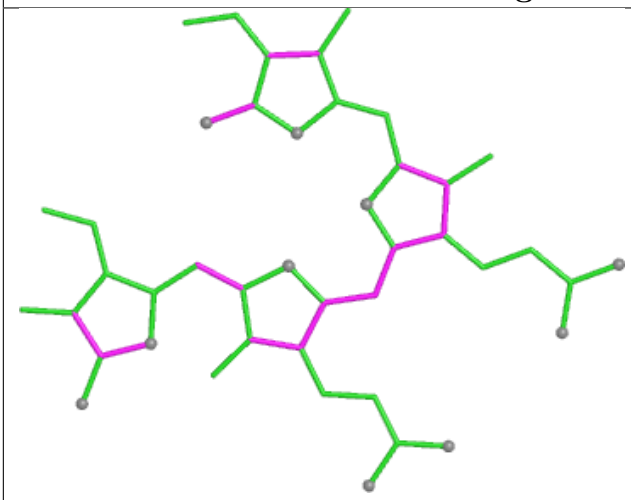


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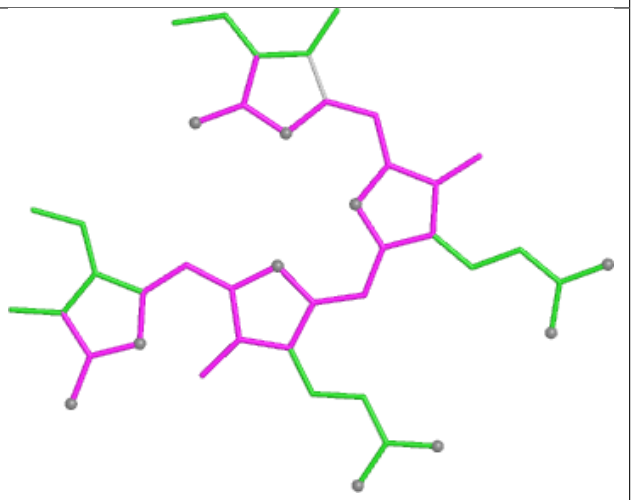


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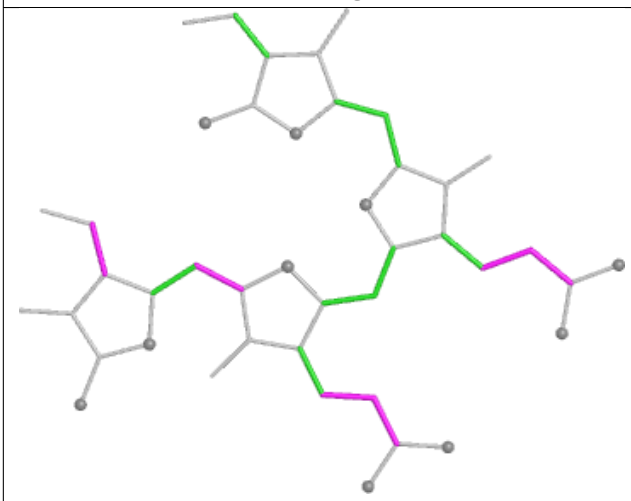
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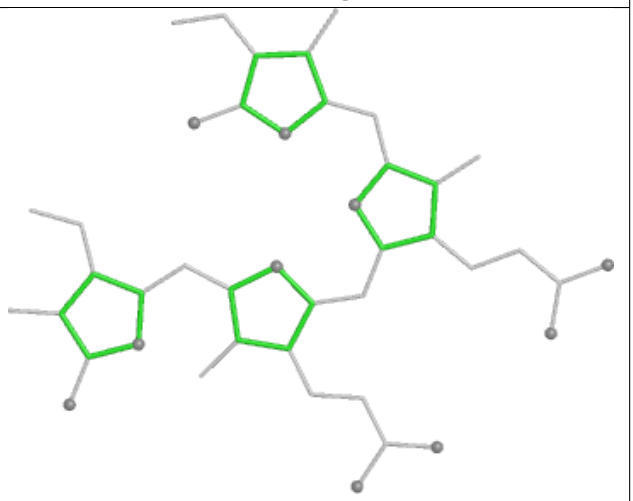
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Bond angles

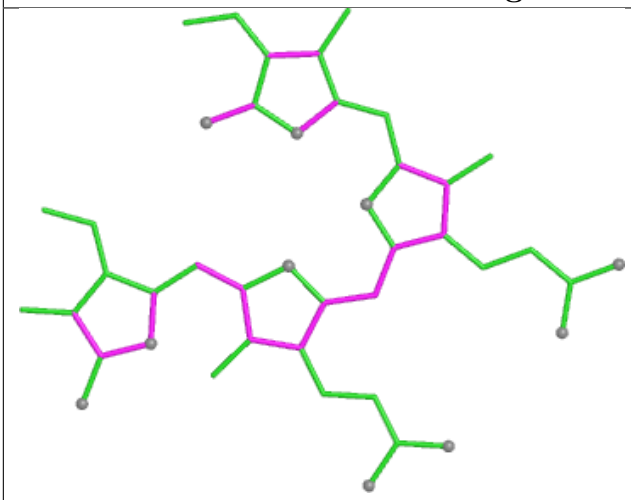


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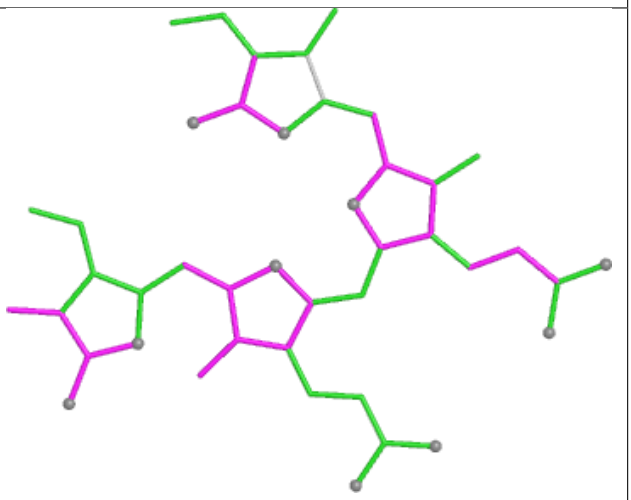


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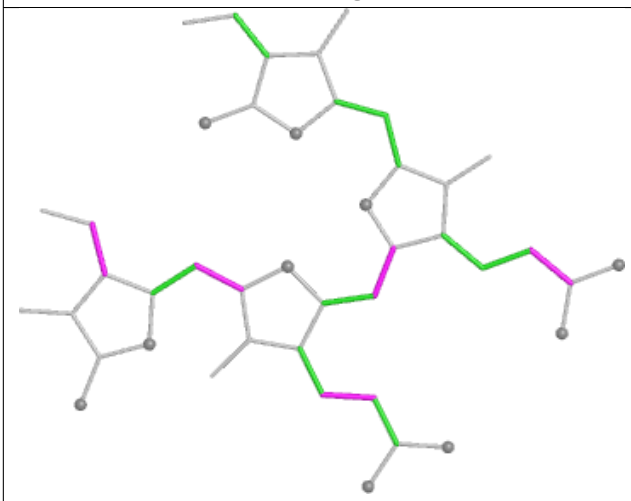
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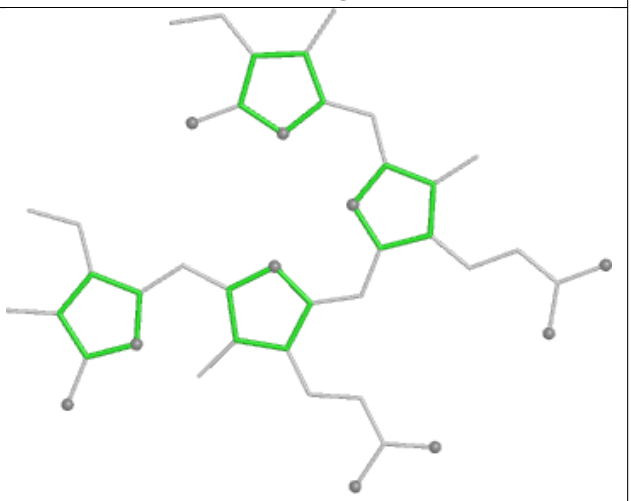
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Bond angles

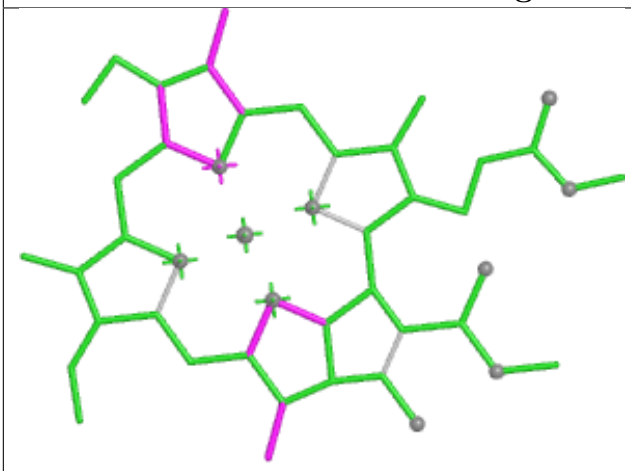


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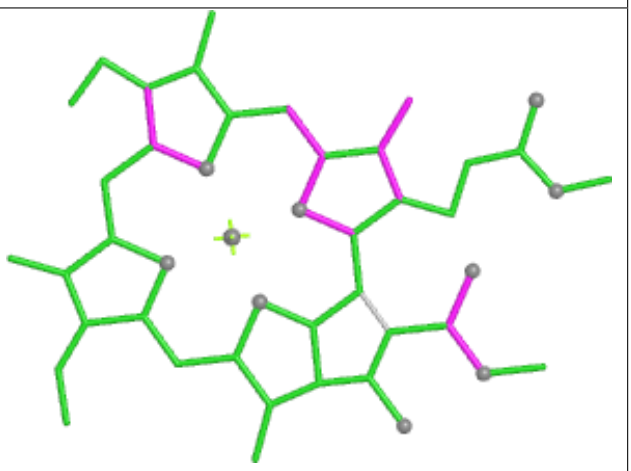


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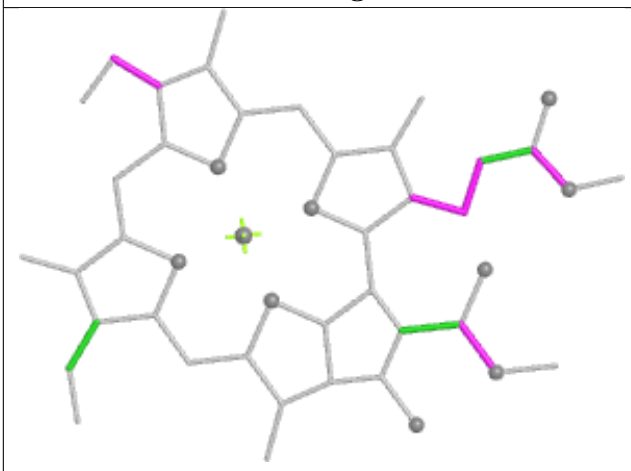
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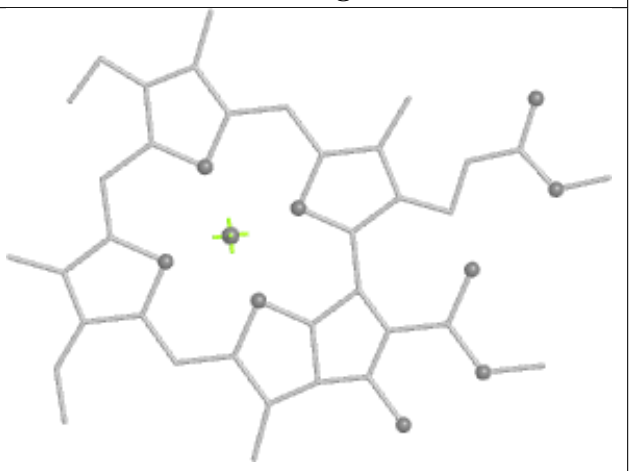
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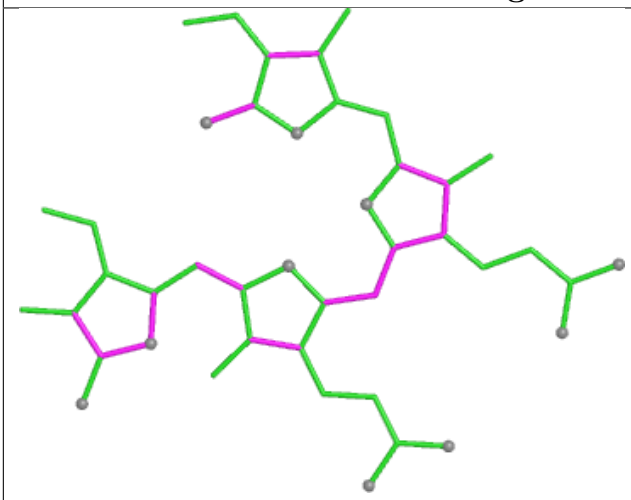


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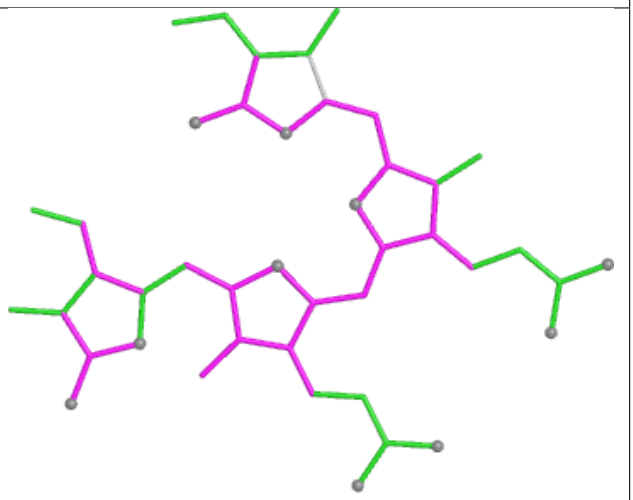


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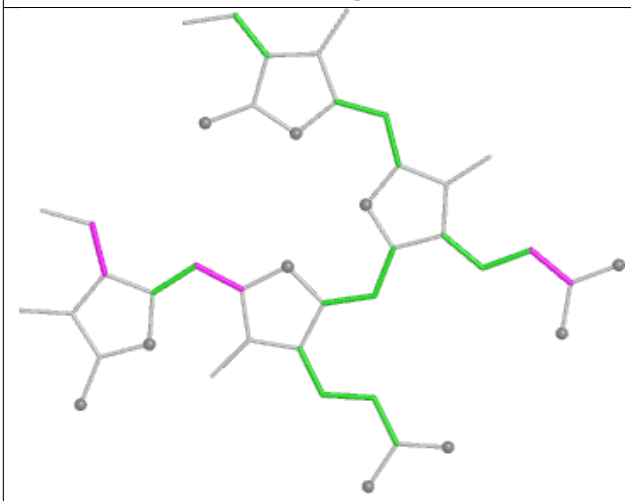
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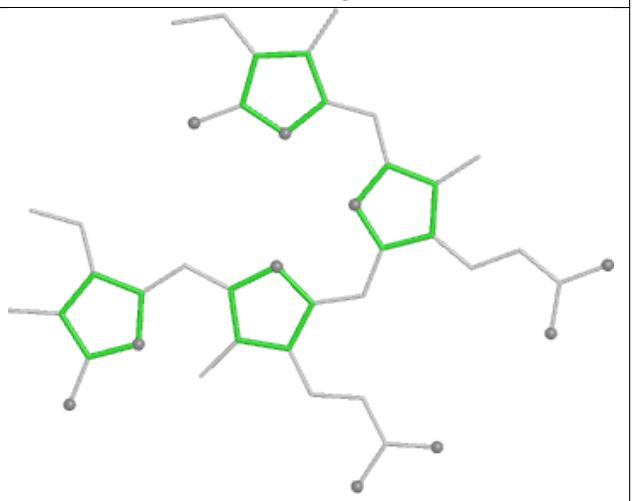
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Bond angles

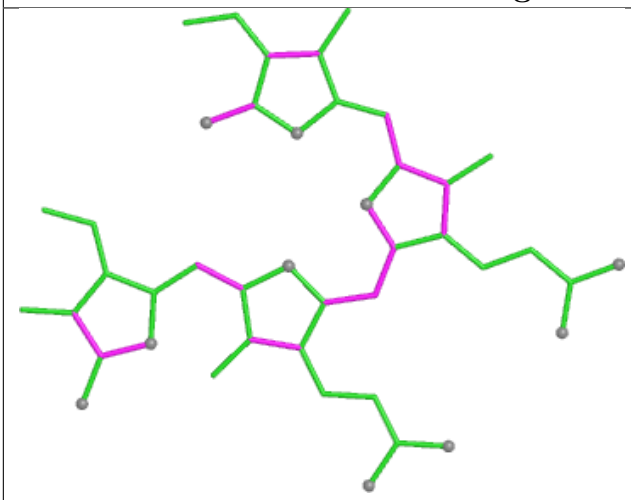


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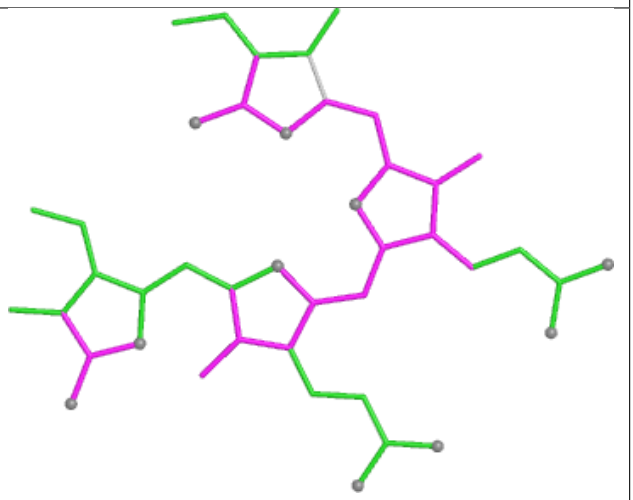


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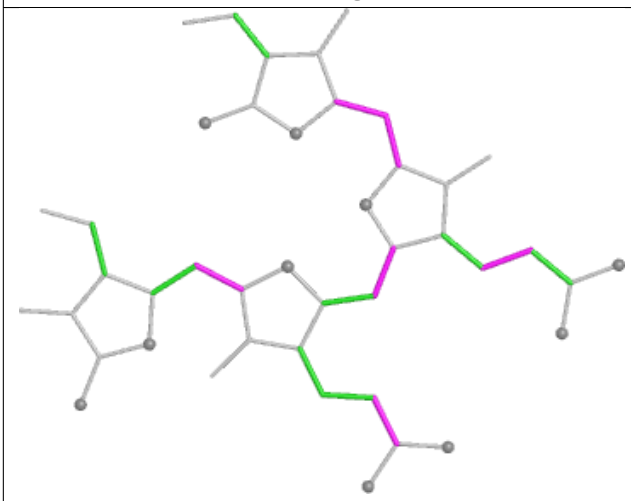
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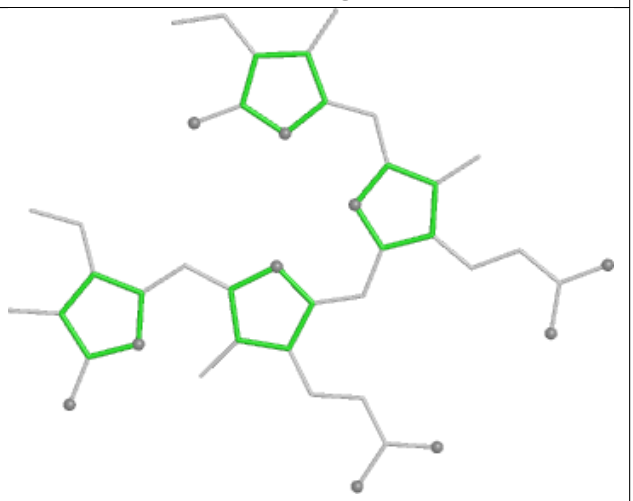
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Bond angles

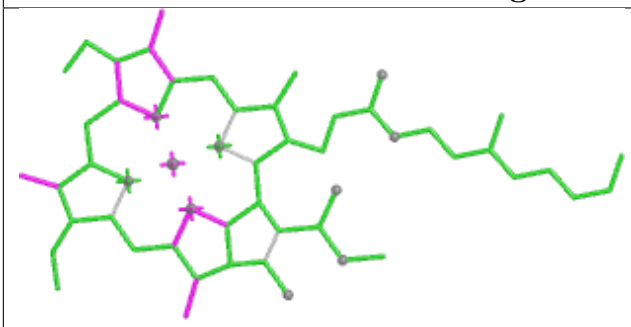


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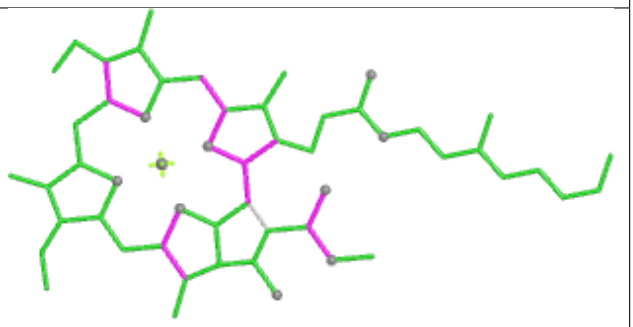


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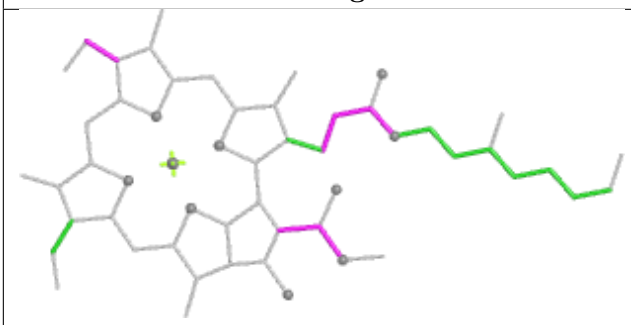
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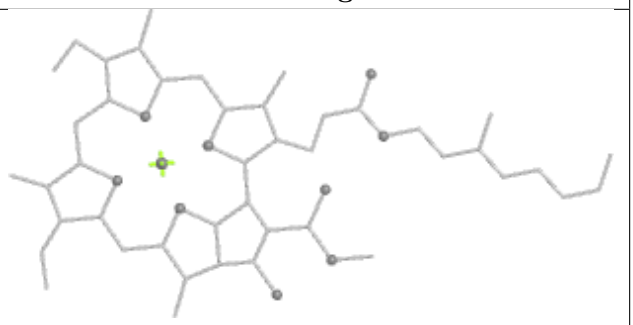
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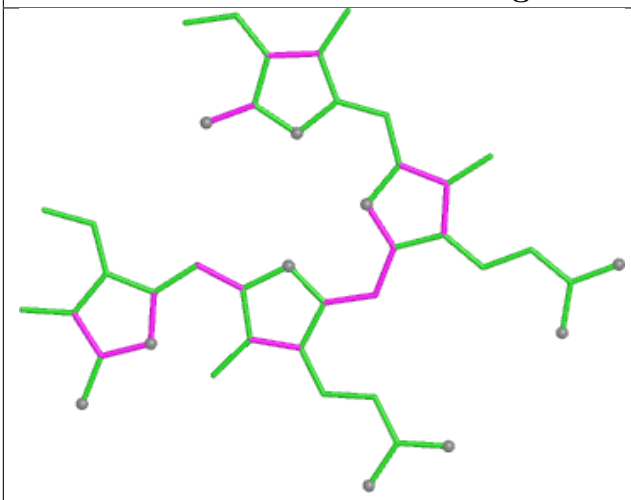


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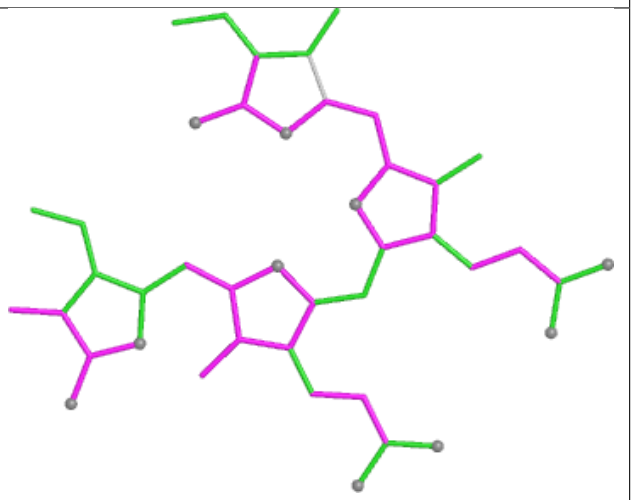


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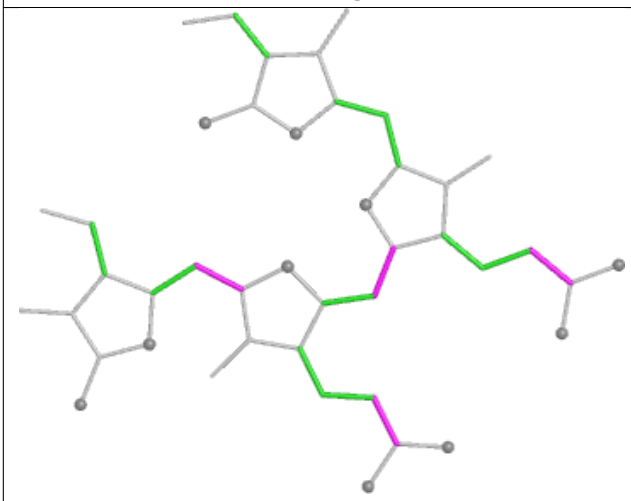
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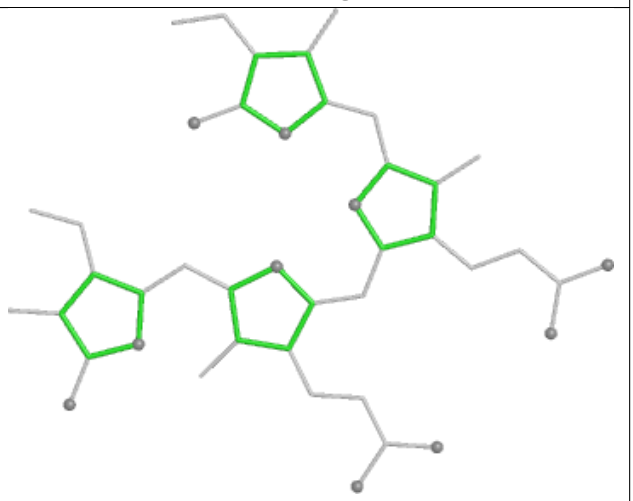
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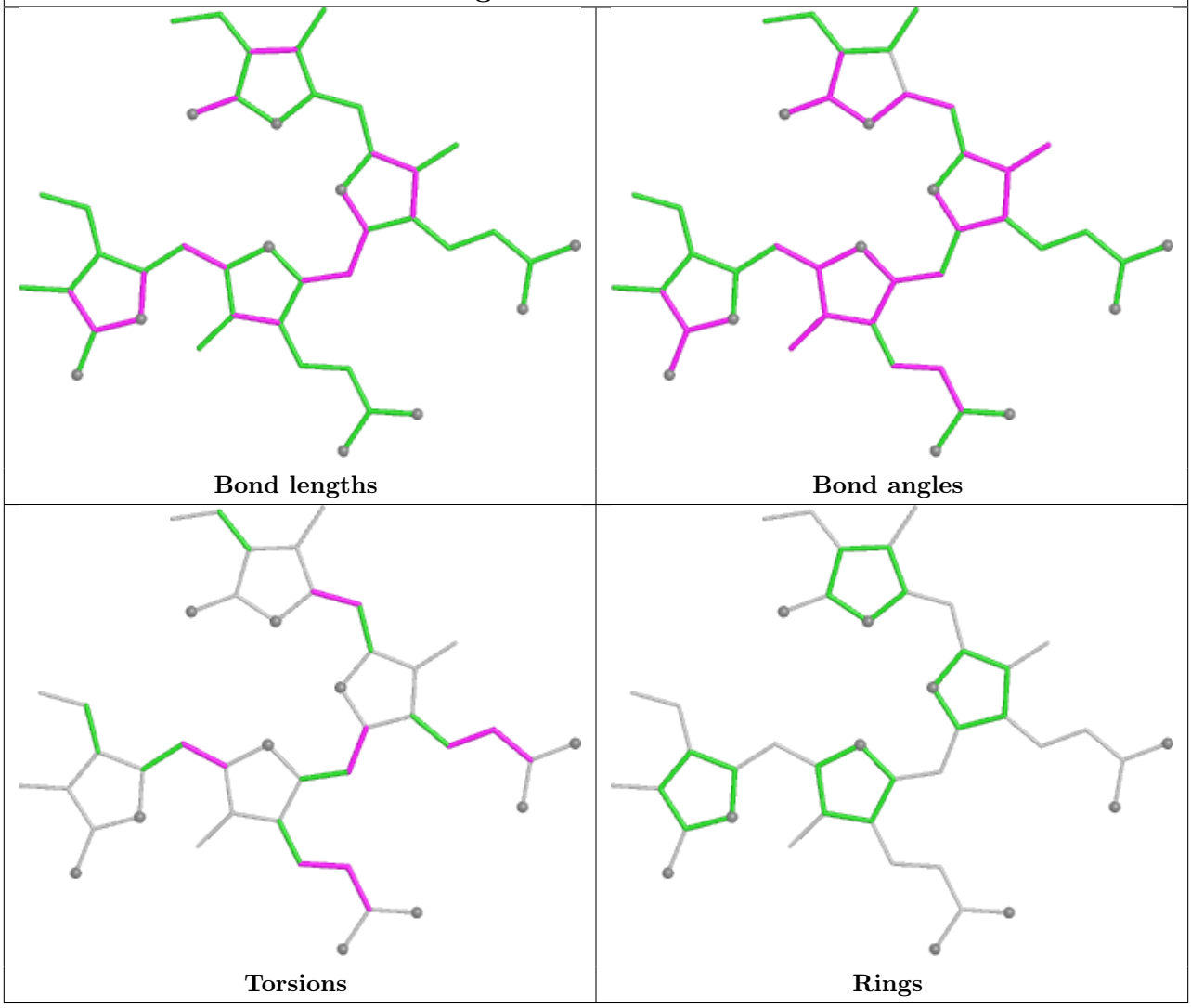


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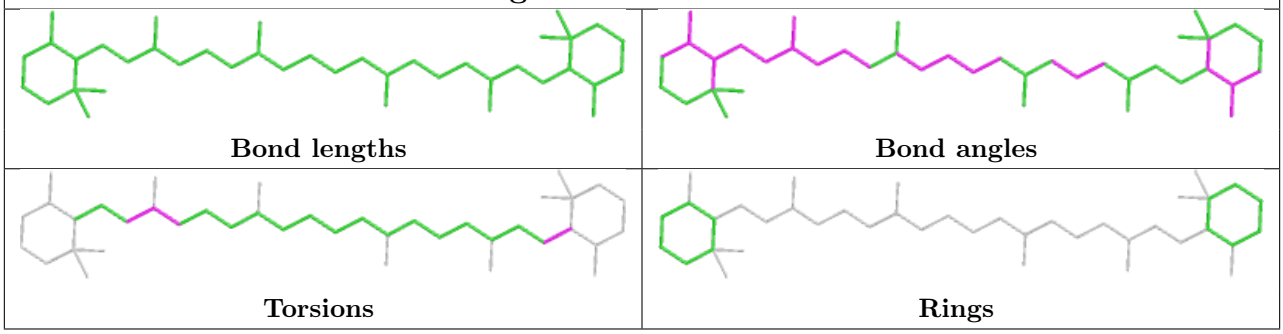


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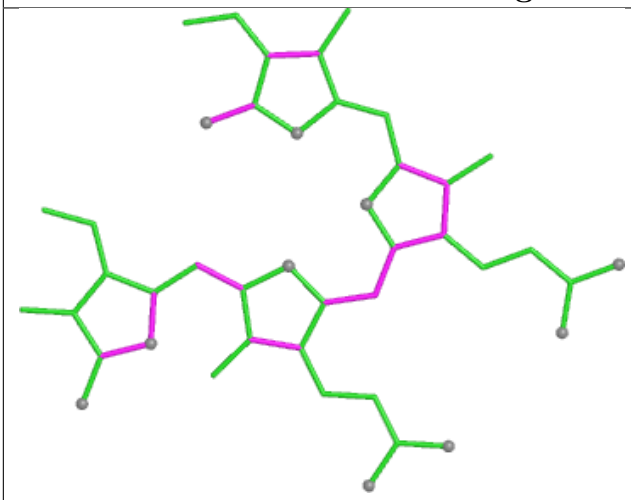
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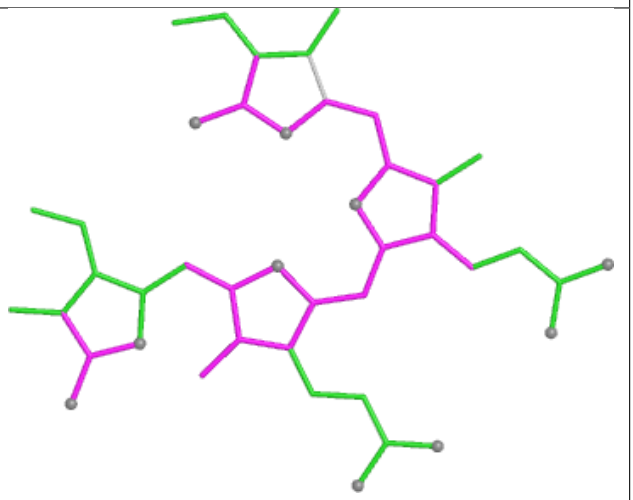
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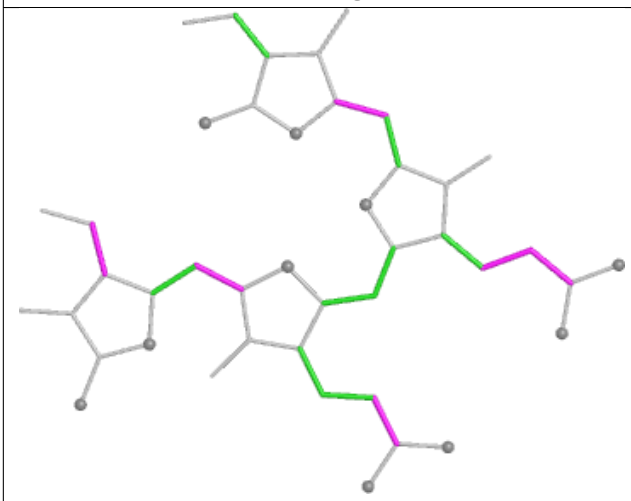
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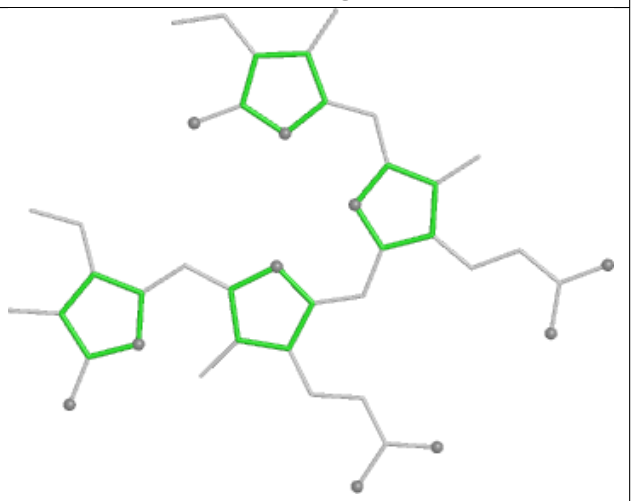
Bond lengths



Bond angles

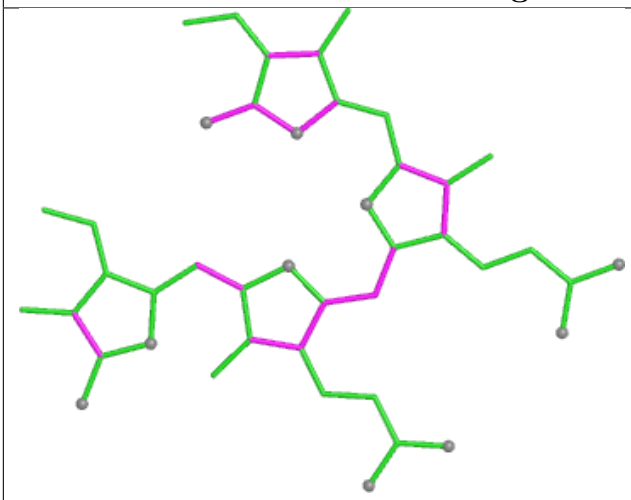


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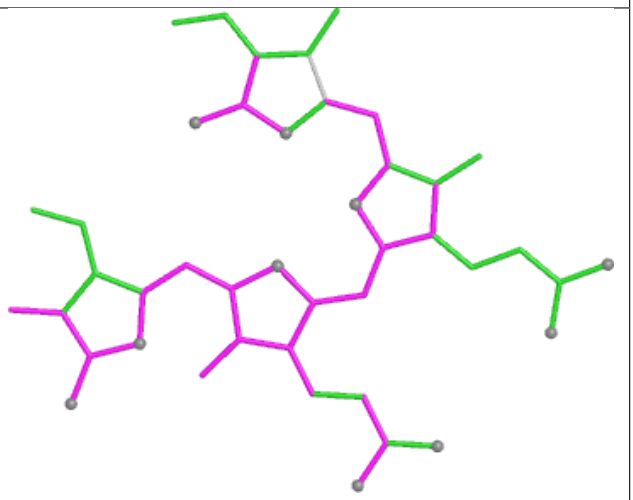


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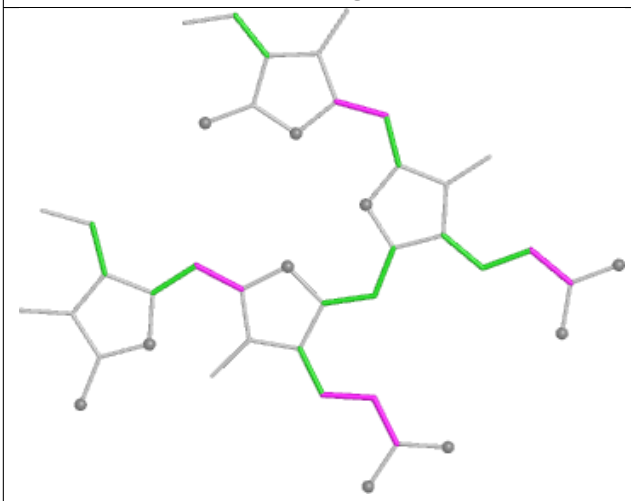
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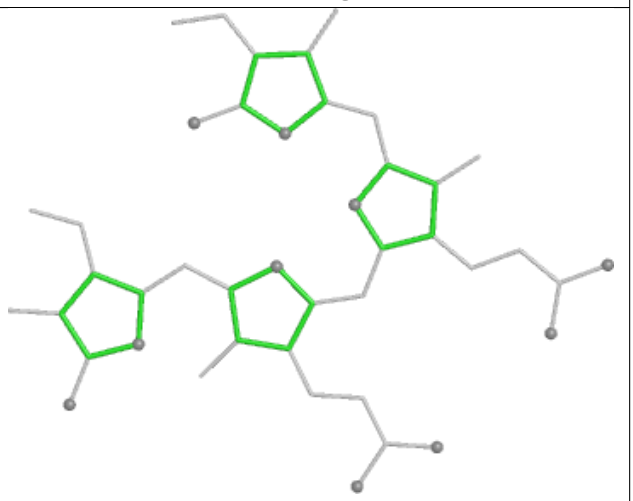
Bond lengths



Bond angles

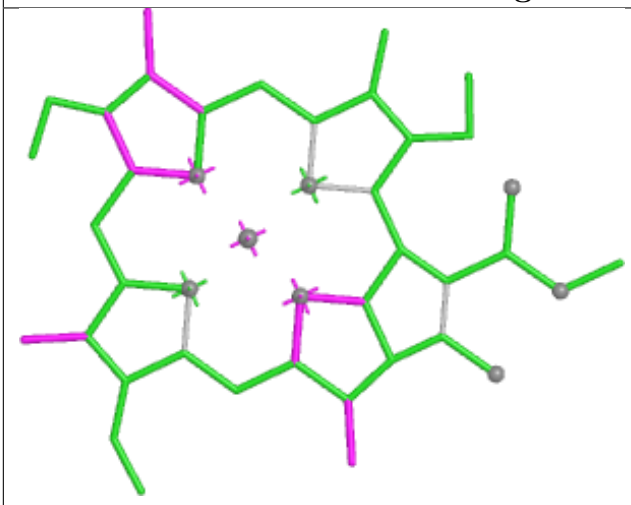


Torsions

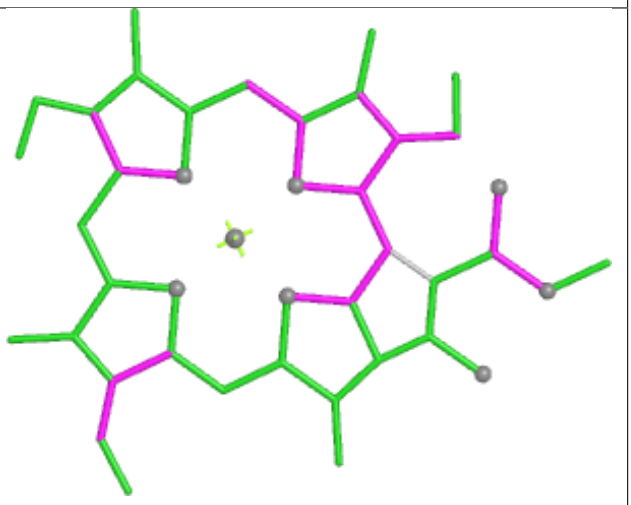


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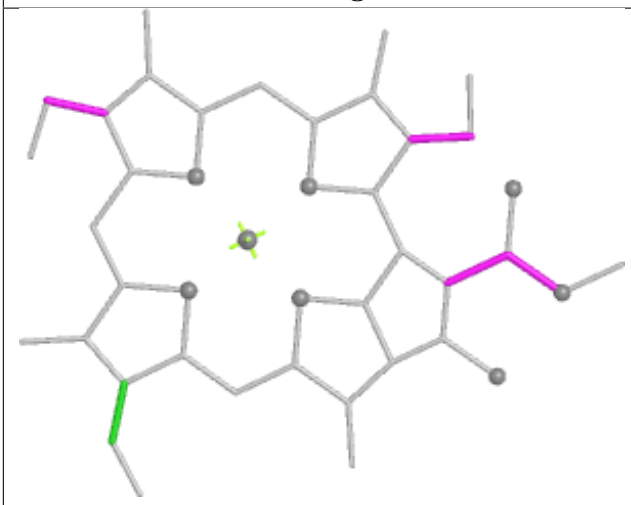
Ligand CLA 7N 604



Bond lengths



Bond angles

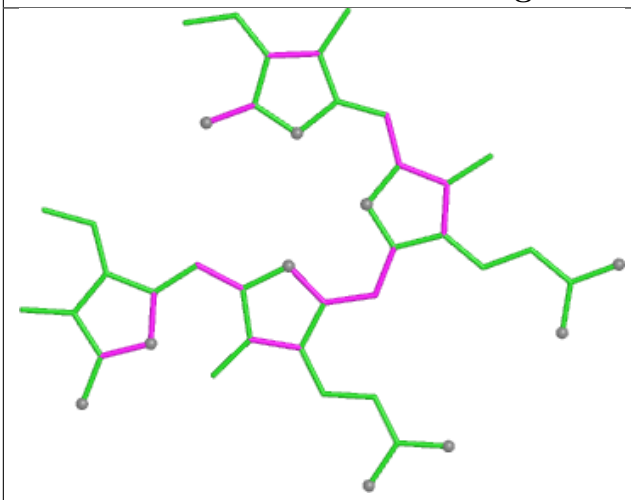


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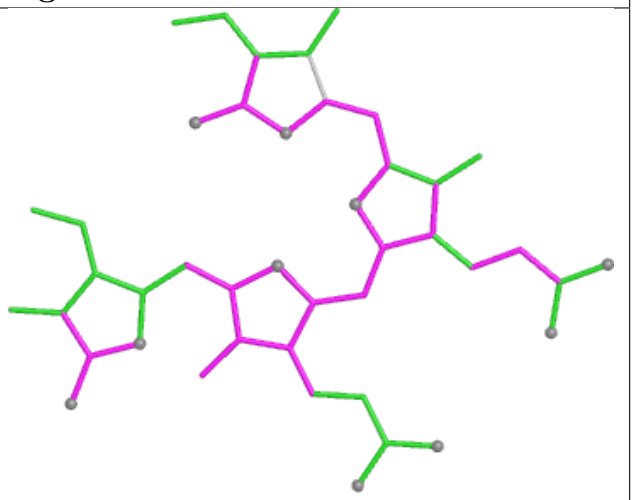


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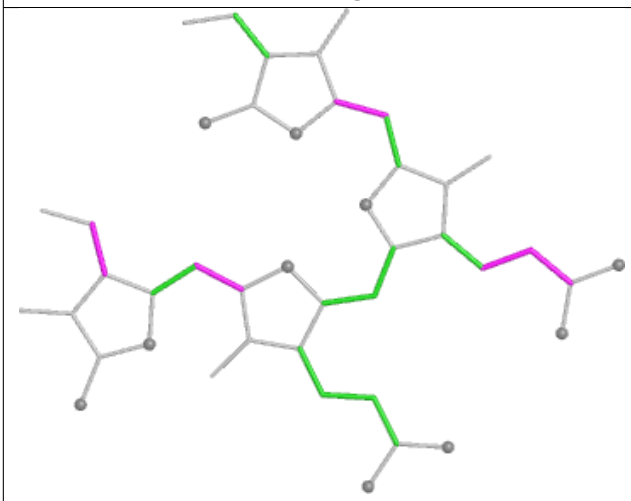
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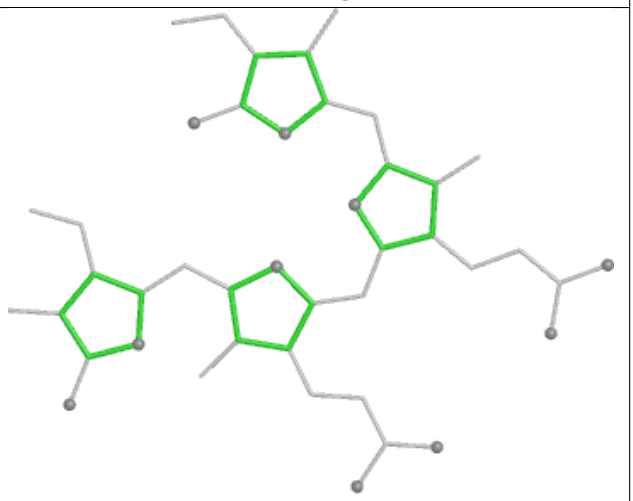
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Bond angles

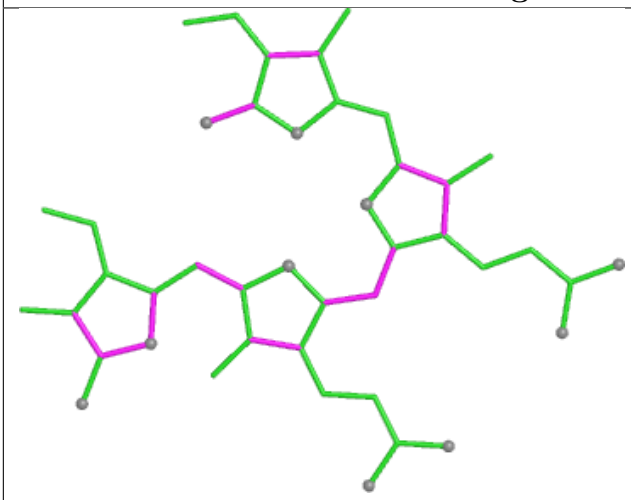


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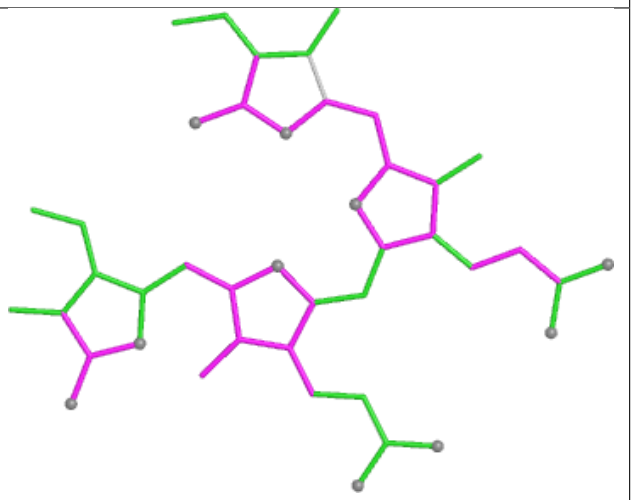


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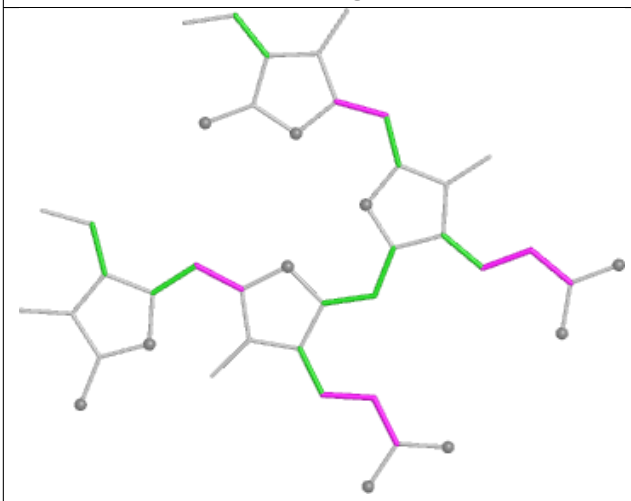
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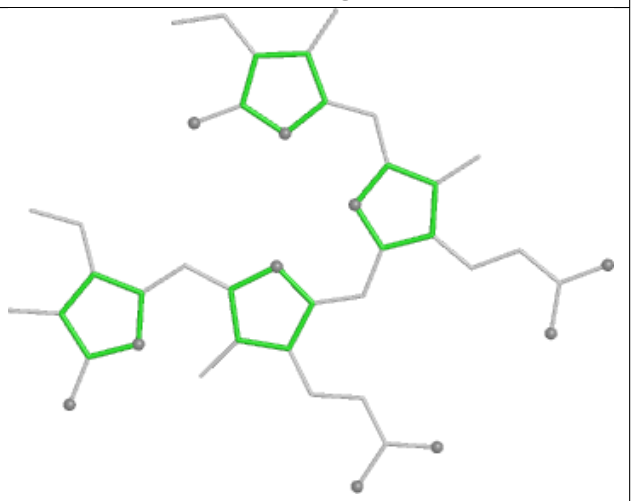
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Bond angles

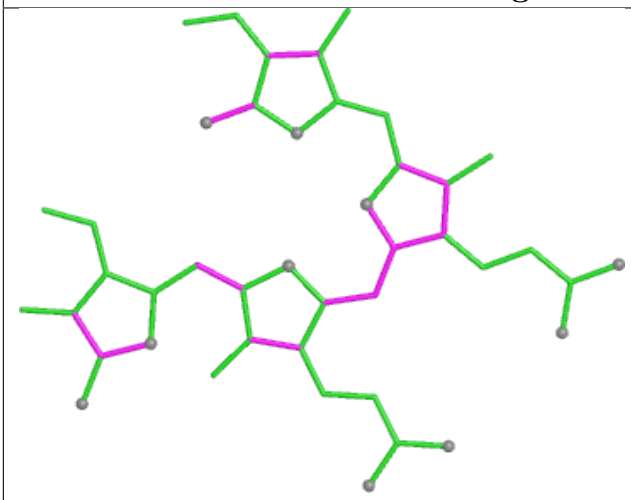


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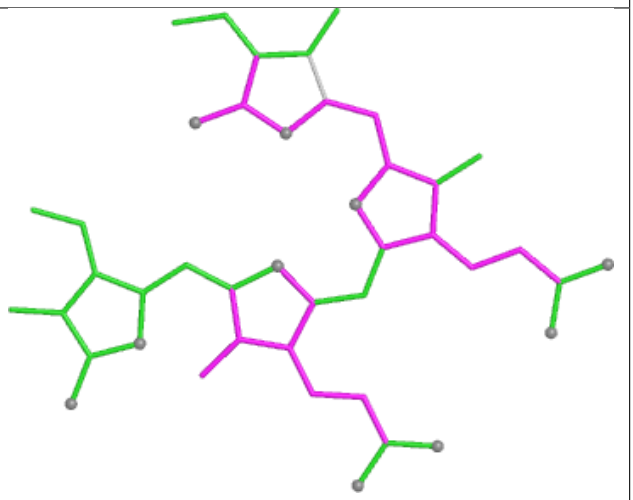


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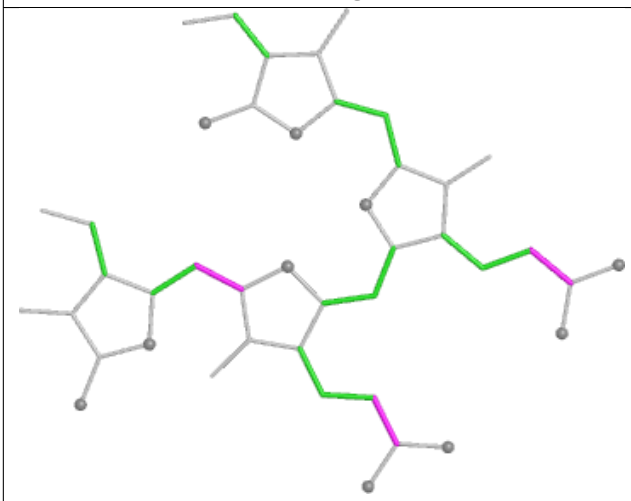
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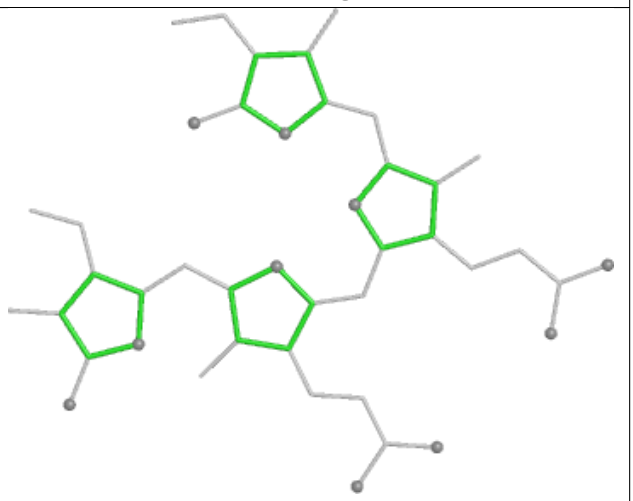
Bond lengths



Bond angles

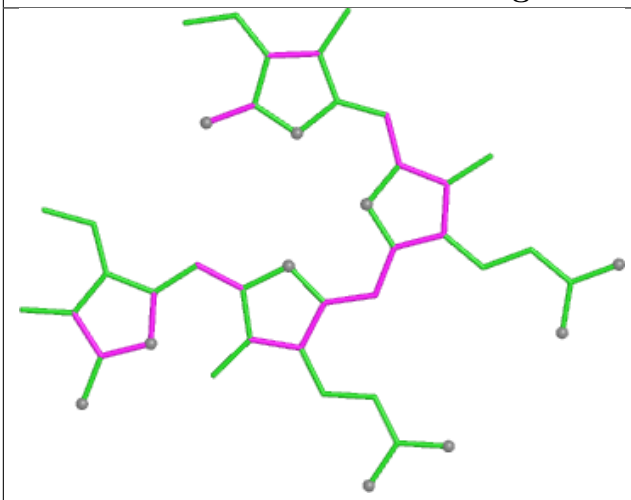


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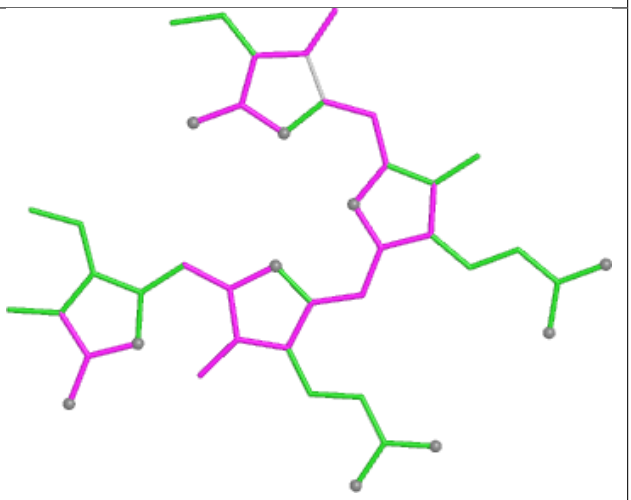


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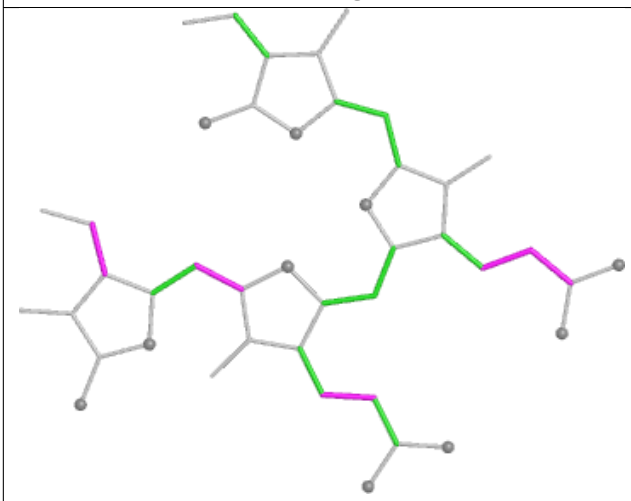
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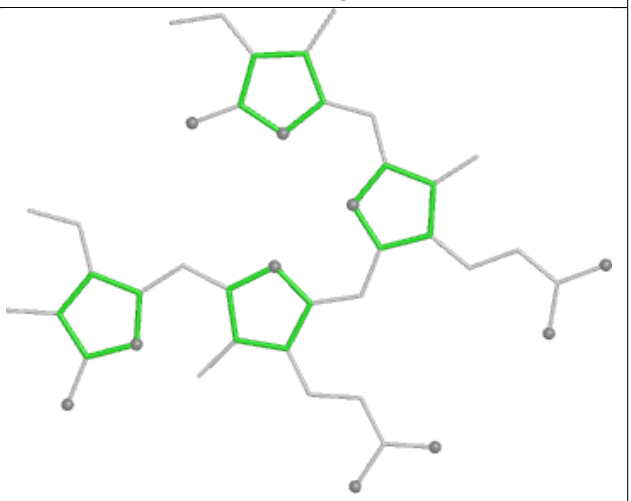
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Bond angles

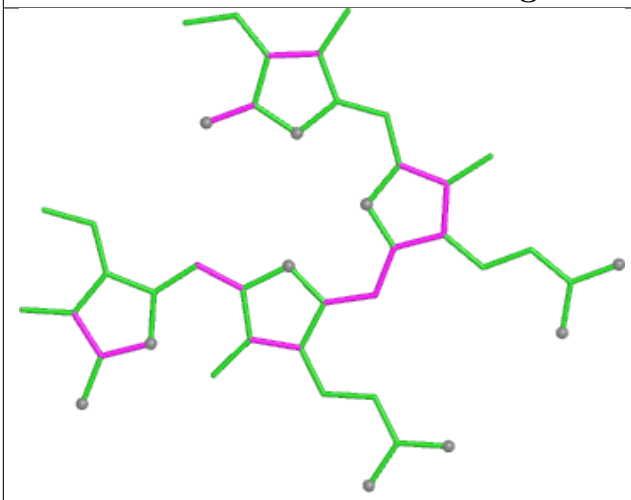


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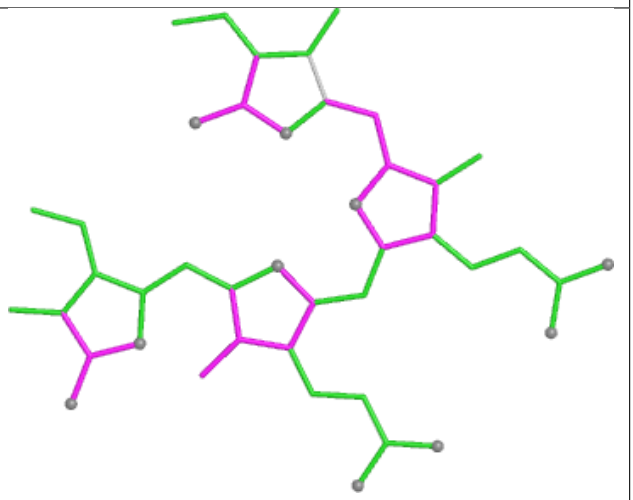


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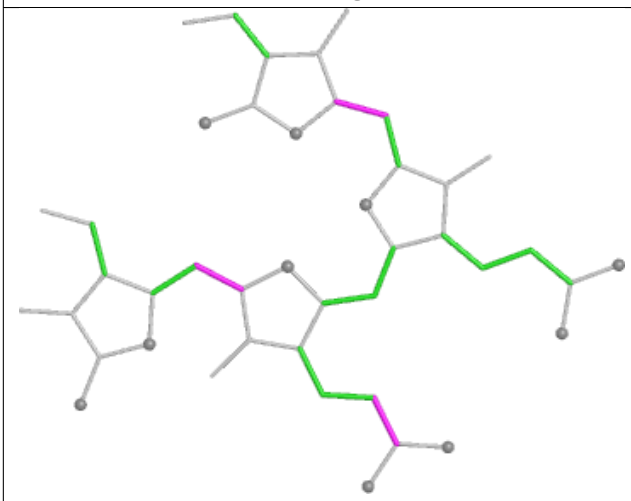
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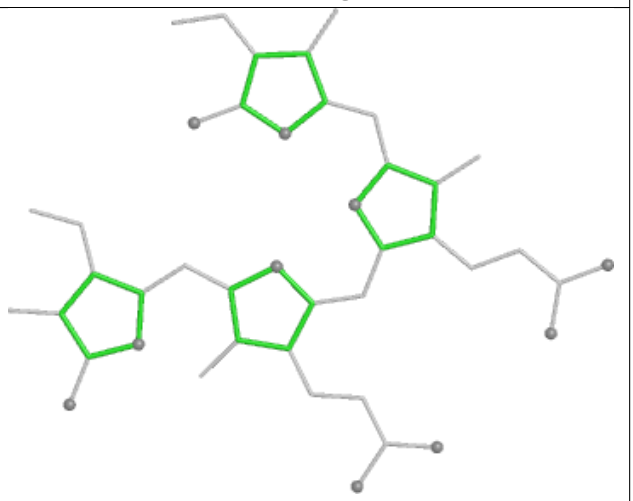
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Bond angles

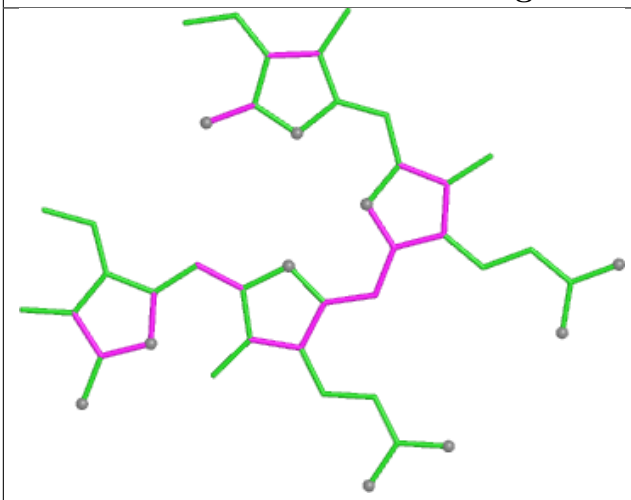


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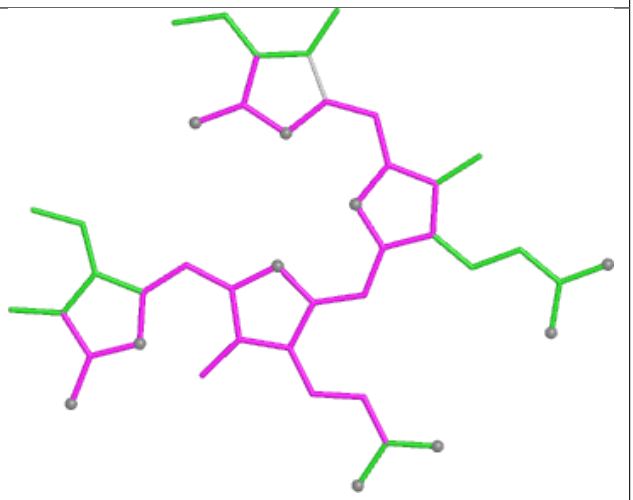


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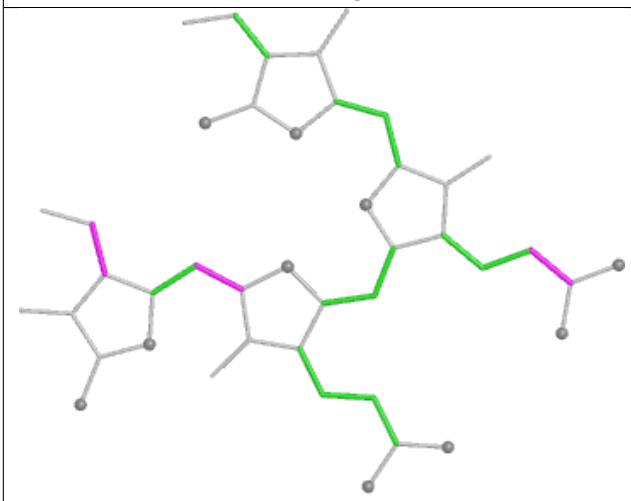
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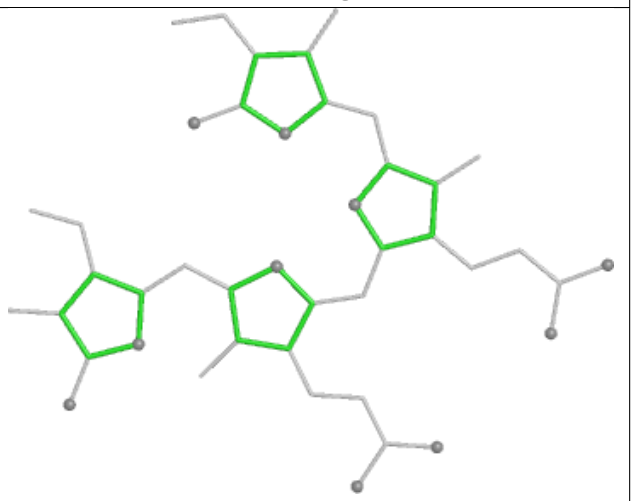
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Bond angles

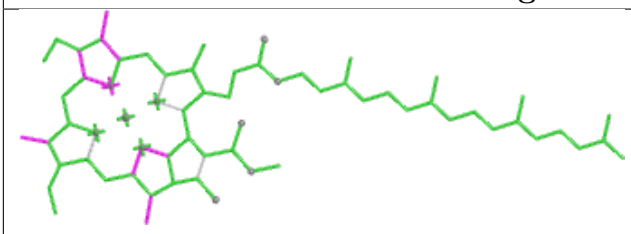


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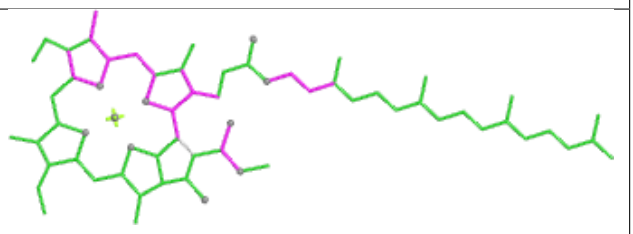


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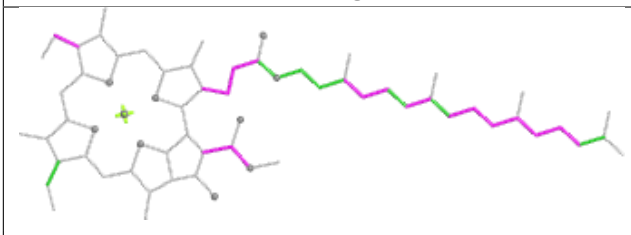
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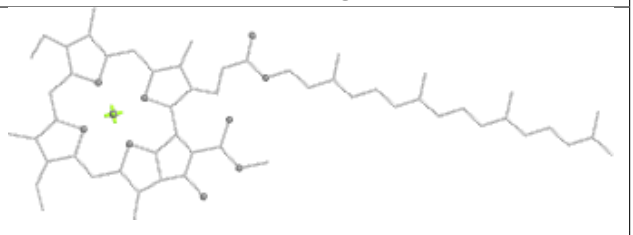
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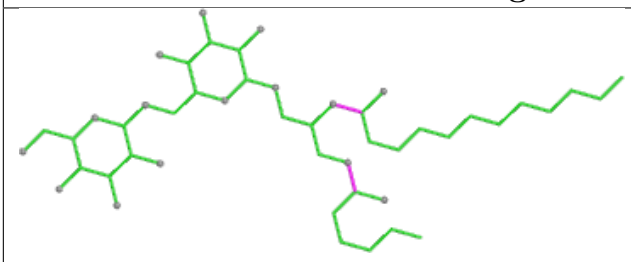


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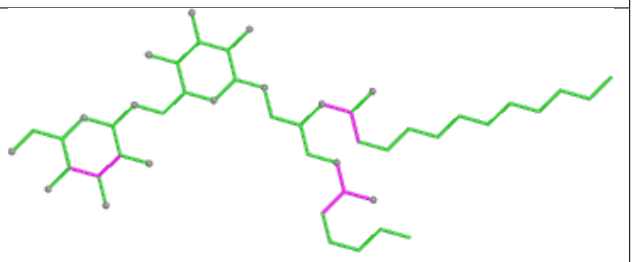


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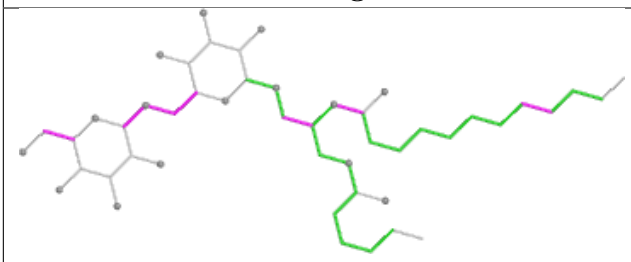
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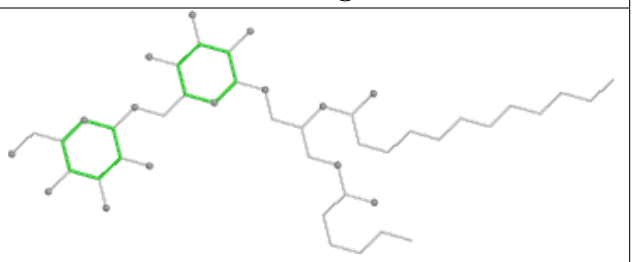
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Bond angles

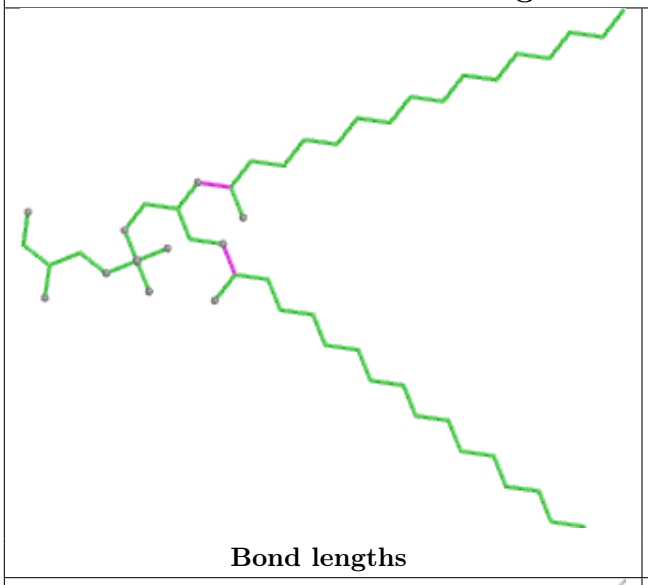


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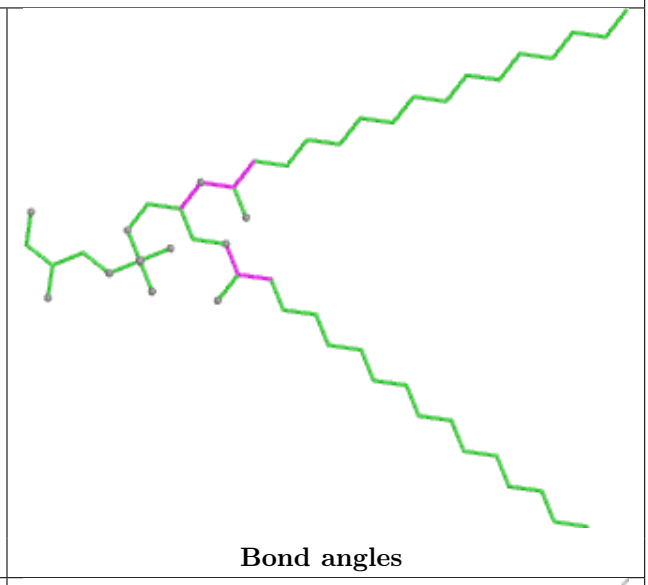


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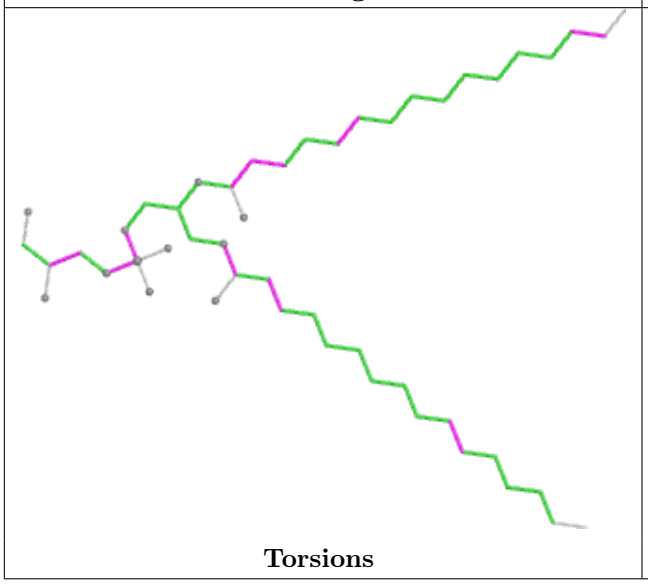
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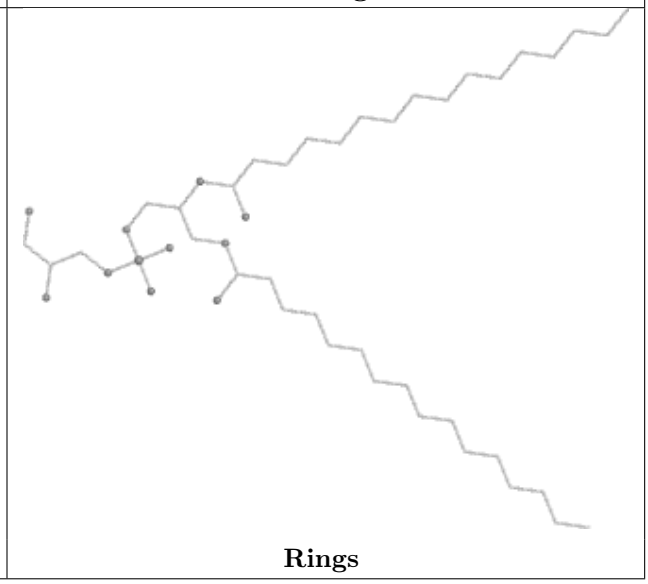
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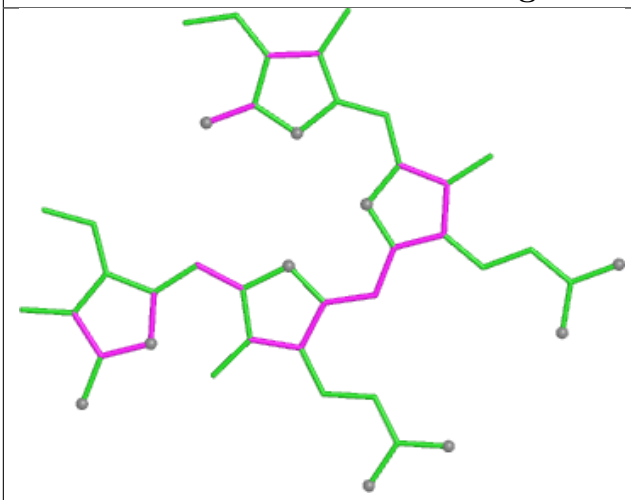


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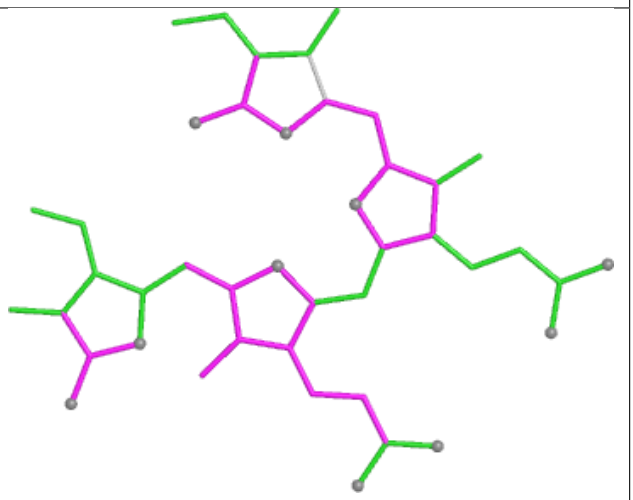


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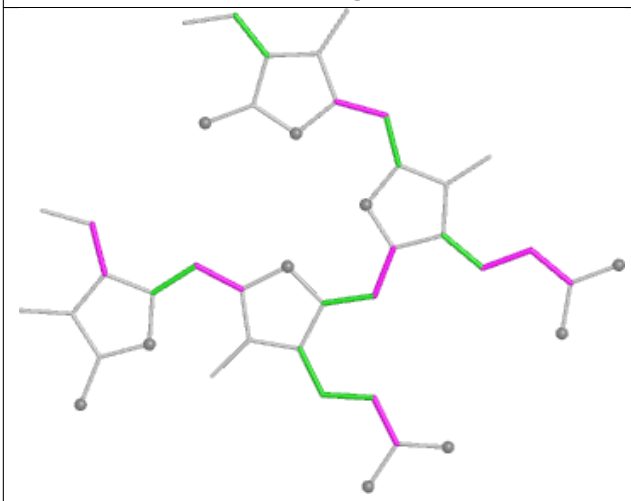
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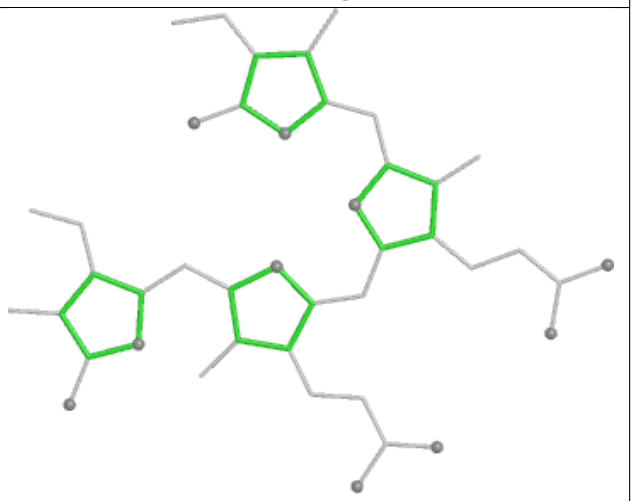
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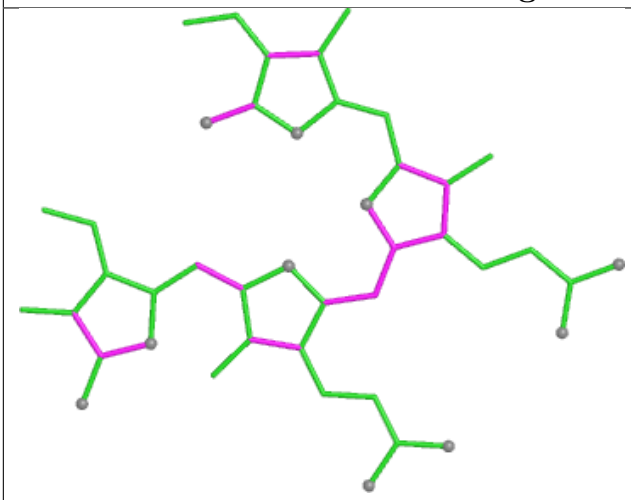


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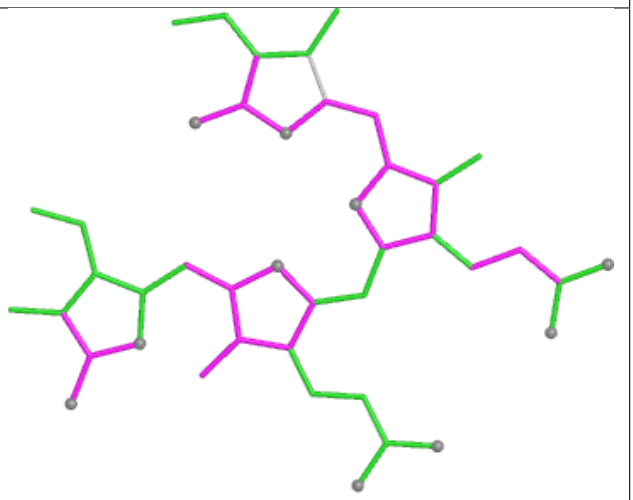


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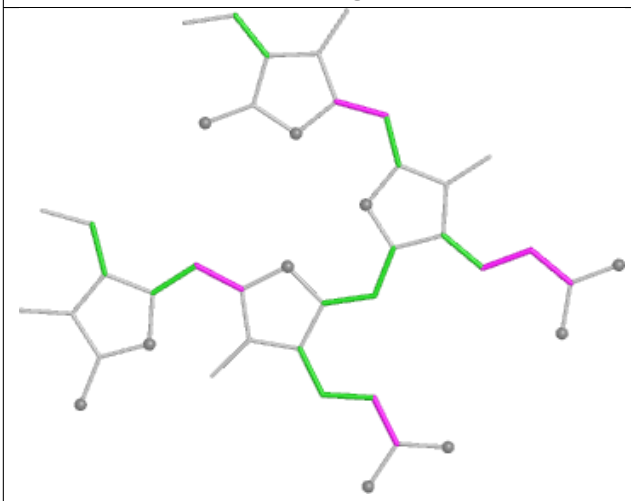
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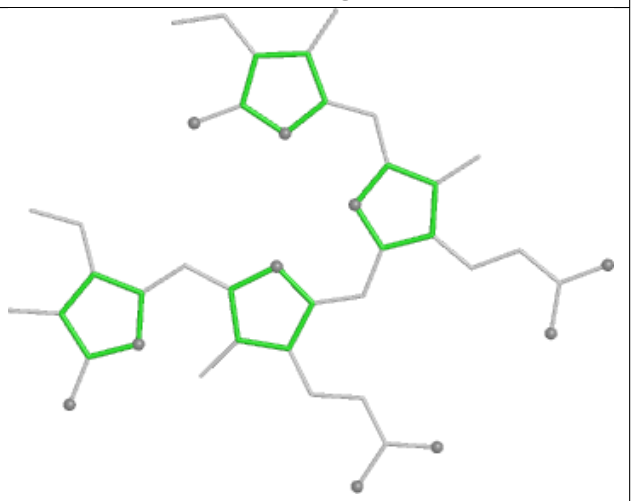
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Bond angles

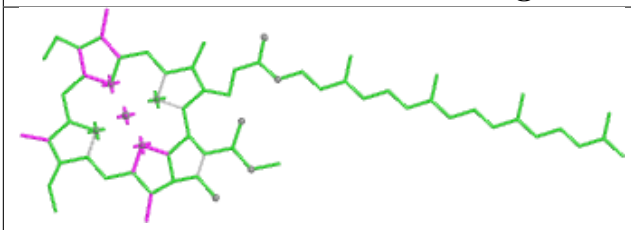


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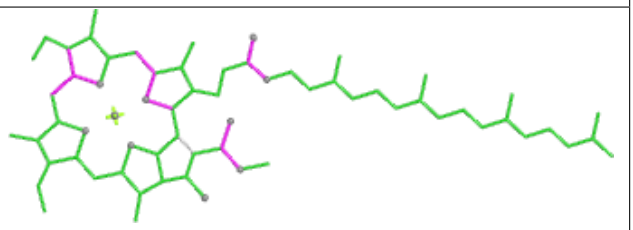


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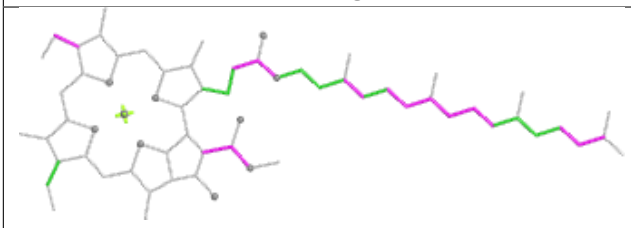
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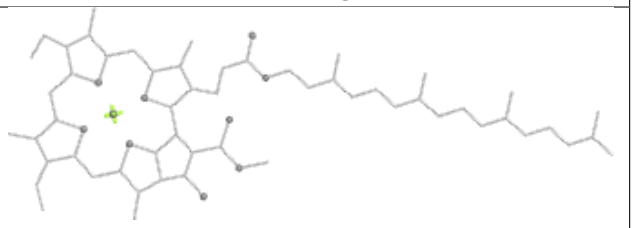
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Bond angles

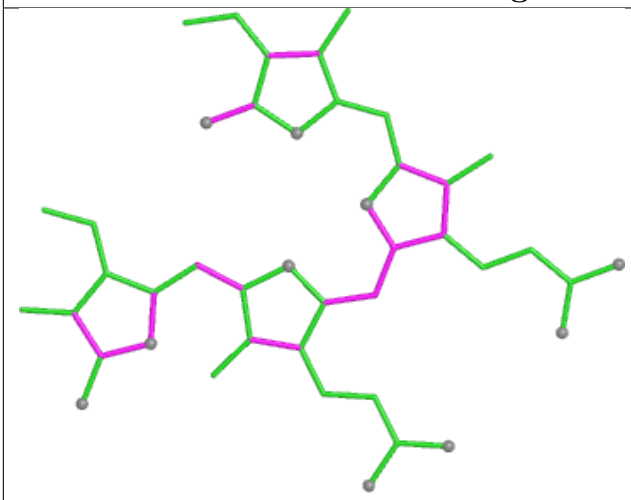


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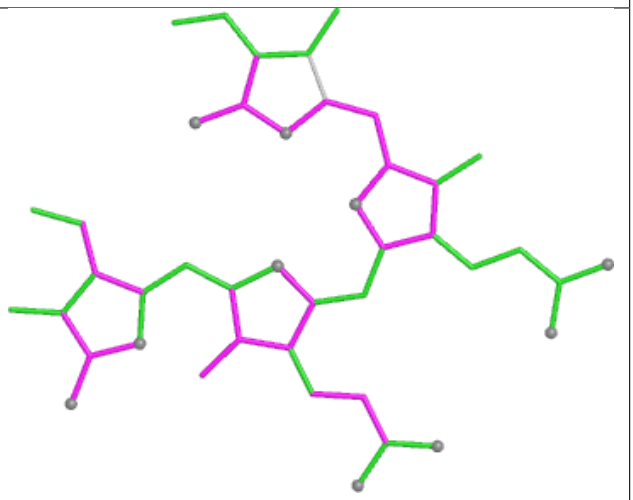


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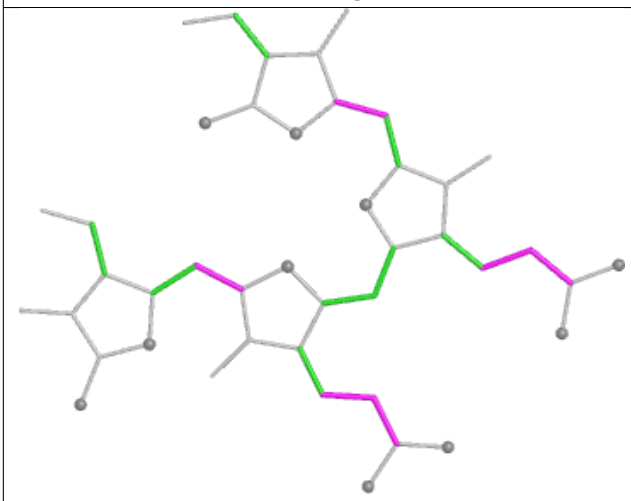
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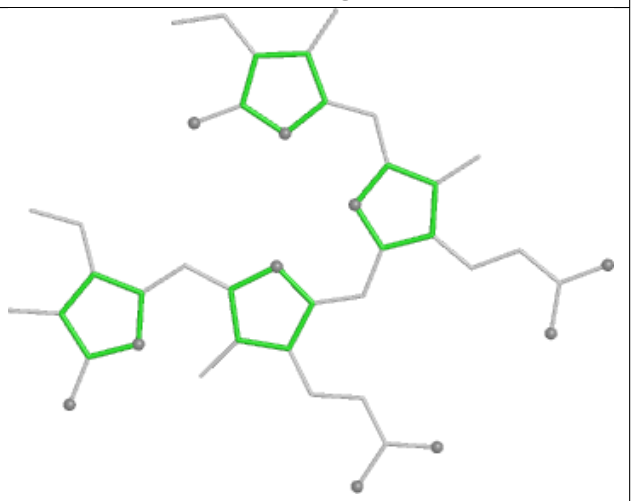
Bond lengths



Bond angles

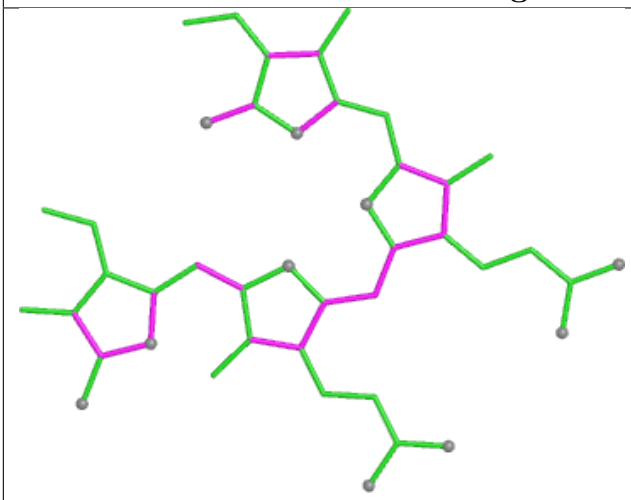


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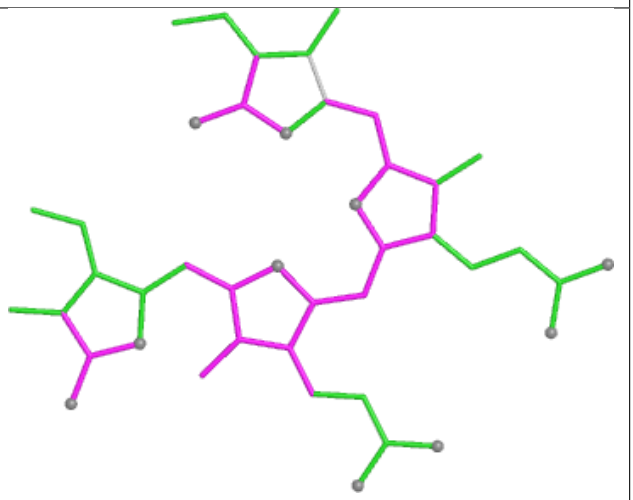


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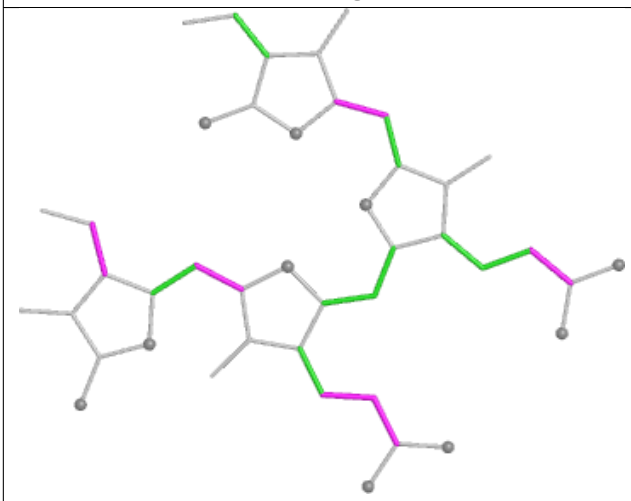
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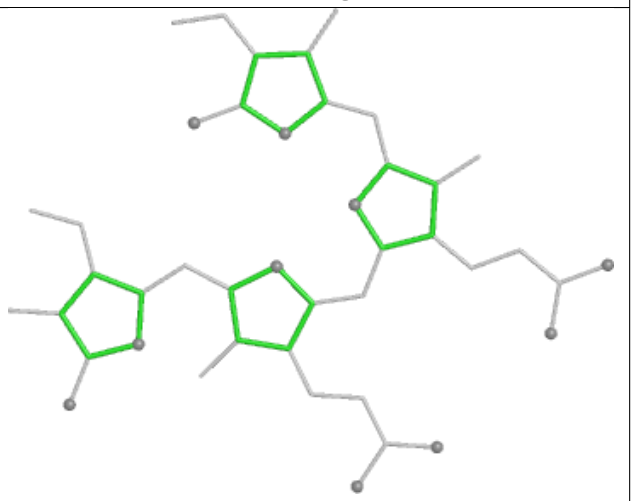
Bond lengths



Bond angles

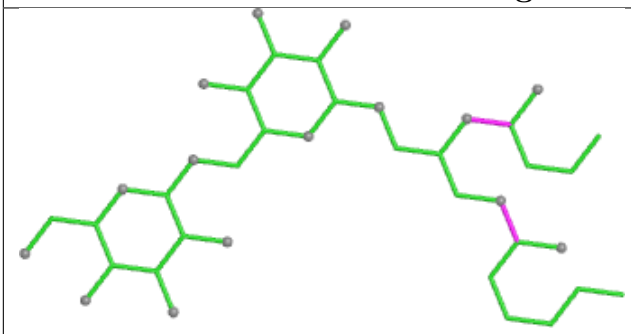


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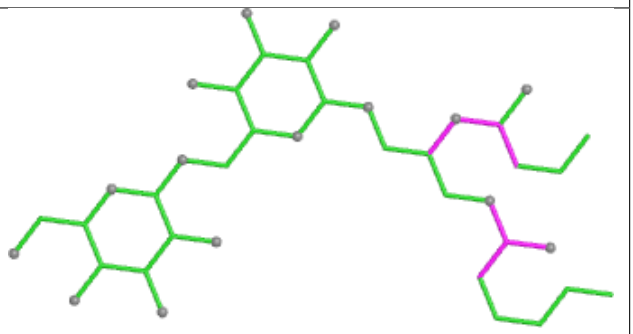


Rings

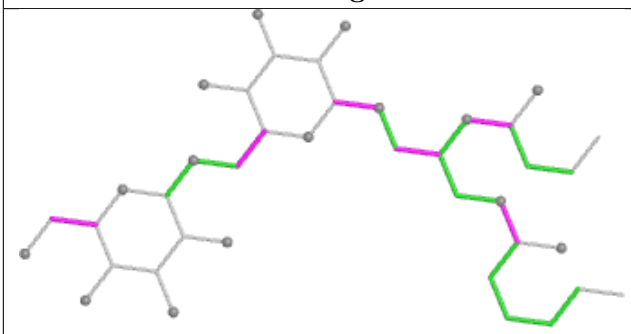
Ligand DGD a6 602



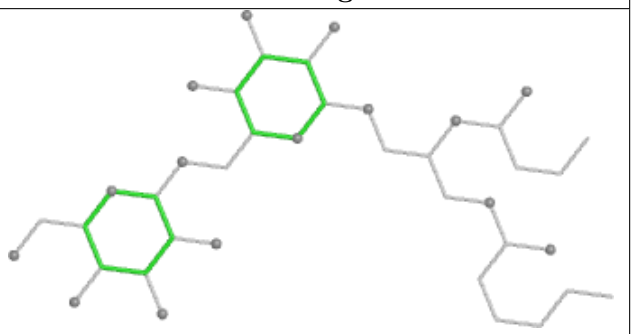
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Bond angles

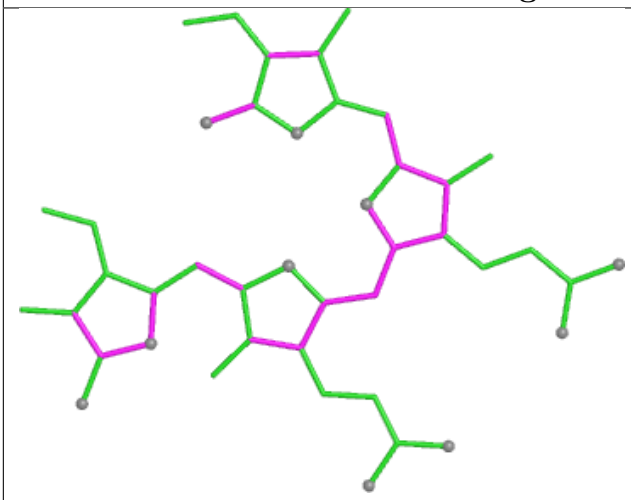


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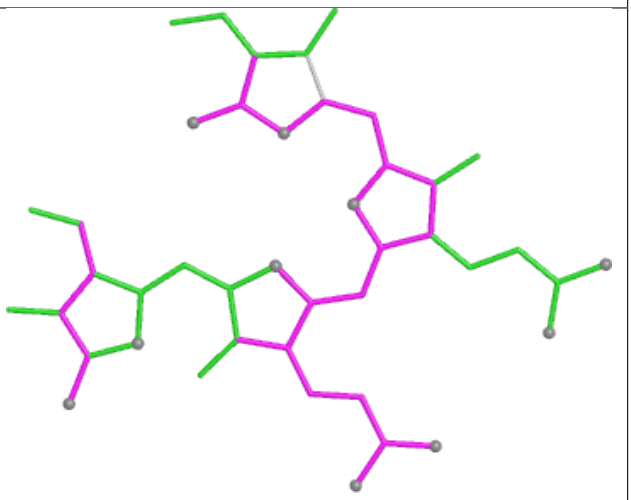


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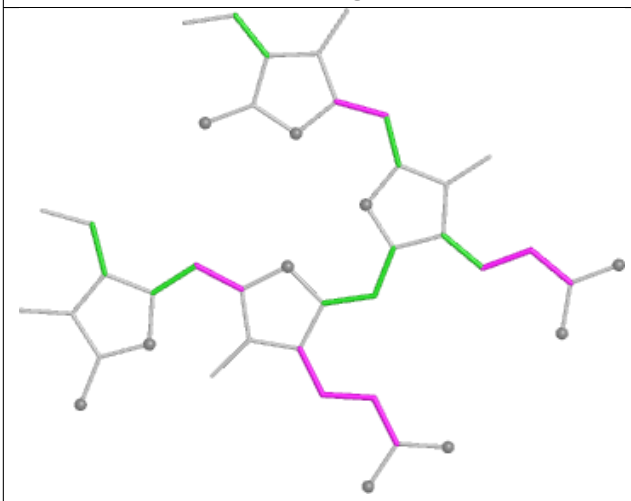
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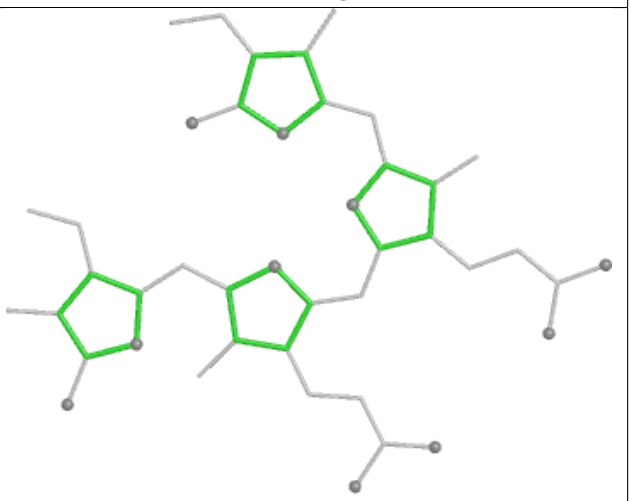
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Bond angles

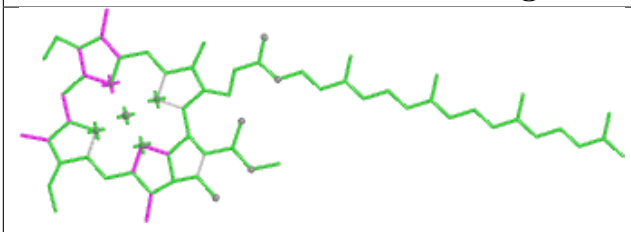


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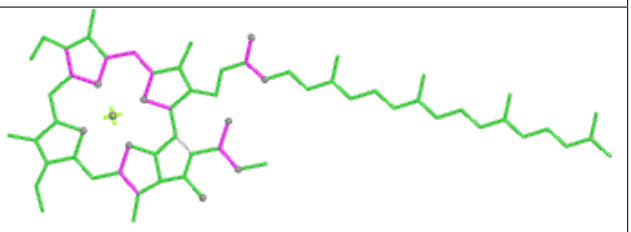


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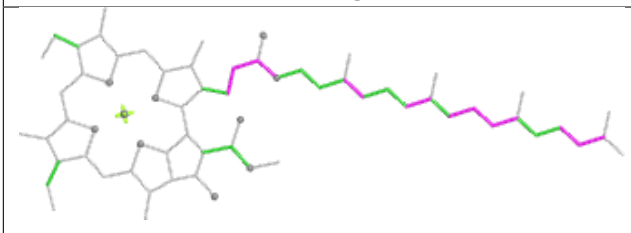
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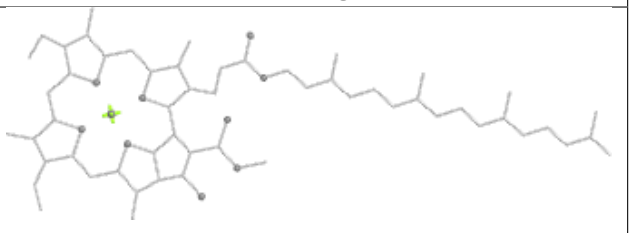
Bond lengths



Bond angles

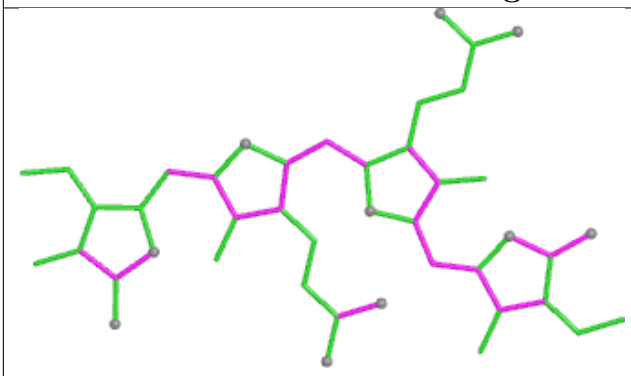


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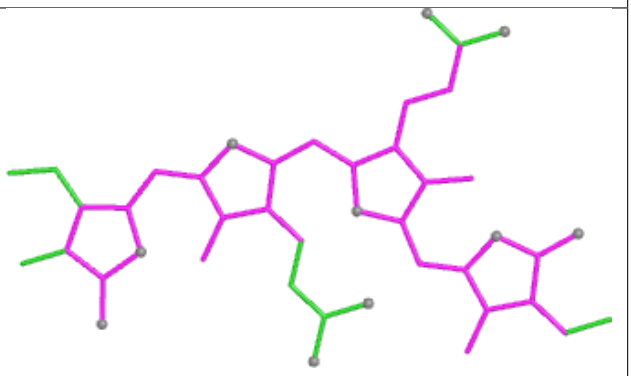


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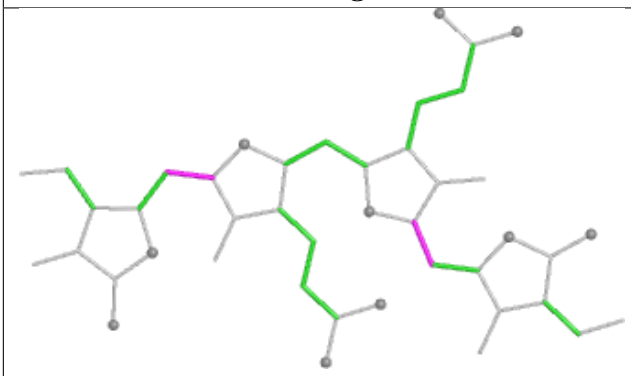
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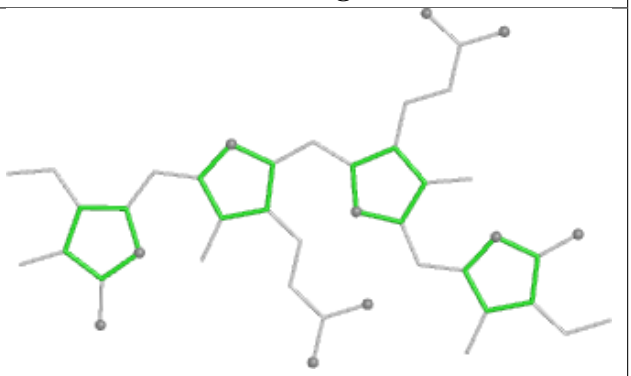
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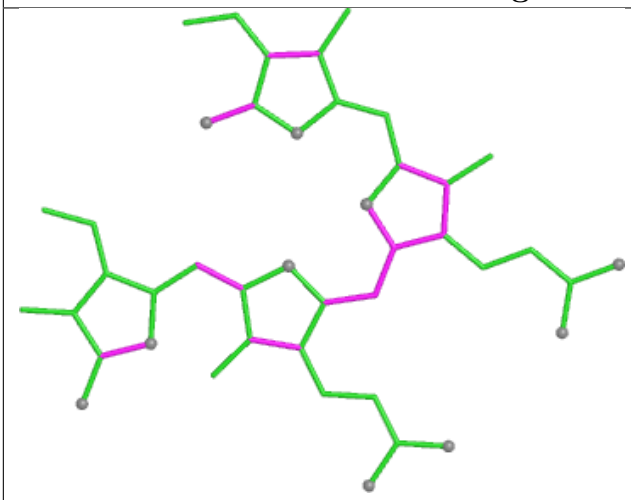


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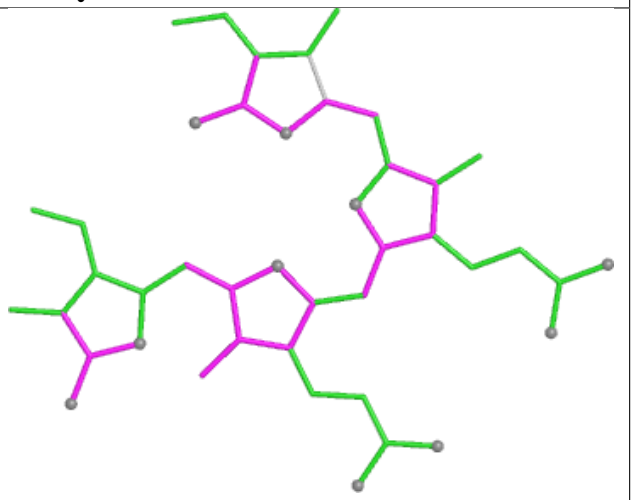


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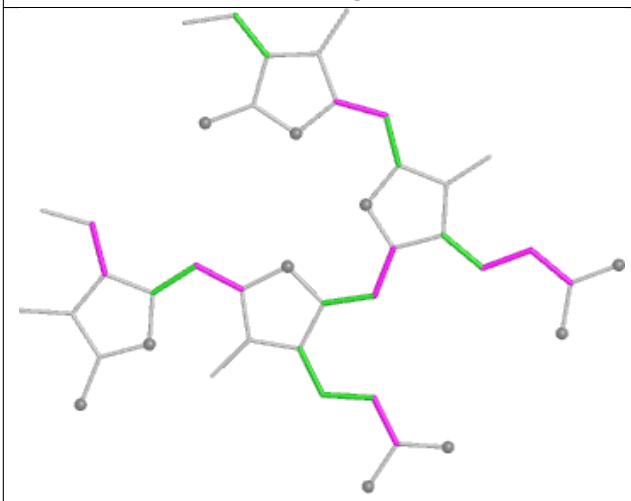
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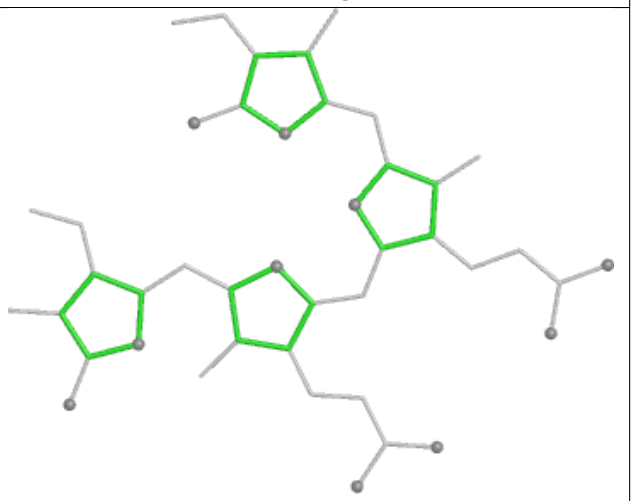
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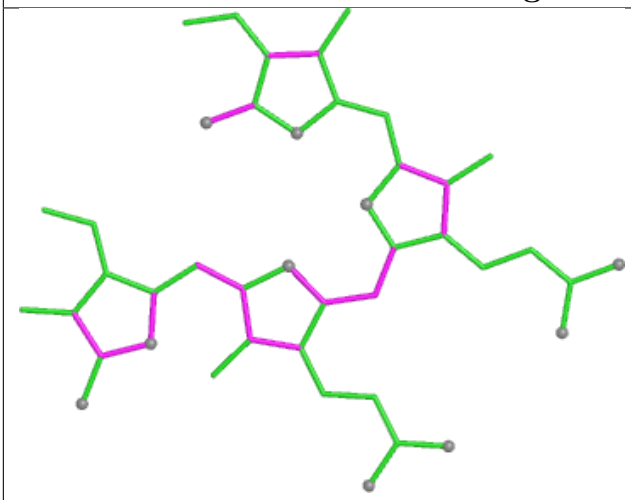


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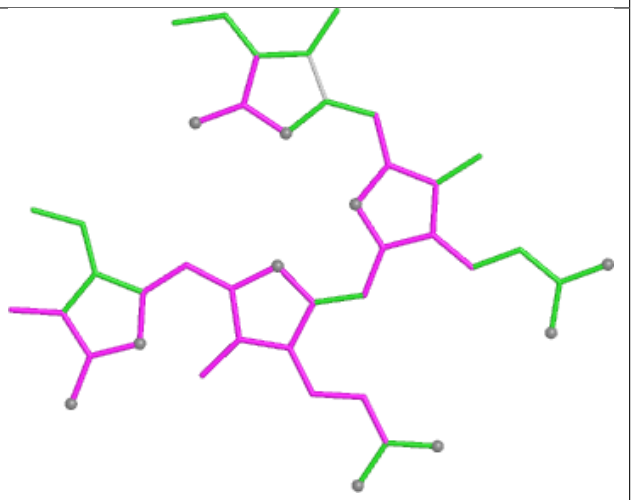


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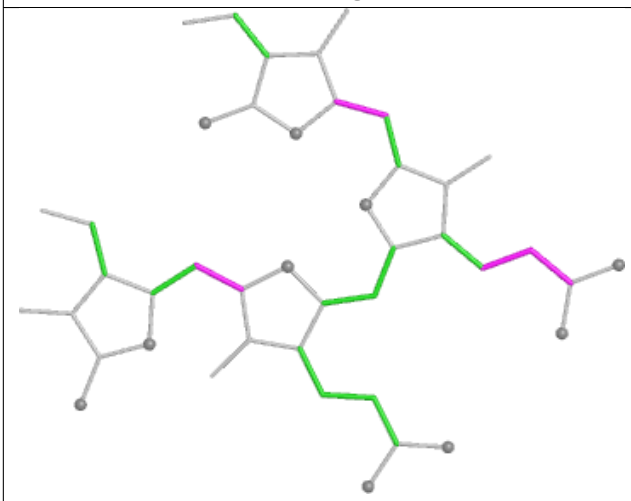
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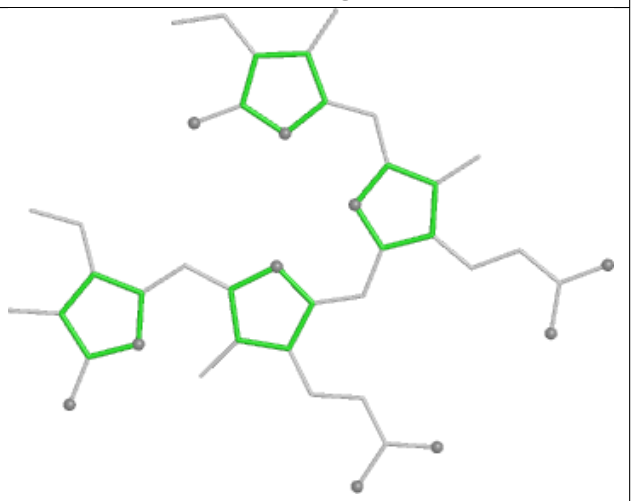
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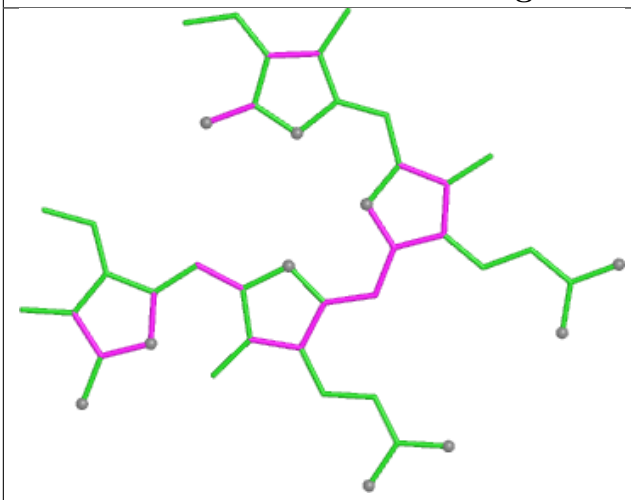


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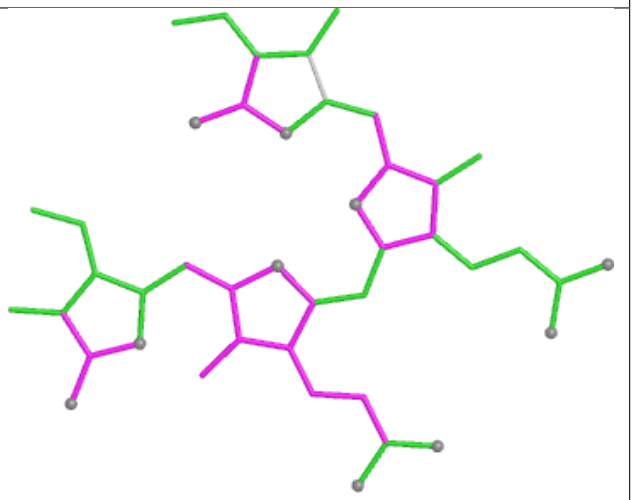


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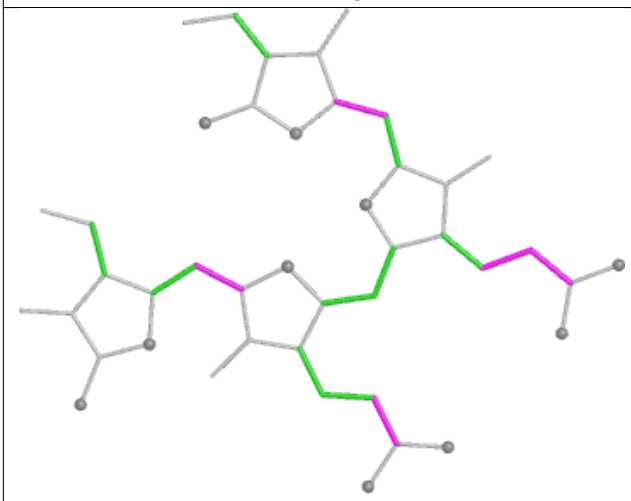
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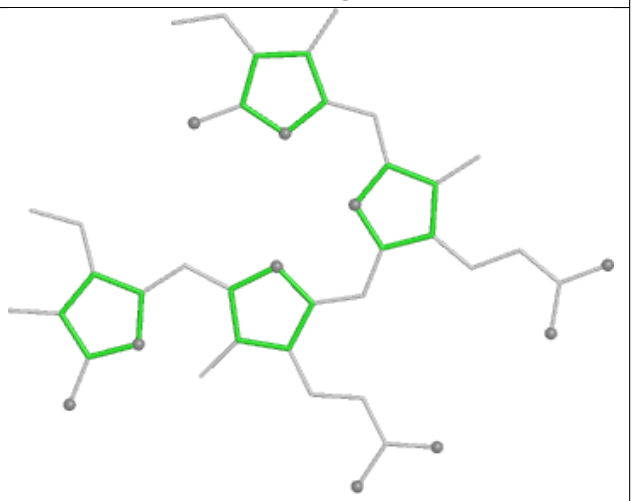
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Bond angles

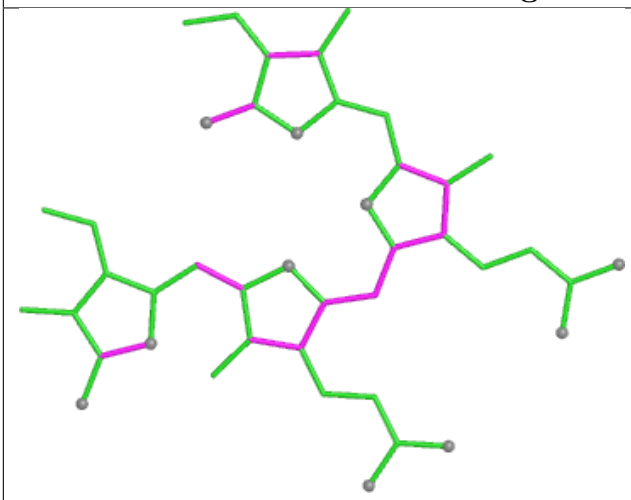


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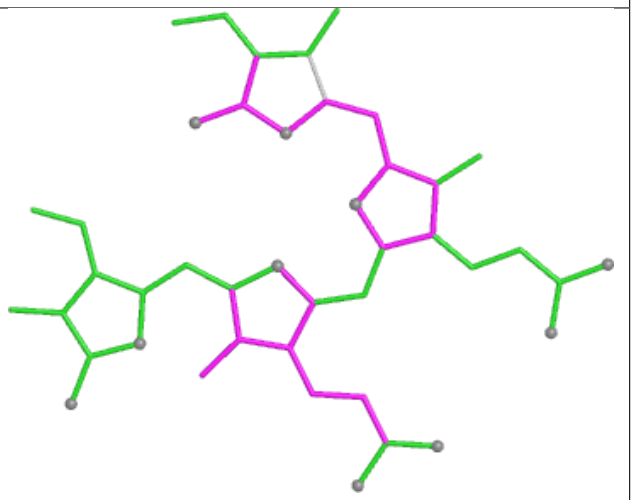


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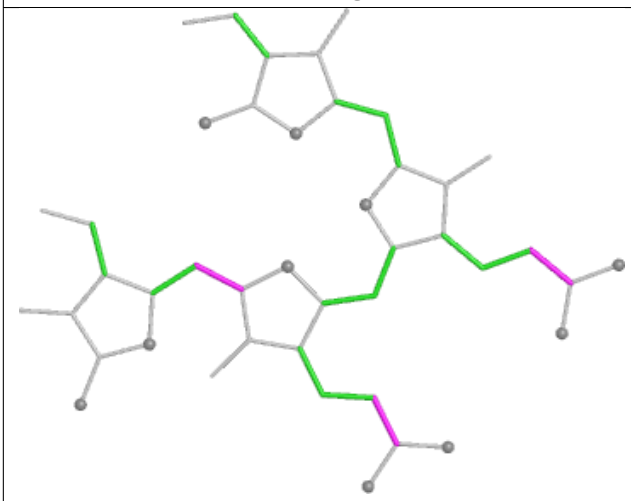
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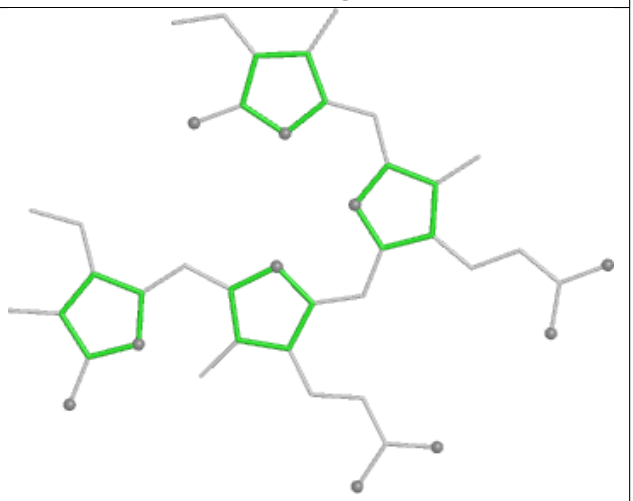
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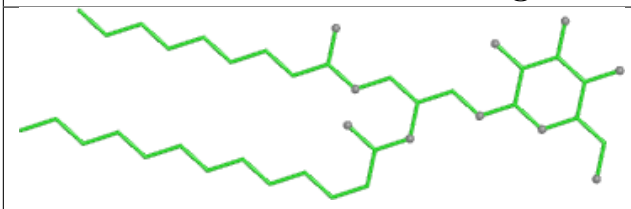


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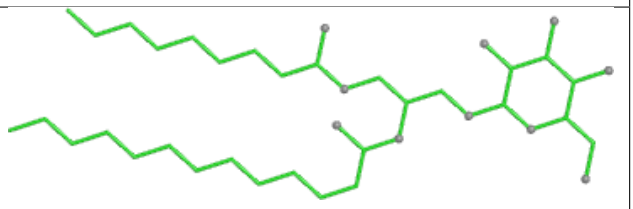


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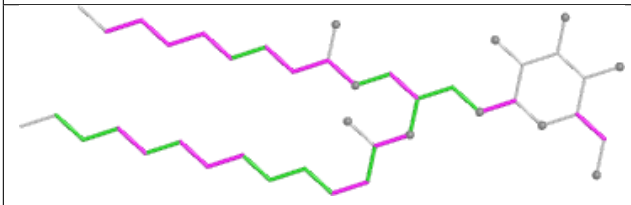
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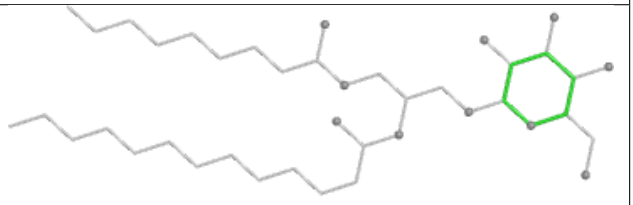
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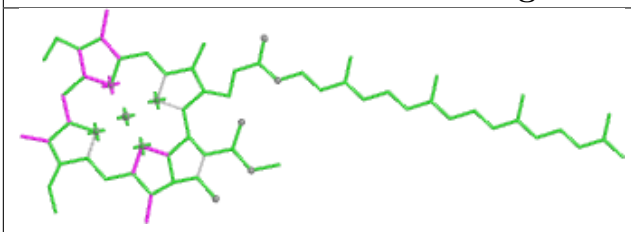


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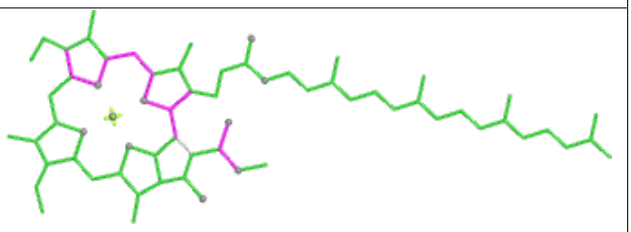


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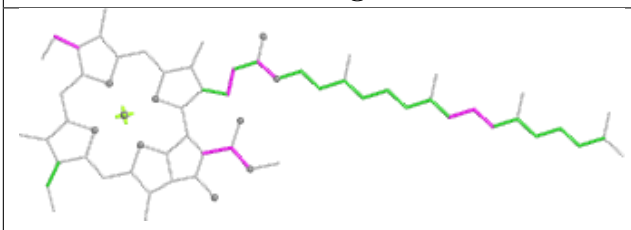
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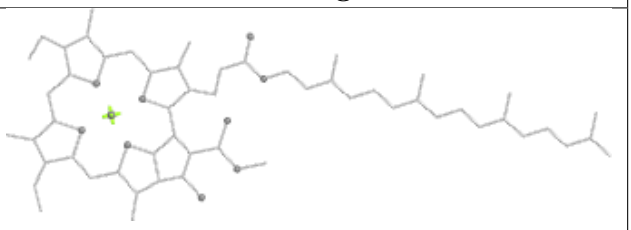
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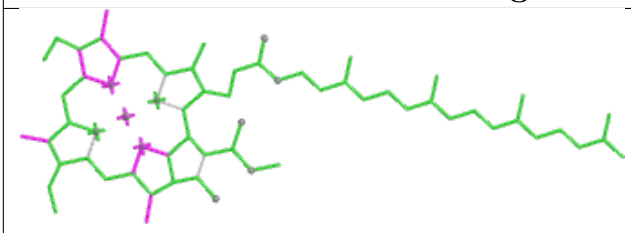


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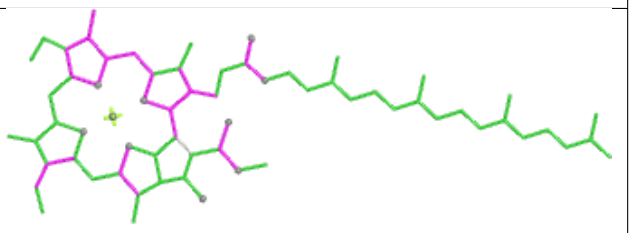


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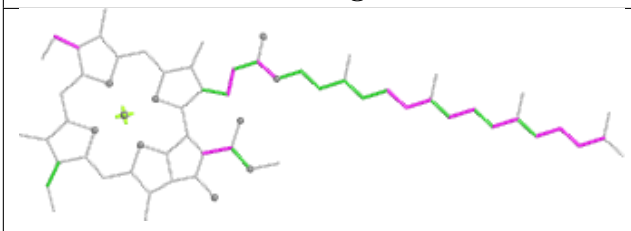
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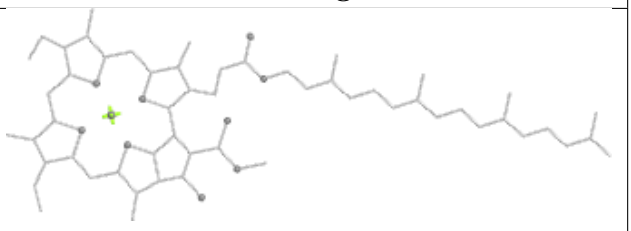
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Bond angles

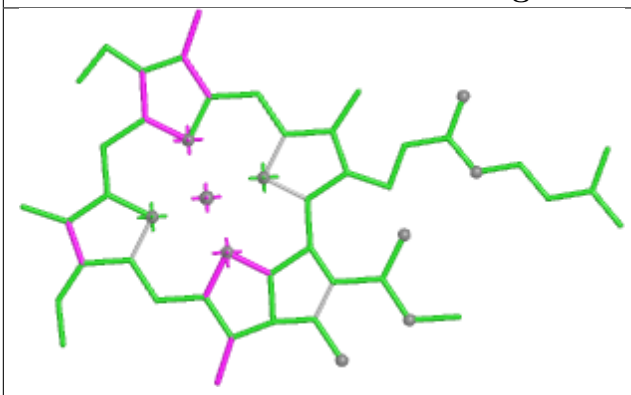


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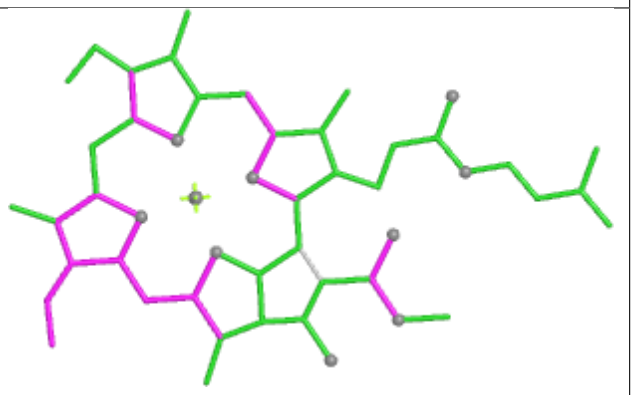


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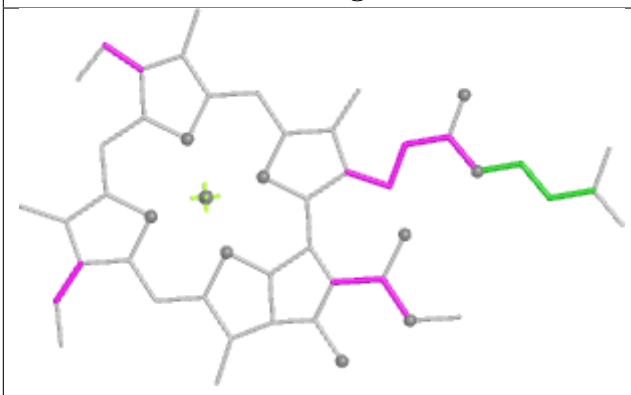
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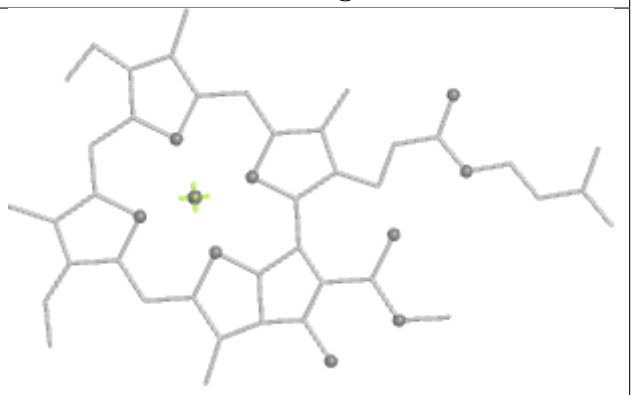
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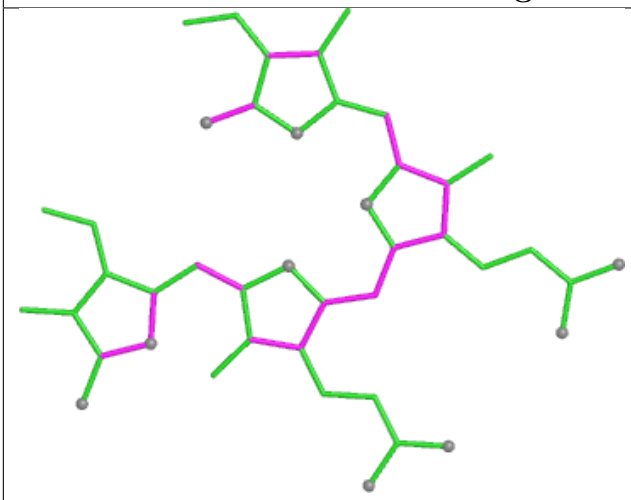


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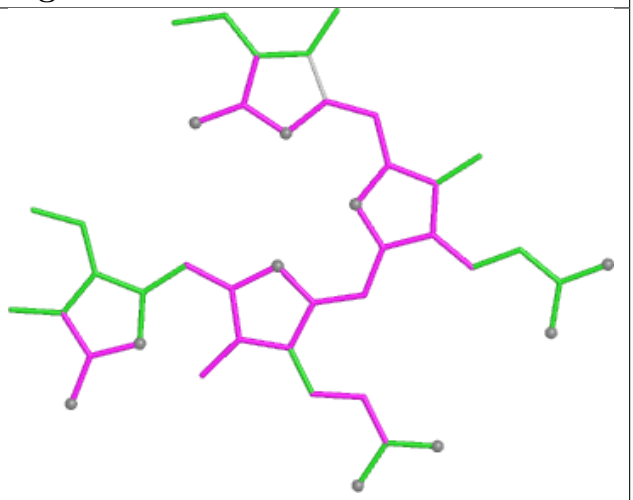


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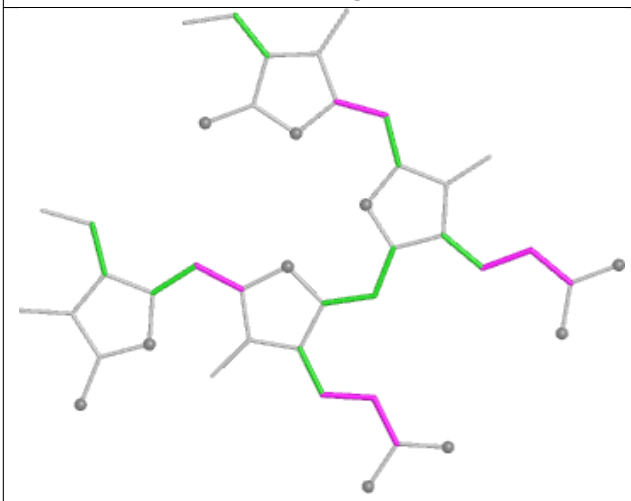
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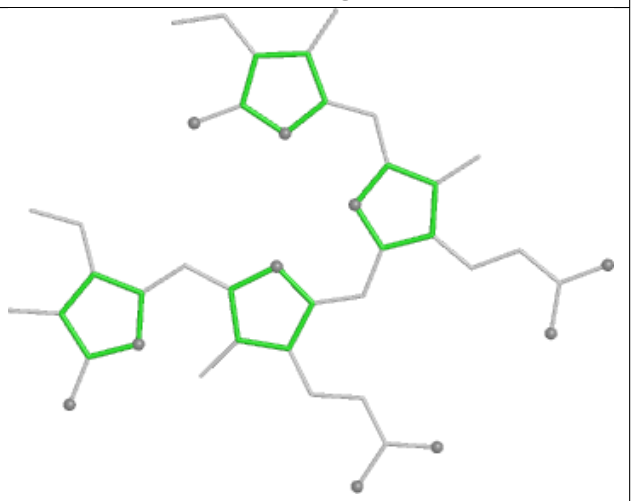
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Bond angles

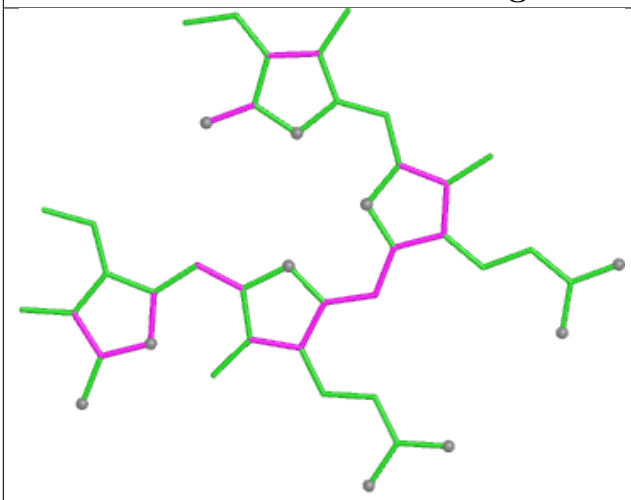


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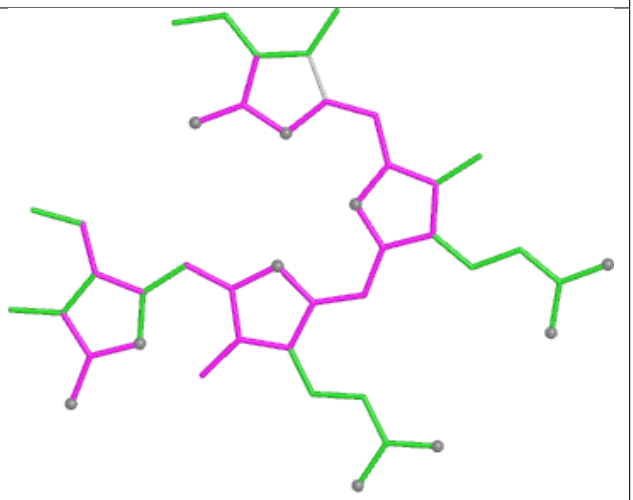


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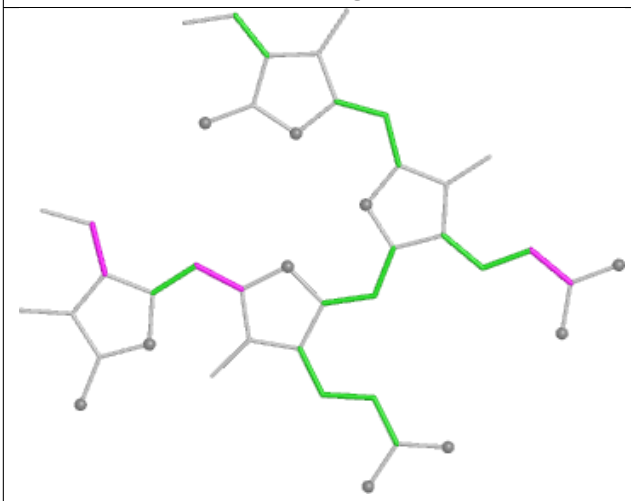
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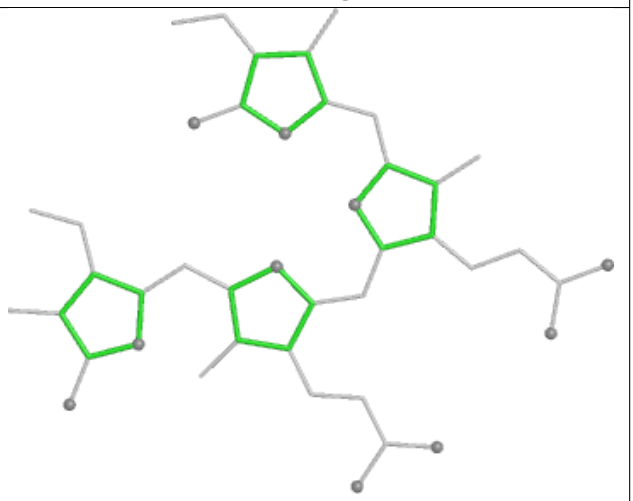
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Bond angles

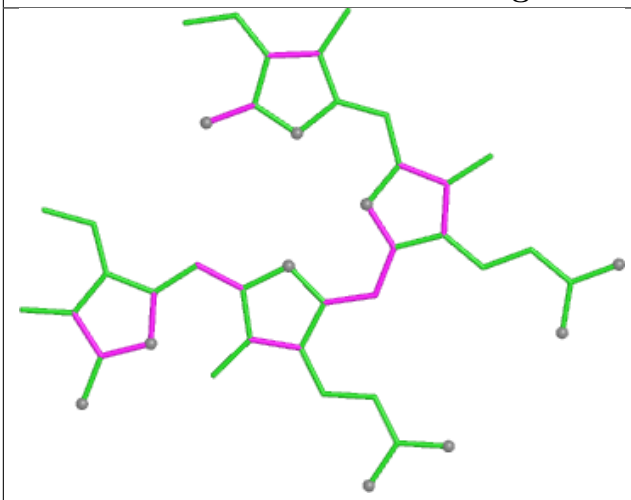


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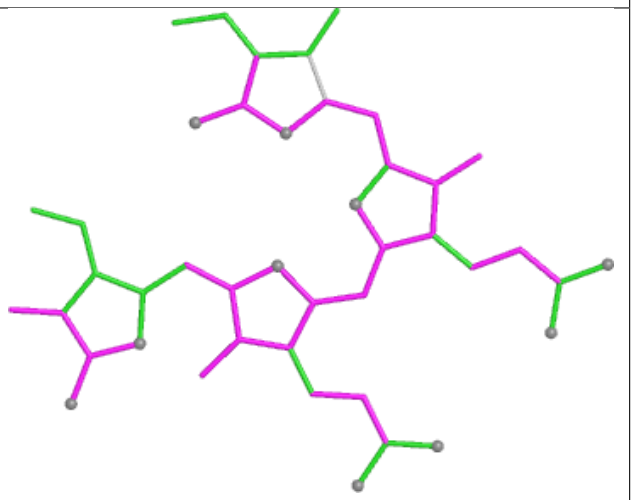


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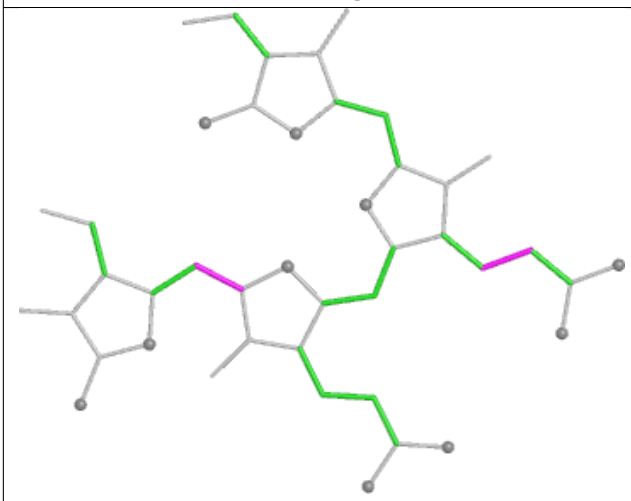
Ligand PEB CB 201



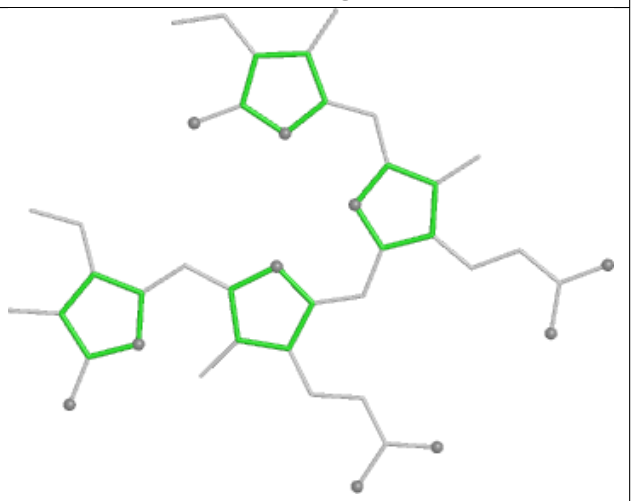
Bond lengths



Bond angles

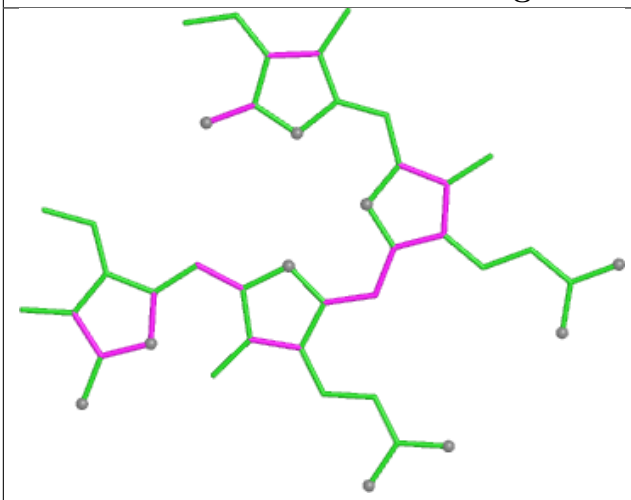


Torsions

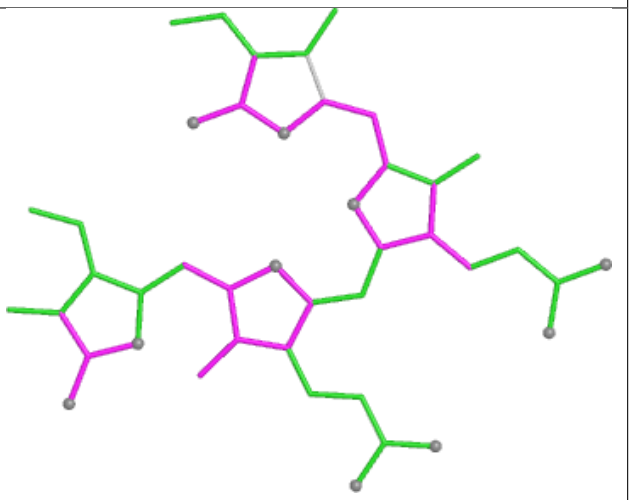


Rings

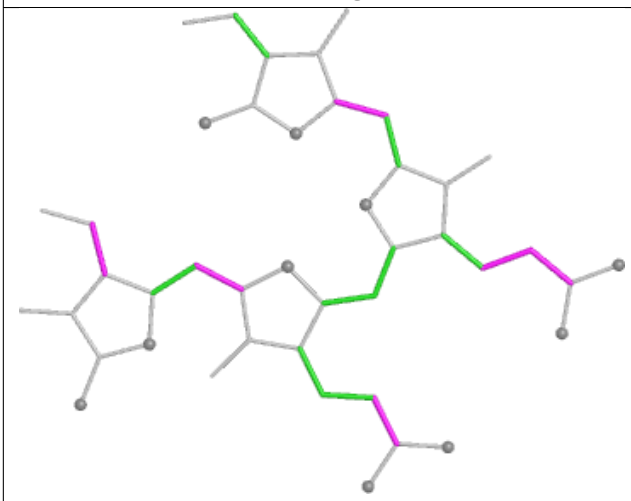
Ligand PEB EP 202



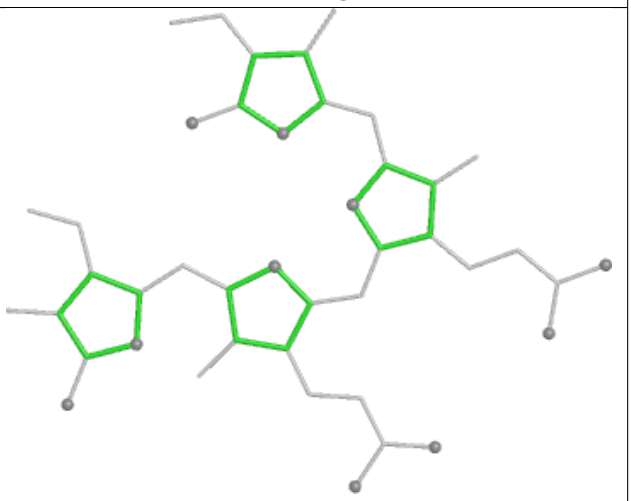
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Bond angles

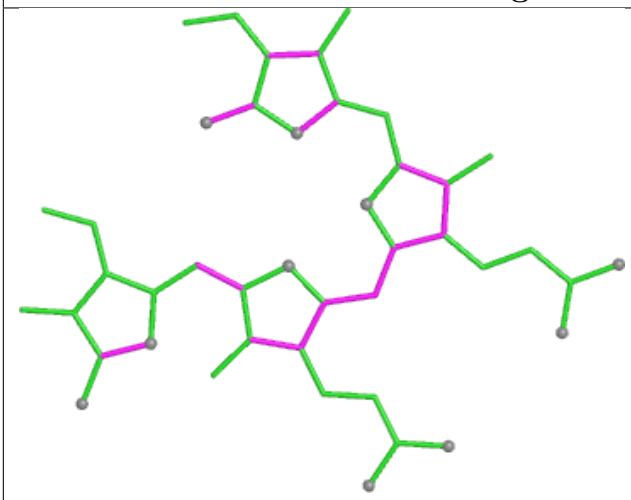


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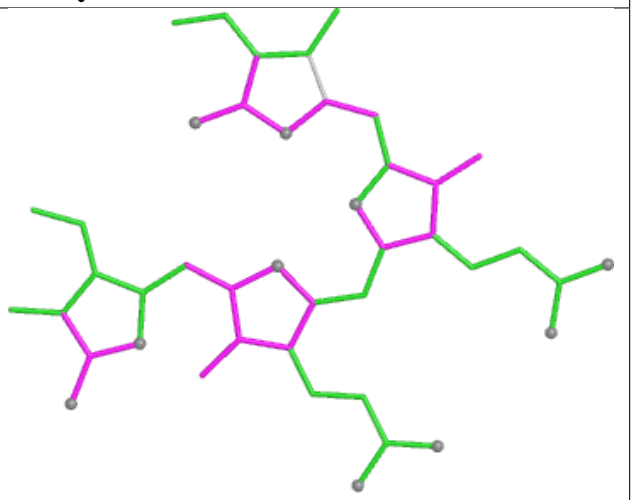


Rings

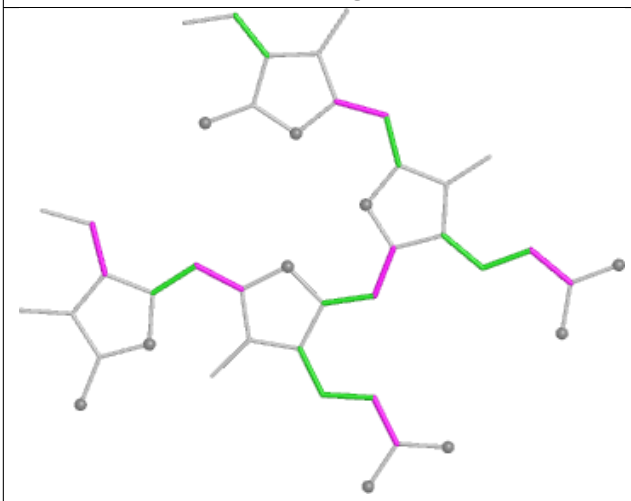
Ligand PEB VQ 202



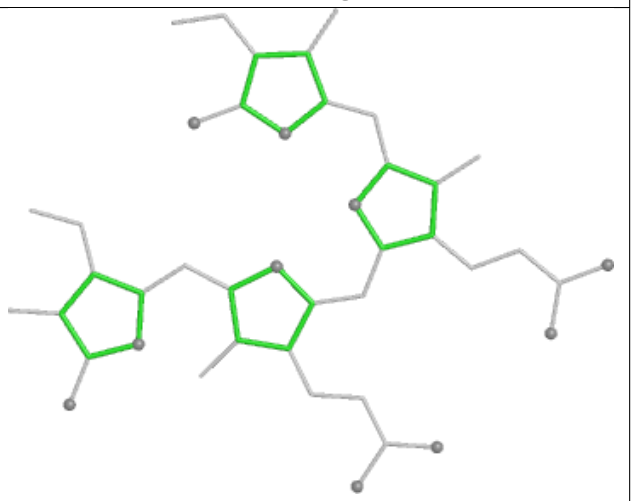
Bond lengths



Bond angles

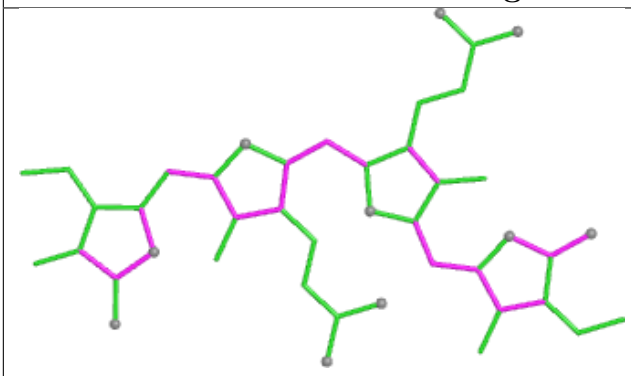


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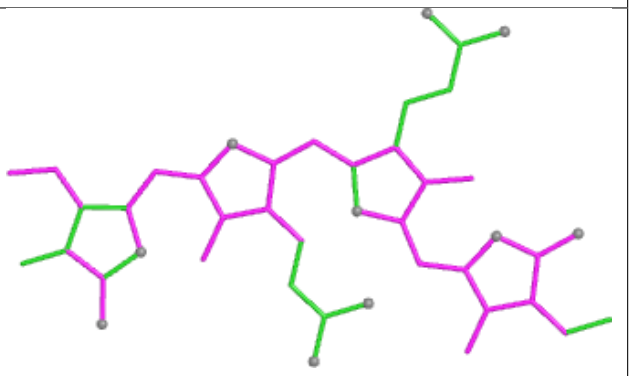


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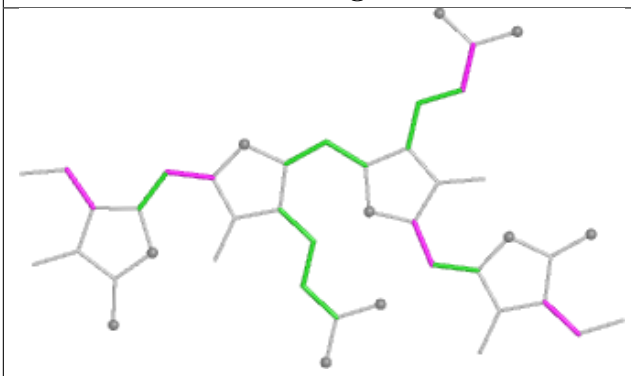
Ligand CYC R3 1001



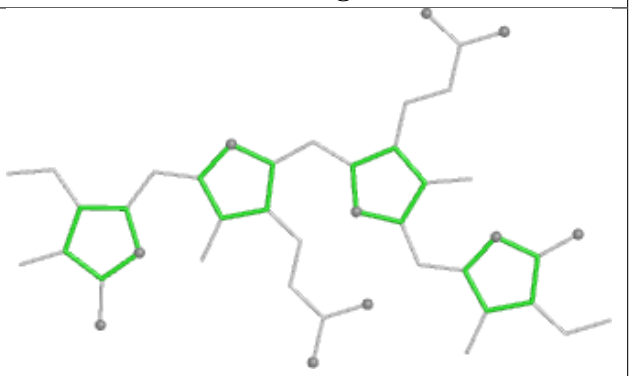
Bond lengths



Bond angles

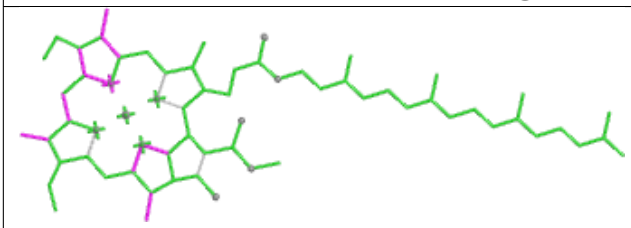


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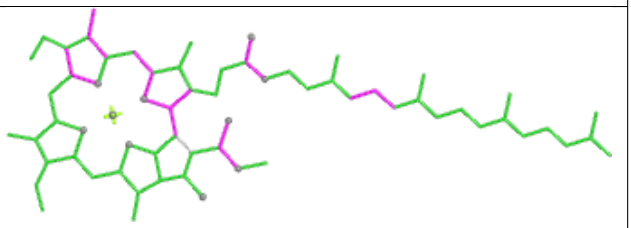


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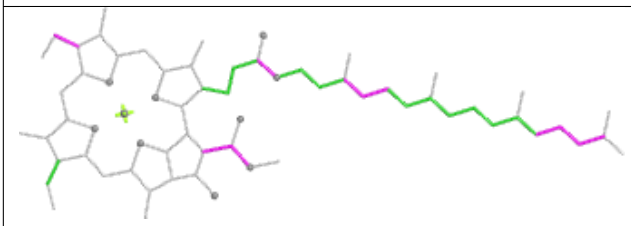
Ligand CLA bL 615



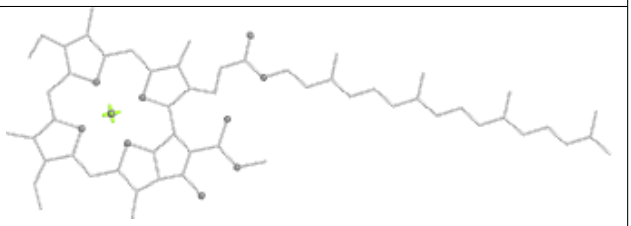
Bond lengths



Bond angles

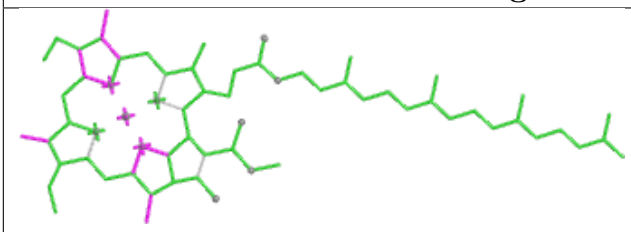


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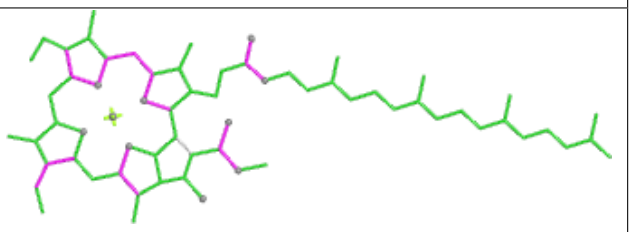


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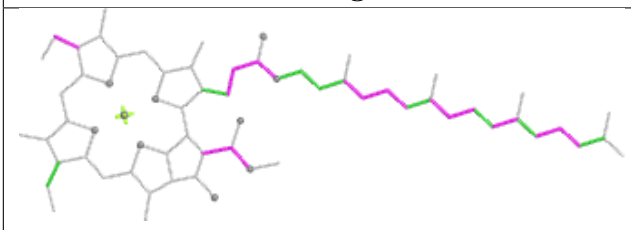
Ligand CLA AN 851



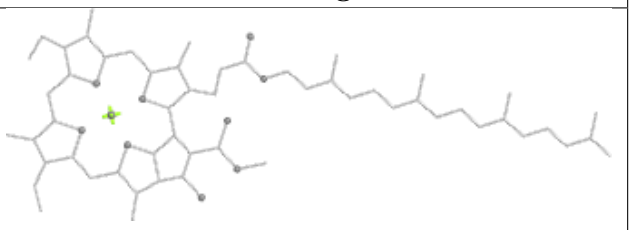
Bond lengths



Bond angles

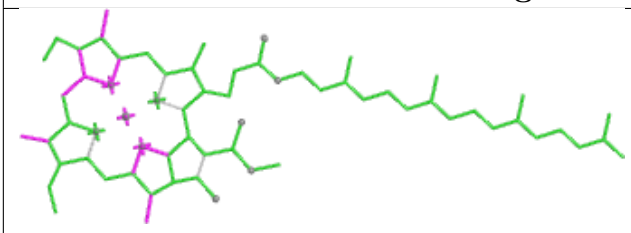


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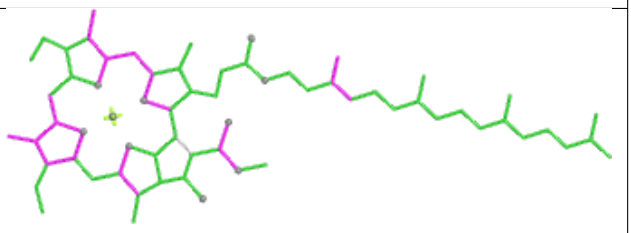


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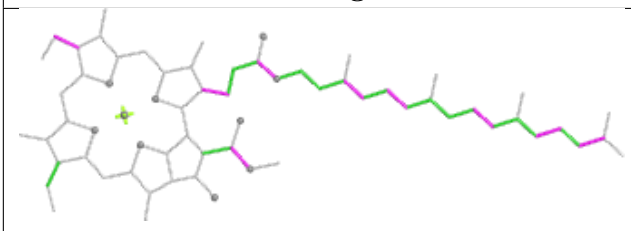
Ligand CLA A2 831



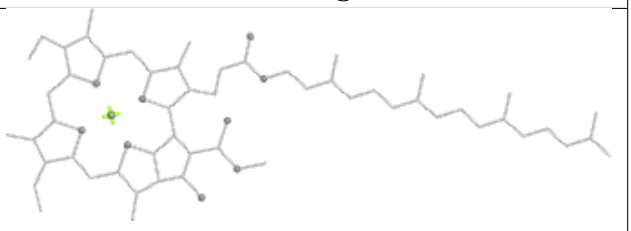
Bond lengths



Bond angles

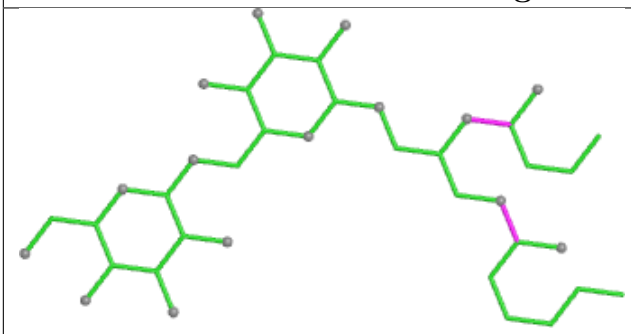


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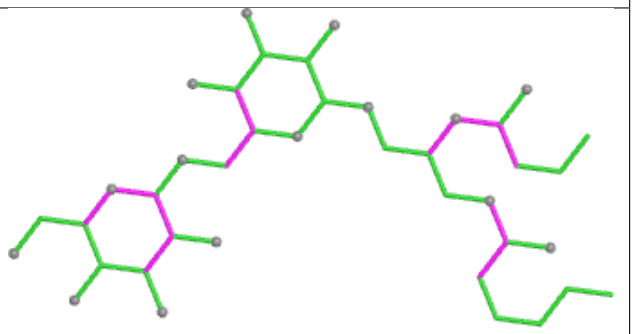


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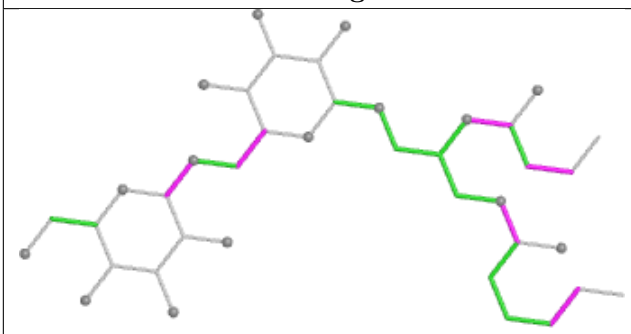
Ligand DGD b6 621



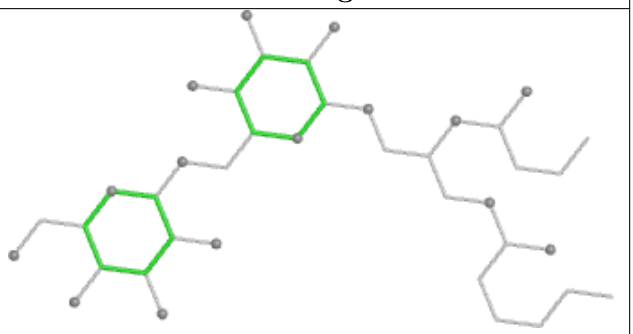
Bond lengths



Bond angles

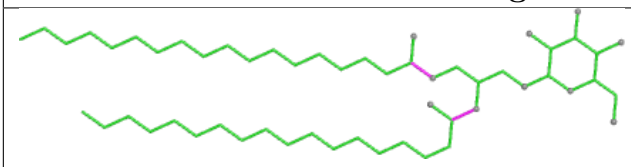


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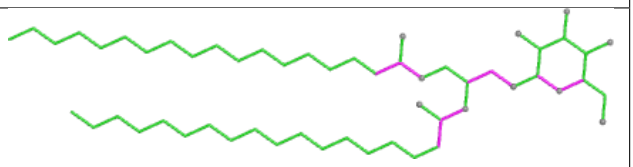


Rings

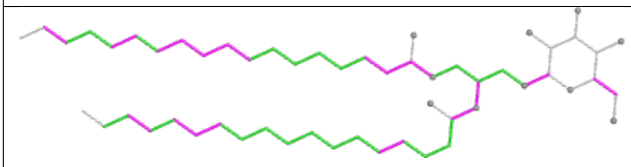
Ligand LMG CL 519



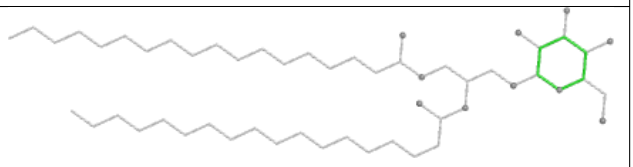
Bond lengths



Bond angles

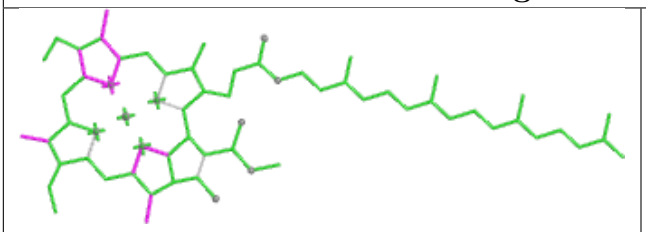


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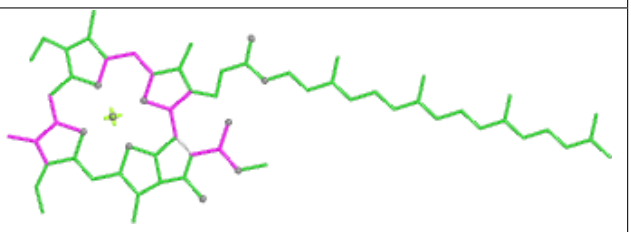


Rings

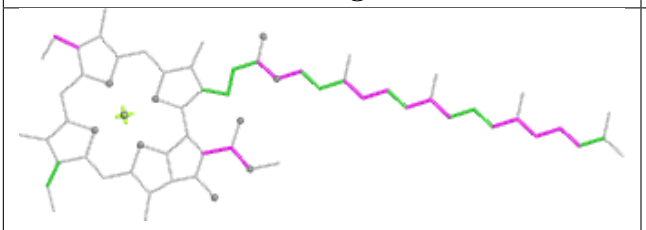
Ligand CLA CL 508



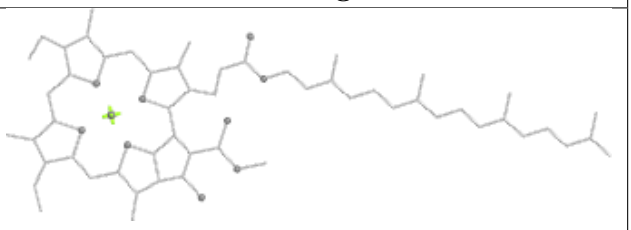
Bond lengths



Bond angles

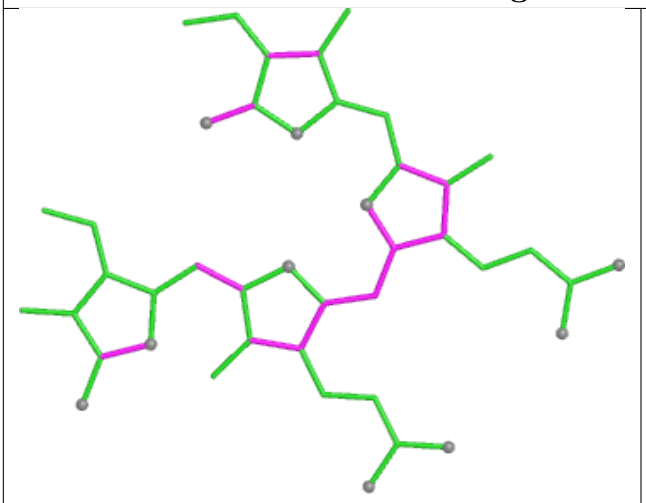


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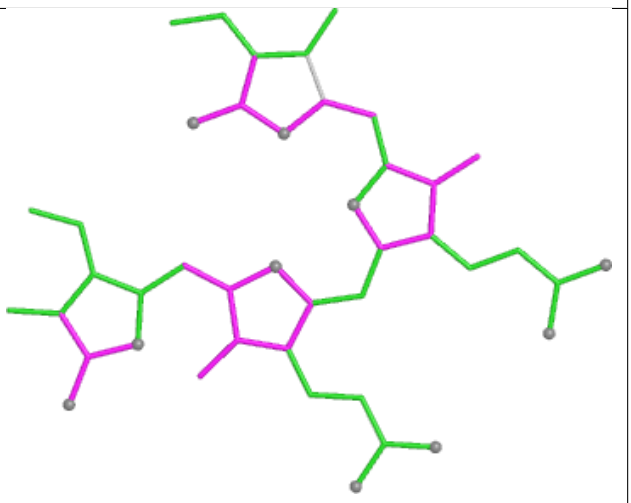


Rings

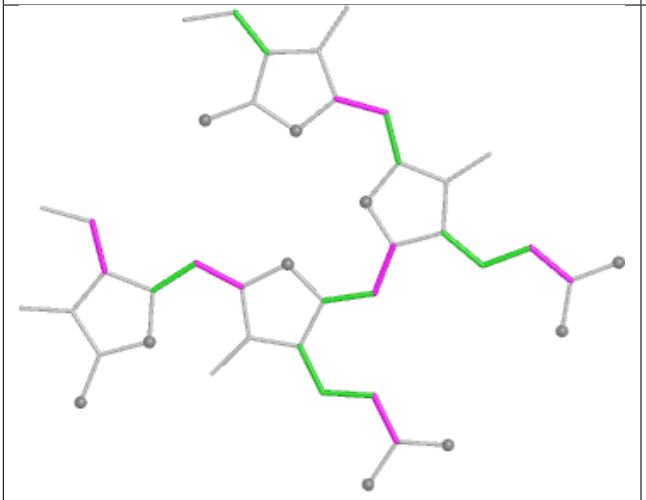
Ligand PEB VD 202



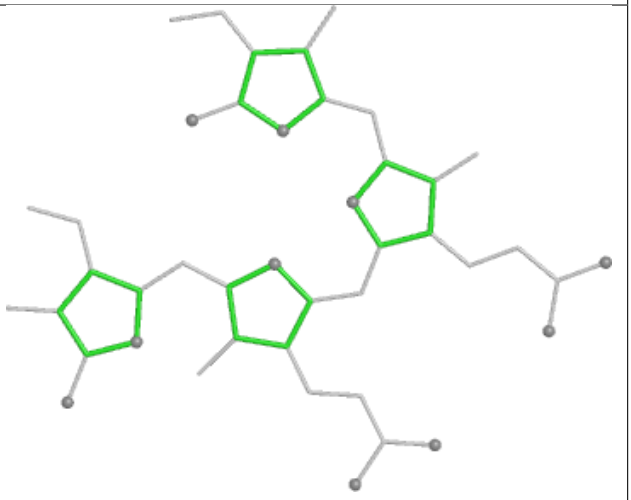
Bond lengths



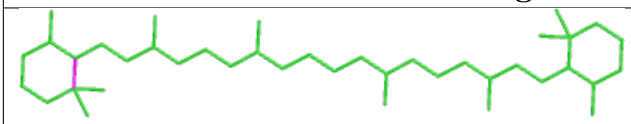
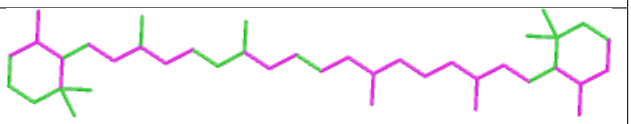
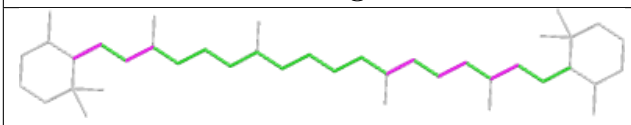
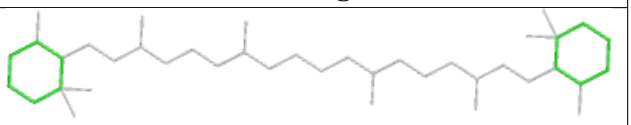
Bond angles

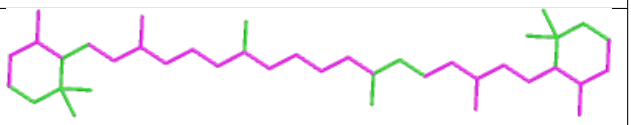
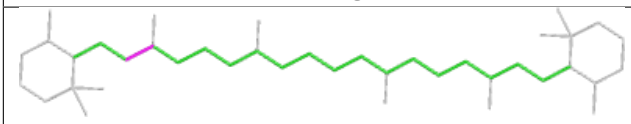
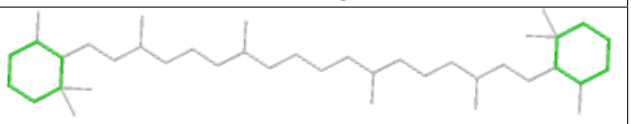


Torsions

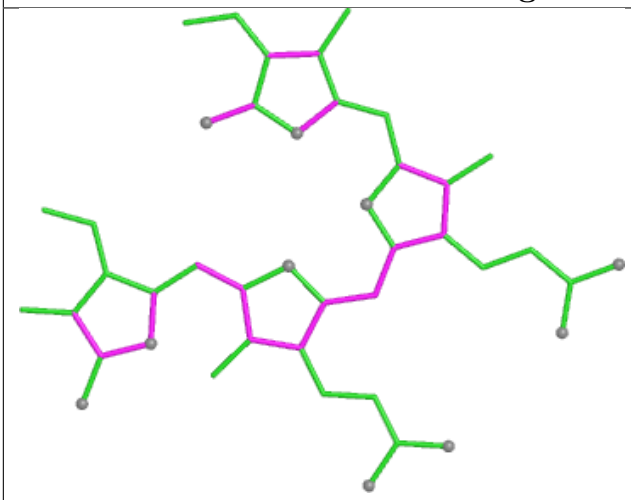


Rings

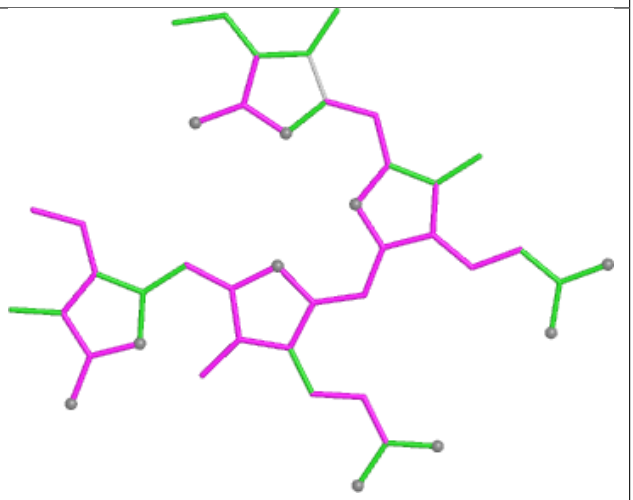
Ligand BCR F6 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR B6 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

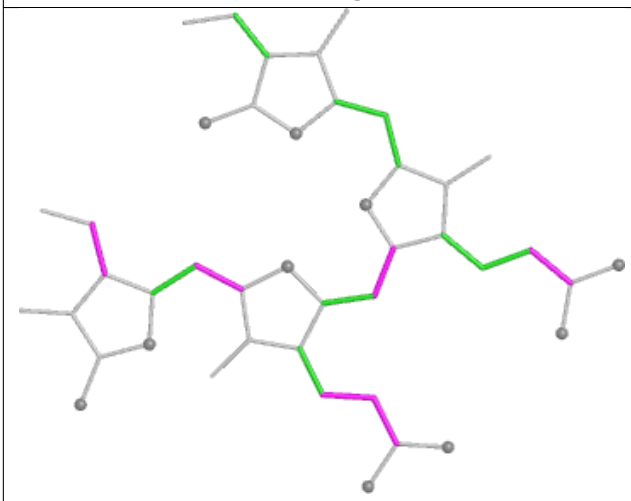
Ligand PEB u8 201



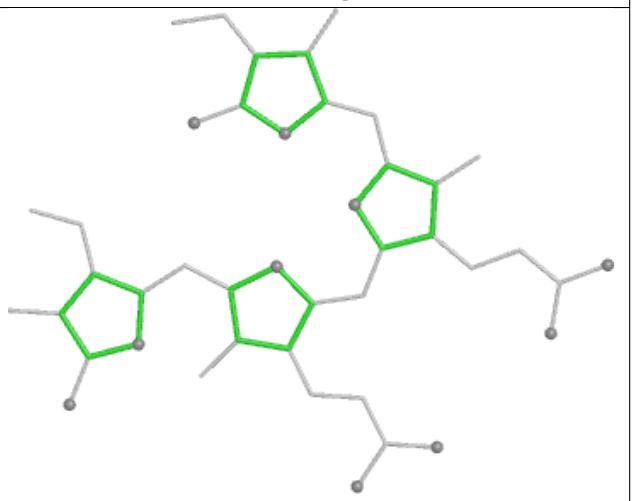
Bond lengths



Bond angles

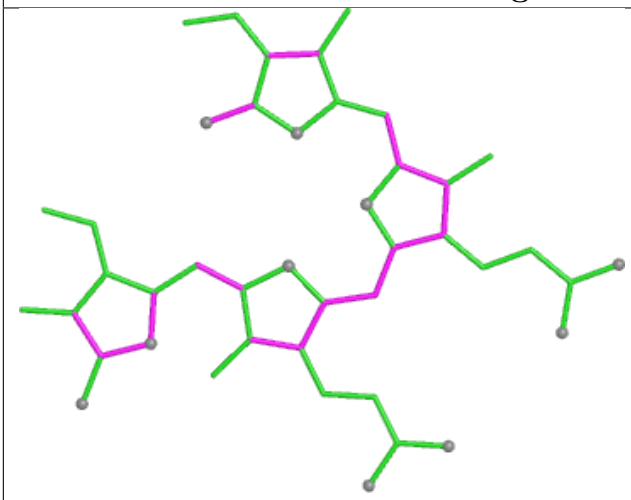


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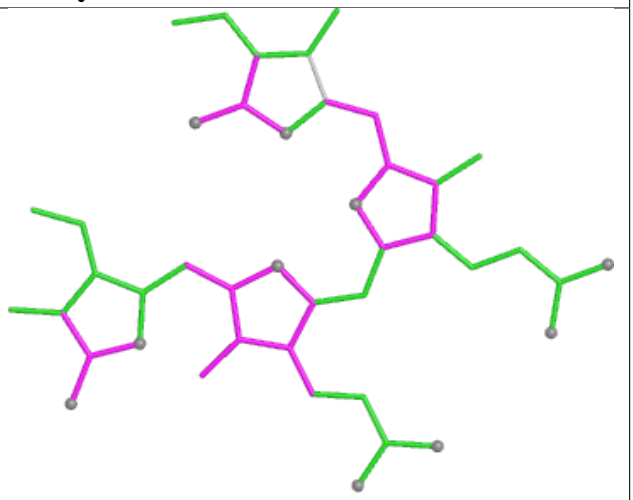


Rings

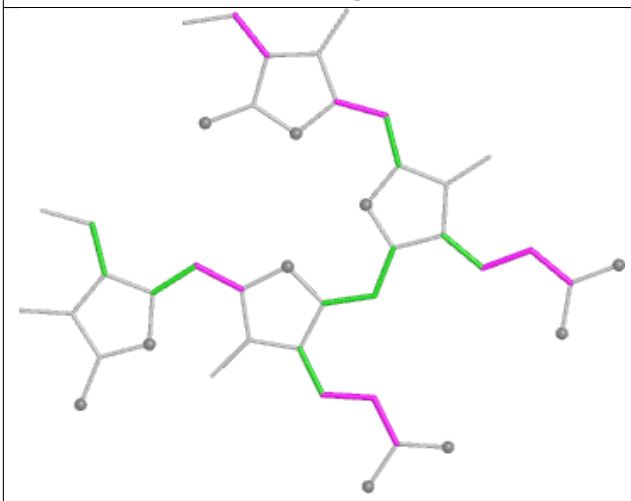
Ligand PEB XQ 202



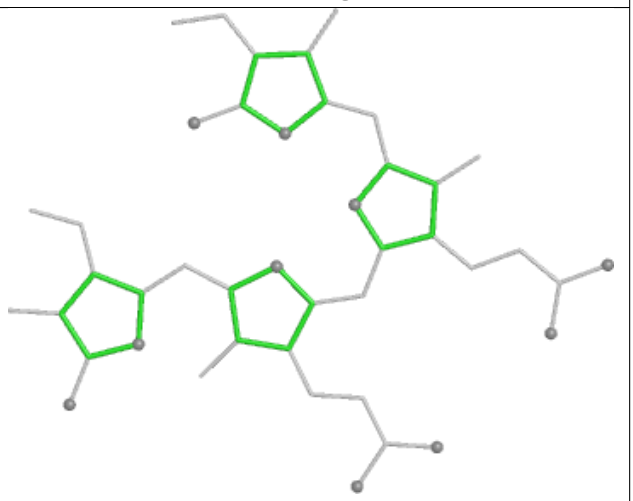
Bond lengths



Bond angles

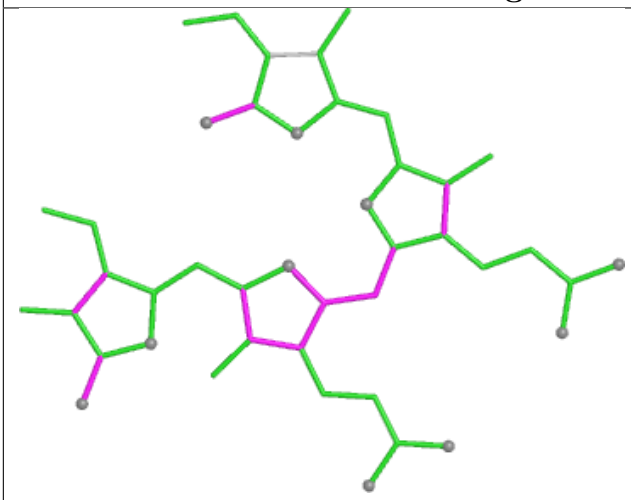


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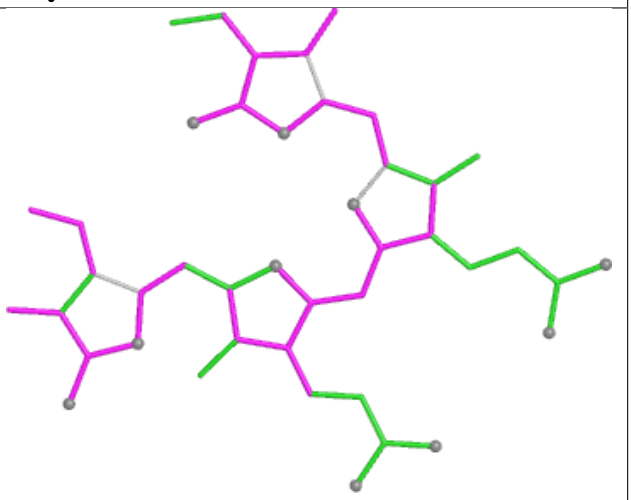


Rings

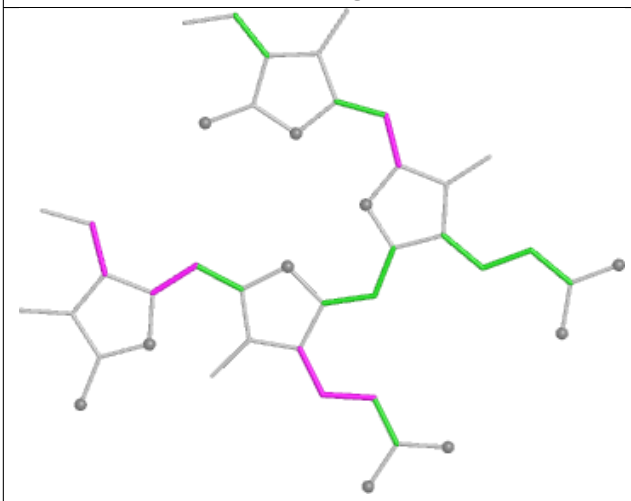
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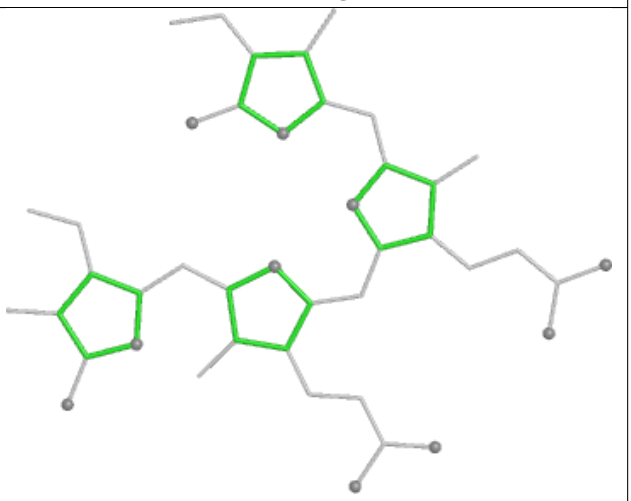
Bond lengths



Bond angles

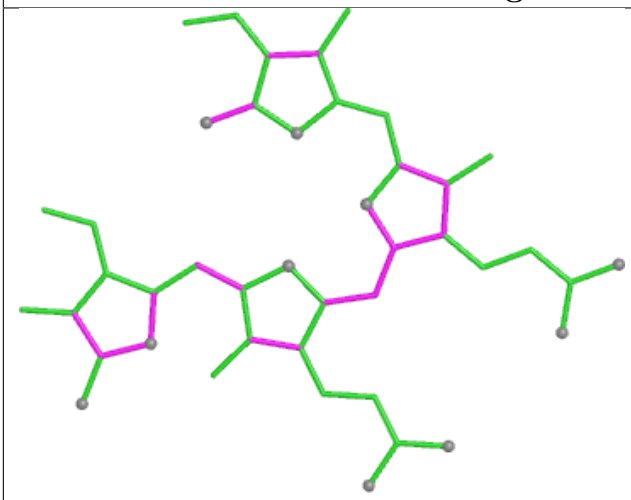


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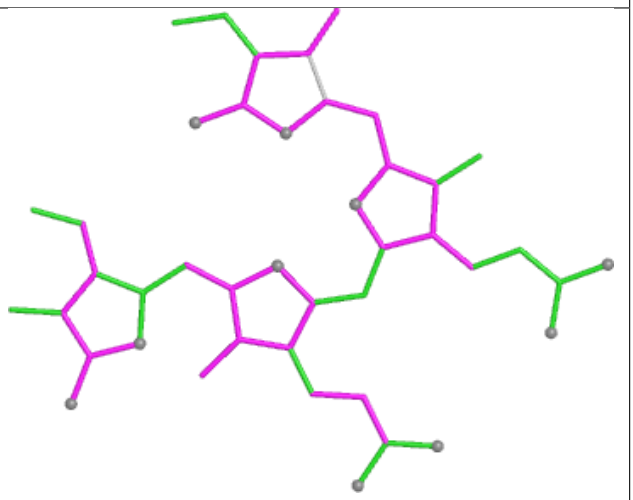


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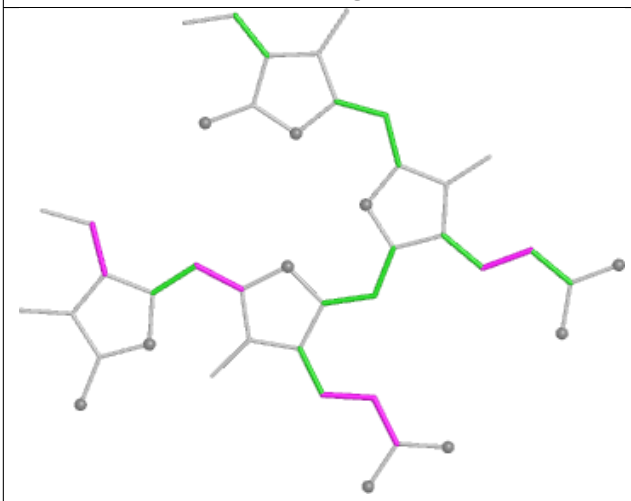
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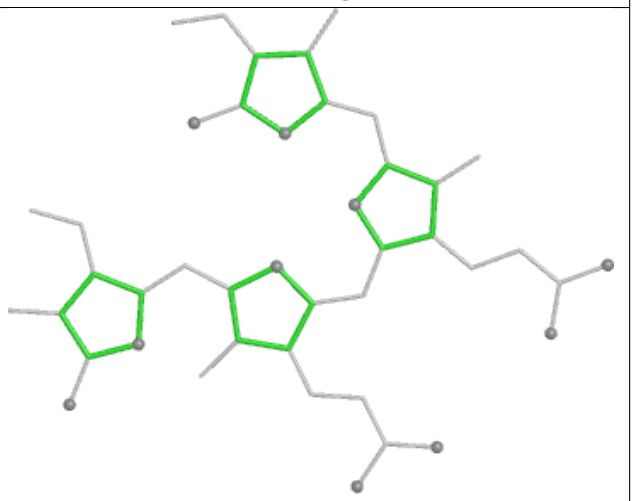
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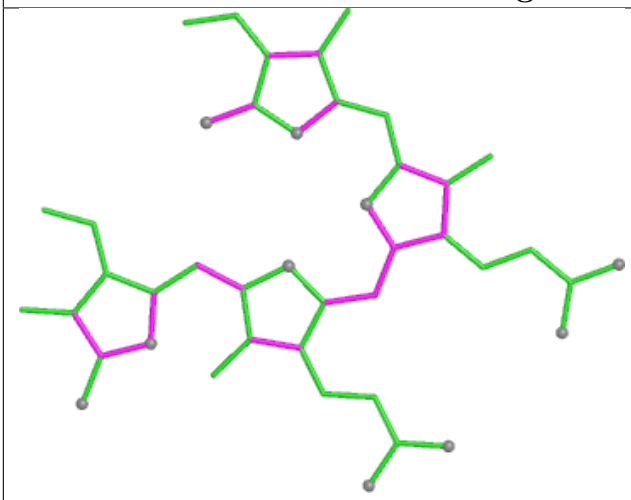


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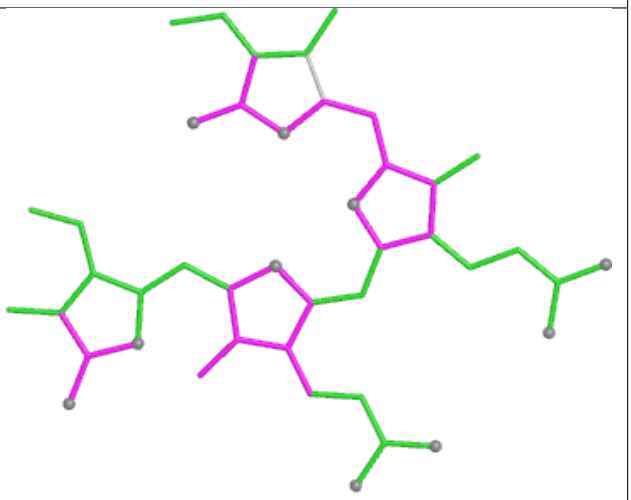


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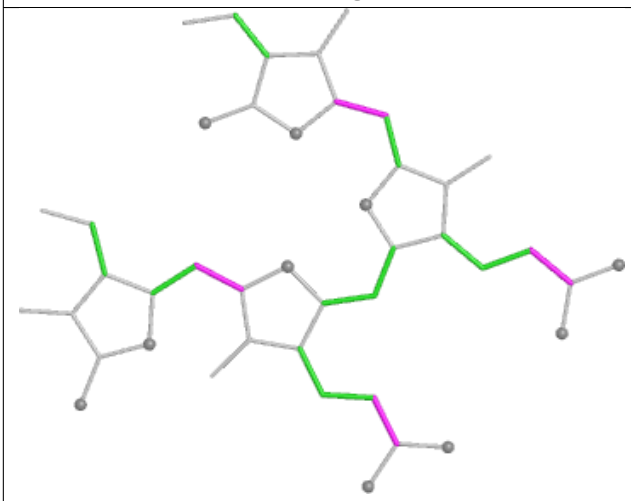
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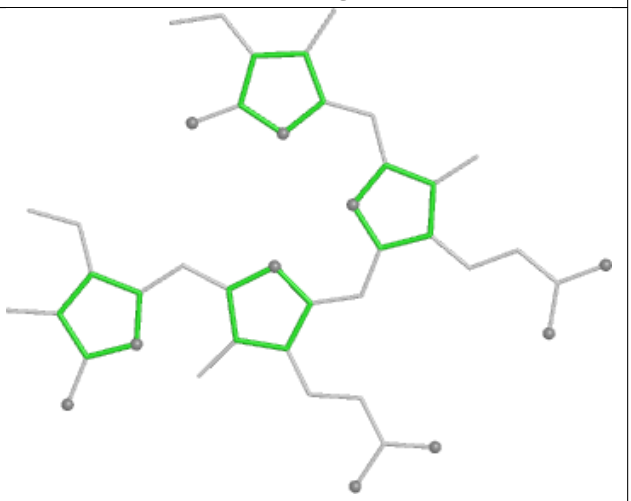
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Bond angles

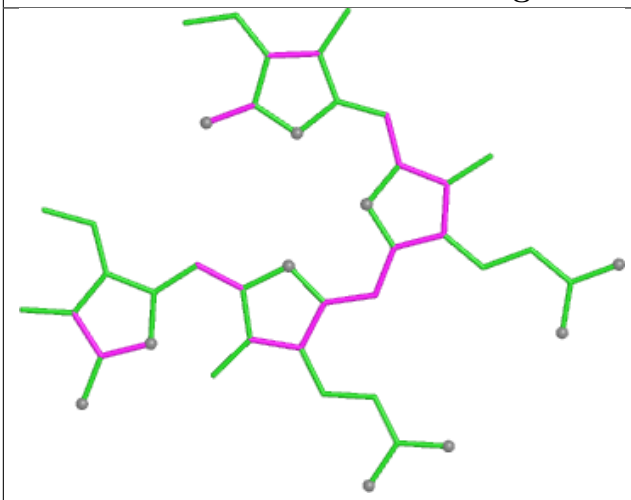


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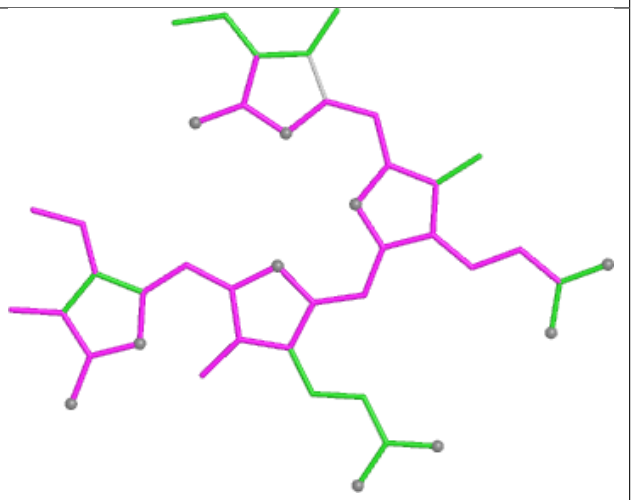


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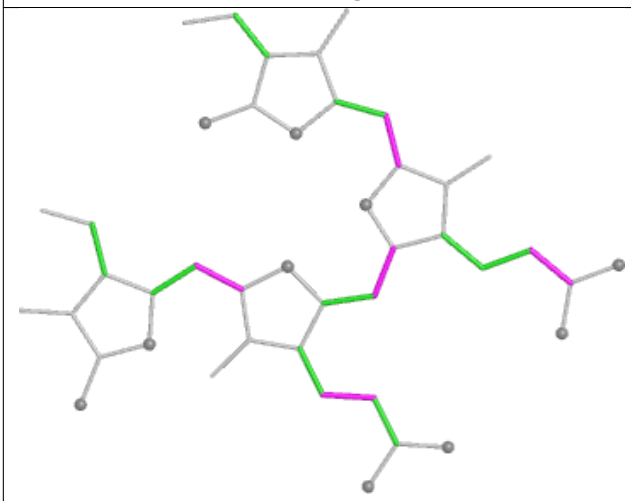
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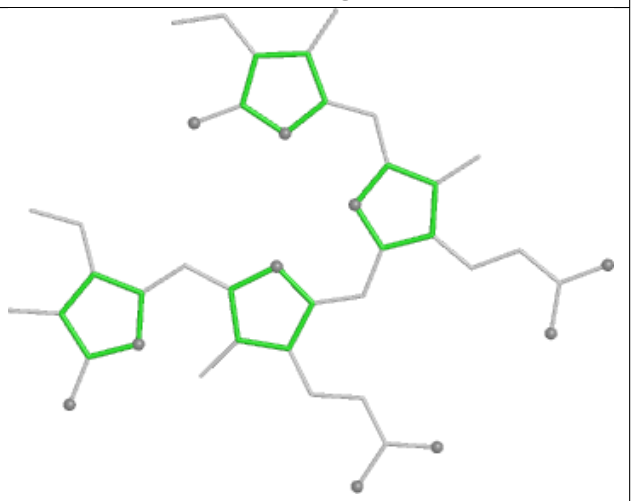
Bond lengths



Bond angles

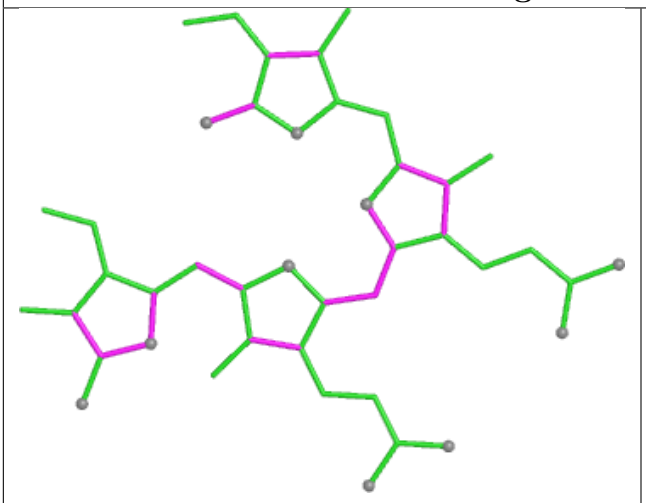


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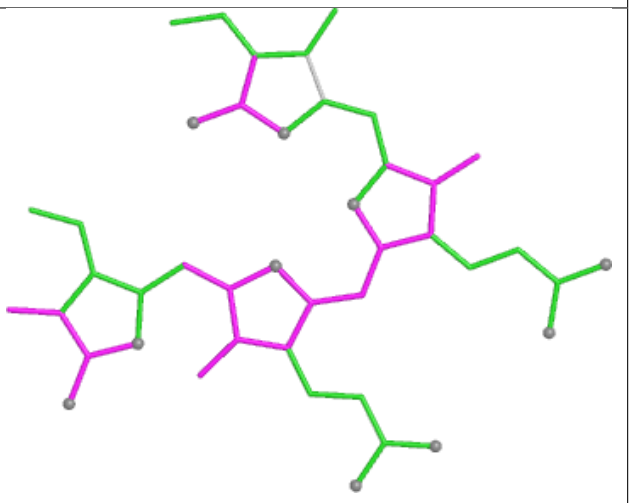


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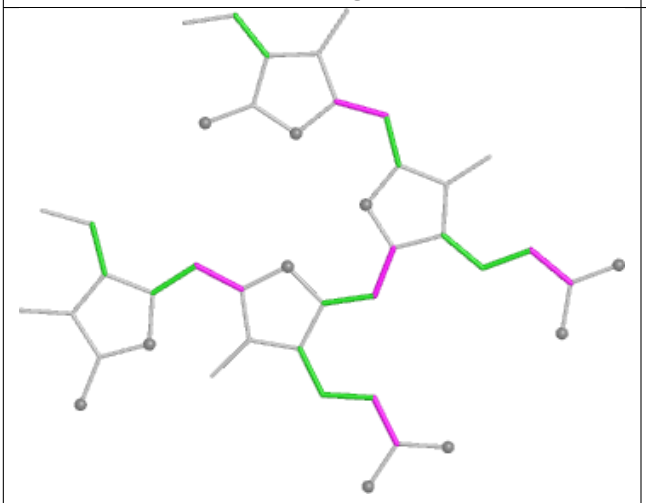
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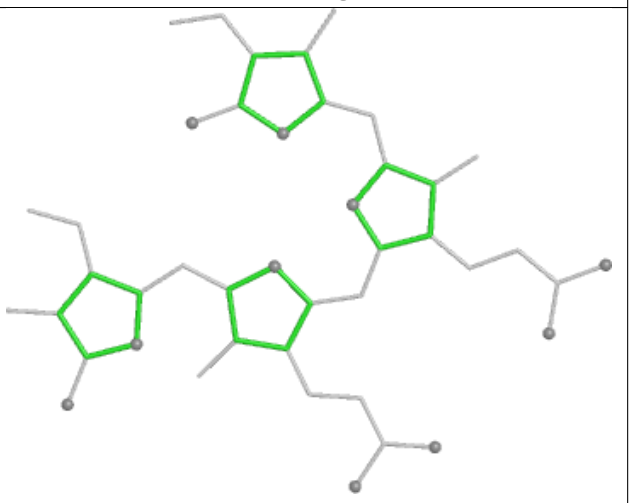
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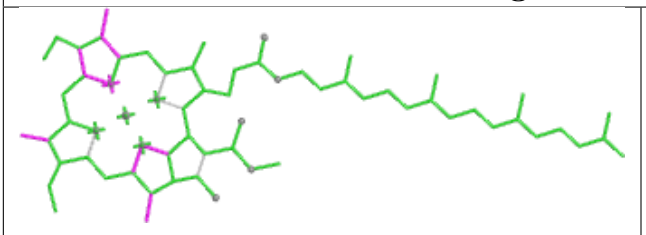


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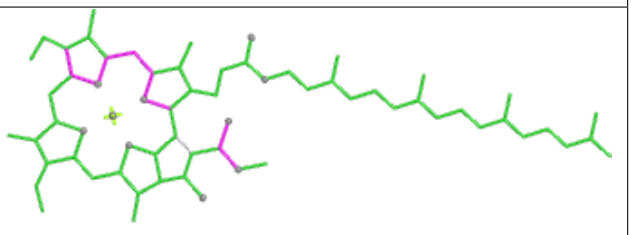


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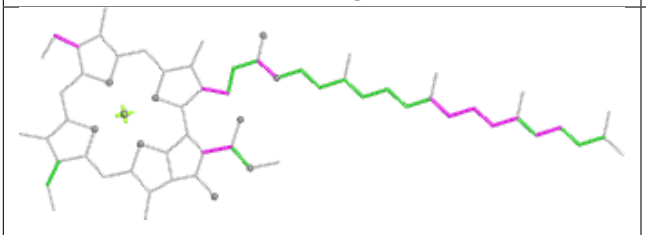
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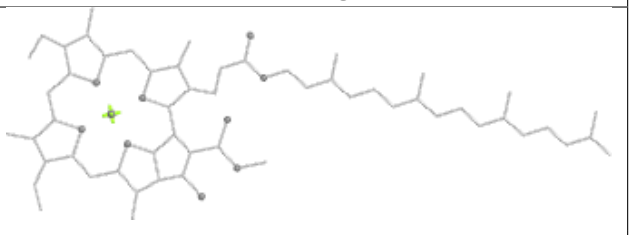
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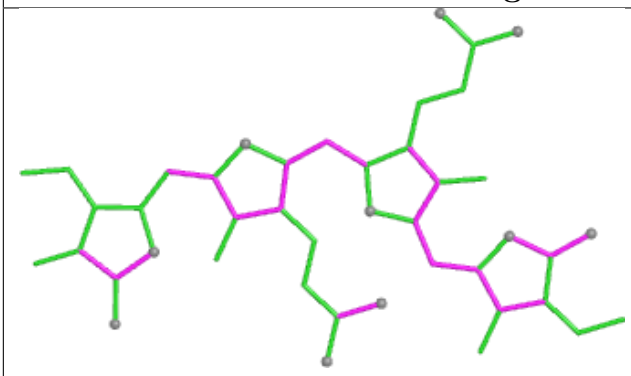


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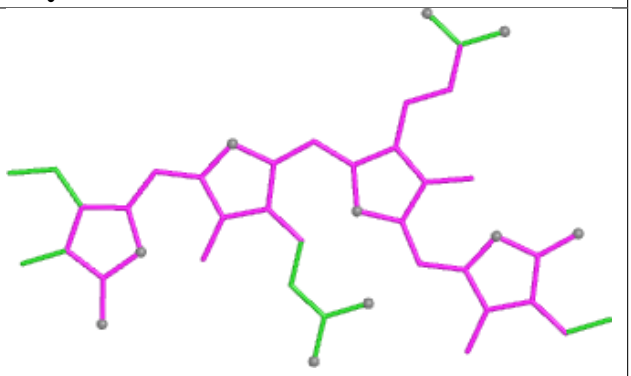


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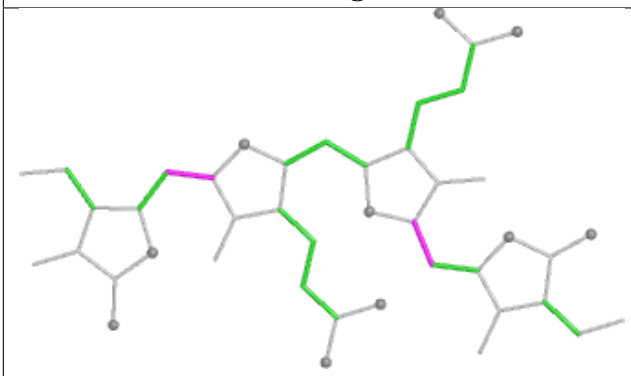
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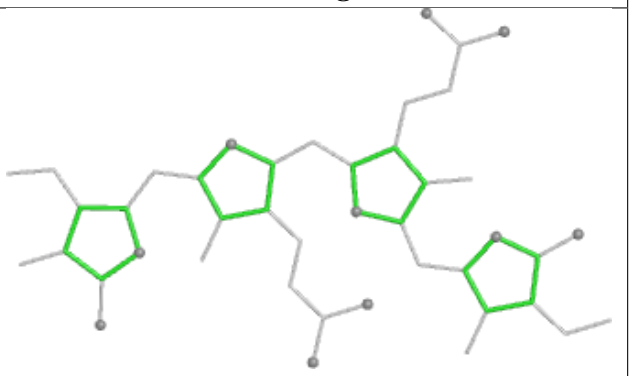
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Bond angles

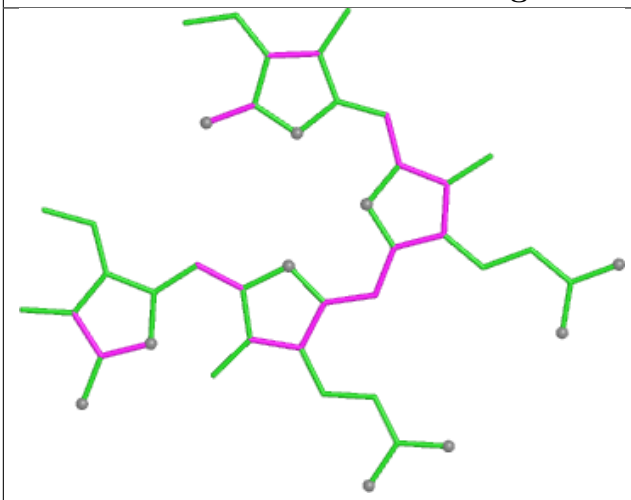


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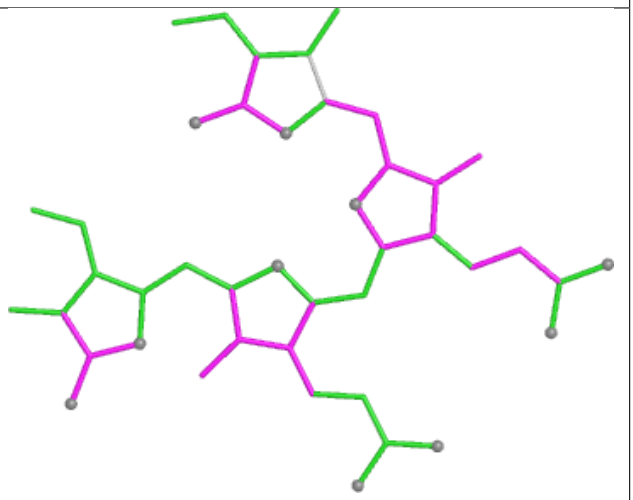


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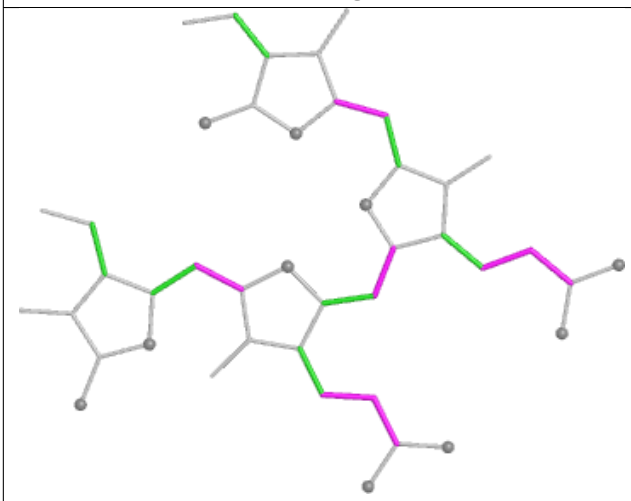
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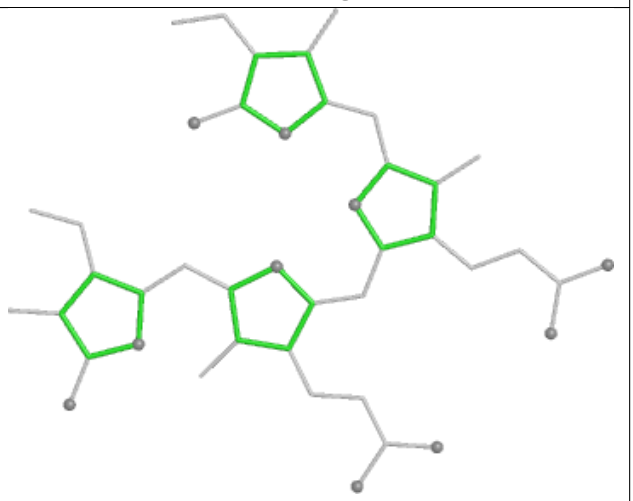
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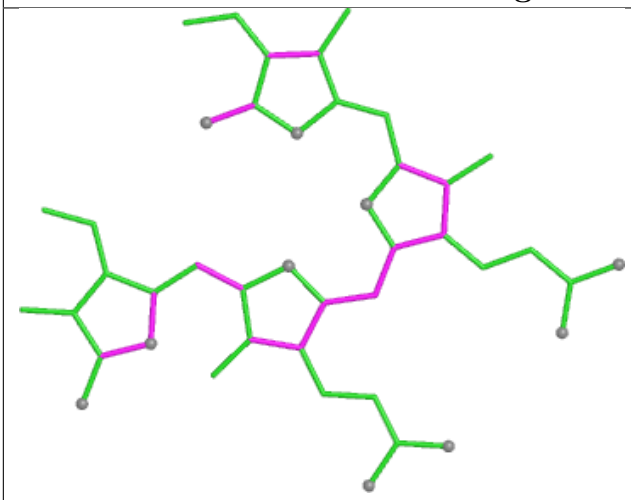


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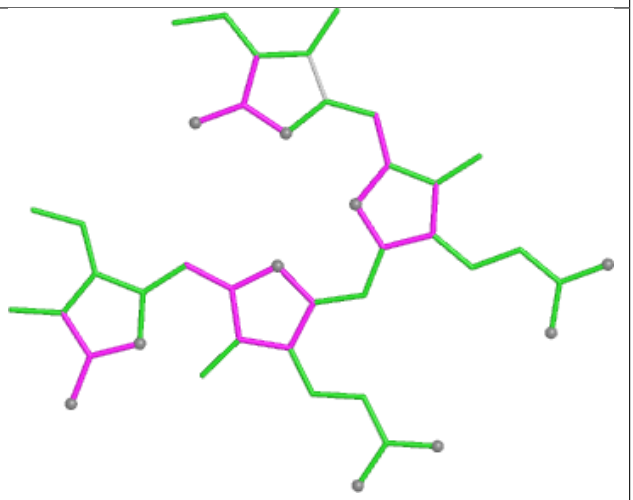


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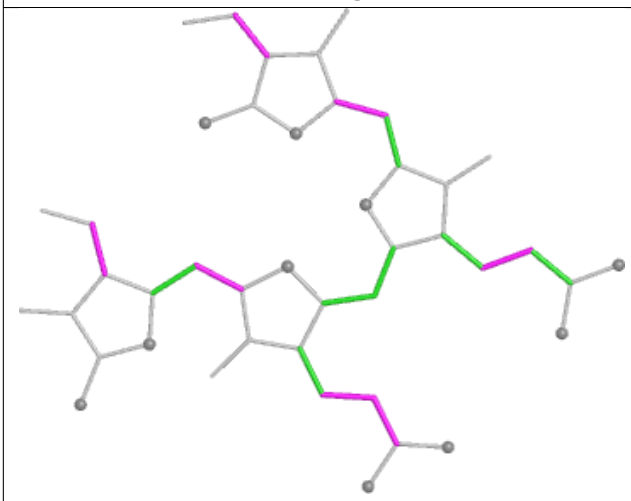
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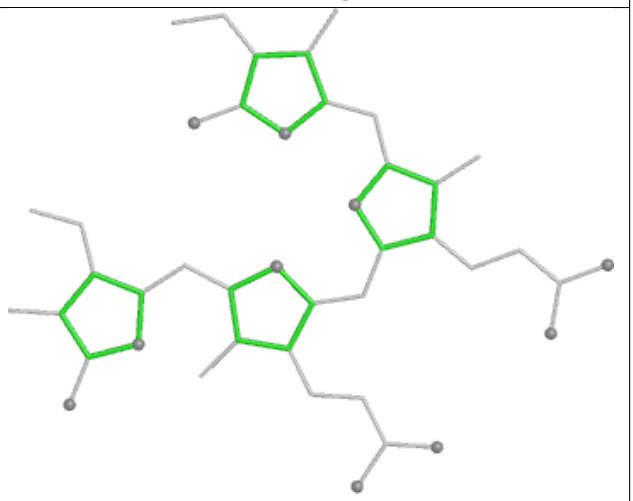
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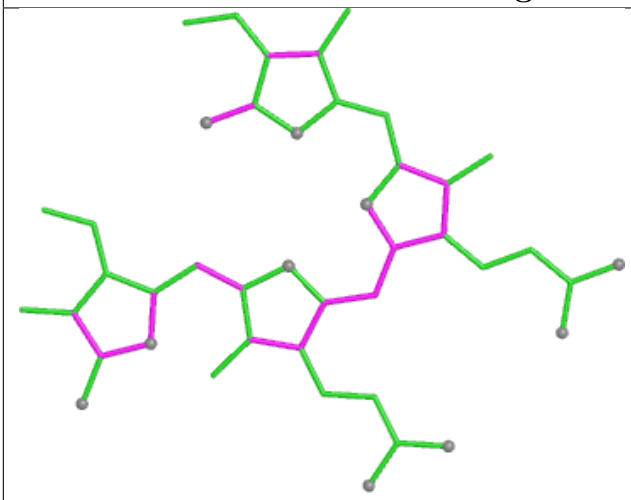


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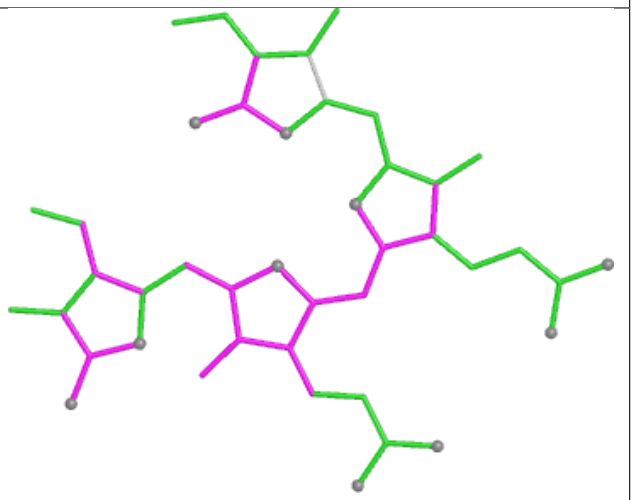


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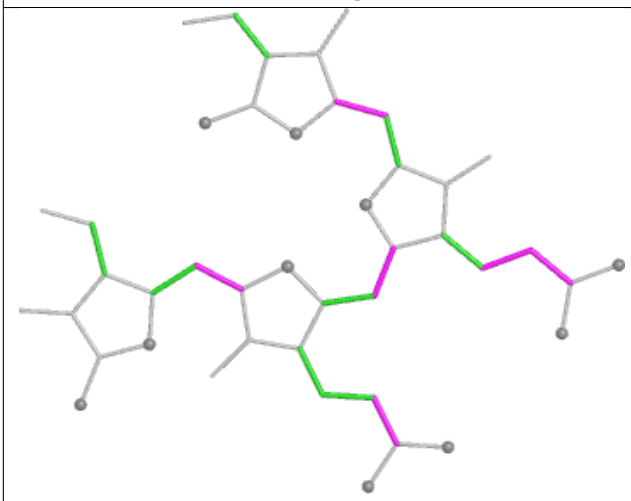
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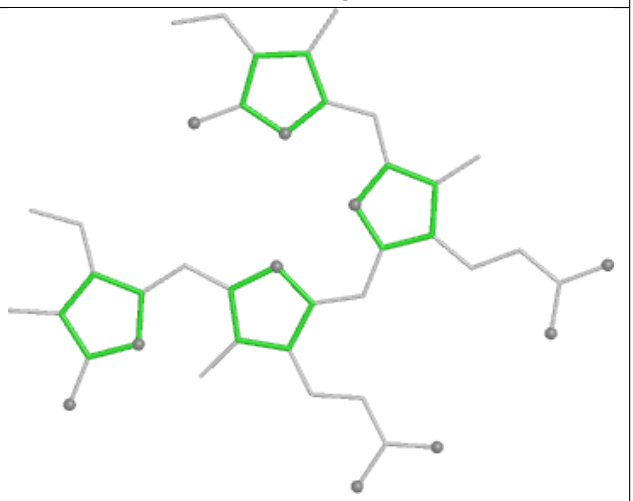
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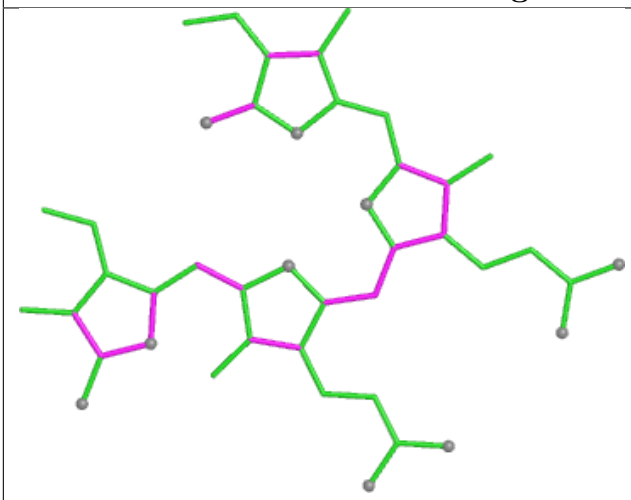


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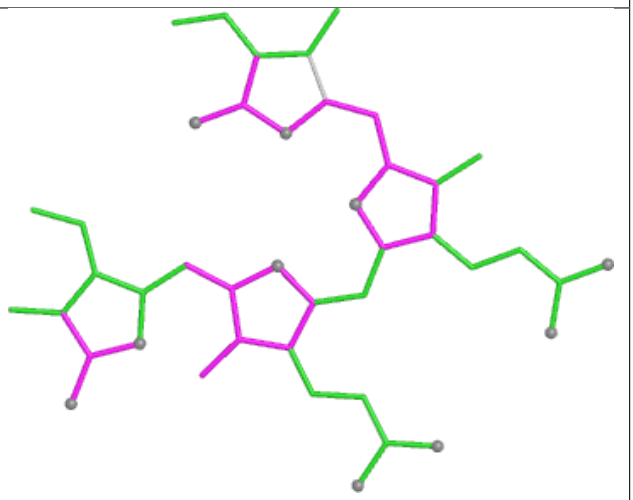


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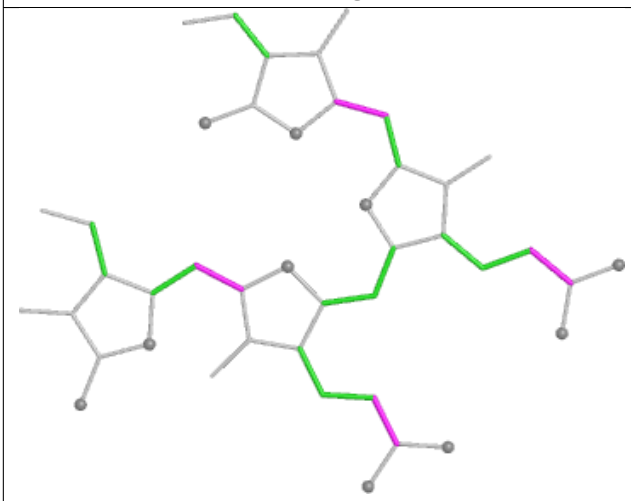
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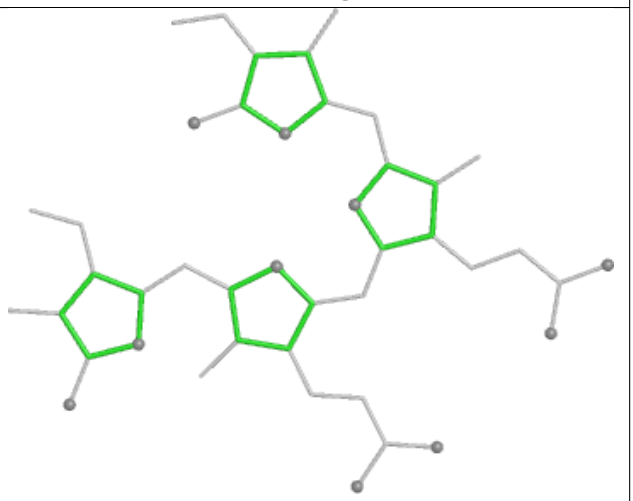
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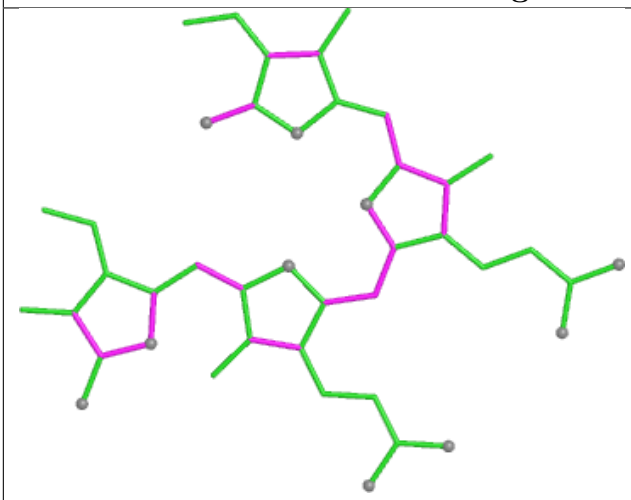


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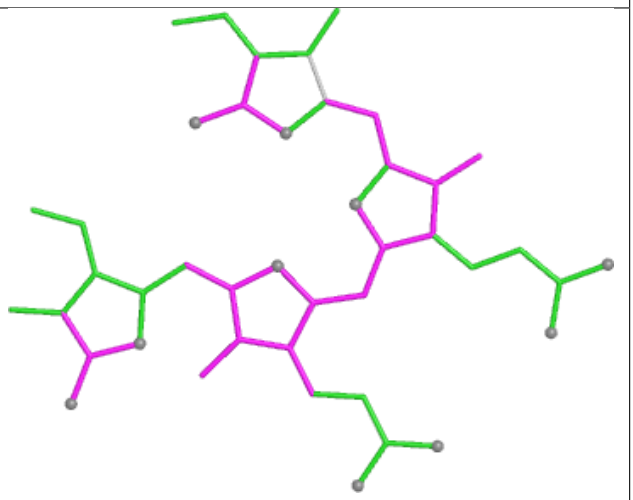


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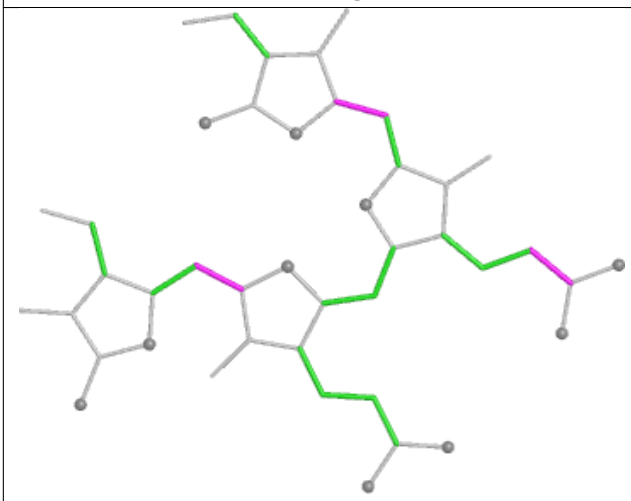
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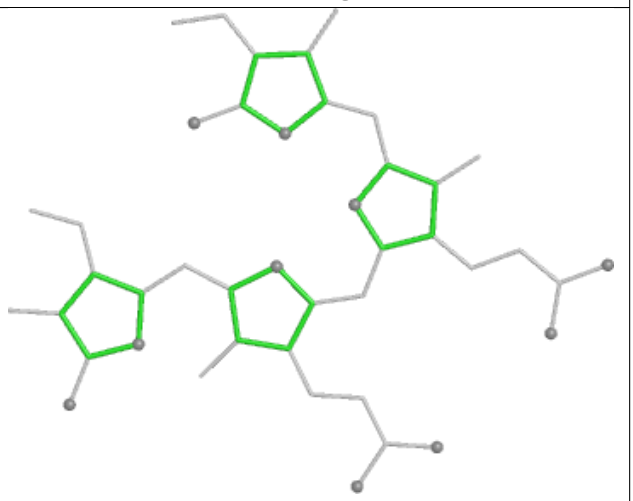
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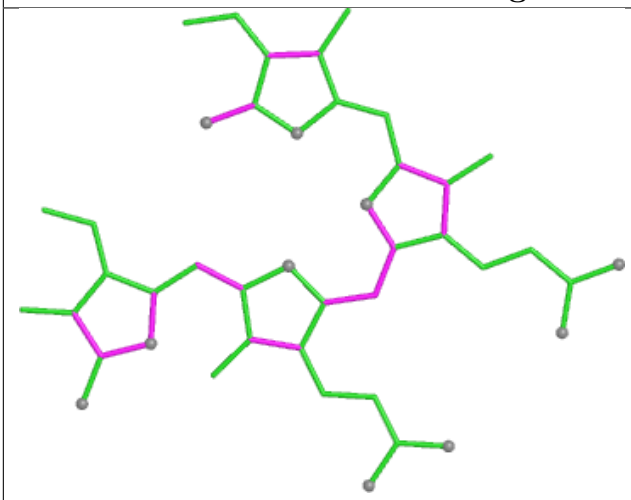


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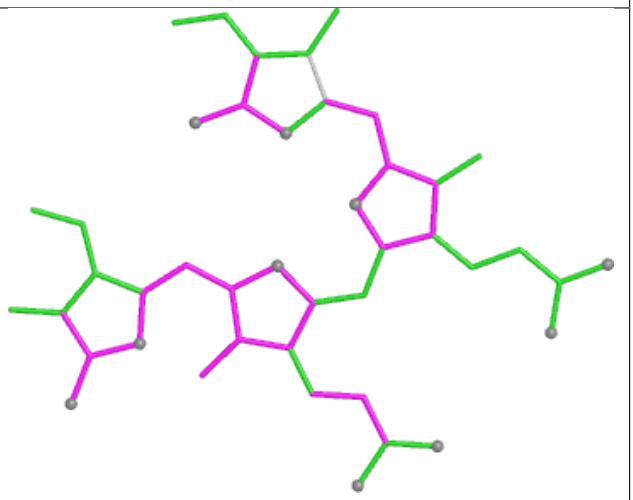


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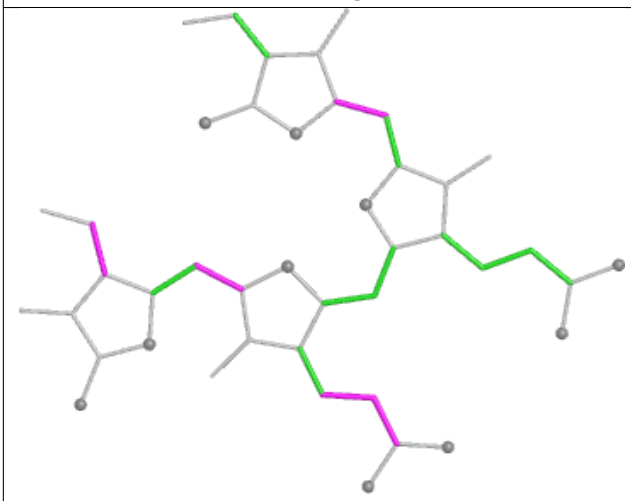
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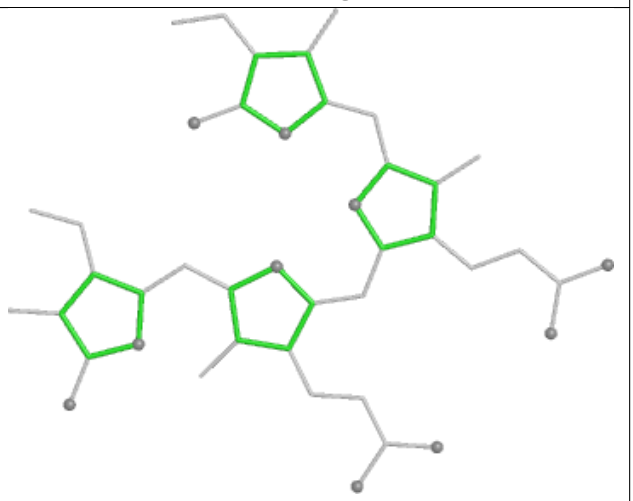
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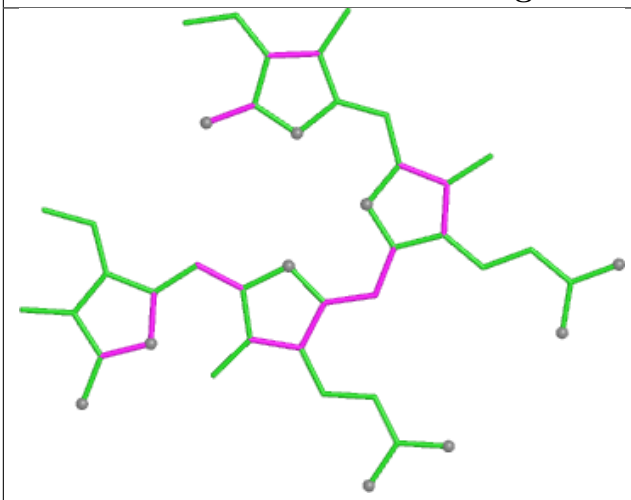


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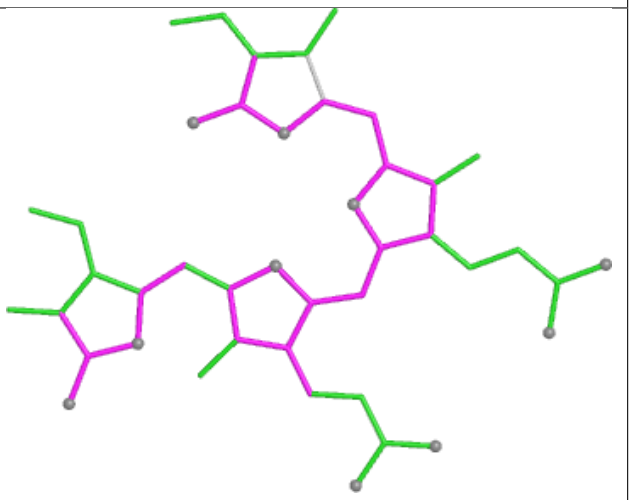


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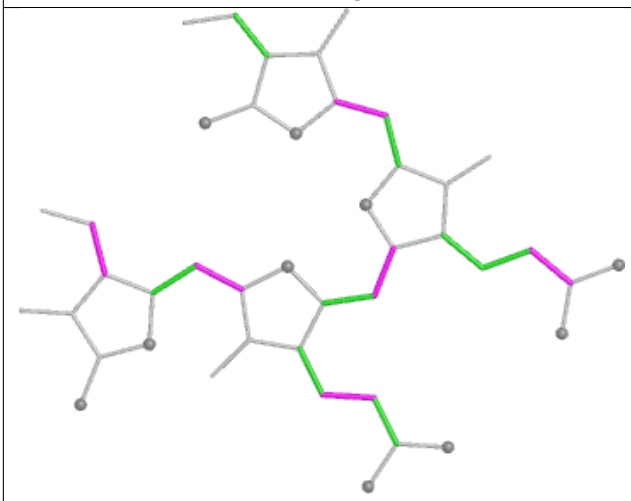
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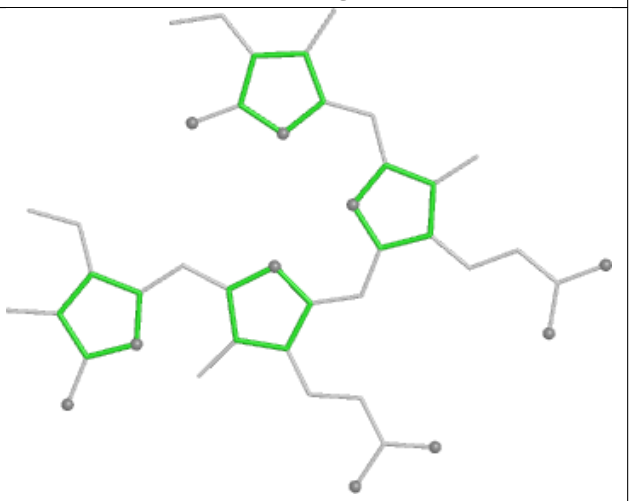
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Bond angles

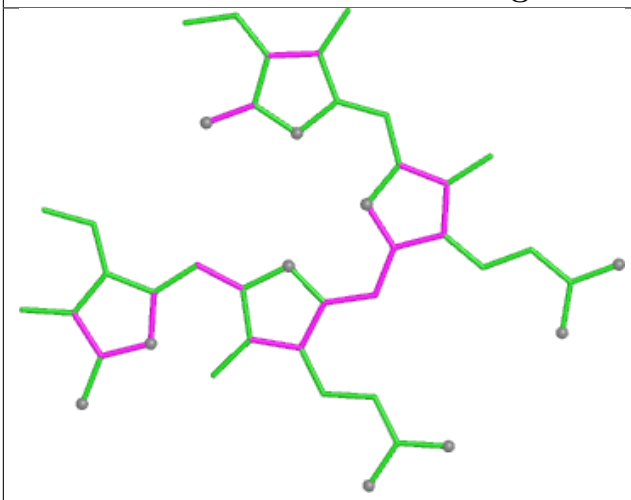


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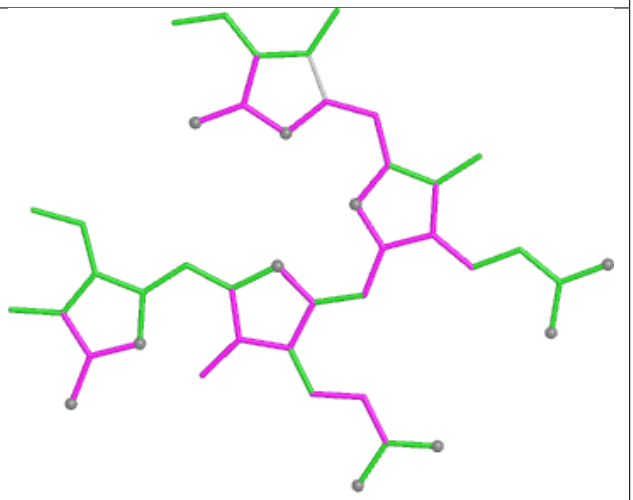


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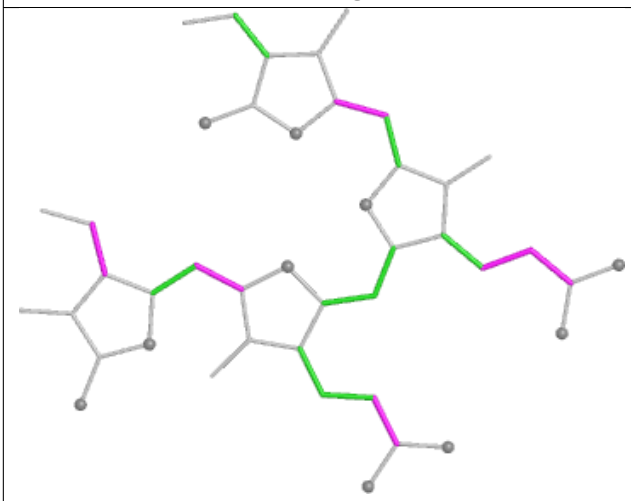
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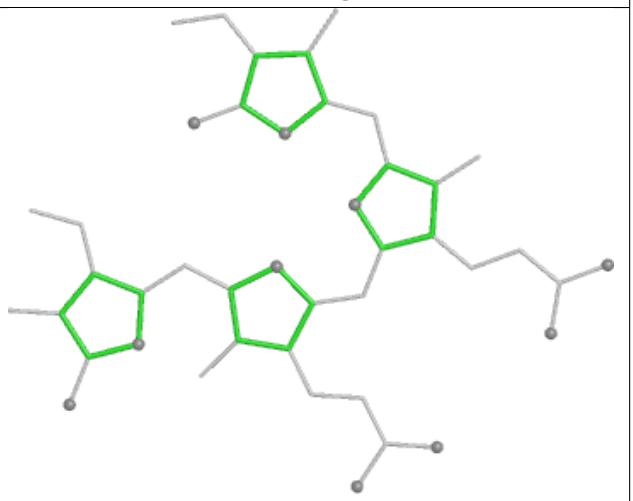
Bond lengths



Bond angles

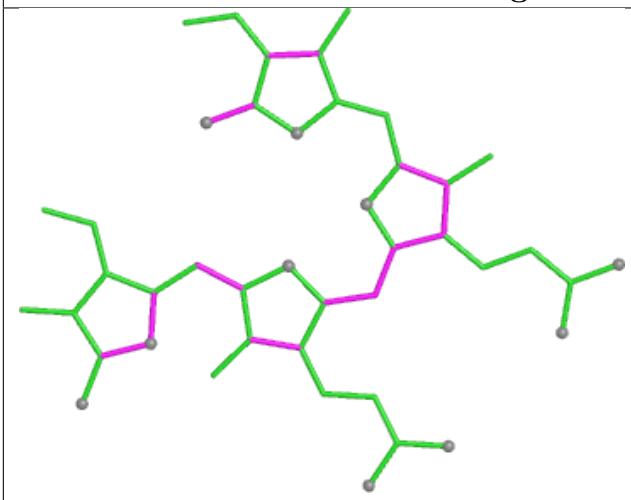


Torsions

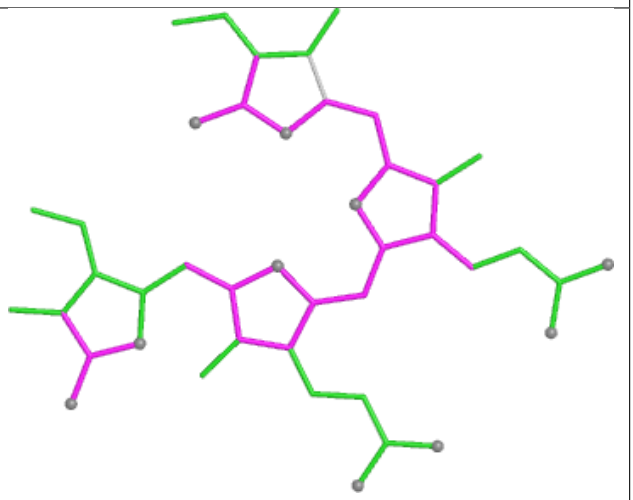


Rings

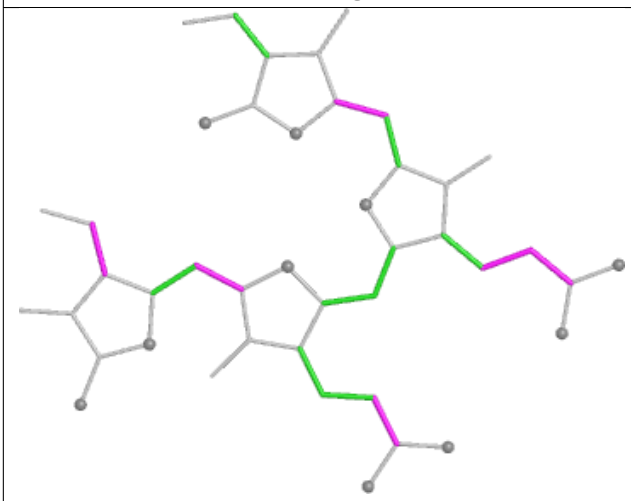
Ligand PEB OH 203



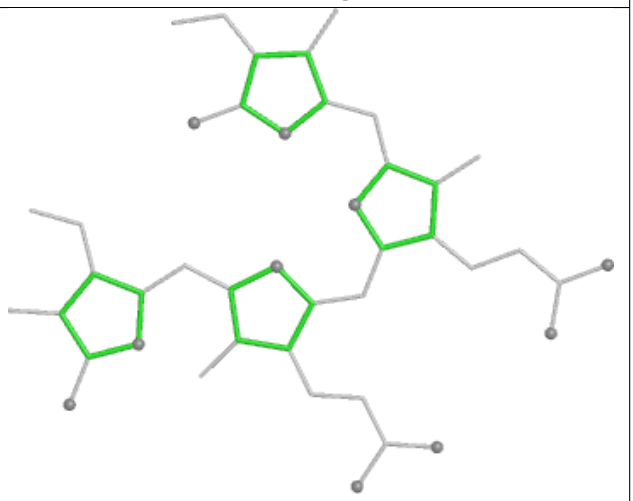
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Bond angles

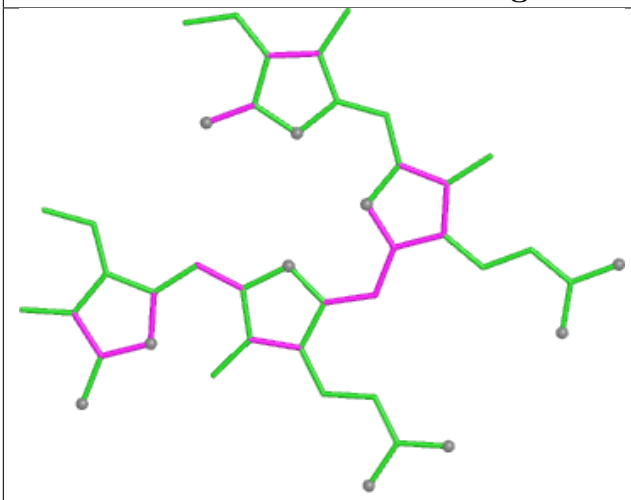


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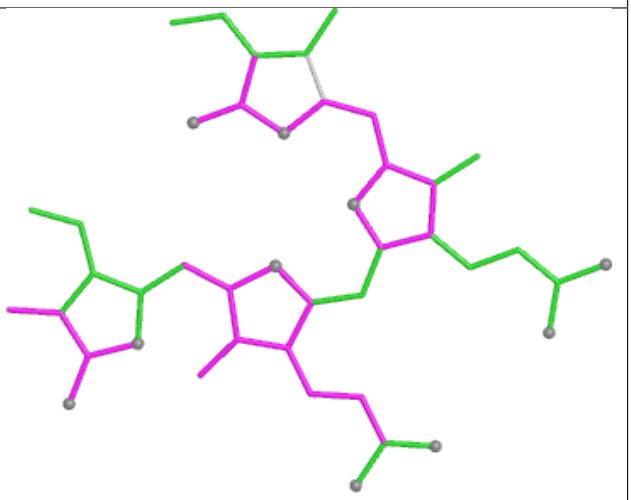


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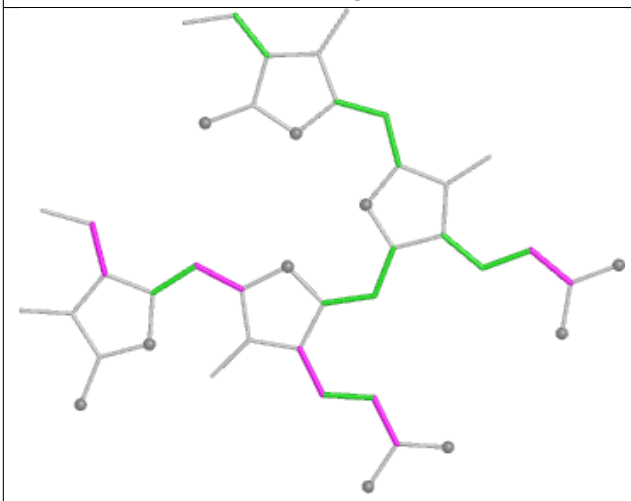
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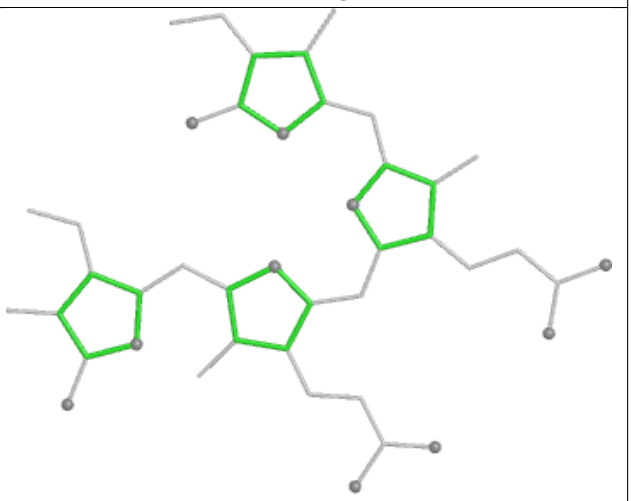
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Bond angles

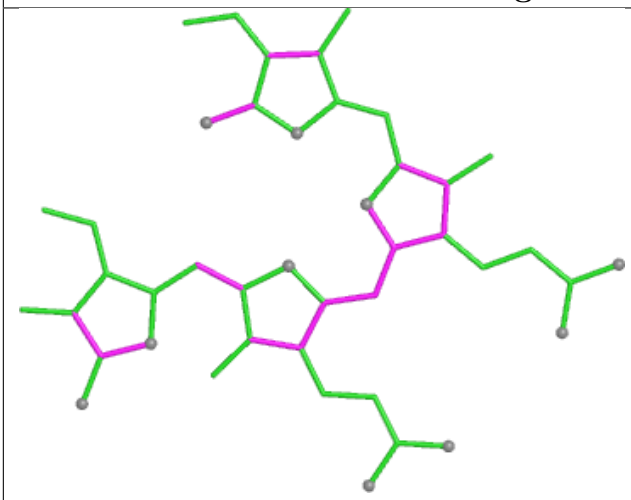


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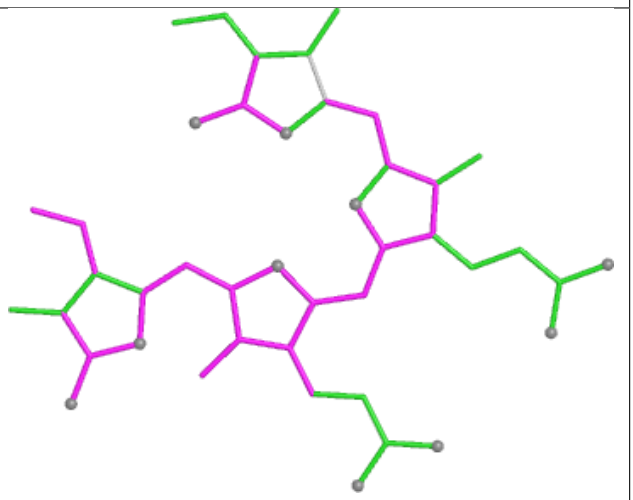


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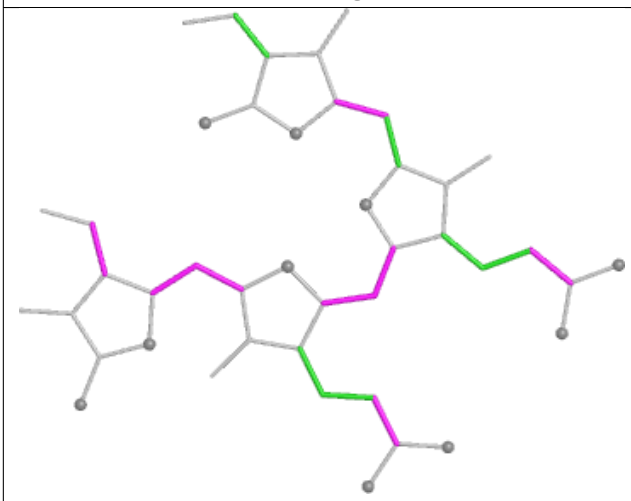
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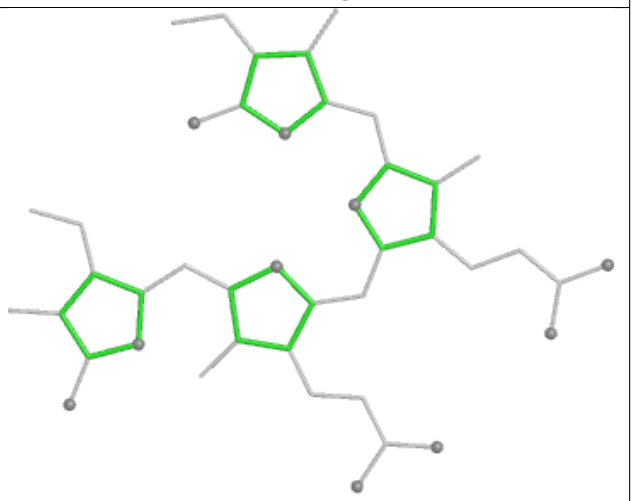
Bond lengths



Bond angles

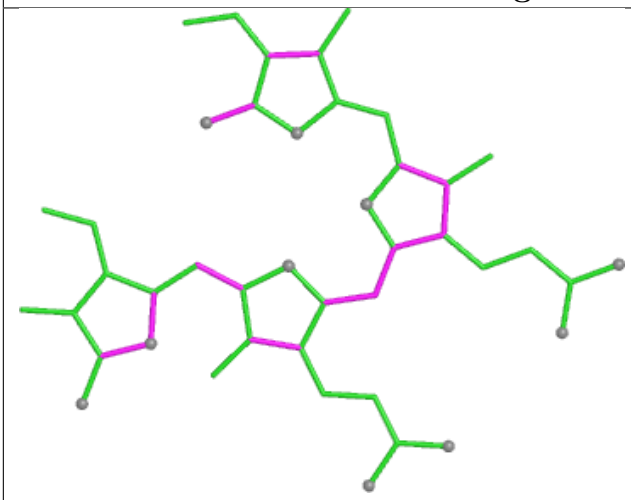


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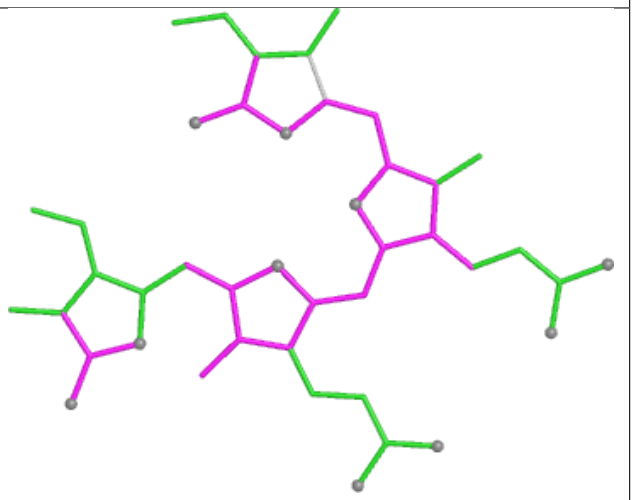


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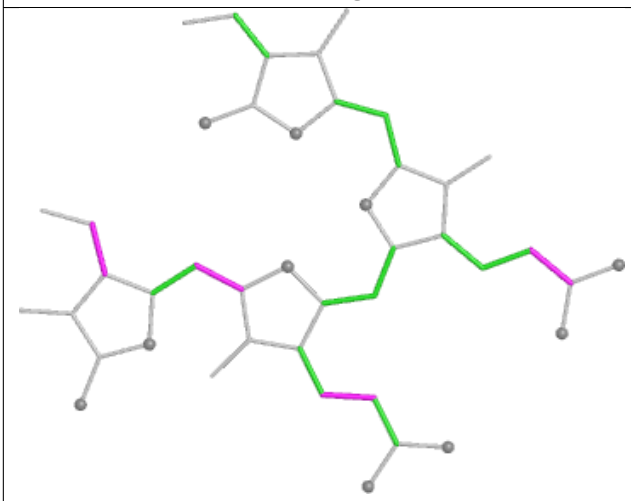
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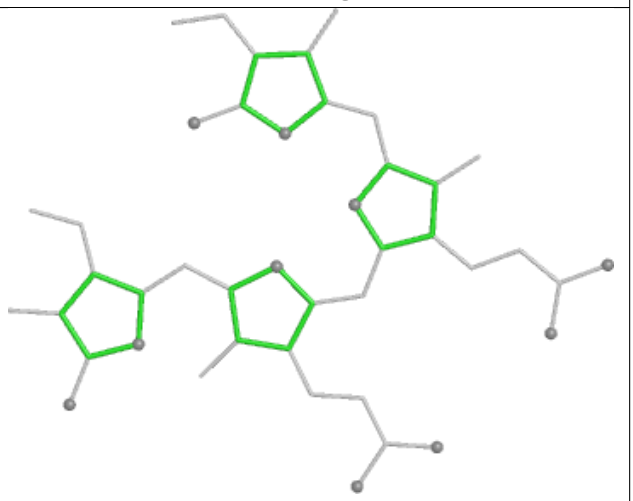
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Bond angles

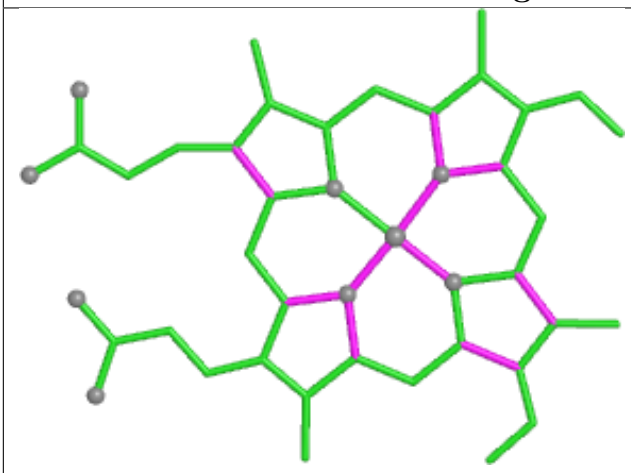


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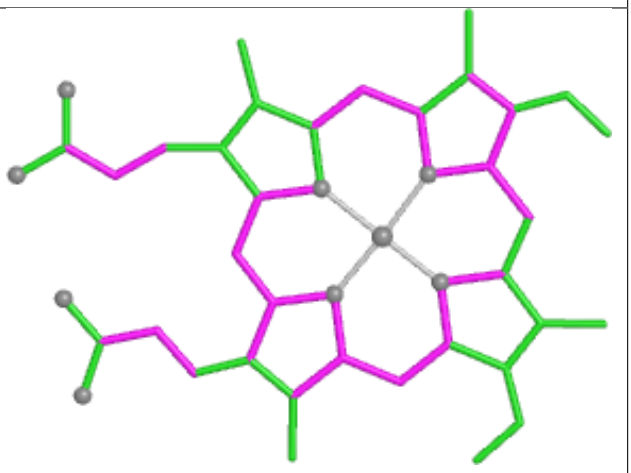


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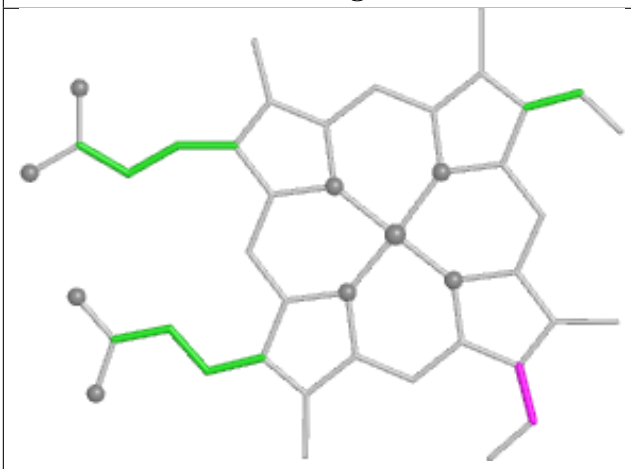
Ligand HEM v6 201



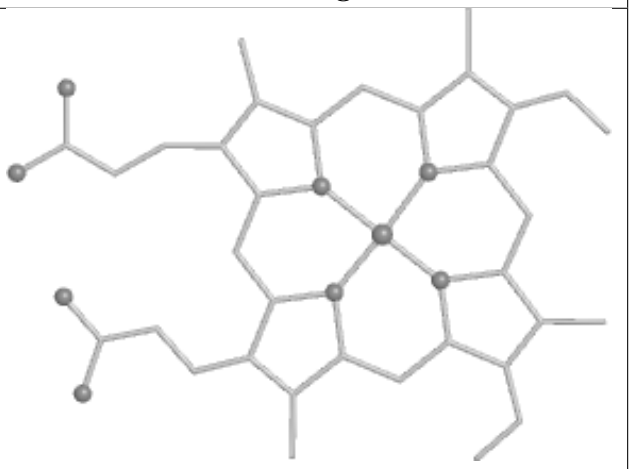
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Bond angles

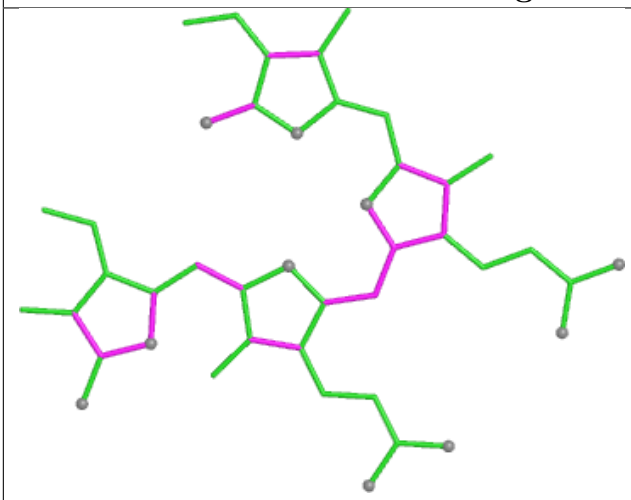


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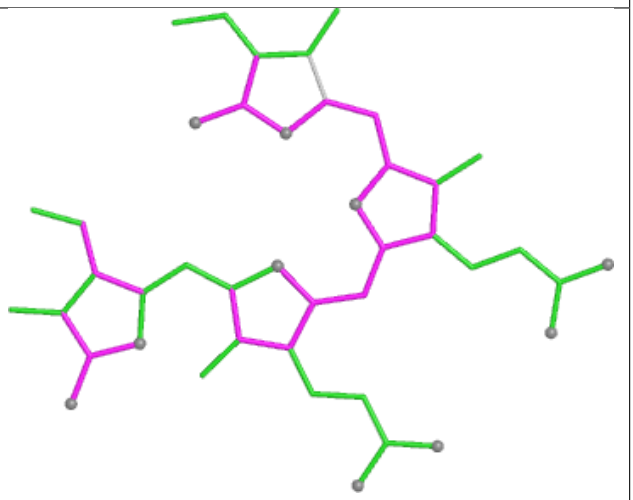


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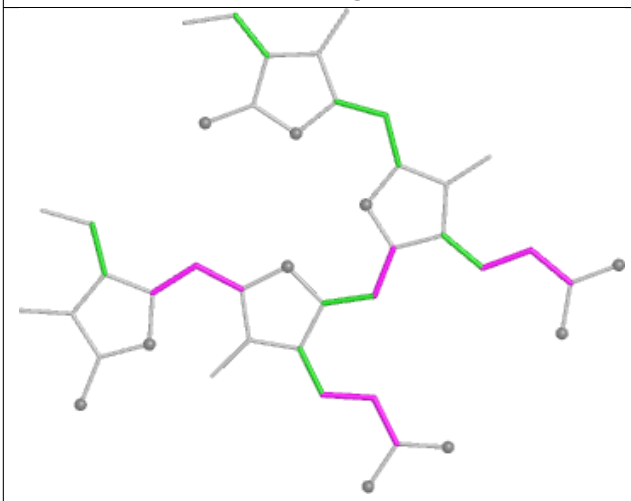
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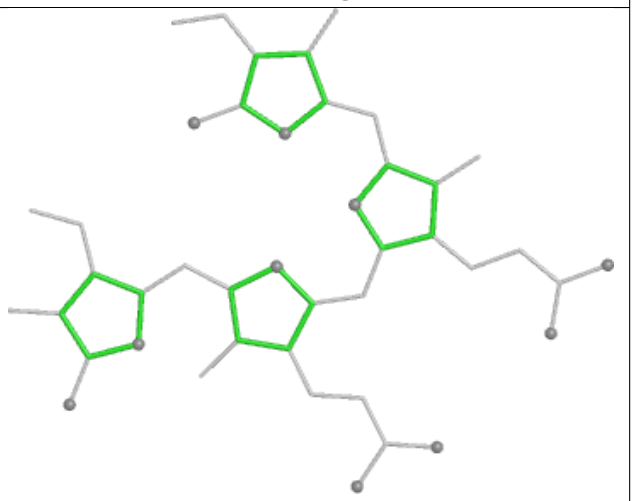
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Bond angles

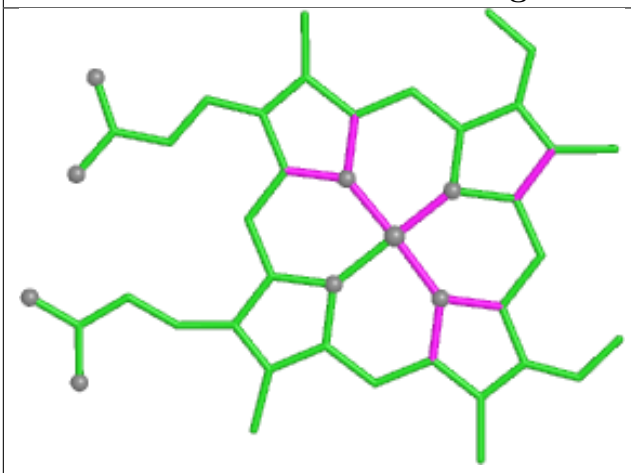


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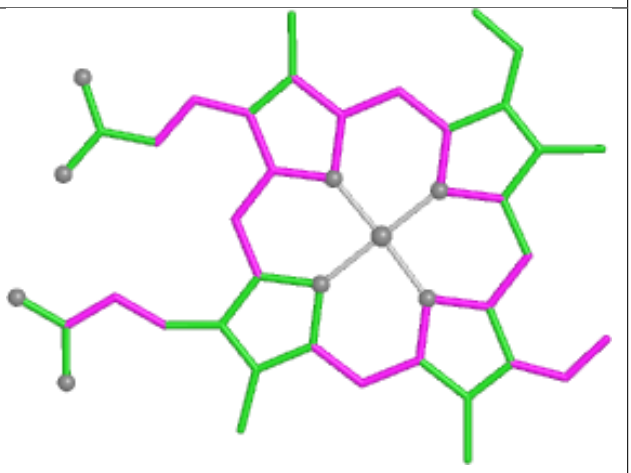


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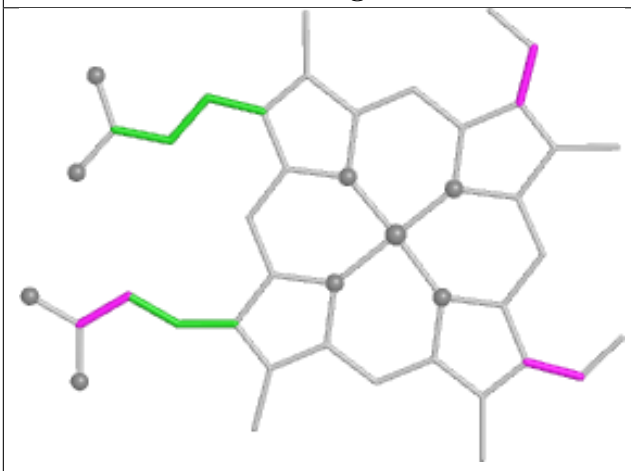
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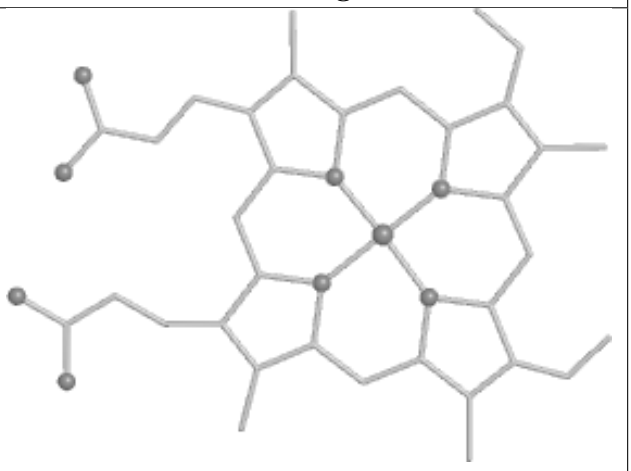
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Bond angles

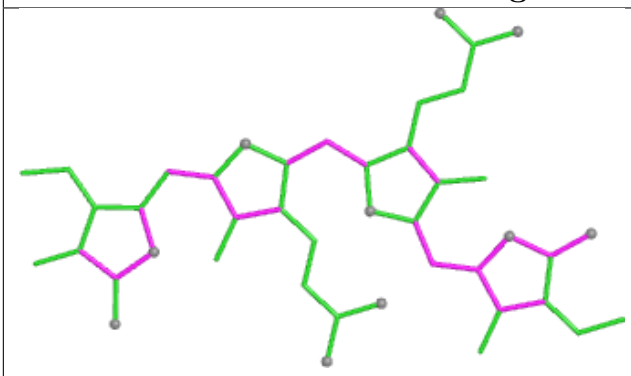


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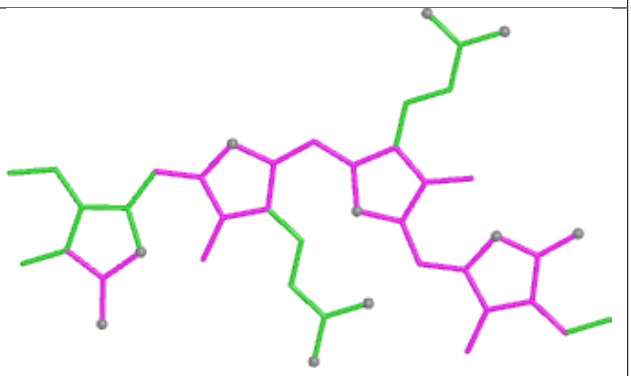


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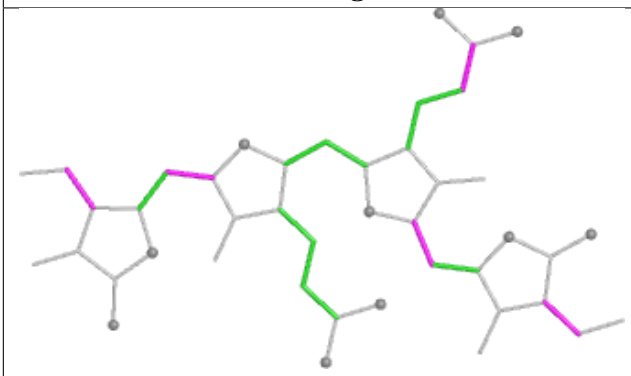
Ligand CYC NE 201



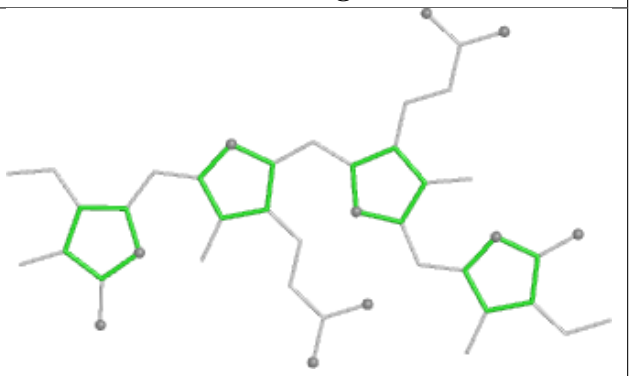
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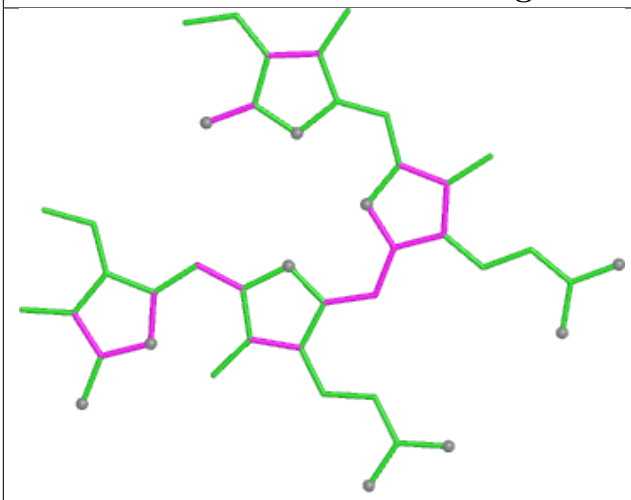


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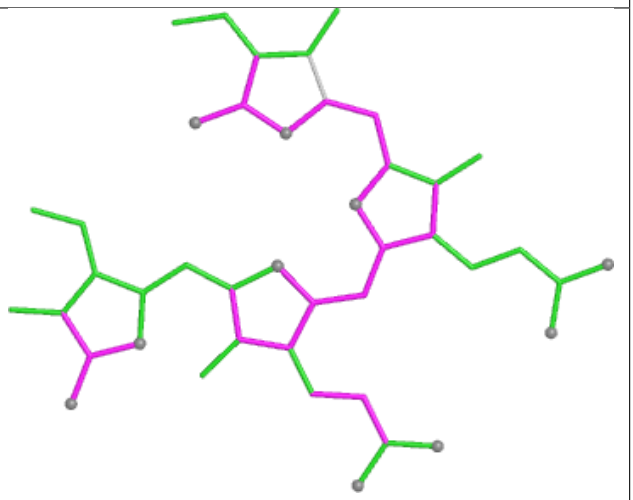


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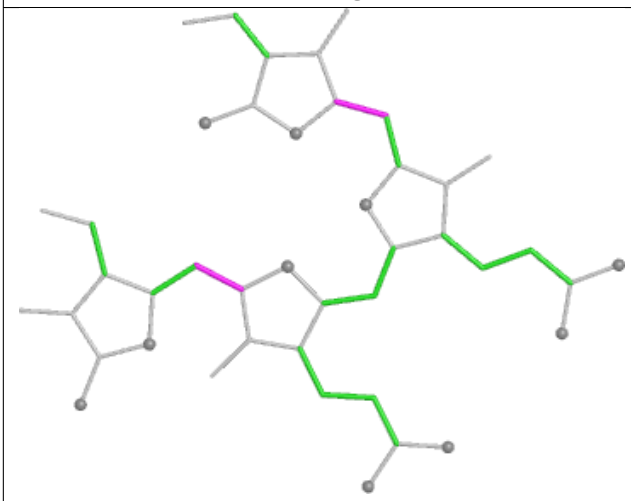
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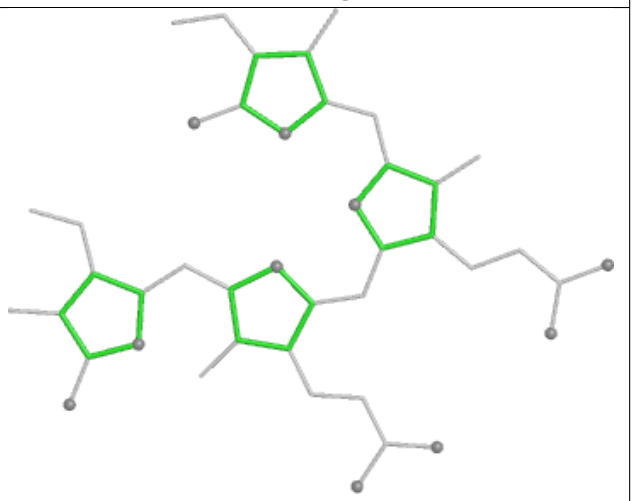
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Bond angles

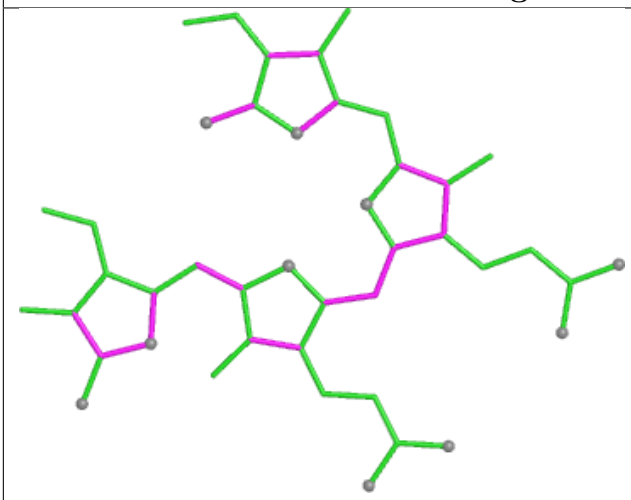


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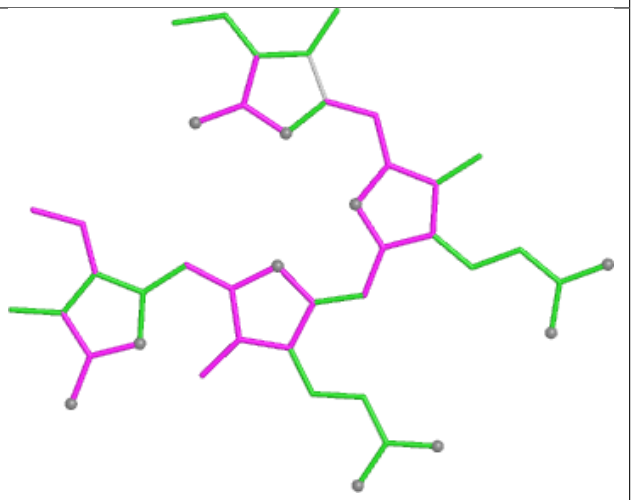


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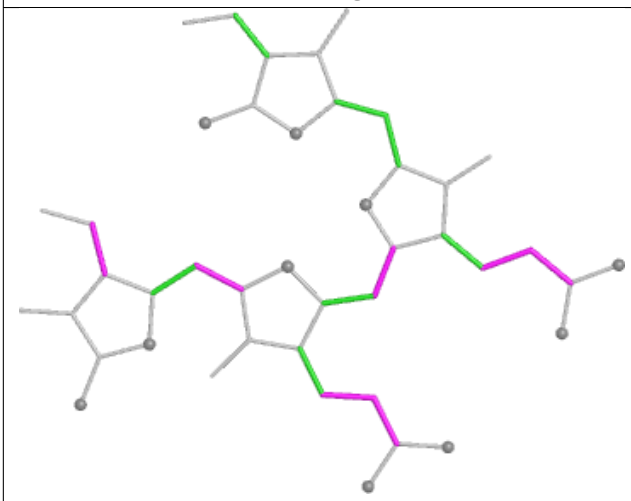
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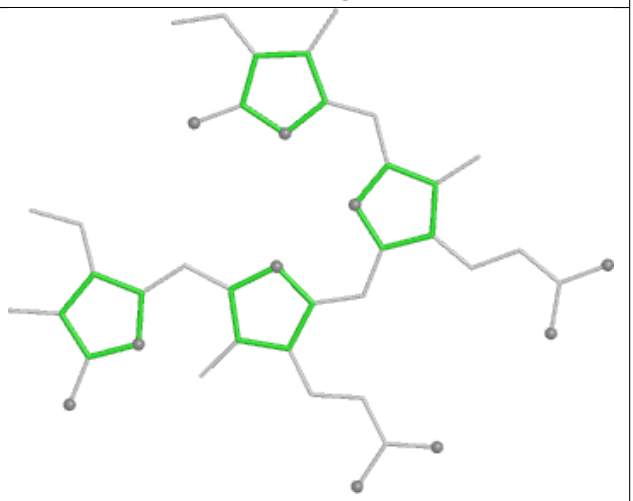
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Bond angles

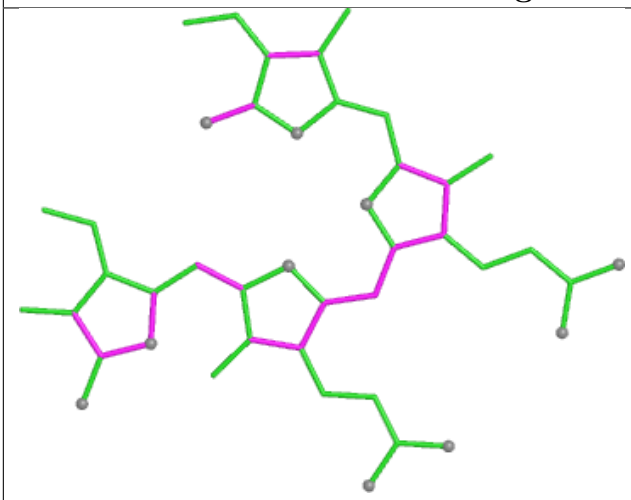


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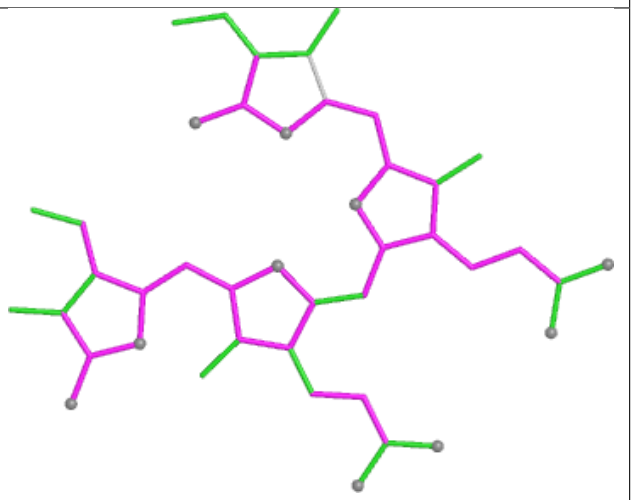


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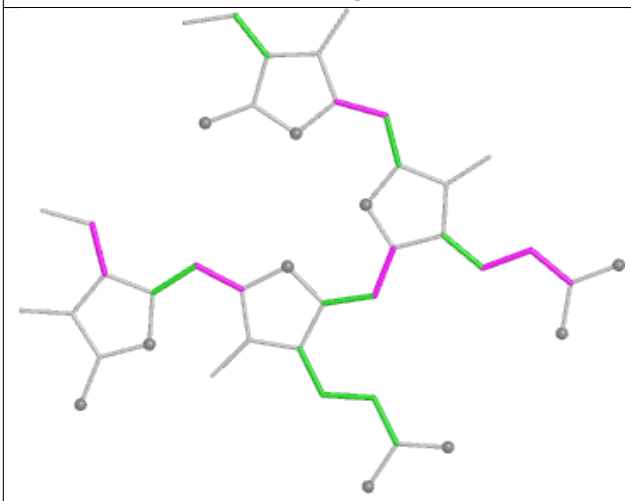
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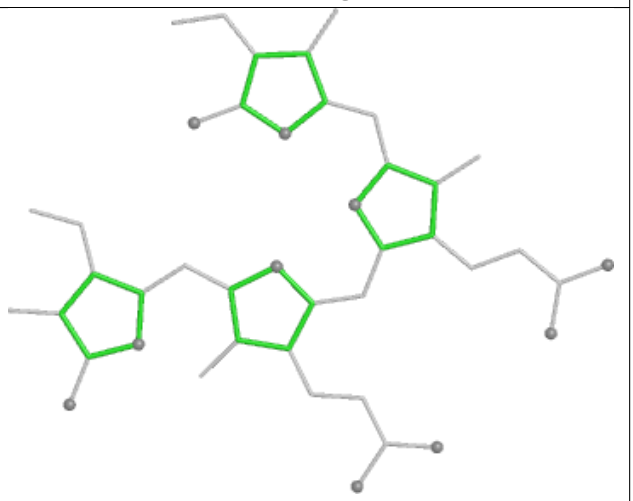
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Bond angles

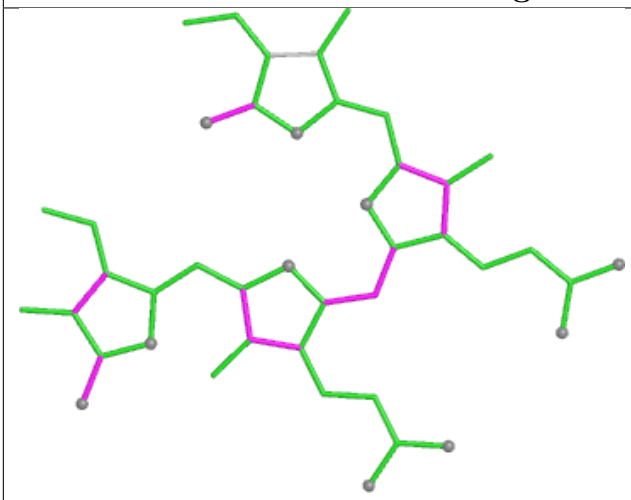


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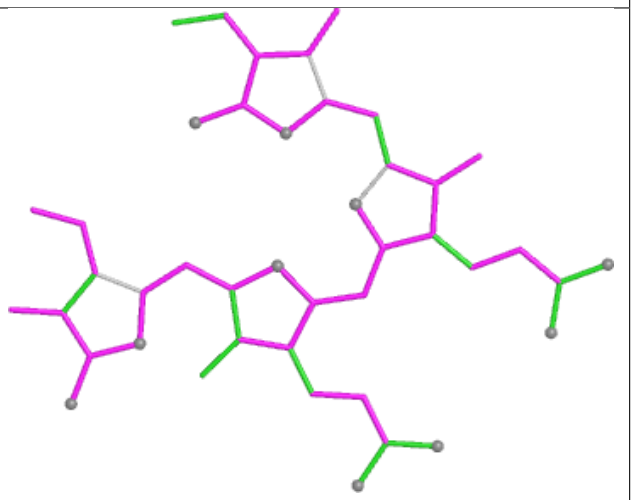


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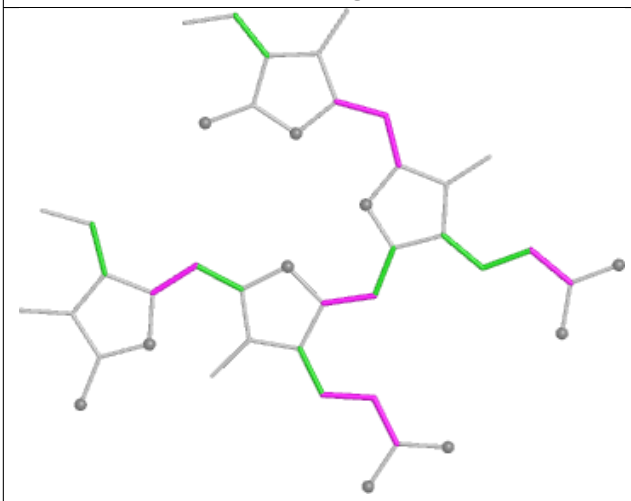
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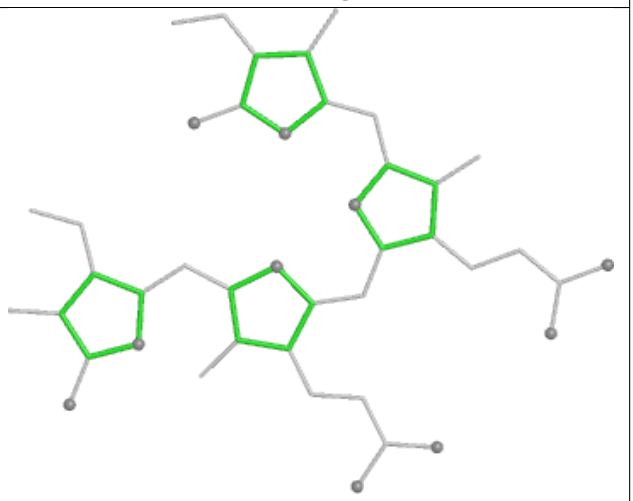
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Bond angles

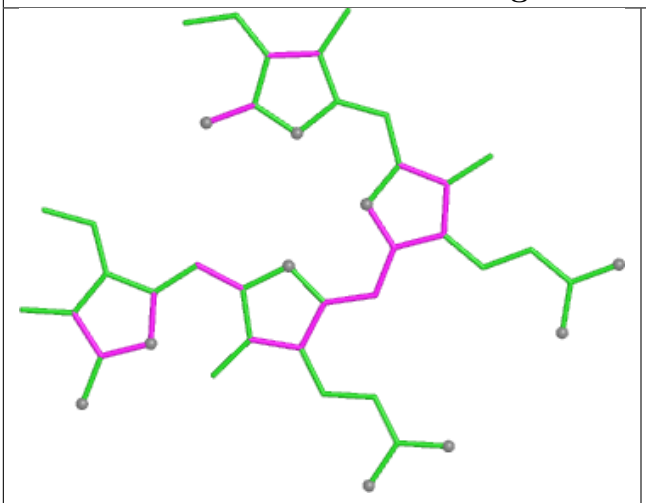


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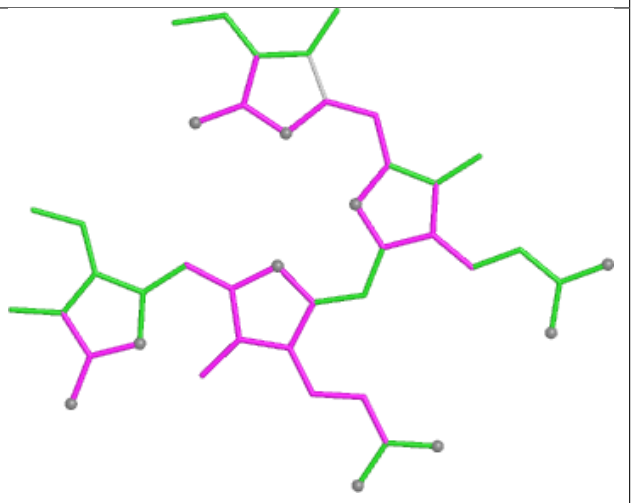


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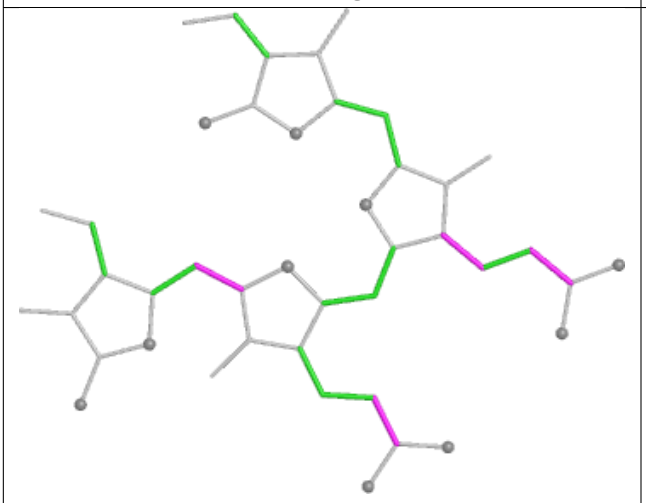
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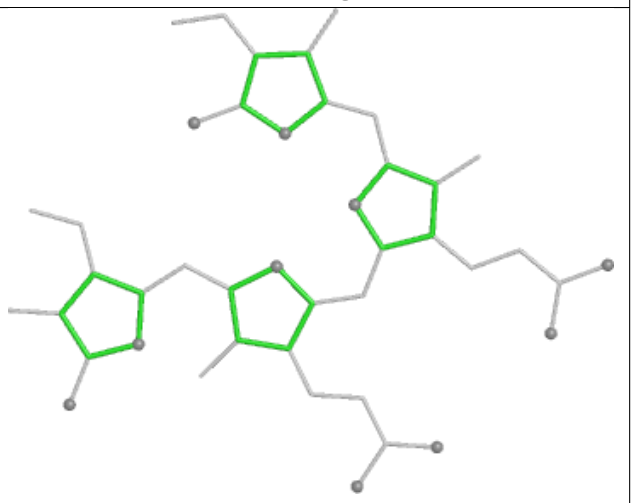
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Bond angles

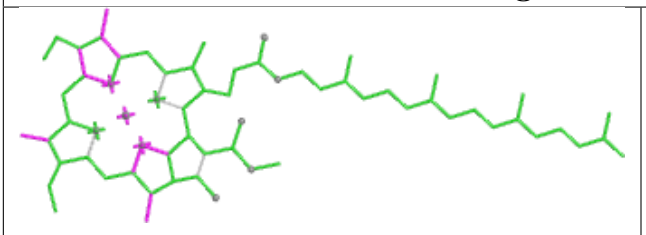


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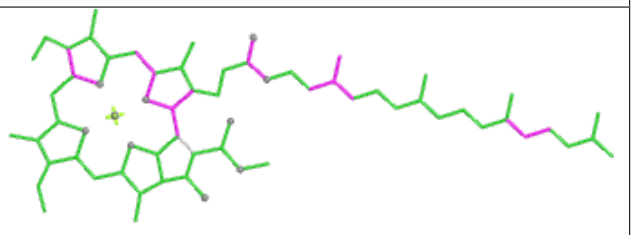


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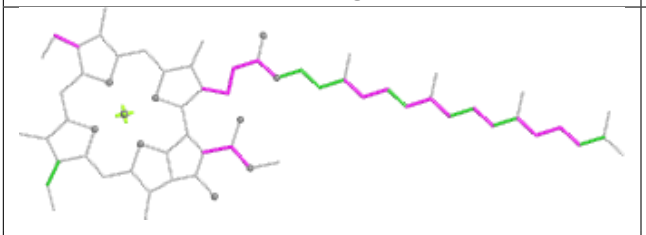
Ligand CLA A2 805



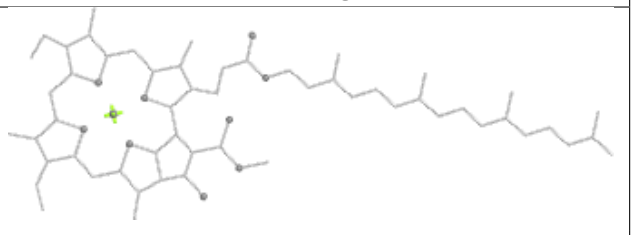
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Bond angles

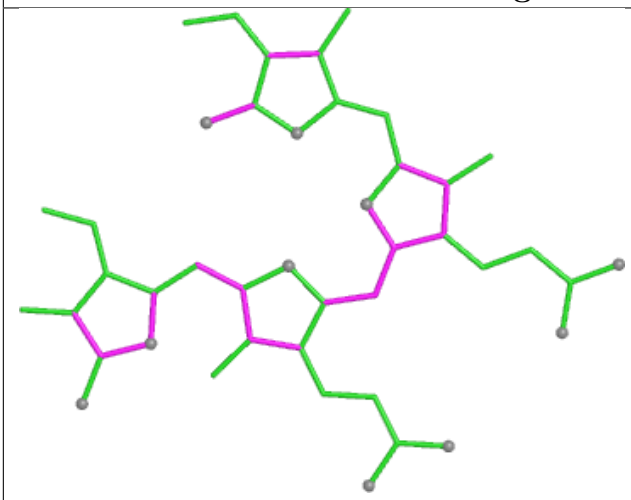


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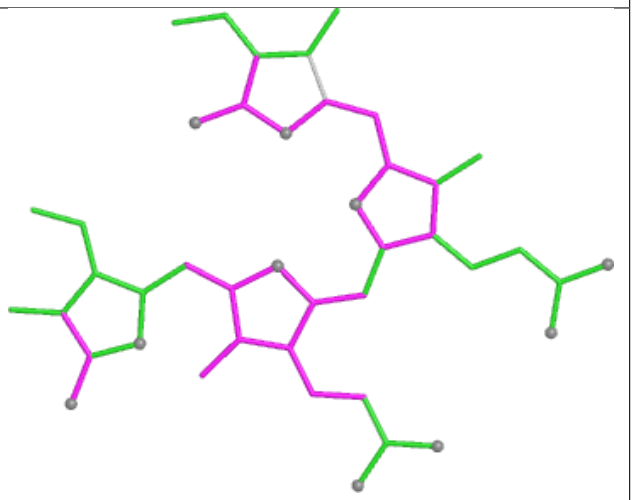


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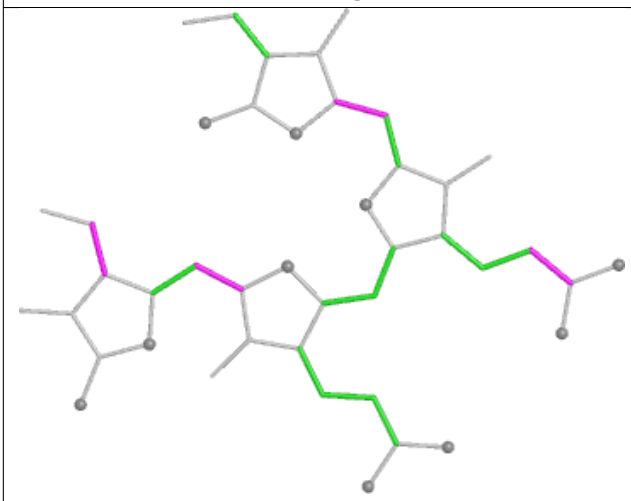
Ligand PEB EP 201



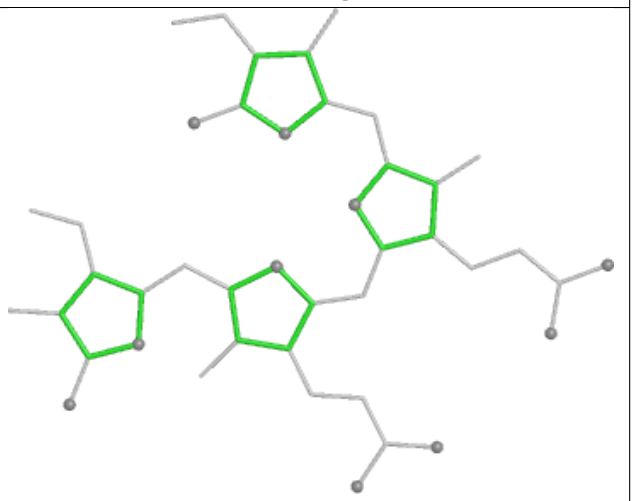
Bond lengths



Bond angles

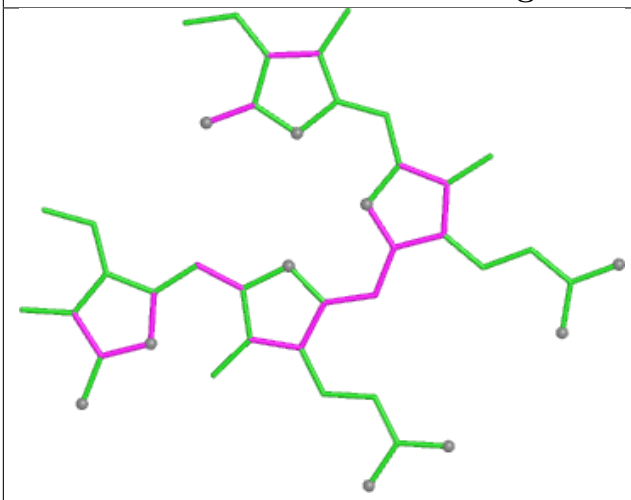


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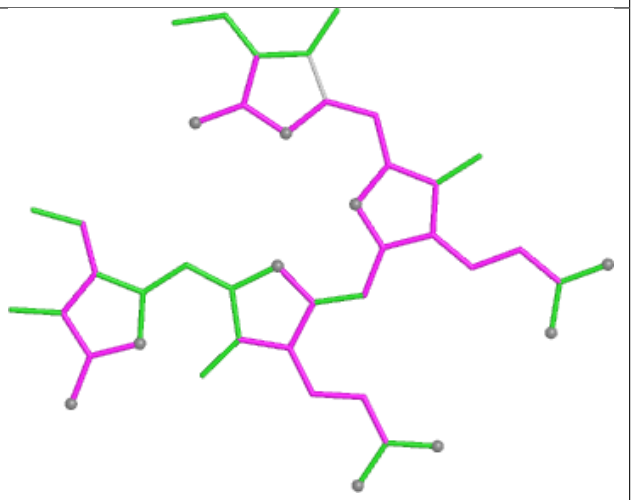


Rings

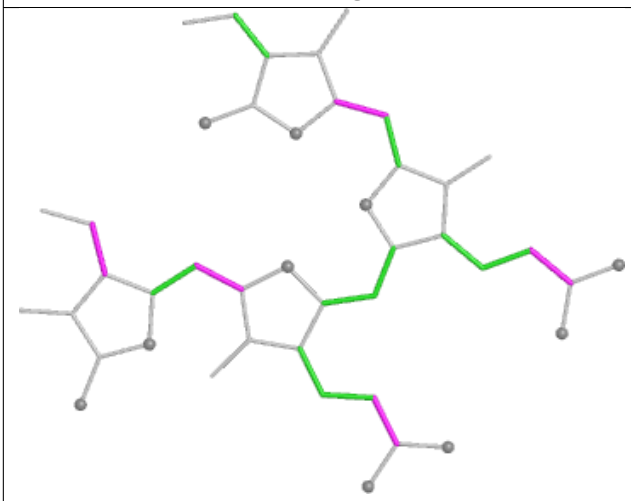
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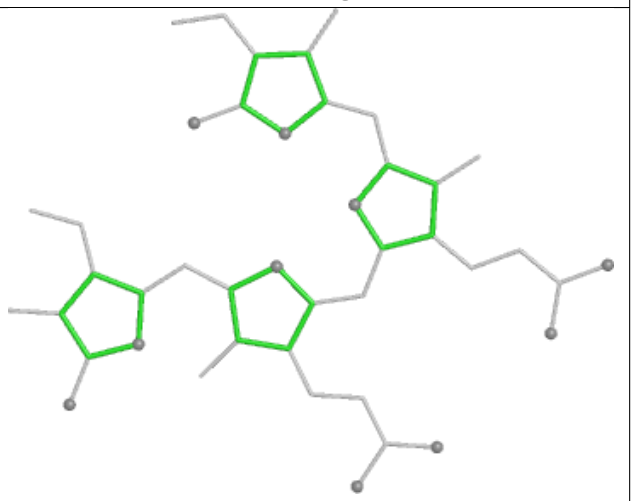
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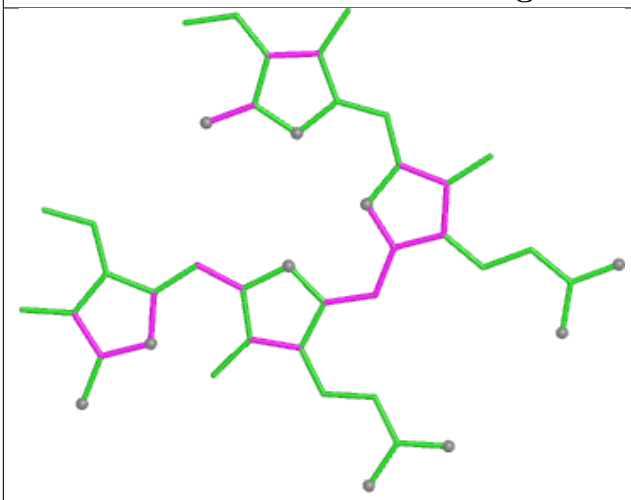


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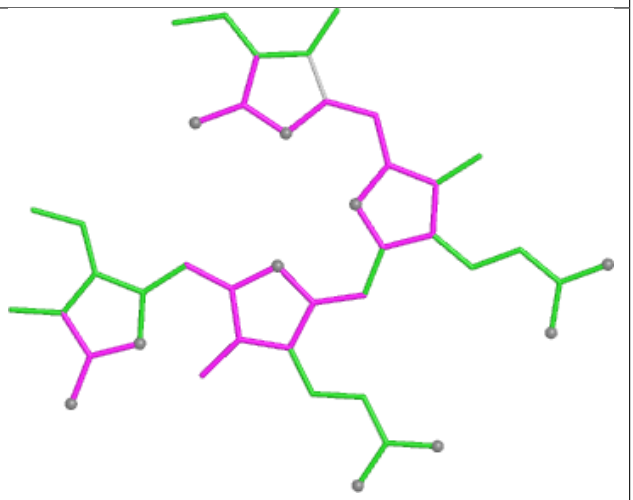


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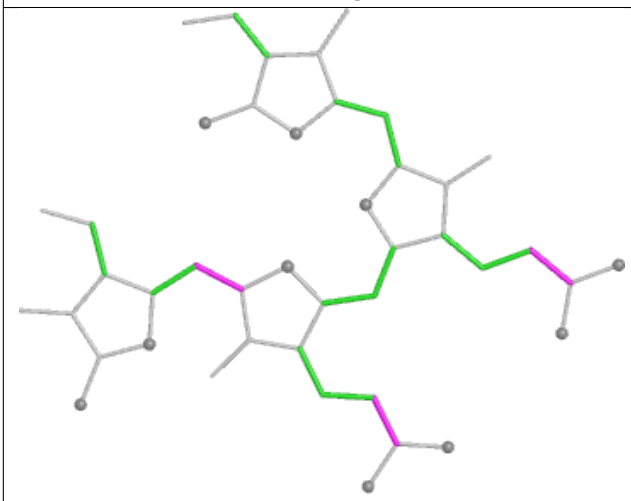
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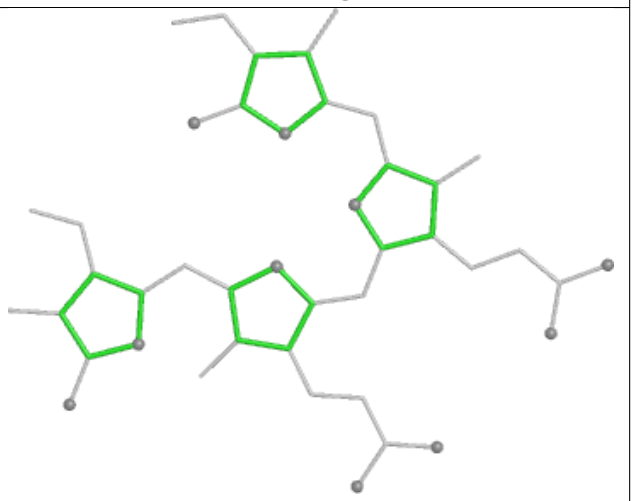
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Bond angles

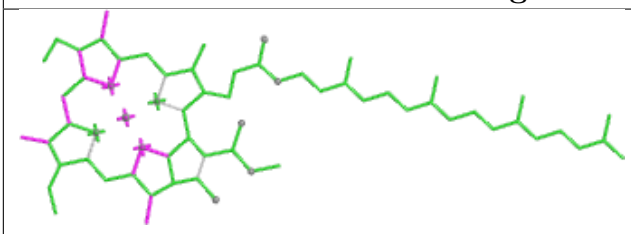


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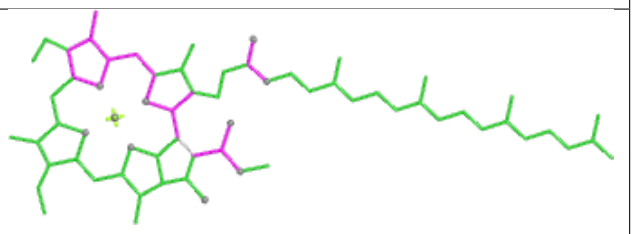


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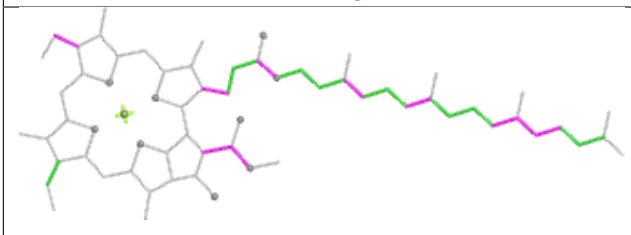
Ligand CLA AN 821



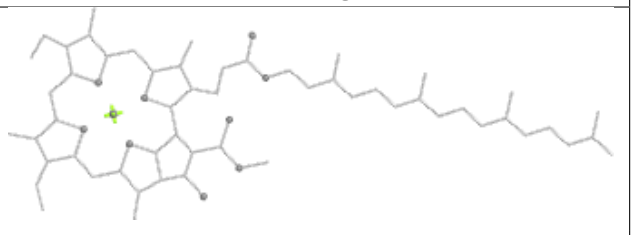
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Bond angles

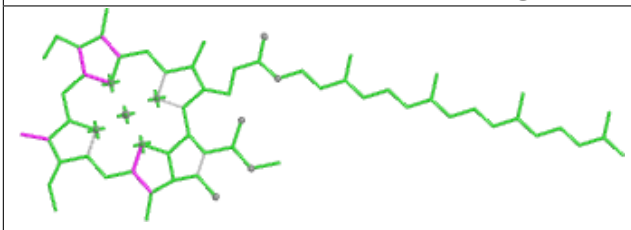


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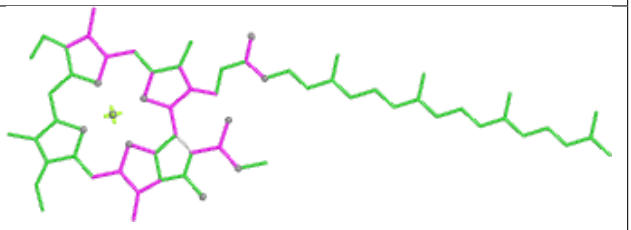


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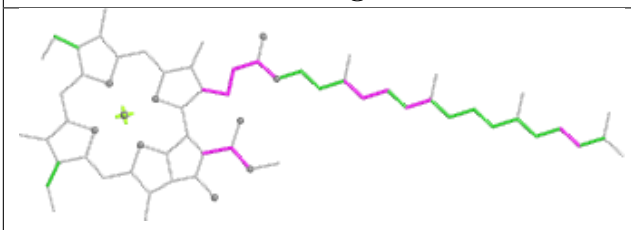
Ligand CLA 2N 303



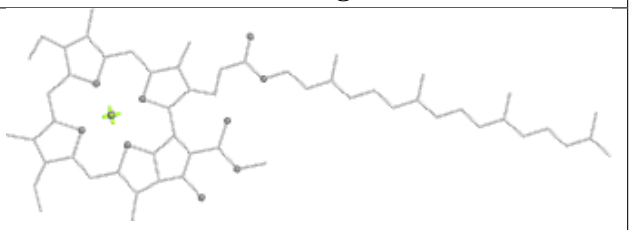
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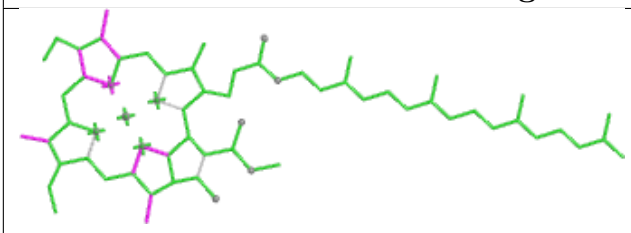


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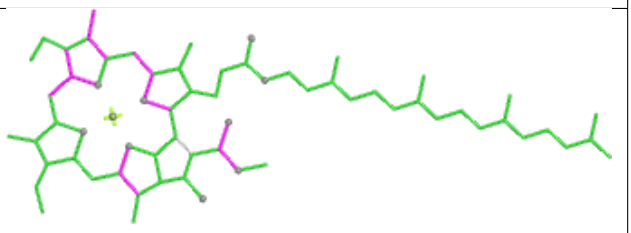


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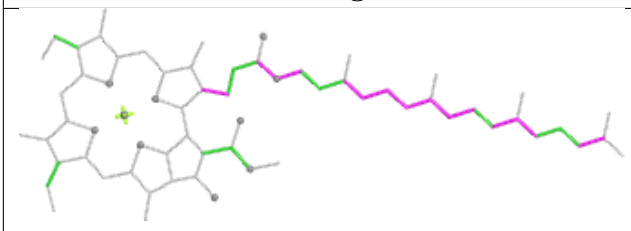
Ligand CLA b6 613



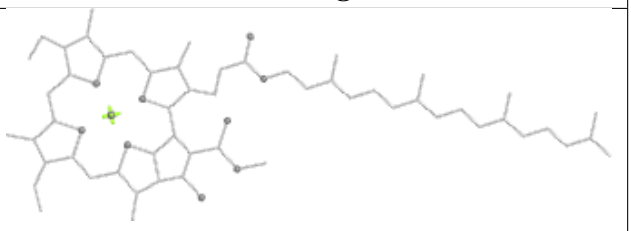
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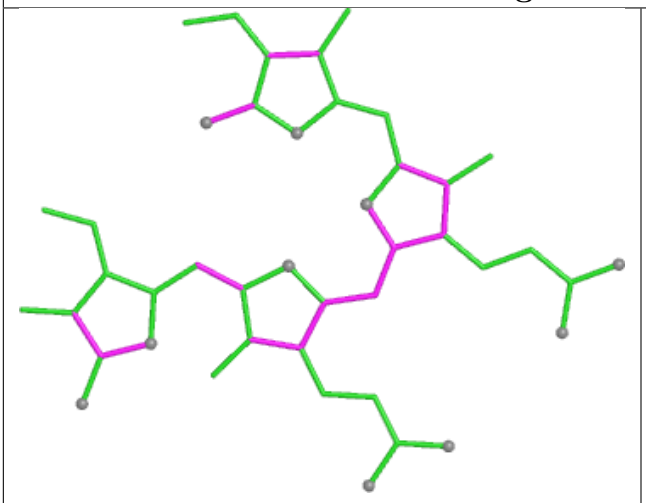


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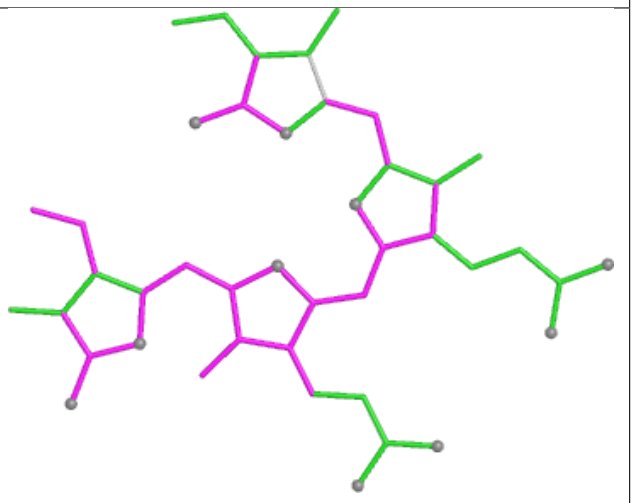


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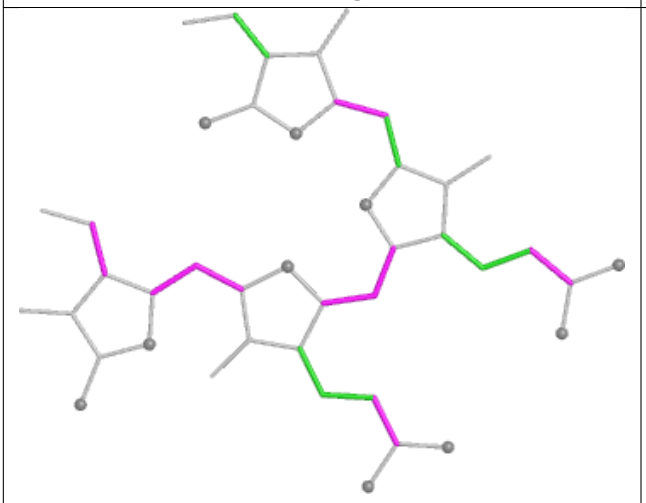
Ligand PEB A9 202



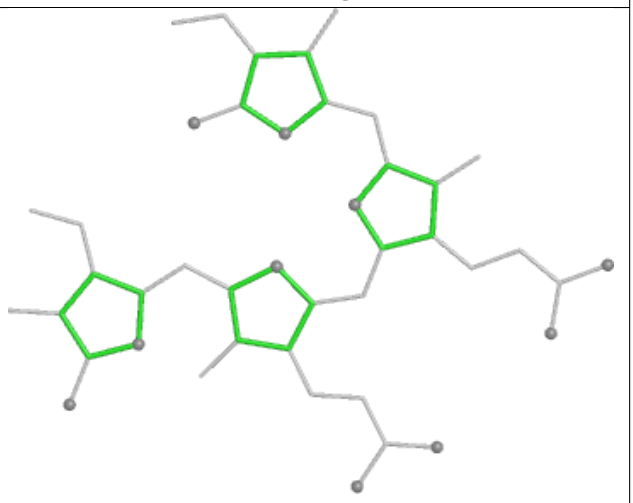
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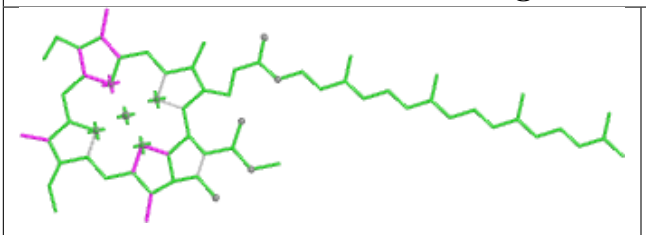


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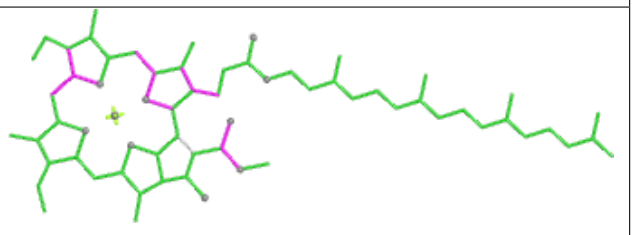


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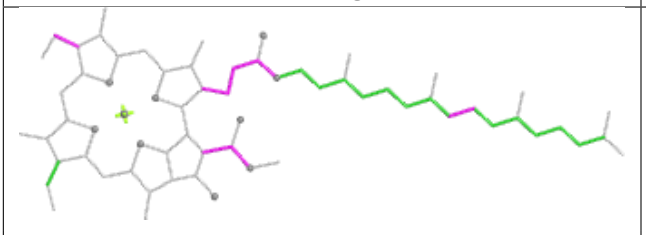
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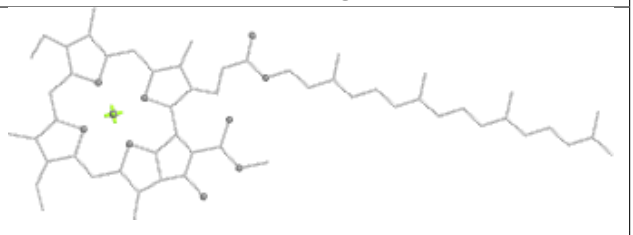
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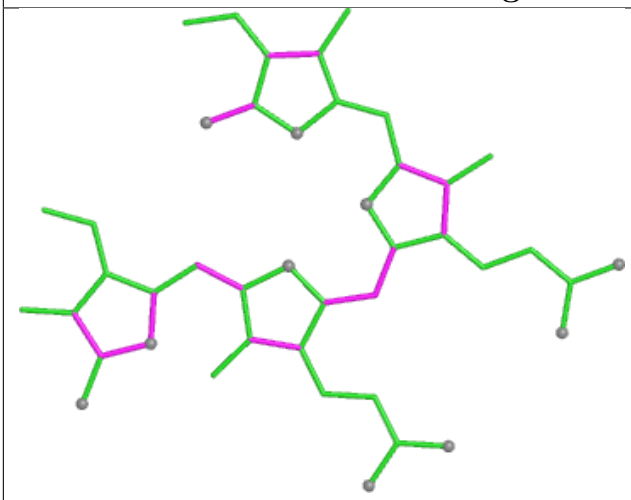


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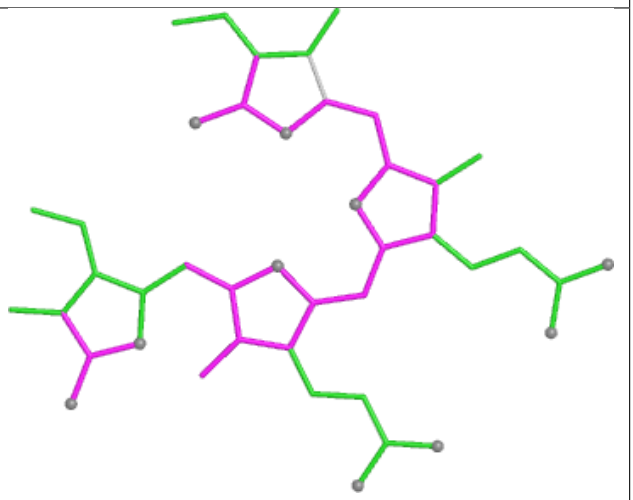


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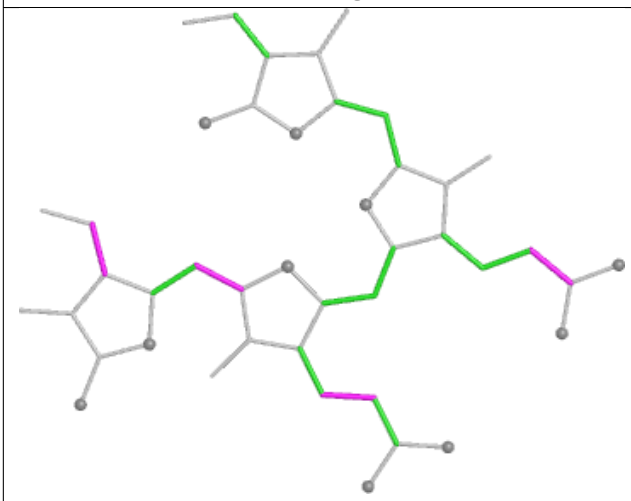
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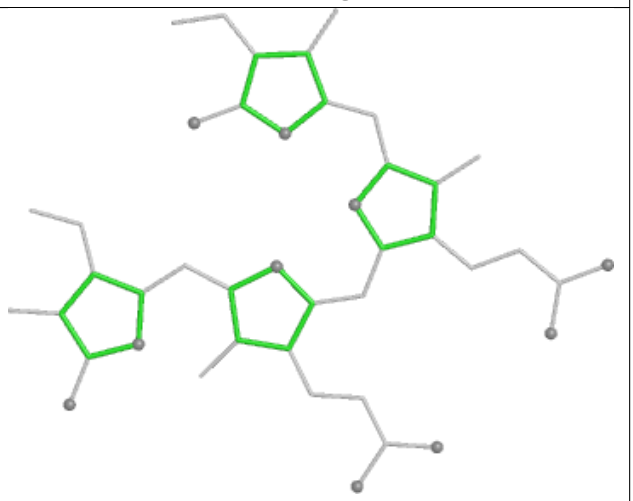
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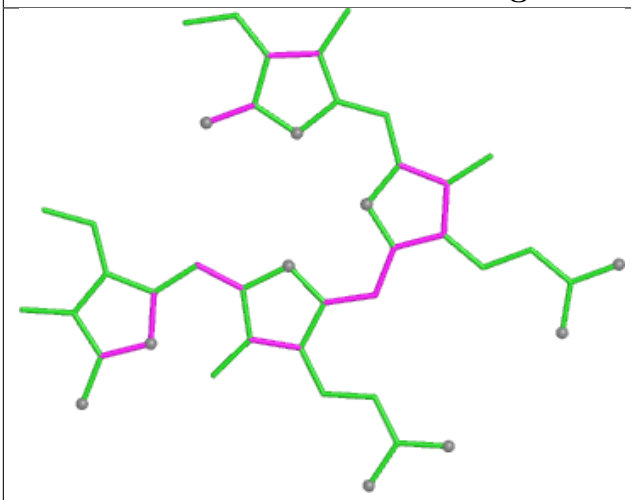


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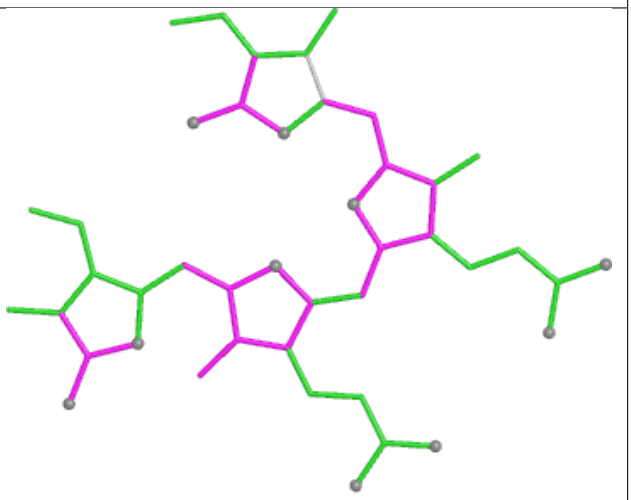


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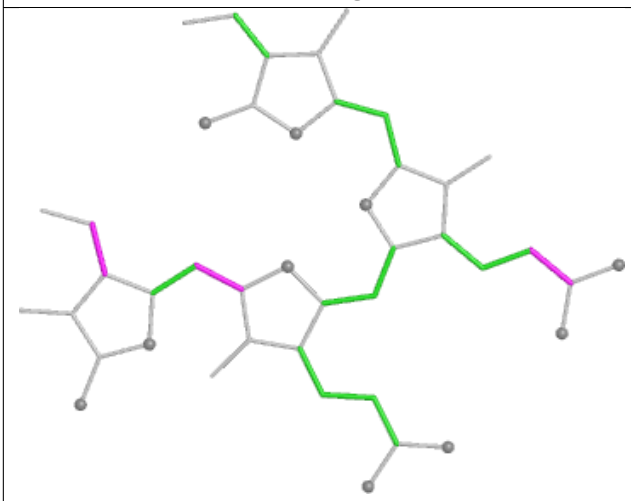
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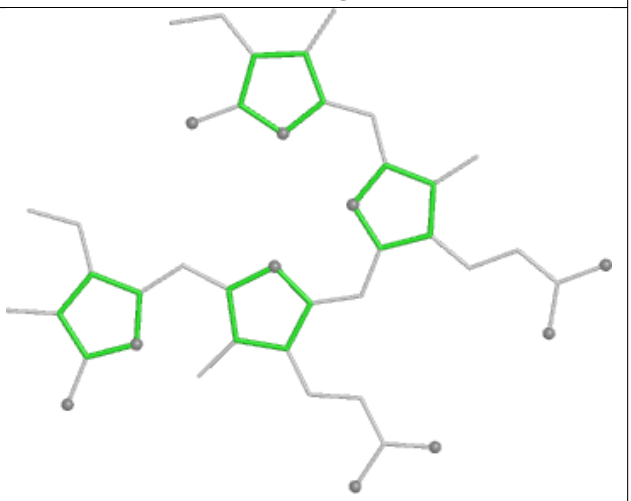
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Bond angles

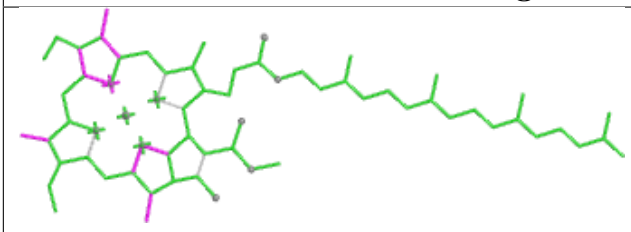


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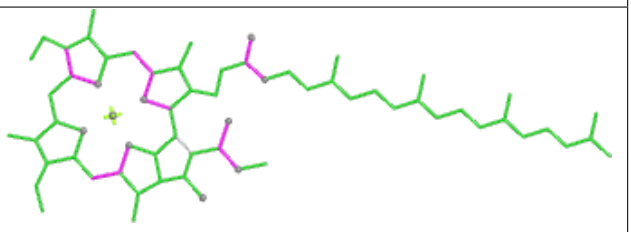


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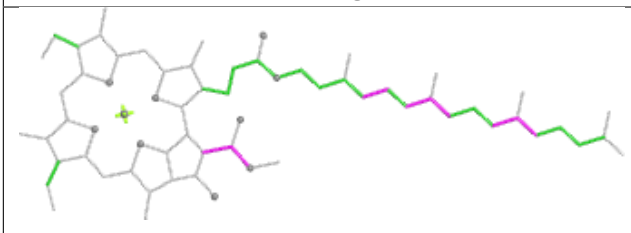
Ligand CLA C6 512



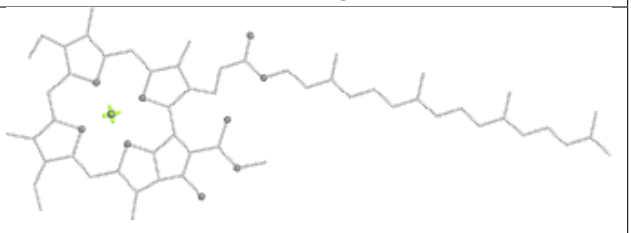
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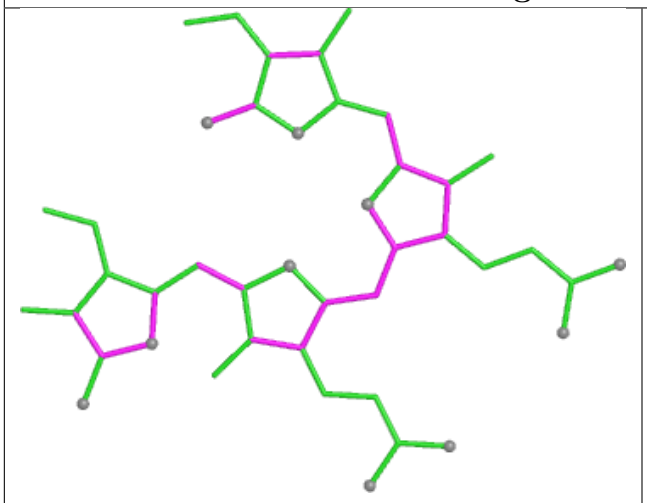


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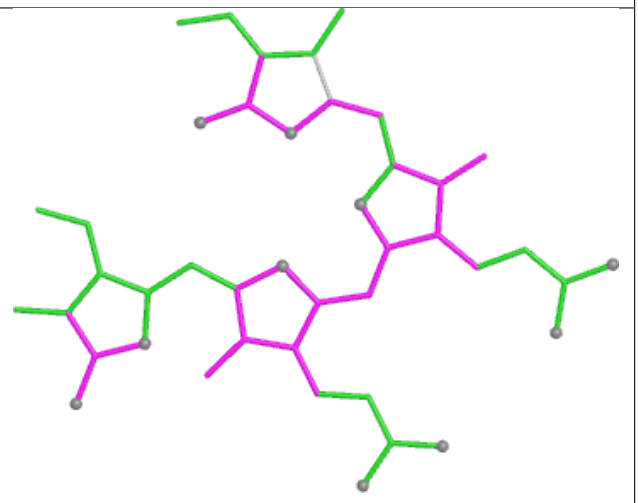


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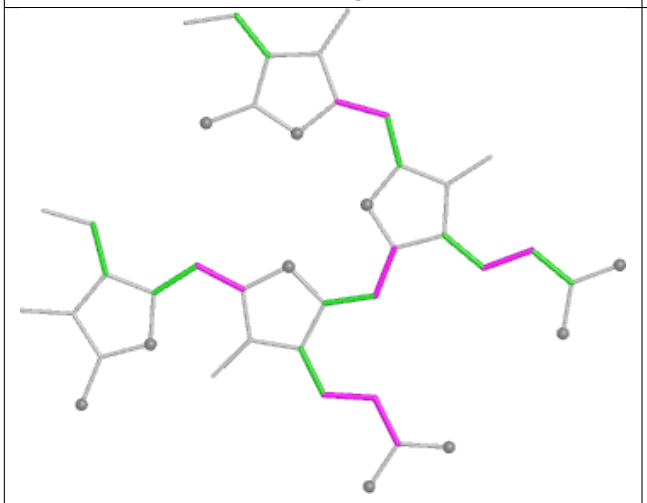
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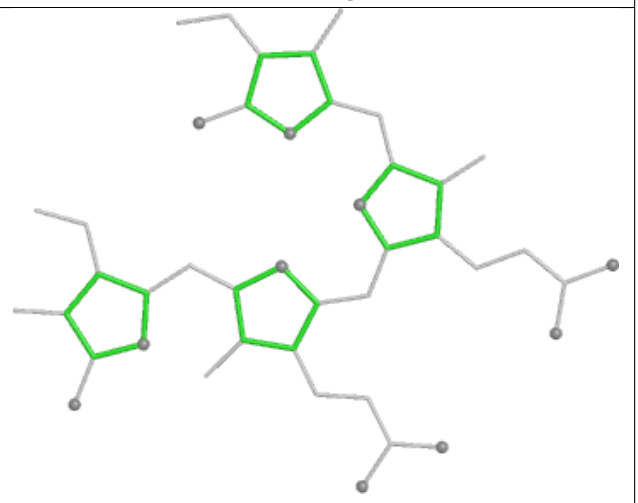
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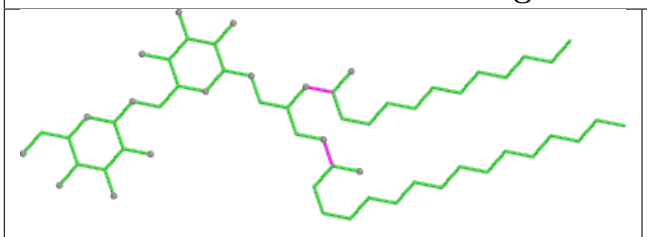


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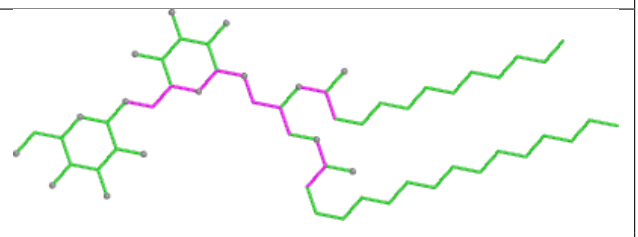


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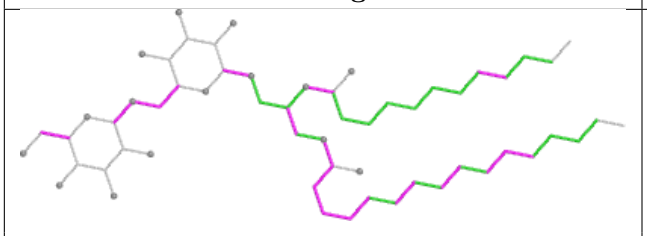
Ligand DGD L6 102



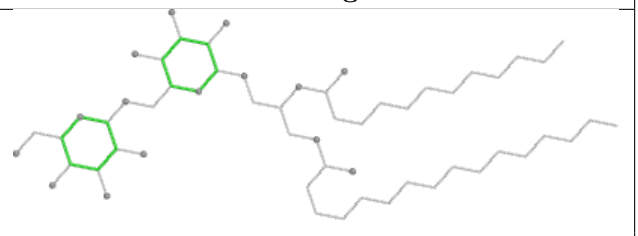
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Bond angles

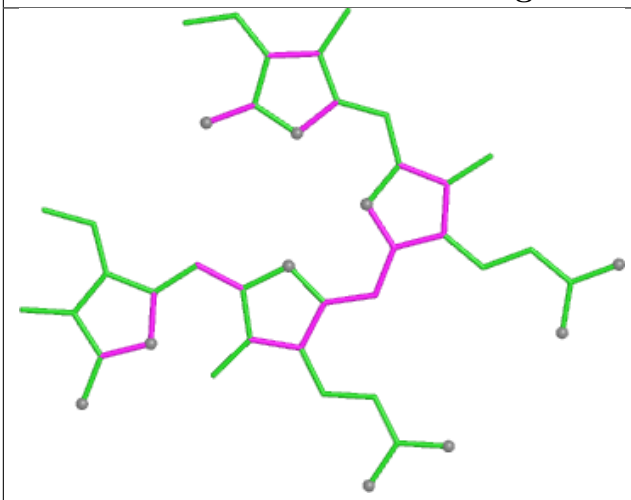


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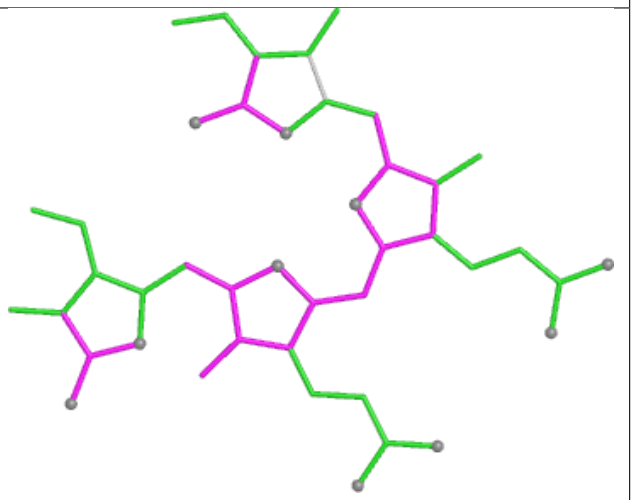


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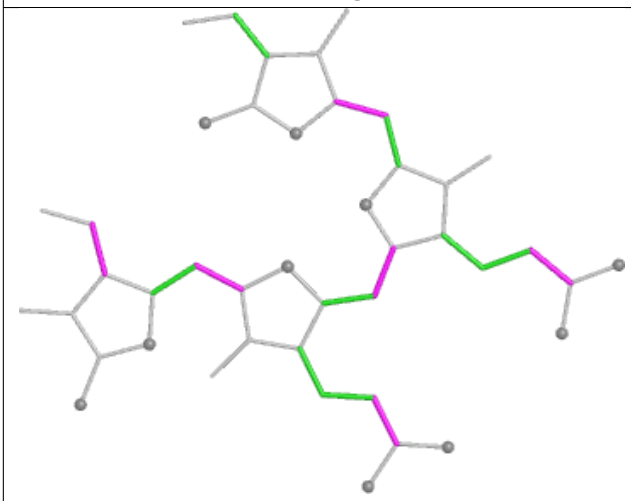
Ligand PEB A1 305



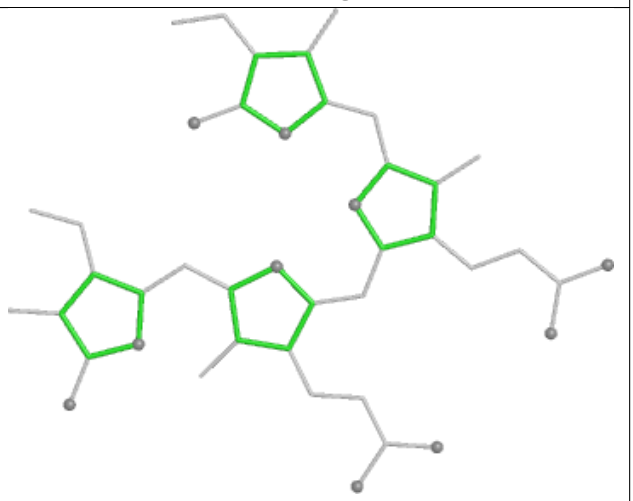
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Bond angles

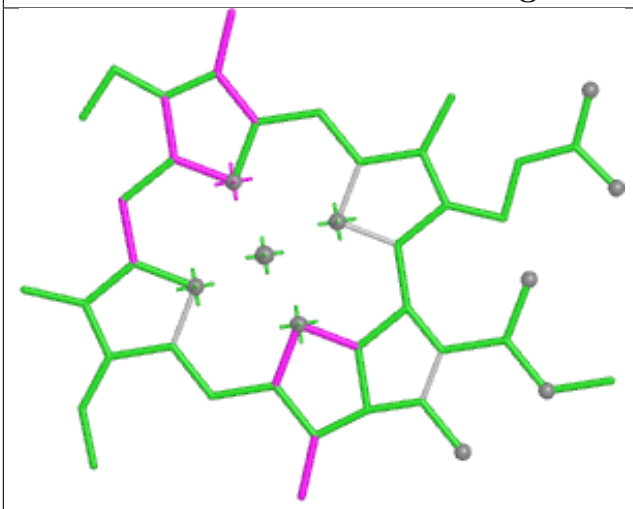


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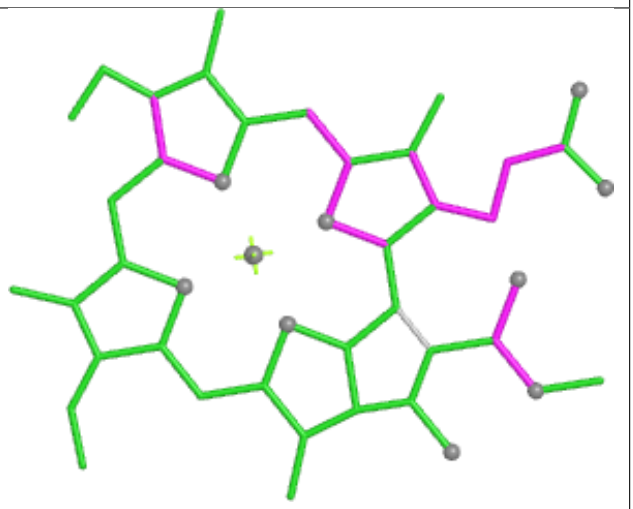


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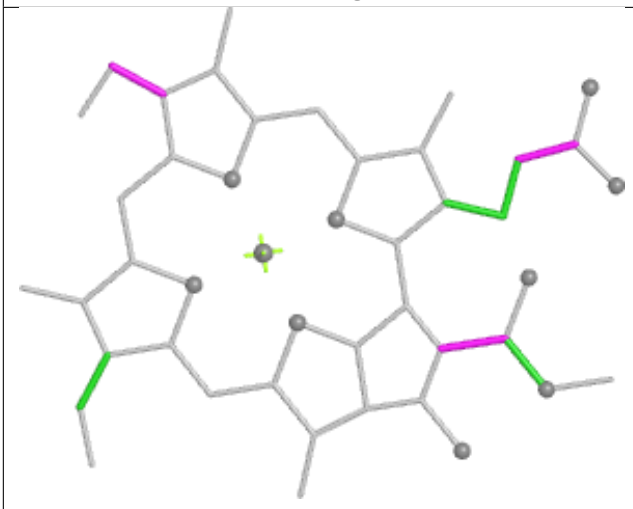
Ligand CLA 52 605



Bond lengths



Bond angles

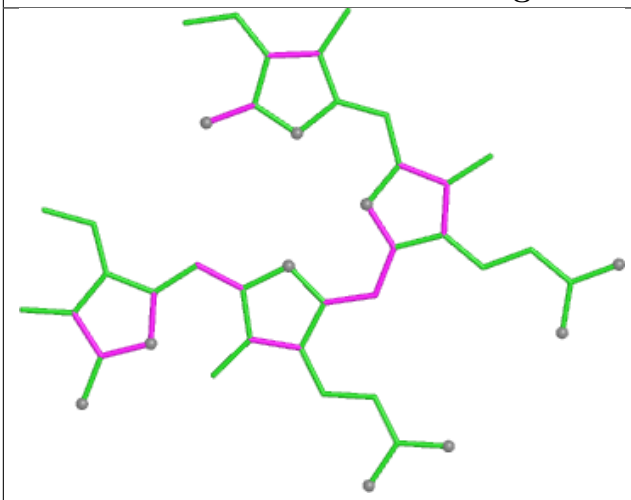


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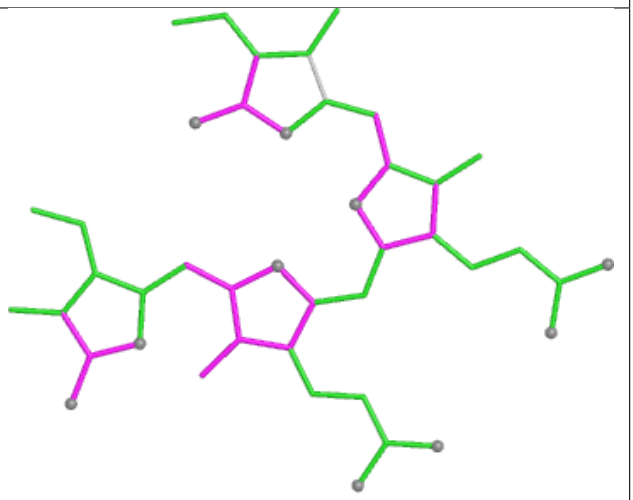


Rings

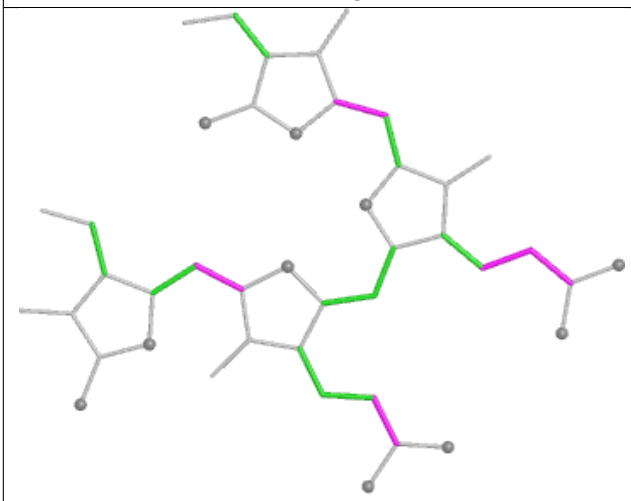
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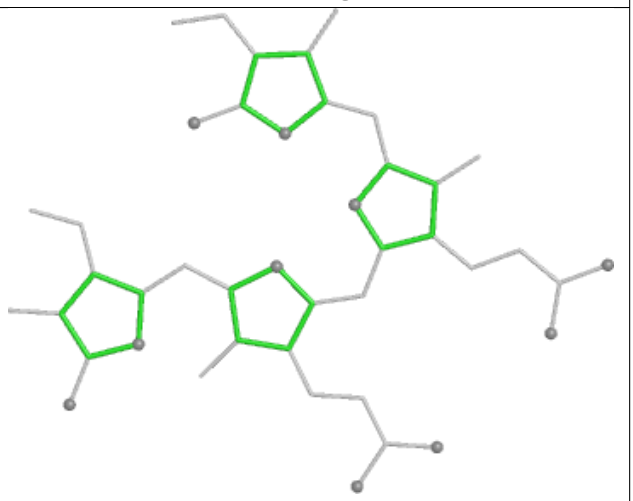
Bond lengths



Bond angles

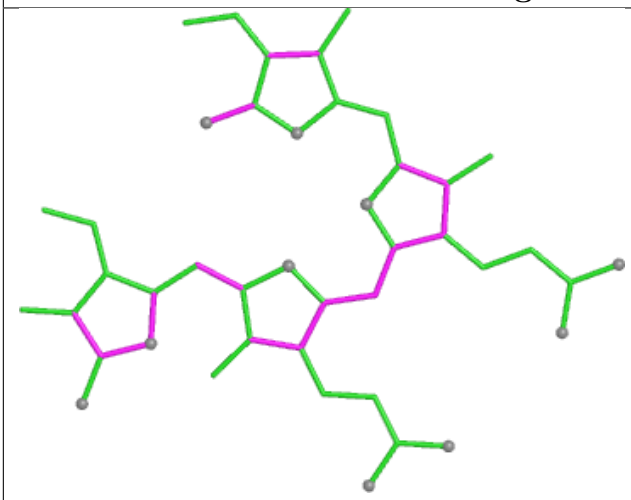


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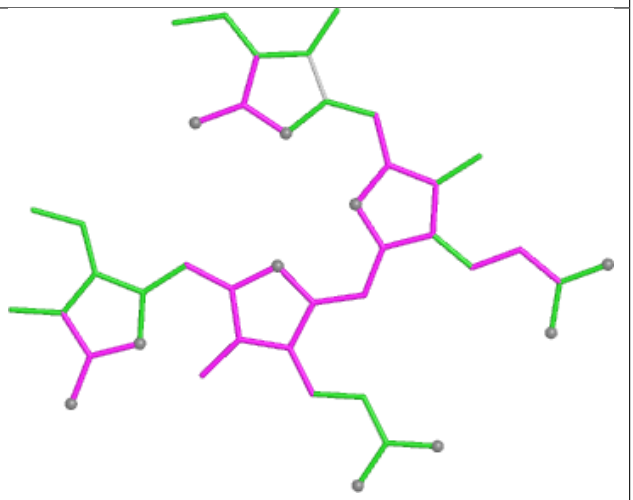


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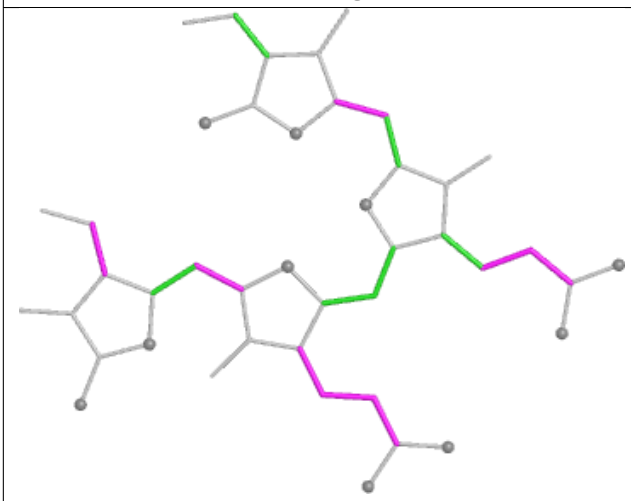
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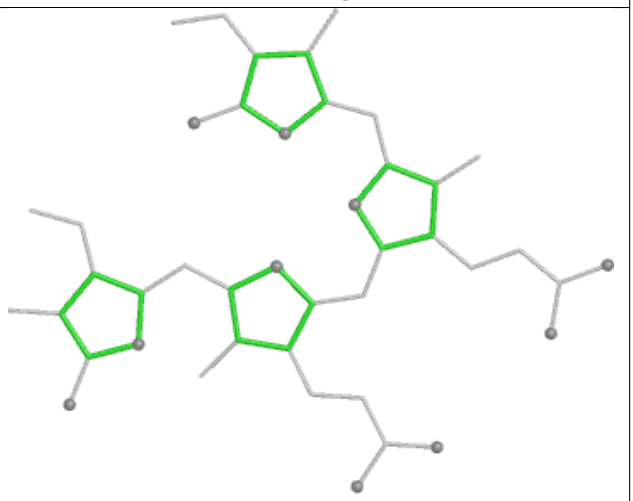
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Bond angles

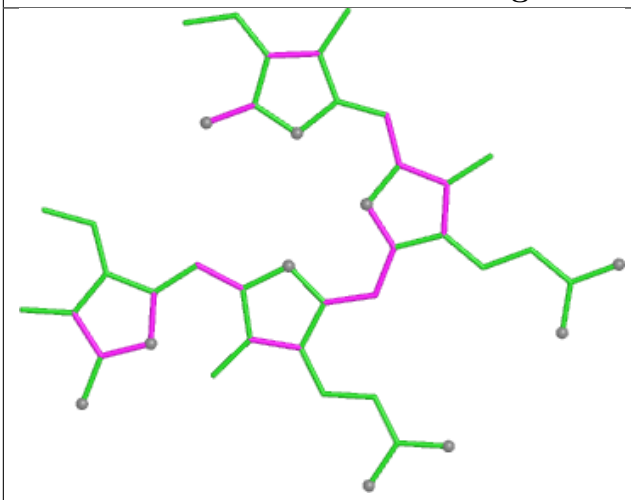


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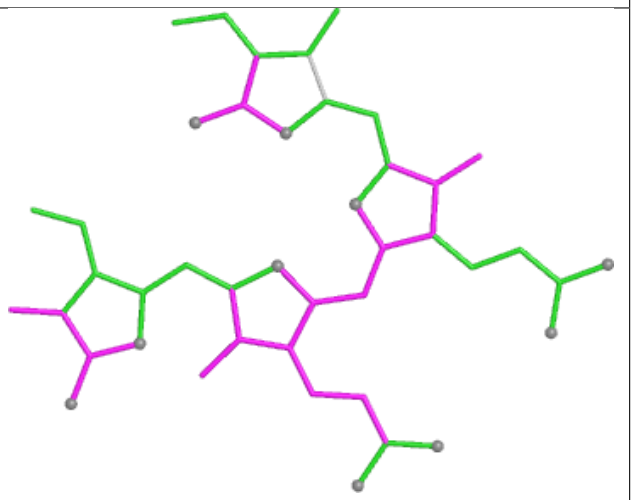


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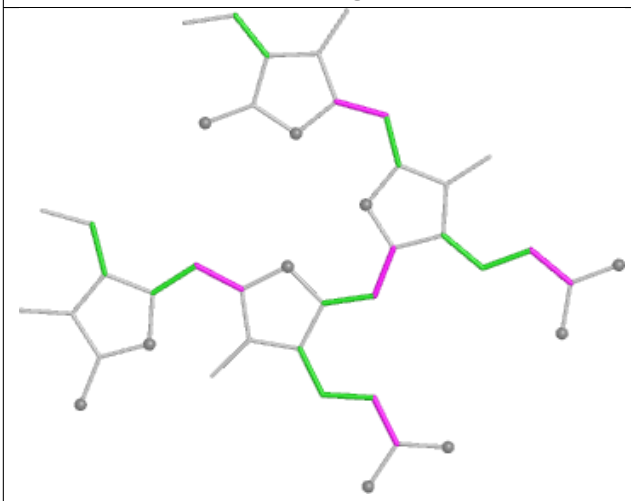
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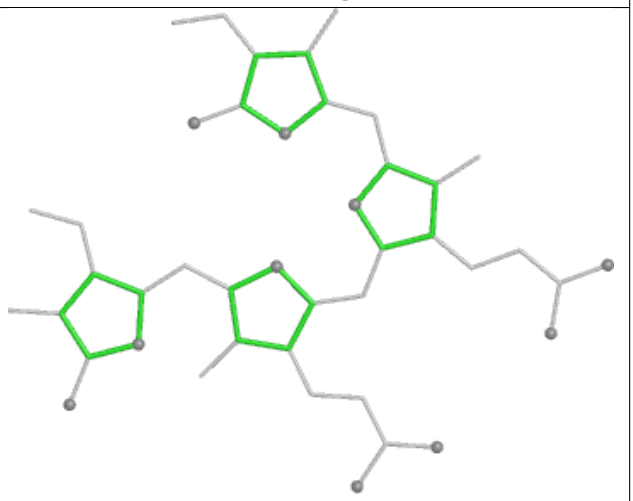
Bond lengths



Bond angles

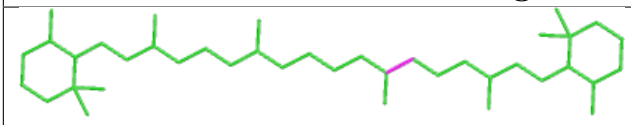


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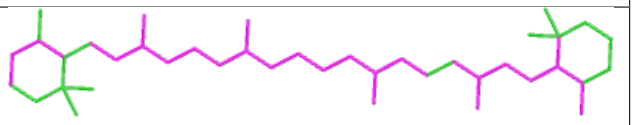


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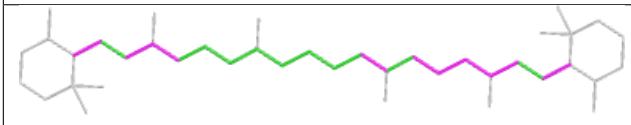
Ligand BCR A2 848



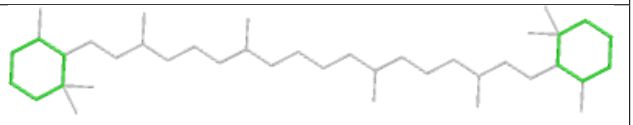
Bond lengths



Bond angles

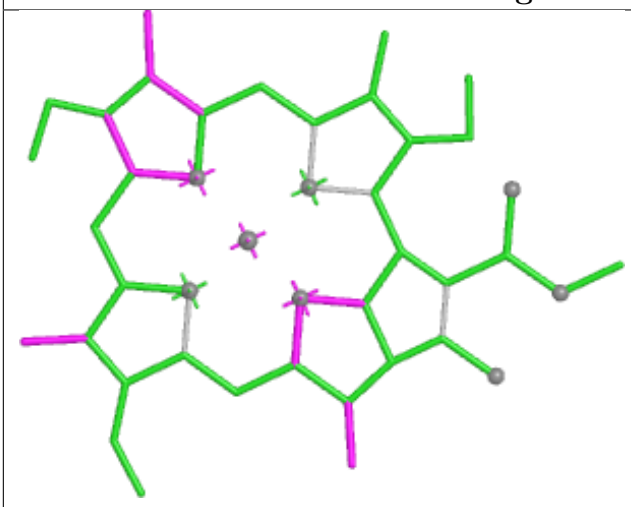


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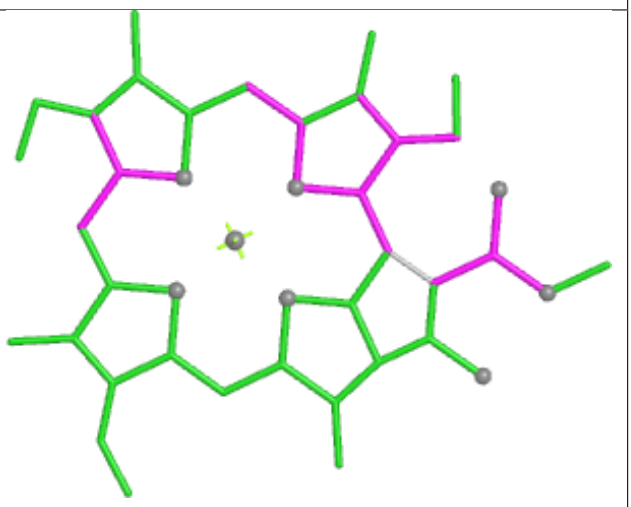


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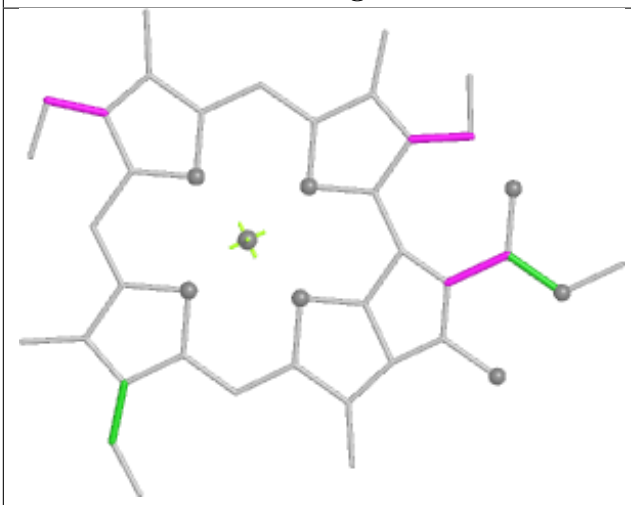
Ligand CLA B2 814



Bond lengths



Bond angles

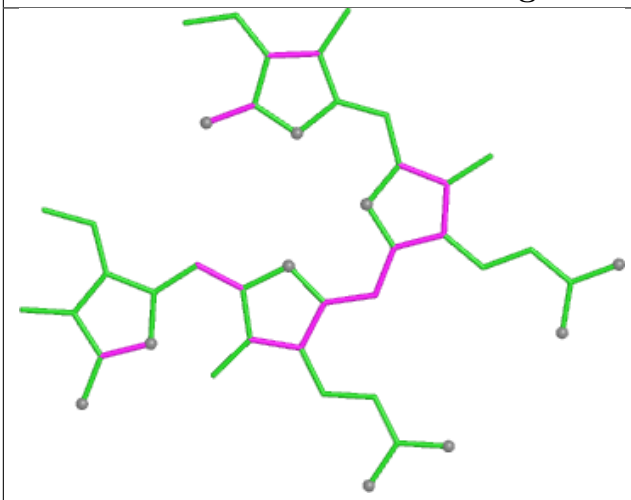


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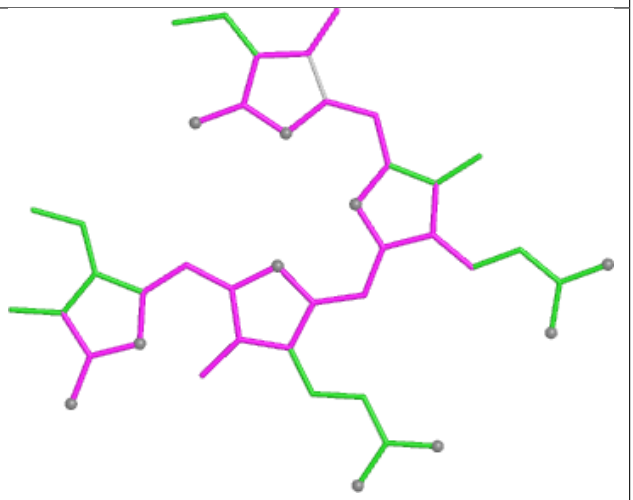


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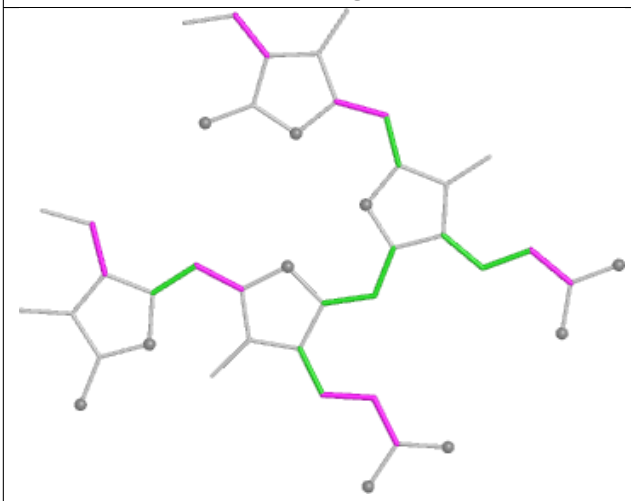
Ligand PEB b1 202



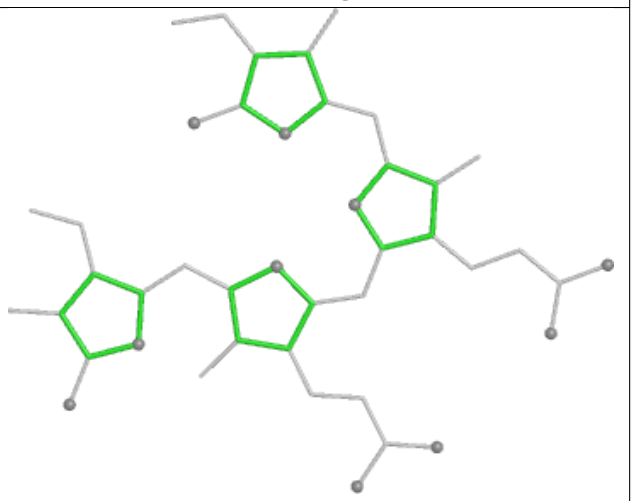
Bond lengths



Bond angles

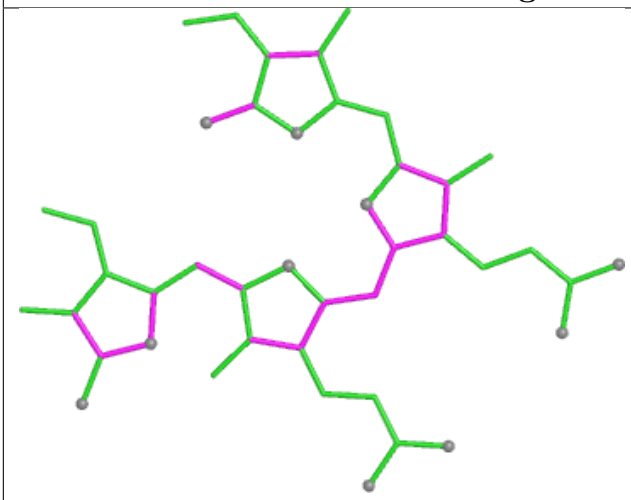


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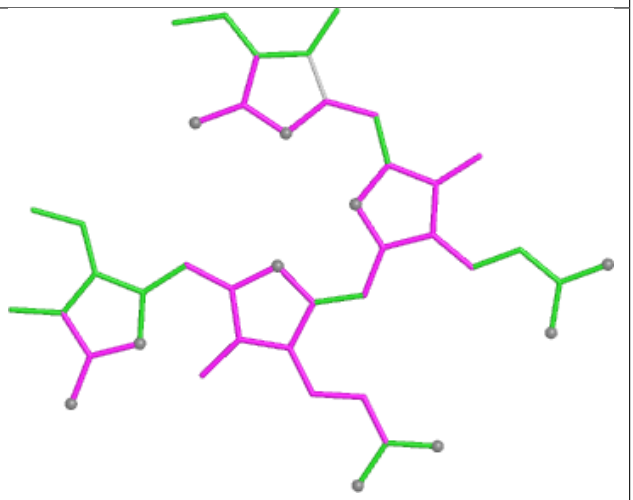


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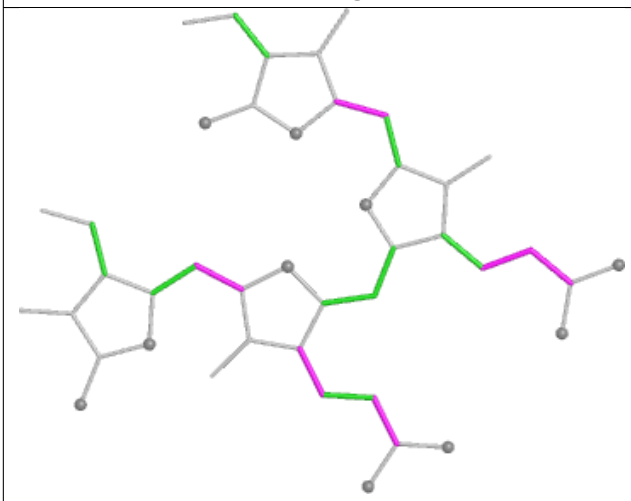
Ligand PEB S5 201



