wwPDB EM Validation Summary Report (i)

Sep 14, 2026 – 01:39 PM JST

PDB ID	:	7Y7B / pdb_00007y7b
EMDB ID	:	EMD-33659
Title	:	Cryo-EM structure of cryptophyte photosystem I
Authors	:	Zhao, L.S.; Li, K.; Zhang, Y.Z.; Liu, L.N.
Deposited on	:	2022-06-22
Resolution	:	2.66 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:

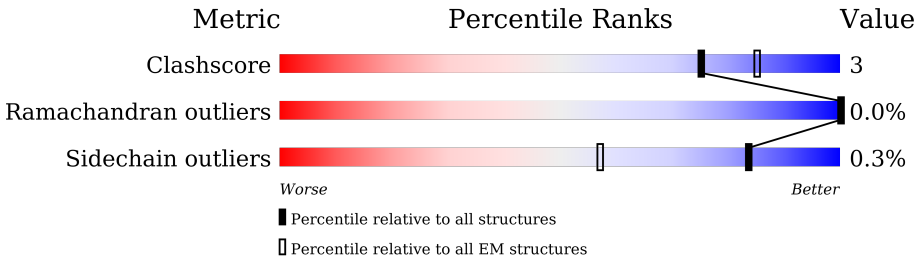
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using 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

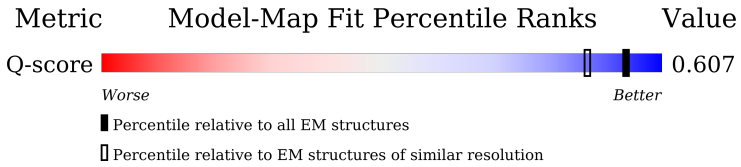
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.66 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	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	9119 (2.16 - 3.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	222	5% 66% 14% 19%
2	2	216	70% 7% 22%
3	3	236	72% 5% 24%
4	4	217	76% 5% 19%

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Mol	Chain	Length	Quality of chain
5	5	229	71% 11% 18%
6	6	215	72% 8% 20%
7	7	230	70% 7% 23%
8	8	227	70% 6% 24%
9	9	220	72% 10% 18%
10	A	752	92% 7%
11	B	734	92% 7%
12	C	81	81% 15%
13	D	141	89% 8%
14	E	64	89% 6% 5%
15	F	183	83% 13%
16	I	36	75% 17% 8%
17	J	42	98%
18	K	87	86% 10%
19	L	153	93% 5%
20	M	30	97%
21	O	99	89% 11%
22	R	133	62% 8% 31%
23	X	164	22% 79% 9% 12%
24	Z	242	59% 37%
25	a	215	74% 5% 20%
25	d	215	76% 20%
26	b	218	76% 5% 19%
27	c	257	72% 11% 16%
28	e	208	73% 7% 19%

2 Entry composition (i)

There are 41 unique types of molecules in this entry. The entry contains 60515 atoms, of which 0 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 ACPI-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1	179	1338	861	227	242	8	0	0

- Molecule 2 is a protein called ACPI-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	2	168	1320	872	215	230	3	0	0

- Molecule 3 is a protein called ACPI-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	3	180	1362	875	231	246	10	0	0

- Molecule 4 is a protein called ACPI-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	4	176	1366	891	224	245	6	0	0

- Molecule 5 is a protein called ACPI-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	5	188	1403	908	234	253	8	0	0

- Molecule 6 is a protein called ACPI-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	6	173	1305	846	217	232	10	0	0

- Molecule 7 is a protein called ACPI-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	177	Total	C	N	O	S	0	0
			1337	861	230	238	8		

- Molecule 8 is a protein called ACPI-8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	8	173	Total	C	N	O	S	0	0
			1298	842	217	235	4		

- Molecule 9 is a protein called ACPI-12.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	9	180	Total	C	N	O	S	0	0
			1349	864	230	243	12		

- Molecule 10 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	A	741	Total	C	N	O	S	0	0
			5824	3804	992	1000	28		

- Molecule 11 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	B	731	Total	C	N	O	S	0	0
			5828	3847	982	984	15		

- Molecule 12 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	C	80	Total	C	N	O	S	0	0
			591	361	103	115	12		

- Molecule 13 is a protein called Photosystem I reaction center subunit II.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	D	137	Total	C	N	O	S	0	0
			1070	685	184	198	3		

- Molecule 14 is a protein called Photosystem I reaction center subunit IV.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	E	61	Total	C	N	O	0	0
			491	312	85	94		

- Molecule 15 is a protein called Photosystem I reaction center subunit III.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	F	160	Total	C	N	O	S	0	0
			1258	814	214	228	2		

- Molecule 16 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I	33	Total	C	N	O	S	0	0
			258	180	34	42	2		

- Molecule 17 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	J	42	Total	C	N	O	S	0	0
			342	232	49	58	3		

- Molecule 18 is a protein called Photosystem I reaction center subunit PsaK.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	K	78	Total	C	N	O	S	0	0
			553	358	90	102	3		

- Molecule 19 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	L	150	Total	C	N	O	S	0	0
			1143	746	184	211	2		

- Molecule 20 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	M	30	Total	C	N	O	S	0	0
			227	152	35	39	1		

- Molecule 21 is a protein called PsaO.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	O	99	Total	C	N	O	S	0	0
			766	518	113	134	1		

- Molecule 22 is a protein called PsaR.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	92	Total	C	N	O	S	0	0
			680	439	112	127	2		

- Molecule 23 is a protein called Unk1.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	X	145	Total	C	N	O	0	0
			725	435	145	145		

- Molecule 24 is a protein called ACPI-S.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Z	153	Total	C	N	O	S	0	0
			1130	721	188	211	10		

- Molecule 25 is a protein called ACPI-13/10.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	a	171	Total	C	N	O	S	0	0
			1271	823	207	231	10		
25	d	171	Total	C	N	O	S	0	0
			1271	823	207	231	10		

- Molecule 26 is a protein called ACPI-14.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	b	176	Total	C	N	O	S	0	0
			1368	891	224	244	9		

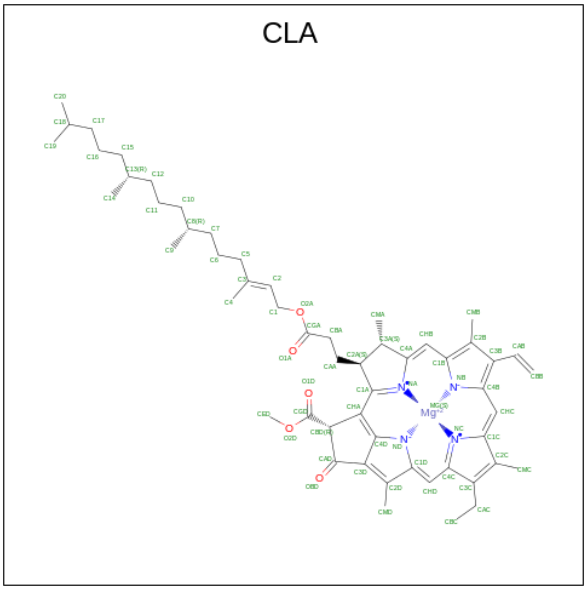
- Molecule 27 is a protein called ACPI-9.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	c	215	Total	C	N	O	S	0	0
			1615	1053	265	283	14		

- Molecule 28 is a protein called ACPI-11.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	e	168	Total	C	N	O	S	0	0
			1288	840	209	227	12		

- Molecule 29 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
29	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	1	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
29	1	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
29	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	1	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
29	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
29	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	2	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
29	2	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
29	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
29	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
29	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
29	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	4	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
29	4	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
29	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	5	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
29	5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	6	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	6	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	6	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	7	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	7	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
29	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
29	7	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	7	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	7	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	7	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
29	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	8	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
29	8	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	8	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	9	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	9	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	9	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
29	9	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	9	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
29	9	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	9	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	9	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
29	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
29	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
29	F	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	F	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	J	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	K	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	K	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	L	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
29	L	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	L	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
29	L	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	O	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	O	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	O	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	R	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	Z	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
29	Z	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	Z	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
29	Z	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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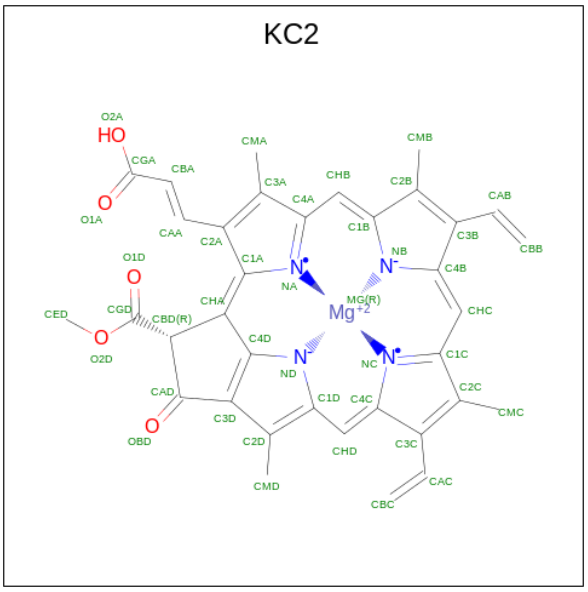
Mol	Chain	Residues	Atoms					AltConf
29	b	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	c	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	d	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
29	d	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
29	d	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	d	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
29	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	d	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	d	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
29	d	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
29	e	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	e	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	e	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
29	e	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	e	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	e	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	e	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	e	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
29	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 30 is Chlorophyll c2 (CCD ID: KC2) (formula: $C_{35}H_{28}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



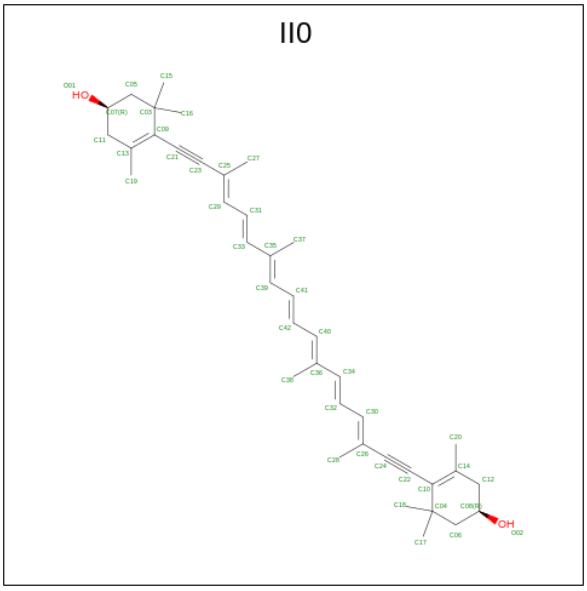
Mol	Chain	Residues	Atoms					AltConf
30	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	Z	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
30	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	e	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	e	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 31 is (1 {R})-3,5,5-trimethyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E})-3,7,12,16-tetramethyl-18-[(4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-3,5,7,9,11,13,15-heptaen-1,17-diynyl]cyclohex-3-en-1-ol (CCD ID: II0) (formula: $C_{40}H_{52}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
31	1	1	Total	C	O	0
			42	40	2	
31	1	1	Total	C	O	0
			42	40	2	
31	1	1	Total	C	O	0
			42	40	2	
31	1	1	Total	C	O	0
			42	40	2	

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Mol	Chain	Residues	Atoms			AltConf
31	2	1	Total	C	O	0
			42	40	2	
31	2	1	Total	C	O	0
			42	40	2	
31	2	1	Total	C	O	0
			42	40	2	
31	3	1	Total	C	O	0
			42	40	2	
31	3	1	Total	C	O	0
			42	40	2	
31	3	1	Total	C	O	0
			42	40	2	
31	3	1	Total	C	O	0
			42	40	2	
31	3	1	Total	C	O	0
			42	40	2	
31	4	1	Total	C	O	0
			42	40	2	
31	4	1	Total	C	O	0
			42	40	2	
31	4	1	Total	C	O	0
			42	40	2	
31	4	1	Total	C	O	0
			42	40	2	
31	5	1	Total	C	O	0
			42	40	2	
31	5	1	Total	C	O	0
			42	40	2	
31	5	1	Total	C	O	0
			42	40	2	
31	5	1	Total	C	O	0
			42	40	2	
31	5	1	Total	C	O	0
			42	40	2	
31	6	1	Total	C	O	0
			42	40	2	
31	6	1	Total	C	O	0
			42	40	2	
31	6	1	Total	C	O	0
			42	40	2	
31	7	1	Total	C	O	0
			42	40	2	

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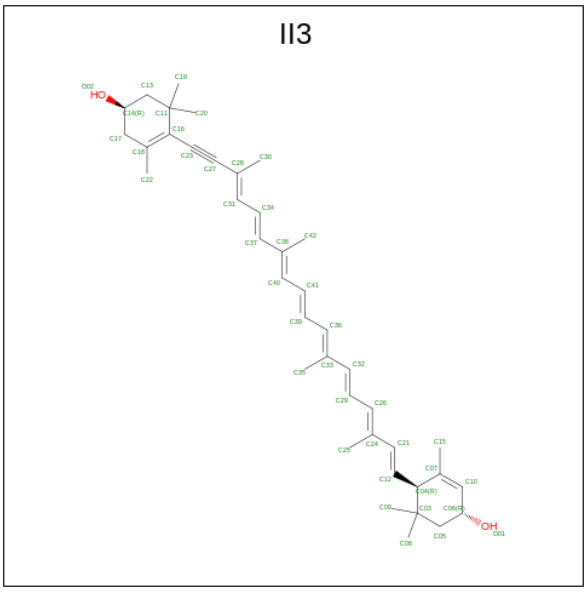
Mol	Chain	Residues	Atoms			AltConf
31	7	1	Total	C	O	0
			42	40	2	
31	7	1	Total	C	O	0
			42	40	2	
31	7	1	Total	C	O	0
			42	40	2	
31	8	1	Total	C	O	0
			42	40	2	
31	8	1	Total	C	O	0
			42	40	2	
31	8	1	Total	C	O	0
			42	40	2	
31	8	1	Total	C	O	0
			42	40	2	
31	9	1	Total	C	O	0
			42	40	2	
31	9	1	Total	C	O	0
			42	40	2	
31	9	1	Total	C	O	0
			42	40	2	
31	9	1	Total	C	O	0
			42	40	2	
31	B	1	Total	C	O	0
			42	40	2	
31	J	1	Total	C	O	0
			42	40	2	
31	O	1	Total	C	O	0
			42	40	2	
31	O	1	Total	C	O	0
			42	40	2	
31	R	1	Total	C	O	0
			42	40	2	
31	a	1	Total	C	O	0
			42	40	2	
31	a	1	Total	C	O	0
			42	40	2	
31	a	1	Total	C	O	0
			42	40	2	
31	a	1	Total	C	O	0
			42	40	2	
31	a	1	Total	C	O	0
			42	40	2	

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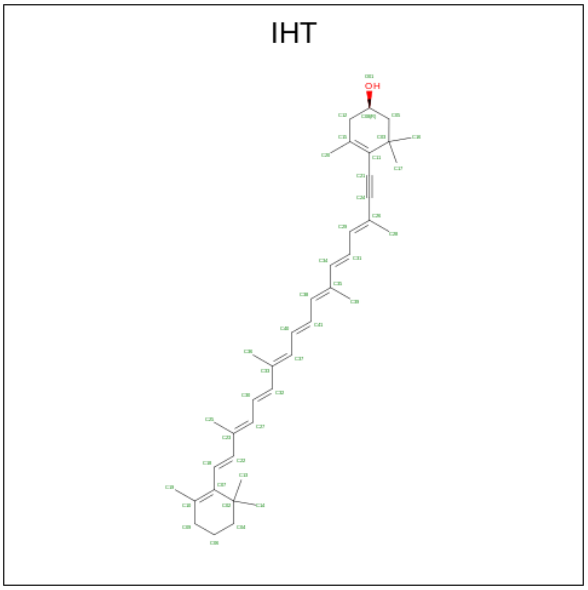
Mol	Chain	Residues	Atoms	AltConf
31	b	1	Total C O 42 40 2	0
31	b	1	Total C O 42 40 2	0
31	c	1	Total C O 42 40 2	0
31	c	1	Total C O 42 40 2	0
31	c	1	Total C O 42 40 2	0
31	c	1	Total C O 42 40 2	0
31	d	1	Total C O 42 40 2	0
31	d	1	Total C O 42 40 2	0
31	d	1	Total C O 42 40 2	0
31	d	1	Total C O 42 40 2	0
31	e	1	Total C O 42 40 2	0
31	e	1	Total C O 42 40 2	0
31	e	1	Total C O 42 40 2	0

- Molecule 32 is (1 {R})-3,5,5-trimethyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(1 {R},4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohex-2-en-1-yl]octadeca-3,5,7,9,11,13,15,17-octaen-1-ynyl]cyclohex-3-en-1-ol (CCD ID: II3) (formula: $C_{40}H_{54}O_2$) (labeled as "Ligand of Interest" by depositor).



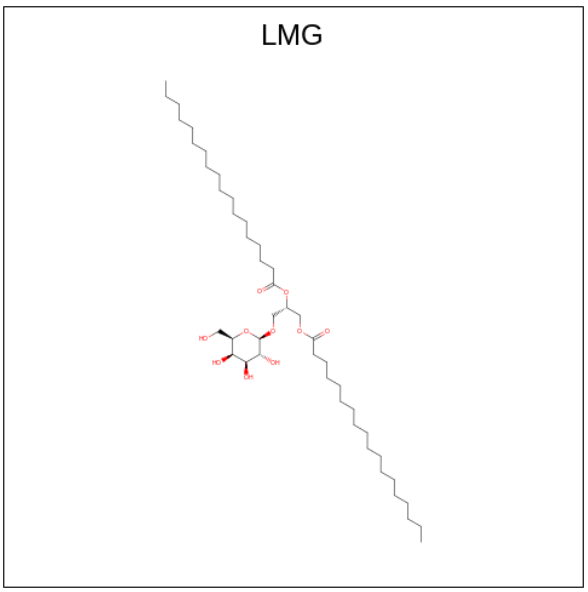
Mol	Chain	Residues	Atoms			AltConf
32	1	1	Total	C	O	0
			42	40	2	
32	b	1	Total	C	O	0
			42	40	2	
32	e	1	Total	C	O	0
			42	40	2	

- Molecule 33 is (1 {R})-3,5,5-trimethyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-(2,6,6-trimethylcyclohexen-1-yl)octadeca-3,5,7,9,11,13,15,17-octaen-1-ynyl]cyclohex-3-en-1-ol (CCD ID: IHT) (formula: $C_{40}H_{54}O$) (labeled as "Ligand of Interest" by depositor).



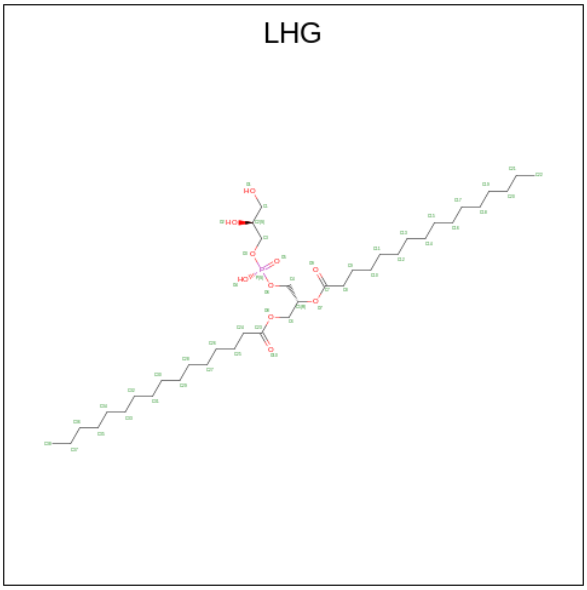
Mol	Chain	Residues	Atoms			AltConf
33	1	1	Total	C	O	0
			41	40	1	
33	2	1	Total	C	O	0
			41	40	1	
33	5	1	Total	C	O	0
			41	40	1	
33	6	1	Total	C	O	0
			41	40	1	
33	8	1	Total	C	O	0
			41	40	1	
33	9	1	Total	C	O	0
			41	40	1	
33	K	1	Total	C	O	0
			41	40	1	
33	L	1	Total	C	O	0
			41	40	1	
33	Z	1	Total	C	O	0
			41	40	1	
33	a	1	Total	C	O	0
			41	40	1	
33	c	1	Total	C	O	0
			41	40	1	
33	d	1	Total	C	O	0
			41	40	1	

- Molecule 34 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms	AltConf
34	2	1	Total C O 36 26 10	0
34	3	1	Total C O 30 20 10	0
34	3	1	Total C O 32 22 10	0
34	6	1	Total C O 32 22 10	0
34	8	1	Total C O 52 42 10	0
34	F	1	Total C O 32 22 10	0
34	I	1	Total C O 51 41 10	0

- Molecule 35 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



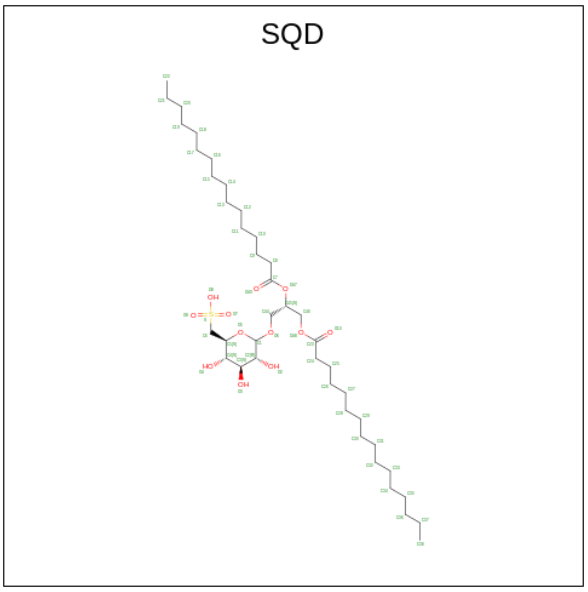
Mol	Chain	Residues	Atoms	AltConf
35	2	1	Total C O P 22 12 9 1	0
35	2	1	Total C O P 39 28 10 1	0
35	2	1	Total C O P 42 31 10 1	0
35	3	1	Total C O P 49 38 10 1	0

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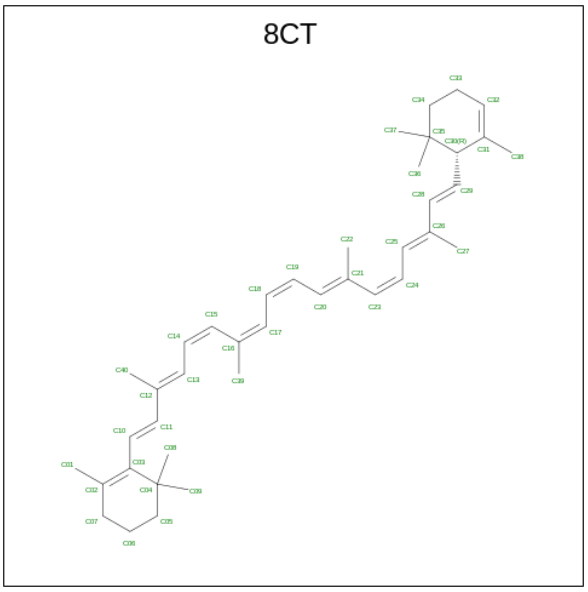
Mol	Chain	Residues	Atoms				AltConf
35	3	1	Total	C	O	P	0
			34	23	10	1	
35	3	1	Total	C	O	P	0
			49	38	10	1	
35	4	1	Total	C	O	P	0
			47	36	10	1	
35	4	1	Total	C	O	P	0
			45	34	10	1	
35	5	1	Total	C	O	P	0
			23	12	10	1	
35	6	1	Total	C	O	P	0
			35	24	10	1	
35	7	1	Total	C	O	P	0
			31	20	10	1	
35	7	1	Total	C	O	P	0
			39	28	10	1	
35	8	1	Total	C	O	P	0
			33	22	10	1	
35	A	1	Total	C	O	P	0
			49	38	10	1	
35	A	1	Total	C	O	P	0
			39	28	10	1	
35	B	1	Total	C	O	P	0
			45	34	10	1	
35	L	1	Total	C	O	P	0
			34	23	10	1	
35	Z	1	Total	C	O	P	0
			46	35	10	1	
35	a	1	Total	C	O	P	0
			29	18	10	1	
35	b	1	Total	C	O	P	0
			49	38	10	1	
35	c	1	Total	C	O	P	0
			29	18	10	1	
35	d	1	Total	C	O	P	0
			23	13	9	1	
35	d	1	Total	C	O	P	0
			39	28	10	1	

- Molecule 36 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms				AltConf
36	3	1	Total 42	C 29	O 12	S 1	0
36	O	1	Total 29	C 16	O 12	S 1	0

- Molecule 37 is (6'R,11cis,11'cis,13cis,15cis)-4',5'-didehydro-5',6'-dihydro-beta,beta-carotene (CCD ID: 8CT) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		AltConf
37	4	1	Total 40	C 40	0

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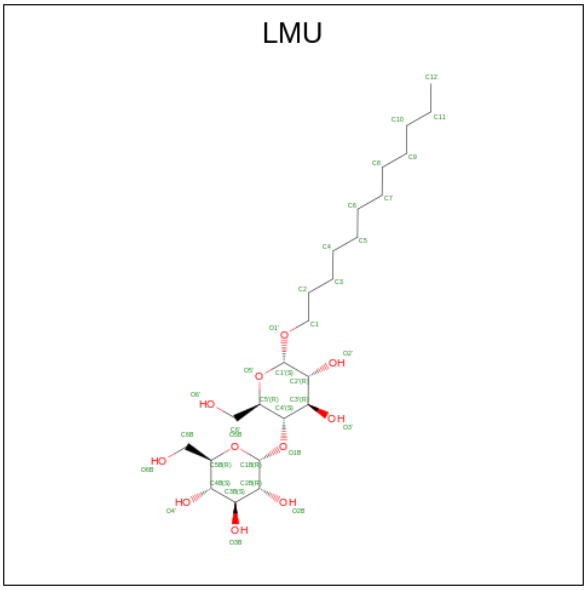
Mol	Chain	Residues	Atoms	AltConf
37	7	1	Total C 40 40	0
37	A	1	Total C 40 40	0
37	A	1	Total C 40 40	0
37	A	1	Total C 40 40	0
37	A	1	Total C 40 40	0
37	A	1	Total C 40 40	0
37	B	1	Total C 40 40	0
37	B	1	Total C 40 40	0
37	B	1	Total C 40 40	0
37	B	1	Total C 40 40	0
37	B	1	Total C 40 40	0
37	B	1	Total C 40 40	0
37	F	1	Total C 40 40	0
37	I	1	Total C 40 40	0
37	J	1	Total C 40 40	0
37	K	1	Total C 40 40	0
37	L	1	Total C 40 40	0
37	M	1	Total C 40 40	0
37	R	1	Total C 40 40	0
37	R	1	Total C 40 40	0
37	Z	1	Total C 40 40	0

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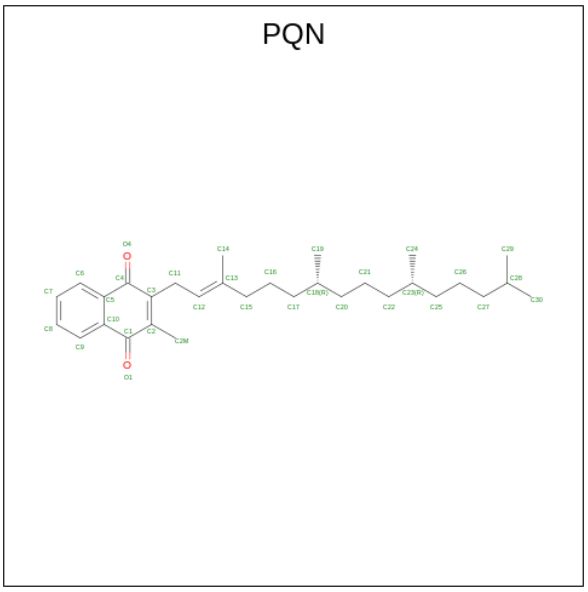
Mol	Chain	Residues	Atoms	AltConf
37	Z	1	Total C 40 40	0
37	b	1	Total C 40 40	0
37	e	1	Total C 40 40	0

- Molecule 38 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$).



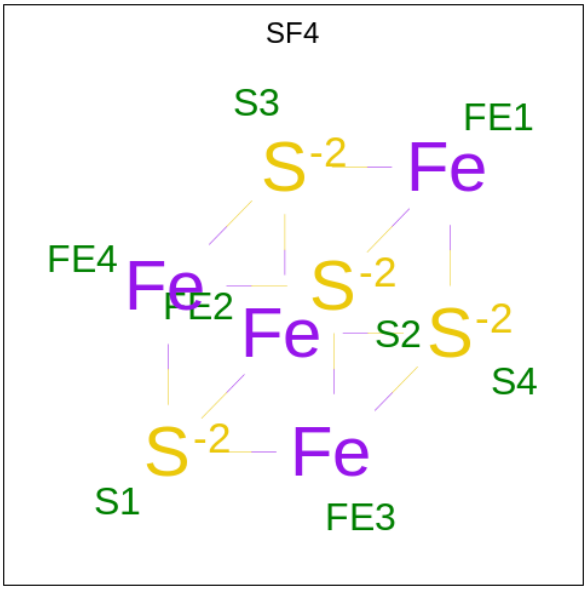
Mol	Chain	Residues	Atoms	AltConf
38	4	1	Total C O 35 24 11	0
38	7	1	Total C O 35 24 11	0
38	J	1	Total C O 31 20 11	0
38	O	1	Total C O 30 19 11	0
38	e	1	Total C O 31 20 11	0

- Molecule 39 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



Mol	Chain	Residues	Atoms			AltConf
39	A	1	Total	C	O	0
			33	31	2	
39	B	1	Total	C	O	0
			33	31	2	

- Molecule 40 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



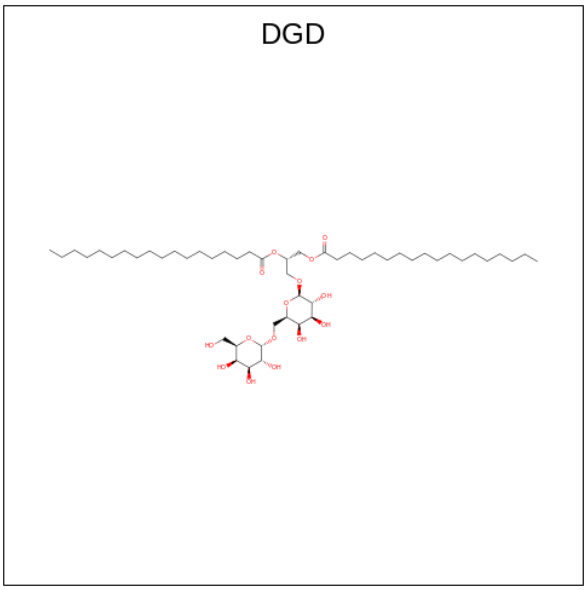
Mol	Chain	Residues	Atoms			AltConf
40	B	1	Total	Fe	S	0
			8	4	4	
40	C	1	Total	Fe	S	0
			8	4	4	

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Mol	Chain	Residues	Atoms			AltConf
40	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 41 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			AltConf
41	B	1	Total	C	O	0
			59	44	15	
41	Z	1	Total	C	O	0
			60	45	15	

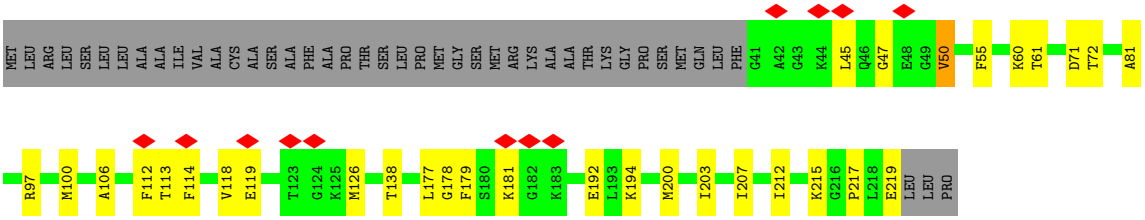
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: ACPI-1

Chain 1:

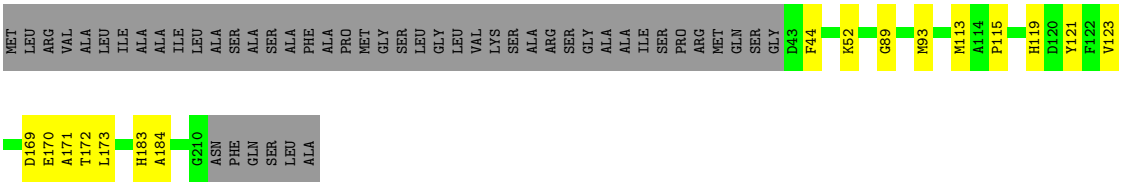




• Molecule 2: ACPI-2

Chain 2:

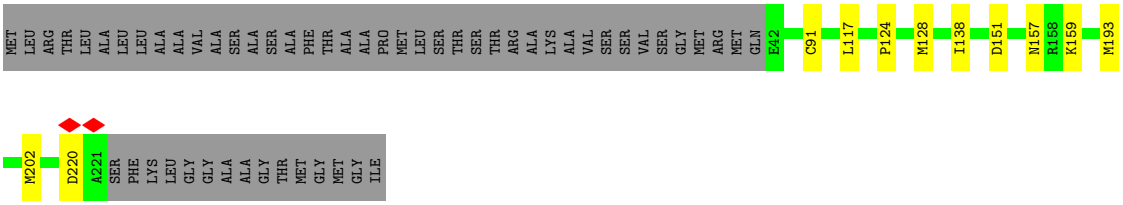




• Molecule 3: ACPI-3

Chain 3:





• Molecule 4: ACPI-4

Chain 4:



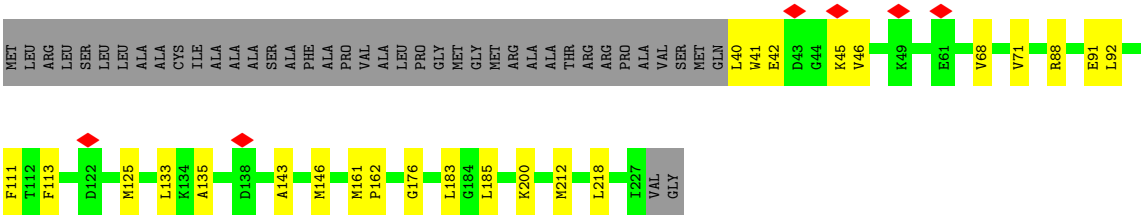




• Molecule 5: ACPI-5

Chain 5:

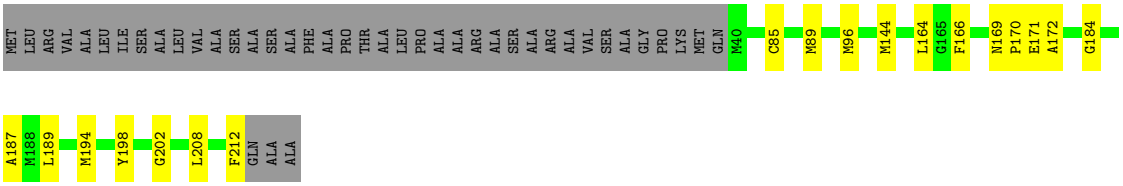




• Molecule 6: ACPI-6

Chain 6:

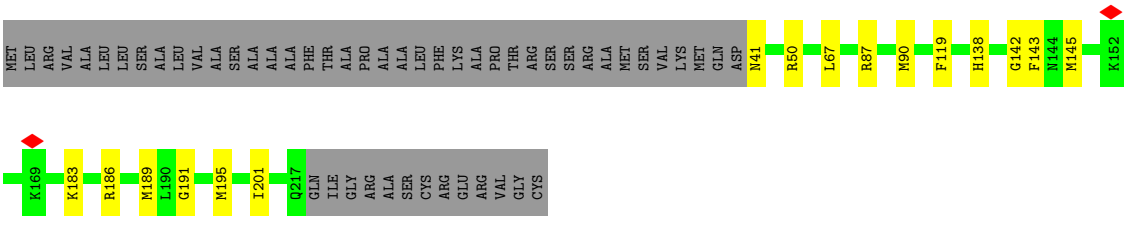




• Molecule 7: ACPI-7

Chain 7:

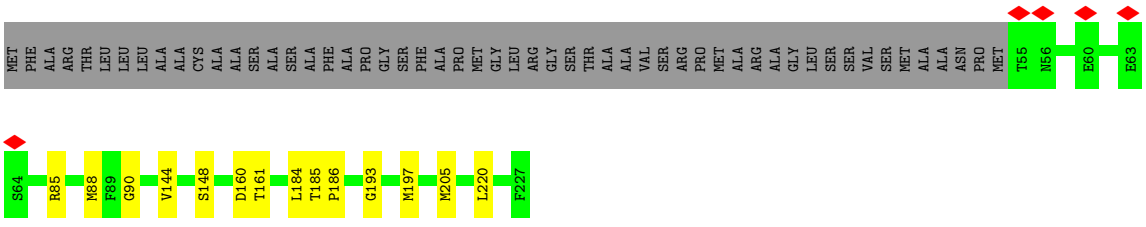




• Molecule 8: ACPI-8

Chain 8:

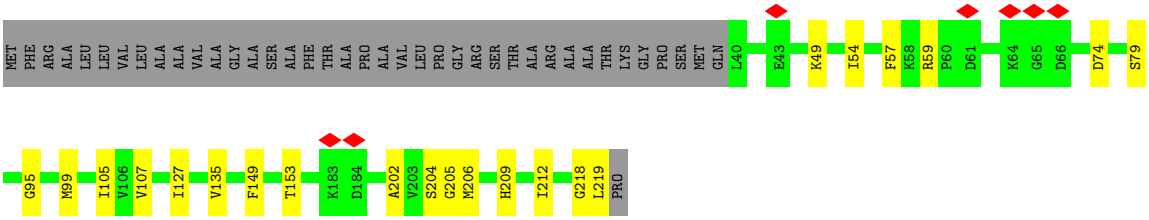




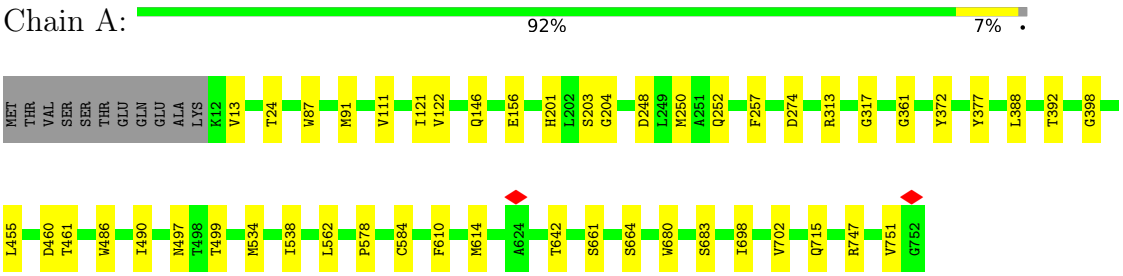
• Molecule 9: ACPI-12

Chain 9:

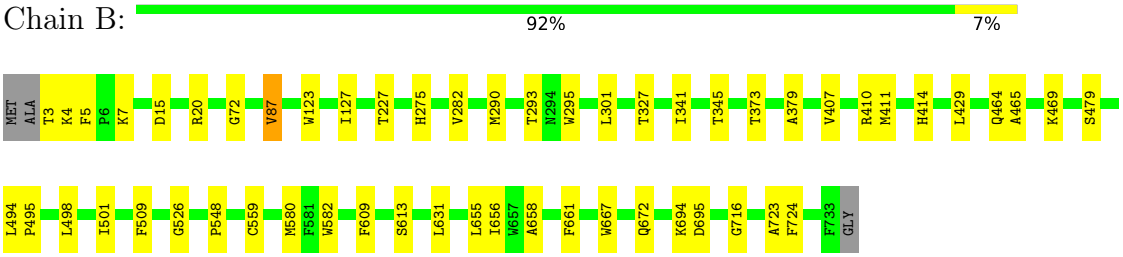




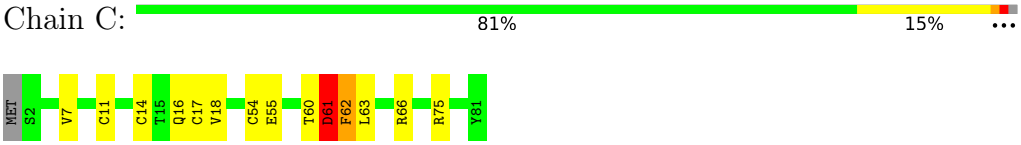
• Molecule 10: Photosystem I P700 chlorophyll a apoprotein A1



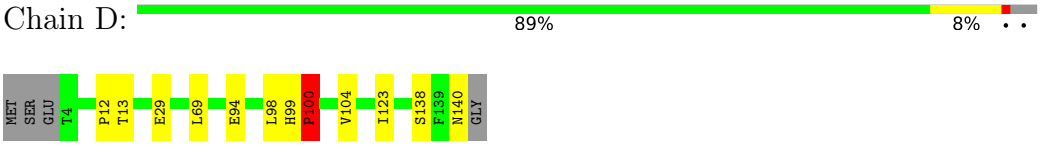
• Molecule 11: Photosystem I P700 chlorophyll a apoprotein A2



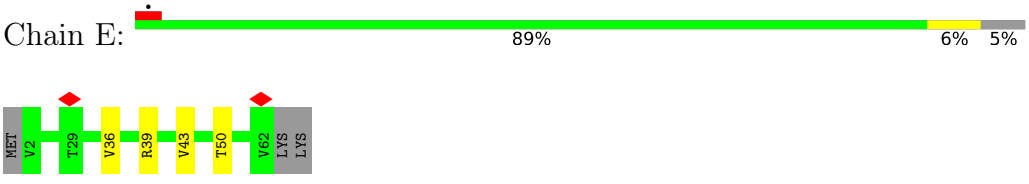
• Molecule 12: Photosystem I iron-sulfur center



• Molecule 13: Photosystem I reaction center subunit II



• Molecule 14: Photosystem I reaction center subunit IV



• Molecule 15: Photosystem I reaction center subunit III

Chain F:

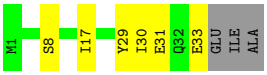




• Molecule 16: Photosystem I reaction center subunit VIII

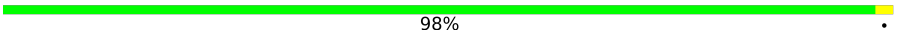
Chain I:





• Molecule 17: Photosystem I reaction center subunit IX

Chain J:

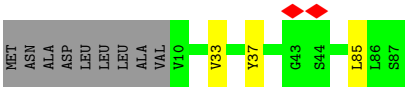




• Molecule 18: Photosystem I reaction center subunit PsaK

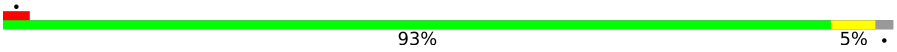
Chain K:

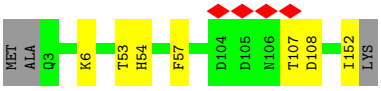




• Molecule 19: Photosystem I reaction center subunit XI

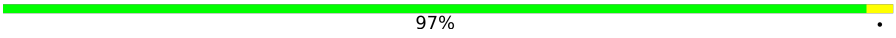
Chain L:





• Molecule 20: Photosystem I reaction center subunit XII

Chain M:

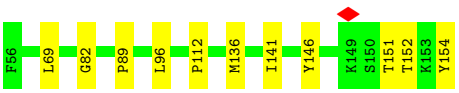




• Molecule 21: PsaO

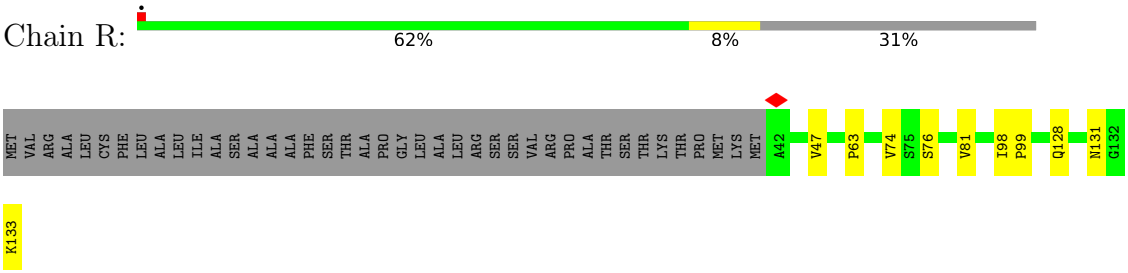
Chain O:





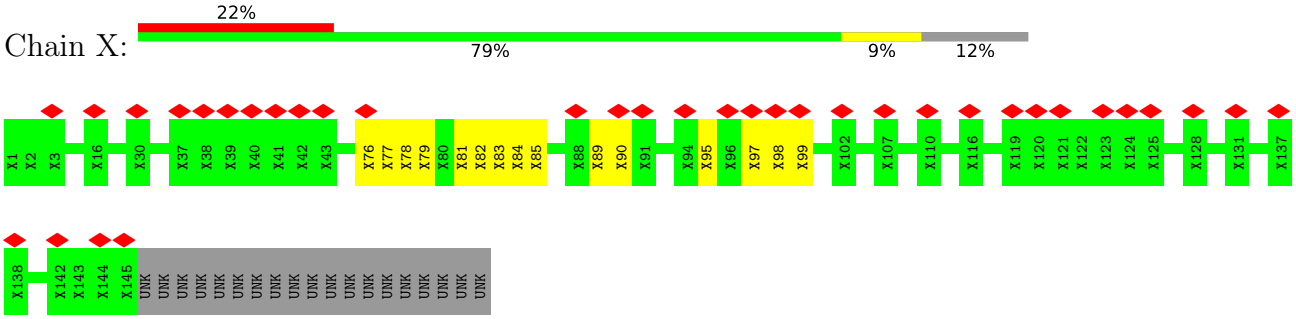
• Molecule 22: PsaR

Chain R:



• Molecule 23: Unk1

Chain X:

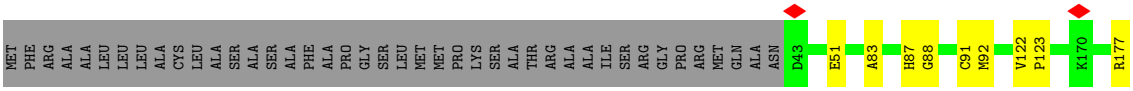

22%
79%
9%
12%
X1 X2 X3 X16 X30 X37 X38 X39 X40 X41 X42 X43 X76 X77 X78 X79 X80 X81 X82 X83 X84 X85 X88 X89 X90 X91 X94 X95 X96 X97 X98 X99 X102 X107 X110 X116 X119 X120 X121 X122 X123 X124 X125 X128 X131 X137
X138 X142 X143 X144 X145 UNK UNK UNK



• Molecule 26: ACPI-14

Chain b:





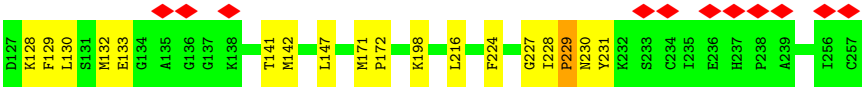


• Molecule 27: ACPI-9

Chain c:



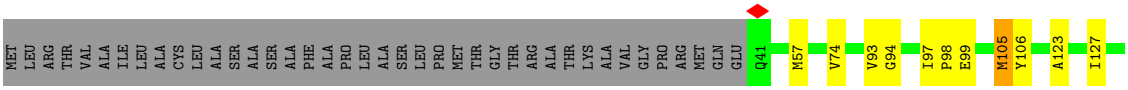




• Molecule 28: ACPI-11

Chain e:







4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	133521	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.411	Depositor
Minimum map value	-0.120	Depositor
Average map value	0.032	Depositor
Map value standard deviation	0.064	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	423.99997, 423.99997, 423.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PQN, KC2, CLA, II0, IHT, DGD, 8CT, LHG, II3, SQD, SF4, LMU, LMG

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 $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	1	0.33	0/1371	0.51	1/1854 (0.1%)
2	2	0.23	0/1356	0.31	0/1835
3	3	0.18	0/1392	0.29	0/1883
4	4	0.18	0/1406	0.32	0/1900
5	5	0.32	0/1438	0.45	0/1940
6	6	0.36	0/1334	0.39	0/1796
7	7	0.22	0/1373	0.35	0/1858
8	8	0.22	0/1326	0.35	0/1804
9	9	0.20	0/1376	0.34	0/1846
10	A	0.23	0/6019	0.35	0/8204
11	B	0.26	0/6046	0.37	1/8254 (0.0%)
12	C	0.48	1/600 (0.2%)	0.64	4/812 (0.5%)
13	D	0.22	0/1094	0.41	0/1476
14	E	0.21	0/499	0.33	0/677
15	F	0.22	0/1290	0.33	0/1745
16	I	0.23	0/266	0.34	0/362
17	J	0.26	0/353	0.34	0/481
18	K	0.23	0/563	0.36	0/768
19	L	0.31	0/1171	0.40	0/1594
20	M	0.19	0/228	0.26	0/310
21	O	0.22	0/796	0.36	0/1091
22	R	0.17	0/700	0.31	0/963
24	Z	0.20	0/1163	0.32	0/1572
25	a	0.21	0/1299	0.33	0/1747
25	d	0.24	0/1299	0.33	0/1747
26	b	0.21	0/1404	0.33	0/1902
27	c	0.29	0/1658	0.45	1/2241 (0.0%)
28	e	0.24	0/1325	0.36	0/1793
All	All	0.25	1/40145 (0.0%)	0.37	7/54455 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	61	ASP	CA-C	-5.09	1.46	1.52

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	C	61	ASP	CA-C-N	-6.23	112.87	122.09
12	C	61	ASP	C-N-CA	-6.23	112.87	122.09
1	1	50	VAL	N-CA-C	6.07	117.42	109.58
27	c	229	PRO	N-CA-C	-5.95	103.24	113.70
12	C	62	PHE	N-CA-CB	5.34	118.88	110.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1338	0	1329	26	0
2	2	1320	0	1309	12	0
3	3	1362	0	1389	8	0
4	4	1366	0	1349	7	0
5	5	1403	0	1398	20	0
6	6	1305	0	1324	16	0
7	7	1337	0	1317	11	0
8	8	1298	0	1322	9	0
9	9	1349	0	1358	15	0
10	A	5824	0	5672	36	0
11	B	5828	0	5626	44	0
12	C	591	0	568	11	0
13	D	1070	0	1076	17	0
14	E	491	0	491	2	0
15	F	1258	0	1266	5	0
16	I	258	0	268	6	0
17	J	342	0	344	1	0
18	K	553	0	581	3	0
19	L	1143	0	1145	5	0
20	M	227	0	257	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	O	766	0	752	10	0
22	R	680	0	674	6	0
23	X	725	0	152	11	0
24	Z	1130	0	1088	6	0
25	a	1271	0	1281	13	0
25	d	1271	0	1281	5	0
26	b	1368	0	1346	10	0
27	c	1615	0	1646	27	0
28	e	1288	0	1282	10	0
29	1	584	0	476	7	0
29	2	547	0	456	1	0
29	3	625	0	596	0	0
29	4	598	0	597	2	0
29	5	563	0	442	6	0
29	6	581	0	514	1	0
29	7	509	0	431	4	0
29	8	496	0	471	4	0
29	9	642	0	539	6	0
29	A	2679	0	2767	11	0
29	B	2406	0	2458	13	0
29	F	160	0	141	0	0
29	J	41	0	29	0	0
29	K	120	0	121	0	0
29	L	267	0	240	2	0
29	O	165	0	147	4	0
29	R	55	0	49	0	0
29	Z	225	0	206	2	0
29	a	645	0	632	1	0
29	b	530	0	525	2	0
29	c	666	0	632	7	0
29	d	589	0	538	1	0
29	e	472	0	414	3	0
30	1	45	0	0	0	0
30	2	45	0	0	0	0
30	3	45	0	0	0	0
30	4	45	0	0	0	0
30	5	45	0	0	0	0
30	6	90	0	0	0	0
30	7	90	0	0	0	0
30	9	45	0	0	0	0
30	Z	45	0	0	0	0
30	a	45	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	b	90	0	0	1	0
30	c	135	0	0	3	0
30	d	45	0	0	0	0
30	e	90	0	0	0	0
31	1	168	0	0	2	0
31	2	126	0	0	1	0
31	3	210	0	0	1	0
31	4	168	0	0	2	0
31	5	210	0	0	3	0
31	6	126	0	0	0	0
31	7	168	0	0	0	0
31	8	168	0	0	1	0
31	9	168	0	0	0	0
31	B	42	0	0	0	0
31	J	42	0	0	0	0
31	O	84	0	0	0	0
31	R	42	0	0	0	0
31	a	210	0	0	2	0
31	b	84	0	0	0	0
31	c	168	0	0	0	0
31	d	168	0	0	0	0
31	e	126	0	0	0	0
32	1	42	0	0	0	0
32	b	42	0	0	1	0
32	e	42	0	0	0	0
33	1	41	0	0	0	0
33	2	41	0	0	1	0
33	5	41	0	0	0	0
33	6	41	0	0	1	0
33	8	41	0	0	0	0
33	9	41	0	0	1	0
33	K	41	0	0	0	0
33	L	41	0	0	0	0
33	Z	41	0	0	0	0
33	a	41	0	0	1	0
33	c	41	0	0	1	0
33	d	41	0	0	1	0
34	2	36	0	42	0	0
34	3	62	0	64	0	0
34	6	32	0	34	0	0
34	8	52	0	77	0	0
34	F	32	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	I	51	0	75	0	0
35	2	103	0	125	0	0
35	3	132	0	186	0	0
35	4	92	0	130	0	0
35	5	23	0	16	0	0
35	6	35	0	40	0	0
35	7	70	0	83	0	0
35	8	33	0	36	0	0
35	A	88	0	122	0	0
35	B	45	0	60	0	0
35	L	34	0	38	1	0
35	Z	46	0	65	0	0
35	a	29	0	28	0	0
35	b	49	0	74	0	0
35	c	29	0	28	0	0
35	d	62	0	73	0	0
36	3	42	0	48	0	0
36	O	29	0	22	0	0
37	4	40	0	0	1	0
37	7	40	0	0	1	0
37	A	200	0	0	0	0
37	B	240	0	0	0	0
37	F	40	0	0	1	0
37	I	40	0	0	0	0
37	J	40	0	0	0	0
37	K	40	0	0	0	0
37	L	40	0	0	0	0
37	M	40	0	0	0	0
37	R	80	0	0	0	0
37	Z	80	0	0	0	0
37	b	40	0	0	0	0
37	e	40	0	0	0	0
38	4	35	0	46	1	0
38	7	35	0	46	1	0
38	J	31	0	35	1	0
38	O	30	0	33	4	0
38	e	31	0	35	0	0
39	A	33	0	46	0	0
39	B	33	0	46	0	0
40	B	8	0	0	0	0
40	C	16	0	0	1	0
41	B	59	0	79	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	Z	60	0	78	1	0
All	All	60515	0	54256	360	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 360 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:a:127:THR:HG23	26:b:218:MET:HE1	1.50	0.93
26:b:177:ARG:NH2	30:b:609:KC2:O1A	2.13	0.81
11:B:609:PHE:O	11:B:613:SER:OG	2.00	0.80
6:6:89:MET:HE3	6:6:184:GLY:HA2	1.64	0.78
38:J:104:LMU:O5B	38:J:104:LMU:O3'	2.03	0.76

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	177/222 (80%)	172 (97%)	5 (3%)	0	100	100
2	2	166/216 (77%)	161 (97%)	5 (3%)	0	100	100
3	3	178/236 (75%)	174 (98%)	4 (2%)	0	100	100
4	4	174/217 (80%)	173 (99%)	1 (1%)	0	100	100
5	5	186/229 (81%)	176 (95%)	10 (5%)	0	100	100
6	6	171/215 (80%)	163 (95%)	8 (5%)	0	100	100
7	7	175/230 (76%)	172 (98%)	3 (2%)	0	100	100
8	8	171/227 (75%)	168 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	9	178/220 (81%)	174 (98%)	4 (2%)	0	100	100
10	A	739/752 (98%)	713 (96%)	26 (4%)	0	100	100
11	B	729/734 (99%)	706 (97%)	23 (3%)	0	100	100
12	C	78/81 (96%)	73 (94%)	4 (5%)	1 (1%)	9	16
13	D	135/141 (96%)	124 (92%)	10 (7%)	1 (1%)	18	30
14	E	59/64 (92%)	57 (97%)	2 (3%)	0	100	100
15	F	158/183 (86%)	152 (96%)	6 (4%)	0	100	100
16	I	31/36 (86%)	29 (94%)	2 (6%)	0	100	100
17	J	40/42 (95%)	40 (100%)	0	0	100	100
18	K	76/87 (87%)	72 (95%)	4 (5%)	0	100	100
19	L	148/153 (97%)	143 (97%)	5 (3%)	0	100	100
20	M	28/30 (93%)	28 (100%)	0	0	100	100
21	O	97/99 (98%)	93 (96%)	4 (4%)	0	100	100
22	R	90/133 (68%)	88 (98%)	2 (2%)	0	100	100
24	Z	151/242 (62%)	150 (99%)	1 (1%)	0	100	100
25	a	169/215 (79%)	165 (98%)	4 (2%)	0	100	100
25	d	169/215 (79%)	166 (98%)	3 (2%)	0	100	100
26	b	174/218 (80%)	171 (98%)	3 (2%)	0	100	100
27	c	213/257 (83%)	203 (95%)	10 (5%)	0	100	100
28	e	166/208 (80%)	165 (99%)	1 (1%)	0	100	100
All	All	5026/5902 (85%)	4871 (97%)	153 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	D	100	PRO
12	C	61	ASP

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	1	130/163 (80%)	130 (100%)	0	100 100
2	2	134/167 (80%)	134 (100%)	0	100 100
3	3	145/183 (79%)	145 (100%)	0	100 100
4	4	139/167 (83%)	139 (100%)	0	100 100
5	5	139/166 (84%)	138 (99%)	1 (1%)	76 86
6	6	134/160 (84%)	134 (100%)	0	100 100
7	7	137/176 (78%)	137 (100%)	0	100 100
8	8	134/169 (79%)	133 (99%)	1 (1%)	76 86
9	9	138/164 (84%)	138 (100%)	0	100 100
10	A	607/617 (98%)	605 (100%)	2 (0%)	86 94
11	B	592/593 (100%)	591 (100%)	1 (0%)	87 95
12	C	66/67 (98%)	66 (100%)	0	100 100
13	D	114/117 (97%)	112 (98%)	2 (2%)	51 72
14	E	56/59 (95%)	55 (98%)	1 (2%)	51 72
15	F	133/154 (86%)	133 (100%)	0	100 100
16	I	27/29 (93%)	27 (100%)	0	100 100
17	J	38/38 (100%)	38 (100%)	0	100 100
18	K	62/69 (90%)	62 (100%)	0	100 100
19	L	126/128 (98%)	125 (99%)	1 (1%)	73 85
20	M	25/25 (100%)	25 (100%)	0	100 100
21	O	81/81 (100%)	81 (100%)	0	100 100
22	R	74/105 (70%)	74 (100%)	0	100 100
24	Z	117/180 (65%)	117 (100%)	0	100 100
25	a	128/153 (84%)	127 (99%)	1 (1%)	73 85
25	d	128/153 (84%)	128 (100%)	0	100 100
26	b	144/173 (83%)	144 (100%)	0	100 100
27	c	169/195 (87%)	169 (100%)	0	100 100
28	e	133/162 (82%)	132 (99%)	1 (1%)	73 85
All	All	4050/4613 (88%)	4039 (100%)	11 (0%)	84 94

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	E	36	VAL
19	L	6	LYS
28	e	105	MET
25	a	129	THR
11	B	87	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
11	B	10	GLN
27	c	223	GLN
11	B	610	ASN
28	e	48	GLN
26	b	199	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