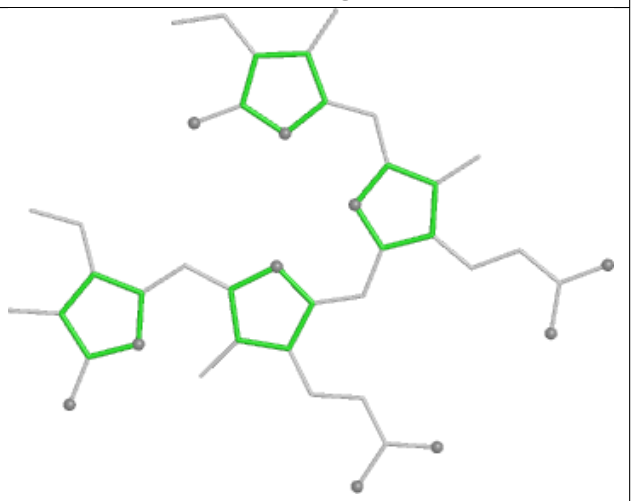
Bond lengths



Bond angles

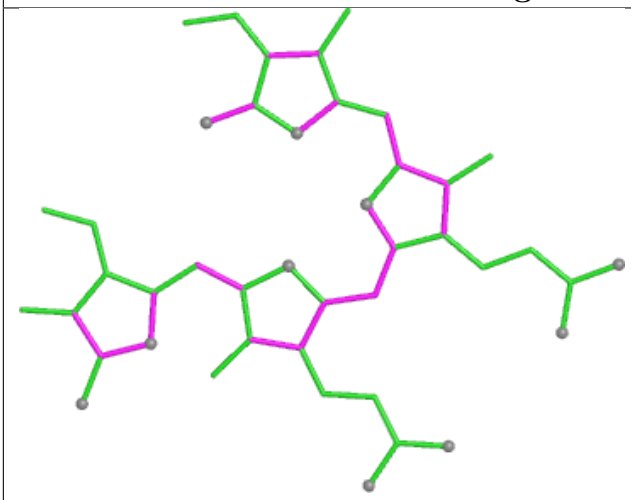


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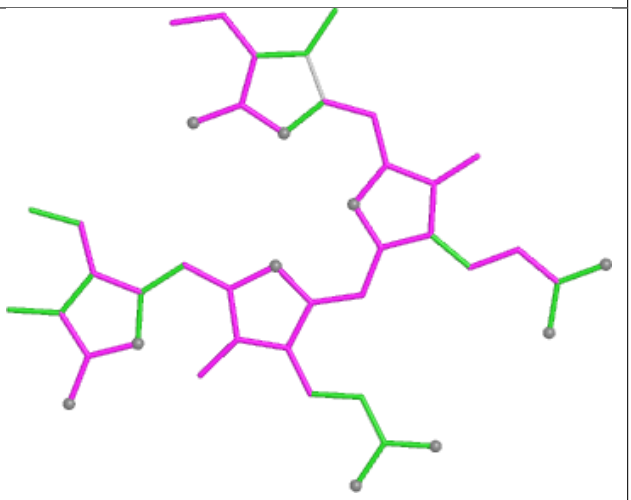


Rings

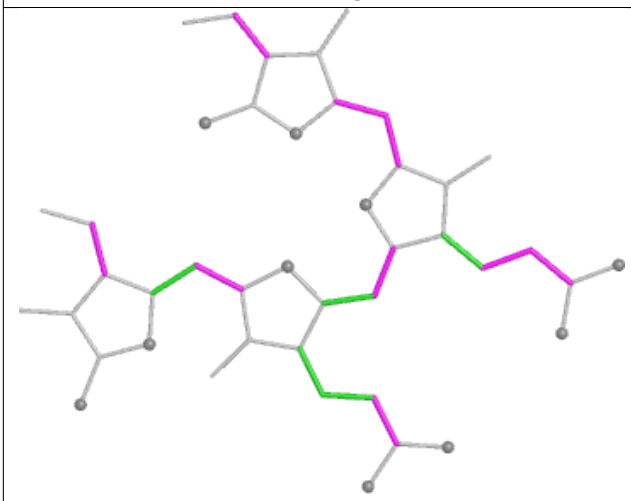
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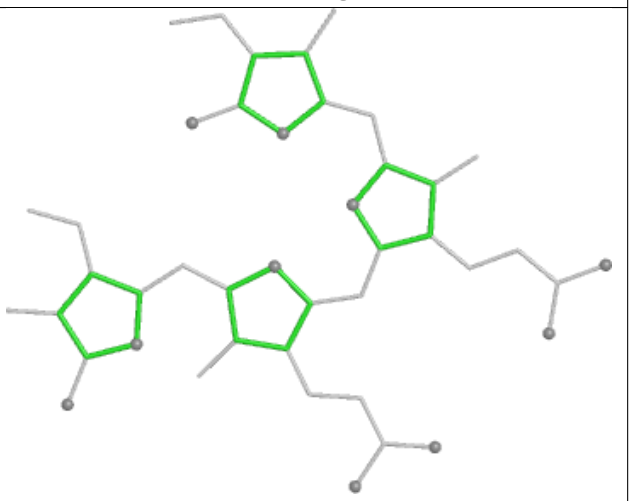
Bond lengths



Bond angles

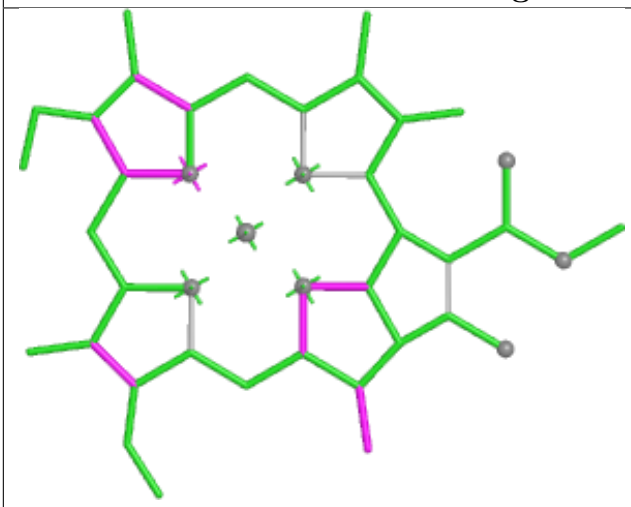


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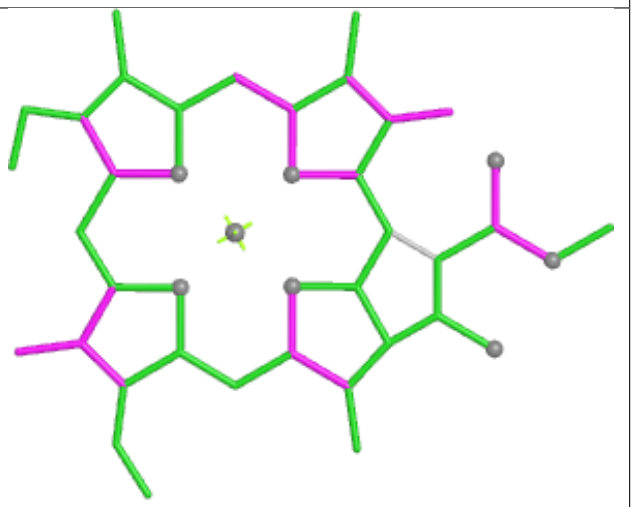


Rings

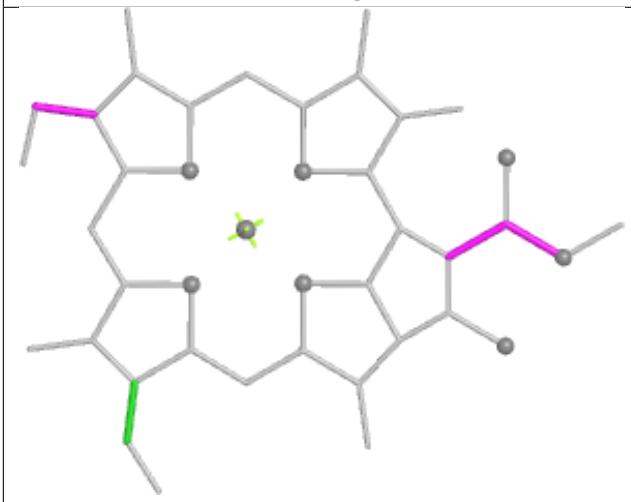
Ligand CLA FN 201



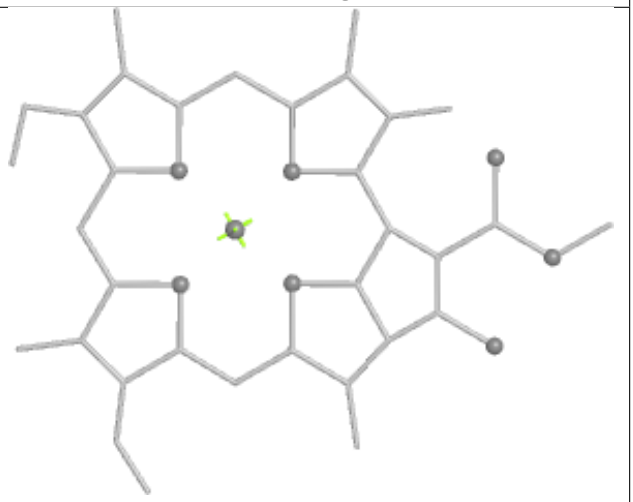
Bond lengths



Bond angles

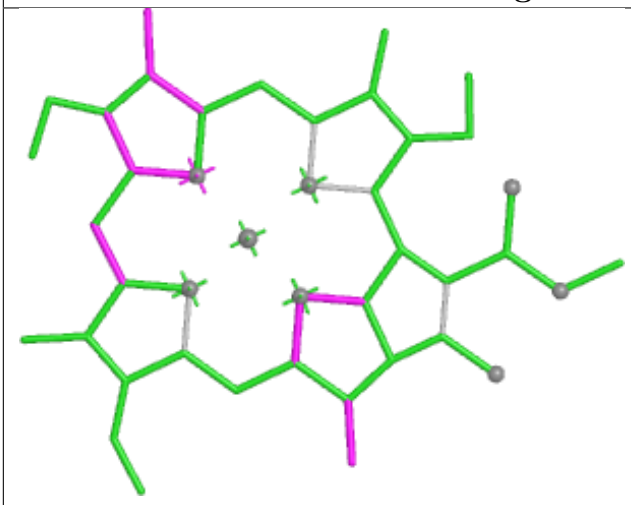


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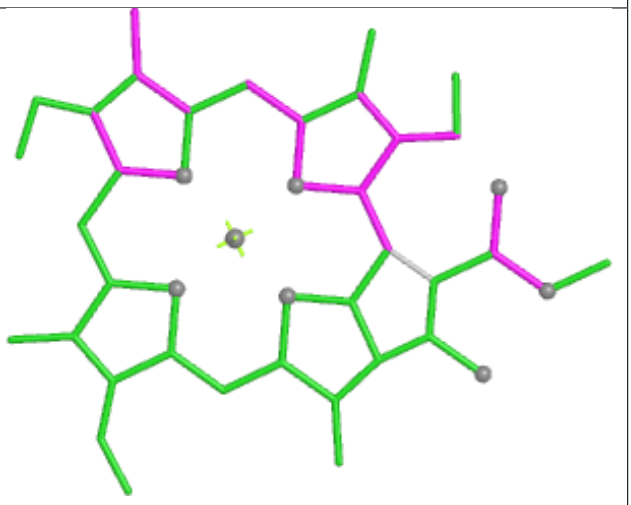


Rings

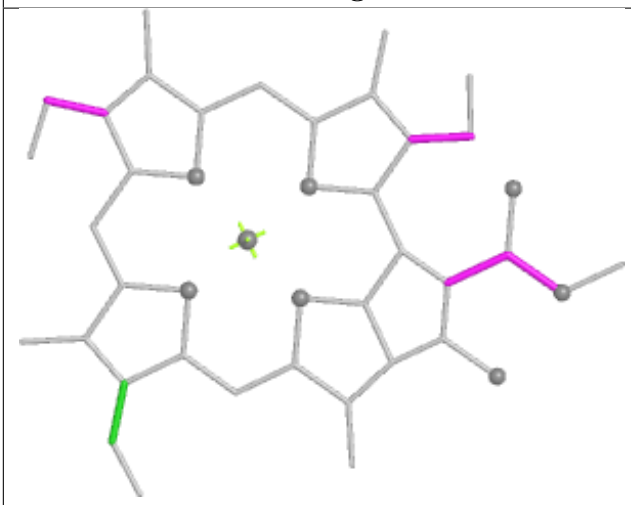
Ligand CLA 2N 311



Bond lengths



Bond angles

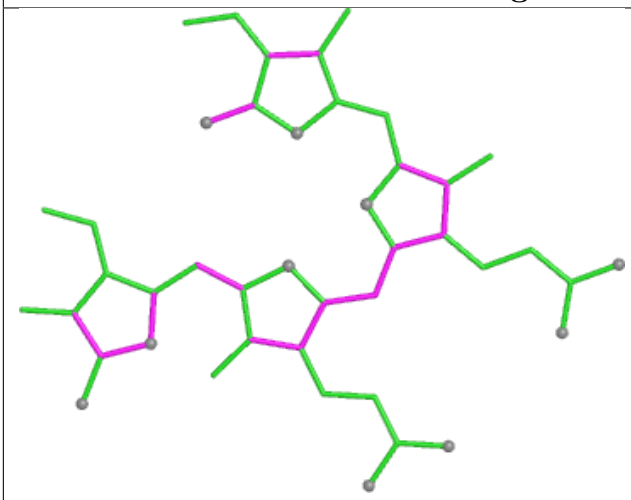


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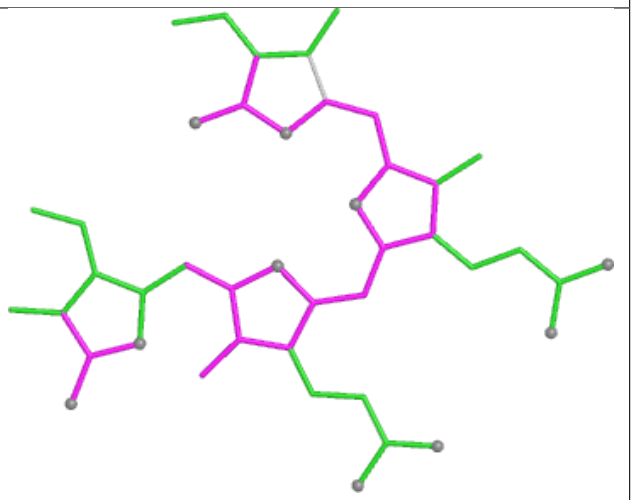


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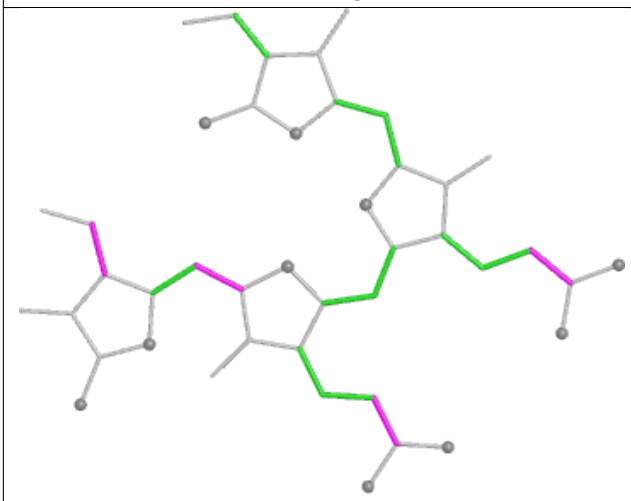
Ligand PEB hM 201



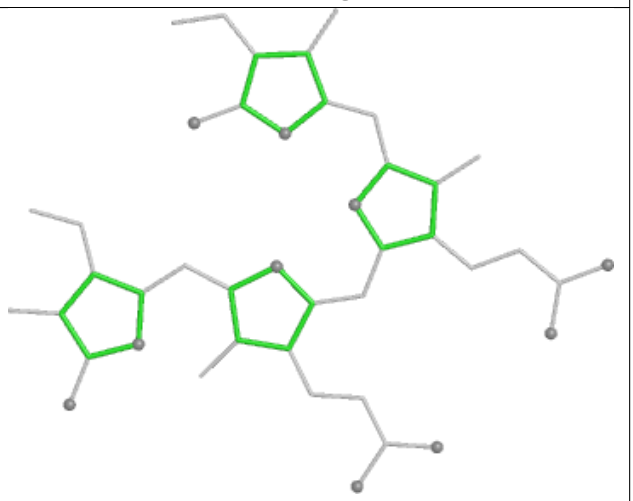
Bond lengths



Bond angles

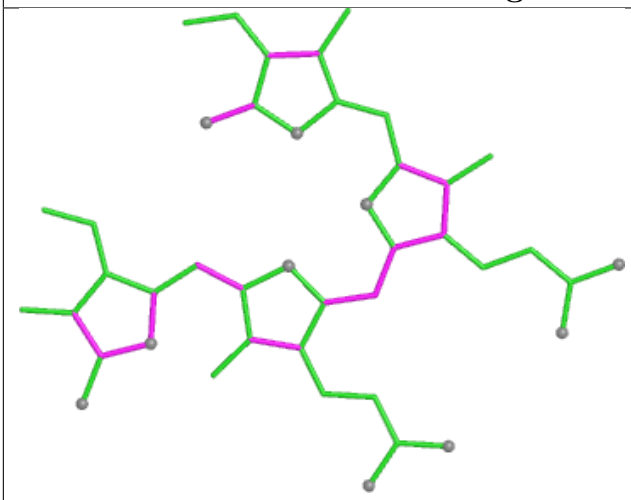


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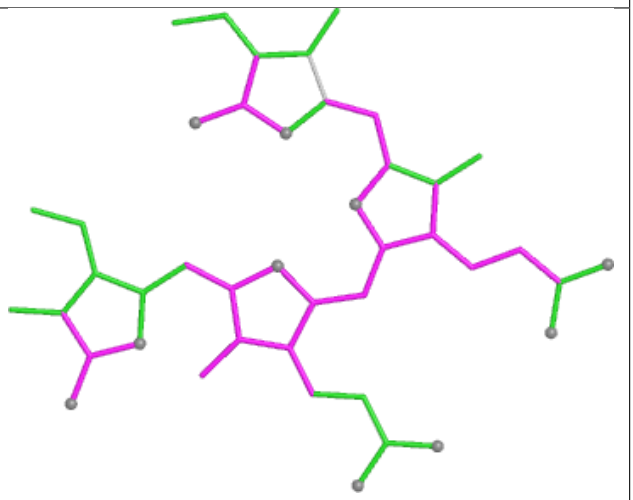


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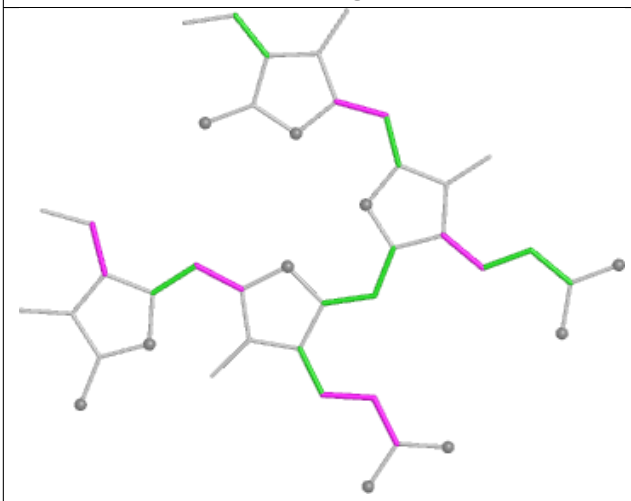
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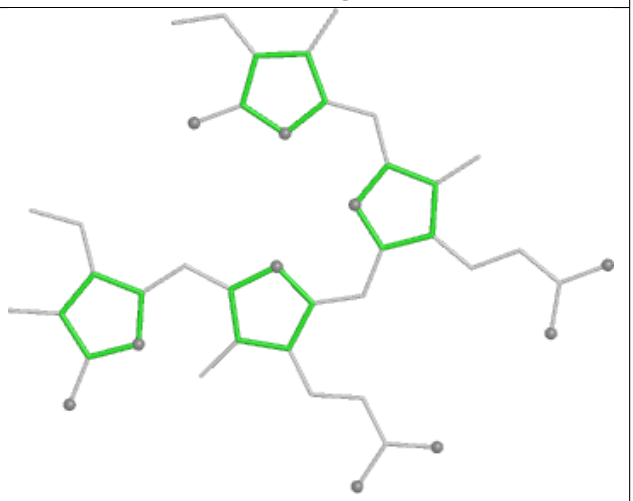
Bond lengths



Bond angles

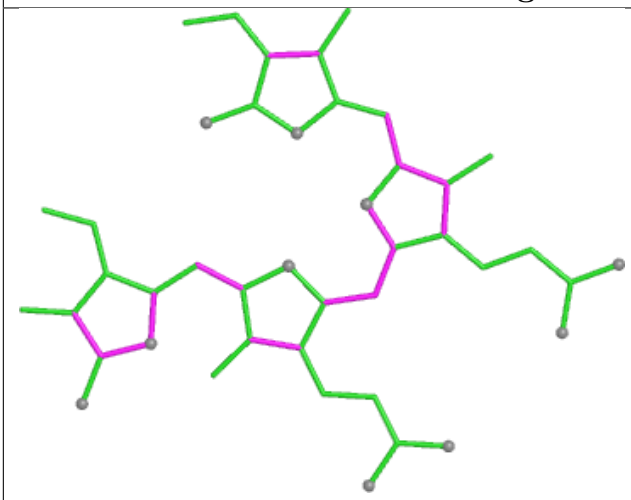


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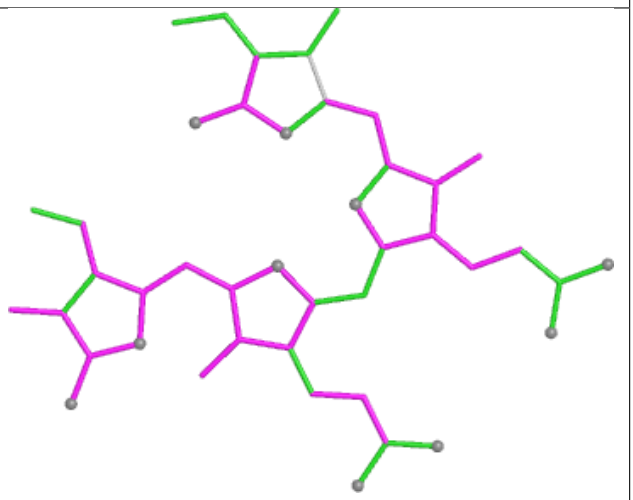


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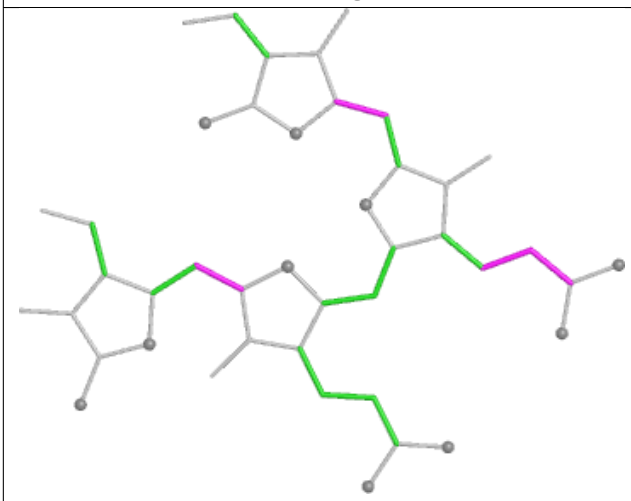
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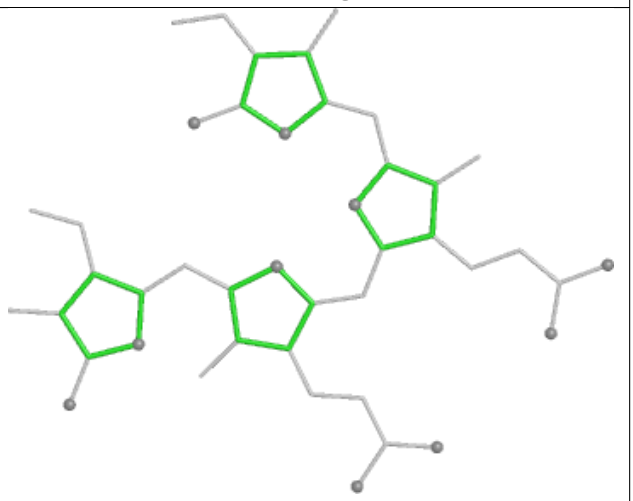
Bond lengths



Bond angles

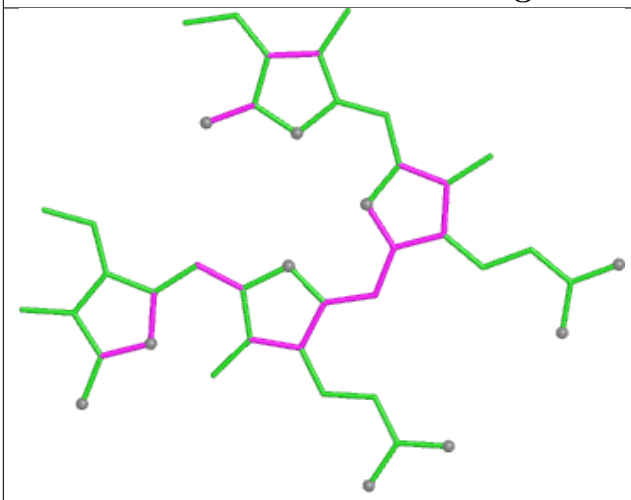


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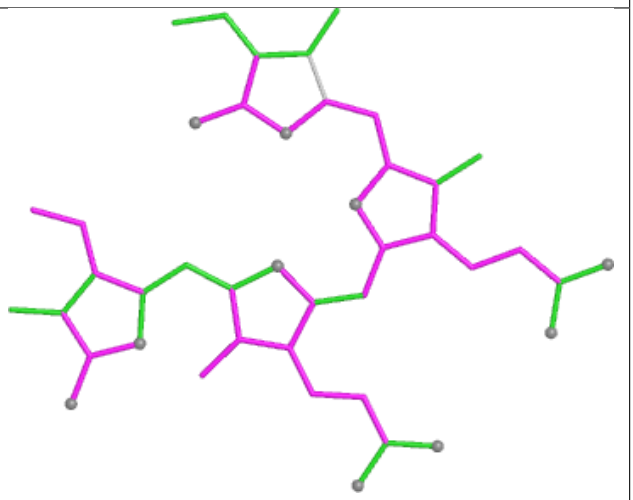


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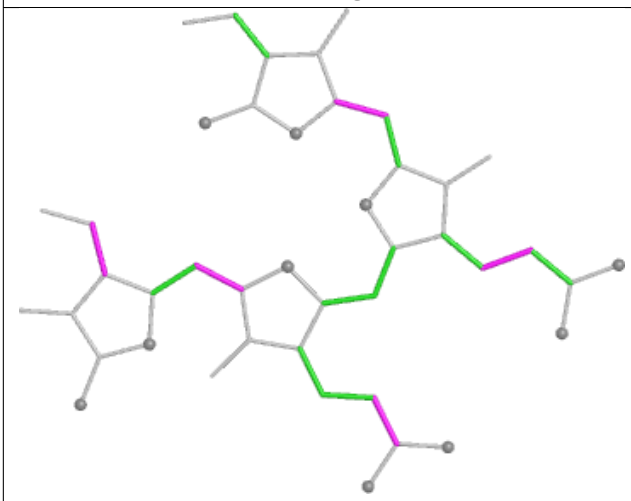
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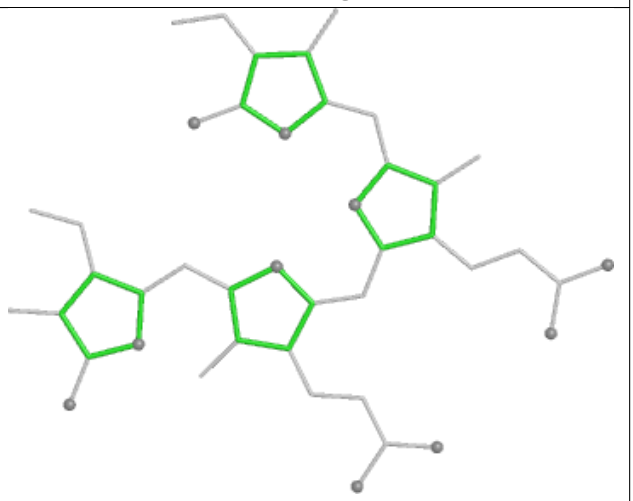
Bond lengths



Bond angles

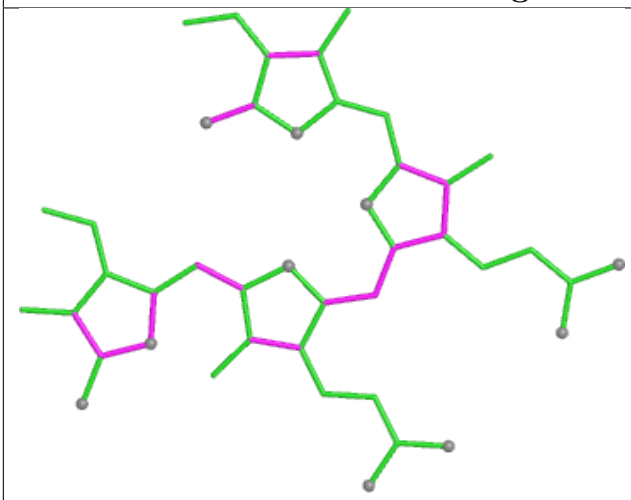


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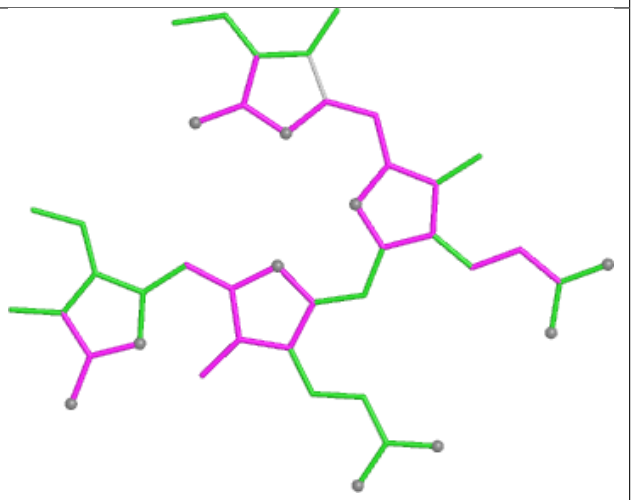


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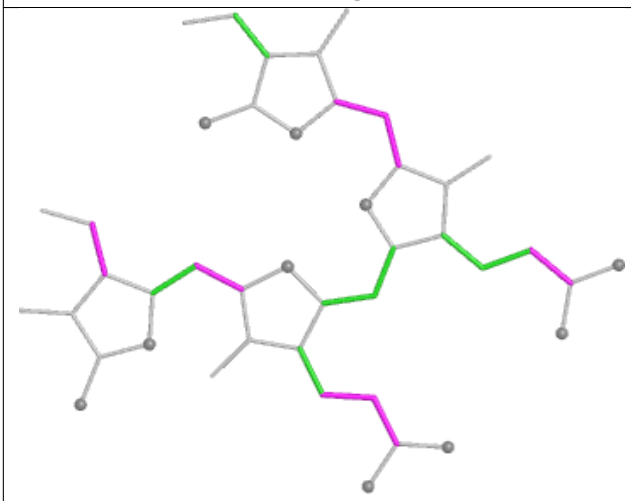
Ligand PEB AO 305



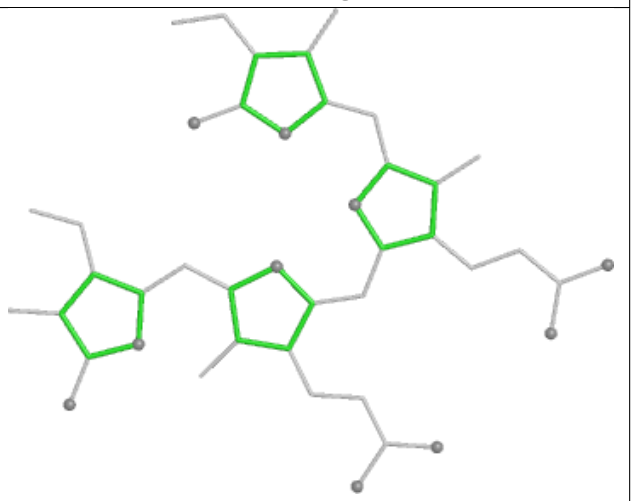
Bond lengths



Bond angles

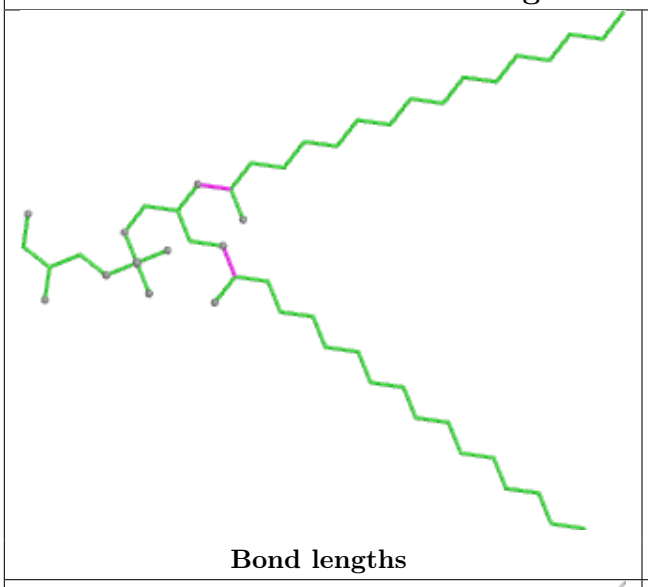


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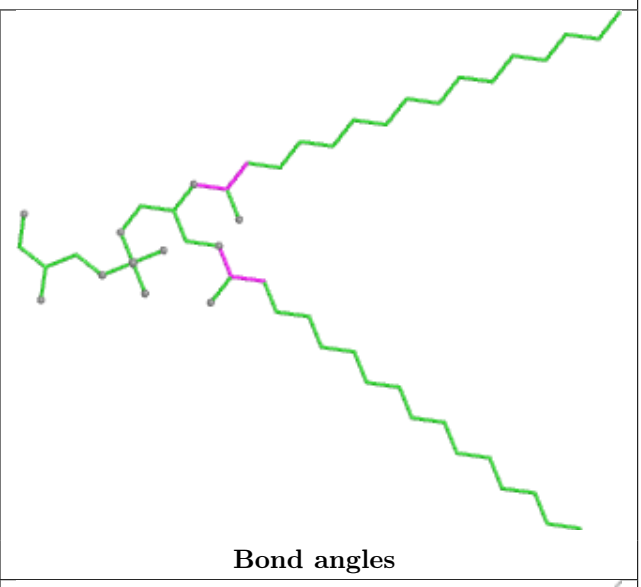


Rings

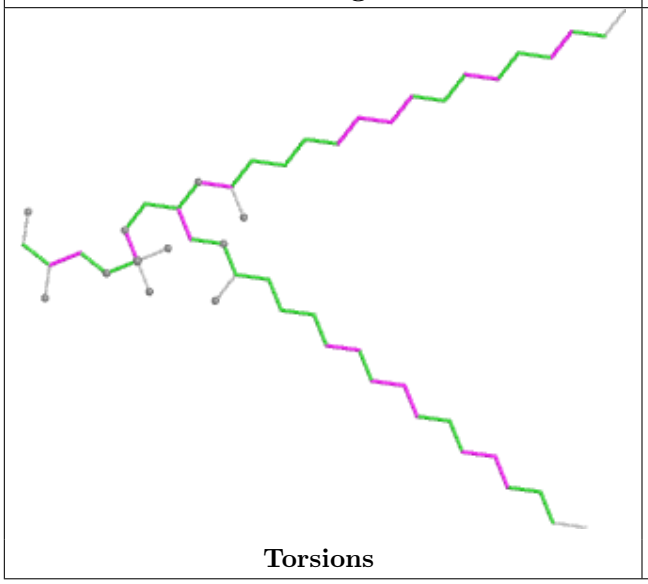
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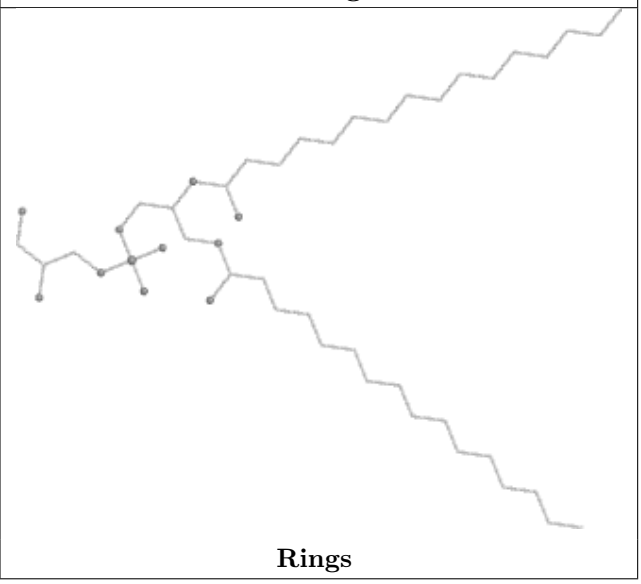
Bond lengths



Bond angles

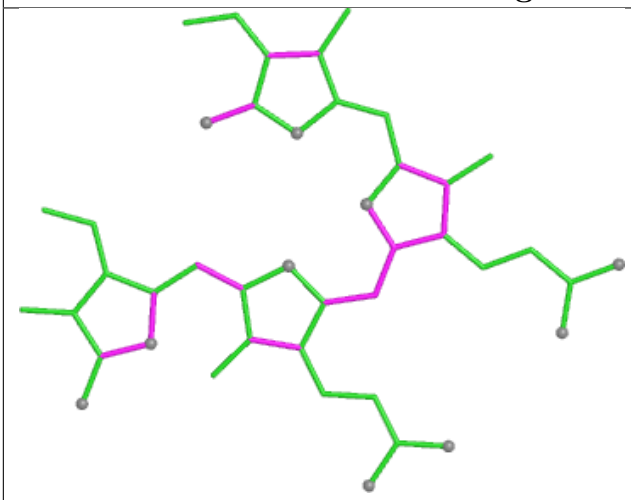


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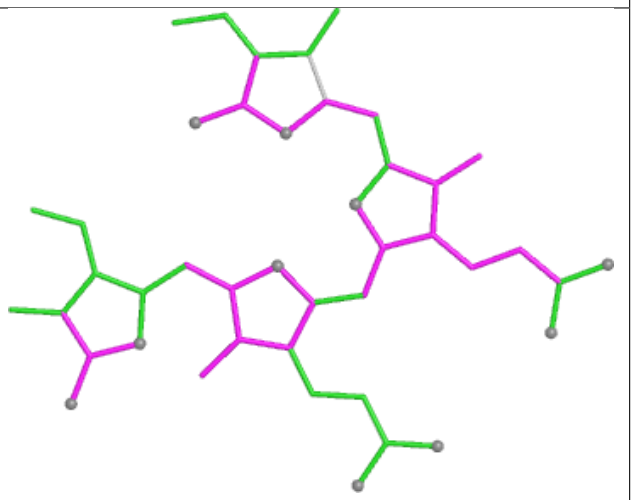


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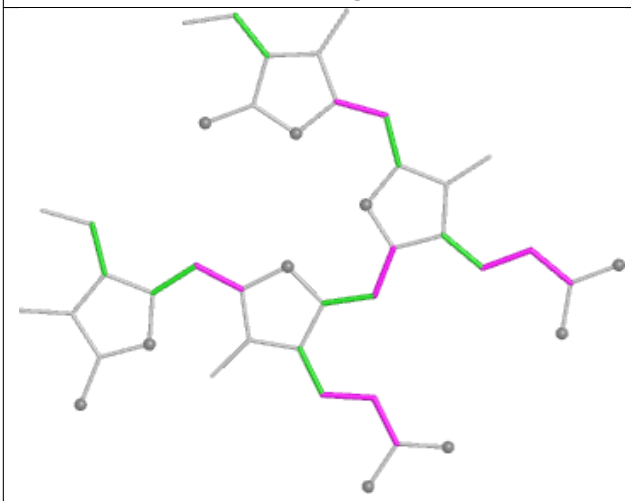
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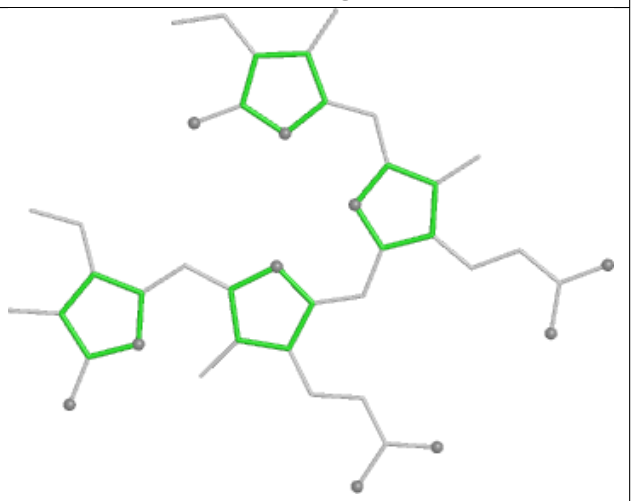
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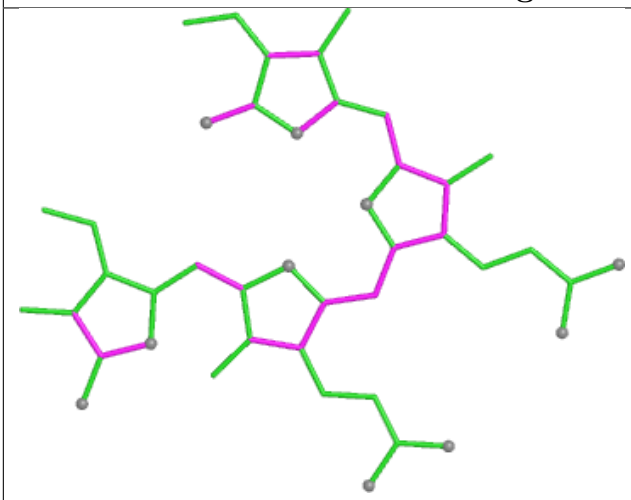


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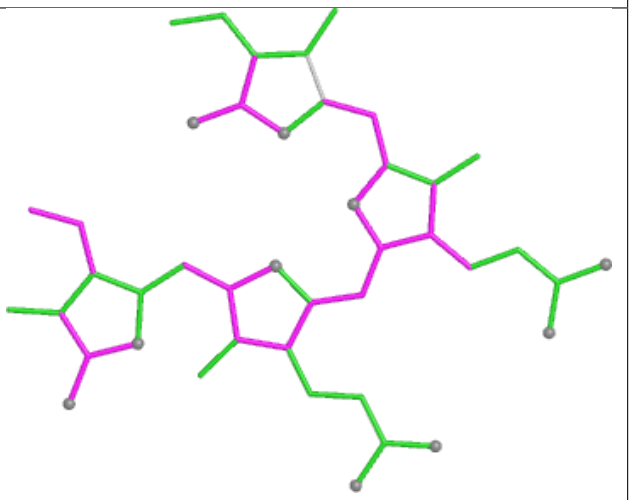


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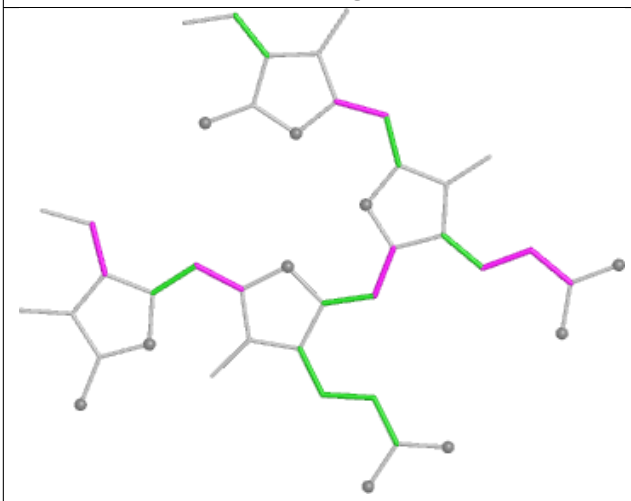
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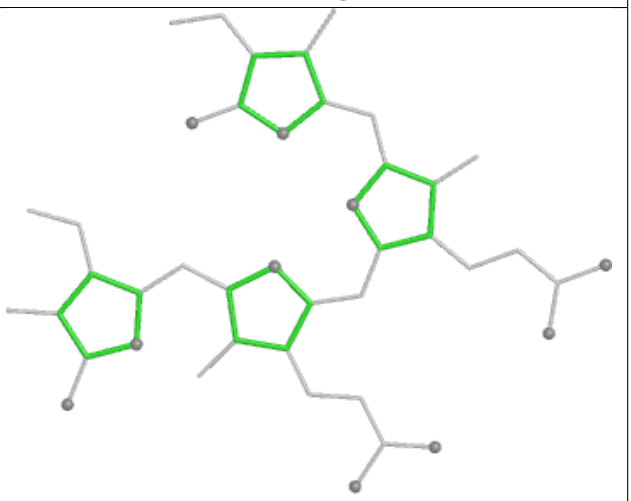
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Bond angles

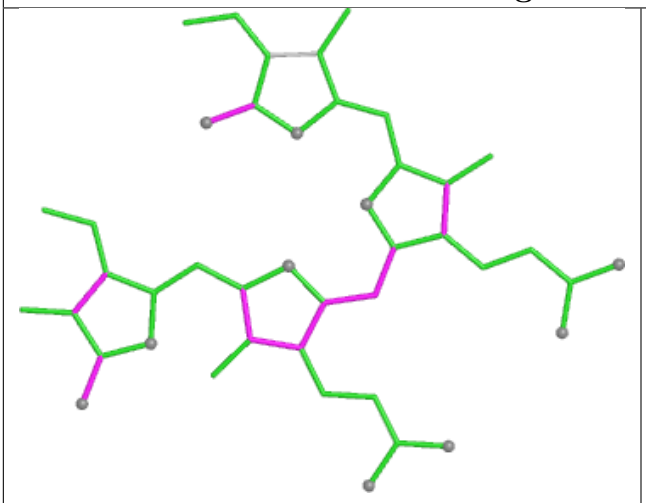


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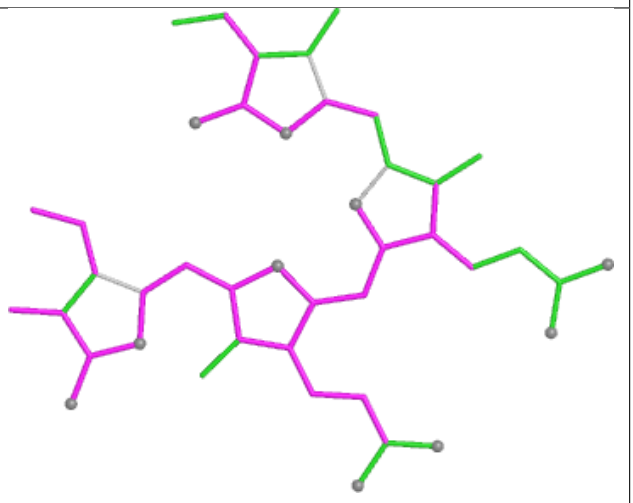


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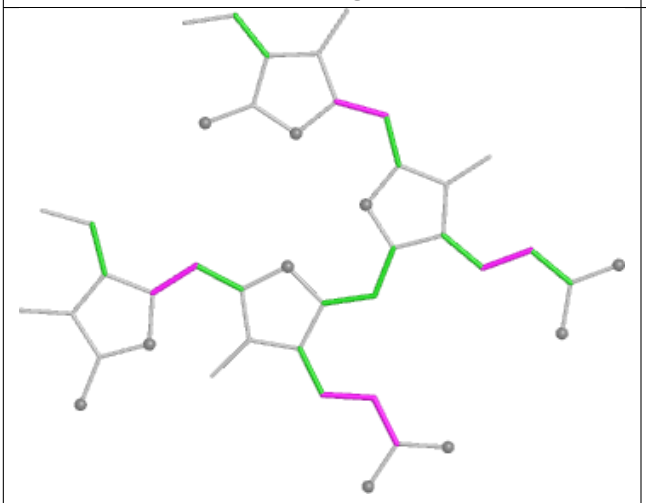
Ligand PUB xF 305



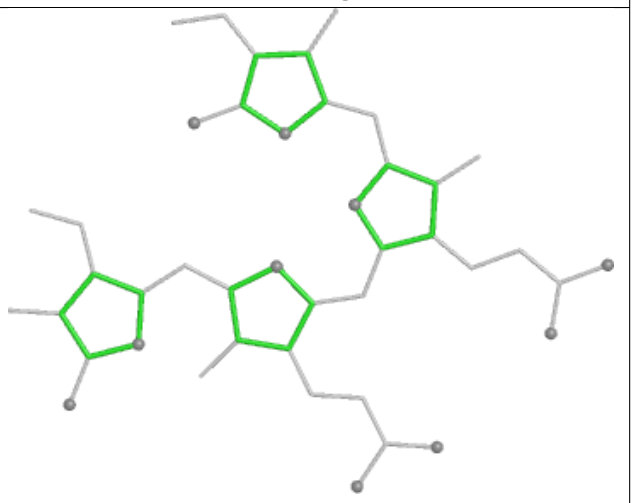
Bond lengths



Bond angles

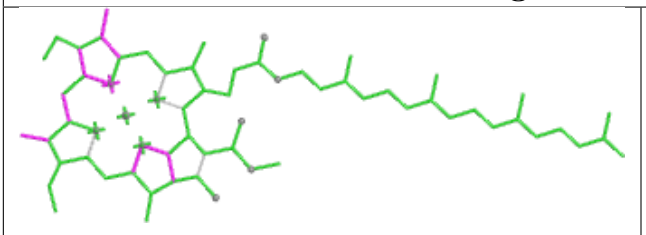


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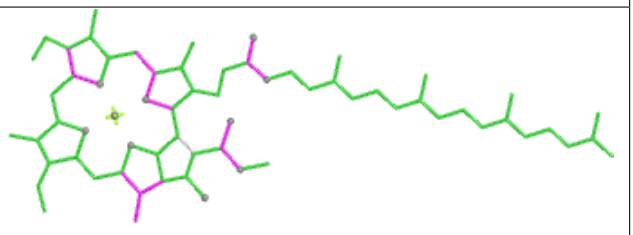


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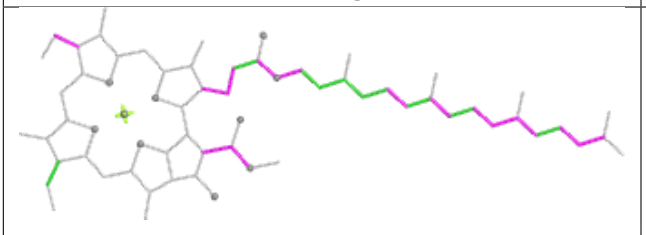
Ligand CLA AN 810



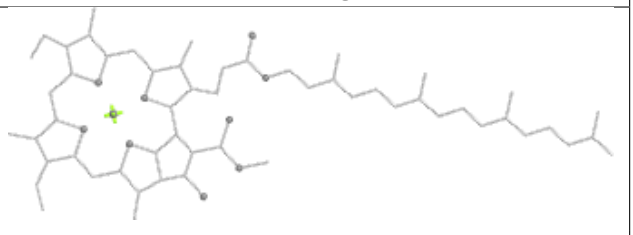
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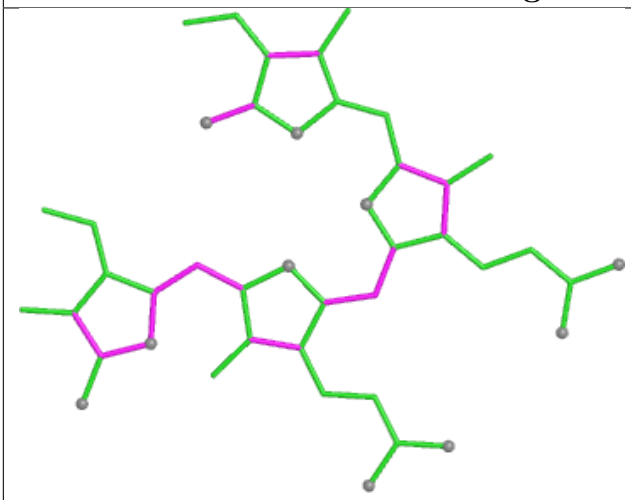


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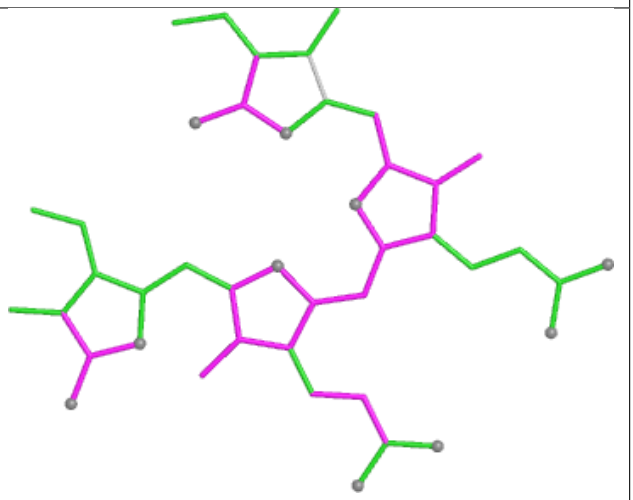


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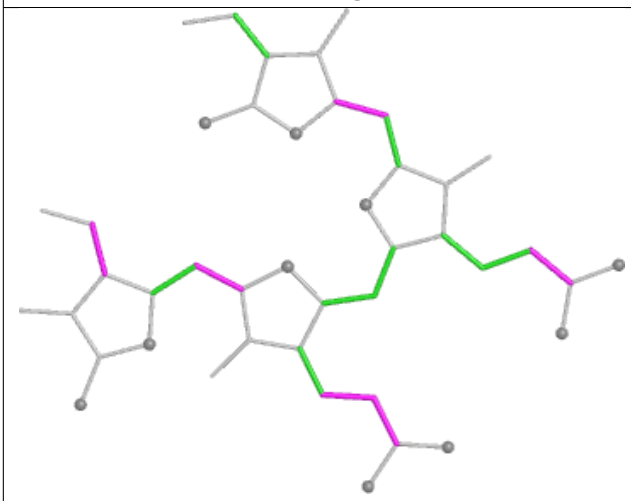
Ligand PEB f4 201



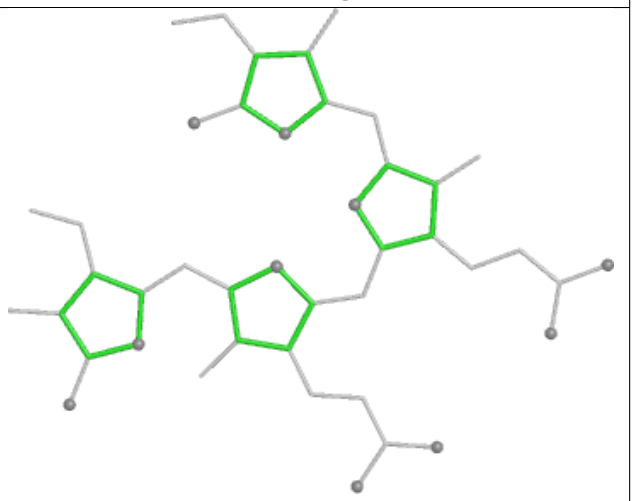
Bond lengths



Bond angles

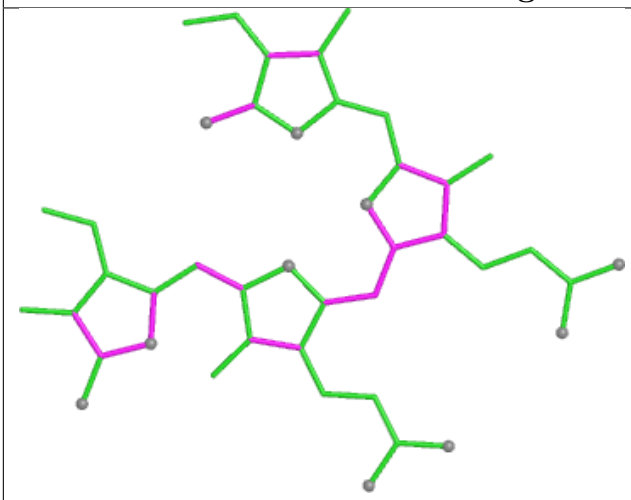


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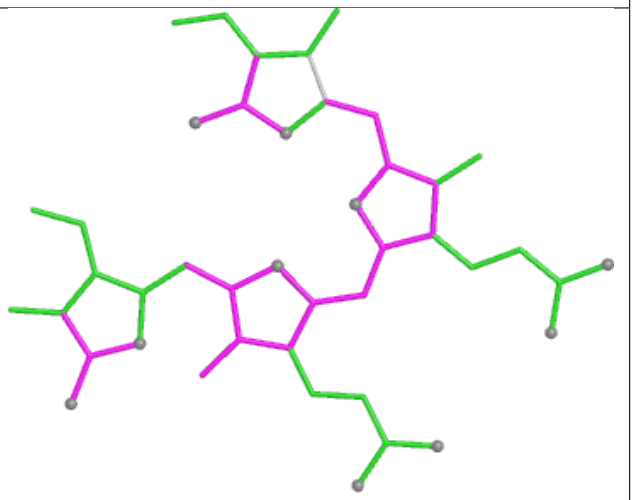


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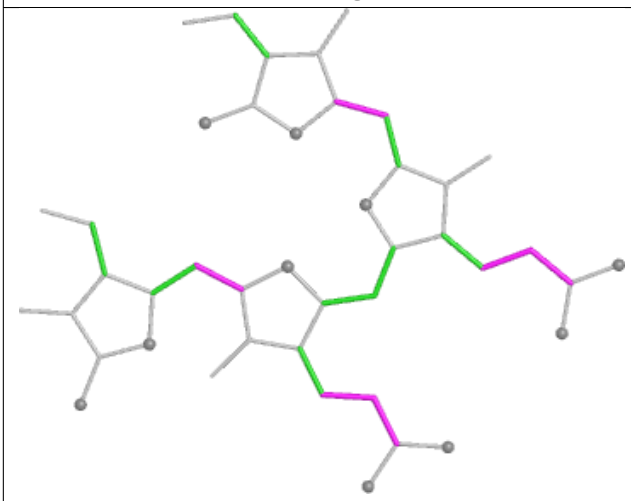
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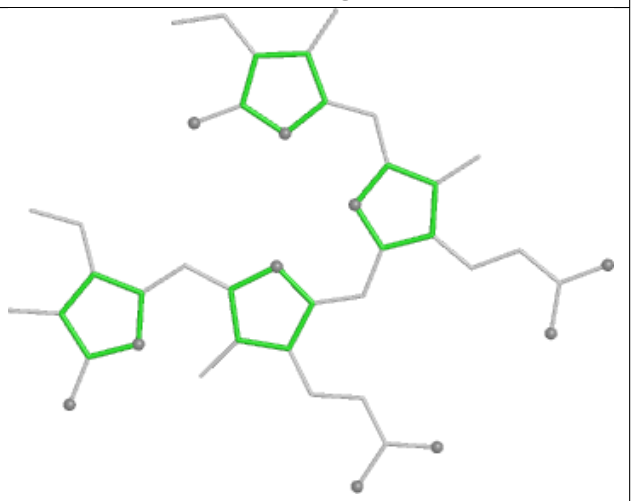
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Bond angles

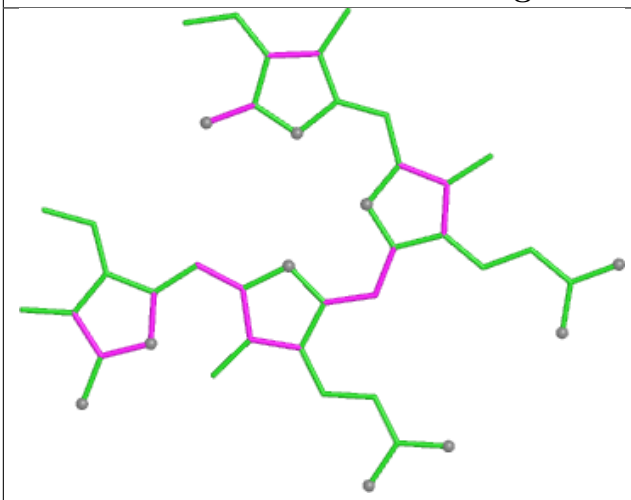


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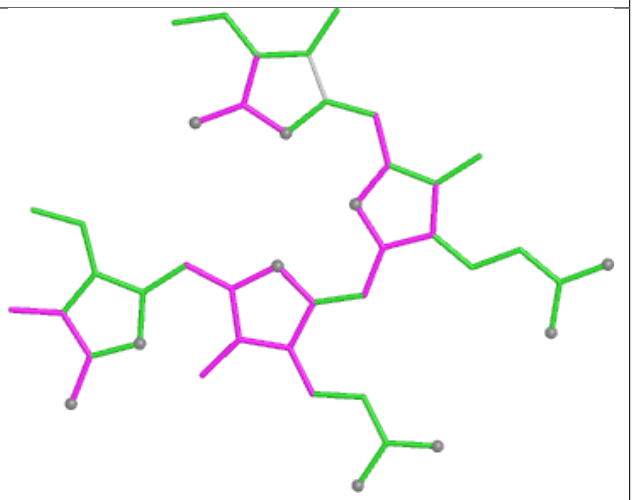


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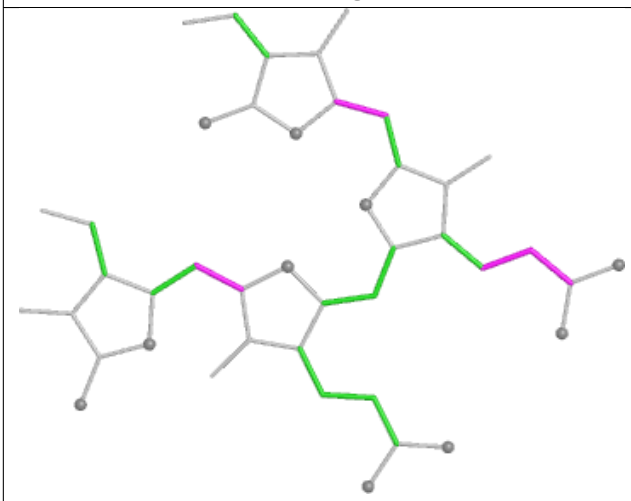
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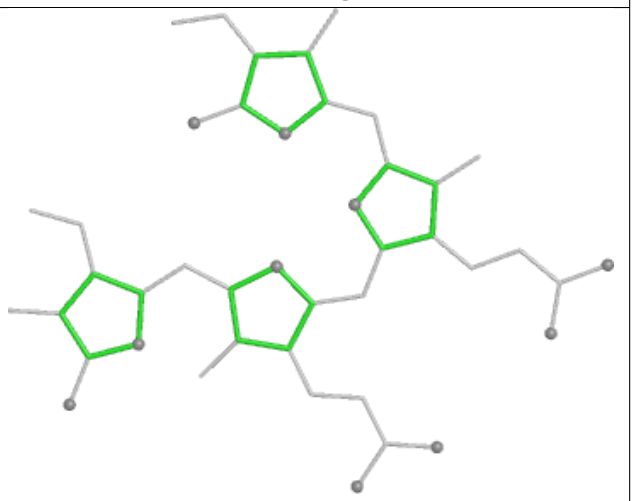
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Bond angles

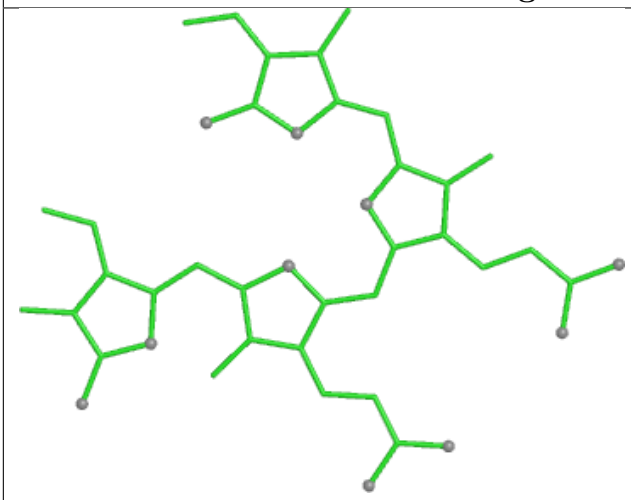


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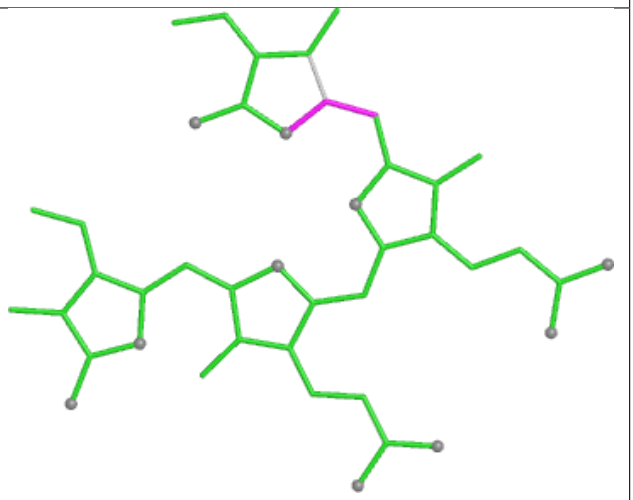


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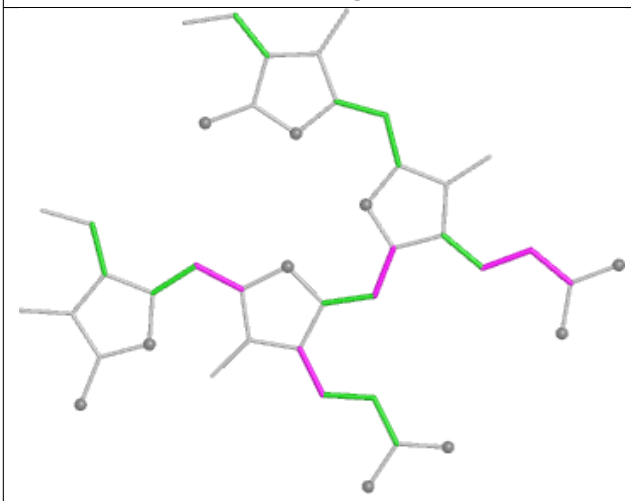
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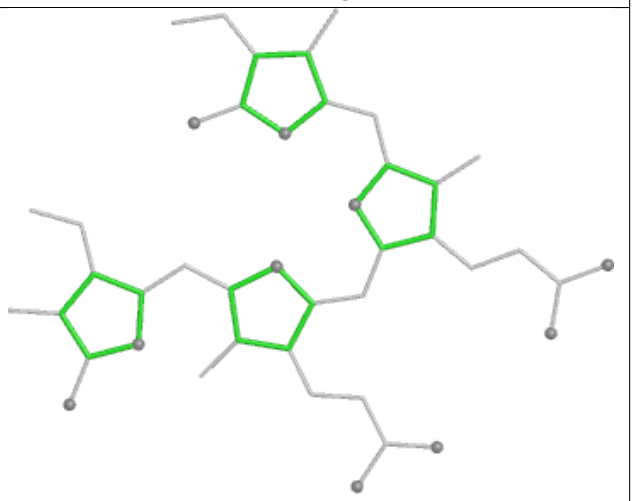
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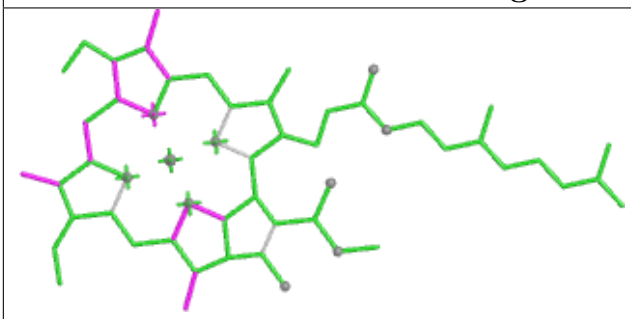


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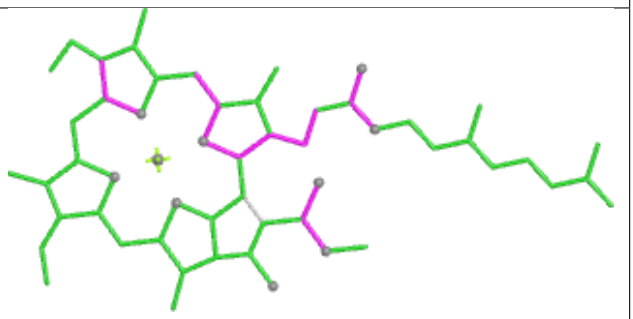


Rings

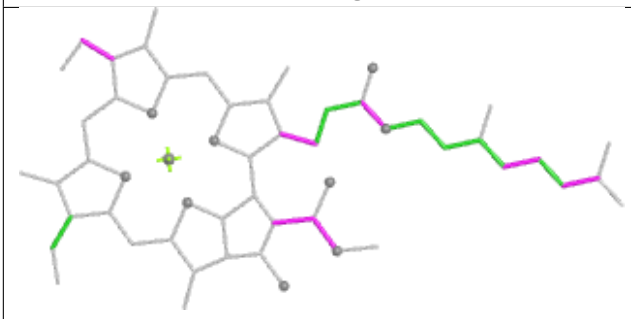
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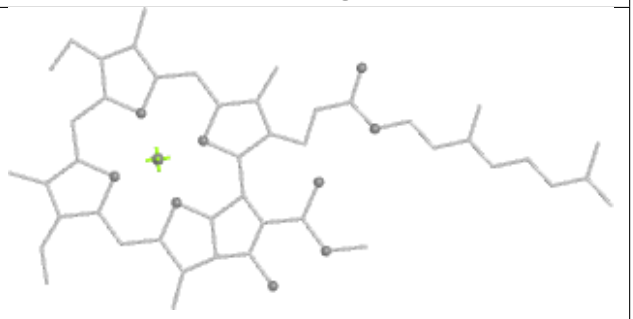
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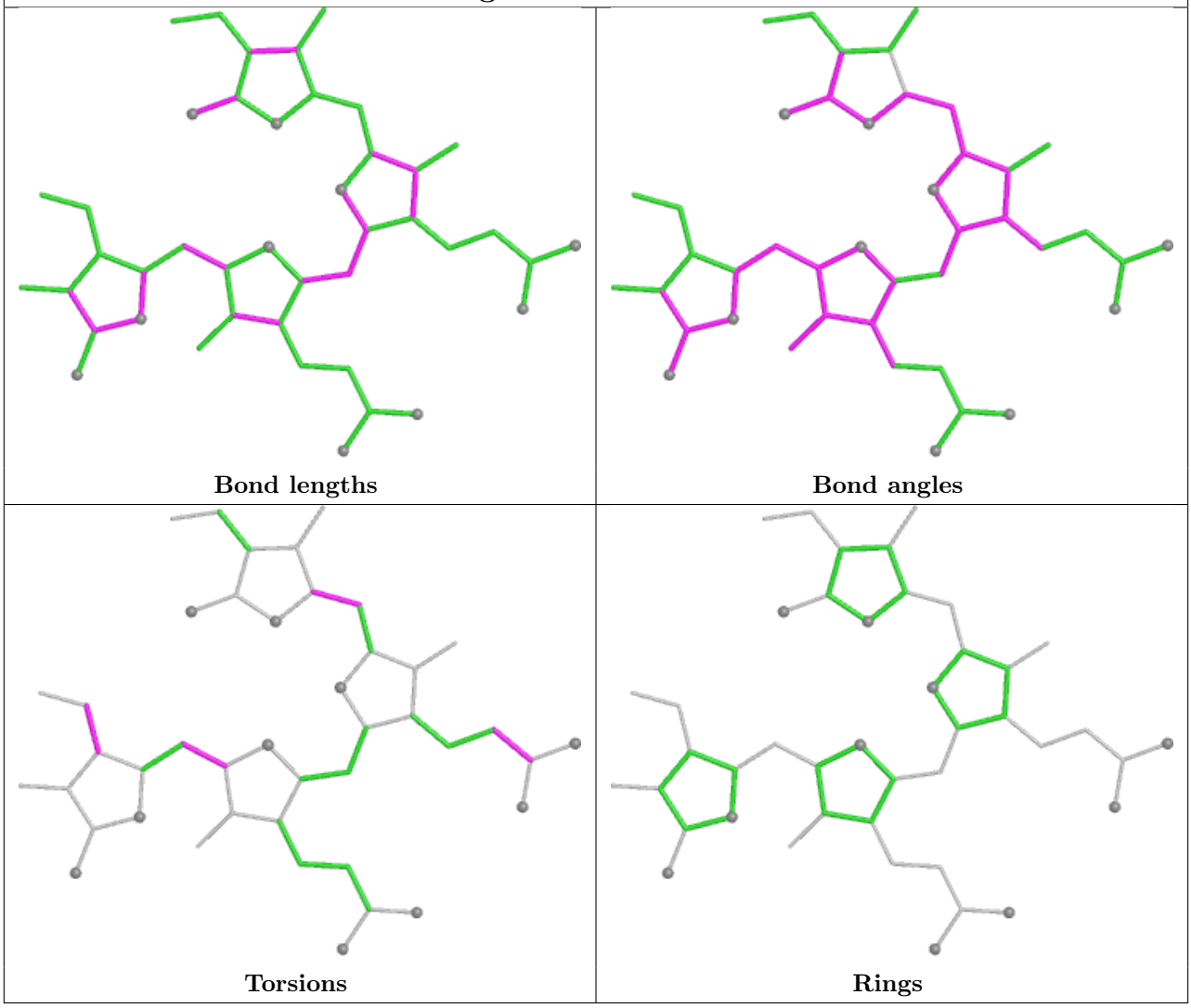


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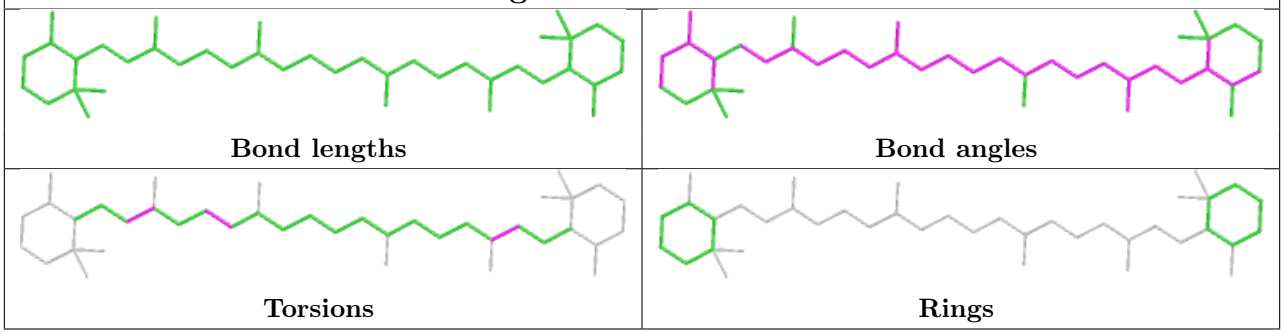


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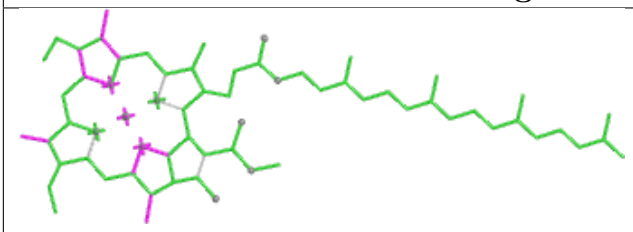
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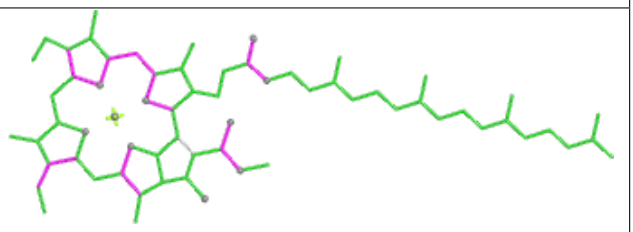
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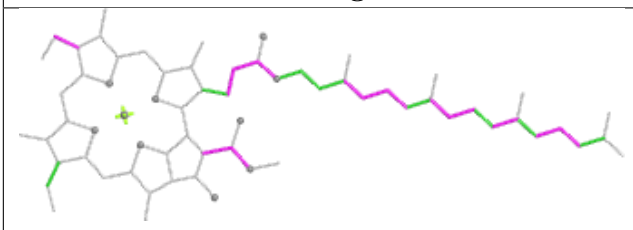
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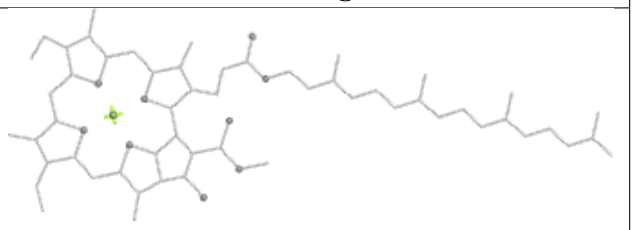
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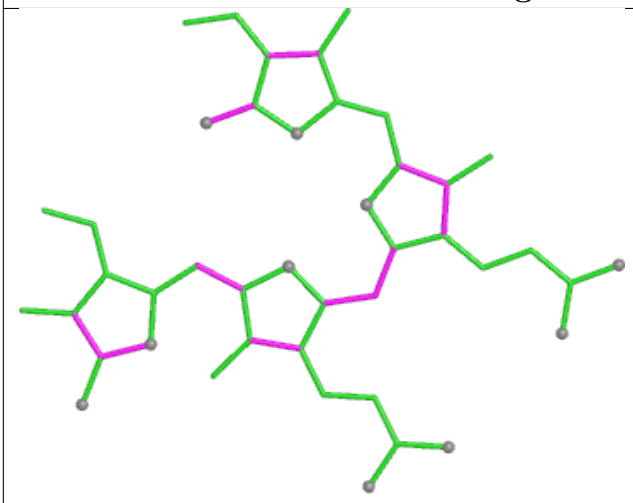


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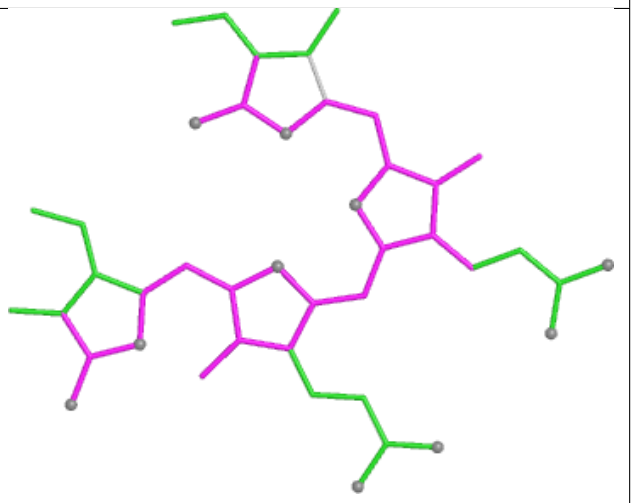


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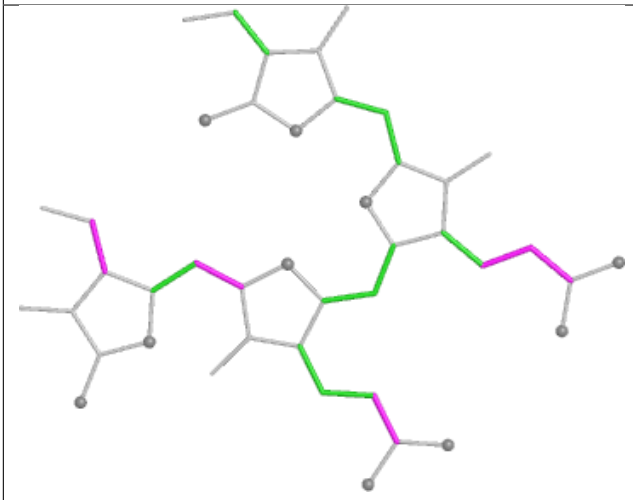
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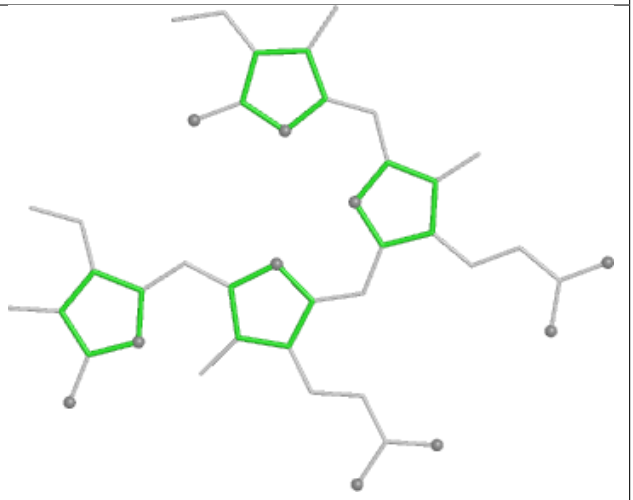
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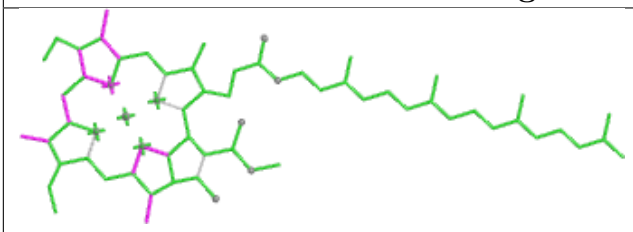


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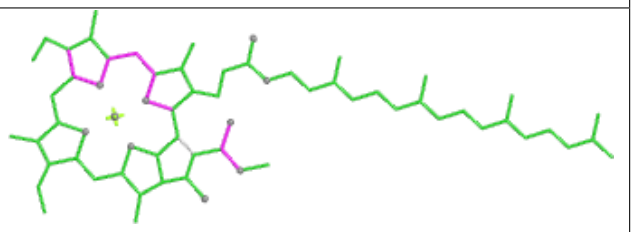


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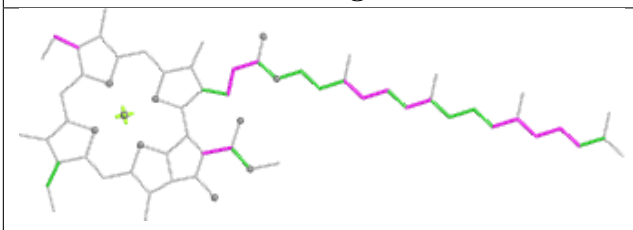
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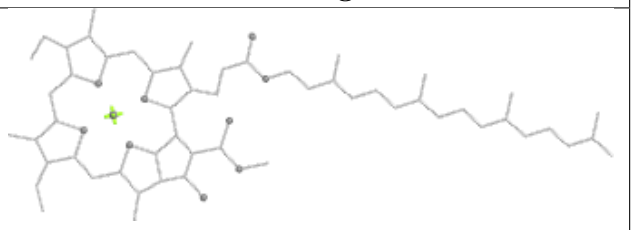
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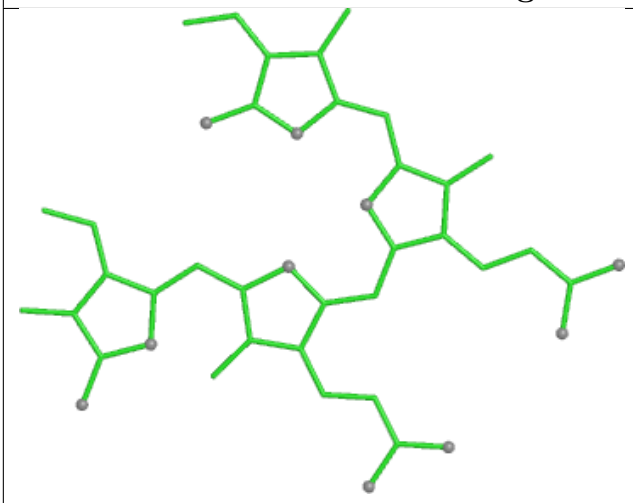


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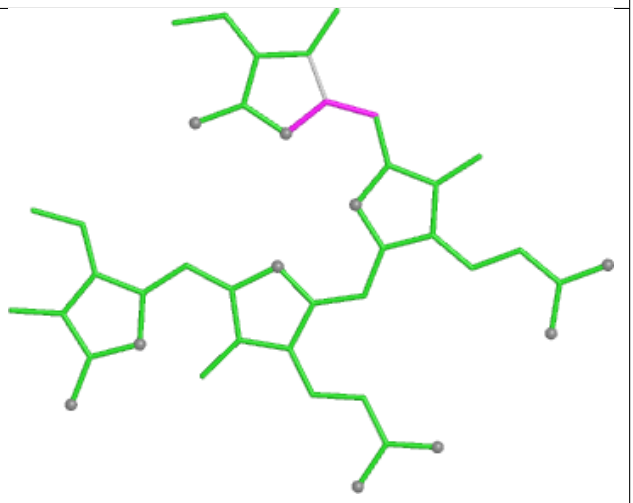


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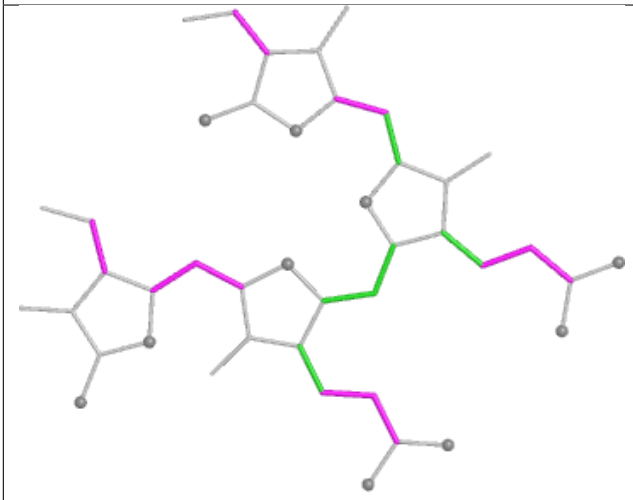
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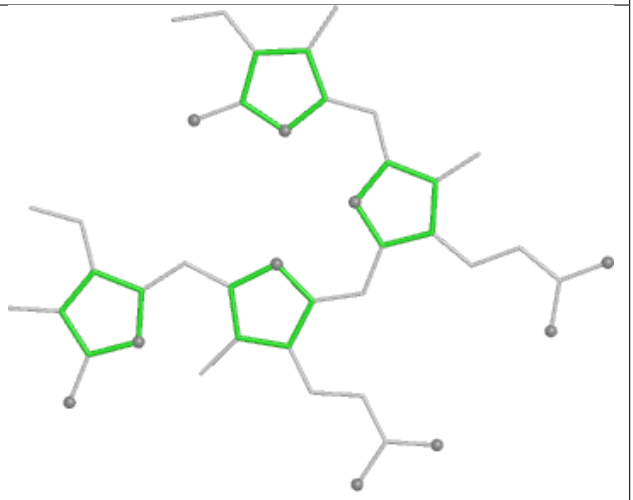
Bond lengths



Bond angles

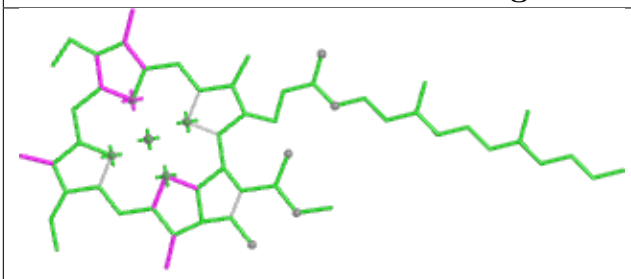


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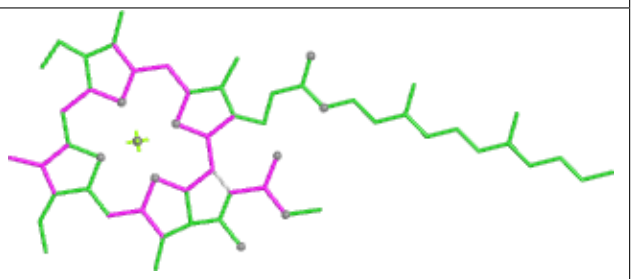


Rings

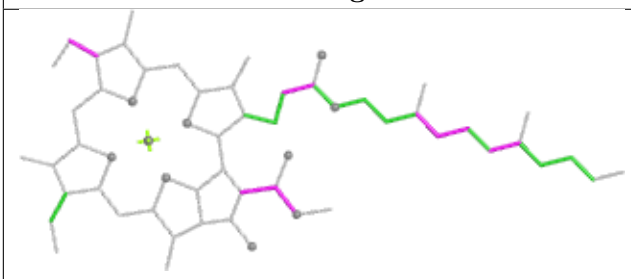
Ligand CLA BN 802



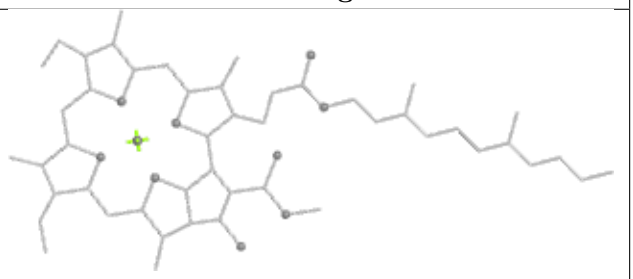
Bond lengths



Bond angles

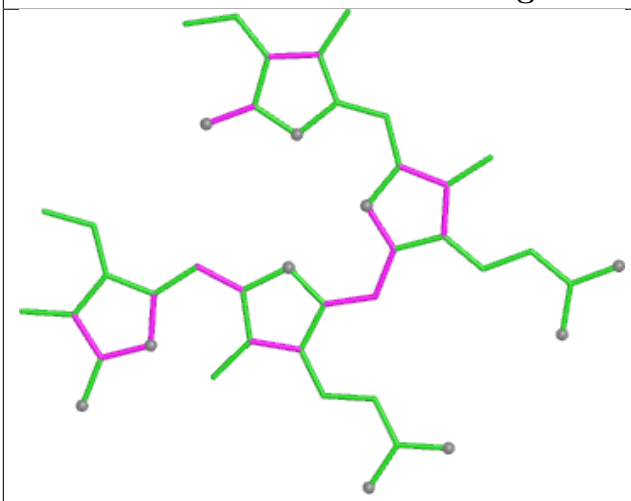


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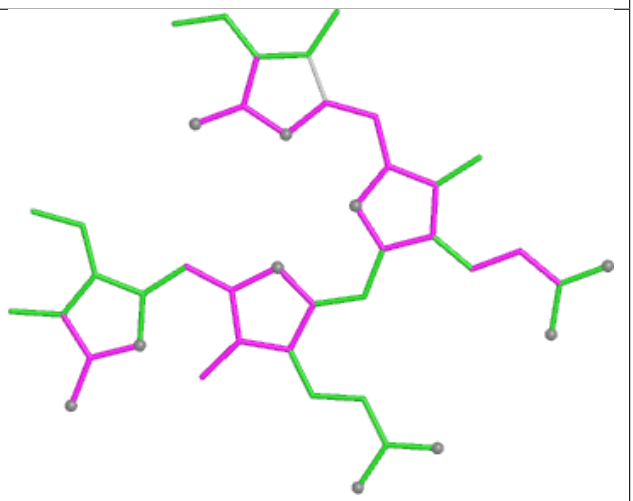


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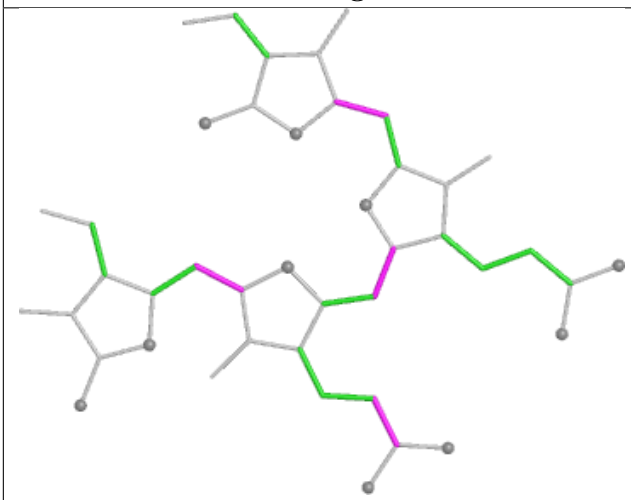
Ligand PEB HI 203



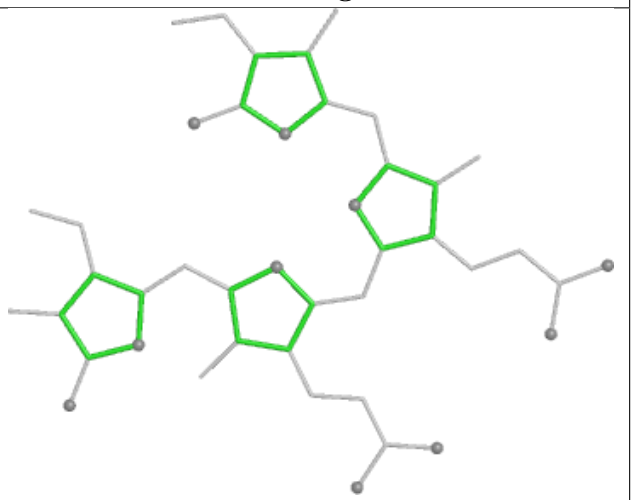
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Bond angles

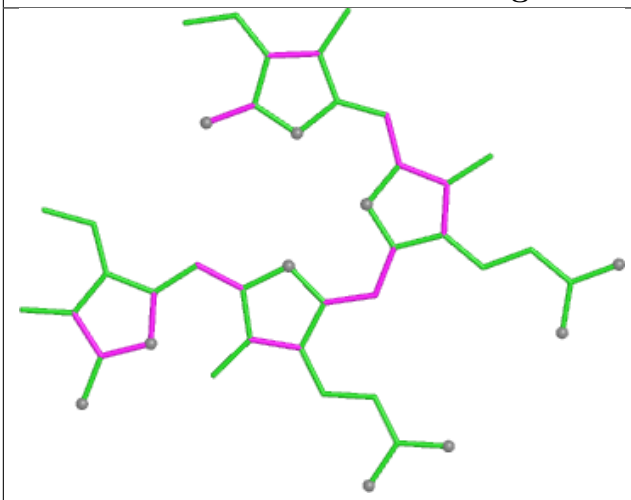


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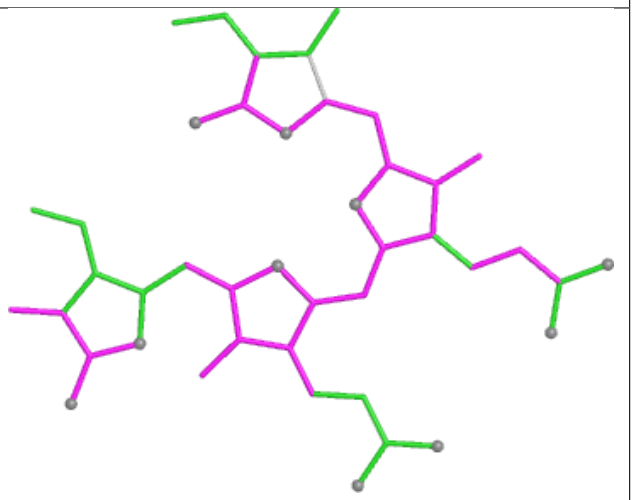


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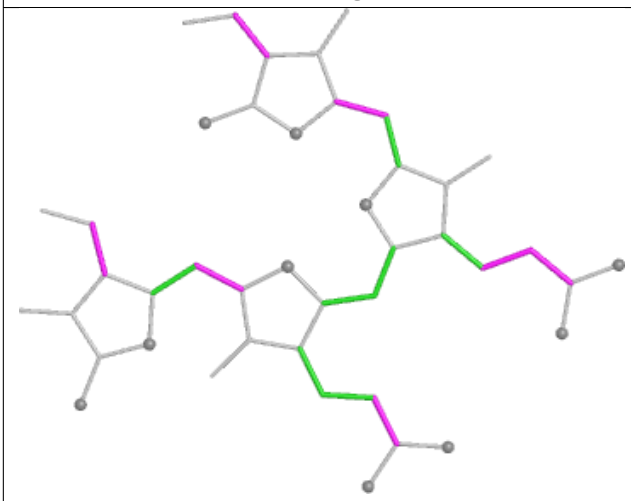
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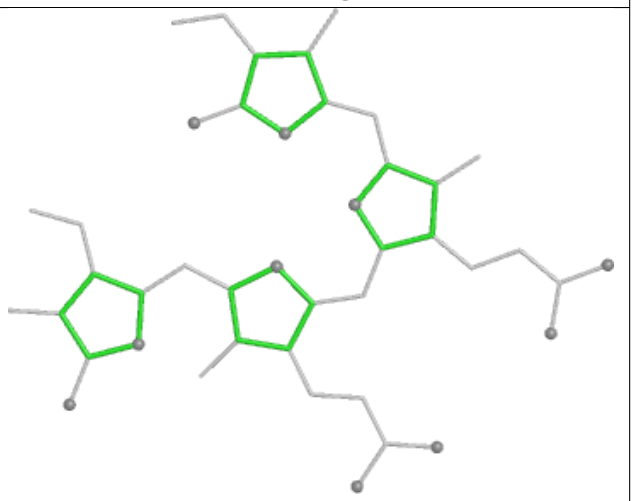
Bond lengths



Bond angles

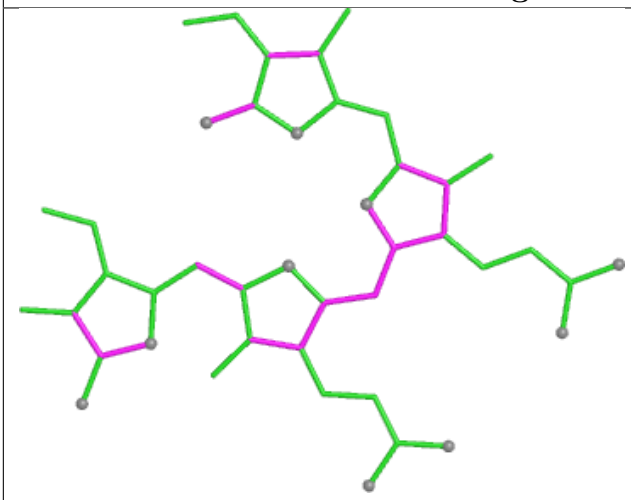


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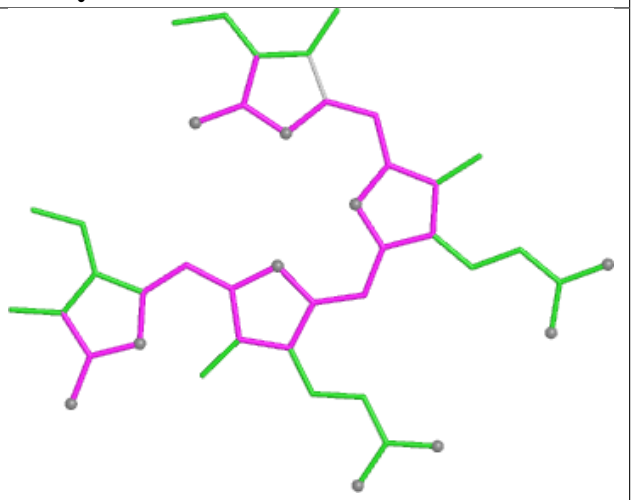


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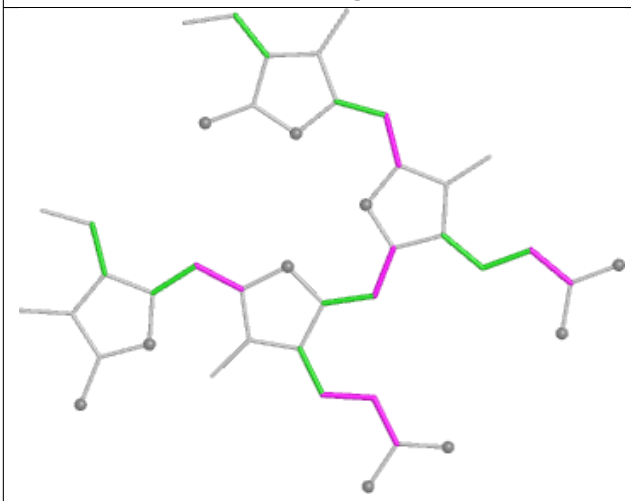
Ligand PEB AQ 304



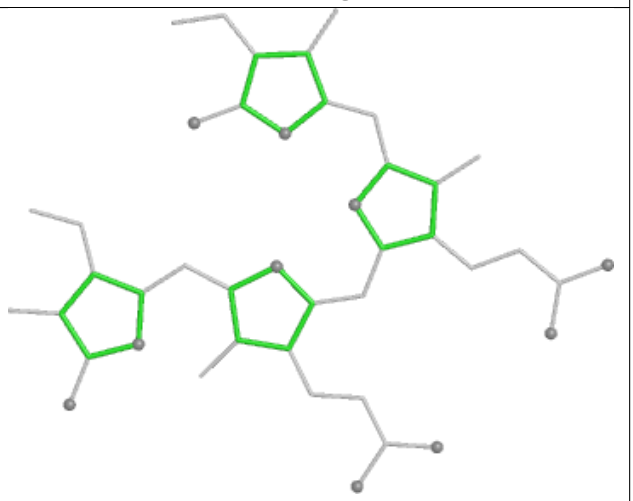
Bond lengths



Bond angles

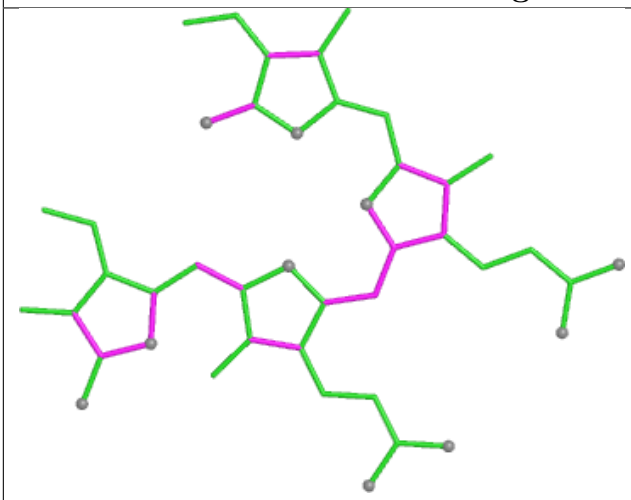


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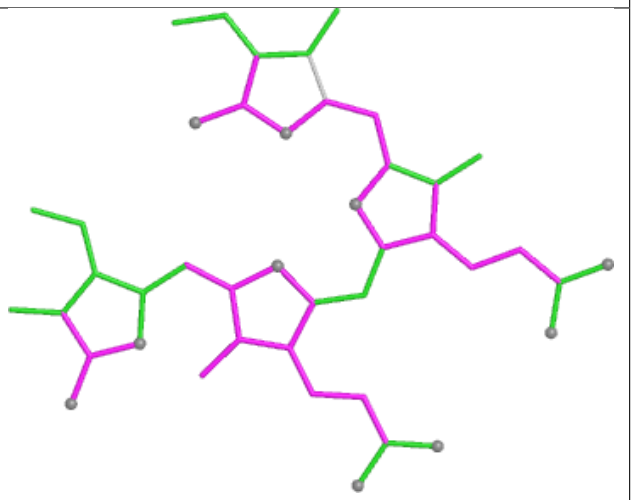


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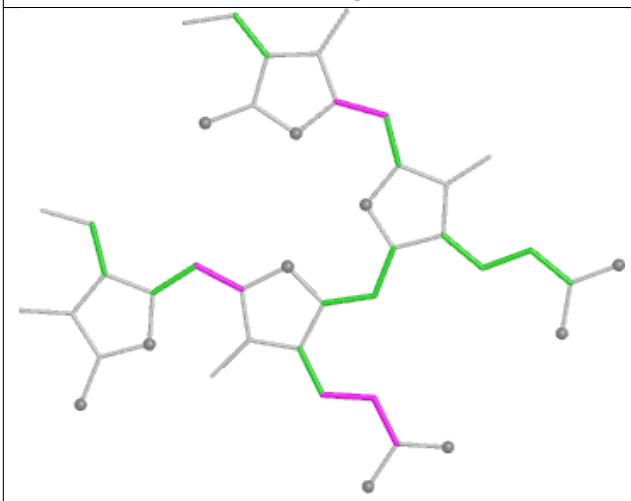
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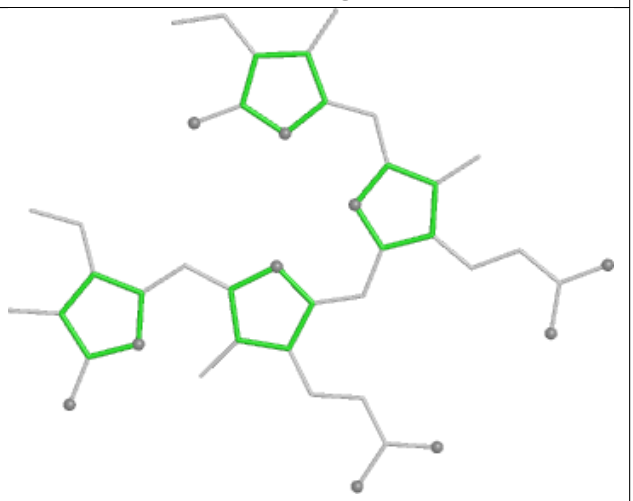
Bond lengths



Bond angles

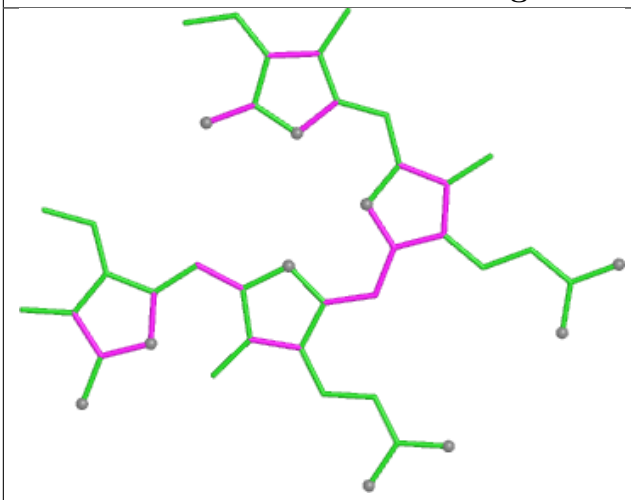


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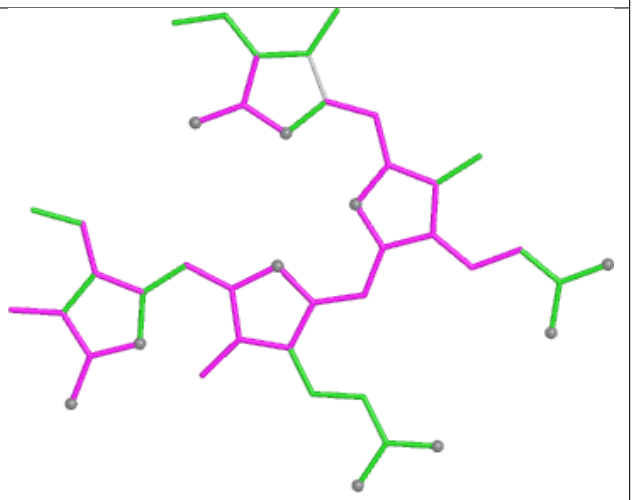


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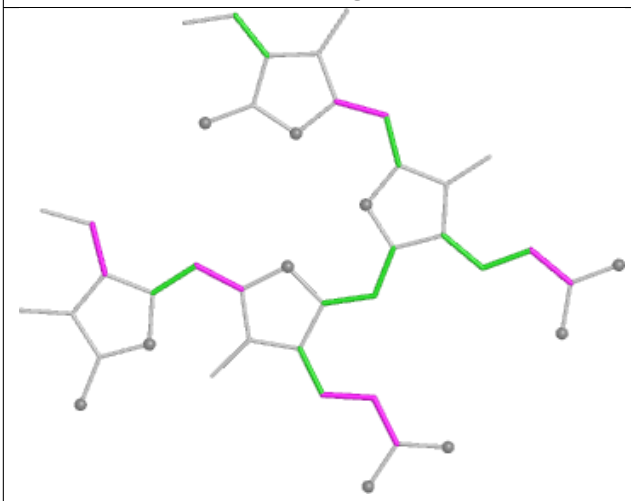
Ligand PEB AD 303



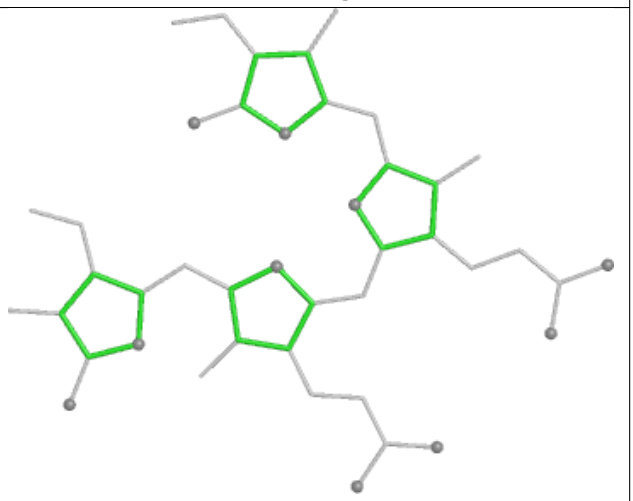
Bond lengths



Bond angles

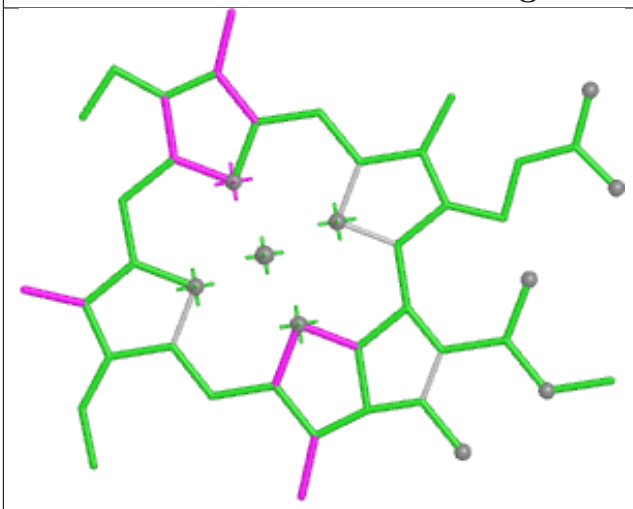


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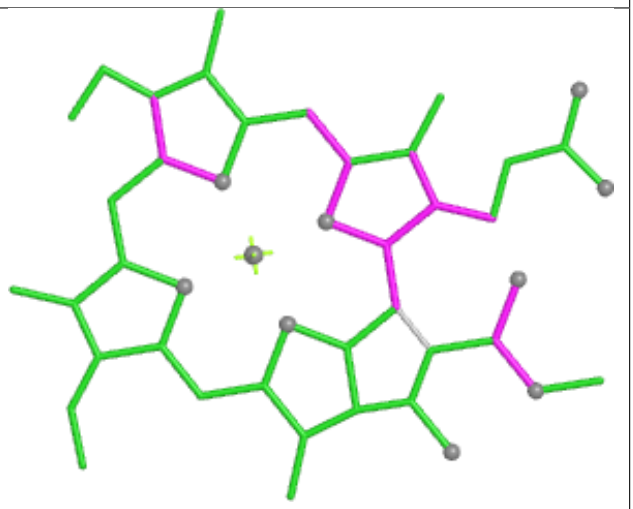


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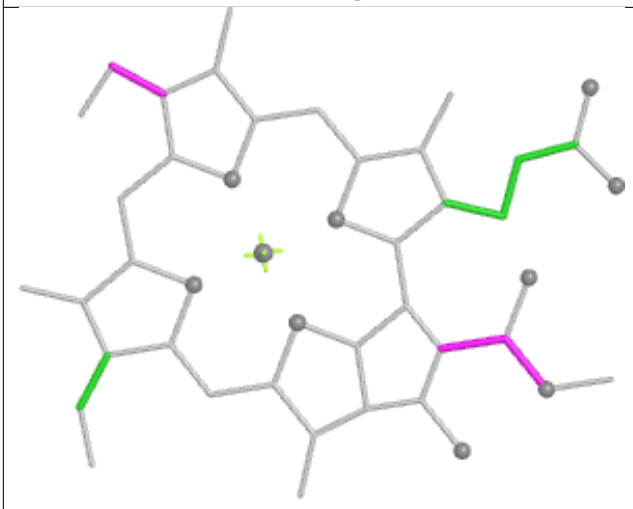
Ligand CLA 72 610



Bond lengths



Bond angles

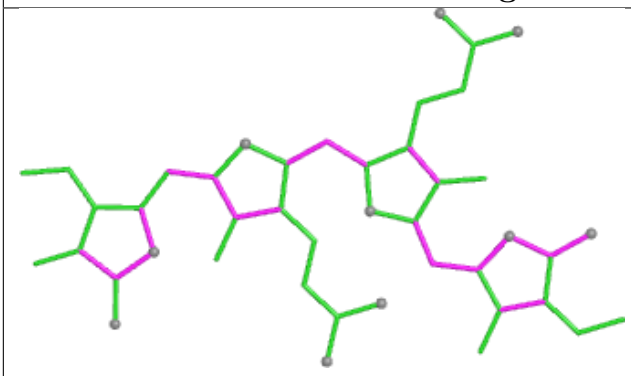


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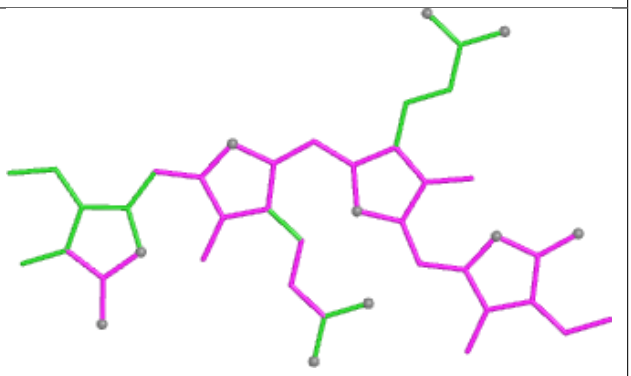


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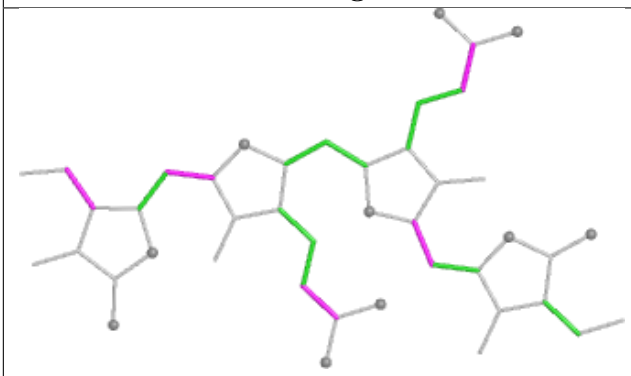
Ligand CYC DO 1001



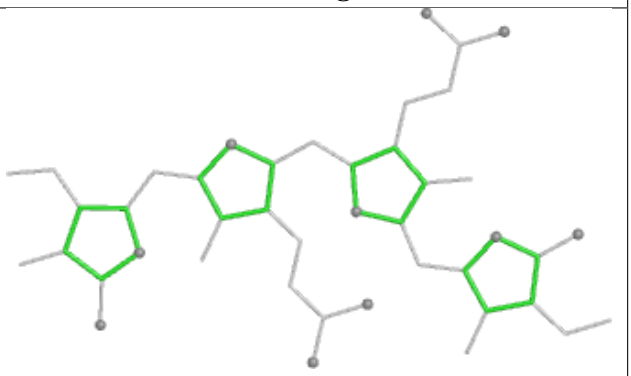
Bond lengths



Bond angles

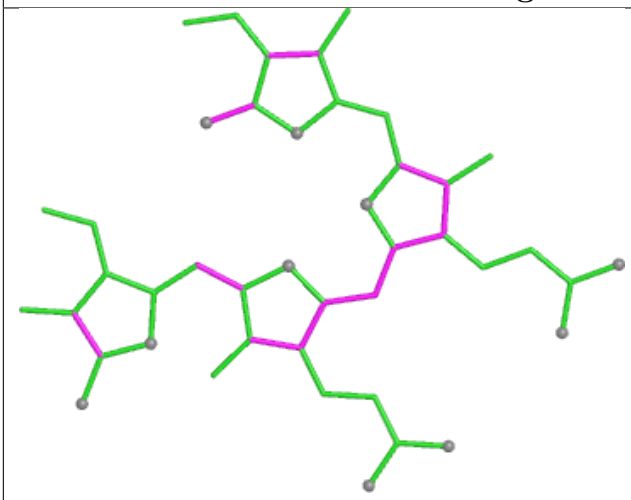


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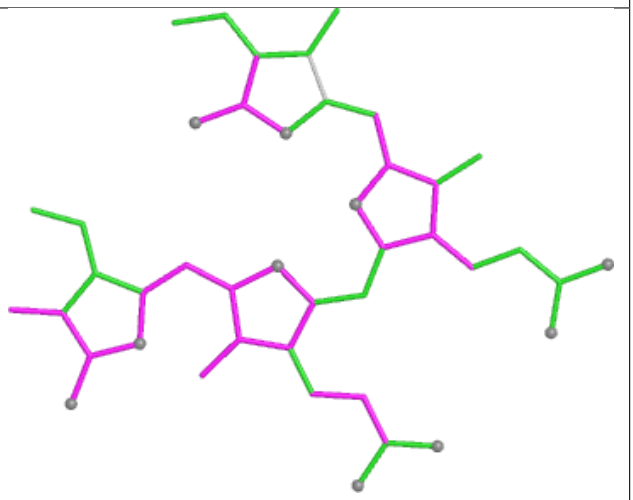


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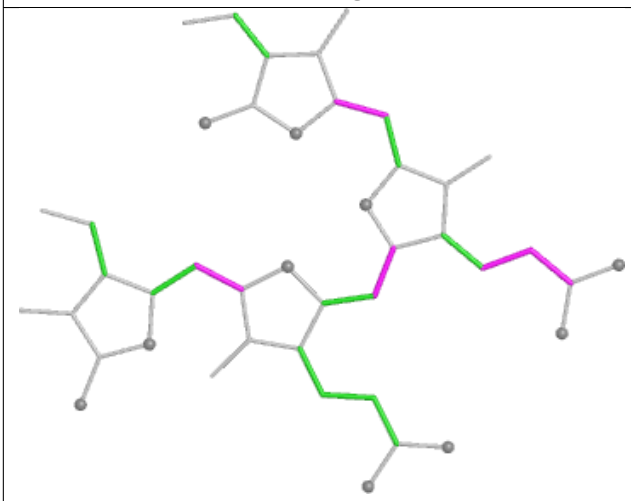
Ligand PEB tK 201



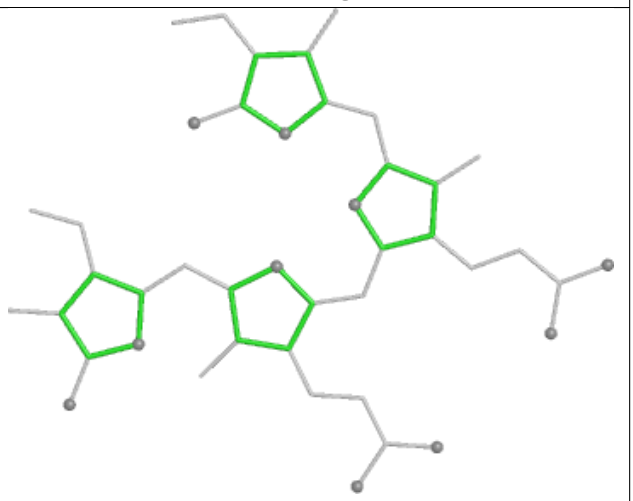
Bond lengths



Bond angles

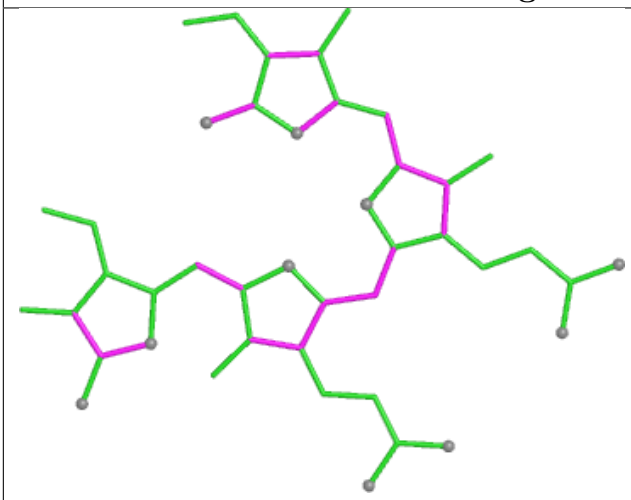


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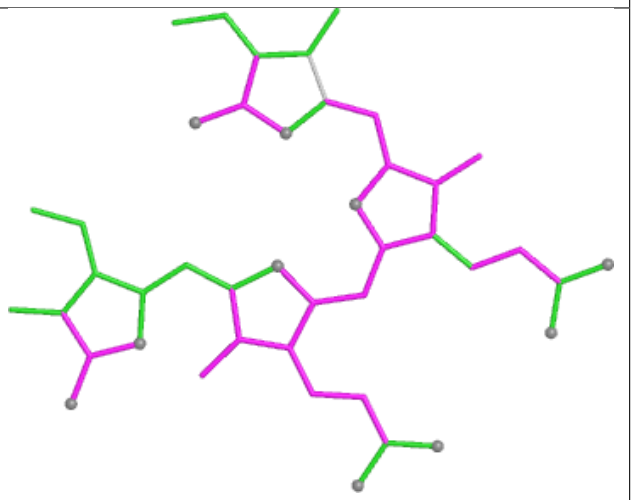


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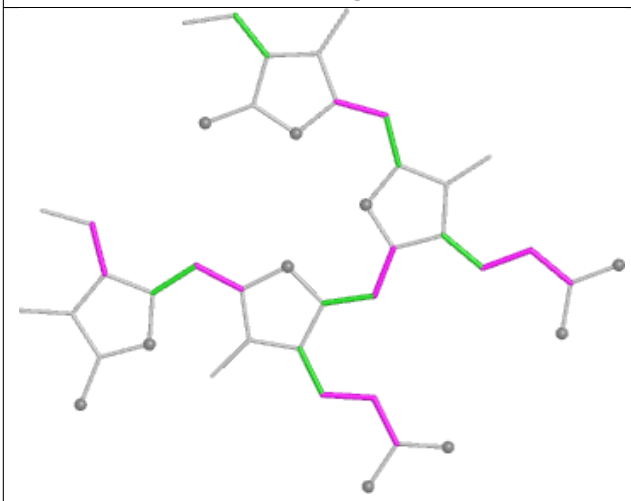
Ligand PEB lK 202



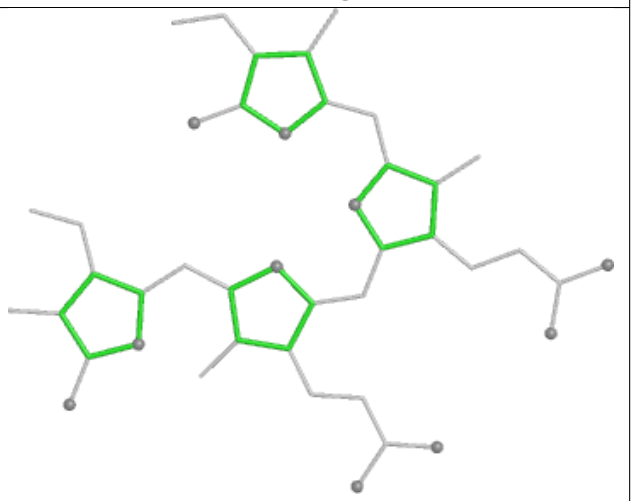
Bond lengths



Bond angles

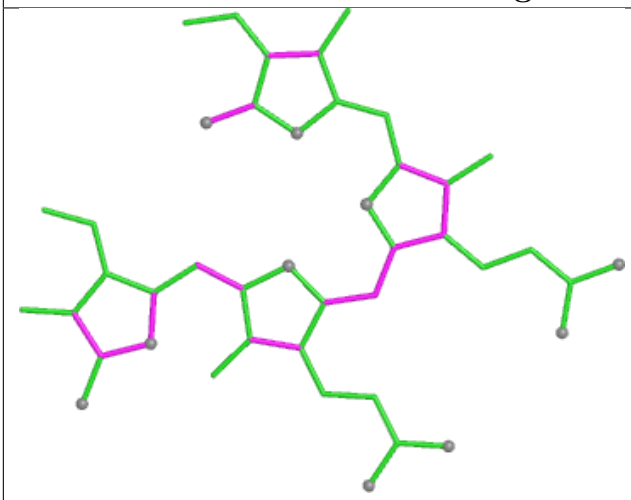


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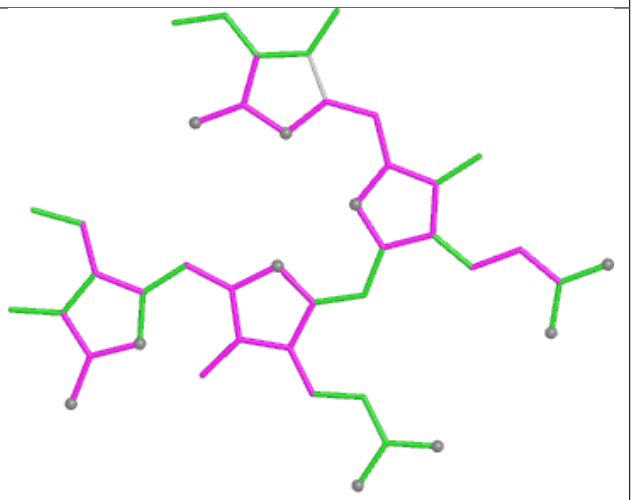


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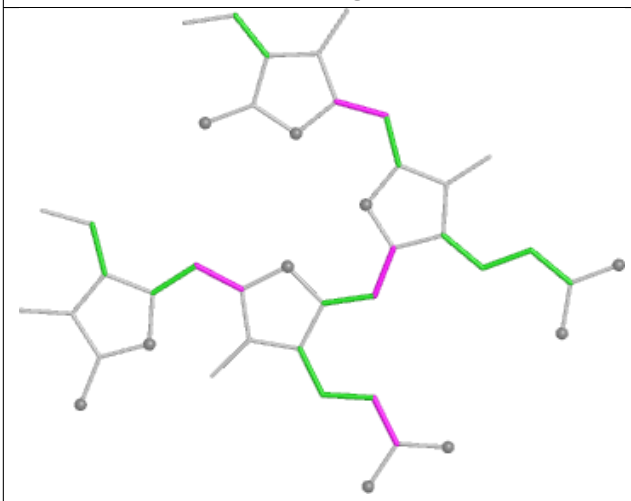
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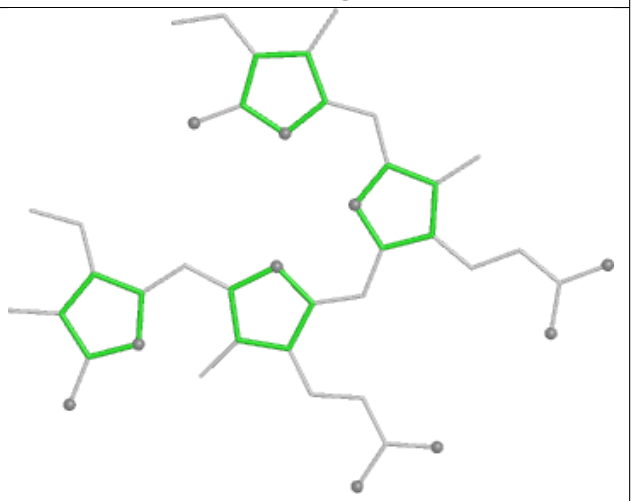
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Bond angles

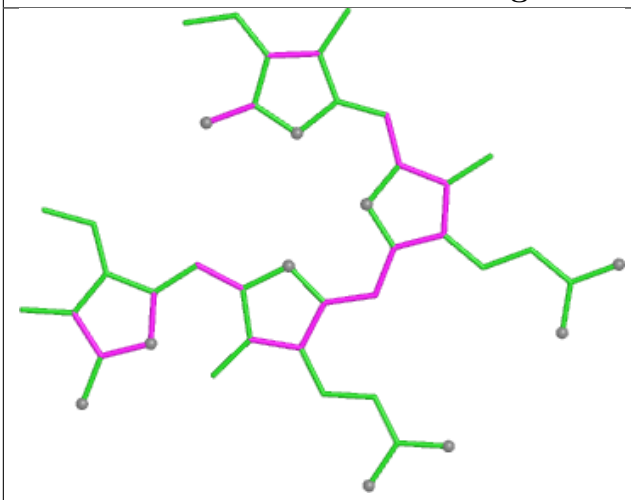


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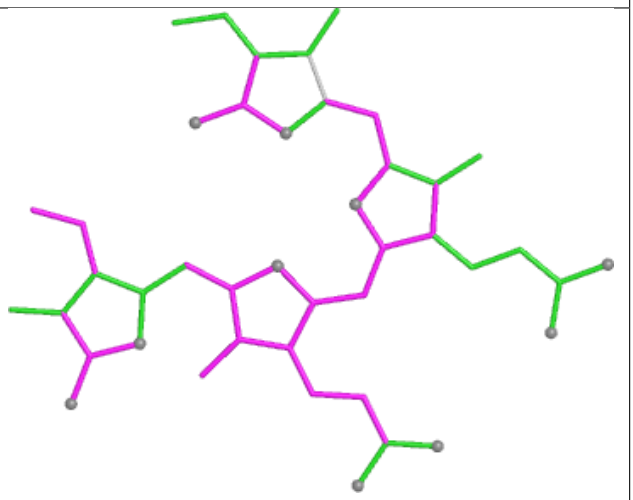


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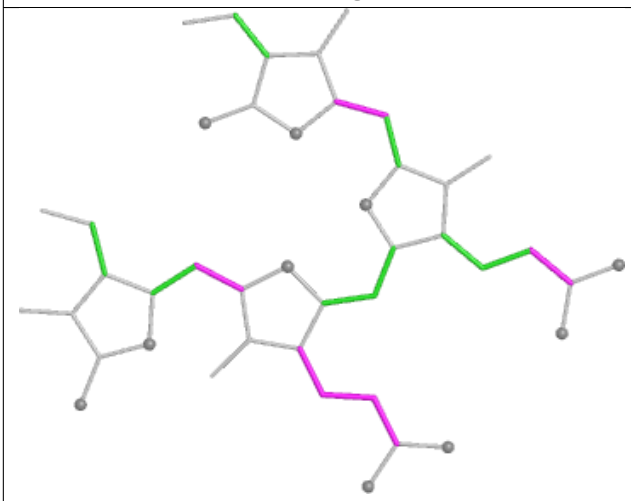
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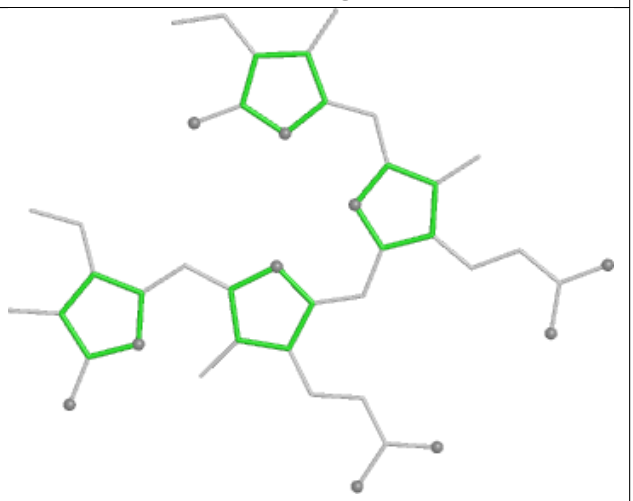
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Bond angles

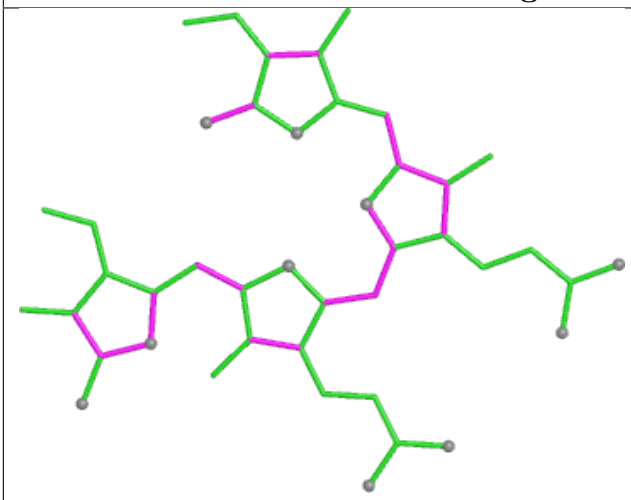


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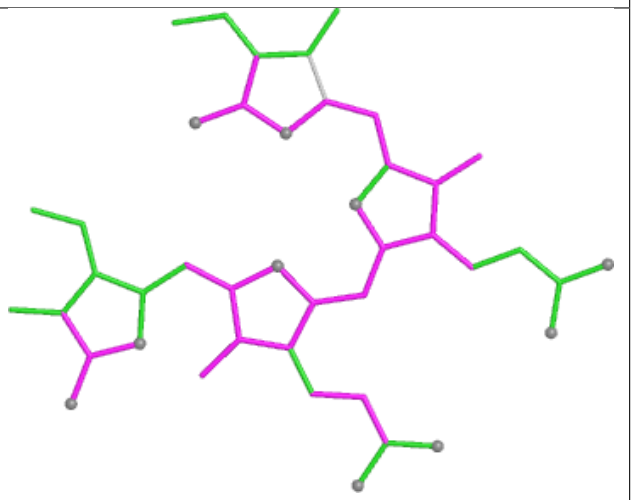


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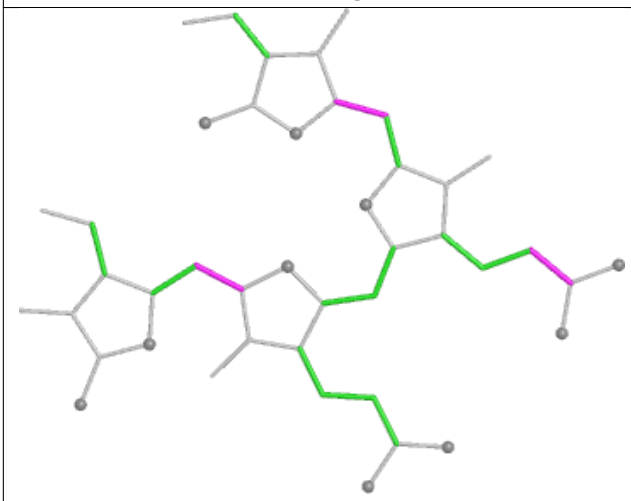
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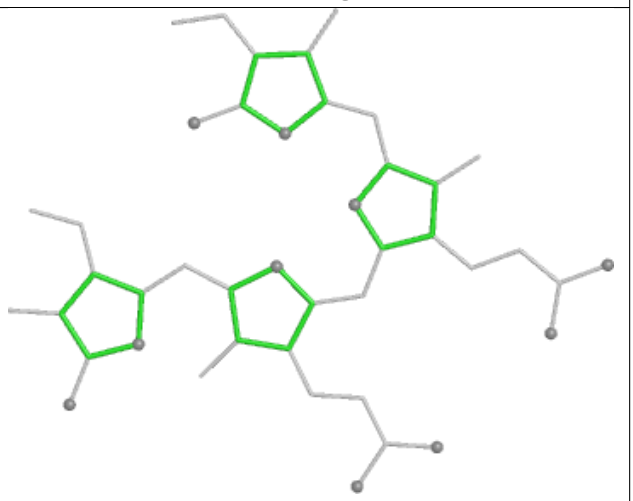
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Bond angles

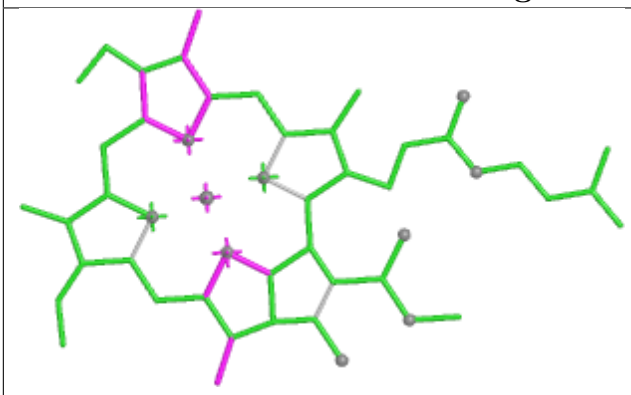


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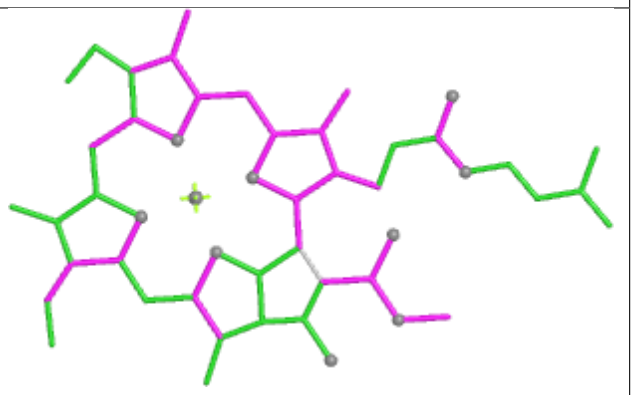


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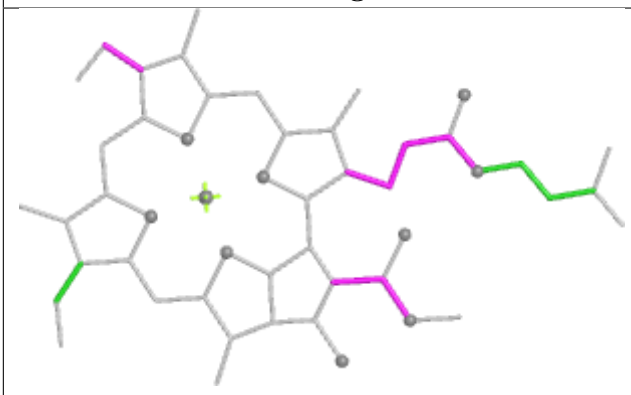
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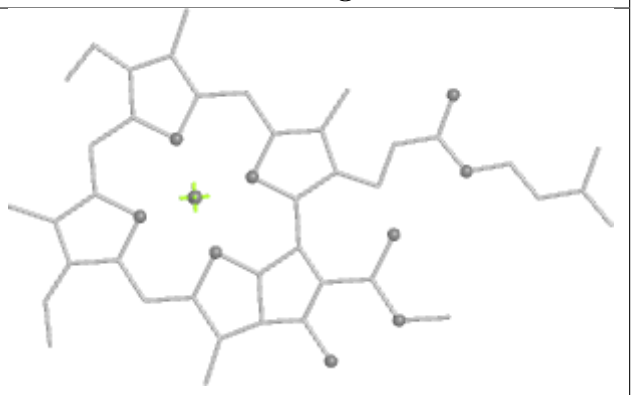
Bond lengths



Bond angles

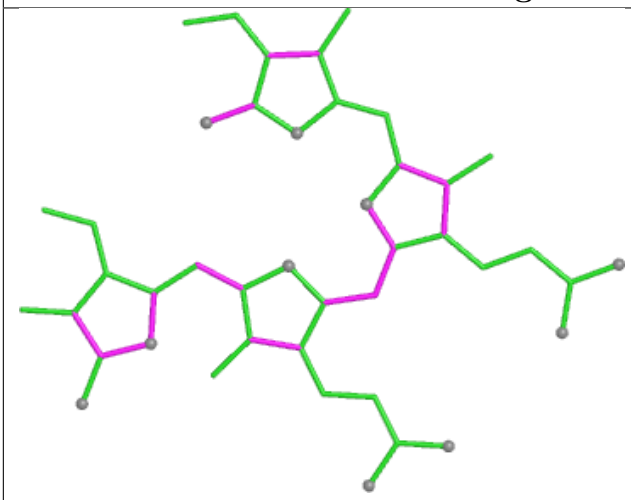


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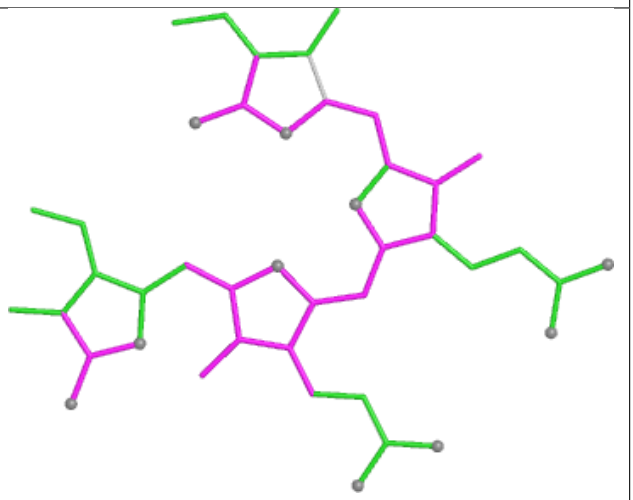


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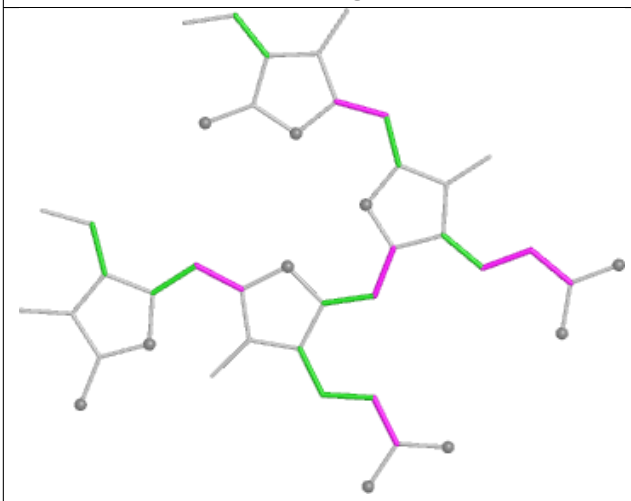
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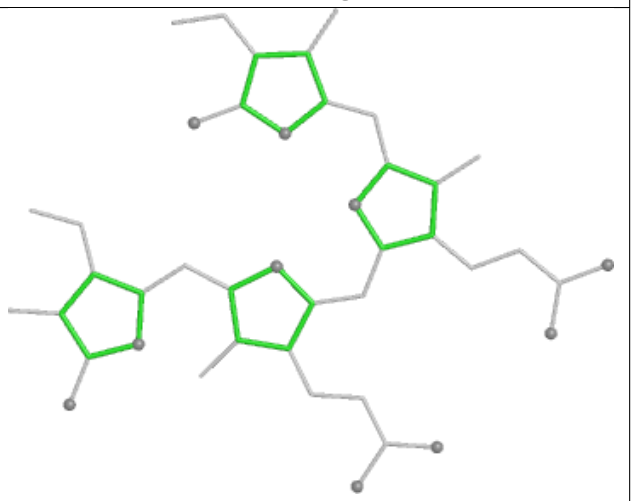
Bond lengths



Bond angles

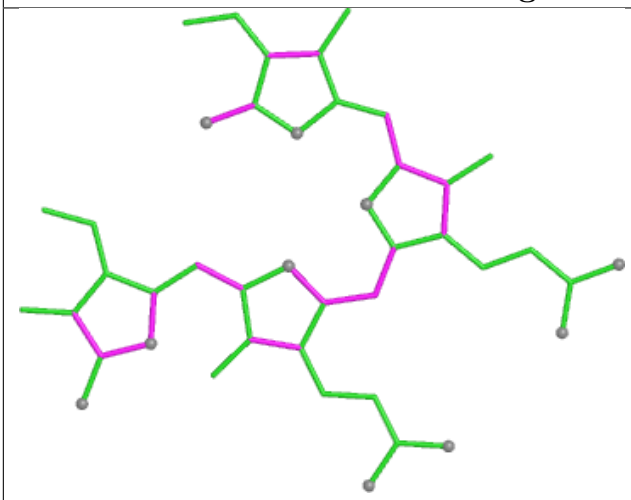


Torsions

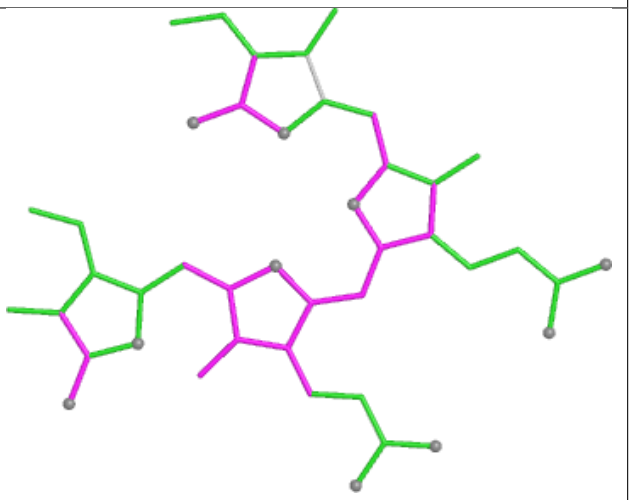


Rings

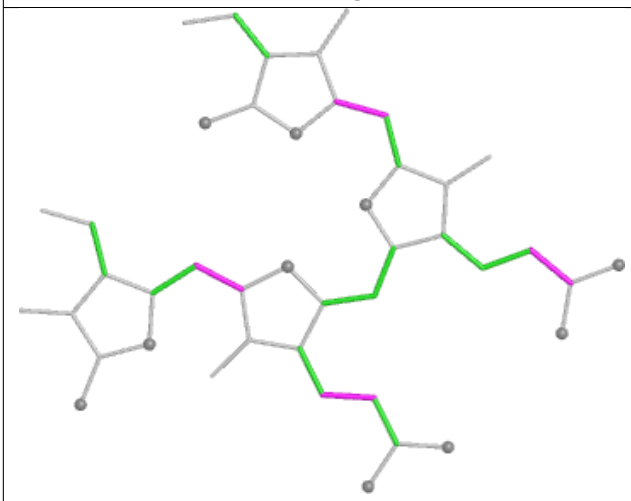
Ligand PEB S1 201



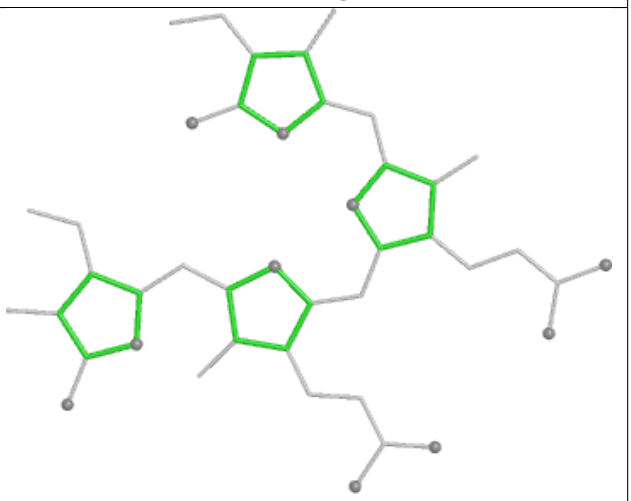
Bond lengths



Bond angles

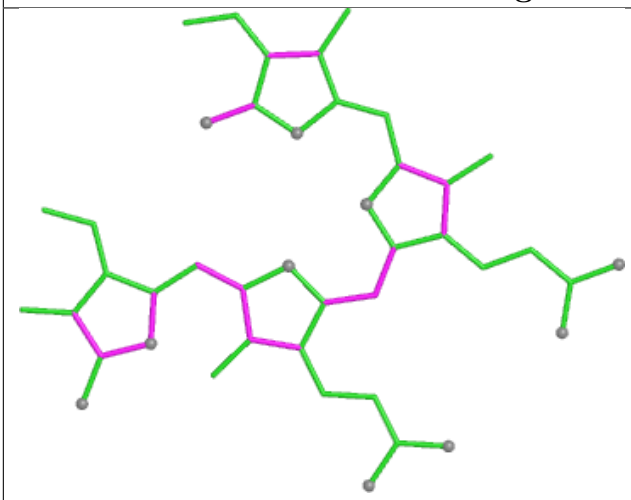


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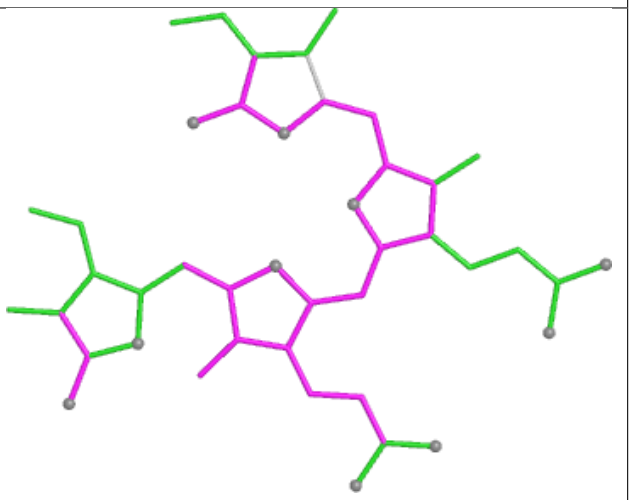


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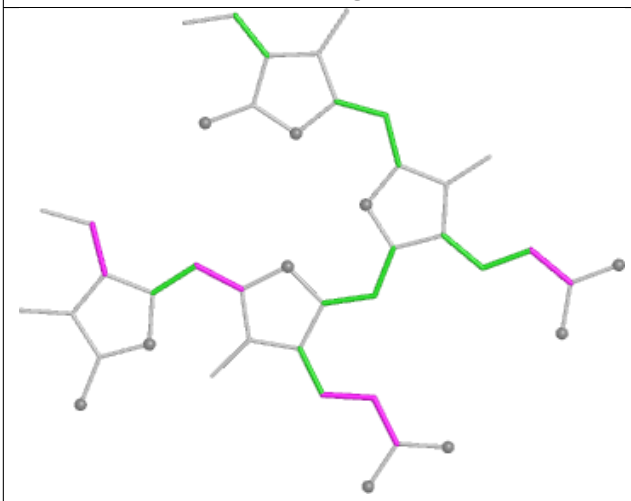
Ligand PEB aK 202



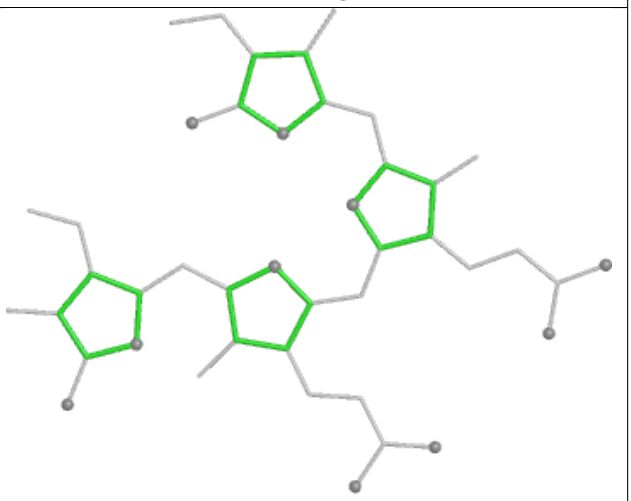
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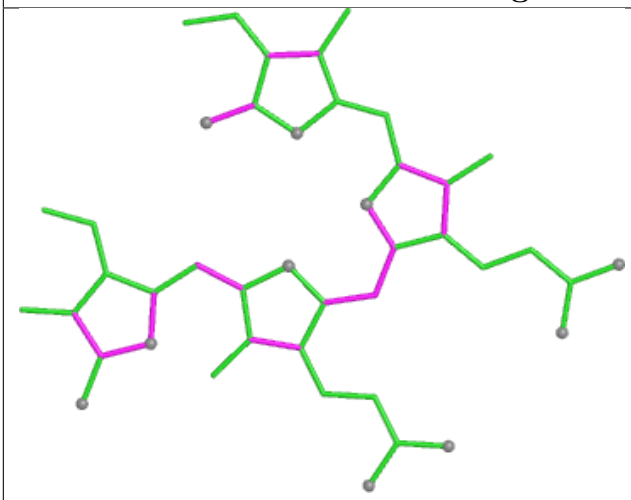


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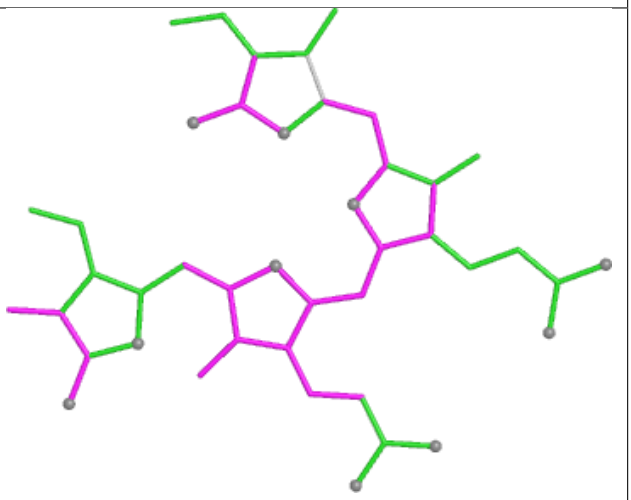


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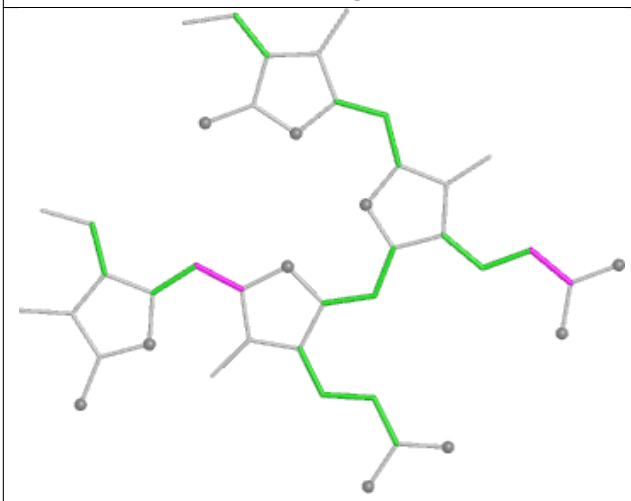
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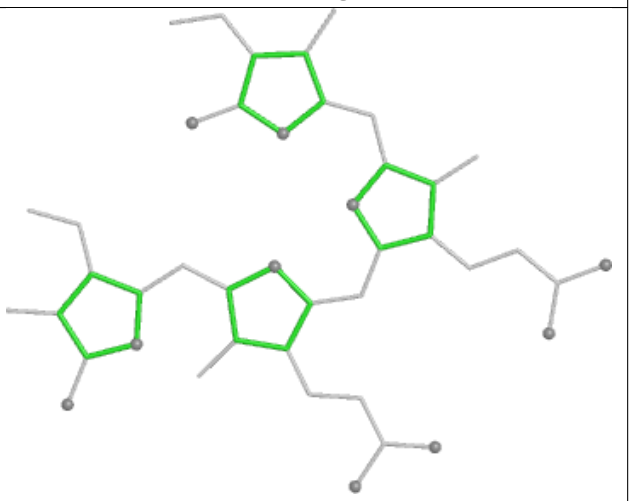
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Bond angles

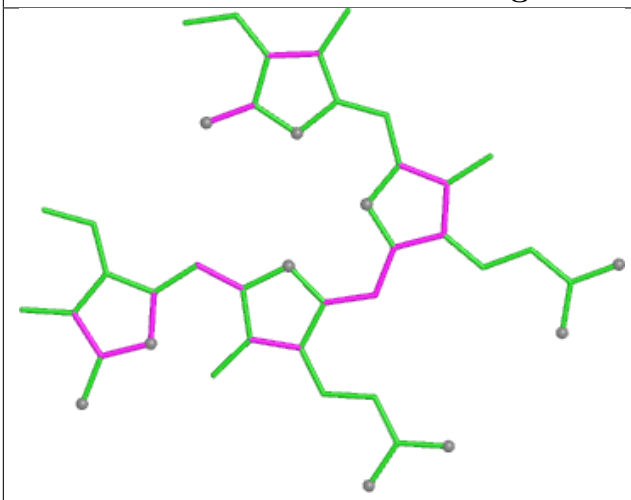


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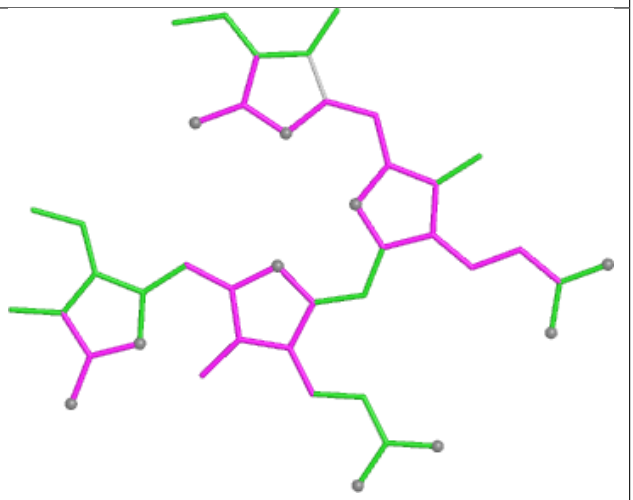


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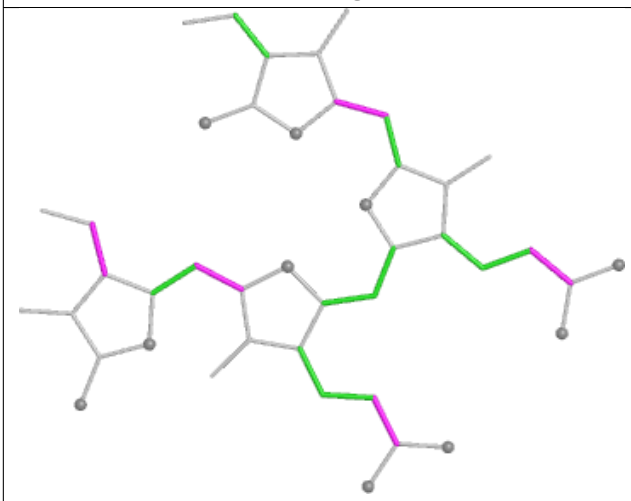
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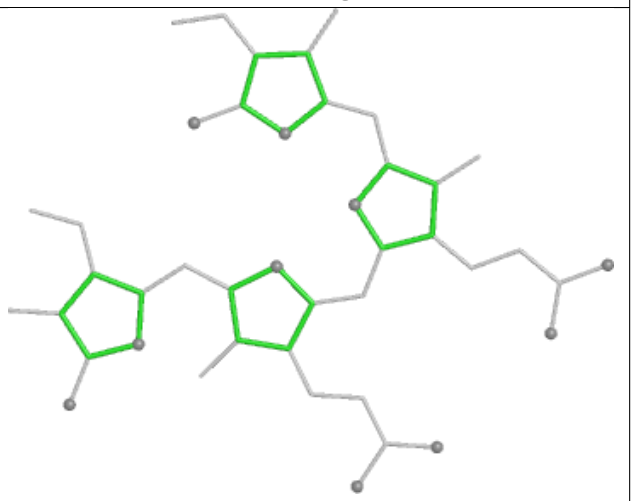
Bond lengths



Bond angles

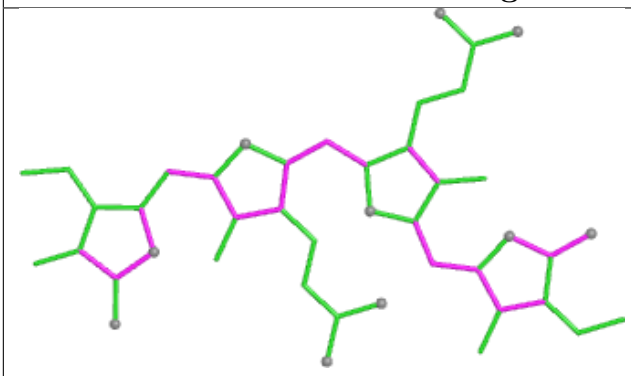


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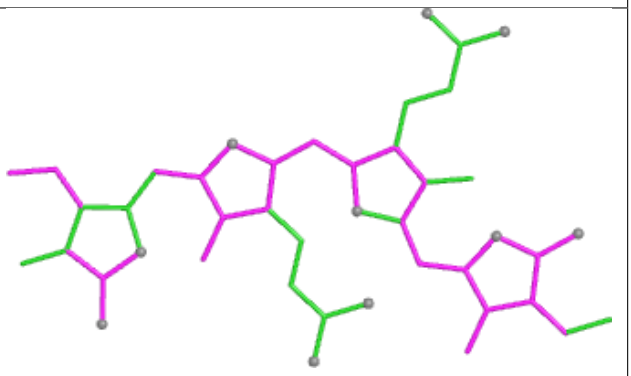


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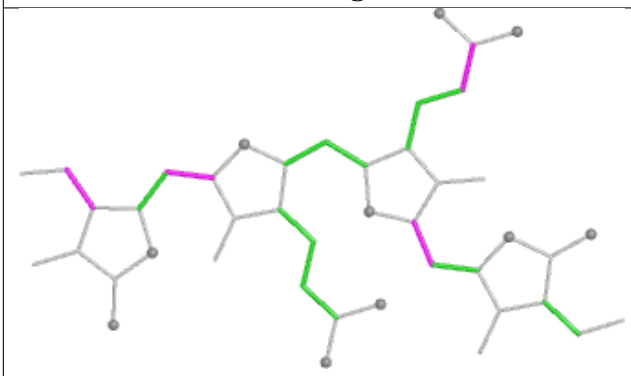
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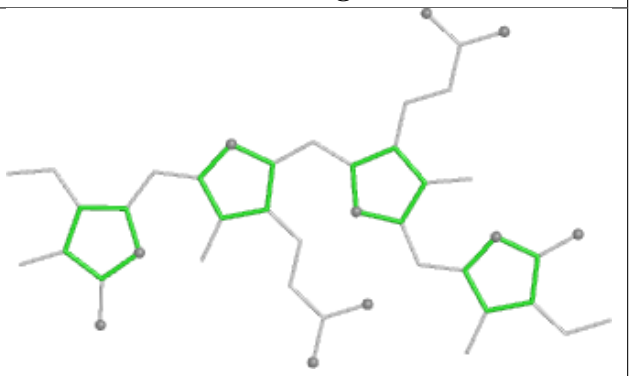
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Bond angles

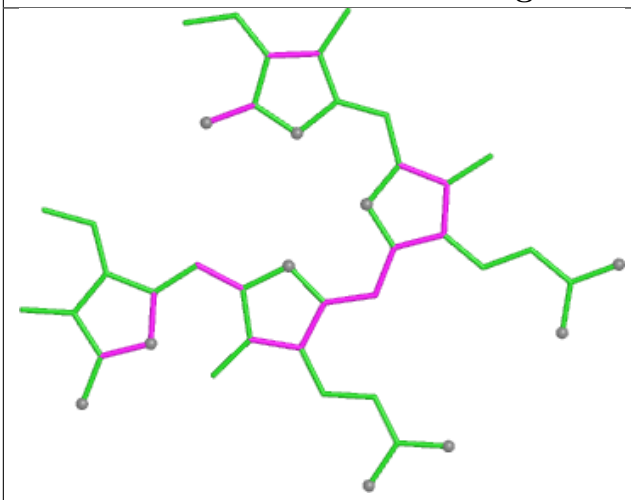


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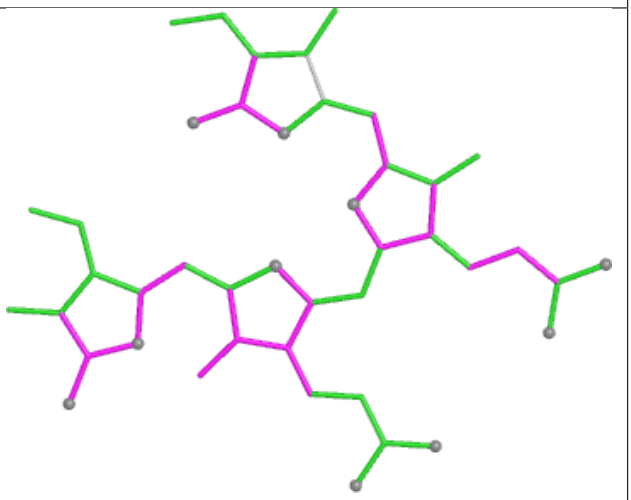


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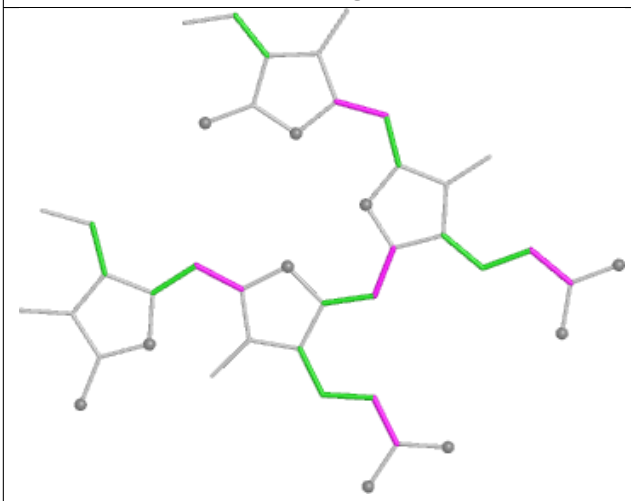
Ligand PEB cG 202



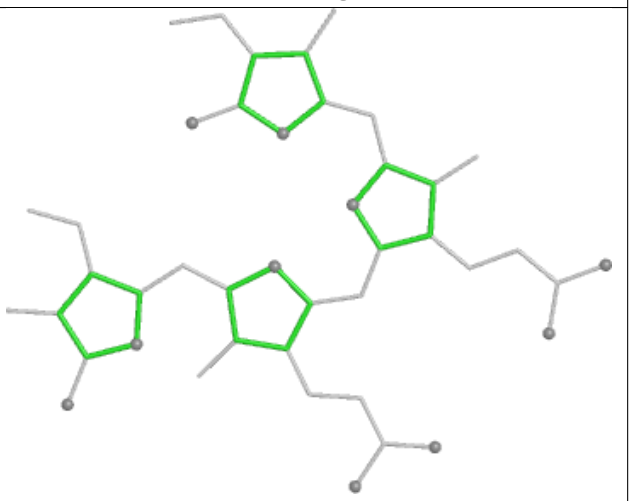
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Bond angles

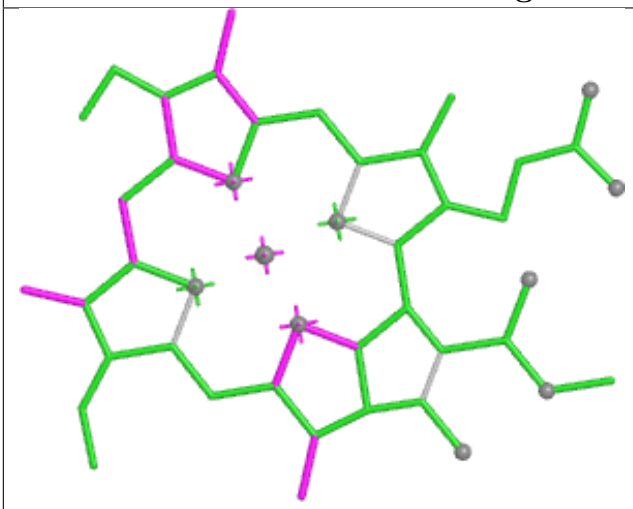


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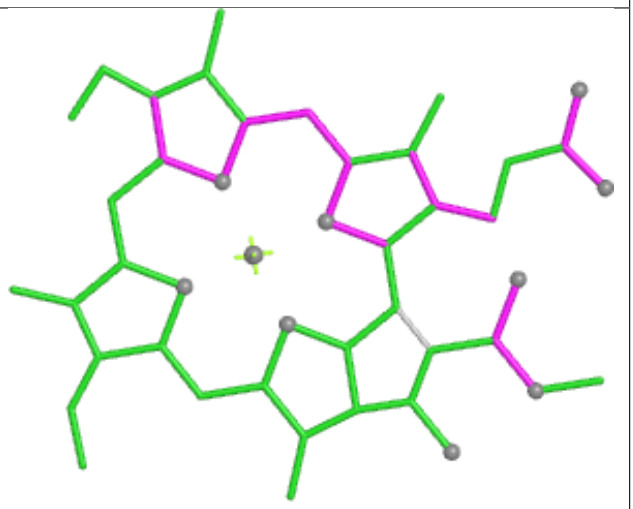


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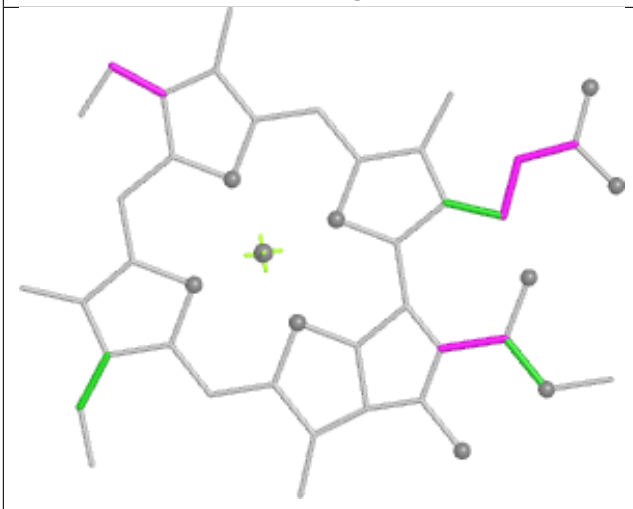
Ligand CLA B2 828



Bond lengths



Bond angles

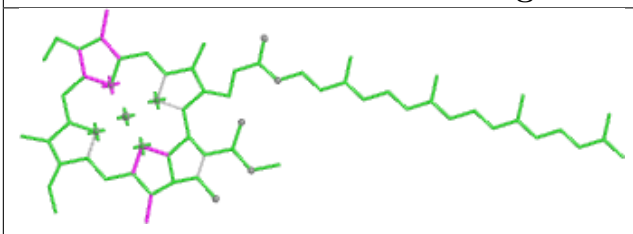


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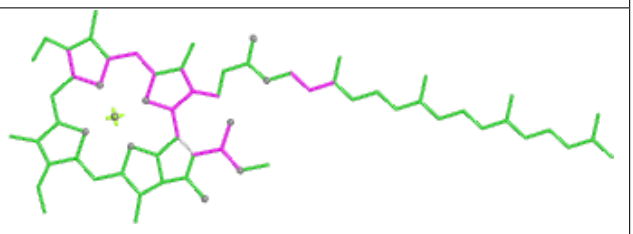


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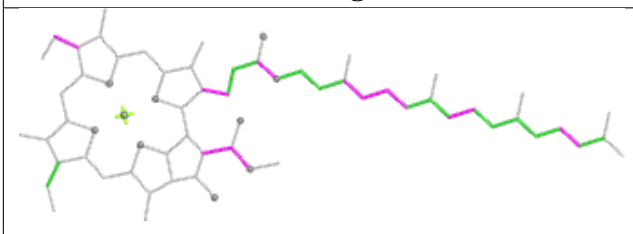
Ligand CLA dL 404



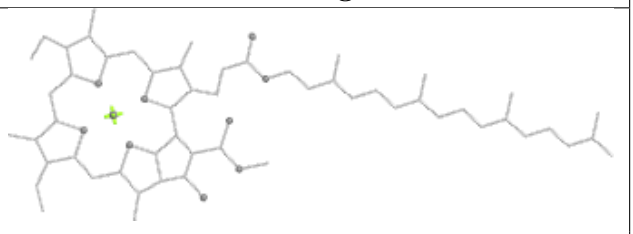
Bond lengths



Bond angles

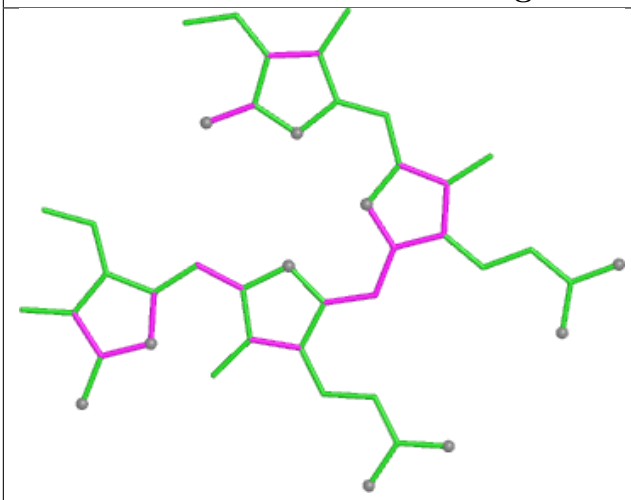


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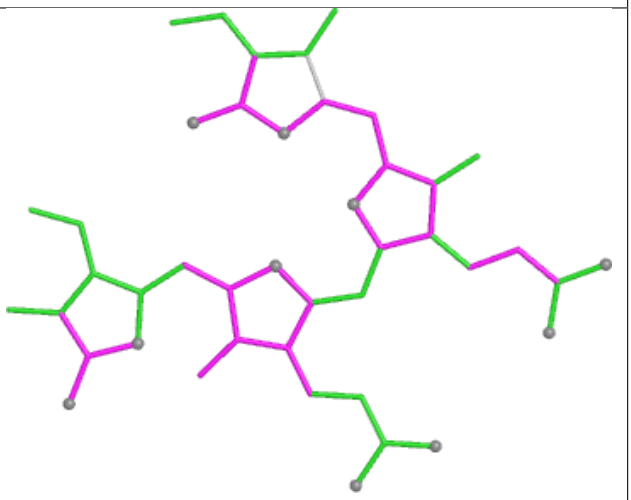


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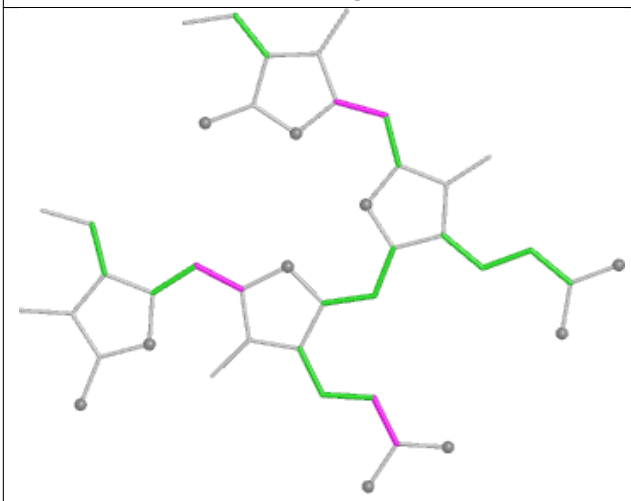
Ligand PEB LP 202



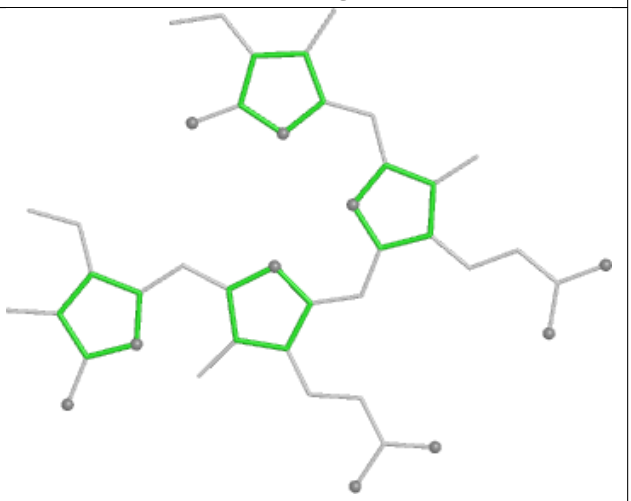
Bond lengths



Bond angles

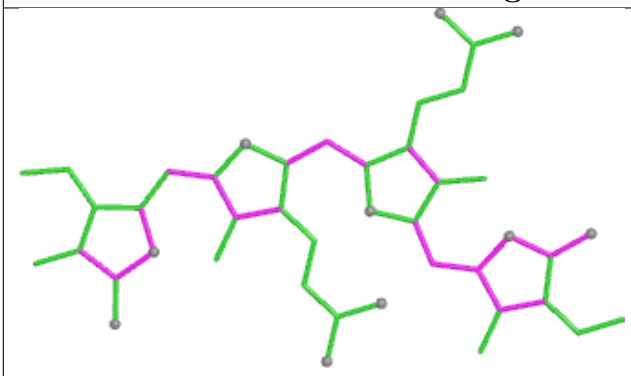


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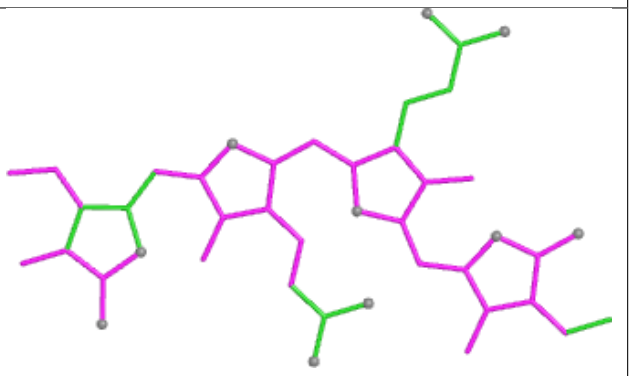


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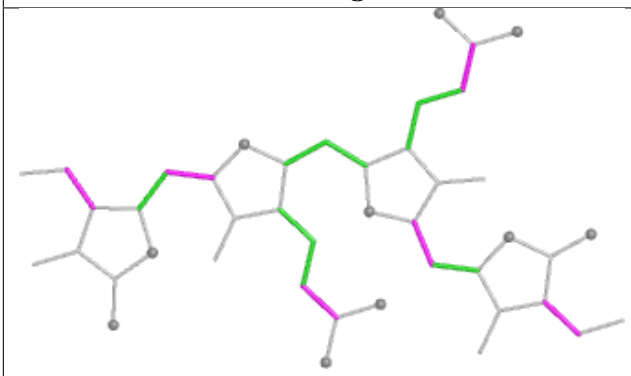
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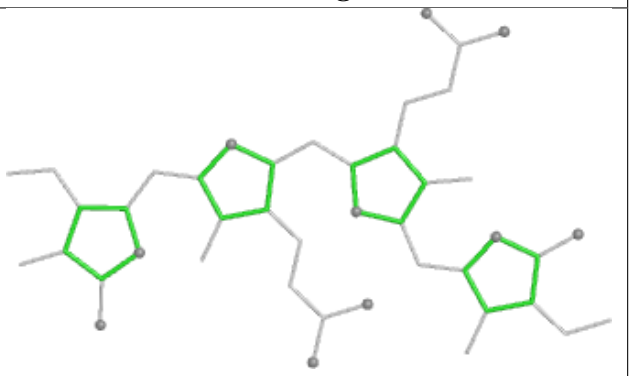
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Bond angles

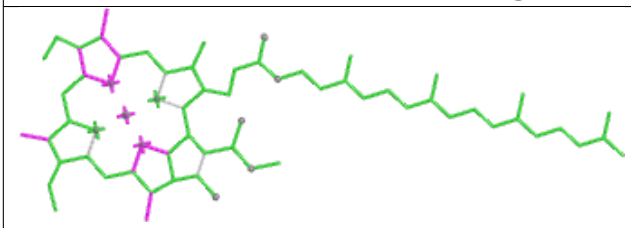


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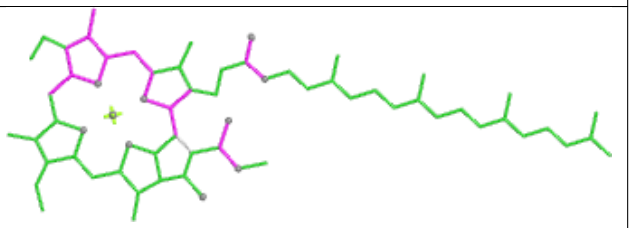


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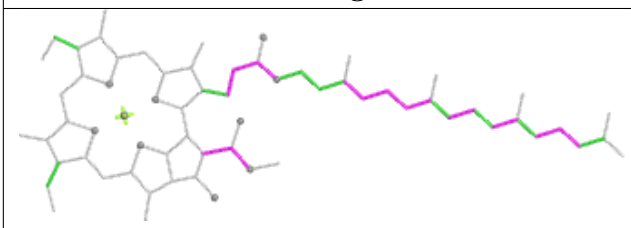
Ligand CLA AN 823



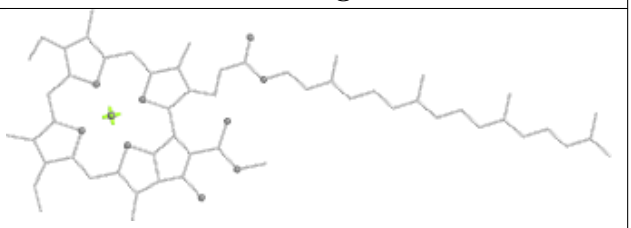
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Bond angles

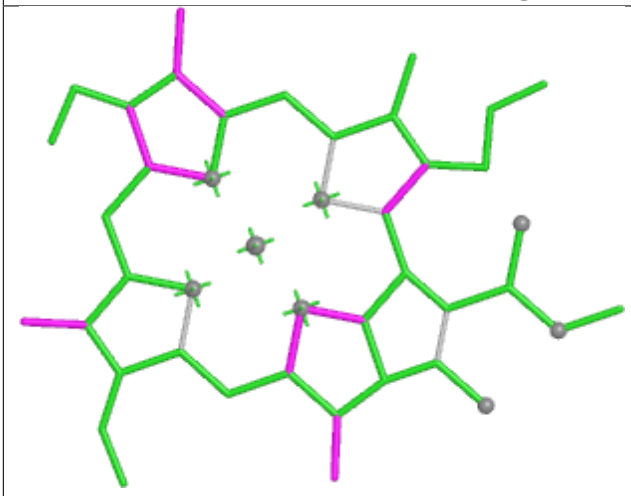


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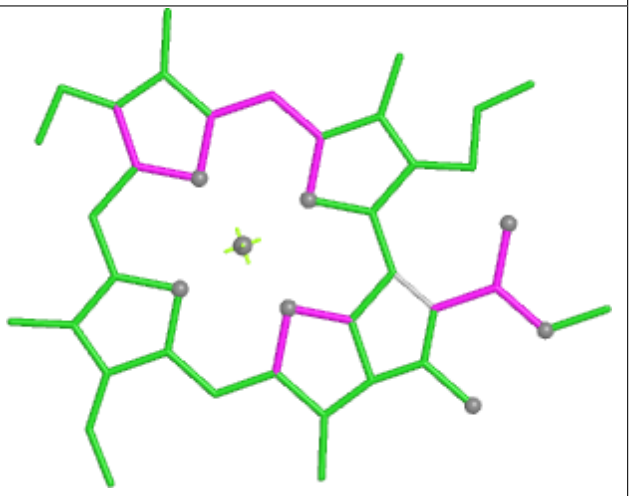


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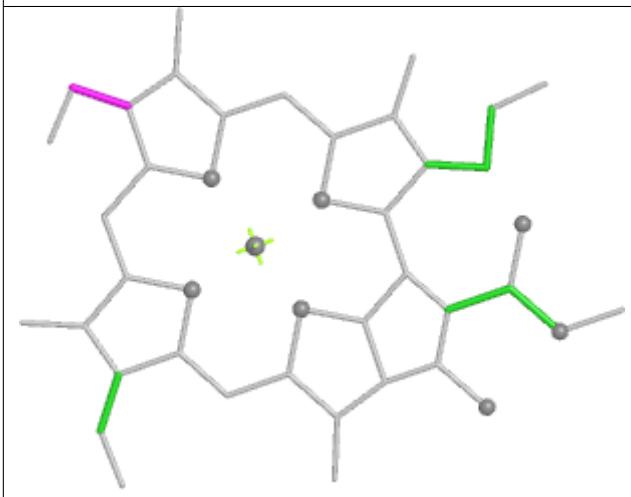
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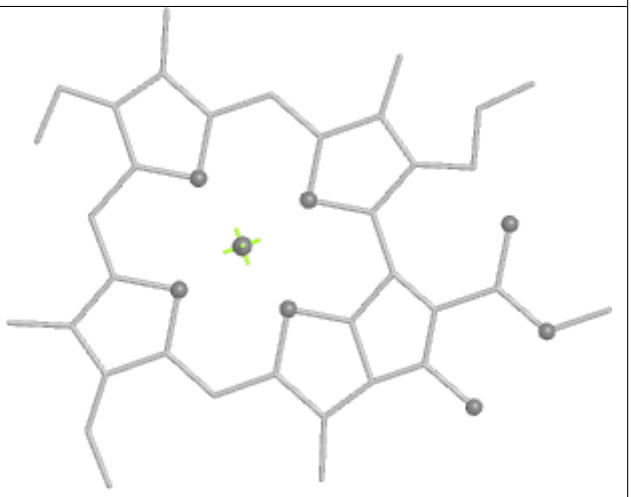
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Bond angles

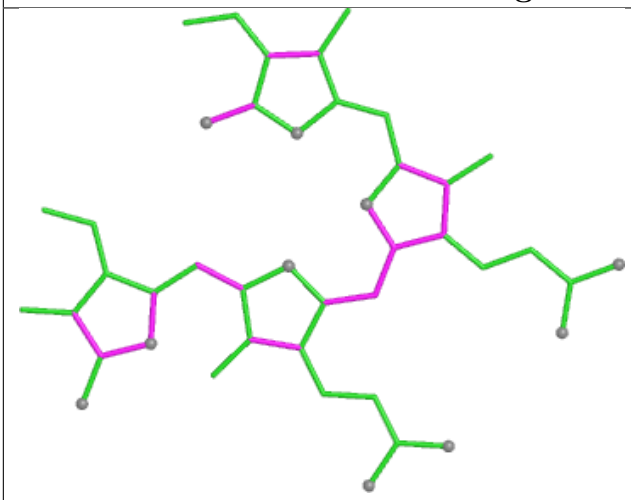


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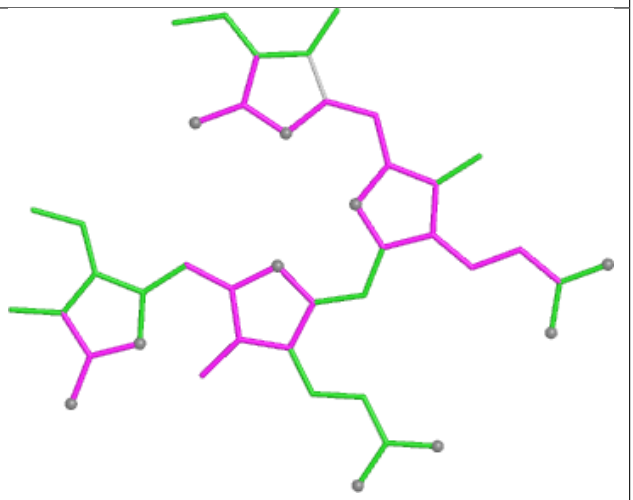


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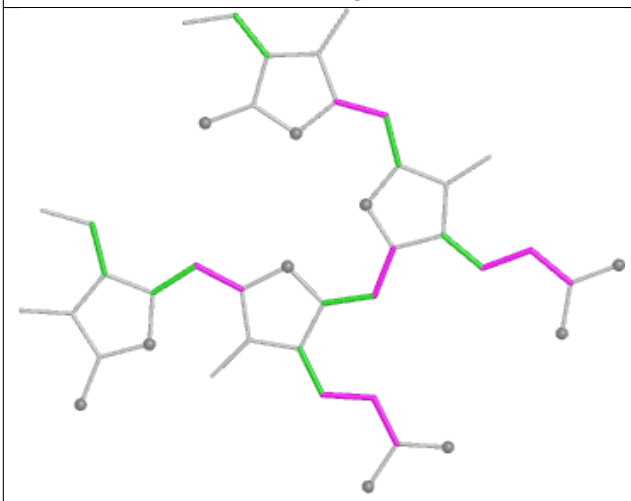
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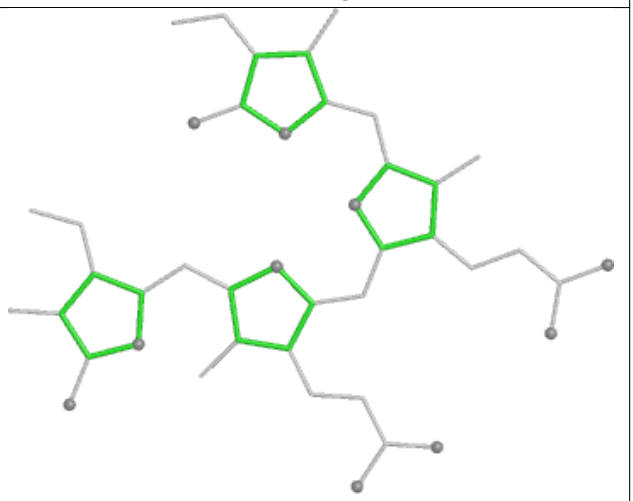
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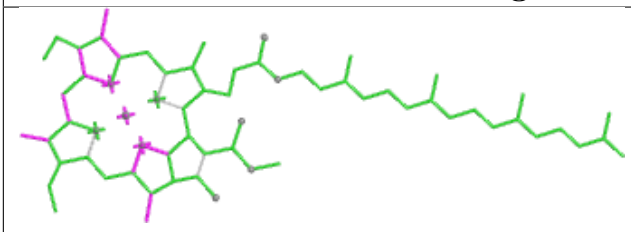


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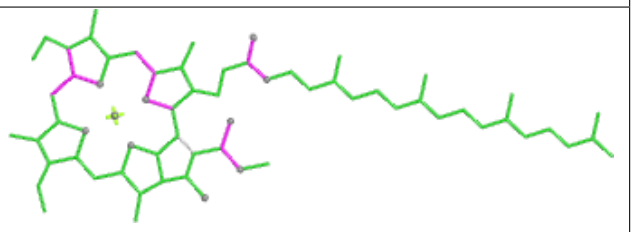


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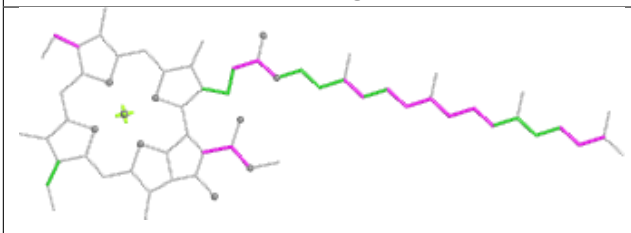
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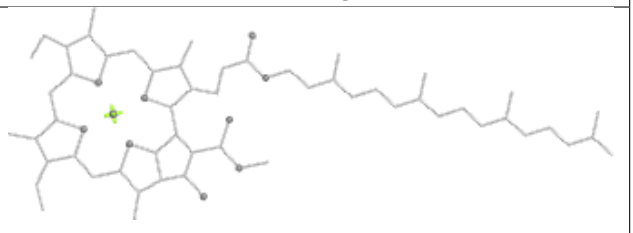
Bond lengths



Bond angles

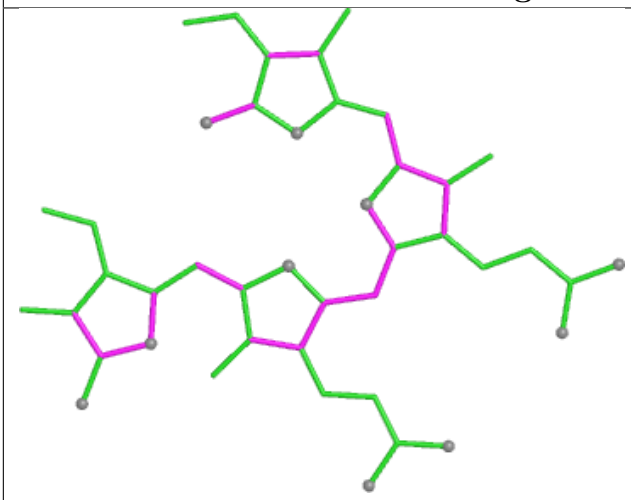


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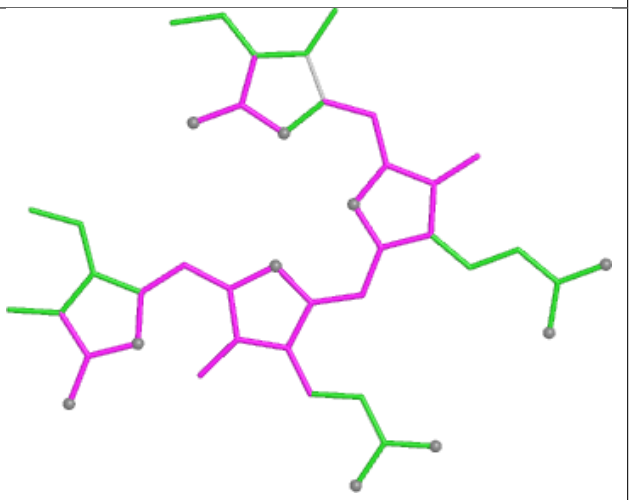


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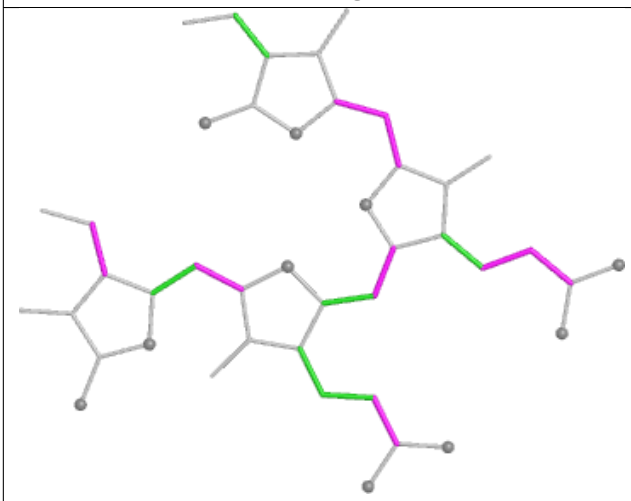
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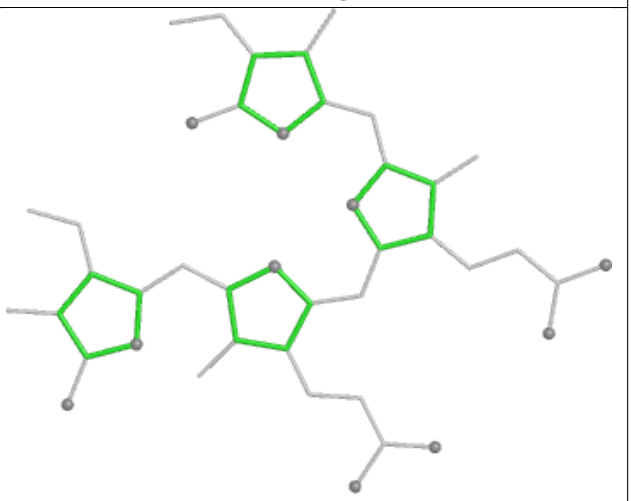
Bond lengths



Bond angles

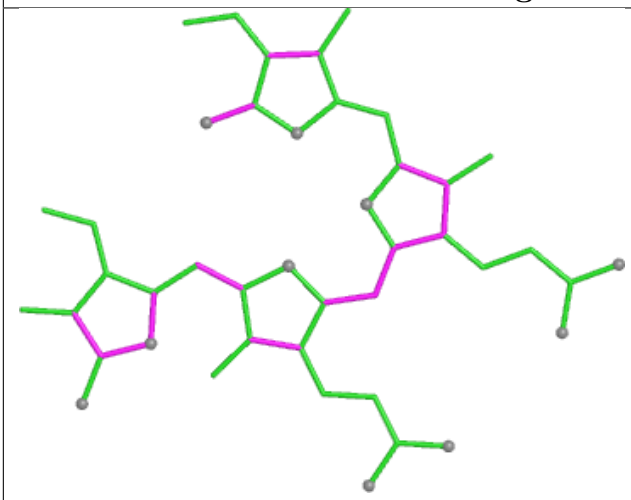


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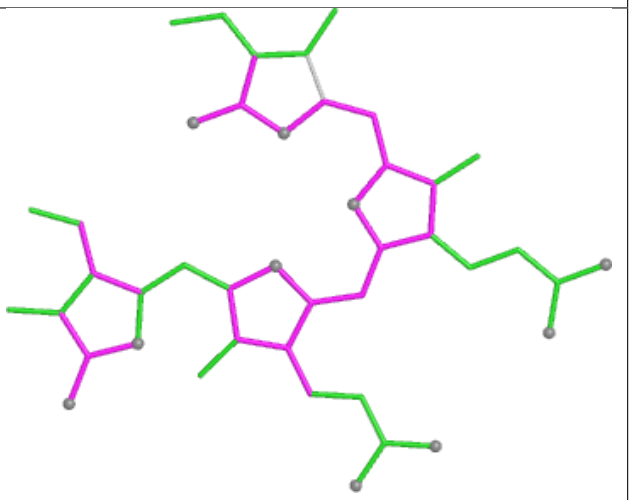


Rings

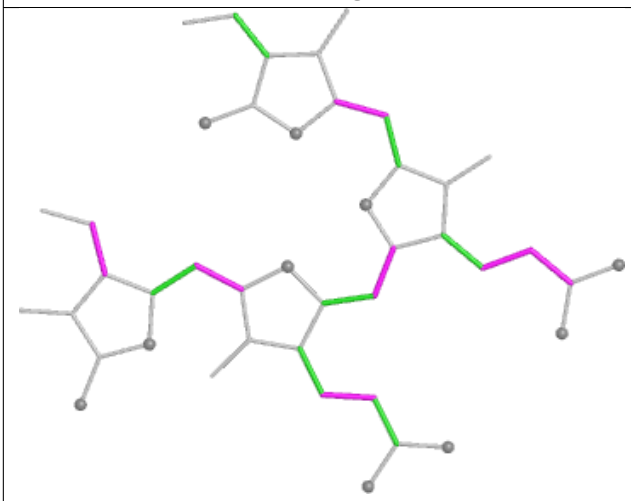
Ligand PEB Y5 202



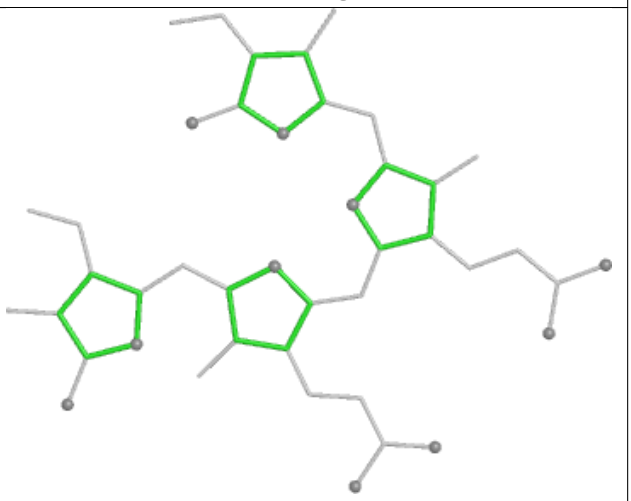
Bond lengths



Bond angles

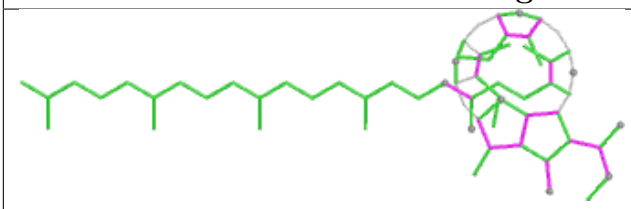


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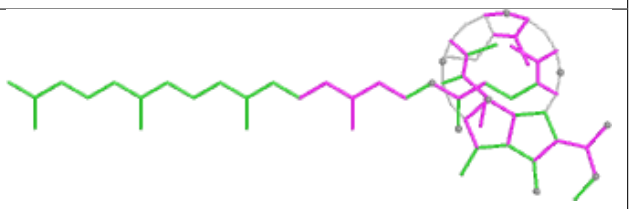


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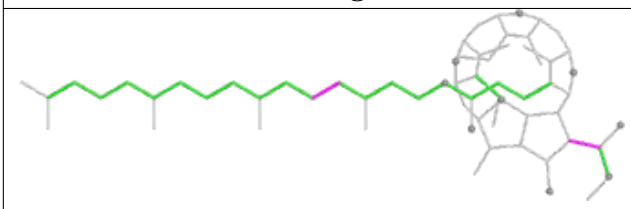
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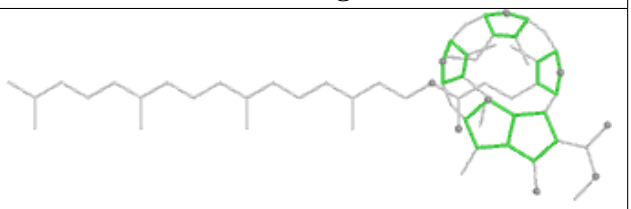
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Bond angles

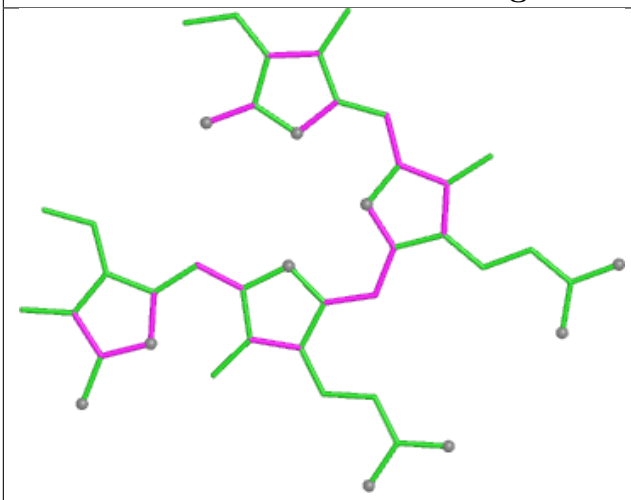


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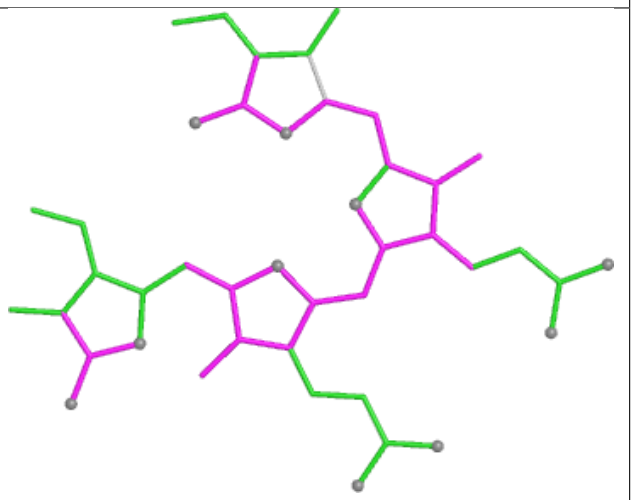


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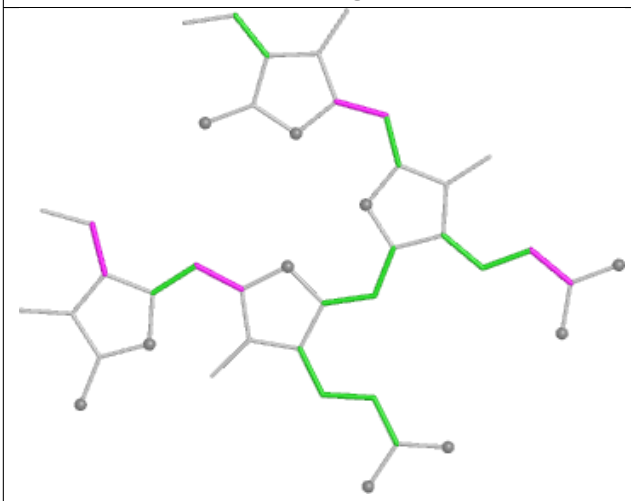
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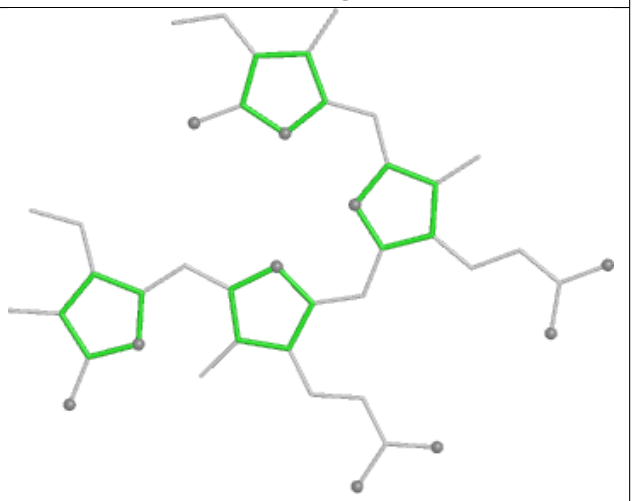
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Bond angles

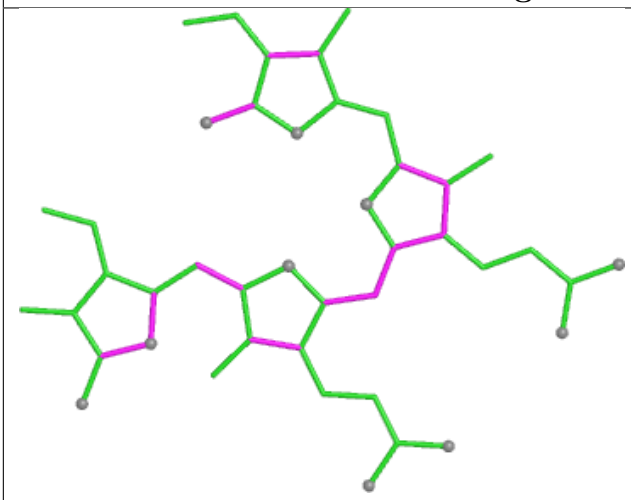


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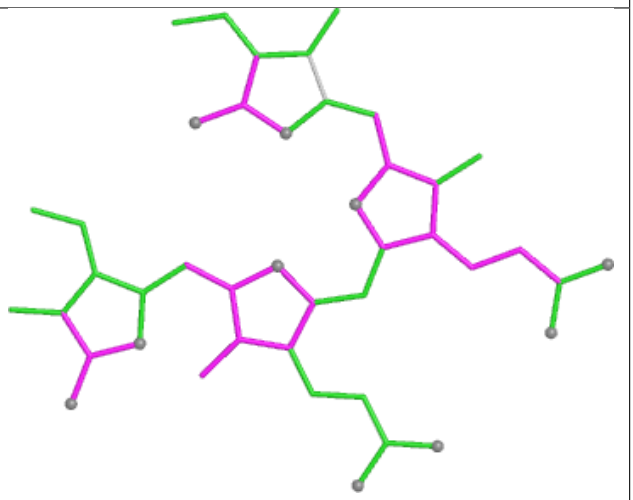


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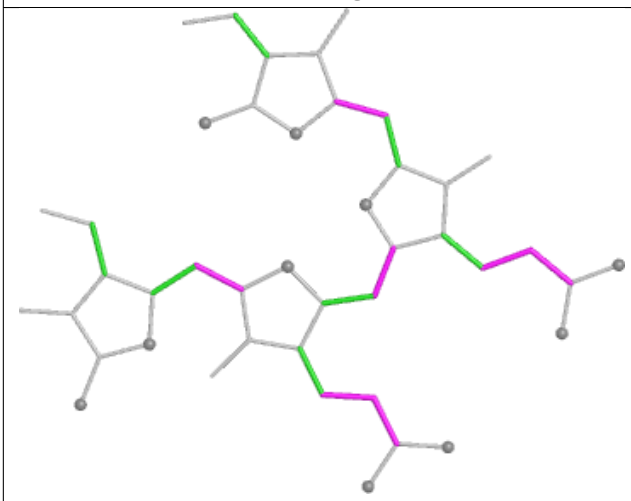
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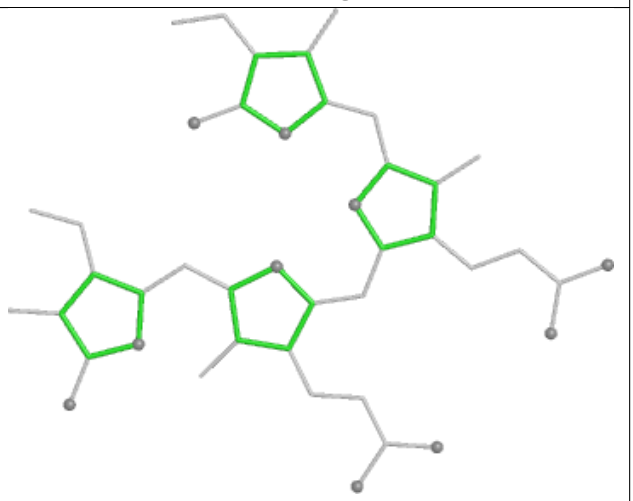
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Bond angles

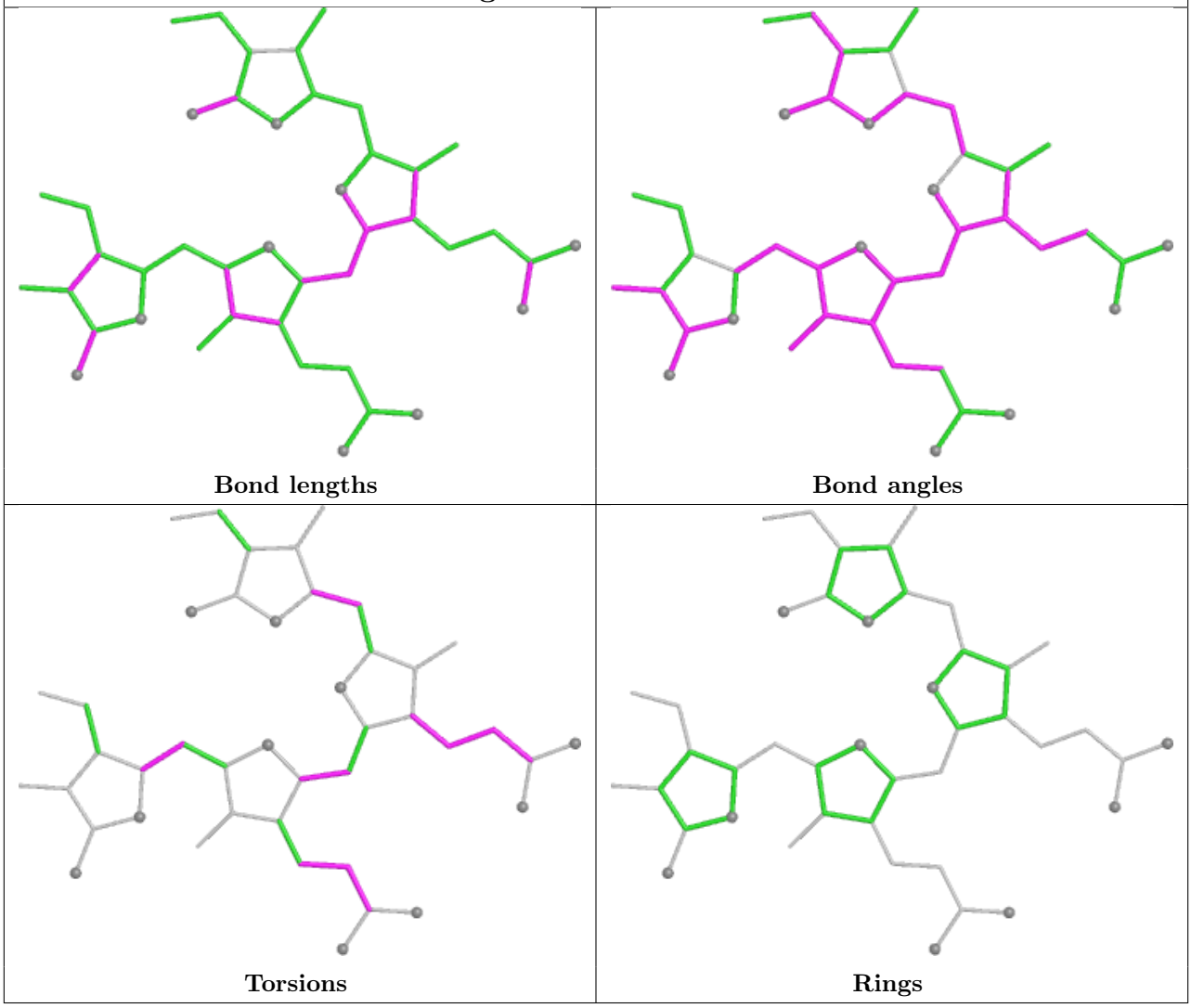


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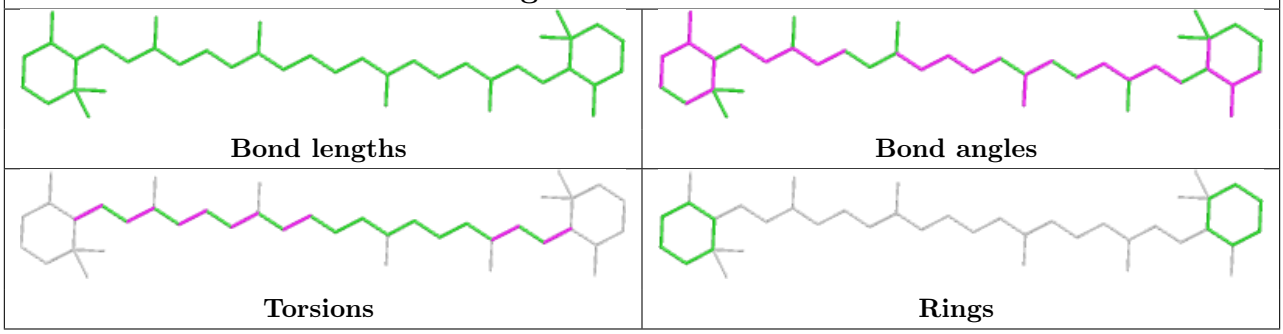


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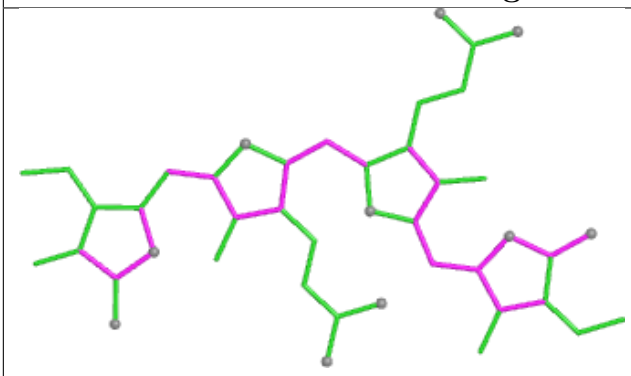
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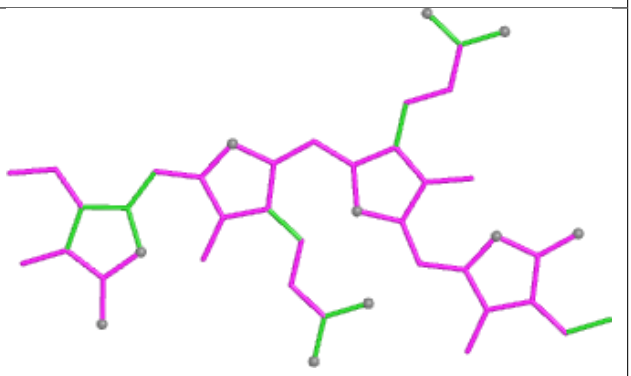
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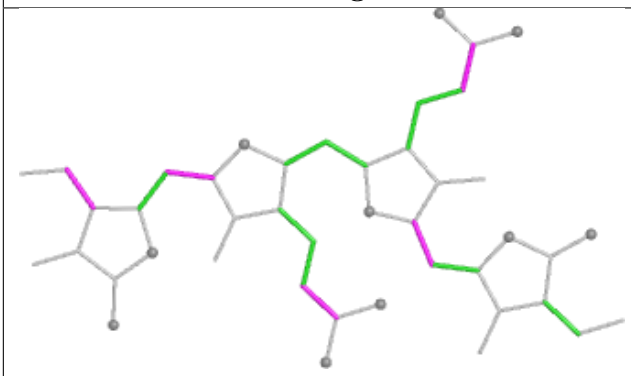
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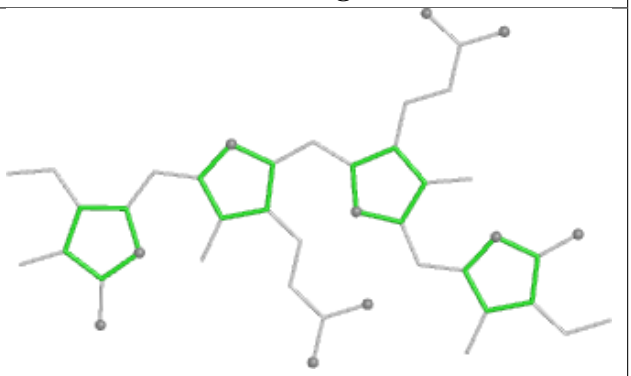
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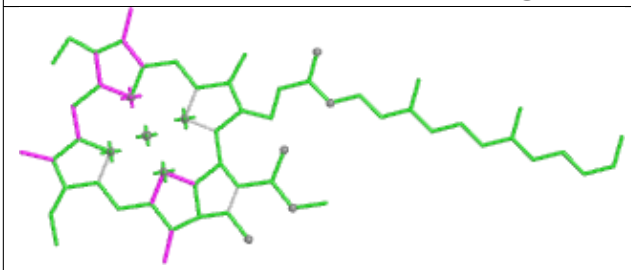


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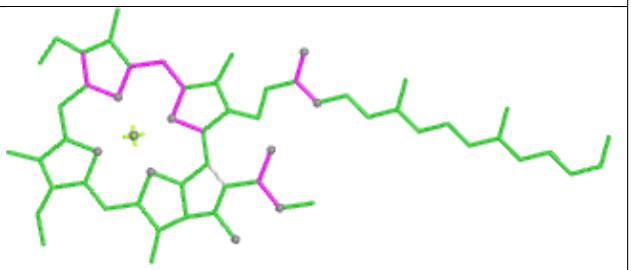


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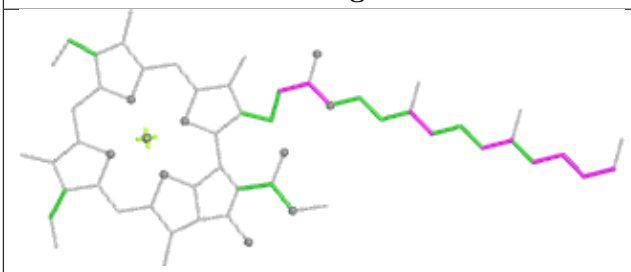
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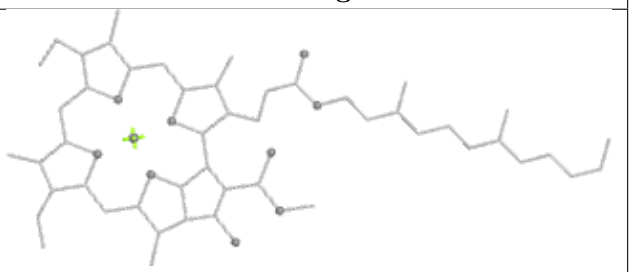
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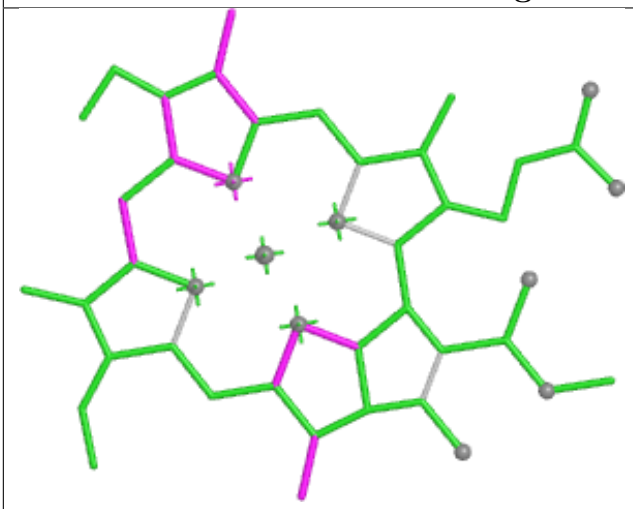


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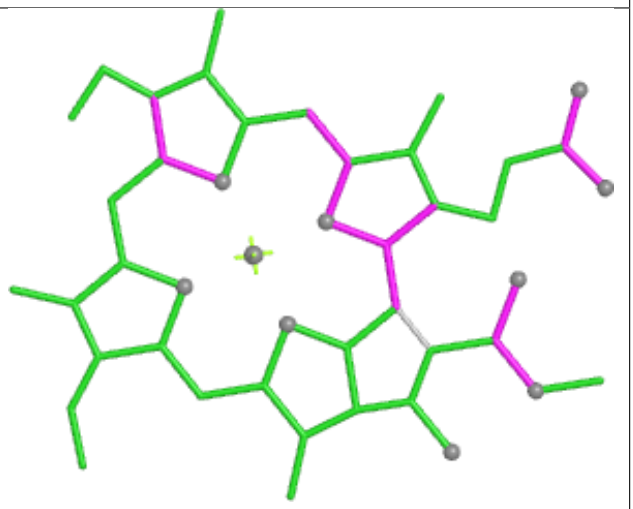


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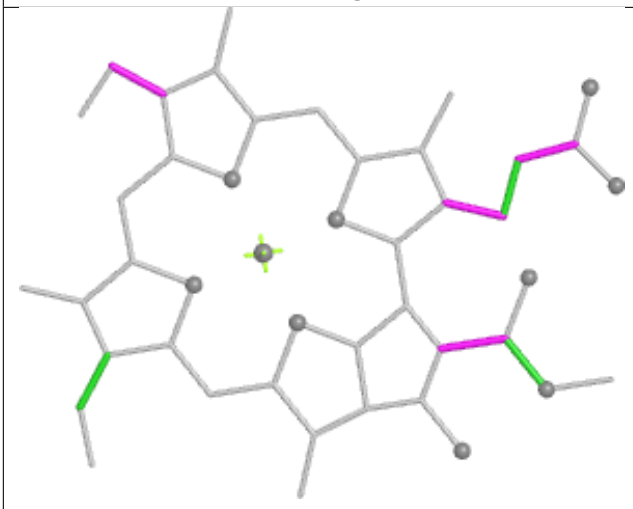
Ligand CLA 7N 606



Bond lengths



Bond angles

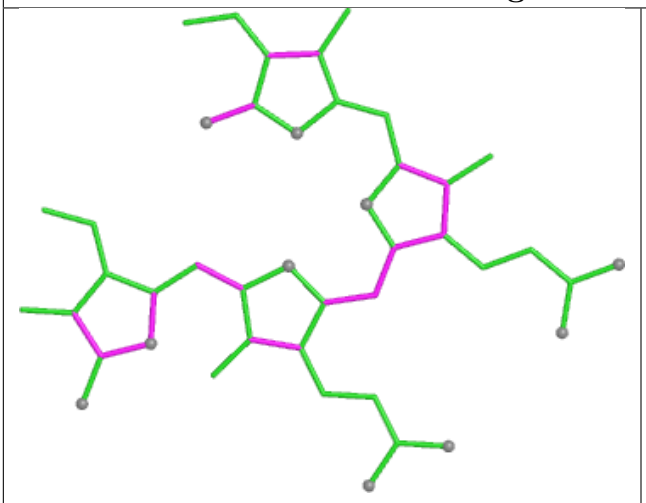


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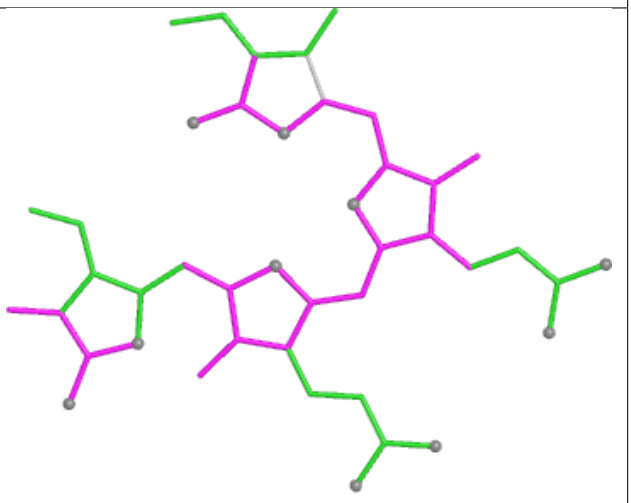


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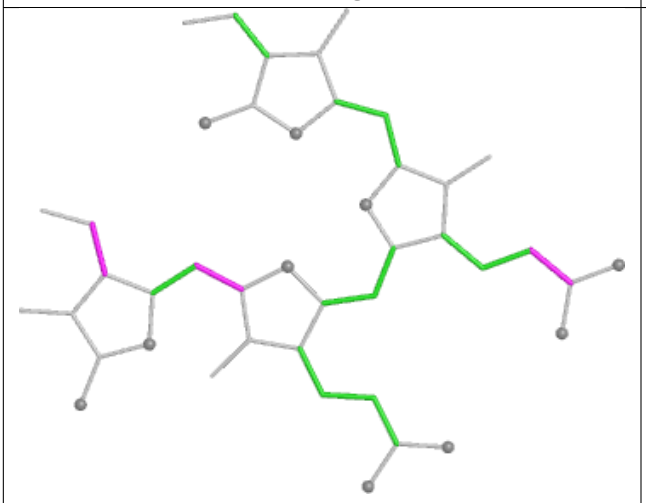
Ligand PEB OM 203



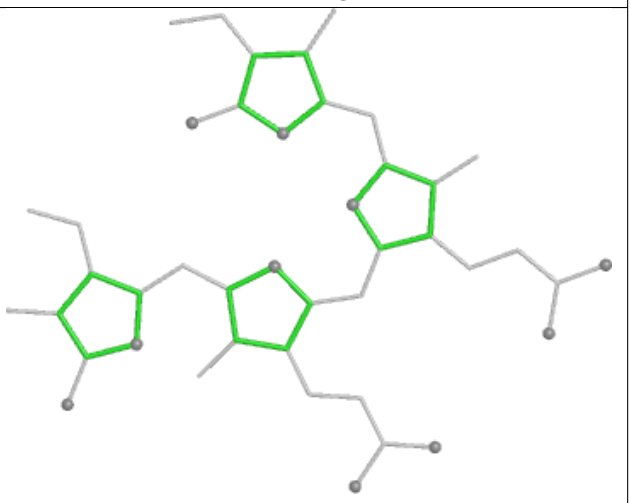
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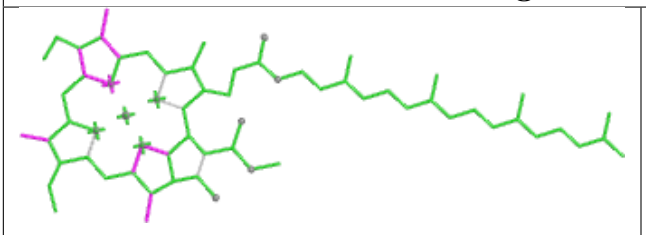


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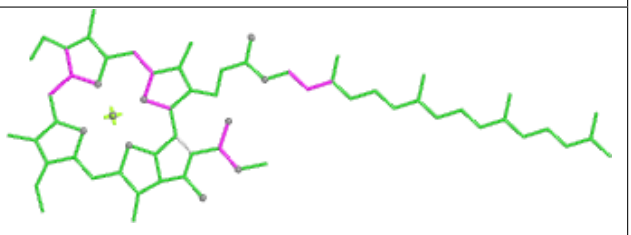


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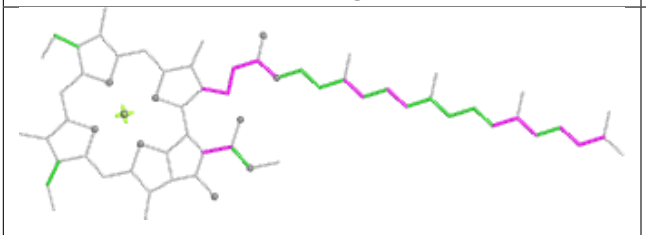
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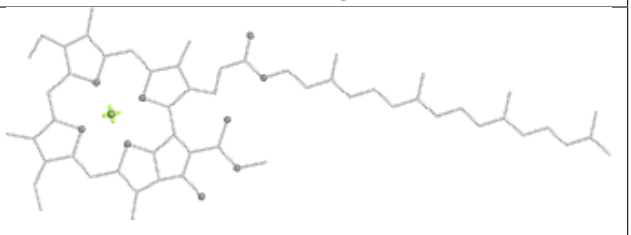
Bond lengths



Bond angles

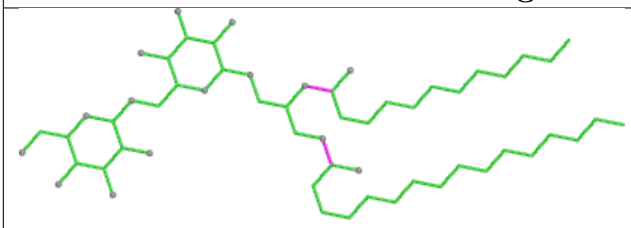


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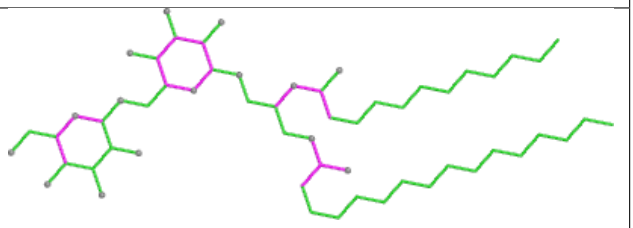


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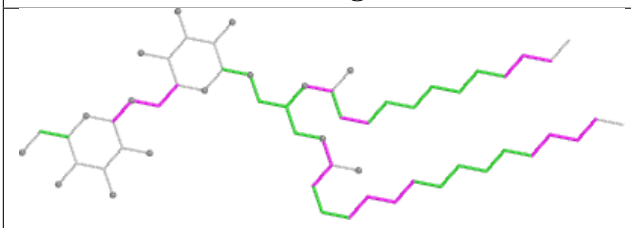
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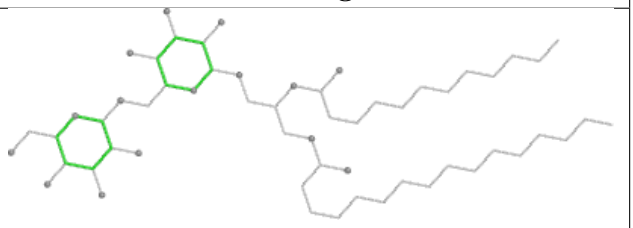
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Bond angles

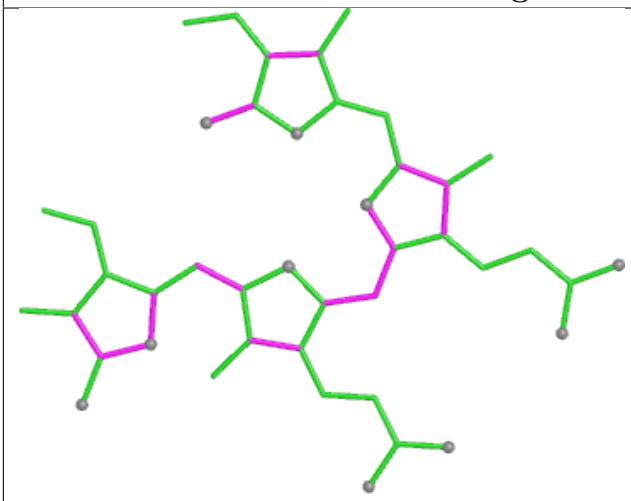


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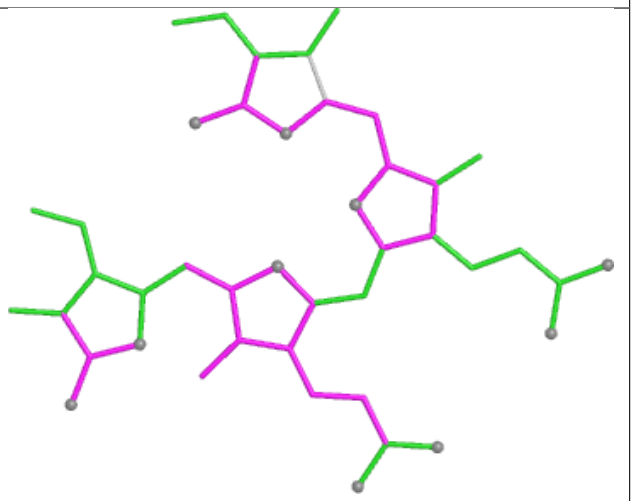


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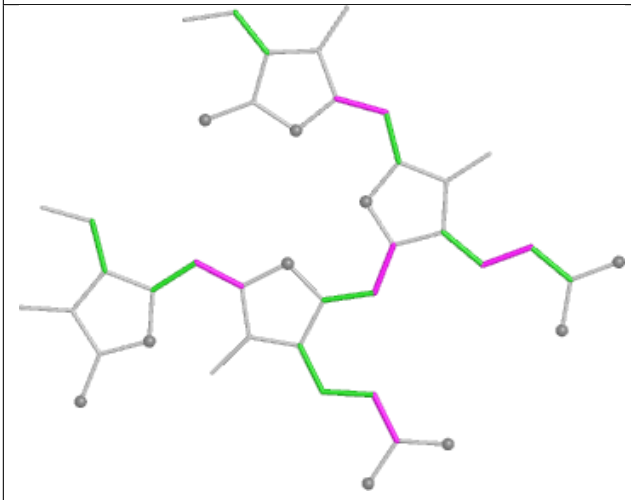
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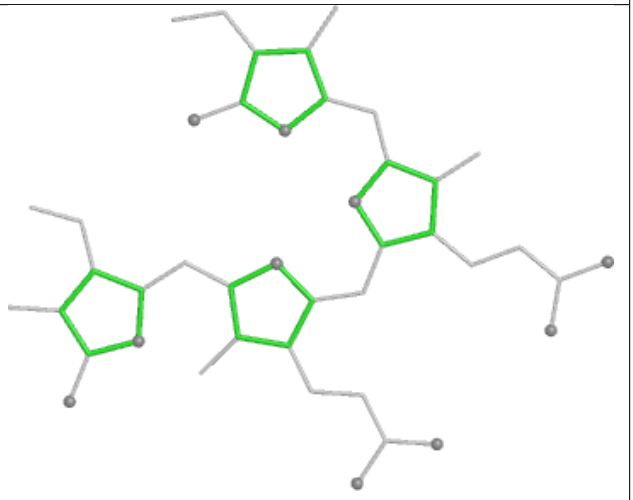
Bond lengths



Bond angles

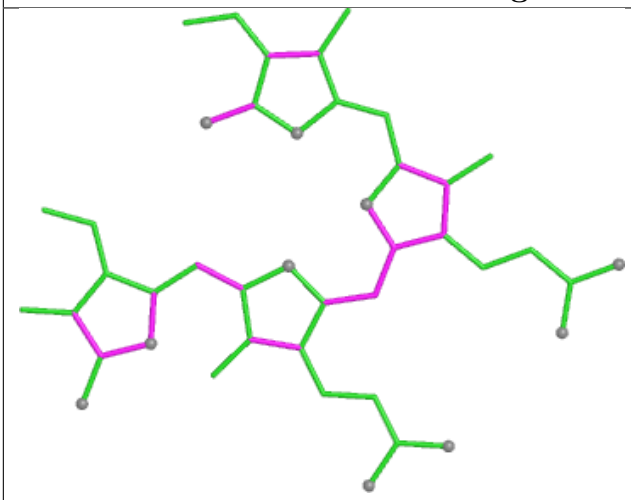


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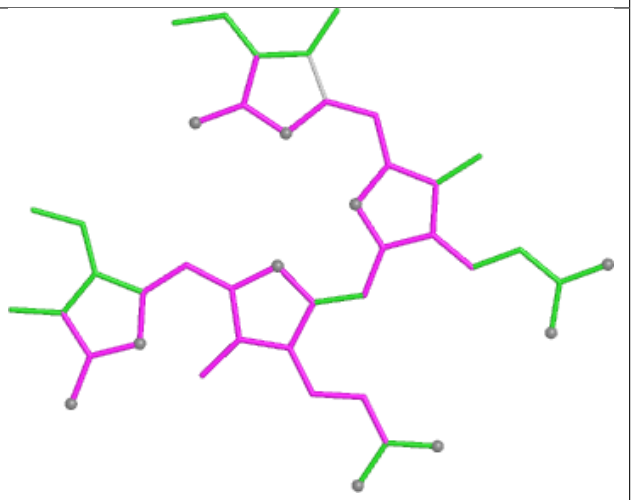


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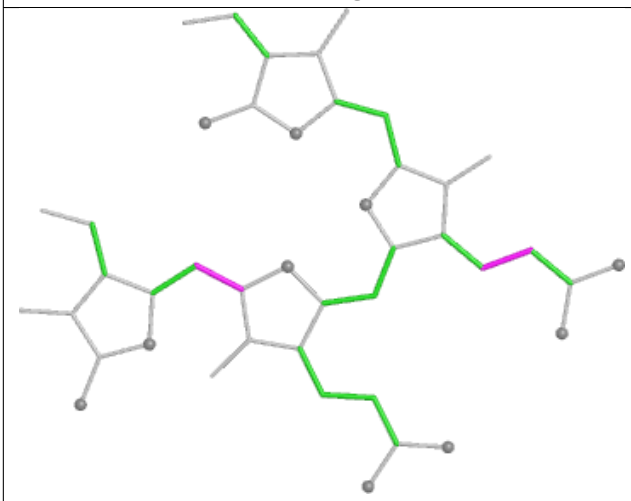
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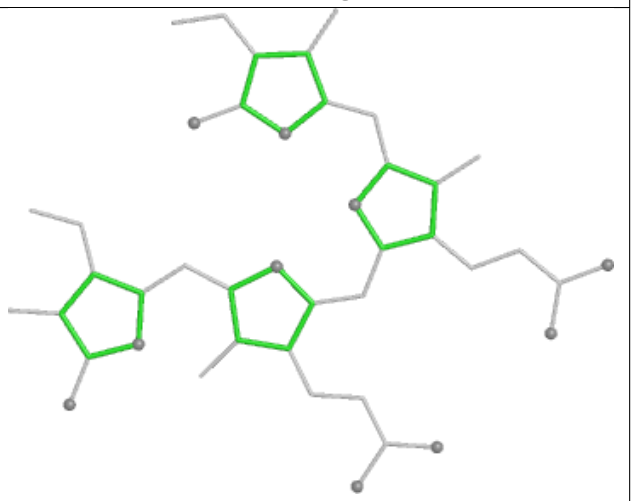
Bond lengths



Bond angles

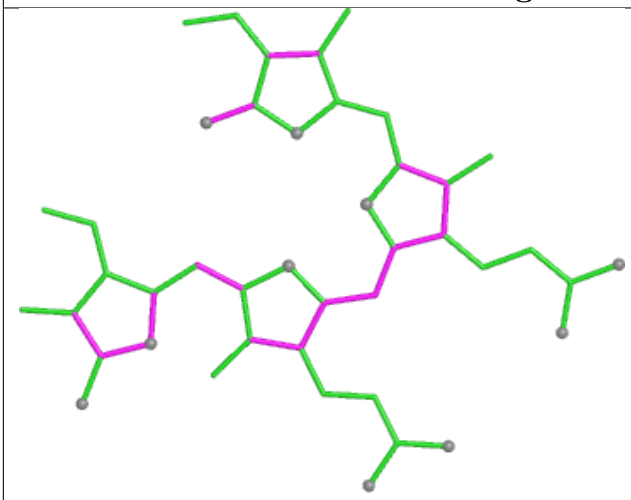


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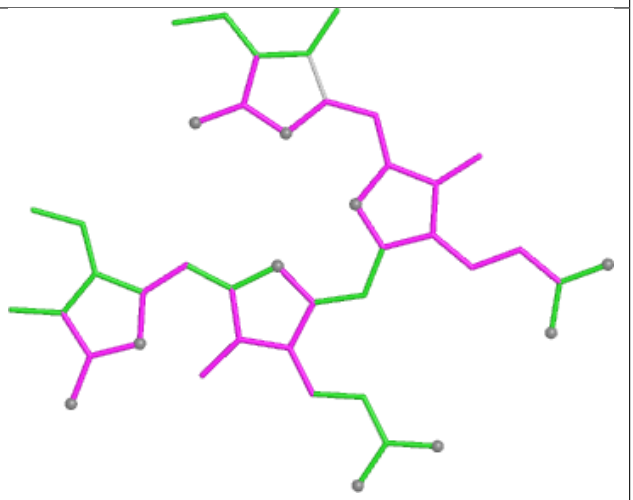


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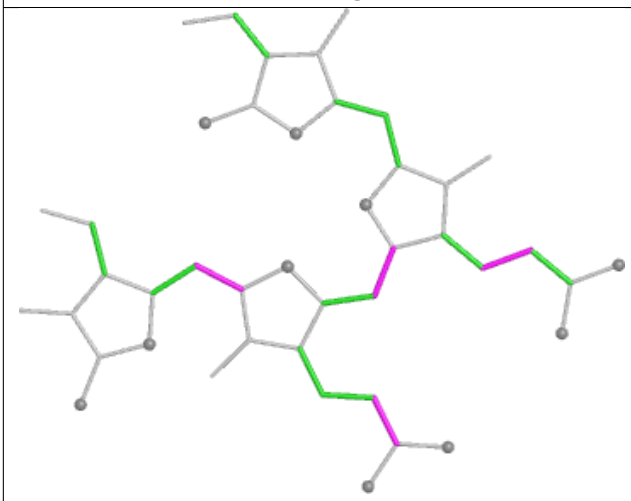
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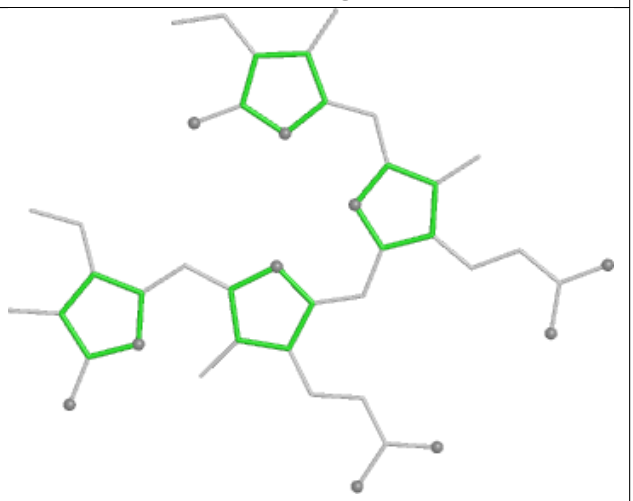
Bond lengths



Bond angles

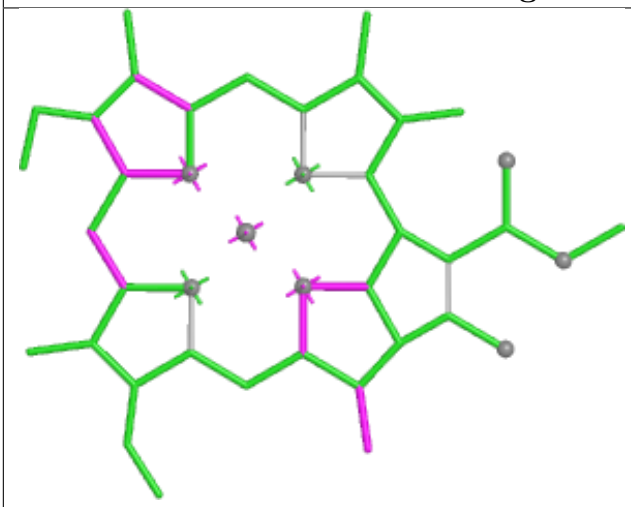


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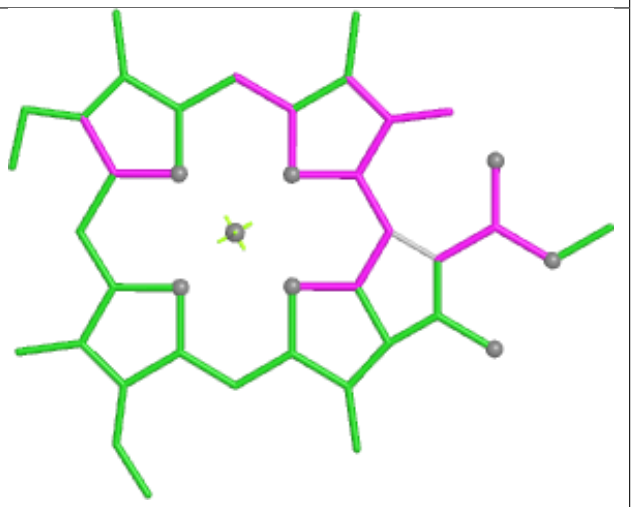


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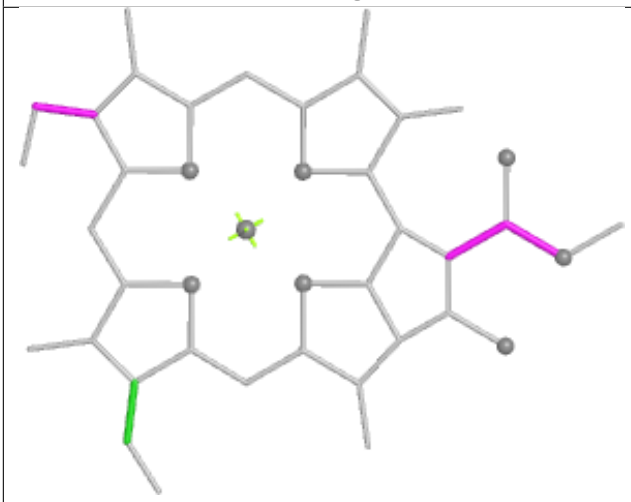
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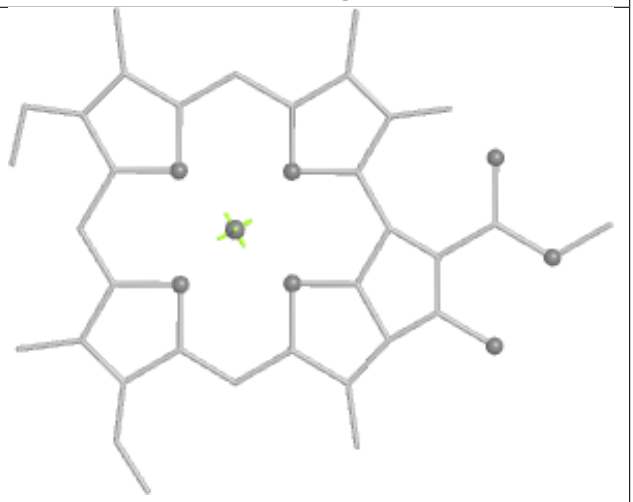
Bond lengths



Bond angles

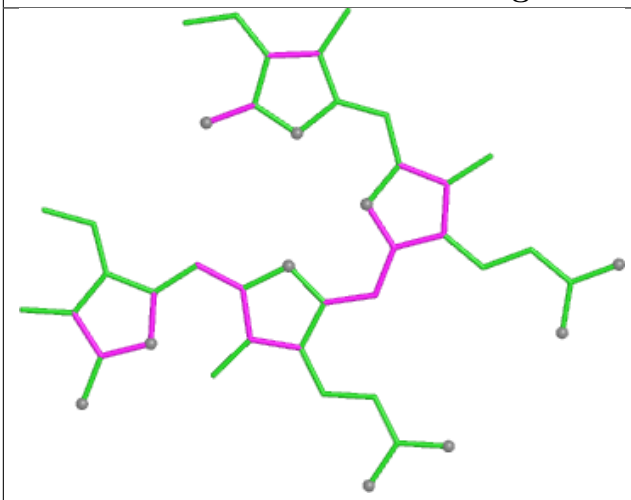


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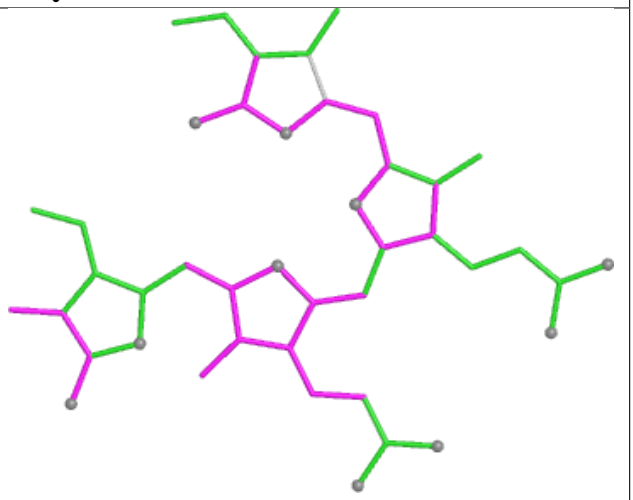


Rings

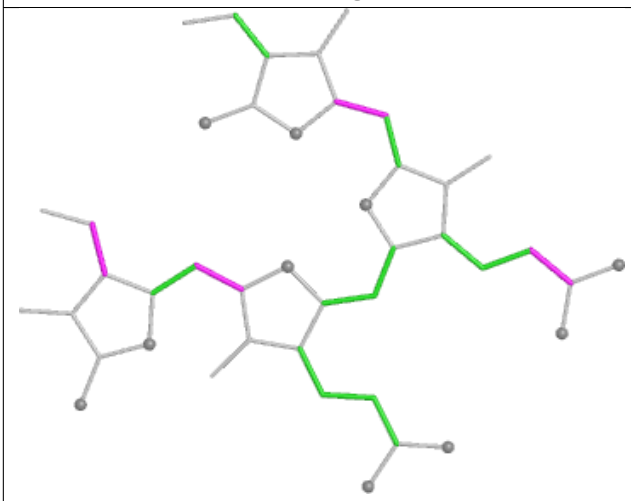
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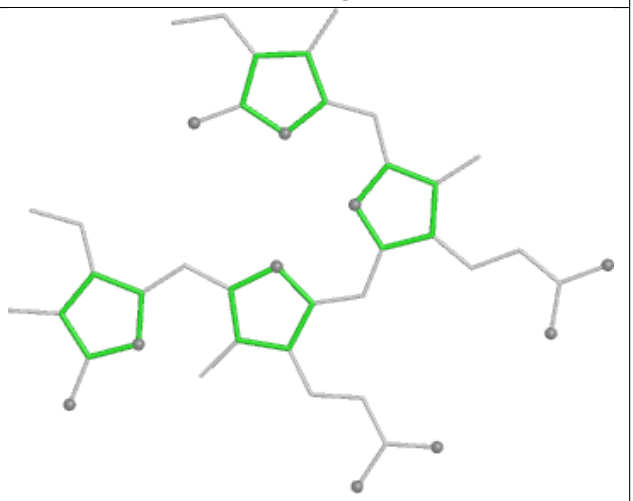
Bond lengths



Bond angles

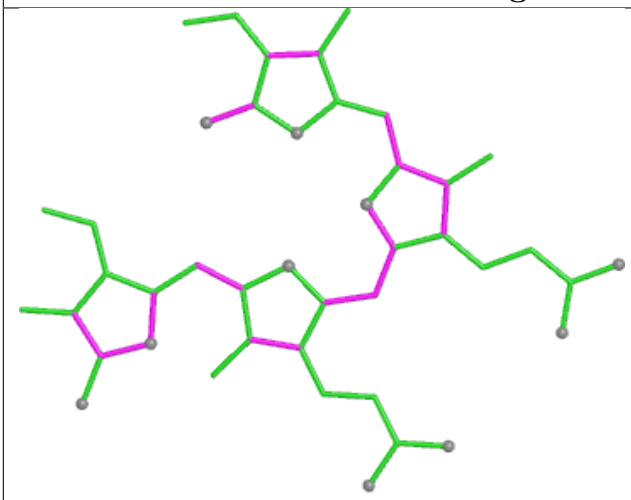


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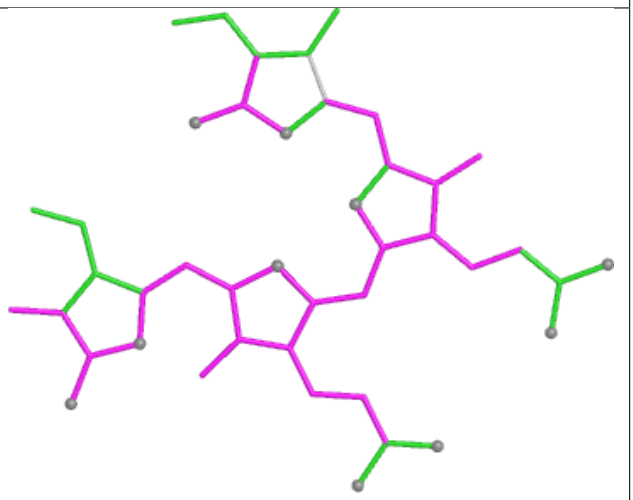


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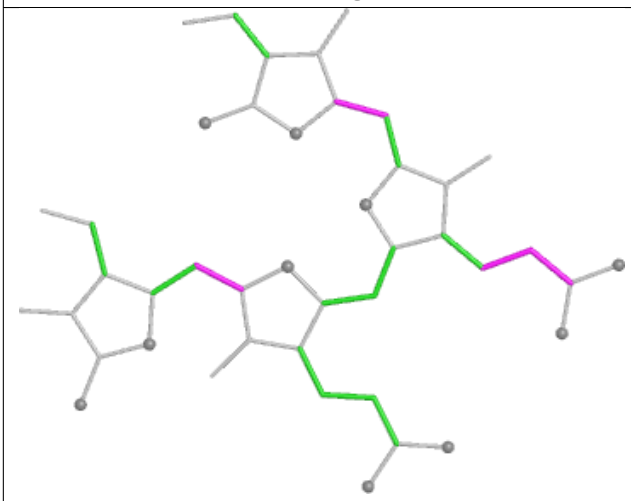
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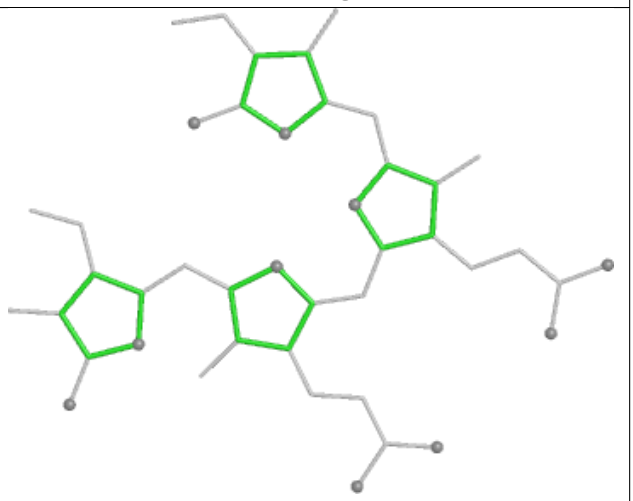
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Bond angles

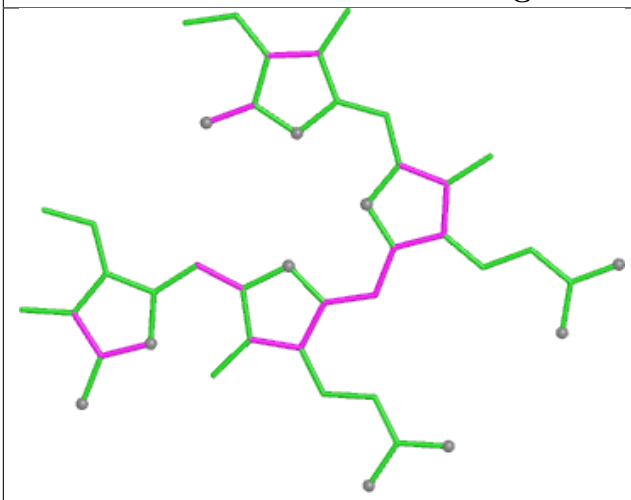


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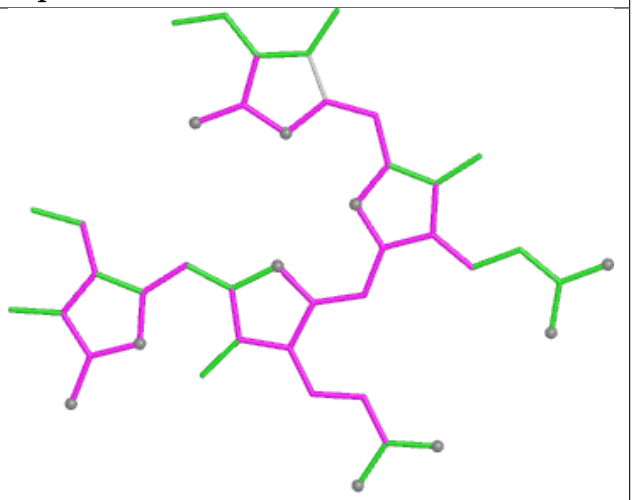


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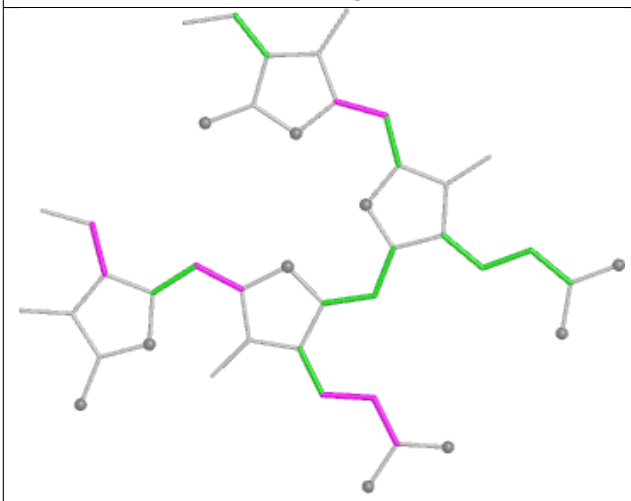
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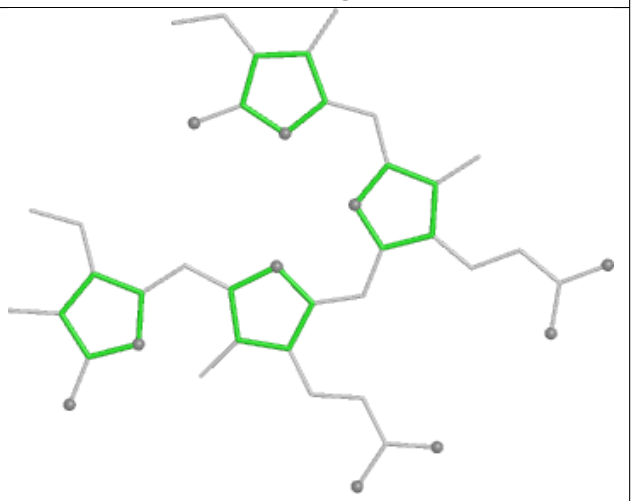
Bond lengths



Bond angles

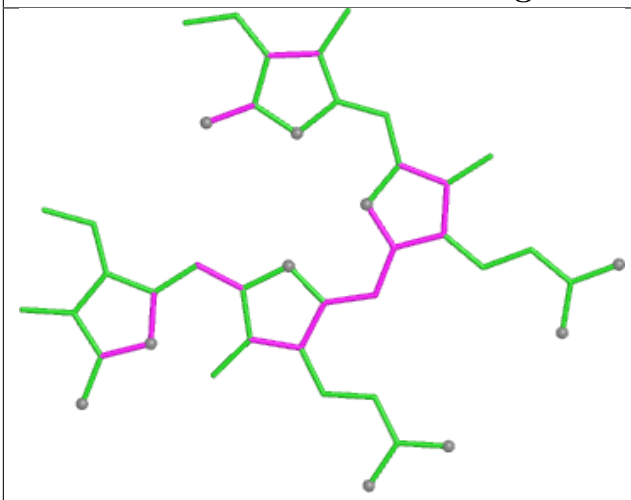


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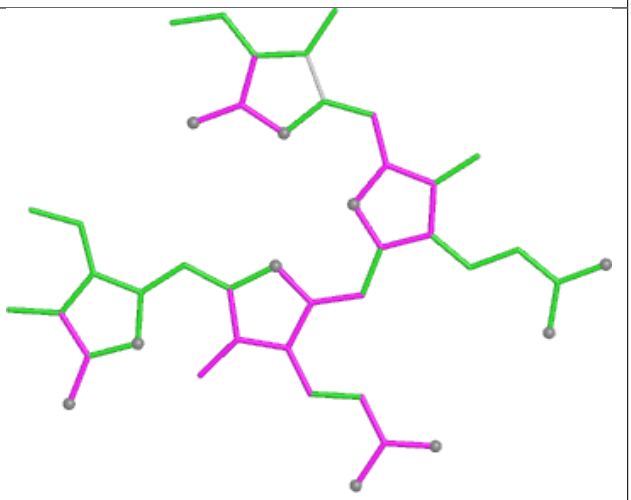


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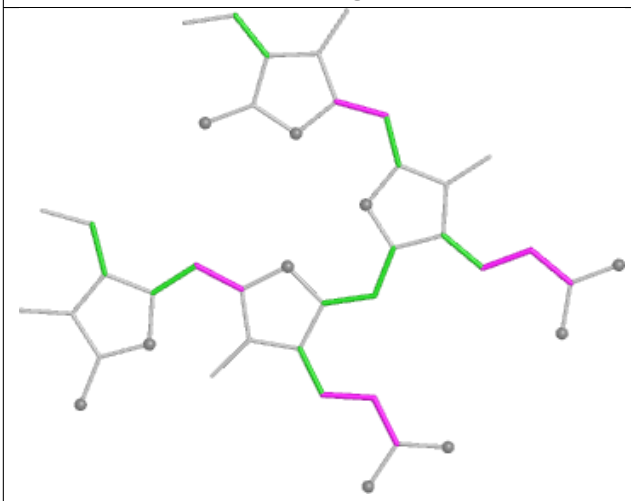
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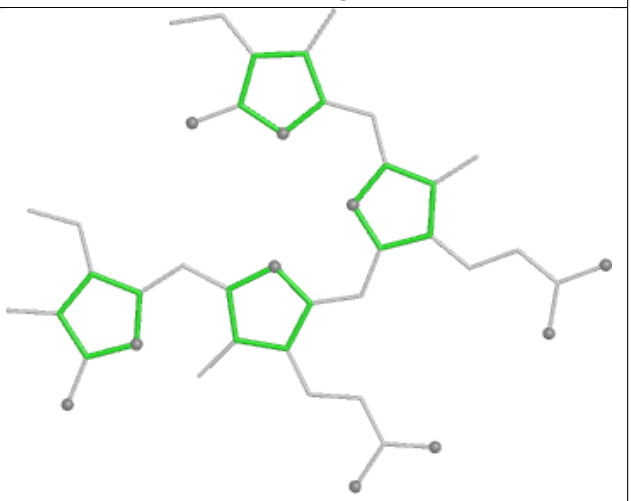
Bond lengths



Bond angles

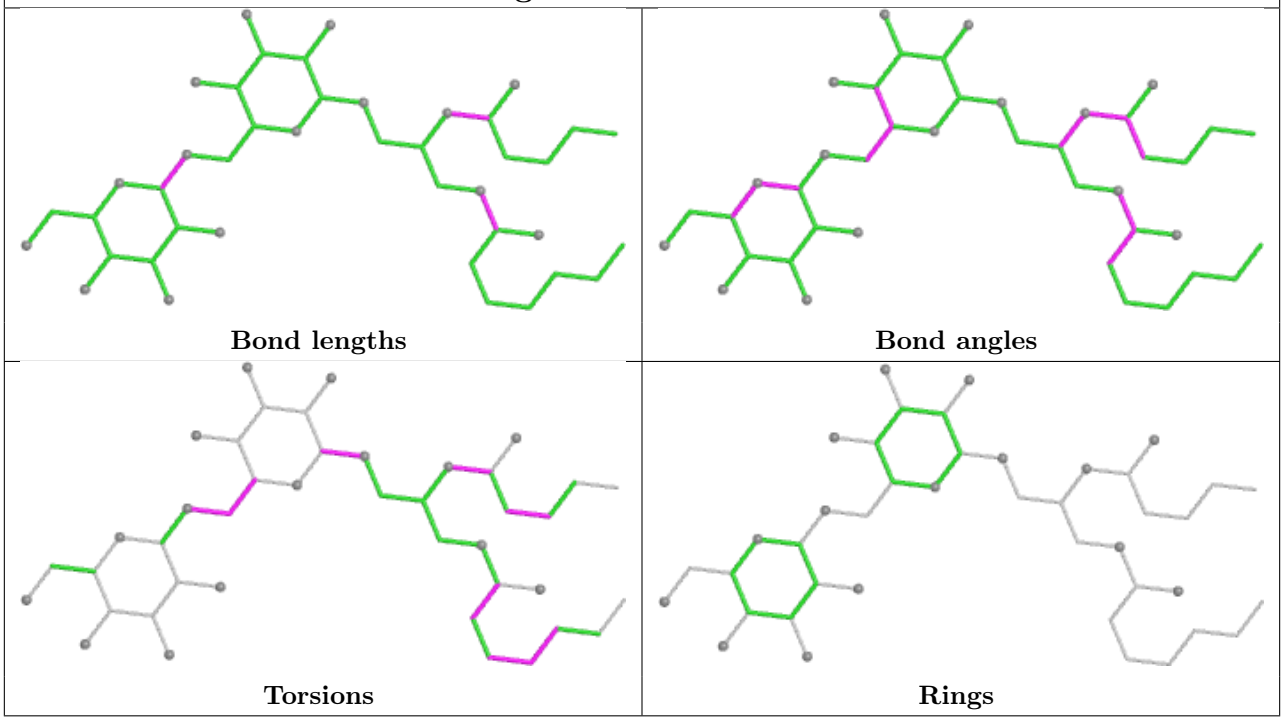


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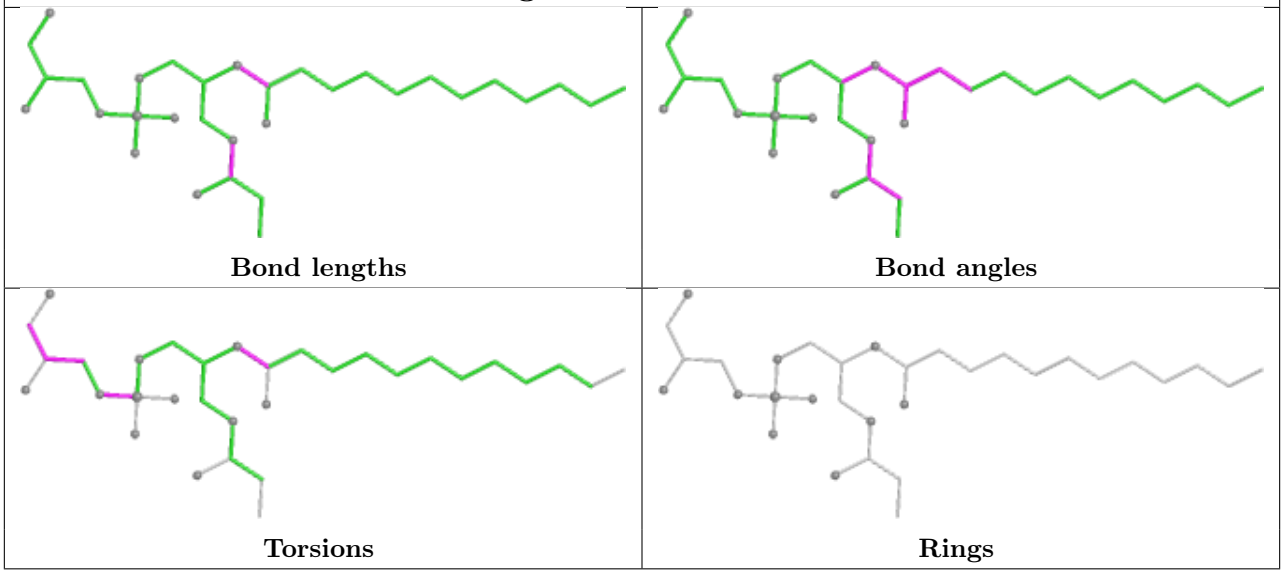


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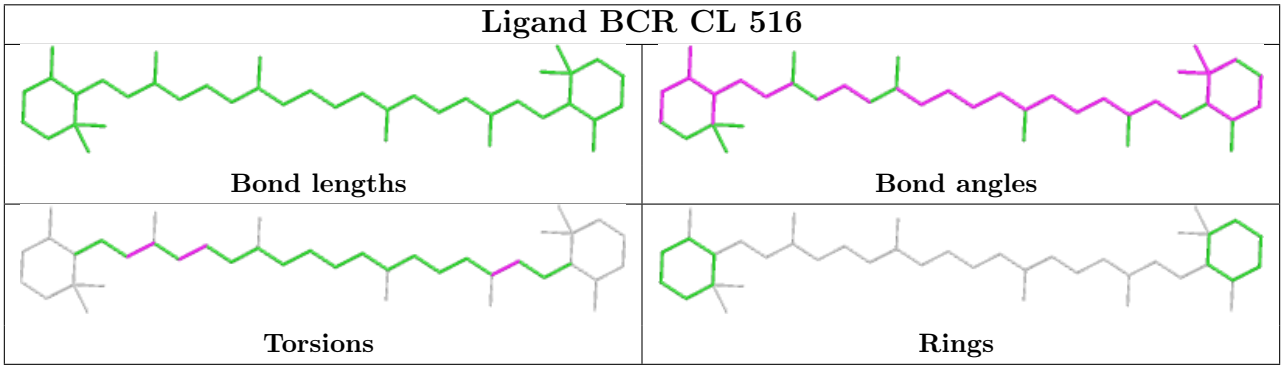
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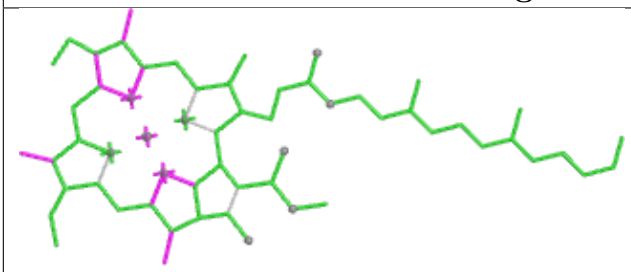
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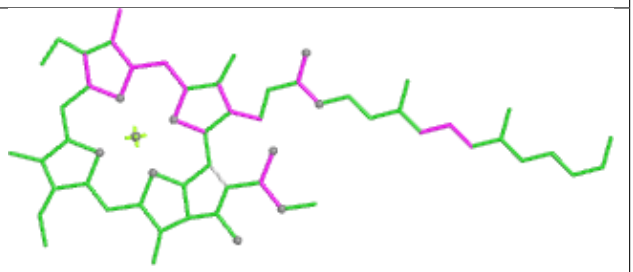
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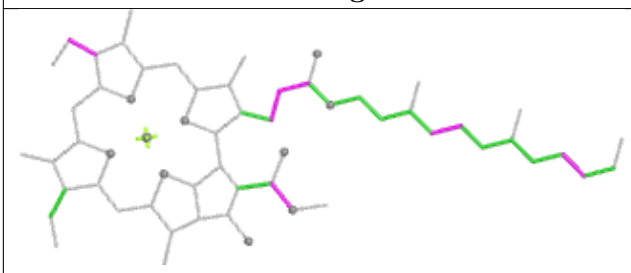
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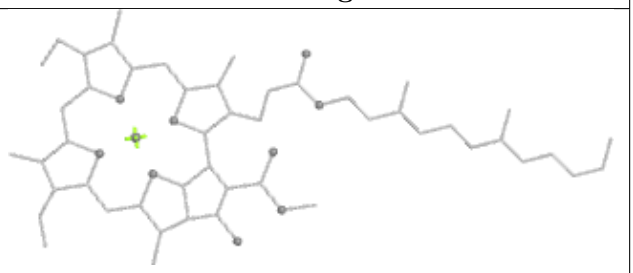
Bond lengths



Bond angles

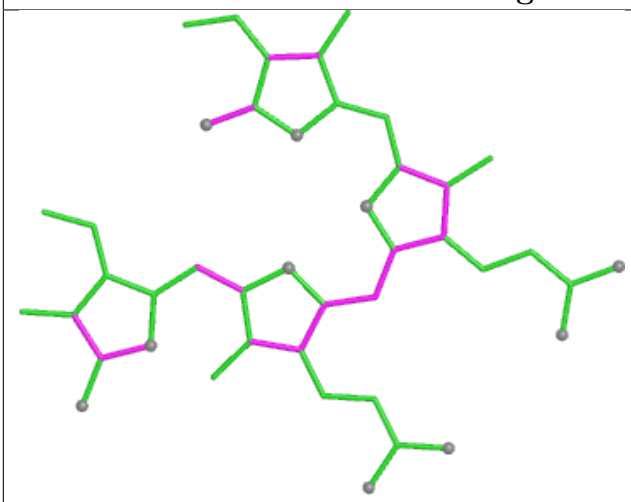


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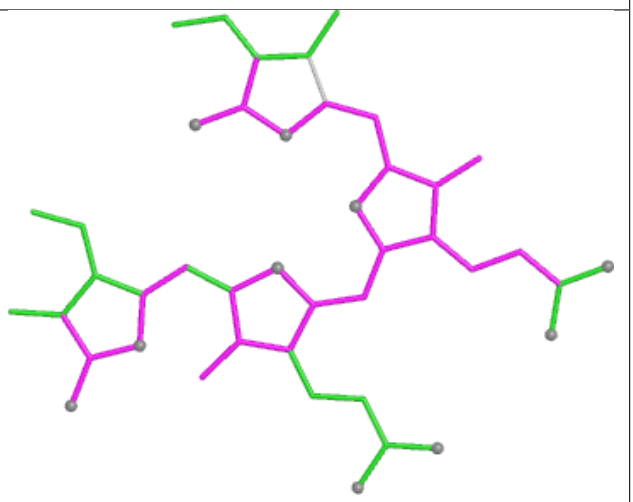


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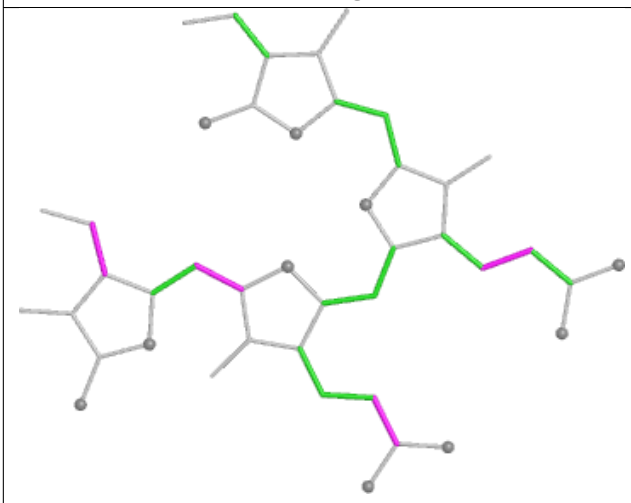
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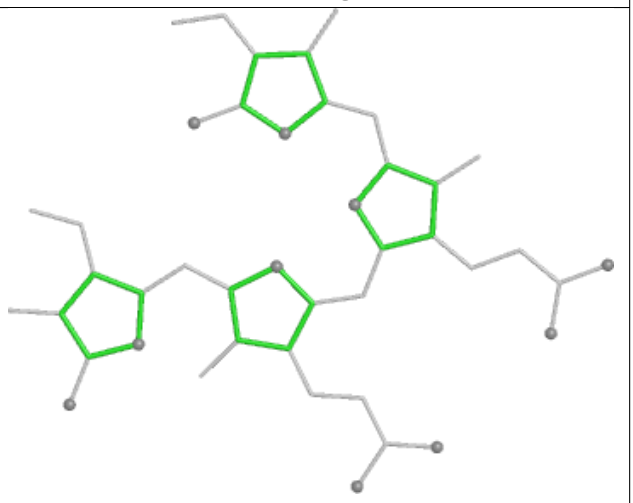
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Bond angles

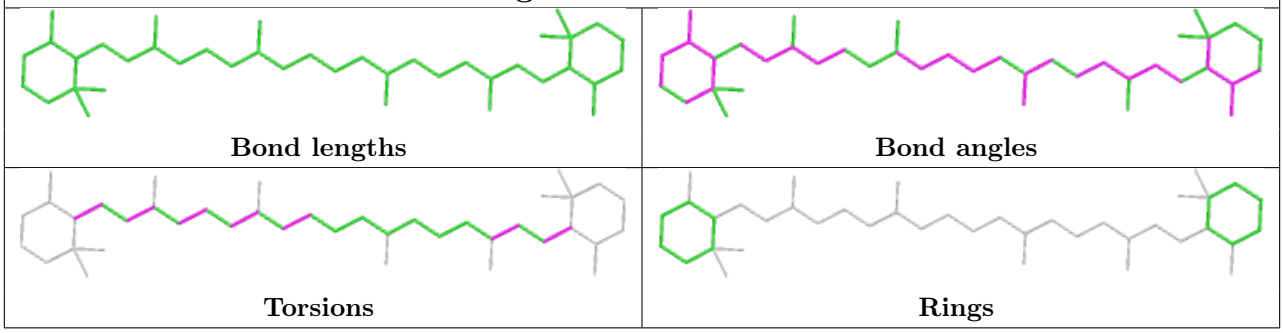


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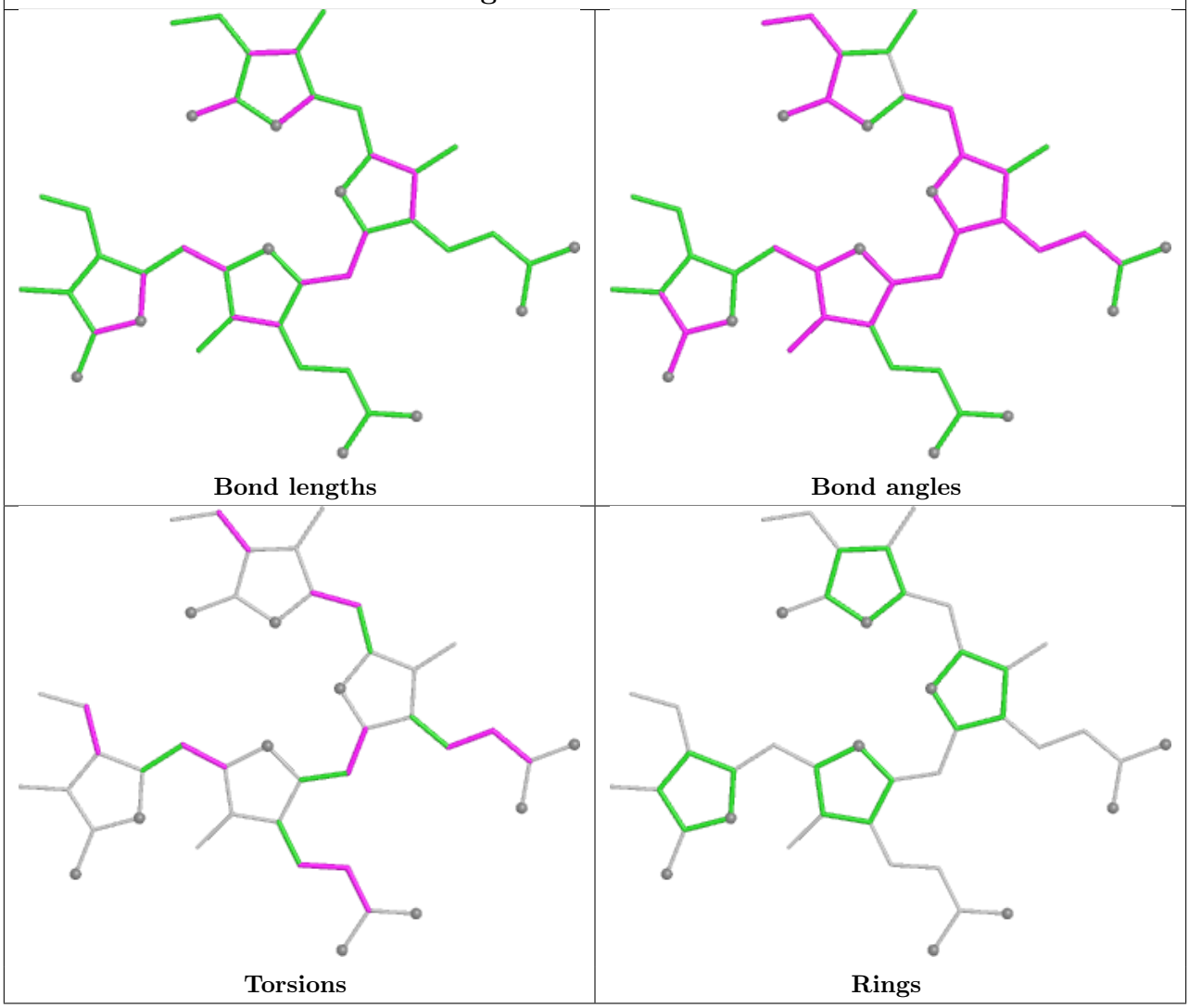


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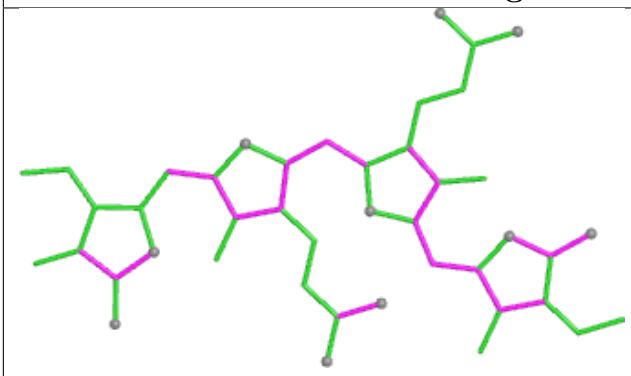
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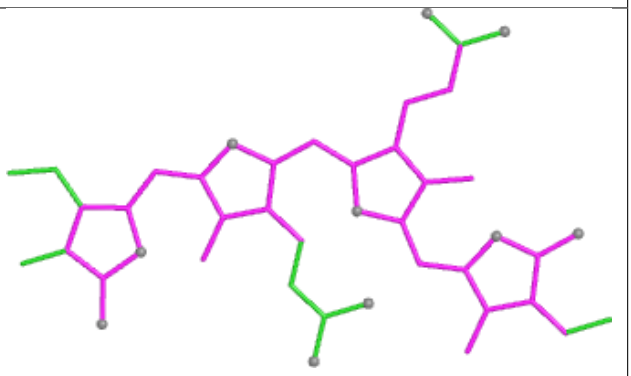
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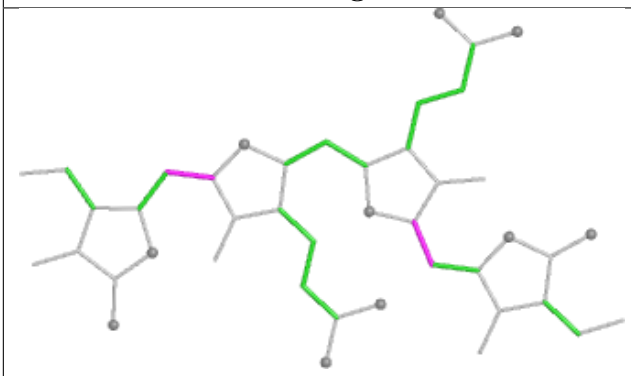
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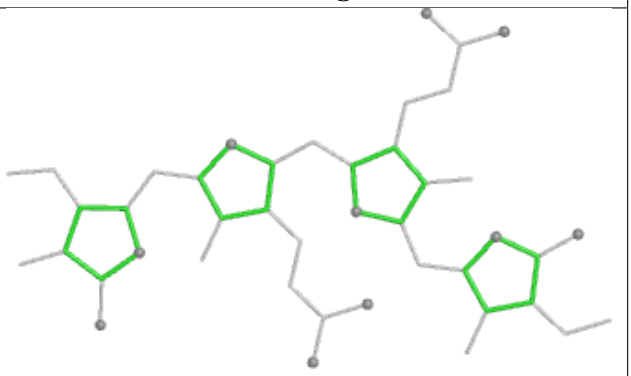
Bond lengths



Bond angles

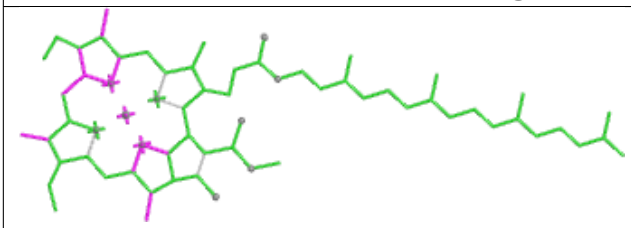


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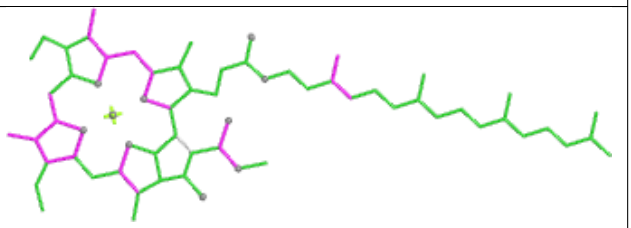


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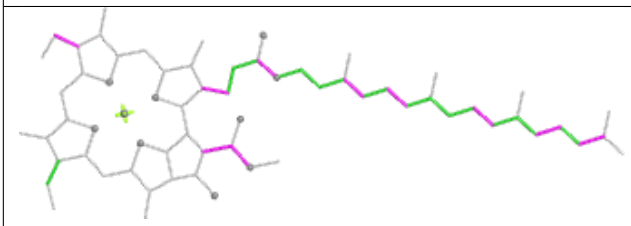
Ligand CLA AN 831



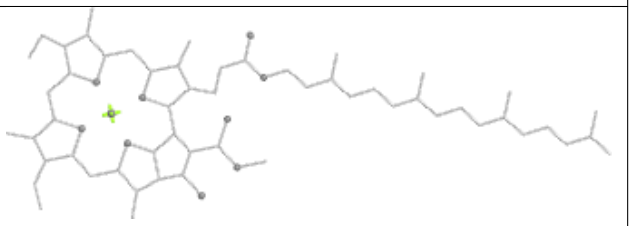
Bond lengths



Bond angles

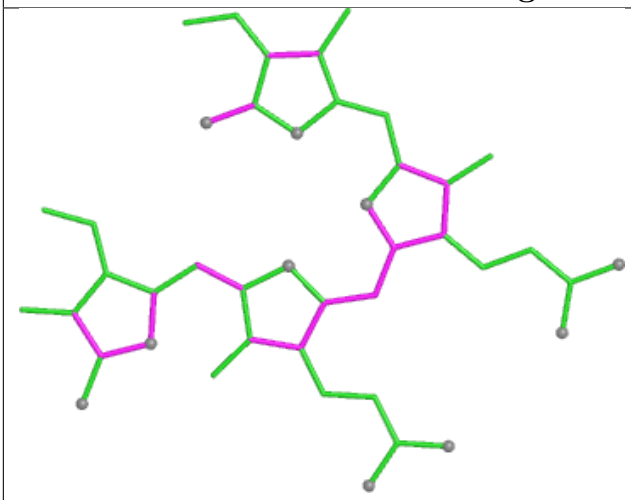


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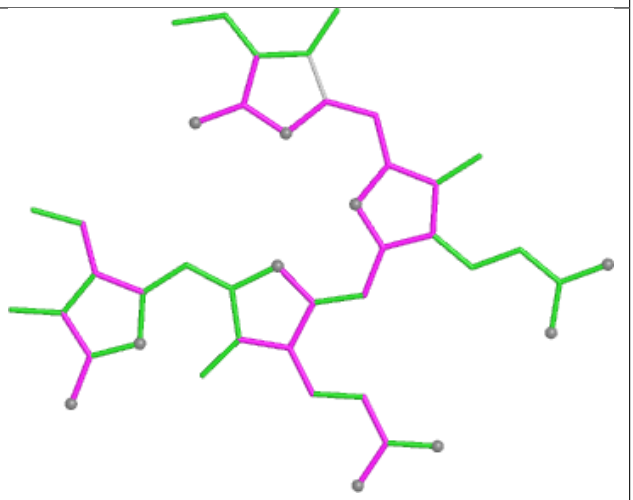


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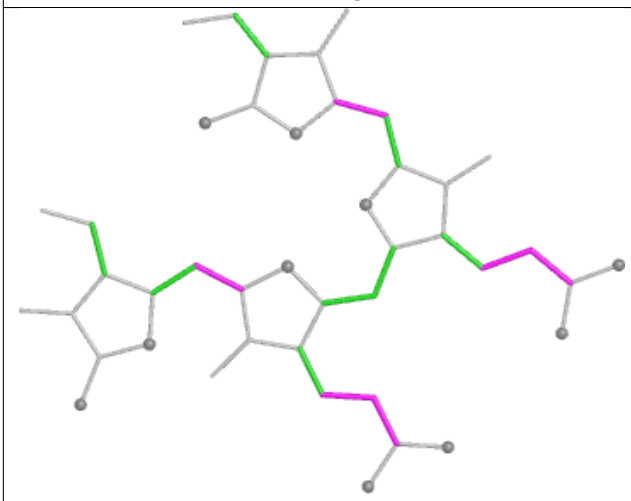
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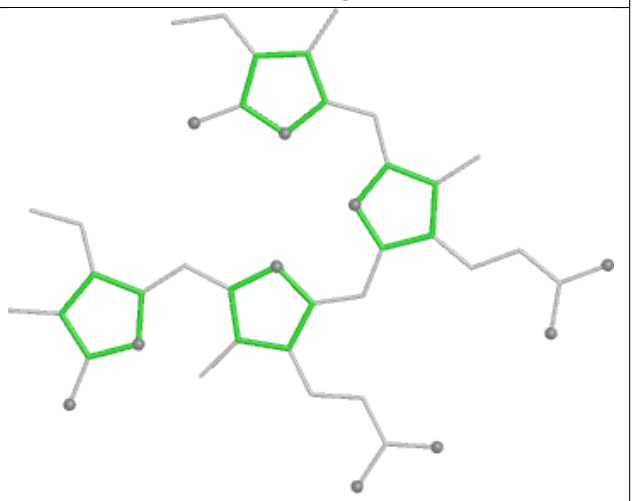
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Bond angles

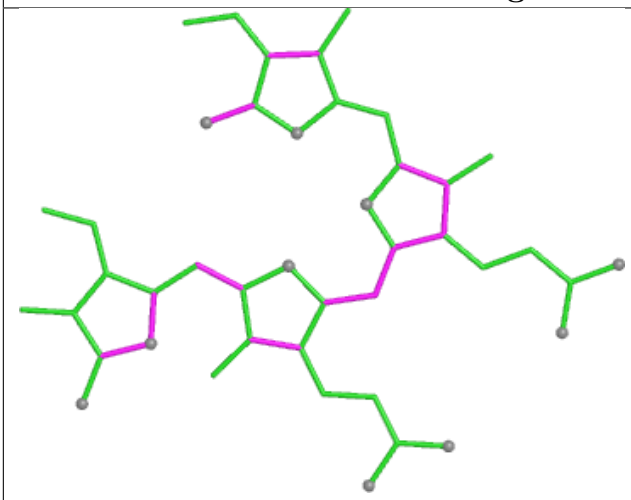


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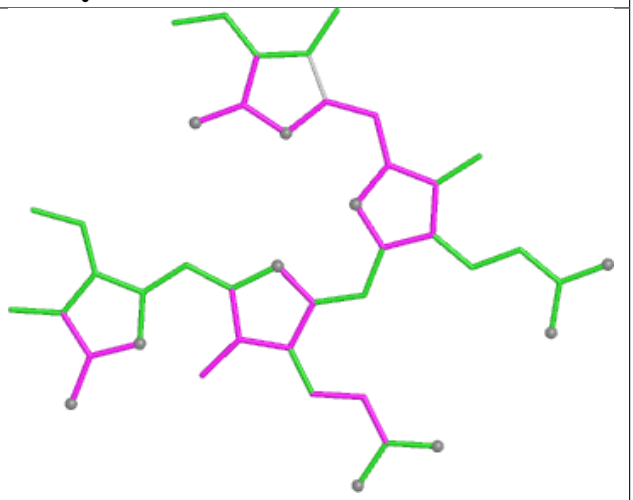


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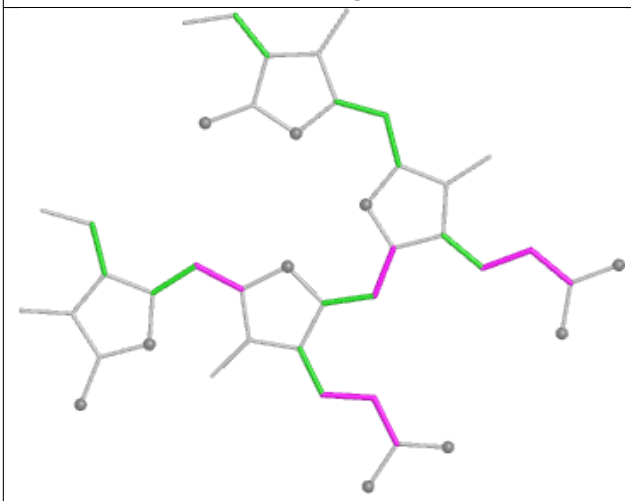
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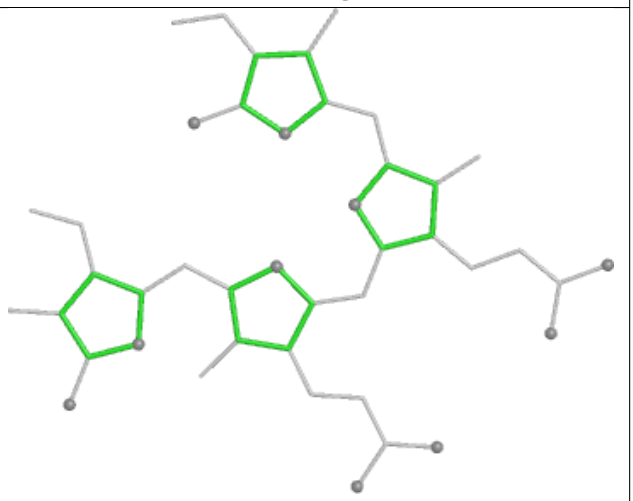
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Bond angles

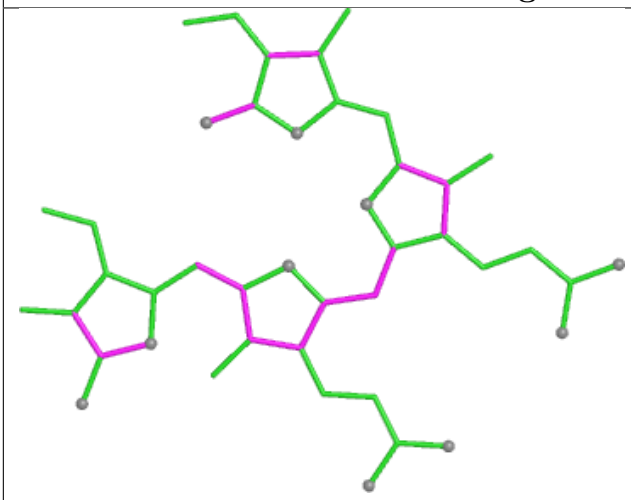


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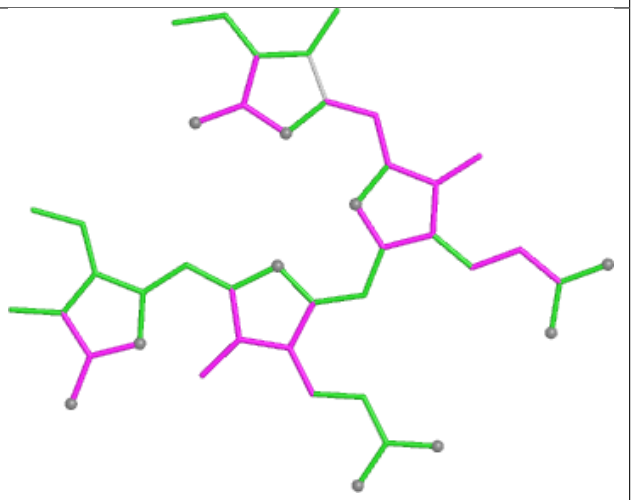


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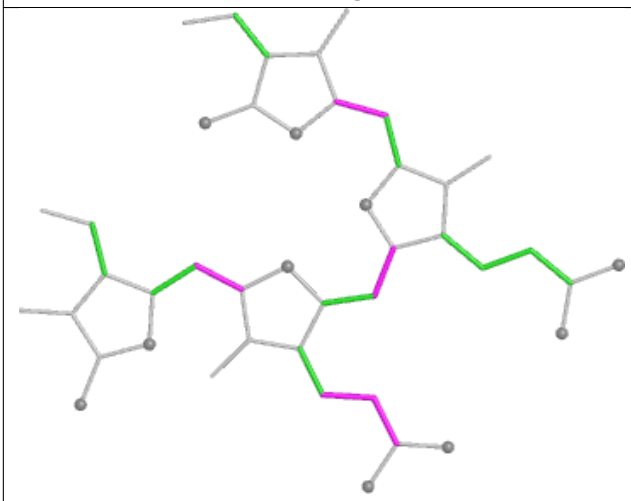
Ligand PEB iH 202



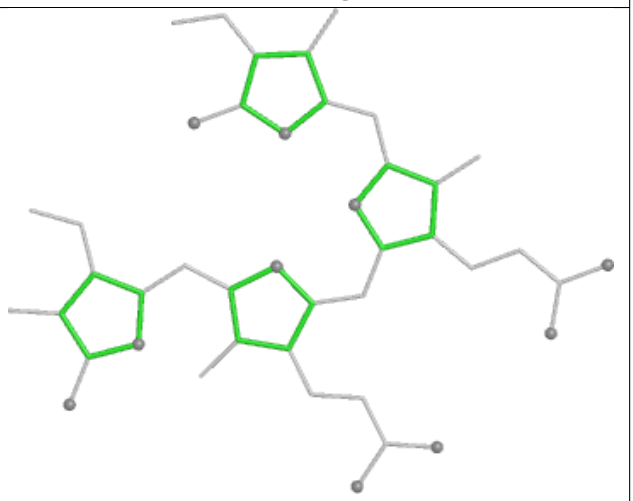
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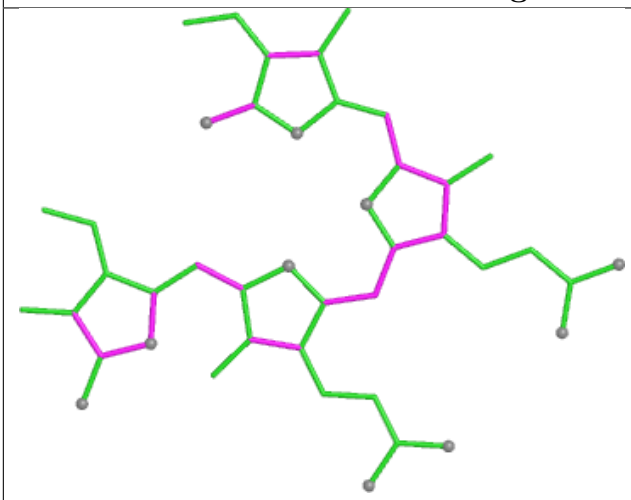


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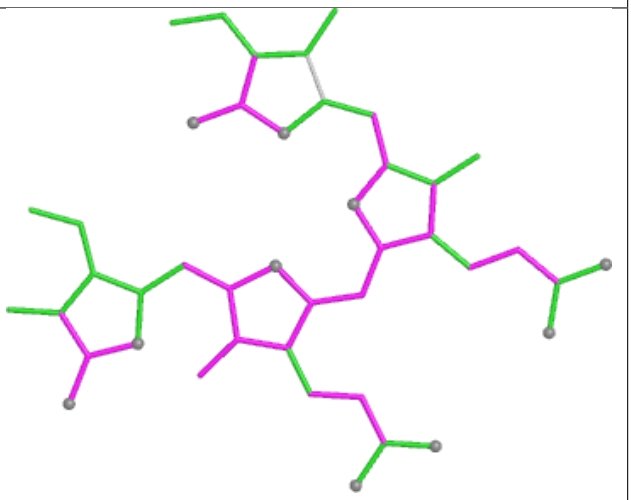


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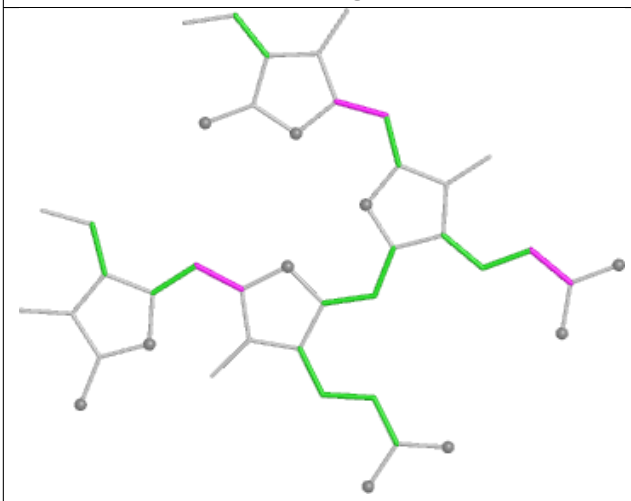
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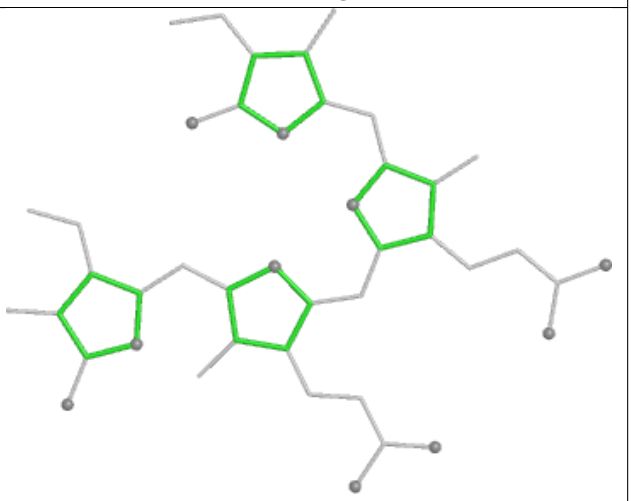
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Bond angles

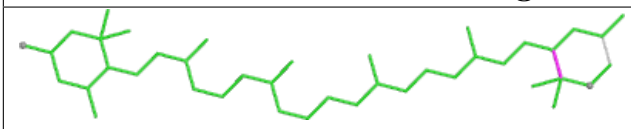


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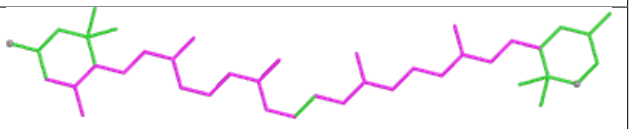


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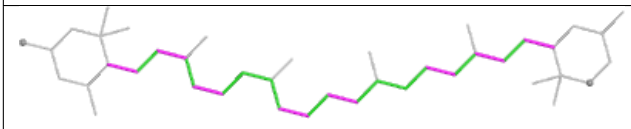
Ligand ZEX 8N 309



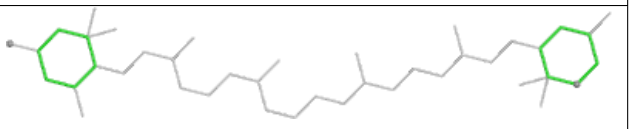
Bond lengths



Bond angles

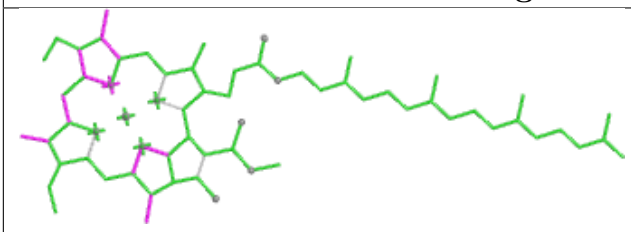


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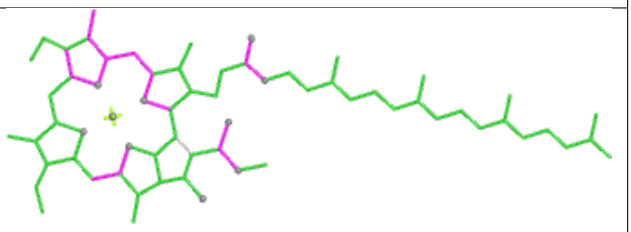


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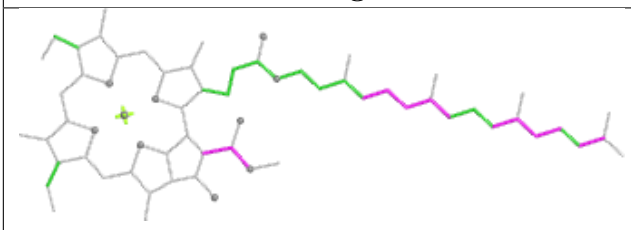
Ligand CLA C6 510



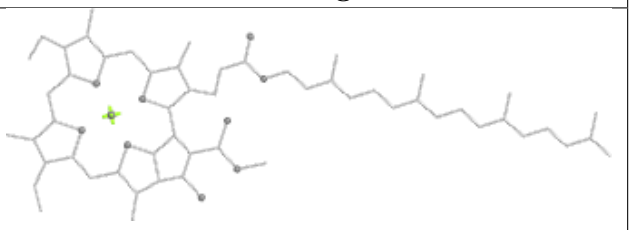
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Bond angles

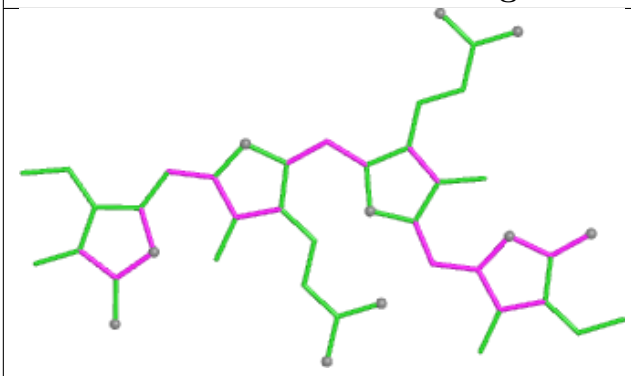


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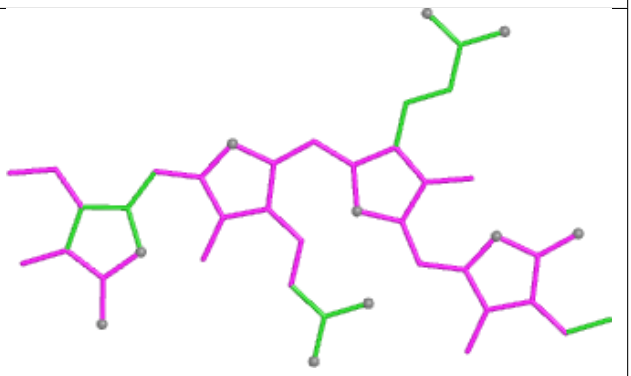


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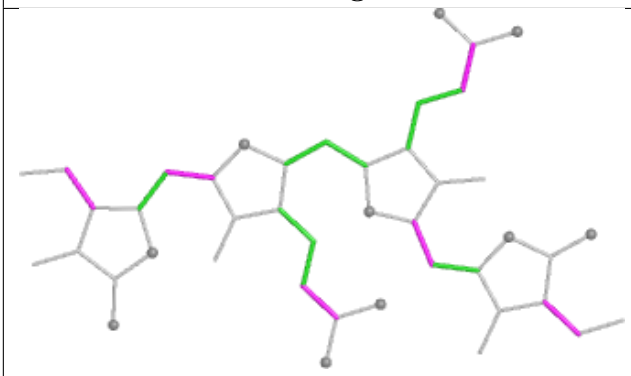
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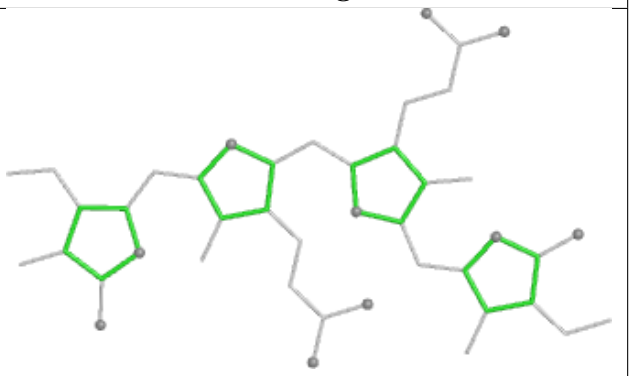
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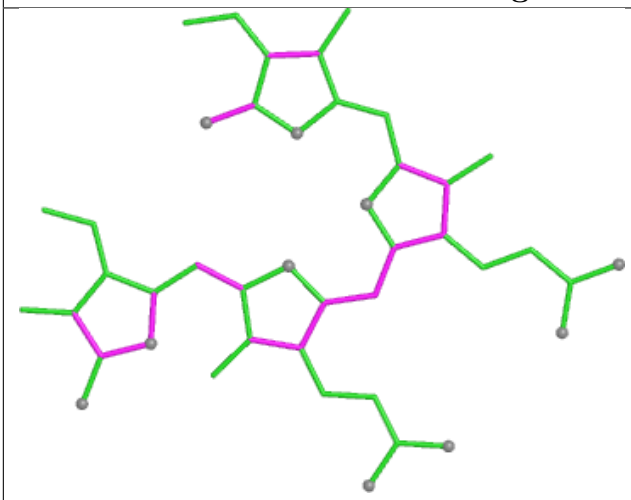


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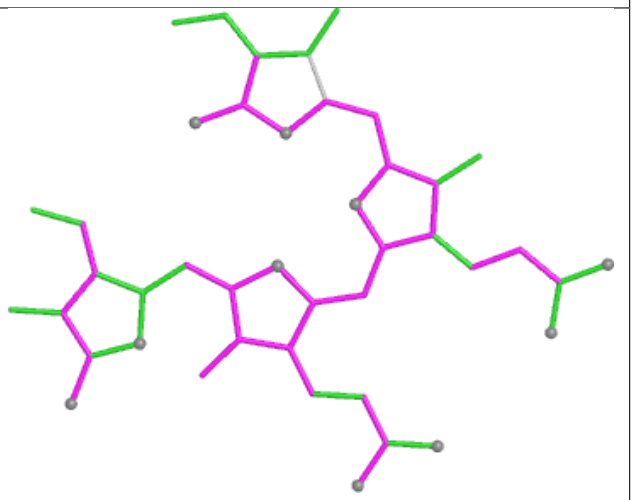


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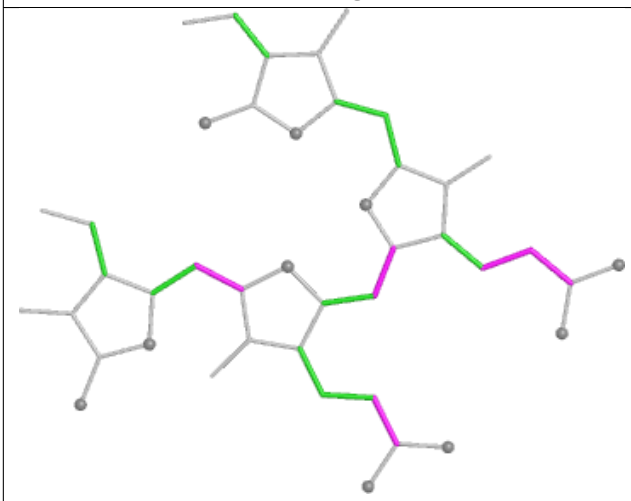
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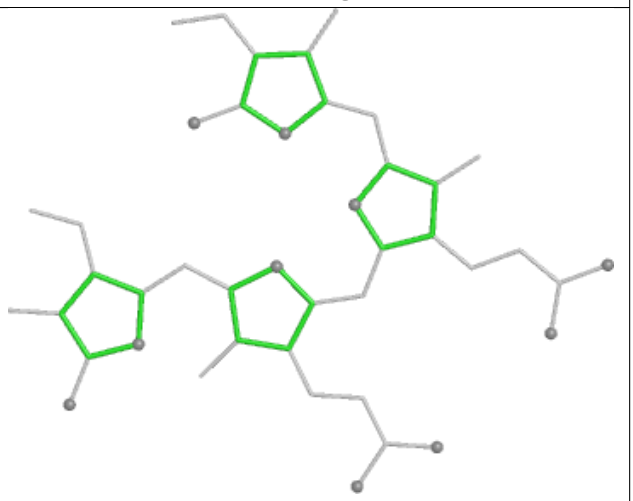
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Bond angles

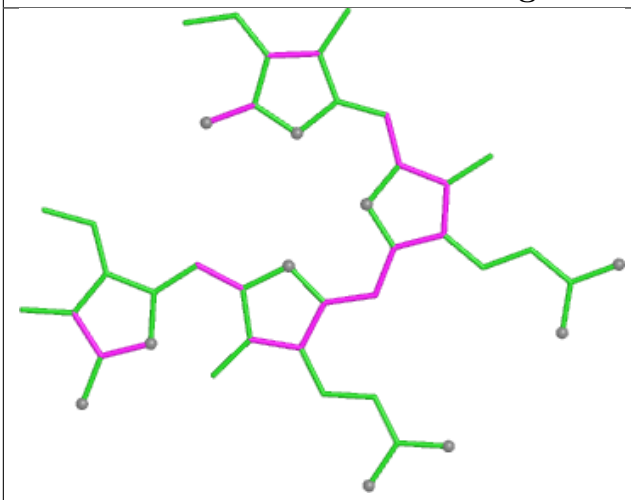


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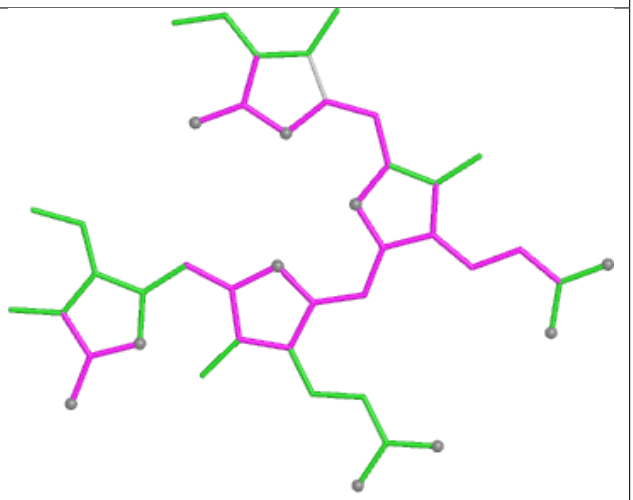


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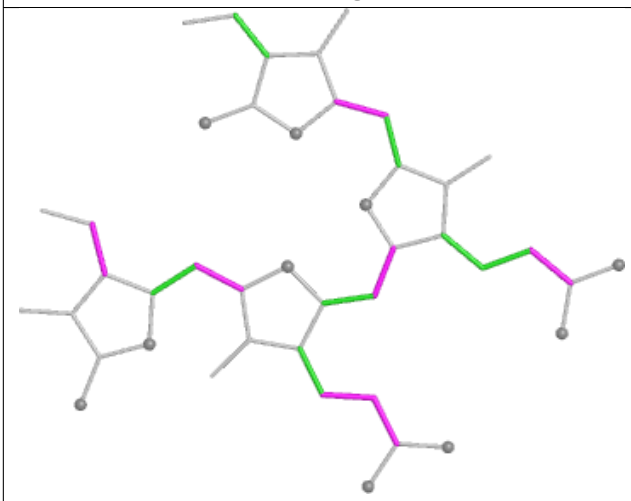
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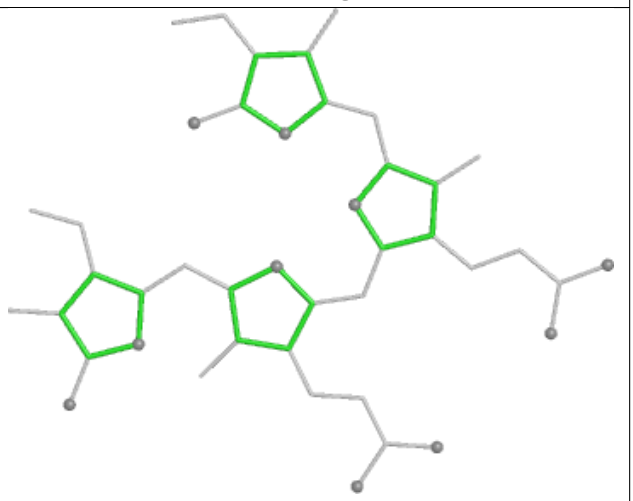
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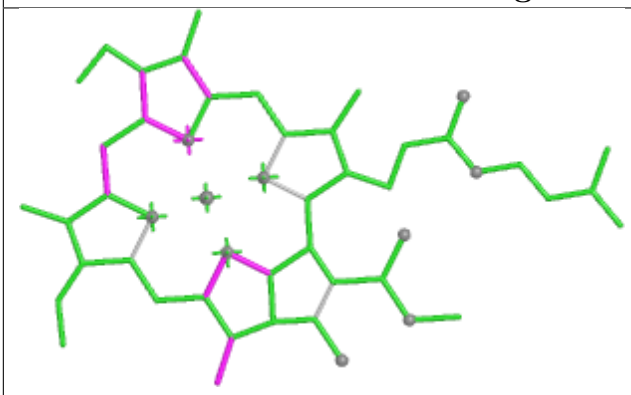


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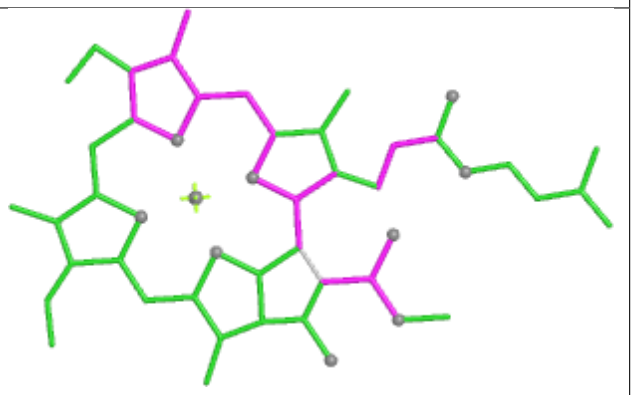


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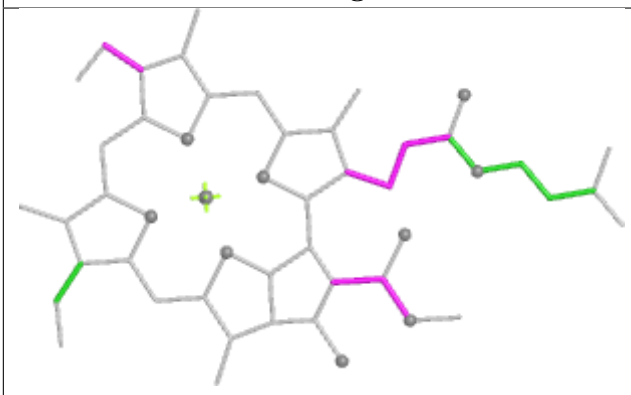
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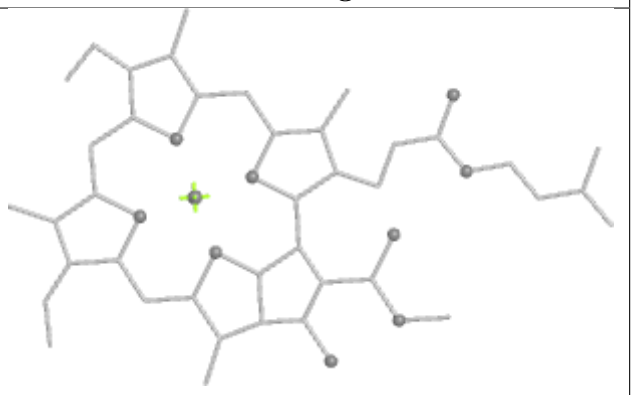
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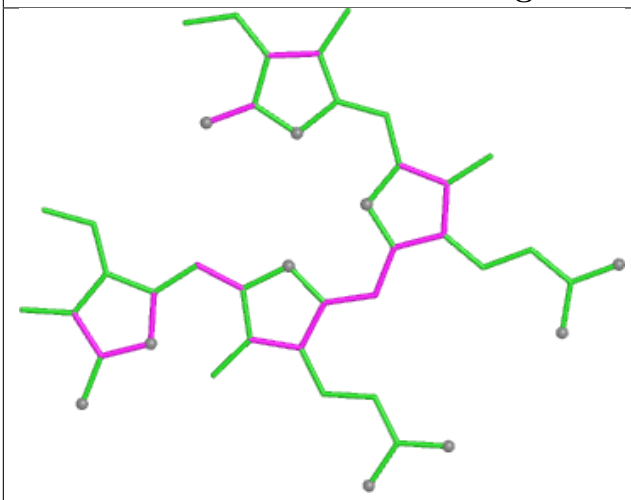


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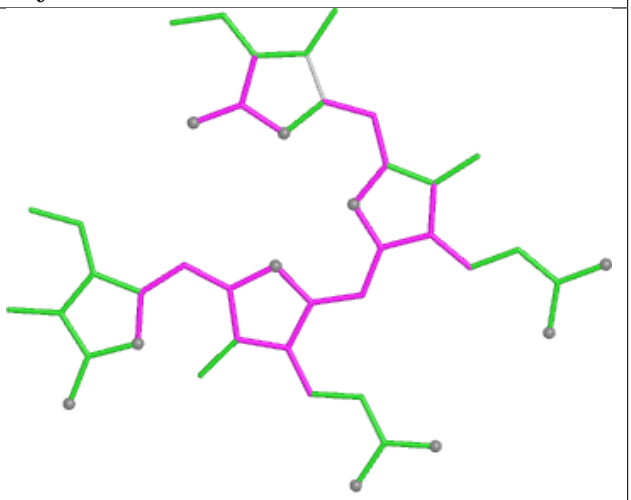


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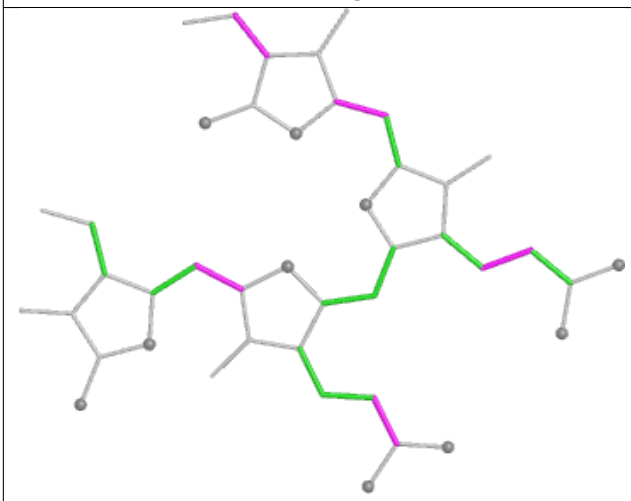
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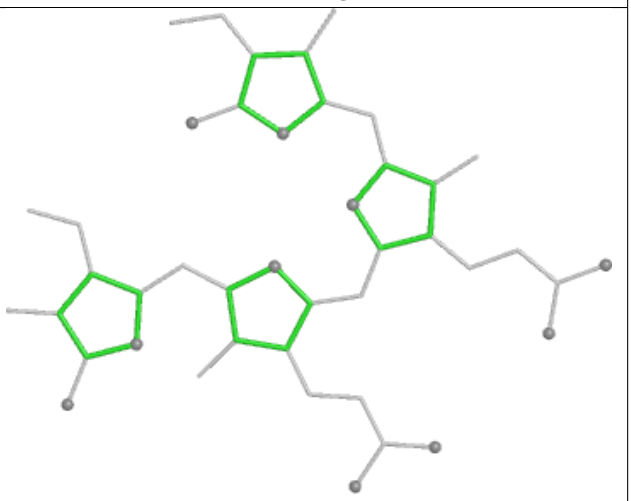
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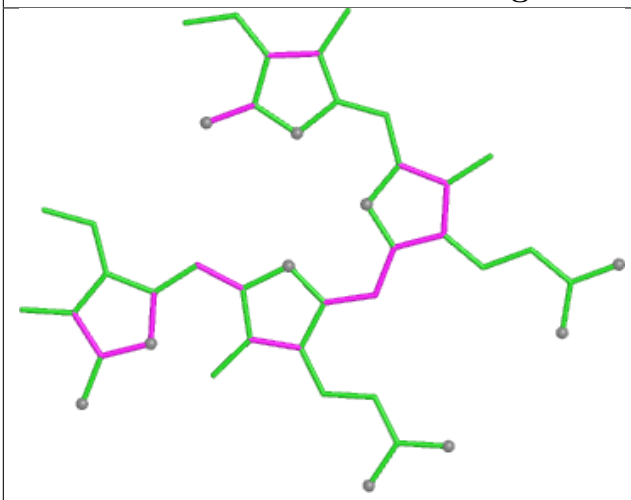


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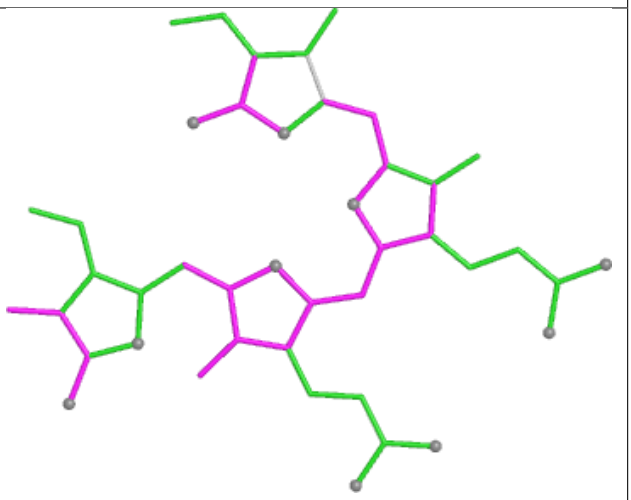


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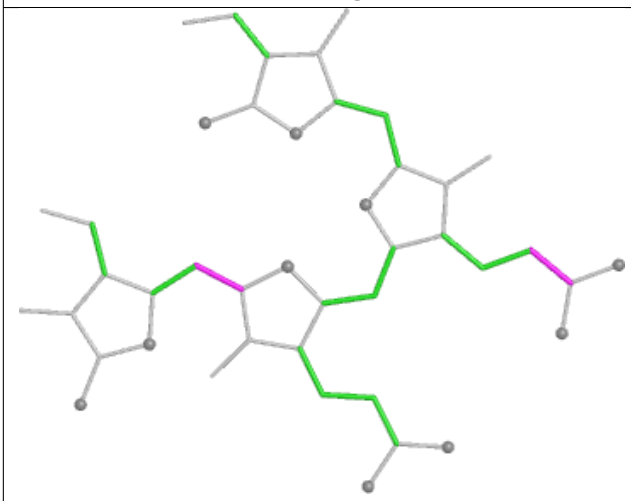
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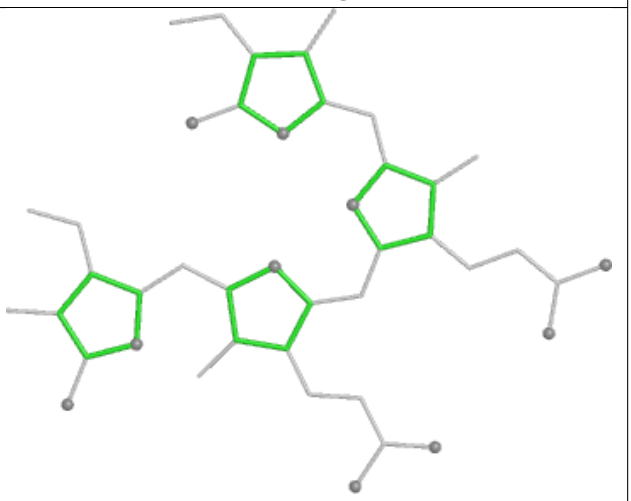
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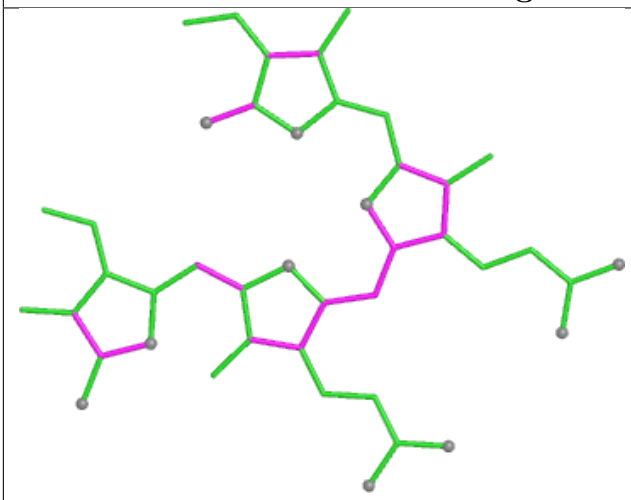


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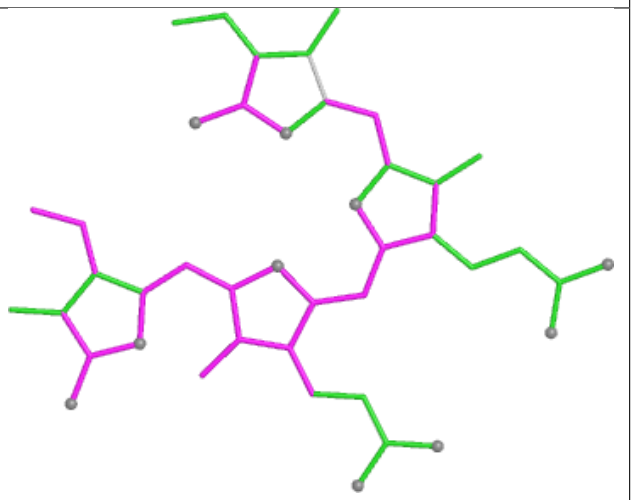


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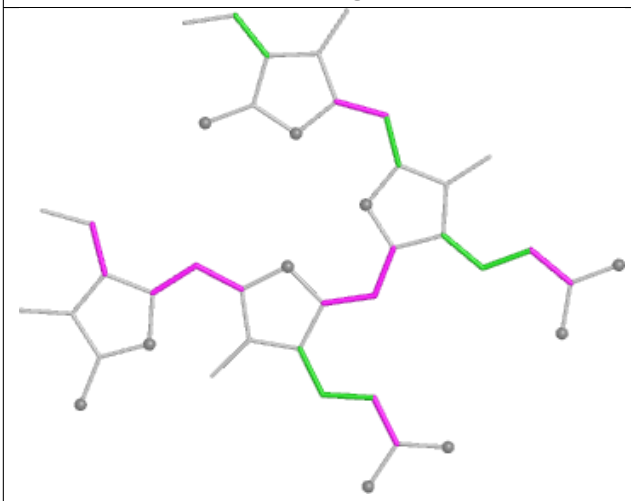
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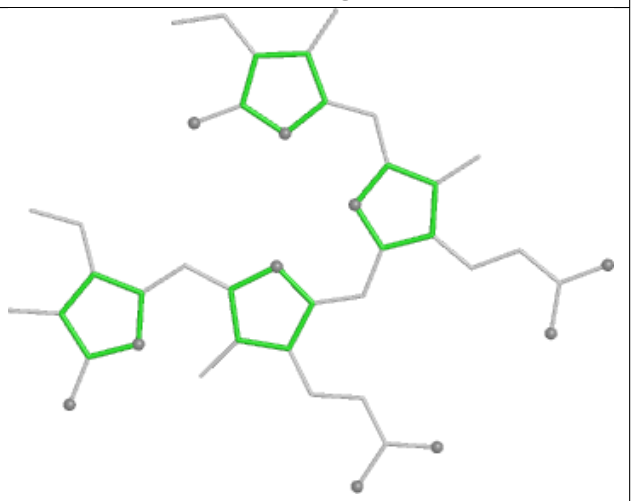
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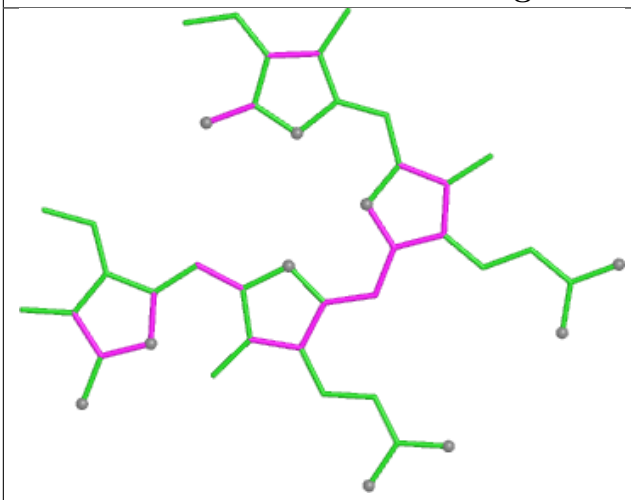


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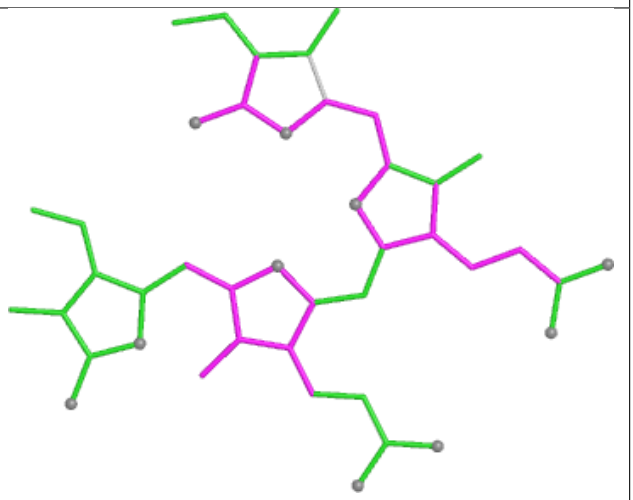


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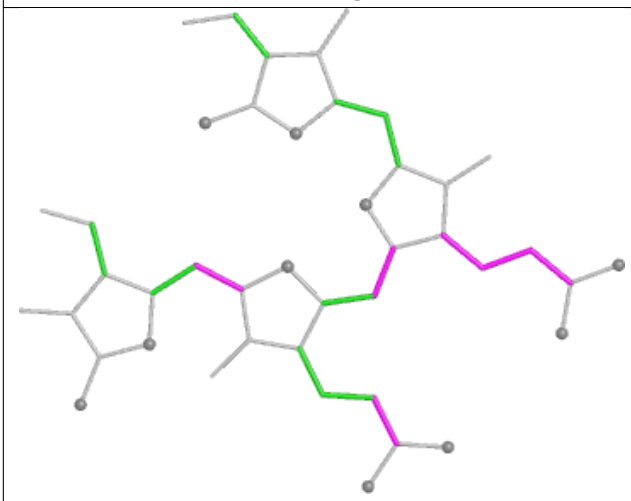
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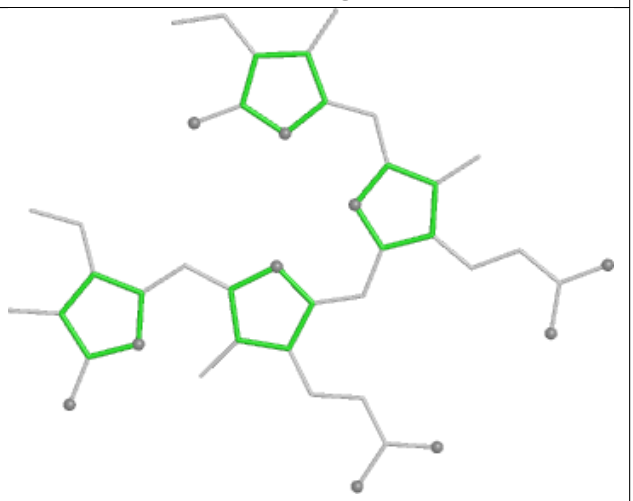
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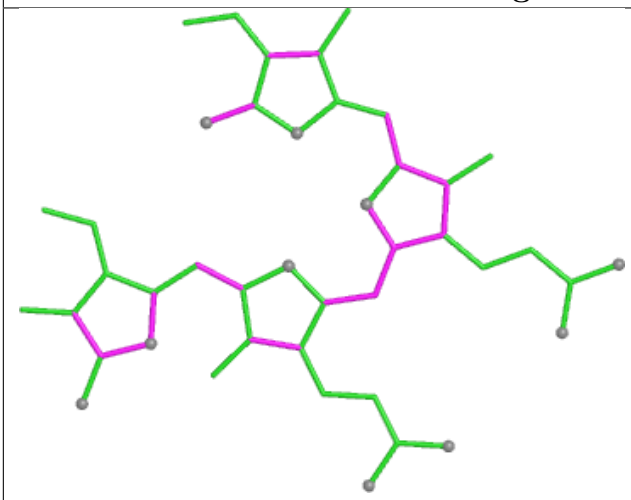


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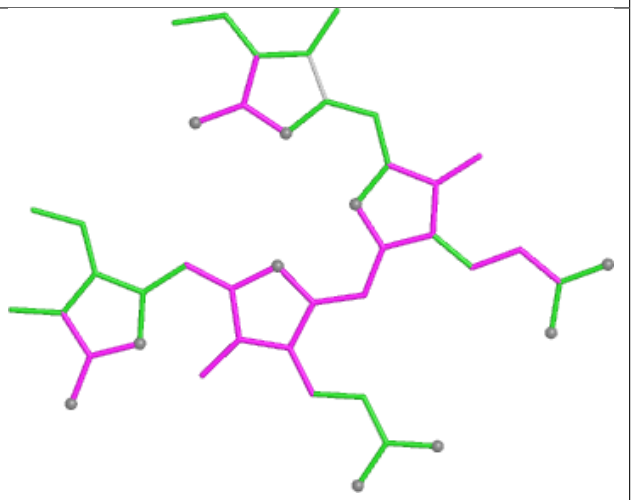


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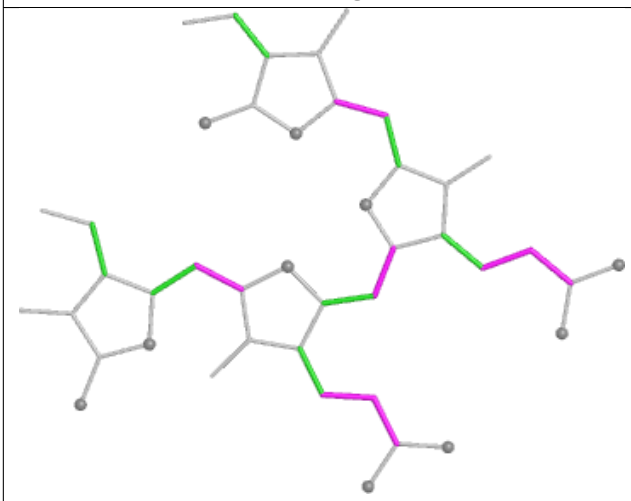
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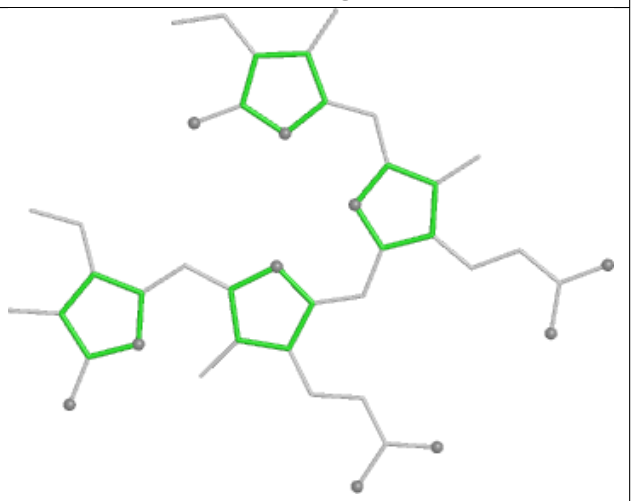
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Bond angles

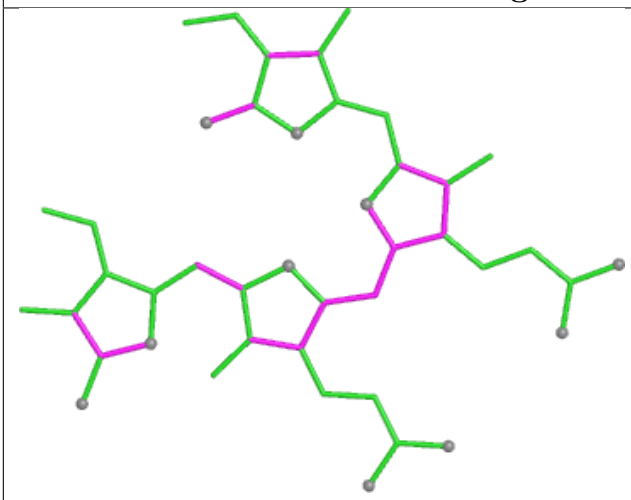


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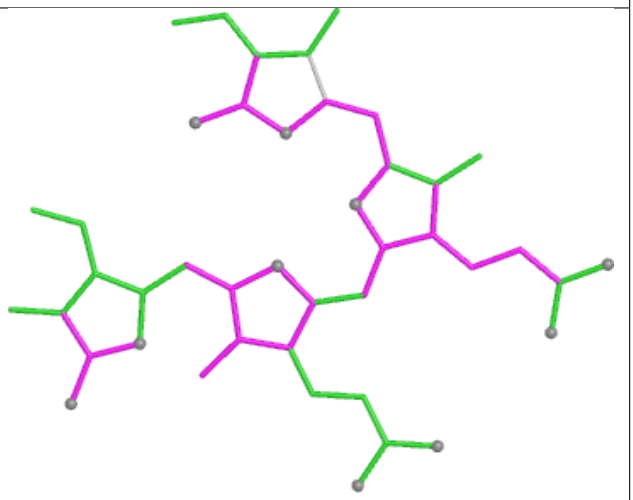


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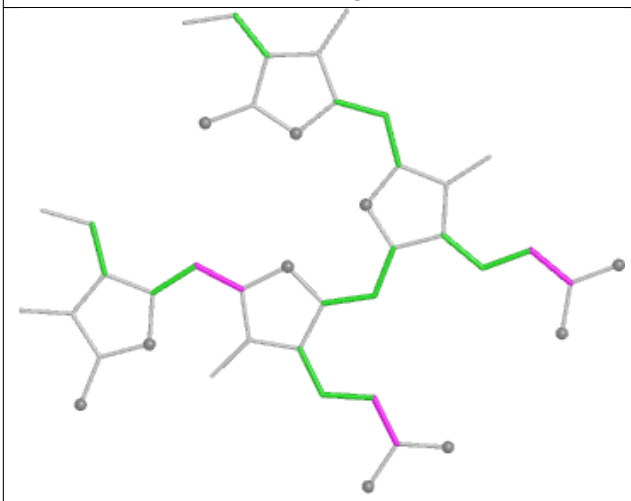
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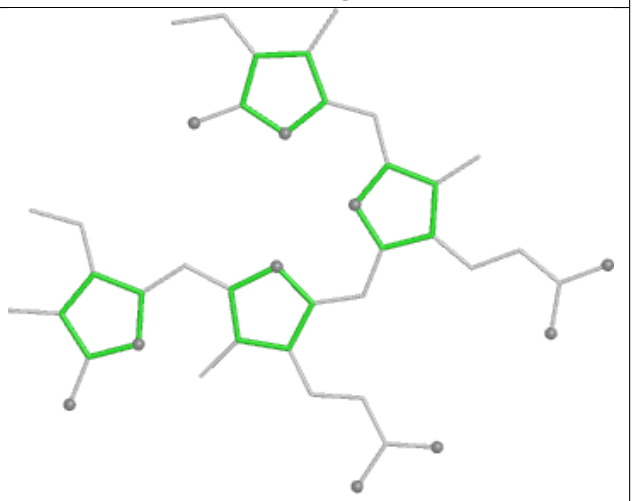
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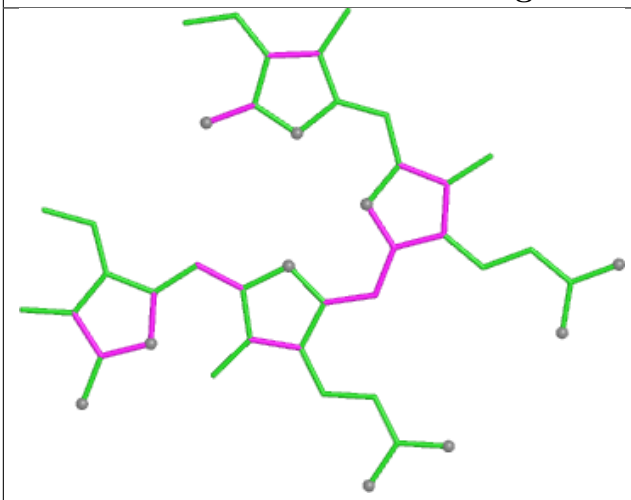


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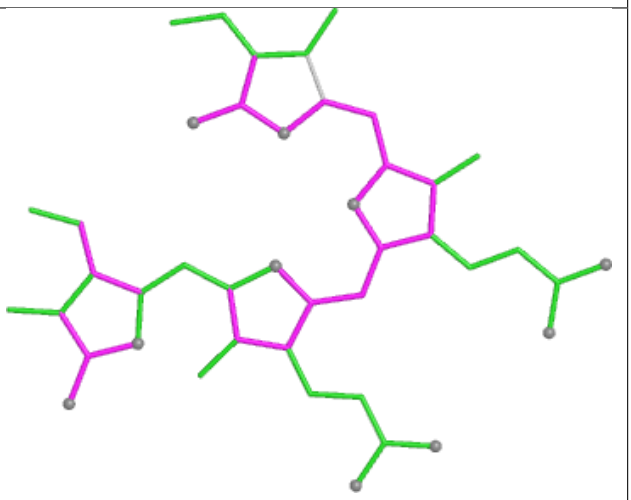


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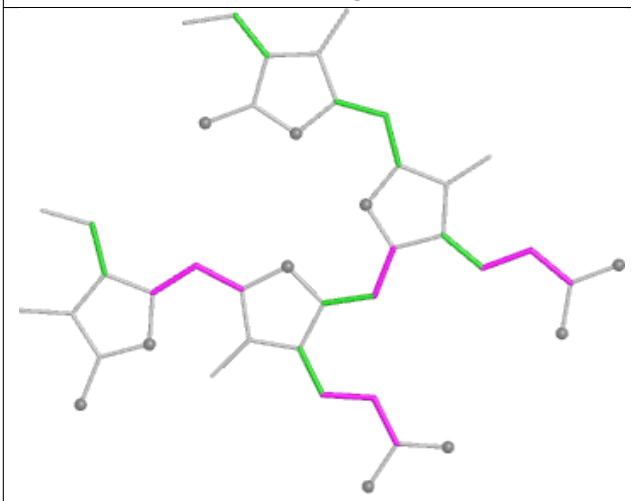
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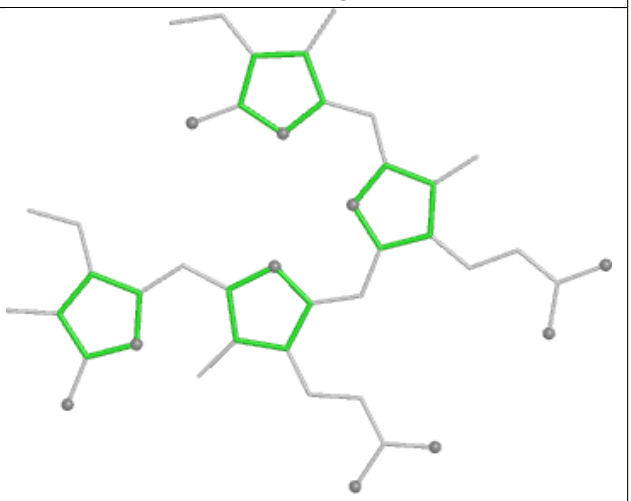
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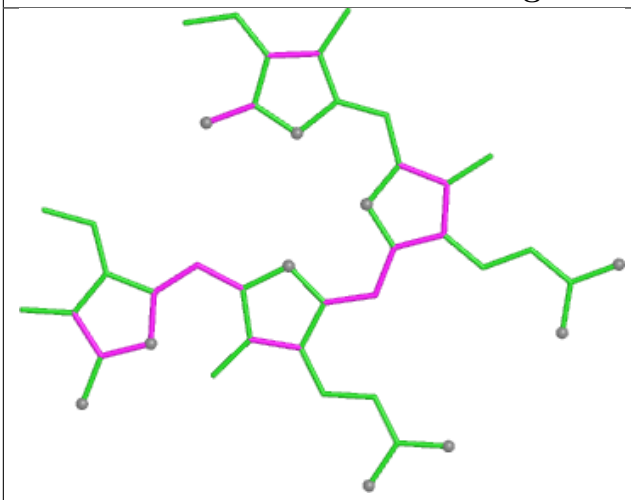


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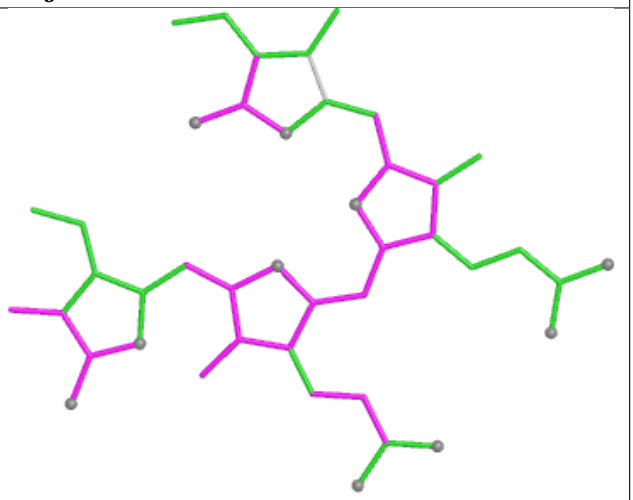


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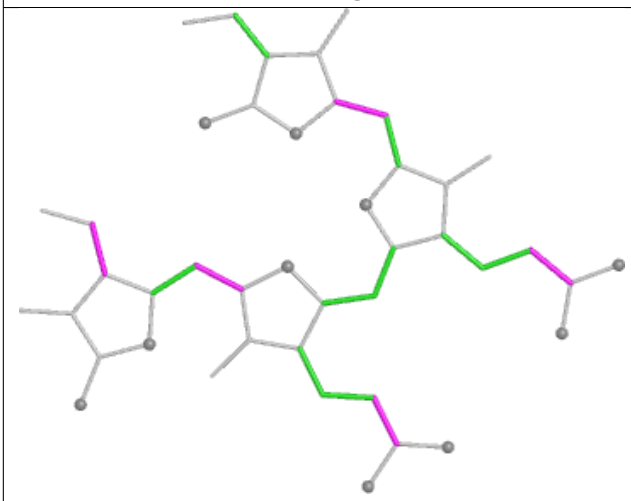
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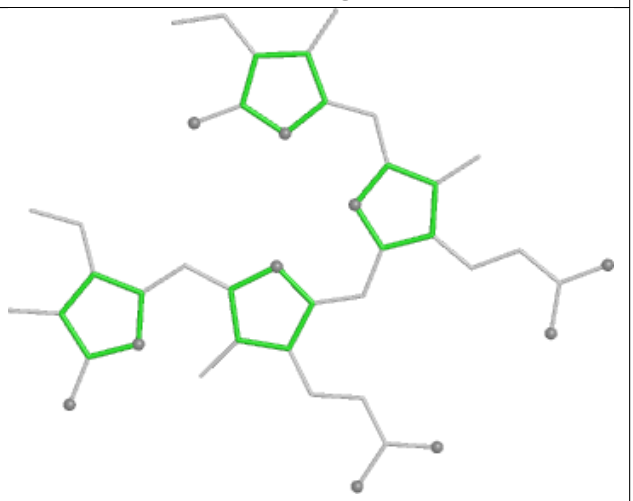
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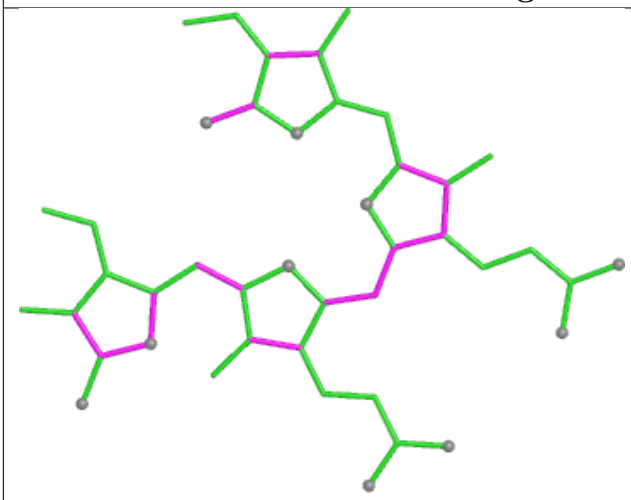


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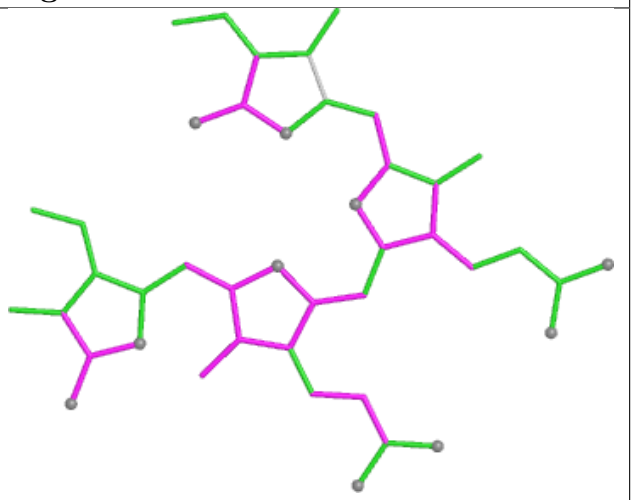


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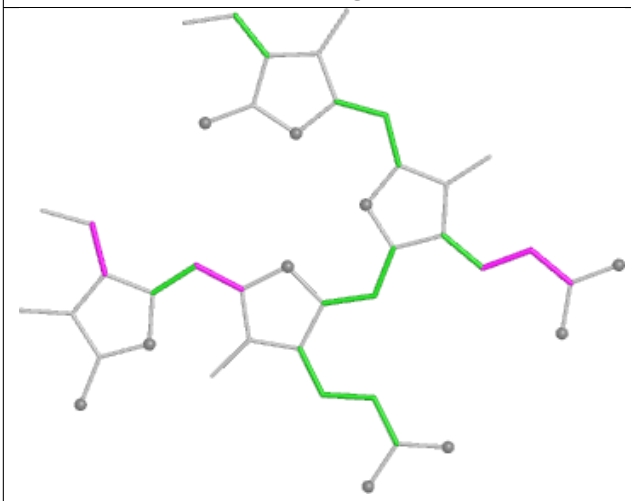
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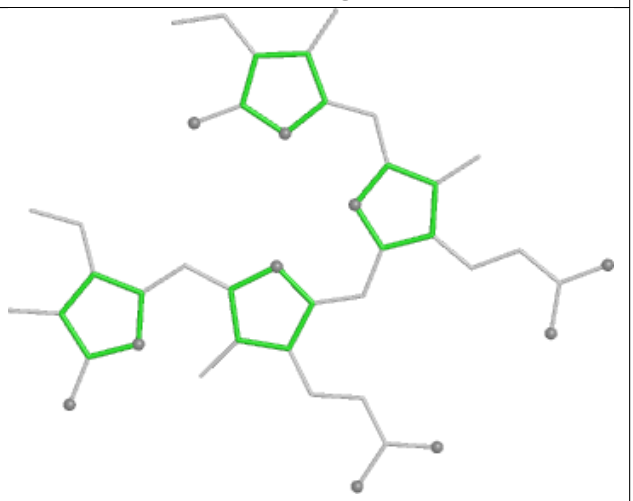
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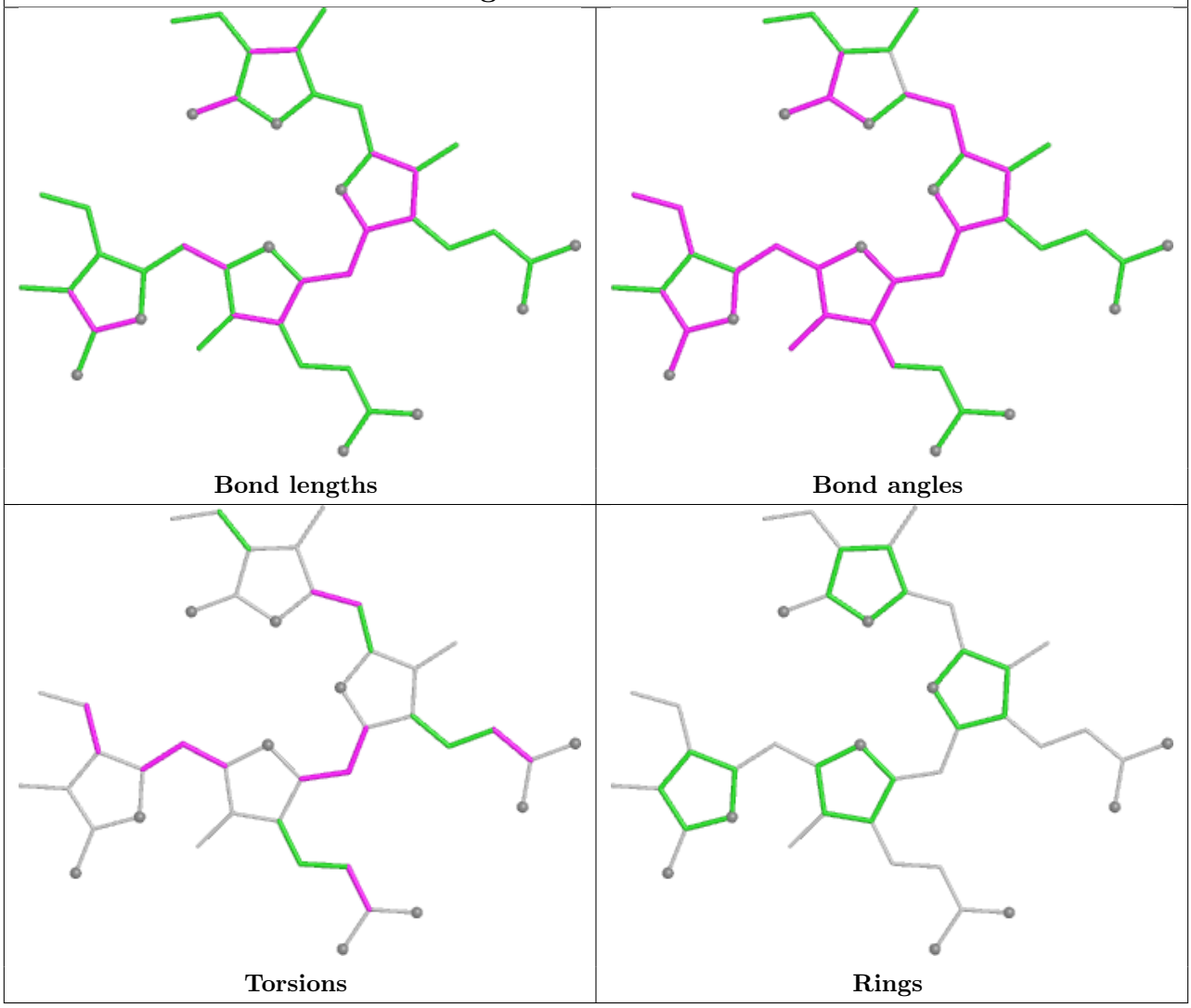


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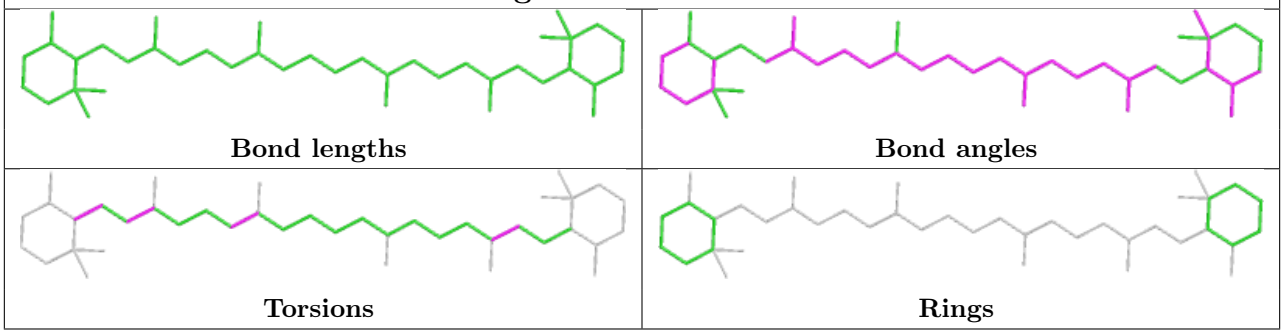


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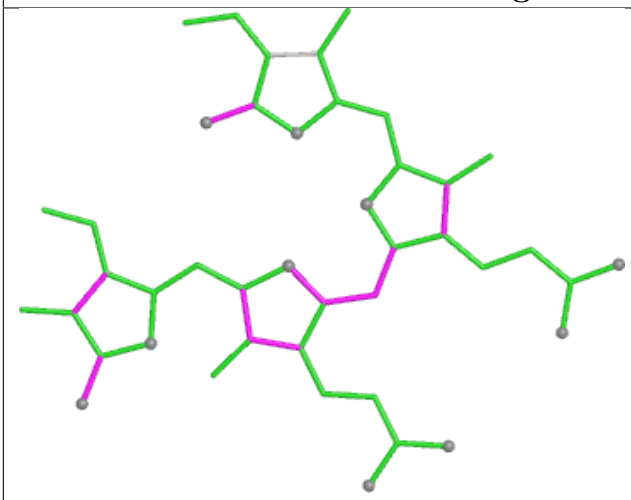
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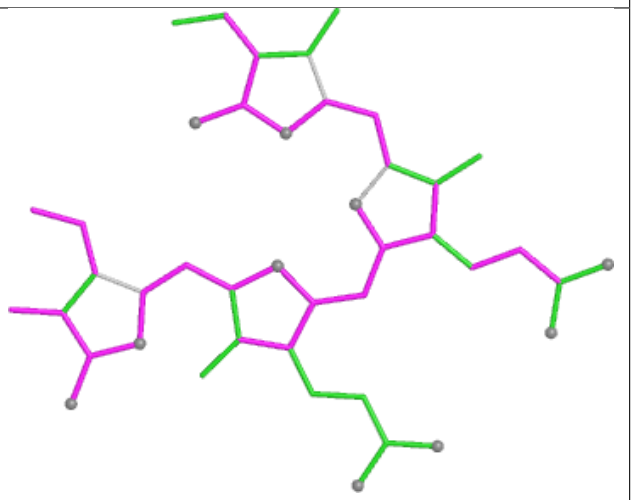
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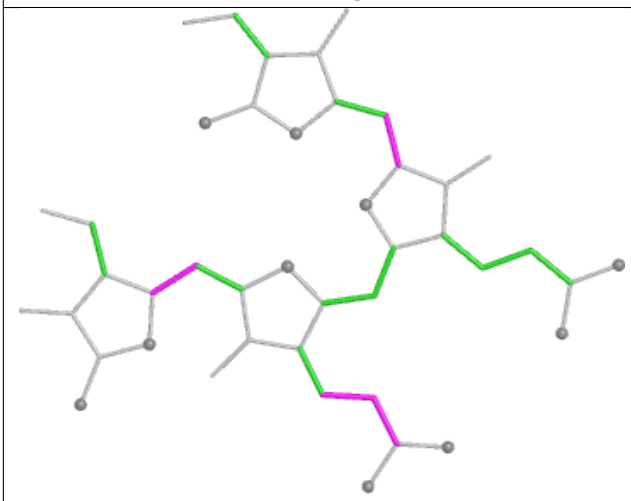
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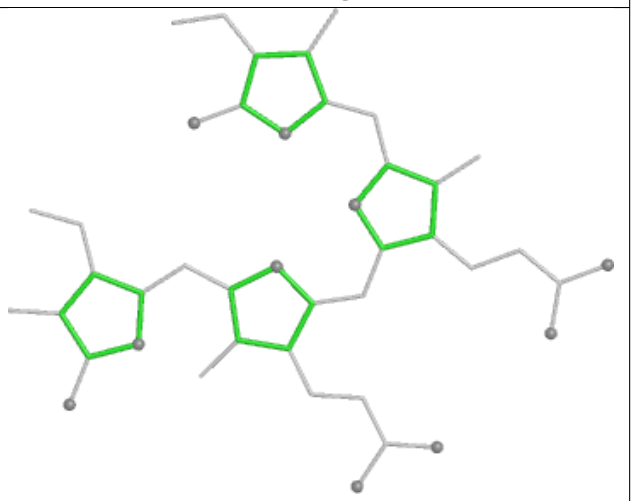
Bond lengths



Bond angles

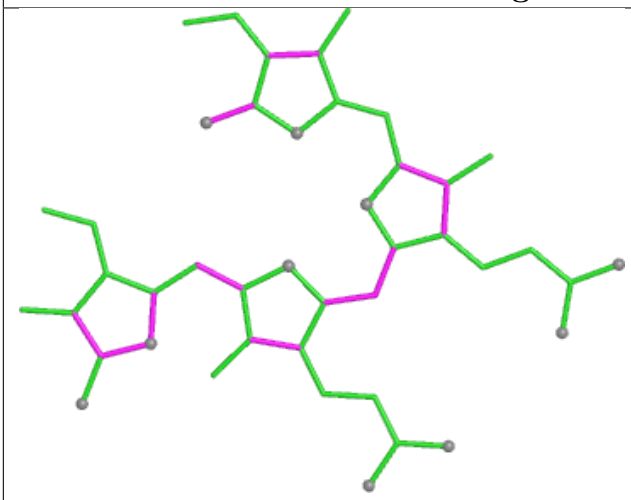


Torsions

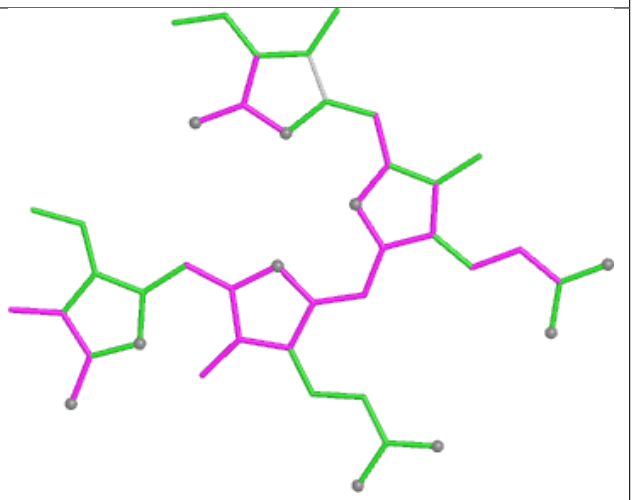


Rings

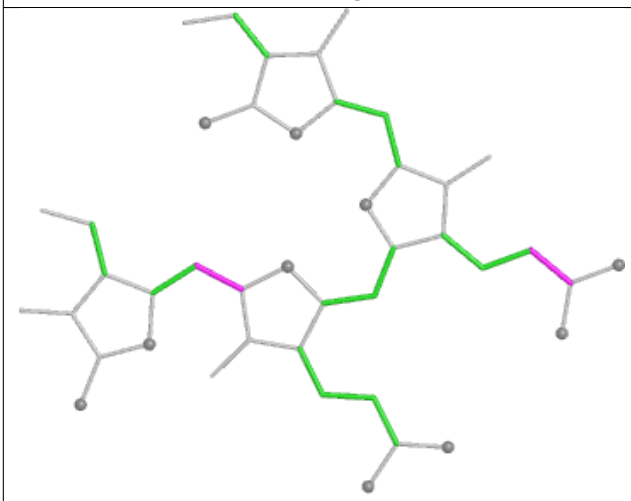
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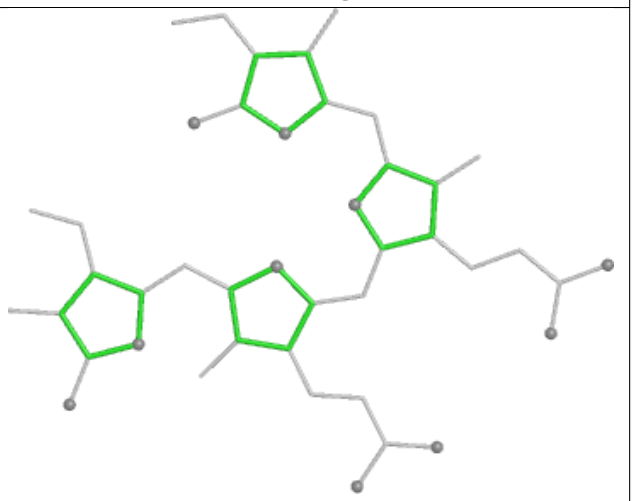
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Bond angles

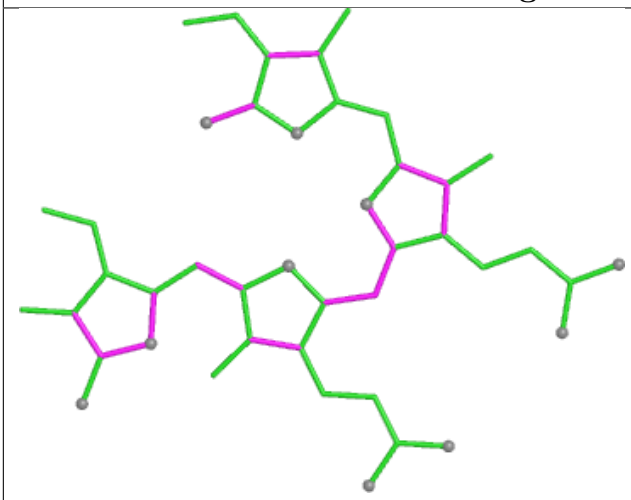


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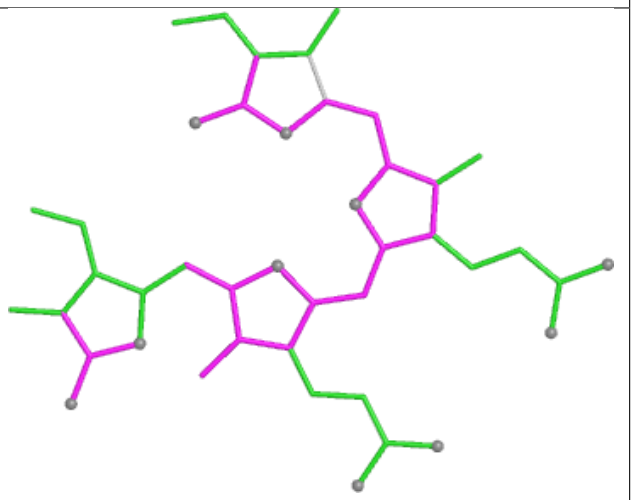


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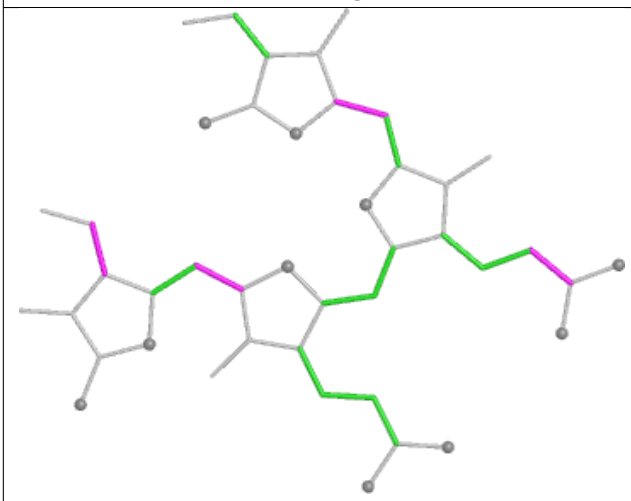
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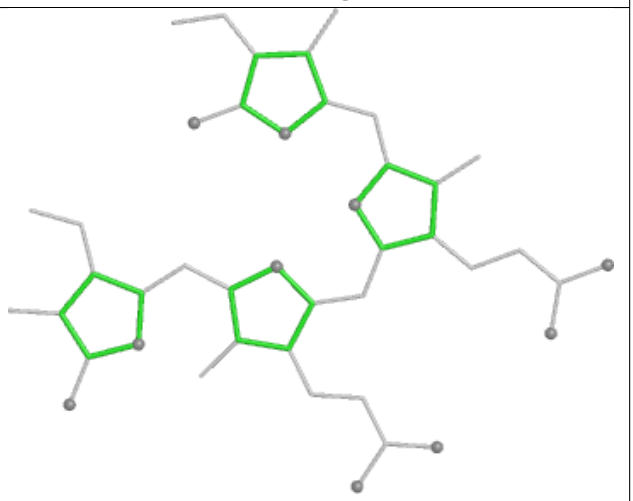
Bond lengths



Bond angles

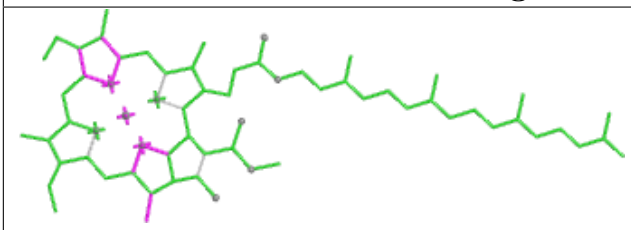


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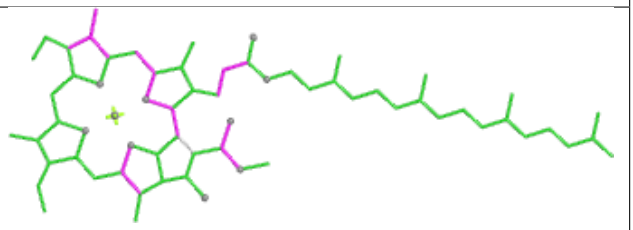


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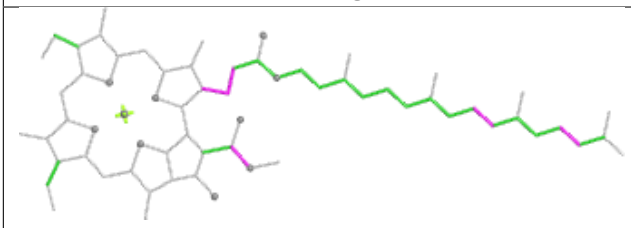
Ligand CLA AN 850



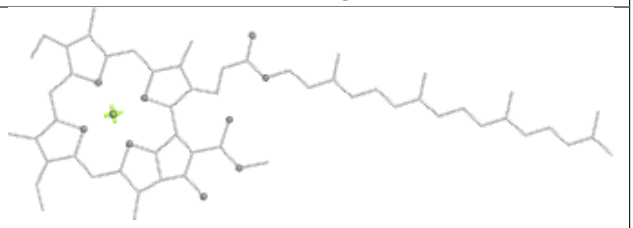
Bond lengths



Bond angles

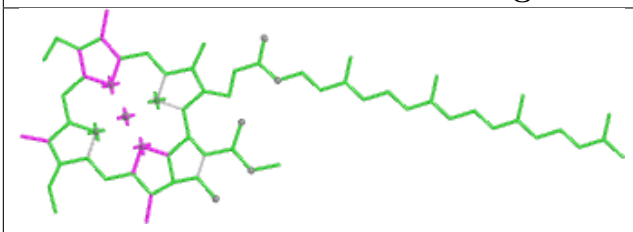


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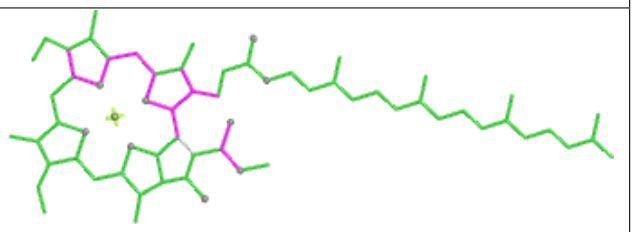


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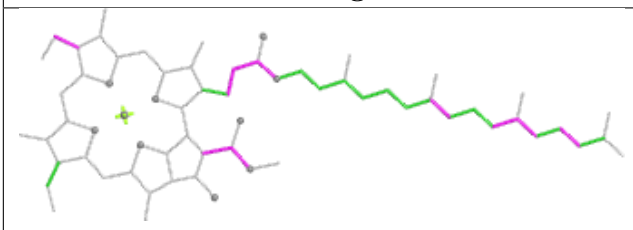
Ligand CLA BL 601



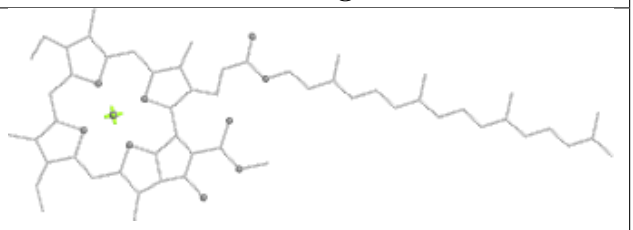
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Bond angles

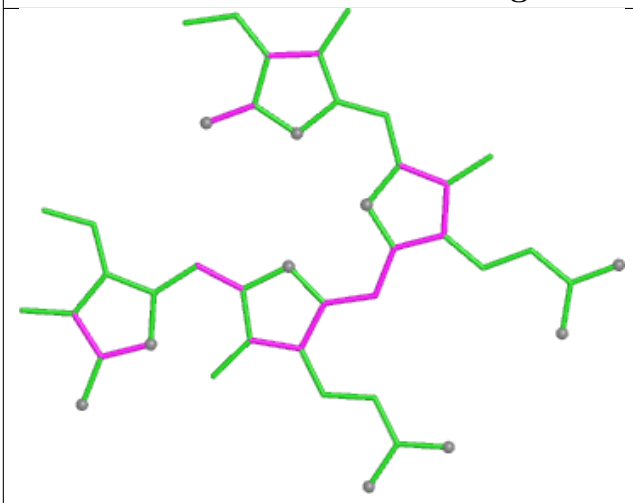


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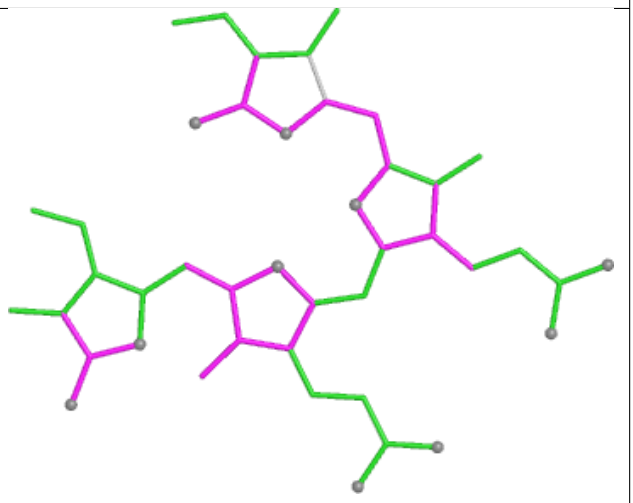


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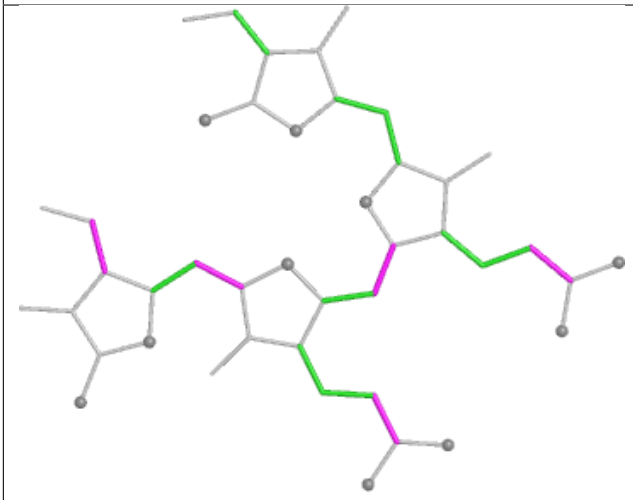
Ligand PEB XD 203



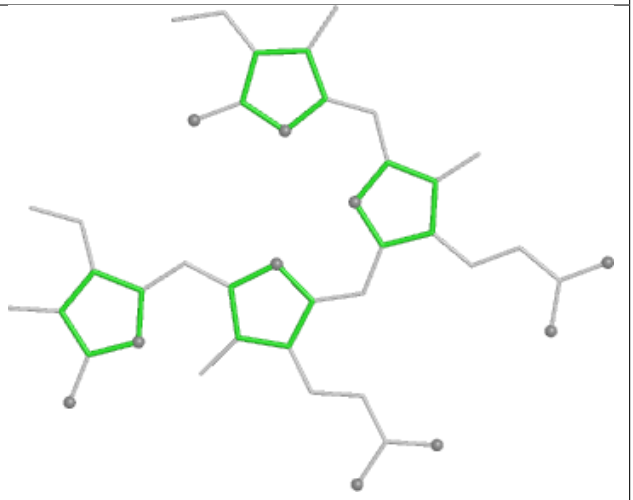
Bond lengths



Bond angles

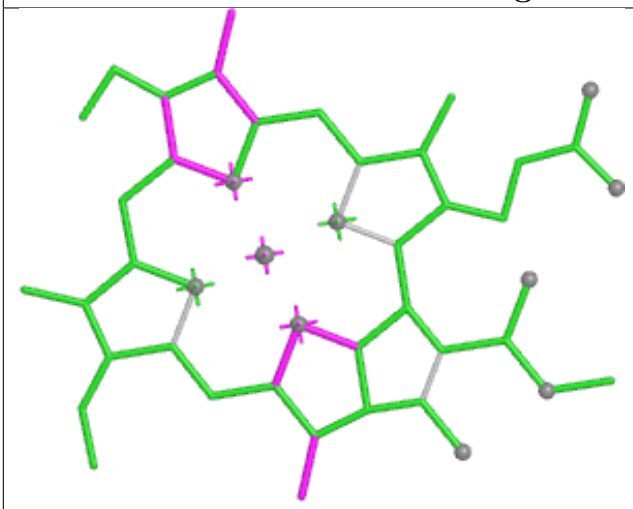


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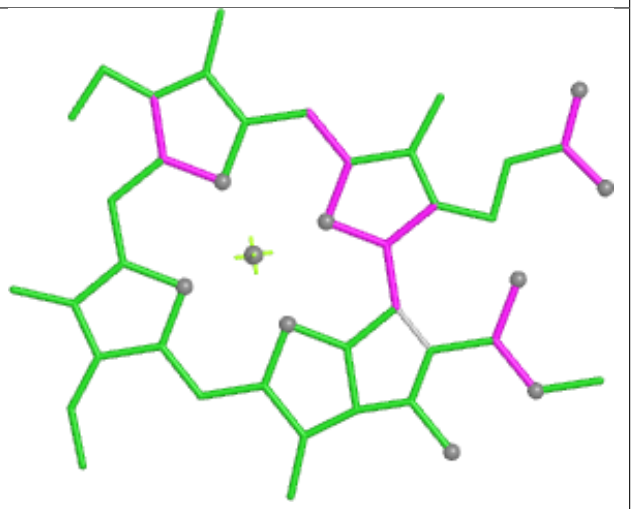


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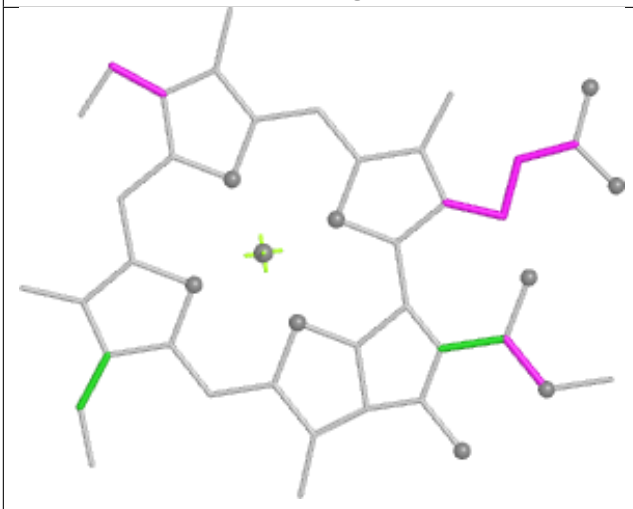
Ligand CLA 3N 312



Bond lengths



Bond angles

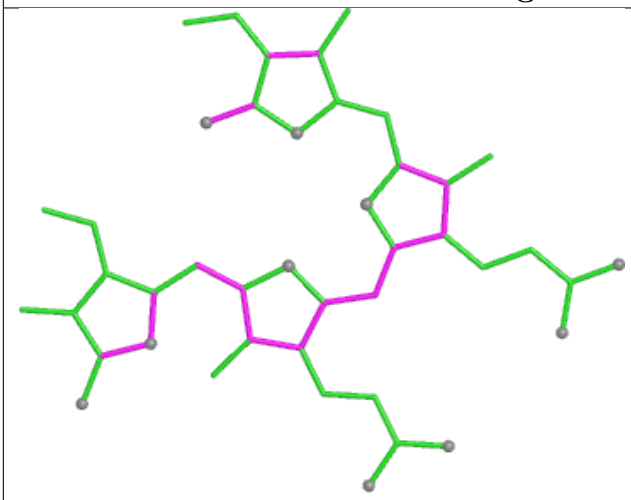


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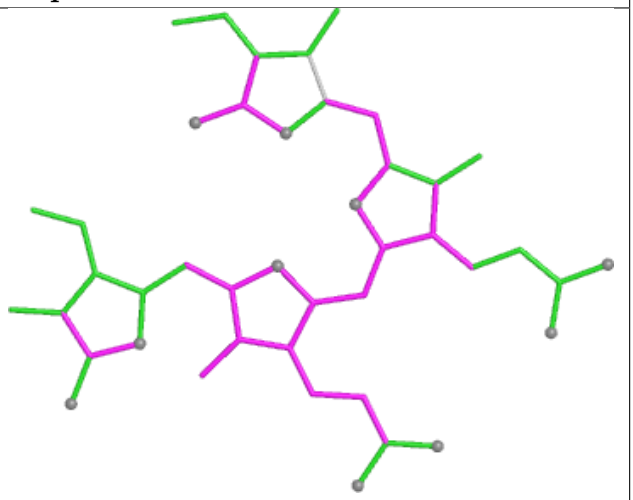


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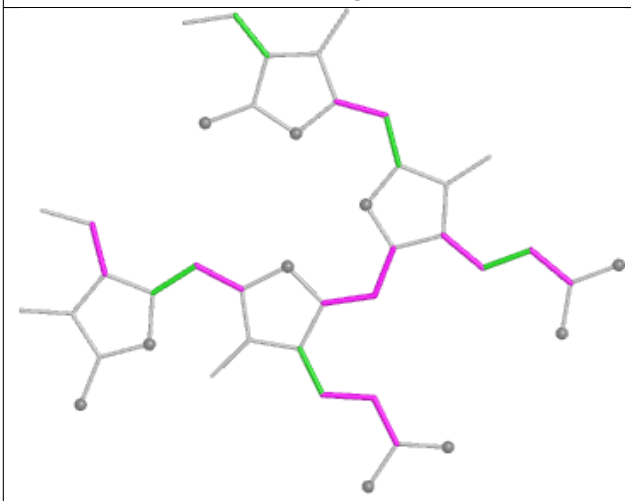
Ligand PEB qF 202



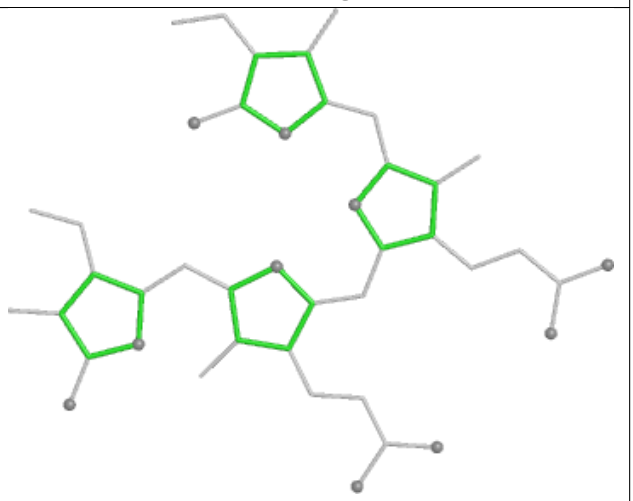
Bond lengths



Bond angles

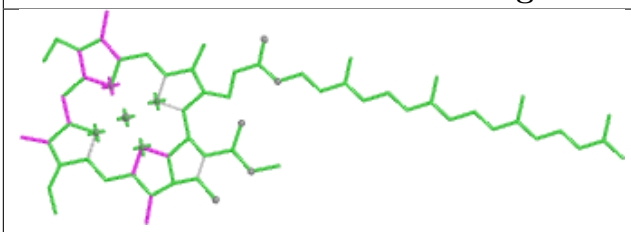


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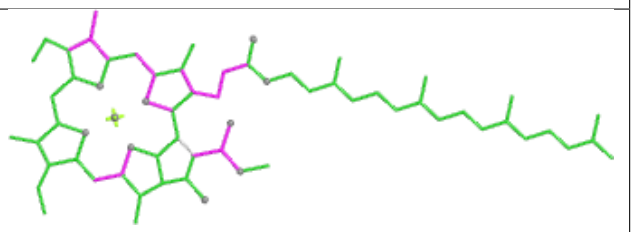


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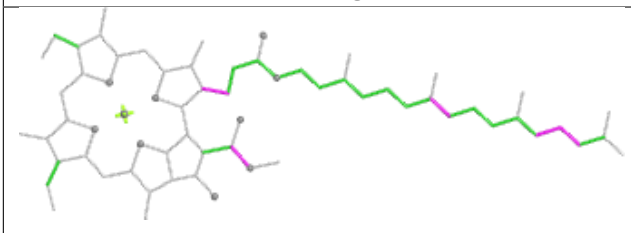
Ligand CLA dL 402



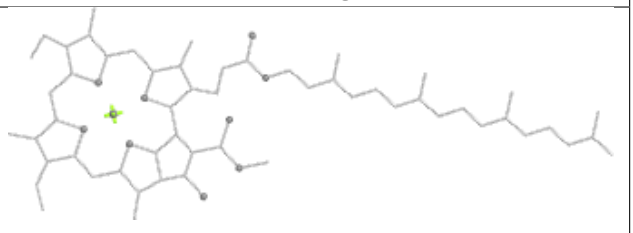
Bond lengths



Bond angles

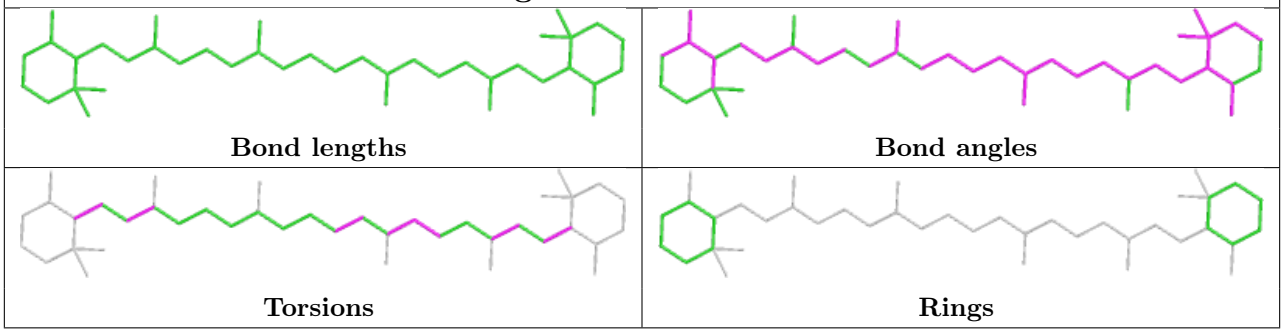


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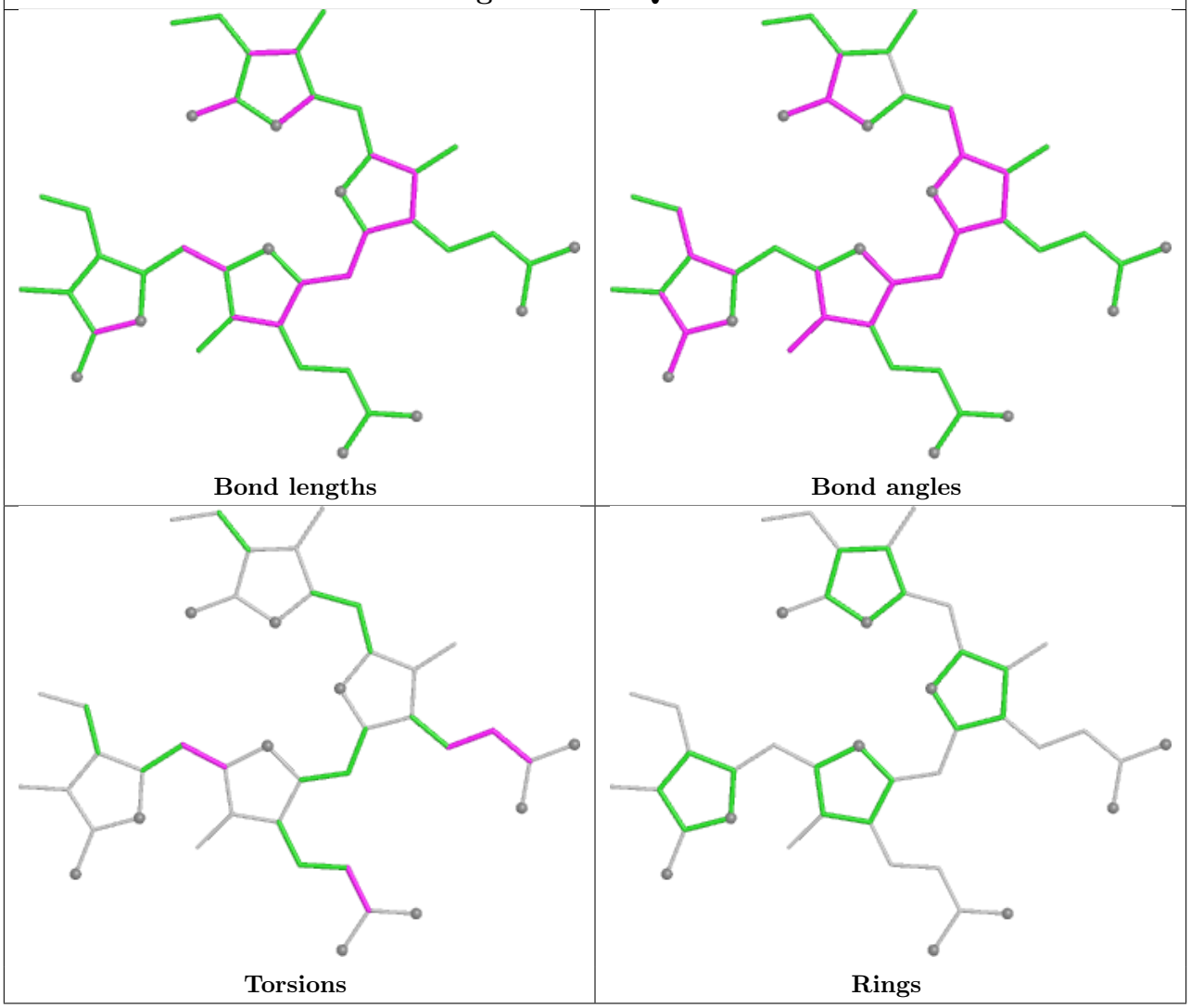


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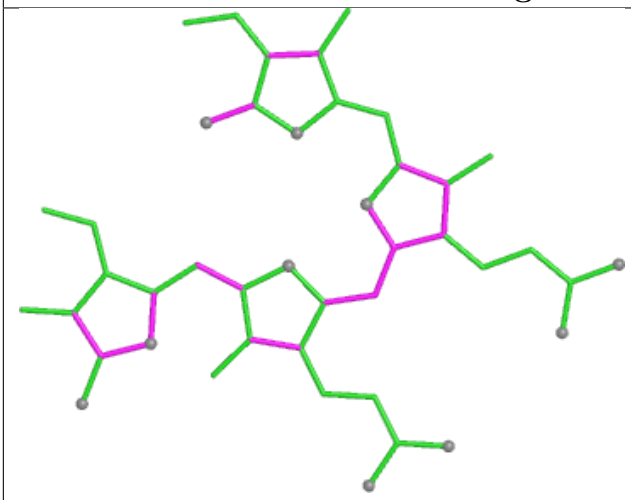
Ligand BCR B2 802



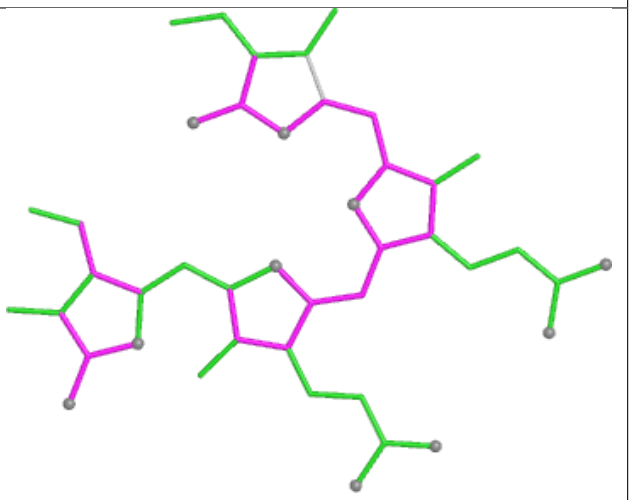
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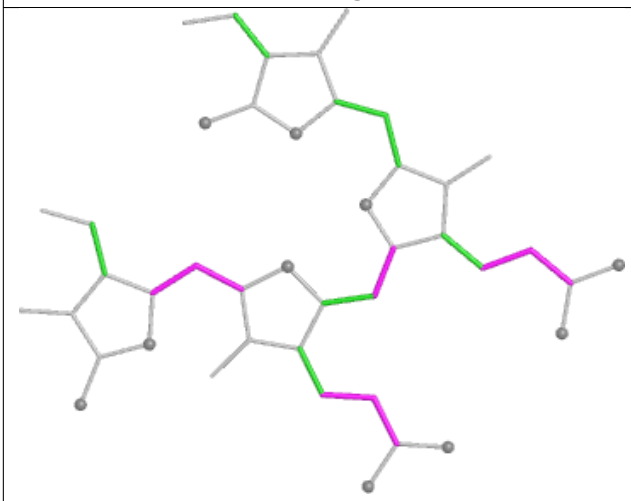
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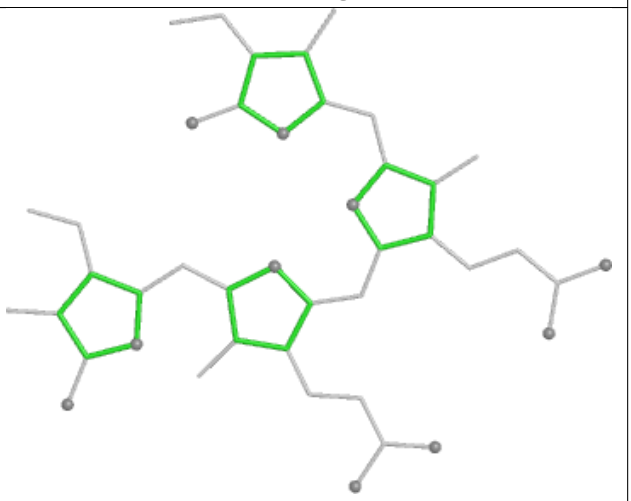
Bond lengths



Bond angles

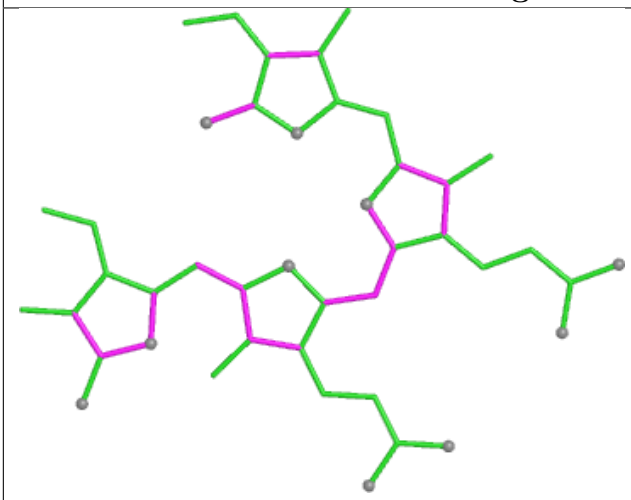


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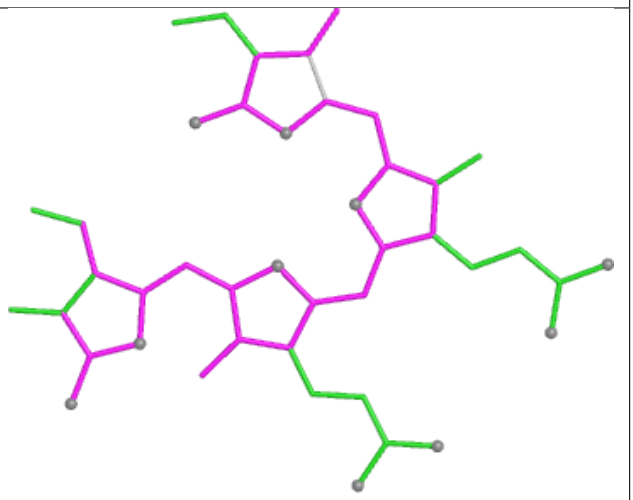


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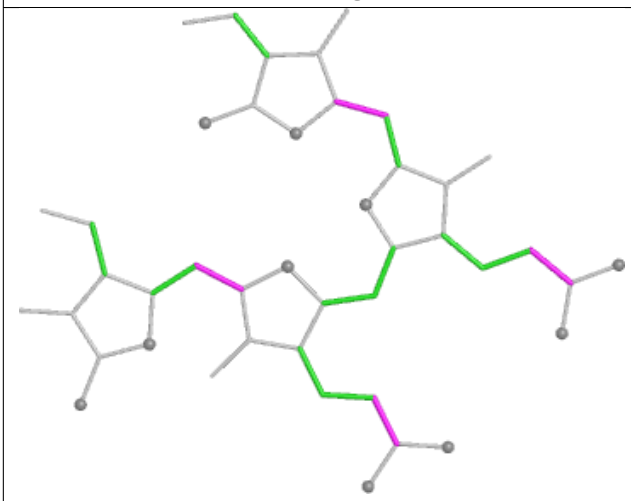
Ligand PEB M5 304



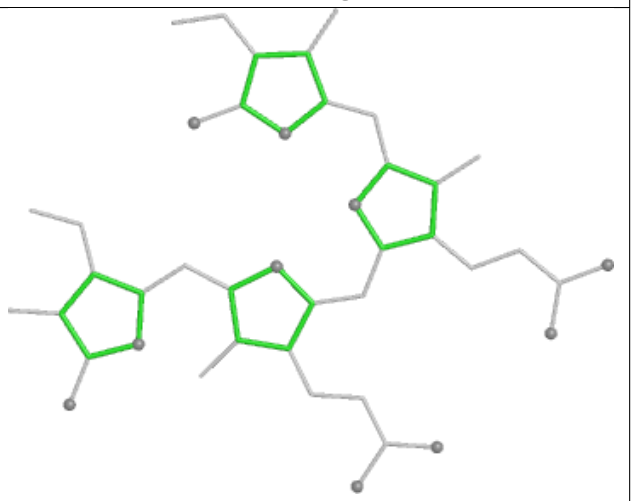
Bond lengths



Bond angles

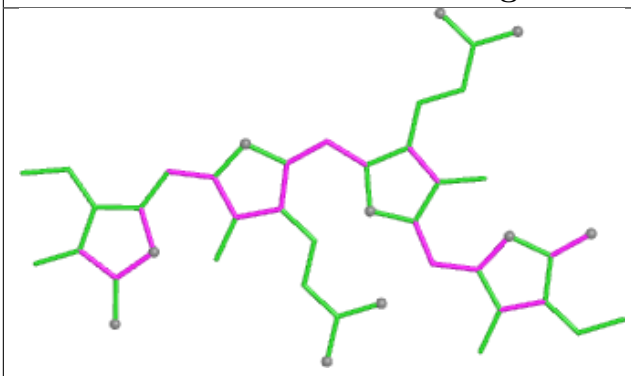


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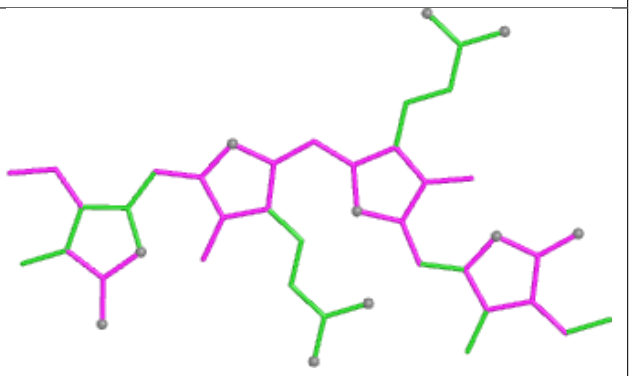


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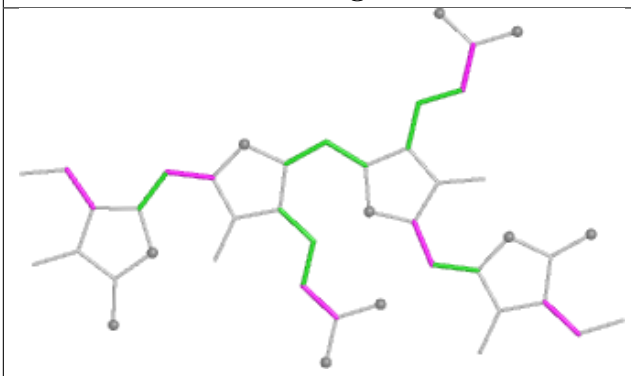
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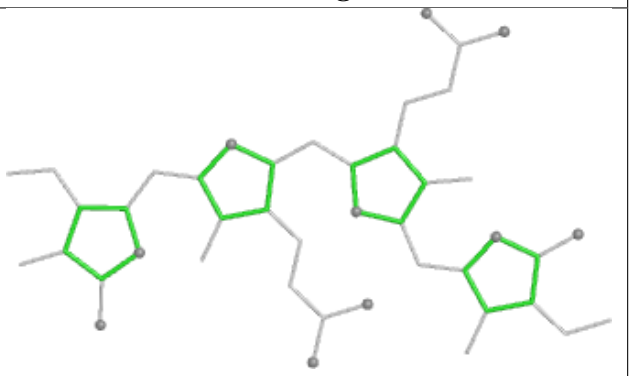
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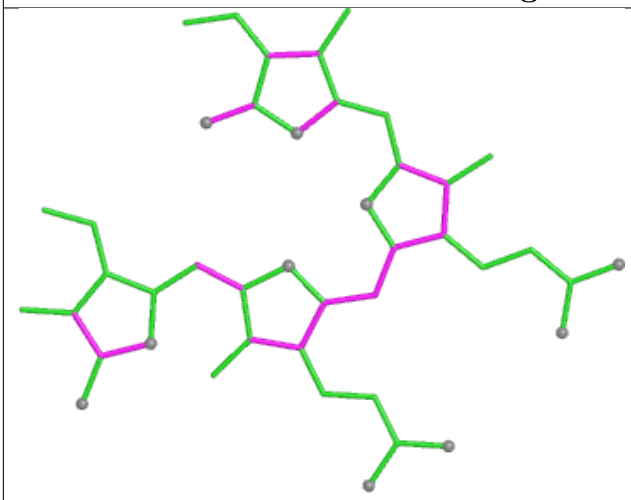


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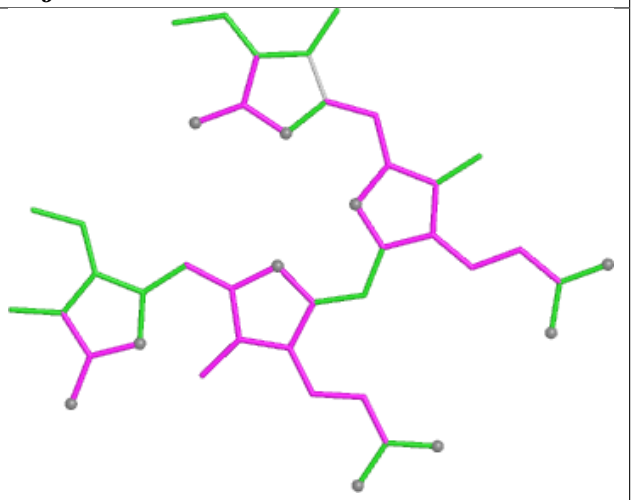


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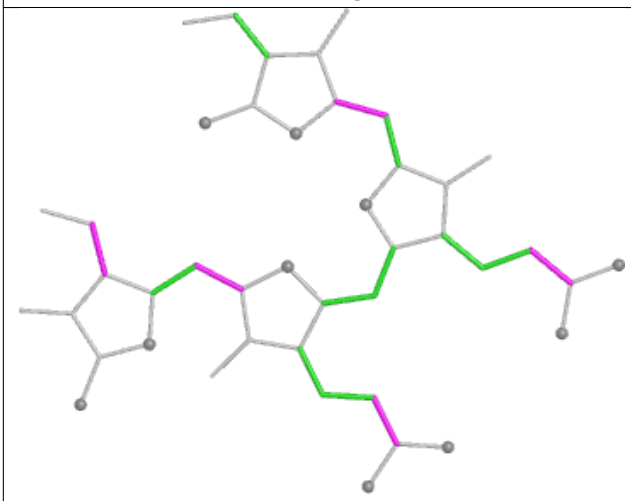
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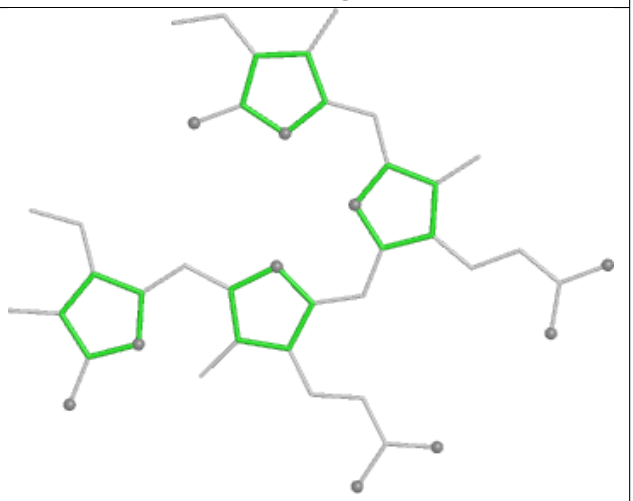
Bond lengths



Bond angles

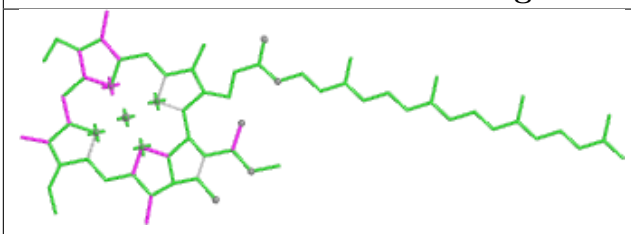


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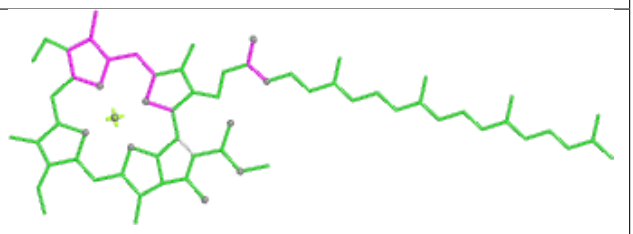


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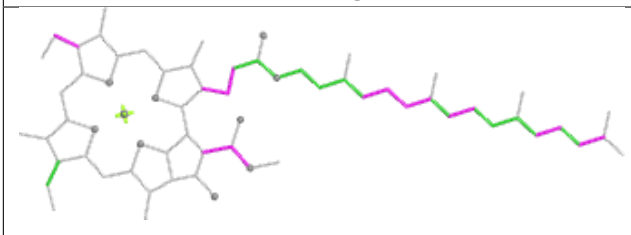
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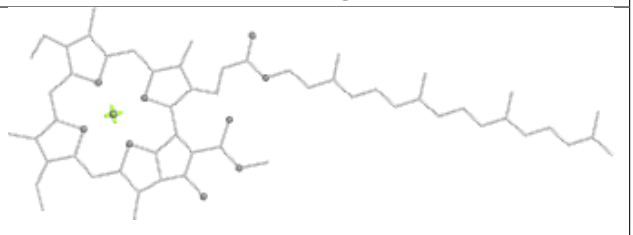
Bond lengths



Bond angles

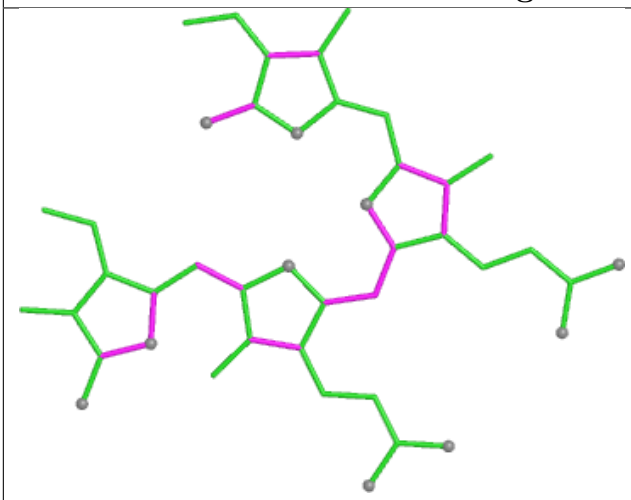


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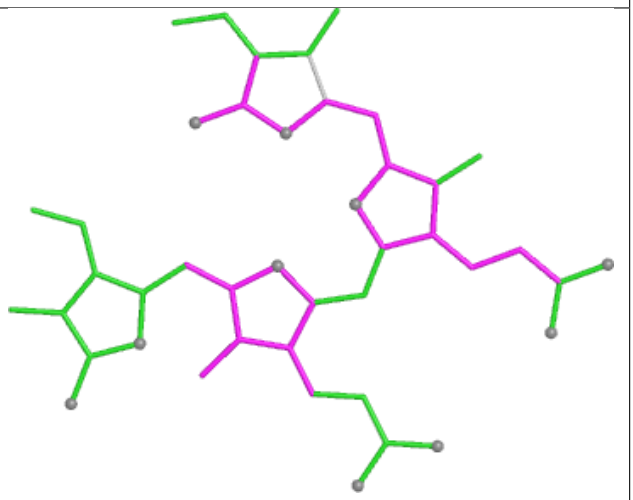


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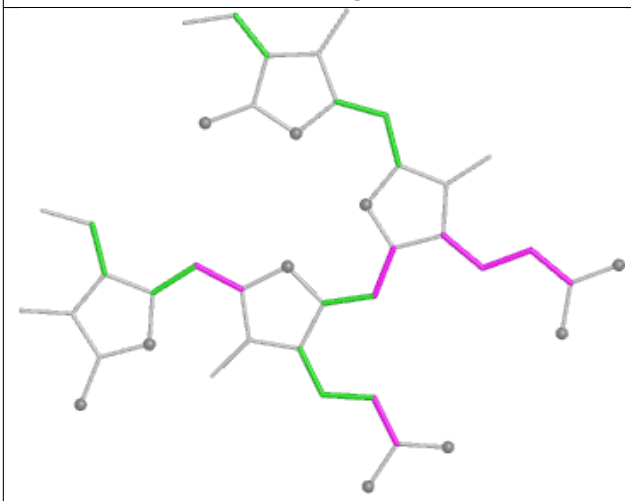
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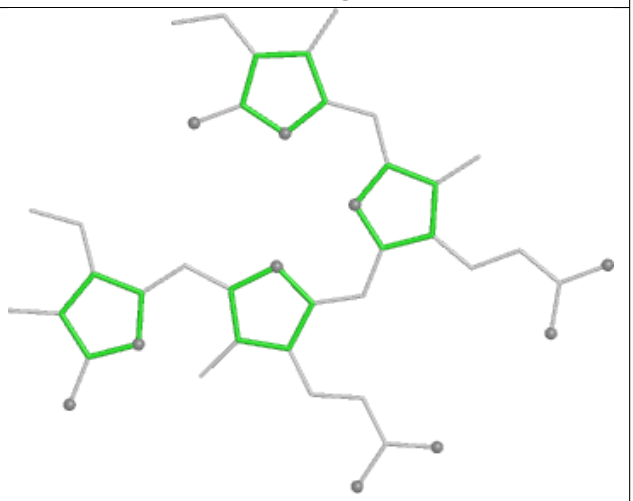
Bond lengths



Bond angles

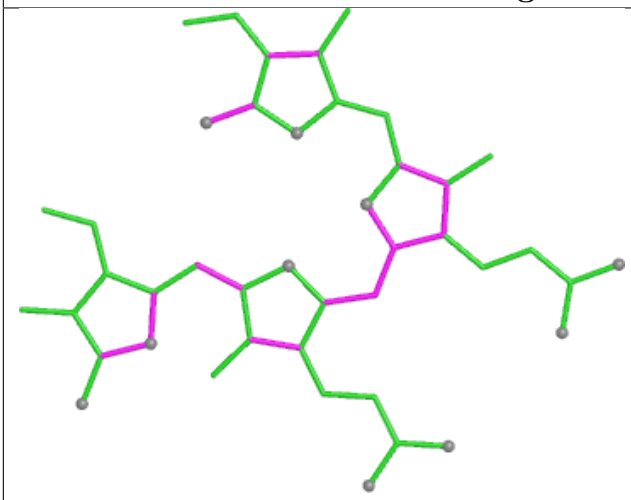


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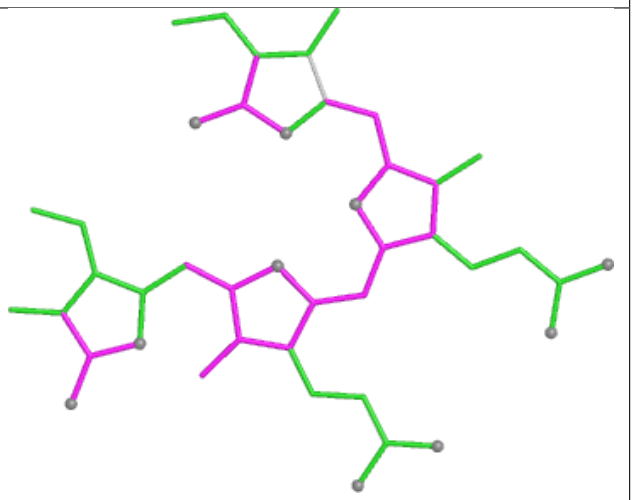


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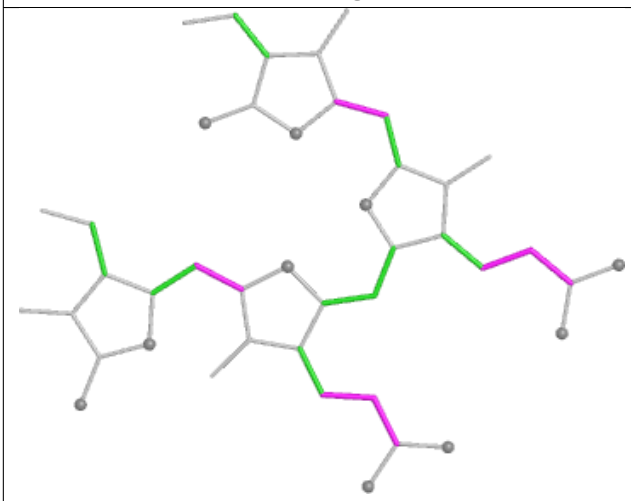
Ligand PEB XI 202



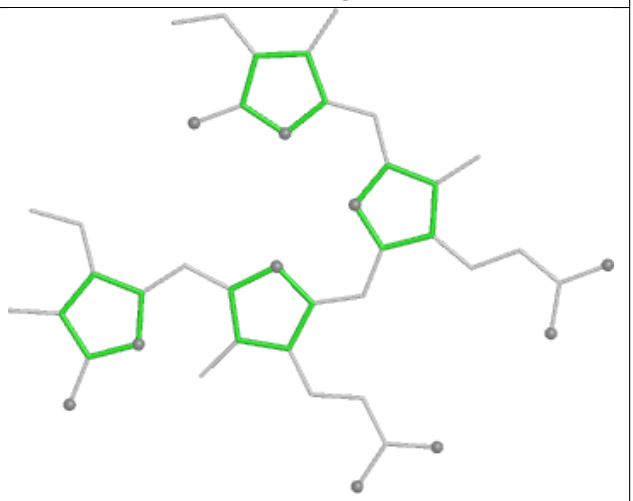
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Bond angles

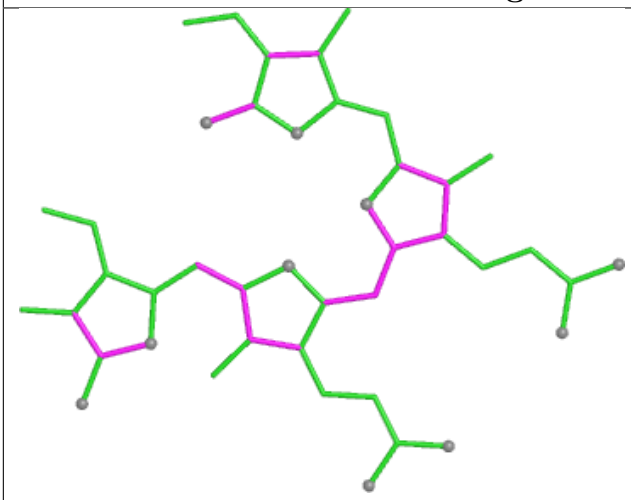


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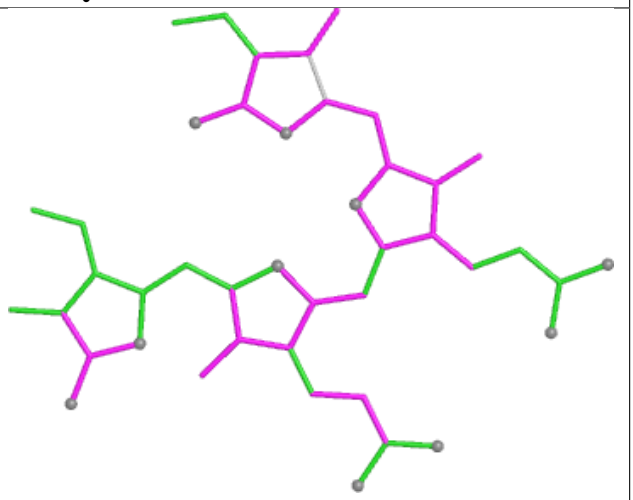


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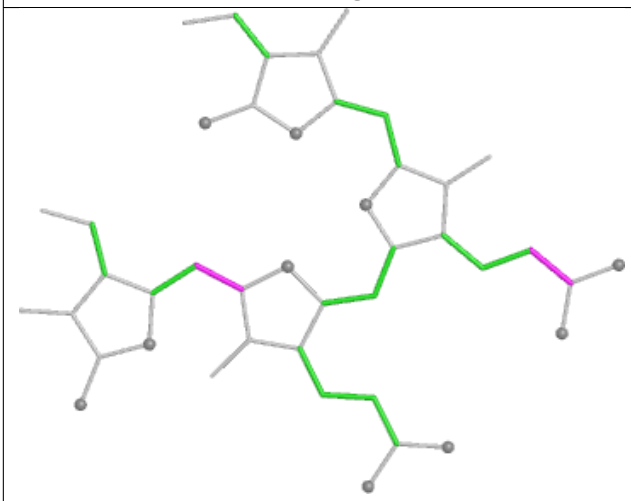
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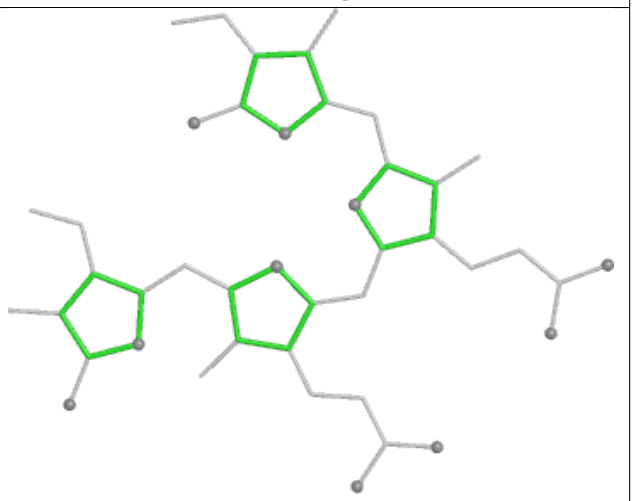
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Bond angles

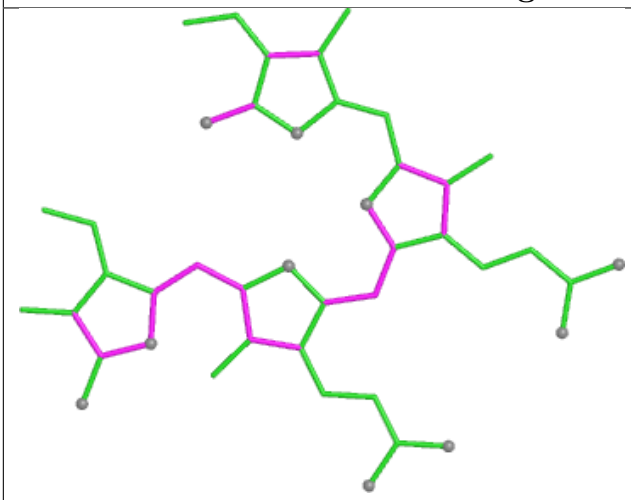


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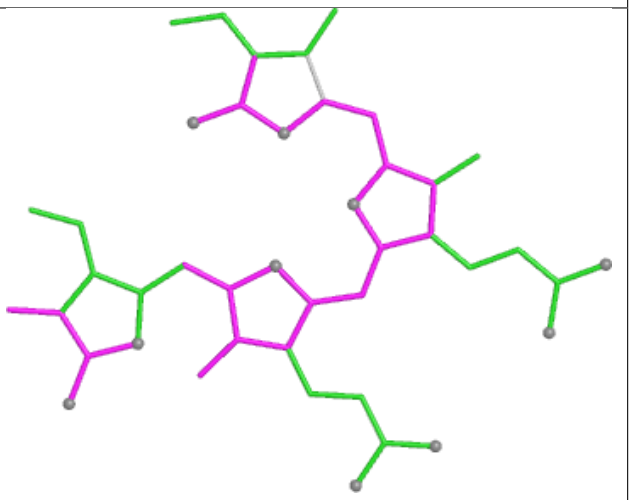


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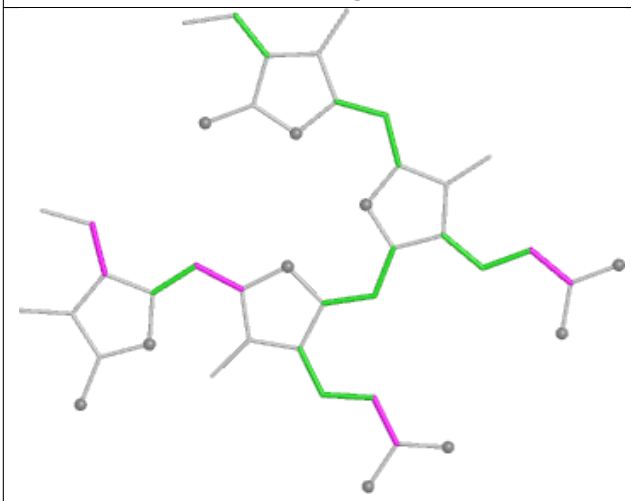
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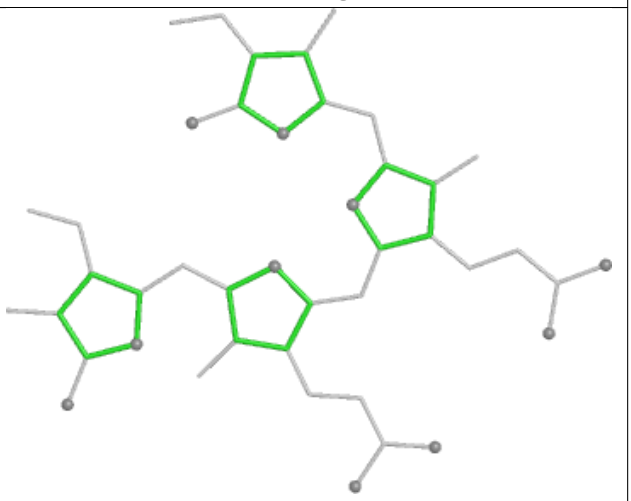
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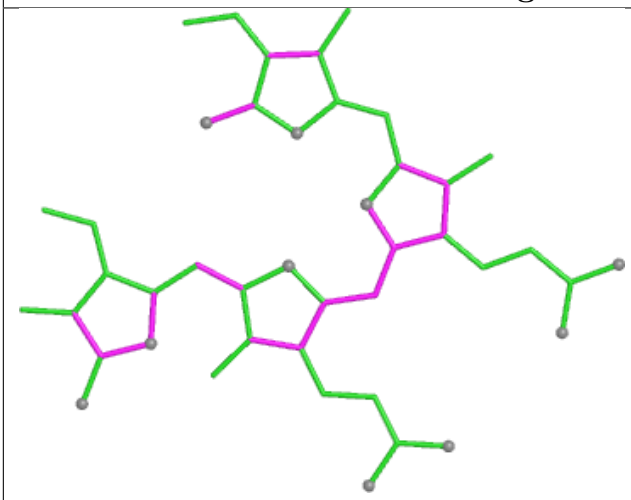


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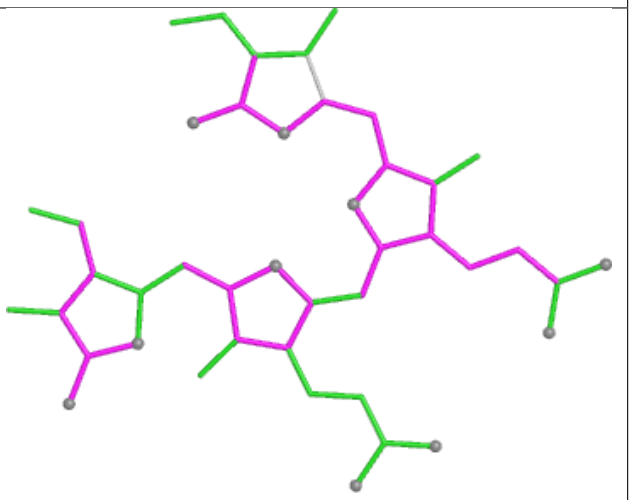


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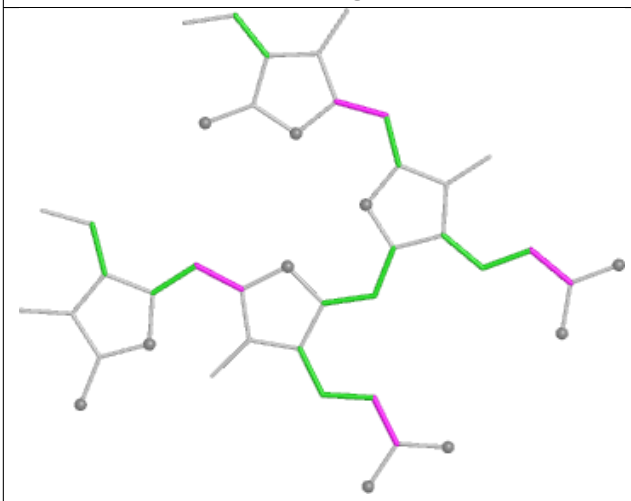
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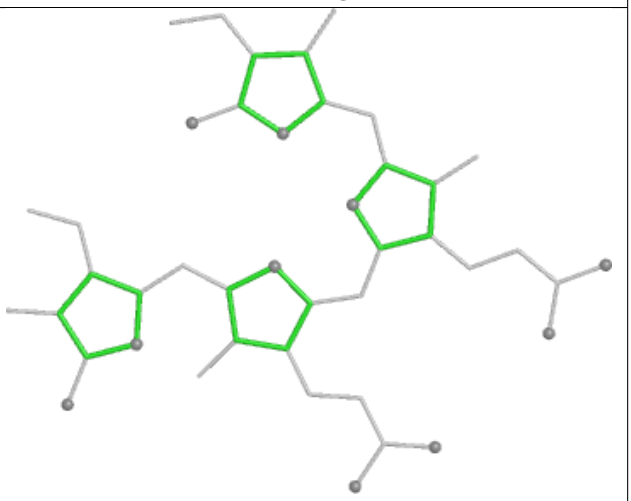
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Bond angles

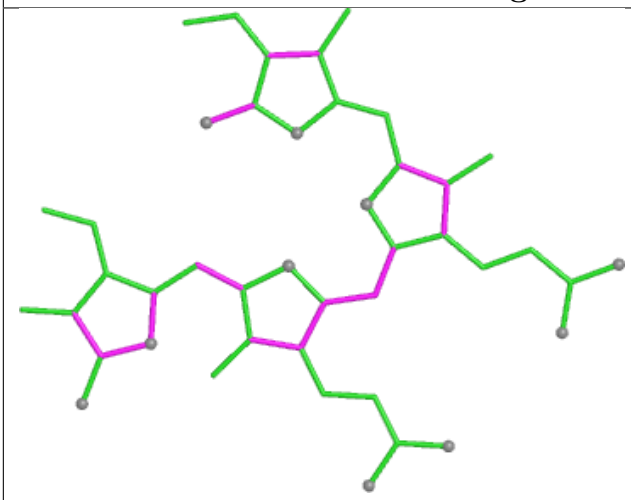


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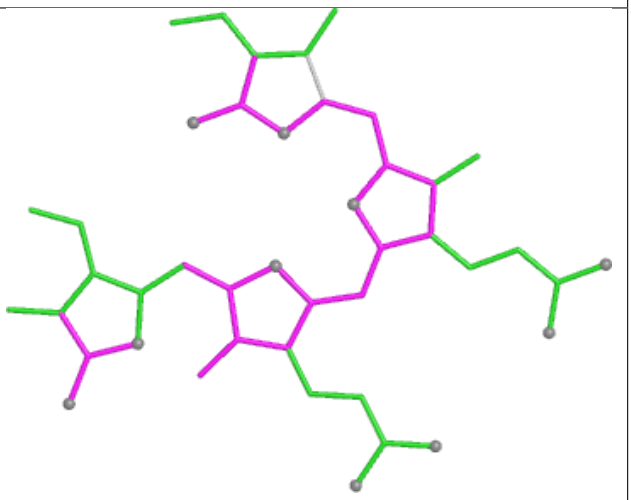


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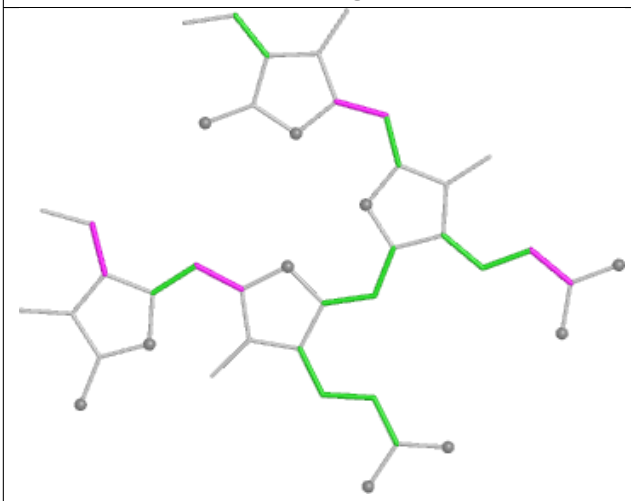
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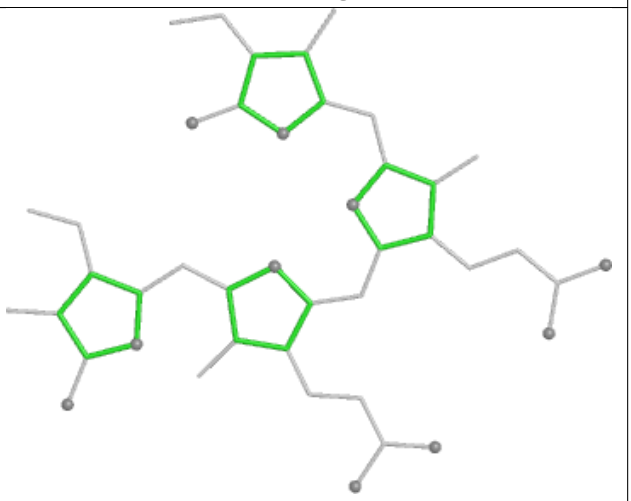
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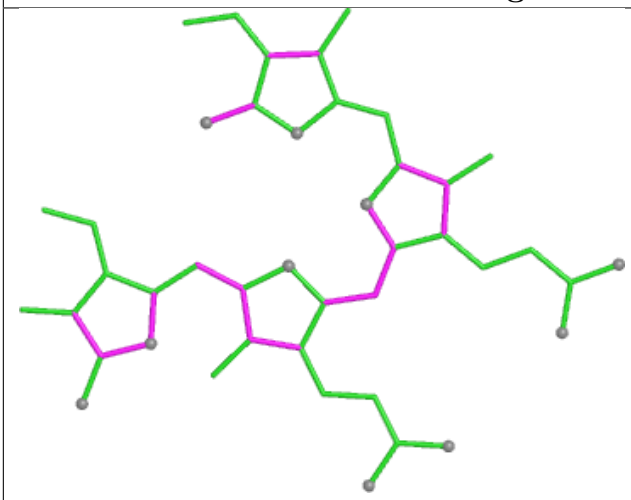


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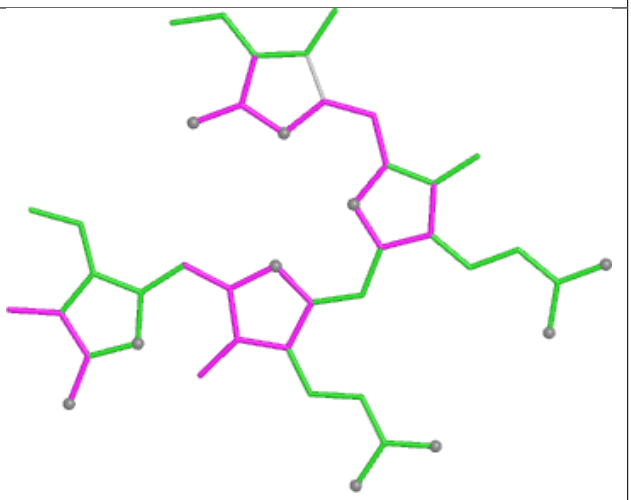


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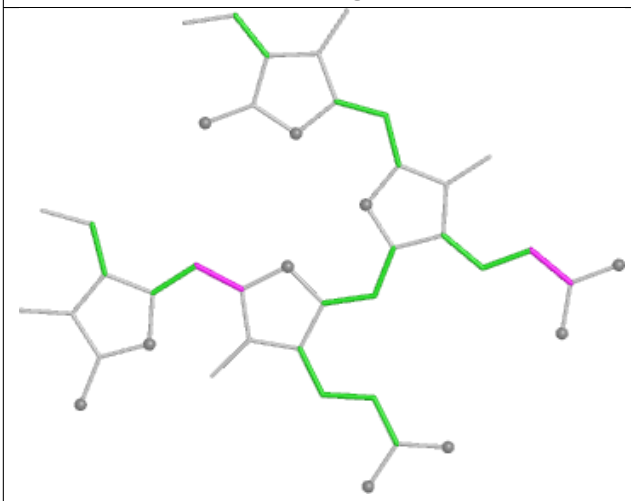
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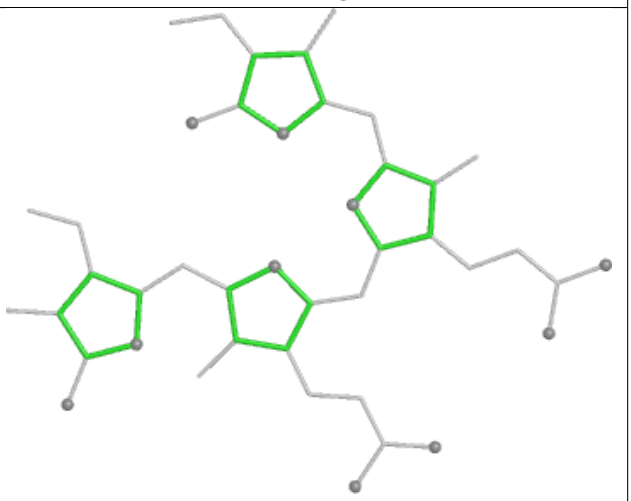
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Bond angles

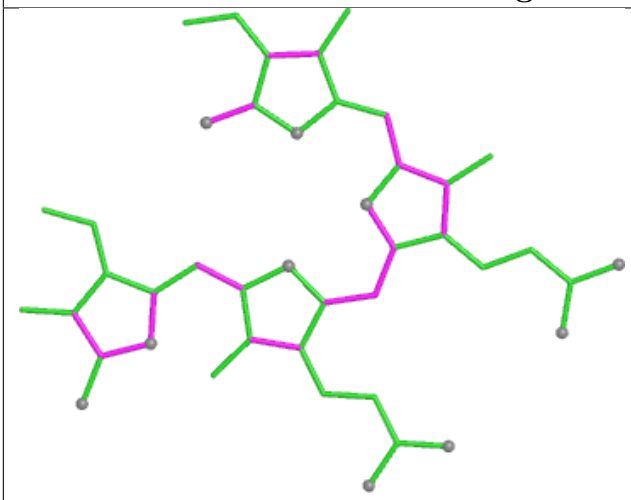


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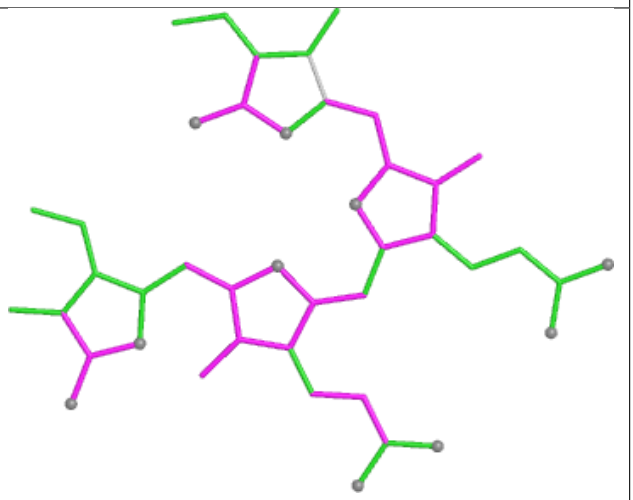


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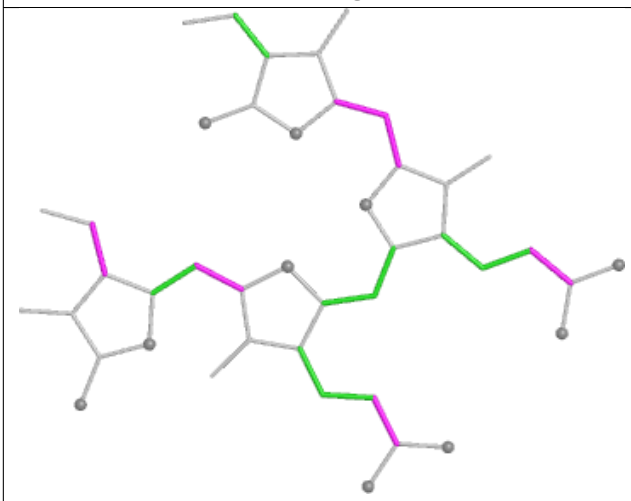
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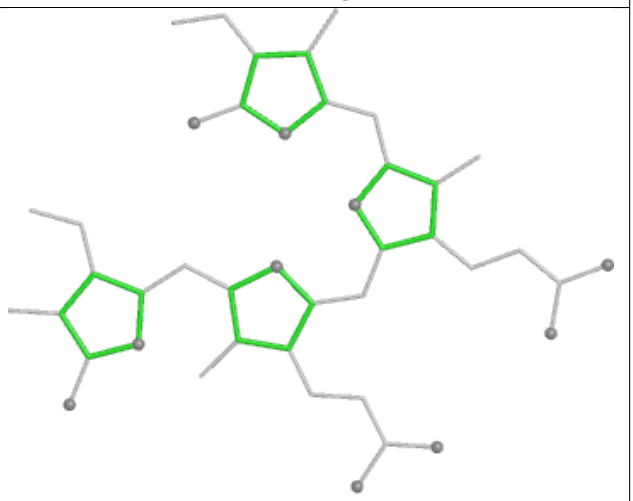
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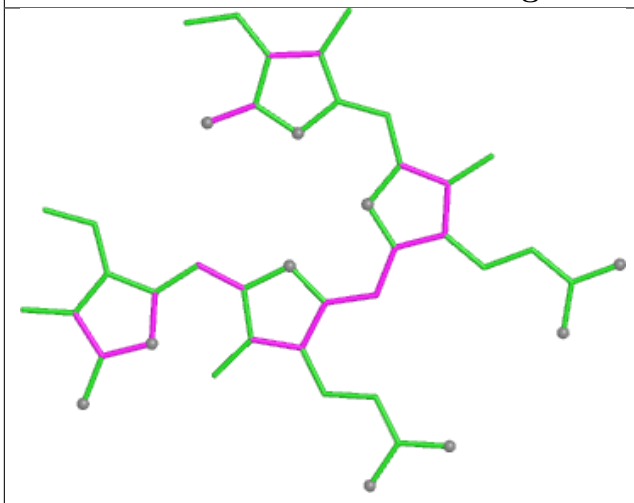


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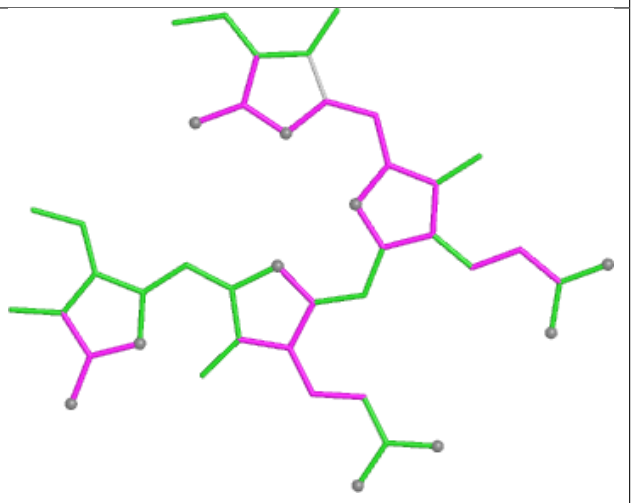


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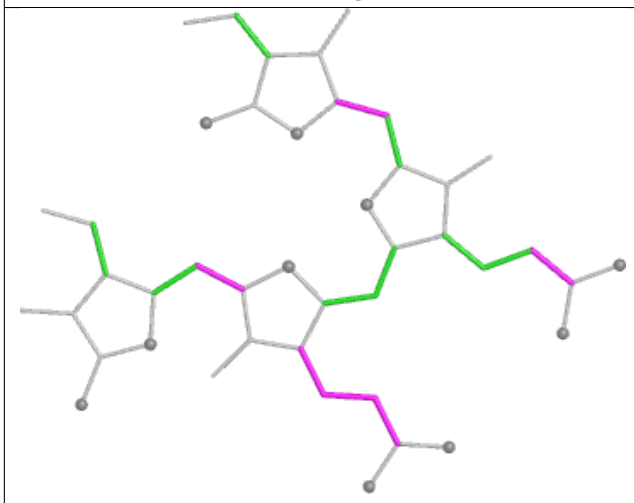
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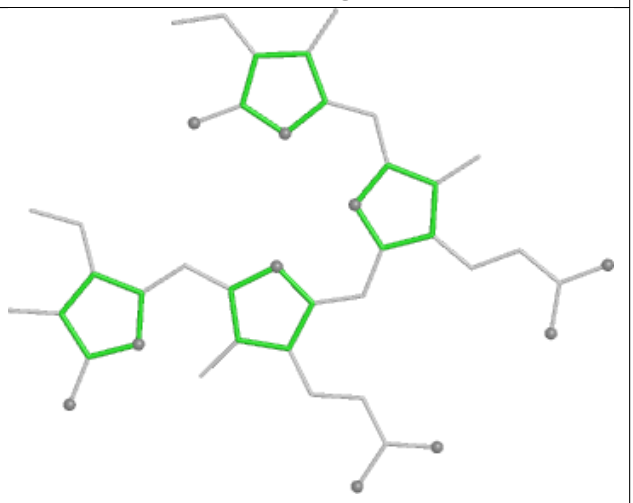
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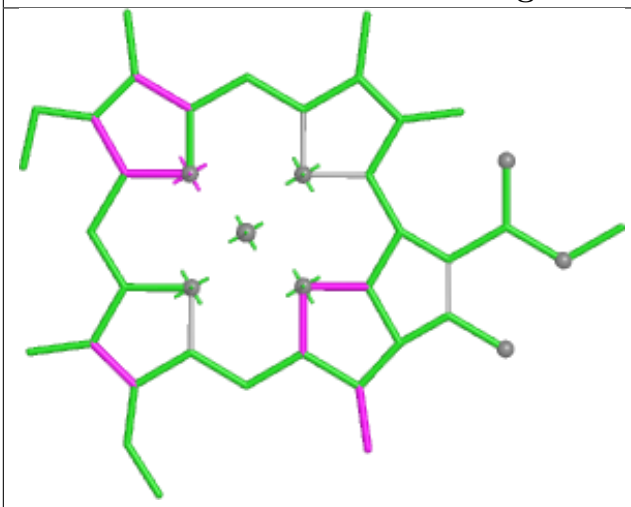


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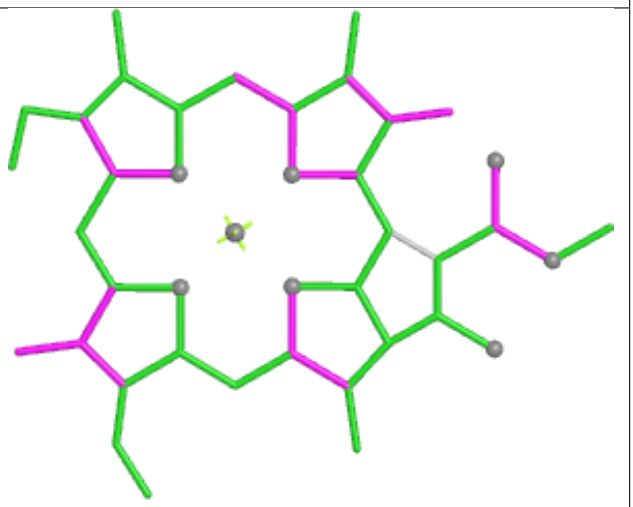


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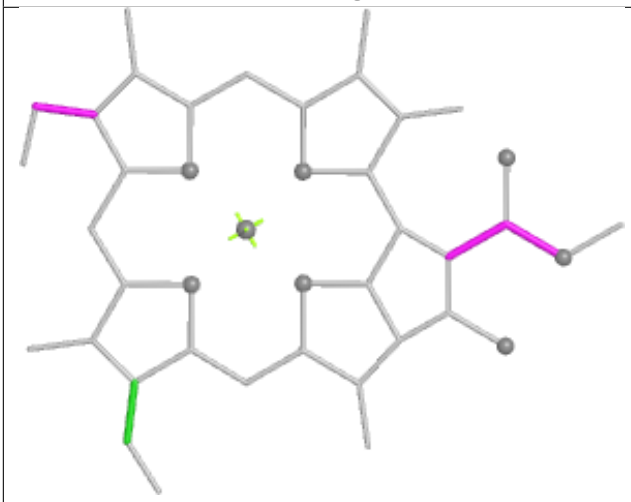
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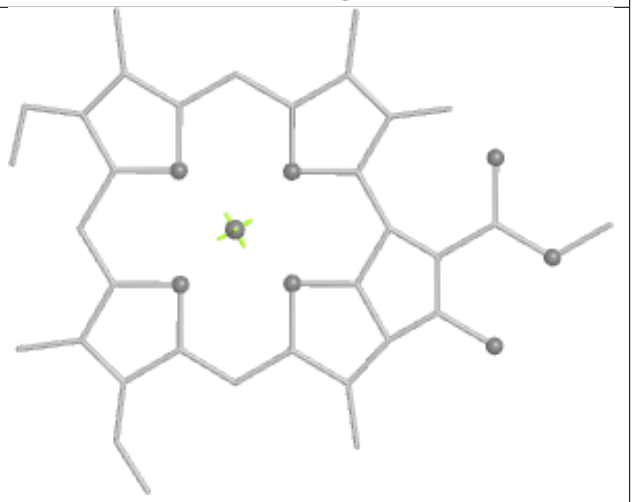
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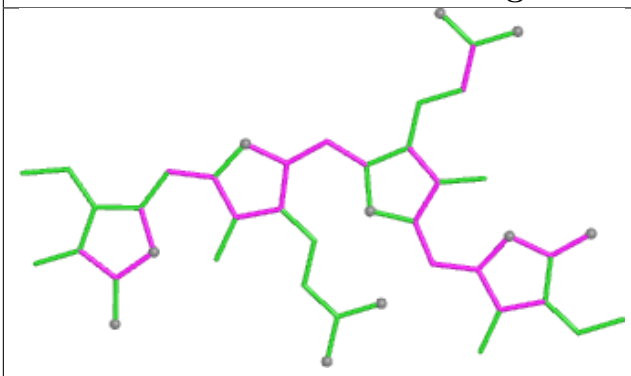


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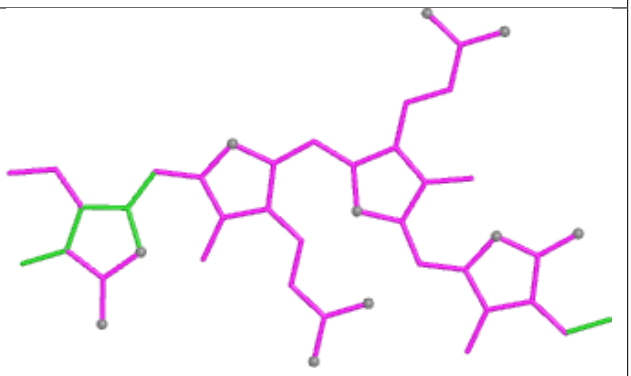


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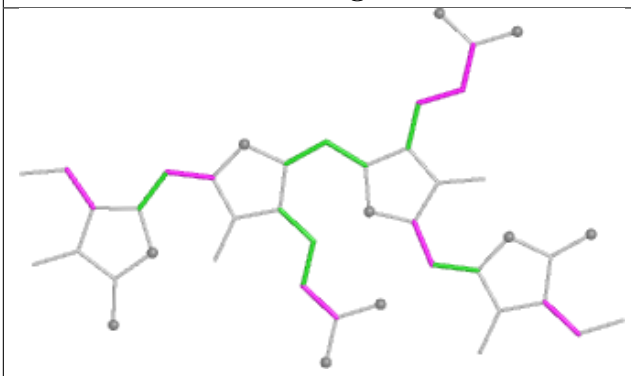
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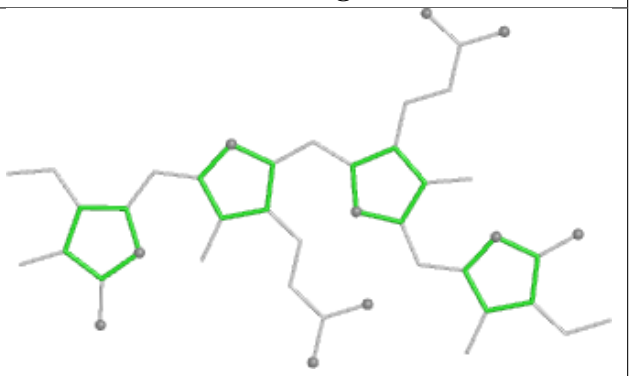
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Bond angles

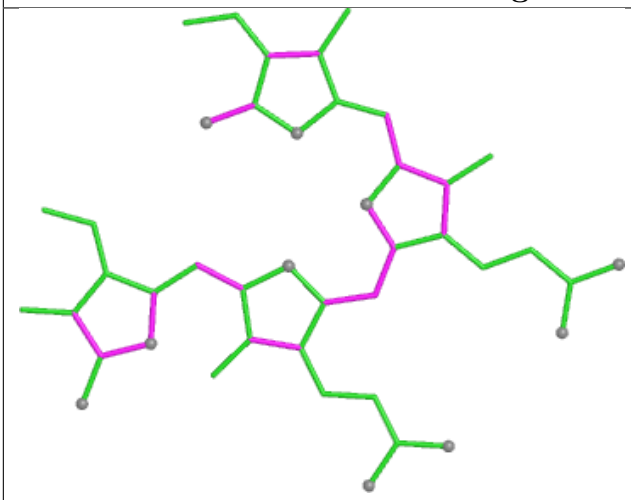


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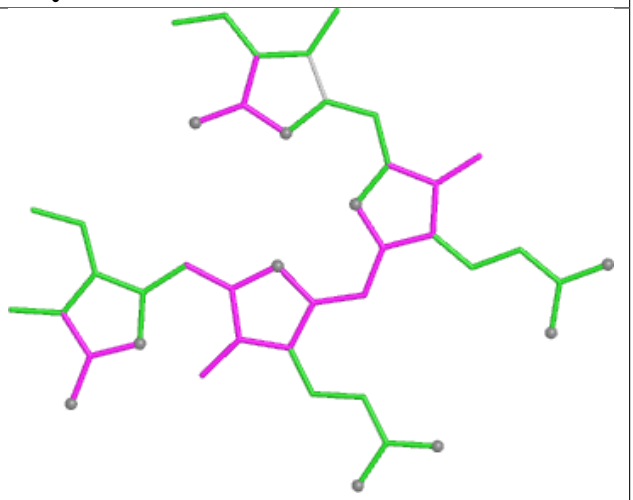


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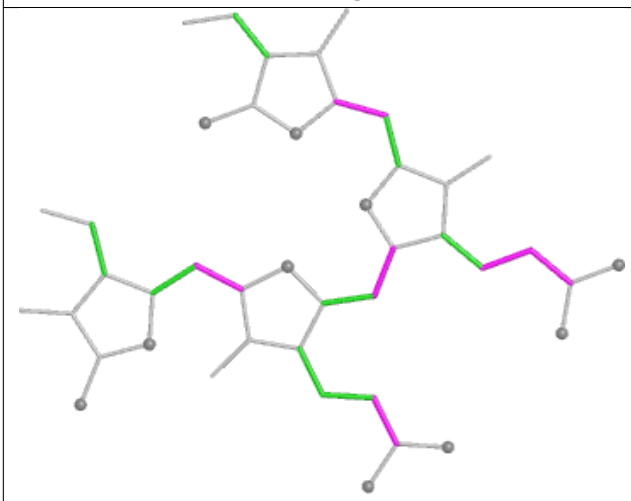
Ligand PEB QB 204



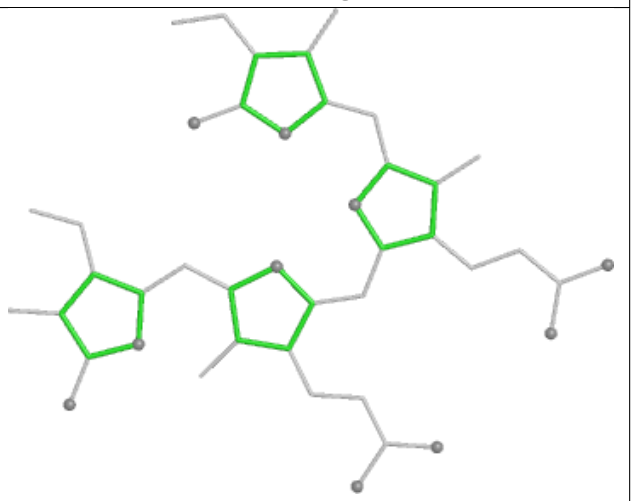
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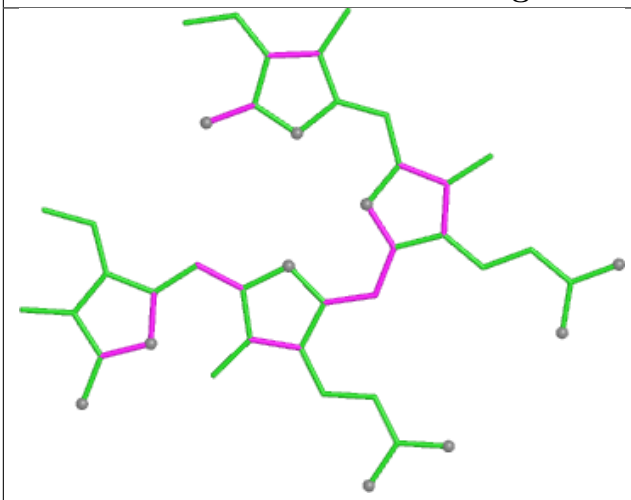


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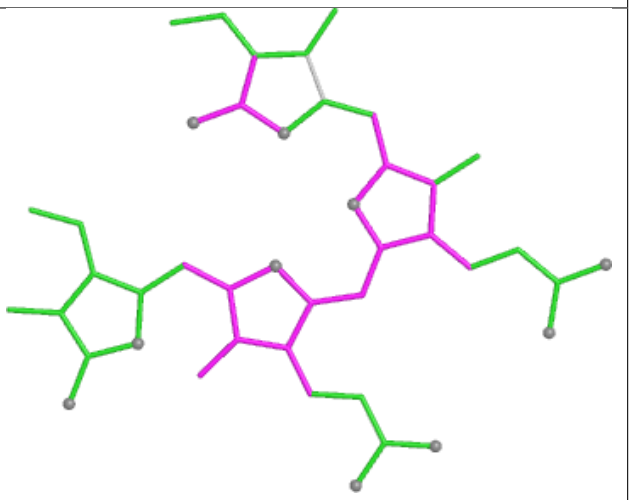


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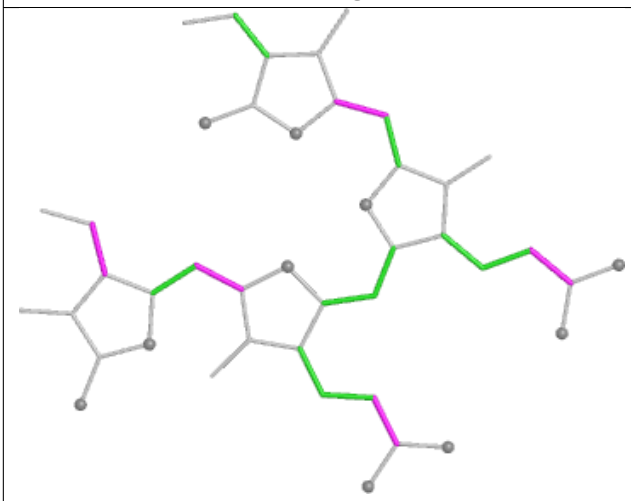
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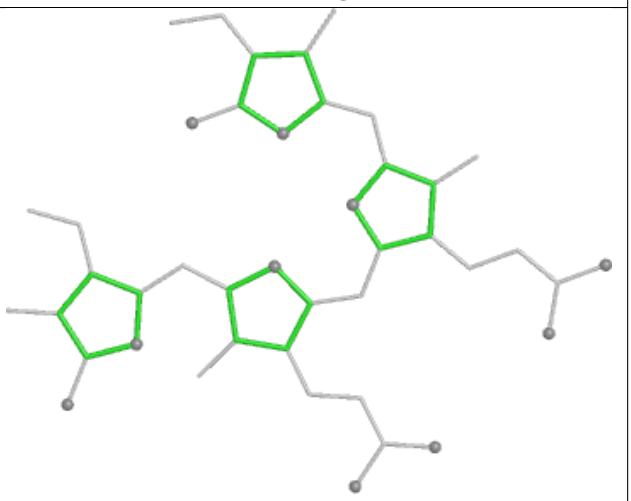
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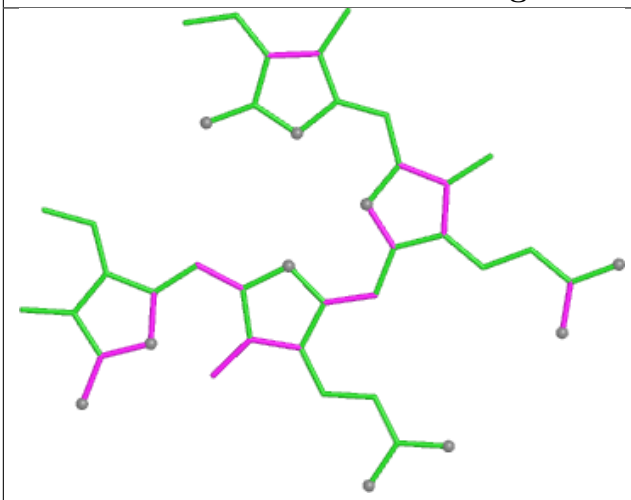


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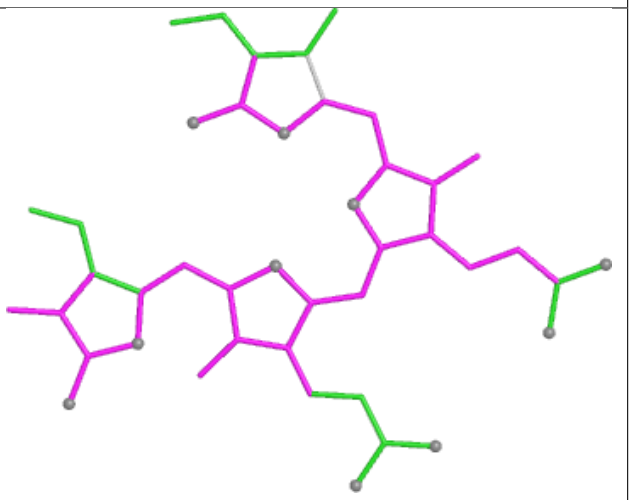


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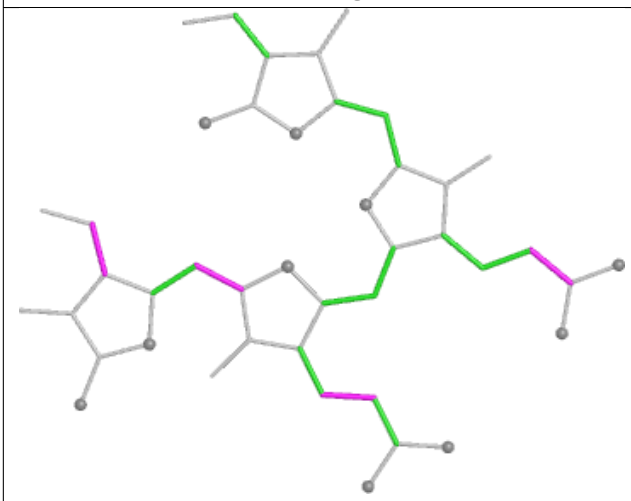
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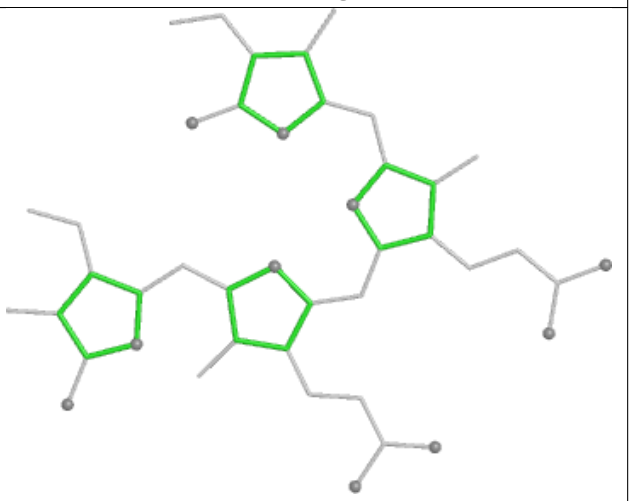
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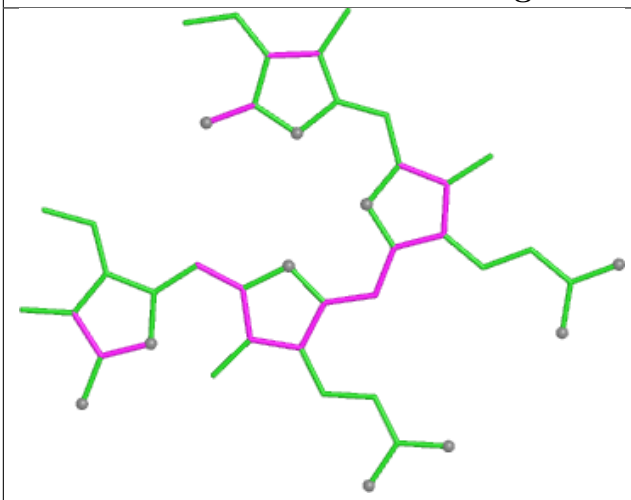


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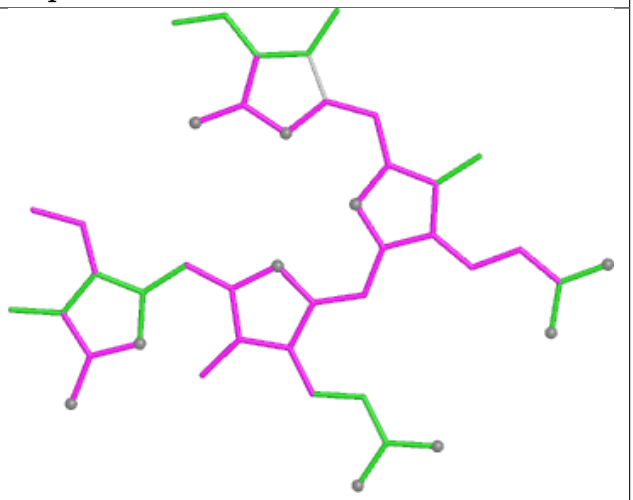


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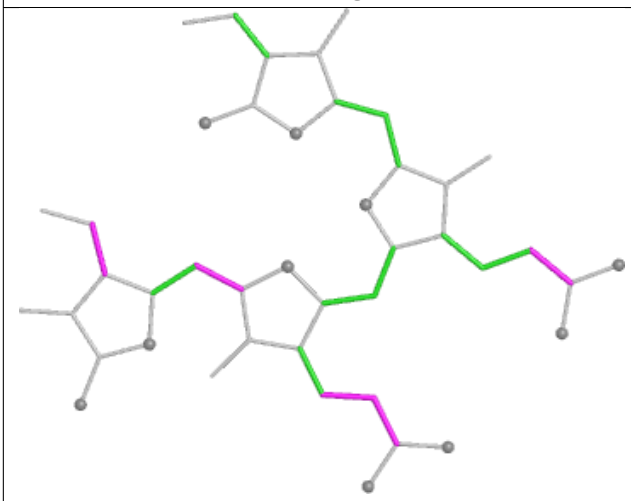
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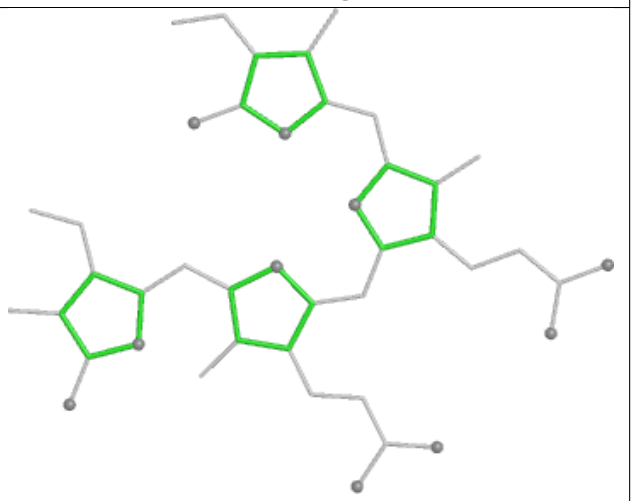
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Bond angles

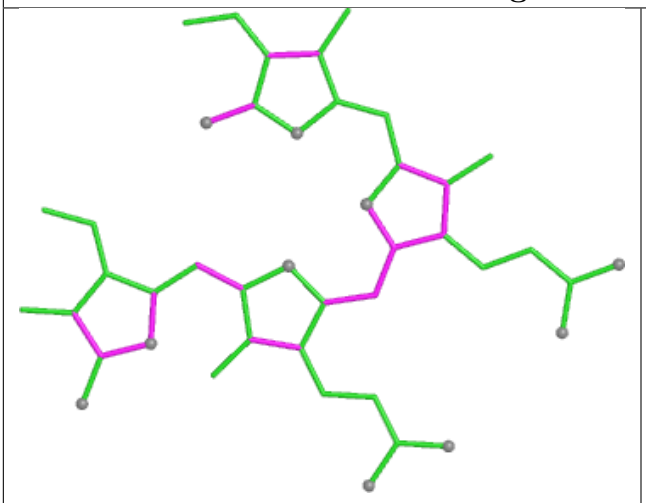


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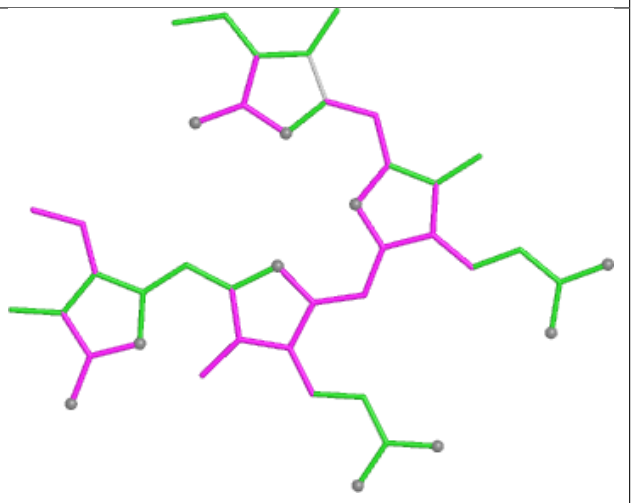


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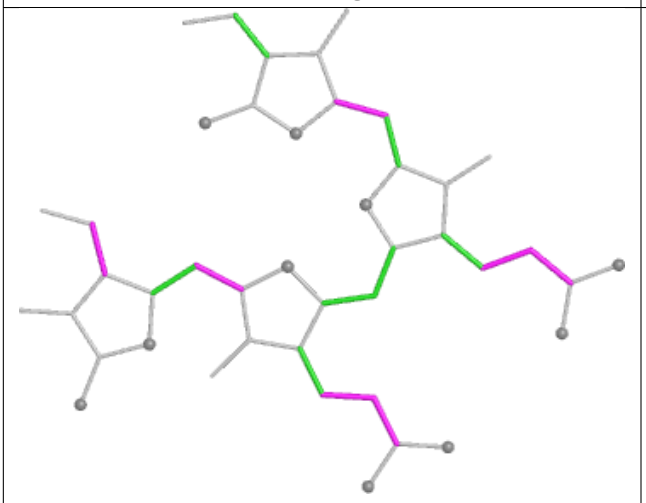
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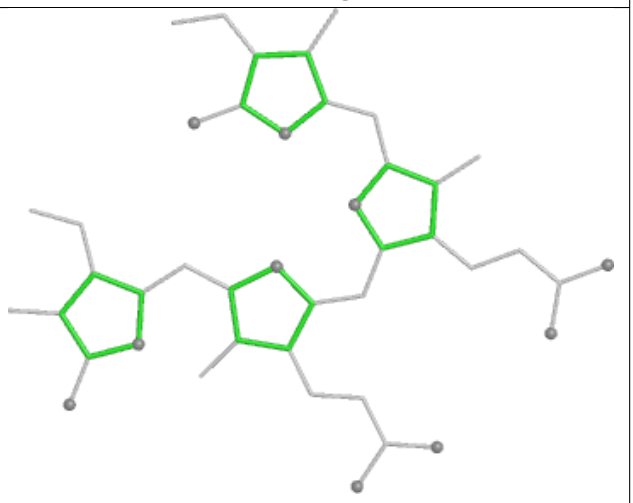
Bond lengths



Bond angles

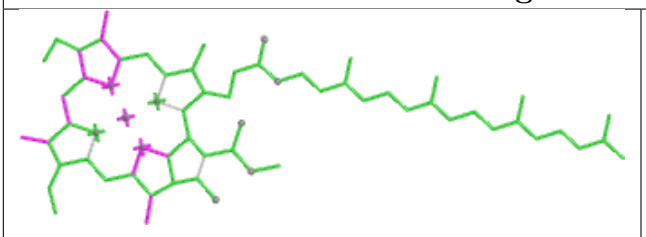


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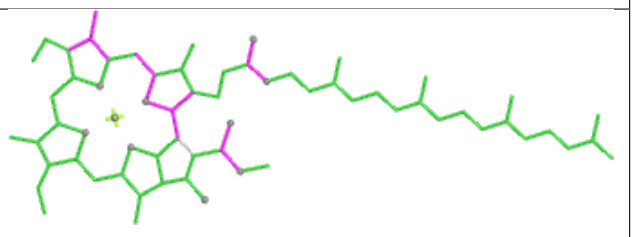


Rings

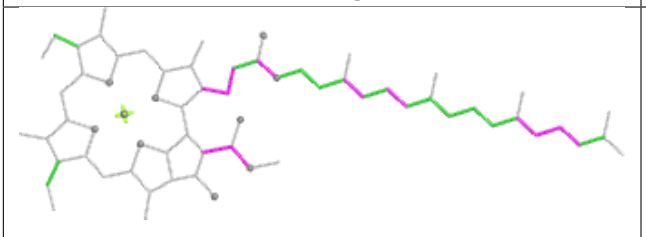
Ligand CLA B2 825



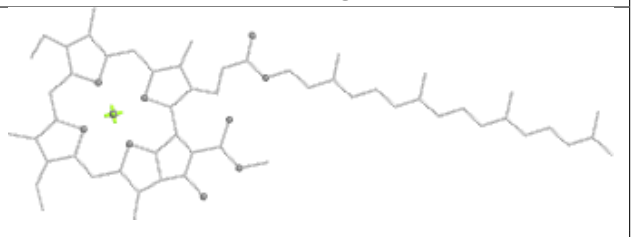
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Bond angles

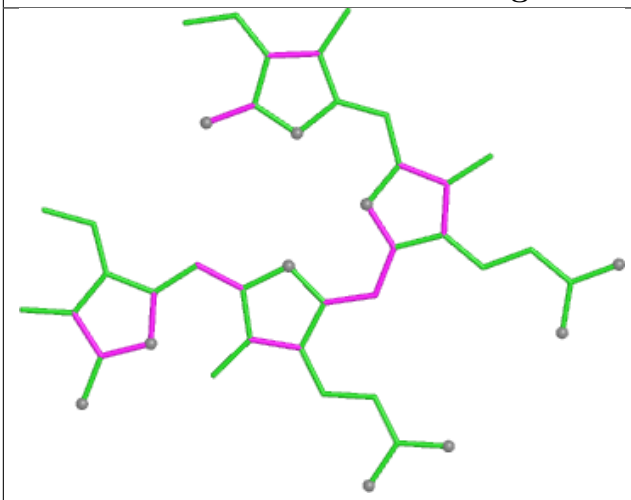


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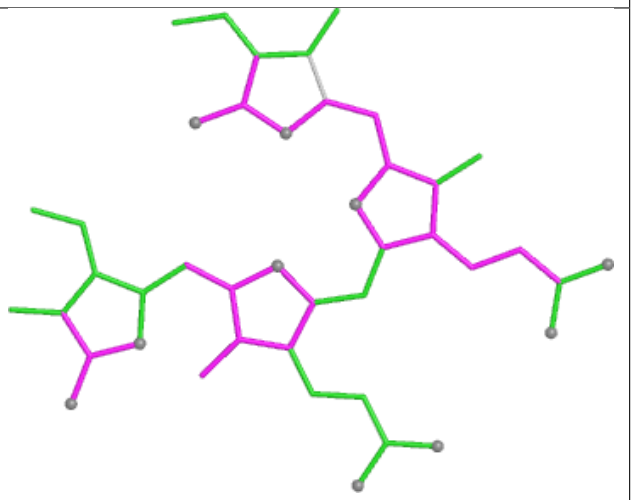


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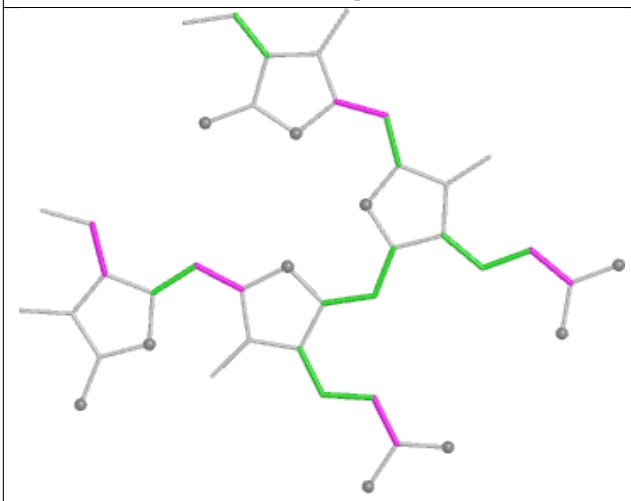
Ligand PEB HB 202



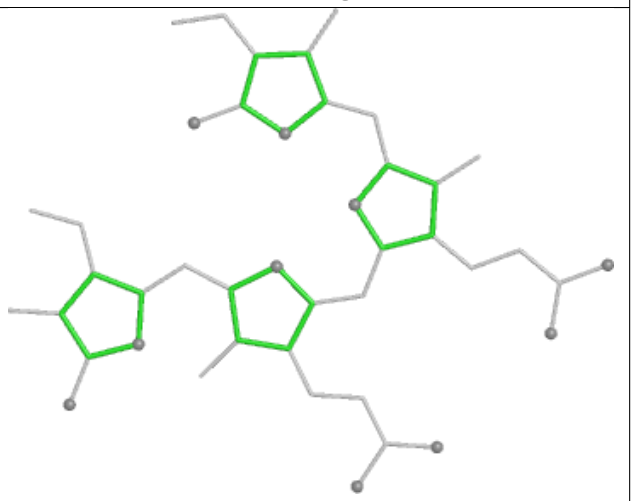
Bond lengths



Bond angles

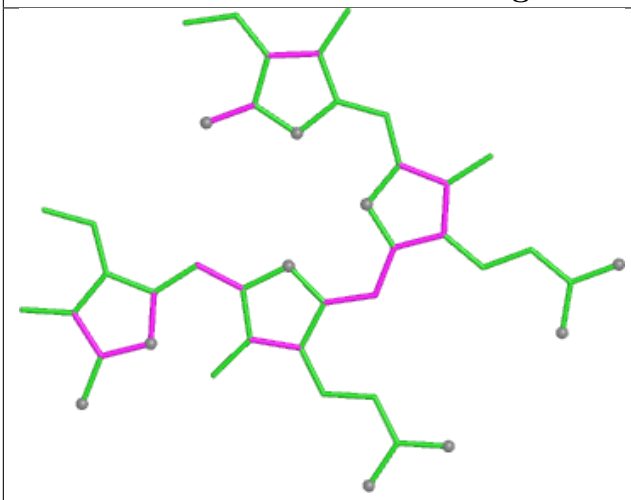


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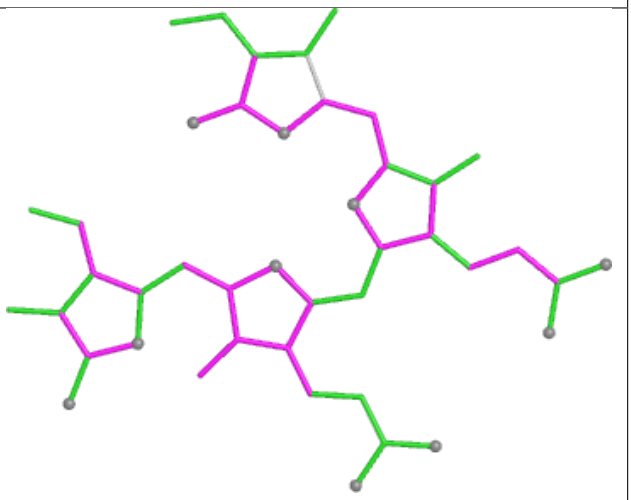


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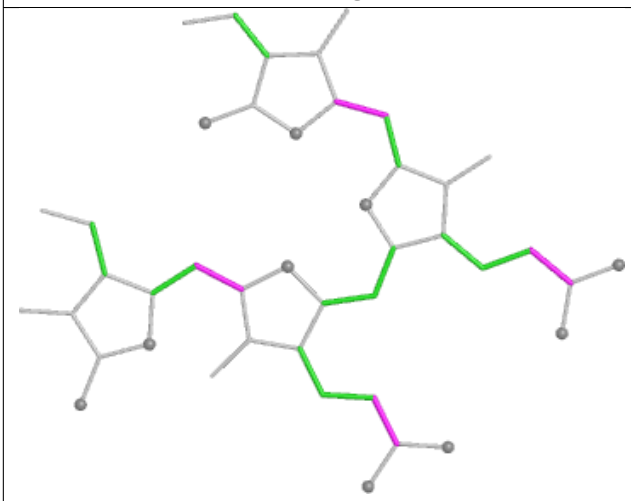
Ligand PEB XP 202



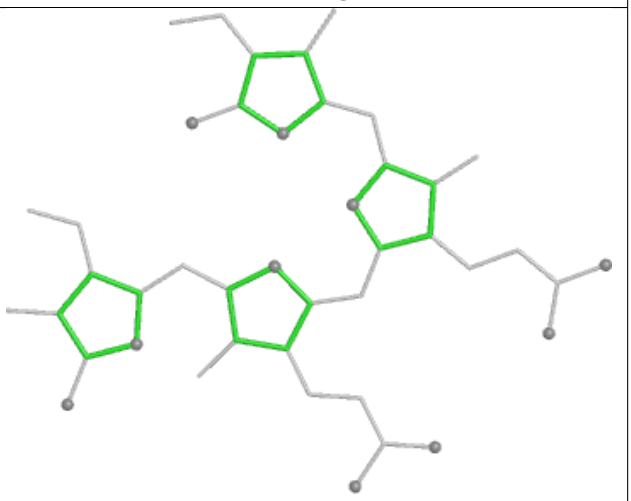
Bond lengths



Bond angles

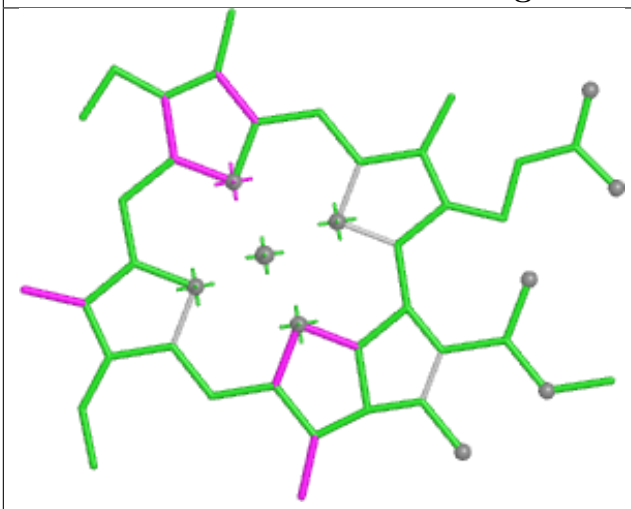


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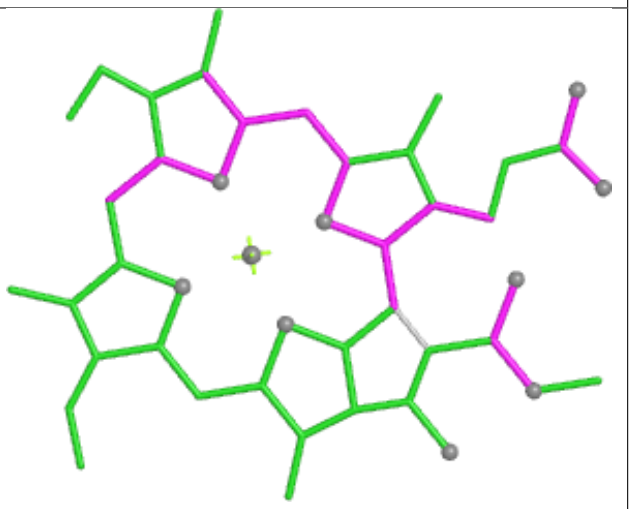


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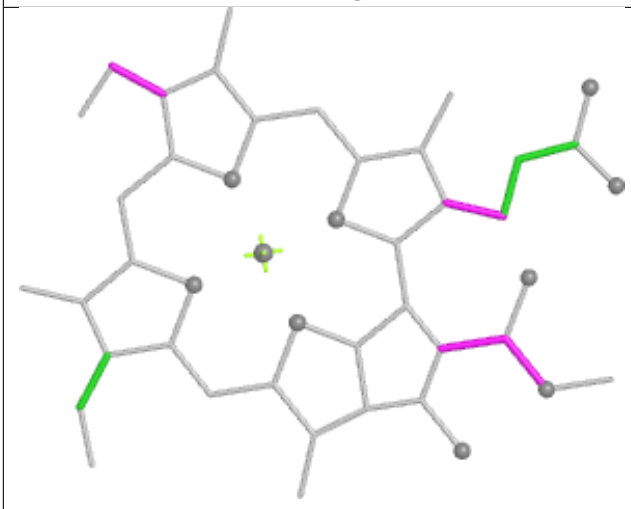
Ligand CLA 2N 308



Bond lengths



Bond angles

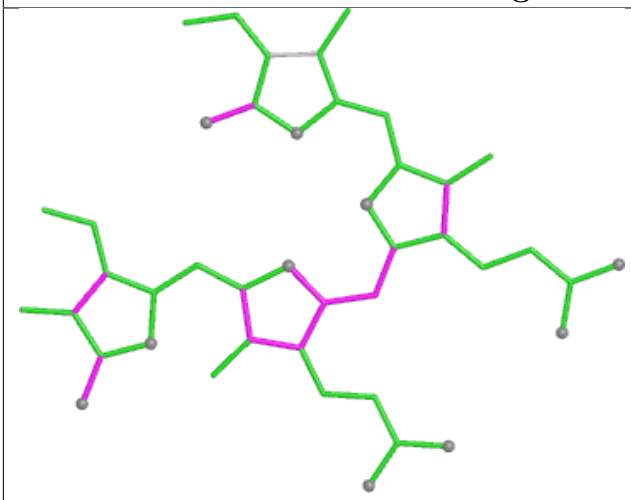


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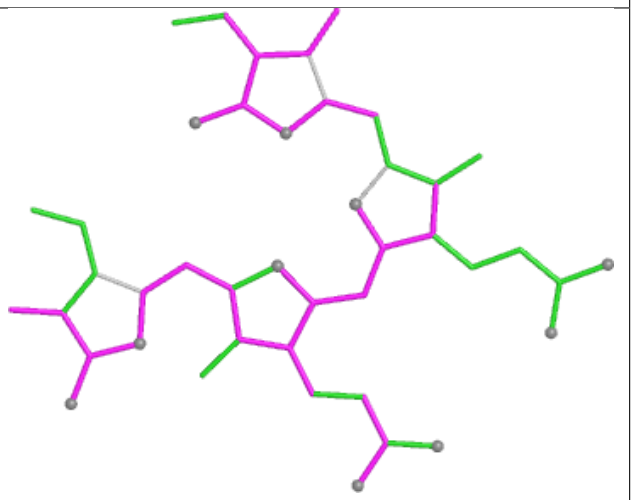


Rings

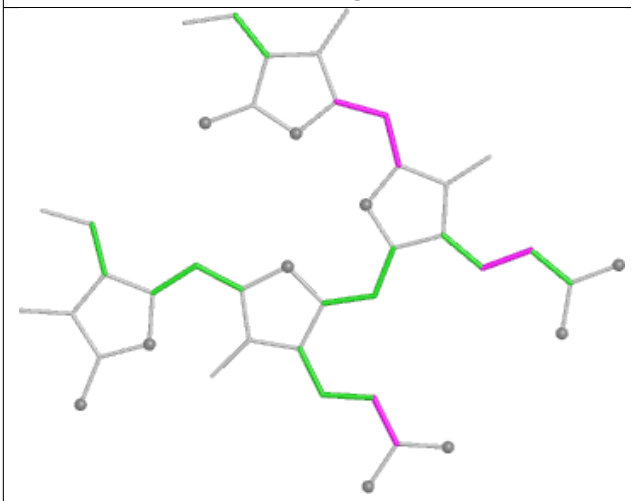
Ligand PUB xK 306



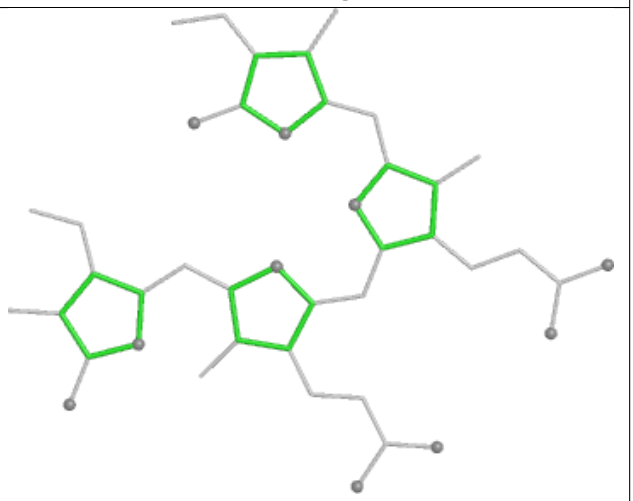
Bond lengths



Bond angles

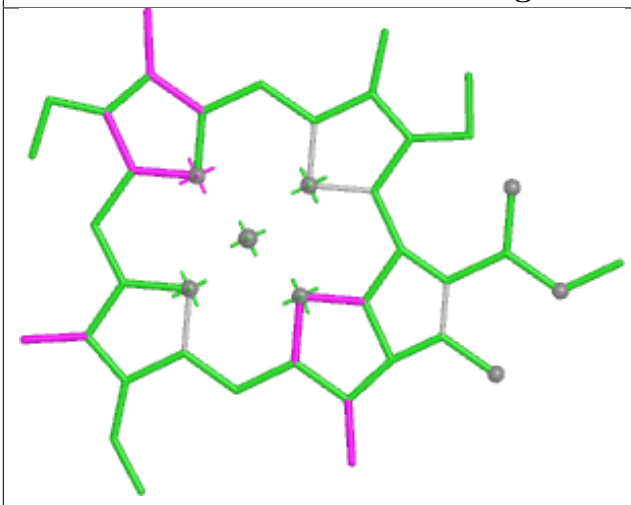


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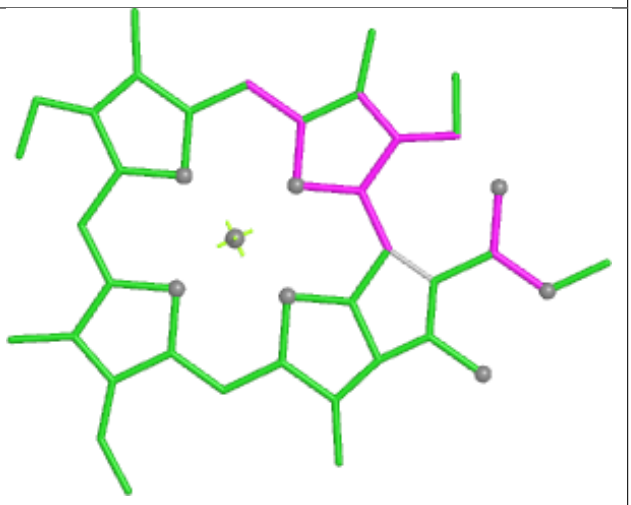


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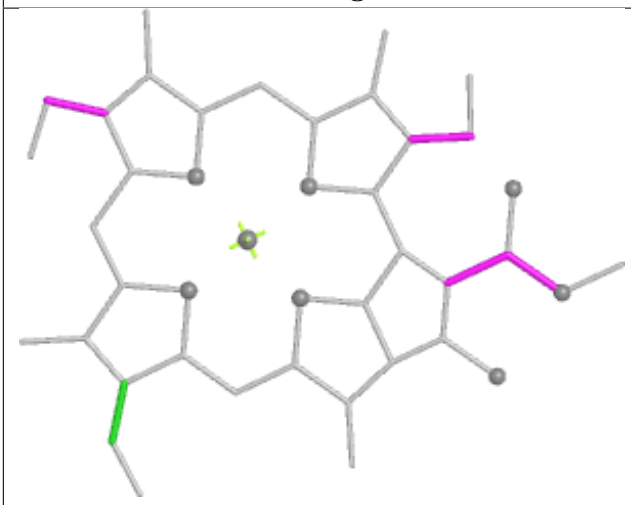
Ligand CLA 5N 609



Bond lengths



Bond angles

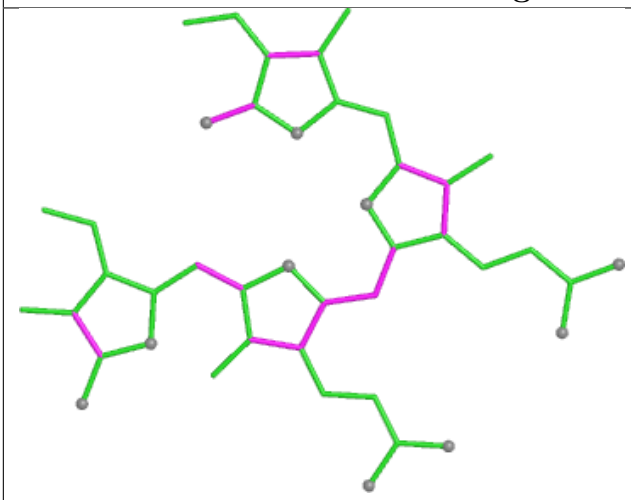


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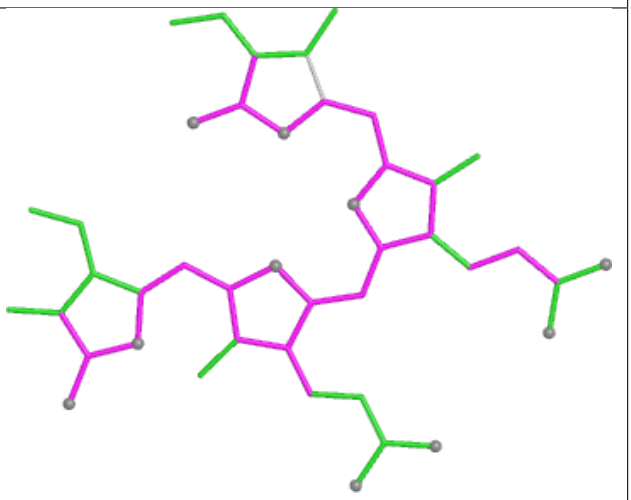


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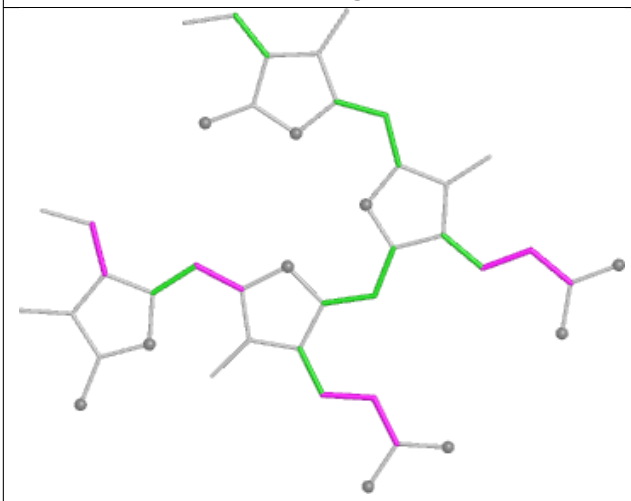
Ligand PEB XF 201



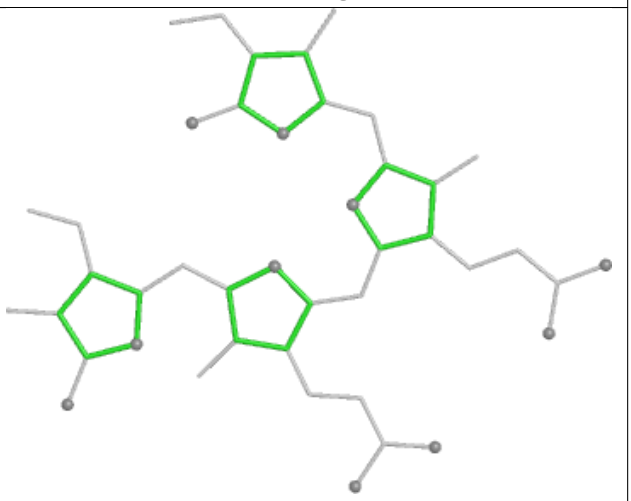
Bond lengths



Bond angles

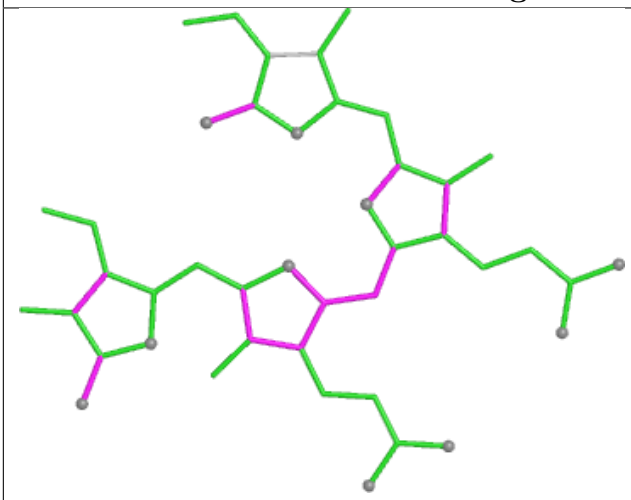


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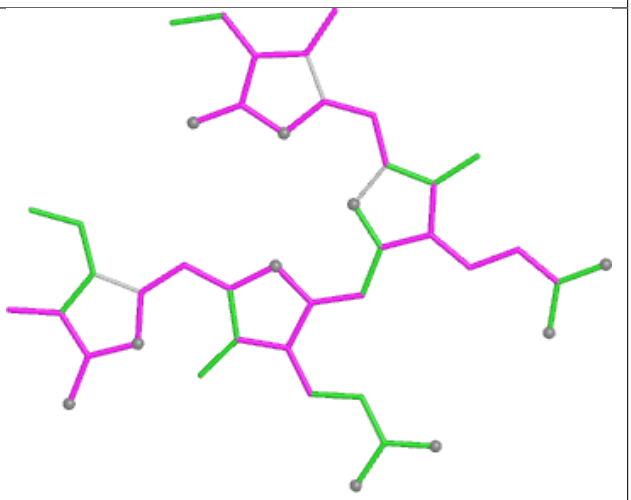


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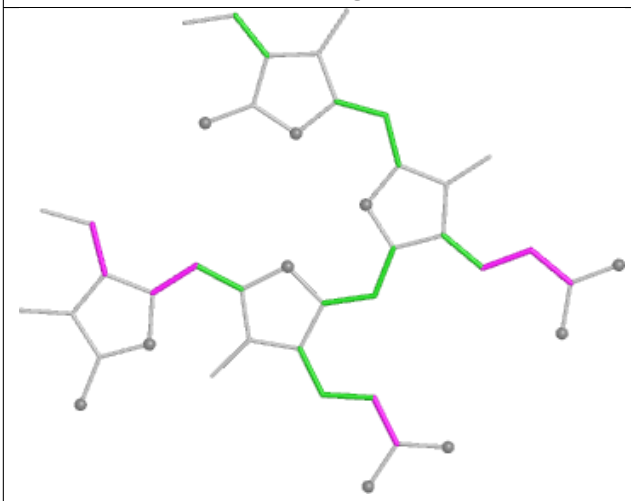
Ligand PUB M5 303



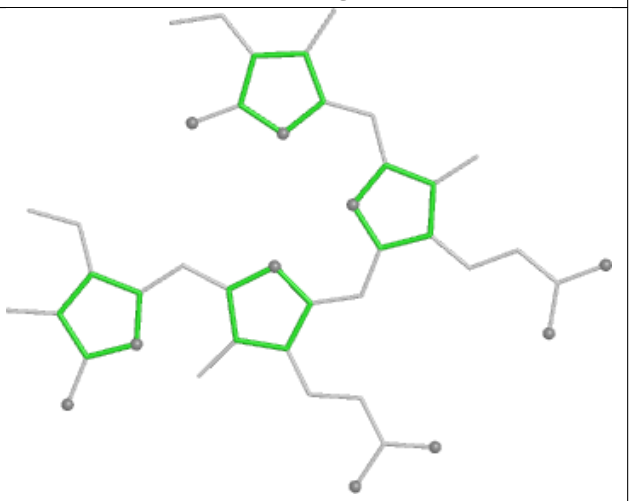
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Bond angles

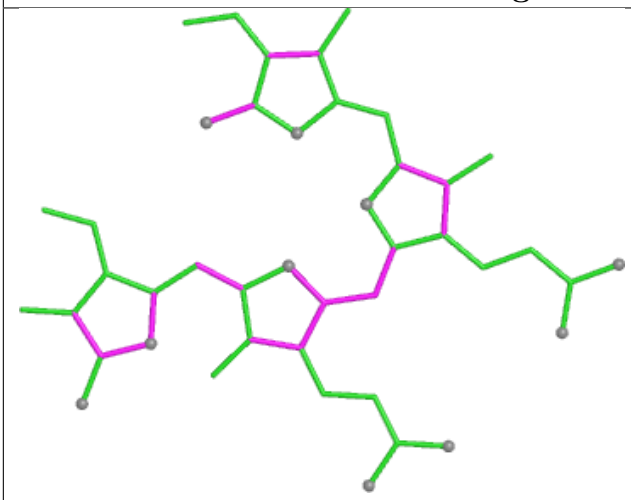


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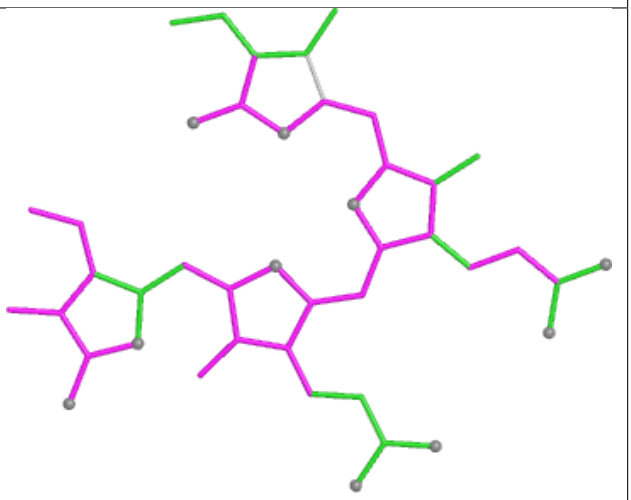


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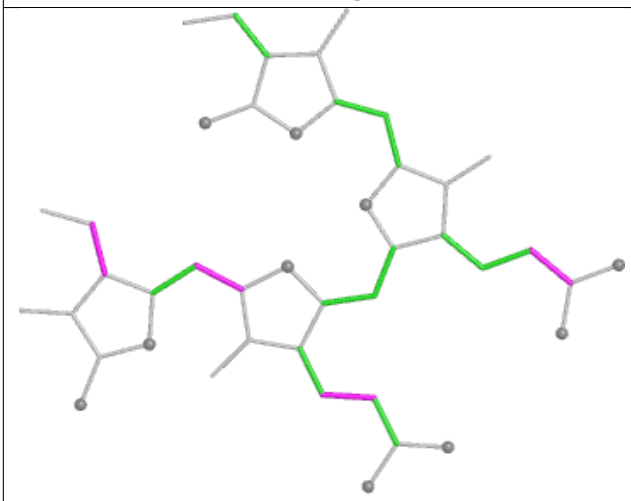
Ligand PEB HF 201



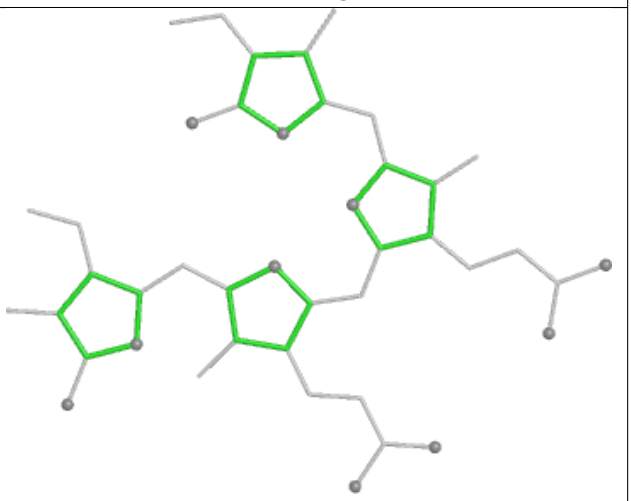
Bond lengths



Bond angles

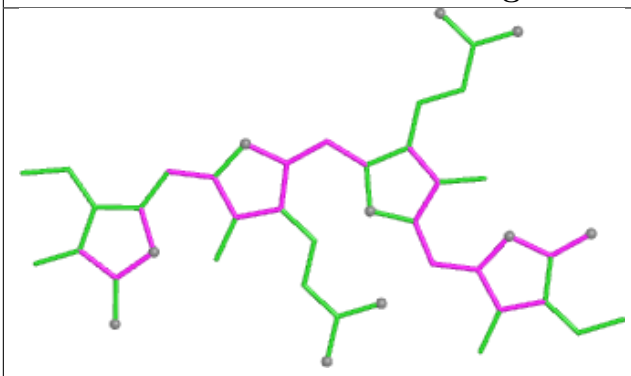


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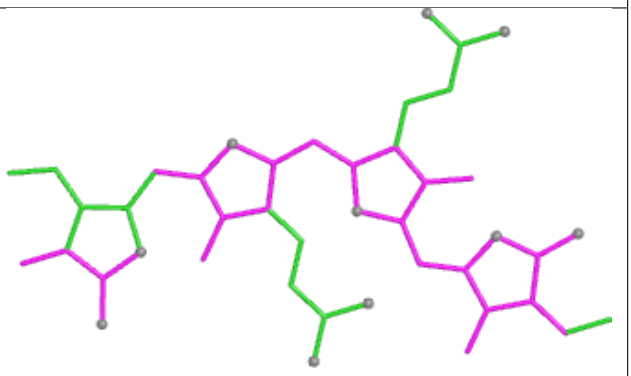


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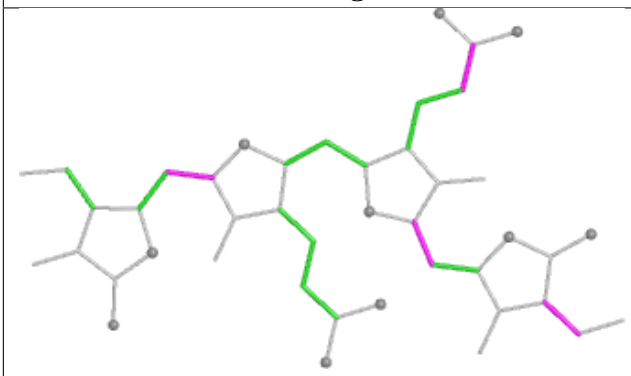
Ligand CYC EE 1001



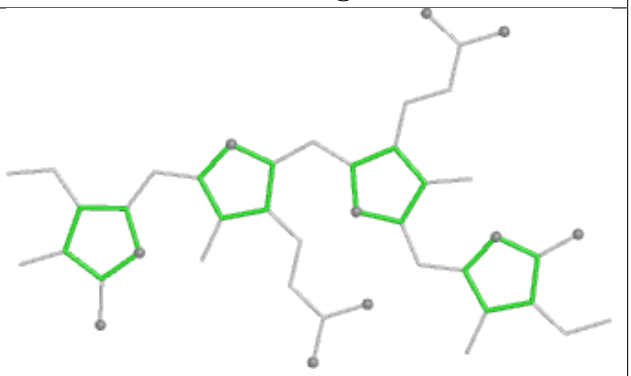
Bond lengths



Bond angles

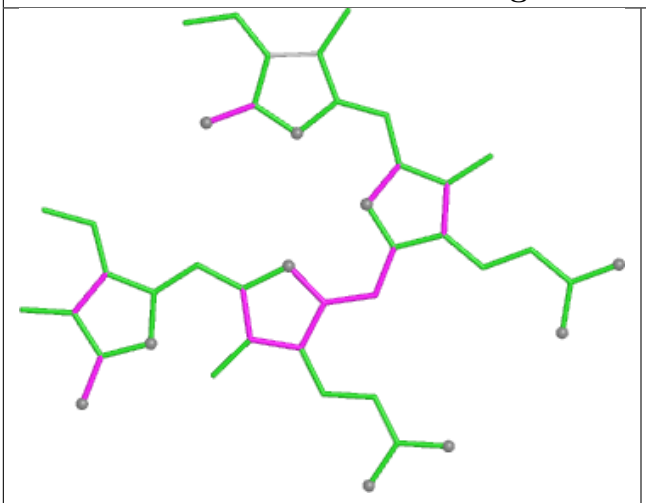


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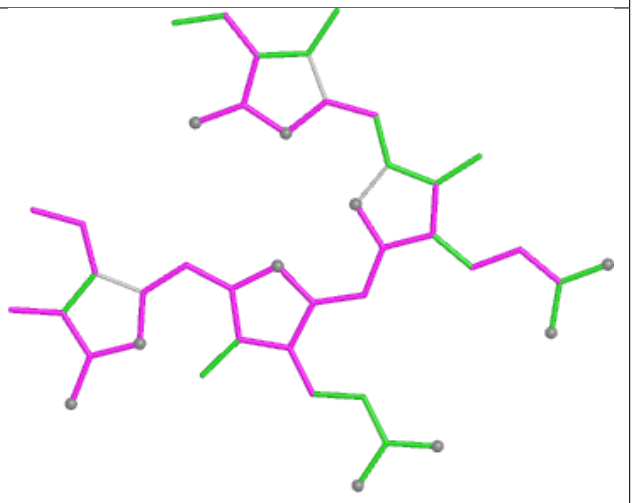


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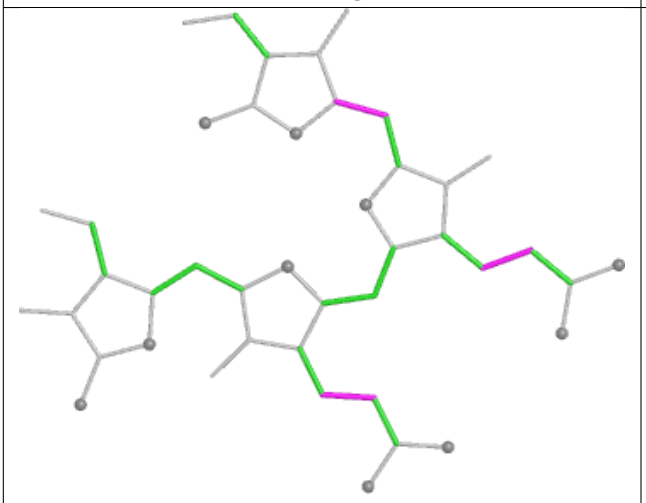
Ligand PUB YA 302



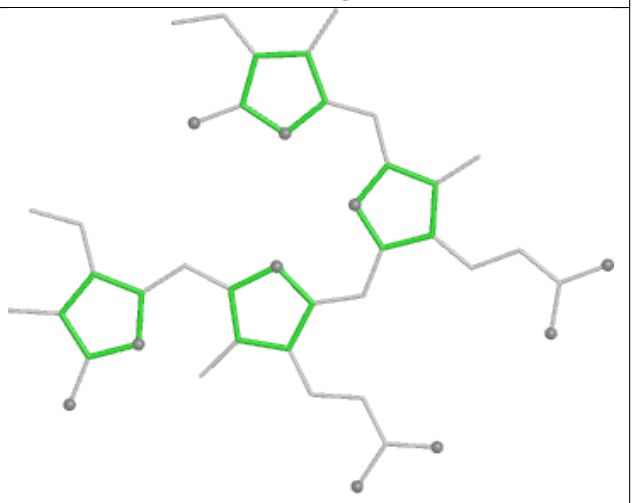
Bond lengths



Bond angles

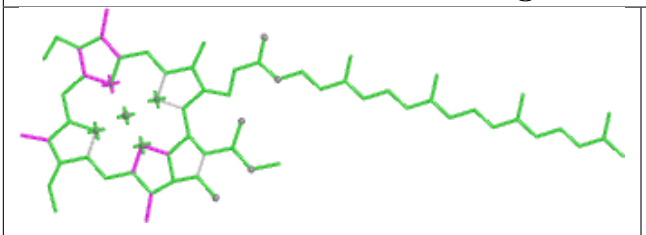


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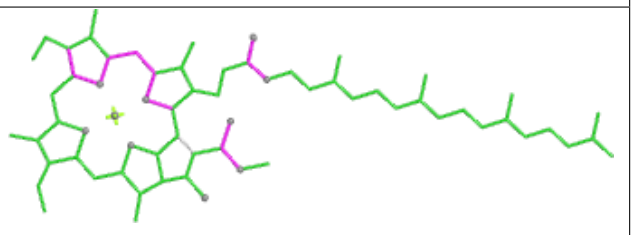


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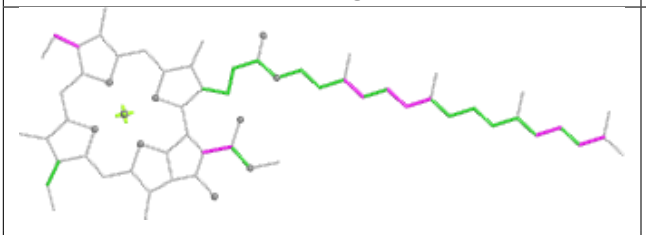
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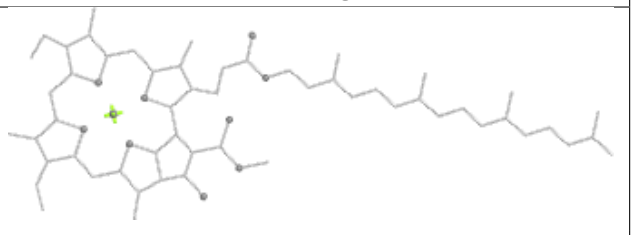
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Bond angles

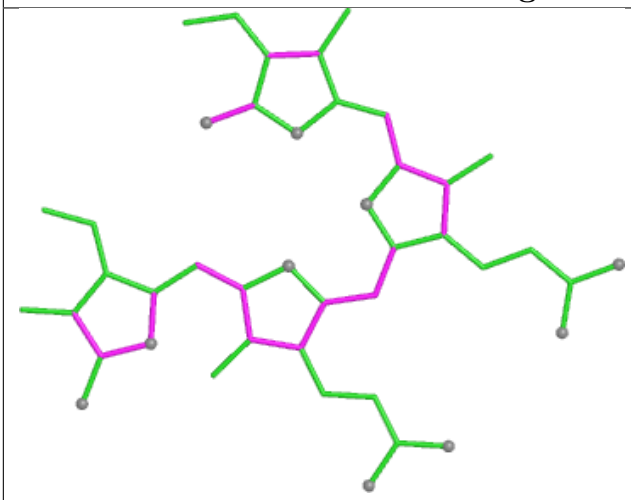


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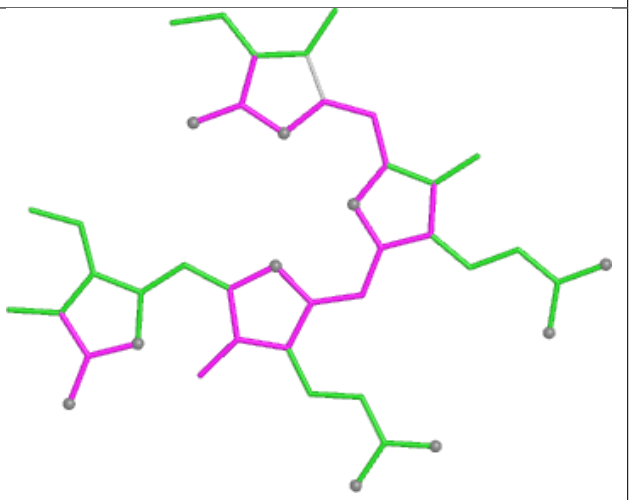


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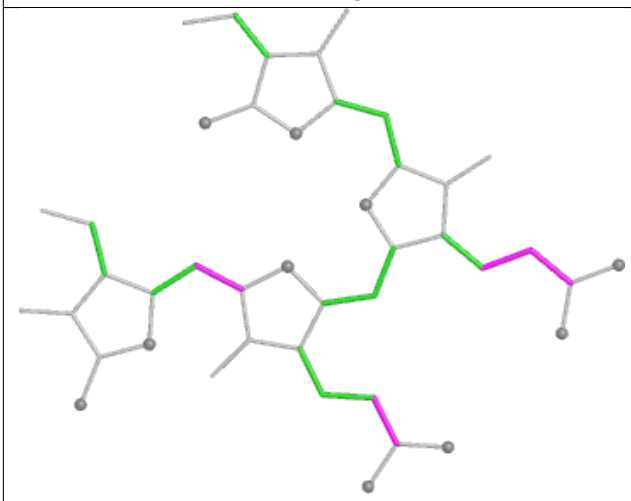
Ligand PEB iH 201



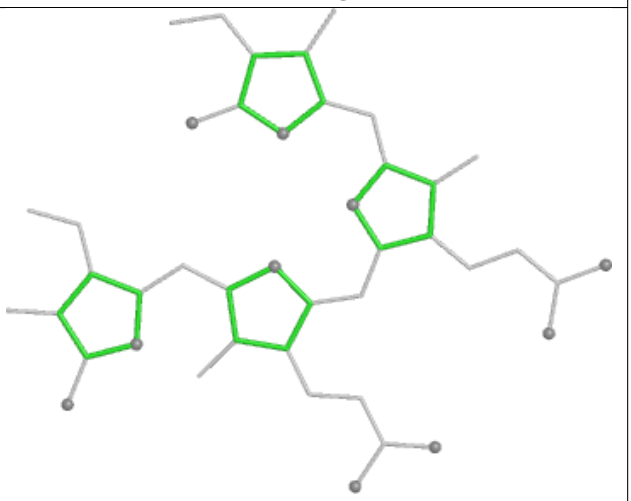
Bond lengths



Bond angles

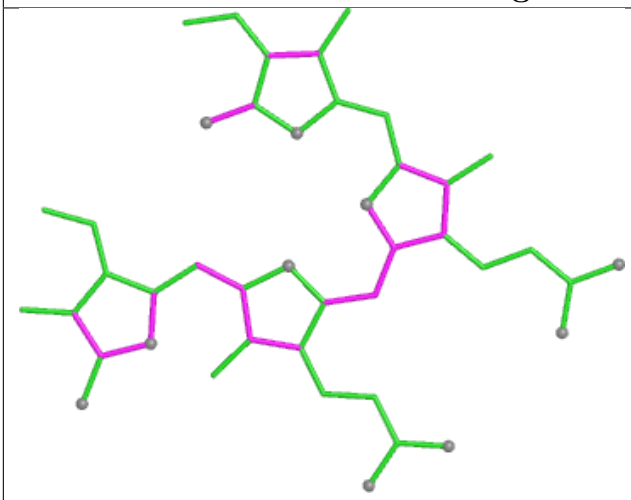


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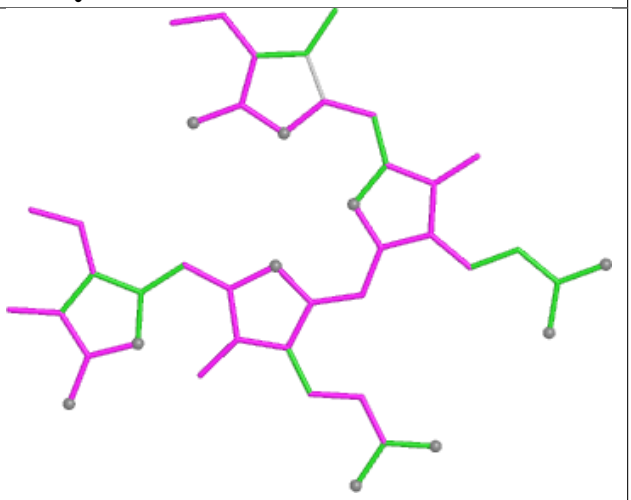


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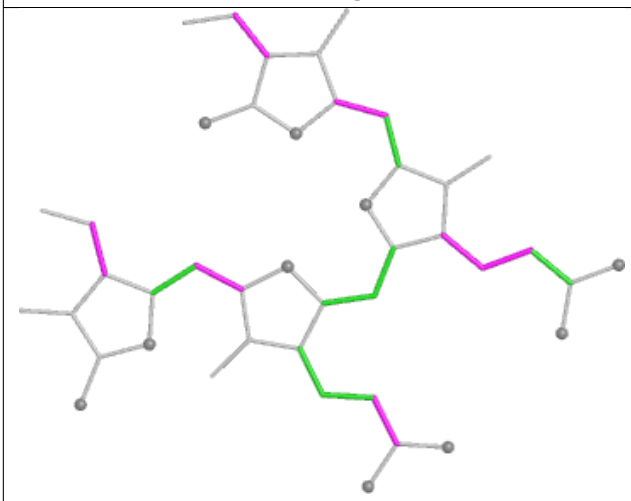
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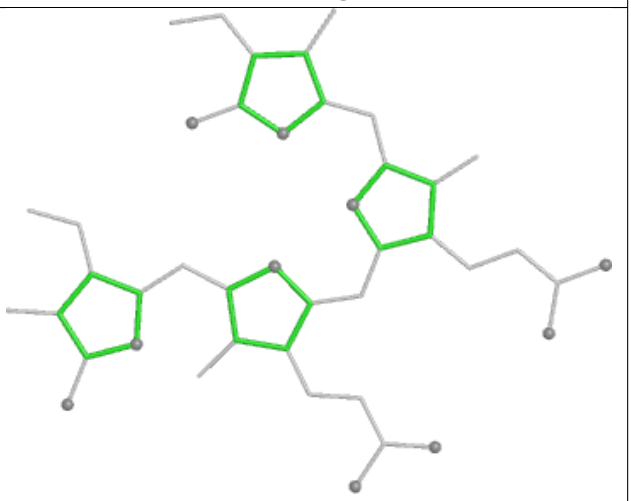
Bond lengths



Bond angles

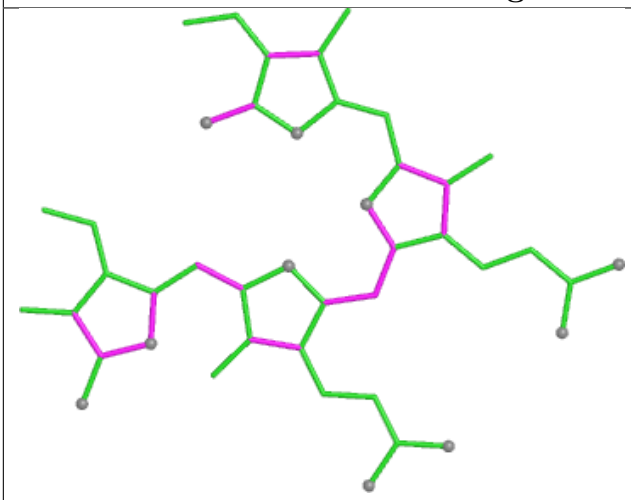


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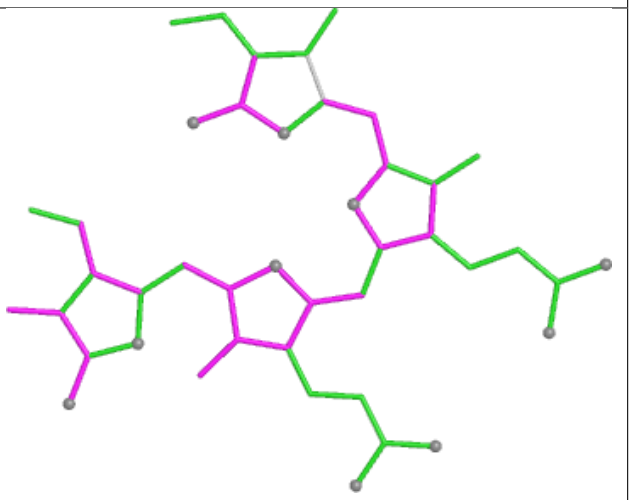


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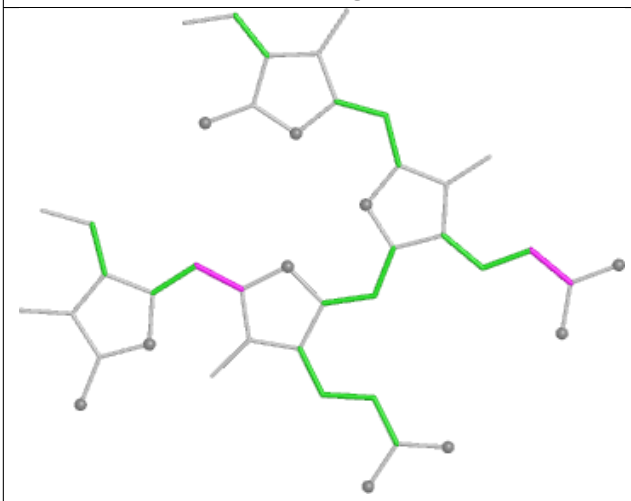
Ligand PEB WP 202



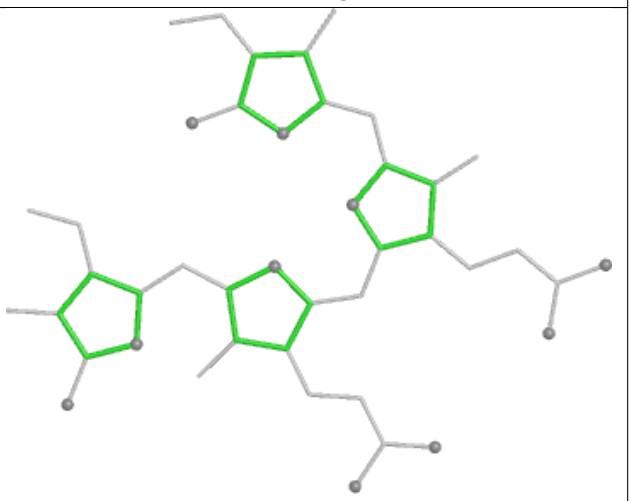
Bond lengths



Bond angles

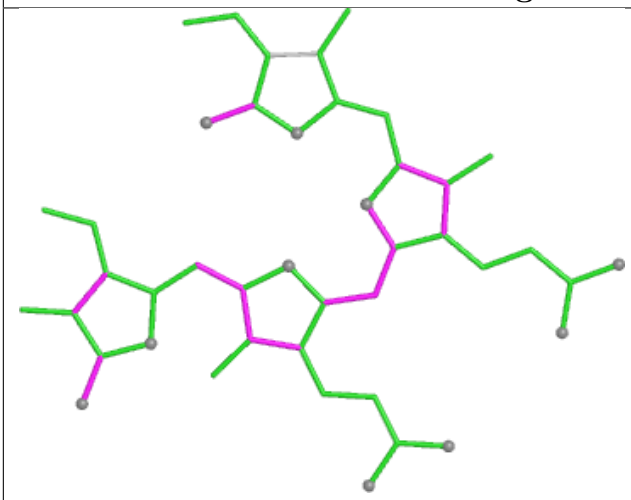


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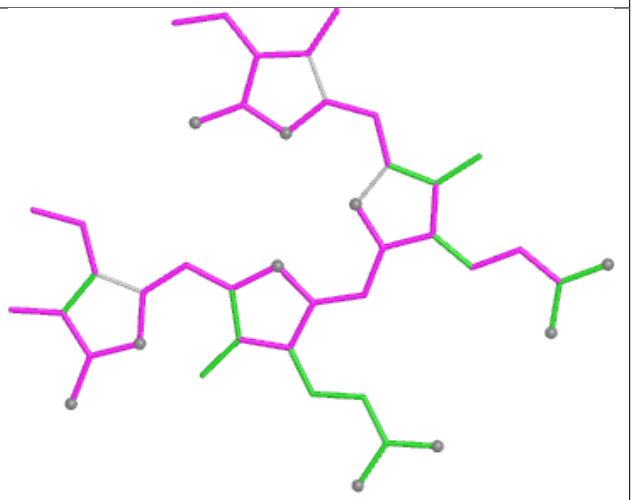


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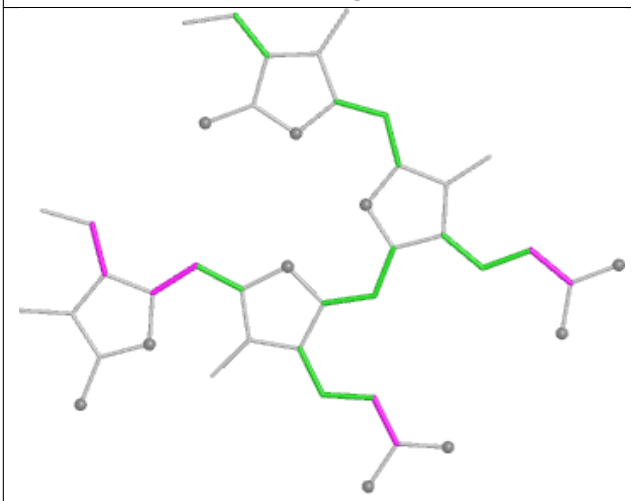
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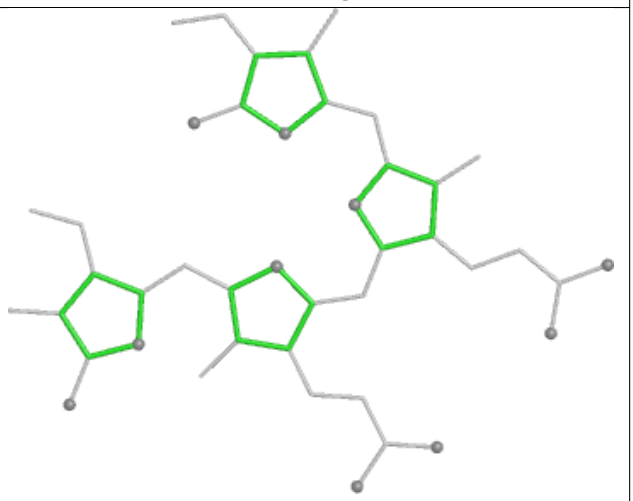
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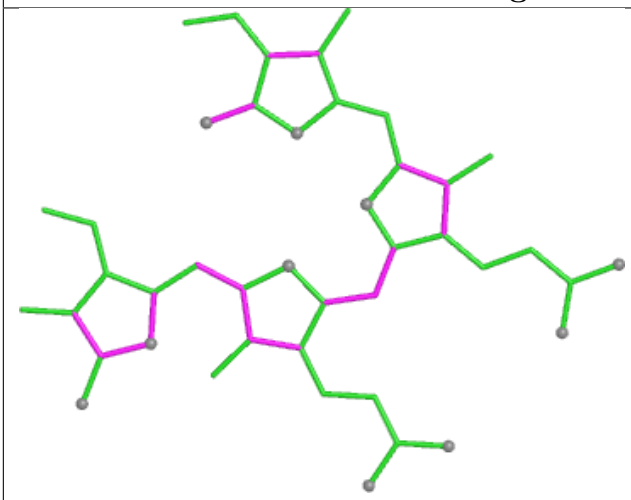


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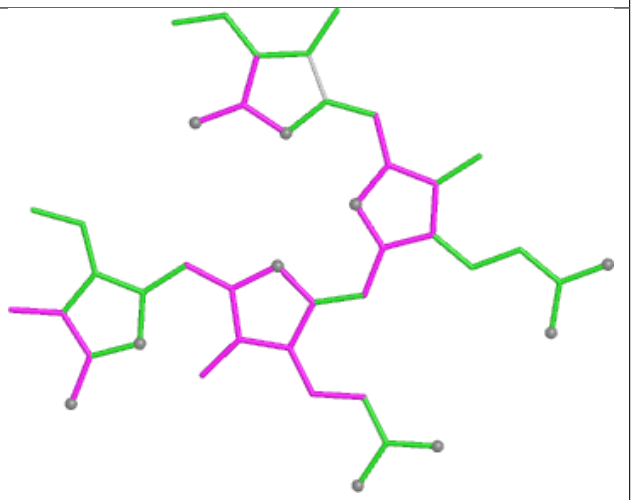


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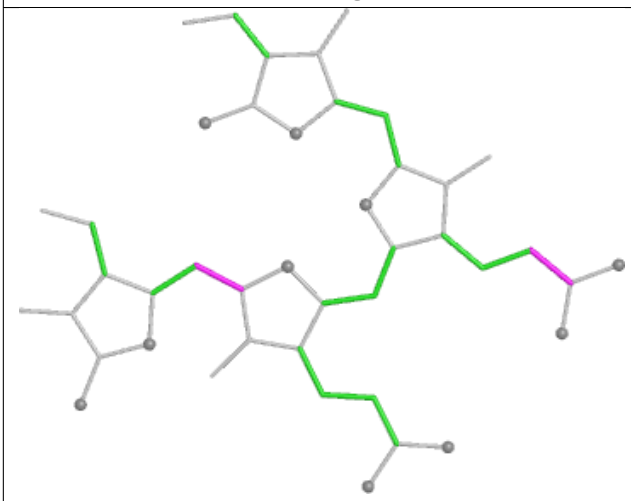
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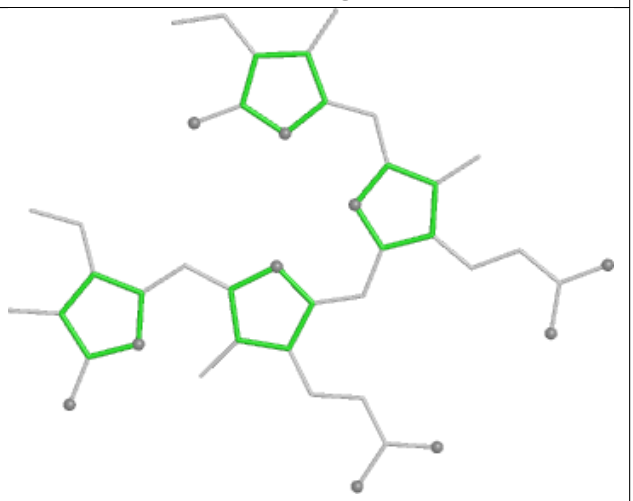
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Bond angles

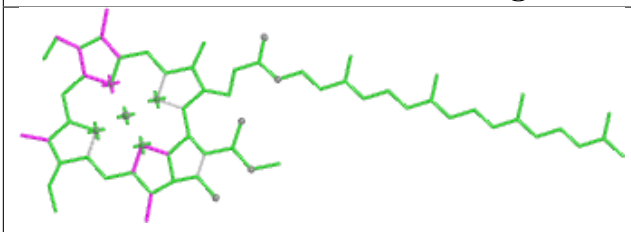


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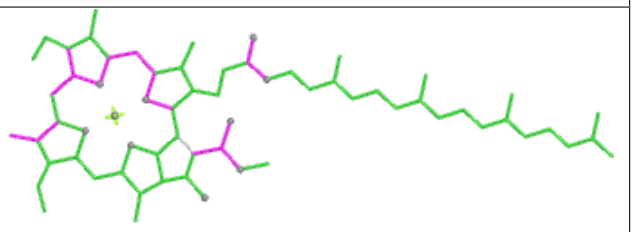


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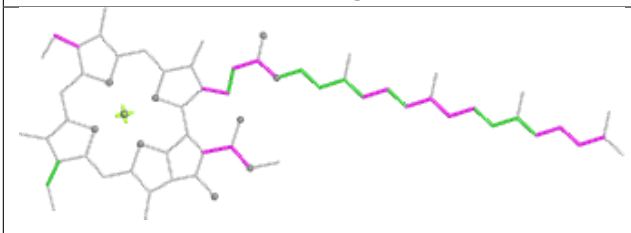
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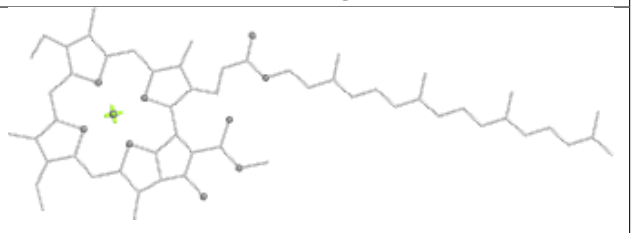
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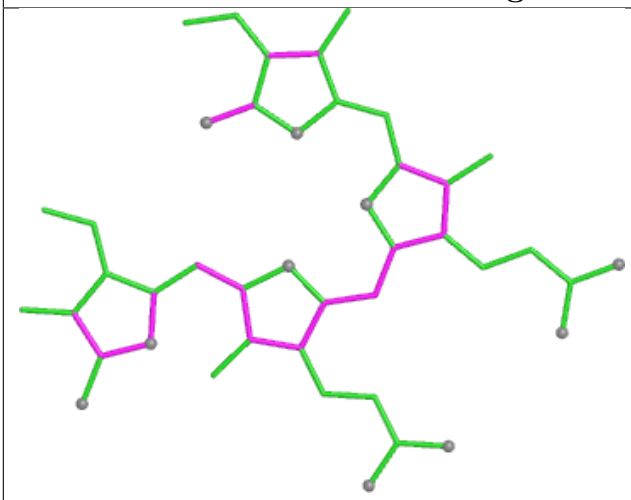


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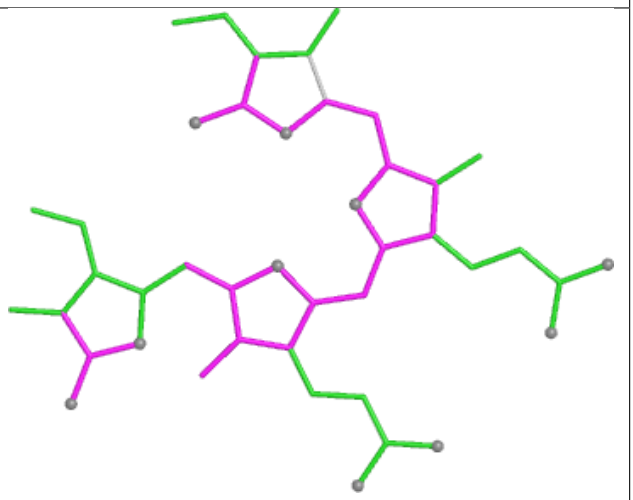


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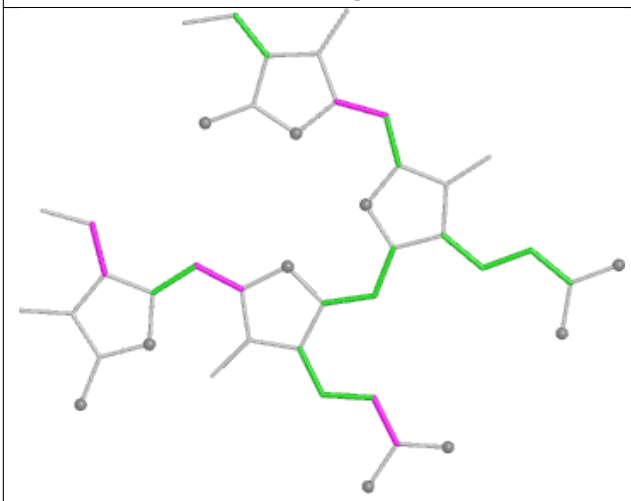
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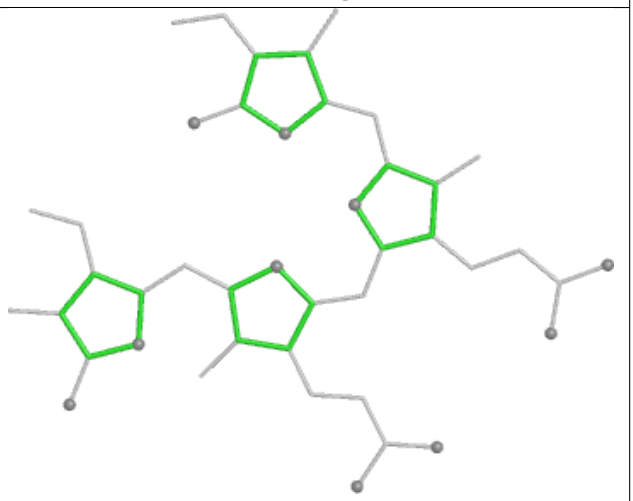
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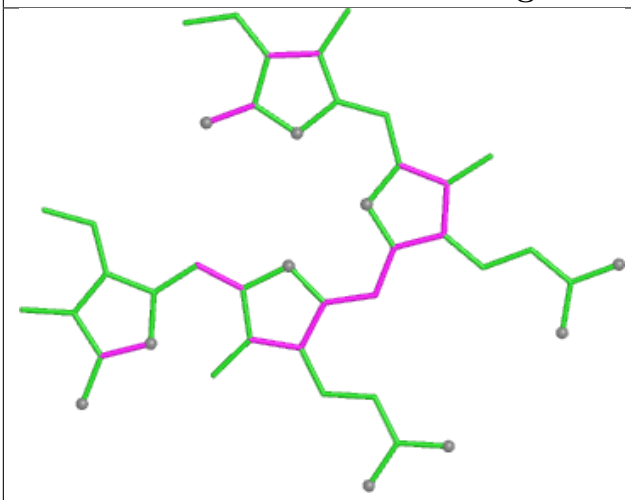


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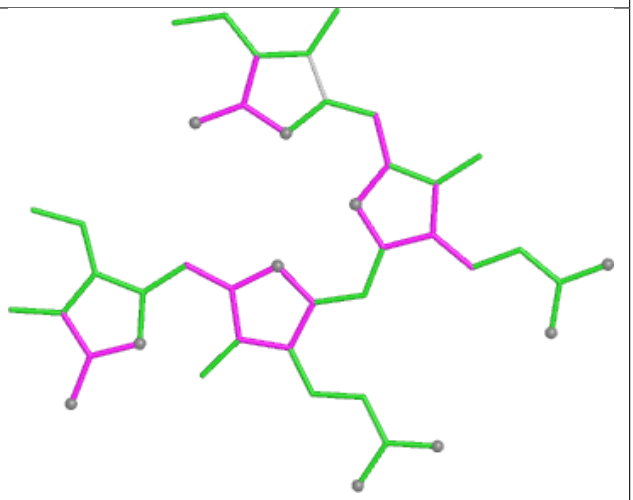


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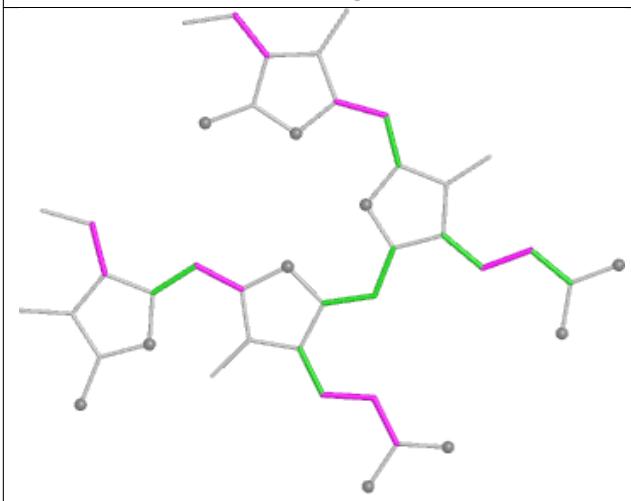
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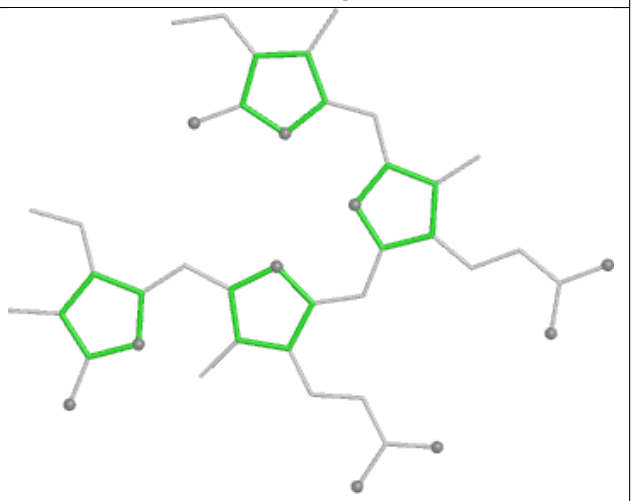
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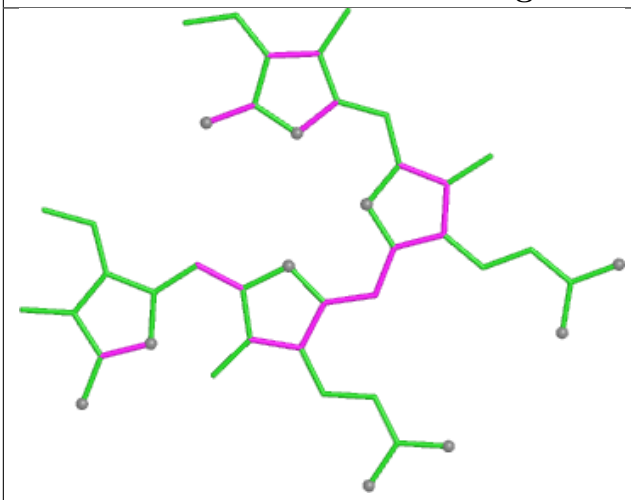


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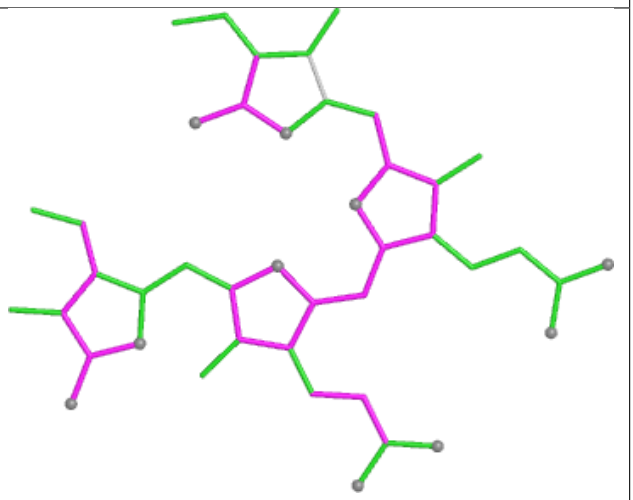


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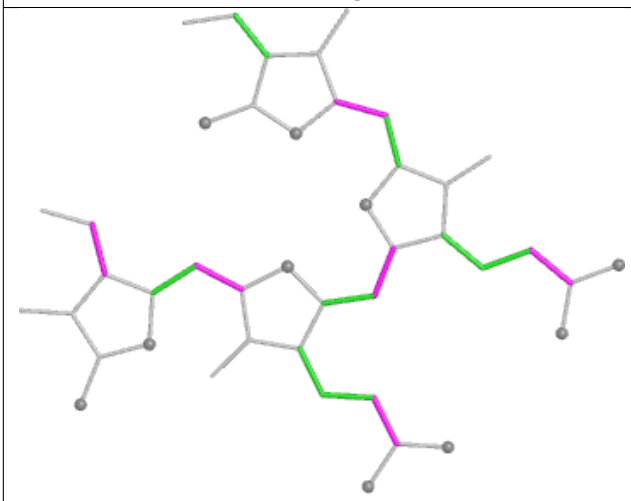
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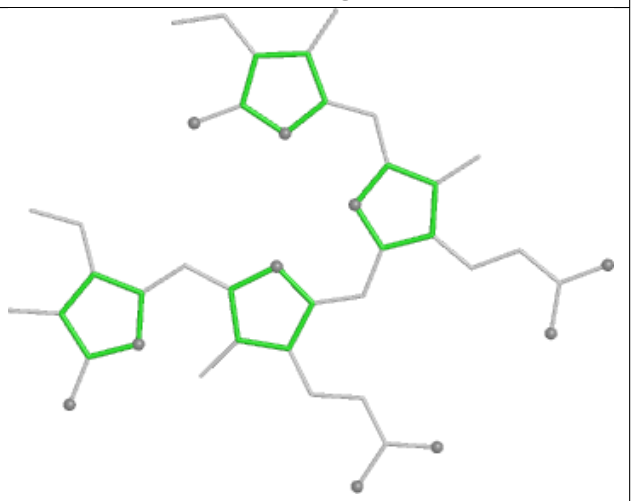
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Bond angles

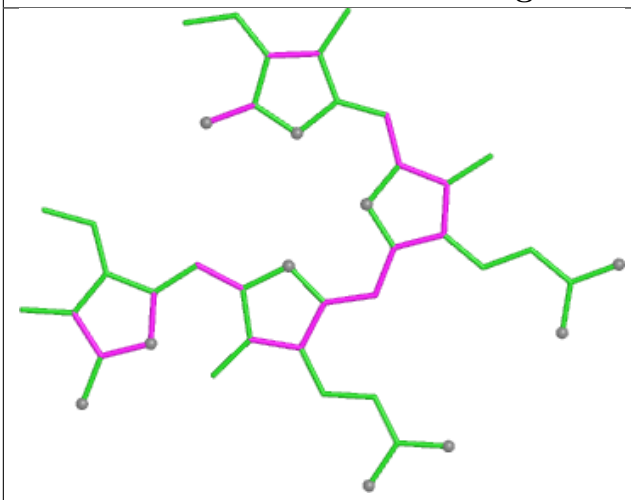


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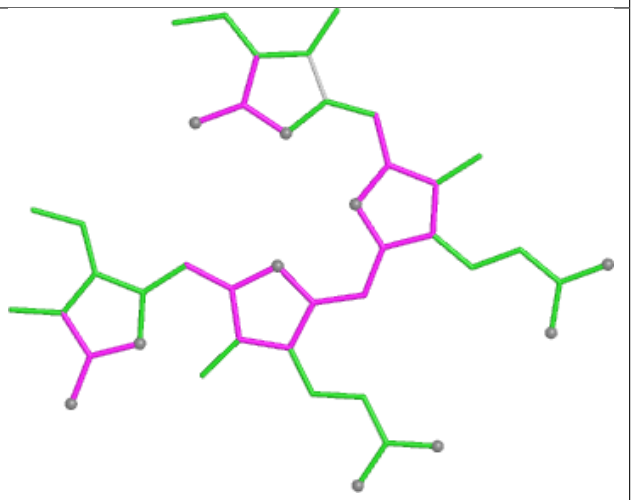


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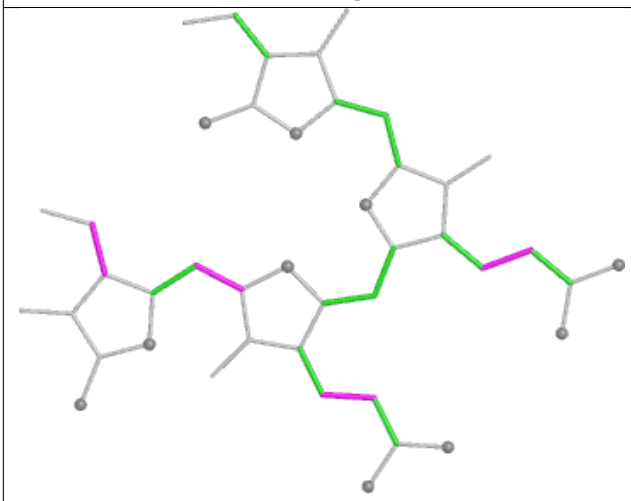
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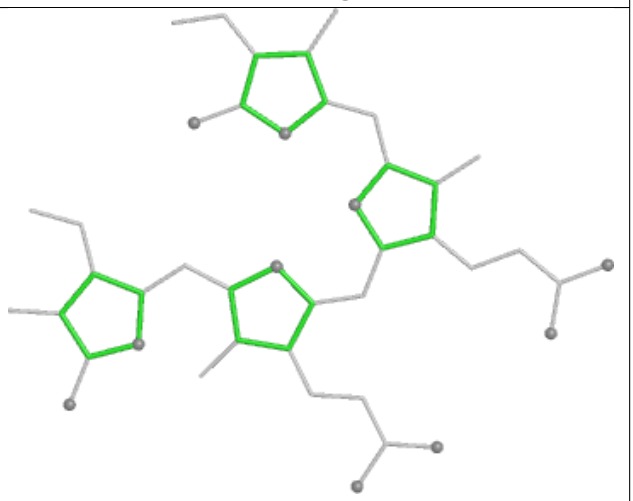
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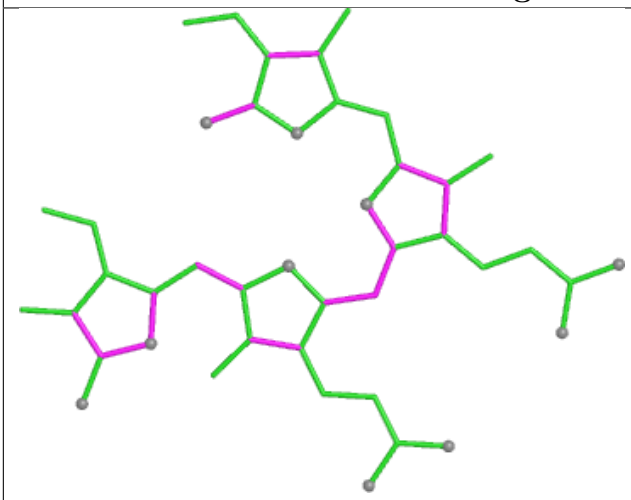


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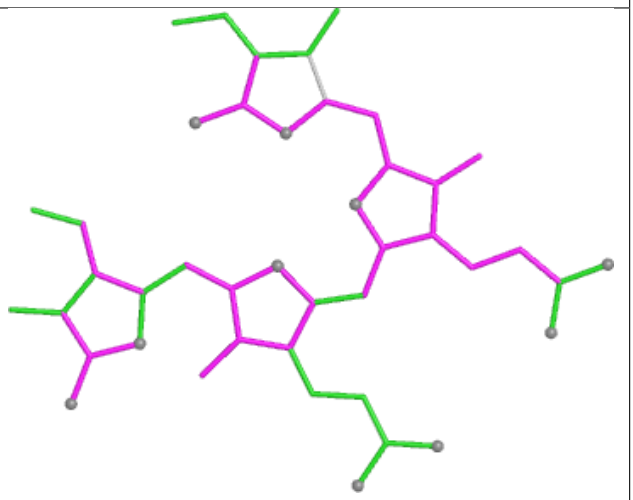


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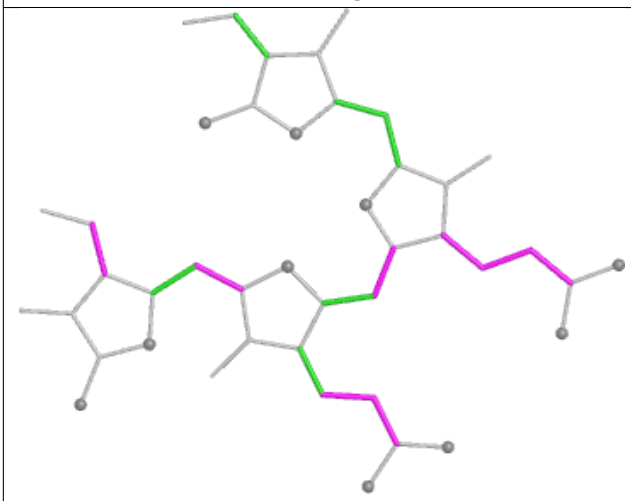
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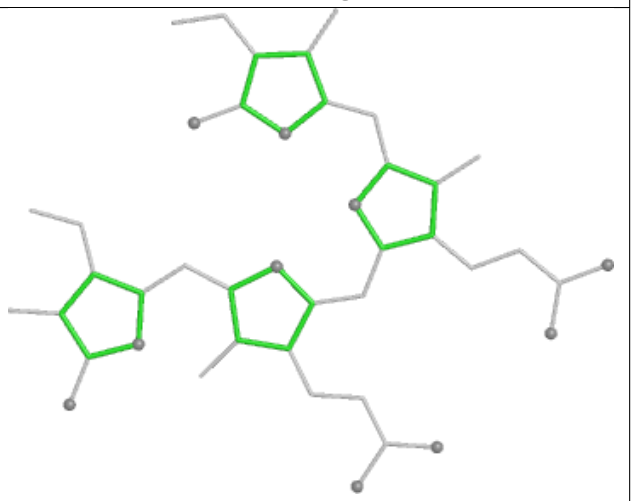
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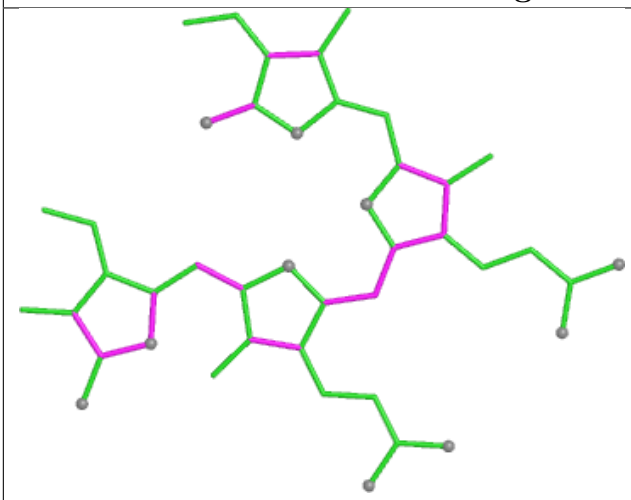


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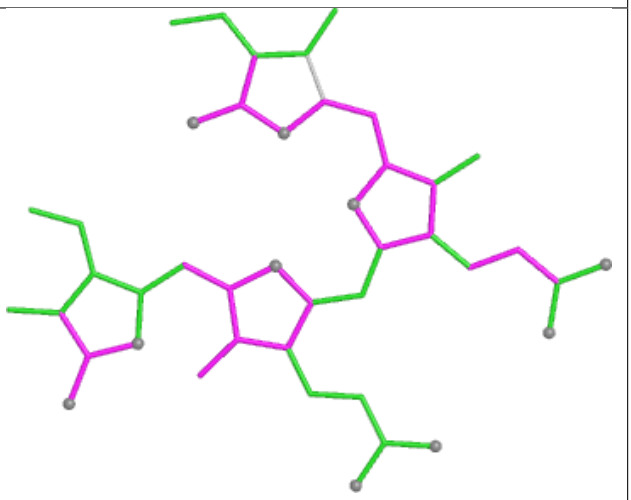


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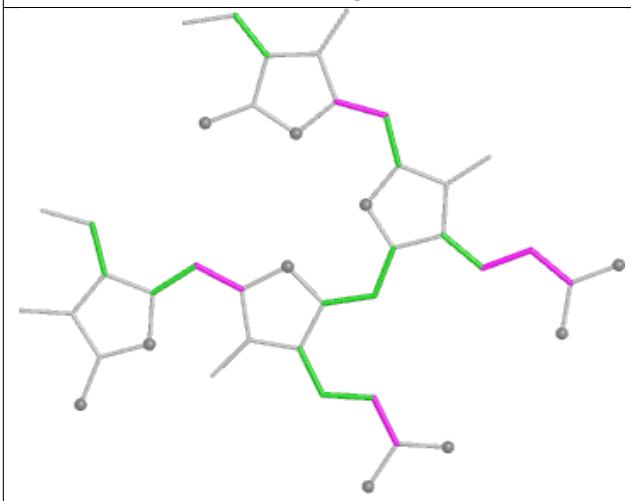
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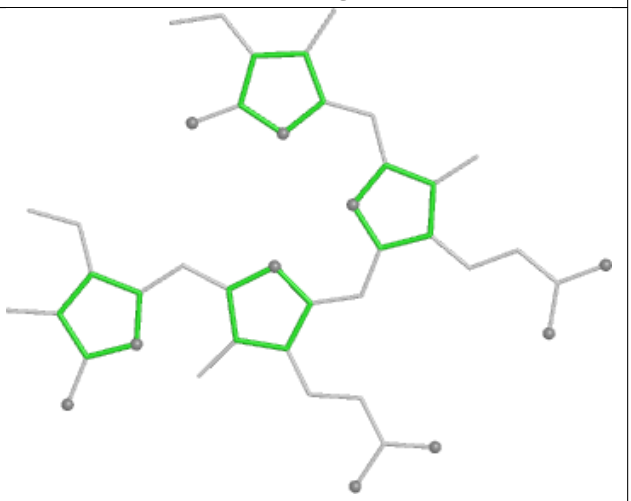
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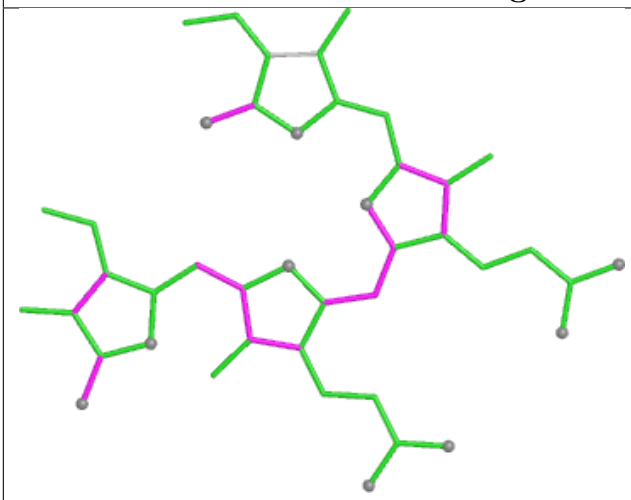


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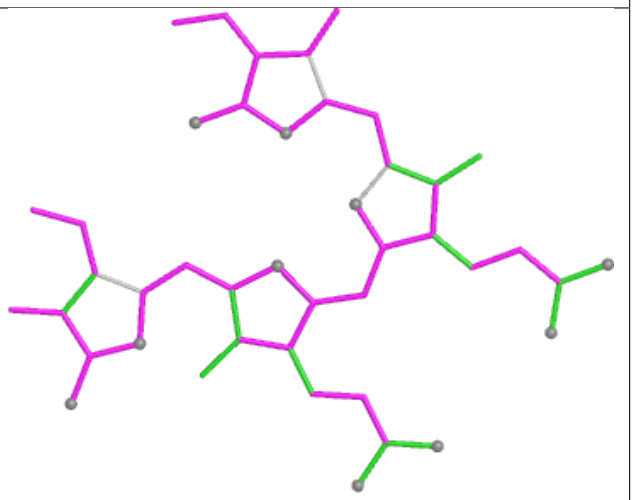


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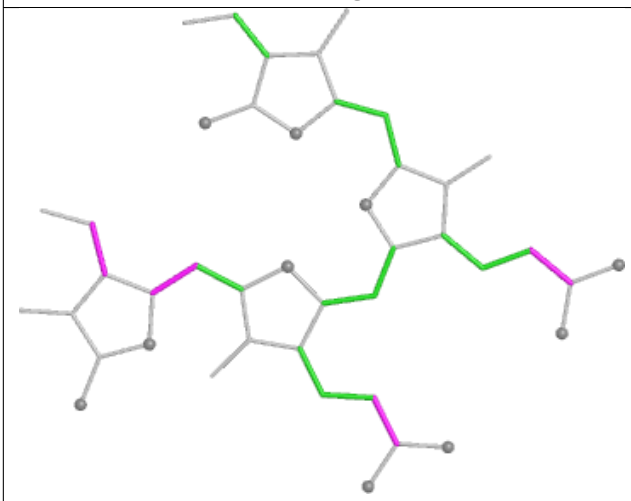
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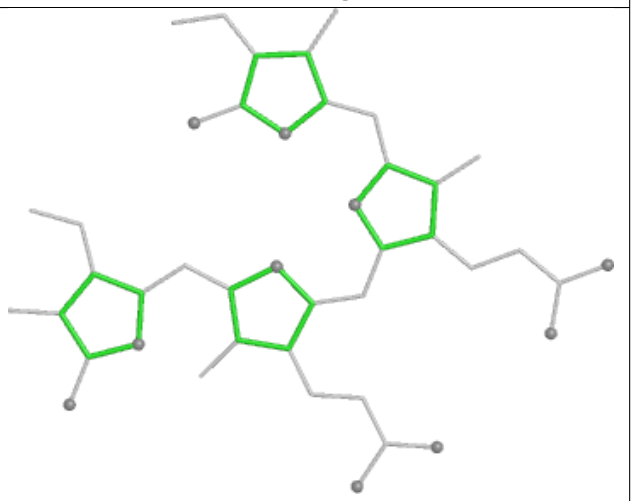
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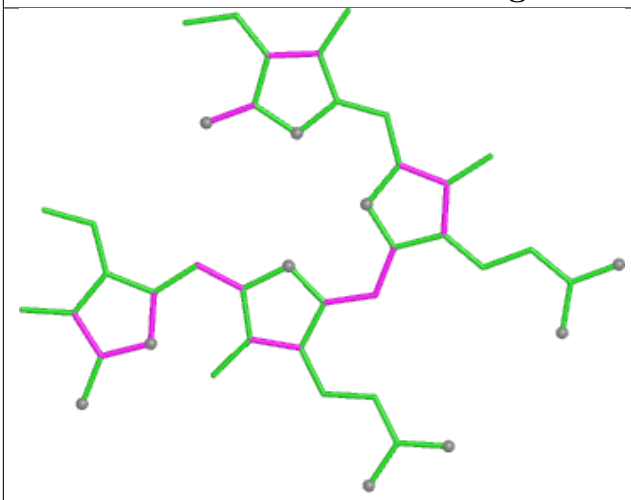


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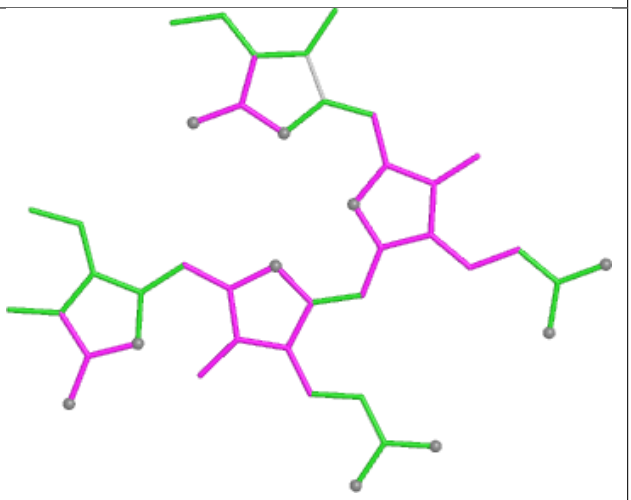


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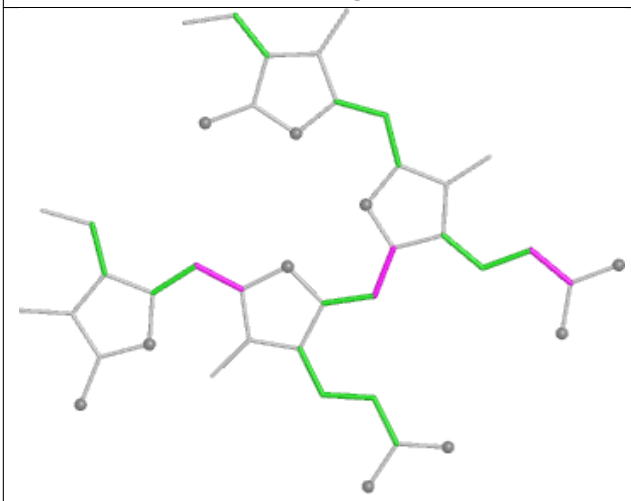
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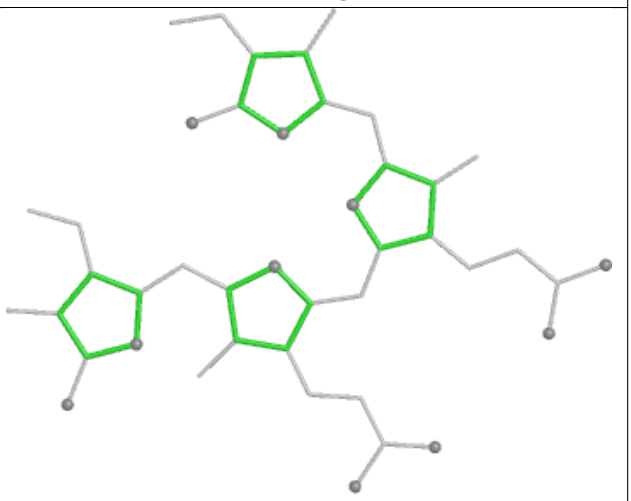
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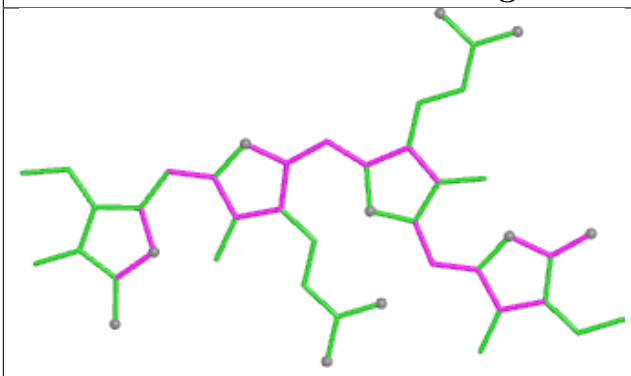


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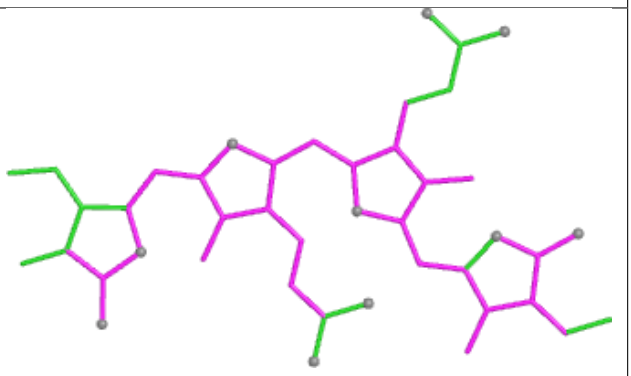


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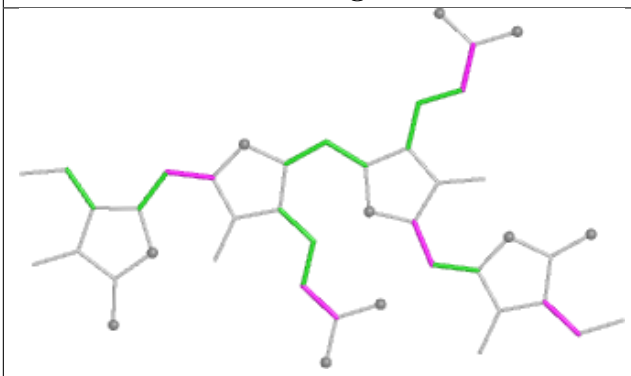
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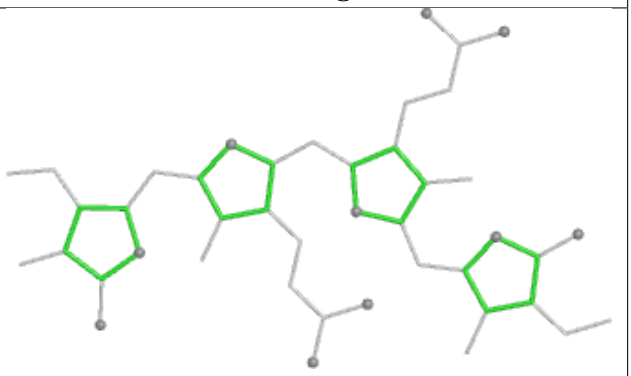
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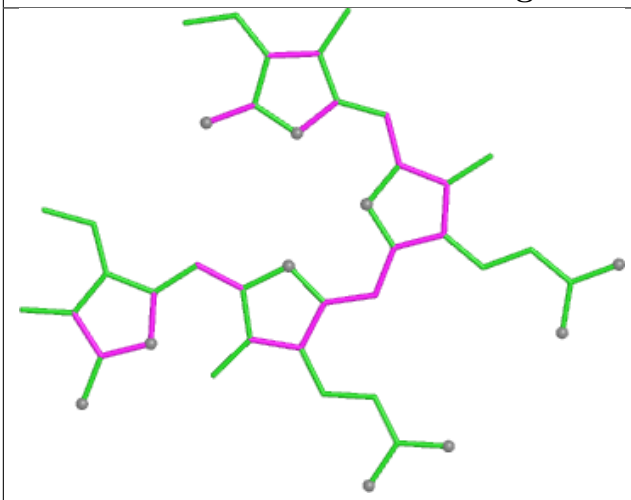


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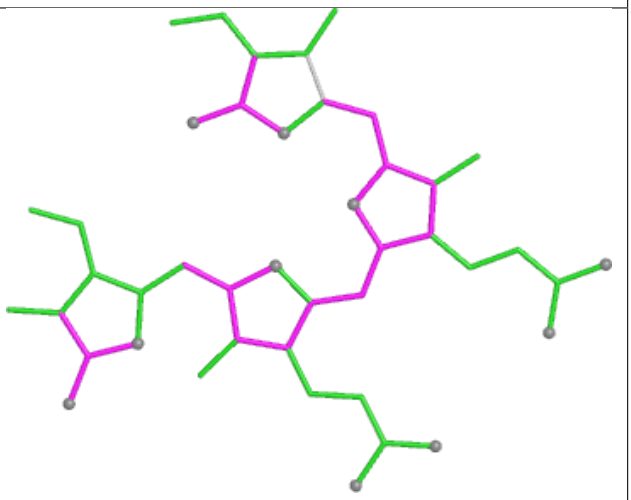


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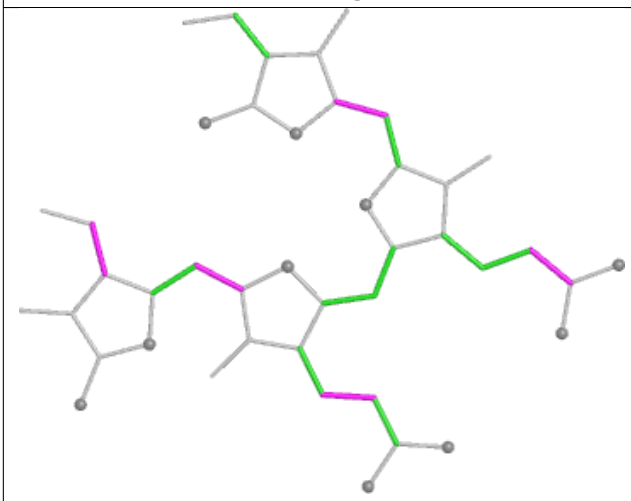
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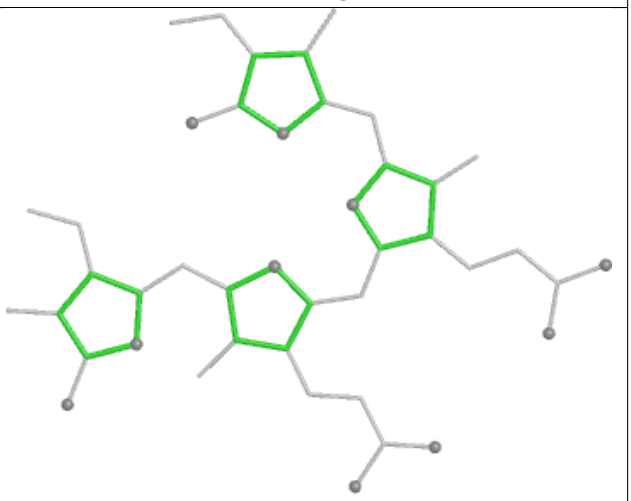
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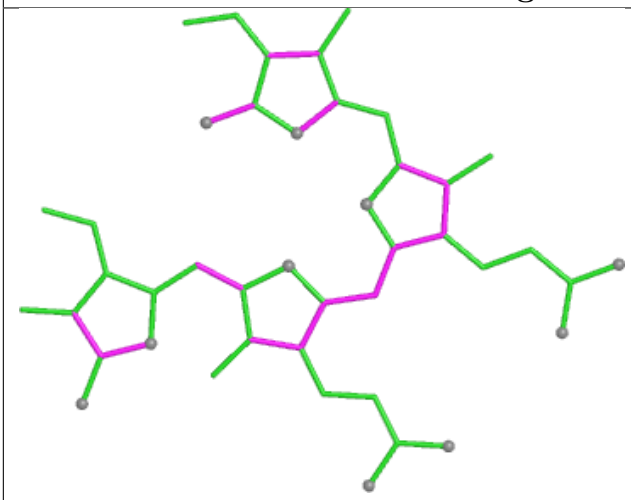


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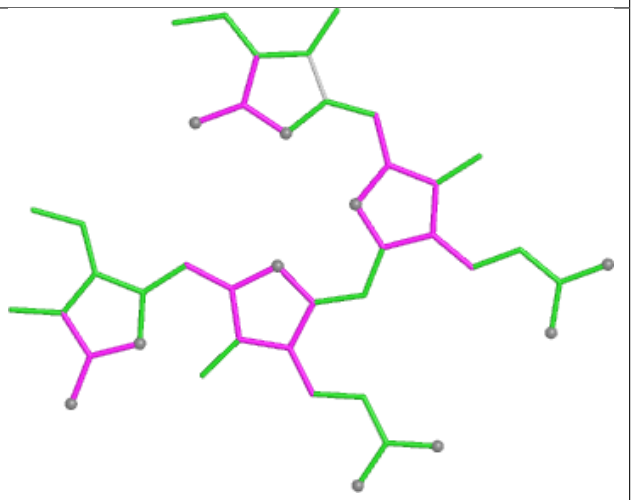


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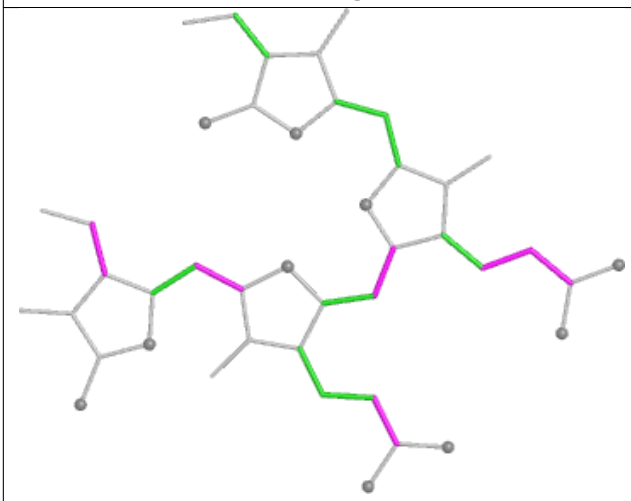
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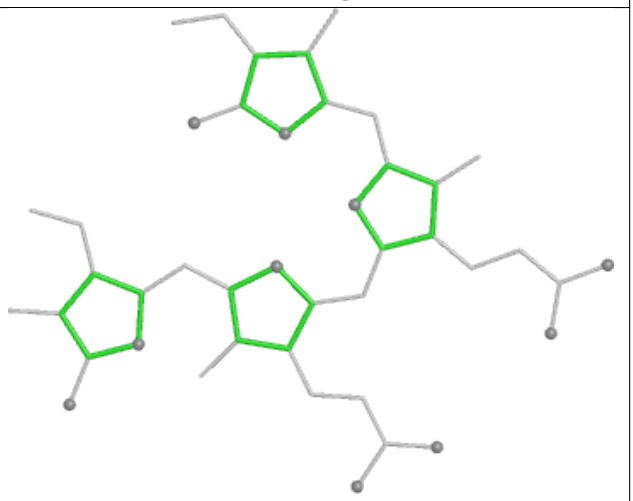
Bond lengths



Bond angles

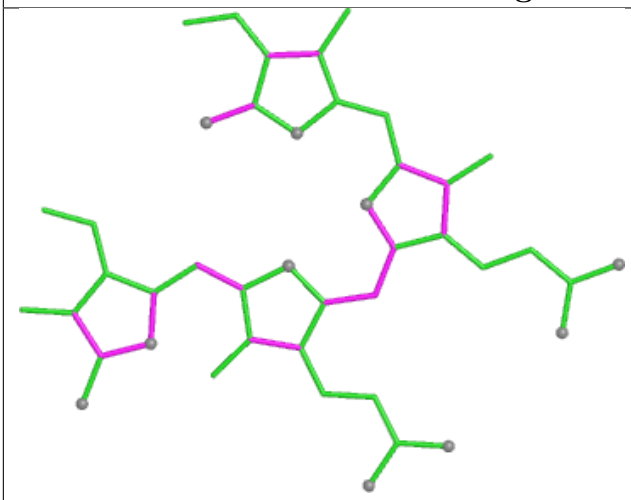


Torsions

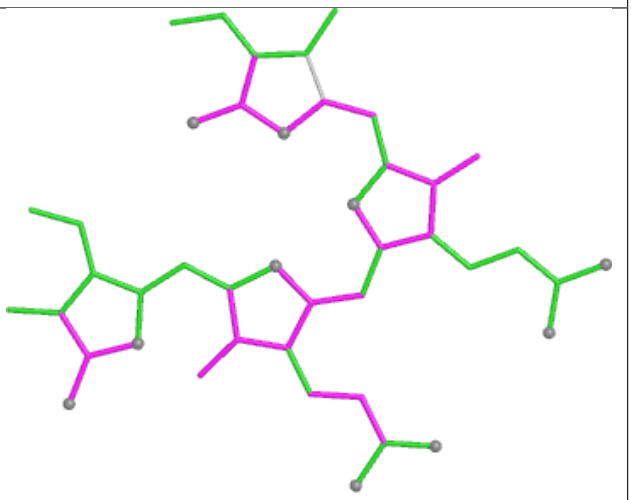


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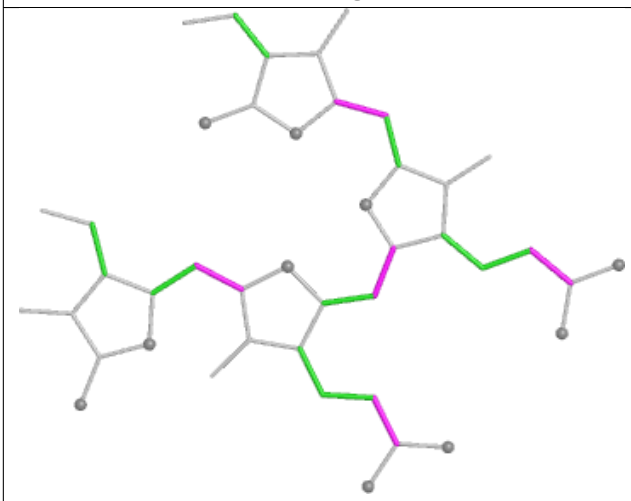
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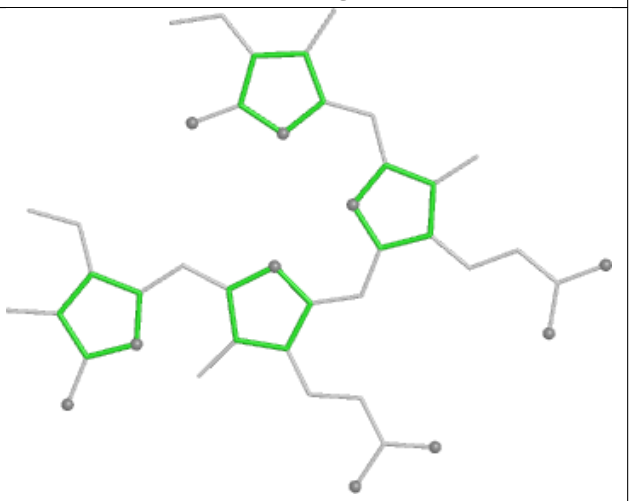
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Bond angles

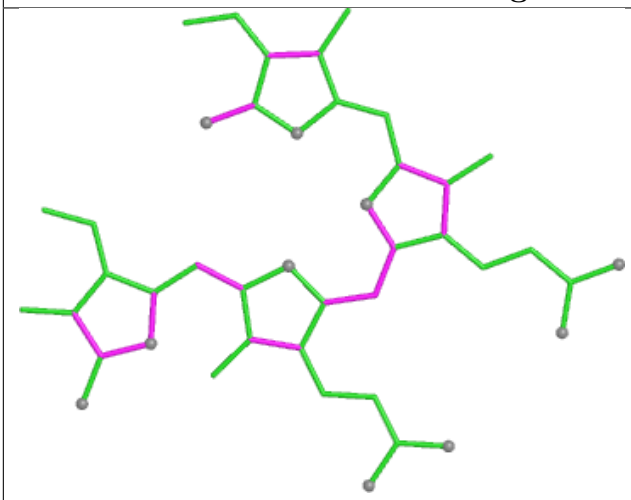


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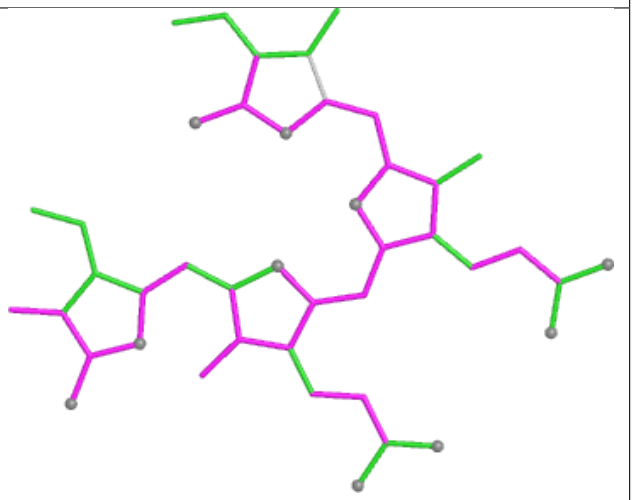


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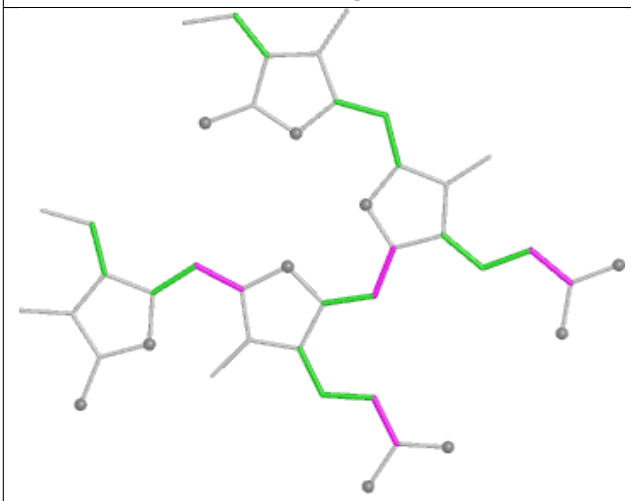
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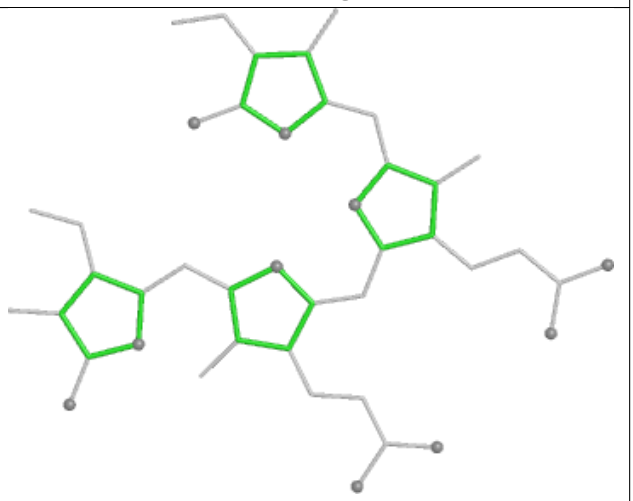
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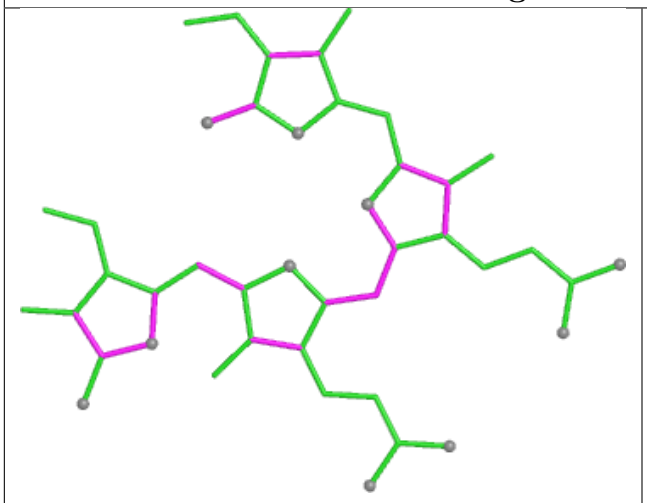


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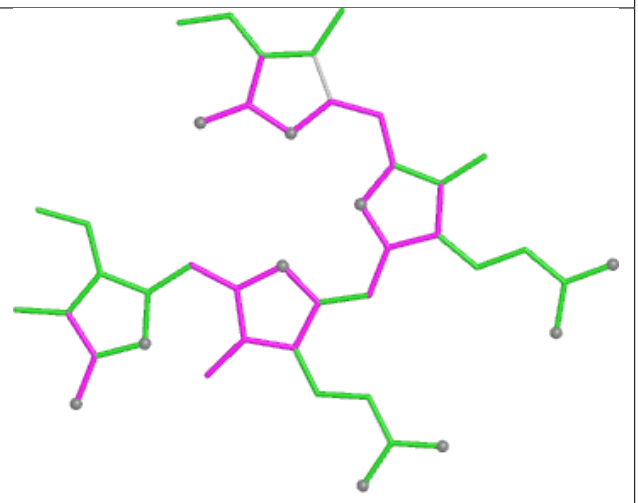


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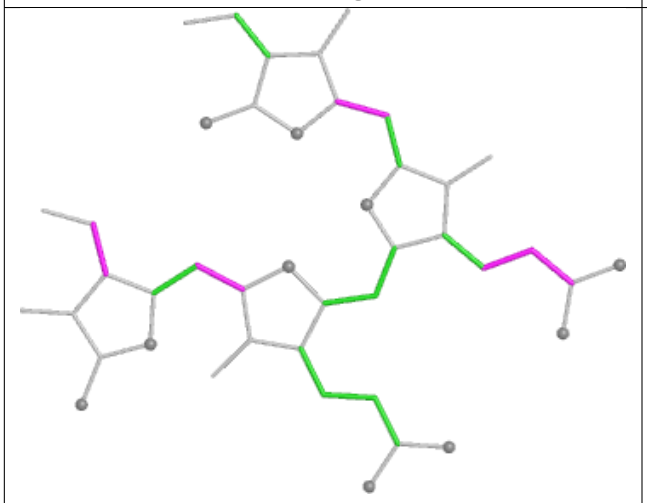
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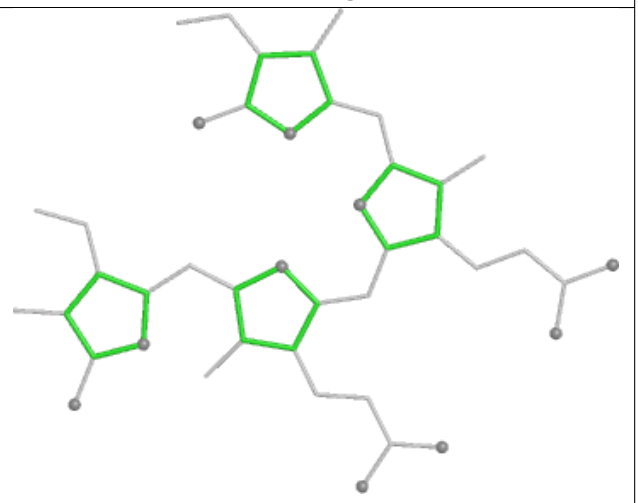
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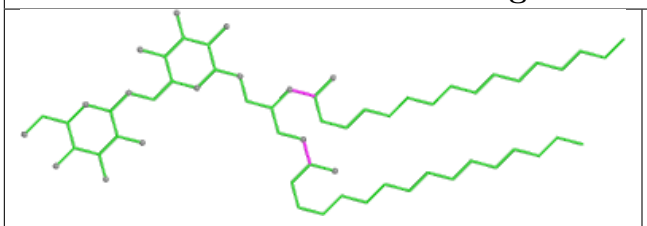


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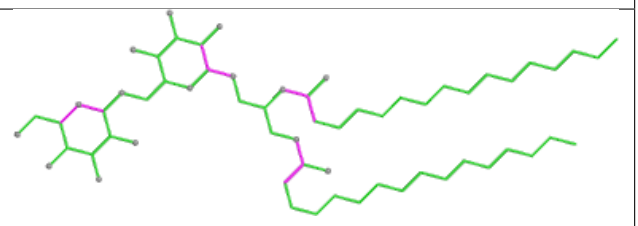


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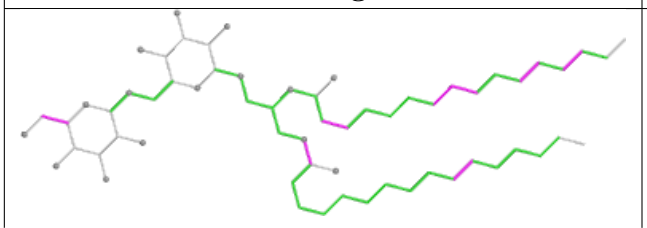
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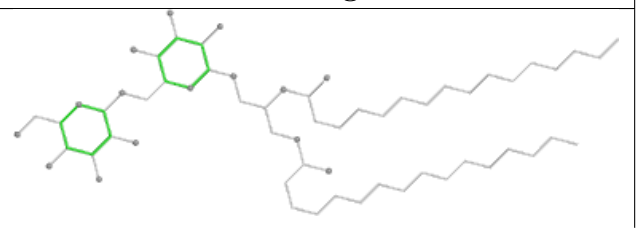
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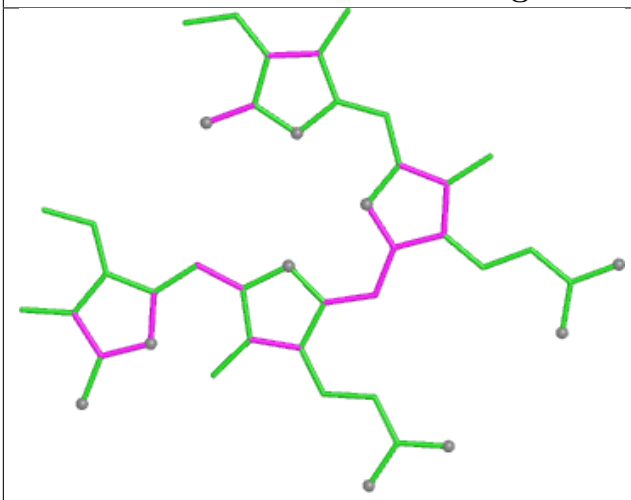


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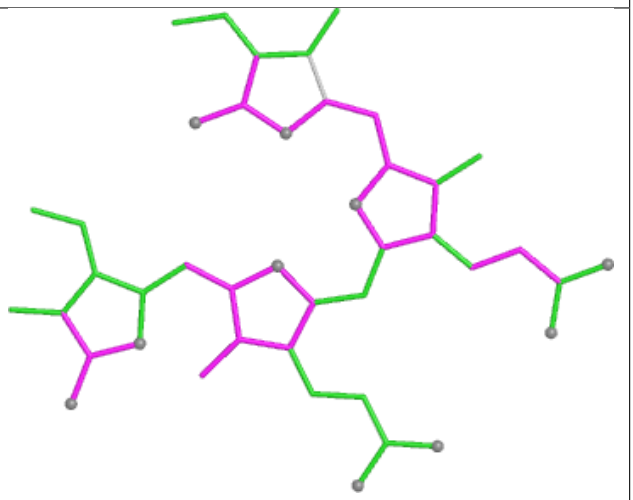


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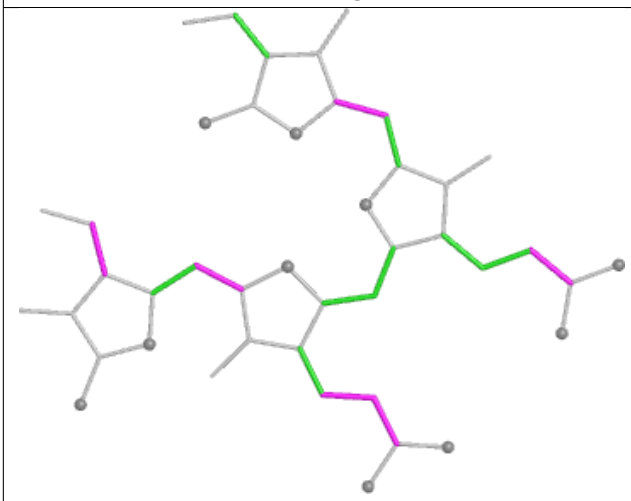
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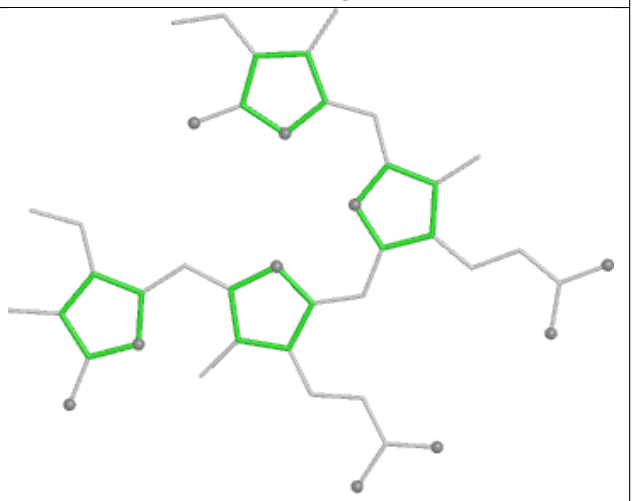
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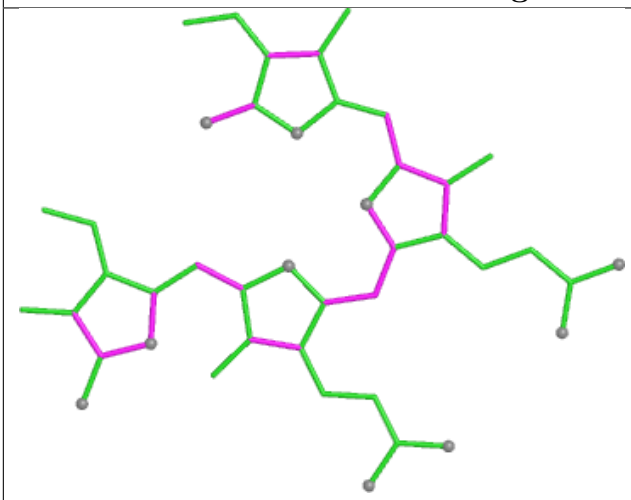


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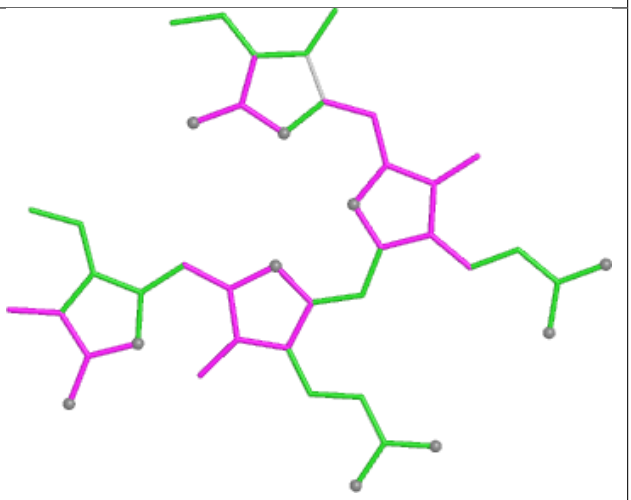


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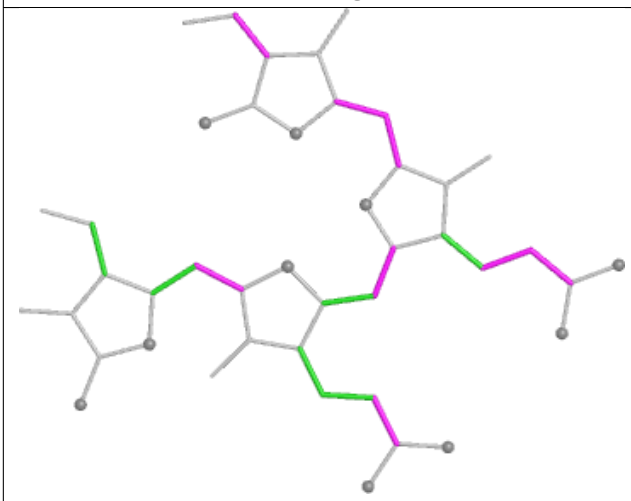
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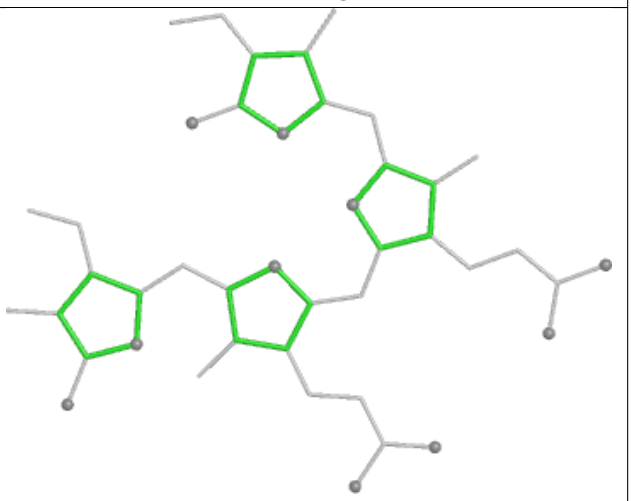
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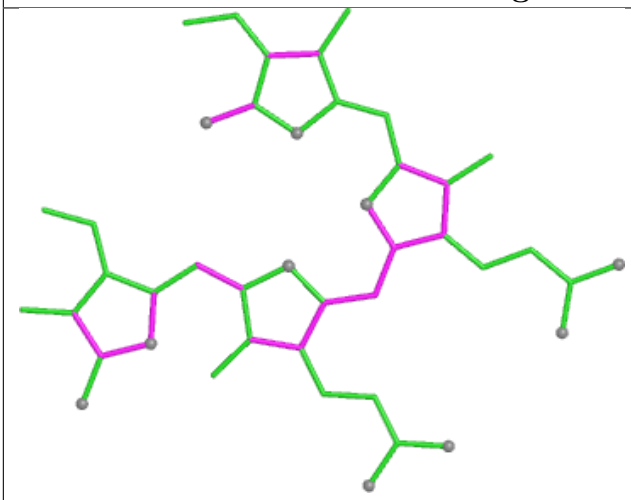


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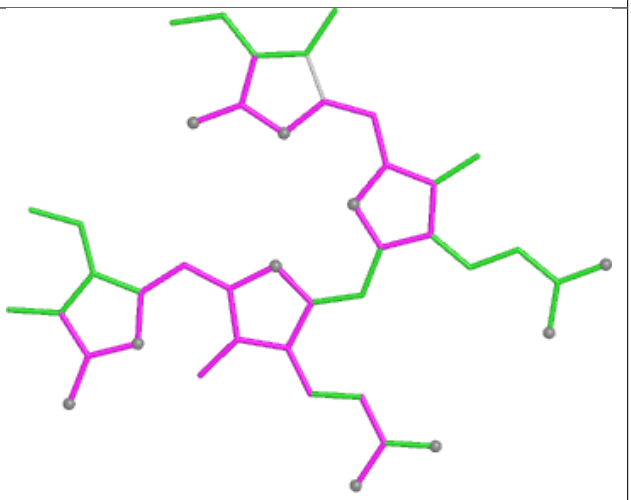


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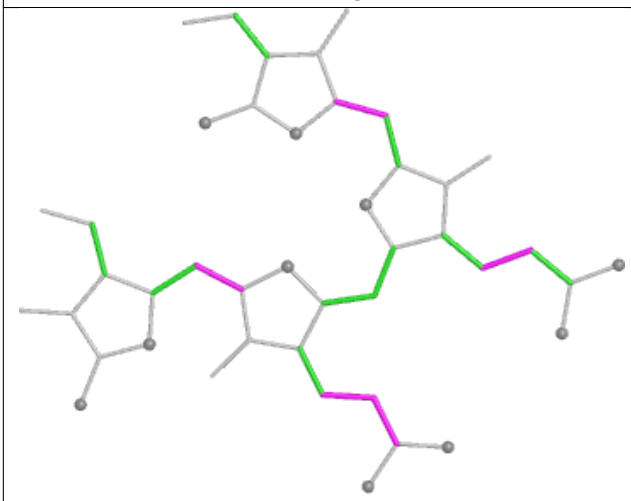
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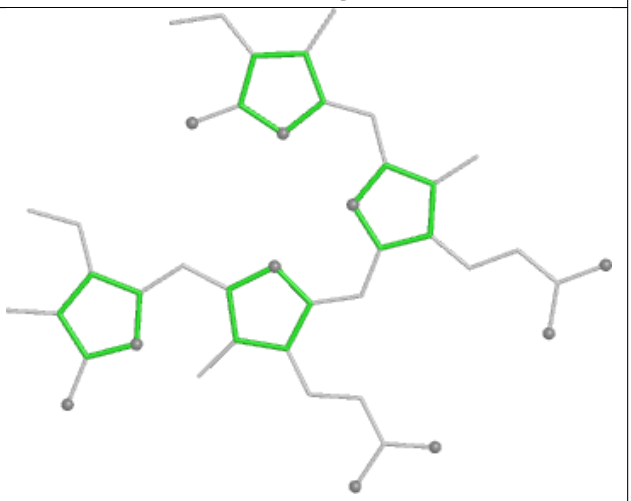
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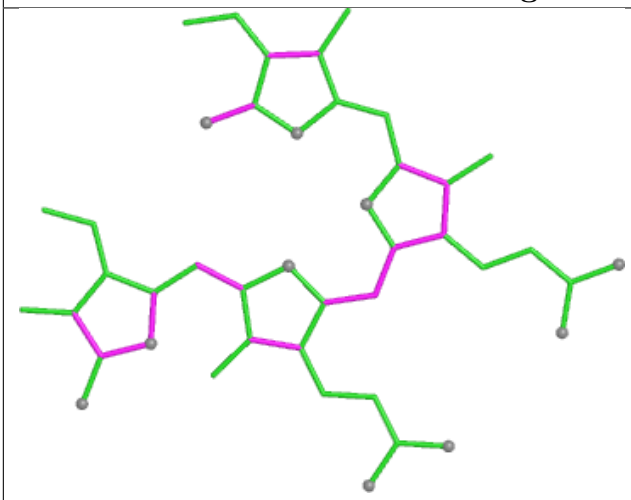


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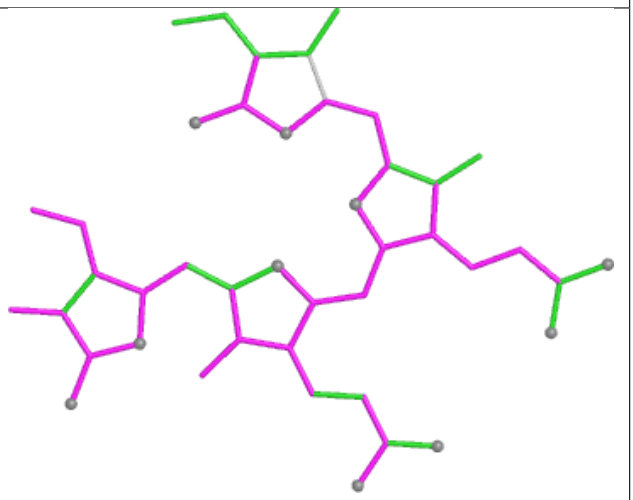


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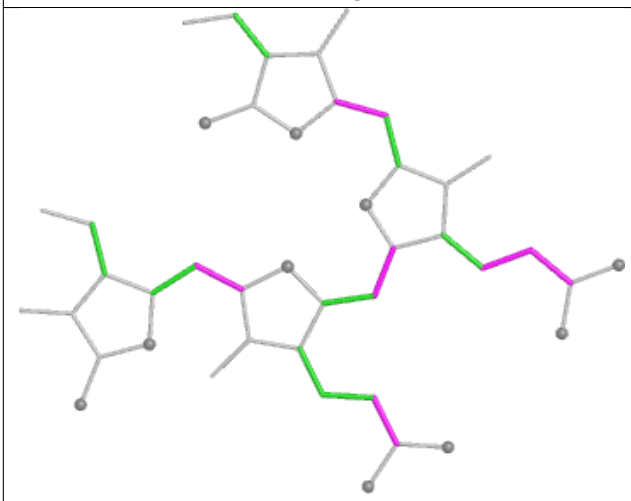
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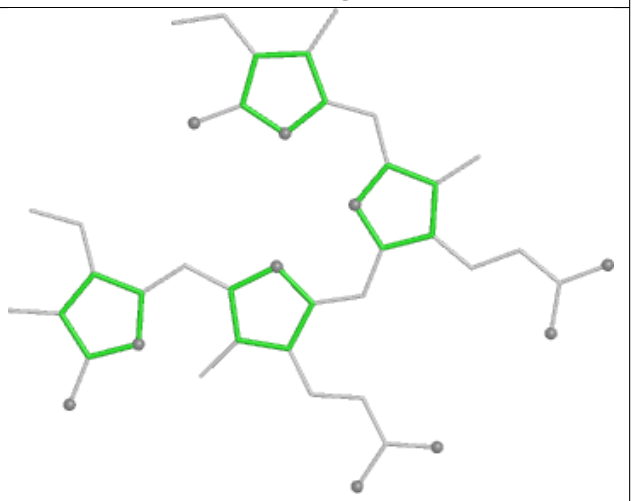
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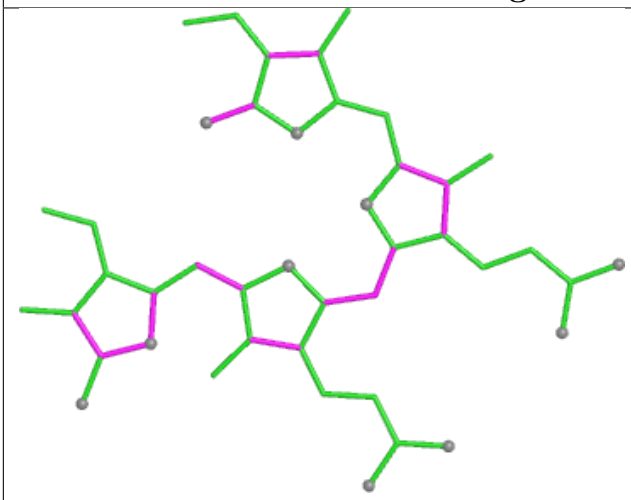


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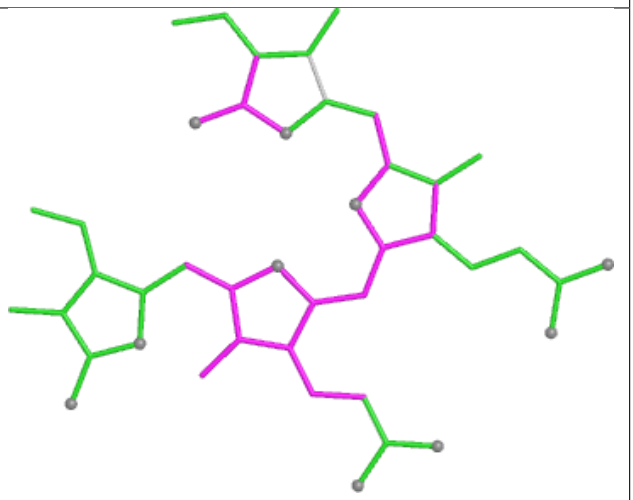


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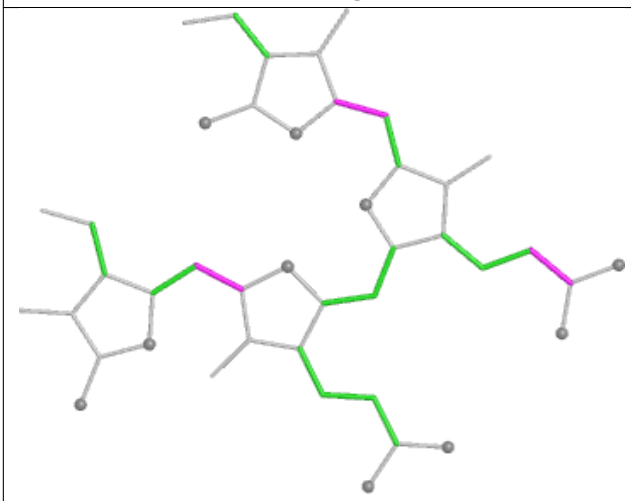
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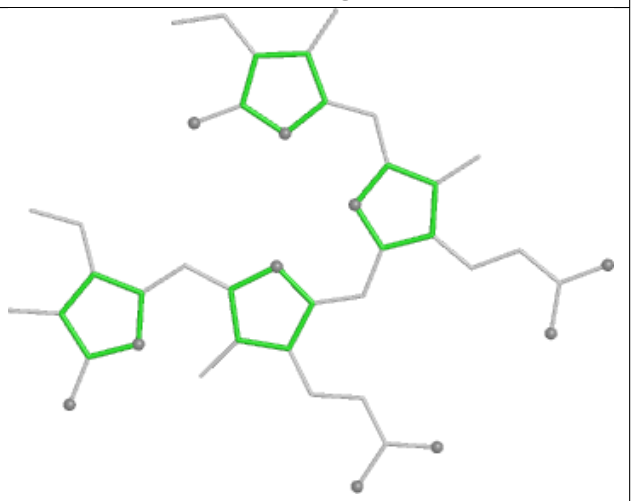
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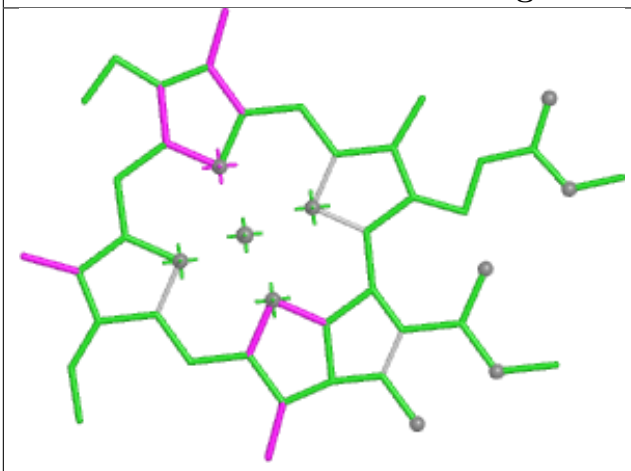


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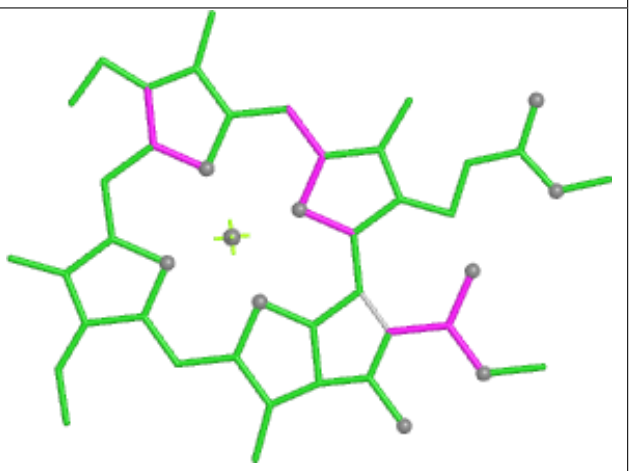


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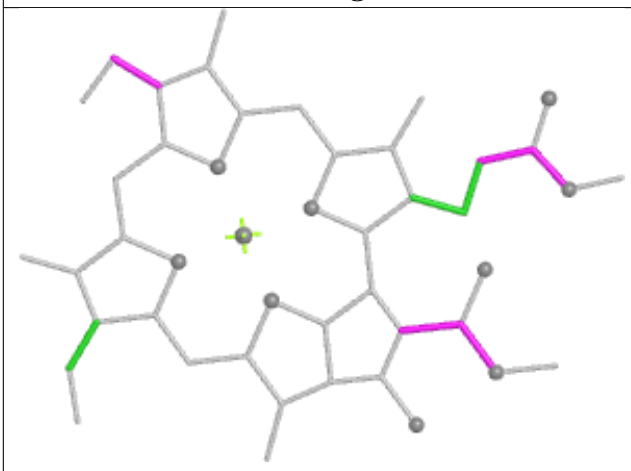
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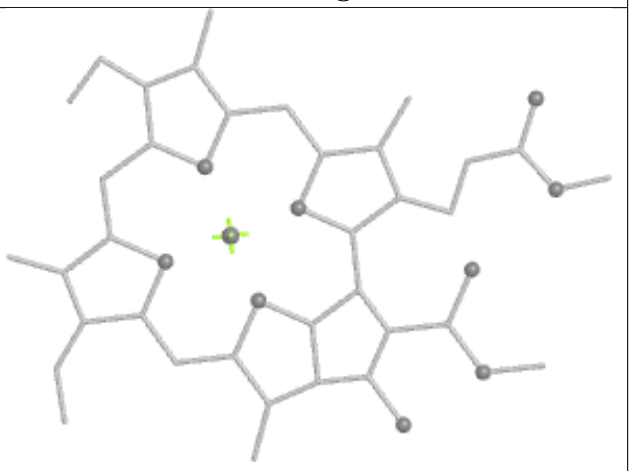
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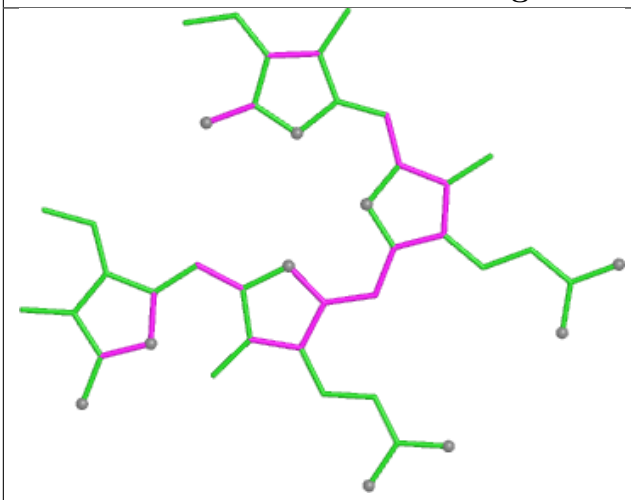


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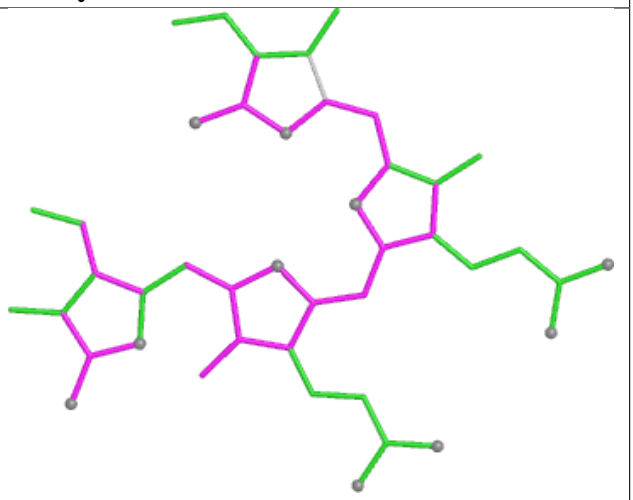


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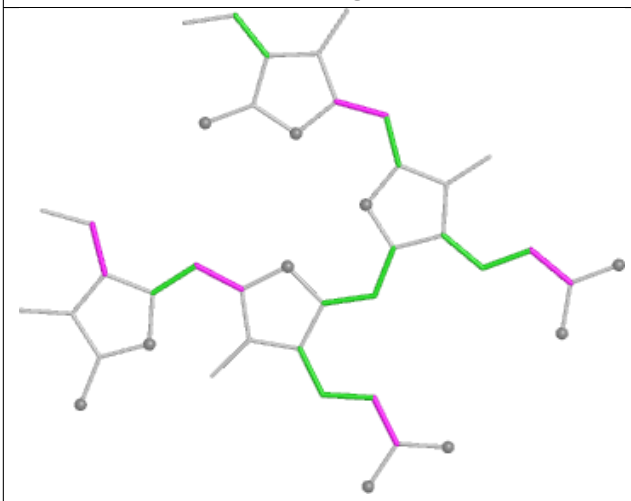
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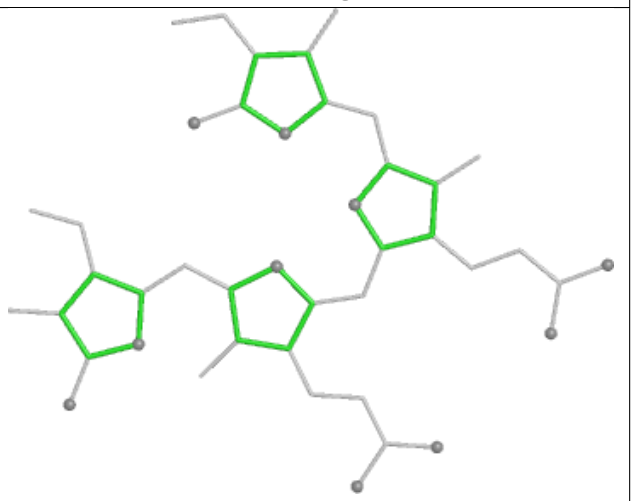
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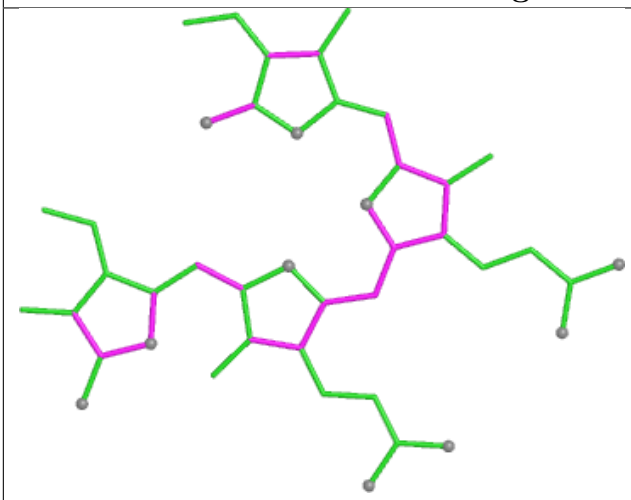


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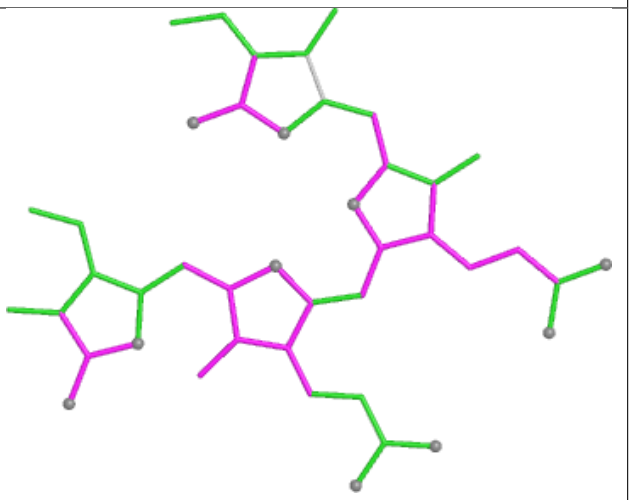


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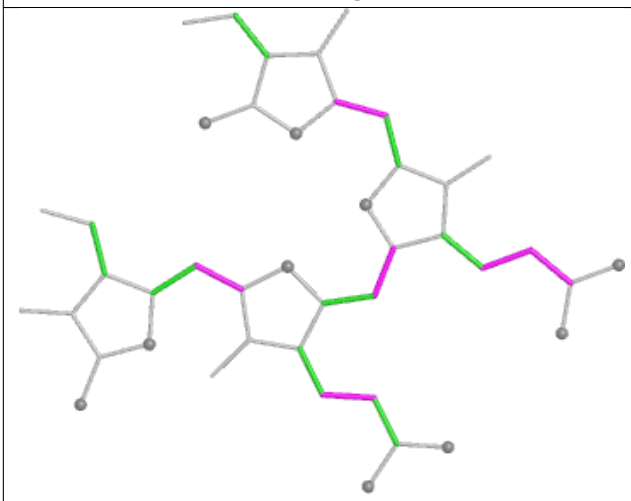
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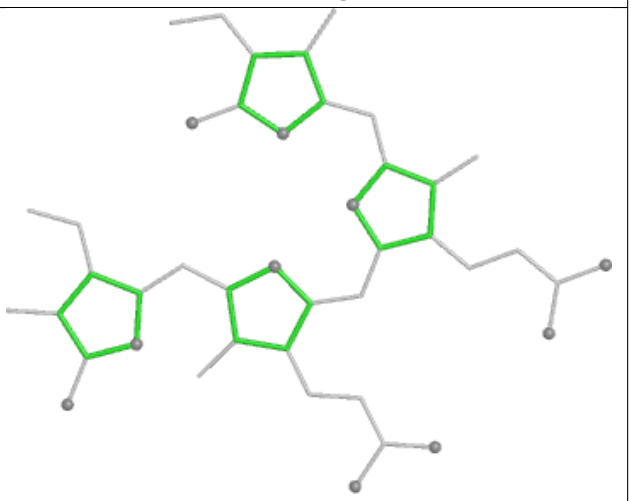
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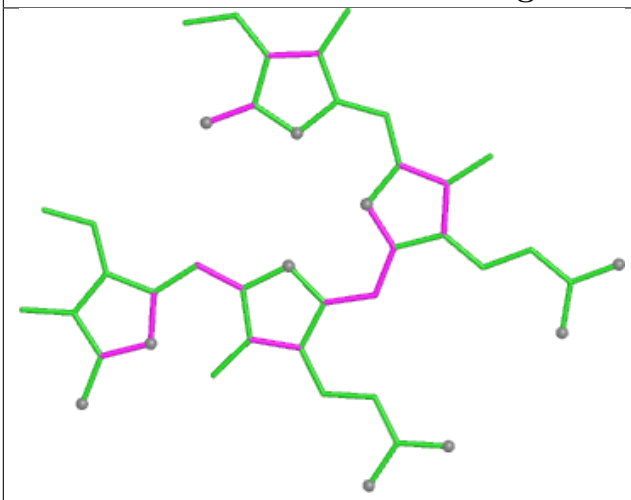


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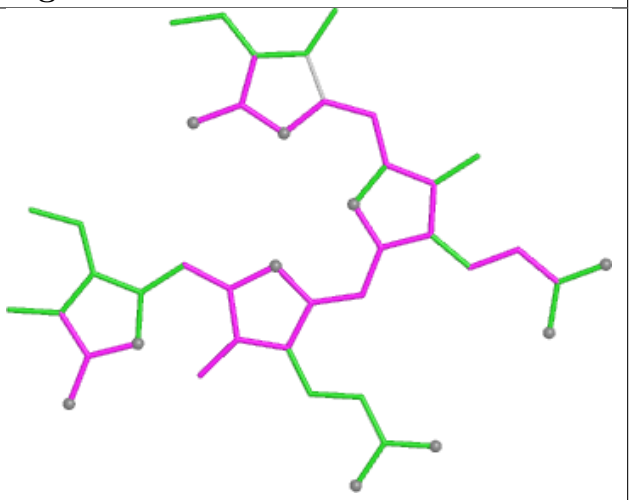


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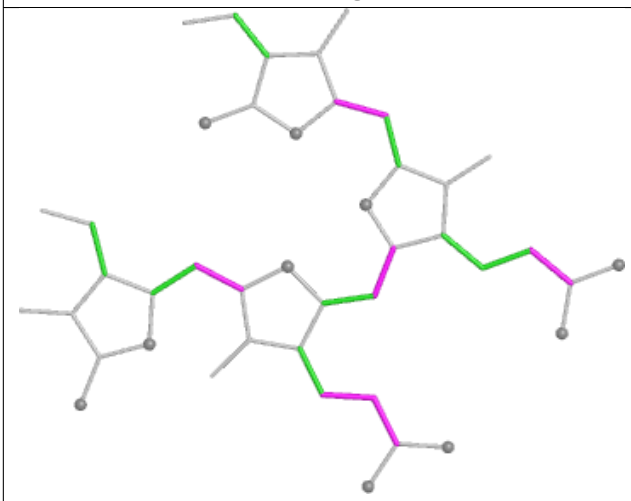
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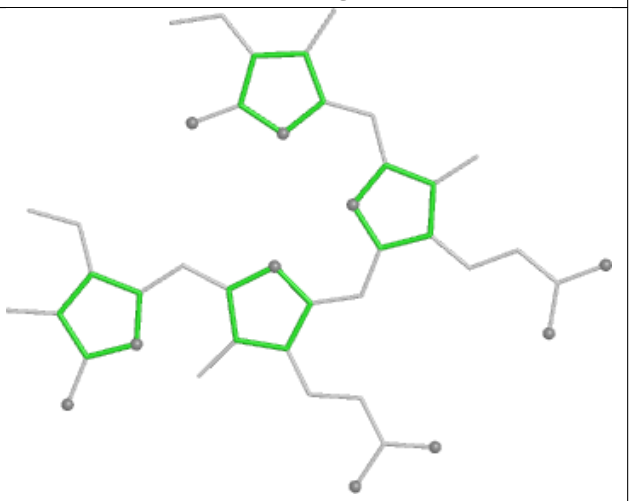
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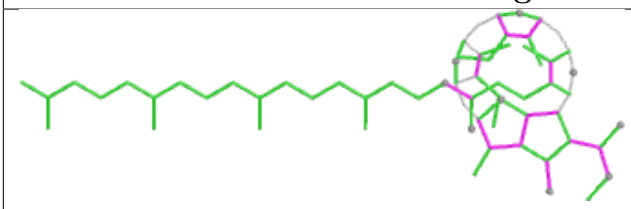


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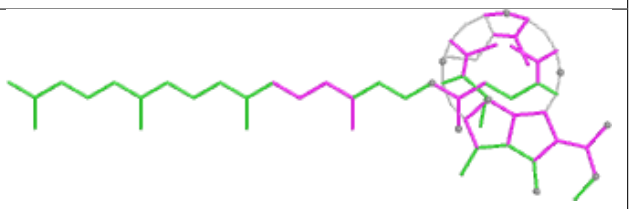


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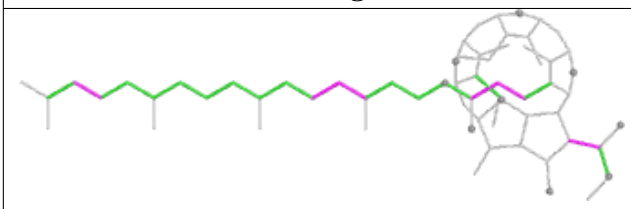
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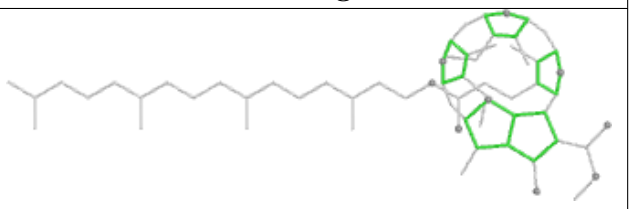
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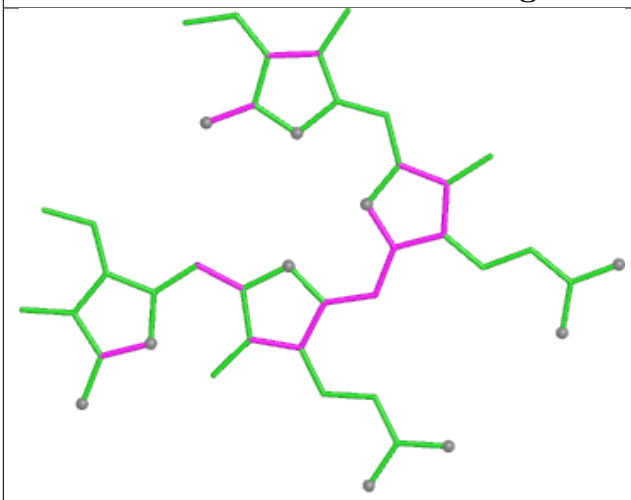


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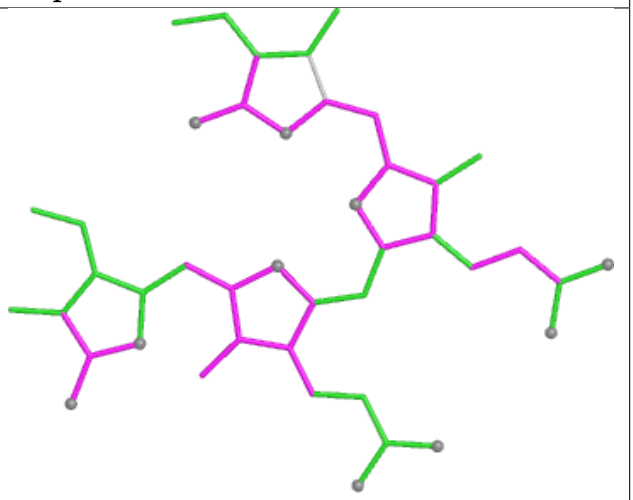


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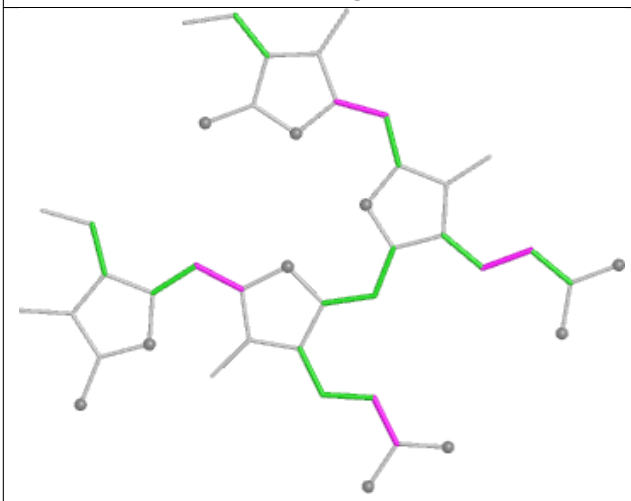
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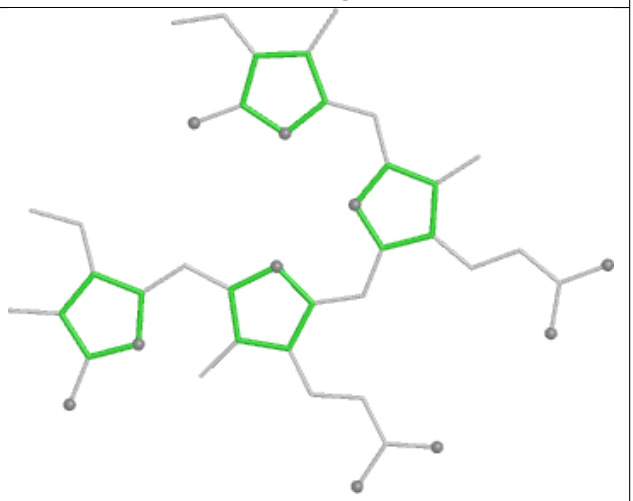
Bond lengths



Bond angles

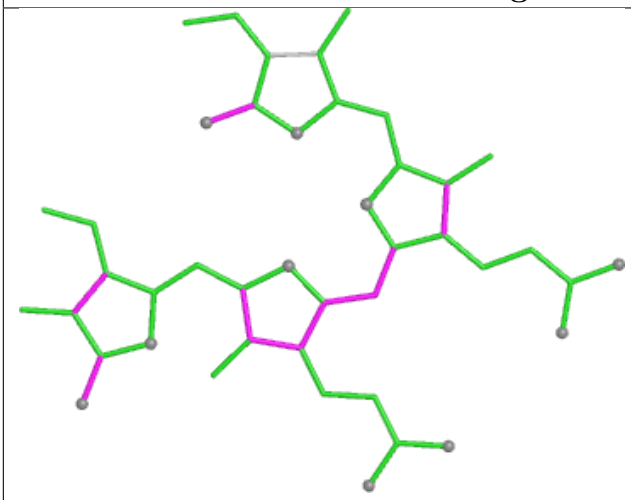


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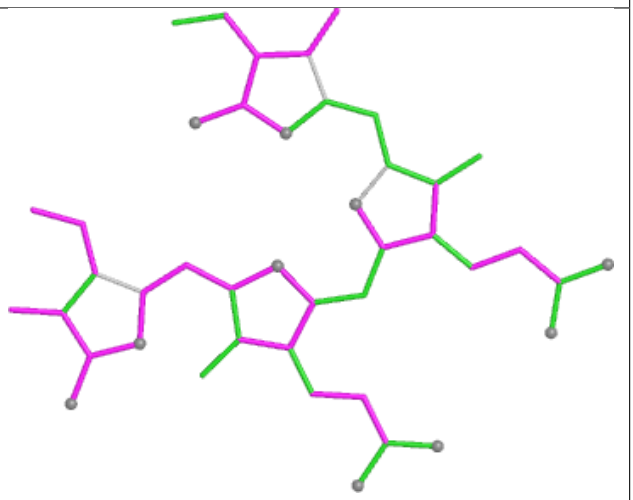


Rings

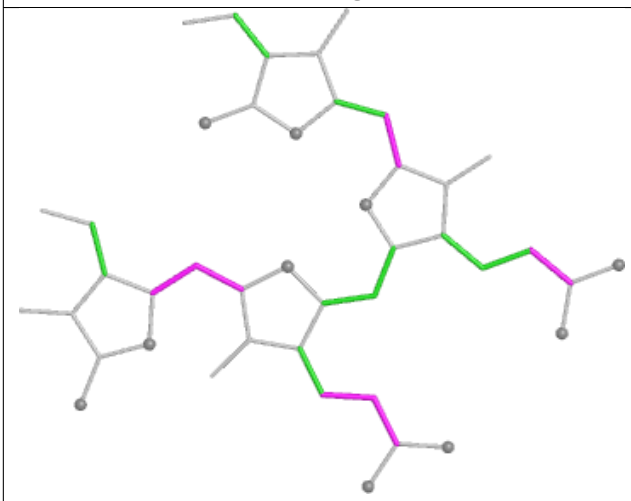
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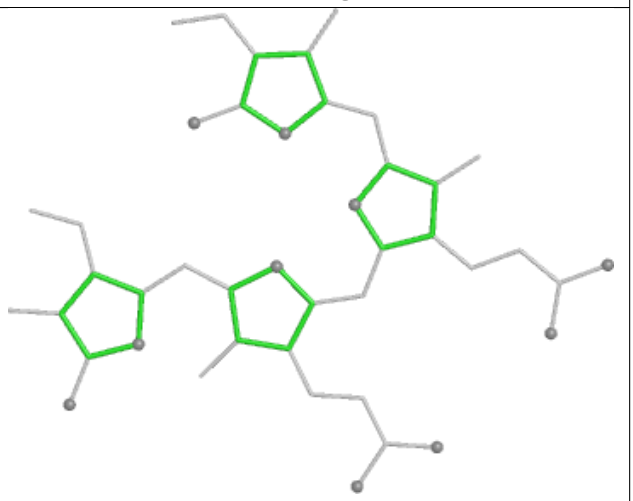
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Bond angles

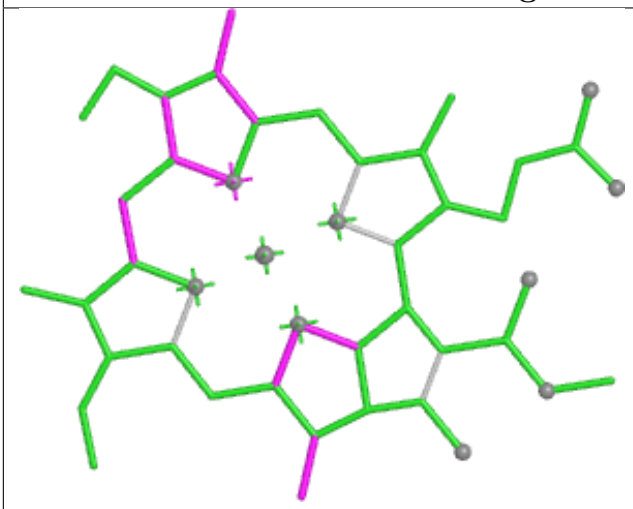


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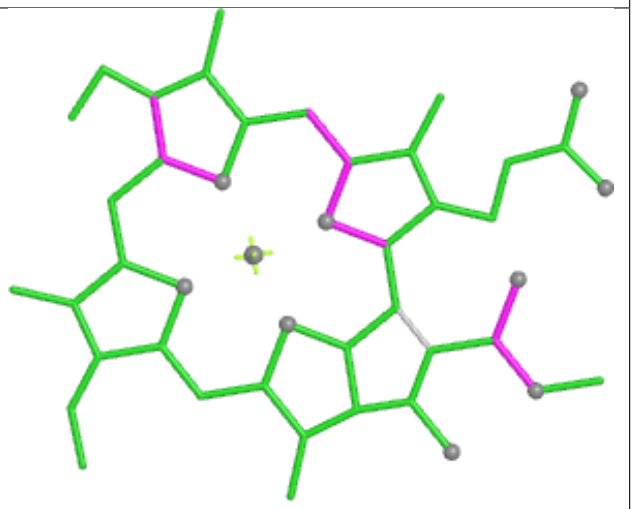


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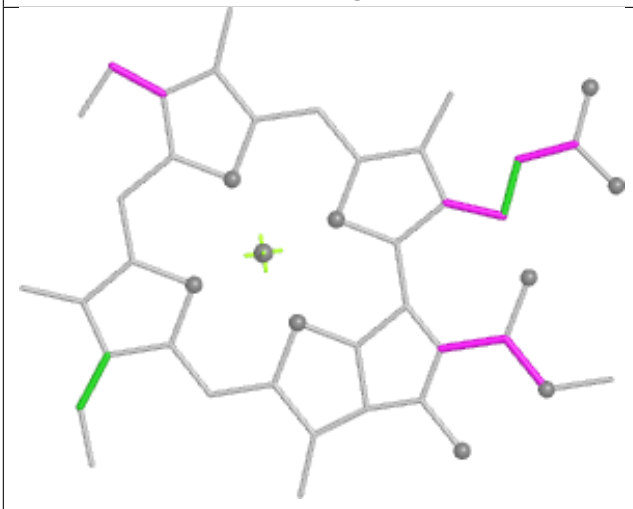
Ligand CLA 62 304



Bond lengths



Bond angles

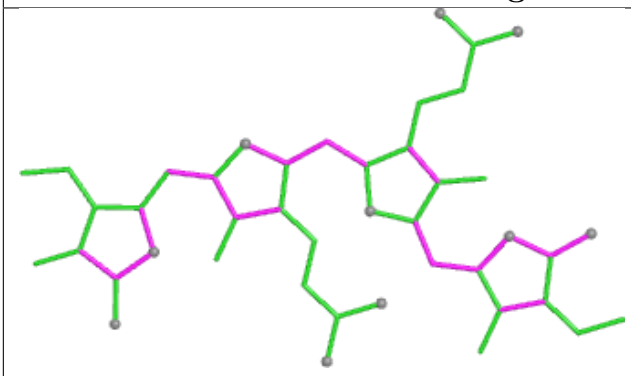


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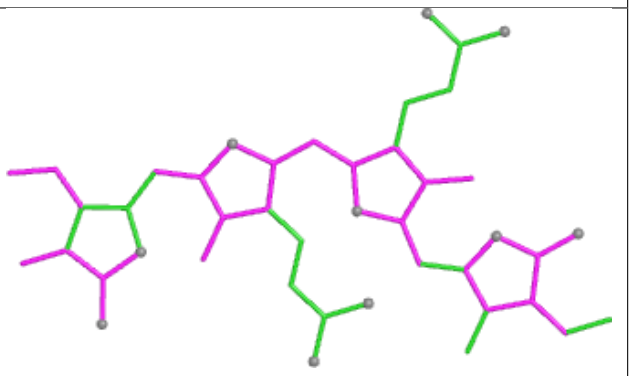


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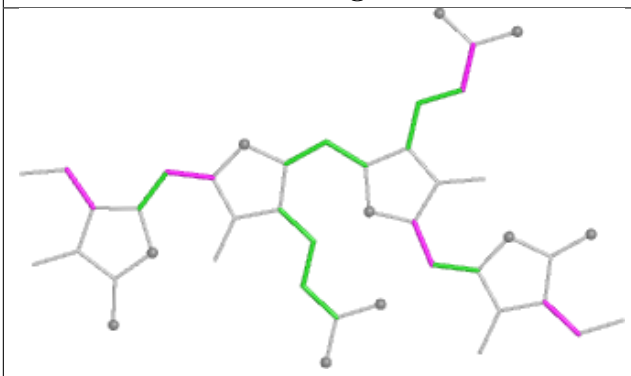
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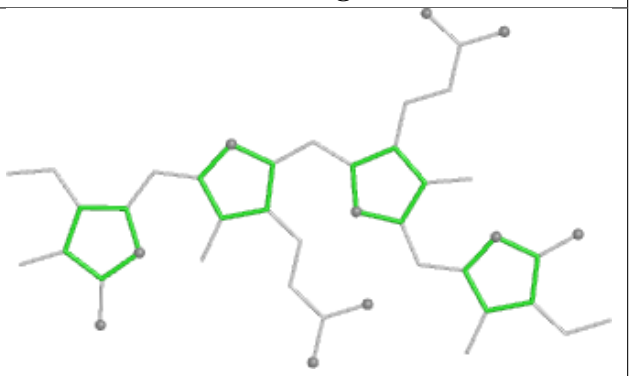
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Bond angles

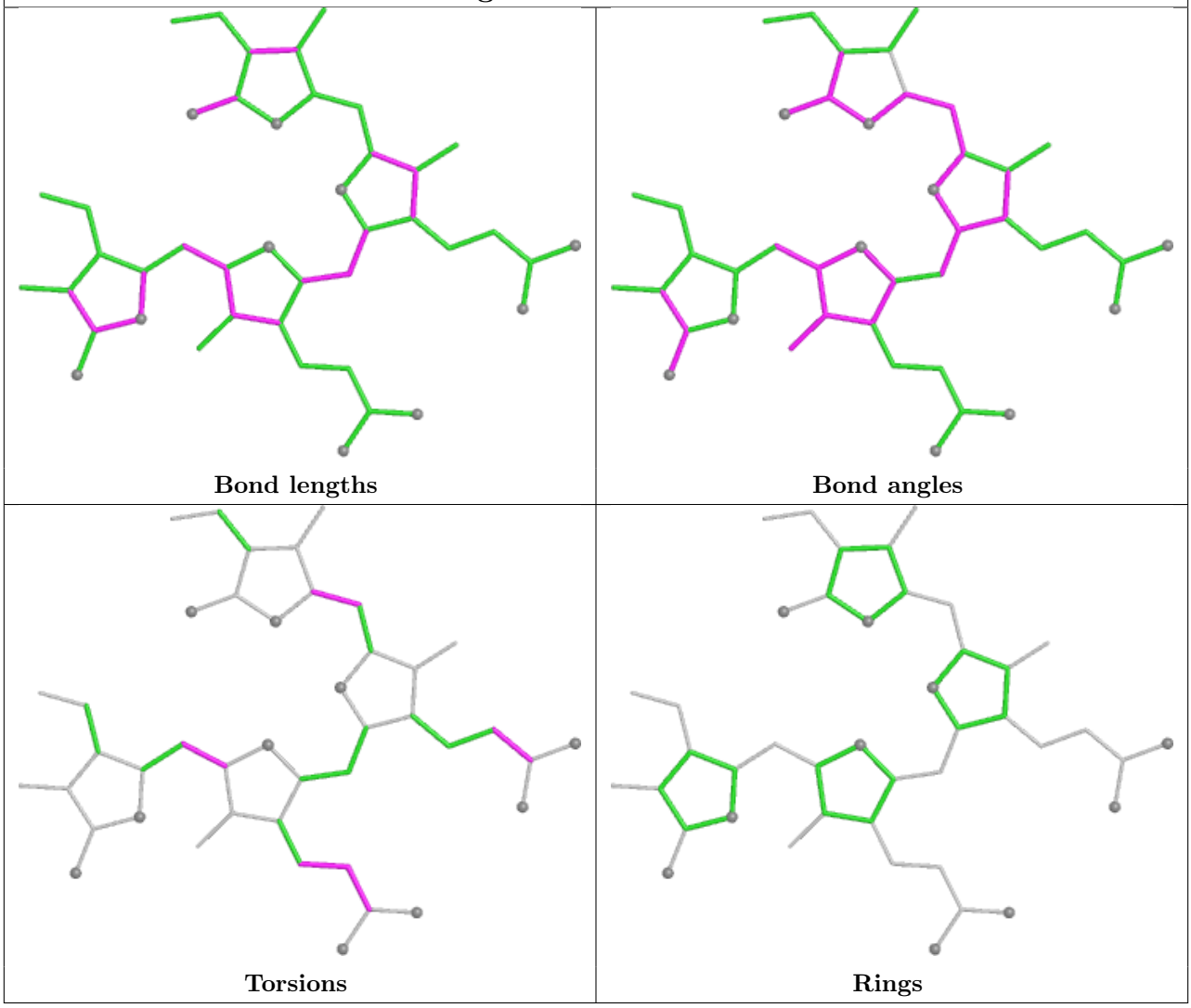


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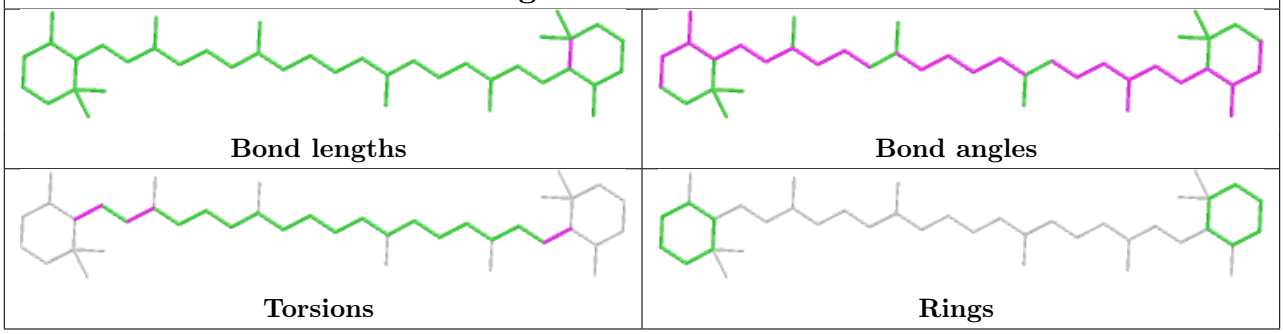


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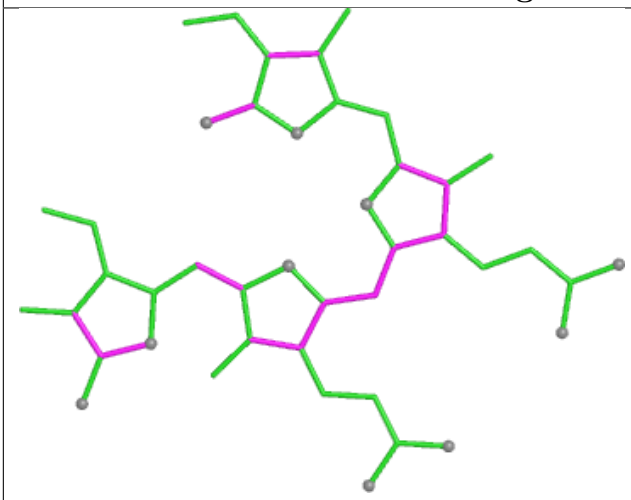
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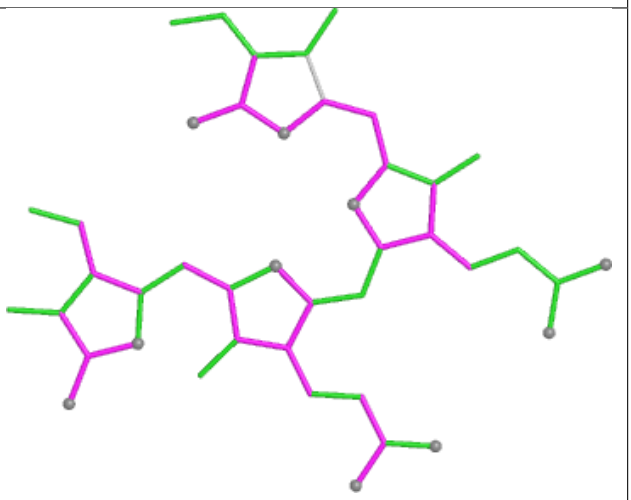
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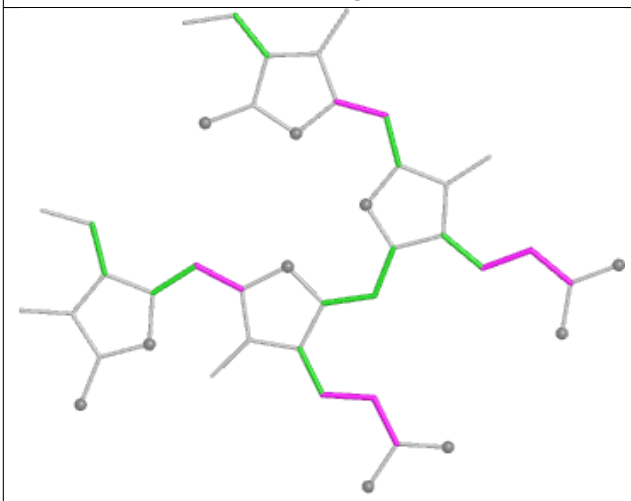
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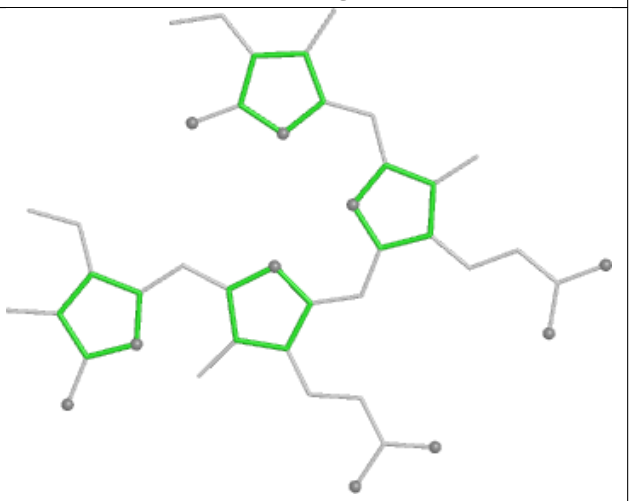
Bond lengths



Bond angles

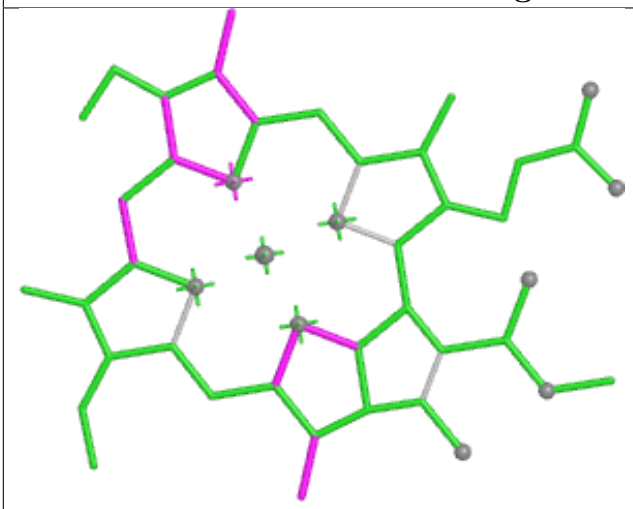


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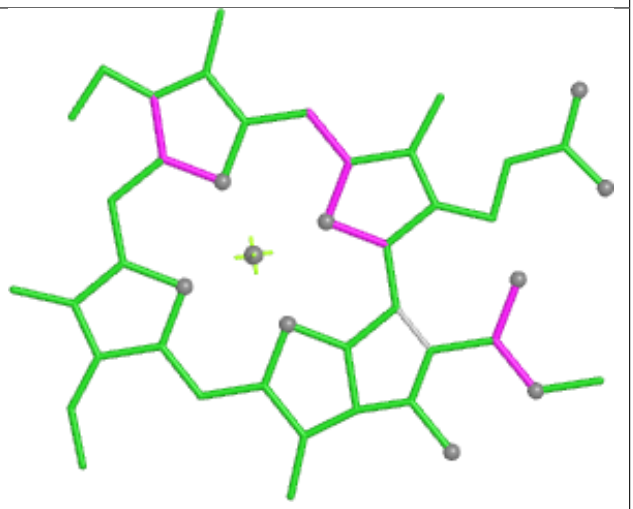


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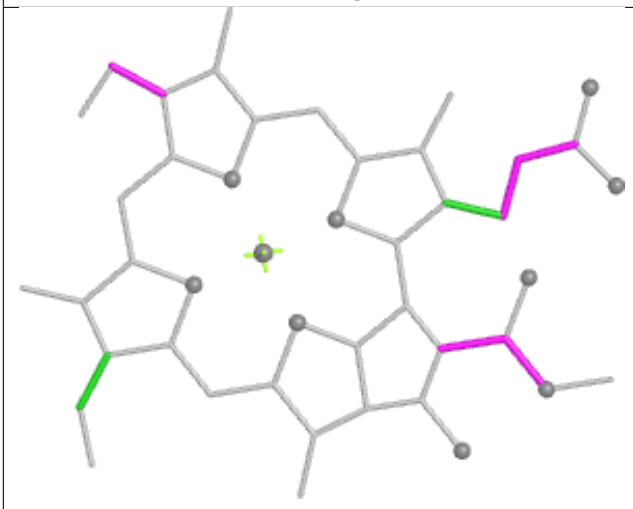
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Bond lengths



Bond angles

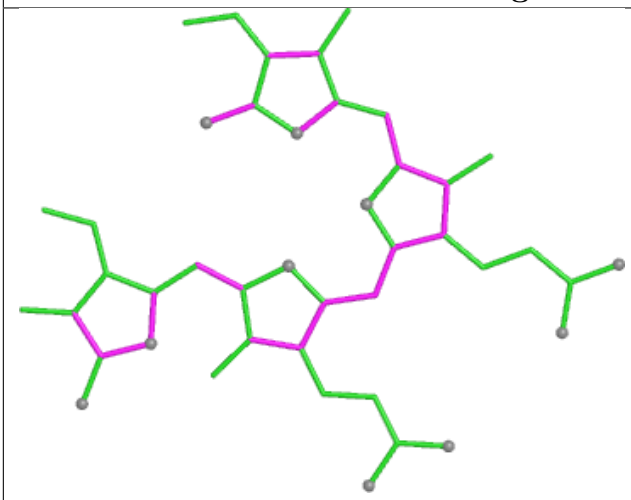


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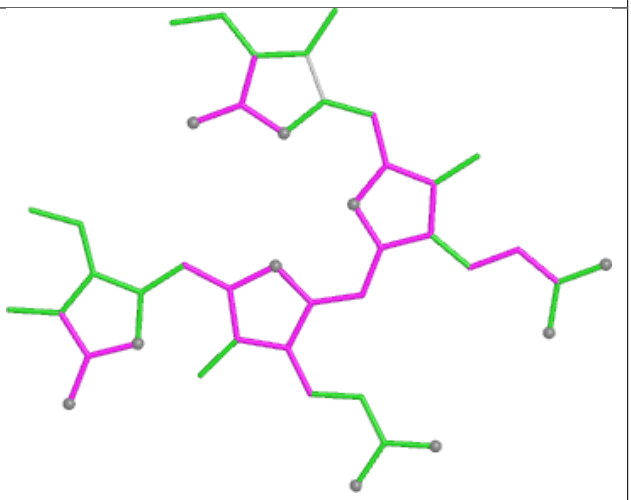


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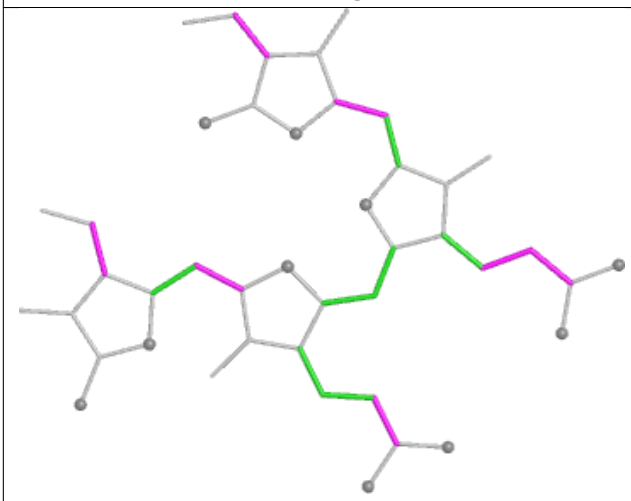
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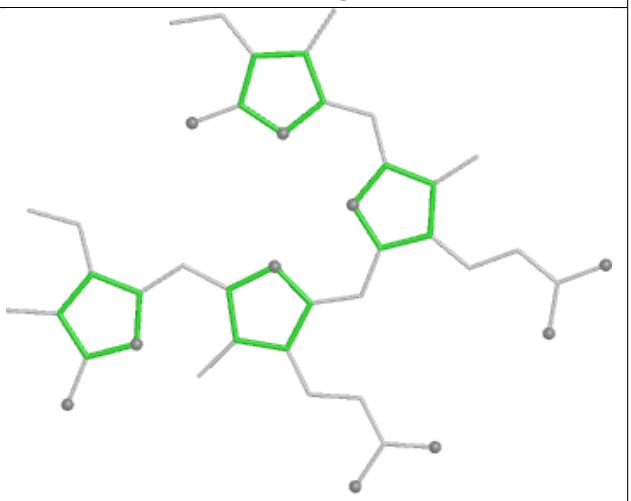
Bond lengths



Bond angles

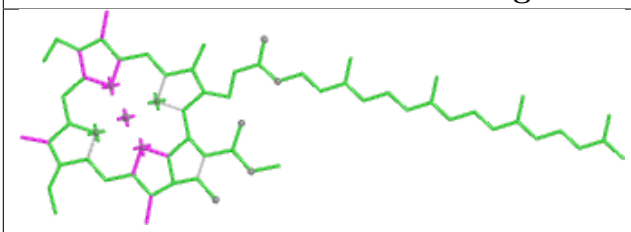


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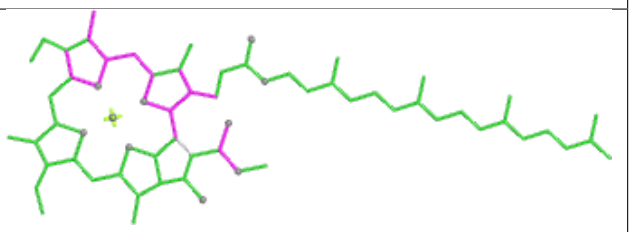


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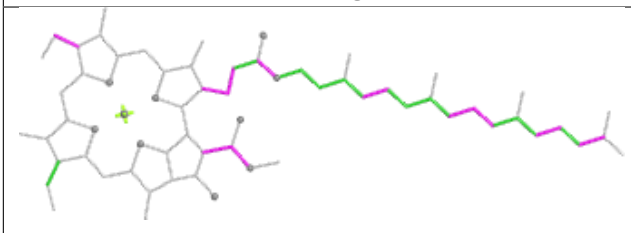
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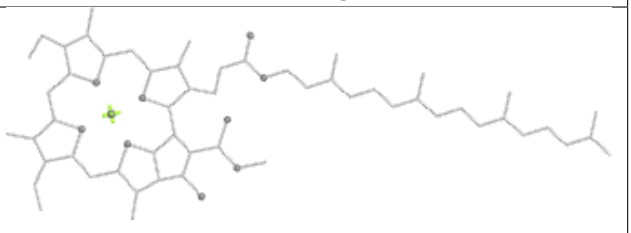
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Bond angles

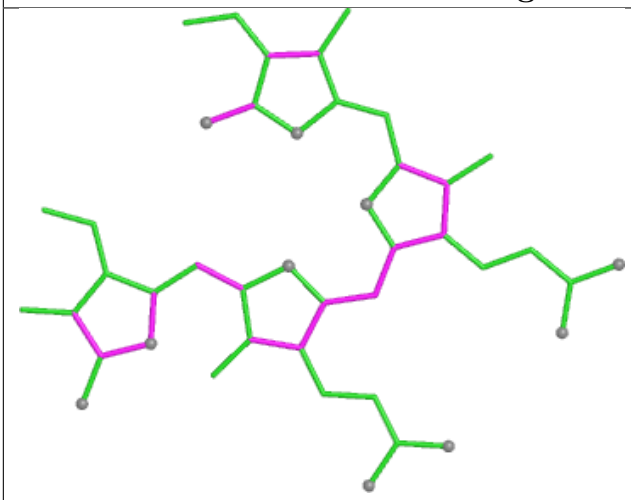


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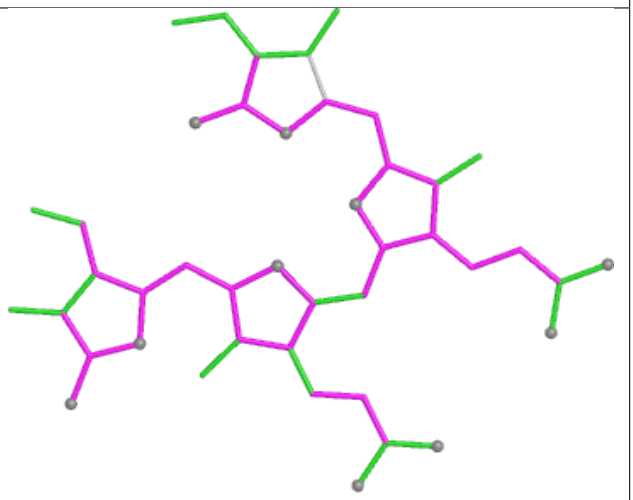


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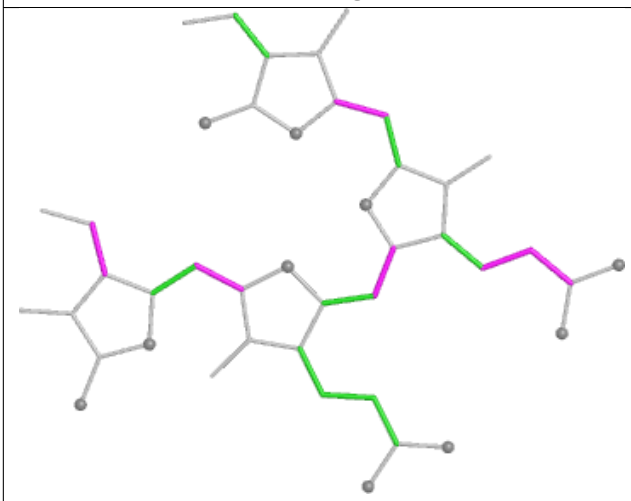
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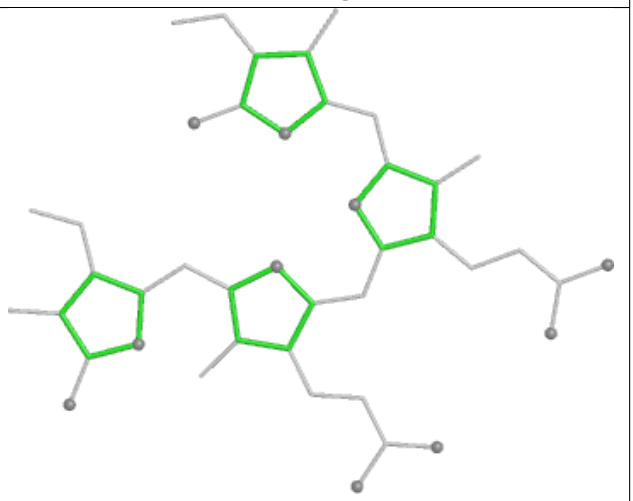
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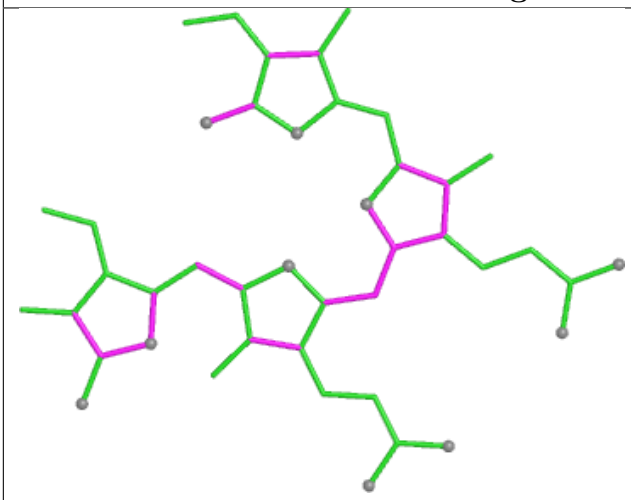


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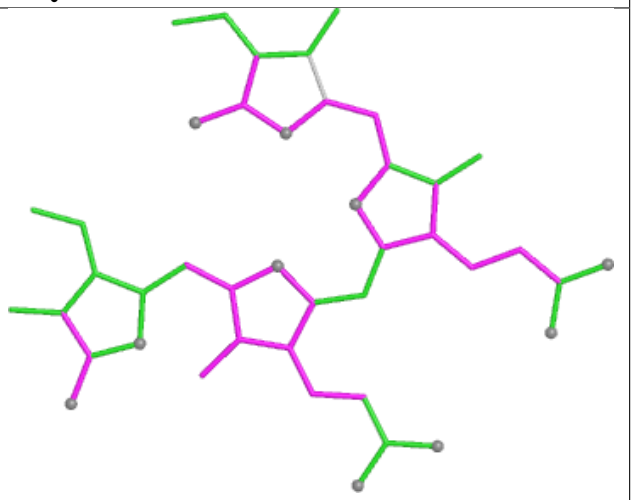


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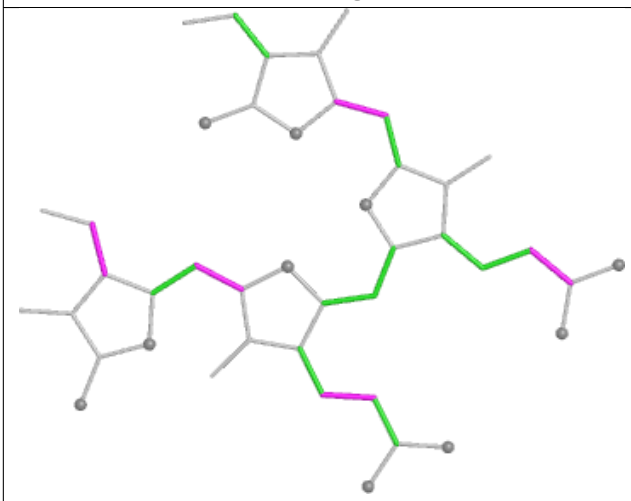
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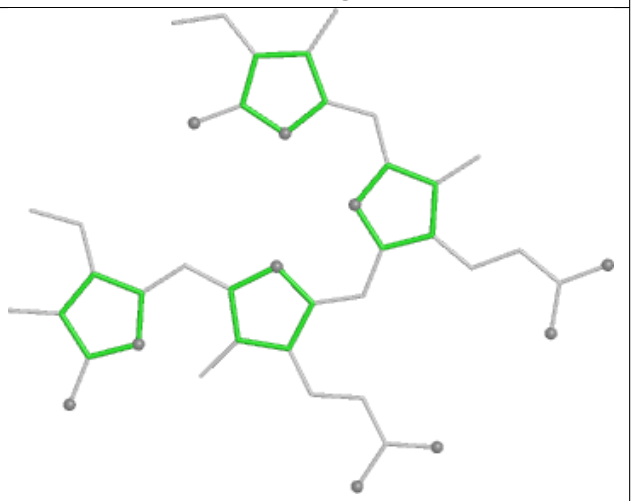
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Bond angles

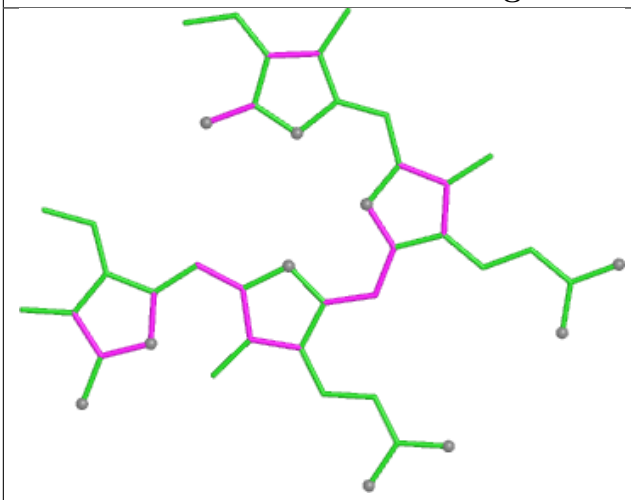


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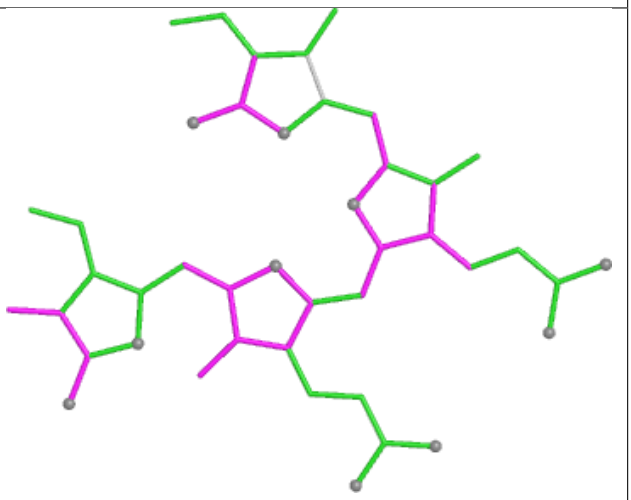


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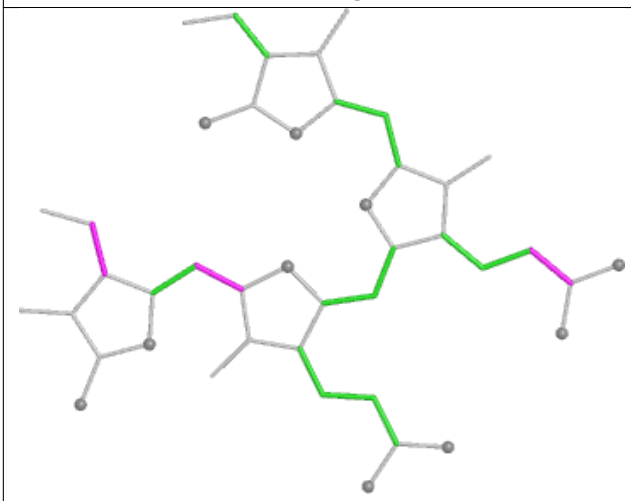
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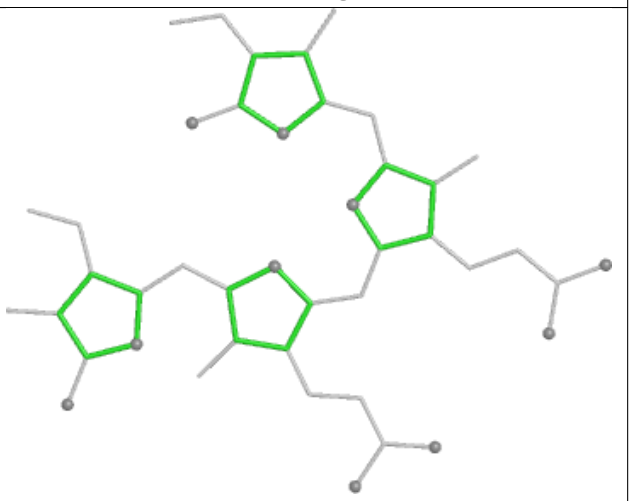
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Bond angles

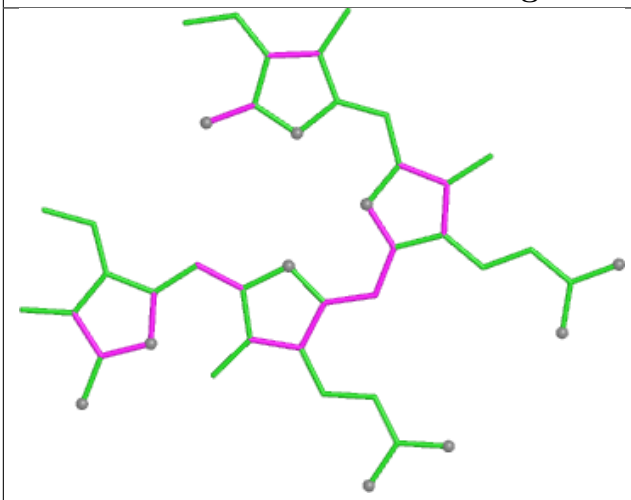


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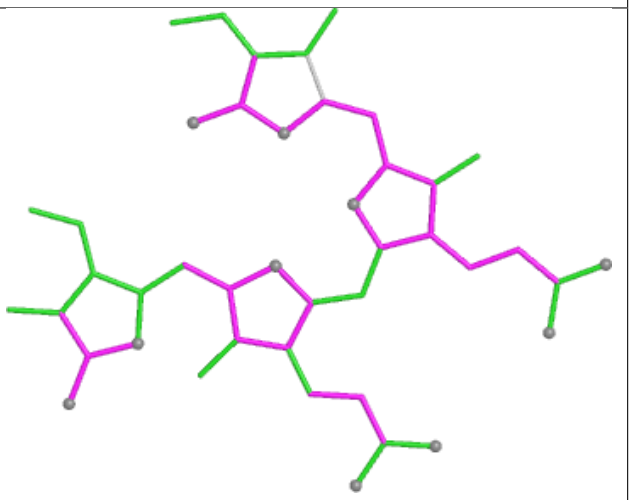


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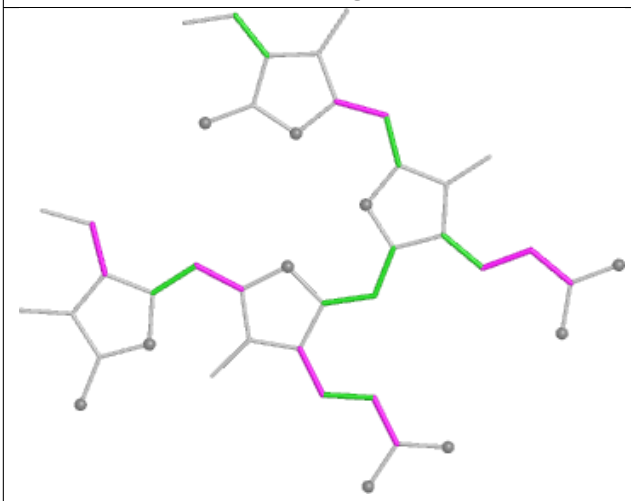
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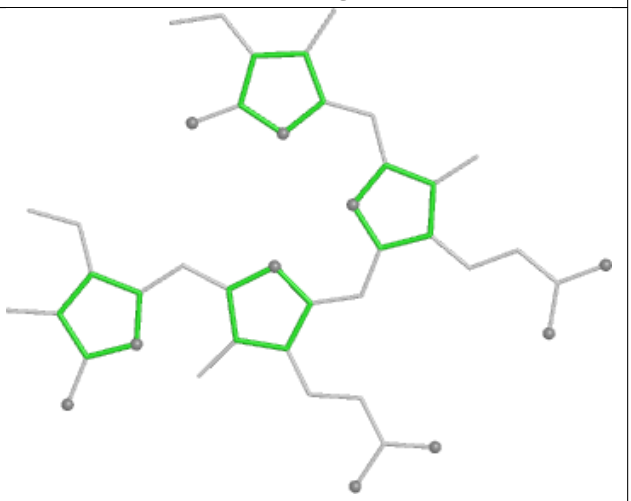
Bond lengths



Bond angles

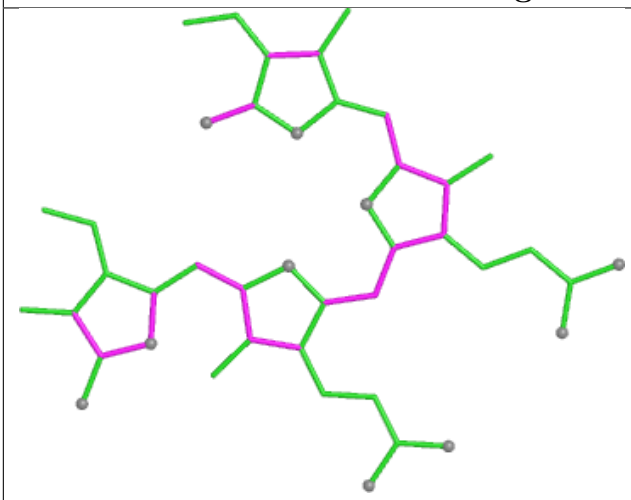


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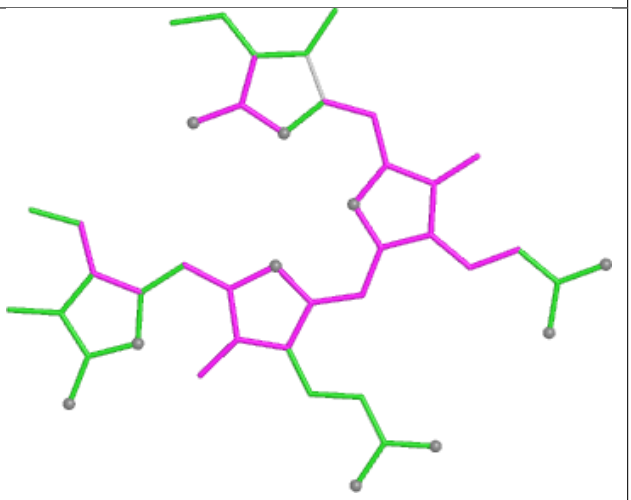


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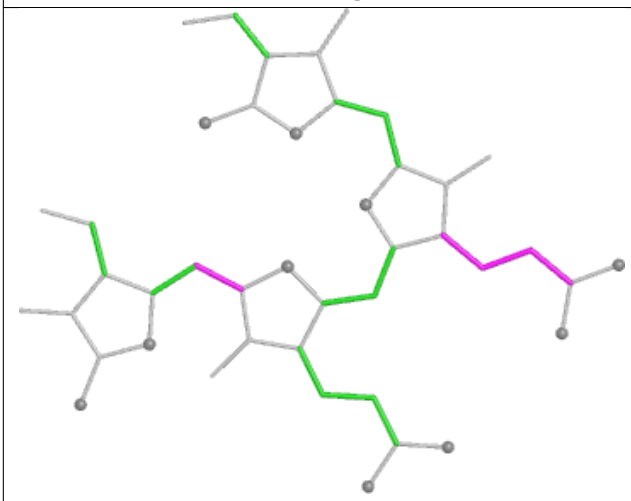
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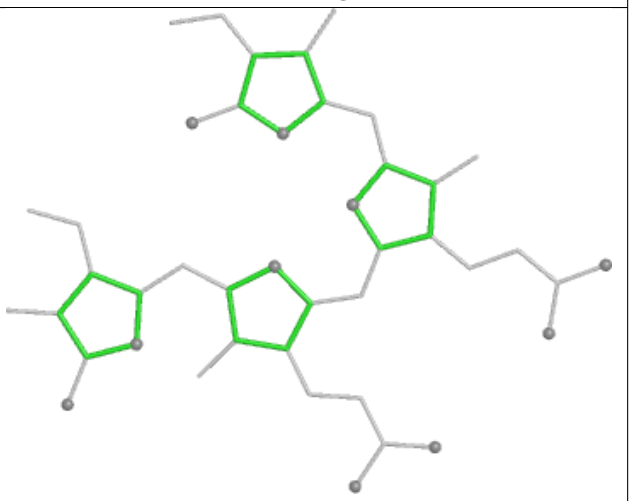
Bond lengths



Bond angles

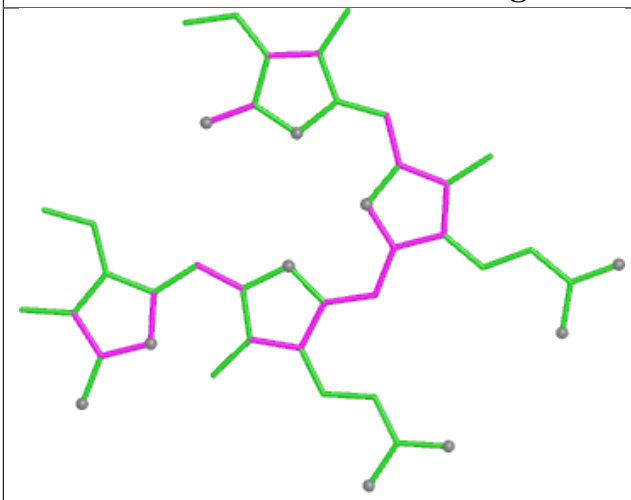


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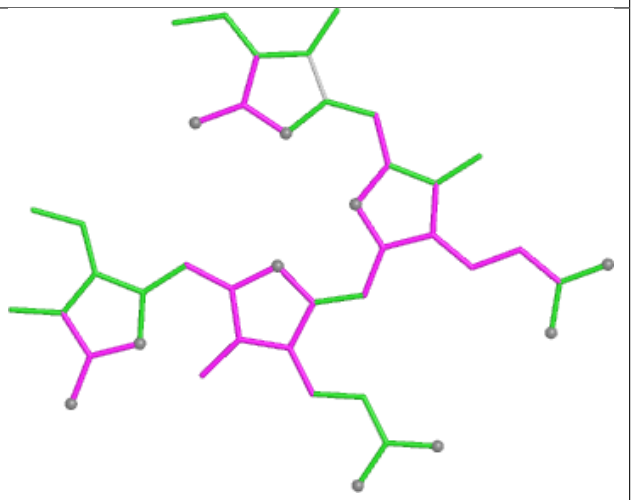


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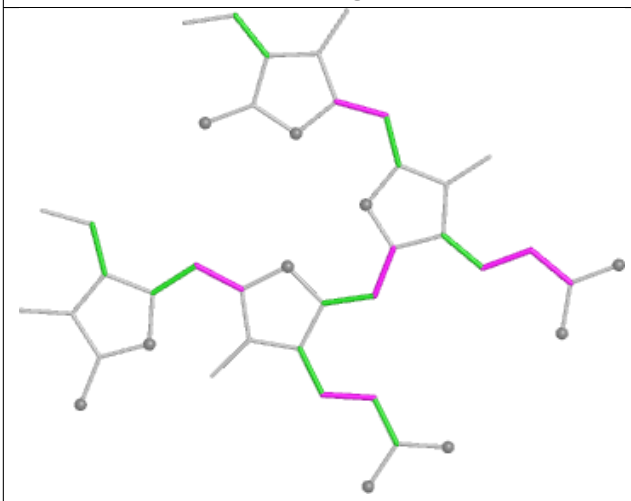
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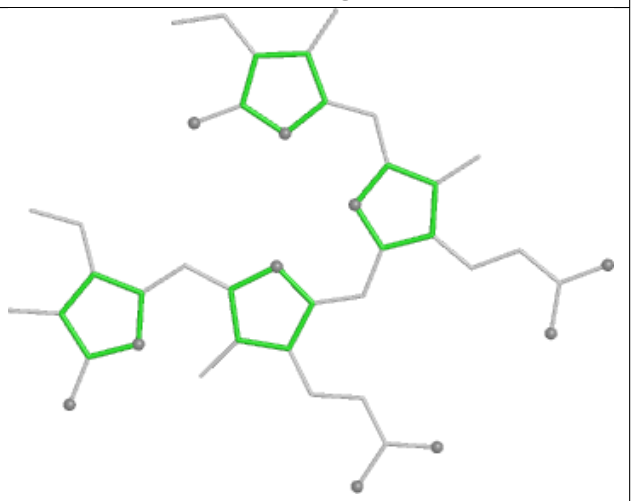
Bond lengths



Bond angles

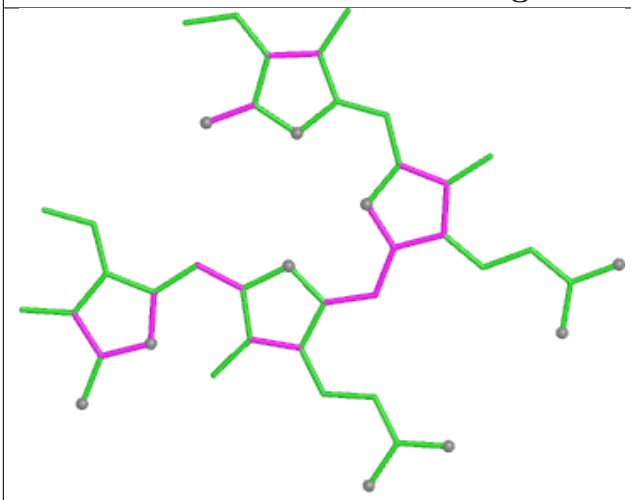


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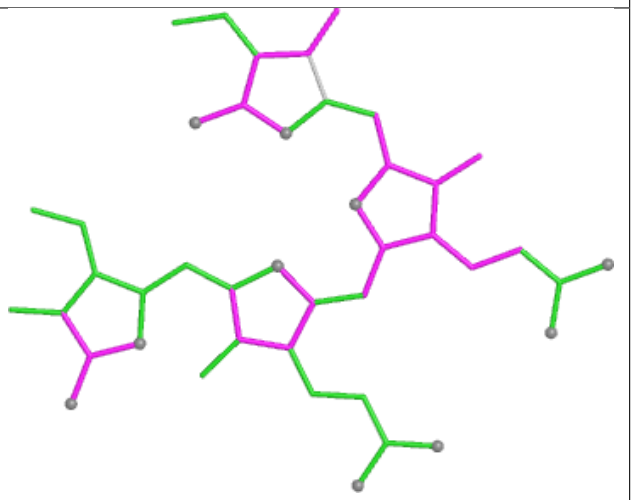


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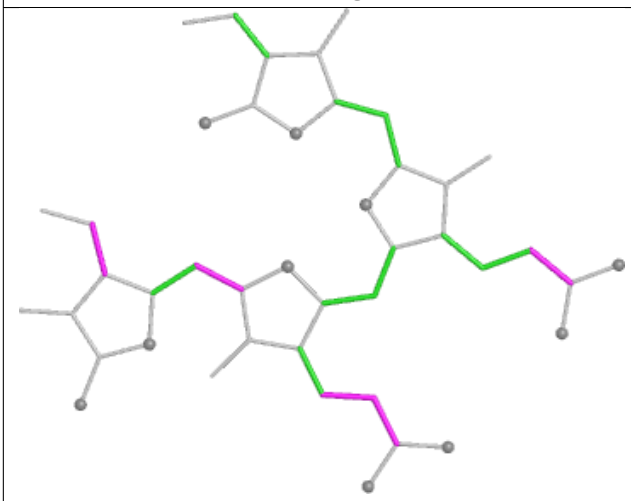
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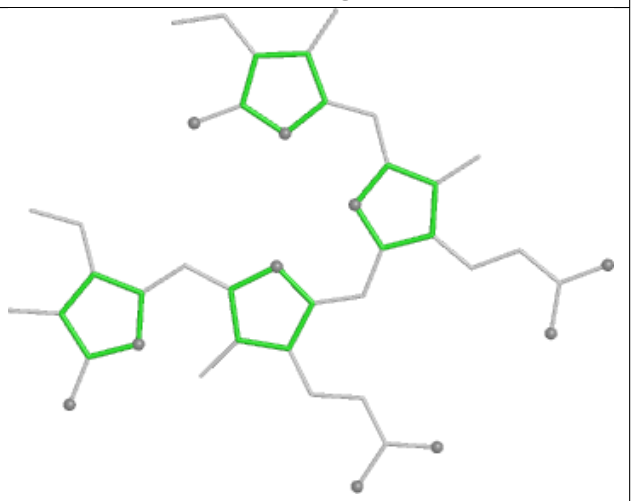
Bond lengths



Bond angles

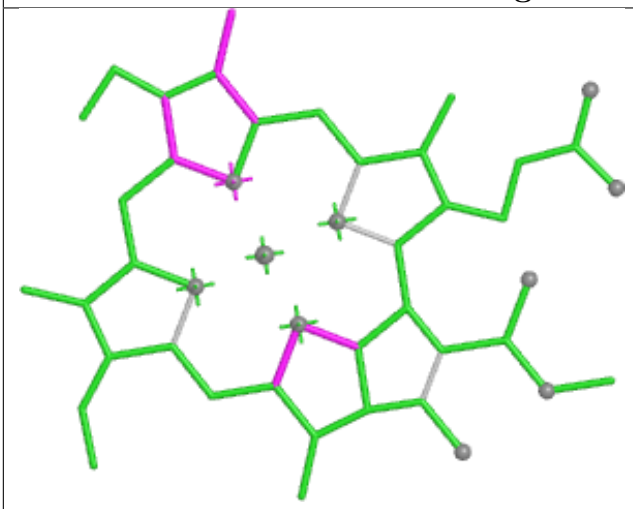


Torsions

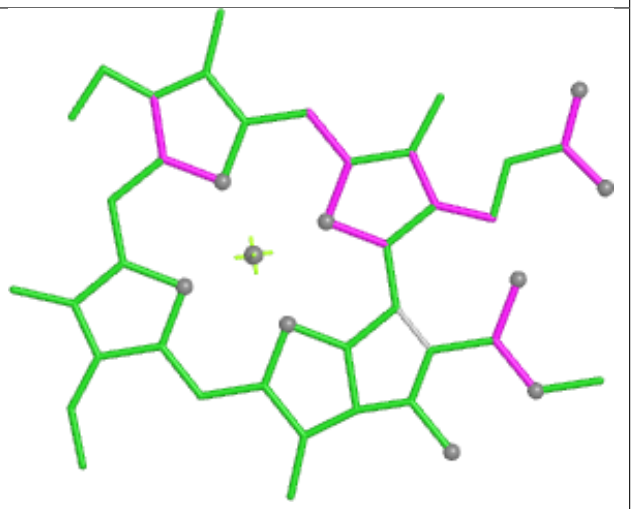


Rings

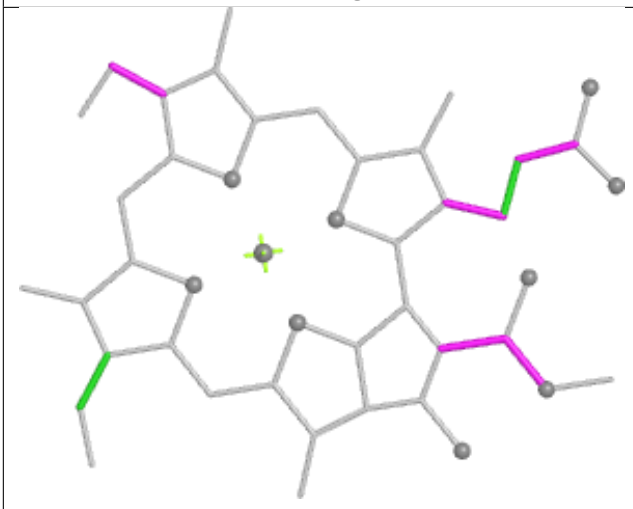
Ligand CLA 1N 605



Bond lengths



Bond angles

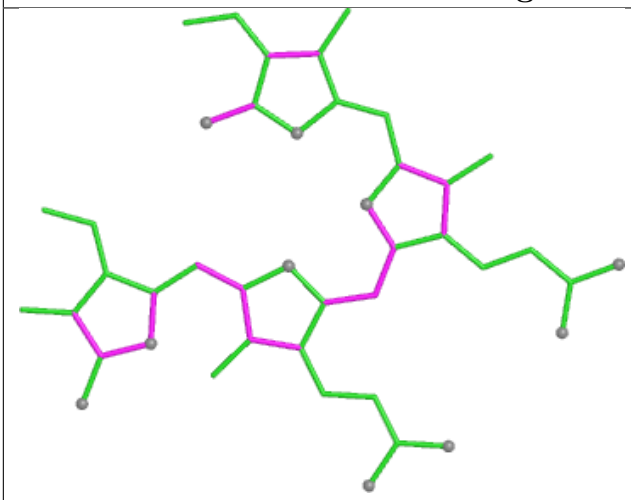


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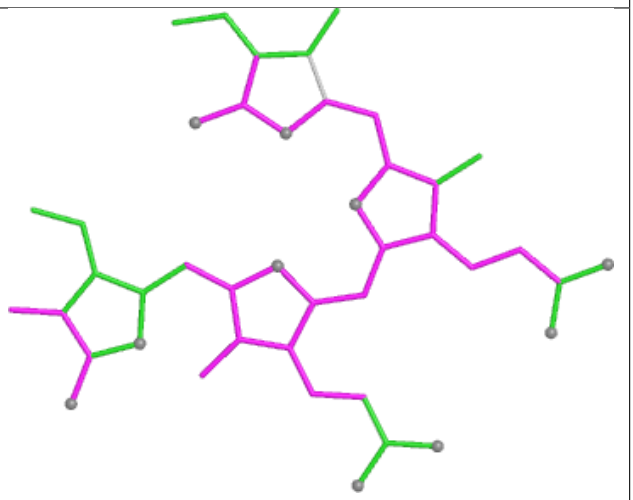


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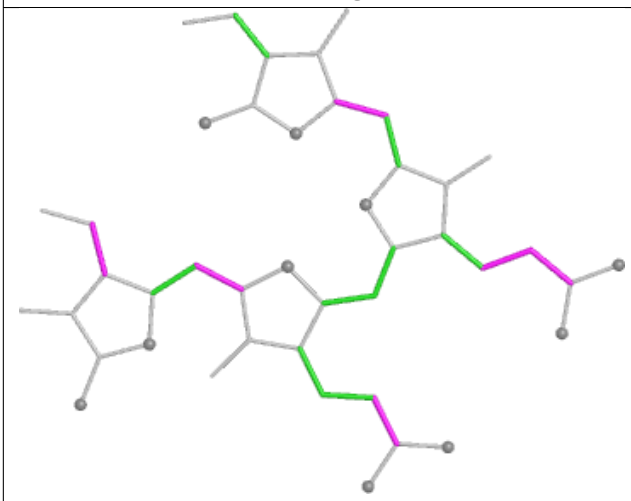
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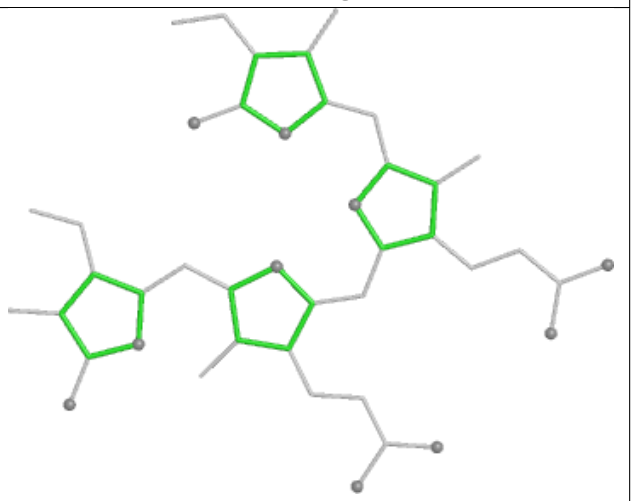
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Bond angles

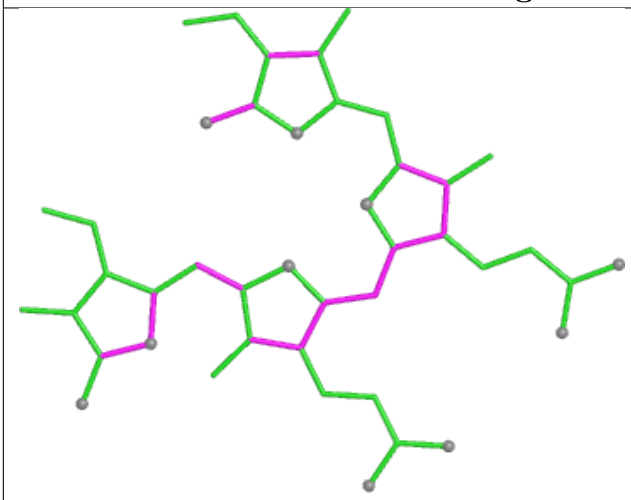


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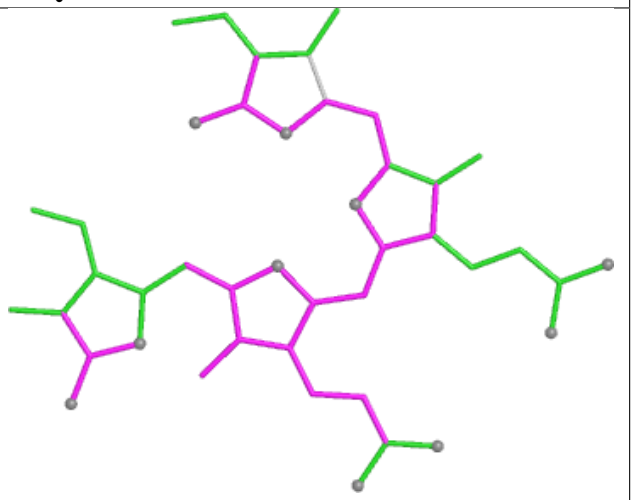


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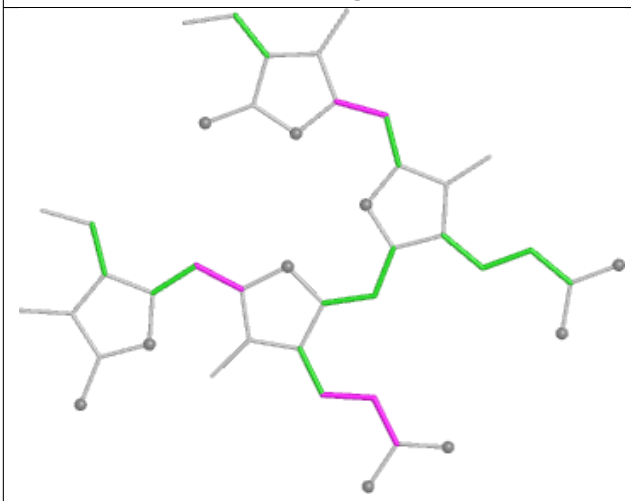
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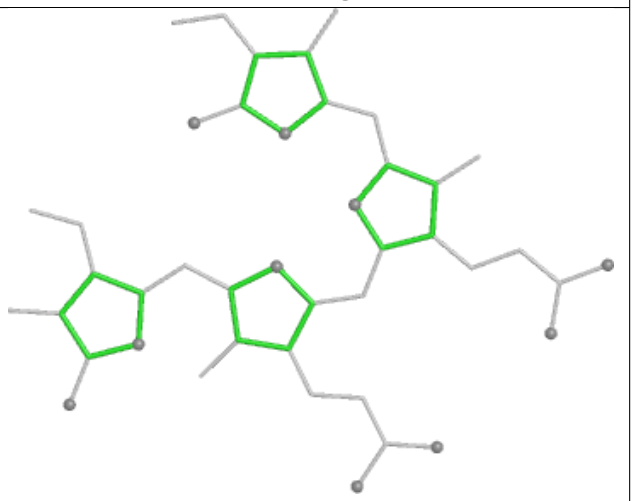
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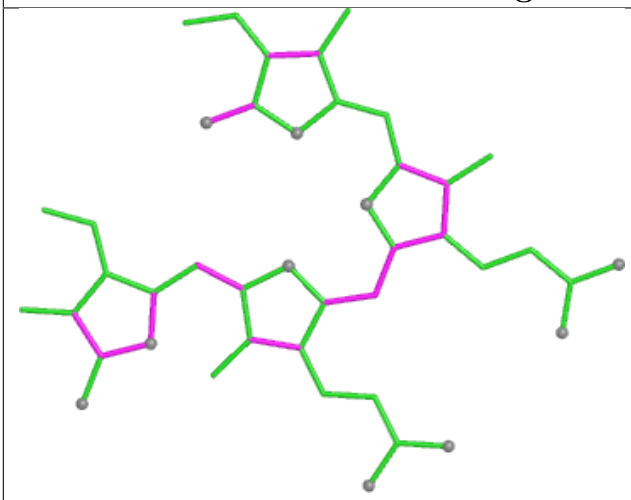


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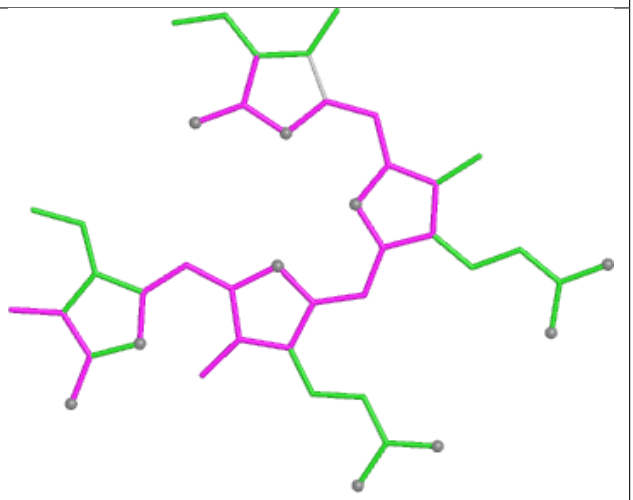


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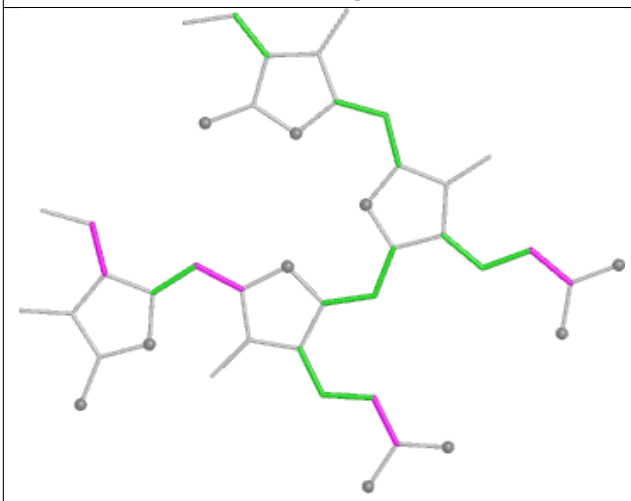
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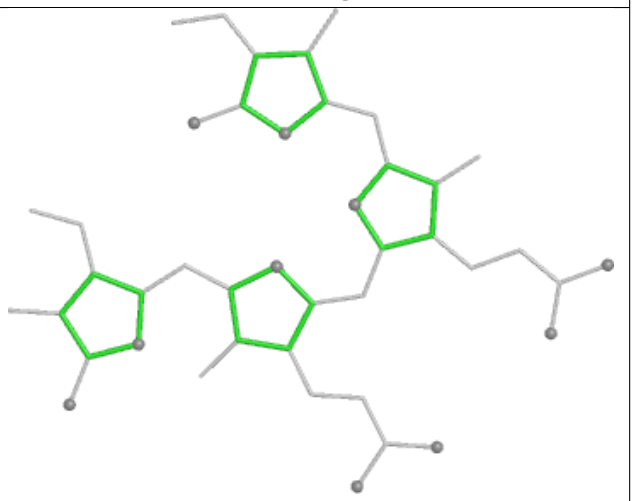
Bond lengths



Bond angles

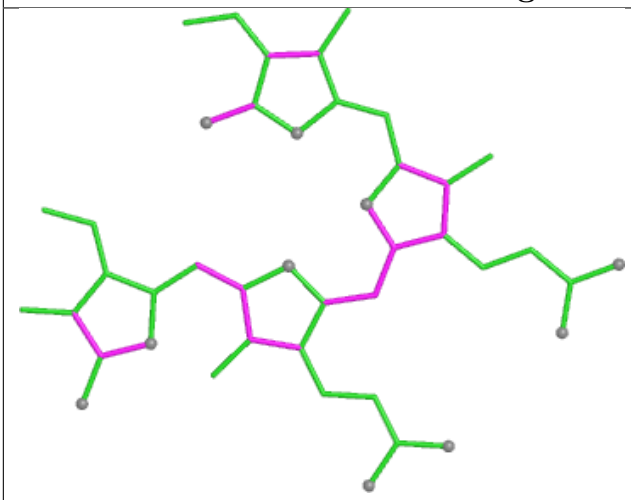


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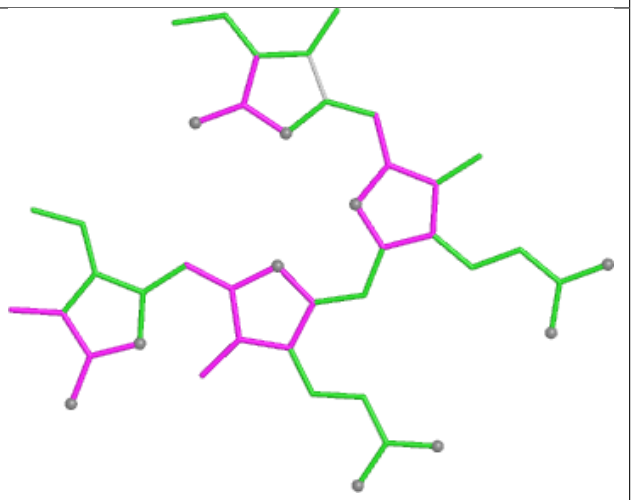


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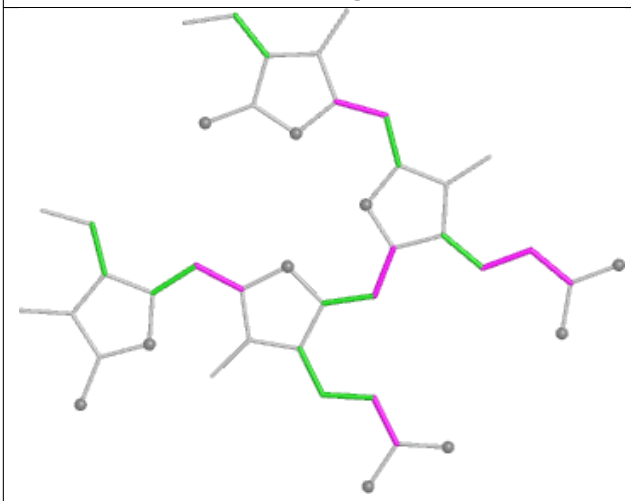
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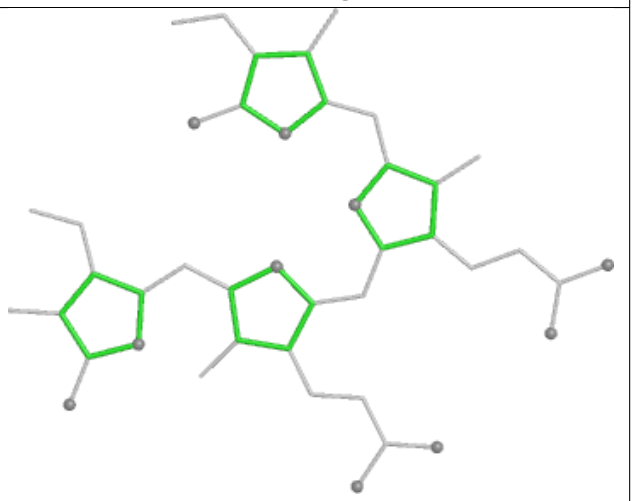
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Bond angles

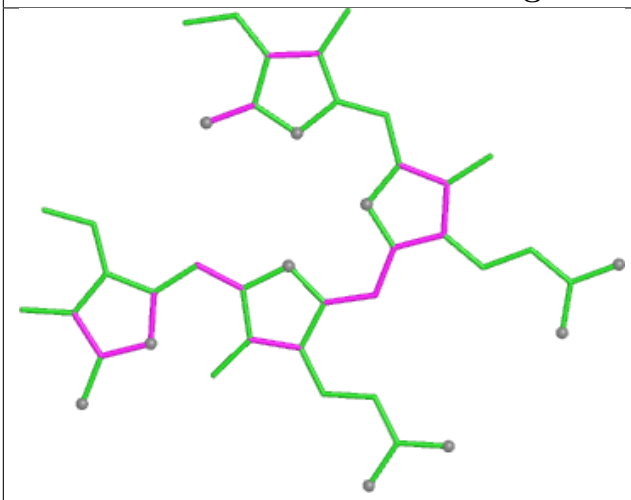


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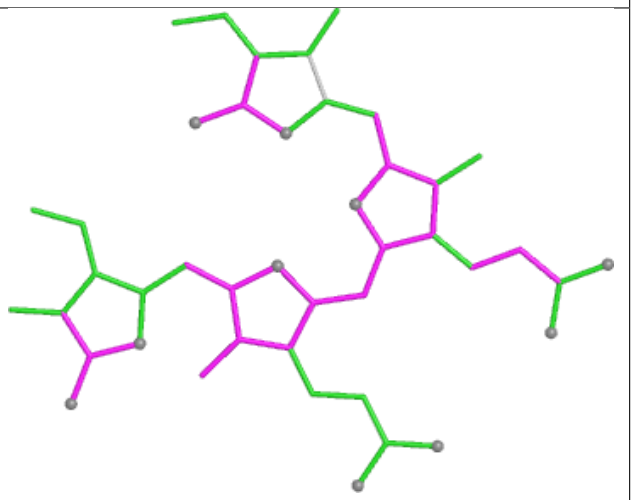


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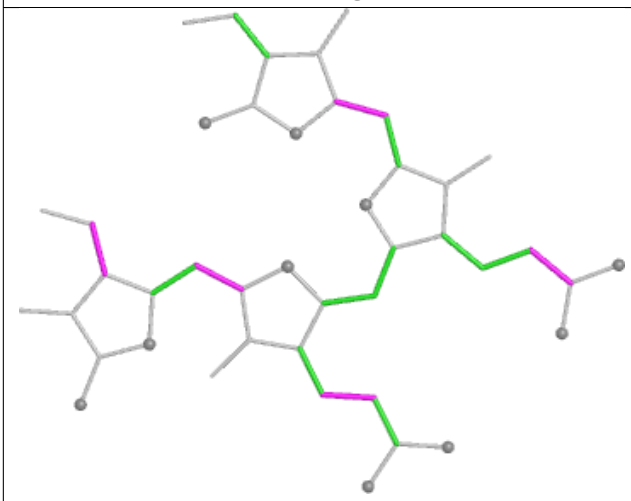
Ligand PEB i4 202



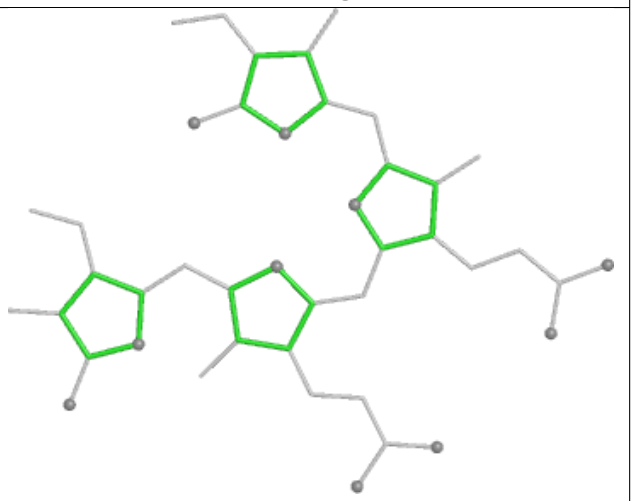
Bond lengths



Bond angles

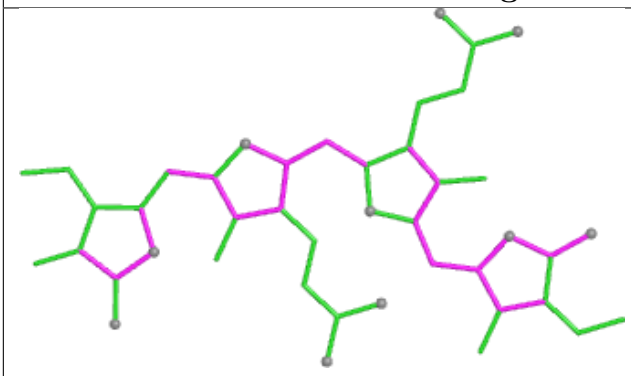


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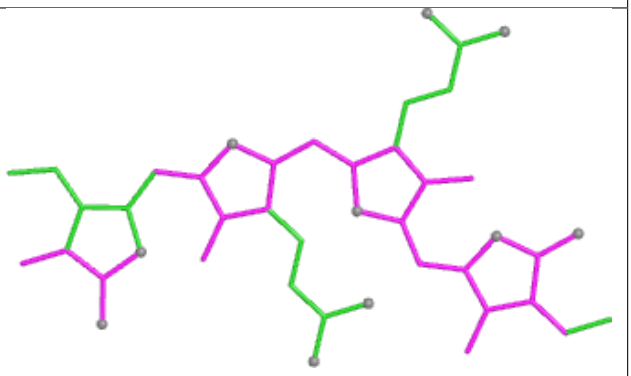


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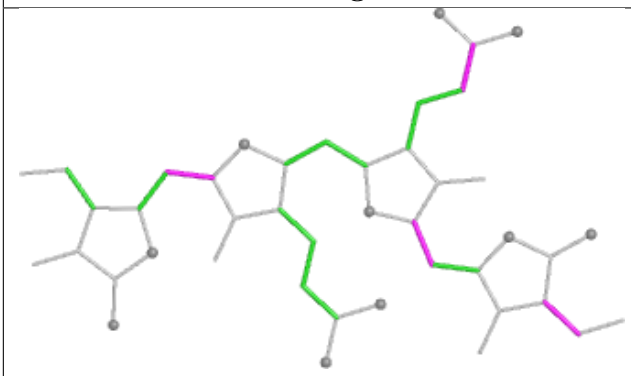
Ligand CYC EG 1001



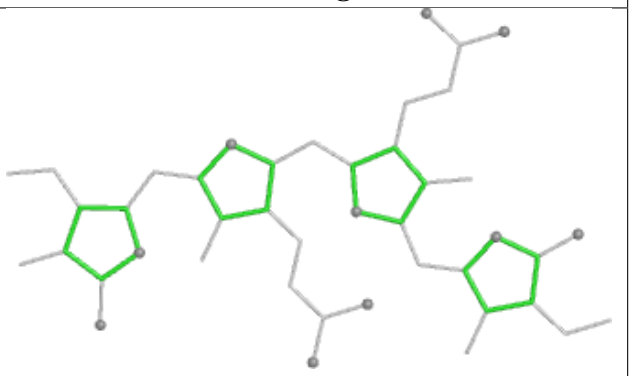
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Bond angles

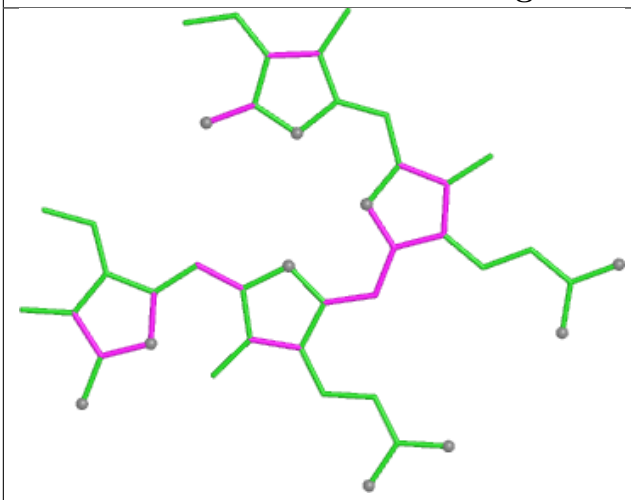


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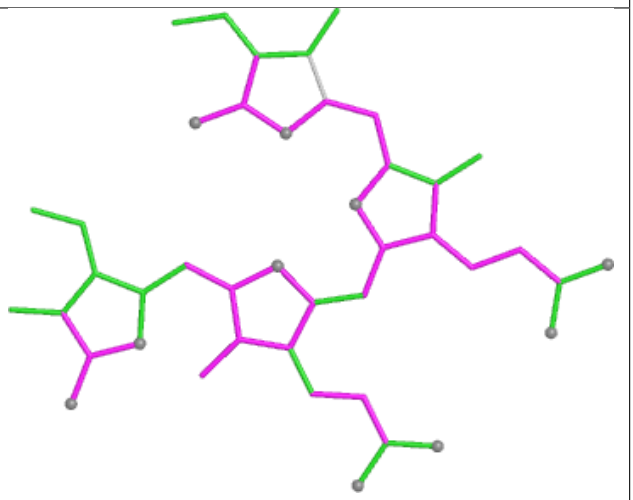