417 ligands 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	$\#\|Z\|>2$
31	II0	4	615	-	39,43,43	2.67	4 (10%)	50,60,60	1.43	6 (12%)
31	II0	O	205	-	39,43,43	2.72	4 (10%)	50,60,60	1.51	11 (22%)
36	SQD	O	206	-	28,29,54	1.63	5 (17%)	37,40,65	1.52	5 (13%)
29	CLA	L	204	-	54,58,73	1.97	9 (16%)	65,95,113	1.65	10 (15%)
29	CLA	Z	305	24	54,58,73	1.96	9 (16%)	65,95,113	1.56	9 (13%)
31	II0	3	614	-	39,43,43	2.71	4 (10%)	50,60,60	1.40	6 (12%)
29	CLA	4	608	35	69,73,73	1.75	9 (13%)	83,113,113	1.37	8 (9%)
37	8CT	b	615	-	40,41,41	0.20	0	50,56,56	0.33	0
29	CLA	5	612	5	49,53,73	2.09	9 (18%)	59,89,113	1.69	10 (16%)
29	CLA	d	605	25	49,53,73	2.12	9 (18%)	59,89,113	1.67	8 (13%)
29	CLA	B	823	-	69,73,73	1.77	9 (13%)	83,113,113	1.38	10 (12%)
31	II0	5	614	-	39,43,43	2.67	4 (10%)	50,60,60	1.39	8 (16%)
29	CLA	c	607	27	69,73,73	1.76	9 (13%)	83,113,113	1.38	9 (10%)
29	CLA	Z	304	24	59,63,73	1.91	9 (15%)	71,101,113	1.47	9 (12%)
35	LHG	b	616	-	48,48,48	0.57	1 (2%)	51,54,54	1.14	4 (7%)
29	CLA	c	605	-	49,53,73	2.08	9 (18%)	59,89,113	1.62	8 (13%)
30	KC2	7	610	7	49,53,53	1.85	4 (8%)	62,89,89	1.39	6 (9%)
30	KC2	6	610	6	49,53,53	1.85	4 (8%)	62,89,89	1.39	7 (11%)
29	CLA	4	602	4	63,67,73	1.84	9 (14%)	75,105,113	1.50	11 (14%)
36	SQD	3	621	-	41,42,54	1.34	4 (9%)	50,53,65	1.12	3 (6%)
40	SF4	C	101	12	0,12,12	-	-	-		
29	CLA	K	101	-	69,73,73	1.76	9 (13%)	83,113,113	1.36	7 (8%)
29	CLA	1	607	1	49,53,73	2.12	9 (18%)	59,89,113	1.64	9 (15%)
29	CLA	B	834	11	59,63,73	1.91	9 (15%)	71,101,113	1.54	10 (14%)
29	CLA	7	609	35	45,49,73	2.26	10 (22%)	54,84,113	1.73	8 (14%)
29	CLA	9	612	-	49,53,73	2.08	9 (18%)	59,89,113	1.62	9 (15%)
29	CLA	B	802	-	69,73,73	1.70	9 (13%)	83,113,113	1.37	9 (10%)
29	CLA	B	820	11	64,68,73	1.83	9 (14%)	77,107,113	1.44	10 (12%)
35	LHG	A	851	-	38,38,48	0.70	1 (2%)	41,44,54	1.25	3 (7%)
30	KC2	c	611	27	49,53,53	1.87	4 (8%)	62,89,89	1.39	8 (12%)
37	8CT	I	101	-	40,41,41	0.27	0	50,56,56	0.46	0
29	CLA	4	611	4	69,73,73	1.74	9 (13%)	83,113,113	1.38	9 (10%)
29	CLA	A	814	-	49,53,73	2.11	9 (18%)	59,89,113	1.65	8 (13%)
29	CLA	9	605	-	49,53,73	2.09	9 (18%)	59,89,113	1.66	9 (15%)
35	LHG	d	618	-	22,22,48	0.80	1 (4%)	24,27,54	1.28	3 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	CLA	O	202	21	59,63,73	1.84	9 (15%)	71,101,113	1.55	10 (14%)
35	LHG	2	619	-	38,38,48	0.68	0	41,44,54	1.24	4 (9%)
29	CLA	Z	301	-	64,68,73	1.85	9 (14%)	77,107,113	1.46	10 (12%)
29	CLA	9	611	9	45,49,73	2.23	10 (22%)	54,84,113	1.74	9 (16%)
34	LMG	3	620	-	32,32,55	0.90	0	40,40,63	1.26	6 (15%)
29	CLA	8	604	8	69,73,73	1.77	9 (13%)	83,113,113	1.41	11 (13%)
29	CLA	B	839	35	69,73,73	1.80	9 (13%)	83,113,113	1.44	10 (12%)
29	CLA	B	816	11	63,67,73	1.84	9 (14%)	75,105,113	1.46	9 (12%)
29	CLA	L	202	19	55,59,73	1.97	9 (16%)	66,96,113	1.57	9 (13%)
29	CLA	3	602	3	59,63,73	1.92	9 (15%)	71,101,113	1.53	9 (12%)
31	II0	c	617	-	39,43,43	2.68	4 (10%)	50,60,60	1.40	7 (14%)
29	CLA	6	602	6	69,73,73	1.81	9 (13%)	83,113,113	1.47	7 (8%)
29	CLA	d	612	-	67,71,73	1.78	9 (13%)	80,110,113	1.37	10 (12%)
29	CLA	e	604	-	64,68,73	1.85	9 (14%)	77,107,113	1.44	8 (10%)
37	8CT	B	845	-	40,41,41	0.39	1 (2%)	50,56,56	0.64	1 (2%)
29	CLA	3	610	3	69,73,73	1.77	9 (13%)	83,113,113	1.44	10 (12%)
38	LMU	O	207	-	31,31,36	0.53	1 (3%)	42,42,47	1.08	2 (4%)
31	II0	d	615	-	39,43,43	2.77	4 (10%)	50,60,60	1.52	7 (14%)
35	LHG	7	618	-	30,30,48	0.74	0	33,36,54	1.19	3 (9%)
31	II0	c	616	-	39,43,43	2.67	4 (10%)	50,60,60	1.27	6 (12%)
41	DGD	B	848	-	60,60,67	0.90	1 (1%)	74,74,81	1.30	6 (8%)
31	II0	5	615	-	39,43,43	2.72	4 (10%)	50,60,60	1.46	7 (14%)
31	II0	2	614	-	39,43,43	2.68	4 (10%)	50,60,60	1.41	7 (14%)
29	CLA	c	601	27	49,53,73	2.14	9 (18%)	59,89,113	1.69	9 (15%)
29	CLA	2	609	-	45,49,73	2.30	10 (22%)	54,84,113	1.78	9 (16%)
29	CLA	B	807	11	69,73,73	1.72	9 (13%)	83,113,113	1.41	10 (12%)
30	KC2	5	610	5	49,53,53	1.86	4 (8%)	62,89,89	1.36	7 (11%)
29	CLA	5	613	5	45,49,73	2.25	10 (22%)	54,84,113	1.71	8 (14%)
31	II0	b	614	-	39,43,43	2.69	4 (10%)	50,60,60	1.43	7 (14%)
29	CLA	7	604	7	57,61,73	1.96	9 (15%)	68,98,113	1.55	9 (13%)
31	II0	c	618	-	39,43,43	2.71	4 (10%)	50,60,60	1.42	8 (16%)
37	8CT	B	851	-	40,41,41	0.25	0	50,56,56	0.42	0
29	CLA	b	607	26	64,68,73	1.85	9 (14%)	77,107,113	1.46	9 (11%)
29	CLA	A	807	10	54,58,73	1.99	9 (16%)	65,95,113	1.60	10 (15%)
33	IHT	K	104	-	40,42,42	2.94	5 (12%)	53,58,58	2.01	18 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	CLA	e	607	28	49,53,73	2.13	9 (18%)	59,89,113	1.68	9 (15%)
29	CLA	A	839	-	69,73,73	1.75	9 (13%)	83,113,113	1.43	10 (12%)
29	CLA	a	604	25	64,68,73	1.87	9 (14%)	77,107,113	1.48	7 (9%)
31	II0	e	614	-	39,43,43	2.78	4 (10%)	50,60,60	1.49	10 (20%)
37	8CT	K	103	-	40,41,41	0.16	0	50,56,56	0.34	0
29	CLA	A	843	10	69,73,73	1.79	9 (13%)	83,113,113	1.46	8 (9%)
40	SF4	C	102	12	0,12,12	-	-	-		
30	KC2	b	609	-	49,53,53	1.88	4 (8%)	62,89,89	1.37	8 (12%)
29	CLA	c	603	27	69,73,73	1.75	9 (13%)	83,113,113	1.41	10 (12%)
30	KC2	b	605	26	49,53,53	1.85	4 (8%)	62,89,89	1.41	9 (14%)
29	CLA	B	840	11	69,73,73	1.72	9 (13%)	83,113,113	1.36	8 (9%)
37	8CT	B	846	-	40,41,41	0.12	0	50,56,56	0.51	0
29	CLA	B	825	11	69,73,73	1.75	9 (13%)	83,113,113	1.38	10 (12%)
29	CLA	B	817	11	64,68,73	1.80	9 (14%)	77,107,113	1.45	8 (10%)
35	LHG	a	618	-	28,28,48	0.81	0	31,34,54	1.31	3 (9%)
29	CLA	a	605	25	59,63,73	1.88	9 (15%)	71,101,113	1.54	9 (12%)
29	CLA	9	601	9	49,53,73	2.10	9 (18%)	59,89,113	1.66	9 (15%)
29	CLA	B	836	11	51,55,73	2.03	9 (17%)	61,91,113	1.60	8 (13%)
31	II0	4	614	-	39,43,43	2.69	4 (10%)	50,60,60	1.34	7 (14%)
35	LHG	6	618	29	34,34,48	0.75	2 (5%)	37,40,54	1.18	3 (8%)
31	II0	2	613	-	39,43,43	2.77	4 (10%)	50,60,60	1.45	10 (20%)
29	CLA	B	805	11	69,73,73	1.75	9 (13%)	83,113,113	1.41	9 (10%)
29	CLA	1	606	-	49,53,73	2.09	9 (18%)	59,89,113	1.67	9 (15%)
29	CLA	A	829	10	54,58,73	1.98	9 (16%)	65,95,113	1.61	9 (13%)
37	8CT	4	616	-	40,41,41	0.20	0	50,56,56	0.35	0
35	LHG	4	619	-	44,44,48	0.65	2 (4%)	47,50,54	1.19	4 (8%)
29	CLA	8	607	8	45,49,73	2.24	10 (22%)	54,84,113	1.74	9 (16%)
33	IHT	5	618	-	40,42,42	2.81	5 (12%)	53,58,58	2.24	16 (30%)
29	CLA	A	809	29	64,68,73	1.87	9 (14%)	77,107,113	1.55	10 (12%)
29	CLA	B	833	-	49,53,73	2.08	9 (18%)	59,89,113	1.59	8 (13%)
29	CLA	c	608	27	64,68,73	1.84	9 (14%)	77,107,113	1.48	9 (11%)
31	II0	b	612	-	39,43,43	2.66	4 (10%)	50,60,60	1.39	8 (16%)
31	II0	O	204	-	39,43,43	2.75	4 (10%)	50,60,60	1.33	5 (10%)
37	8CT	M	101	-	40,41,41	0.19	0	50,56,56	0.87	1 (2%)
29	CLA	O	203	-	59,63,73	1.86	9 (15%)	71,101,113	1.60	10 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	II0	a	615	-	39,43,43	2.72	4 (10%)	50,60,60	1.43	9 (18%)
29	CLA	2	601	2	46,50,73	2.19	9 (19%)	55,85,113	1.77	9 (16%)
29	CLA	2	611	-	49,53,73	2.11	9 (18%)	59,89,113	1.64	10 (16%)
35	LHG	3	622	30	33,33,48	0.71	0	36,39,54	1.25	3 (8%)
40	SF4	B	801	10,11	0,12,12	-	-	-		
34	LMG	8	614	-	52,52,55	0.84	3 (5%)	60,60,63	1.28	6 (10%)
29	CLA	a	606	-	69,73,73	1.75	9 (13%)	83,113,113	1.42	9 (10%)
29	CLA	A	834	10	59,63,73	1.89	9 (15%)	71,101,113	1.50	12 (16%)
29	CLA	5	607	5	49,53,73	2.08	9 (18%)	59,89,113	1.61	8 (13%)
29	CLA	4	609	4	64,68,73	1.84	9 (14%)	77,107,113	1.46	8 (10%)
33	IHT	6	617	-	40,42,42	2.81	4 (10%)	53,58,58	2.16	16 (30%)
29	CLA	e	602	28	59,63,73	1.93	9 (15%)	71,101,113	1.61	10 (14%)
29	CLA	Z	306	24	64,68,73	1.81	9 (14%)	77,107,113	1.47	8 (10%)
31	II0	d	614	-	39,43,43	2.71	4 (10%)	50,60,60	1.42	7 (14%)
29	CLA	e	610	-	55,59,73	2.00	9 (16%)	66,96,113	1.58	10 (15%)
29	CLA	c	614	-	59,63,73	1.90	9 (15%)	71,101,113	1.45	7 (9%)
29	CLA	a	607	25	69,73,73	1.75	9 (13%)	83,113,113	1.39	8 (9%)
29	CLA	c	613	27	49,53,73	2.13	9 (18%)	59,89,113	1.60	8 (13%)
31	II0	e	612	-	39,43,43	2.69	4 (10%)	50,60,60	1.43	10 (20%)
29	CLA	B	821	-	64,68,73	1.80	9 (14%)	77,107,113	1.47	9 (11%)
35	LHG	d	619	-	38,38,48	0.70	1 (2%)	41,44,54	1.16	2 (4%)
31	II0	3	617	-	39,43,43	2.71	4 (10%)	50,60,60	1.35	5 (10%)
29	CLA	7	608	7	59,63,73	1.90	9 (15%)	71,101,113	1.62	8 (11%)
29	CLA	6	609	35	45,49,73	2.27	10 (22%)	54,84,113	1.75	8 (14%)
29	CLA	6	605	6	59,63,73	1.88	9 (15%)	71,101,113	1.46	9 (12%)
29	CLA	A	837	10	69,73,73	1.71	9 (13%)	83,113,113	1.37	8 (9%)
29	CLA	e	608	-	45,49,73	2.27	10 (22%)	54,84,113	1.73	9 (16%)
29	CLA	A	817	10	69,73,73	1.77	9 (13%)	83,113,113	1.51	9 (10%)
29	CLA	A	802	10,29	59,63,73	1.86	9 (15%)	71,101,113	1.49	9 (12%)
37	8CT	R	201	-	40,41,41	0.19	0	50,56,56	0.42	0
30	KC2	6	613	6	49,53,53	1.84	4 (8%)	62,89,89	1.37	7 (11%)
29	CLA	5	605	5	49,53,73	2.09	9 (18%)	59,89,113	1.61	9 (15%)
37	8CT	B	850	-	40,41,41	0.37	1 (2%)	50,56,56	0.74	1 (2%)
29	CLA	2	606	-	49,53,73	2.10	9 (18%)	59,89,113	1.62	9 (15%)
29	CLA	a	602	25	59,63,73	1.92	9 (15%)	71,101,113	1.58	9 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	CLA	8	606	8	59,63,73	1.91	9 (15%)	71,101,113	1.51	9 (12%)
34	LMG	2	617	-	36,36,55	0.85	0	44,44,63	1.21	3 (6%)
38	LMU	4	618	-	36,36,36	0.48	1 (2%)	47,47,47	0.94	3 (6%)
37	8CT	A	848	-	40,41,41	0.37	0	50,56,56	0.57	0
29	CLA	d	609	-	45,49,73	2.24	10 (22%)	54,84,113	1.71	9 (16%)
29	CLA	c	609	-	45,49,73	2.25	10 (22%)	54,84,113	1.72	9 (16%)
31	II0	7	614	-	39,43,43	2.68	4 (10%)	50,60,60	1.48	7 (14%)
29	CLA	9	603	9	49,53,73	2.12	9 (18%)	59,89,113	1.65	9 (15%)
29	CLA	b	608	-	69,73,73	1.76	9 (13%)	83,113,113	1.37	9 (10%)
31	II0	9	617	-	39,43,43	2.71	4 (10%)	50,60,60	1.45	7 (14%)
29	CLA	5	606	-	49,53,73	2.09	9 (18%)	59,89,113	1.66	10 (16%)
31	II0	a	614	-	39,43,43	2.71	4 (10%)	50,60,60	1.40	7 (14%)
37	8CT	A	852	-	40,41,41	0.24	0	50,56,56	0.64	1 (2%)
29	CLA	5	611	5	49,53,73	2.10	9 (18%)	59,89,113	1.61	8 (13%)
29	CLA	3	603	3	64,68,73	1.83	9 (14%)	77,107,113	1.47	9 (11%)
31	II0	8	612	-	39,43,43	2.69	4 (10%)	50,60,60	1.39	6 (12%)
29	CLA	1	601	1	49,53,73	2.16	9 (18%)	59,89,113	1.74	10 (16%)
29	CLA	6	603	6	49,53,73	2.16	9 (18%)	59,89,113	1.67	8 (13%)
29	CLA	B	819	11	64,68,73	1.85	9 (14%)	77,107,113	1.54	11 (14%)
29	CLA	9	607	9	69,73,73	1.73	9 (13%)	83,113,113	1.38	10 (12%)
29	CLA	3	605	3	59,63,73	1.91	9 (15%)	71,101,113	1.54	8 (11%)
29	CLA	L	201	11	69,73,73	1.78	9 (13%)	83,113,113	1.44	11 (13%)
31	II0	9	615	-	39,43,43	2.70	4 (10%)	50,60,60	1.44	9 (18%)
33	IHT	a	617	-	40,42,42	2.81	4 (10%)	53,58,58	2.30	17 (32%)
37	8CT	A	847	-	40,41,41	0.24	0	50,56,56	0.76	1 (2%)
29	CLA	1	605	-	45,50,73	2.15	9 (20%)	53,85,113	1.65	7 (13%)
29	CLA	c	604	-	64,68,73	1.87	9 (14%)	77,107,113	1.47	9 (11%)
29	CLA	8	602	8	49,53,73	2.11	9 (18%)	59,89,113	1.55	6 (10%)
31	II0	6	615	-	39,43,43	2.69	4 (10%)	50,60,60	1.36	6 (12%)
29	CLA	9	606	-	68,72,73	1.75	9 (13%)	81,111,113	1.44	10 (12%)
29	CLA	B	815	11	69,73,73	1.80	9 (13%)	83,113,113	1.42	9 (10%)
35	LHG	3	619	-	48,48,48	0.60	0	51,54,54	1.21	6 (11%)
29	CLA	1	603	1	56,60,73	1.97	9 (16%)	67,97,113	1.52	9 (13%)
31	II0	5	617	-	39,43,43	2.70	4 (10%)	50,60,60	1.56	8 (16%)
29	CLA	6	606	-	59,63,73	1.93	9 (15%)	71,101,113	1.57	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	CLA	A	833	10	69,73,73	1.76	9 (13%)	83,113,113	1.41	8 (9%)
29	CLA	5	602	5	59,63,73	1.93	9 (15%)	71,101,113	1.53	9 (12%)
37	8CT	L	206	-	40,41,41	0.21	0	50,56,56	0.44	0
29	CLA	2	605	2	64,68,73	1.80	9 (14%)	77,107,113	1.42	8 (10%)
37	8CT	e	616	-	40,41,41	0.16	0	50,56,56	0.36	0
39	PQN	B	842	-	34,34,34	0.37	0	42,45,45	0.65	1 (2%)
31	II0	a	616	-	39,43,43	2.80	4 (10%)	50,60,60	1.54	8 (16%)
30	KC2	d	610	25	49,53,53	1.87	4 (8%)	62,89,89	1.41	6 (9%)
29	CLA	A	818	10	69,73,73	1.75	9 (13%)	83,113,113	1.41	8 (9%)
31	II0	6	616	-	39,43,43	2.71	4 (10%)	50,60,60	1.60	11 (22%)
29	CLA	L	207	-	45,49,73	2.27	10 (22%)	54,84,113	1.78	8 (14%)
29	CLA	A	805	10	54,58,73	1.99	9 (16%)	65,95,113	1.60	9 (13%)
29	CLA	d	611	-	54,58,73	2.00	9 (16%)	65,95,113	1.63	10 (15%)
29	CLA	a	609	-	64,68,73	1.81	9 (14%)	77,107,113	1.50	9 (11%)
37	8CT	A	845	-	40,41,41	0.26	0	50,56,56	0.35	0
30	KC2	Z	307	24	49,53,53	1.84	4 (8%)	62,89,89	1.38	8 (12%)
29	CLA	8	603	-	69,73,73	1.78	9 (13%)	83,113,113	1.41	8 (9%)
29	CLA	9	604	-	59,63,73	1.92	9 (15%)	71,101,113	1.49	8 (11%)
29	CLA	5	601	5	45,49,73	2.29	10 (22%)	54,84,113	1.82	9 (16%)
29	CLA	B	828	11	69,73,73	1.75	9 (13%)	83,113,113	1.36	8 (9%)
31	II0	c	619	-	39,43,43	2.72	4 (10%)	50,60,60	1.43	8 (16%)
33	IHT	8	609	-	40,42,42	2.80	4 (10%)	53,58,58	2.35	16 (30%)
29	CLA	d	606	-	45,49,73	2.22	10 (22%)	54,84,113	1.75	11 (20%)
29	CLA	6	601	6	49,53,73	2.08	9 (18%)	59,89,113	1.63	9 (15%)
29	CLA	3	612	3	49,53,73	2.07	9 (18%)	59,89,113	1.61	8 (13%)
33	IHT	9	619	-	40,42,42	2.80	4 (10%)	53,58,58	2.44	14 (26%)
34	LMG	3	618	-	30,30,55	0.96	1 (3%)	38,38,63	1.20	5 (13%)
29	CLA	A	831	10	69,73,73	1.74	9 (13%)	83,113,113	1.35	8 (9%)
31	II0	3	616	-	39,43,43	2.70	4 (10%)	50,60,60	1.38	6 (12%)
29	CLA	8	601	8	49,53,73	2.09	9 (18%)	59,89,113	1.61	8 (13%)
37	8CT	Z	308	-	40,41,41	0.16	0	50,56,56	0.32	0
29	CLA	1	611	1	49,53,73	2.15	9 (18%)	59,89,113	1.66	8 (13%)
29	CLA	5	603	5	49,53,73	2.10	9 (18%)	59,89,113	1.63	9 (15%)
32	II3	e	613	-	40,43,43	2.00	3 (7%)	47,60,60	1.66	13 (27%)
29	CLA	4	610	4	69,73,73	1.74	9 (13%)	83,113,113	1.38	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
35	LHG	Z	310	-	45,45,48	0.63	0	48,51,54	1.19	4 (8%)
31	II0	R	204	-	39,43,43	2.71	4 (10%)	50,60,60	1.44	8 (16%)
29	CLA	B	835	11	69,73,73	1.80	9 (13%)	83,113,113	1.52	9 (10%)
29	CLA	3	601	3	49,53,73	2.11	9 (18%)	59,89,113	1.64	8 (13%)
29	CLA	A	813	10	46,50,73	2.16	9 (19%)	55,85,113	1.73	8 (14%)
29	CLA	c	606	-	69,73,73	1.77	9 (13%)	83,113,113	1.43	10 (12%)
29	CLA	A	815	10	66,70,73	1.82	9 (13%)	79,109,113	1.39	8 (10%)
29	CLA	3	611	3	54,58,73	2.00	9 (16%)	65,95,113	1.56	9 (13%)
29	CLA	B	826	11	69,73,73	1.73	9 (13%)	83,113,113	1.38	8 (9%)
31	II0	4	613	-	39,43,43	2.71	4 (10%)	50,60,60	1.37	6 (12%)
39	PQN	A	849	-	34,34,34	0.37	0	42,45,45	0.74	1 (2%)
33	IHT	Z	302	-	40,42,42	2.83	4 (10%)	53,58,58	2.15	15 (28%)
29	CLA	A	816	10	64,68,73	1.79	9 (14%)	77,107,113	1.46	8 (10%)
29	CLA	b	604	-	69,73,73	1.77	9 (13%)	83,113,113	1.37	9 (10%)
29	CLA	A	838	-	69,73,73	1.76	9 (13%)	83,113,113	1.38	8 (9%)
33	IHT	c	620	-	40,42,42	2.76	4 (10%)	53,58,58	2.17	15 (28%)
29	CLA	A	810	10	69,73,73	1.74	9 (13%)	83,113,113	1.40	11 (13%)
29	CLA	B	837	-	69,73,73	1.78	9 (13%)	83,113,113	1.36	9 (10%)
33	IHT	L	205	-	40,42,42	2.85	4 (10%)	53,58,58	2.24	16 (30%)
29	CLA	7	612	7	54,58,73	2.00	9 (16%)	65,95,113	1.59	9 (13%)
29	CLA	B	831	11	59,63,73	1.94	9 (15%)	71,101,113	1.61	10 (14%)
35	LHG	8	613	-	32,32,48	0.76	1 (3%)	35,38,54	1.18	2 (5%)
29	CLA	1	613	-	49,53,73	2.15	9 (18%)	59,89,113	1.68	10 (16%)
29	CLA	A	804	10	69,73,73	1.76	9 (13%)	83,113,113	1.39	10 (12%)
29	CLA	A	832	-	69,73,73	1.75	9 (13%)	83,113,113	1.36	8 (9%)
29	CLA	B	806	11	69,73,73	1.75	9 (13%)	83,113,113	1.41	11 (13%)
31	II0	5	620	-	39,43,43	2.75	4 (10%)	50,60,60	1.55	8 (16%)
34	LMG	6	619	-	32,32,55	0.97	1 (3%)	40,40,63	1.22	4 (10%)
29	CLA	6	608	6	64,68,73	1.82	9 (14%)	77,107,113	1.49	10 (12%)
29	CLA	4	606	4	64,68,73	1.85	9 (14%)	77,107,113	1.44	9 (11%)
29	CLA	B	830	11	64,68,73	1.82	9 (14%)	77,107,113	1.47	8 (10%)
31	II0	9	616	-	39,43,43	2.70	4 (10%)	50,60,60	1.37	9 (18%)
29	CLA	A	825	10	69,73,73	1.76	9 (13%)	83,113,113	1.39	10 (12%)
29	CLA	A	811	10	69,73,73	1.79	9 (13%)	83,113,113	1.45	8 (9%)
41	DGD	Z	303	-	61,61,67	0.95	3 (4%)	75,75,81	1.36	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
33	IHT	d	617	-	40,42,42	2.75	4 (10%)	53,58,58	2.25	15 (28%)
29	CLA	A	830	10	64,68,73	1.83	9 (14%)	77,107,113	1.45	8 (10%)
29	CLA	9	613	9	49,53,73	2.12	9 (18%)	59,89,113	1.61	9 (15%)
29	CLA	7	611	-	59,63,73	1.92	9 (15%)	71,101,113	1.50	8 (11%)
29	CLA	R	202	-	59,63,73	1.92	9 (15%)	71,101,113	1.65	11 (15%)
29	CLA	6	611	-	59,63,73	1.90	9 (15%)	71,101,113	1.53	10 (14%)
29	CLA	8	605	8	54,58,73	2.00	9 (16%)	65,95,113	1.65	11 (16%)
35	LHG	c	621	-	28,28,48	0.78	0	31,34,54	1.26	3 (9%)
31	II0	4	612	-	39,43,43	2.68	4 (10%)	50,60,60	1.42	8 (16%)
29	CLA	e	603	28	54,58,73	2.02	9 (16%)	65,95,113	1.61	8 (12%)
29	CLA	B	824	-	64,68,73	1.84	9 (14%)	77,107,113	1.51	9 (11%)
34	LMG	F	205	-	32,32,55	0.84	0	40,40,63	1.29	6 (15%)
31	II0	2	615	-	39,43,43	2.73	4 (10%)	50,60,60	1.57	10 (20%)
29	CLA	2	603	2	54,58,73	2.01	9 (16%)	65,95,113	1.56	10 (15%)
29	CLA	1	608	1	64,68,73	1.83	9 (14%)	77,107,113	1.48	9 (11%)
31	II0	d	613	-	39,43,43	2.69	4 (10%)	50,60,60	1.38	6 (12%)
30	KC2	3	606	35	49,53,53	1.83	4 (8%)	62,89,89	1.43	9 (14%)
29	CLA	A	824	-	69,73,73	1.78	9 (13%)	83,113,113	1.40	8 (9%)
29	CLA	3	609	-	69,73,73	1.75	9 (13%)	83,113,113	1.34	7 (8%)
30	KC2	7	606	-	49,53,53	1.87	4 (8%)	62,89,89	1.45	8 (12%)
38	LMU	e	617	-	32,32,36	0.40	0	43,43,47	1.05	2 (4%)
29	CLA	9	614	-	45,49,73	2.30	10 (22%)	54,84,113	1.80	9 (16%)
29	CLA	B	808	11	69,73,73	1.73	9 (13%)	83,113,113	1.35	8 (9%)
31	II0	B	843	-	39,43,43	2.73	4 (10%)	50,60,60	1.37	5 (10%)
33	IHT	2	616	-	40,42,42	2.86	4 (10%)	53,58,58	2.27	17 (32%)
35	LHG	4	617	29	46,46,48	0.61	0	49,52,54	1.19	4 (8%)
29	CLA	A	836	10	59,63,73	1.89	9 (15%)	71,101,113	1.49	8 (11%)
29	CLA	B	811	11	59,63,73	1.90	9 (15%)	71,101,113	1.52	8 (11%)
35	LHG	5	619	-	22,22,48	0.88	1 (4%)	25,28,54	1.32	3 (12%)
29	CLA	A	821	10	59,63,73	1.89	9 (15%)	71,101,113	1.57	9 (12%)
29	CLA	1	602	1	63,67,73	1.85	9 (14%)	75,105,113	1.49	10 (13%)
29	CLA	A	808	10	59,63,73	1.89	9 (15%)	71,101,113	1.53	10 (14%)
29	CLA	A	822	10	69,73,73	1.76	9 (13%)	83,113,113	1.40	9 (10%)
29	CLA	d	607	25	69,73,73	1.75	9 (13%)	83,113,113	1.42	10 (12%)
37	8CT	F	201	-	40,41,41	0.46	1 (2%)	50,56,56	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	II0	a	619	-	39,43,43	2.69	4 (10%)	50,60,60	1.40	8 (16%)
37	8CT	B	847	-	40,41,41	0.16	0	50,56,56	0.49	0
29	CLA	4	604	-	59,63,73	1.91	9 (15%)	71,101,113	1.47	8 (11%)
29	CLA	F	203	-	49,53,73	2.09	9 (18%)	59,89,113	1.60	8 (13%)
29	CLA	2	607	2	49,53,73	2.09	9 (18%)	59,89,113	1.66	10 (16%)
35	LHG	7	619	29	38,38,48	0.65	0	41,44,54	1.16	3 (7%)
29	CLA	A	803	10	69,73,73	1.74	9 (13%)	83,113,113	1.45	10 (12%)
29	CLA	A	801	-	69,73,73	1.71	8 (11%)	83,113,113	1.35	10 (12%)
30	KC2	e	609	-	49,53,53	1.86	4 (8%)	62,89,89	1.38	7 (11%)
29	CLA	e	611	28	69,73,73	1.78	9 (13%)	83,113,113	1.36	10 (12%)
29	CLA	6	604	6	64,68,73	1.85	9 (14%)	77,107,113	1.47	9 (11%)
35	LHG	B	849	29	44,44,48	0.66	1 (2%)	47,50,54	1.20	5 (10%)
29	CLA	7	603	7	59,63,73	1.92	9 (15%)	71,101,113	1.52	9 (12%)
31	II0	7	613	-	39,43,43	2.67	4 (10%)	50,60,60	1.44	8 (16%)
31	II0	1	616	-	39,43,43	2.67	4 (10%)	50,60,60	1.46	8 (16%)
29	CLA	A	827	-	69,73,73	1.73	9 (13%)	83,113,113	1.36	9 (10%)
29	CLA	4	601	4	59,63,73	1.89	9 (15%)	71,101,113	1.47	9 (12%)
29	CLA	a	608	25	64,68,73	1.82	9 (14%)	77,107,113	1.49	8 (10%)
37	8CT	B	844	-	40,41,41	0.23	0	50,56,56	0.62	0
29	CLA	b	603	26	64,68,73	1.83	9 (14%)	77,107,113	1.48	9 (11%)
29	CLA	3	604	-	69,73,73	1.77	9 (13%)	83,113,113	1.39	8 (9%)
29	CLA	A	842	10	69,73,73	1.77	9 (13%)	83,113,113	1.44	10 (12%)
38	LMU	7	620	-	36,36,36	0.39	0	47,47,47	1.05	3 (6%)
31	II0	8	610	-	39,43,43	2.78	4 (10%)	50,60,60	1.51	9 (18%)
29	CLA	A	812	10	59,63,73	1.89	9 (15%)	71,101,113	1.54	11 (15%)
29	CLA	2	608	2	64,68,73	1.83	9 (14%)	77,107,113	1.48	9 (11%)
29	CLA	d	603	25	54,58,73	2.00	9 (16%)	65,95,113	1.57	9 (13%)
29	CLA	d	604	-	64,68,73	1.87	9 (14%)	77,107,113	1.48	8 (10%)
29	CLA	5	609	-	45,49,73	2.26	10 (22%)	54,84,113	1.71	8 (14%)
29	CLA	9	609	-	45,49,73	2.26	10 (22%)	54,84,113	1.74	11 (20%)
30	KC2	e	605	28	49,53,53	1.86	4 (8%)	62,89,89	1.38	8 (12%)
31	II0	8	611	-	39,43,43	2.76	4 (10%)	50,60,60	1.39	7 (14%)
35	LHG	A	850	-	48,48,48	0.60	0	51,54,54	1.15	4 (7%)
29	CLA	3	607	3	64,68,73	1.83	9 (14%)	77,107,113	1.44	9 (11%)
29	CLA	O	201	-	59,63,73	1.89	9 (15%)	71,101,113	1.54	10 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	CLA	2	602	2	63,67,73	1.86	9 (14%)	75,105,113	1.59	12 (16%)
37	8CT	7	617	-	40,41,41	0.40	1 (2%)	50,56,56	0.58	0
29	CLA	B	827	-	69,73,73	1.75	9 (13%)	83,113,113	1.40	8 (9%)
29	CLA	4	607	4	64,68,73	1.83	9 (14%)	77,107,113	1.47	10 (12%)
29	CLA	A	823	-	69,73,73	1.77	9 (13%)	83,113,113	1.36	9 (10%)
29	CLA	B	838	-	69,73,73	1.77	9 (13%)	83,113,113	1.43	11 (13%)
29	CLA	B	803	-	69,73,73	1.75	9 (13%)	83,113,113	1.34	11 (13%)
29	CLA	d	601	25	49,53,73	2.10	9 (18%)	59,89,113	1.64	8 (13%)
29	CLA	7	605	7	49,53,73	2.13	9 (18%)	59,89,113	1.65	8 (13%)
35	LHG	L	208	-	33,33,48	0.74	1 (3%)	36,39,54	1.19	2 (5%)
29	CLA	A	828	10	69,73,73	1.76	9 (13%)	83,113,113	1.35	8 (9%)
29	CLA	A	844	-	69,73,73	1.67	9 (13%)	83,113,113	1.45	9 (10%)
31	II0	e	615	-	39,43,43	2.71	4 (10%)	50,60,60	1.42	7 (14%)
29	CLA	1	612	1	64,68,73	1.81	9 (14%)	77,107,113	1.40	9 (11%)
29	CLA	b	611	26	59,63,73	1.88	9 (15%)	71,101,113	1.50	9 (12%)
29	CLA	8	608	-	69,73,73	1.78	9 (13%)	83,113,113	1.39	8 (9%)
29	CLA	B	829	11	49,53,73	2.13	9 (18%)	59,89,113	1.76	10 (16%)
29	CLA	K	102	18	59,63,73	1.92	9 (15%)	71,101,113	1.52	10 (14%)
30	KC2	c	615	-	49,53,53	1.85	4 (8%)	62,89,89	1.39	8 (12%)
29	CLA	e	606	28	64,68,73	1.82	9 (14%)	77,107,113	1.40	10 (12%)
29	CLA	B	809	11	69,73,73	1.72	9 (13%)	83,113,113	1.36	8 (9%)
29	CLA	5	604	5	59,63,73	1.95	9 (15%)	71,101,113	1.55	8 (11%)
29	CLA	A	835	10	64,68,73	1.82	9 (14%)	77,107,113	1.44	8 (10%)
29	CLA	B	841	-	56,60,73	1.95	9 (16%)	67,97,113	1.55	9 (13%)
37	8CT	R	203	-	40,41,41	0.18	0	50,56,56	0.55	1 (2%)
29	CLA	7	607	7	49,53,73	2.12	9 (18%)	59,89,113	1.68	9 (15%)
29	CLA	A	806	10	69,73,73	1.75	9 (13%)	83,113,113	1.38	9 (10%)
31	II0	d	616	-	39,43,43	2.69	4 (10%)	50,60,60	1.65	11 (22%)
29	CLA	B	822	11	69,73,73	1.73	9 (13%)	83,113,113	1.40	10 (12%)
37	8CT	Z	309	-	40,41,41	0.24	0	50,56,56	0.67	1 (2%)
29	CLA	5	608	-	64,68,73	1.84	9 (14%)	77,107,113	1.61	10 (12%)
29	CLA	9	608	9	59,63,73	1.91	9 (15%)	71,101,113	1.56	10 (14%)
31	II0	7	615	-	39,43,43	2.74	4 (10%)	50,60,60	1.45	10 (20%)
30	KC2	c	610	27	49,53,53	1.82	4 (8%)	62,89,89	1.41	9 (14%)
29	CLA	3	608	3	64,68,73	1.85	9 (14%)	77,107,113	1.47	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	II0	3	615	-	39,43,43	2.72	4 (10%)	50,60,60	1.38	7 (14%)
31	II0	1	617	-	39,43,43	2.73	4 (10%)	50,60,60	1.45	9 (18%)
29	CLA	c	612	27	59,63,73	1.89	9 (15%)	71,101,113	1.60	11 (15%)
29	CLA	A	820	10	69,73,73	1.78	9 (13%)	83,113,113	1.38	8 (9%)
29	CLA	A	819	-	69,73,73	1.77	9 (13%)	83,113,113	1.44	10 (12%)
29	CLA	e	601	28	49,53,73	2.10	9 (18%)	59,89,113	1.64	8 (13%)
29	CLA	B	812	11	69,73,73	1.75	9 (13%)	83,113,113	1.41	10 (12%)
29	CLA	2	604	2	59,63,73	1.93	9 (15%)	71,101,113	1.50	9 (12%)
31	II0	J	101	-	39,43,43	2.71	4 (10%)	50,60,60	1.47	9 (18%)
29	CLA	2	612	2	49,53,73	2.08	9 (18%)	59,89,113	1.66	8 (13%)
29	CLA	9	602	9	59,63,73	1.92	9 (15%)	71,101,113	1.57	10 (14%)
29	CLA	B	814	-	46,50,73	2.18	9 (19%)	55,85,113	1.73	9 (16%)
29	CLA	J	102	17	45,49,73	2.29	10 (22%)	54,84,113	1.75	10 (18%)
30	KC2	1	610	1	49,53,53	1.87	4 (8%)	62,89,89	1.36	7 (11%)
29	CLA	8	615	-	69,73,73	1.77	9 (13%)	83,113,113	1.40	10 (12%)
31	II0	1	614	-	39,43,43	2.71	4 (10%)	50,60,60	1.39	6 (12%)
29	CLA	a	603	25	64,68,73	1.83	9 (14%)	77,107,113	1.45	9 (11%)
29	CLA	7	602	7	69,73,73	1.78	9 (13%)	83,113,113	1.43	11 (13%)
29	CLA	b	602	26	68,72,73	1.80	9 (13%)	81,111,113	1.50	11 (13%)
31	II0	a	613	-	39,43,43	2.70	4 (10%)	50,60,60	1.41	8 (16%)
29	CLA	1	609	-	45,49,73	2.26	10 (22%)	54,84,113	1.74	8 (14%)
35	LHG	2	618	-	21,21,48	0.76	0	23,26,54	1.24	2 (8%)
31	II0	8	616	-	39,43,43	2.63	4 (10%)	50,60,60	1.56	7 (14%)
30	KC2	9	610	9	49,53,53	1.85	4 (8%)	62,89,89	1.39	9 (14%)
29	CLA	d	608	25	69,73,73	1.78	9 (13%)	83,113,113	1.44	10 (12%)
32	II3	1	615	-	40,43,43	2.01	3 (7%)	47,60,60	1.61	12 (25%)
29	CLA	A	841	-	69,73,73	1.75	9 (13%)	83,113,113	1.39	9 (10%)
29	CLA	7	601	7	49,53,73	2.09	9 (18%)	59,89,113	1.62	8 (13%)
29	CLA	4	603	4	58,62,73	1.94	9 (15%)	69,99,113	1.56	8 (11%)
31	II0	9	618	-	39,43,43	2.69	4 (10%)	50,60,60	1.37	8 (16%)
31	II0	1	619	-	39,43,43	2.78	4 (10%)	50,60,60	1.53	11 (22%)
37	8CT	J	103	-	40,41,41	0.19	0	50,56,56	0.39	0
29	CLA	a	601	25	49,53,73	2.09	9 (18%)	59,89,113	1.64	8 (13%)
29	CLA	6	612	-	49,53,73	2.07	9 (18%)	59,89,113	1.63	8 (13%)
35	LHG	2	620	-	41,41,48	0.65	0	44,47,54	1.20	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	II0	5	616	-	39,43,43	2.74	4 (10%)	50,60,60	1.44	9 (18%)
33	IHT	1	618	-	40,42,42	2.84	4 (10%)	53,58,58	2.09	14 (26%)
29	CLA	B	804	-	49,53,73	2.08	9 (18%)	59,89,113	1.60	9 (15%)
29	CLA	B	813	11	65,69,73	1.77	9 (13%)	78,108,113	1.45	9 (11%)
29	CLA	F	202	-	64,68,73	1.84	9 (14%)	77,107,113	1.44	10 (12%)
29	CLA	a	612	25	69,73,73	1.73	9 (13%)	83,113,113	1.38	9 (10%)
29	CLA	d	602	25	68,72,73	1.79	9 (13%)	81,111,113	1.46	11 (13%)
29	CLA	c	602	27	69,73,73	1.78	9 (13%)	83,113,113	1.42	9 (10%)
34	LMG	I	102	-	51,51,55	0.71	0	59,59,63	1.30	6 (10%)
29	CLA	L	203	-	64,68,73	1.85	9 (14%)	77,107,113	1.47	10 (12%)
30	KC2	a	610	-	49,53,53	1.86	4 (8%)	62,89,89	1.35	7 (11%)
29	CLA	F	204	15	59,63,73	1.90	9 (15%)	71,101,113	1.49	9 (12%)
29	CLA	B	818	-	64,68,73	1.82	9 (14%)	77,107,113	1.47	8 (10%)
29	CLA	b	601	26	49,53,73	2.09	9 (18%)	59,89,113	1.65	8 (13%)
30	KC2	2	610	2	49,53,53	1.86	4 (8%)	62,89,89	1.37	7 (11%)
31	II0	7	616	-	39,43,43	2.70	4 (10%)	50,60,60	1.46	9 (18%)
35	LHG	3	623	-	48,48,48	0.61	1 (2%)	51,54,54	1.20	5 (9%)
29	CLA	B	810	-	64,68,73	1.79	9 (14%)	77,107,113	1.47	9 (11%)
29	CLA	1	604	1	49,53,73	2.15	9 (18%)	59,89,113	1.63	9 (15%)
29	CLA	b	610	26	55,59,73	2.00	9 (16%)	66,96,113	1.60	9 (13%)
29	CLA	a	611	-	59,63,73	1.92	9 (15%)	71,101,113	1.52	9 (12%)
30	KC2	4	605	4	49,53,53	1.86	4 (8%)	62,89,89	1.39	7 (11%)
29	CLA	A	840	-	59,63,73	1.85	9 (15%)	71,101,113	1.55	8 (11%)
38	LMU	J	104	-	32,32,36	0.41	0	43,43,47	1.04	2 (4%)
37	8CT	A	846	-	40,41,41	0.16	0	50,56,56	0.35	0
29	CLA	B	832	-	69,73,73	1.75	9 (13%)	83,113,113	1.38	9 (10%)
31	II0	3	613	-	39,43,43	2.67	4 (10%)	50,60,60	1.34	6 (12%)
29	CLA	6	607	6	59,63,73	1.89	9 (15%)	71,101,113	1.49	9 (12%)
31	II0	6	614	-	39,43,43	2.69	4 (10%)	50,60,60	1.44	8 (16%)
29	CLA	A	826	10	69,73,73	1.72	9 (13%)	83,113,113	1.35	9 (10%)
29	CLA	b	606	26	69,73,73	1.76	9 (13%)	83,113,113	1.37	8 (9%)
32	II3	b	613	-	40,43,43	2.02	3 (7%)	47,60,60	1.68	14 (29%)

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
31	II0	4	615	-	-	1/21/67/67	0/2/2/2
31	II0	O	205	-	-	1/21/67/67	0/2/2/2
36	SQD	O	206	-	-	11/24/44/69	0/1/1/1
29	CLA	L	204	-	-	7/21/97/115	-
29	CLA	Z	305	24	-	3/21/97/115	-
31	II0	3	614	-	-	0/21/67/67	0/2/2/2
29	CLA	4	608	35	-	4/39/115/115	-
37	8CT	b	615	-	-	6/29/63/63	0/2/2/2
29	CLA	5	612	5	-	5/15/91/115	-
29	CLA	d	605	25	-	5/15/91/115	-
29	CLA	B	823	-	-	11/39/115/115	-
31	II0	5	614	-	-	2/21/67/67	0/2/2/2
29	CLA	c	607	27	-	11/39/115/115	-
29	CLA	Z	304	24	-	3/27/103/115	-
35	LHG	b	616	-	-	27/53/53/53	-
29	CLA	c	605	-	-	7/15/91/115	-
30	KC2	7	610	7	-	6/15/71/71	-
30	KC2	6	610	6	-	6/15/71/71	-
29	CLA	4	602	4	-	3/32/108/115	-
36	SQD	3	621	-	-	16/37/57/69	0/1/1/1
40	SF4	C	101	12	-	-	0/6/5/5
29	CLA	K	101	-	-	8/39/115/115	-
29	CLA	1	607	1	-	0/15/91/115	-
29	CLA	B	834	11	-	3/27/103/115	-
29	CLA	7	609	35	-	2/10/86/115	-
29	CLA	9	612	-	-	3/15/91/115	-
29	CLA	B	802	-	-	6/39/115/115	-
29	CLA	B	820	11	-	11/33/109/115	-
35	LHG	A	851	-	-	21/43/43/53	-
30	KC2	c	611	27	-	5/15/71/71	-
37	8CT	I	101	-	-	3/29/63/63	0/2/2/2
29	CLA	4	611	4	-	11/39/115/115	-
29	CLA	A	814	-	-	5/15/91/115	-
29	CLA	9	605	-	-	0/15/91/115	-
35	LHG	d	618	-	-	8/26/26/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	O	202	21	-	9/27/103/115	-
35	LHG	2	619	-	-	18/43/43/53	-
29	CLA	Z	301	-	-	13/33/109/115	-
29	CLA	9	611	9	-	3/10/86/115	-
34	LMG	3	620	-	-	12/27/47/70	0/1/1/1
29	CLA	8	604	8	-	7/39/115/115	-
29	CLA	B	839	35	-	5/39/115/115	-
29	CLA	B	816	11	-	14/32/108/115	-
29	CLA	L	202	19	-	1/23/99/115	-
29	CLA	3	602	3	-	4/27/103/115	-
31	II0	c	617	-	-	0/21/67/67	0/2/2/2
29	CLA	6	602	6	-	7/39/115/115	-
29	CLA	d	612	-	-	5/37/113/115	-
29	CLA	e	604	-	-	3/33/109/115	-
37	8CT	B	845	-	-	8/29/63/63	0/2/2/2
29	CLA	3	610	3	-	9/39/115/115	-
38	LMU	O	207	-	-	9/16/56/61	0/2/2/2
31	II0	d	615	-	-	2/21/67/67	0/2/2/2
35	LHG	7	618	-	-	9/35/35/53	-
31	II0	c	616	-	-	2/21/67/67	0/2/2/2
41	DGD	B	848	-	-	17/48/88/95	0/2/2/2
31	II0	5	615	-	-	2/21/67/67	0/2/2/2
31	II0	2	614	-	-	0/21/67/67	0/2/2/2
29	CLA	c	601	27	-	2/15/91/115	-
29	CLA	2	609	-	-	1/10/86/115	-
29	CLA	B	807	11	-	7/39/115/115	-
30	KC2	5	610	5	-	4/15/71/71	-
29	CLA	5	613	5	-	3/10/86/115	-
31	II0	b	614	-	-	1/21/67/67	0/2/2/2
29	CLA	7	604	7	-	8/25/101/115	-
31	II0	c	618	-	-	2/21/67/67	0/2/2/2
37	8CT	B	851	-	-	9/29/63/63	0/2/2/2
29	CLA	b	607	26	-	7/33/109/115	-
29	CLA	A	807	10	-	2/21/97/115	-
33	IHT	K	104	-	-	2/25/65/65	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	e	607	28	-	3/15/91/115	-
29	CLA	A	839	-	-	12/39/115/115	-
29	CLA	a	604	25	-	13/33/109/115	-
31	II0	e	614	-	-	1/21/67/67	0/2/2/2
37	8CT	K	103	-	-	2/29/63/63	0/2/2/2
29	CLA	A	843	10	-	10/39/115/115	-
40	SF4	C	102	12	-	-	0/6/5/5
30	KC2	b	609	-	-	2/15/71/71	-
29	CLA	c	603	27	-	14/39/115/115	-
30	KC2	b	605	26	-	7/15/71/71	-
29	CLA	B	840	11	-	2/39/115/115	-
37	8CT	B	846	-	-	8/29/63/63	0/2/2/2
29	CLA	B	825	11	-	4/39/115/115	-
29	CLA	B	817	11	-	1/33/109/115	-
35	LHG	a	618	-	-	17/33/33/53	-
29	CLA	a	605	25	-	13/27/103/115	-
29	CLA	9	601	9	-	6/15/91/115	-
29	CLA	B	836	11	-	3/18/94/115	-
31	II0	4	614	-	-	1/21/67/67	0/2/2/2
35	LHG	6	618	29	-	15/39/39/53	-
31	II0	2	613	-	-	2/21/67/67	0/2/2/2
29	CLA	B	805	11	-	11/39/115/115	-
29	CLA	1	606	-	-	0/15/91/115	-
29	CLA	A	829	10	-	8/21/97/115	-
37	8CT	4	616	-	-	5/29/63/63	0/2/2/2
35	LHG	4	619	-	-	17/49/49/53	-
29	CLA	8	607	8	-	3/10/86/115	-
33	IHT	5	618	-	-	1/25/65/65	0/2/2/2
29	CLA	A	809	29	-	6/33/109/115	-
29	CLA	B	833	-	-	3/15/91/115	-
29	CLA	c	608	27	-	9/33/109/115	-
31	II0	b	612	-	-	1/21/67/67	0/2/2/2
31	II0	O	204	-	-	2/21/67/67	0/2/2/2
37	8CT	M	101	-	-	5/29/63/63	0/2/2/2
29	CLA	O	203	-	-	10/27/103/115	-
31	II0	a	615	-	-	1/21/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	2	601	2	-	5/12/88/115	-
29	CLA	2	611	-	-	2/15/91/115	-
35	LHG	3	622	30	-	13/38/38/53	-
40	SF4	B	801	10,11	-	-	0/6/5/5
34	LMG	8	614	-	-	23/47/67/70	0/1/1/1
29	CLA	a	606	-	-	7/39/115/115	-
29	CLA	A	834	10	-	7/27/103/115	-
29	CLA	5	607	5	-	2/15/91/115	-
29	CLA	4	609	4	-	5/33/109/115	-
33	IHT	6	617	-	-	3/25/65/65	0/2/2/2
29	CLA	e	602	28	-	10/27/103/115	-
29	CLA	Z	306	24	-	13/33/109/115	-
31	II0	d	614	-	-	2/21/67/67	0/2/2/2
29	CLA	e	610	-	-	6/23/99/115	-
29	CLA	c	614	-	-	7/27/103/115	-
29	CLA	a	607	25	-	4/39/115/115	-
29	CLA	c	613	27	-	9/15/91/115	-
31	II0	e	612	-	-	0/21/67/67	0/2/2/2
29	CLA	B	821	-	-	11/33/109/115	-
35	LHG	d	619	-	-	20/43/43/53	-
31	II0	3	617	-	-	2/21/67/67	0/2/2/2
29	CLA	7	608	7	-	12/27/103/115	-
29	CLA	6	609	35	-	2/10/86/115	-
29	CLA	6	605	6	-	7/27/103/115	-
29	CLA	A	837	10	-	12/39/115/115	-
29	CLA	e	608	-	-	2/10/86/115	-
29	CLA	A	817	10	-	13/39/115/115	-
29	CLA	A	802	10,29	-	5/27/103/115	-
37	8CT	R	201	-	-	7/29/63/63	0/2/2/2
30	KC2	6	613	6	-	7/15/71/71	-
29	CLA	5	605	5	-	4/15/91/115	-
37	8CT	B	850	-	-	4/29/63/63	0/2/2/2
29	CLA	2	606	-	-	1/15/91/115	-
29	CLA	a	602	25	-	10/27/103/115	-
29	CLA	8	606	8	-	4/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	LMG	2	617	-	-	8/31/51/70	0/1/1/1
38	LMU	4	618	-	-	12/21/61/61	0/2/2/2
37	8CT	A	848	-	-	0/29/63/63	0/2/2/2
29	CLA	d	609	-	-	0/10/86/115	-
29	CLA	c	609	-	-	2/10/86/115	-
31	II0	7	614	-	-	1/21/67/67	0/2/2/2
29	CLA	9	603	9	-	6/15/91/115	-
29	CLA	b	608	-	-	12/39/115/115	-
31	II0	9	617	-	-	2/21/67/67	0/2/2/2
29	CLA	5	606	-	-	5/15/91/115	-
31	II0	a	614	-	-	1/21/67/67	0/2/2/2
37	8CT	A	852	-	-	6/29/63/63	0/2/2/2
29	CLA	5	611	5	-	8/15/91/115	-
29	CLA	3	603	3	-	4/33/109/115	-
31	II0	8	612	-	-	1/21/67/67	0/2/2/2
29	CLA	1	601	1	-	6/15/91/115	-
29	CLA	6	603	6	-	7/15/91/115	-
29	CLA	B	819	11	-	9/33/109/115	-
29	CLA	9	607	9	-	11/39/115/115	-
29	CLA	3	605	3	-	4/27/103/115	-
29	CLA	L	201	11	-	10/39/115/115	-
31	II0	9	615	-	-	2/21/67/67	0/2/2/2
33	IHT	a	617	-	-	4/25/65/65	0/2/2/2
37	8CT	A	847	-	-	8/29/63/63	0/2/2/2
29	CLA	1	605	-	-	3/11/87/115	-
29	CLA	c	604	-	-	5/33/109/115	-
29	CLA	8	602	8	-	4/15/91/115	-
31	II0	6	615	-	-	2/21/67/67	0/2/2/2
29	CLA	9	606	-	-	11/38/114/115	-
29	CLA	B	815	11	-	10/39/115/115	-
35	LHG	3	619	-	-	23/53/53/53	-
29	CLA	1	603	1	-	6/24/100/115	-
31	II0	5	617	-	-	2/21/67/67	0/2/2/2
29	CLA	6	606	-	-	8/27/103/115	-
29	CLA	A	833	10	-	8/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	5	602	5	-	7/27/103/115	-
37	8CT	L	206	-	-	3/29/63/63	0/2/2/2
29	CLA	2	605	2	-	7/33/109/115	-
37	8CT	e	616	-	-	1/29/63/63	0/2/2/2
39	PQN	B	842	-	-	5/23/43/43	0/2/2/2
31	II0	a	616	-	-	1/21/67/67	0/2/2/2
30	KC2	d	610	25	-	5/15/71/71	-
29	CLA	A	818	10	-	9/39/115/115	-
31	II0	6	616	-	-	2/21/67/67	0/2/2/2
29	CLA	L	207	-	-	4/10/86/115	-
29	CLA	A	805	10	-	3/21/97/115	-
29	CLA	d	611	-	-	7/21/97/115	-
29	CLA	a	609	-	-	8/33/109/115	-
37	8CT	A	845	-	-	1/29/63/63	0/2/2/2
30	KC2	Z	307	24	-	6/15/71/71	-
29	CLA	8	603	-	-	11/39/115/115	-
29	CLA	9	604	-	-	3/27/103/115	-
29	CLA	5	601	5	-	2/10/86/115	-
29	CLA	B	828	11	-	10/39/115/115	-
31	II0	c	619	-	-	2/21/67/67	0/2/2/2
33	IHT	8	609	-	-	1/25/65/65	0/2/2/2
29	CLA	d	606	-	-	1/10/86/115	-
29	CLA	6	601	6	-	4/15/91/115	-
29	CLA	3	612	3	-	6/15/91/115	-
33	IHT	9	619	-	-	4/25/65/65	0/2/2/2
34	LMG	3	618	-	-	10/25/45/70	0/1/1/1
29	CLA	A	831	10	-	11/39/115/115	-
31	II0	3	616	-	-	2/21/67/67	0/2/2/2
29	CLA	8	601	8	-	2/15/91/115	-
37	8CT	Z	308	-	-	4/29/63/63	0/2/2/2
29	CLA	1	611	1	-	3/15/91/115	-
29	CLA	5	603	5	-	3/15/91/115	-
32	II3	e	613	-	-	3/25/67/67	0/2/2/2
29	CLA	4	610	4	-	7/39/115/115	-
35	LHG	Z	310	-	-	23/50/50/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	II0	R	204	-	-	1/21/67/67	0/2/2/2
29	CLA	B	835	11	-	8/39/115/115	-
29	CLA	3	601	3	-	5/15/91/115	-
29	CLA	A	813	10	-	0/12/88/115	-
29	CLA	c	606	-	-	14/39/115/115	-
29	CLA	A	815	10	-	2/36/112/115	-
29	CLA	3	611	3	-	4/21/97/115	-
29	CLA	B	826	11	-	12/39/115/115	-
31	II0	4	613	-	-	0/21/67/67	0/2/2/2
39	PQN	A	849	-	-	11/23/43/43	0/2/2/2
33	IHT	Z	302	-	-	2/25/65/65	0/2/2/2
29	CLA	A	816	10	-	9/33/109/115	-
29	CLA	b	604	-	-	17/39/115/115	-
29	CLA	A	838	-	-	7/39/115/115	-
33	IHT	c	620	-	-	1/25/65/65	0/2/2/2
29	CLA	A	810	10	-	20/39/115/115	-
29	CLA	B	837	-	-	6/39/115/115	-
33	IHT	L	205	-	-	2/25/65/65	0/2/2/2
29	CLA	7	612	7	-	8/21/97/115	-
29	CLA	B	831	11	-	10/27/103/115	-
35	LHG	8	613	-	-	23/37/37/53	-
29	CLA	1	613	-	-	6/15/91/115	-
29	CLA	A	804	10	-	15/39/115/115	-
29	CLA	A	832	-	-	8/39/115/115	-
29	CLA	B	806	11	-	12/39/115/115	-
31	II0	5	620	-	-	1/21/67/67	0/2/2/2
34	LMG	6	619	-	-	5/27/47/70	0/1/1/1
29	CLA	6	608	6	-	7/33/109/115	-
29	CLA	4	606	4	-	8/33/109/115	-
29	CLA	B	830	11	-	1/33/109/115	-
31	II0	9	616	-	-	2/21/67/67	0/2/2/2
29	CLA	A	825	10	-	9/39/115/115	-
29	CLA	A	811	10	-	13/39/115/115	-
41	DGD	Z	303	-	-	27/49/89/95	0/2/2/2
33	IHT	d	617	-	-	1/25/65/65	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	A	830	10	-	5/33/109/115	-
29	CLA	9	613	9	-	5/15/91/115	-
29	CLA	7	611	-	-	5/27/103/115	-
29	CLA	R	202	-	-	10/27/103/115	-
29	CLA	6	611	-	-	3/27/103/115	-
29	CLA	8	605	8	-	3/21/97/115	-
35	LHG	c	621	-	-	16/33/33/53	-
31	II0	4	612	-	-	2/21/67/67	0/2/2/2
29	CLA	e	603	28	-	6/21/97/115	-
29	CLA	B	824	-	-	5/33/109/115	-
34	LMG	F	205	-	-	13/27/47/70	0/1/1/1
31	II0	2	615	-	-	2/21/67/67	0/2/2/2
29	CLA	2	603	2	-	5/21/97/115	-
29	CLA	1	608	1	-	5/33/109/115	-
31	II0	d	613	-	-	2/21/67/67	0/2/2/2
30	KC2	3	606	35	-	9/15/71/71	-
29	CLA	A	824	-	-	7/39/115/115	-
29	CLA	3	609	-	-	3/39/115/115	-
30	KC2	7	606	-	-	8/15/71/71	-
38	LMU	e	617	-	-	8/17/57/61	0/2/2/2
29	CLA	9	614	-	-	3/10/86/115	-
29	CLA	B	808	11	-	13/39/115/115	-
31	II0	B	843	-	-	2/21/67/67	0/2/2/2
33	IHT	2	616	-	-	2/25/65/65	0/2/2/2
35	LHG	4	617	29	-	18/51/51/53	-
29	CLA	A	836	10	-	2/27/103/115	-
29	CLA	B	811	11	-	9/27/103/115	-
35	LHG	5	619	-	-	14/26/26/53	-
29	CLA	A	821	10	-	3/27/103/115	-
29	CLA	1	602	1	-	6/32/108/115	-
29	CLA	A	808	10	-	1/27/103/115	-
29	CLA	A	822	10	-	10/39/115/115	-
29	CLA	d	607	25	-	8/39/115/115	-
37	8CT	F	201	-	-	3/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	II0	a	619	-	-	1/21/67/67	0/2/2/2
37	8CT	B	847	-	-	3/29/63/63	0/2/2/2
29	CLA	4	604	-	-	11/27/103/115	-
29	CLA	F	203	-	-	3/15/91/115	-
29	CLA	2	607	2	-	2/15/91/115	-
35	LHG	7	619	29	-	19/43/43/53	-
29	CLA	A	803	10	-	9/39/115/115	-
29	CLA	A	801	-	-	8/39/115/115	-
30	KC2	e	609	-	-	7/15/71/71	-
29	CLA	e	611	28	-	11/39/115/115	-
29	CLA	6	604	6	-	5/33/109/115	-
35	LHG	B	849	29	-	22/49/49/53	-
29	CLA	7	603	7	-	3/27/103/115	-
31	II0	7	613	-	-	1/21/67/67	0/2/2/2
31	II0	1	616	-	-	1/21/67/67	0/2/2/2
29	CLA	A	827	-	-	4/39/115/115	-
29	CLA	4	601	4	-	7/27/103/115	-
29	CLA	a	608	25	-	4/33/109/115	-
37	8CT	B	844	-	-	4/29/63/63	0/2/2/2
29	CLA	b	603	26	-	7/33/109/115	-
29	CLA	3	604	-	-	4/39/115/115	-
29	CLA	A	842	10	-	5/39/115/115	-
38	LMU	7	620	-	-	8/21/61/61	0/2/2/2
31	II0	8	610	-	-	2/21/67/67	0/2/2/2
29	CLA	A	812	10	-	4/27/103/115	-
29	CLA	2	608	2	-	8/33/109/115	-
29	CLA	d	603	25	-	2/21/97/115	-
29	CLA	d	604	-	-	6/33/109/115	-
29	CLA	5	609	-	-	3/10/86/115	-
29	CLA	9	609	-	-	3/10/86/115	-
30	KC2	e	605	28	-	5/15/71/71	-
31	II0	8	611	-	-	2/21/67/67	0/2/2/2
35	LHG	A	850	-	-	22/53/53/53	-
29	CLA	3	607	3	-	5/33/109/115	-
29	CLA	O	201	-	-	3/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	2	602	2	-	14/32/108/115	-
37	8CT	7	617	-	-	9/29/63/63	0/2/2/2
29	CLA	B	827	-	-	5/39/115/115	-
29	CLA	4	607	4	-	7/33/109/115	-
29	CLA	A	823	-	-	13/39/115/115	-
29	CLA	B	838	-	-	5/39/115/115	-
29	CLA	B	803	-	-	12/39/115/115	-
29	CLA	d	601	25	-	5/15/91/115	-
29	CLA	7	605	7	-	6/15/91/115	-
35	LHG	L	208	-	-	15/38/38/53	-
29	CLA	A	828	10	-	7/39/115/115	-
29	CLA	A	844	-	-	7/39/115/115	-
31	II0	e	615	-	-	0/21/67/67	0/2/2/2
29	CLA	1	612	1	-	10/33/109/115	-
29	CLA	b	611	26	-	3/27/103/115	-
29	CLA	8	608	-	-	7/39/115/115	-
29	CLA	B	829	11	-	0/15/91/115	-
29	CLA	K	102	18	-	4/27/103/115	-
30	KC2	c	615	-	-	6/15/71/71	-
29	CLA	e	606	28	-	9/33/109/115	-
29	CLA	B	809	11	-	9/39/115/115	-
29	CLA	5	604	5	-	7/27/103/115	-
29	CLA	A	835	10	-	6/33/109/115	-
29	CLA	B	841	-	-	8/24/100/115	-
37	8CT	R	203	-	-	4/29/63/63	0/2/2/2
29	CLA	7	607	7	-	2/15/91/115	-
29	CLA	A	806	10	-	8/39/115/115	-
31	II0	d	616	-	-	4/21/67/67	0/2/2/2
29	CLA	B	822	11	-	12/39/115/115	-
37	8CT	Z	309	-	-	6/29/63/63	0/2/2/2
29	CLA	5	608	-	-	13/33/109/115	-
29	CLA	9	608	9	-	10/27/103/115	-
31	II0	7	615	-	-	2/21/67/67	0/2/2/2
30	KC2	c	610	27	-	4/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	3	608	3	-	6/33/109/115	-
31	II0	3	615	-	-	1/21/67/67	0/2/2/2
31	II0	1	617	-	-	1/21/67/67	0/2/2/2
29	CLA	c	612	27	-	5/27/103/115	-
29	CLA	A	820	10	-	7/39/115/115	-
29	CLA	A	819	-	-	8/39/115/115	-
29	CLA	e	601	28	-	5/15/91/115	-
29	CLA	B	812	11	-	16/39/115/115	-
29	CLA	2	604	2	-	2/27/103/115	-
31	II0	J	101	-	-	1/21/67/67	0/2/2/2
29	CLA	2	612	2	-	5/15/91/115	-
29	CLA	9	602	9	-	9/27/103/115	-
29	CLA	B	814	-	-	4/12/88/115	-
29	CLA	J	102	17	-	2/10/86/115	-
30	KC2	1	610	1	-	7/15/71/71	-
29	CLA	8	615	-	-	9/39/115/115	-
31	II0	1	614	-	-	1/21/67/67	0/2/2/2
29	CLA	a	603	25	-	8/33/109/115	-
29	CLA	7	602	7	-	8/39/115/115	-
29	CLA	b	602	26	-	16/38/114/115	-
31	II0	a	613	-	-	1/21/67/67	0/2/2/2
29	CLA	1	609	-	-	3/10/86/115	-
35	LHG	2	618	-	-	10/24/24/53	-
31	II0	8	616	-	-	0/21/67/67	0/2/2/2
30	KC2	9	610	9	-	5/15/71/71	-
29	CLA	d	608	25	-	5/39/115/115	-
32	II3	1	615	-	-	1/25/67/67	0/2/2/2
29	CLA	A	841	-	-	5/39/115/115	-
29	CLA	7	601	7	-	2/15/91/115	-
29	CLA	4	603	4	-	7/26/102/115	-
31	II0	9	618	-	-	2/21/67/67	0/2/2/2
31	II0	1	619	-	-	2/21/67/67	0/2/2/2
37	8CT	J	103	-	-	7/29/63/63	0/2/2/2
29	CLA	a	601	25	-	4/15/91/115	-
29	CLA	6	612	-	-	6/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	LHG	2	620	-	-	17/46/46/53	-
31	II0	5	616	-	-	0/21/67/67	0/2/2/2
33	IHT	1	618	-	-	2/25/65/65	0/2/2/2
29	CLA	B	804	-	-	3/15/91/115	-
29	CLA	B	813	11	-	11/35/111/115	-
29	CLA	F	202	-	-	13/33/109/115	-
29	CLA	a	612	25	-	7/39/115/115	-
29	CLA	d	602	25	-	11/38/114/115	-
29	CLA	c	602	27	-	10/39/115/115	-
34	LMG	I	102	-	-	22/46/66/70	0/1/1/1
29	CLA	L	203	-	-	9/33/109/115	-
30	KC2	a	610	-	-	2/15/71/71	-
29	CLA	F	204	15	-	7/27/103/115	-
29	CLA	B	818	-	-	7/33/109/115	-
29	CLA	b	601	26	-	4/15/91/115	-
30	KC2	2	610	2	-	7/15/71/71	-
31	II0	7	616	-	-	2/21/67/67	0/2/2/2
35	LHG	3	623	-	-	25/53/53/53	-
29	CLA	B	810	-	-	6/33/109/115	-
29	CLA	1	604	1	-	3/15/91/115	-
29	CLA	b	610	26	-	8/23/99/115	-
29	CLA	a	611	-	-	6/27/103/115	-
30	KC2	4	605	4	-	7/15/71/71	-
29	CLA	A	840	-	-	5/27/103/115	-
38	LMU	J	104	-	-	10/17/57/61	0/2/2/2
37	8CT	A	846	-	-	4/29/63/63	0/2/2/2
29	CLA	B	832	-	-	15/39/115/115	-
31	II0	3	613	-	-	2/21/67/67	0/2/2/2
29	CLA	6	607	6	-	4/27/103/115	-
31	II0	6	614	-	-	1/21/67/67	0/2/2/2
29	CLA	A	826	10	-	5/39/115/115	-
29	CLA	b	606	26	-	7/39/115/115	-
32	II3	b	613	-	-	1/25/67/67	0/2/2/2

The worst 5 of 2714 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	b	609	KC2	MG-ND	-10.26	1.85	2.05
33	K	104	IHT	C10-C07	10.23	1.52	1.34
30	3	606	KC2	MG-ND	-10.16	1.85	2.05
30	2	610	KC2	MG-ND	-10.14	1.85	2.05
30	6	613	KC2	MG-ND	-10.04	1.85	2.05

The worst 5 of 3286 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	8	609	IHT	C02-C07-C10	-10.25	108.18	122.61
33	9	619	IHT	C02-C07-C10	-10.19	108.27	122.61
33	d	617	IHT	C02-C07-C10	-9.38	109.40	122.61
33	5	618	IHT	C02-C07-C10	-8.97	109.98	122.61
33	L	205	IHT	C02-C07-C10	-8.87	110.12	122.61

There are no chirality outliers.

5 of 2649 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
29	1	603	CLA	C1A-C2A-CAA-CBA
29	1	605	CLA	C2B-C3B-CAB-CBB
29	1	605	CLA	C4B-C3B-CAB-CBB
29	2	601	CLA	C3A-C2A-CAA-CBA
29	2	601	CLA	CHA-CBD-CGD-O1D

There are no ring outliers.

90 monomers are involved in 102 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	3	614	II0	1	0
29	5	612	CLA	1	0
29	B	823	CLA	1	0
31	5	614	II0	2	0
29	Z	304	CLA	1	0
29	B	834	CLA	1	0
29	7	609	CLA	1	0
30	c	611	KC2	3	0
29	4	611	CLA	2	0
29	9	611	CLA	2	0
29	B	816	CLA	2	0
29	L	202	CLA	1	0
29	d	612	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	O	207	LMU	4	0
31	2	614	II0	1	0
29	c	601	CLA	2	0
40	C	102	SF4	1	0
30	b	609	KC2	1	0
31	4	614	II0	1	0
37	4	616	8CT	1	0
29	O	203	CLA	2	0
31	a	615	II0	1	0
29	A	834	CLA	1	0
33	6	617	IHT	1	0
29	Z	306	CLA	1	0
29	e	610	CLA	1	0
29	c	614	CLA	2	0
38	4	618	LMU	1	0
29	c	609	CLA	1	0
29	1	601	CLA	1	0
29	L	201	CLA	1	0
33	a	617	IHT	1	0
29	1	605	CLA	1	0
29	9	606	CLA	1	0
29	B	815	CLA	1	0
31	a	616	II0	1	0
29	8	603	CLA	1	0
29	9	604	CLA	2	0
33	9	619	IHT	1	0
29	1	611	CLA	2	0
29	B	835	CLA	1	0
29	B	826	CLA	1	0
31	4	613	II0	1	0
29	b	604	CLA	1	0
33	c	620	IHT	1	0
29	A	810	CLA	2	0
29	7	612	CLA	1	0
29	1	613	CLA	1	0
31	5	620	II0	1	0
41	Z	303	DGD	1	0
33	d	617	IHT	1	0
29	7	611	CLA	2	0
29	8	605	CLA	1	0
29	A	824	CLA	1	0
29	B	808	CLA	1	0

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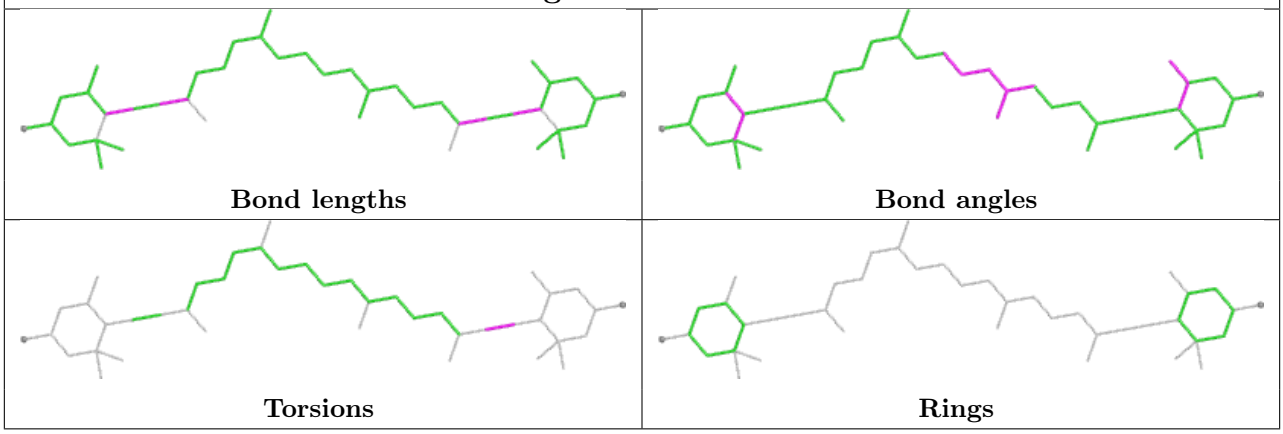
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	2	616	IHT	1	0
29	A	836	CLA	2	0
29	A	821	CLA	1	0
37	F	201	8CT	1	0
29	e	611	CLA	2	0
29	A	842	CLA	1	0
38	7	620	LMU	1	0
31	8	610	II0	1	0
29	5	609	CLA	2	0
29	O	201	CLA	2	0
37	7	617	8CT	1	0
29	A	823	CLA	1	0
29	B	803	CLA	1	0
35	L	208	LHG	1	0
29	A	844	CLA	1	0
29	8	608	CLA	1	0
29	B	809	CLA	1	0
29	5	604	CLA	2	0
29	5	608	CLA	1	0
29	9	608	CLA	1	0
29	c	612	CLA	1	0
29	2	612	CLA	1	0
29	8	615	CLA	1	0
31	1	614	II0	2	0
29	a	603	CLA	1	0
29	1	609	CLA	1	0
29	6	612	CLA	1	0
29	c	602	CLA	1	0
29	B	818	CLA	3	0
29	1	604	CLA	1	0
29	b	610	CLA	1	0
38	J	104	LMU	1	0
29	B	832	CLA	1	0
29	A	826	CLA	2	0
32	b	613	II3	1	0

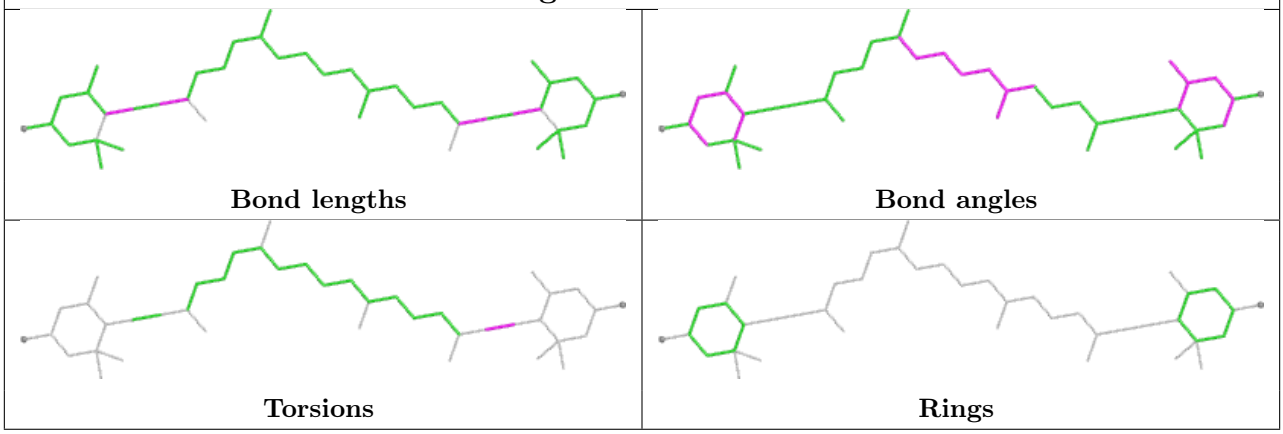
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

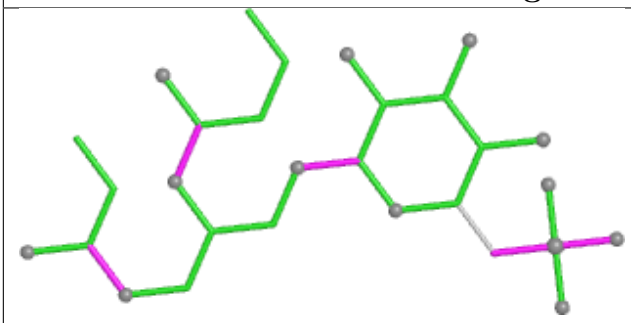
Ligand II0 4 615



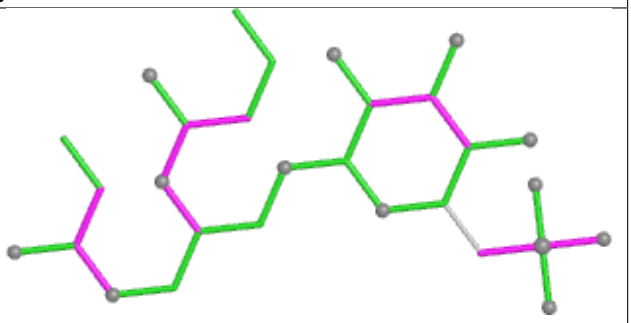
Ligand II0 O 205



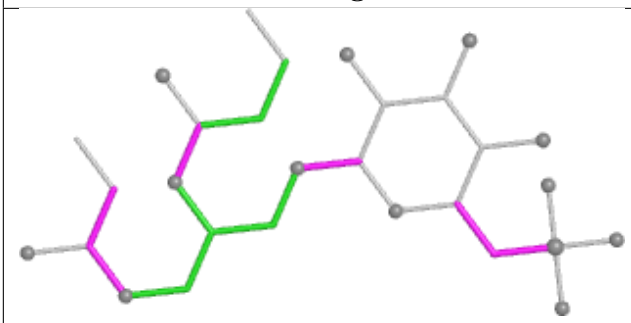
Ligand SQD O 206



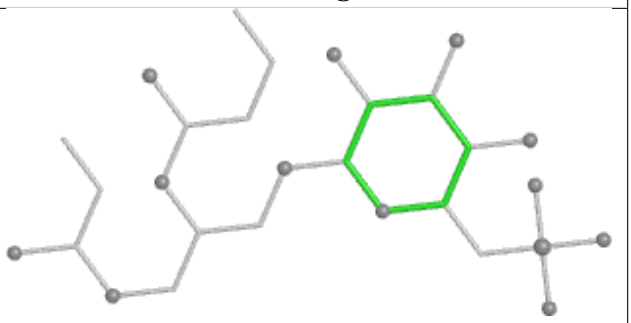
Bond lengths



Bond angles

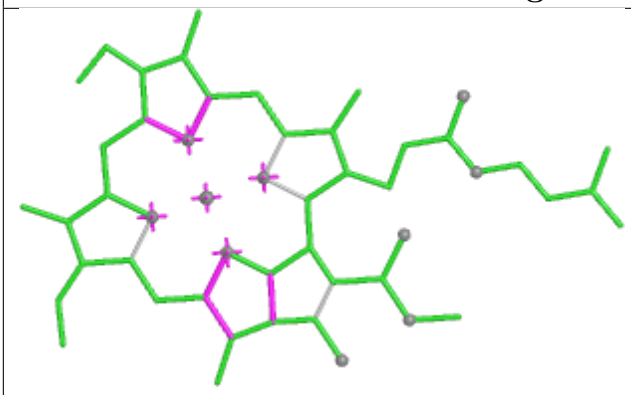


Torsions

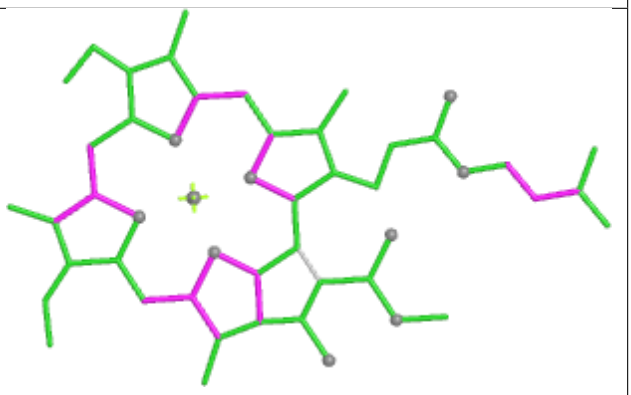


Rings

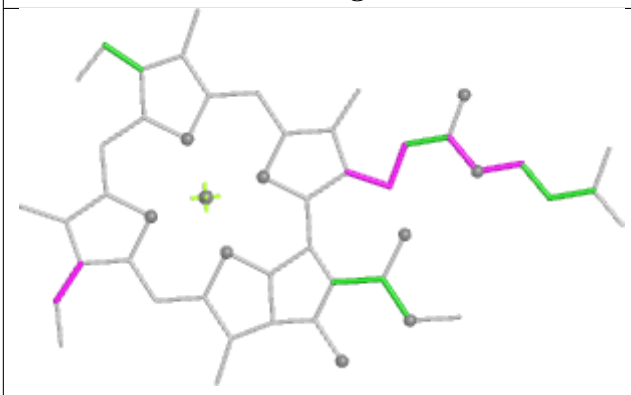
Ligand CLA L 204



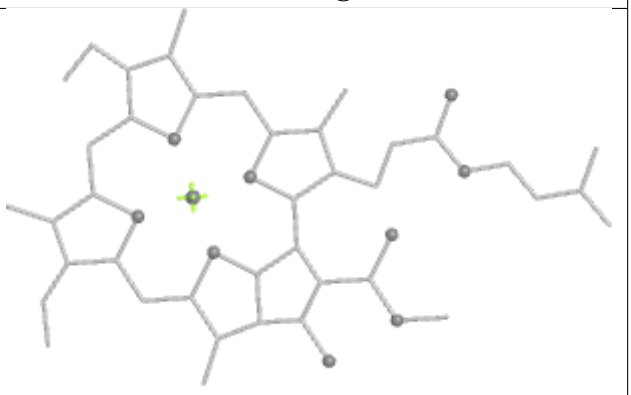
Bond lengths



Bond angles

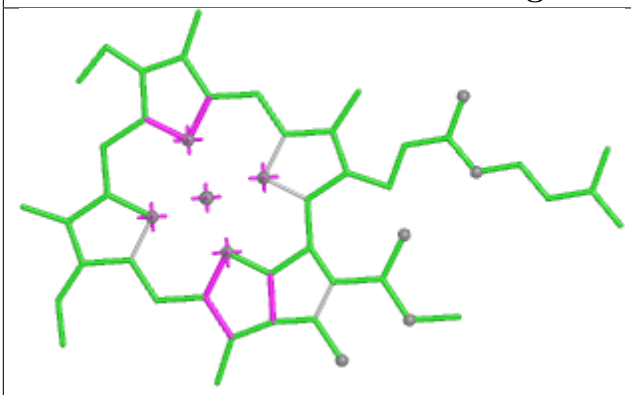


Torsions

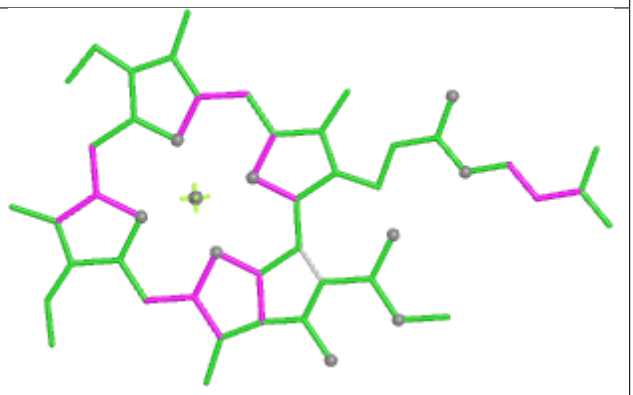


Rings

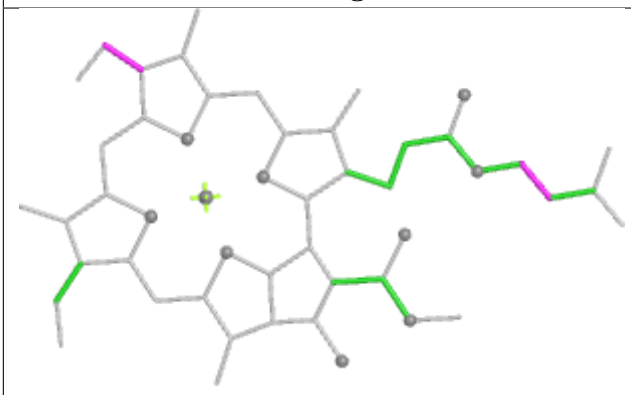
Ligand CLA Z 305



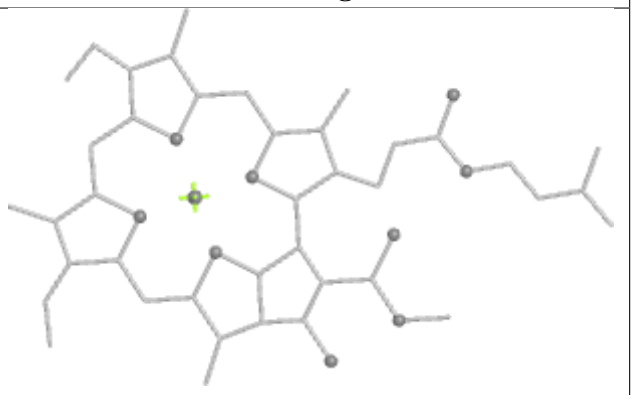
Bond lengths



Bond angles

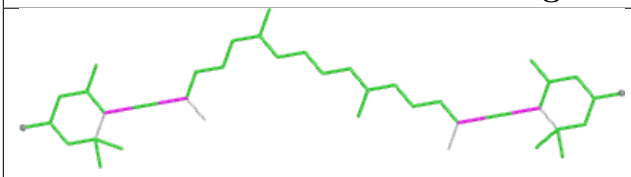


Torsions

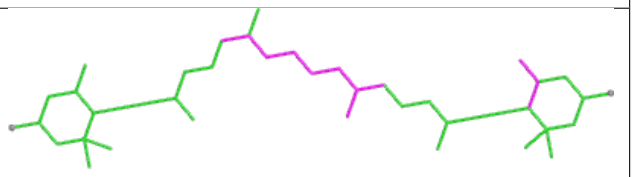


Rings

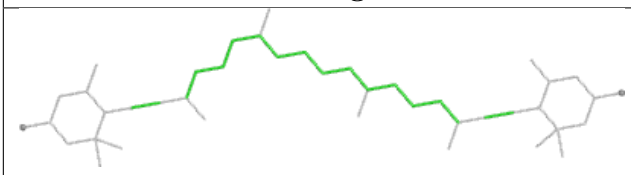
Ligand II0 3 614



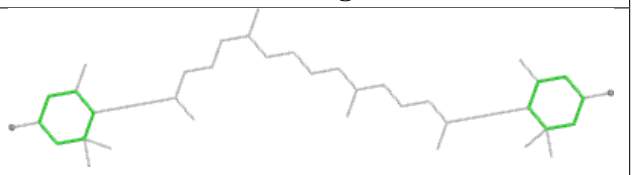
Bond lengths



Bond angles

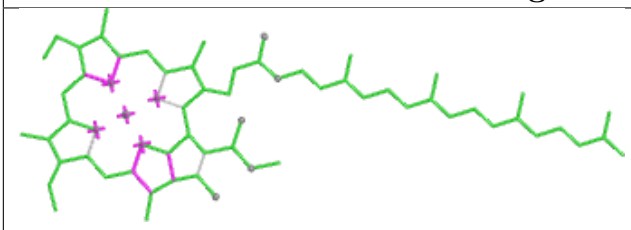


Torsions

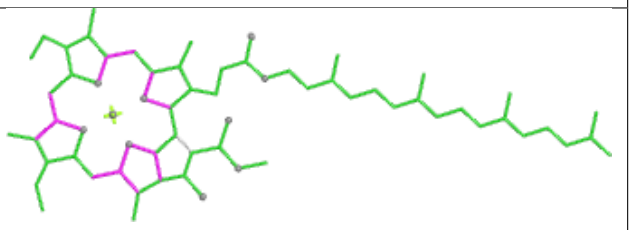


Rings

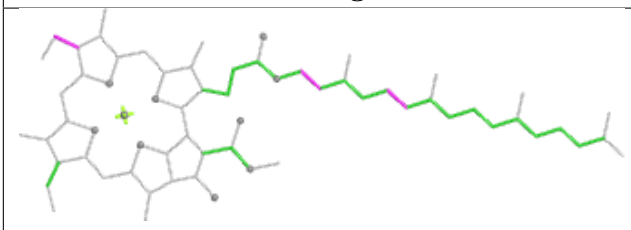
Ligand CLA 4 608



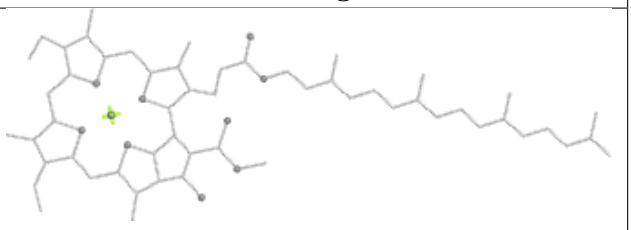
Bond lengths



Bond angles

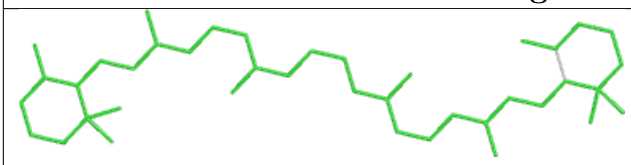


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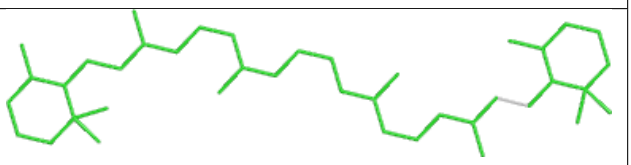