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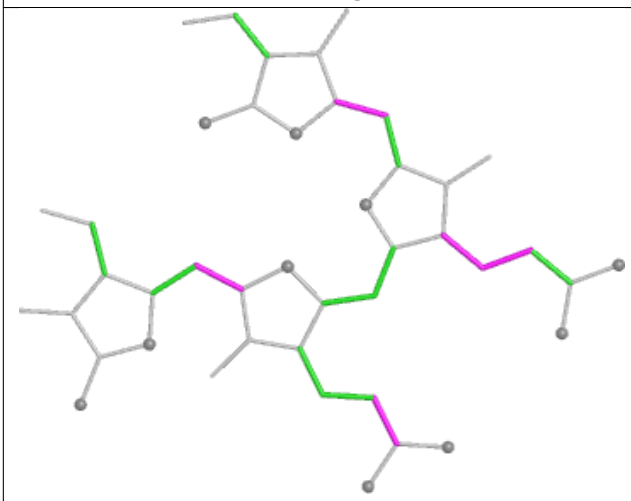
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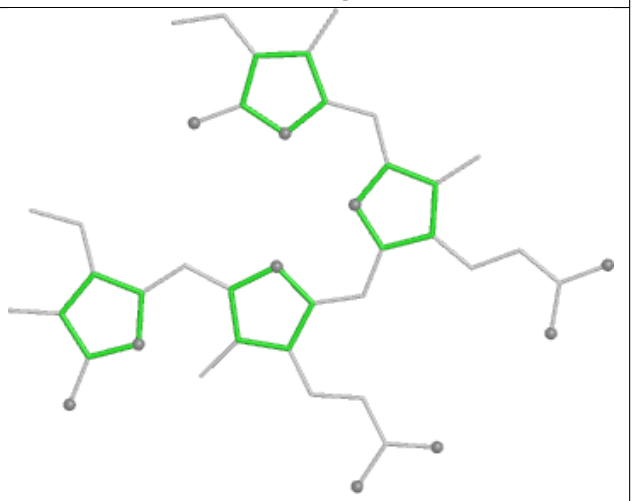
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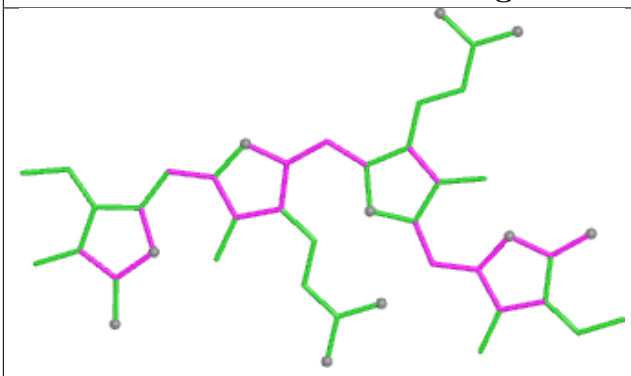


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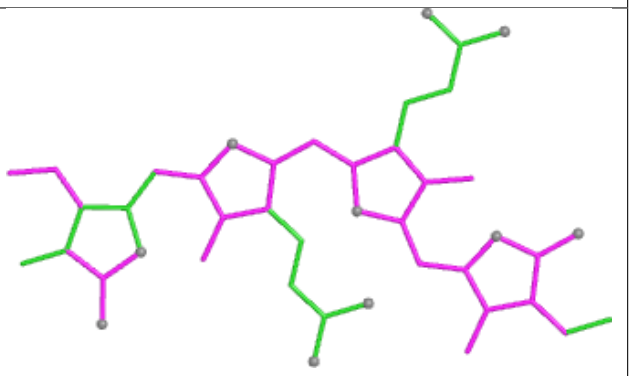


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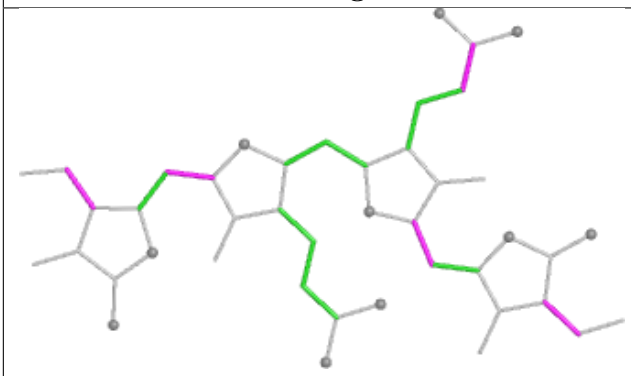
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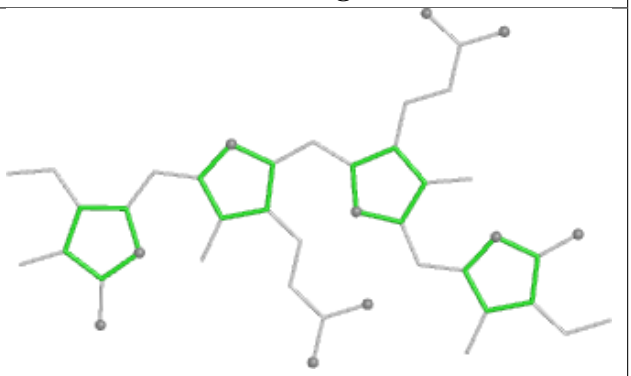
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Bond angles

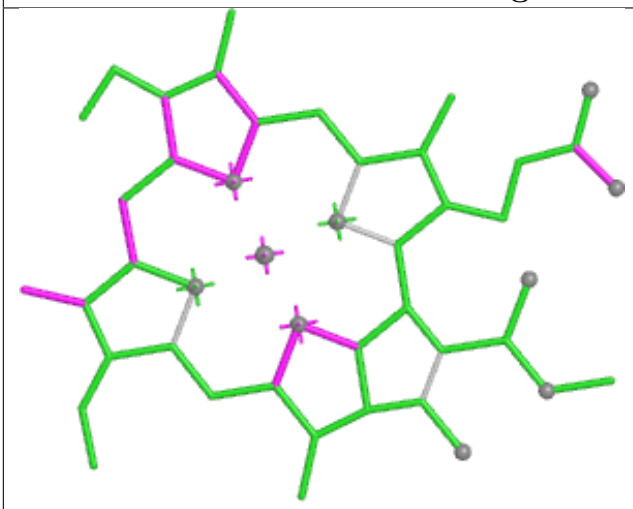


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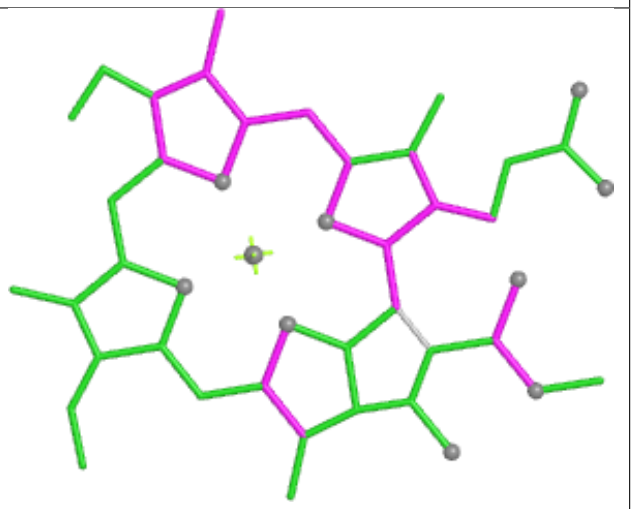


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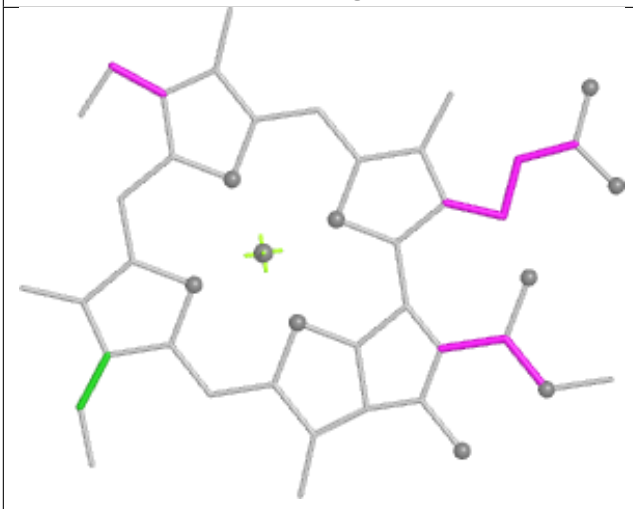
Ligand CLA M2 101



Bond lengths



Bond angles

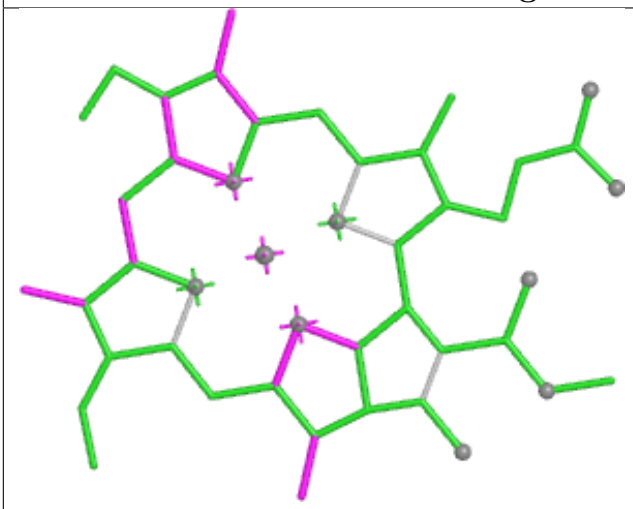


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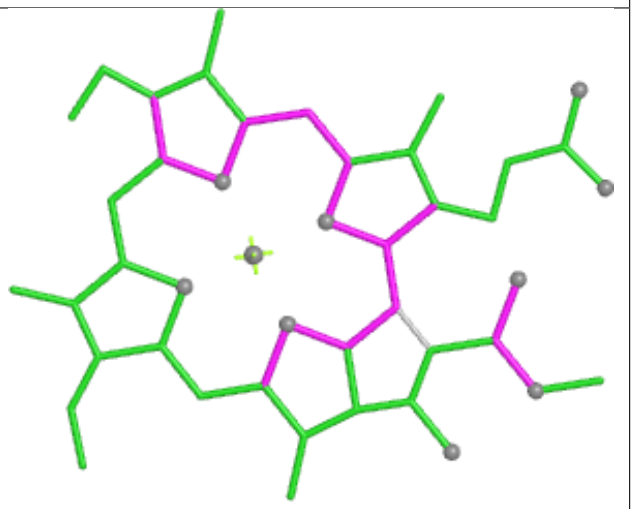


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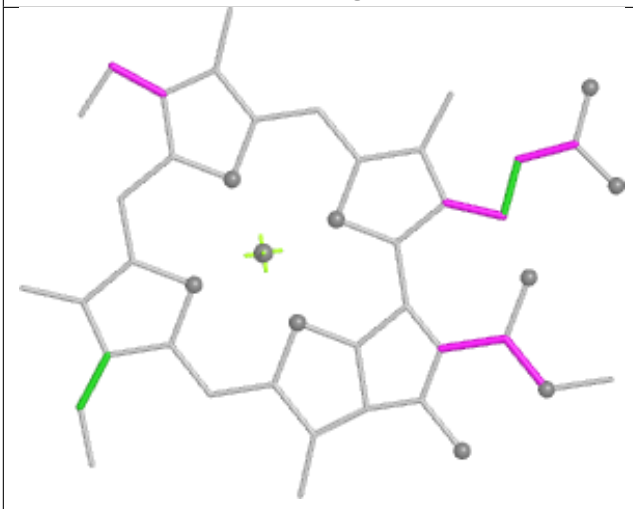
Ligand CLA 82 301



Bond lengths



Bond angles

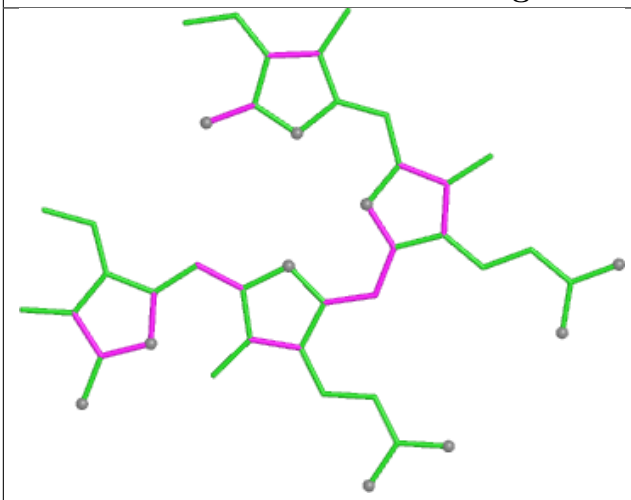


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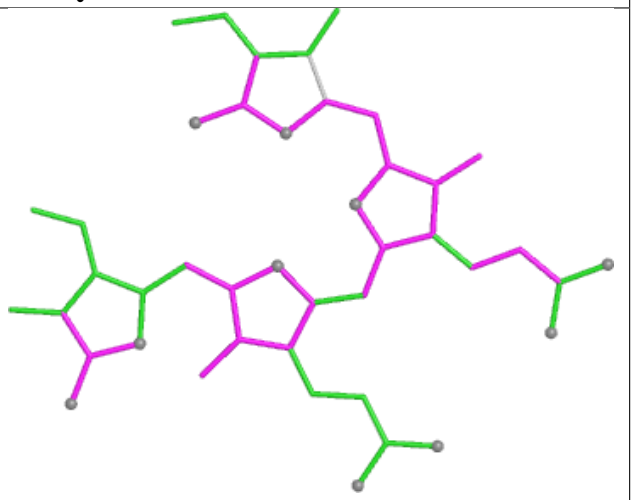


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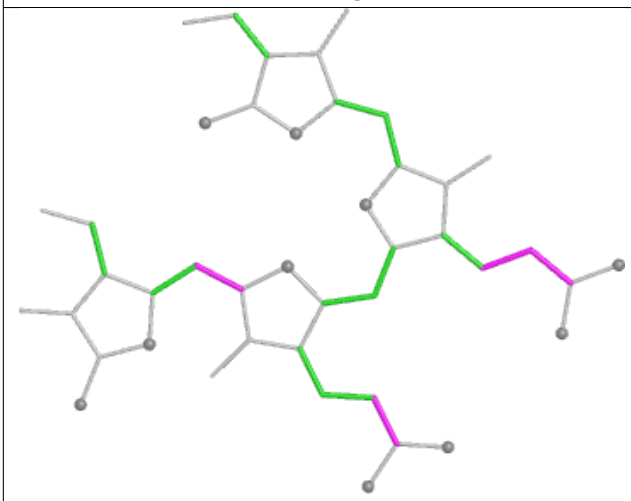
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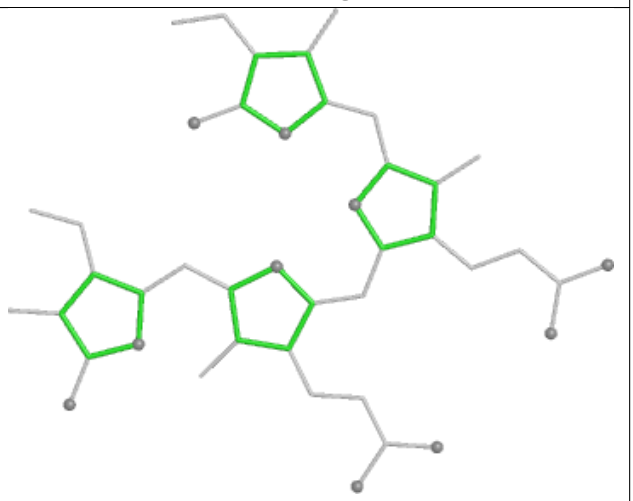
Bond lengths



Bond angles

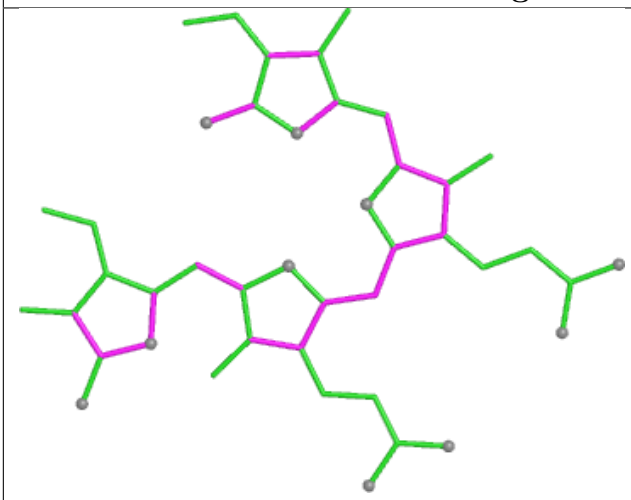


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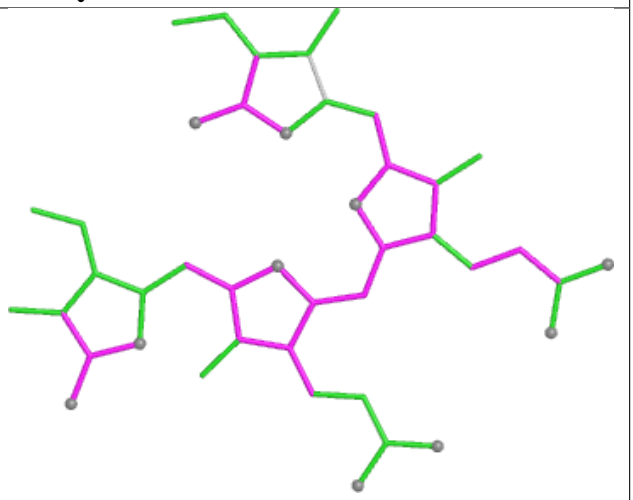


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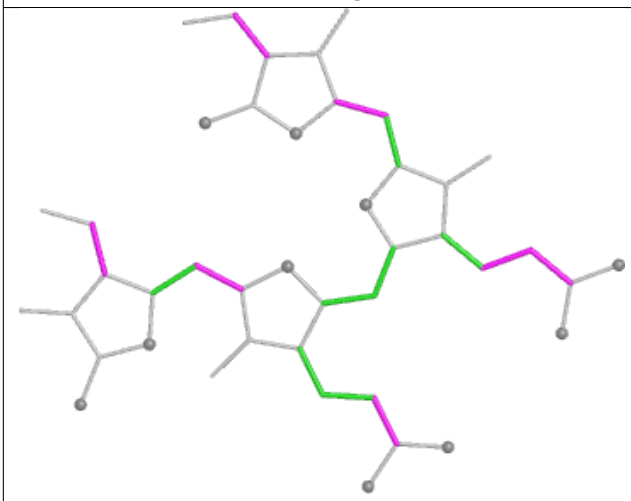
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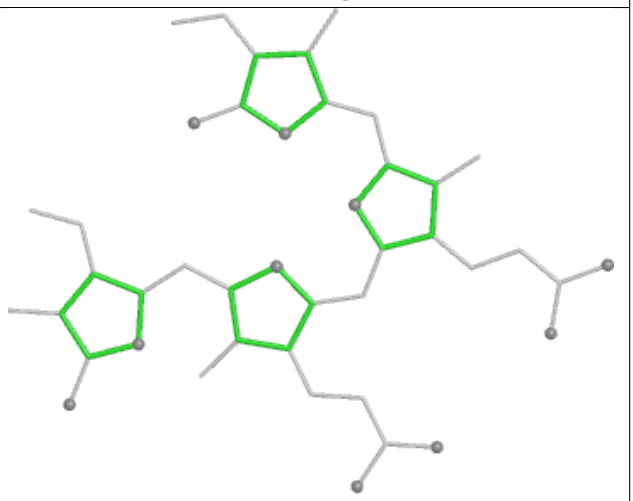
Bond lengths



Bond angles

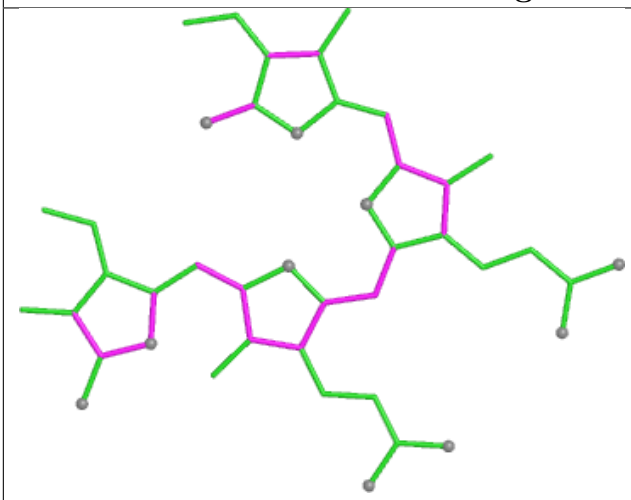


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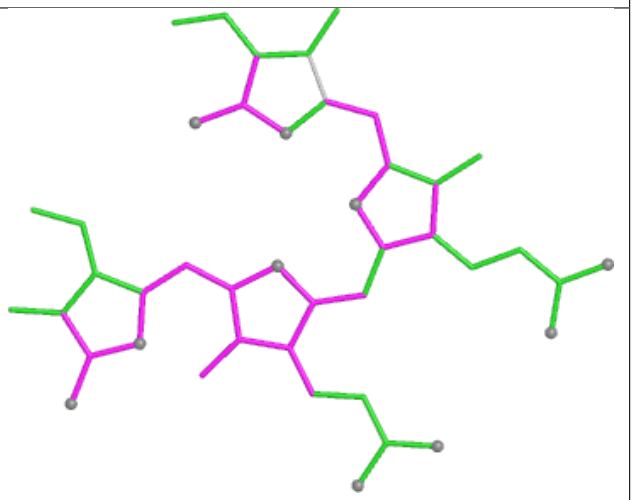


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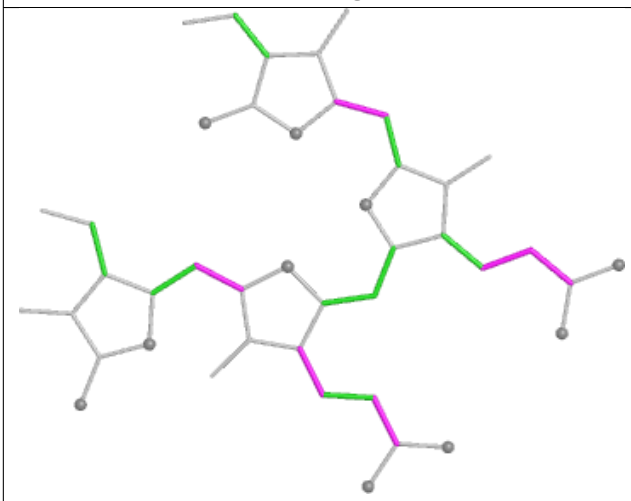
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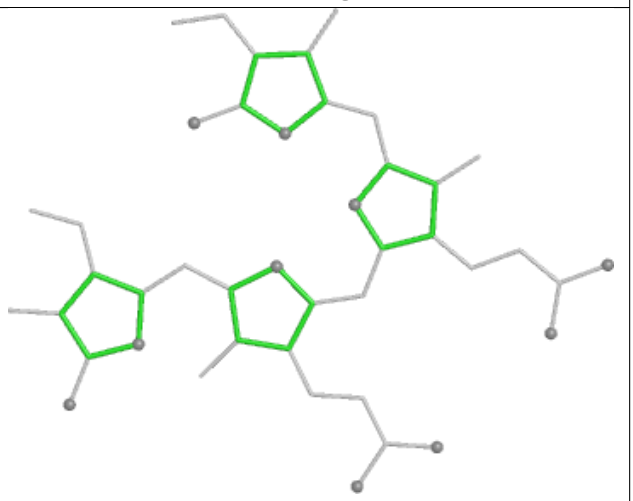
Bond lengths



Bond angles

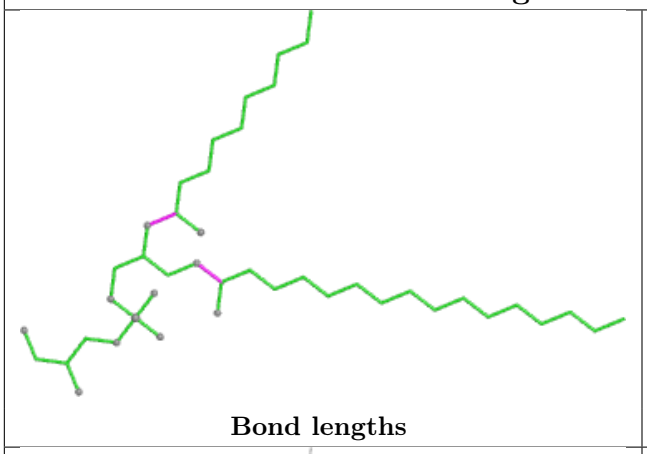


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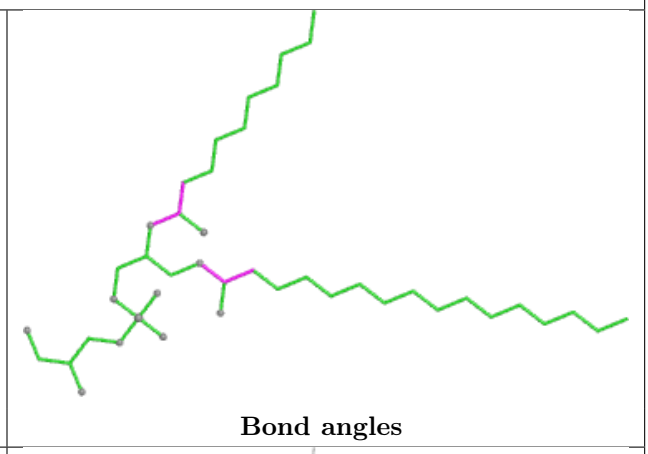


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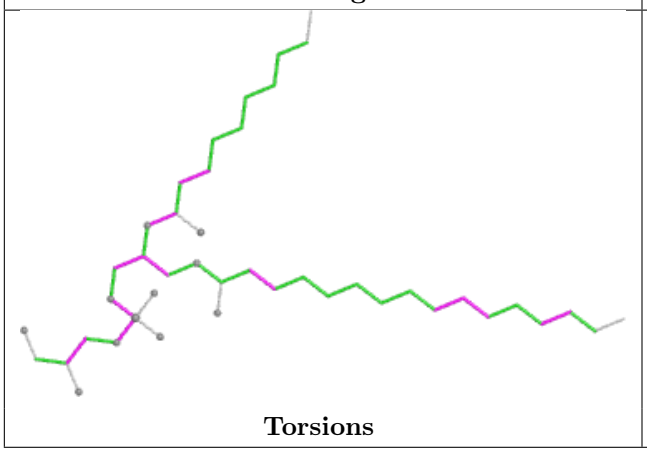
Ligand LHG AL 407



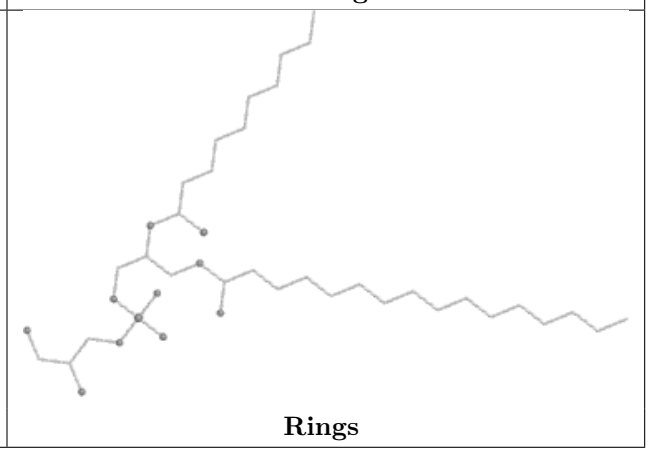
Bond lengths



Bond angles

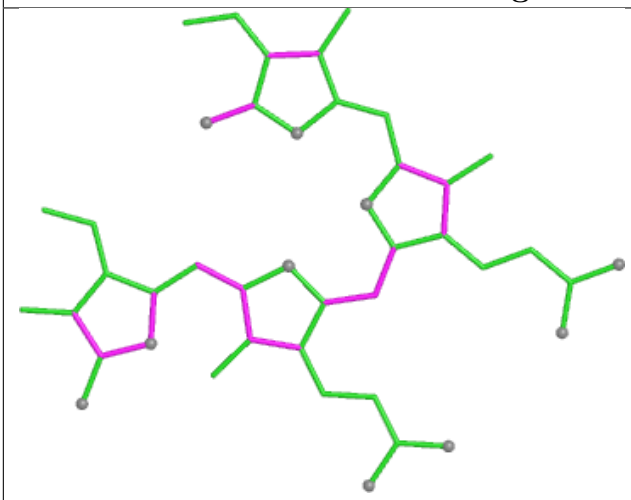


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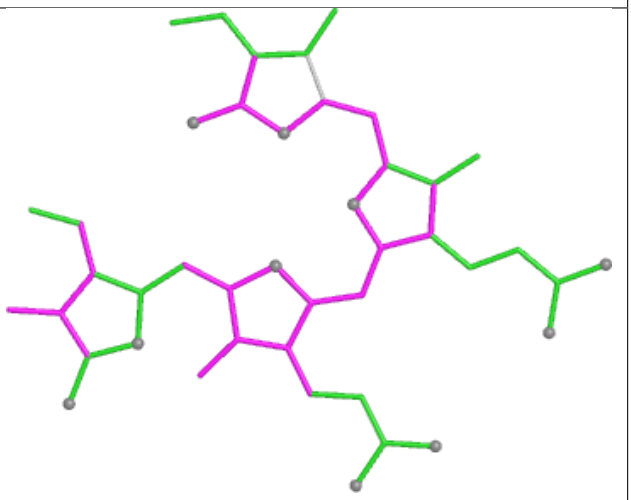


Rings

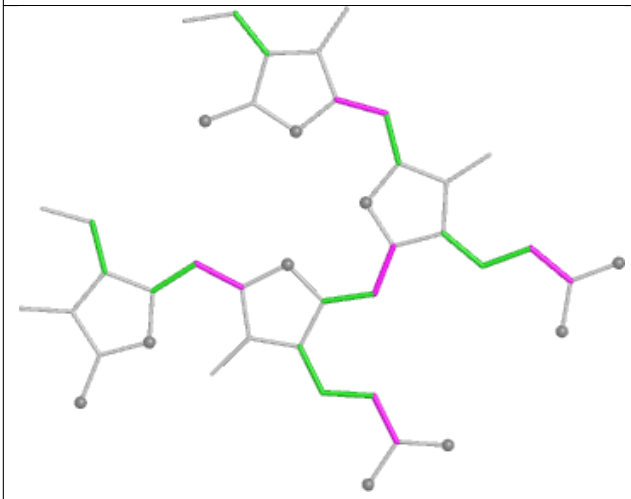
Ligand PEB PD 202



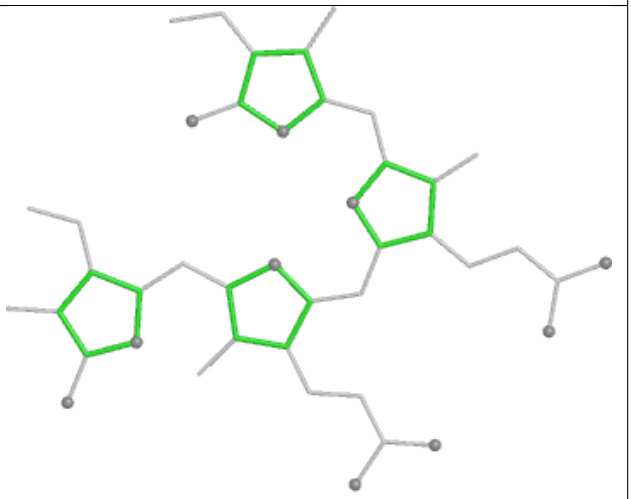
Bond lengths



Bond angles

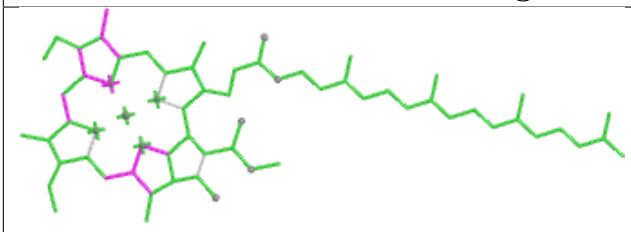


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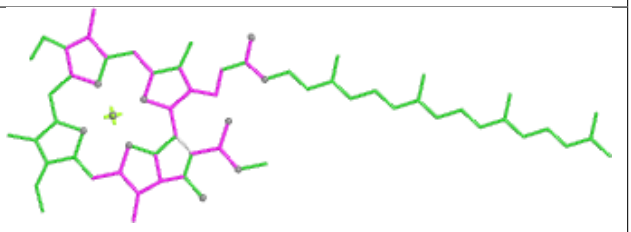


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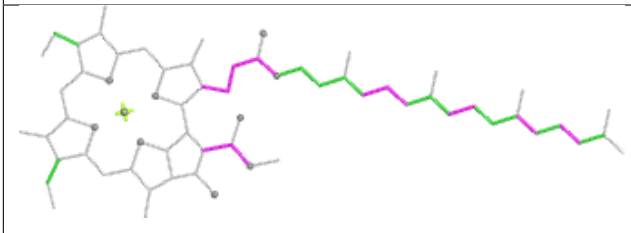
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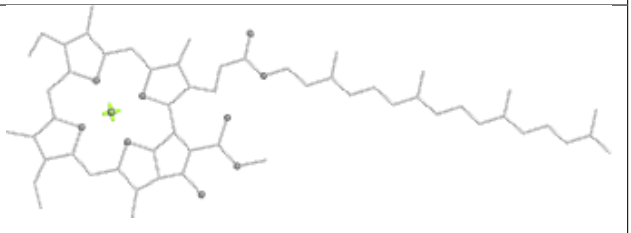
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Bond angles

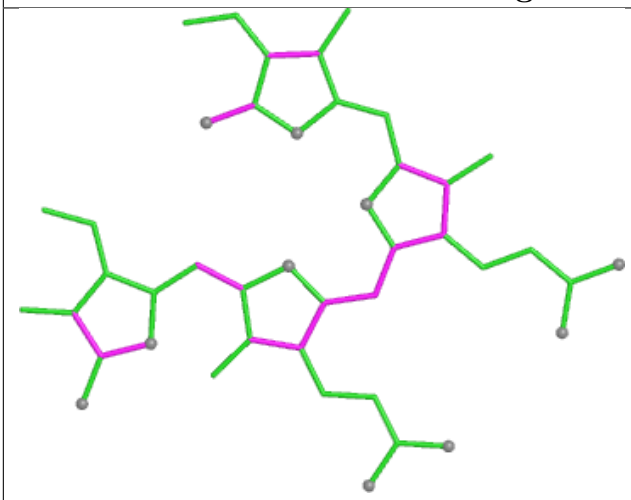


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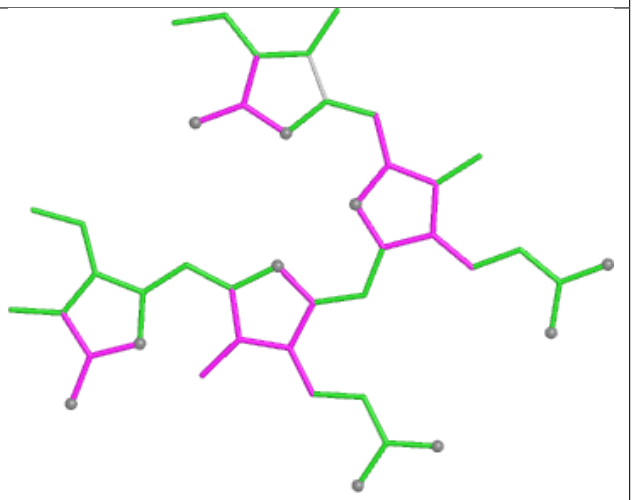


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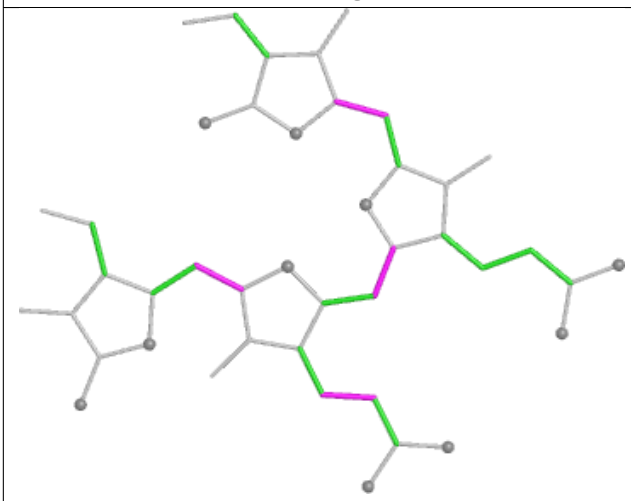
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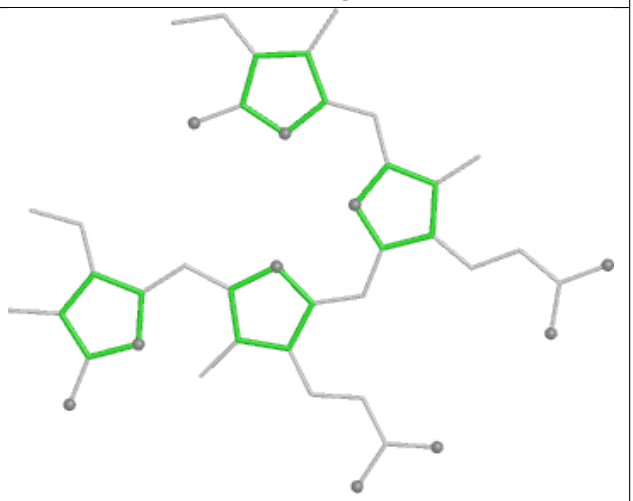
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Bond angles

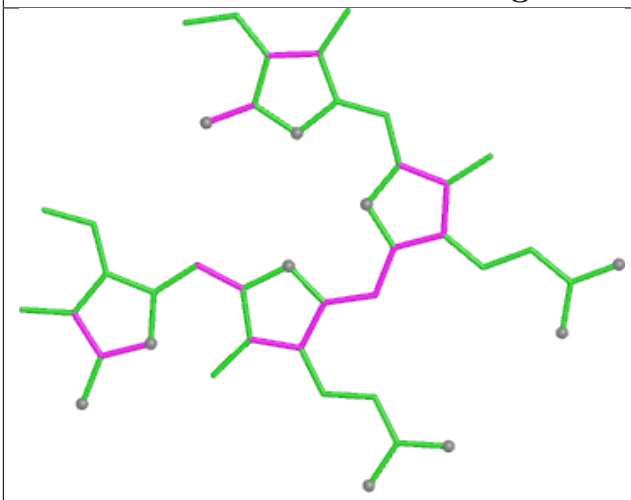


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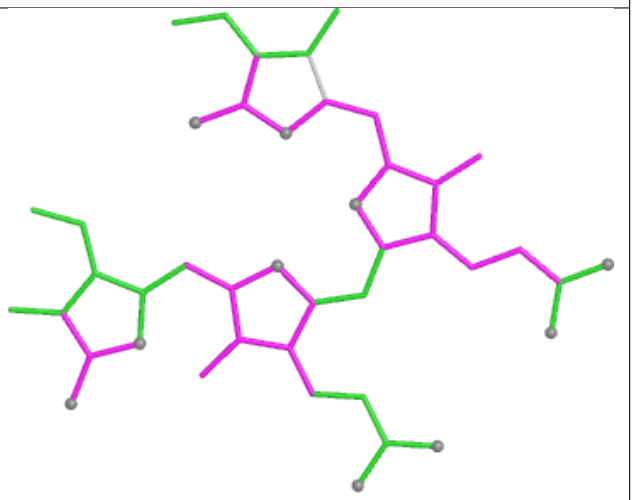


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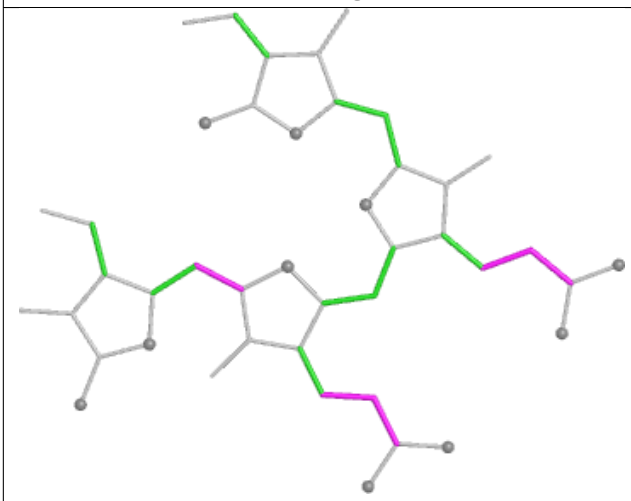
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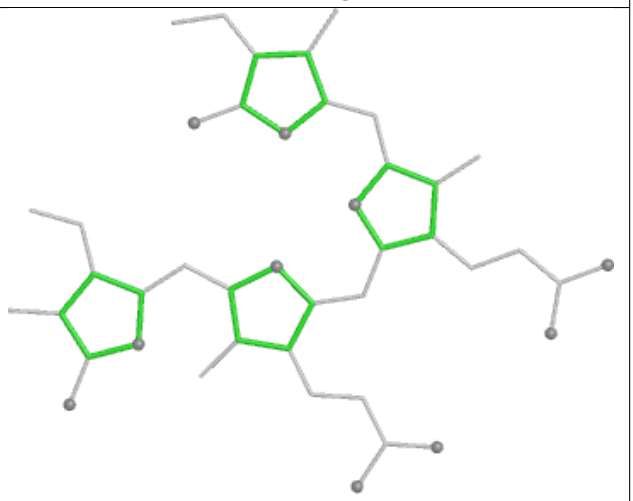
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Bond angles

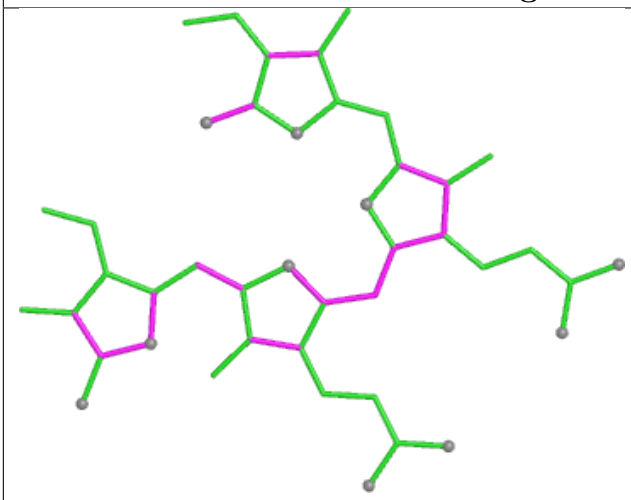


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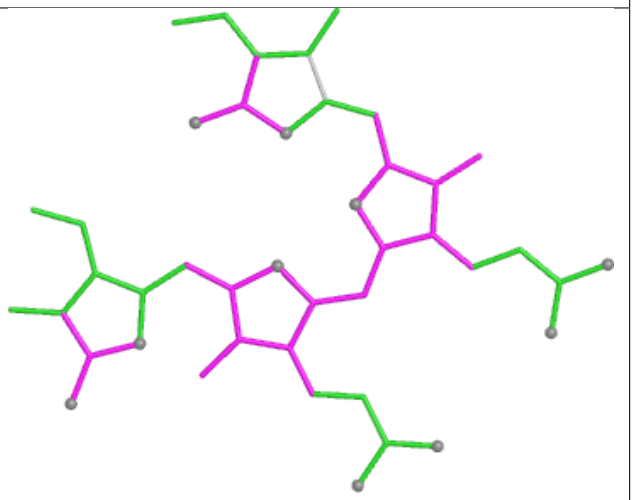


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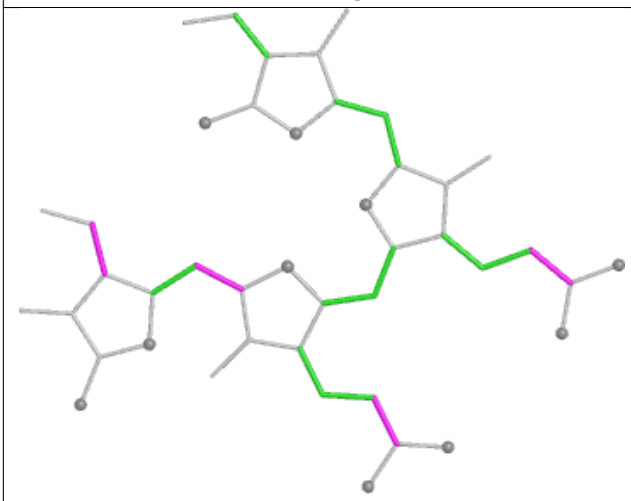
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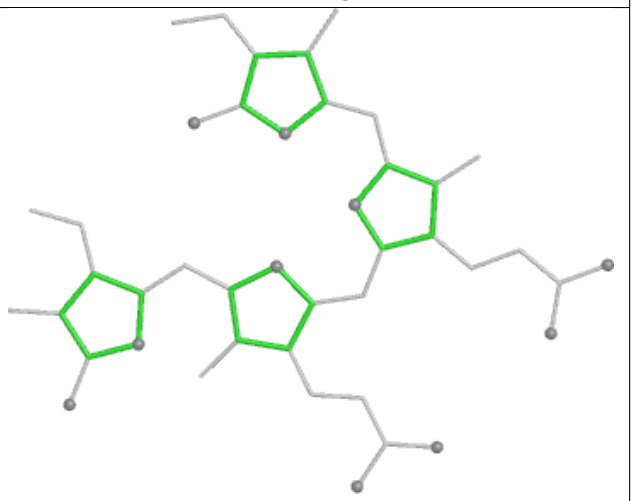
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Bond angles

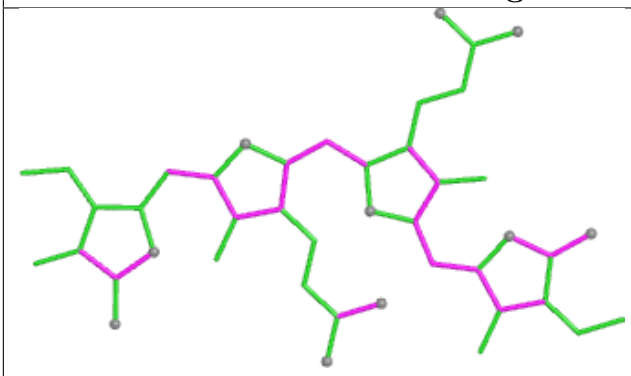


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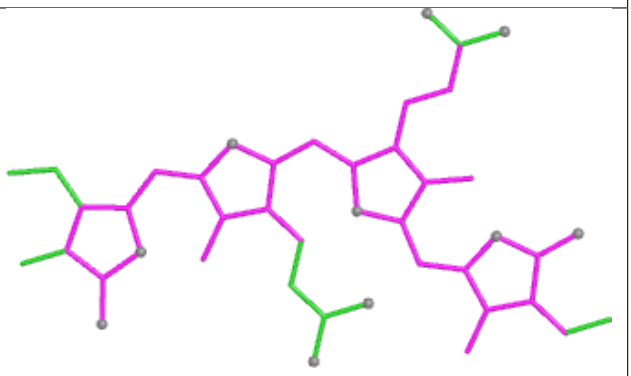


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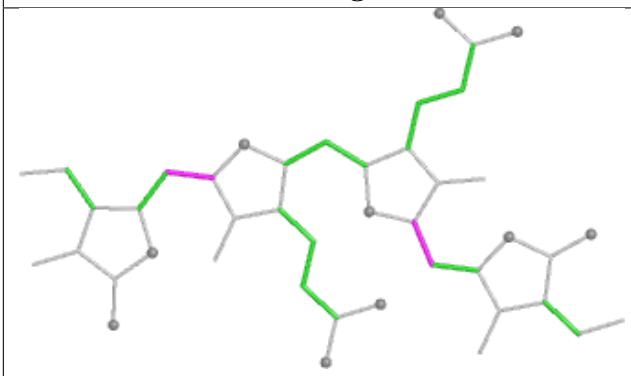
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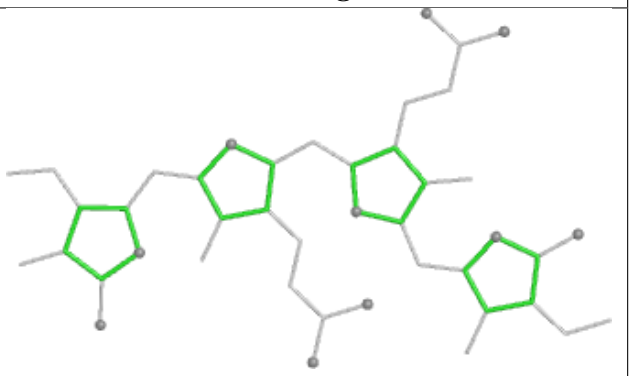
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Bond angles

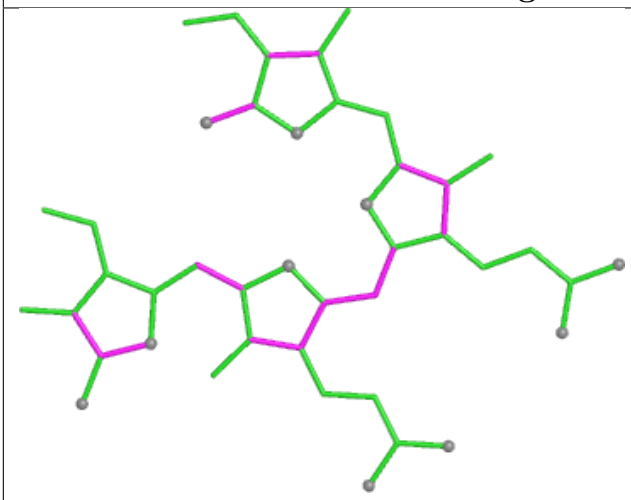


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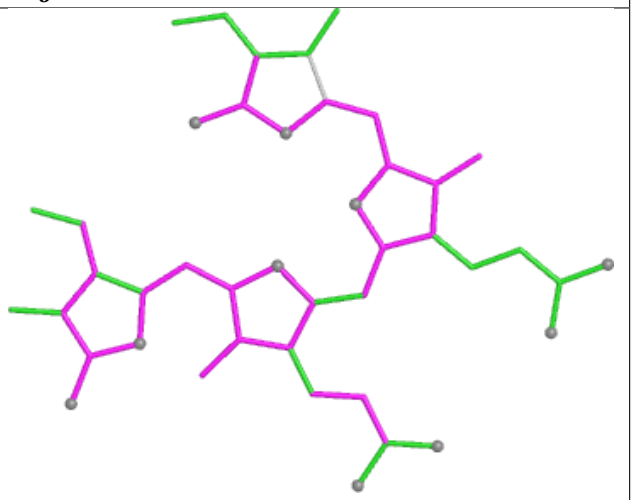


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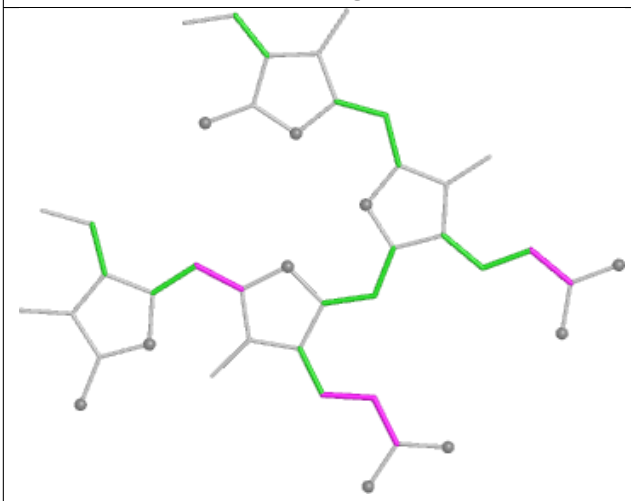
Ligand PEB jK 201



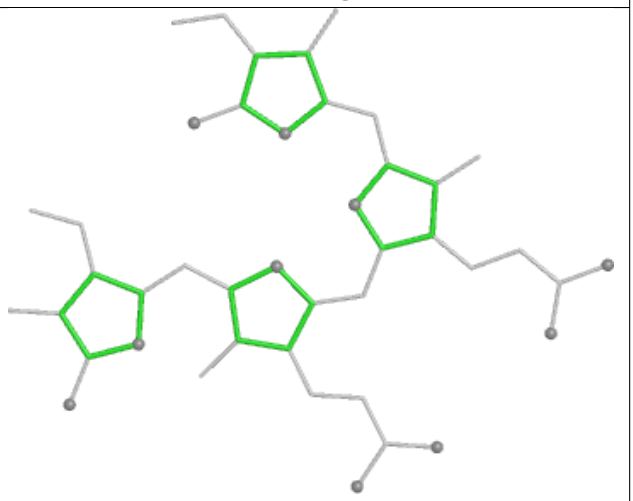
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Bond angles

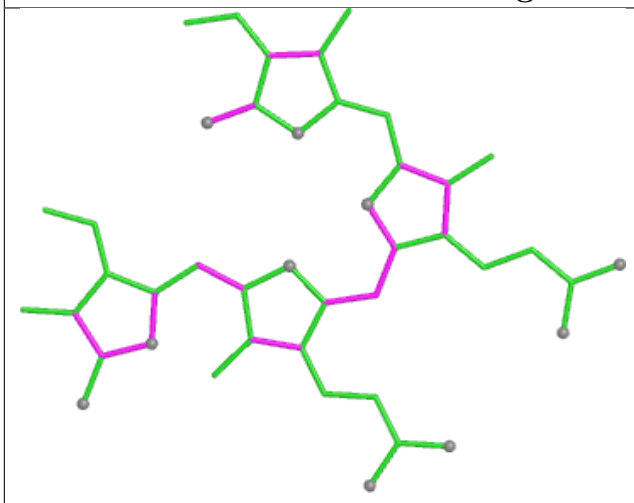


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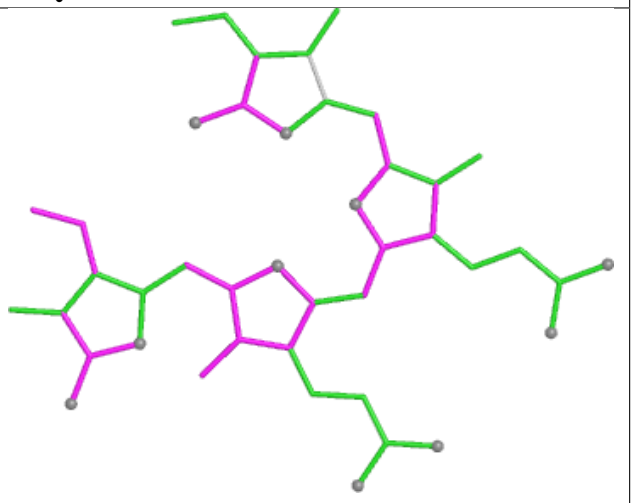


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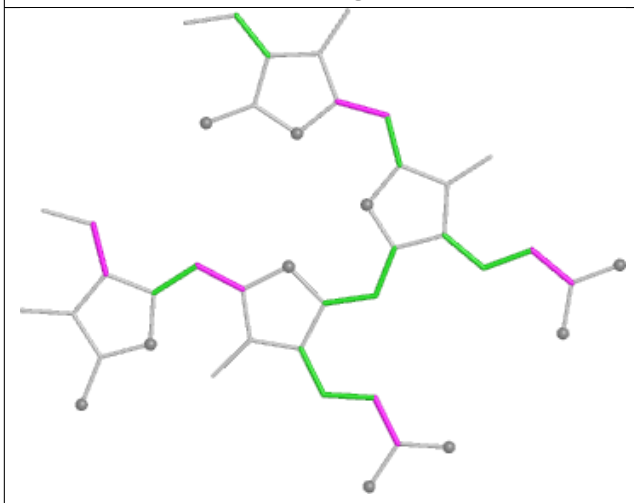
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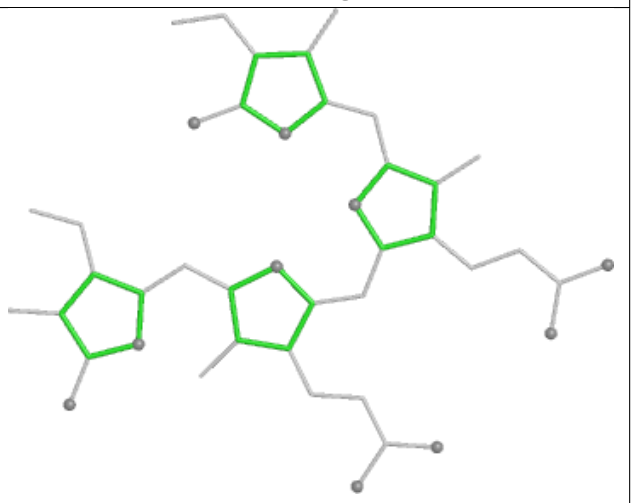
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Bond angles



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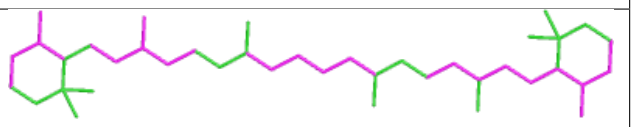


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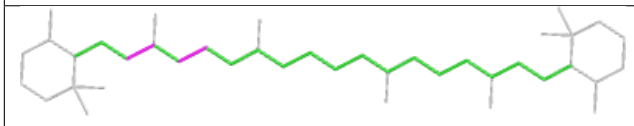
Ligand BCR h6 102



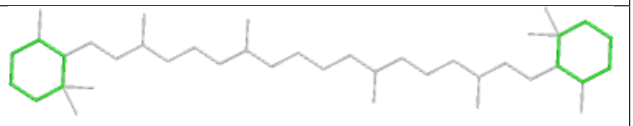
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Bond angles

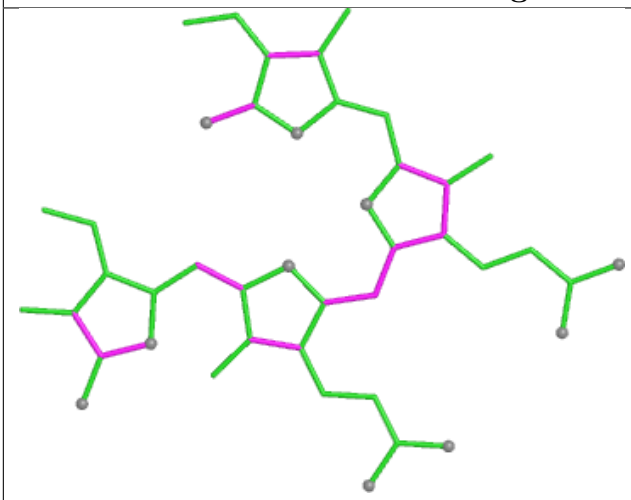


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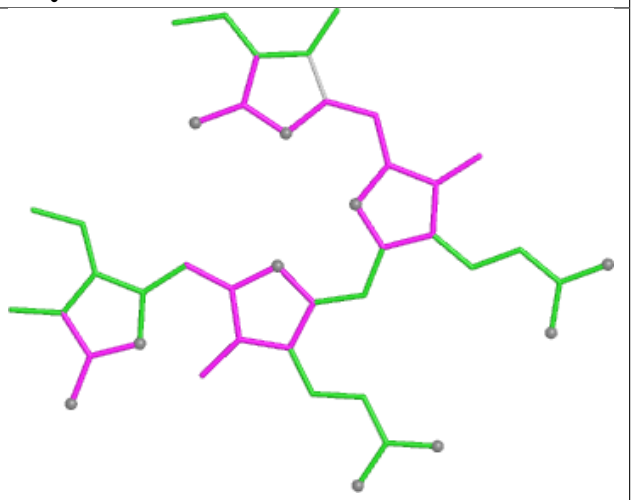


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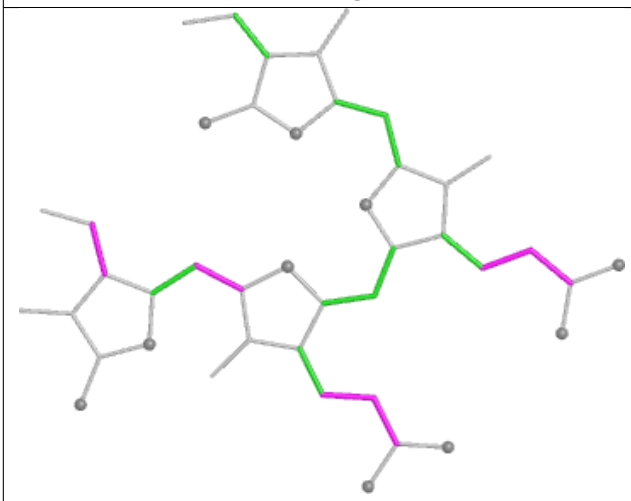
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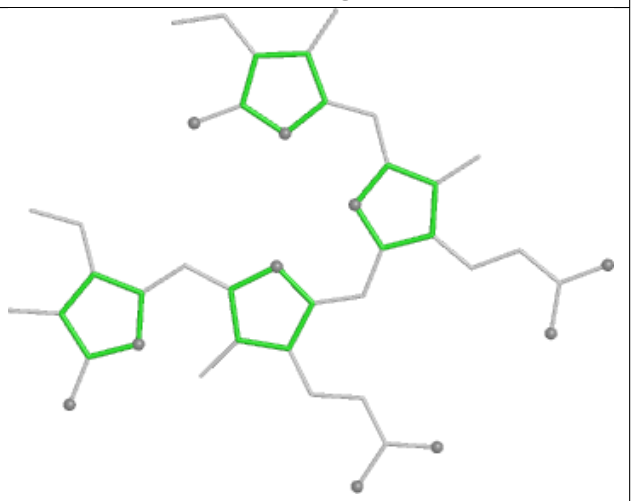
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Bond angles

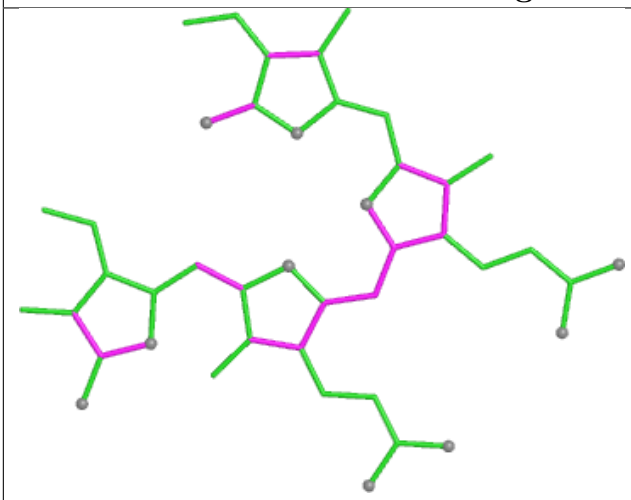


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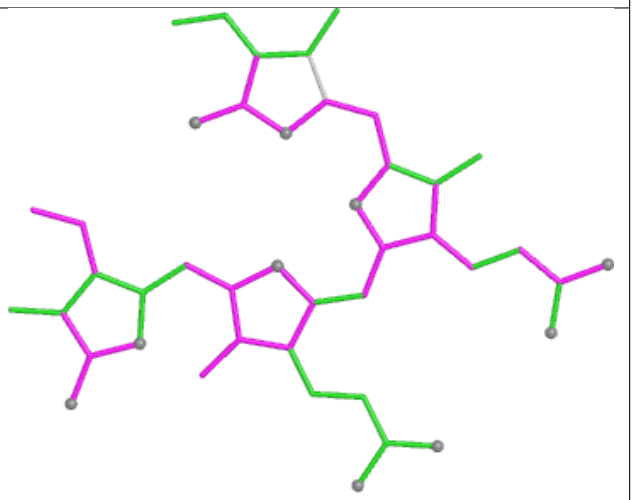


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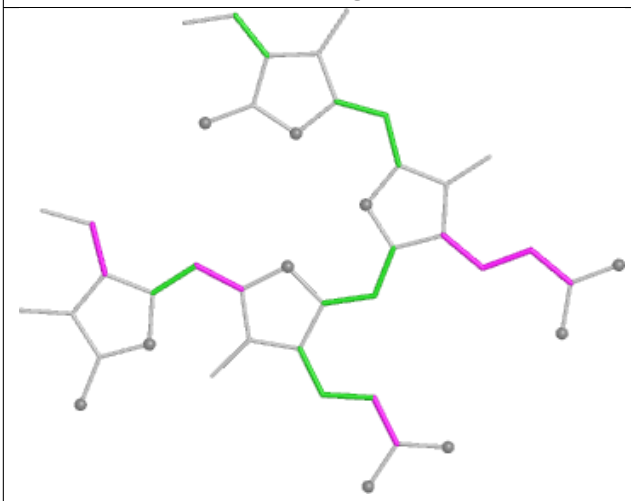
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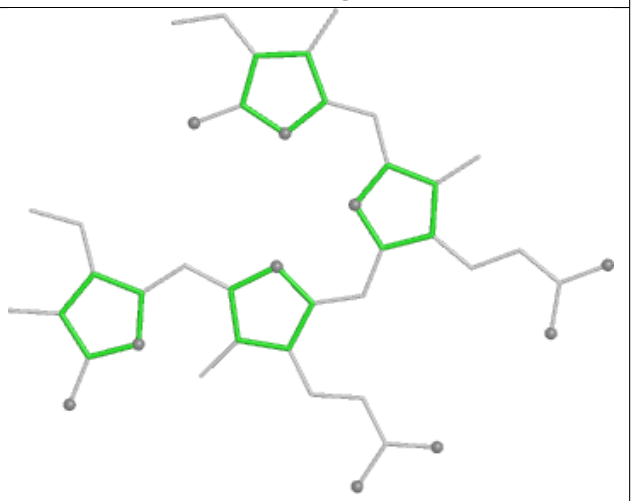
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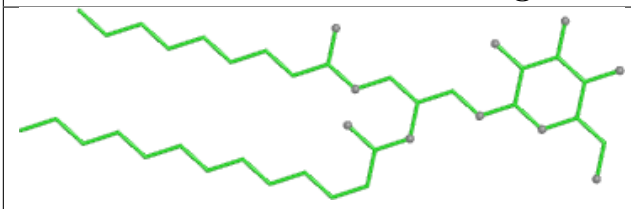


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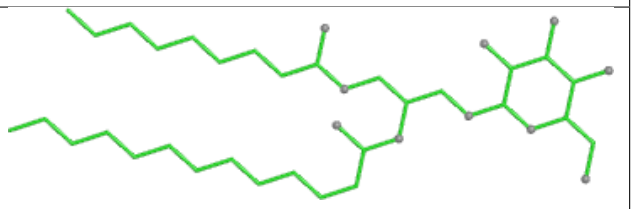


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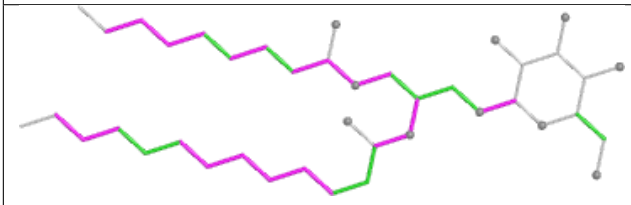
Ligand LMG b6 623



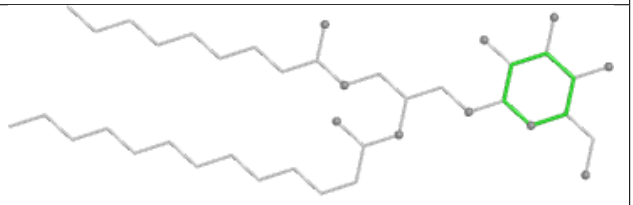
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Bond angles

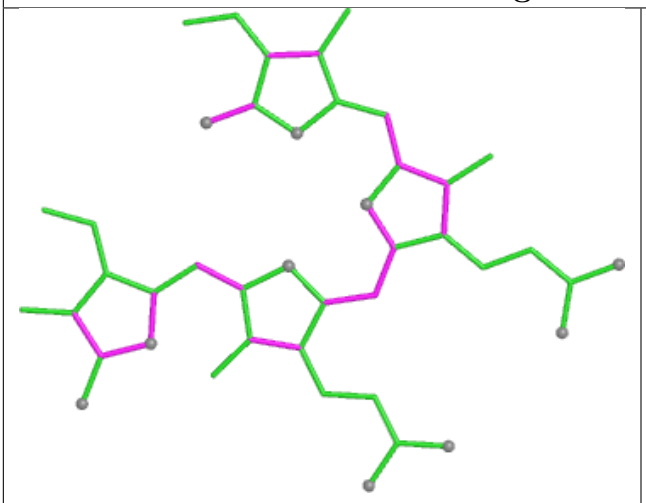


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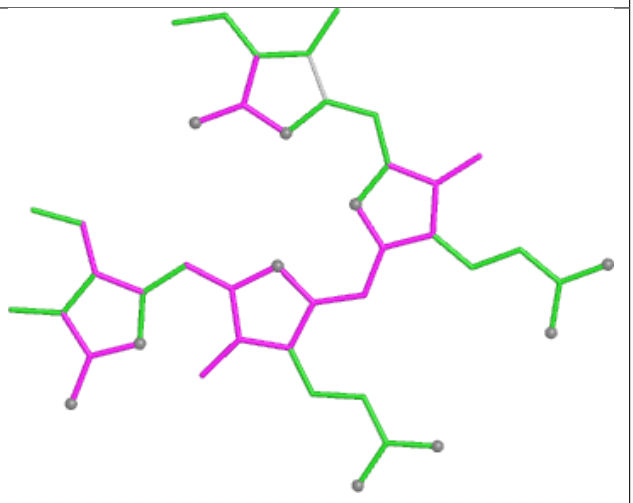


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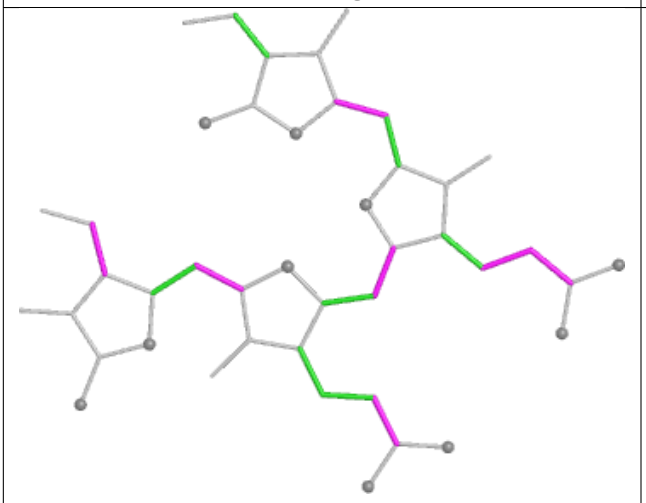
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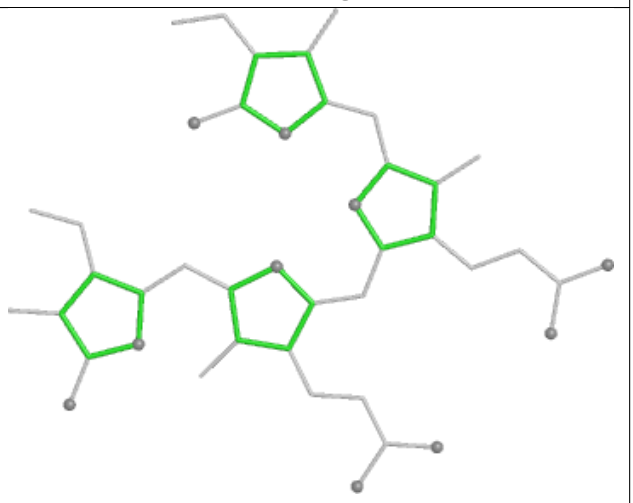
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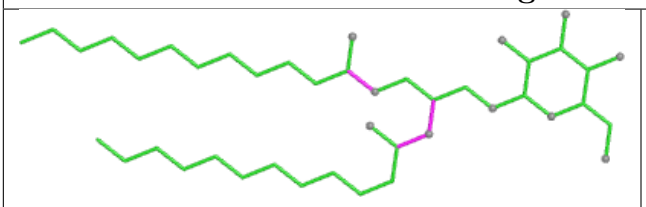


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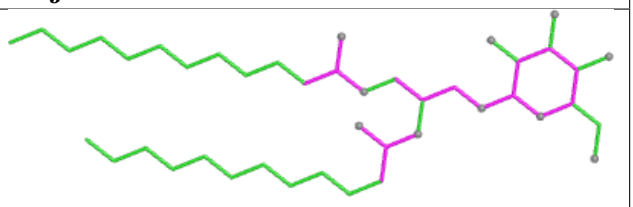


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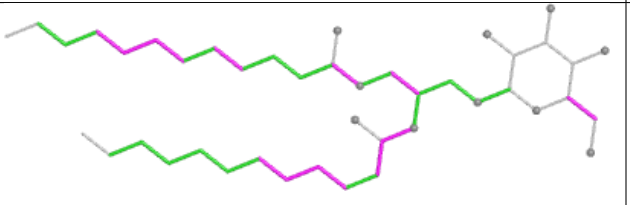
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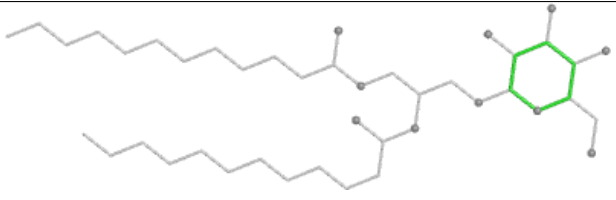
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Bond angles

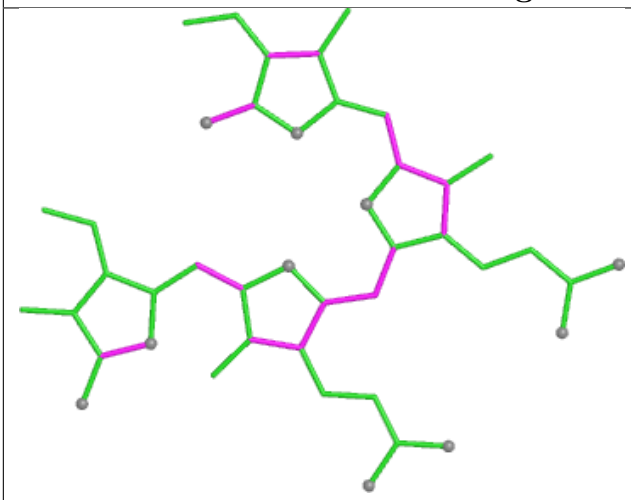


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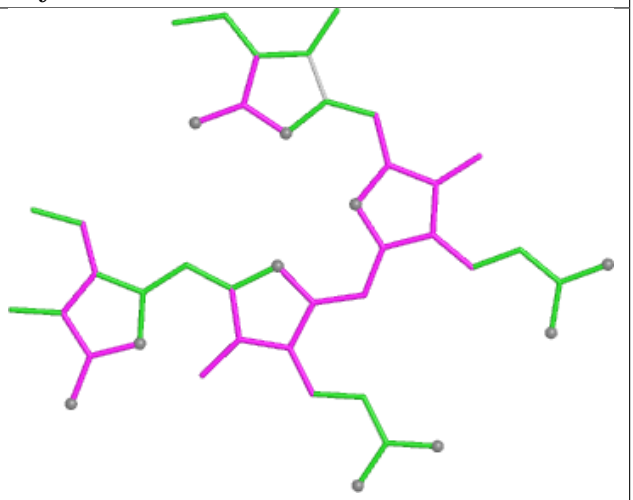


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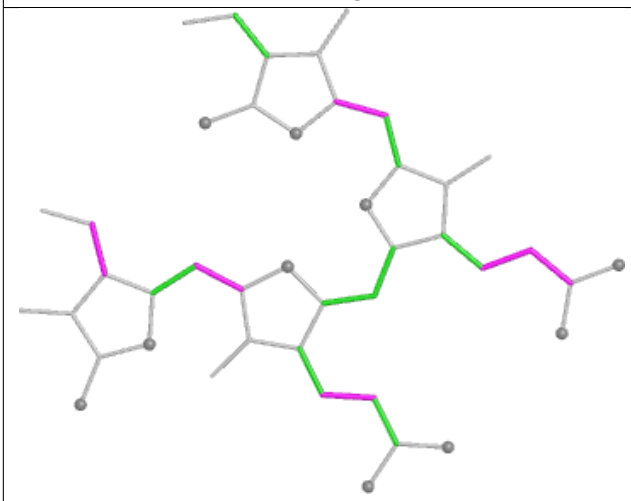
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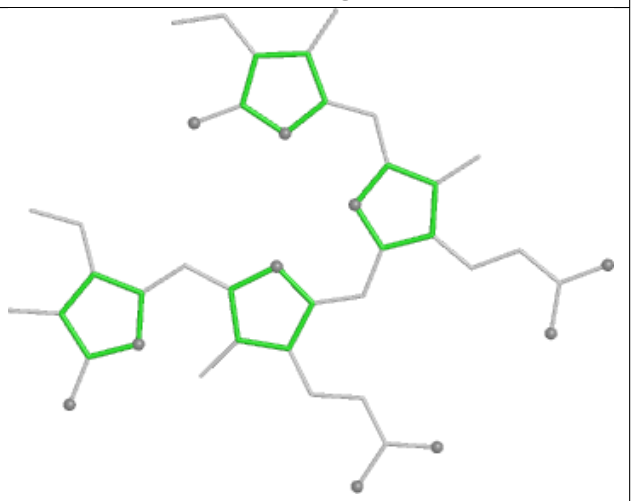
Bond lengths



Bond angles

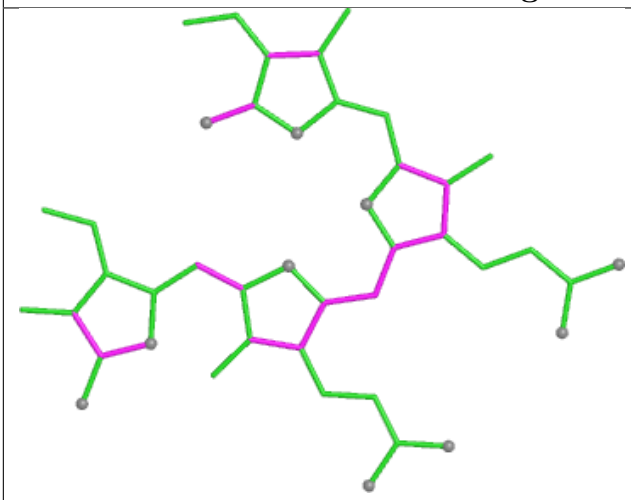


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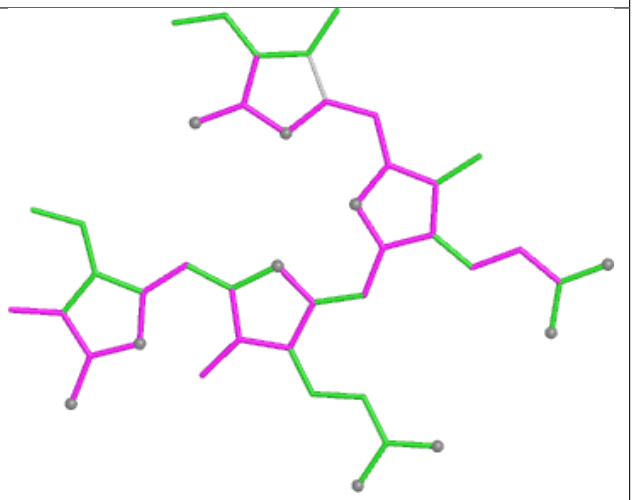


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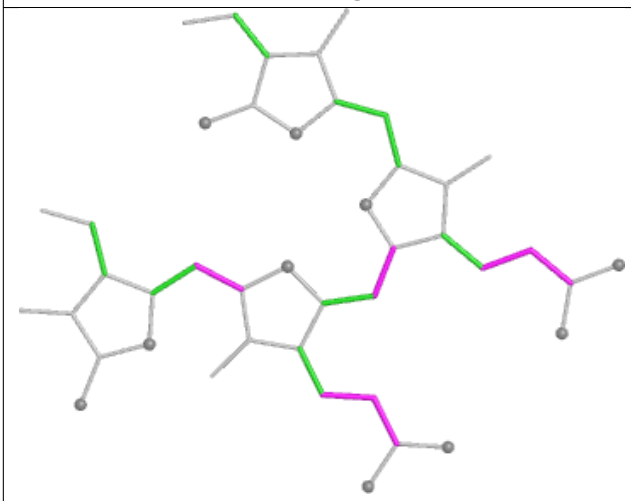
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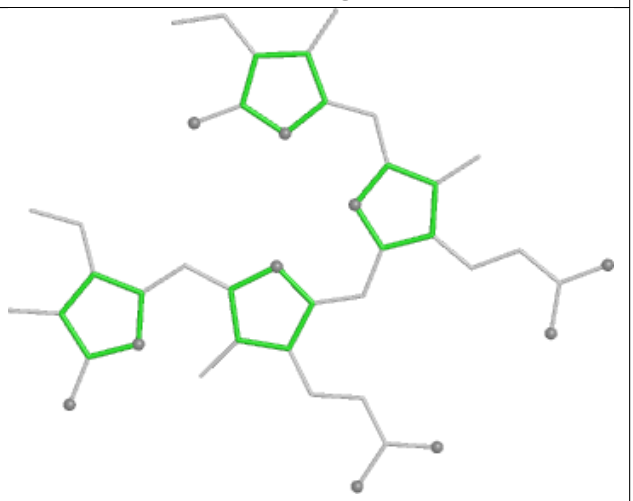
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Bond angles

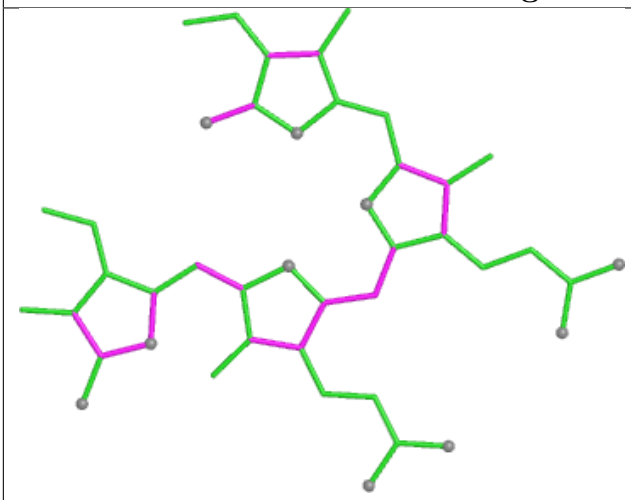


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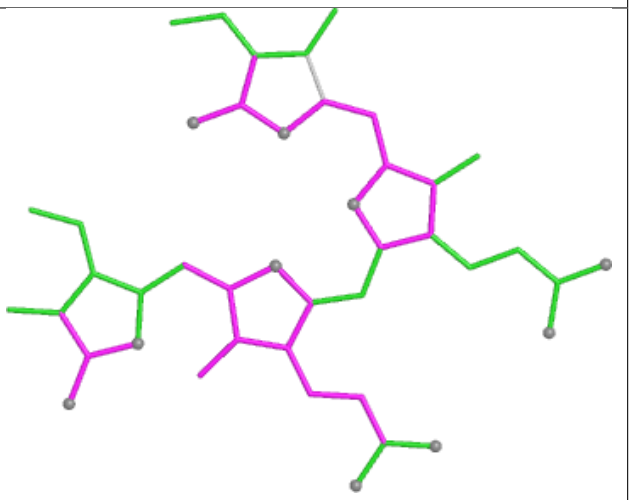


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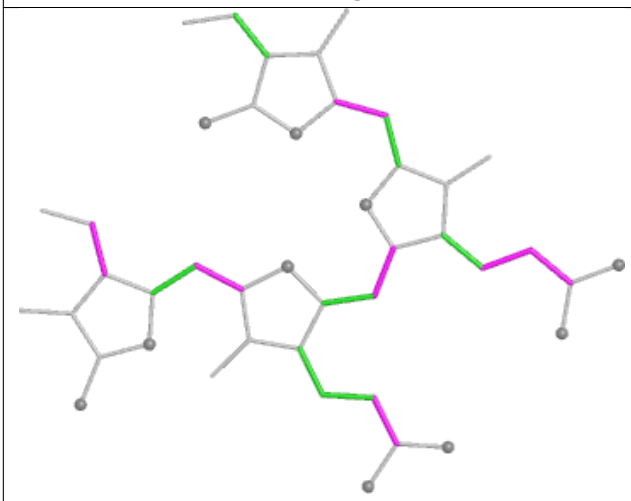
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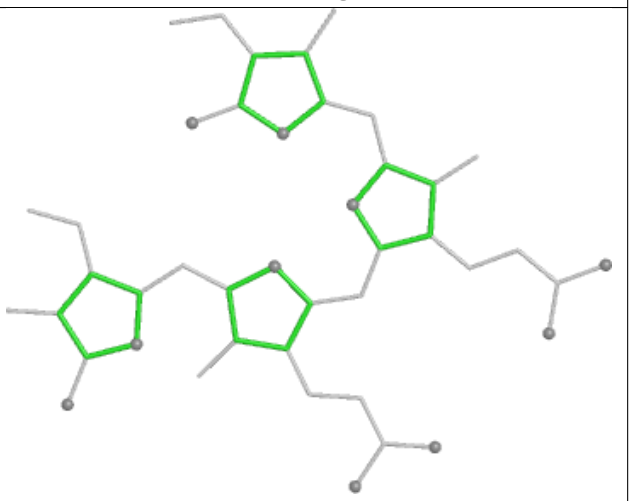
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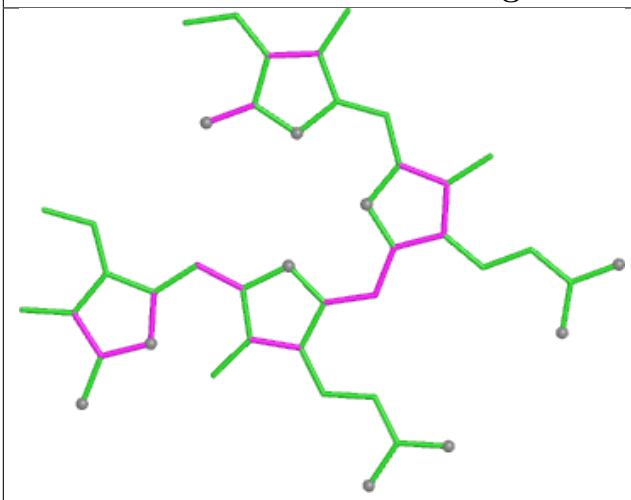


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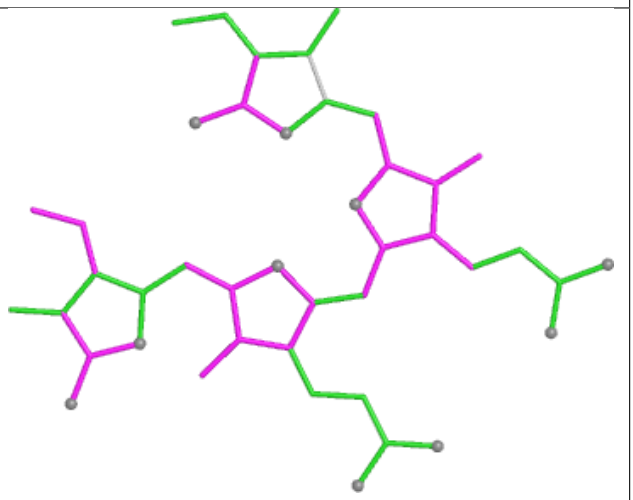


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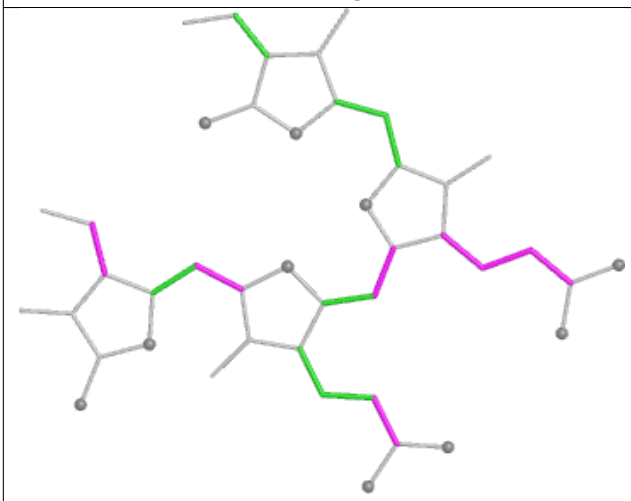
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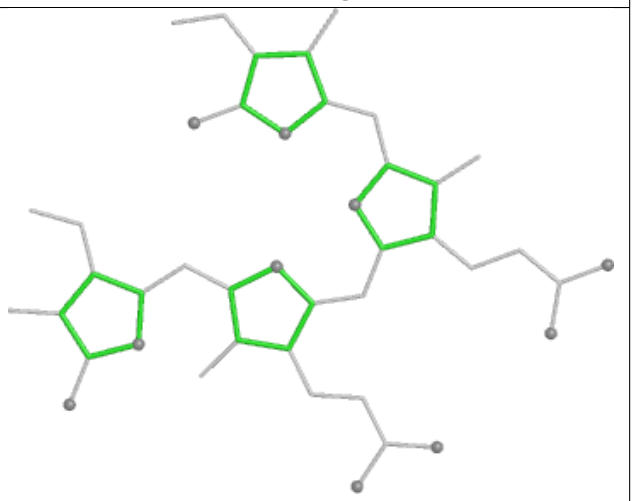
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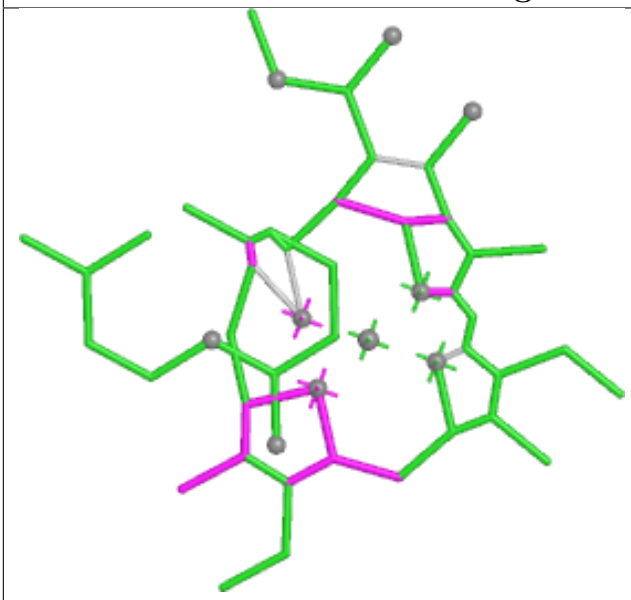


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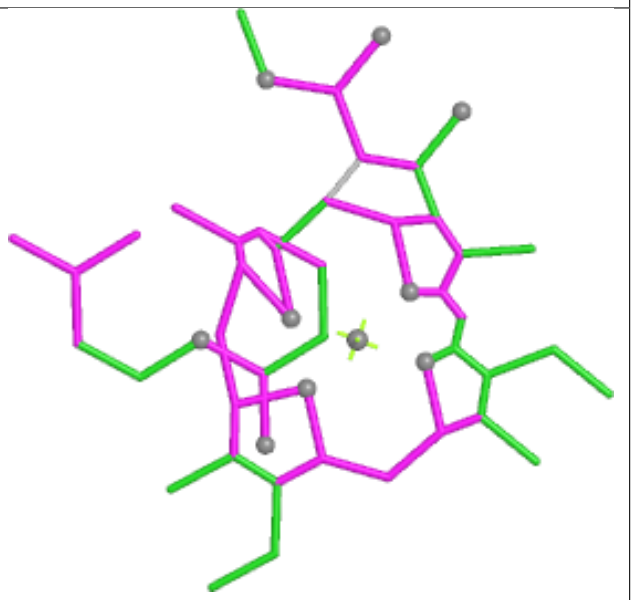


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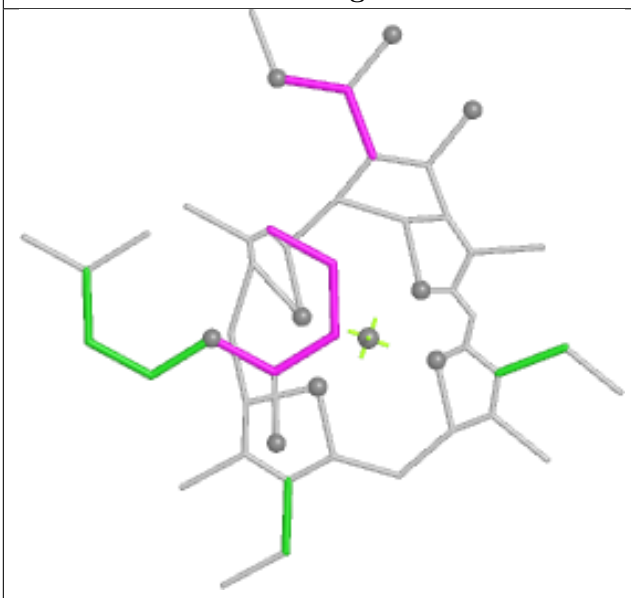
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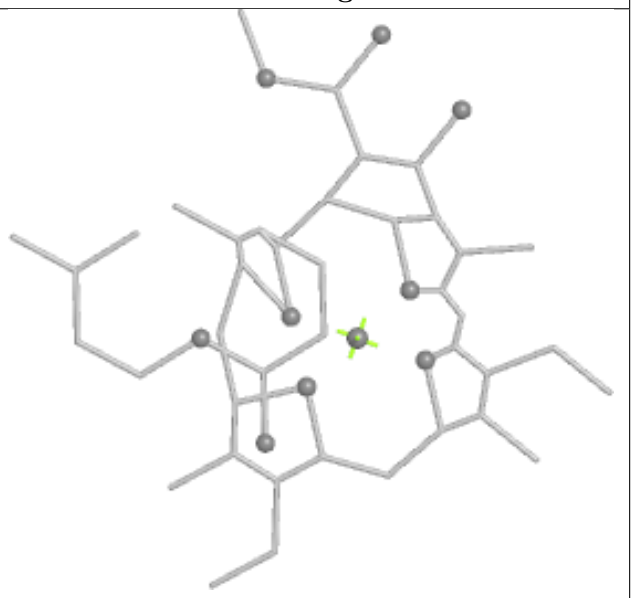
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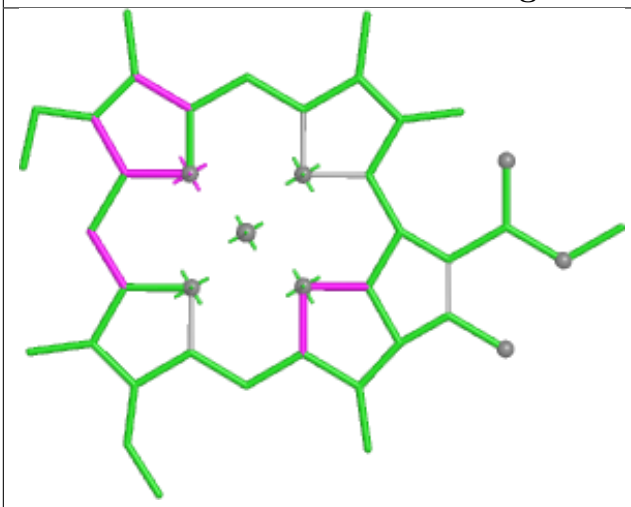


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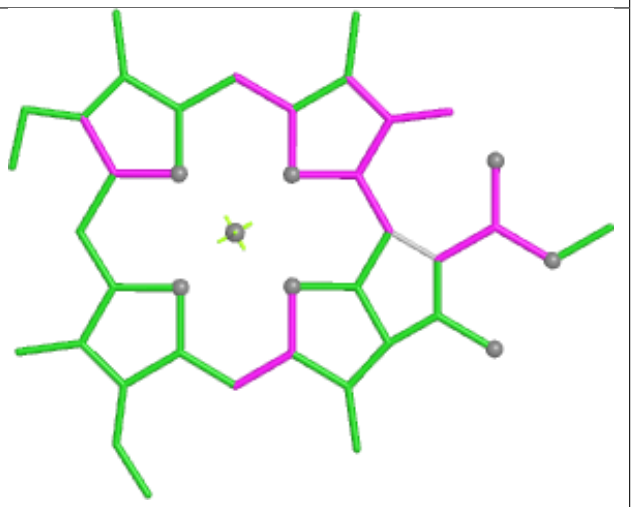


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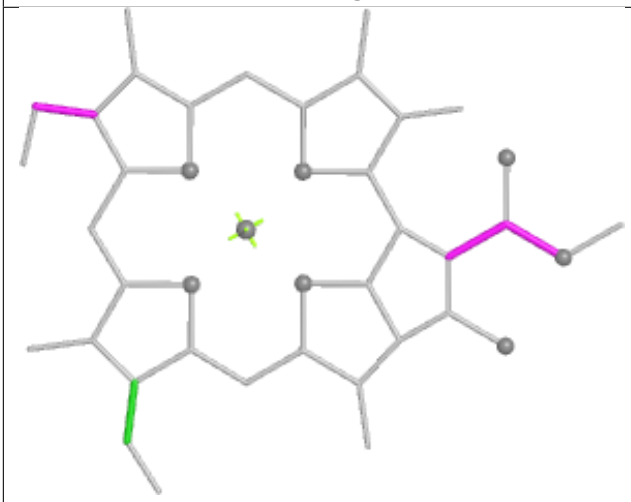
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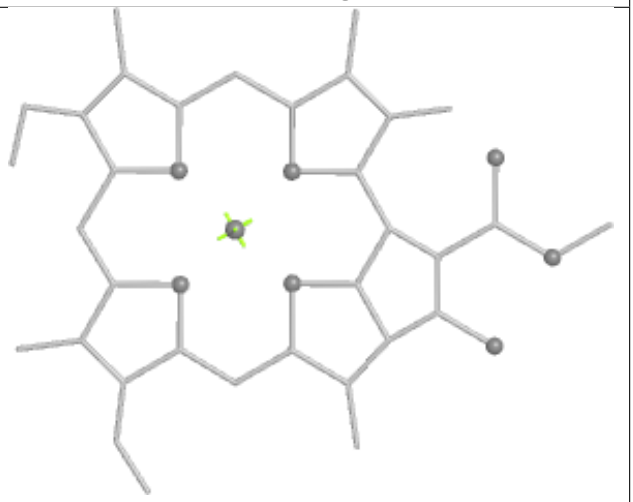
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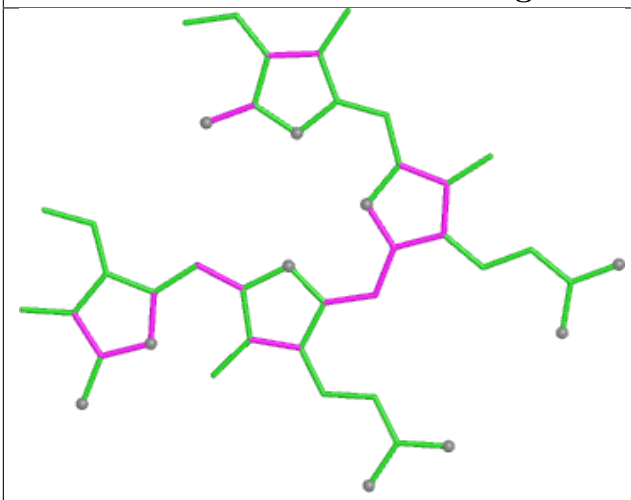


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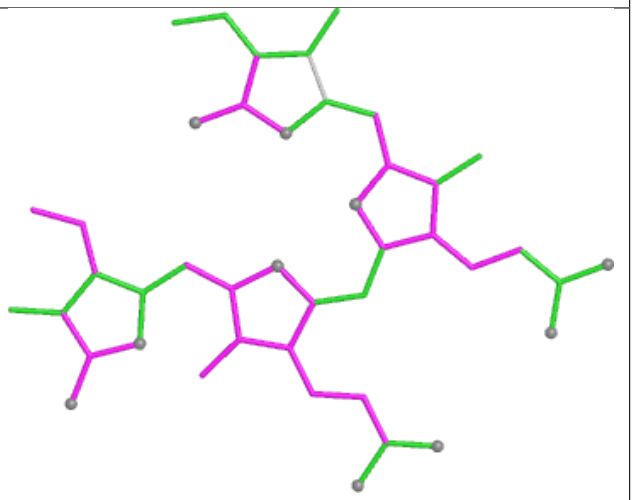


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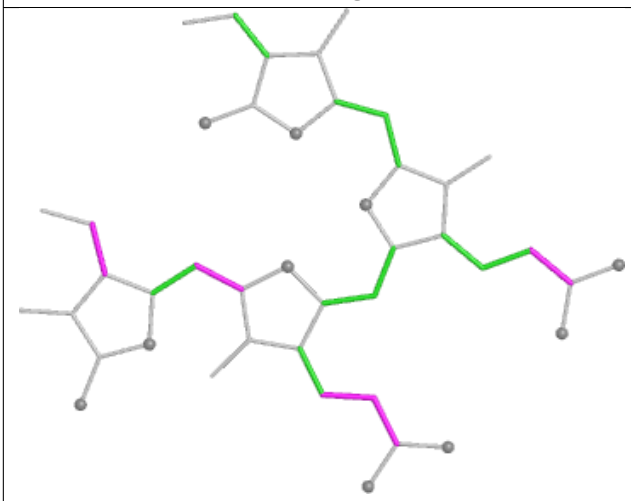
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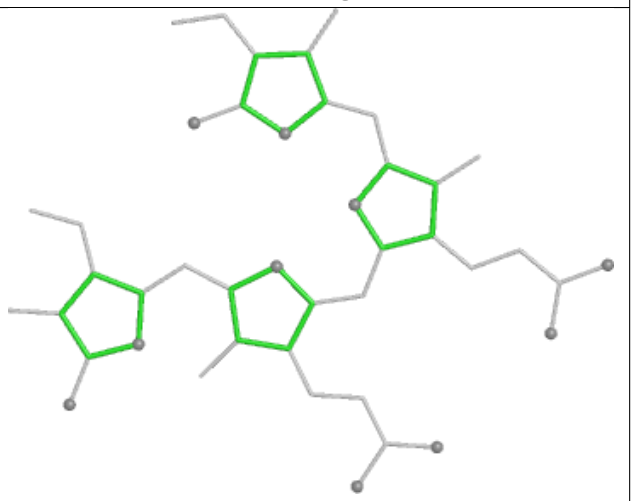
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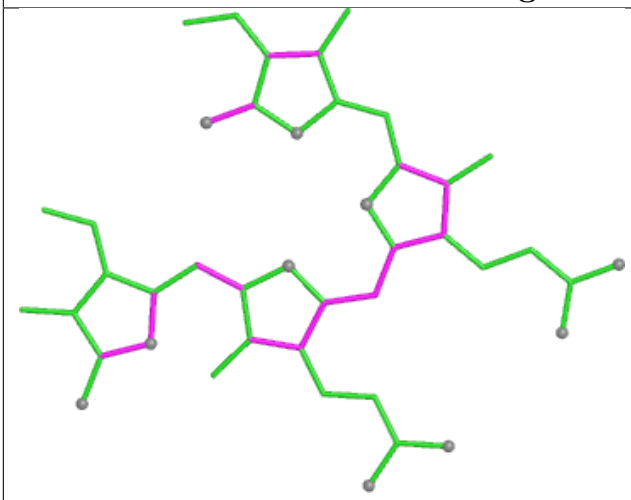


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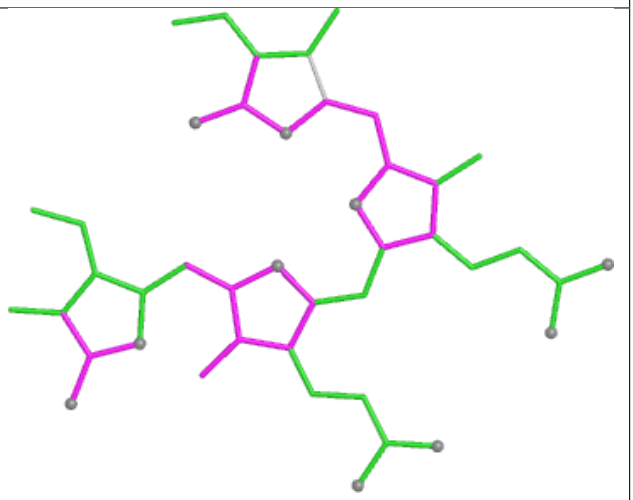


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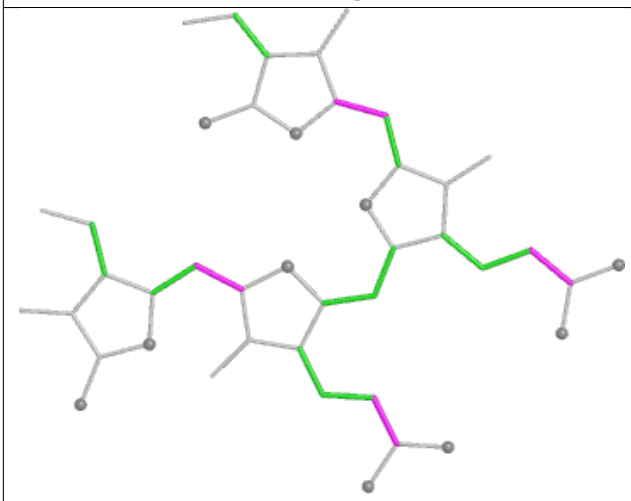
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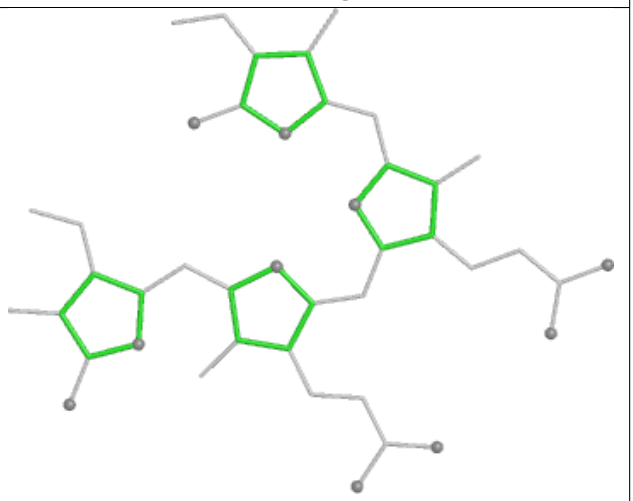
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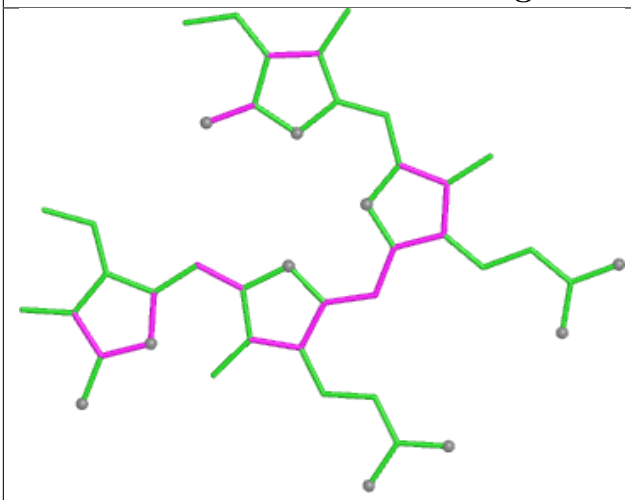


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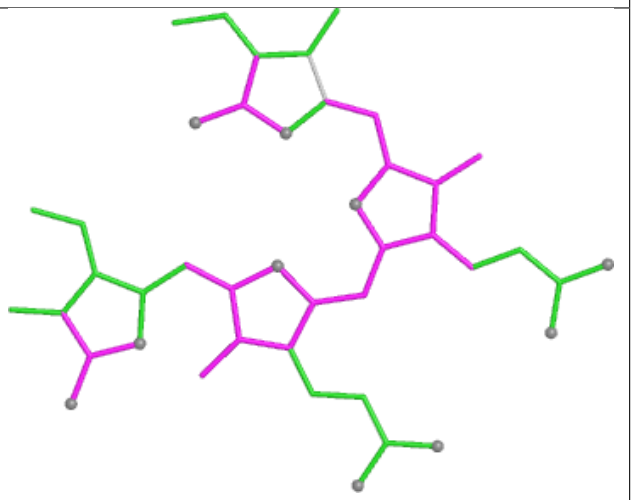


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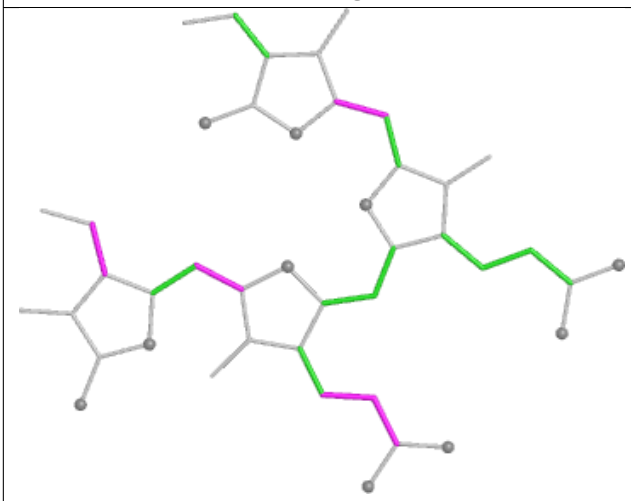
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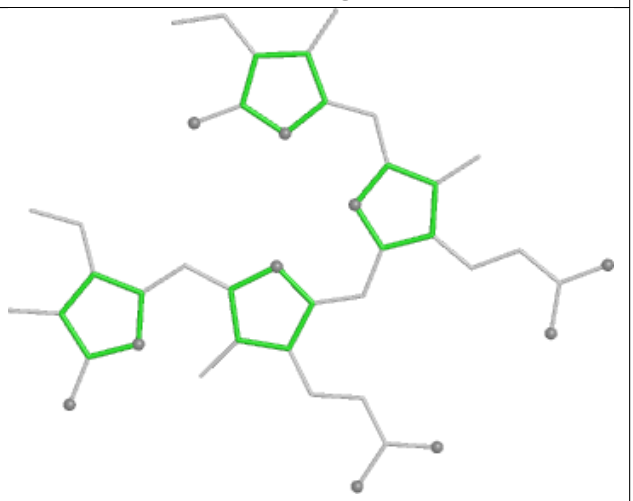
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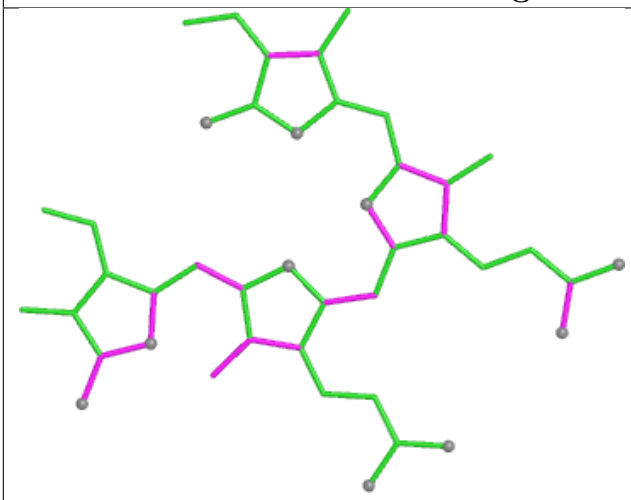


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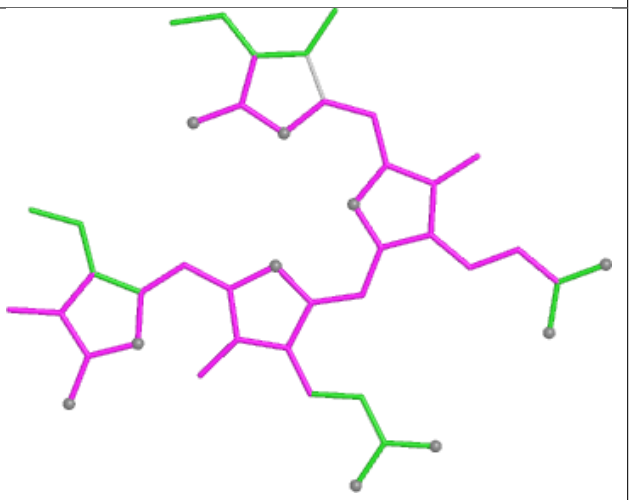


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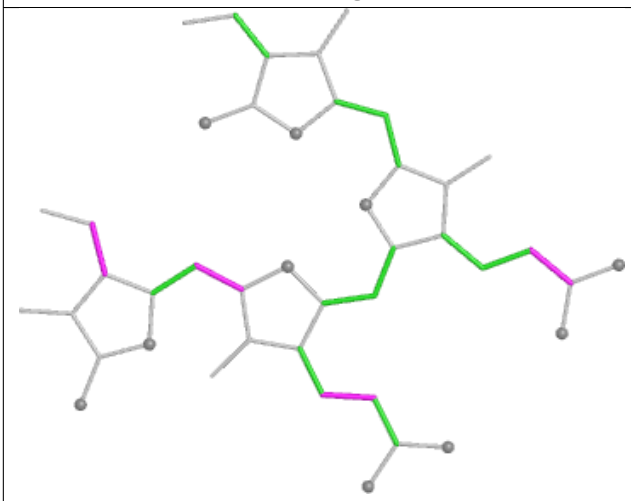
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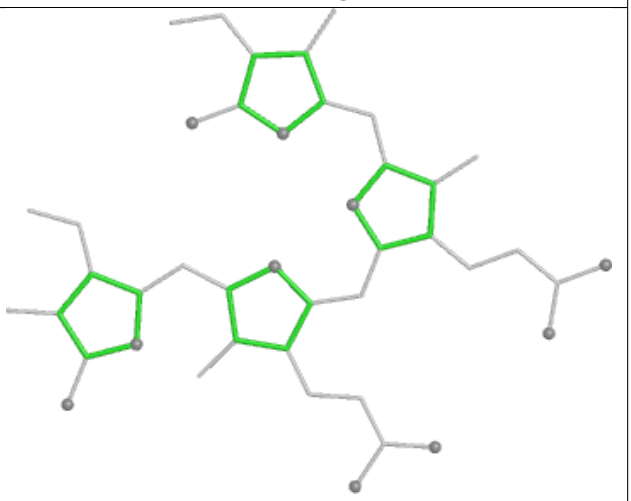
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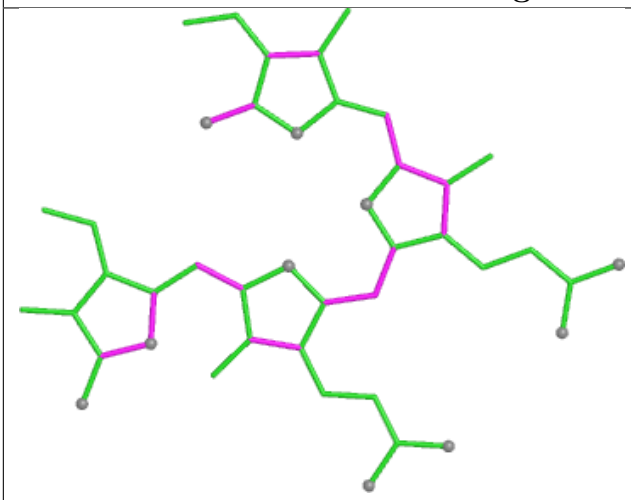


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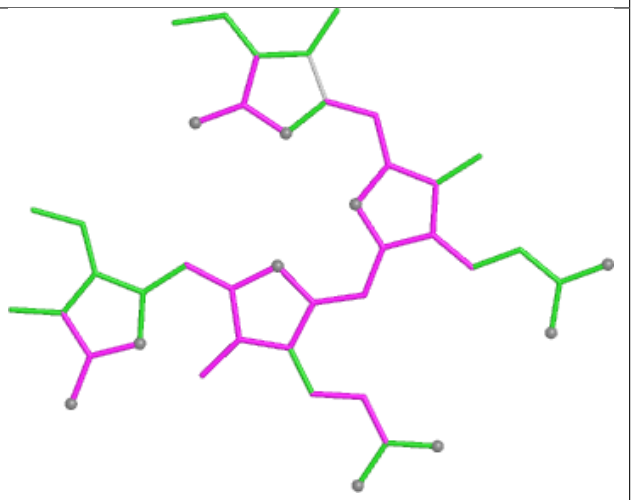


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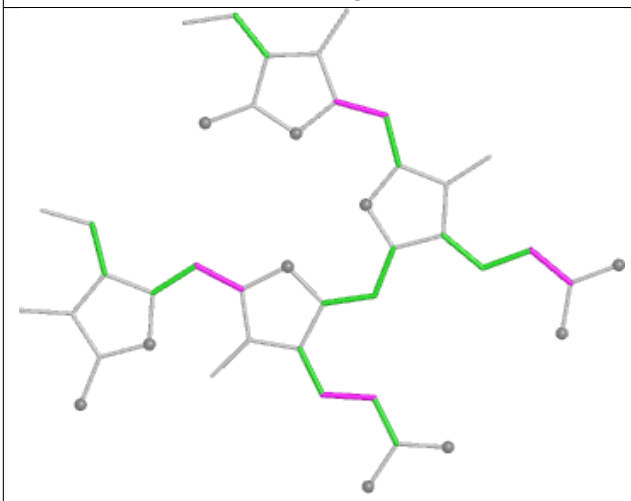
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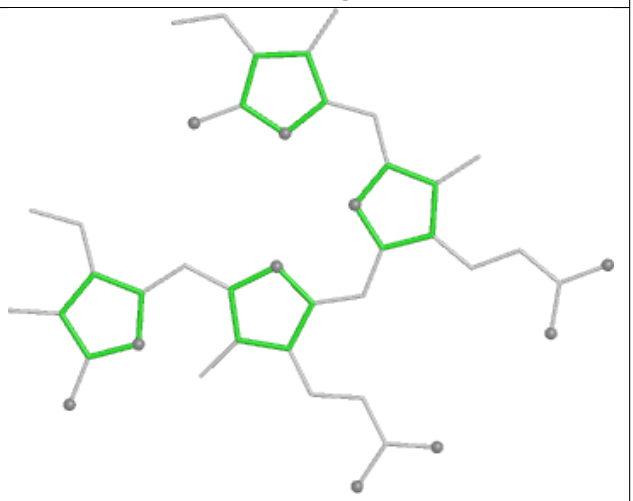
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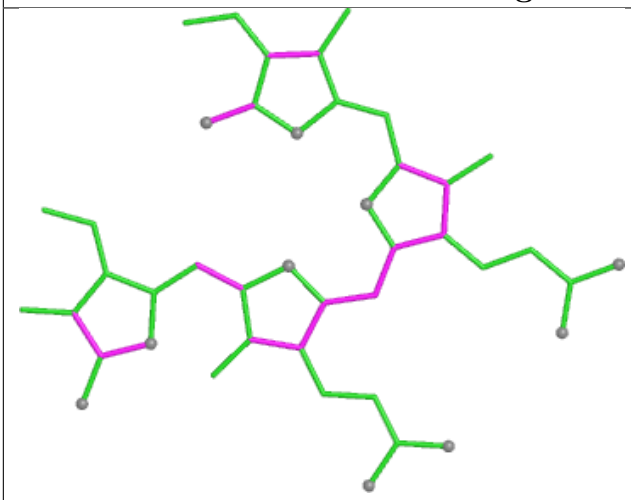


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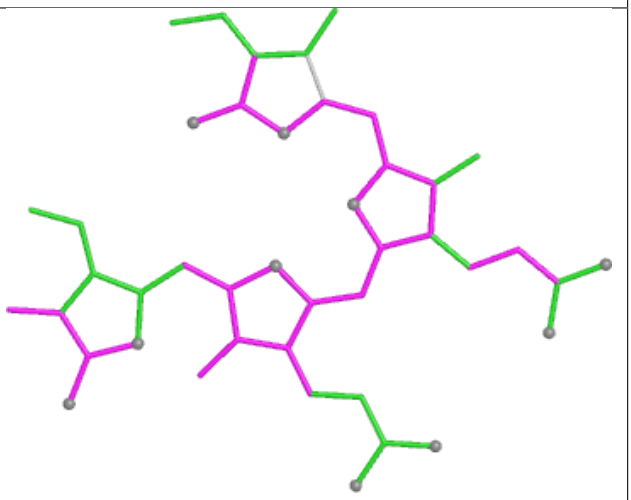


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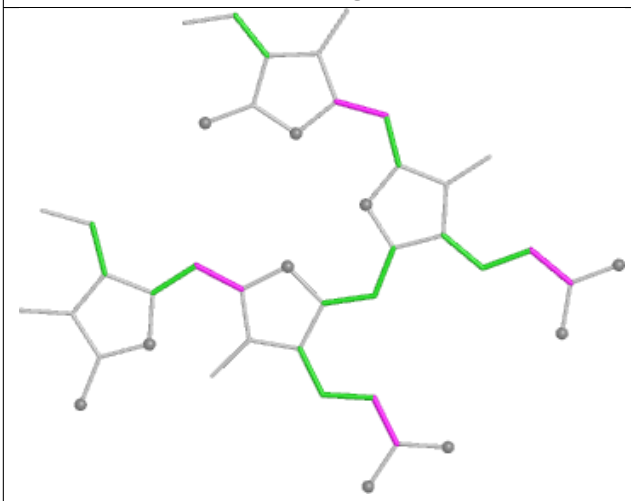
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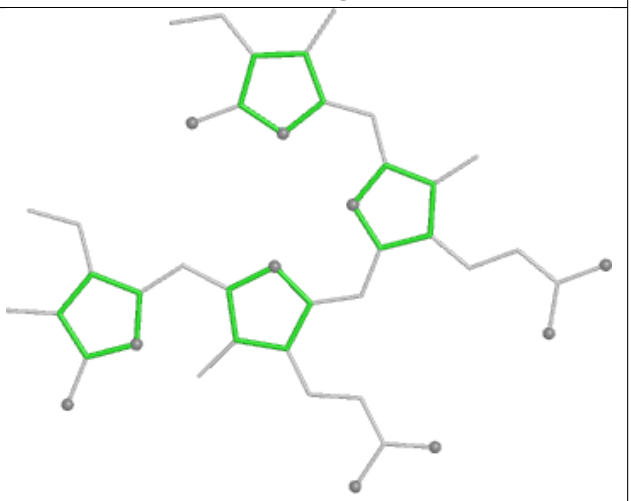
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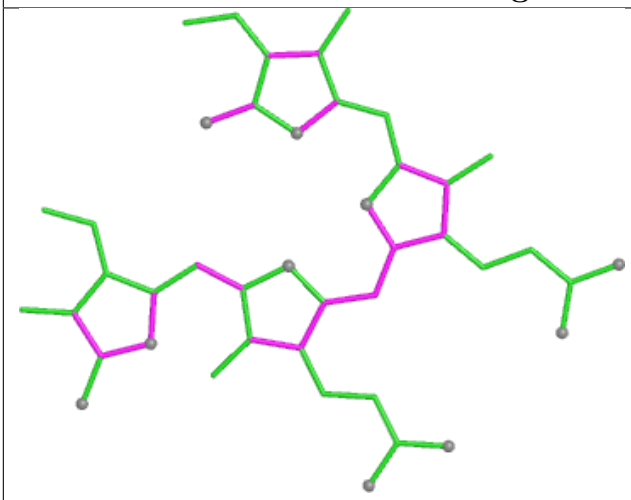


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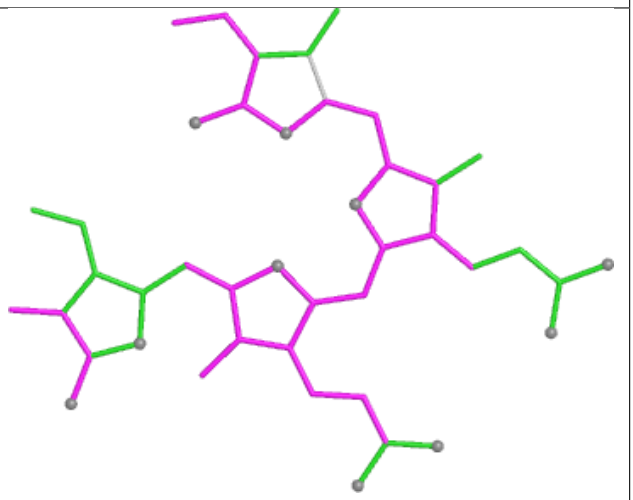


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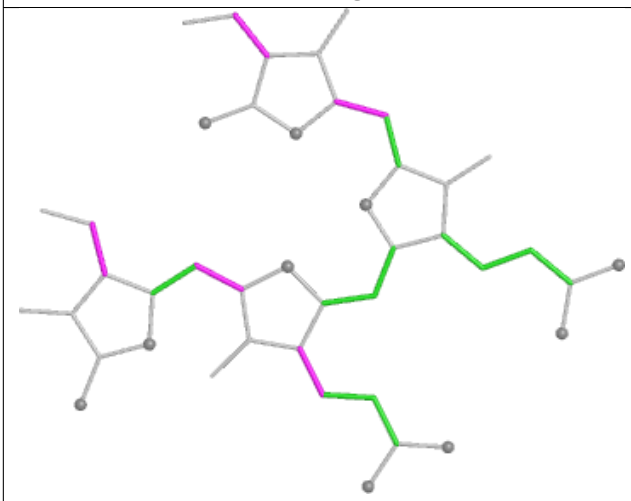
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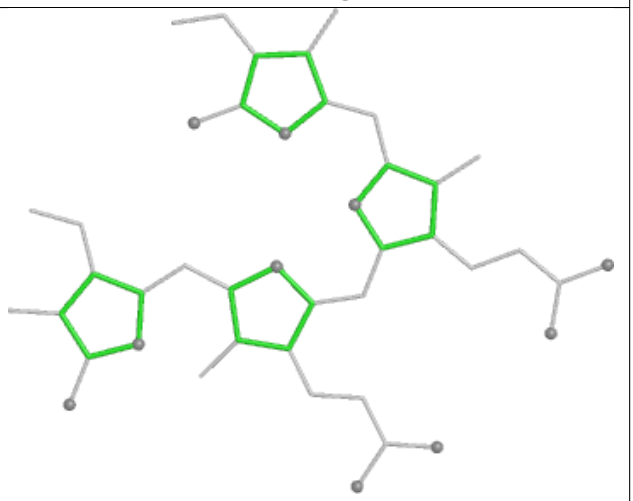
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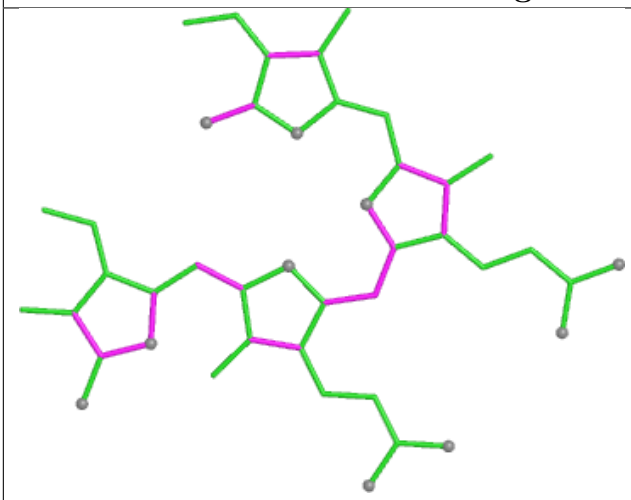


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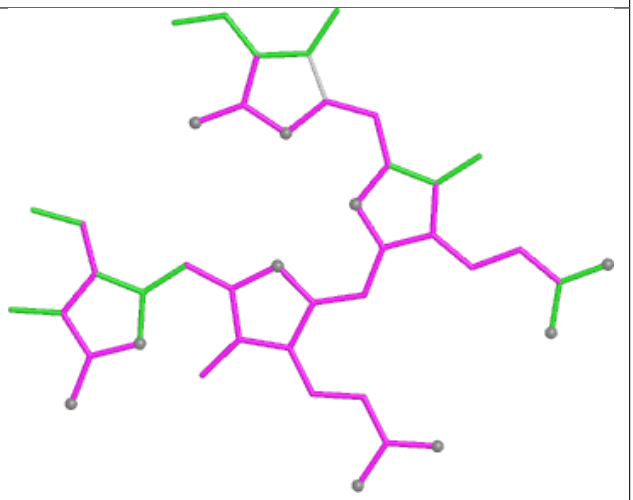


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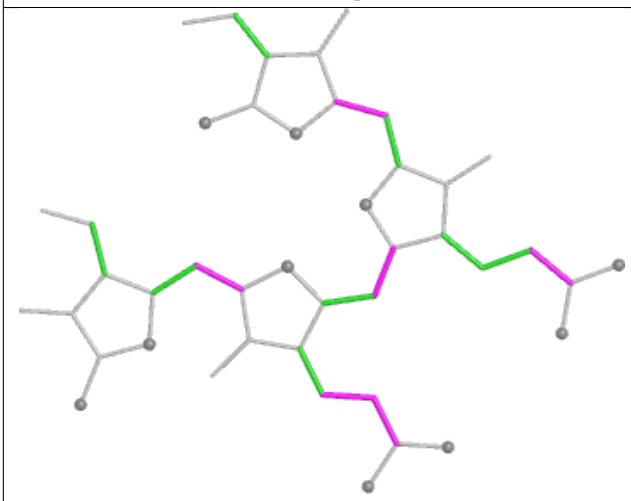
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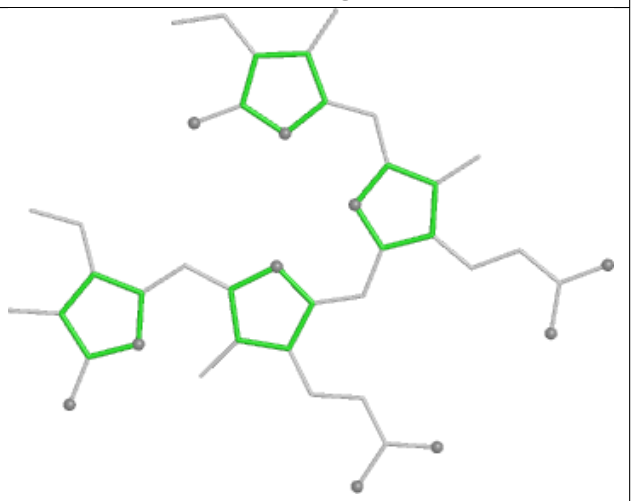
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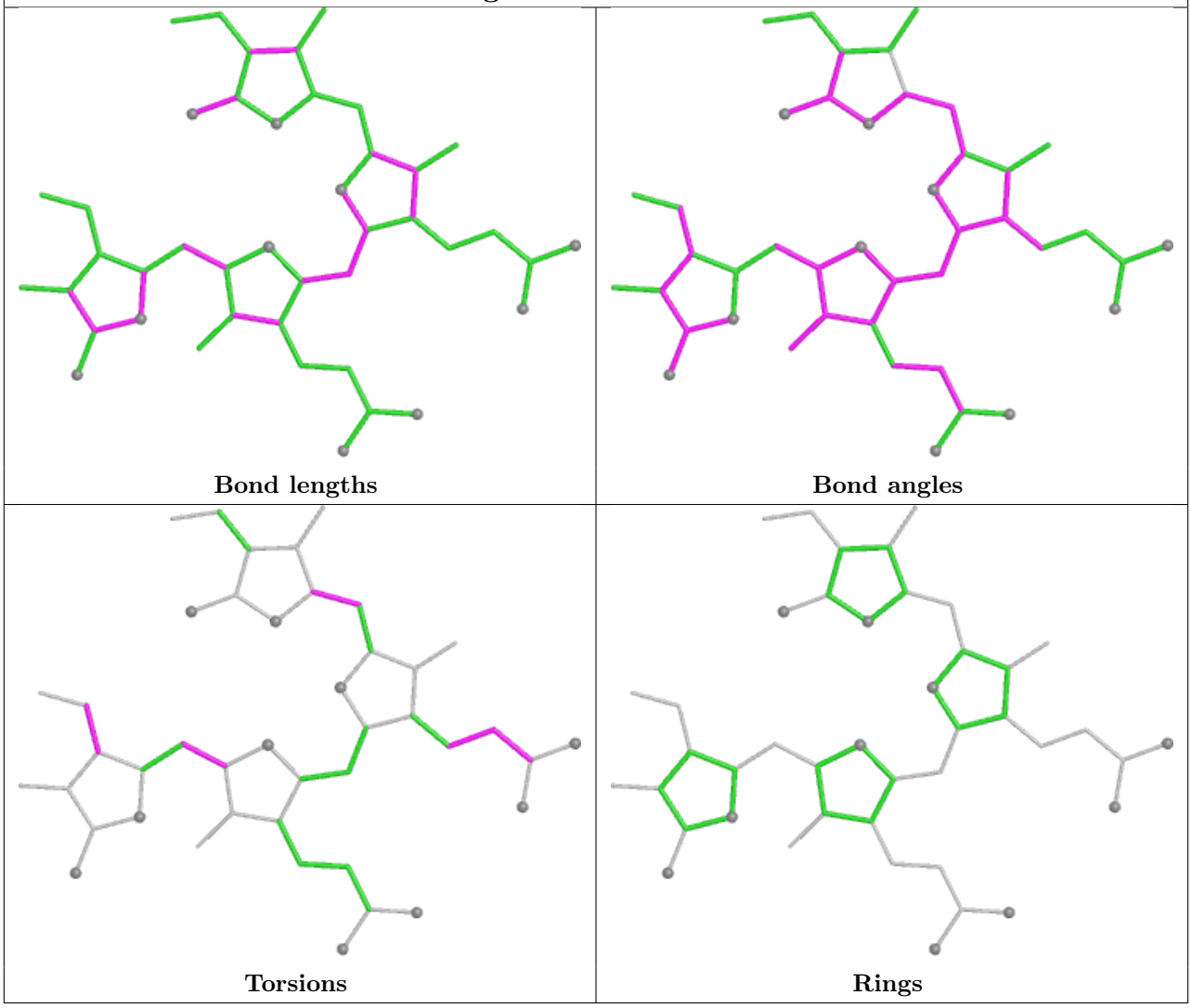


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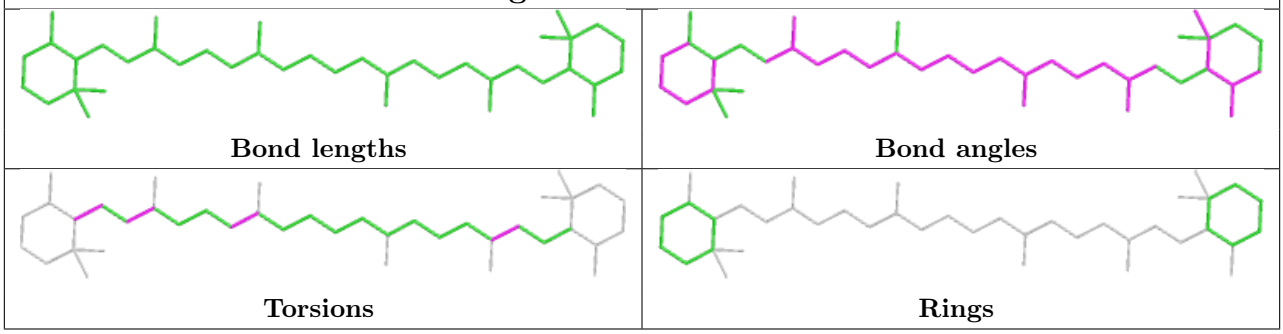


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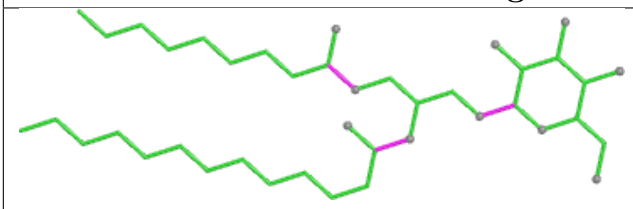
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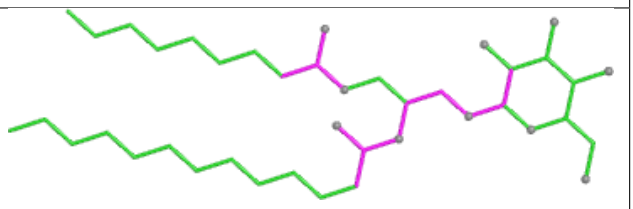
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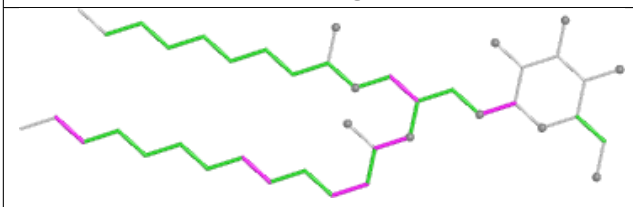
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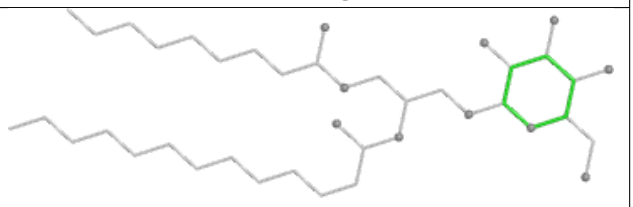
Bond lengths



Bond angles

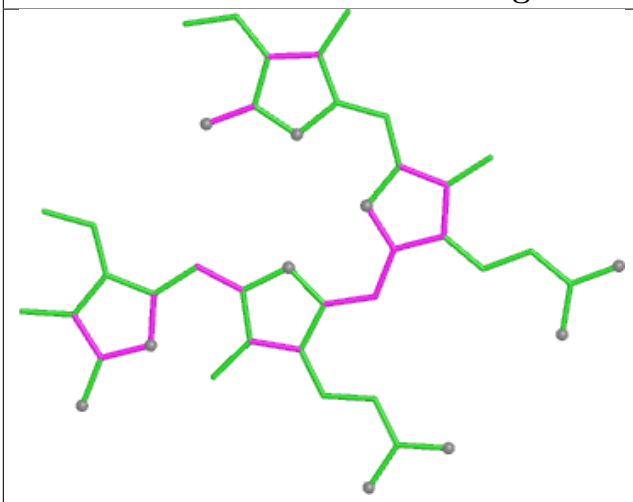


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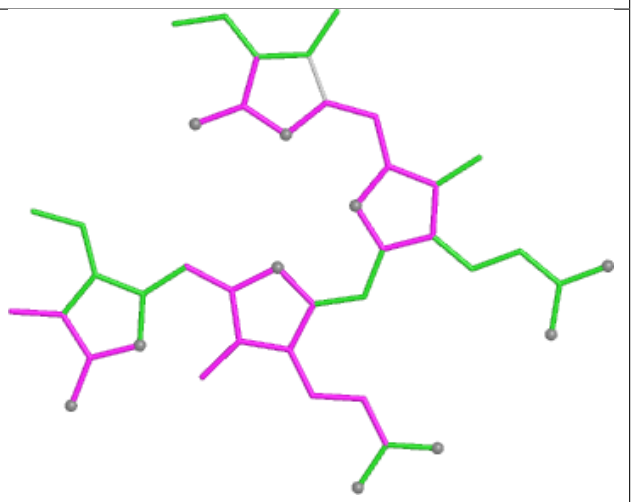


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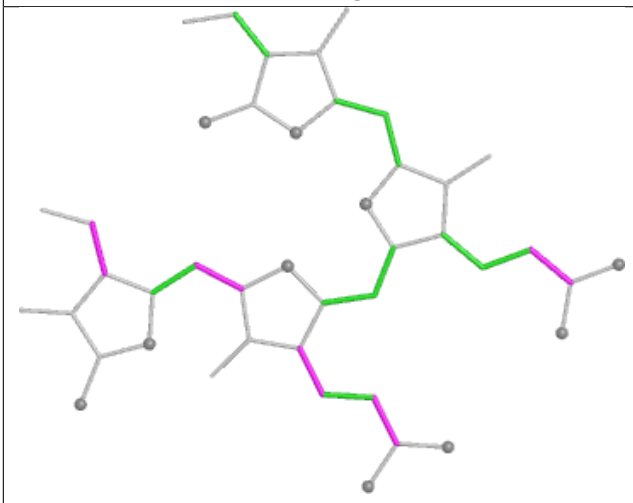
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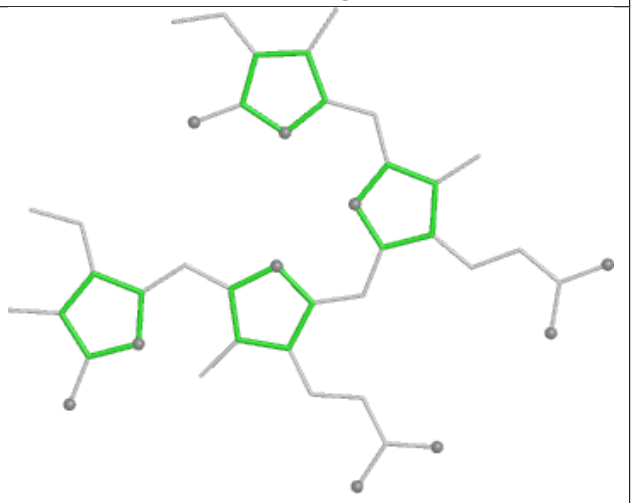
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Bond angles

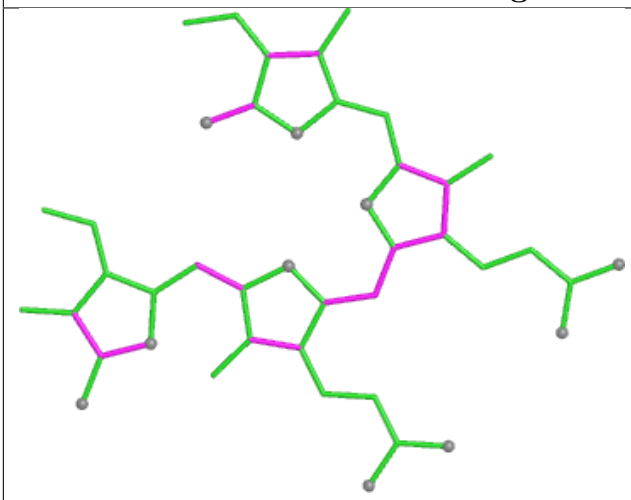


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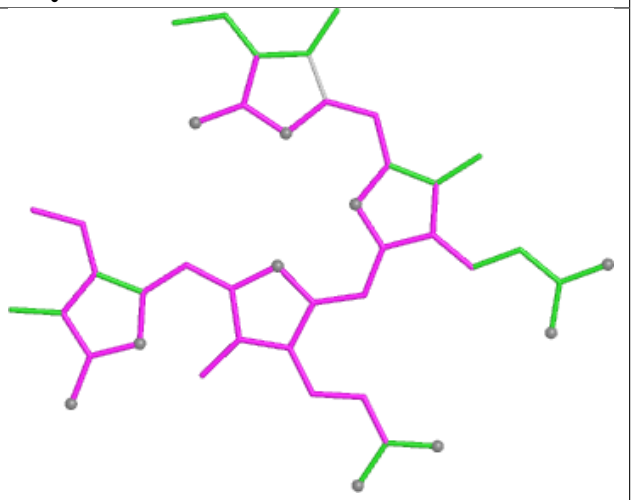


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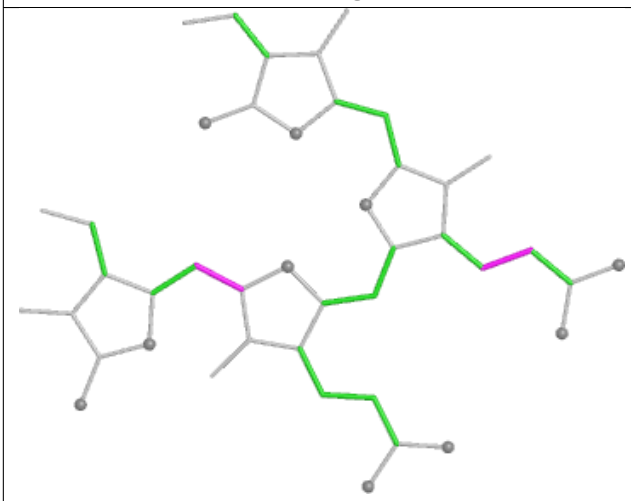
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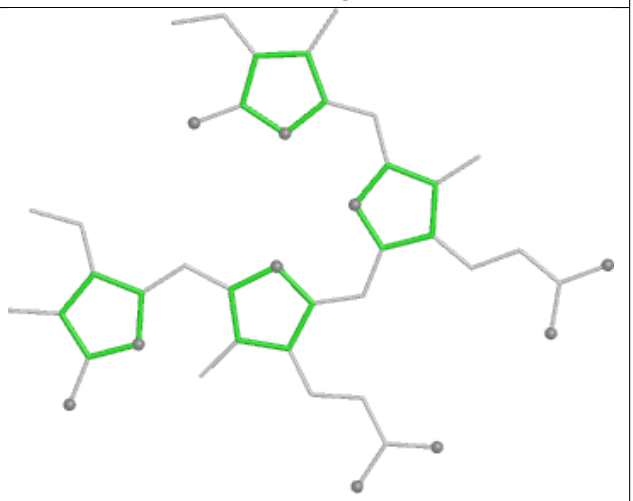
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Bond angles

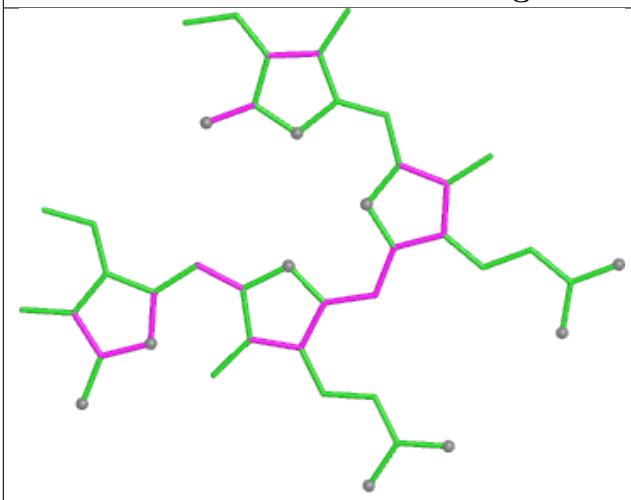


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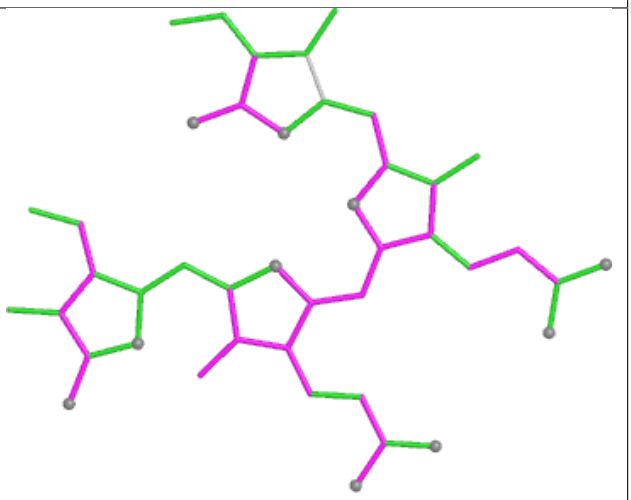


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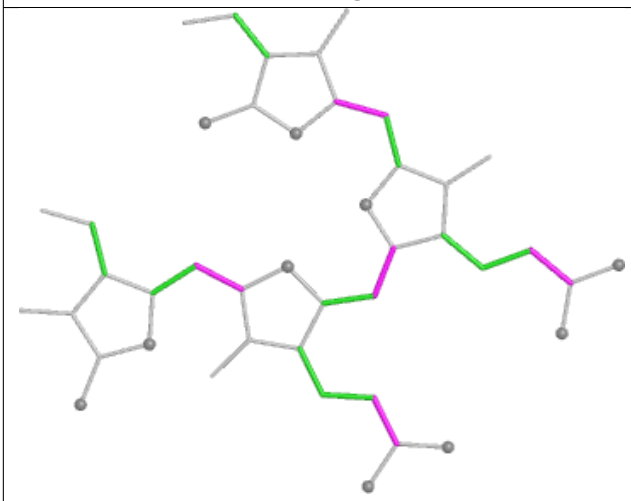
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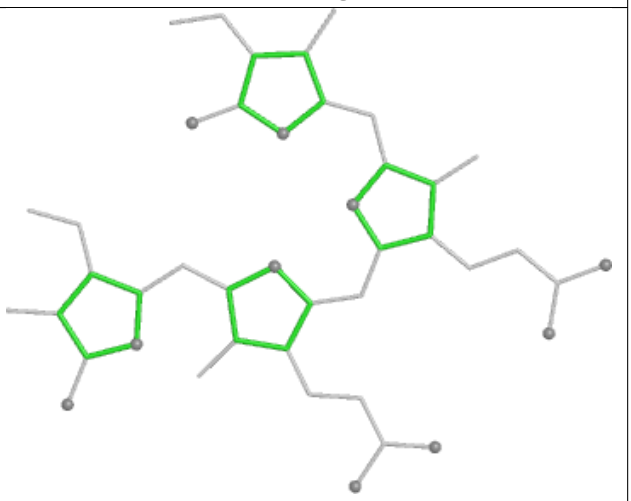
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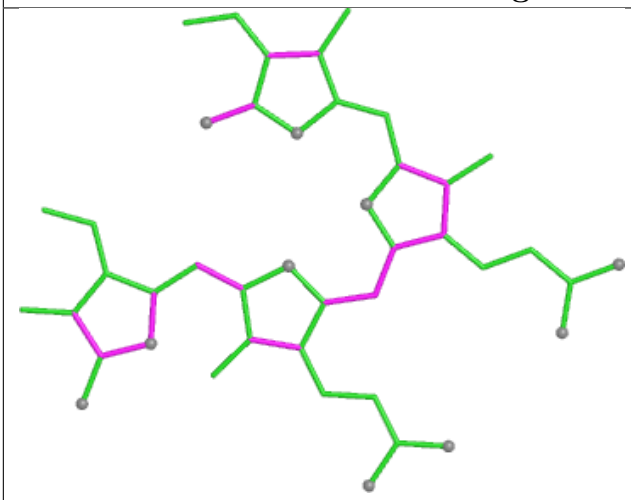


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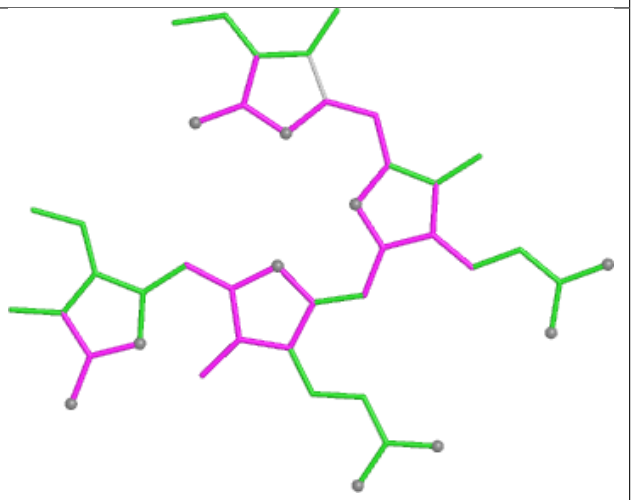


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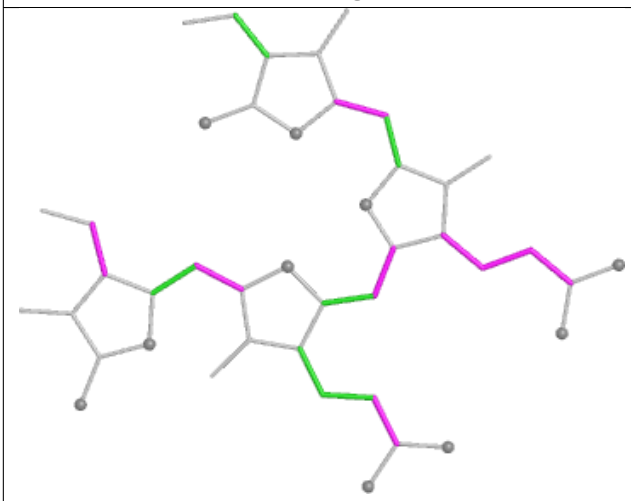
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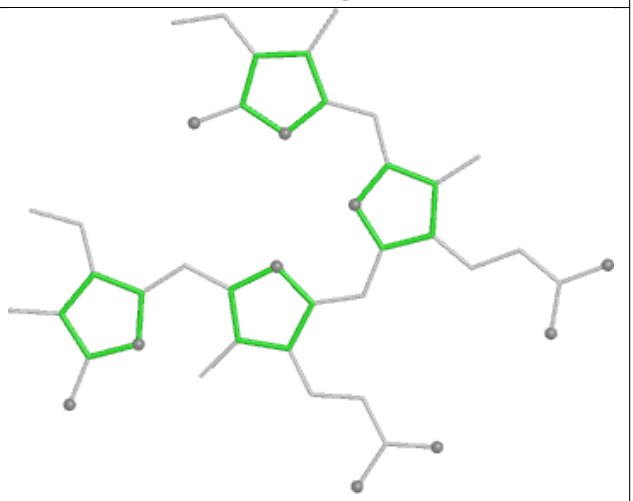
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Bond angles

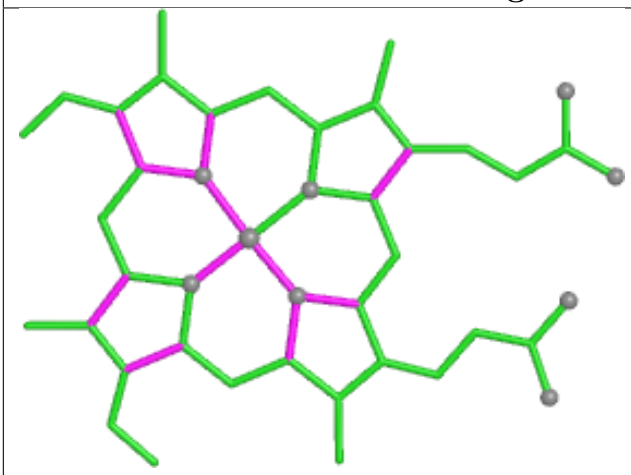


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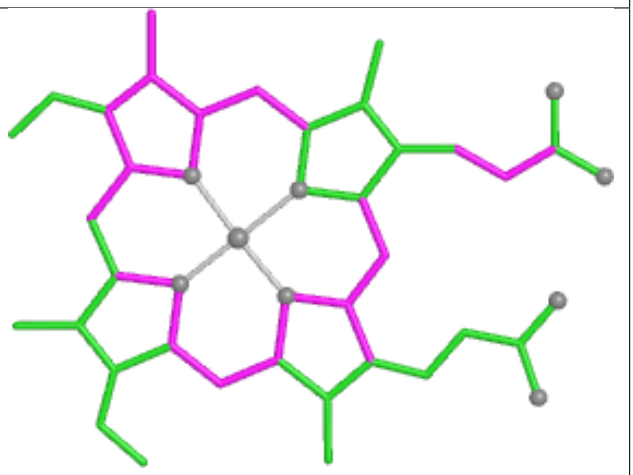


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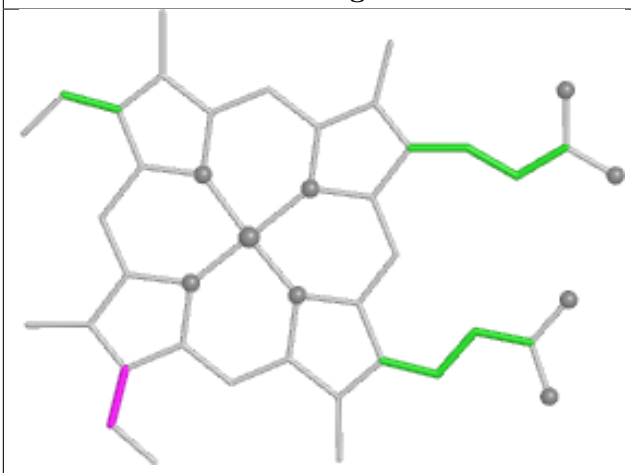
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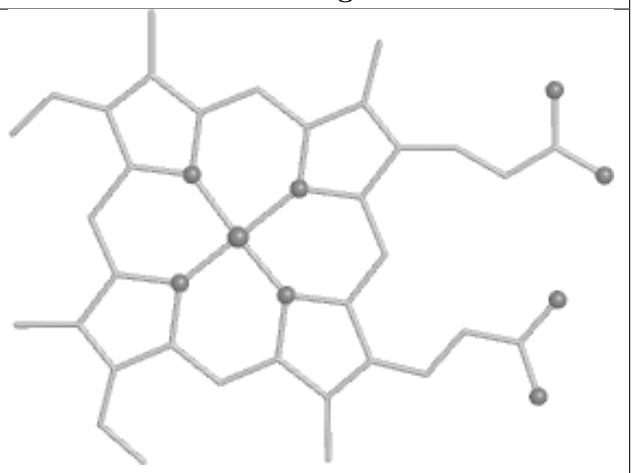
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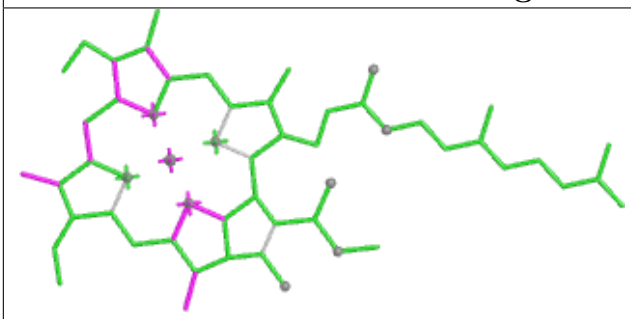


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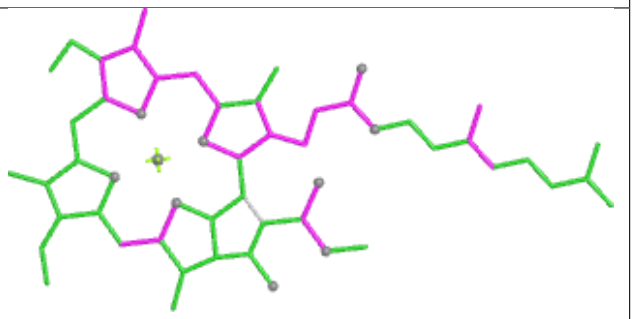


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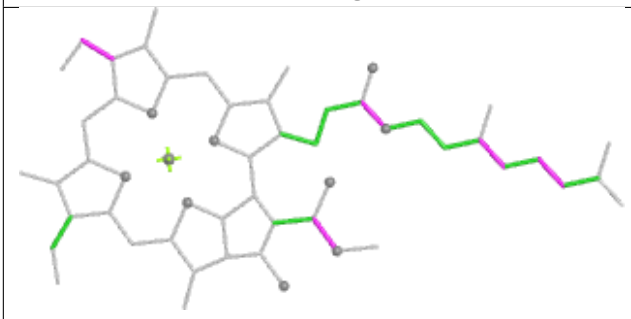
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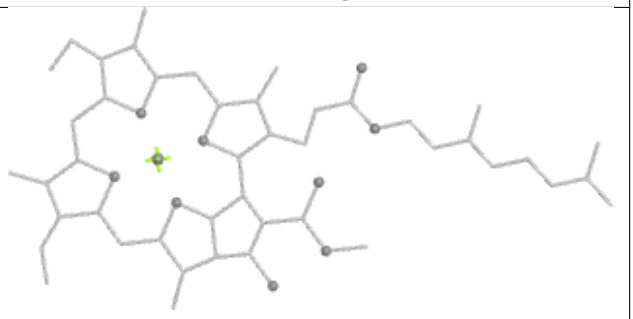
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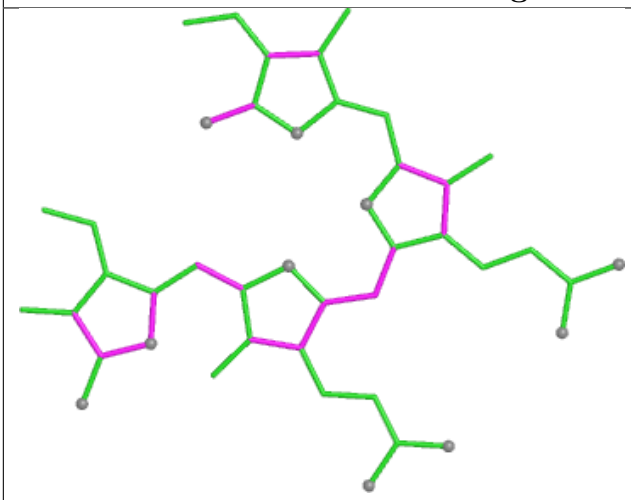


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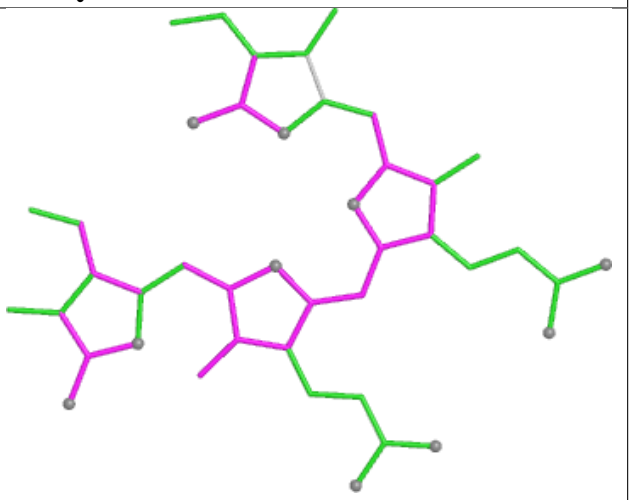


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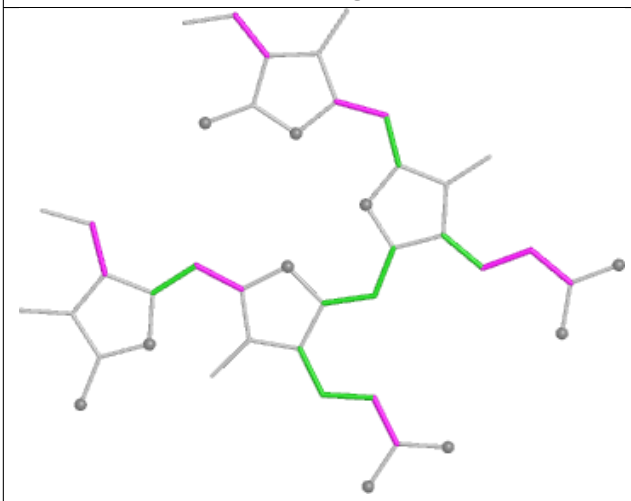
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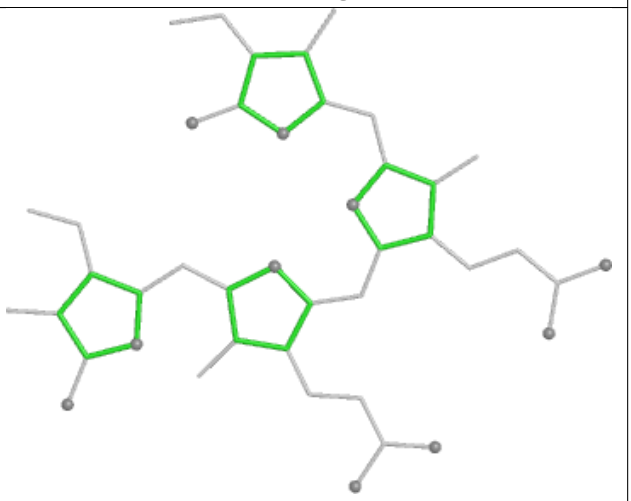
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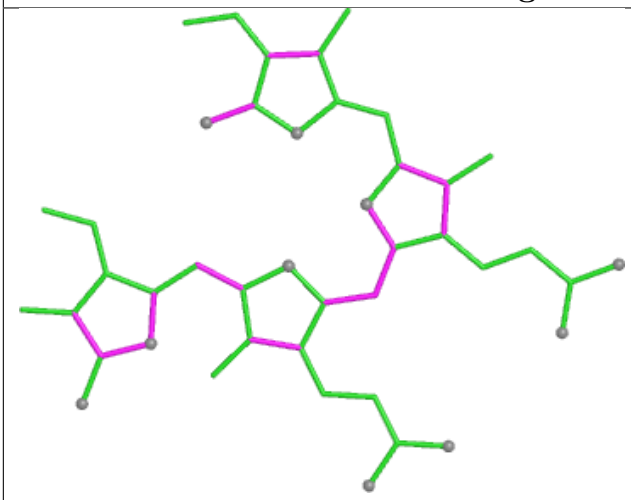


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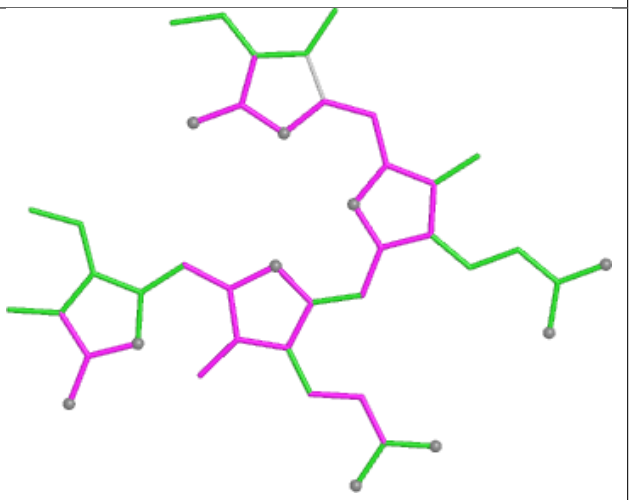


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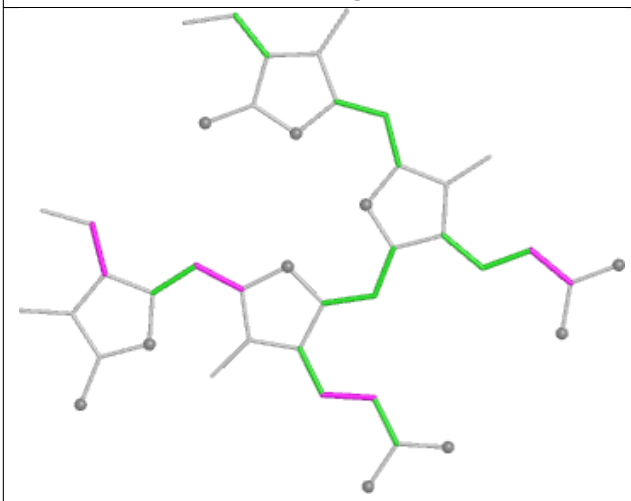
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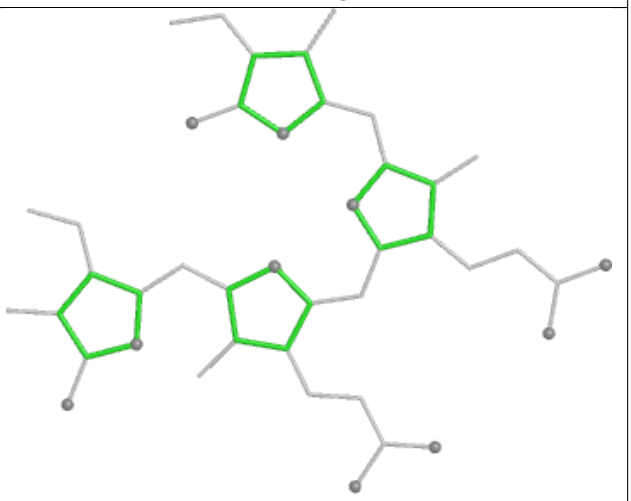
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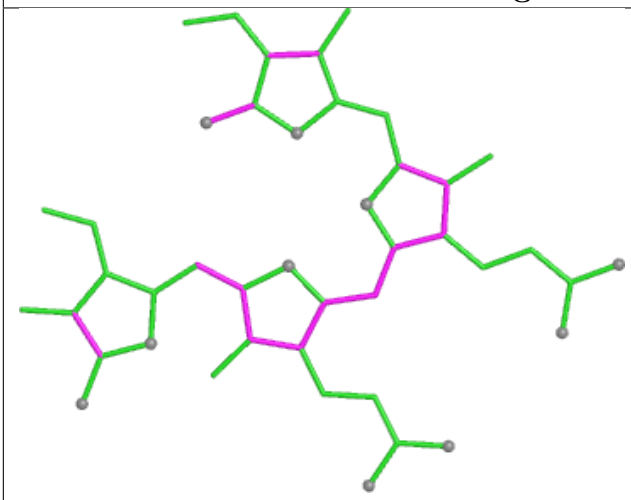


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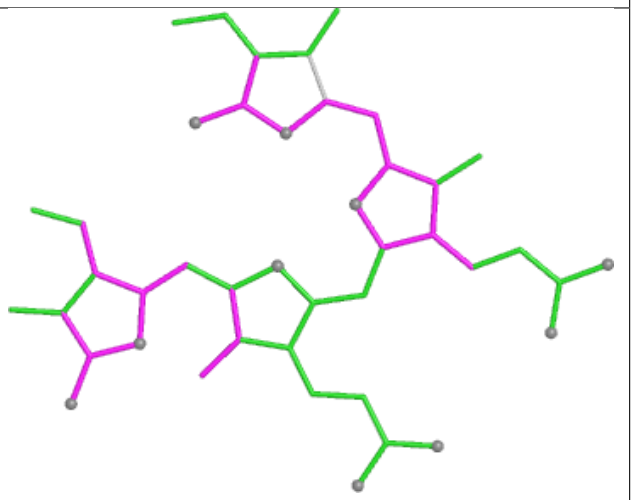


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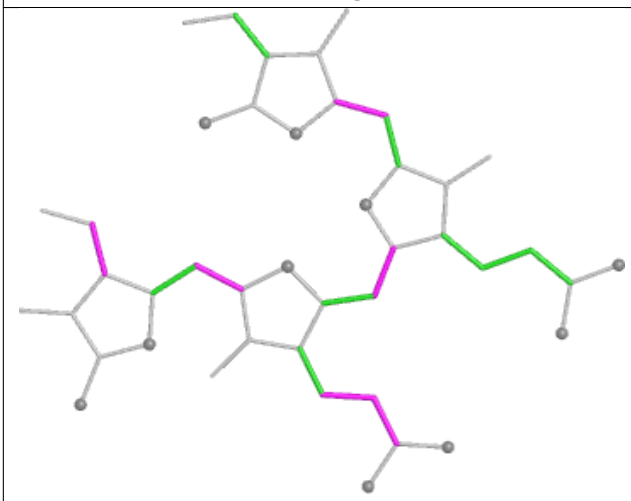
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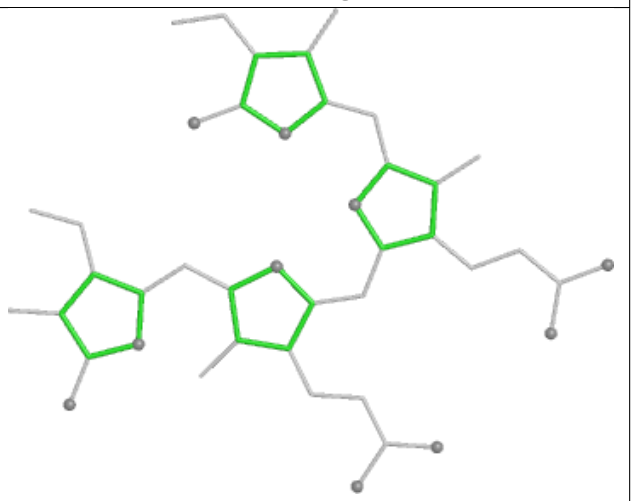
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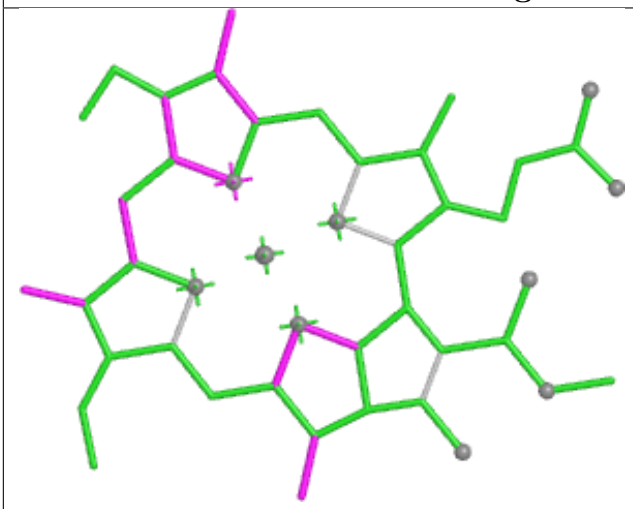


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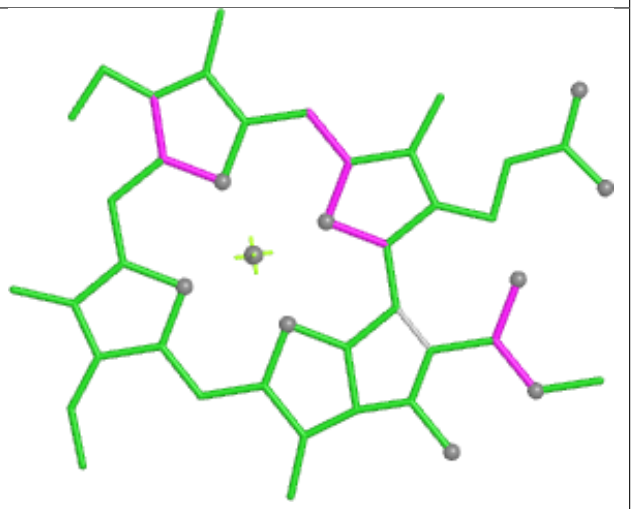


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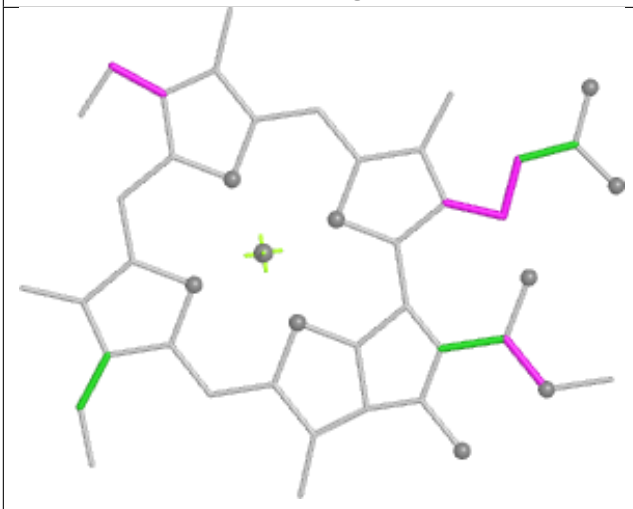
Ligand CLA 4N 611



Bond lengths



Bond angles

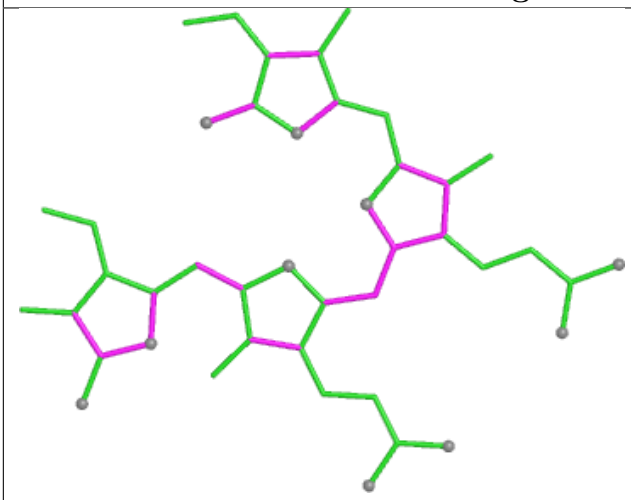


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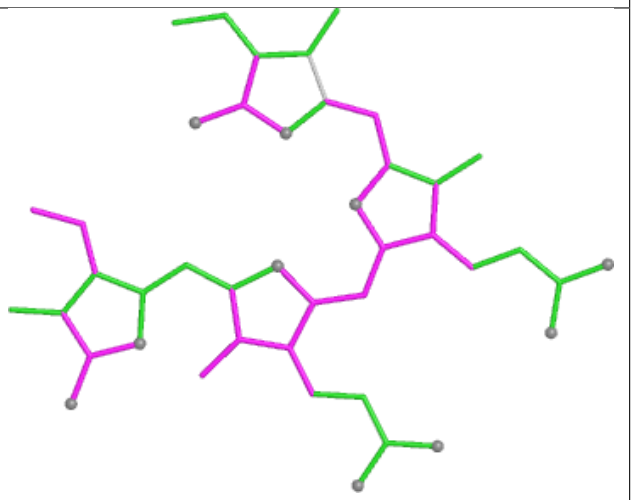


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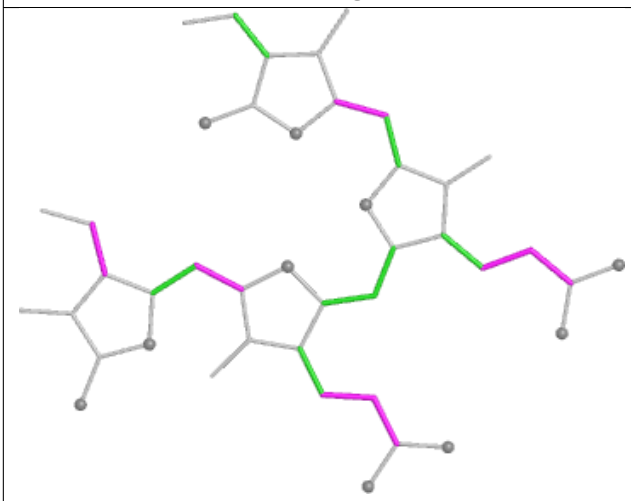
Ligand PEB UE 203



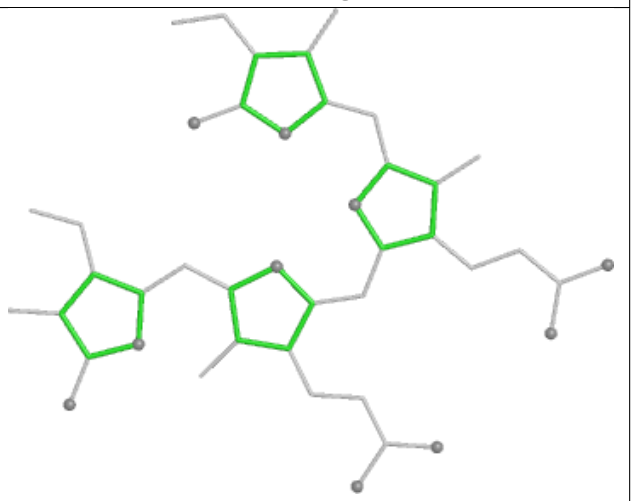
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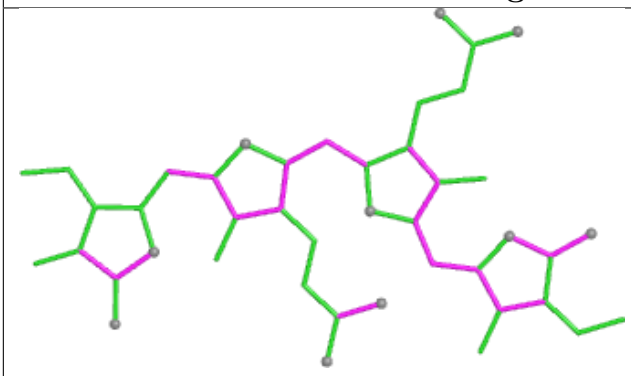


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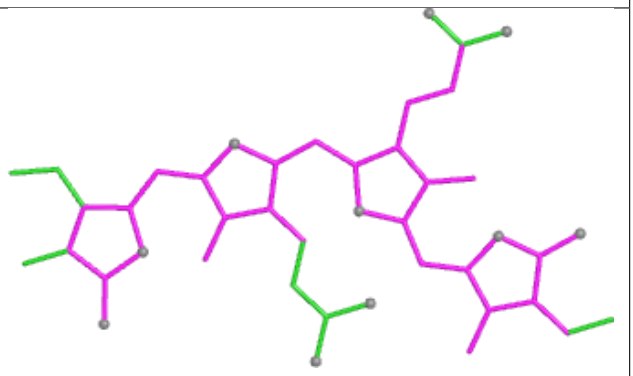


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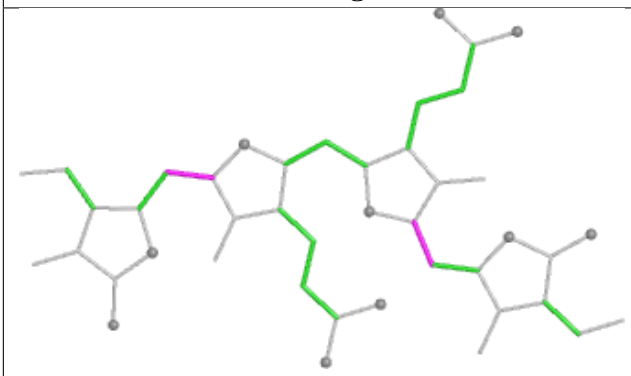
Ligand CYC h3 1001



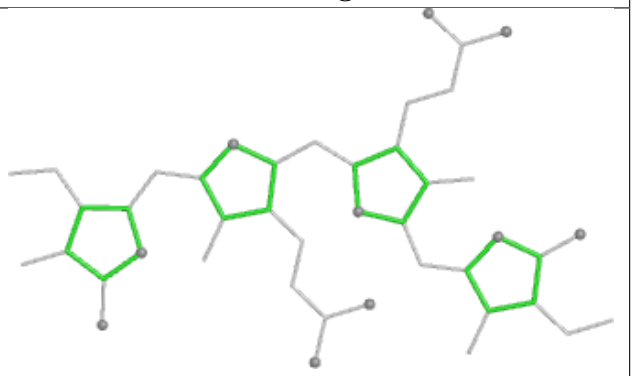
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Bond angles

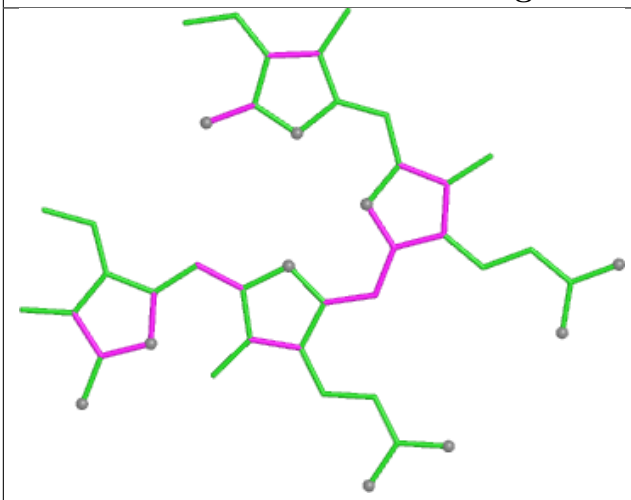


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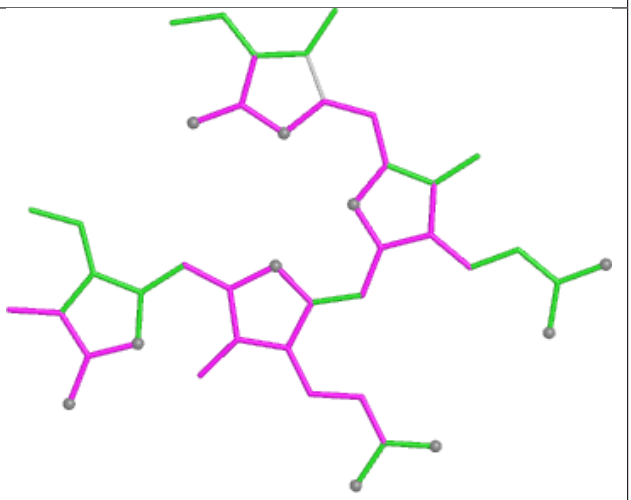


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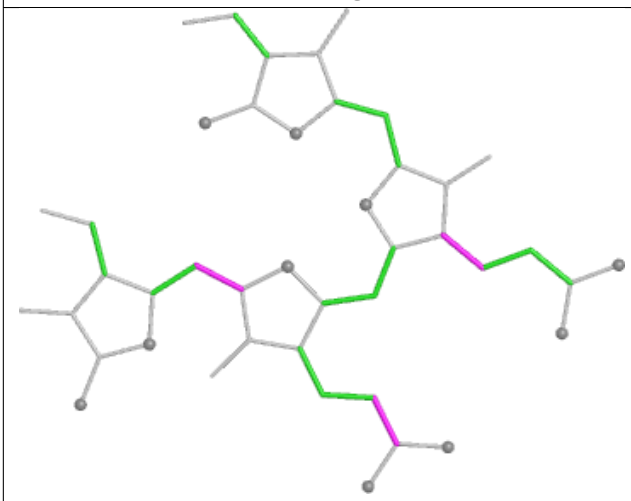
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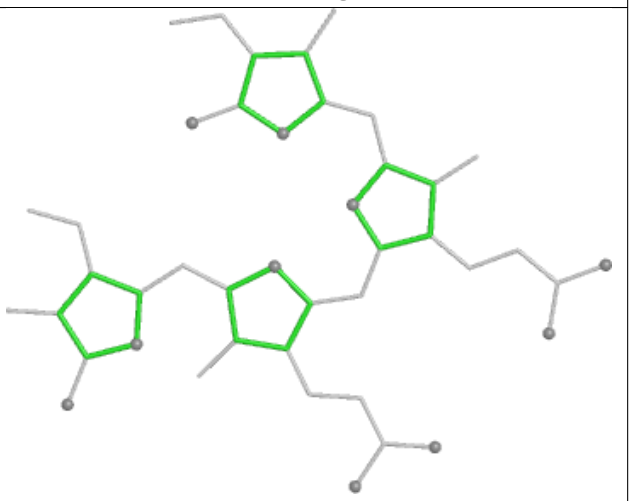
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Bond angles

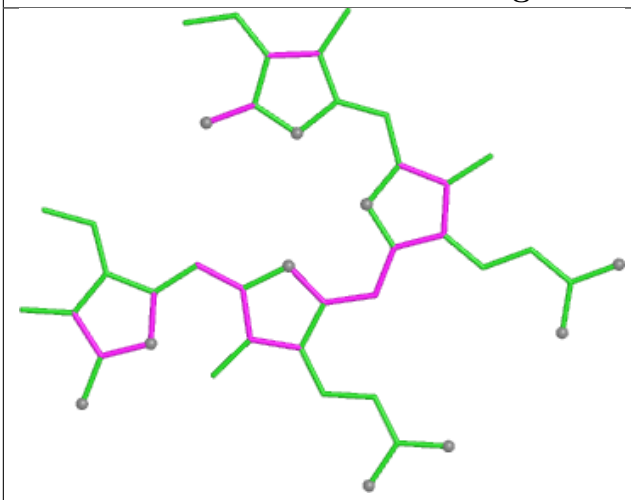


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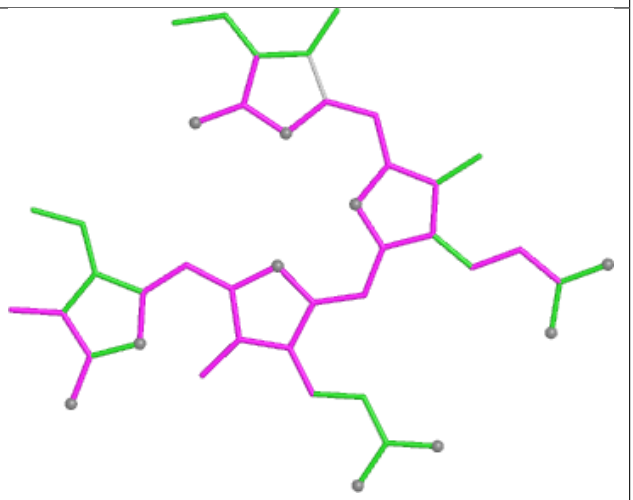


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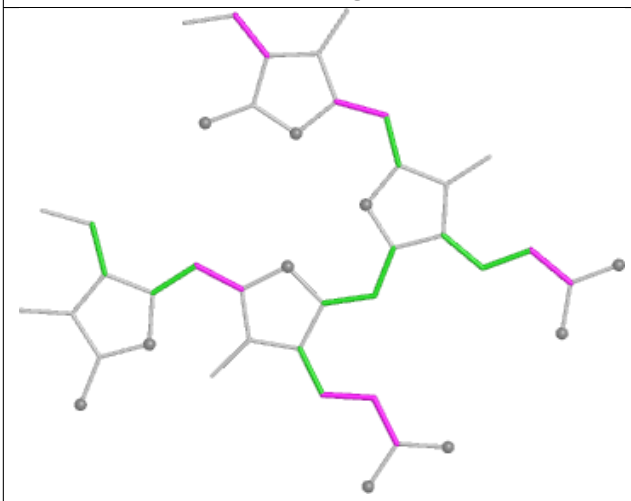
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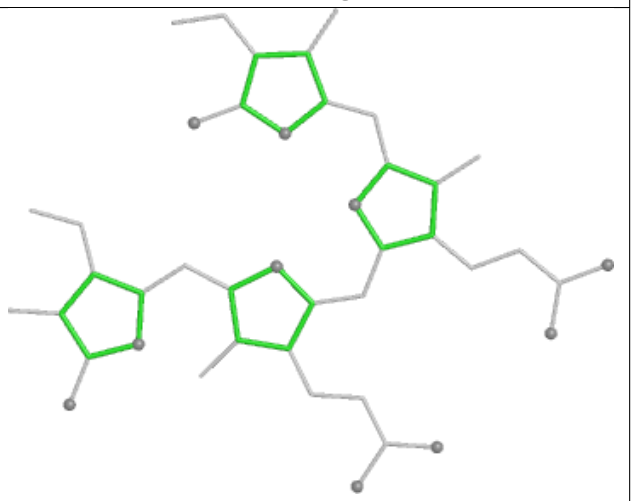
Bond lengths



Bond angles

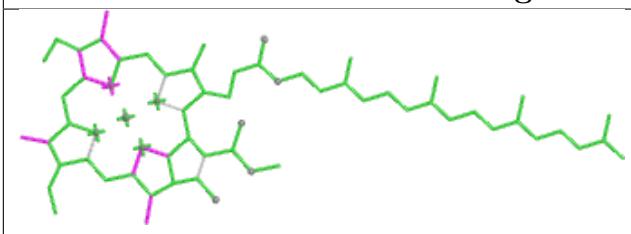


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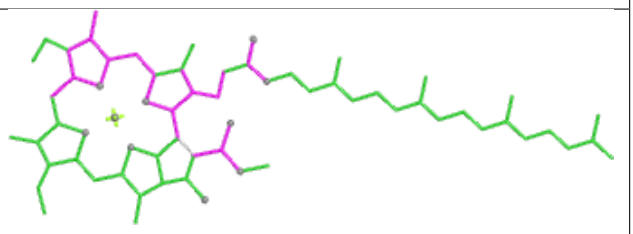


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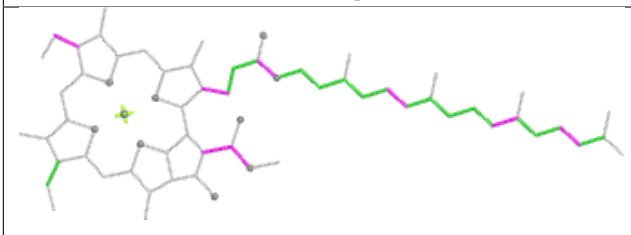
Ligand CLA A2 809



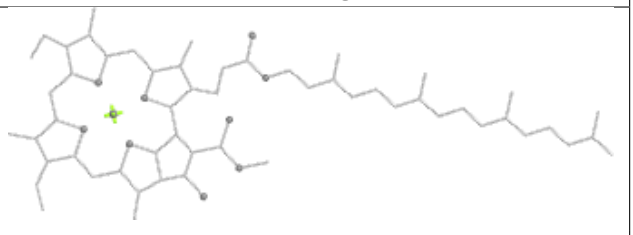
Bond lengths



Bond angles

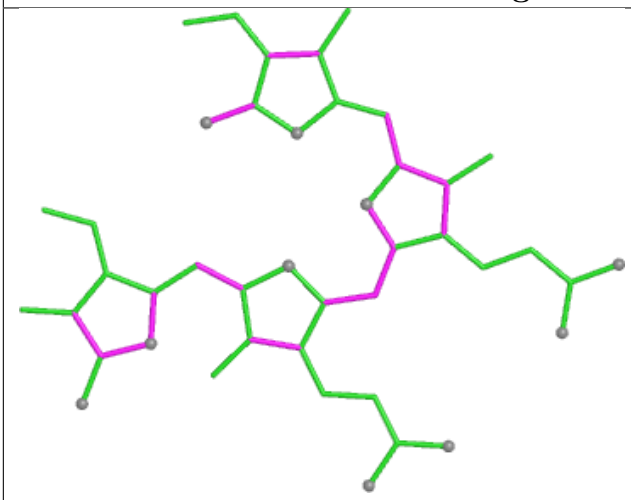


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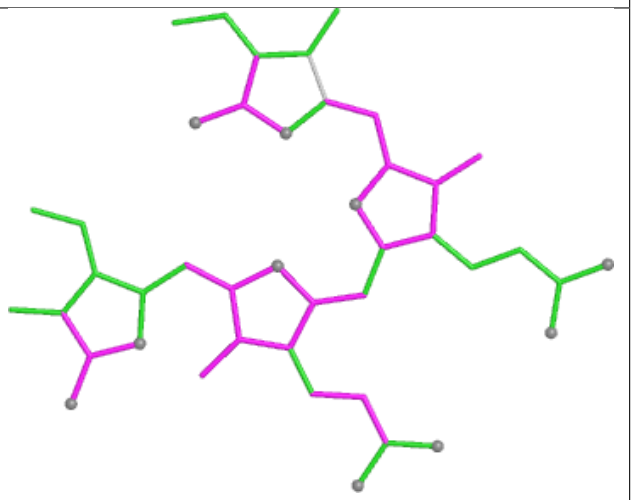


Rings

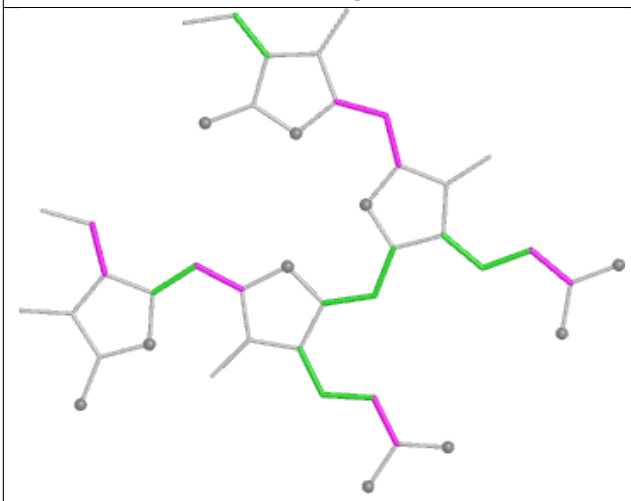
Ligand PEB TB 202



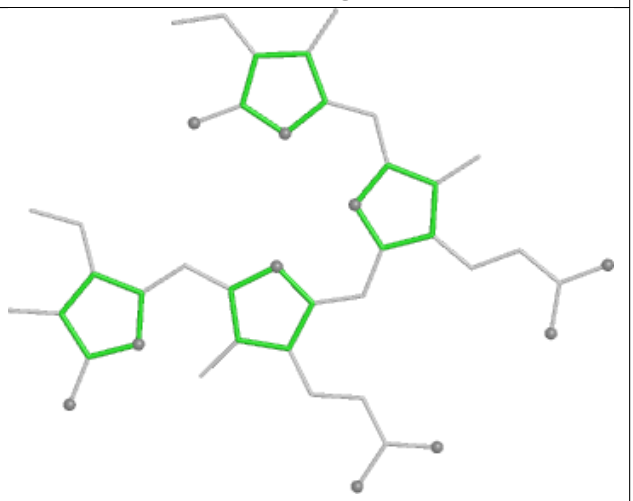
Bond lengths



Bond angles

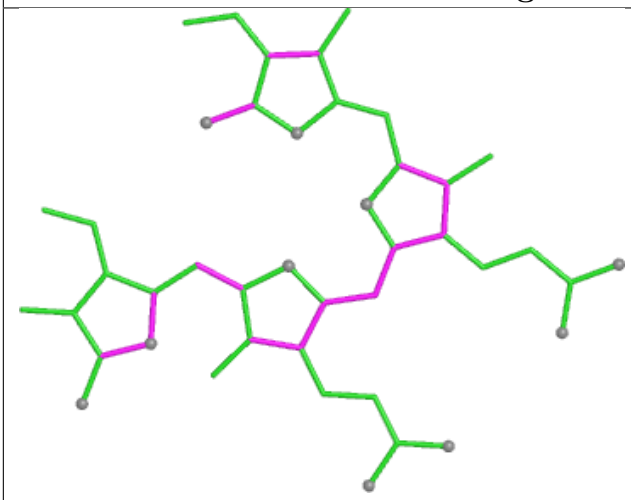


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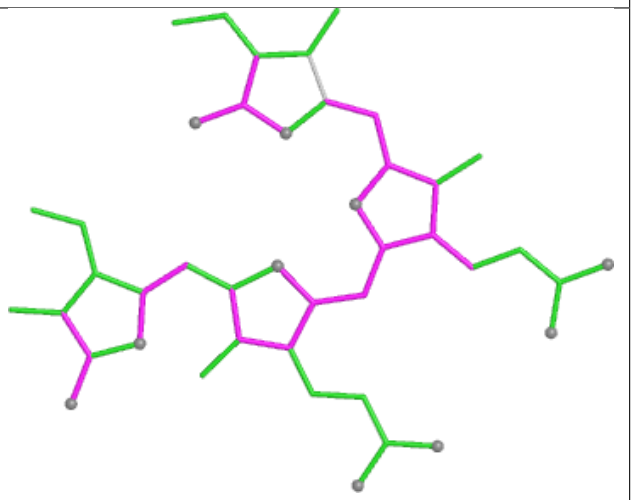


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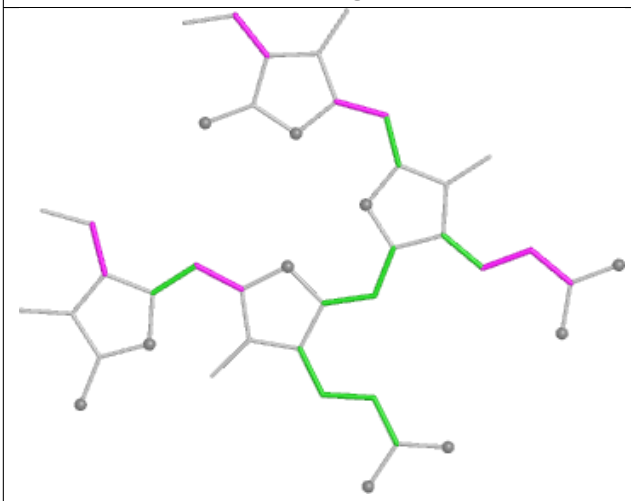
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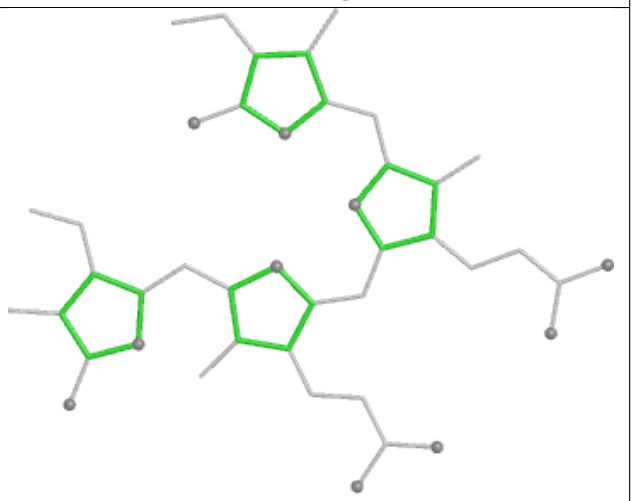
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Bond angles

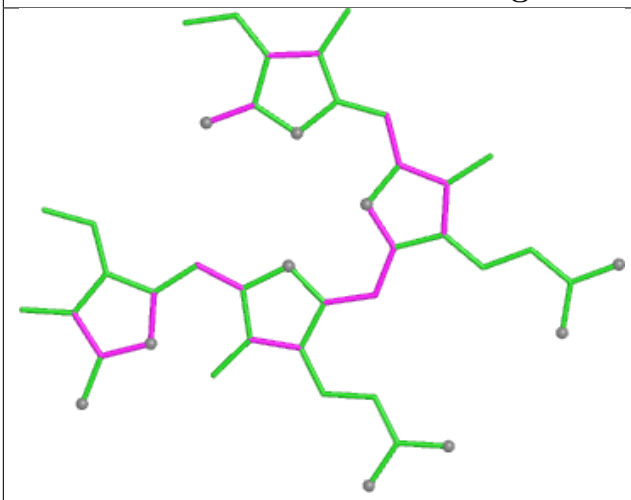


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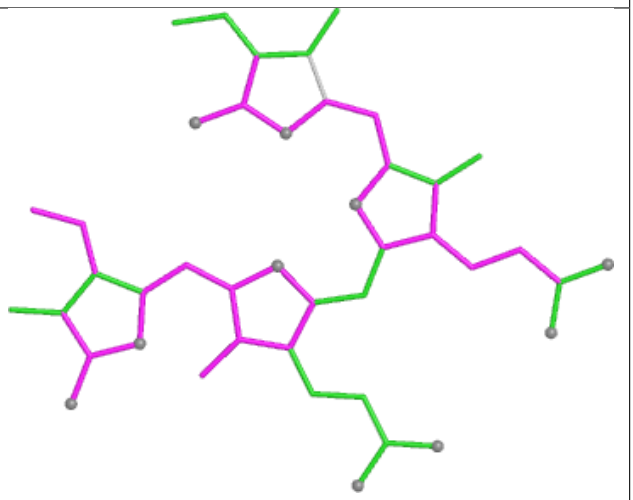


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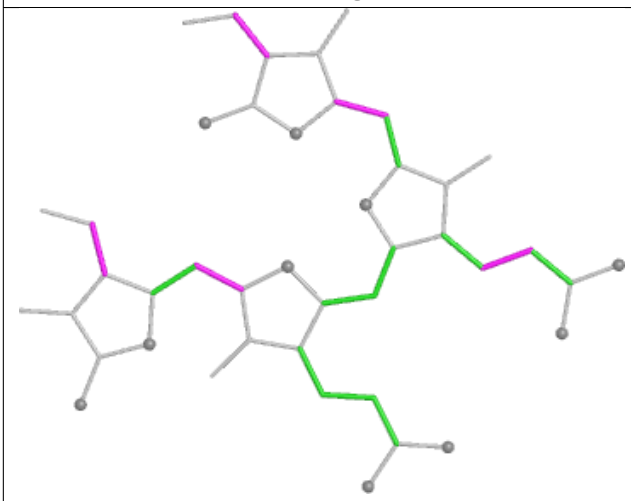
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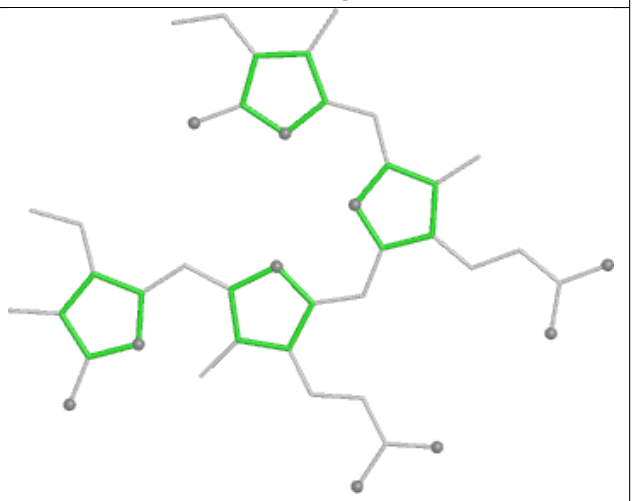
Bond lengths



Bond angles

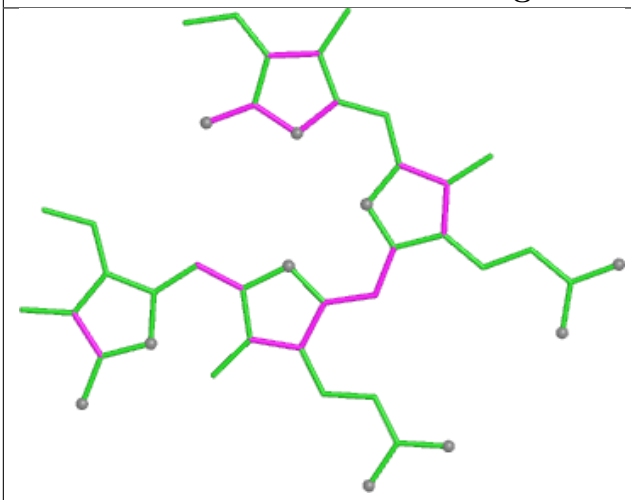


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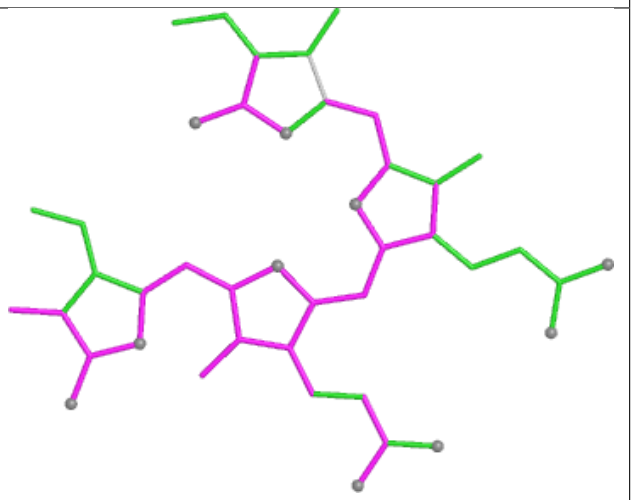


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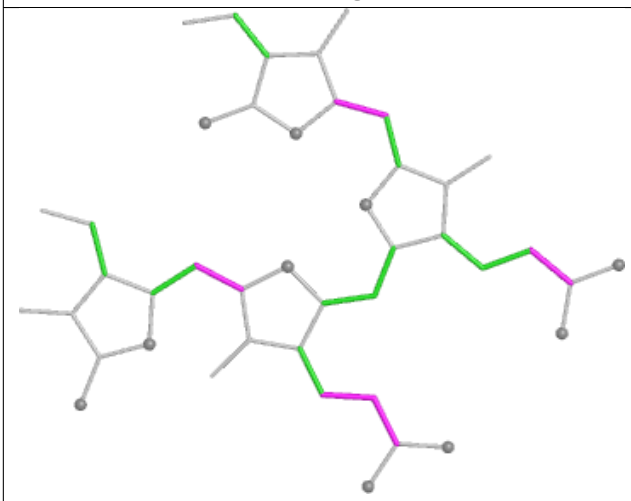
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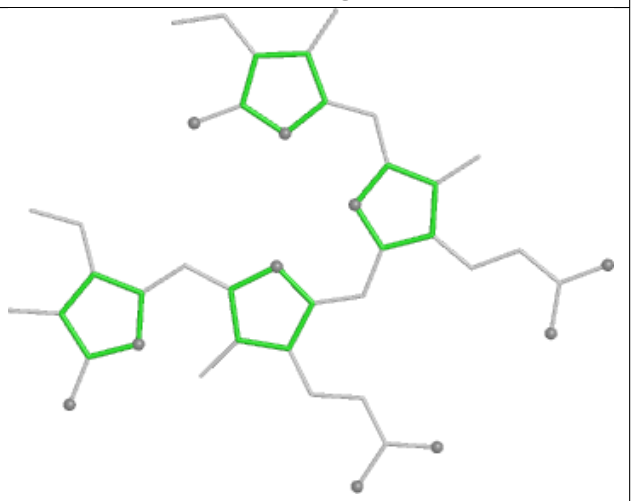
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Bond angles

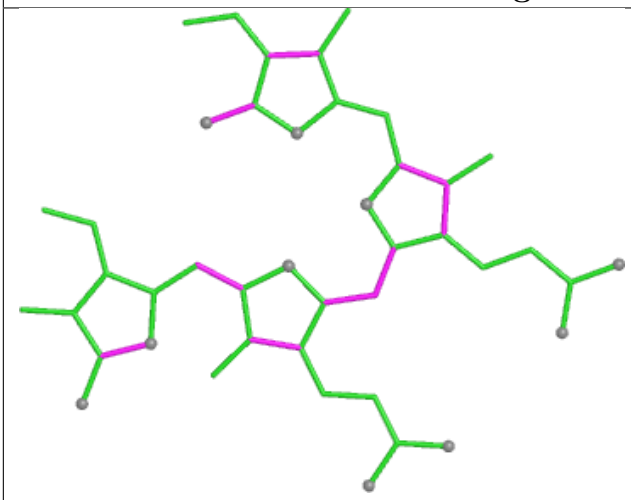


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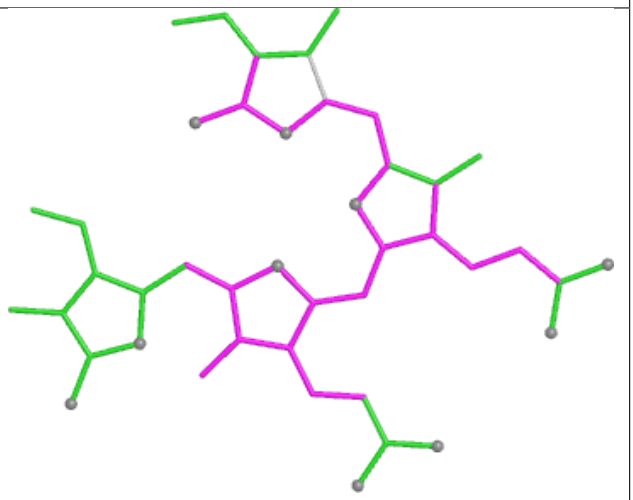


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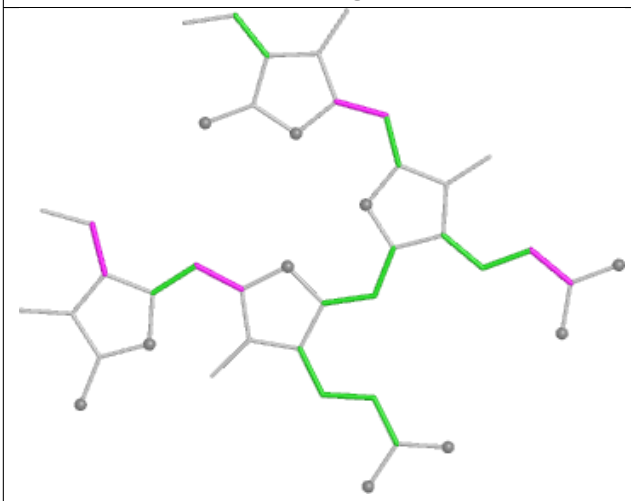
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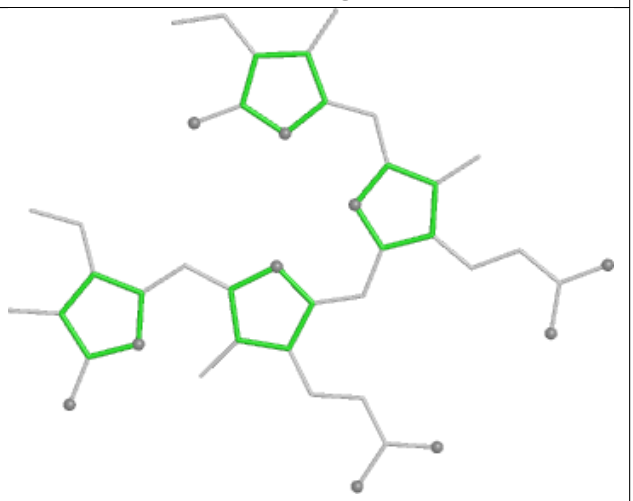
Bond lengths



Bond angles

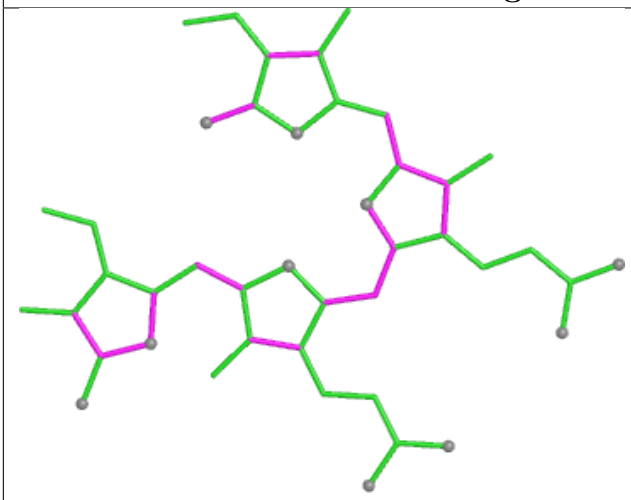


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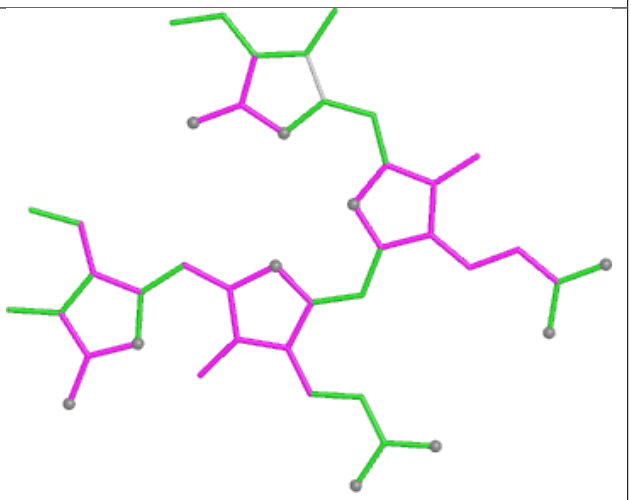


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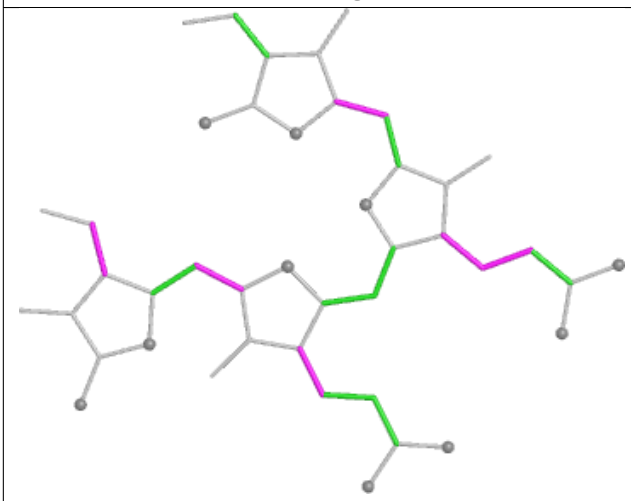
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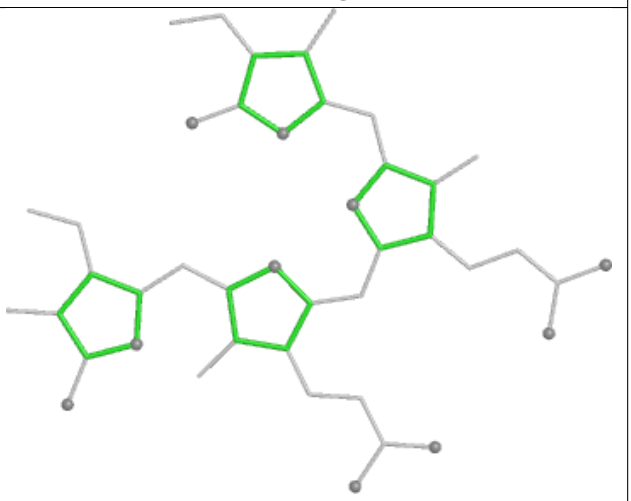
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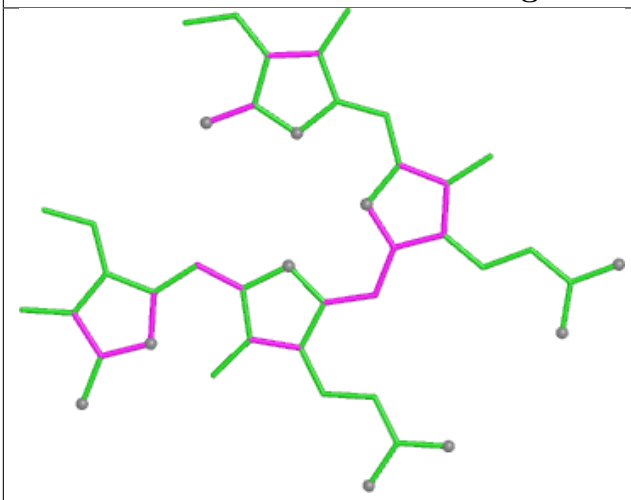


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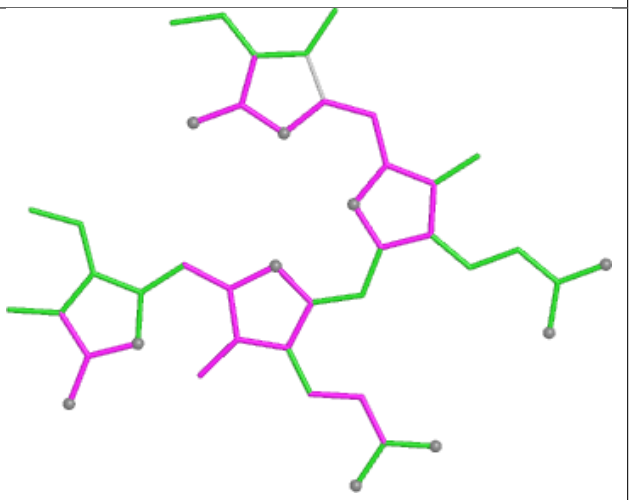


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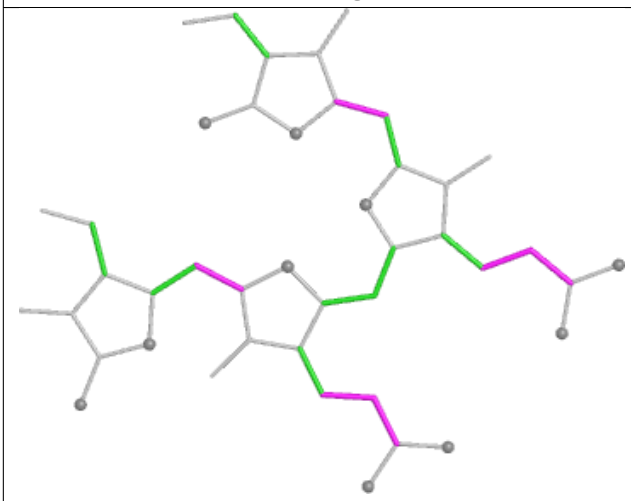
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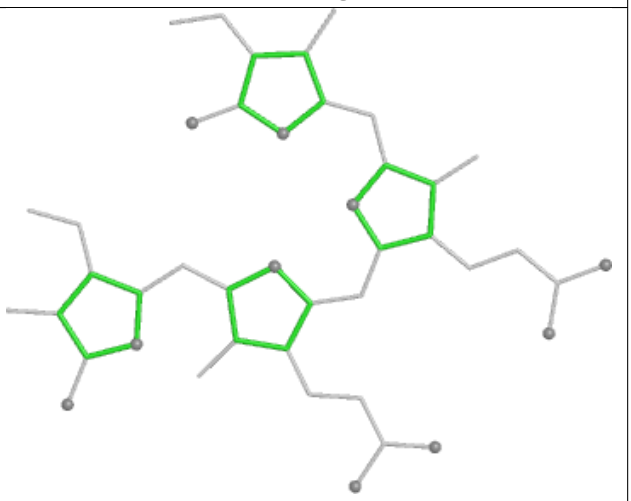
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Bond angles

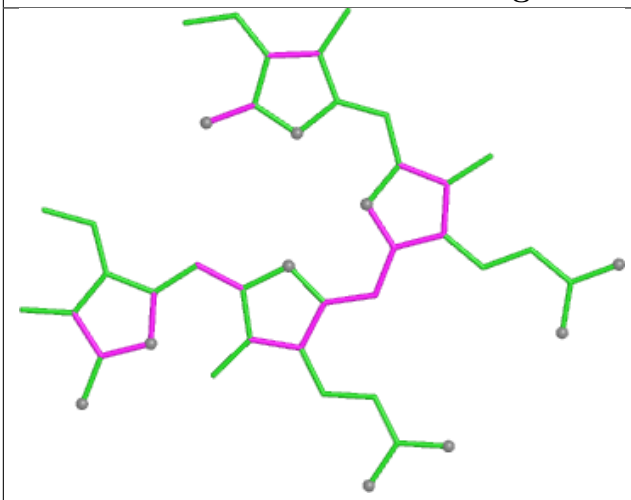


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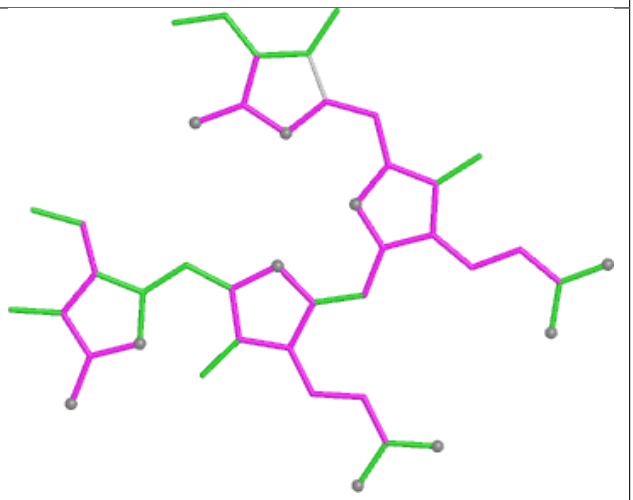


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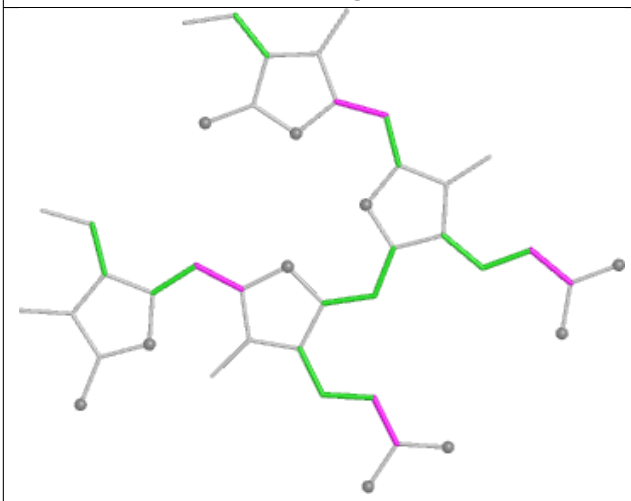
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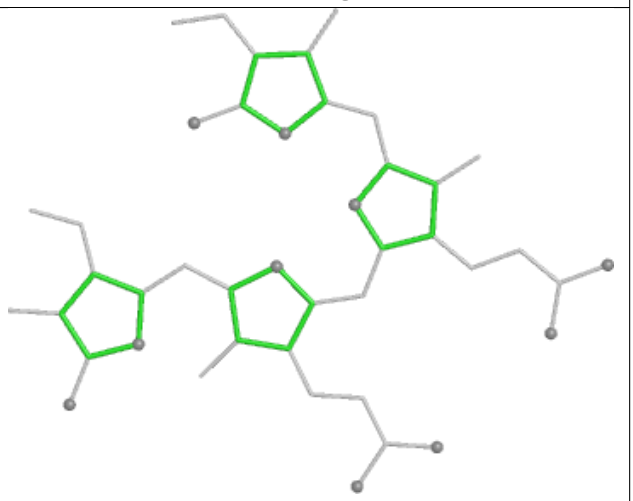
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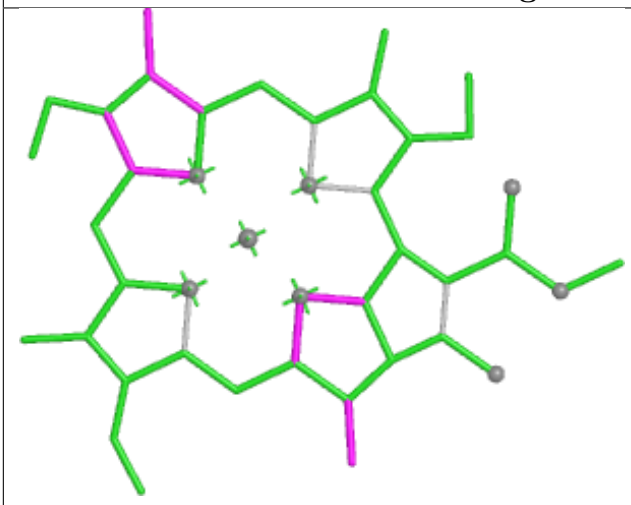


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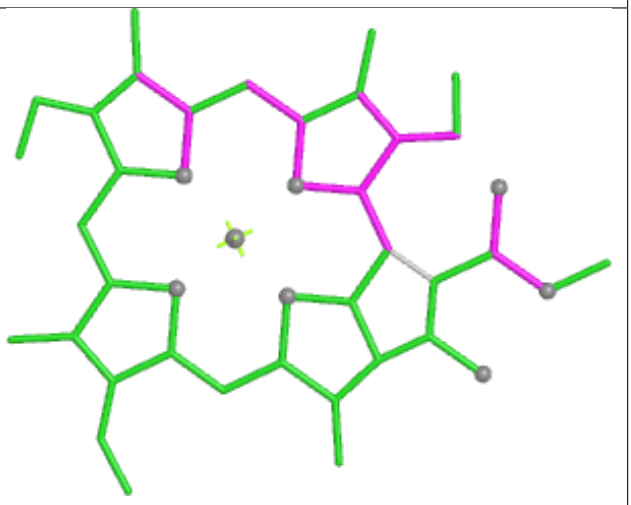


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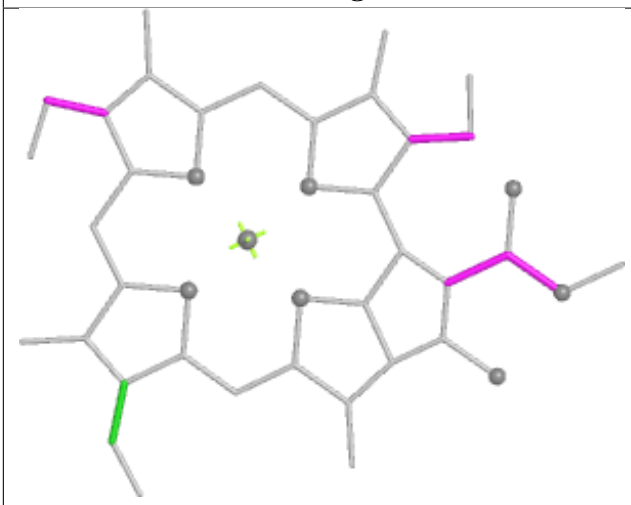
Ligand CLA 42 610



Bond lengths



Bond angles

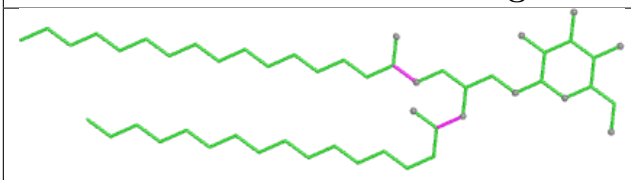


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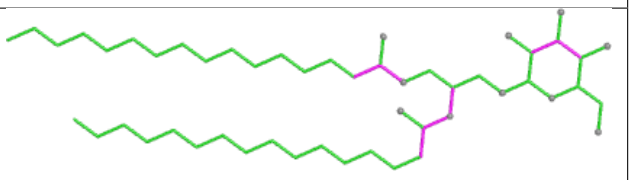


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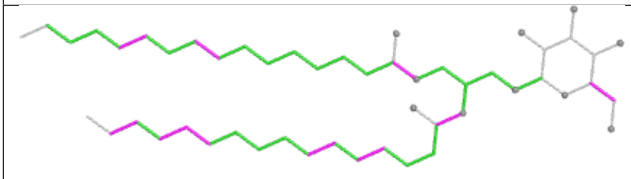
Ligand LMG AL 411



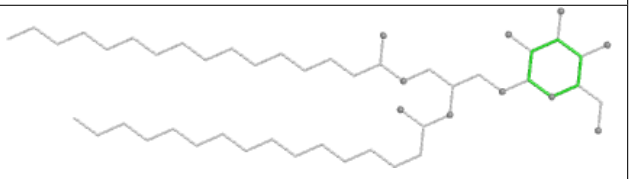
Bond lengths



Bond angles

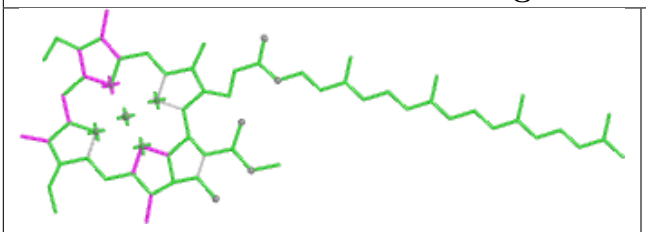


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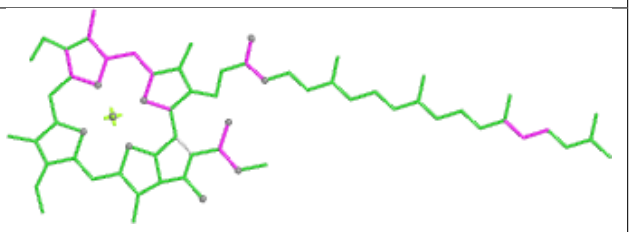


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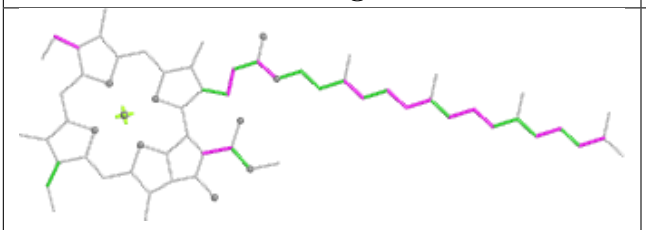
Ligand CLA BL 609



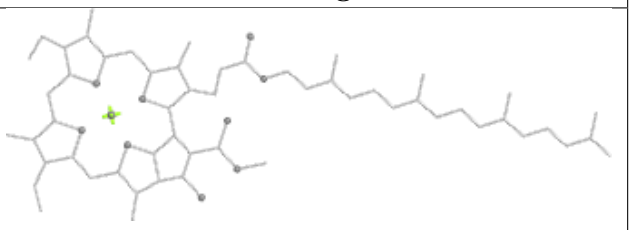
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Bond angles

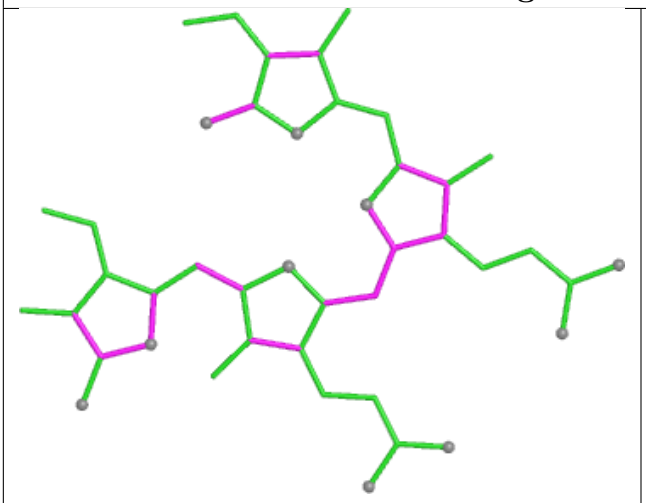


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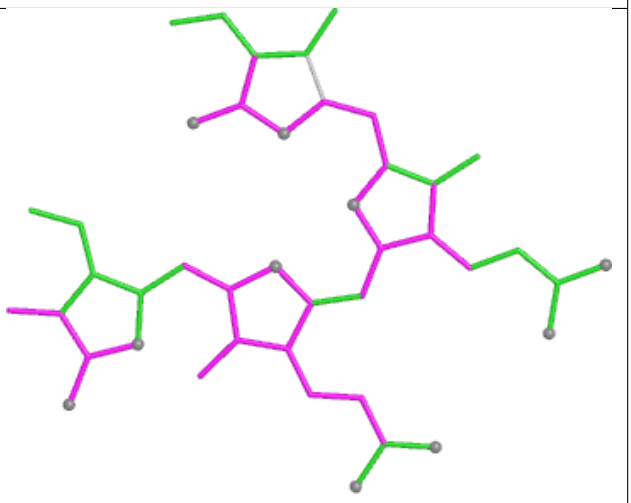


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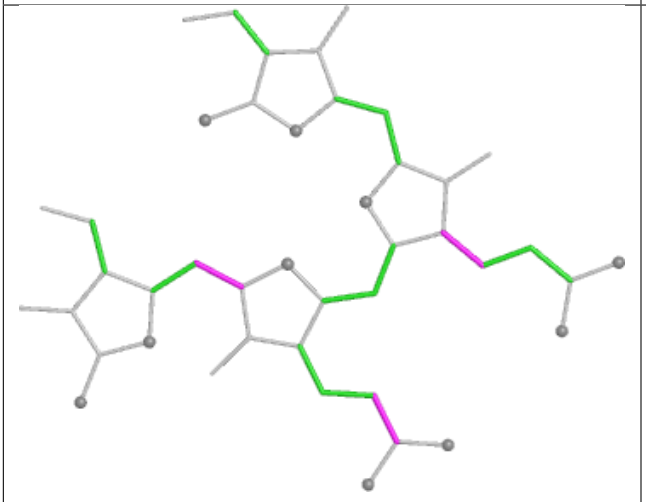
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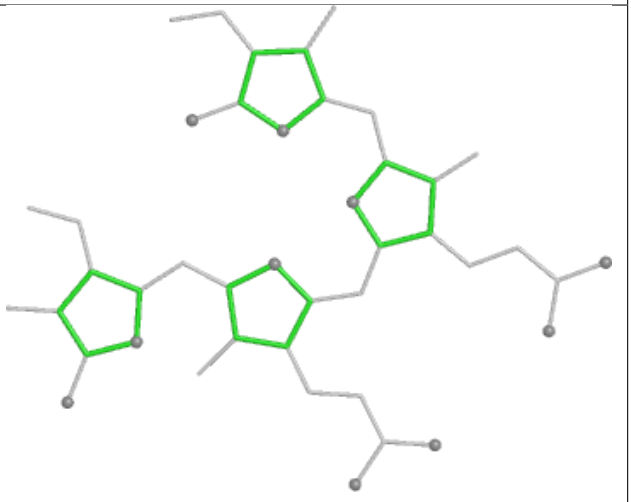
Bond lengths



Bond angles

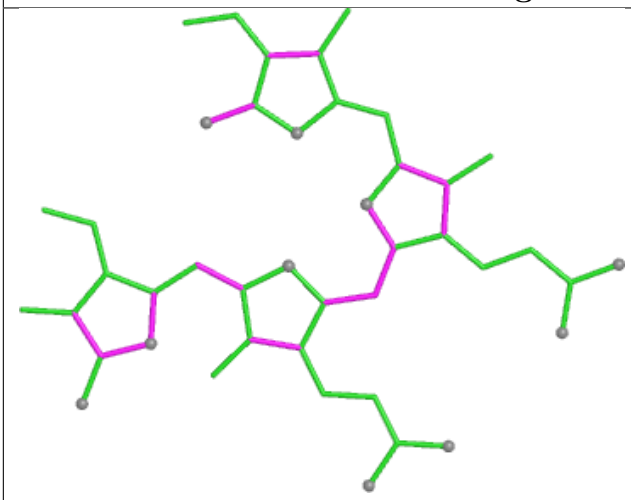


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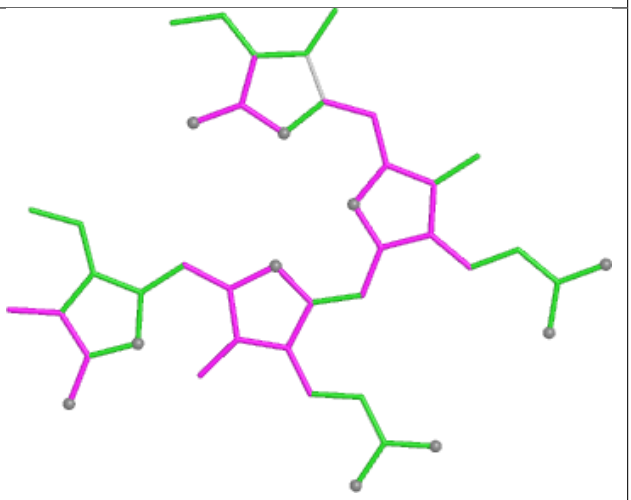


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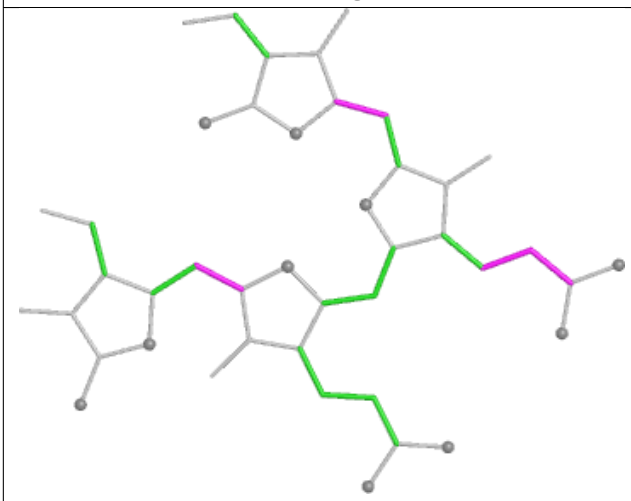
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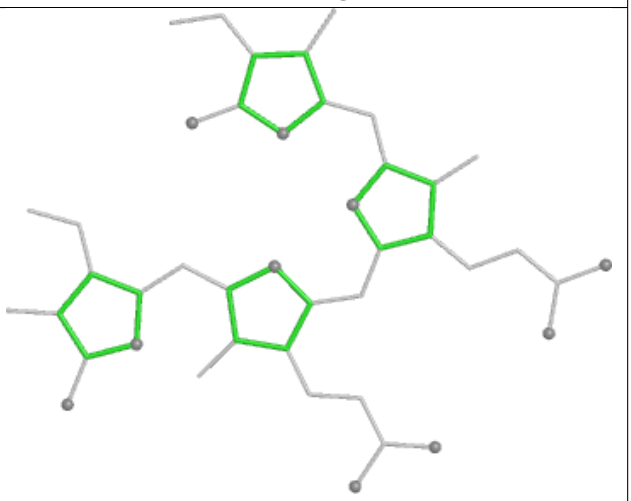
Bond lengths



Bond angles

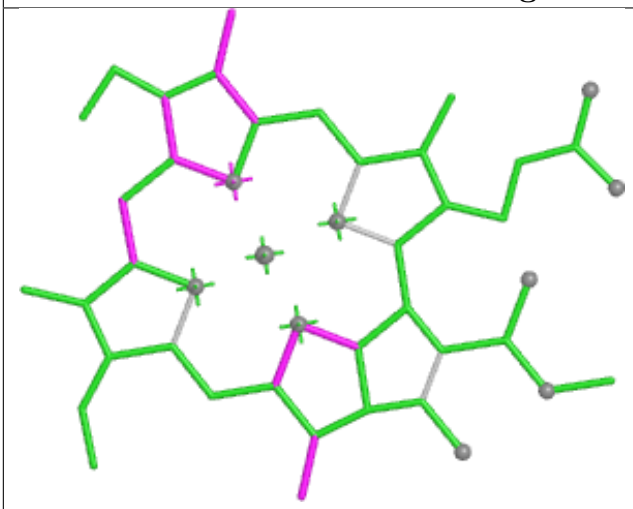


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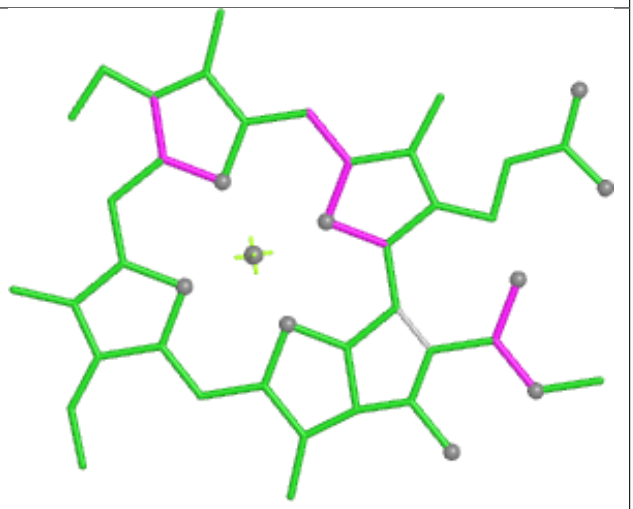


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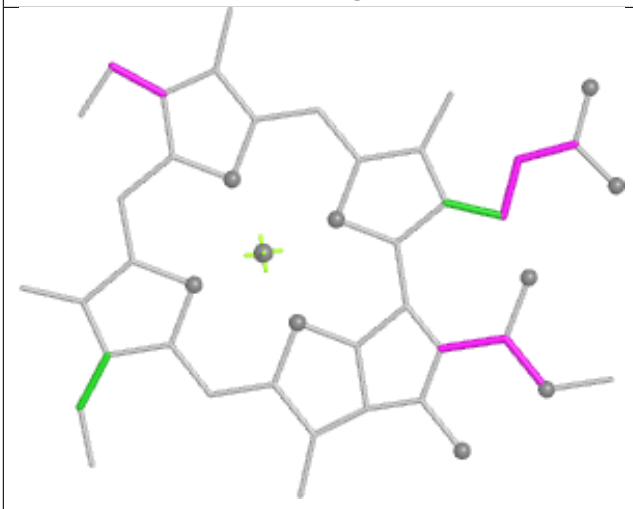
Ligand CLA 52 603



Bond lengths



Bond angles

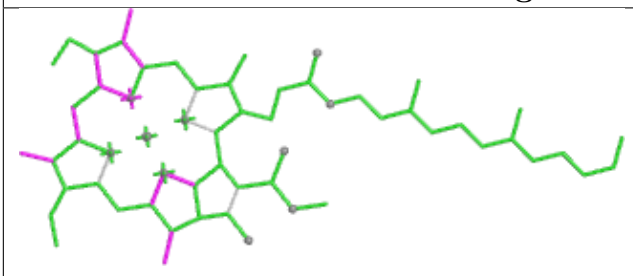


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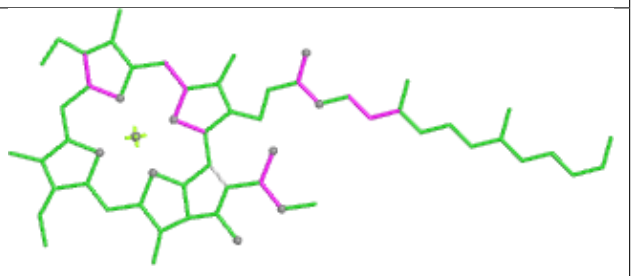


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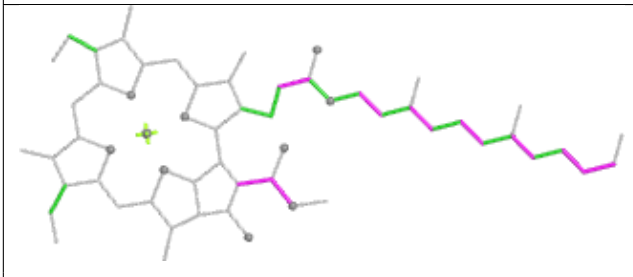
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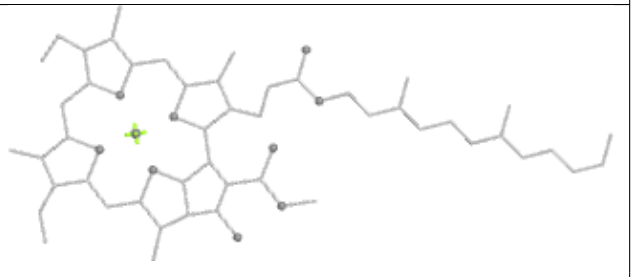
Bond lengths



Bond angles

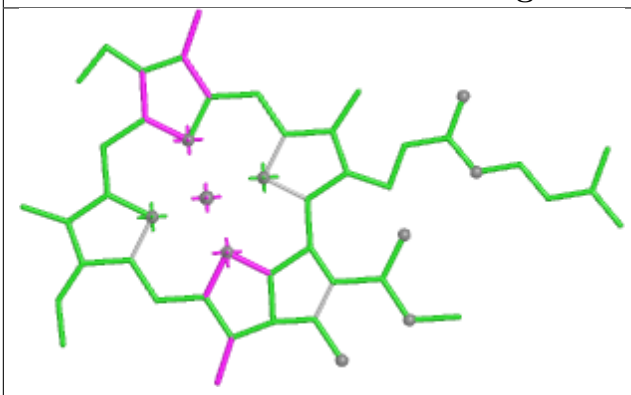


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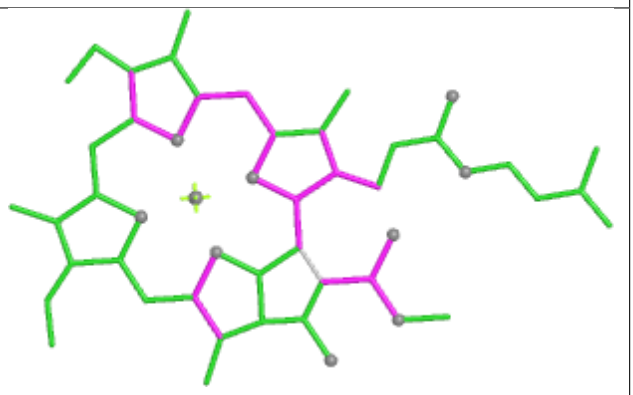


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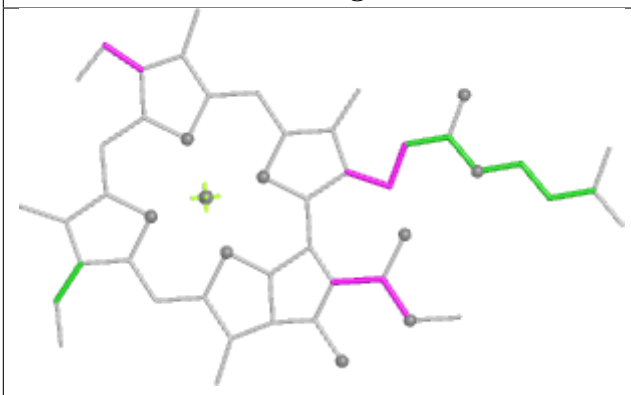
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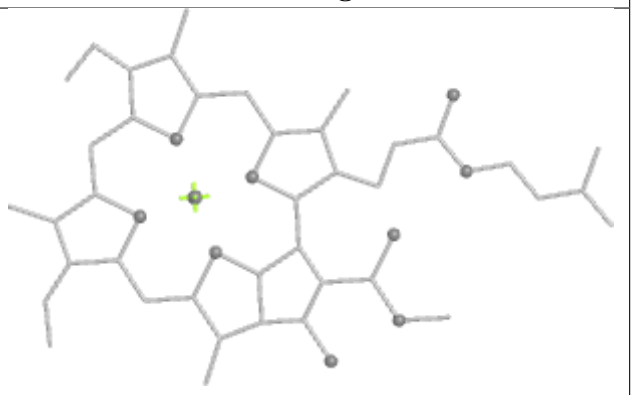
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Bond angles

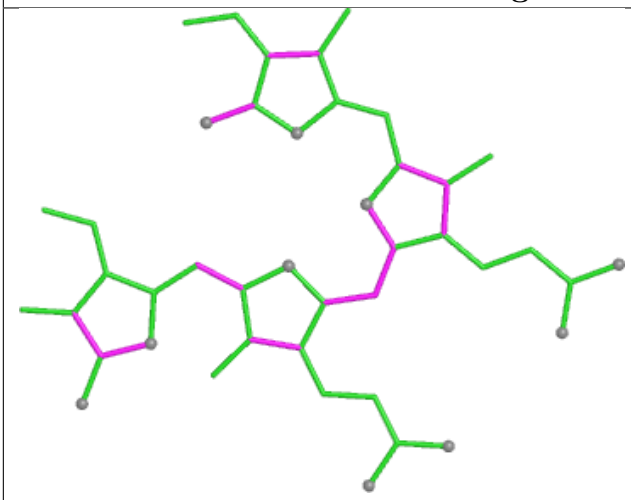


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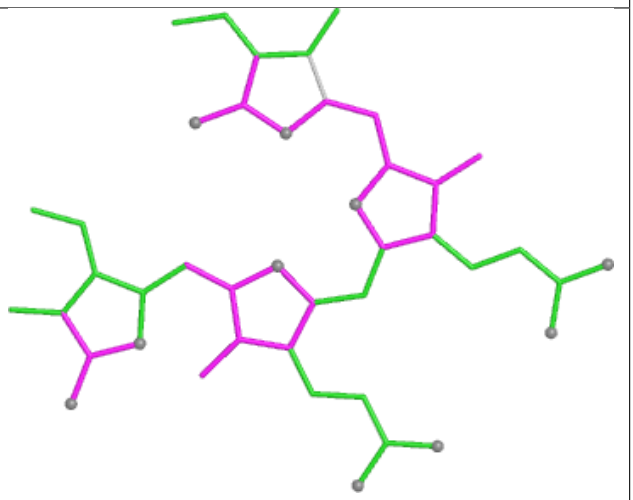


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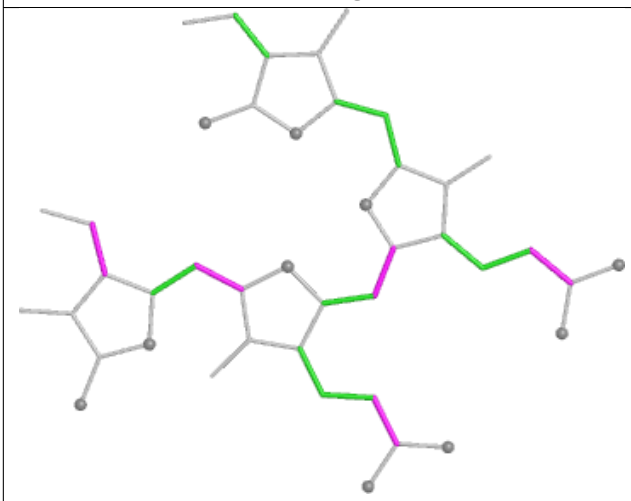
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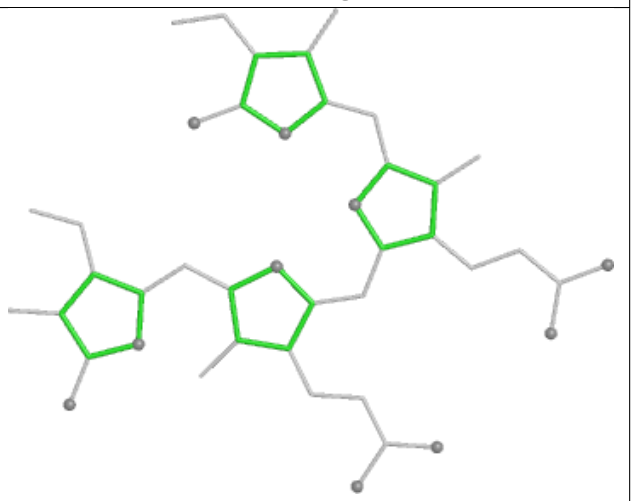
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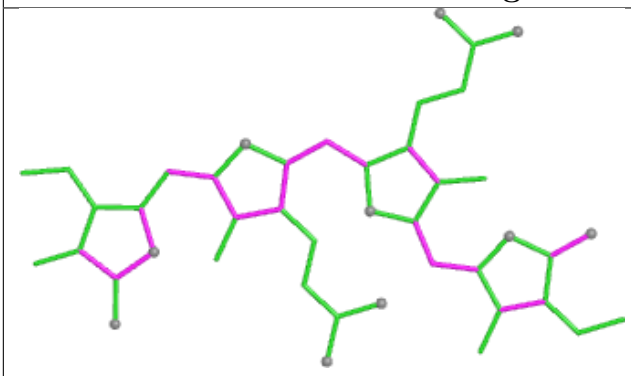


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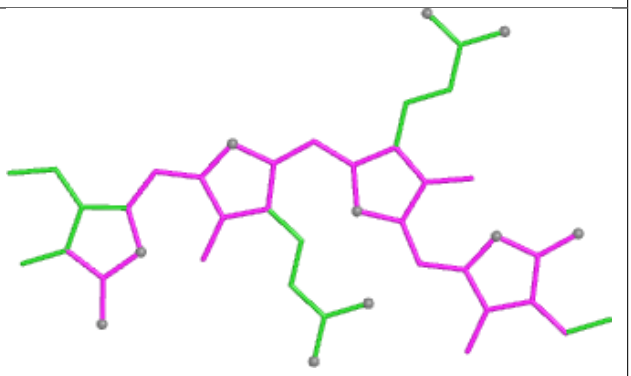


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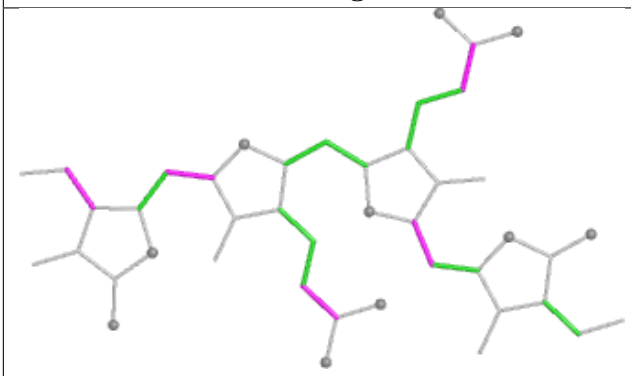
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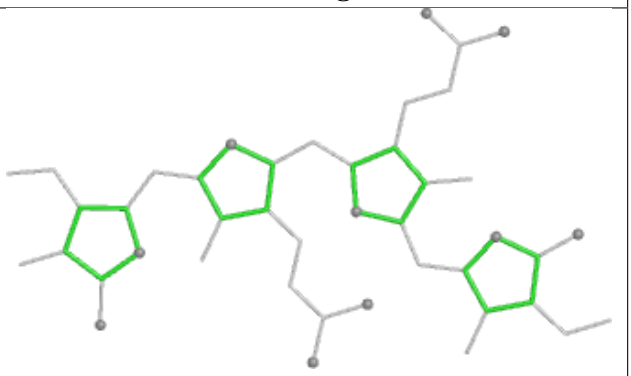
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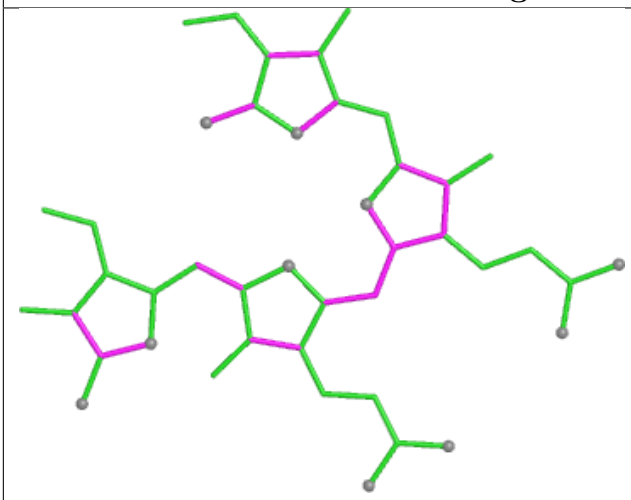


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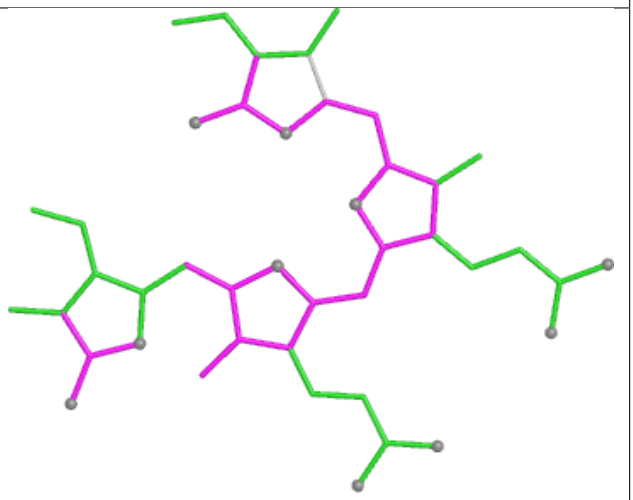


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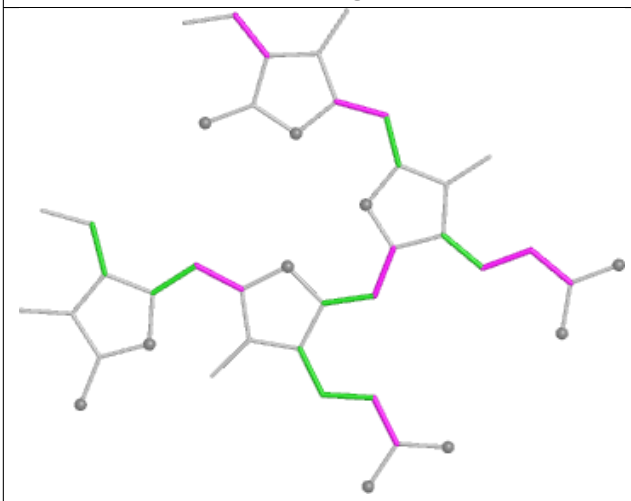
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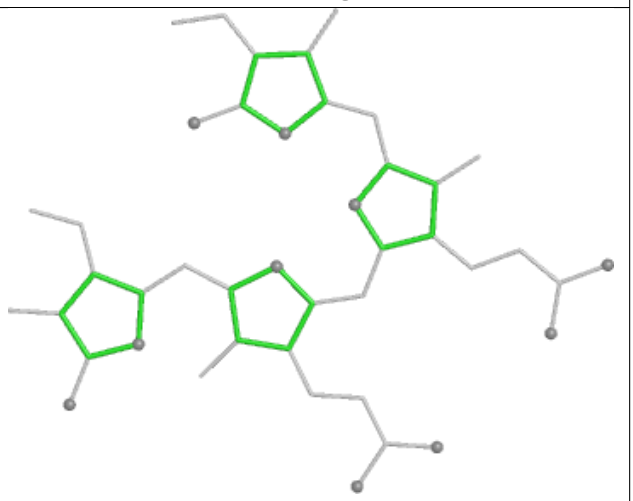
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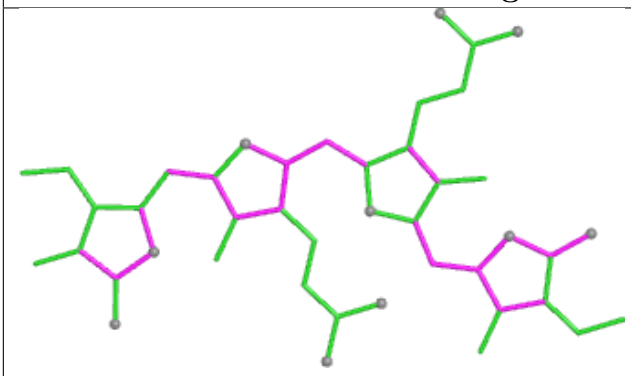


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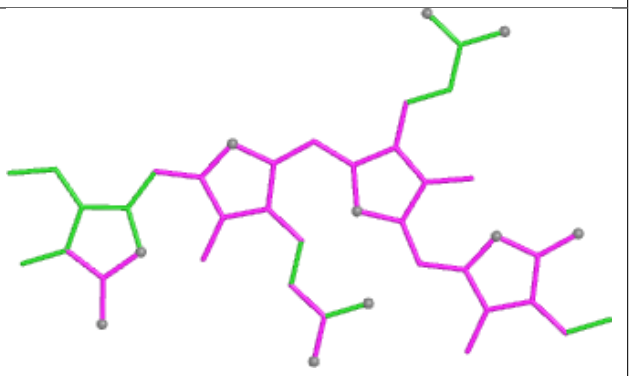


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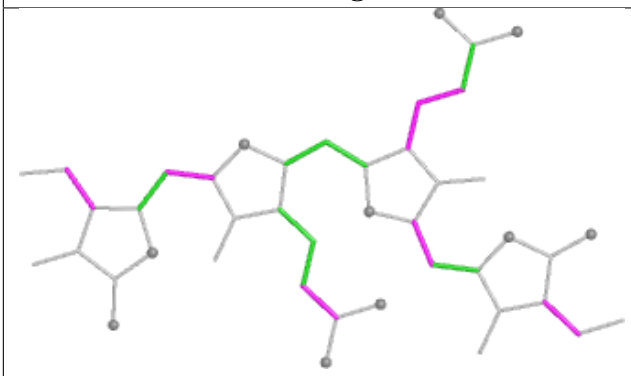
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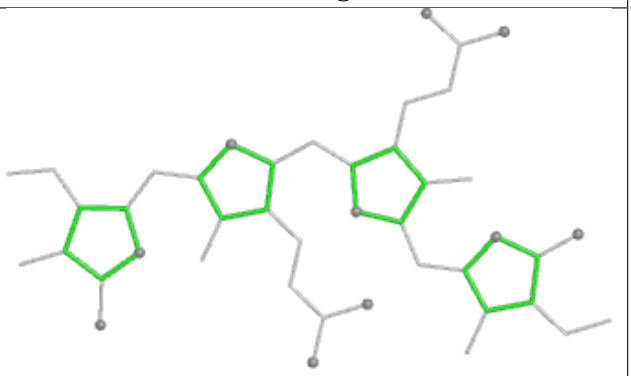
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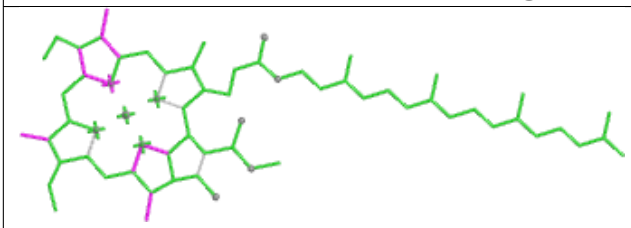


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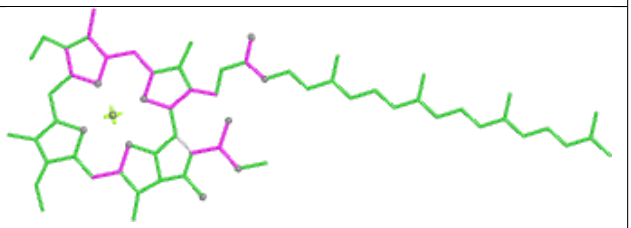


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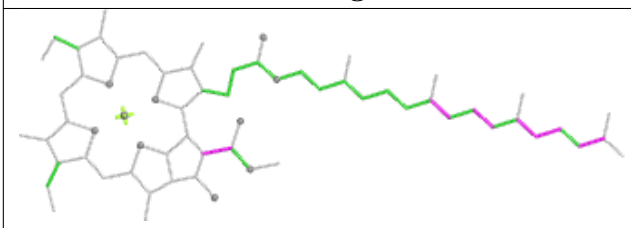
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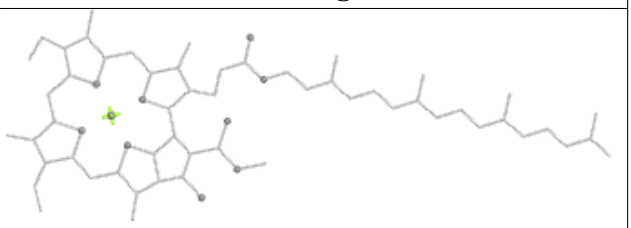
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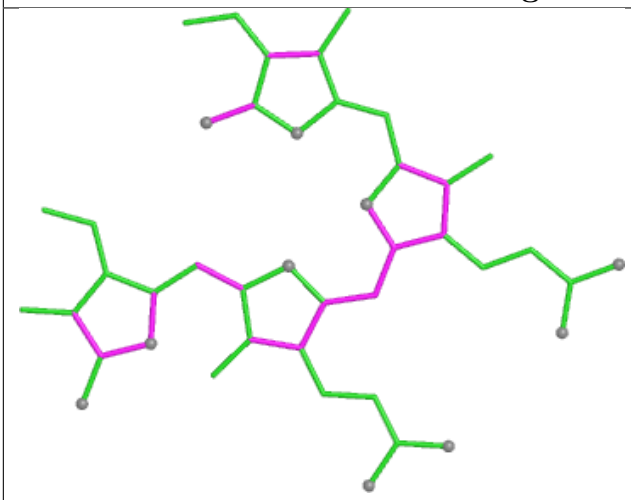


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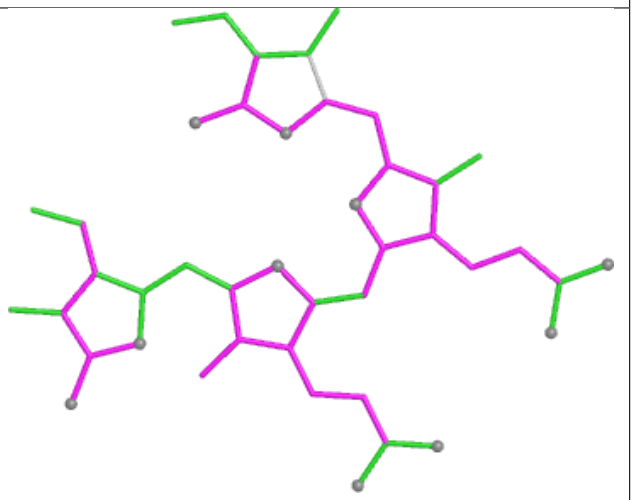


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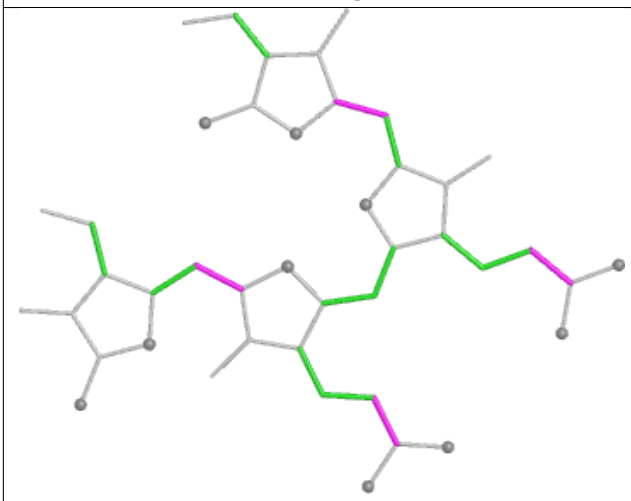
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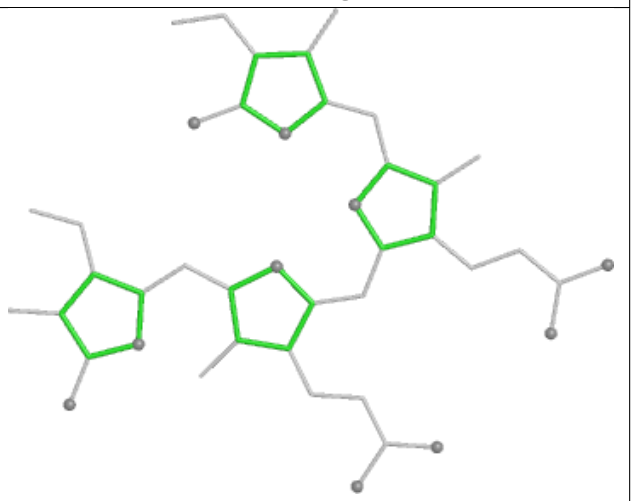
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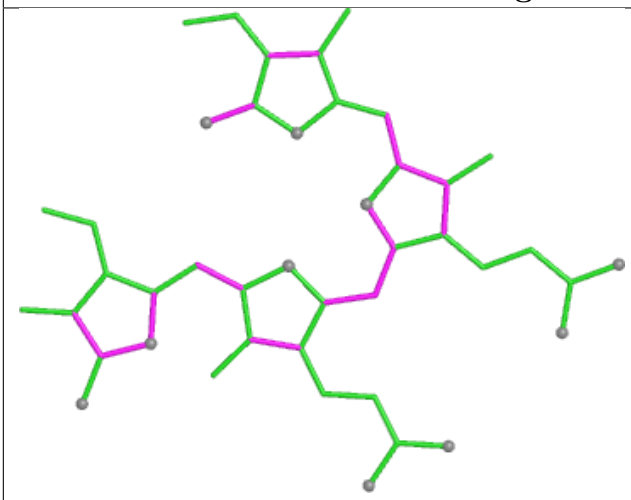


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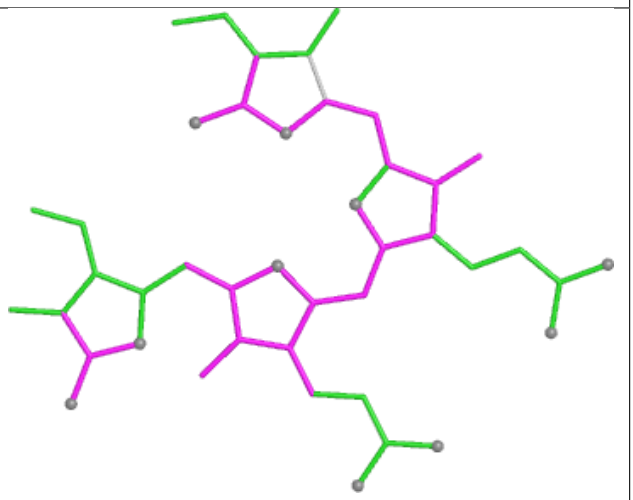


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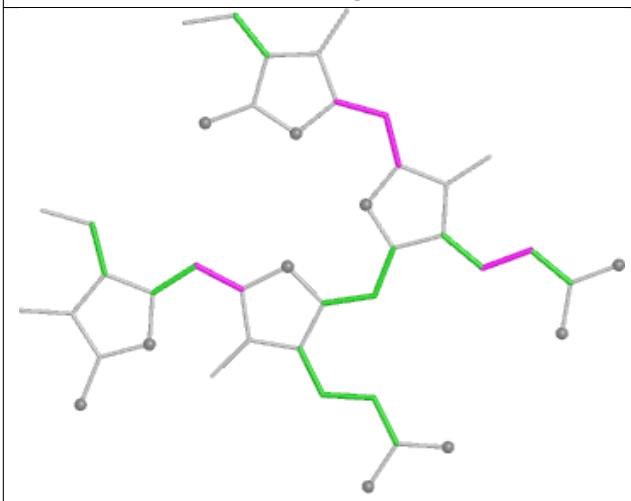
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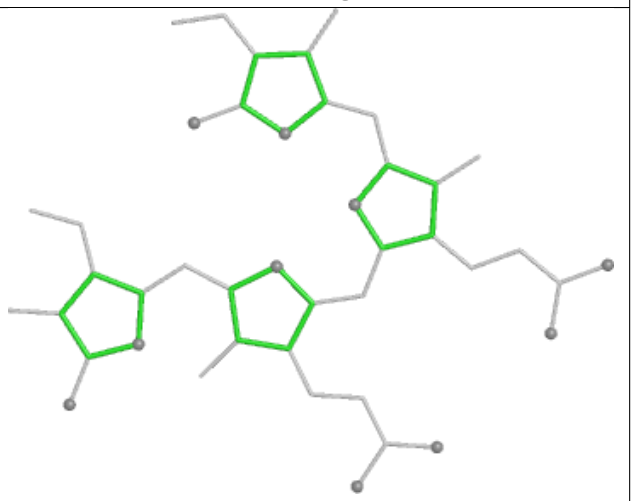
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Bond angles

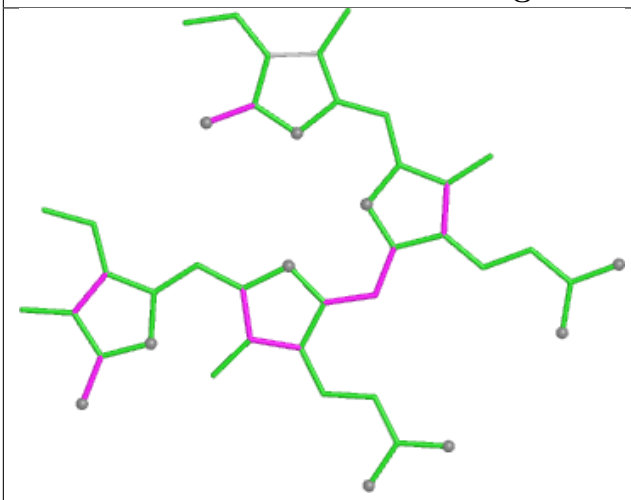


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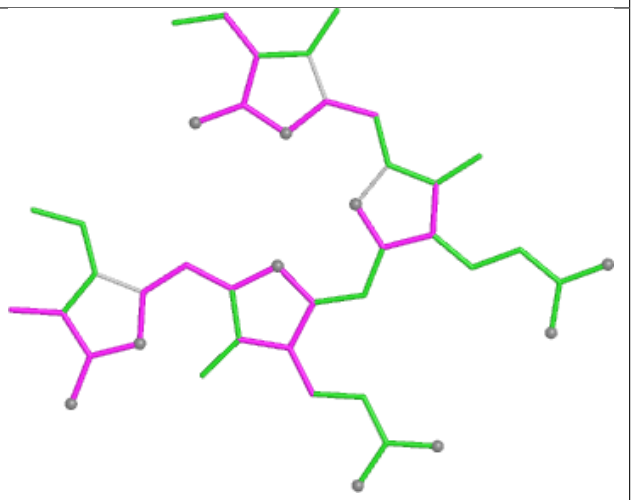


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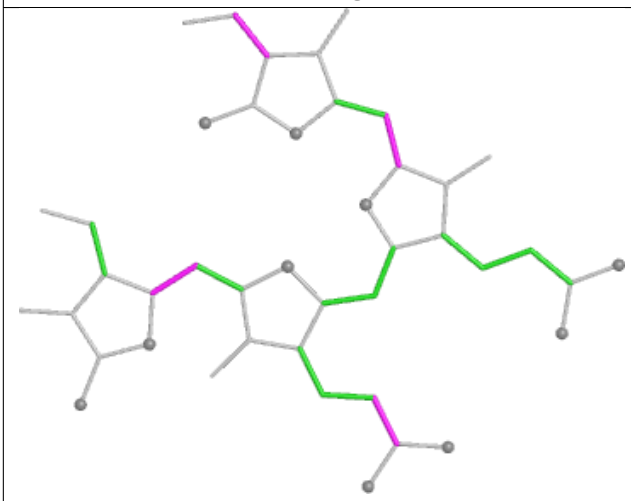
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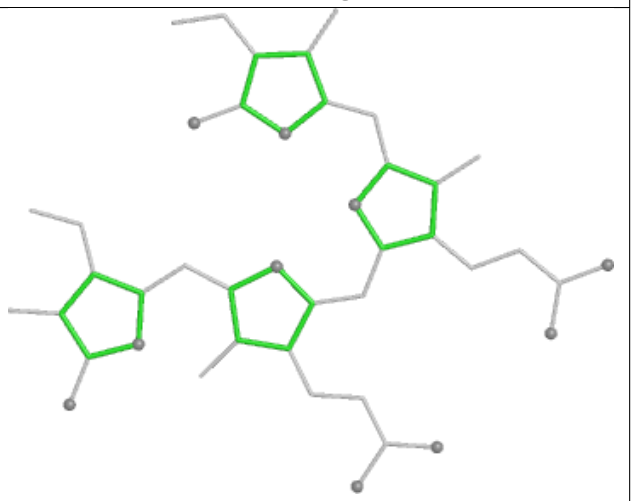
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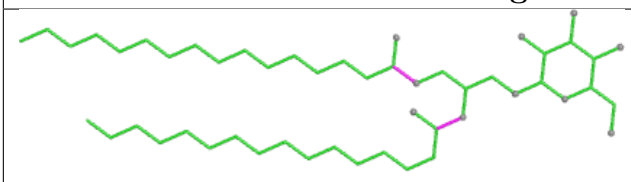


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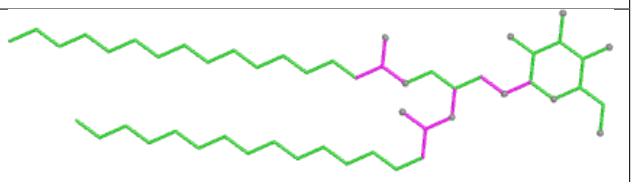


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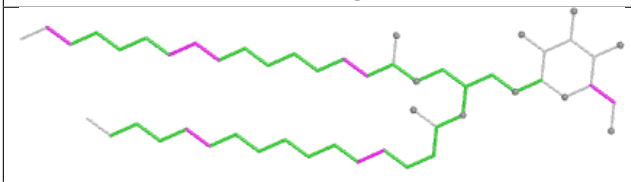
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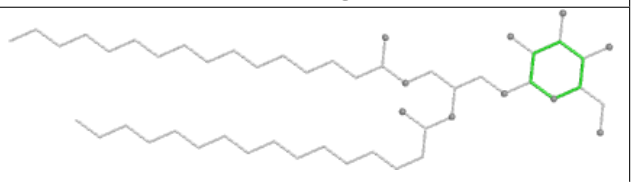
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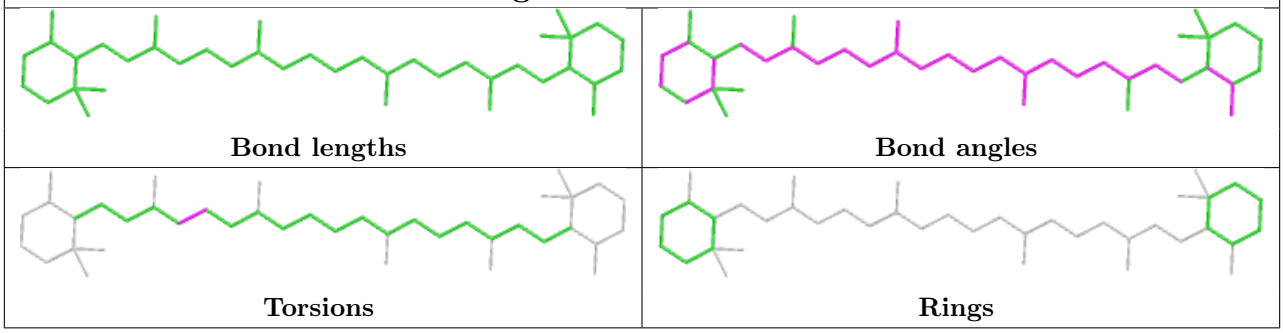


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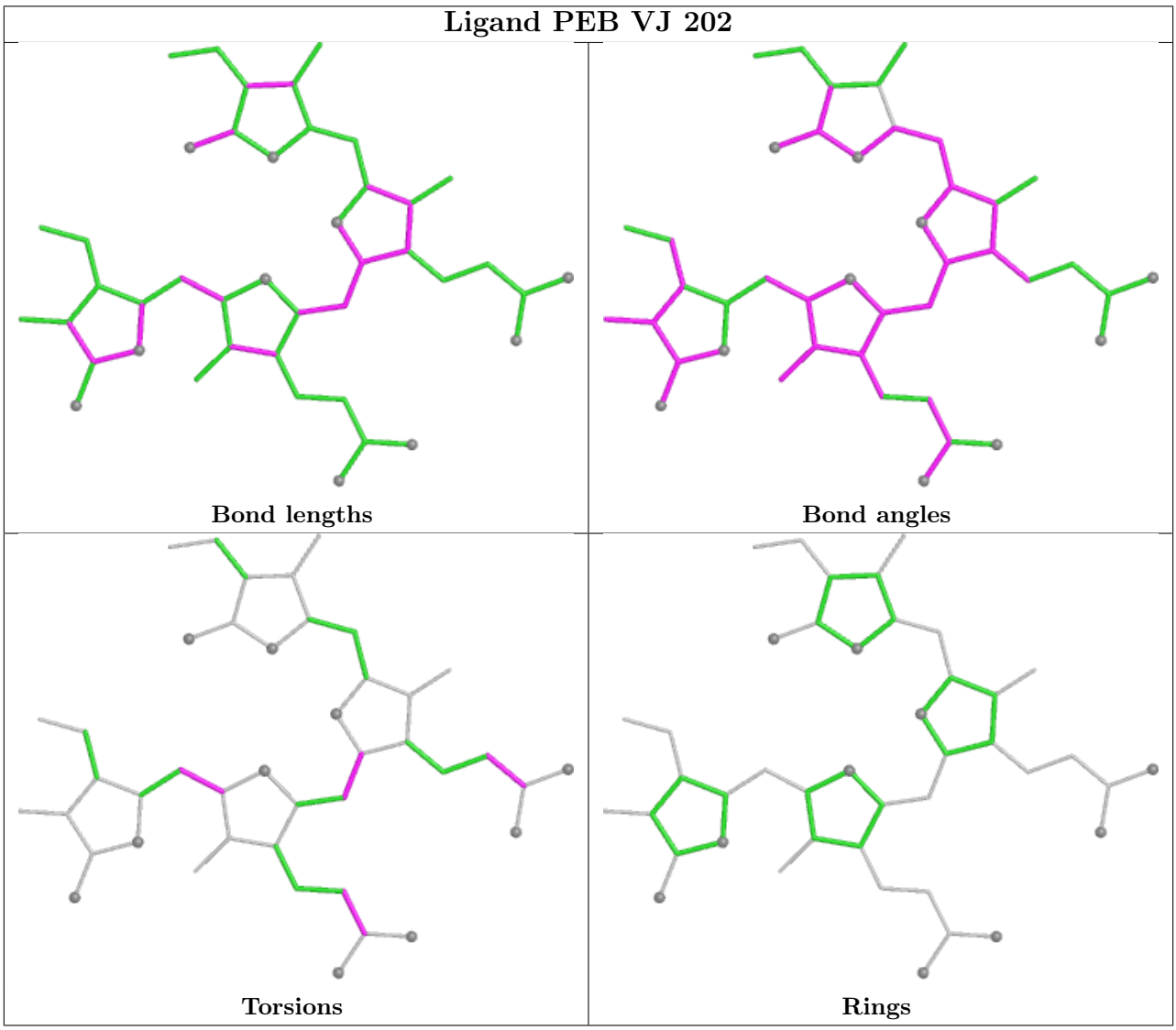


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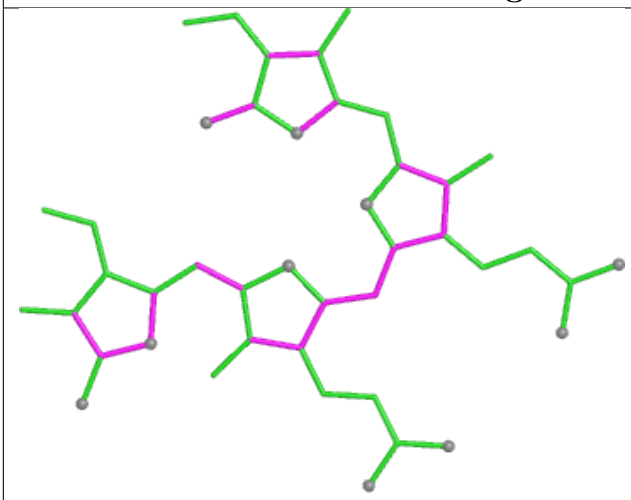
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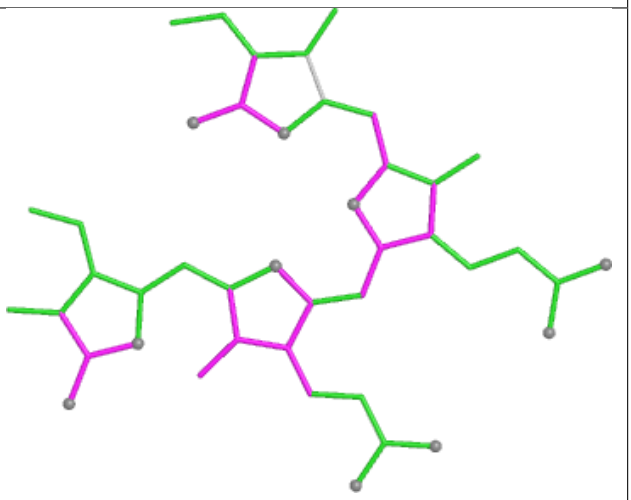
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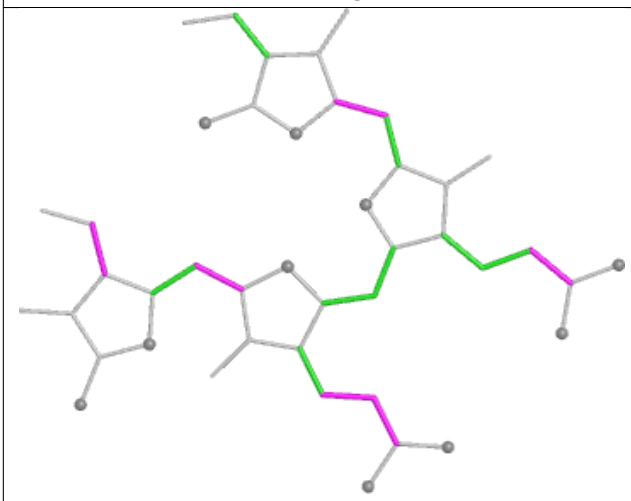
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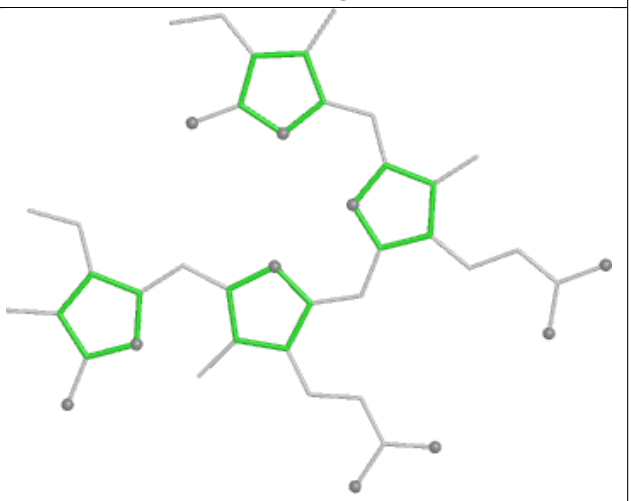
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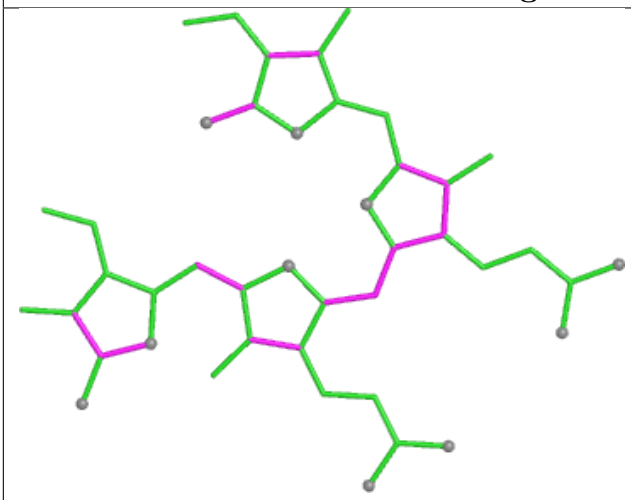


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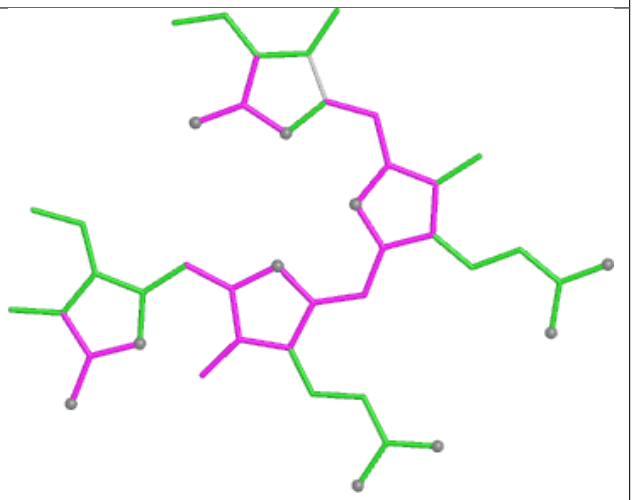


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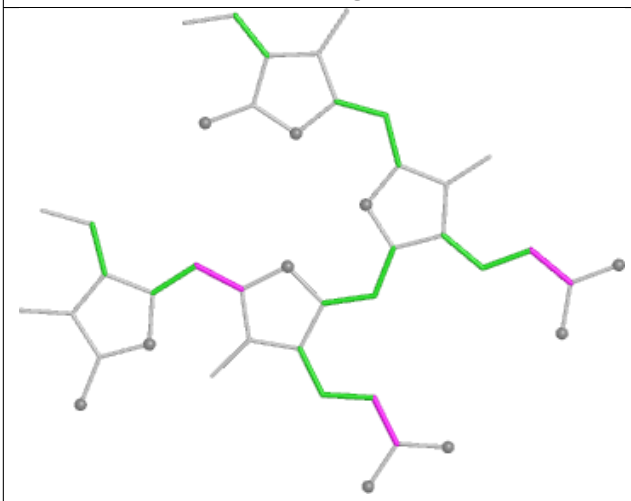
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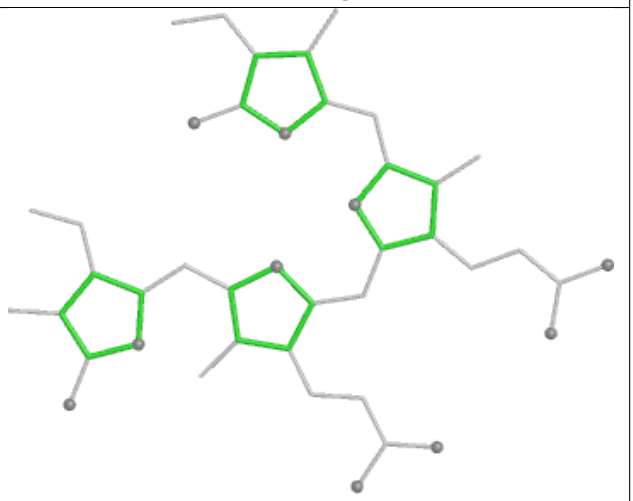
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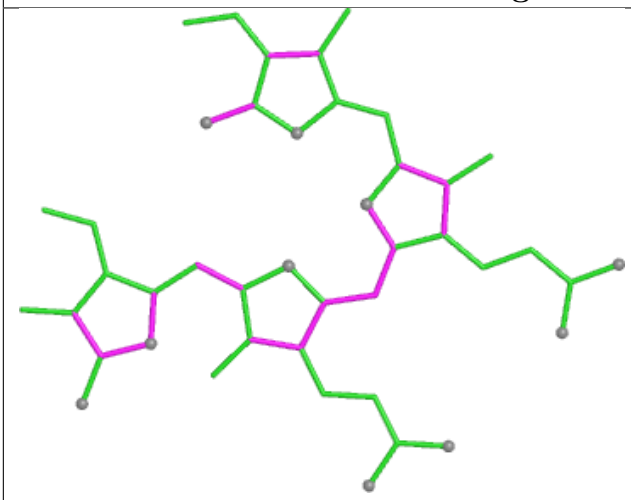


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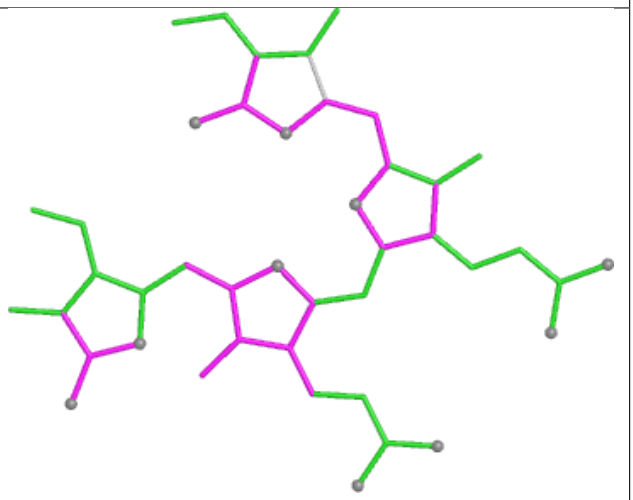


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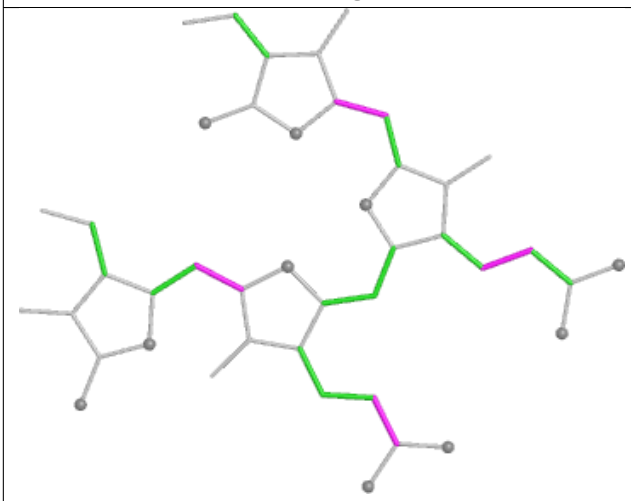
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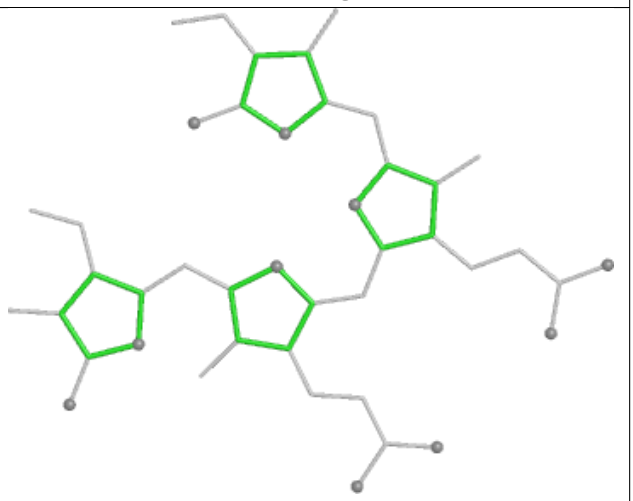
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Bond angles

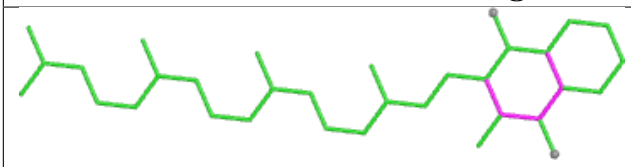


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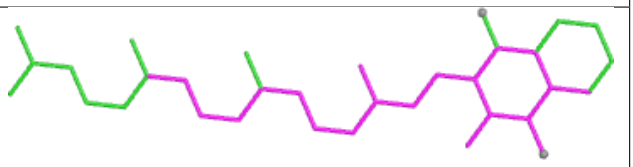


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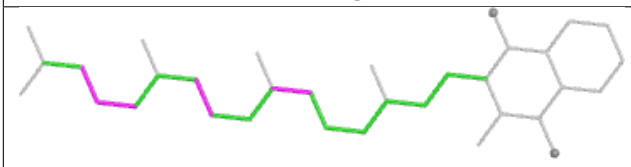
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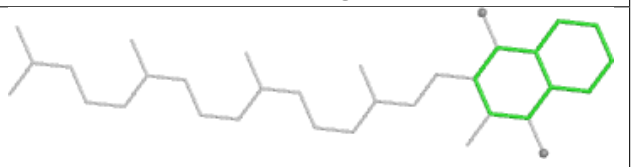
Bond lengths



Bond angles

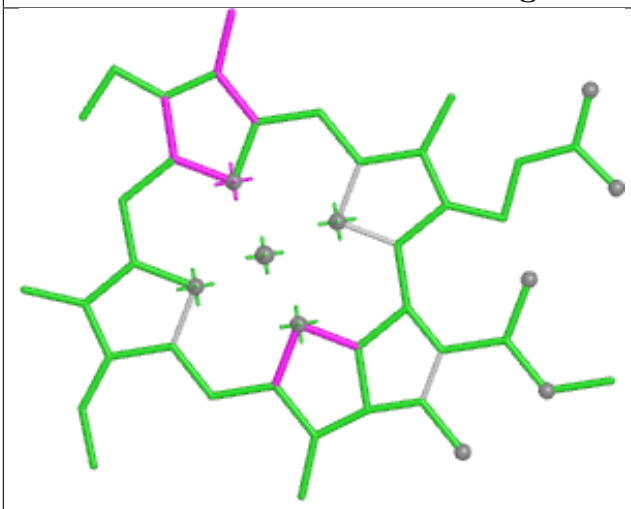


Torsions

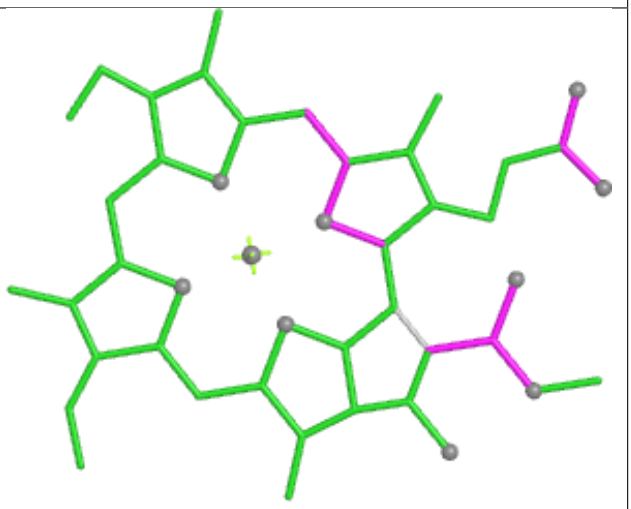


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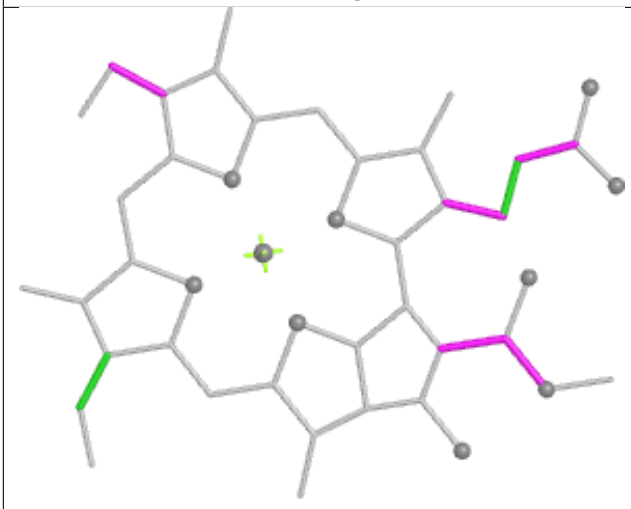
Ligand CLA 22 606



Bond lengths



Bond angles

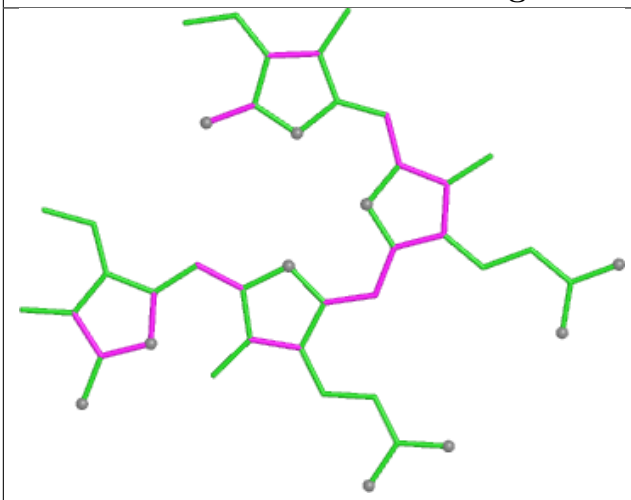


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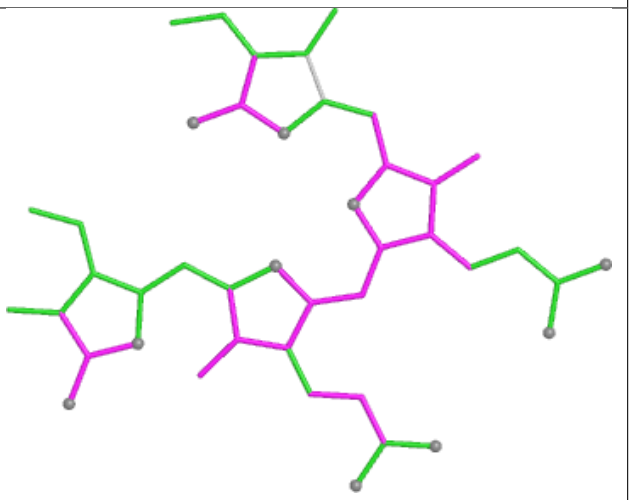


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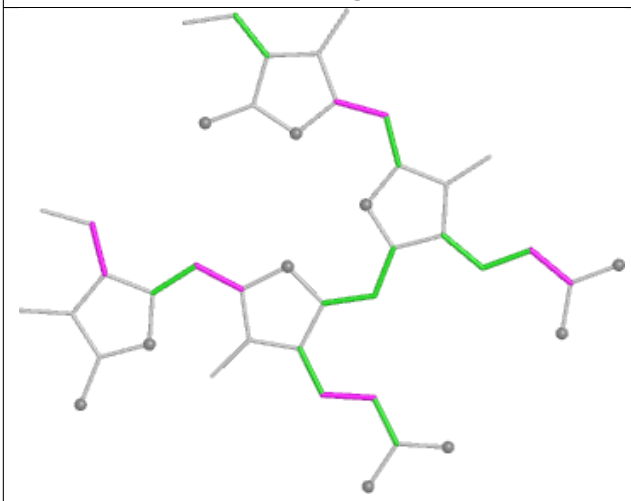
Ligand PEB mG 202



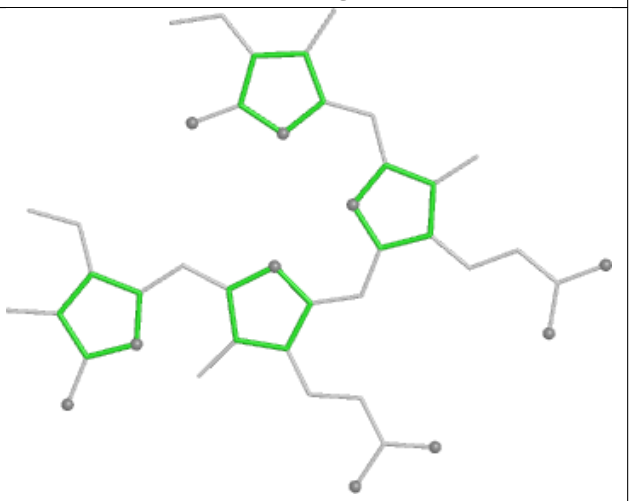
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Bond angles

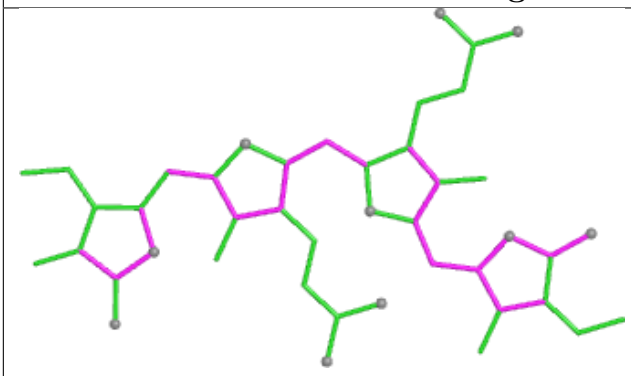


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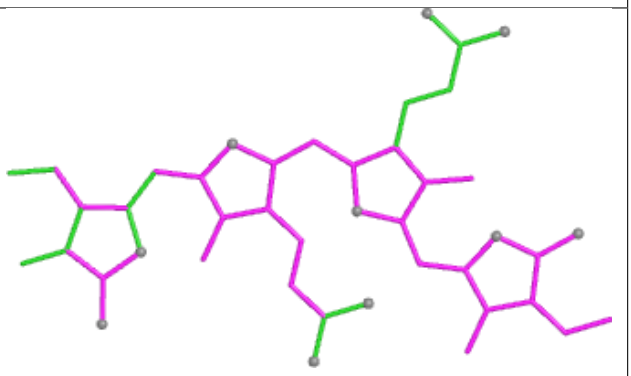


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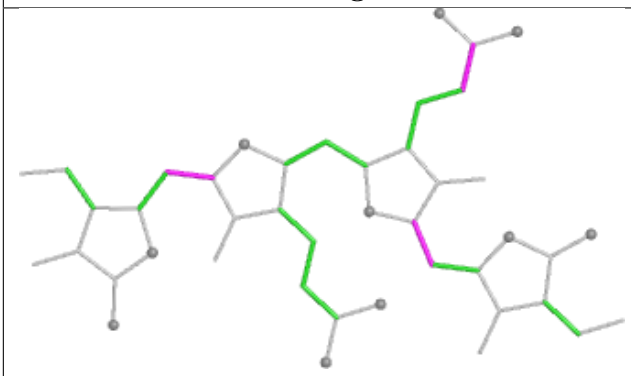
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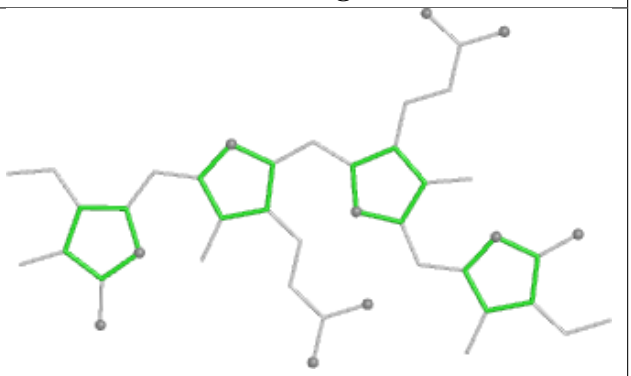
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Bond angles

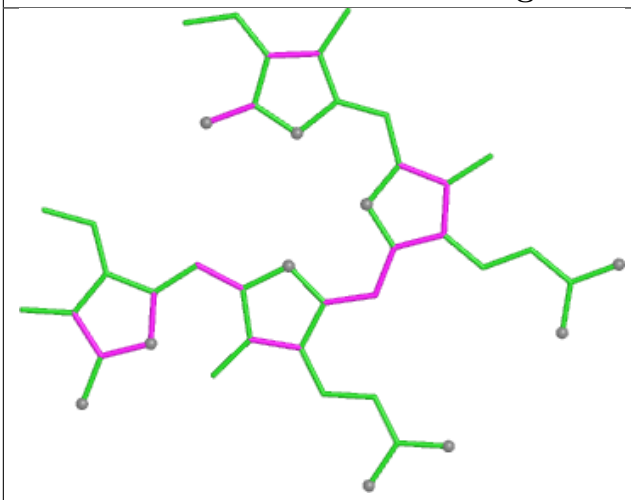


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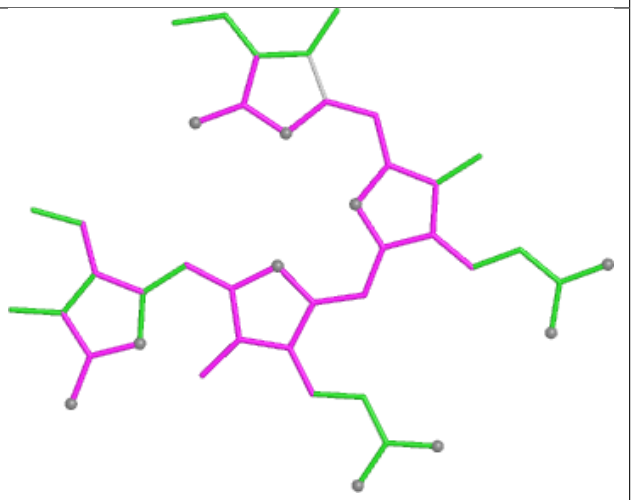


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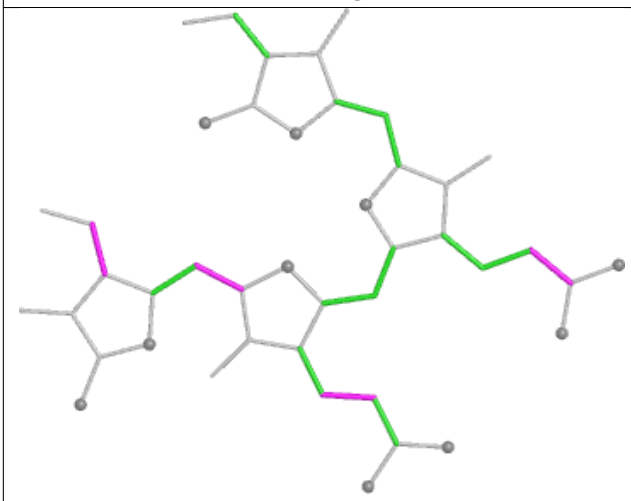
Ligand PEB EJ 201



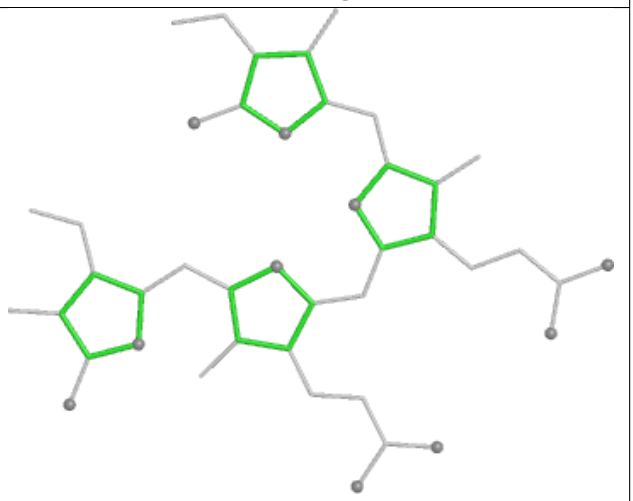
Bond lengths



Bond angles

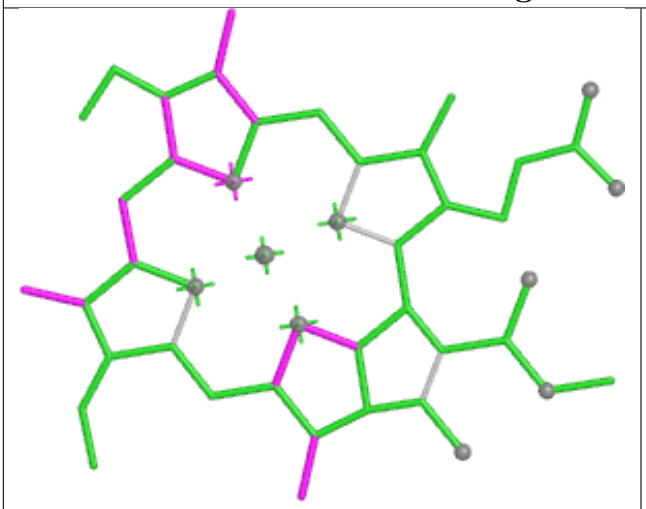


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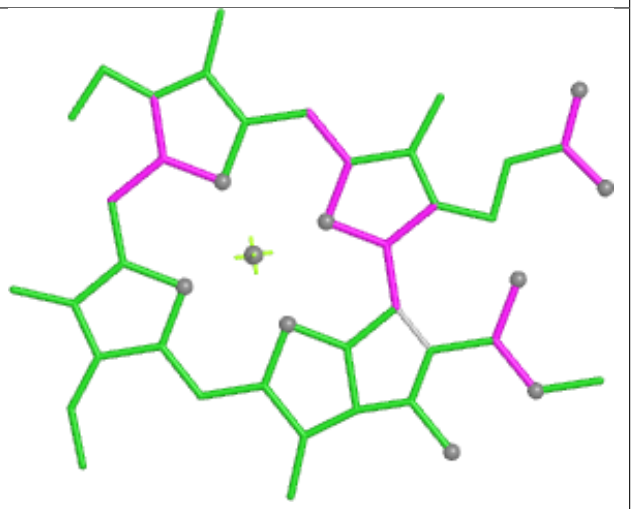


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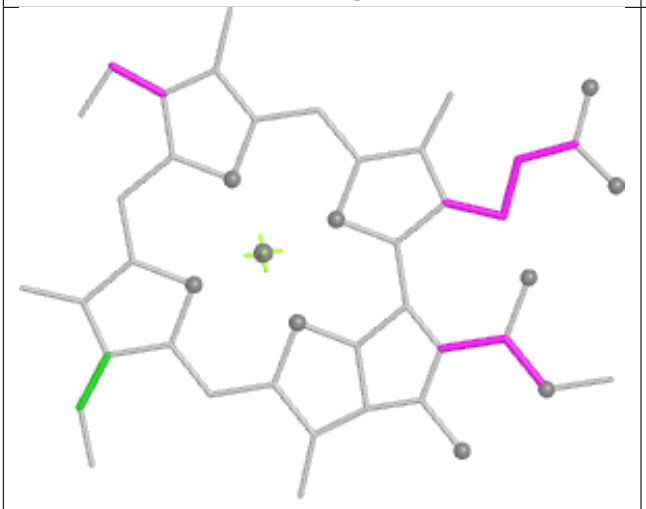
Ligand CLA R2 204



Bond lengths



Bond angles

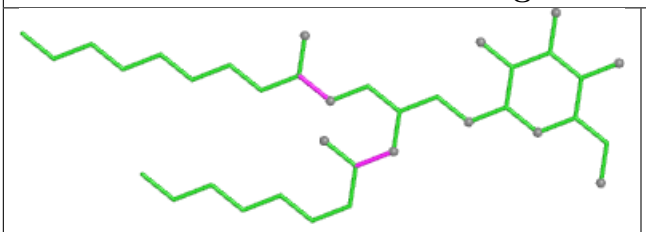


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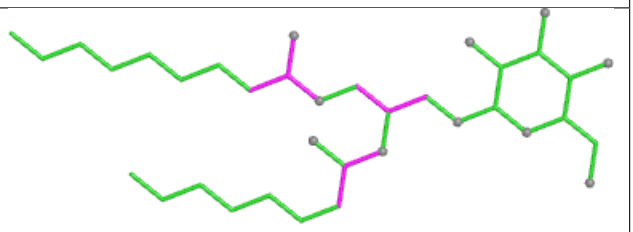


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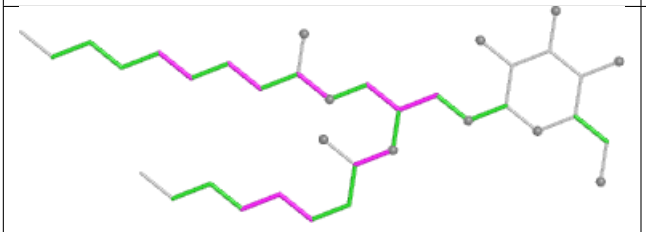
Ligand LMG b6 624



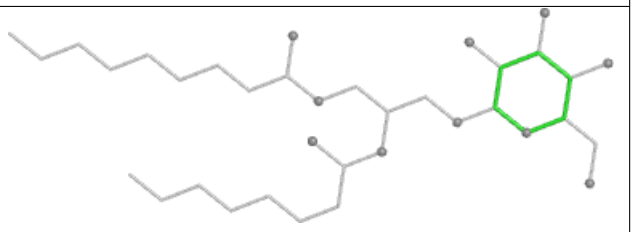
Bond lengths



Bond angles

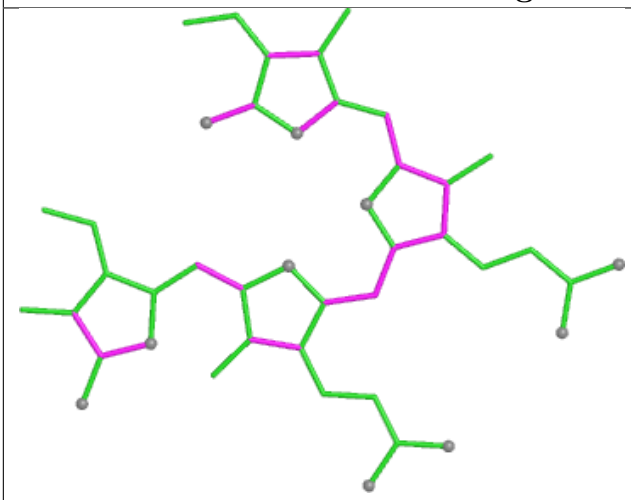


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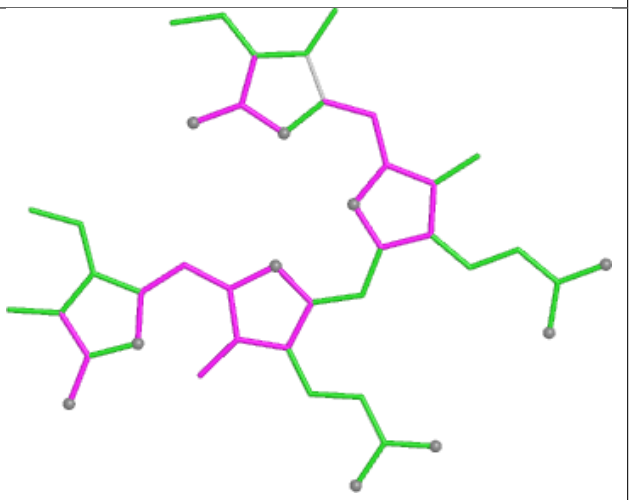


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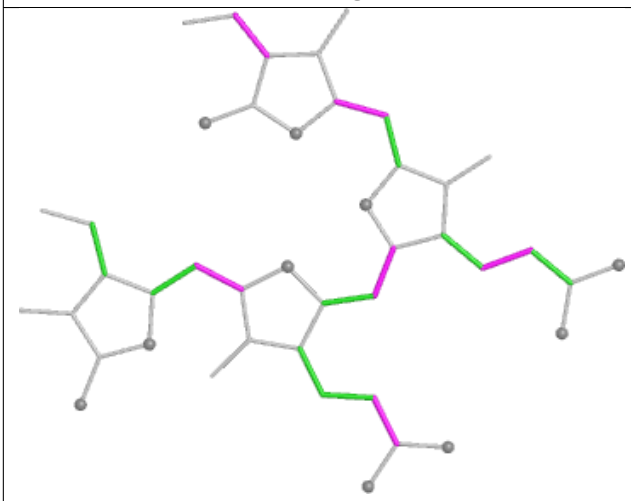
Ligand PEB eH 202



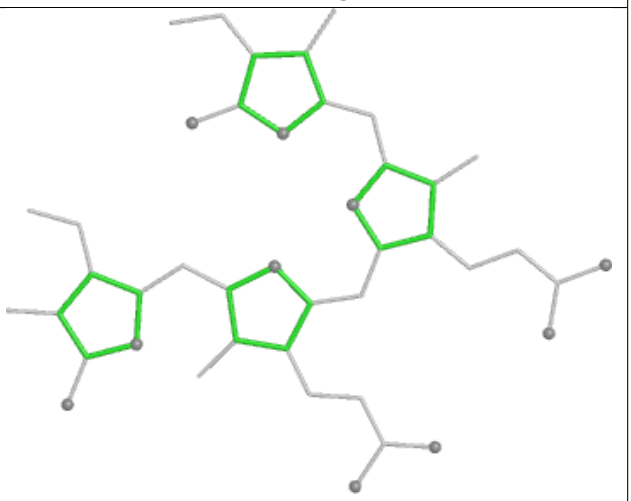
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Bond angles

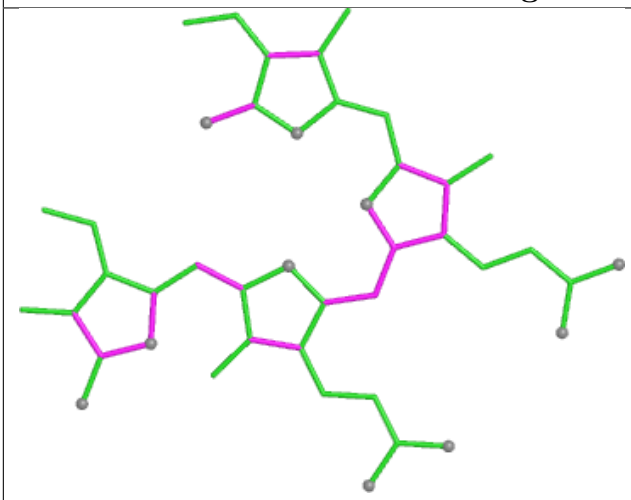


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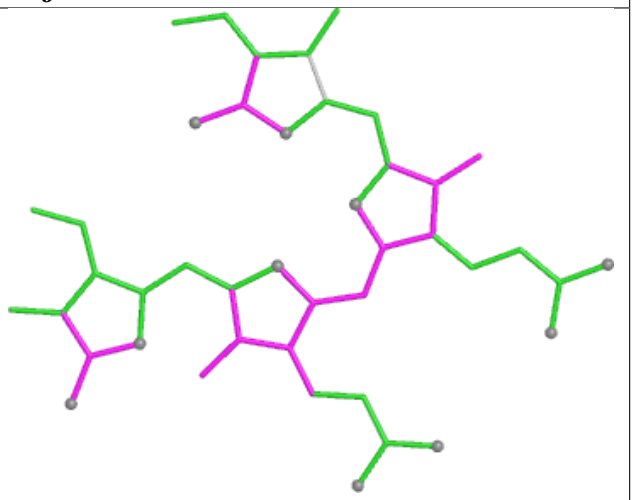


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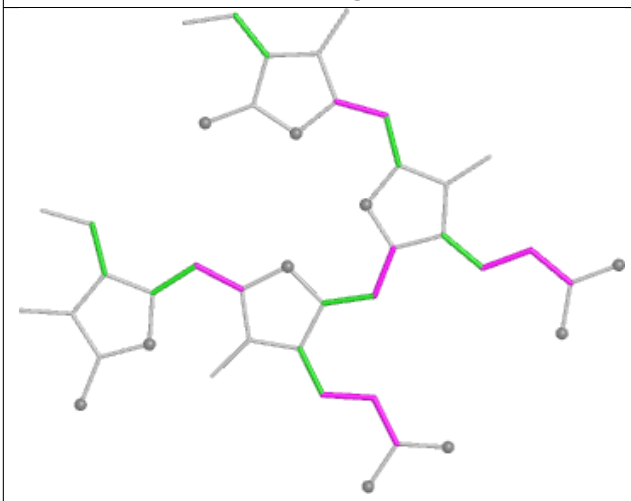
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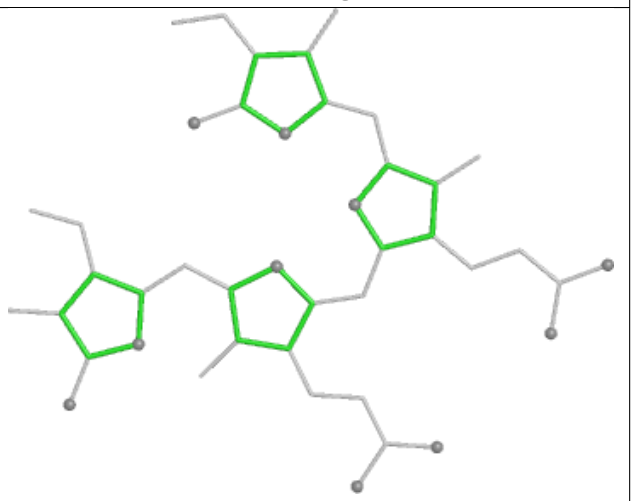
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Bond angles

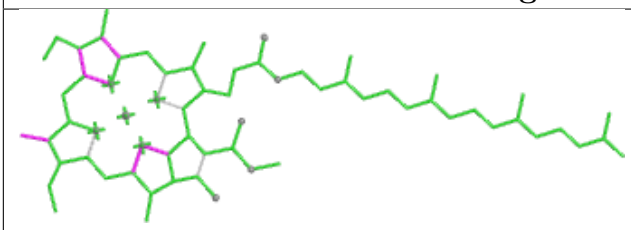


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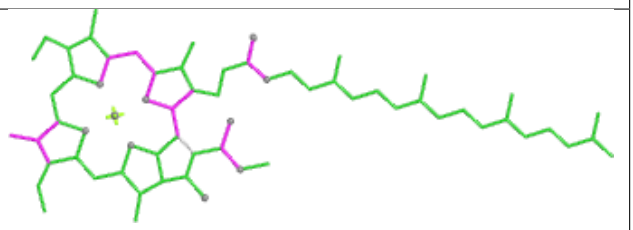


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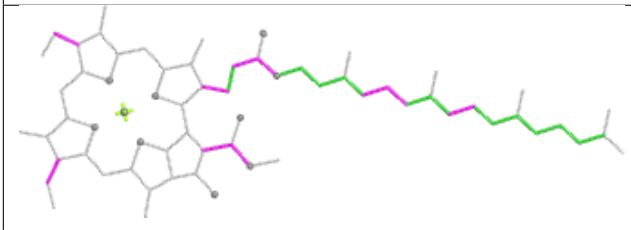
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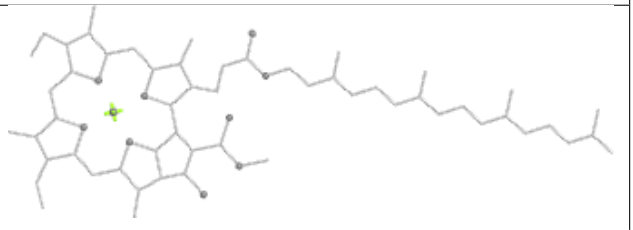
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Bond angles

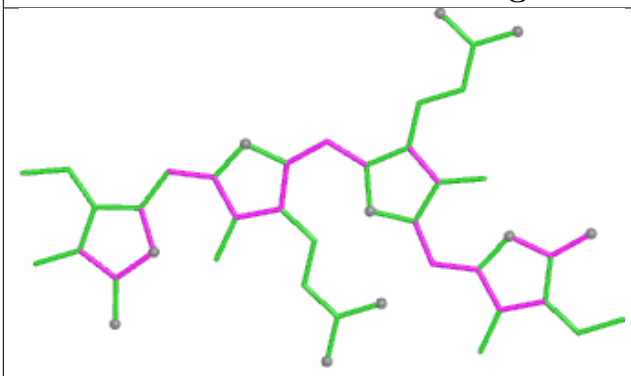


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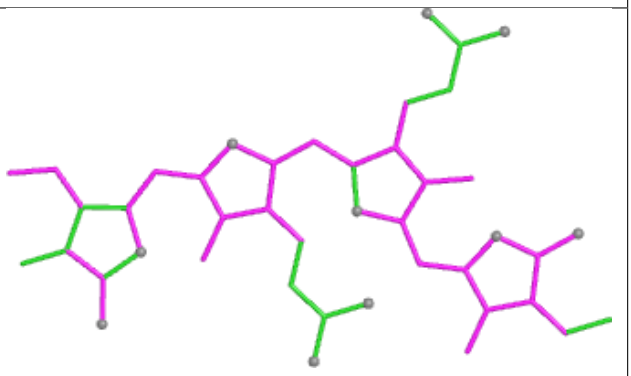


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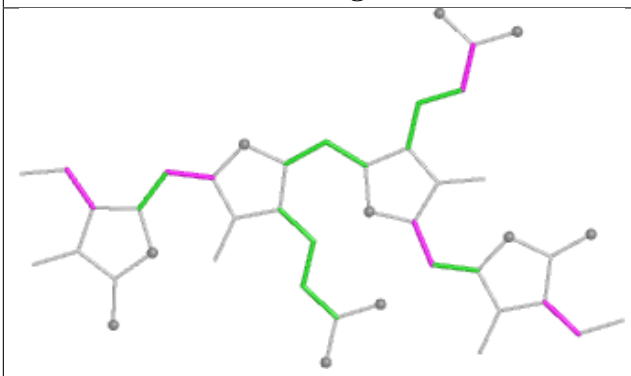
Ligand CYC e3 1001



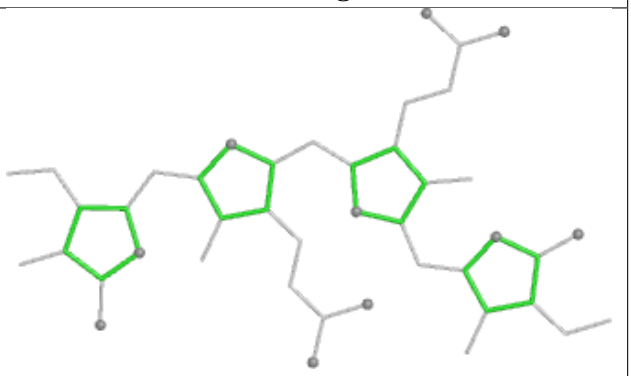
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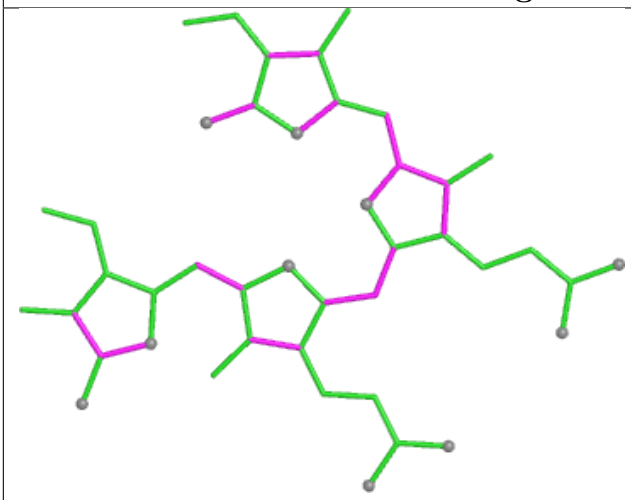


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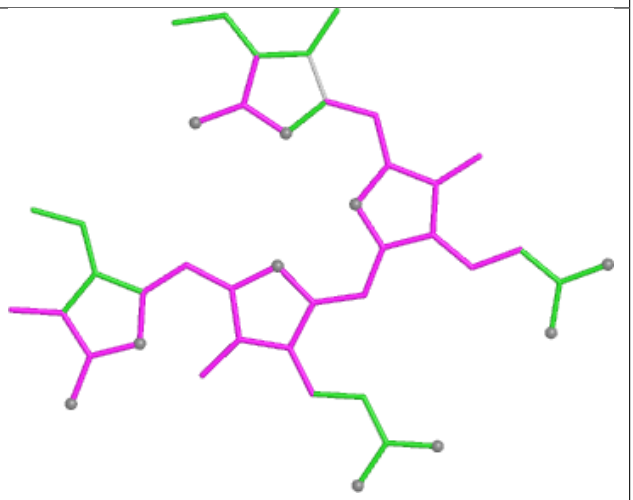


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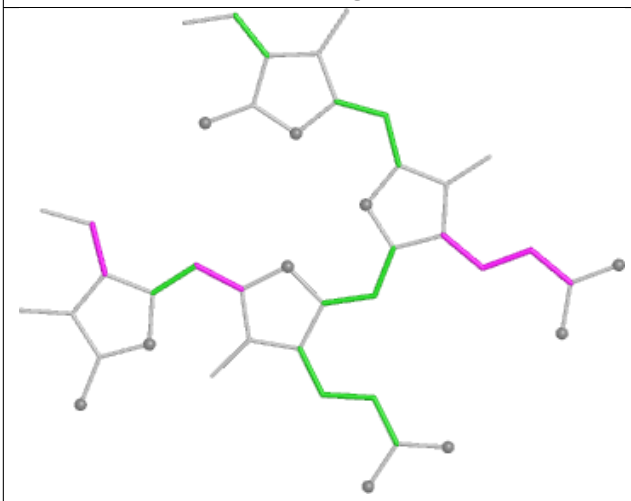
Ligand PEB O9 202



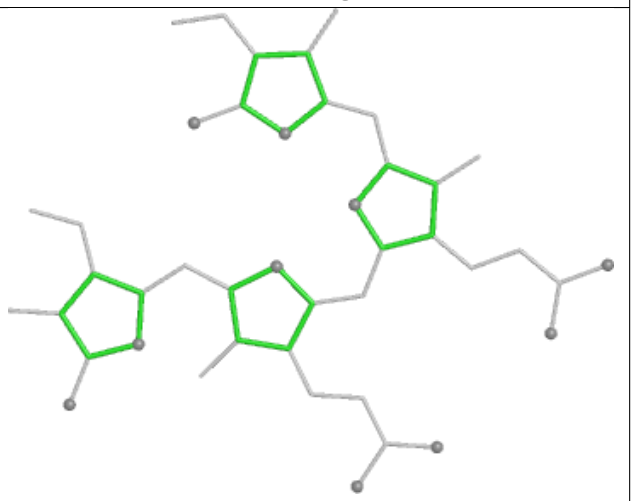
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Bond angles

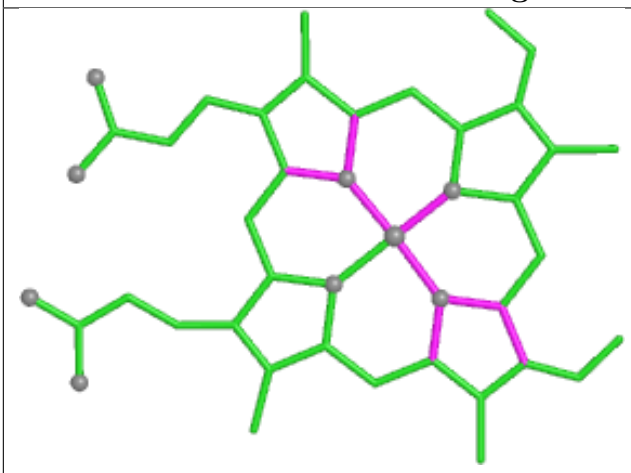


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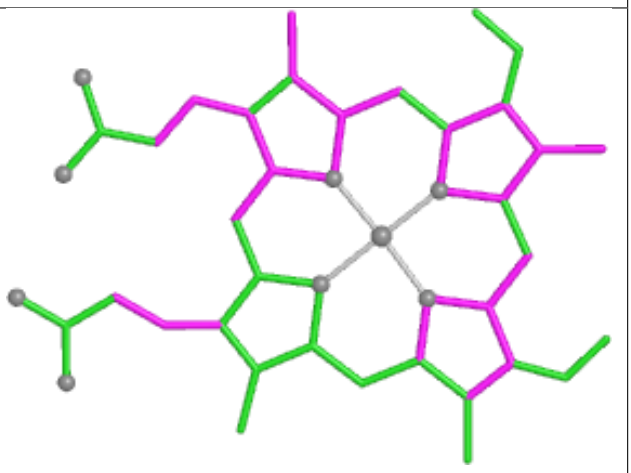


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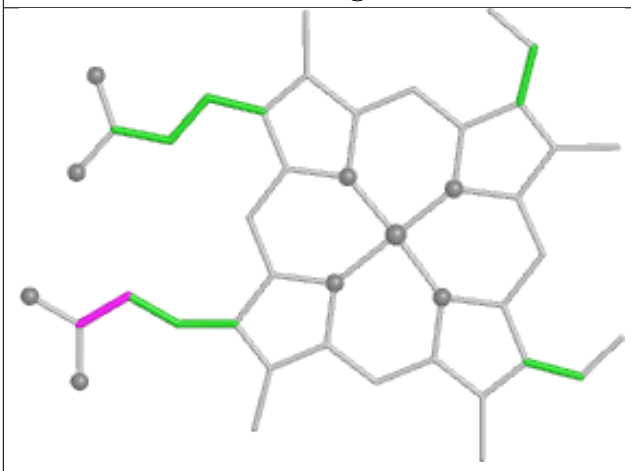
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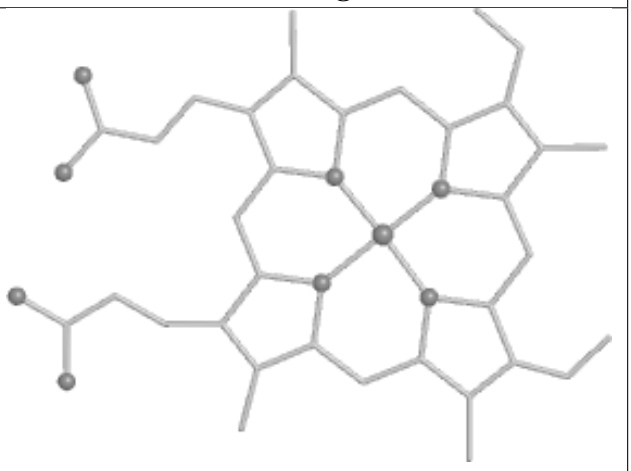
Bond lengths



Bond angles

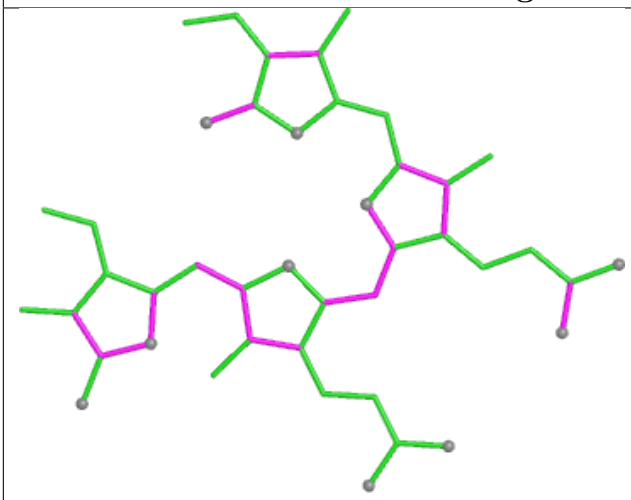


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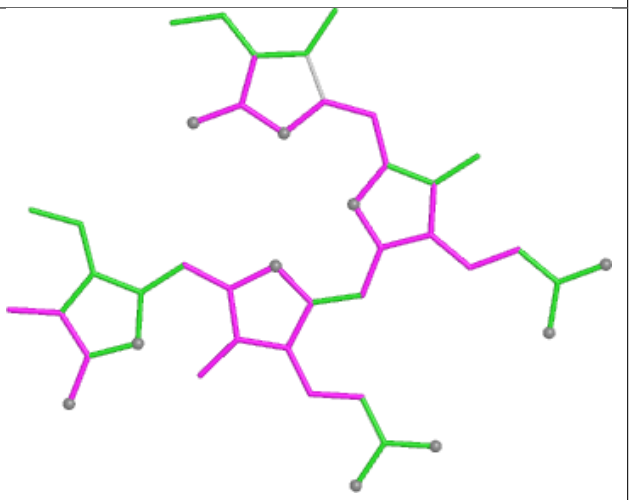


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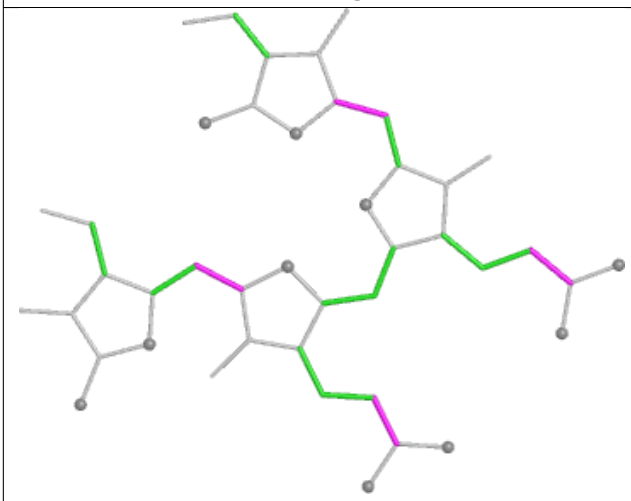
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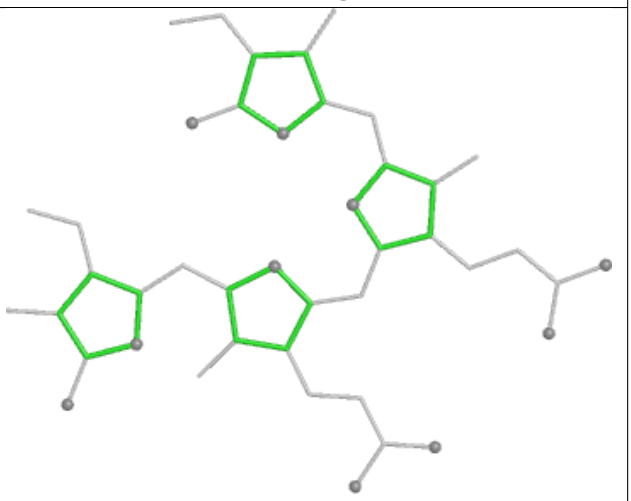
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Bond angles

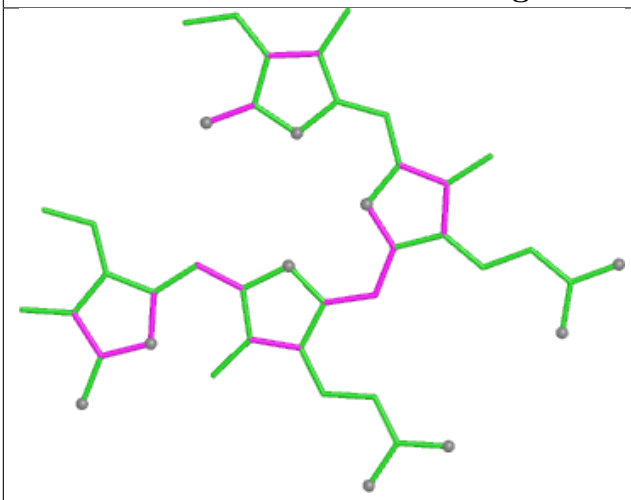


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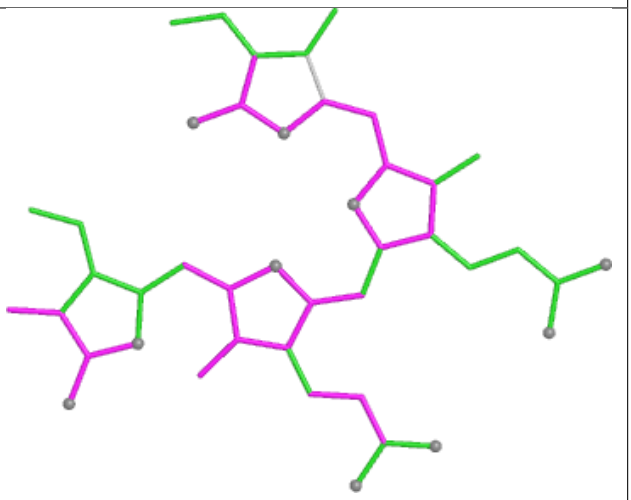


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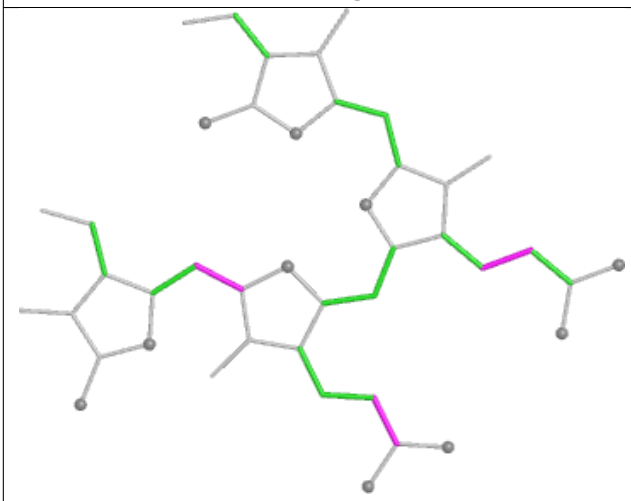
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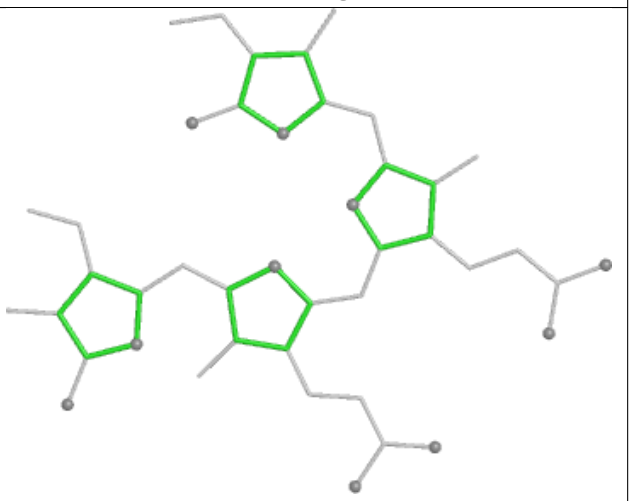
Bond lengths



Bond angles

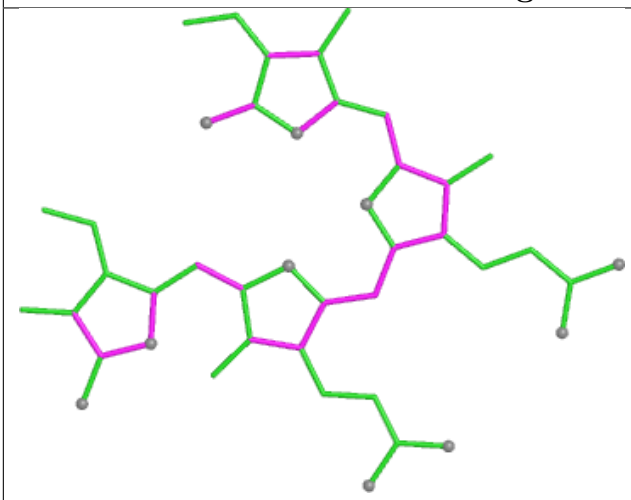


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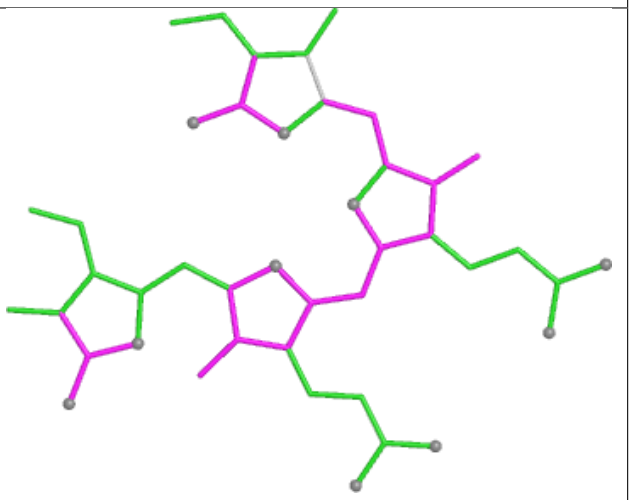


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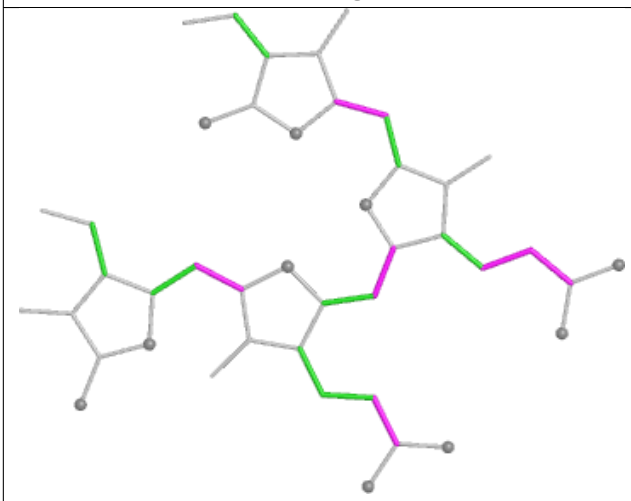
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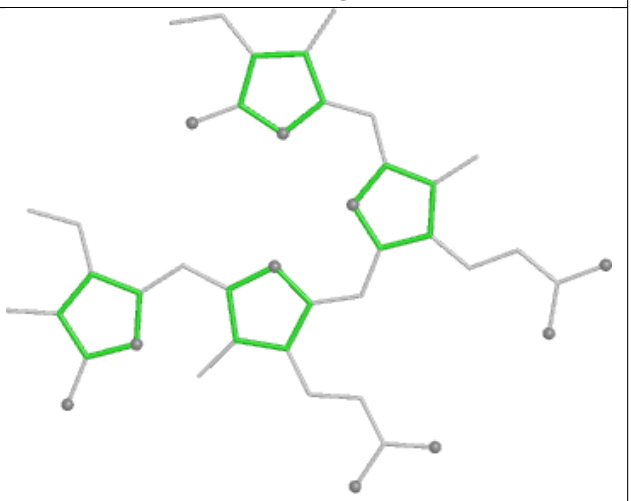
Bond lengths



Bond angles

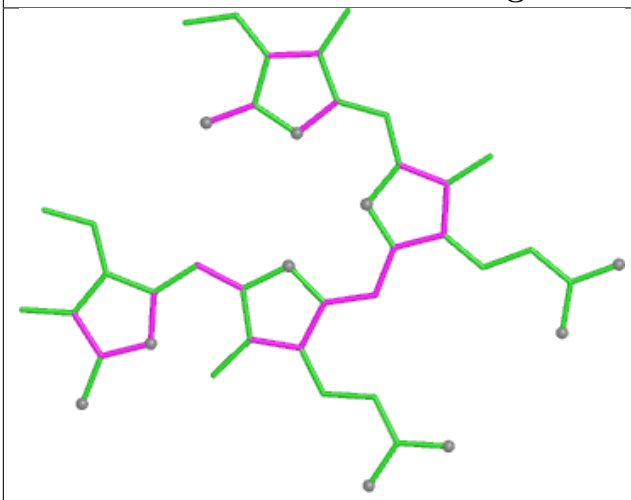


Torsions

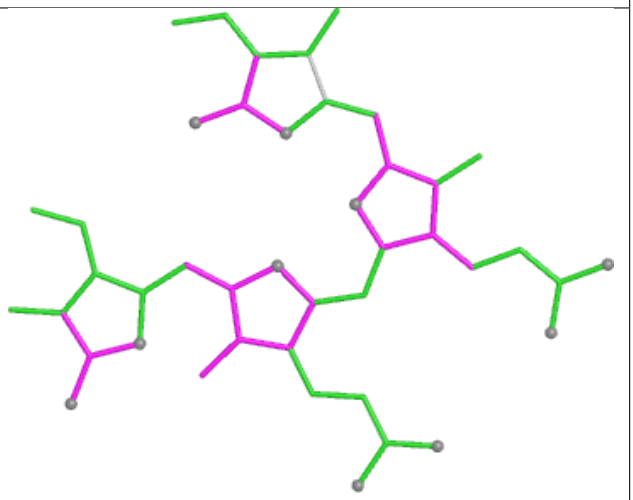


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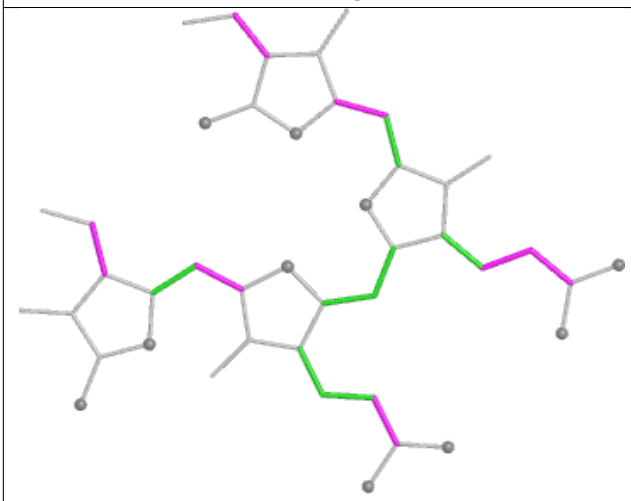
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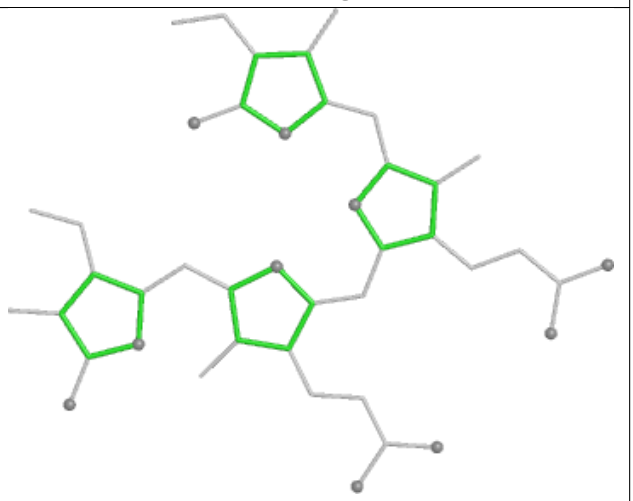
Bond lengths



Bond angles

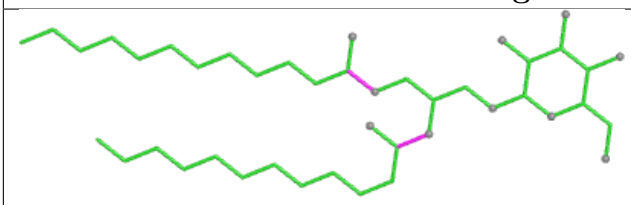


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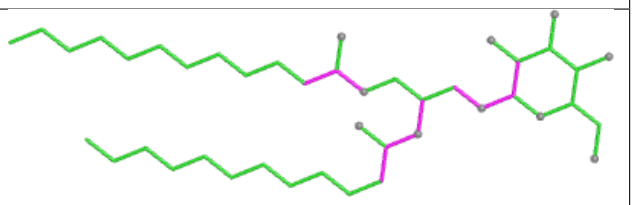


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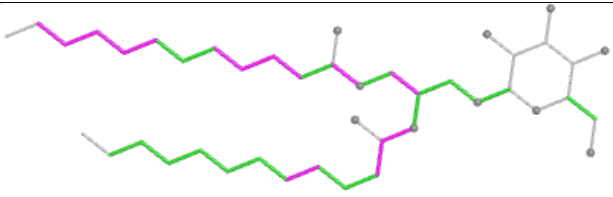
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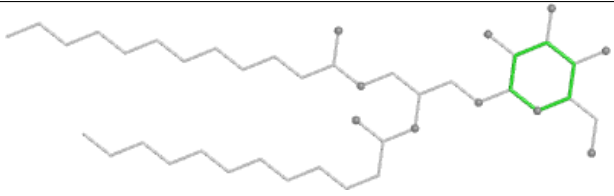
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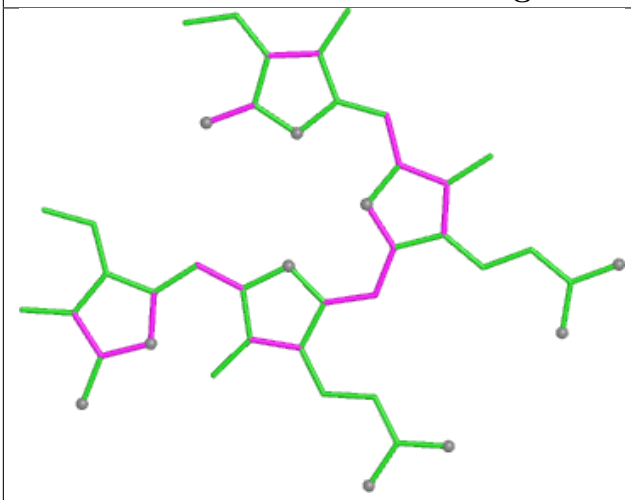


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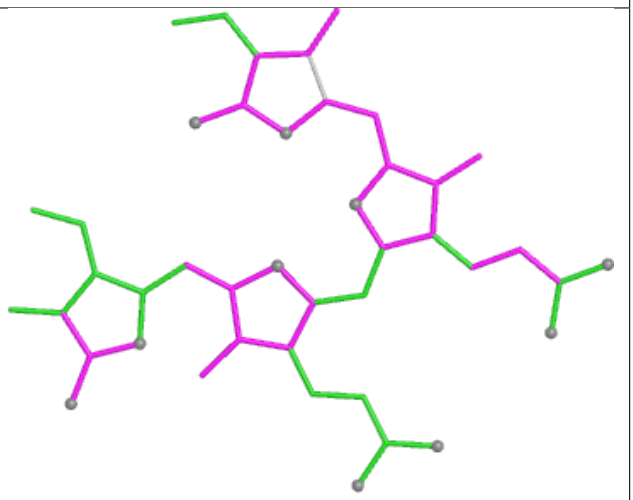


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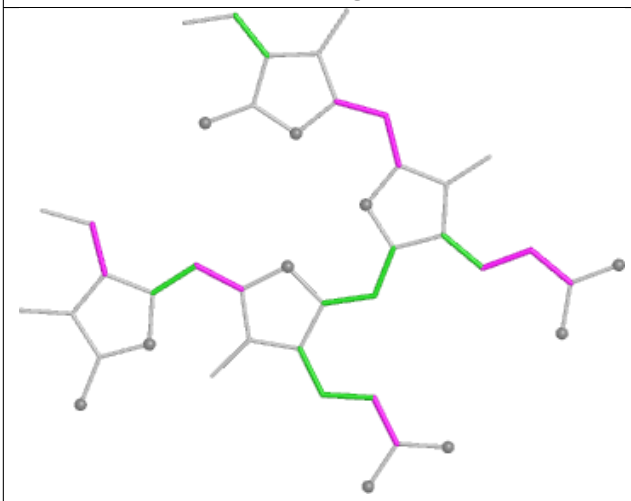
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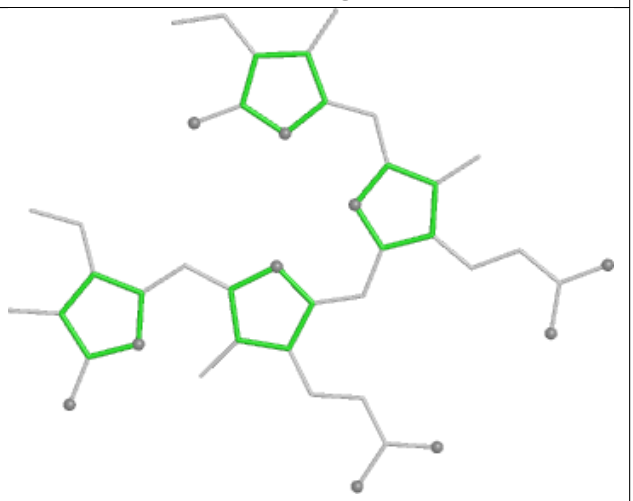
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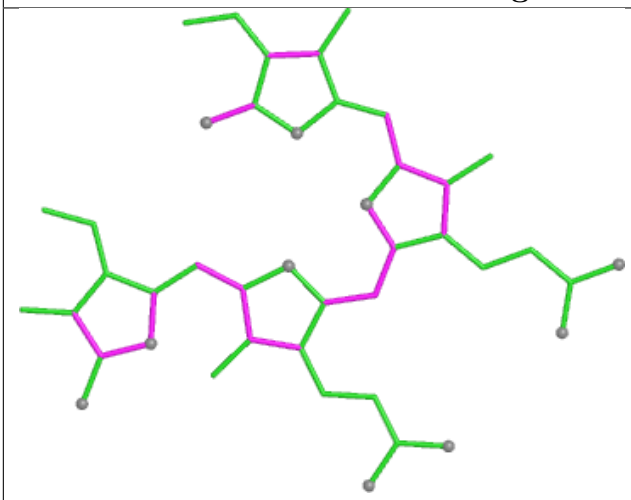


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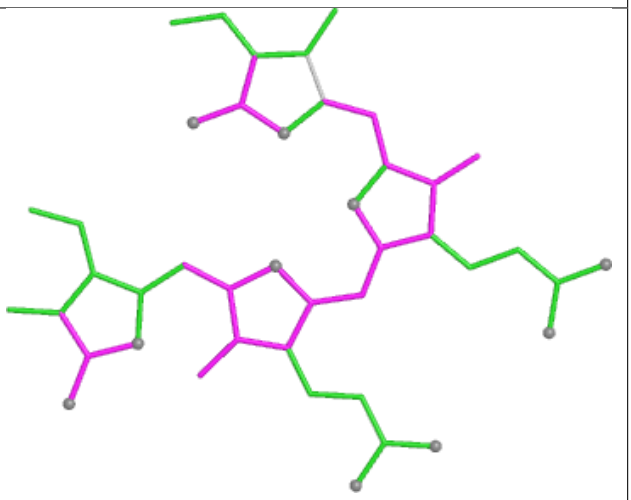


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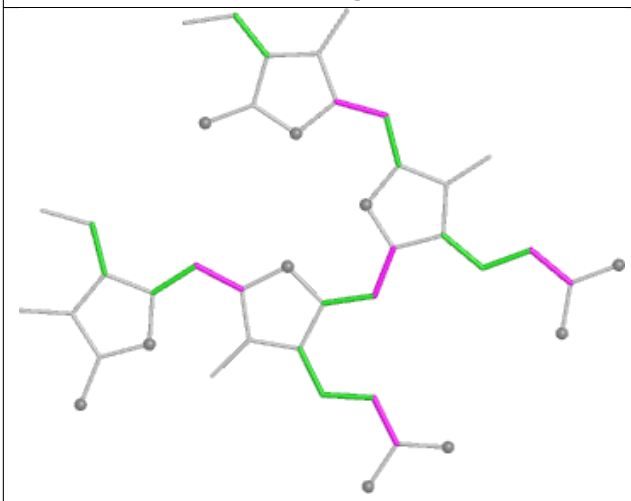
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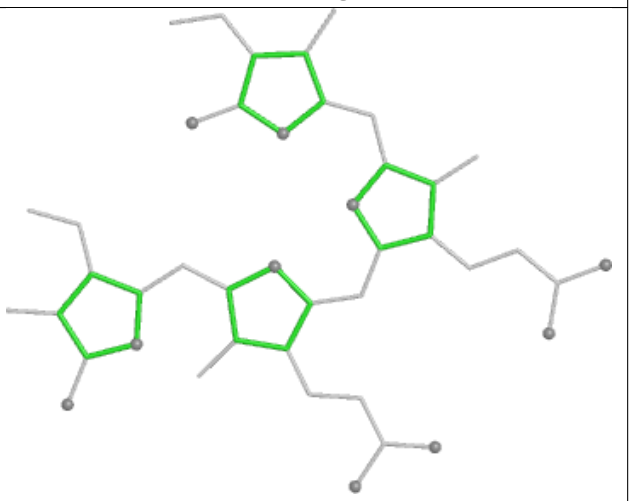
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Bond angles

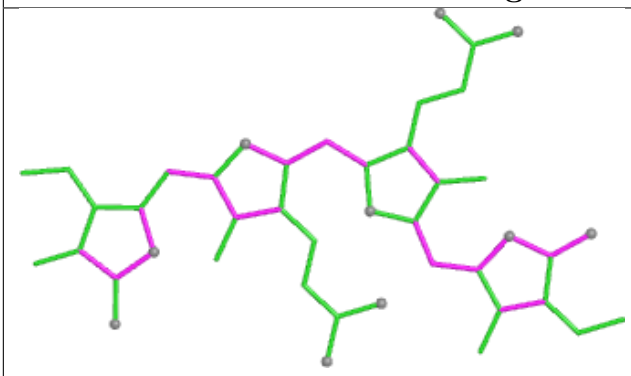


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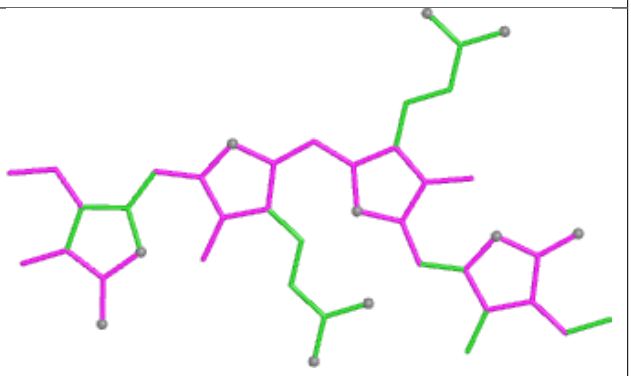