Rings

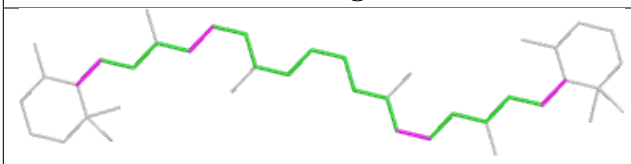
Ligand 8CT b 615



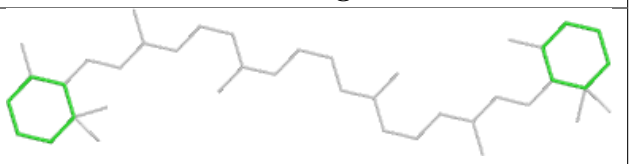
Bond lengths



Bond angles

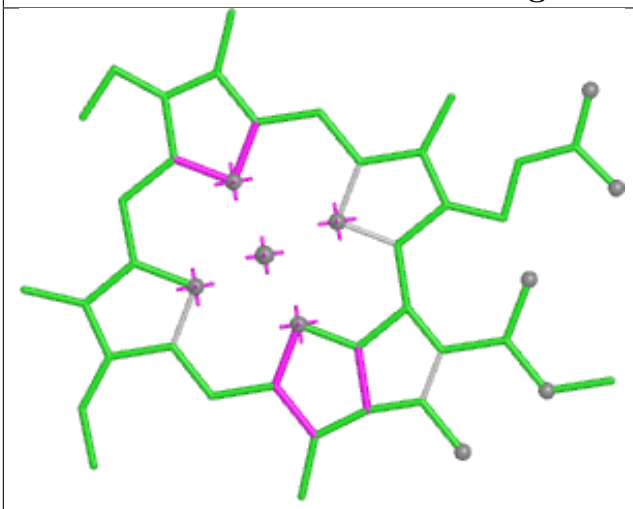


Torsions

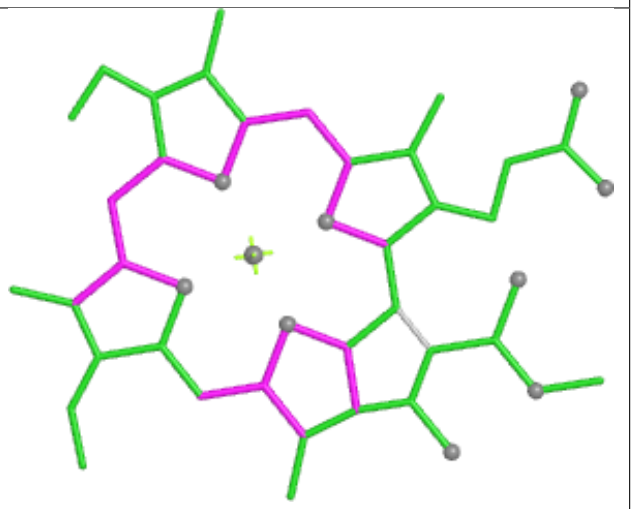


Rings

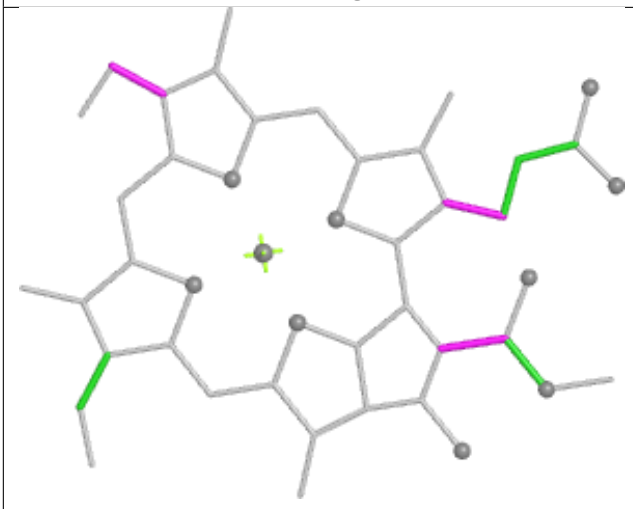
Ligand CLA 5 612



Bond lengths



Bond angles

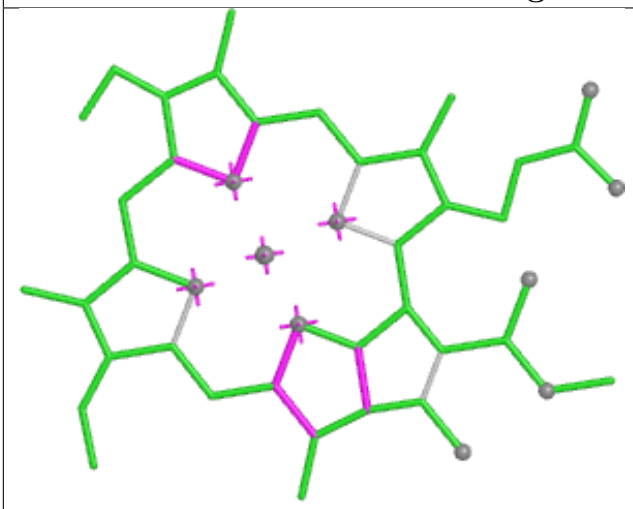


Torsions

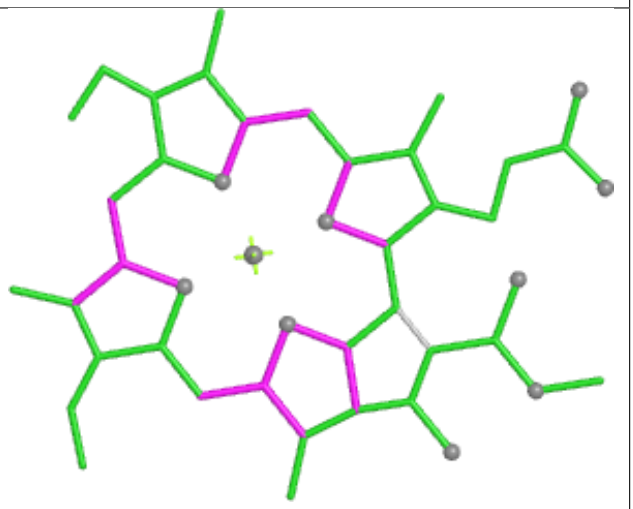


Rings

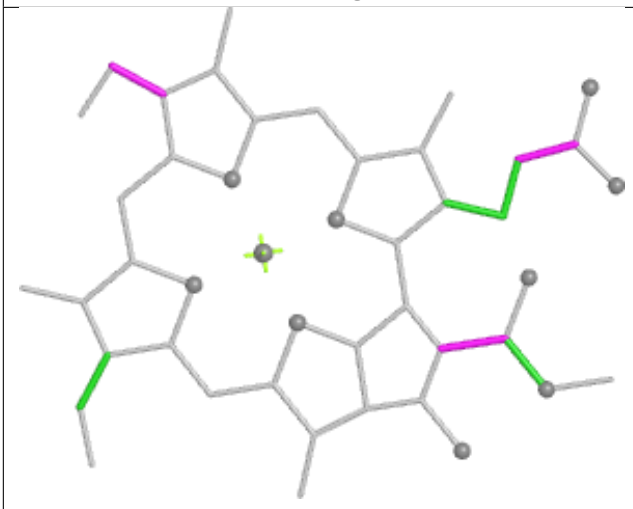
Ligand CLA d 605



Bond lengths



Bond angles

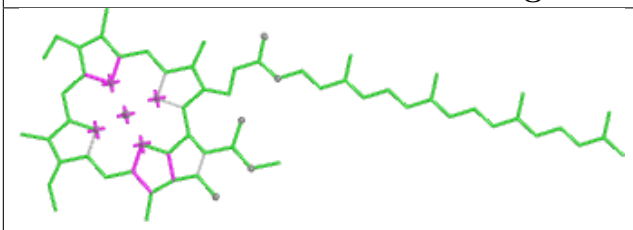


Torsions

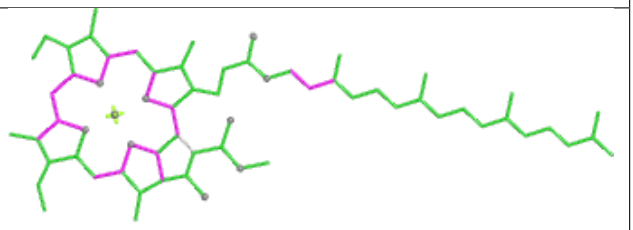


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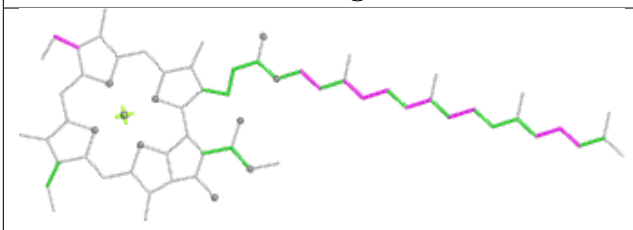
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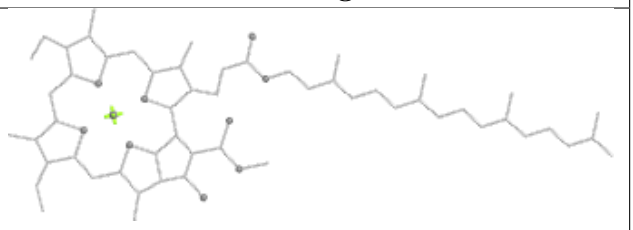
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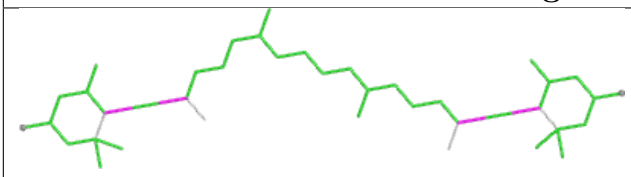
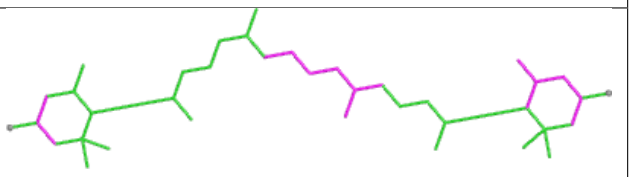
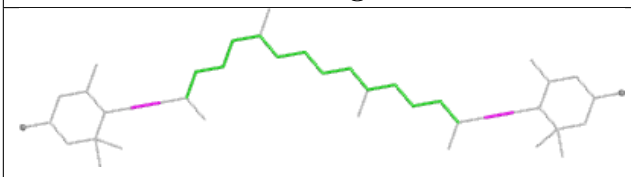
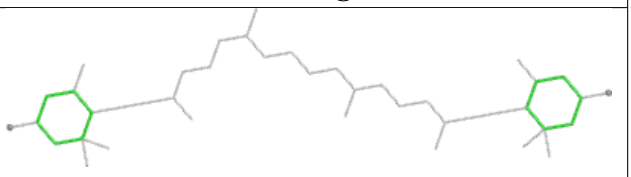
Bond angles

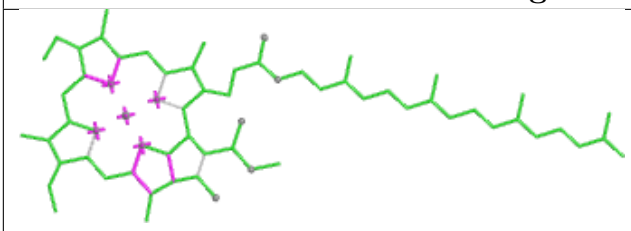
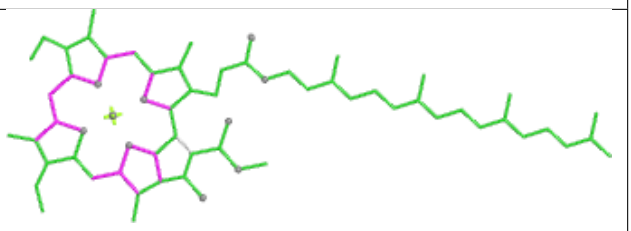
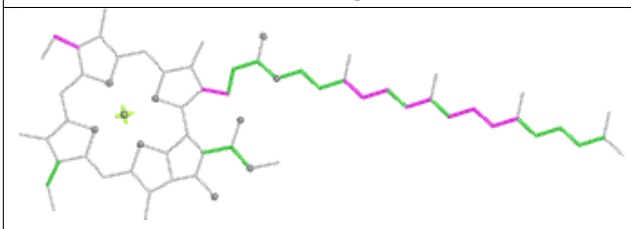
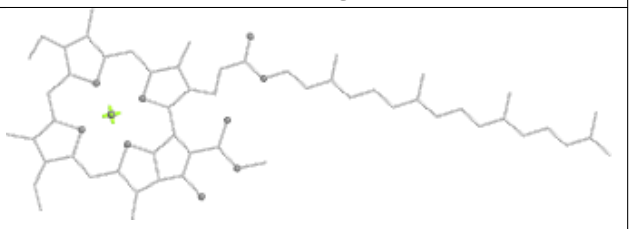


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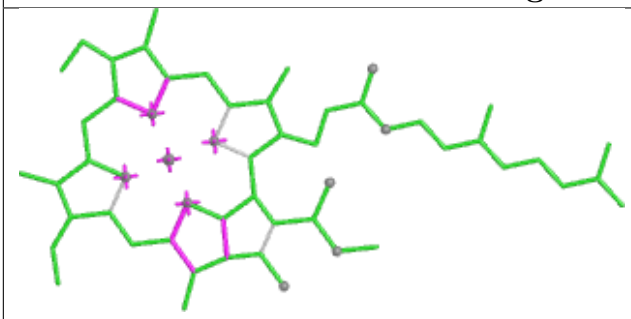


Rings

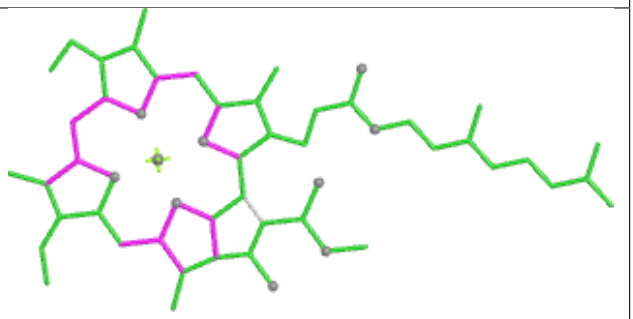
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 Bond lengths	 Bond angles
 Torsions	 Rings

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 Bond lengths	 Bond angles
 Torsions	 Rings

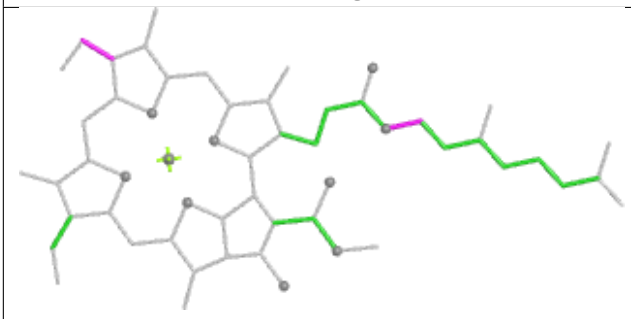
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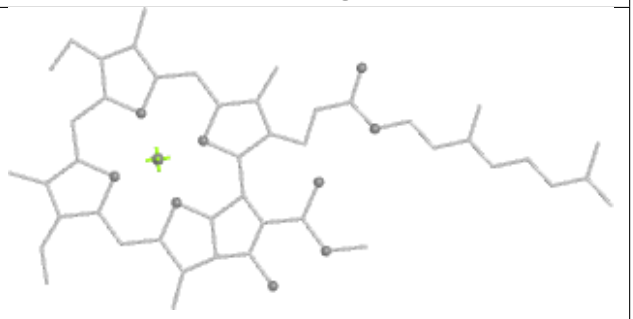
Bond lengths



Bond angles

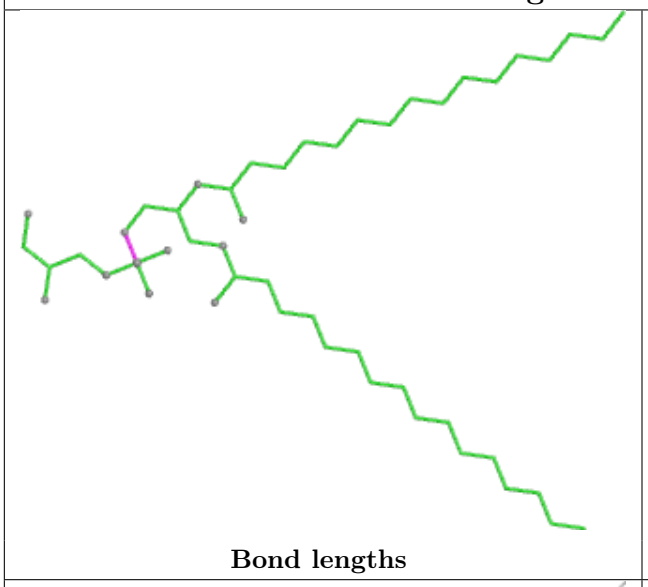


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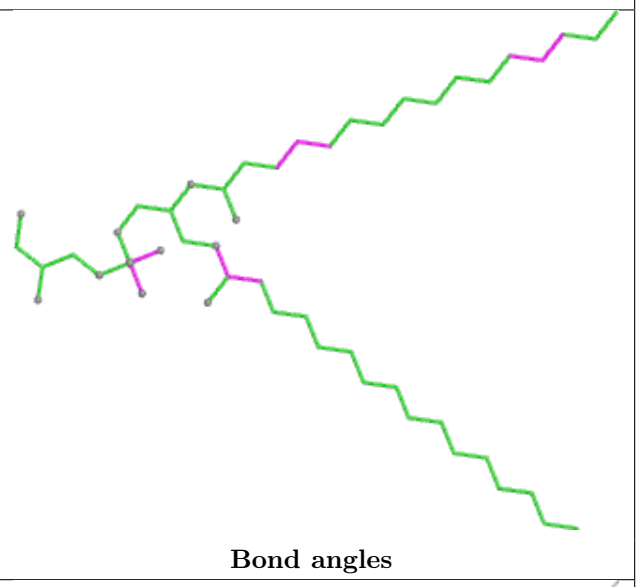


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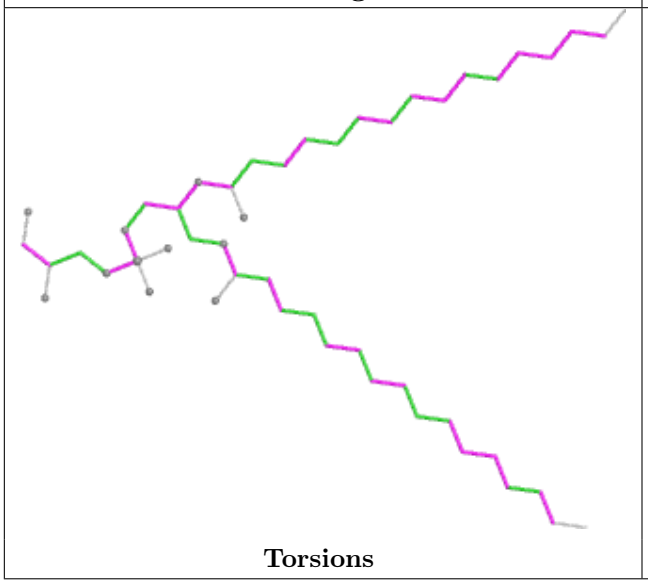
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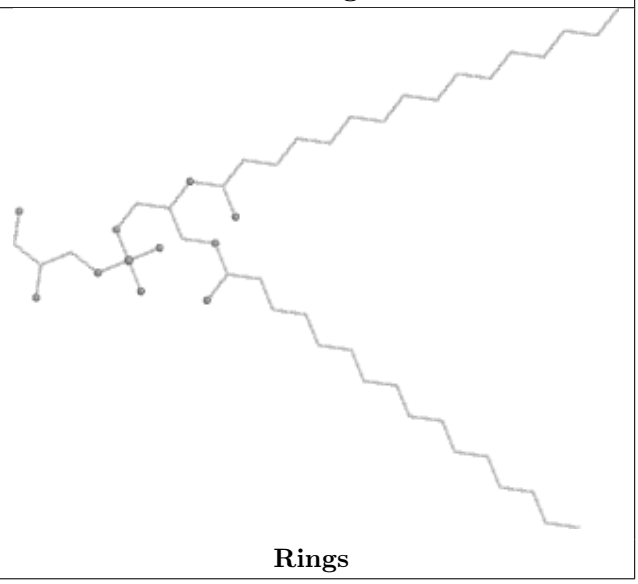
Bond lengths



Bond angles

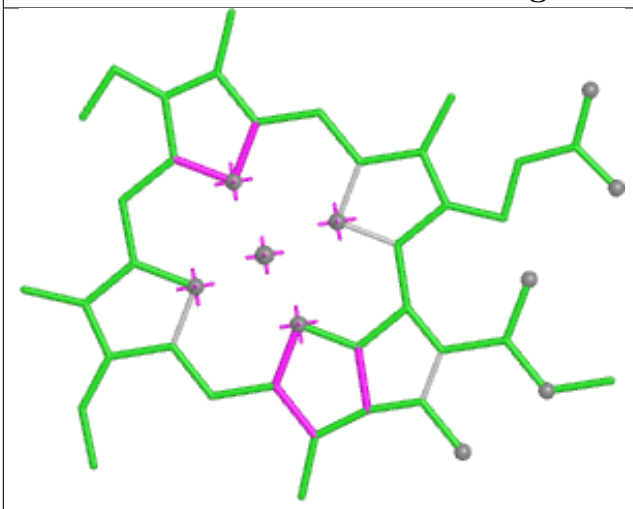


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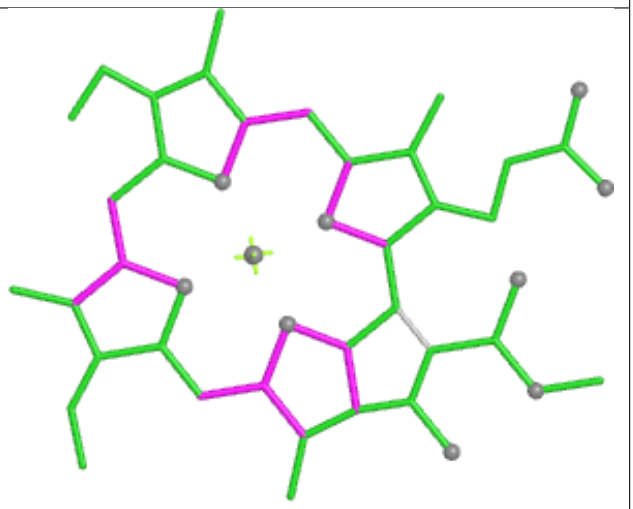


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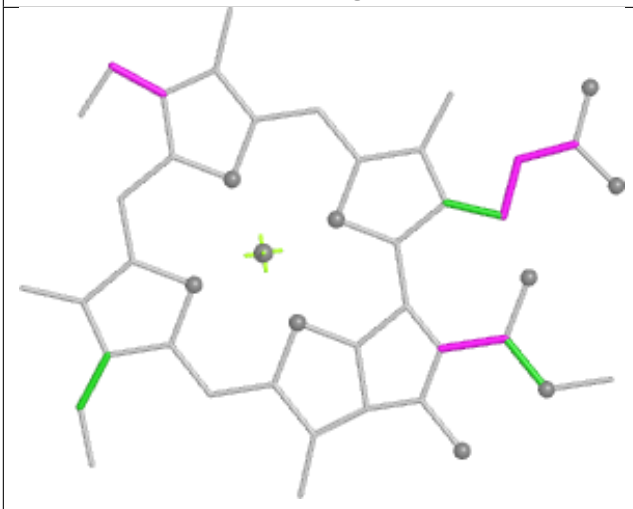
Ligand CLA c 605



Bond lengths



Bond angles

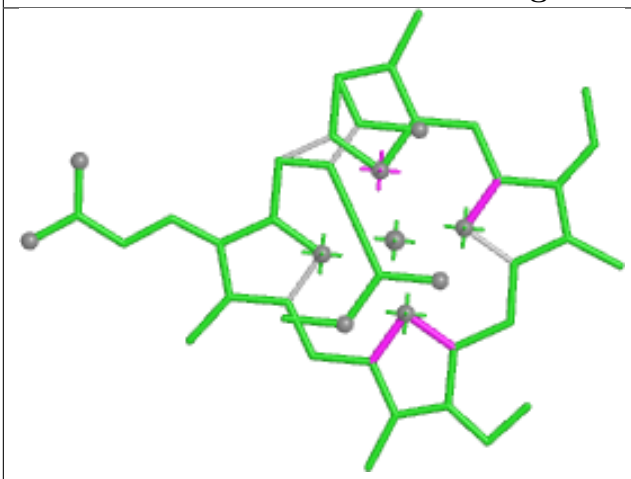


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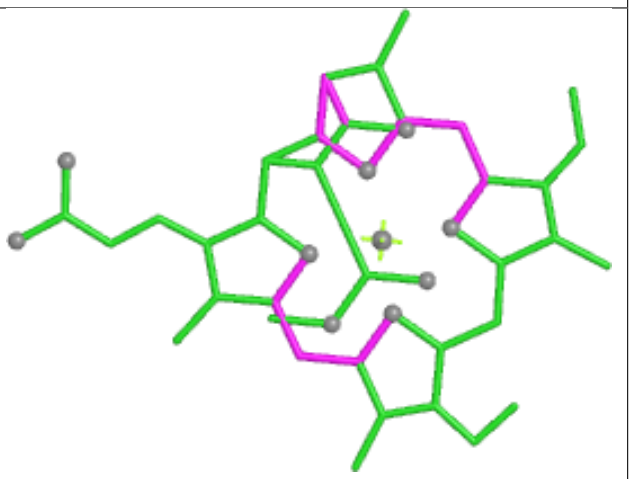


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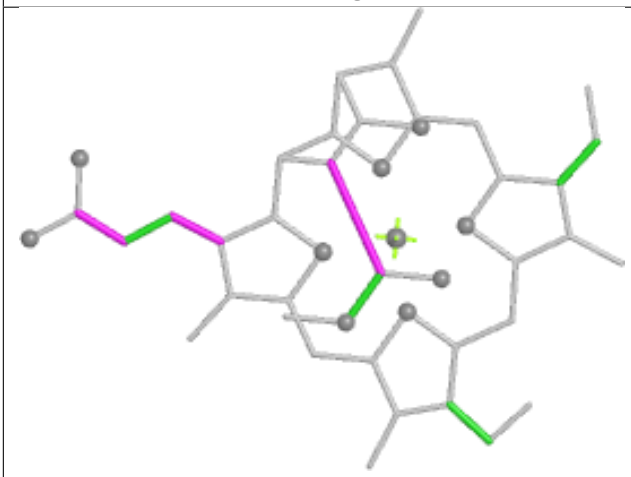
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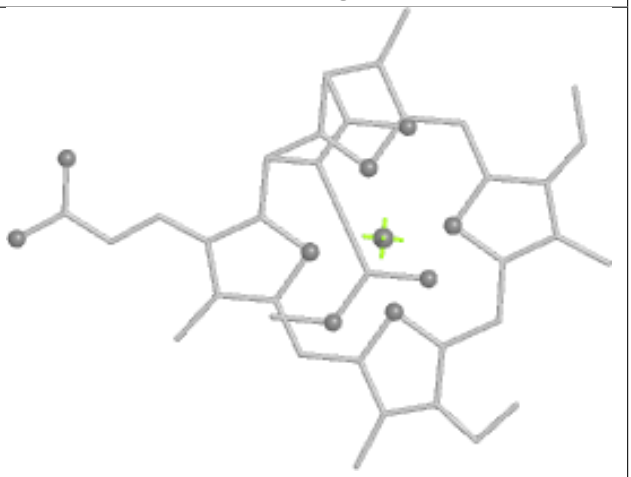
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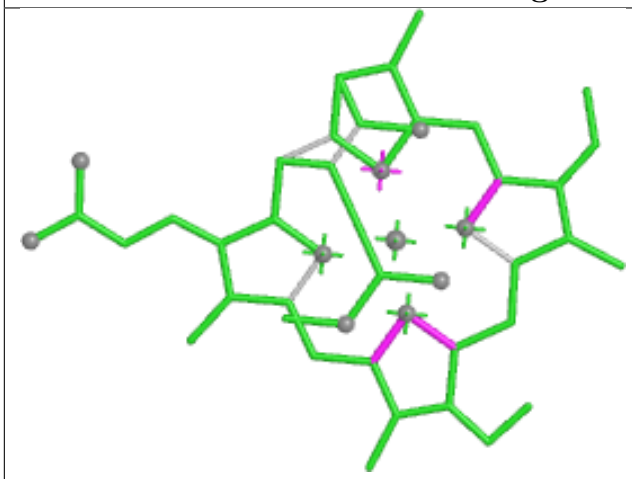


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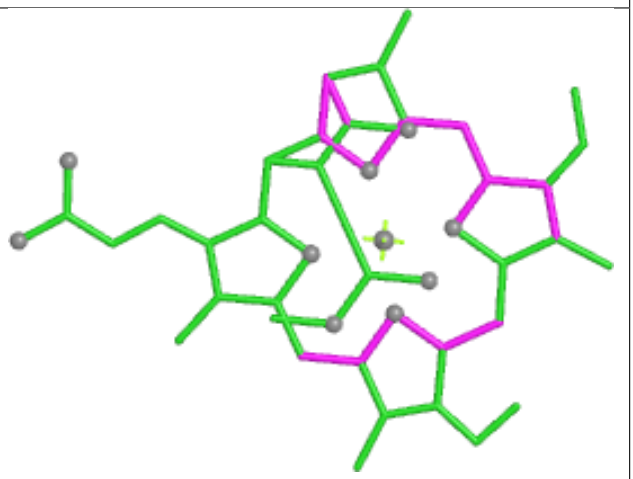


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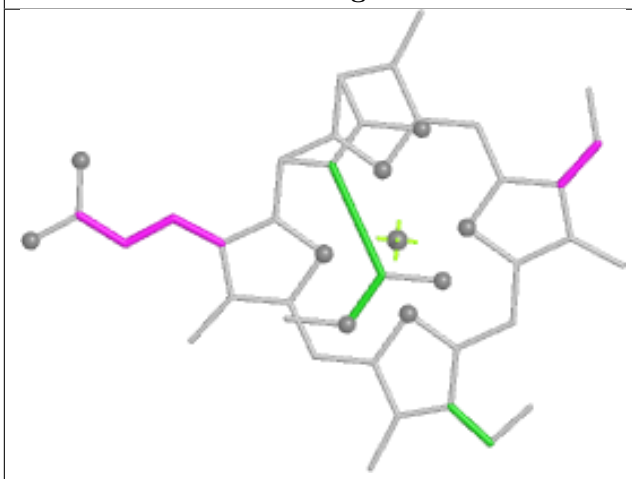
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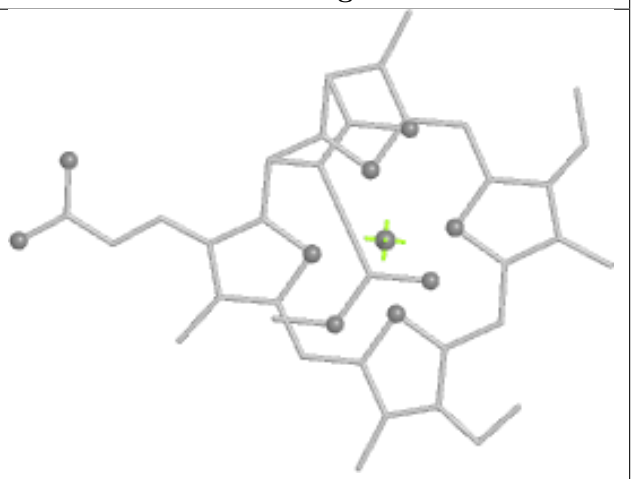
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Bond angles

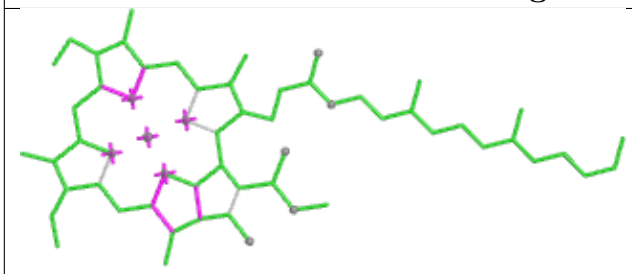


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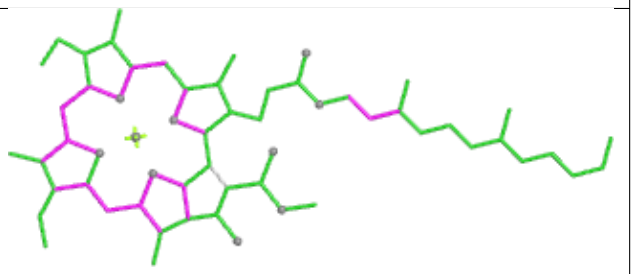


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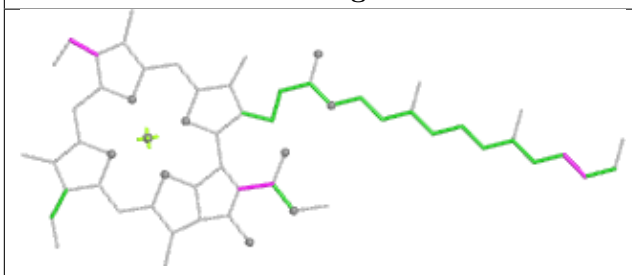
Ligand CLA 4 602



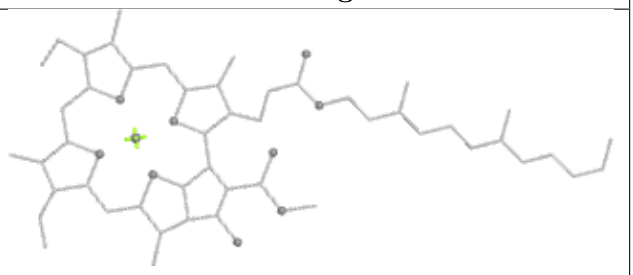
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Bond angles

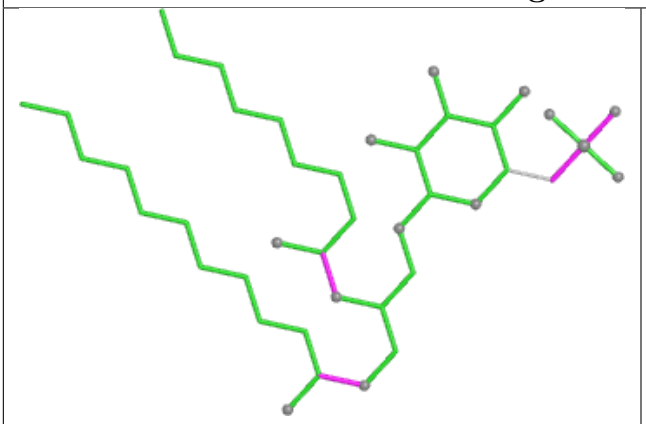


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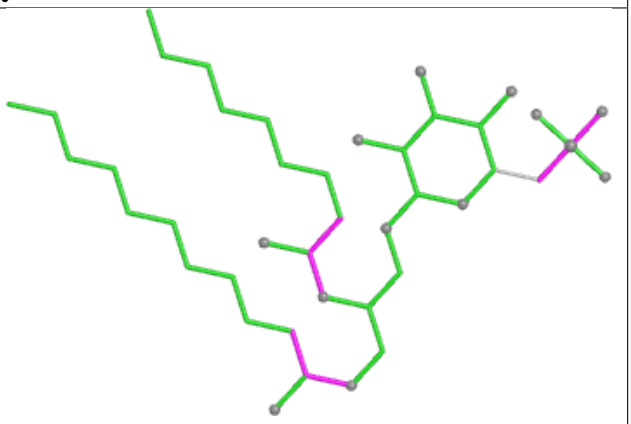


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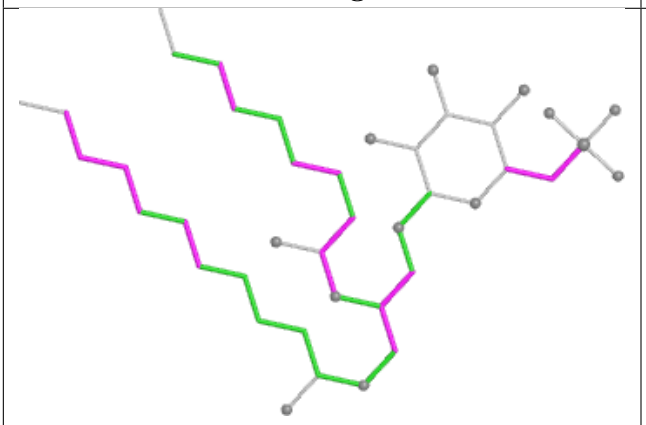
Ligand SQD 3 621



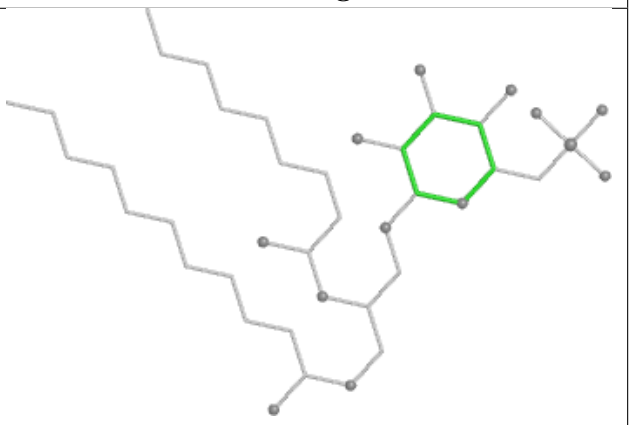
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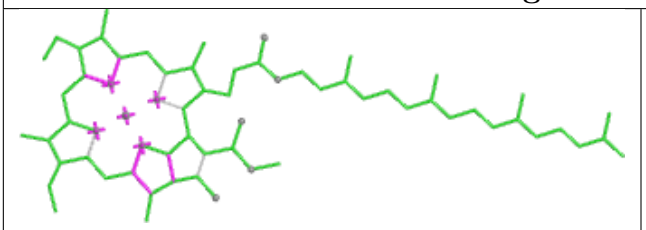


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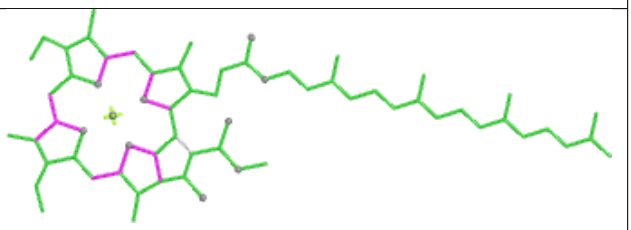


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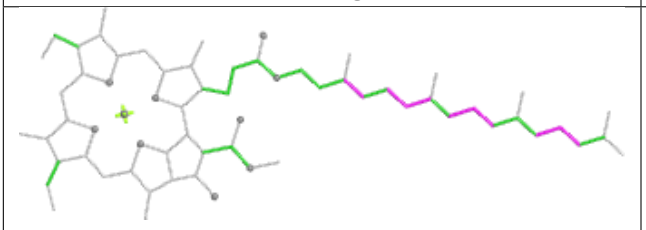
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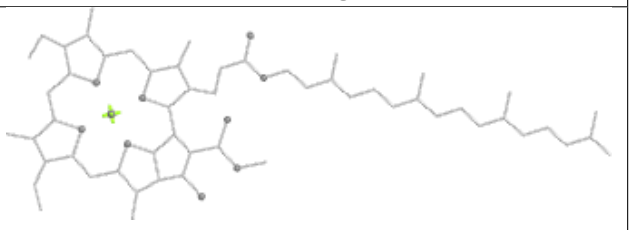
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Bond angles

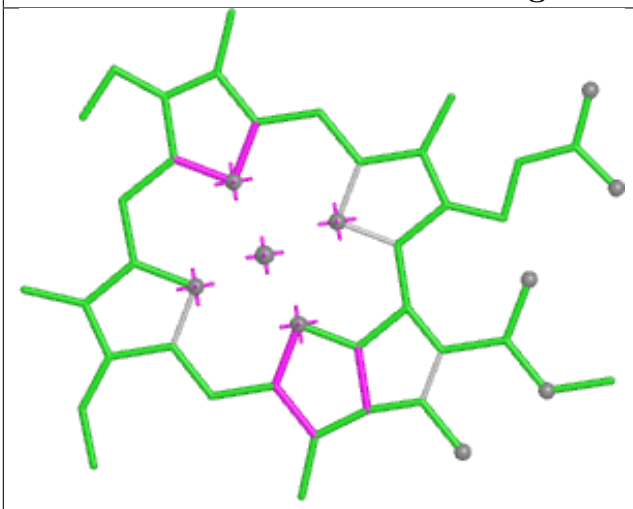


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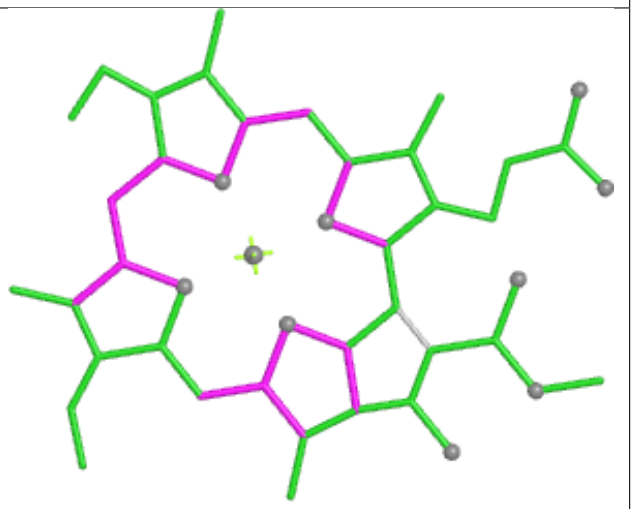


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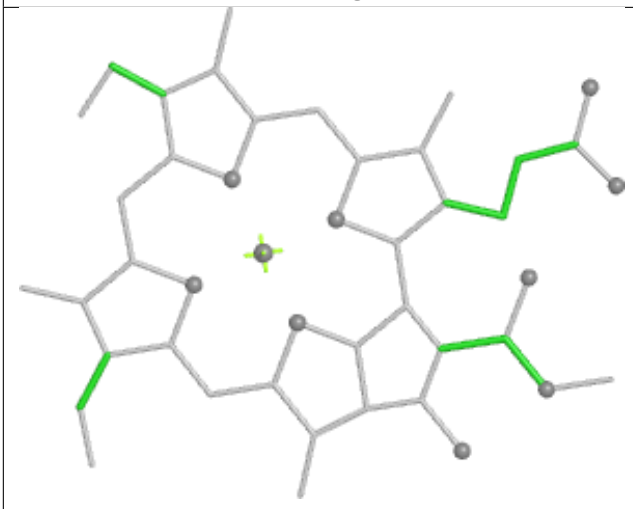
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Bond lengths



Bond angles

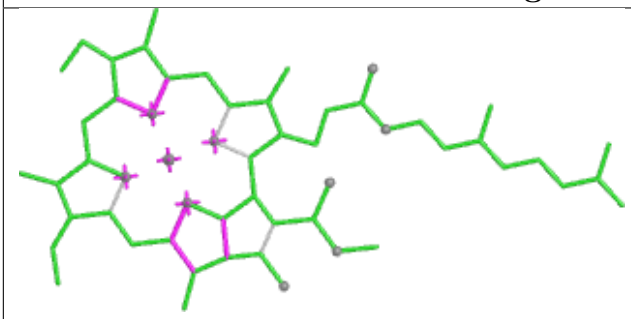


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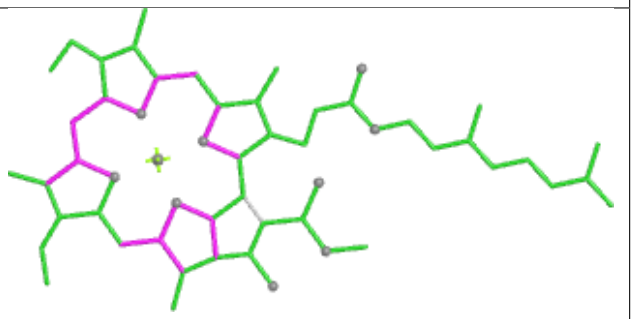


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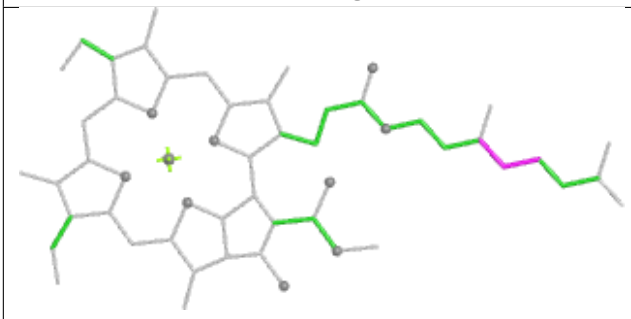
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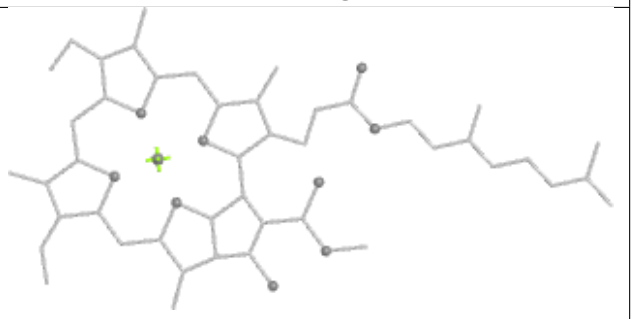
Bond lengths



Bond angles

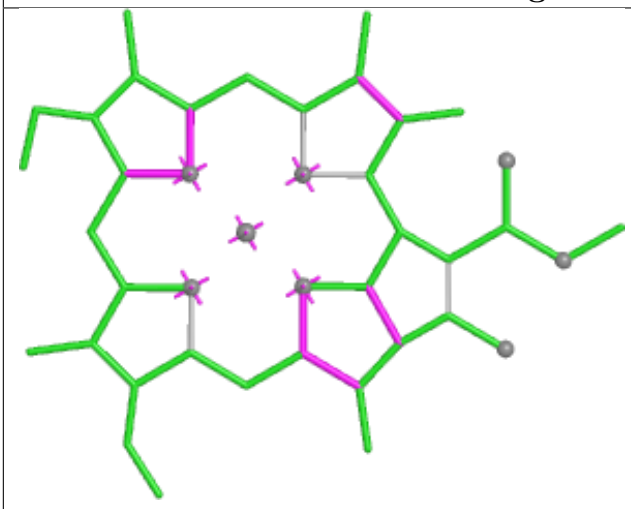


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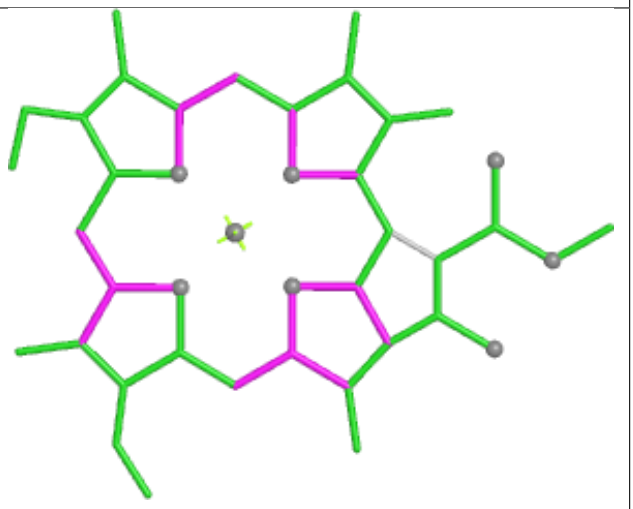


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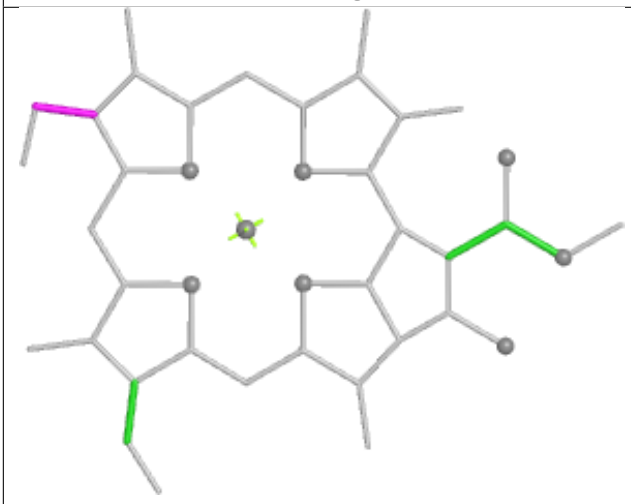
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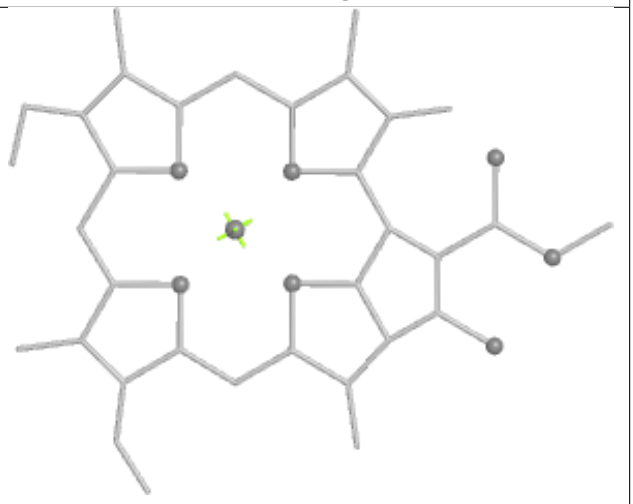
Bond lengths



Bond angles

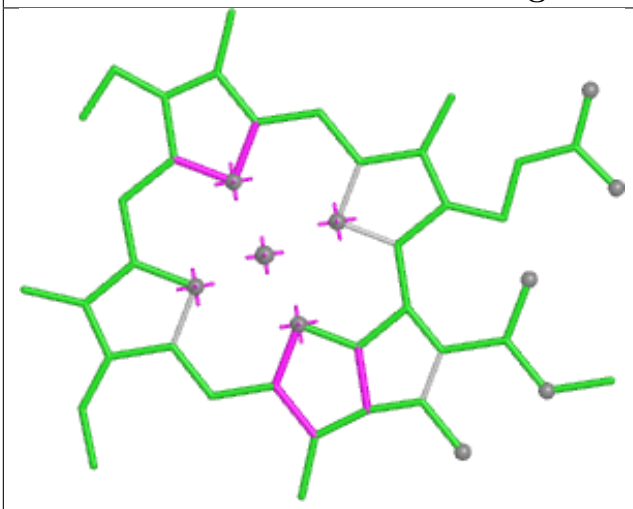


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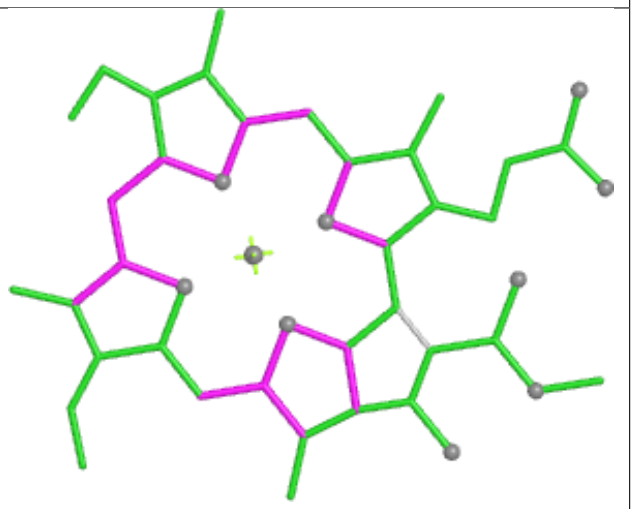


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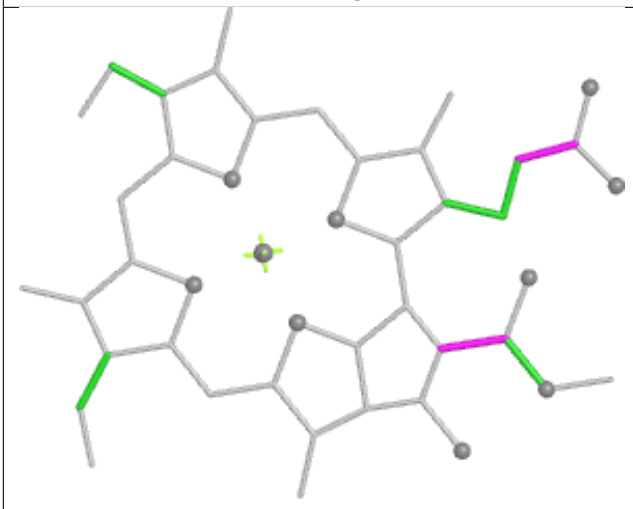
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Bond lengths



Bond angles

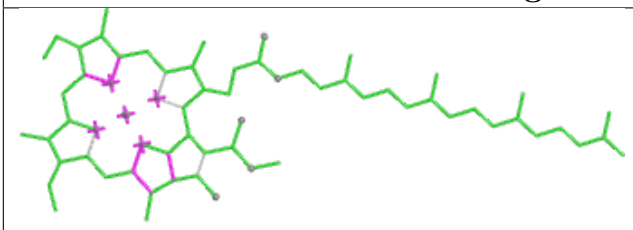


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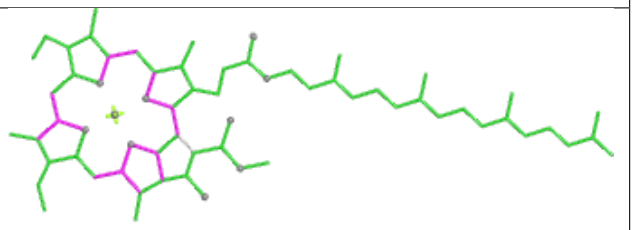


Rings

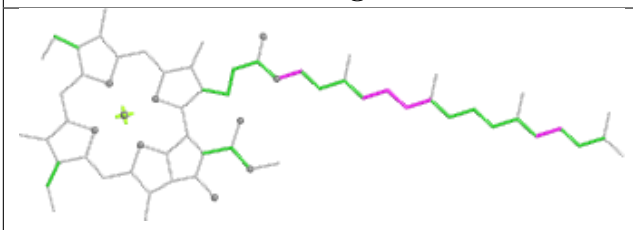
Ligand CLA B 802



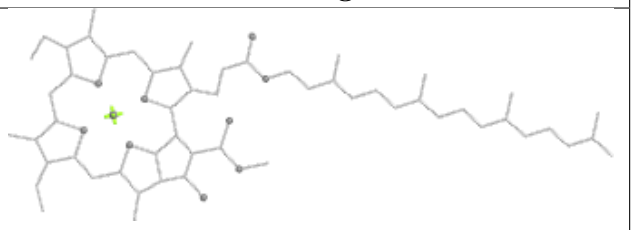
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Bond angles

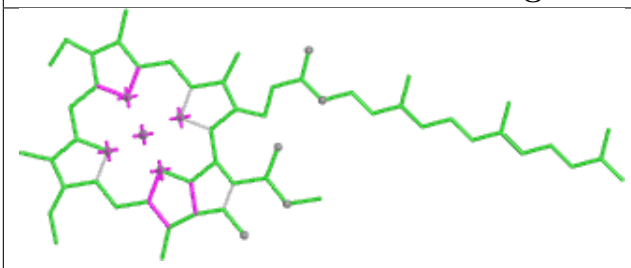


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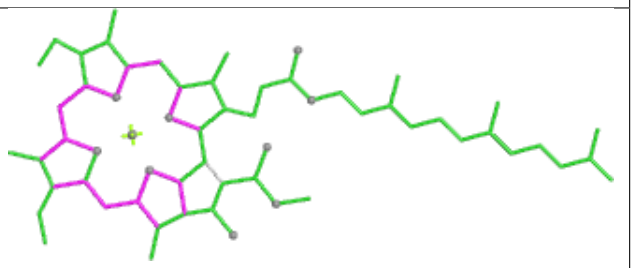


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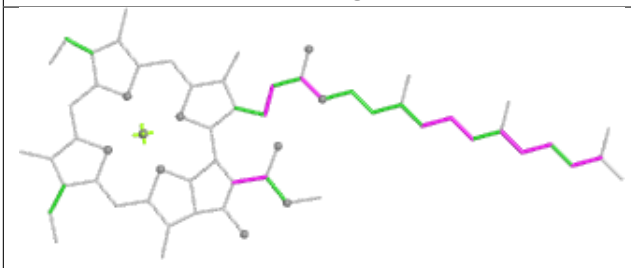
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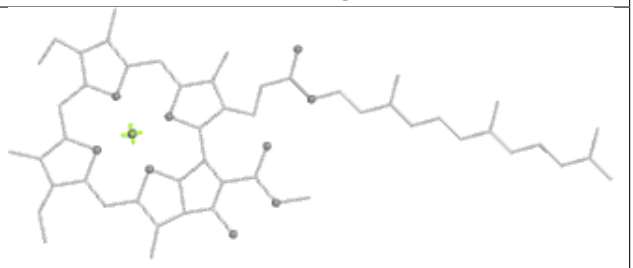
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Bond angles

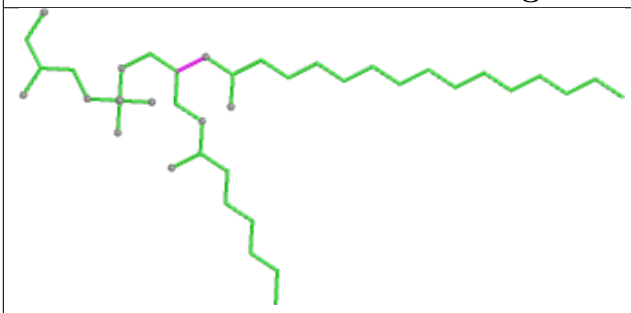


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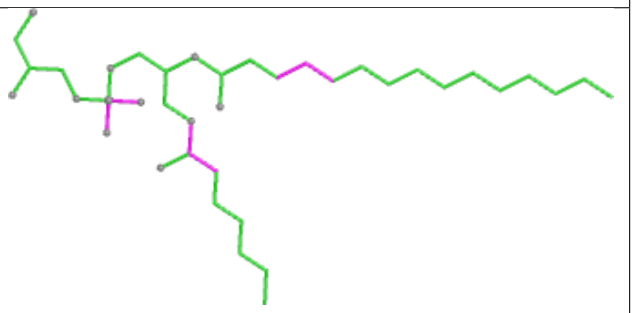


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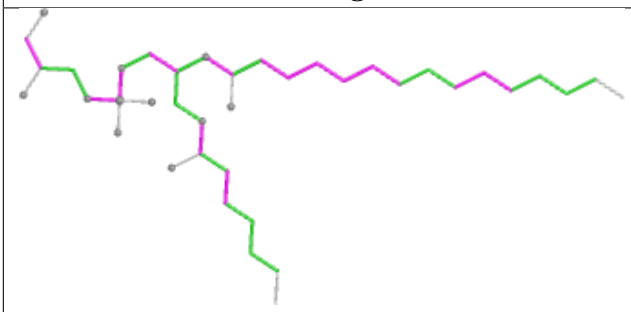
Ligand LHG A 851



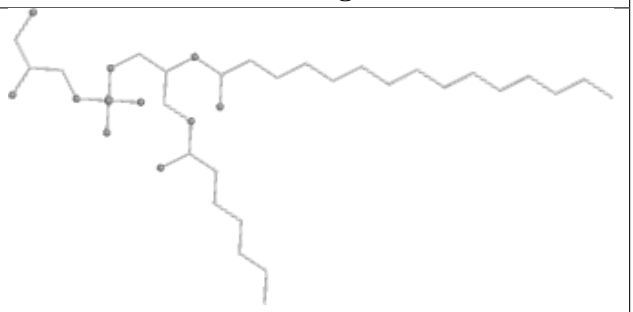
Bond lengths



Bond angles

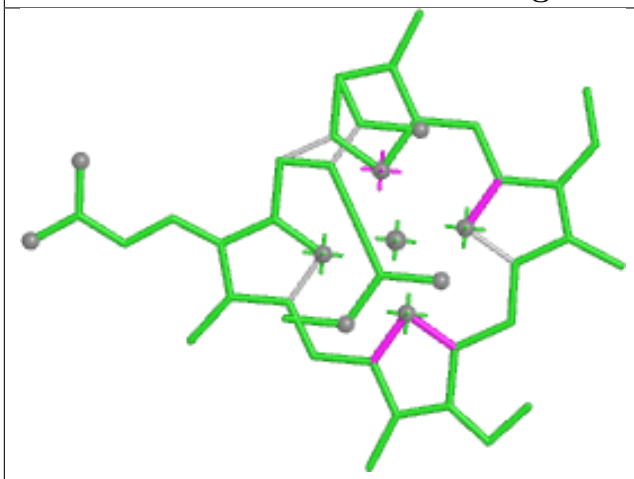


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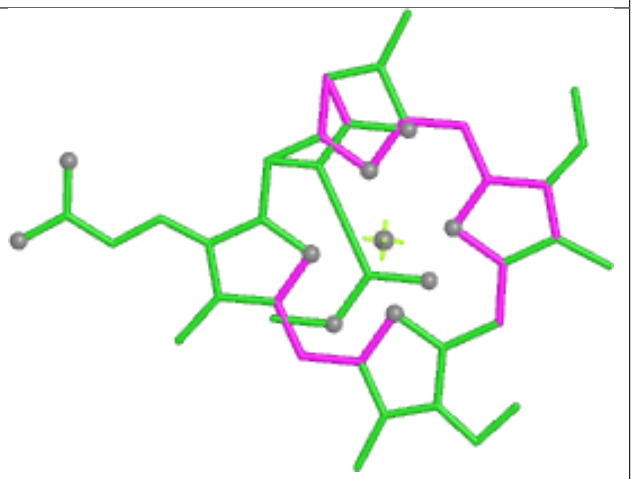


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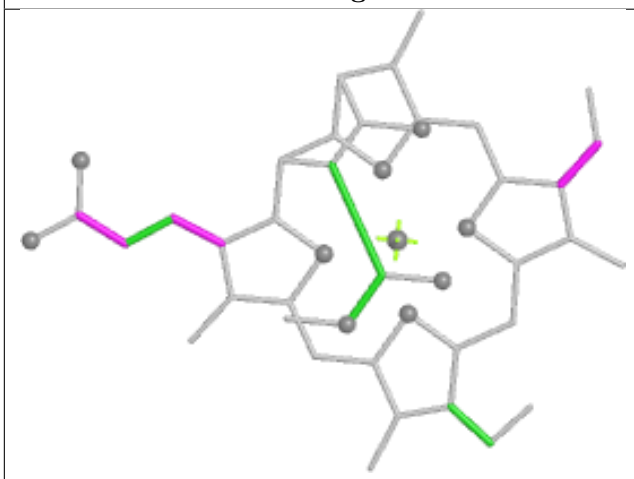
Ligand KC2 c 611



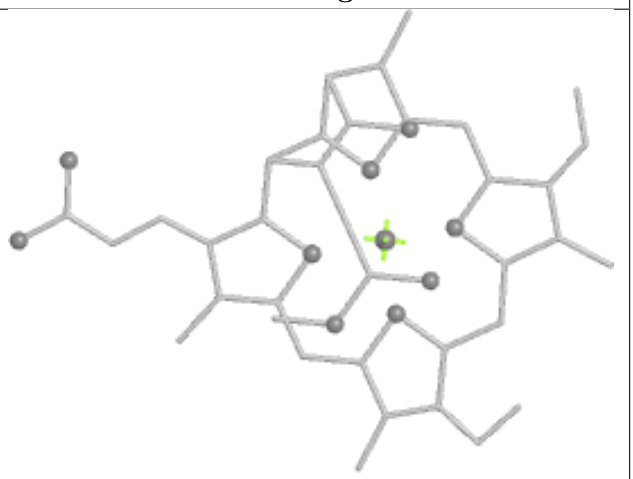
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Bond angles



Torsions



Rings

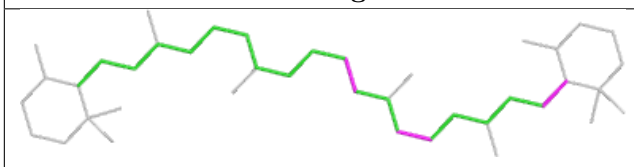
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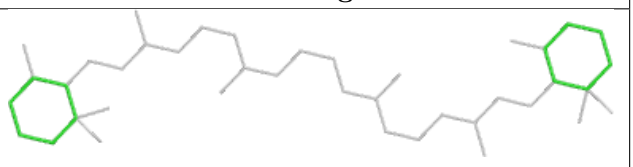
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Bond angles

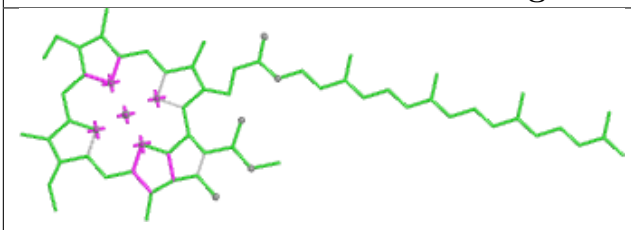


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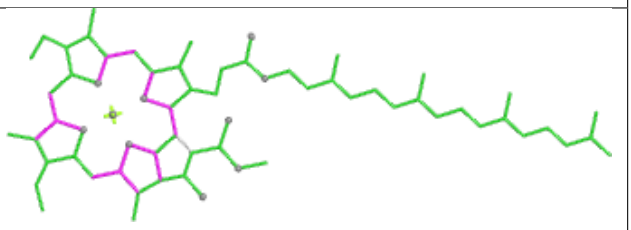


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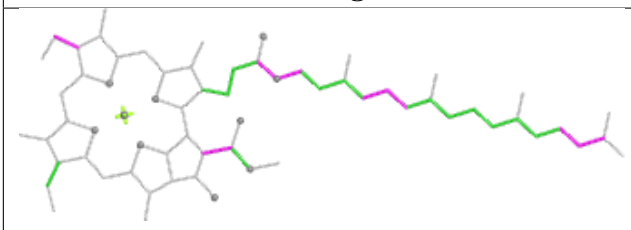
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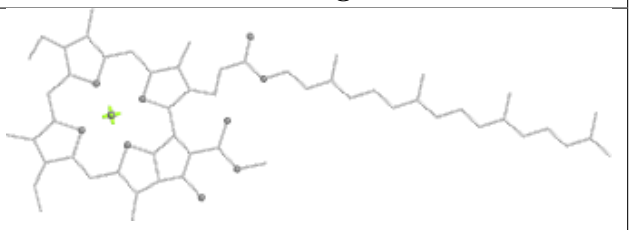
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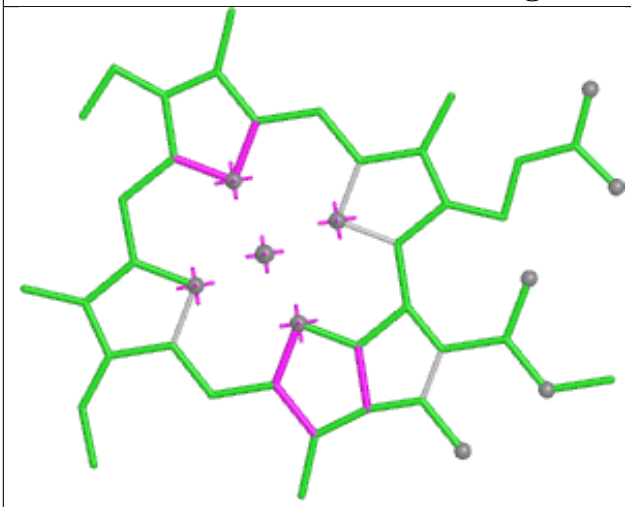


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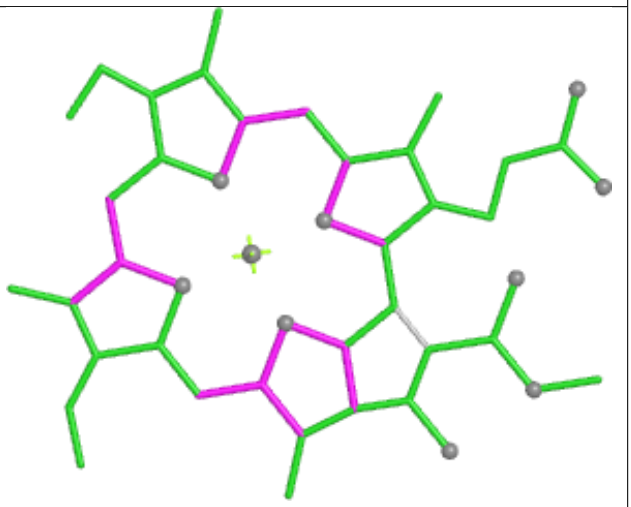


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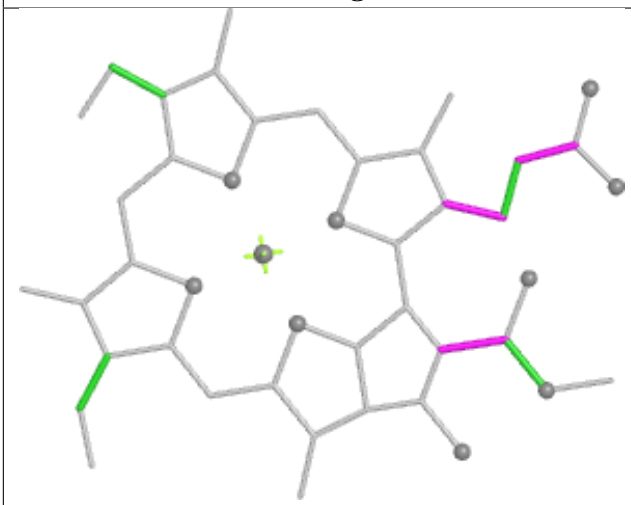
Ligand CLA A 814



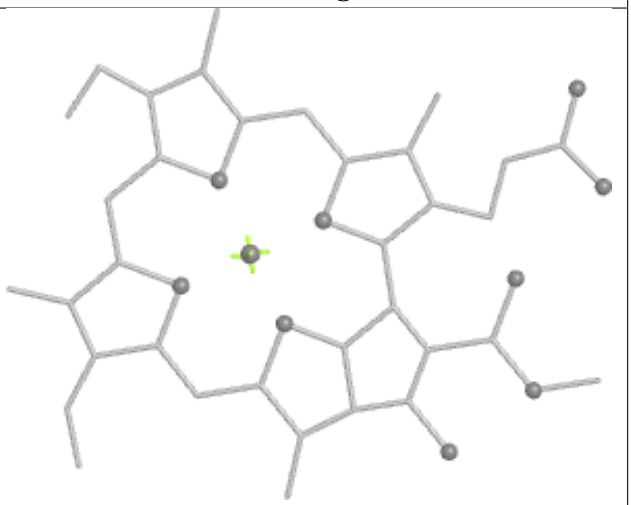
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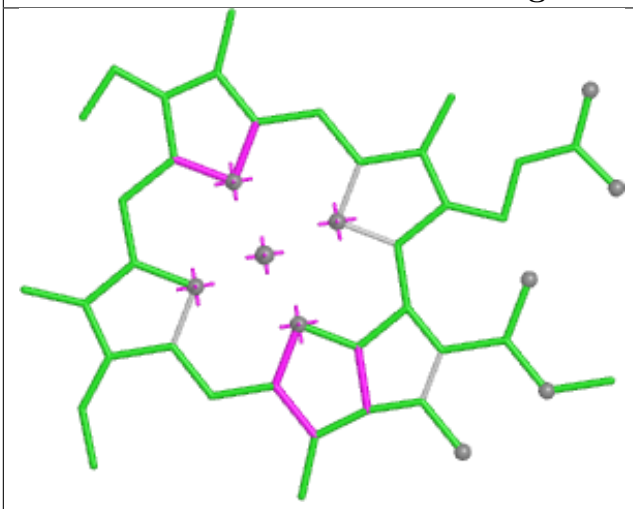


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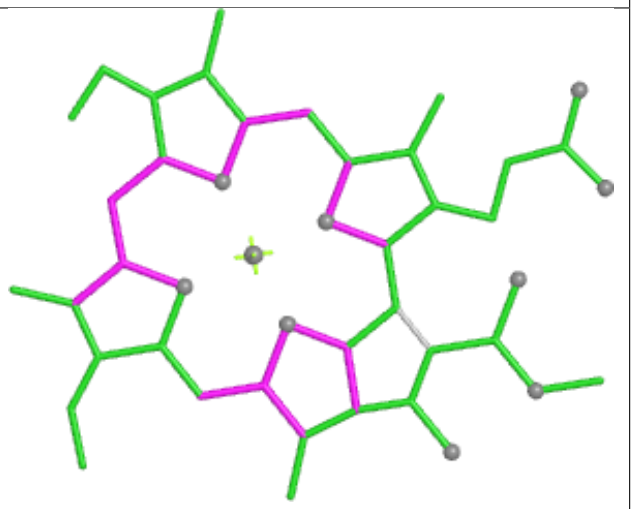


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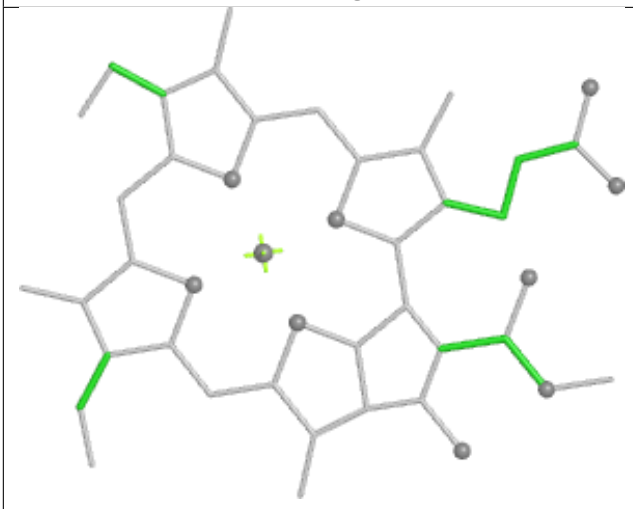
Ligand CLA 9 605



Bond lengths



Bond angles

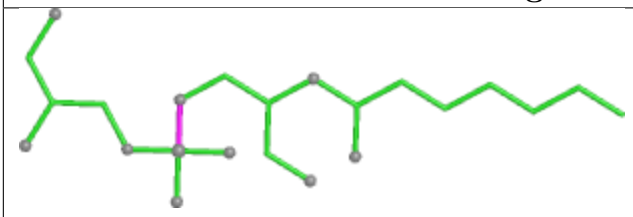


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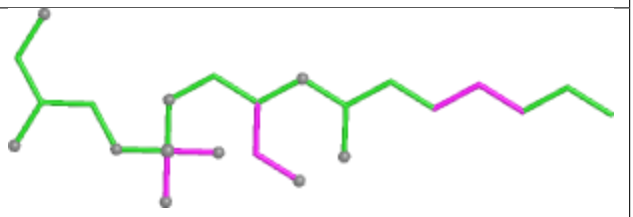


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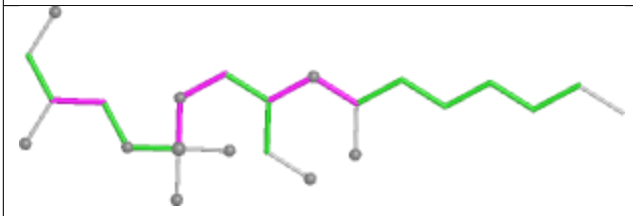
Ligand LHG d 618



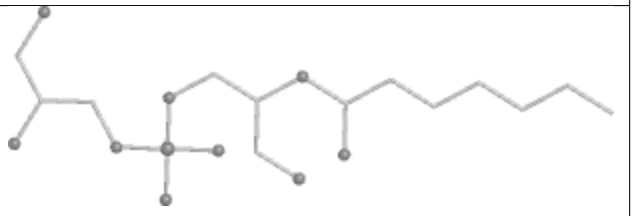
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Bond angles

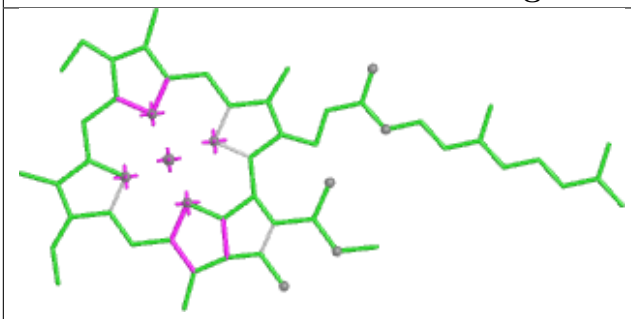


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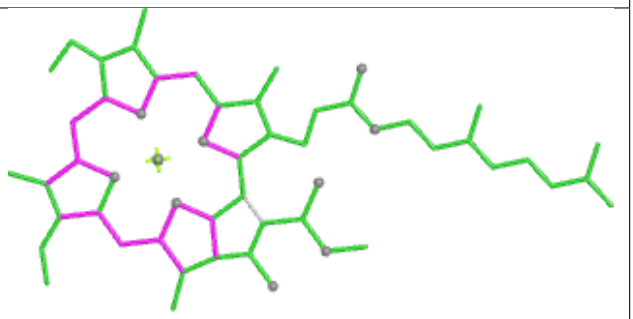


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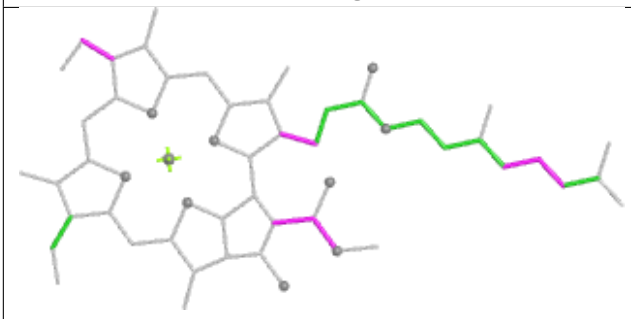
Ligand CLA O 202



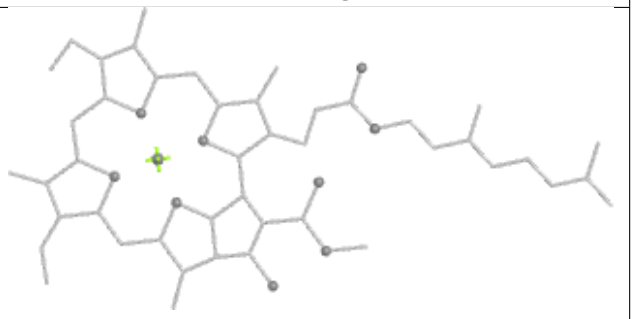
Bond lengths



Bond angles

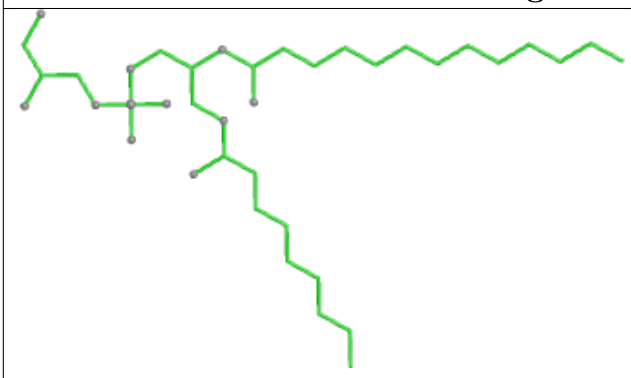


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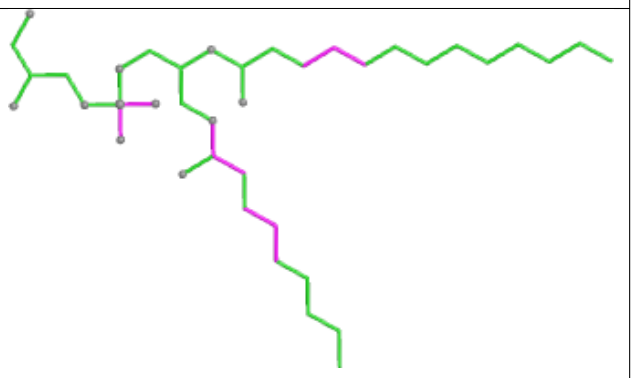


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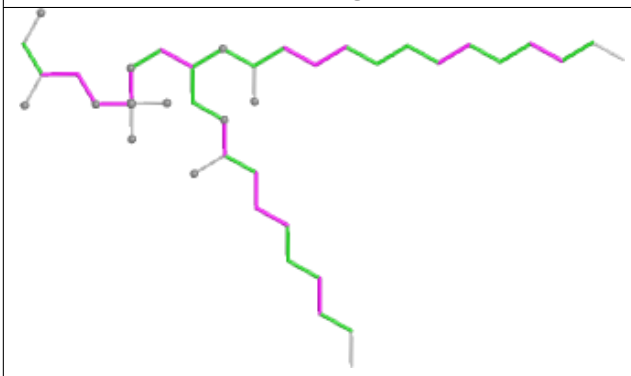
Ligand LHG 2 619



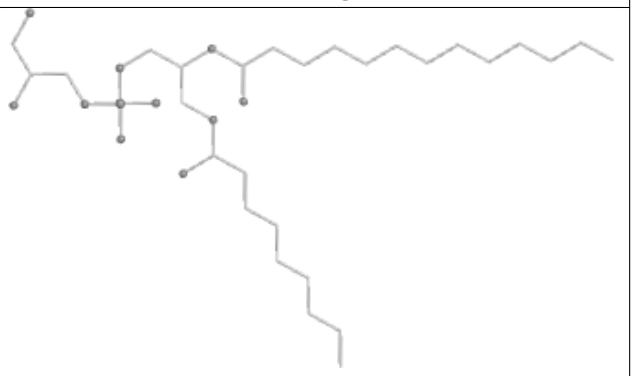
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Bond angles

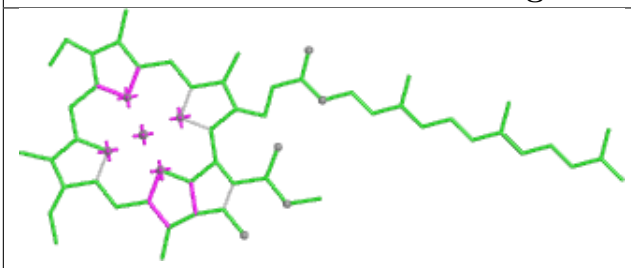


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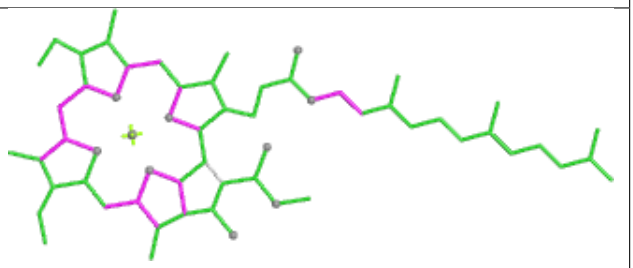


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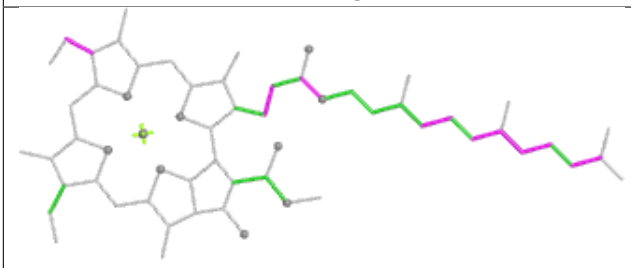
Ligand CLA Z 301