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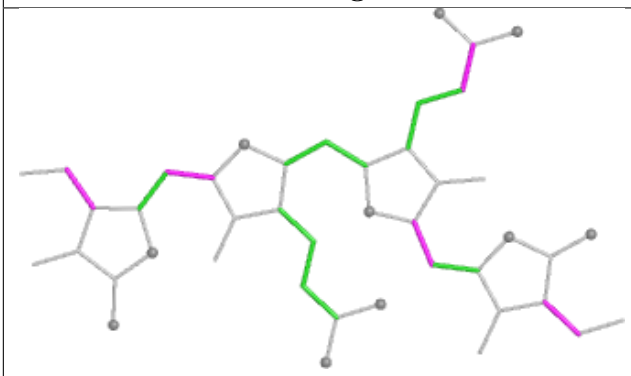
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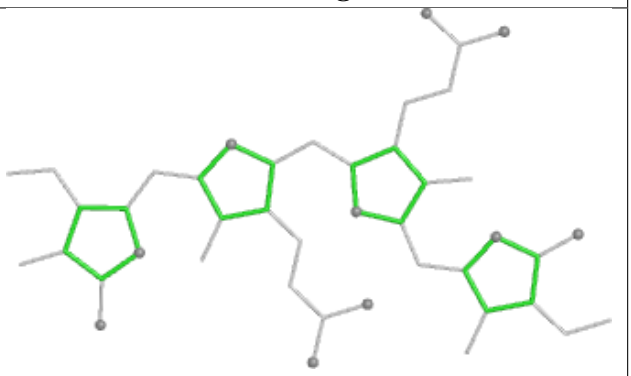
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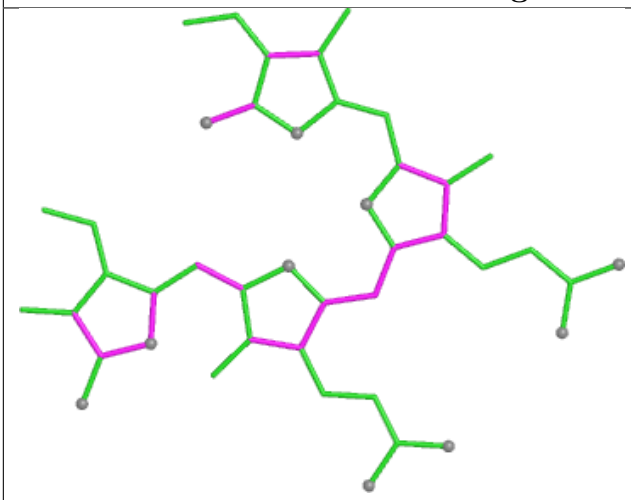


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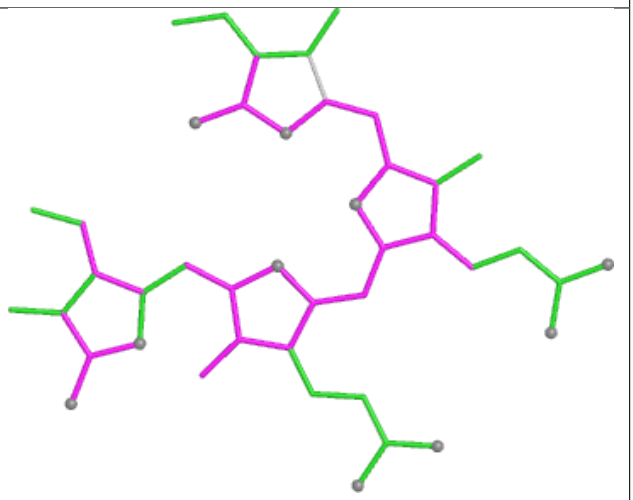


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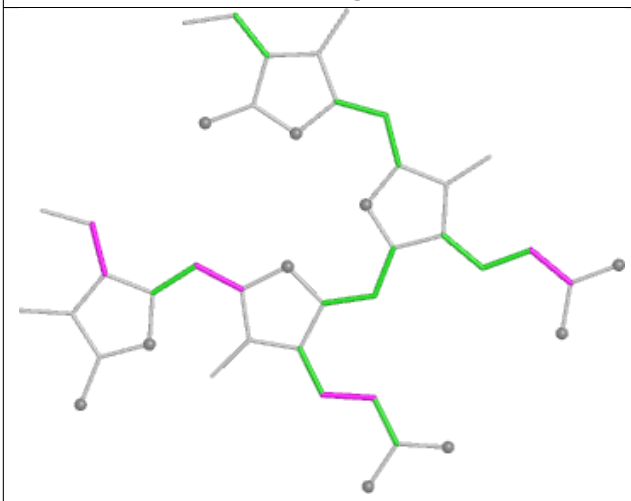
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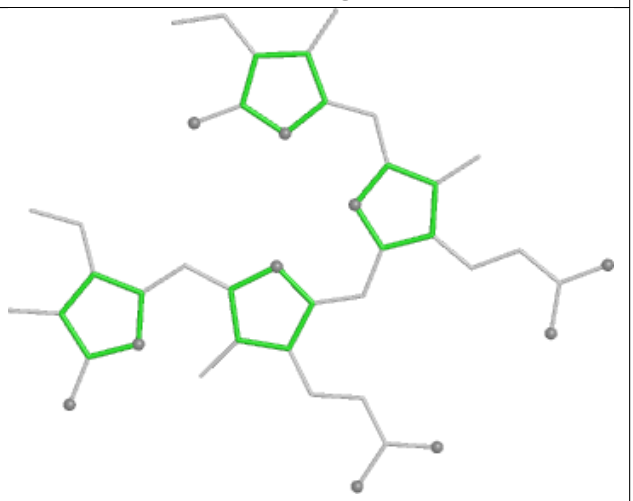
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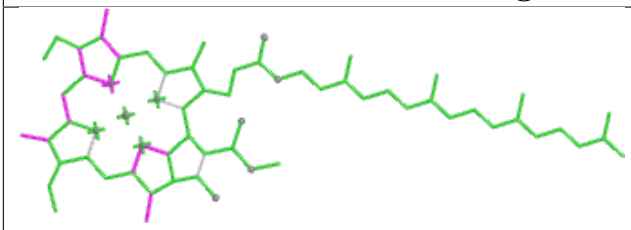


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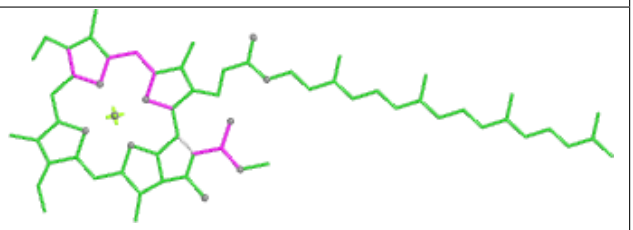


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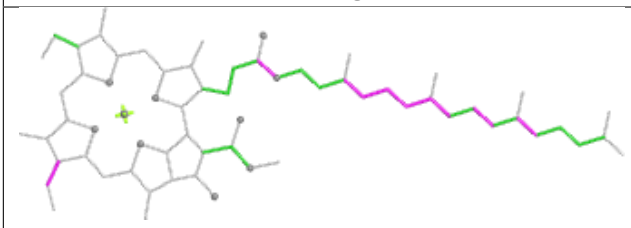
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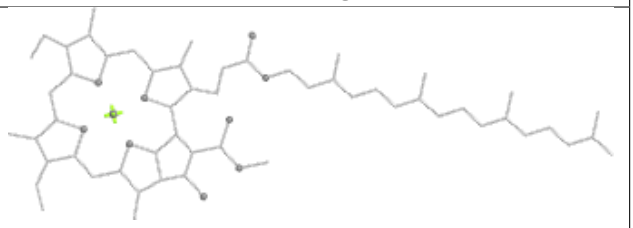
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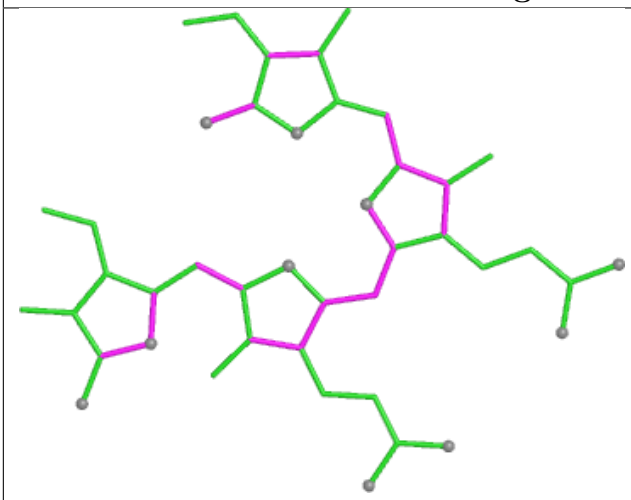


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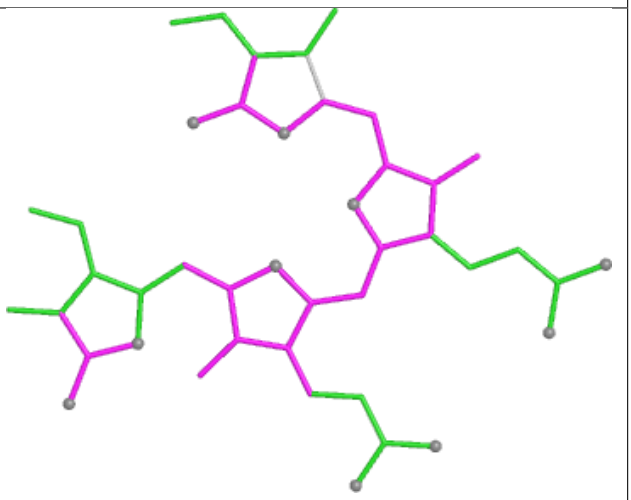


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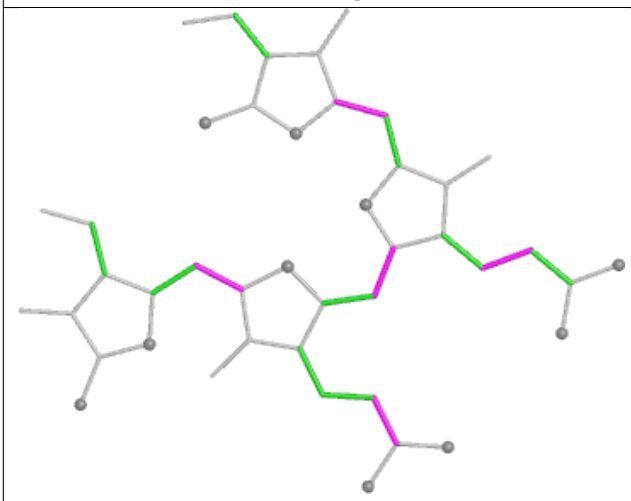
Ligand PEB hK 202



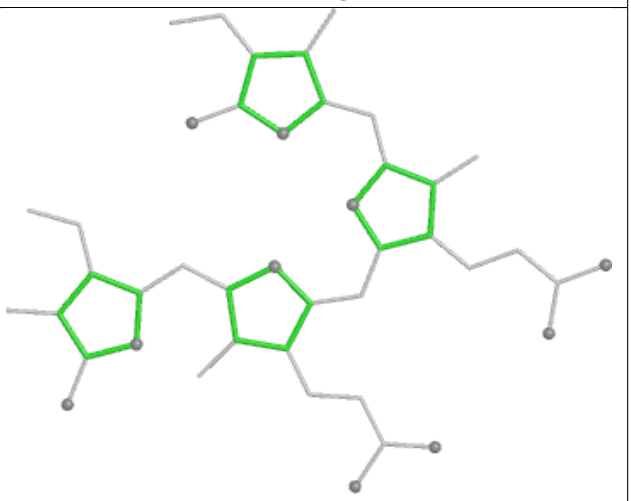
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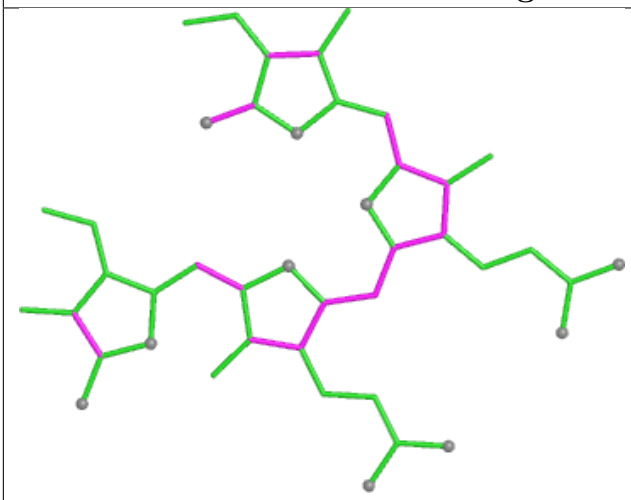


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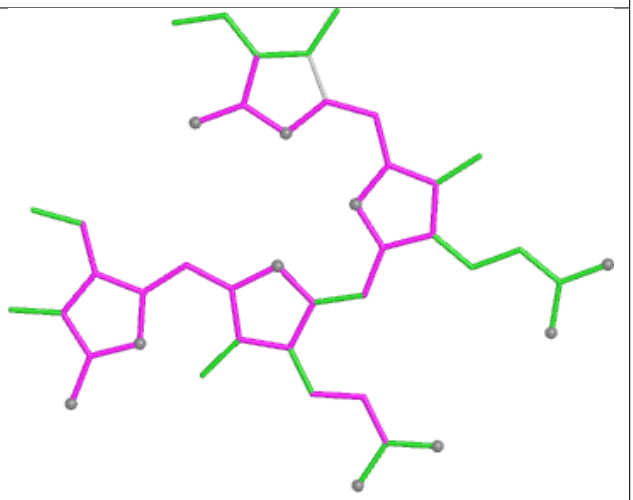


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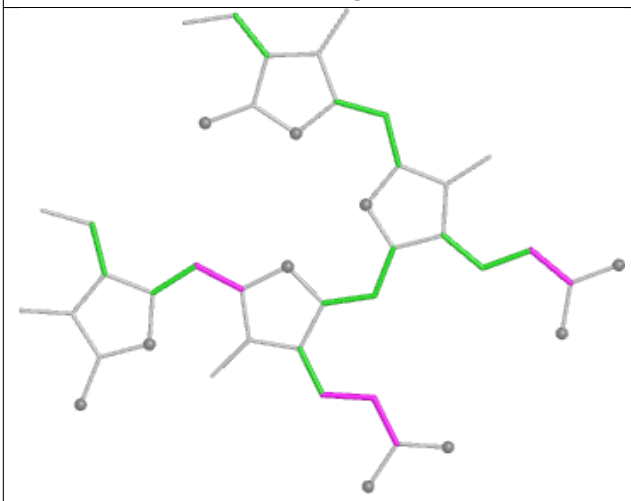
Ligand PEB vF 201



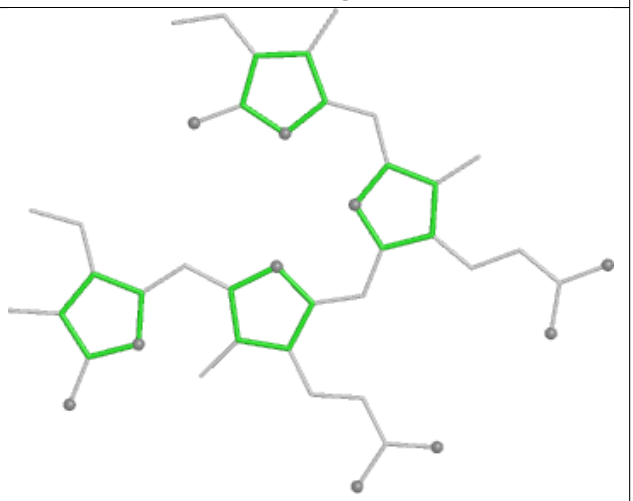
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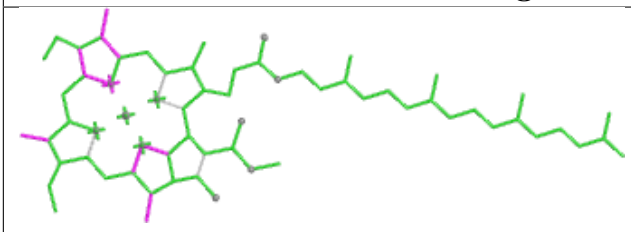


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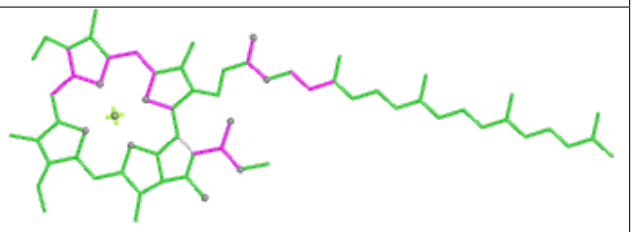


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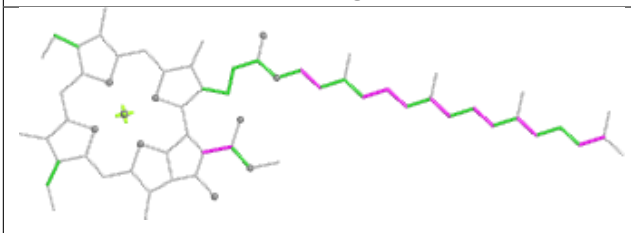
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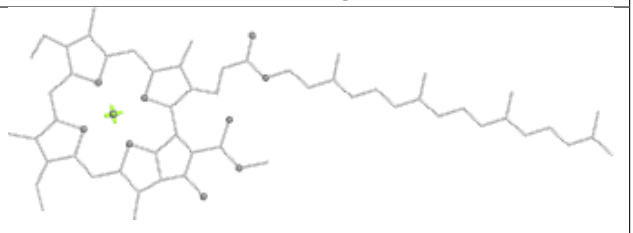
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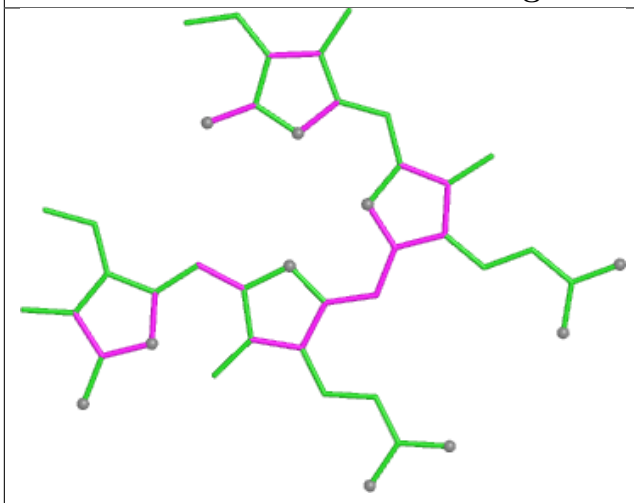


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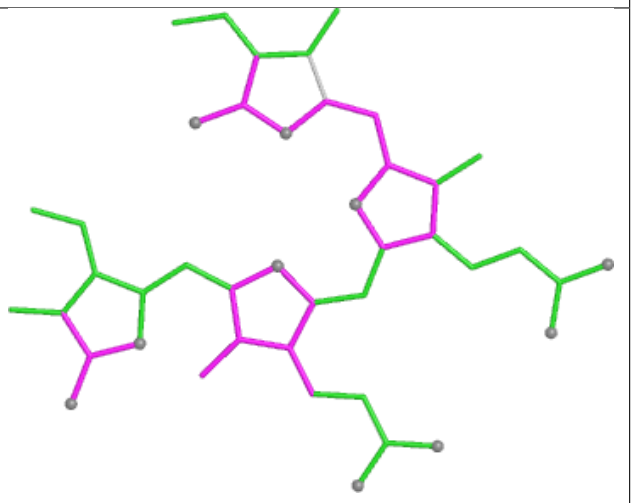


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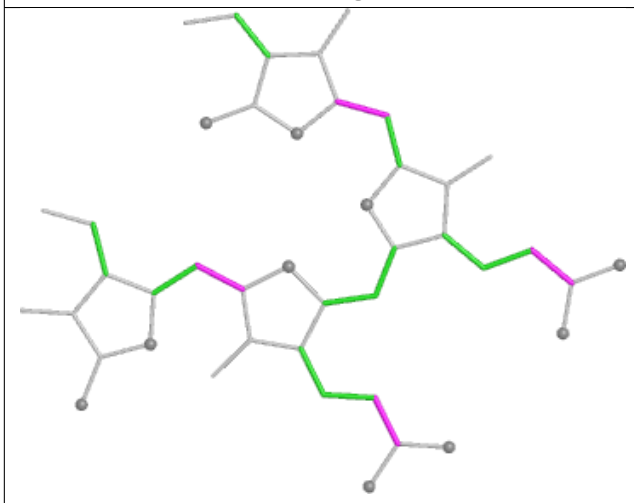
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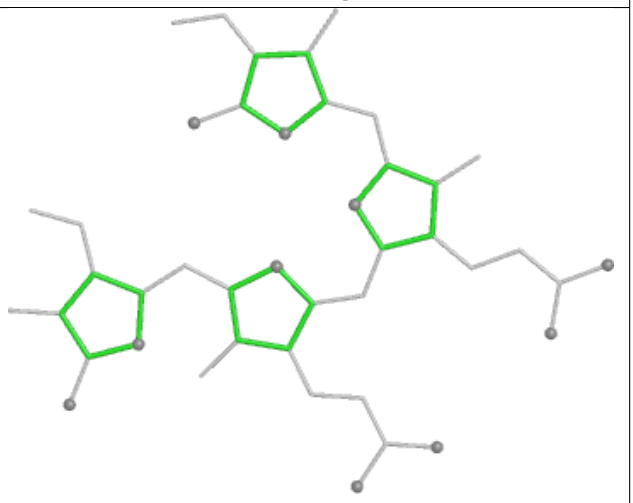
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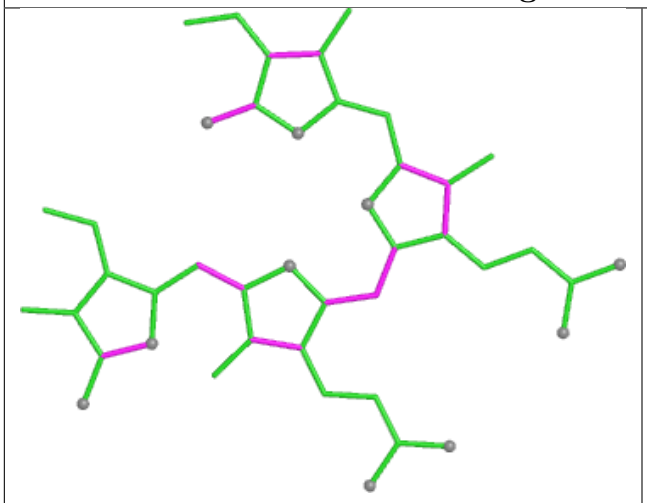


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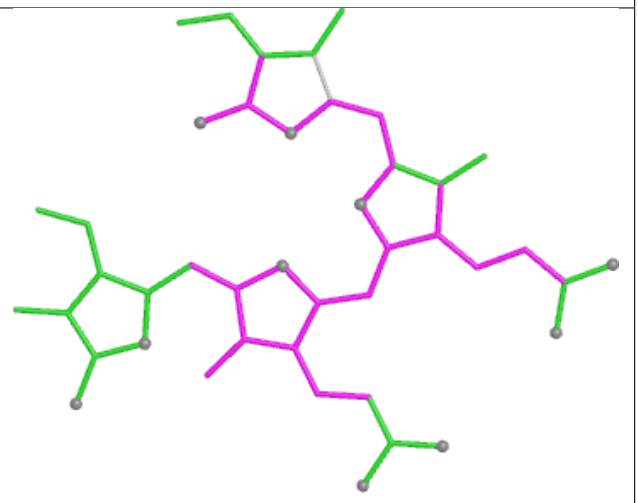


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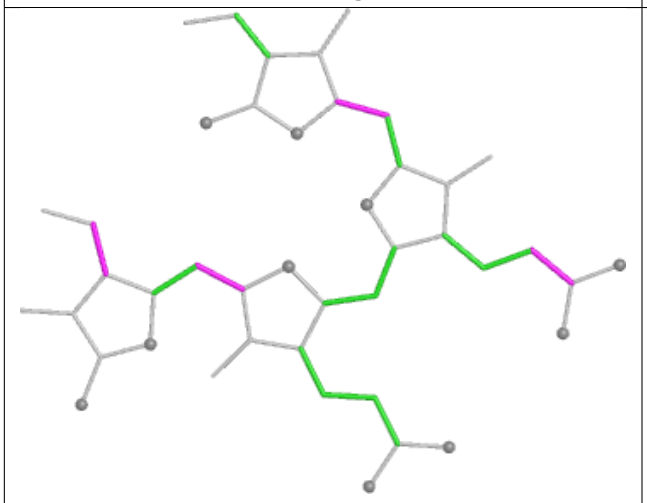
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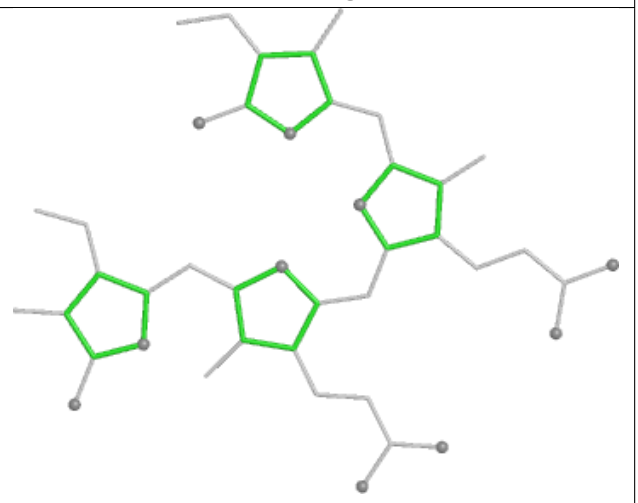
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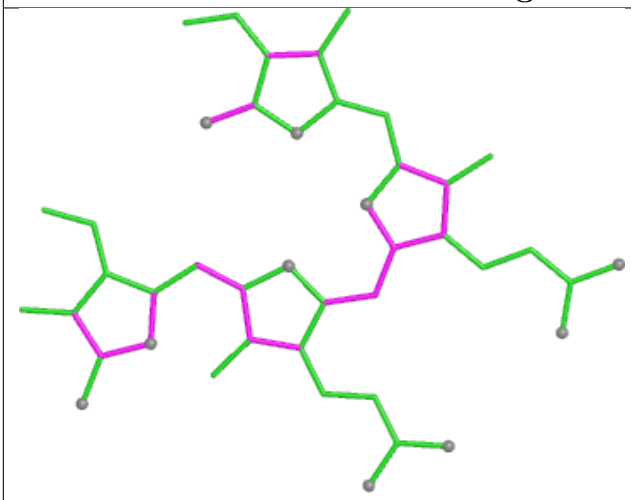


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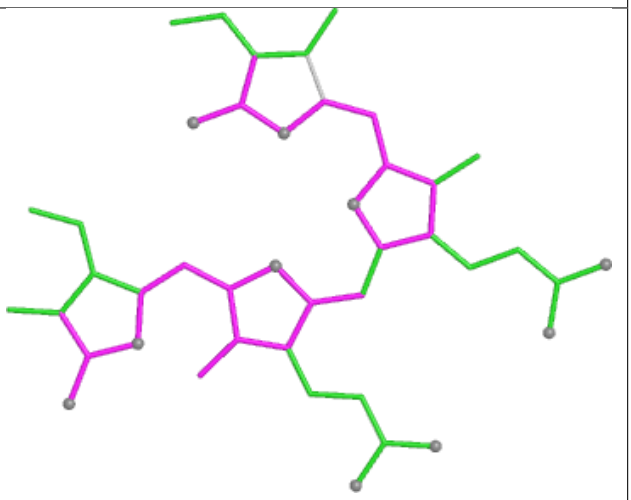


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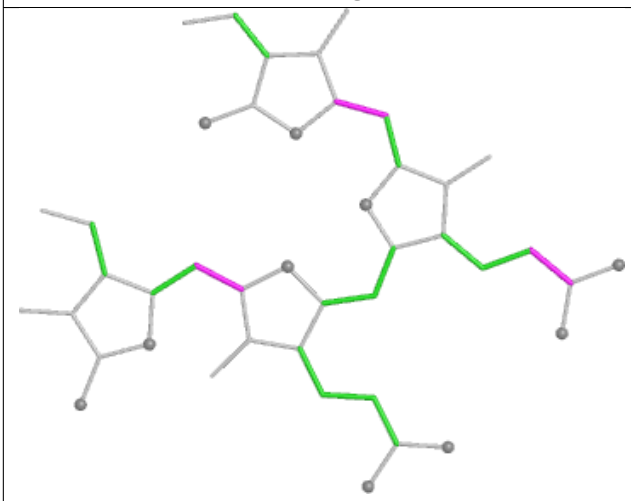
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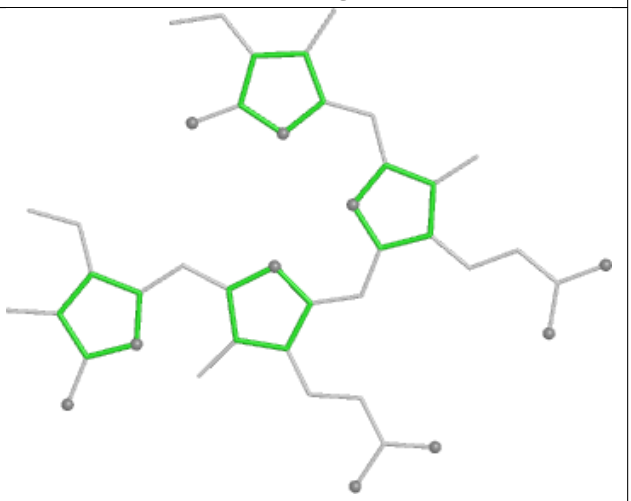
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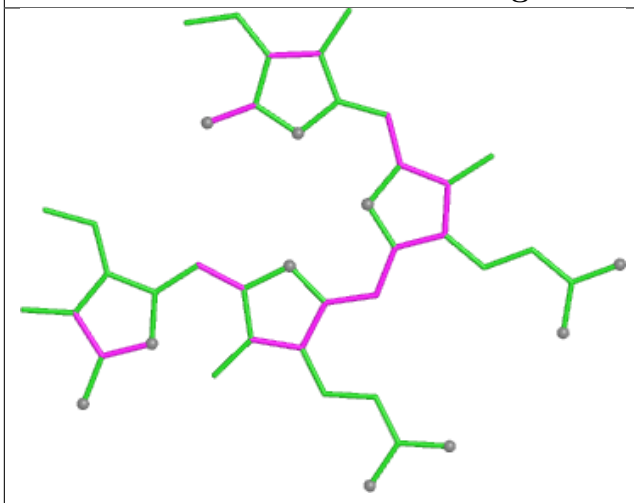


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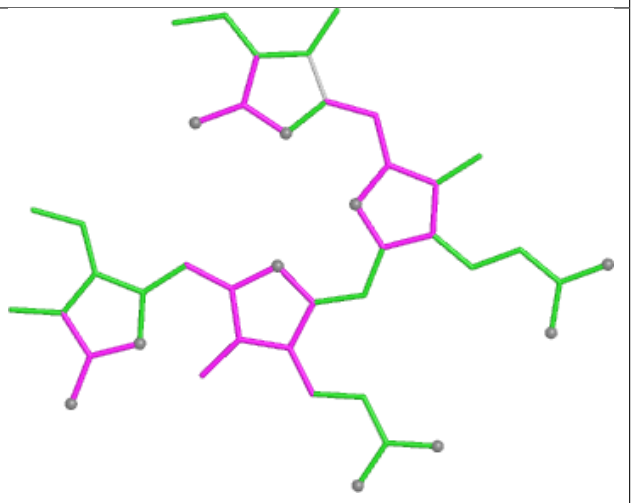


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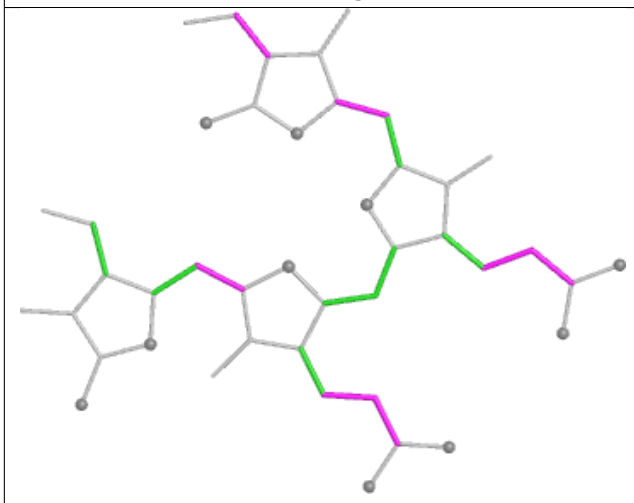
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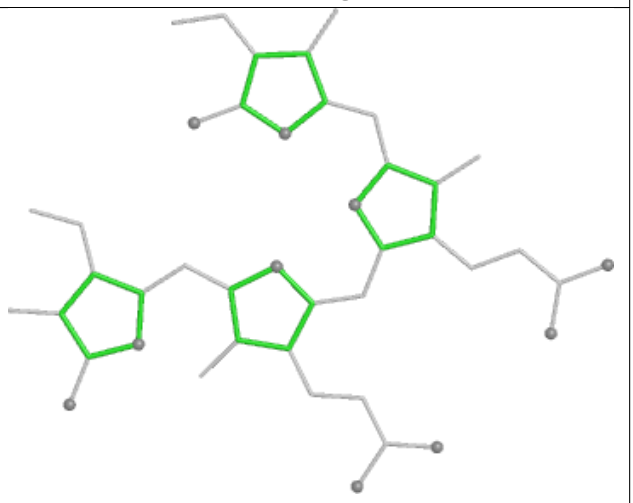
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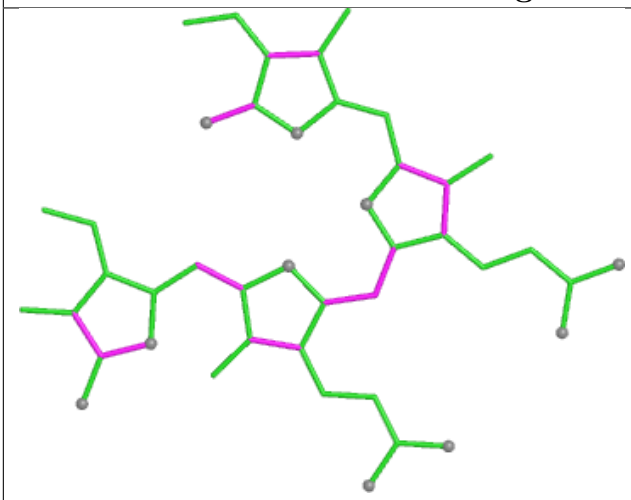


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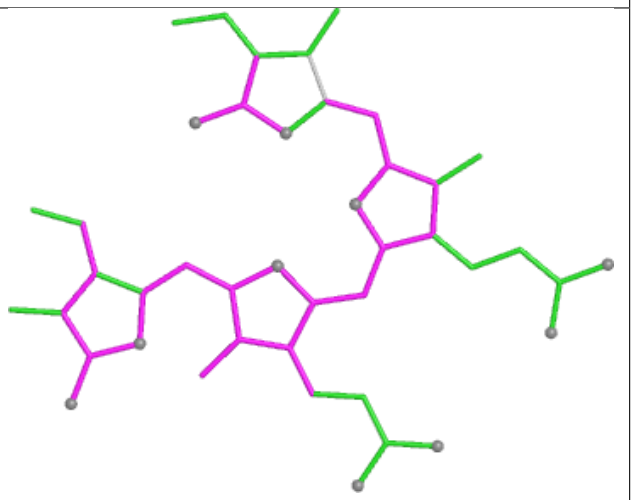


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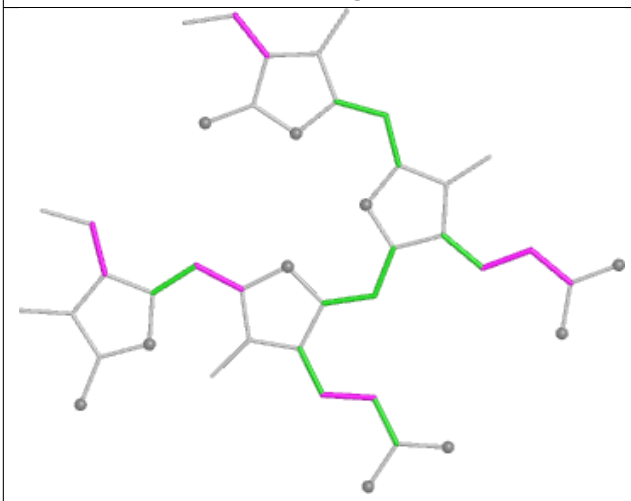
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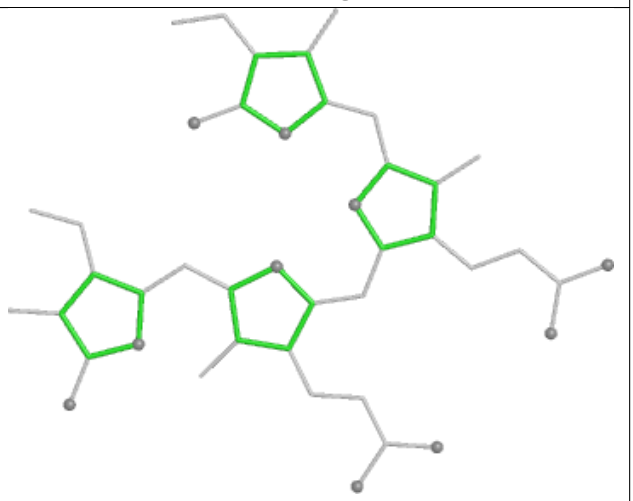
Bond lengths



Bond angles

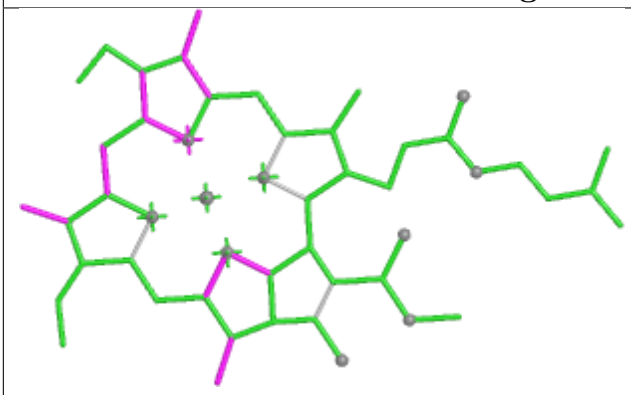


Torsions

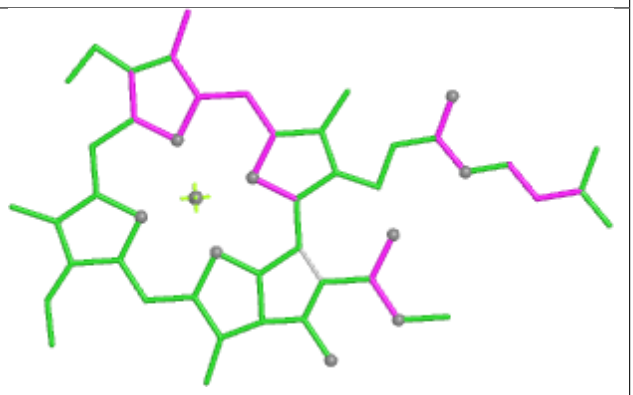


Rings

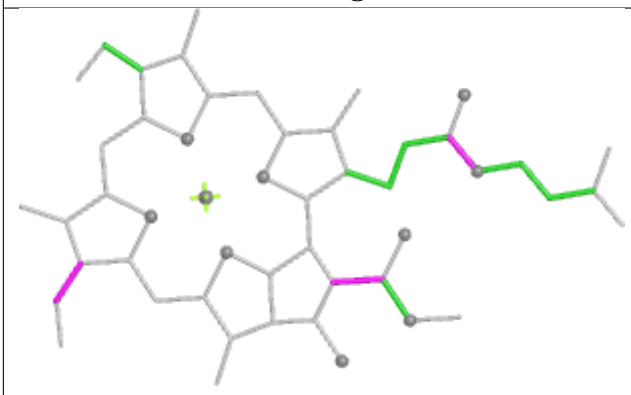
Ligand CLA a6 609



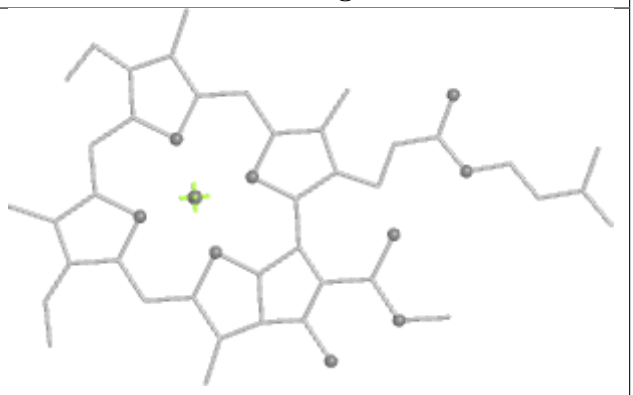
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Bond angles

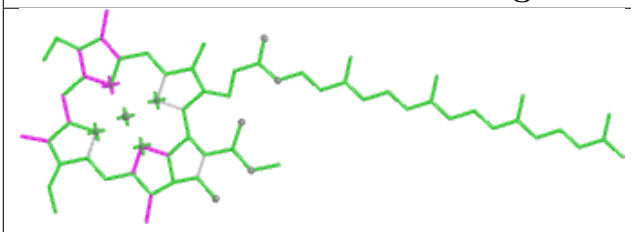


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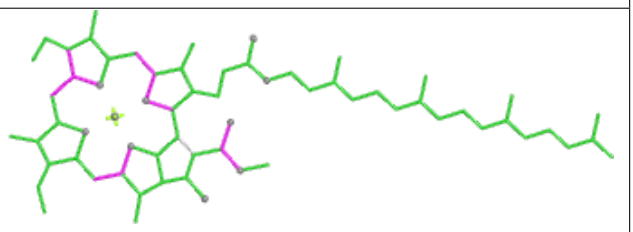


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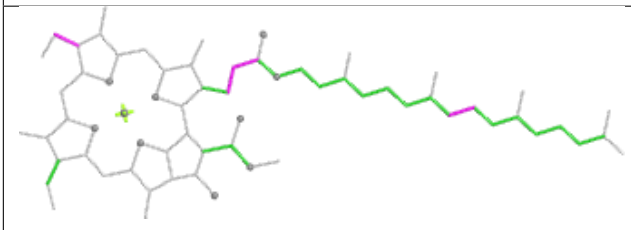
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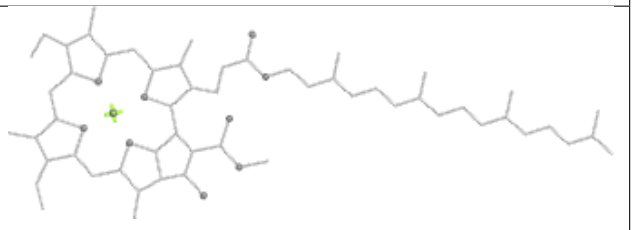
Bond lengths



Bond angles

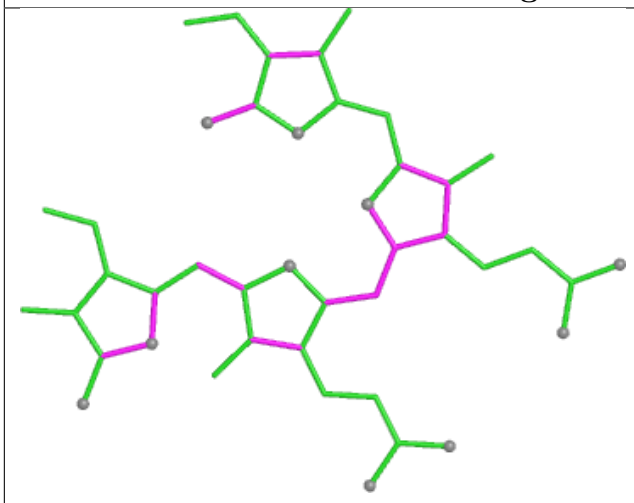


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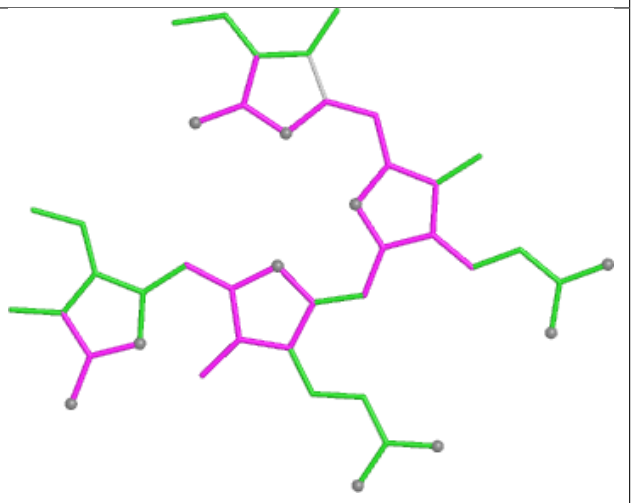


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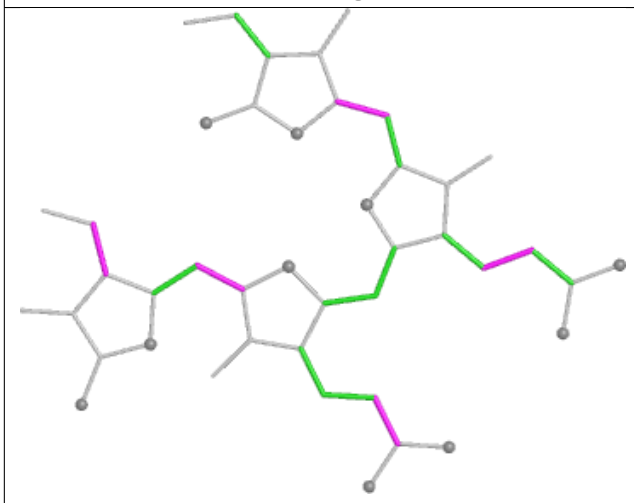
Ligand PEB EI 201



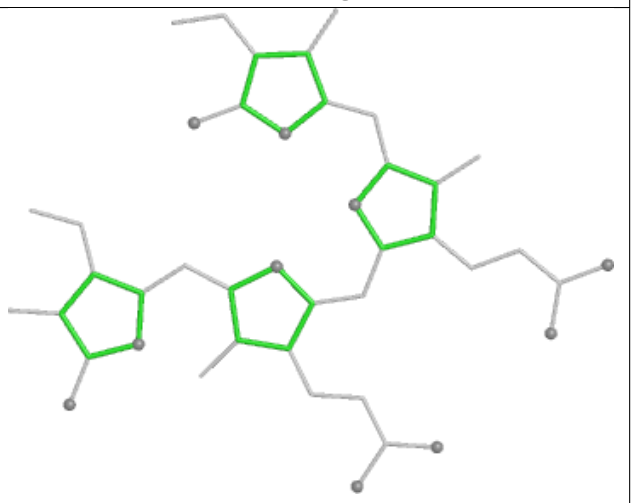
Bond lengths



Bond angles

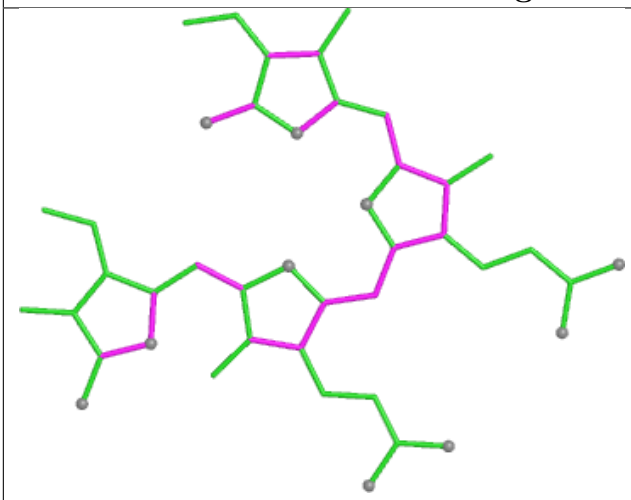


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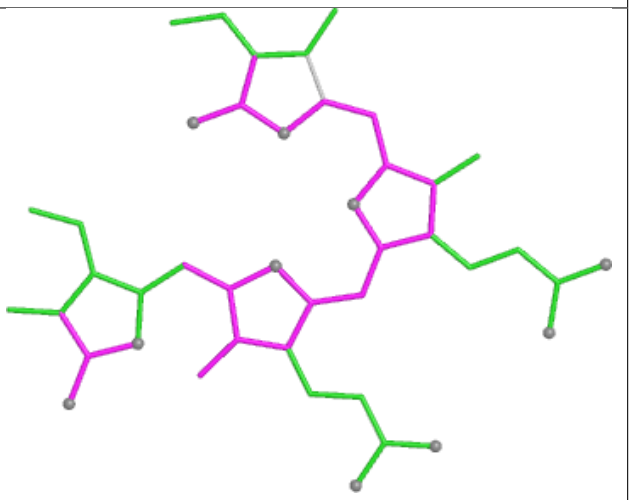


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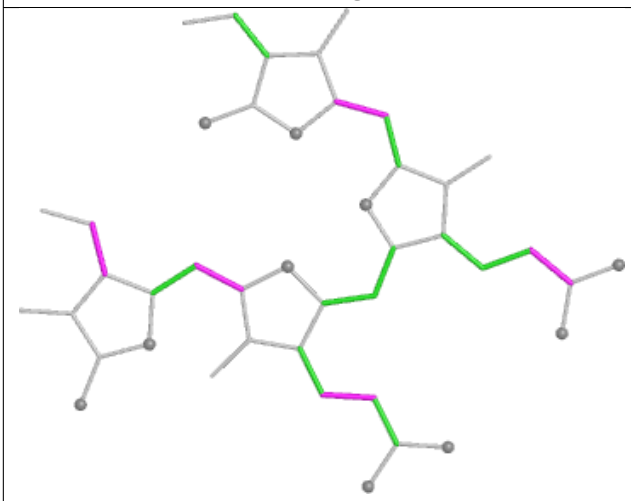
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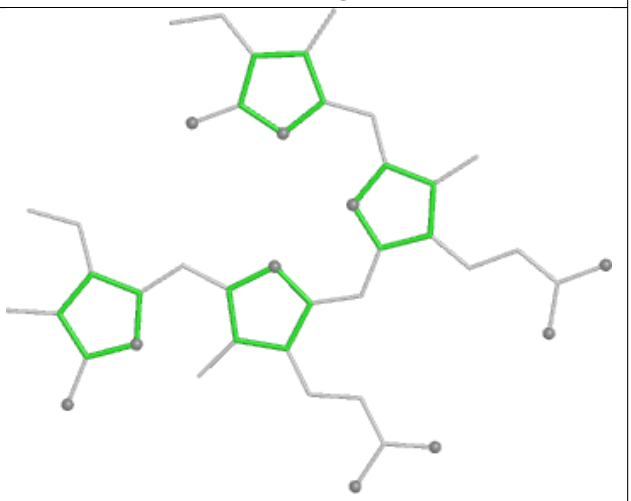
Bond lengths



Bond angles

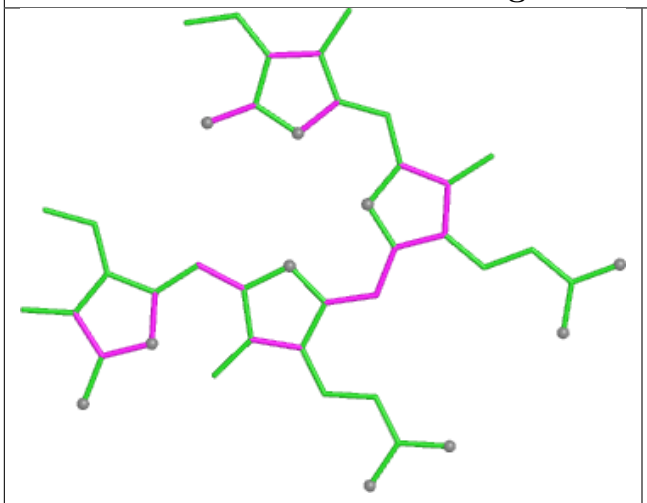


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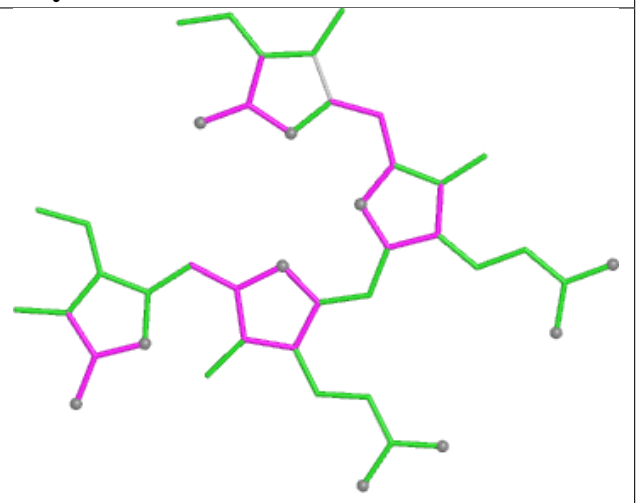


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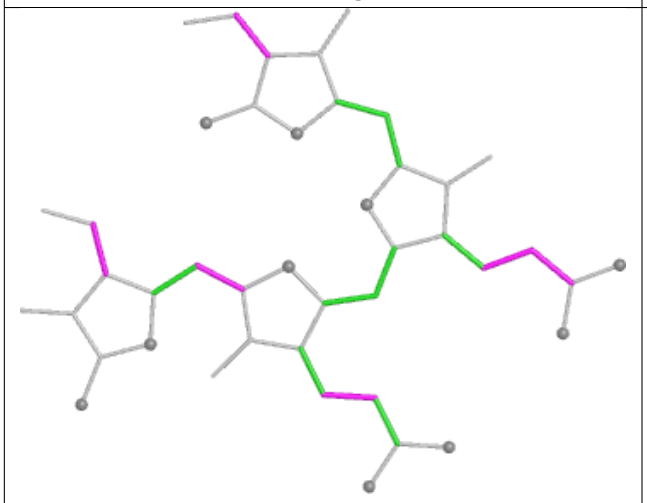
Ligand PEB QM 204



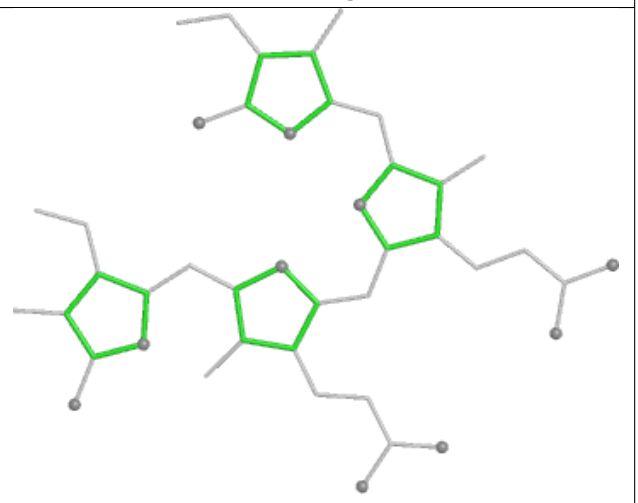
Bond lengths



Bond angles

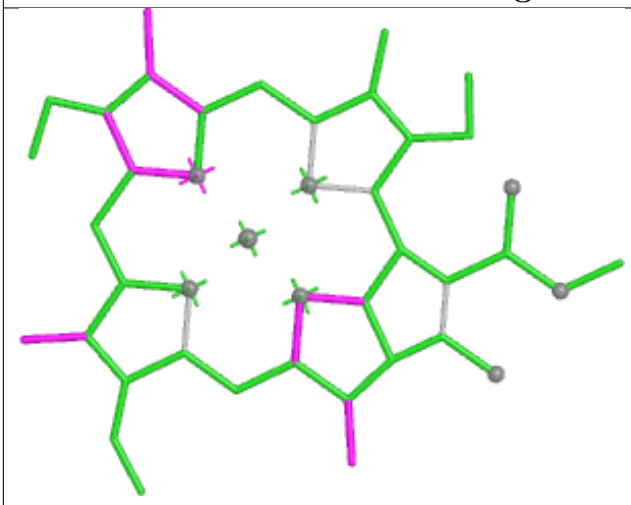


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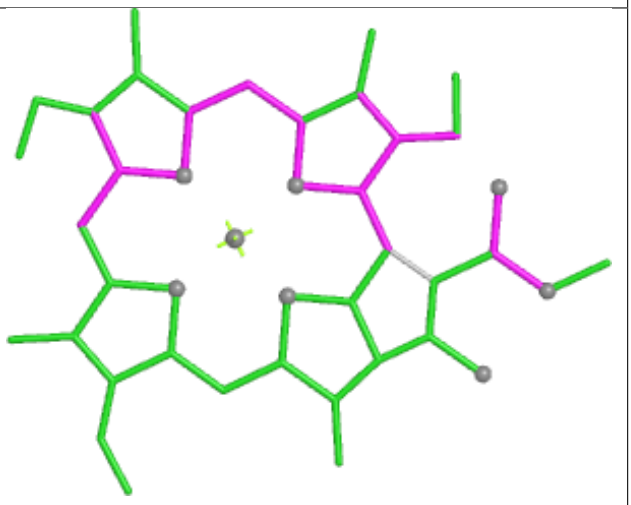


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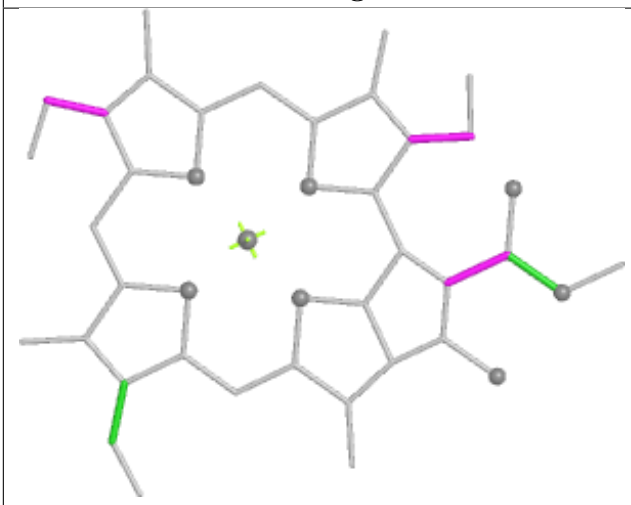
Ligand CLA 3N 307



Bond lengths



Bond angles

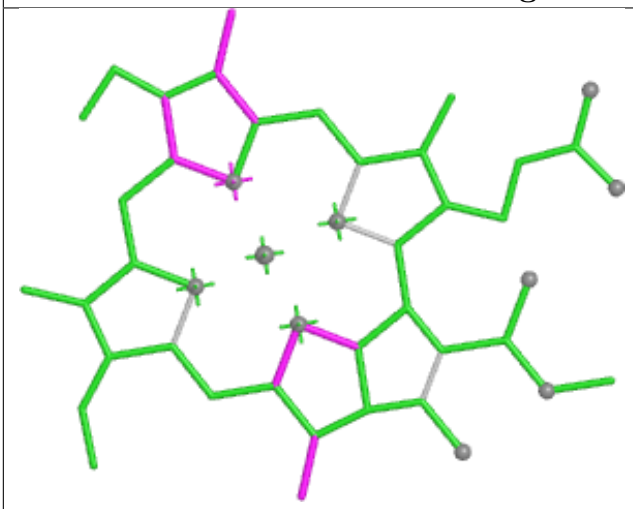


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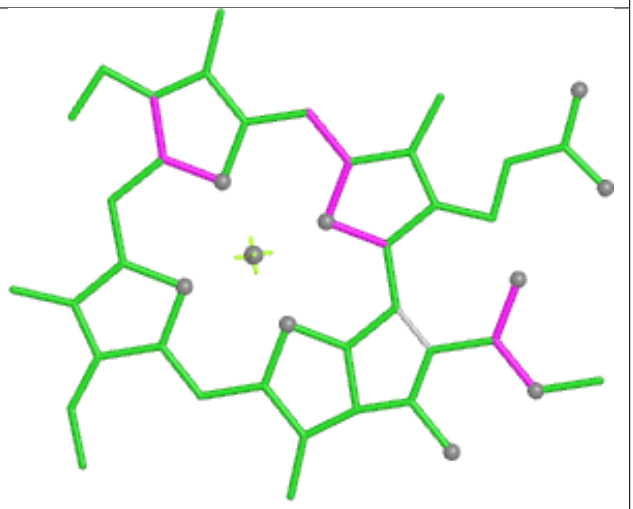


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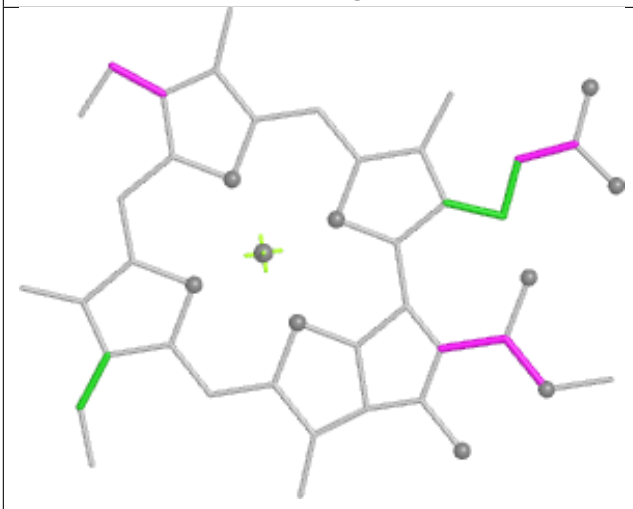
Ligand CLA 22 603



Bond lengths



Bond angles

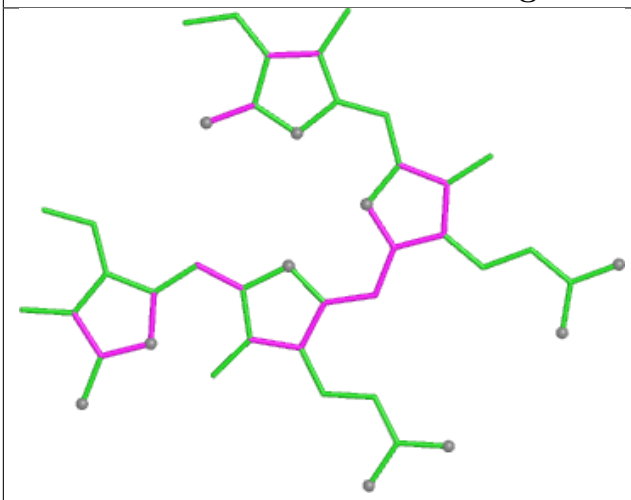


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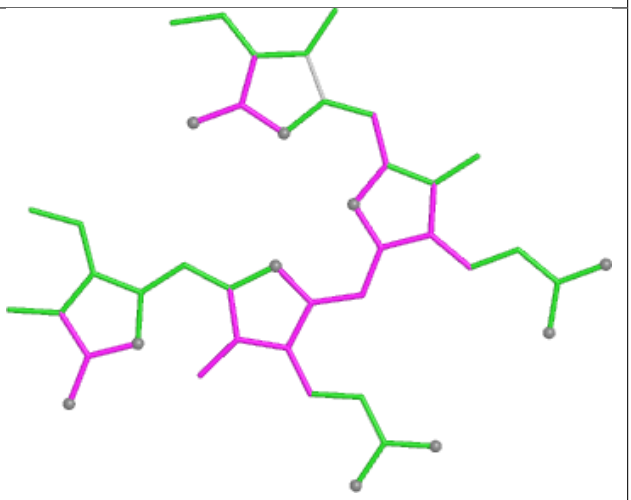


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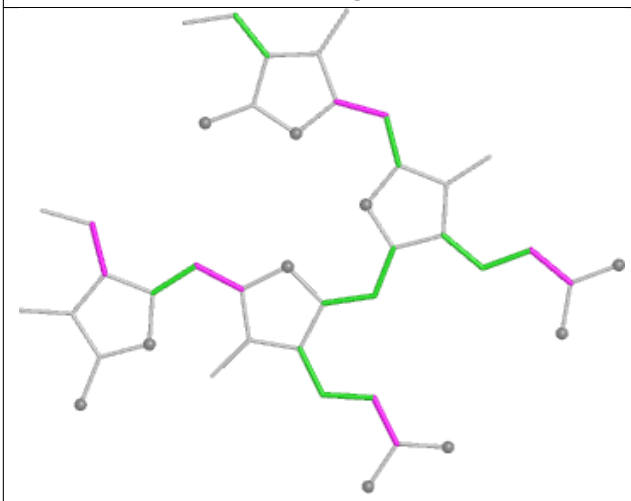
Ligand PEB v8 201



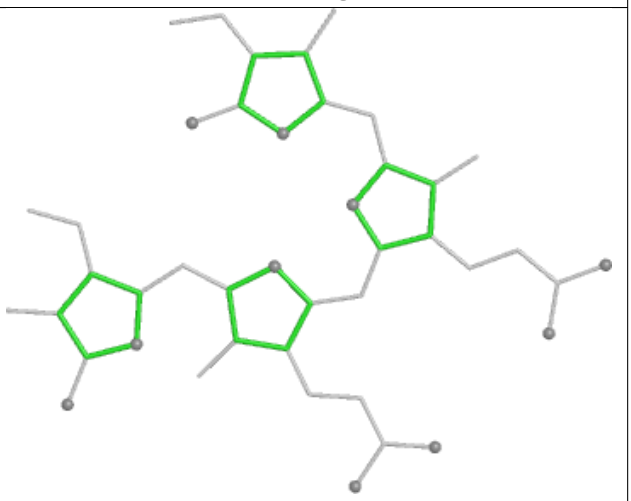
Bond lengths



Bond angles

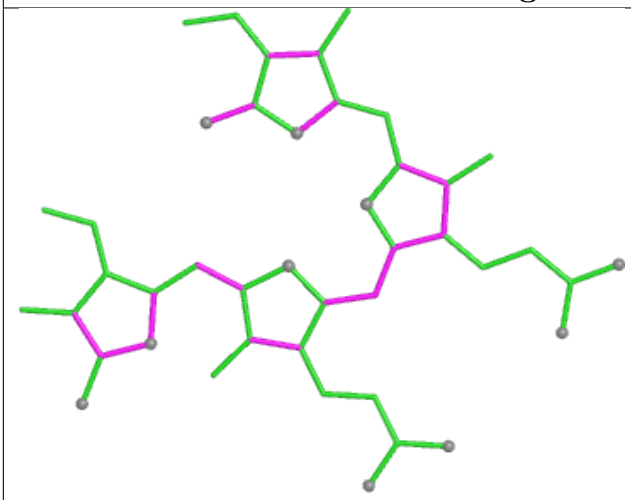


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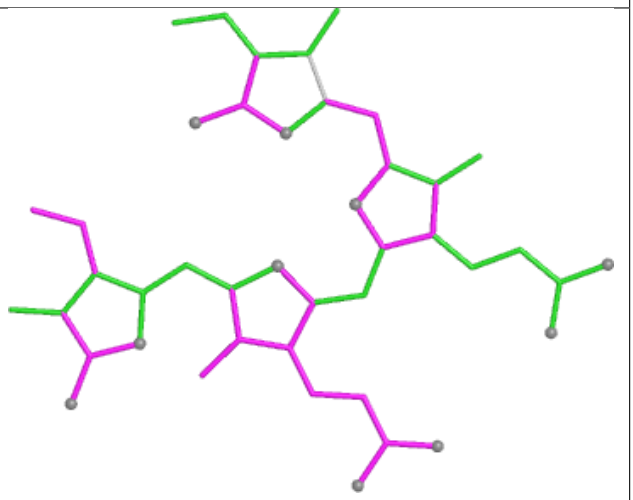


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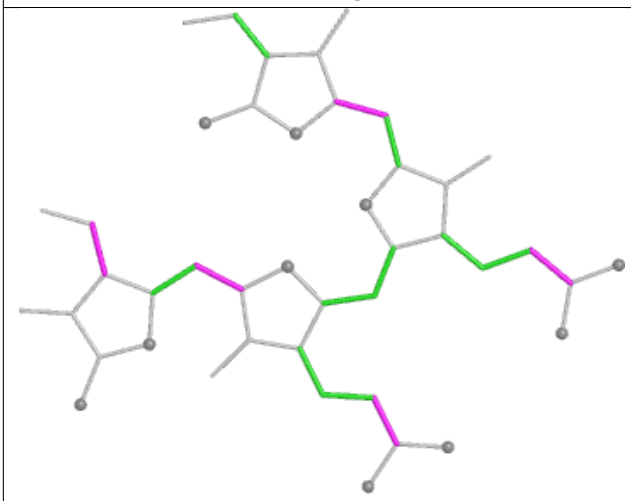
Ligand PEB lO 202



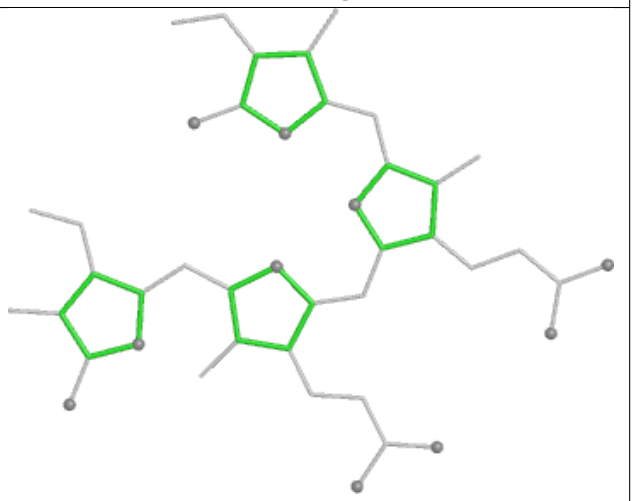
Bond lengths



Bond angles

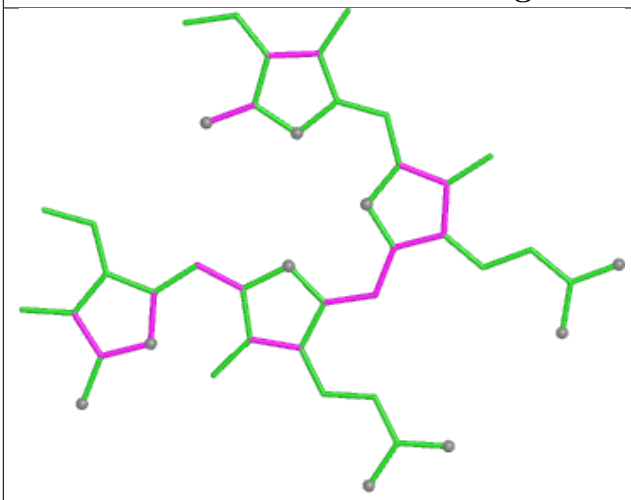


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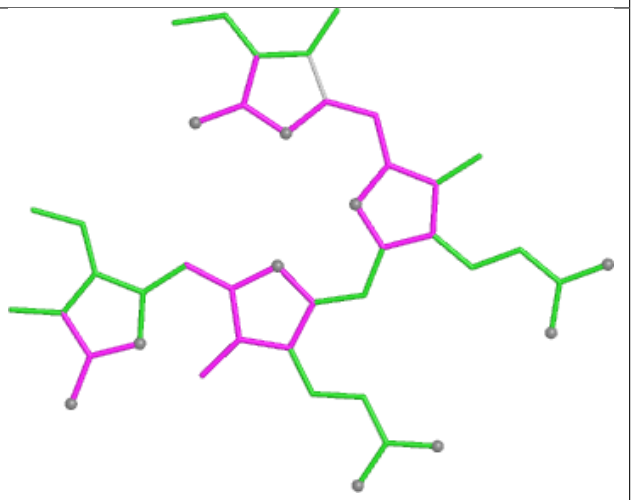


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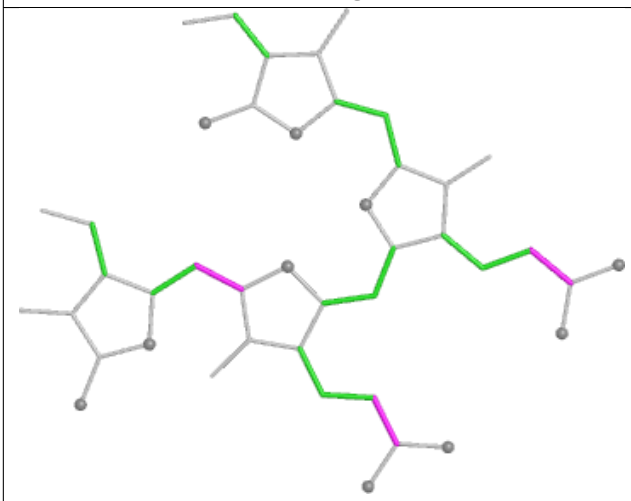
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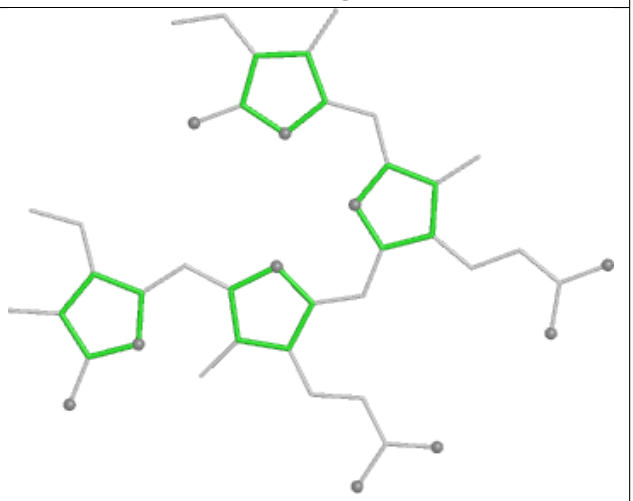
Bond lengths



Bond angles

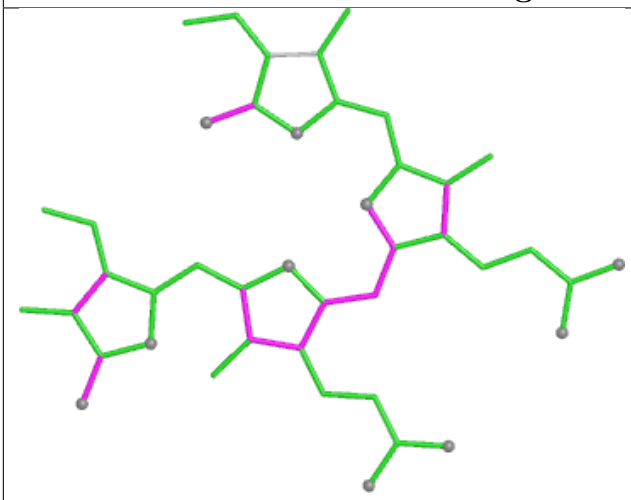


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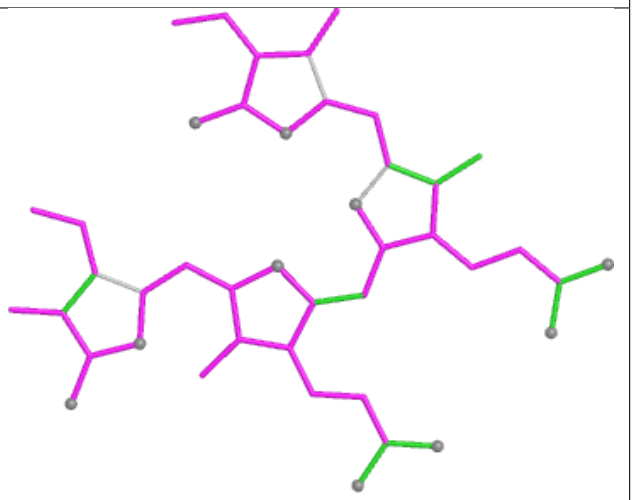


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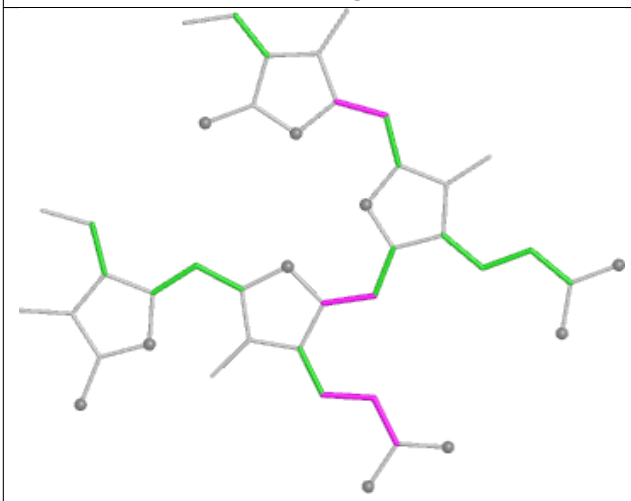
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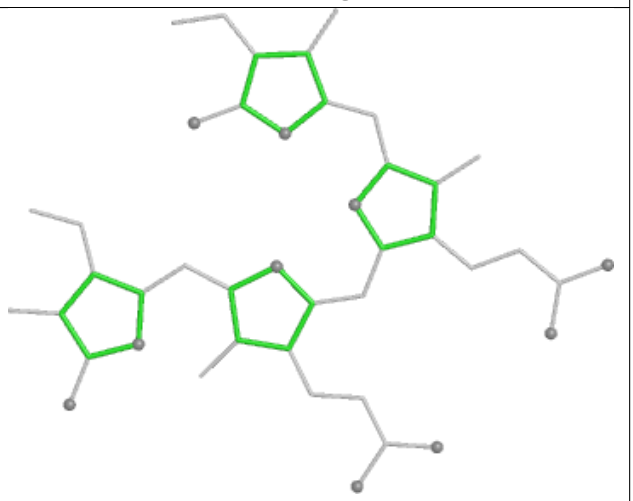
Bond lengths



Bond angles

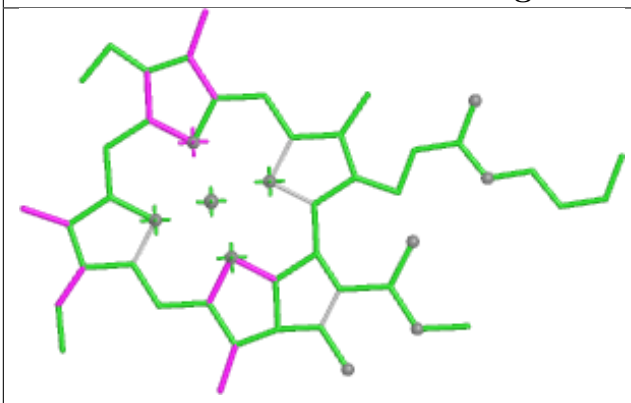


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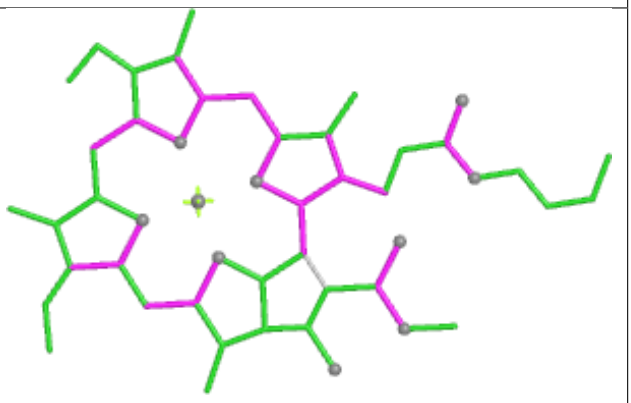


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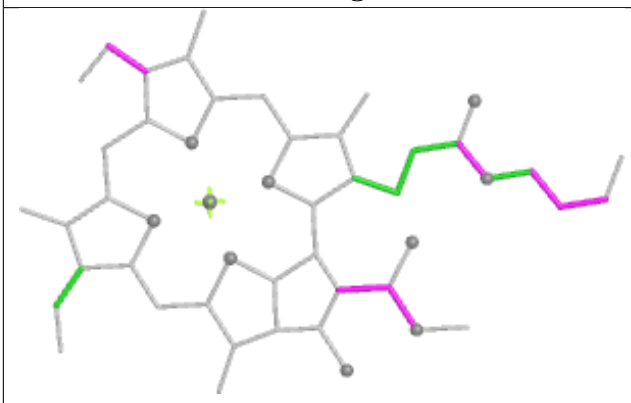
Ligand CLA K2 106



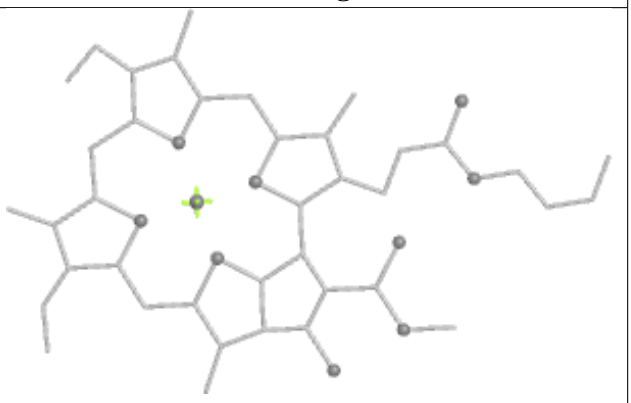
Bond lengths



Bond angles

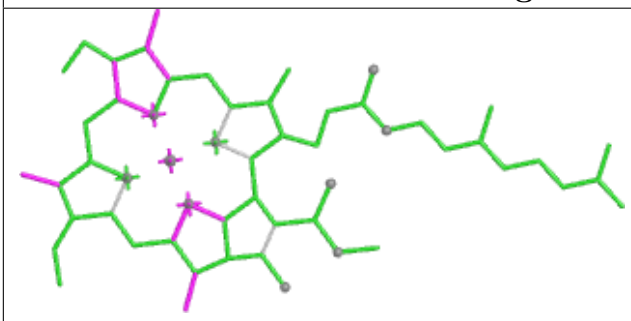


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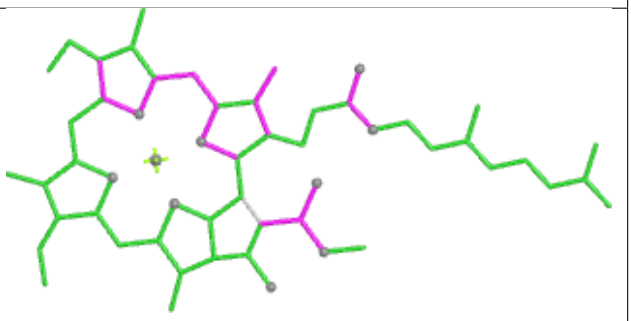


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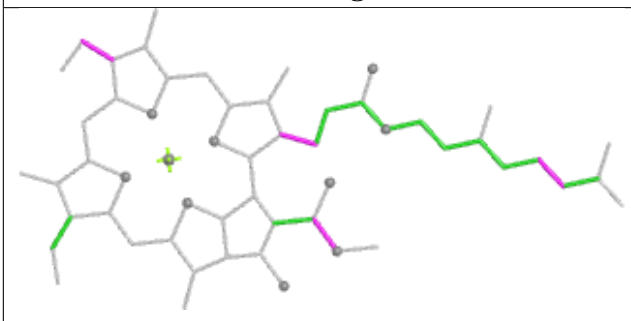
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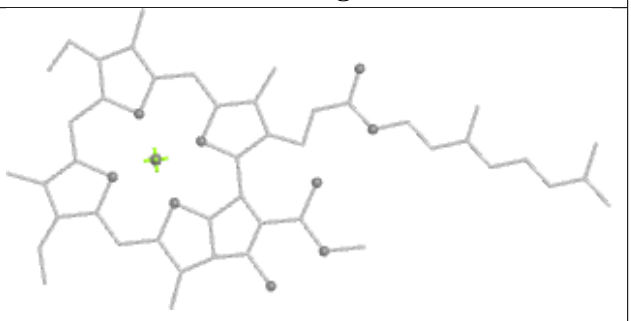
Bond lengths



Bond angles

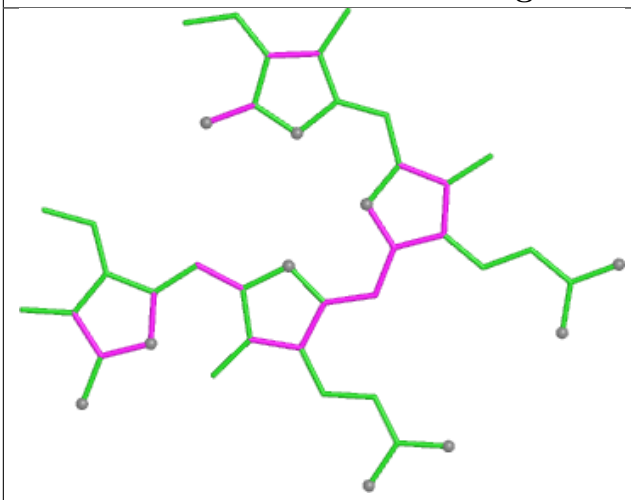


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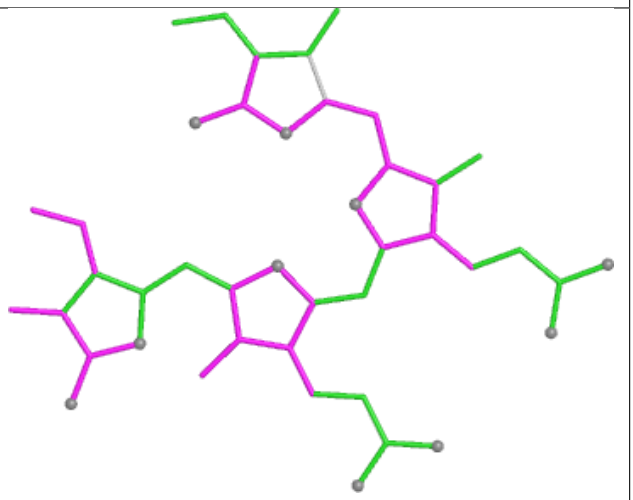


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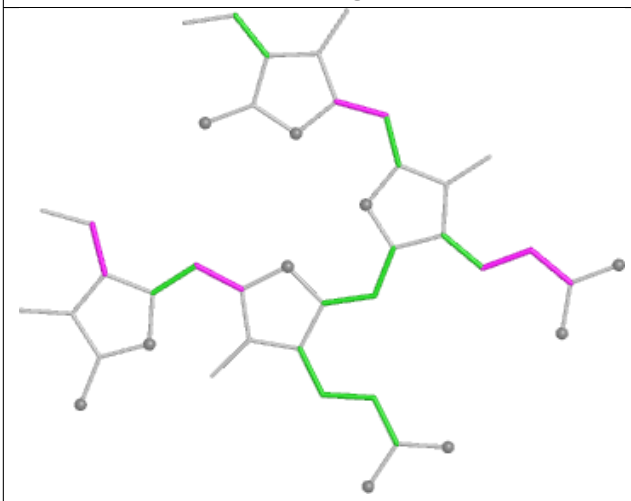
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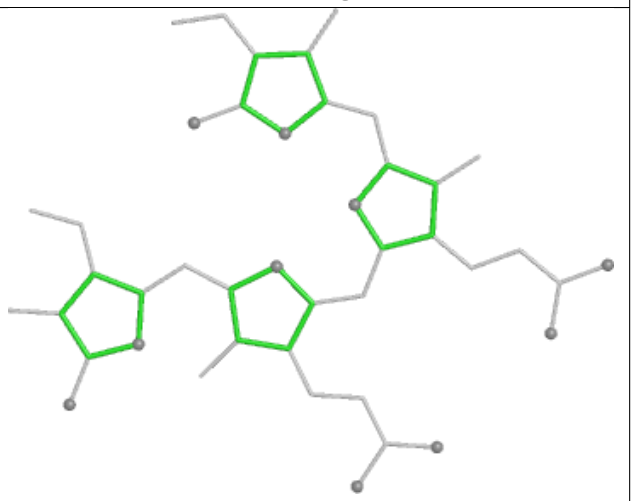
Bond lengths



Bond angles

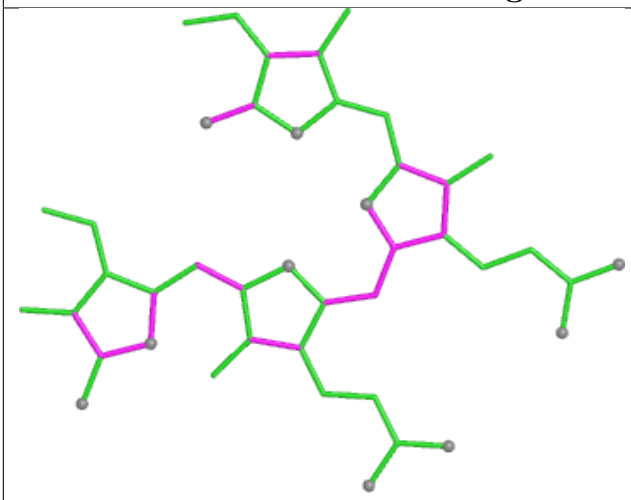


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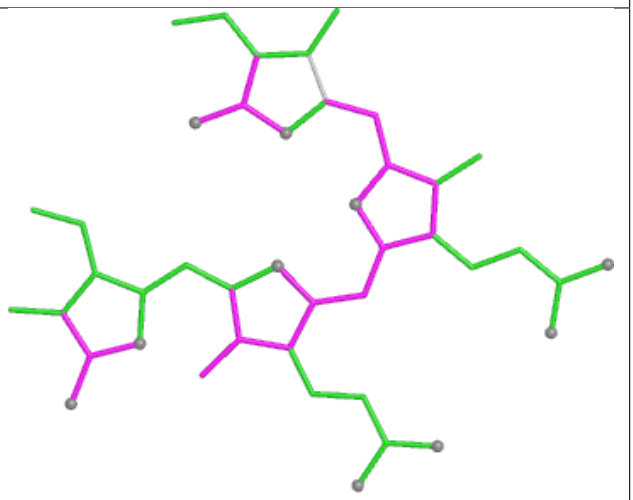


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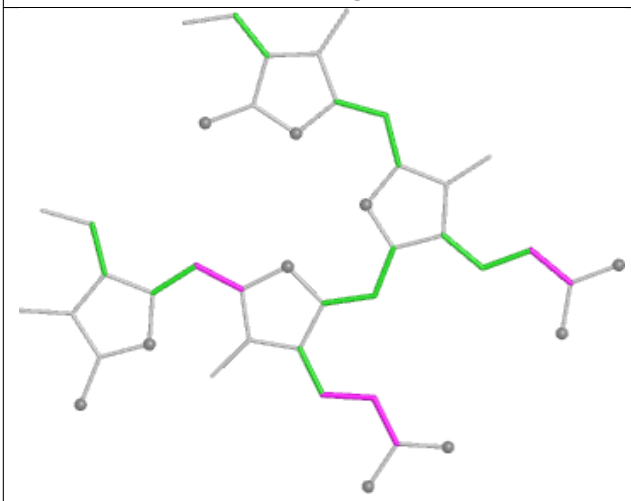
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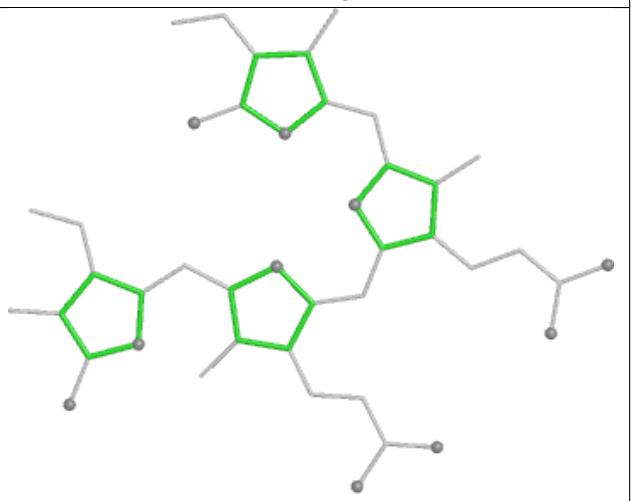
Bond lengths



Bond angles

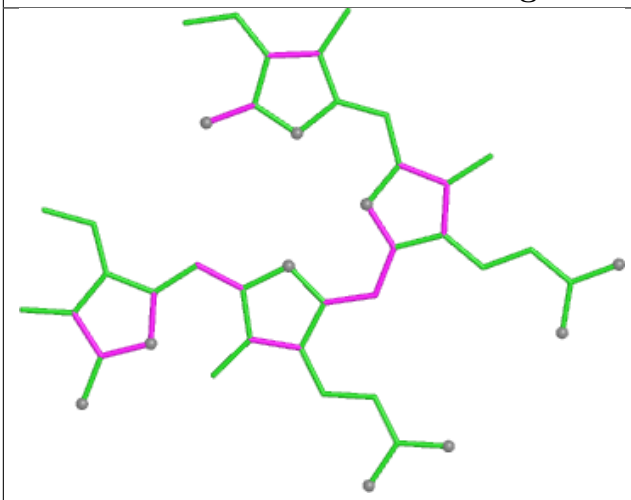


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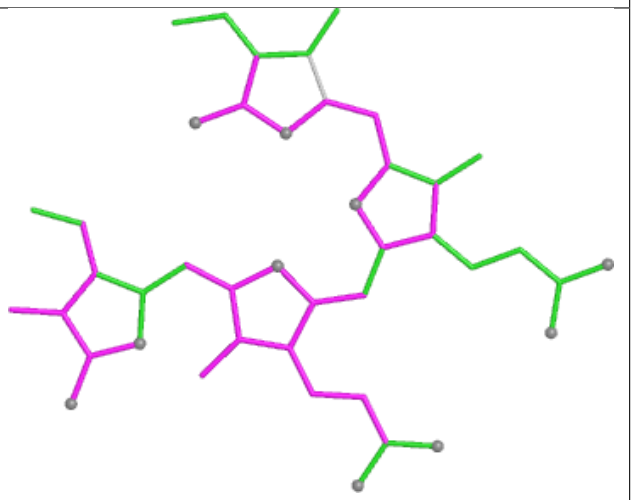


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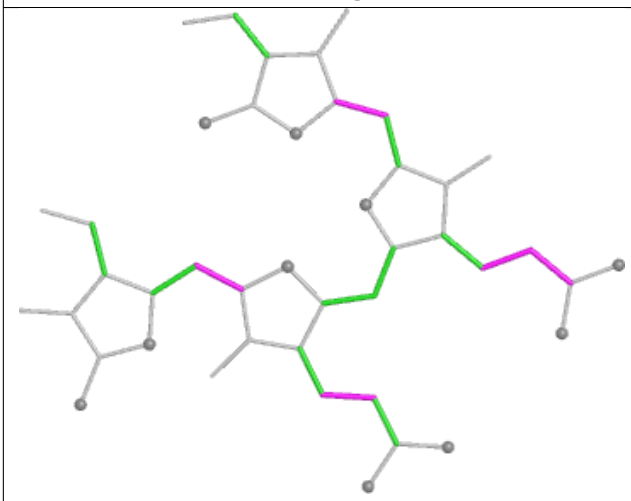
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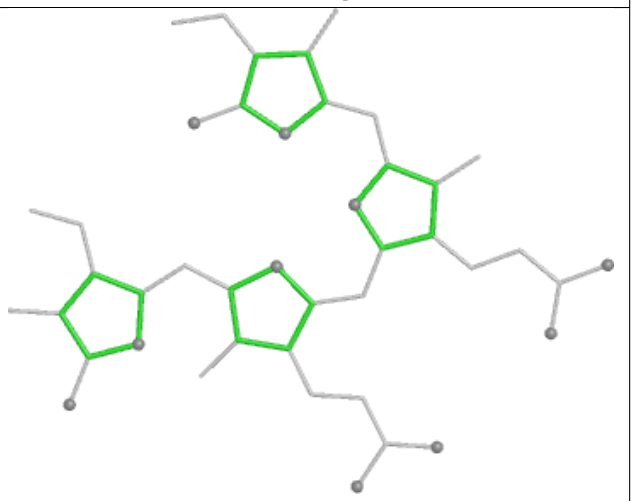
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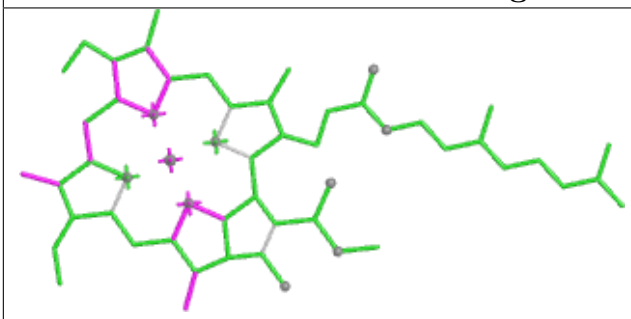


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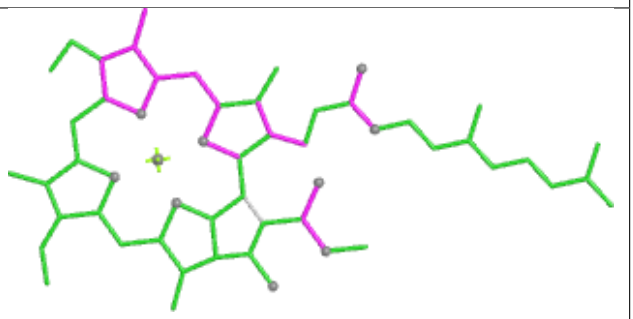


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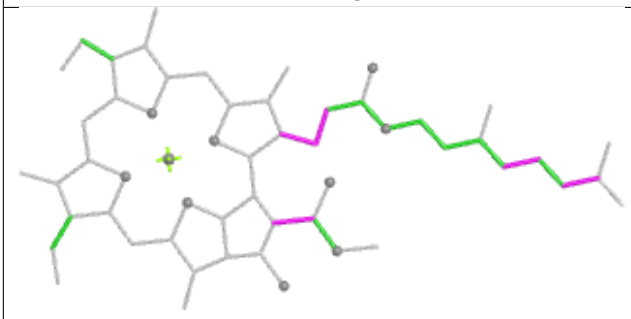
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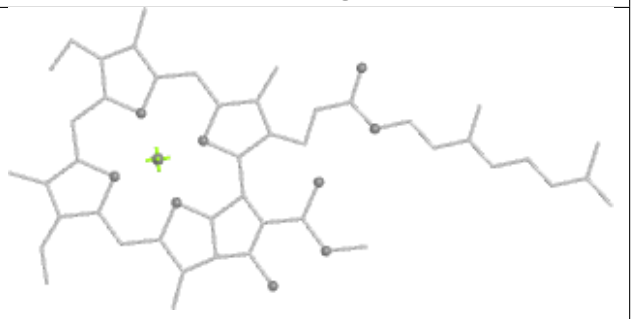
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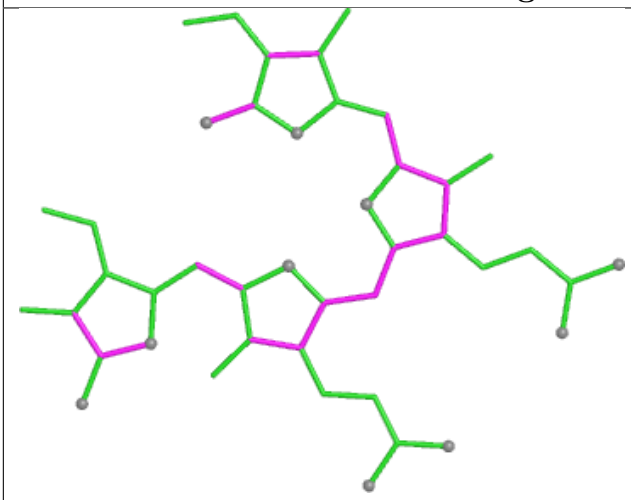


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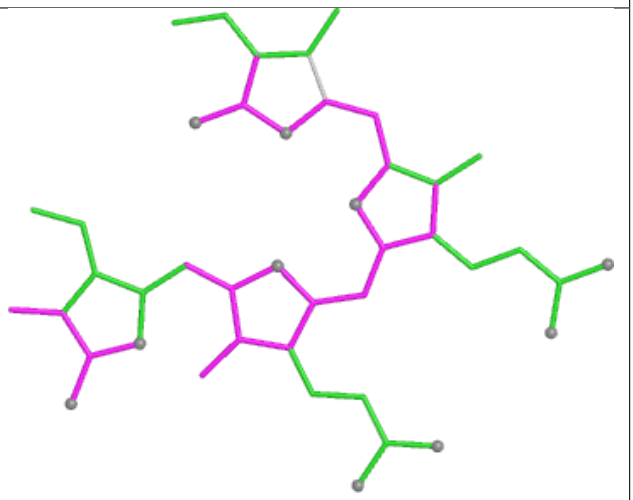


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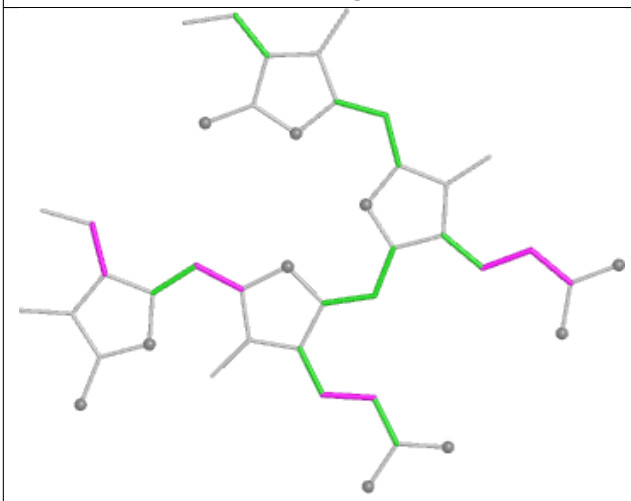
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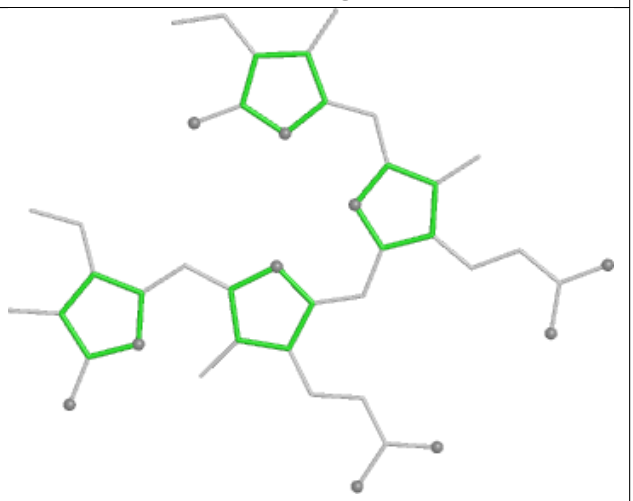
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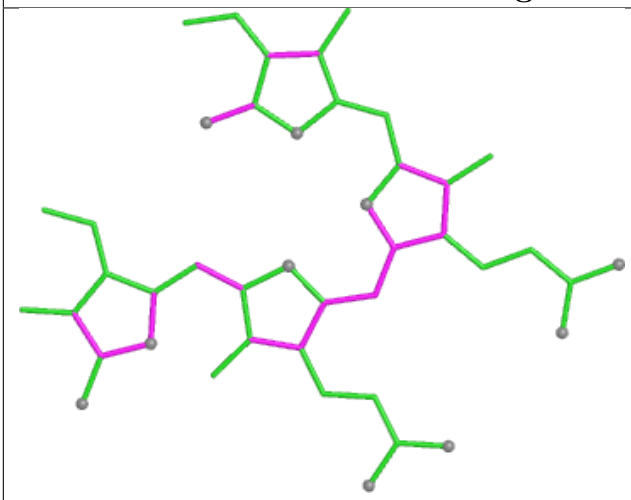


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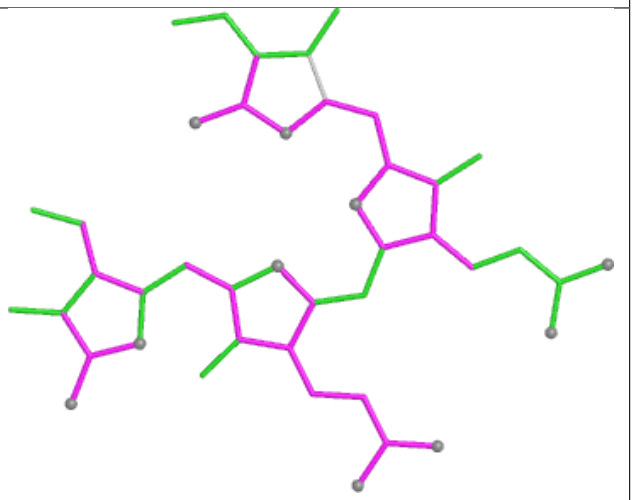


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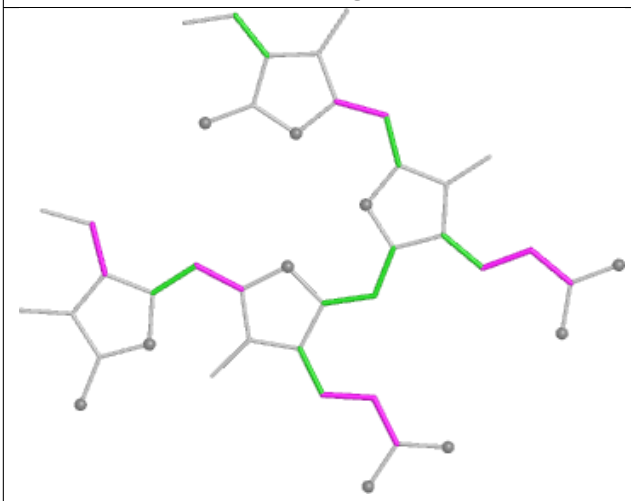
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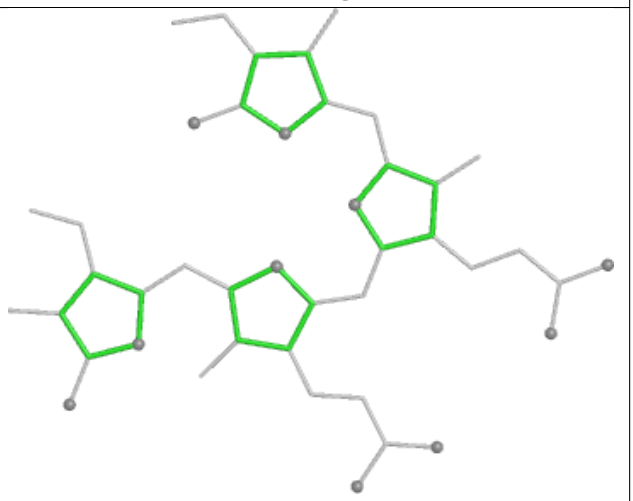
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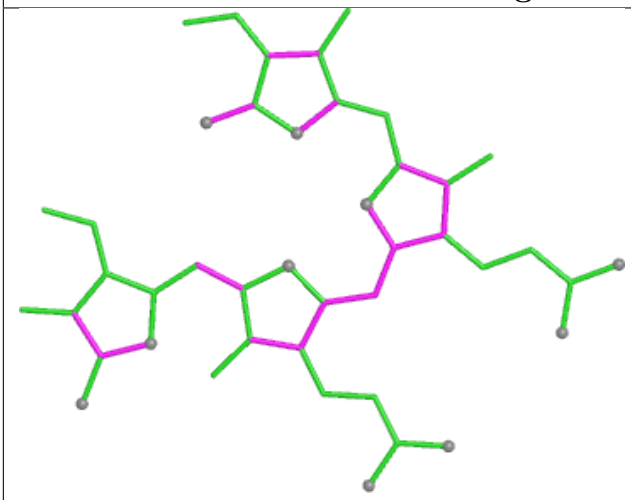


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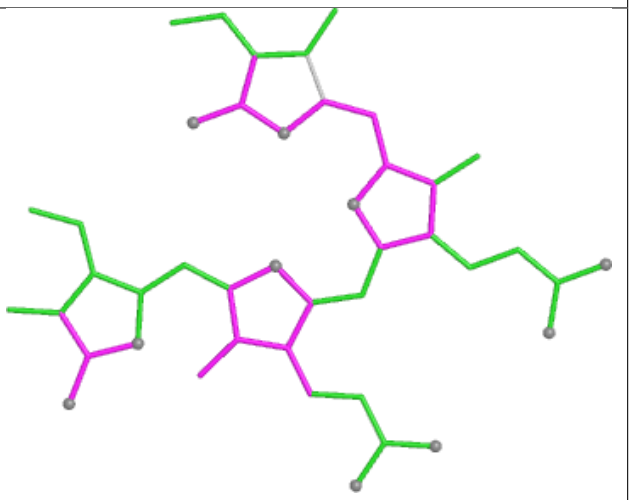


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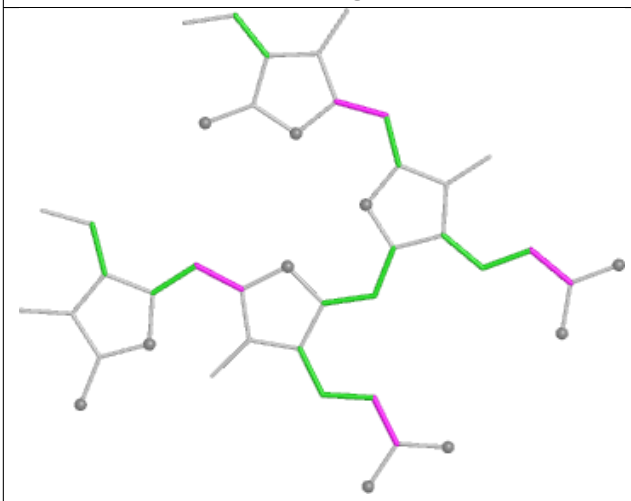
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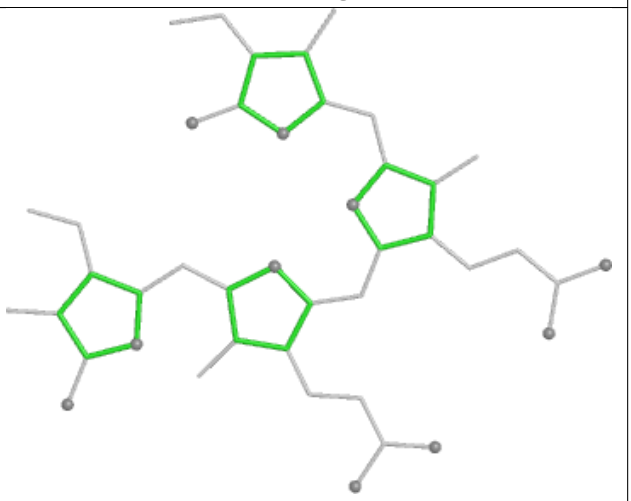
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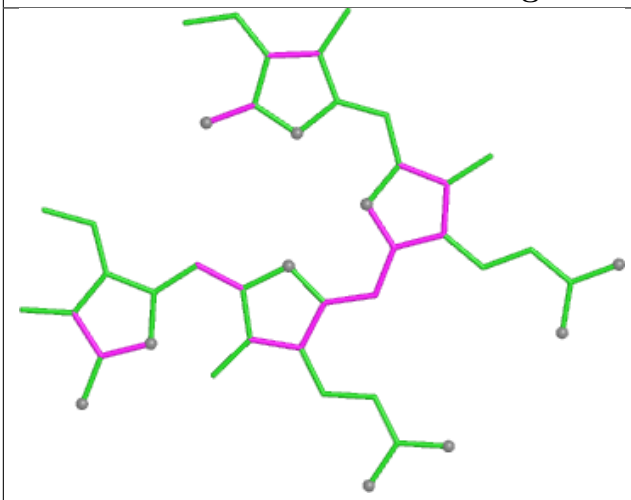


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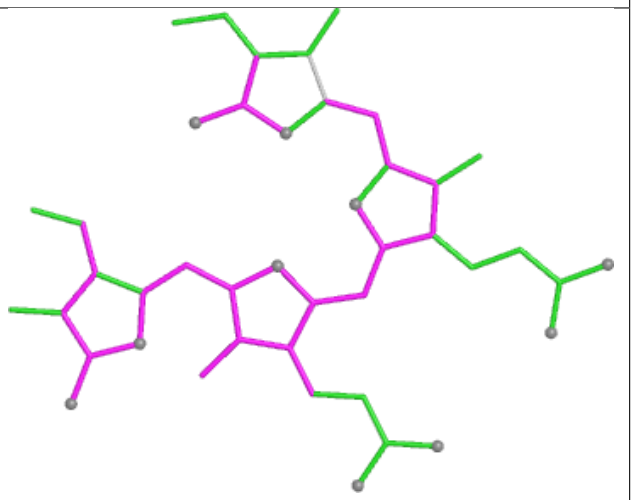


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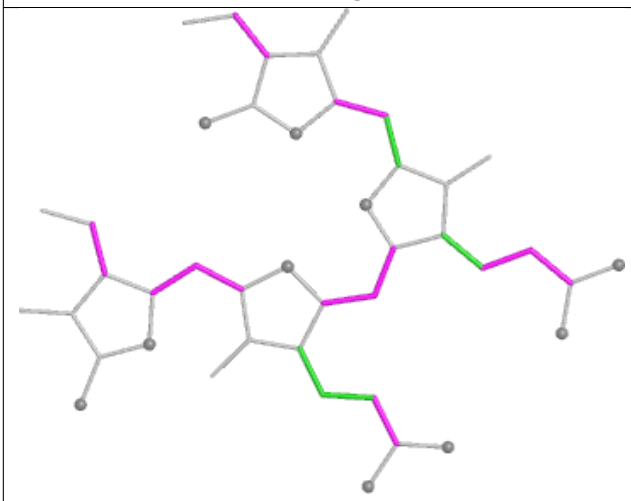
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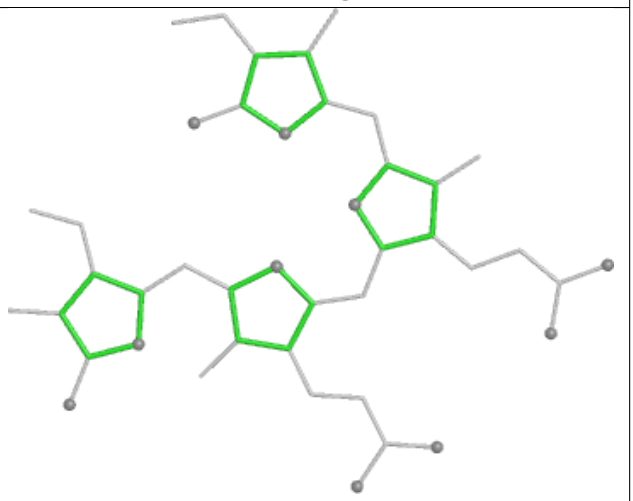
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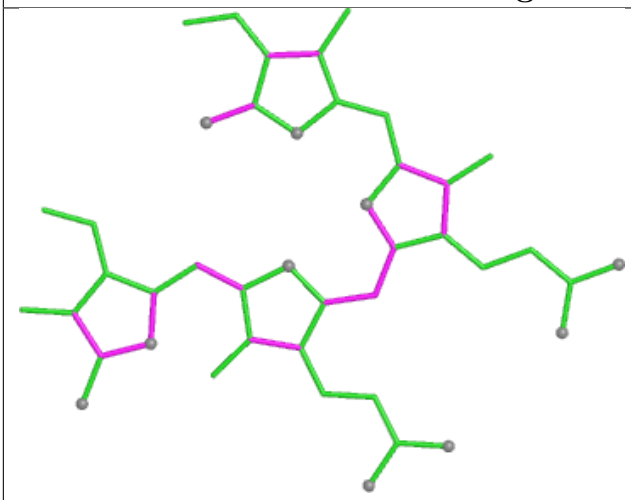


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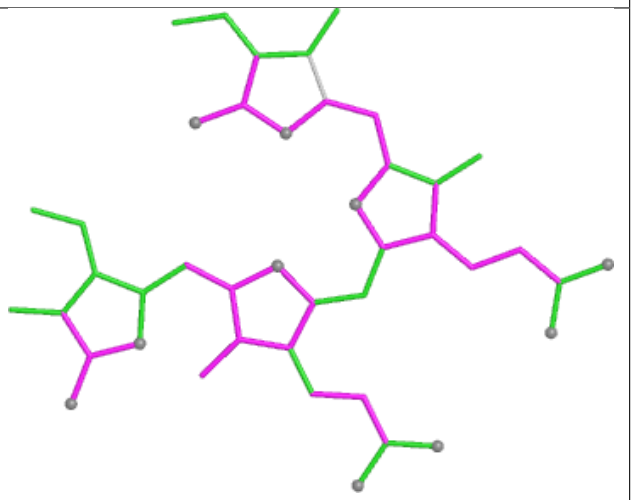


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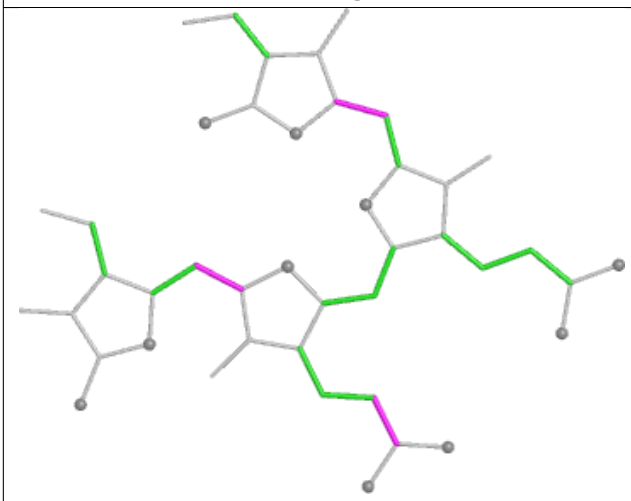
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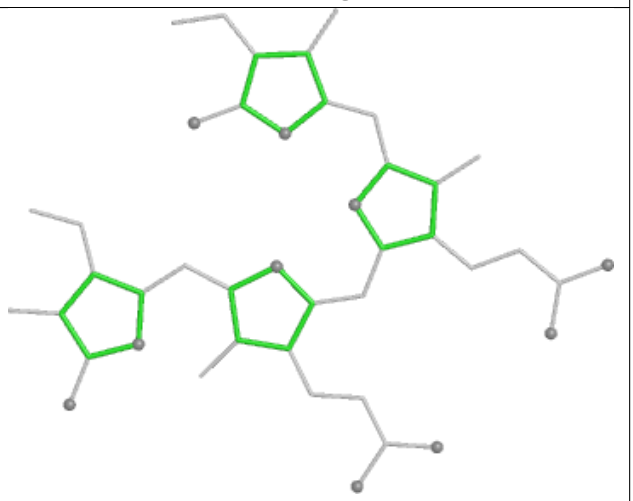
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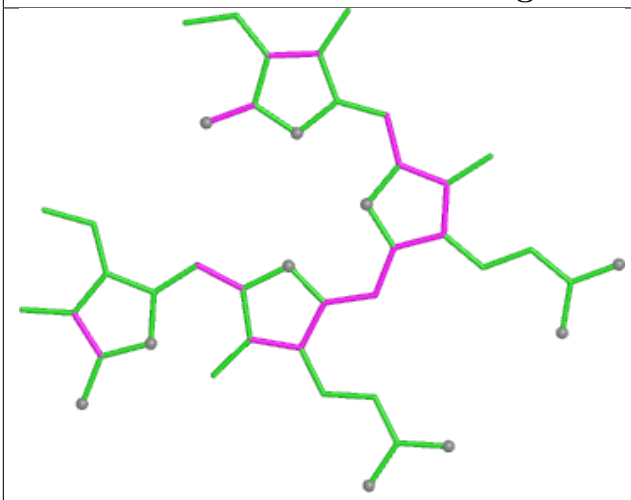


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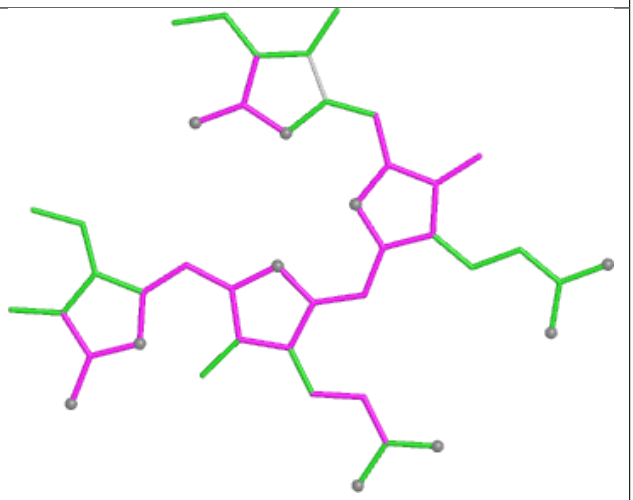


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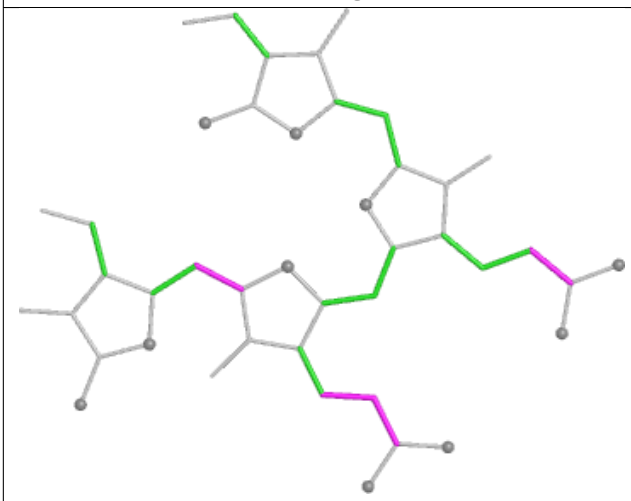
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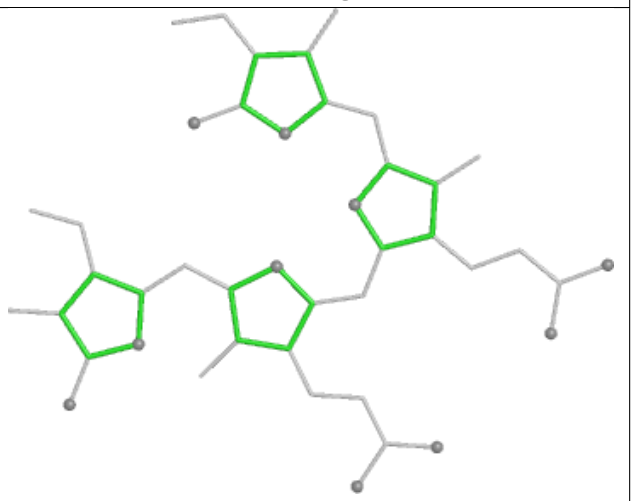
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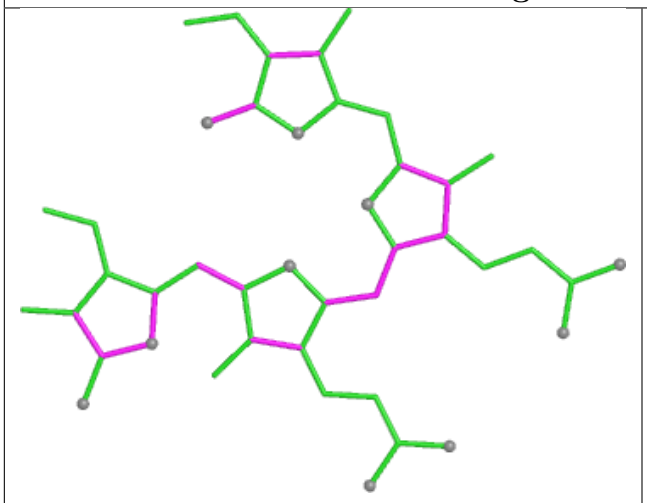


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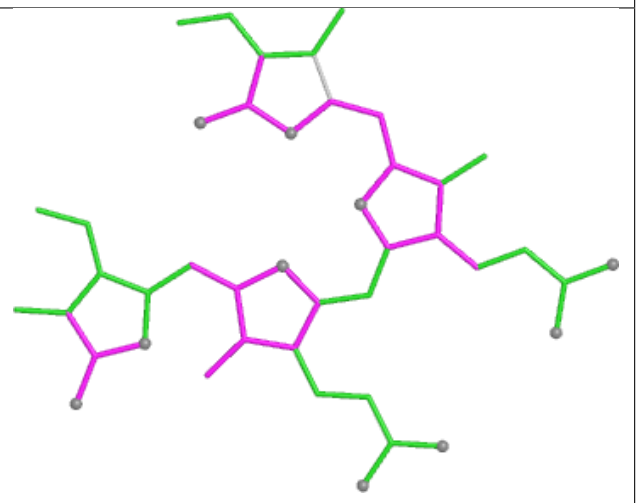


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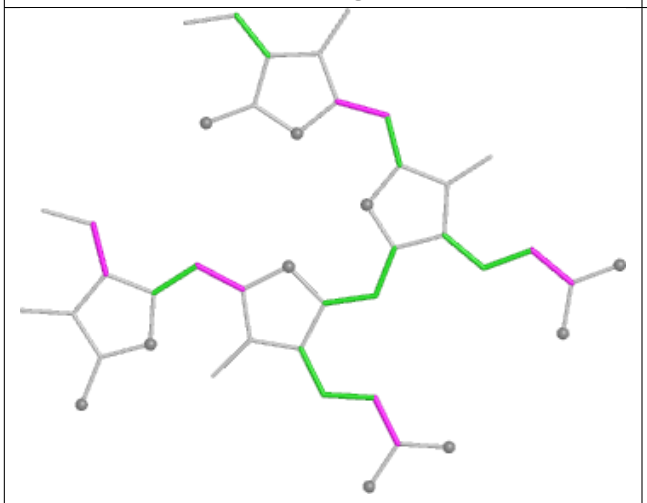
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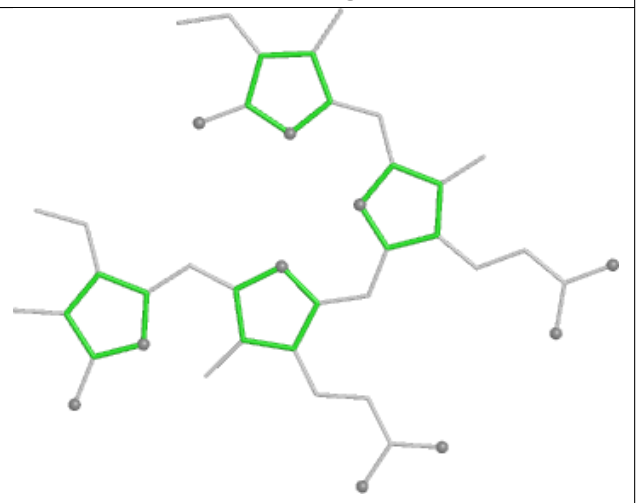
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Bond angles

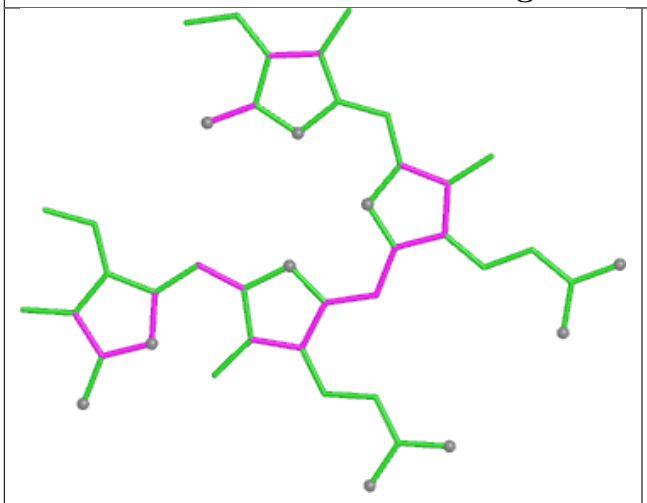


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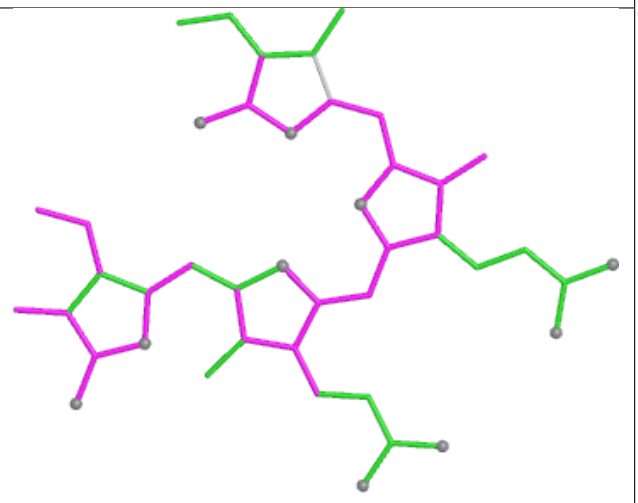


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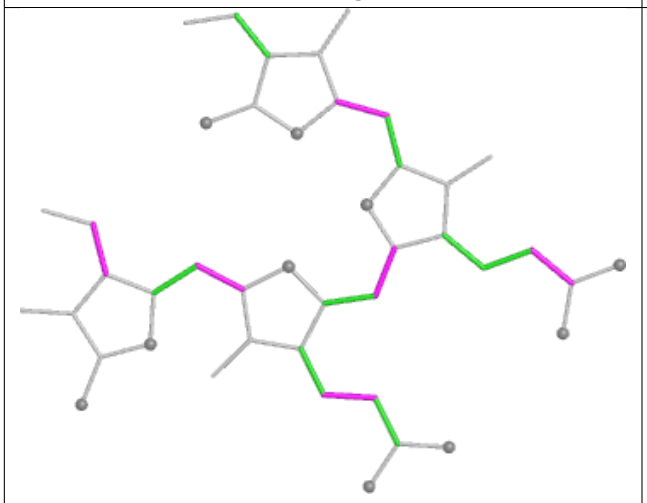
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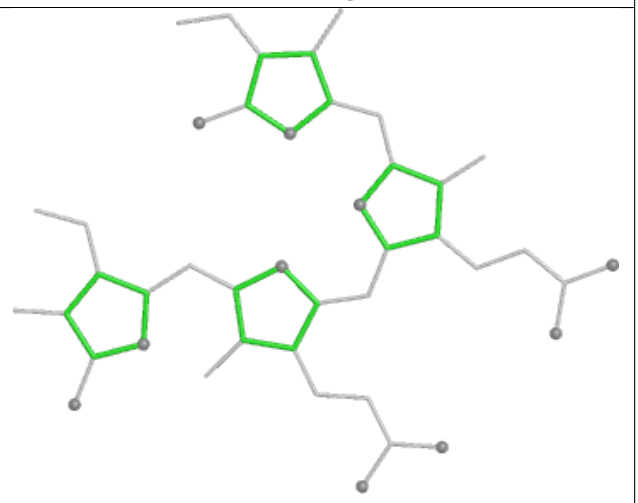
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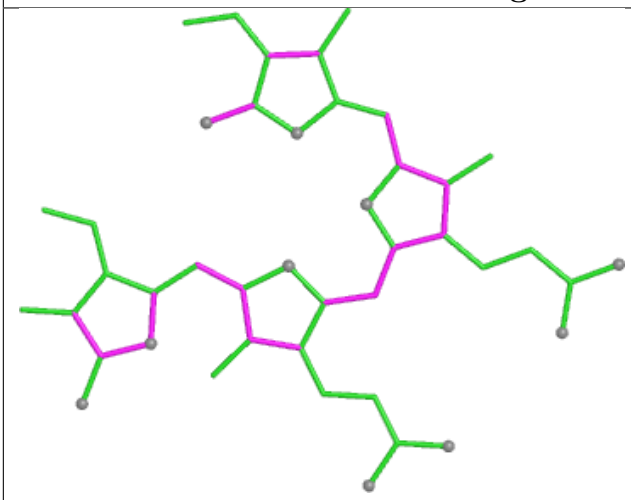


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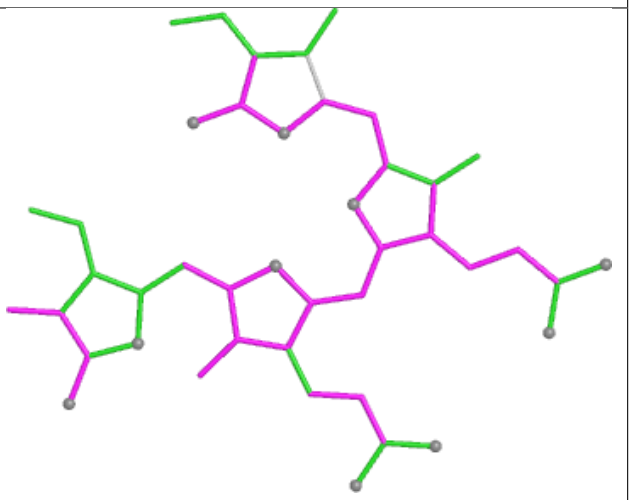


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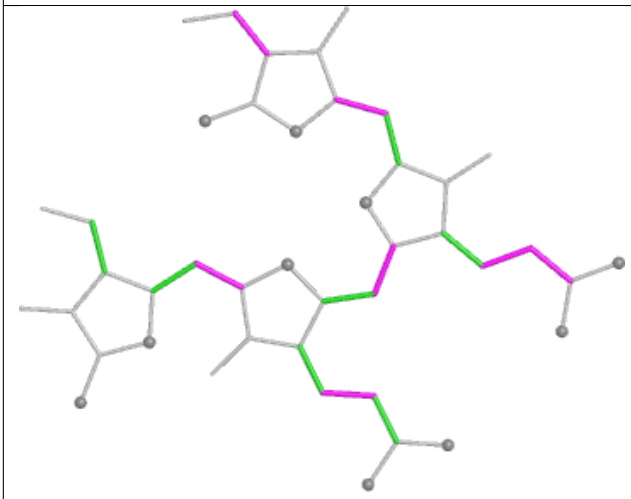
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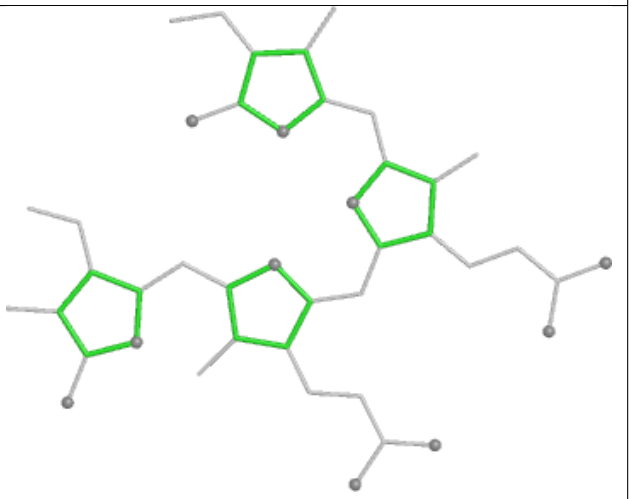
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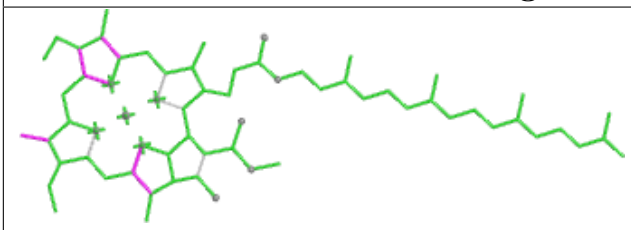


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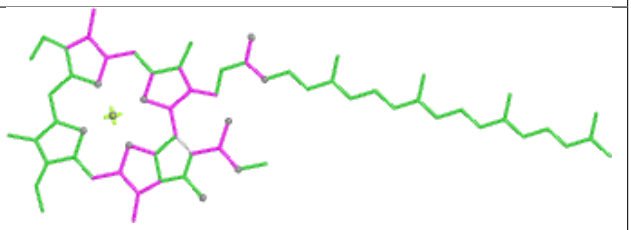


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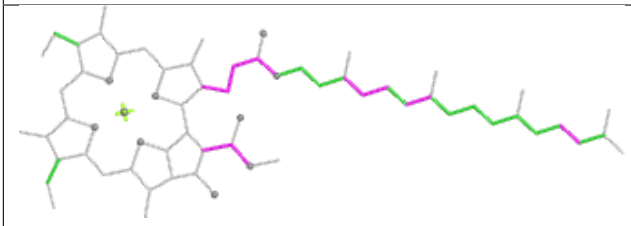
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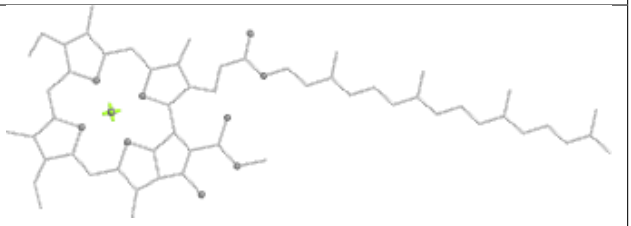
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Bond angles

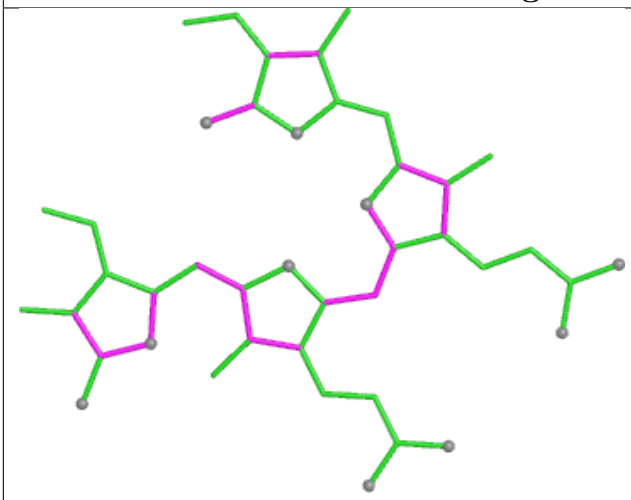


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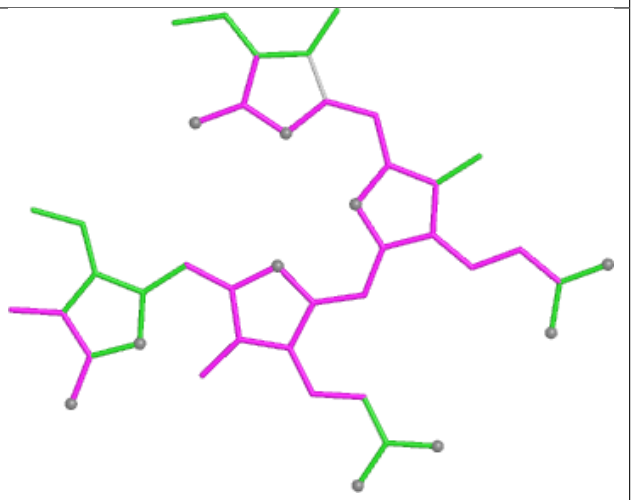


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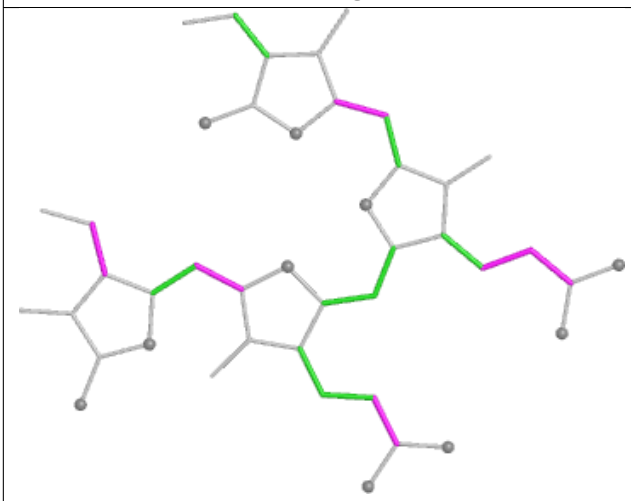
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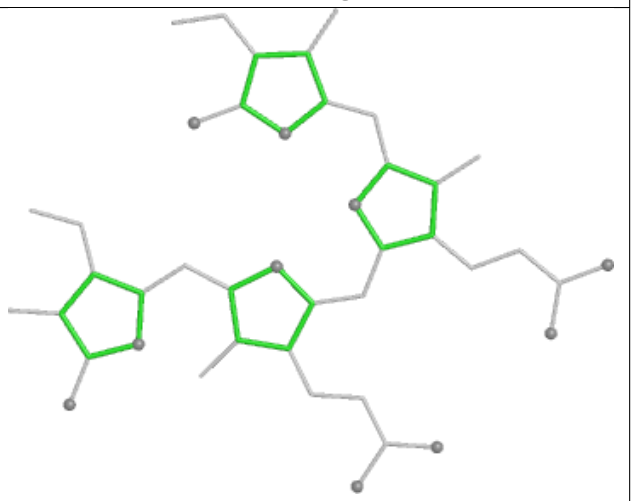
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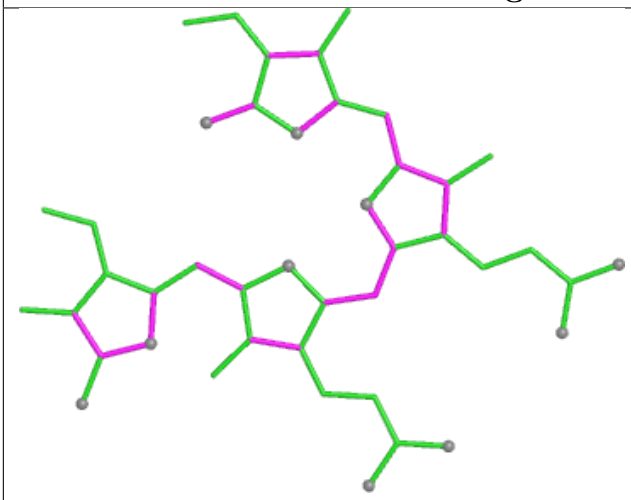


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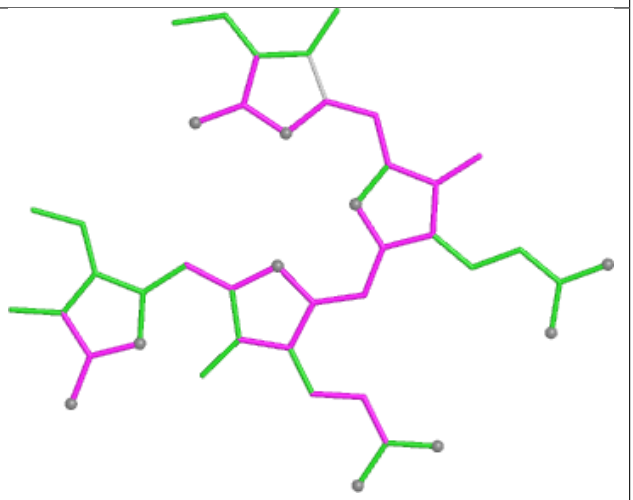


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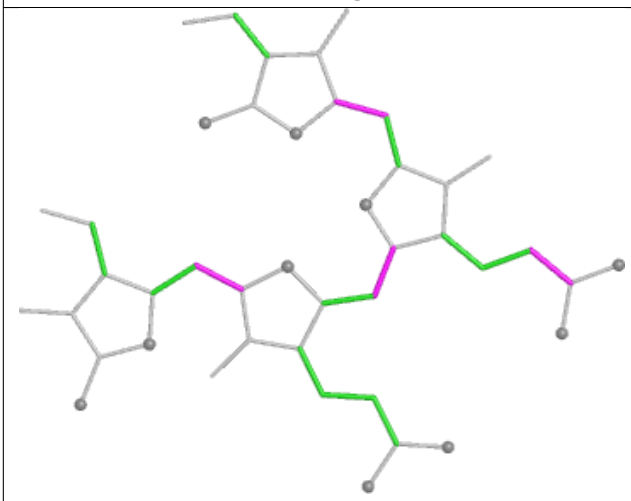
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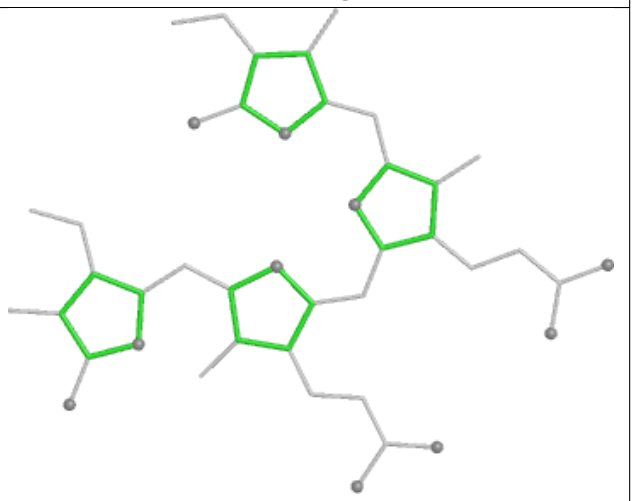
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Bond angles

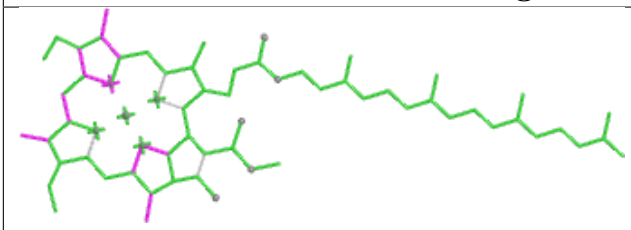


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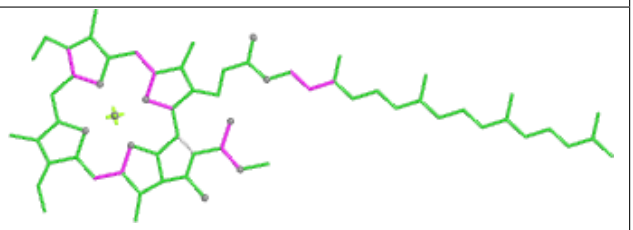


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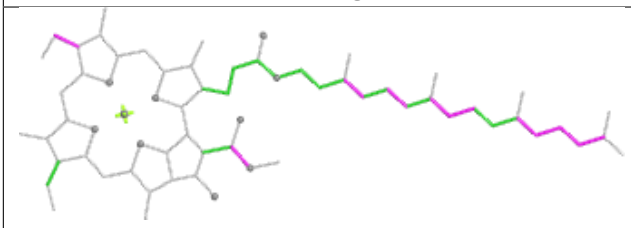
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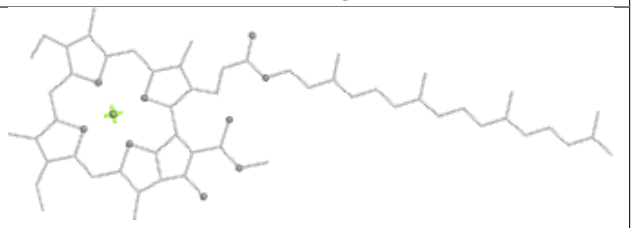
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Bond angles

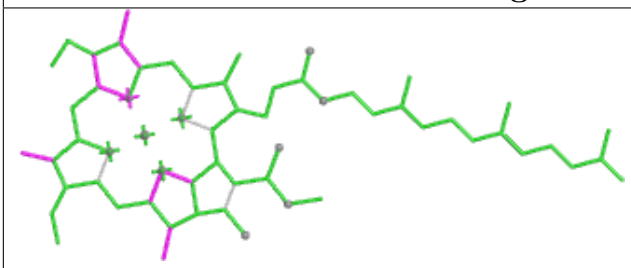


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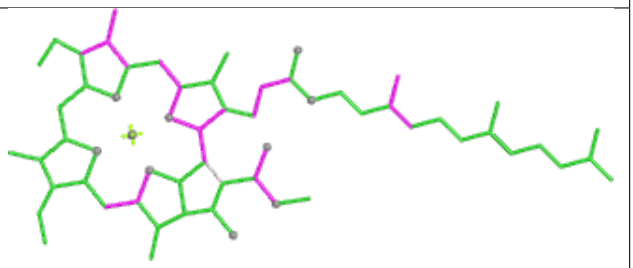


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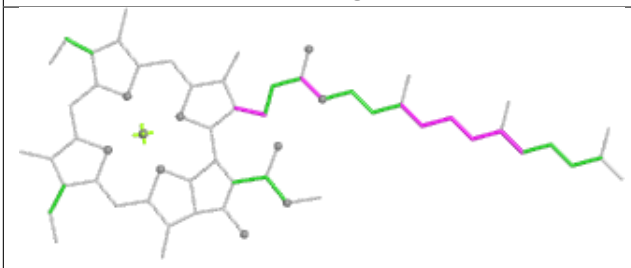
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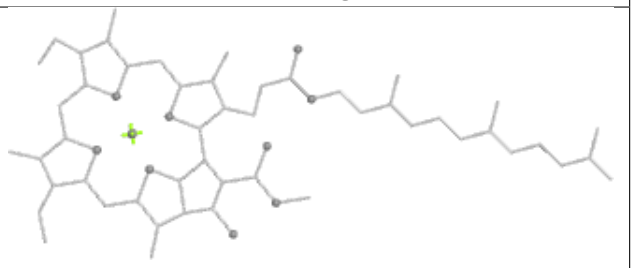
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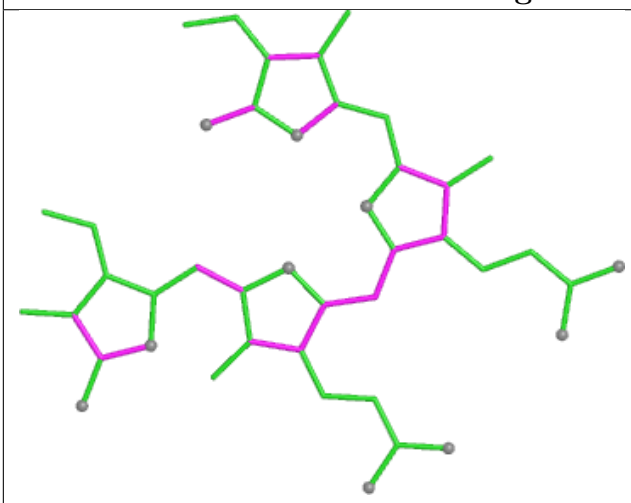


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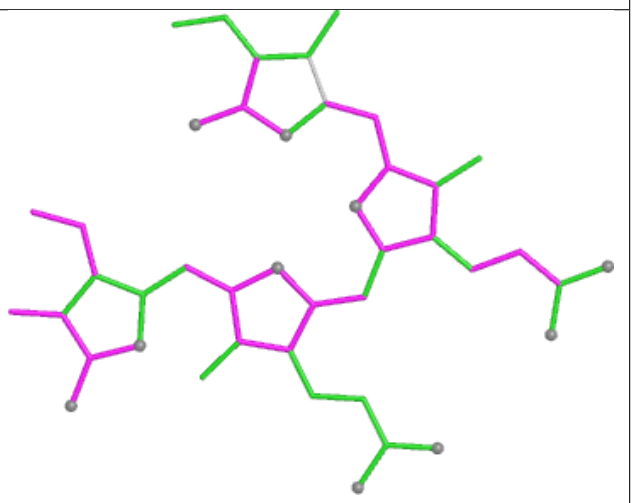


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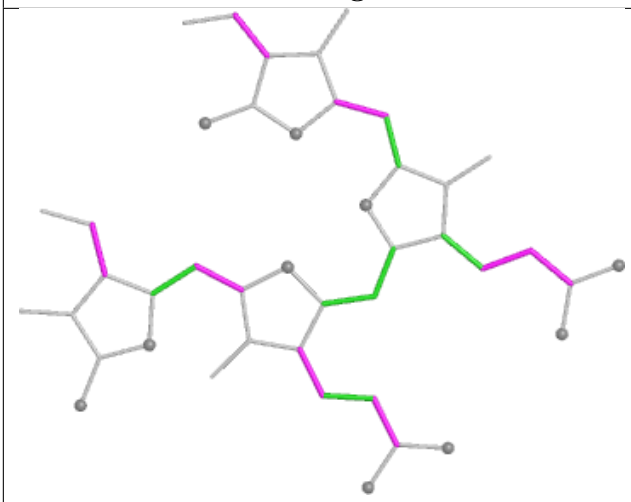
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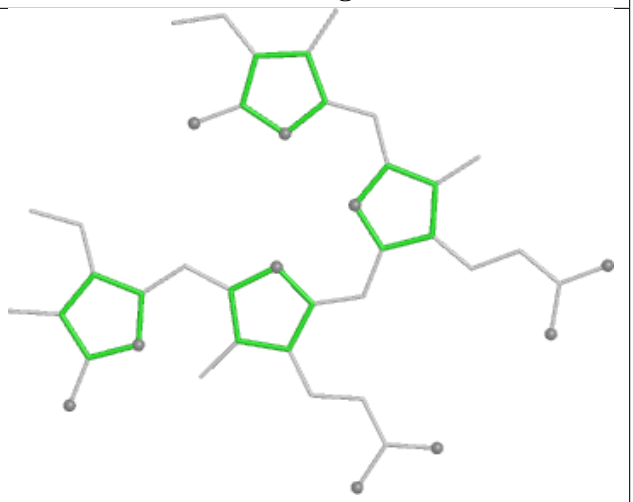
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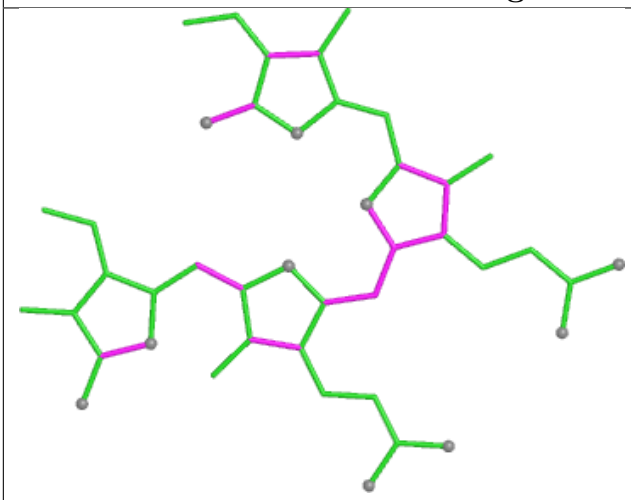


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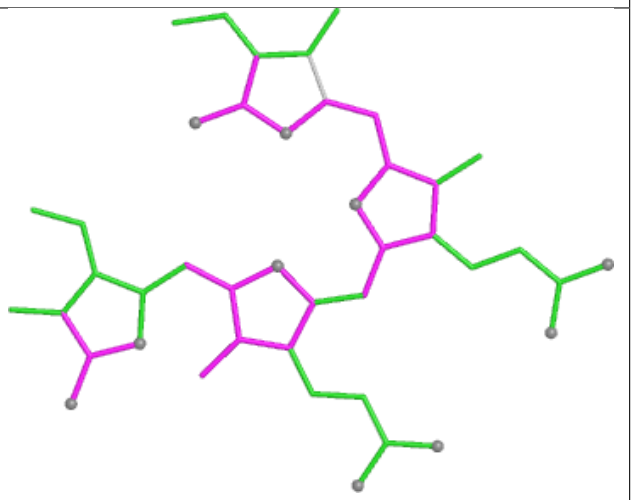


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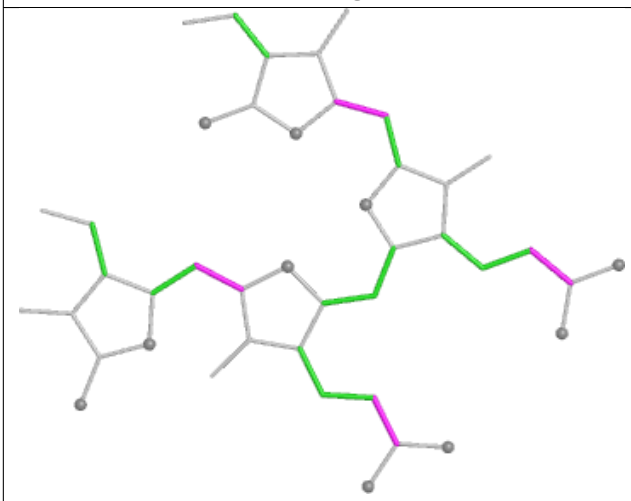
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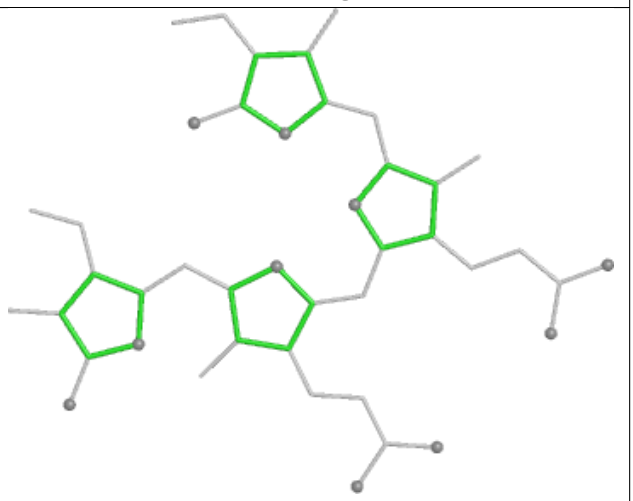
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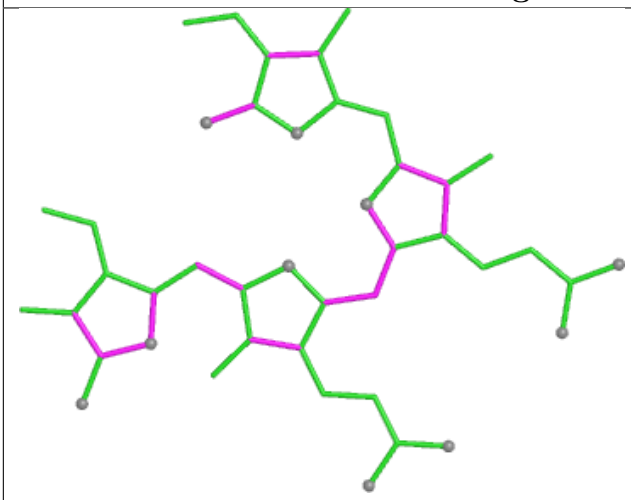


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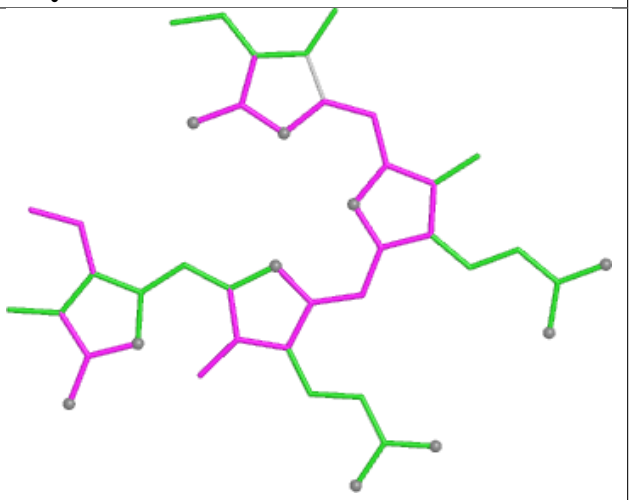


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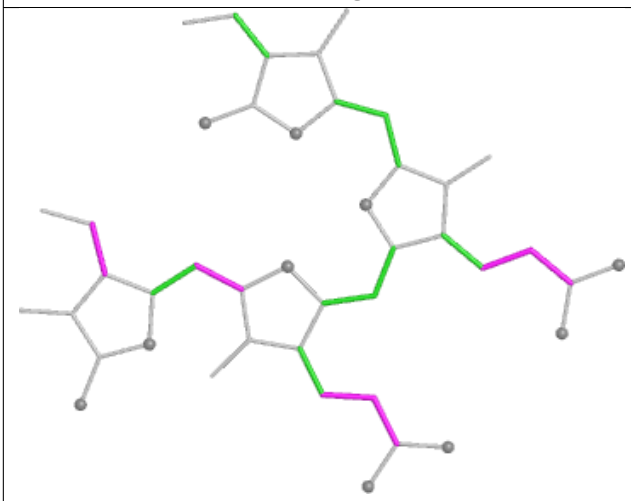
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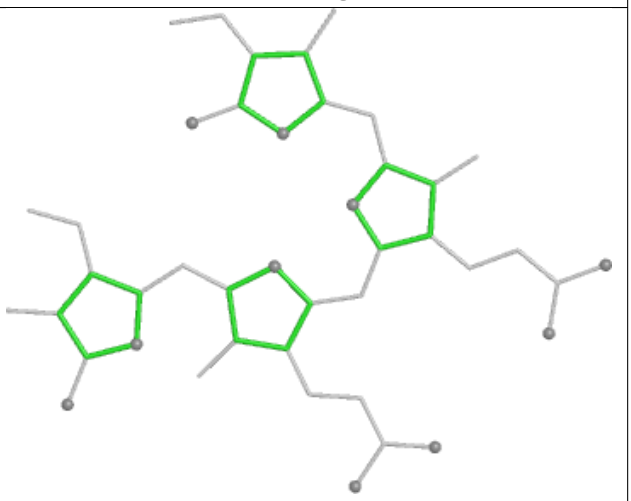
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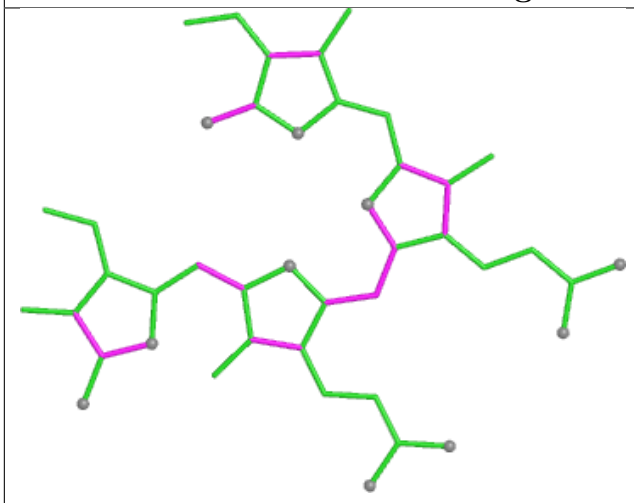


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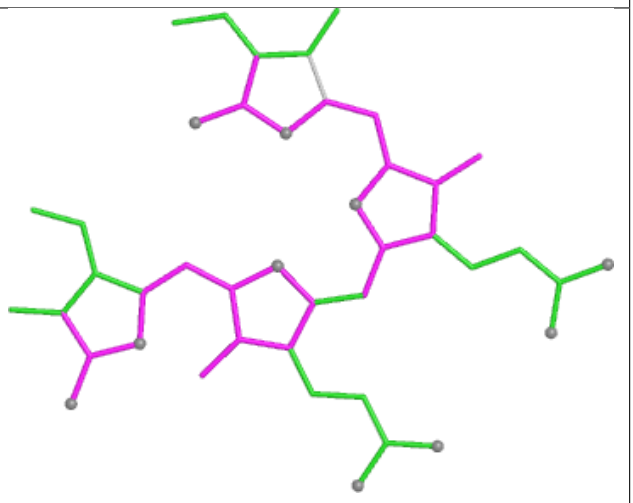


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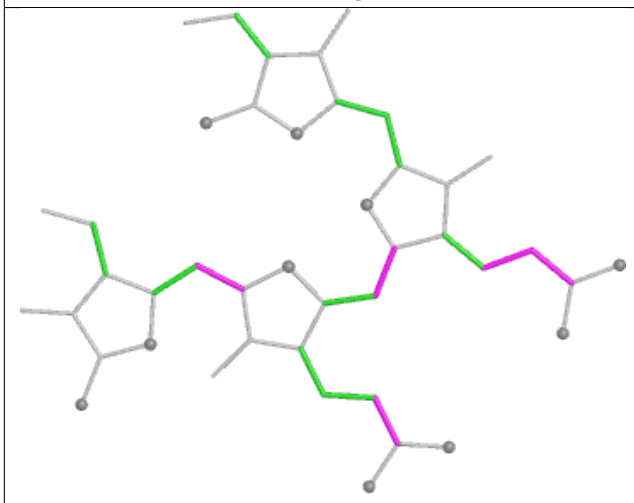
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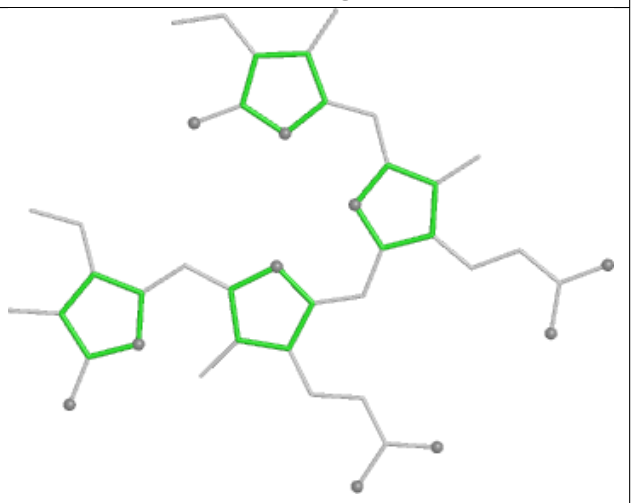
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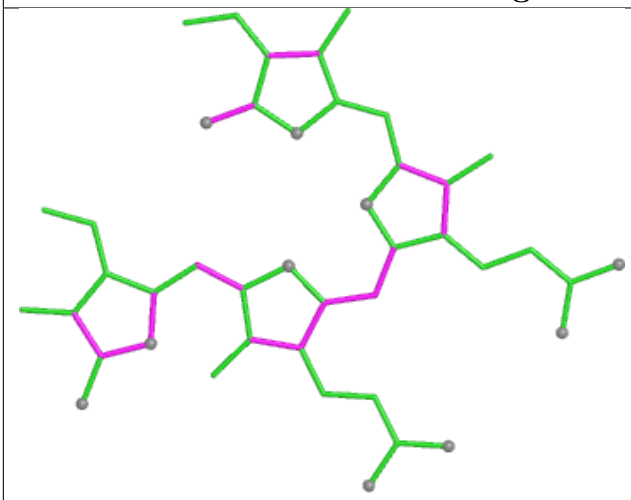


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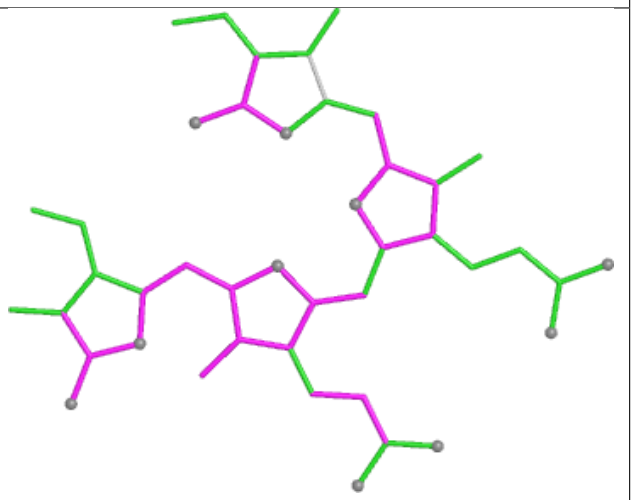


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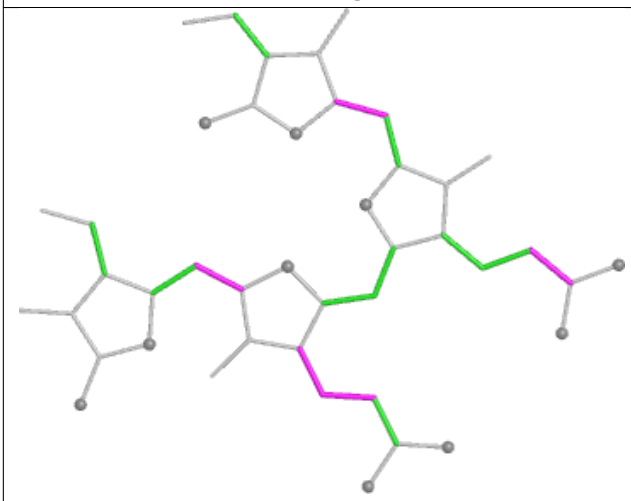
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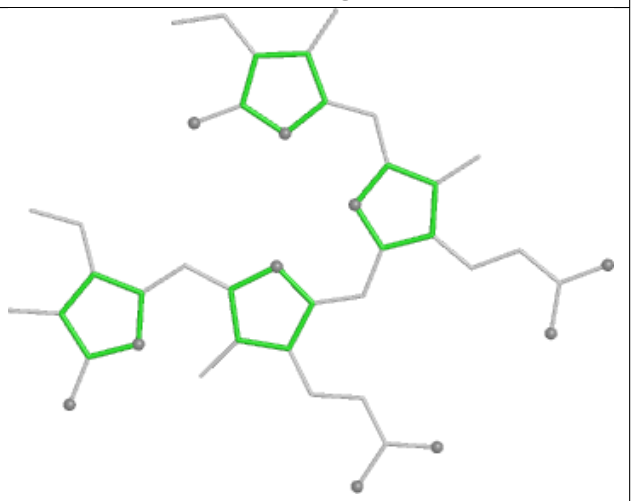
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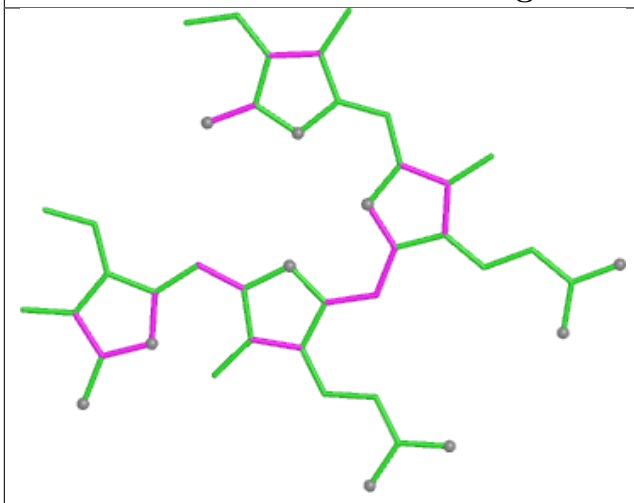


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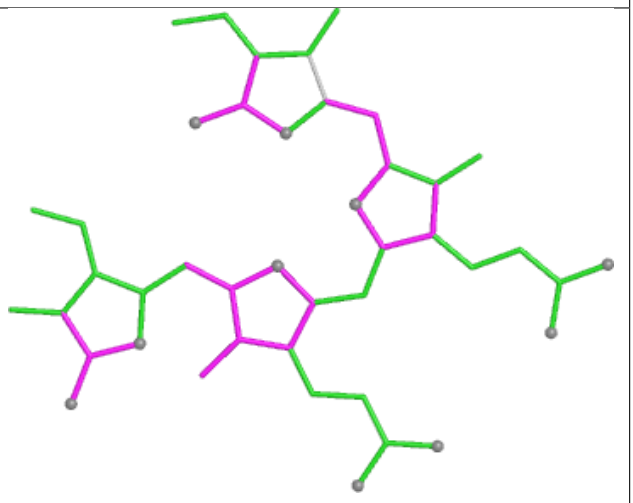


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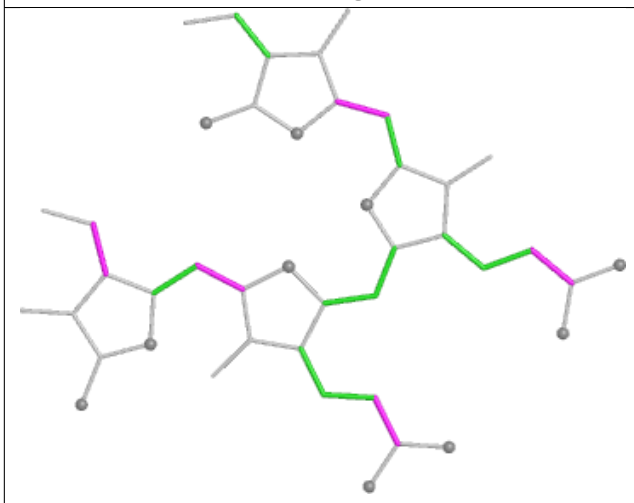
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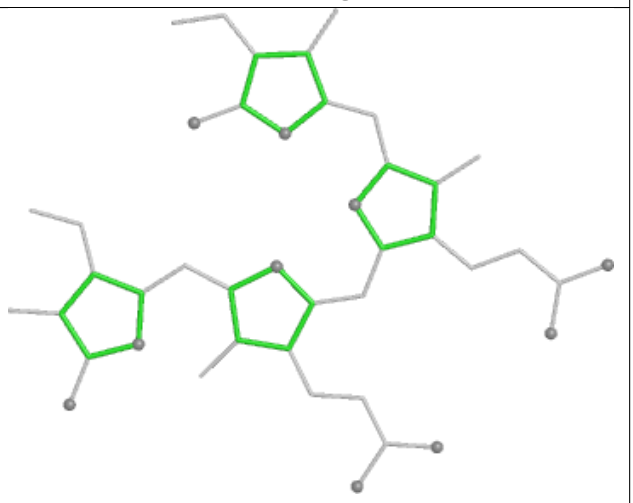
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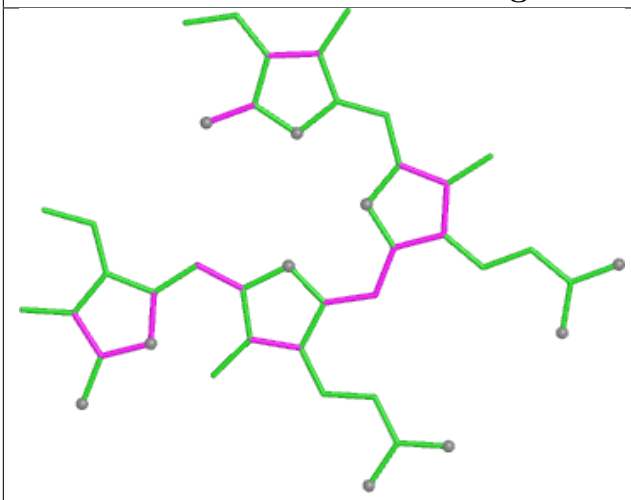


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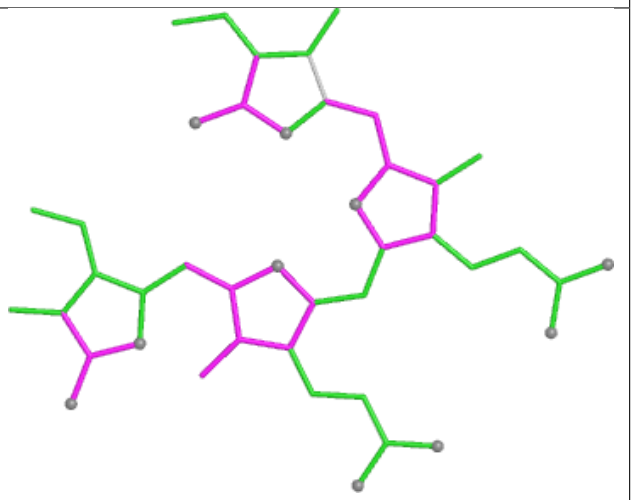


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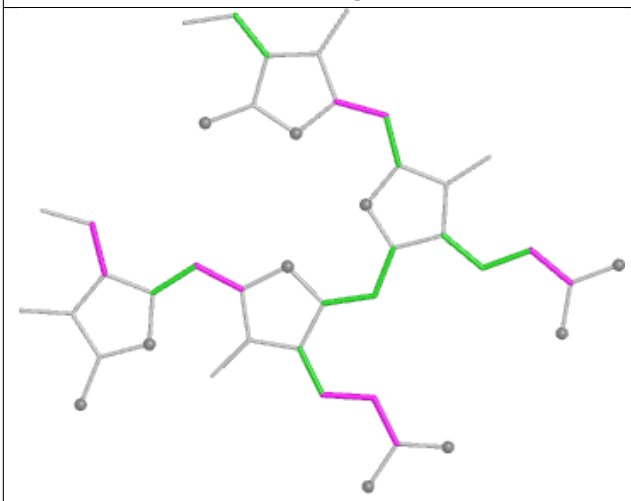
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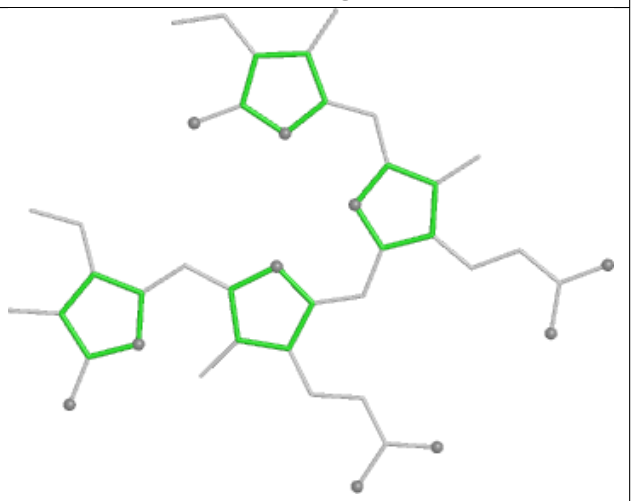
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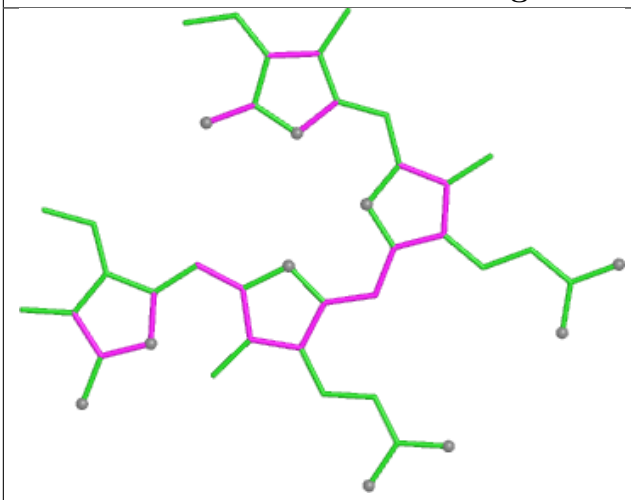


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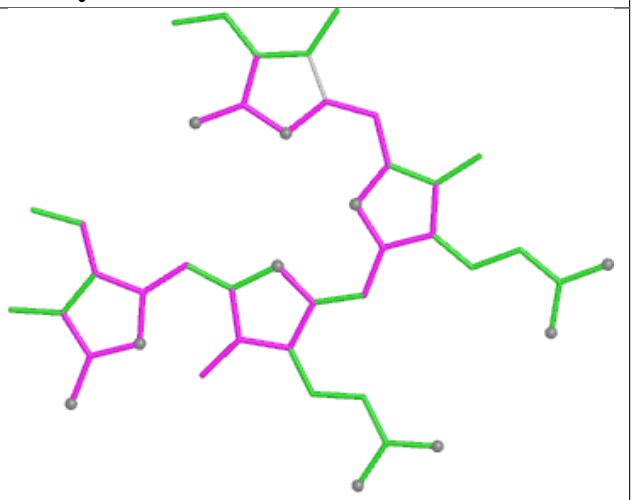


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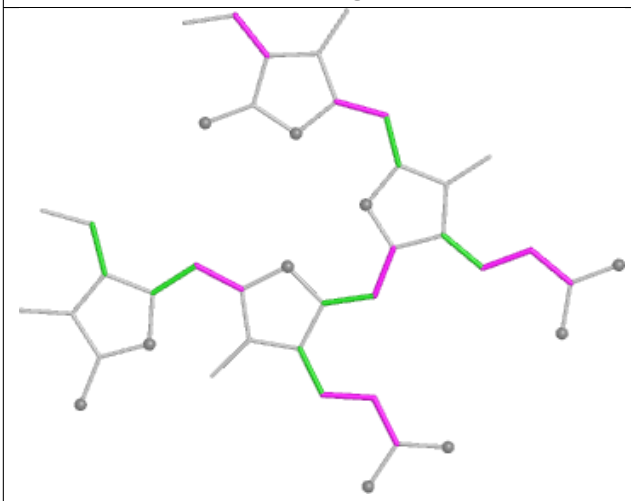
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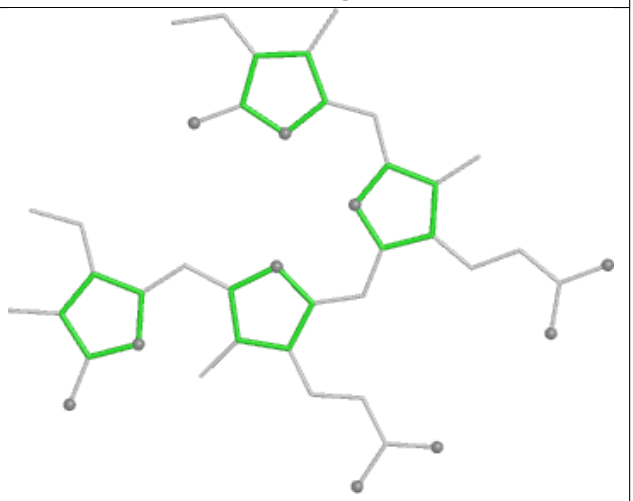
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Bond angles

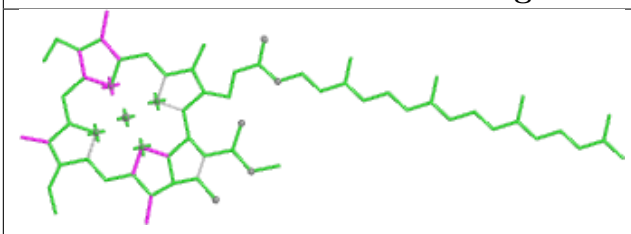


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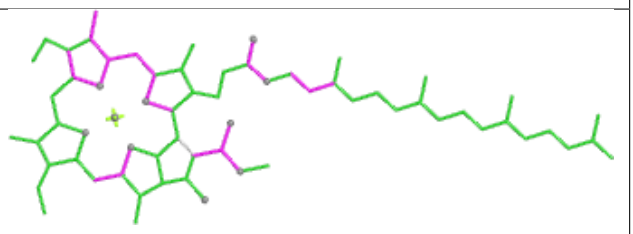


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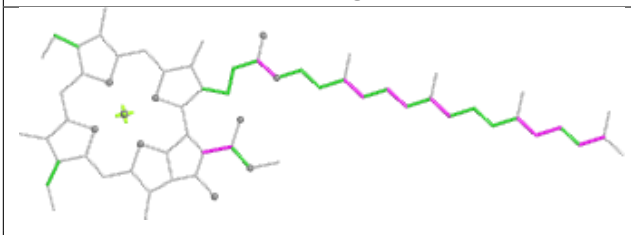
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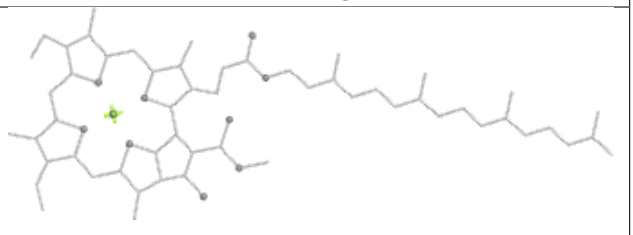
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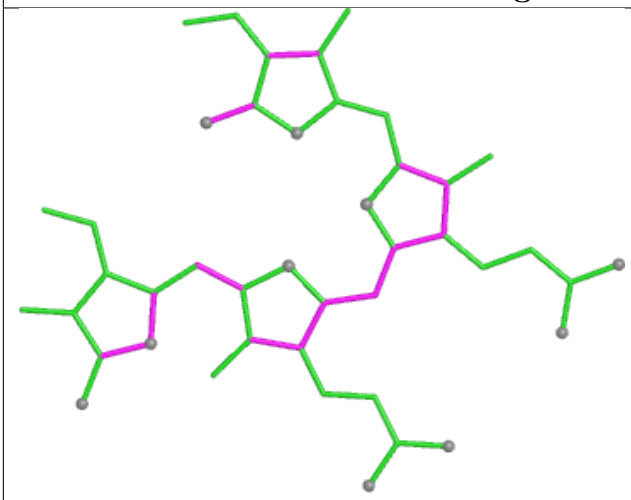


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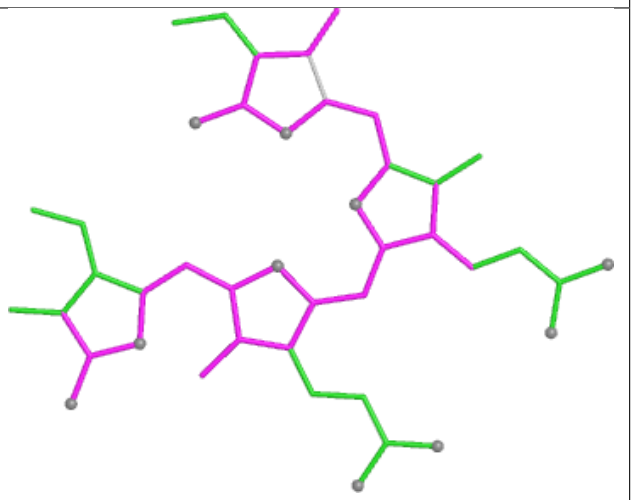


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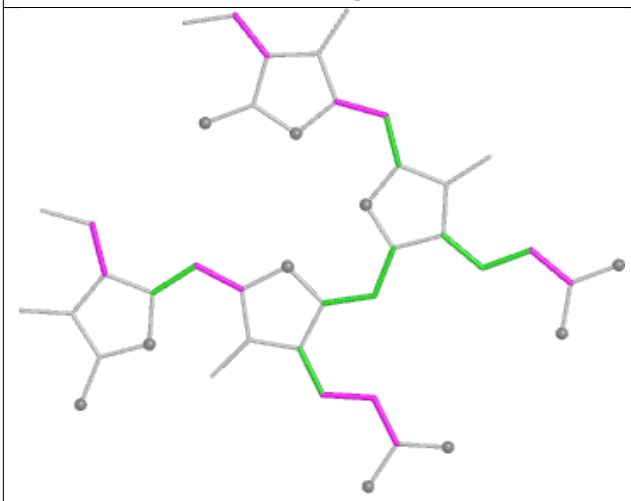
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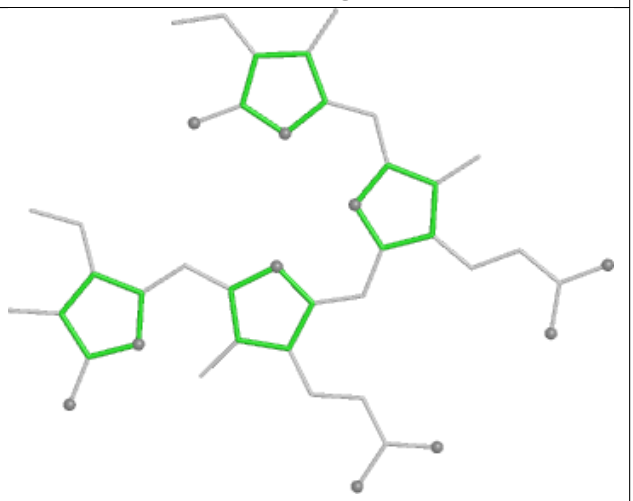
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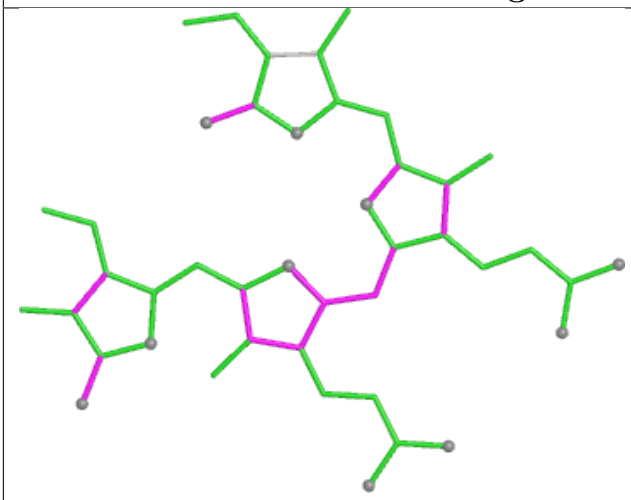


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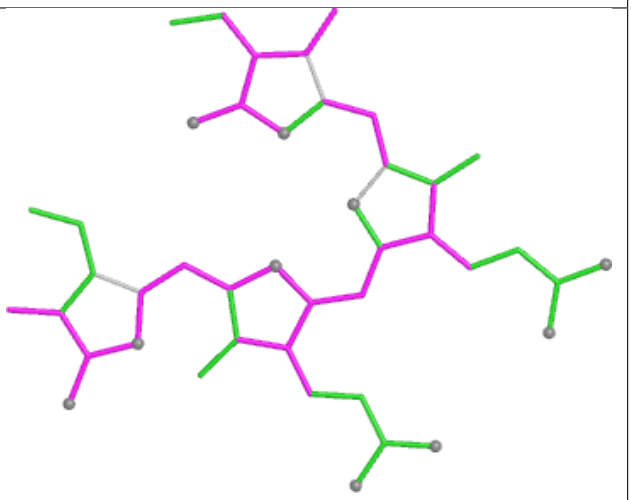


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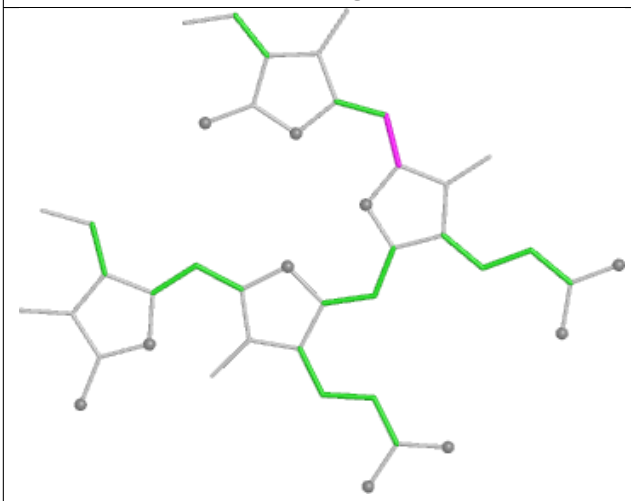
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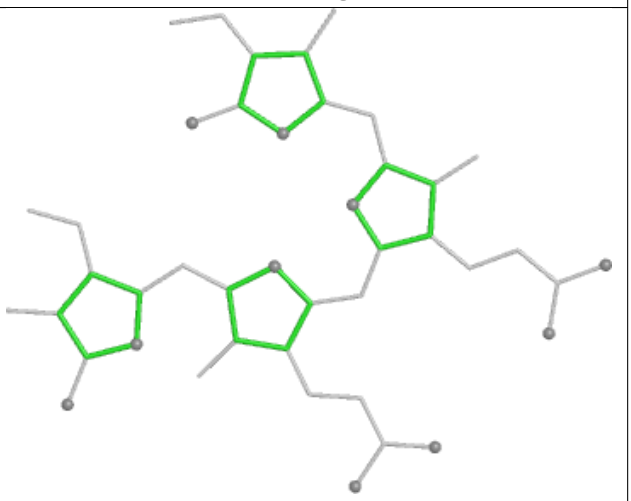
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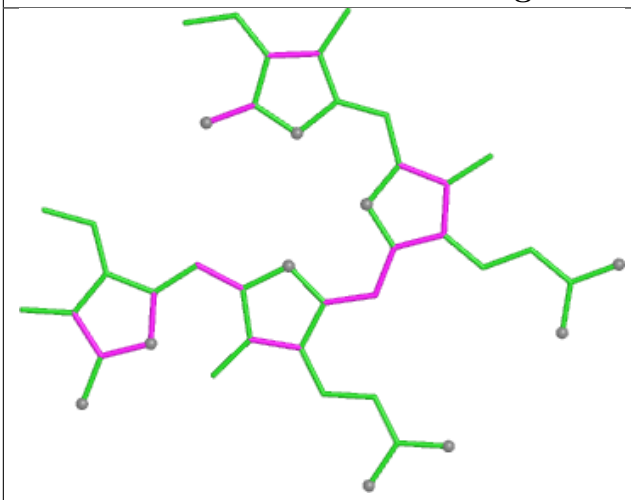


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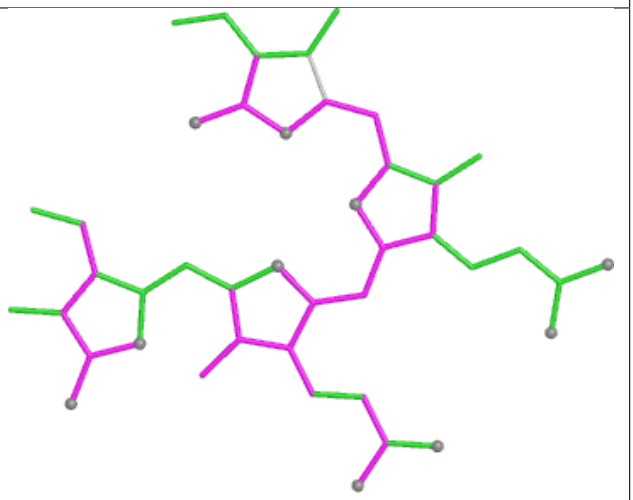


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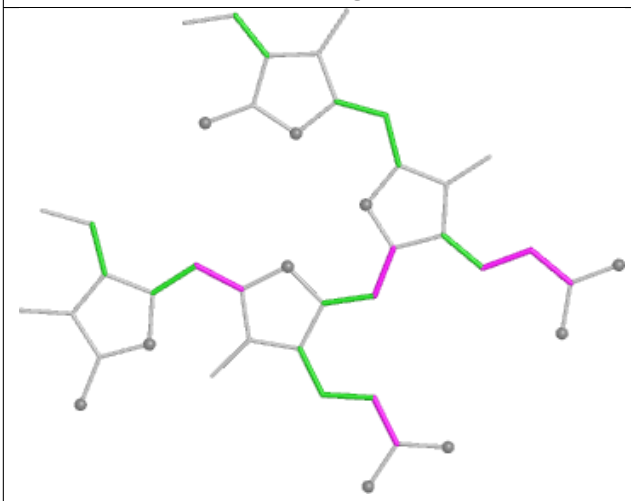
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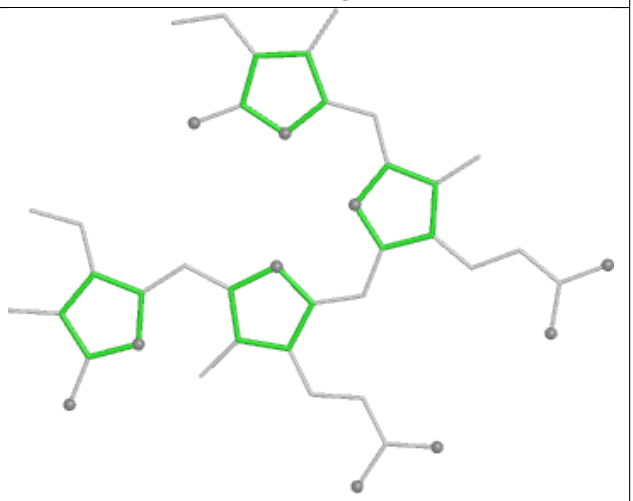
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Bond angles

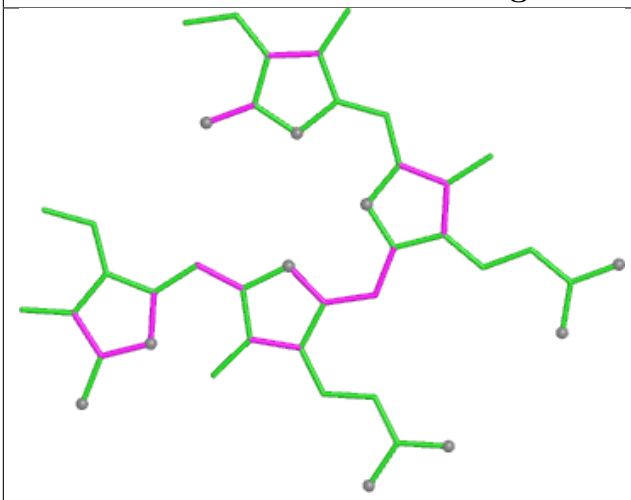


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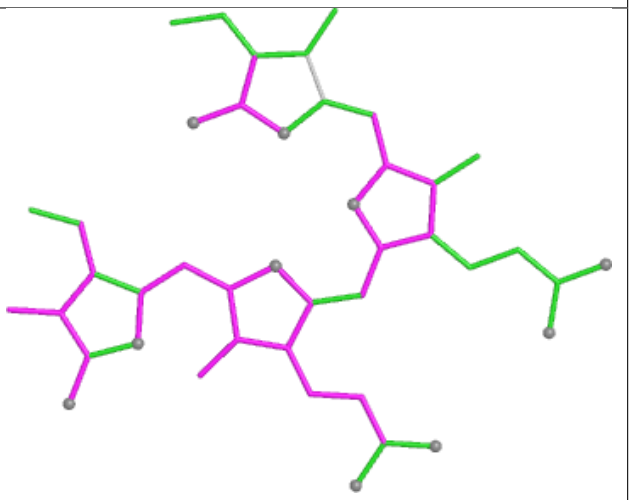


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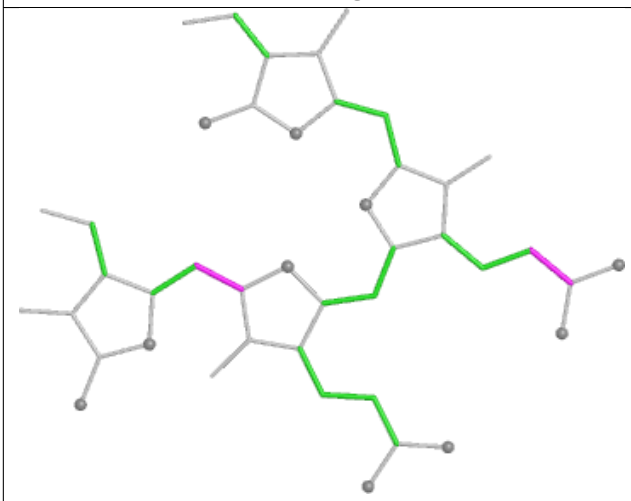
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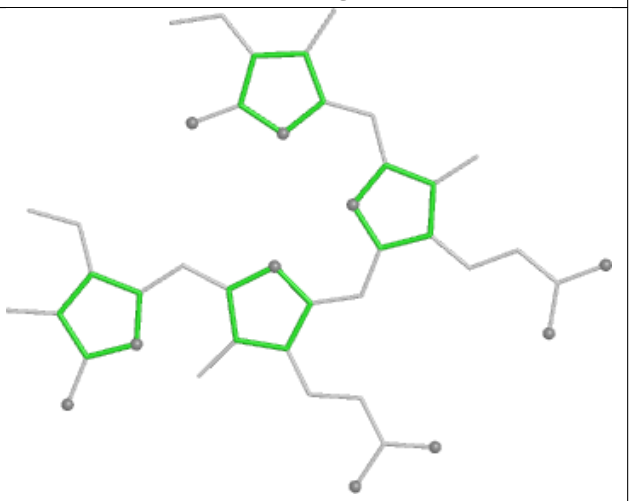
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Bond angles

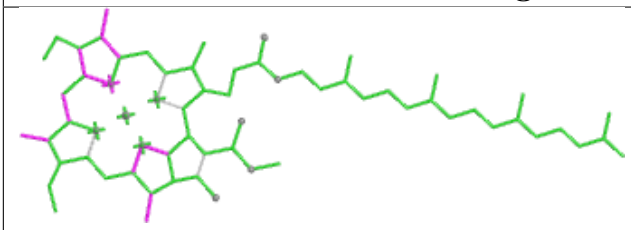


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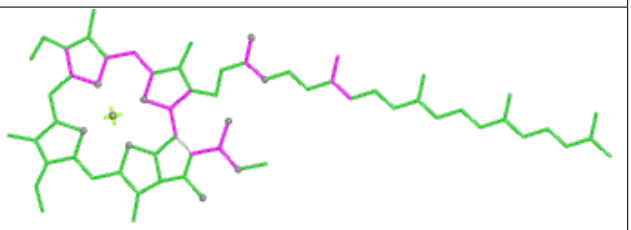


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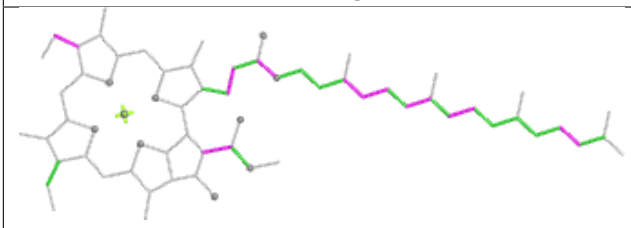
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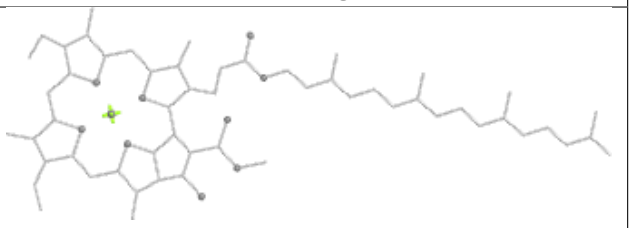
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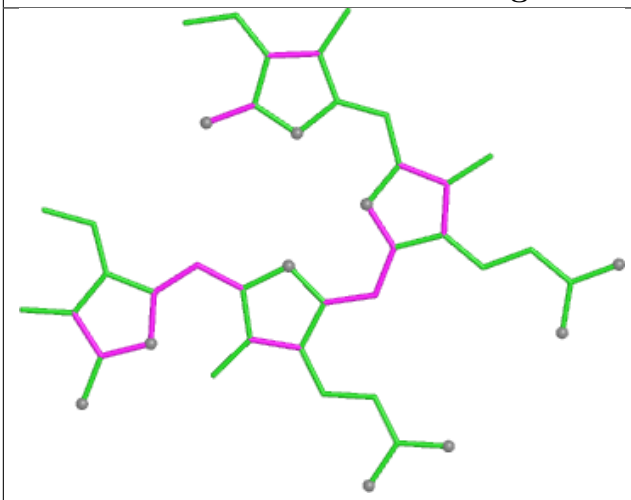


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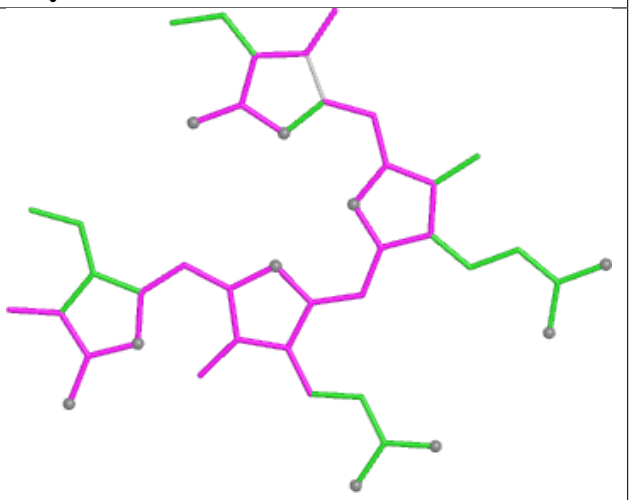


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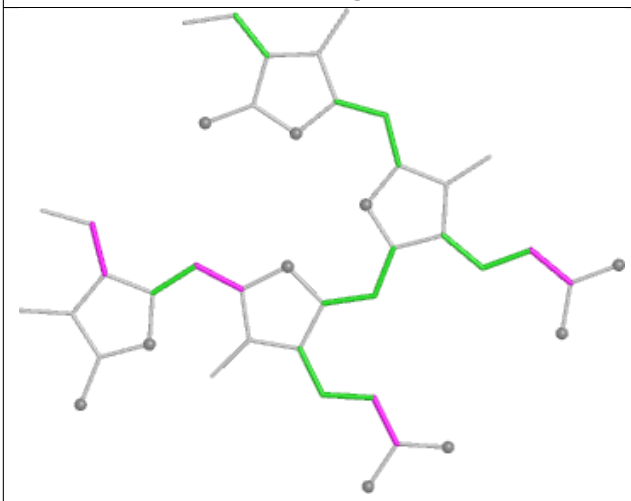
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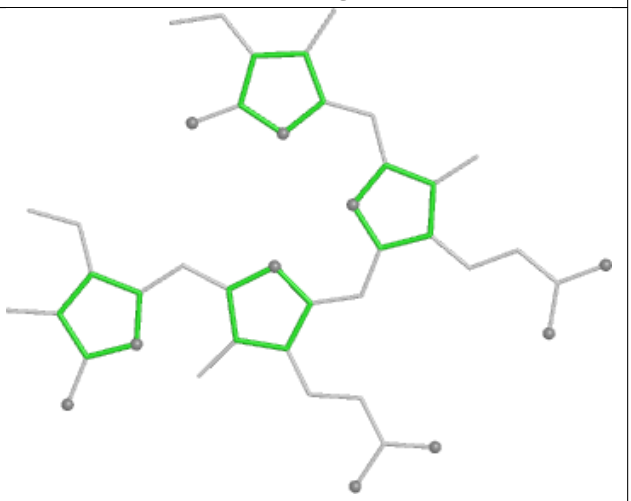
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Bond angles

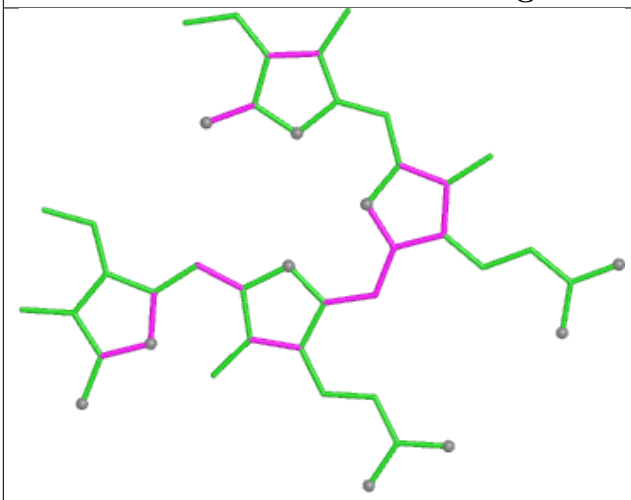


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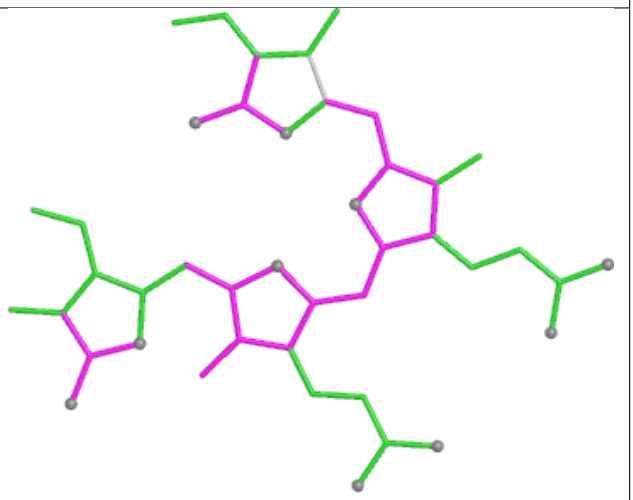


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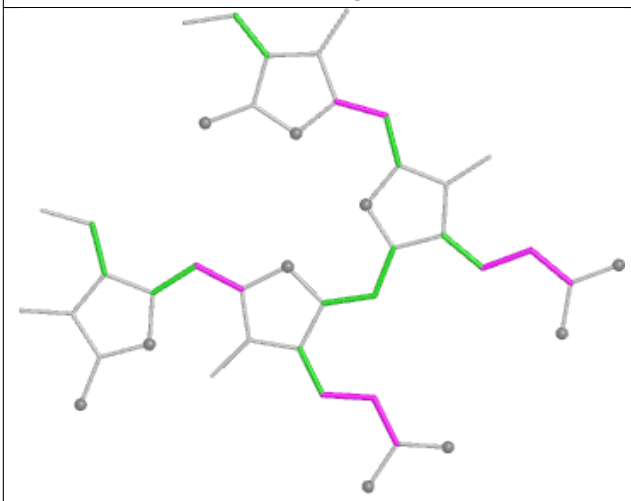
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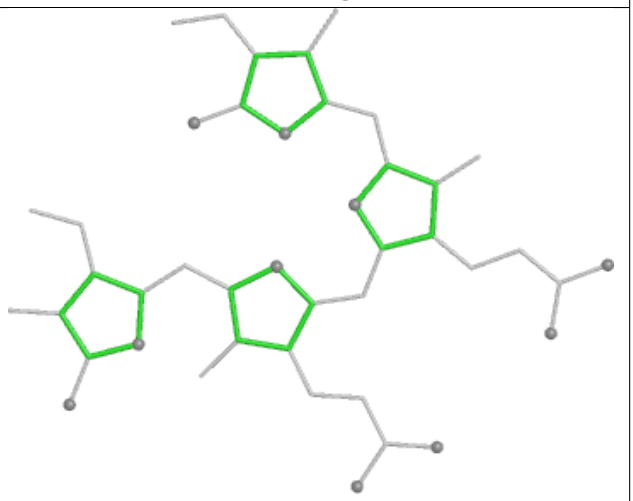
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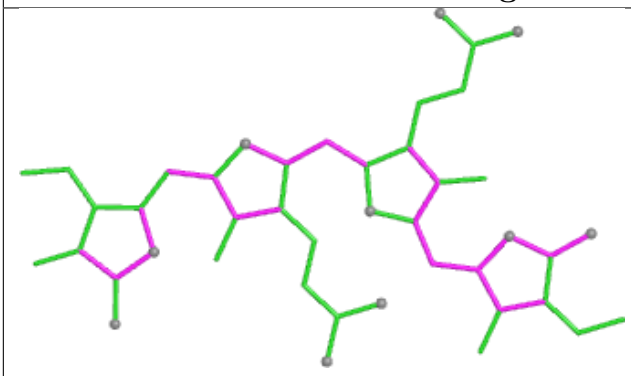


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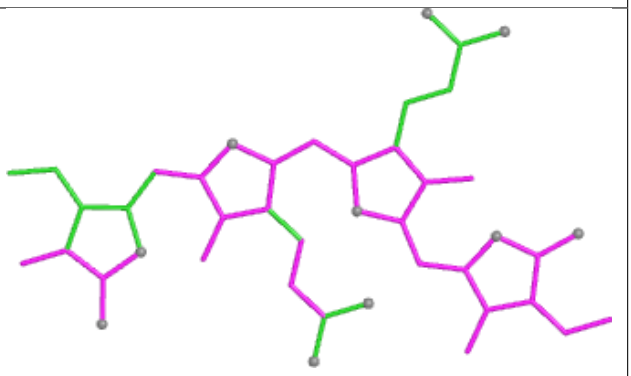


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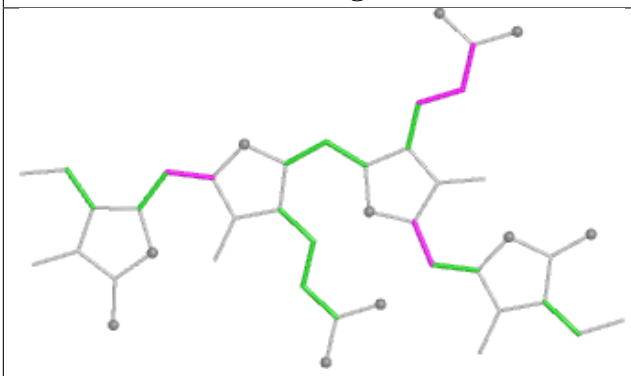
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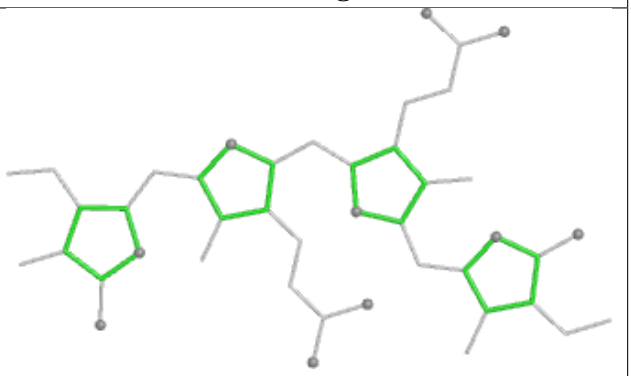
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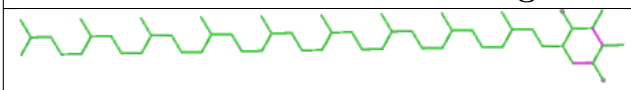


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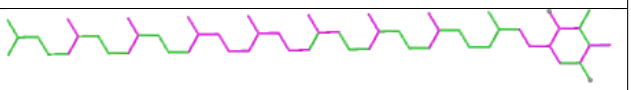


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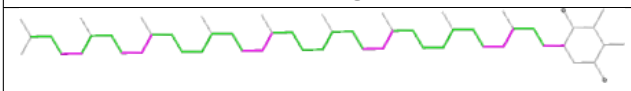
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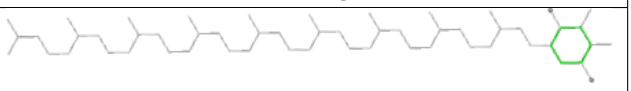
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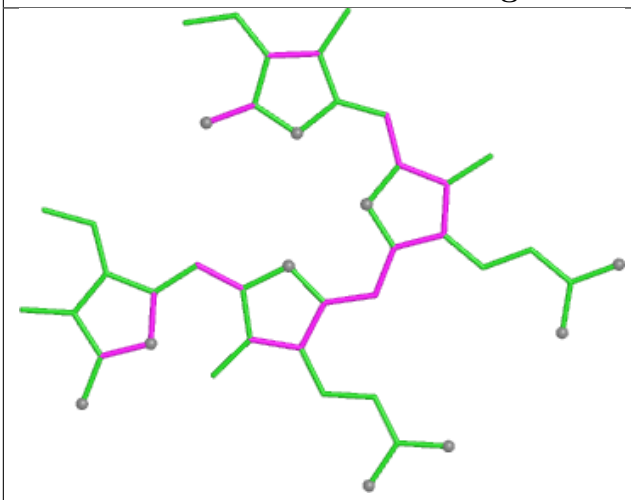


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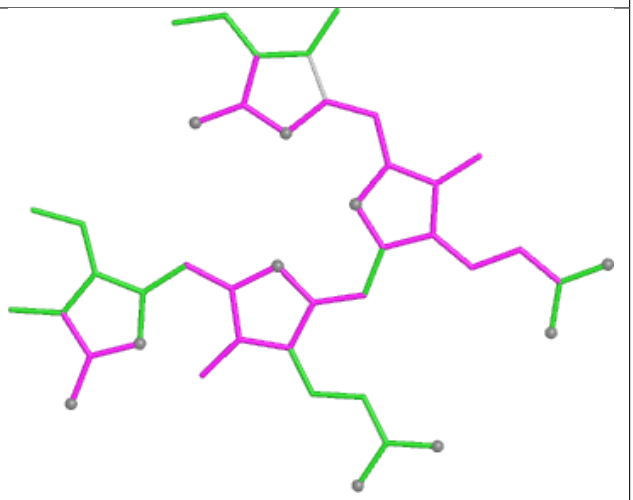


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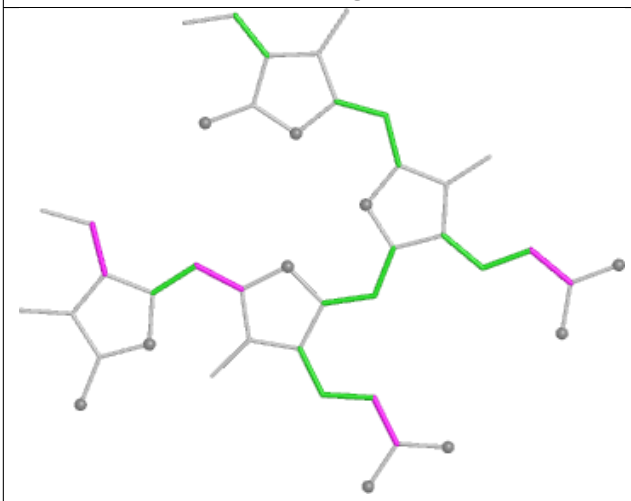
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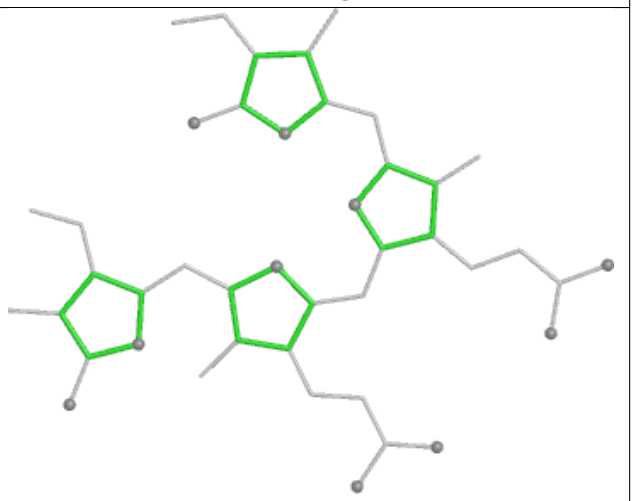
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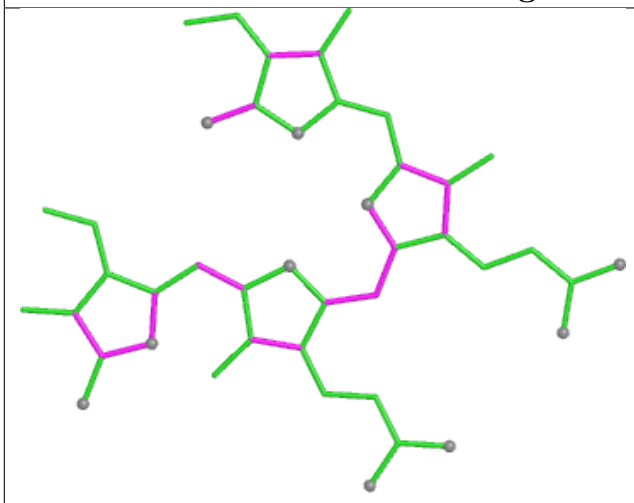


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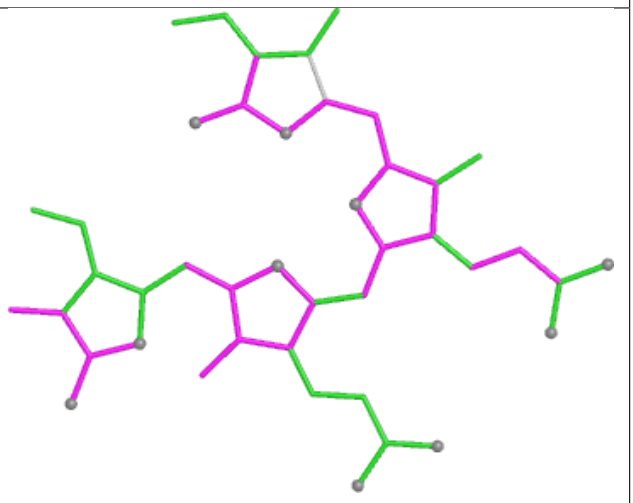


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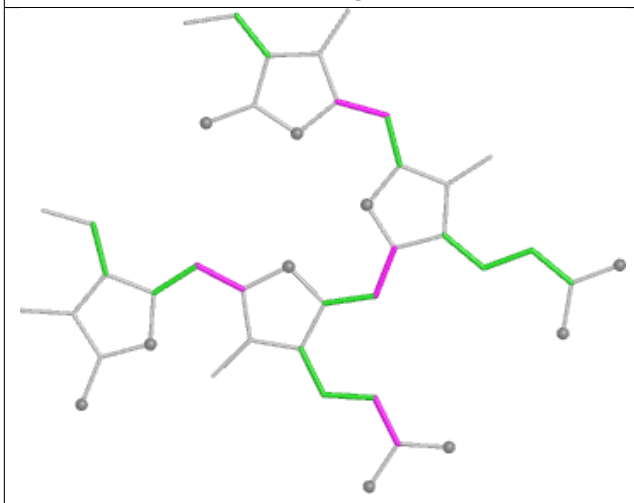
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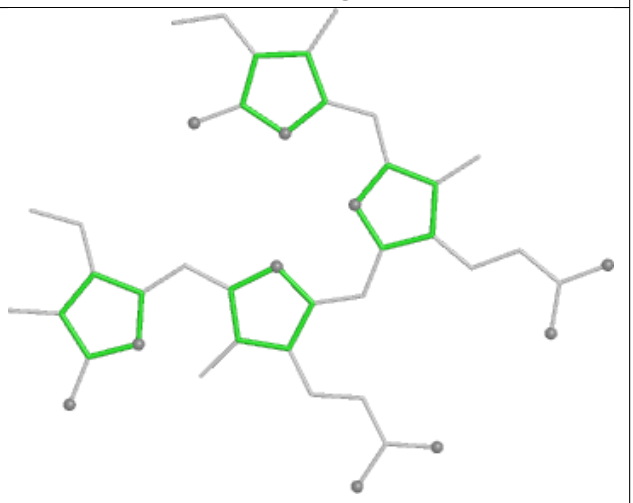
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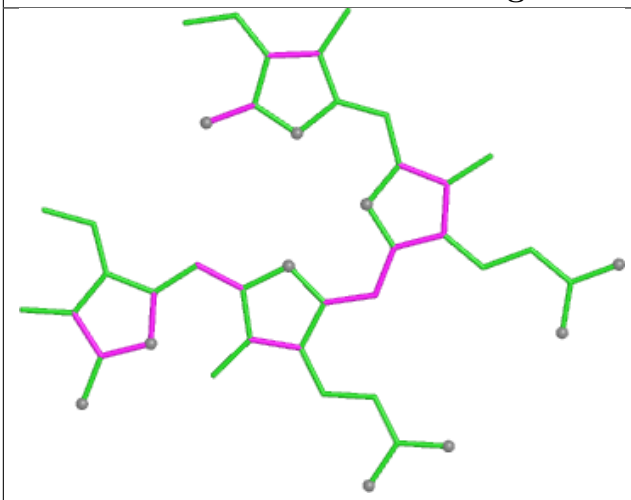


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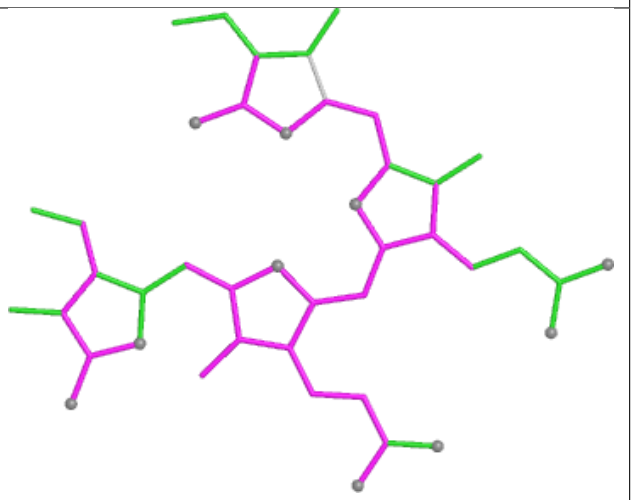


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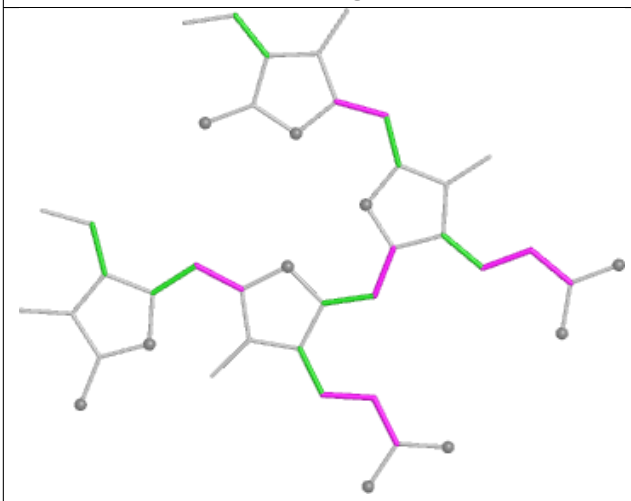
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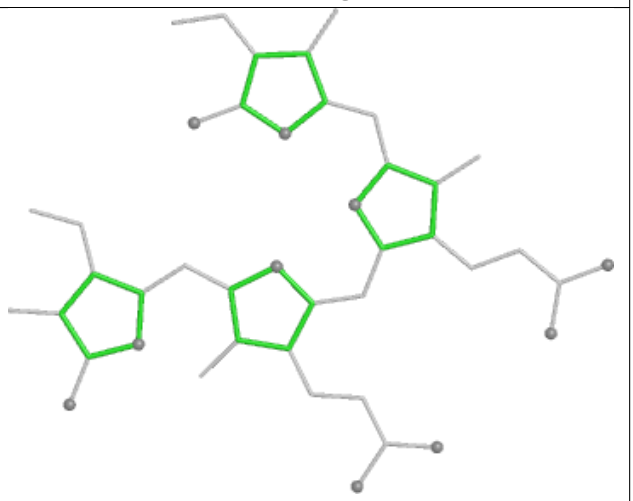
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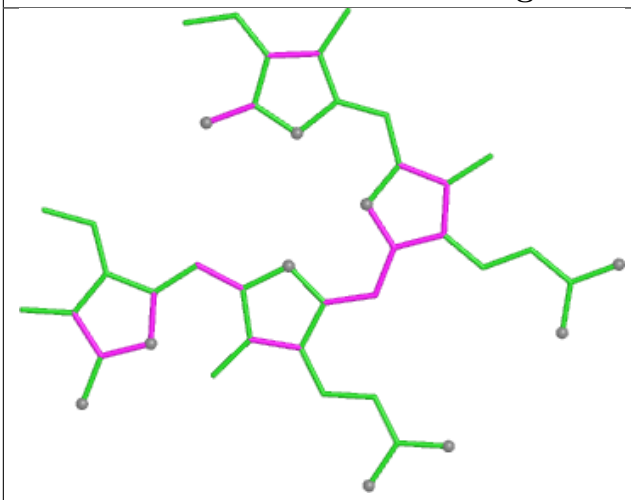


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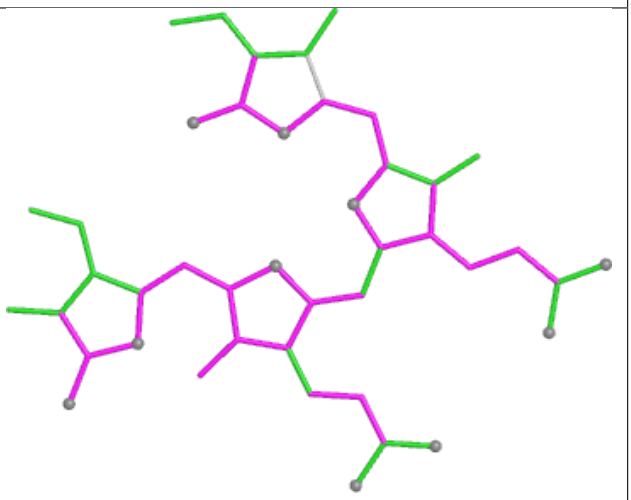


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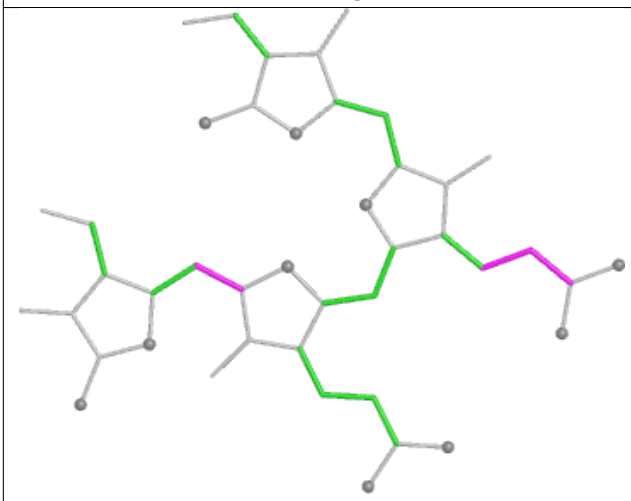
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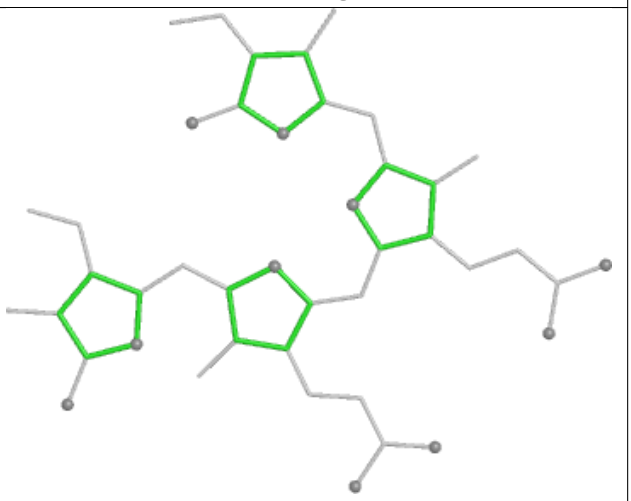
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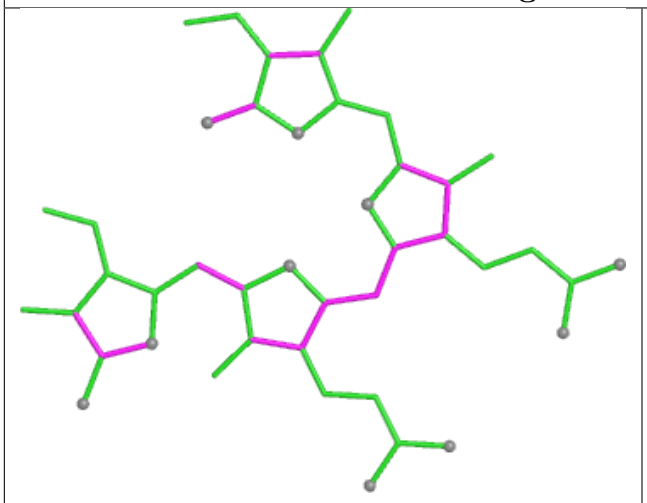


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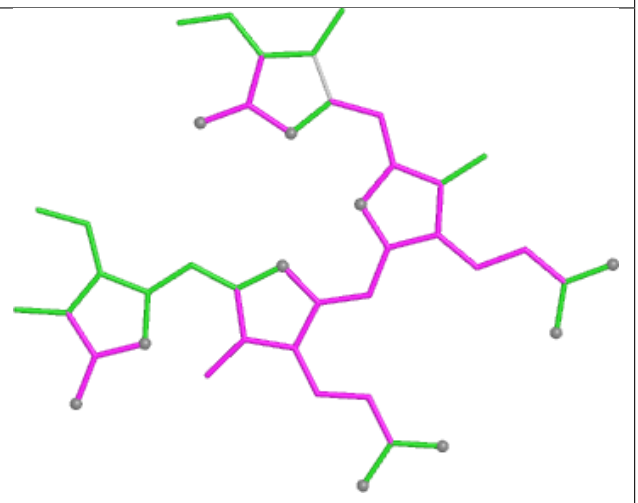


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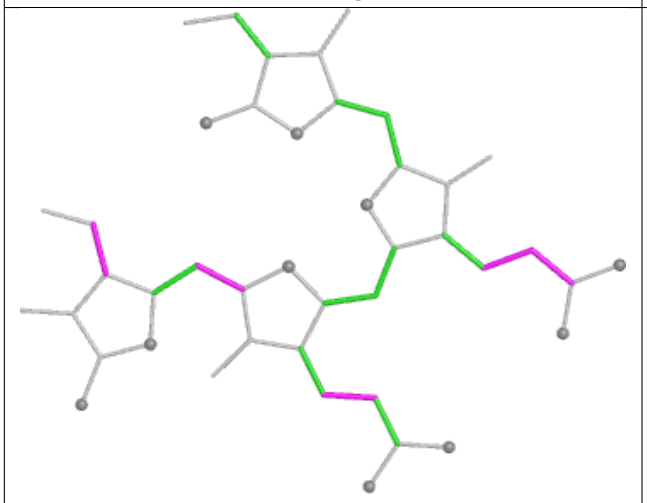
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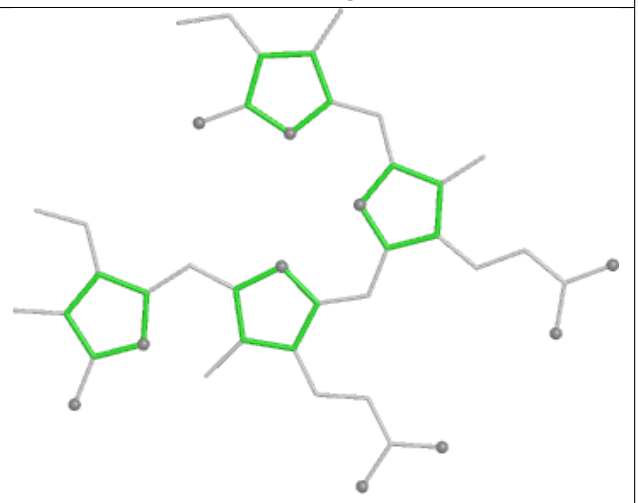
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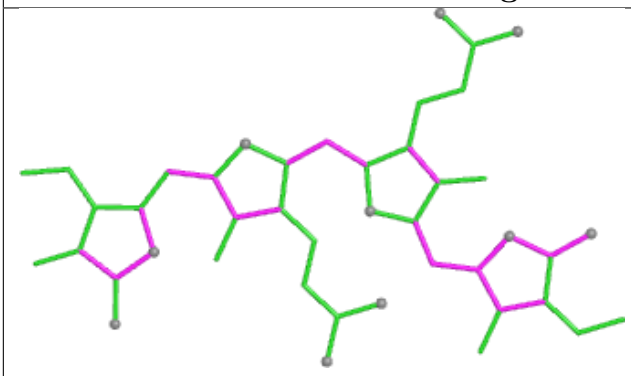


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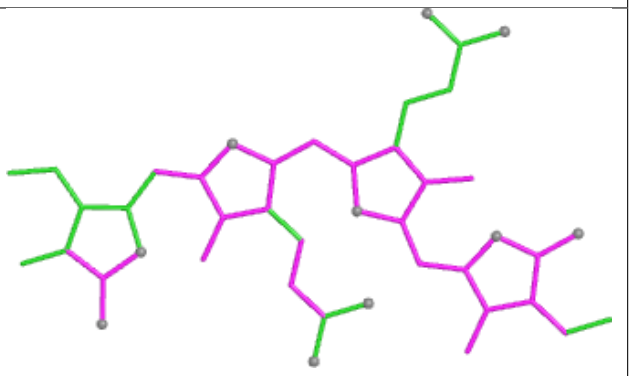


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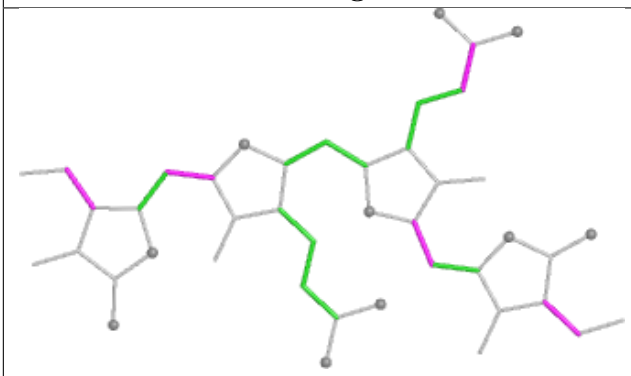
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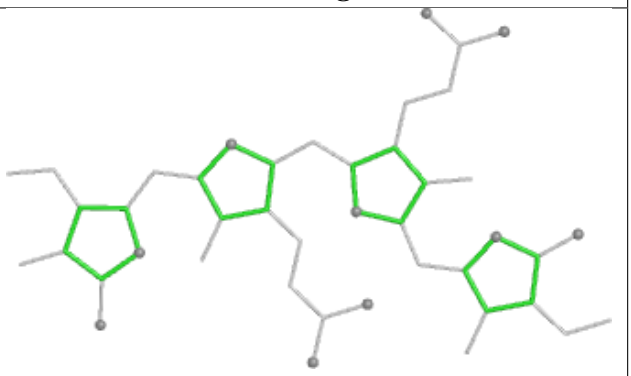
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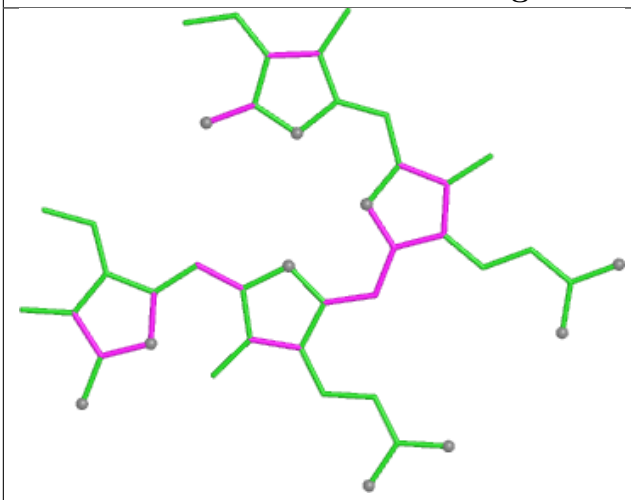


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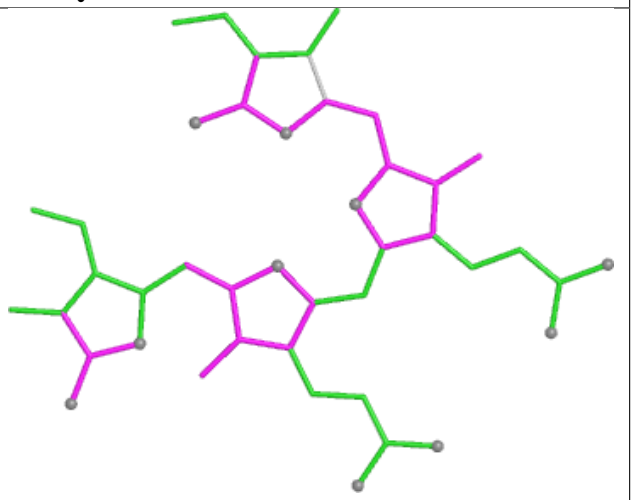


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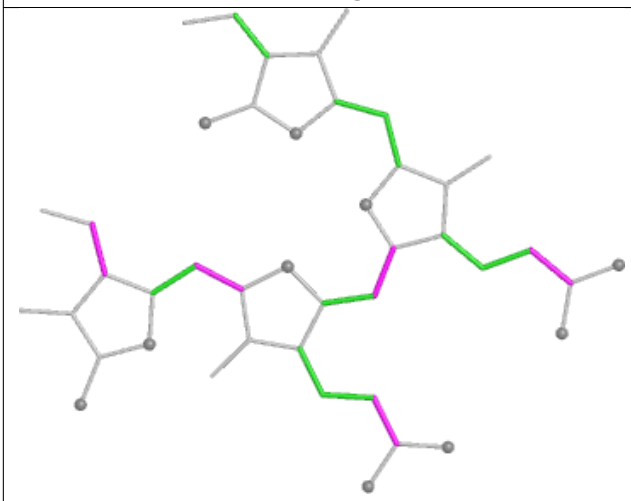
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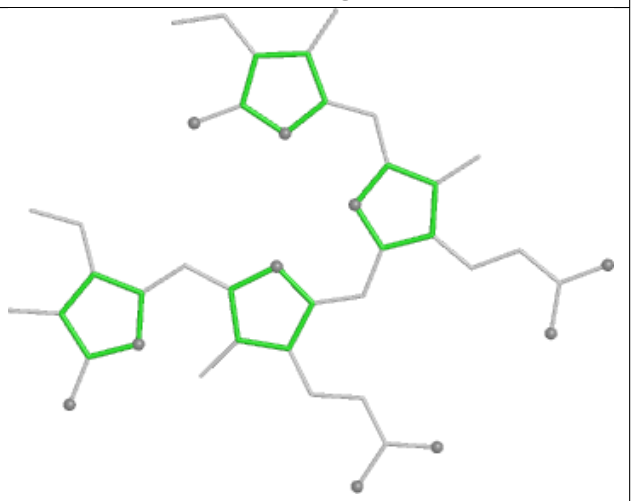
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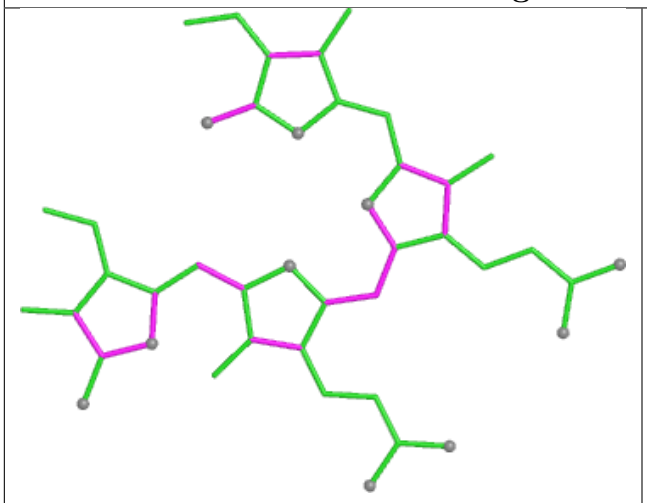


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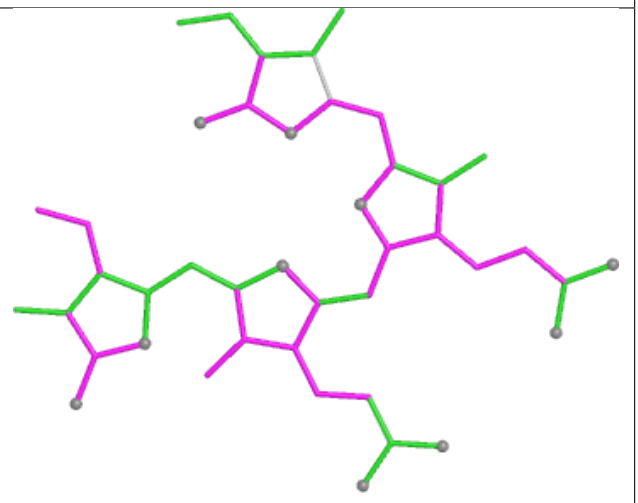


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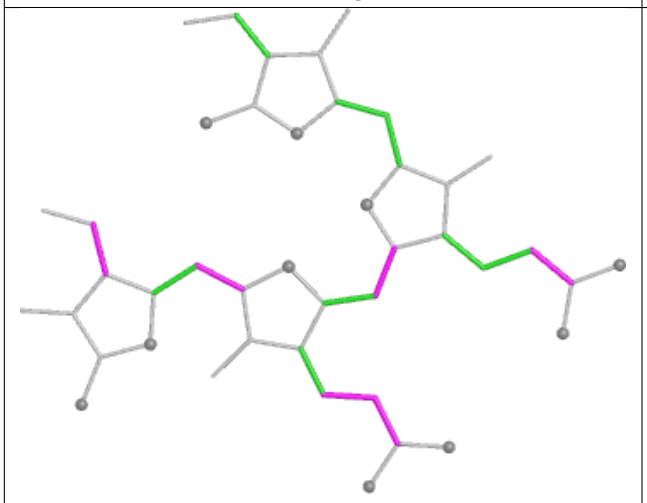
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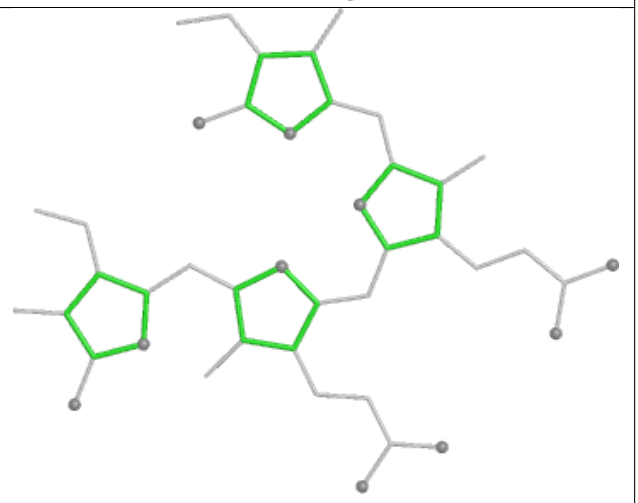
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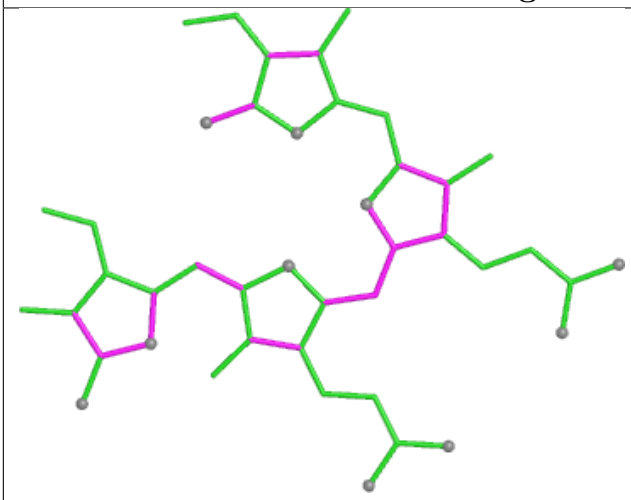


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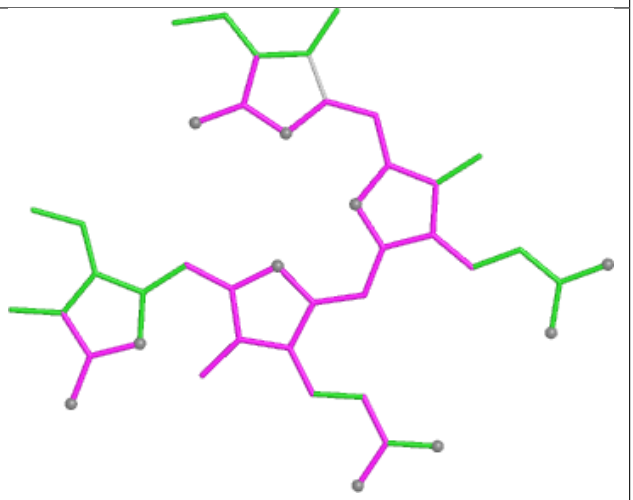


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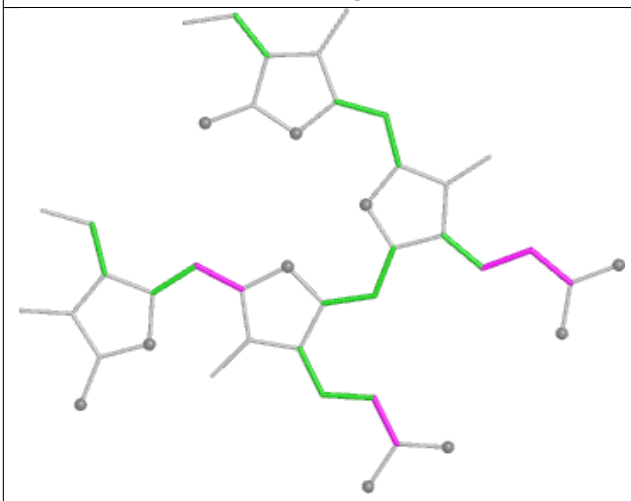
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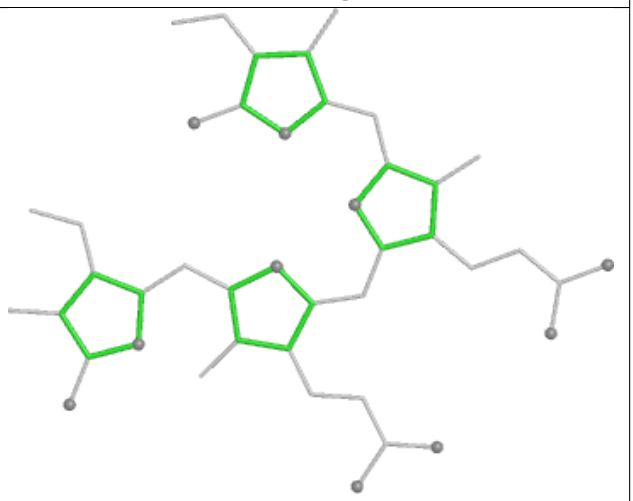
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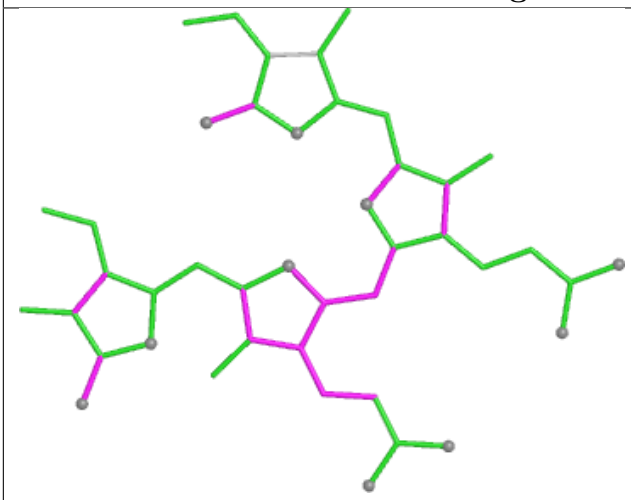


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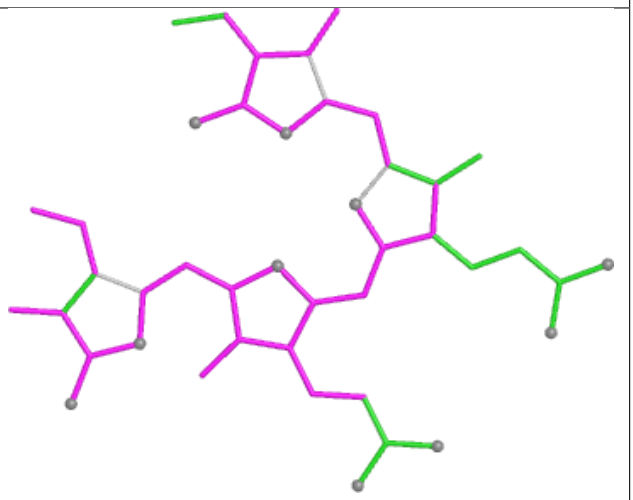


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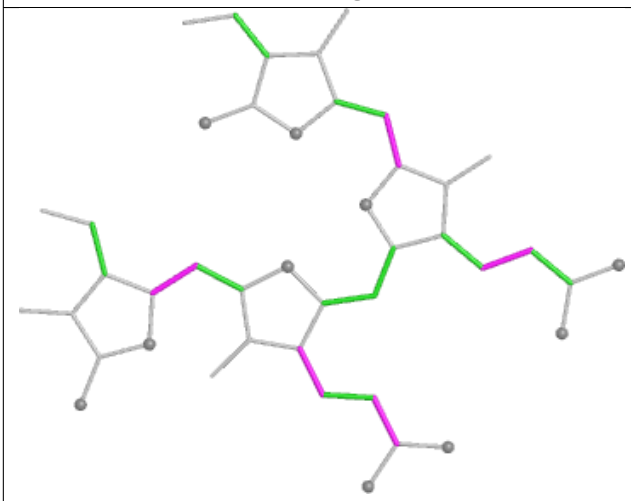
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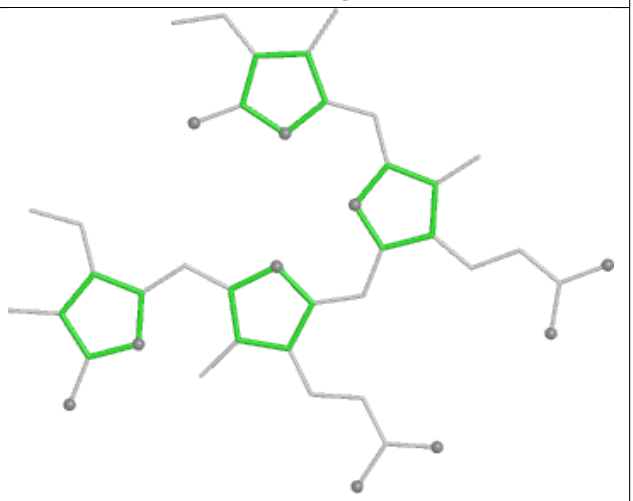
Bond lengths



Bond angles

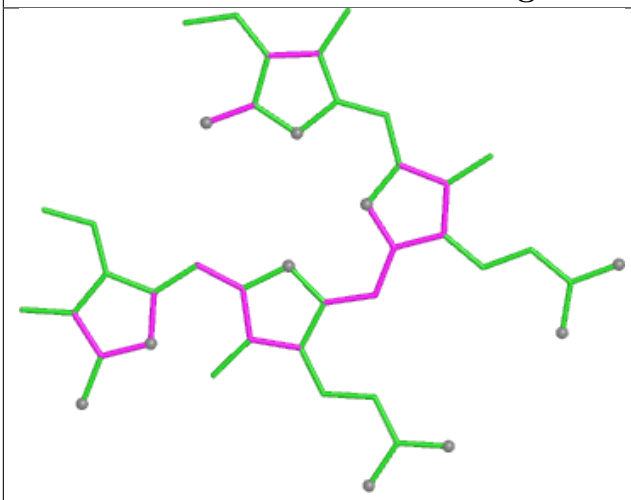


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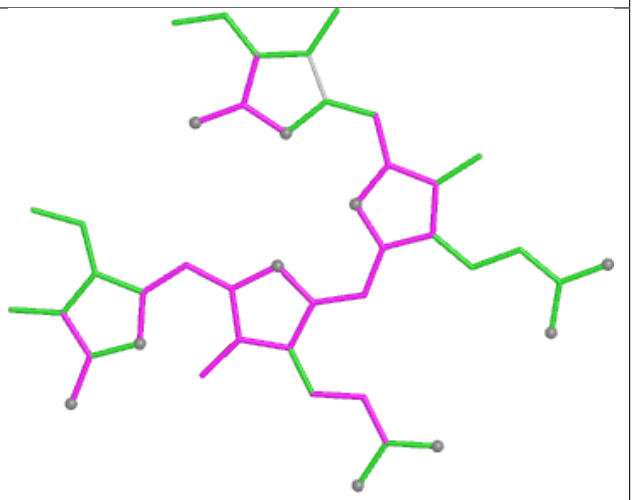


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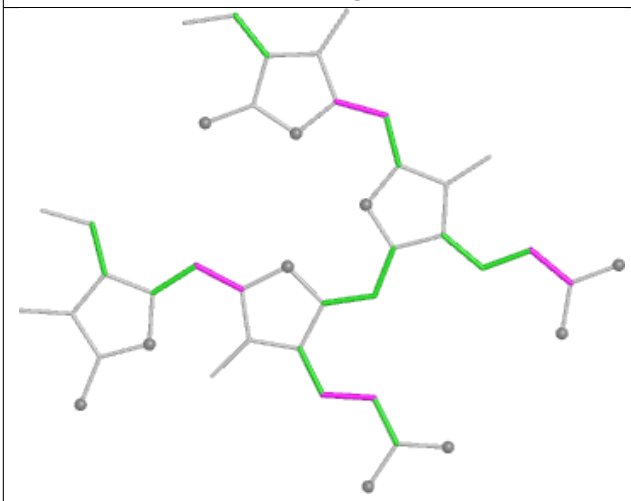
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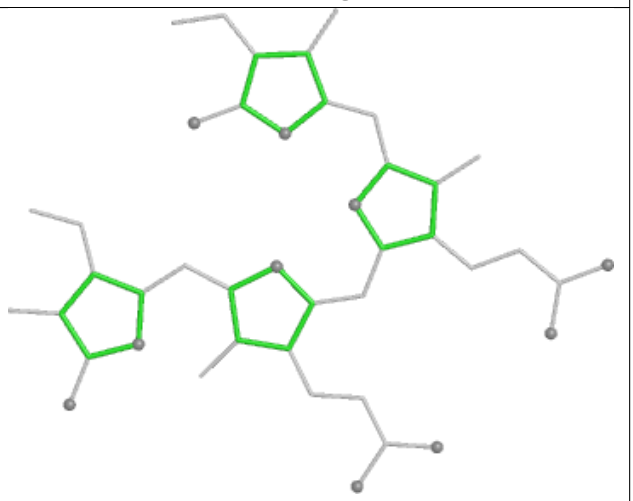
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Bond angles

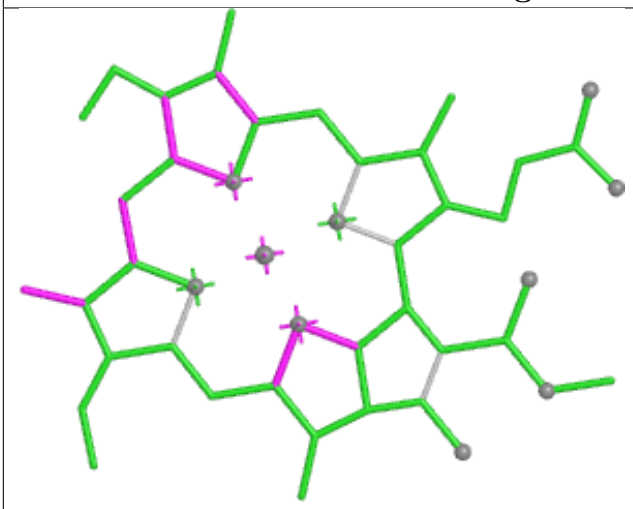


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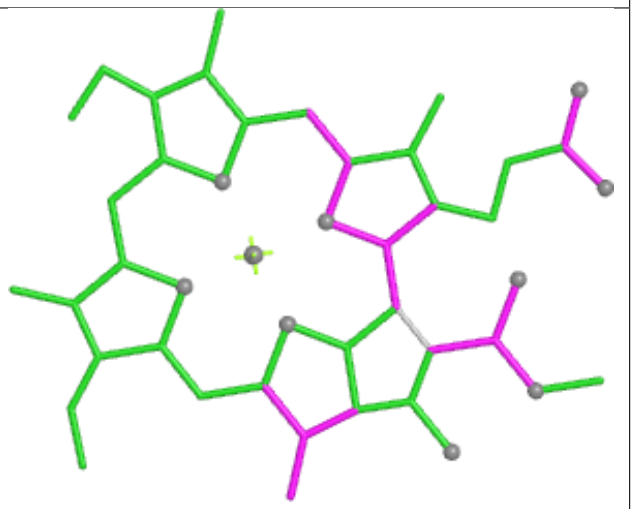


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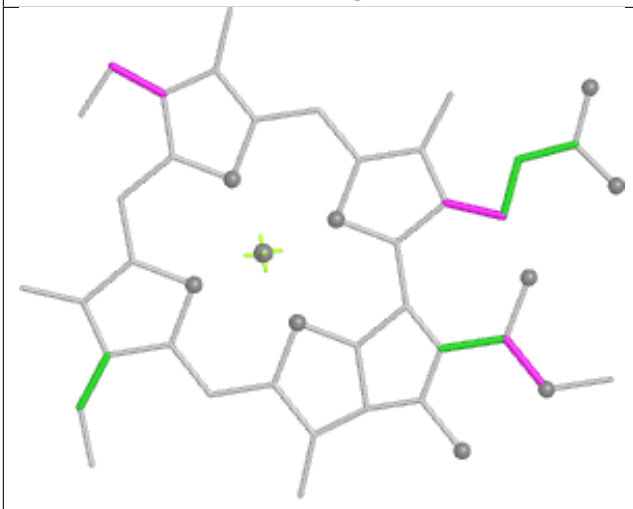
Ligand CLA 3N 301



Bond lengths



Bond angles

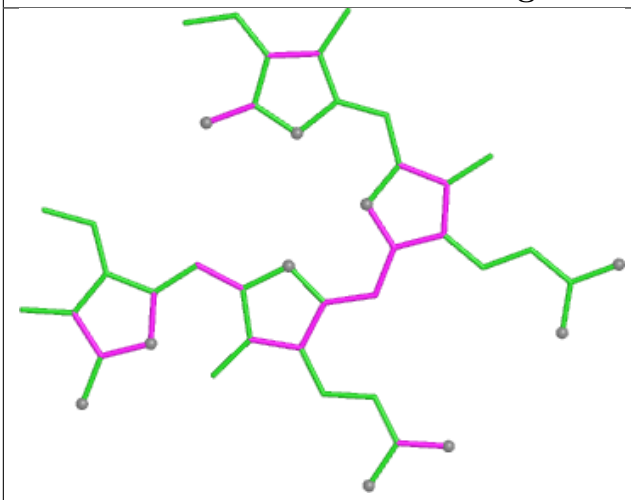


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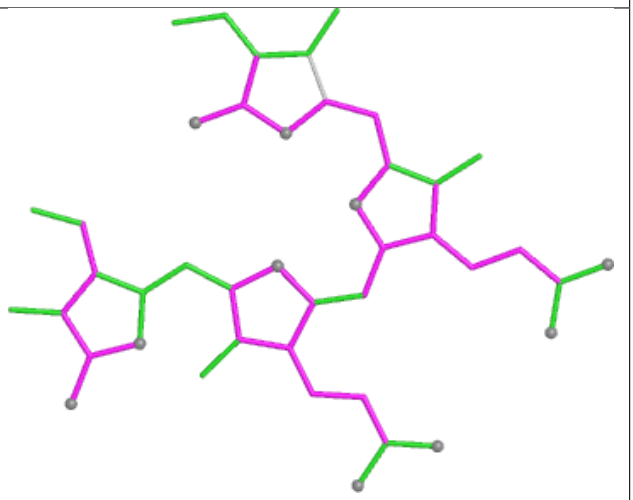


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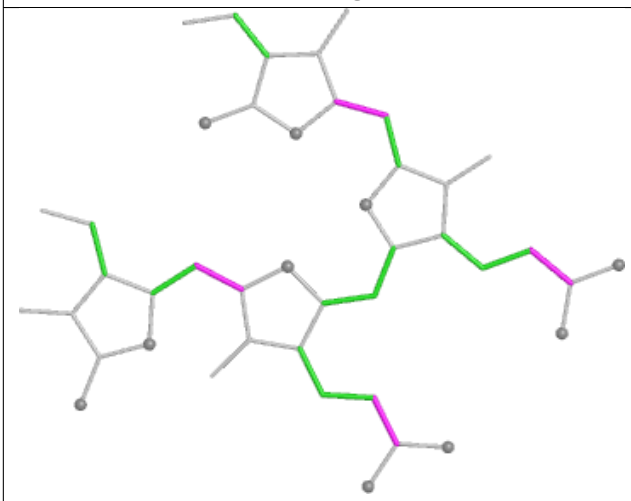
Ligand PEB OI 201



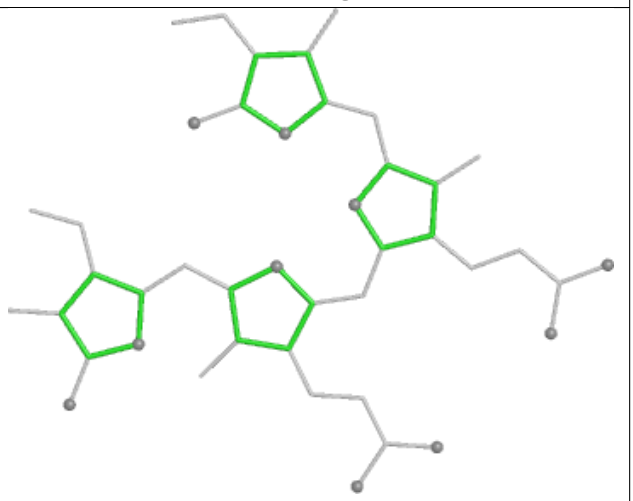
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Bond angles

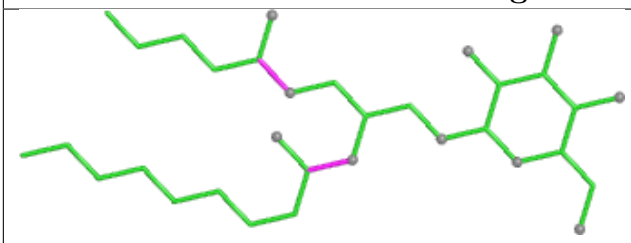


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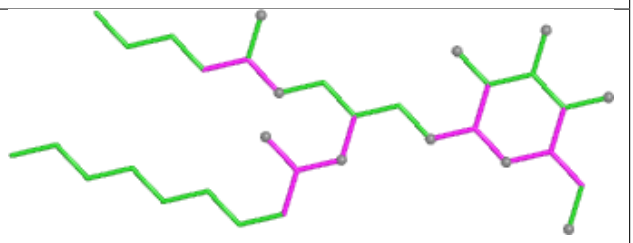


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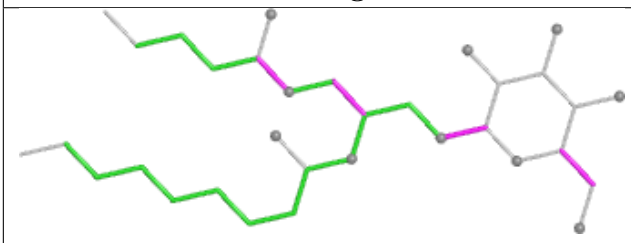
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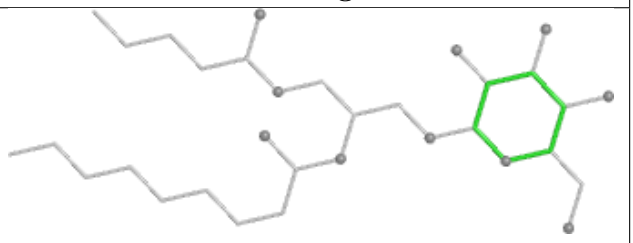
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Bond angles

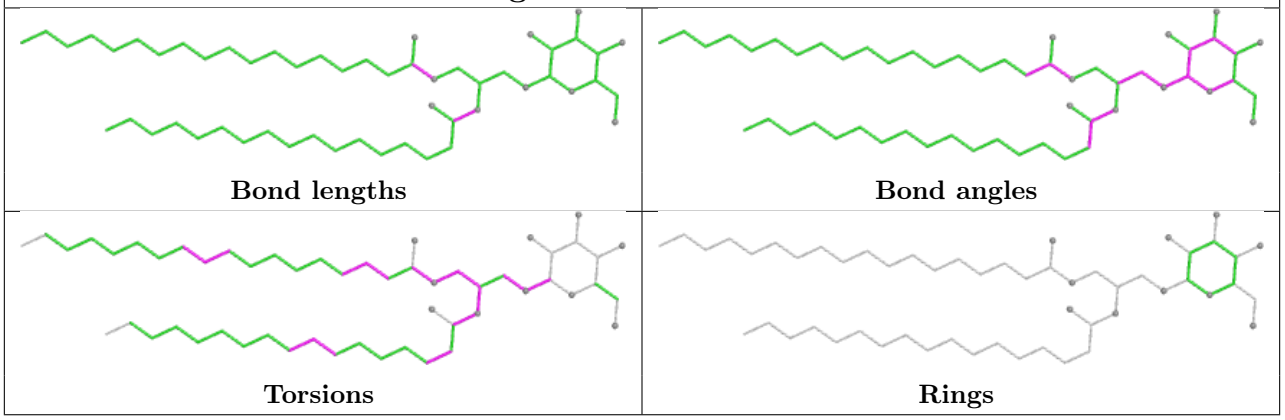


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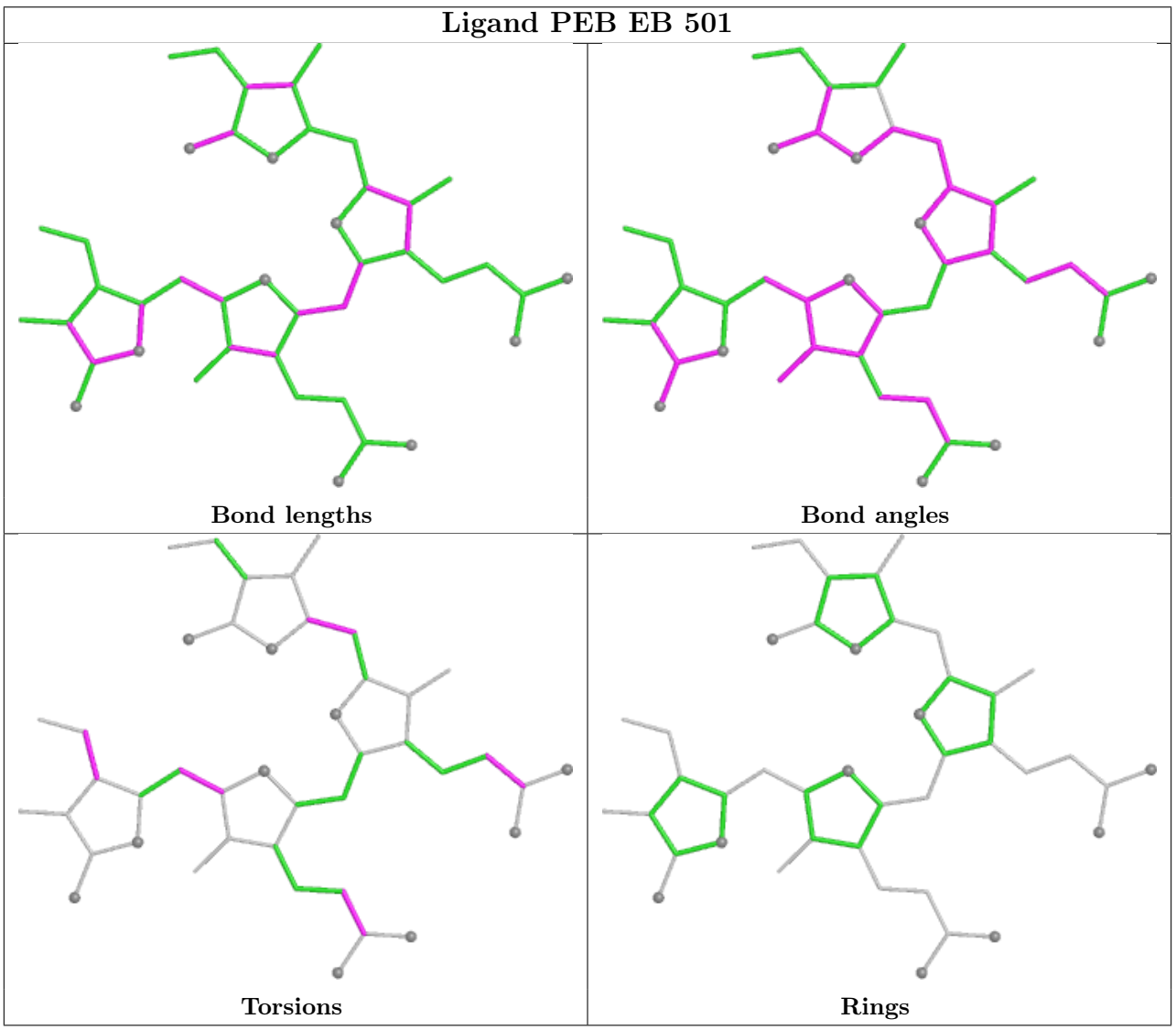


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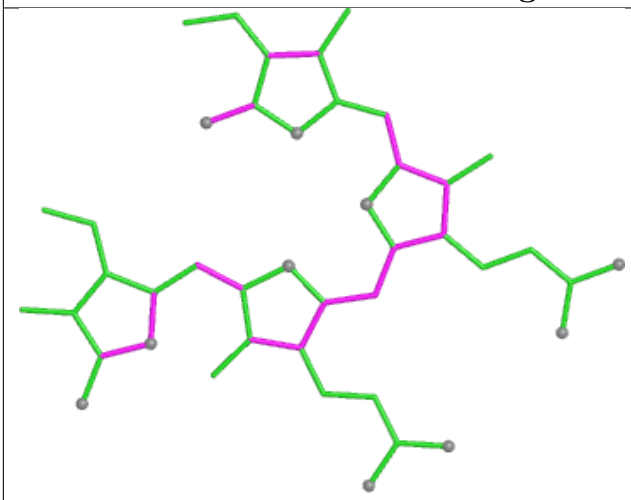
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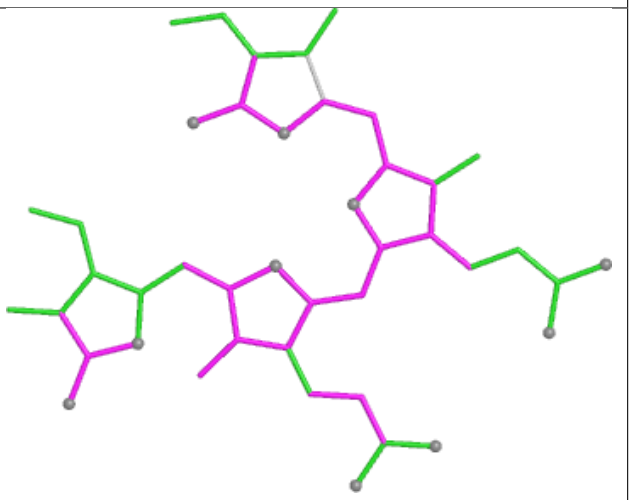
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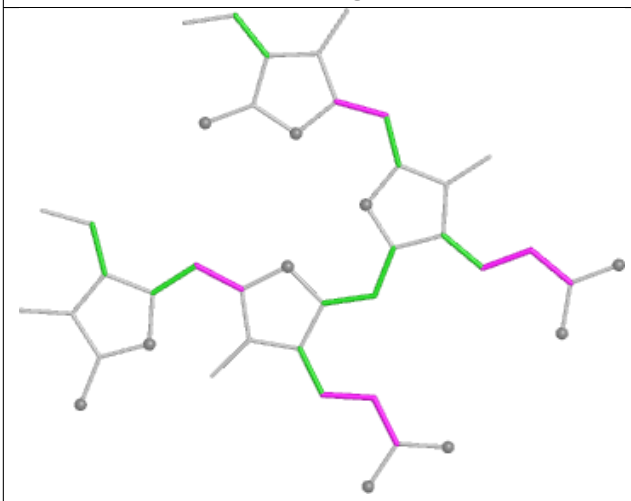
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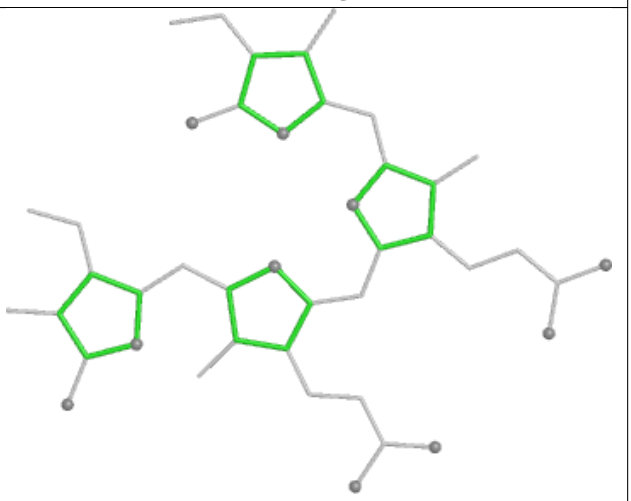
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Bond angles

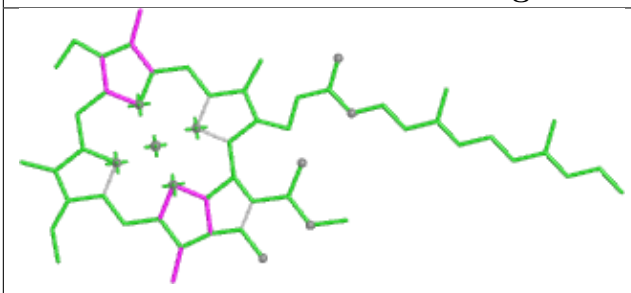


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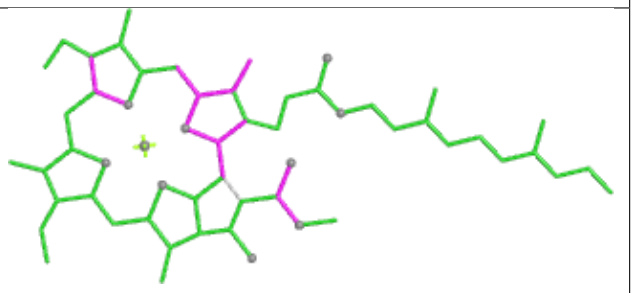


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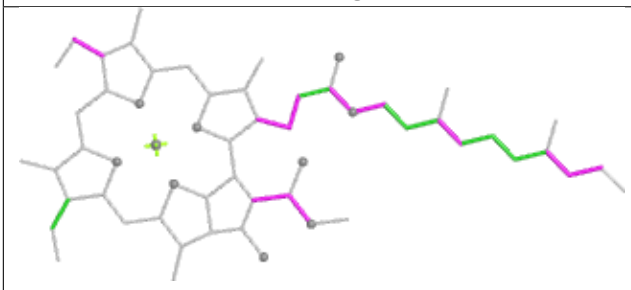
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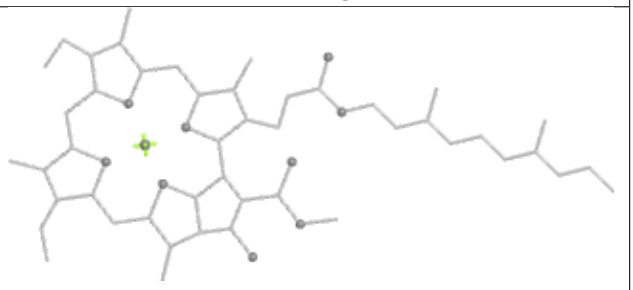
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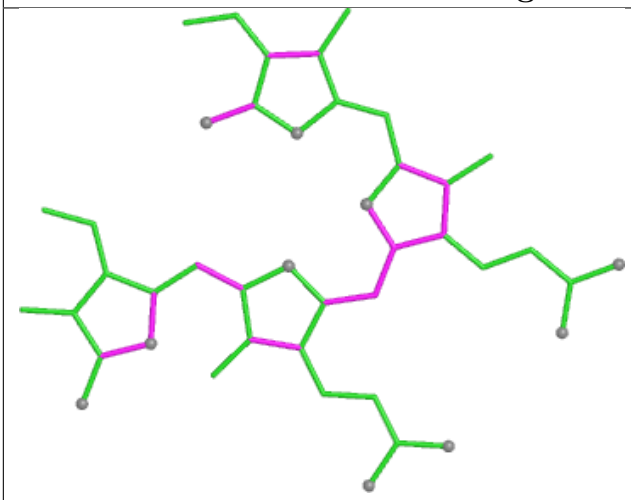


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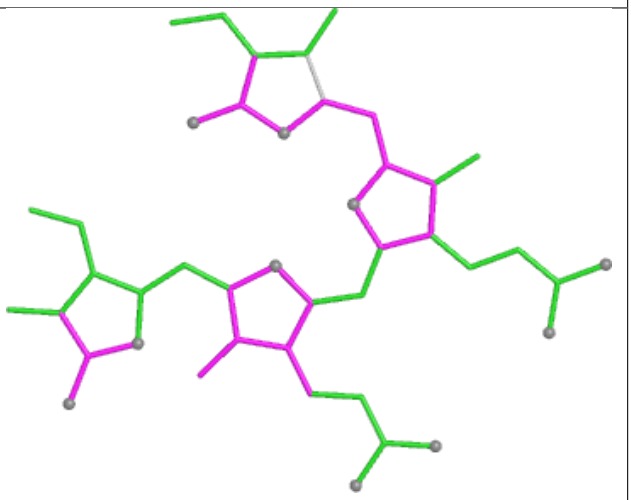


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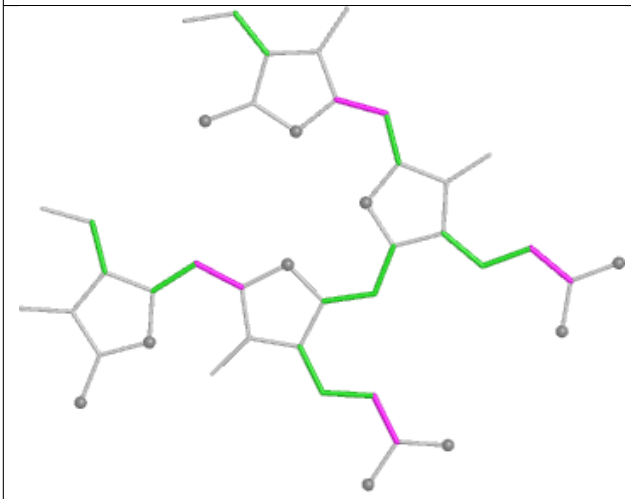
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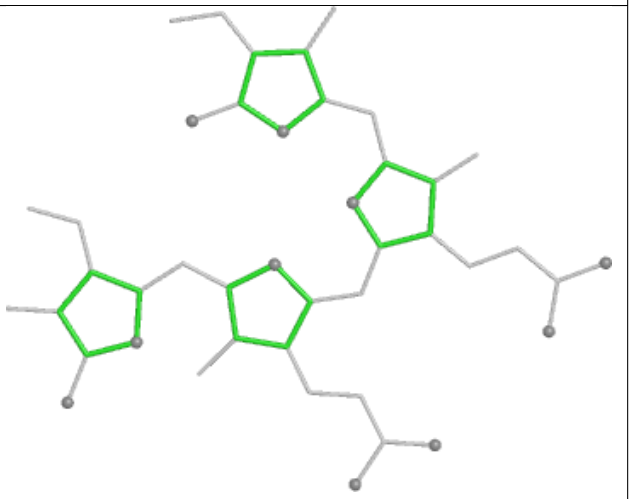
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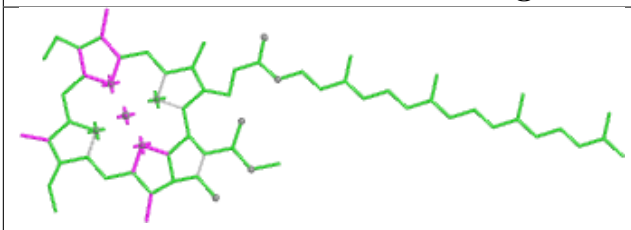


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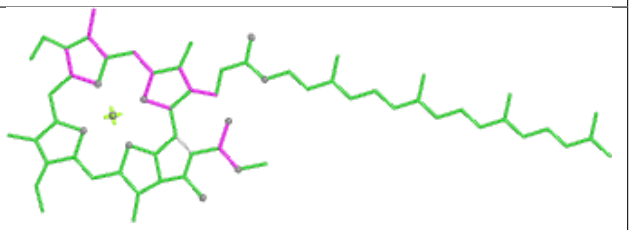


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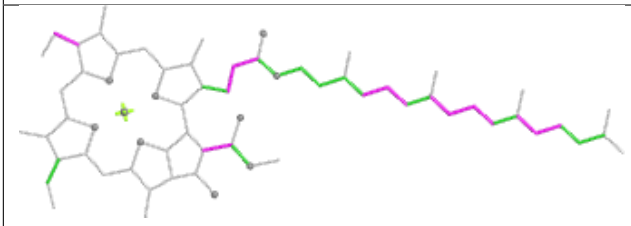
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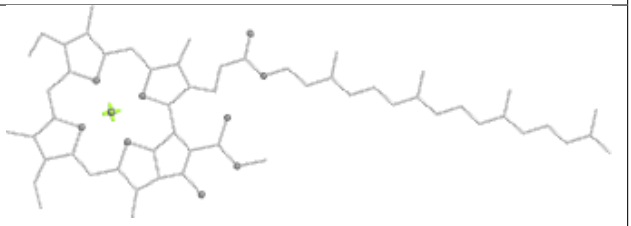
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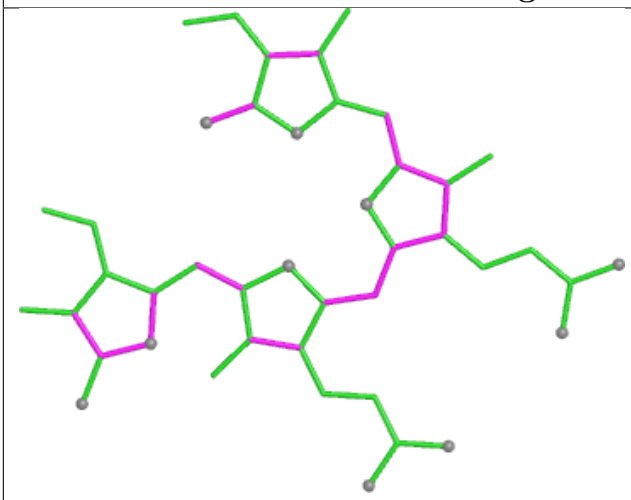


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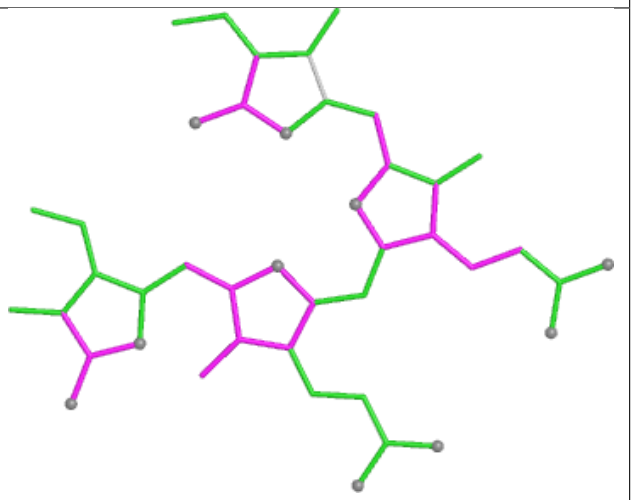


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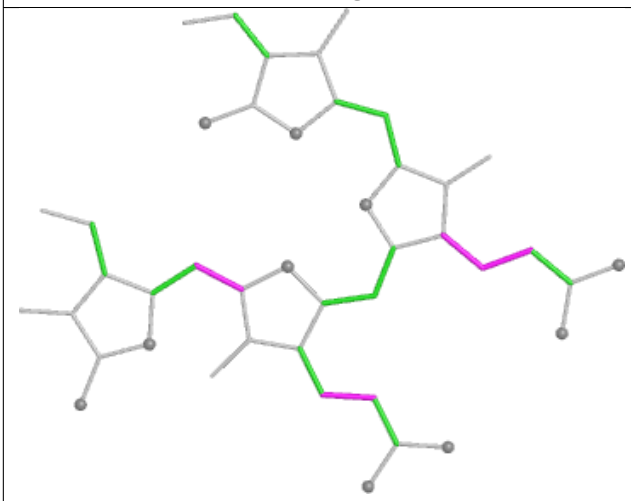
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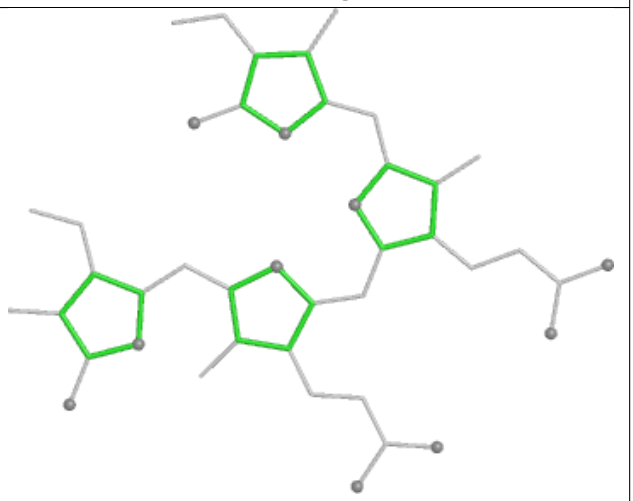
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Bond angles

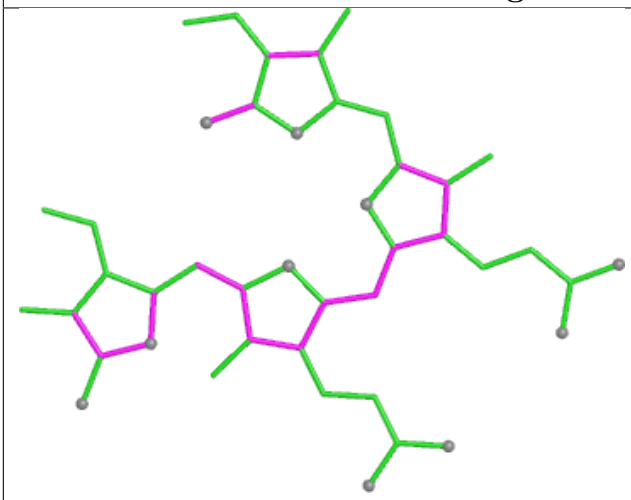


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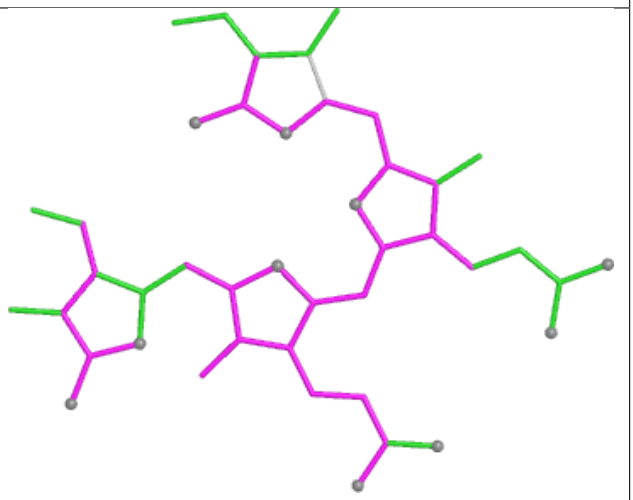


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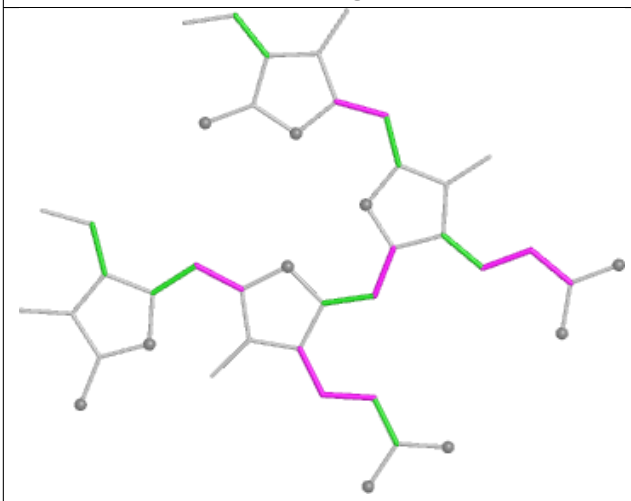
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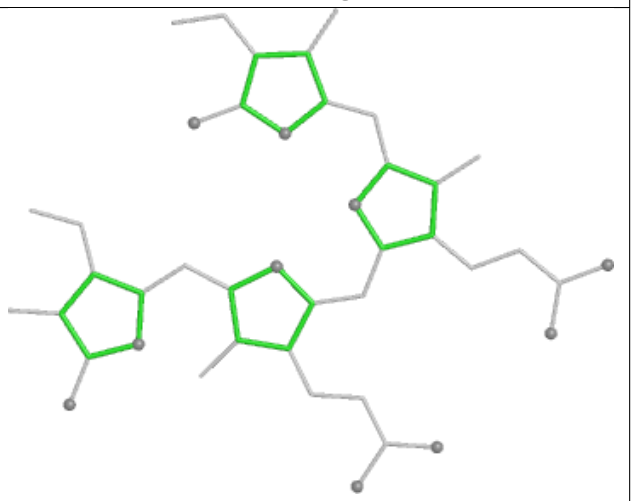
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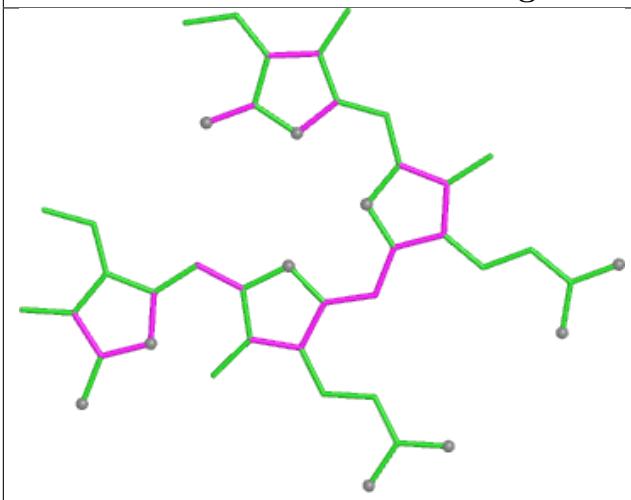


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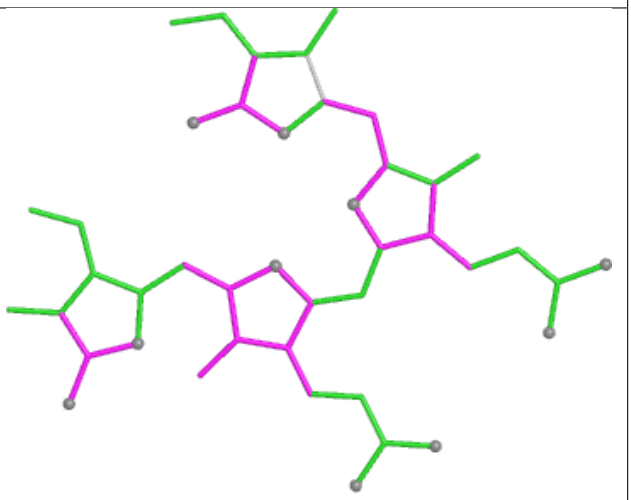


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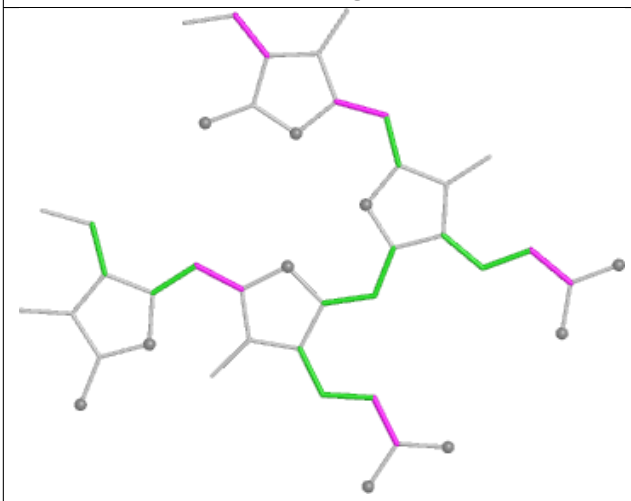
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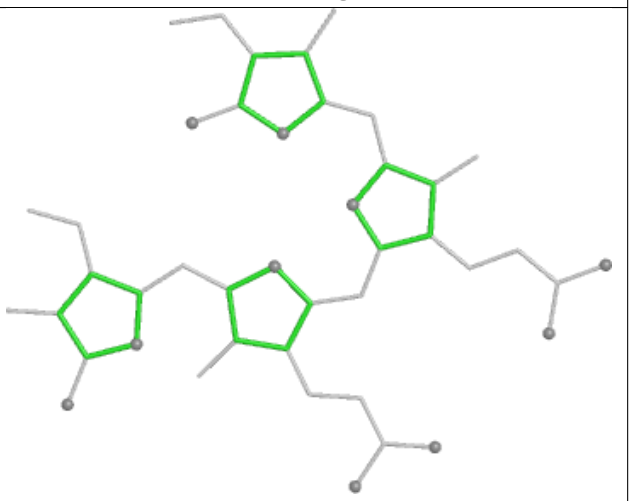
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Bond angles

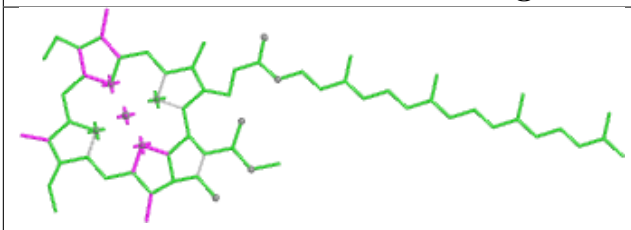


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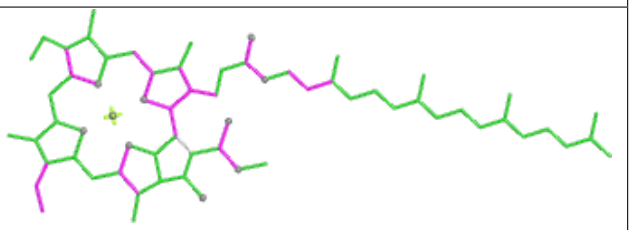


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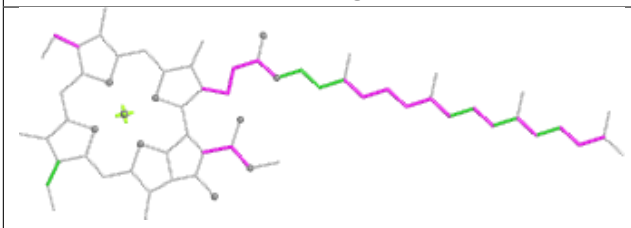
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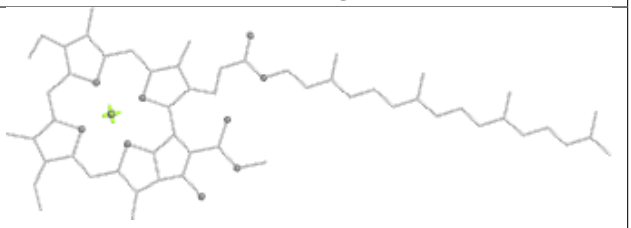
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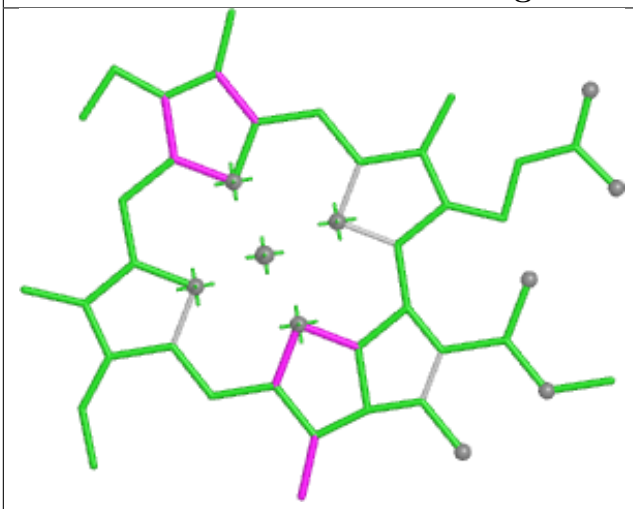


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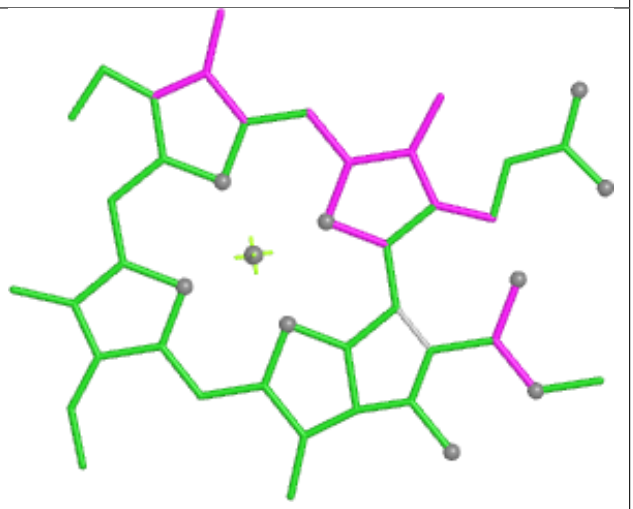


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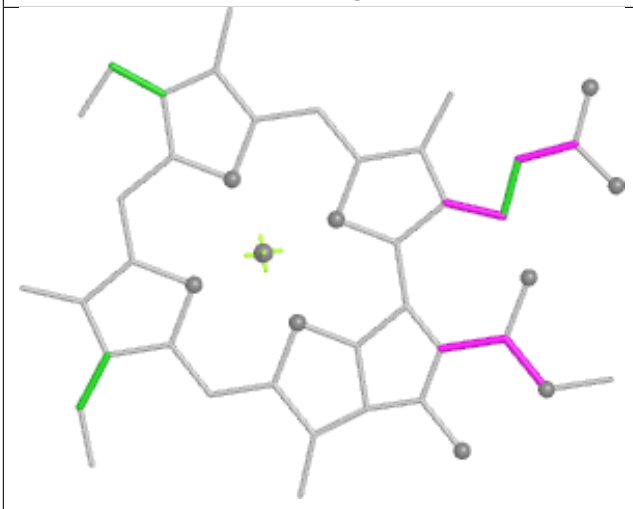
Ligand CLA 5N 606



Bond lengths



Bond angles

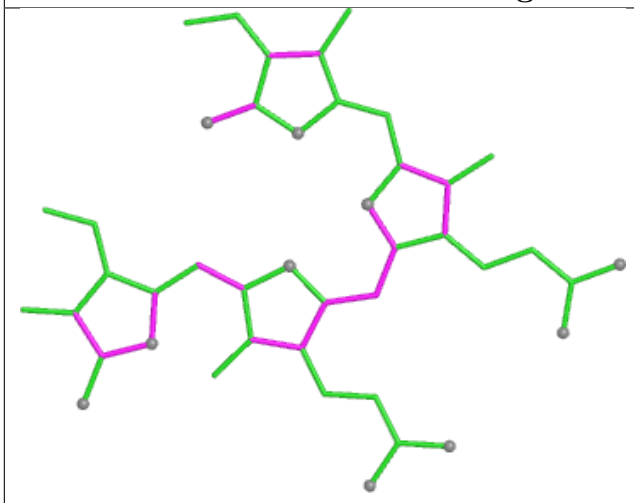


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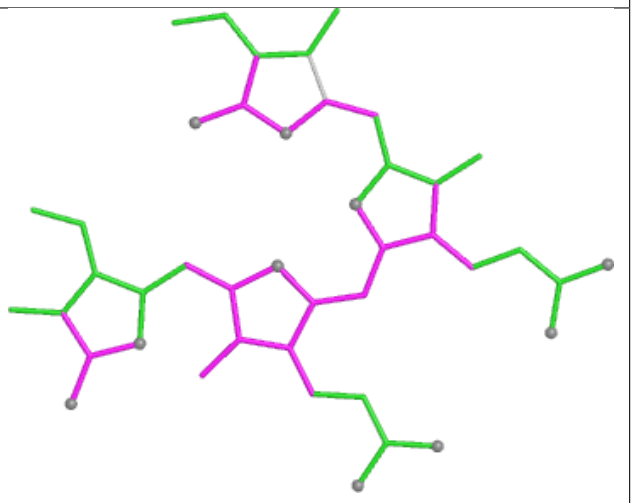


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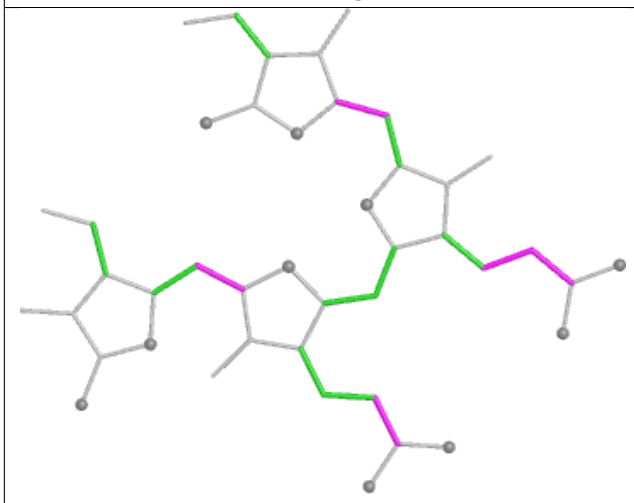
Ligand PEB O5 201



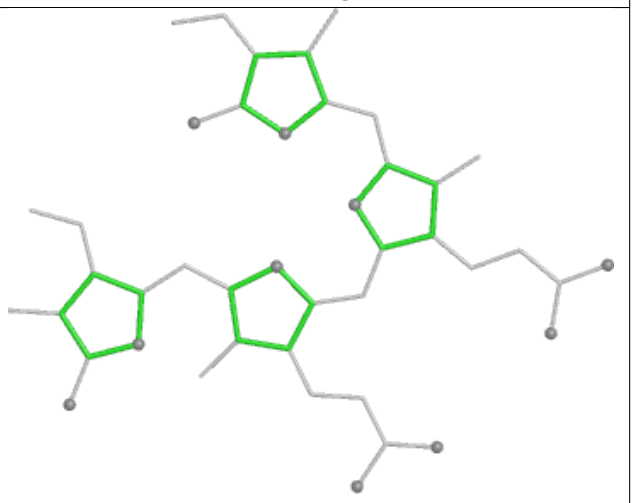
Bond lengths



Bond angles

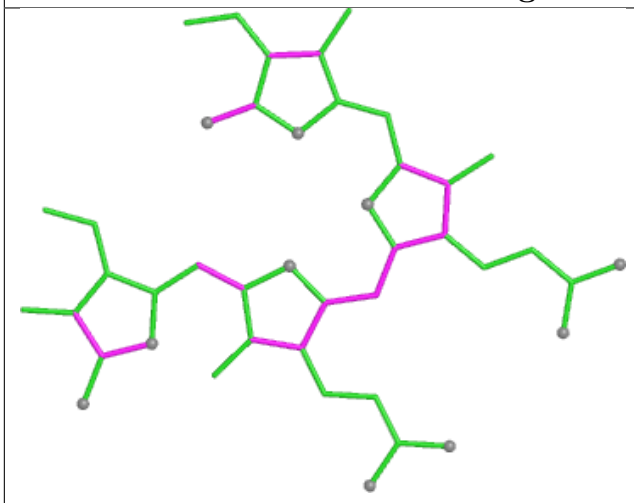


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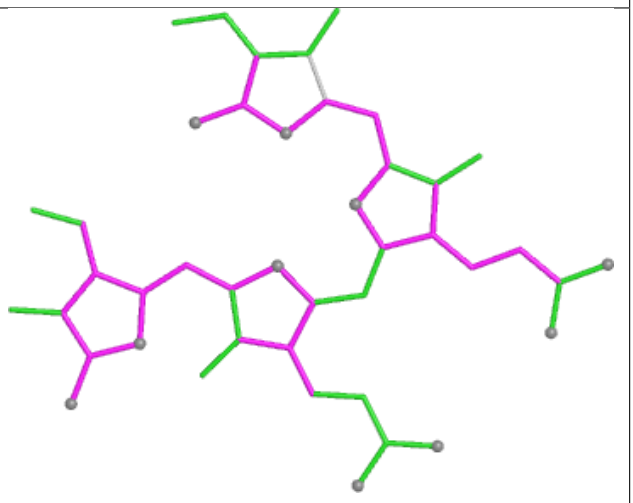


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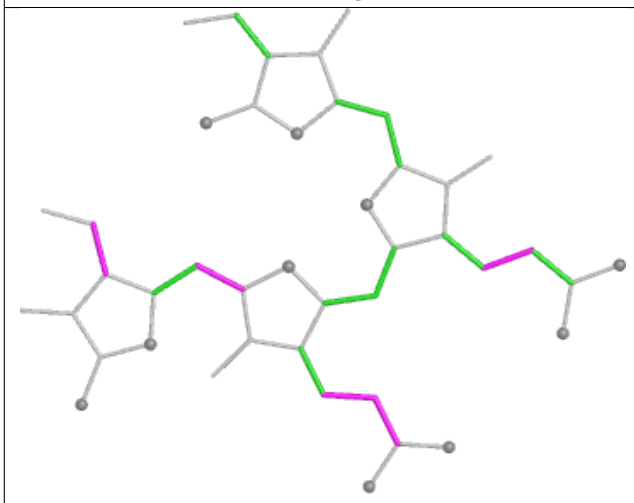
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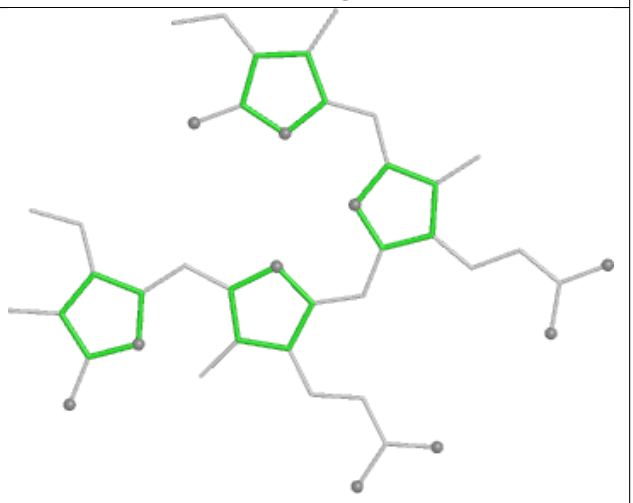
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Bond angles

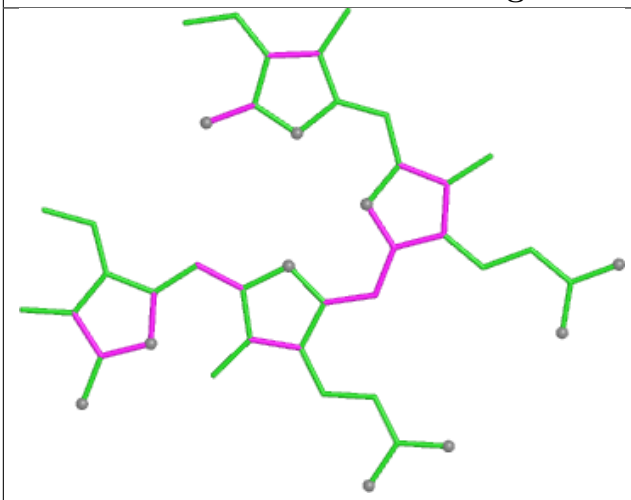


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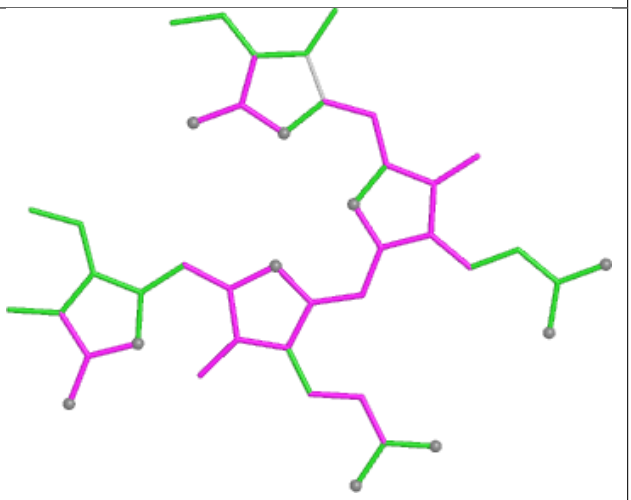


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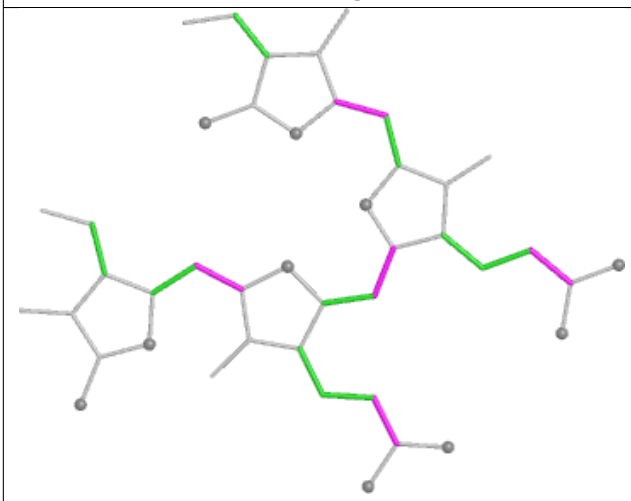
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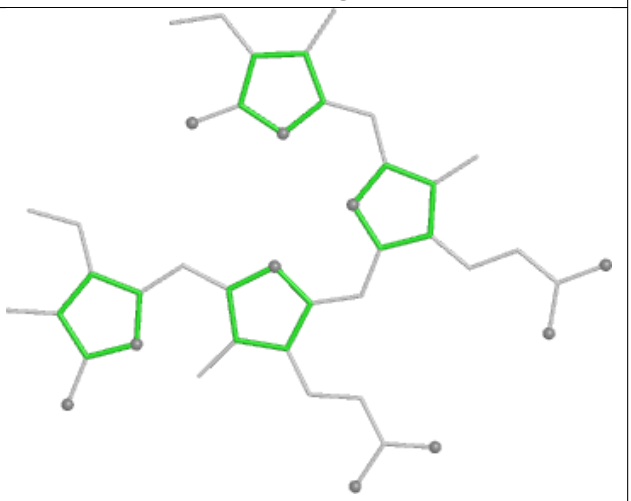
Bond lengths



Bond angles

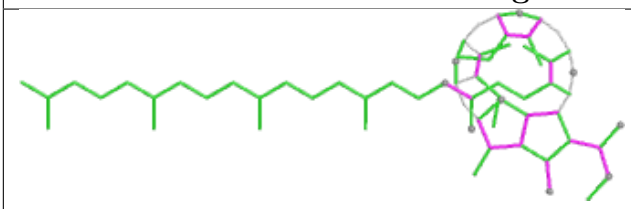


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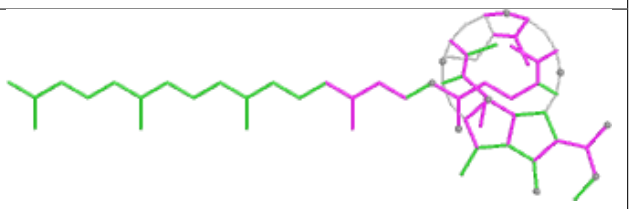


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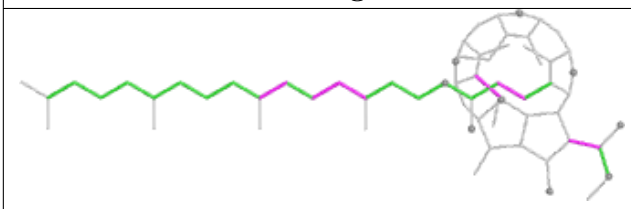
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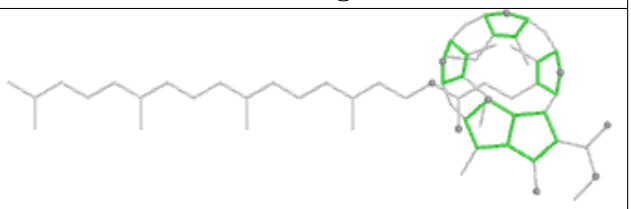
Bond lengths



Bond angles

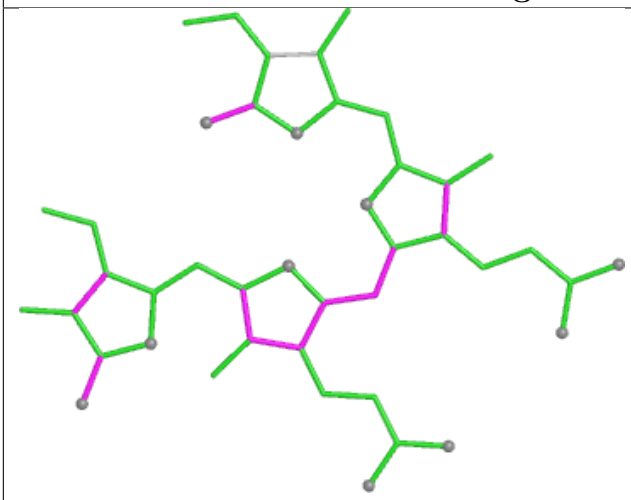


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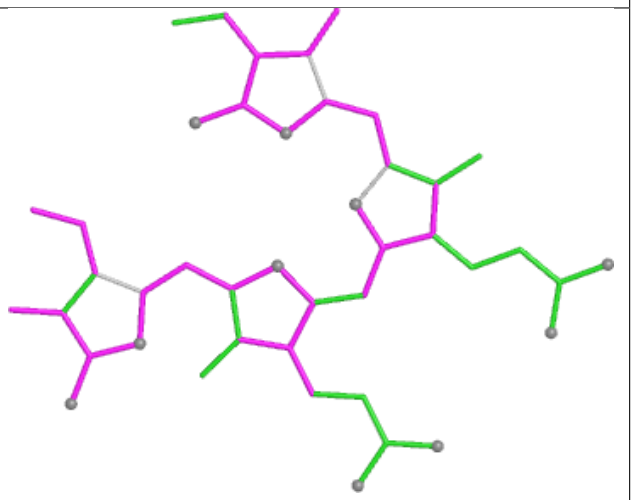


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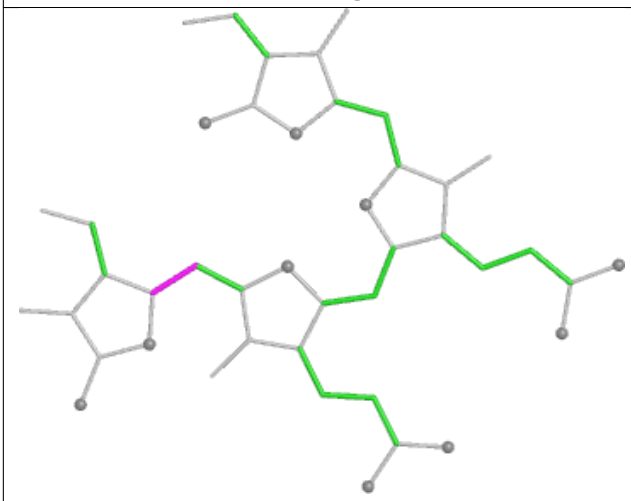
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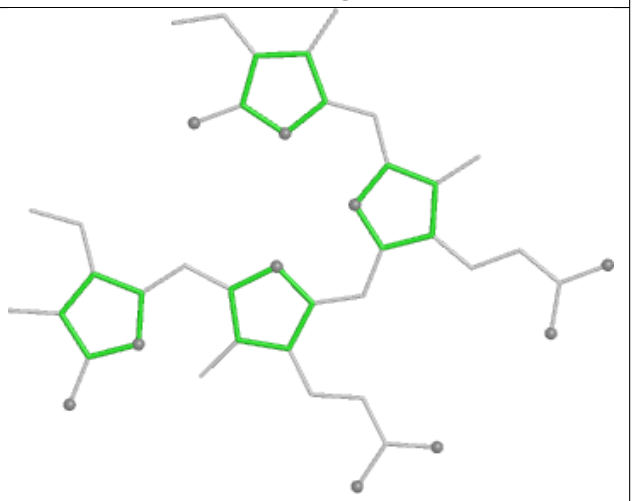
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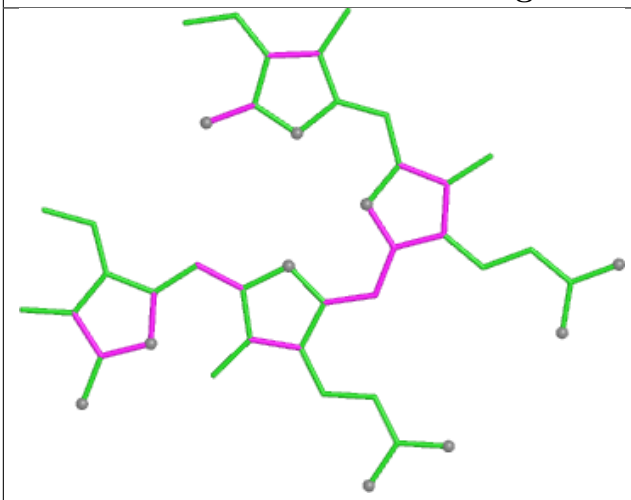


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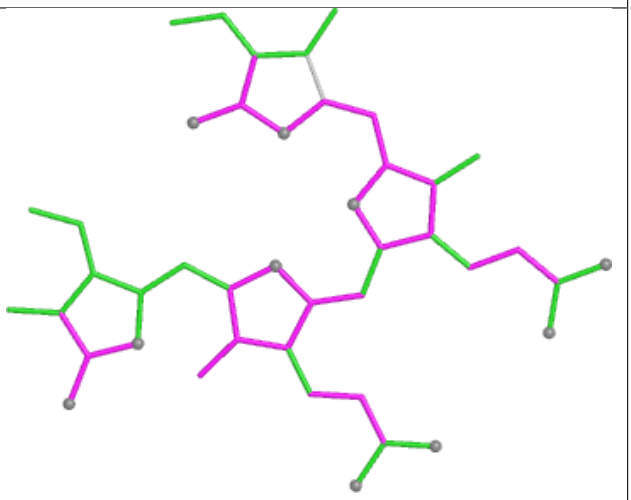


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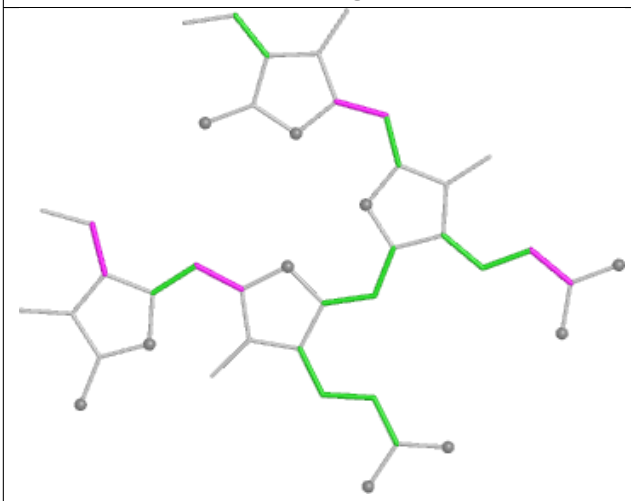
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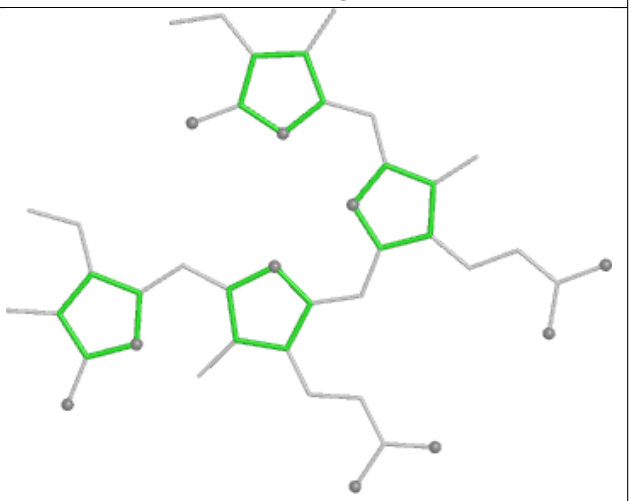
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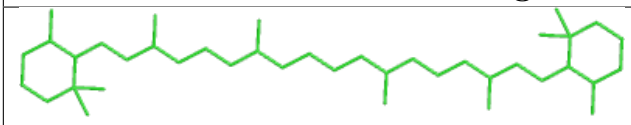


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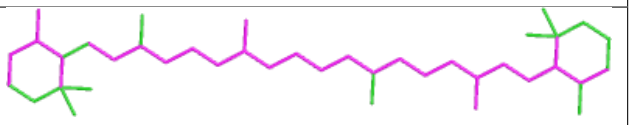


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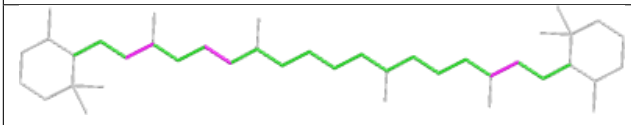
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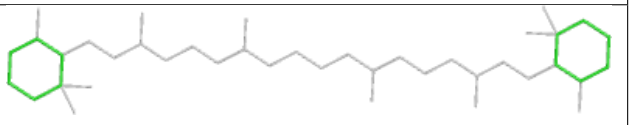
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Bond angles

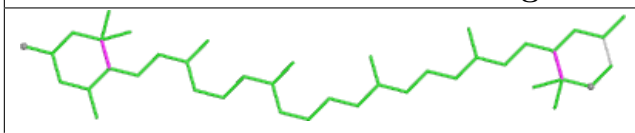


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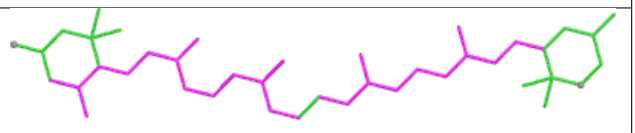


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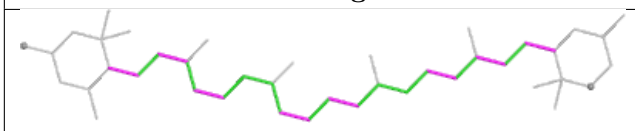
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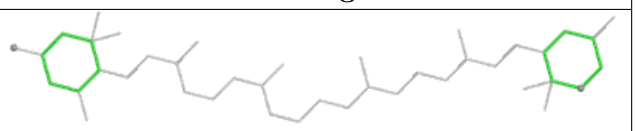
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Bond angles

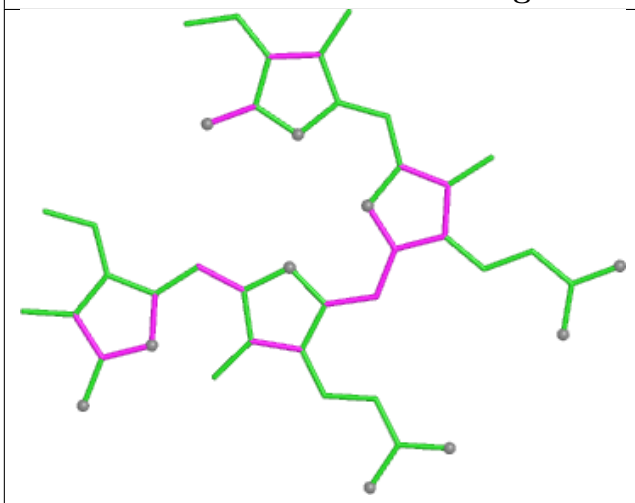


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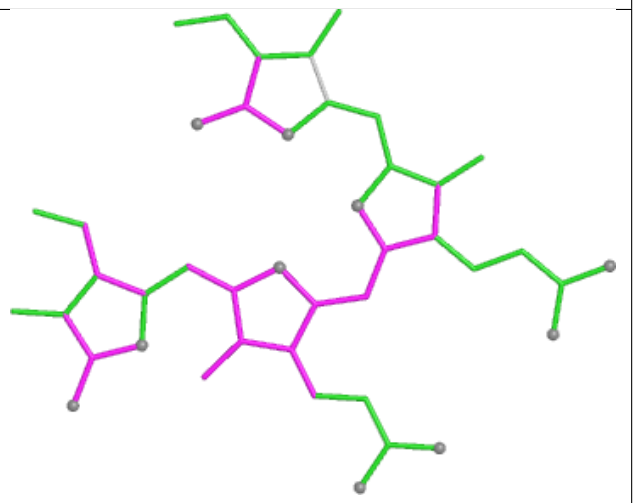


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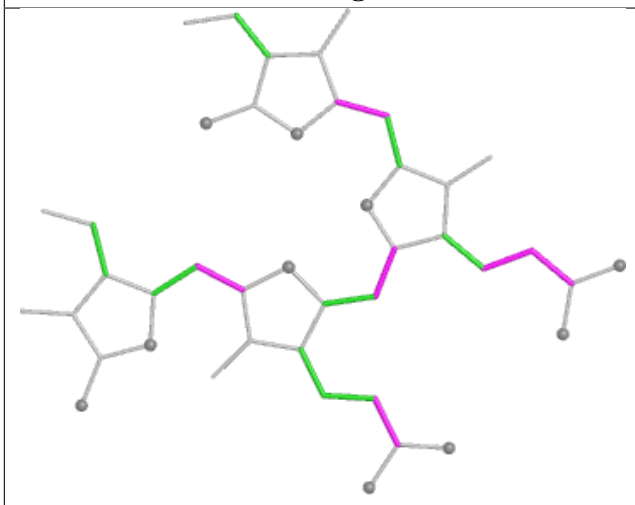
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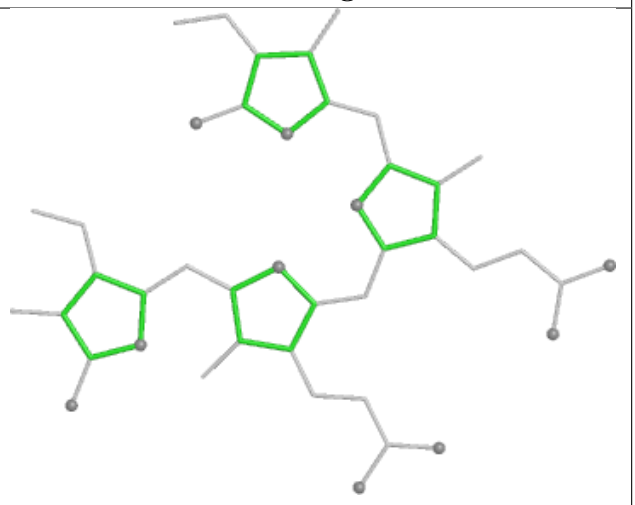
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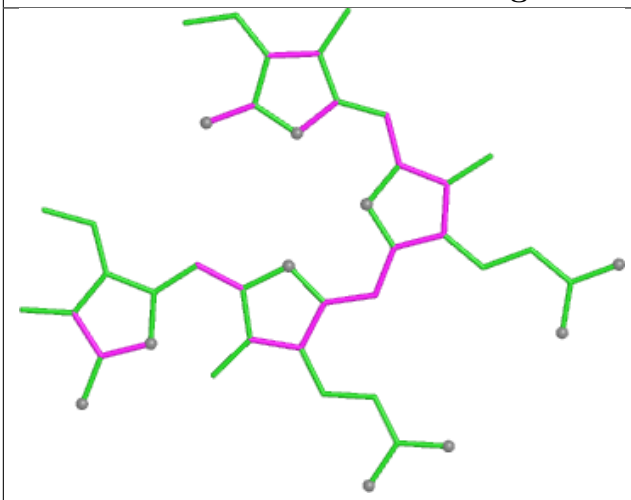


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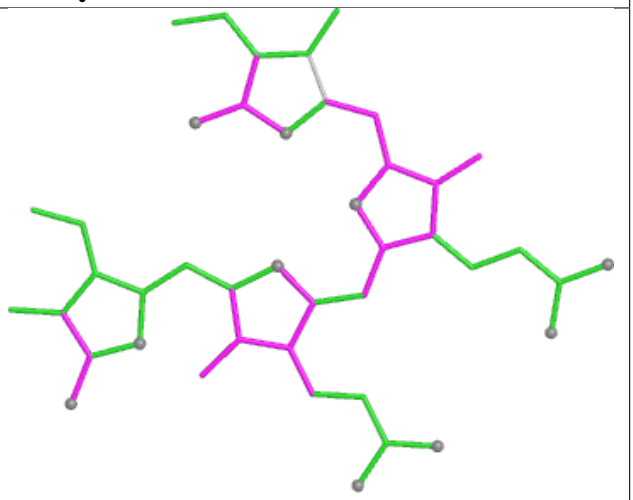


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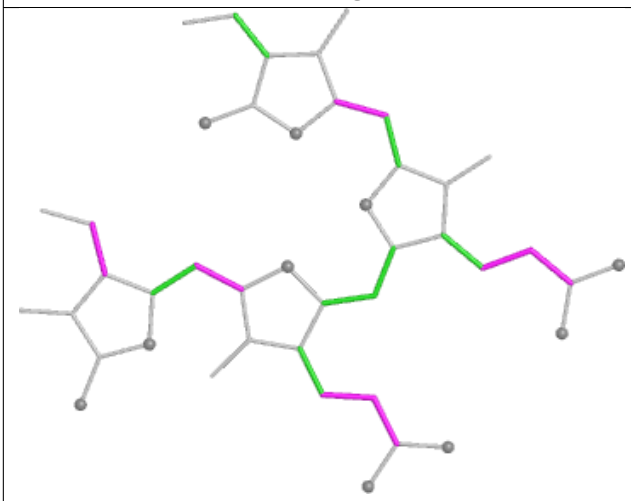
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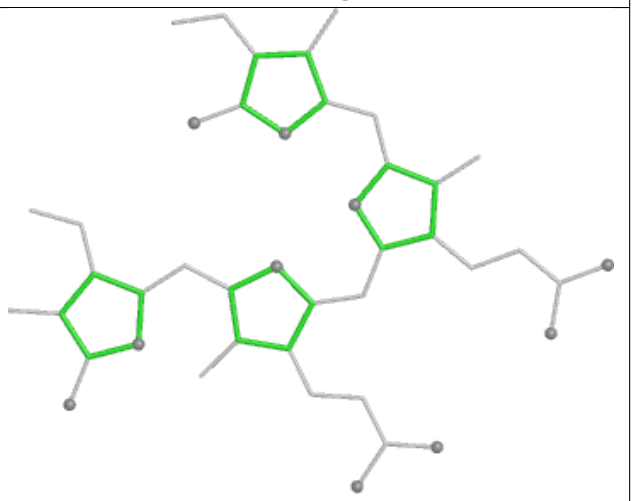
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Bond angles

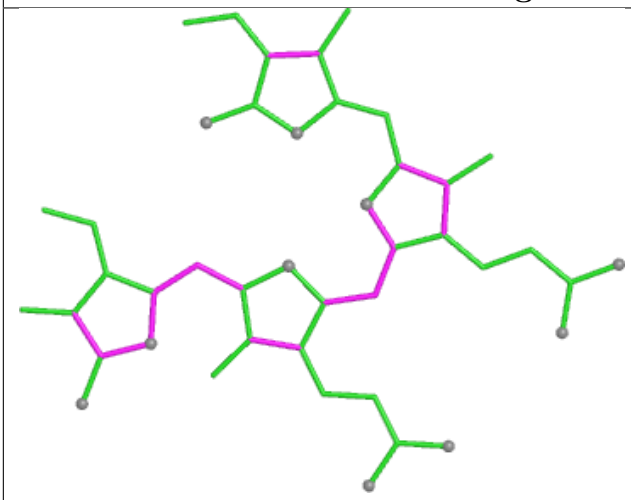


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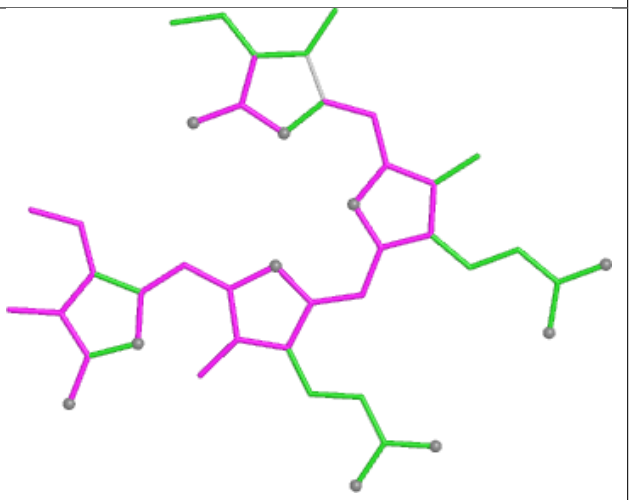


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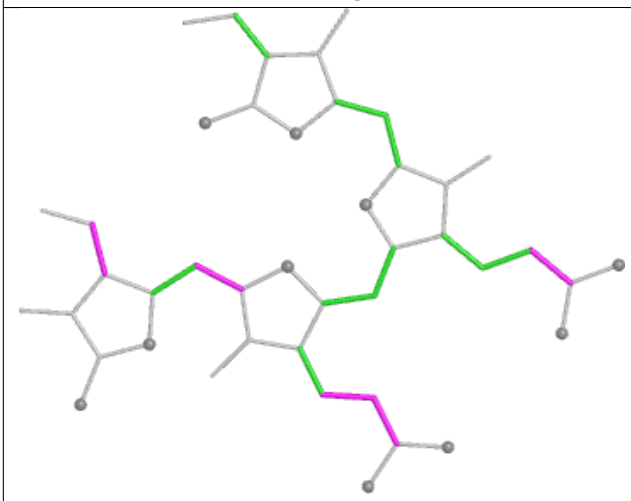
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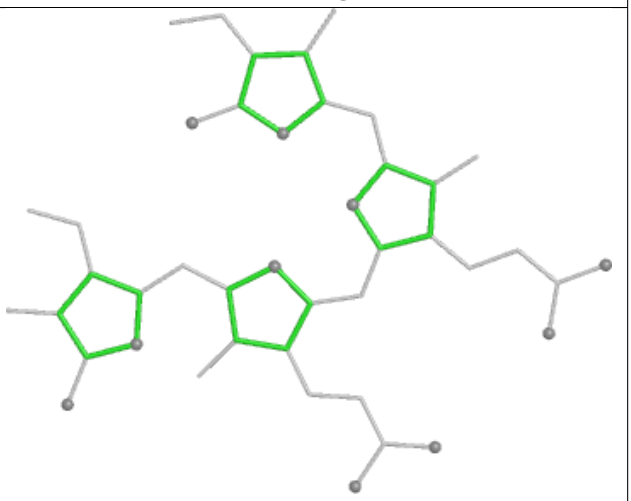
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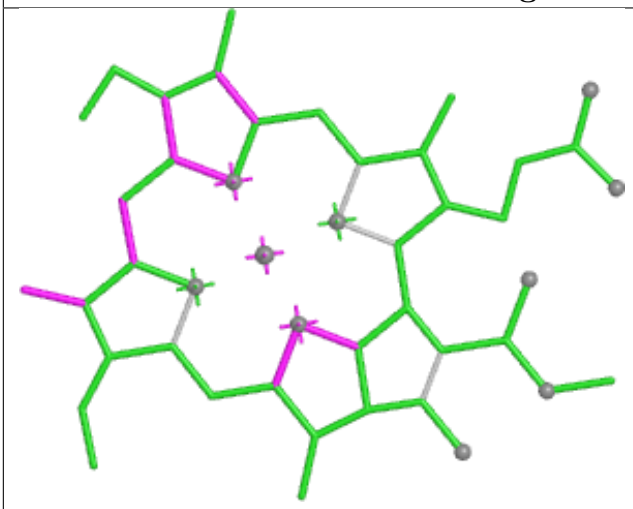


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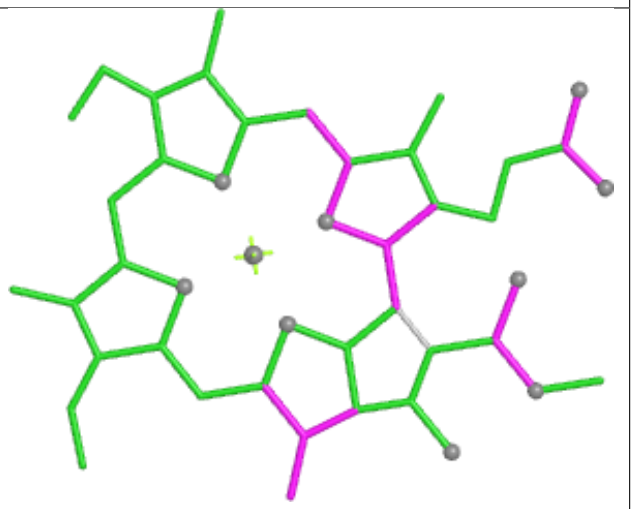


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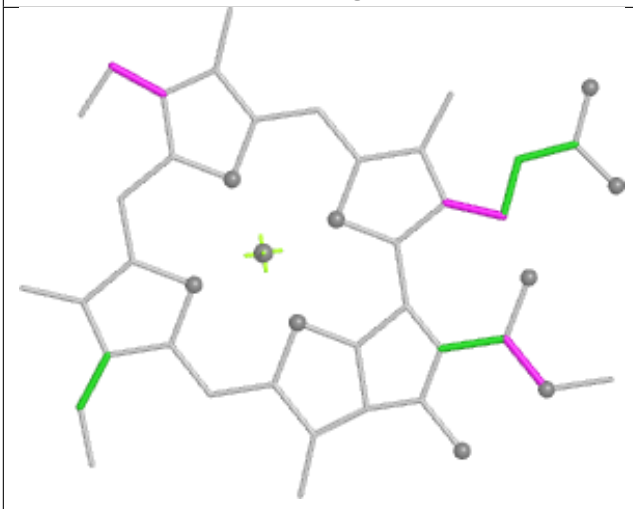
Ligand CLA 32 308



Bond lengths



Bond angles

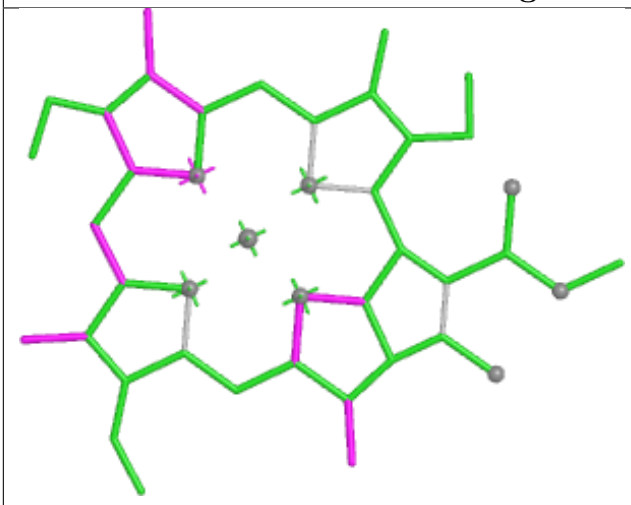


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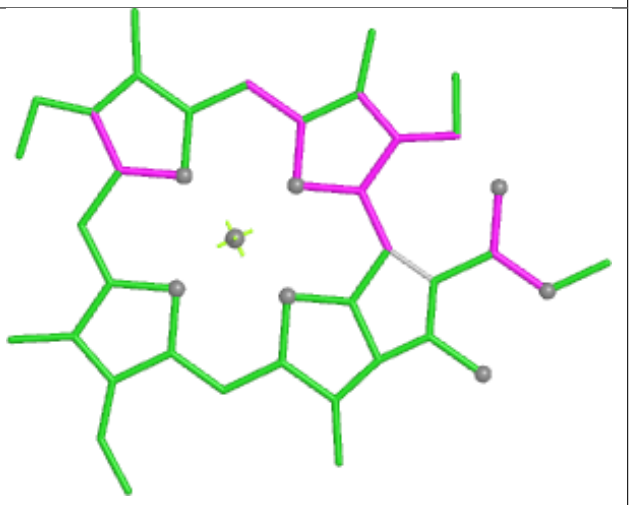


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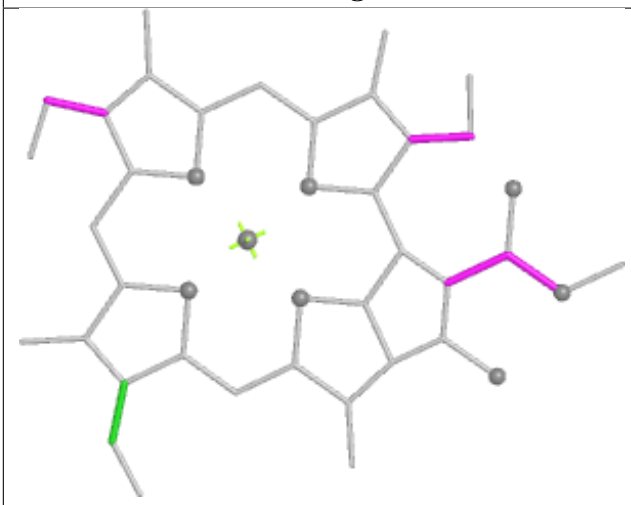
Ligand CLA 52 604



Bond lengths



Bond angles

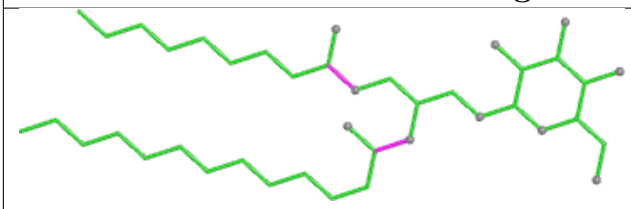


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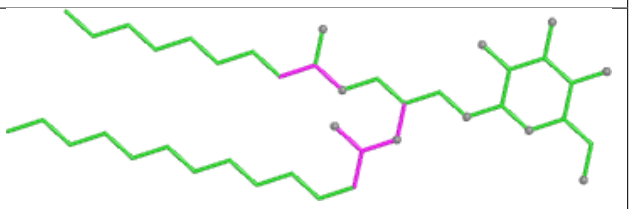


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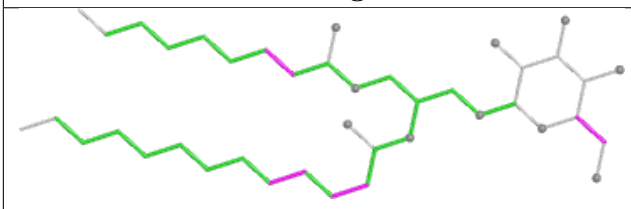
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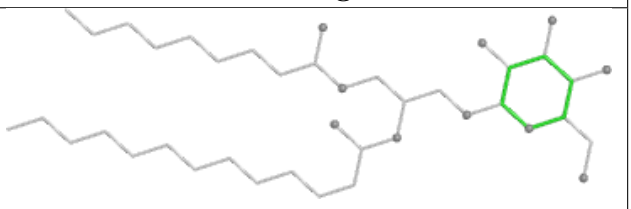
Bond lengths



Bond angles

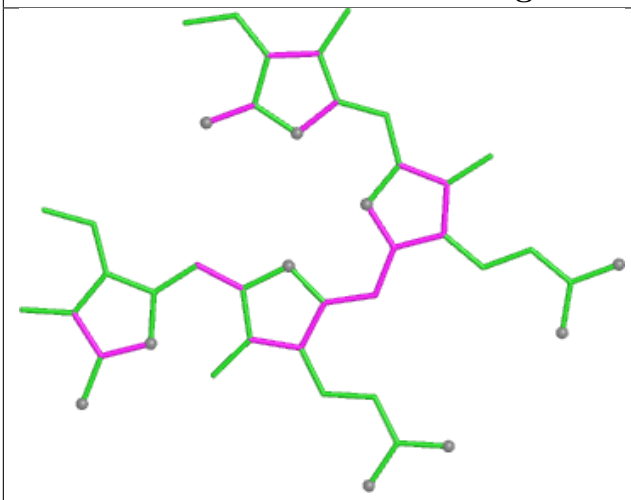


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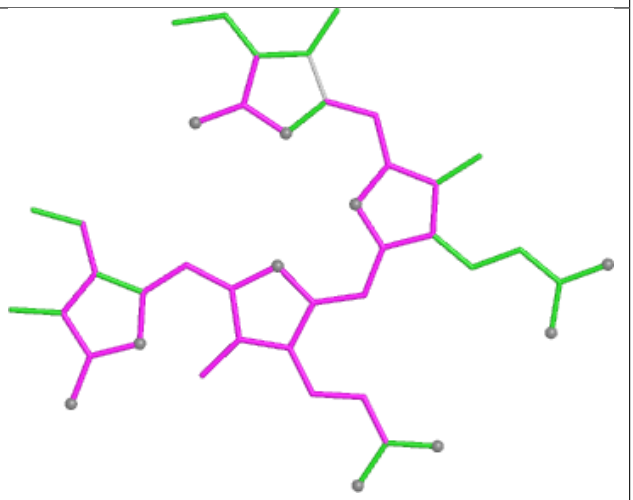


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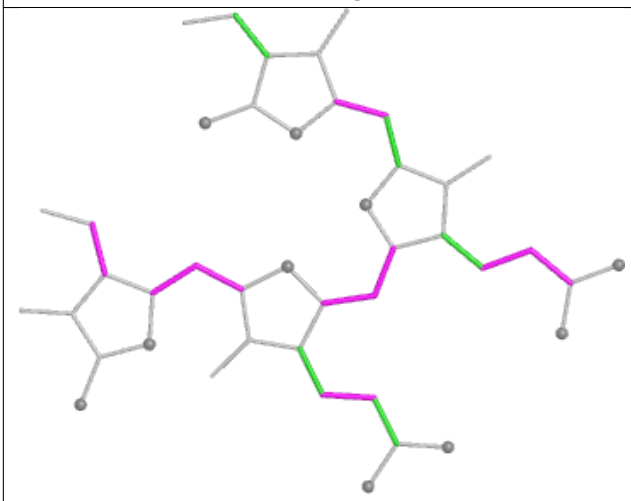
Ligand PEB vC 202



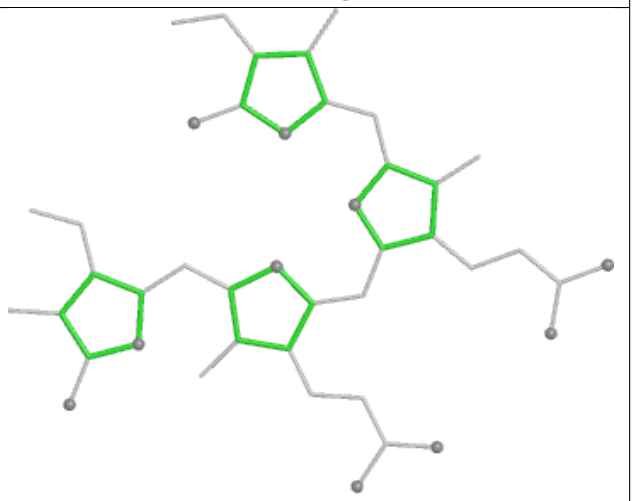
Bond lengths



Bond angles

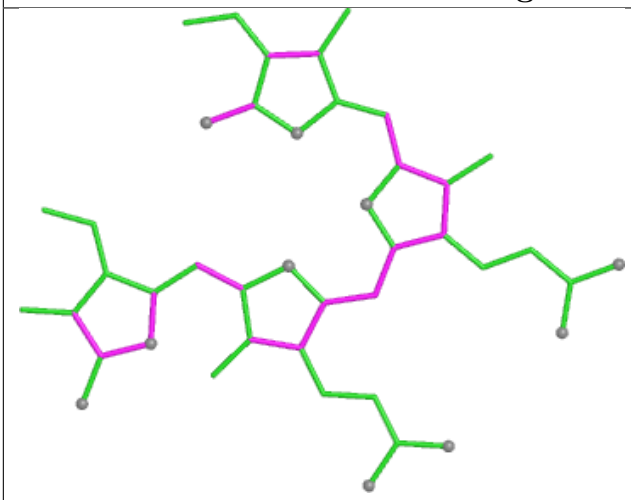


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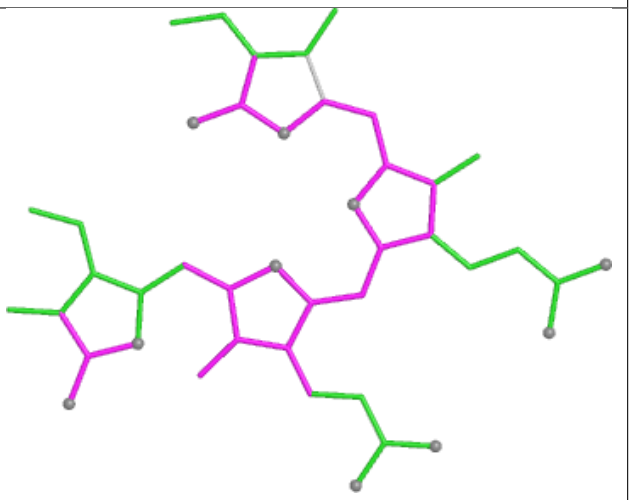


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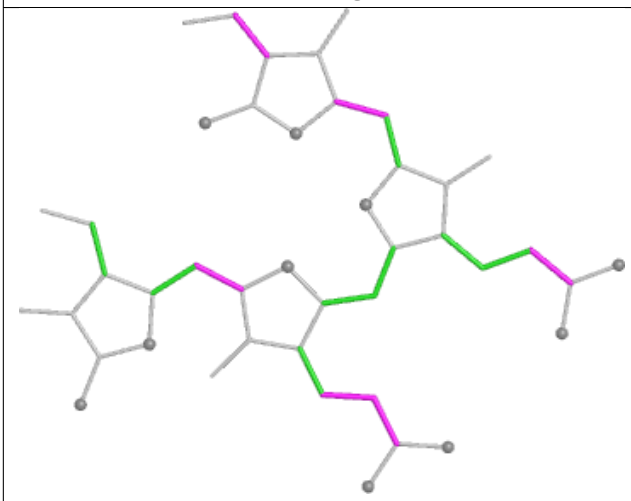
Ligand PEB cO 202



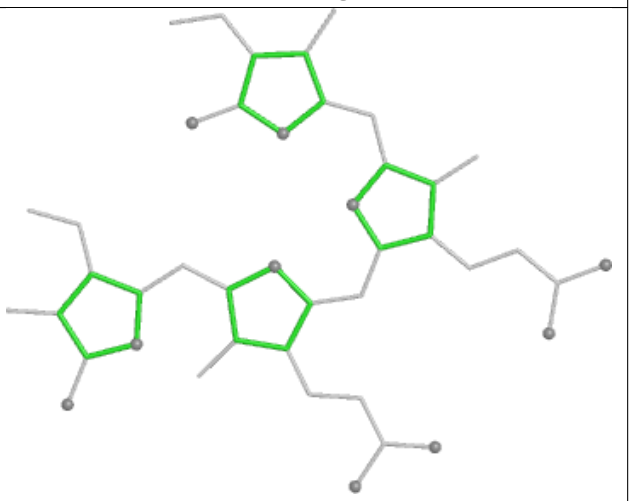
Bond lengths



Bond angles

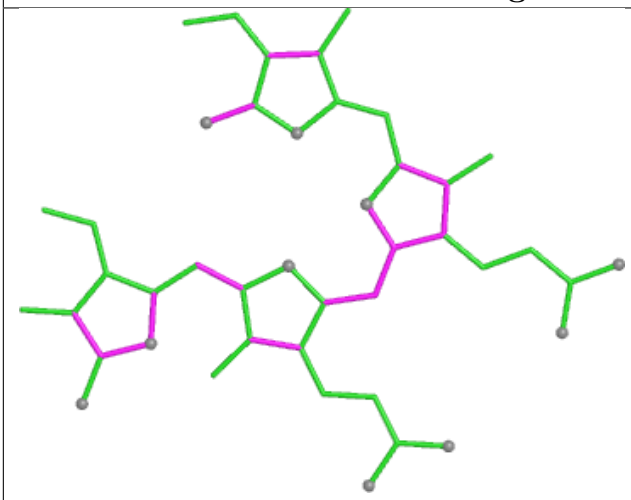


Torsions

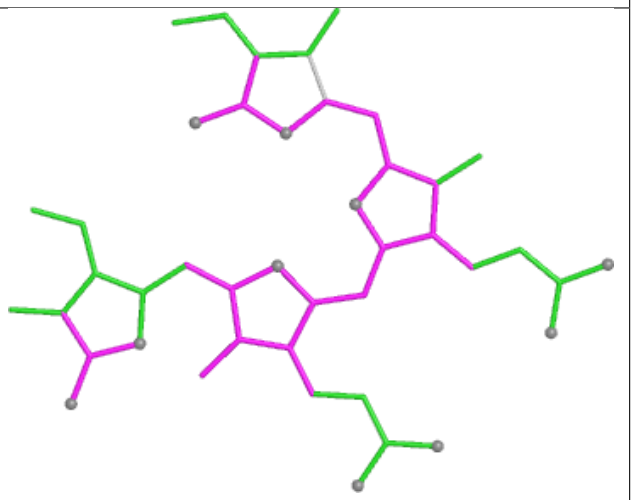


Rings

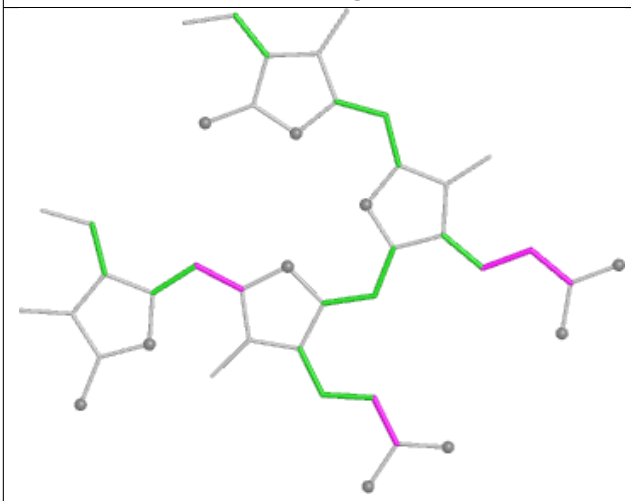
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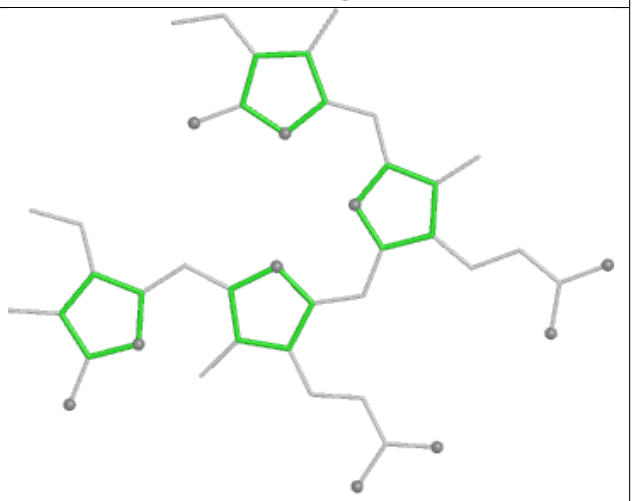
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Bond angles

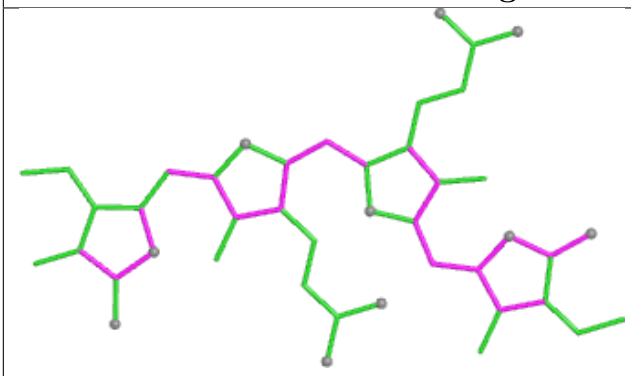


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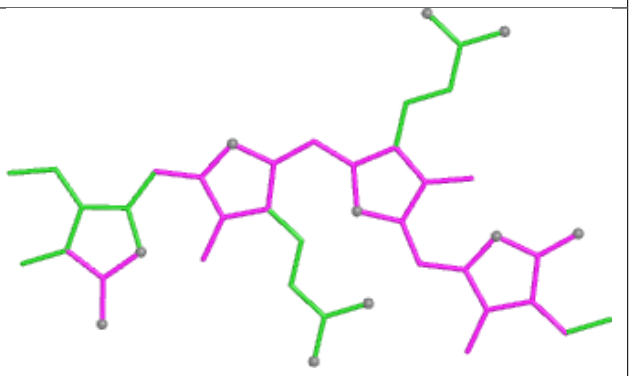


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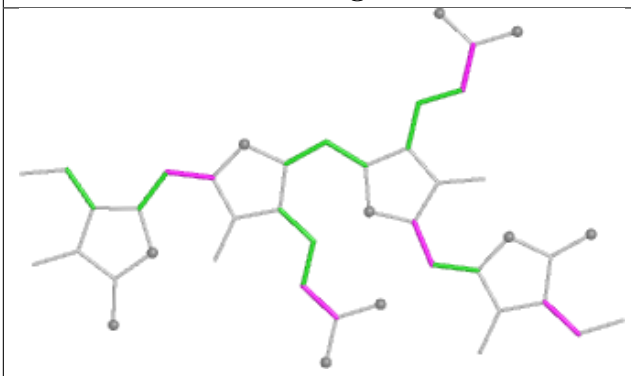
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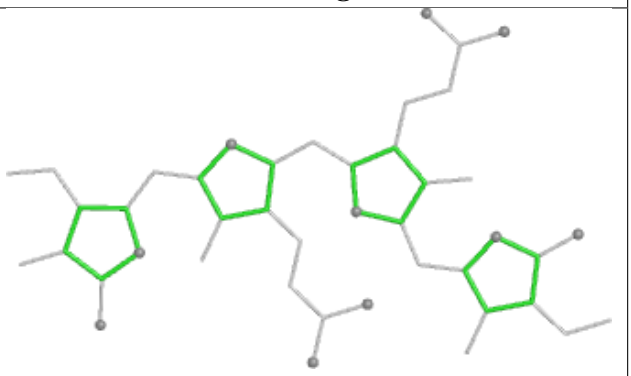
Bond lengths



Bond angles

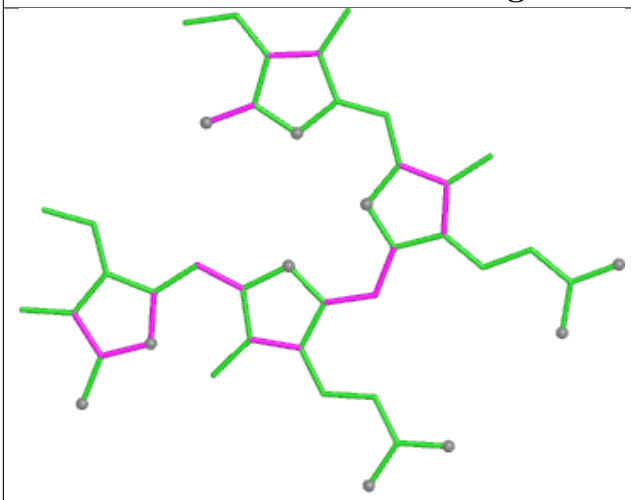


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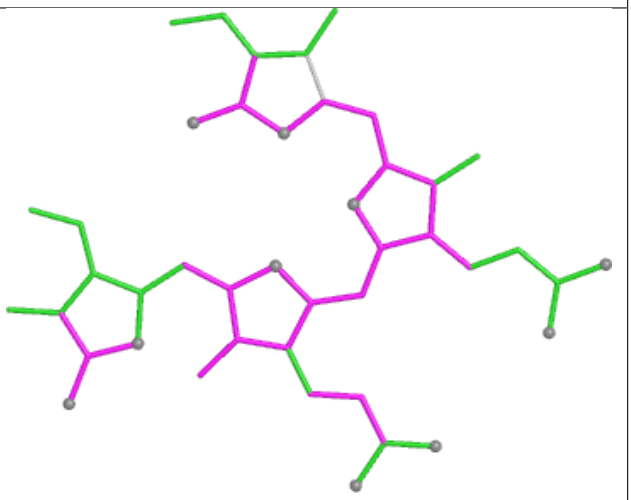