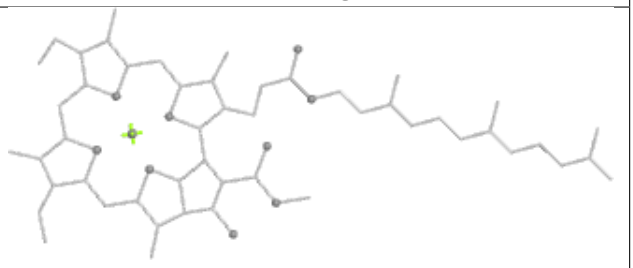
Bond lengths



Bond angles

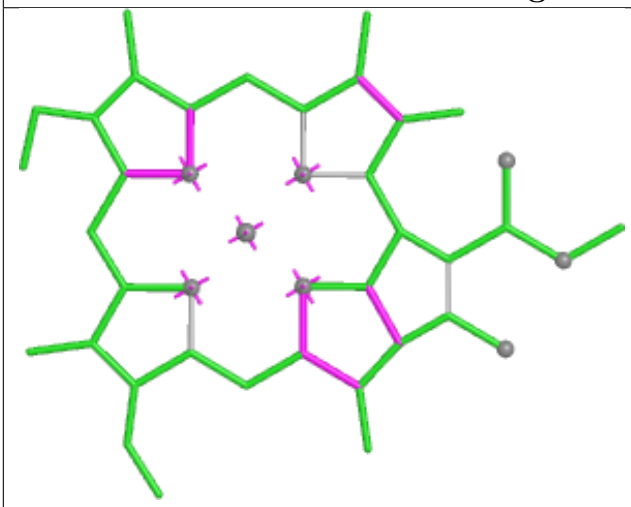


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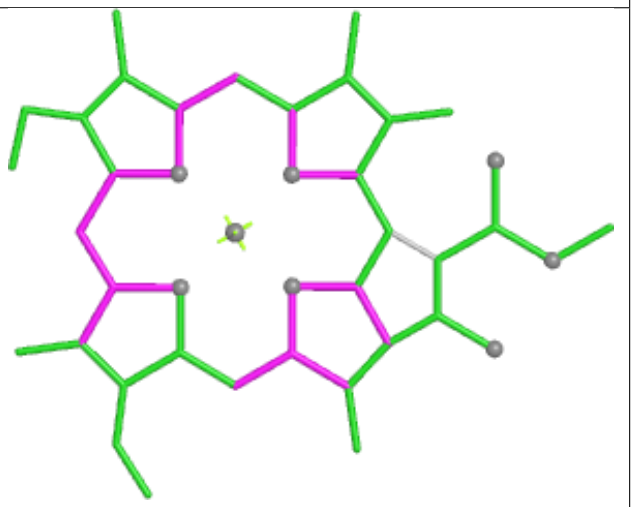


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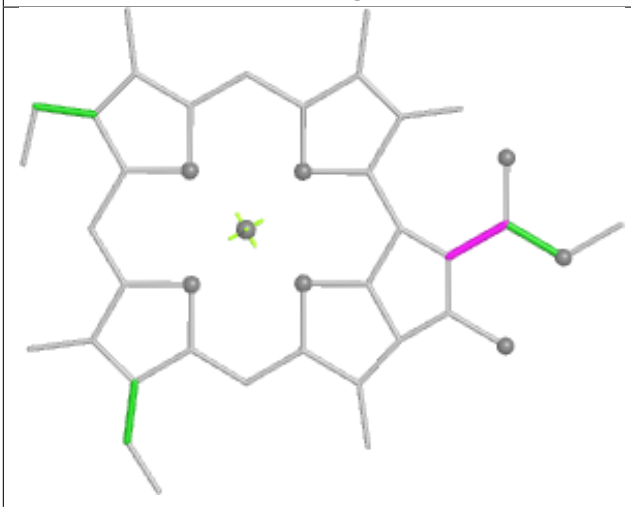
Ligand CLA 9 611



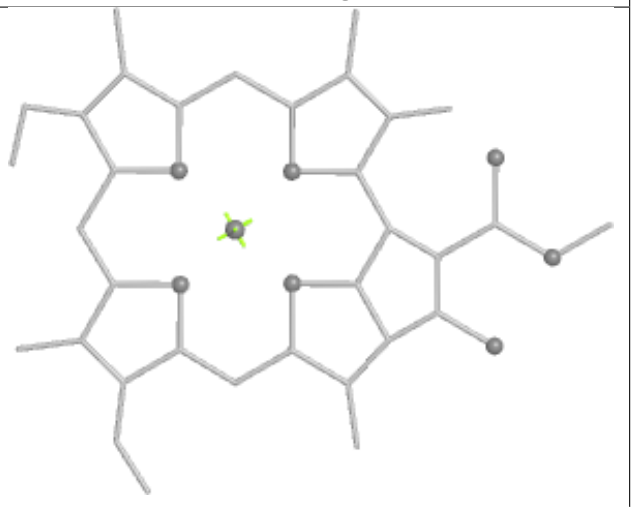
Bond lengths



Bond angles

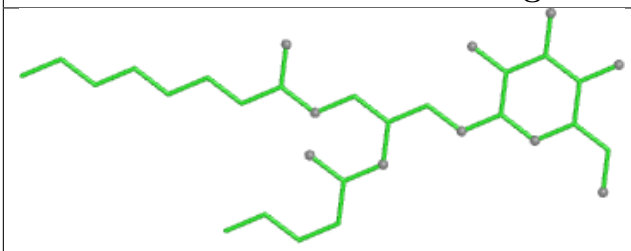


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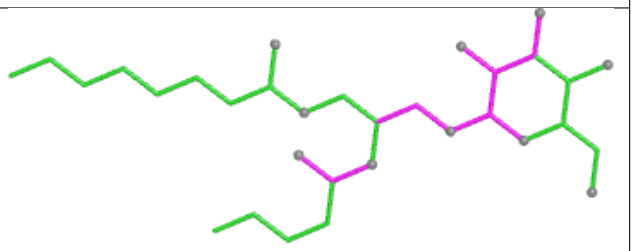


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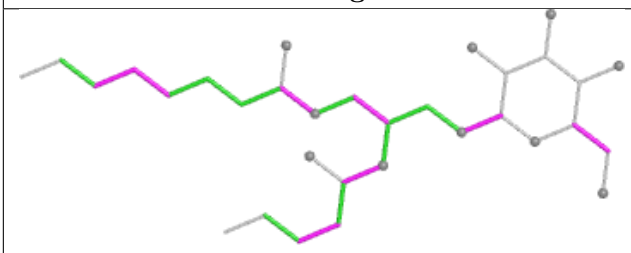
Ligand LMG 3 620



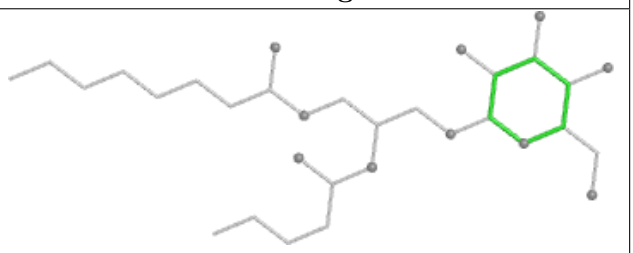
Bond lengths



Bond angles

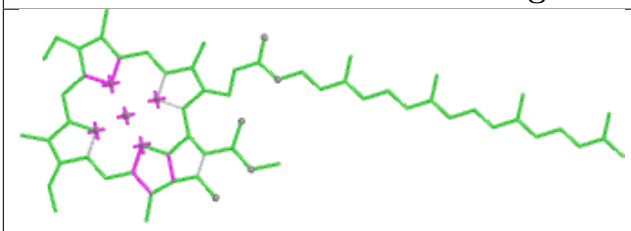


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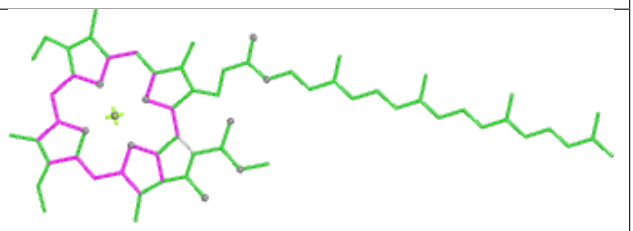


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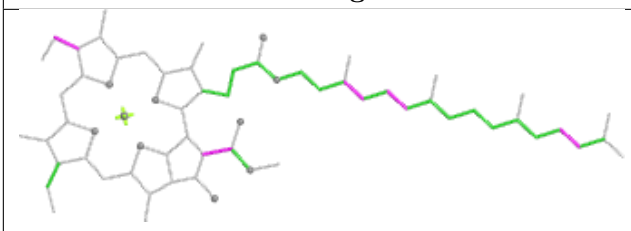
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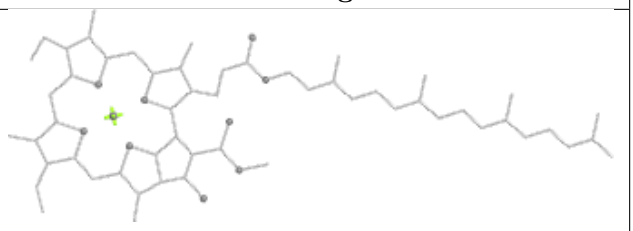
Bond lengths



Bond angles

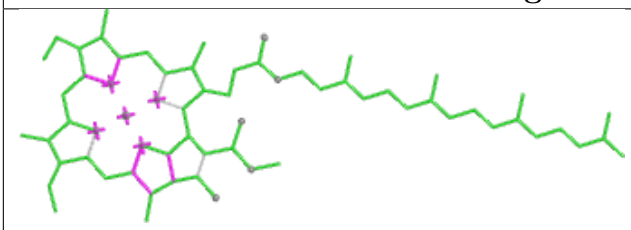


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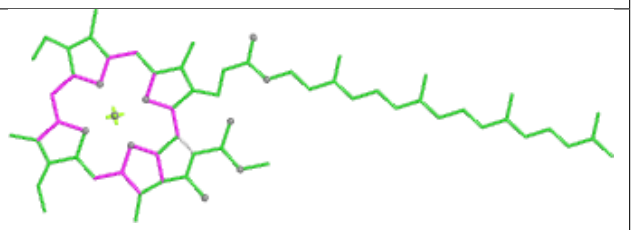


Rings

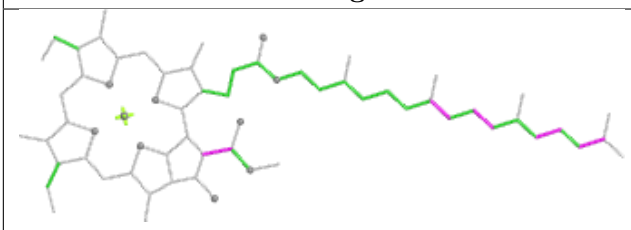
Ligand CLA B 839



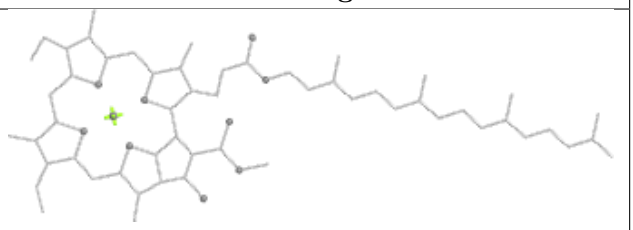
Bond lengths



Bond angles

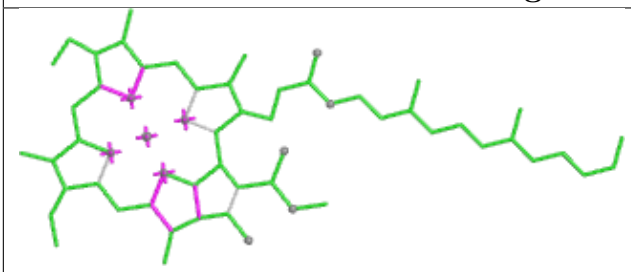


Torsions

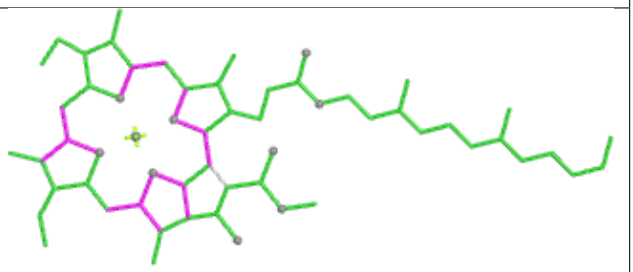


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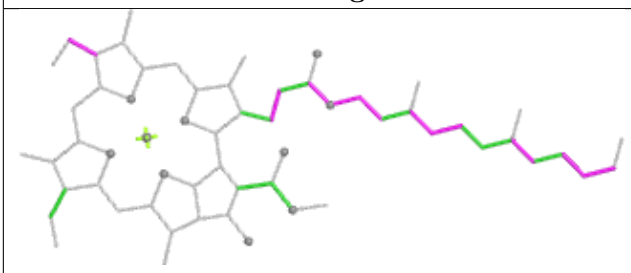
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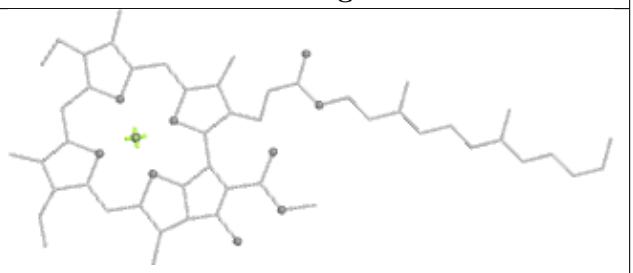
Bond lengths



Bond angles

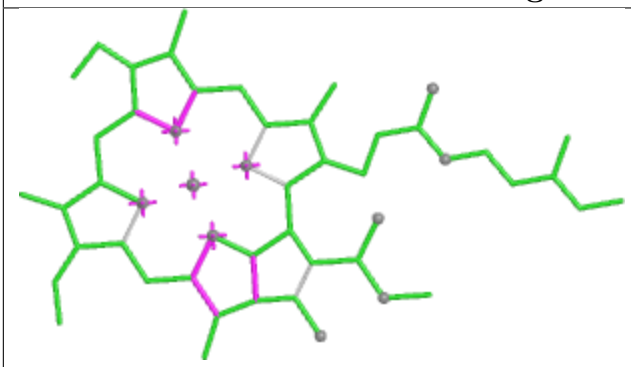


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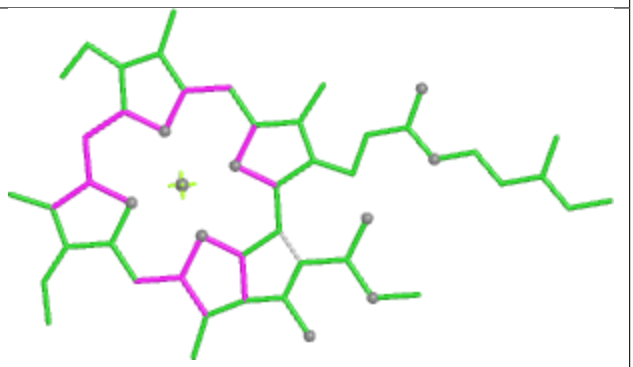


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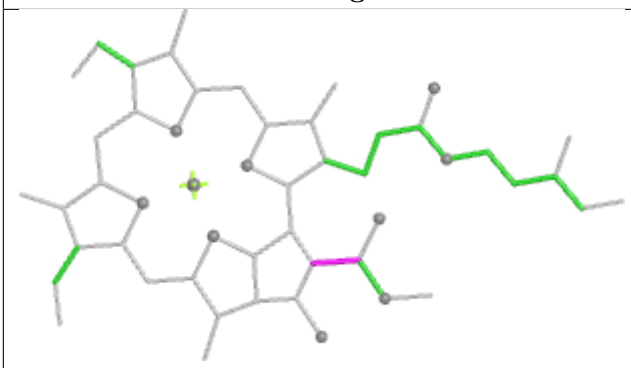
Ligand CLA L 202



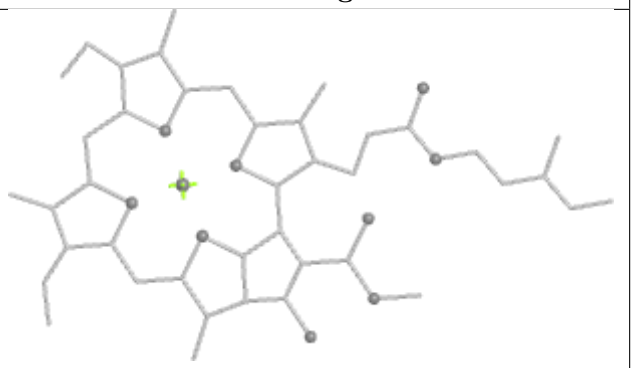
Bond lengths



Bond angles

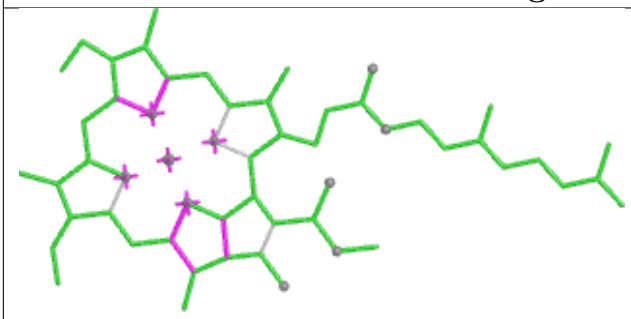


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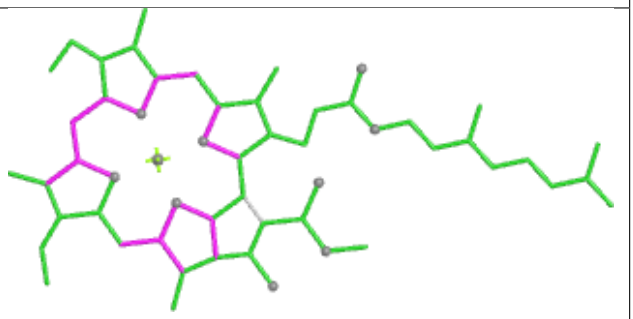


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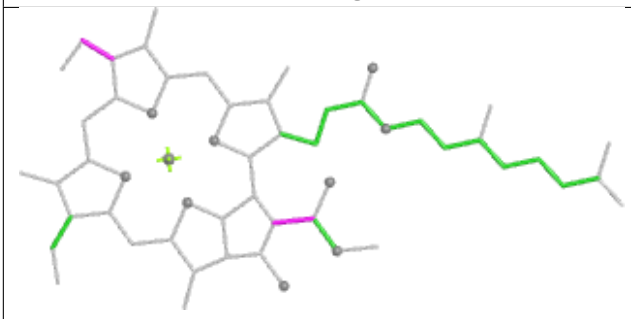
Ligand CLA 3 602



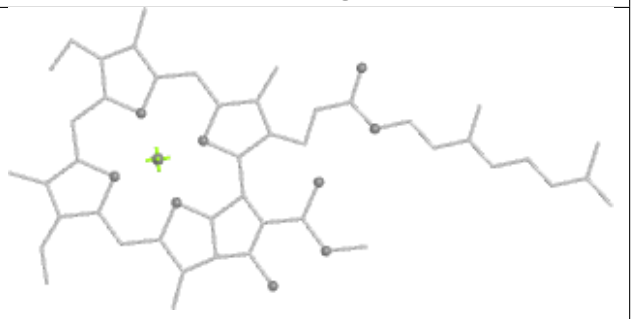
Bond lengths



Bond angles

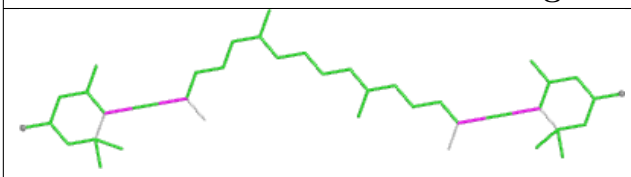


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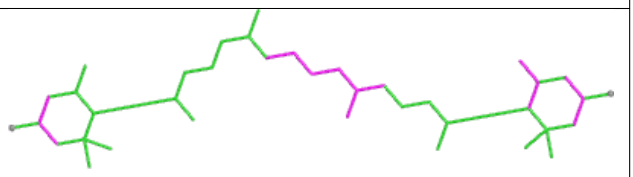


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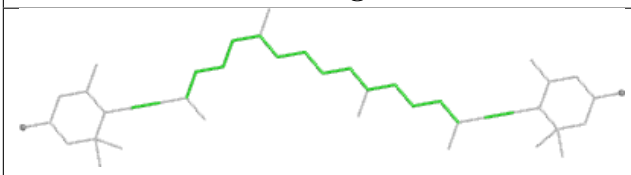
Ligand II0 c 617



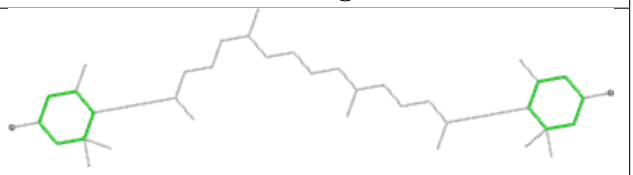
Bond lengths



Bond angles

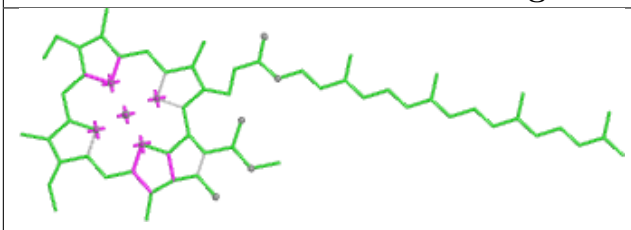


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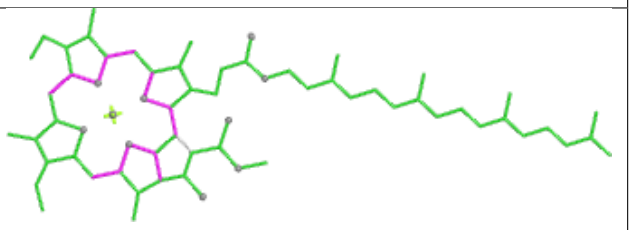


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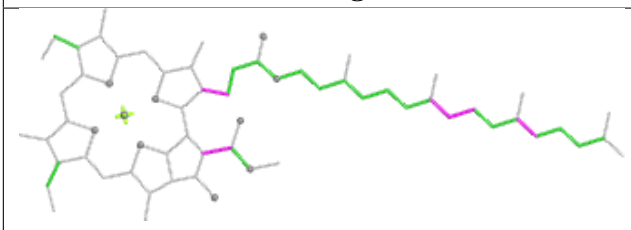
Ligand CLA 6 602



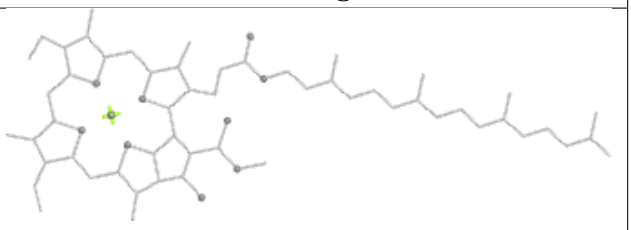
Bond lengths



Bond angles

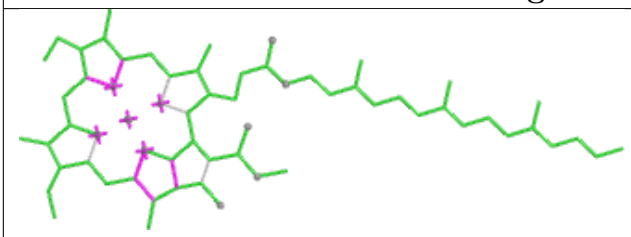


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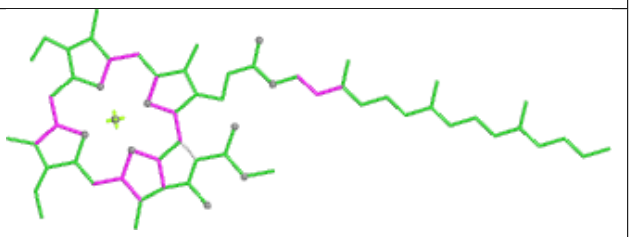


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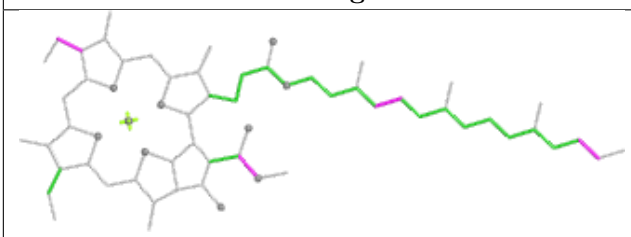
Ligand CLA d 612



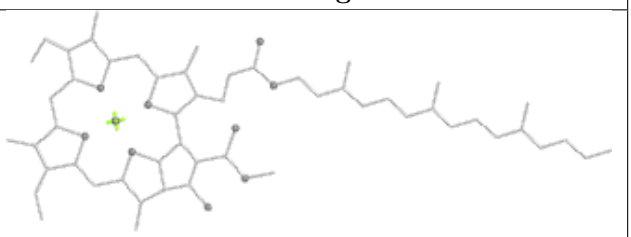
Bond lengths



Bond angles

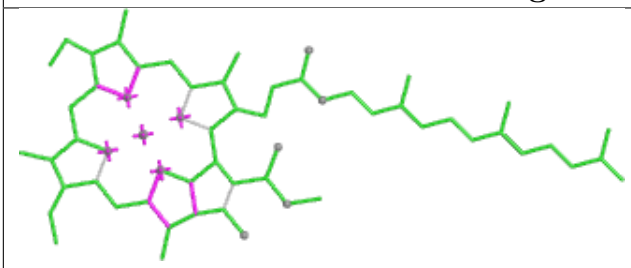


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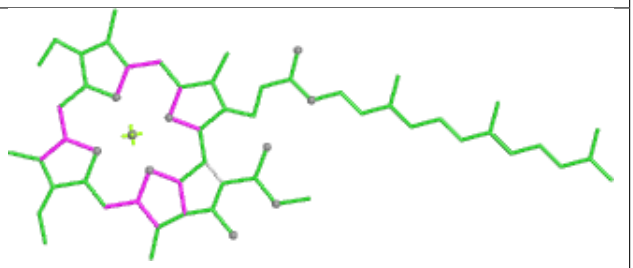


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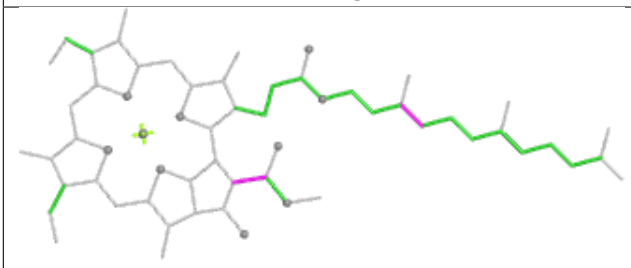
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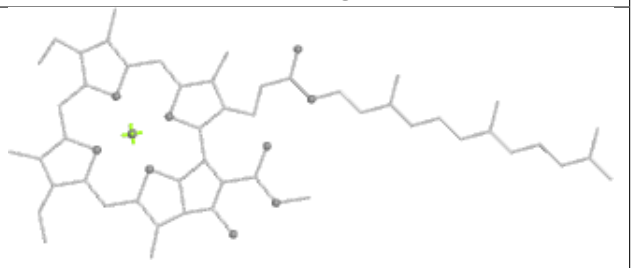
Bond lengths



Bond angles

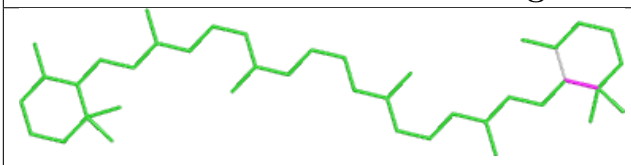


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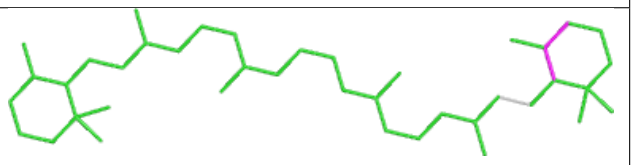


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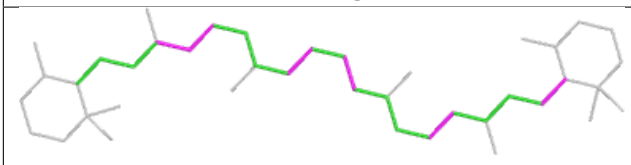
Ligand 8CT B 845



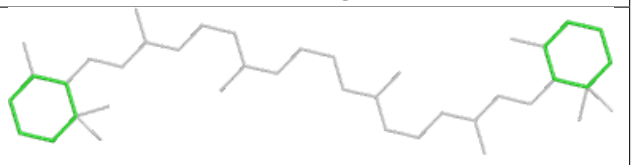
Bond lengths



Bond angles

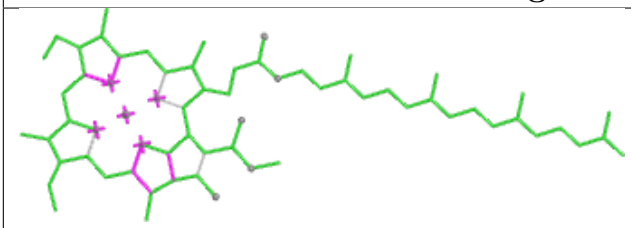


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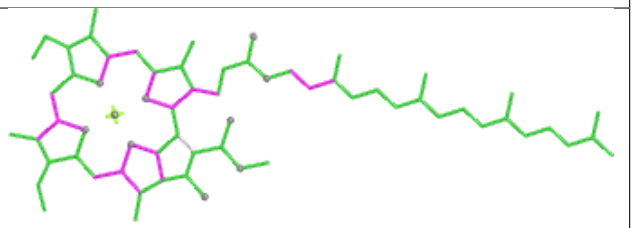


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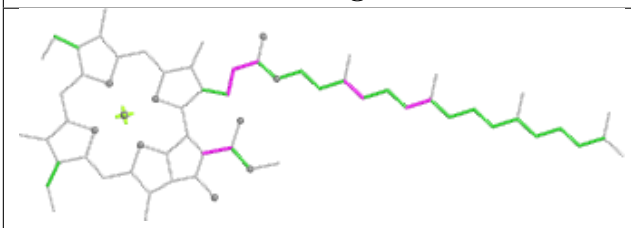
Ligand CLA 3 610



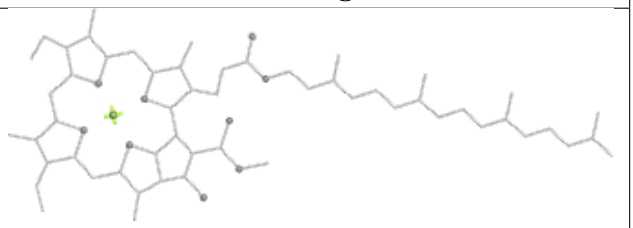
Bond lengths



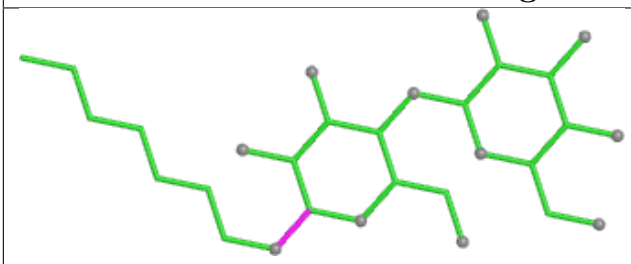
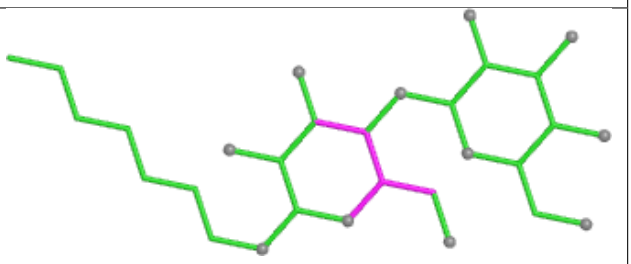
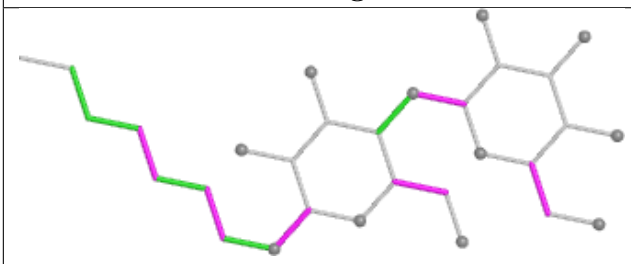
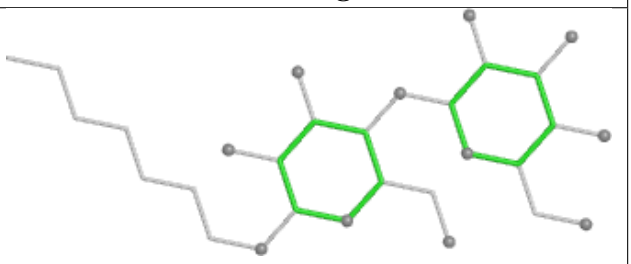
Bond angles

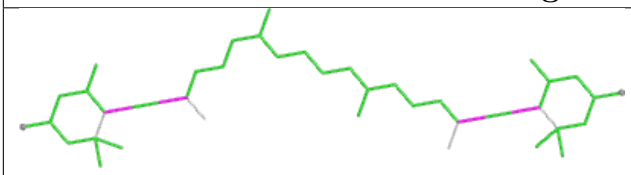
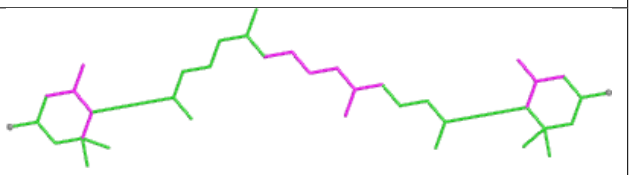
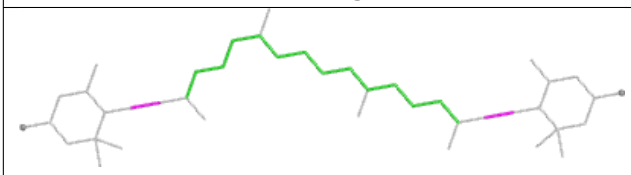
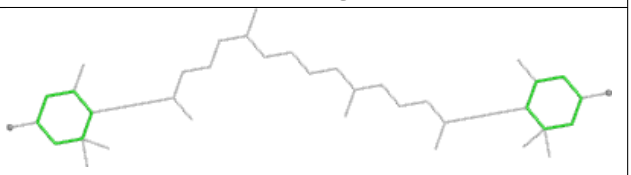


Torsions

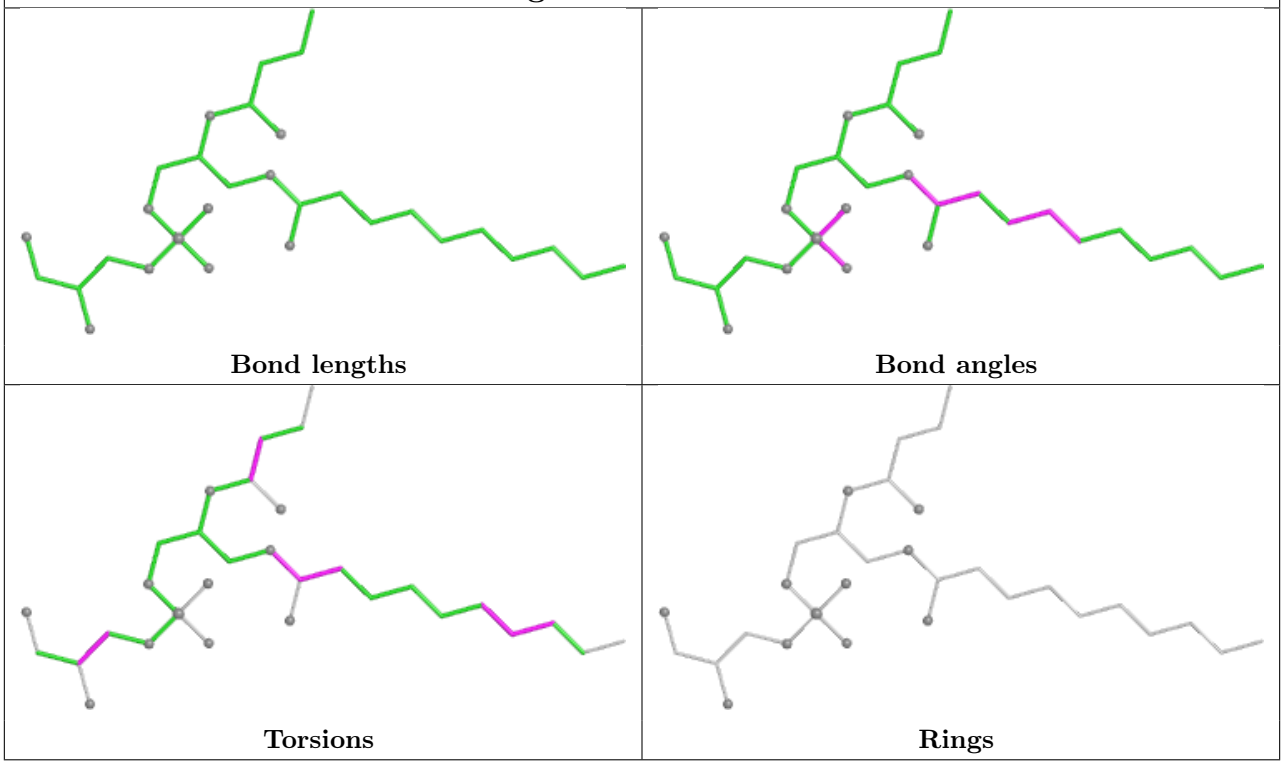


Rings

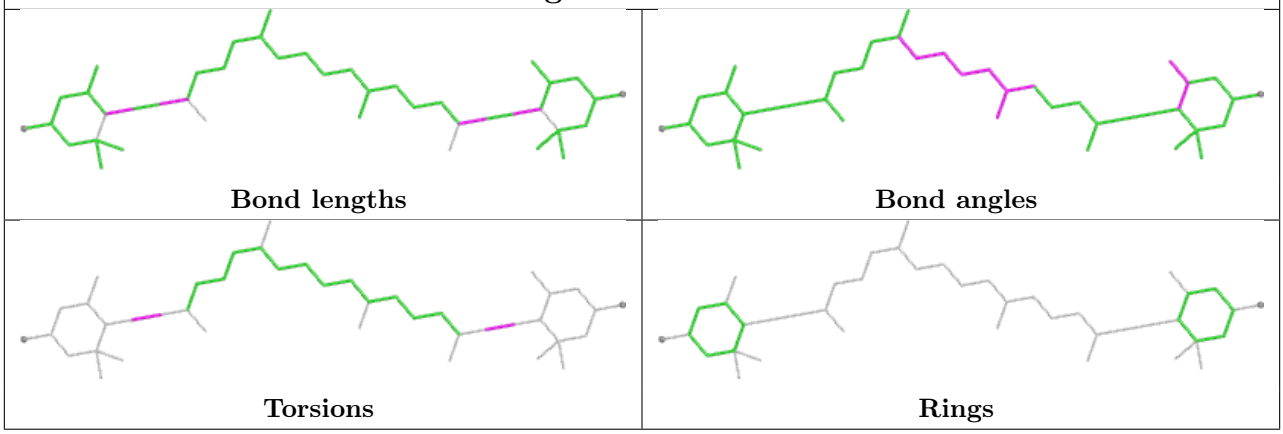
Ligand LMU O 207	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand II0 d 615	
 Bond lengths	 Bond angles
 Torsions	 Rings

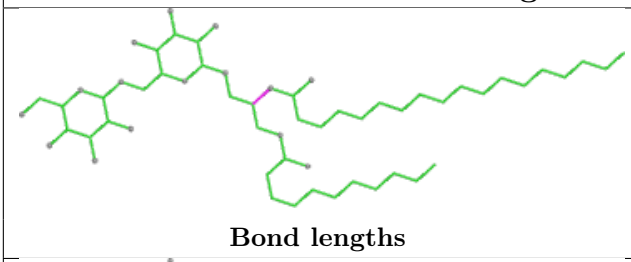
Ligand LHG 7 618



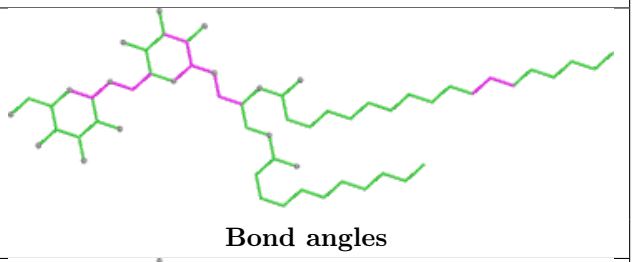
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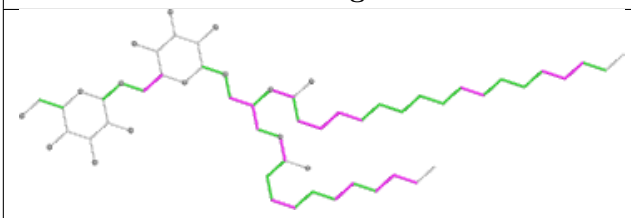
Ligand DGD B 848



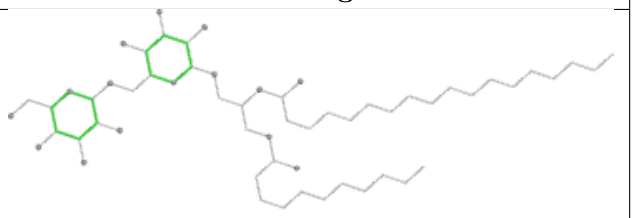
Bond lengths



Bond angles

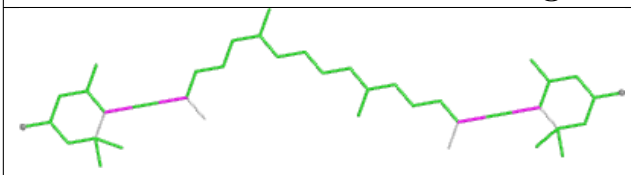


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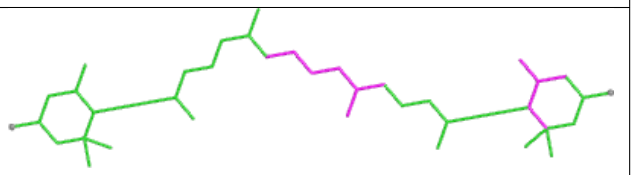


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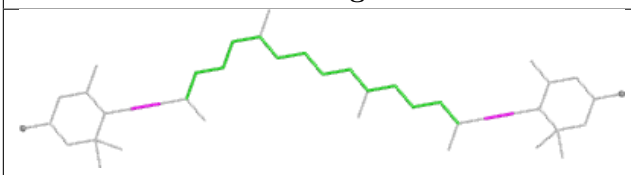
Ligand II0 5 615



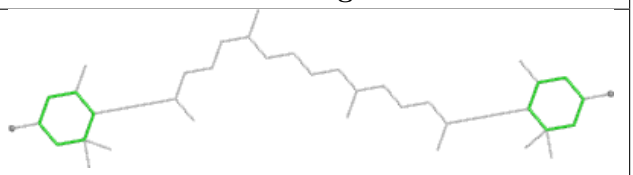
Bond lengths



Bond angles

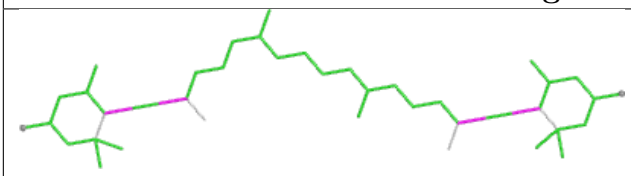


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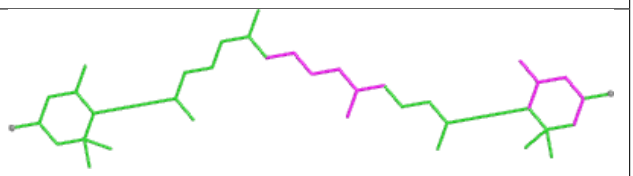


Rings

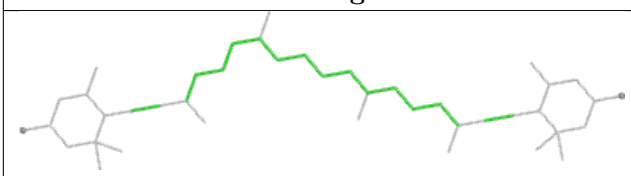
Ligand II0 2 614



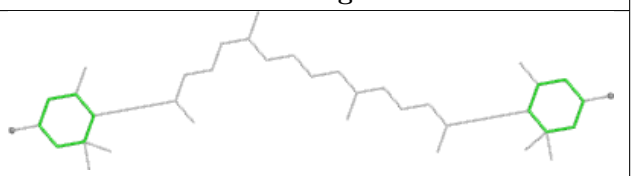
Bond lengths



Bond angles

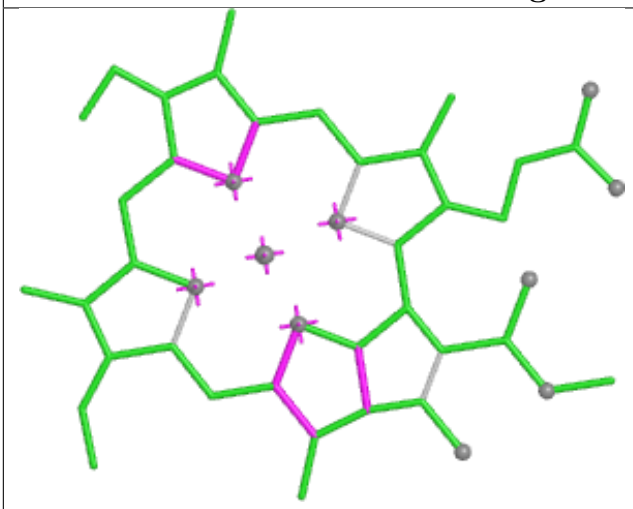


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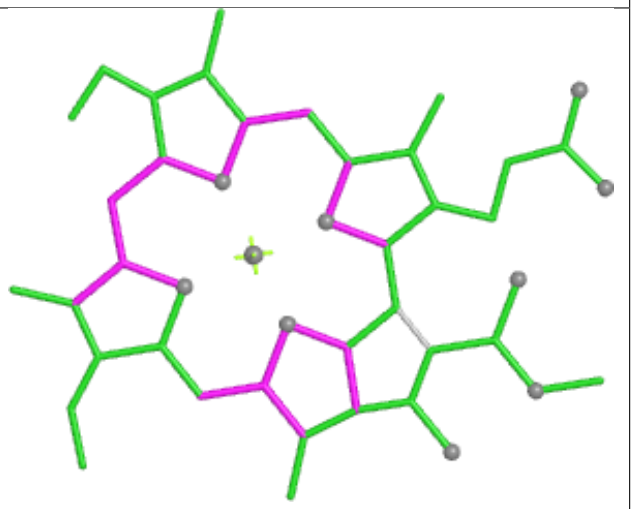


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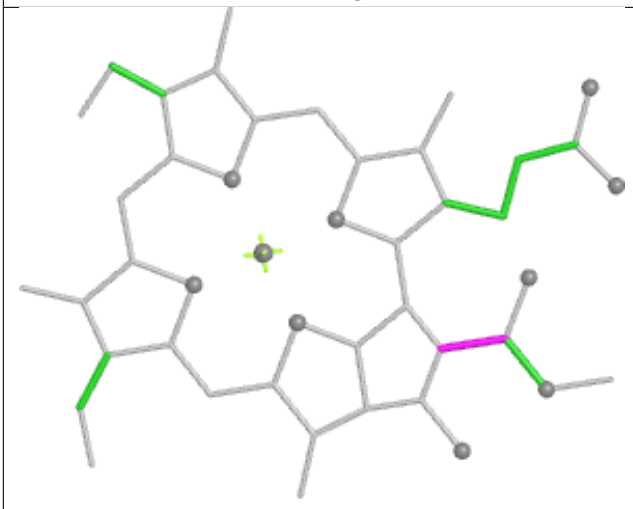
Ligand CLA c 601



Bond lengths



Bond angles

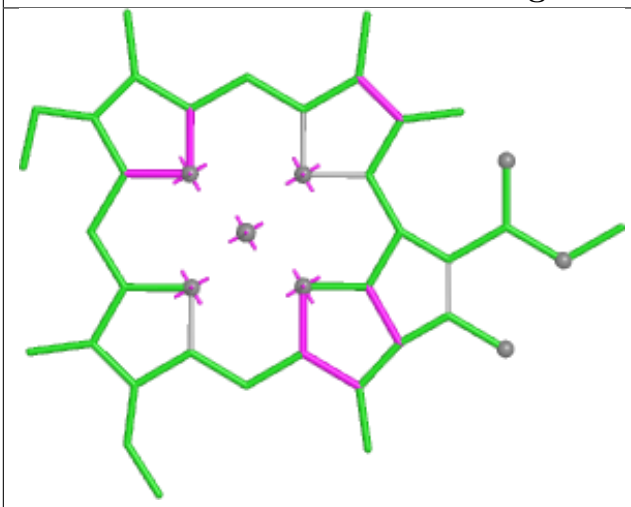


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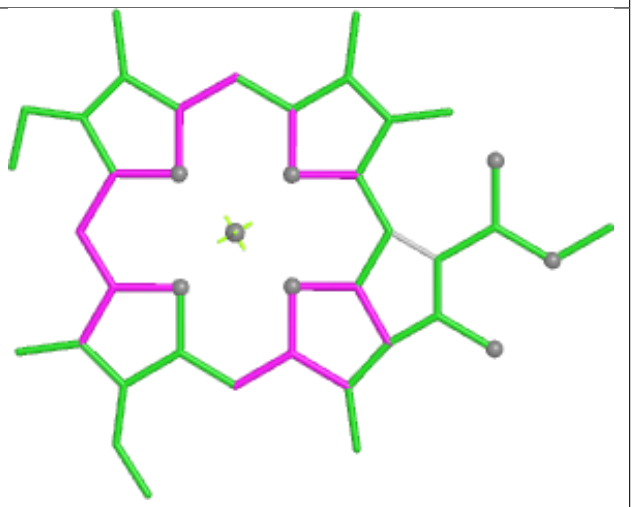


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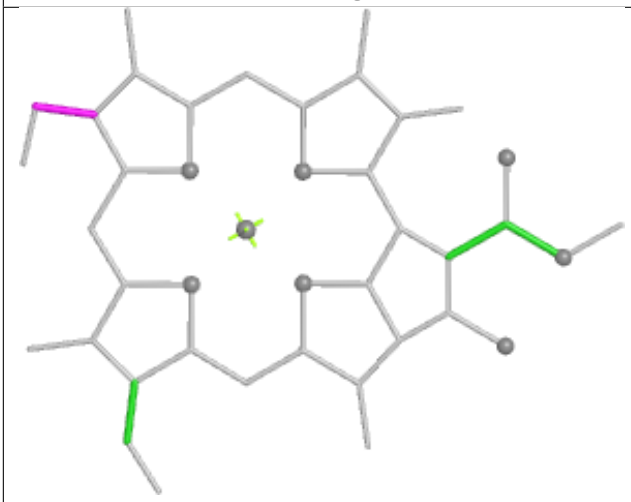
Ligand CLA 2 609



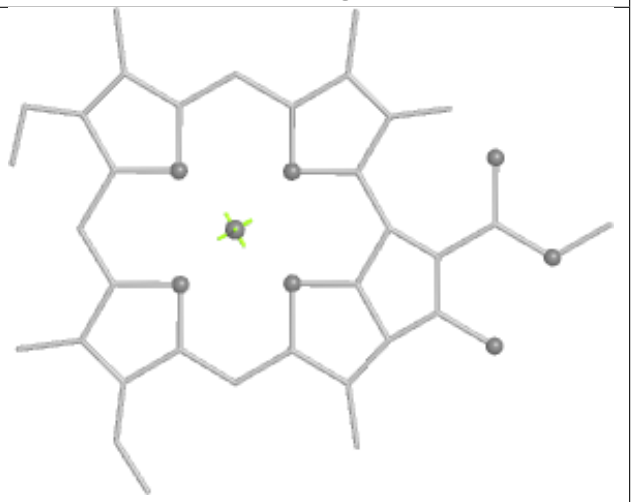
Bond lengths



Bond angles

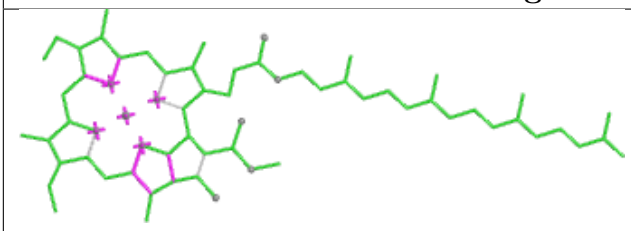


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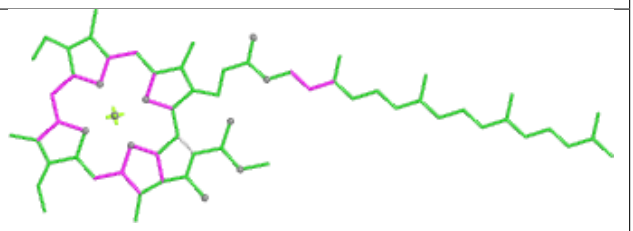


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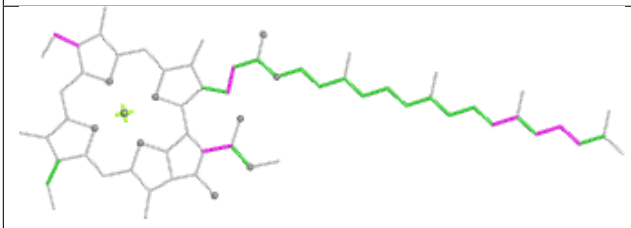
Ligand CLA B 807



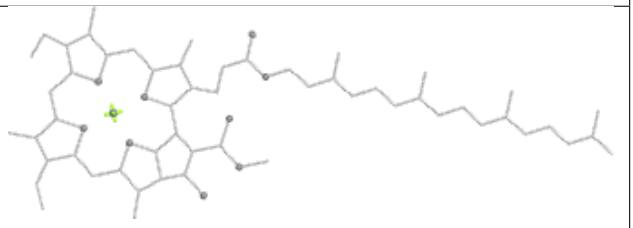
Bond lengths



Bond angles

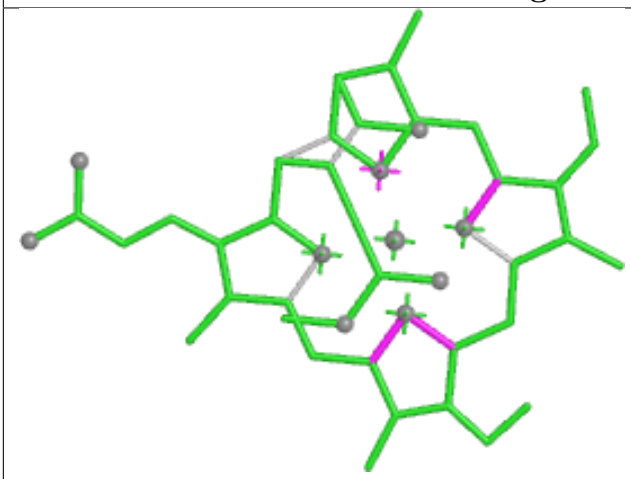


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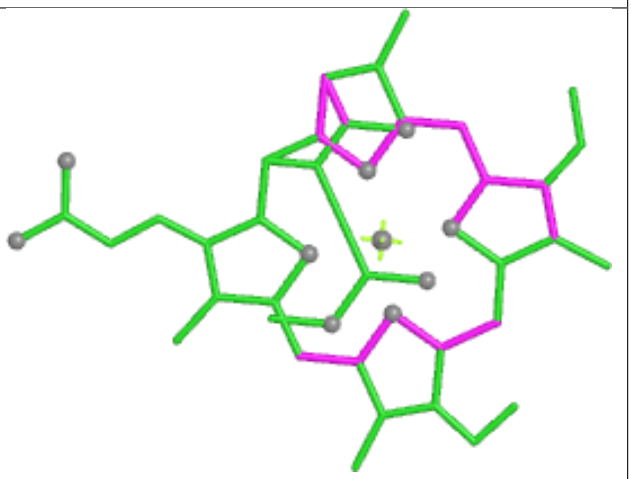


Rings

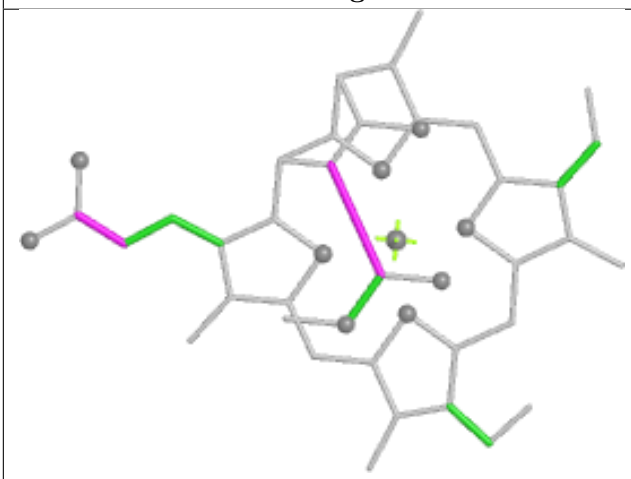
Ligand KC2 5 610



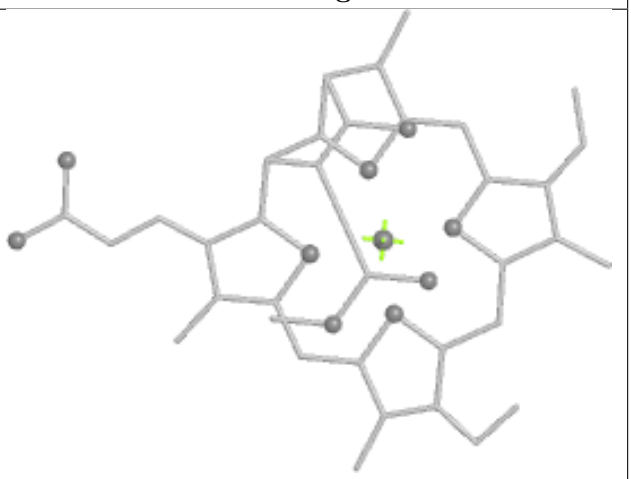
Bond lengths



Bond angles

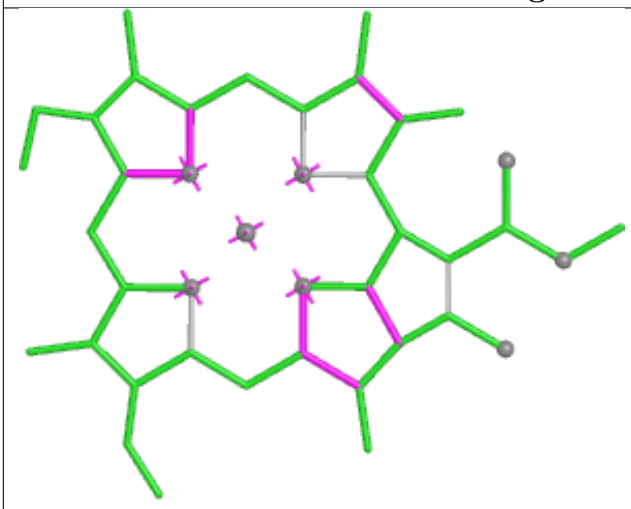


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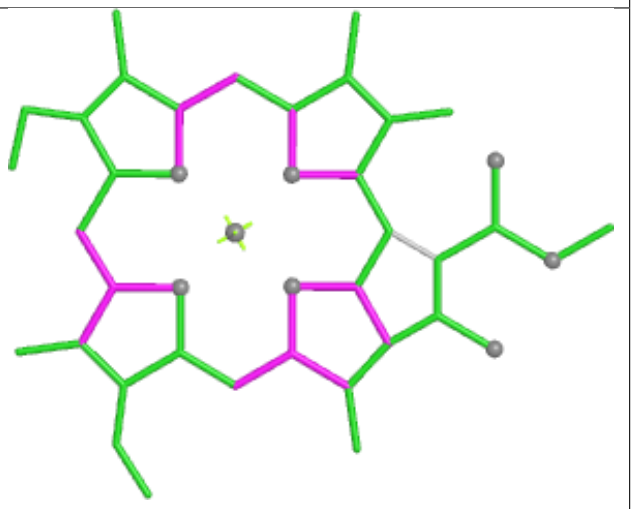


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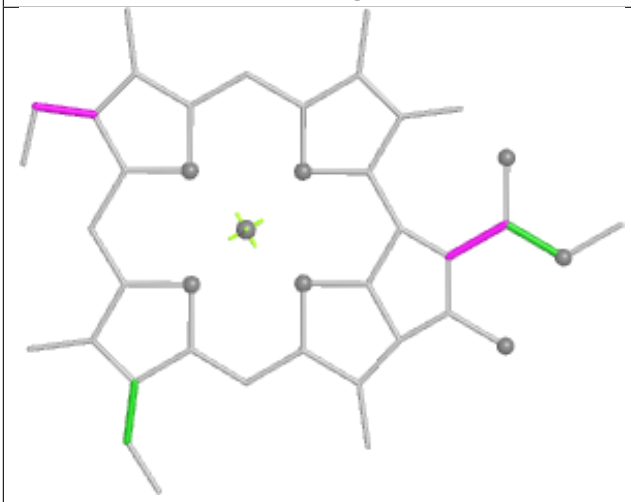
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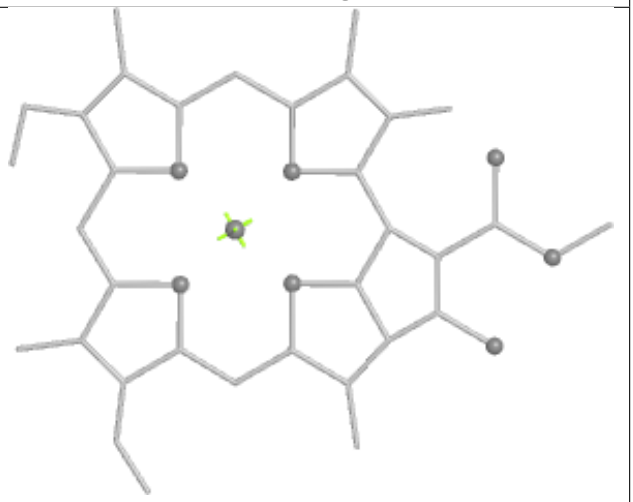
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Bond angles

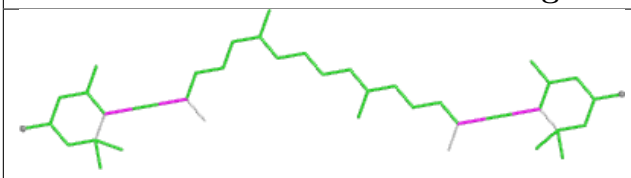


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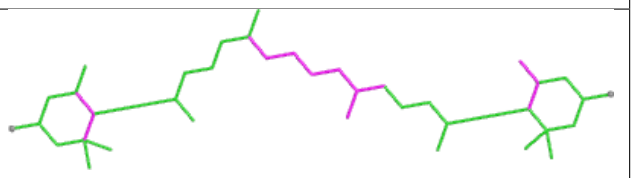


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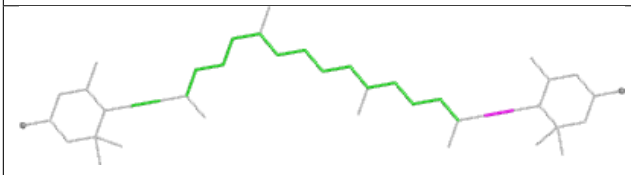
Ligand II0 b 614



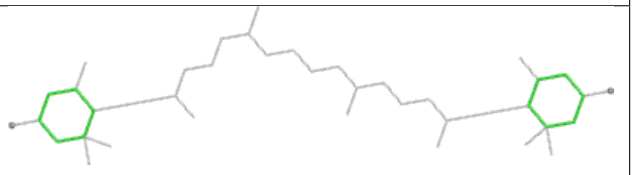
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Bond angles

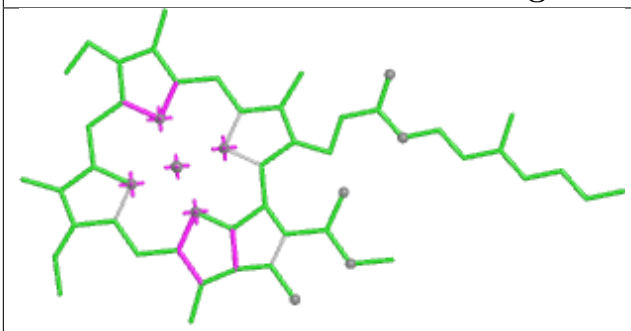


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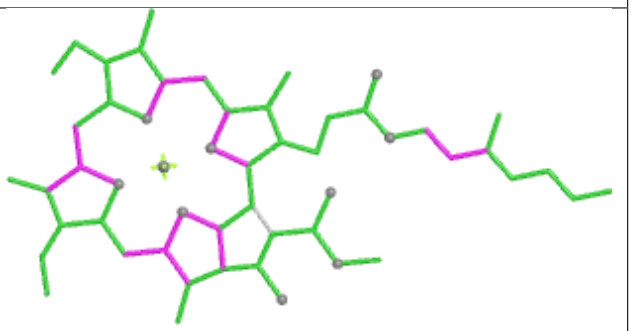


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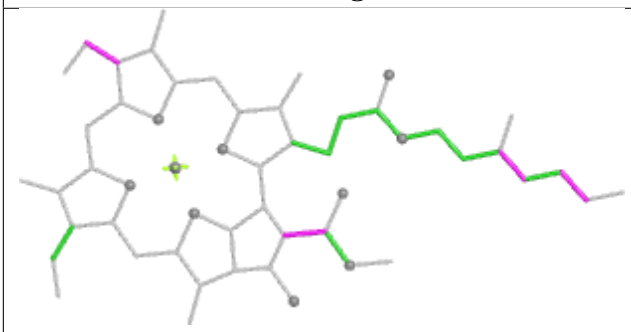
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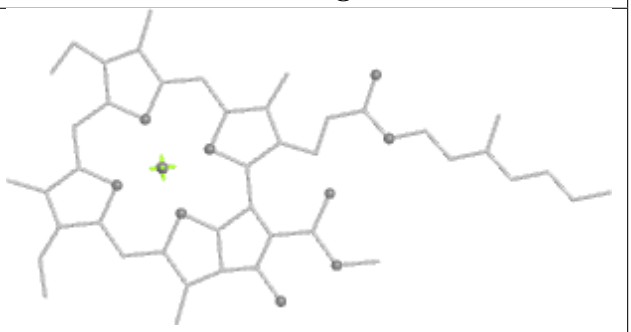
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Bond angles

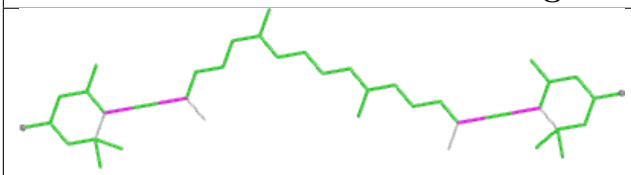


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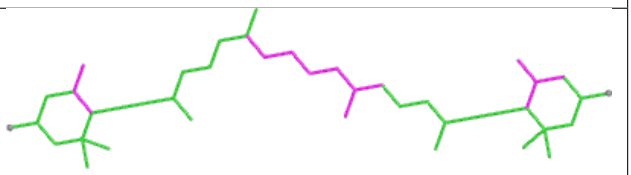


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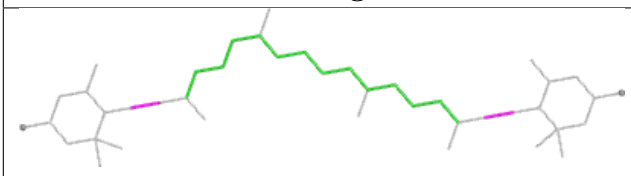
Ligand II0 c 618



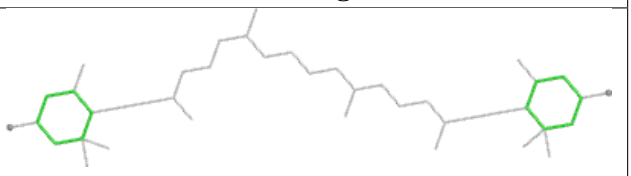
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Bond angles

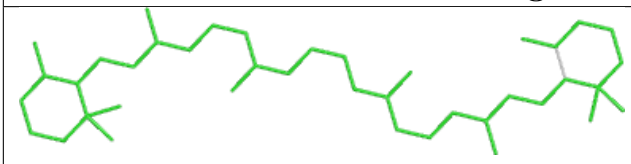


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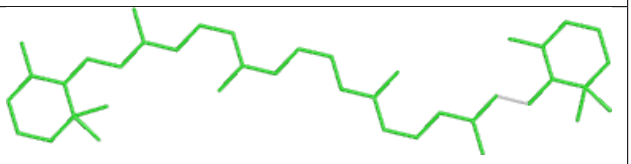


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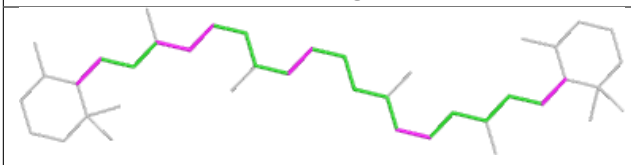
Ligand 8CT B 851



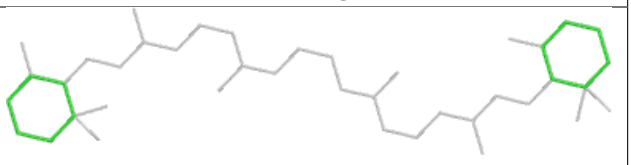
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Bond angles

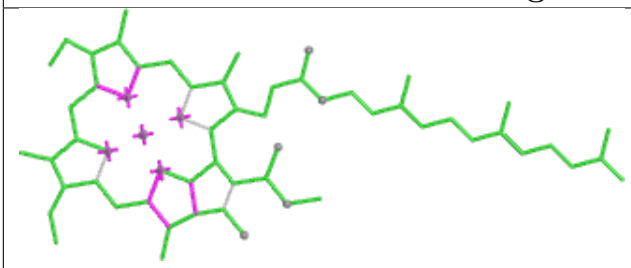


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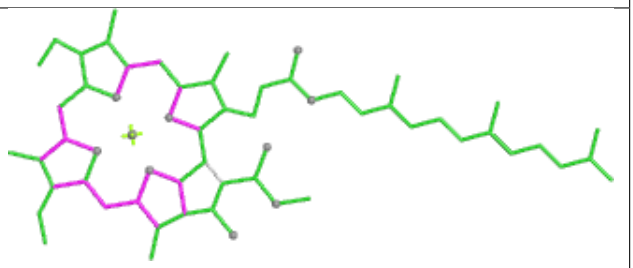


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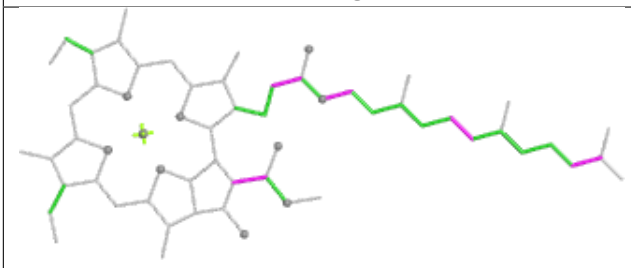
Ligand CLA b 607



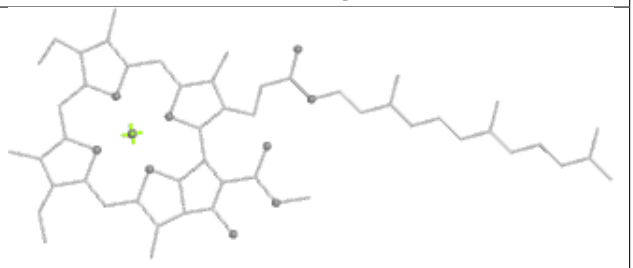
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Bond angles

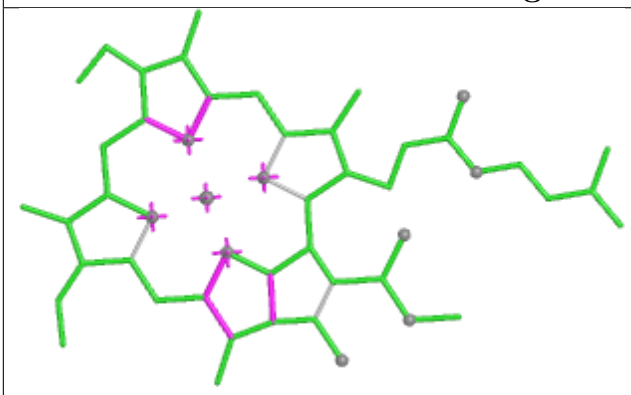


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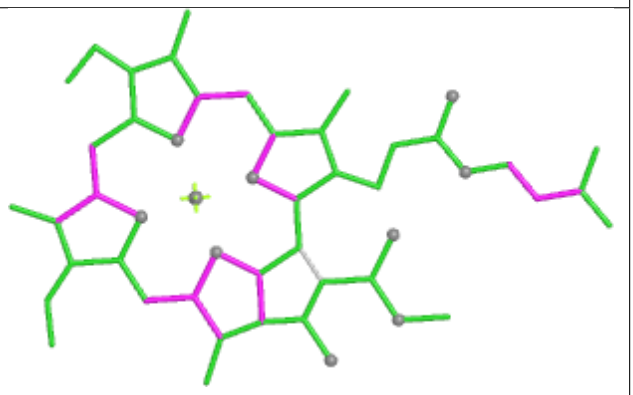


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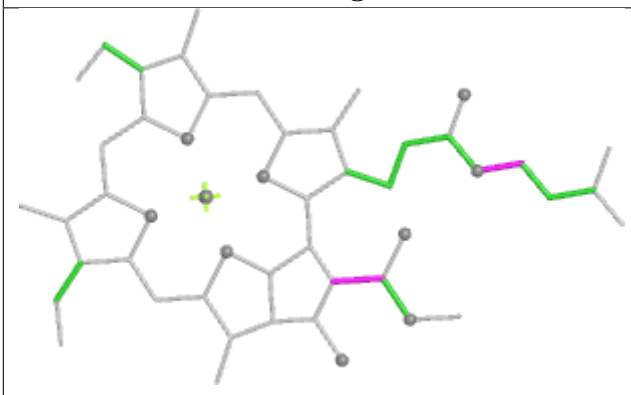
Ligand CLA A 807



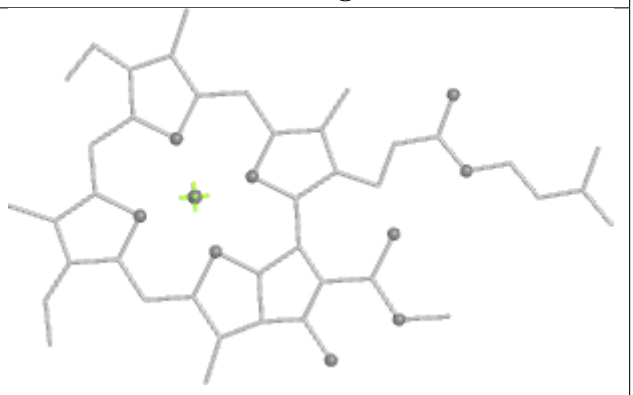
Bond lengths



Bond angles

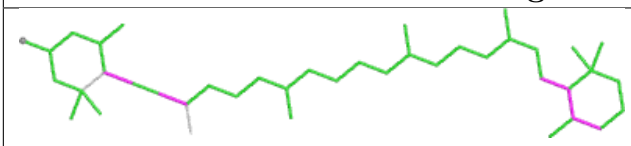


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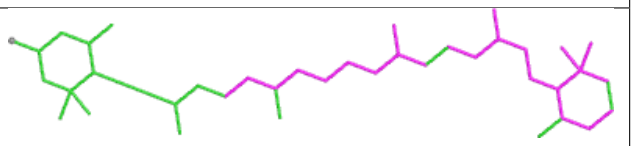


Rings

Ligand IHT K 104



Bond lengths



Bond angles

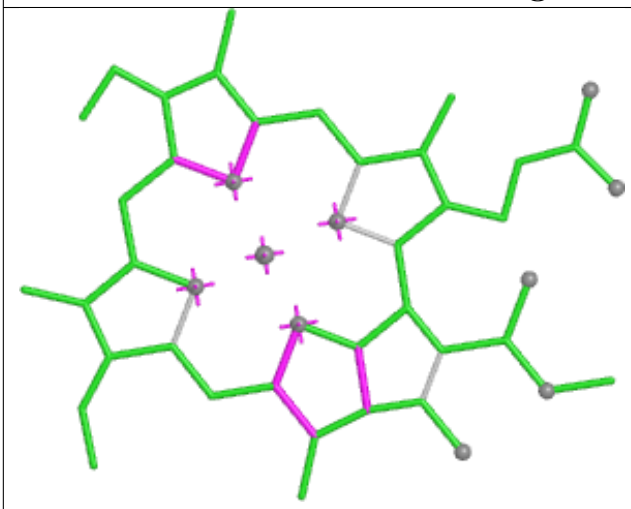


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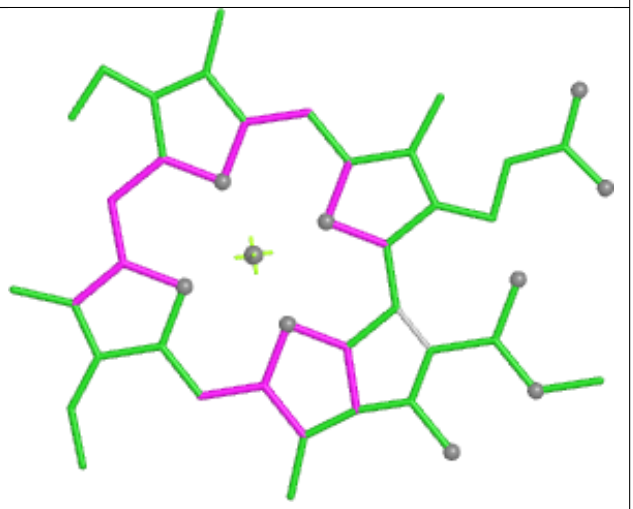