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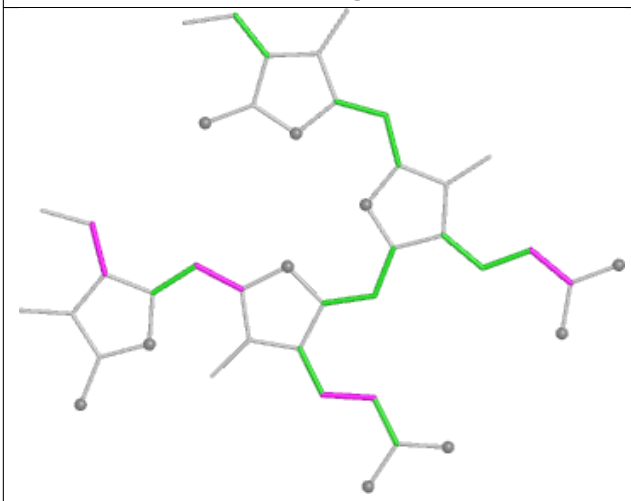
Ligand PEB WE 203



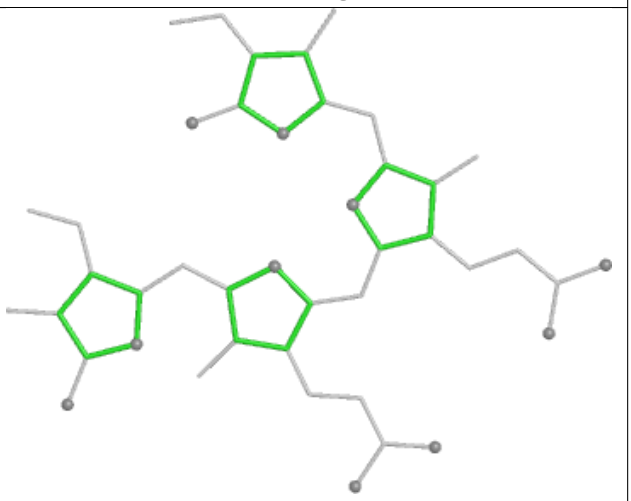
Bond lengths



Bond angles

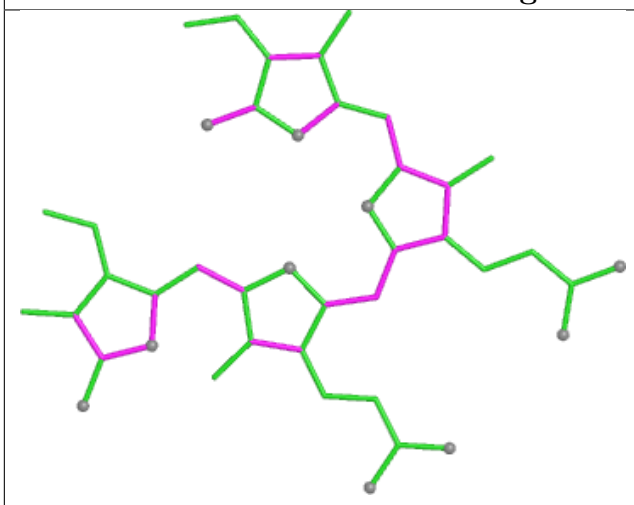


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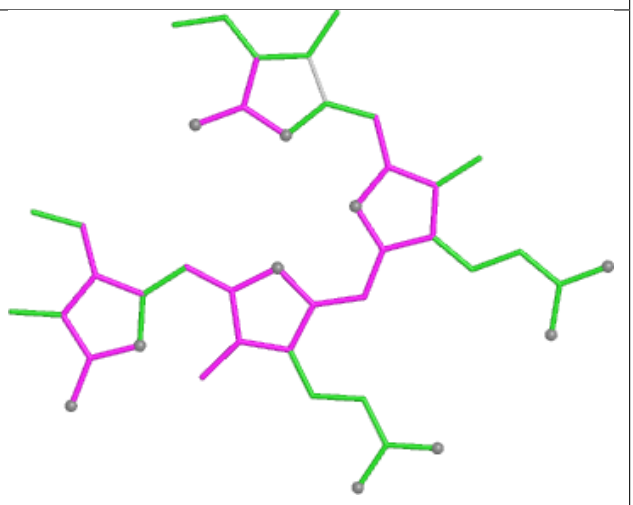


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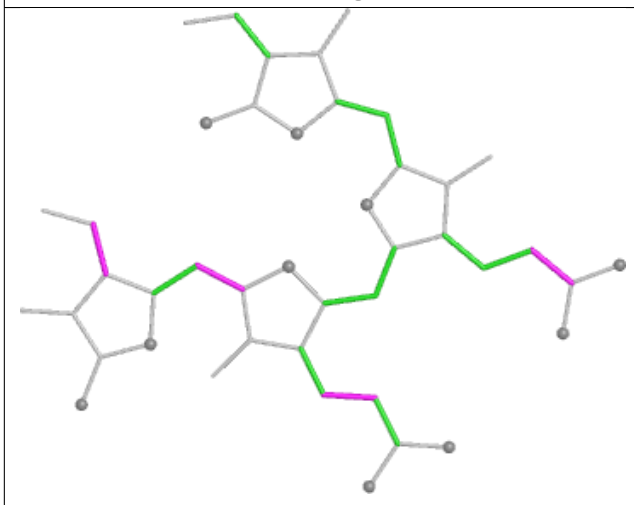
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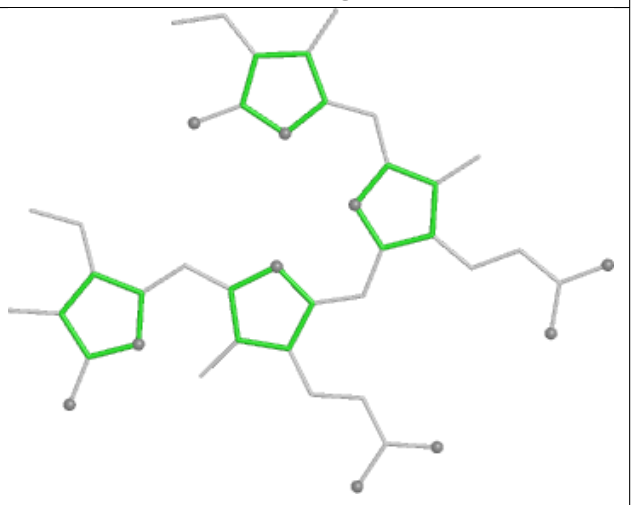
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Bond angles

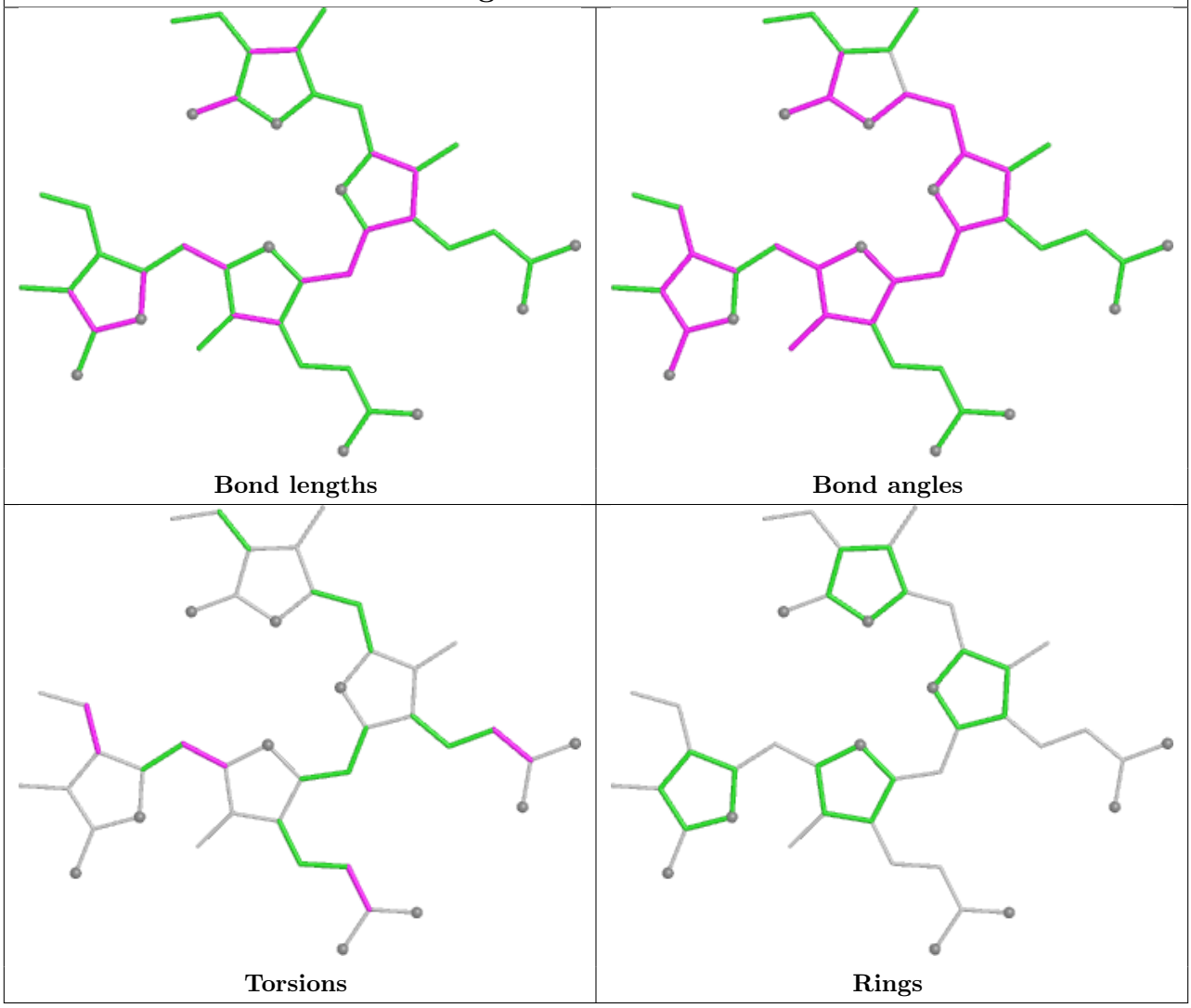


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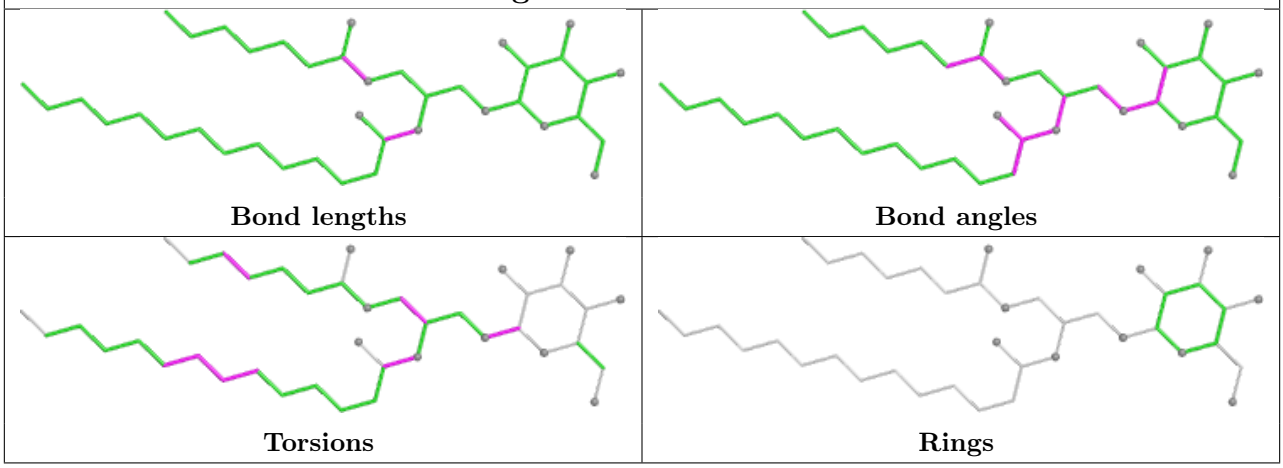


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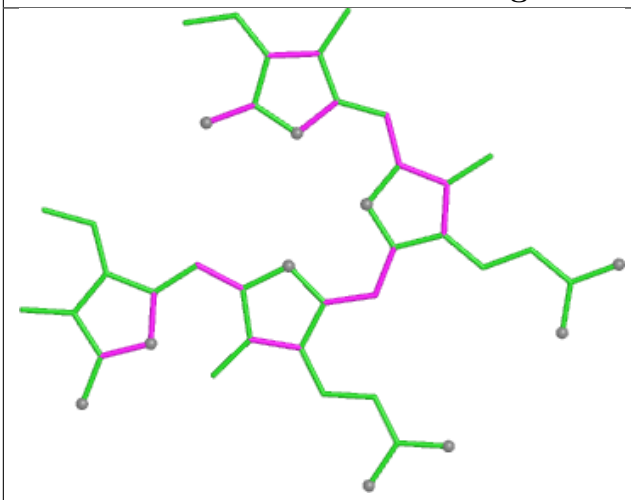
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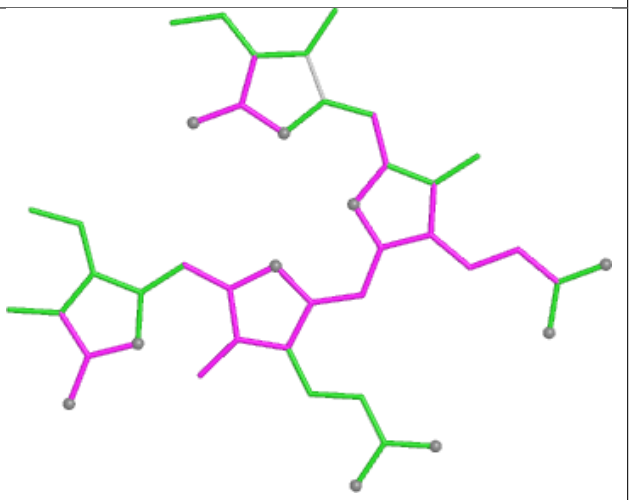
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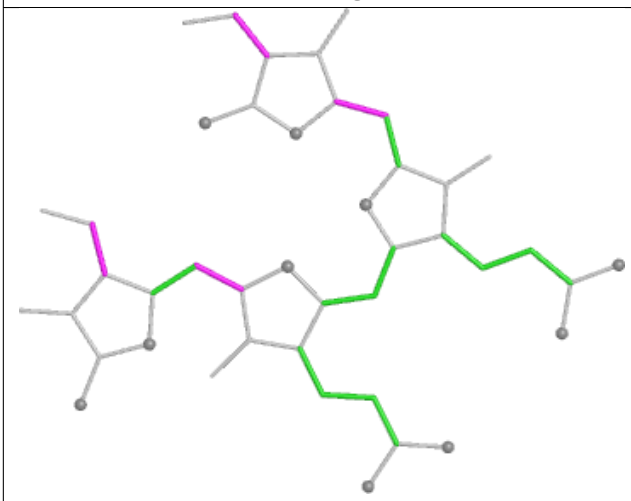
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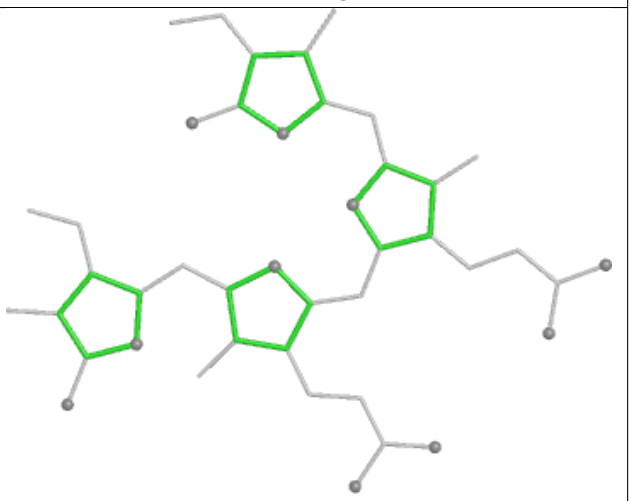
Bond lengths



Bond angles

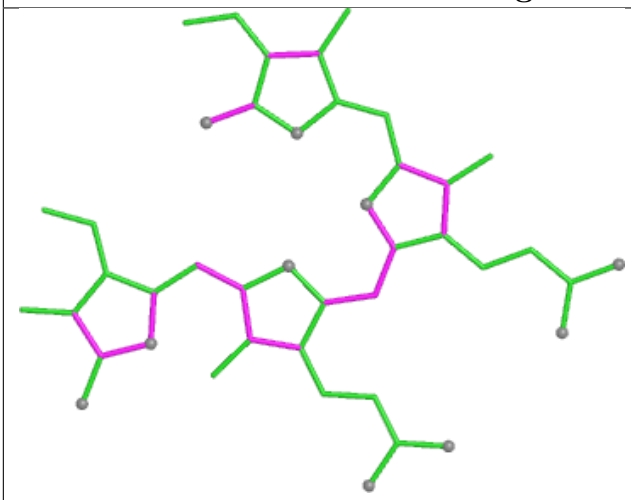


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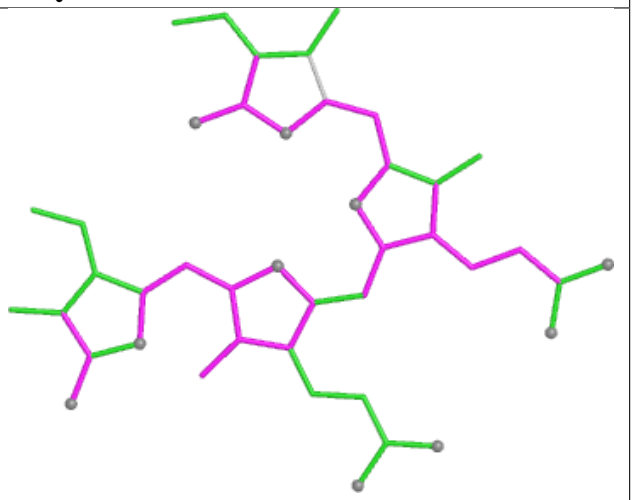


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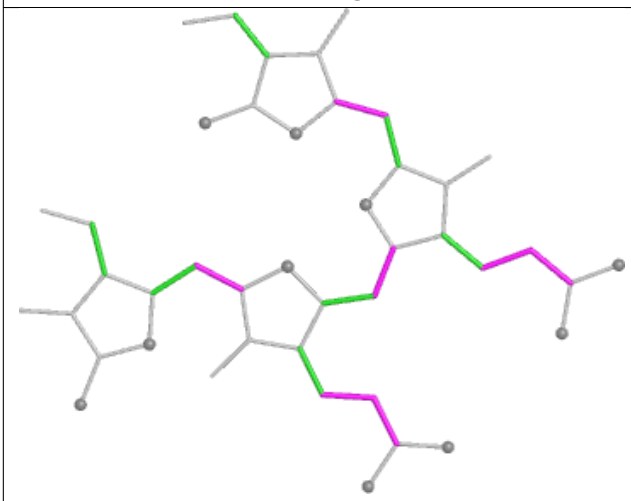
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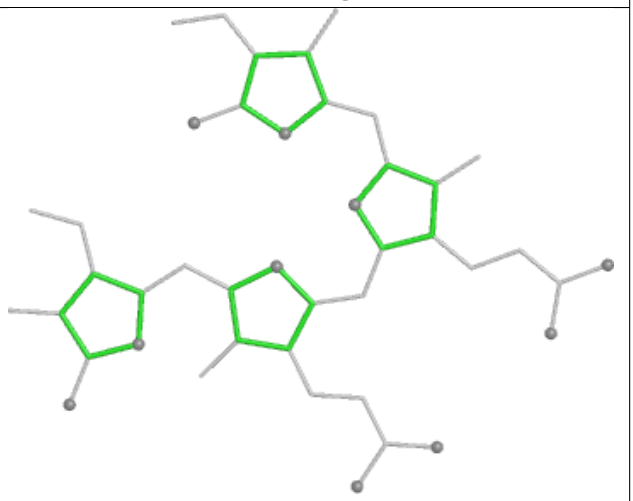
Bond lengths



Bond angles

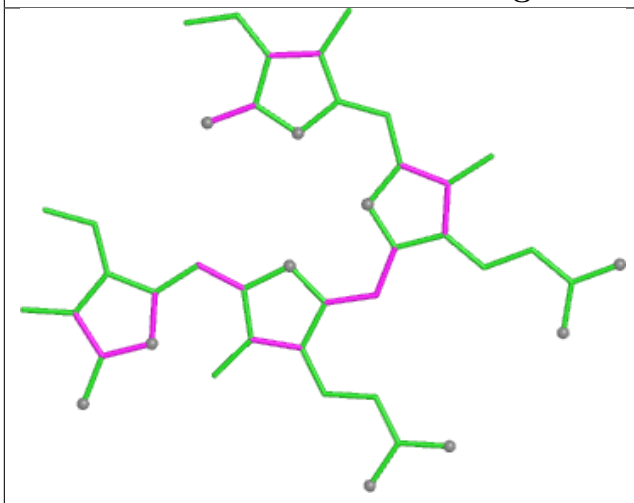


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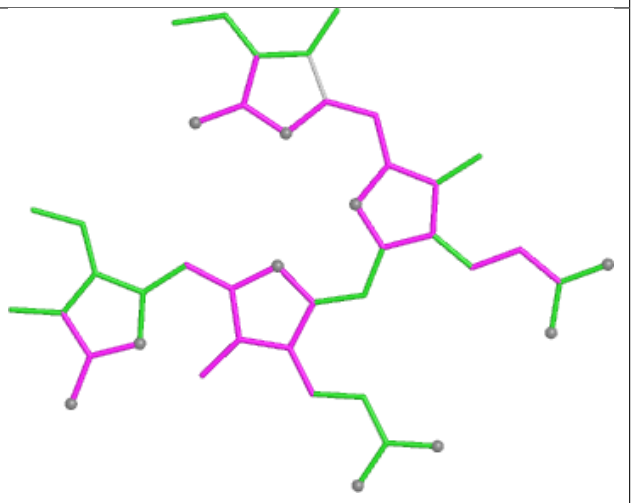


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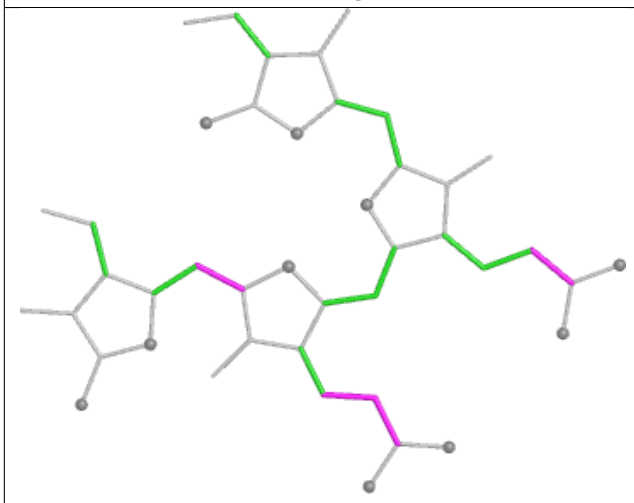
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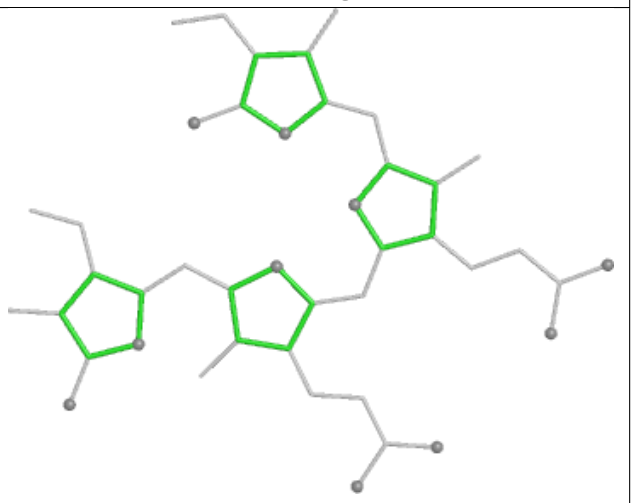
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Bond angles

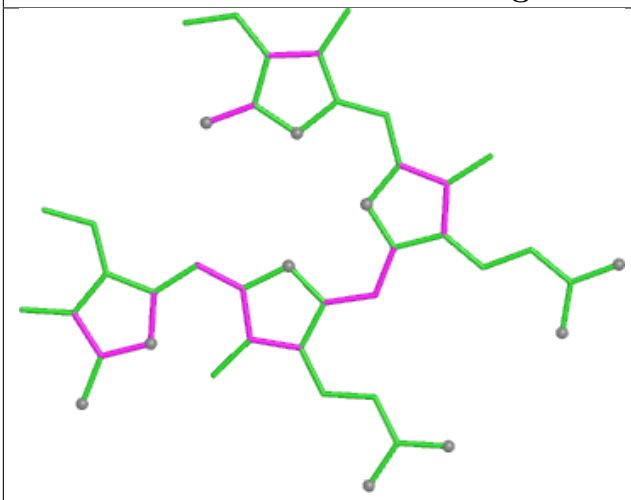


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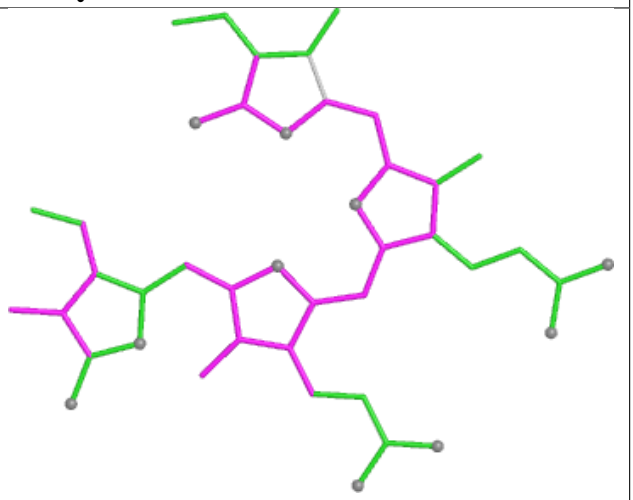


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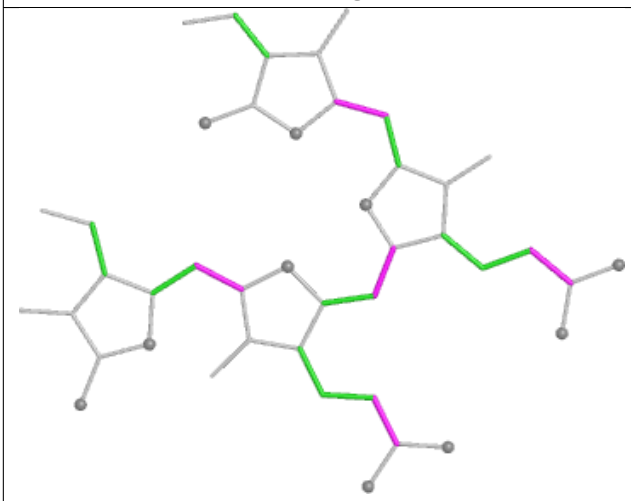
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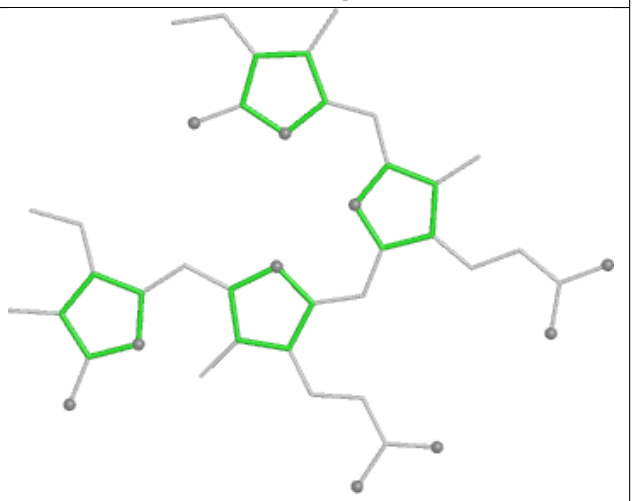
Bond lengths



Bond angles

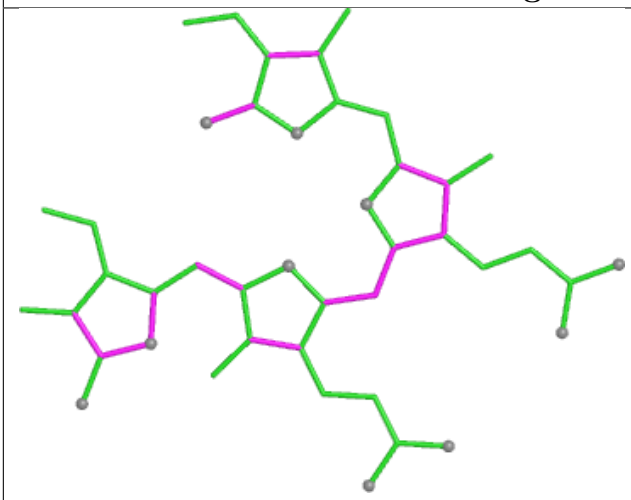


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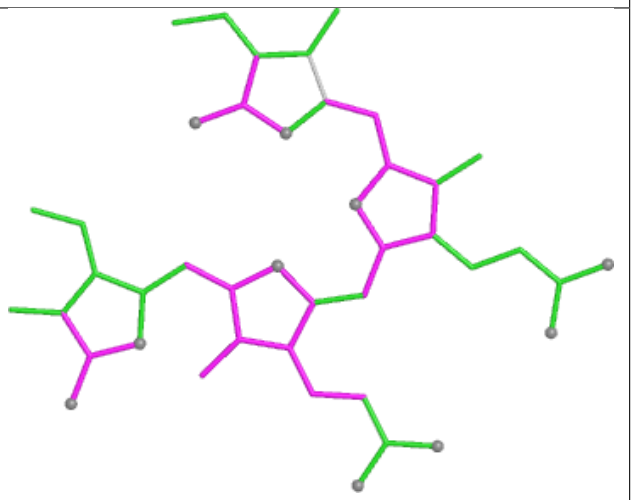


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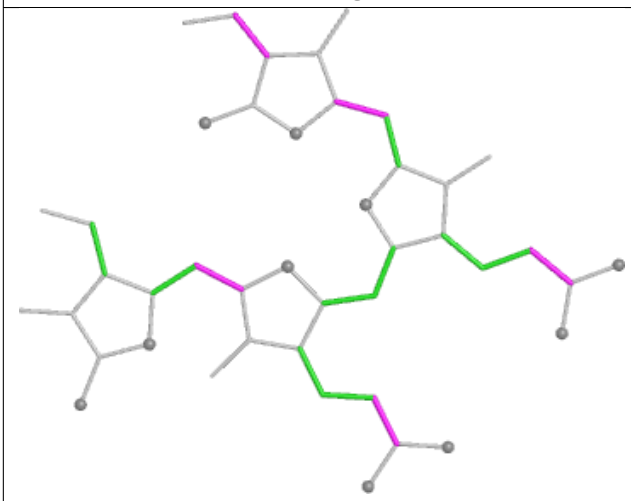
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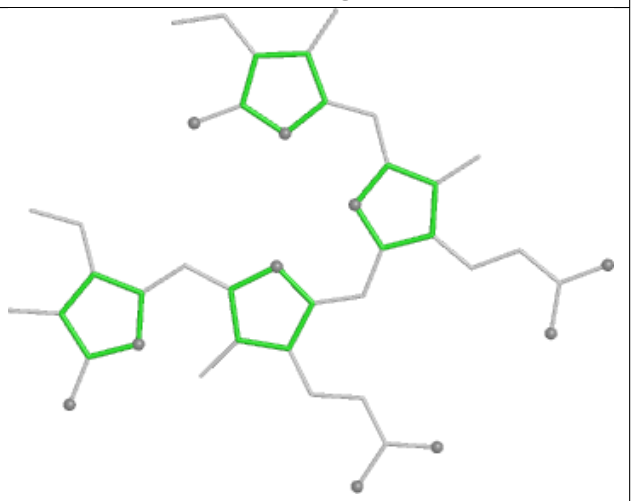
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Bond angles

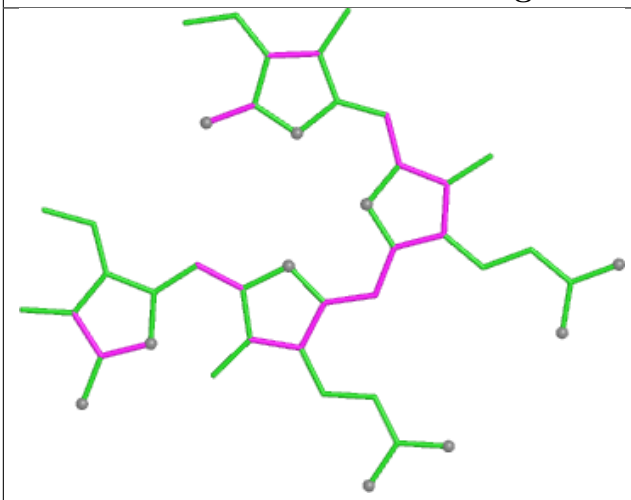


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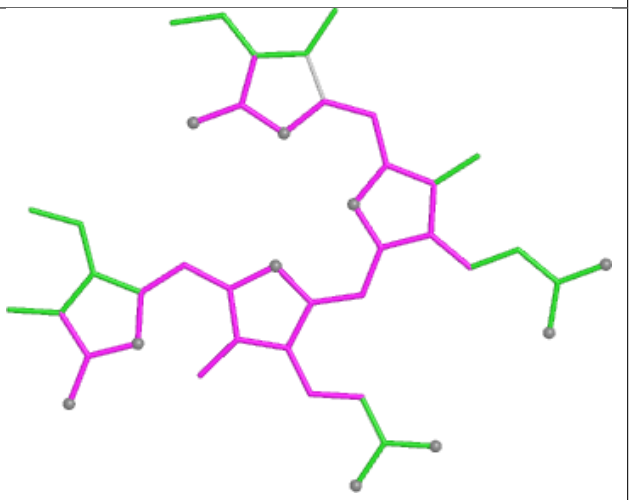


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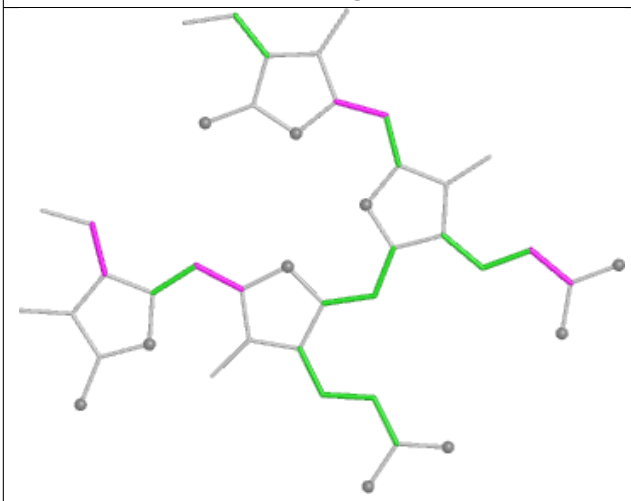
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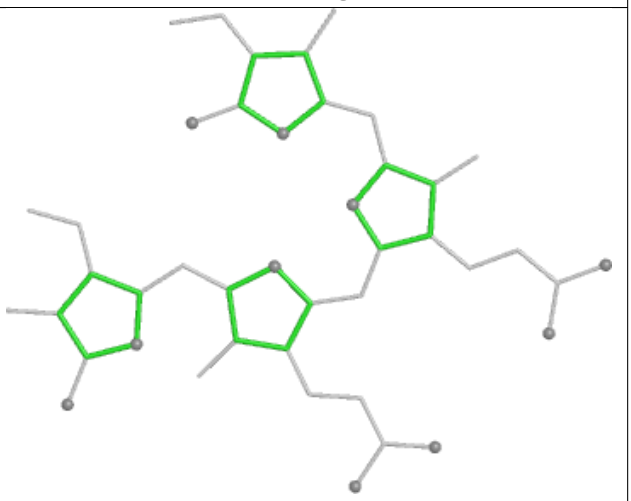
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Bond angles

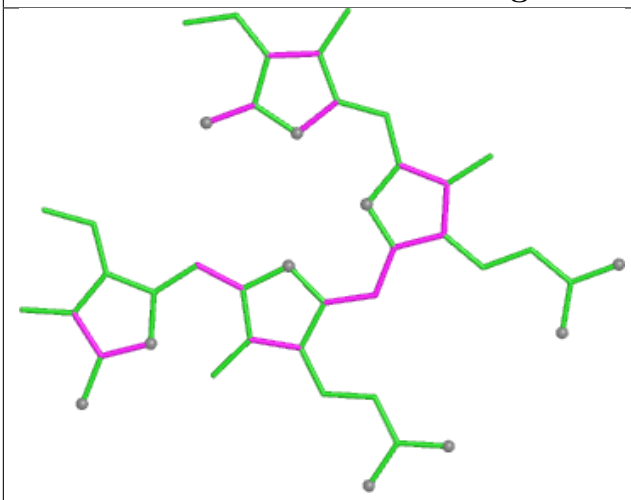


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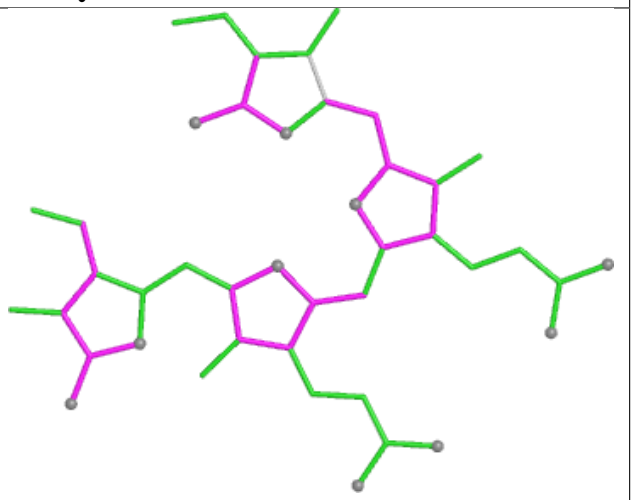


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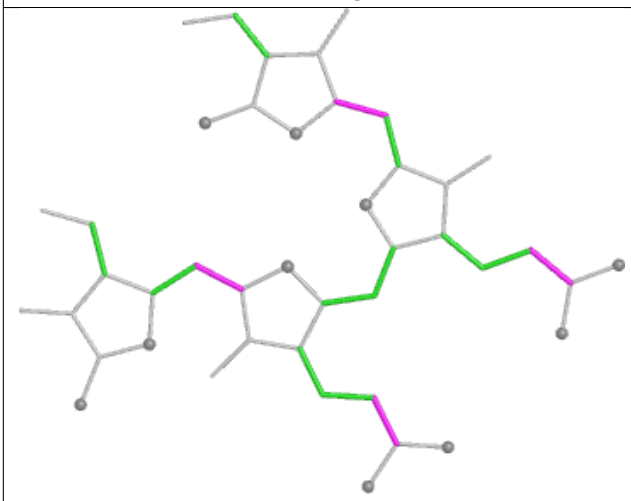
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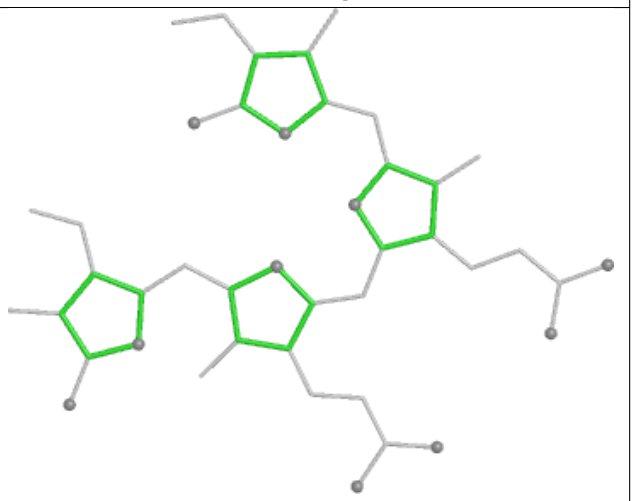
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Bond angles

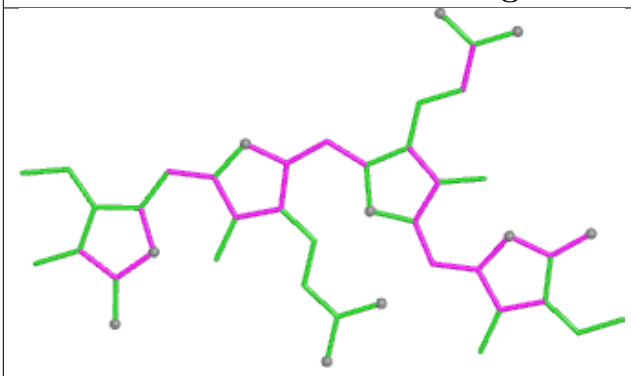


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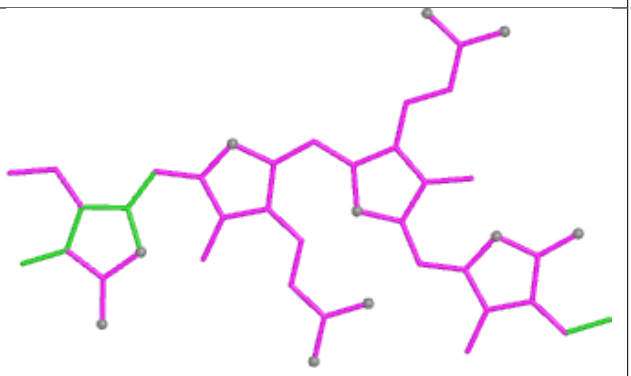


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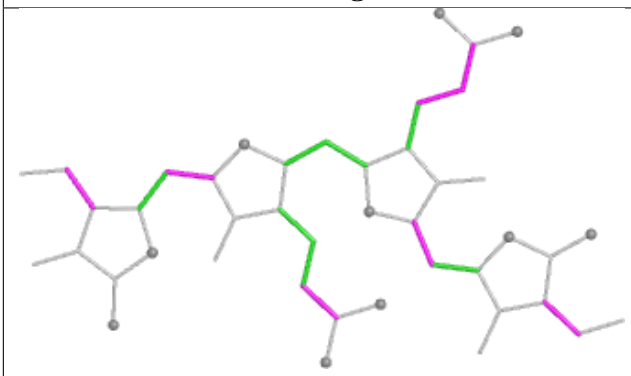
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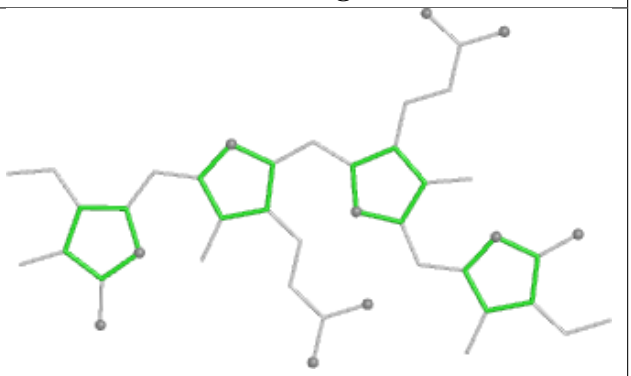
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Bond angles

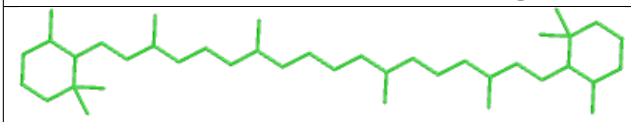


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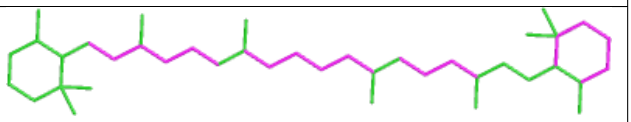


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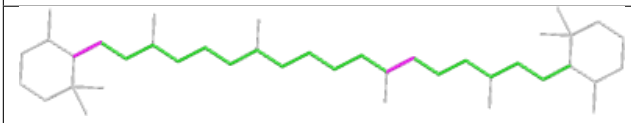
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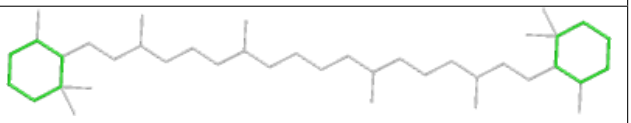
Bond lengths



Bond angles

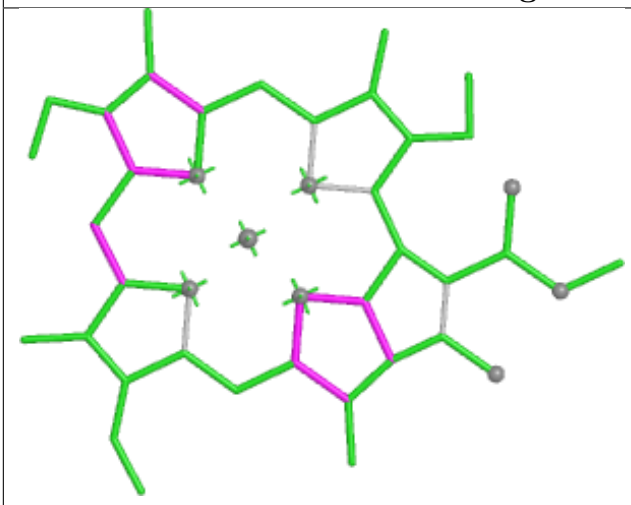


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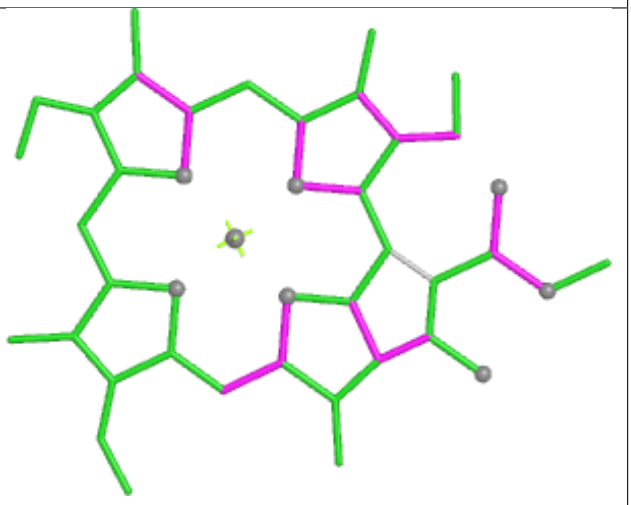


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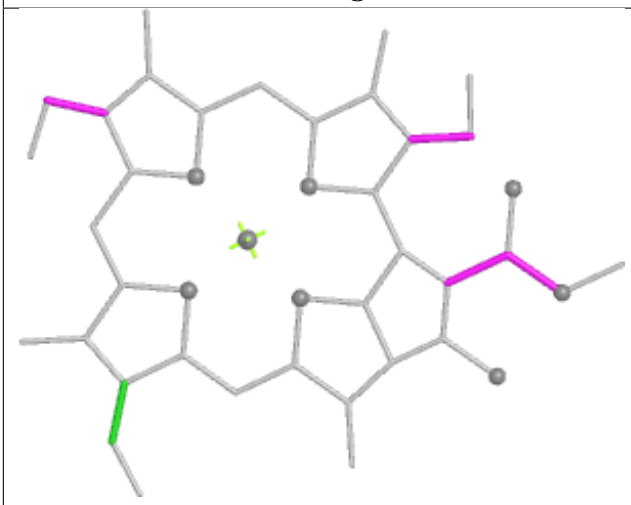
Ligand CLA 62 305



Bond lengths



Bond angles

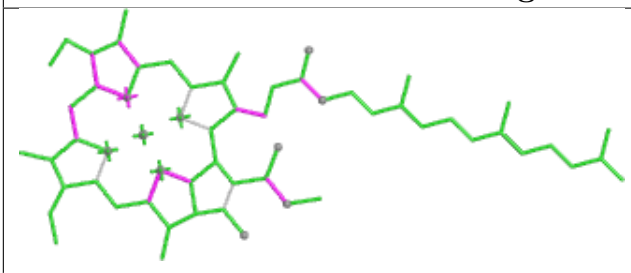


Torsions

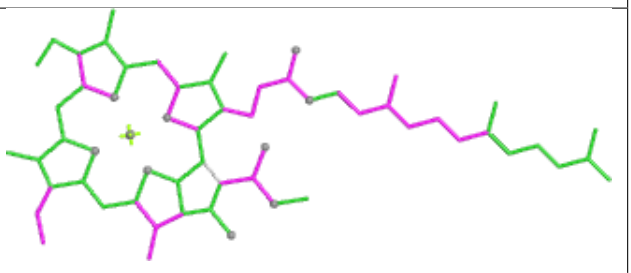


Rings

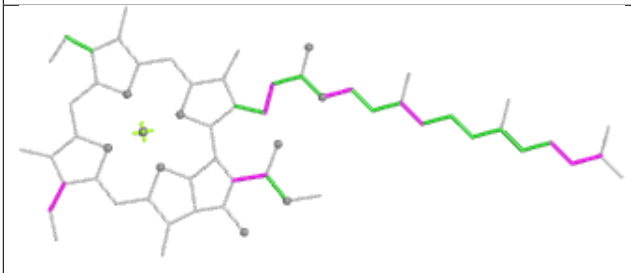
Ligand CLA aL 606



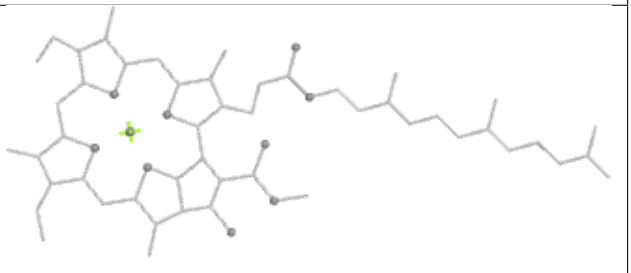
Bond lengths



Bond angles

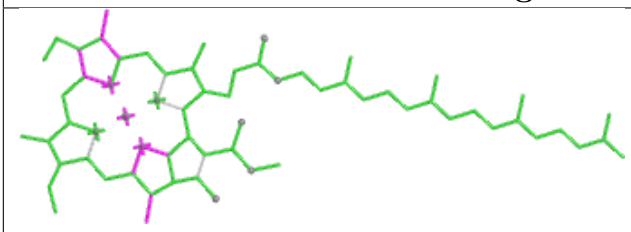


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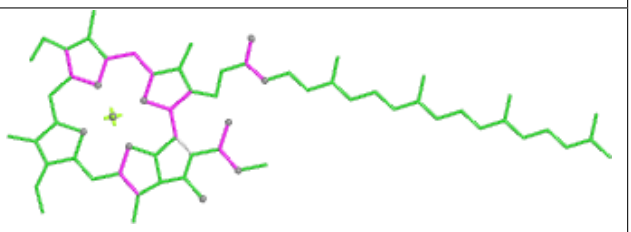


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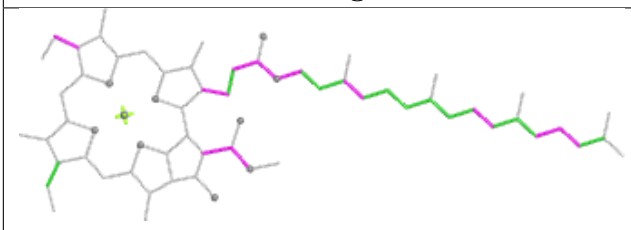
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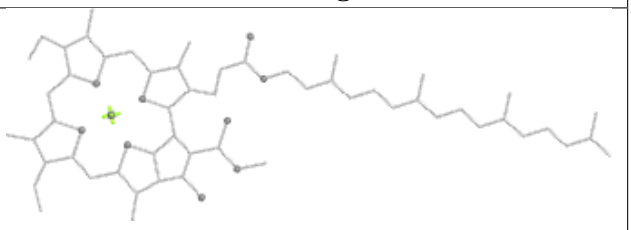
Bond lengths



Bond angles



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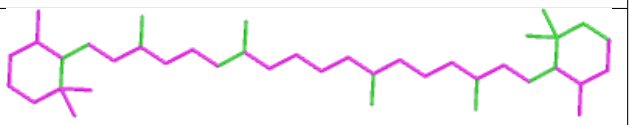


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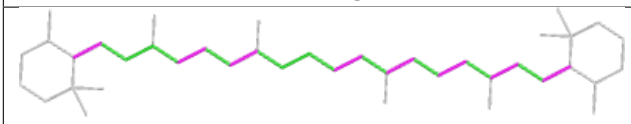
Ligand BCR J2 103



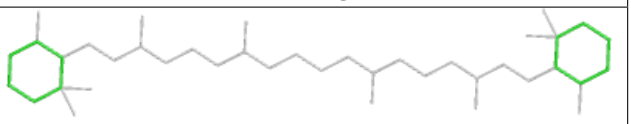
Bond lengths



Bond angles

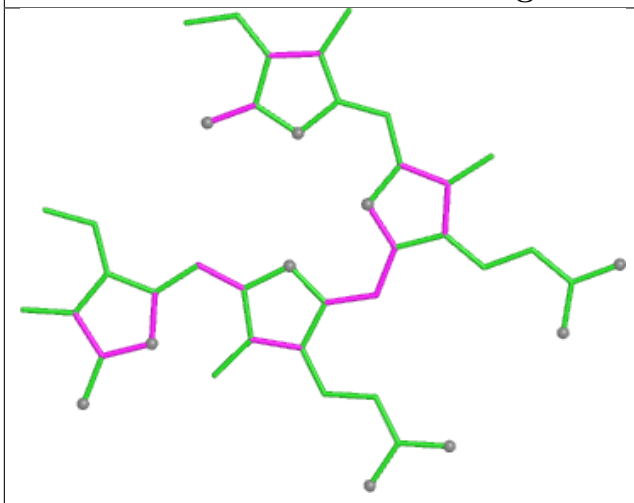


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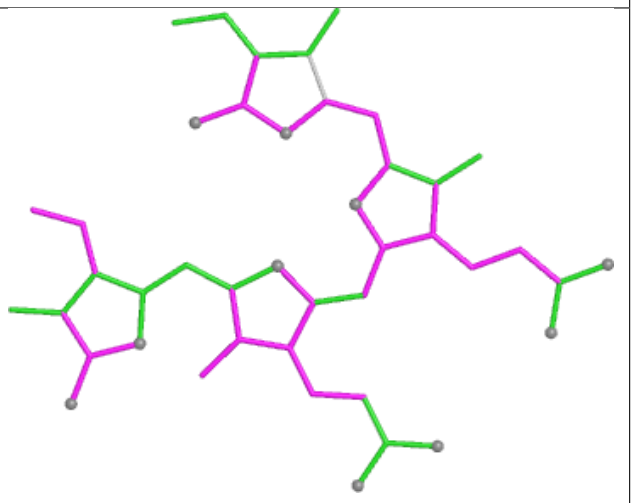


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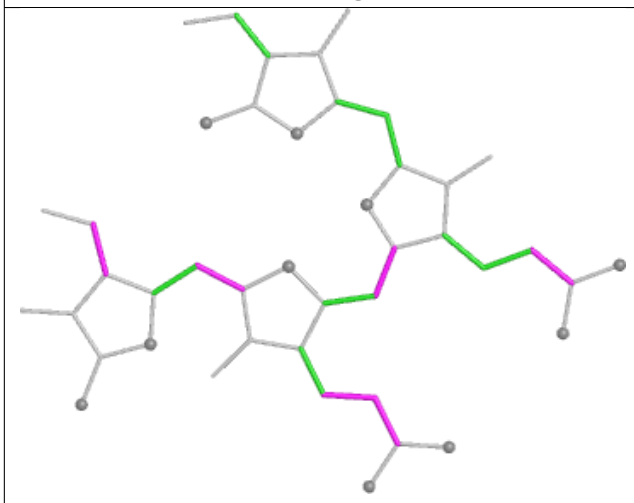
Ligand PEB O7 202



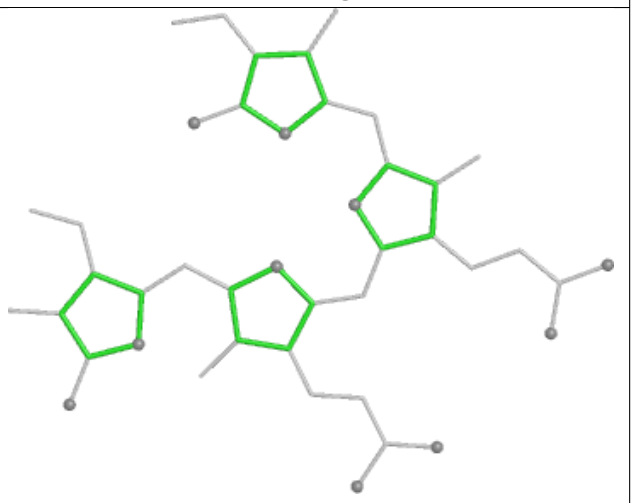
Bond lengths



Bond angles

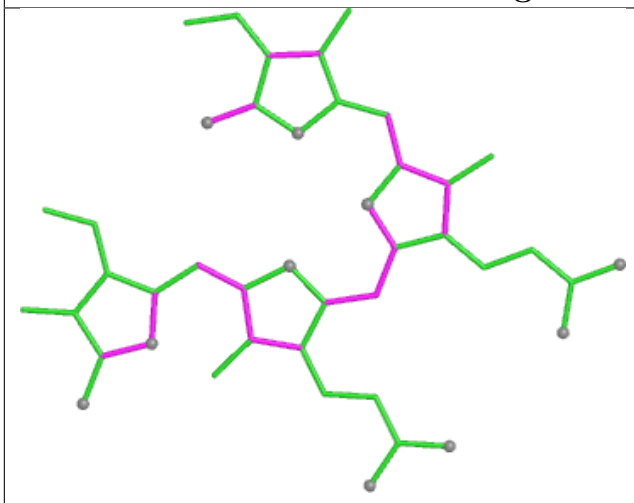


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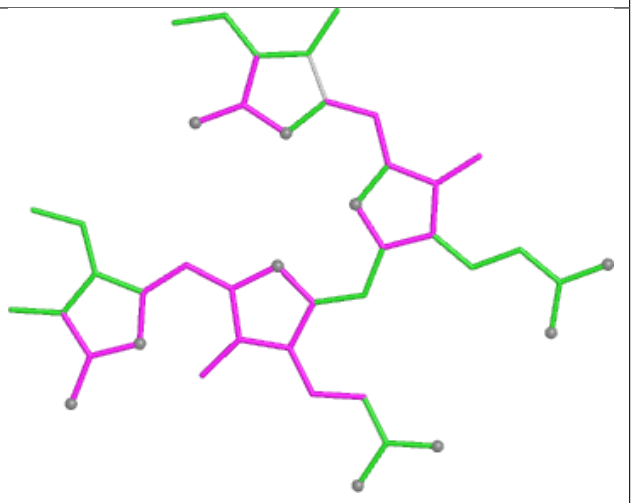


Rings

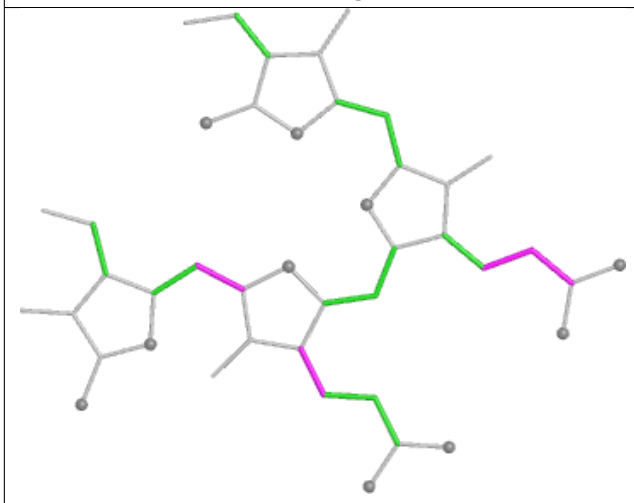
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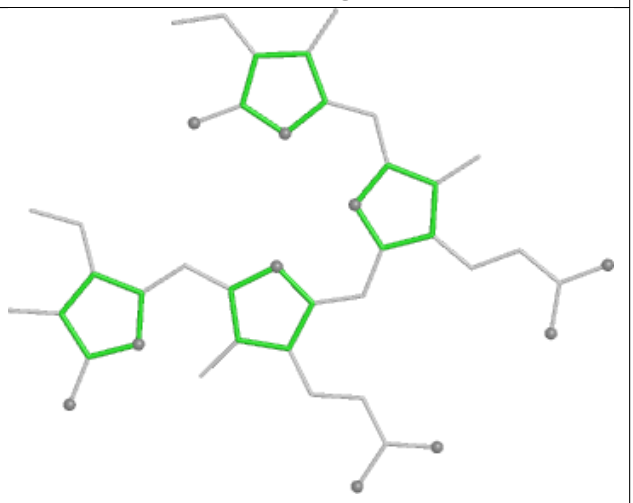
Bond lengths



Bond angles

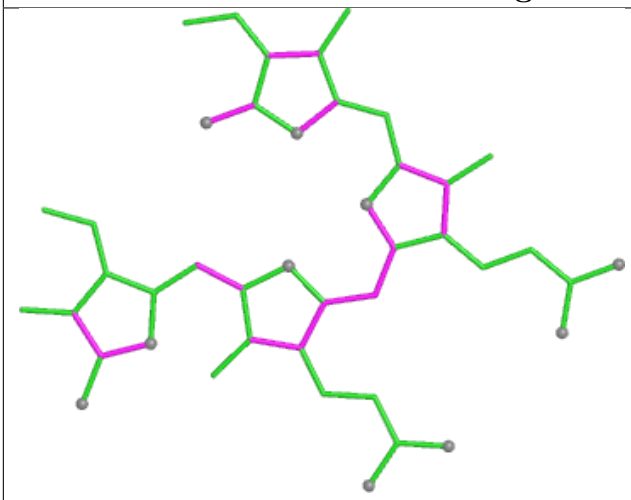


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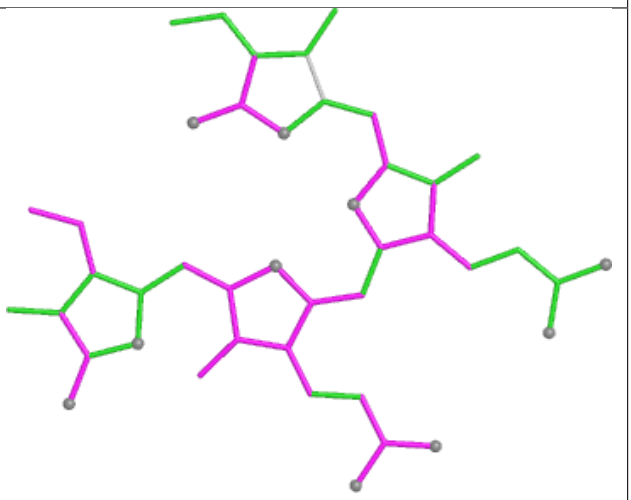


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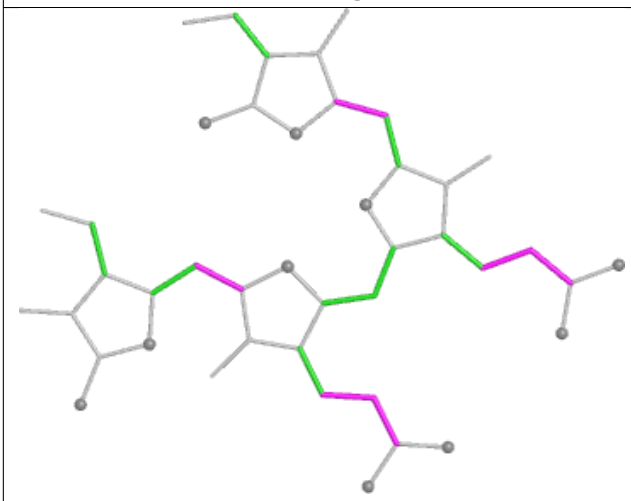
Ligand PEB D9 201



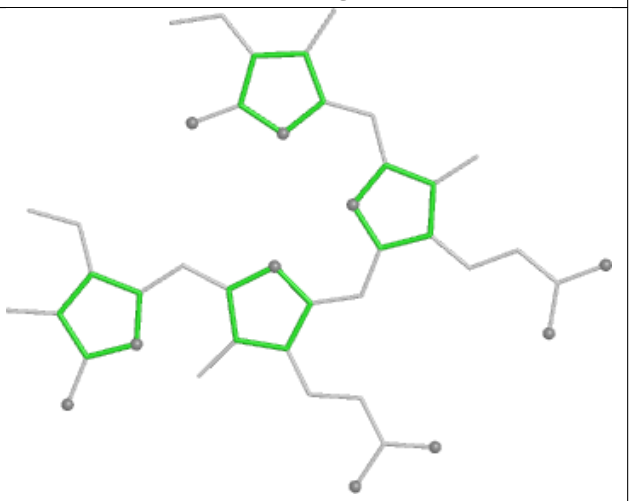
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Bond angles

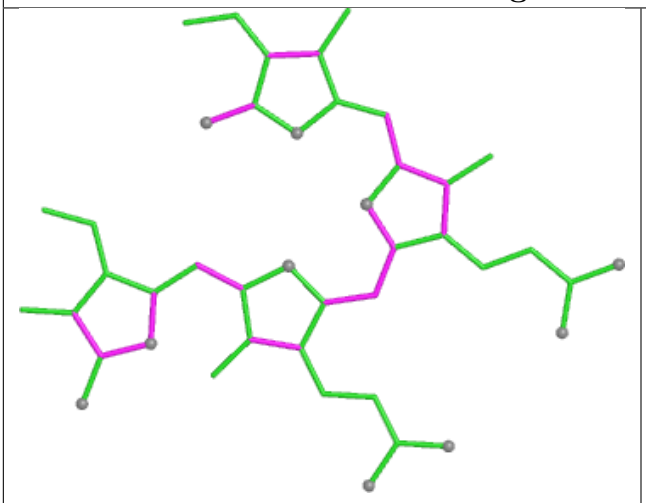


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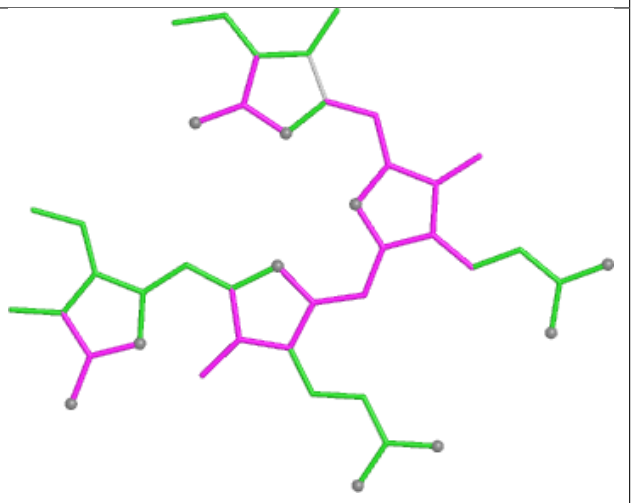


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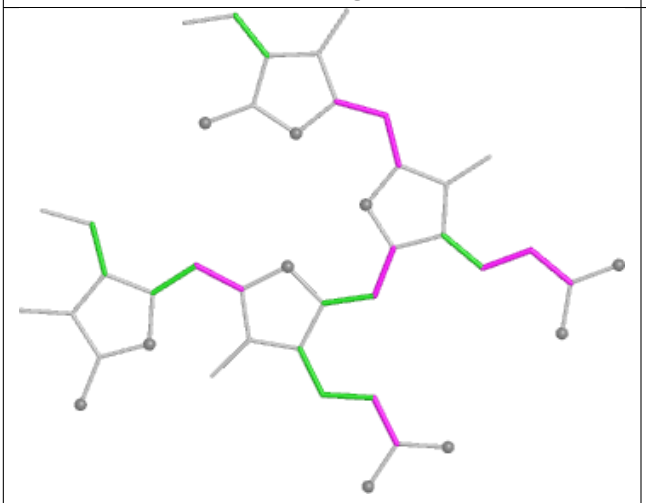
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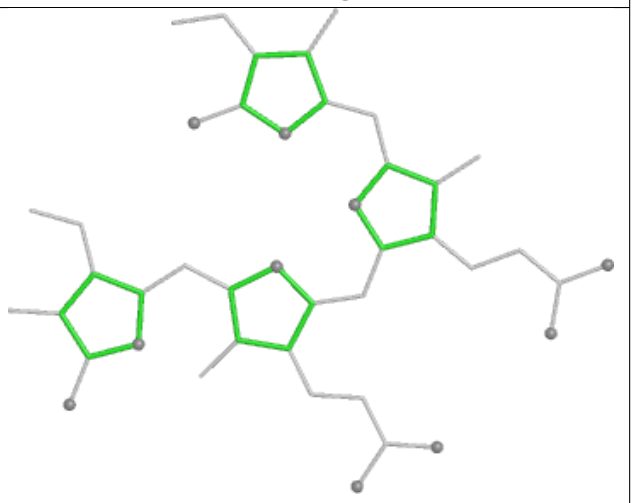
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Bond angles

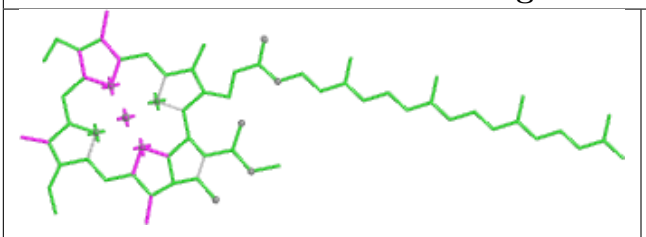


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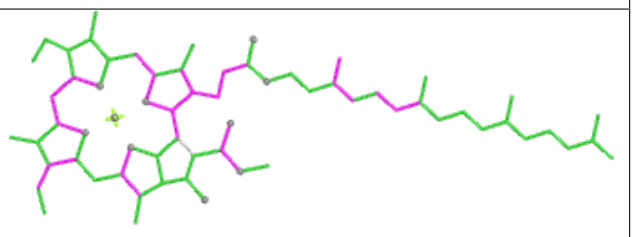


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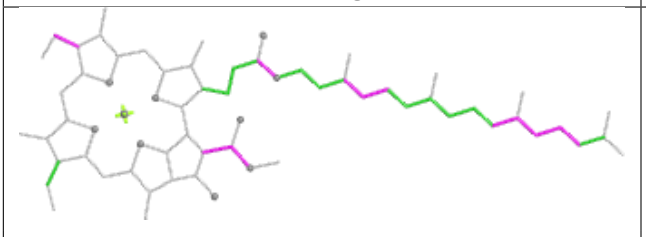
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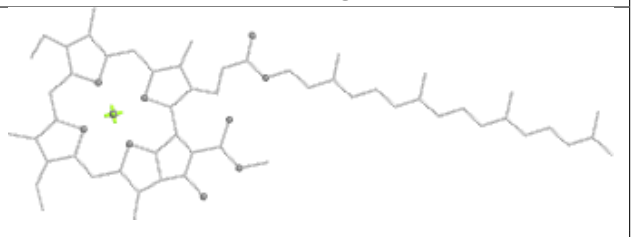
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Bond angles

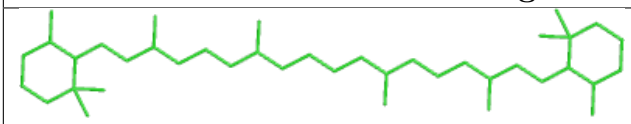


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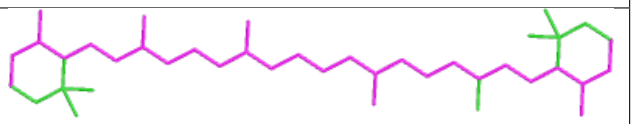


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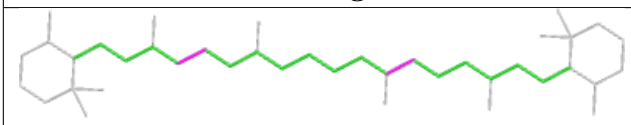
Ligand BCR c6 602



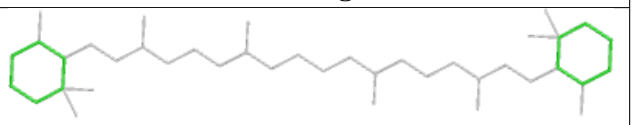
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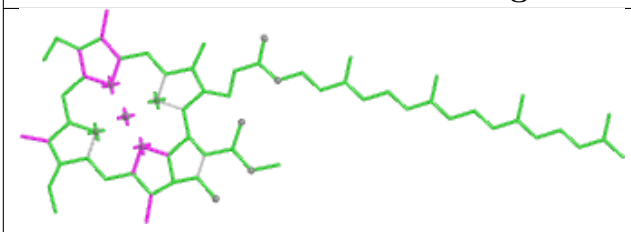


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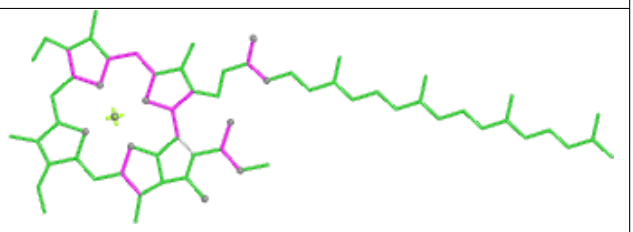


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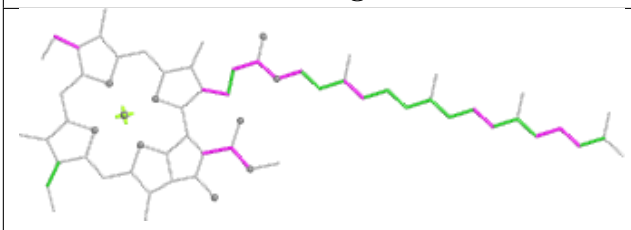
Ligand CLA BN 826



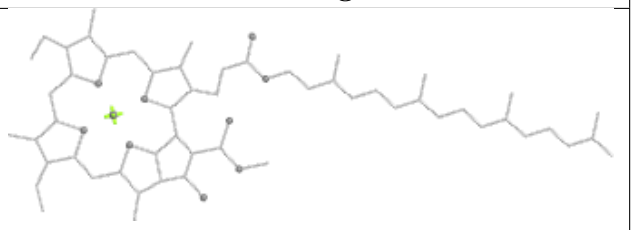
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Bond angles

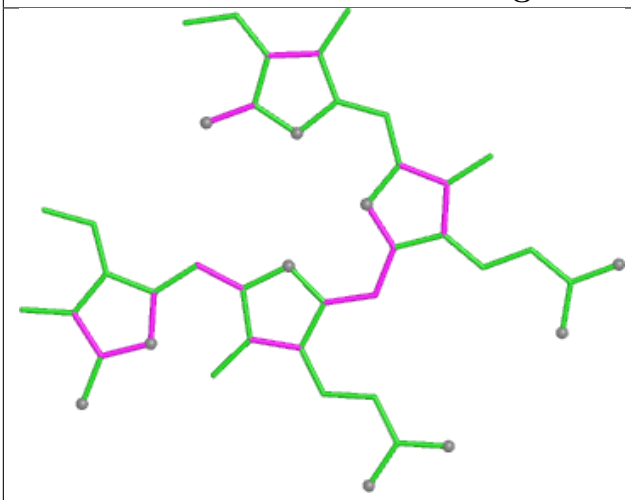


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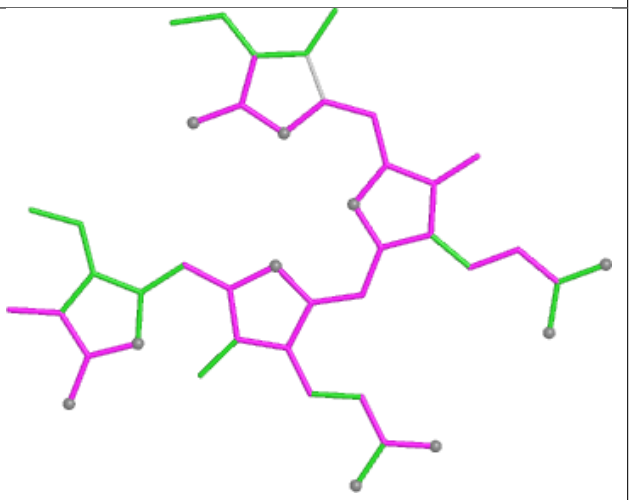


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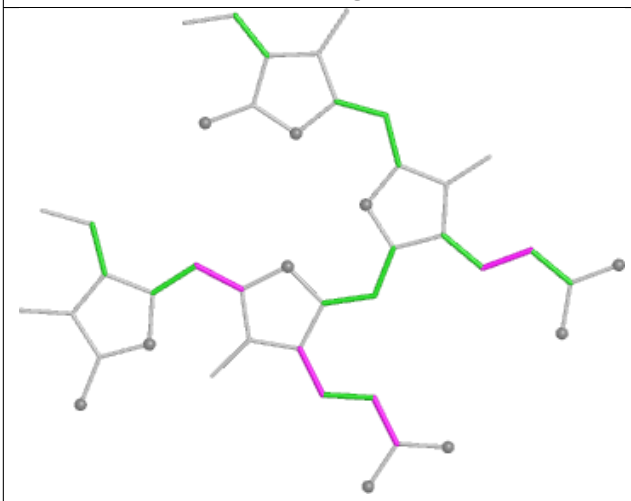
Ligand PEB TA 203



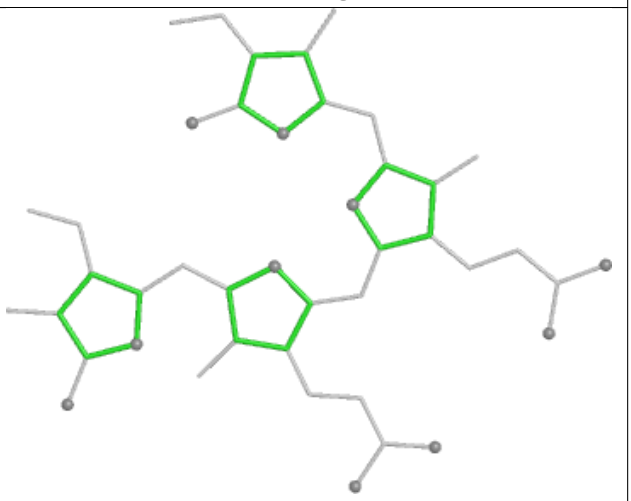
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Bond angles

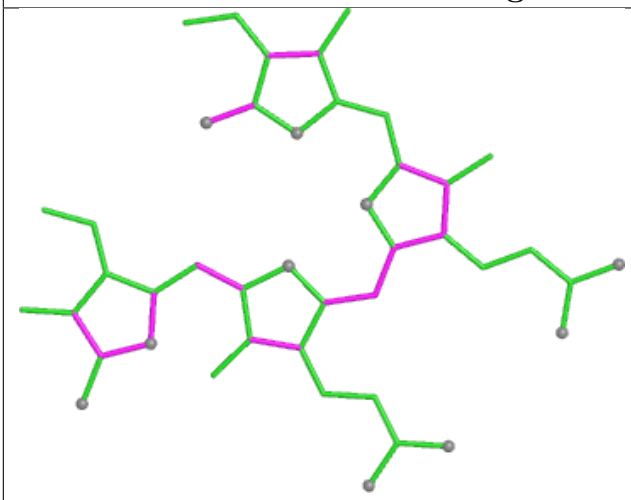


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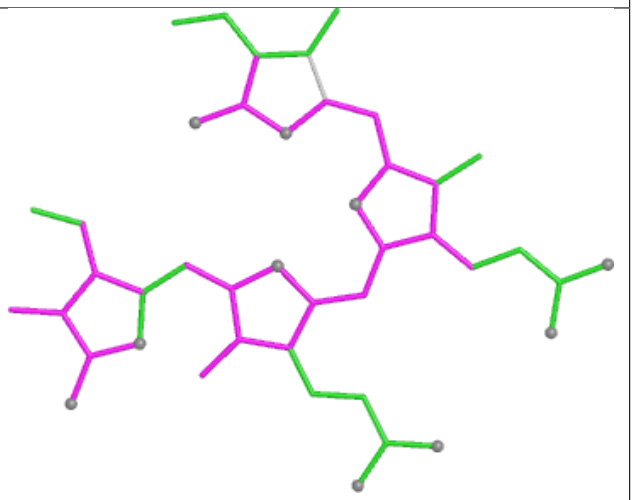


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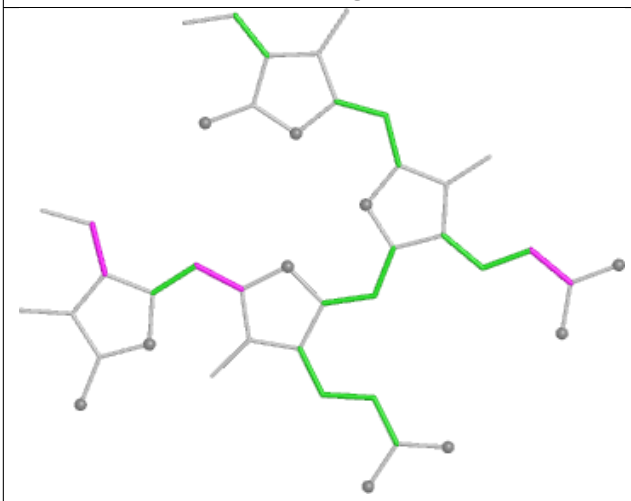
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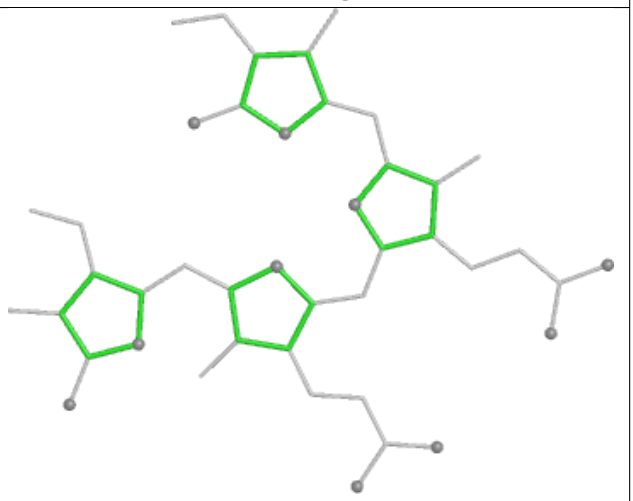
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Bond angles

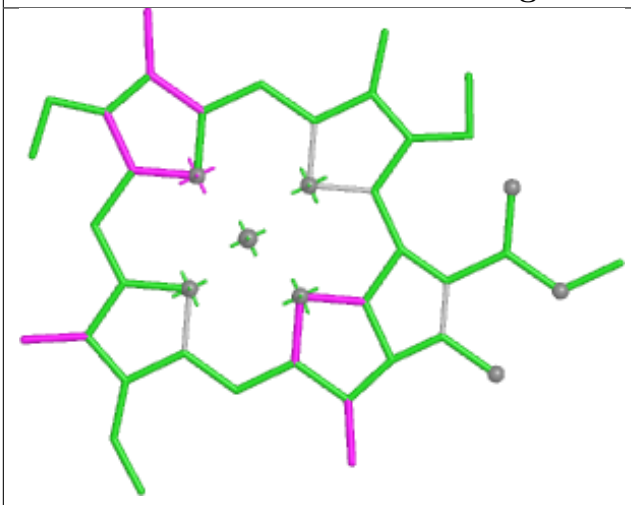


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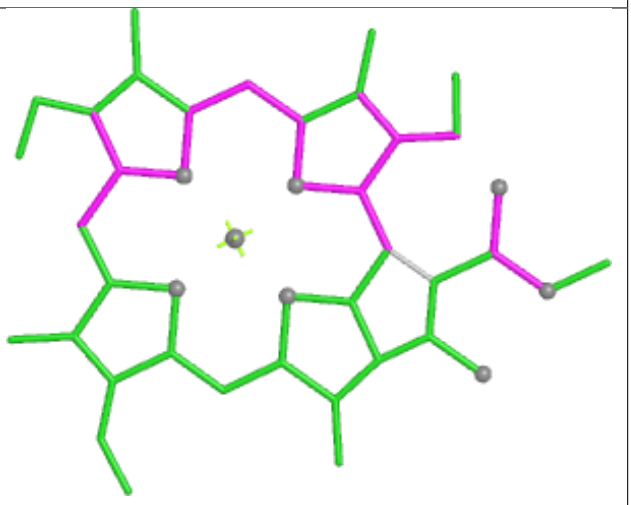


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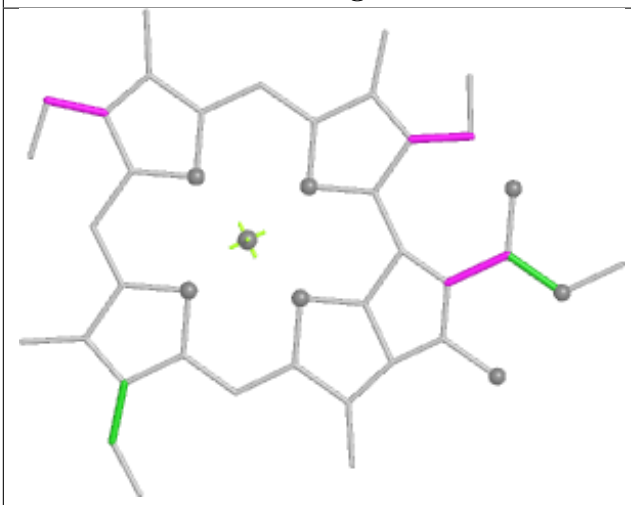
Ligand CLA 32 306



Bond lengths



Bond angles

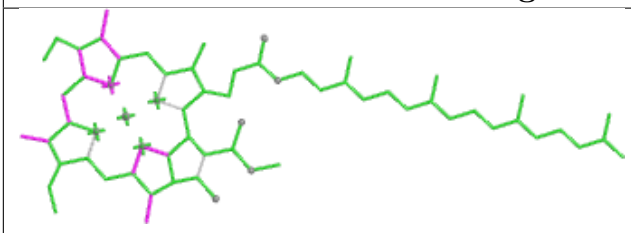


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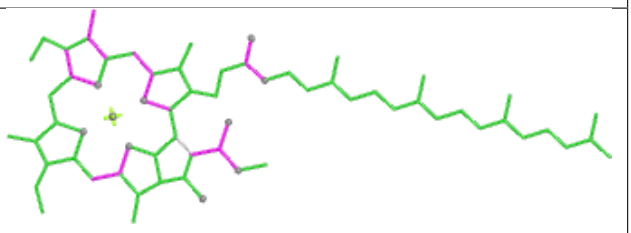


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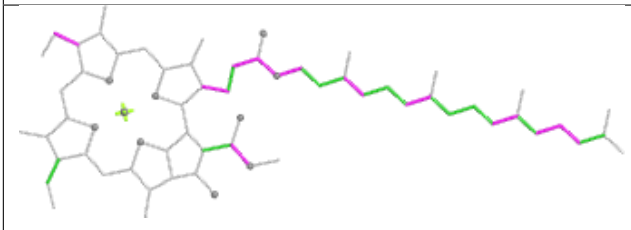
Ligand CLA d6 403



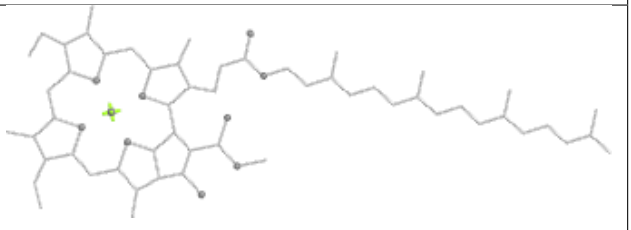
Bond lengths



Bond angles

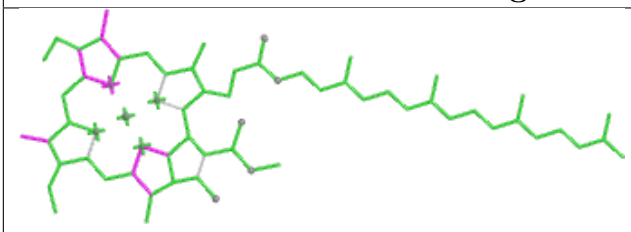


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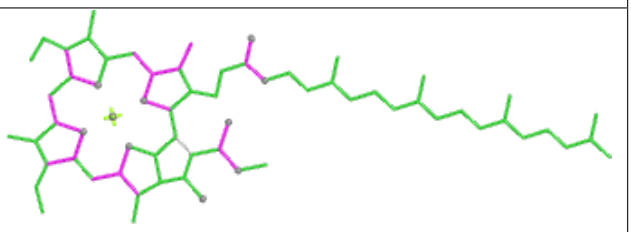


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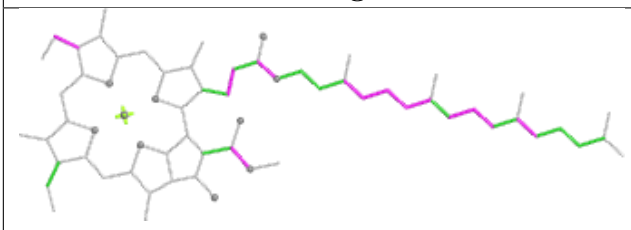
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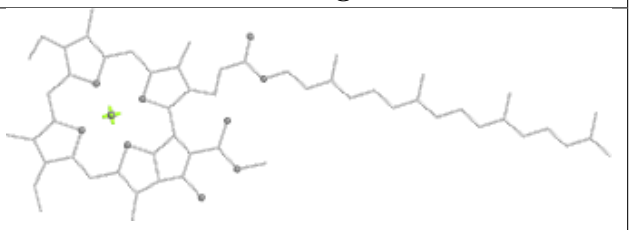
Bond lengths



Bond angles

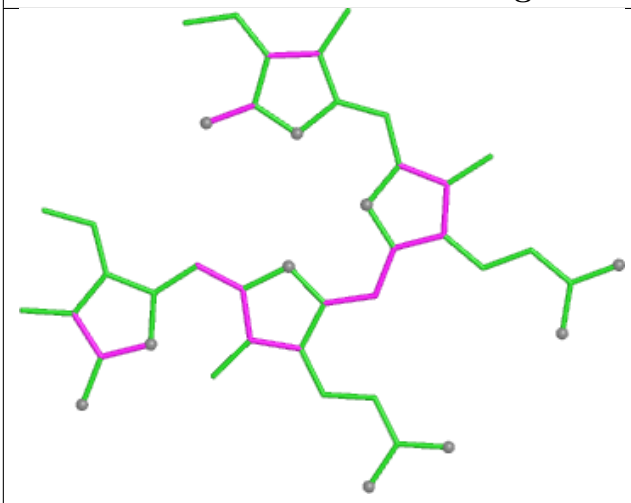


Torsions

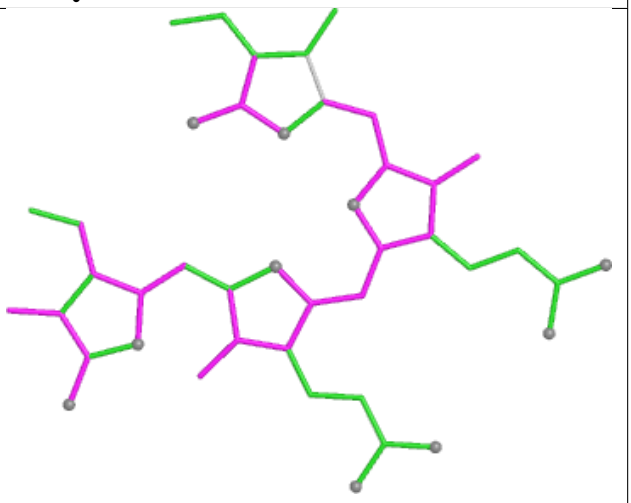


Rings

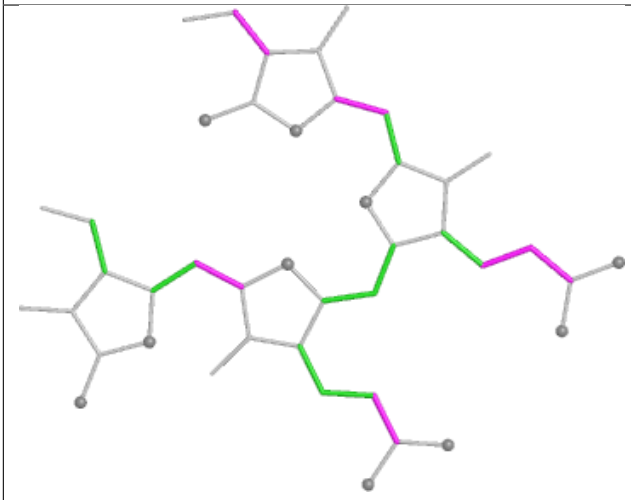
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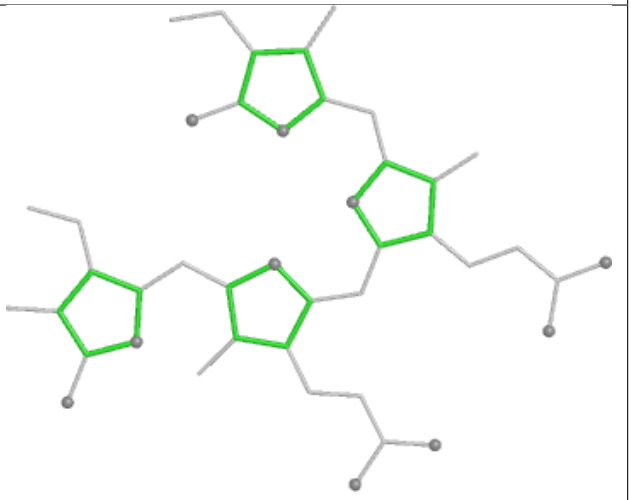
Bond lengths



Bond angles

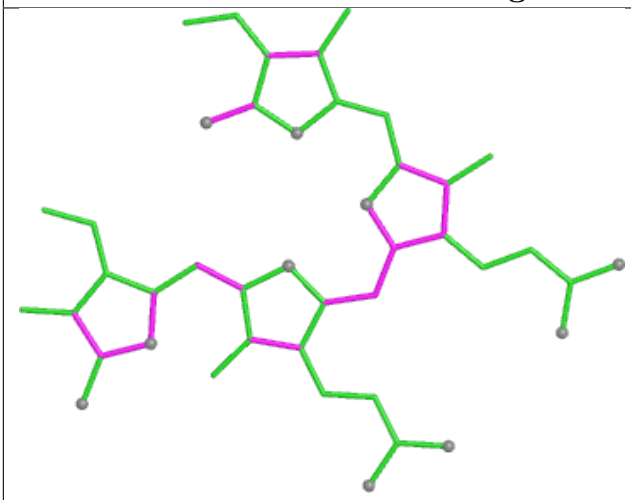


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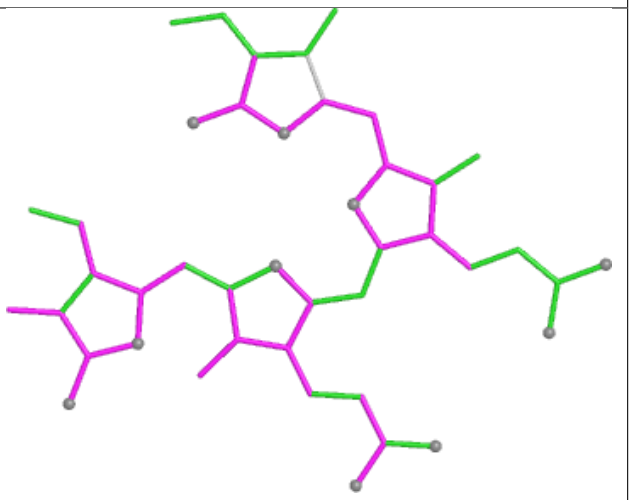


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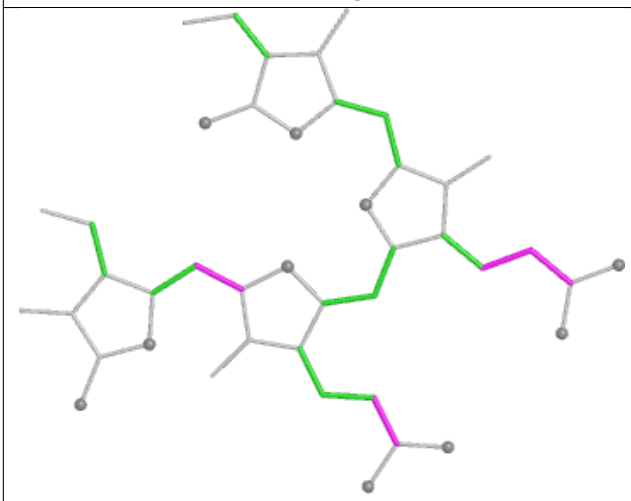
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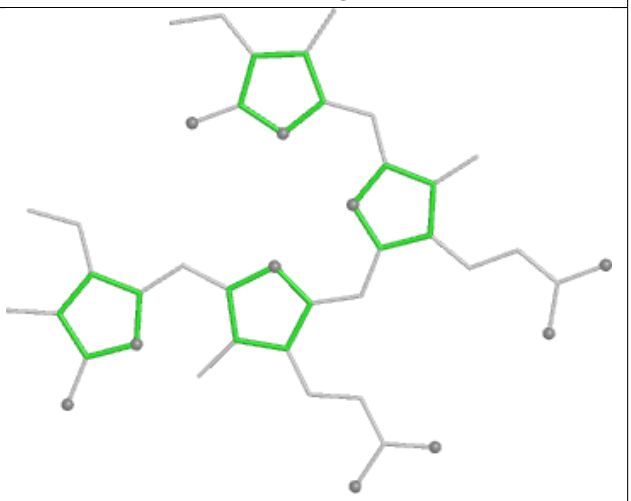
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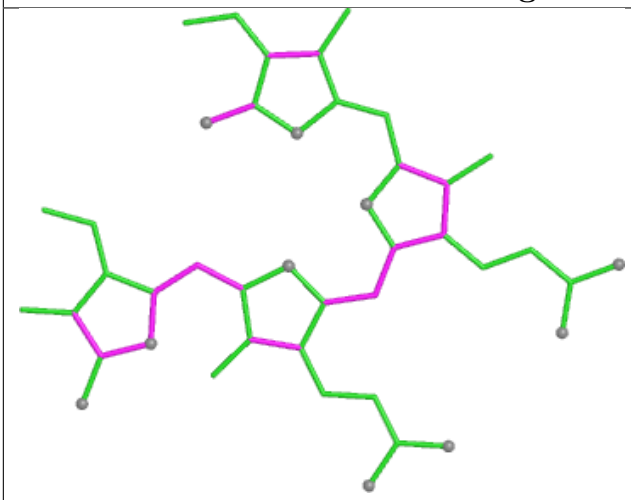


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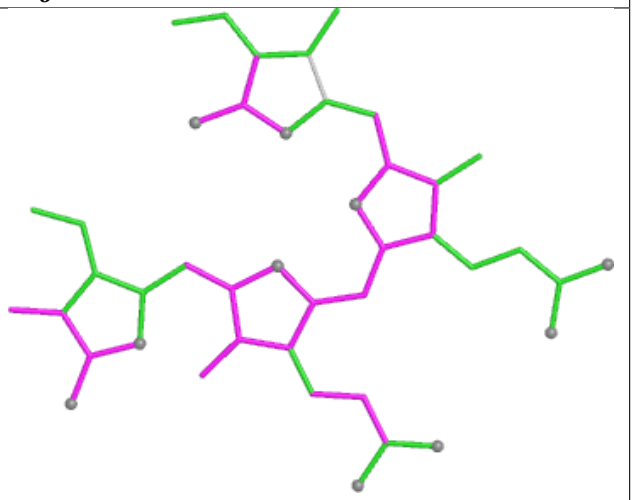


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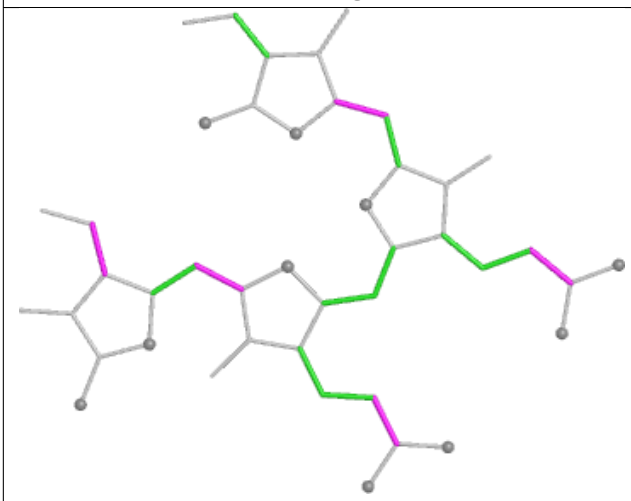
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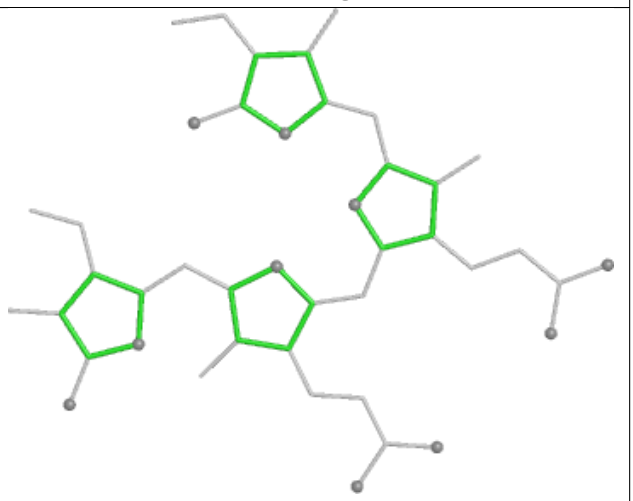
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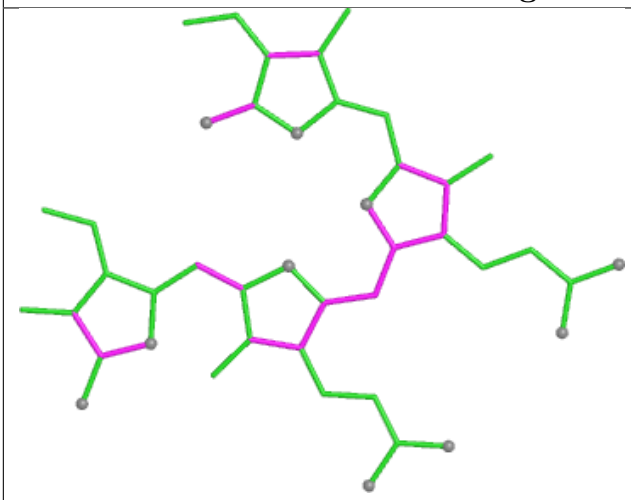


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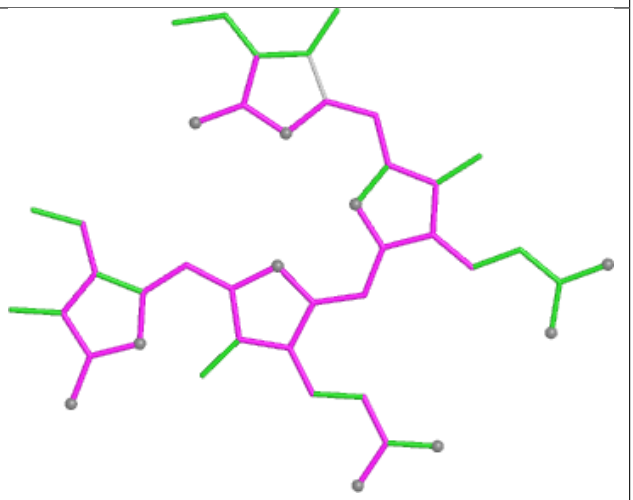


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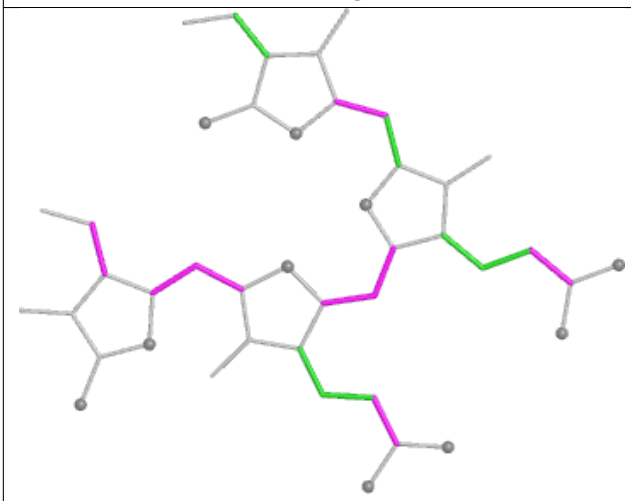
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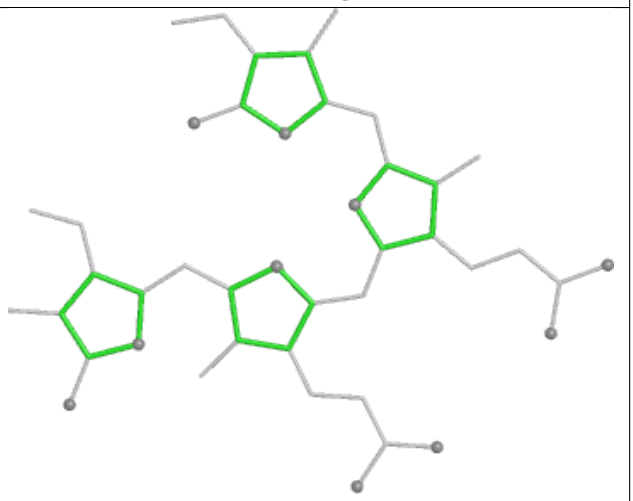
Bond lengths



Bond angles

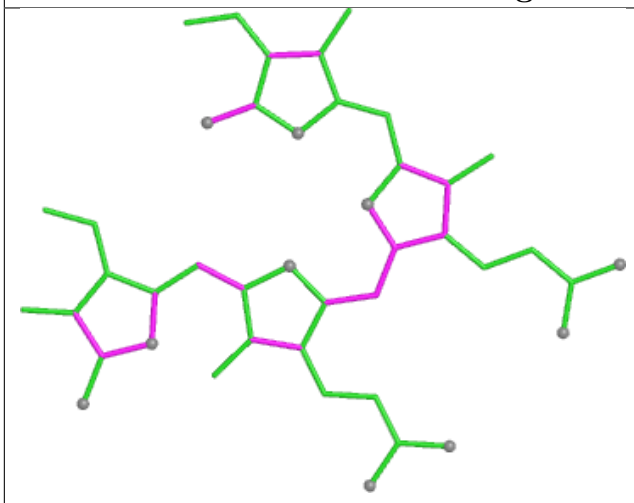


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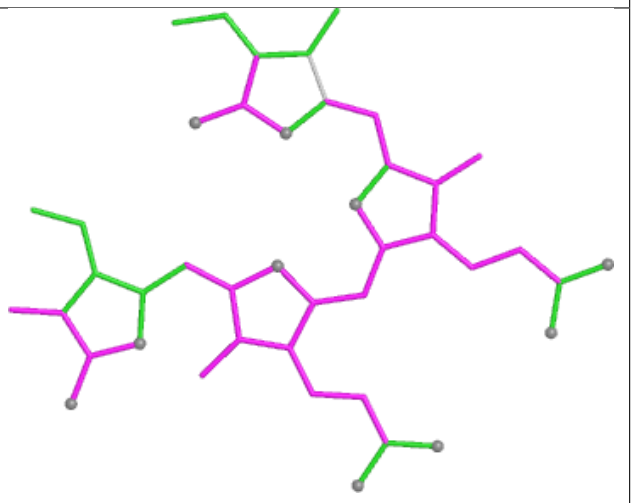


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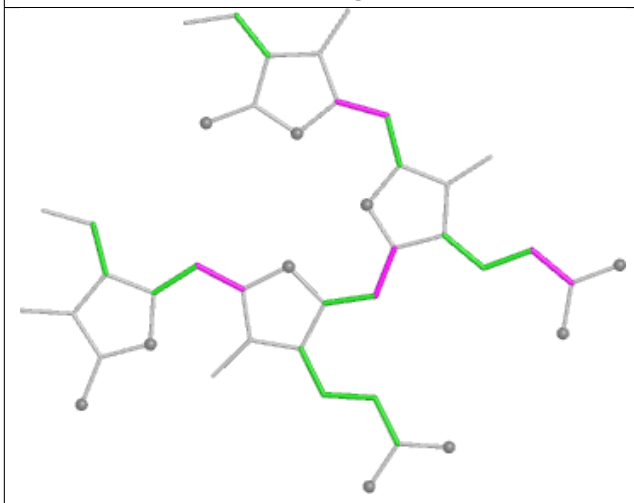
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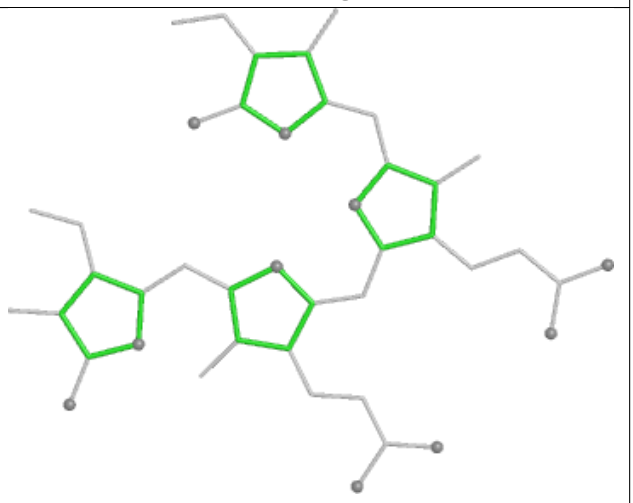
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Bond angles



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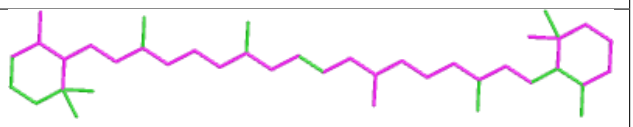


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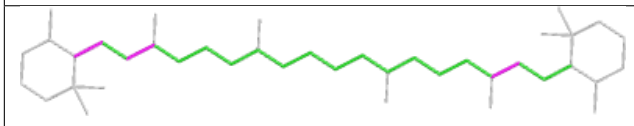
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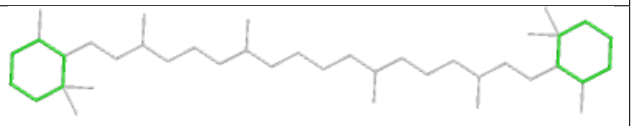
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Bond angles

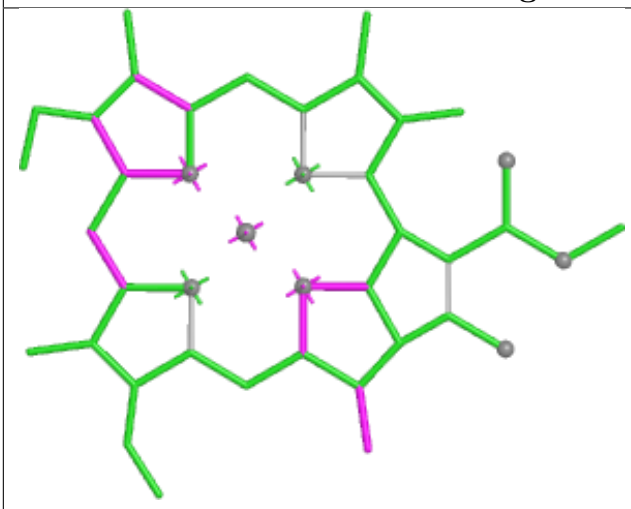


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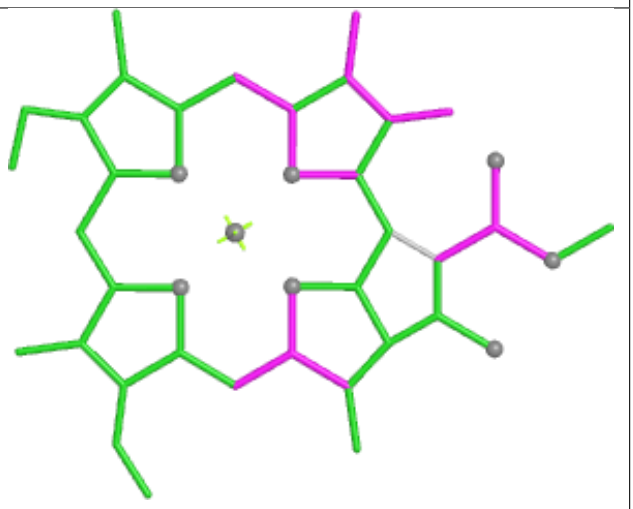


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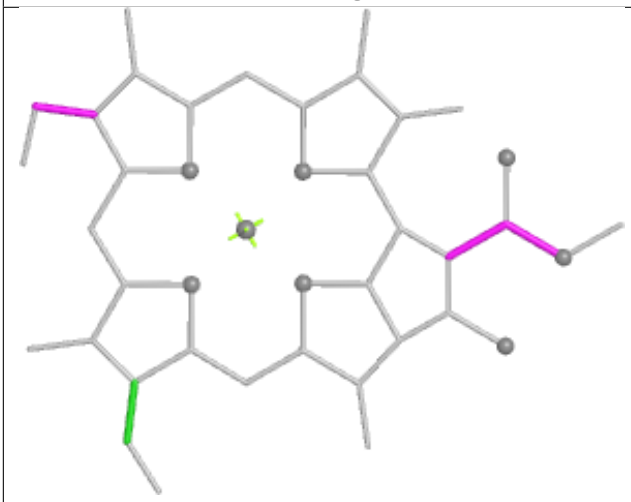
Ligand CLA 52 608



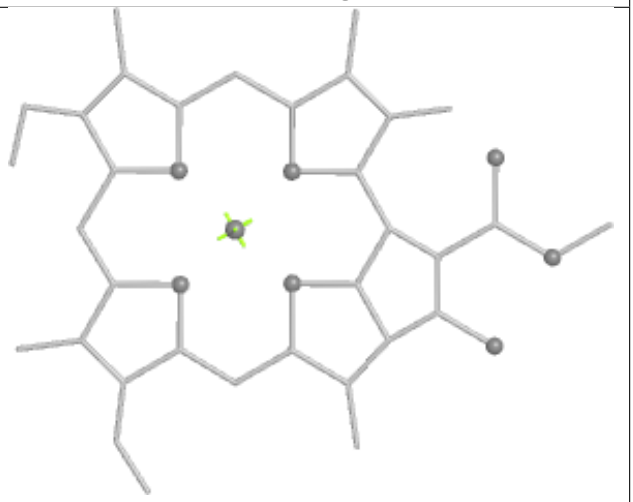
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Bond angles

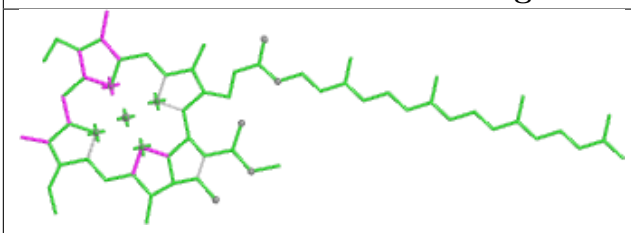


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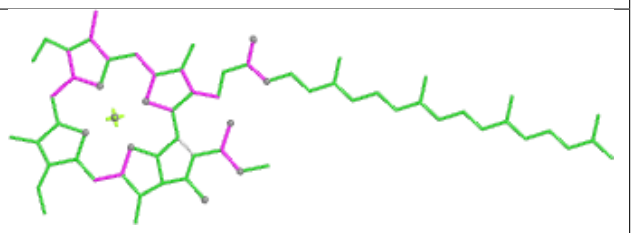


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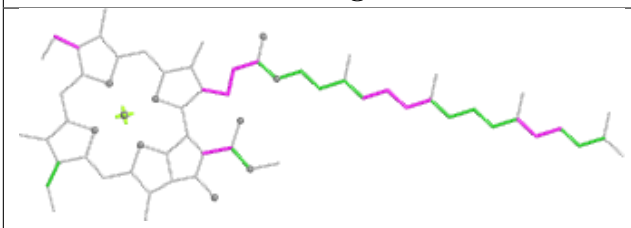
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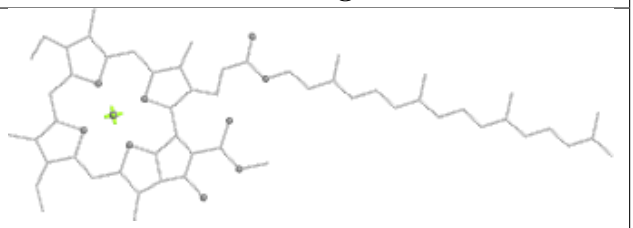
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Bond angles

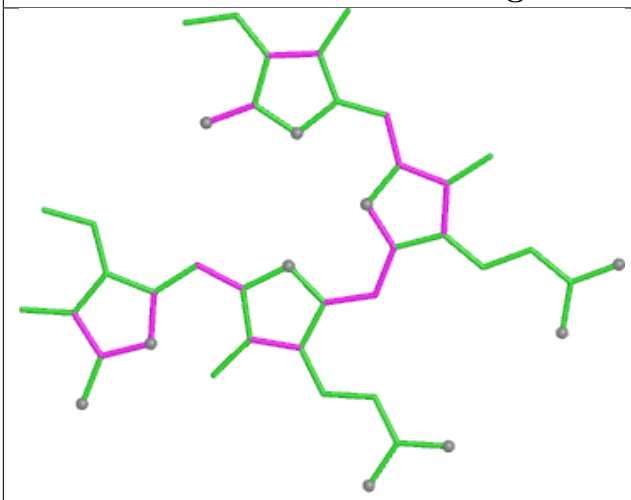


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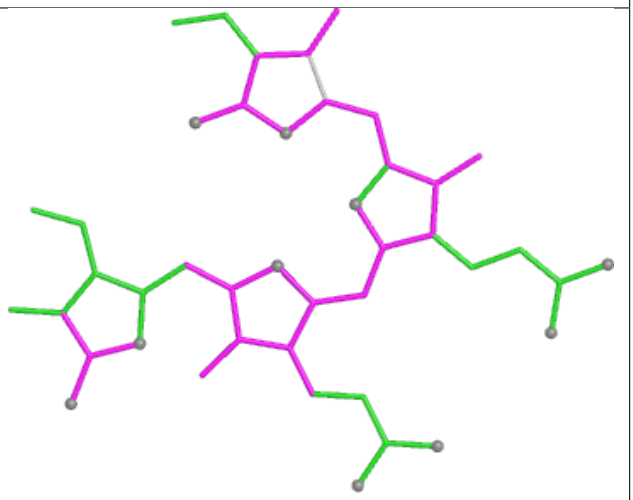


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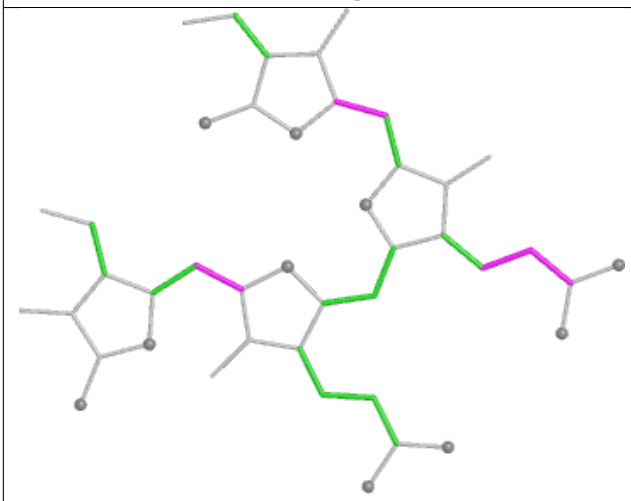
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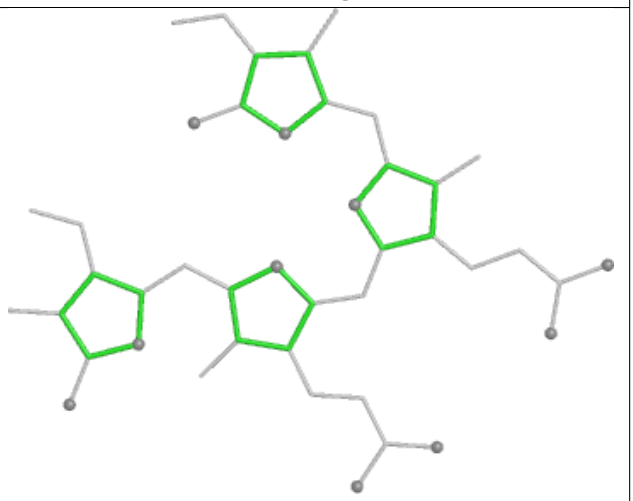
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Bond angles

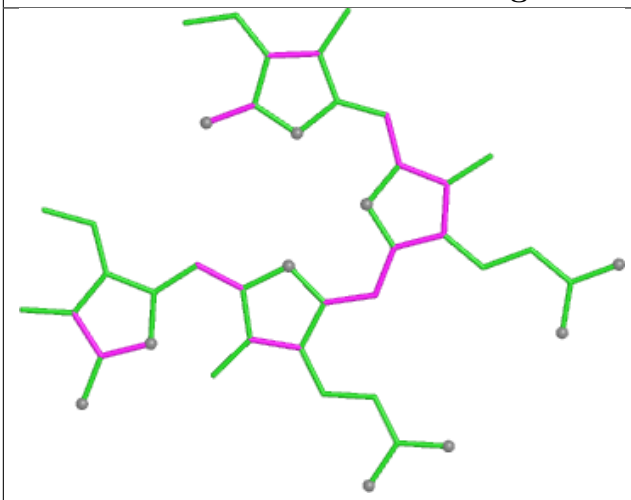


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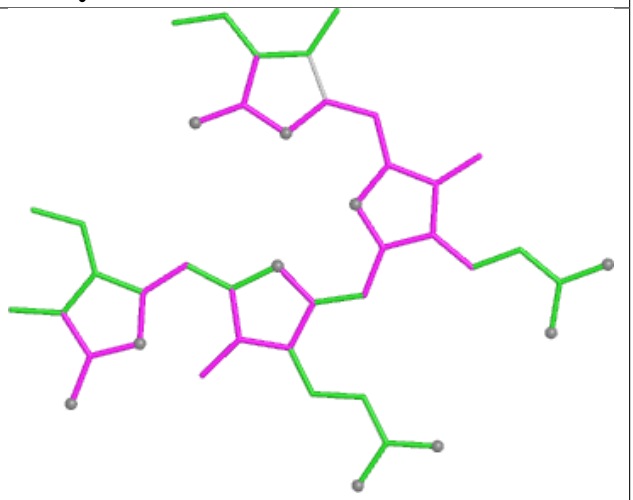


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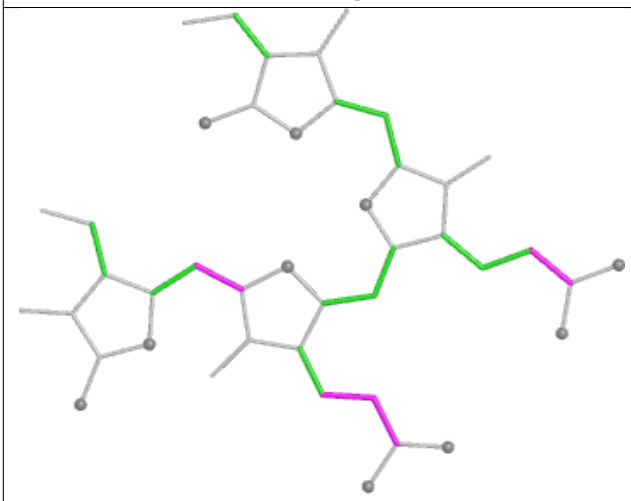
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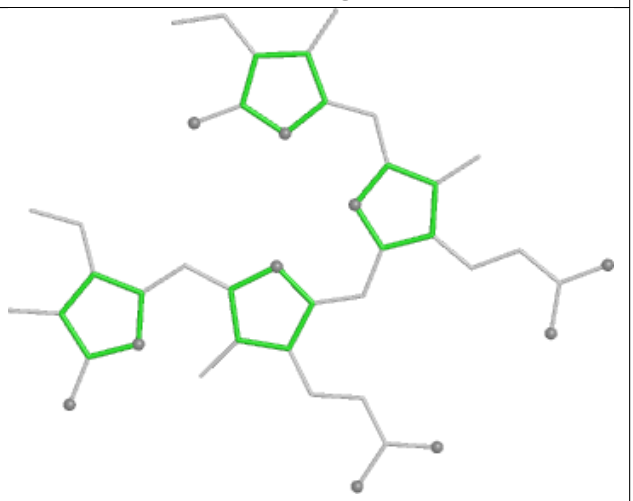
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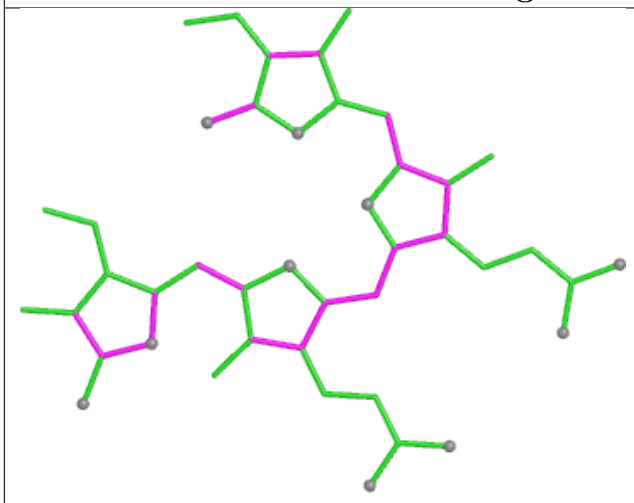


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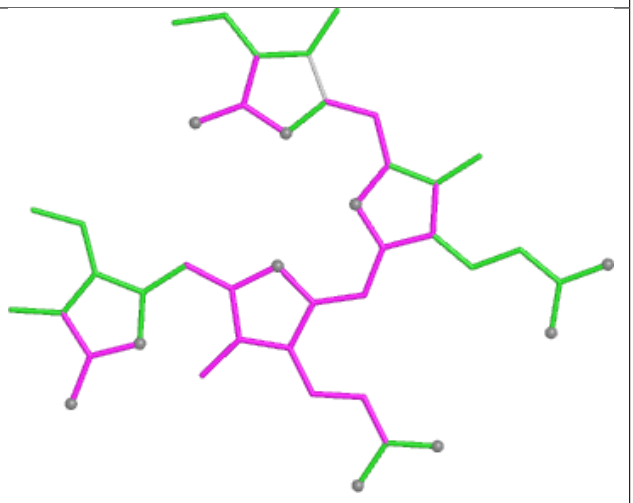


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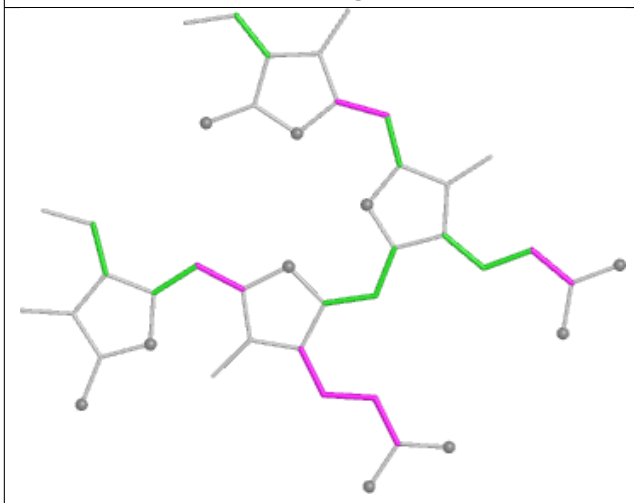
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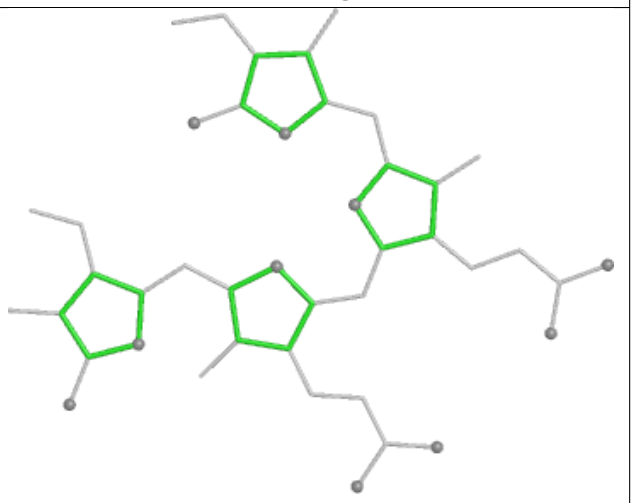
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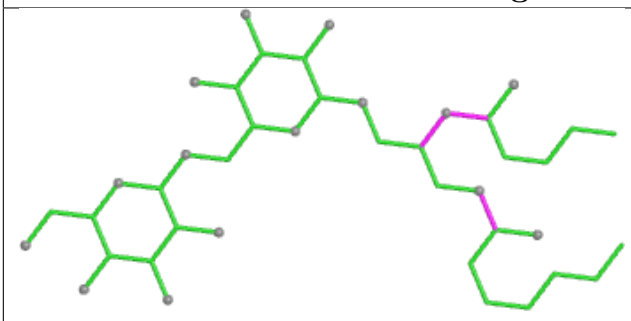


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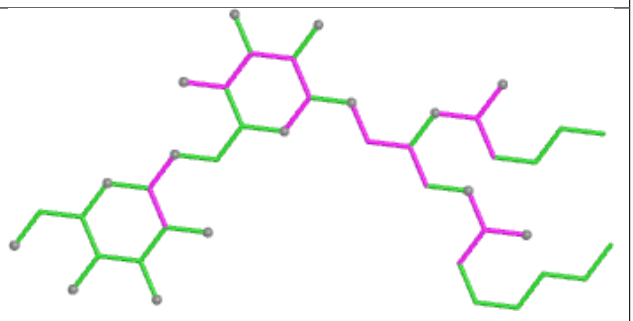


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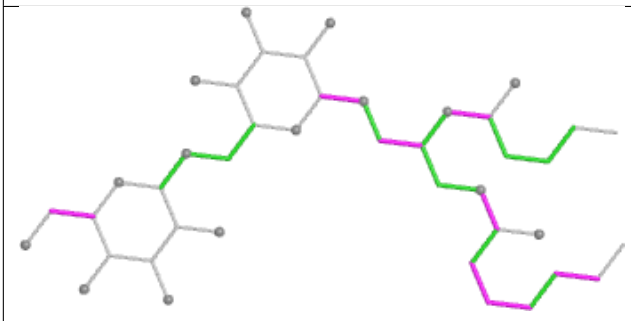
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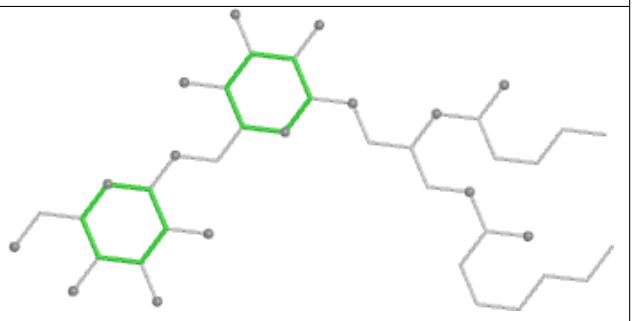
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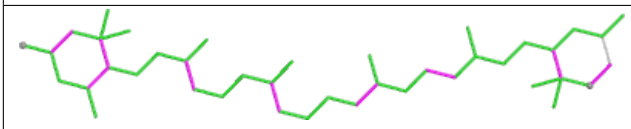


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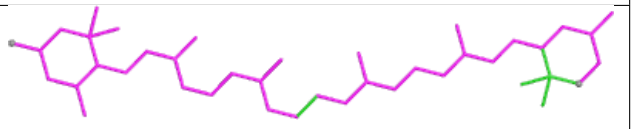


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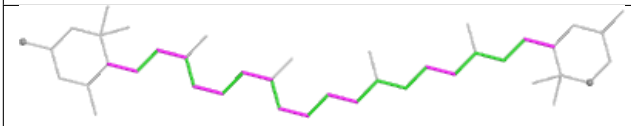
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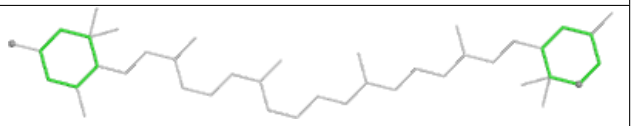
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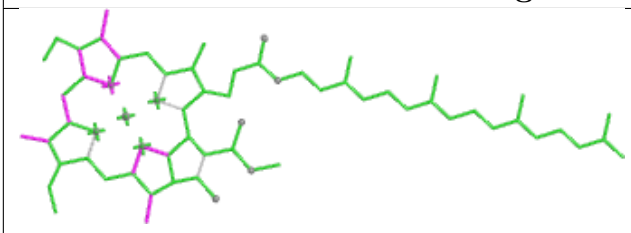


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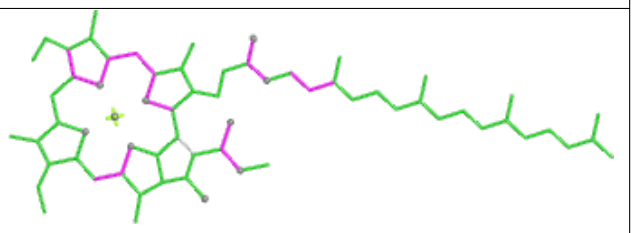


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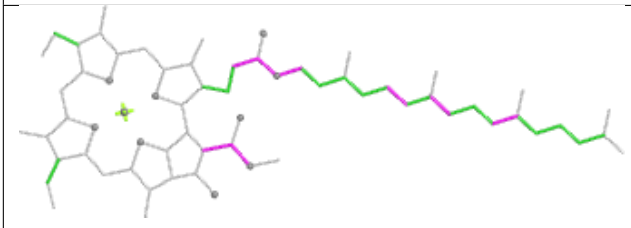
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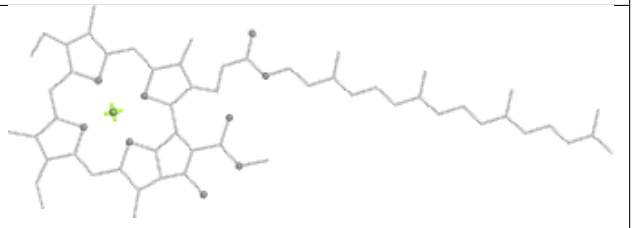
Bond lengths



Bond angles

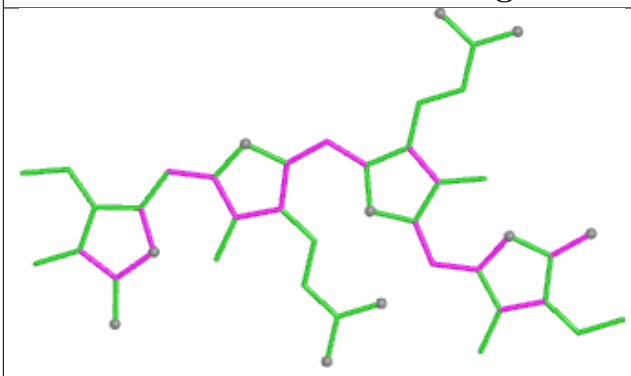


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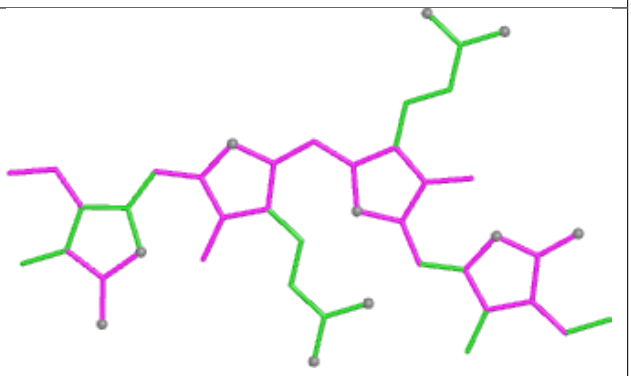


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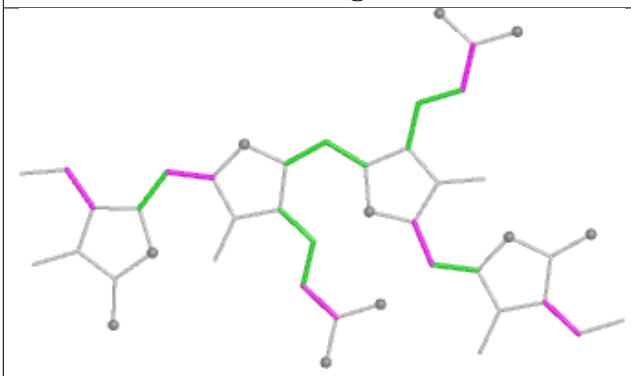
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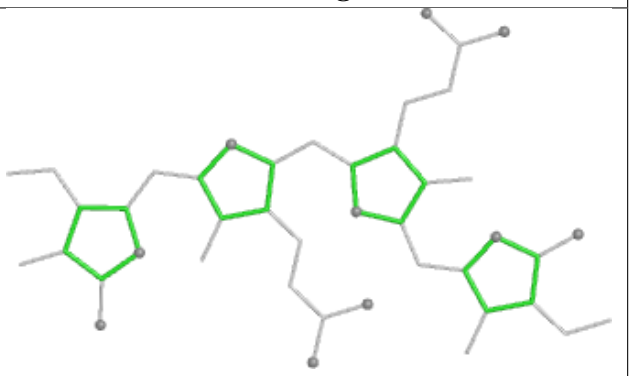
Bond lengths



Bond angles

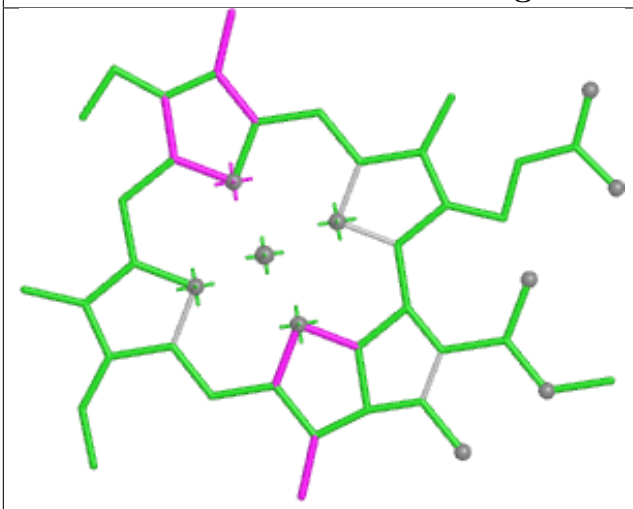


Torsions

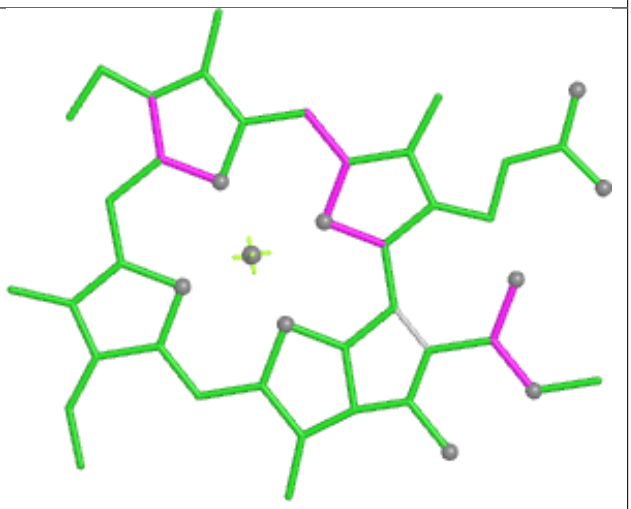


Rings

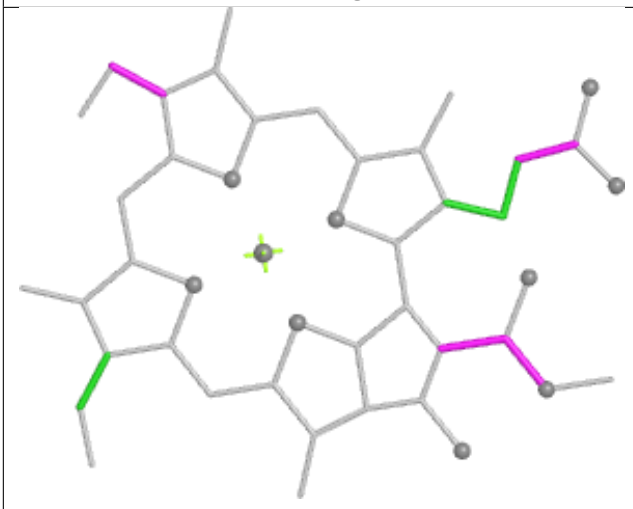
Ligand CLA 2N 304



Bond lengths



Bond angles

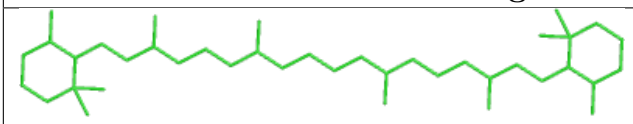


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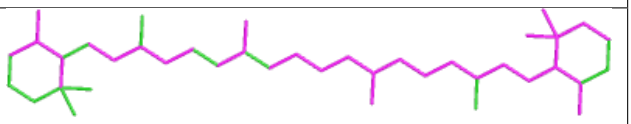


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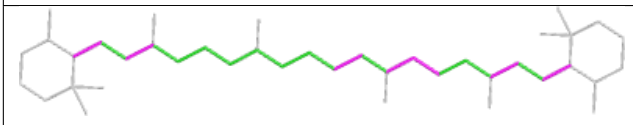
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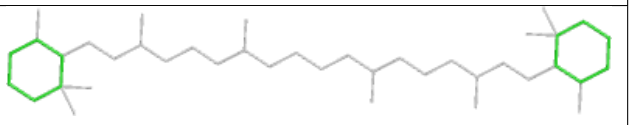
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Bond angles

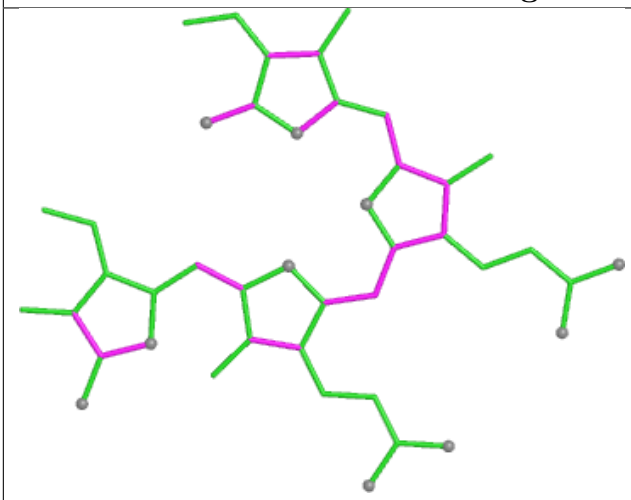


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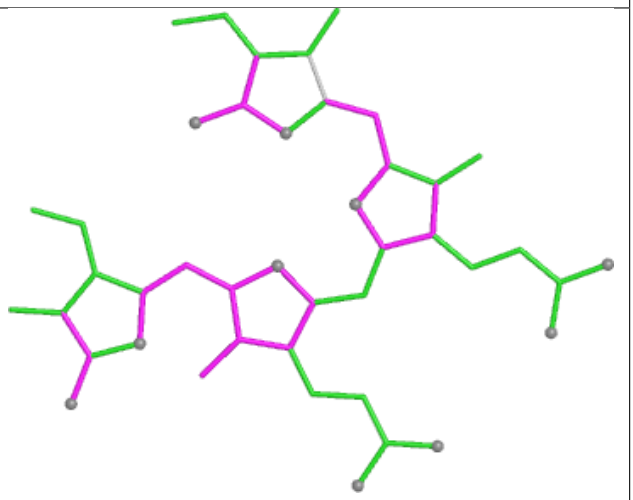


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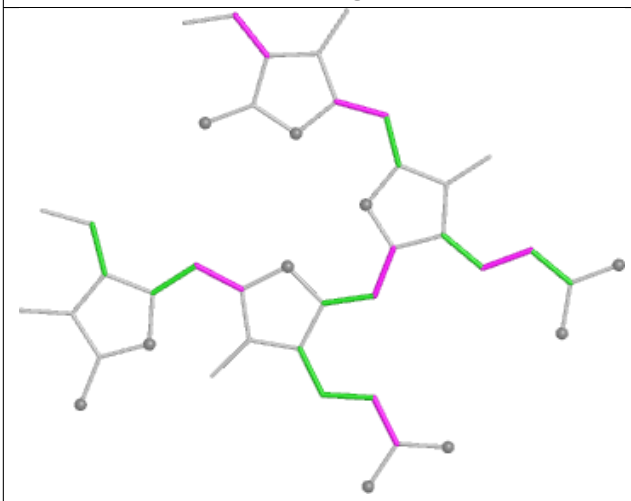
Ligand PEB e1 202



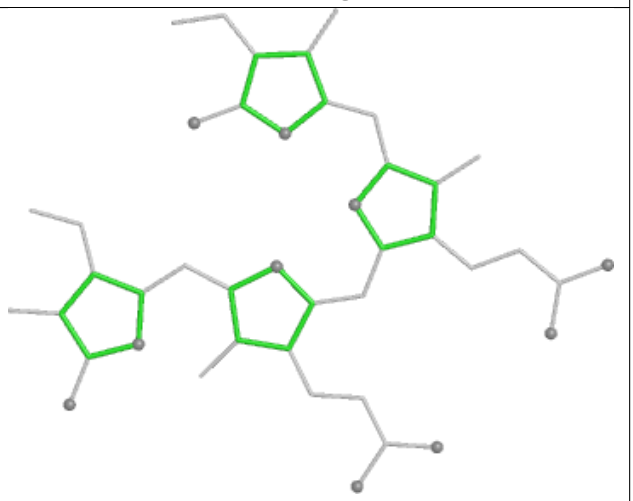
Bond lengths



Bond angles

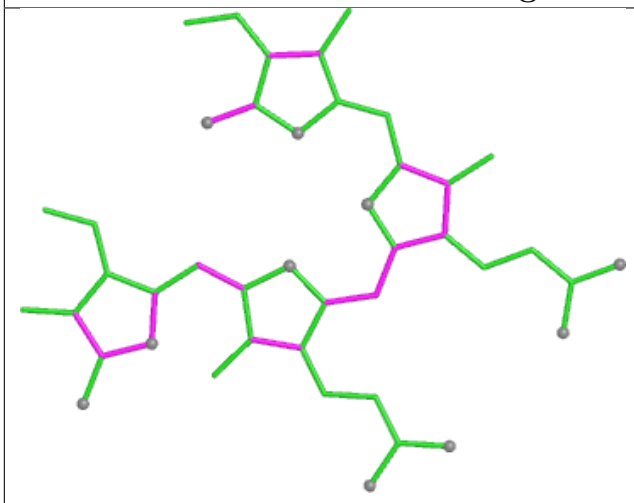


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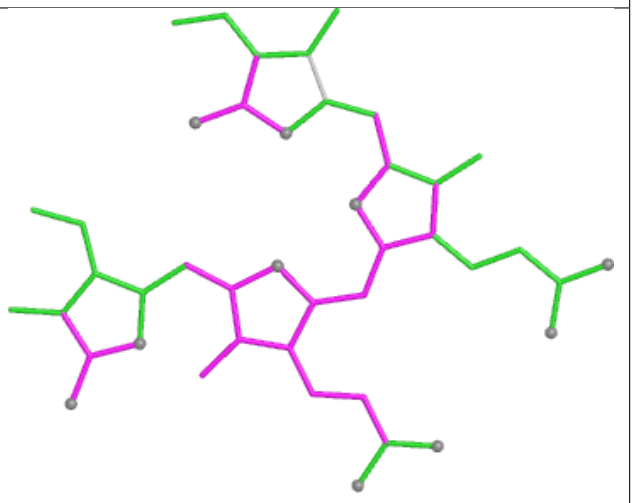


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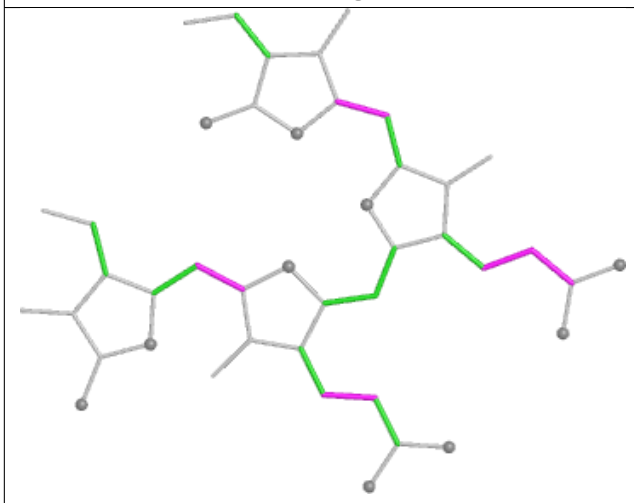
Ligand PEB SJ 201



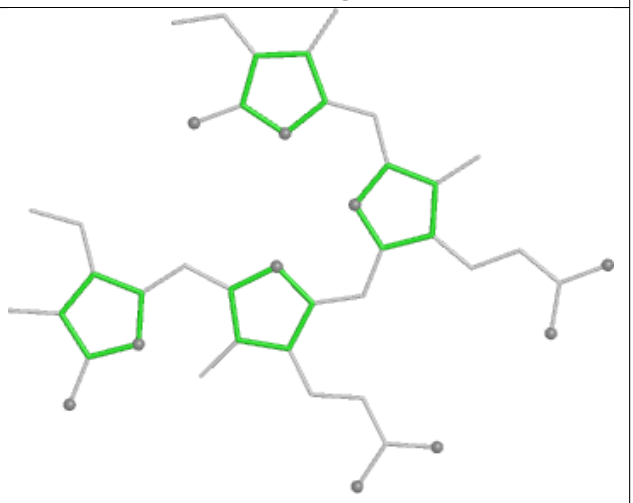
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Bond angles

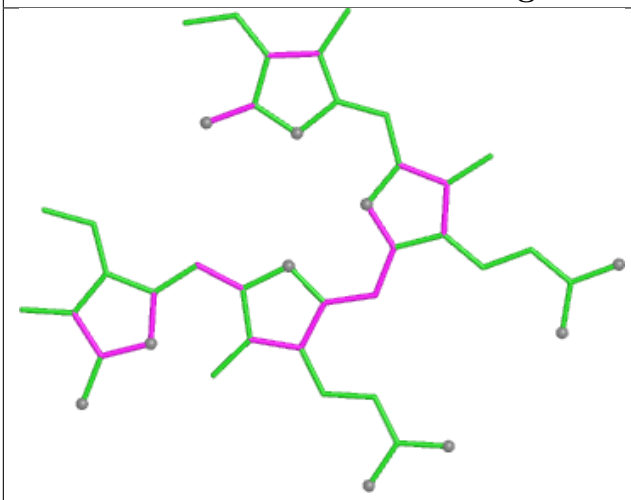


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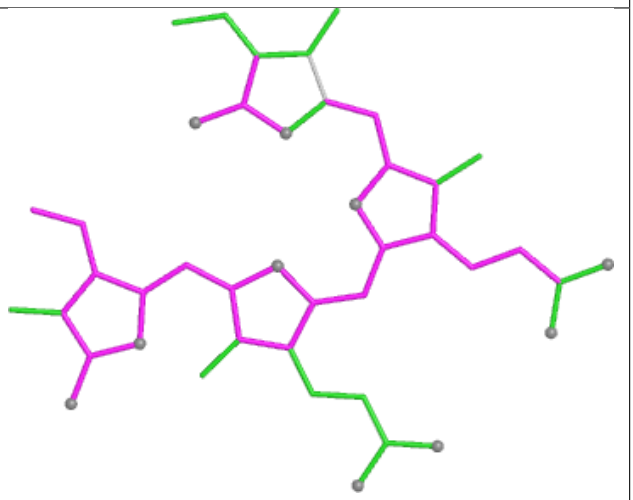


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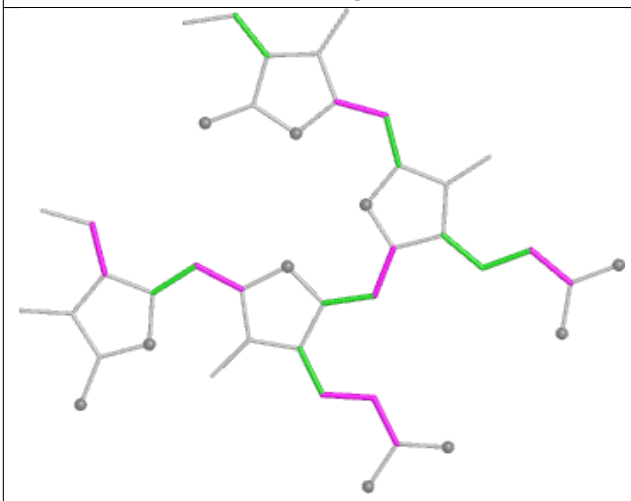
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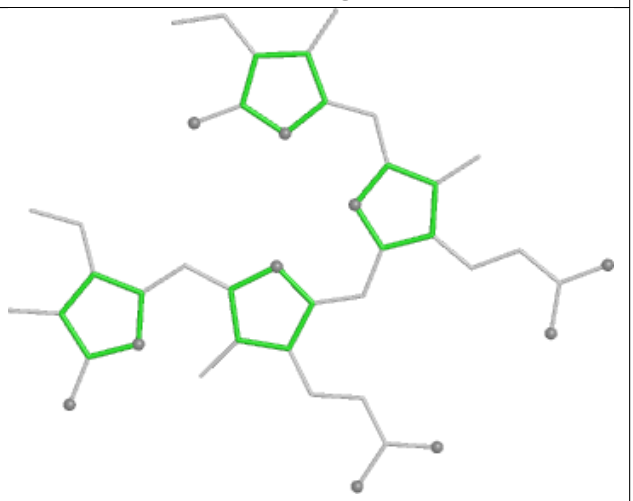
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Bond angles

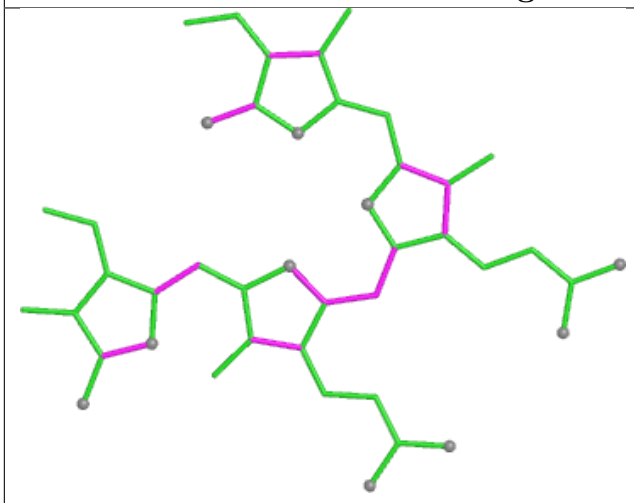


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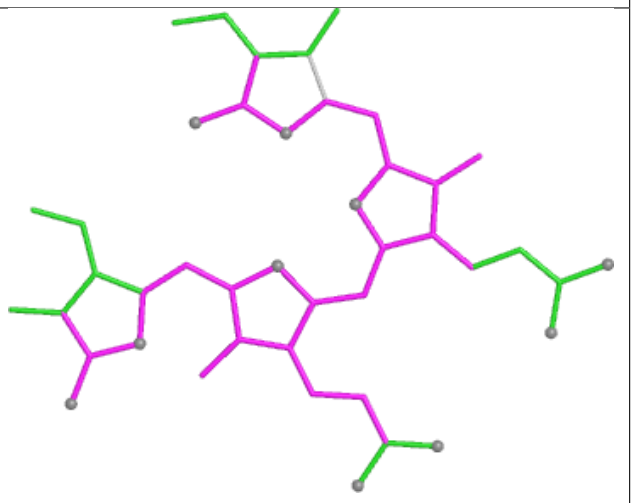


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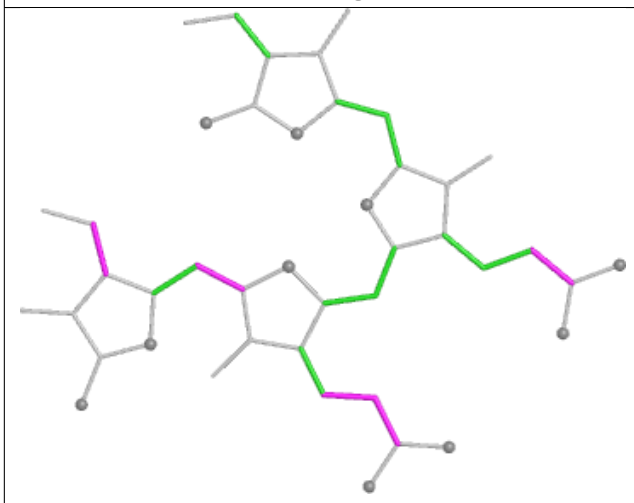
Ligand PEB T7 202



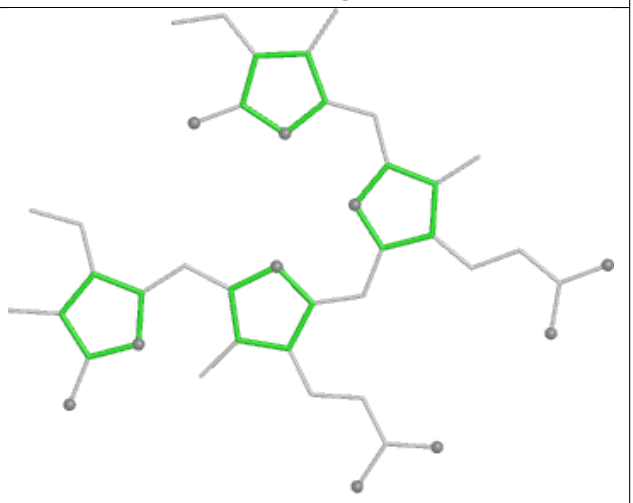
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Bond angles

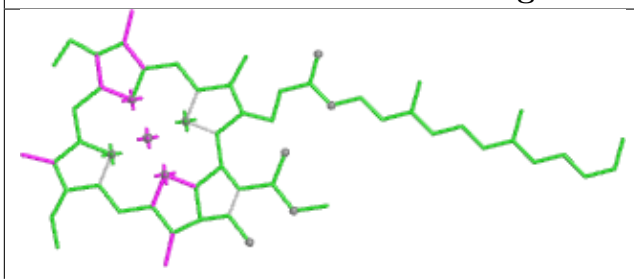


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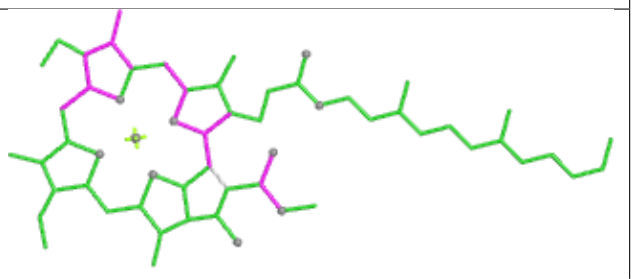


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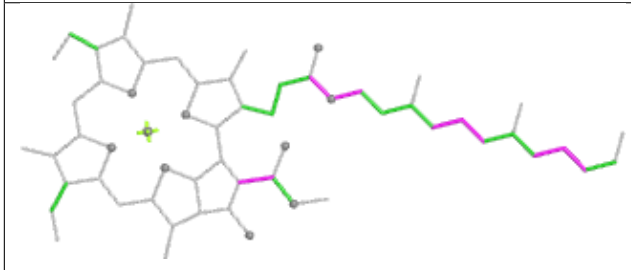
Ligand CLA bL 619



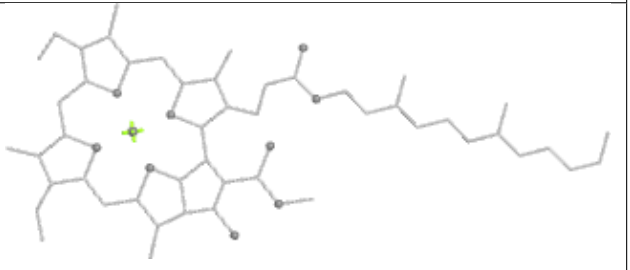
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Bond angles

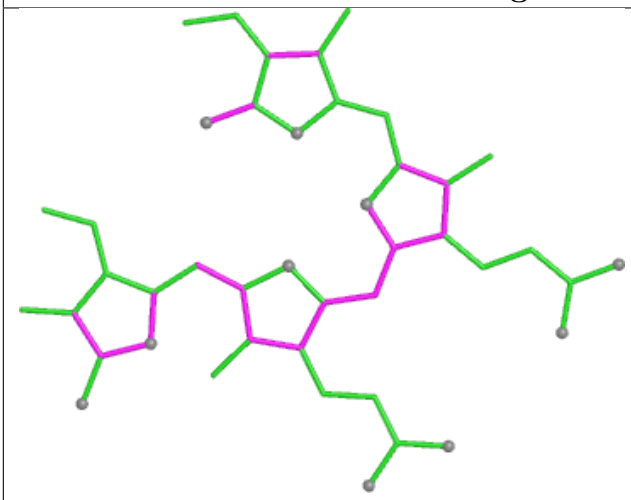


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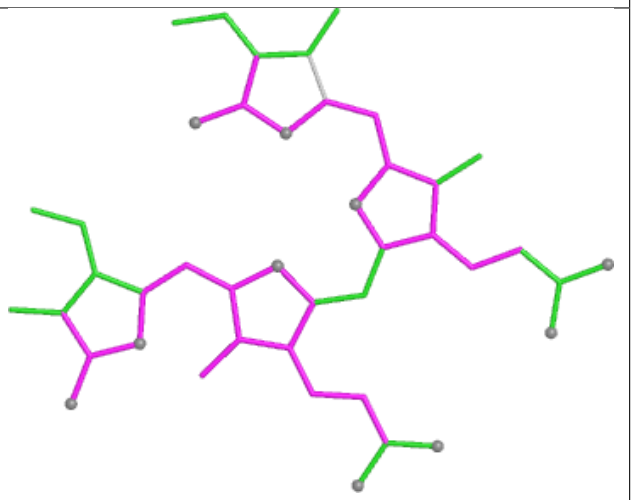


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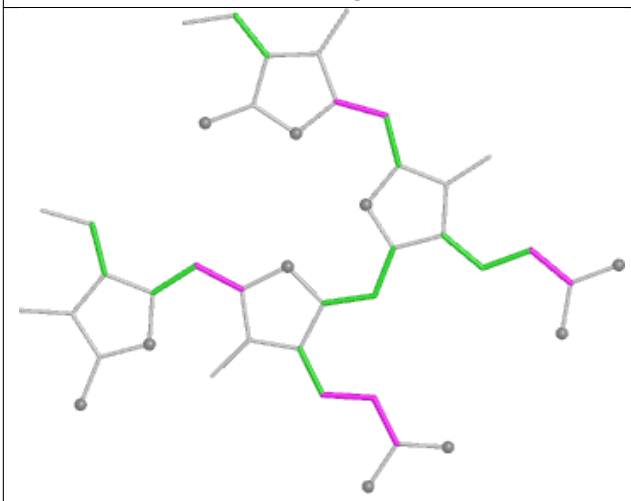
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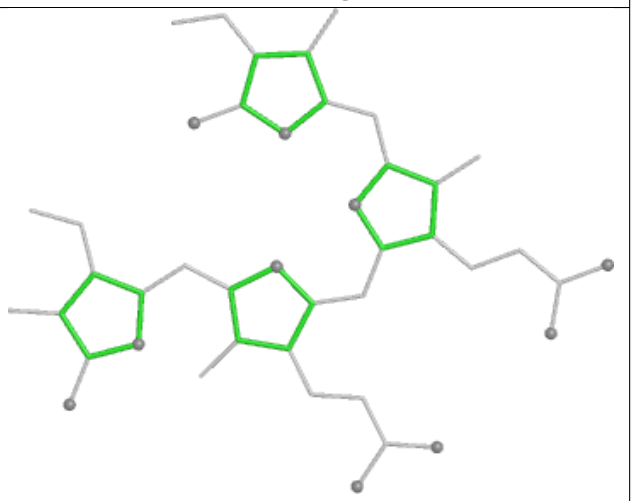
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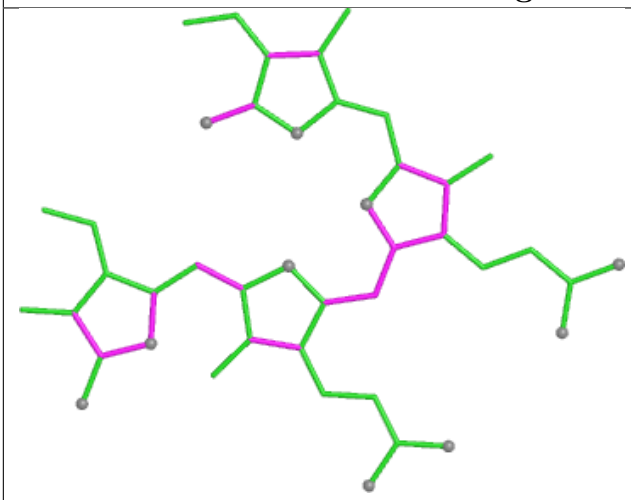


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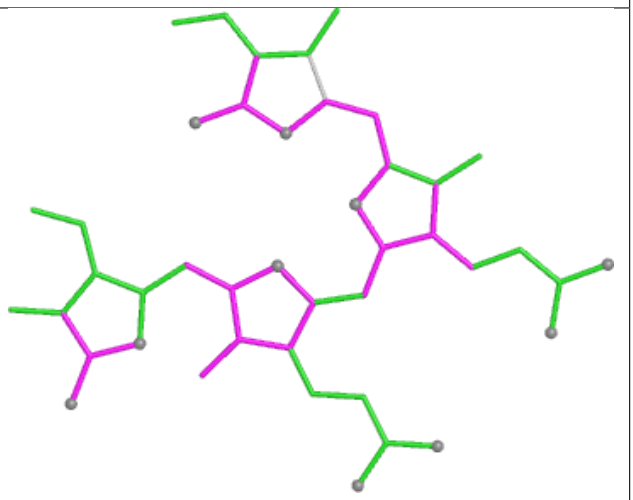


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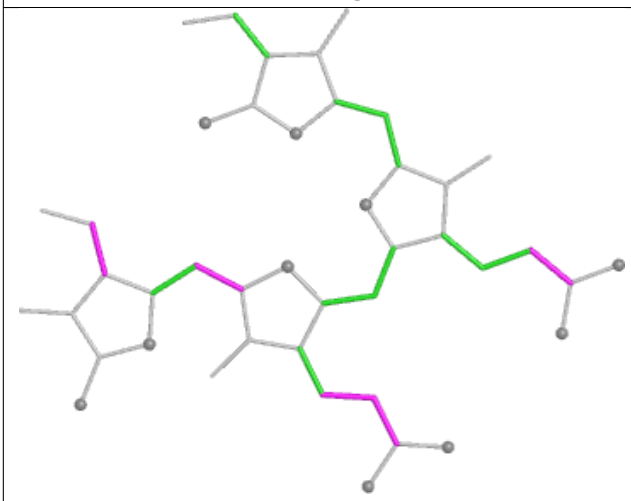
Ligand PEB A4 304



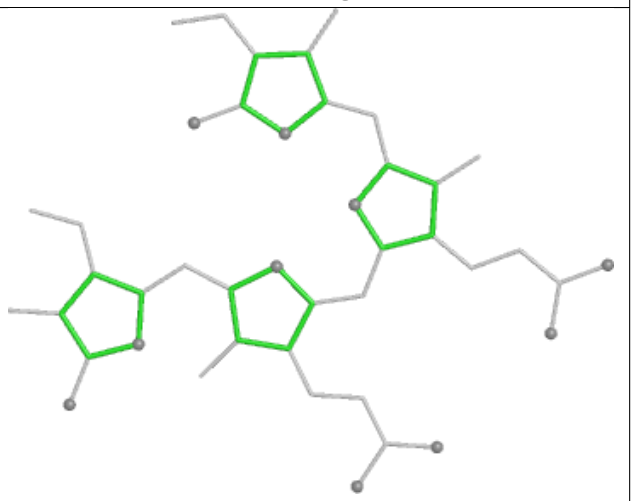
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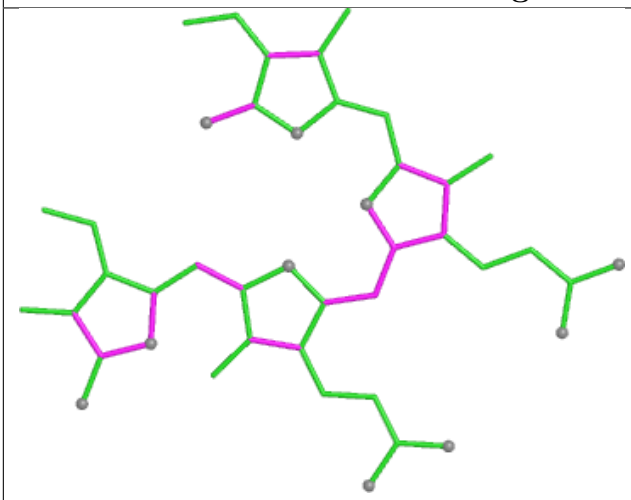


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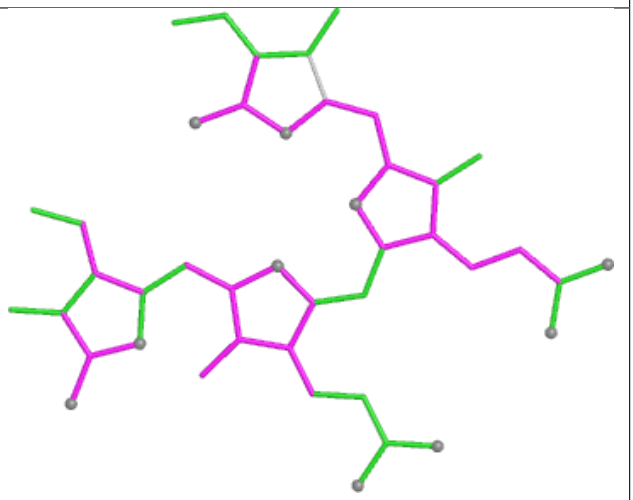


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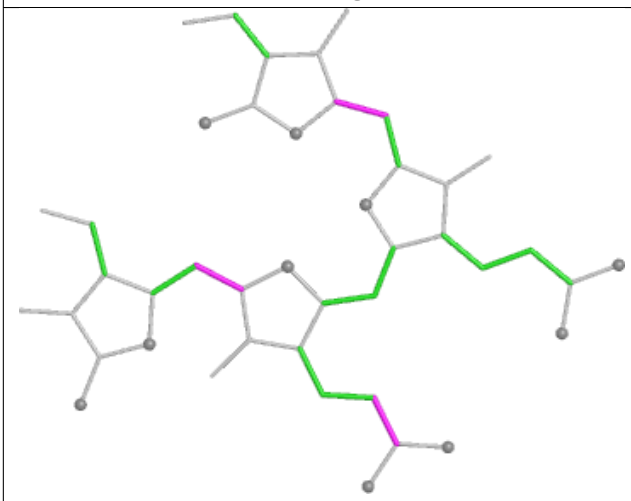
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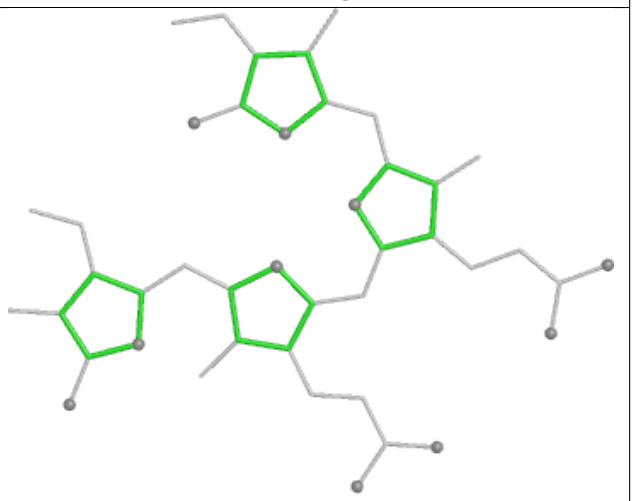
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Bond angles

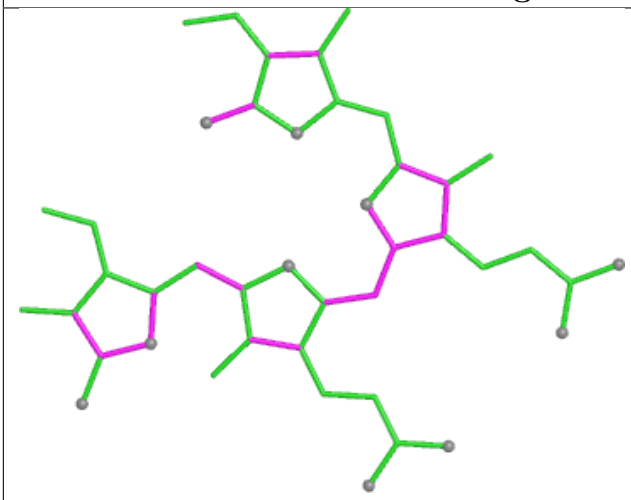


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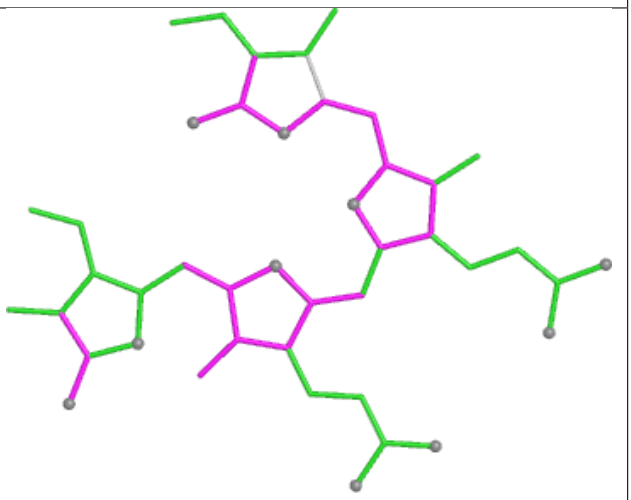


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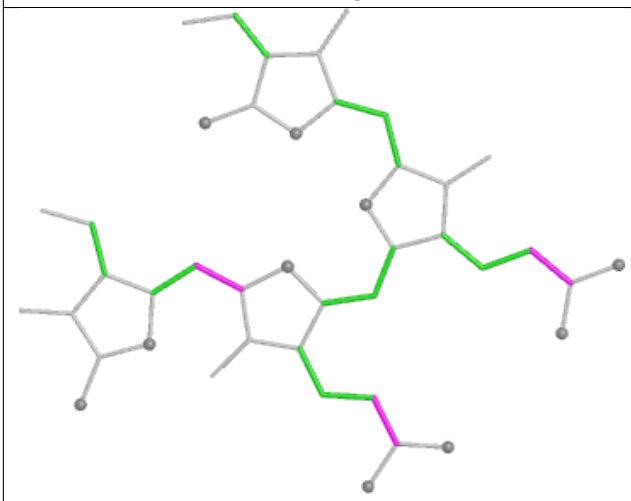
Ligand PEB bG 201



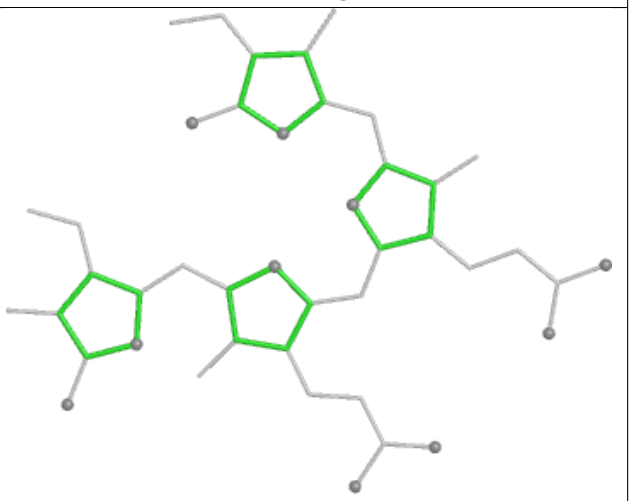
Bond lengths



Bond angles

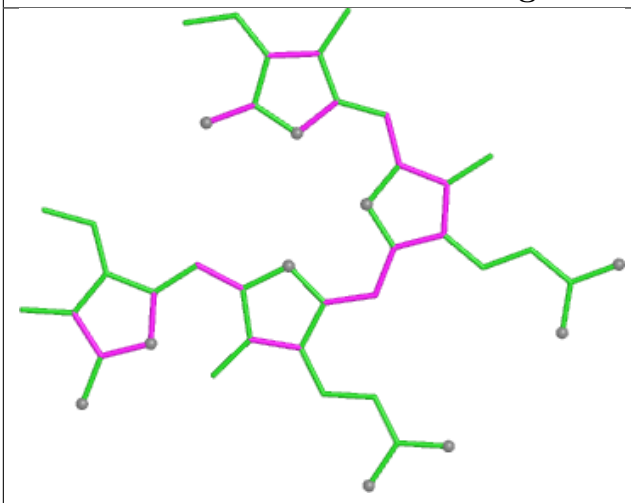


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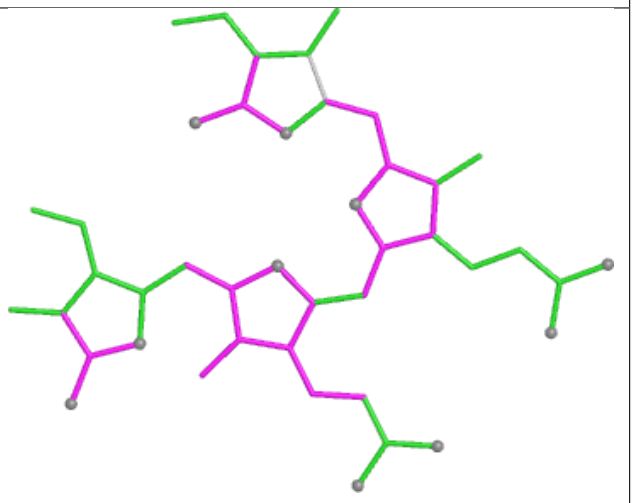


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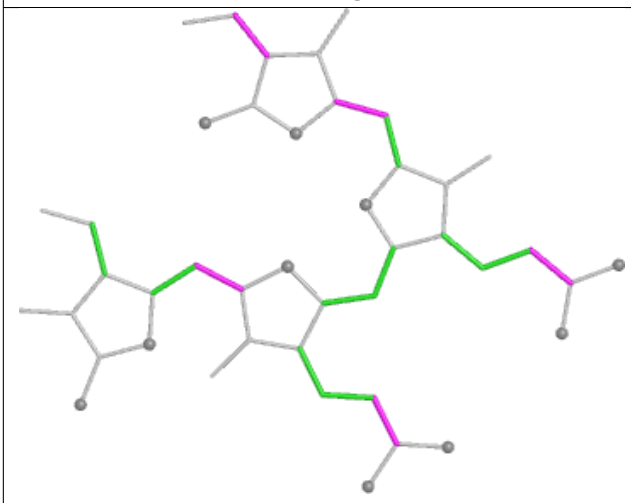
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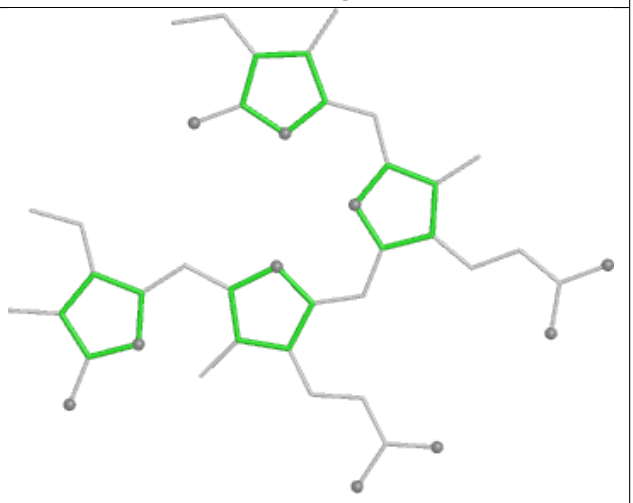
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Bond angles

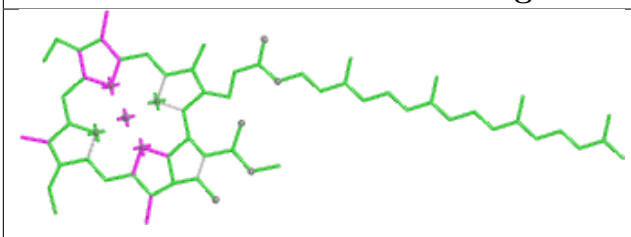


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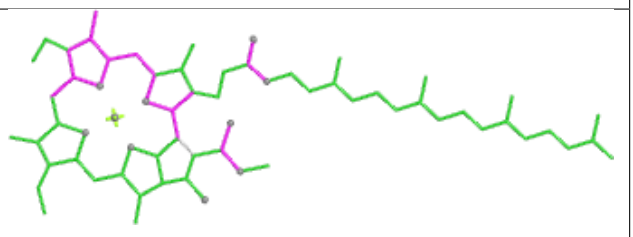


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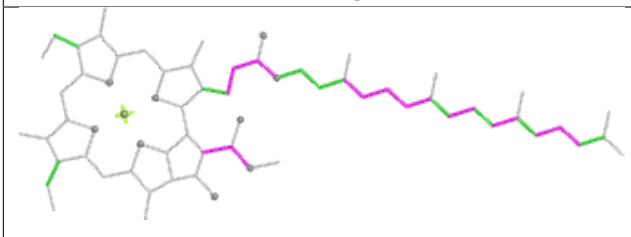
Ligand CLA A2 823



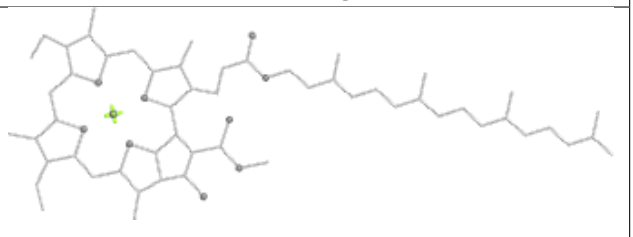
Bond lengths



Bond angles

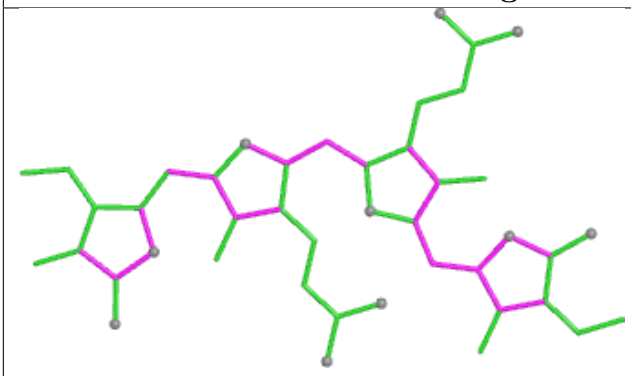


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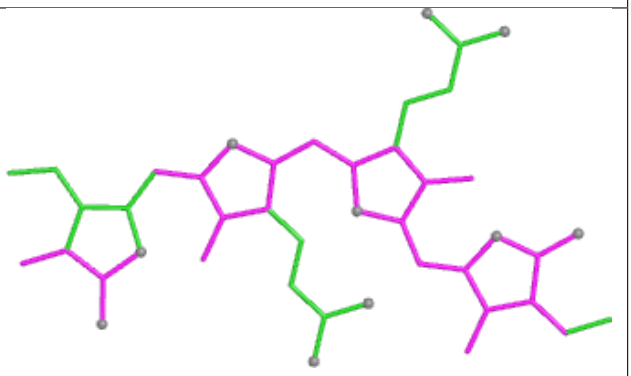


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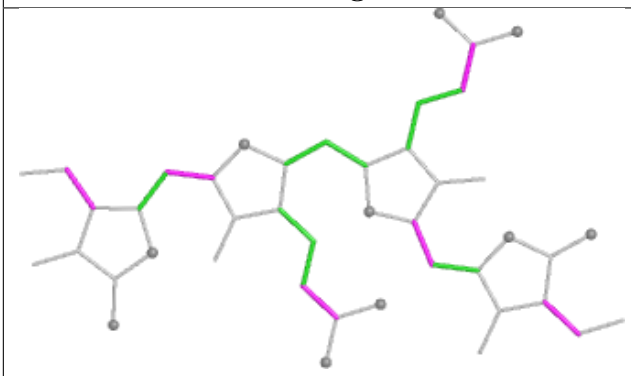
Ligand CYC EH 1001



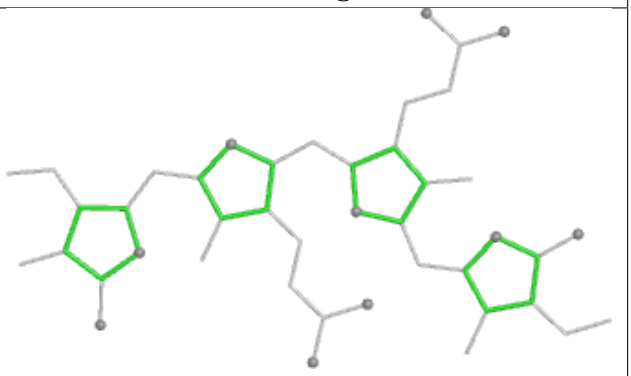
Bond lengths



Bond angles

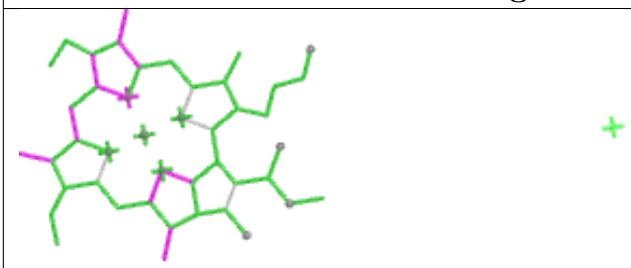


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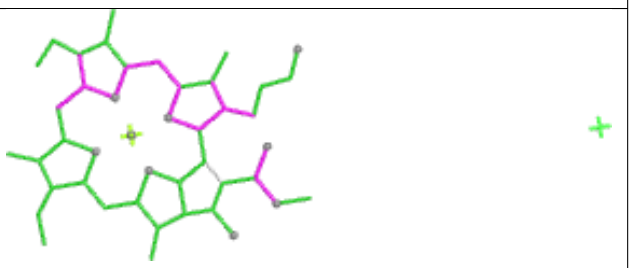


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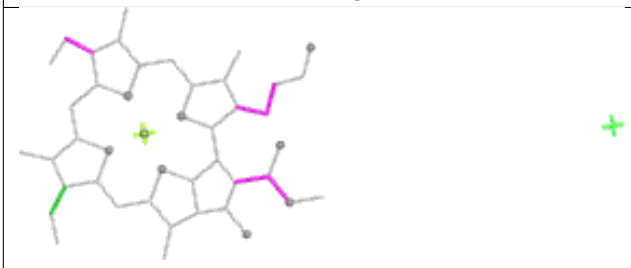
Ligand CLA AN 801



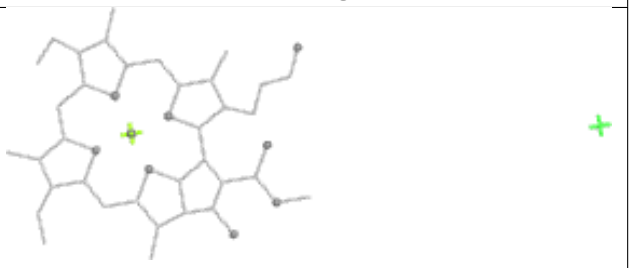
Bond lengths



Bond angles

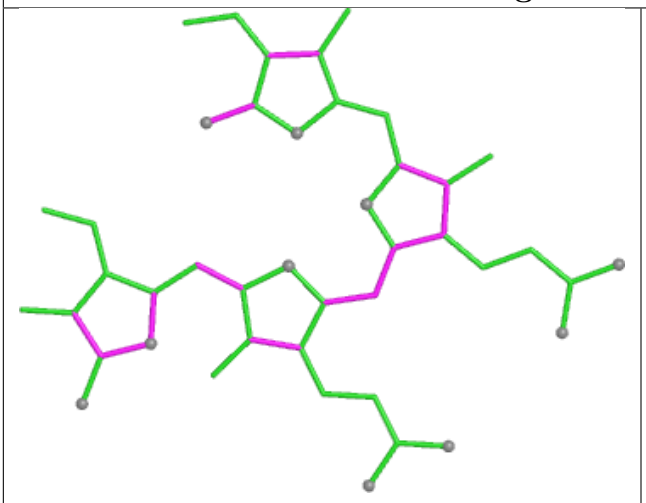


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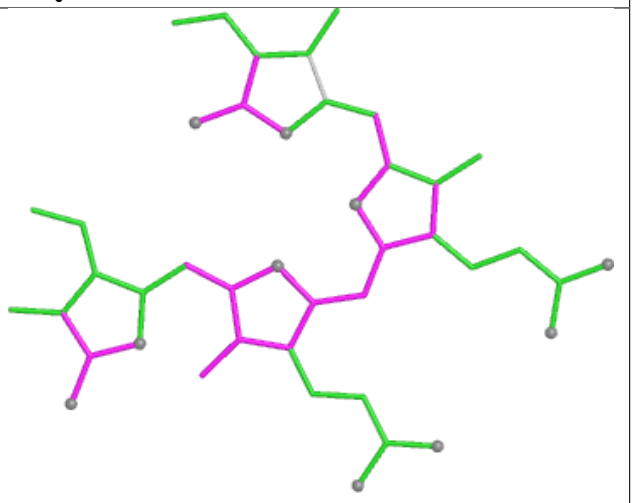


Rings

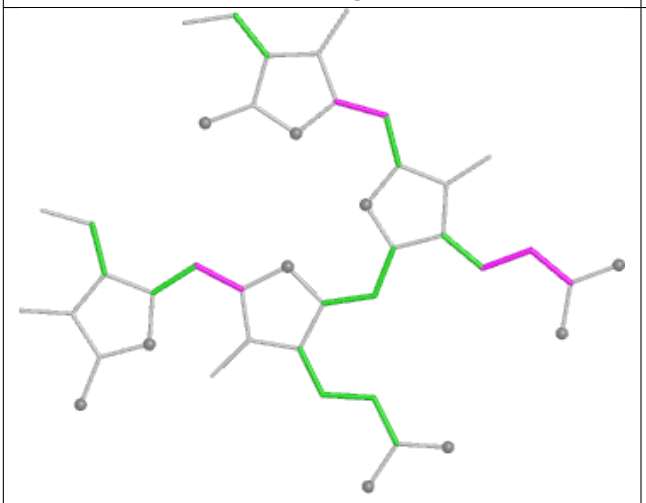
Ligand PEB QJ 203



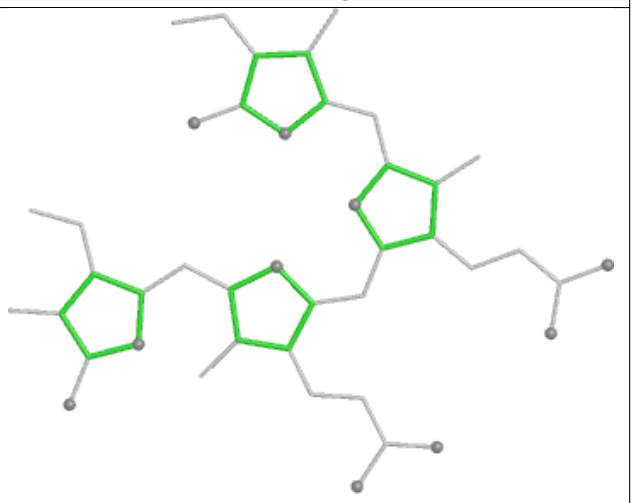
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Bond angles

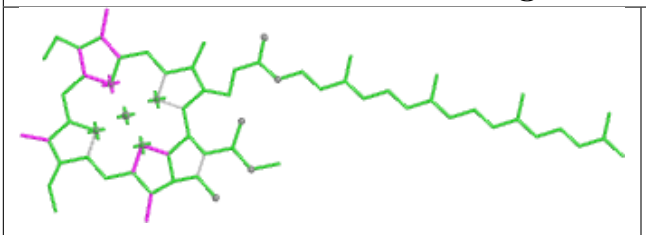


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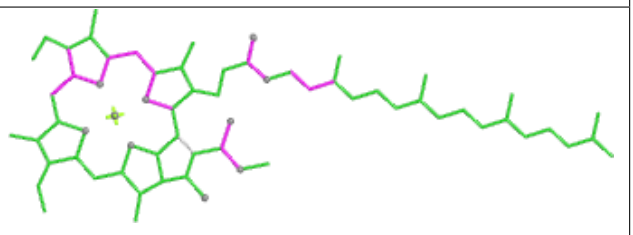


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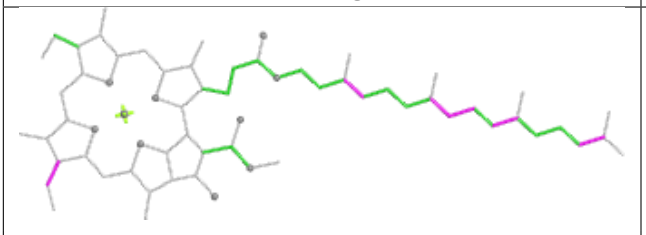
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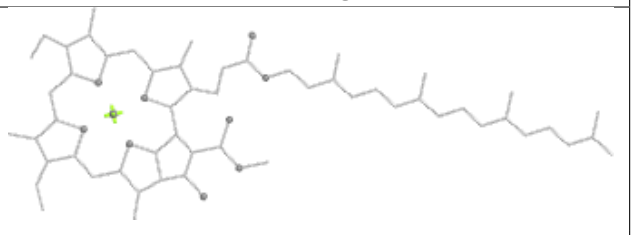
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Bond angles

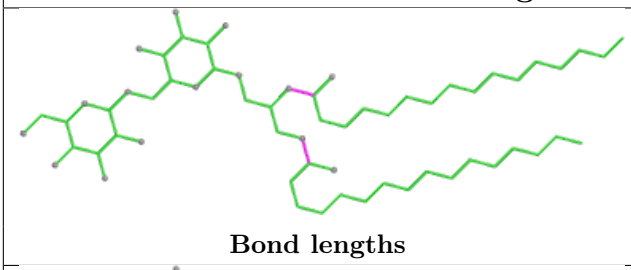


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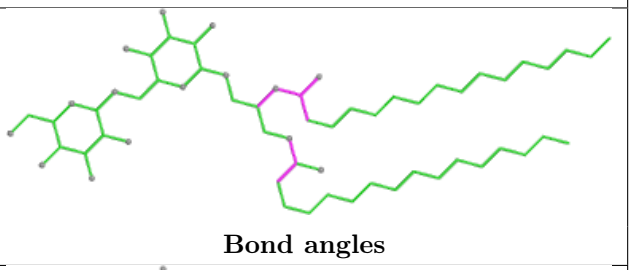


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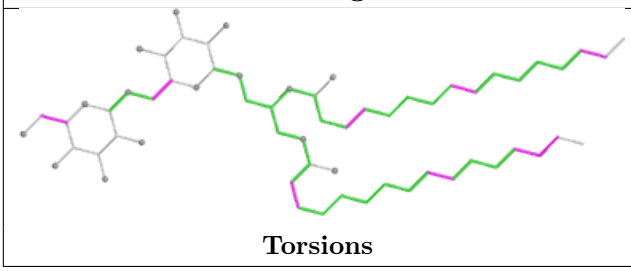
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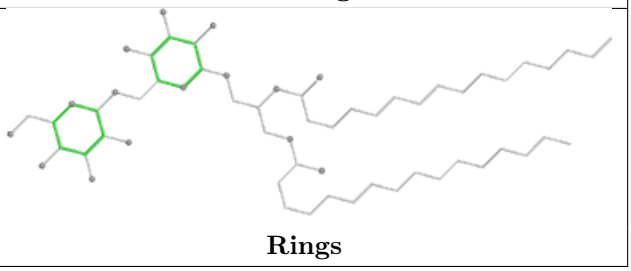
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Bond angles

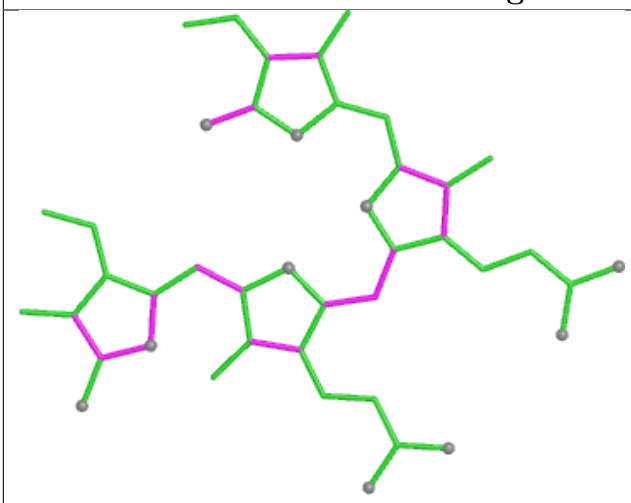


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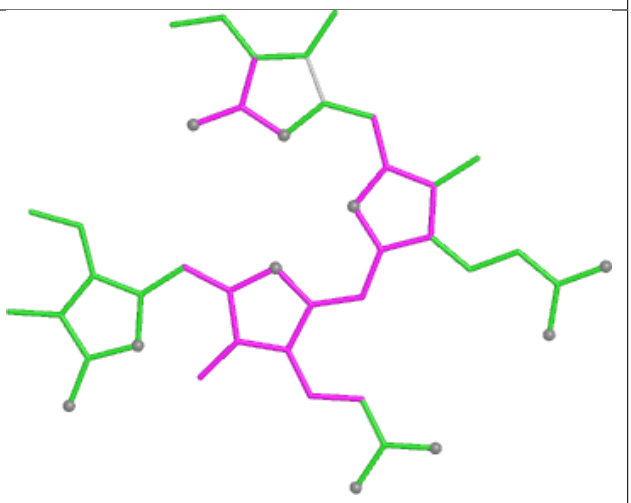


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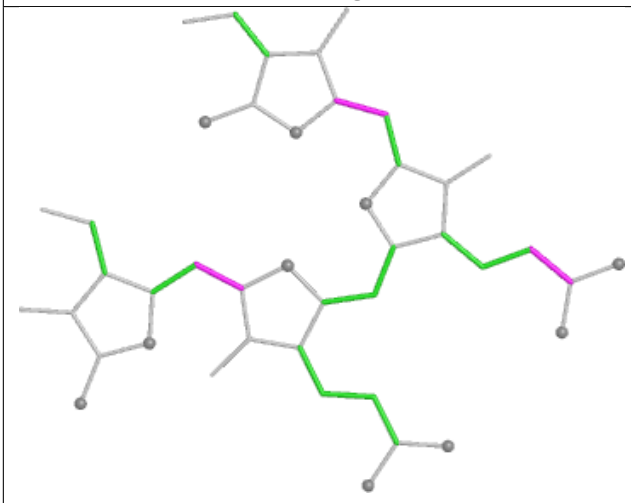
Ligand PEB MK 201



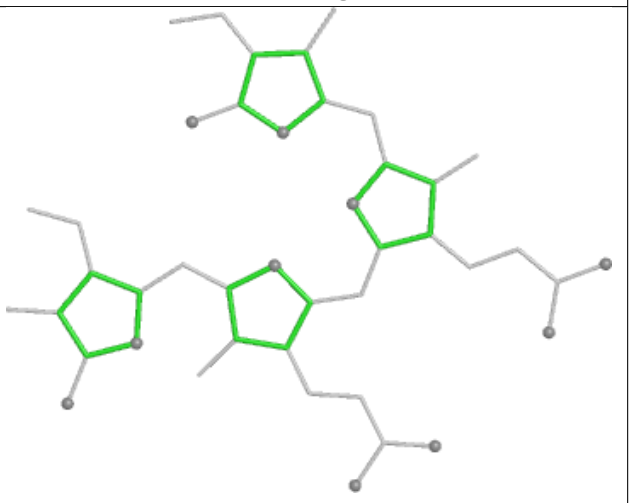
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Bond angles

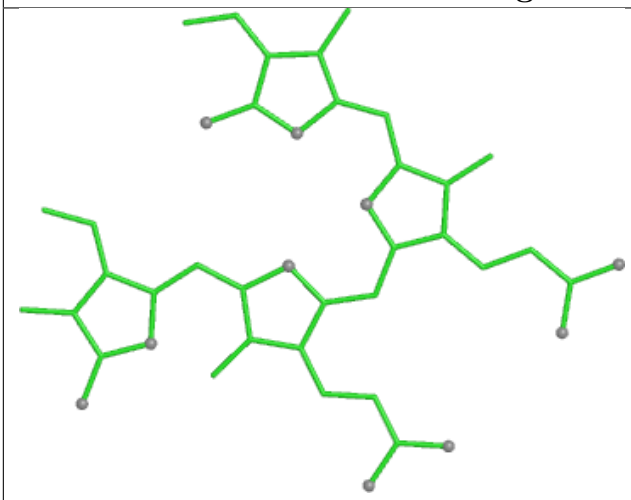


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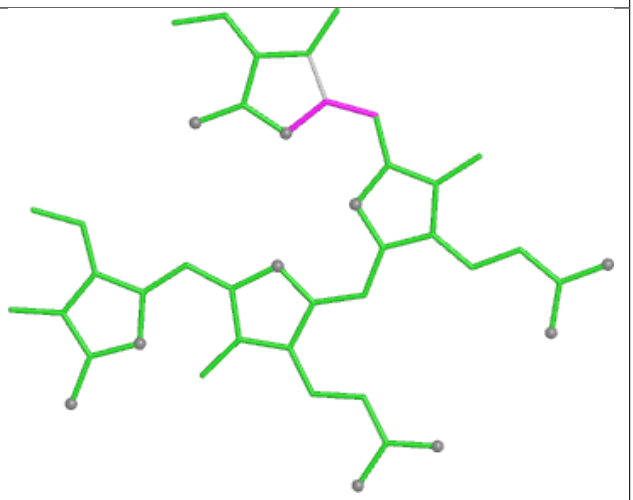


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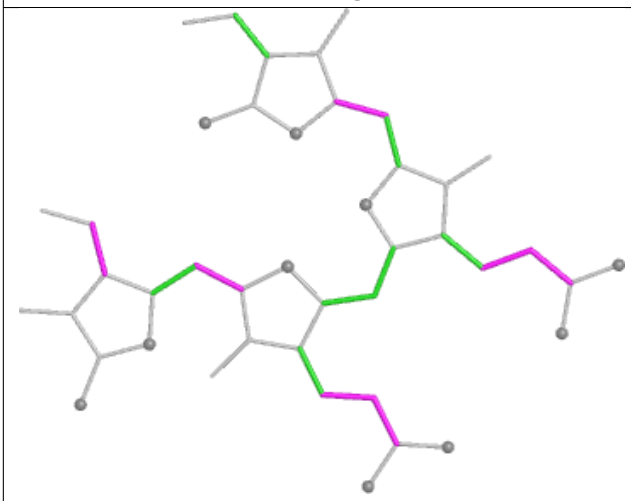
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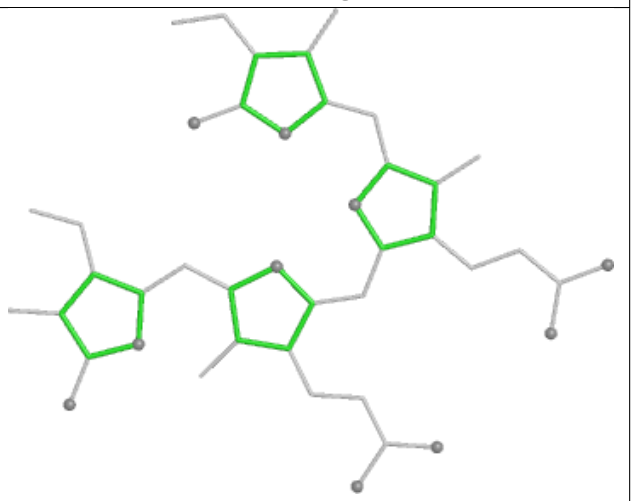
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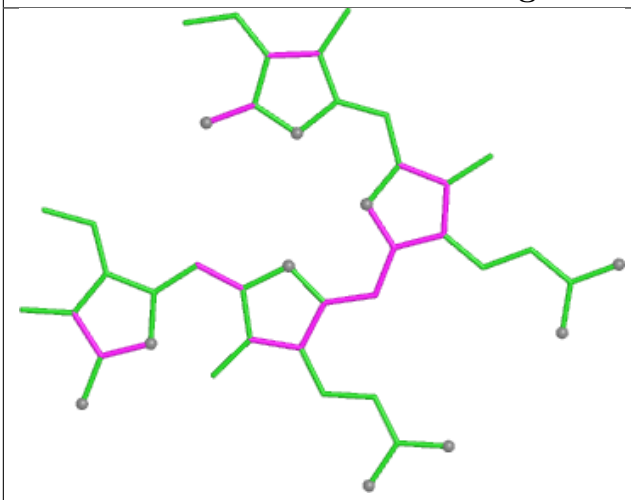


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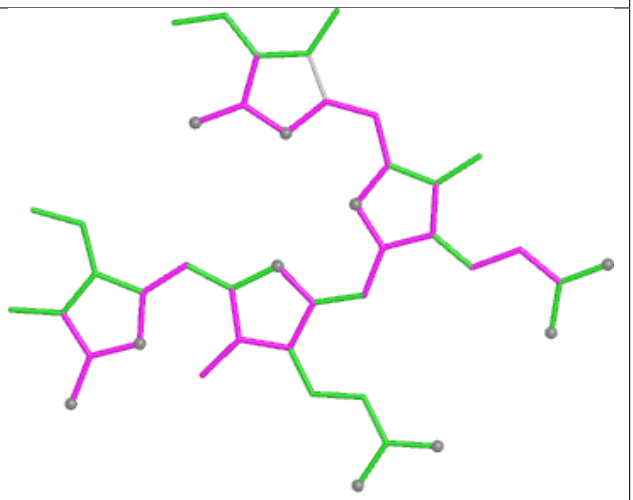


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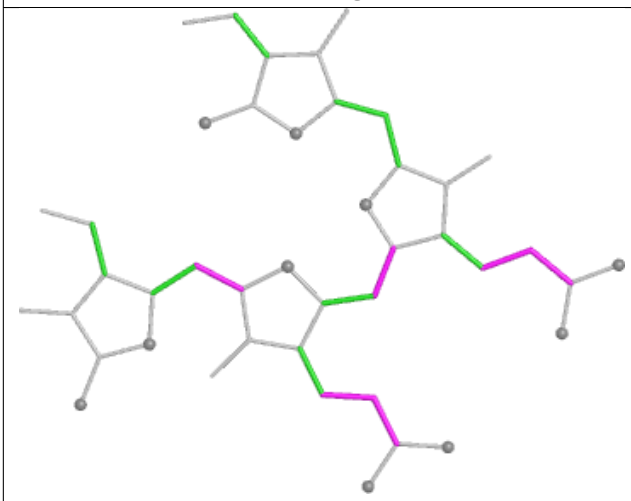
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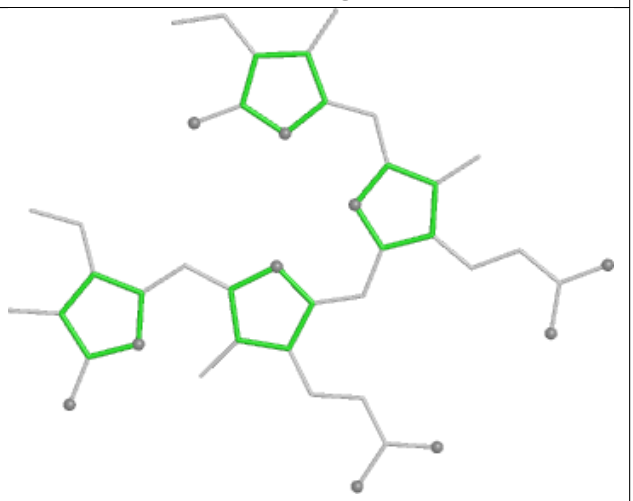
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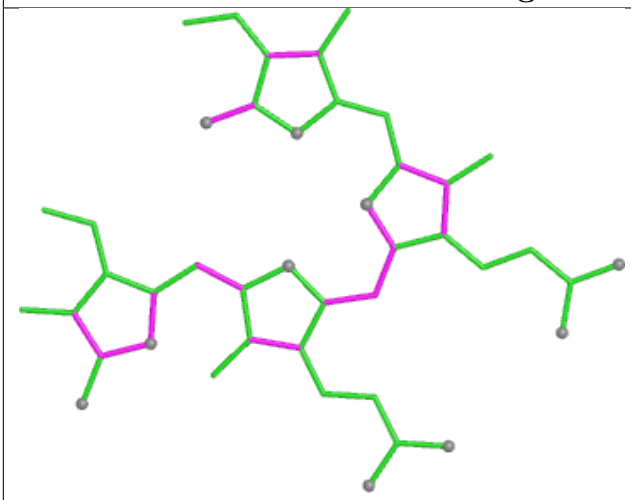


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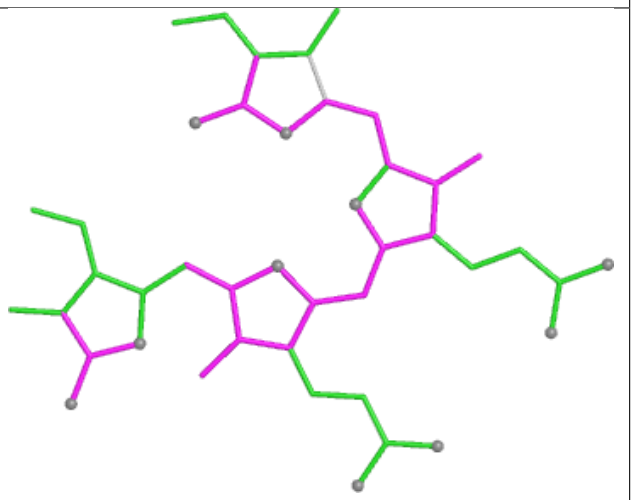


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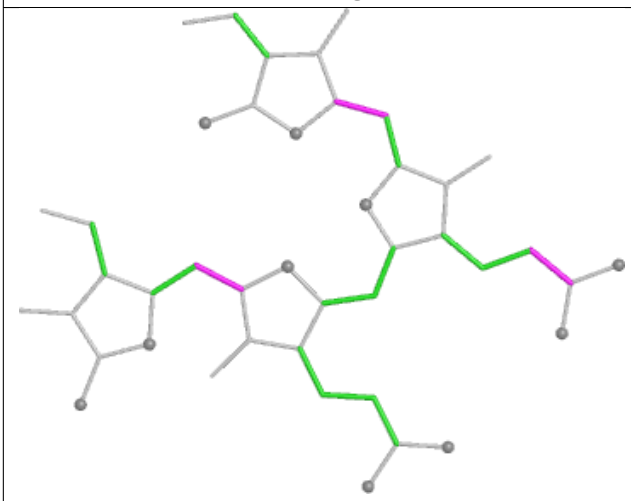
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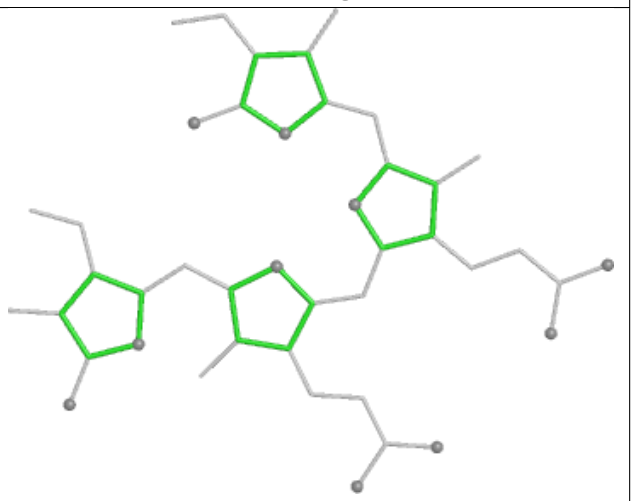
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Bond angles

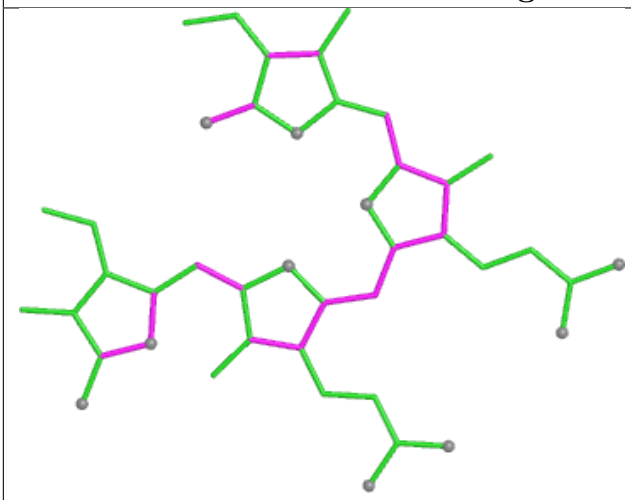


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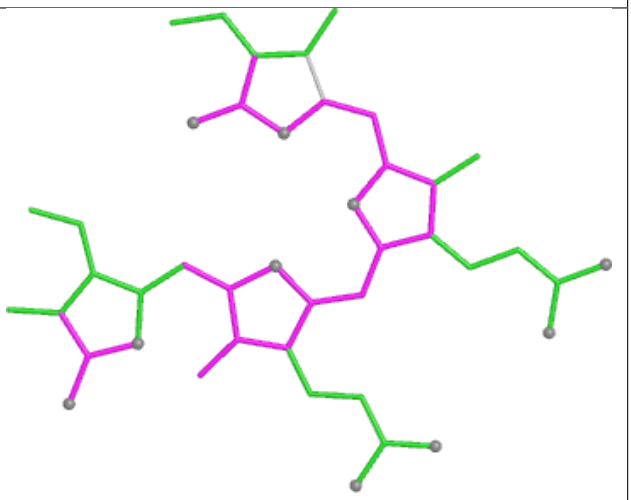


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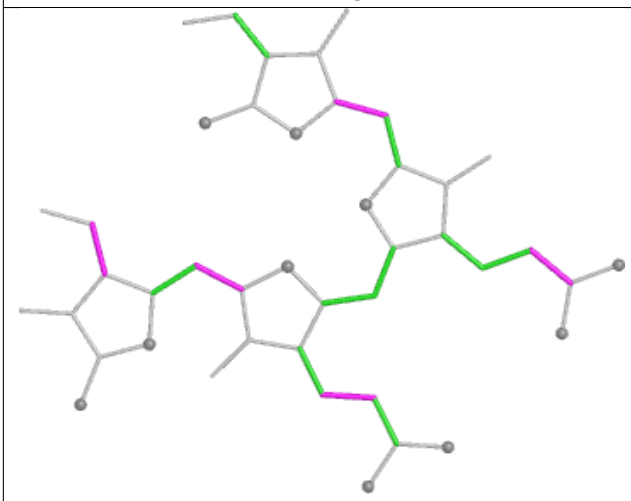
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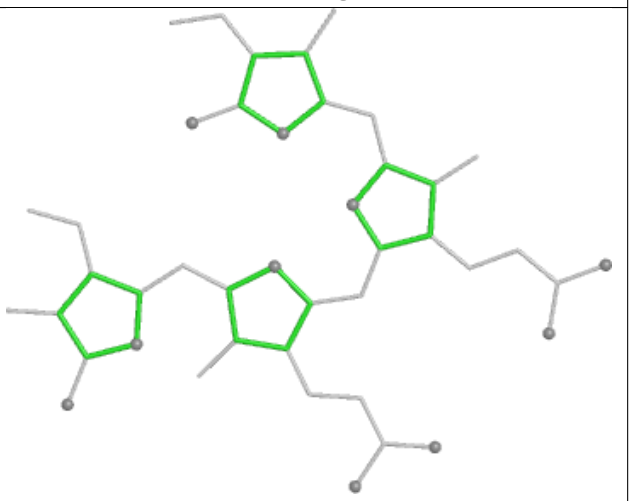
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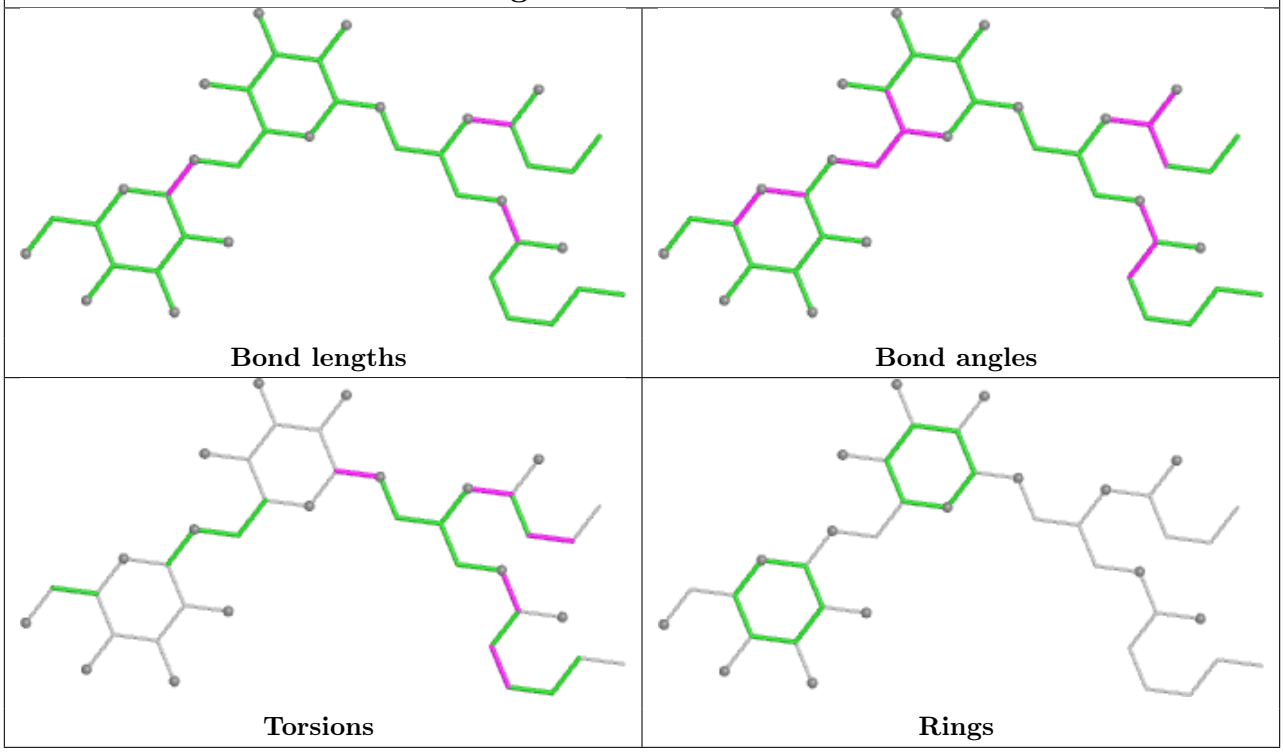


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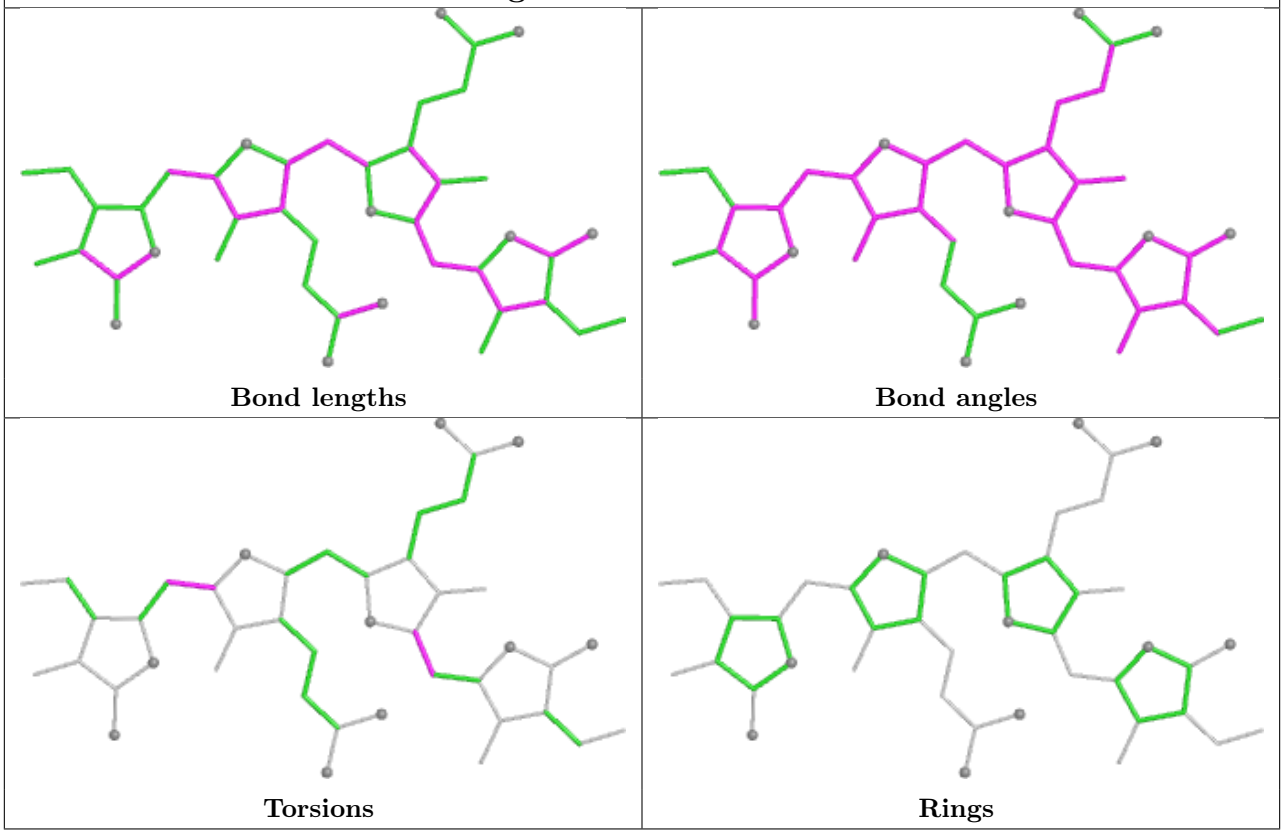


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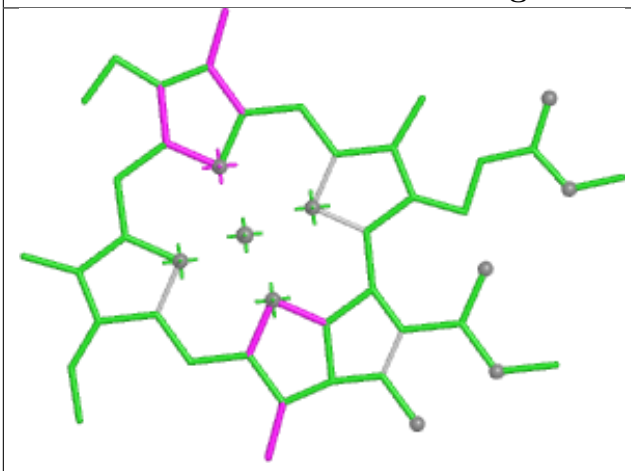
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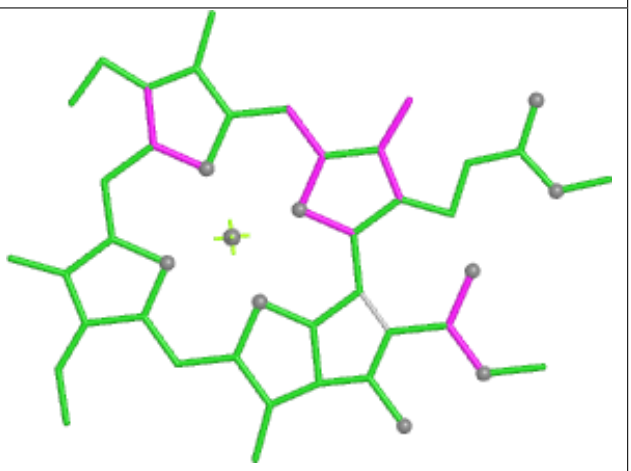
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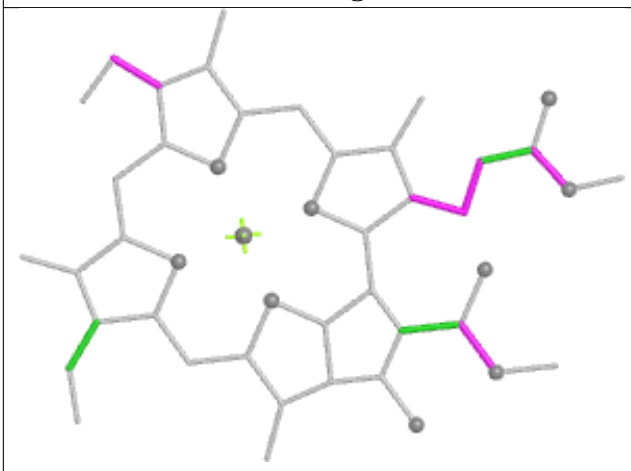
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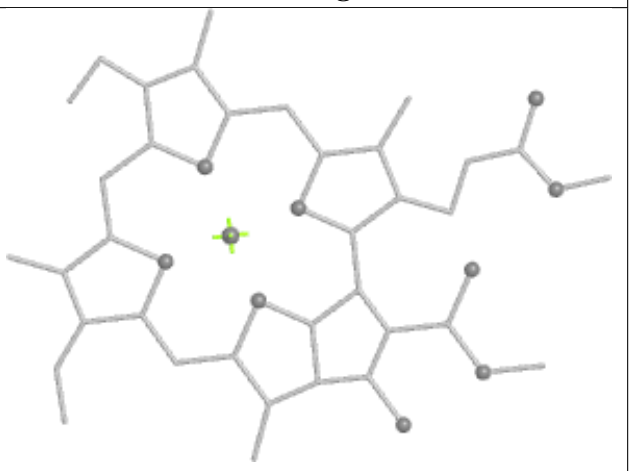
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Bond angles

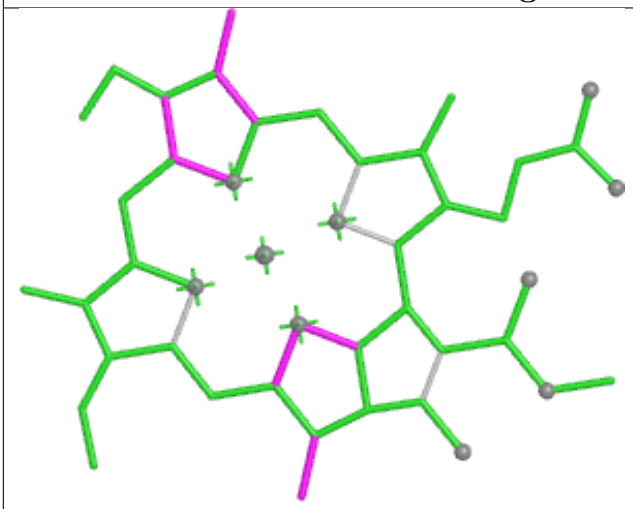


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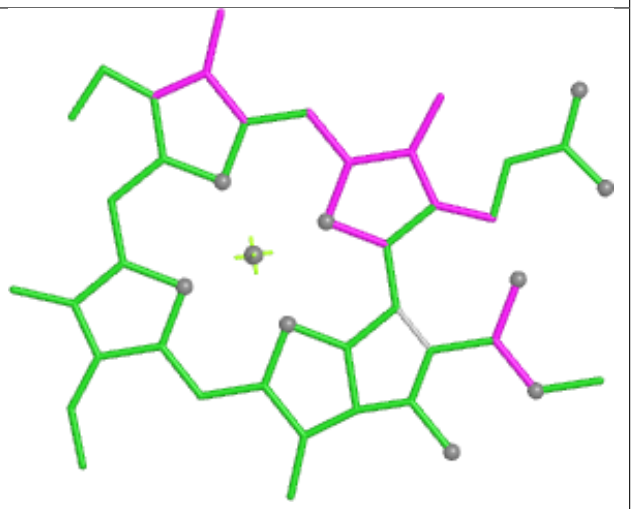


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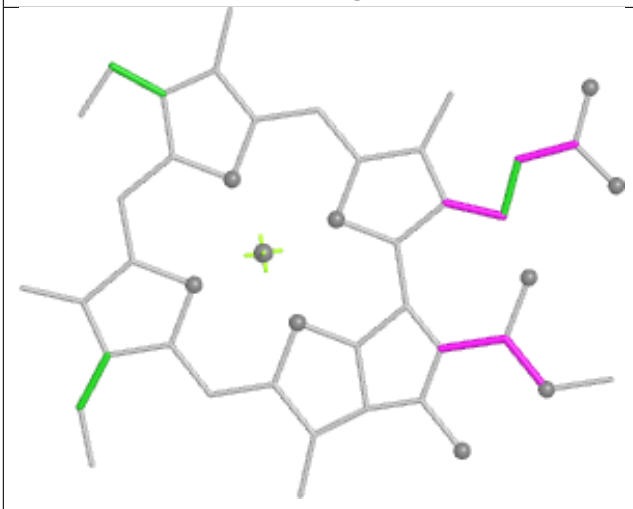
Ligand CLA 52 606



Bond lengths



Bond angles

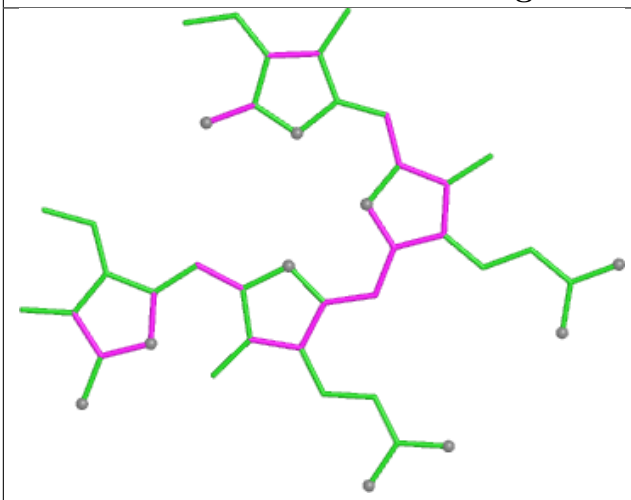


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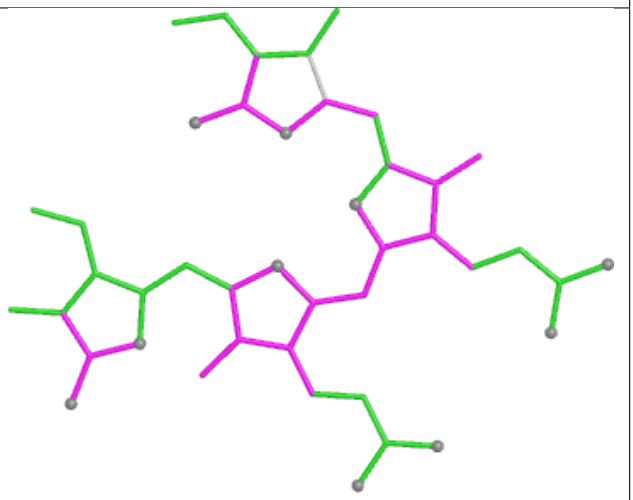


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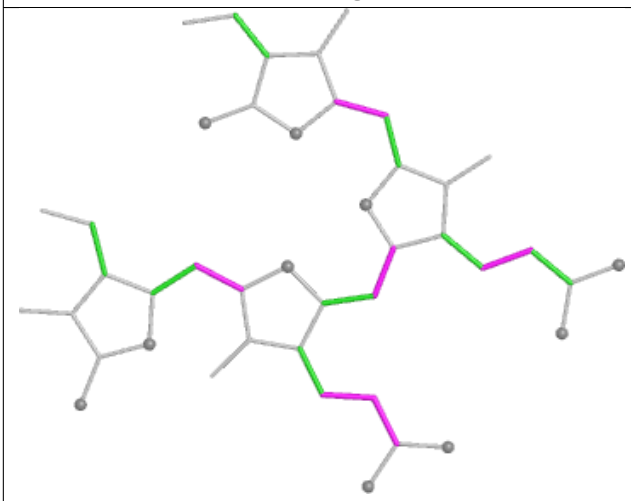
Ligand PEB ZF 202



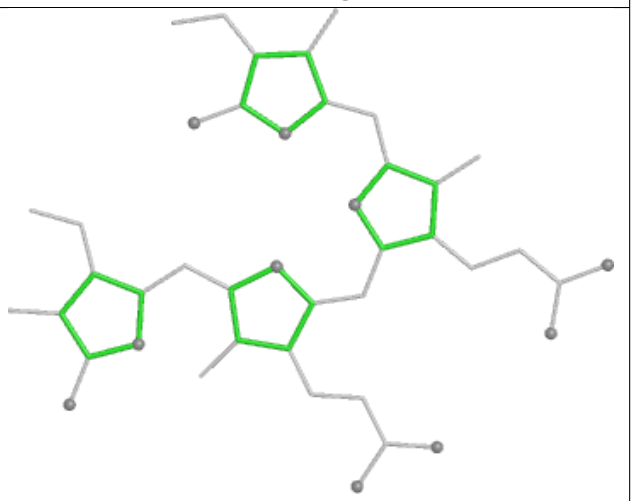
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Bond angles

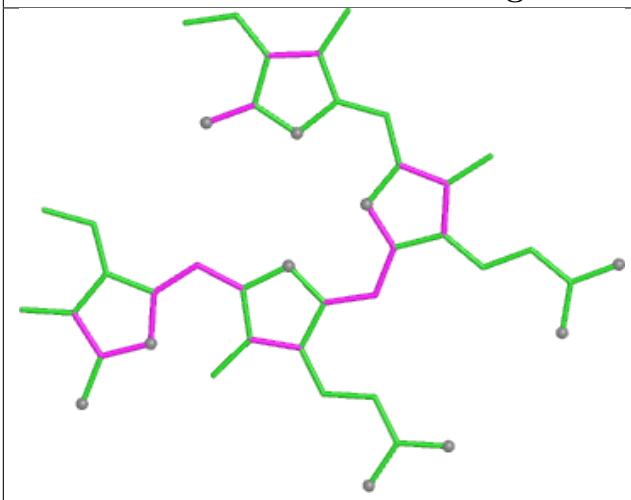


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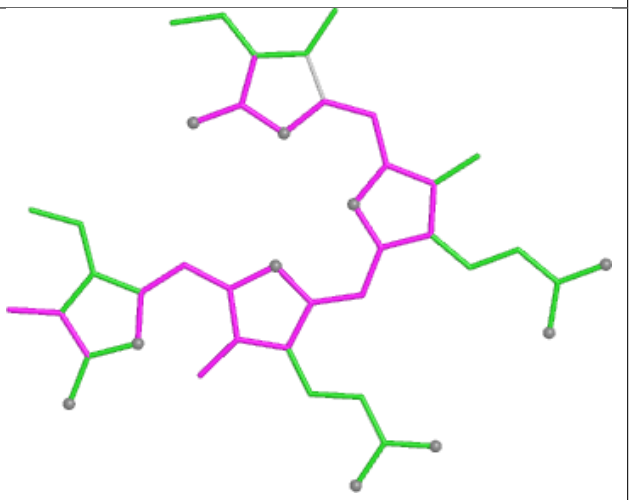


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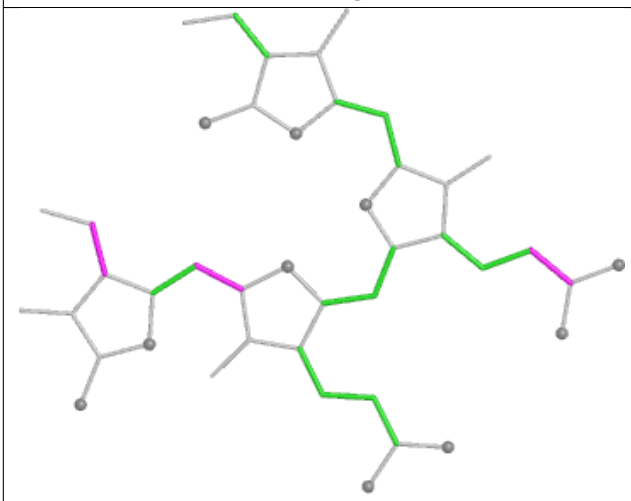
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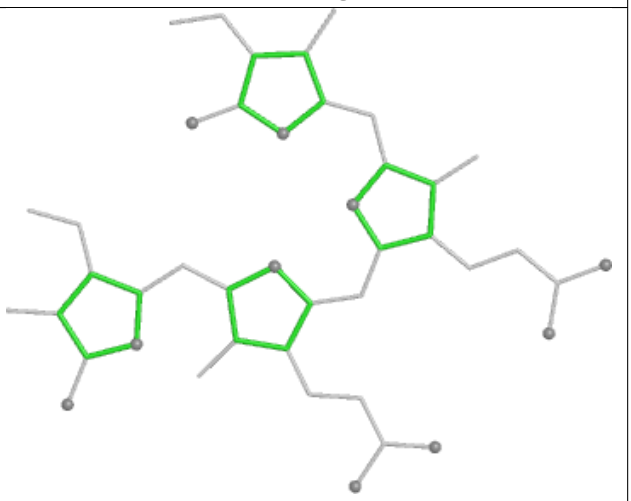
Bond lengths



Bond angles

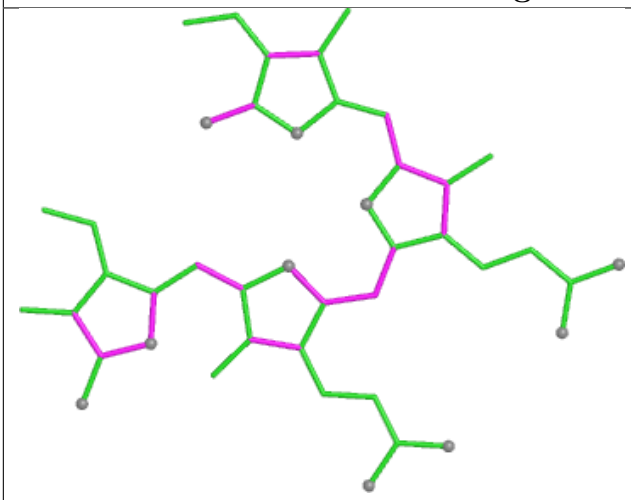


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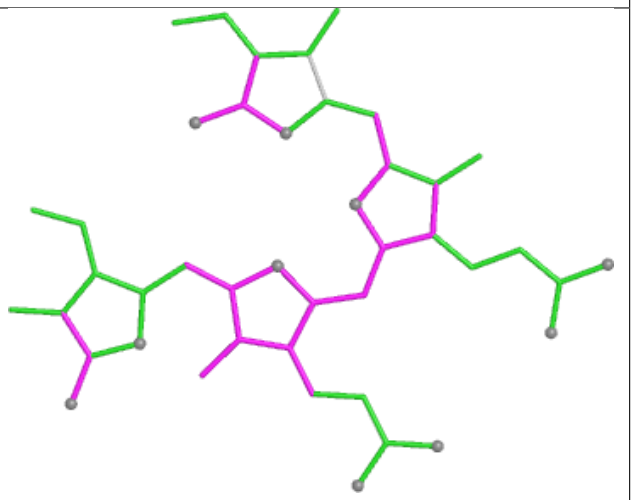


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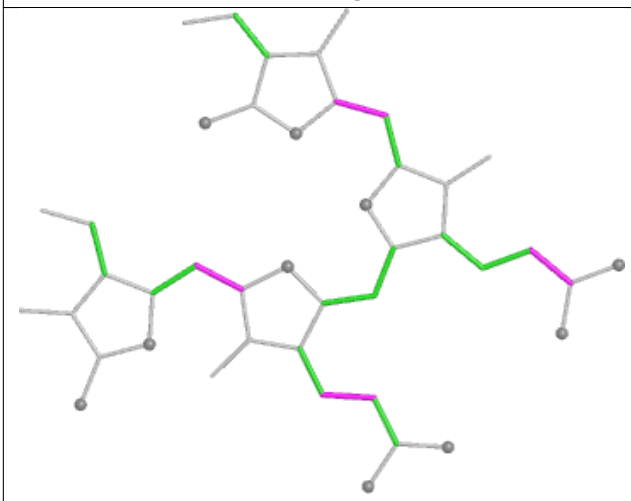
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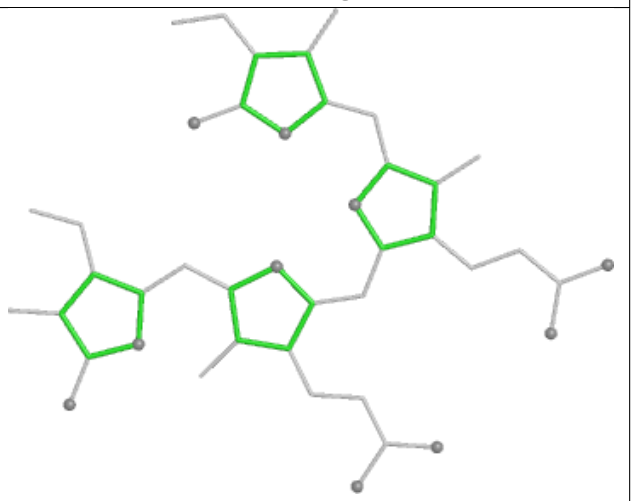
Bond lengths



Bond angles

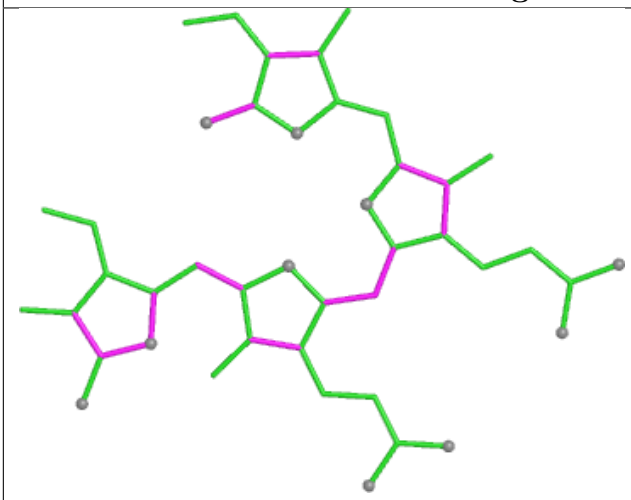


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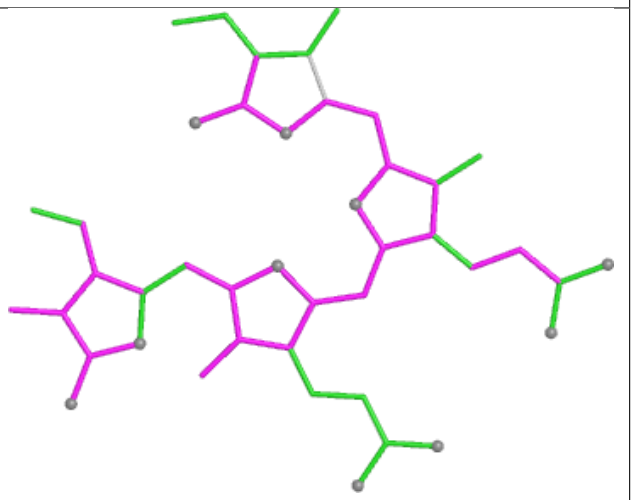


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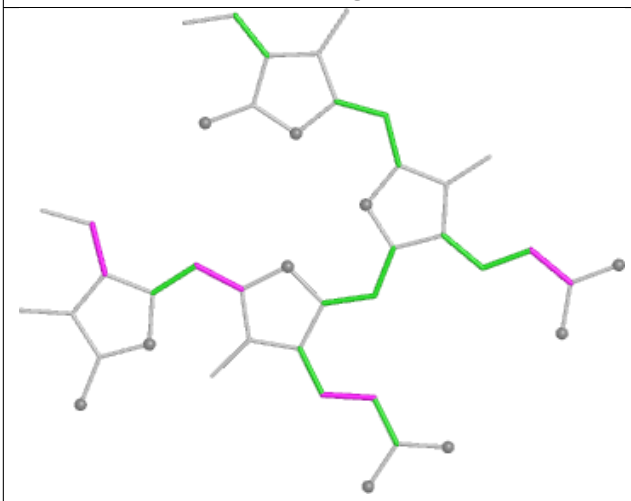
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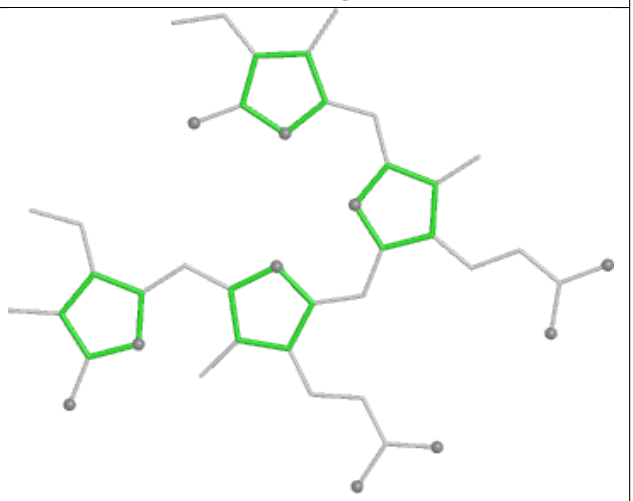
Bond lengths



Bond angles

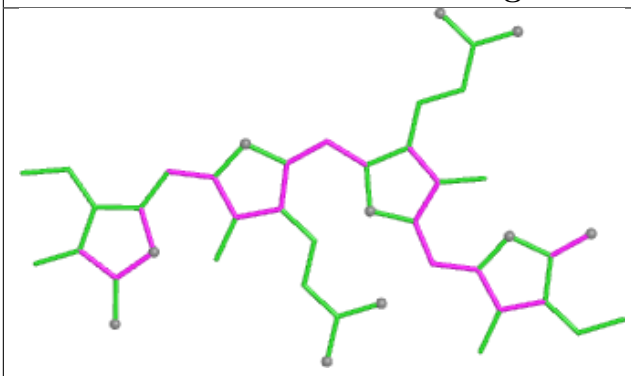


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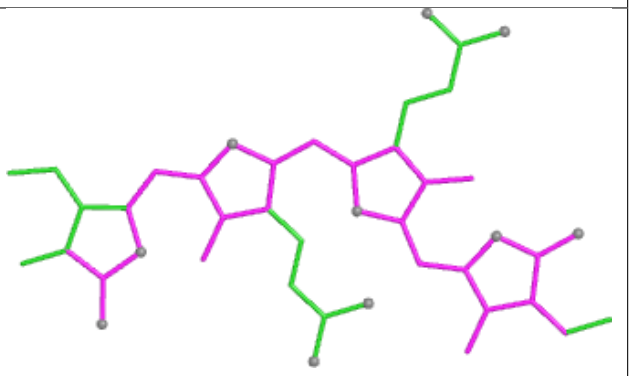


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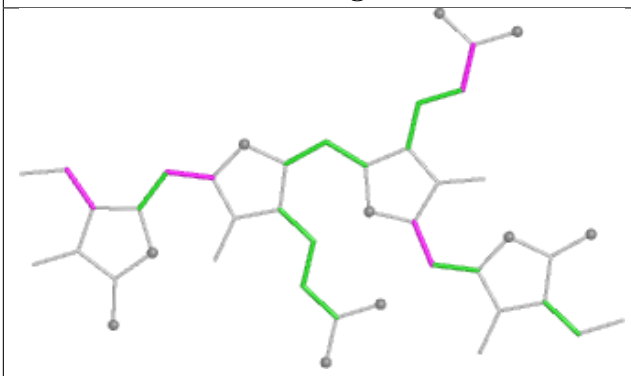
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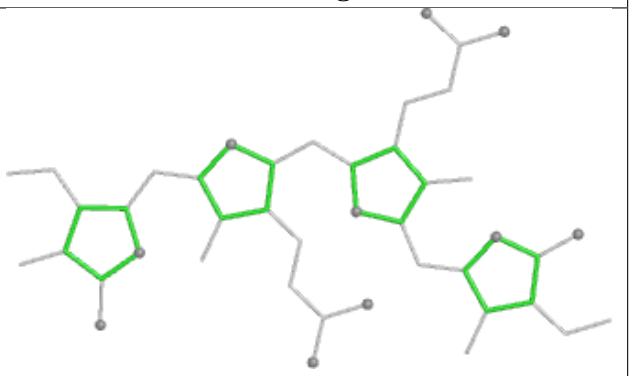
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Bond angles

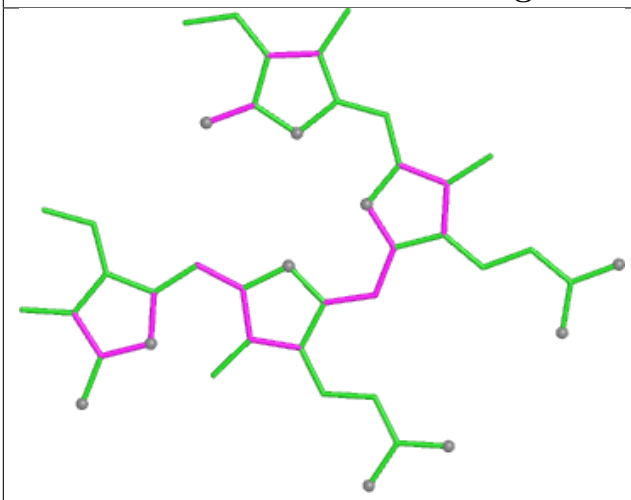


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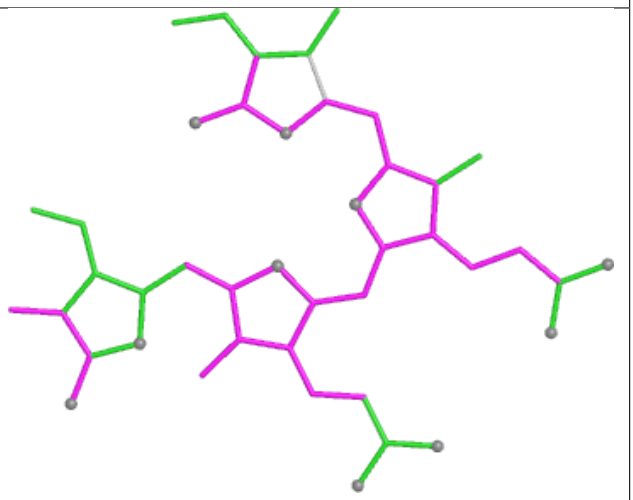


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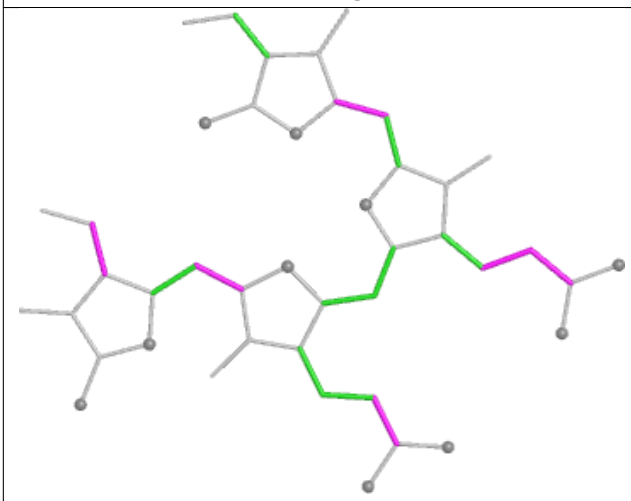
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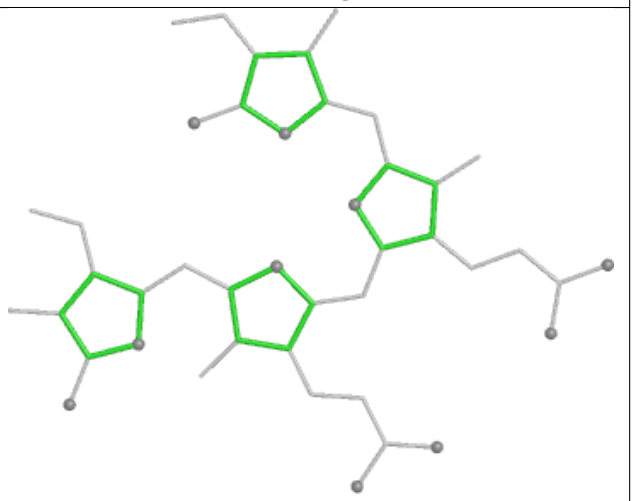
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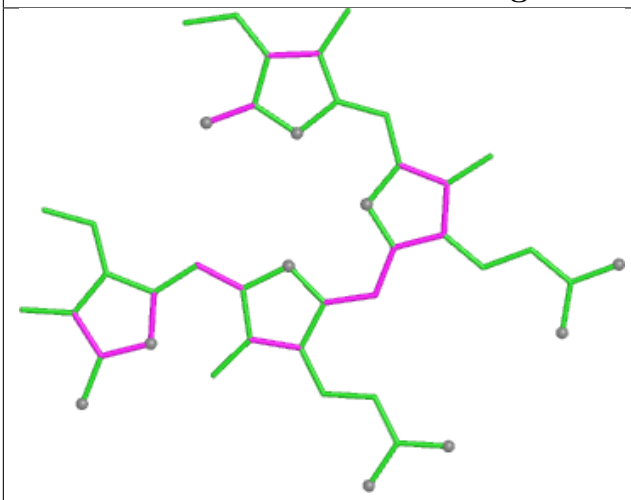


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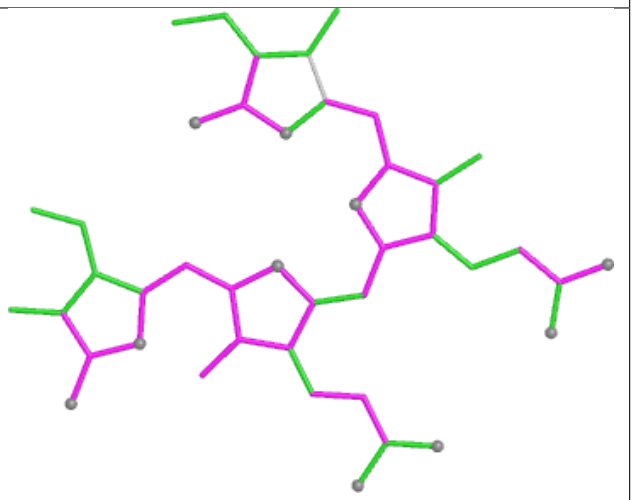


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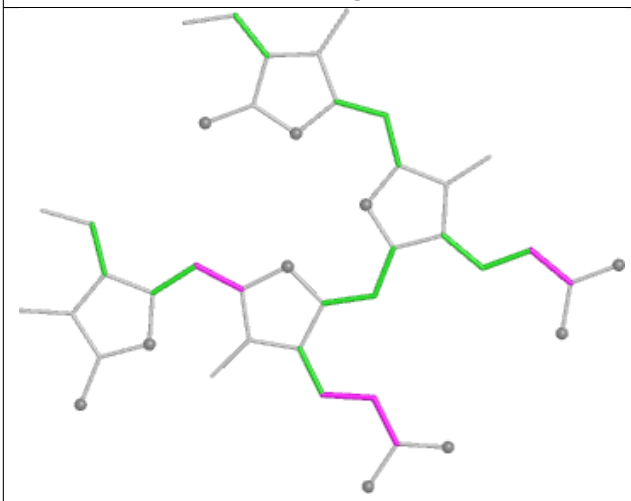
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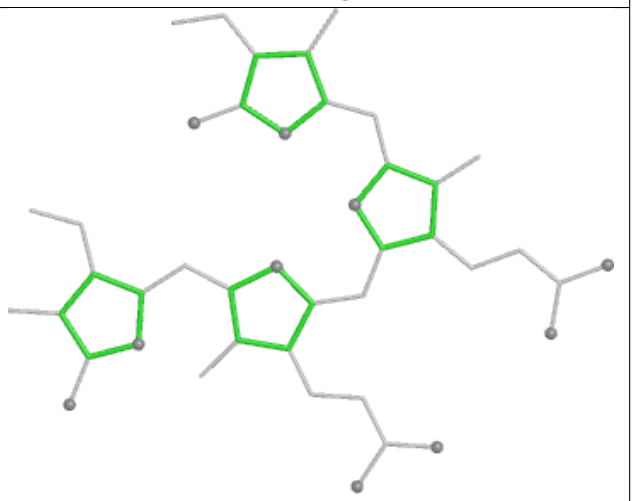
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Bond angles

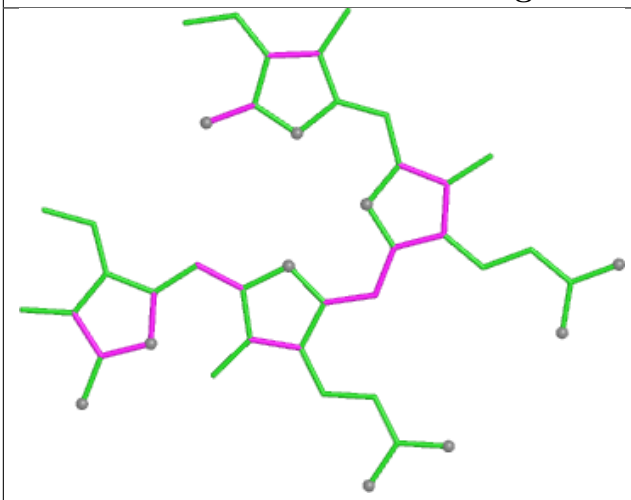


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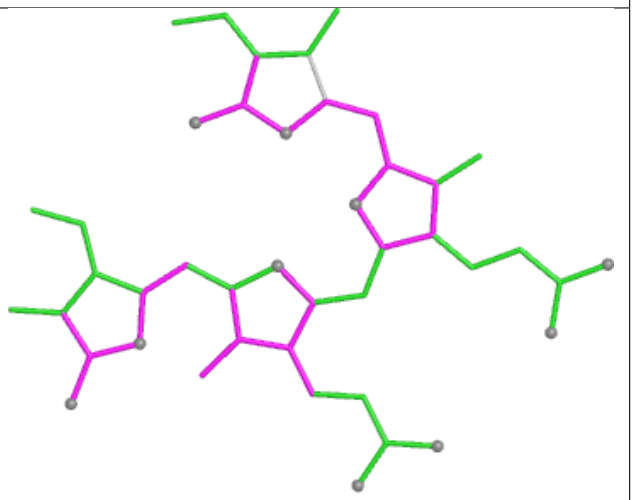


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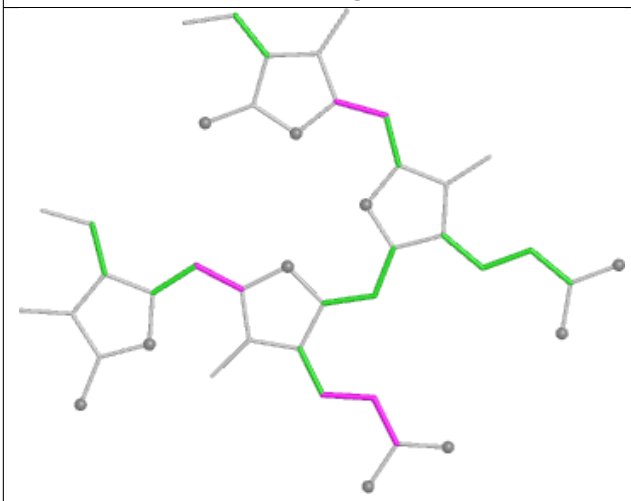
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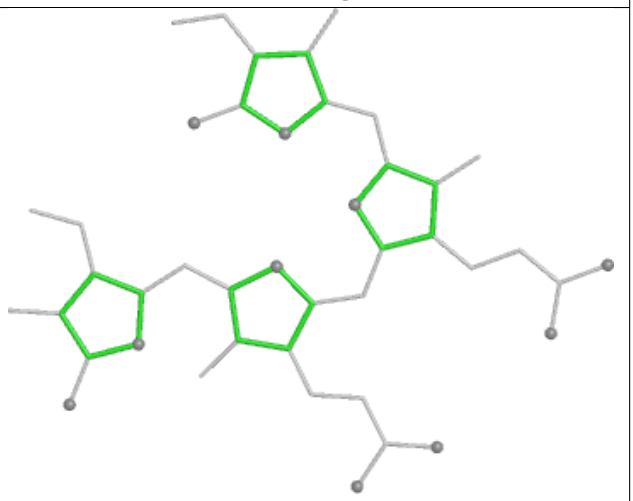
Bond lengths



Bond angles

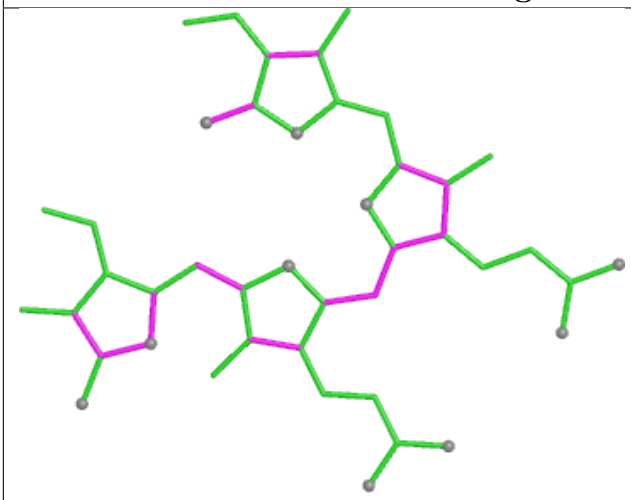


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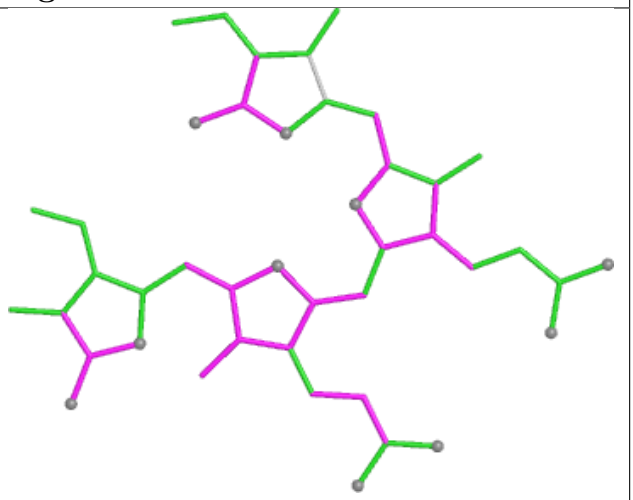


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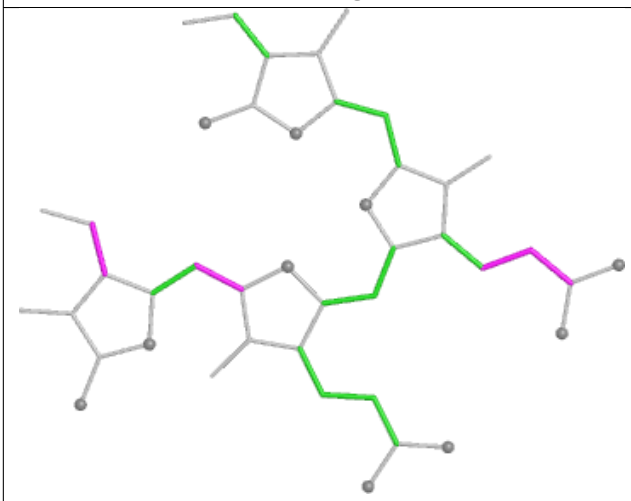
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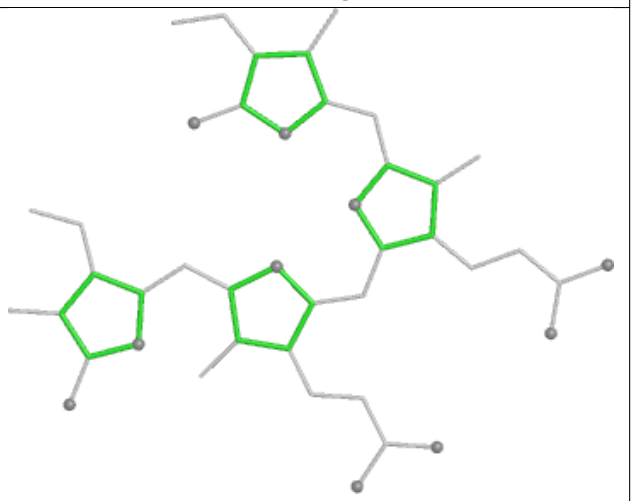
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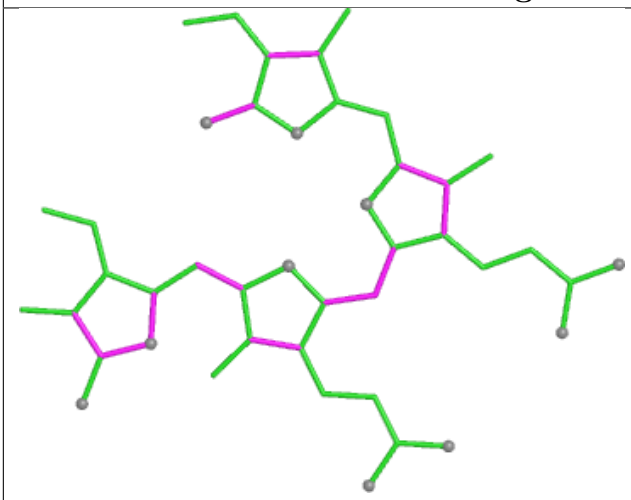


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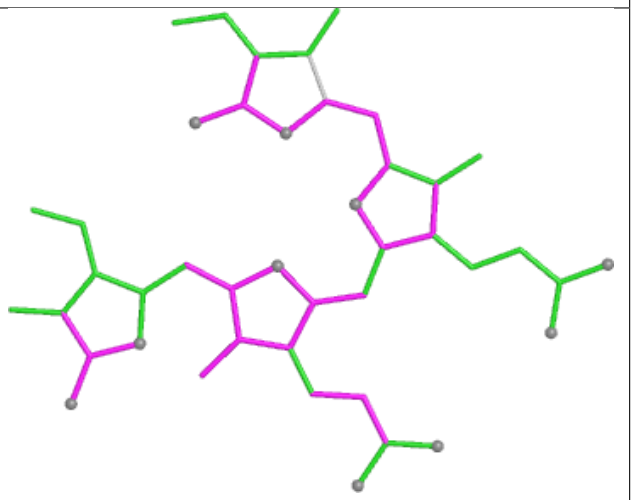


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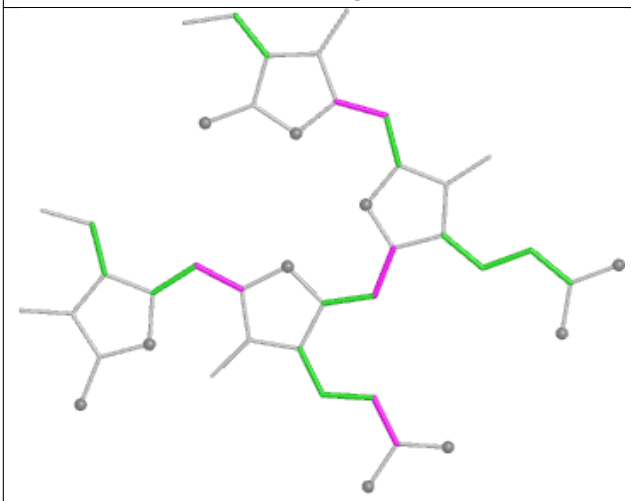
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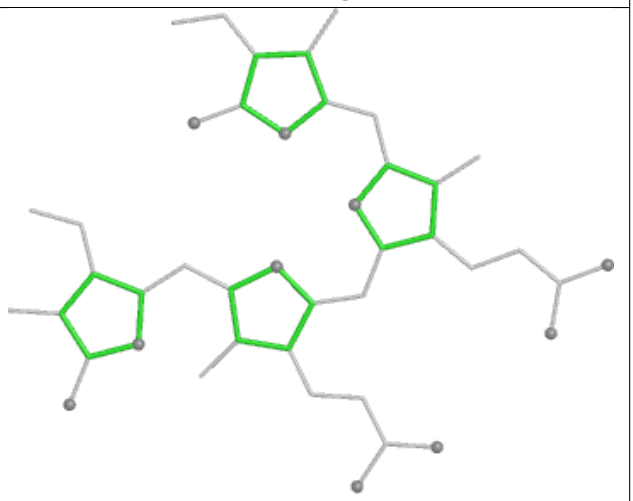
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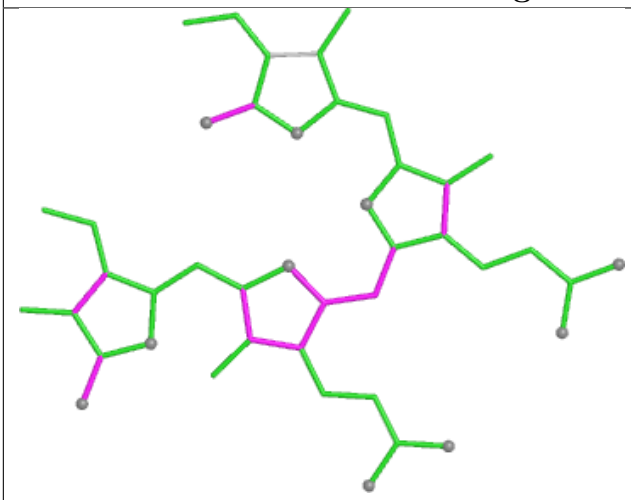


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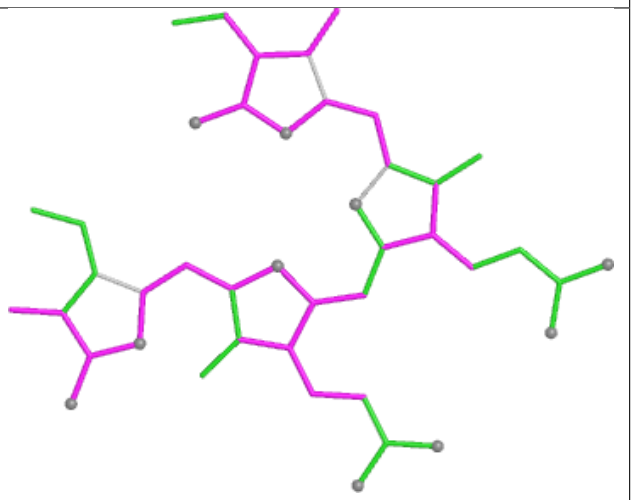


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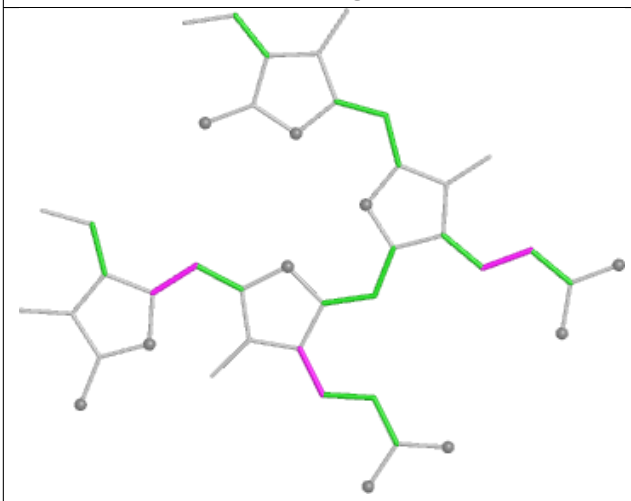
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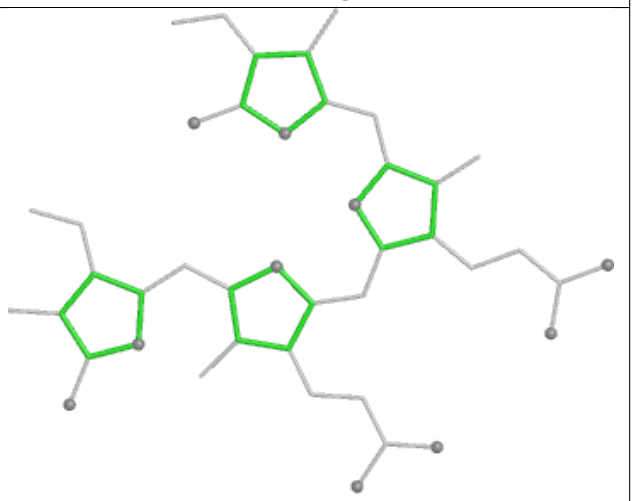
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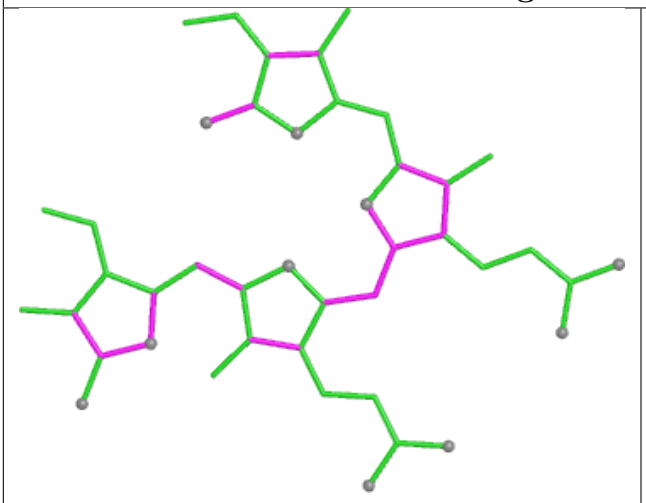


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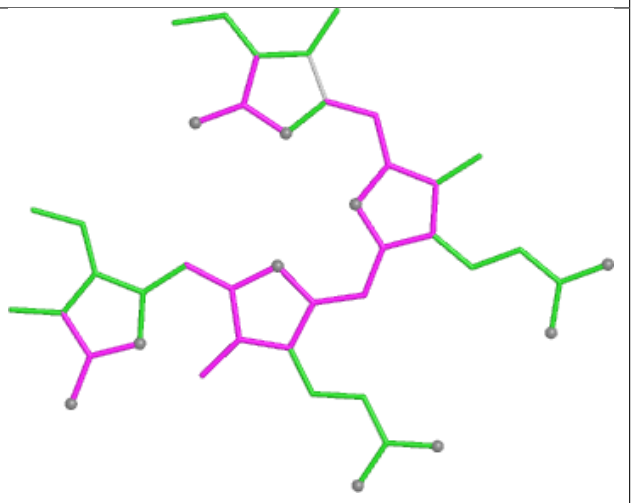


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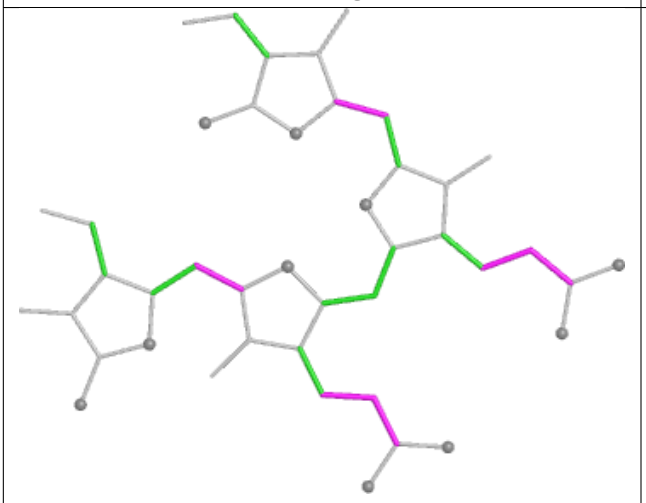
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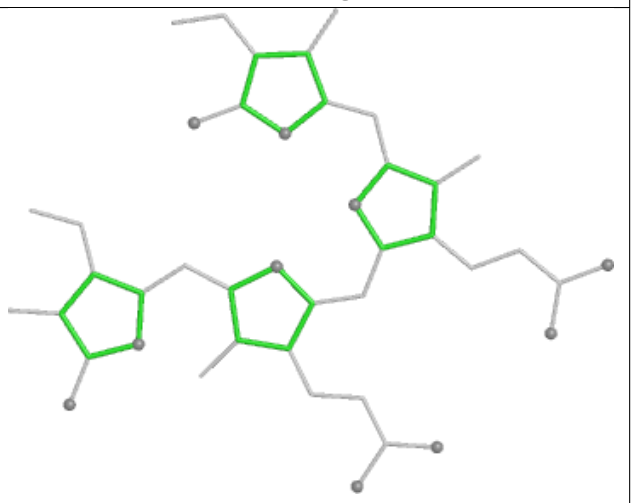
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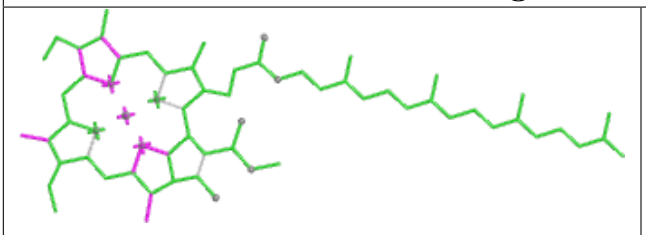


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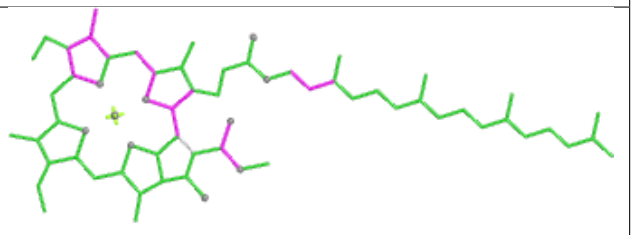


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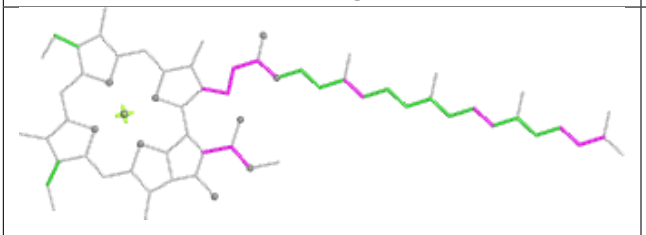
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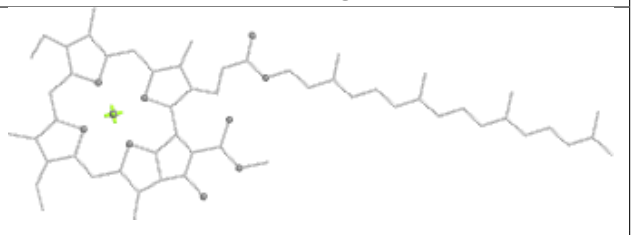
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Bond angles

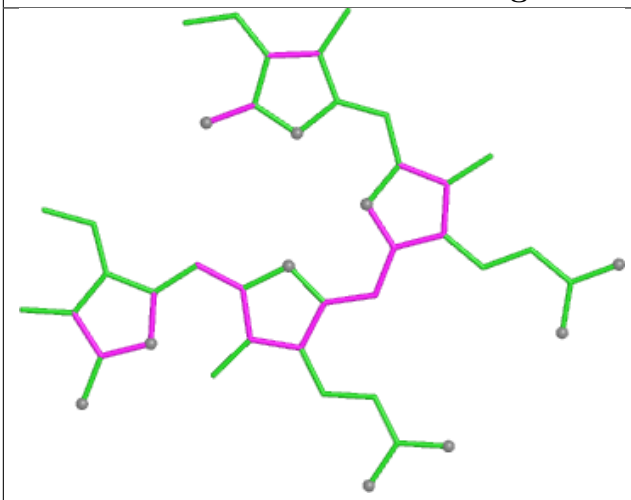


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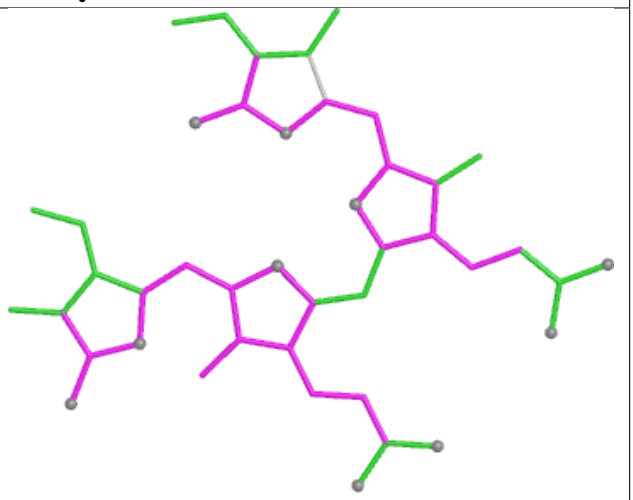


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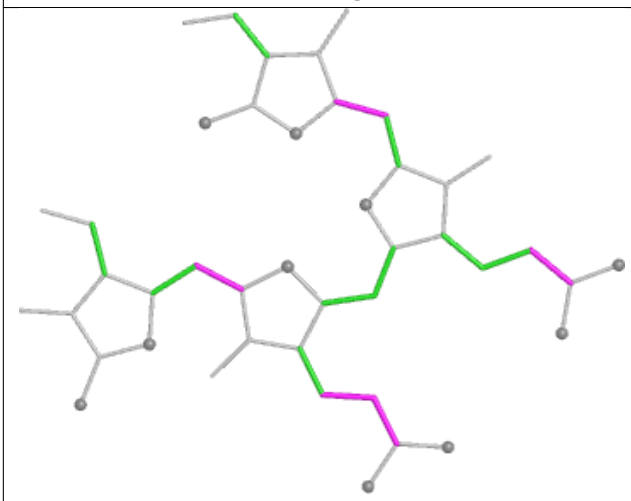
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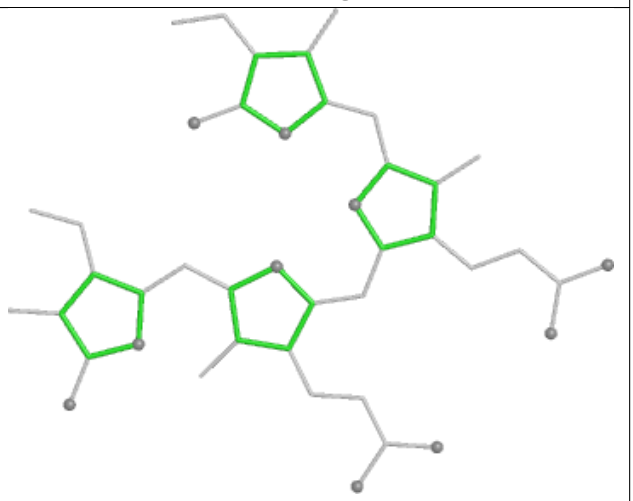
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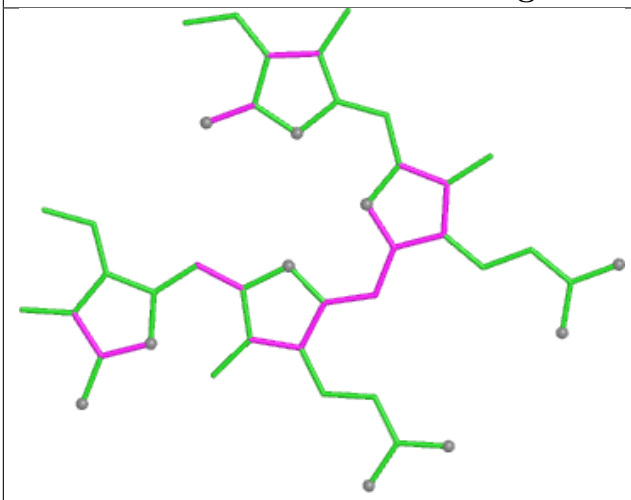


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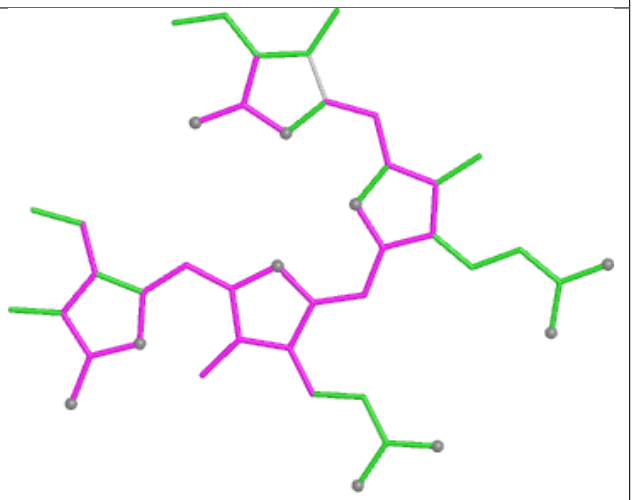


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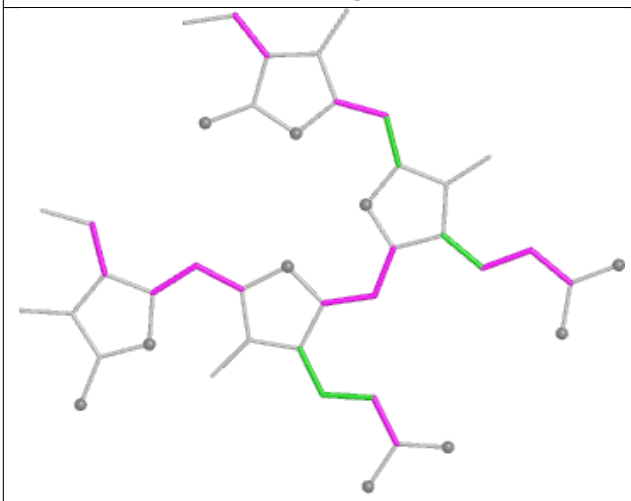
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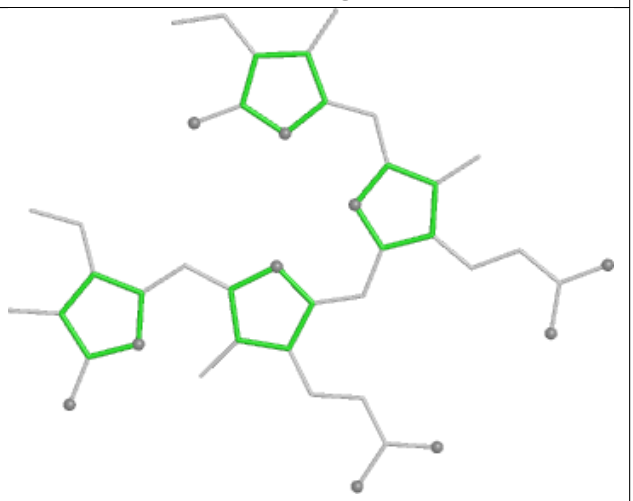
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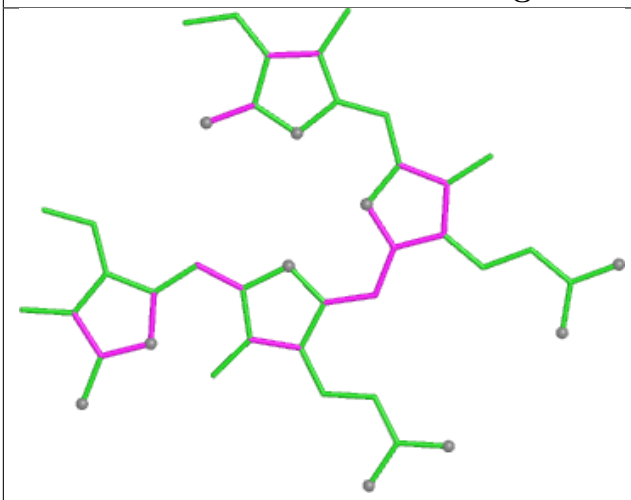


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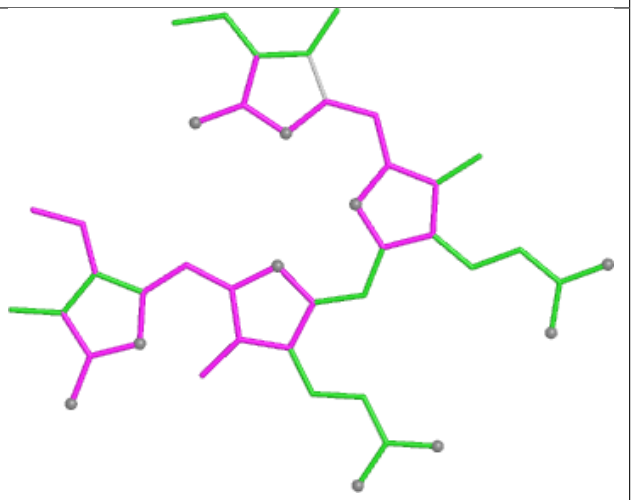


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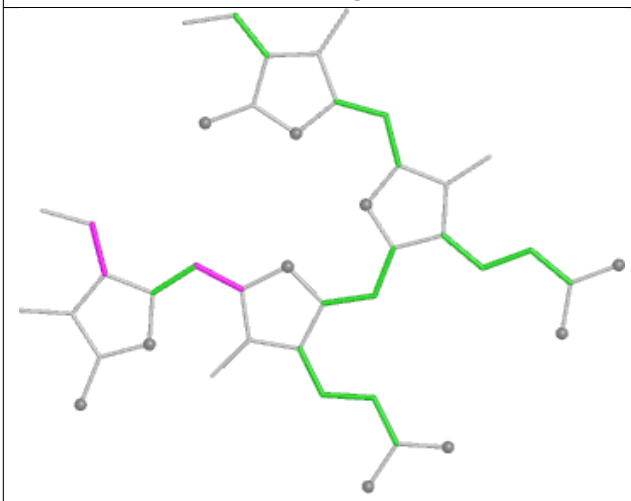
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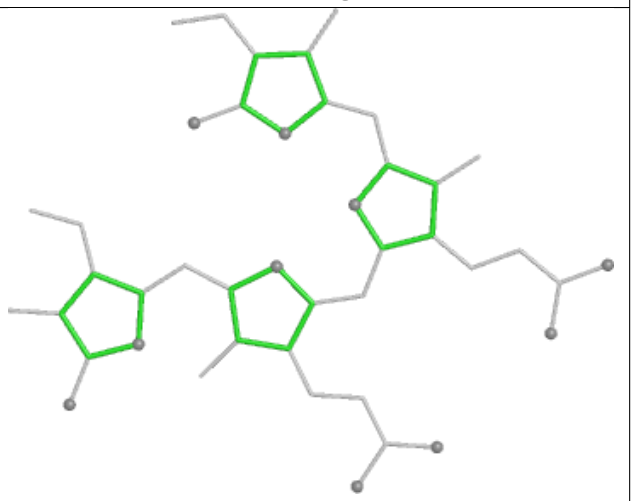
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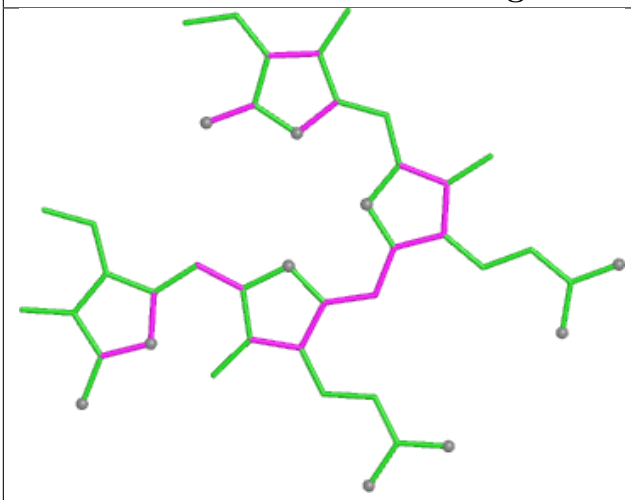


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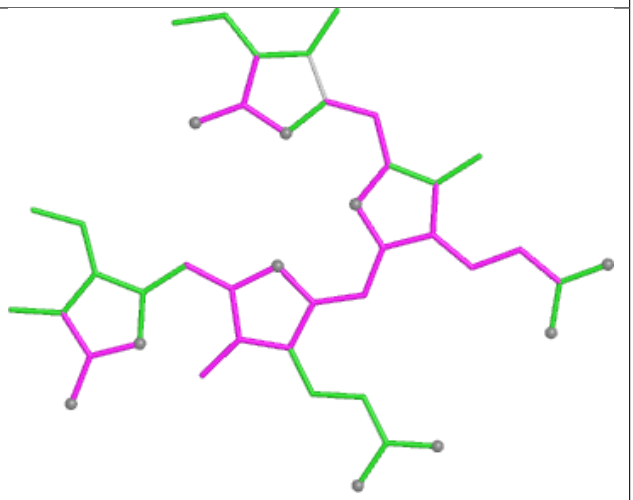


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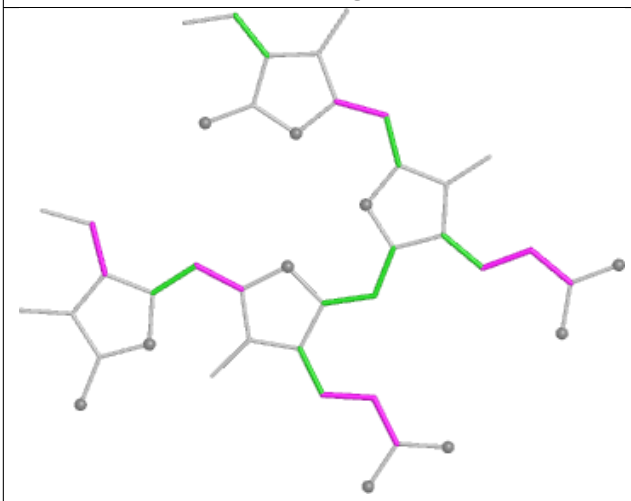
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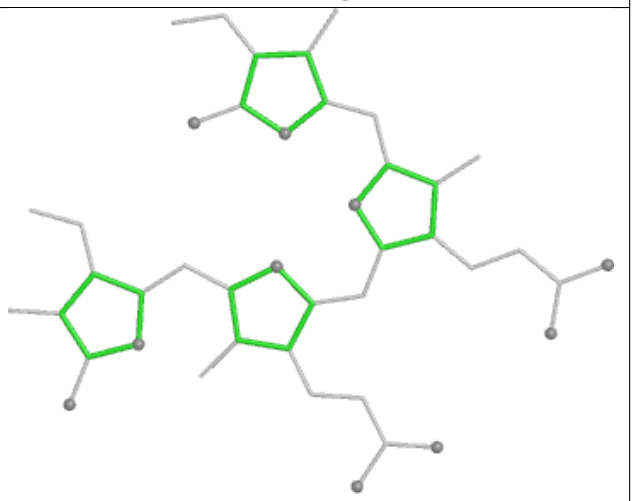
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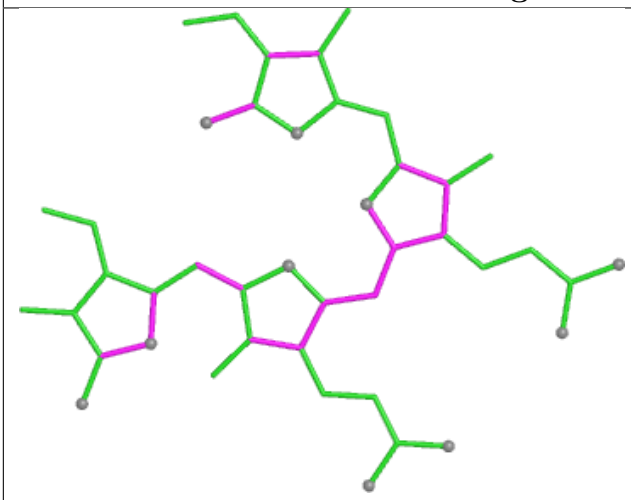


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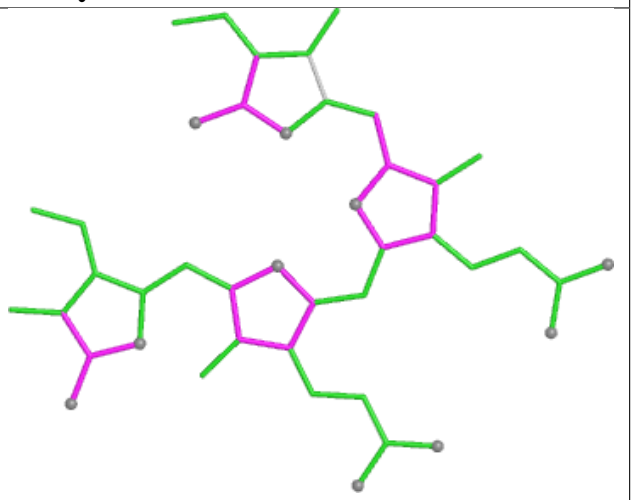


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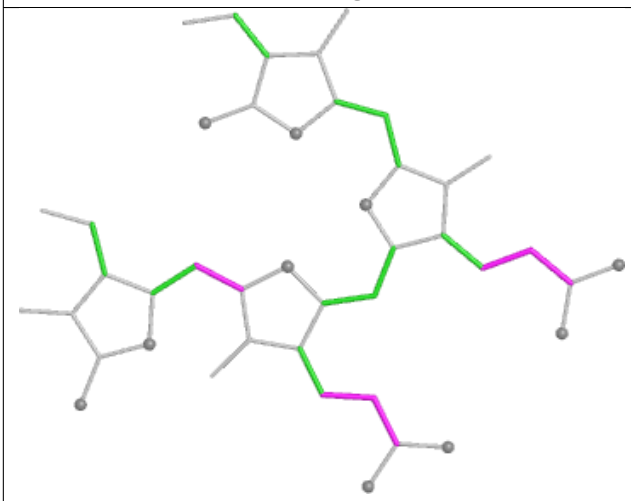
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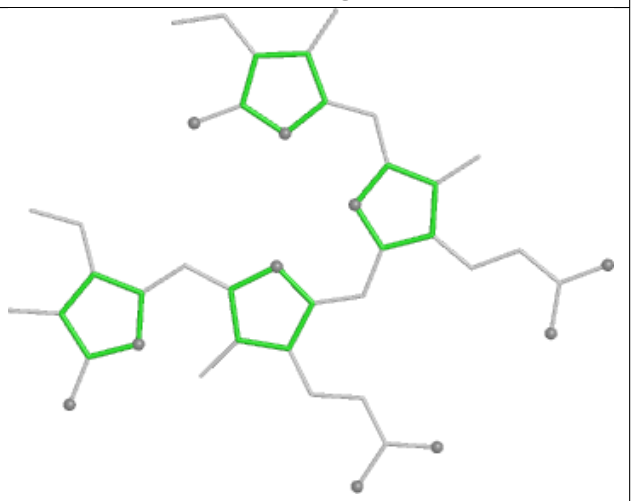
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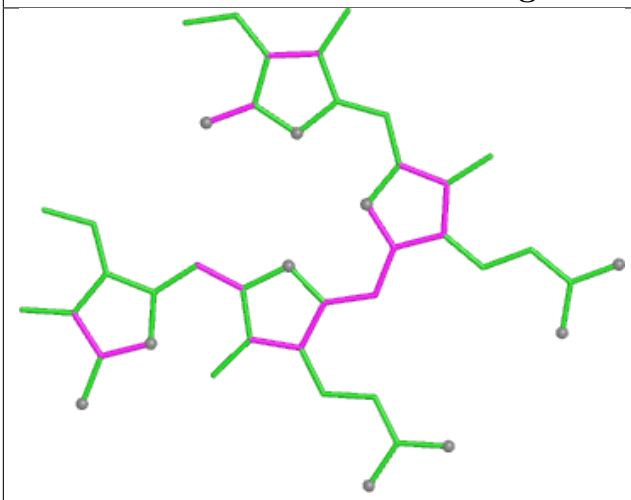


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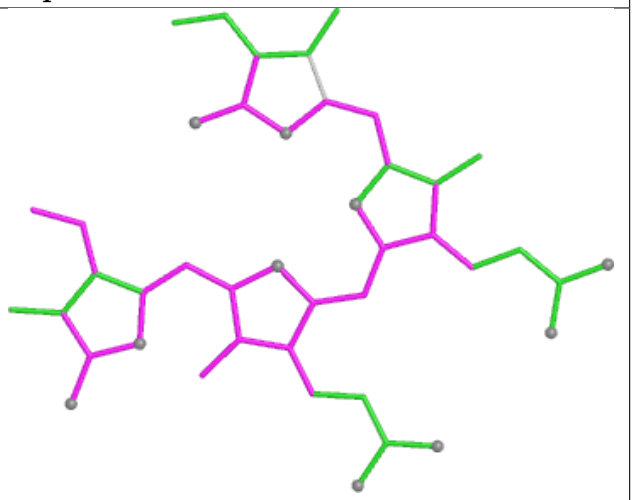


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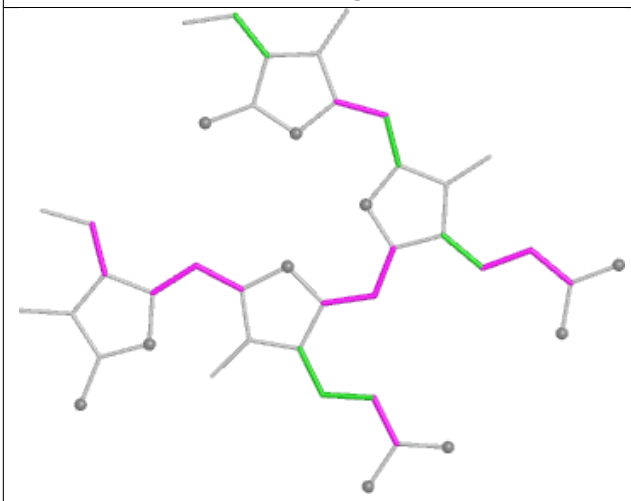
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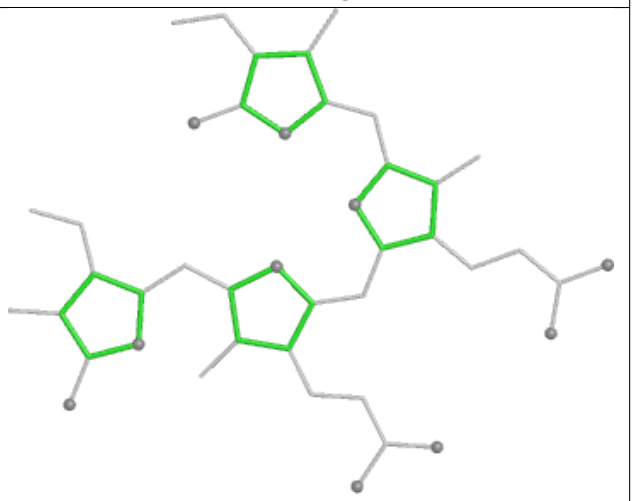
Bond lengths



Bond angles

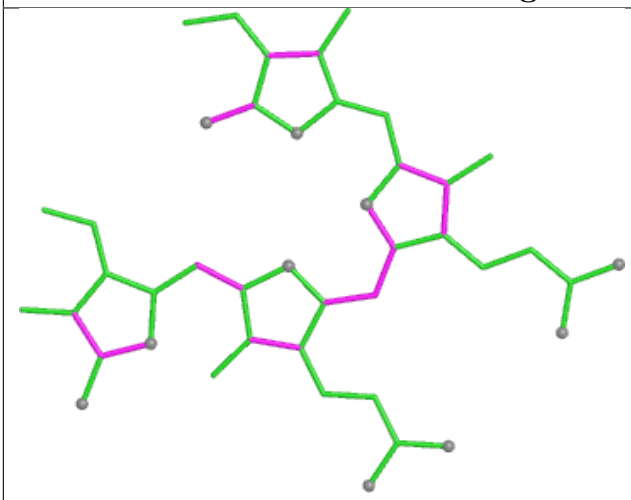


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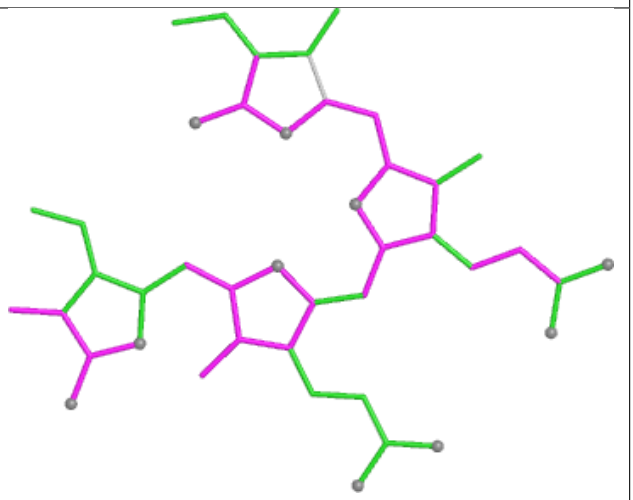


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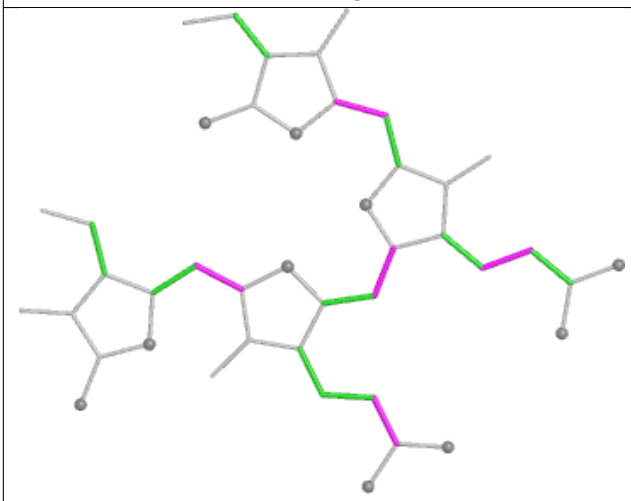
Ligand PEB FI 202



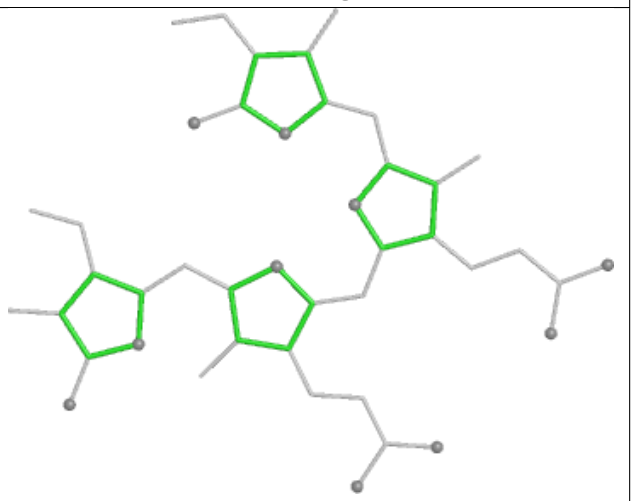
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Bond angles

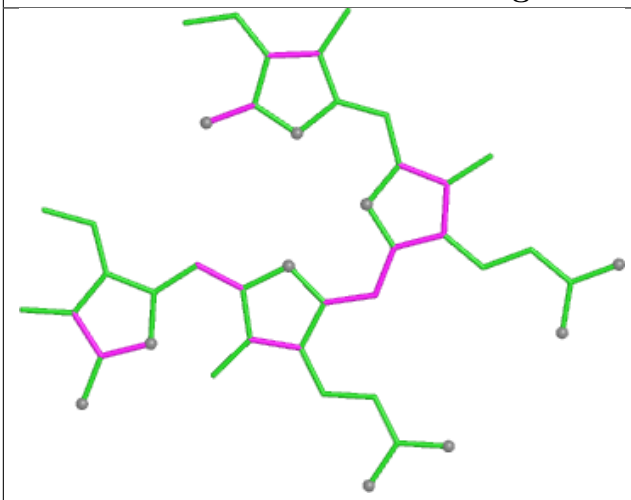


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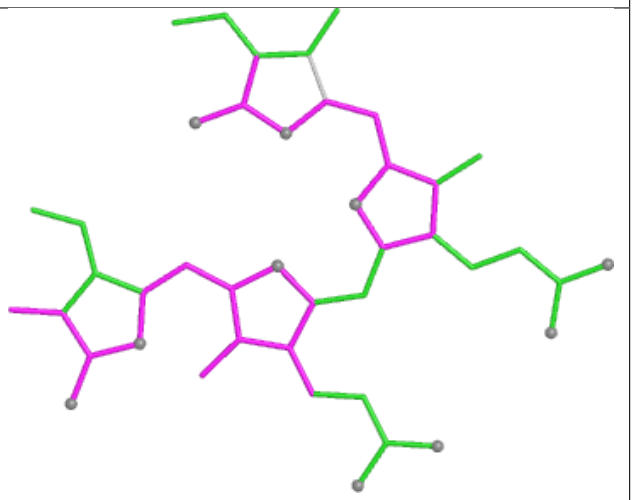


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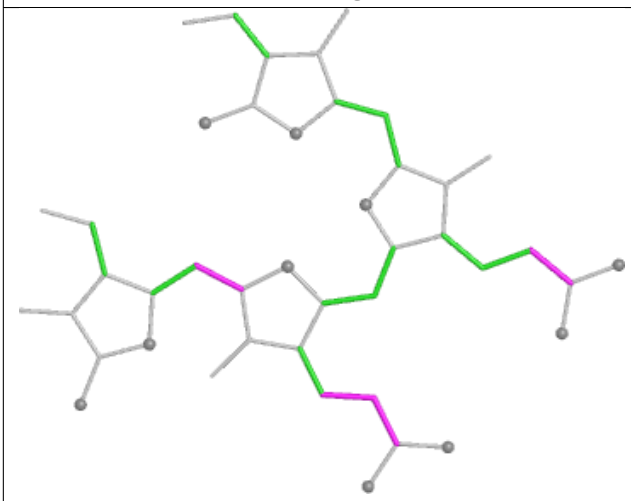
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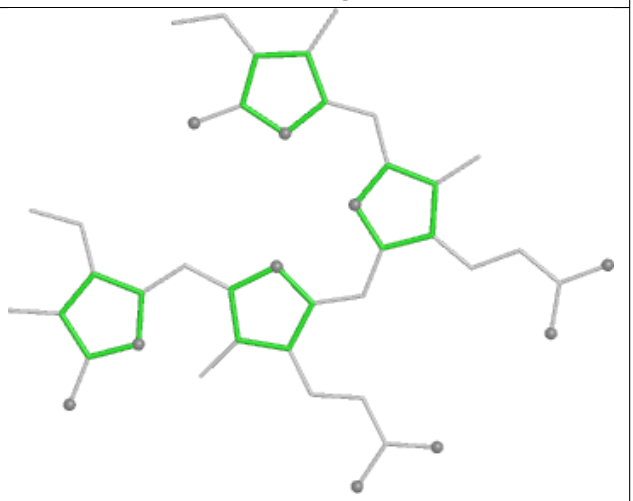
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Bond angles

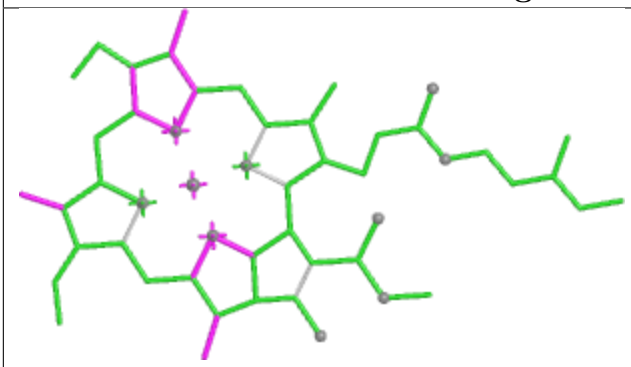


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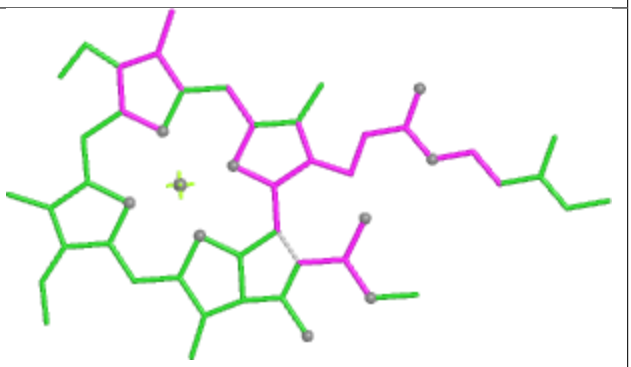


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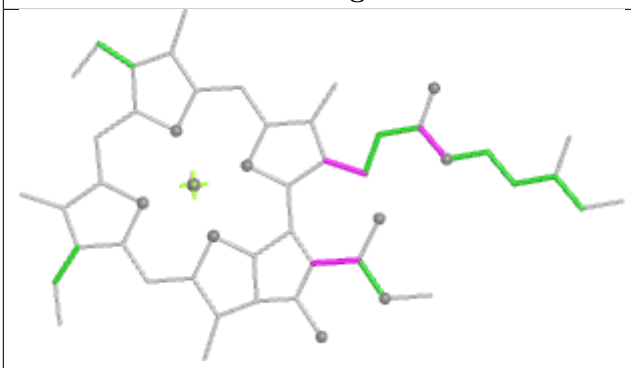
Ligand CLA A2 837



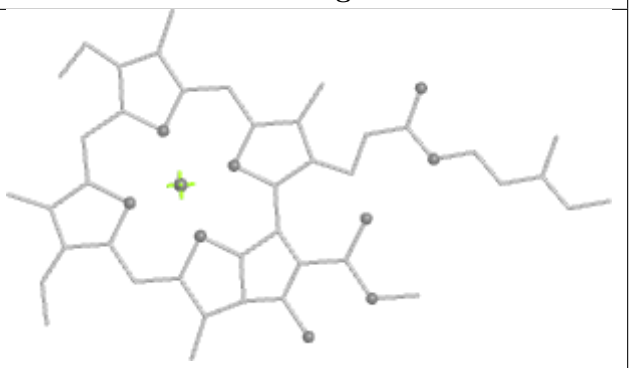
Bond lengths



Bond angles

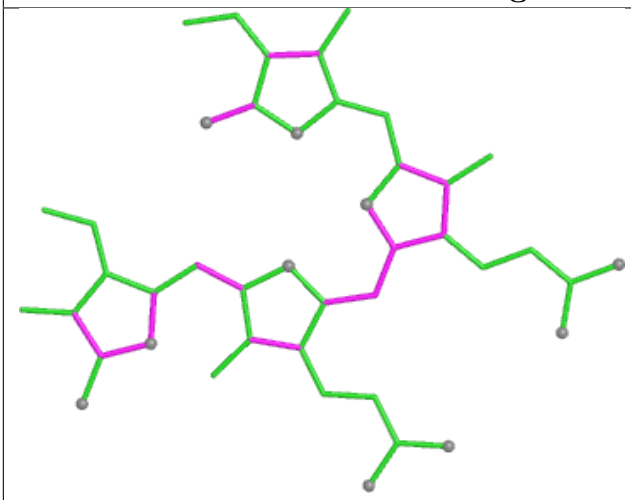


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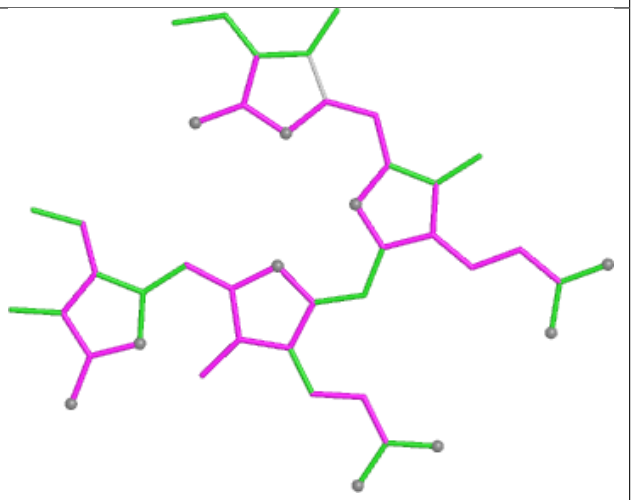


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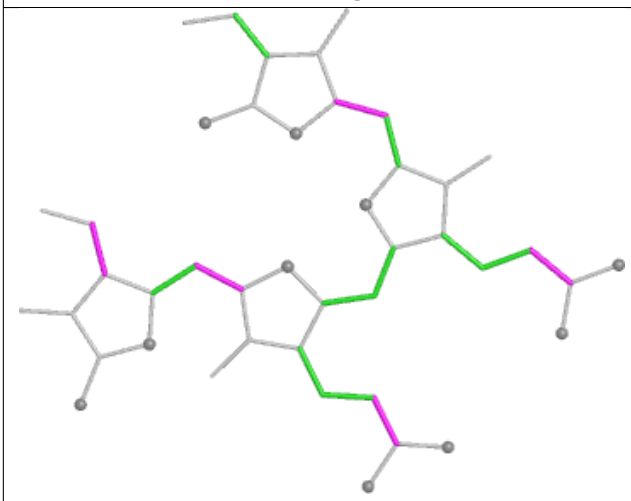
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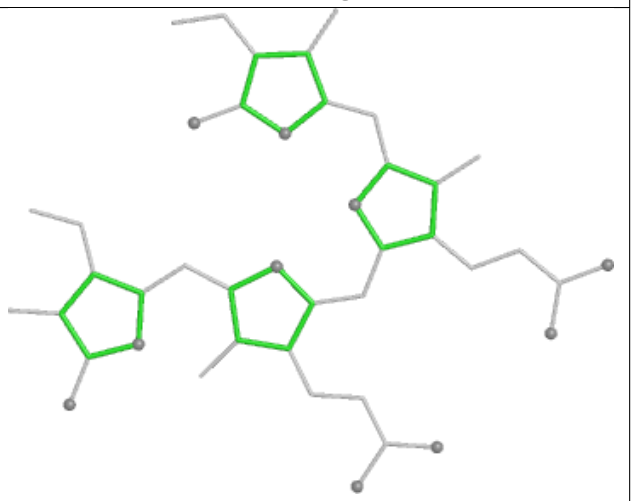
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Bond angles

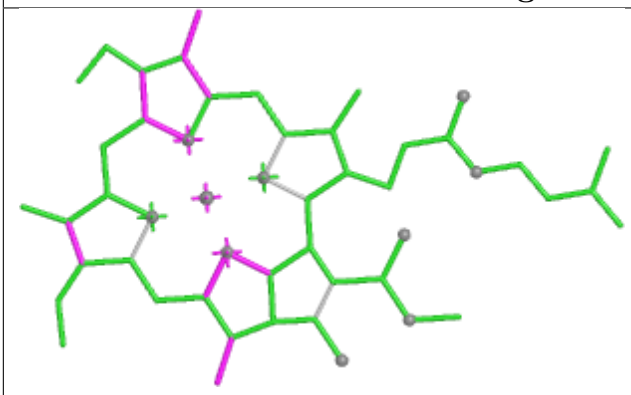


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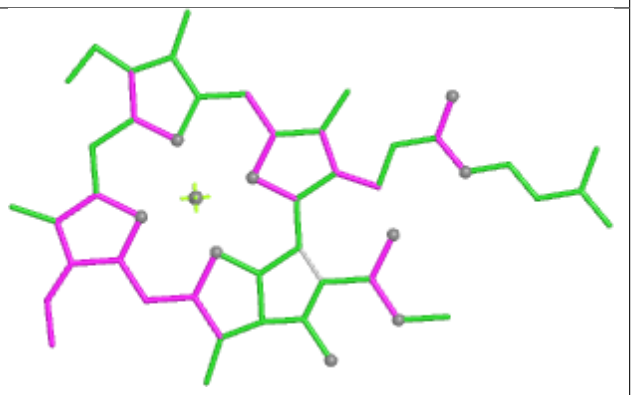


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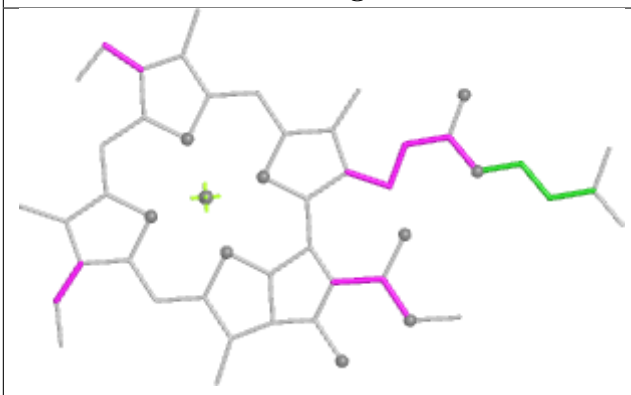
Ligand CLA L2 204



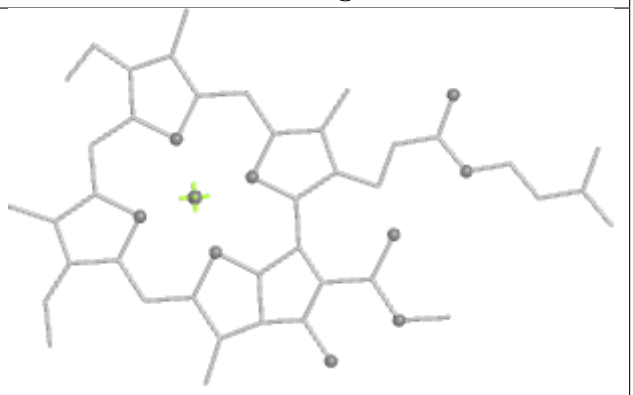
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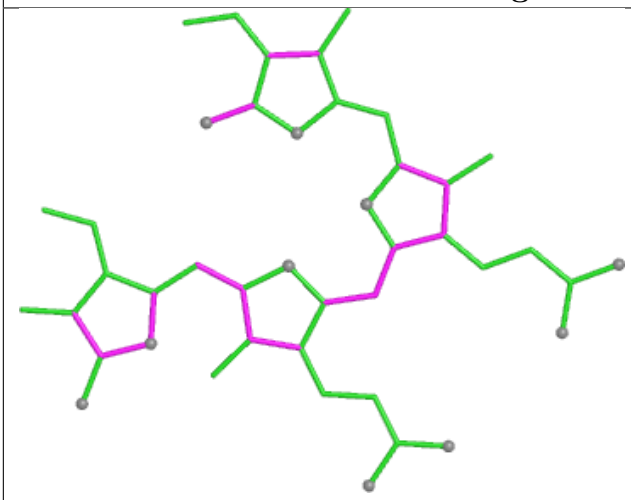


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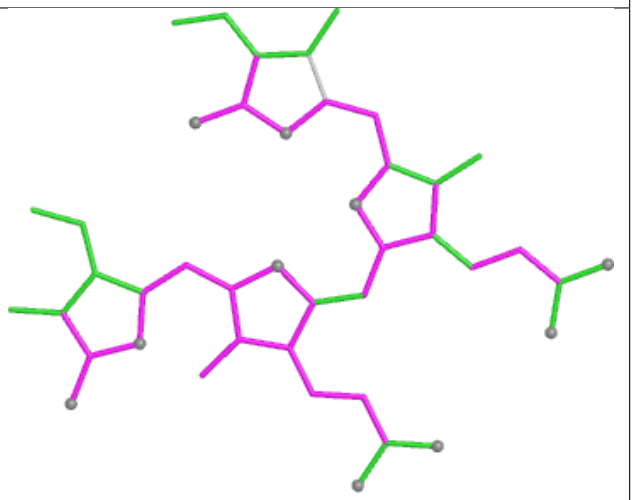


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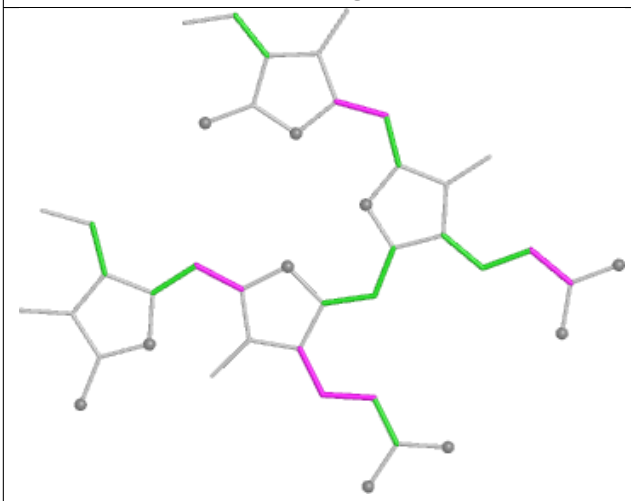
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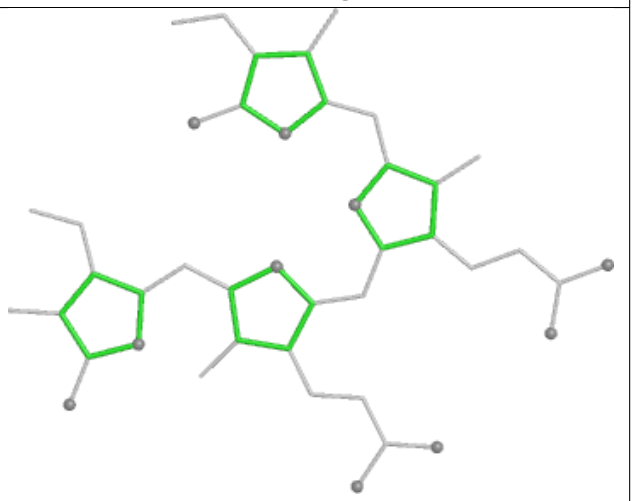
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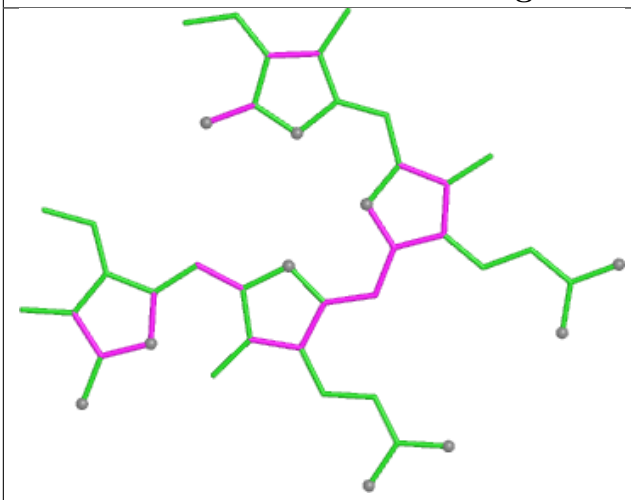


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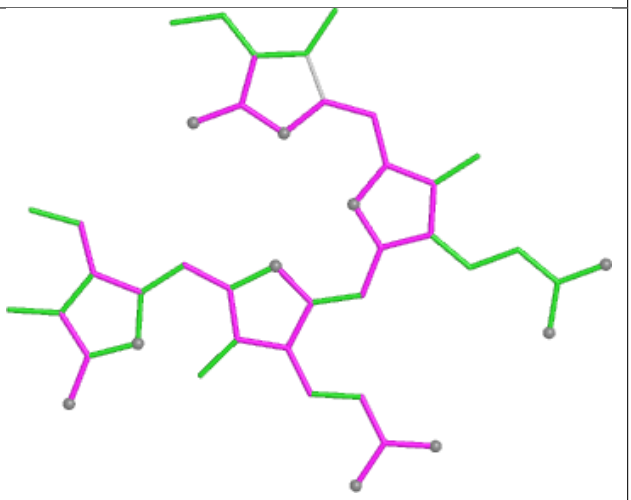


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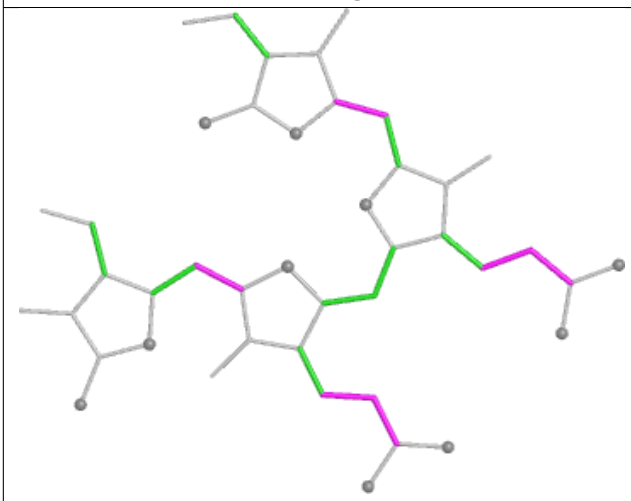
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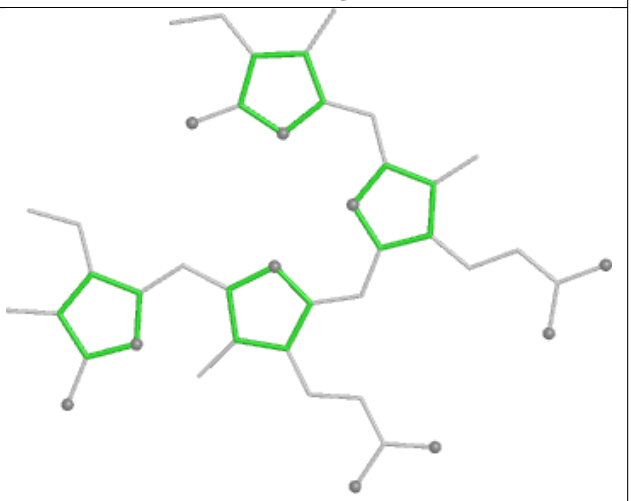
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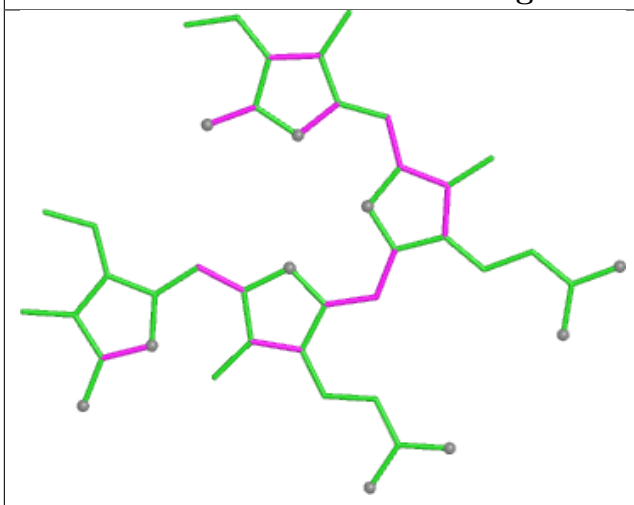


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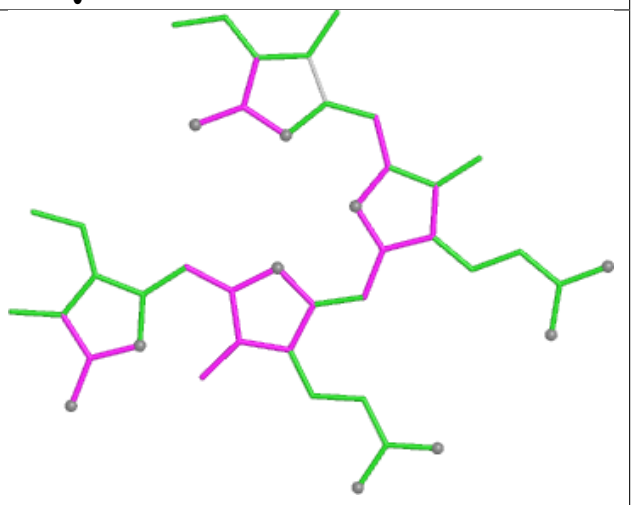


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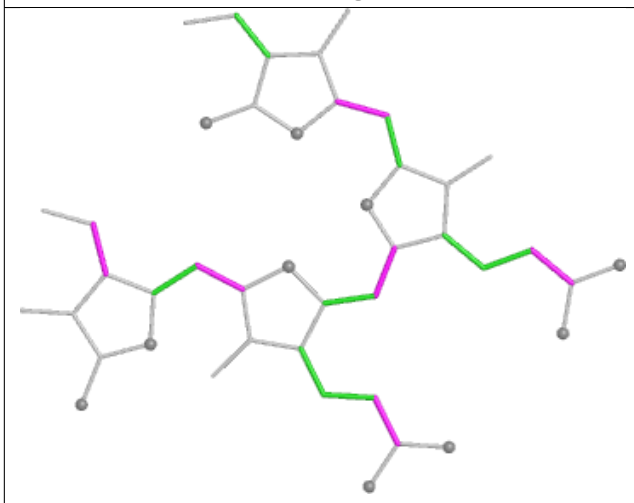
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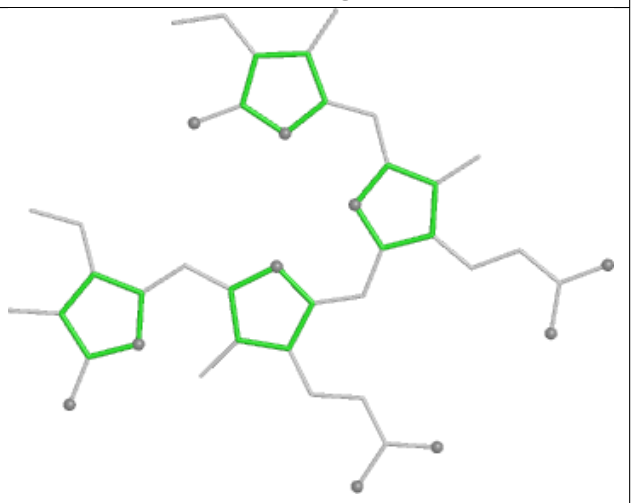
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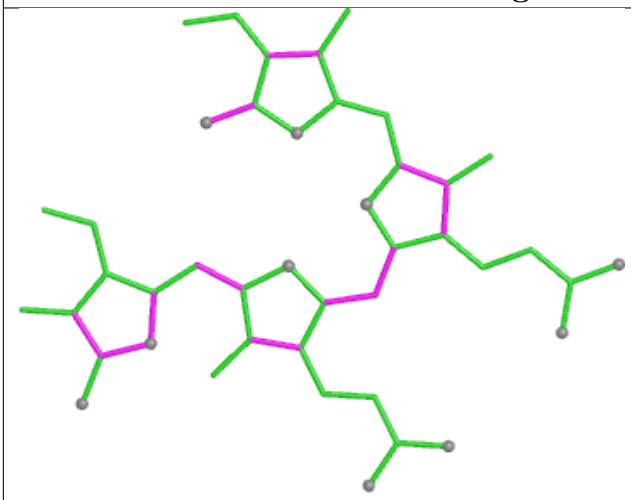


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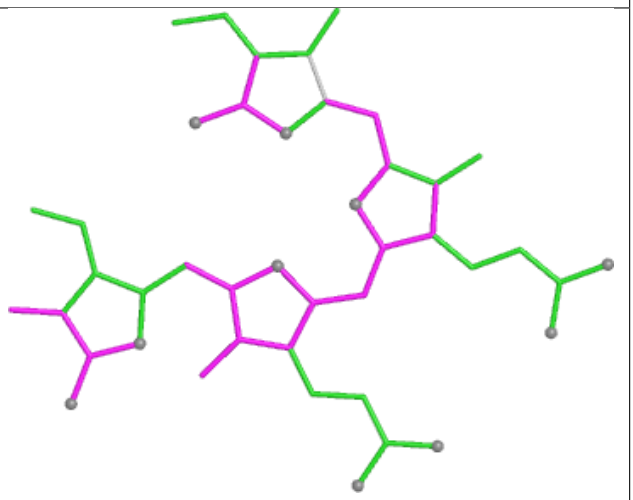


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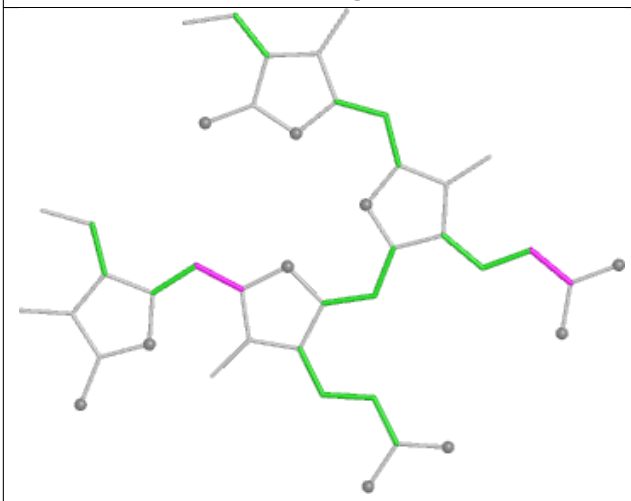
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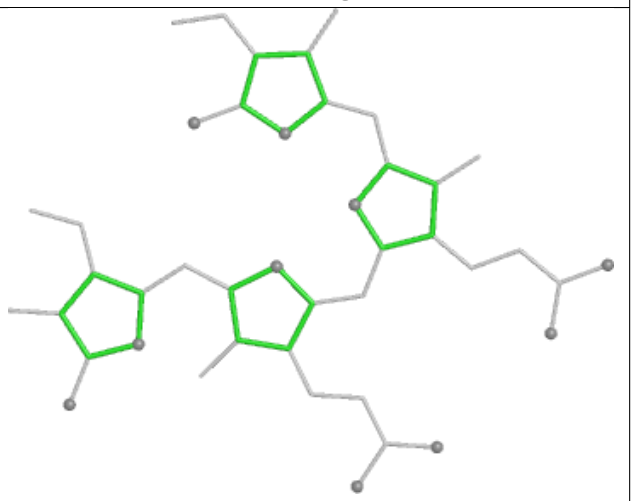
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Bond angles

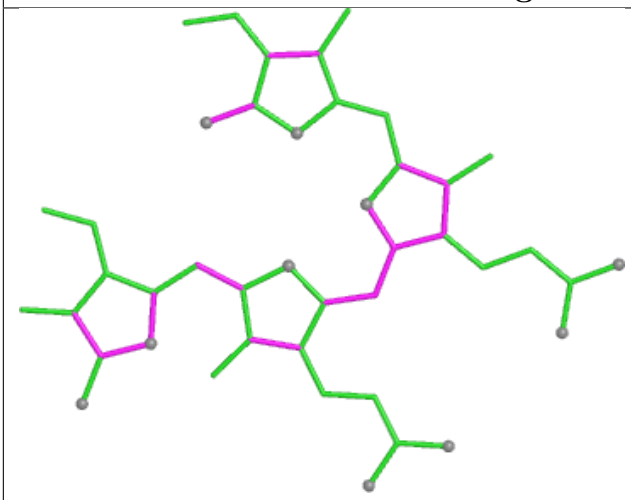


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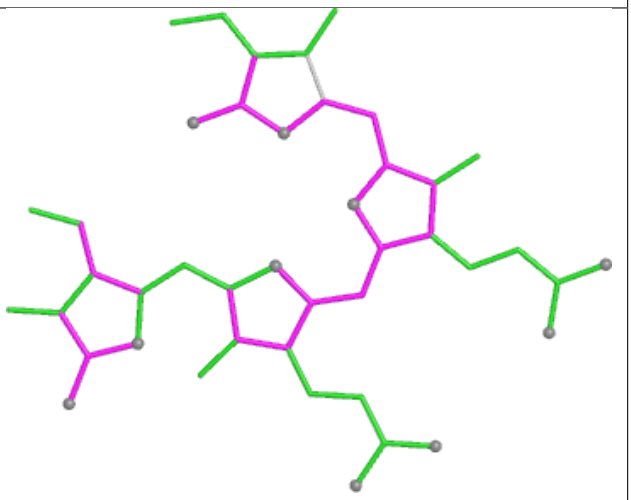


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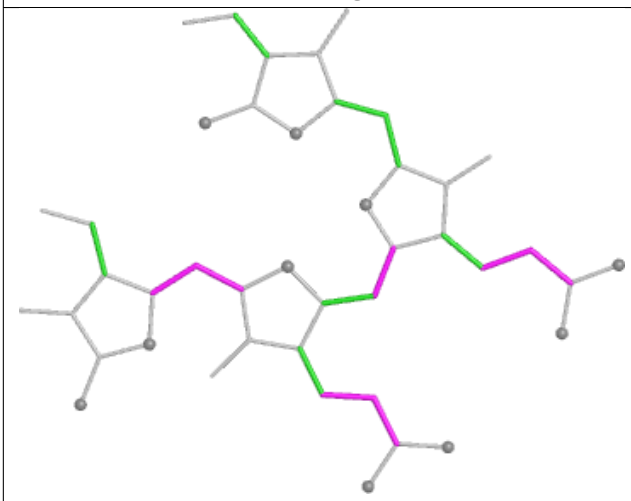
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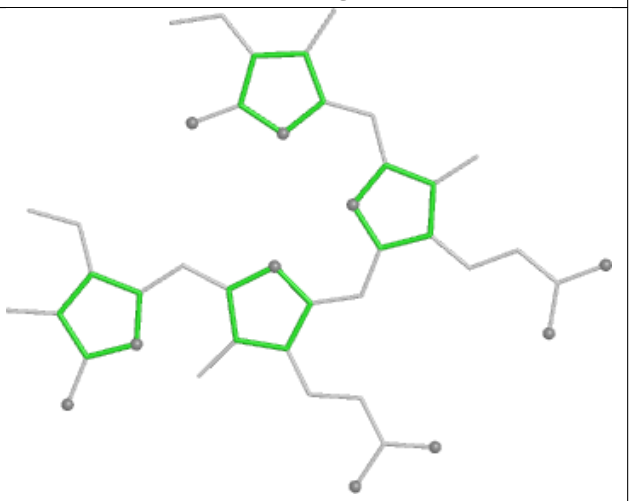
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Bond angles

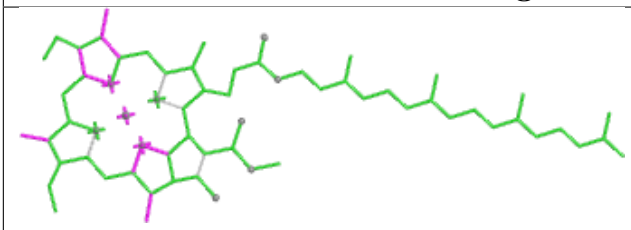


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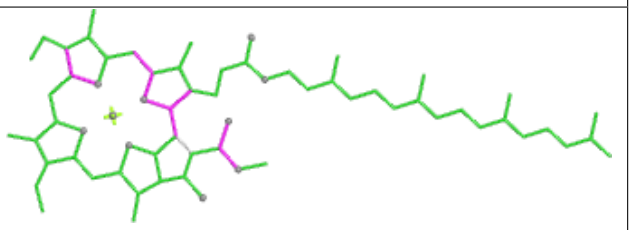


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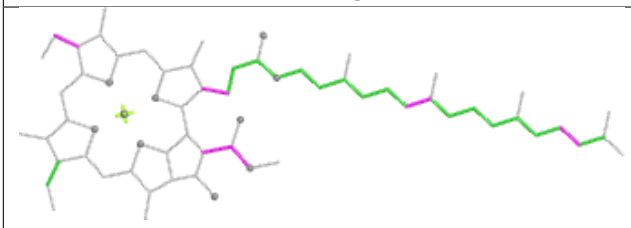
Ligand CLA B2 807



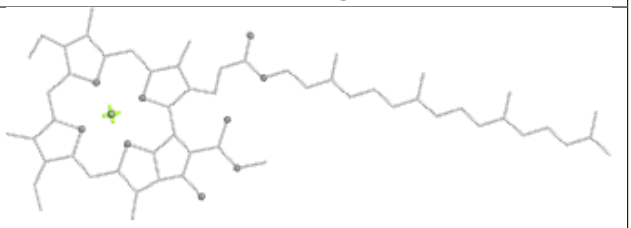
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Bond angles

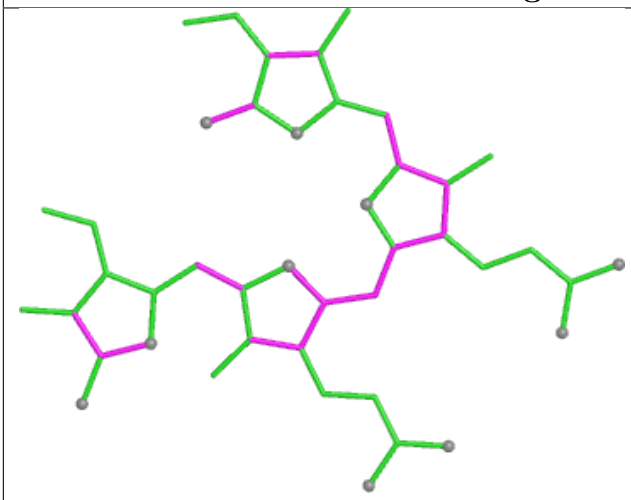


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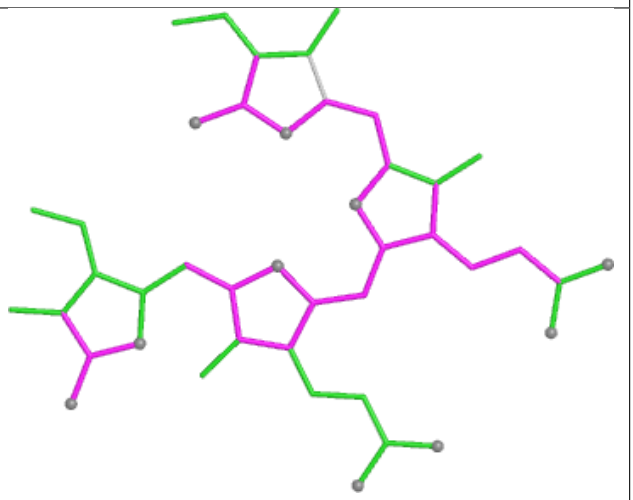


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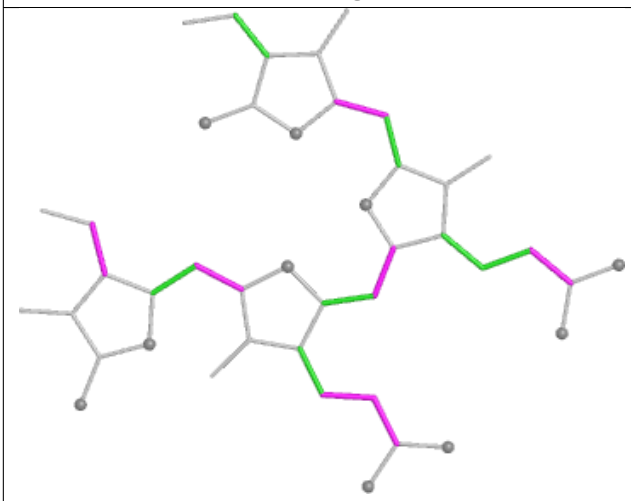
Ligand PEB l1 203



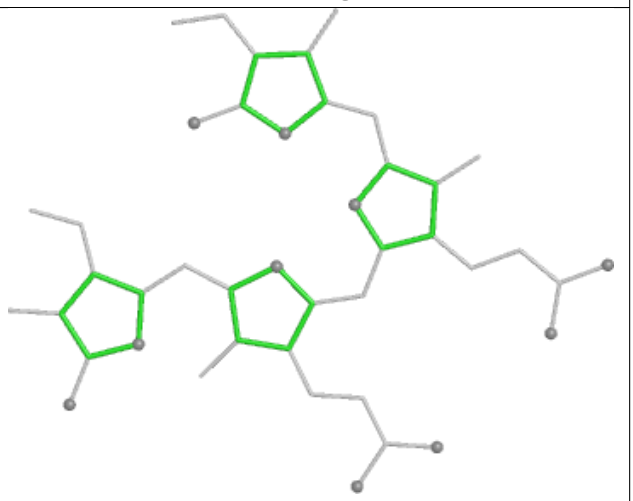
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Bond angles

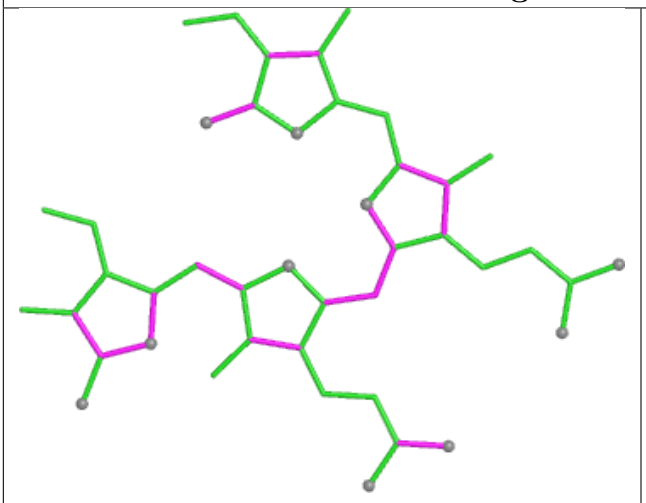


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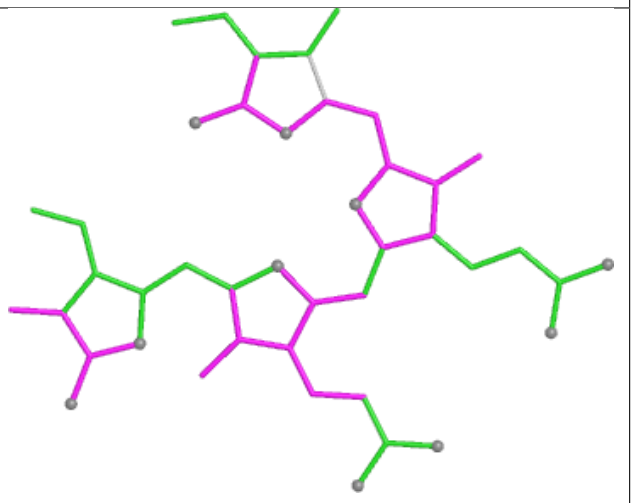


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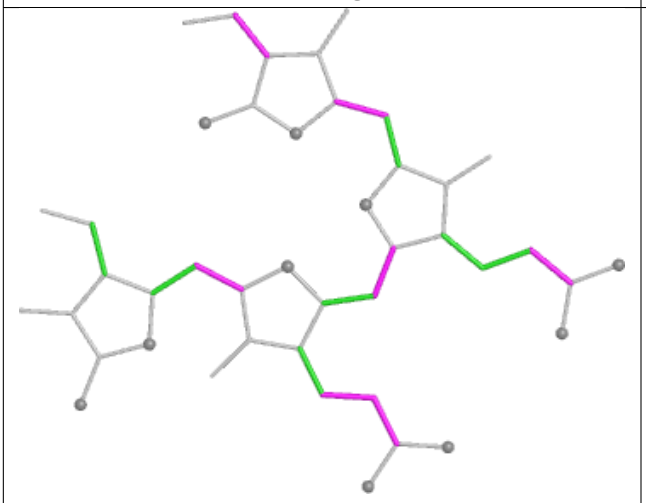
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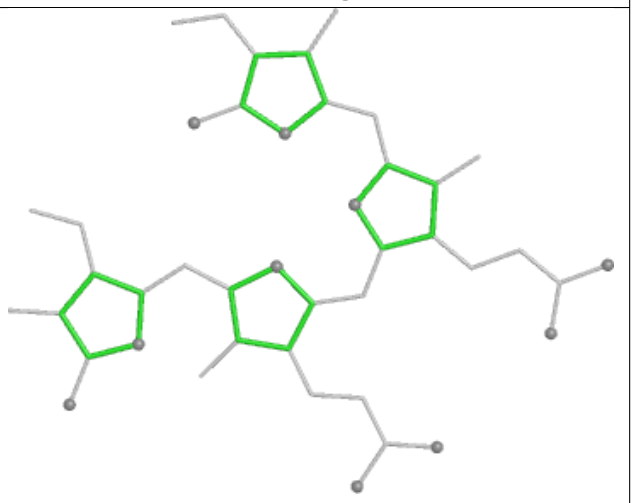
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Bond angles

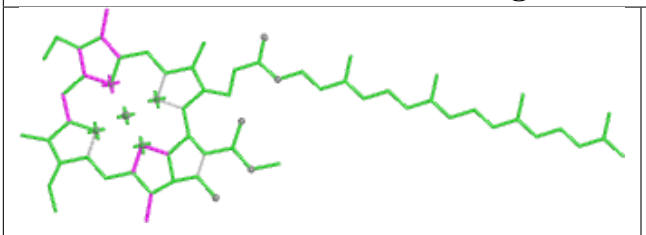


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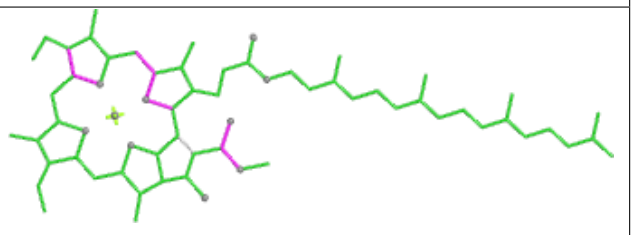


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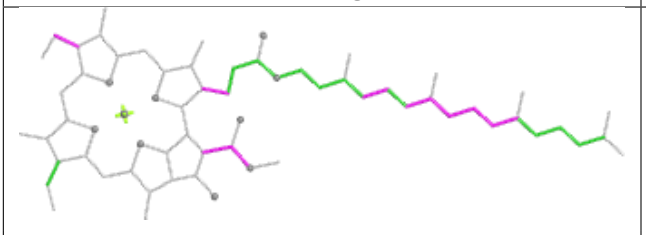
Ligand CLA BN 830



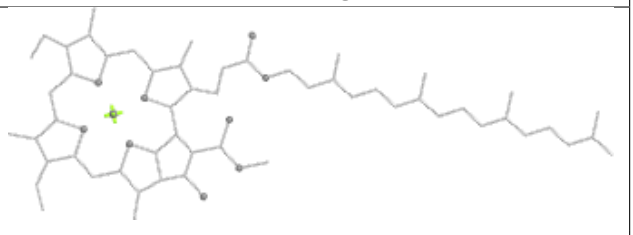
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Bond angles

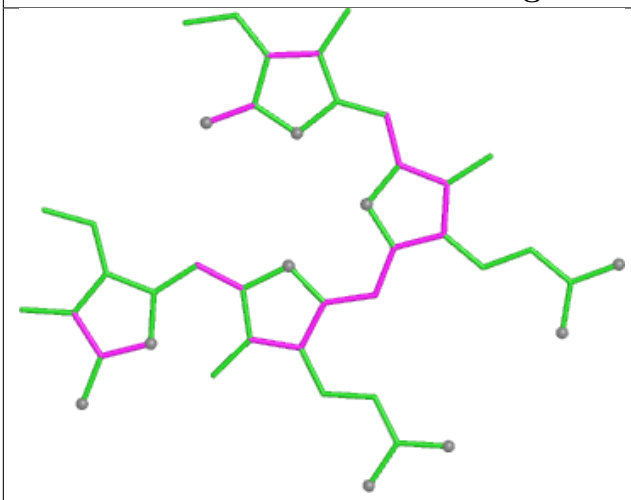


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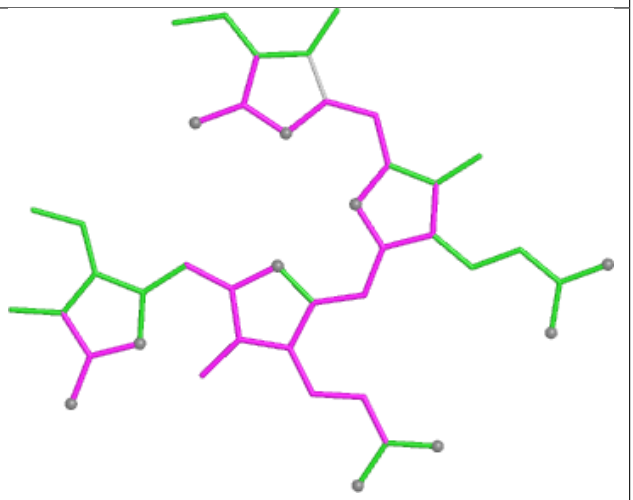


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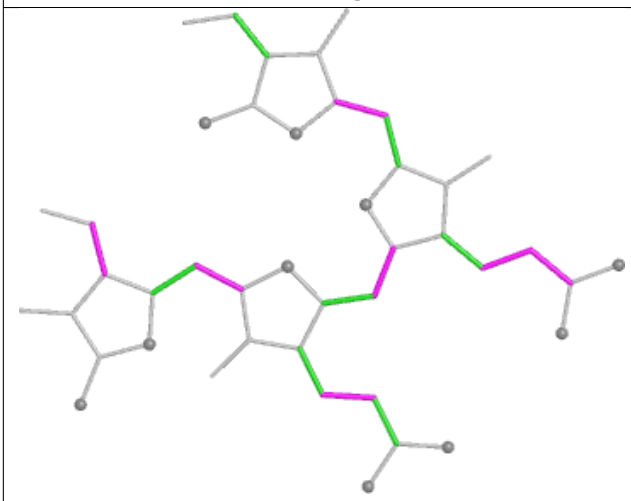
Ligand PEB f1 203



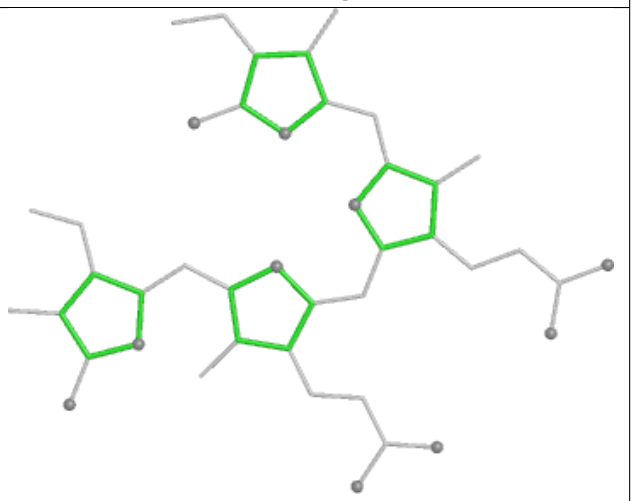
Bond lengths



Bond angles

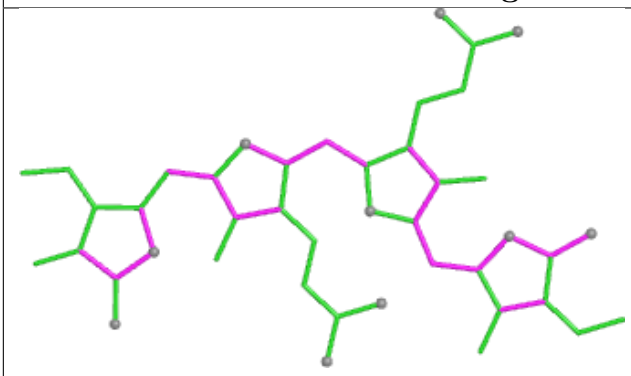


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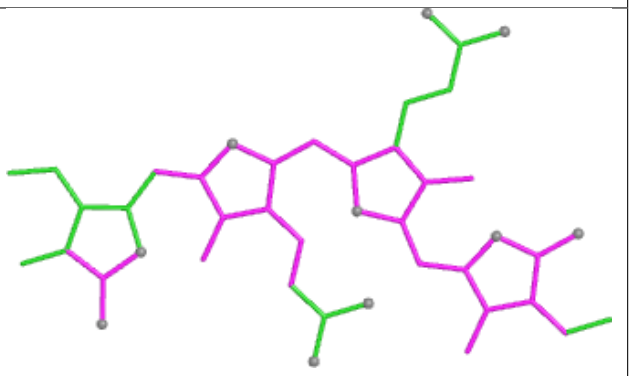


Rings

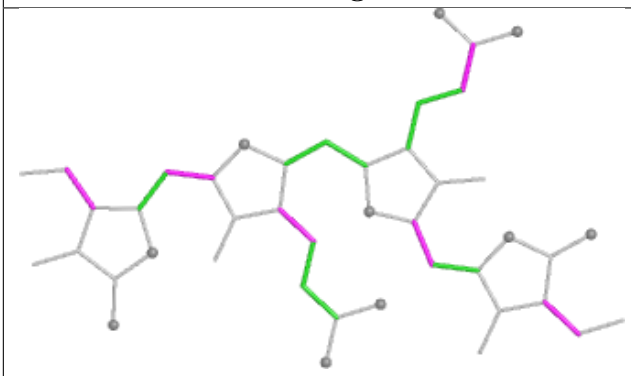
Ligand CYC LG 1001



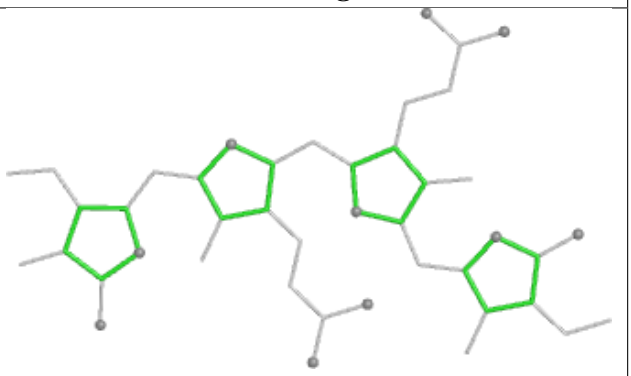
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Bond angles

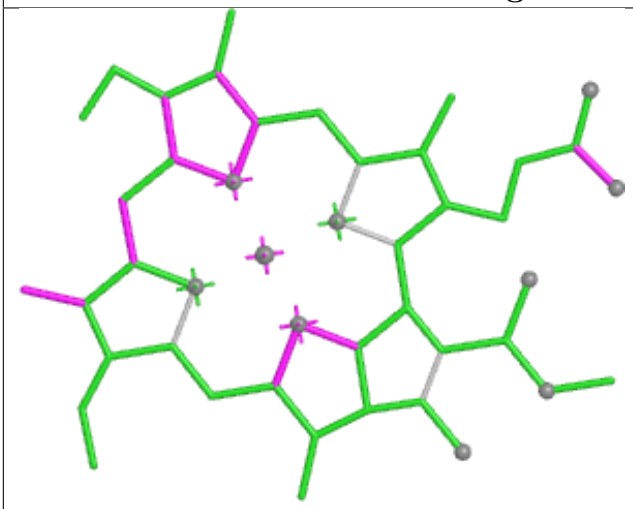


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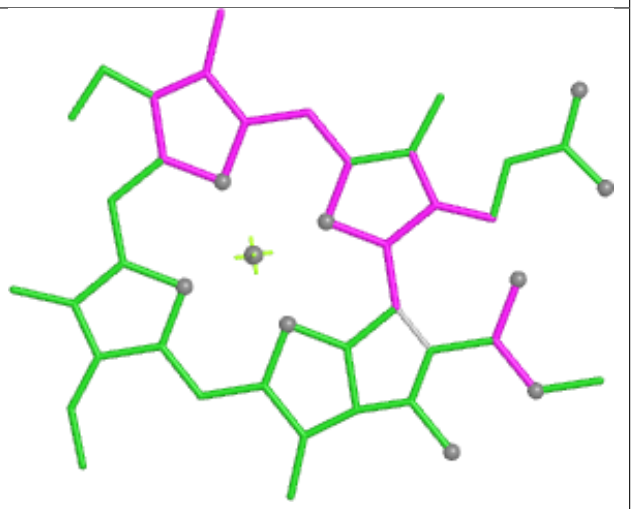


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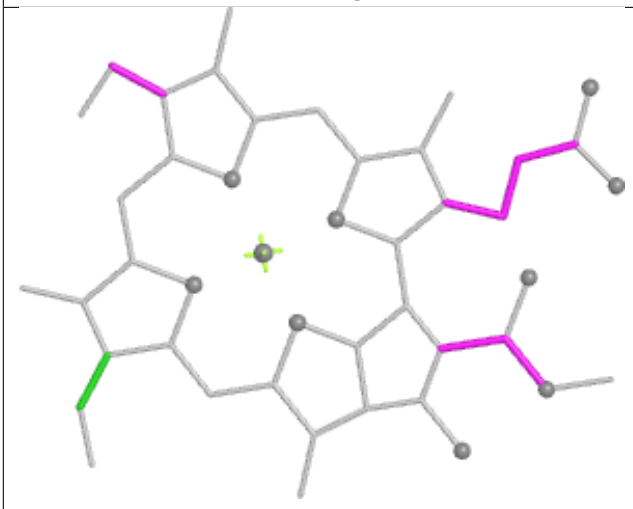
Ligand CLA MN 101



Bond lengths



Bond angles

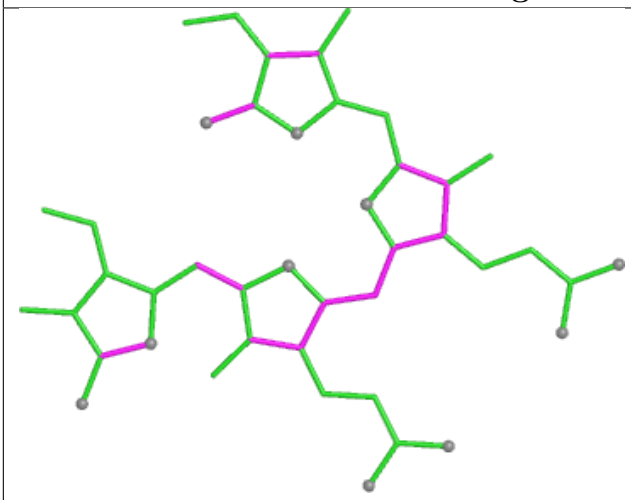


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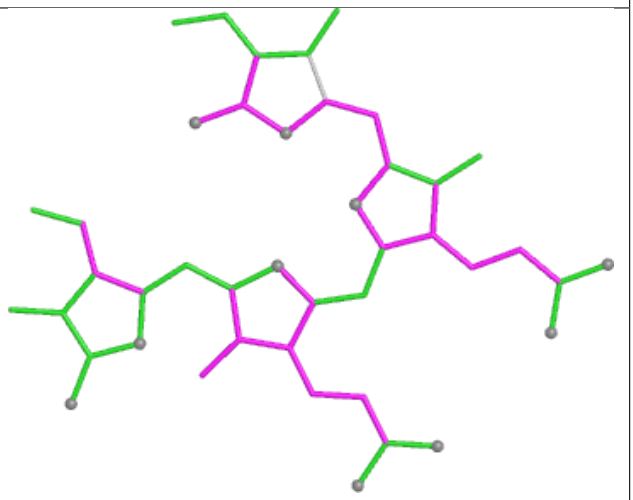


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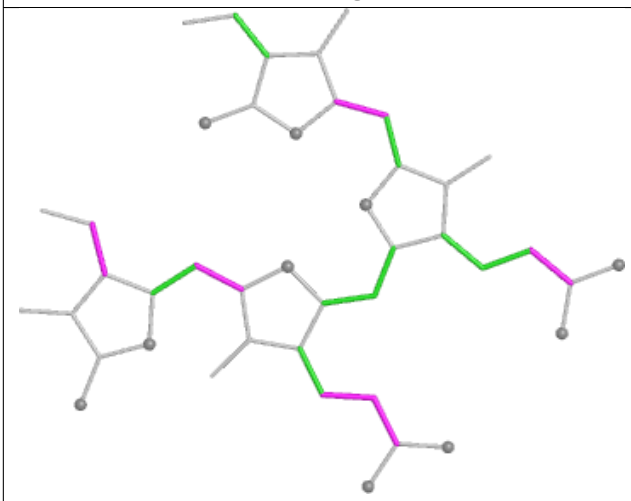
Ligand PEB TO 203



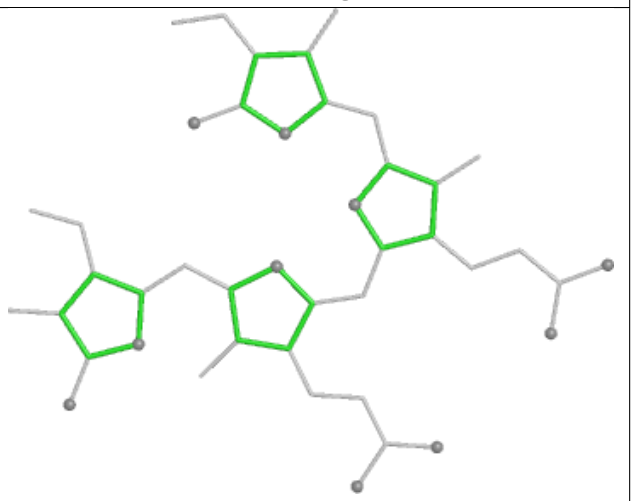
Bond lengths



Bond angles

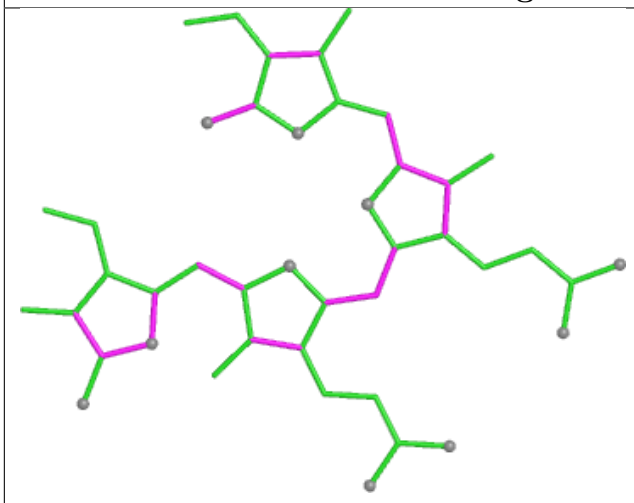


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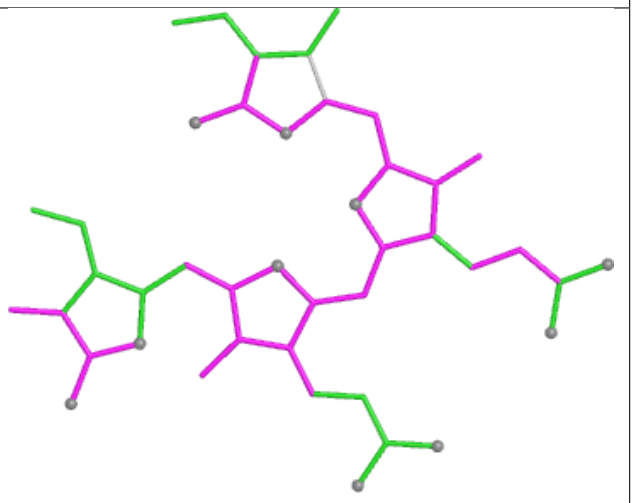


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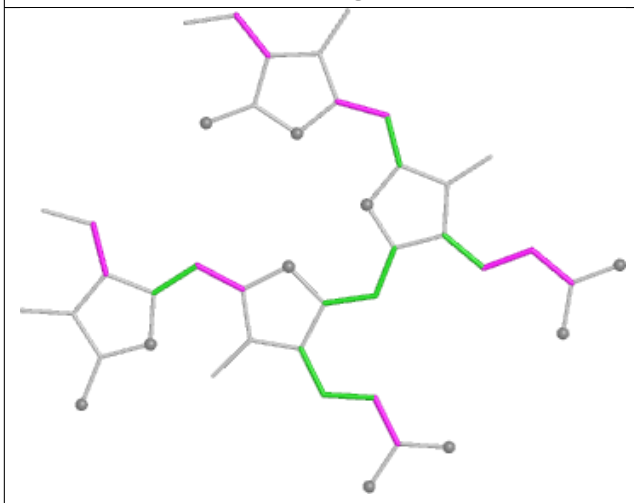
Ligand PEB V4 202



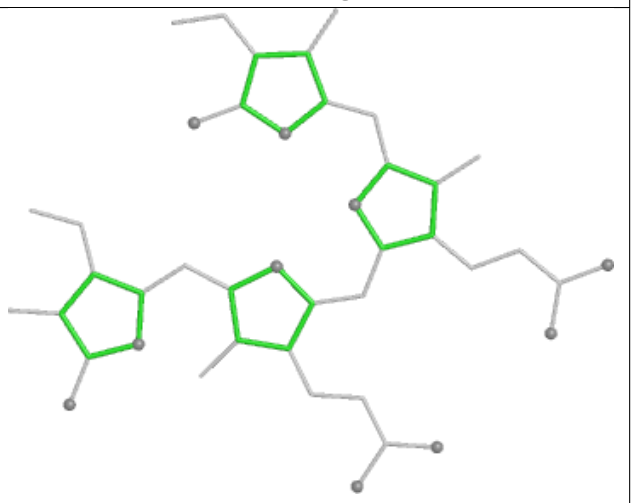
Bond lengths



Bond angles

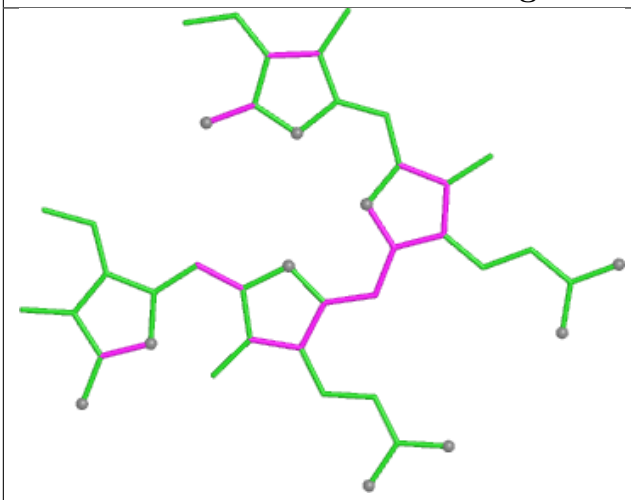


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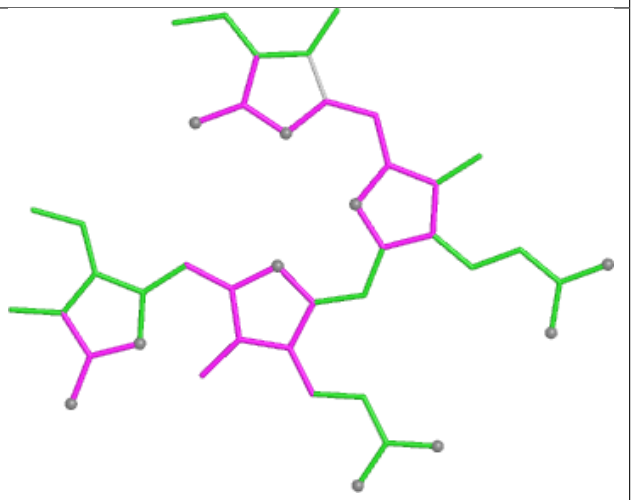


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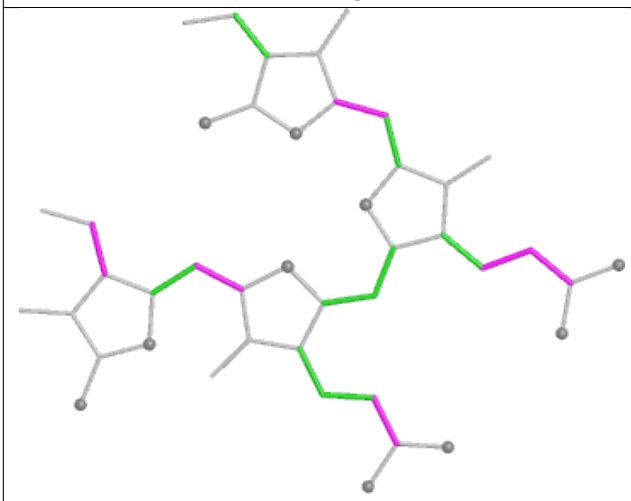
Ligand PEB x8 201



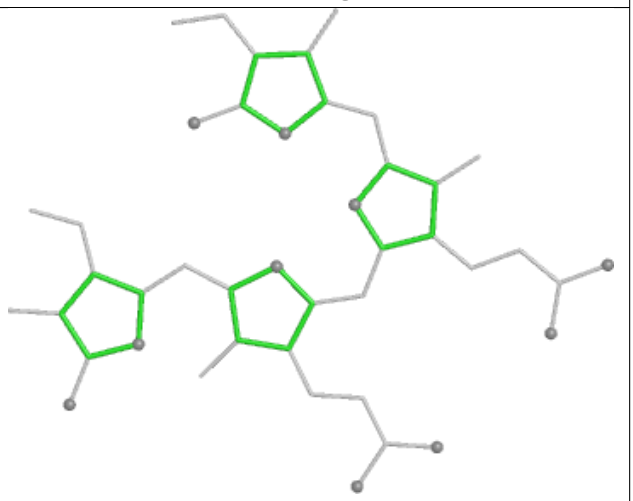
Bond lengths



Bond angles

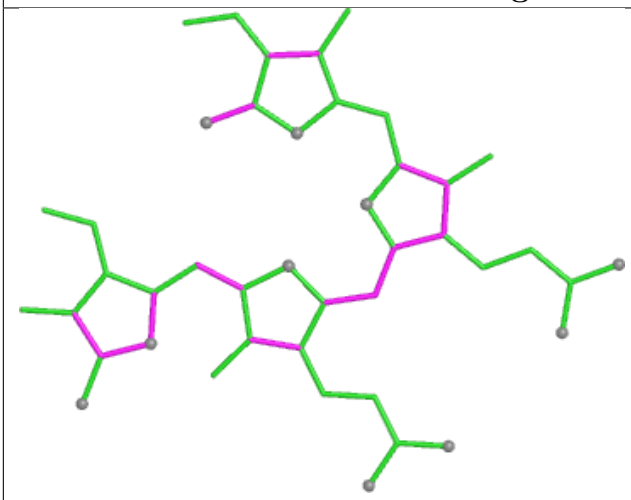


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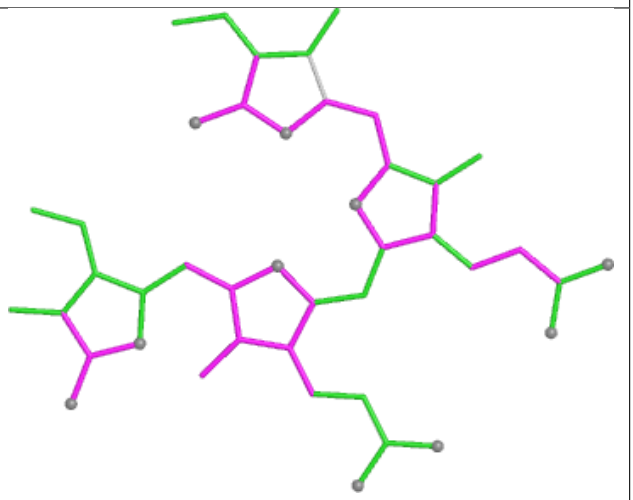


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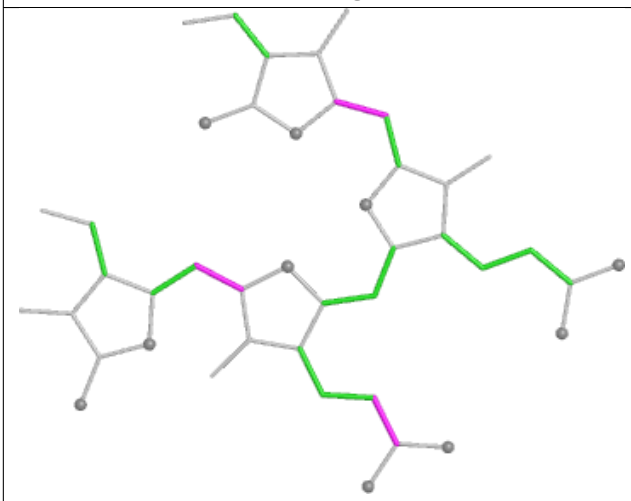
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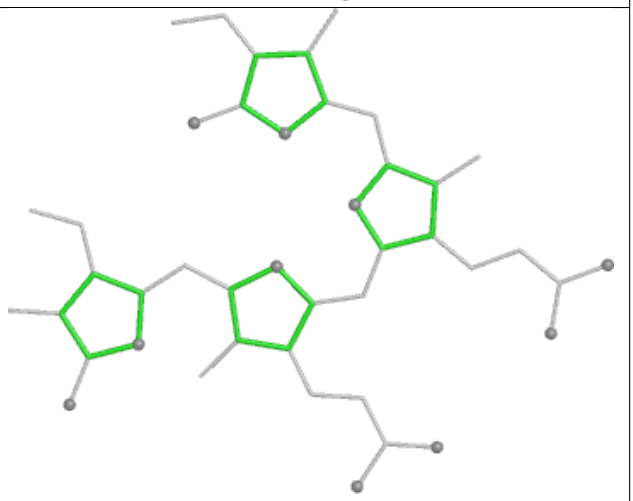
Bond lengths



Bond angles

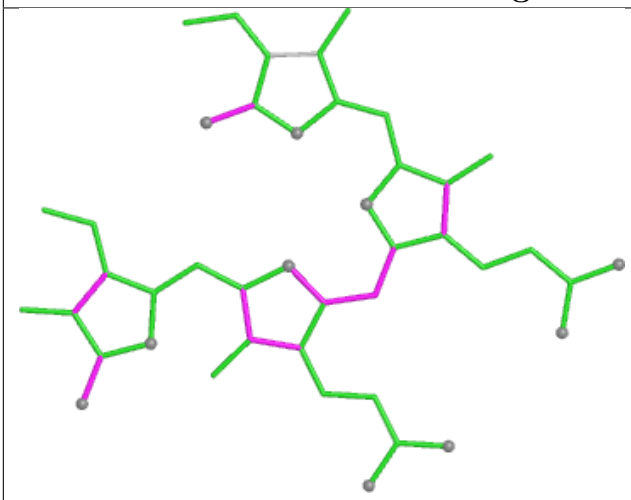


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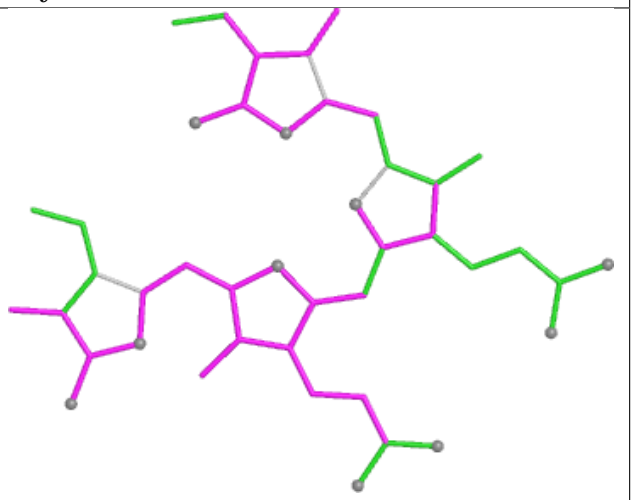


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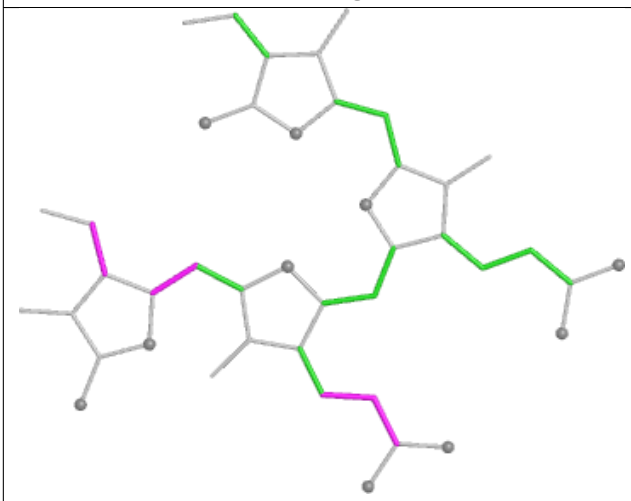
Ligand PUB yK 303



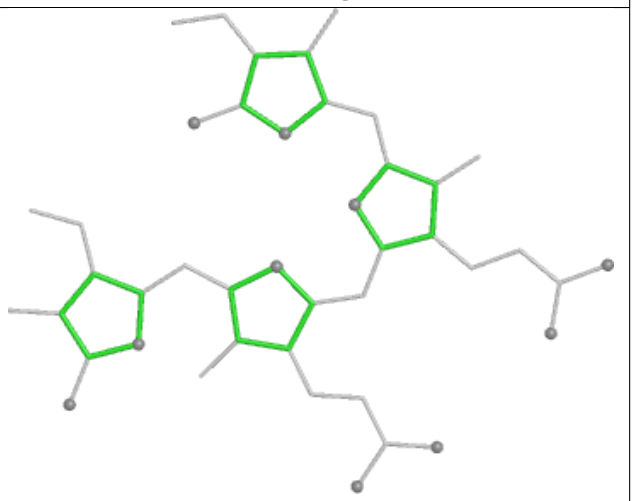
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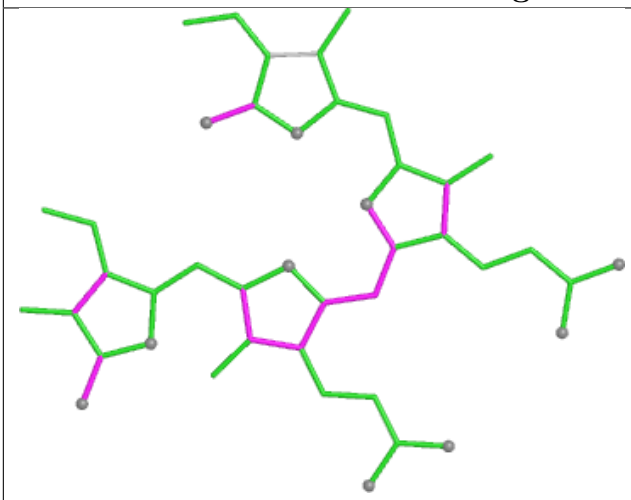


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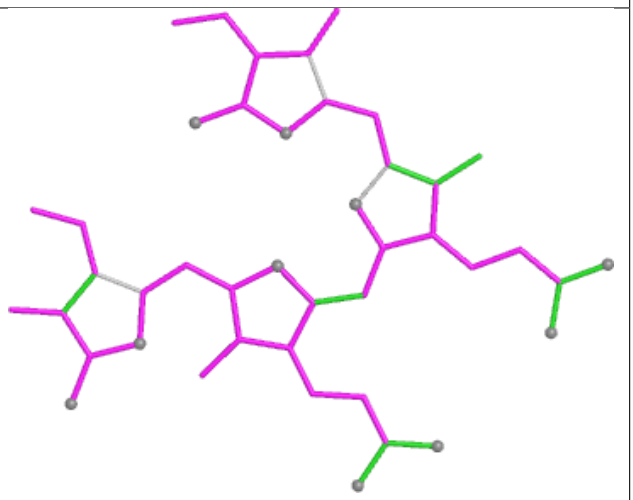


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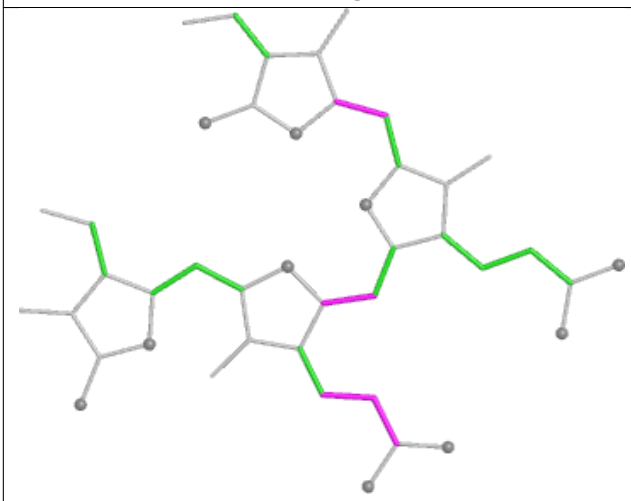
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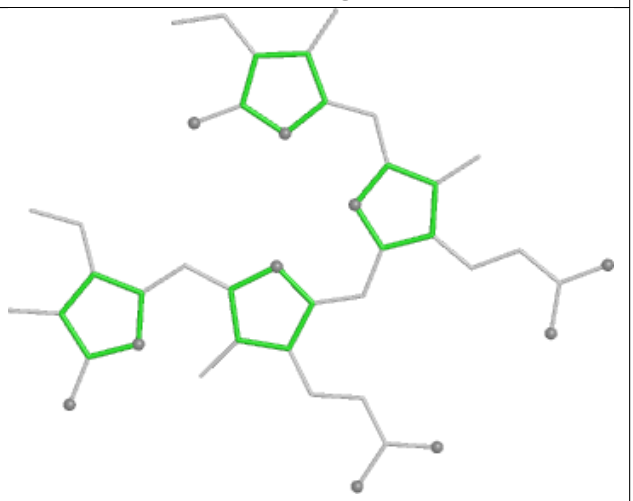
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Bond angles

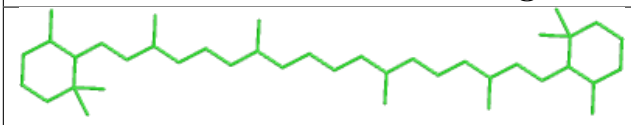


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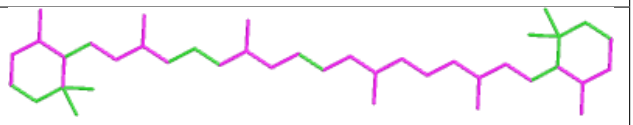


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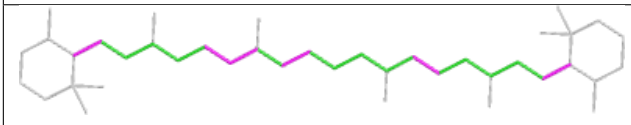
Ligand BCR c6 617



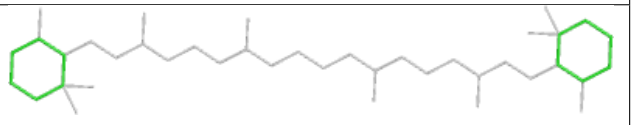
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Bond angles

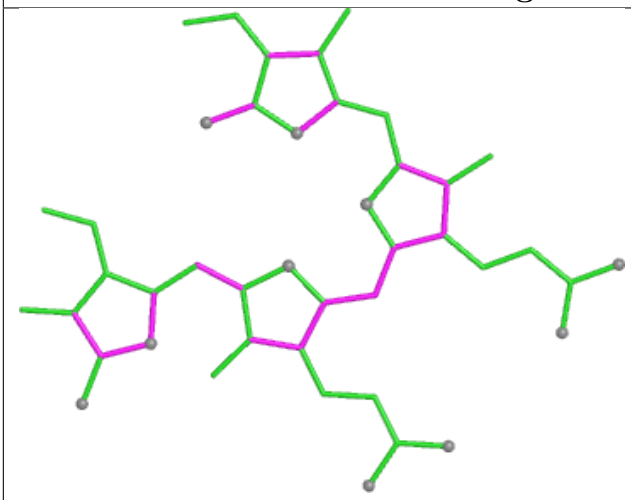


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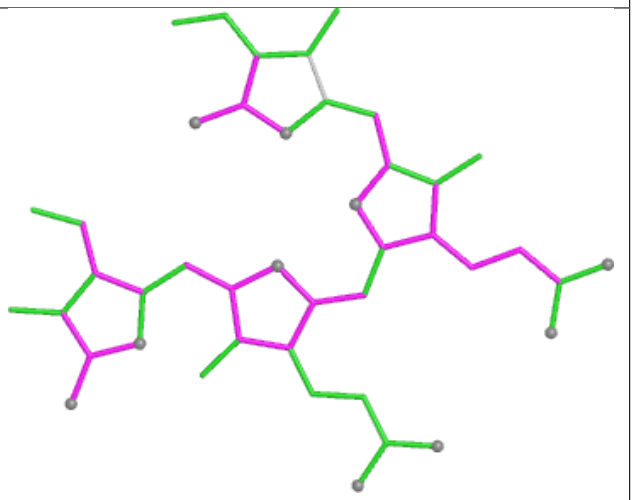


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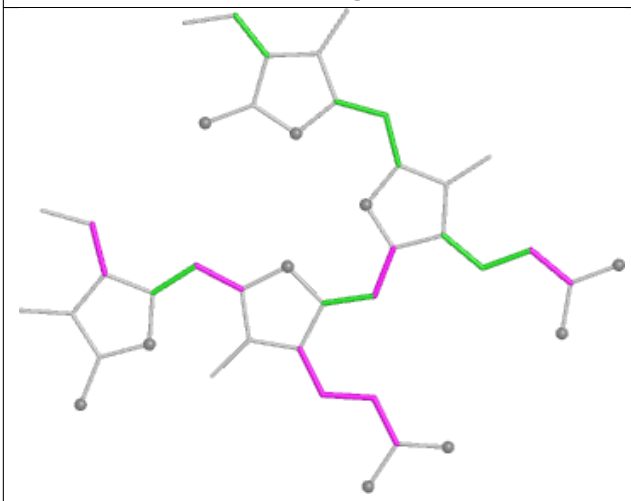
Ligand PEB dE 204



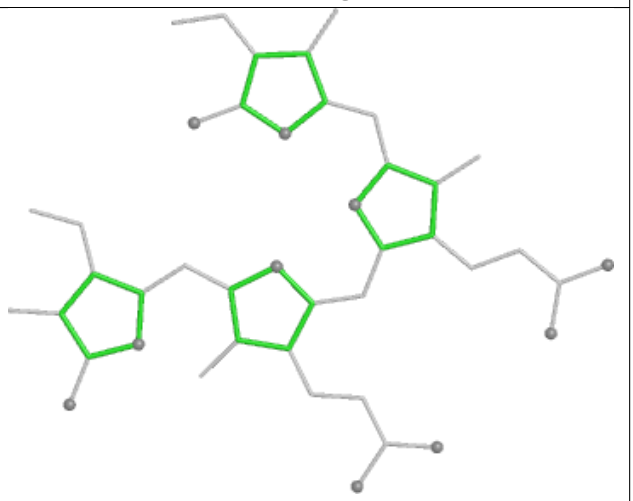
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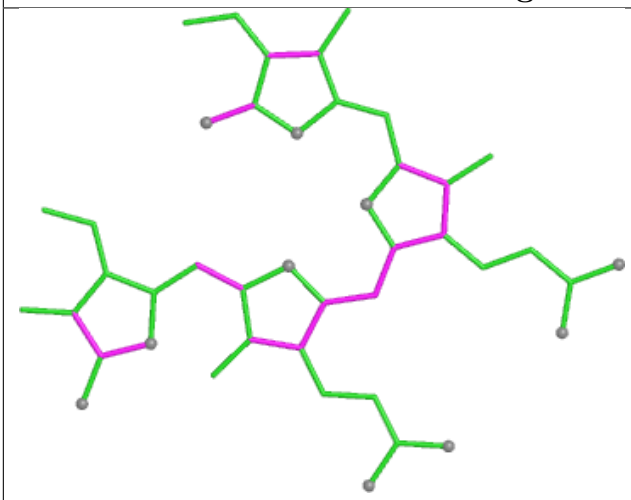


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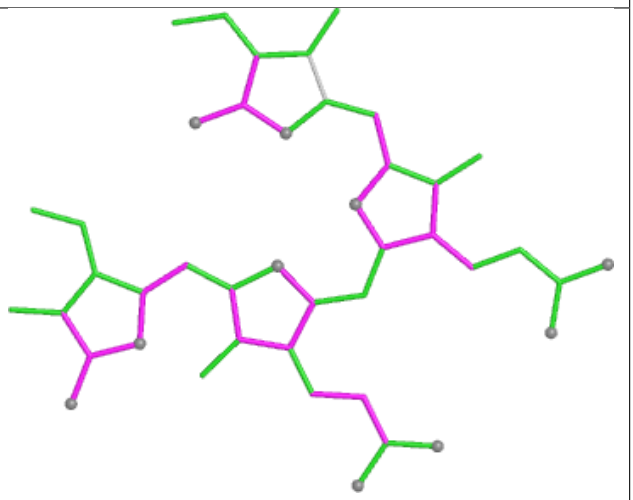


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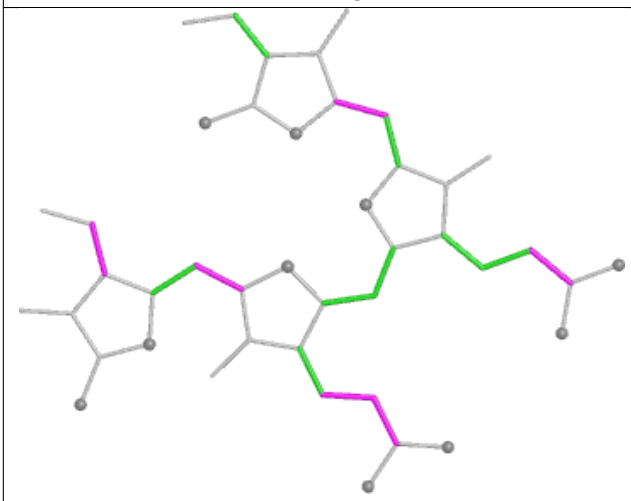
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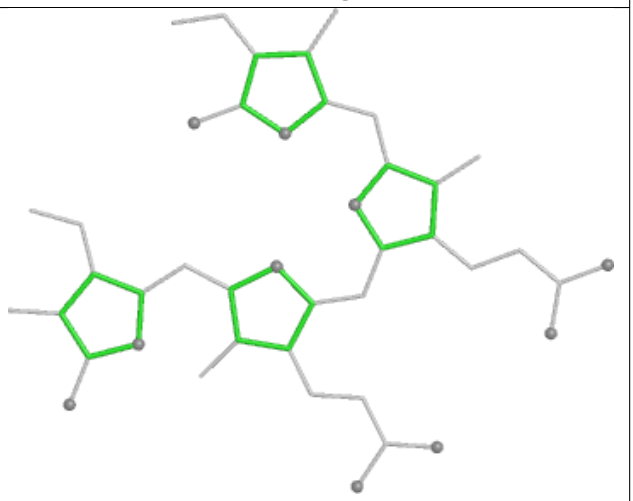
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Bond angles

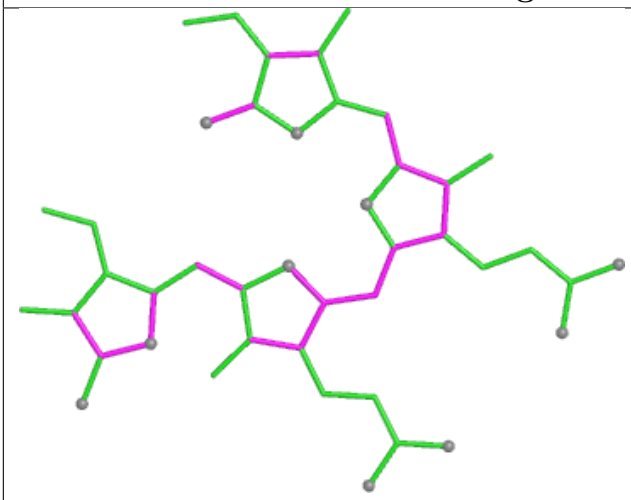


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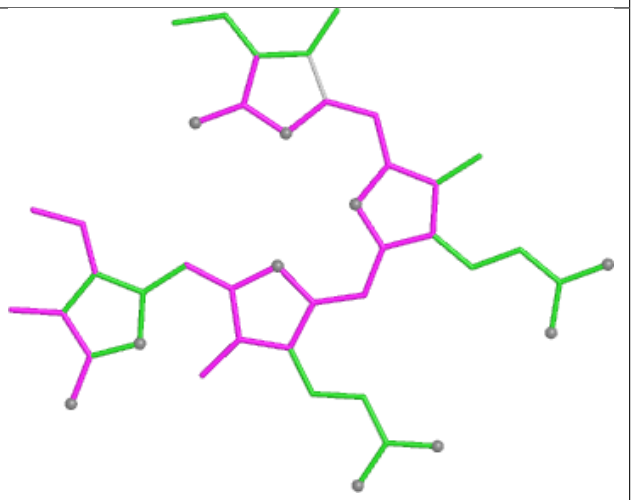


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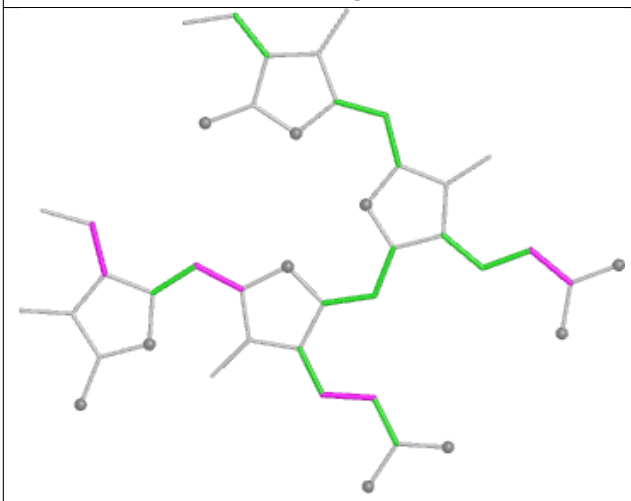
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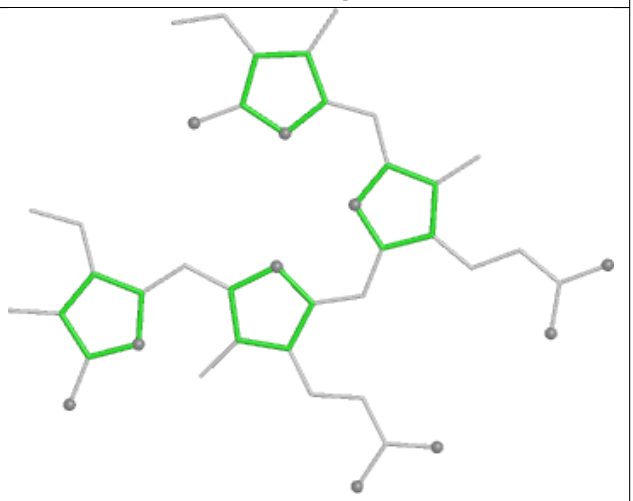
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Bond angles

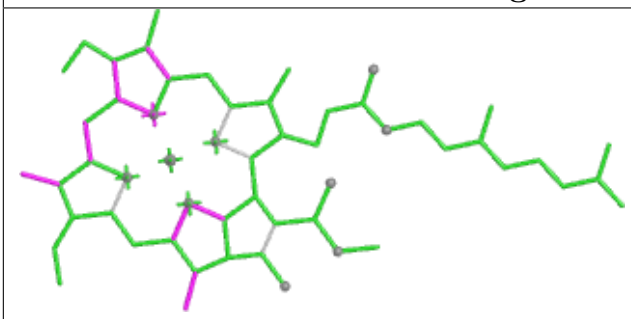


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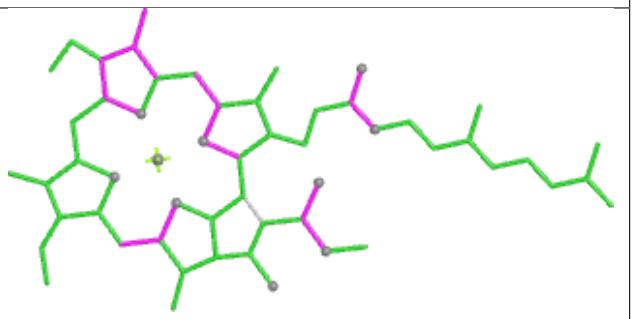


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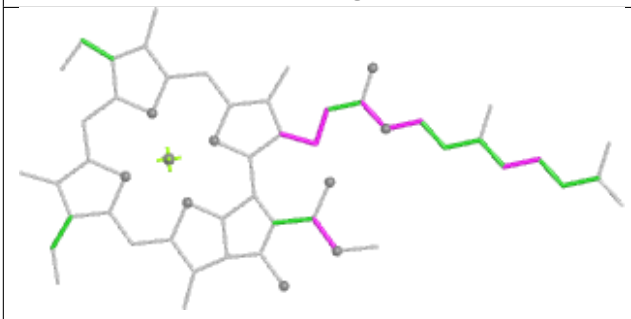
Ligand CLA AN 806



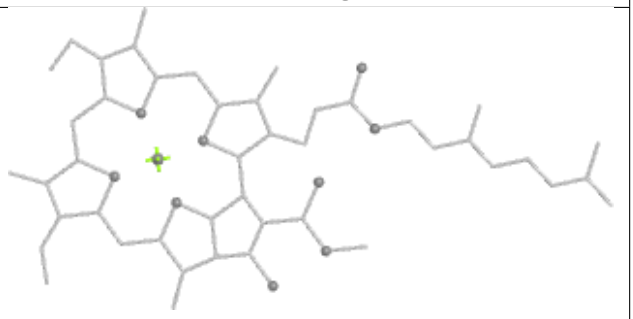
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Bond angles

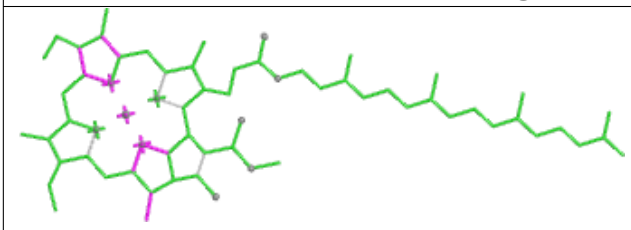


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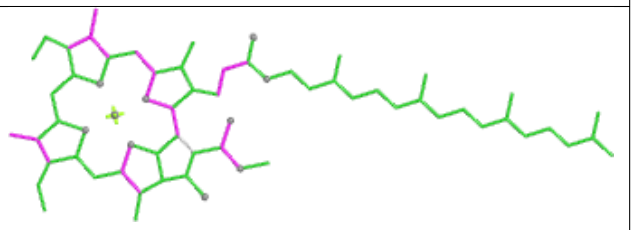


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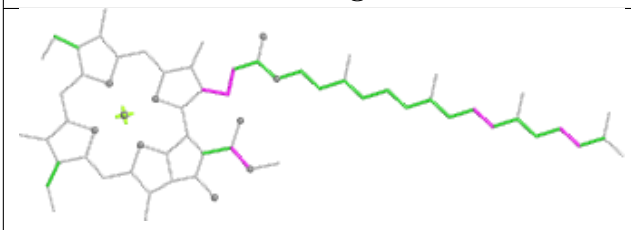
Ligand CLA A2 850



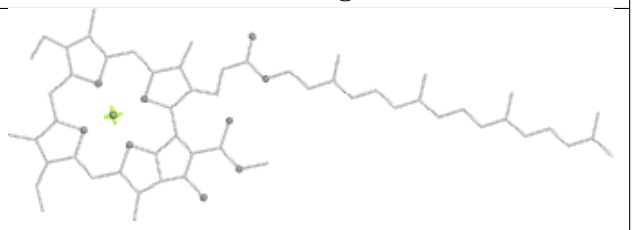
Bond lengths



Bond angles

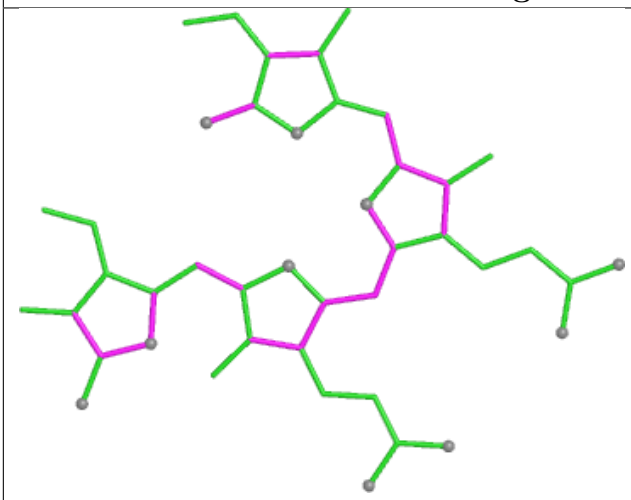


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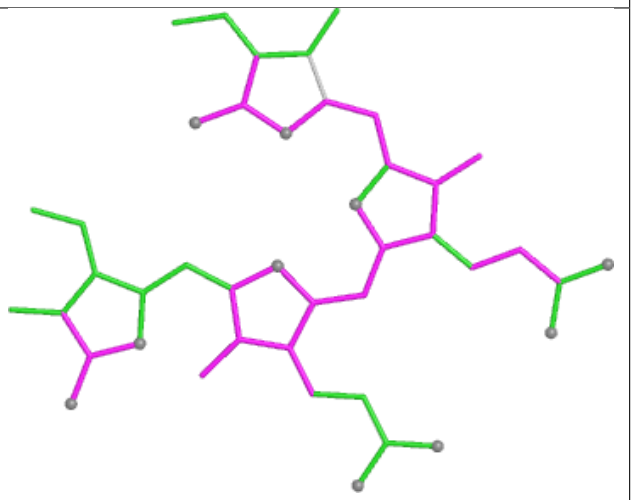


Rings

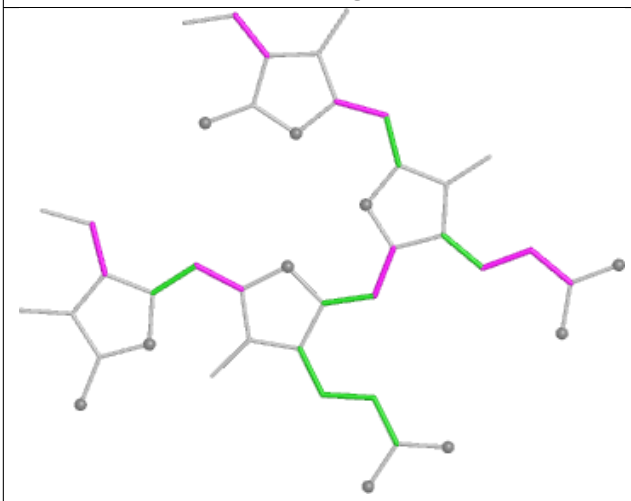
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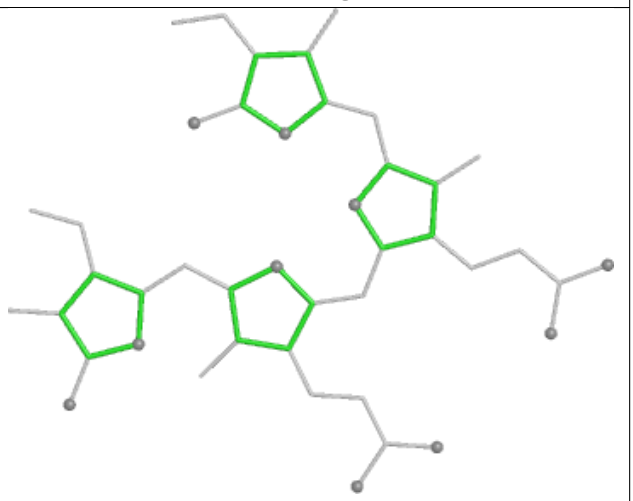
Bond lengths



Bond angles

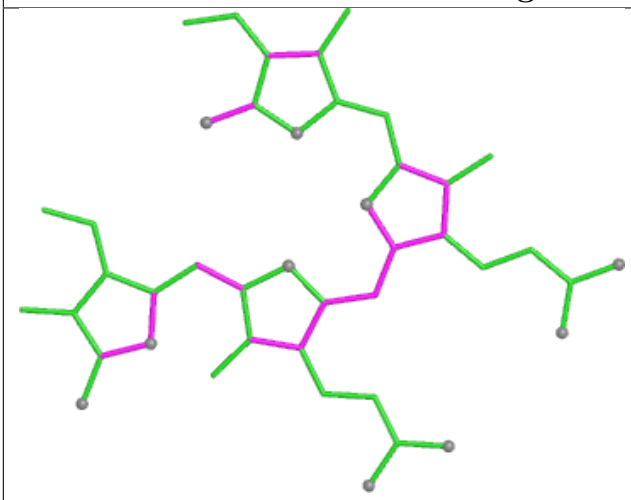


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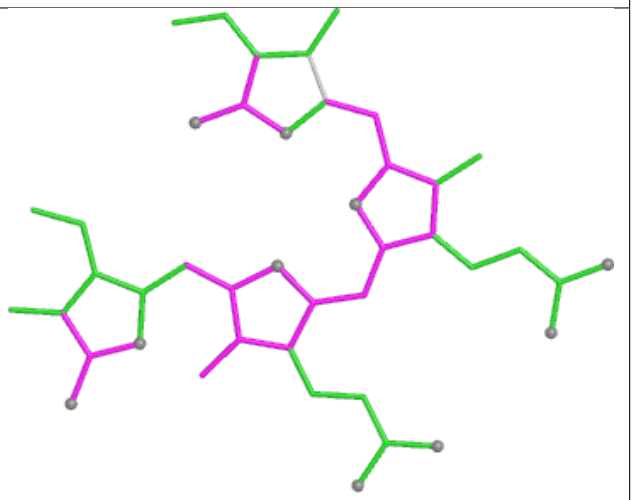


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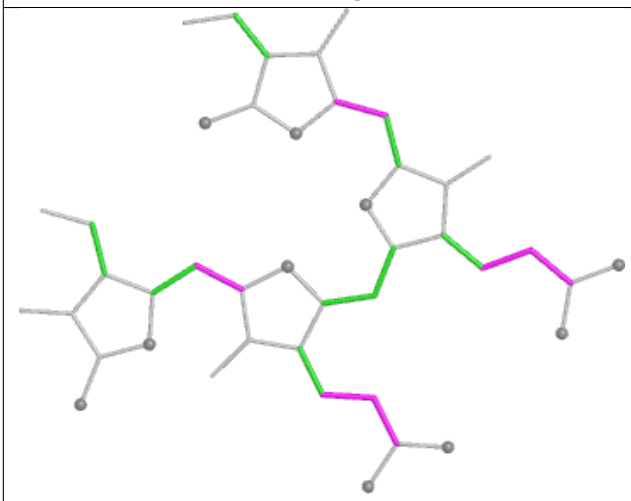
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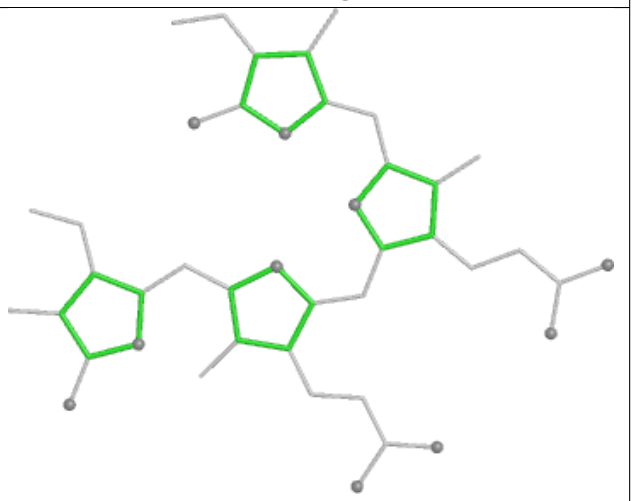
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Bond angles

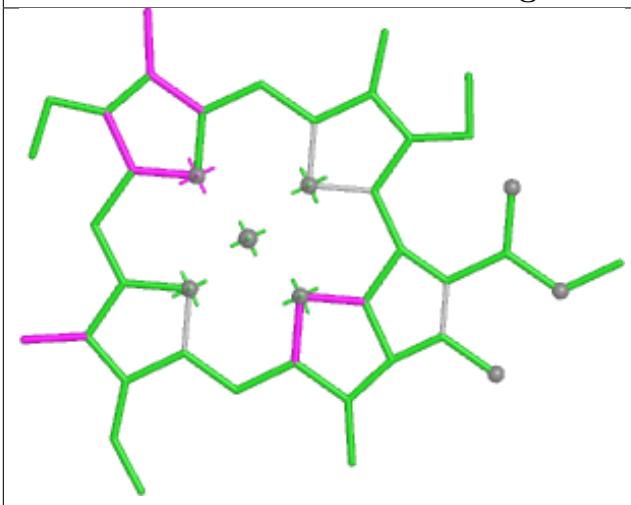


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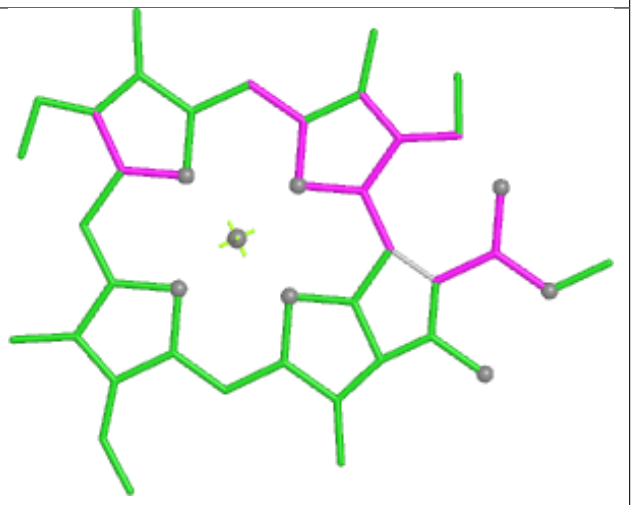


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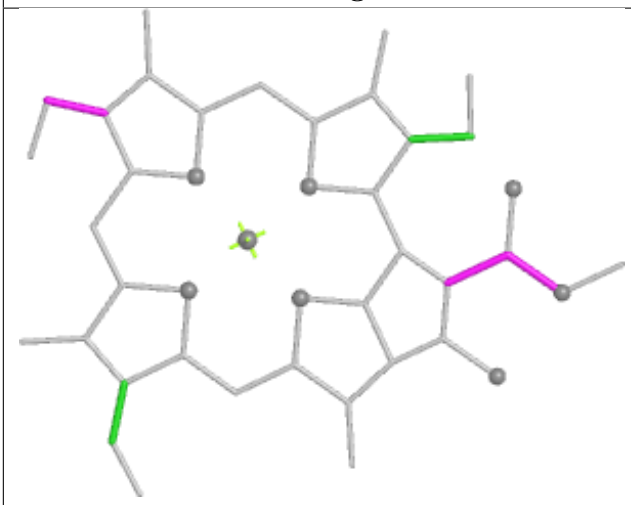
Ligand CLA 62 311



Bond lengths



Bond angles

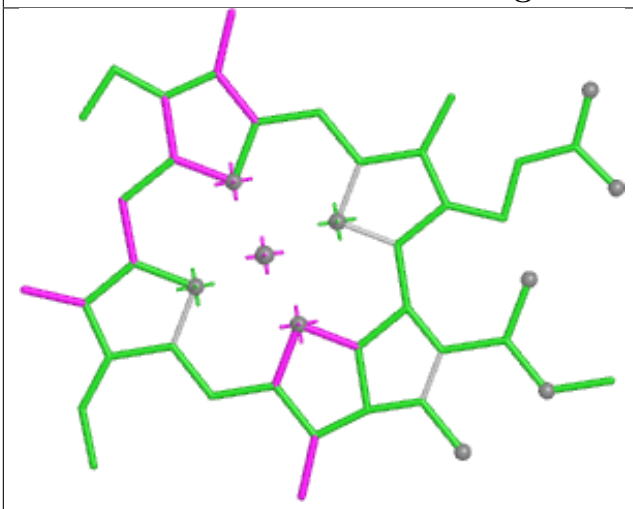


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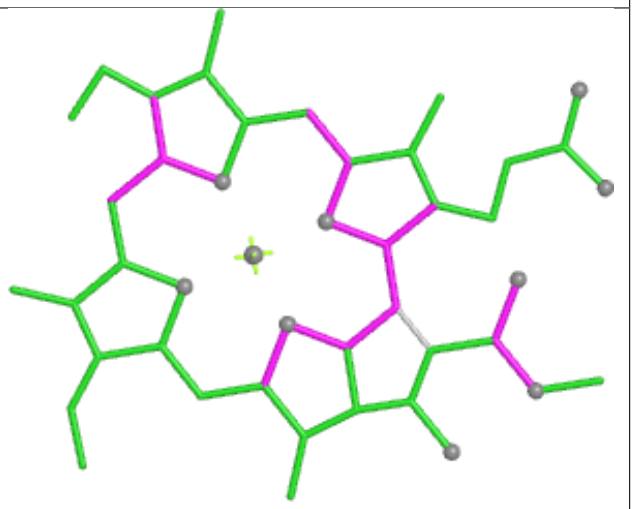


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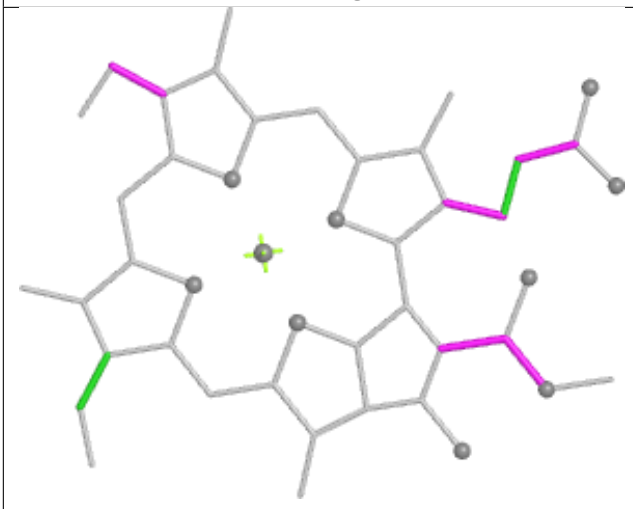
Ligand CLA 8N 302



Bond lengths



Bond angles

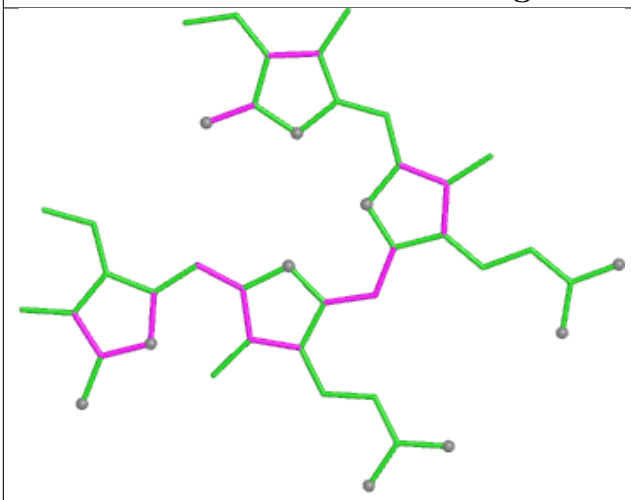


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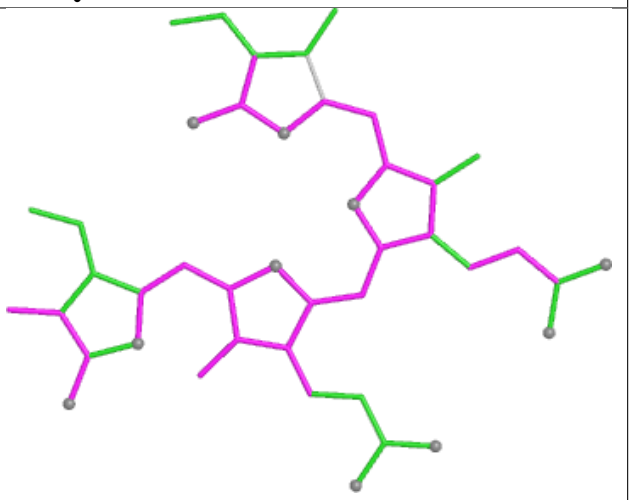


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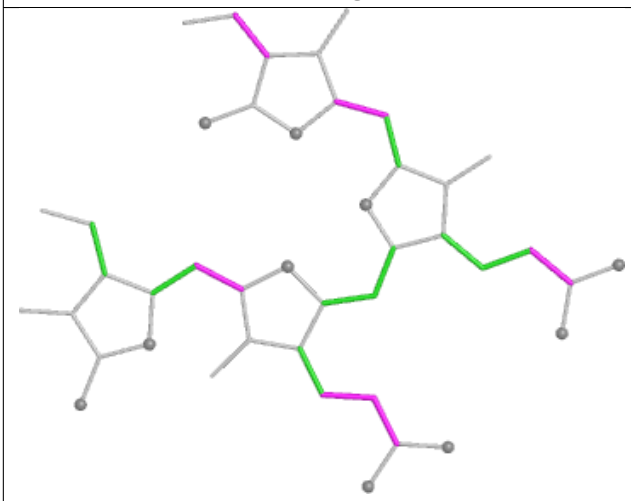
Ligand PEB FQ 201



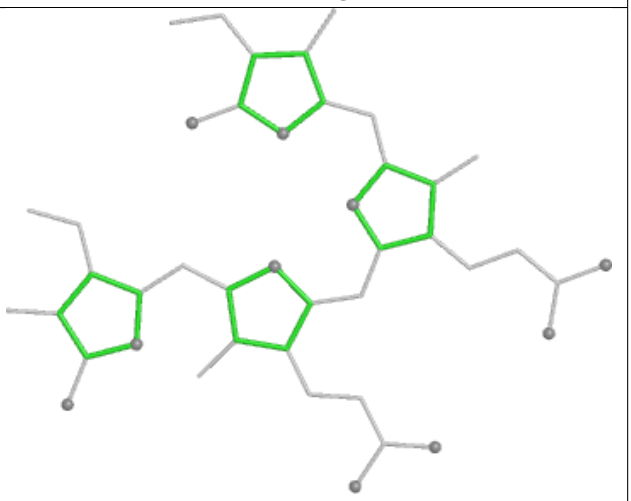
Bond lengths



Bond angles

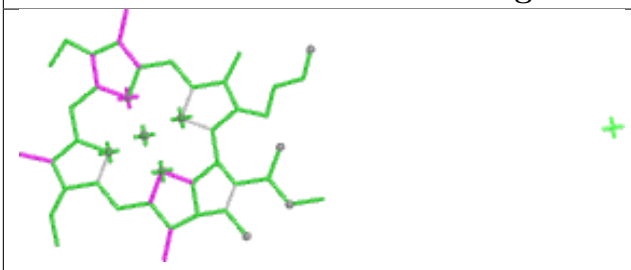


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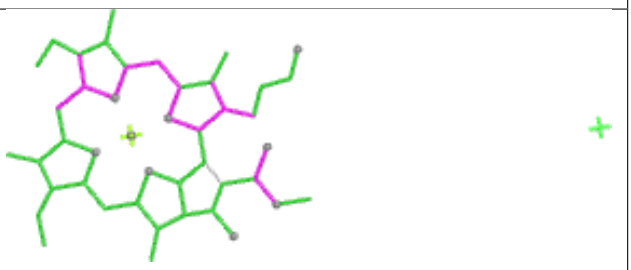


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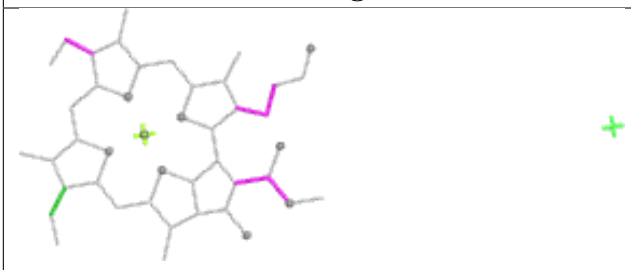
Ligand CLA A2 802



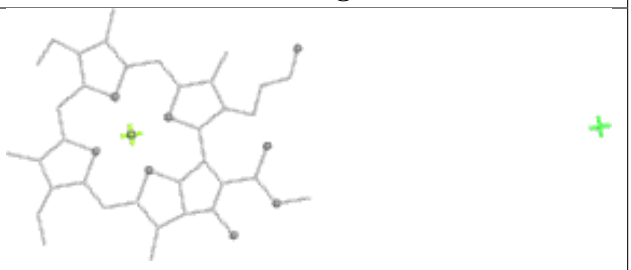
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Bond angles

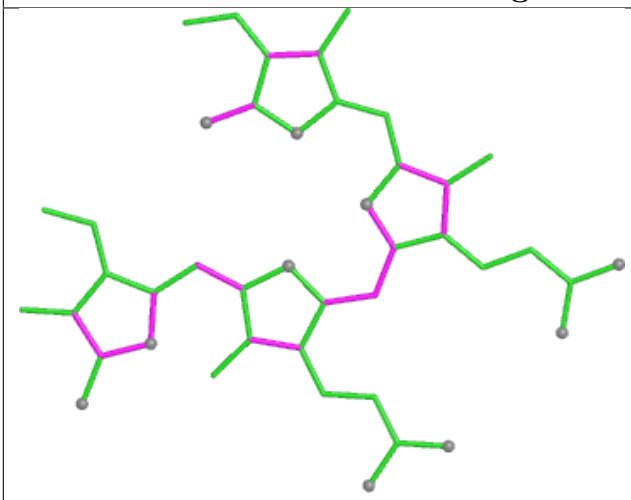


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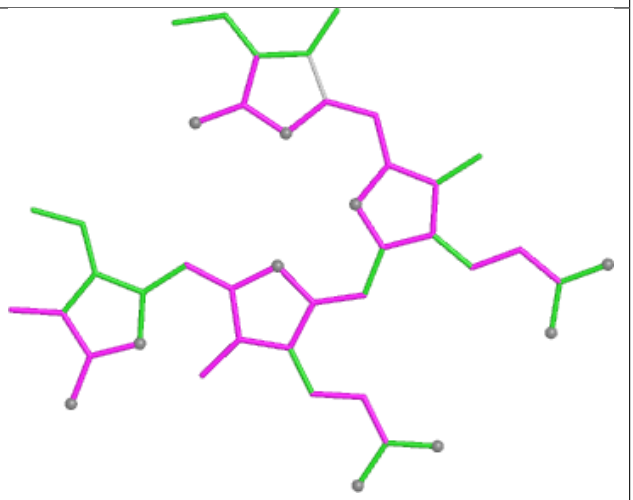


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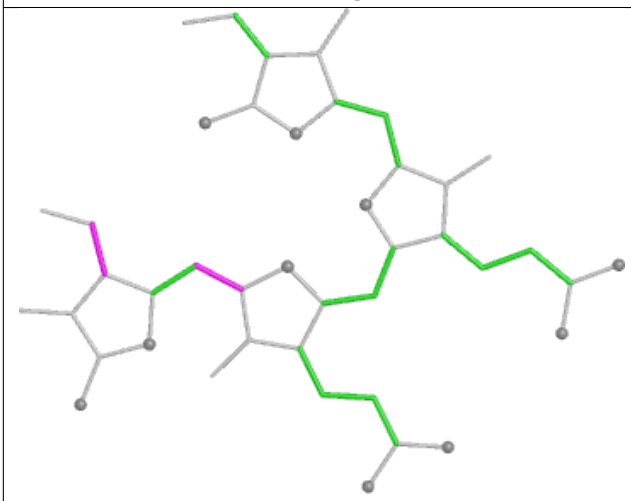
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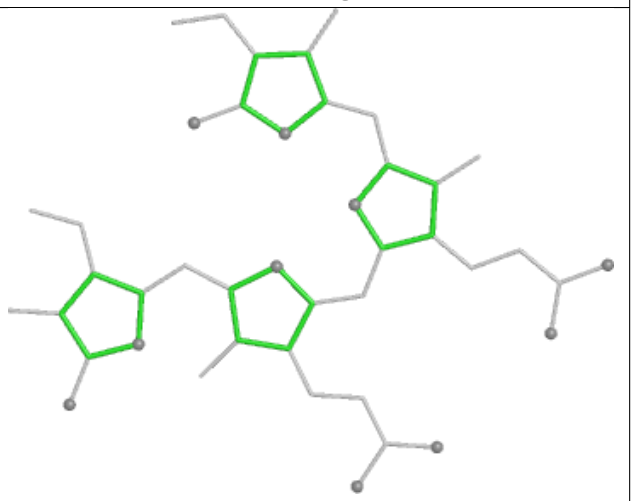
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Bond angles

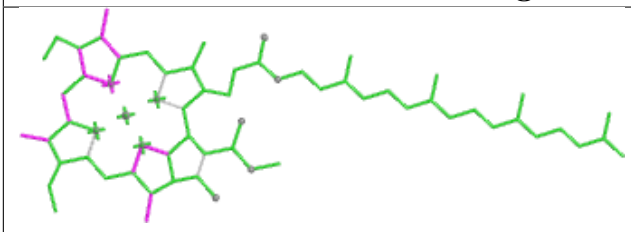


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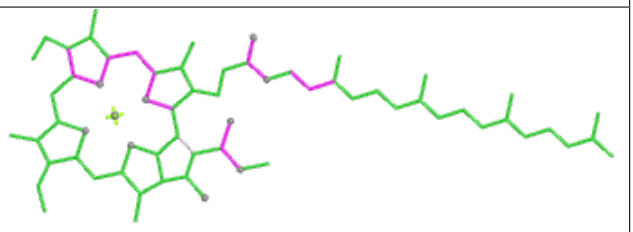


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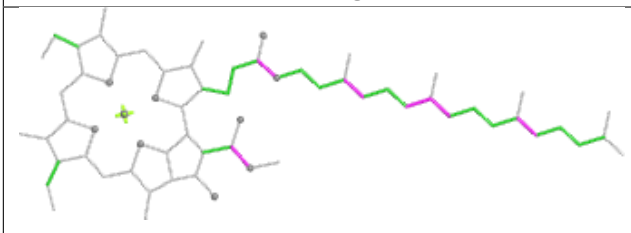
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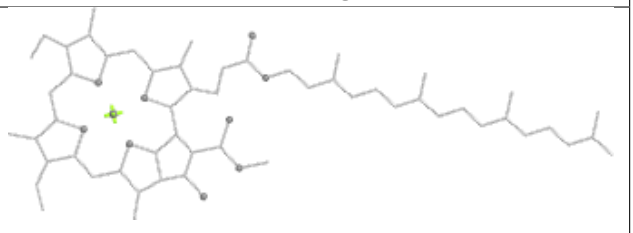
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Bond angles

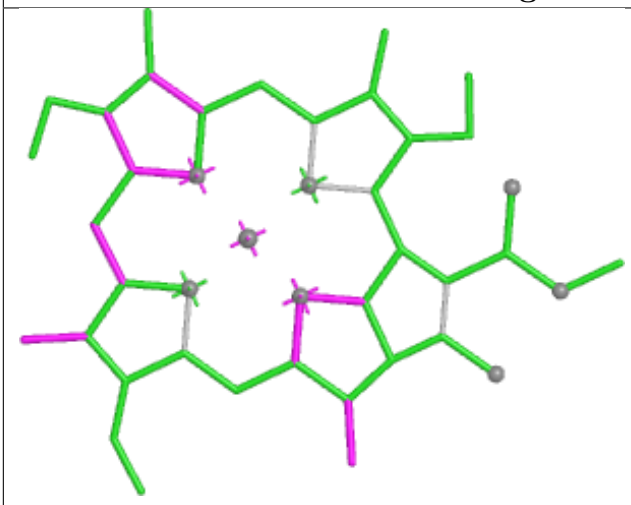


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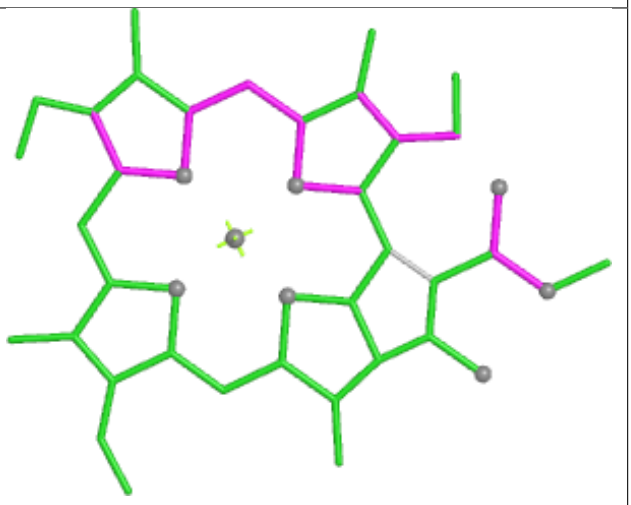


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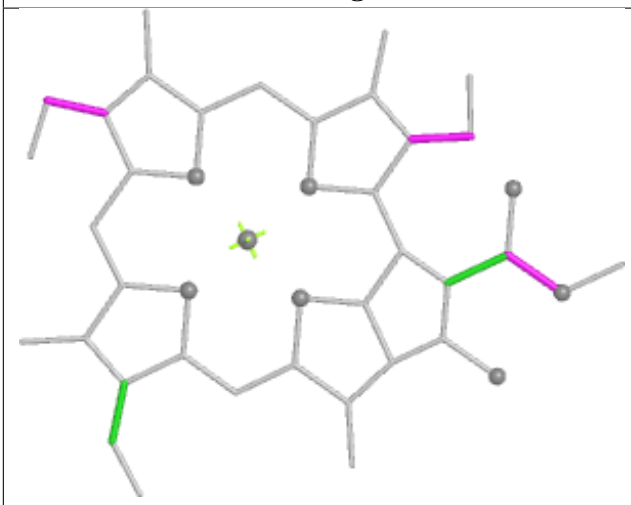
Ligand CLA 82 307



Bond lengths



Bond angles

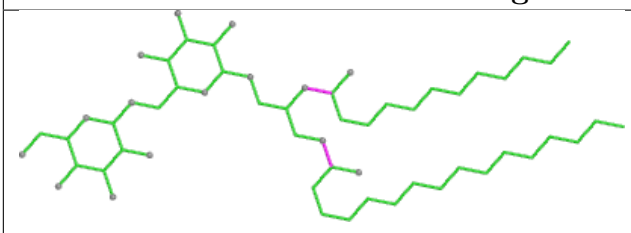


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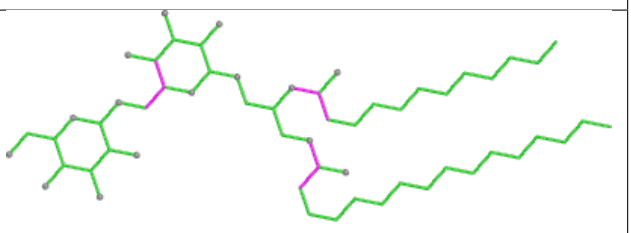


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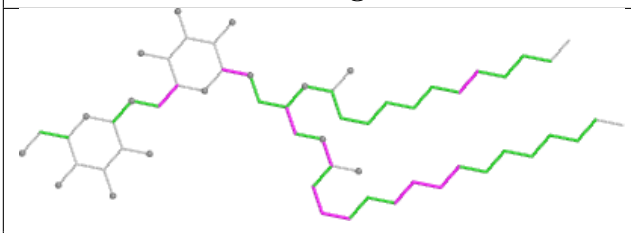
Ligand DGD B6 620



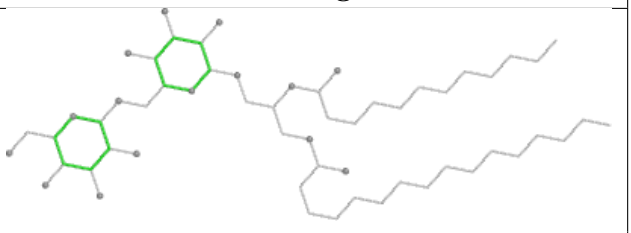
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Bond angles

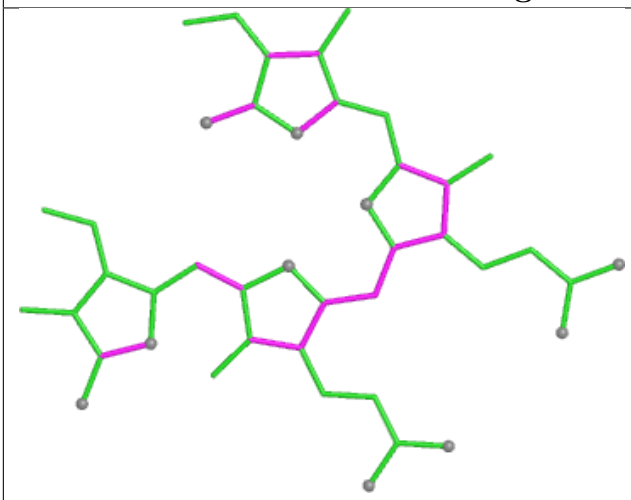


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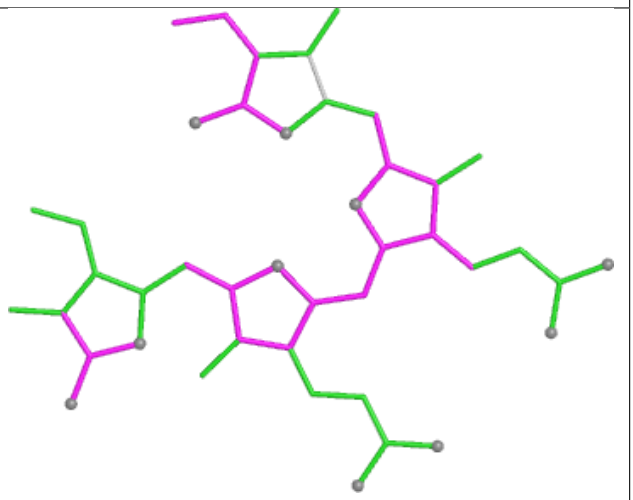


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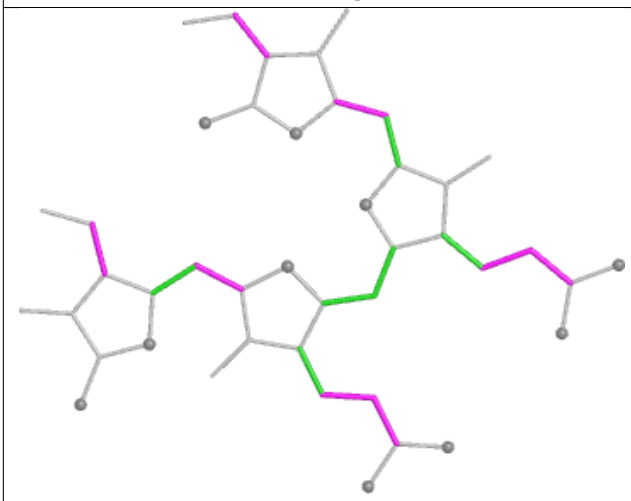
Ligand PEB JD 203



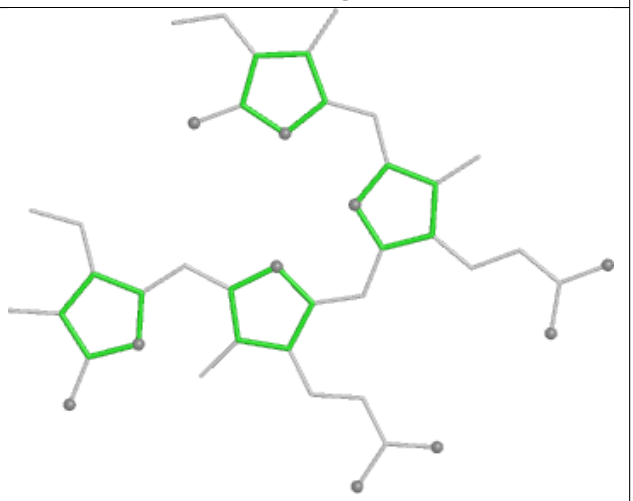
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Bond angles

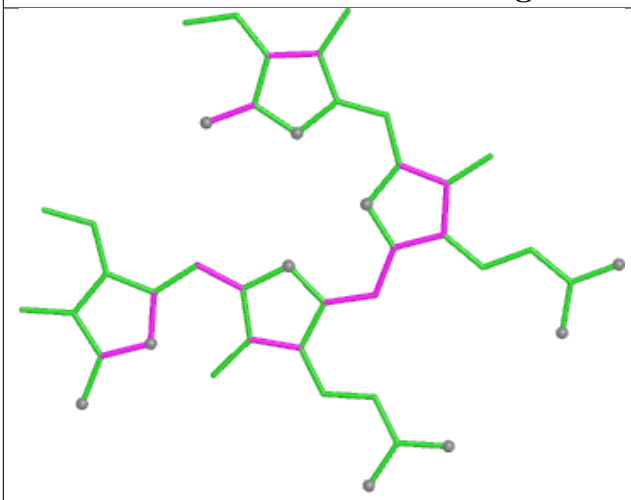


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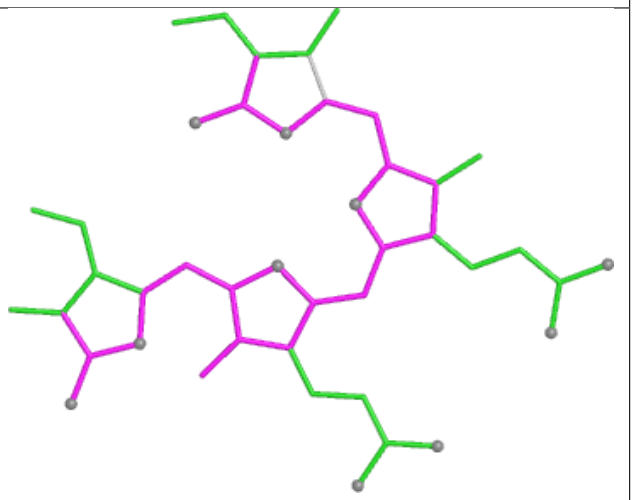


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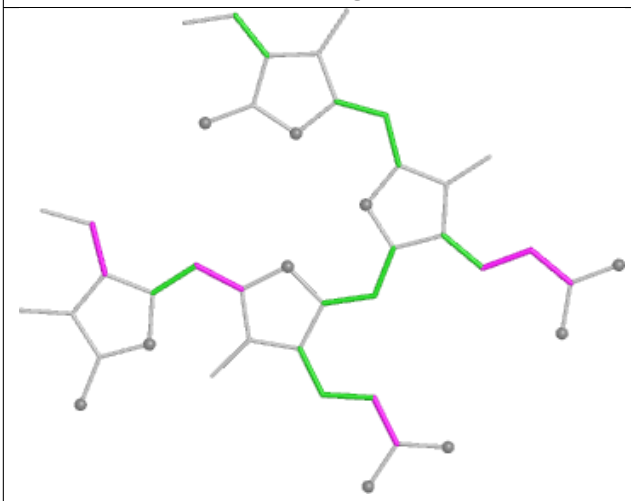
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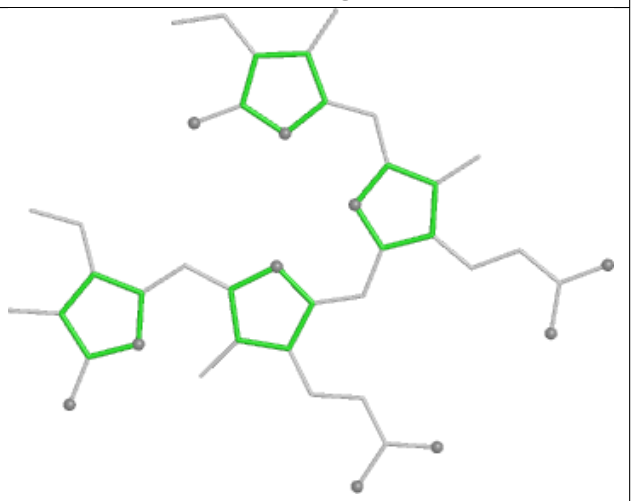
Bond lengths



Bond angles

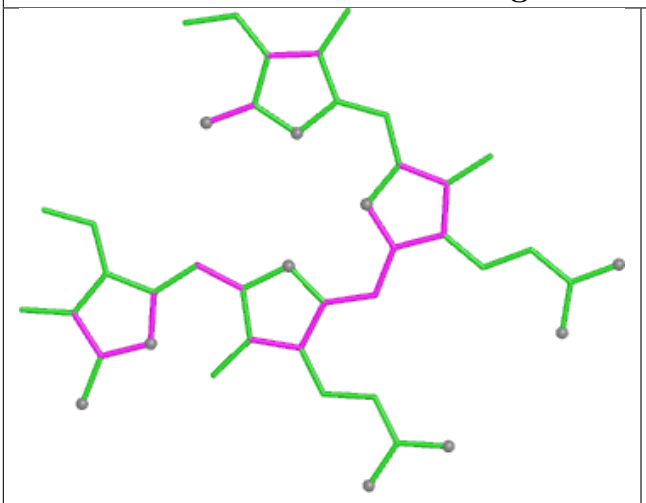


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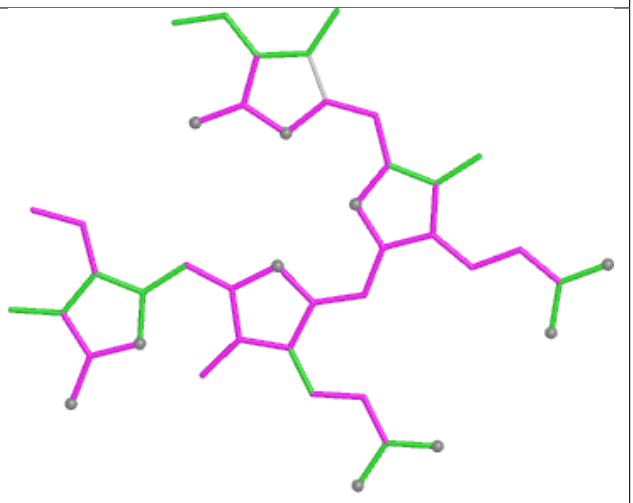


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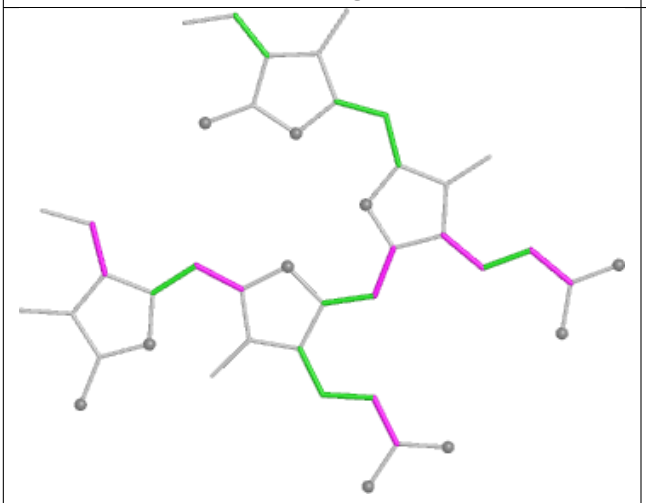
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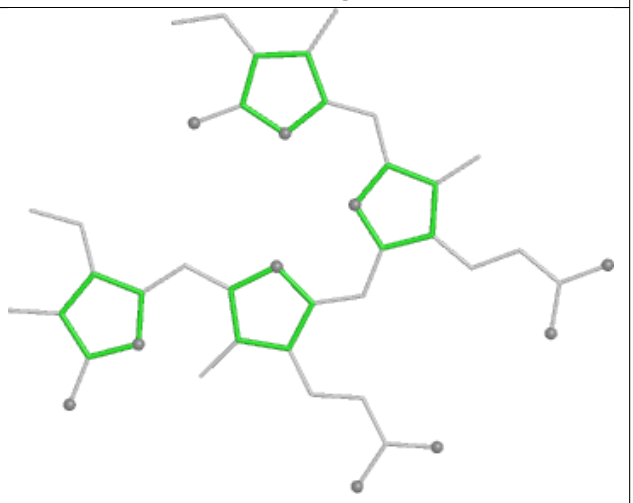
Bond lengths



Bond angles

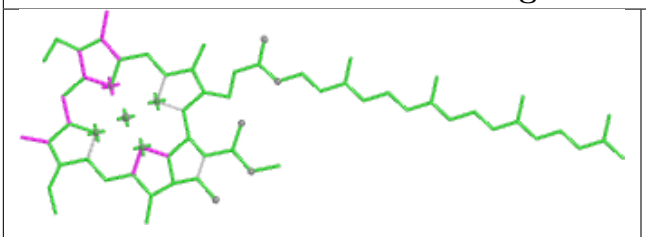


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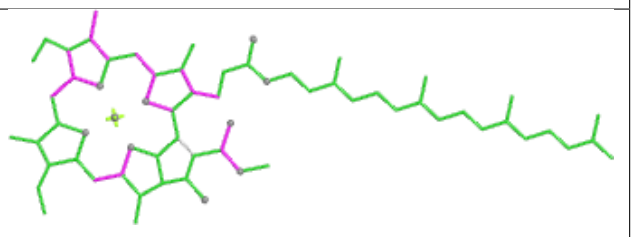


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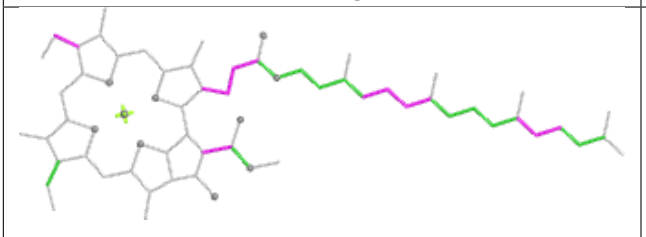
Ligand CLA 52 602



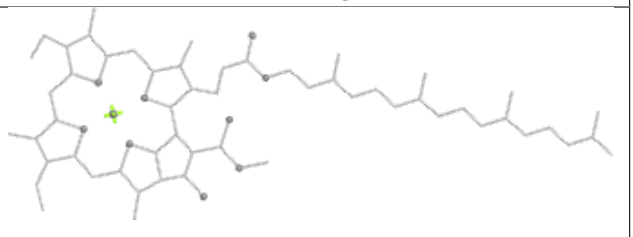
Bond lengths



Bond angles

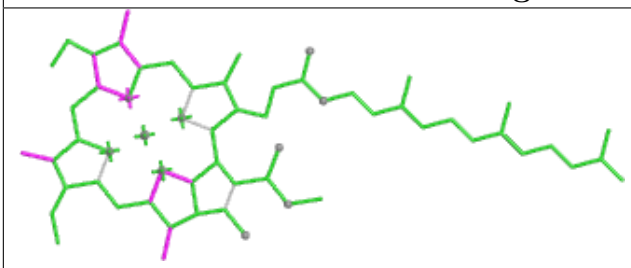


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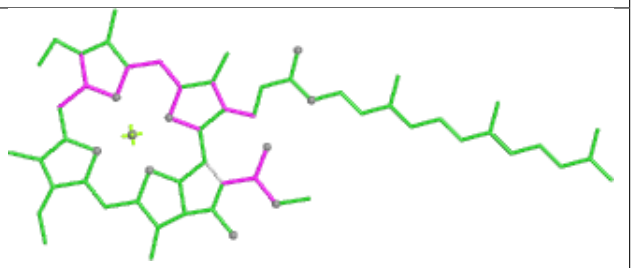


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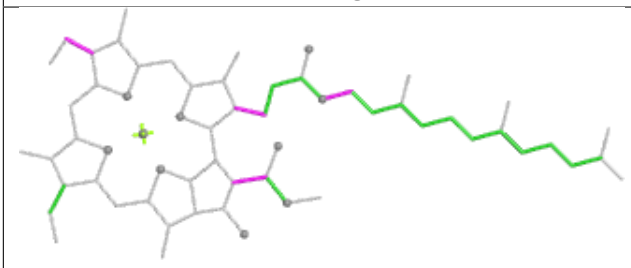
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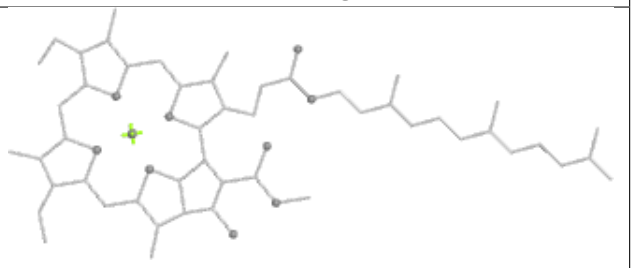
Bond lengths



Bond angles

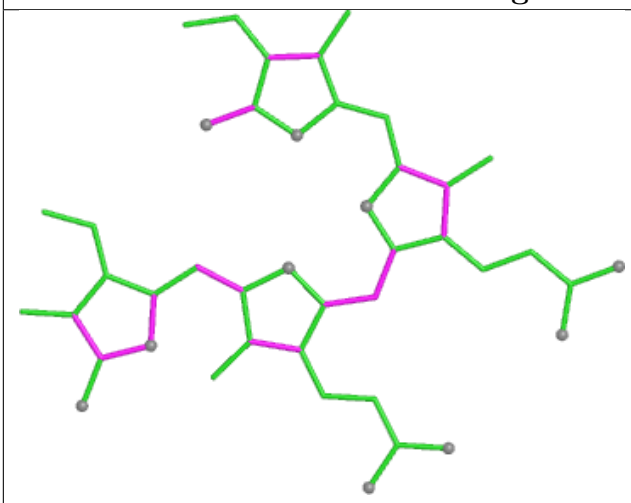


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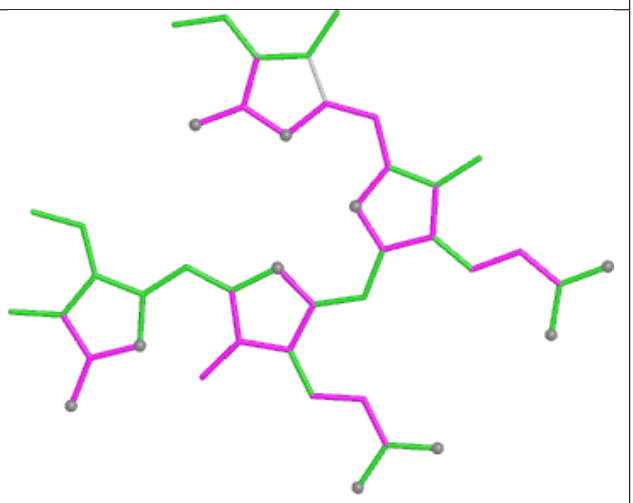


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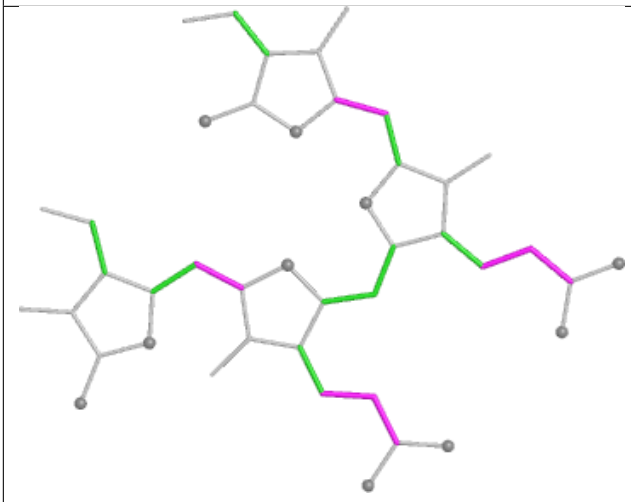
Ligand PEB VB 202



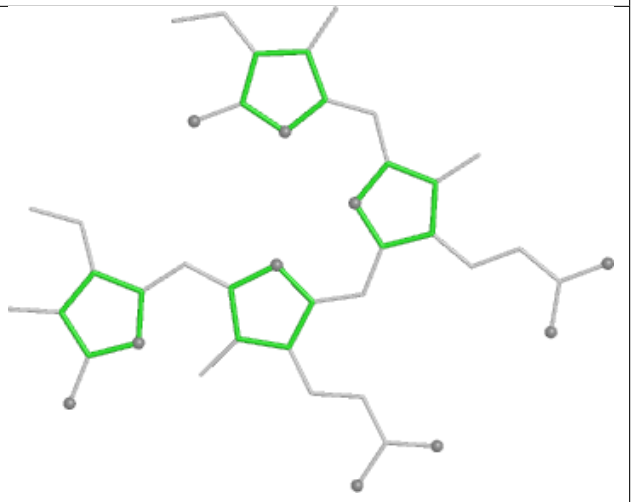
Bond lengths



Bond angles

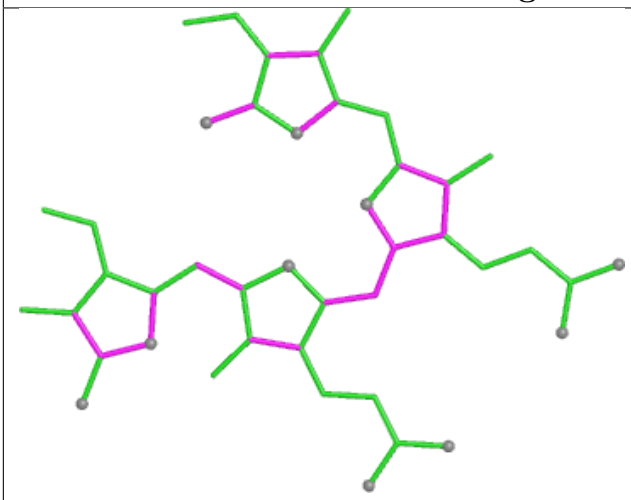


Torsions

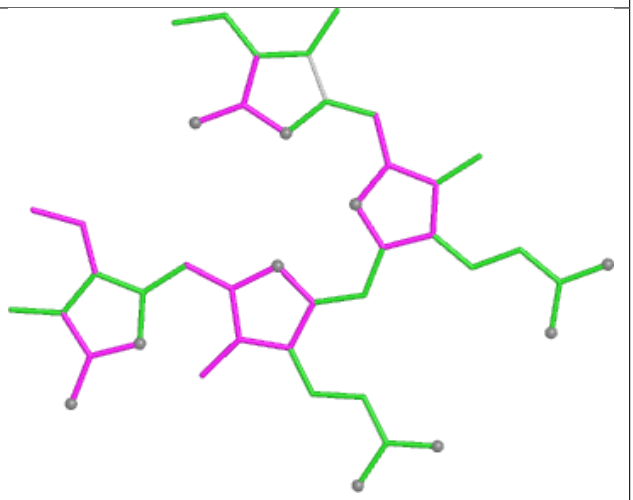


Rings

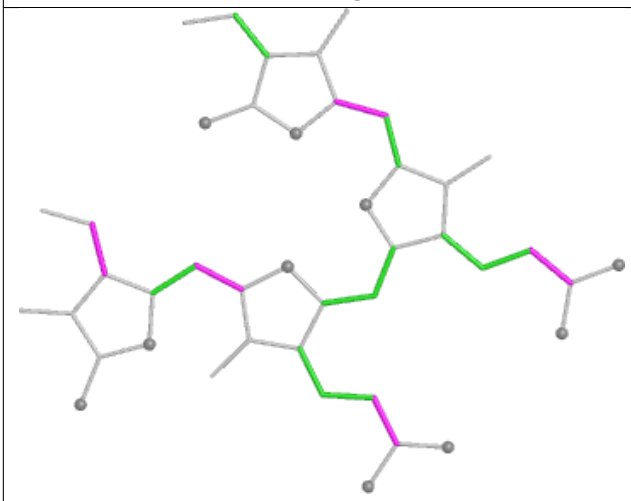
Ligand PEB S4 202



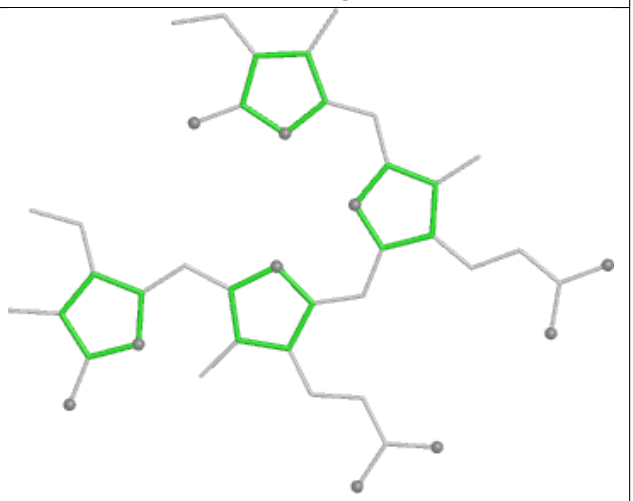
Bond lengths



Bond angles

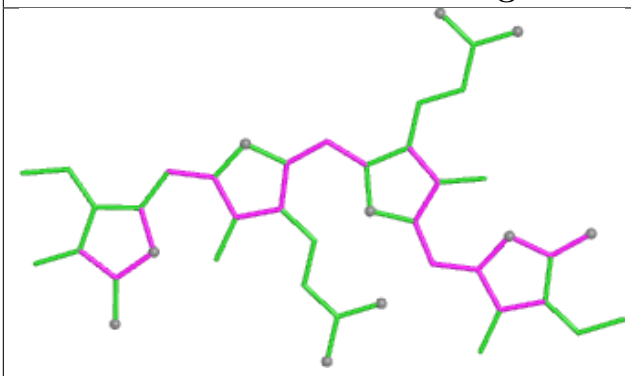


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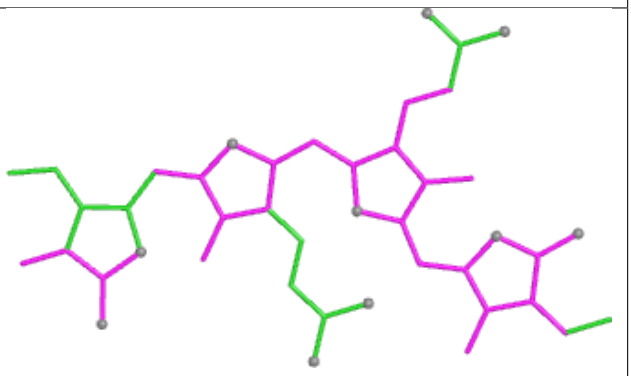


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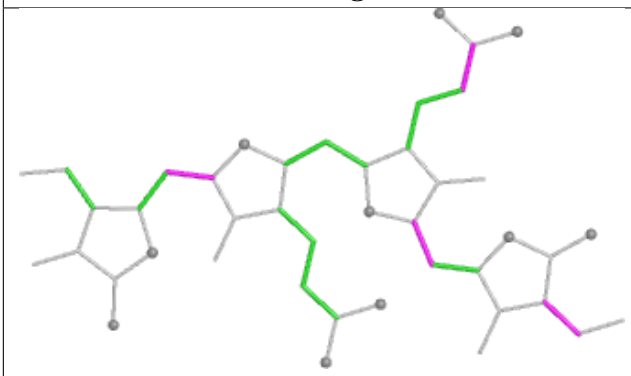
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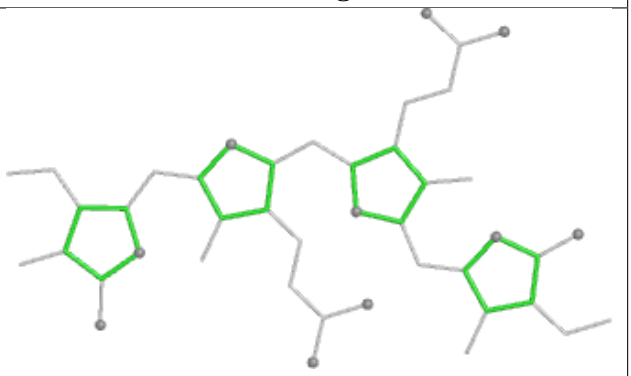
Bond lengths



Bond angles

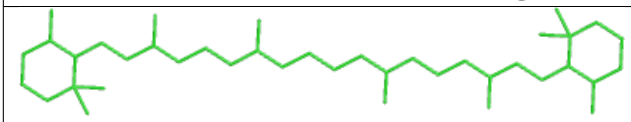


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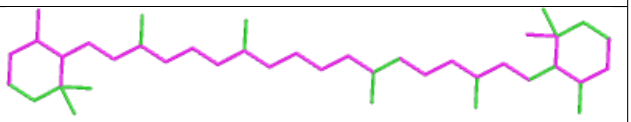


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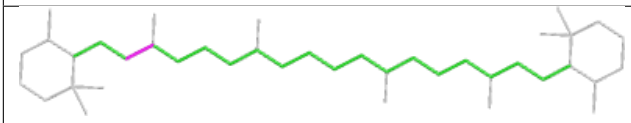
Ligand BCR A2 804



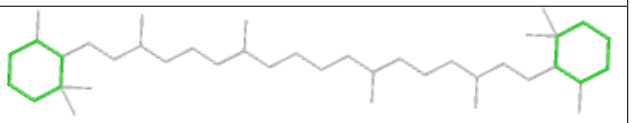
Bond lengths



Bond angles

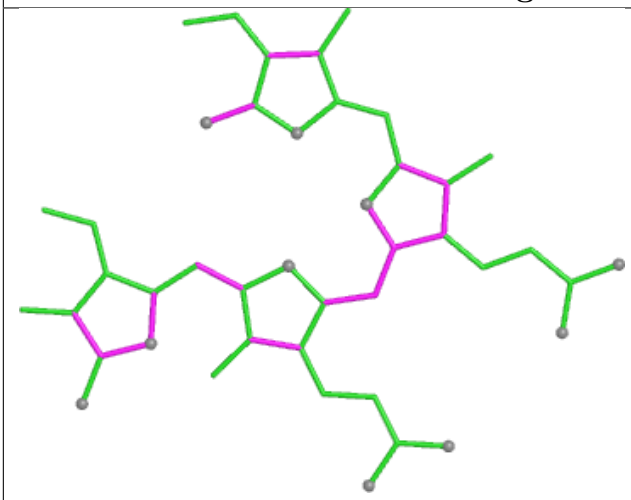


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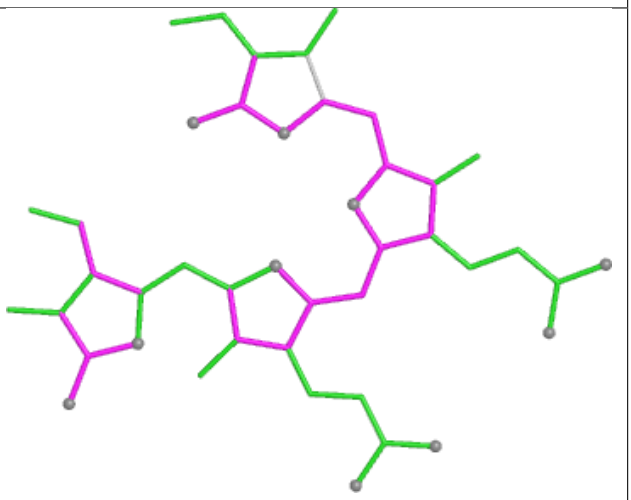


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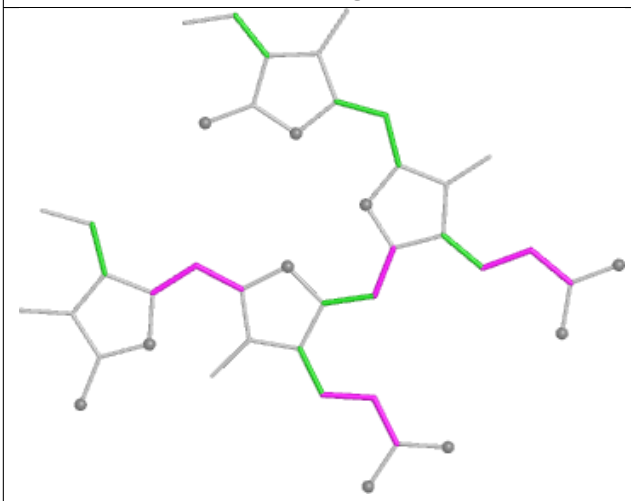
Ligand PEB P5 202



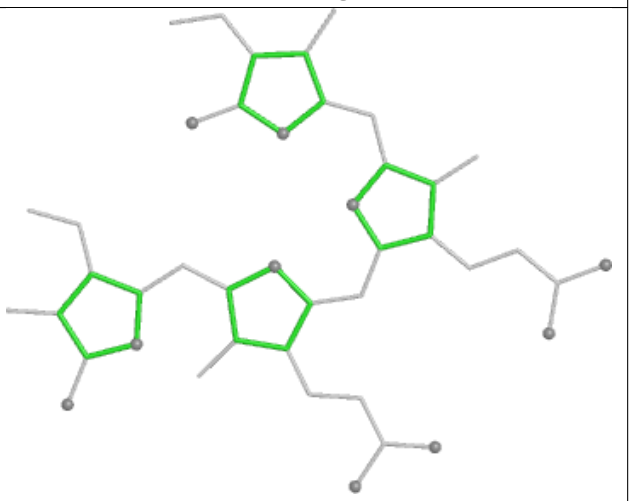
Bond lengths



Bond angles

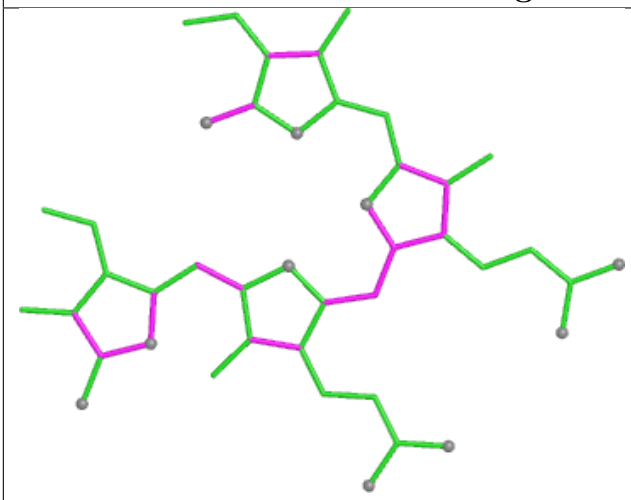


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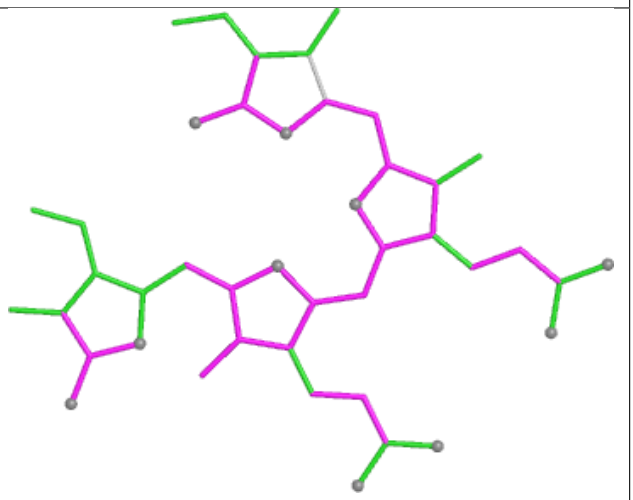


Rings

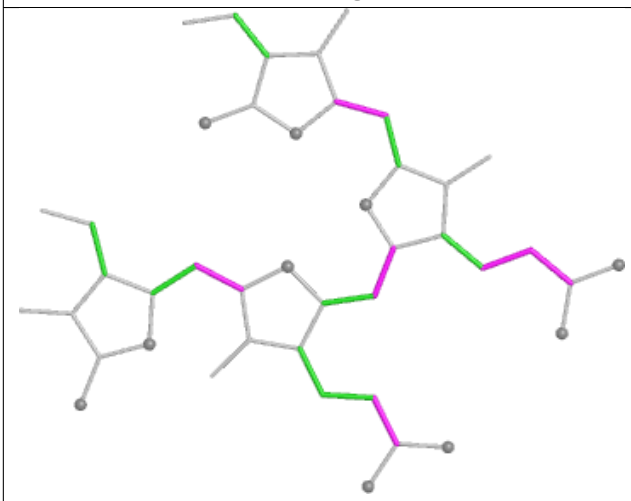
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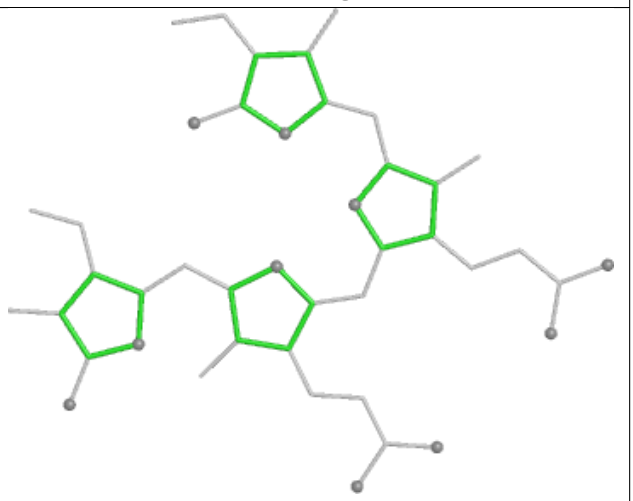
Bond lengths



Bond angles

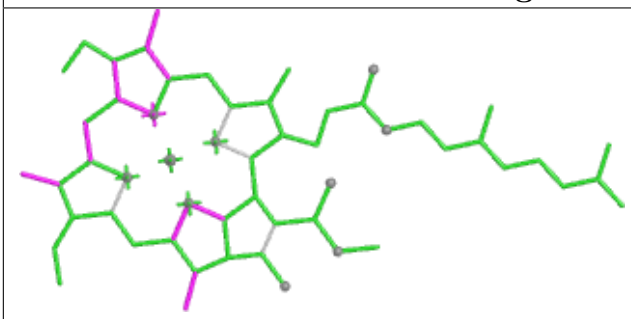


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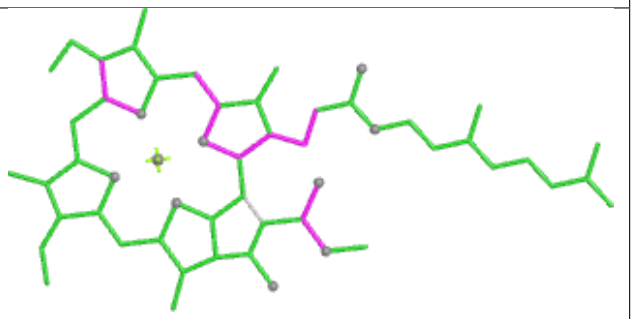


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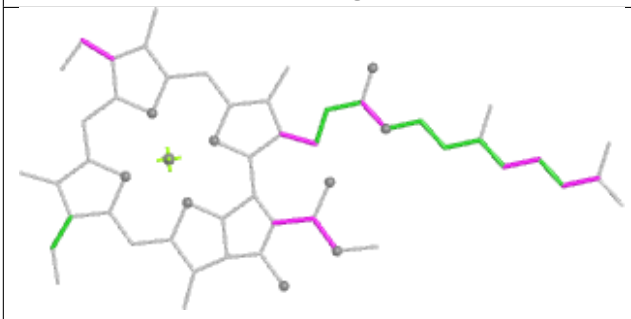
Ligand CLA B2 821



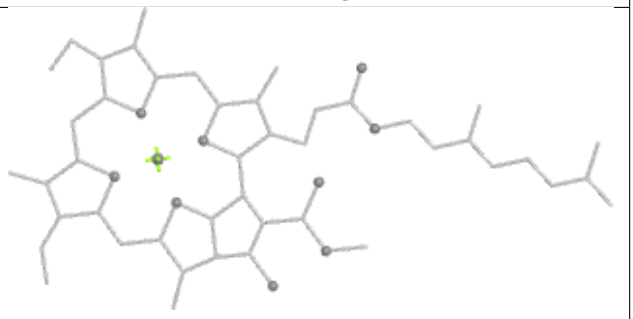
Bond lengths



Bond angles

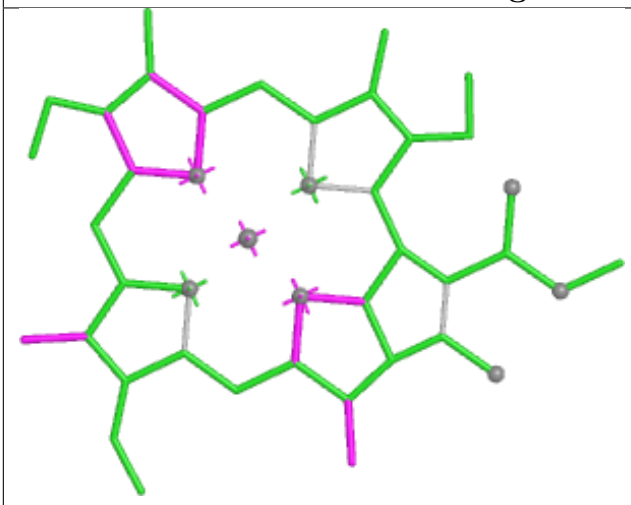


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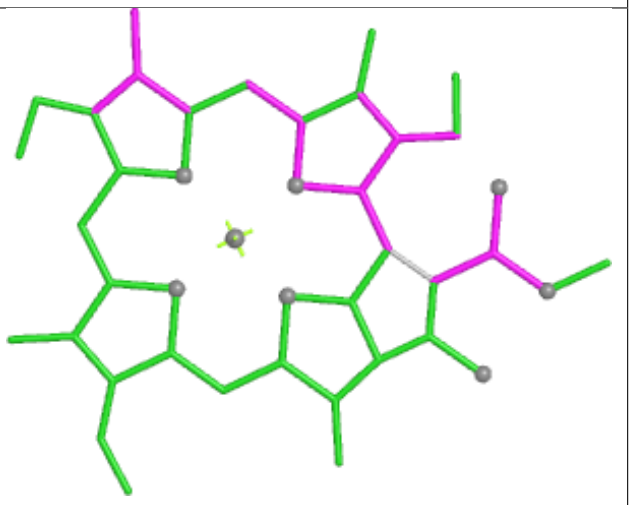


Rings

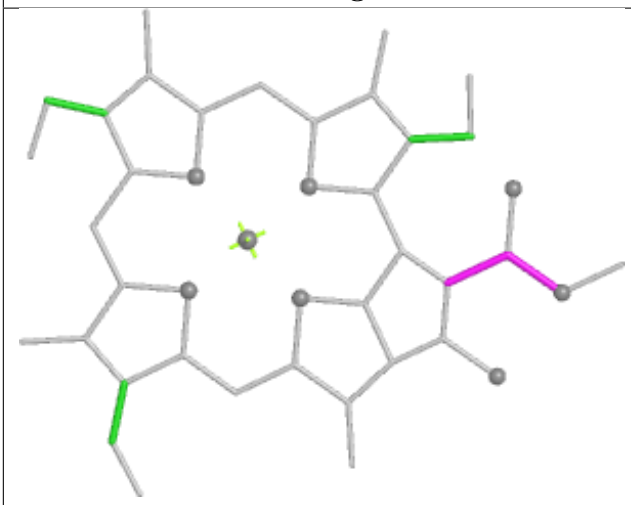
Ligand CLA KN 103



Bond lengths



Bond angles

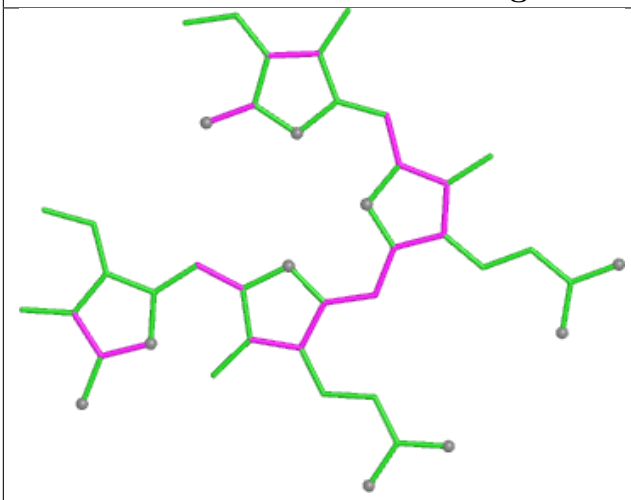


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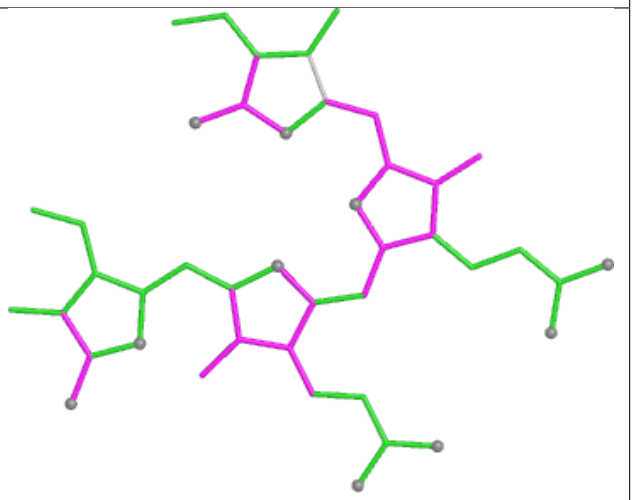


Rings

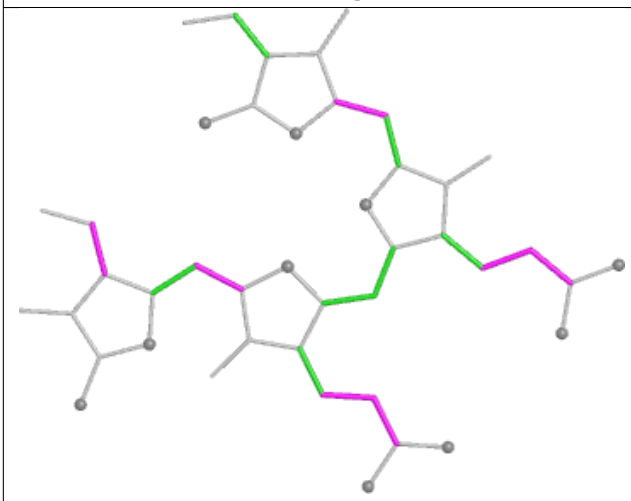
Ligand PEB ND 202



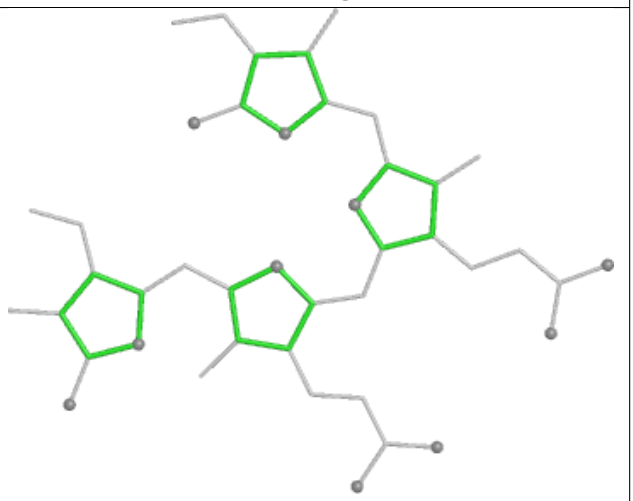
Bond lengths



Bond angles

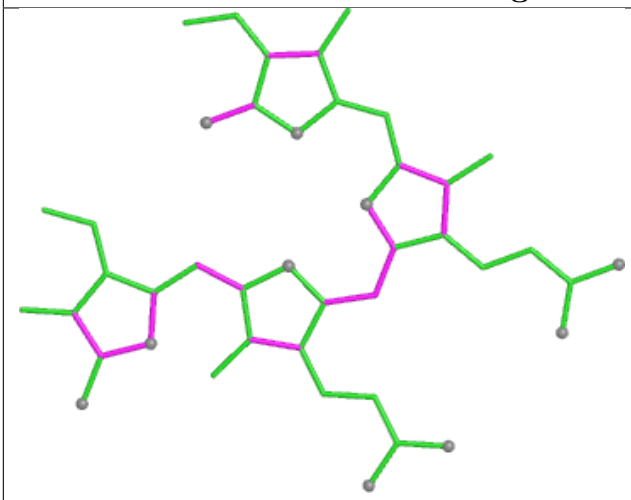


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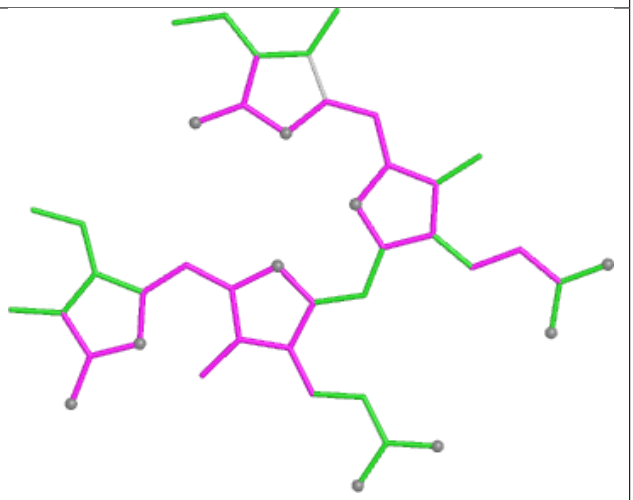


Rings

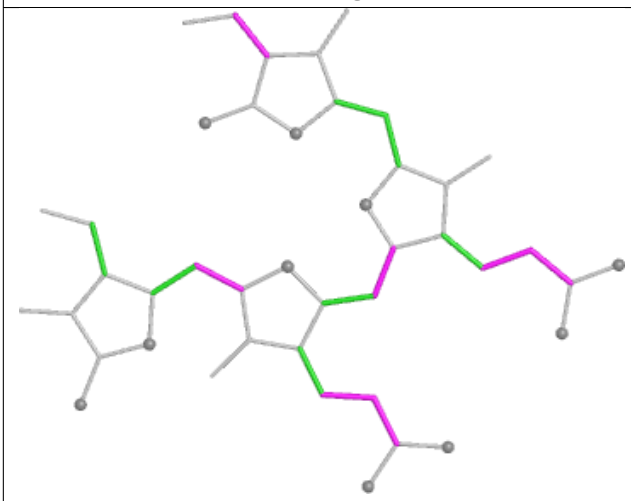
Ligand PEB GB 203



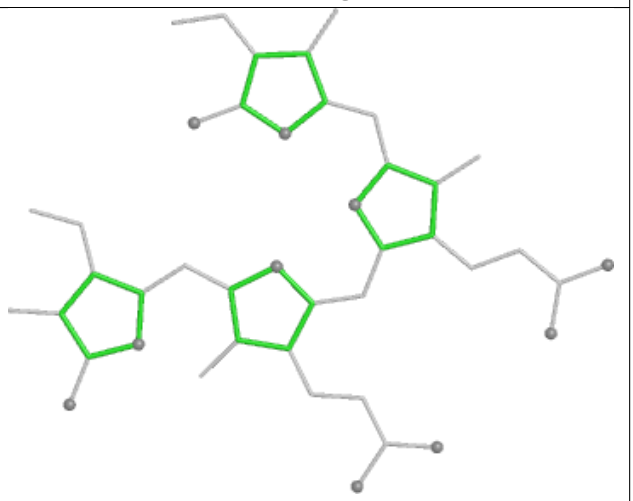
Bond lengths



Bond angles

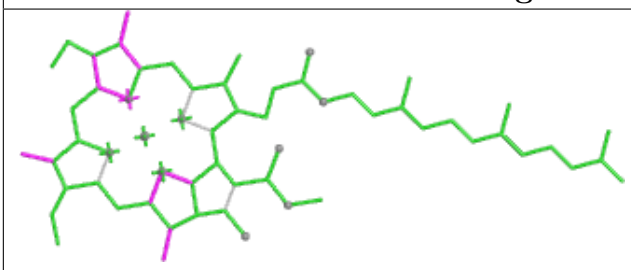


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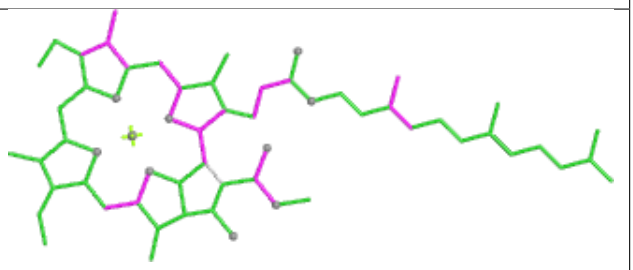


Rings

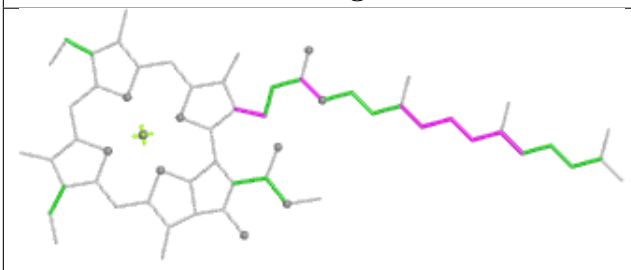
Ligand CLA B2 817



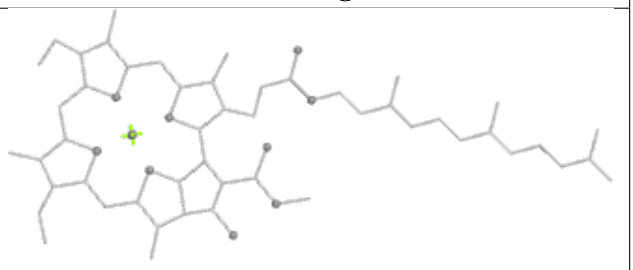
Bond lengths



Bond angles

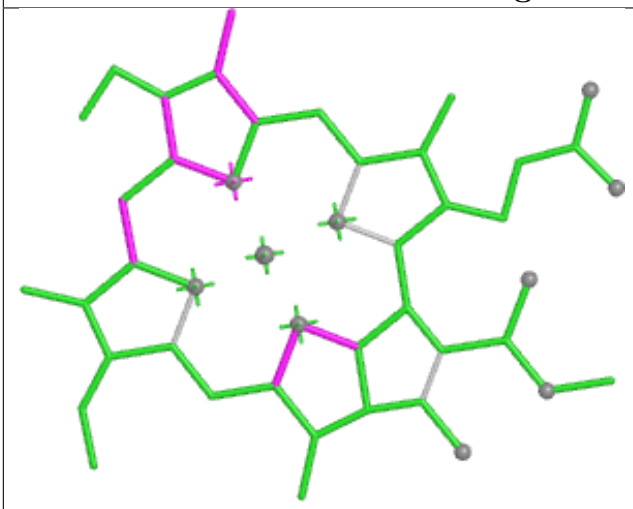


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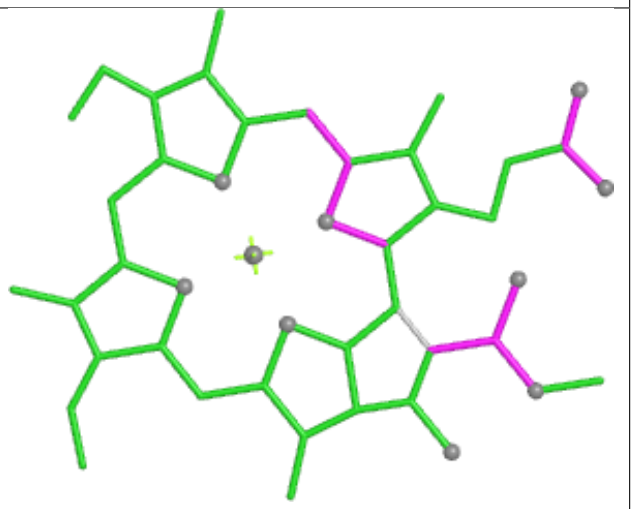


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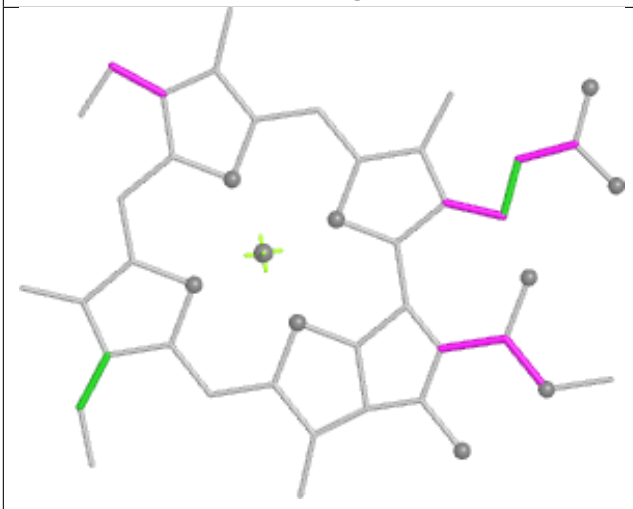
Ligand CLA 2N 306



Bond lengths



Bond angles

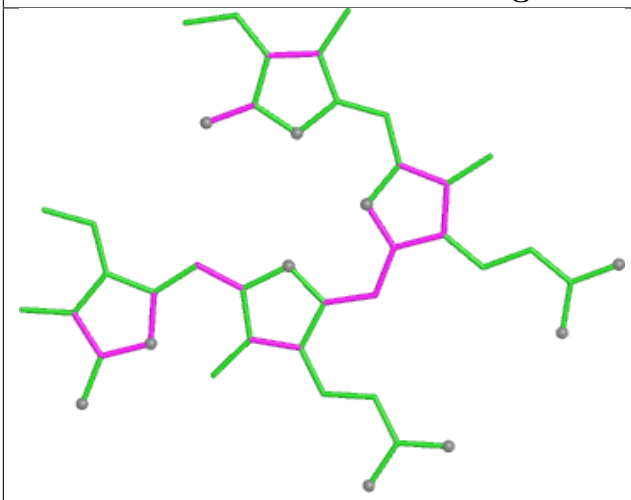


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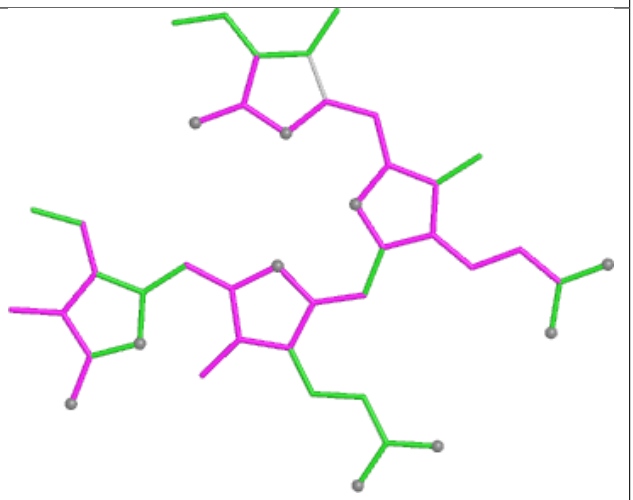


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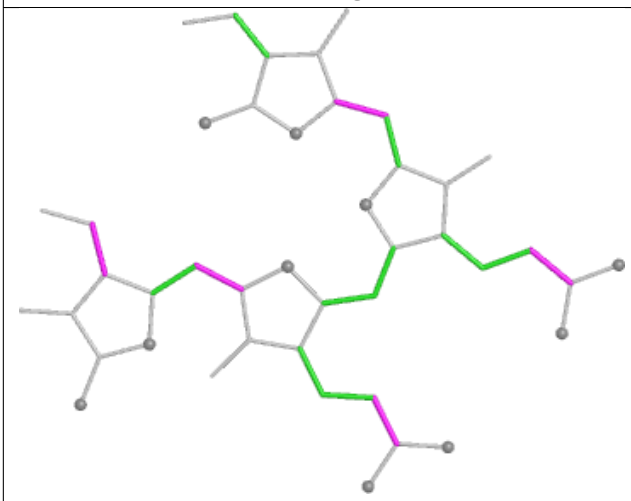
Ligand PEB OE 201



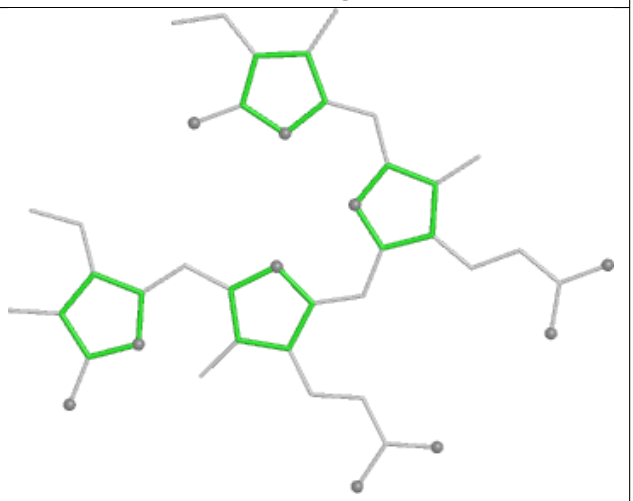
Bond lengths



Bond angles

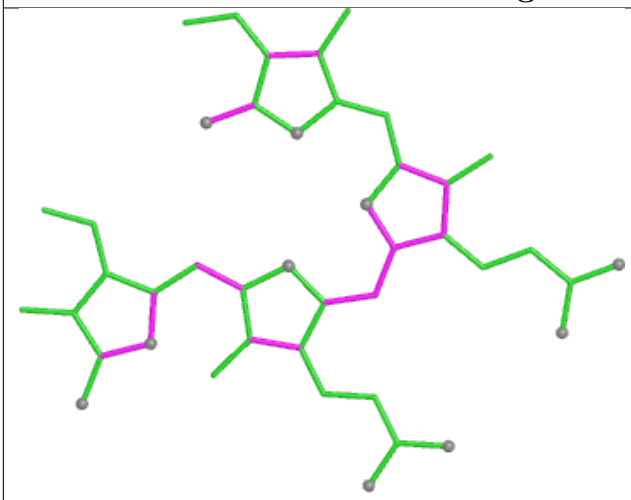


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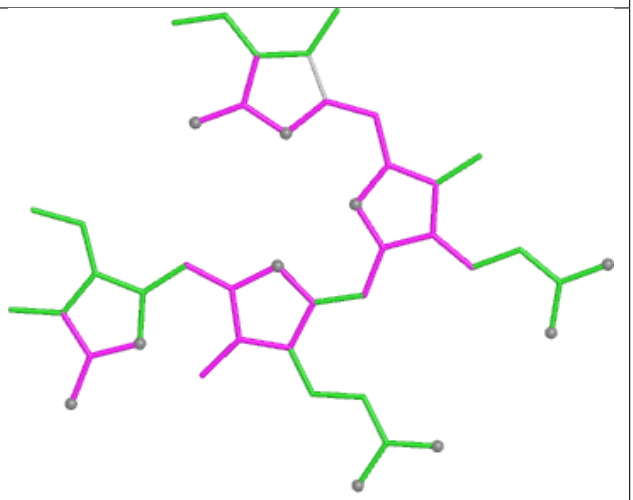


Rings

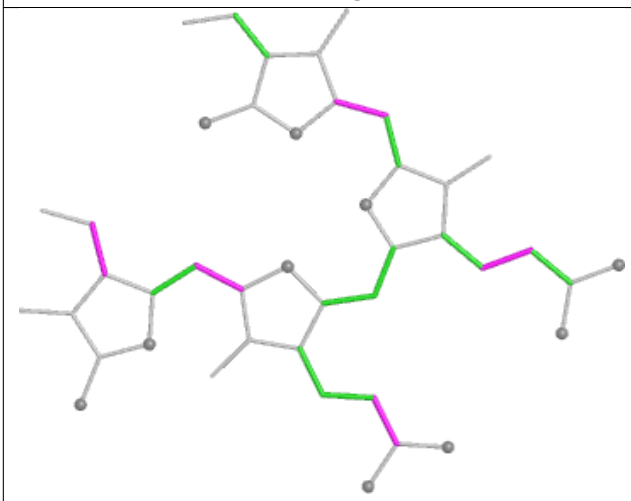
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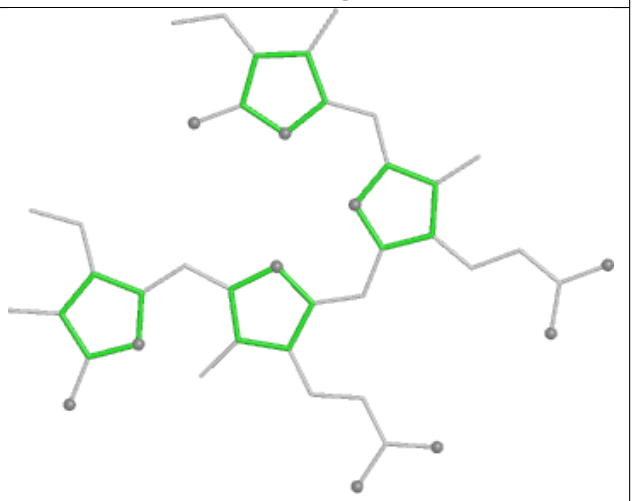
Bond lengths



Bond angles

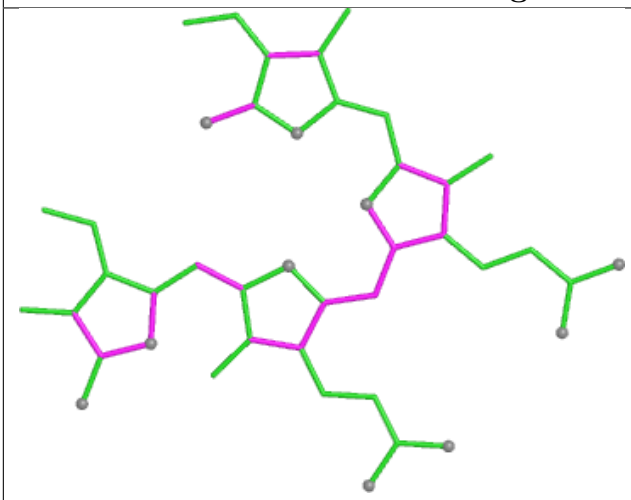


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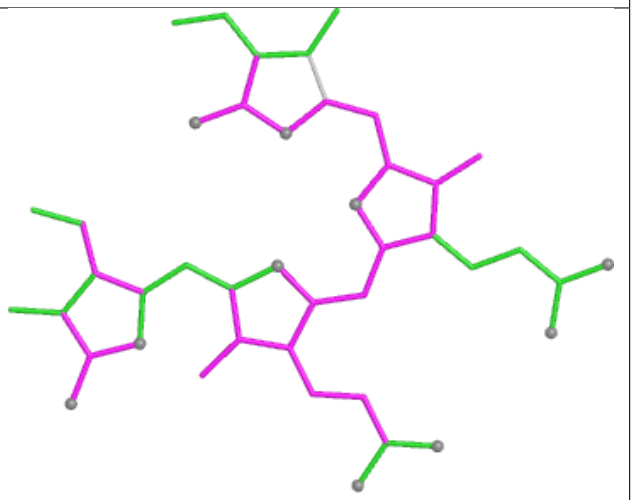


Rings

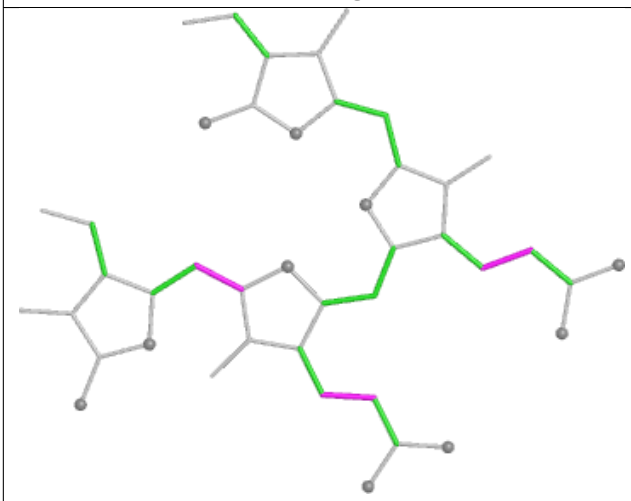
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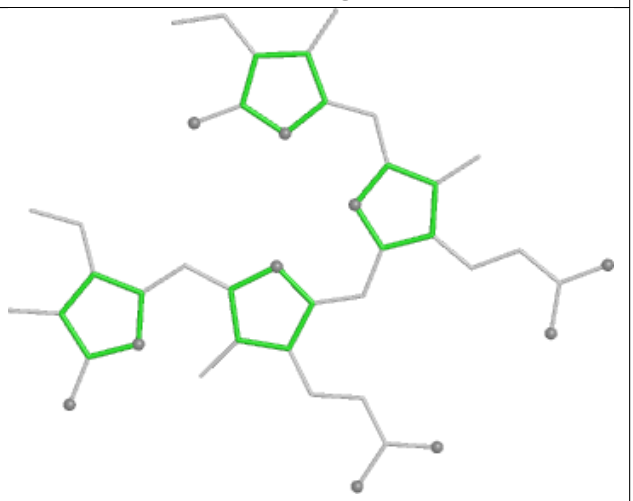
Bond lengths



Bond angles

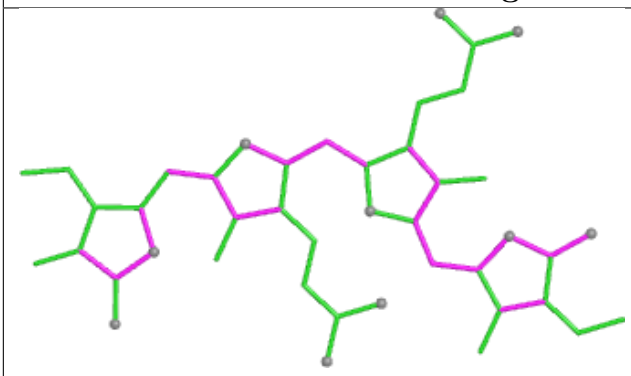


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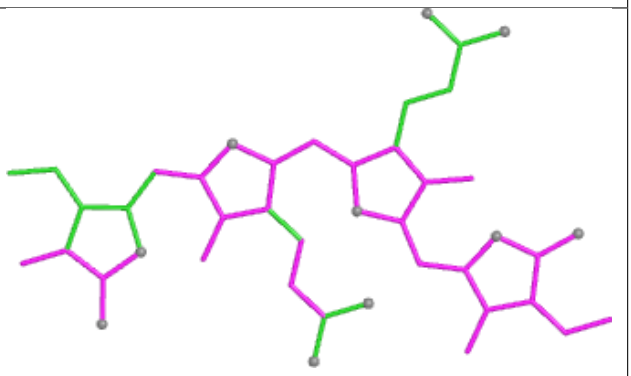


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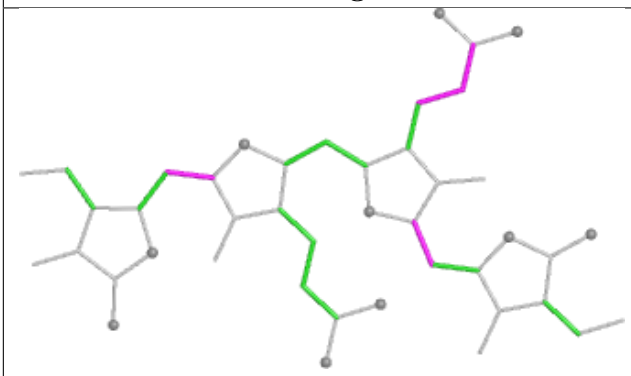
Ligand CYC BE 1002



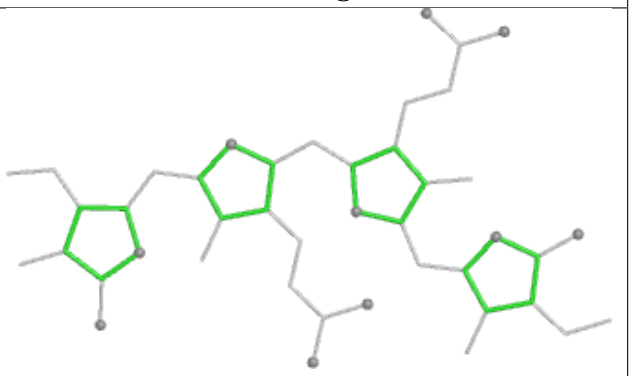
Bond lengths



Bond angles

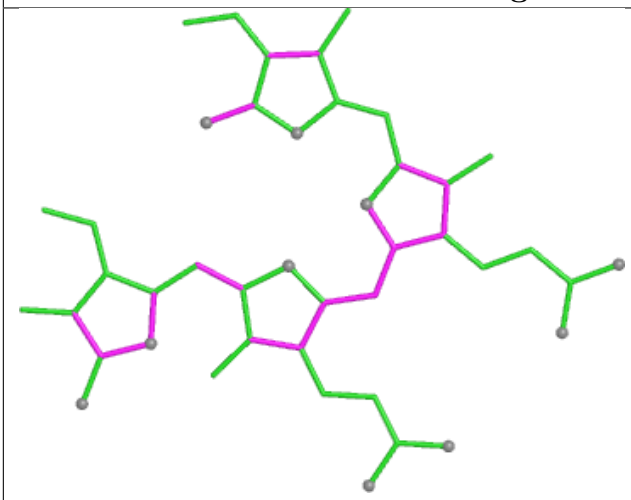


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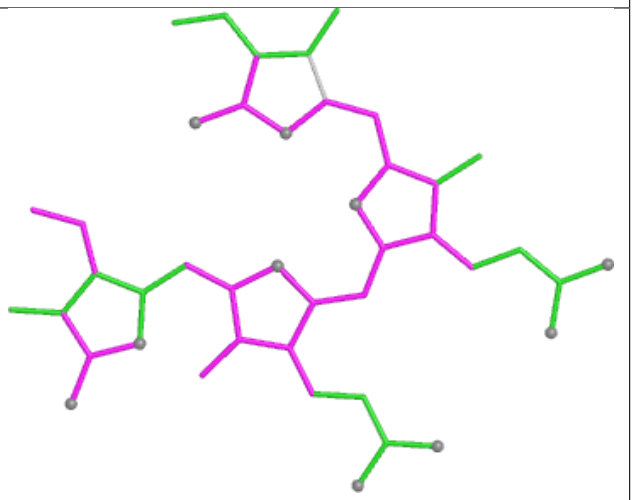


Rings

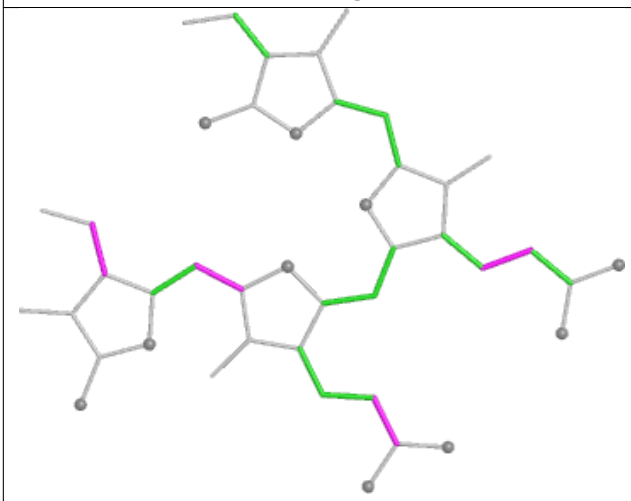
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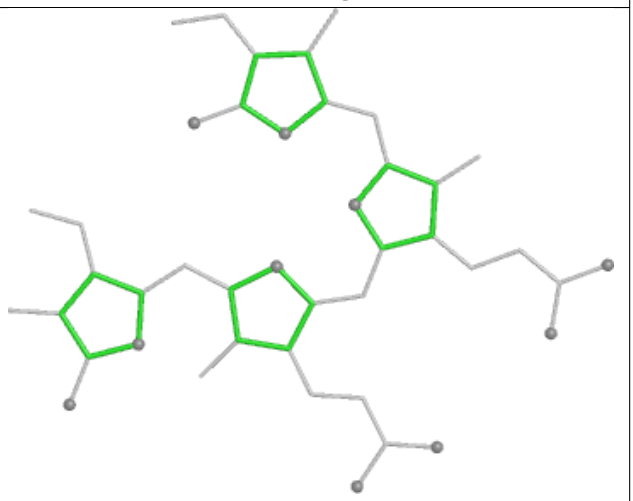
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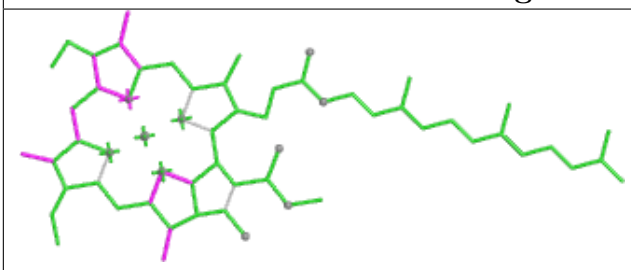


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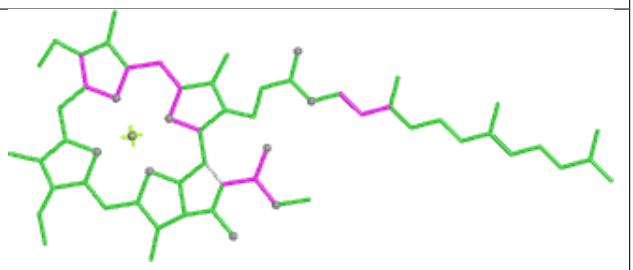


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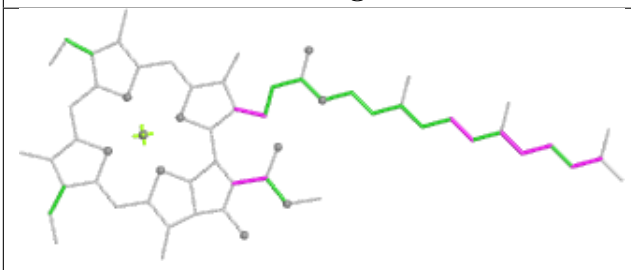
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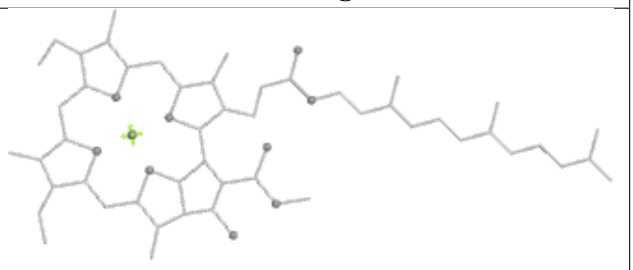
Bond lengths



Bond angles

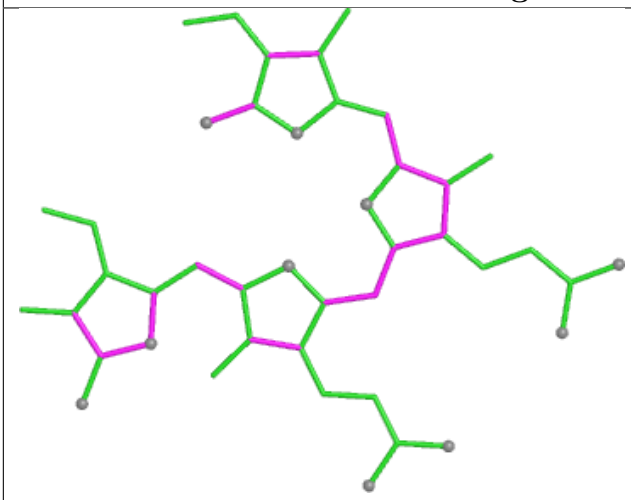


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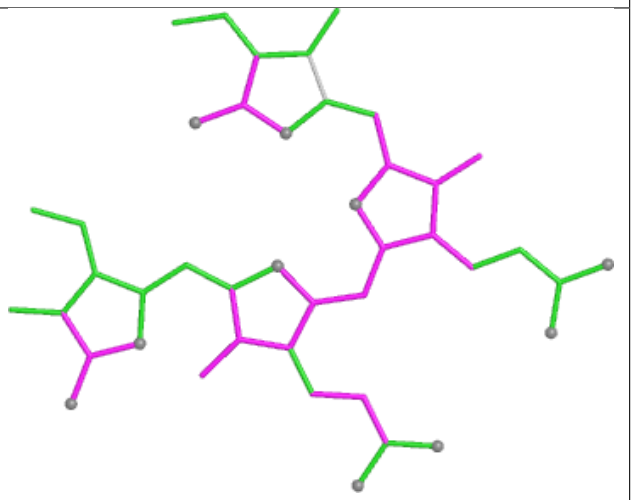


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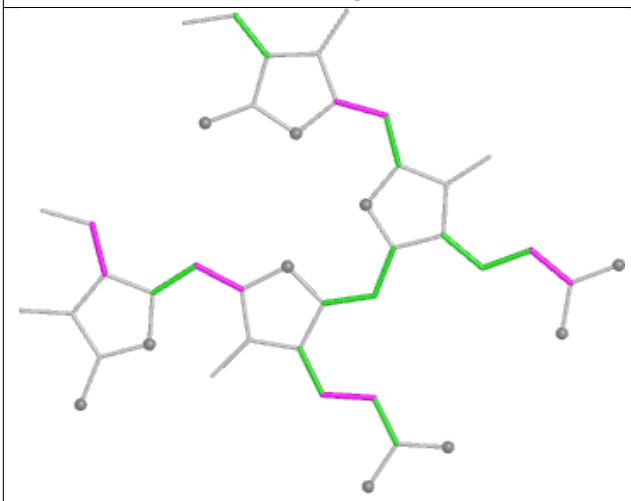
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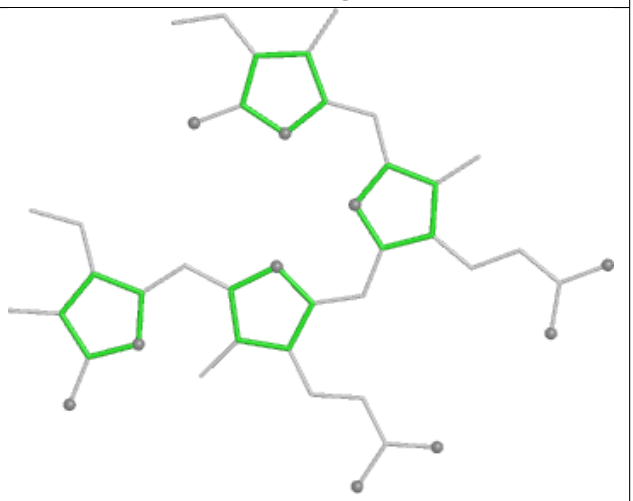
Bond lengths



Bond angles

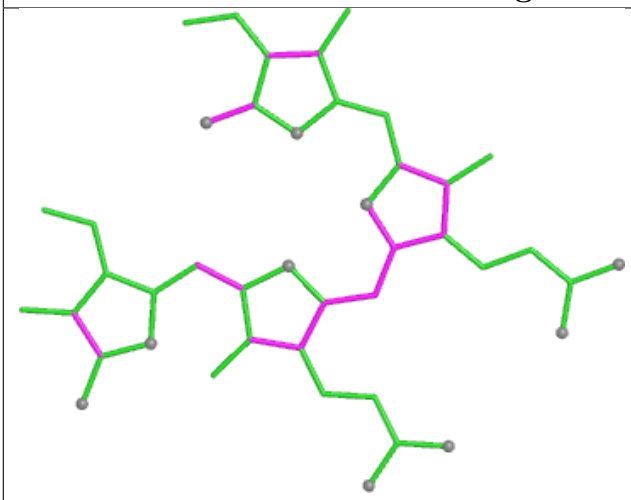


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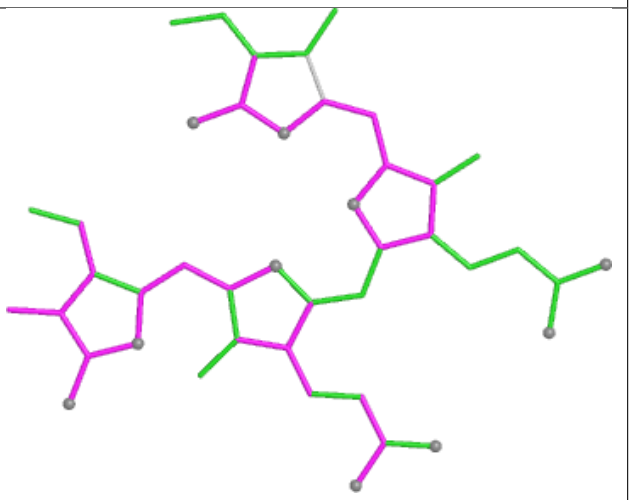


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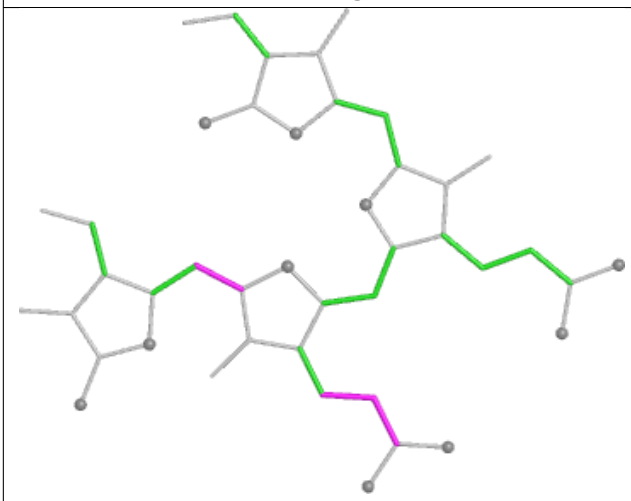
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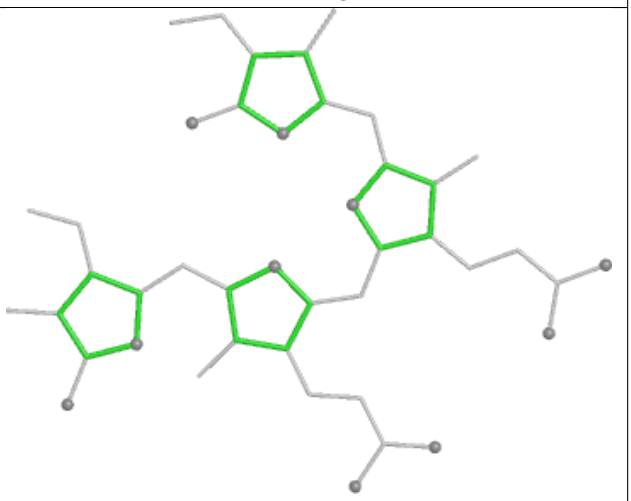
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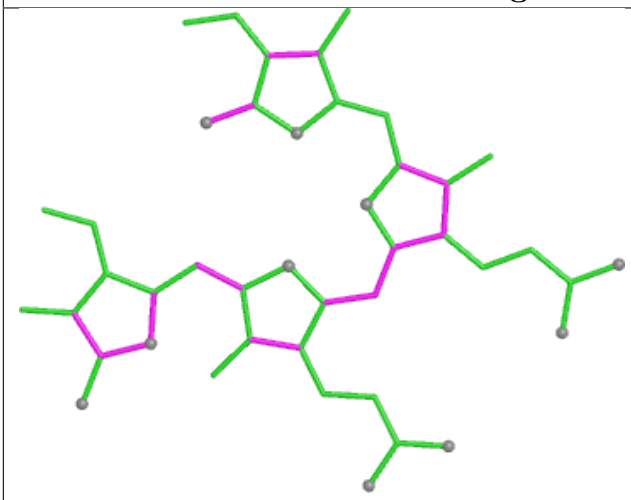


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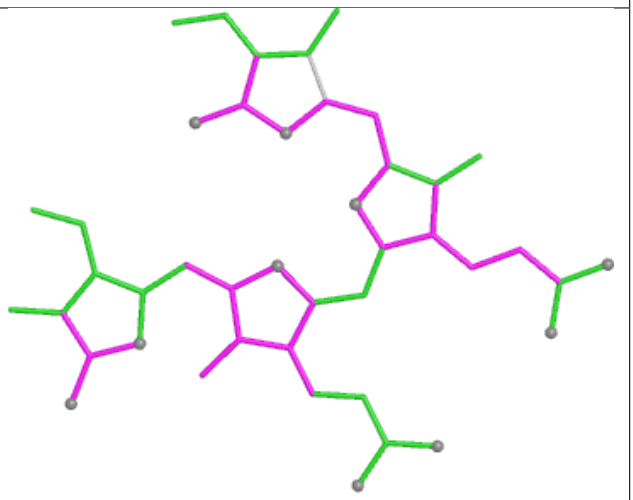


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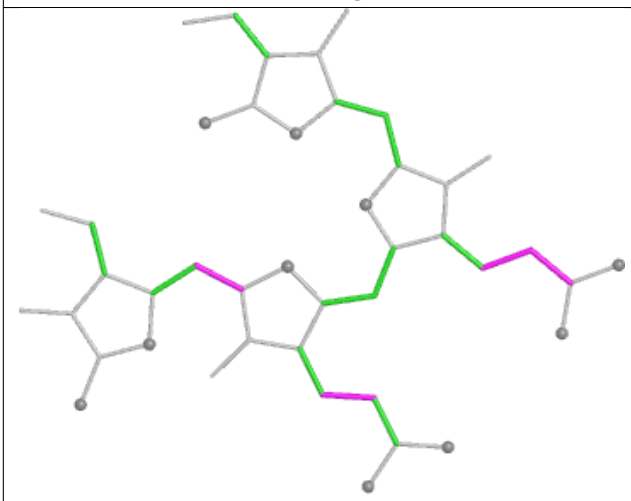
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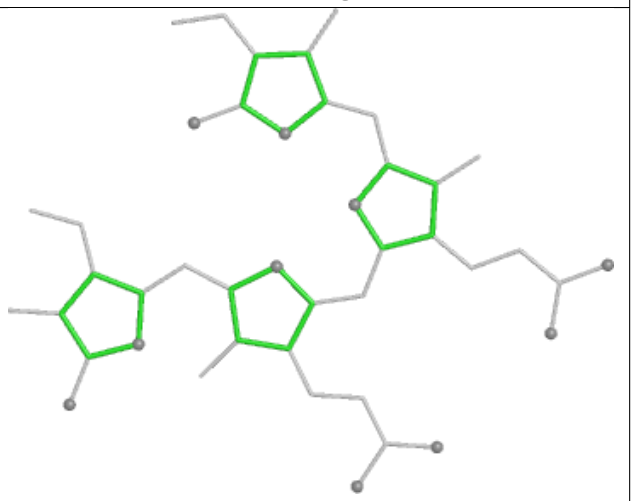
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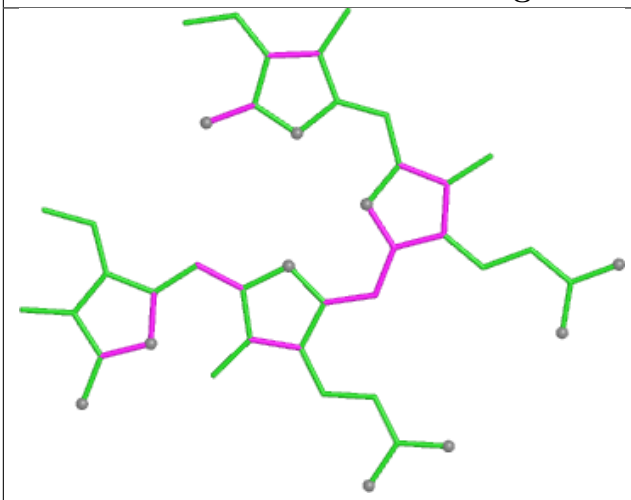


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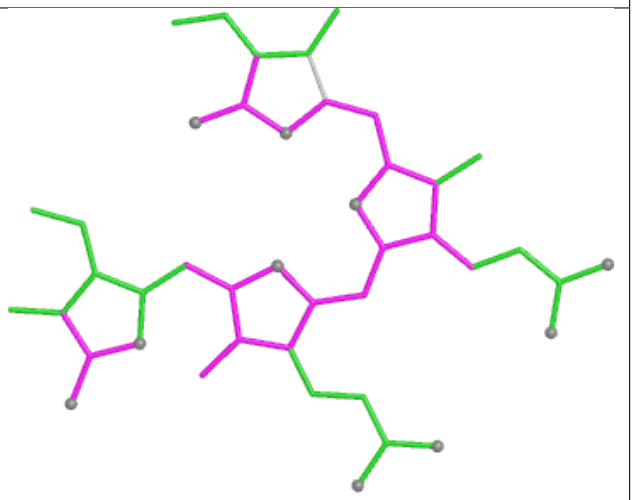


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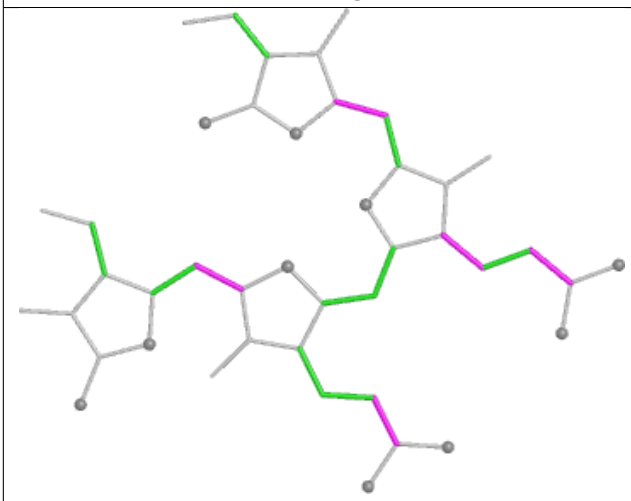
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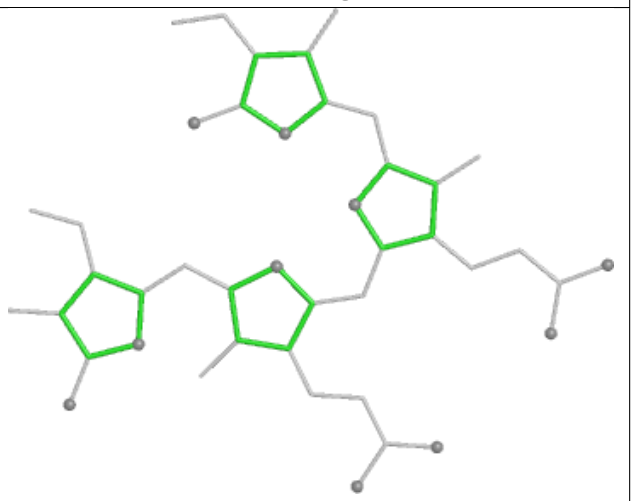
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Bond angles

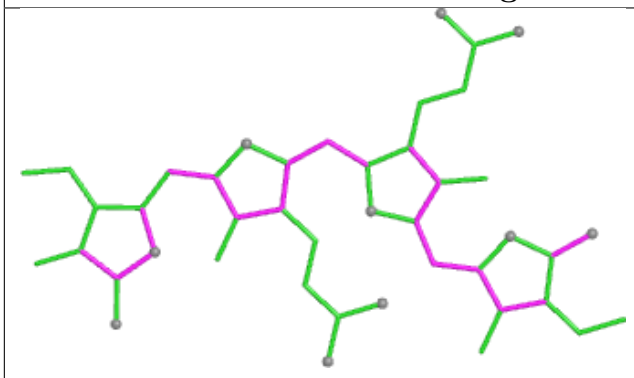


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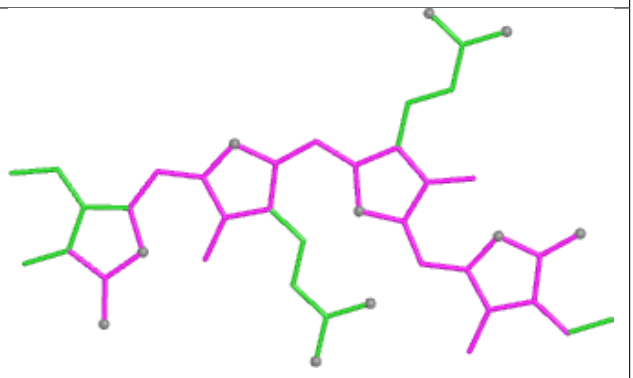


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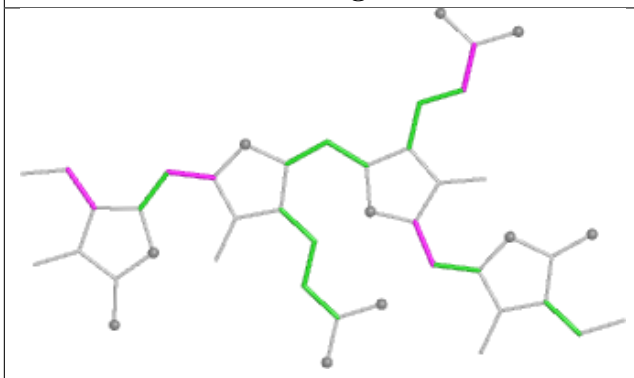
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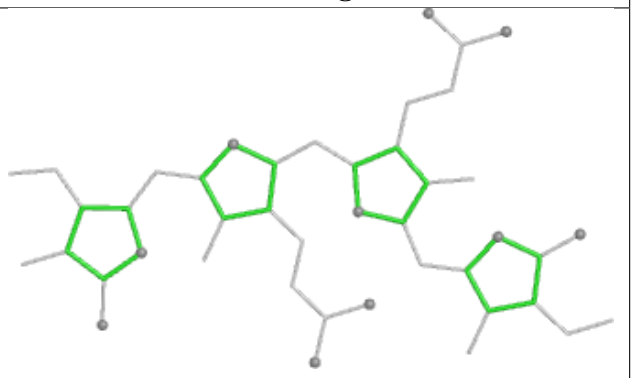
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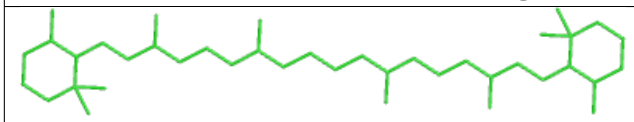


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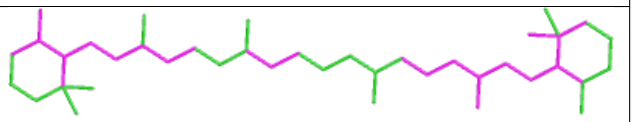


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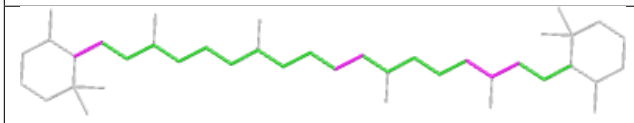
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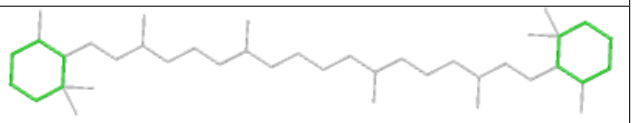
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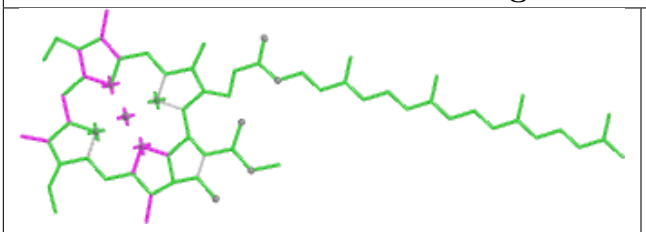


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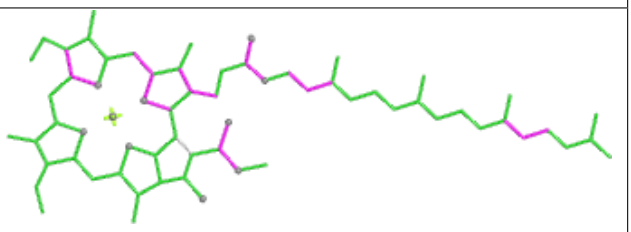


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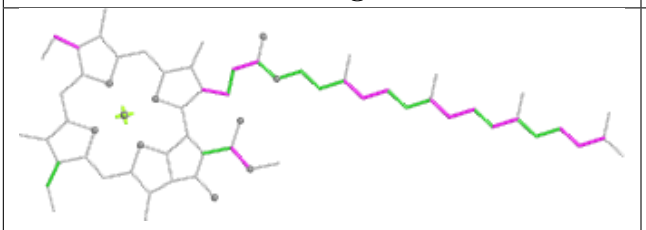
Ligand CLA AN 808



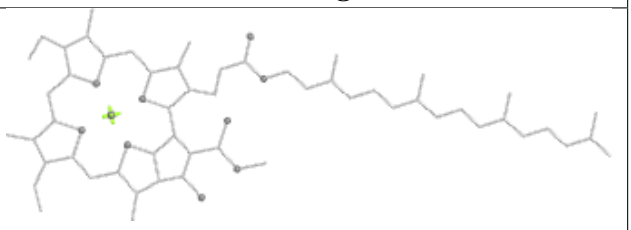
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Bond angles

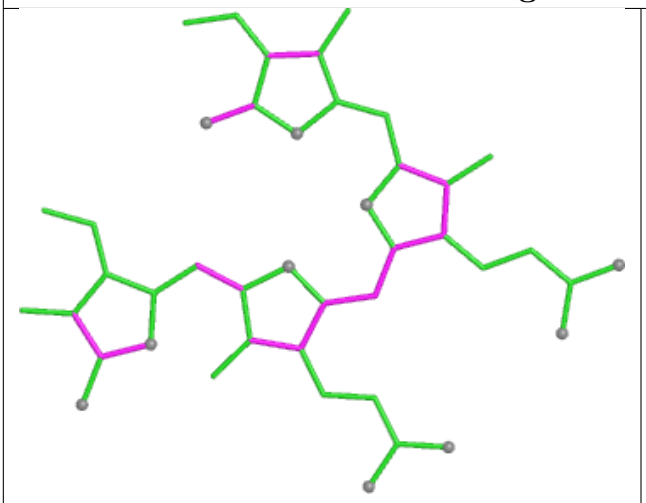


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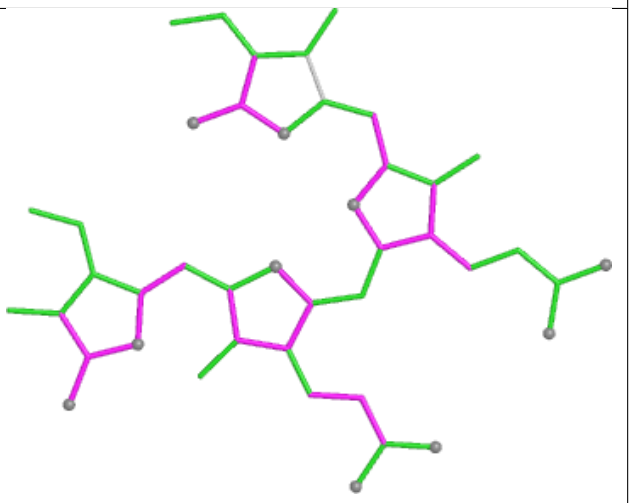


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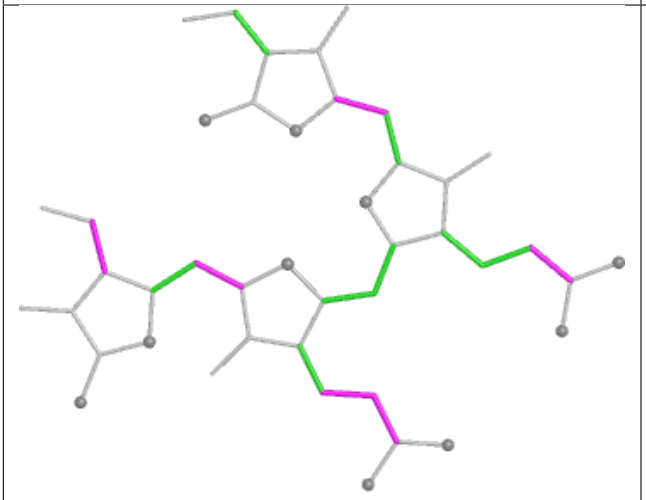
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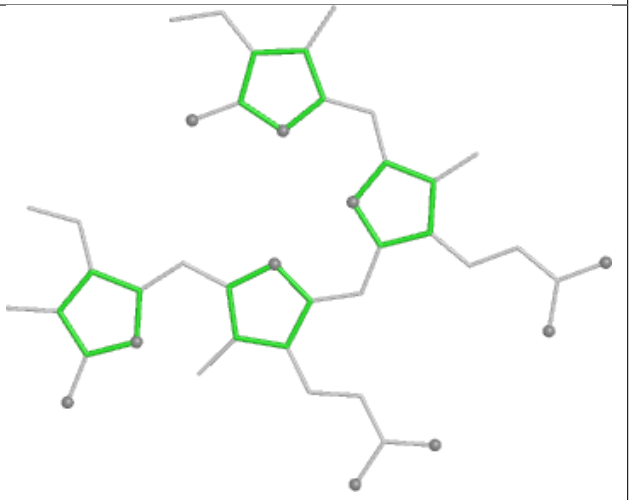
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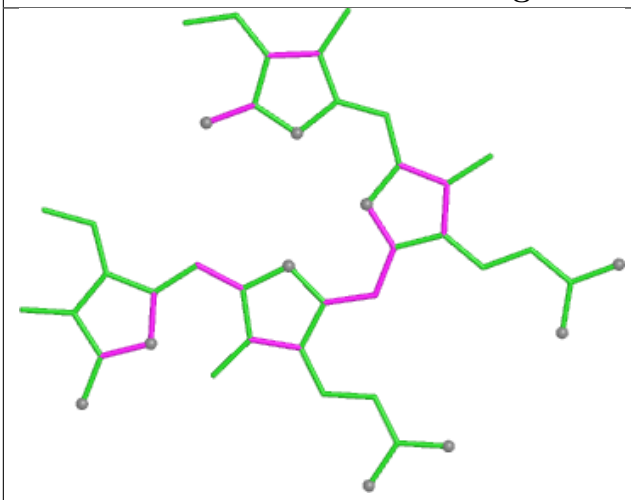


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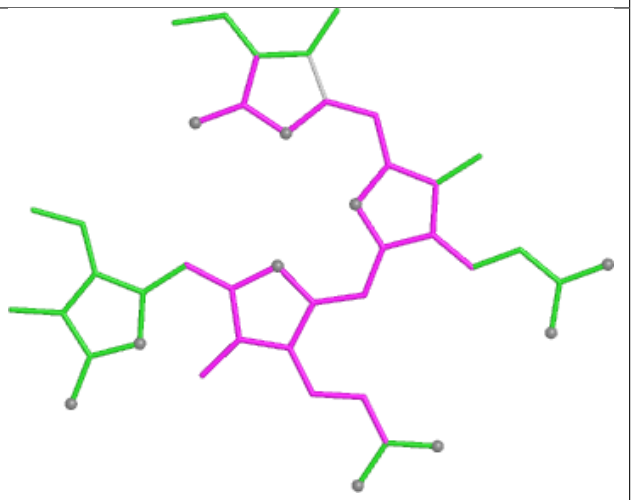


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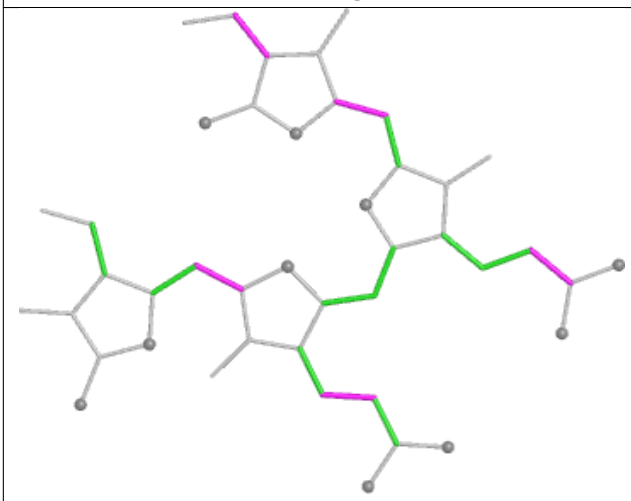
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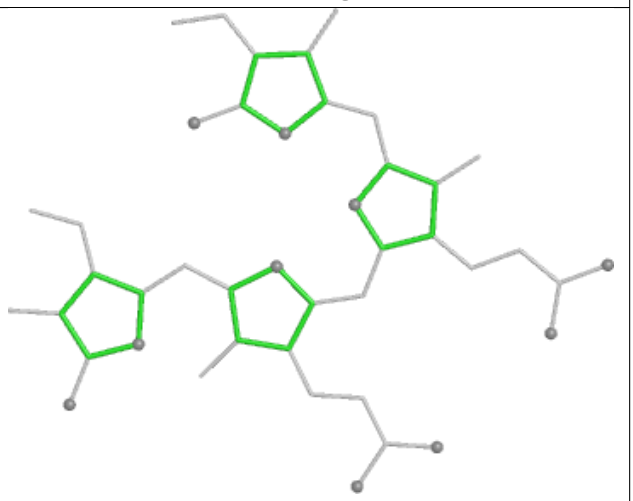
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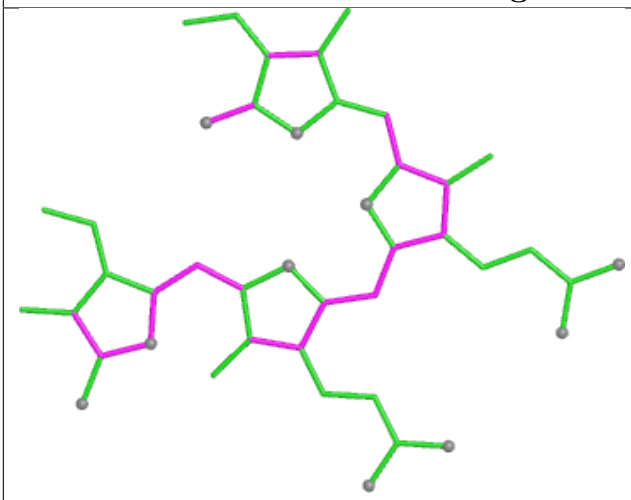


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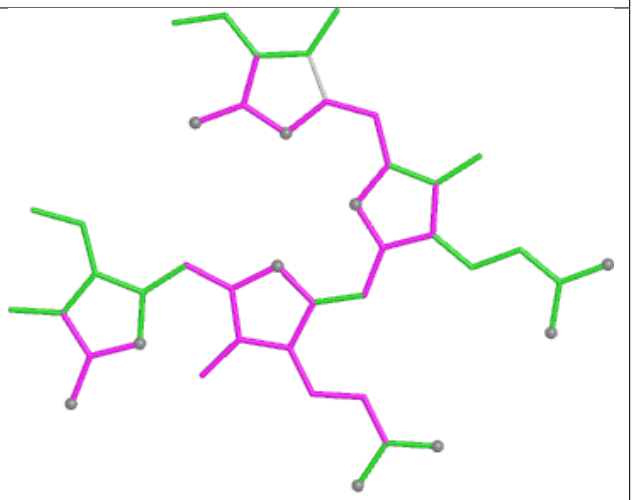


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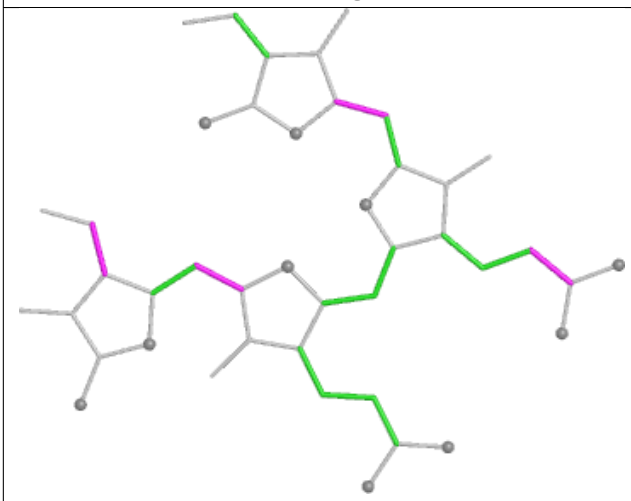
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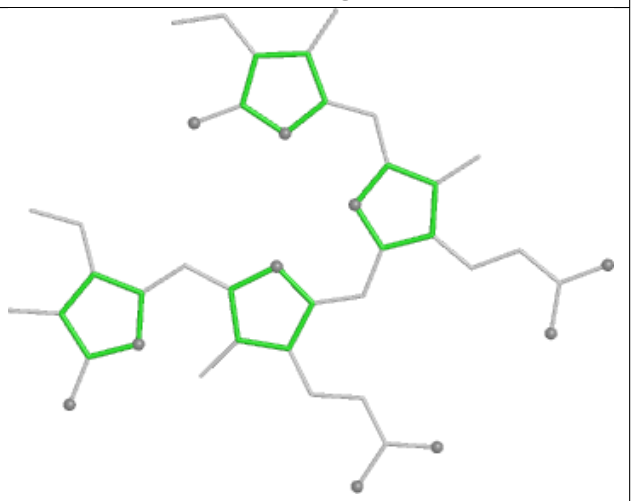
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Bond angles

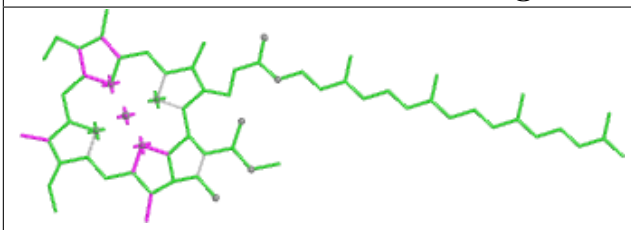


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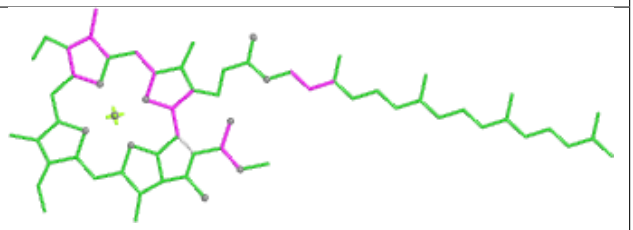


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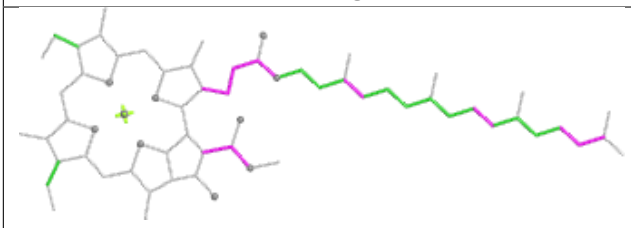
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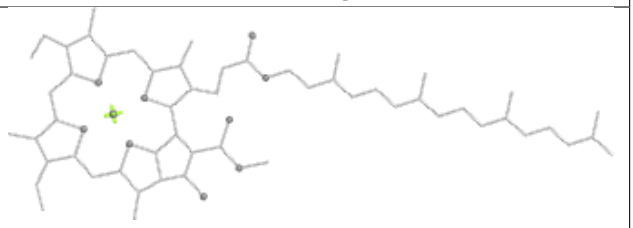
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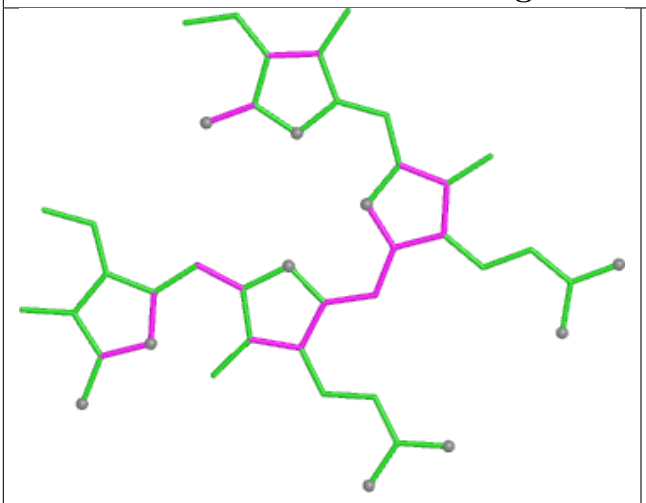


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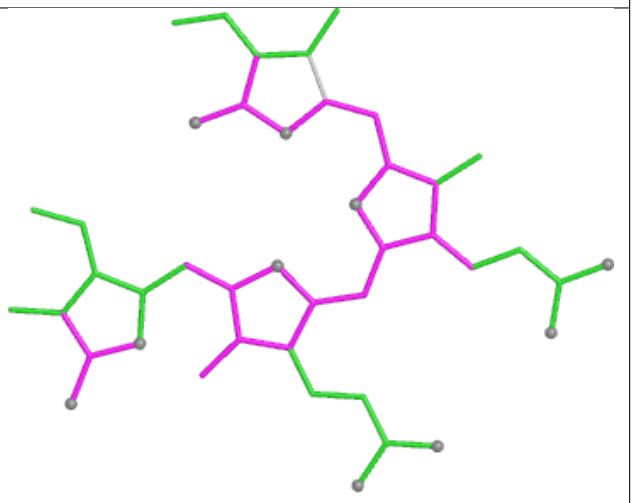


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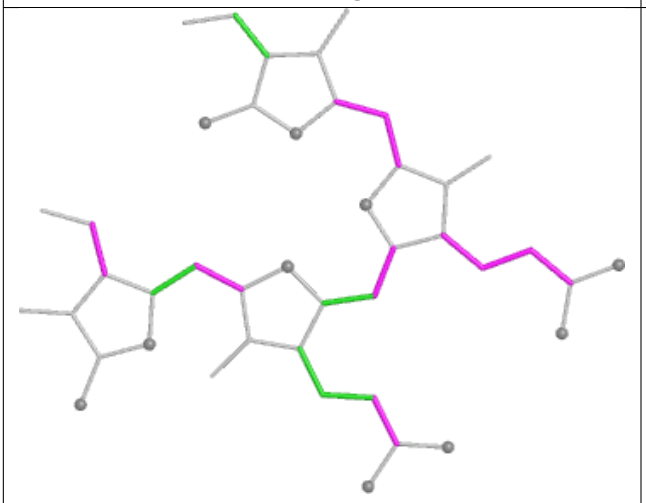
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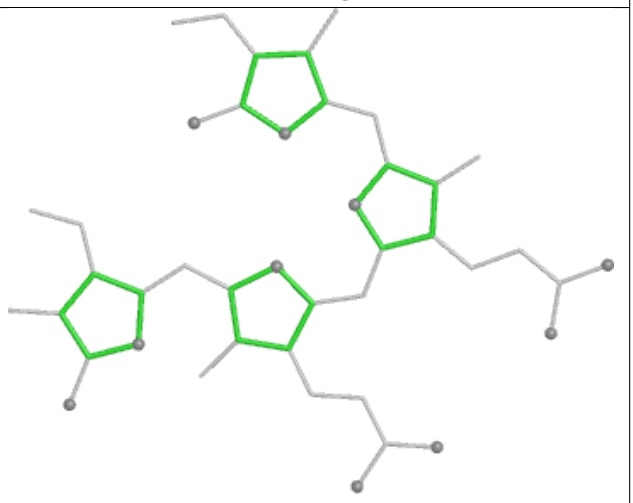
Bond lengths



Bond angles

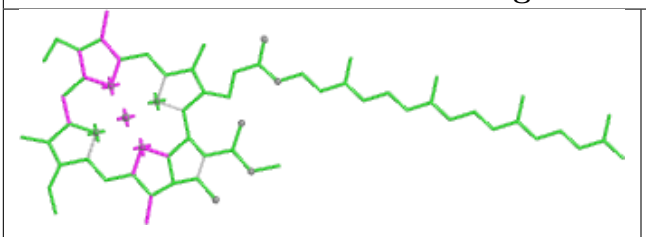


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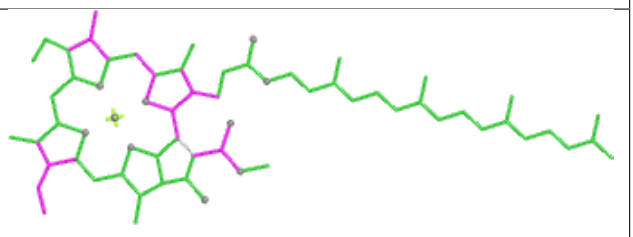


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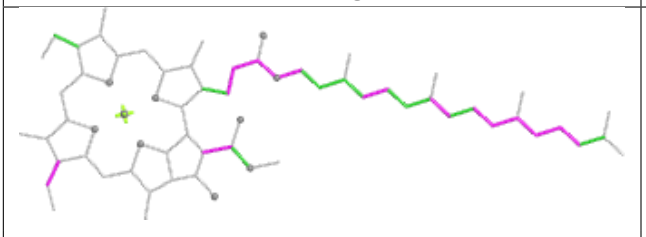
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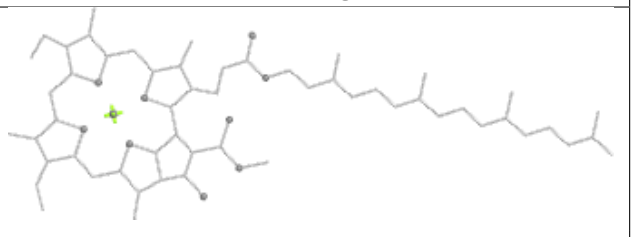
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Bond angles

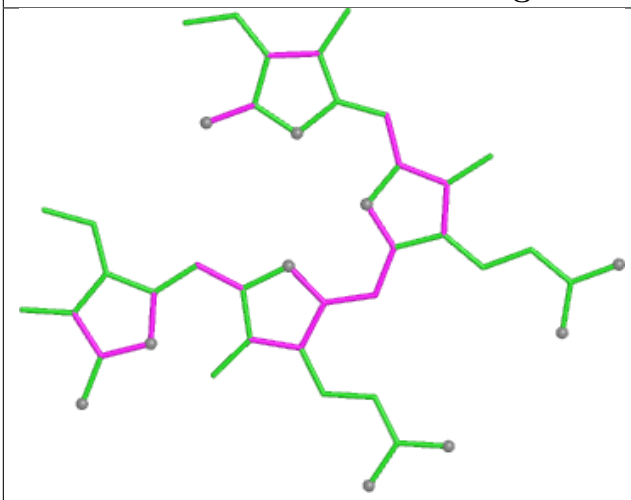


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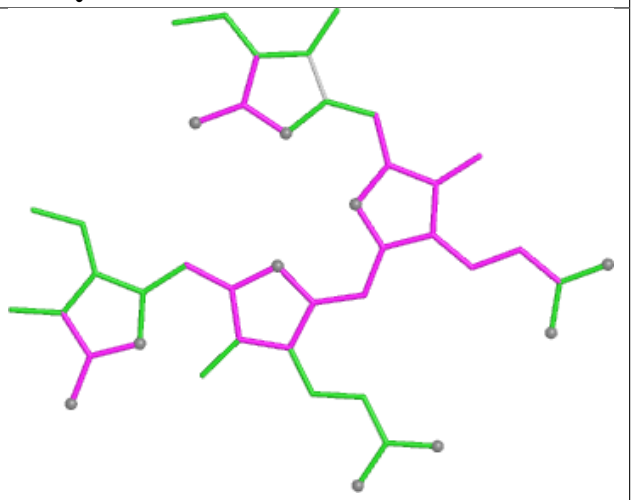


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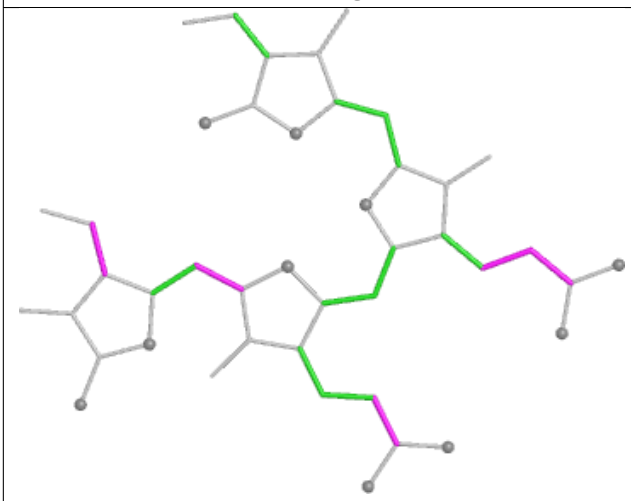
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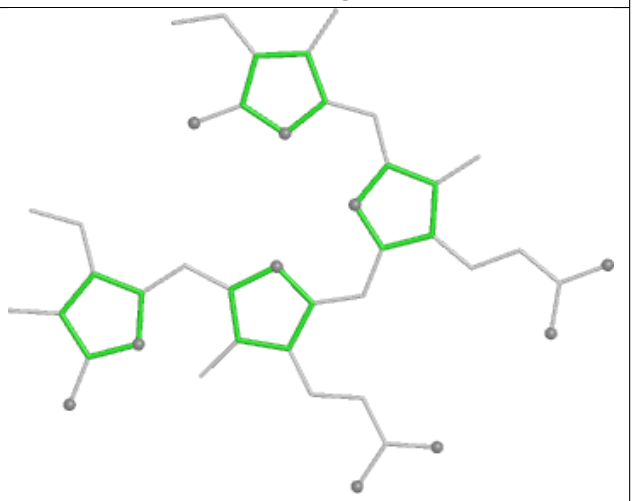
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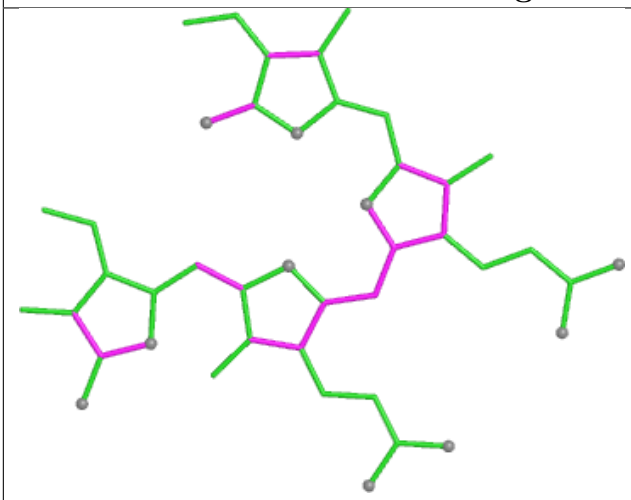


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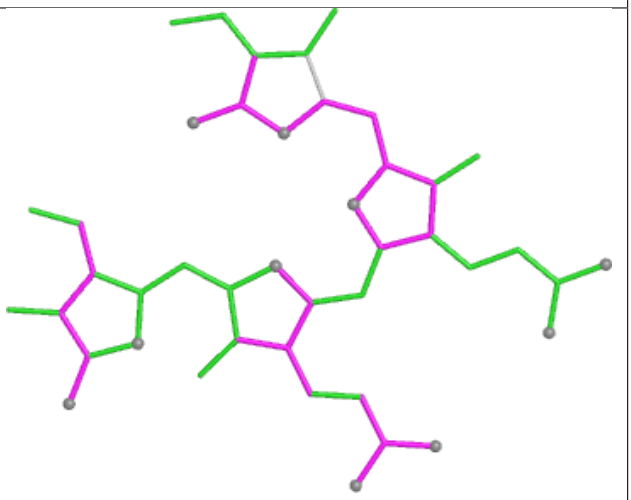


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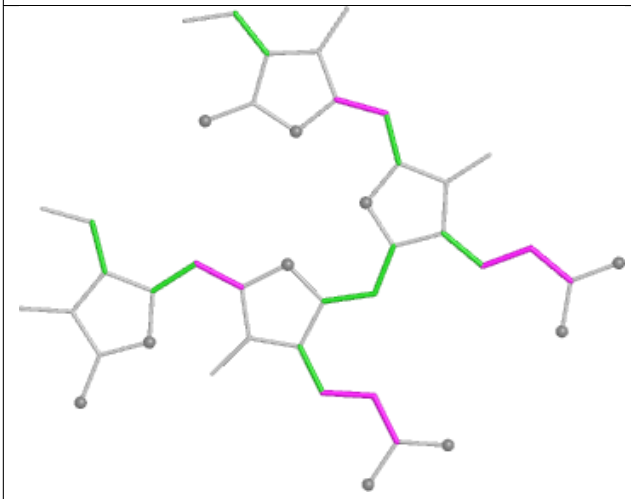
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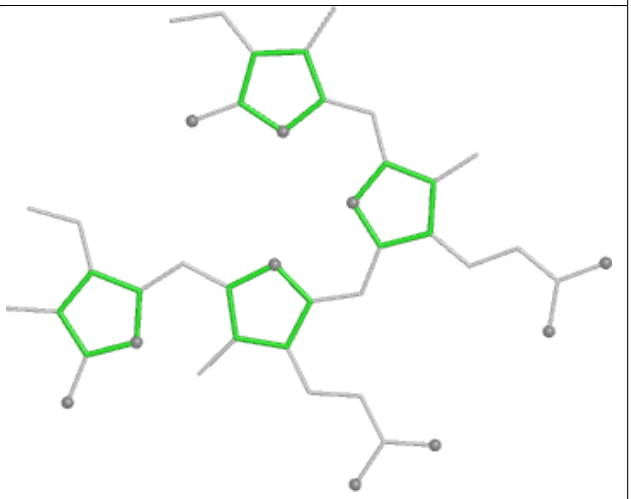
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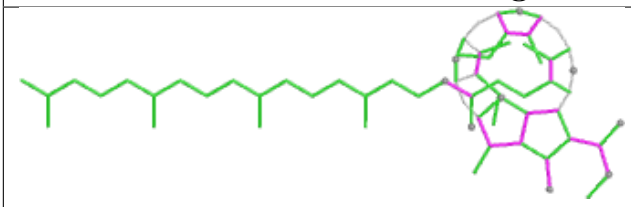


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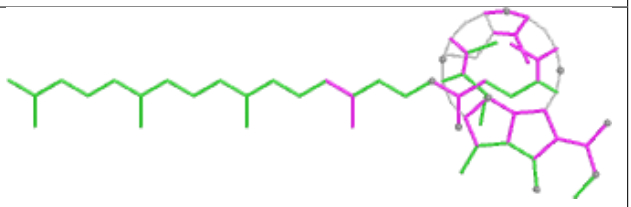


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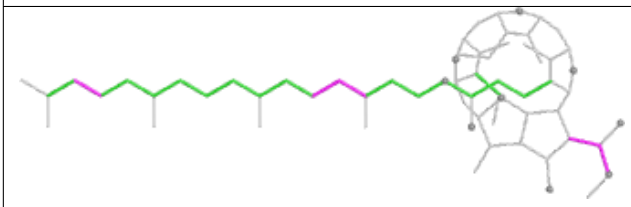
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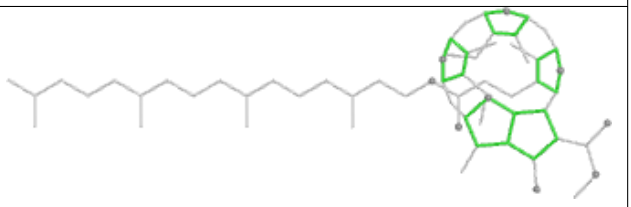
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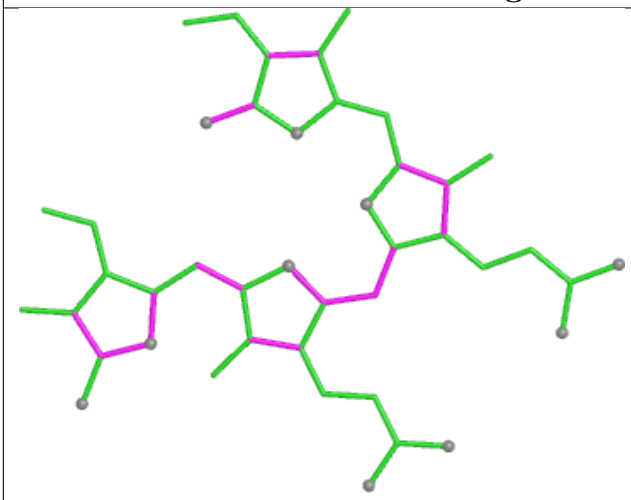


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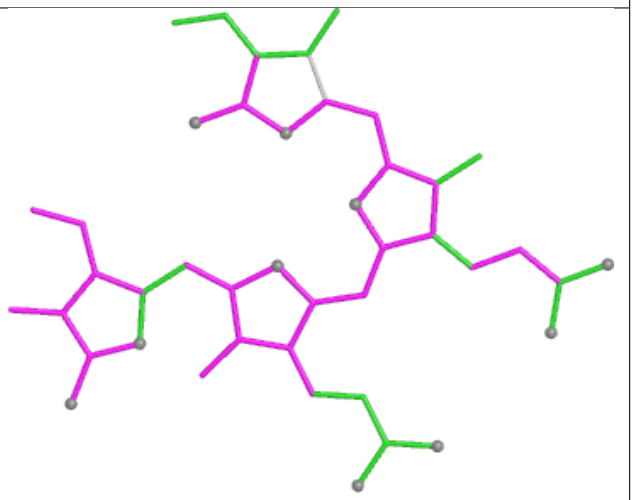


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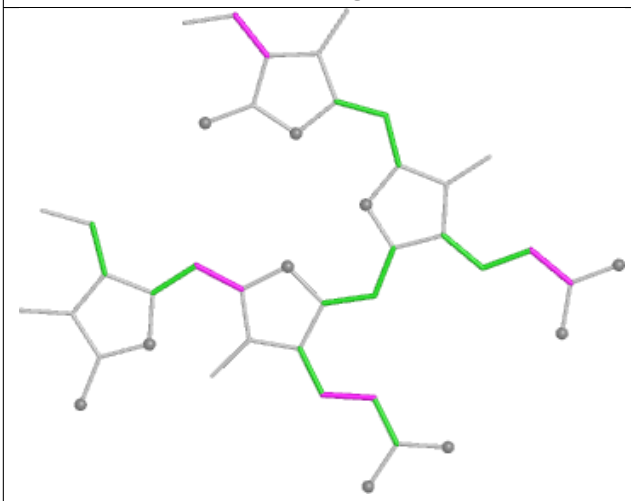
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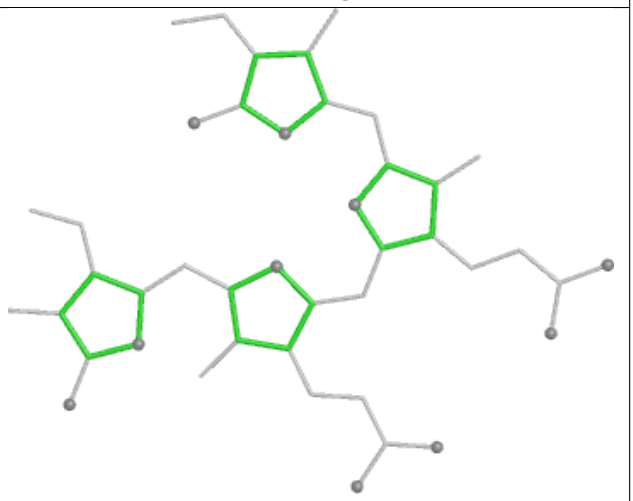
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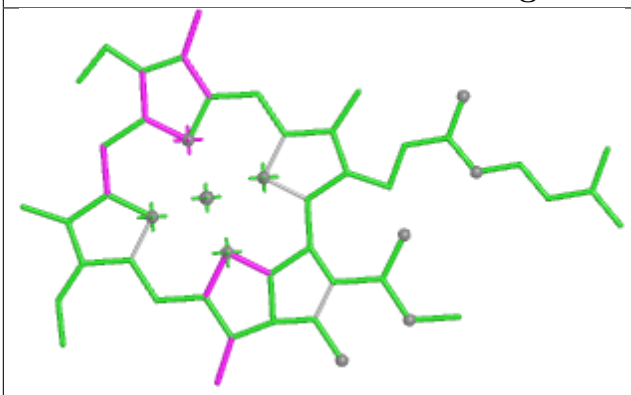


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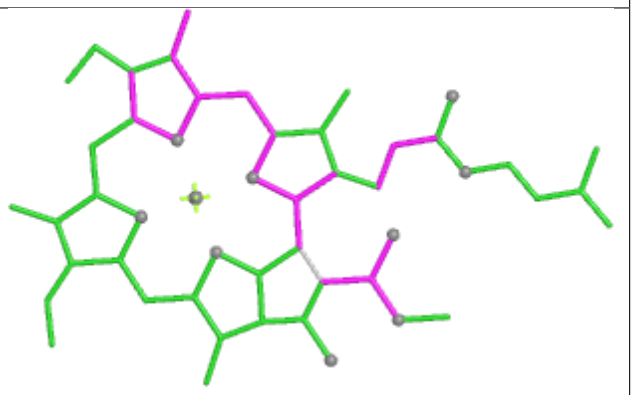


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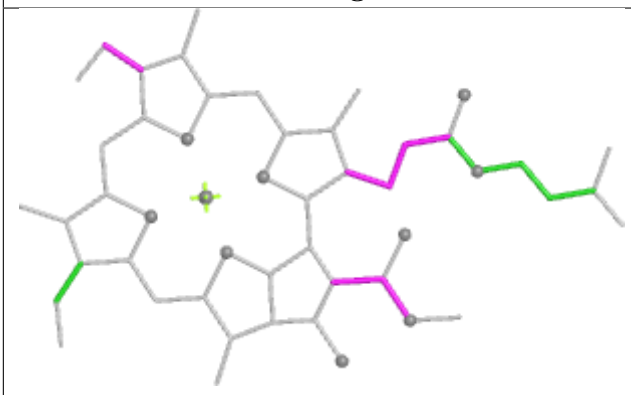
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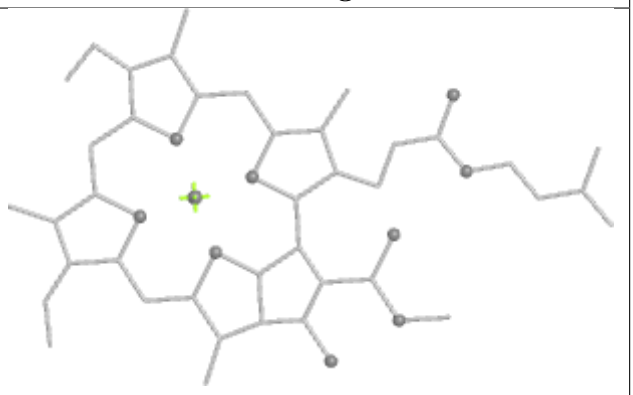
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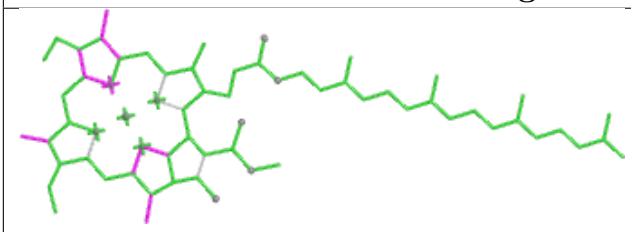


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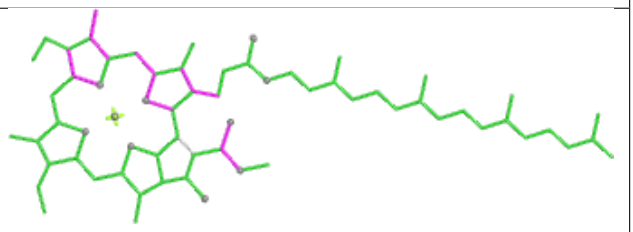


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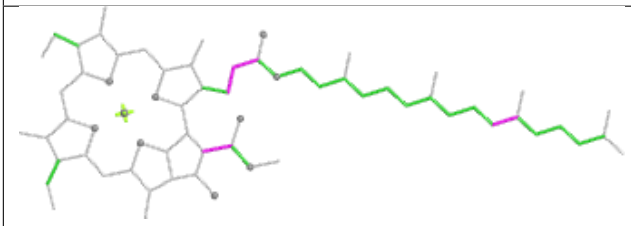
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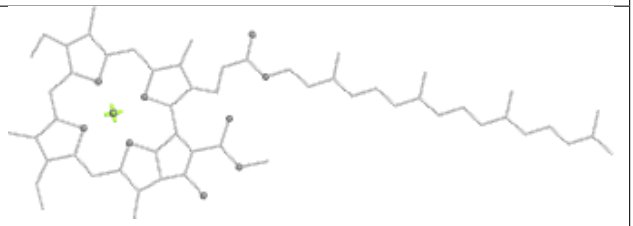
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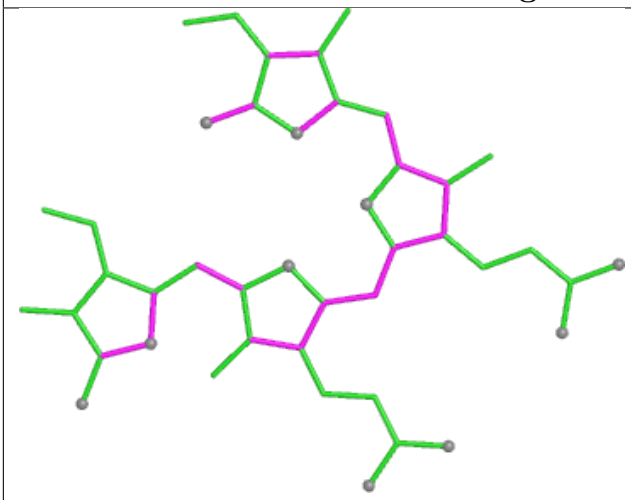


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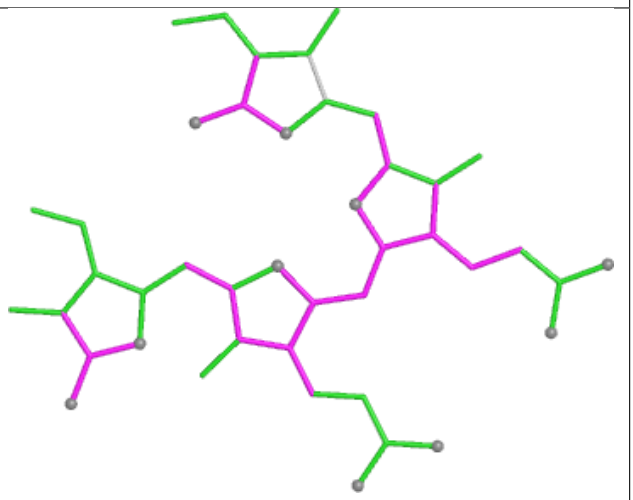


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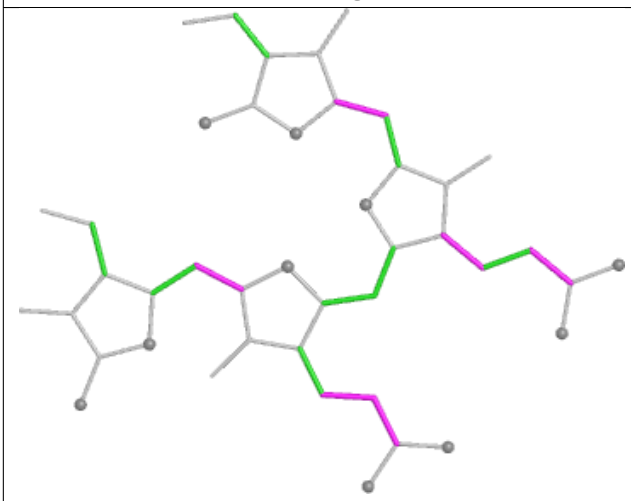
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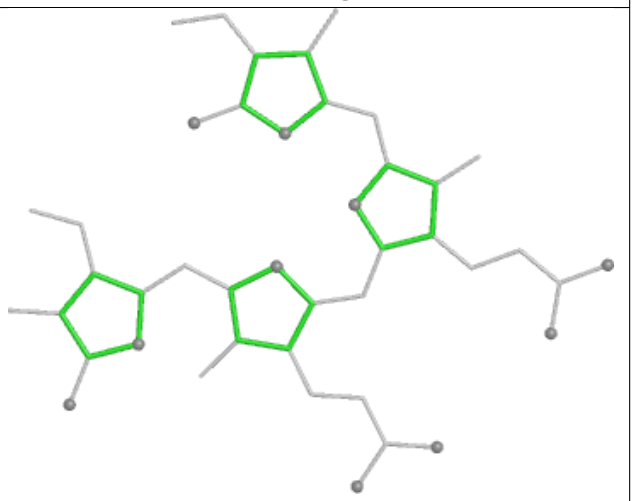
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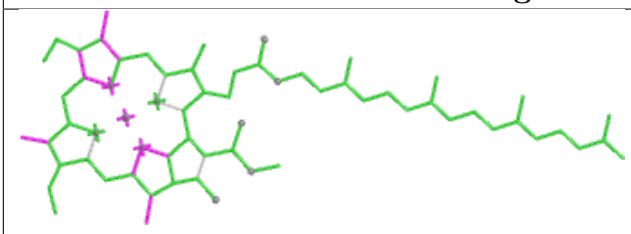


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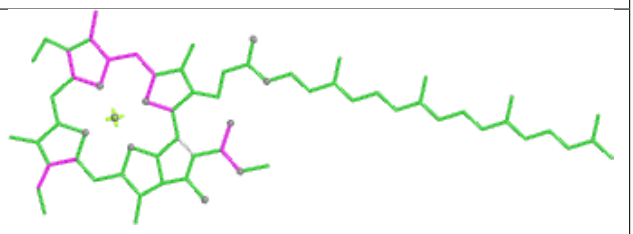


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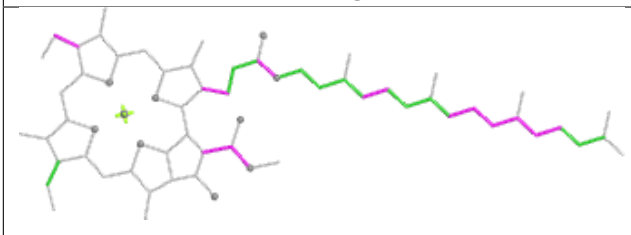
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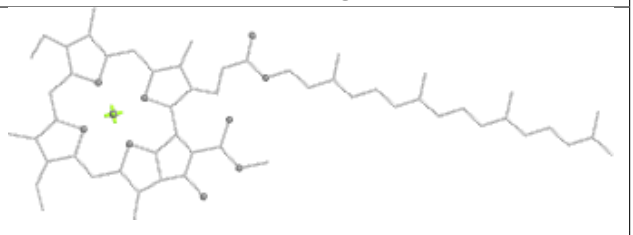
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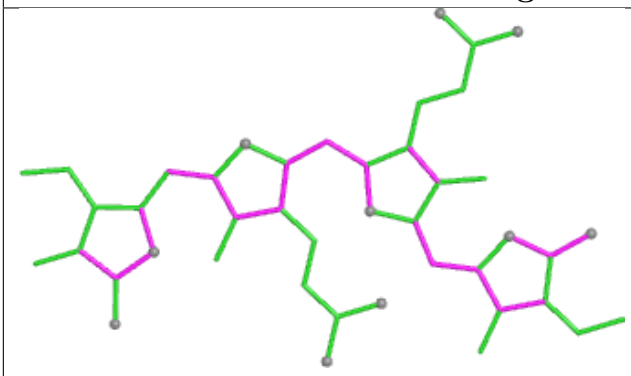


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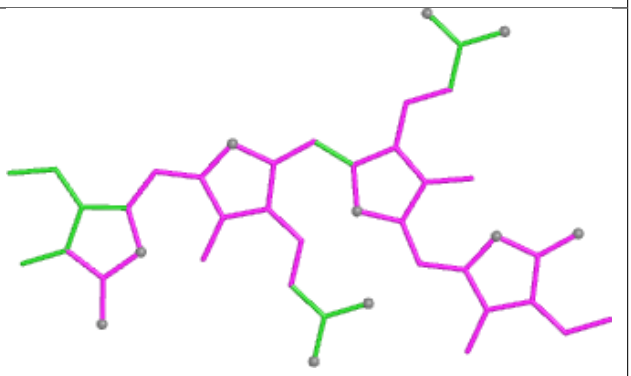


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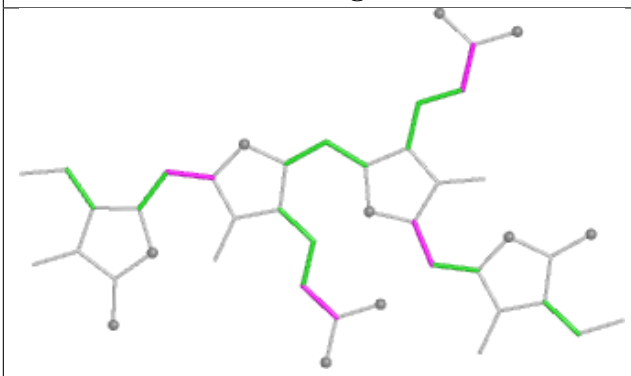
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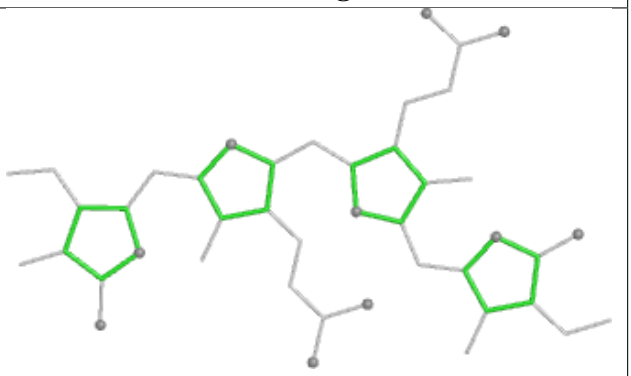
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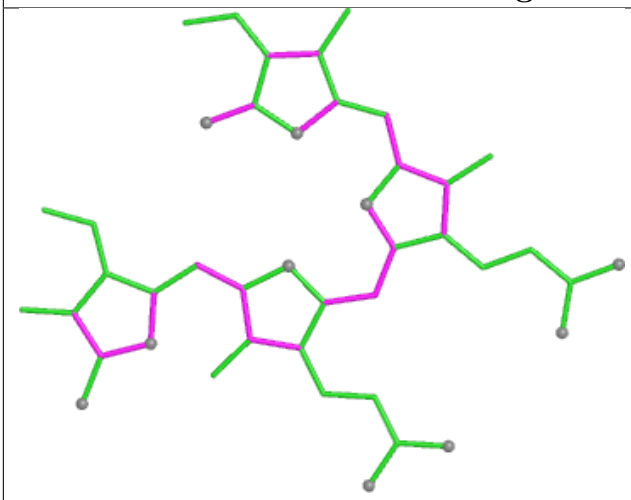


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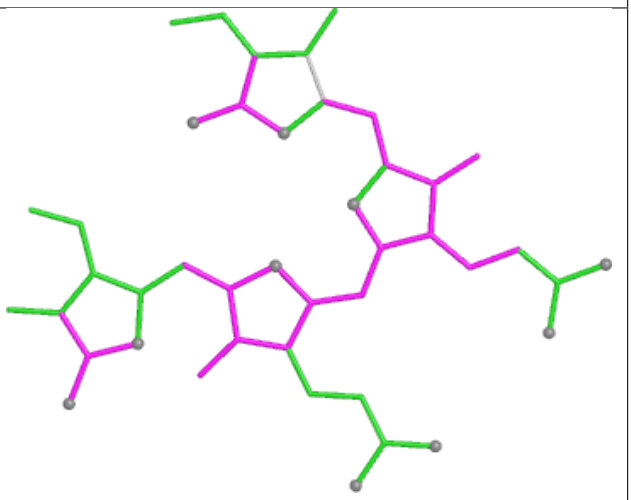


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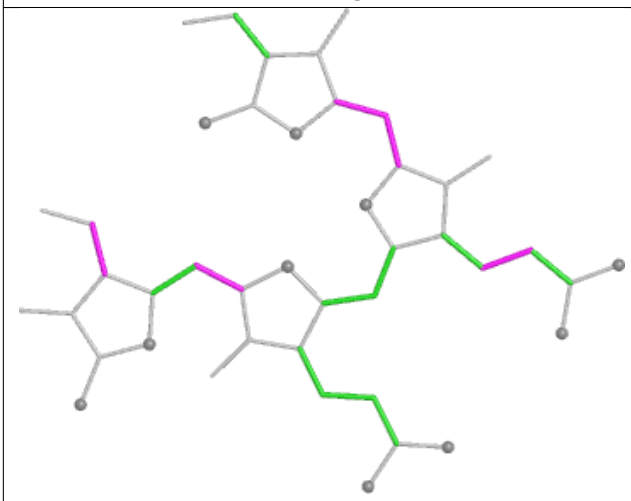
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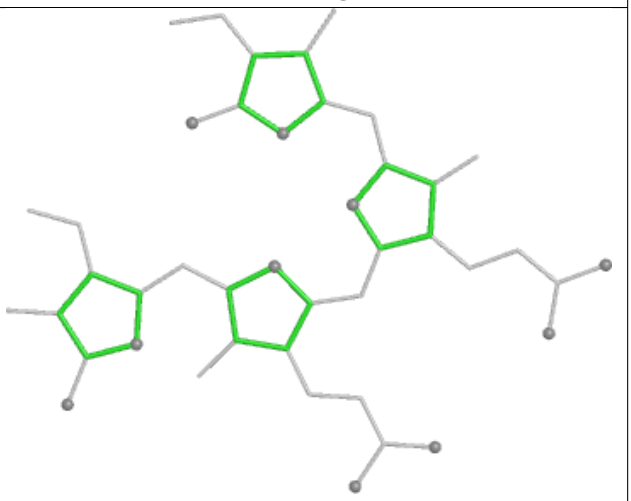
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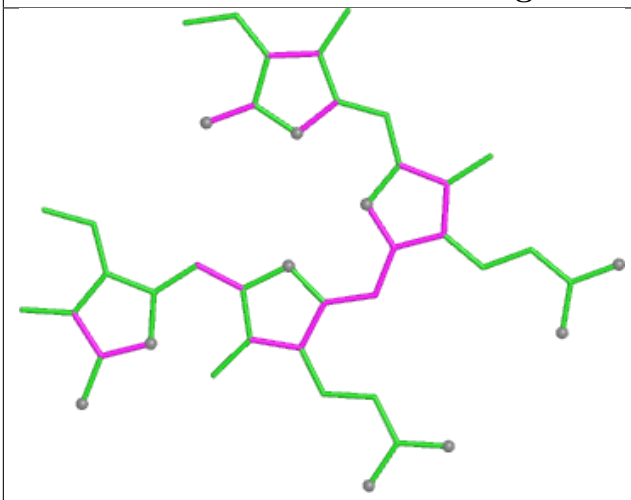


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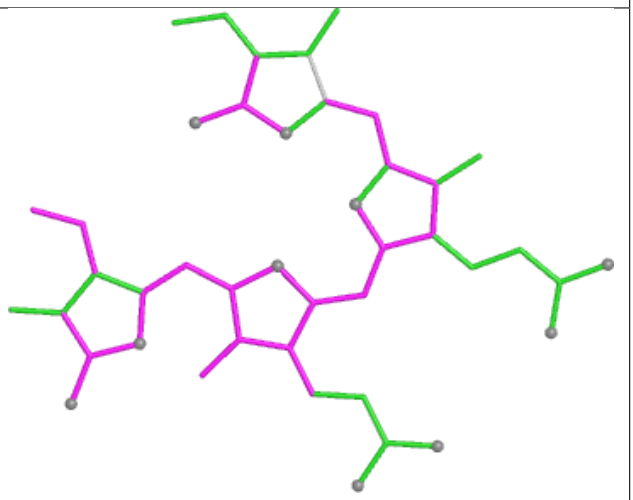


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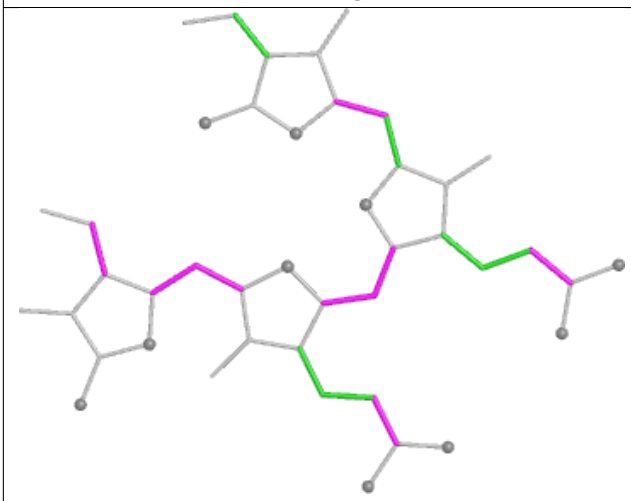
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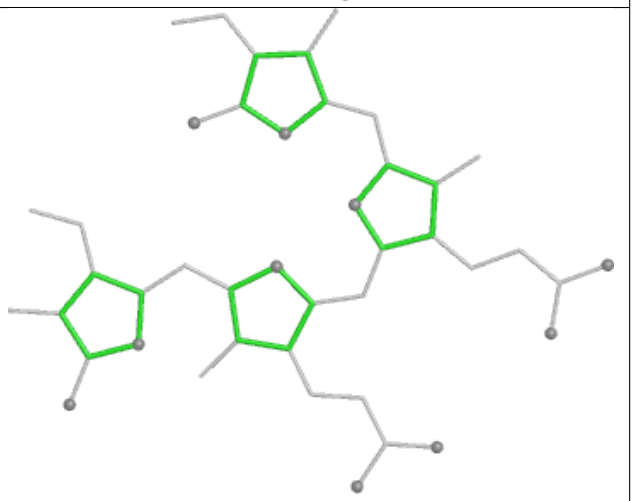
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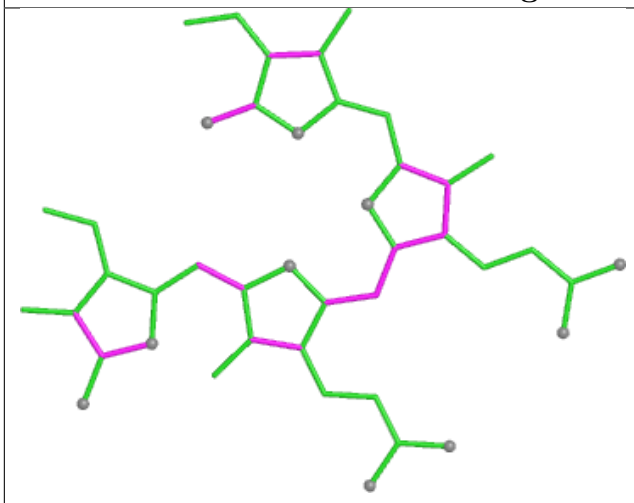


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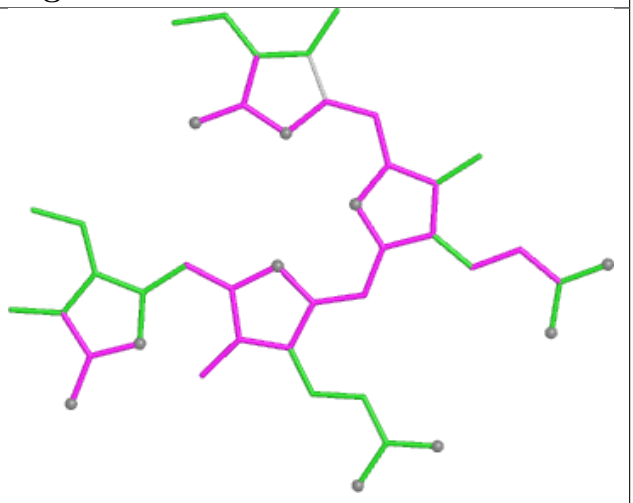


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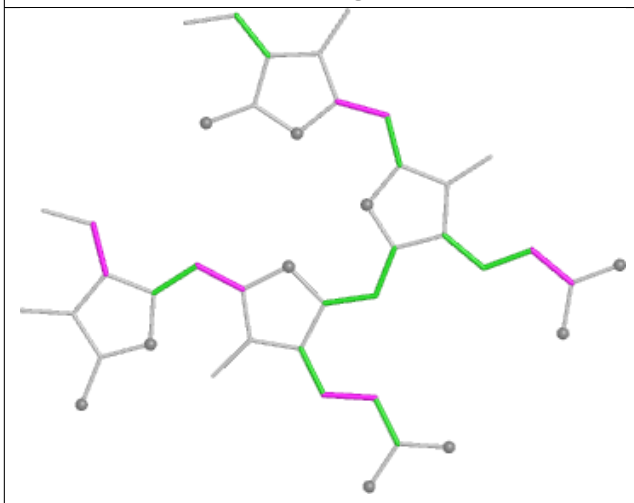
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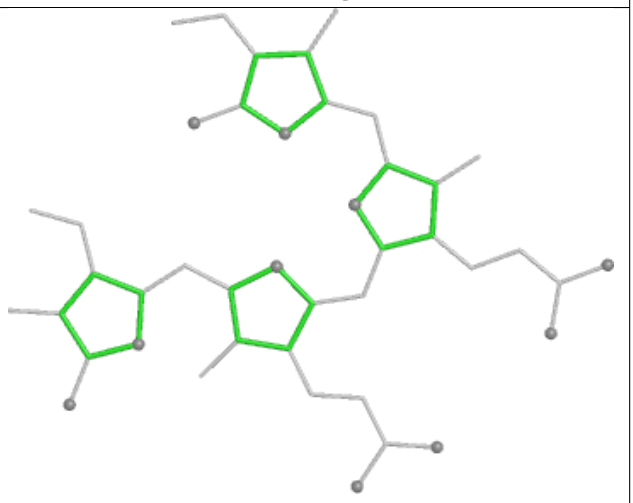
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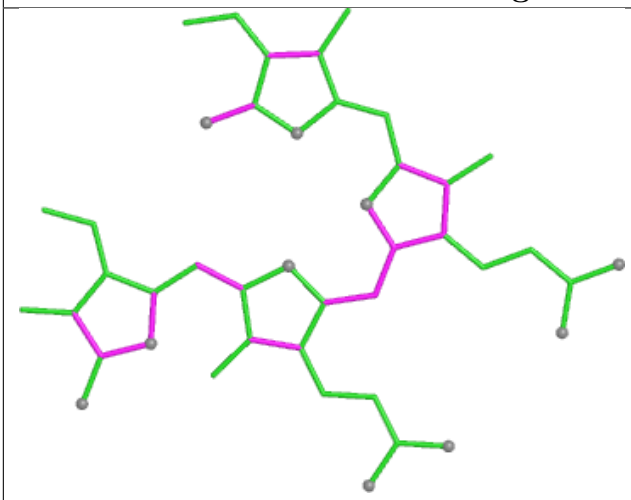


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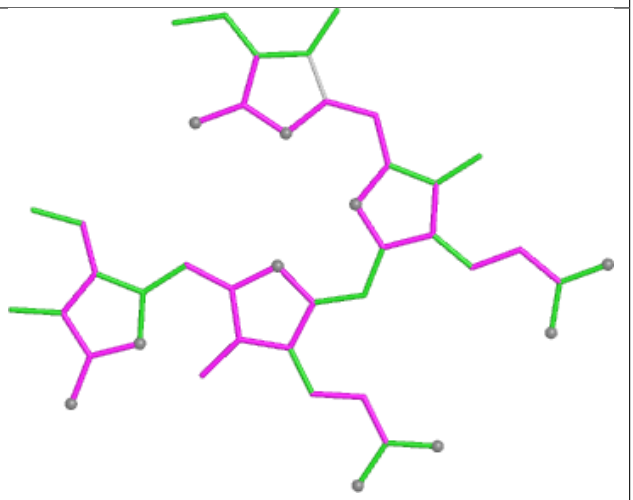


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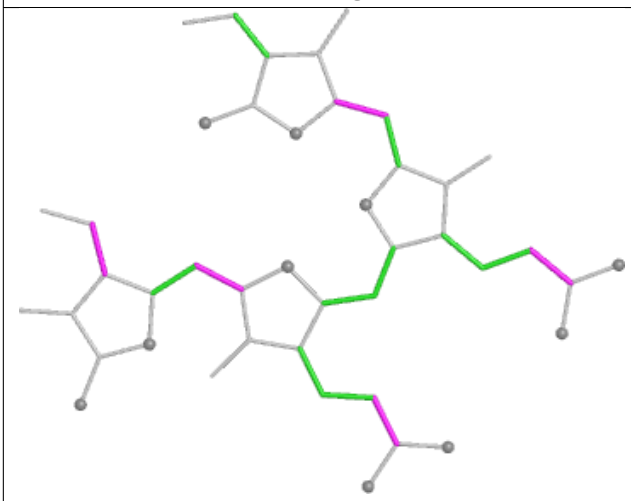
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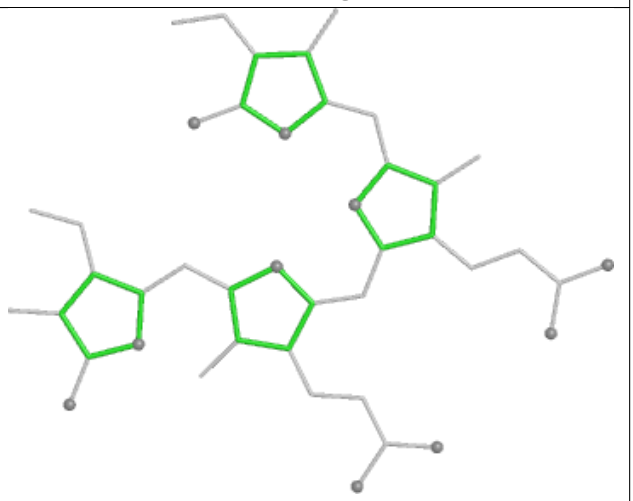
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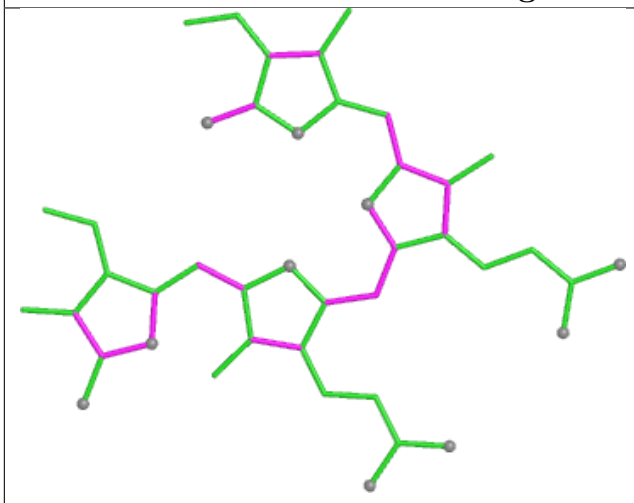


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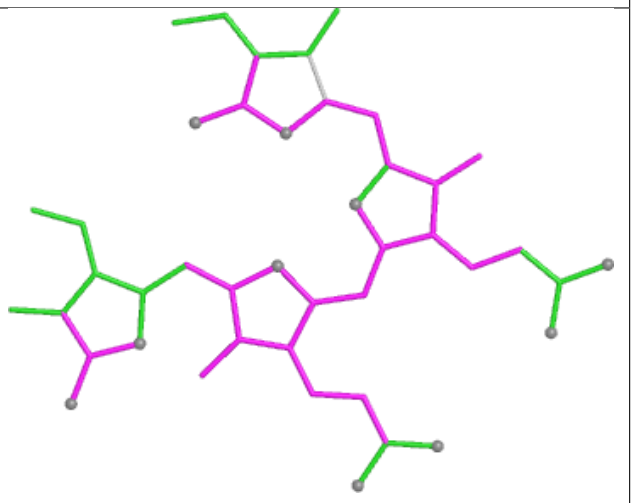


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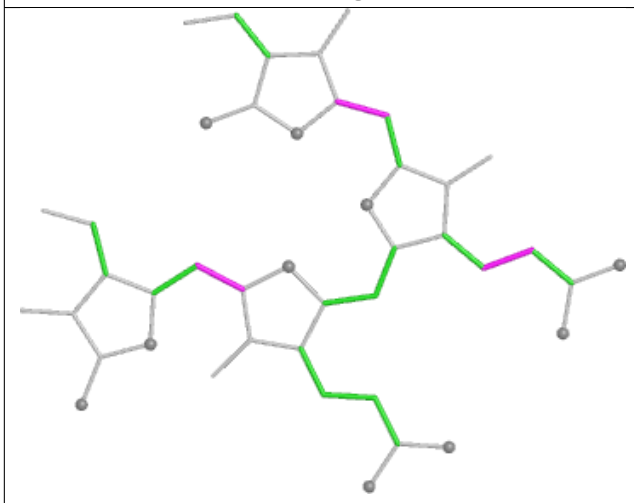
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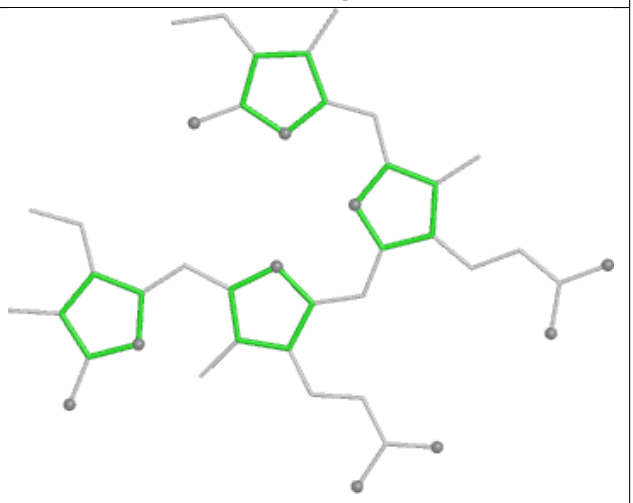
Bond lengths



Bond angles

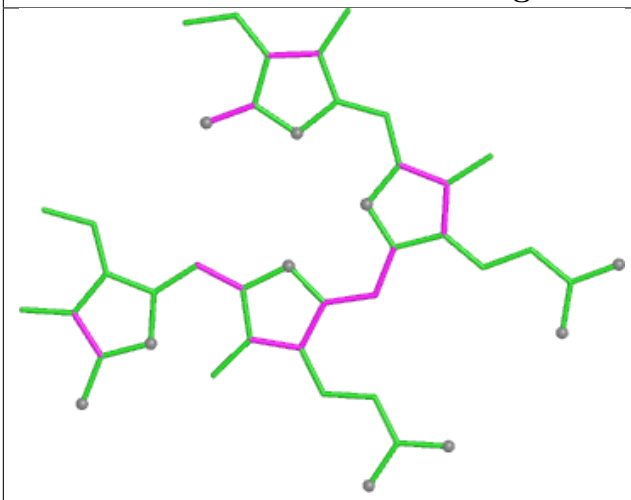


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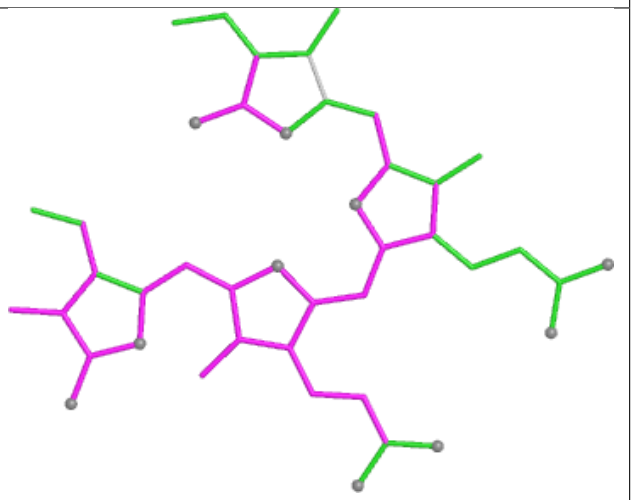


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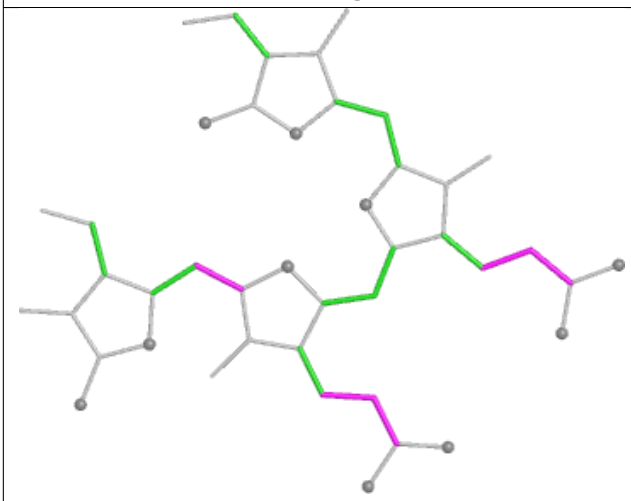
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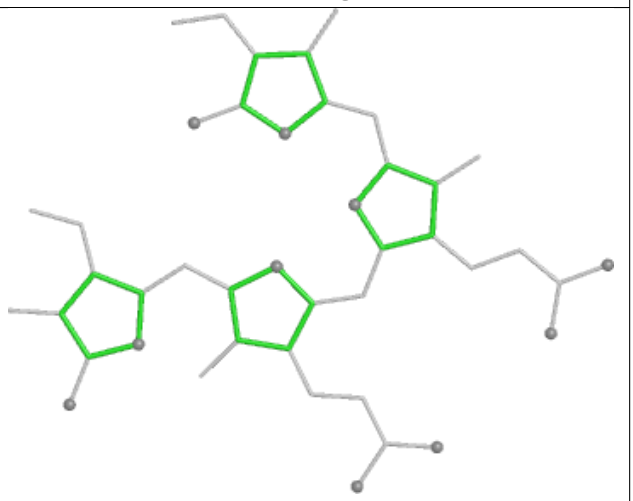
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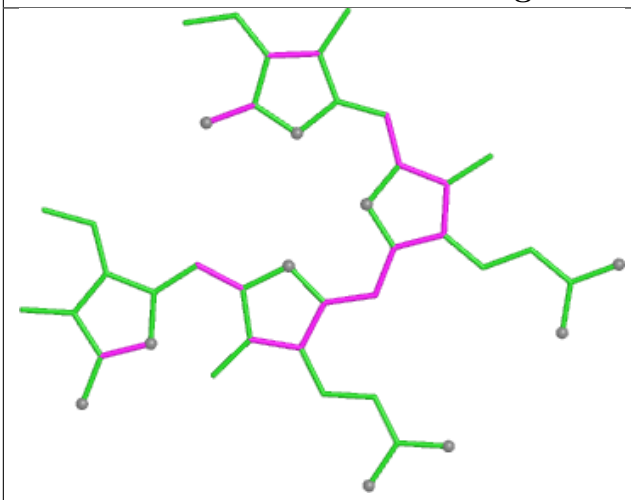


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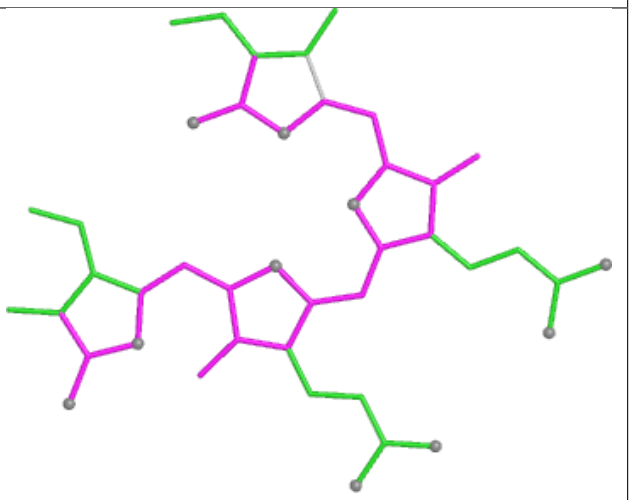


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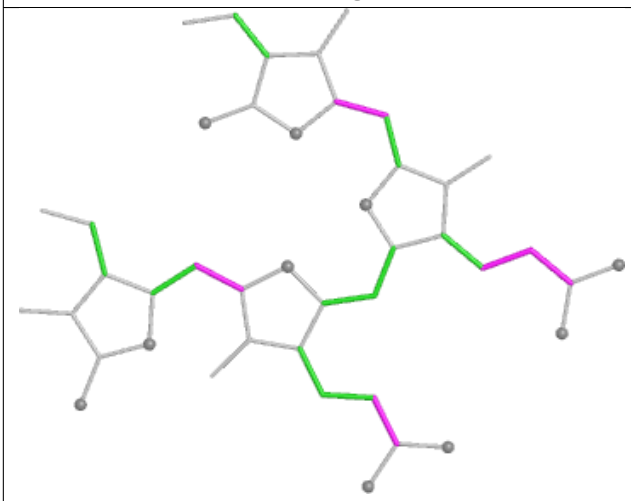
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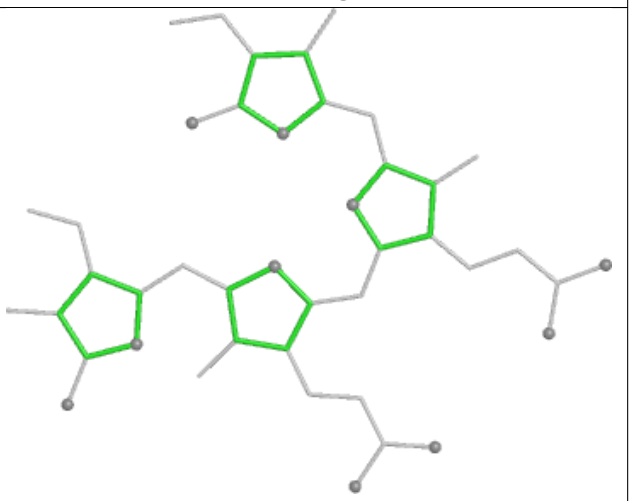
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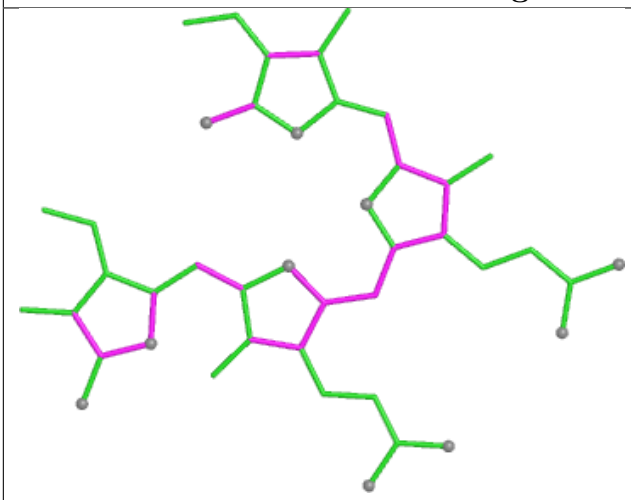


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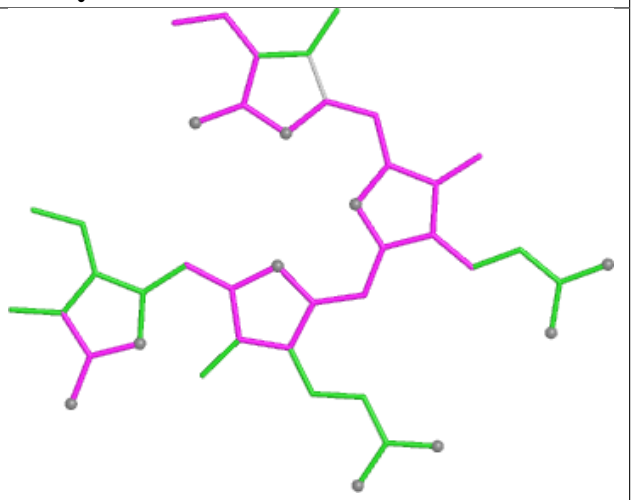


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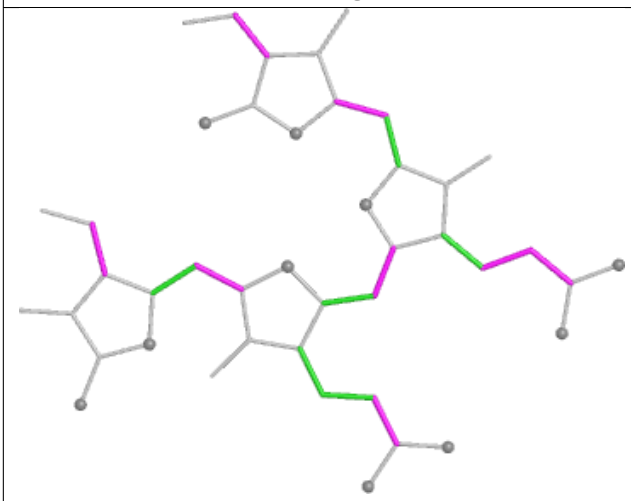
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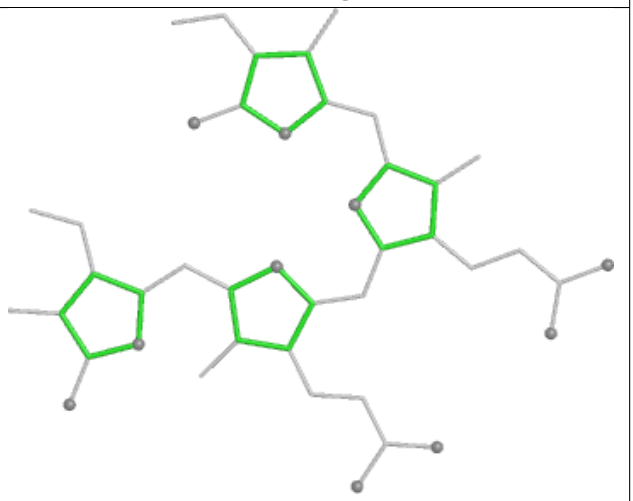
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Bond angles

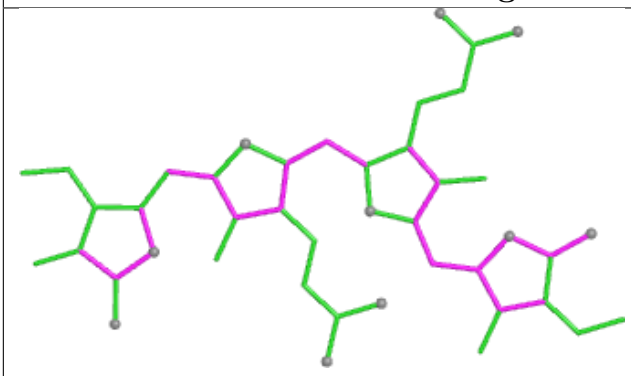


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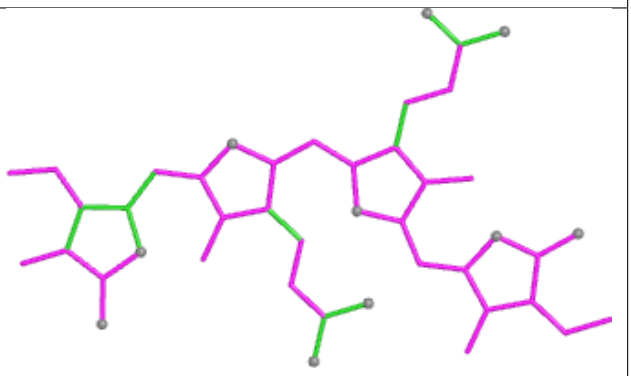


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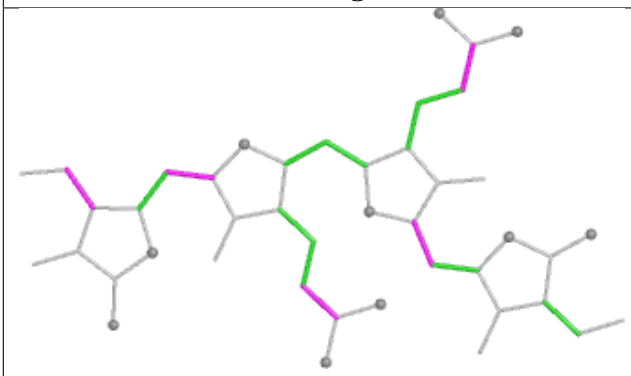
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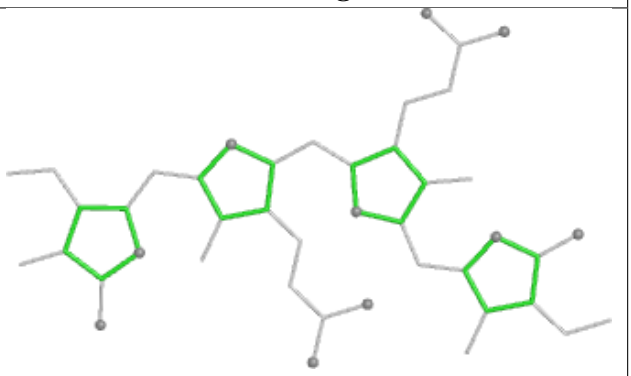
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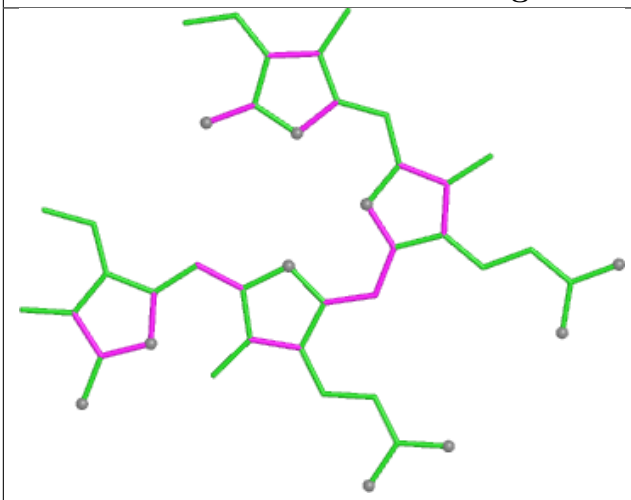


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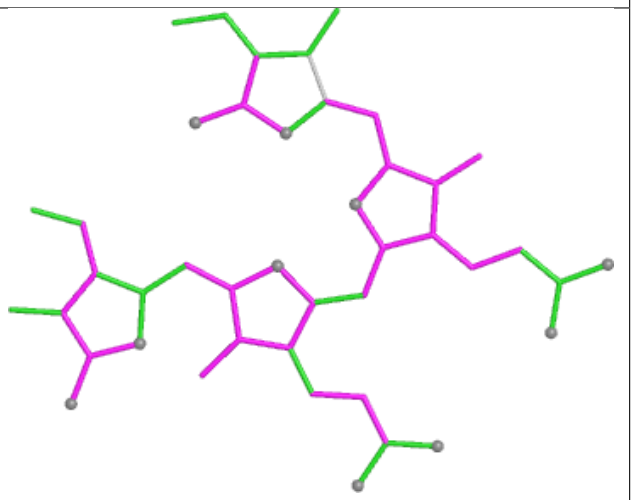


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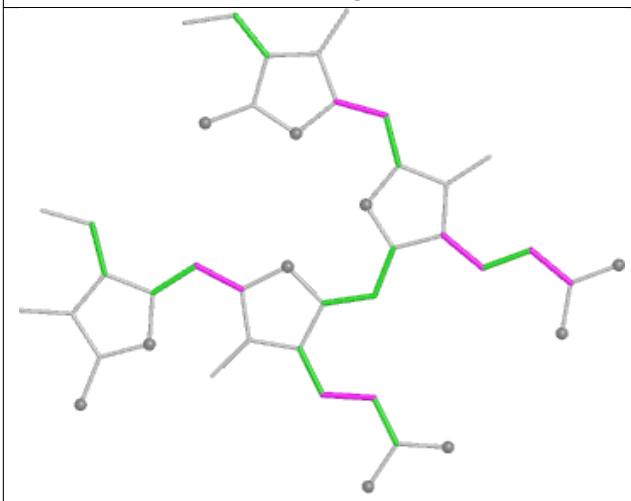
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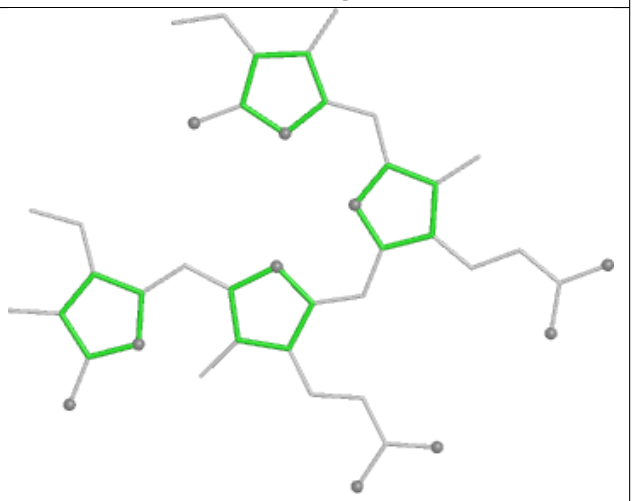
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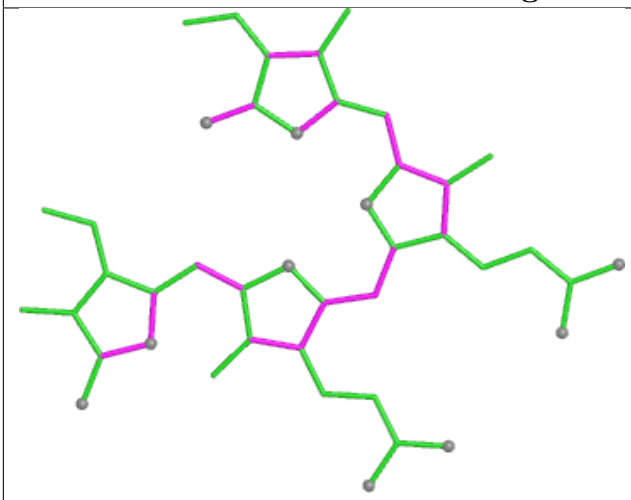


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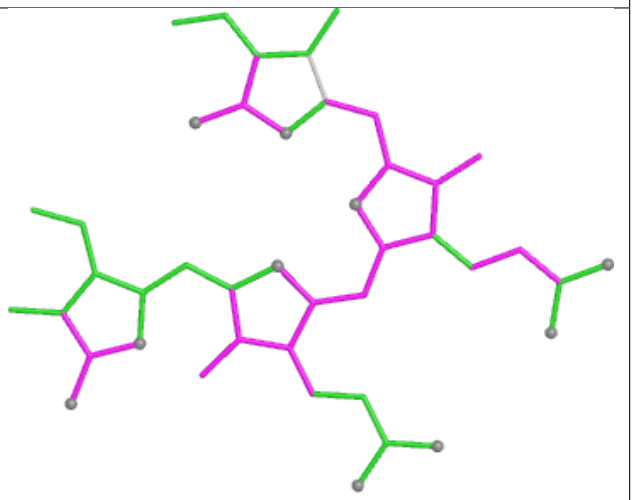


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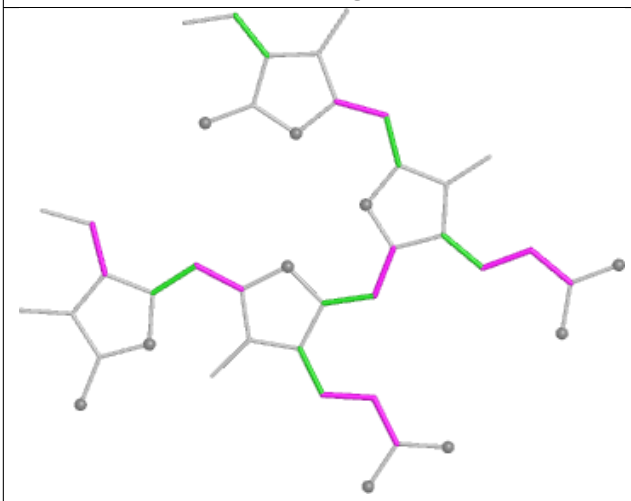
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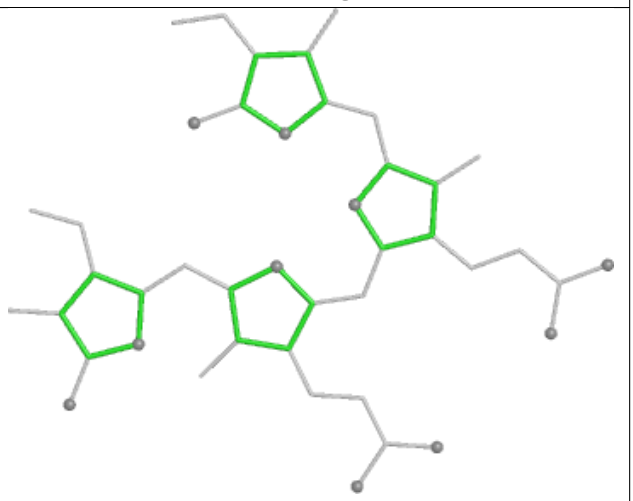
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Bond angles

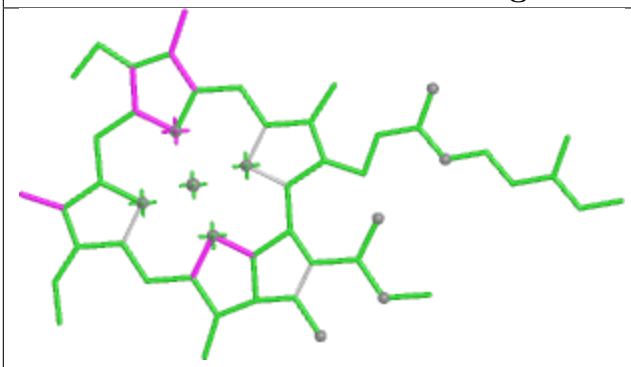


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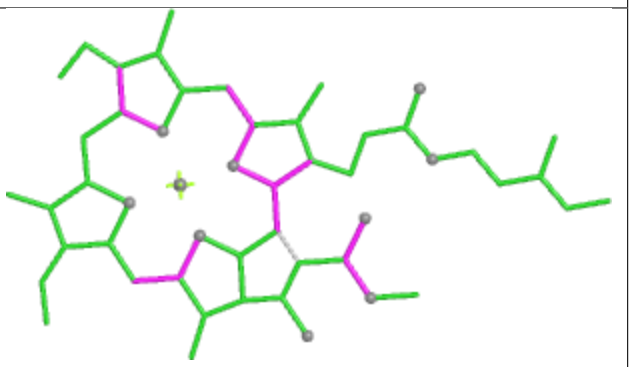


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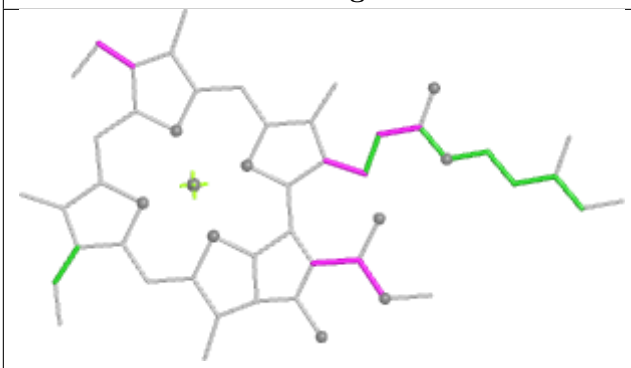
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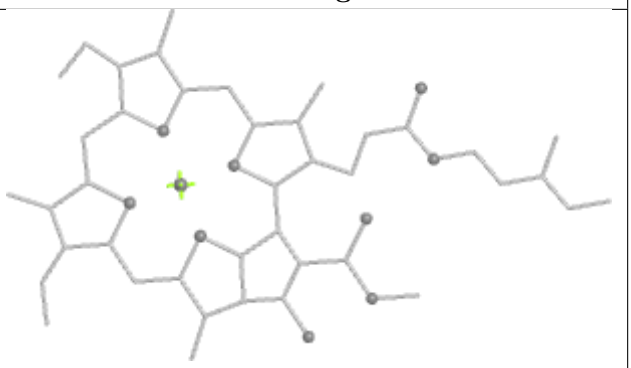
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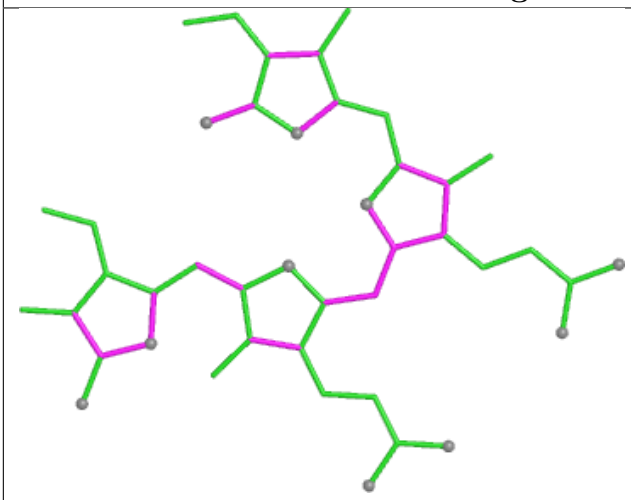


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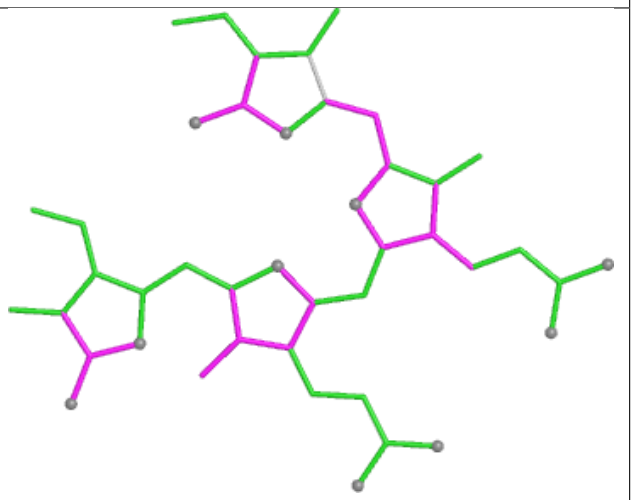


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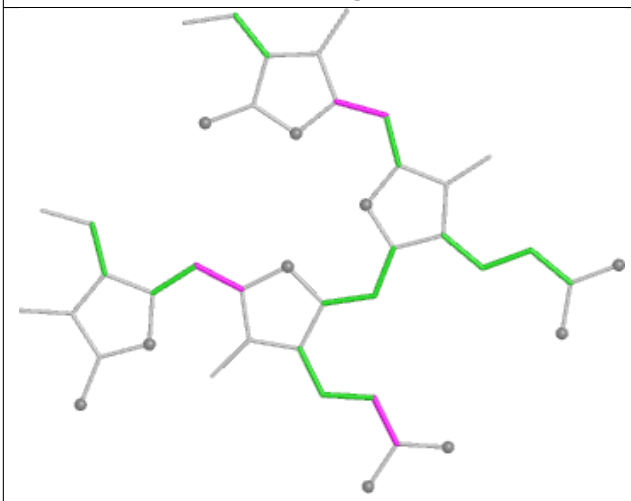
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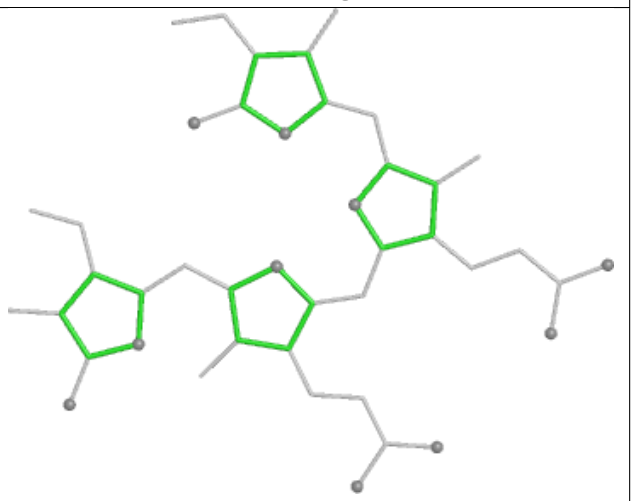
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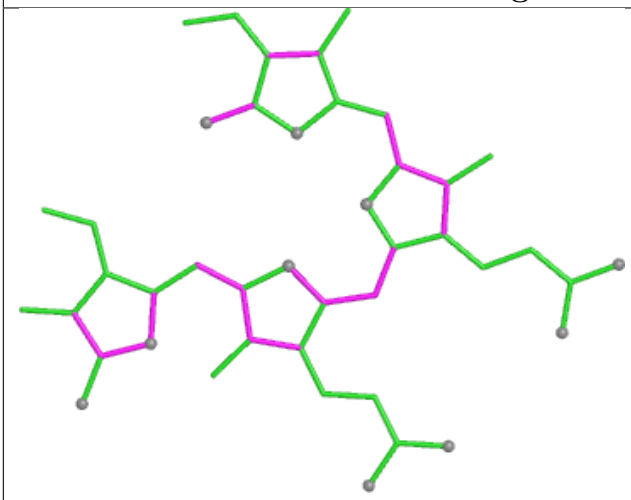


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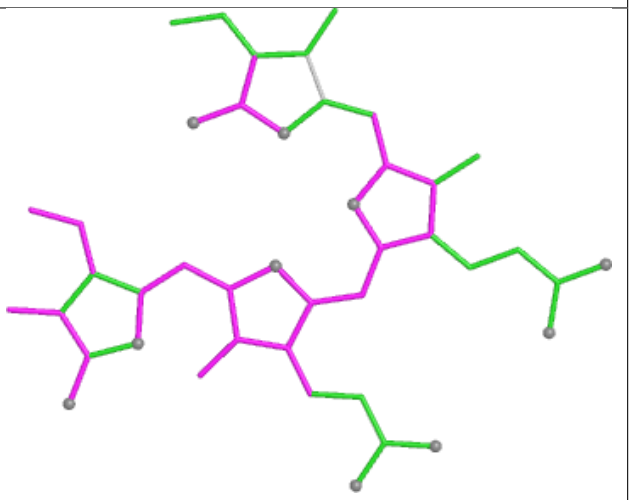


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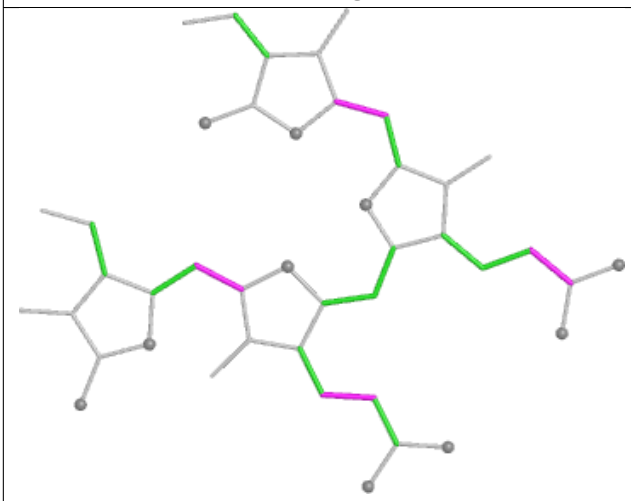
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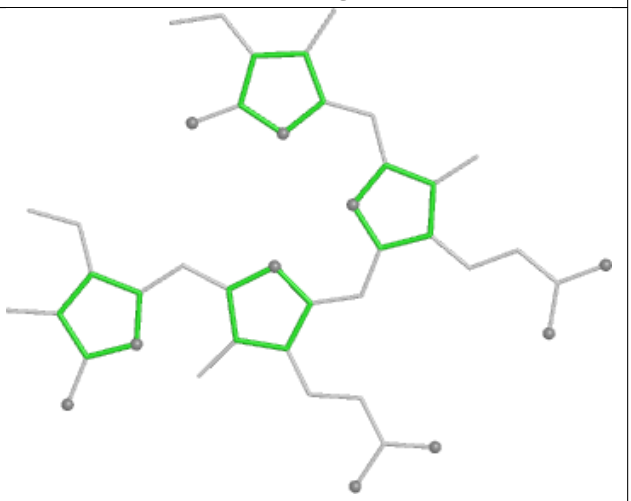
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Bond angles

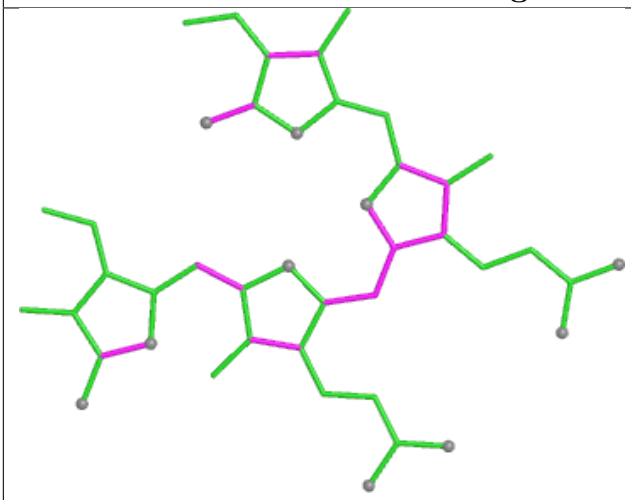


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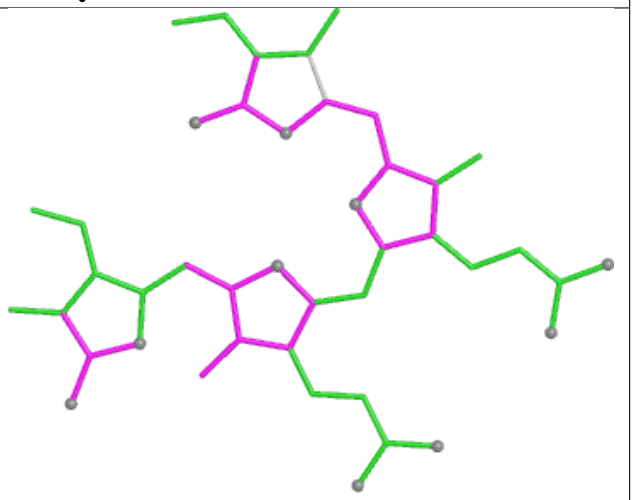


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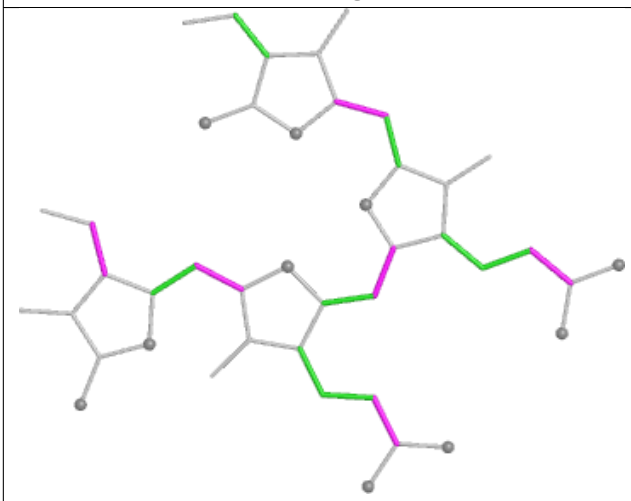
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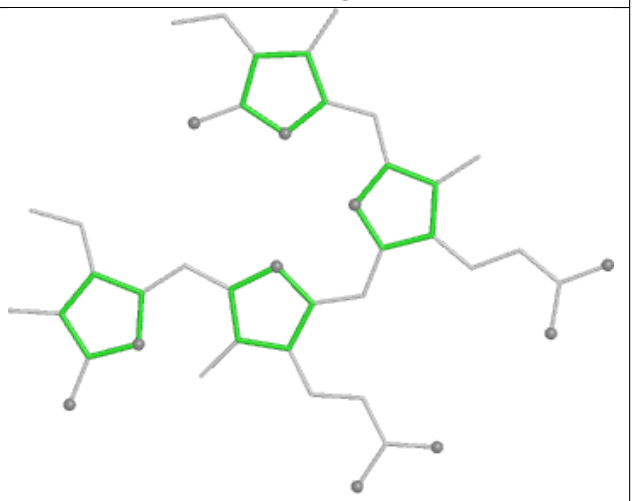
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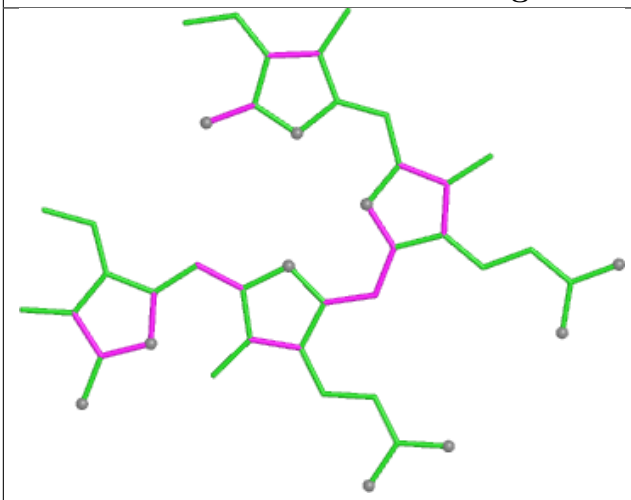


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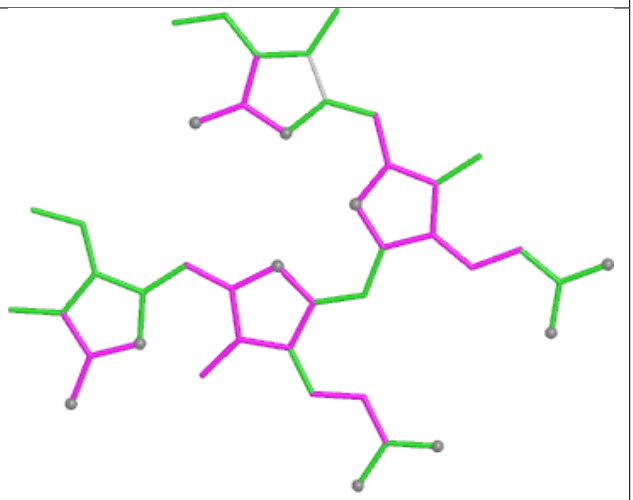


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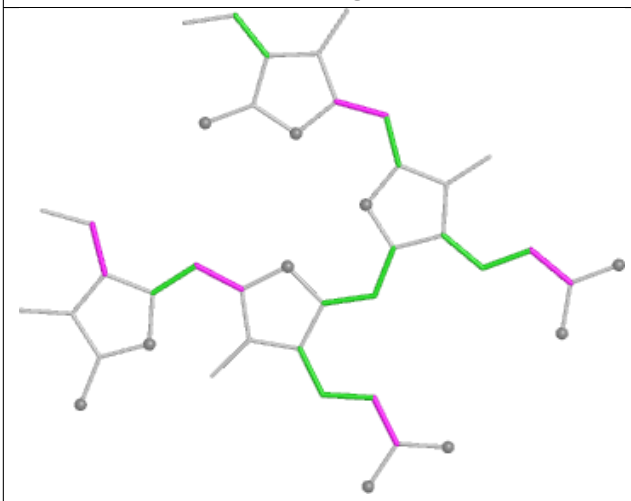
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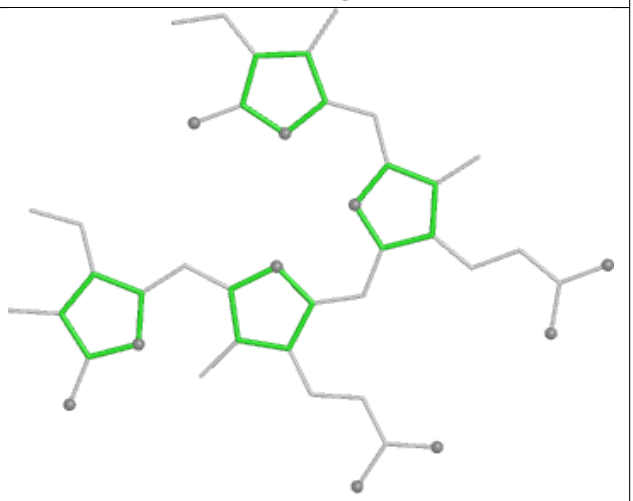
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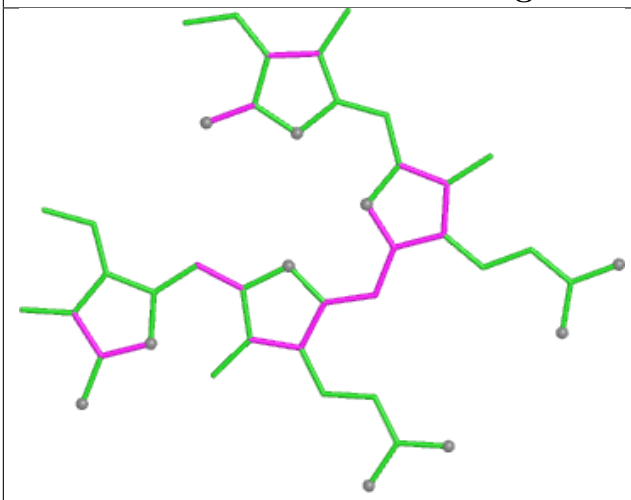


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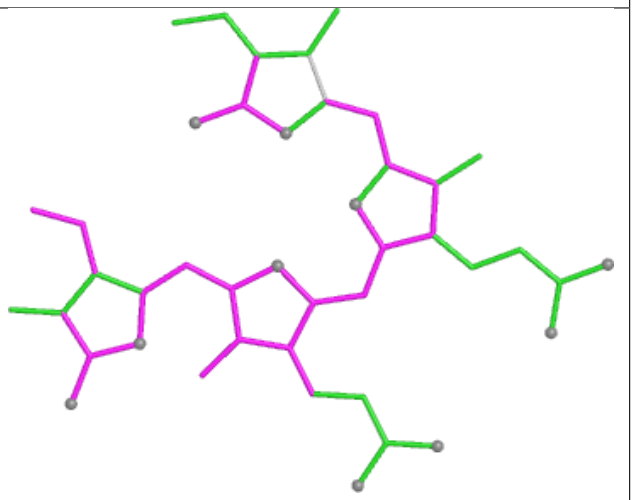


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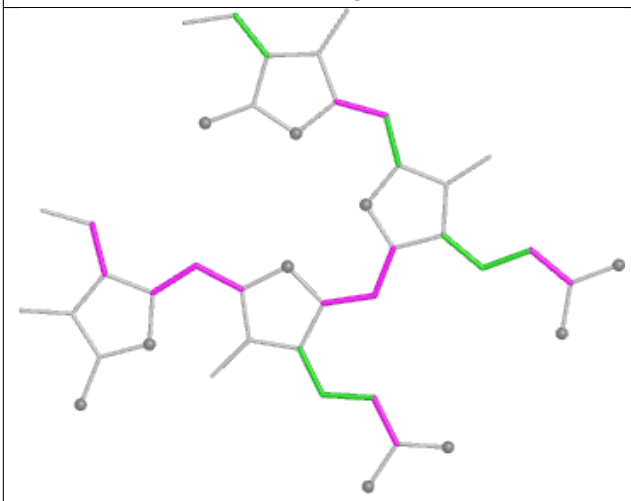
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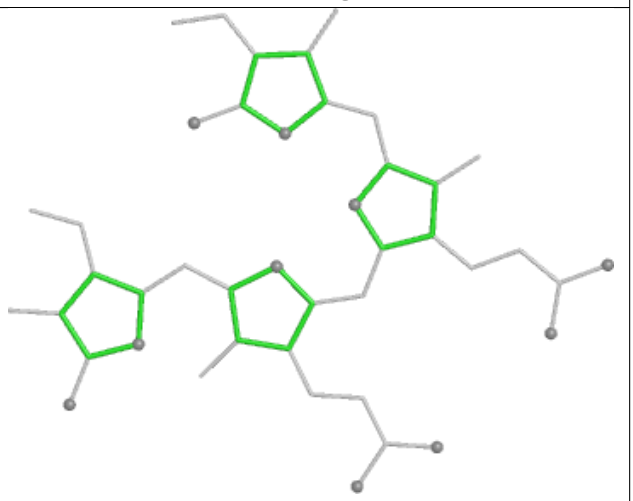
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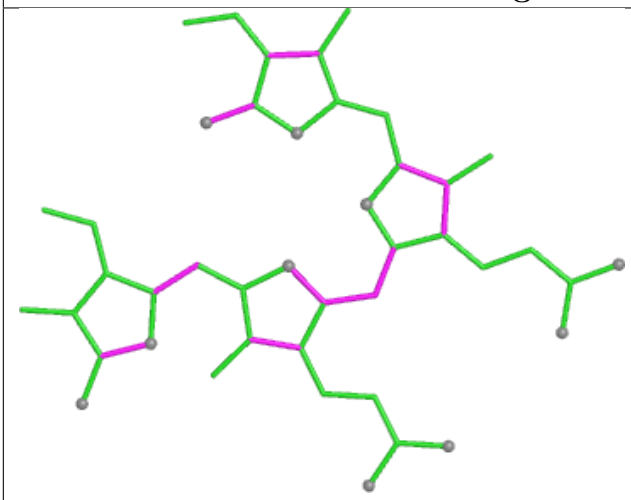


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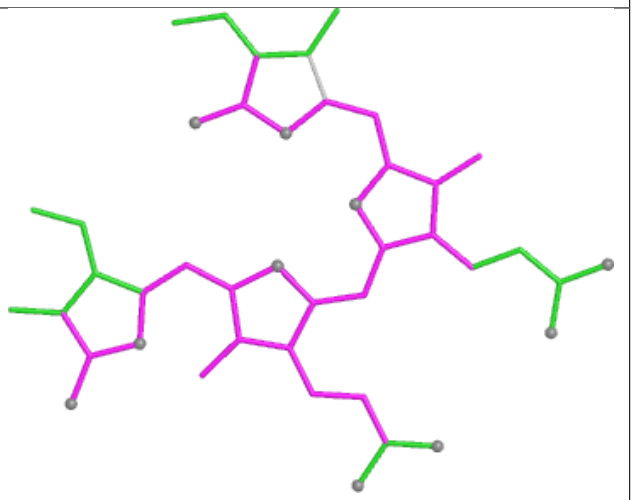


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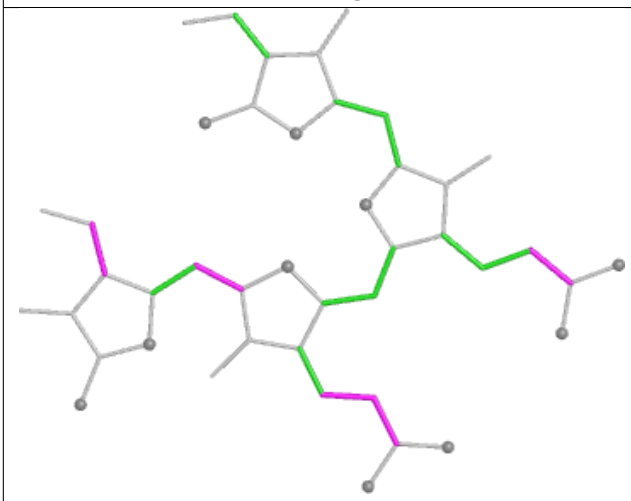
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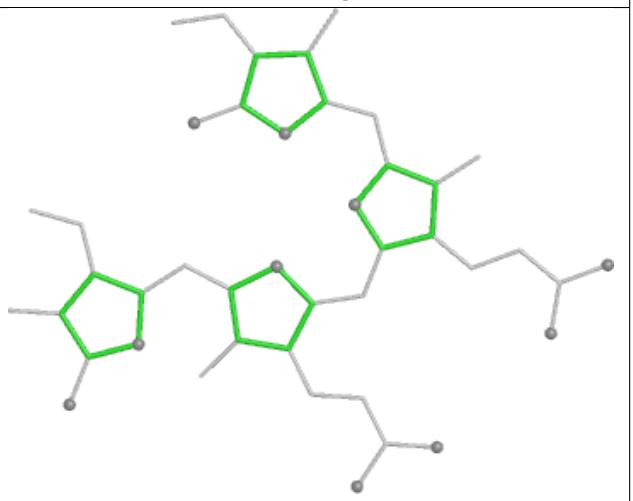
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Bond angles

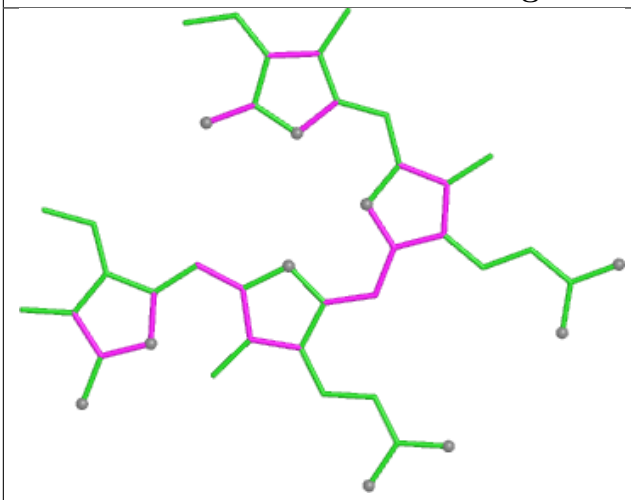


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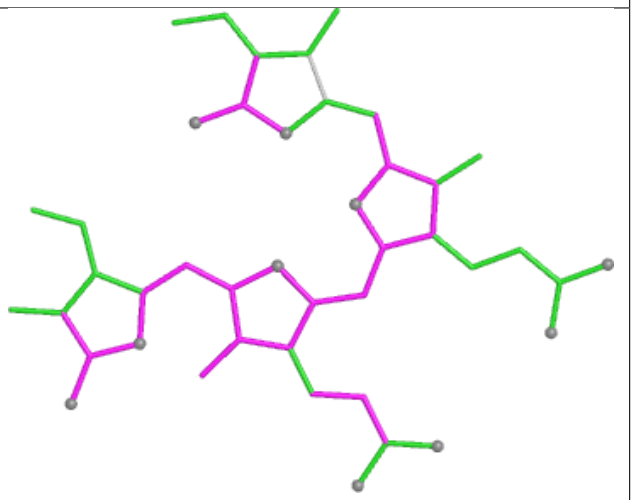


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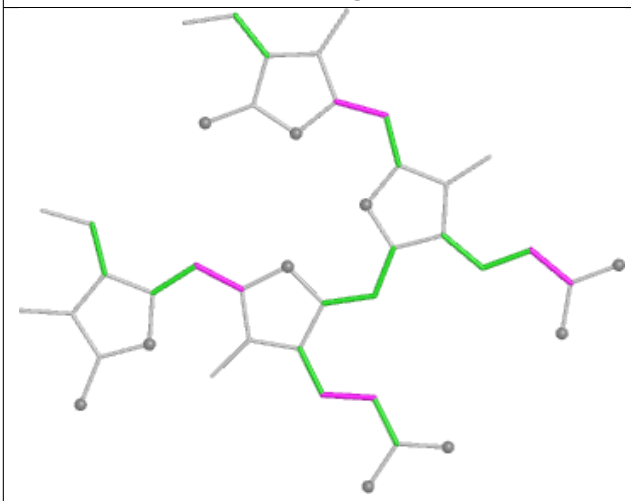
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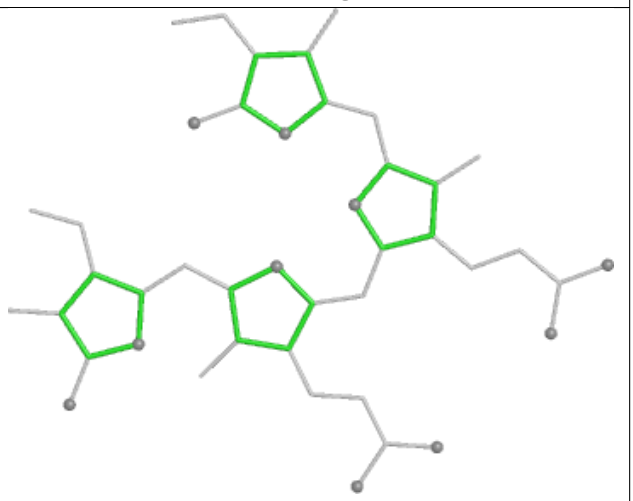
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Bond angles

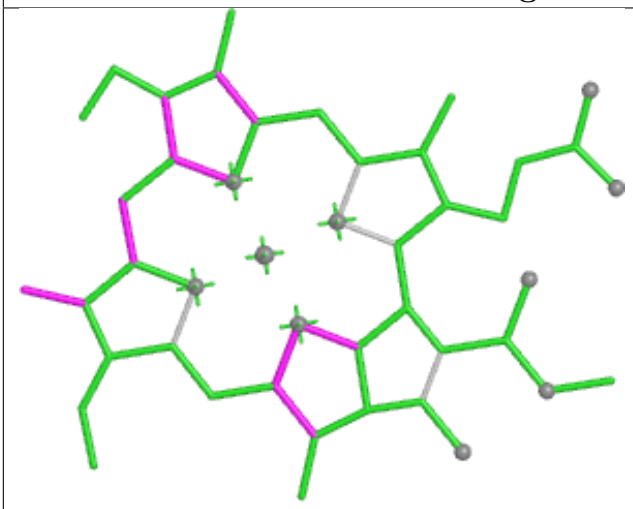


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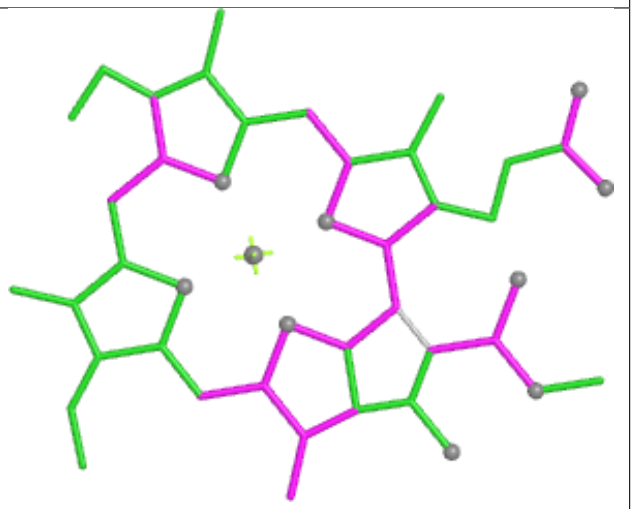


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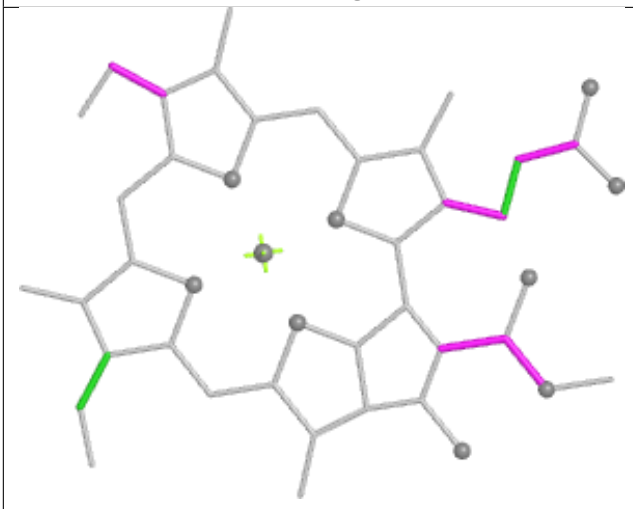
Ligand CLA 62 313



Bond lengths



Bond angles

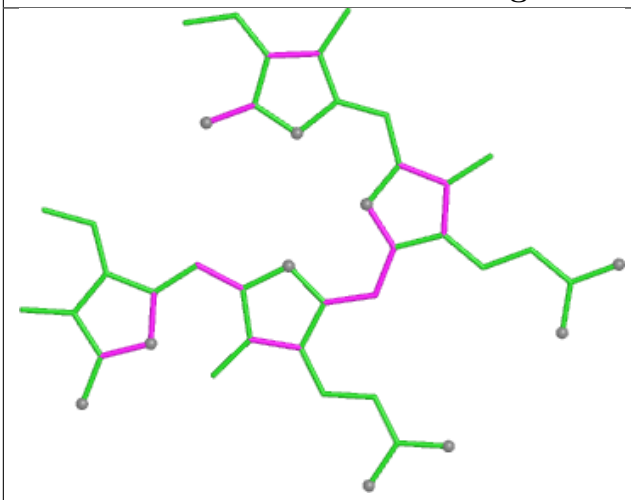


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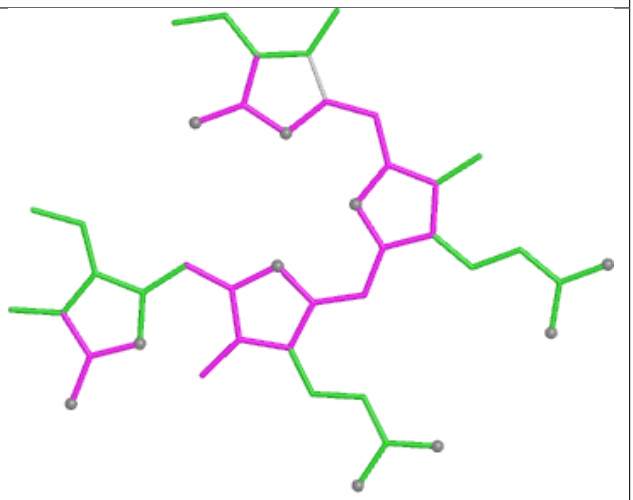


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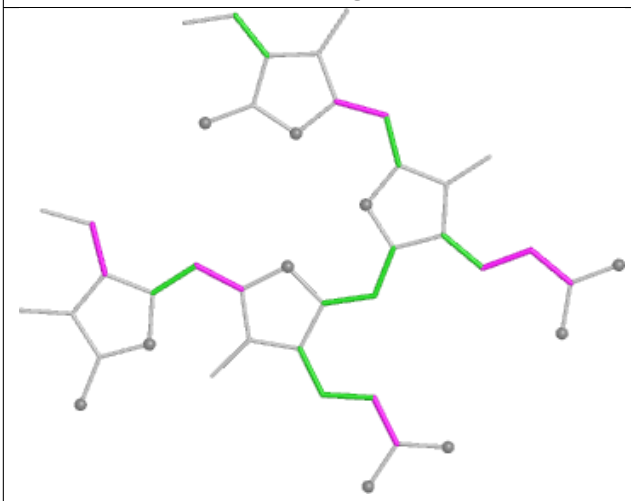
Ligand PEB UK 202



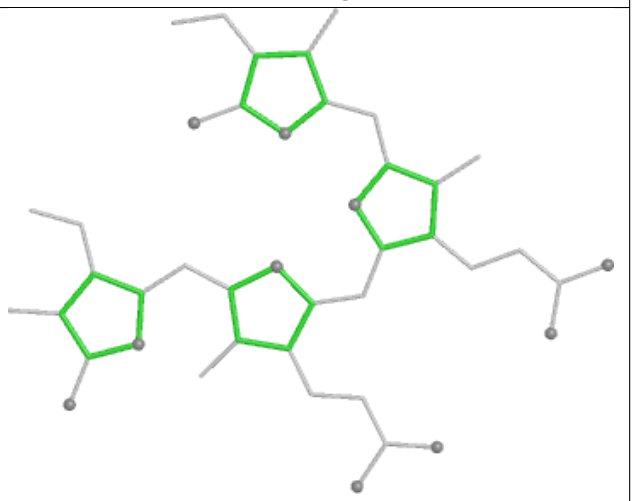
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Bond angles

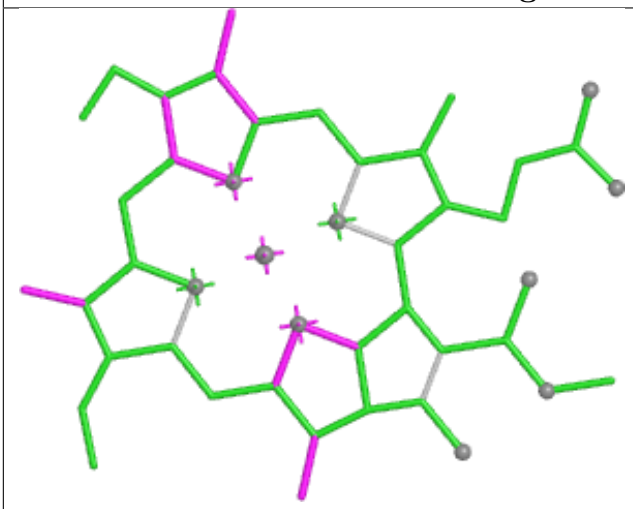


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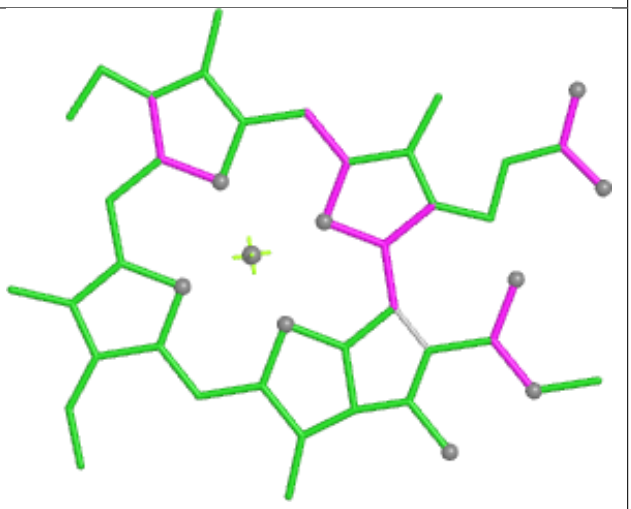


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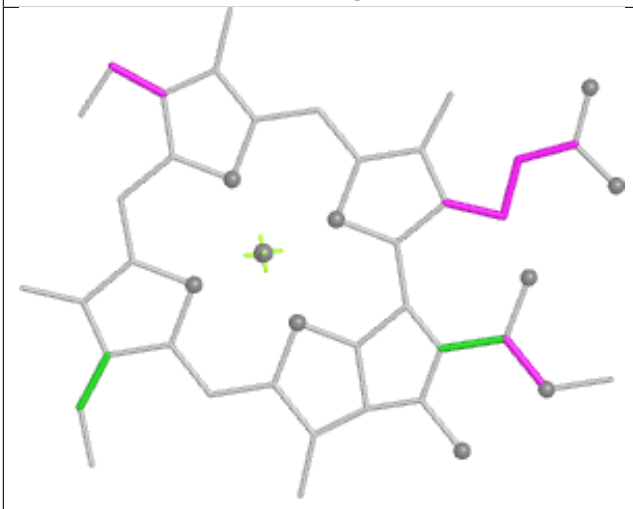
Ligand CLA 32 312



Bond lengths



Bond angles

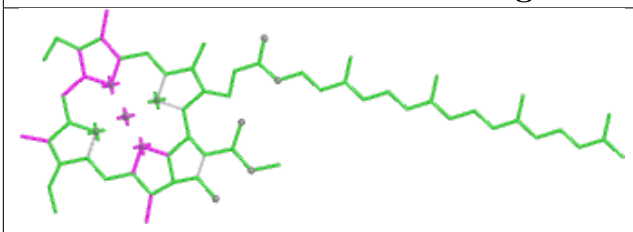


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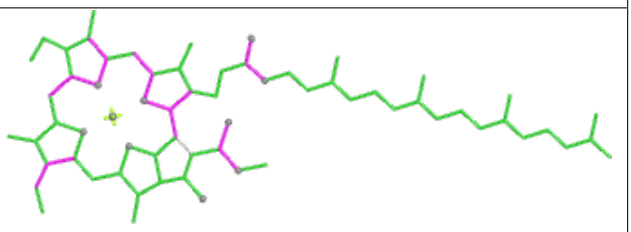


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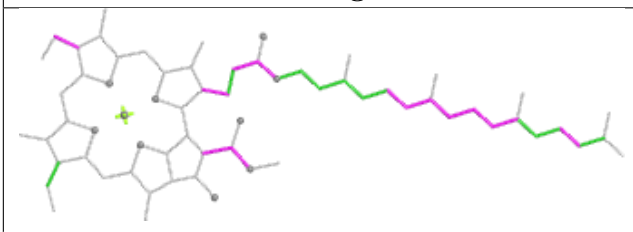
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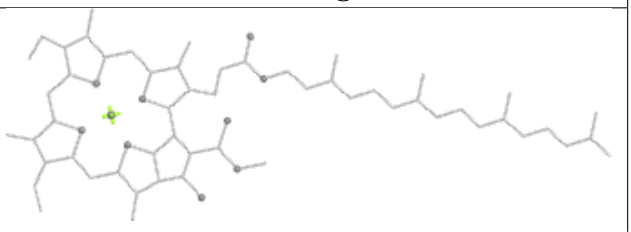
Bond lengths



Bond angles

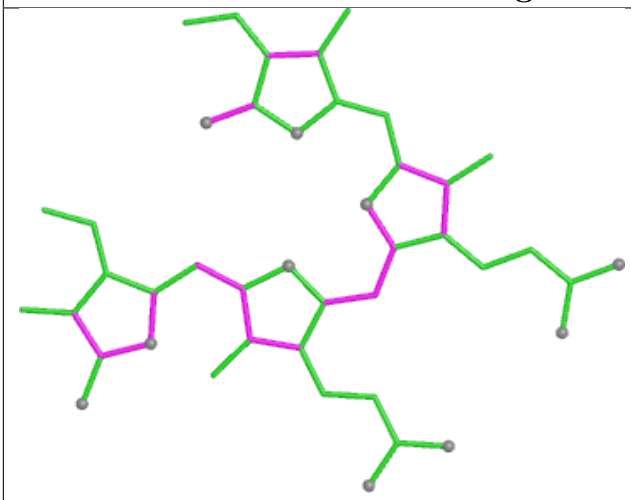


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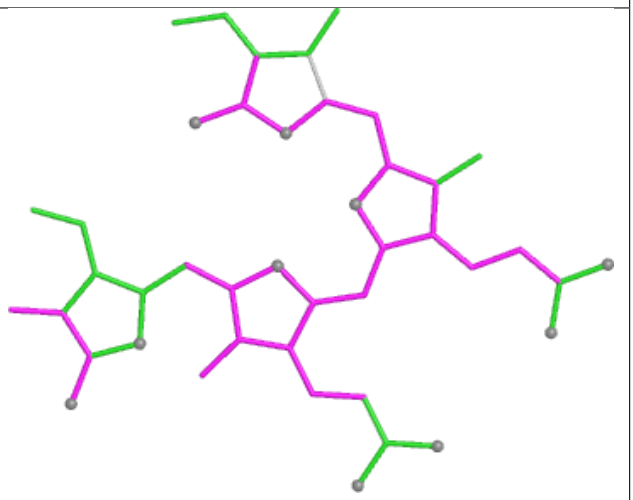


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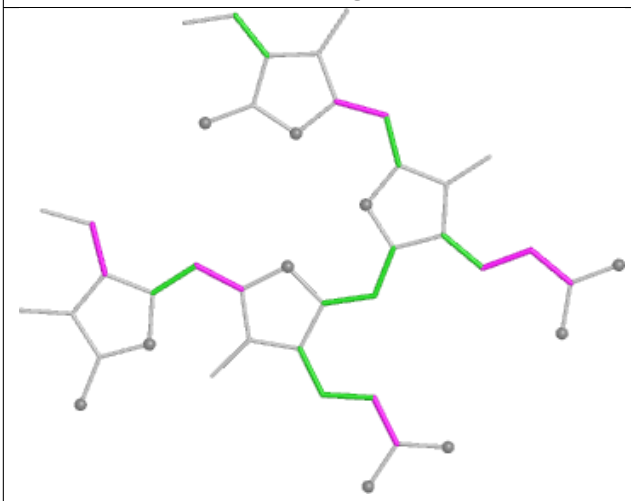
Ligand PEB A5 201



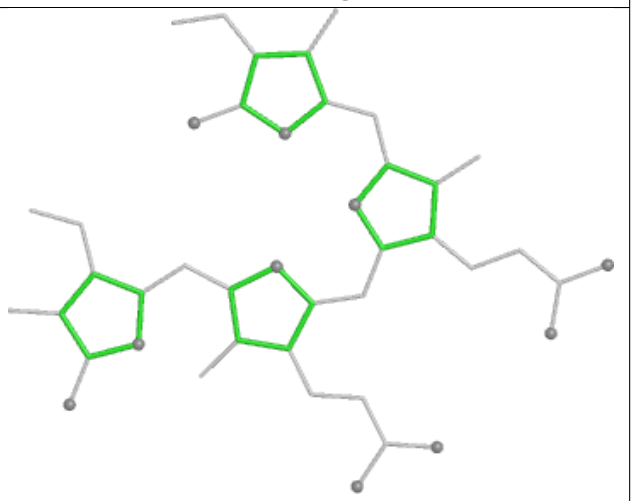
Bond lengths



Bond angles

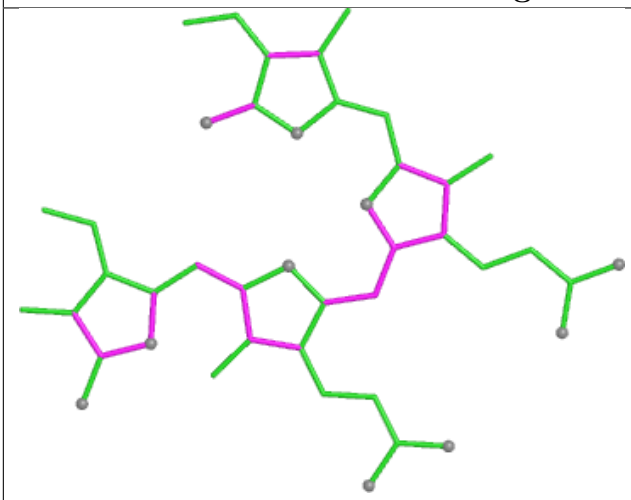


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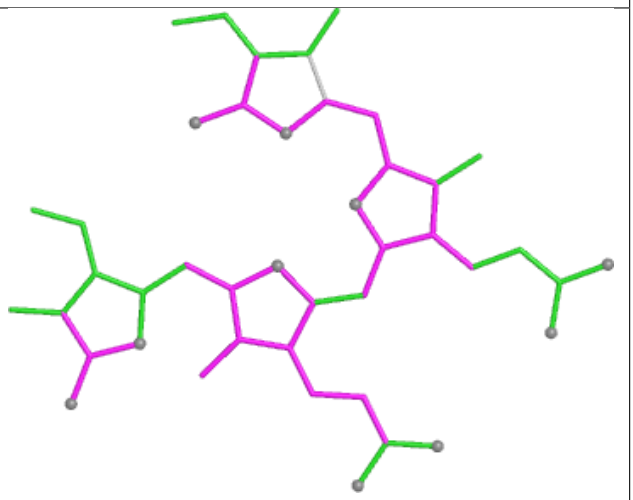


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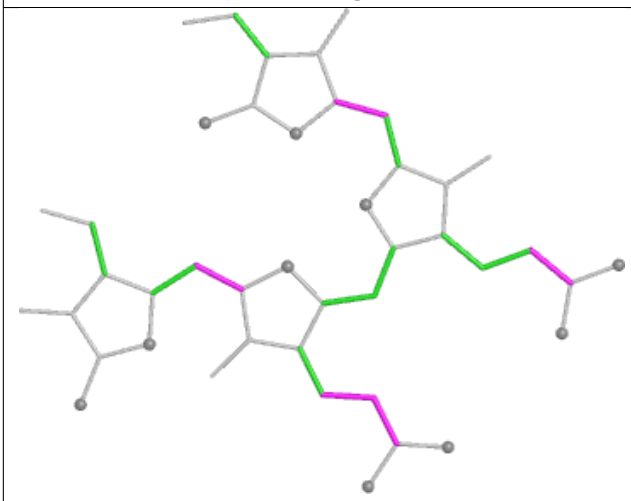
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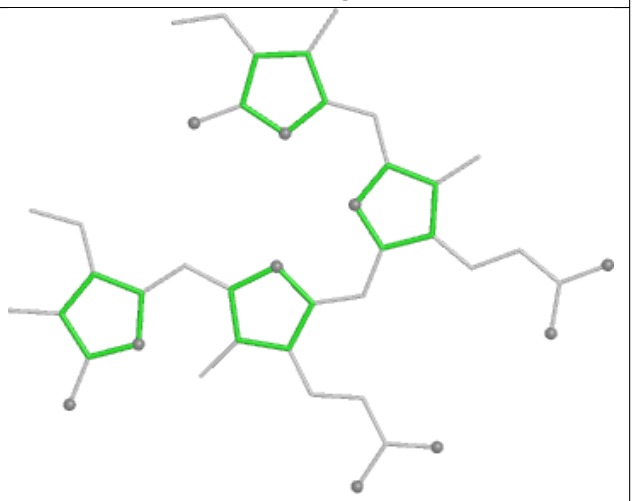
Bond lengths



Bond angles

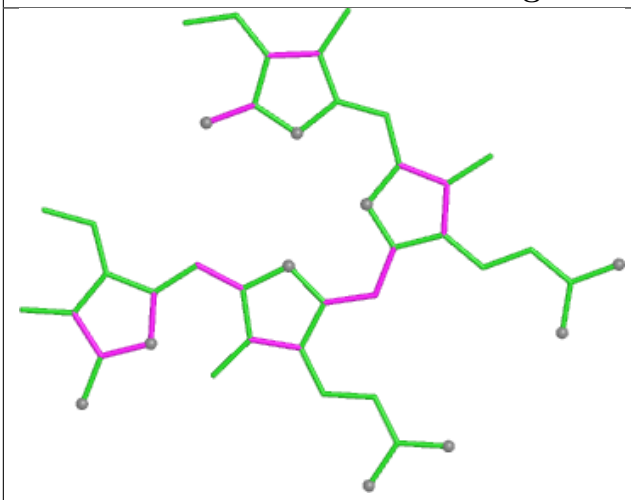


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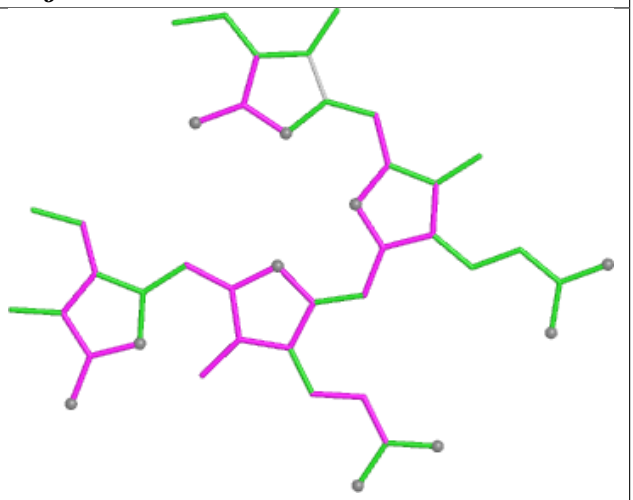


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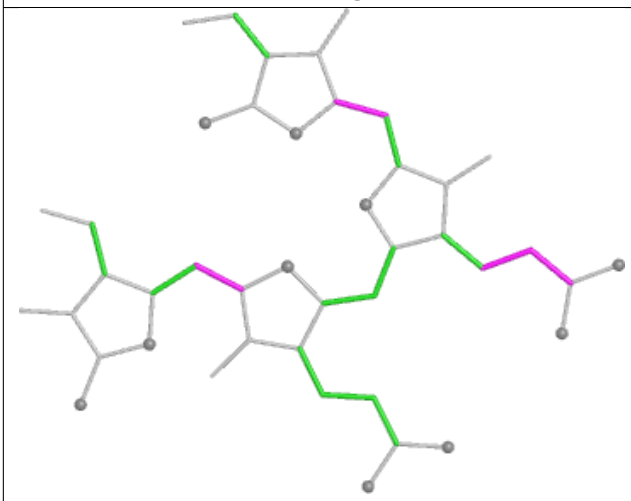
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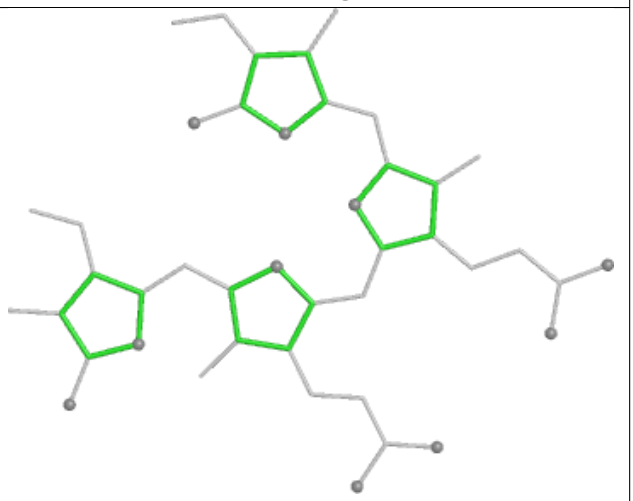
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Bond angles

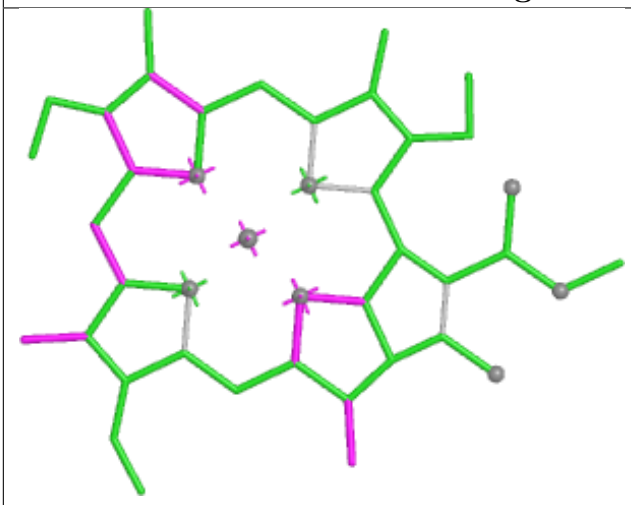


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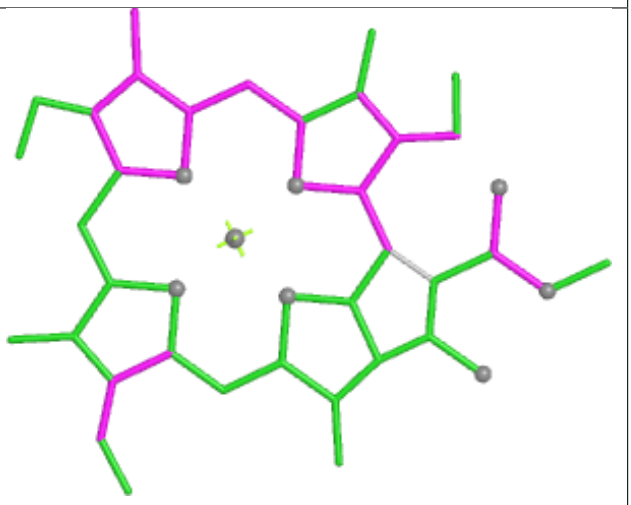


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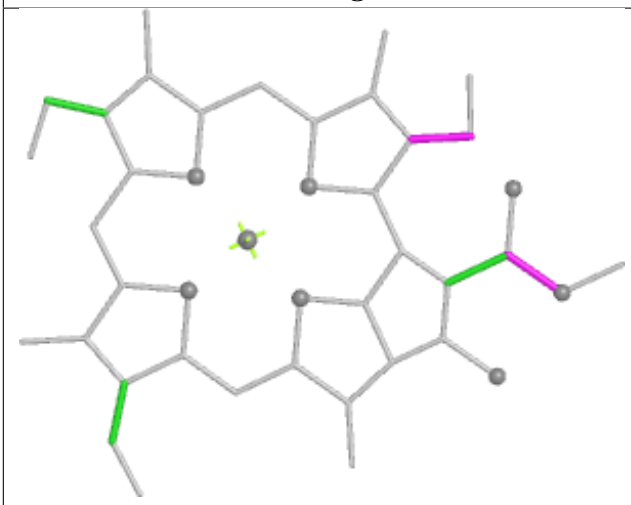
Ligand CLA 2N 305



Bond lengths



Bond angles

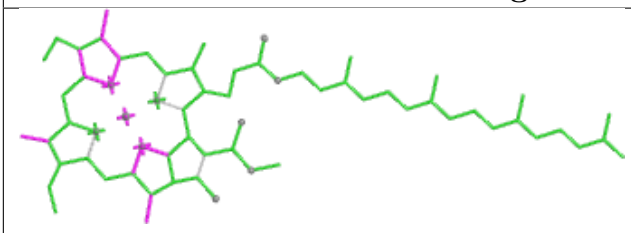


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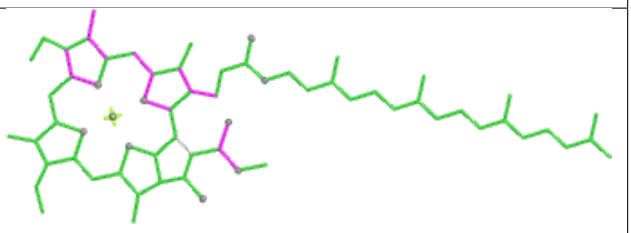


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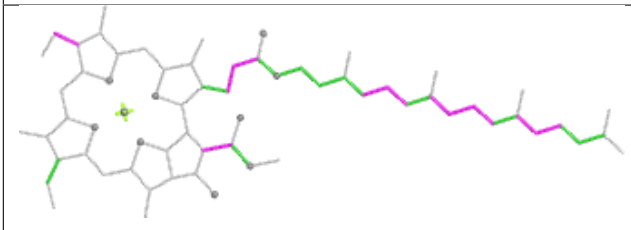
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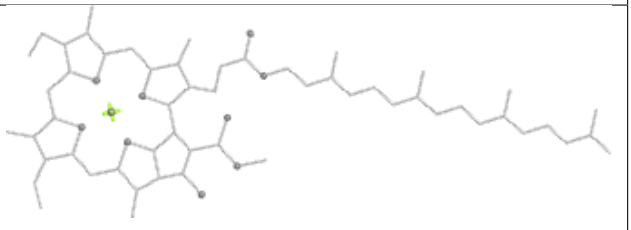
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Bond angles

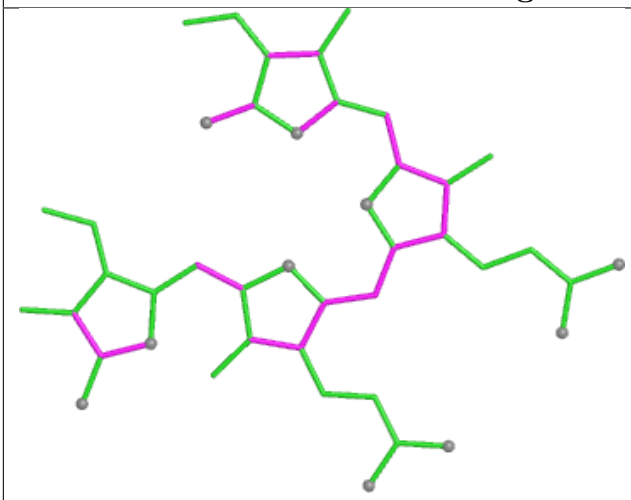


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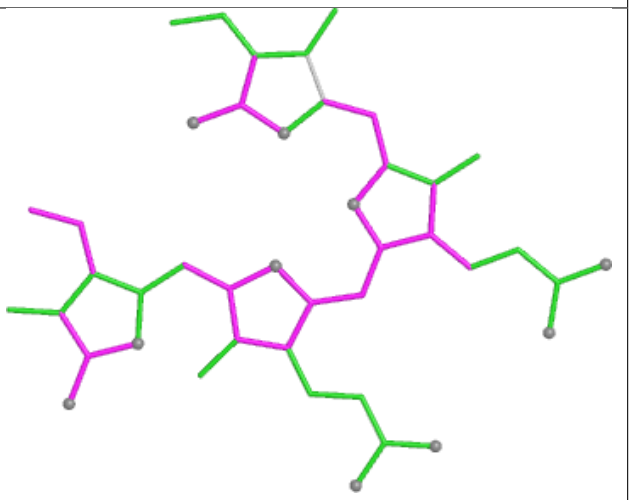


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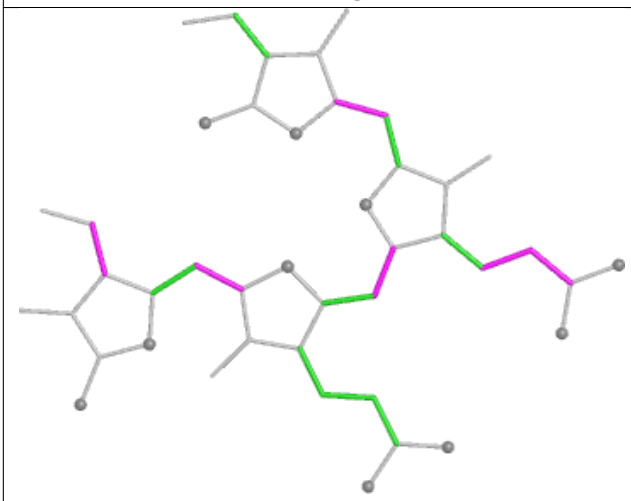
Ligand PEB tK 203



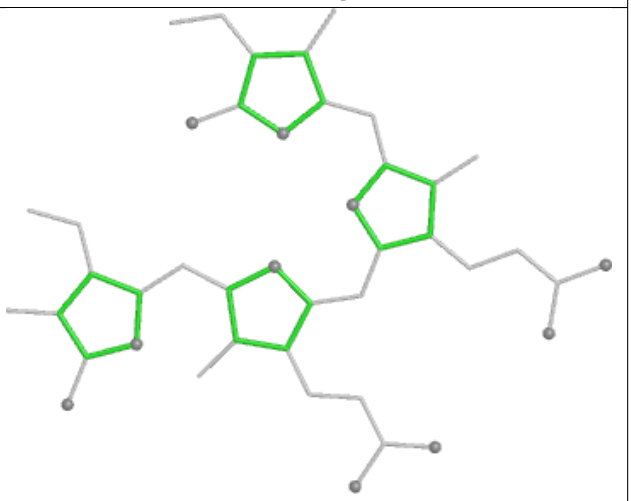
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Bond angles

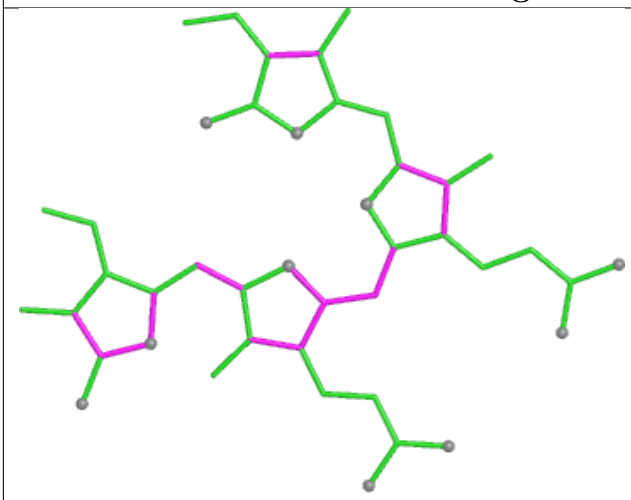


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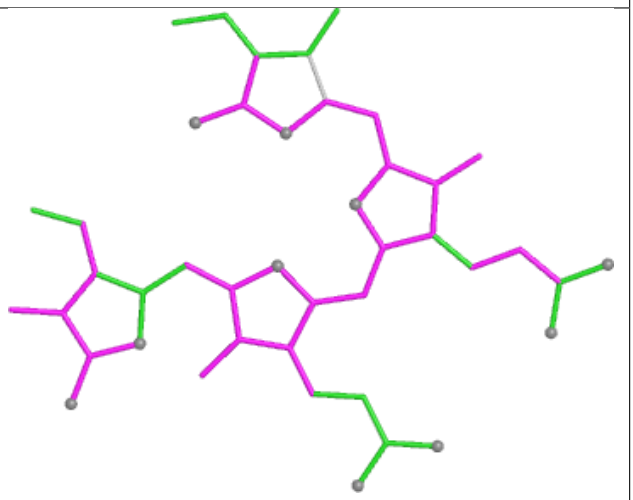


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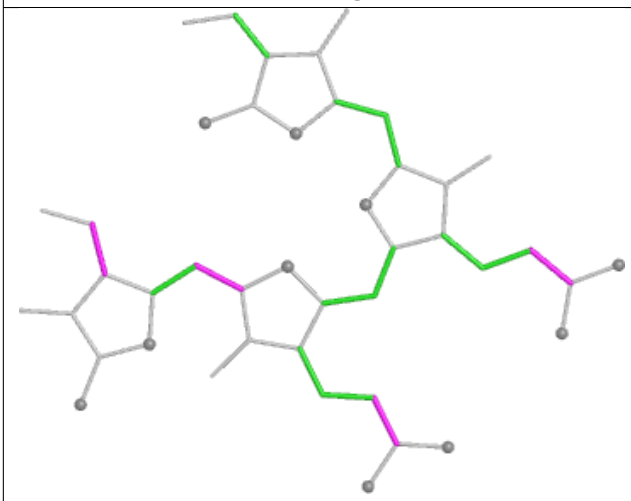
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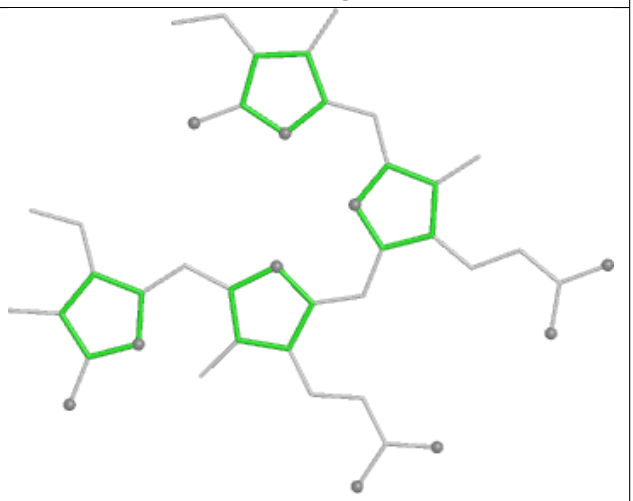
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Bond angles

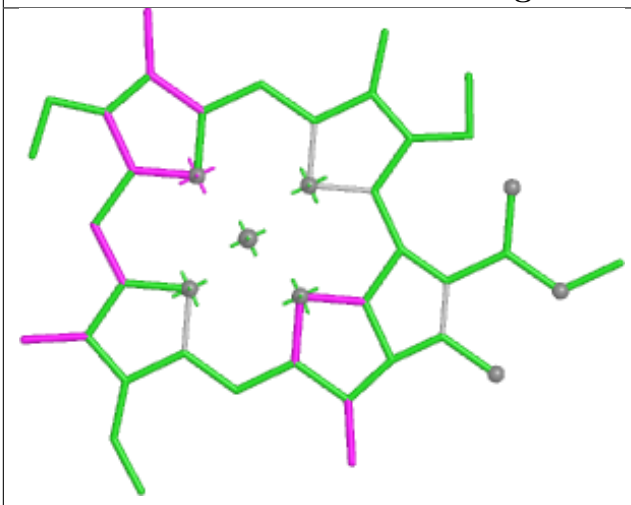


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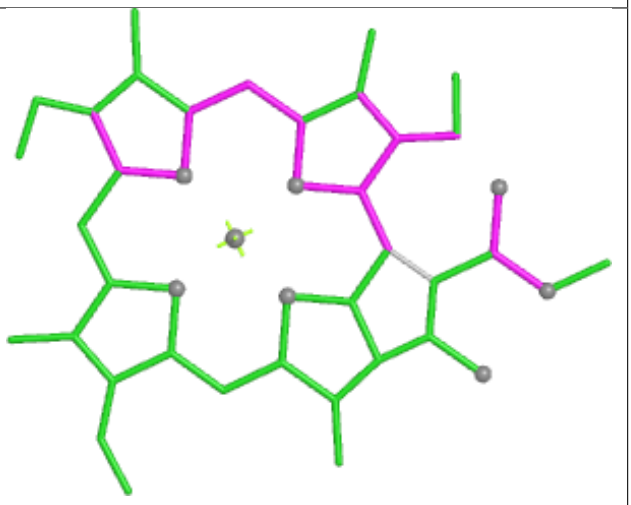


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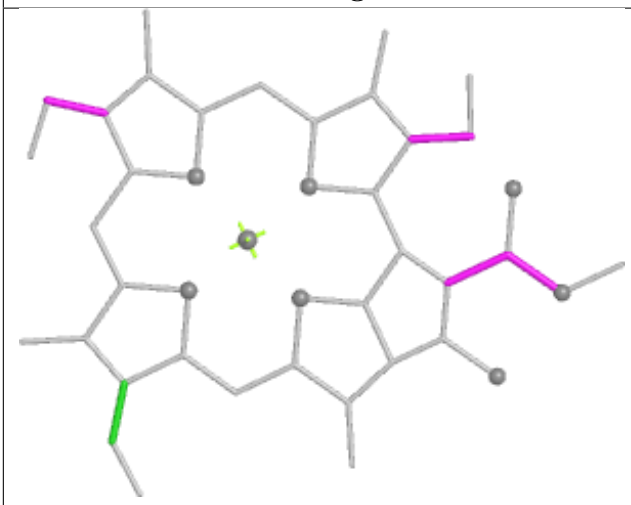
Ligand CLA 3N 311



Bond lengths



Bond angles

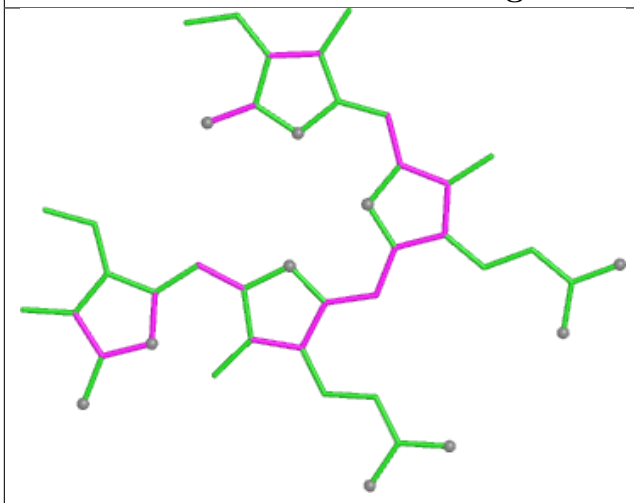


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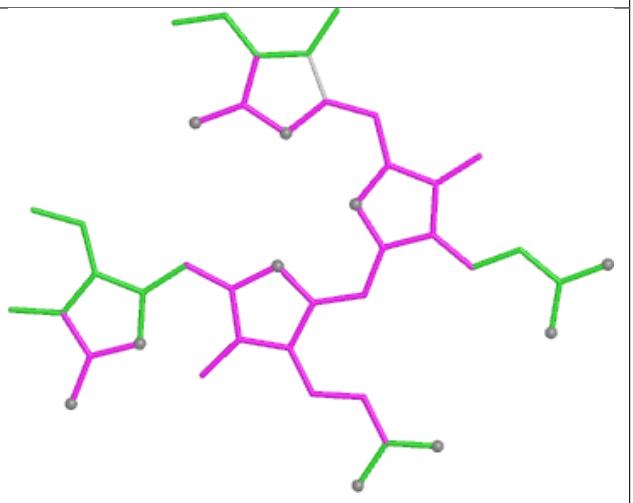


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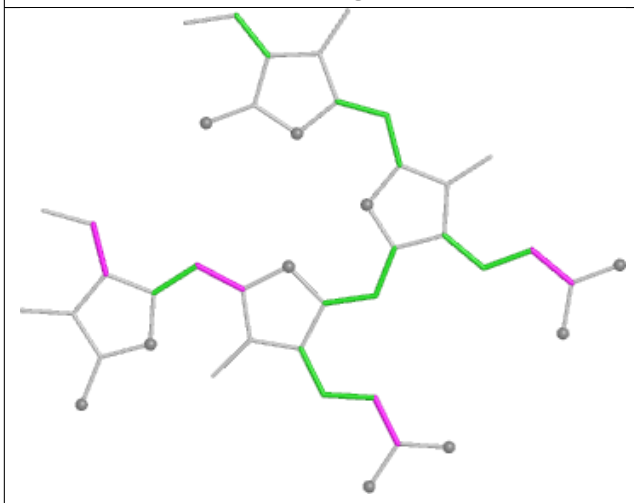
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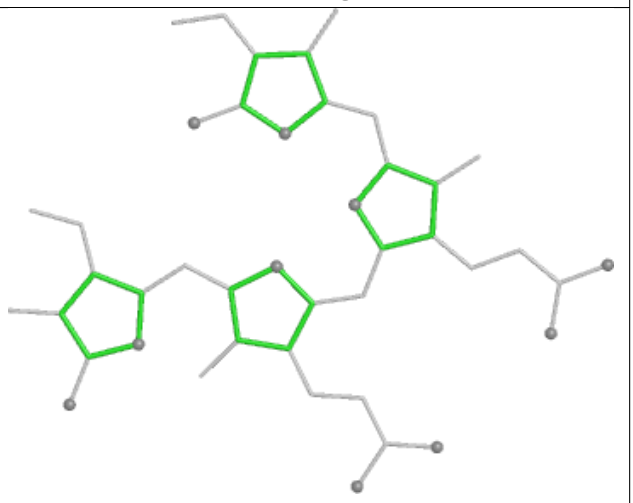
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Bond angles

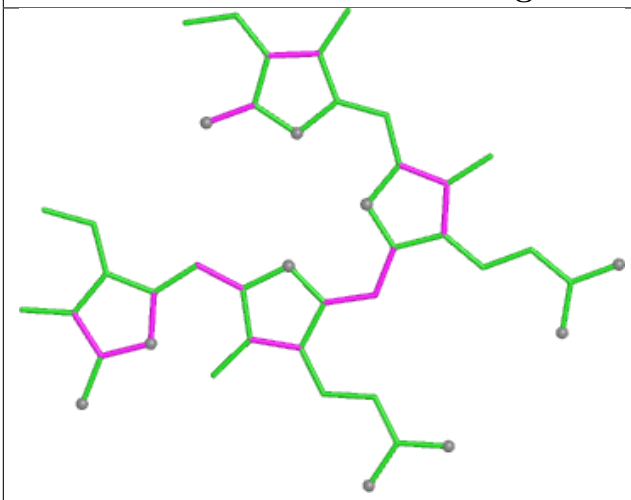


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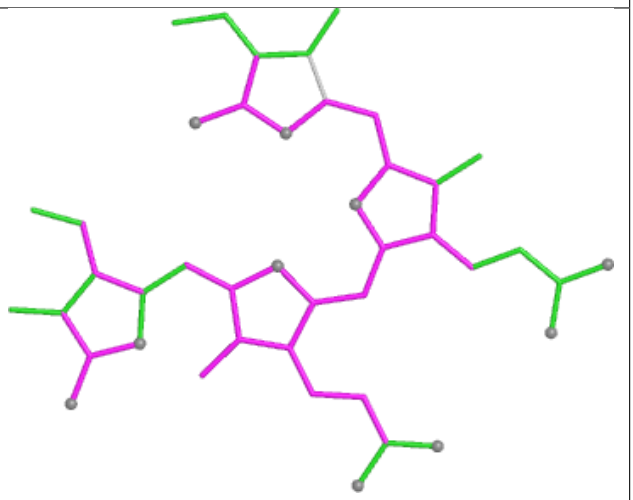


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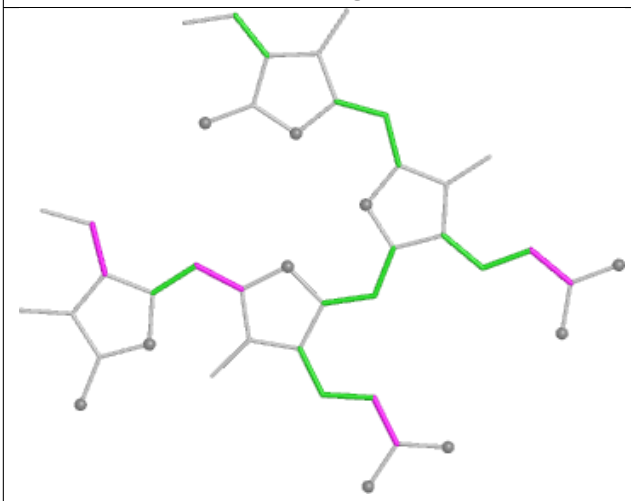
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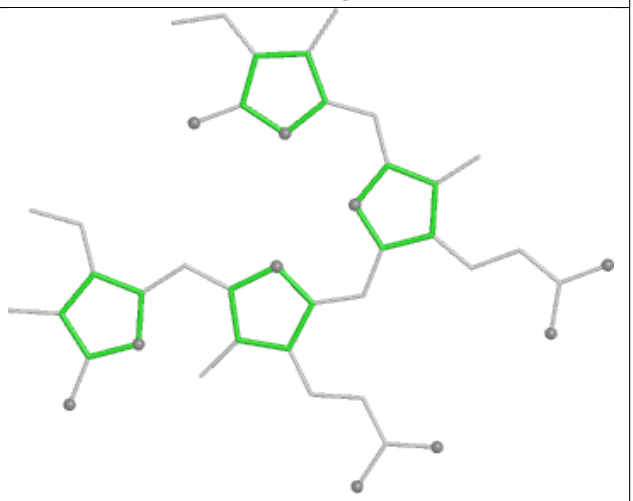
Bond lengths



Bond angles

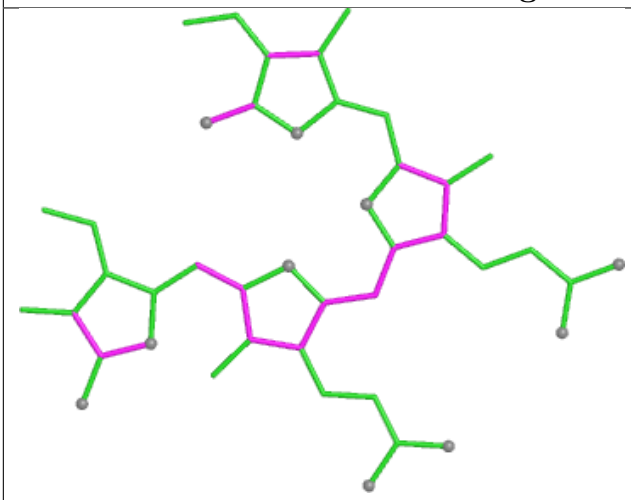


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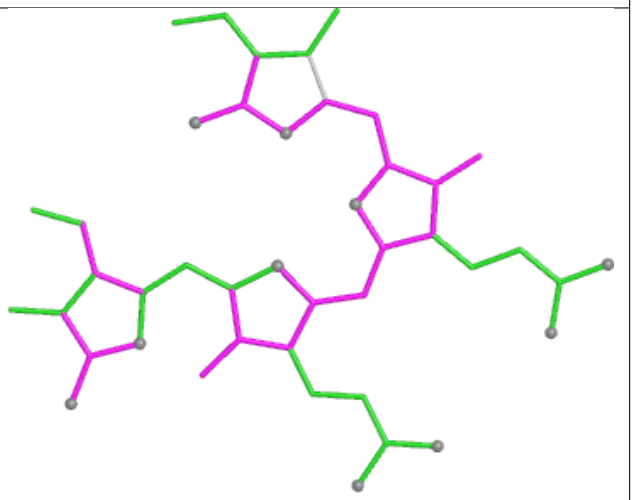


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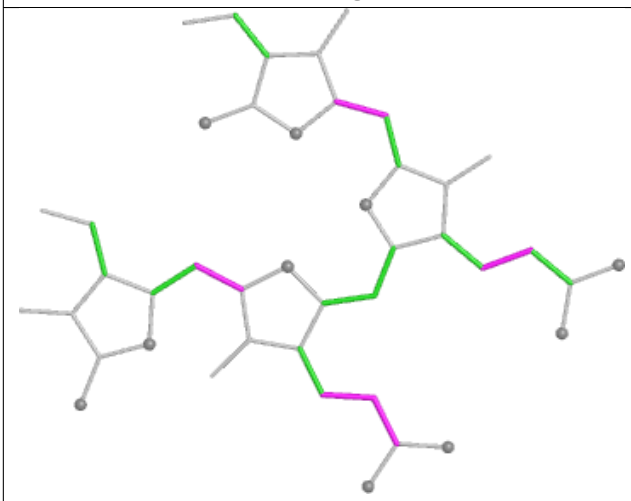
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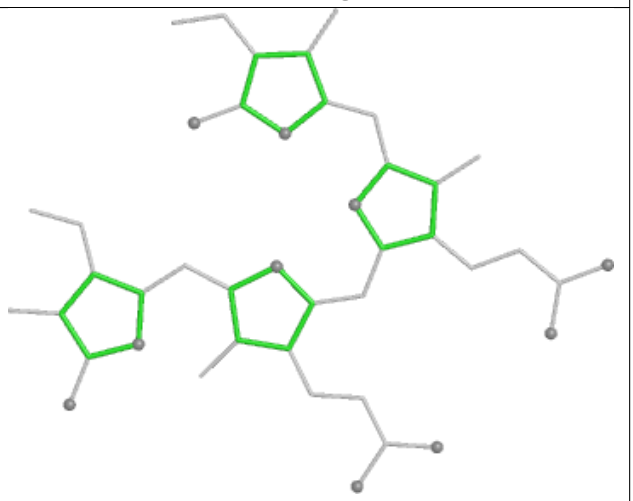
Bond lengths



Bond angles

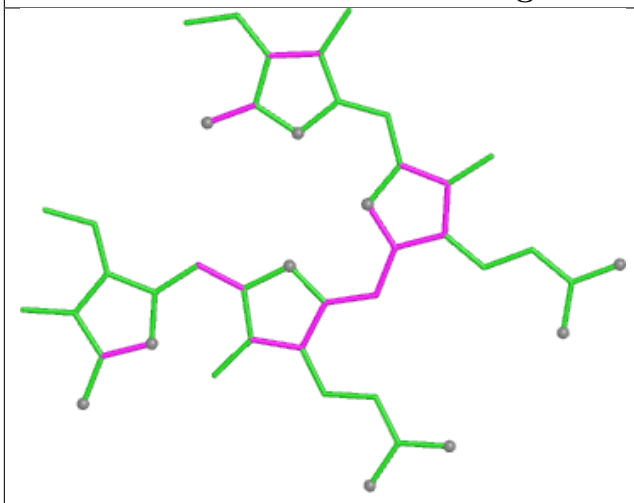


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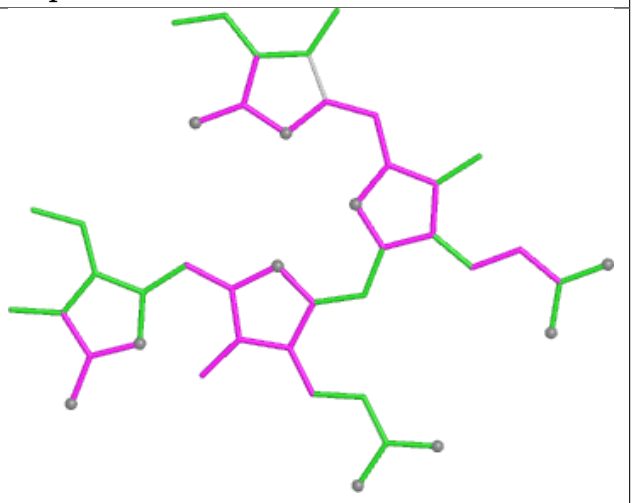


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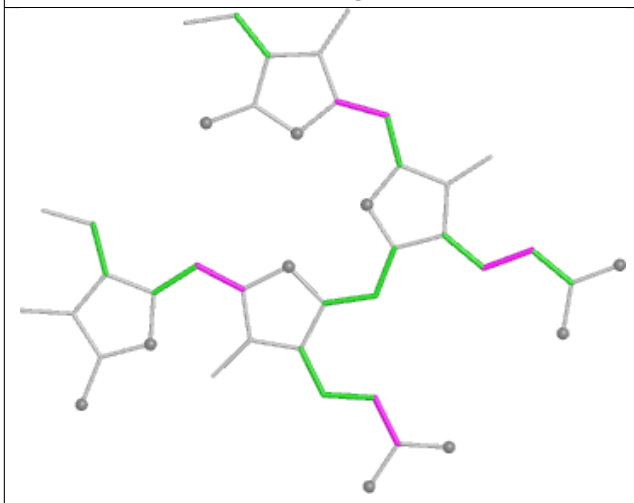
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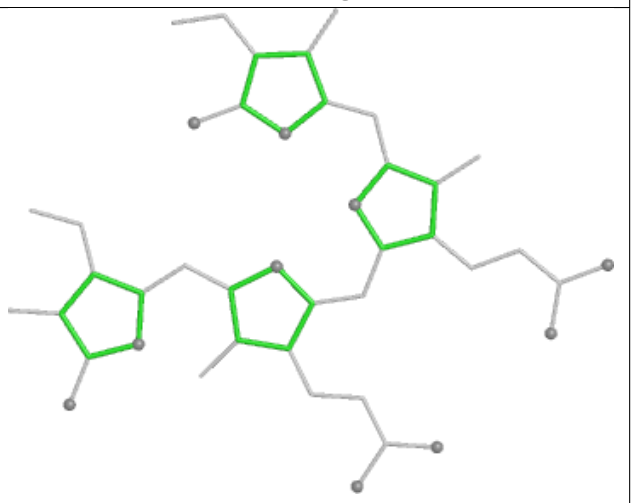
Bond lengths



Bond angles

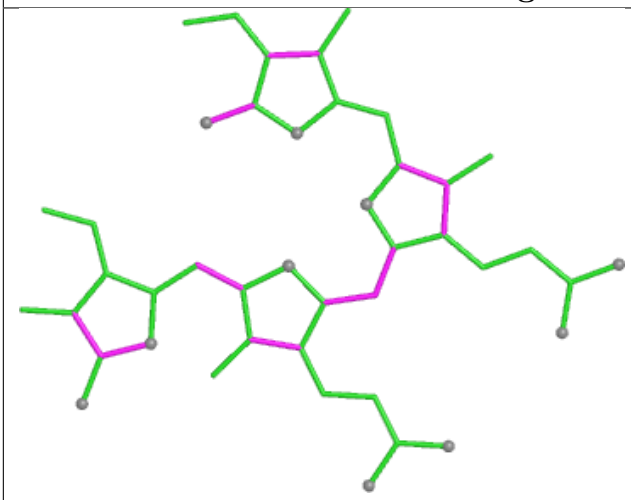


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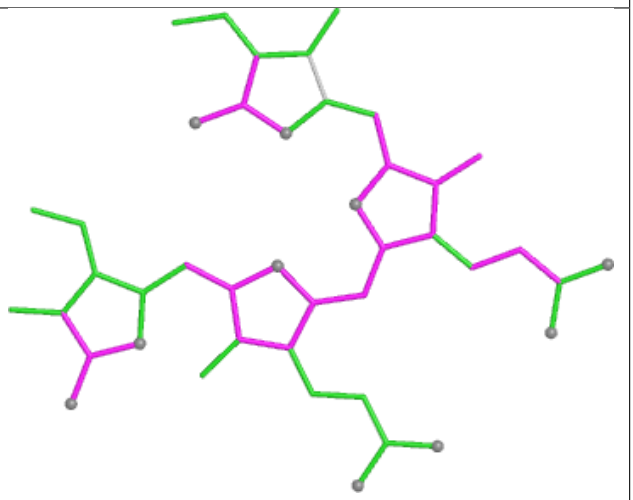


Rings

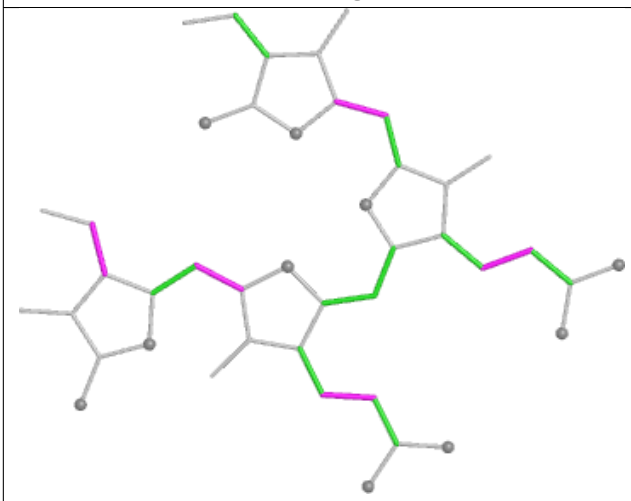
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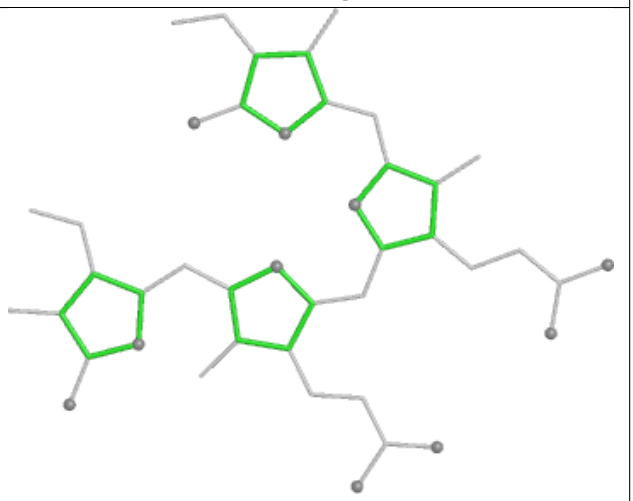
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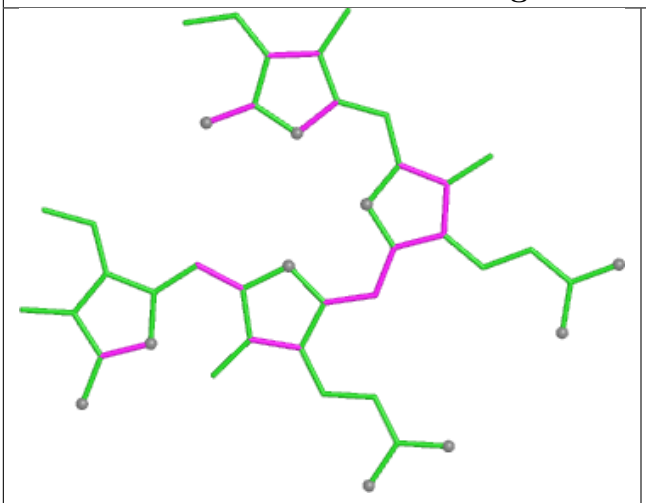


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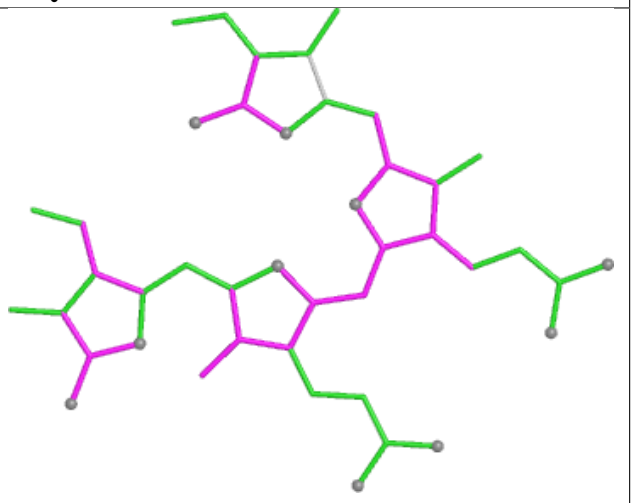