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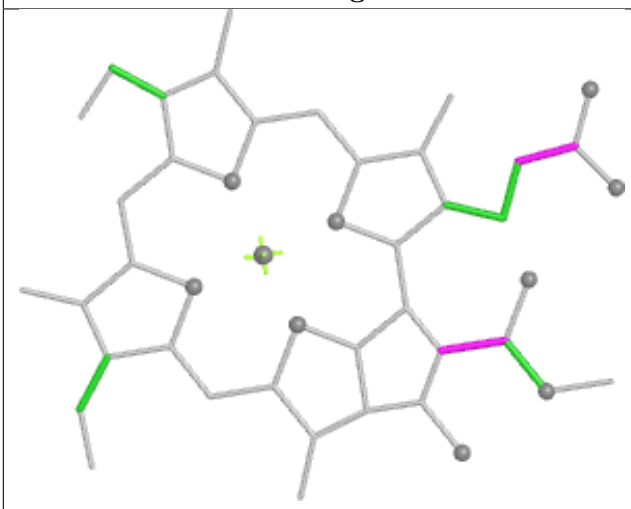
Ligand CLA e 607



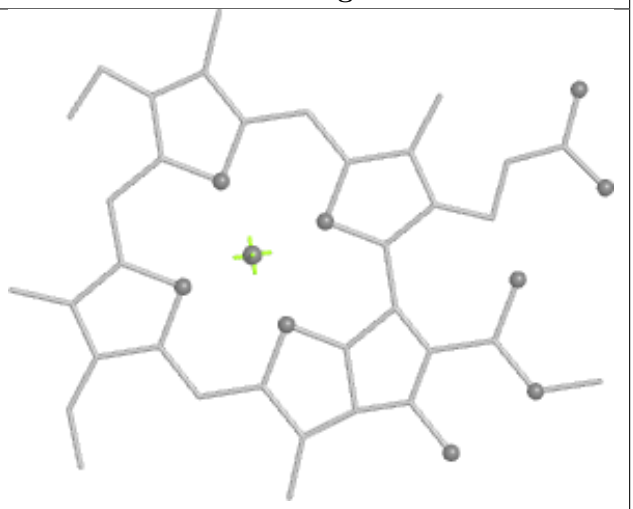
Bond lengths



Bond angles

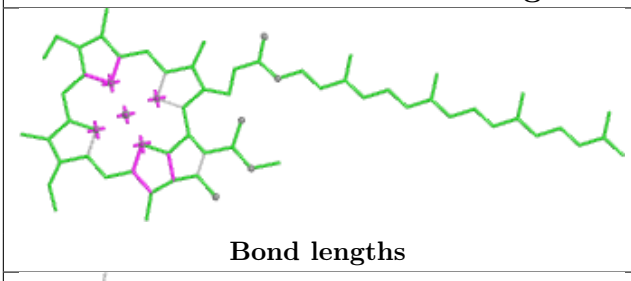


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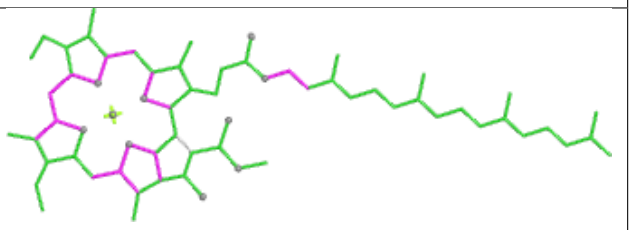


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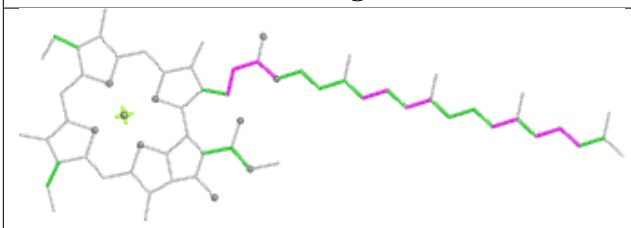
Ligand CLA A 839



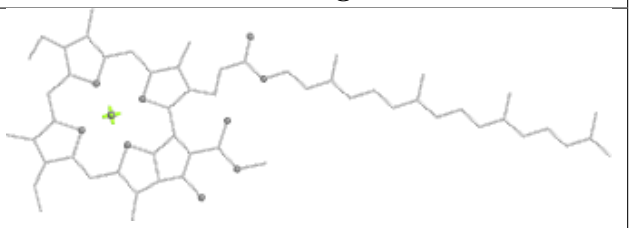
Bond lengths



Bond angles

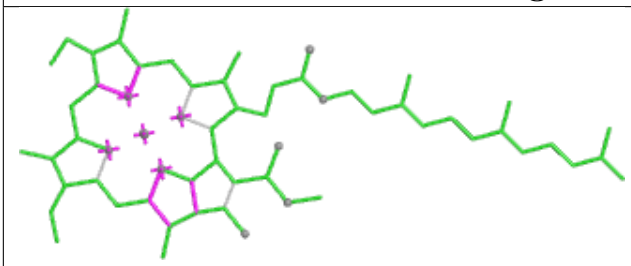


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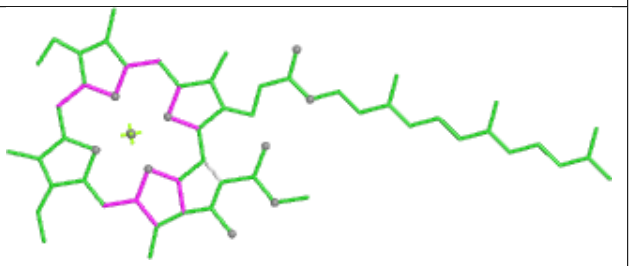


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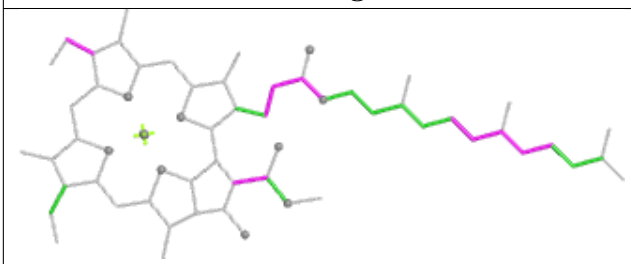
Ligand CLA a 604



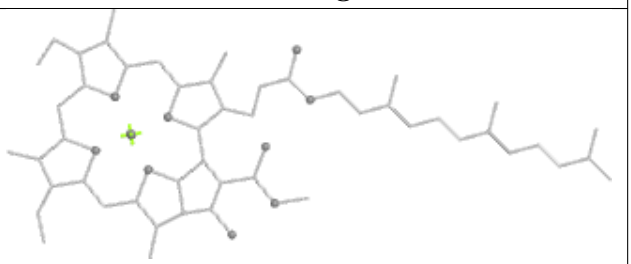
Bond lengths



Bond angles

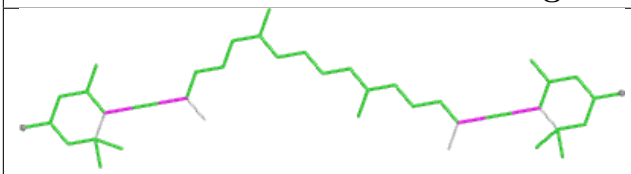


Torsions

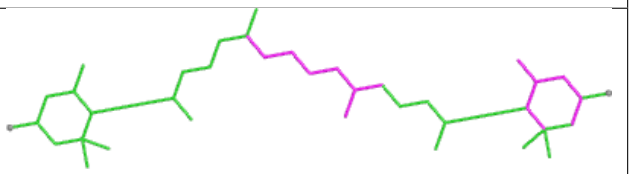


Rings

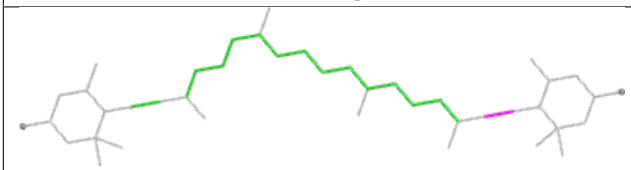
Ligand II0 e 614



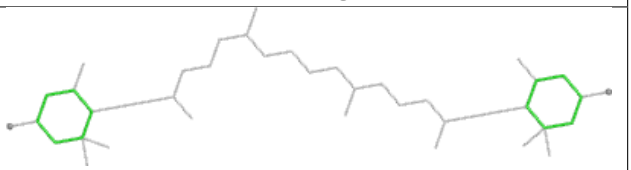
Bond lengths



Bond angles

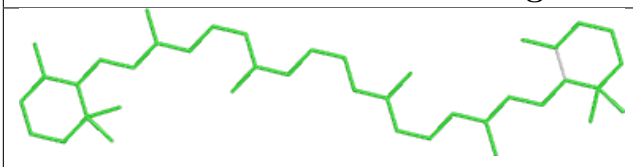


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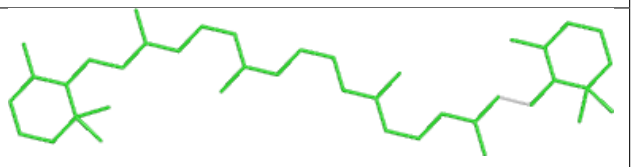


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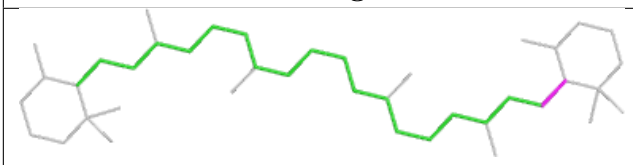
Ligand 8CT K 103



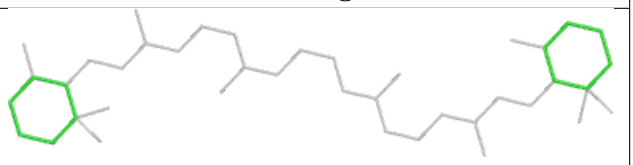
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Bond angles

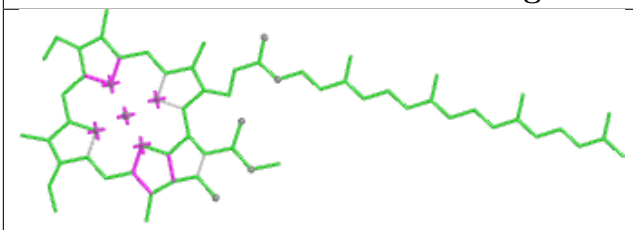


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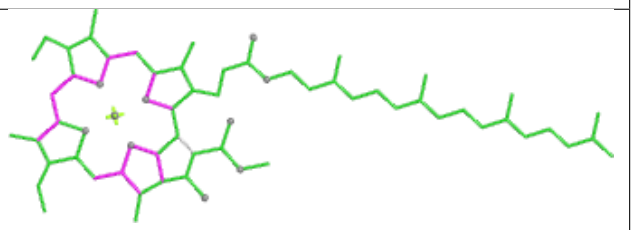


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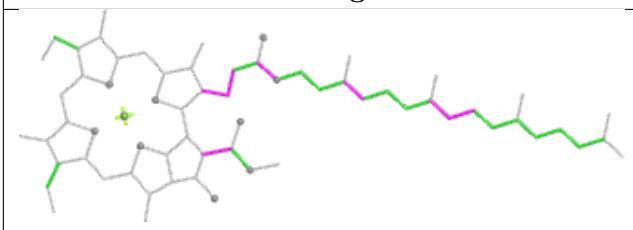
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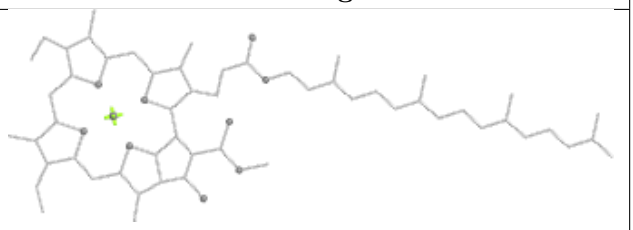
Bond lengths



Bond angles

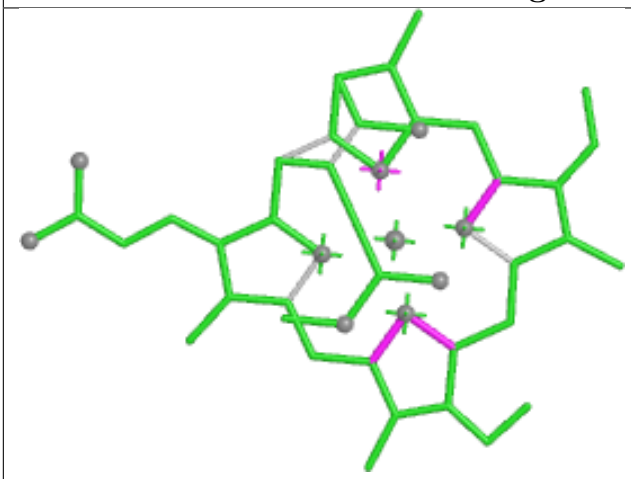


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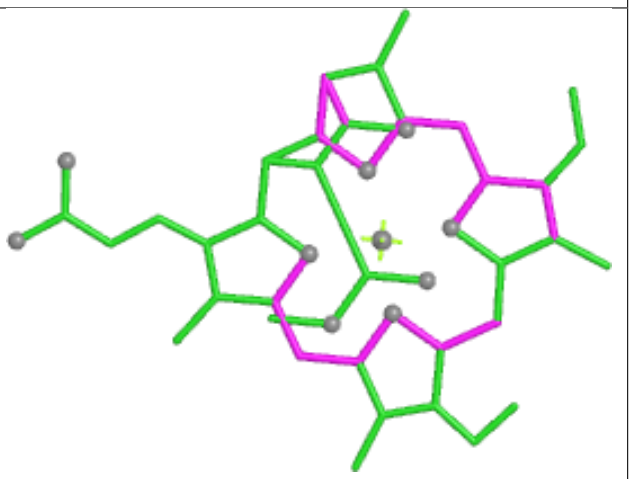


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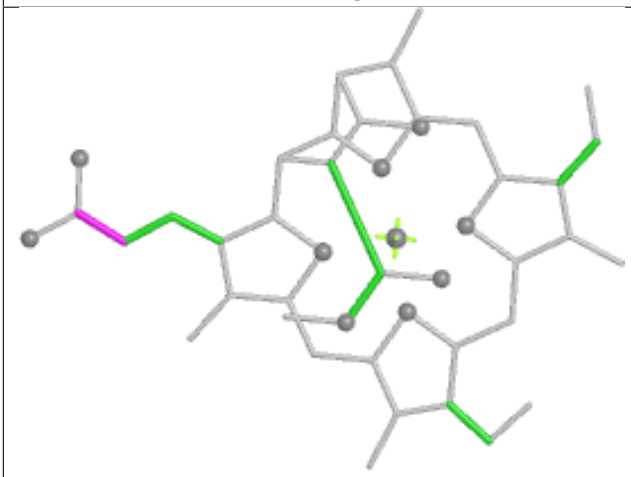
Ligand KC2 b 609



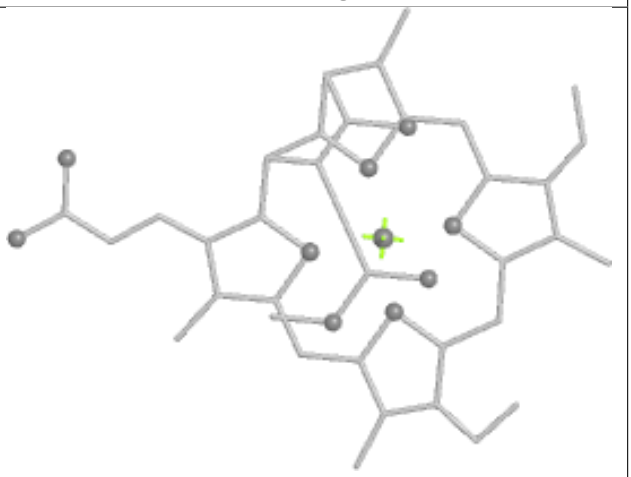
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Bond angles

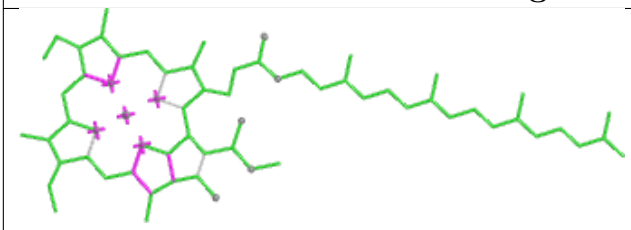


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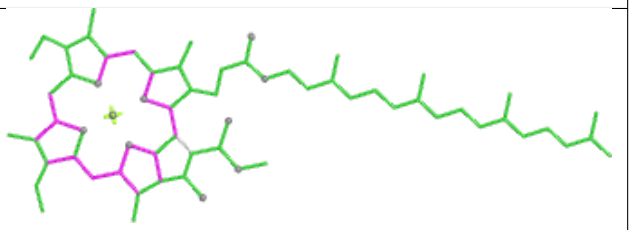


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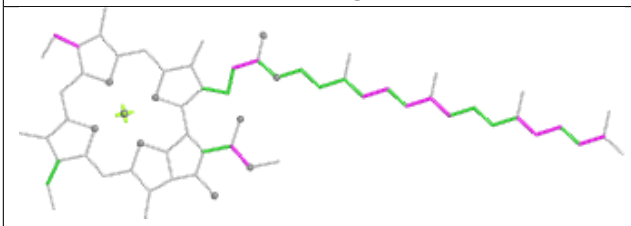
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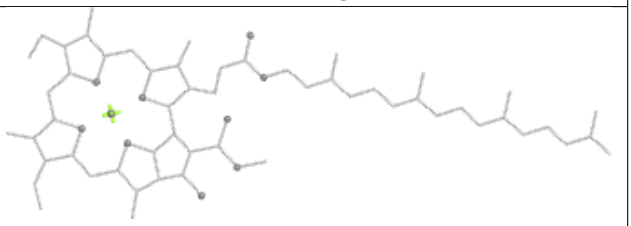
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Bond angles

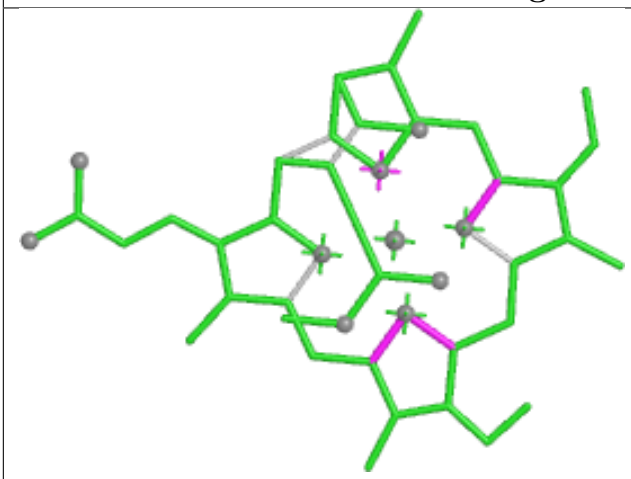


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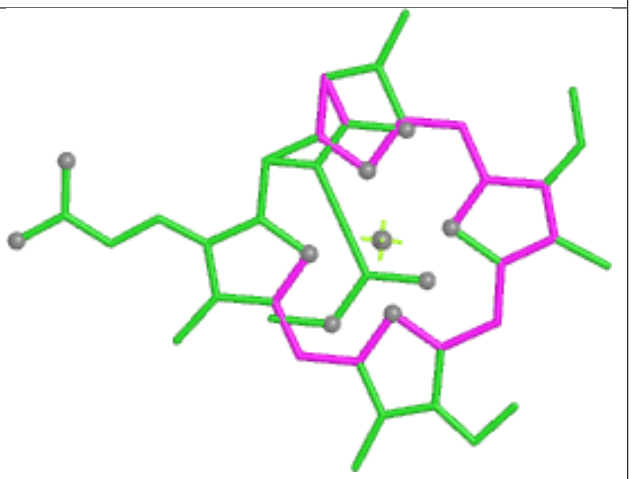


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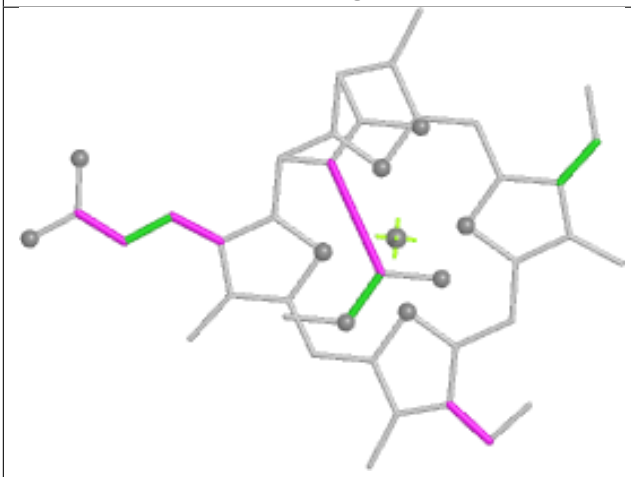
Ligand KC2 b 605



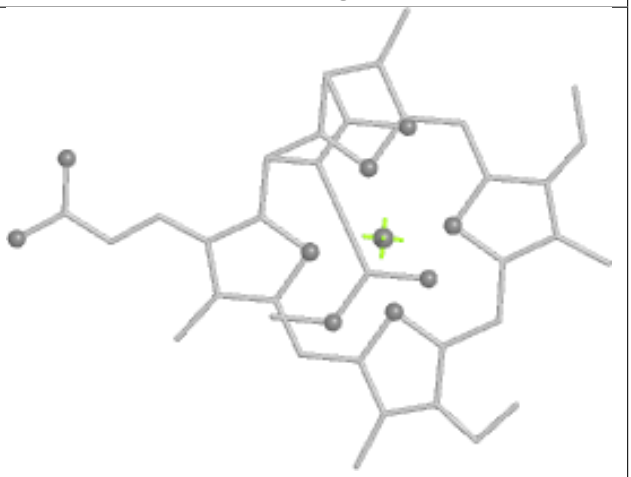
Bond lengths



Bond angles

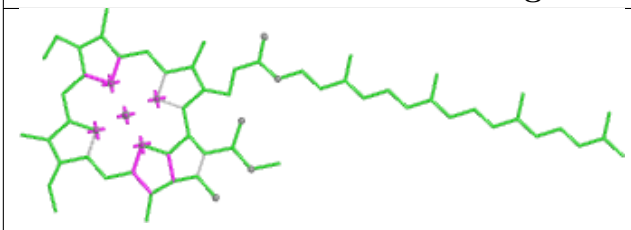


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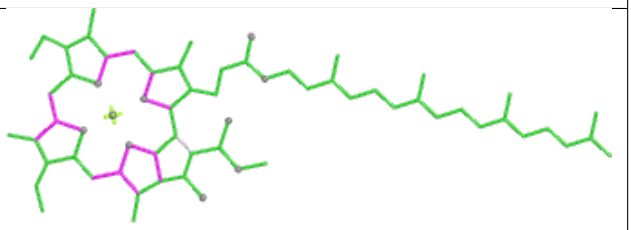


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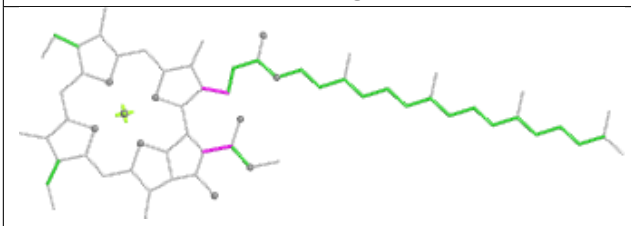
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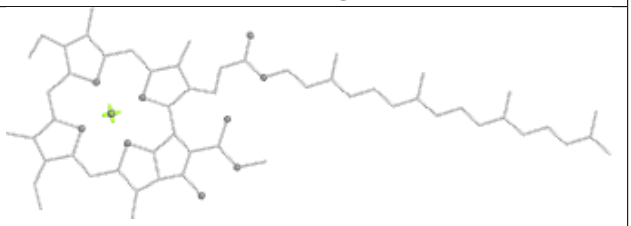
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Bond angles

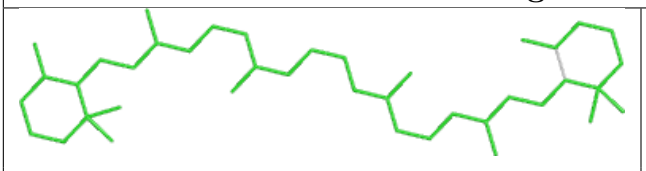


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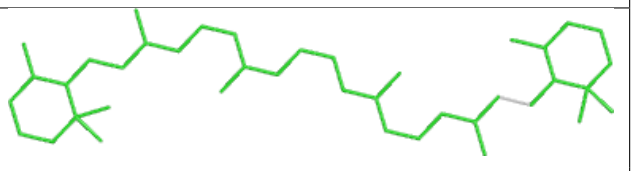


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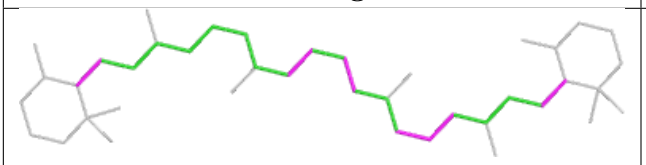
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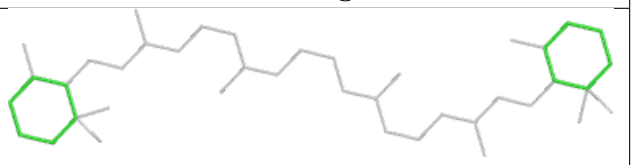
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Bond angles

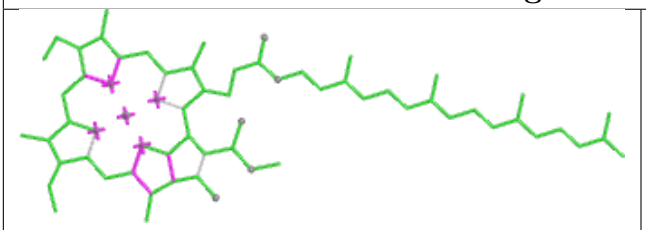


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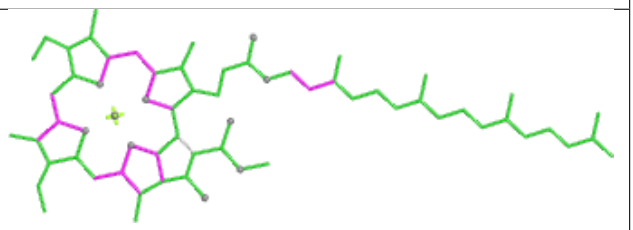


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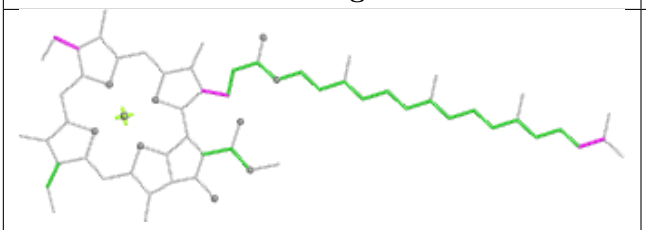
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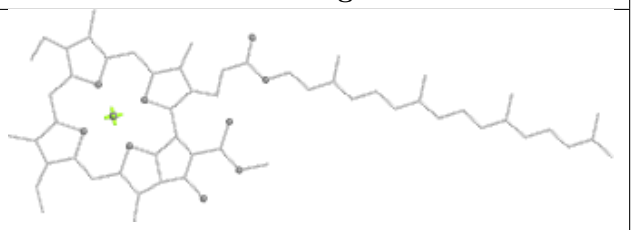
Bond lengths



Bond angles

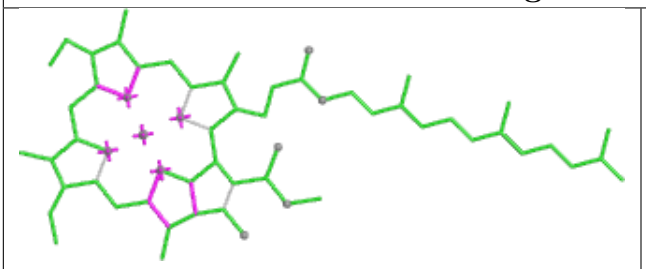


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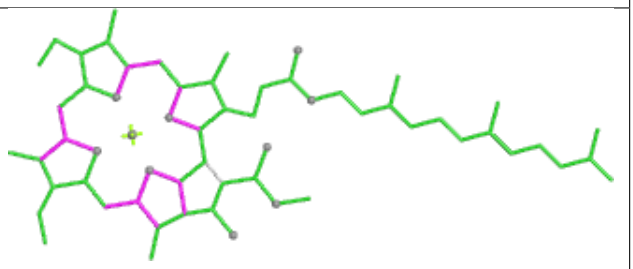


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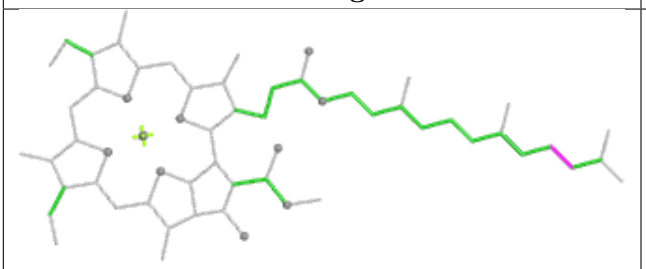
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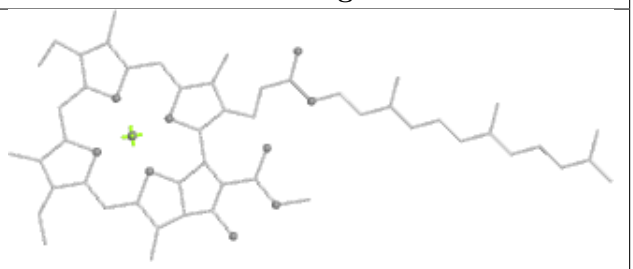
Bond lengths



Bond angles

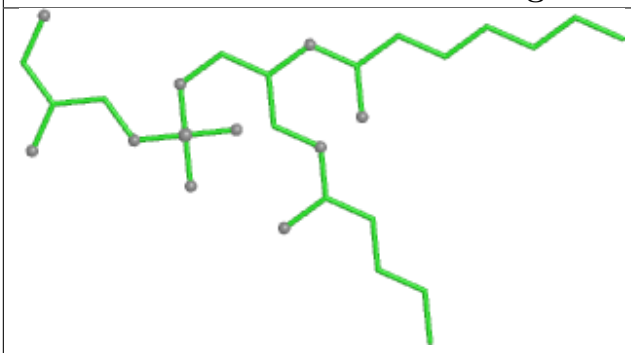


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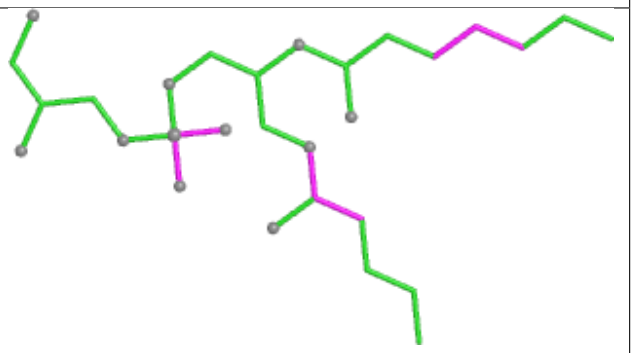


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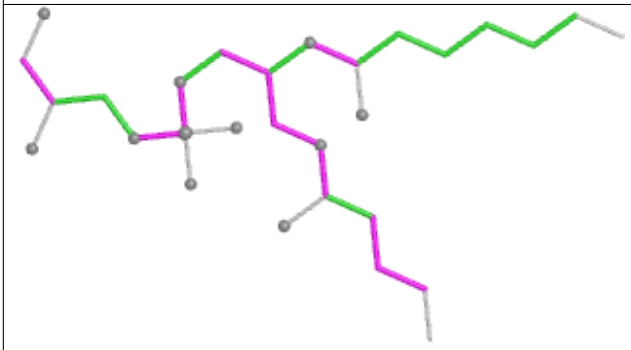
Ligand LHG a 618



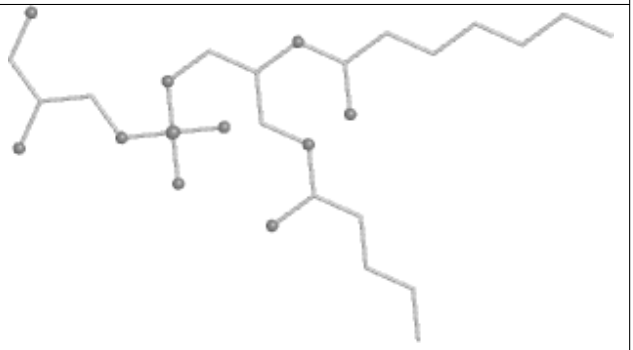
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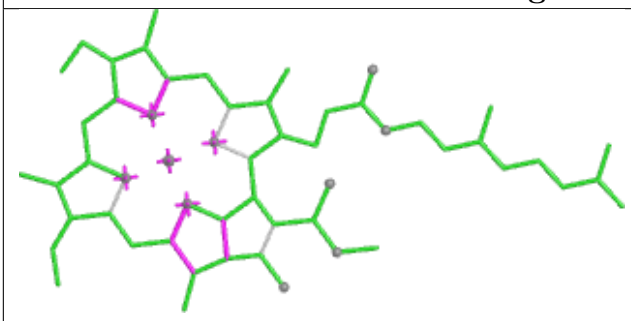


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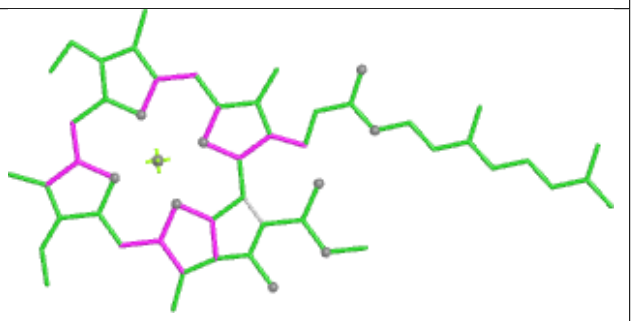


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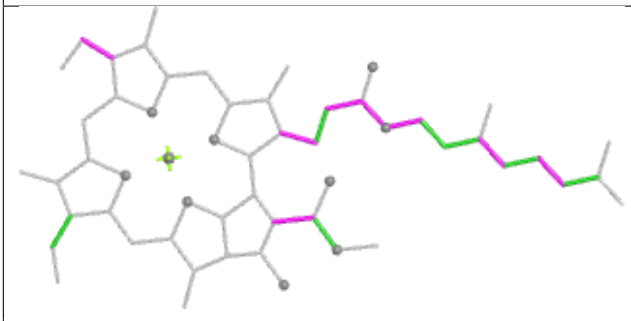
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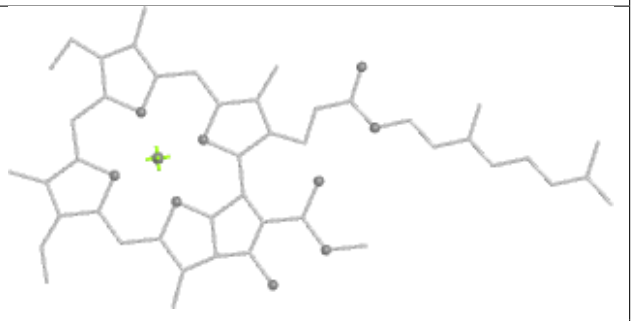
Bond lengths



Bond angles

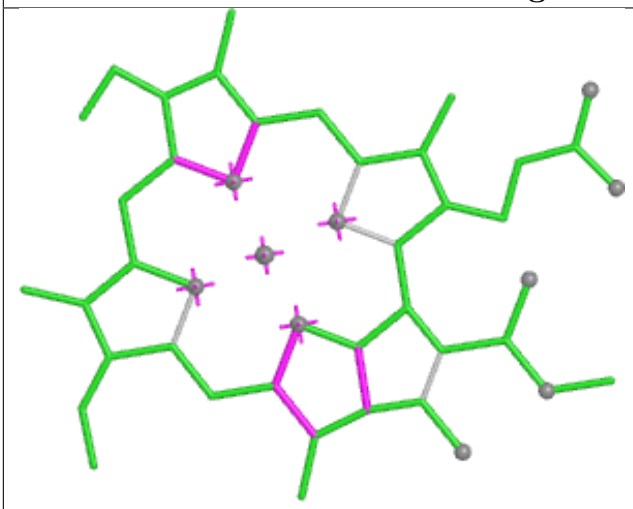


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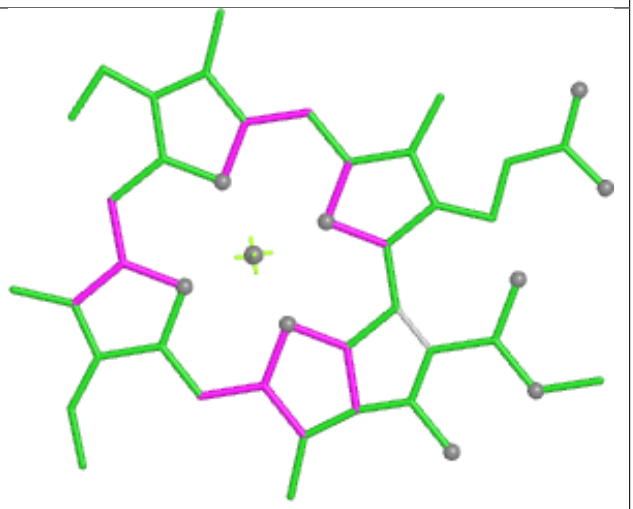


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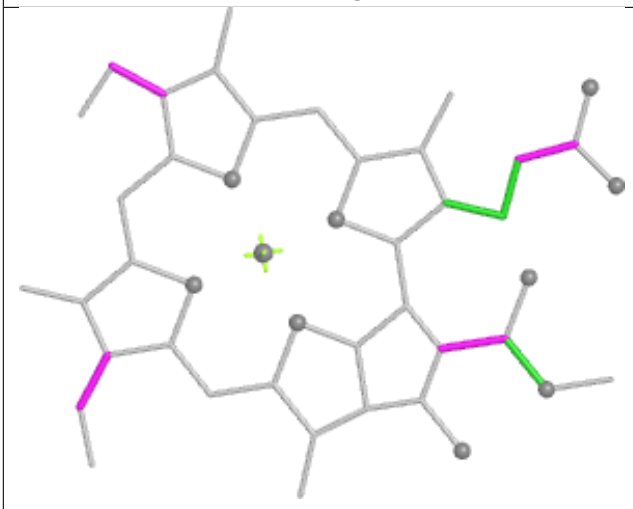
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Bond lengths



Bond angles

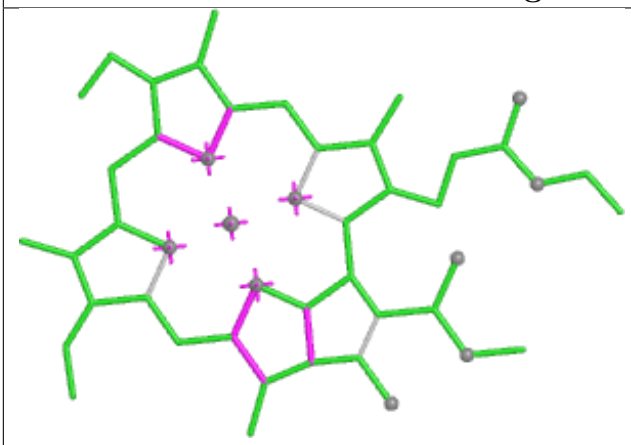


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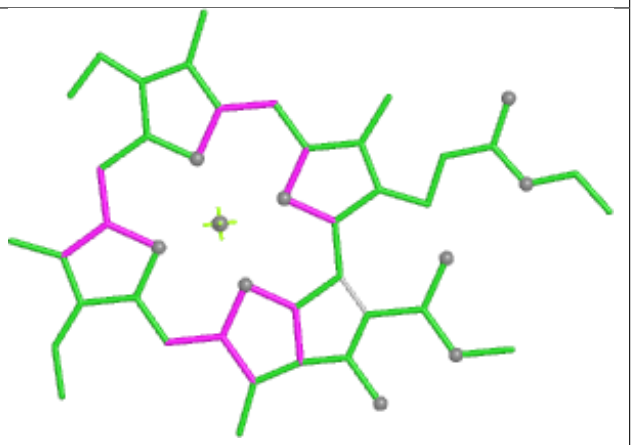


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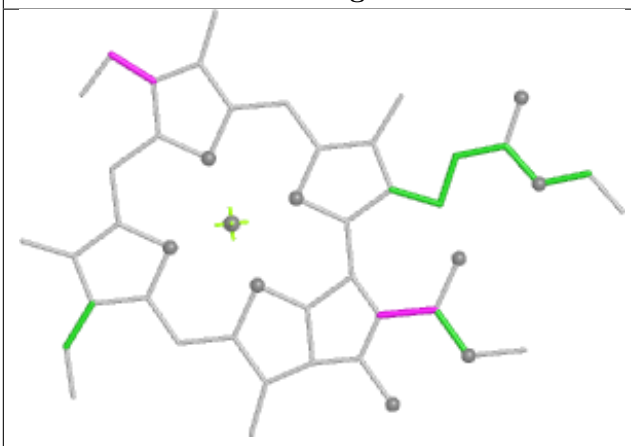
Ligand CLA B 836



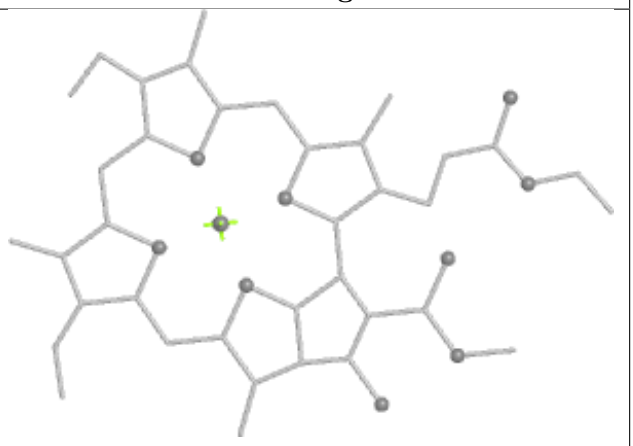
Bond lengths



Bond angles

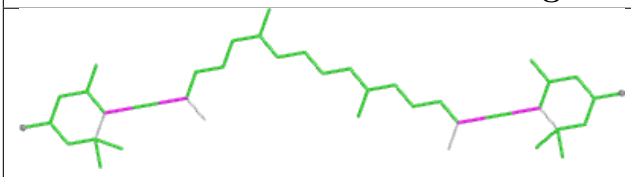


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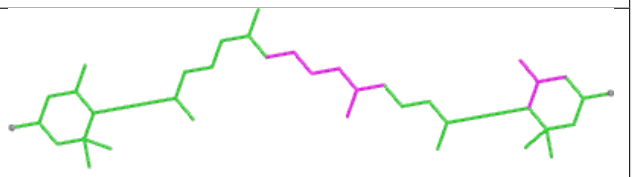


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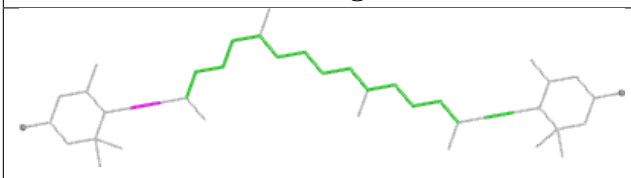
Ligand II0 4 614



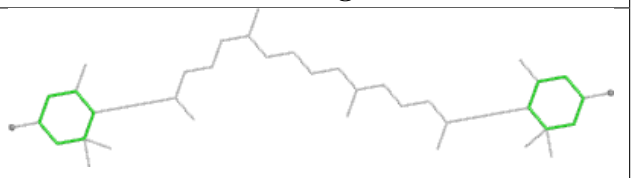
Bond lengths



Bond angles

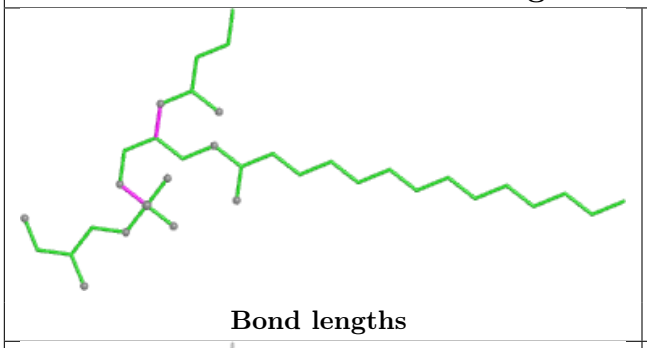


Torsions

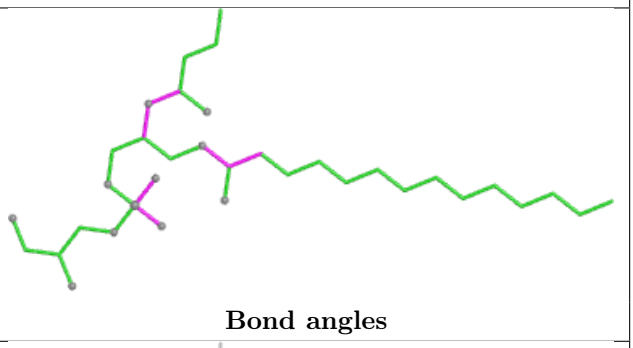


Rings

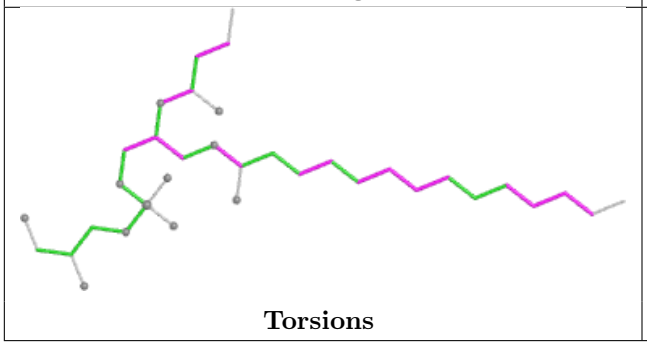
Ligand LHG 6 618



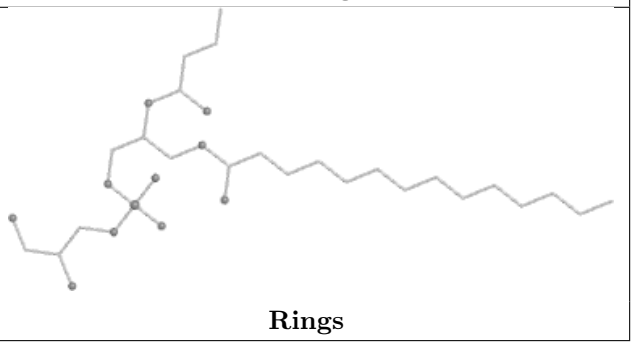
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Bond angles

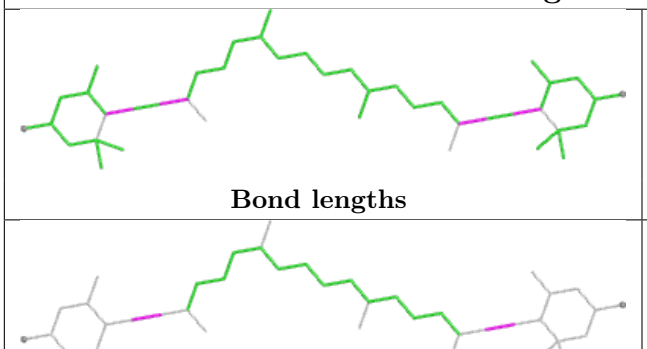


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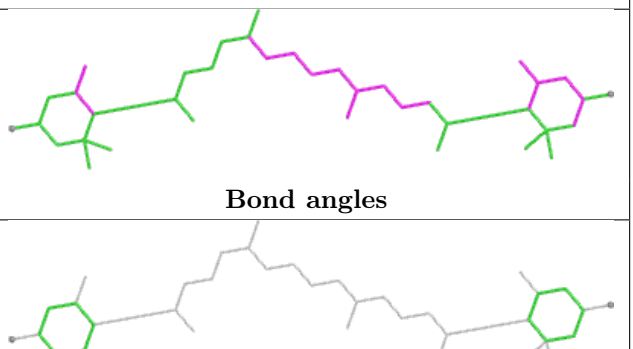


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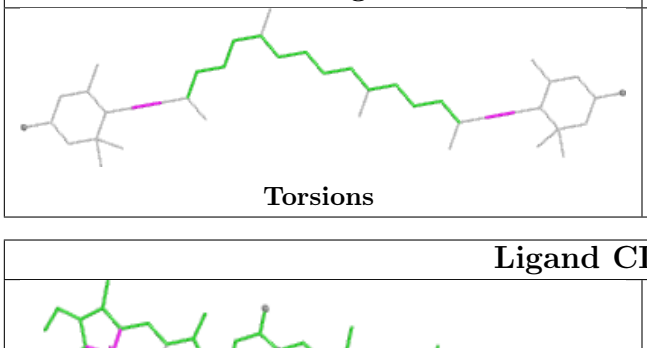
Ligand II0 2 613



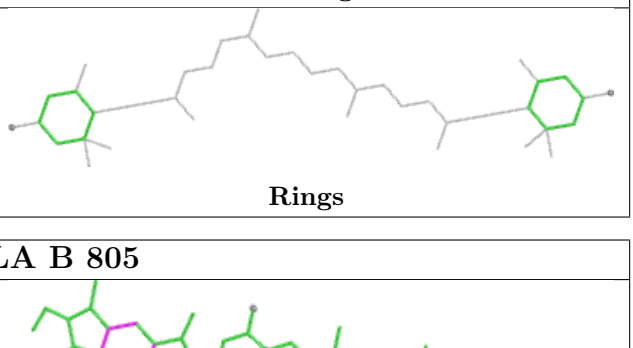
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Bond angles

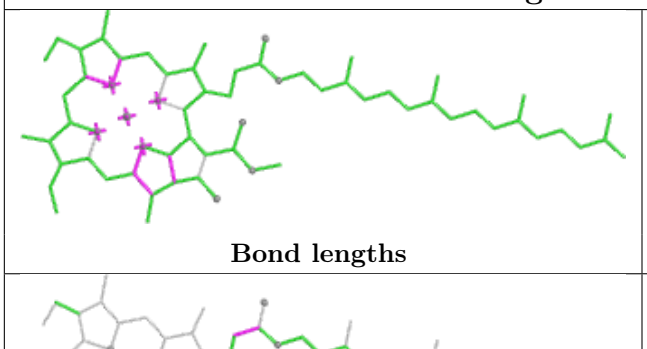


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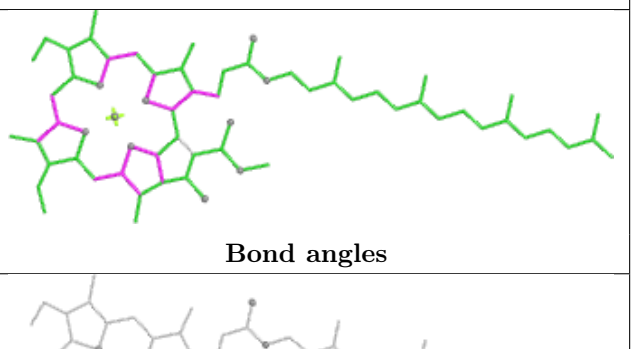


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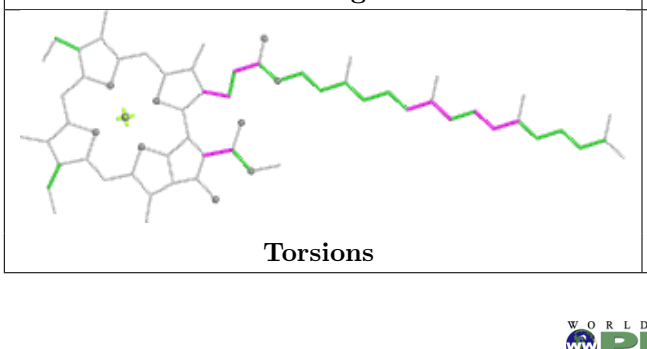
Ligand CLA B 805



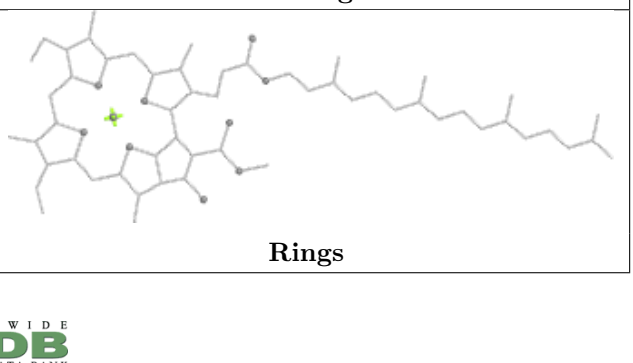
Bond lengths



Bond angles

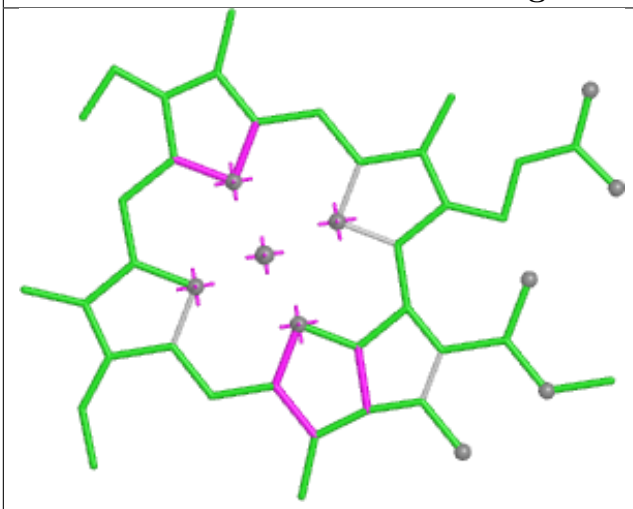


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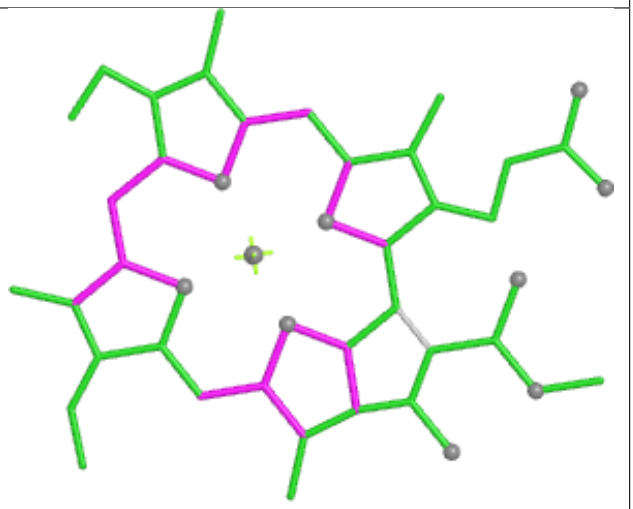


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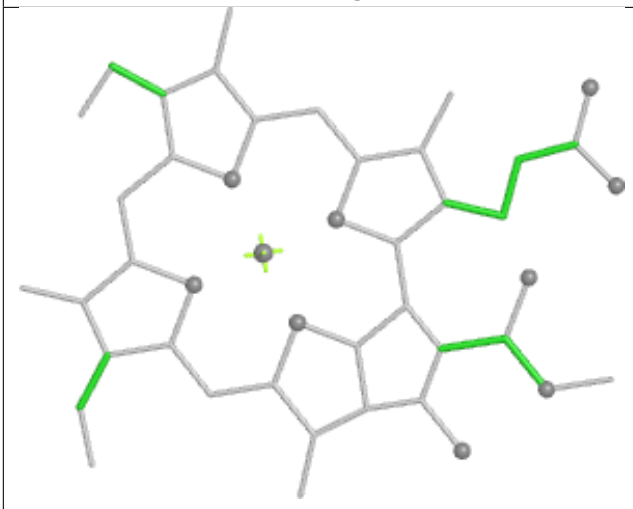
Ligand CLA 1 606



Bond lengths



Bond angles

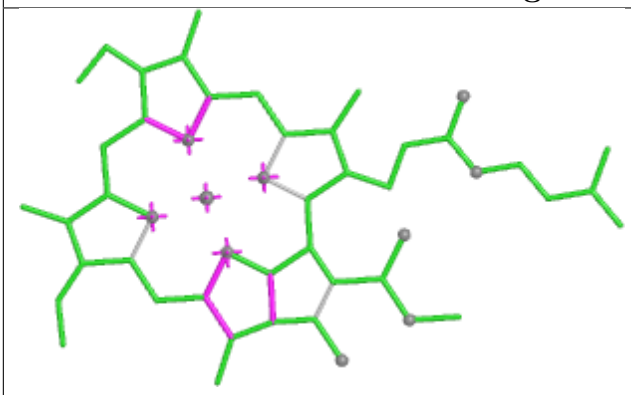


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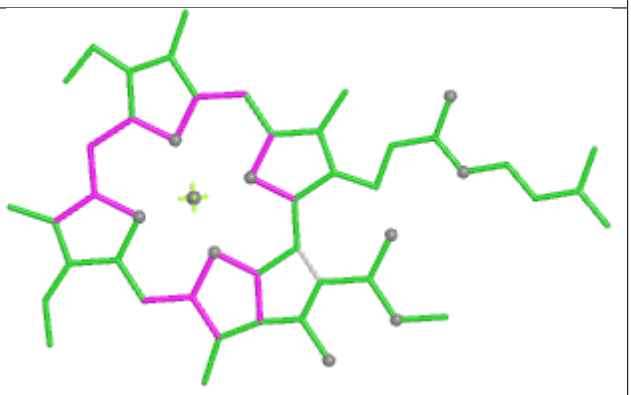


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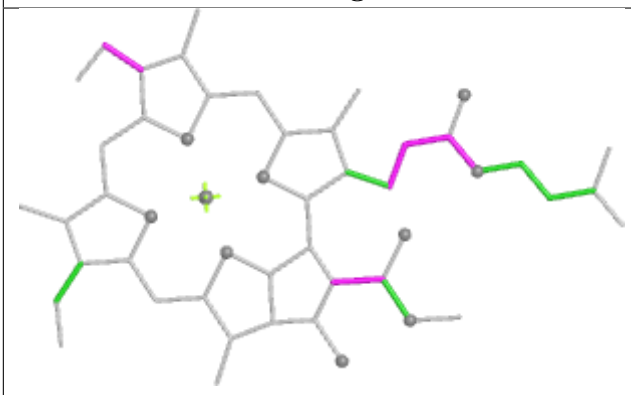
Ligand CLA A 829



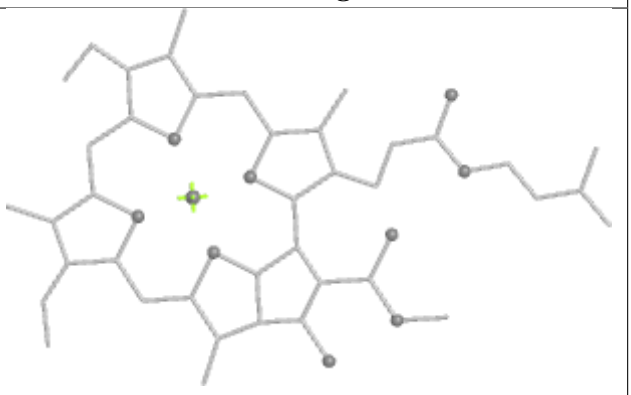
Bond lengths



Bond angles

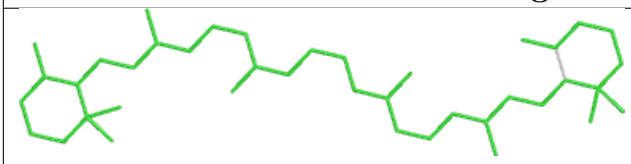


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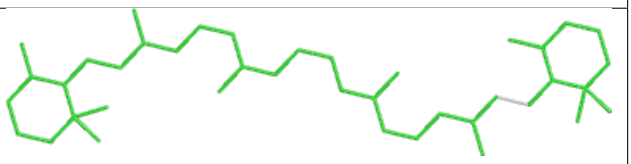


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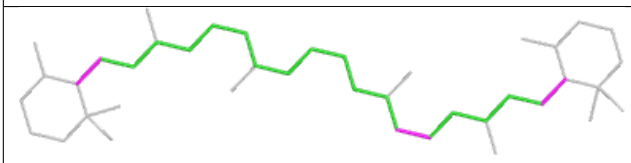
Ligand 8CT 4 616



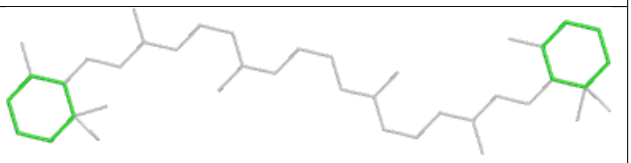
Bond lengths



Bond angles

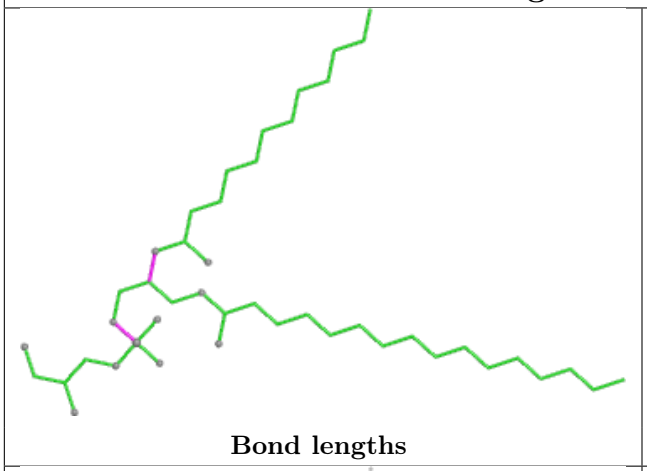


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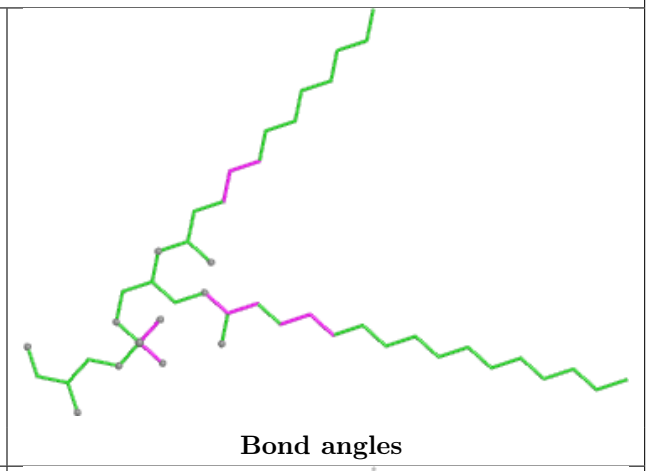


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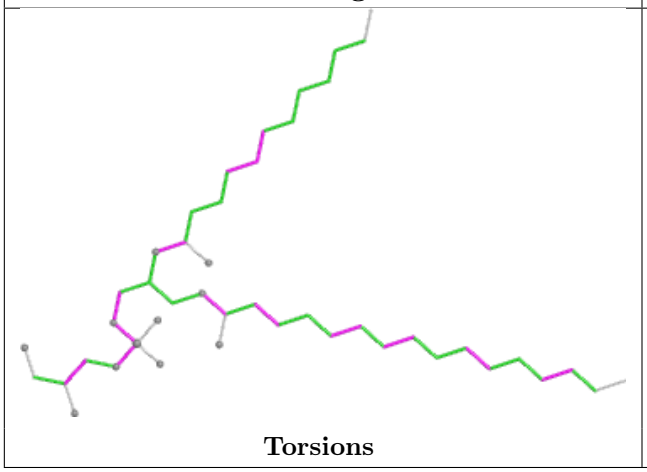
Ligand LHG 4 619



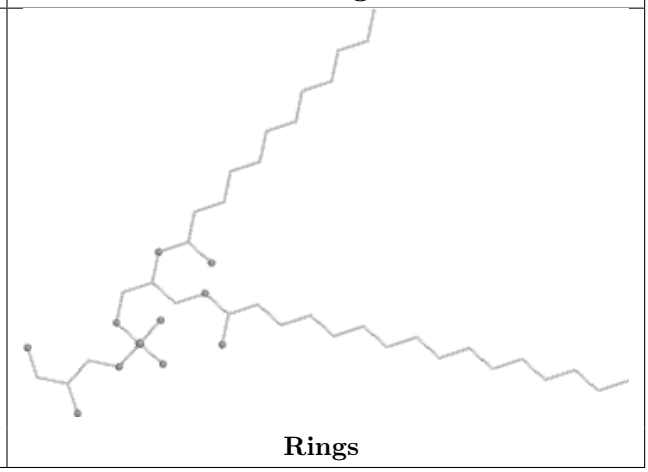
Bond lengths



Bond angles

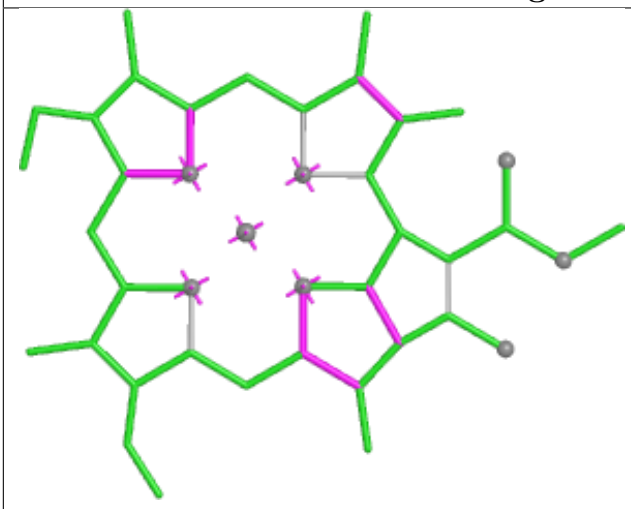


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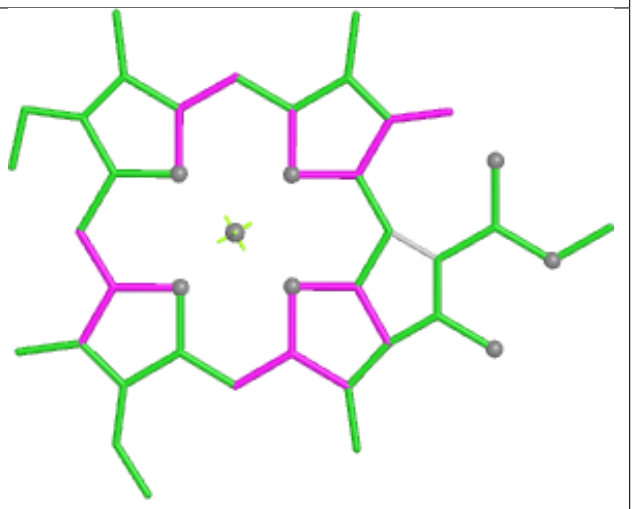


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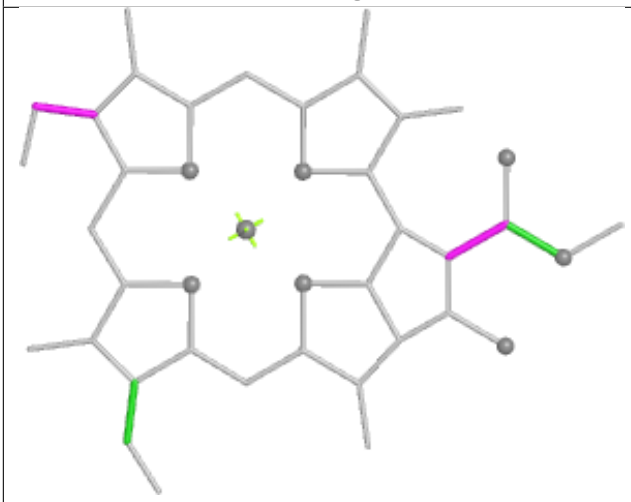
Ligand CLA 8 607



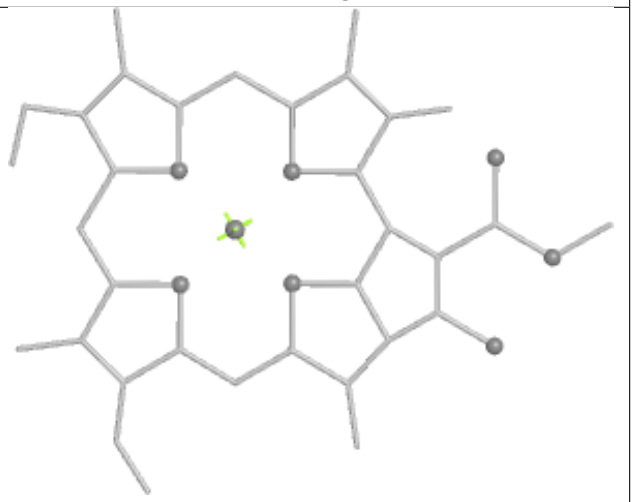
Bond lengths



Bond angles



Torsions

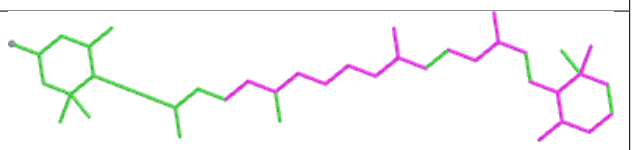


Rings

Ligand IHT 5 618



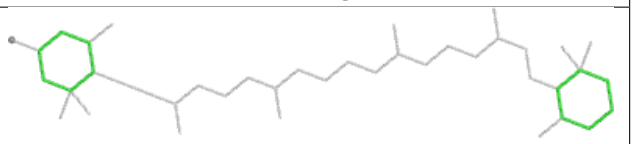
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Bond angles

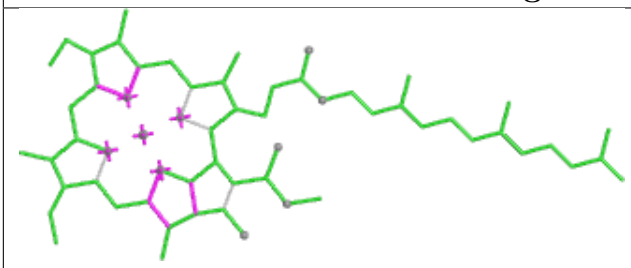


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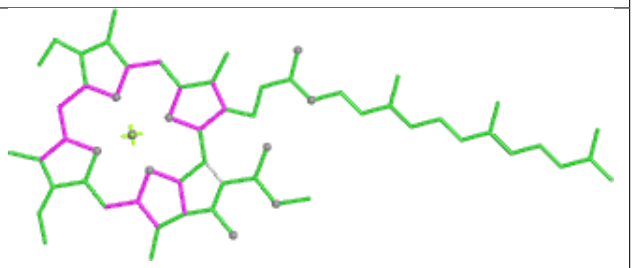


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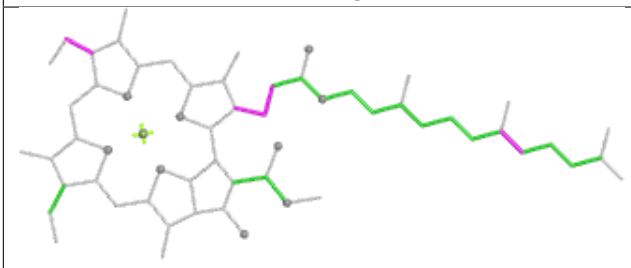
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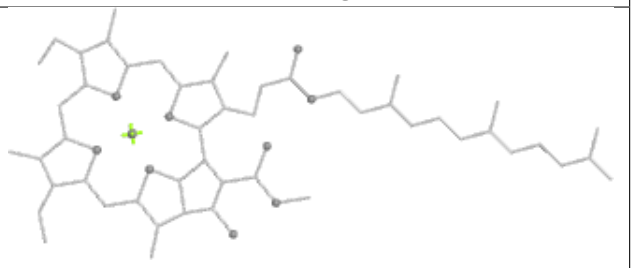
Bond lengths



Bond angles

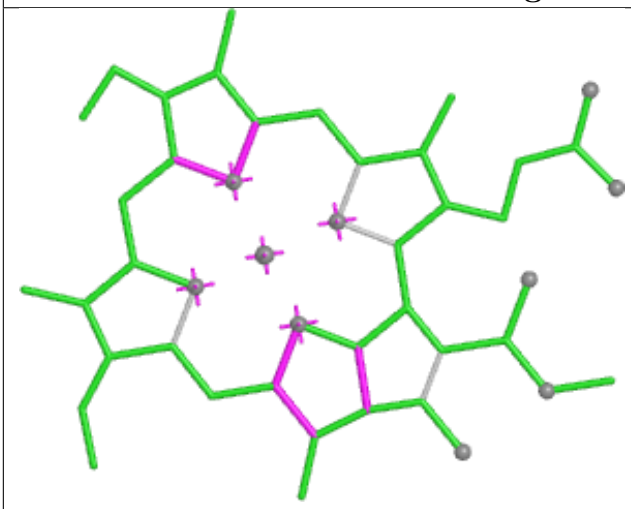


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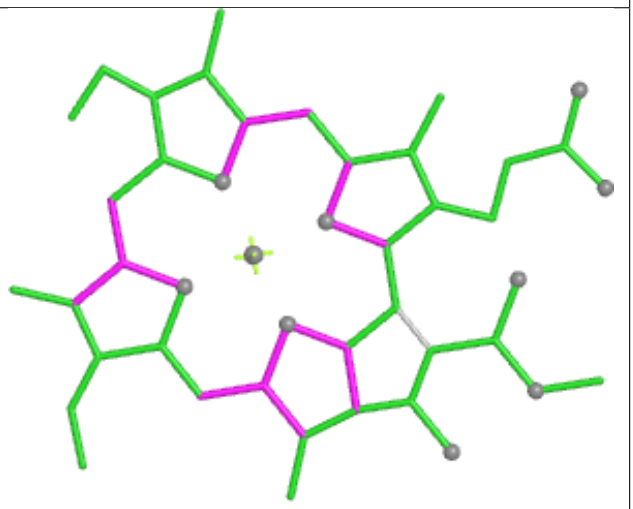


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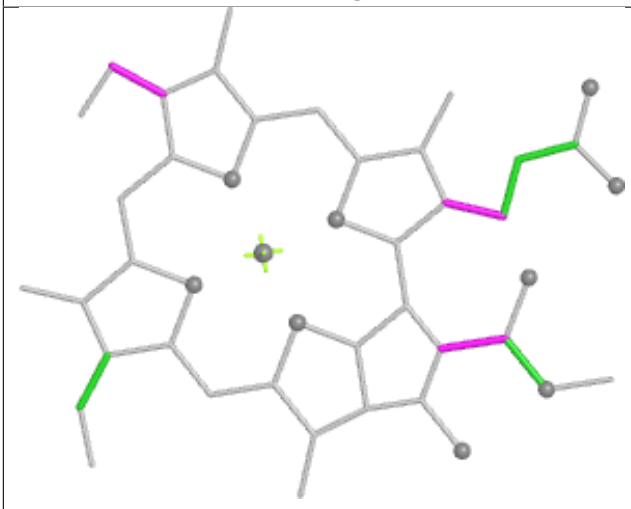
Ligand CLA B 833



Bond lengths



Bond angles

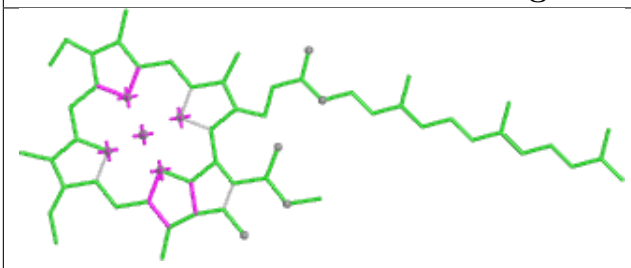


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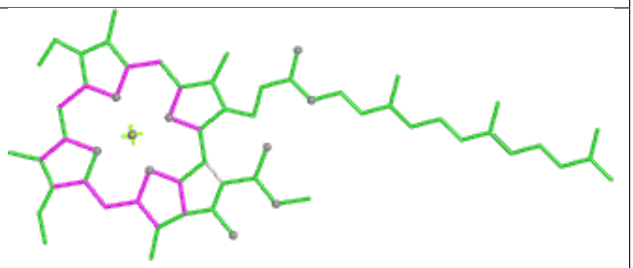


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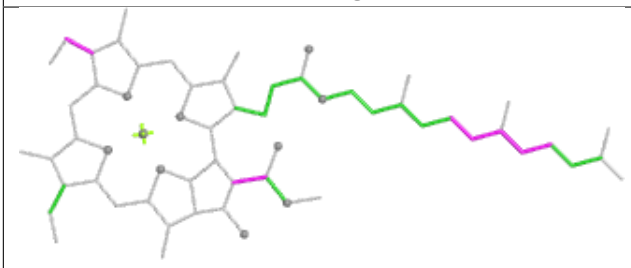
Ligand CLA c 608



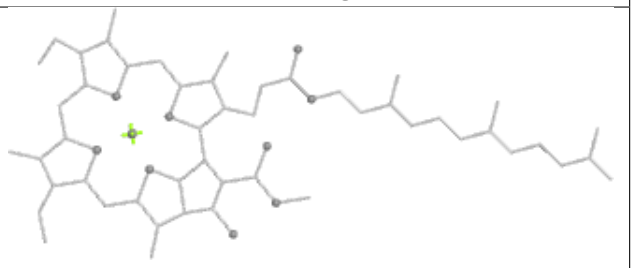
Bond lengths



Bond angles

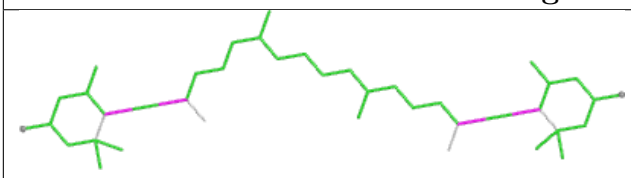


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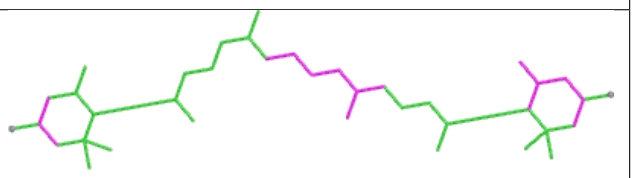


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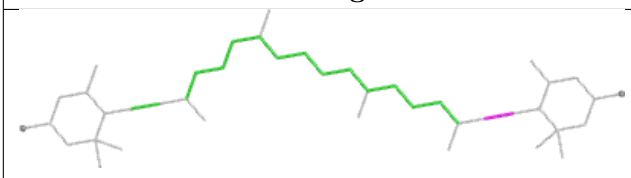
Ligand II0 b 612



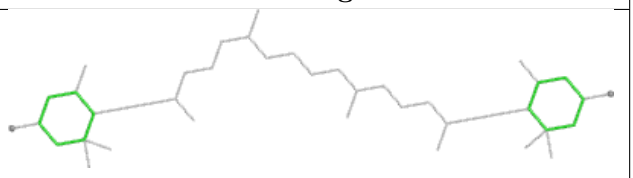
Bond lengths



Bond angles

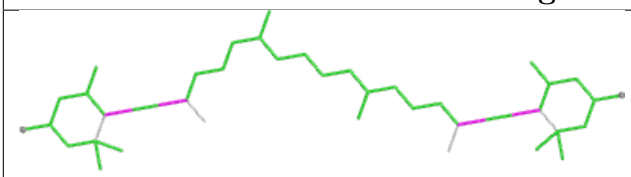


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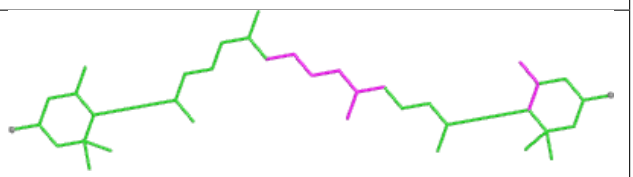


Rings

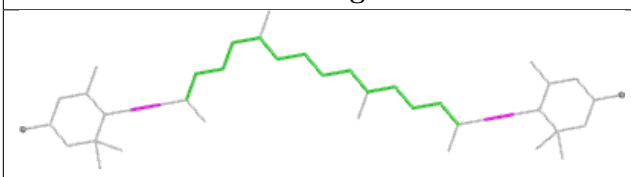
Ligand II0 O 204



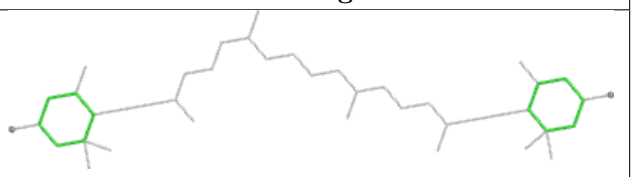
Bond lengths



Bond angles

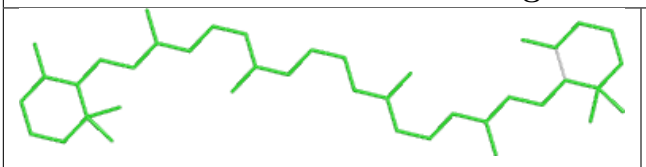


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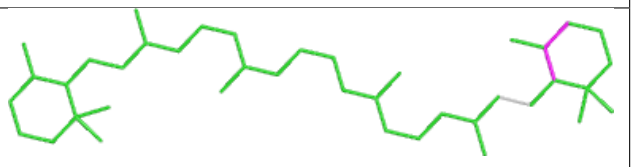


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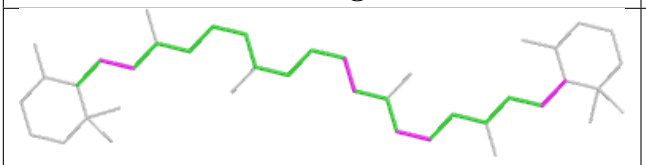
Ligand 8CT M 101



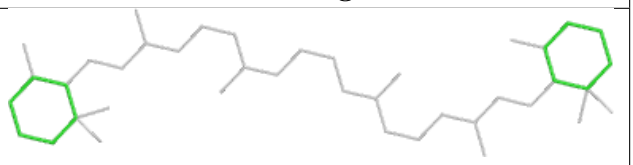
Bond lengths



Bond angles

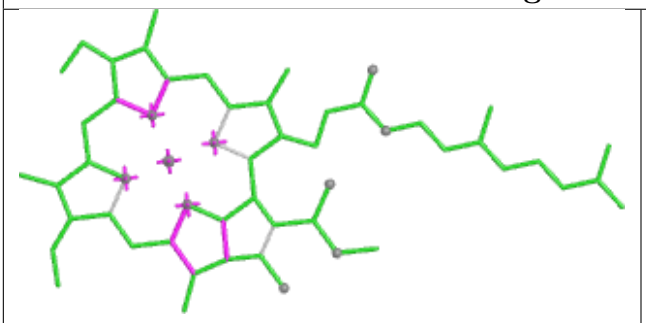


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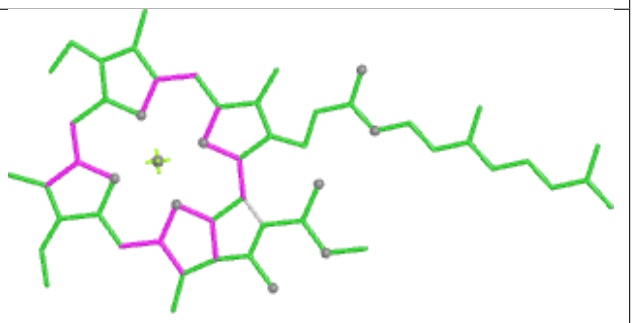


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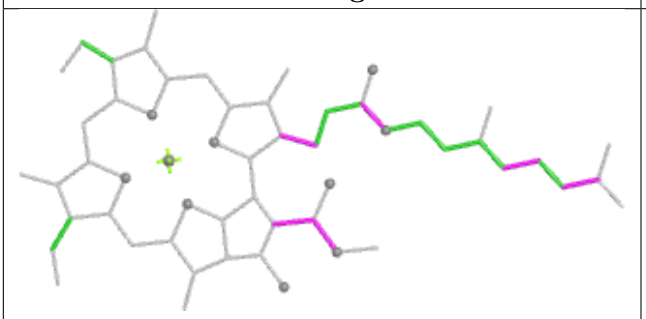
Ligand CLA O 203



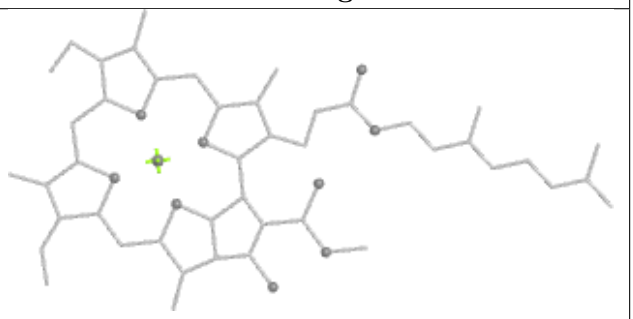
Bond lengths



Bond angles

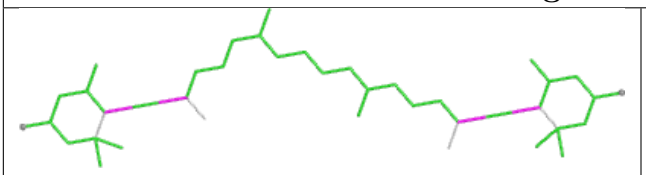


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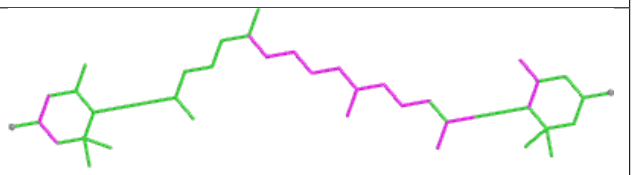


Rings

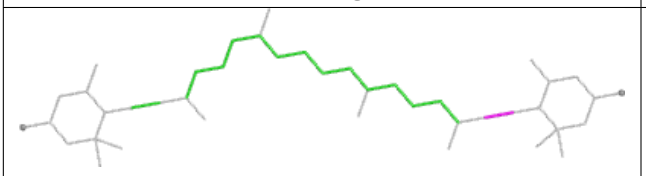
Ligand II0 a 615



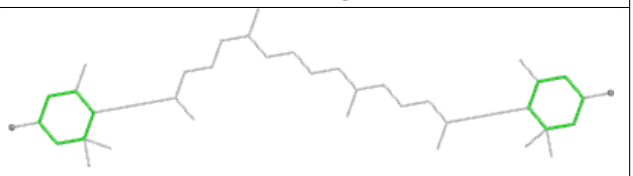
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Bond angles

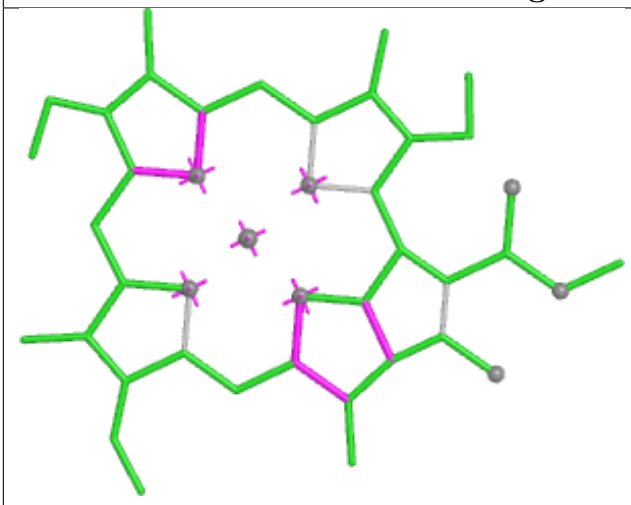


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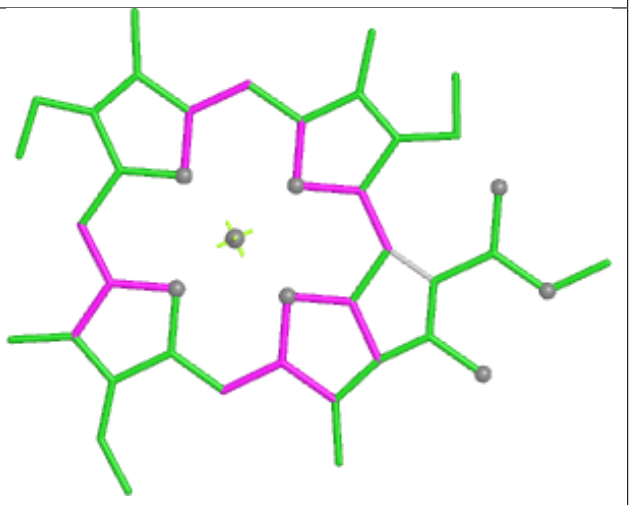


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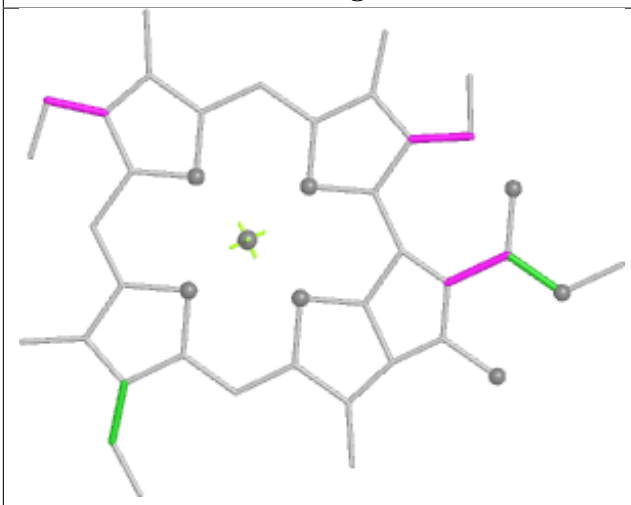
Ligand CLA 2 601



Bond lengths



Bond angles

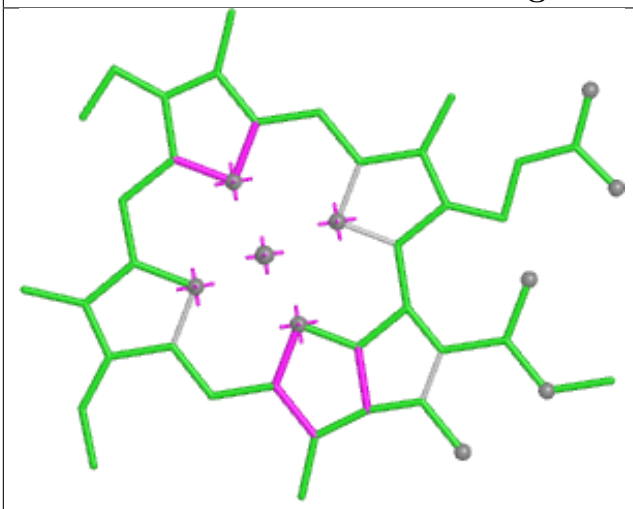


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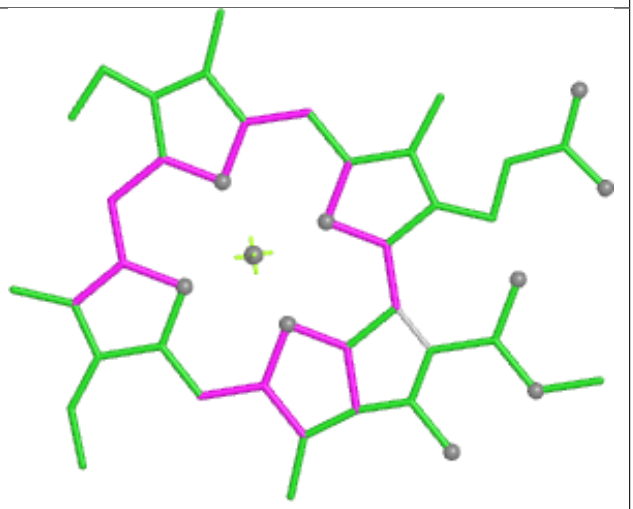


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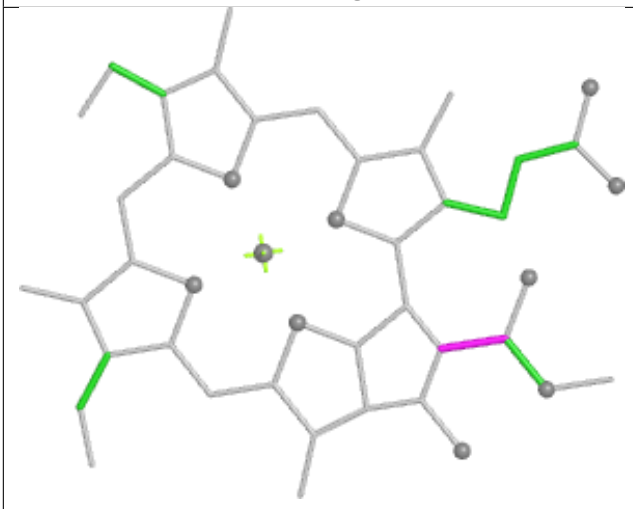
Ligand CLA 2 611



Bond lengths



Bond angles

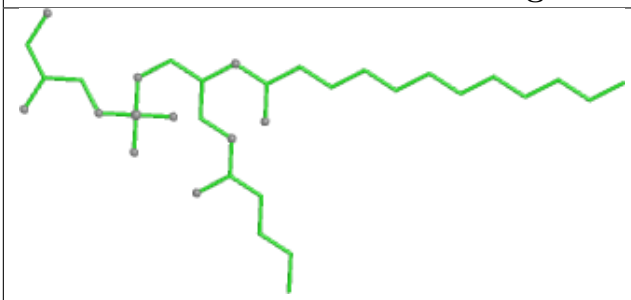


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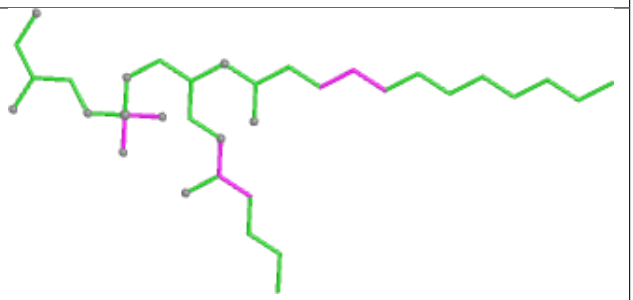


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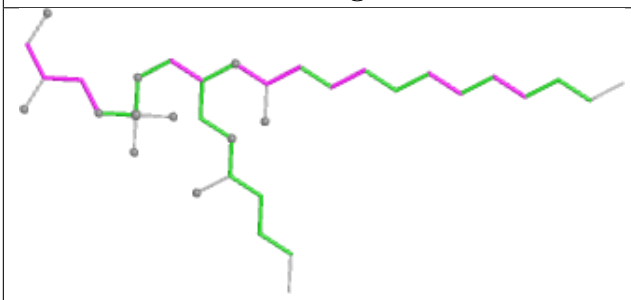
Ligand LHG 3 622



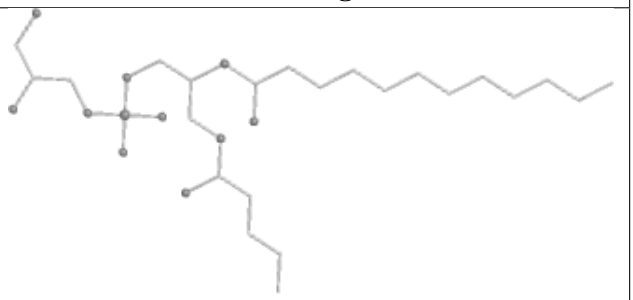
Bond lengths



Bond angles

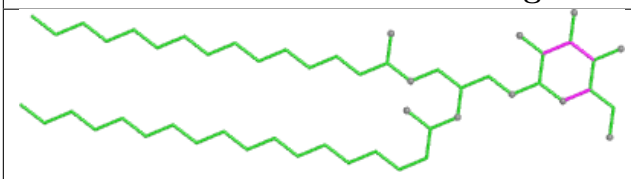


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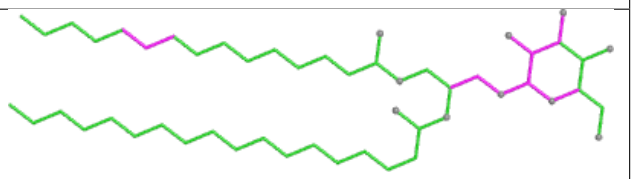


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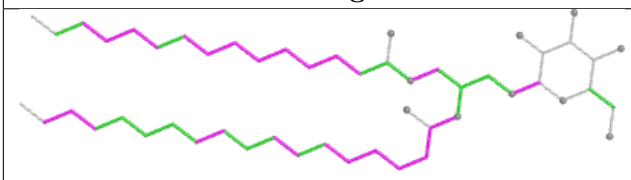
Ligand LMG 8 614



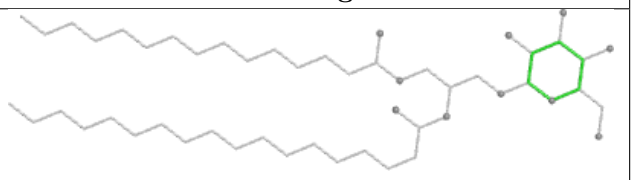
Bond lengths



Bond angles

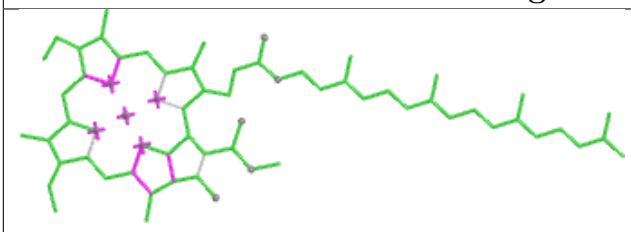


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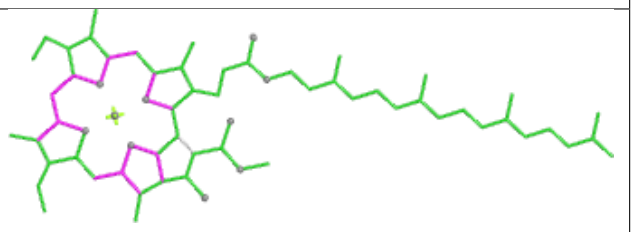


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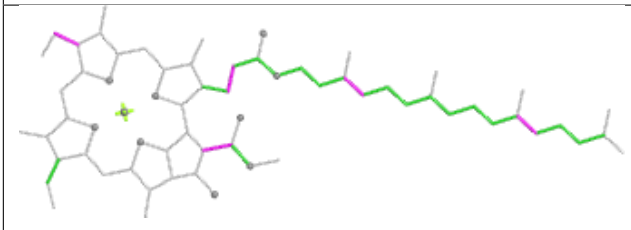
Ligand CLA a 606



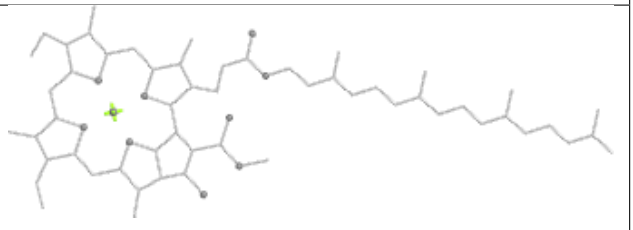
Bond lengths



Bond angles

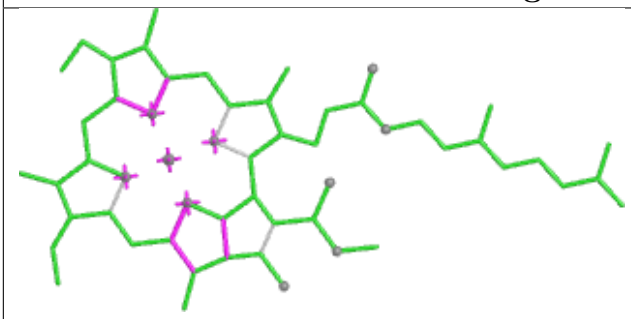


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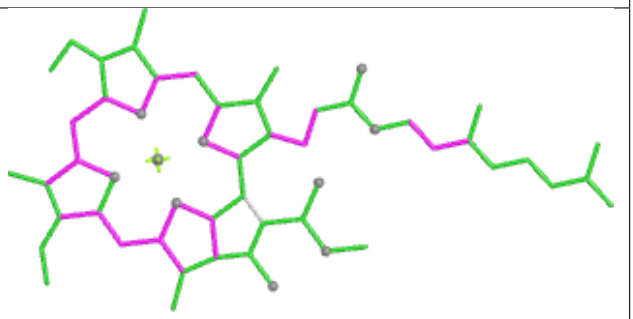


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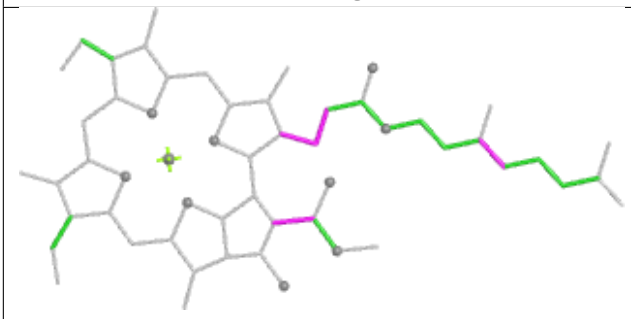
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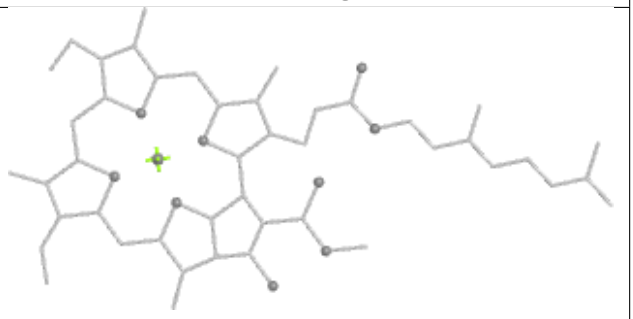
Bond lengths



Bond angles

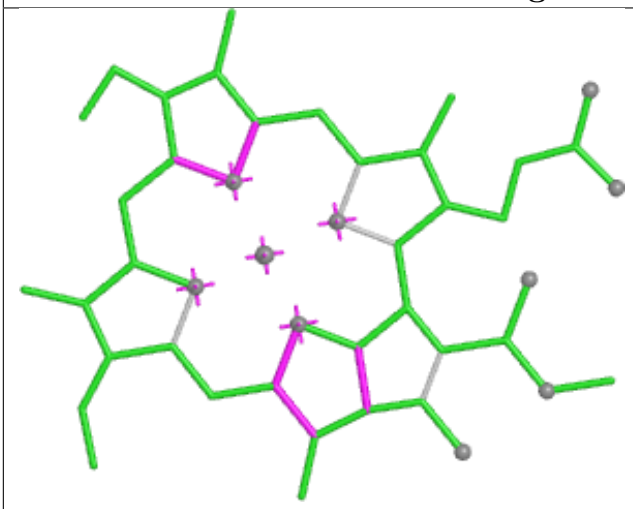


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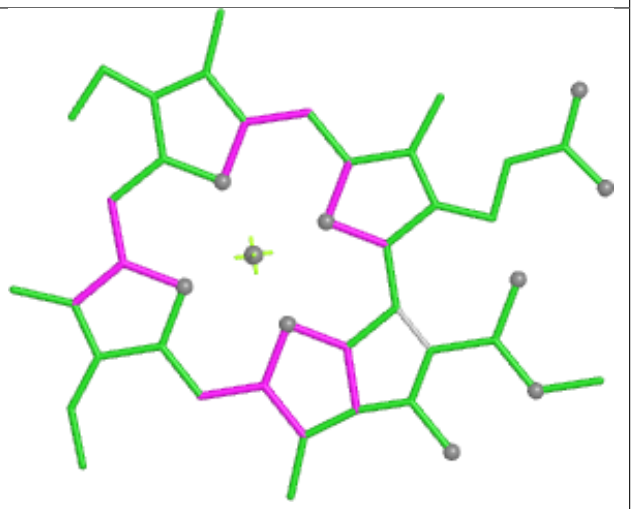


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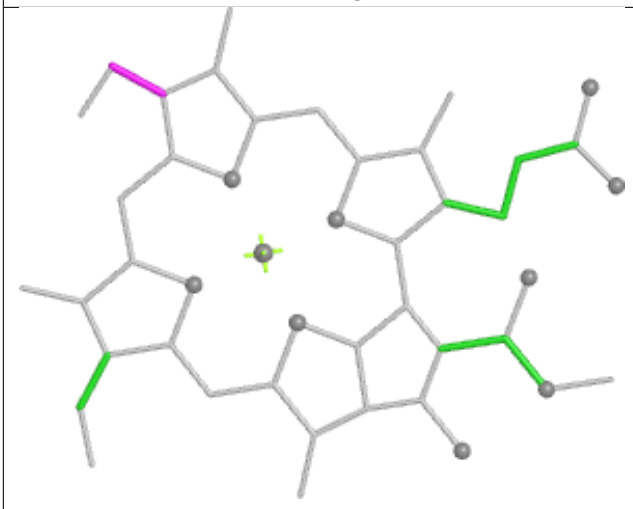
Ligand CLA 5 607



Bond lengths



Bond angles

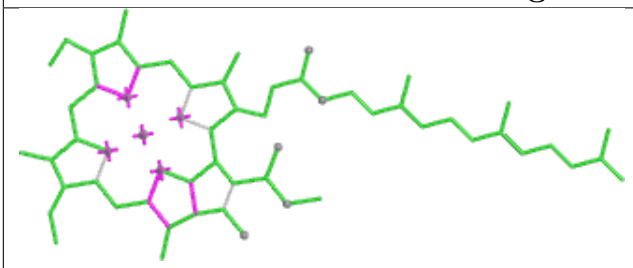


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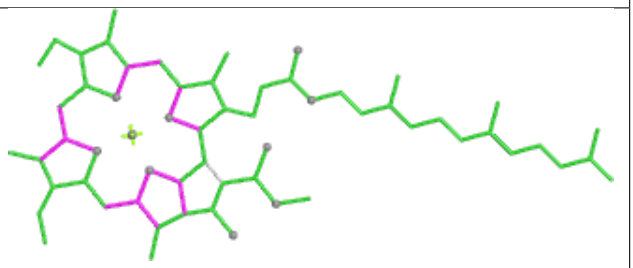


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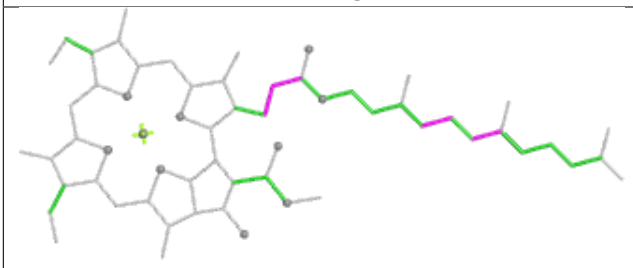
Ligand CLA 4 609



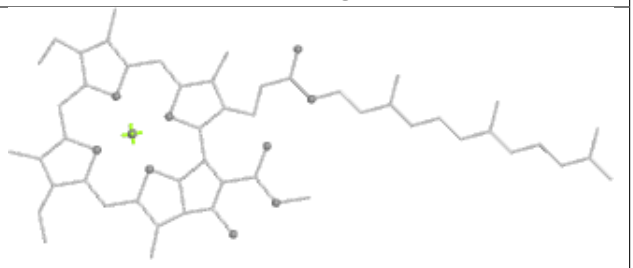
Bond lengths



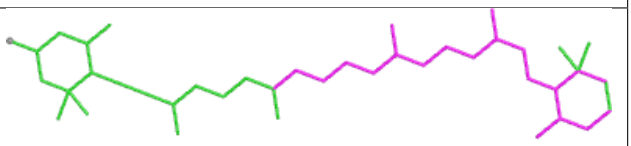
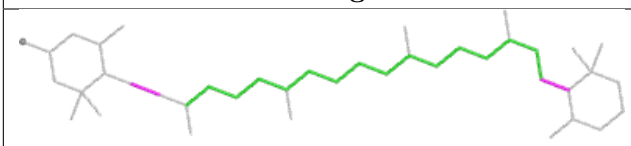
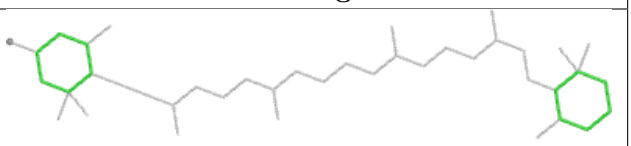
Bond angles

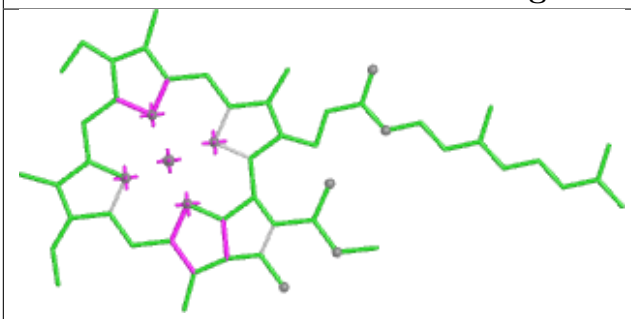
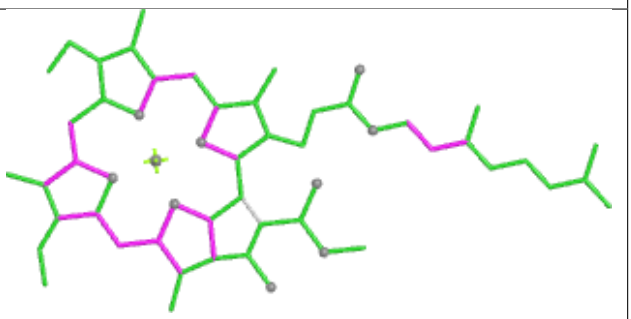
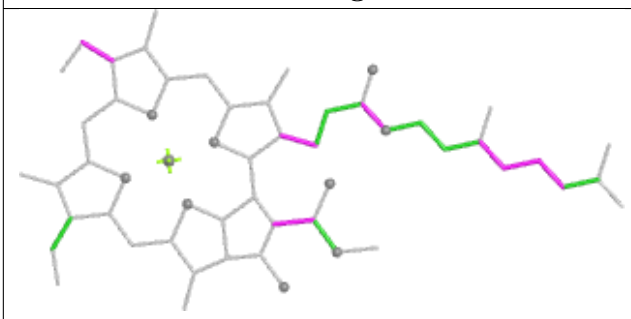
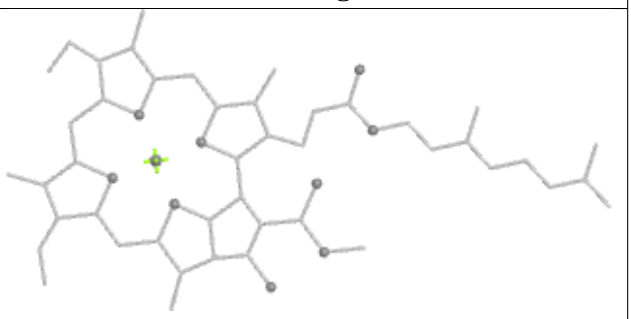


Torsions

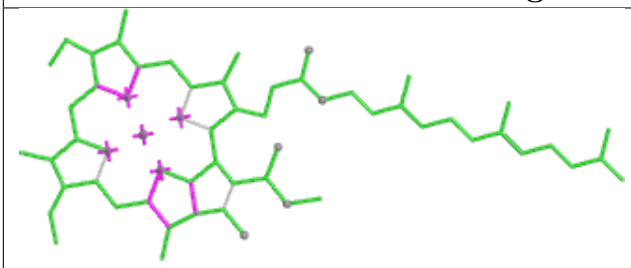


Rings

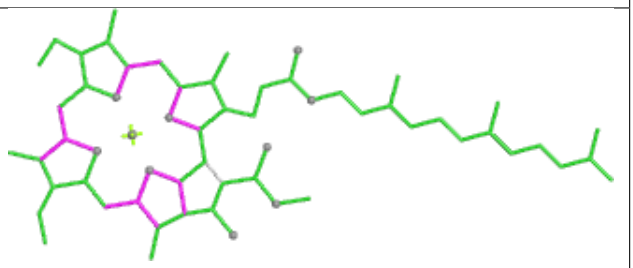
Ligand IHT 6 617	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA e 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

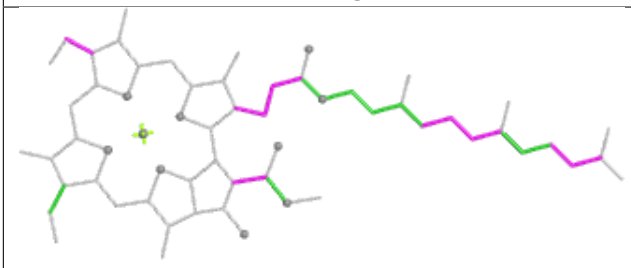
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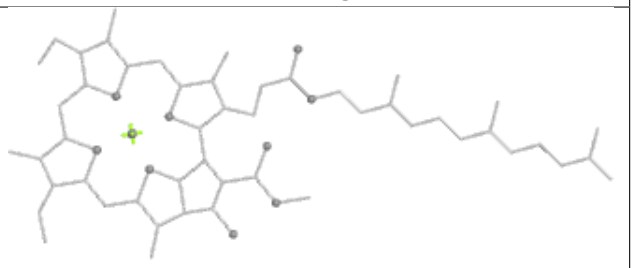
Bond lengths



Bond angles

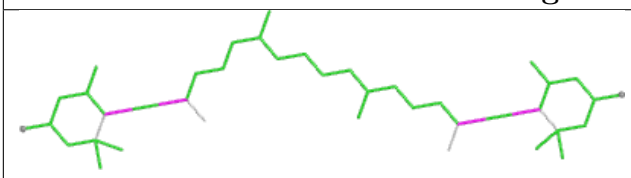


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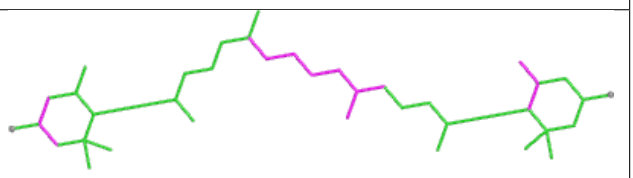


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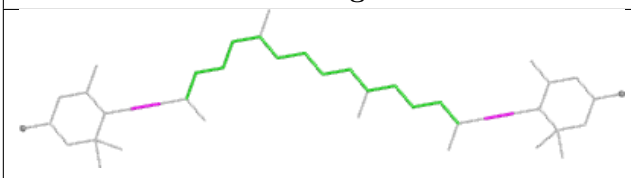
Ligand II0 d 614



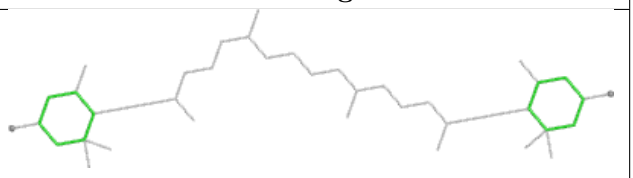
Bond lengths



Bond angles

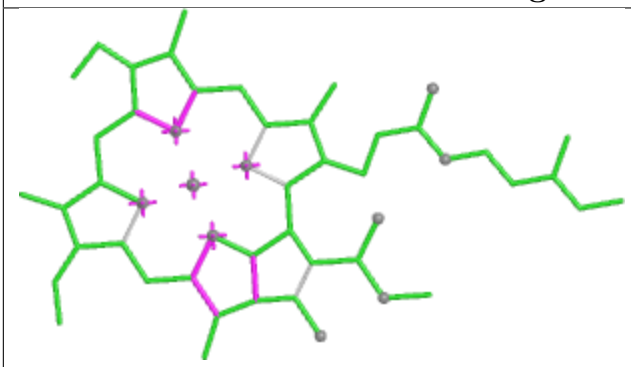


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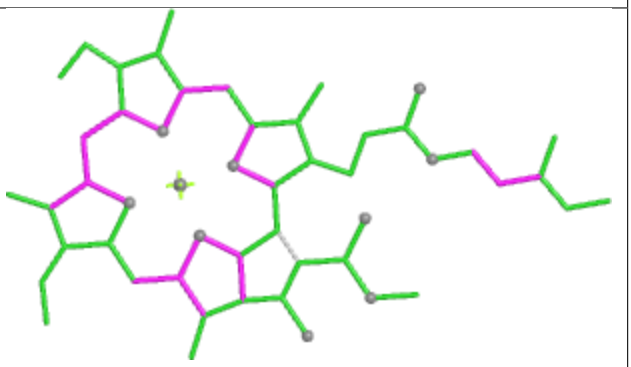


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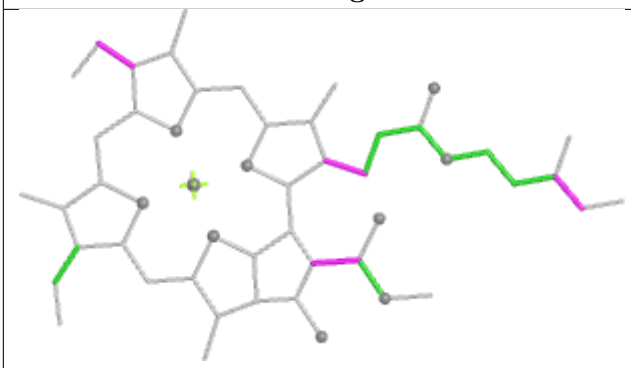
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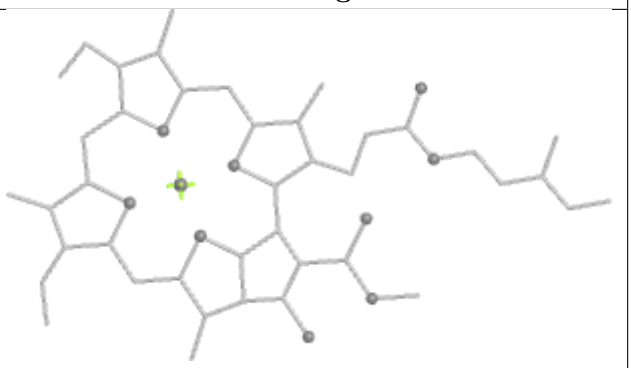
Bond lengths



Bond angles

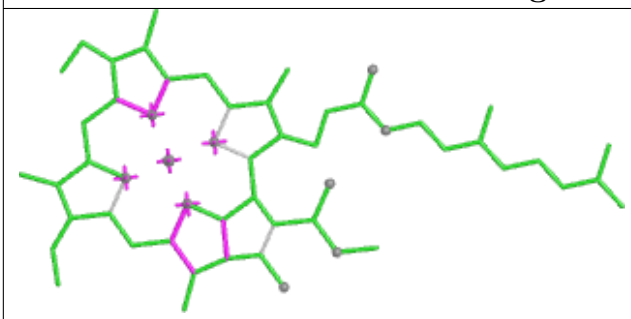


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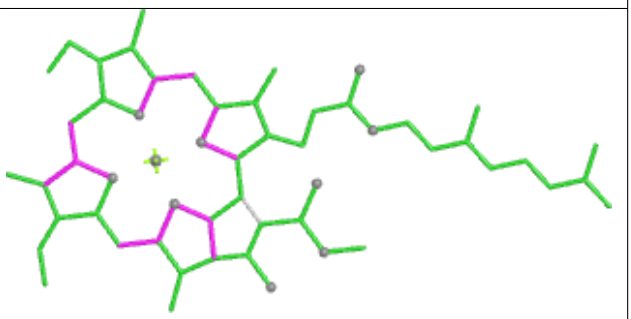


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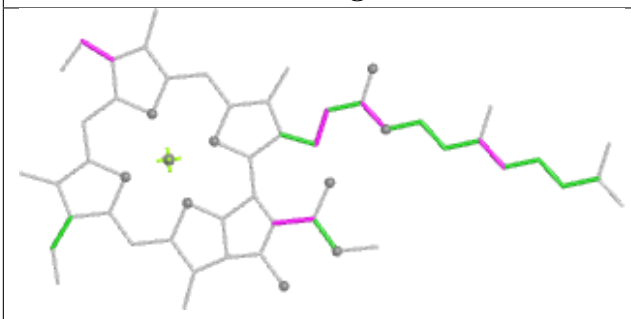
Ligand CLA c 614



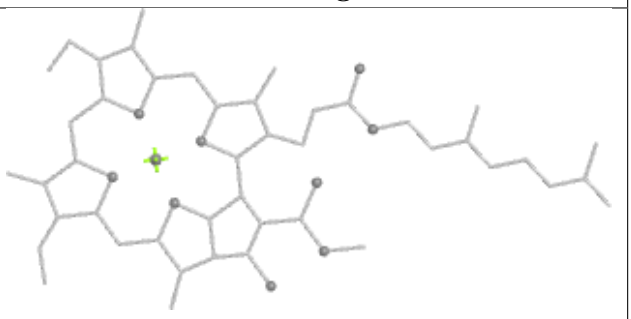
Bond lengths



Bond angles

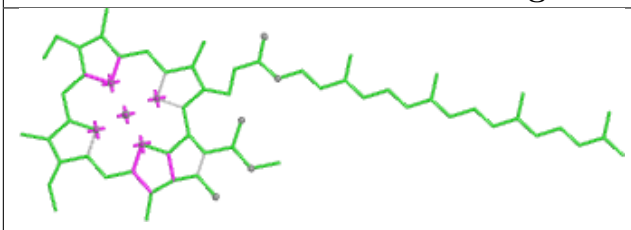


Torsions

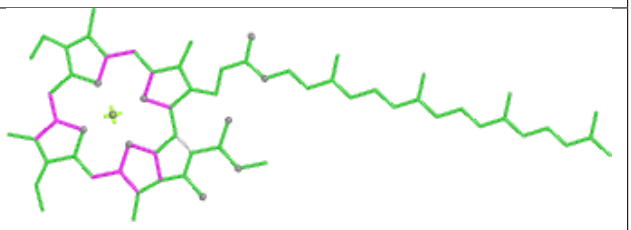


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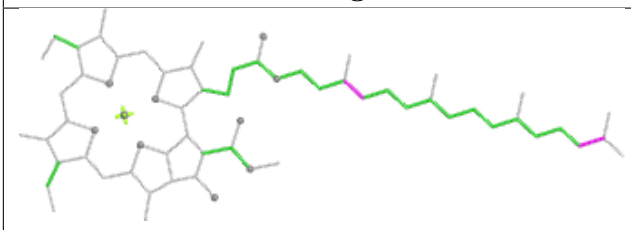
Ligand CLA a 607



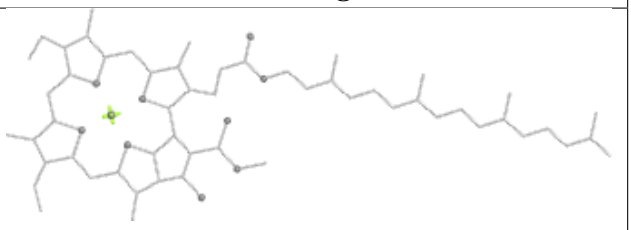
Bond lengths



Bond angles

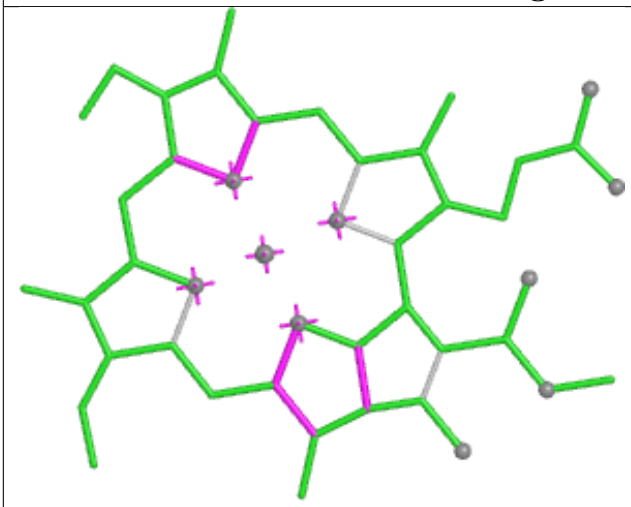


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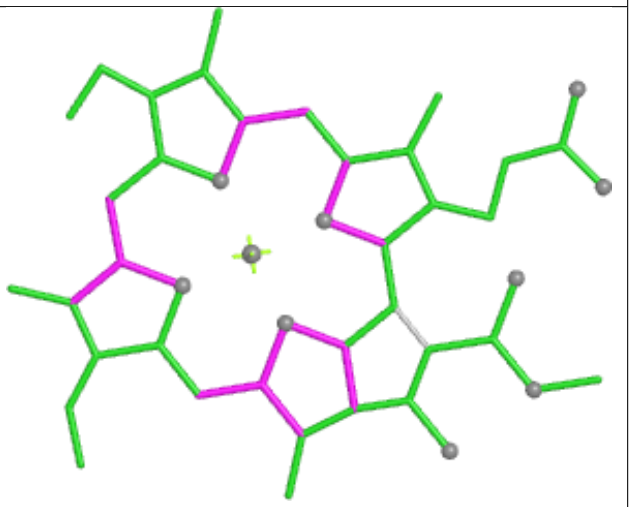


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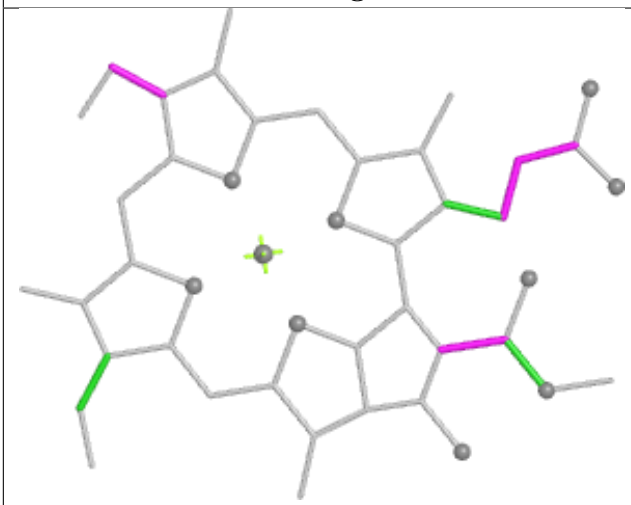
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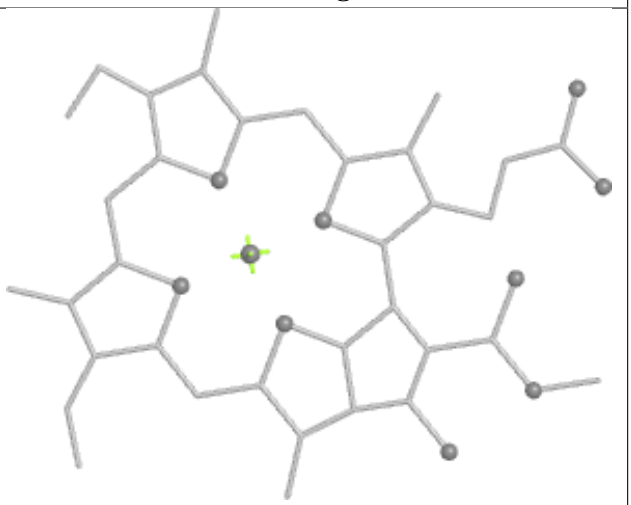
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Bond angles

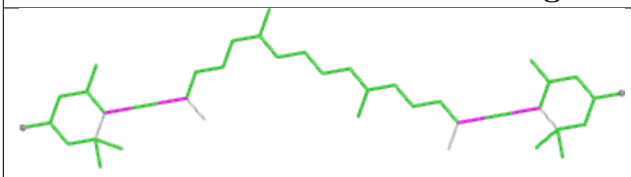


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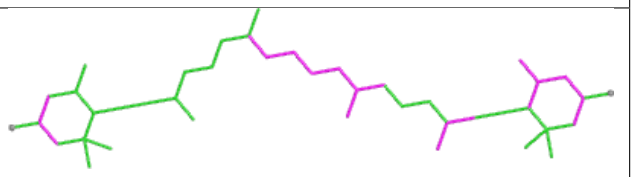


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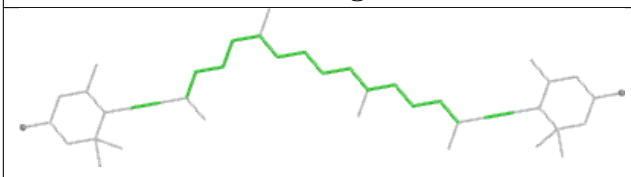
Ligand II0 e 612



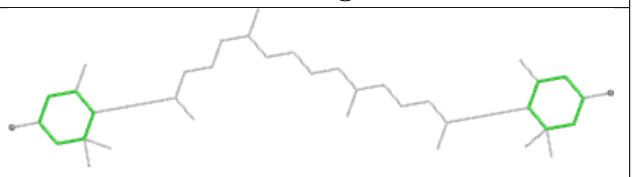
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Bond angles

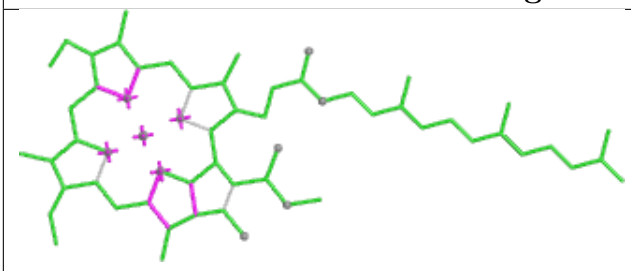


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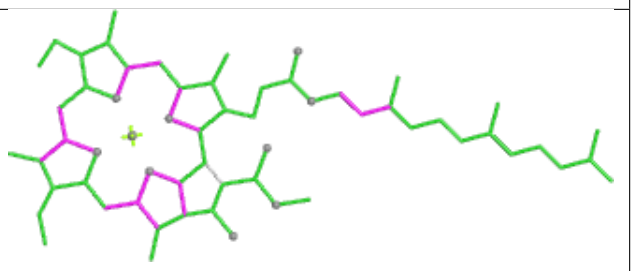


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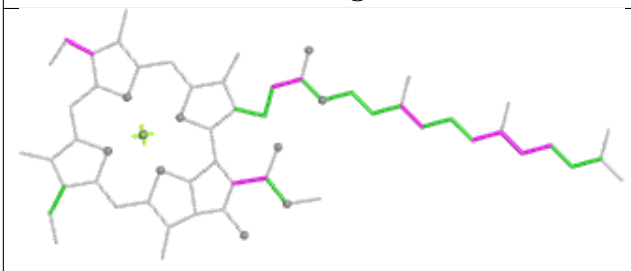
Ligand CLA B 821



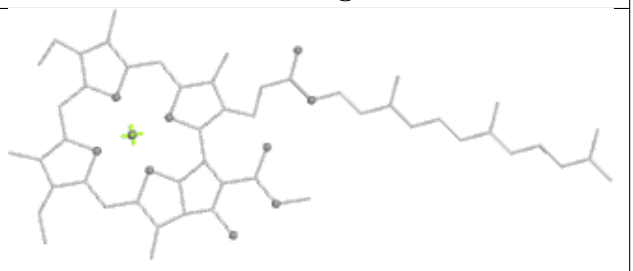
Bond lengths



Bond angles

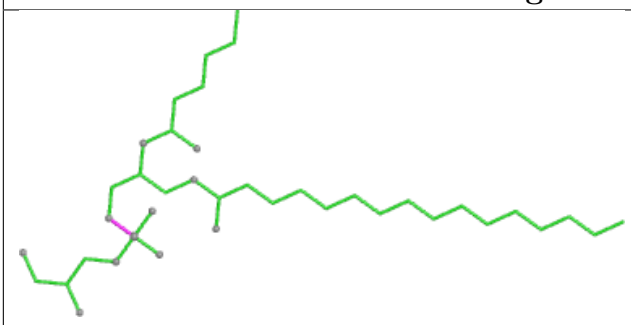


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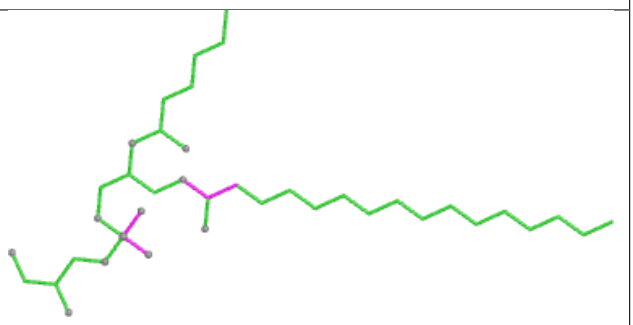


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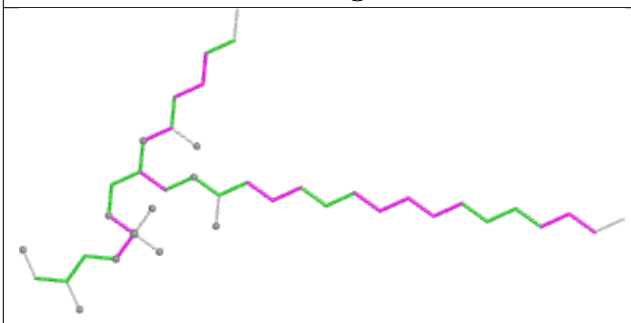
Ligand LHG d 619



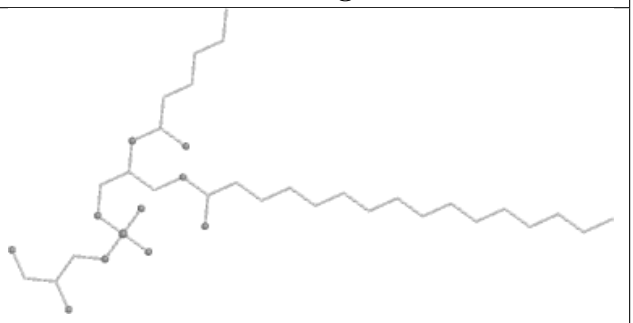
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Bond angles

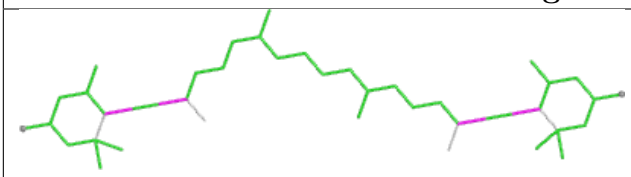


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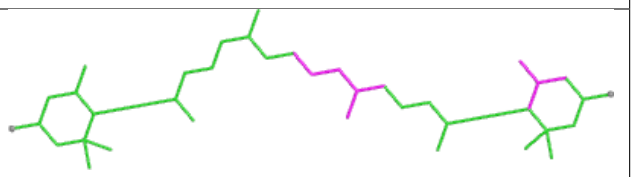


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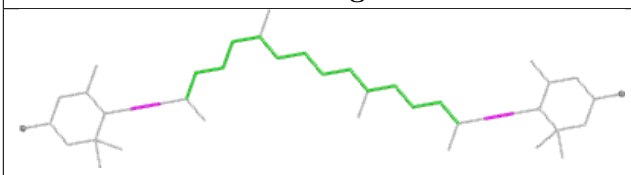
Ligand II0 3 617



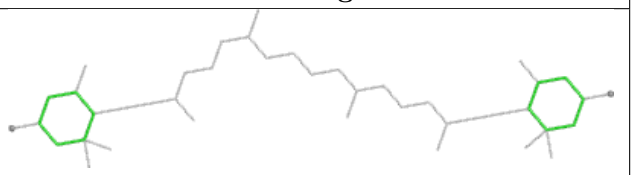
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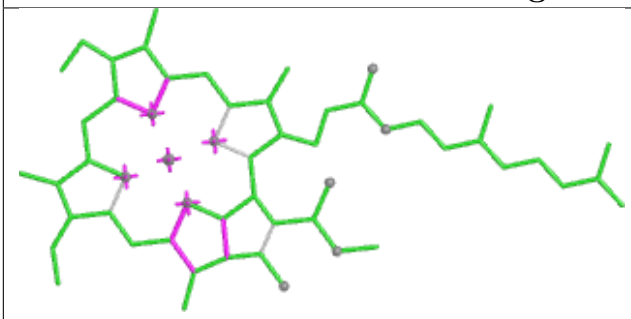


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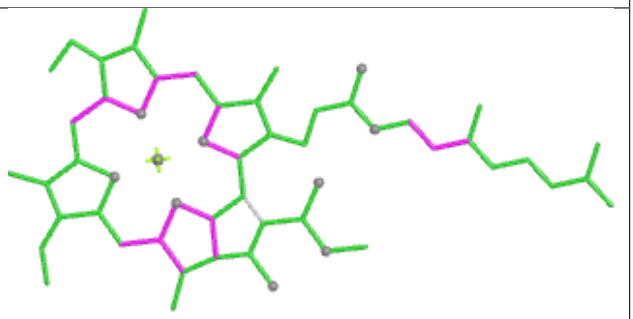


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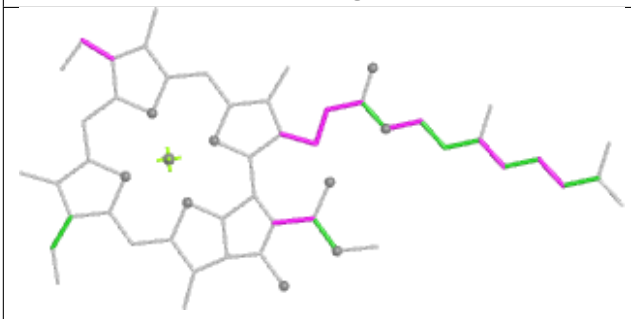
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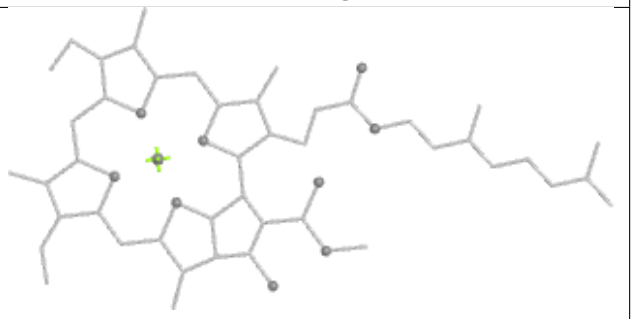
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Bond angles

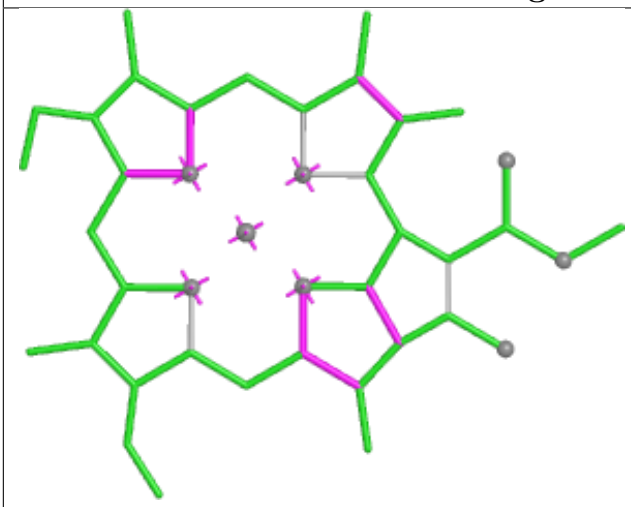


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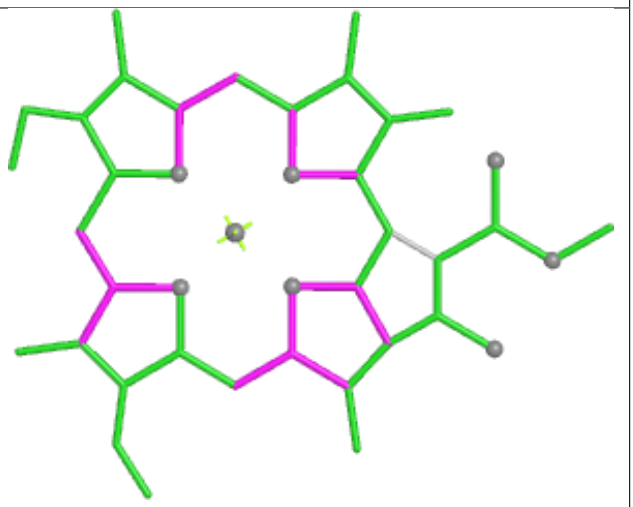


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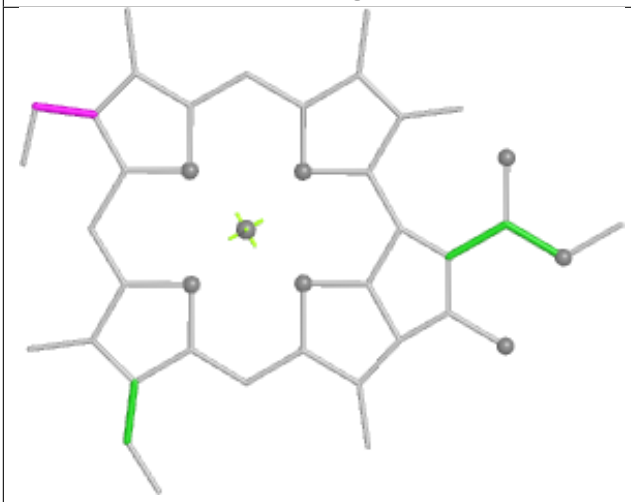
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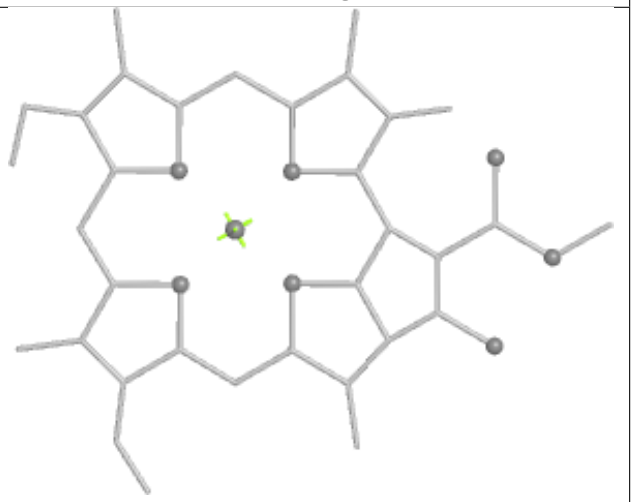
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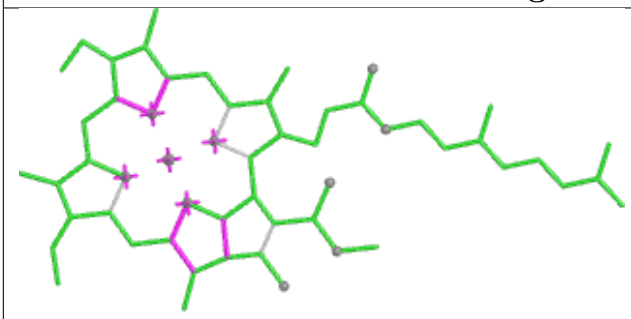
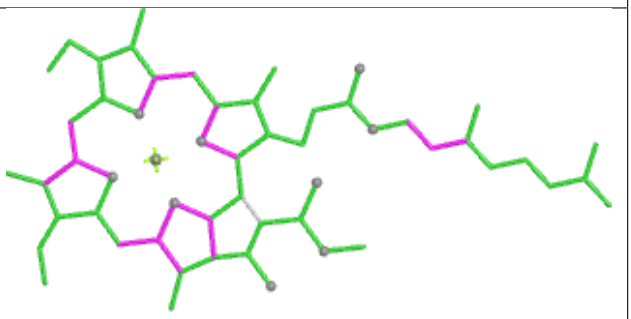
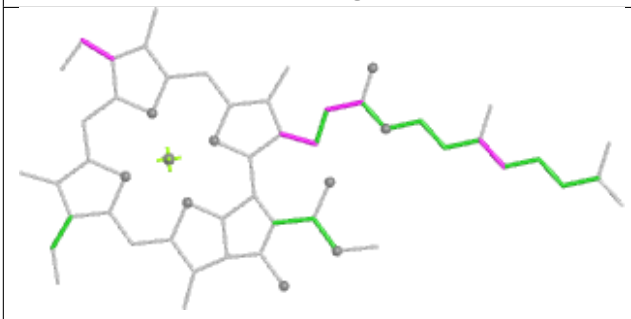
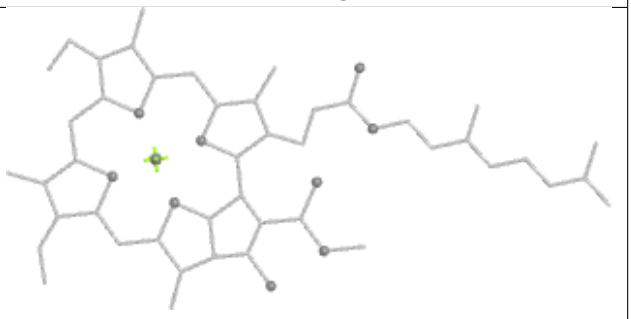
Bond angles

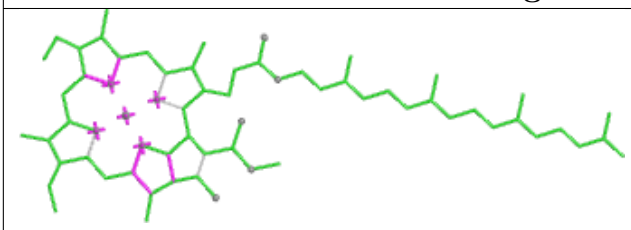
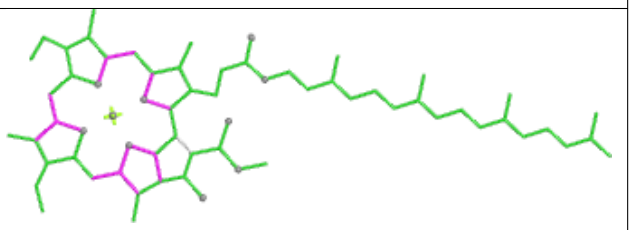
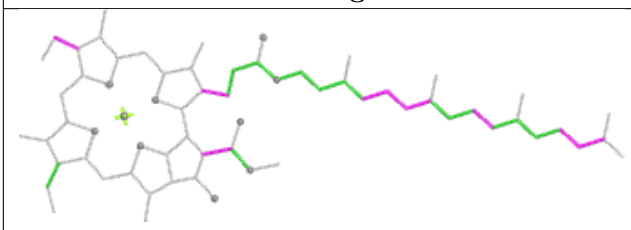
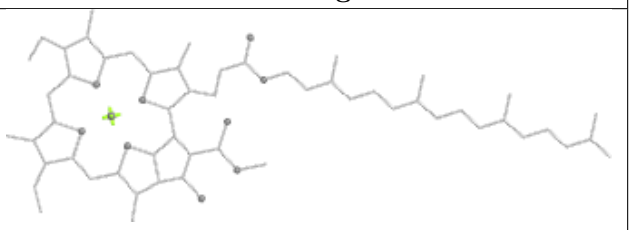


Torsions

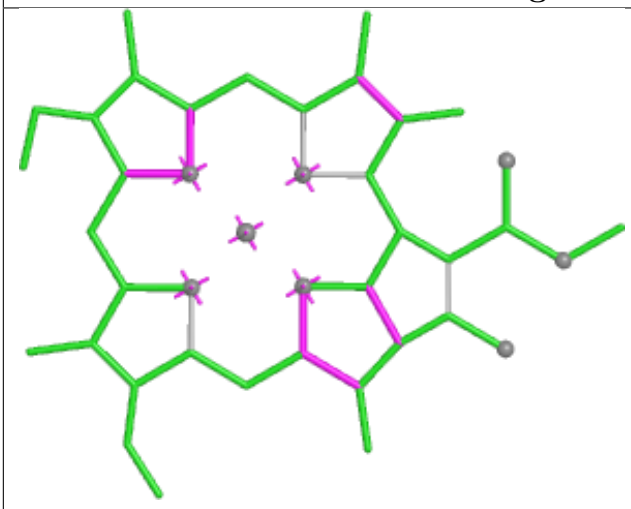


Rings

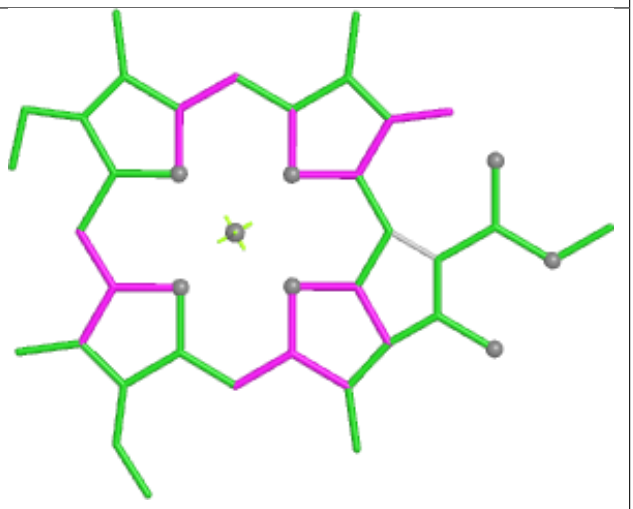
Ligand CLA 6 605	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 837	
	
Bond lengths	Bond angles
	
Torsions	Rings

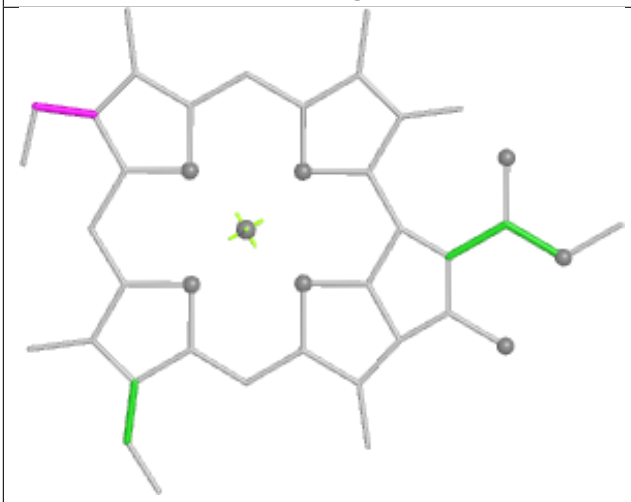
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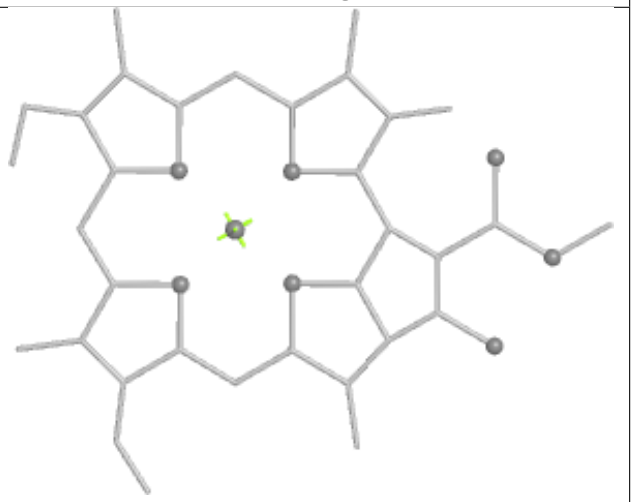
Bond lengths



Bond angles

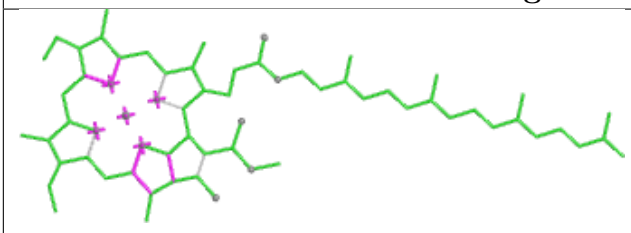


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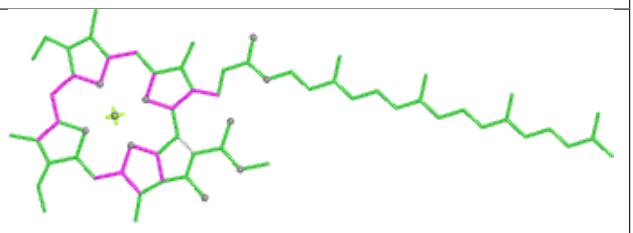


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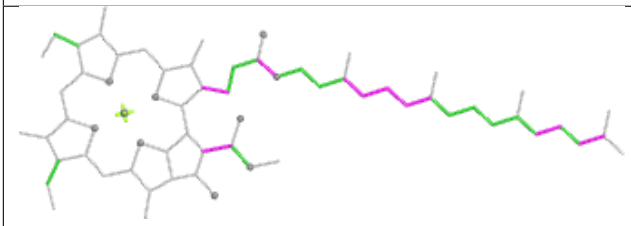
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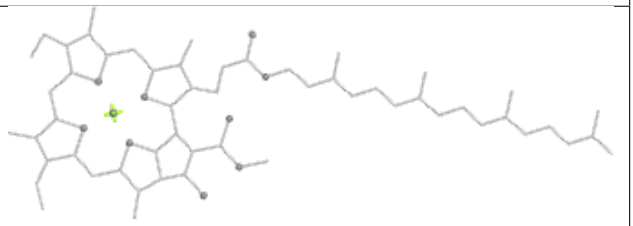
Bond lengths



Bond angles

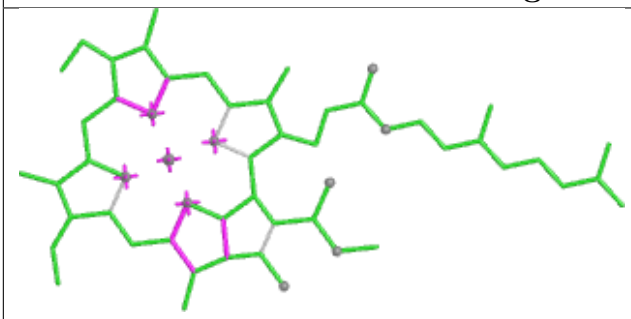


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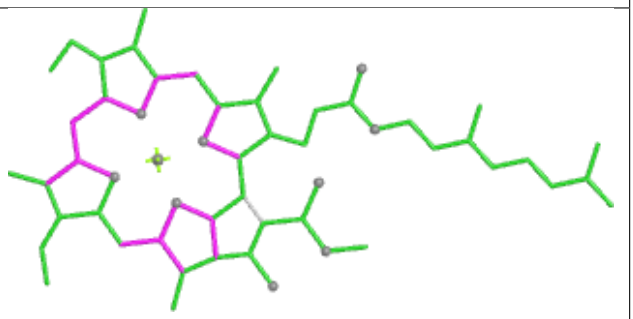


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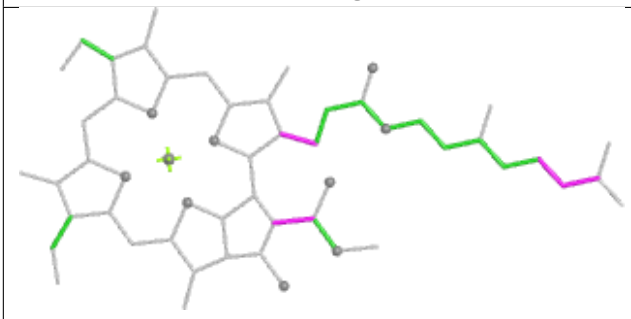
Ligand CLA A 802



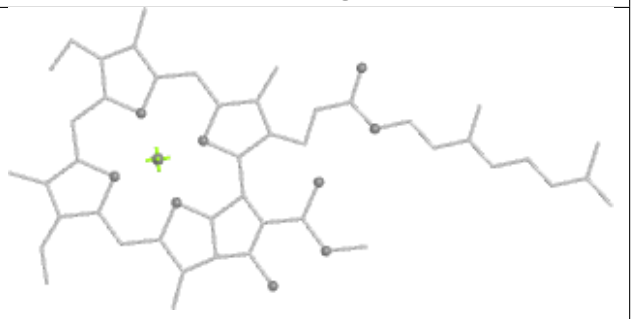
Bond lengths



Bond angles

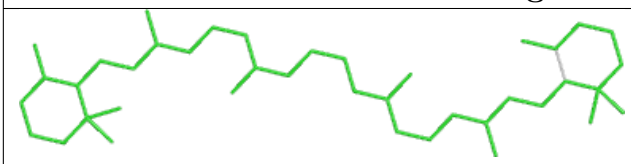


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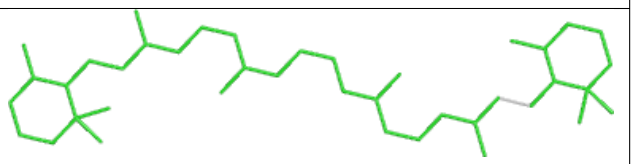