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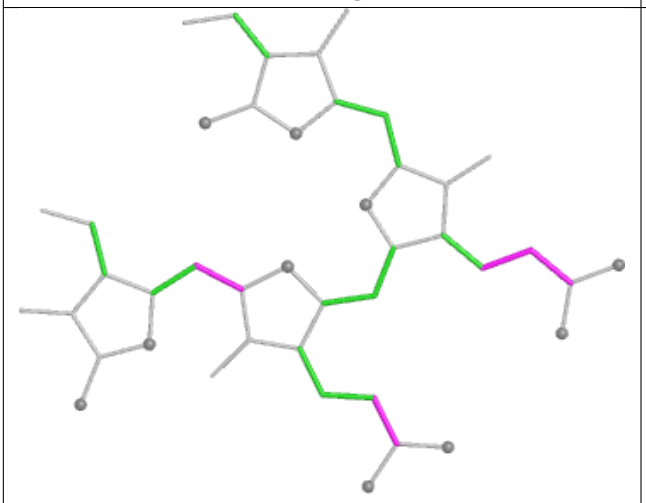
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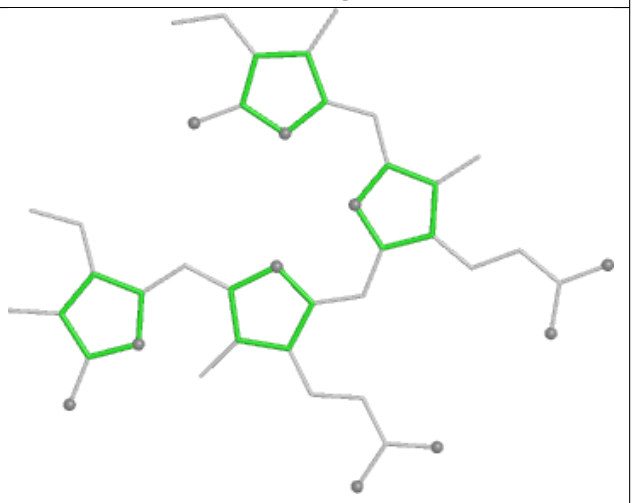
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Bond angles

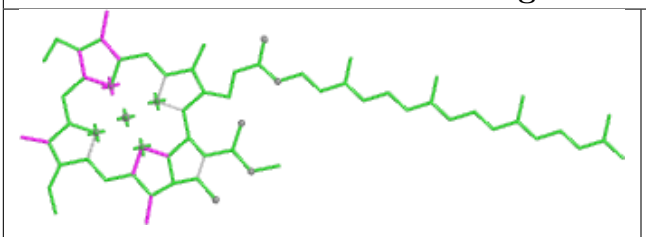


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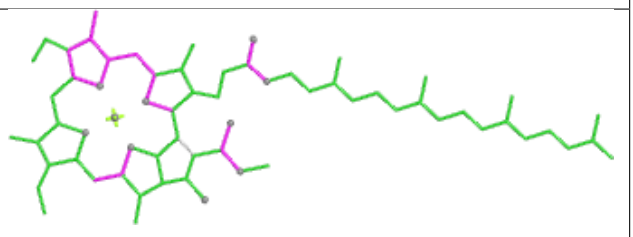


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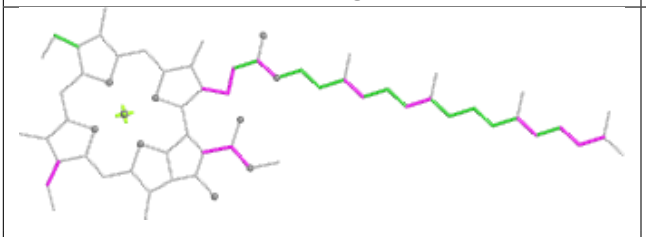
Ligand CLA b6 609



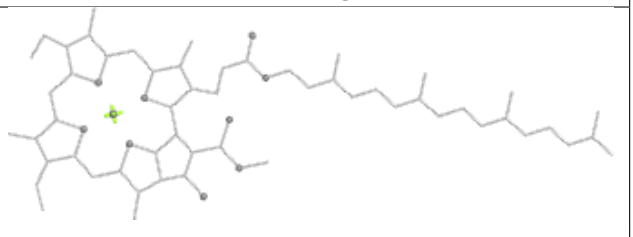
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Bond angles

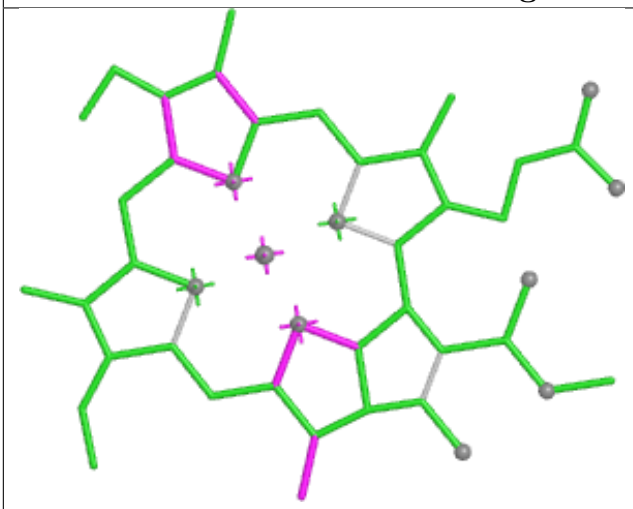


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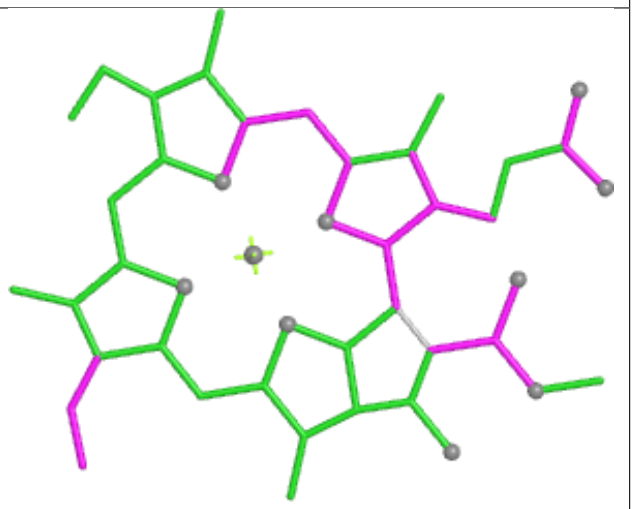


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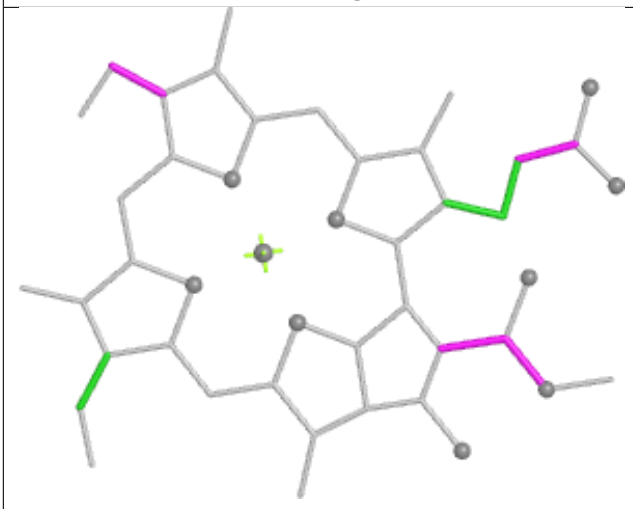
Ligand CLA 22 607



Bond lengths



Bond angles

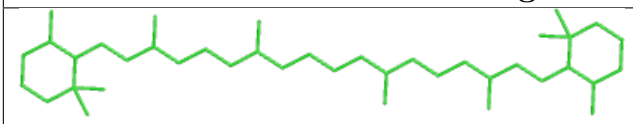


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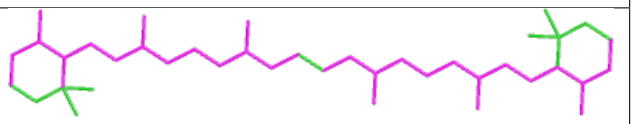


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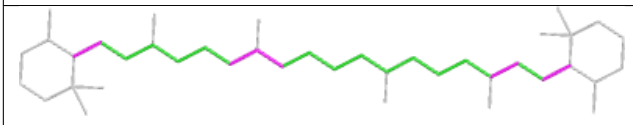
Ligand BCR c6 603



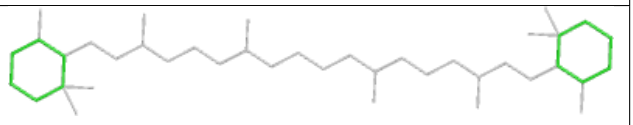
Bond lengths



Bond angles

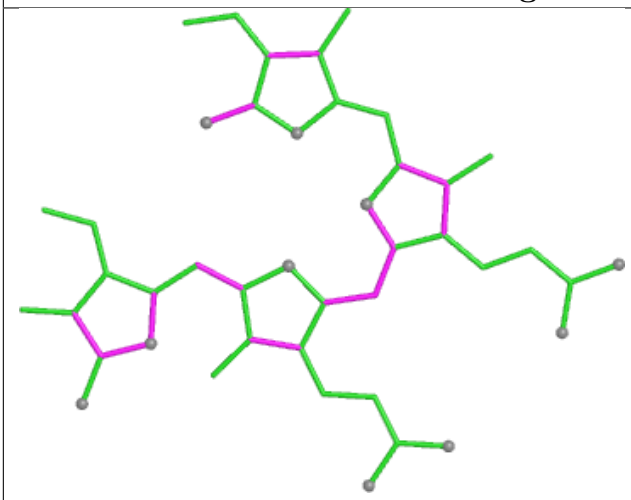


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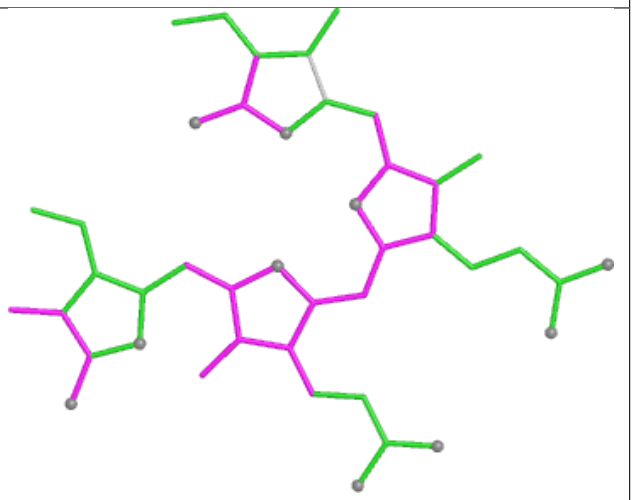


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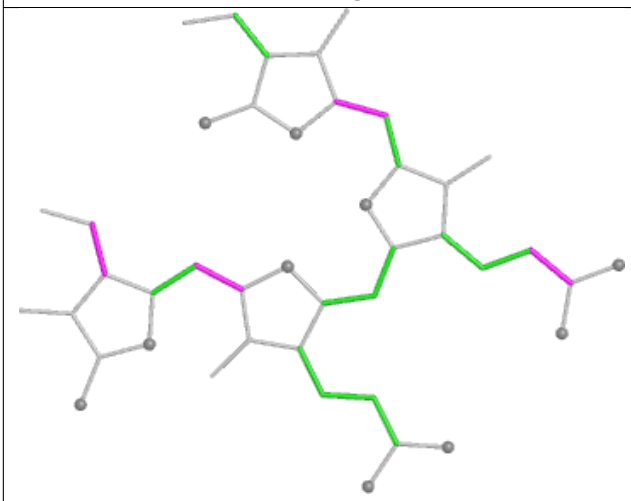
Ligand PEB lO 201



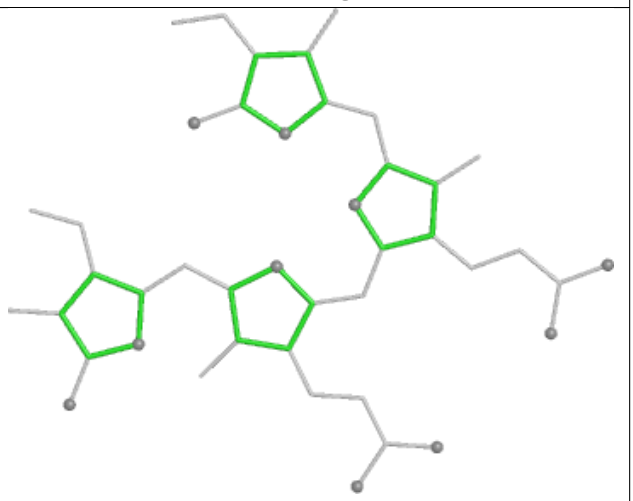
Bond lengths



Bond angles

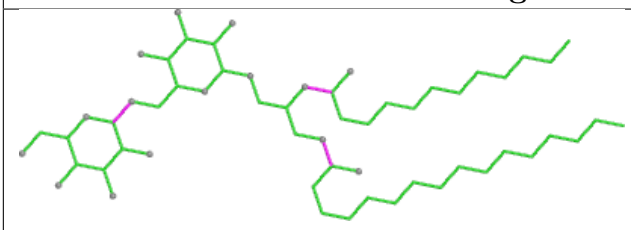


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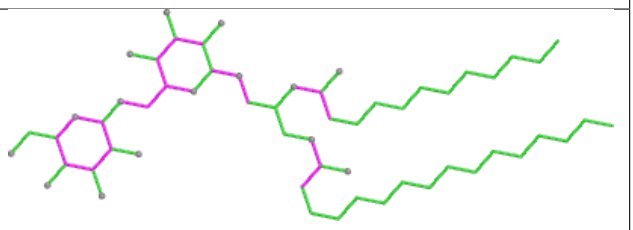


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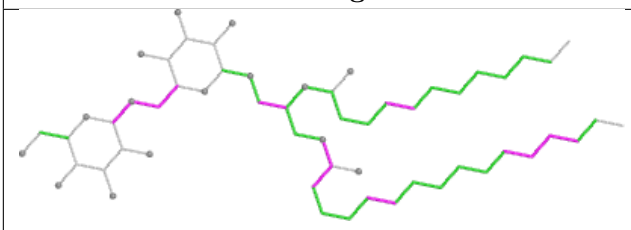
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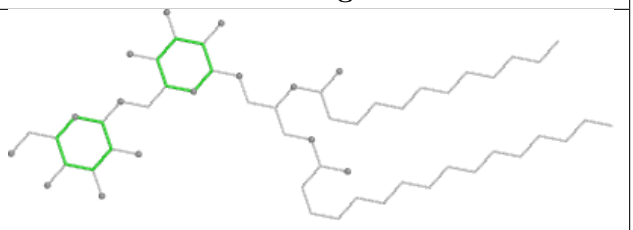
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Bond angles

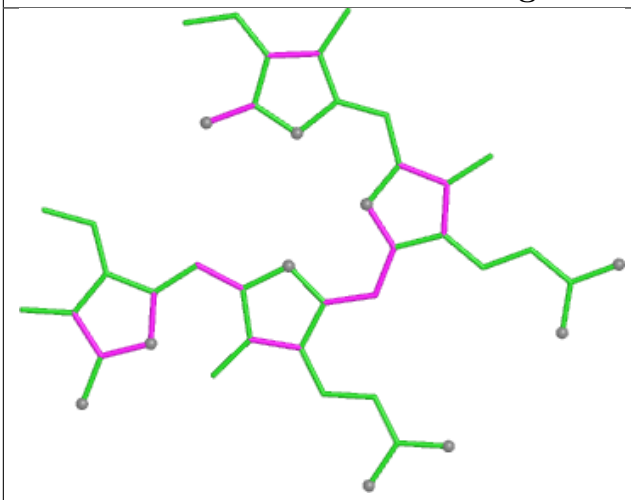


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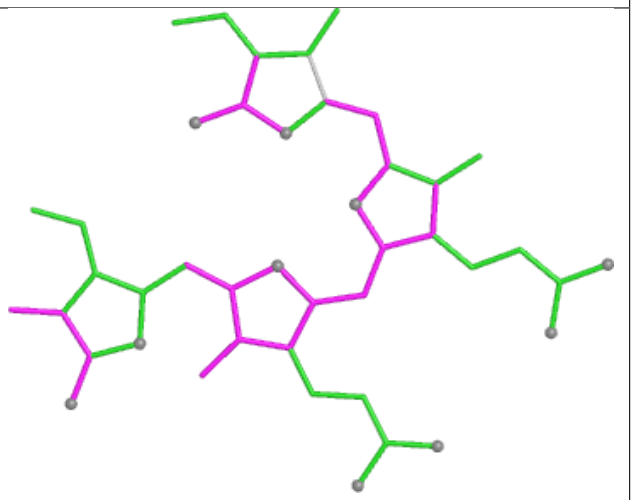


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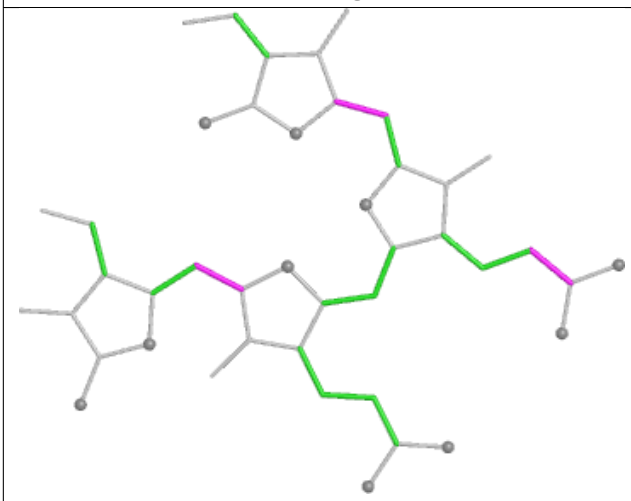
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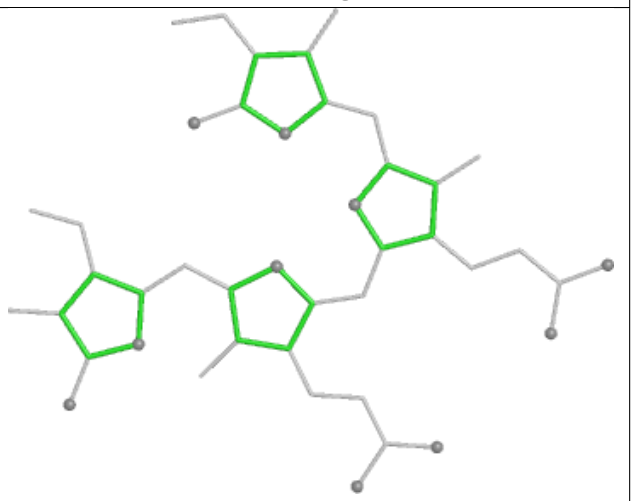
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Bond angles

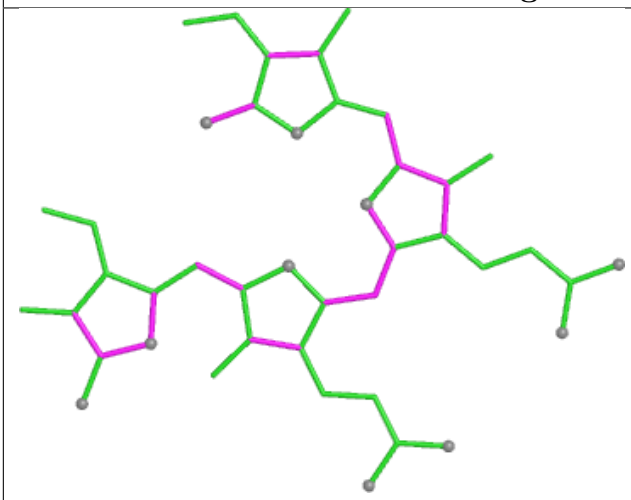


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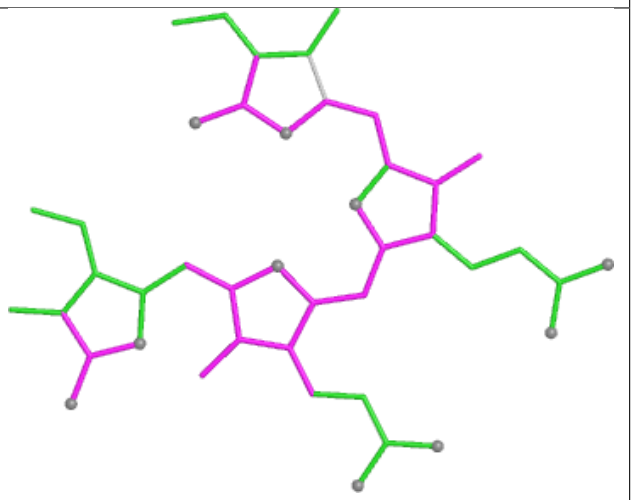


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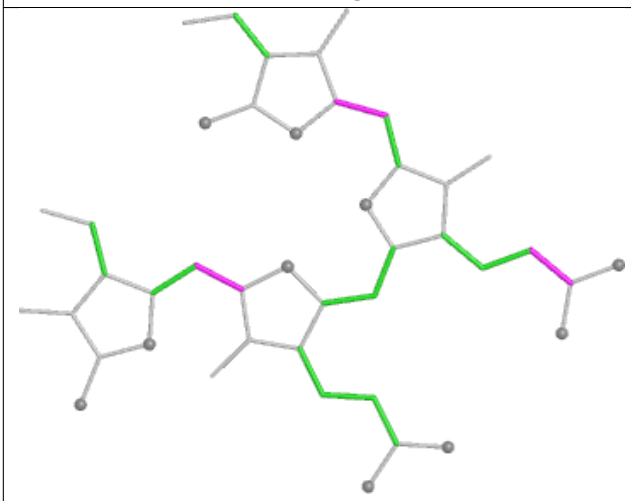
Ligand PEB cJ 201



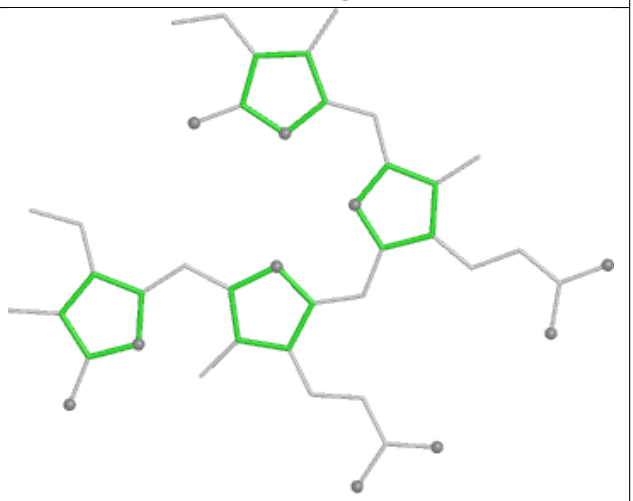
Bond lengths



Bond angles

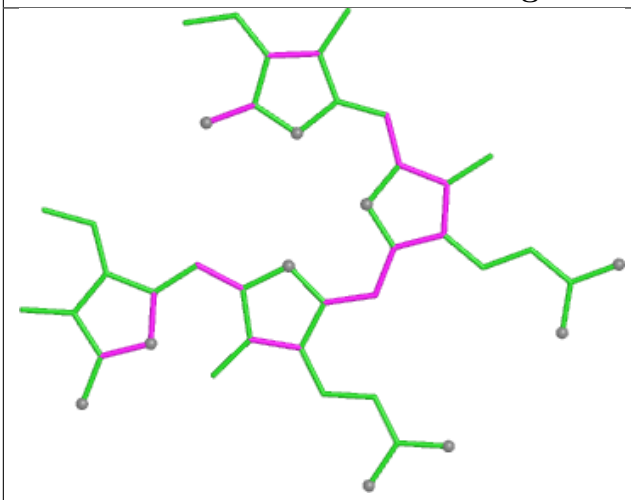


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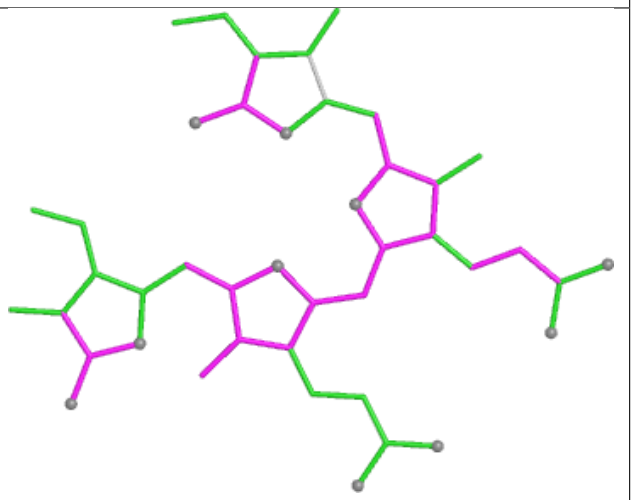


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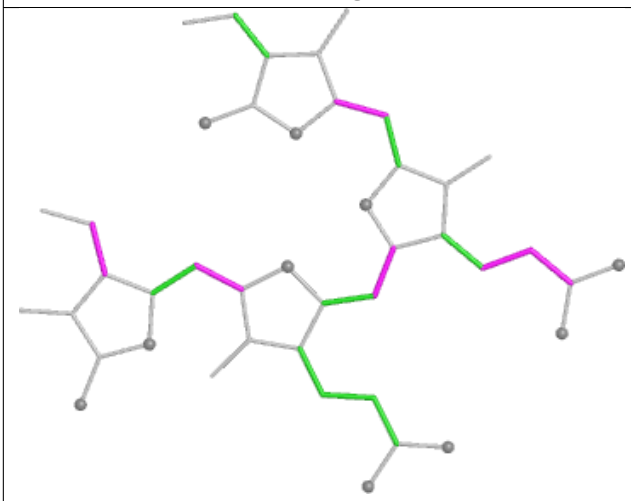
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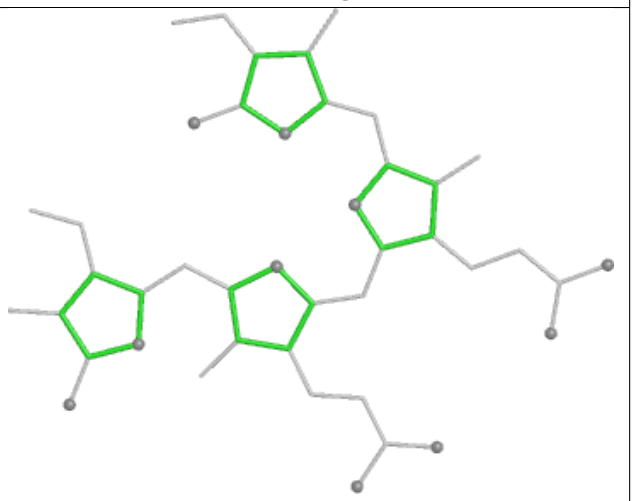
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Bond angles

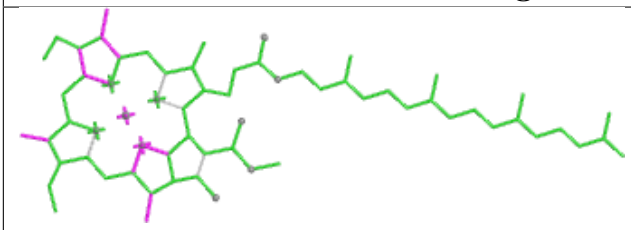


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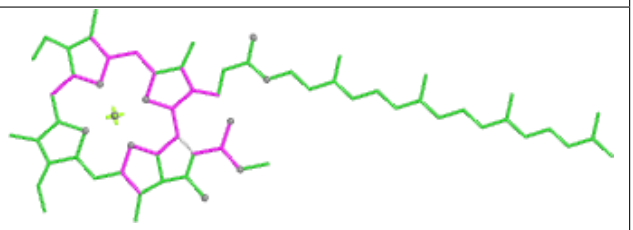


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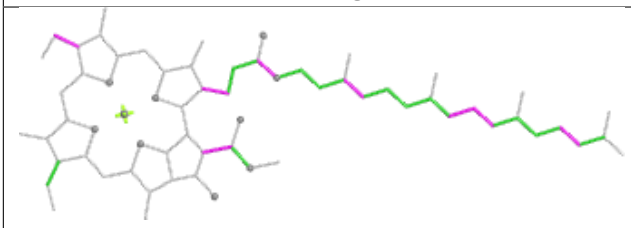
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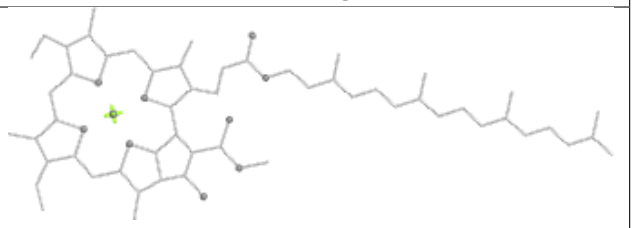
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Bond angles

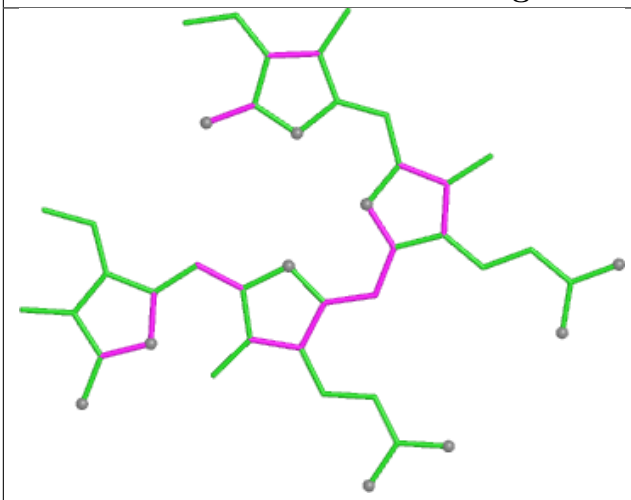


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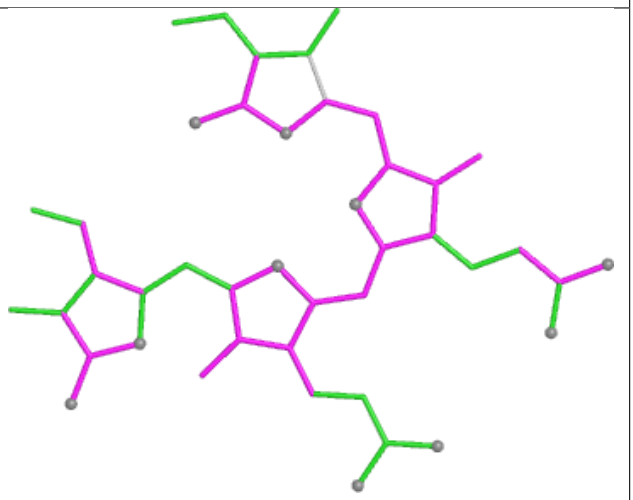


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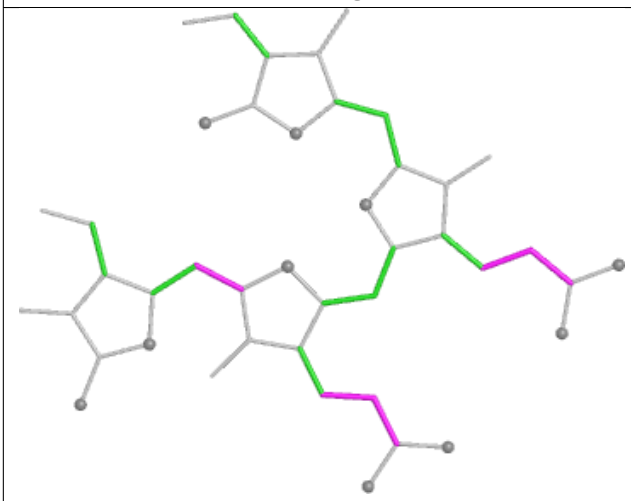
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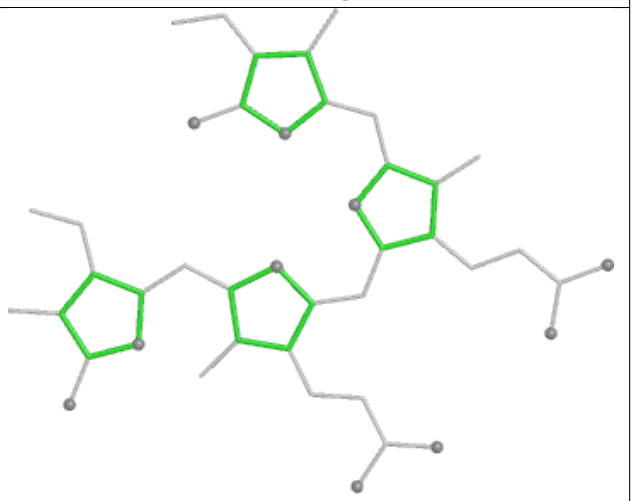
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Bond angles

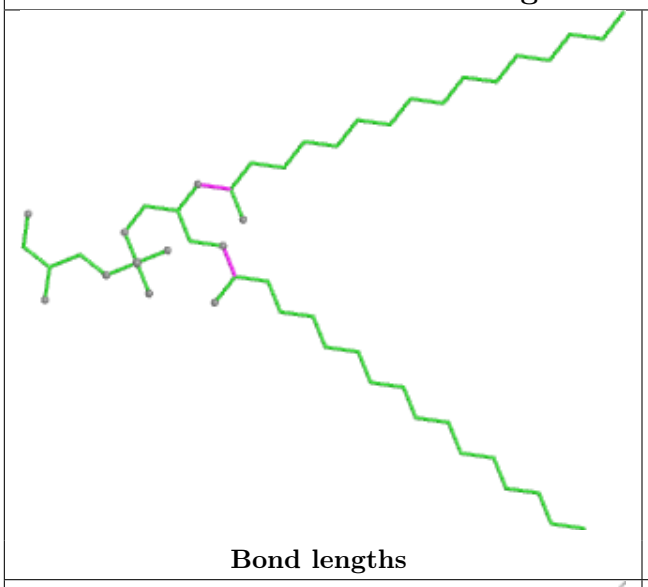


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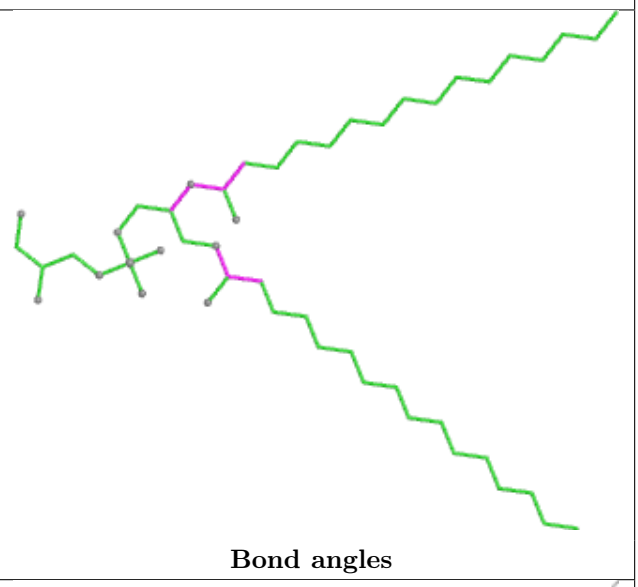


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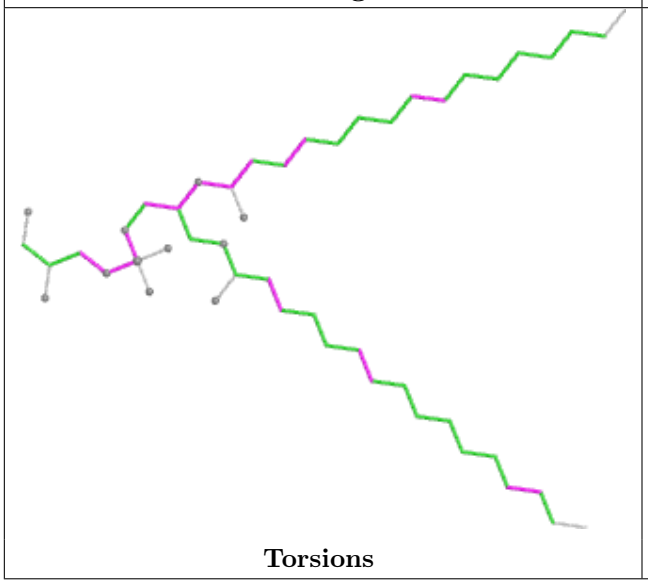
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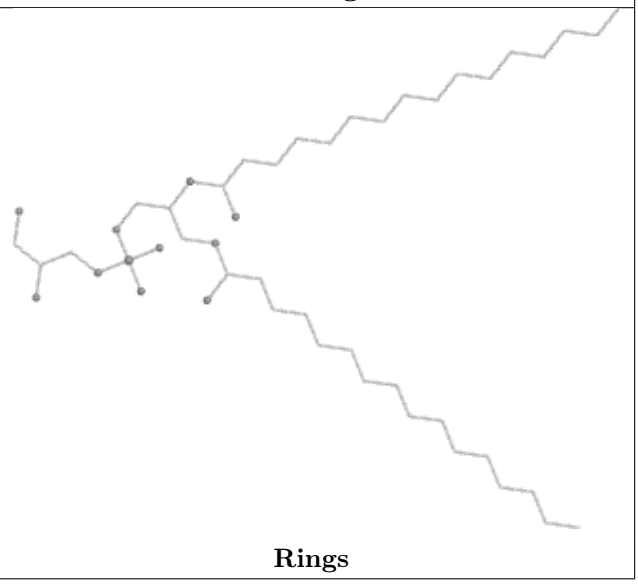
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Bond angles

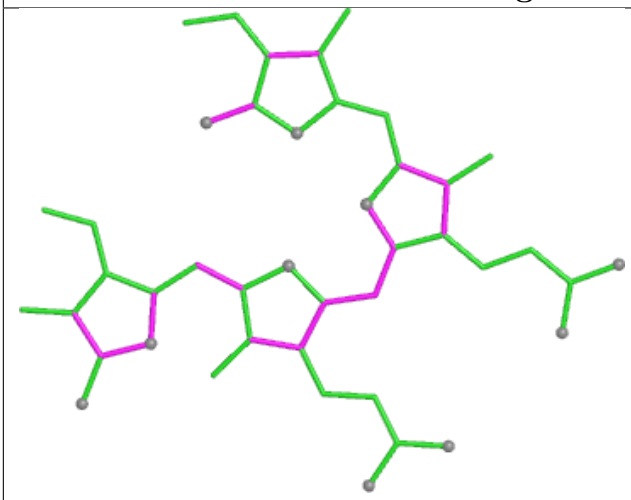


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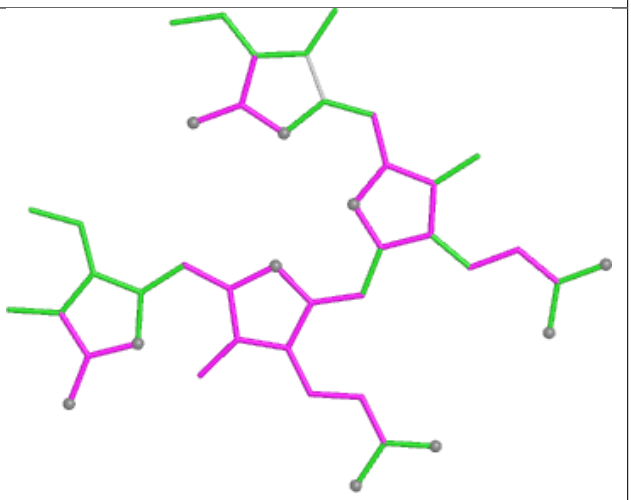


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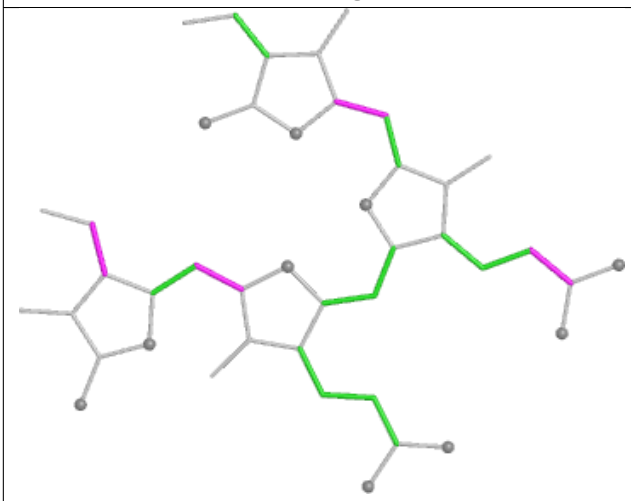
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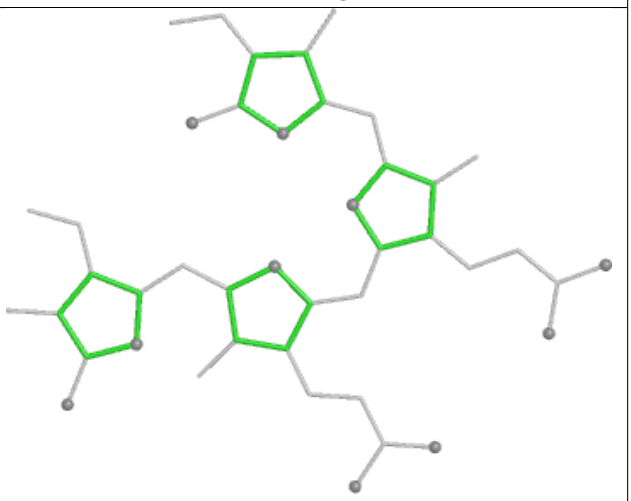
Bond lengths



Bond angles

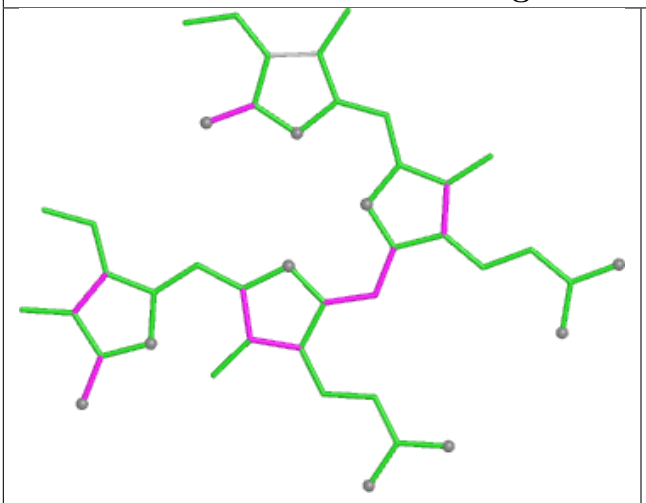


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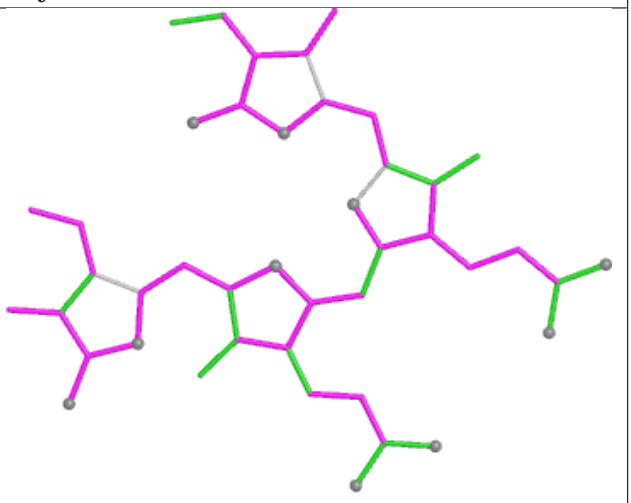


Rings

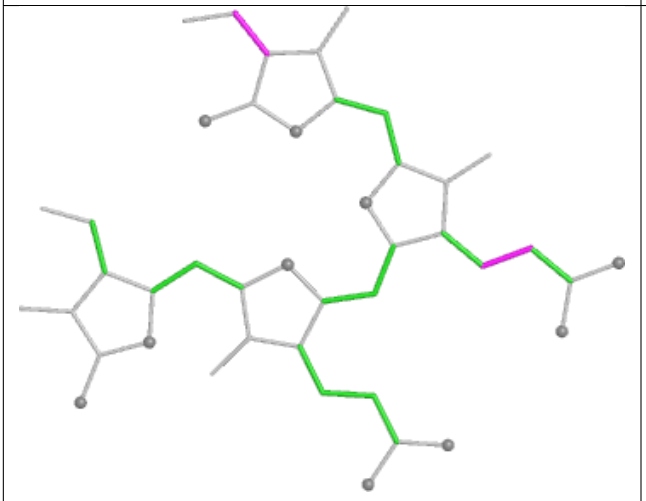
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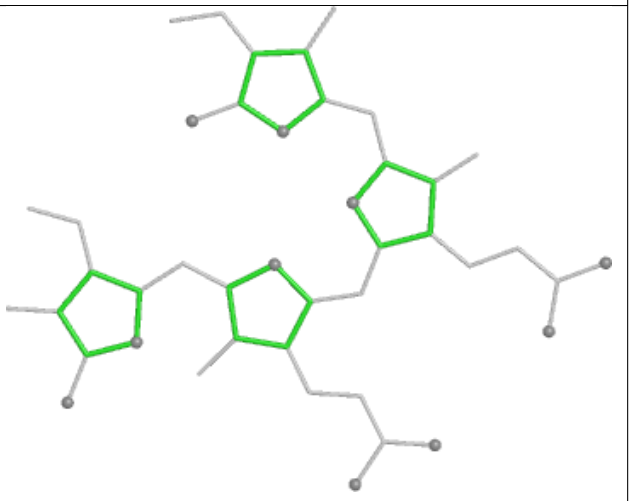
Bond lengths



Bond angles

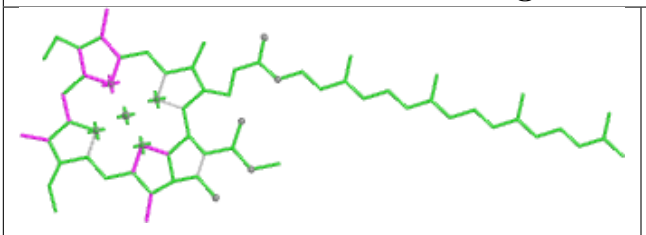


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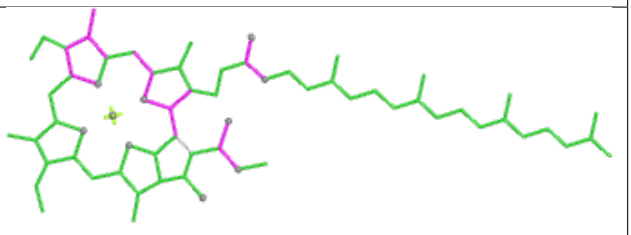


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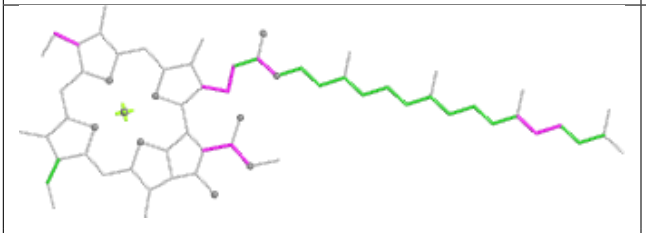
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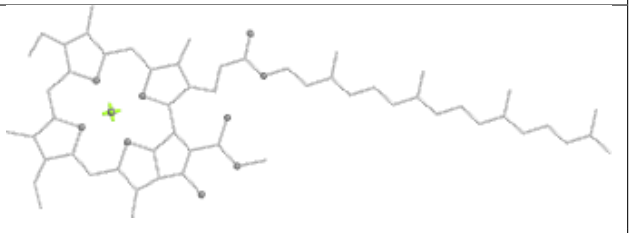
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Bond angles

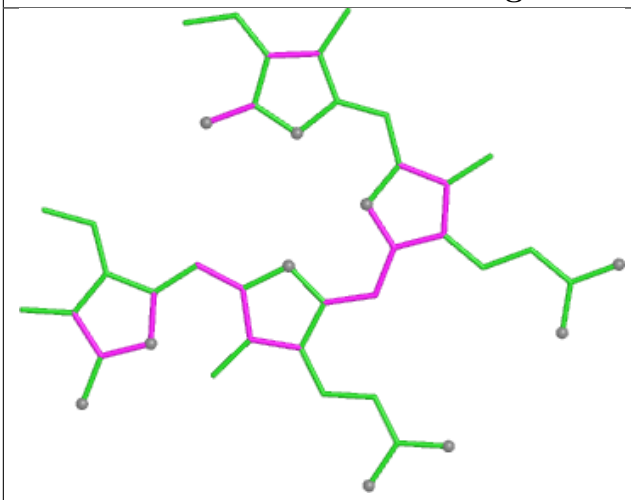


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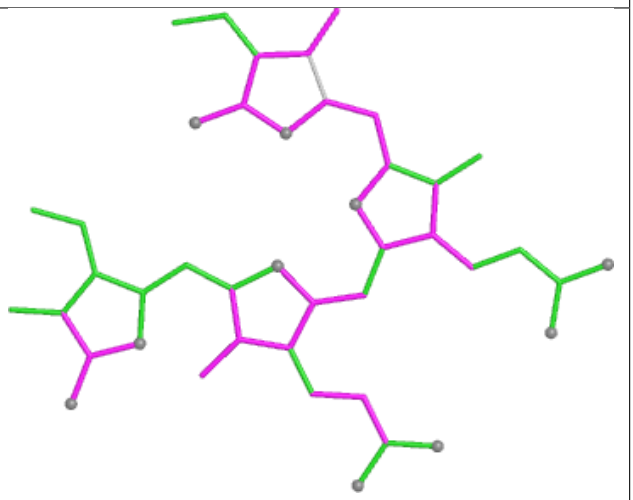


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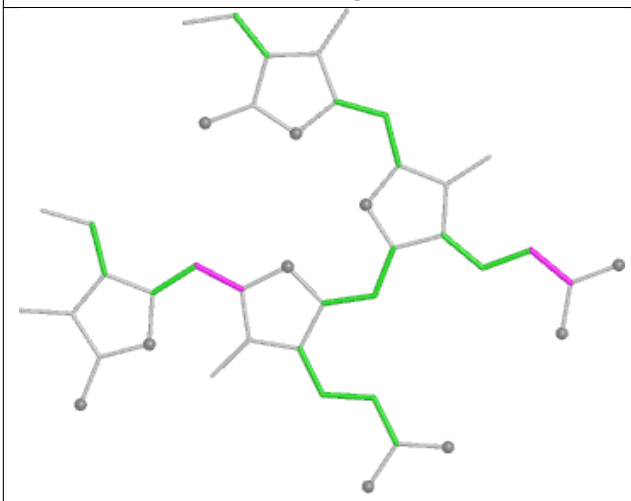
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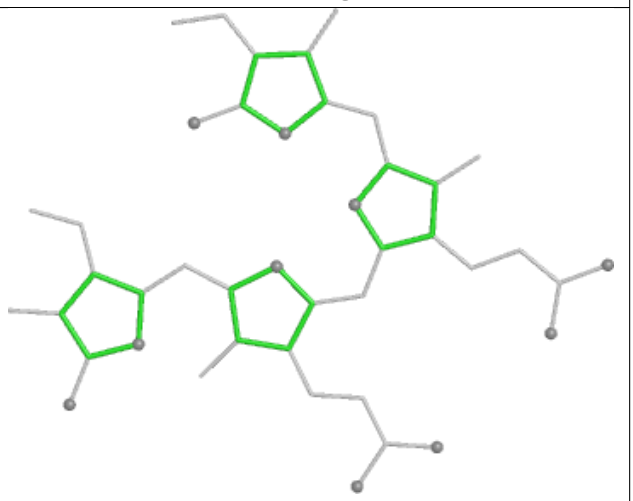
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Bond angles

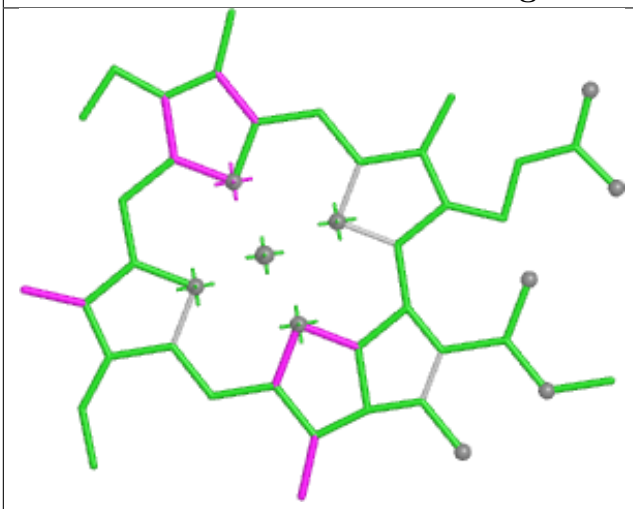


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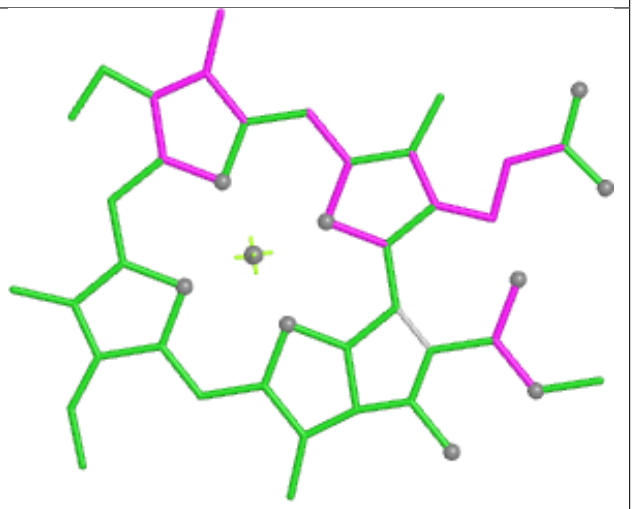


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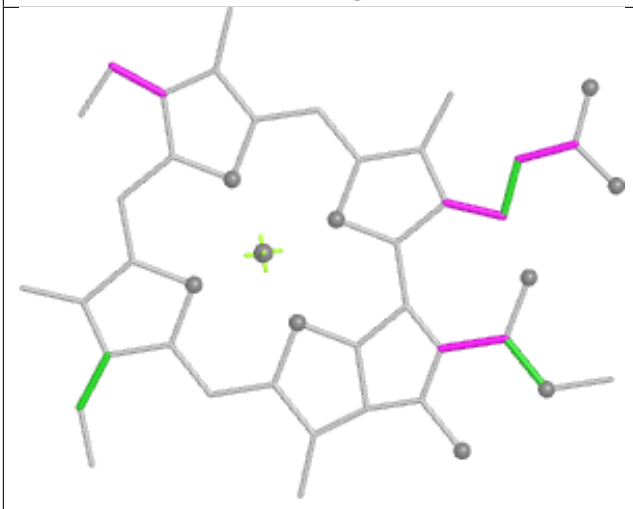
Ligand CLA 32 305



Bond lengths



Bond angles

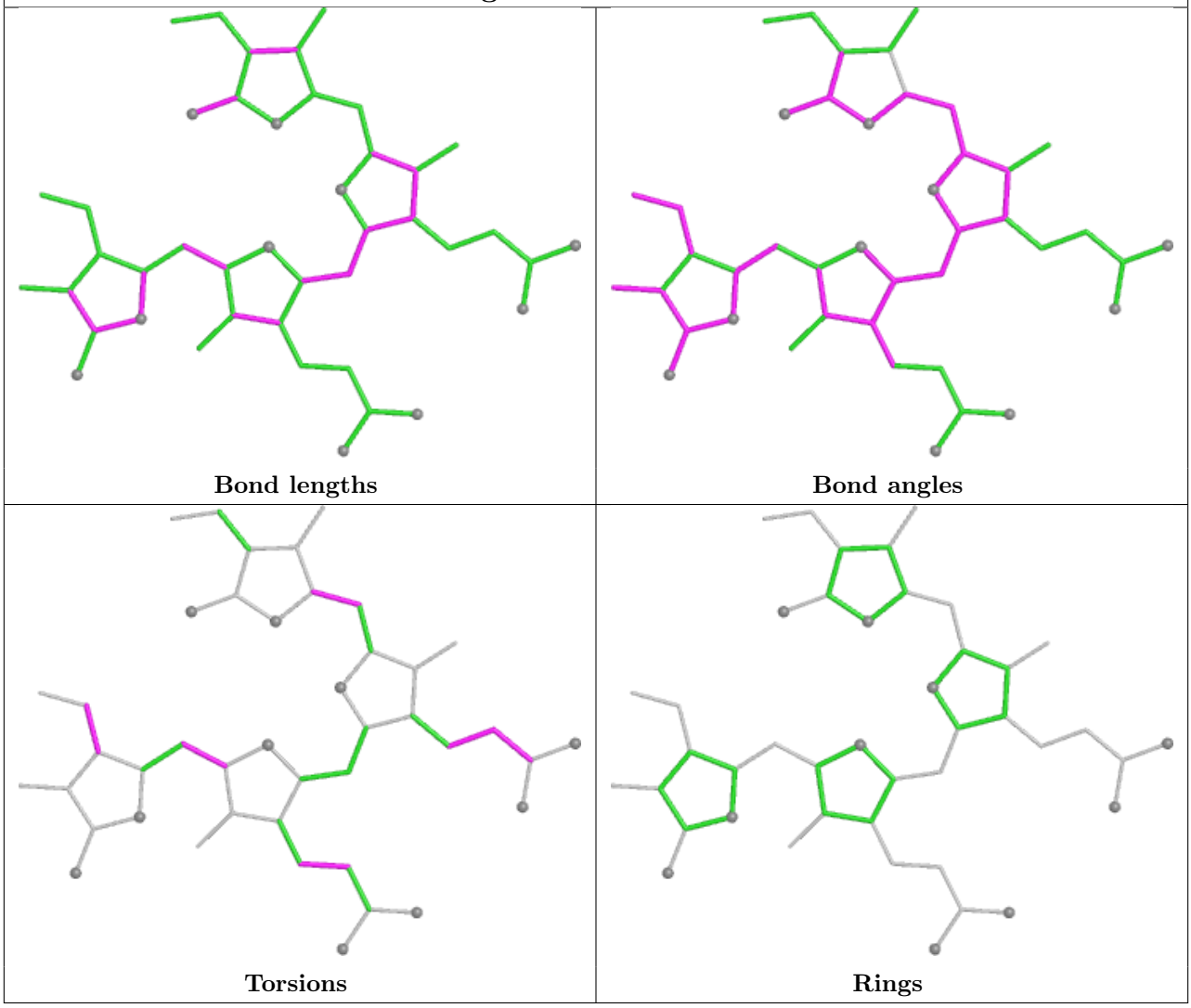


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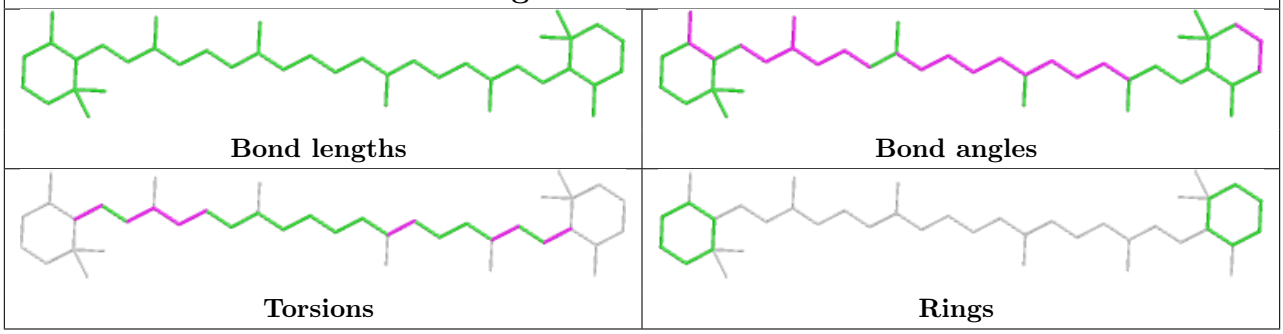


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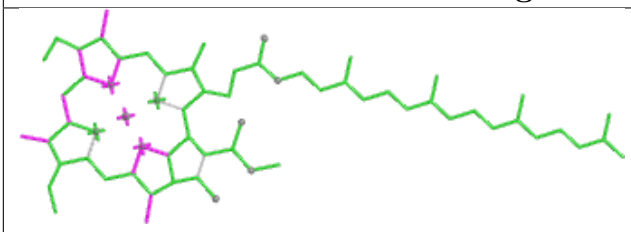
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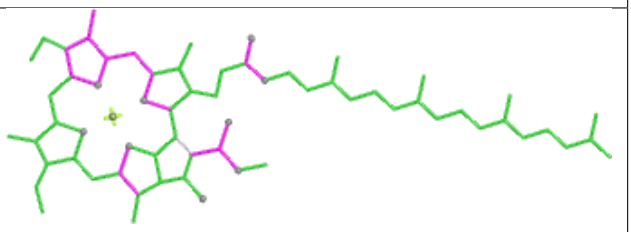
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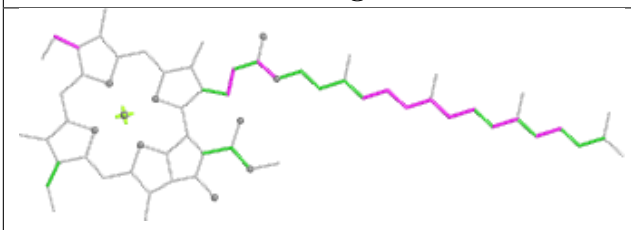
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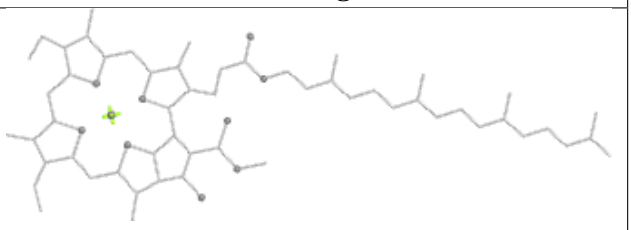
Bond lengths



Bond angles

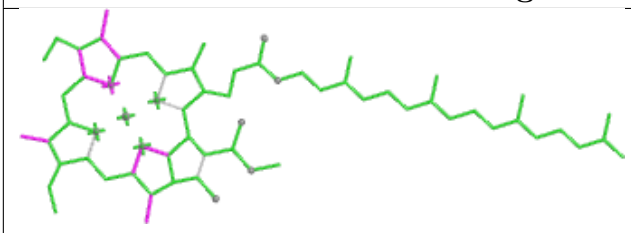


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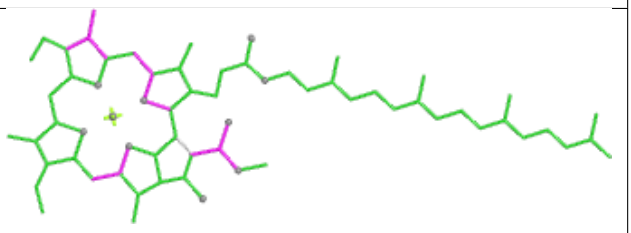


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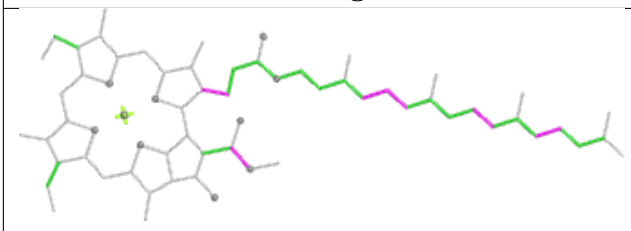
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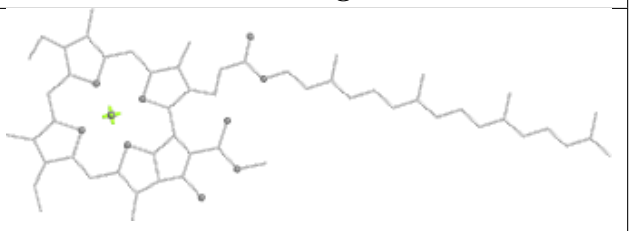
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Bond angles

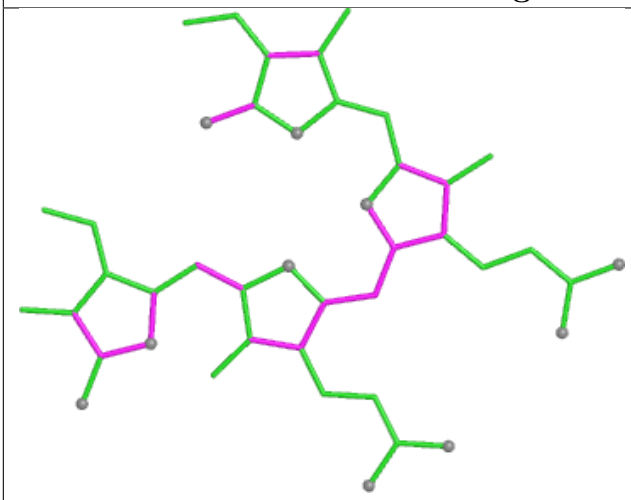


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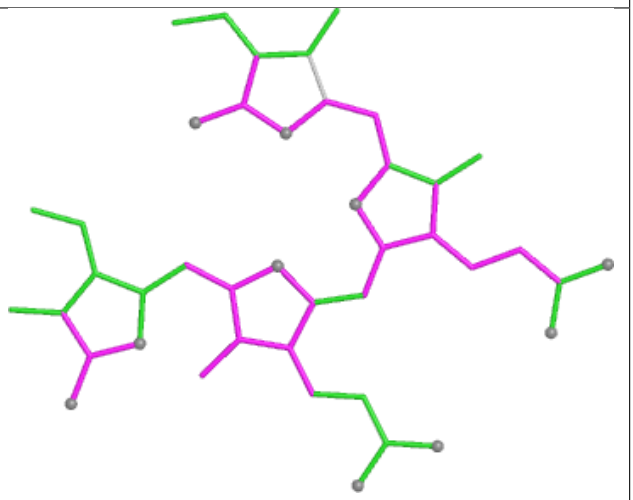


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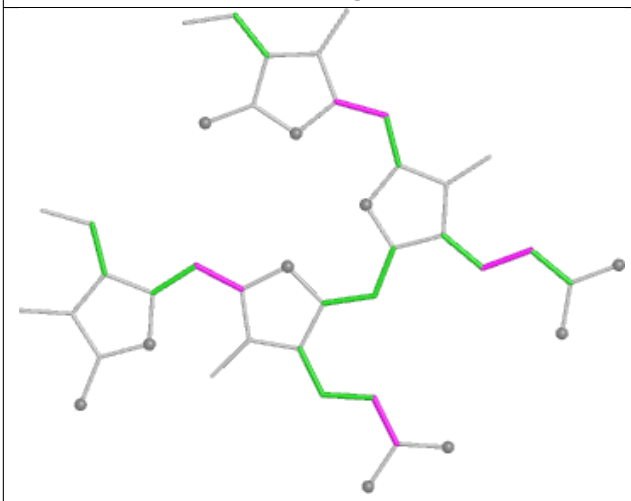
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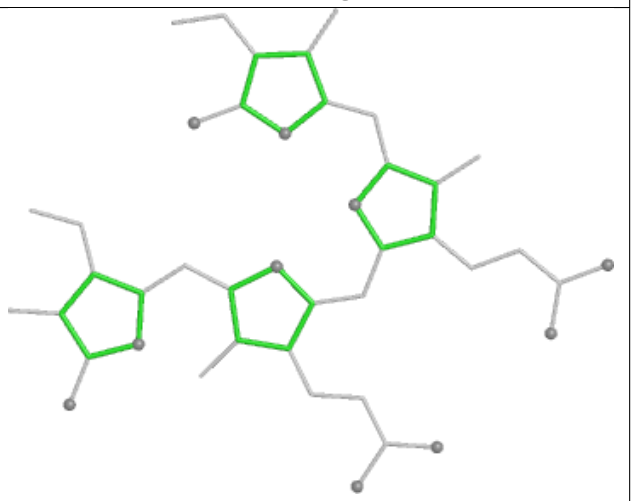
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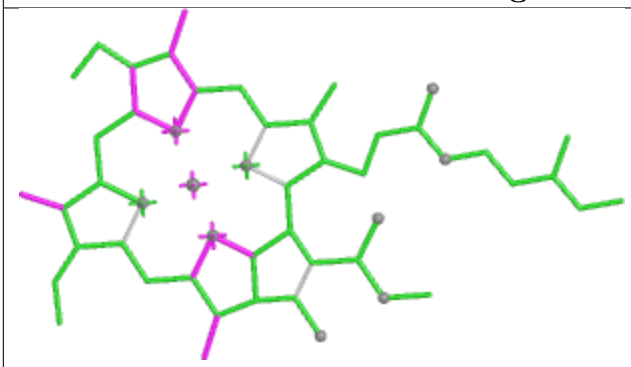


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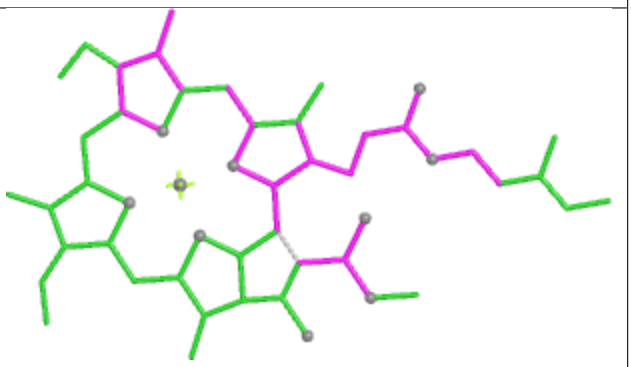


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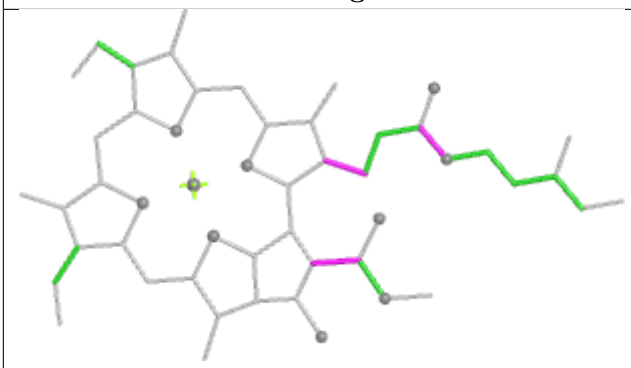
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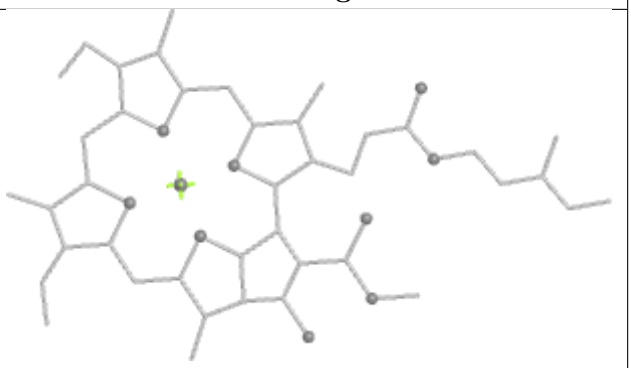
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Bond angles

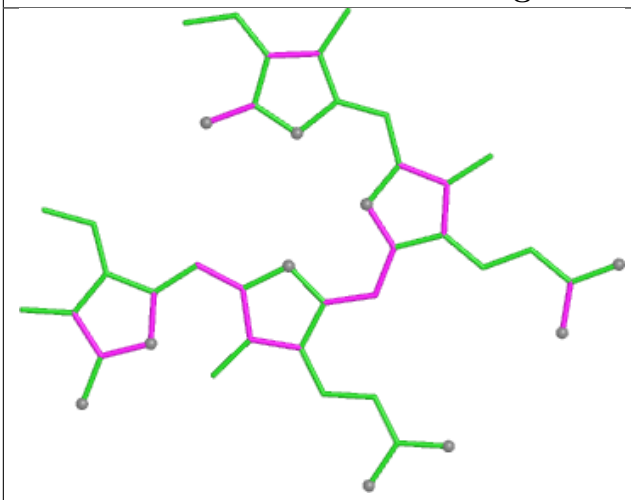


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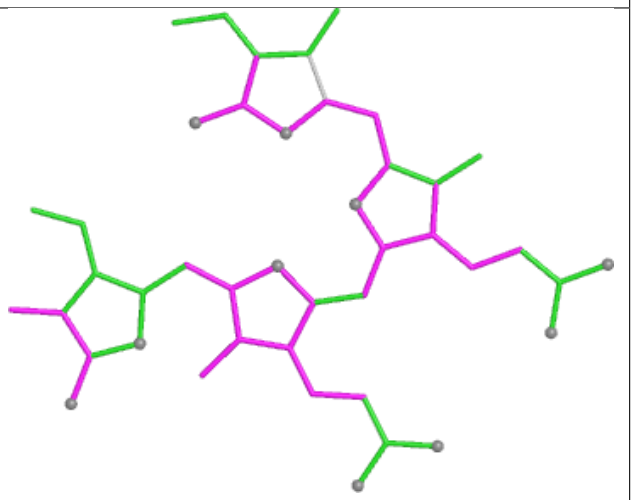


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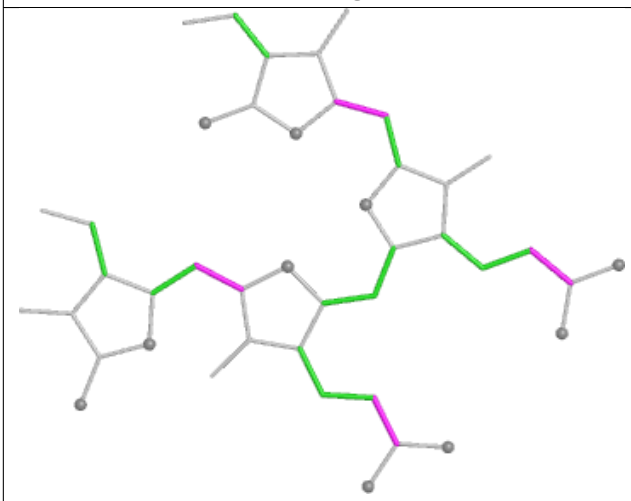
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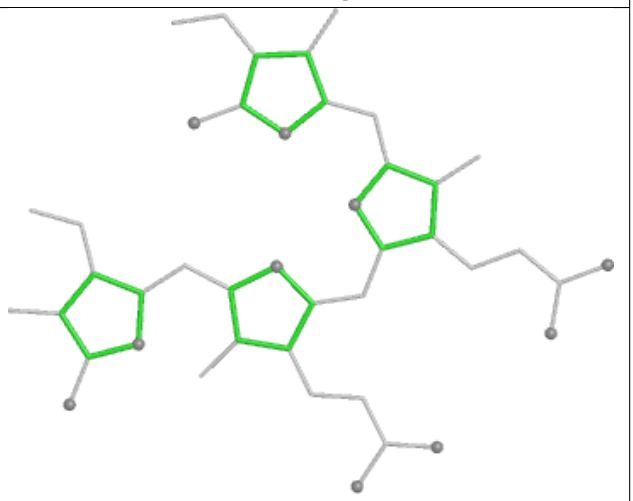
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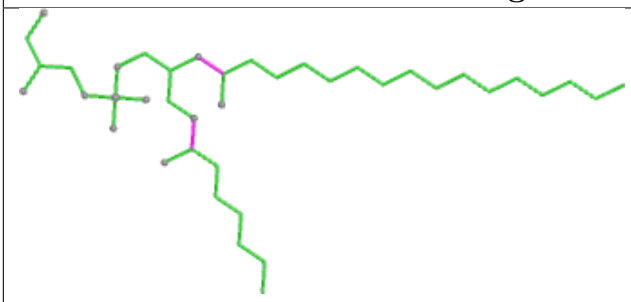


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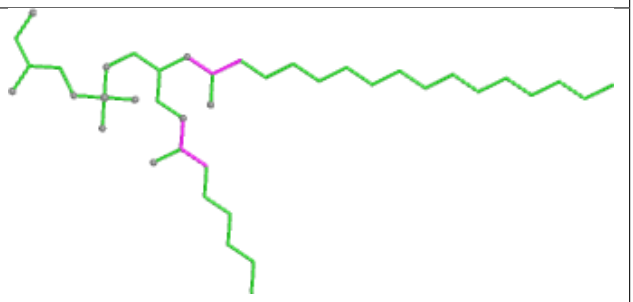


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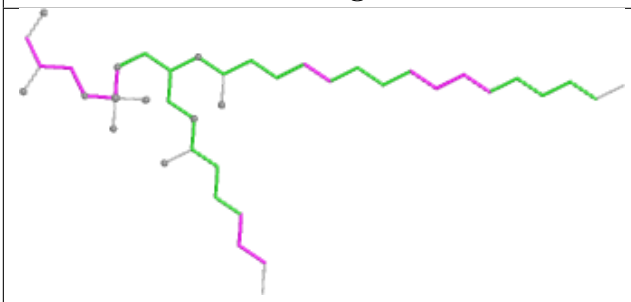
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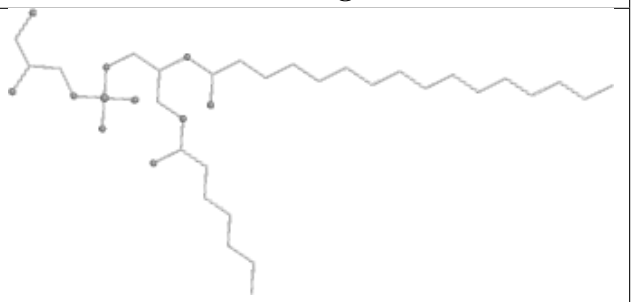
Bond lengths



Bond angles

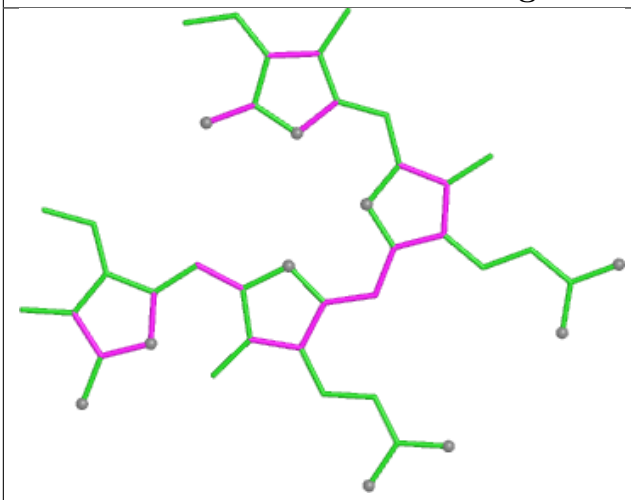


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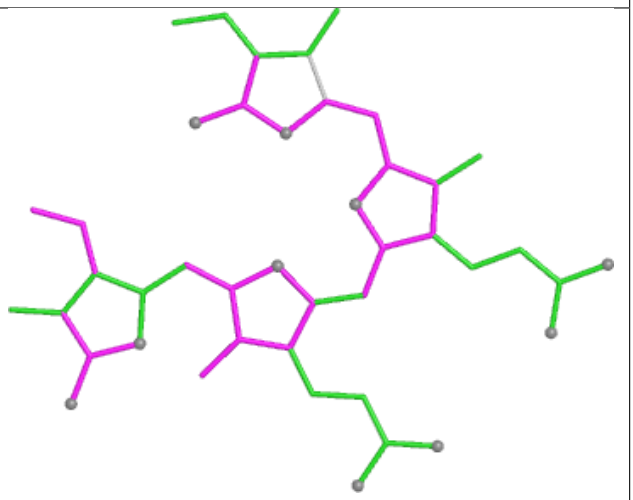


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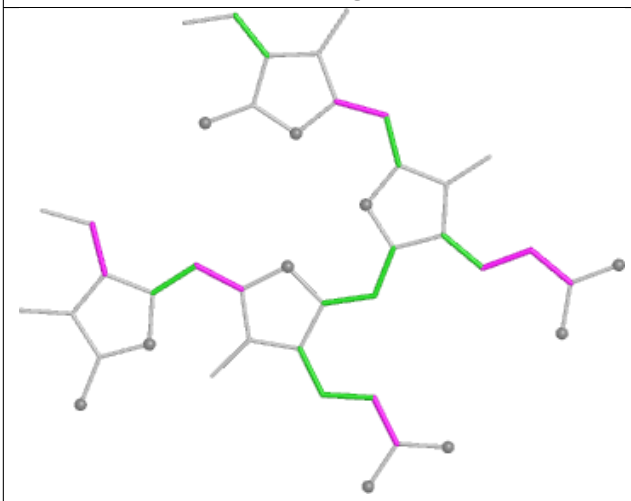
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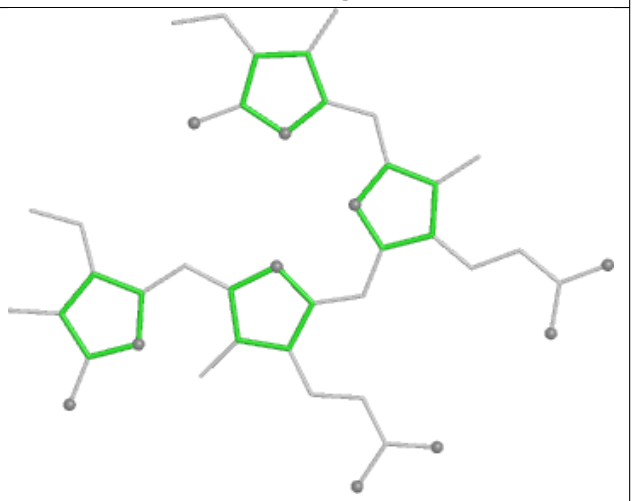
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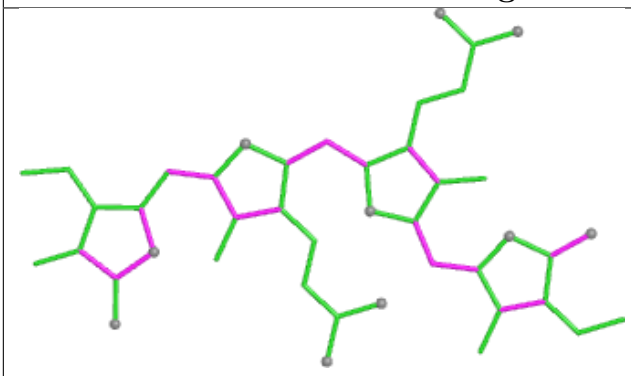


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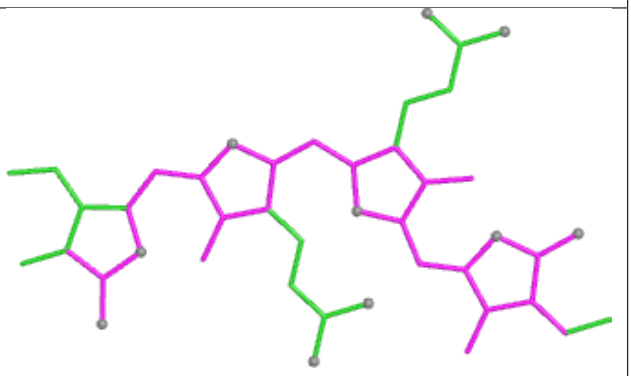


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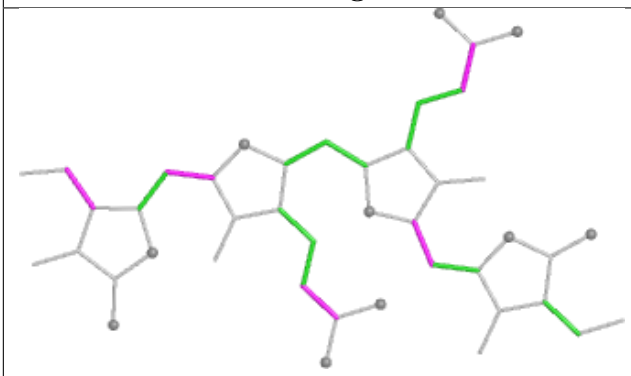
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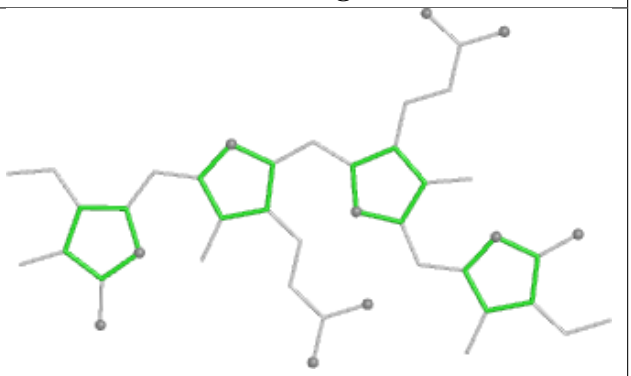
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Bond angles

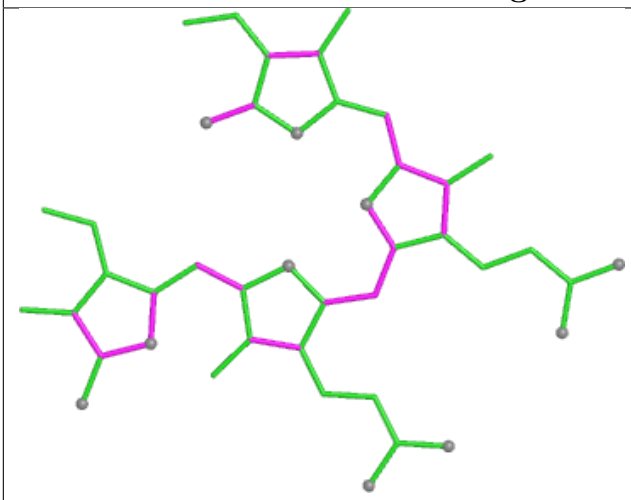


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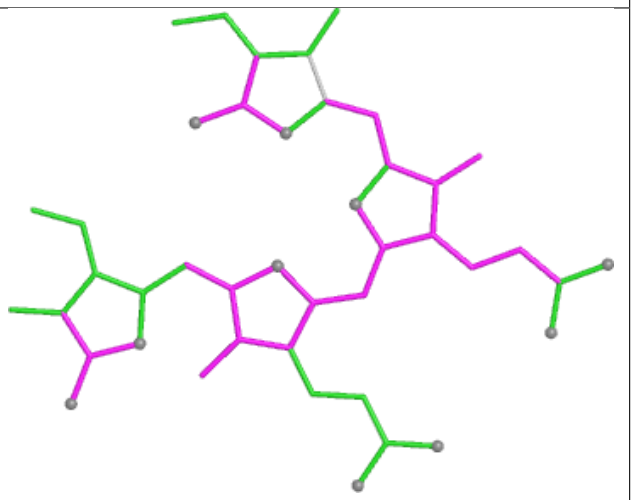


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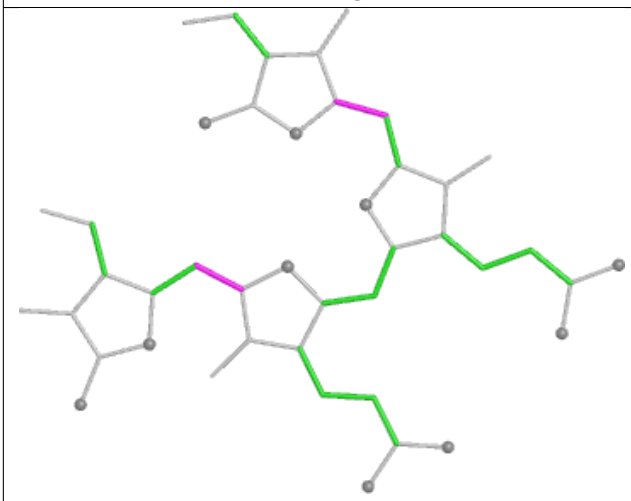
Ligand PEB LM 201



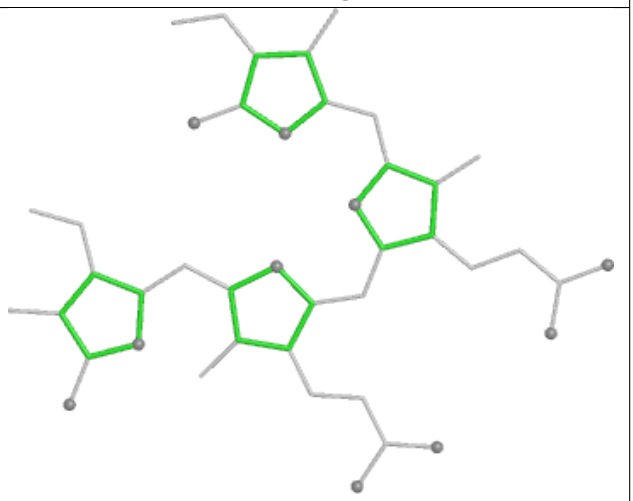
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Bond angles

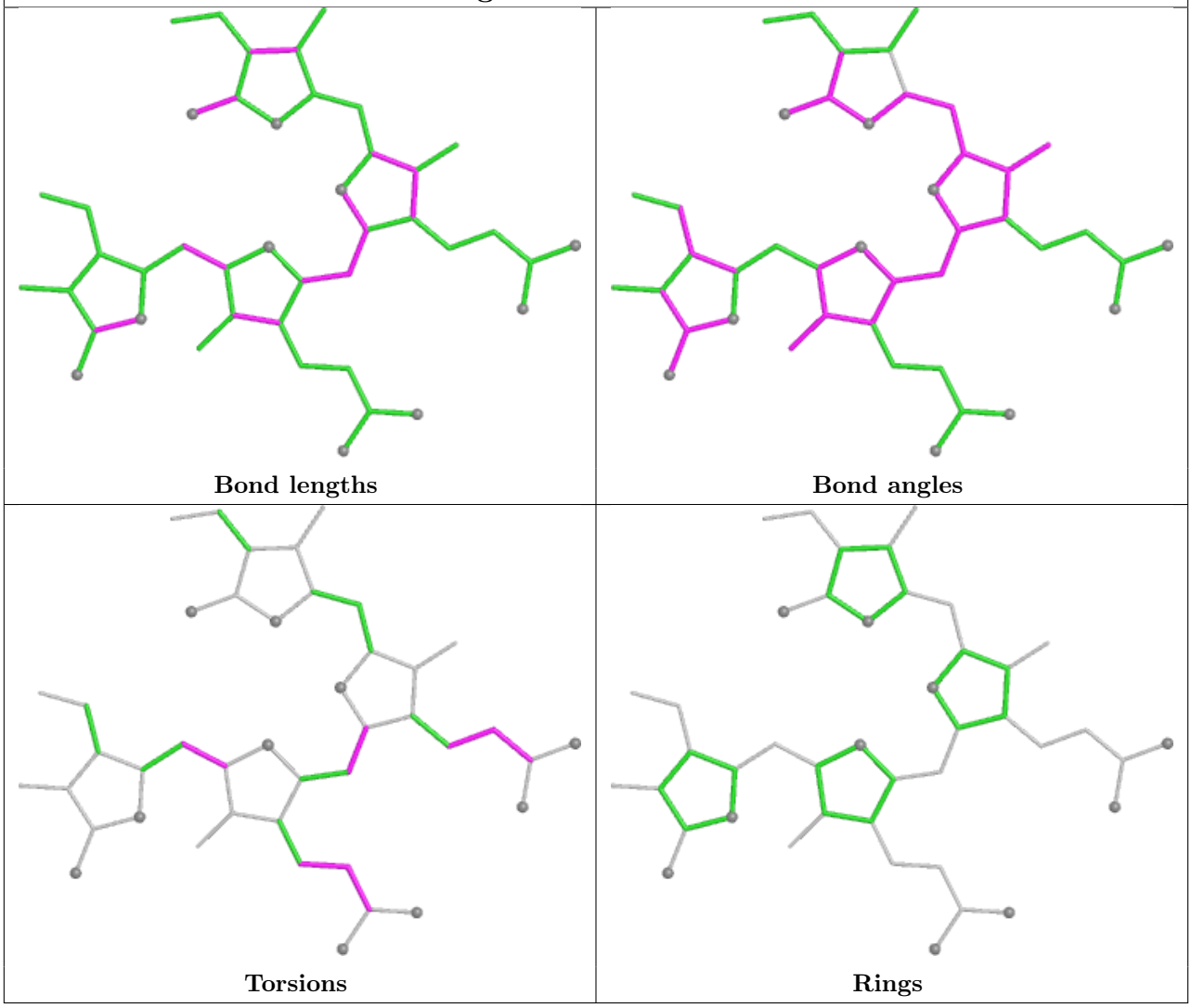


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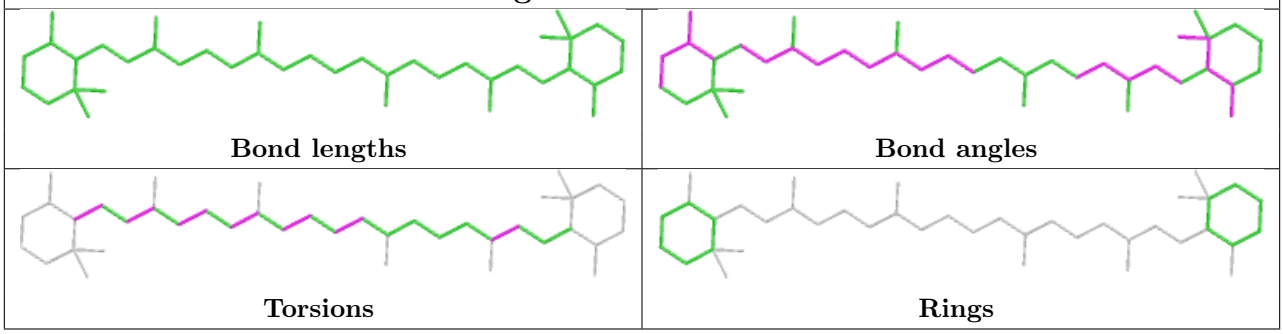


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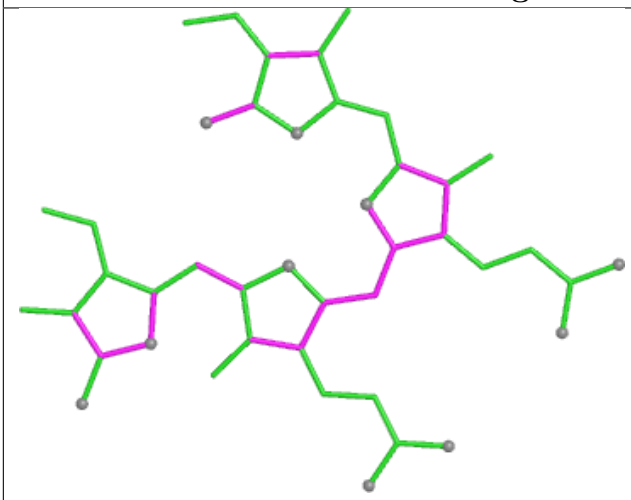
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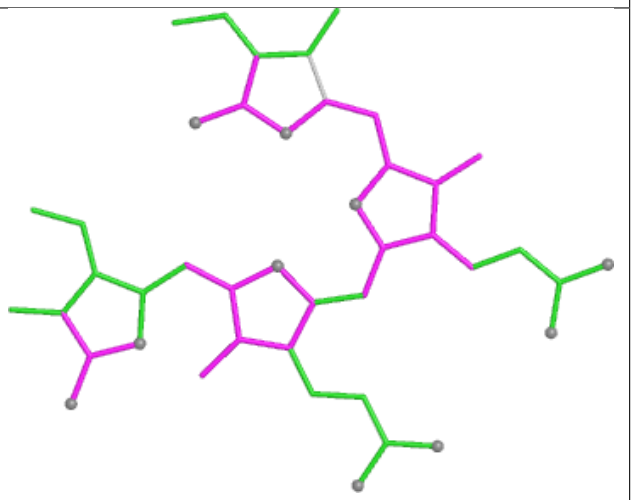
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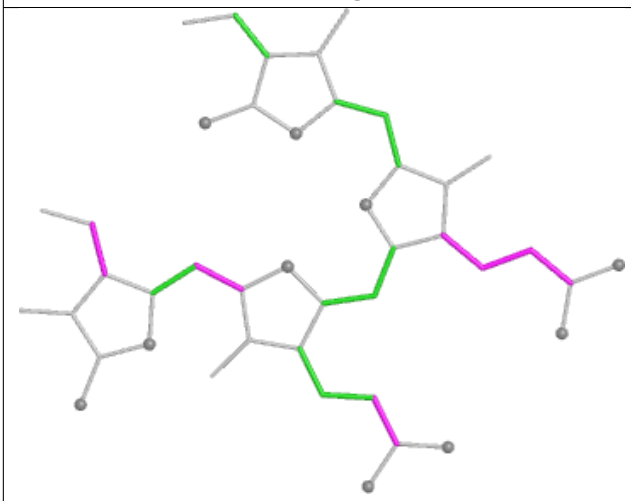
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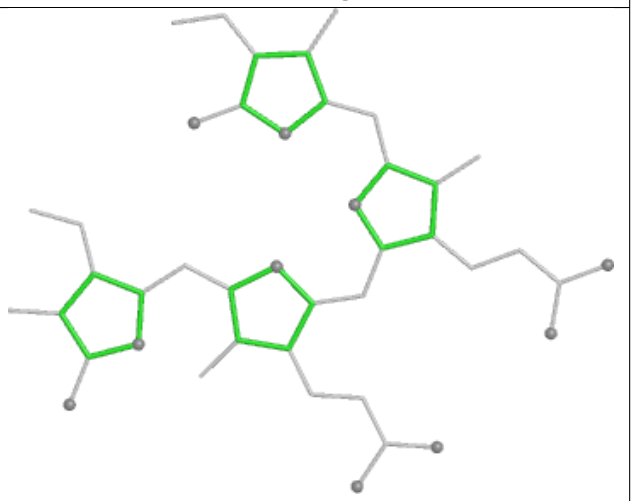
Bond lengths



Bond angles

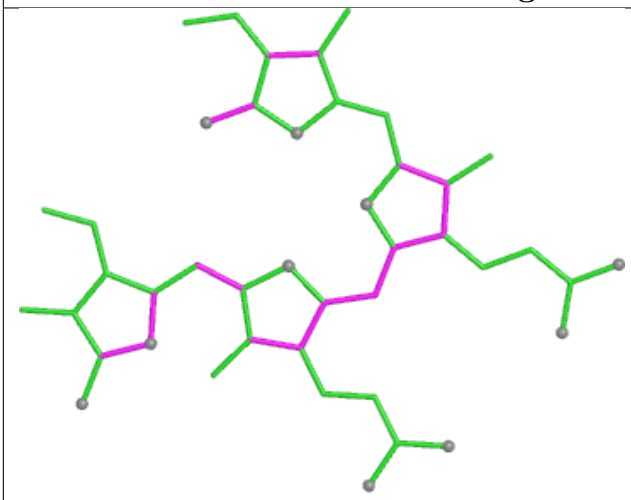


Torsions

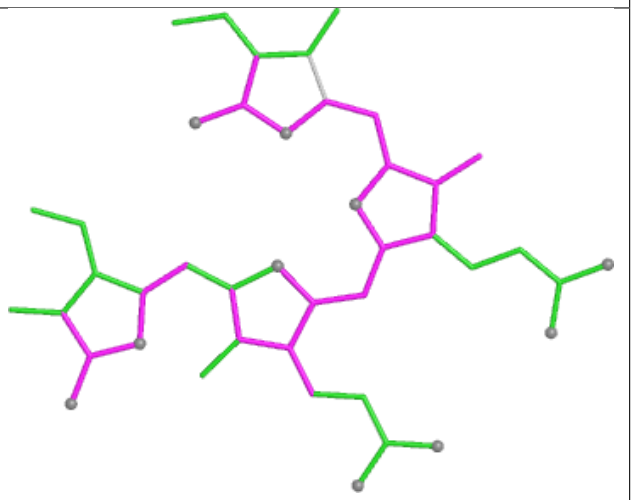


Rings

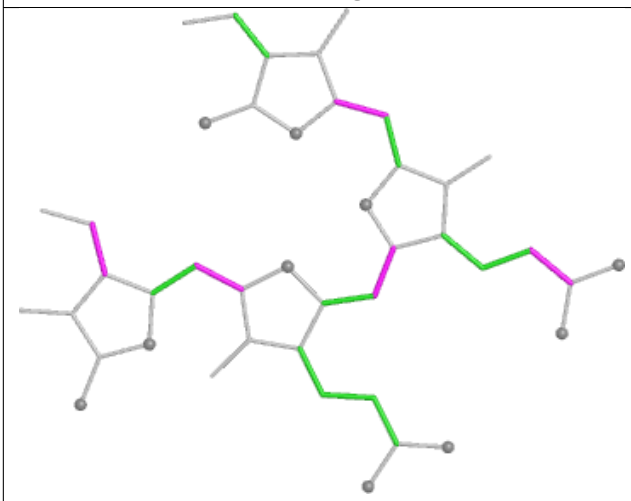
Ligand PEB L5 202



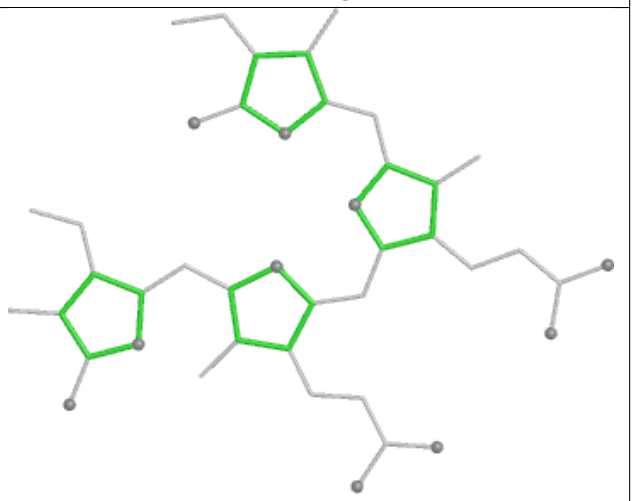
Bond lengths



Bond angles

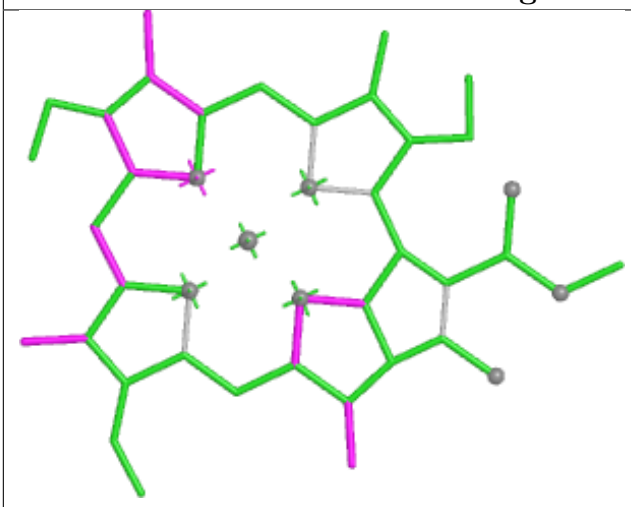


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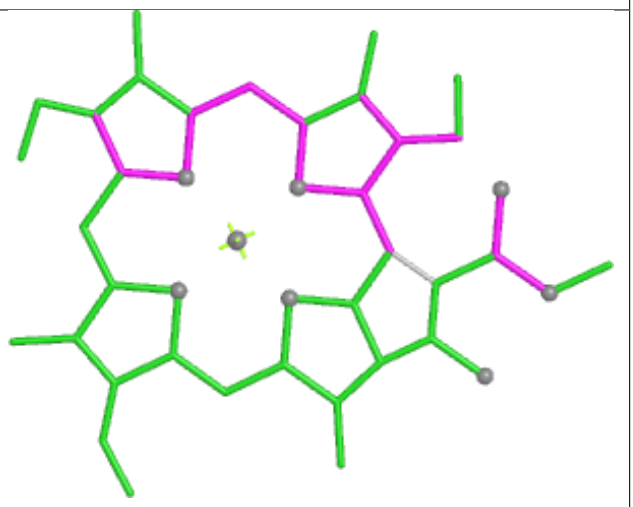


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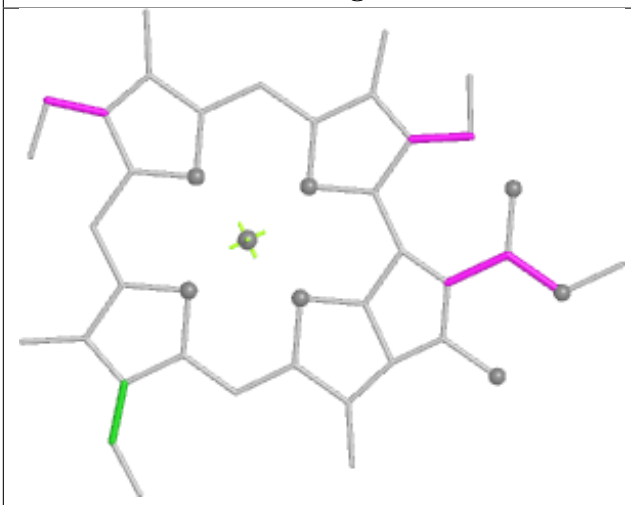
Ligand CLA 32 311



Bond lengths



Bond angles

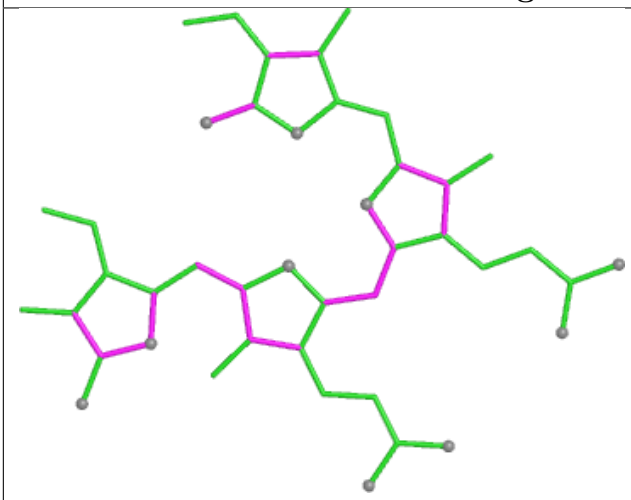


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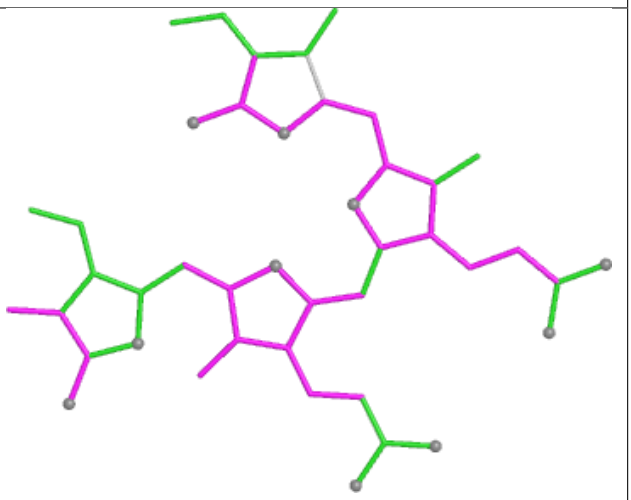


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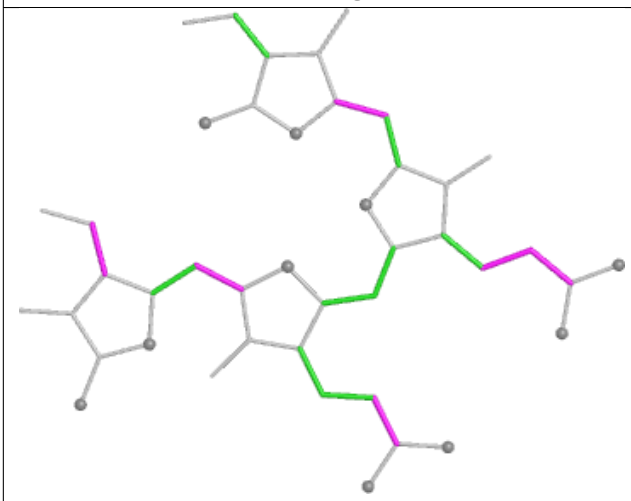
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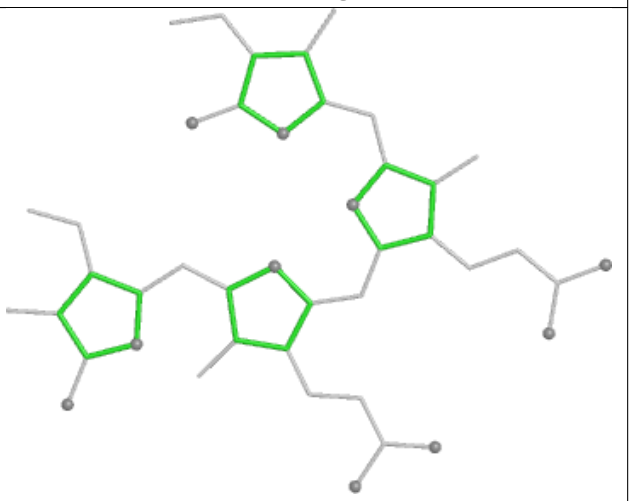
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Bond angles

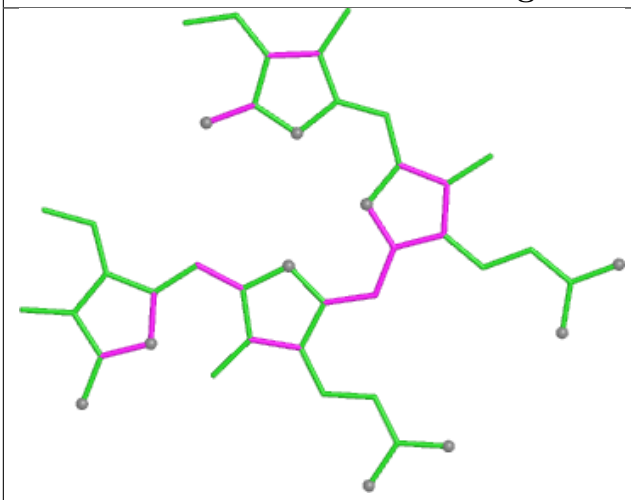


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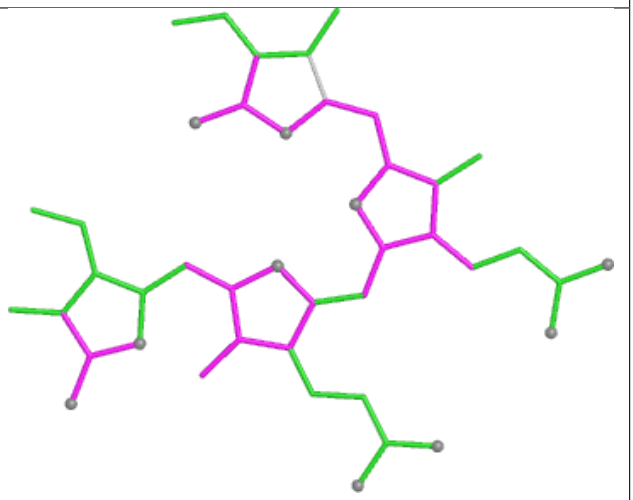


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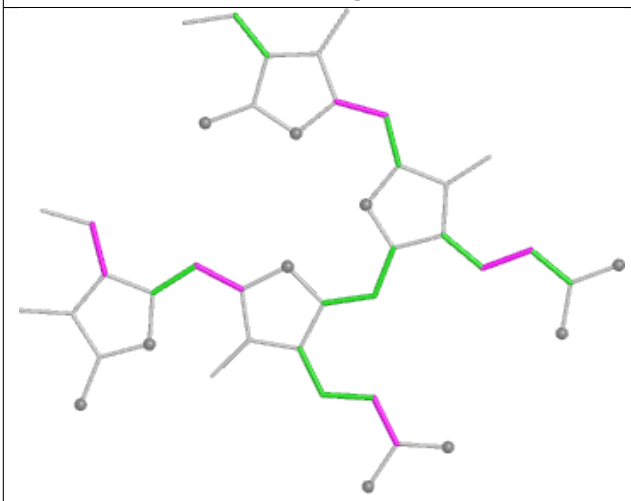
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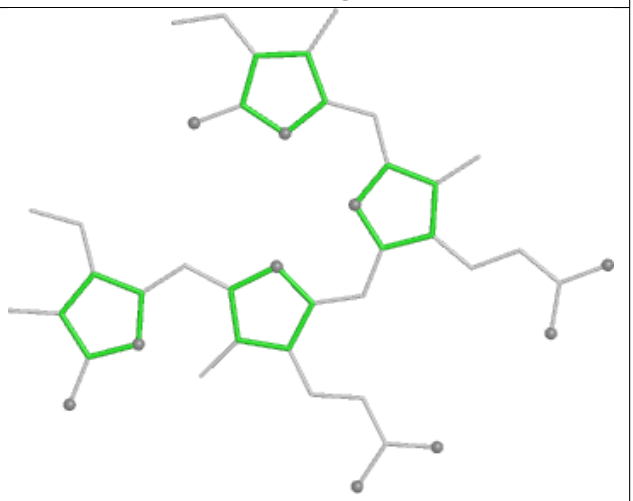
Bond lengths



Bond angles

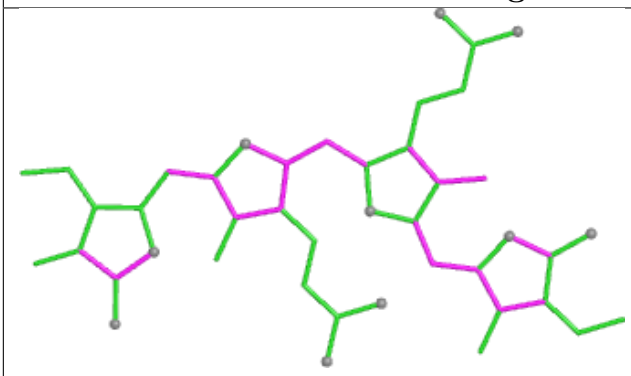


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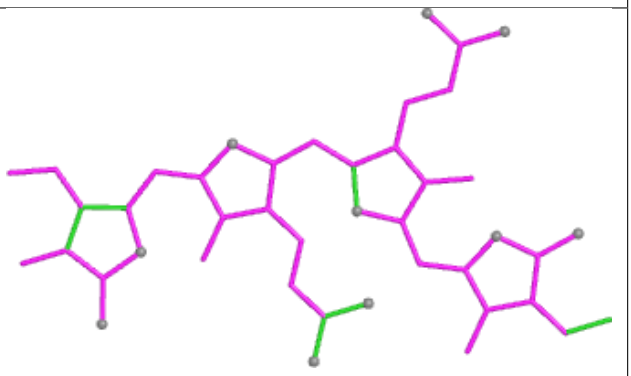


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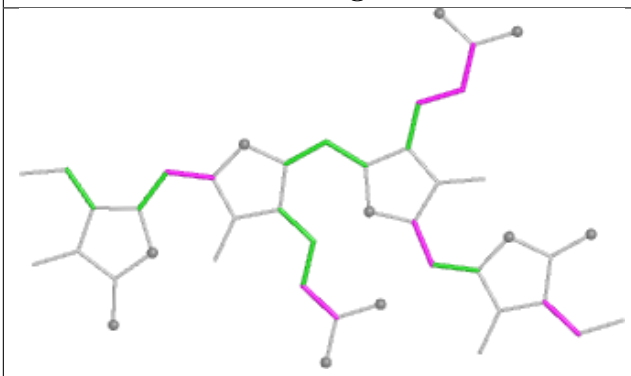
Ligand CYC x3 1001



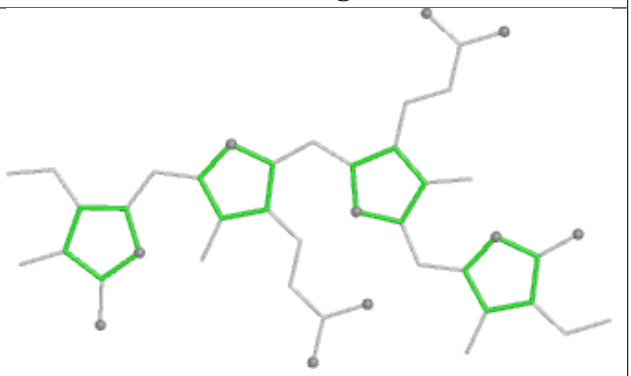
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Bond angles

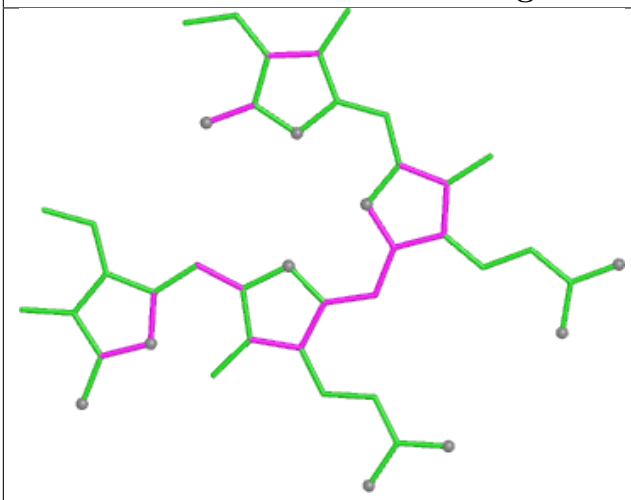


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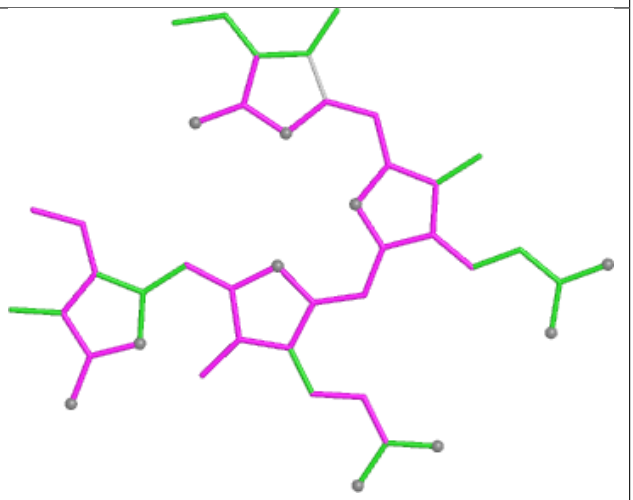


Rings

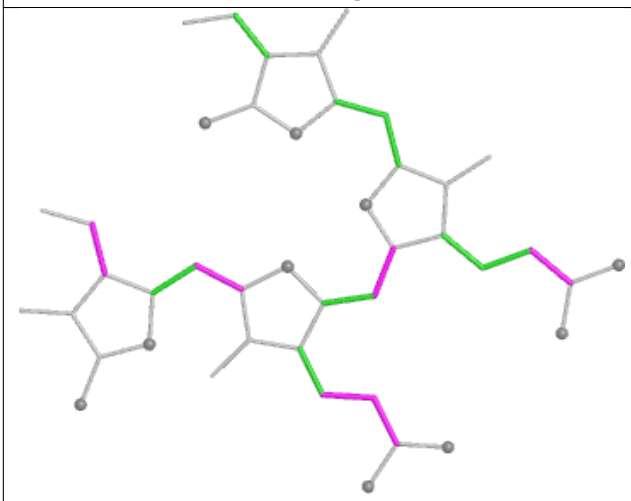
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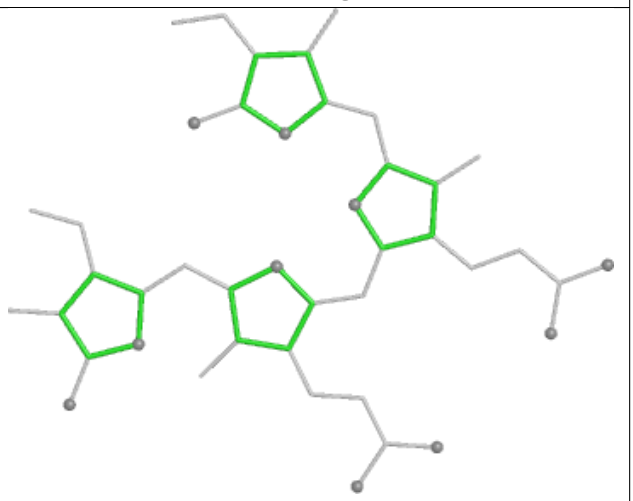
Bond lengths



Bond angles

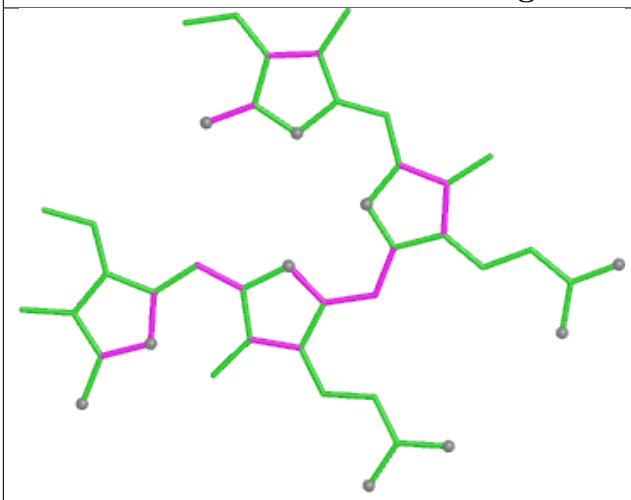


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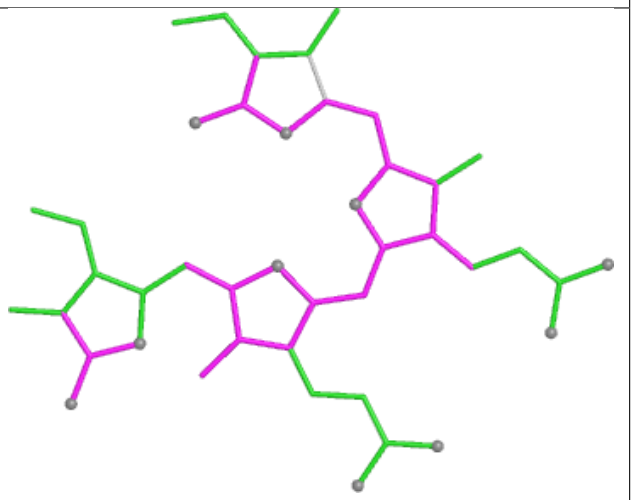


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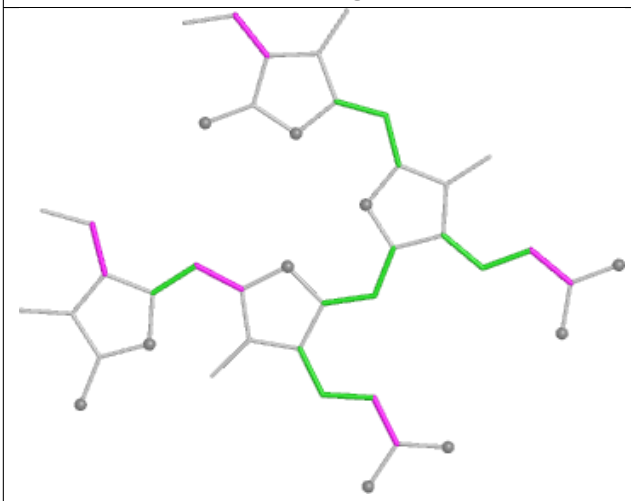
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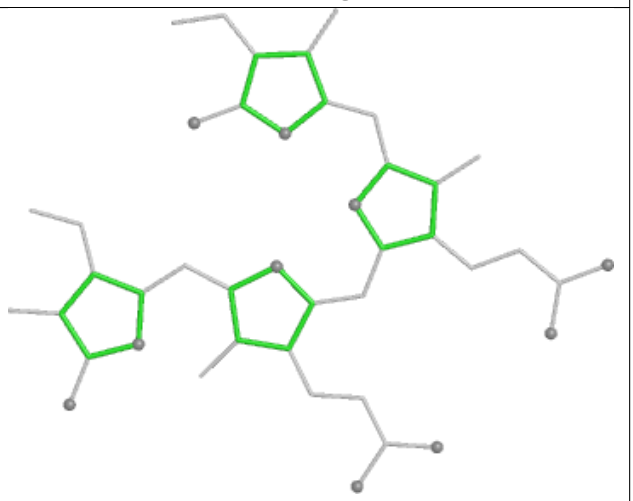
Bond lengths



Bond angles

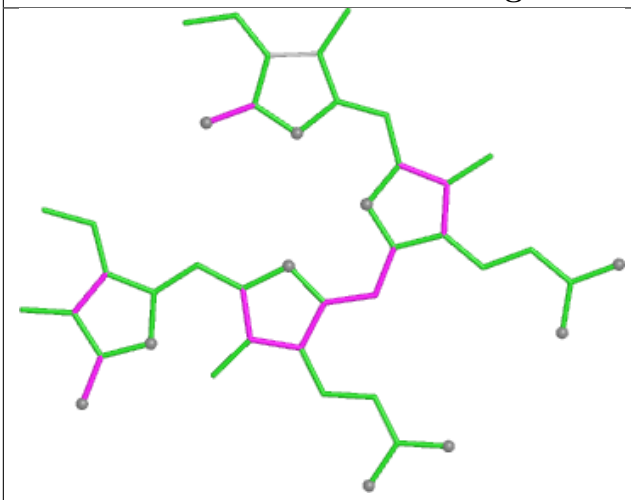


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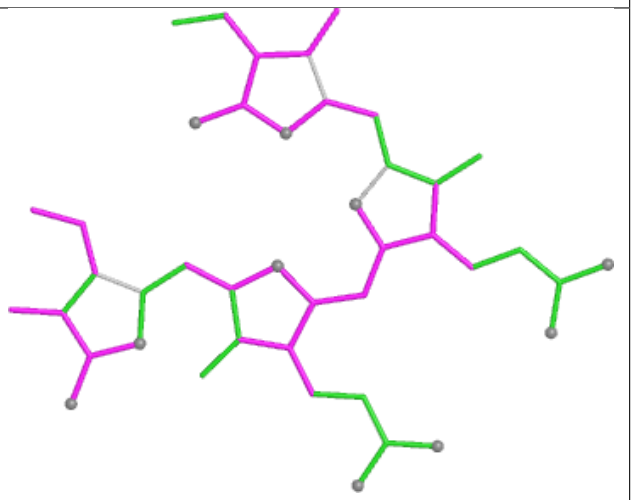


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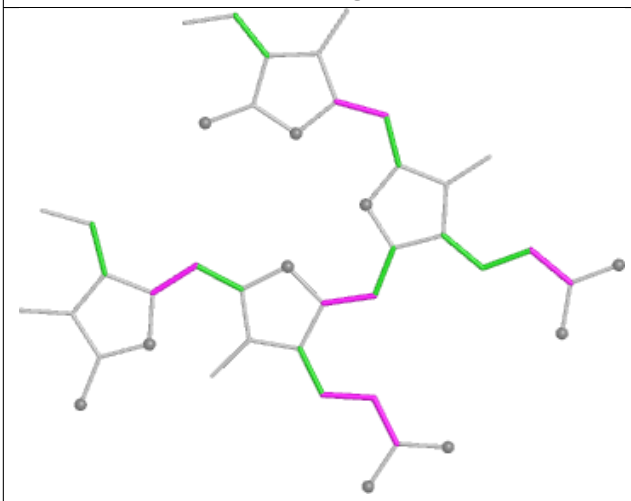
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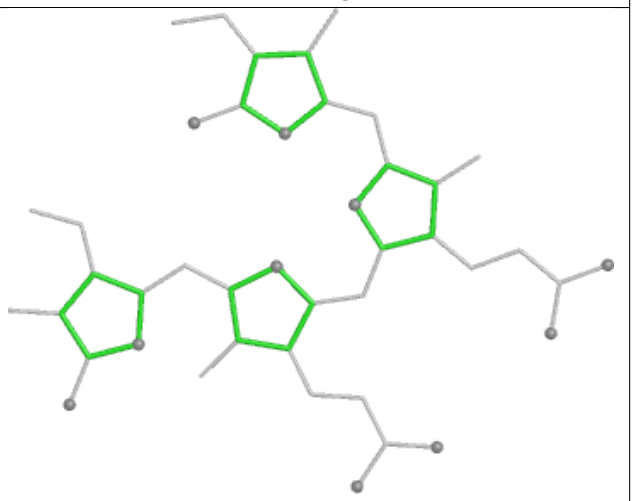
Bond lengths



Bond angles

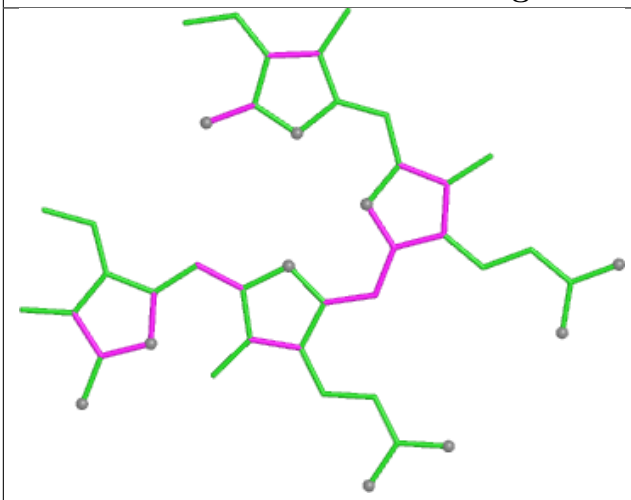


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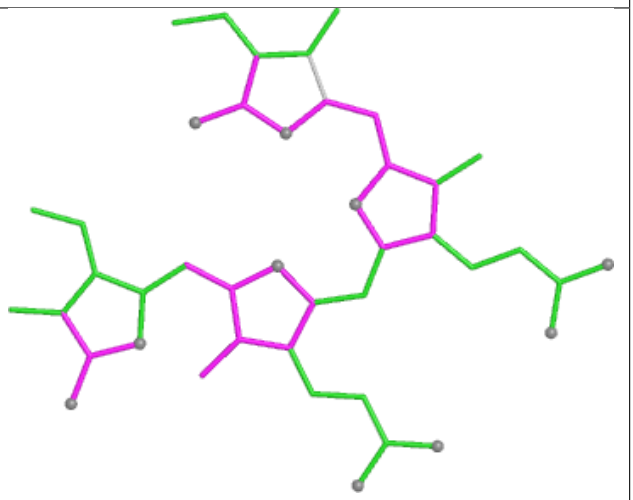


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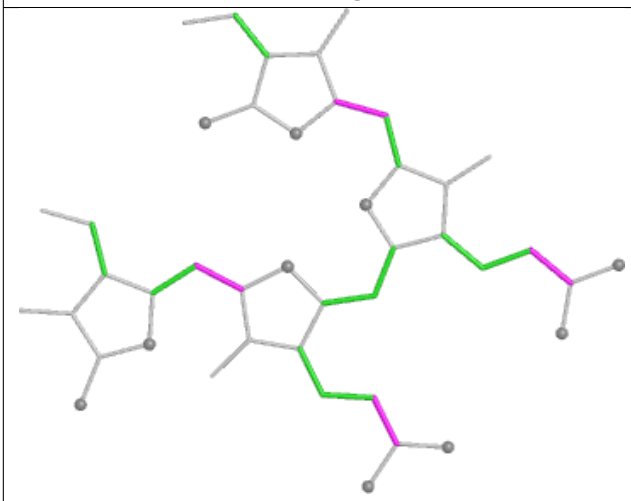
Ligand PEB YP 503



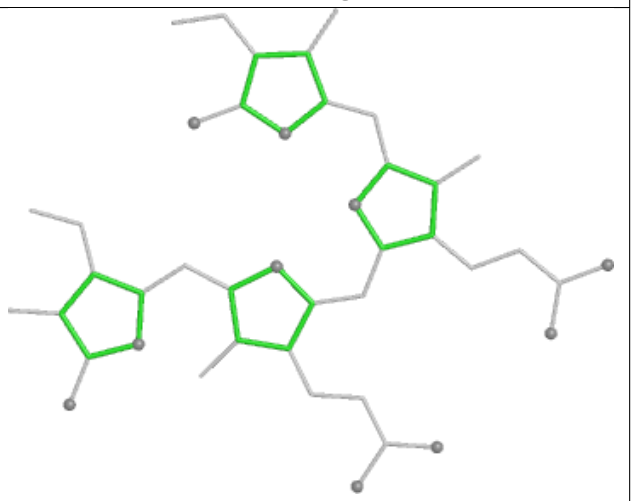
Bond lengths



Bond angles

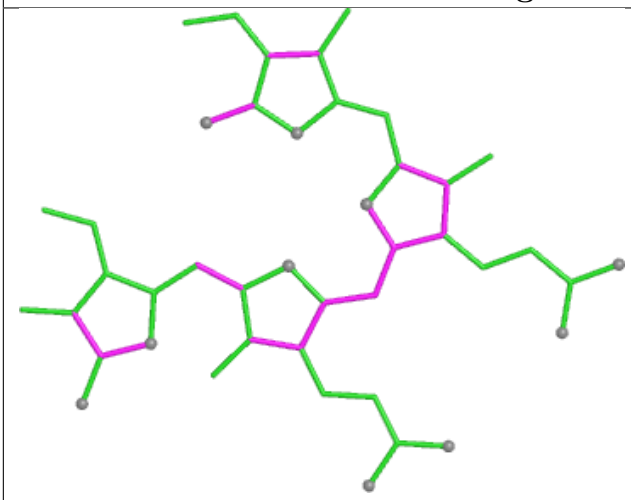


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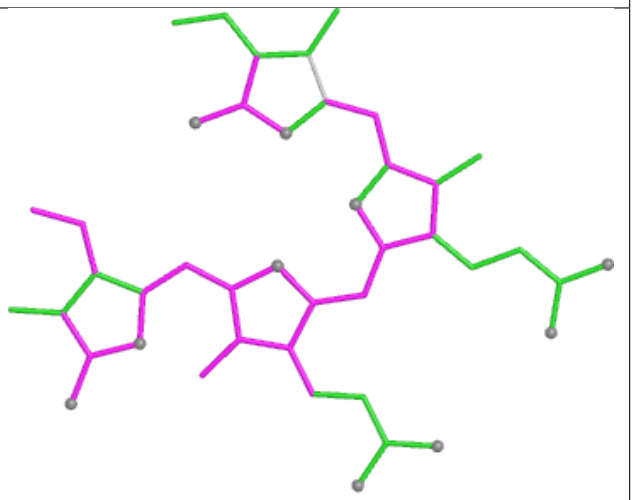


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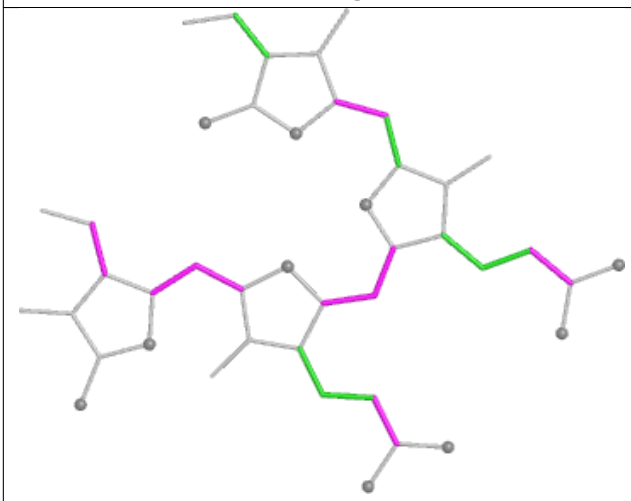
Ligand PEB T9 202



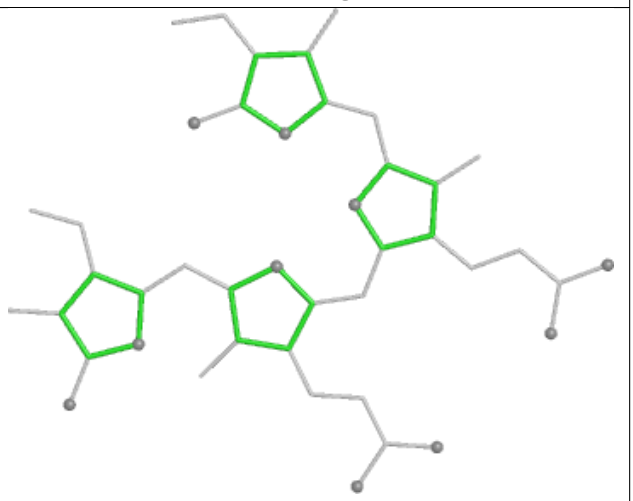
Bond lengths



Bond angles

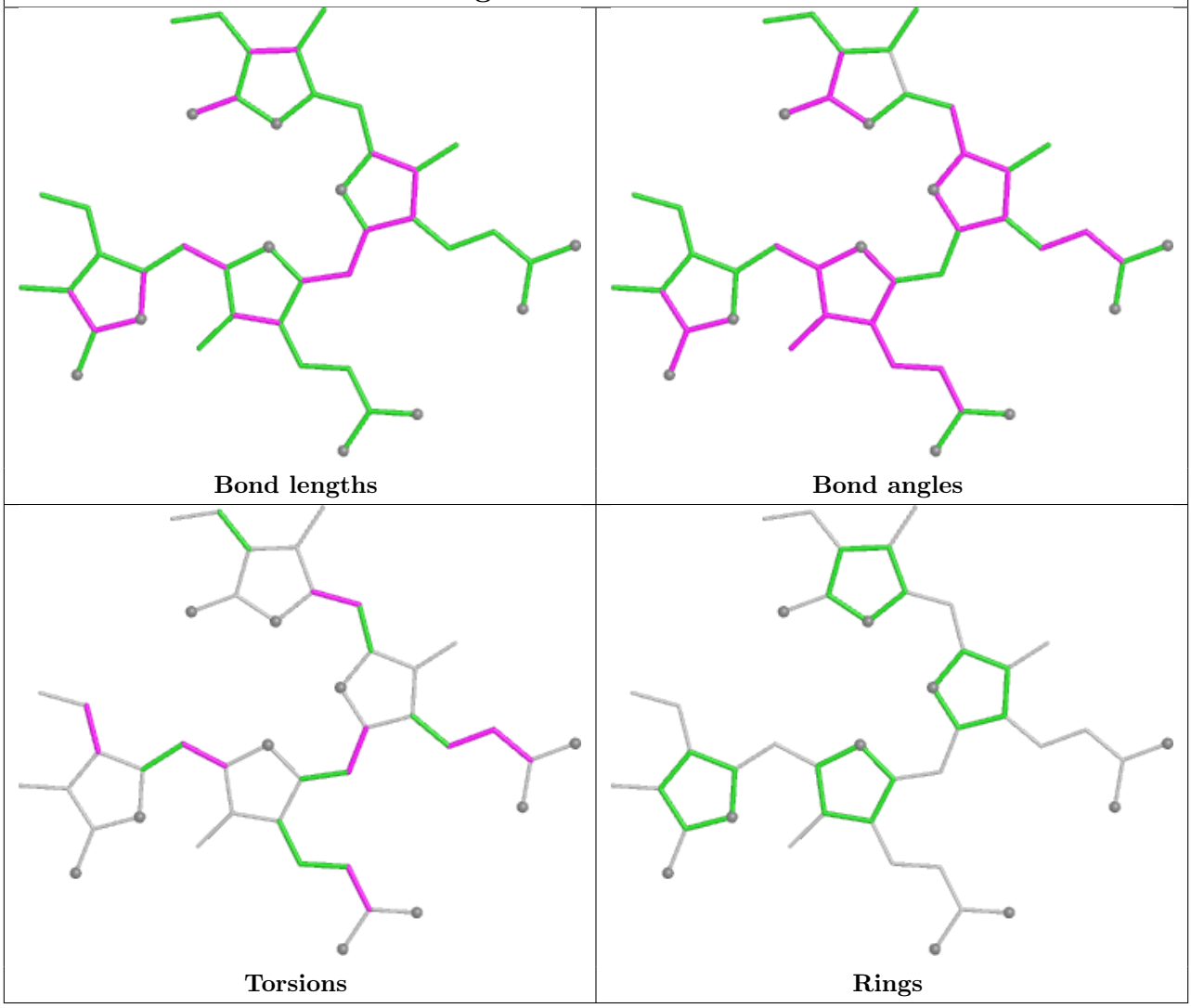


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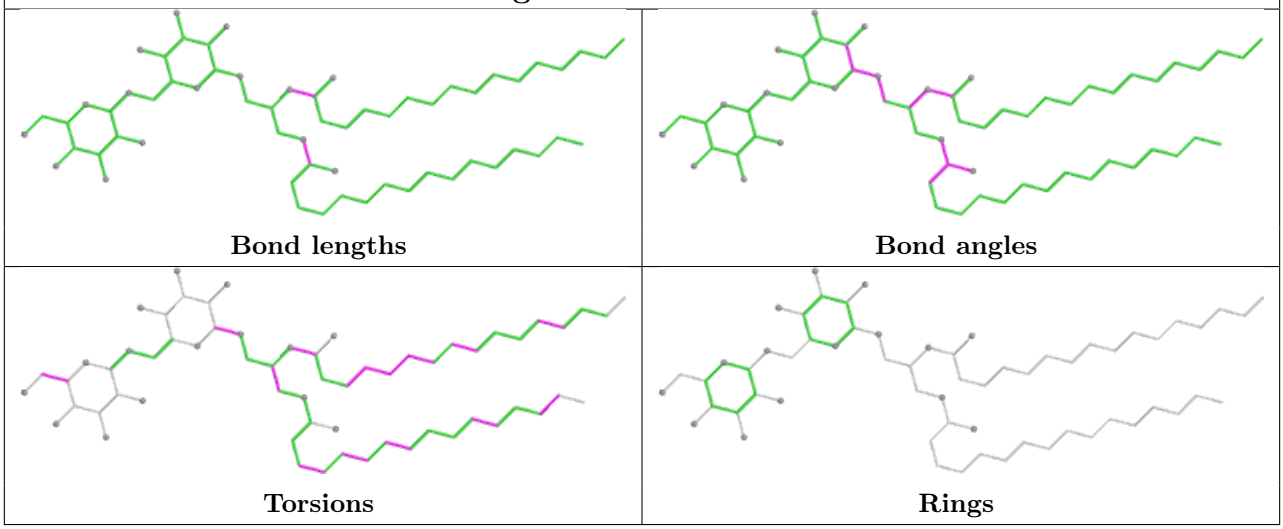


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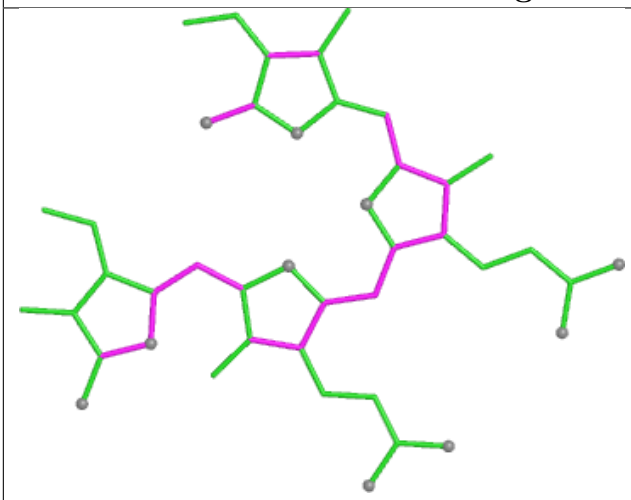
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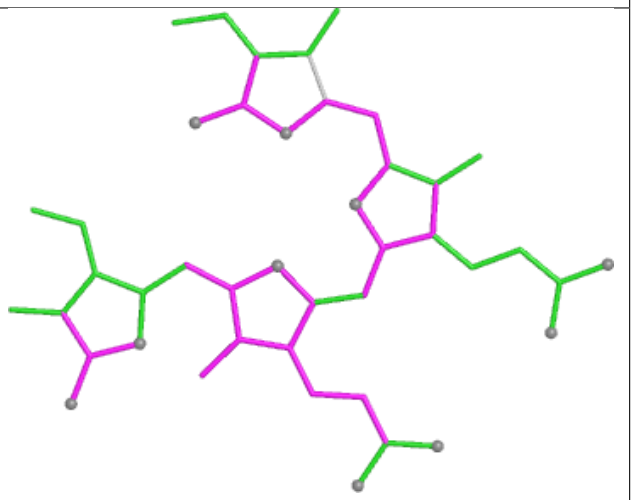
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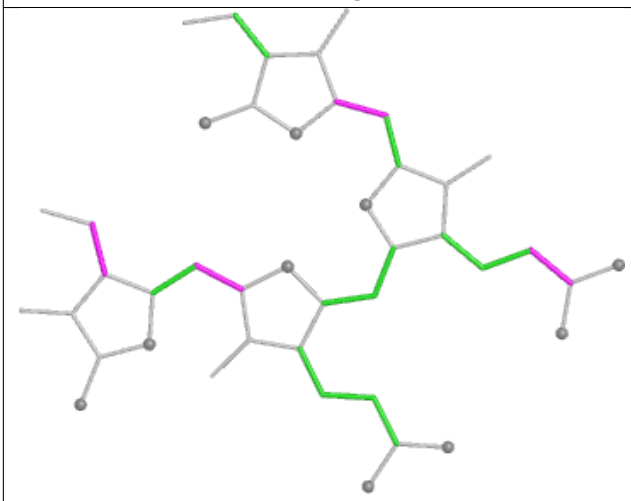
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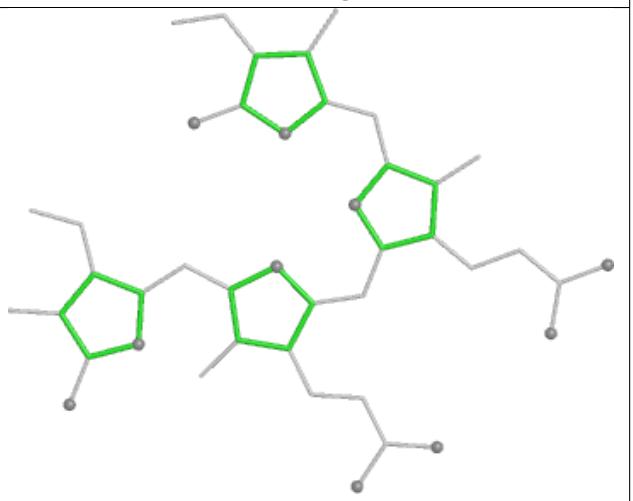
Bond lengths



Bond angles

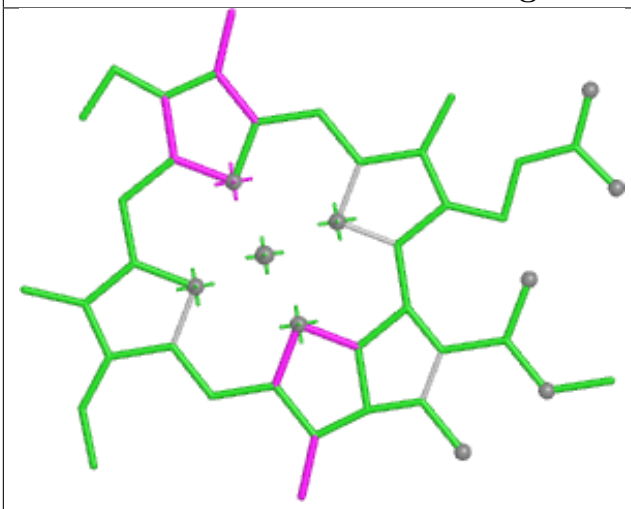


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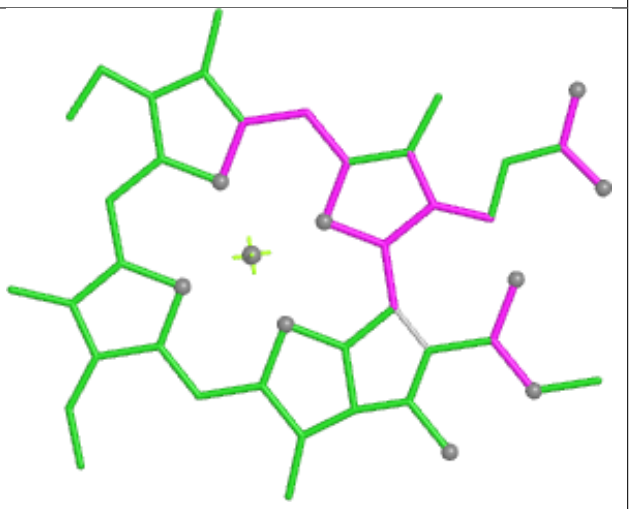


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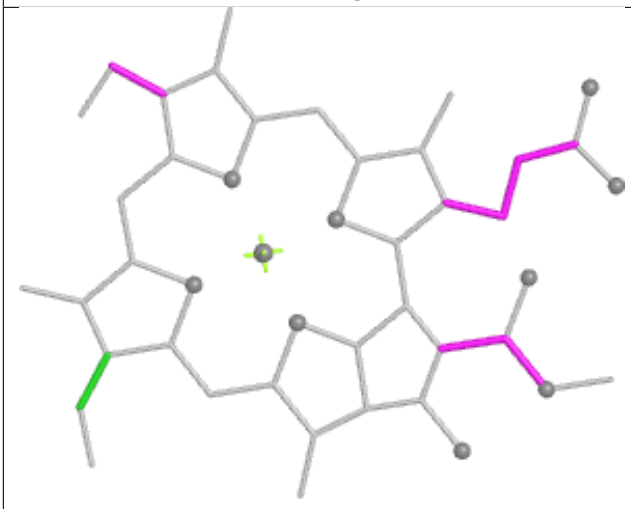
Ligand CLA 52 611



Bond lengths



Bond angles

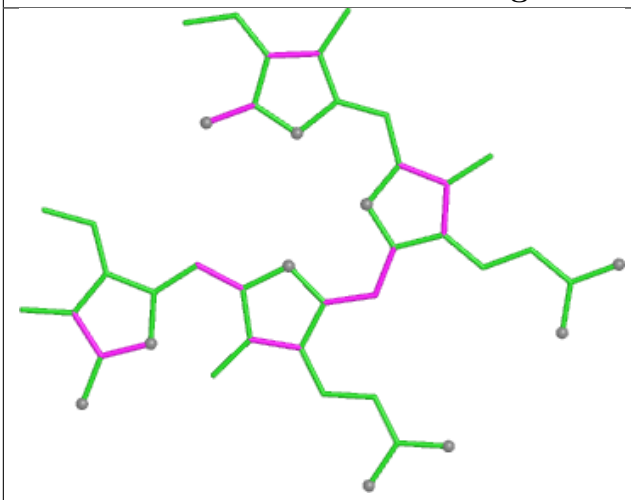


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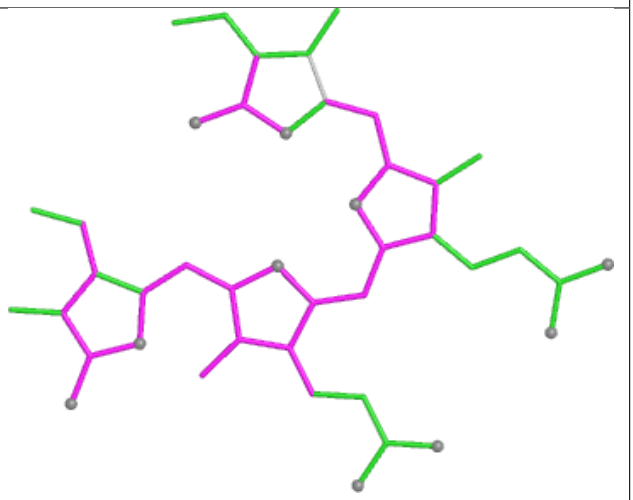


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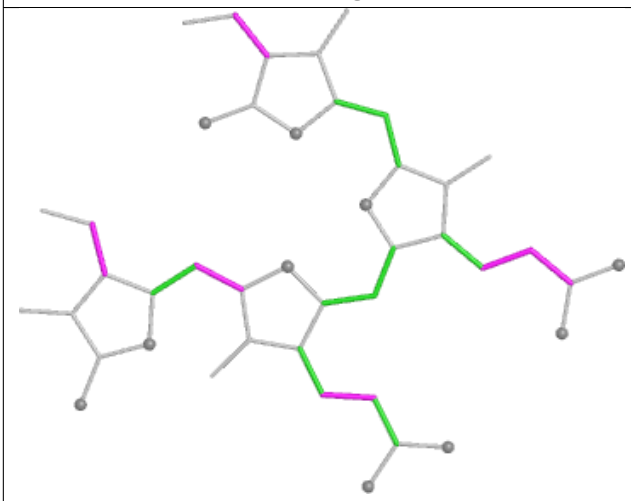
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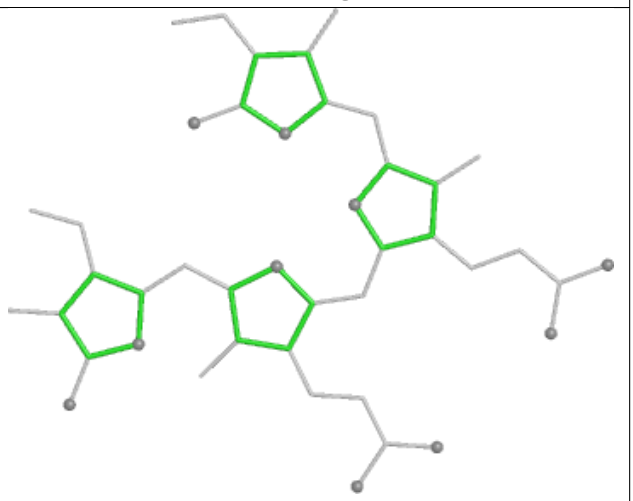
Bond lengths



Bond angles

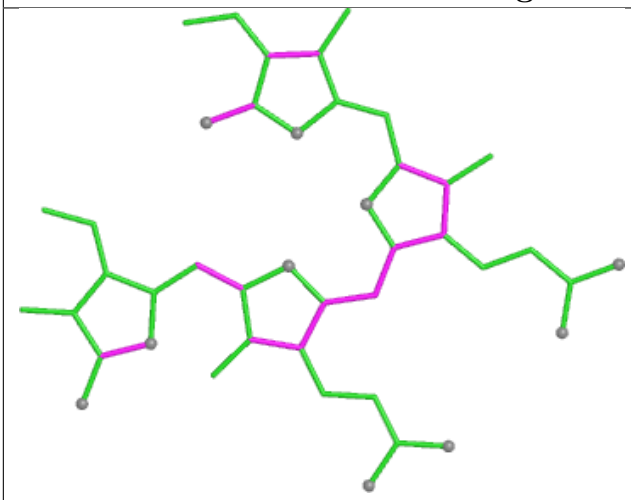


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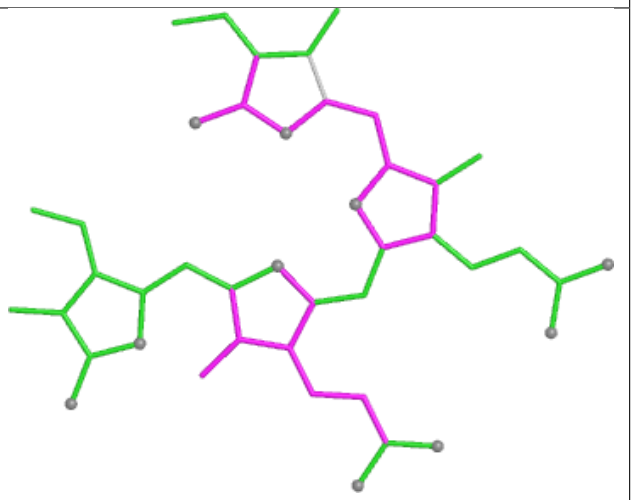


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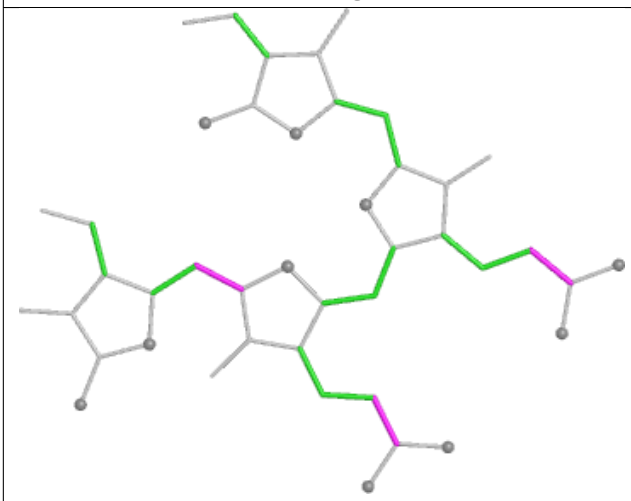
Ligand PEB eO 203



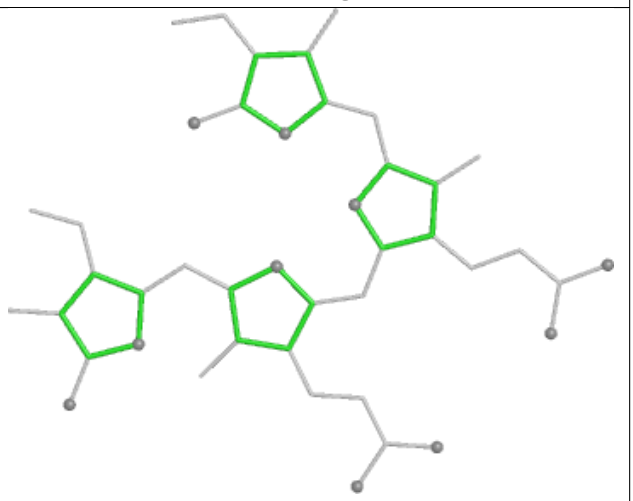
Bond lengths



Bond angles

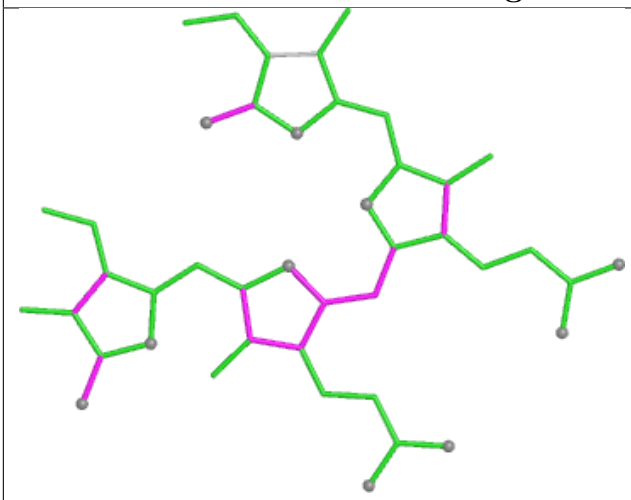


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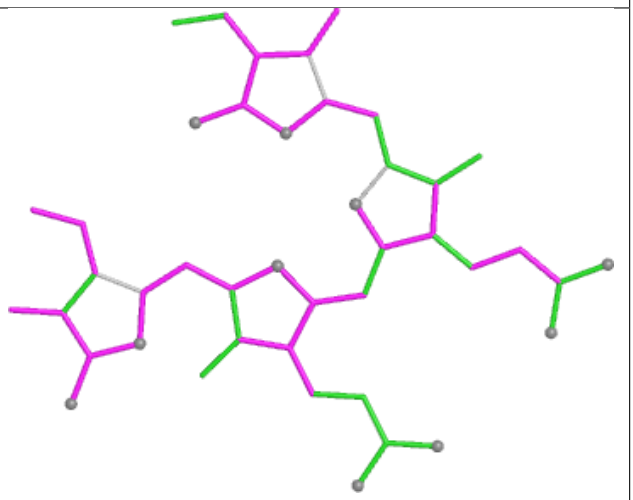


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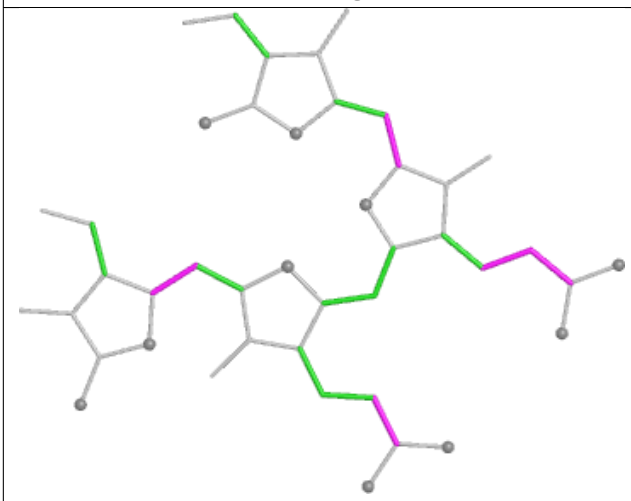
Ligand PUB AM 304



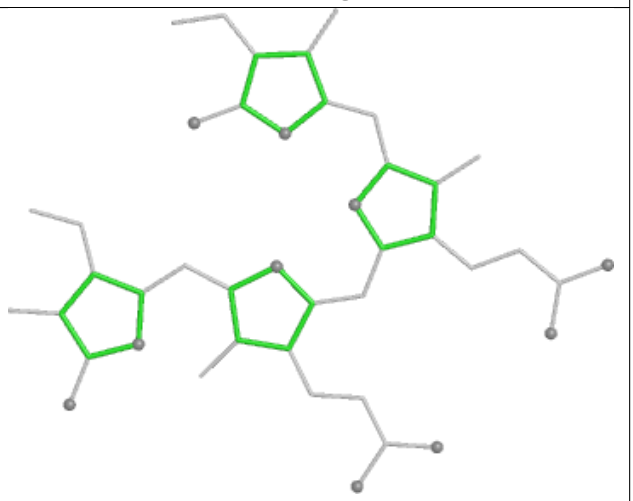
Bond lengths



Bond angles

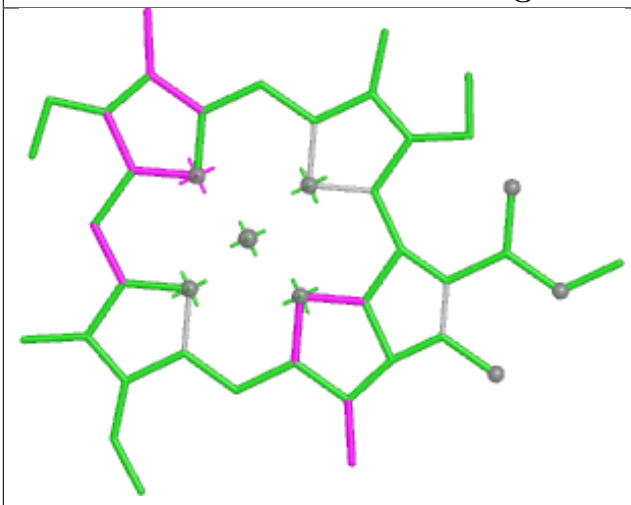


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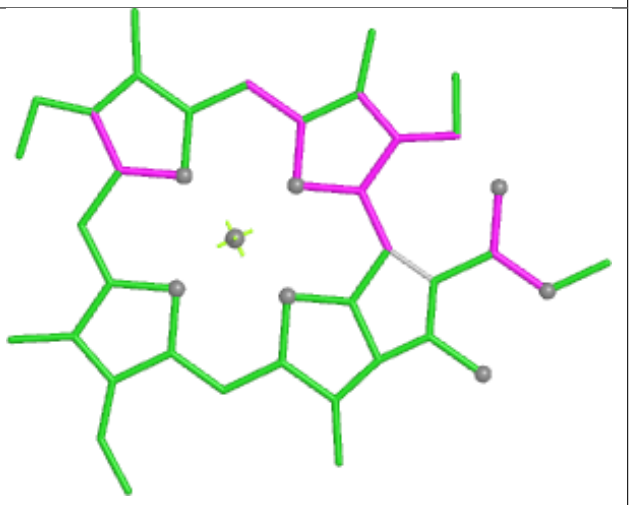


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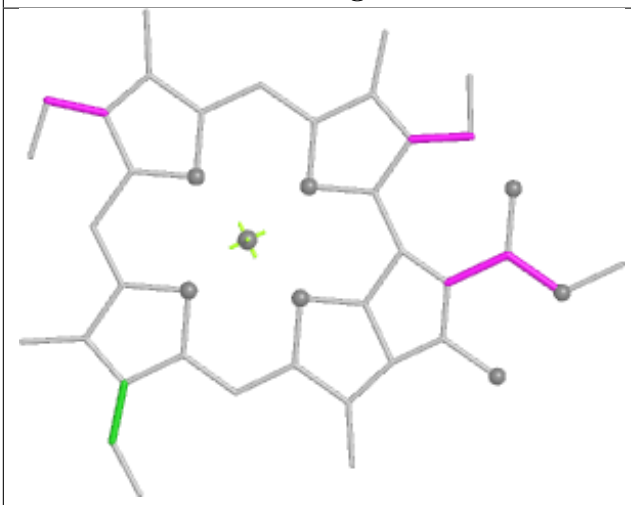
Ligand CLA 7N 609



Bond lengths



Bond angles

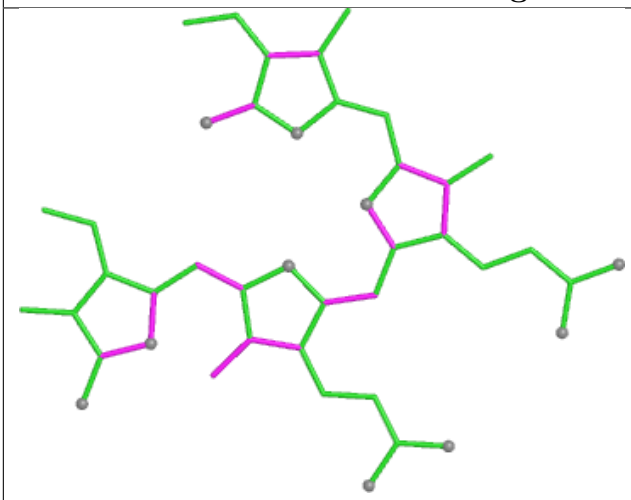


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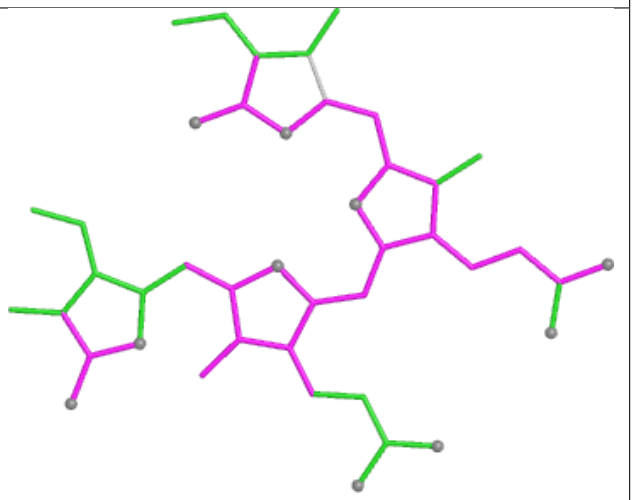


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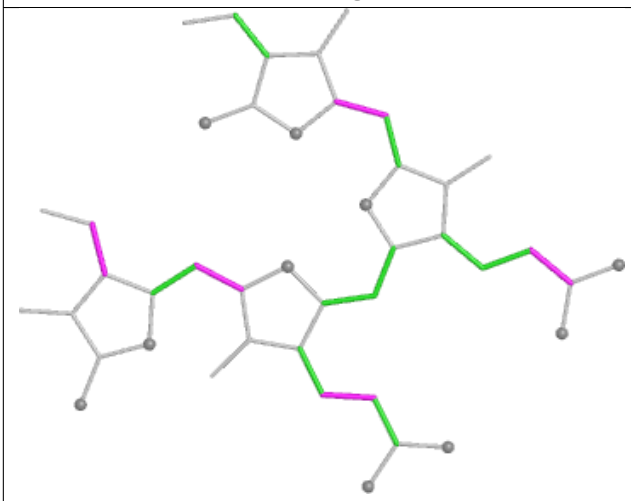
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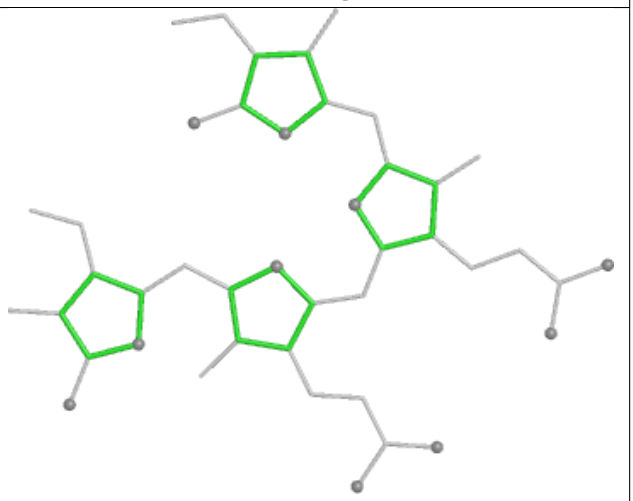
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Bond angles

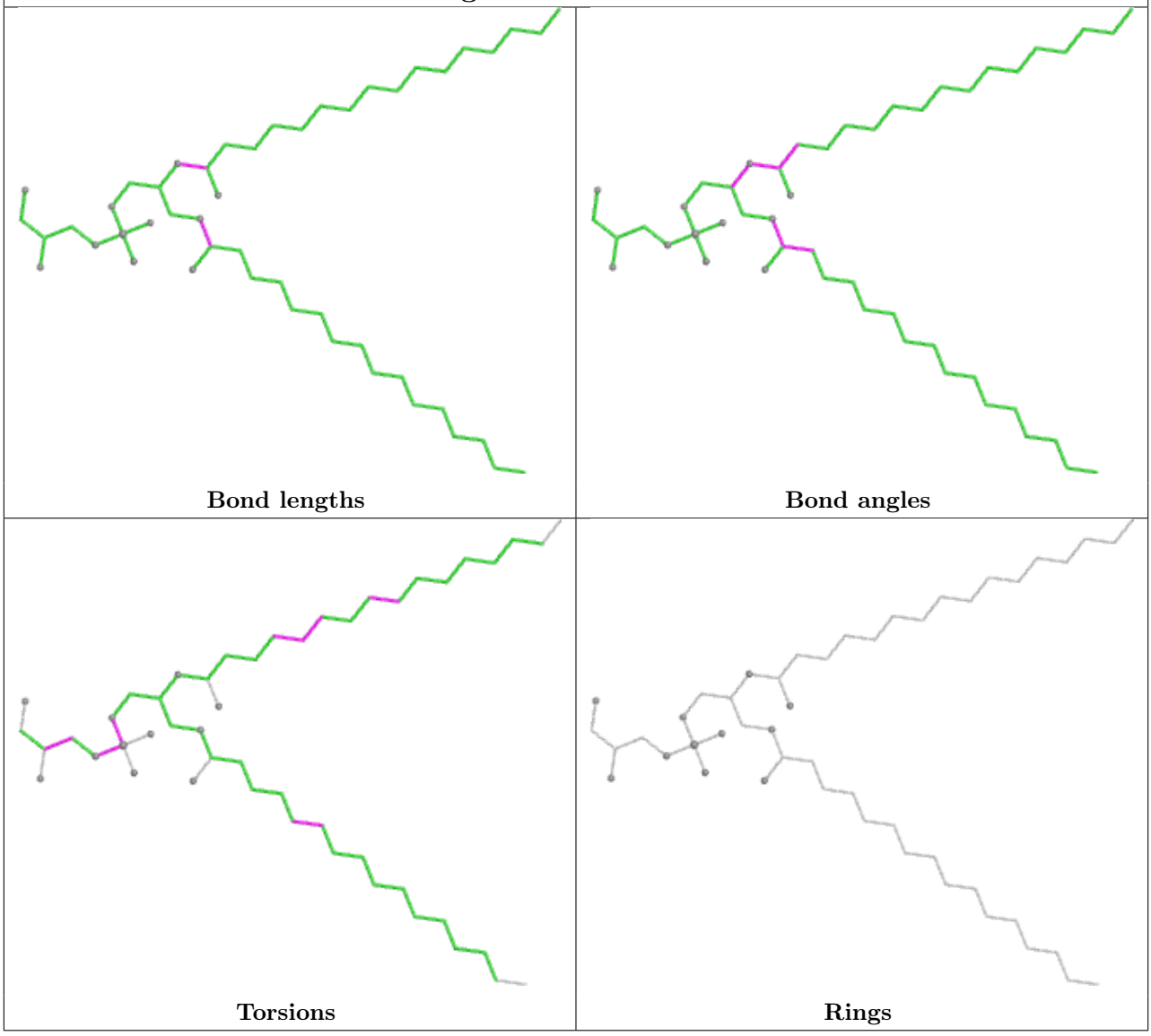


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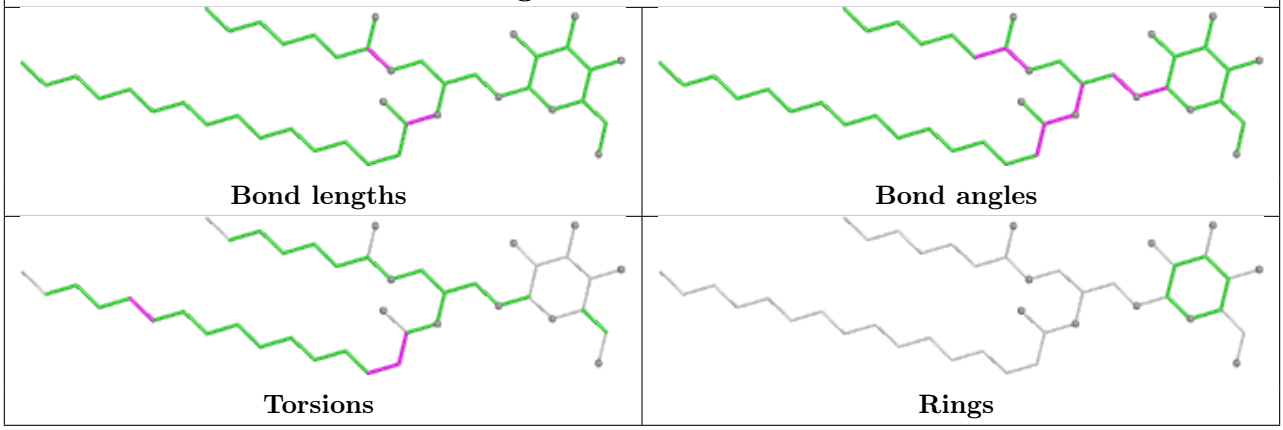


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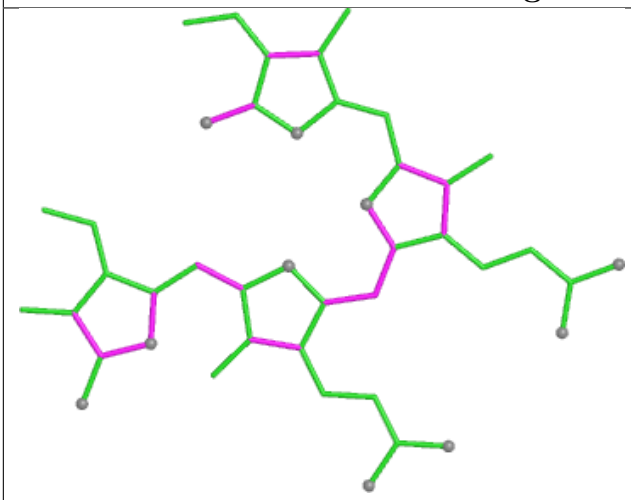
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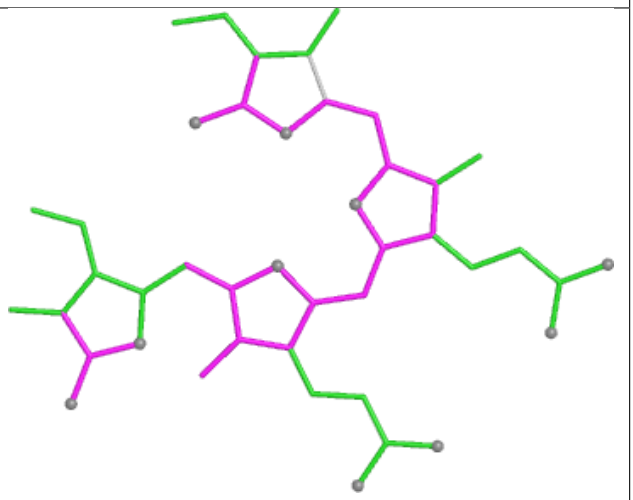
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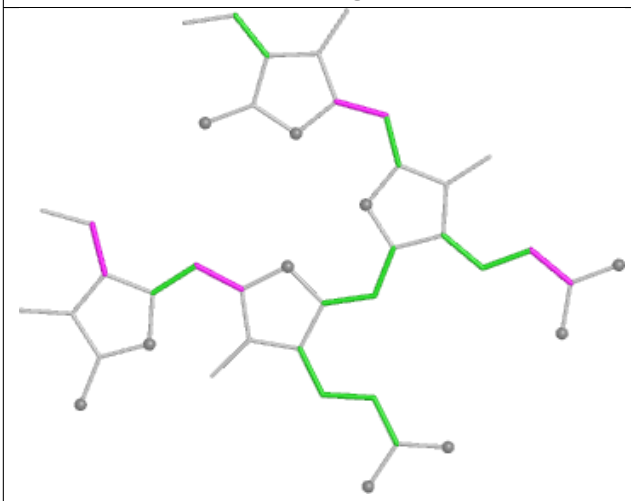
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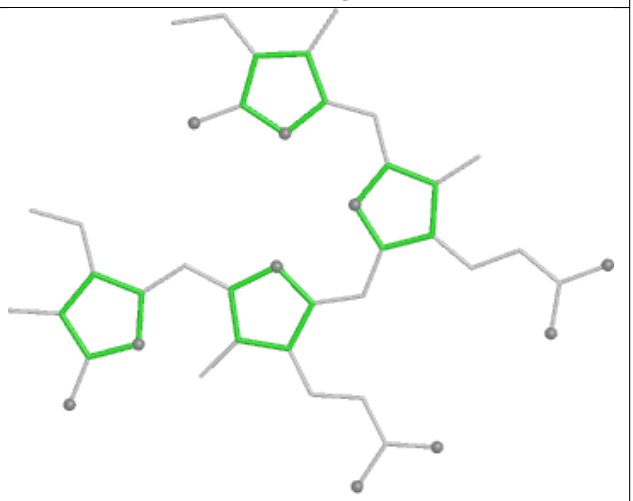
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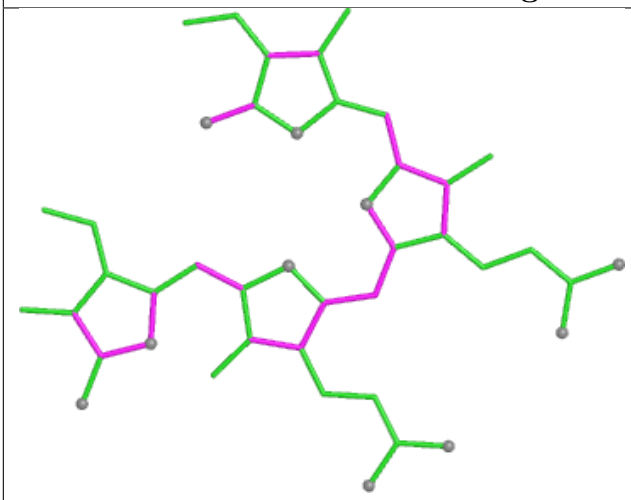


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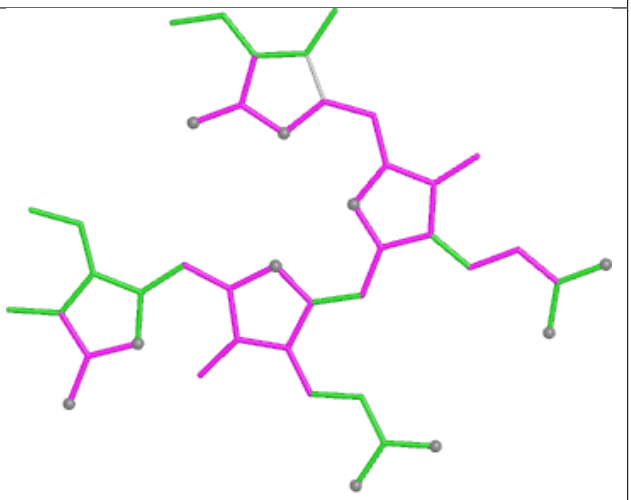


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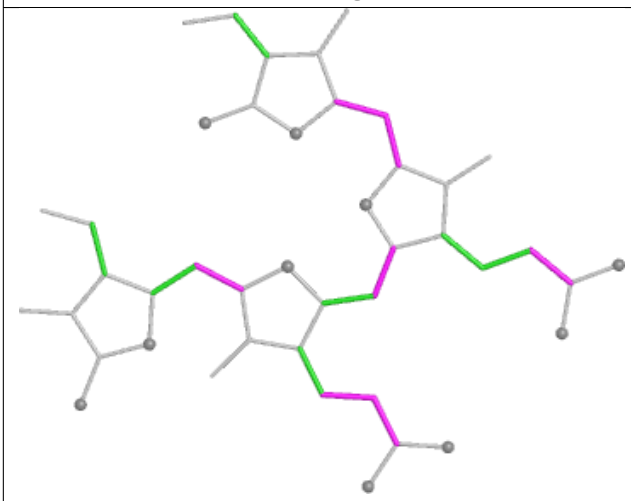
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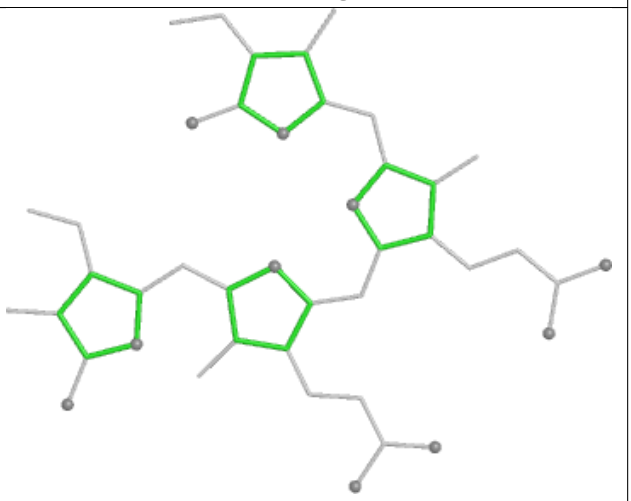
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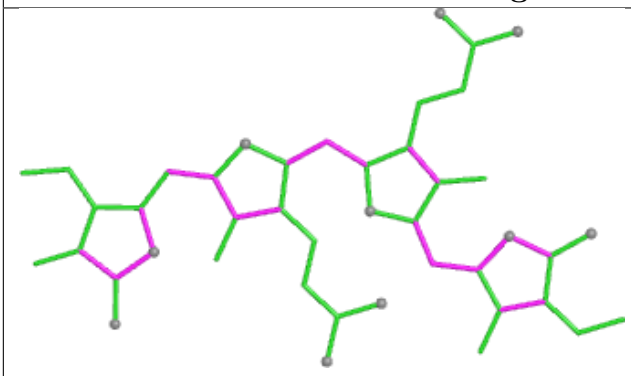


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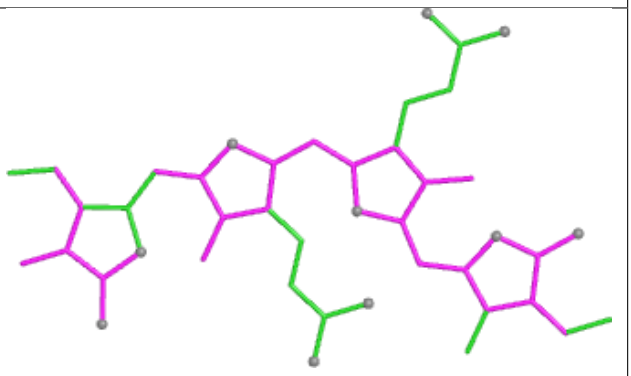


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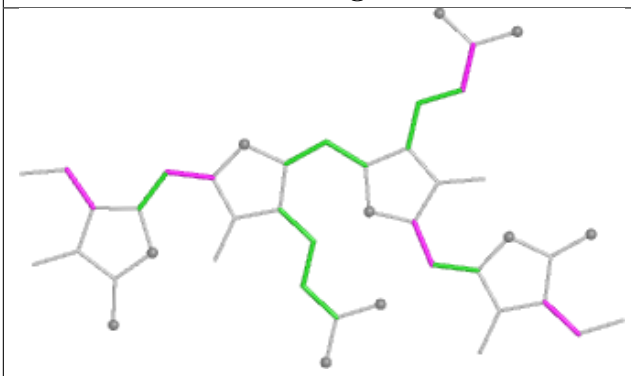
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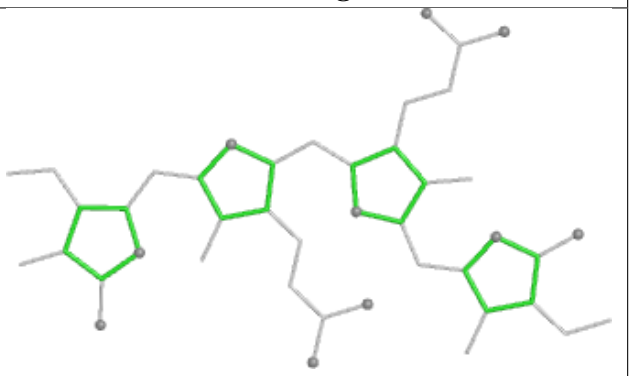
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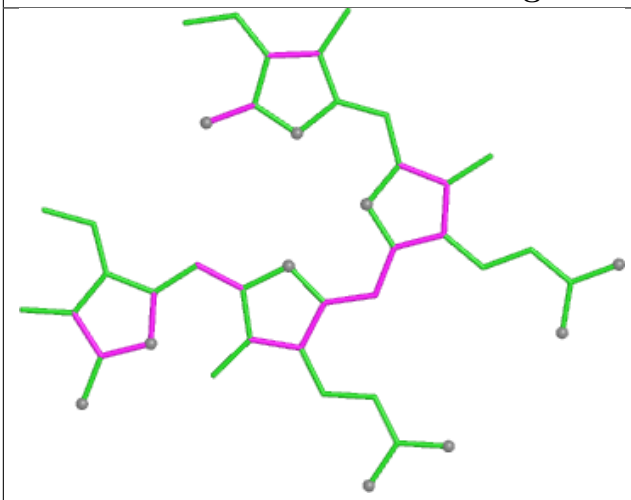


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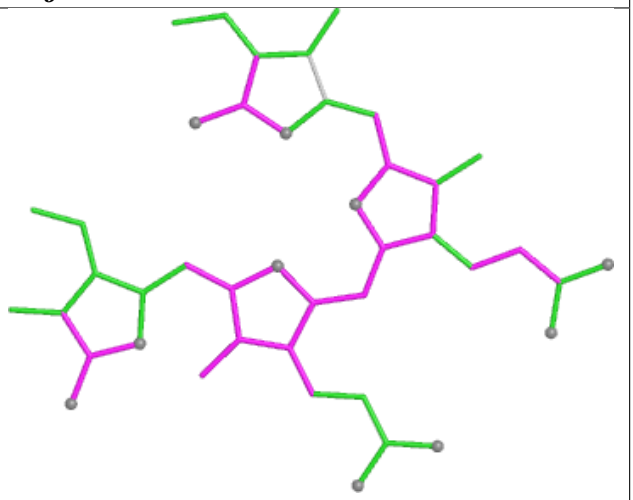


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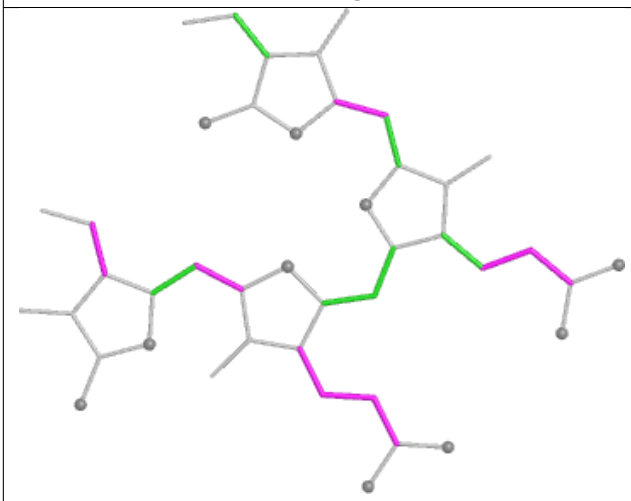
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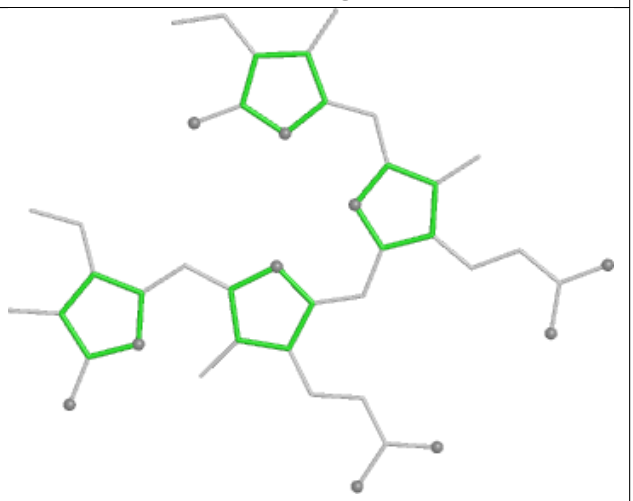
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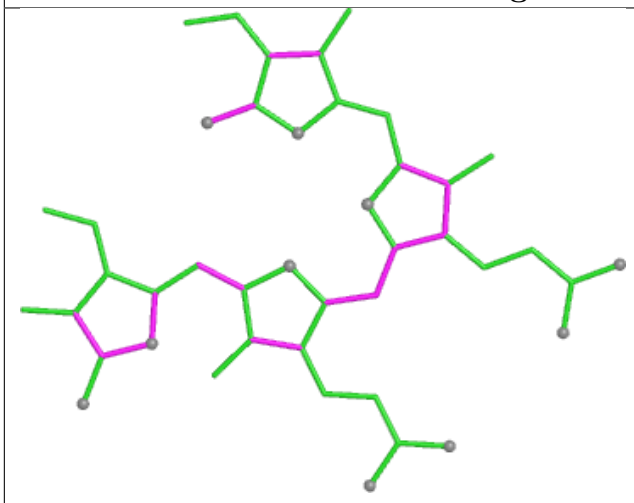


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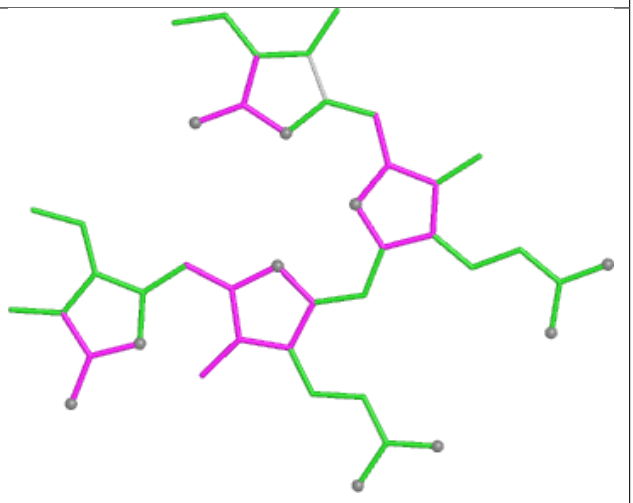


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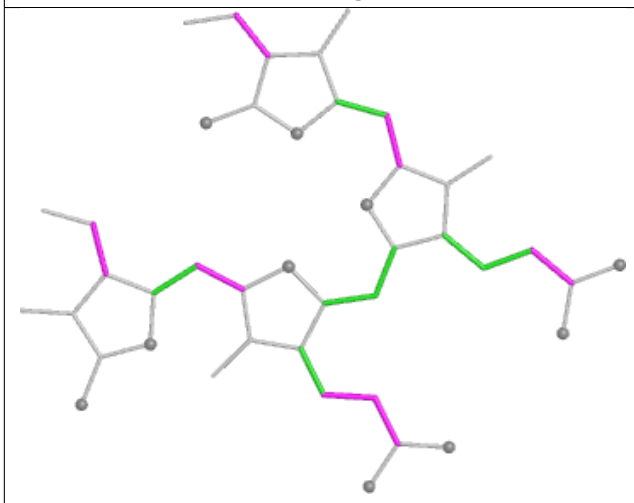
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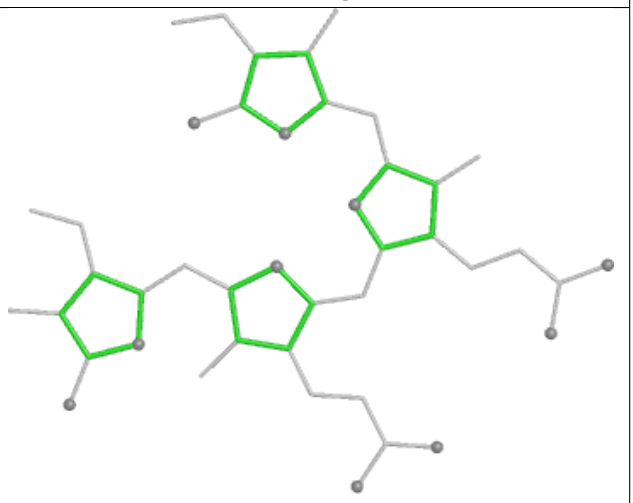
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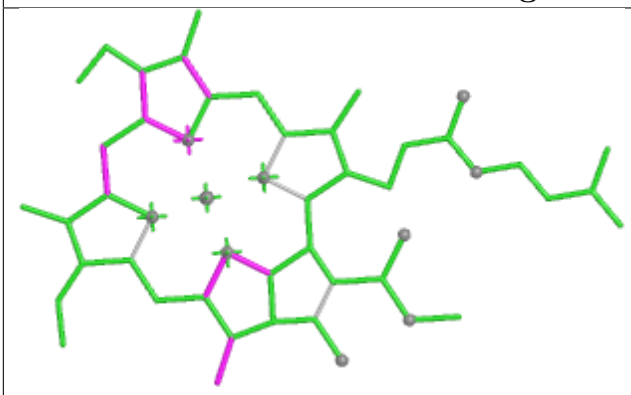


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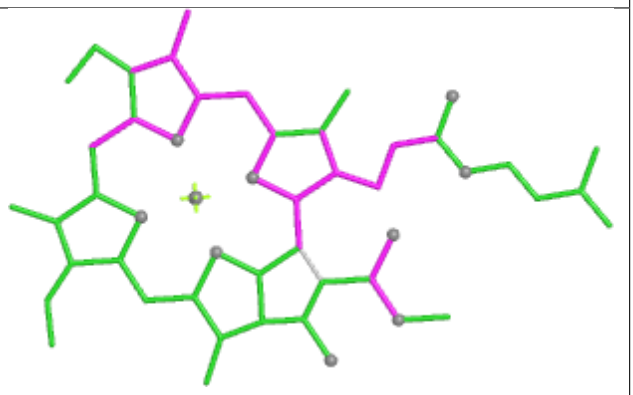


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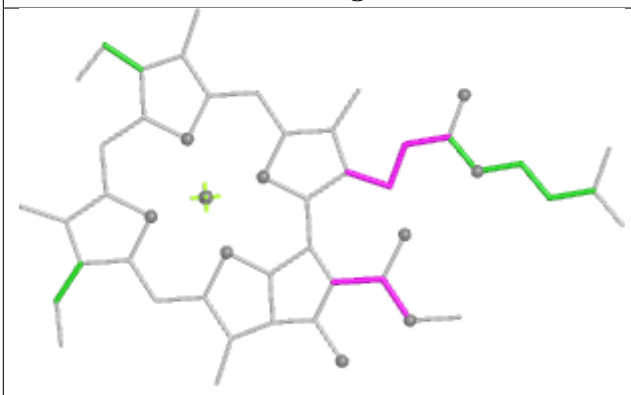
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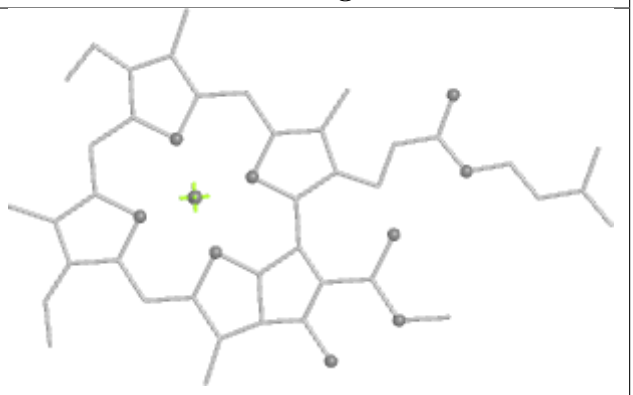
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Bond angles

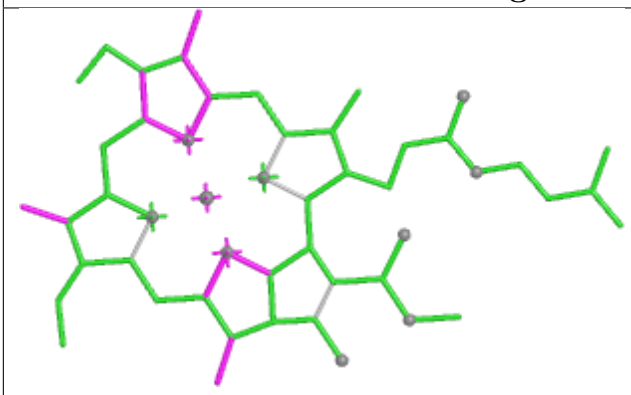


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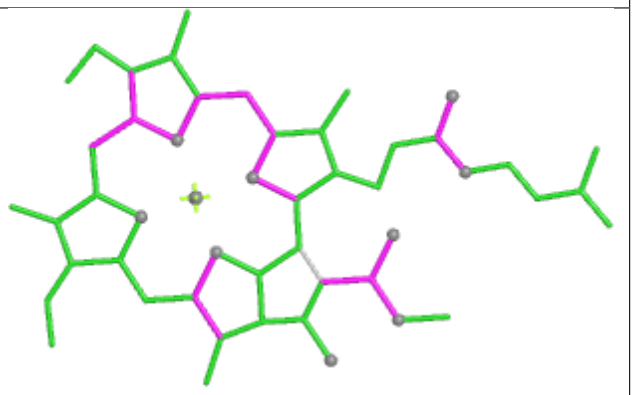


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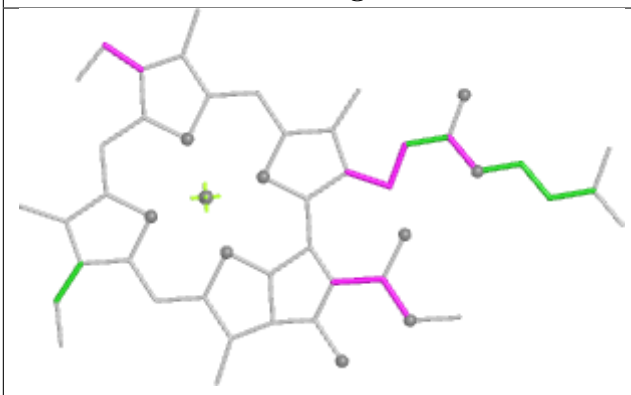
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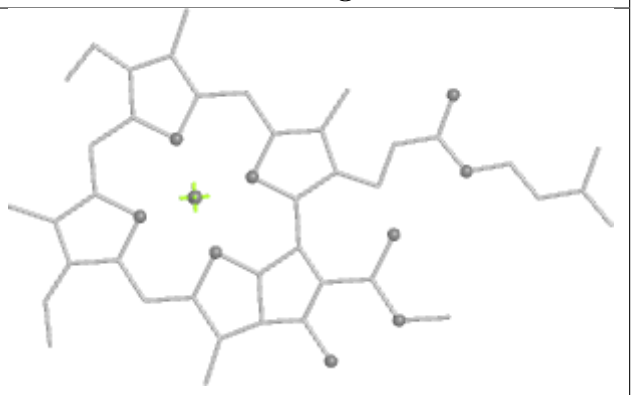
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Bond angles

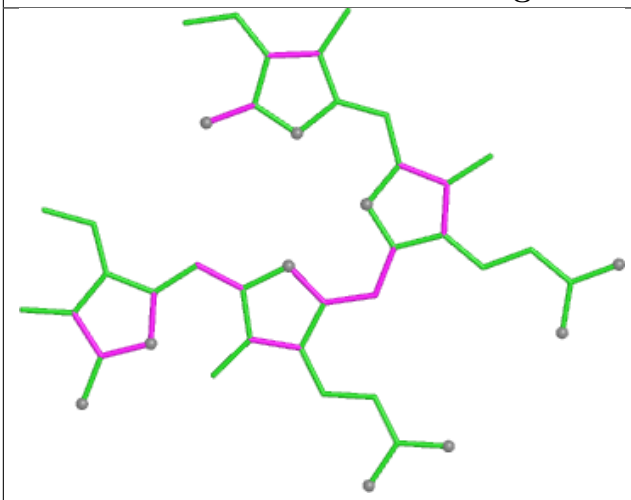


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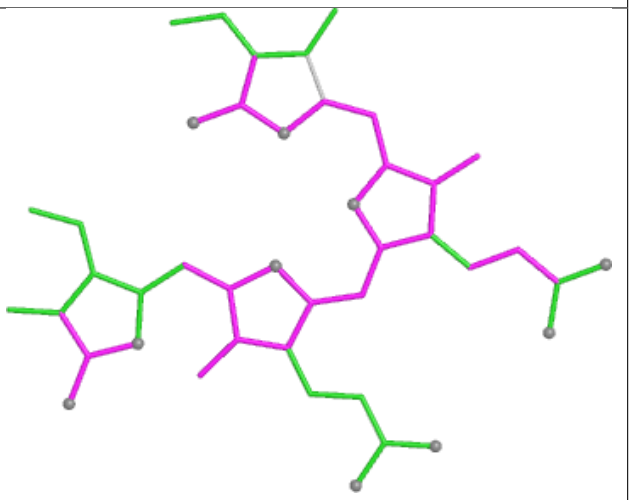


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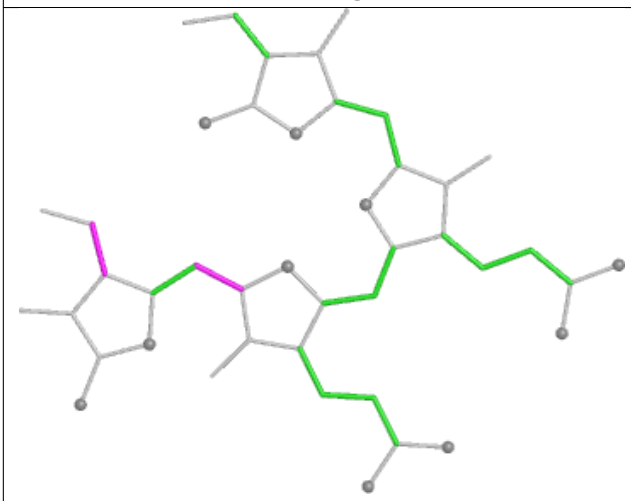
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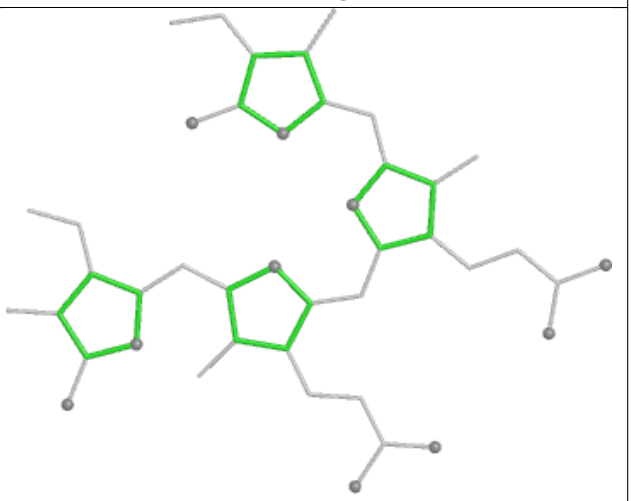
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Bond angles

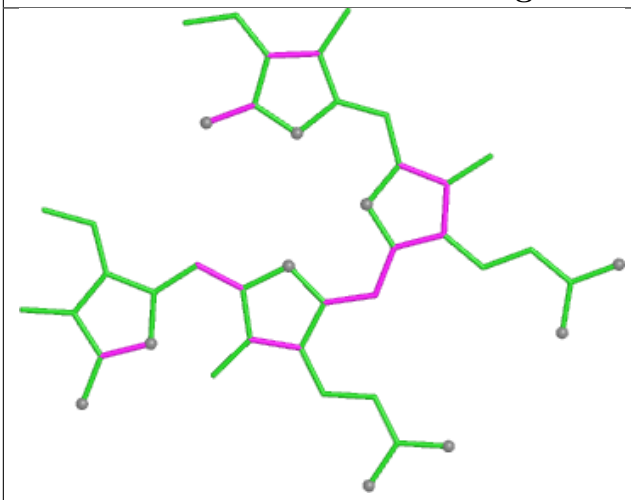


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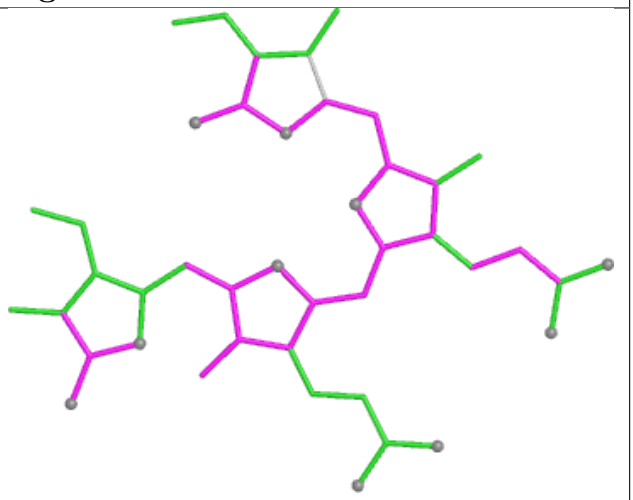


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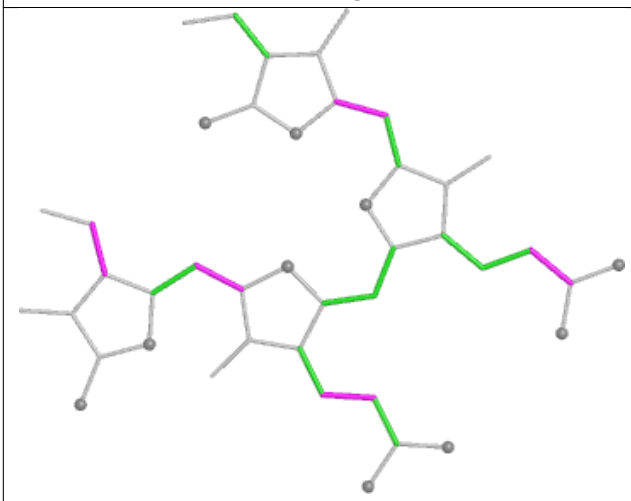
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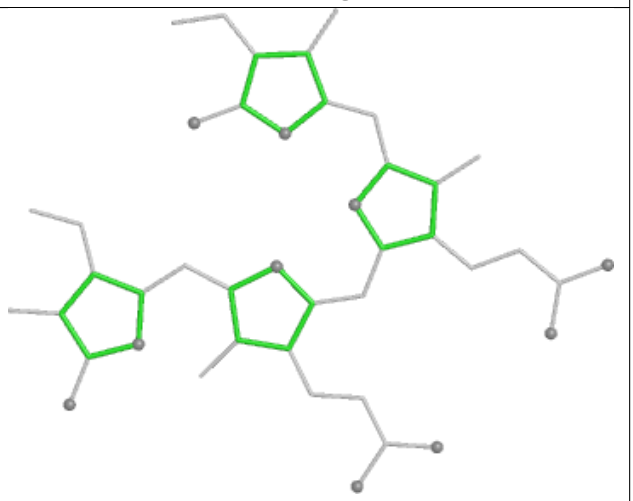
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Bond angles

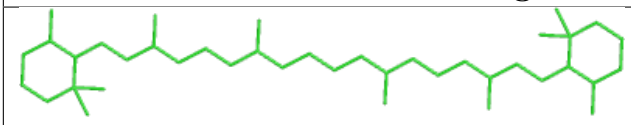


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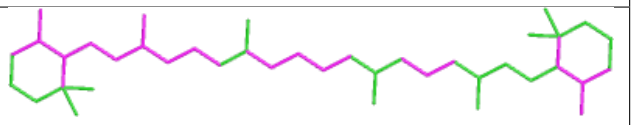


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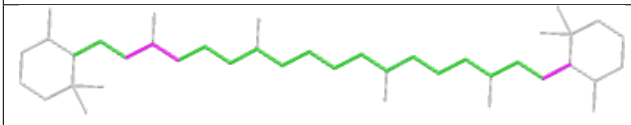
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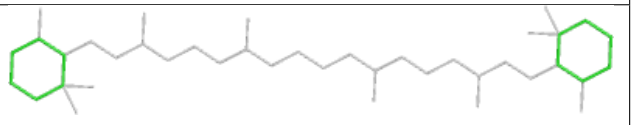
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Bond angles

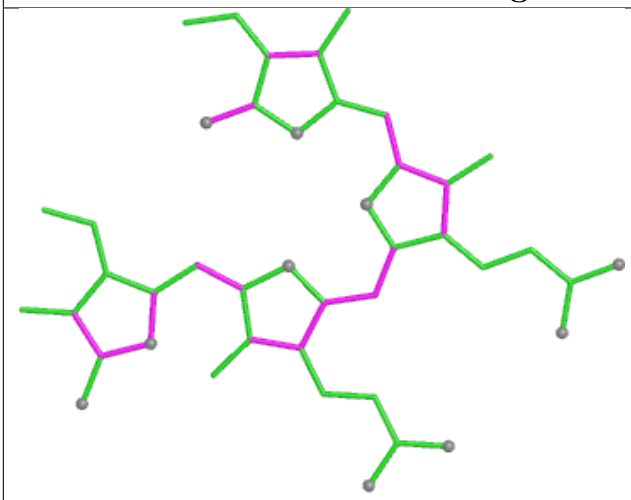


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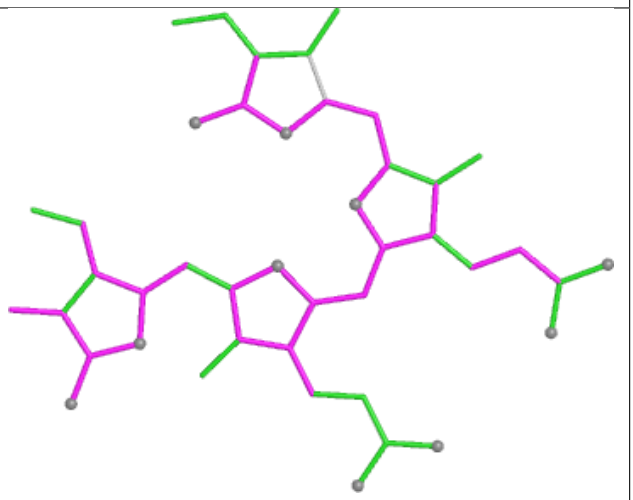


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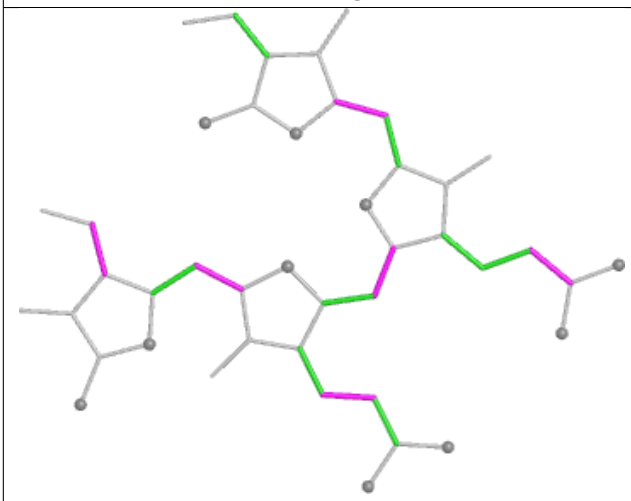
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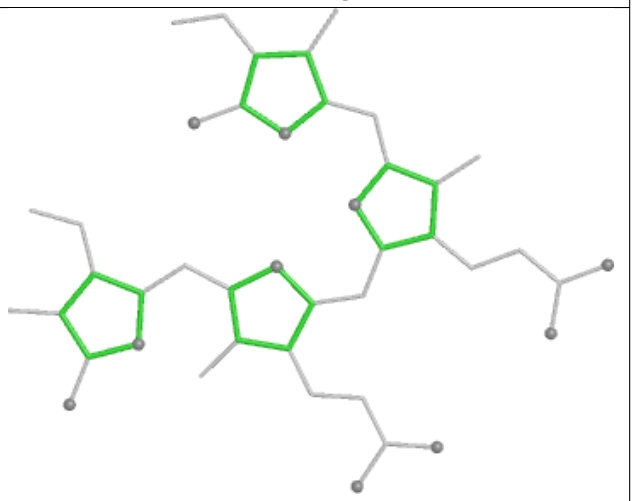
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Bond angles

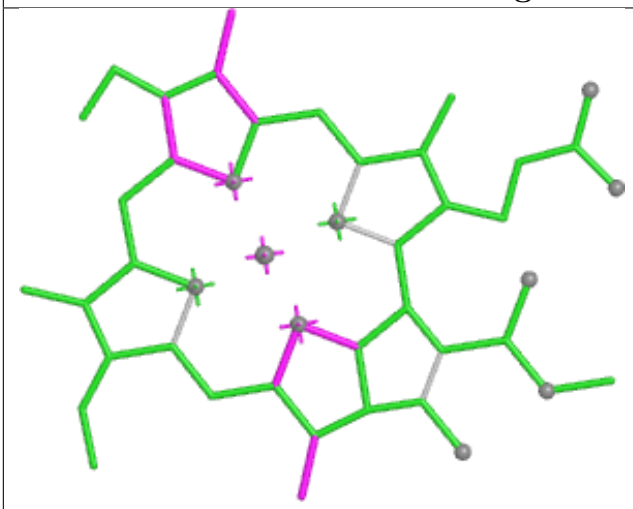


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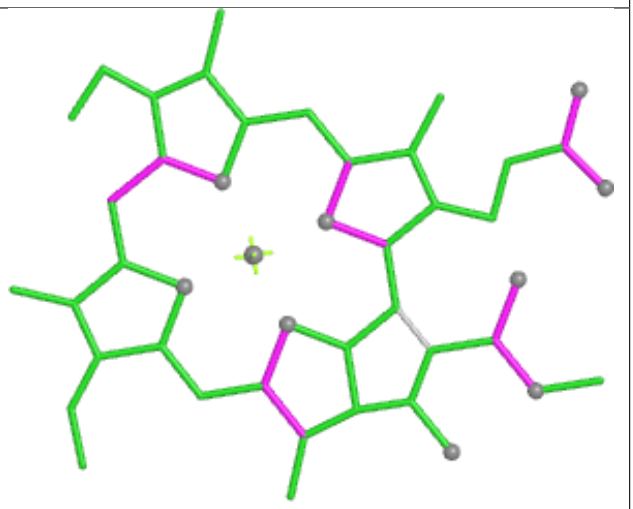


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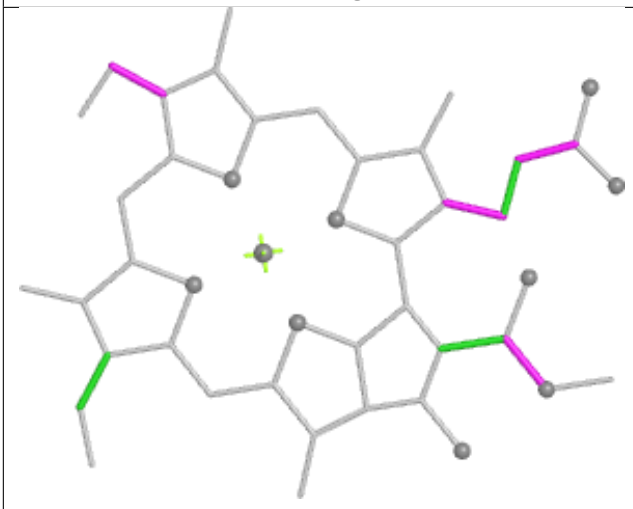
Ligand CLA 1N 606



Bond lengths



Bond angles

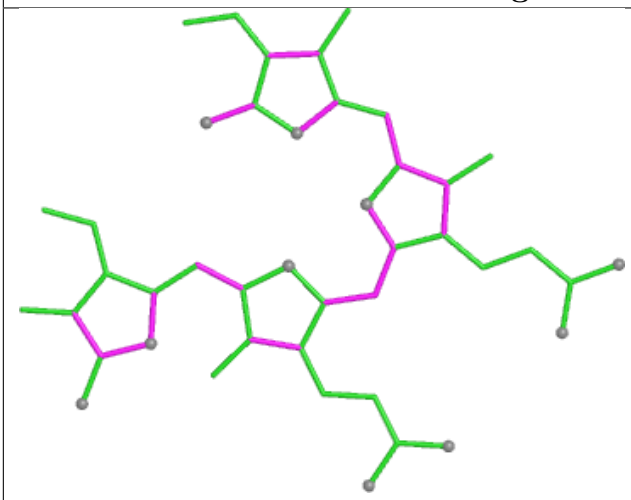


Torsions

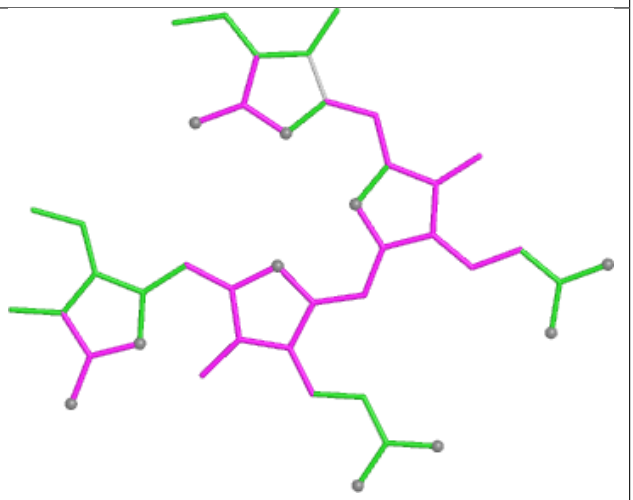


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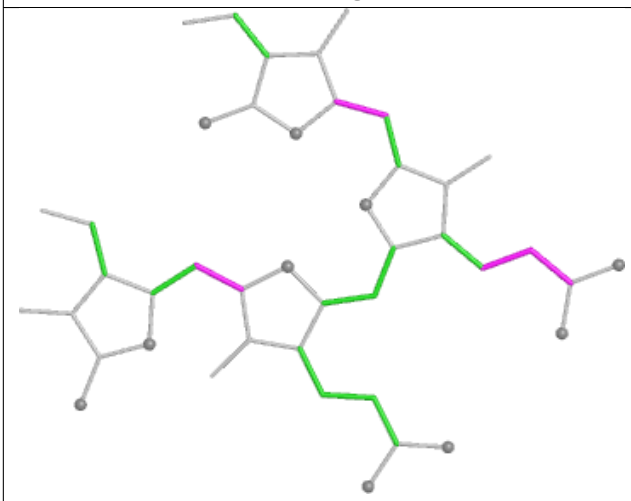
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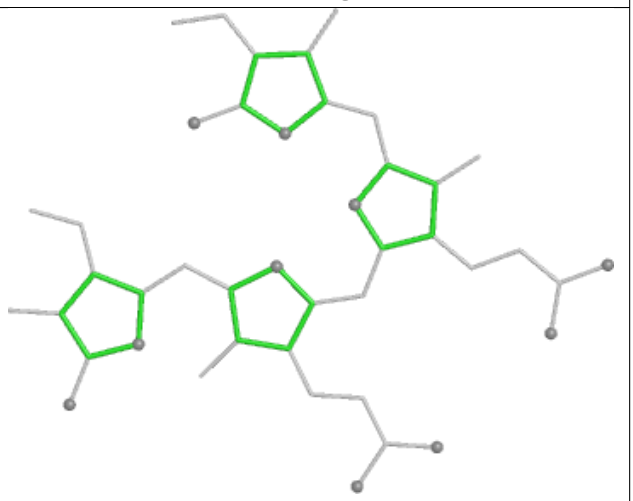
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Bond angles

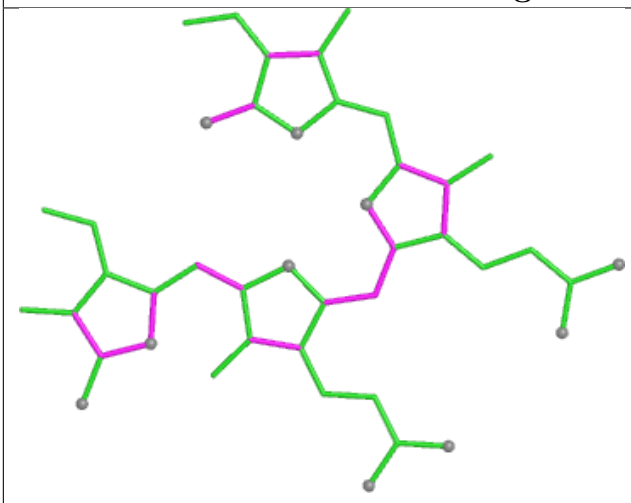


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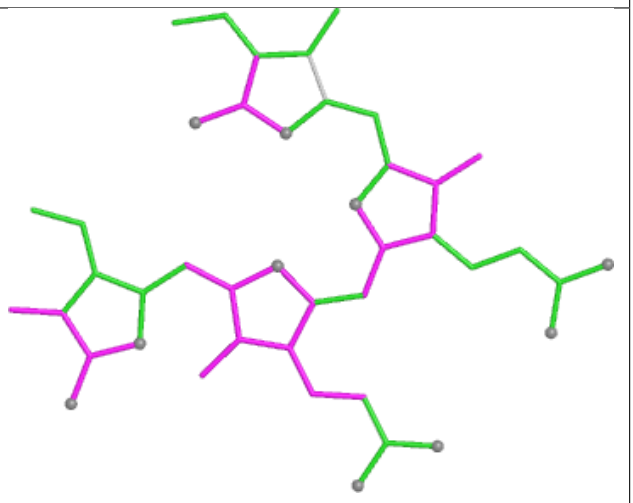


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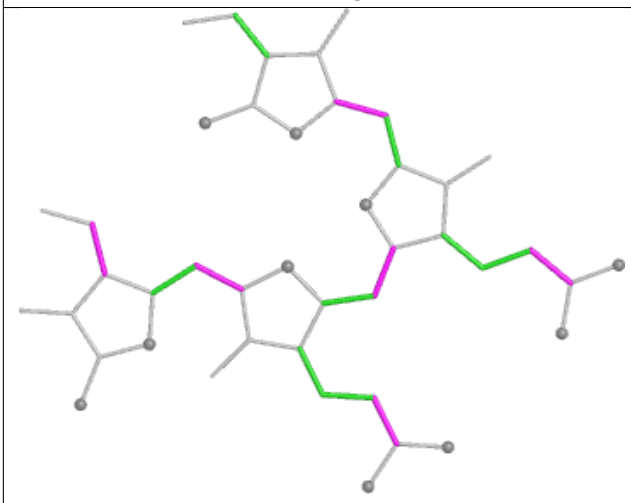
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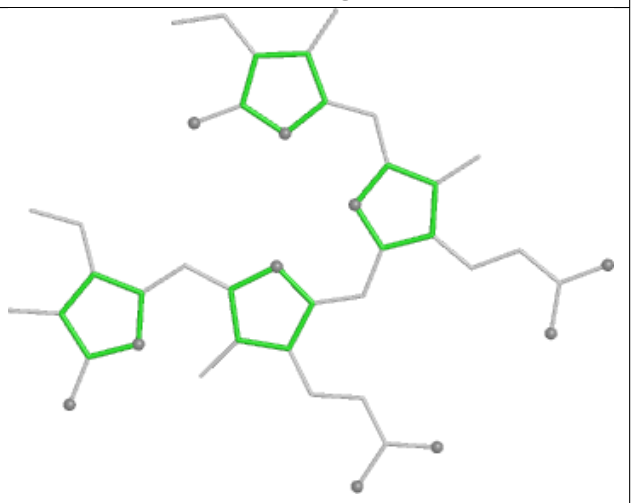
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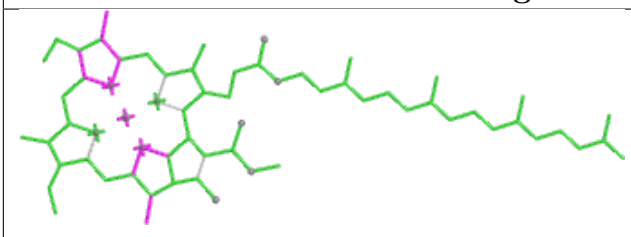


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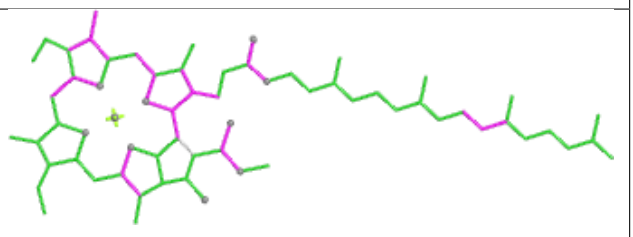


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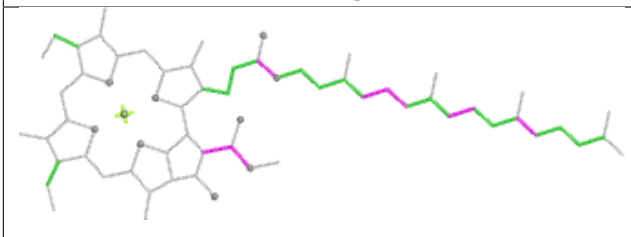
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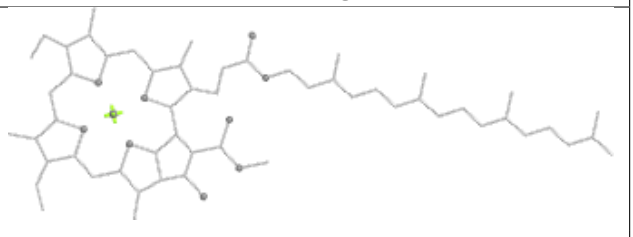
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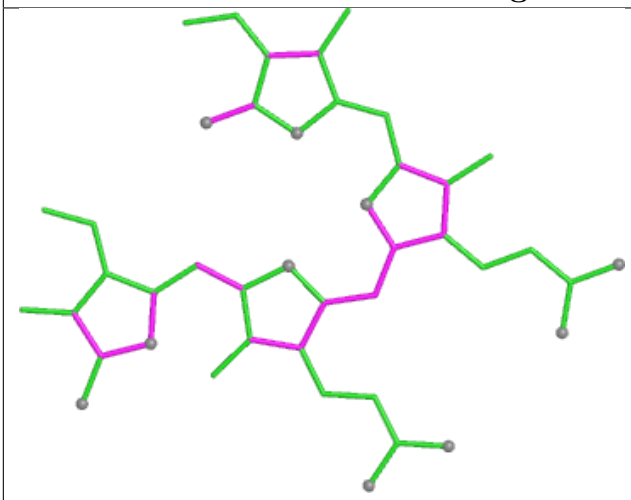


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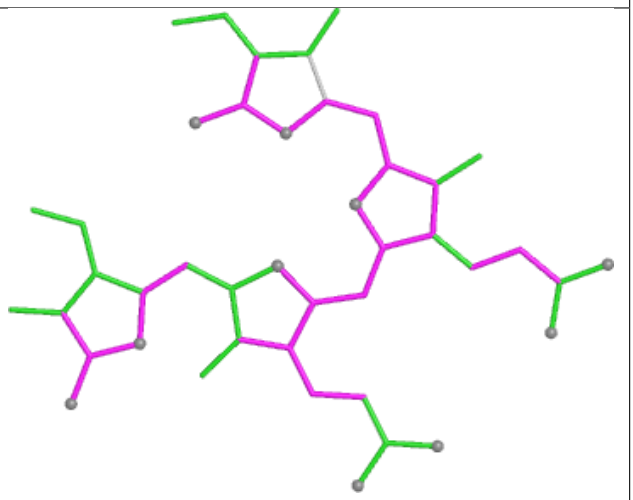


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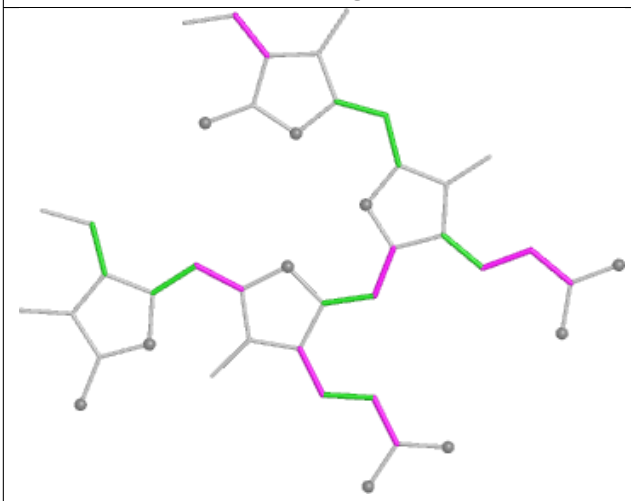
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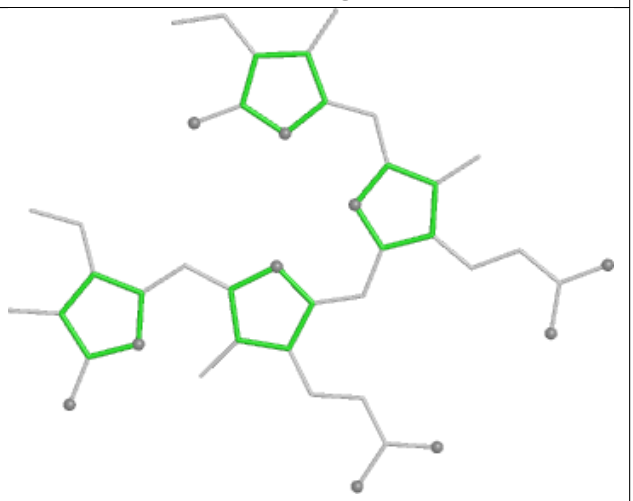
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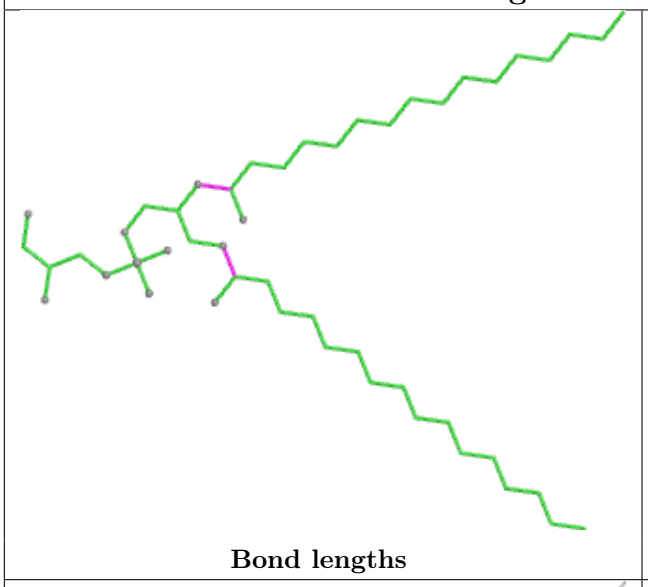


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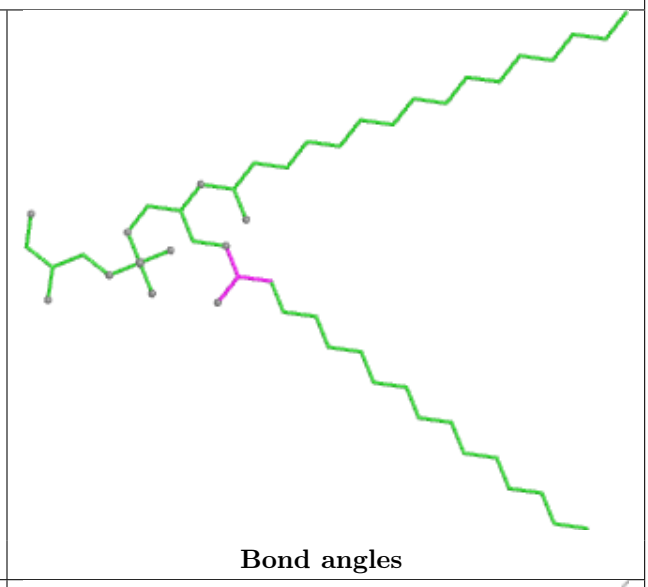


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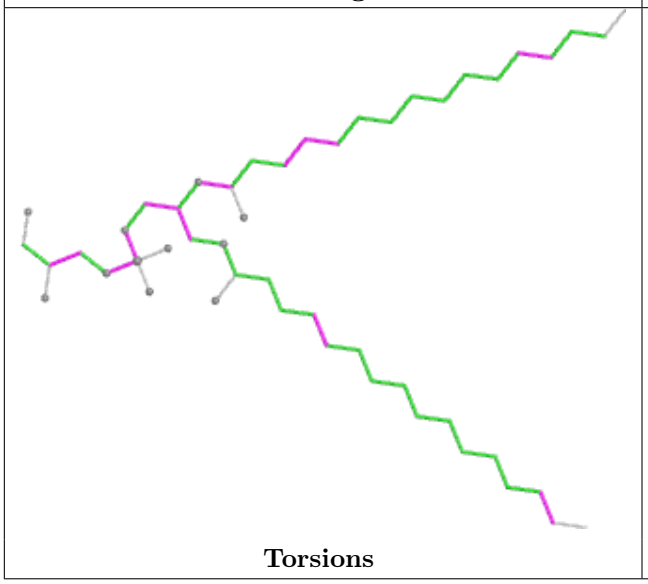
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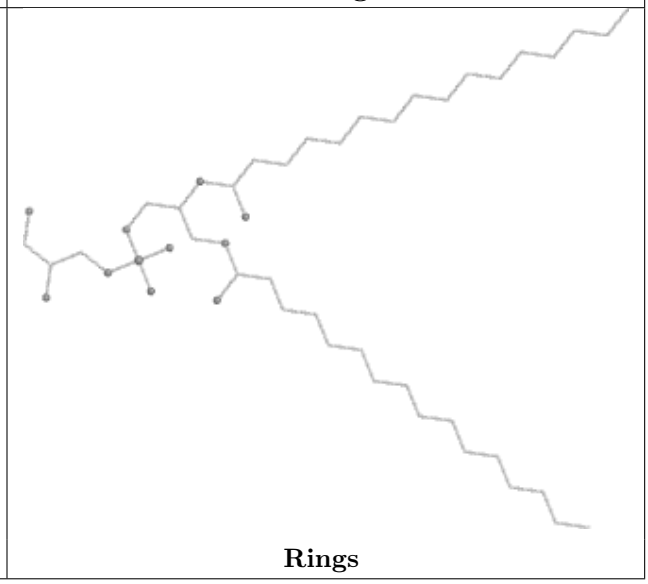
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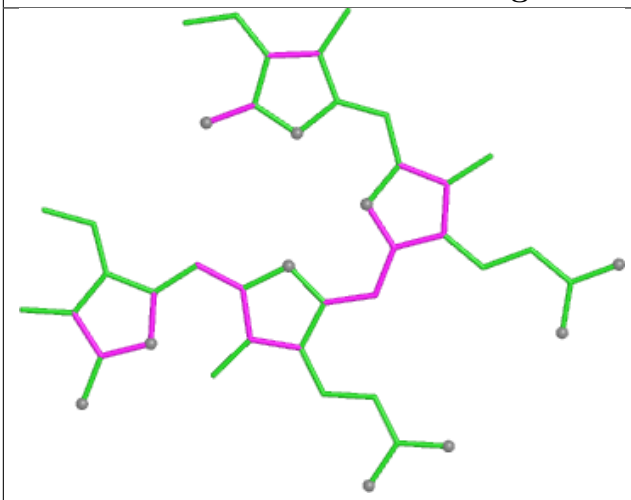


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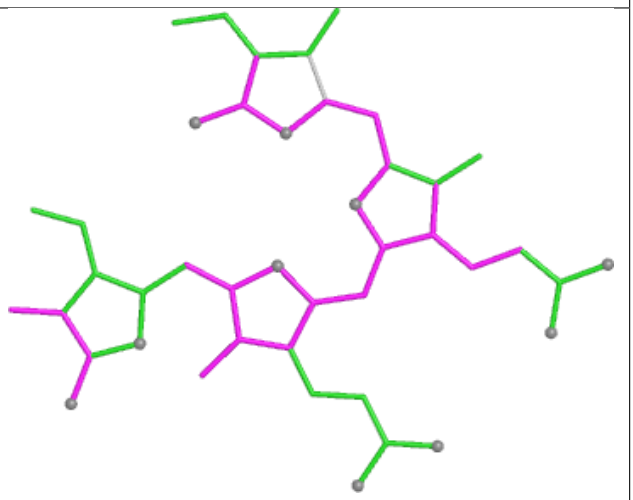


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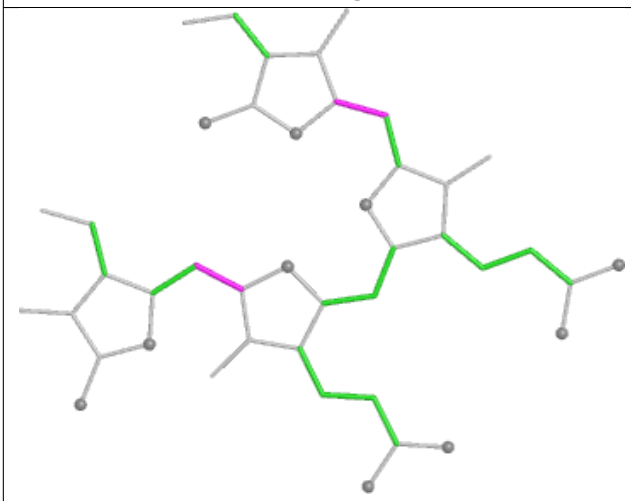
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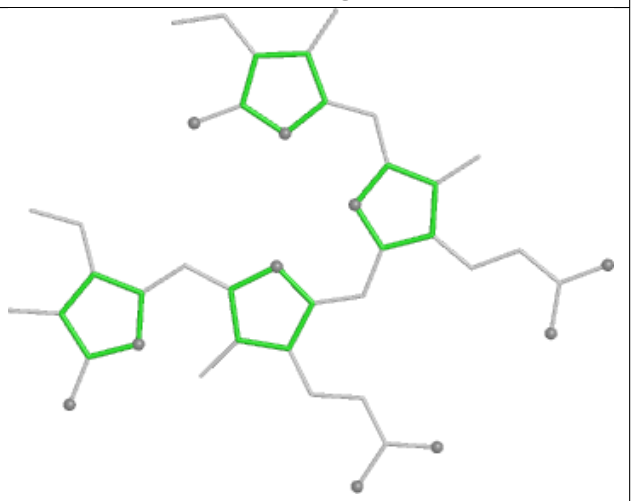
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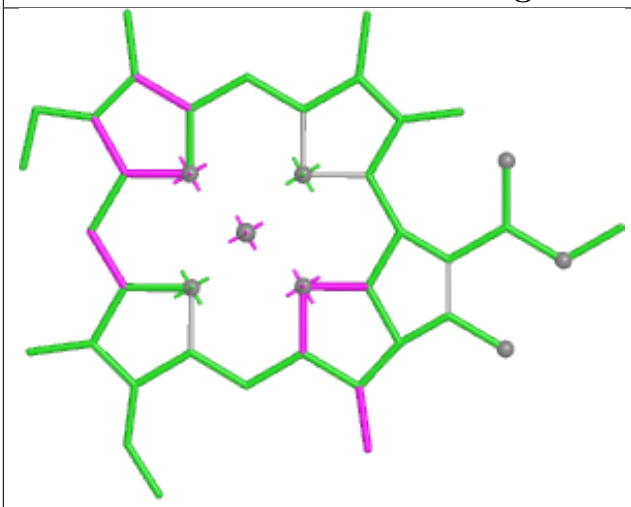


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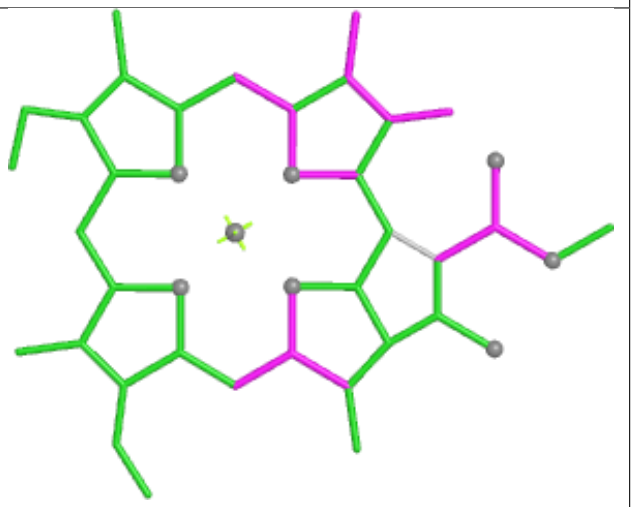


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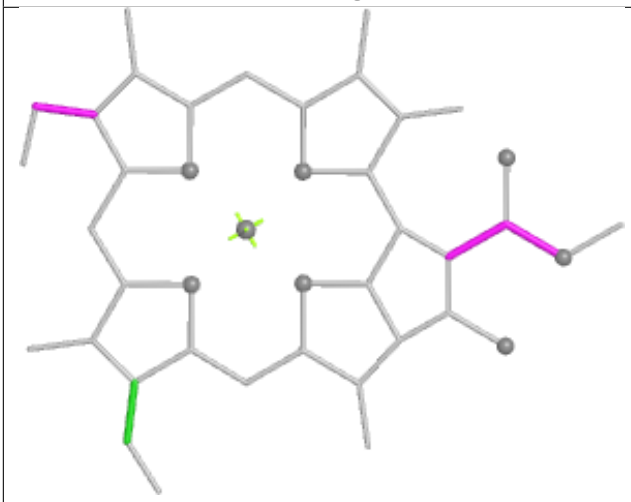
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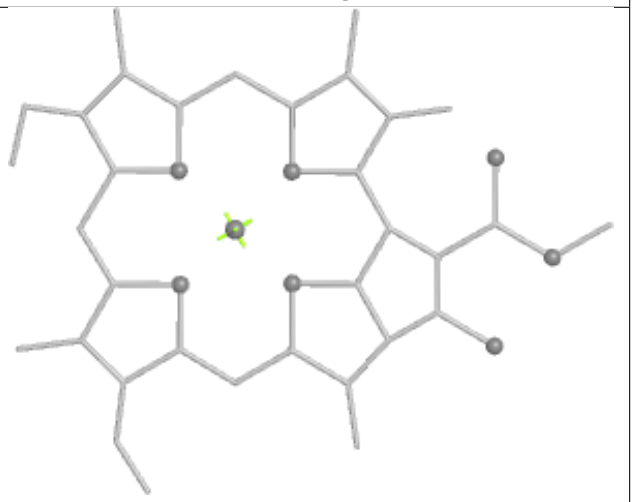
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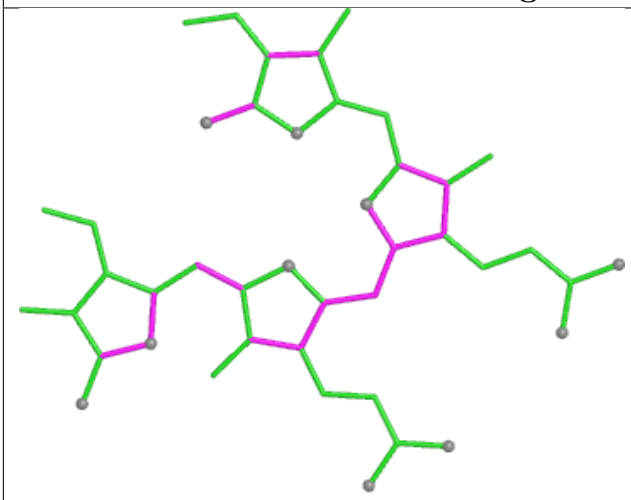


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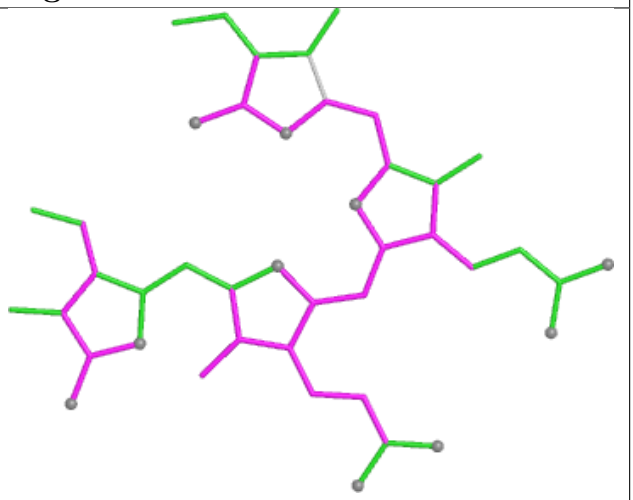


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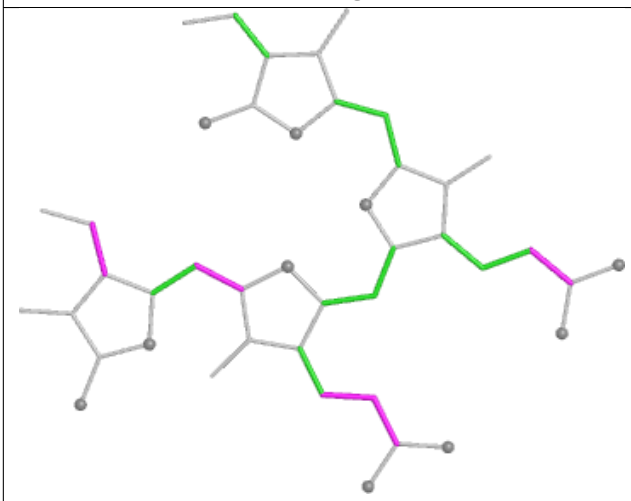
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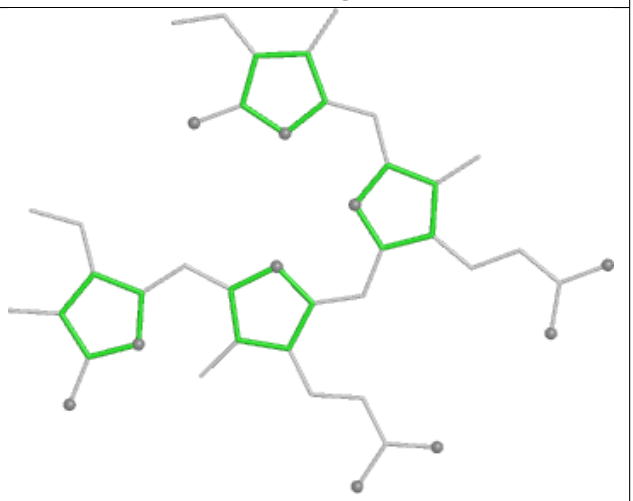
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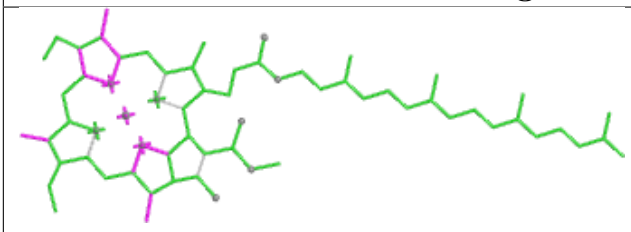


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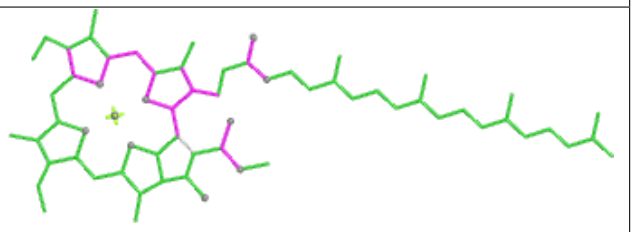


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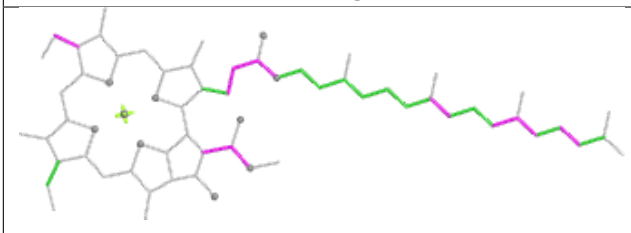
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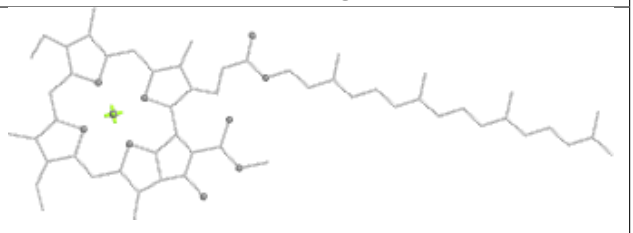
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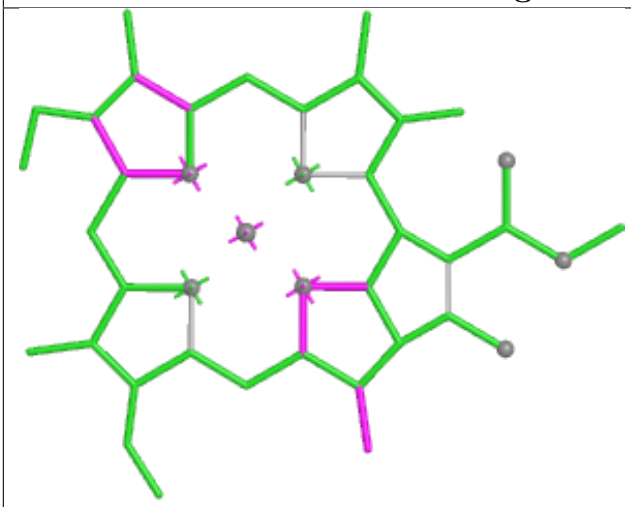


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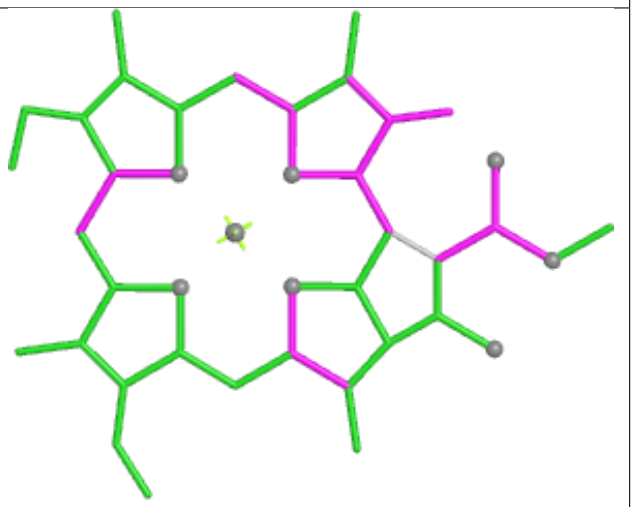


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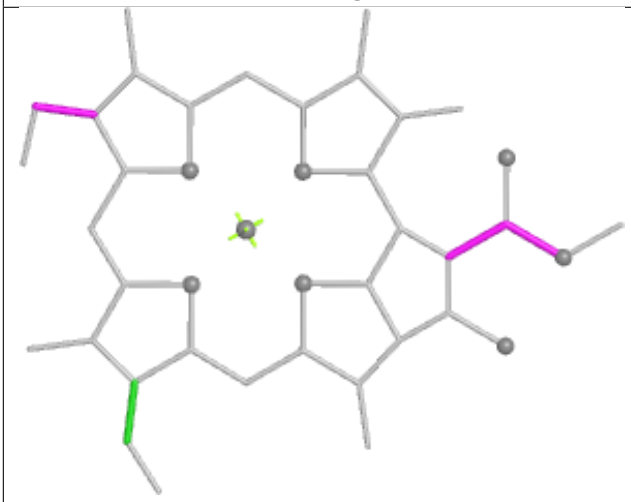
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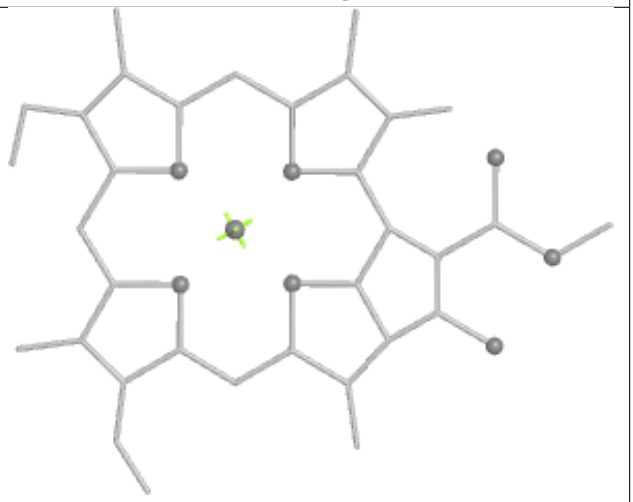
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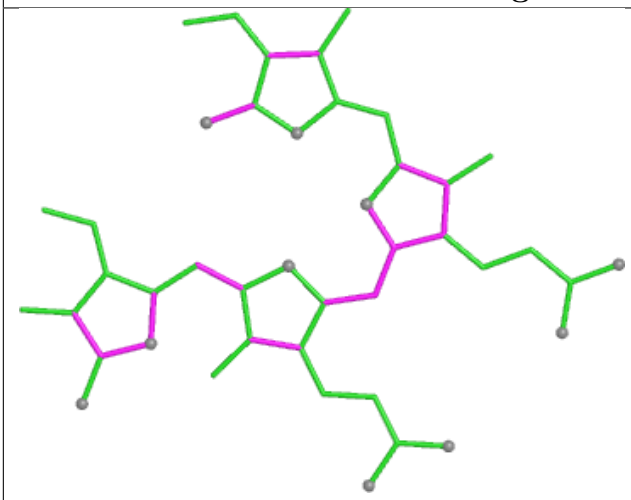


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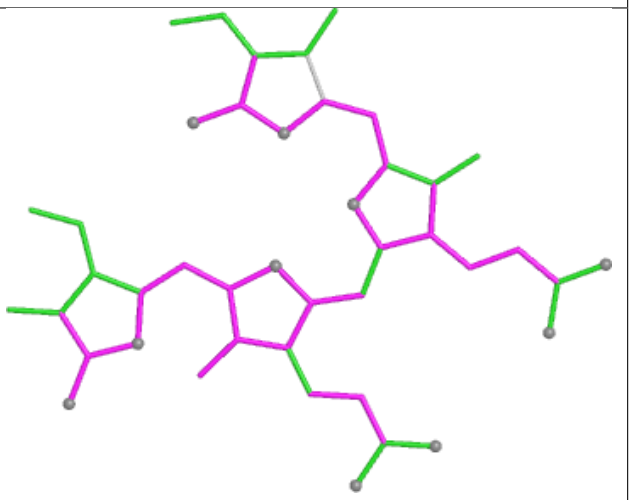


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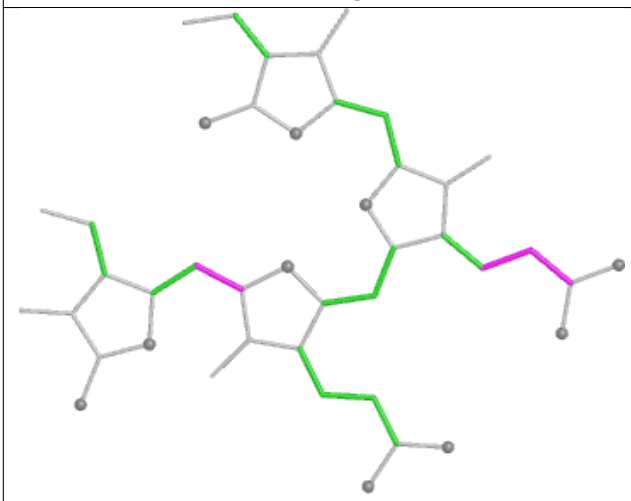
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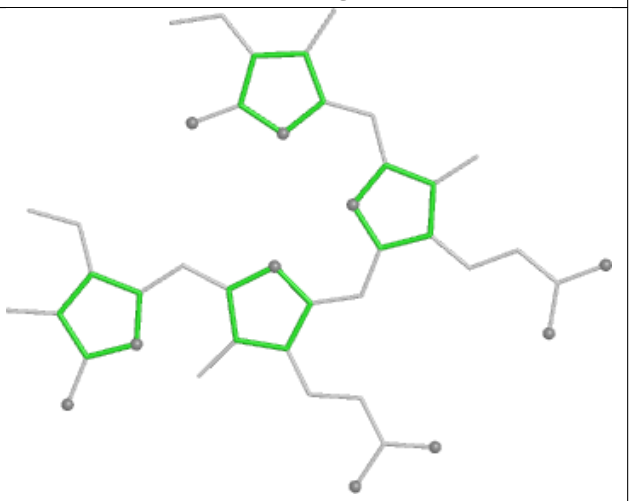
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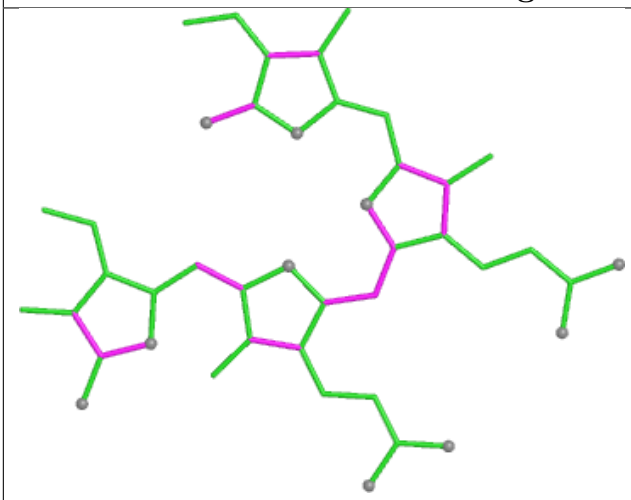


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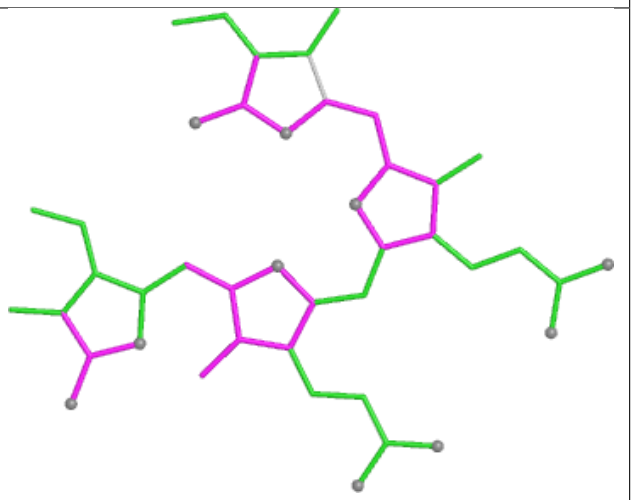


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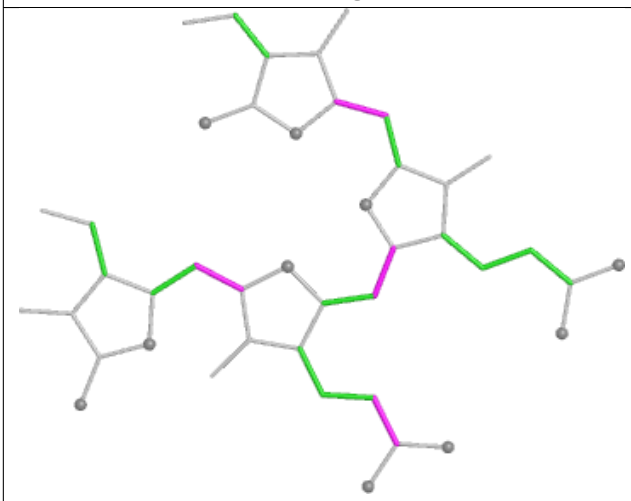
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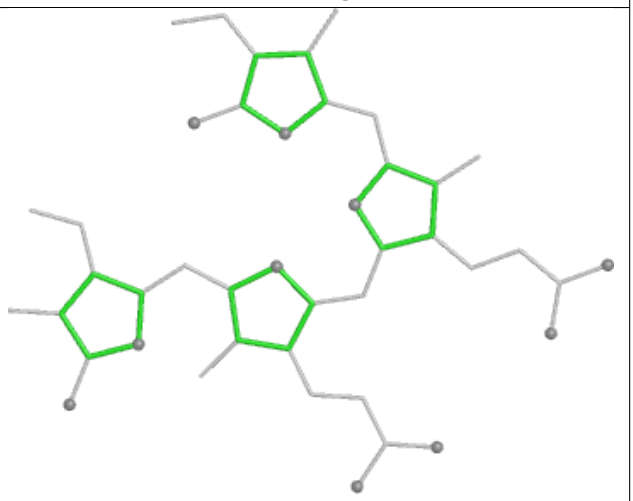
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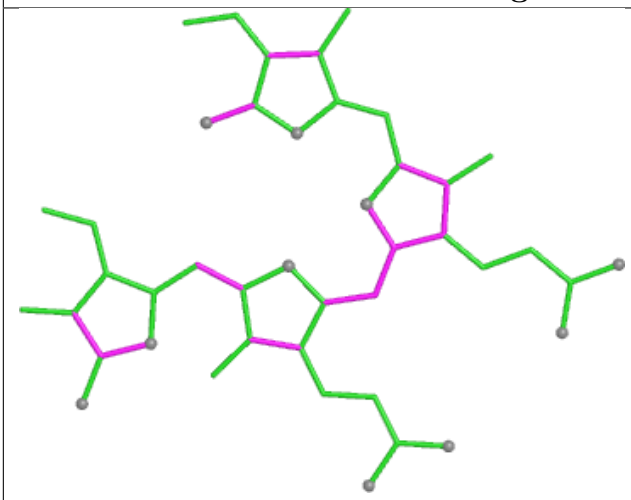


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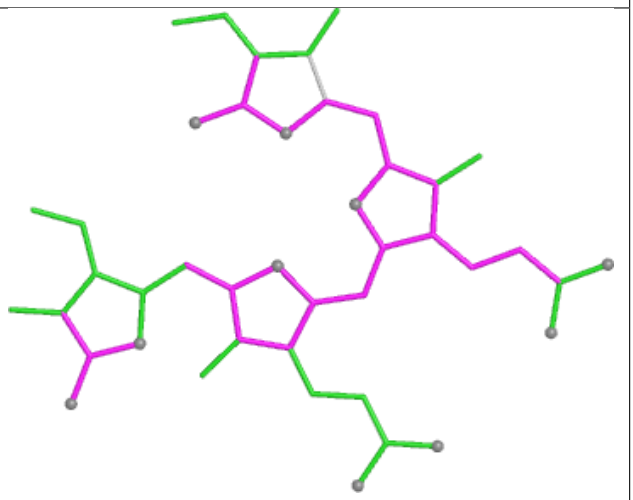


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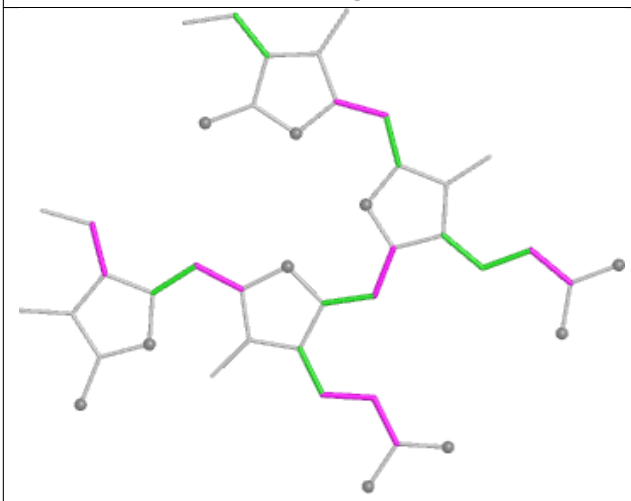
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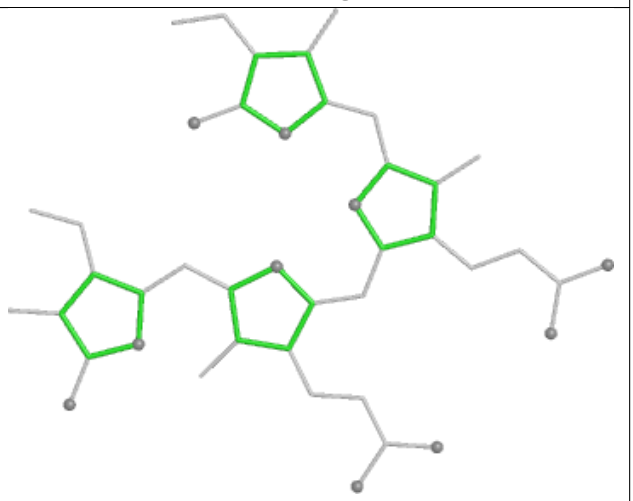
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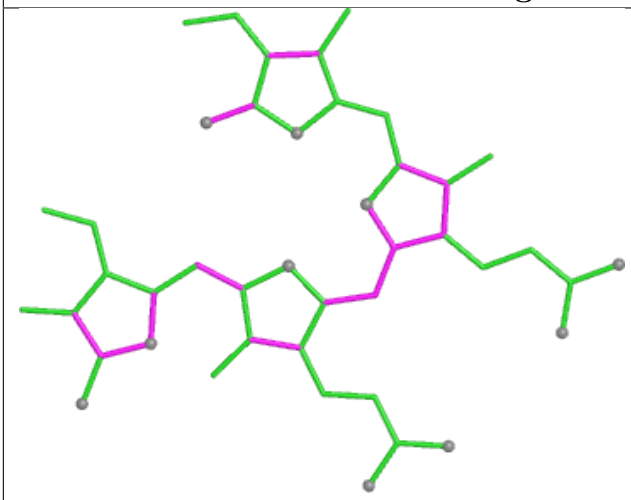


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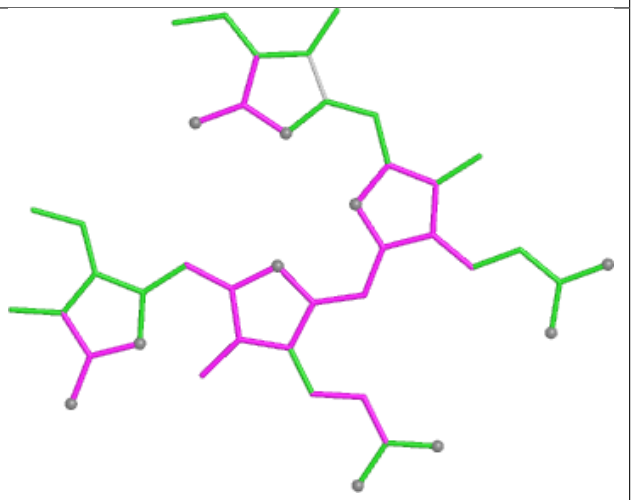


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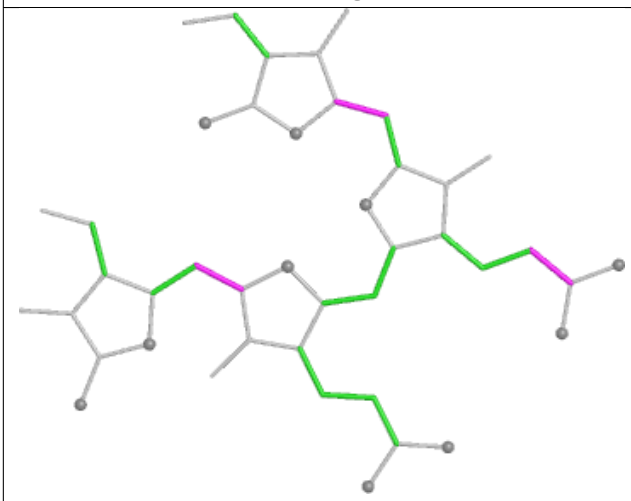
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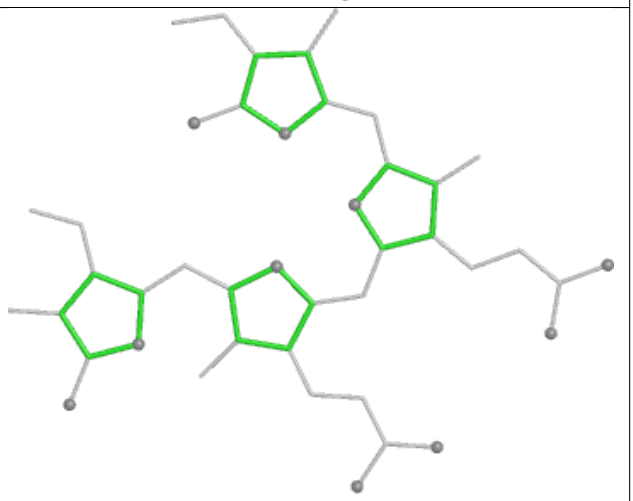
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Bond angles

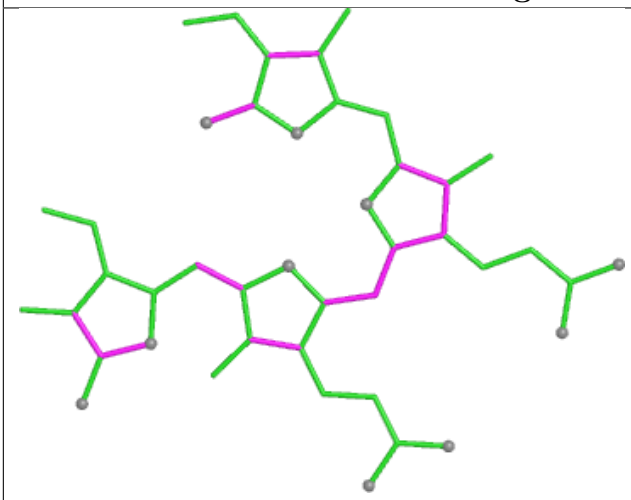


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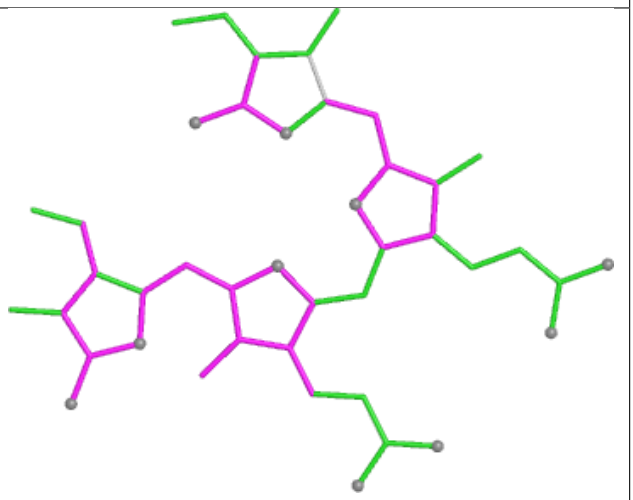


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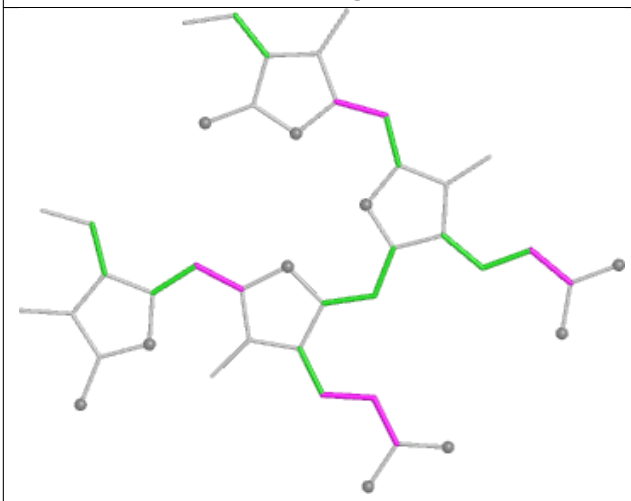
Ligand PEB dK 201



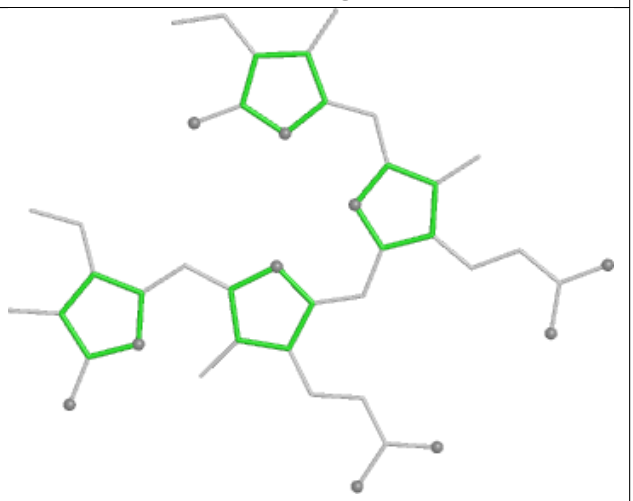
Bond lengths



Bond angles

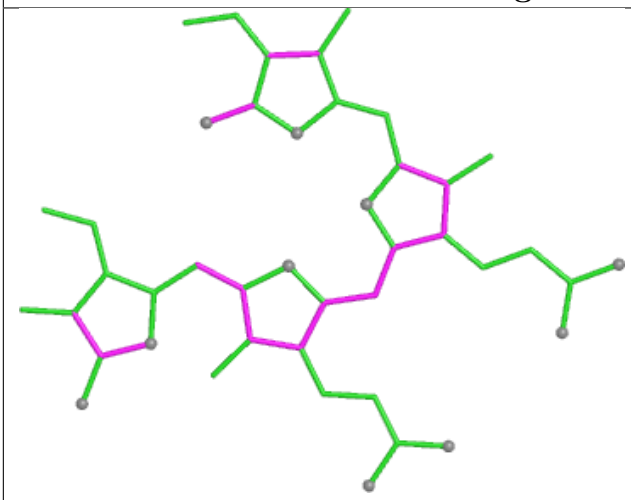


Torsions

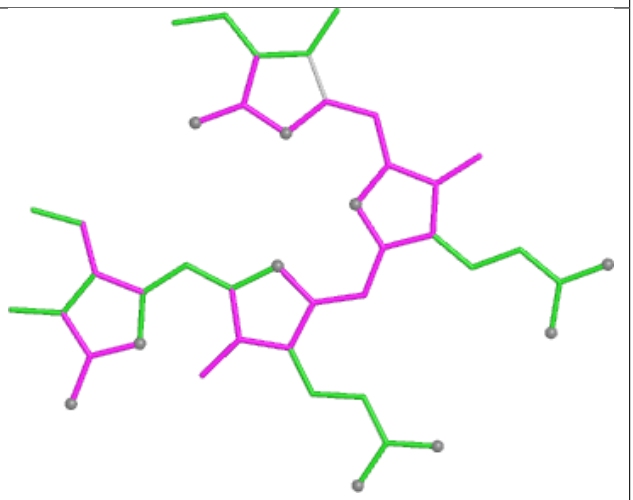


Rings

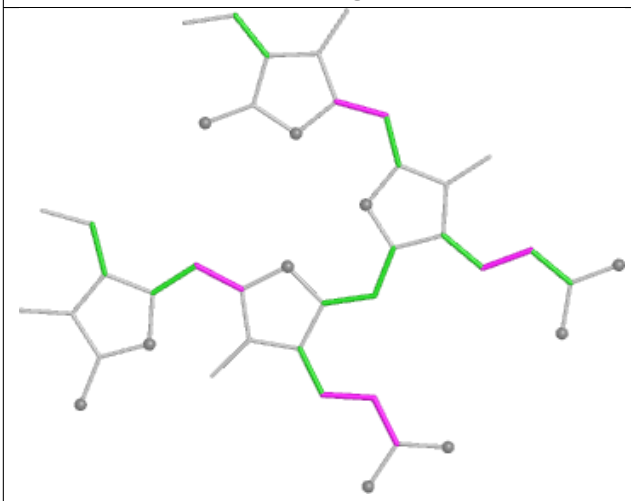
Ligand PEB kH 202



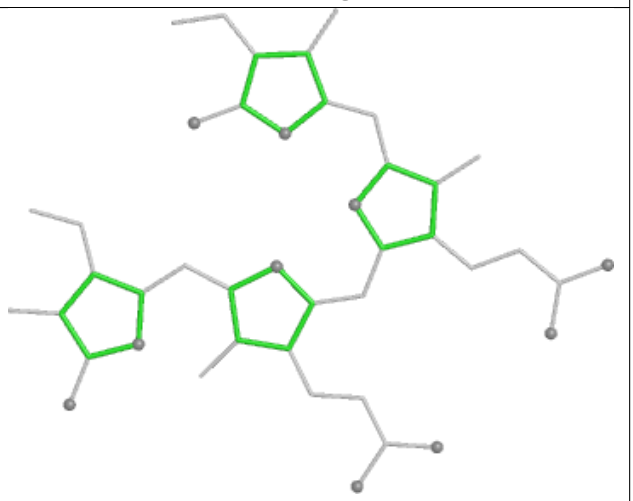
Bond lengths



Bond angles

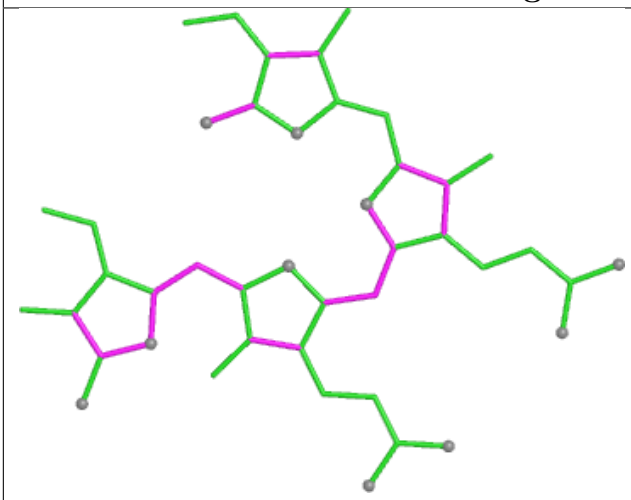


Torsions

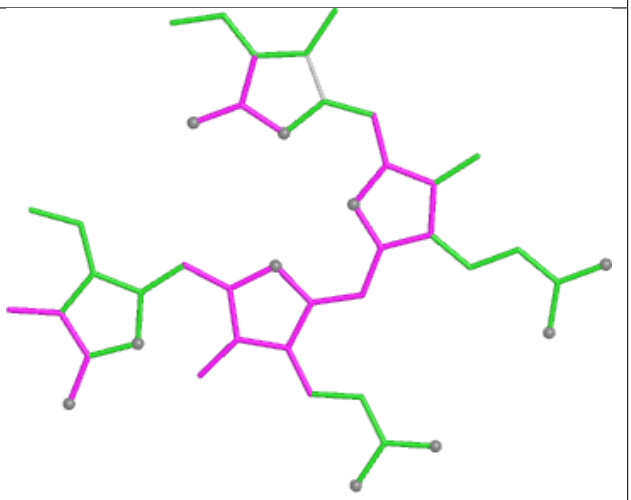


Rings

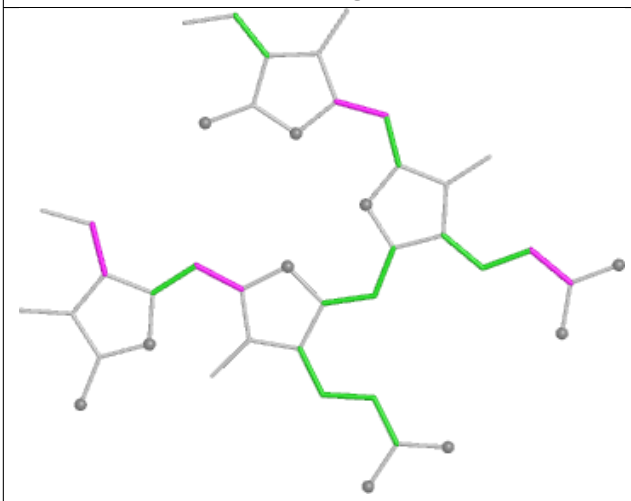
Ligand PEB l4 201



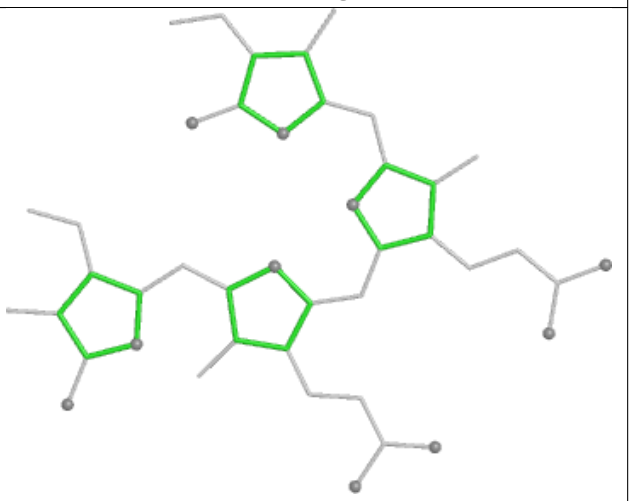
Bond lengths



Bond angles

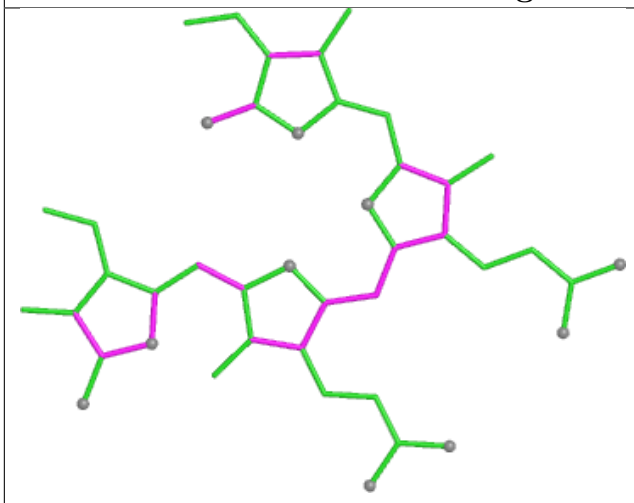


Torsions

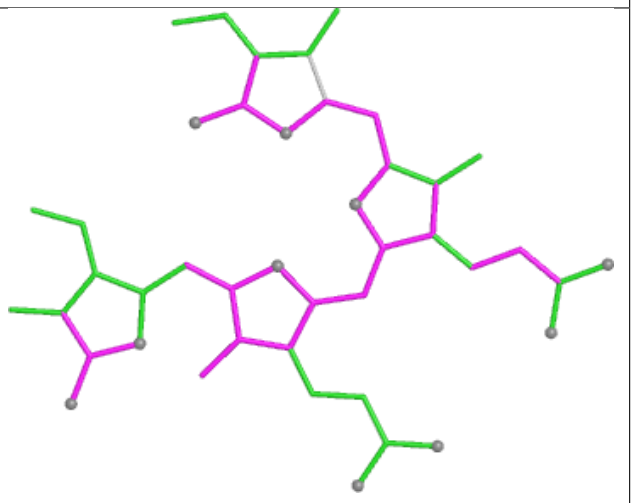


Rings

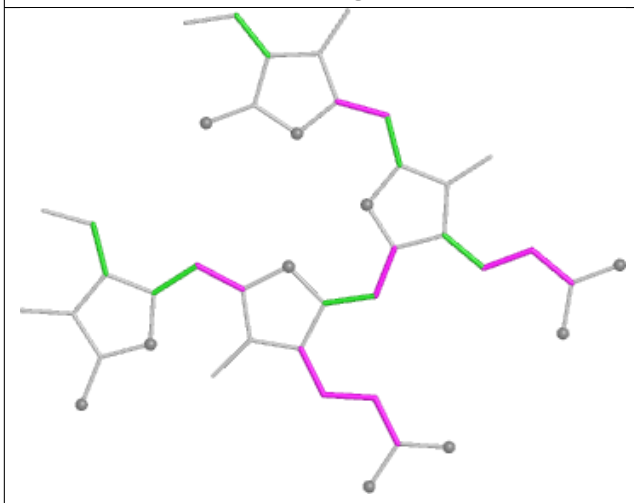
Ligand PEB aG 202



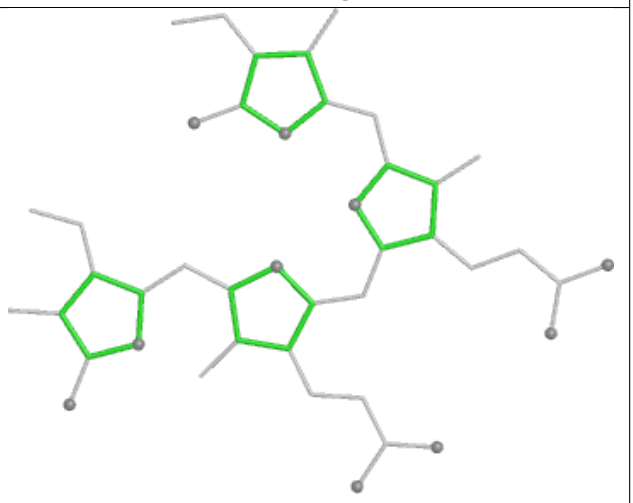
Bond lengths



Bond angles

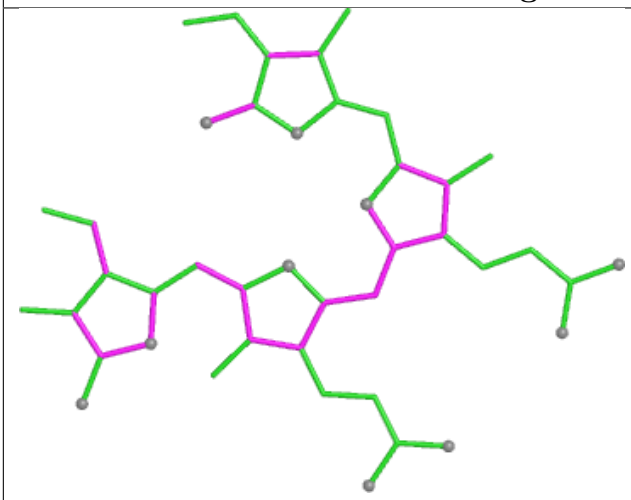


Torsions

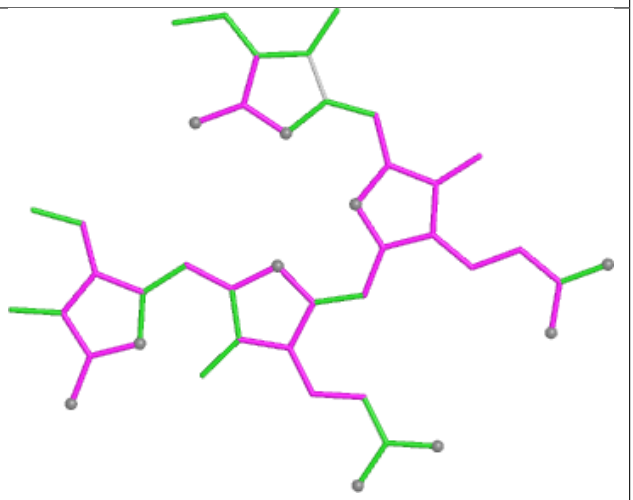


Rings

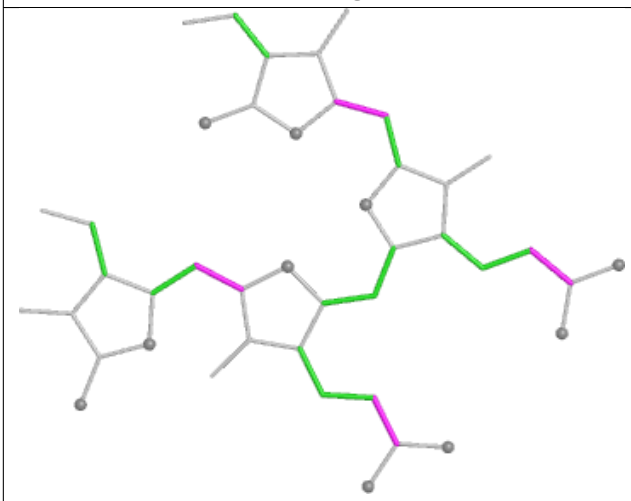
Ligand PEB ZI 401



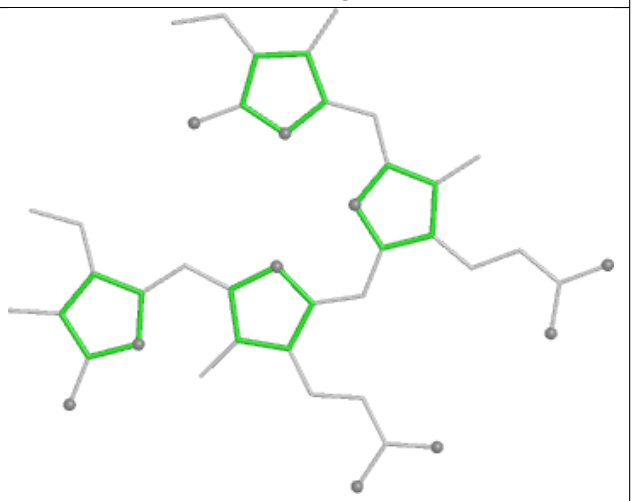
Bond lengths



Bond angles

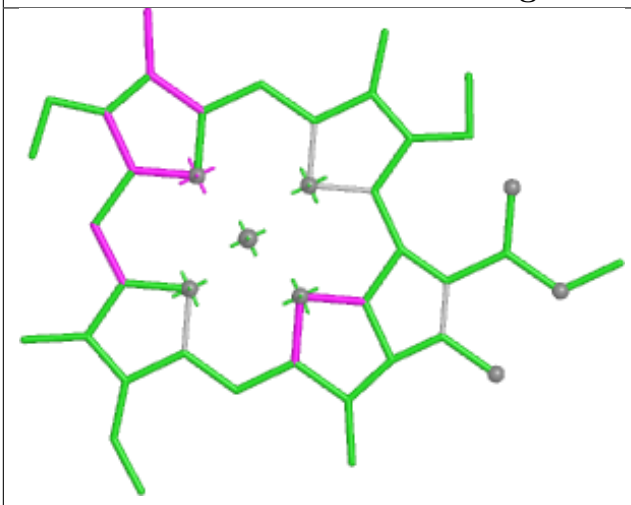


Torsions

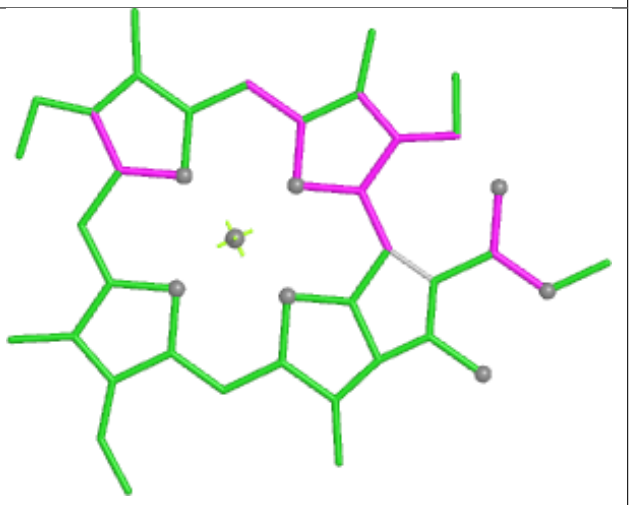


Rings

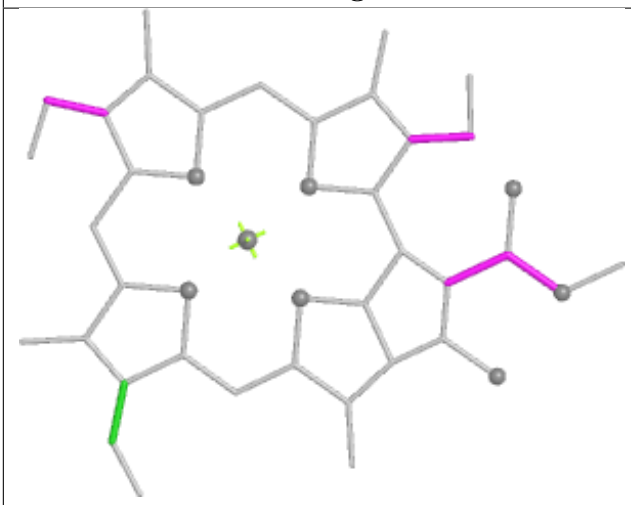
Ligand CLA 72 609



Bond lengths



Bond angles

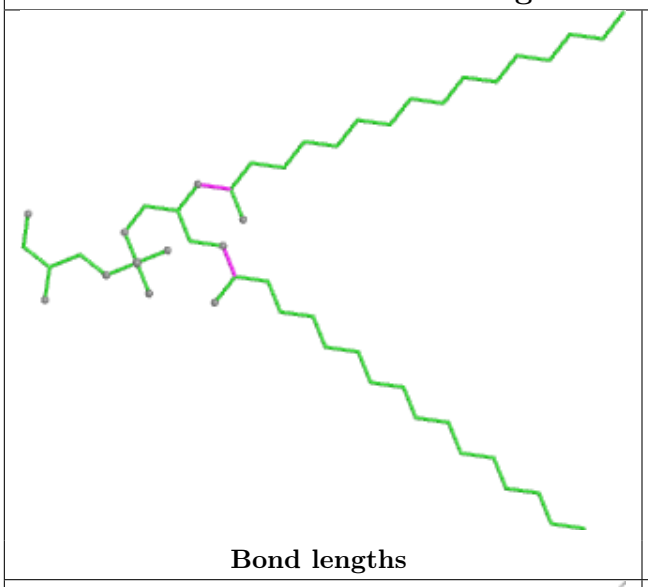


Torsions

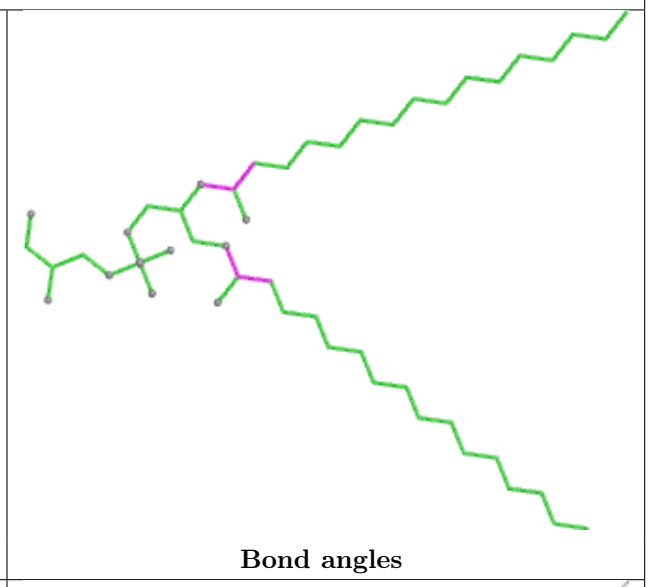


Rings

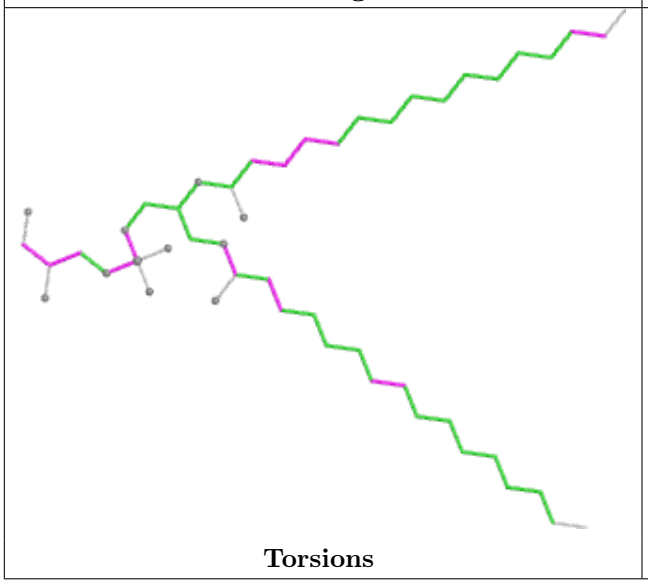
Ligand LHG B6 617



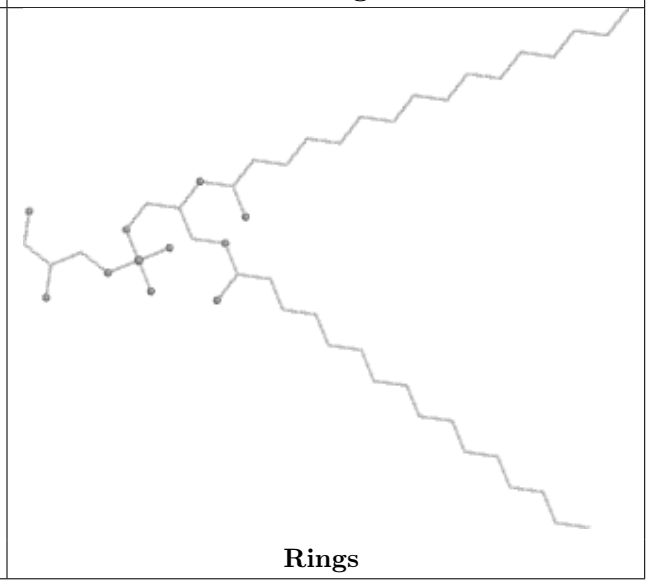
Bond lengths



Bond angles

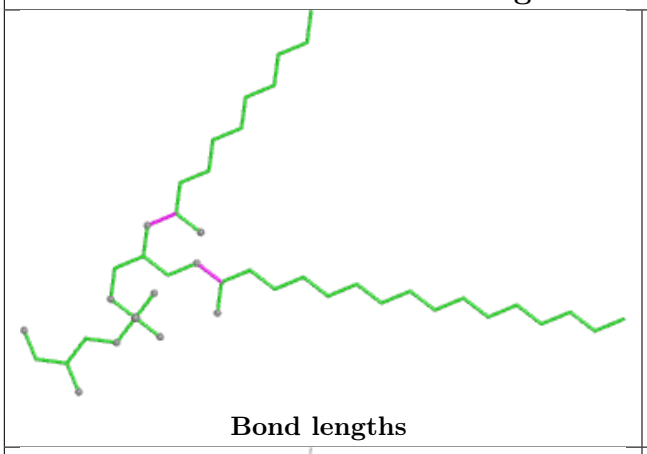


Torsions

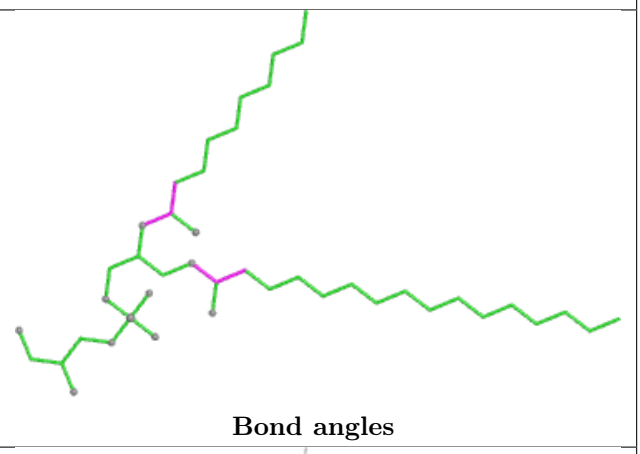


Rings

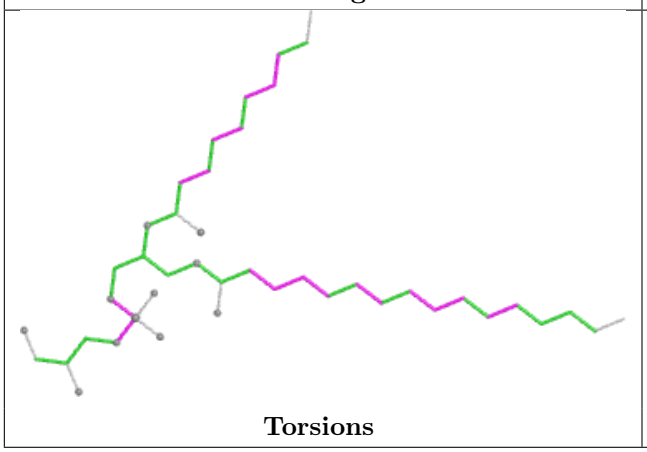
Ligand LHG D6 401



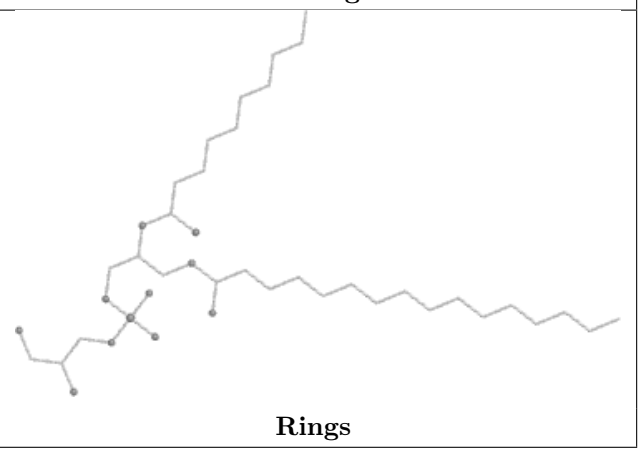
Bond lengths



Bond angles

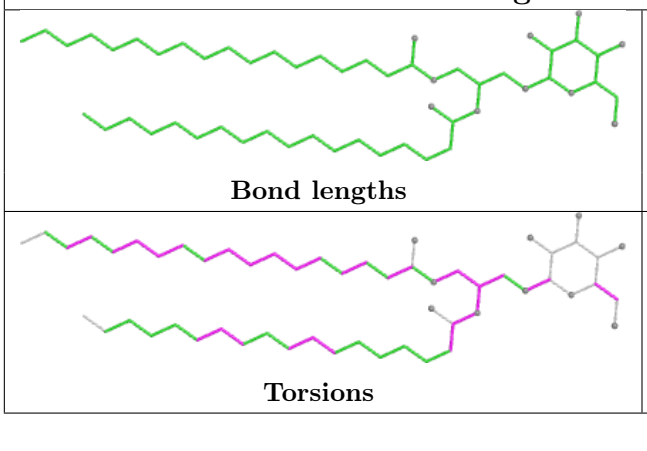


Torsions

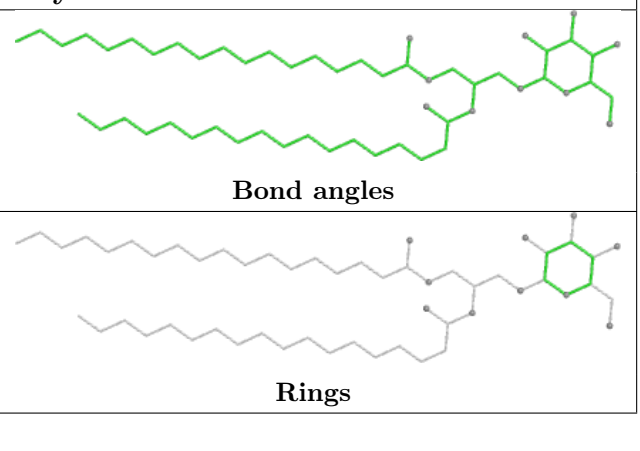


Rings

Ligand LMG yL 101



Bond lengths



Bond angles

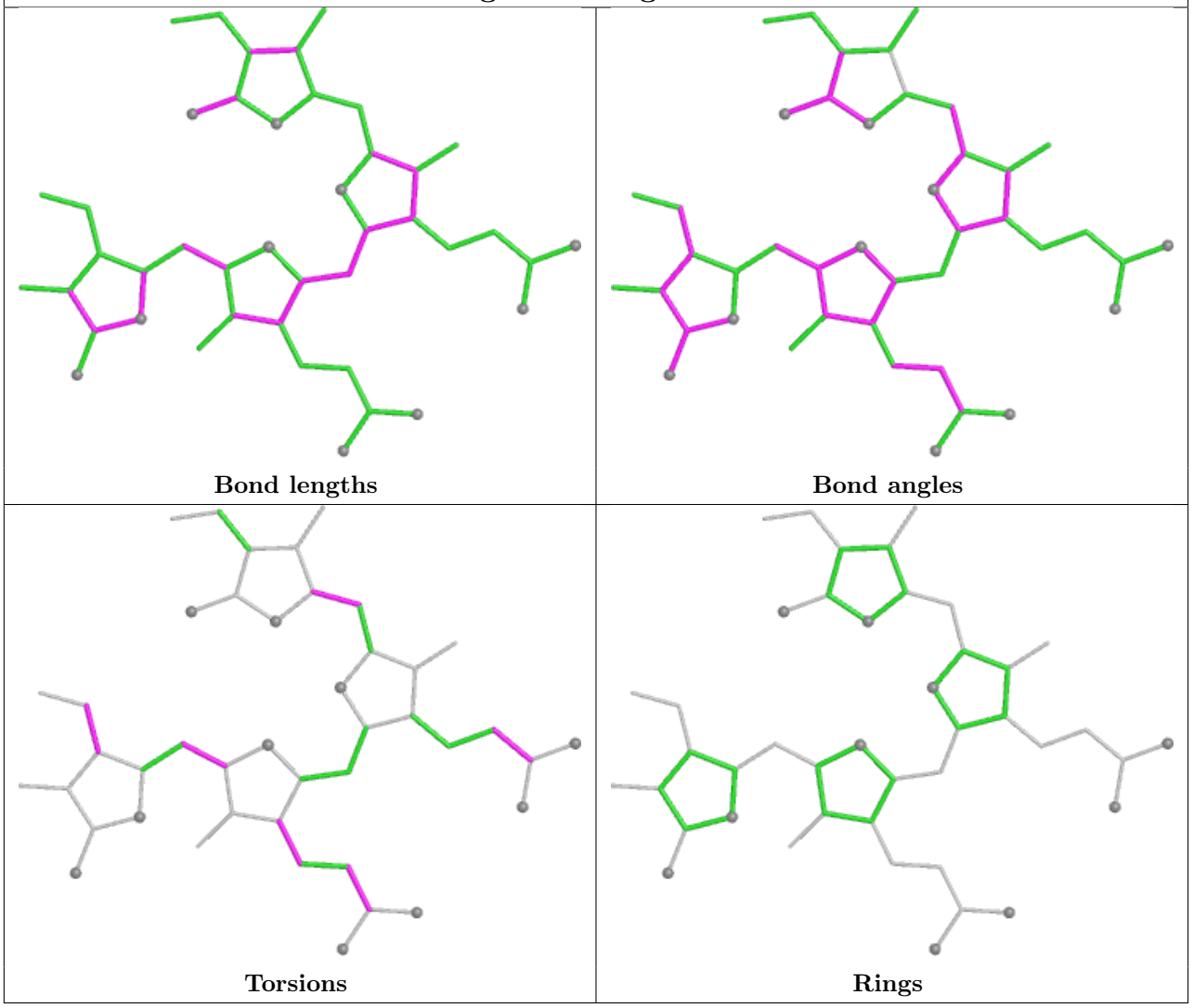


Torsions



Rings

Ligand PEB gB 201



4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

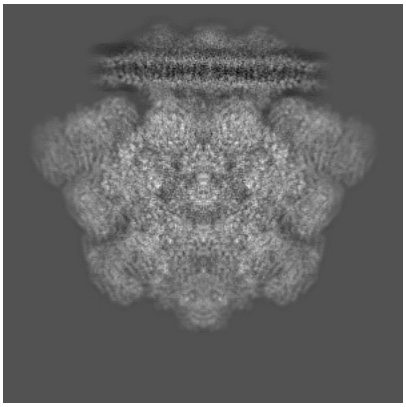
5 Map visualisation

This section contains visualisations of the EMDB entry EMD-33618. These allow visual inspection of the internal detail of the map and identification of artifacts.

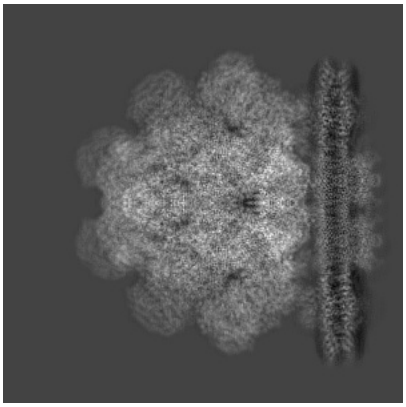
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

5.1 Orthogonal projections

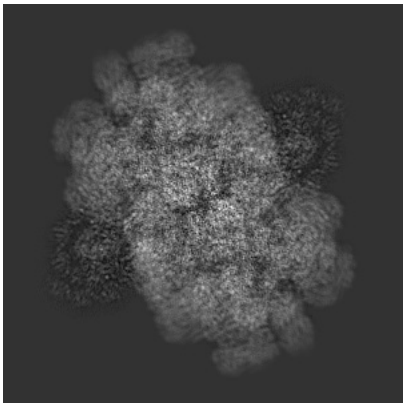
5.1.1 Primary map



X



Y

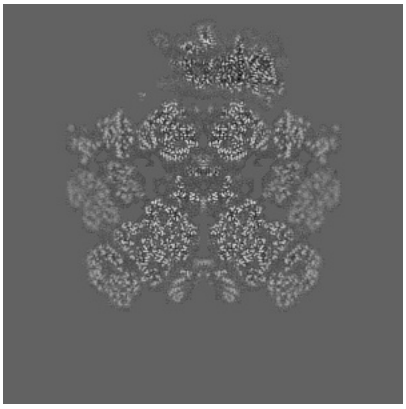


Z

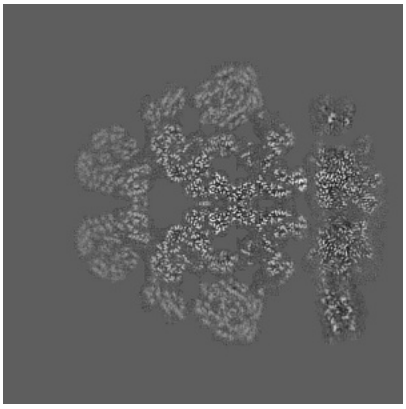
The images above show the map projected in three orthogonal directions.

5.2 Central slices

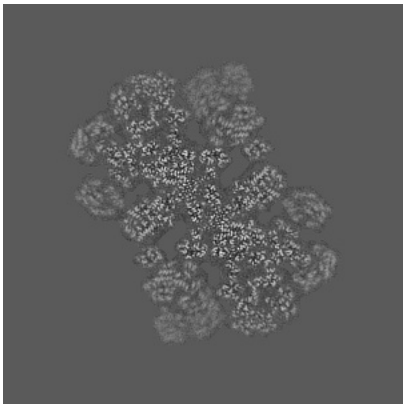
5.2.1 Primary map



X Index: 192



Y Index: 192

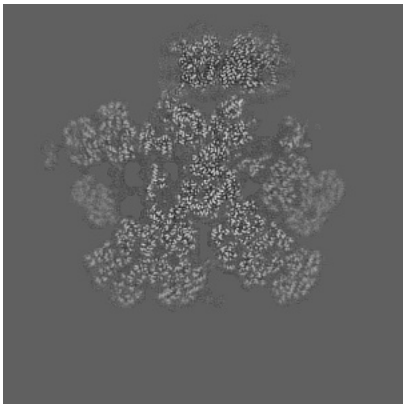


Z Index: 192

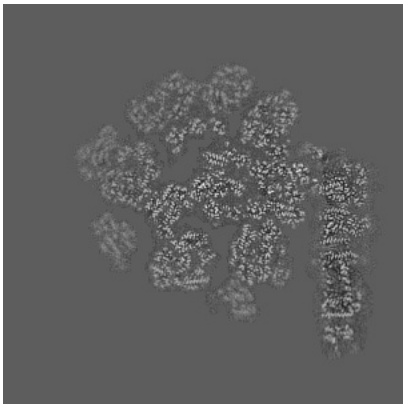
The images above show central slices of the map in three orthogonal directions.

5.3 Largest variance slices (i)

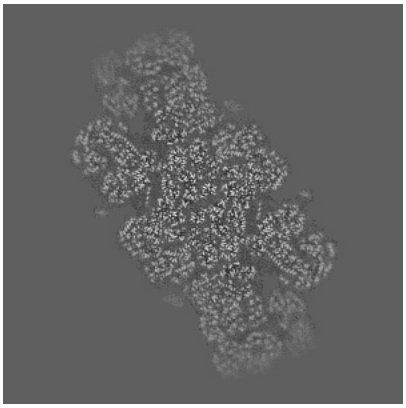
5.3.1 Primary map



X Index: 200



Y Index: 174

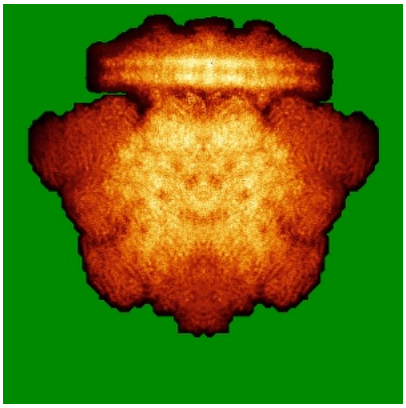


Z Index: 251

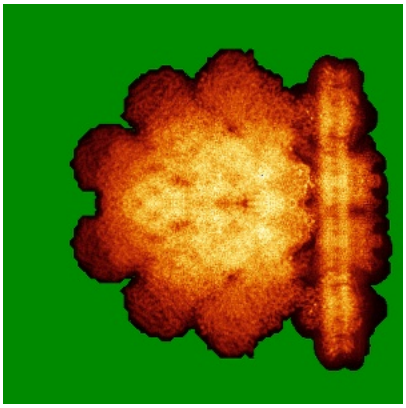
The images above show the largest variance slices of the map in three orthogonal directions.

5.4 Orthogonal standard-deviation projections (False-color) (i)

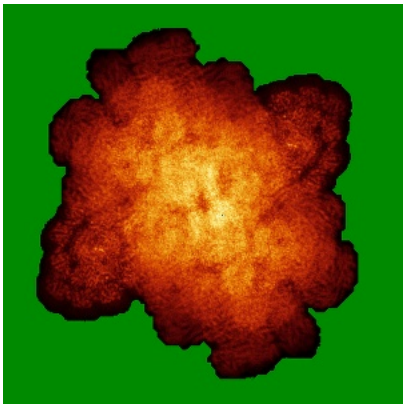
5.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

5.5 Orthogonal surface views (i)

5.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 1.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

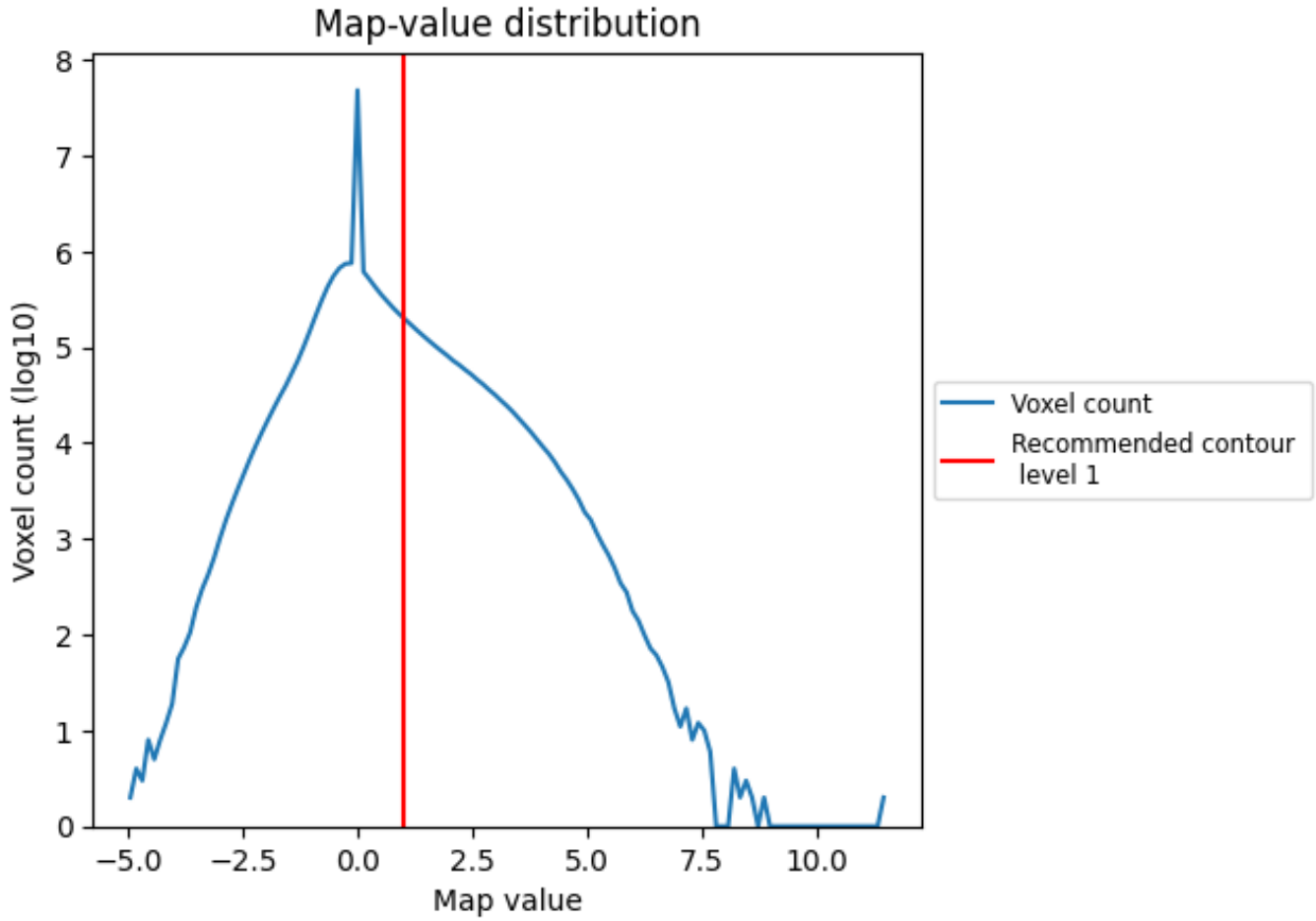
5.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

6 Map analysis

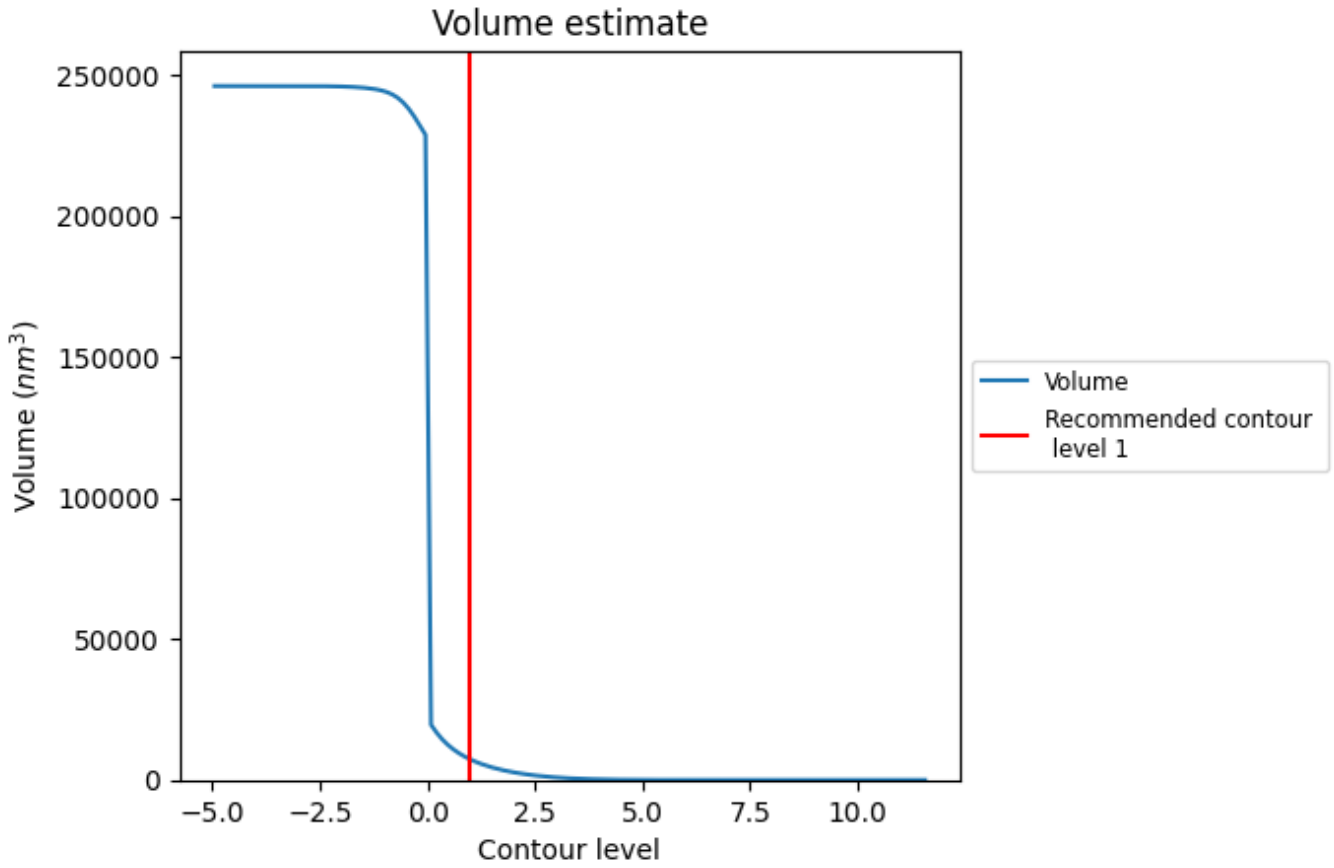
This section contains the results of statistical analysis of the map.

6.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

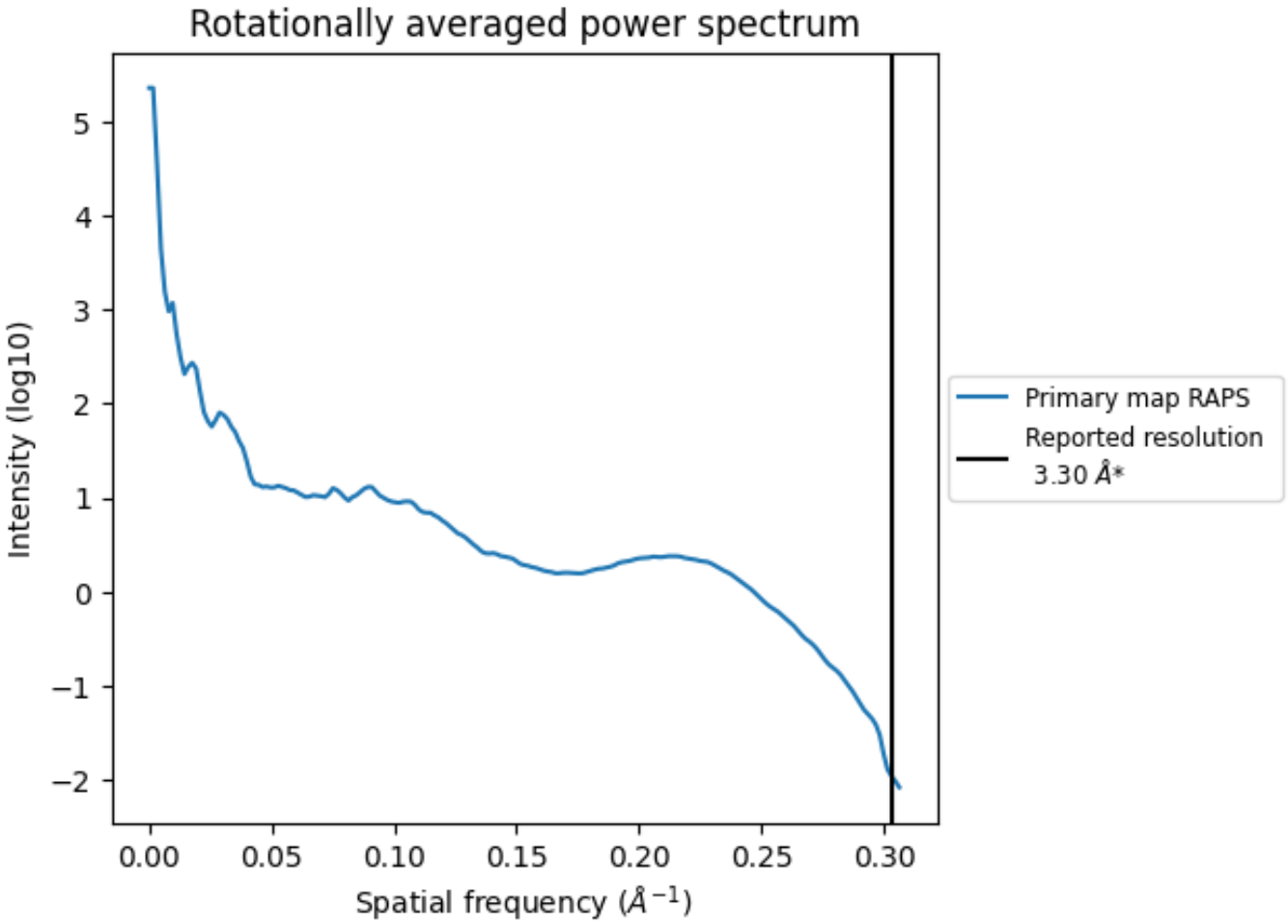
6.2 Volume estimate (i)



The volume at the recommended contour level is 7288 nm^3; this corresponds to an approximate mass of 6584 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

6.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

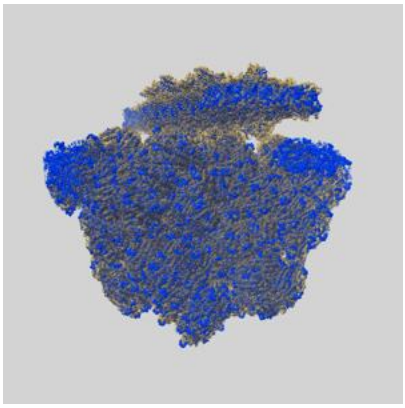
7 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

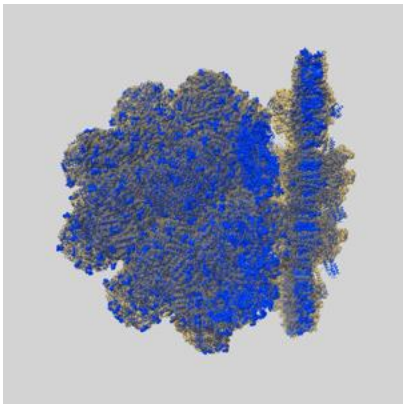
8 Map-model fit

This section contains information regarding the fit between EMDB map EMD-33618 and PDB model 7Y5E. Per-residue inclusion information can be found in section ?? on page ??.

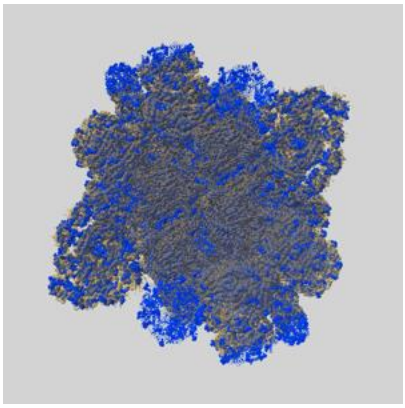
8.1 Map-model overlay



X



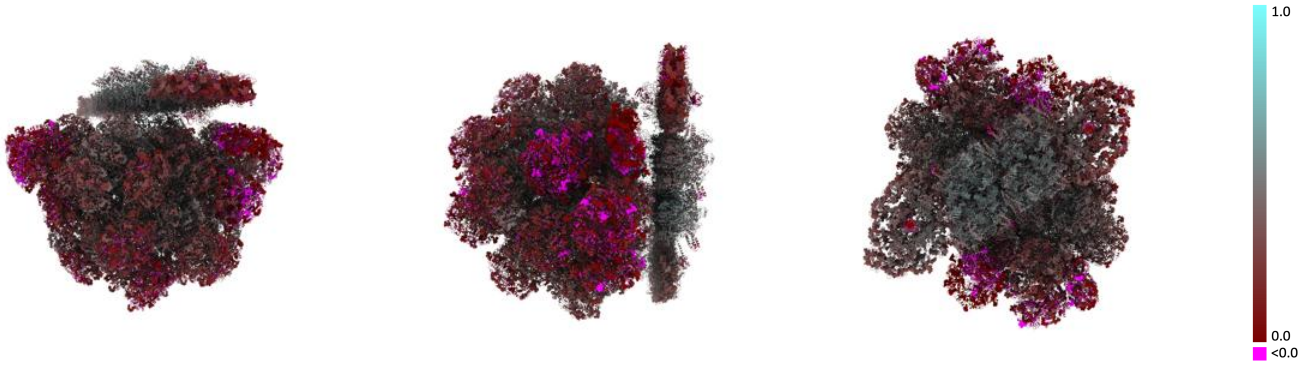
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

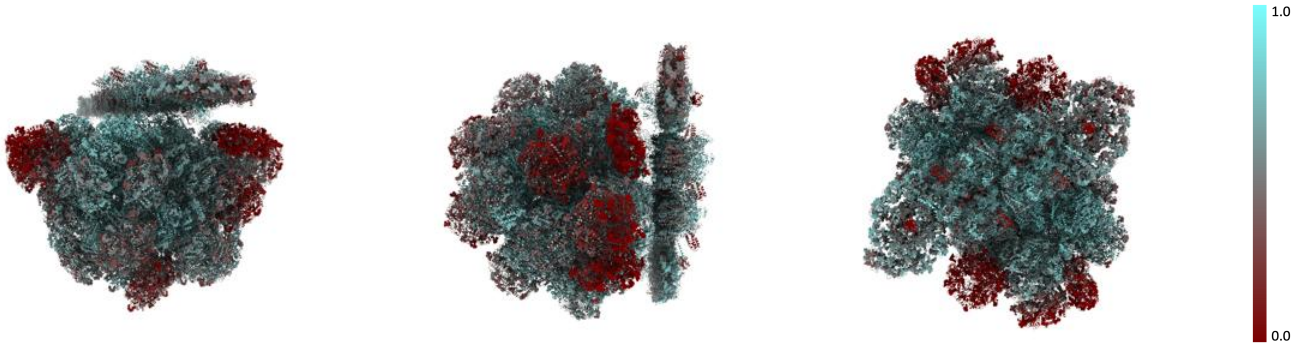
8.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

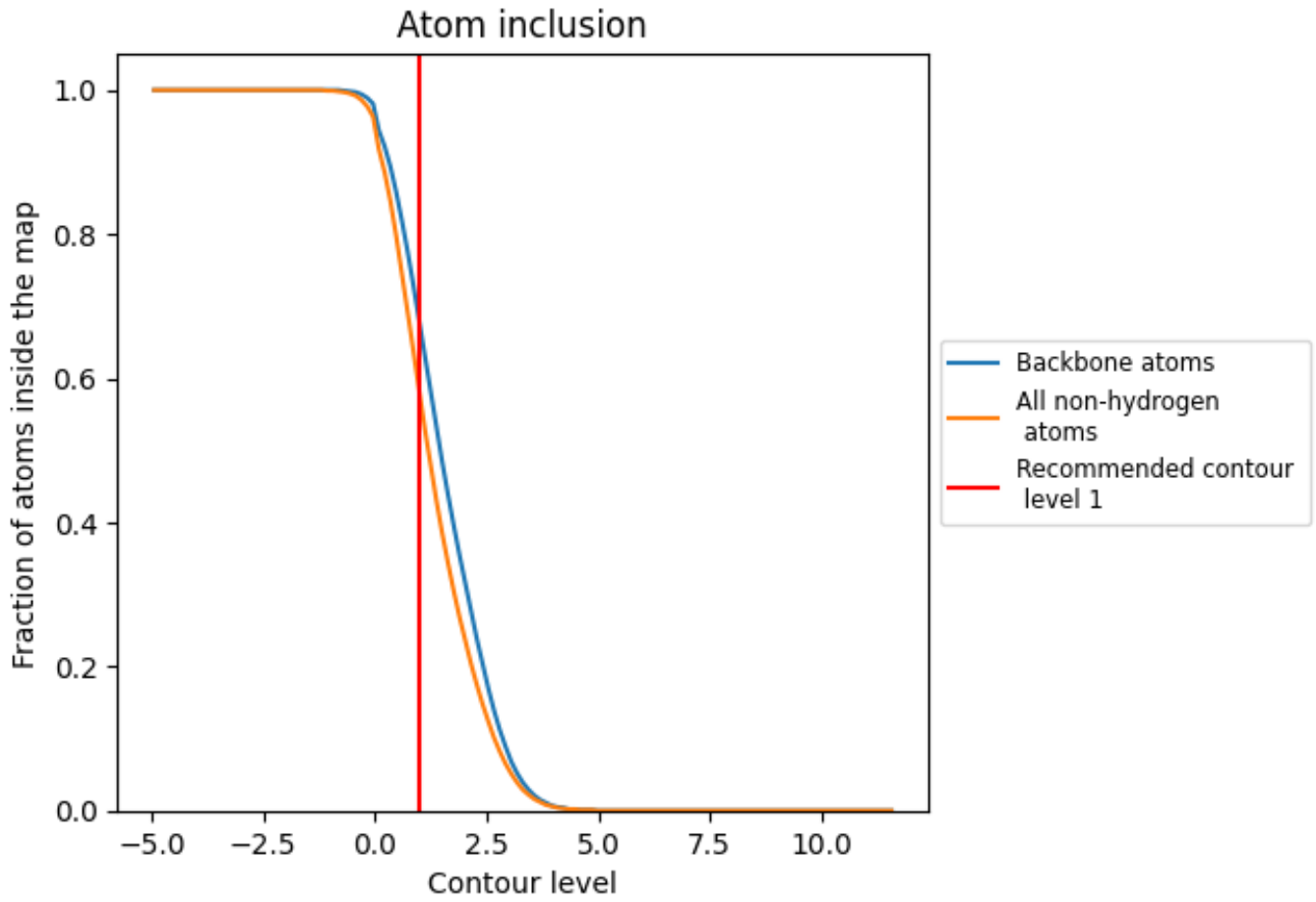
8.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1).

8.4 Atom inclusion (i)



At the recommended contour level, 68% of all backbone atoms, 58% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5780	0.3180
12	0.4390	0.1560
16	0.6930	0.3980
18	0.0110	-0.0030
1C	0.0170	-0.0110
1L	0.7440	0.3220
1N	0.5630	0.3160
22	0.4570	0.2120
23	0.7100	0.4200
2N	0.5750	0.3340
32	0.5830	0.3060
33	0.7710	0.4620
3N	0.6100	0.3390
42	0.5180	0.2400
43	0.7670	0.4570
46	0.6220	0.3040
4L	0.7420	0.3330
4N	0.6040	0.3430
52	0.4250	0.1850
53	0.5220	0.3660
5N	0.5400	0.3230
62	0.2890	0.1130
63	0.7710	0.4570
6N	0.4040	0.3020
72	0.3360	0.1330
73	0.7600	0.4500
7N	0.4790	0.3070
82	0.5420	0.3030
8N	0.6140	0.3720
A1	0.2940	0.1230
A2	0.5660	0.3550
A3	0.7480	0.4250
A4	0.6230	0.2700
A5	0.4380	0.2330
A6	0.7110	0.5100



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Chain	Atom inclusion	Q-score
A7	0.4250	0.1810
A8	0.0280	0.0110
A9	0.0050	0.0550
AA	0.4270	0.1540
AB	0.7440	0.4230
AC	0.0050	0.0160
AD	0.3150	0.1960
AE	0.6080	0.2810
AF	0.6700	0.3390
AG	0.6080	0.2770
AH	0.2880	0.1260
AI	0.4730	0.1950
AJ	0.6220	0.3700
AK	0.6660	0.3200
AL	0.7190	0.4980
AM	0.5900	0.3450
AN	0.5700	0.3960
AO	0.6270	0.2740
AP	0.7570	0.4450
AQ	0.3140	0.1880
B1	0.6570	0.3550
B2	0.5120	0.2830
B3	0.7720	0.4310
B4	0.7680	0.4330
B5	0.4910	0.2780
B6	0.6820	0.4980
B7	0.4380	0.1570
B9	0.0710	0.1180
BA	0.4400	0.1630
BB	0.7280	0.4430
BD	0.6180	0.3060
BE	0.7100	0.3920
BF	0.6910	0.3840
BG	0.7080	0.3940
BH	0.6550	0.3530
BI	0.5150	0.2070
BJ	0.7100	0.4380
BK	0.6790	0.3580
BL	0.7160	0.4930
BM	0.6970	0.4280
BN	0.5750	0.3930
BO	0.7710	0.4350

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Chain	Atom inclusion	Q-score
BP	0.7680	0.4370
BQ	0.6120	0.3060
C1	0.6210	0.2880
C2	0.7000	0.2570
C3	0.7960	0.3880
C4	0.7610	0.4170
C5	0.4900	0.1950
C6	0.6720	0.5120
C7	0.5040	0.2400
C9	0.0110	0.0710
CA	0.4910	0.2550
CB	0.7160	0.3770
CD	0.6560	0.3670
CE	0.7220	0.3850
CF	0.6920	0.3250
CG	0.7280	0.3970
CH	0.6140	0.2740
CI	0.5440	0.2480
CJ	0.7800	0.4500
CK	0.6720	0.3040
CL	0.7230	0.4980
CM	0.7670	0.4340
CN	0.7970	0.3750
CO	0.7530	0.4070
CP	0.7120	0.3890
CQ	0.6590	0.3630
D1	0.6280	0.2840
D2	0.7190	0.2960
D3	0.7460	0.4070
D4	0.7450	0.4460
D5	0.4860	0.2430
D6	0.6750	0.5030
D7	0.5410	0.2910
D9	0.0320	0.0840
DA	0.5090	0.2690
DB	0.7450	0.4660
DD	0.6850	0.3910
DE	0.7470	0.4180
DF	0.6900	0.3330
DG	0.7480	0.4270
DH	0.6310	0.2850
DI	0.5530	0.2840

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Chain	Atom inclusion	Q-score
DJ	0.7490	0.4190
DK	0.6790	0.3140
DL	0.7190	0.5040
DM	0.7490	0.4140
DN	0.7970	0.3960
DO	0.7500	0.4520
DP	0.7680	0.4440
DQ	0.6870	0.3870
E1	0.7200	0.4030
E2	0.6670	0.2100
E3	0.7260	0.4050
E4	0.7210	0.3840
E5	0.5170	0.2380
E6	0.6500	0.4730
E7	0.4670	0.2150
E9	0.2320	0.1390
EA	0.4640	0.2190
EB	0.7650	0.4090
ED	0.6680	0.3760
EE	0.7490	0.4070
EF	0.6980	0.3540
EG	0.7560	0.4000
EH	0.7310	0.4080
EI	0.4870	0.2160
EJ	0.7680	0.3980
EK	0.7070	0.3560
EL	0.7140	0.4750
EM	0.7710	0.3980
EN	0.7540	0.3700
EO	0.7330	0.3910
EP	0.7240	0.3840
EQ	0.6710	0.3740
F1	0.6780	0.3980
F2	0.4910	0.2310
F3	0.7630	0.4560
F4	0.7390	0.4120
F5	0.5900	0.3360
F6	0.6270	0.4700
F7	0.4130	0.1770
F9	0.3980	0.2610
FA	0.4070	0.1570
FB	0.6520	0.4040

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Chain	Atom inclusion	Q-score
FD	0.6570	0.3510
FE	0.7380	0.4040
FF	0.7200	0.4140
FG	0.7370	0.4110
FH	0.6850	0.3850
FI	0.5210	0.2390
FJ	0.7950	0.4480
FK	0.7370	0.4340
FL	0.6950	0.4770
FM	0.8000	0.4450
FN	0.5630	0.3470
FO	0.7420	0.4180
FP	0.7410	0.4150
FQ	0.6740	0.3560
G1	0.6390	0.2780
G2	0.0110	0.0720
G3	0.7550	0.4300
G4	0.7530	0.4220
G5	0.5760	0.2980
G6	0.0600	0.3190
G7	0.4500	0.2370
G9	0.3250	0.1930
GA	0.4390	0.2220
GB	0.7290	0.4480
GD	0.6260	0.3100
GE	0.7740	0.4330
GF	0.6890	0.3570
GG	0.7610	0.4270
GH	0.6540	0.2780
GI	0.5480	0.2920
GJ	0.7400	0.3910
GK	0.6980	0.3740
GL	0.2180	0.3740
GM	0.7420	0.3840
GN	0.0060	0.0830
GO	0.7570	0.4260
GP	0.7150	0.3730
GQ	0.6320	0.3200
H1	0.6460	0.3120
H3	0.7880	0.4350
H4	0.7270	0.4210
H5	0.5440	0.2540

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Chain	Atom inclusion	Q-score
H6	0.6180	0.4890
H7	0.5480	0.3290
H9	0.2580	0.1700
HA	0.5300	0.3250
HB	0.7410	0.4420
HD	0.6410	0.2980
HE	0.7390	0.4350
HF	0.7230	0.3570
HG	0.7460	0.4320
HH	0.6530	0.3250
HI	0.5360	0.2960
HJ	0.7300	0.4350
HK	0.7270	0.3650
HL	0.6780	0.4770
HM	0.7090	0.4300
HO	0.7270	0.4240
HP	0.7250	0.3940
HQ	0.6350	0.2910
I1	0.6600	0.3090
I2	0.4960	0.3430
I3	0.7740	0.4590
I4	0.7210	0.3640
I5	0.5170	0.2950
I6	0.6460	0.4830
I7	0.4220	0.1720
I9	0.2770	0.1560
IA	0.4090	0.1640
IB	0.7670	0.4570
ID	0.7130	0.3890
IE	0.7650	0.4080
IF	0.7220	0.4070
IG	0.7610	0.3980
IH	0.6700	0.3230
II	0.5320	0.2740
IJ	0.7390	0.4290
IK	0.7330	0.4050
IL	0.7450	0.4990
IM	0.7390	0.4260
IN	0.5260	0.4050
IO	0.7170	0.3660
IP	0.7410	0.4200
IQ	0.7220	0.3940

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Chain	Atom inclusion	Q-score
J1	0.6520	0.2870
J2	0.4720	0.3000
J3	0.7620	0.4380
J4	0.7090	0.3750
J5	0.4780	0.3140
J6	0.5690	0.4910
J7	0.4290	0.1720
J9	0.1950	0.1400
JA	0.4210	0.1550
JB	0.7690	0.4640
JD	0.5980	0.2520
JE	0.7390	0.3780
JF	0.7260	0.4140
JG	0.7420	0.3780
JH	0.6790	0.3180
JI	0.4530	0.1860
JJ	0.7820	0.4220
JK	0.7240	0.4020
JL	0.6670	0.5040
JM	0.7830	0.4260
JN	0.4900	0.3870
JO	0.7110	0.3720
JP	0.7920	0.4610
JQ	0.6080	0.2440
K1	0.6710	0.3640
K2	0.5780	0.3520
K3	0.7840	0.4200
K4	0.7250	0.3600
K5	0.4820	0.2770
K6	0.6160	0.4950
K7	0.4440	0.1950
K9	0.1260	0.0840
KA	0.4240	0.1810
KB	0.6620	0.4160
KD	0.6150	0.2870
KE	0.7080	0.3380
KF	0.6890	0.3600
KG	0.7070	0.3390
KH	0.6480	0.3400
KI	0.4650	0.2090
KJ	0.7480	0.4680
KK	0.6650	0.3460

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Chain	Atom inclusion	Q-score
KL	0.6760	0.4910
KM	0.7440	0.4560
KN	0.6150	0.3590
KO	0.7090	0.3410
KP	0.7760	0.4570
KQ	0.6130	0.2900
L1	0.6910	0.3750
L2	0.5930	0.3790
L3	0.8090	0.4610
L4	0.6930	0.3380
L5	0.5480	0.2920
L6	0.5980	0.4920
L7	0.5000	0.2640
L9	0.2430	0.1370
LA	0.5010	0.2610
LB	0.7090	0.3730
LD	0.6180	0.2740
LE	0.7280	0.3730
LF	0.7210	0.3700
LG	0.7210	0.3780
LH	0.6710	0.3580
LI	0.5870	0.3410
LJ	0.7500	0.4680
LK	0.7140	0.3750
LL	0.7250	0.4950
LM	0.7580	0.4700
LN	0.6400	0.4050
LO	0.6800	0.3310
LP	0.7710	0.4400
LQ	0.6110	0.2800
M1	0.6630	0.2500
M2	0.5290	0.3000
M3	0.7490	0.4190
M4	0.7530	0.4140
M5	0.5460	0.3270
M6	0.5600	0.4780
M7	0.6690	0.3310
M9	0.3150	0.2180
MA	0.6500	0.3180
MB	0.7320	0.3950
MD	0.6320	0.3020
ME	0.7460	0.3930

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Chain	Atom inclusion	Q-score
MF	0.6270	0.2830
MG	0.7450	0.3990
MH	0.6430	0.2570
MI	0.5700	0.3280
MJ	0.7810	0.4760
MK	0.6000	0.2580
ML	0.5600	0.4780
MM	0.7760	0.4710
MN	0.5750	0.3730
MO	0.7370	0.4010
MP	0.7790	0.4490
MQ	0.6320	0.2990
N1	0.6430	0.2840
N2	0.2940	0.1860
N3	0.7790	0.4520
N4	0.7210	0.3850
N5	0.4200	0.2170
N6	0.8690	0.4710
N7	0.7080	0.3850
N9	0.0070	0.0600
NA	0.6920	0.3590
NB	0.7470	0.4600
ND	0.2390	0.1150
NE	0.7060	0.3660
NF	0.6310	0.3190
NG	0.7120	0.3740
NH	0.6210	0.2680
NI	0.4880	0.1890
NJ	0.7880	0.4800
NK	0.6070	0.2930
NL	0.8760	0.4730
NM	0.7700	0.4780
NN	0.3500	0.2660
NO	0.7180	0.3740
NP	0.7720	0.4450
NQ	0.2230	0.0980
O1	0.5620	0.2530
O2	0.6240	0.3700
O3	0.8180	0.4250
O4	0.7110	0.3840
O5	0.4900	0.2910
O6	0.6570	0.4820

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Chain	Atom inclusion	Q-score
O7	0.7180	0.3890
O9	0.0700	0.1180
OA	0.7220	0.3910
OB	0.6480	0.4070
OD	0.2720	0.1190
OE	0.7270	0.3900
OF	0.6450	0.3220
OG	0.7250	0.4040
OH	0.5310	0.2350
OI	0.5140	0.2040
OJ	0.7210	0.4020
OK	0.6360	0.3080
OL	0.6790	0.4520
OM	0.7160	0.3900
ON	0.7070	0.3790
OO	0.7190	0.3810
OP	0.7180	0.4080
OQ	0.2750	0.1040
P1	0.6430	0.3680
P3	0.7890	0.4340
P4	0.7260	0.3910
P5	0.4720	0.2080
P7	0.7030	0.3710
P9	0.0110	0.0580
PA	0.6890	0.3660
PB	0.7740	0.4450
PD	0.2960	0.1730
PE	0.7400	0.4270
PF	0.6850	0.3610
PG	0.7460	0.4340
PH	0.6260	0.3510
PI	0.5370	0.2330
PJ	0.6950	0.4030
PK	0.6740	0.3390
PM	0.6820	0.3860
PO	0.7150	0.3920
PP	0.7730	0.4490
PQ	0.3180	0.1880
Q1	0.5540	0.2570
Q3	0.7810	0.4540
Q4	0.7310	0.4040
Q5	0.5010	0.2450

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Chain	Atom inclusion	Q-score
Q6	0.5820	0.4370
Q7	0.7230	0.4150
Q9	0.0320	0.1040
QA	0.7170	0.4150
QB	0.7290	0.4300
QD	0.3580	0.2180
QE	0.6920	0.3540
QF	0.6570	0.3490
QG	0.6870	0.3520
QH	0.5560	0.2480
QI	0.5570	0.2900
QJ	0.6900	0.3780
QK	0.6570	0.3490
QL	0.6490	0.4210
QM	0.7060	0.3730
QO	0.7210	0.4130
QP	0.7160	0.3810
QQ	0.3470	0.1910
R1	0.5010	0.2200
R2	0.4400	0.1690
R3	0.7570	0.4320
R4	0.7600	0.4430
R5	0.5290	0.2510
R6	0.4860	0.4130
R7	0.7100	0.4050
R9	0.2250	0.1540
RA	0.7070	0.4070
RB	0.7010	0.3170
RD	0.2840	0.1240
RE	0.7020	0.3700
RF	0.6800	0.3790
RG	0.7040	0.3800
RH	0.4700	0.2060
RI	0.4840	0.2220
RJ	0.7320	0.4260
RK	0.6820	0.3980
RL	0.6040	0.4280
RM	0.7260	0.4150
RN	0.5810	0.3530
RO	0.7550	0.4460
RP	0.7510	0.4180
RQ	0.3010	0.1230

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Chain	Atom inclusion	Q-score
S1	0.5600	0.2580
S3	0.7940	0.4500
S4	0.7240	0.3950
S5	0.5870	0.3280
S6	0.7500	0.4170
S7	0.7270	0.4040
S9	0.3910	0.2720
SA	0.7240	0.4080
SB	0.7720	0.4590
SD	0.2880	0.0990
SE	0.6850	0.3570
SF	0.7100	0.3950
SG	0.6740	0.3520
SH	0.5710	0.2700
SI	0.5190	0.2630
SJ	0.6880	0.3830
SK	0.7030	0.4000
SL	0.8170	0.4300
SM	0.6690	0.3700
SO	0.7280	0.3990
SP	0.7230	0.3830
SQ	0.3060	0.0970
T1	0.6080	0.2940
T3	0.7820	0.4270
T4	0.7220	0.3960
T5	0.5800	0.3030
T6	0.6100	0.4700
T7	0.7410	0.4240
T9	0.3250	0.1890
TA	0.7430	0.4340
TB	0.7690	0.4630
TD	0.3060	0.1040
TE	0.7310	0.4150
TF	0.6970	0.4080
TG	0.7340	0.4120
TH	0.6150	0.3040
TI	0.5680	0.3210
TJ	0.7290	0.4280
TK	0.7050	0.4180
TL	0.6510	0.4900
TM	0.6960	0.4160
TO	0.7150	0.4010

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Chain	Atom inclusion	Q-score
TP	0.7320	0.4010
TQ	0.2830	0.1160
U1	0.5340	0.1900
U3	0.7820	0.4650
U4	0.7320	0.4020
U5	0.5610	0.2720
U6	0.7230	0.4830
U7	0.6800	0.3500
U9	0.2560	0.1650
UA	0.6880	0.3560
UB	0.6830	0.4220
UD	0.4010	0.2320
UE	0.6980	0.3480
UF	0.6920	0.3810
UG	0.6940	0.3470
UH	0.5370	0.2140
UI	0.5470	0.3030
UJ	0.7210	0.4320
UK	0.7040	0.3850
UL	0.7660	0.4570
UM	0.7060	0.4210
UO	0.7360	0.4050
UP	0.7560	0.4300
UQ	0.4260	0.2460
V1	0.4730	0.2170
V3	0.8100	0.4390
V4	0.7420	0.4440
V5	0.5380	0.3090
V6	0.6850	0.4510
V7	0.6740	0.3450
V9	0.2730	0.1480
VA	0.6570	0.3360
VB	0.6540	0.3360
VD	0.3050	0.1070
VE	0.6780	0.3410
VF	0.6560	0.3460
VG	0.6740	0.3320
VH	0.4940	0.2210
VI	0.5540	0.2830
VJ	0.6940	0.4060
VK	0.6560	0.3400
VL	0.7370	0.4530

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Chain	Atom inclusion	Q-score
VM	0.6860	0.3990
VO	0.7490	0.4440
VP	0.7910	0.4630
VQ	0.3050	0.1000
W1	0.6000	0.2190
W3	0.7840	0.4530
W4	0.7160	0.3830
W5	0.4850	0.3140
W6	0.7740	0.4690
W7	0.6740	0.3180
W9	0.1900	0.1360
WA	0.6700	0.3220
WB	0.7040	0.3740
WD	0.2690	0.1110
WE	0.6920	0.3710
WF	0.6780	0.3460
WG	0.6910	0.3630
WH	0.5950	0.2170
WI	0.4620	0.2090
WJ	0.7530	0.4700
WK	0.6620	0.3250
WL	0.8010	0.4500
WM	0.7430	0.4610
WO	0.7130	0.3890
WP	0.7880	0.4570
WQ	0.2750	0.1110
X1	0.6160	0.3490
X3	0.8020	0.4840
X4	0.7710	0.4640
X5	0.4750	0.2740
X6	0.5860	0.4440
X7	0.7050	0.3670
X9	0.1420	0.0960
XA	0.7210	0.3700
XB	0.7170	0.3530
XD	0.2630	0.1340
XE	0.7670	0.4540
XF	0.7190	0.4280
XG	0.7620	0.4510
XH	0.6100	0.3470
XI	0.4900	0.2240
XJ	0.7290	0.4450

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Chain	Atom inclusion	Q-score
XK	0.7210	0.4190
XL	0.6160	0.4550
XM	0.7170	0.4360
XO	0.7770	0.4670
XP	0.7590	0.4410
XQ	0.2550	0.1350
Y1	0.6040	0.2850
Y3	0.6630	0.4760
Y4	0.7260	0.3940
Y5	0.5360	0.2940
Y6	0.5320	0.3820
Y7	0.5110	0.2800
Y9	0.2760	0.1570
YA	0.4970	0.2620
YB	0.7460	0.4220
YD	0.3790	0.2160
YE	0.7450	0.4360
YF	0.4110	0.1010
YG	0.7530	0.4280
YH	0.5790	0.2800
YI	0.5910	0.3400
YJ	0.7360	0.4560
YK	0.3940	0.0840
YL	0.6120	0.4690
YM	0.7280	0.4450
YO	0.7410	0.4070
YP	0.7620	0.4350
YQ	0.3590	0.1990
Z1	0.5160	0.1800
Z2	0.5880	0.3520
Z3	0.7080	0.4380
Z4	0.7520	0.4260
Z5	0.5570	0.3260
Z6	0.5430	0.4400
Z9	0.3130	0.2170
ZB	0.3370	0.3380
ZE	0.6890	0.3630
ZF	0.3780	0.1060
ZG	0.7090	0.3870
ZH	0.5000	0.1630
ZI	0.5750	0.3260
ZJ	0.7490	0.4650

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Chain	Atom inclusion	Q-score
ZK	0.3720	0.0990
ZL	0.6150	0.4430
ZM	0.7350	0.4600
ZN	0.7540	0.3610
ZO	0.7500	0.4240
a1	0.4870	0.1970
a3	0.7590	0.4700
a4	0.7470	0.4510
a6	0.6530	0.4980
a8	0.3520	0.1150
aB	0.7600	0.4400
aC	0.4990	0.2680
aE	0.6870	0.3650
aF	0.4650	0.1710
aG	0.6980	0.3610
aH	0.5020	0.1950
aJ	0.6280	0.3560
aK	0.4670	0.1670
aL	0.6750	0.4680
aM	0.6250	0.3570
aO	0.7510	0.4570
b1	0.2820	0.0700
b3	0.7410	0.4140
b4	0.5530	0.1820
b6	0.7000	0.5180
bB	0.6790	0.2930
bE	0.5870	0.2540
bF	0.5440	0.2490
bG	0.5980	0.2500
bH	0.3100	0.1050
bJ	0.7500	0.4510
bK	0.5350	0.2350
bL	0.7050	0.4850
bM	0.7550	0.4560
bO	0.5600	0.2040
bP	0.7650	0.4340
c1	0.3740	0.1170
c3	0.7530	0.4250
c4	0.5110	0.1600
c6	0.5880	0.4770
cB	0.6940	0.3560
cE	0.6150	0.2870

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Chain	Atom inclusion	Q-score
cF	0.4670	0.1850
cG	0.6130	0.2790
cH	0.3750	0.1200
cJ	0.5680	0.2760
cK	0.4690	0.1880
cL	0.6040	0.4370
cM	0.5850	0.2810
cO	0.5120	0.1570
d1	0.3150	0.0630
d3	0.7390	0.4060
d4	0.5890	0.2480
d6	0.6840	0.5120
dB	0.7020	0.3360
dD	0.6800	0.3680
dE	0.5500	0.1940
dF	0.4750	0.2030
dG	0.5540	0.1990
dH	0.3010	0.0640
dJ	0.6050	0.3480
dK	0.4800	0.2070
dL	0.6780	0.4700
dM	0.5890	0.3400
dO	0.5780	0.2480
dQ	0.6790	0.3750
e1	0.1700	0.0350
e3	0.7820	0.4020
e4	0.6330	0.3020
e6	0.6610	0.4780
e7	0.7190	0.4040
eA	0.7160	0.4020
eB	0.7150	0.4150
eE	0.5290	0.1890
eF	0.5100	0.2410
eG	0.5360	0.1760
eH	0.1840	0.0490
eJ	0.6650	0.4260
eK	0.5230	0.2470
eL	0.6540	0.4300
eM	0.6600	0.4170
eO	0.6450	0.3050
f1	0.3020	0.0670
f3	0.7700	0.4550

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Chain	Atom inclusion	Q-score
f4	0.5350	0.1820
f6	0.6670	0.4760
fB	0.7800	0.4790
fE	0.5450	0.2170
fF	0.5540	0.2740
fG	0.5830	0.2330
fH	0.2930	0.0670
fJ	0.5410	0.2610
fK	0.5740	0.2830
fL	0.6650	0.4550
fM	0.5590	0.2650
fO	0.5420	0.1840
g1	0.3550	0.1320
g3	0.7320	0.4180
g4	0.5190	0.1580
g6	0.1460	0.3750
gB	0.3370	0.3270
gE	0.6220	0.2890
gF	0.5370	0.2350
gG	0.6220	0.2810
gH	0.3590	0.1340
gJ	0.5380	0.2730
gK	0.5500	0.2540
gL	0.1350	0.2730
gM	0.5300	0.2490
gO	0.5360	0.1690
h1	0.1530	0.0680
h3	0.7840	0.4290
h4	0.5810	0.2240
h6	0.6870	0.5110
hB	0.7750	0.4690
hE	0.5610	0.1810
hF	0.4540	0.1450
hG	0.5630	0.1860
hH	0.1470	0.0530
hJ	0.5750	0.2870
hK	0.4440	0.1600
hL	0.6820	0.4680
hM	0.5780	0.2870
hO	0.6020	0.2400
i1	0.2370	0.0570
i3	0.7630	0.4330

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Chain	Atom inclusion	Q-score
i4	0.6200	0.2860
i6	0.5540	0.4770
iE	0.5320	0.1660
iF	0.5480	0.2250
iG	0.5300	0.1730
iH	0.2440	0.0330
iJ	0.6000	0.3470
iK	0.5290	0.2060
iL	0.5990	0.4500
iM	0.6070	0.3320
iO	0.6270	0.2990
j1	0.1260	0.0900
j3	0.7850	0.4290
j4	0.5630	0.2040
j6	0.5490	0.4700
jE	0.5570	0.2150
jF	0.6300	0.3420
jG	0.5630	0.1980
jH	0.1190	0.0950
jJ	0.5700	0.2810
jK	0.6280	0.3390
jL	0.5800	0.4240
jM	0.5800	0.2830
jO	0.5660	0.1960
k1	0.3170	0.1100
k3	0.7730	0.4580
k4	0.5600	0.1920
k6	0.4880	0.4630
kE	0.6310	0.2800
kF	0.1260	0.0090
kG	0.6190	0.2790
kH	0.3100	0.1000
kJ	0.6510	0.3190
kK	0.1400	0.0080
kL	0.5420	0.4120
kM	0.6160	0.3000
kO	0.5320	0.1710
l1	0.0490	0.0540
l3	0.7490	0.4410
l4	0.6070	0.2620
l6	0.6450	0.4930
lE	0.5820	0.2340

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Chain	Atom inclusion	Q-score
lF	0.2230	0.0570
lG	0.5750	0.2080
lH	0.0360	0.0630
lJ	0.6840	0.3750
lK	0.1910	0.0440
lL	0.6850	0.4840
lM	0.6700	0.3800
lO	0.6140	0.2670
m1	0.0030	0.0570
m3	0.7860	0.4220
m4	0.6430	0.2930
m6	0.5060	0.5010
mE	0.5030	0.1390
mF	0.2190	0.0680
mG	0.4910	0.1360
mH	0.0010	0.0610
mJ	0.6390	0.3770
mK	0.2040	0.0440
mL	0.5840	0.4760
mM	0.6320	0.3620
mO	0.6480	0.3050
n3	0.8230	0.4560
n6	0.7480	0.4930
nF	0.1830	0.0400
nK	0.1850	0.0390
nL	0.7400	0.4950
o3	0.7540	0.4240
o6	0.6360	0.4400
oF	0.2140	0.0770
oK	0.2130	0.0680
oL	0.6450	0.4420
p3	0.7700	0.4460
p8	0.0000	0.0000
pC	0.0000	0.0000
pF	0.2600	0.0810
pK	0.2460	0.0740
q3	0.8340	0.4000
q6	0.5180	0.3830
q8	0.0000	-0.0000
qC	0.0000	0.0000
qF	0.2580	0.0910
qK	0.2640	0.1010

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Chain	Atom inclusion	Q-score
qL	0.5460	0.3710
r3	0.7860	0.4390
r6	0.4940	0.3860
r8	0.0000	0.0000
rC	0.0000	0.0000
rF	0.2750	0.1310
rK	0.2770	0.1490
rL	0.5570	0.3750
s3	0.7800	0.4480
s8	0.0000	-0.0000
sC	0.0000	-0.0000
sF	0.2400	0.0460
sK	0.2430	0.0370
t3	0.7600	0.4320
t6	0.6020	0.4910
t8	0.0020	-0.0030
tC	0.0000	-0.0030
tF	0.1870	0.0300
tK	0.1840	0.0350
tL	0.6100	0.4580
u3	0.7720	0.4450
u6	0.6870	0.4520
u8	0.0040	-0.0200
uC	0.0010	-0.0140
uF	0.2050	0.0130
uK	0.1930	0.0330
uL	0.7000	0.4250
v3	0.7830	0.4250
v6	0.6570	0.4320
v8	0.0140	-0.0030
vC	0.0150	0.0020
vF	0.3260	0.1030
vK	0.3180	0.0950
vL	0.6930	0.4120
w3	0.7830	0.4690
w6	0.7610	0.4330
w8	0.0000	-0.0090
wC	0.0000	-0.0120
wF	0.5660	0.2820
wK	0.5630	0.2810
wL	0.8010	0.4000
x3	0.8550	0.4420

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Chain	Atom inclusion	Q-score
x6	0.5890	0.4660
x8	0.0080	0.0150
xC	0.0090	0.0240
xF	0.2050	0.0790
xK	0.2060	0.0810
xL	0.6010	0.3920
y3	0.8030	0.4660
y6	0.4120	0.3390
y8	0.0010	-0.0210
yC	0.0030	-0.0150
yF	0.7090	0.4320
yK	0.7040	0.4190
yL	0.4430	0.3820
z3	0.7840	0.4810
z6	0.4230	0.3880
z8	0.0010	-0.0000
zC	0.0010	-0.0100
zF	0.5460	0.2600
zK	0.6340	0.3350
zL	0.4610	0.3670