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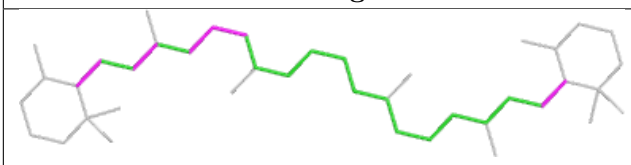
Ligand 8CT R 201



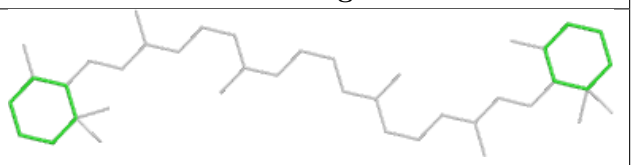
Bond lengths



Bond angles

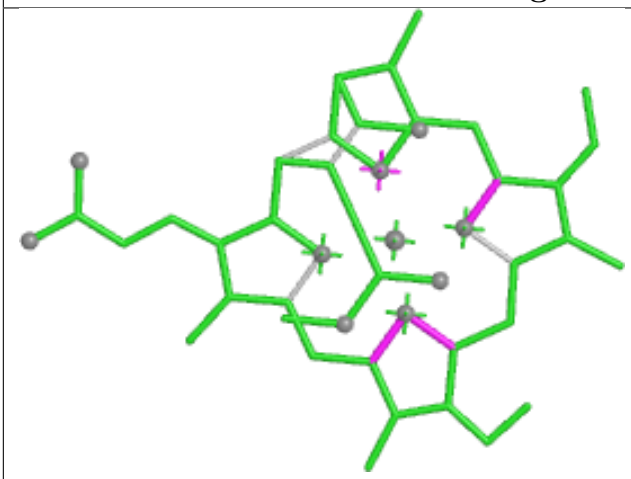


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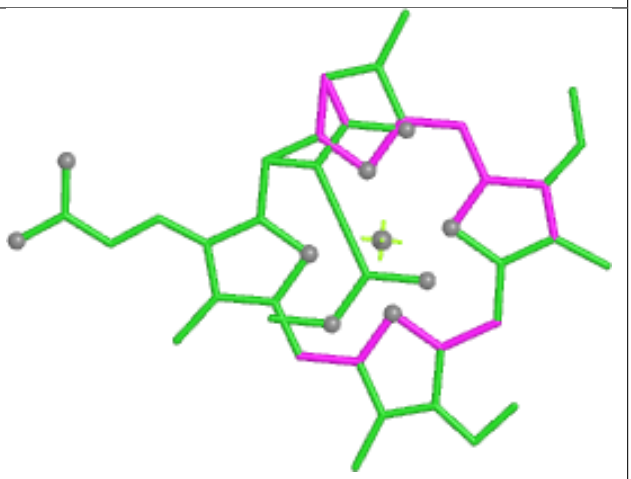


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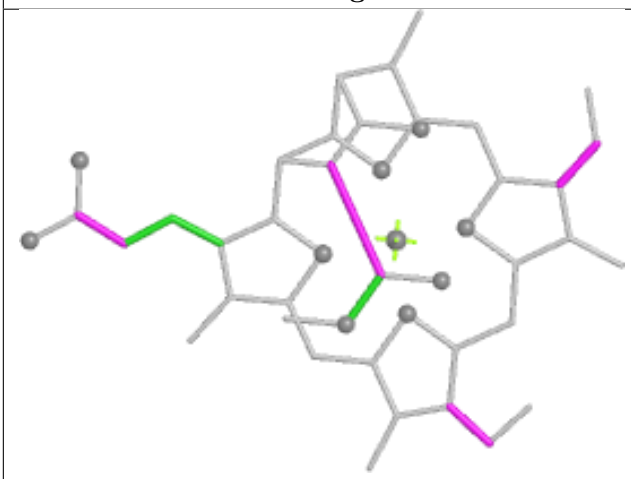
Ligand KC2 6 613



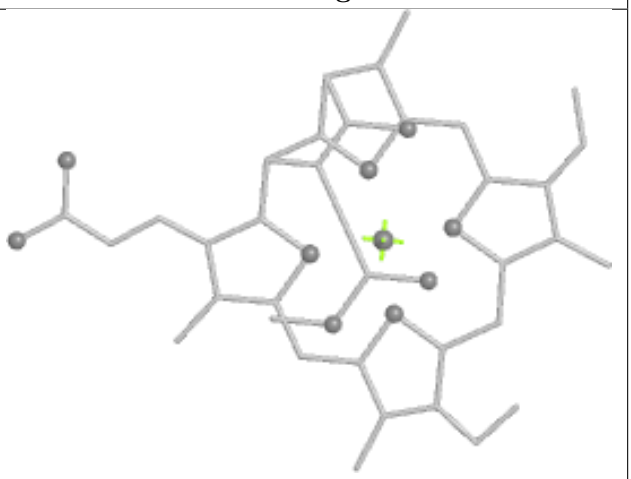
Bond lengths



Bond angles

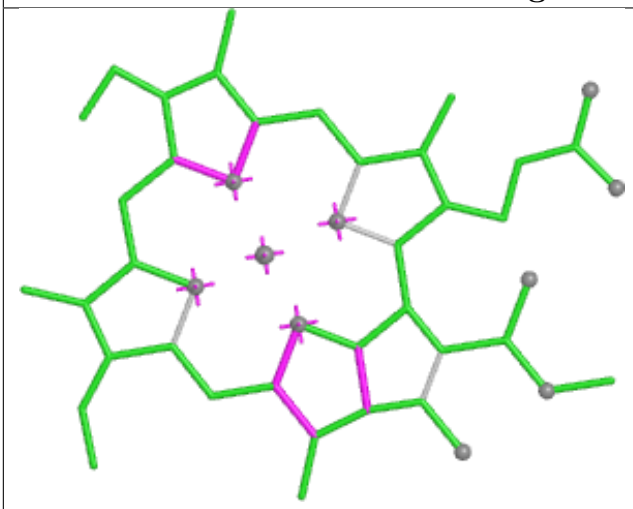


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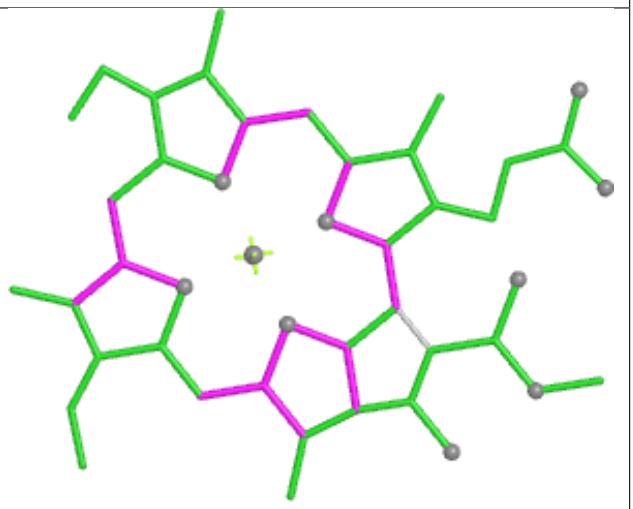


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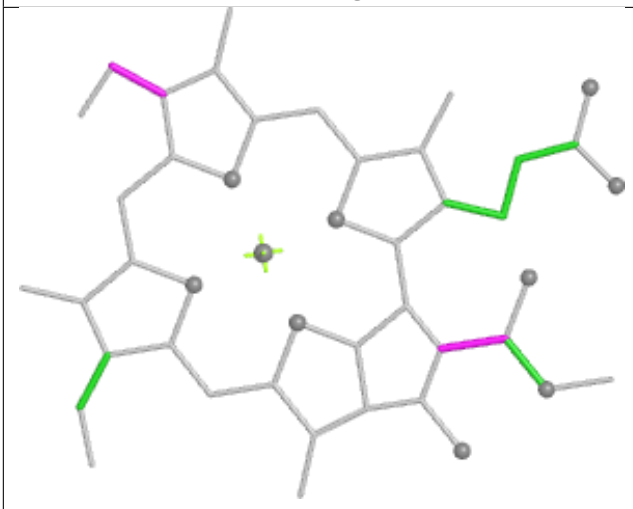
Ligand CLA 5 605



Bond lengths



Bond angles

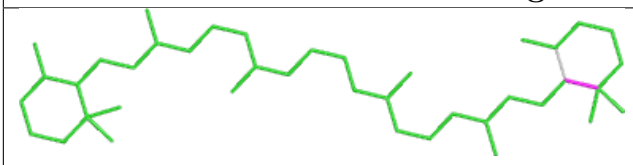


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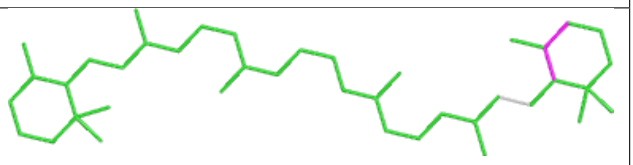


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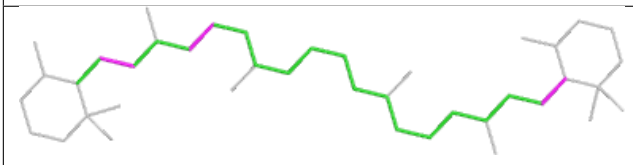
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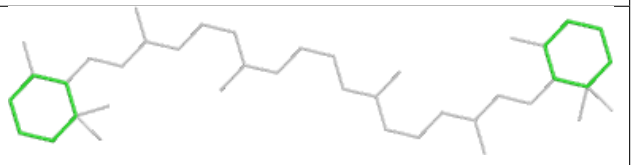
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Bond angles

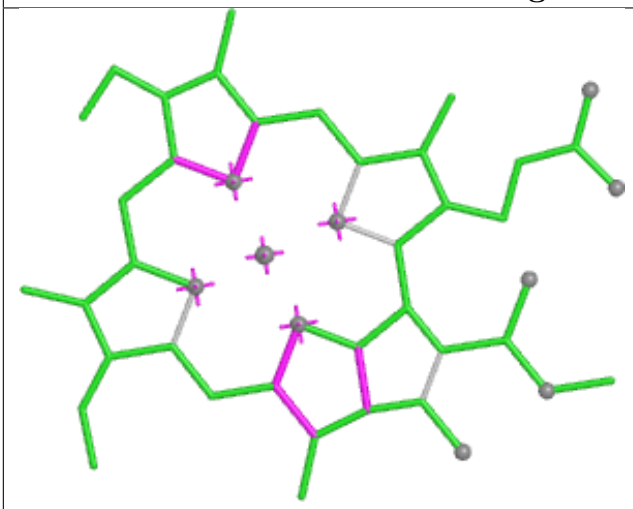


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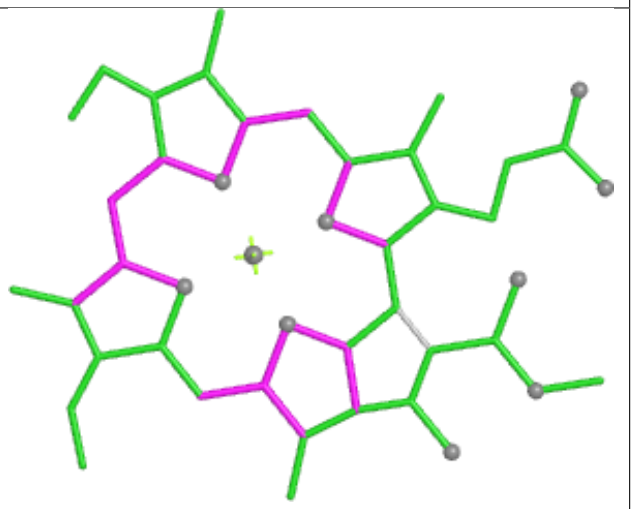


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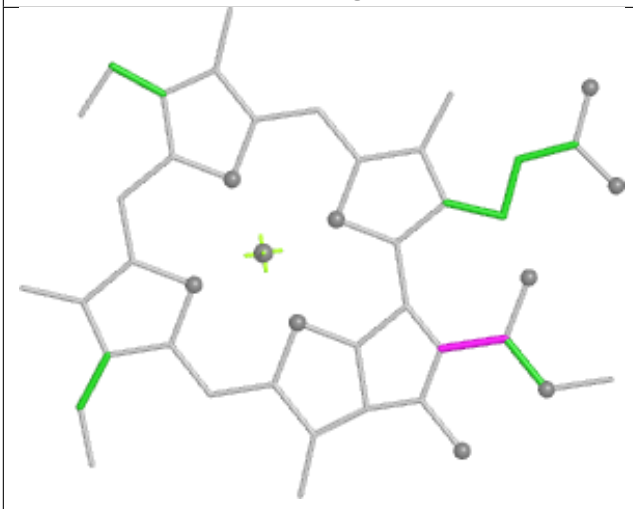
Ligand CLA 2 606



Bond lengths



Bond angles

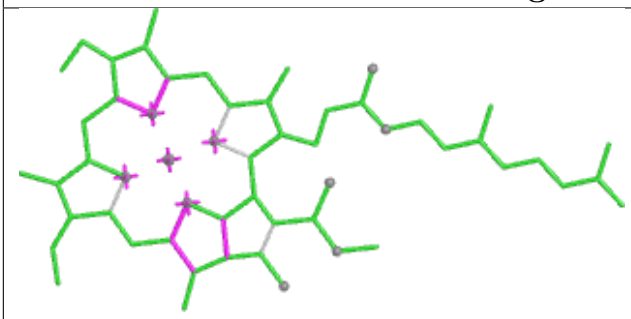


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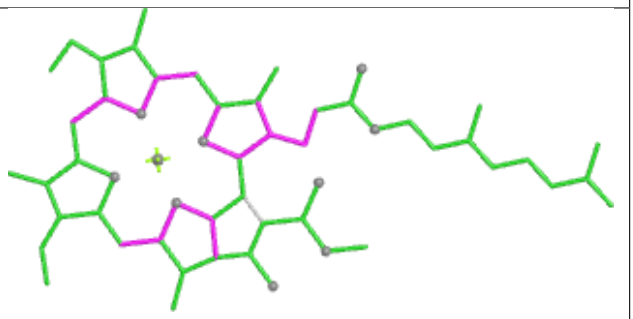


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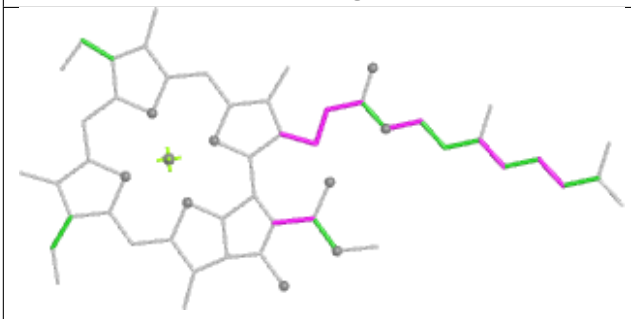
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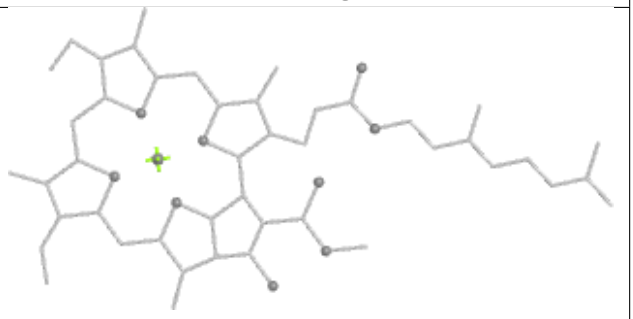
Bond lengths



Bond angles

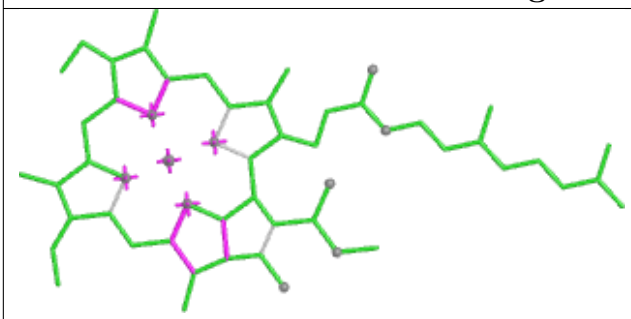


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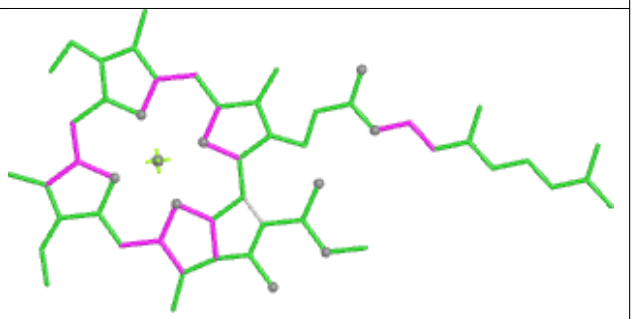


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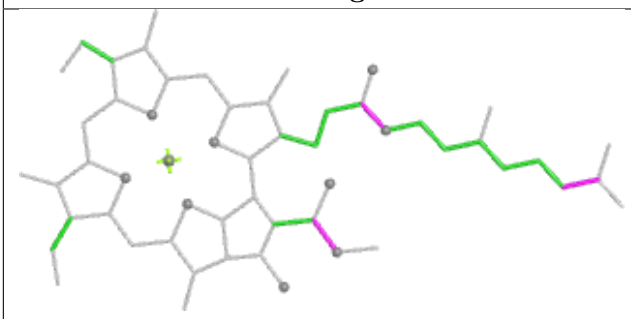
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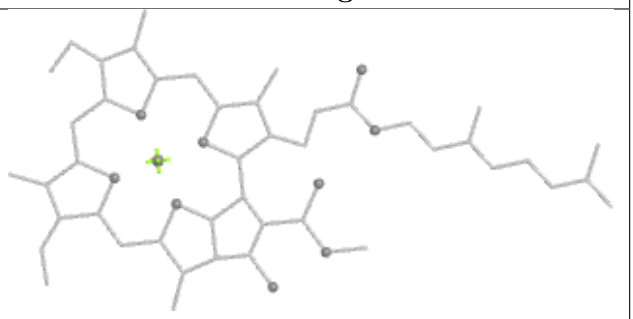
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Bond angles

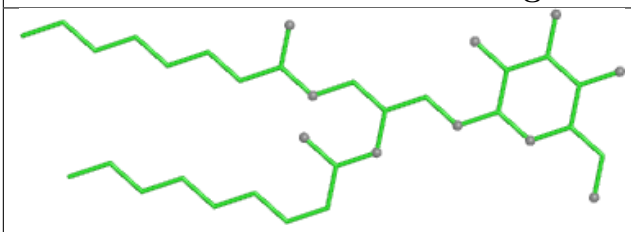


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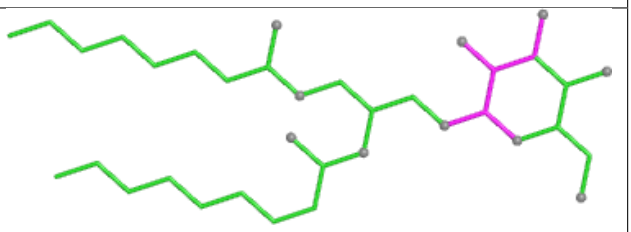


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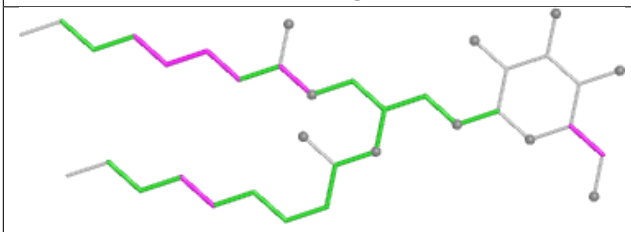
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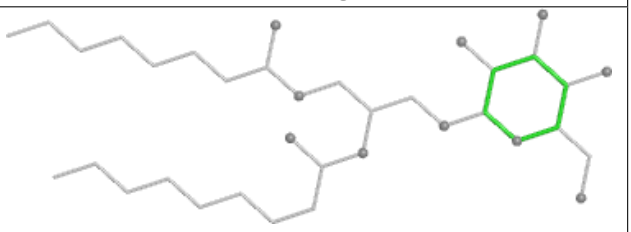
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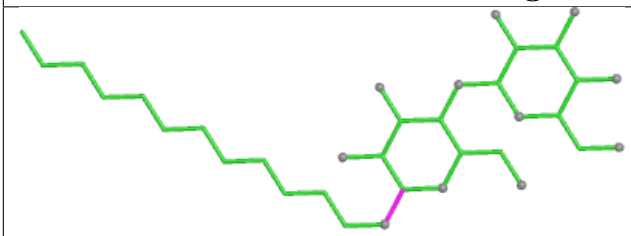


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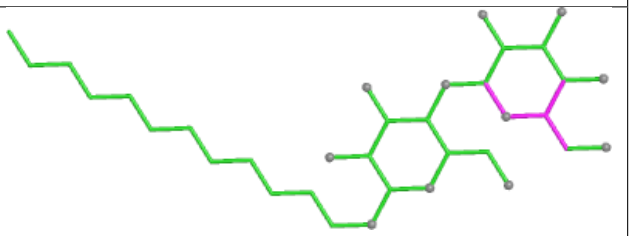


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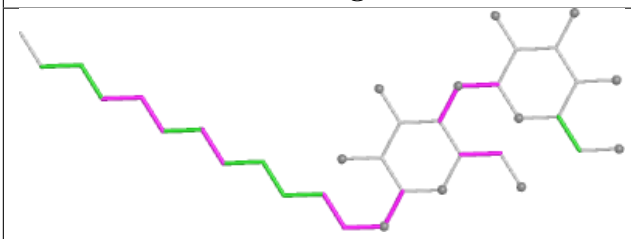
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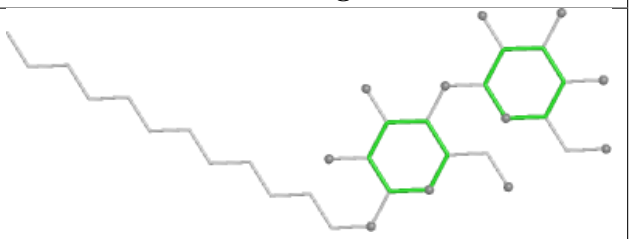
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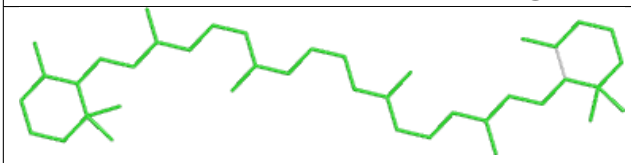


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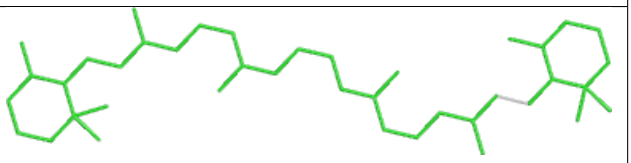


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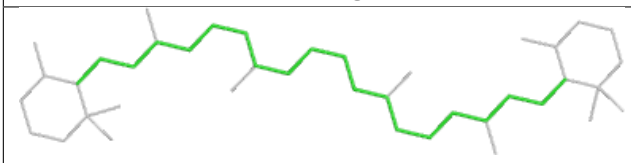
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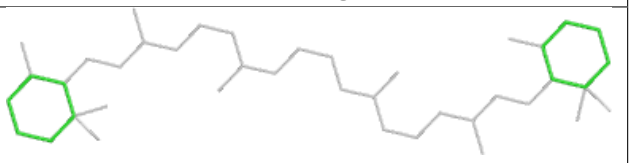
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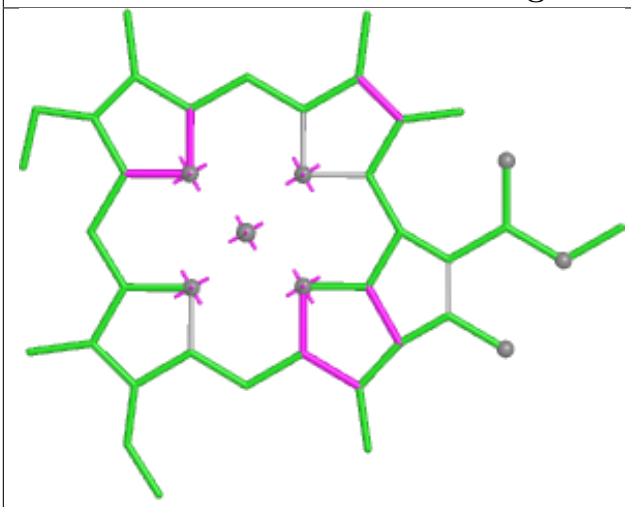


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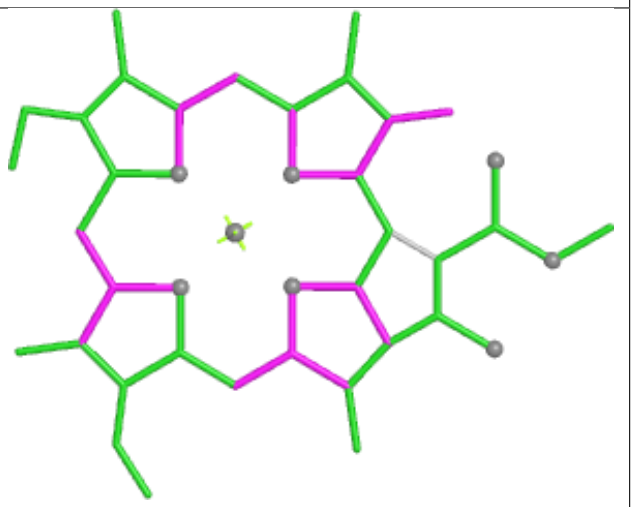


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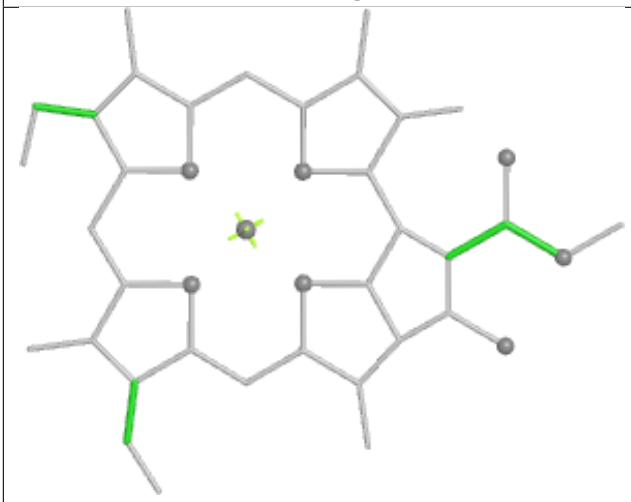
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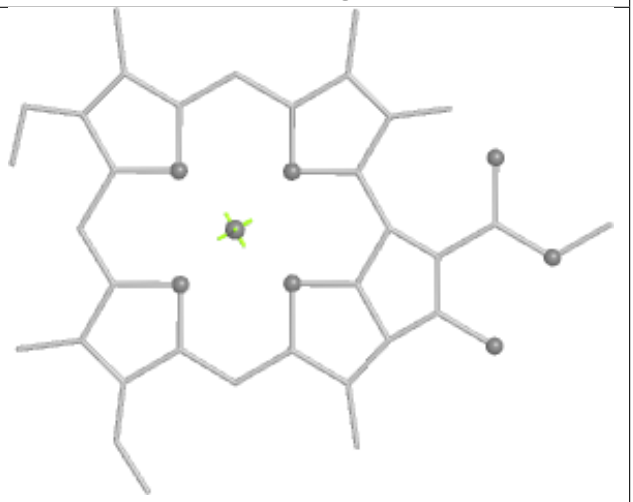
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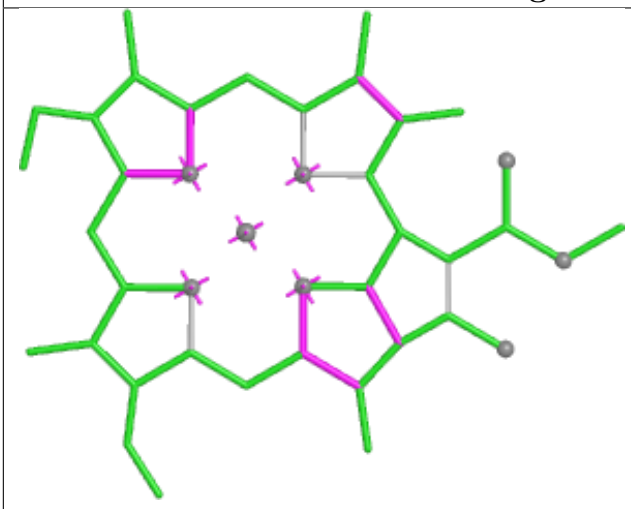


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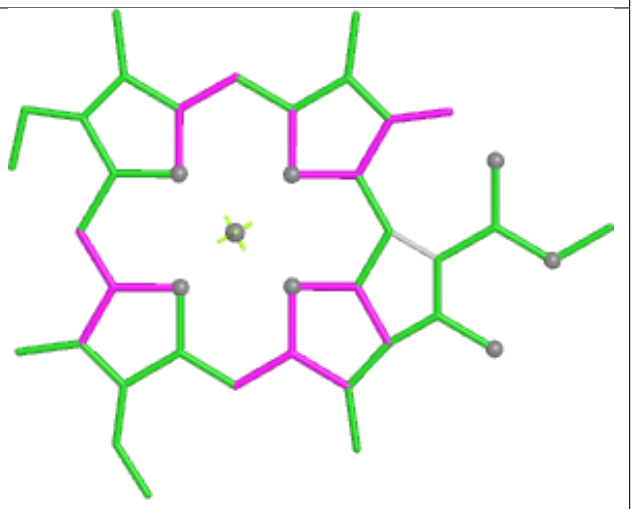


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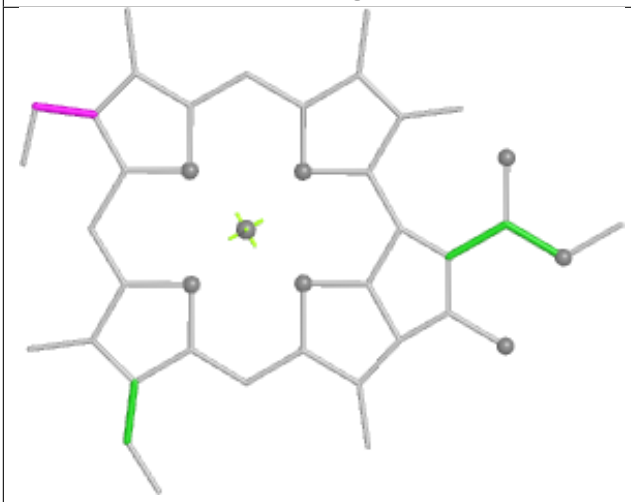
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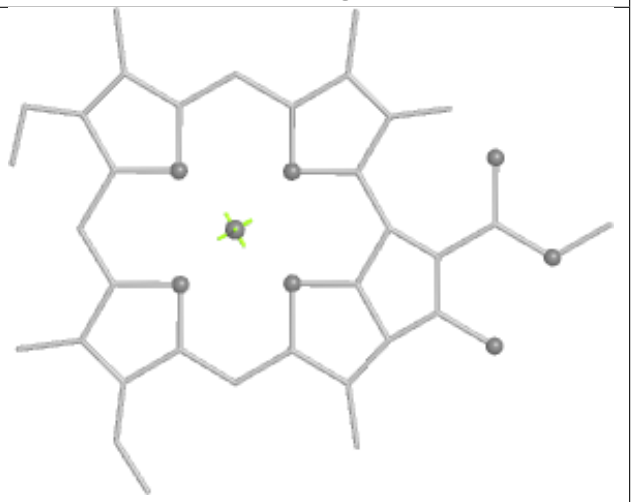
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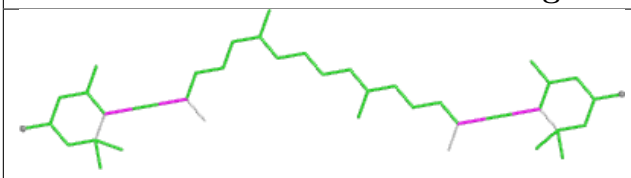


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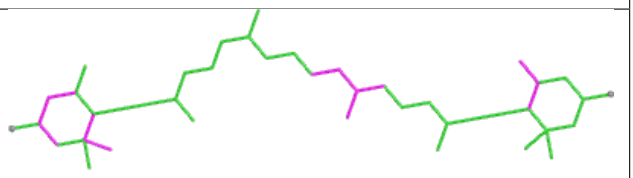


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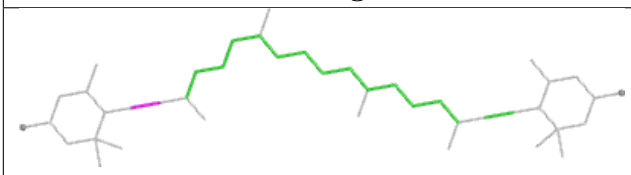
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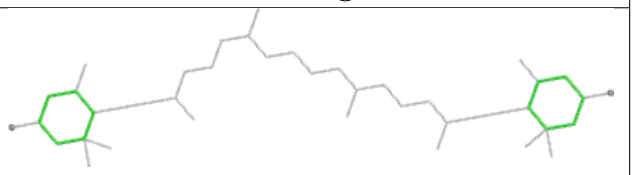
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Bond angles

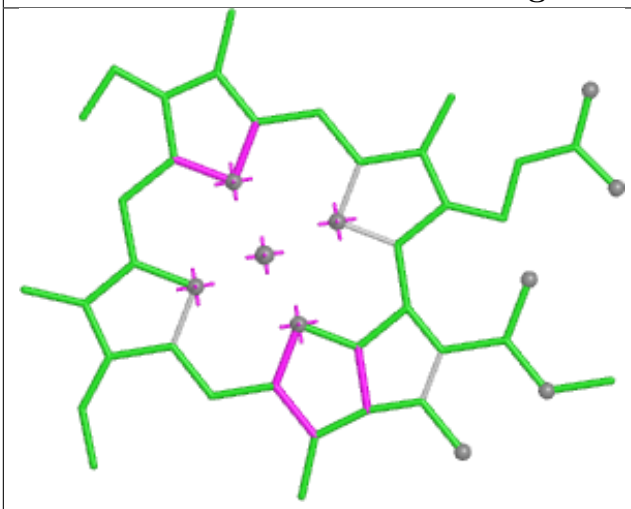


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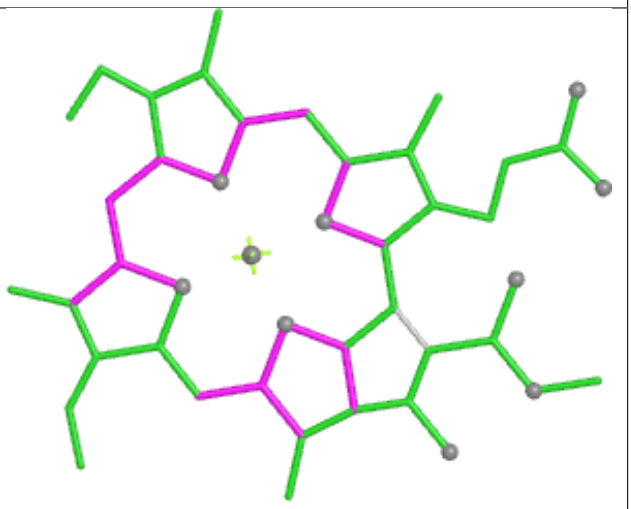


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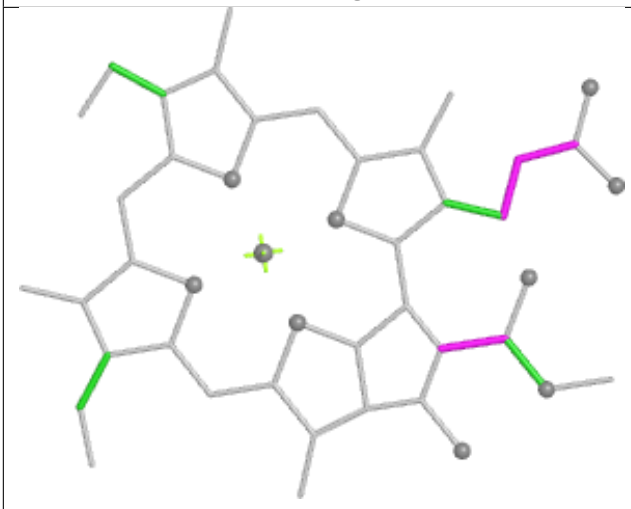
Ligand CLA 9 603



Bond lengths



Bond angles

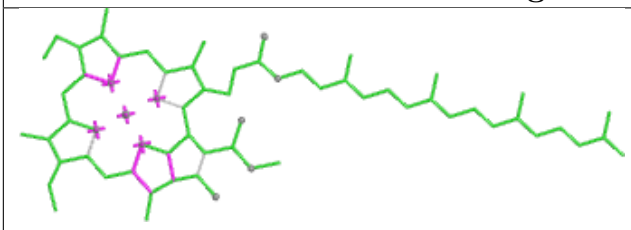


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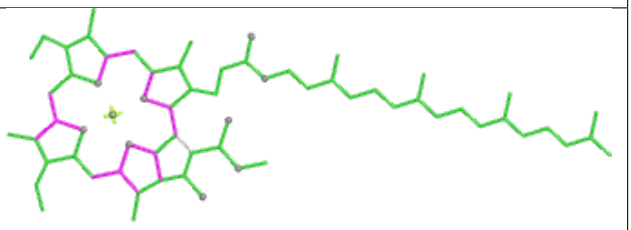


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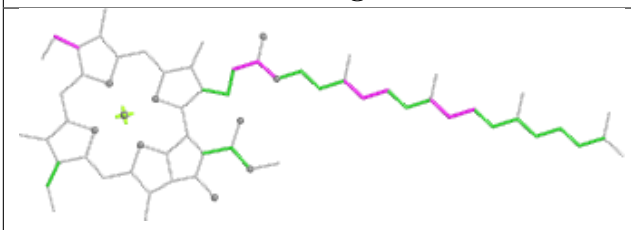
Ligand CLA b 608



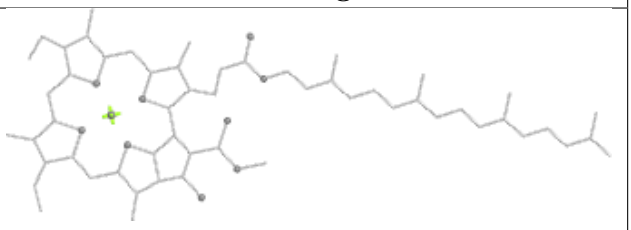
Bond lengths



Bond angles

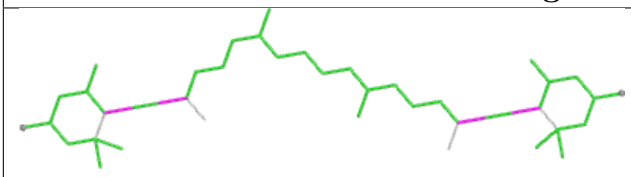


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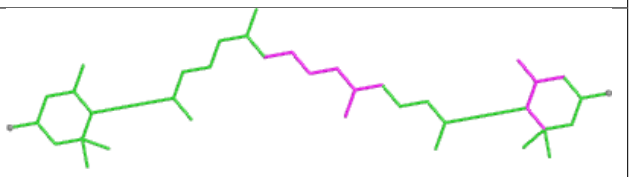


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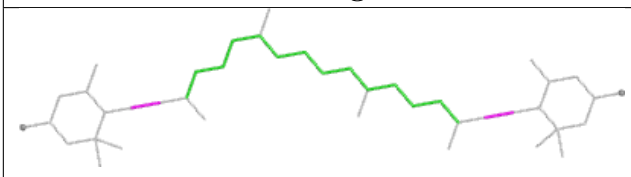
Ligand II0 9 617



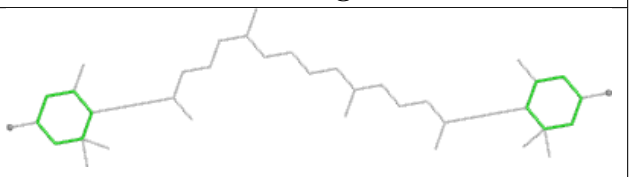
Bond lengths



Bond angles

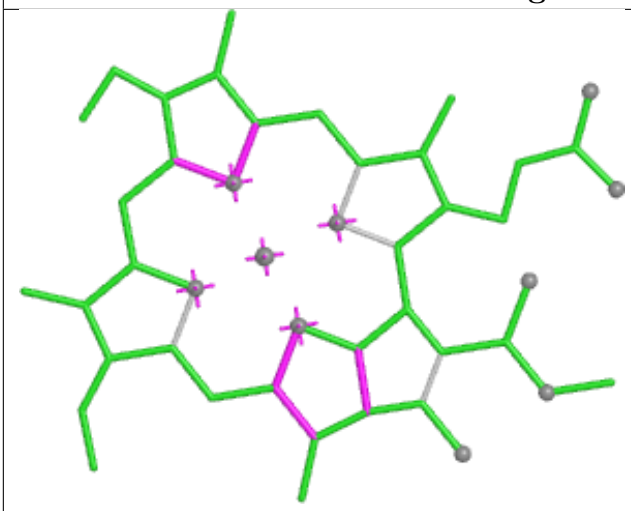


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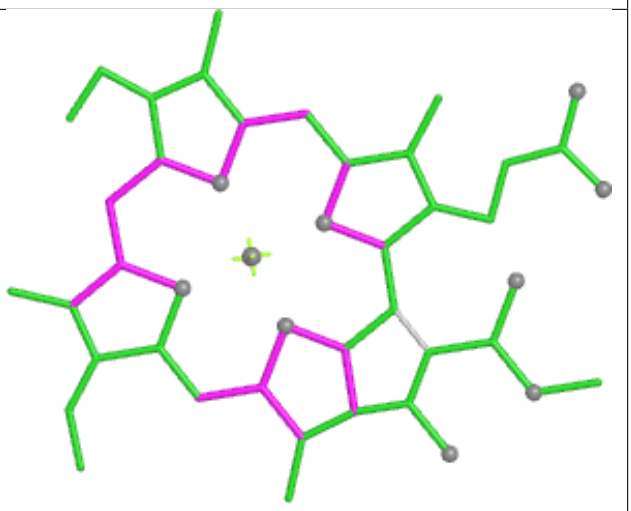


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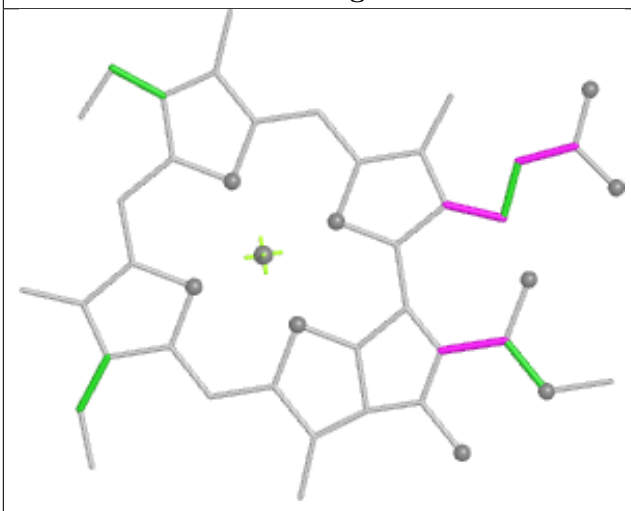
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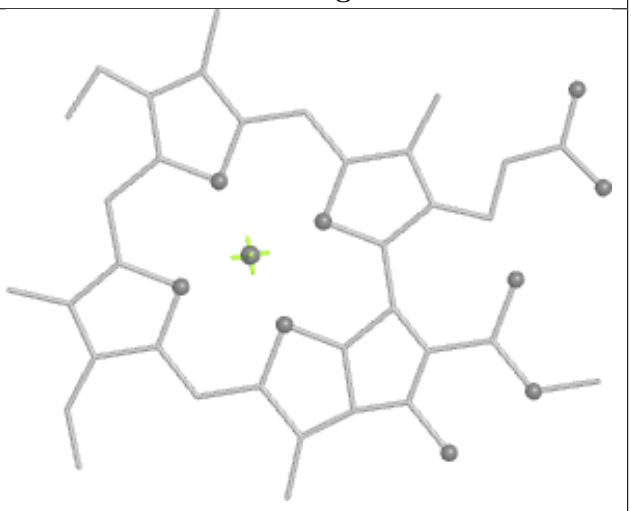
Bond lengths



Bond angles

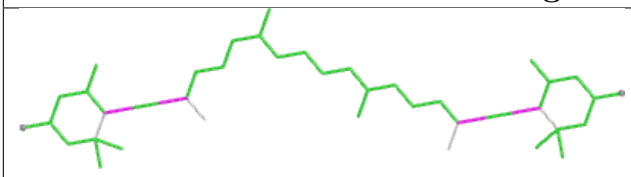


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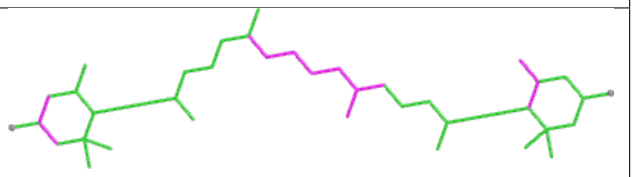


Rings

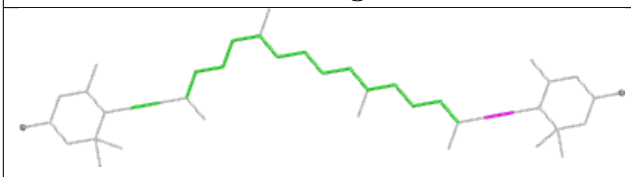
Ligand II0 a 614



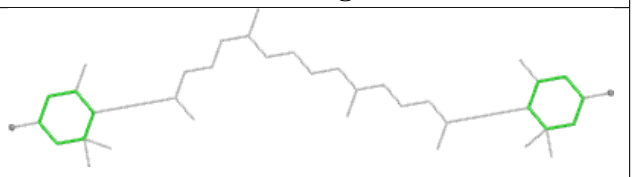
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Bond angles

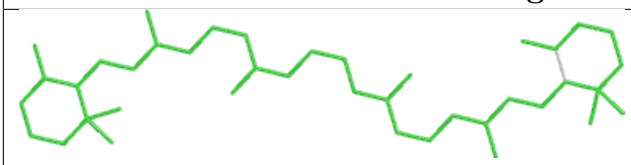


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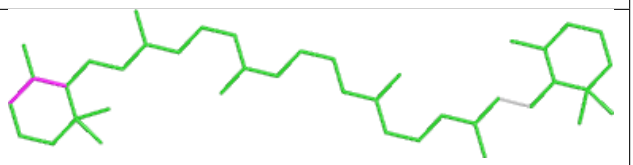


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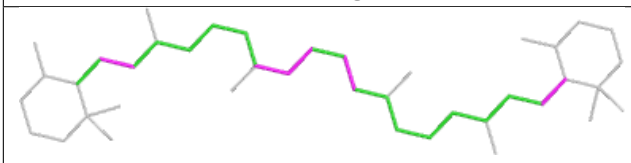
Ligand 8CT A 852



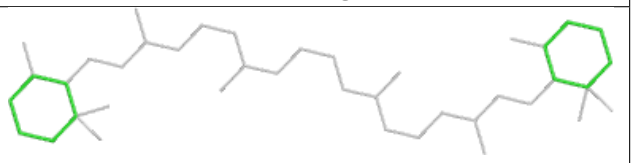
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Bond angles

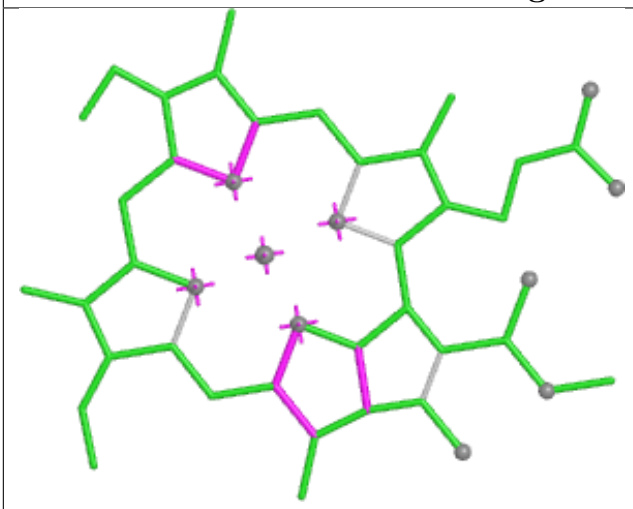


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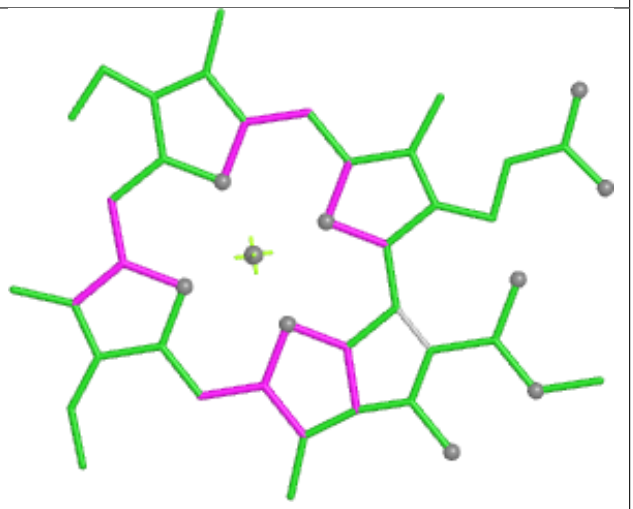


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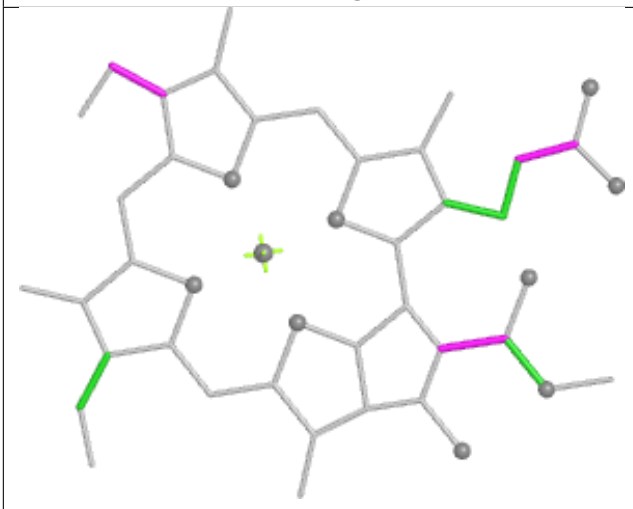
Ligand CLA 5 611



Bond lengths



Bond angles

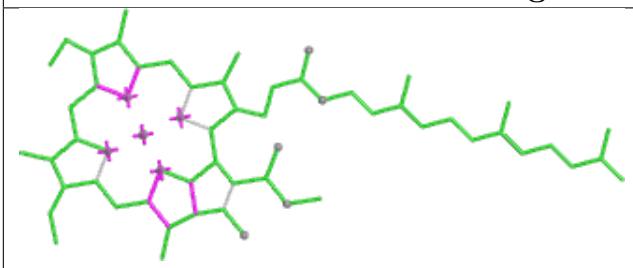


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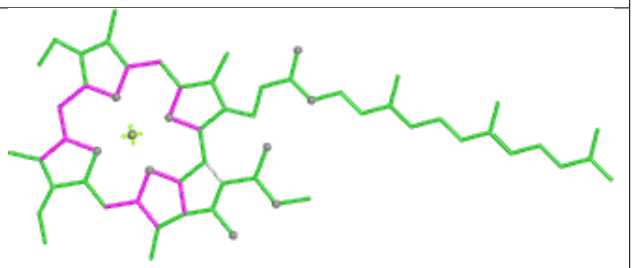


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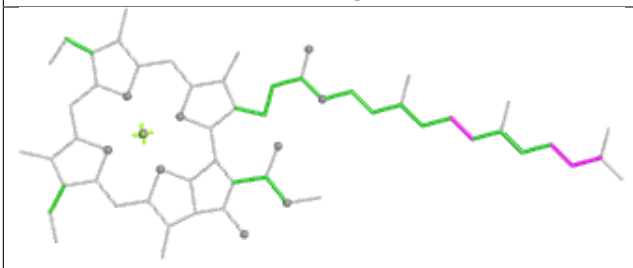
Ligand CLA 3 603



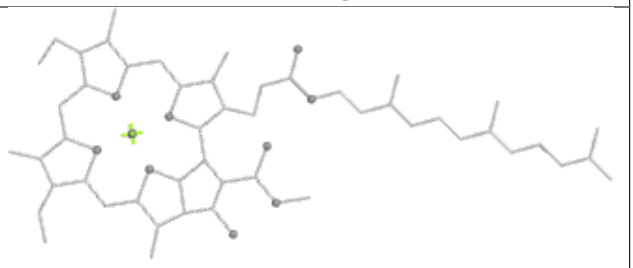
Bond lengths



Bond angles

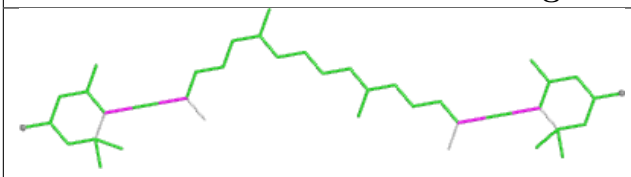


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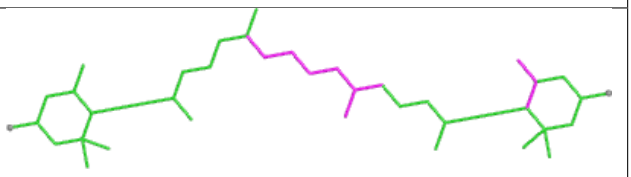


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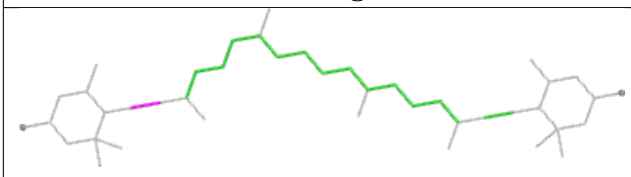
Ligand II0 8 612



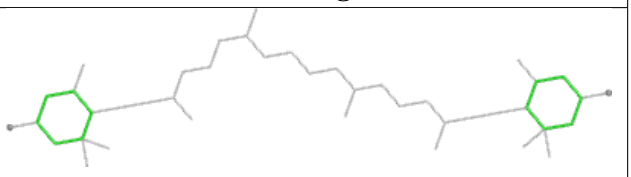
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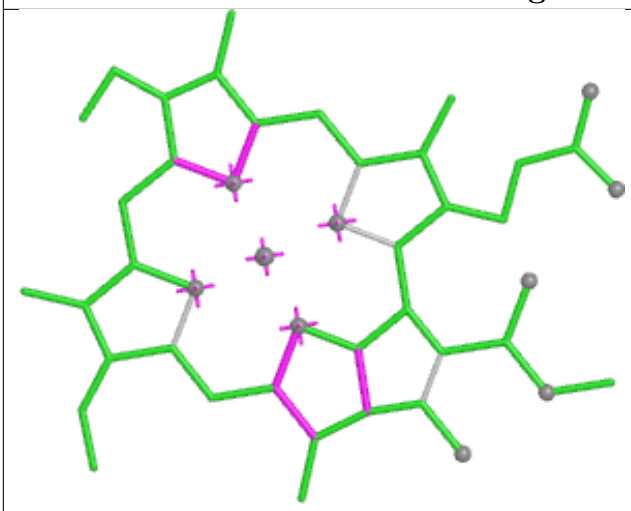


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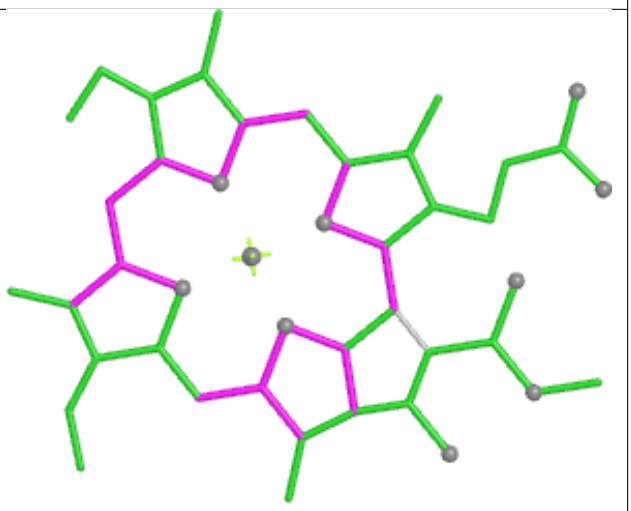


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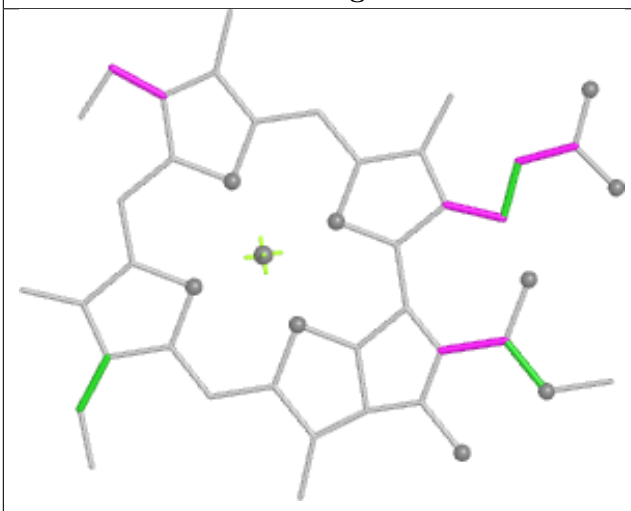
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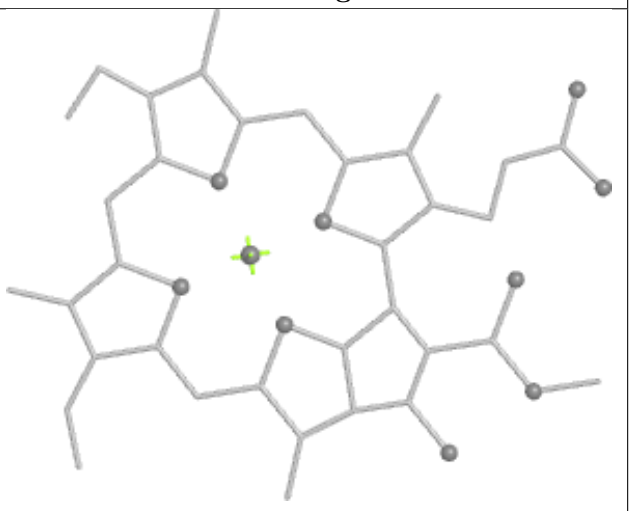
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Bond angles

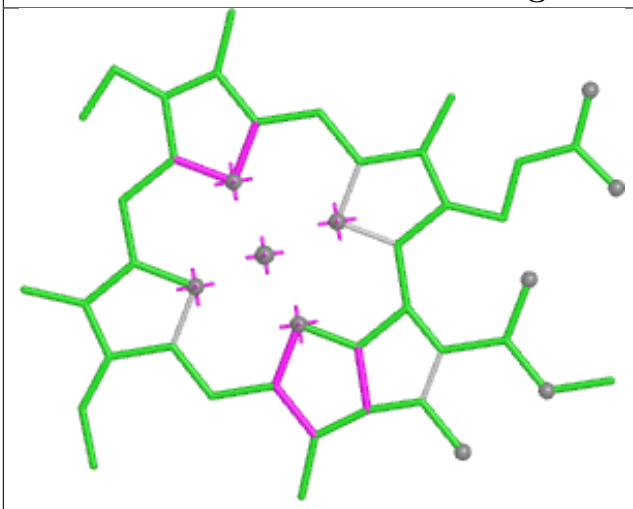


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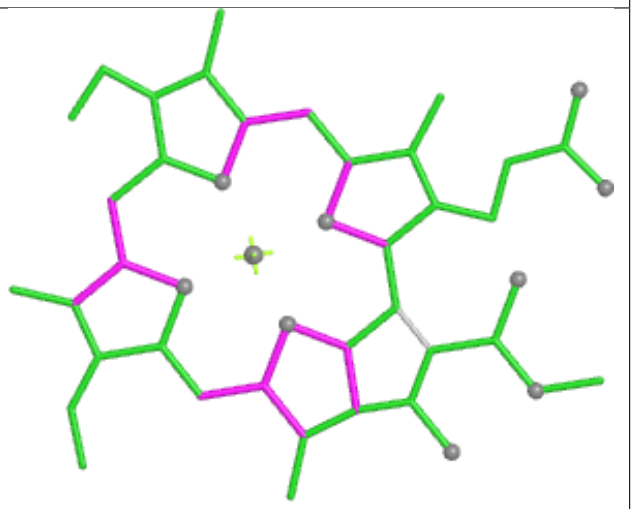


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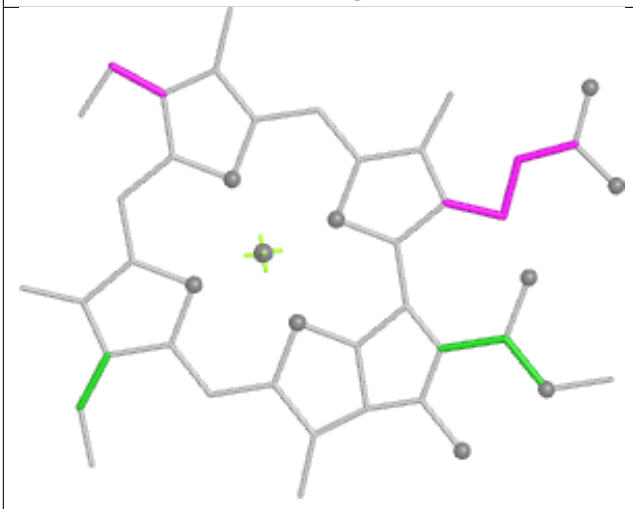
Ligand CLA 6 603



Bond lengths



Bond angles

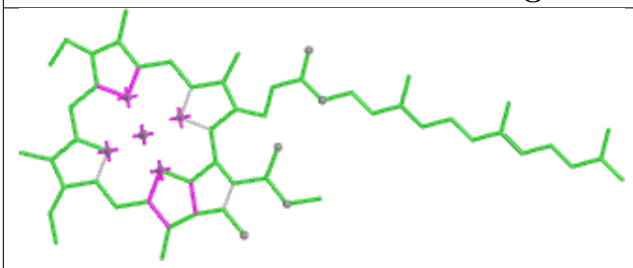


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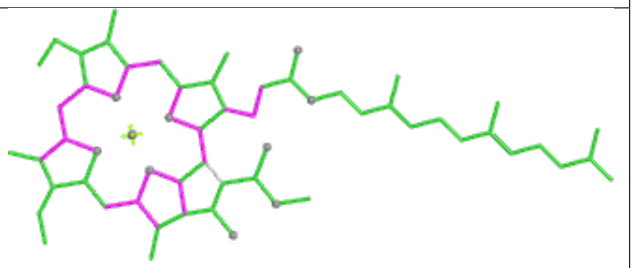


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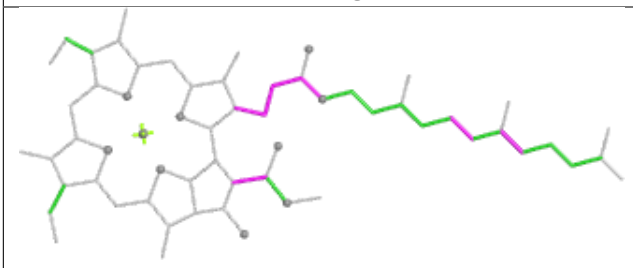
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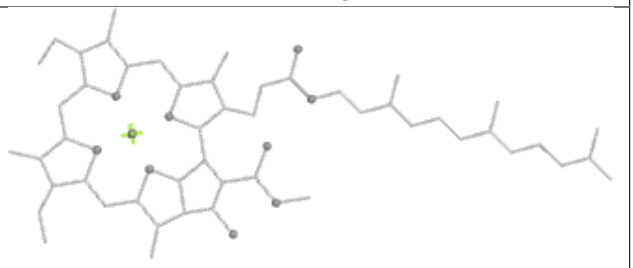
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Bond angles

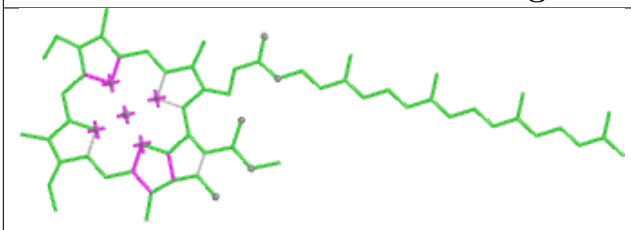


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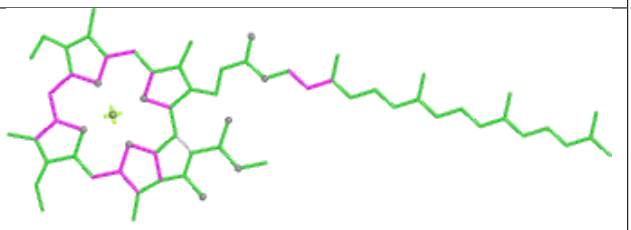


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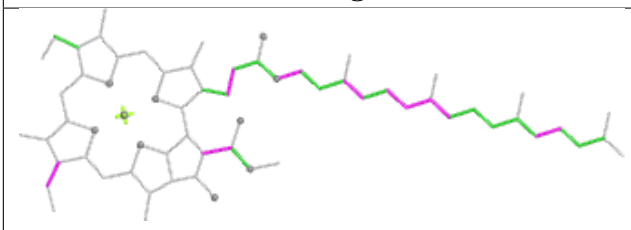
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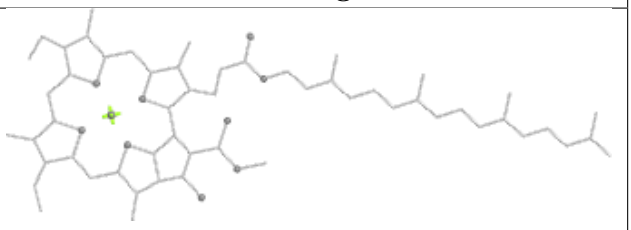
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Bond angles

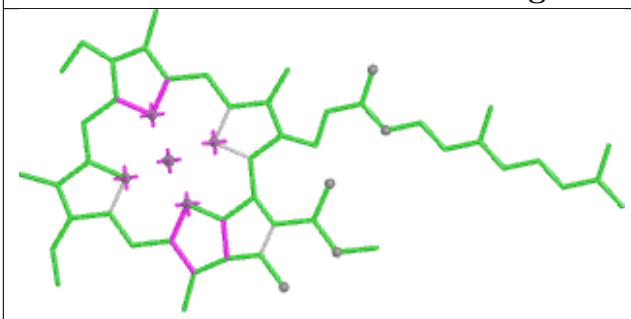


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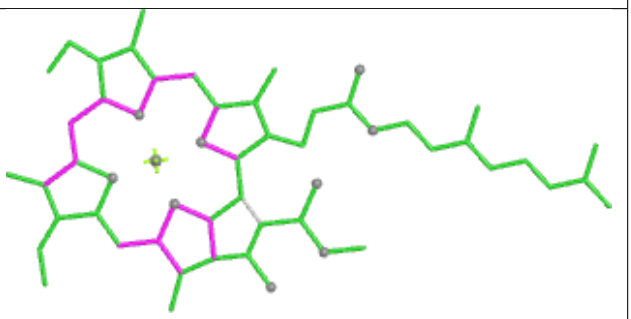


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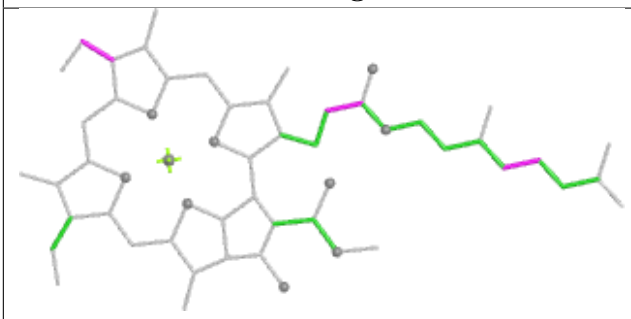
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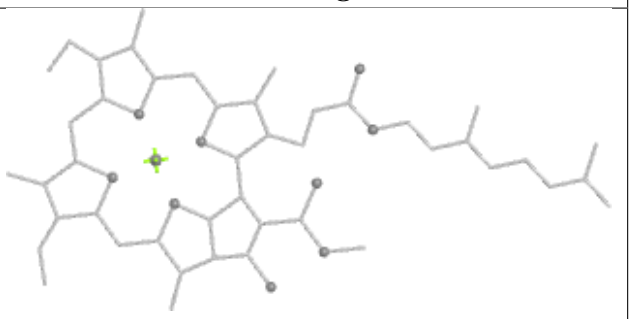
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Bond angles

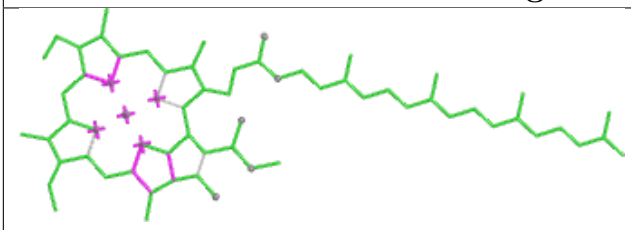


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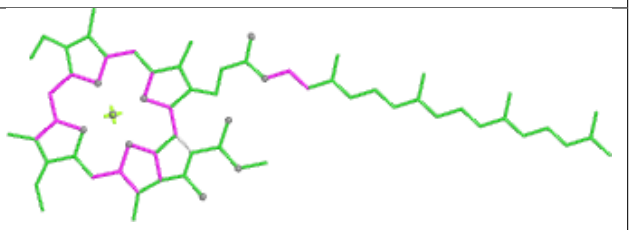


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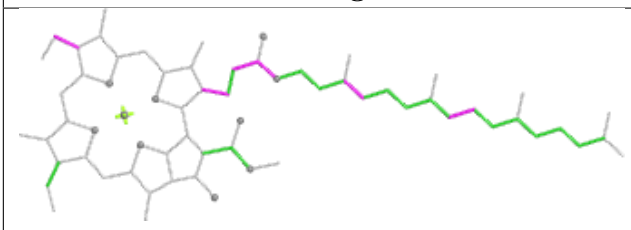
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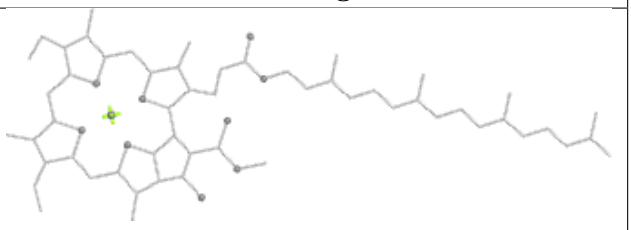
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Bond angles

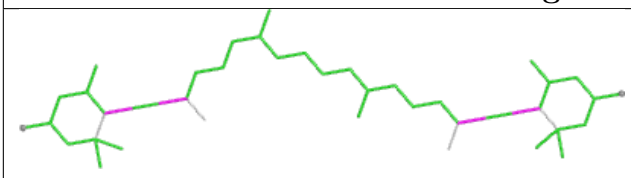


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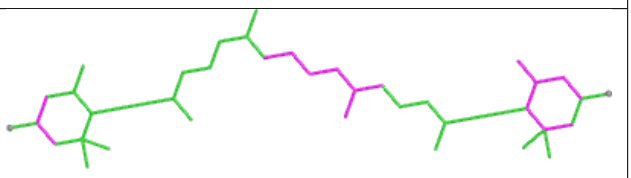


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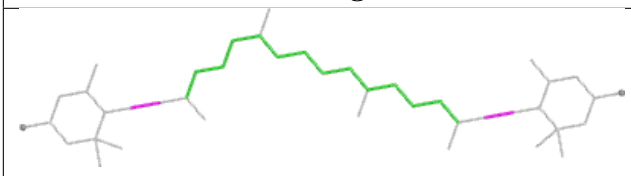
Ligand II0 9 615



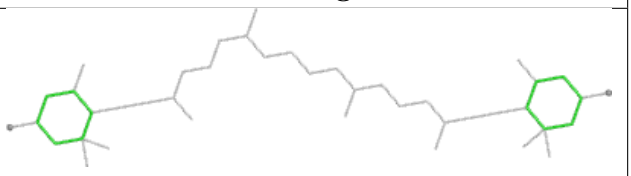
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Bond angles



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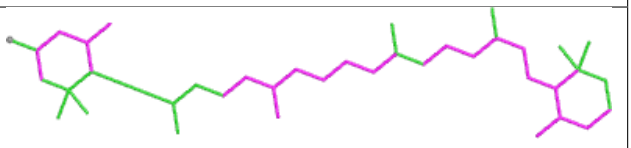


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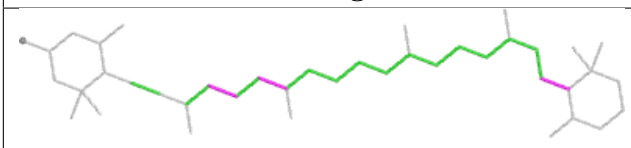
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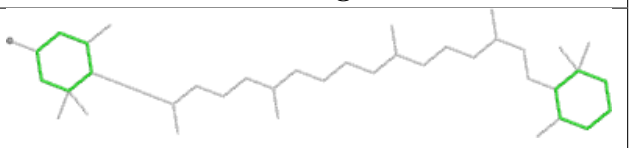
Bond lengths



Bond angles

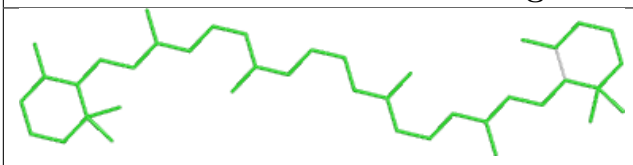


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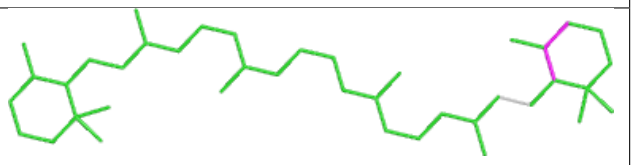


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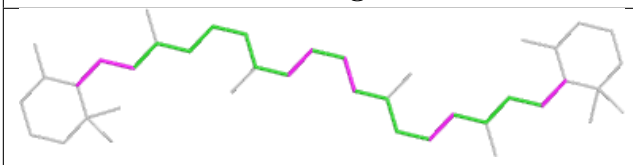
Ligand 8CT A 847



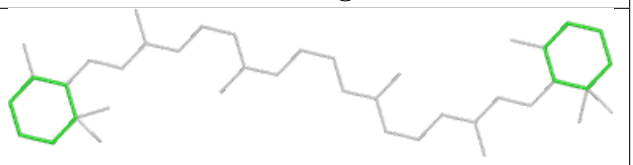
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Bond angles

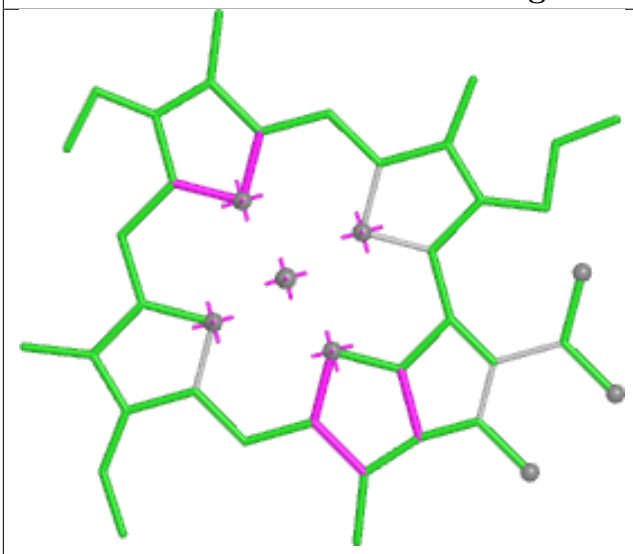


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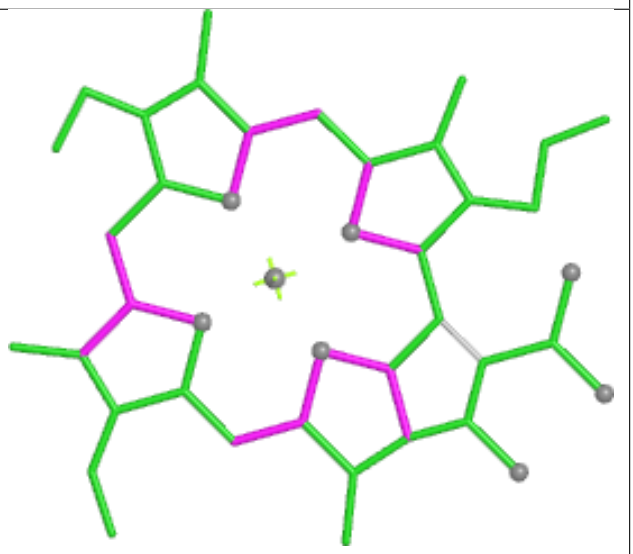


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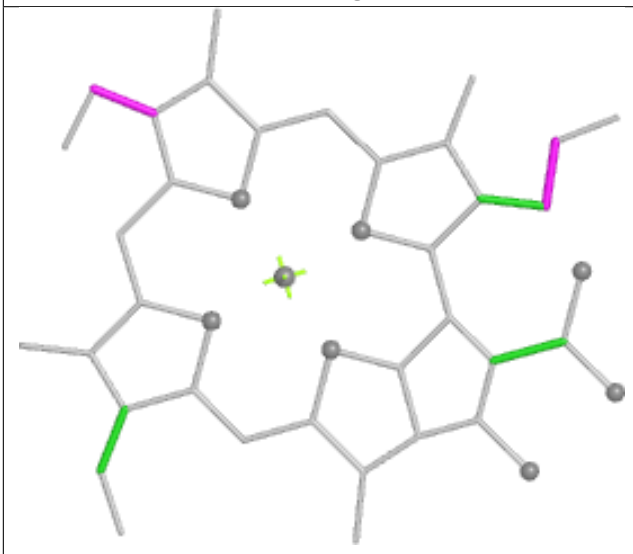
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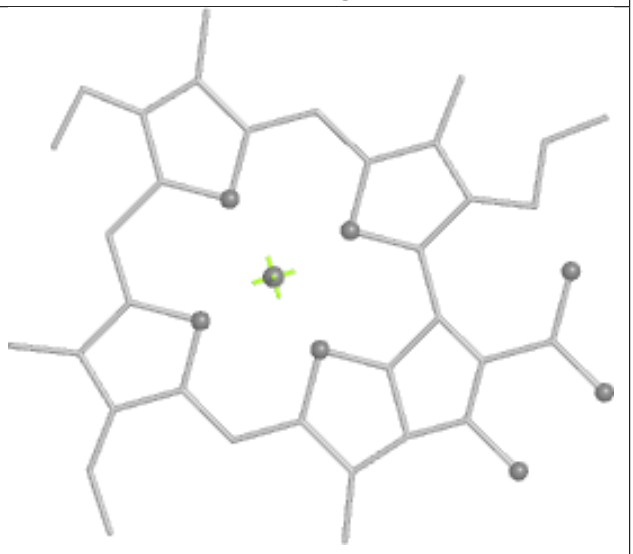
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Bond angles

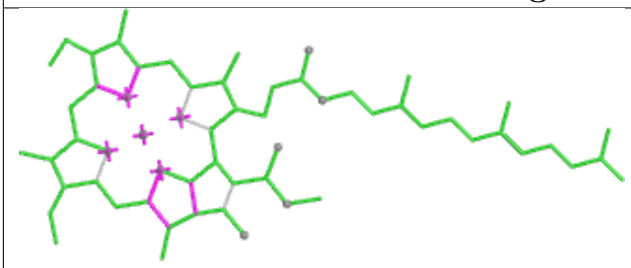


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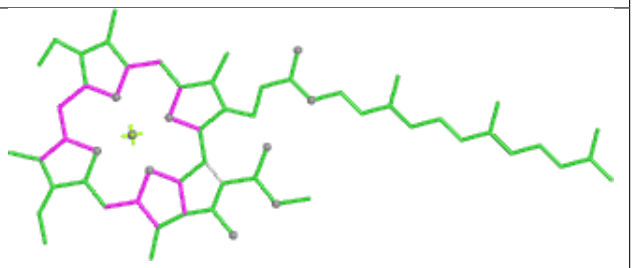


Rings

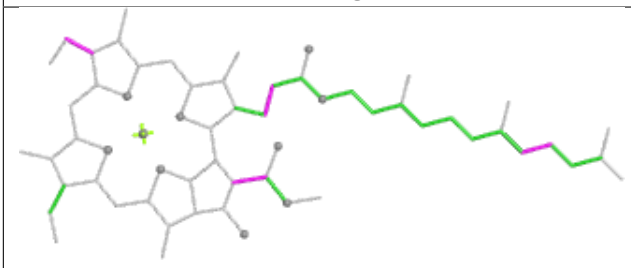
Ligand CLA c 604



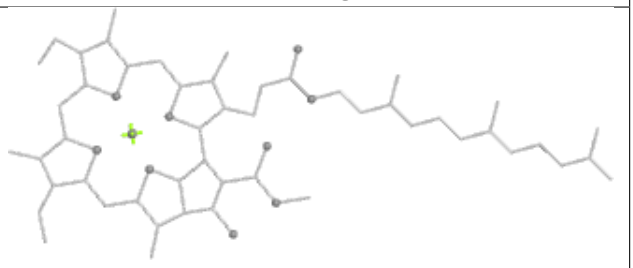
Bond lengths



Bond angles

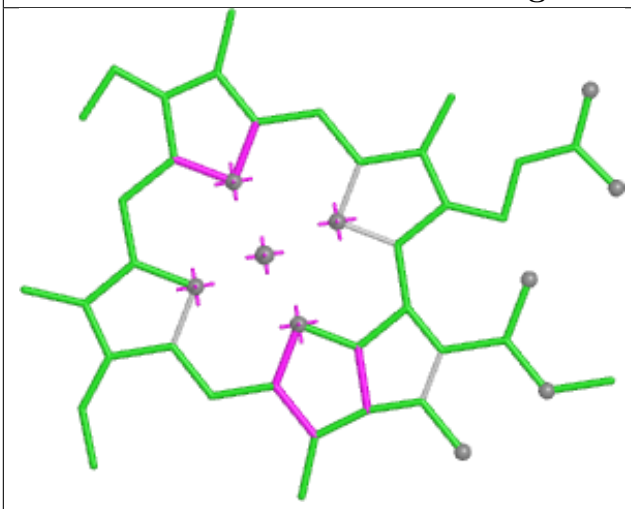


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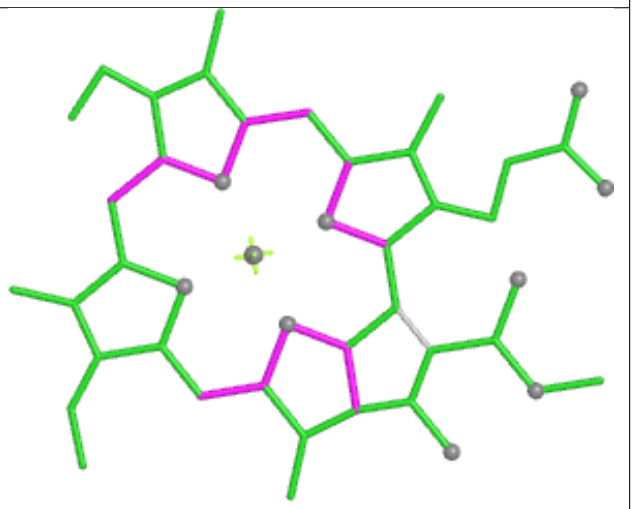


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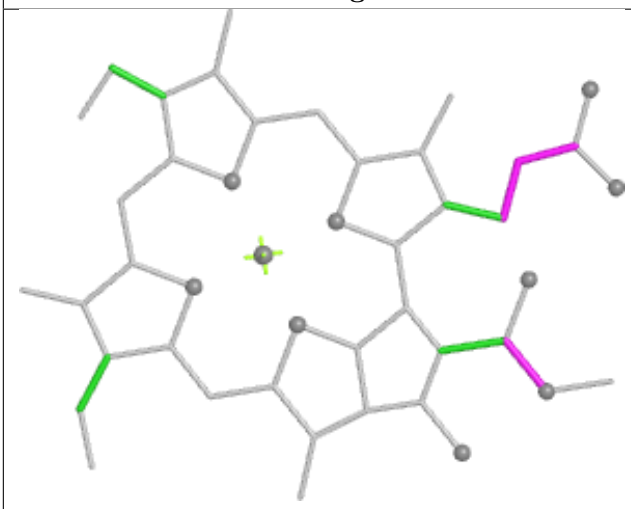
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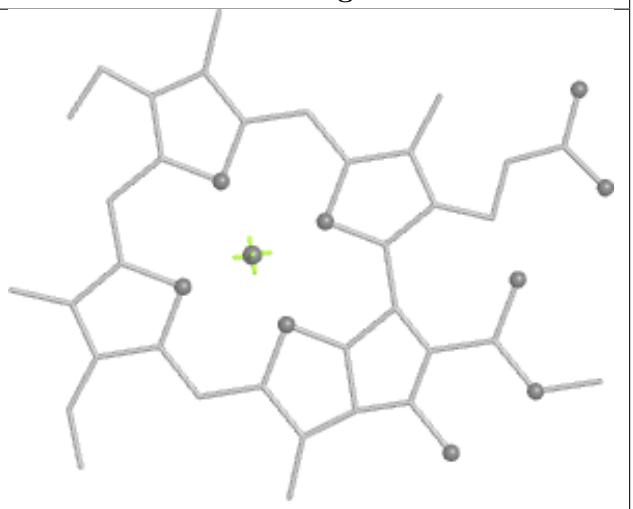
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Bond angles

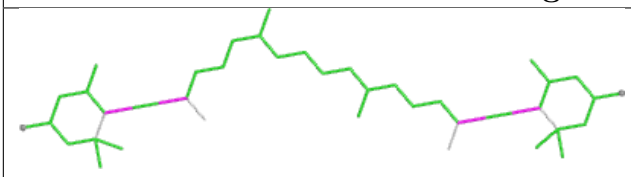


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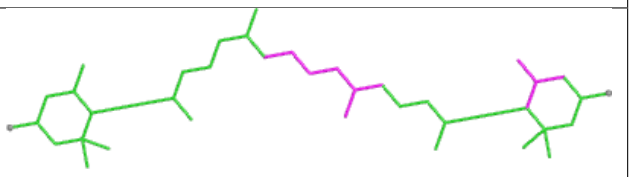


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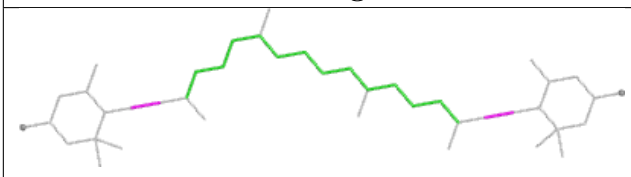
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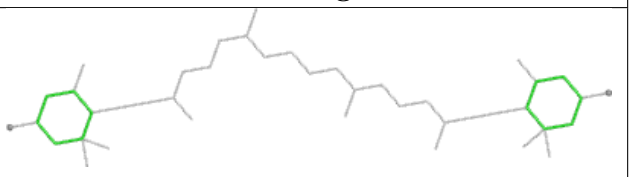
Bond lengths



Bond angles

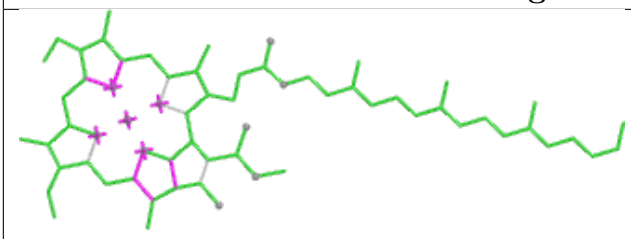


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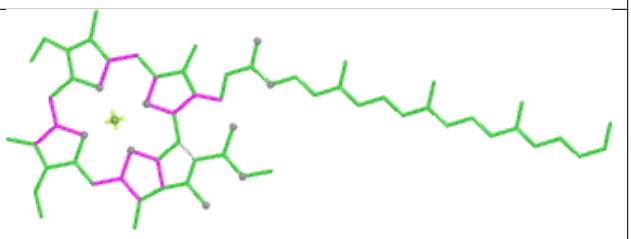


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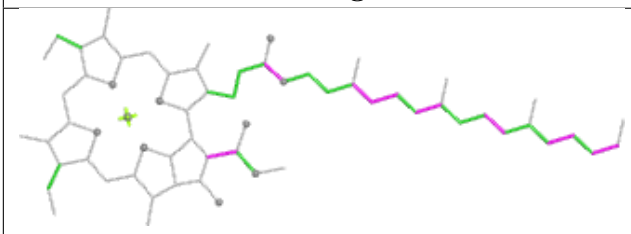
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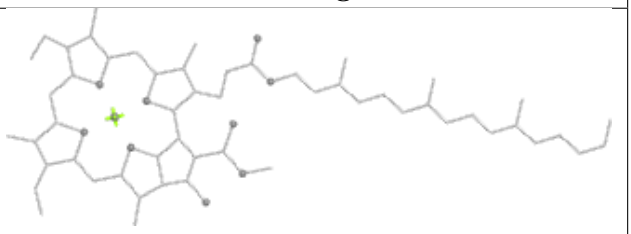
Bond lengths



Bond angles

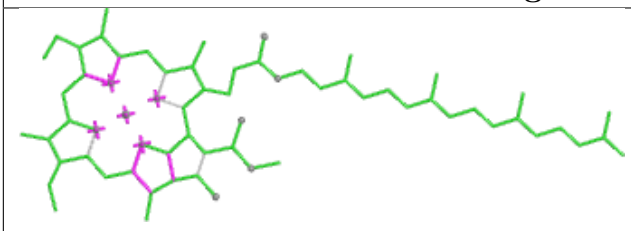


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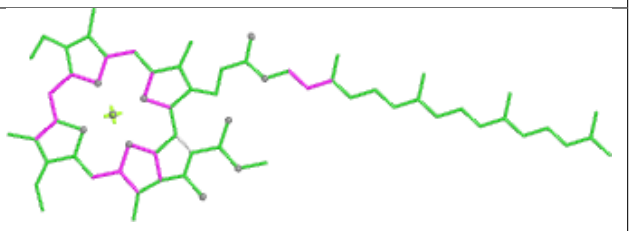


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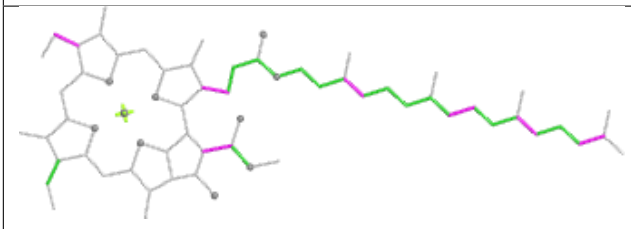
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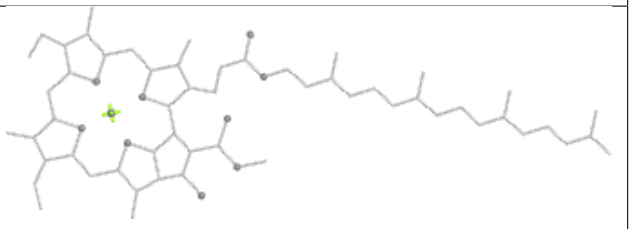
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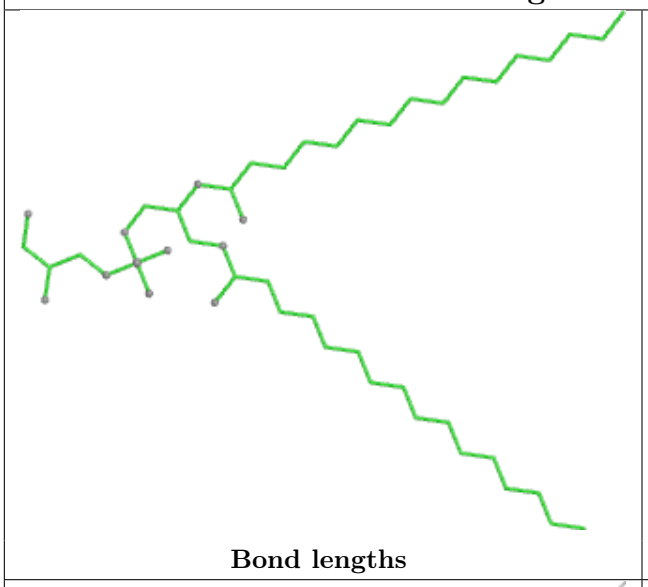


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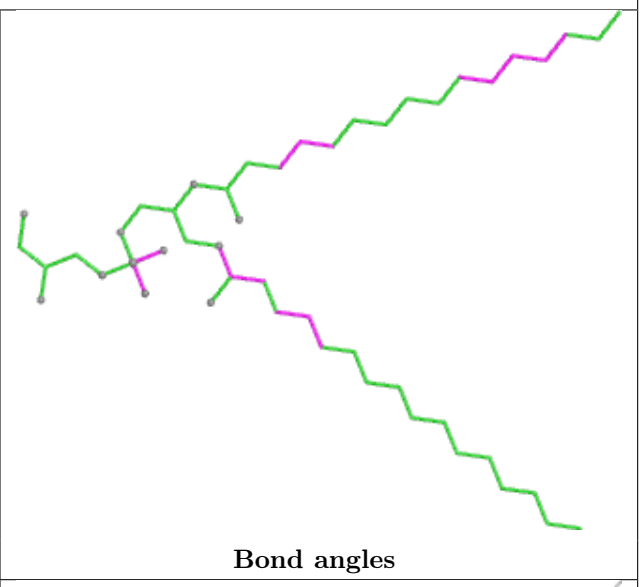


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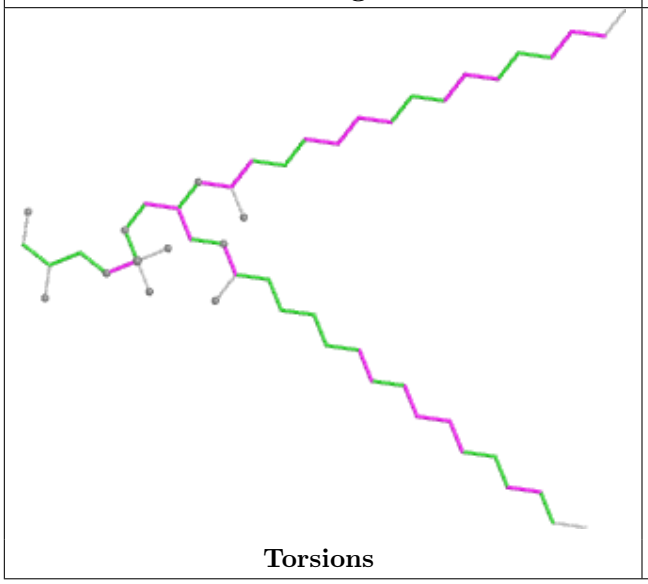
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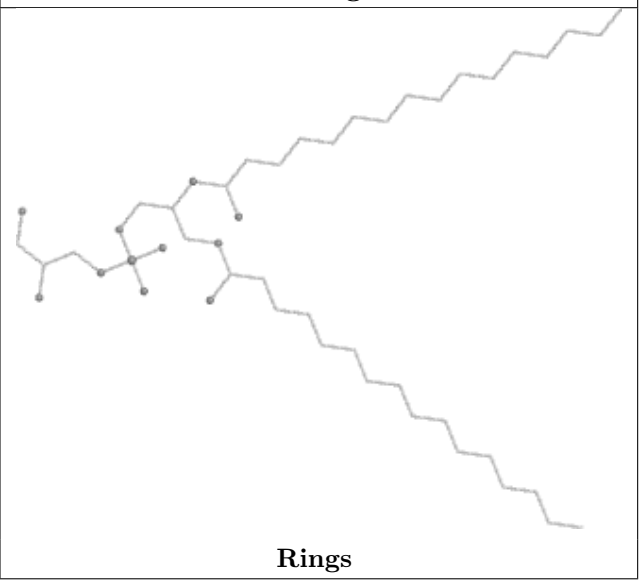
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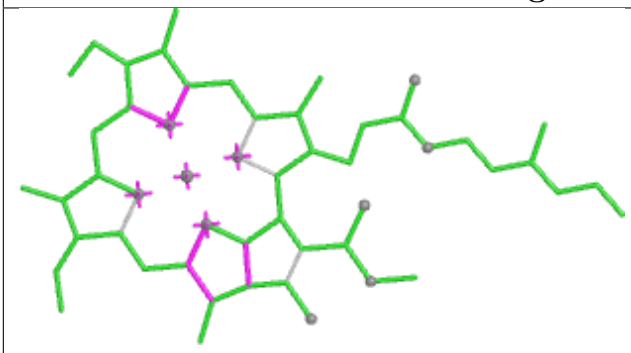


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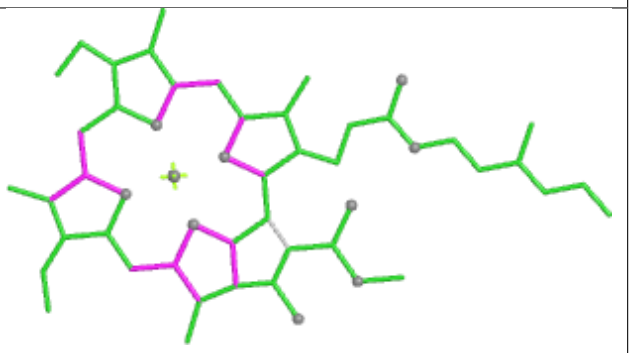


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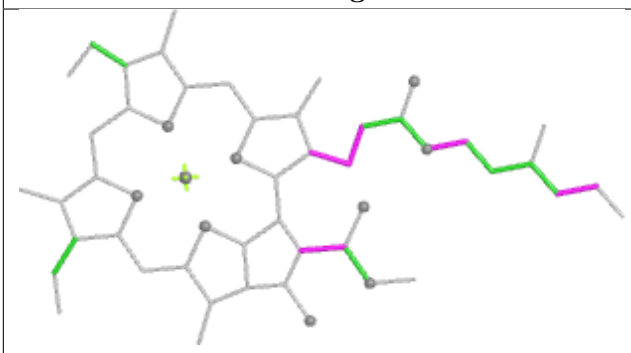
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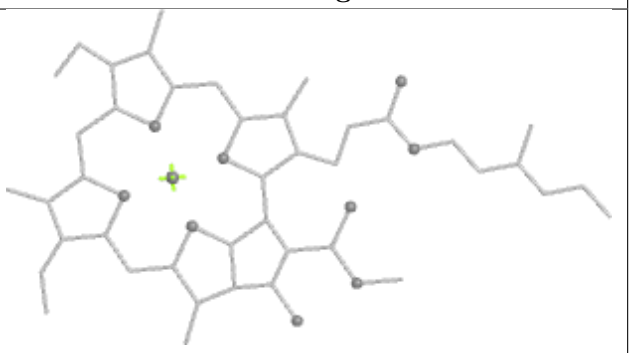
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Bond angles

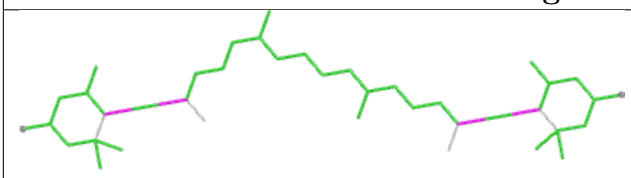


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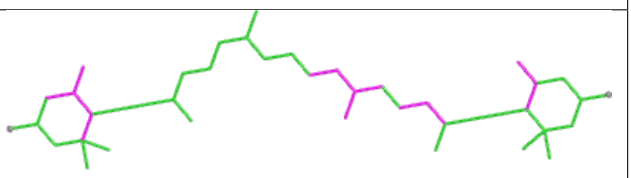


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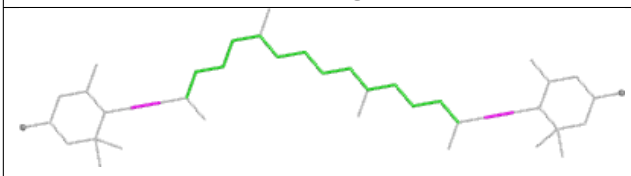
Ligand II0 5 617



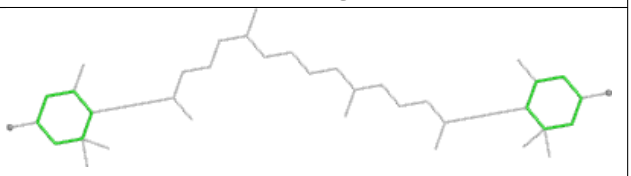
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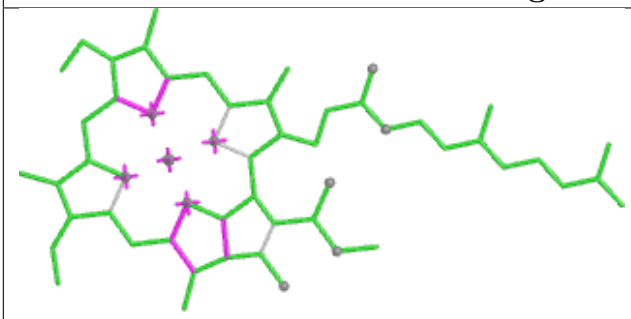
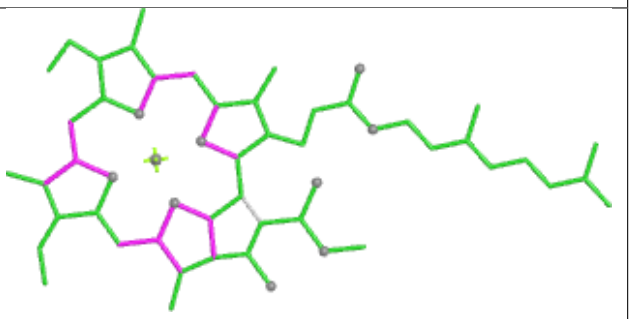
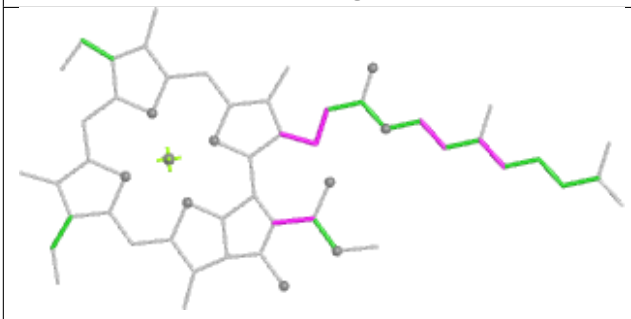
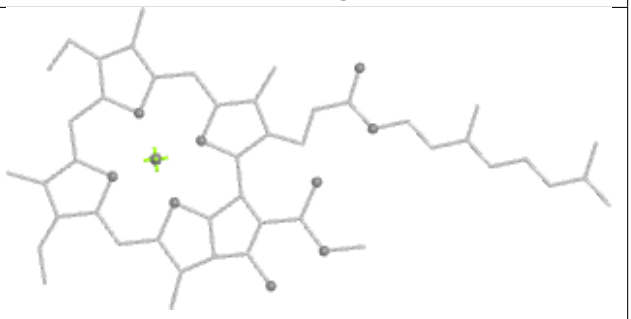
Bond angles

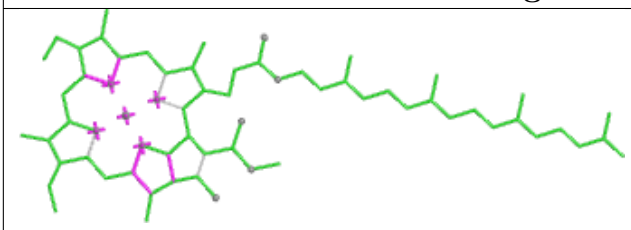
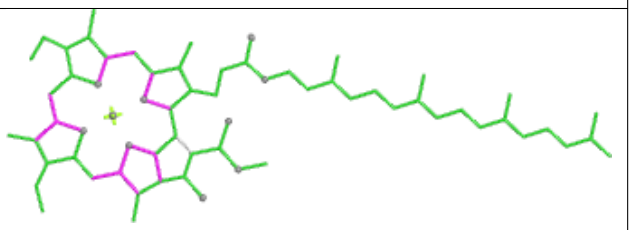
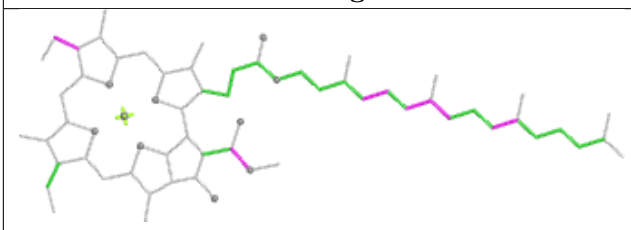
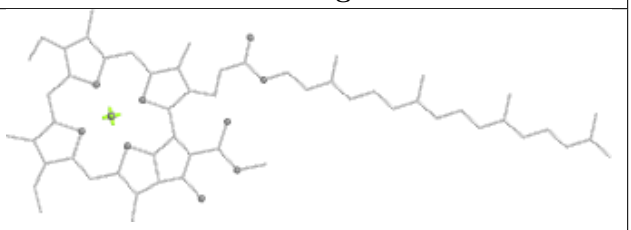


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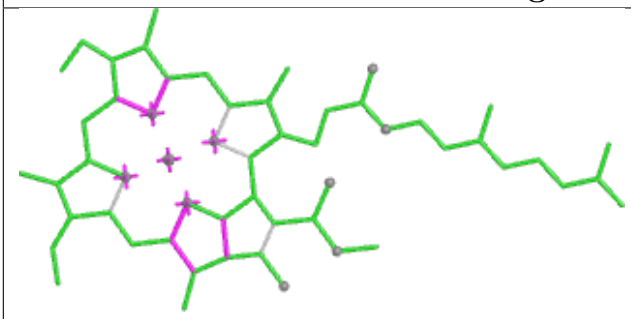


Rings

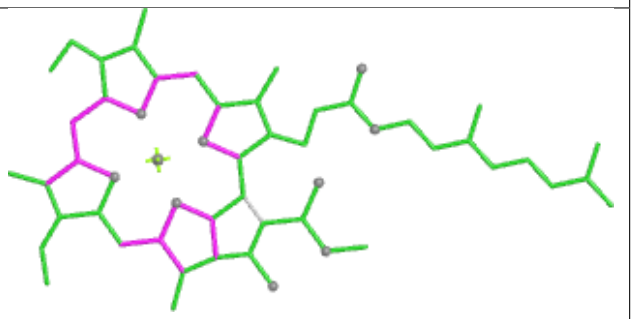
Ligand CLA 6 606	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 833	
	
Bond lengths	Bond angles
	
Torsions	Rings

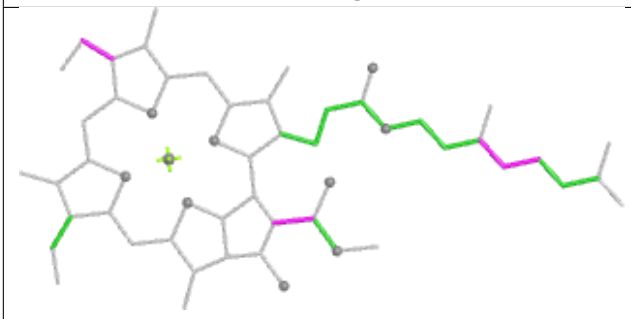
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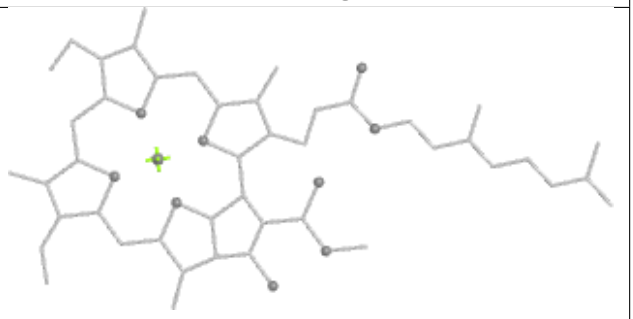
Bond lengths



Bond angles

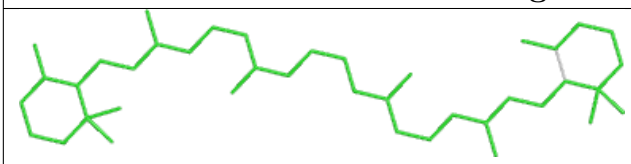


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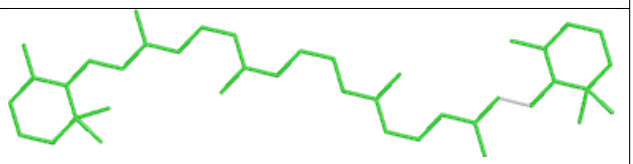


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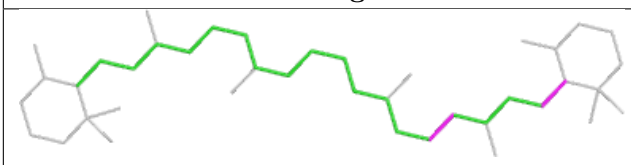
Ligand 8CT L 206



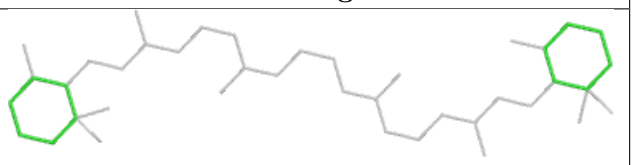
Bond lengths



Bond angles

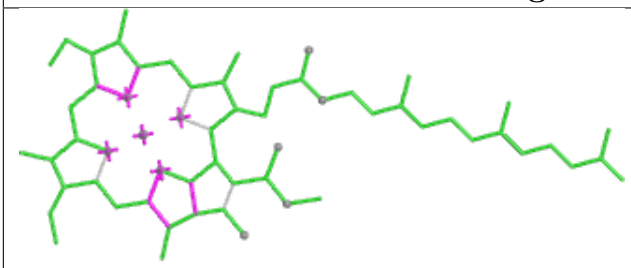


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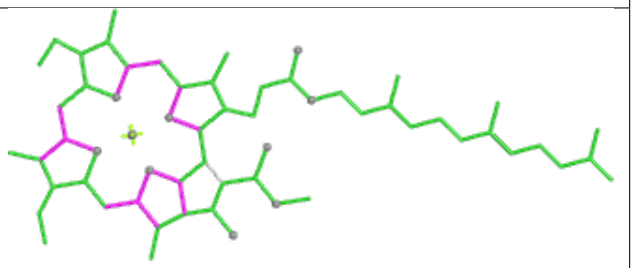


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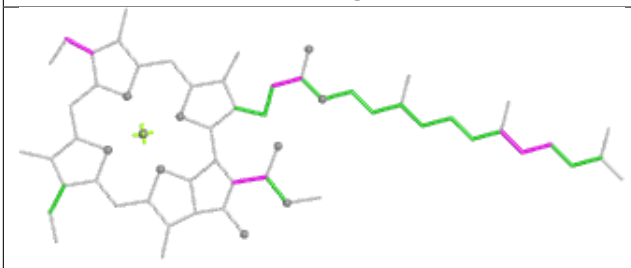
Ligand CLA 2 605



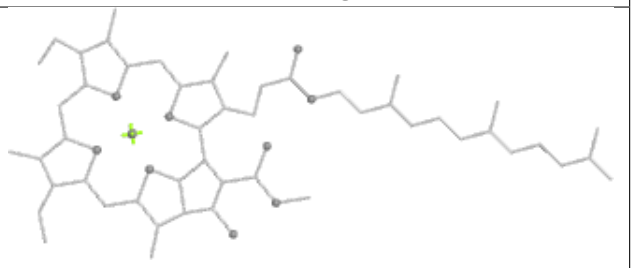
Bond lengths



Bond angles

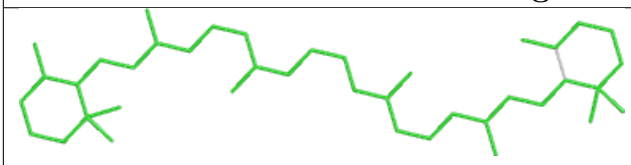


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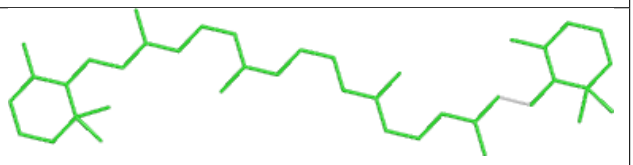


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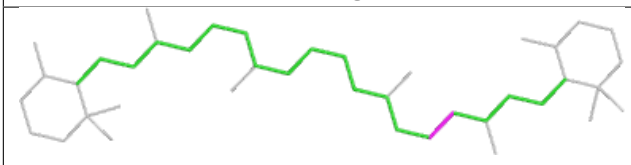
Ligand 8CT e 616



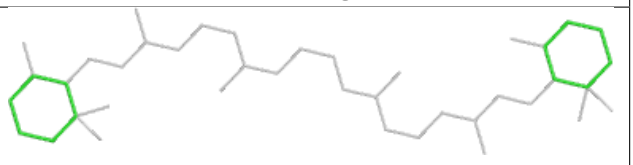
Bond lengths



Bond angles

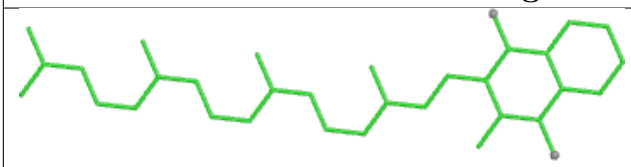


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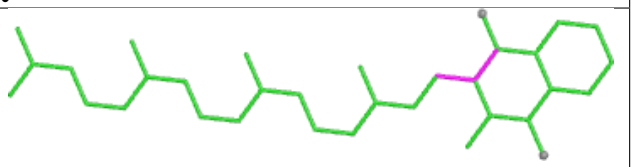


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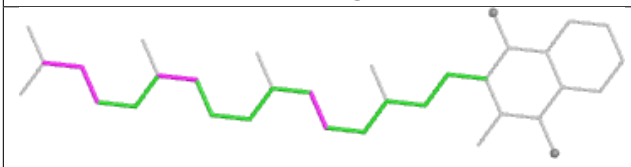
Ligand PQN B 842



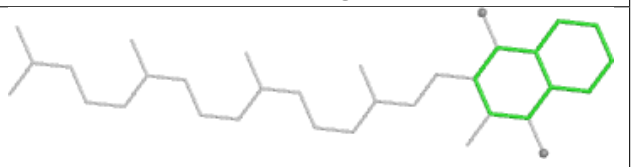
Bond lengths



Bond angles

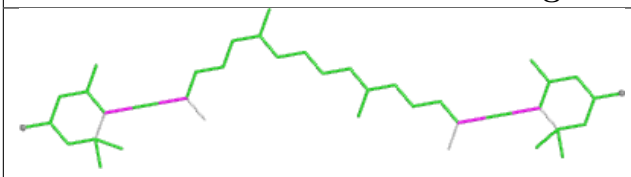


Torsions

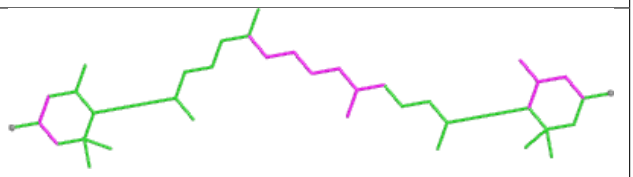


Rings

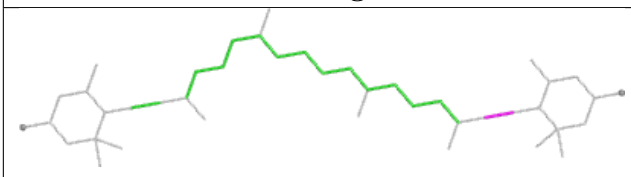
Ligand II0 a 616



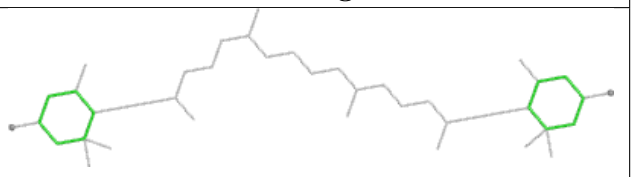
Bond lengths



Bond angles

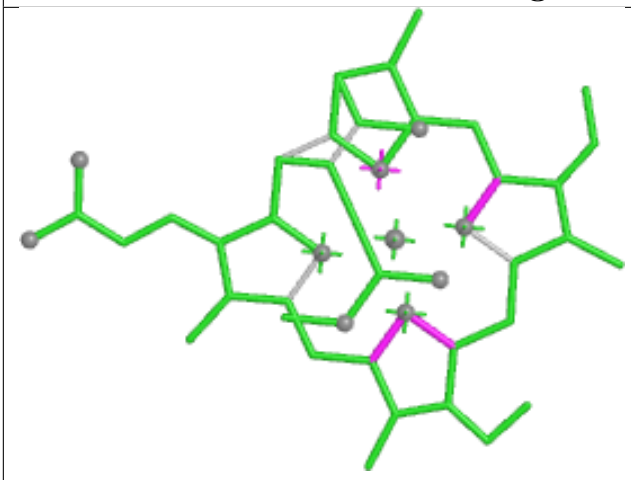


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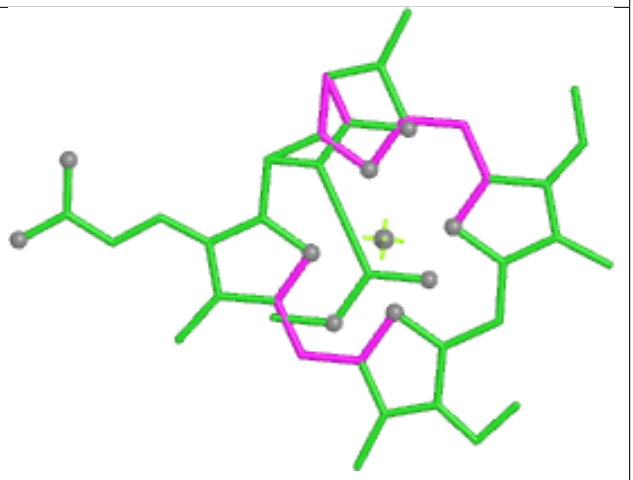


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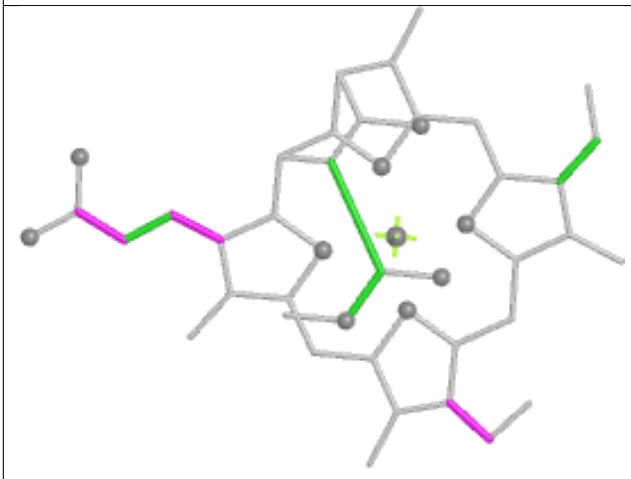
Ligand KC2 d 610



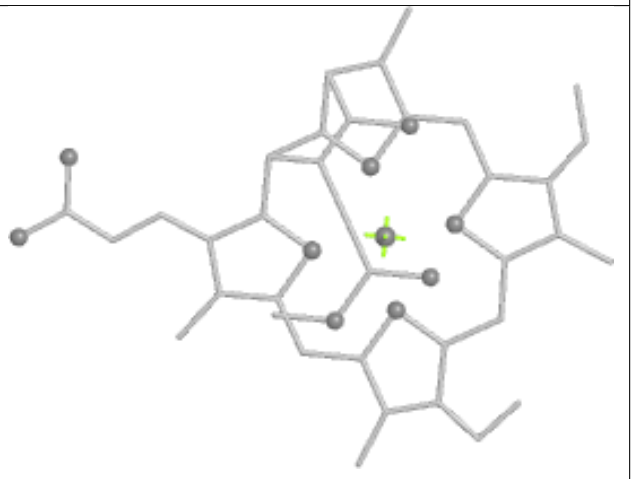
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Bond angles

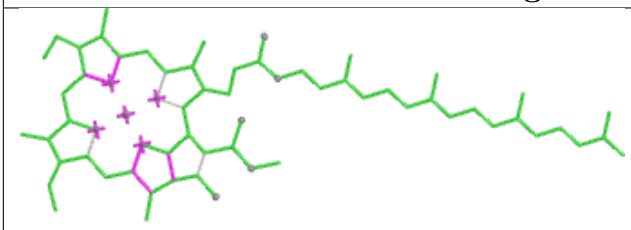


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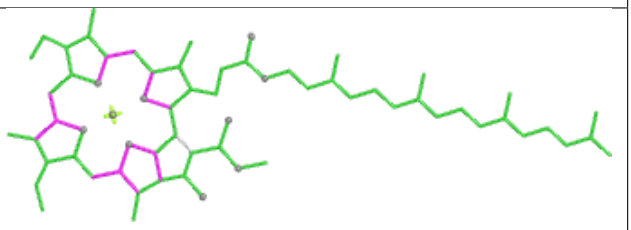


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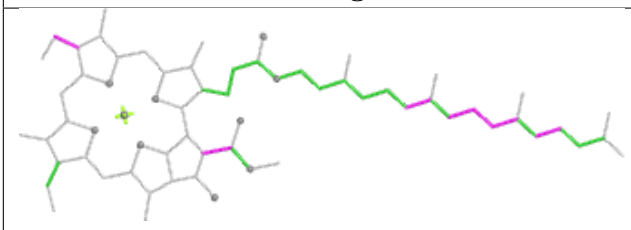
Ligand CLA A 818



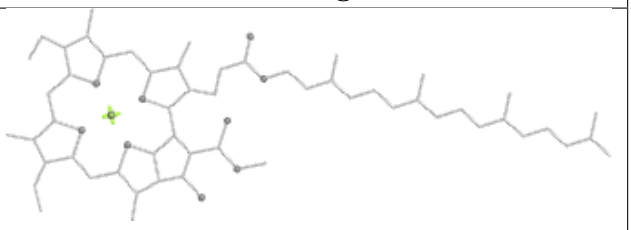
Bond lengths



Bond angles

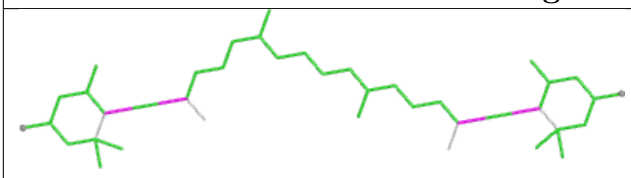


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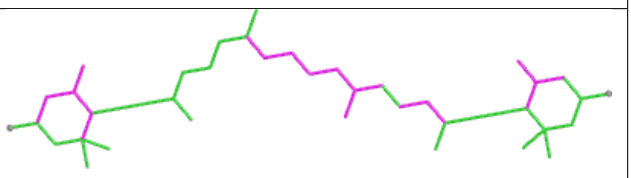


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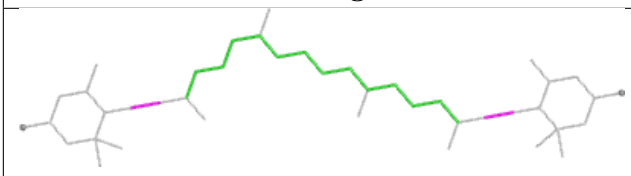
Ligand II0 6 616



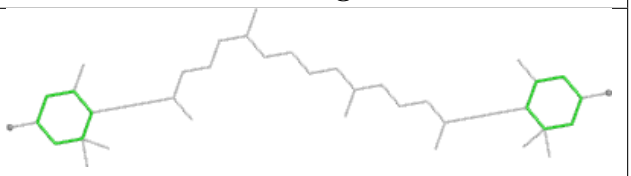
Bond lengths



Bond angles

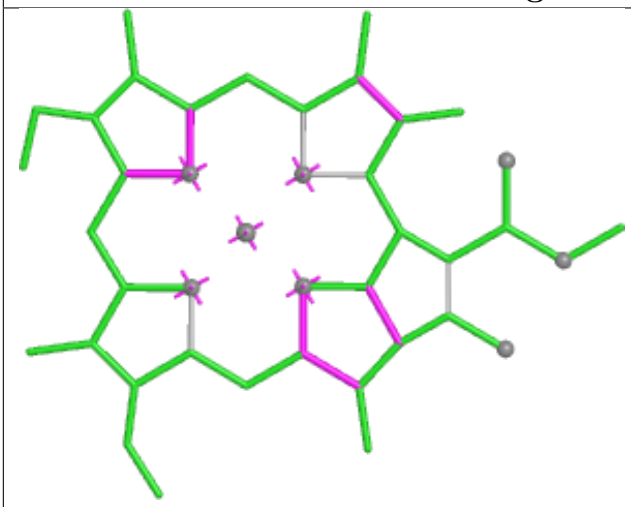


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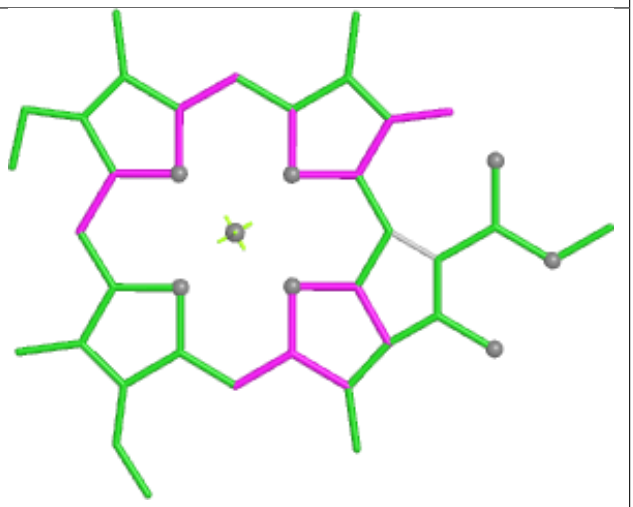


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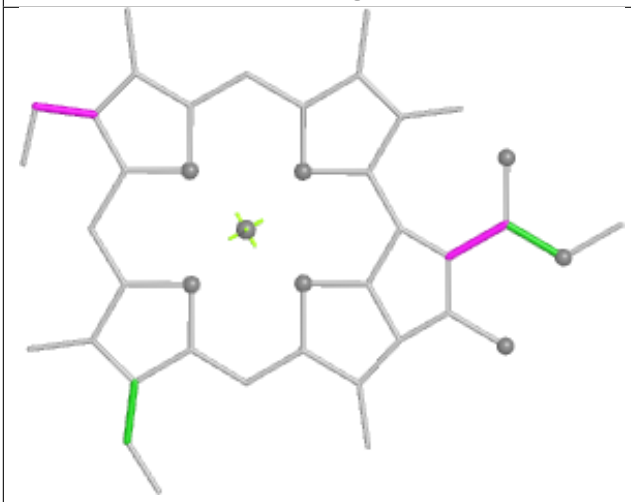
Ligand CLA L 207



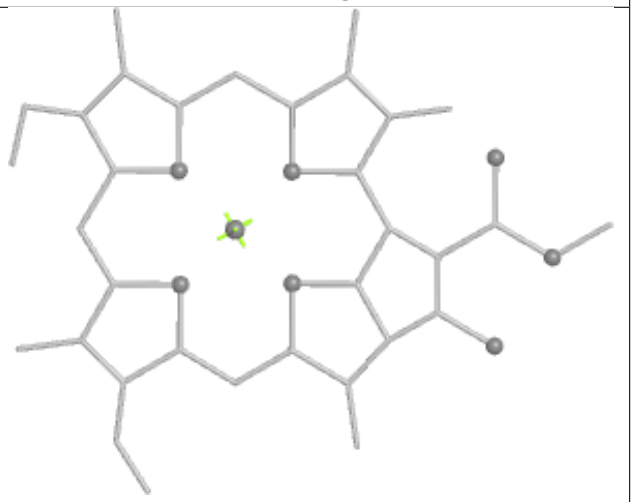
Bond lengths



Bond angles

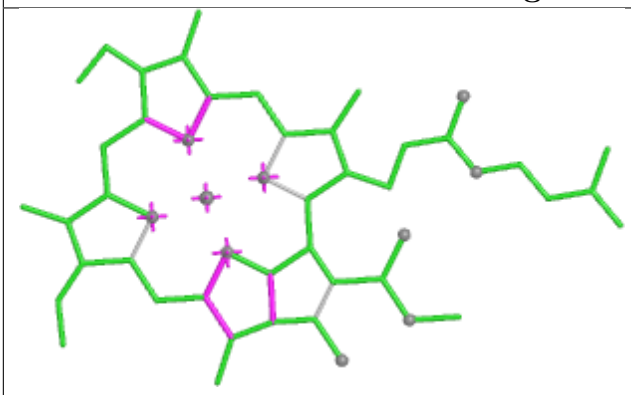


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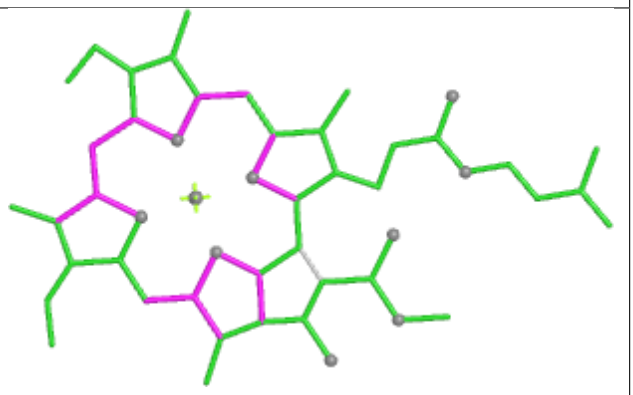


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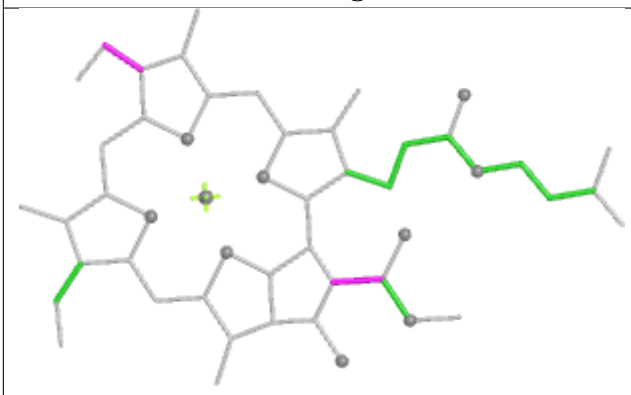
Ligand CLA A 805



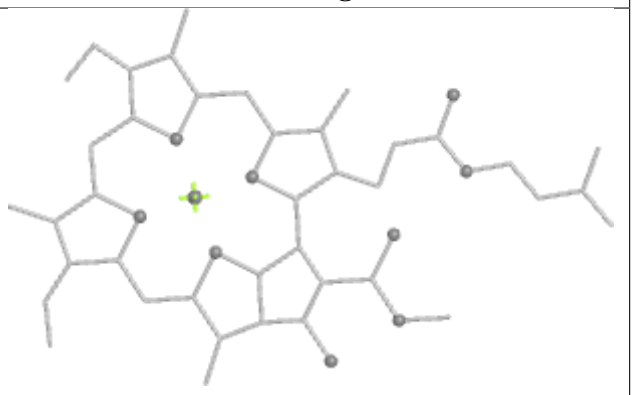
Bond lengths



Bond angles

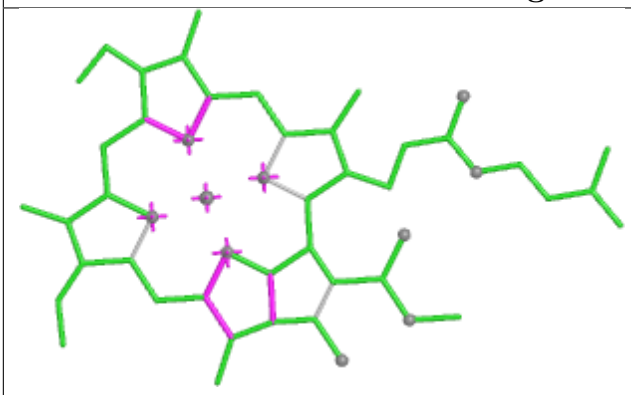


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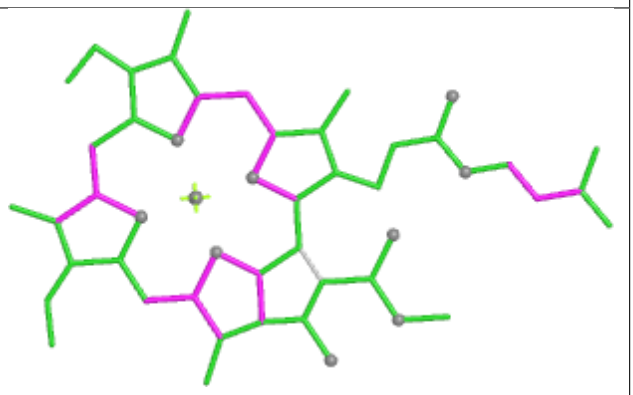


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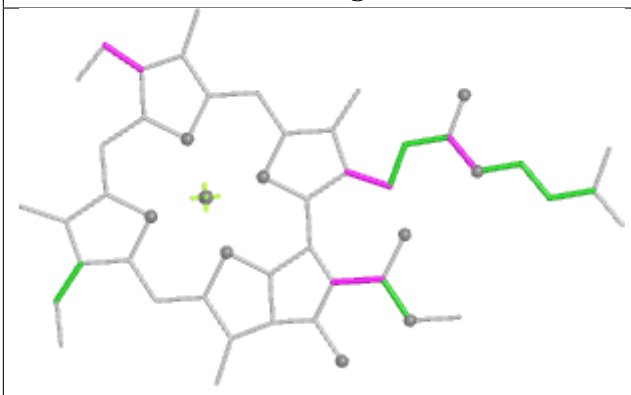
Ligand CLA d 611



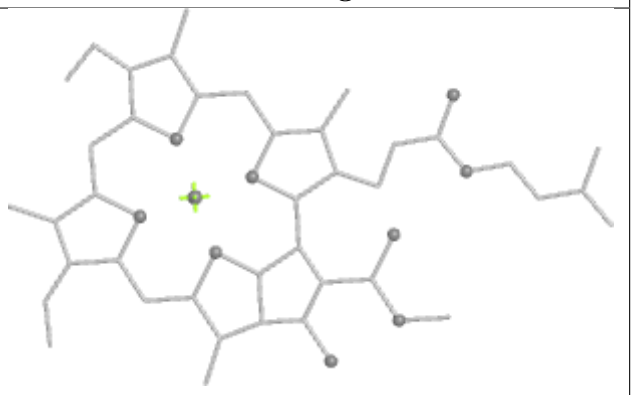
Bond lengths



Bond angles

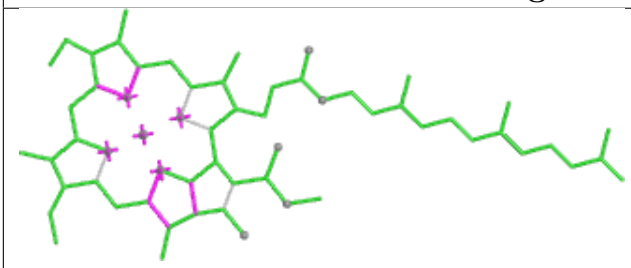


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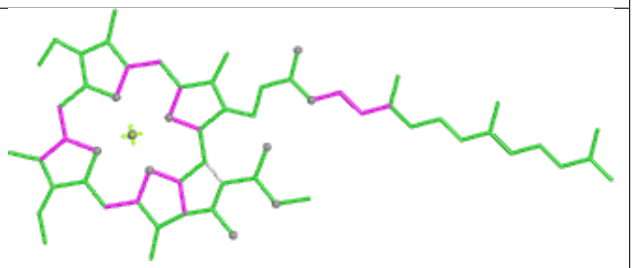


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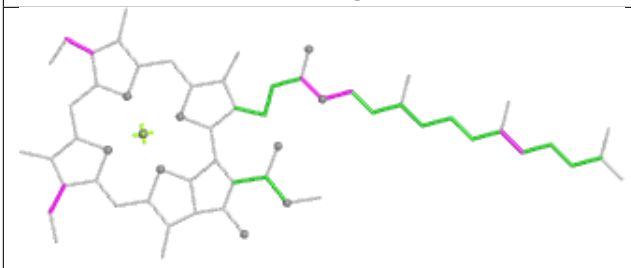
Ligand CLA a 609



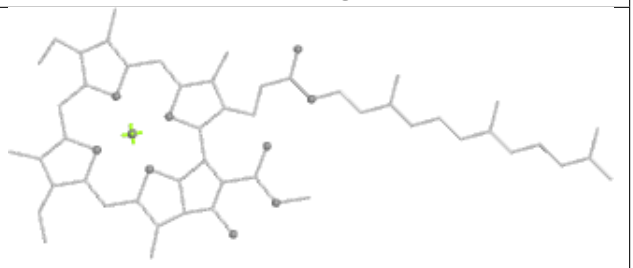
Bond lengths



Bond angles

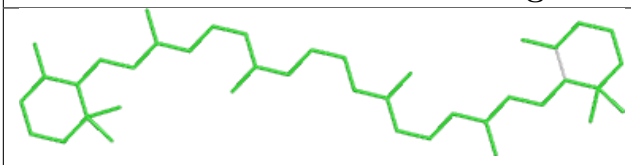


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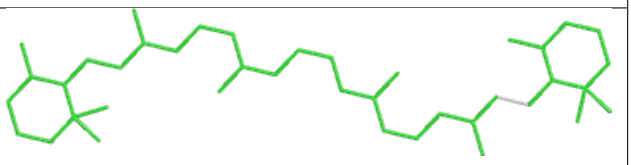


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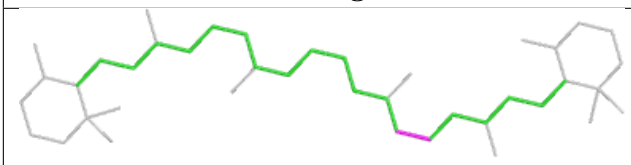
Ligand 8CT A 845



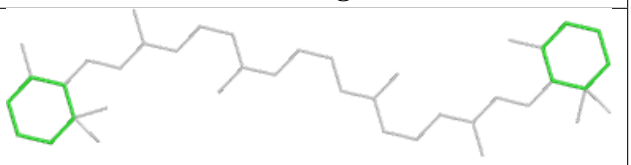
Bond lengths



Bond angles

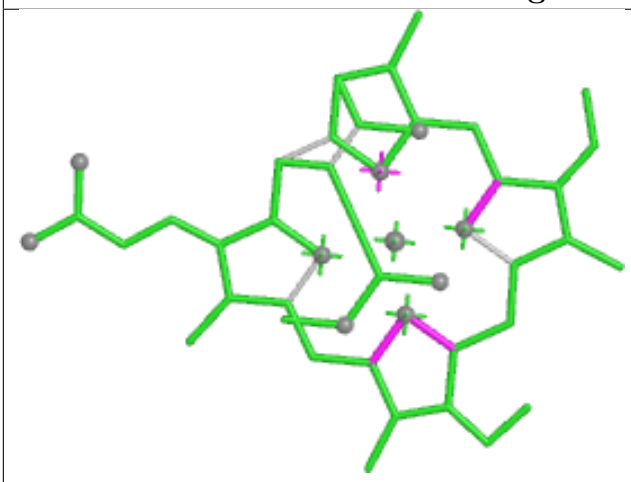


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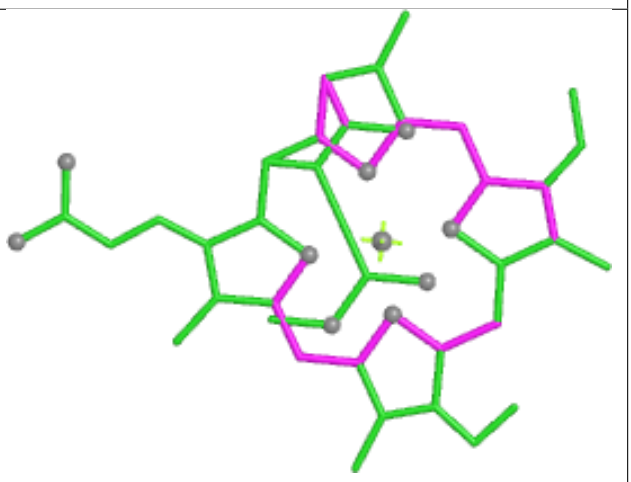


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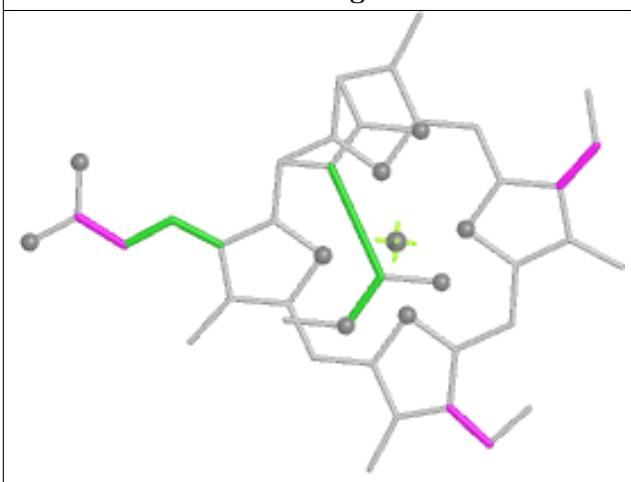
Ligand KC2 Z 307



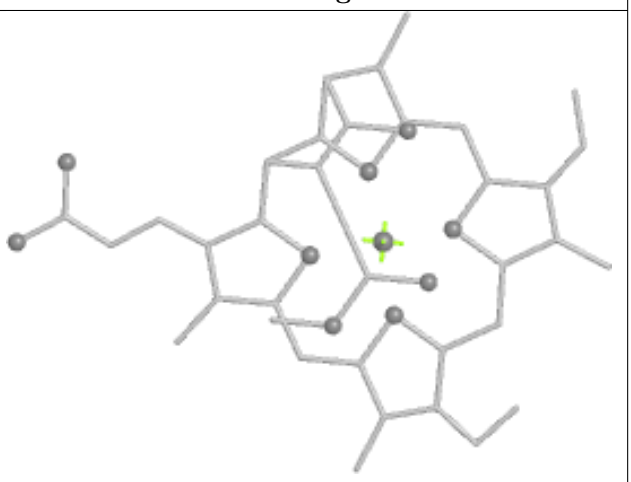
Bond lengths



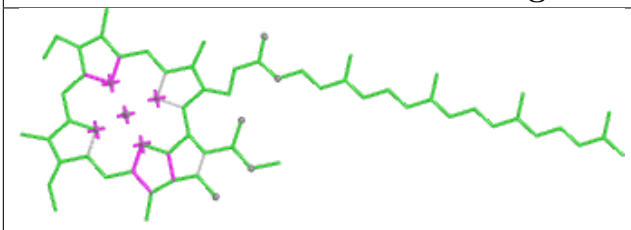
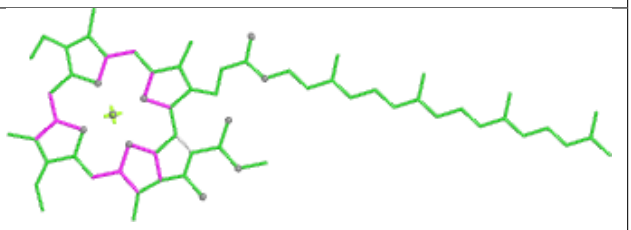
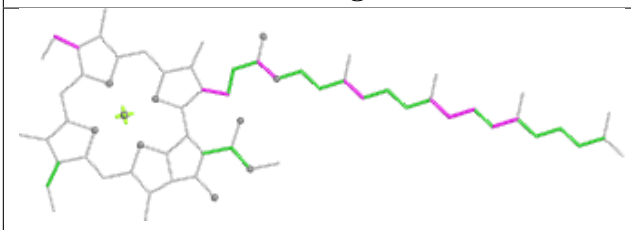
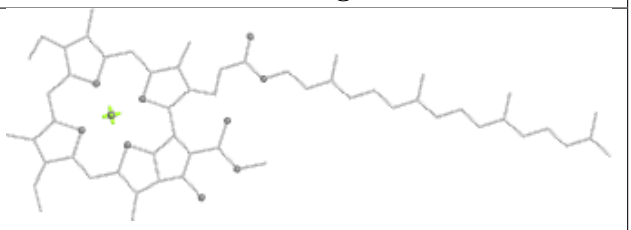
Bond angles

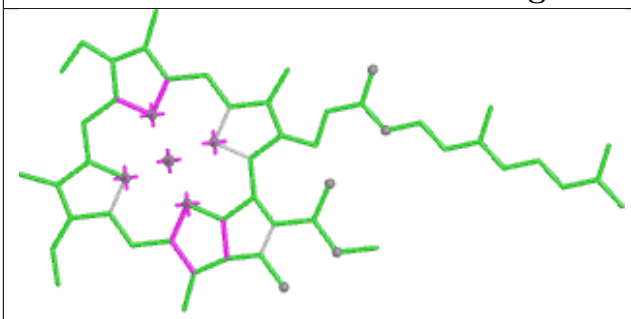
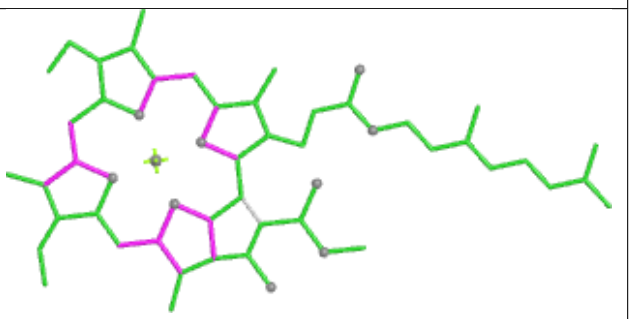
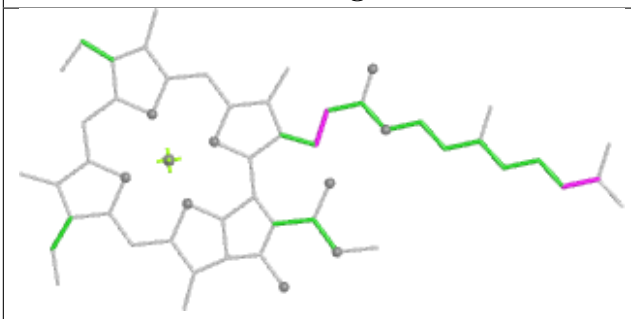
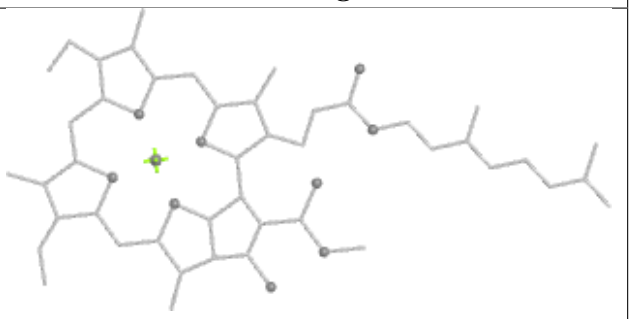


Torsions

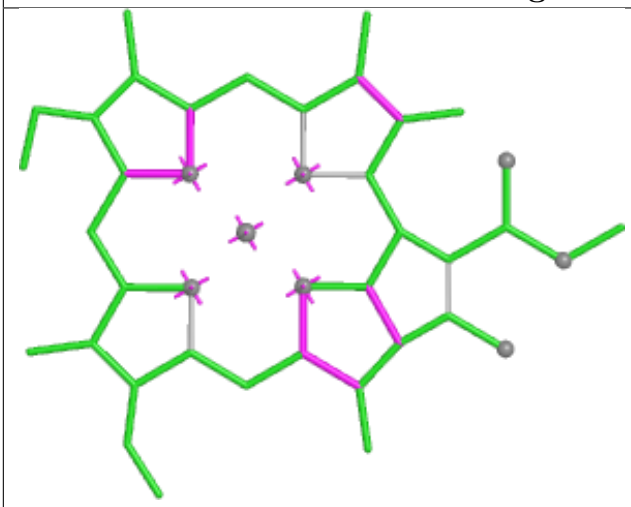


Rings

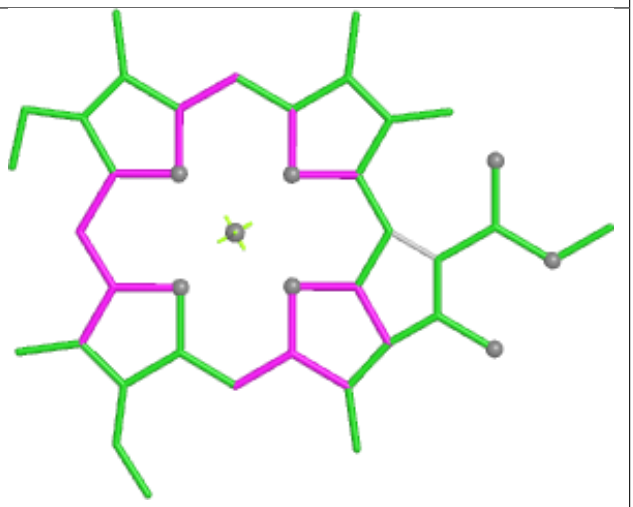
Ligand CLA 8 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 9 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

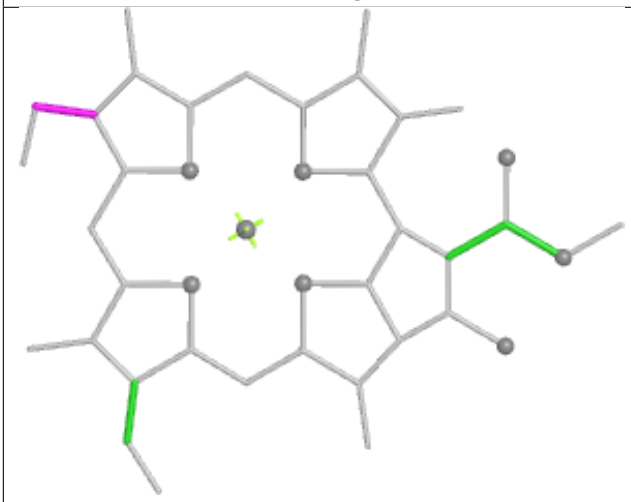
Ligand CLA 5 601



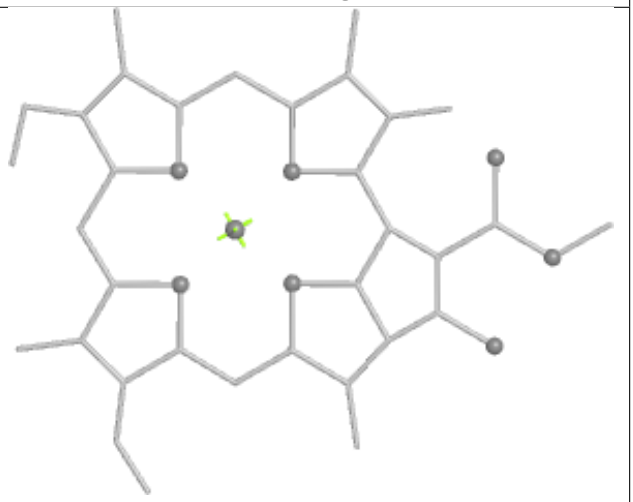
Bond lengths



Bond angles

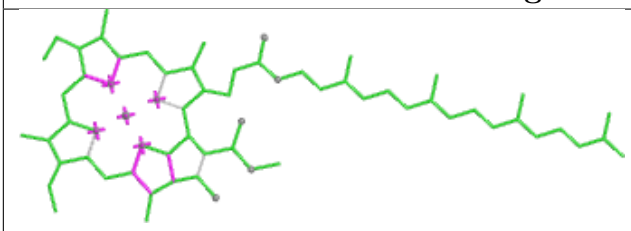


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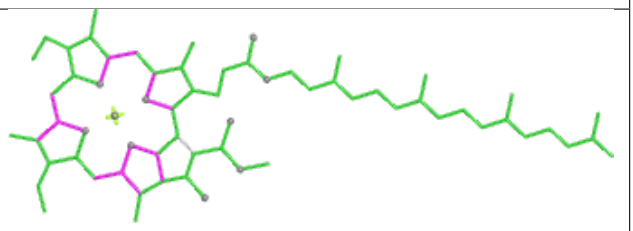


Rings

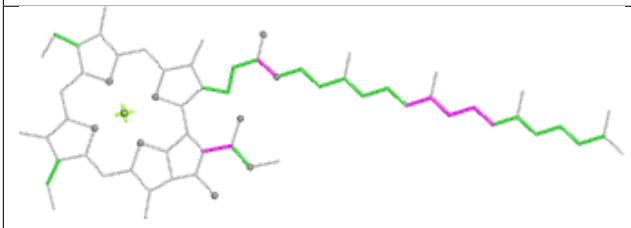
Ligand CLA B 828



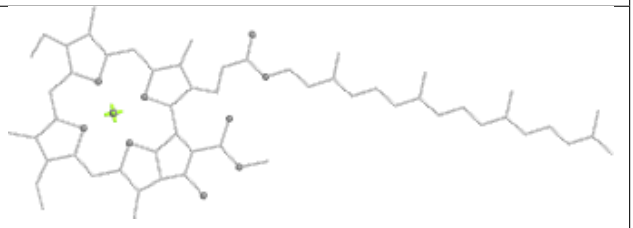
Bond lengths



Bond angles

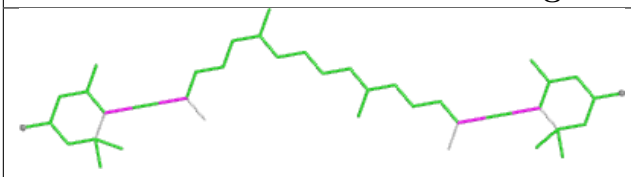


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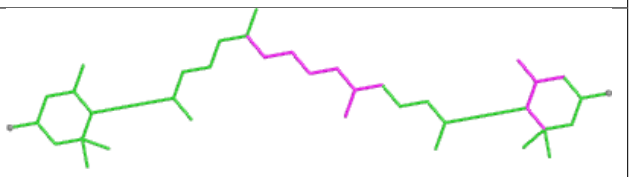


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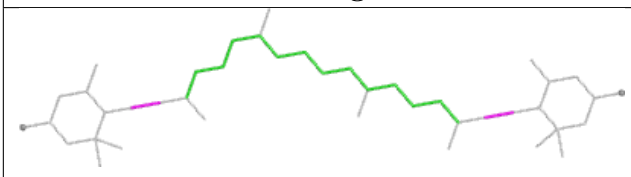
Ligand II0 c 619



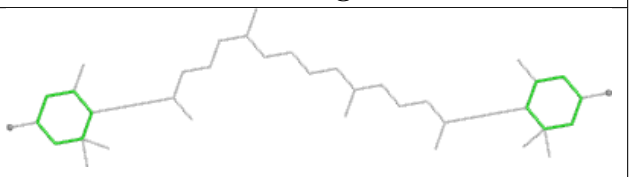
Bond lengths



Bond angles

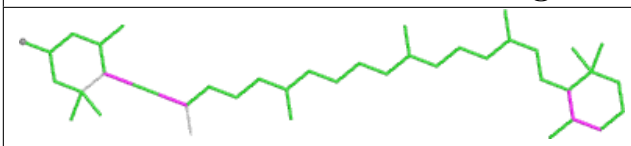


Torsions

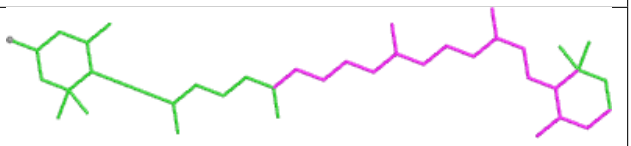


Rings

Ligand IHT 8 609



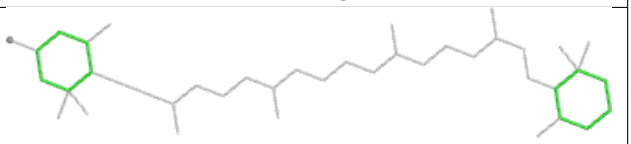
Bond lengths



Bond angles

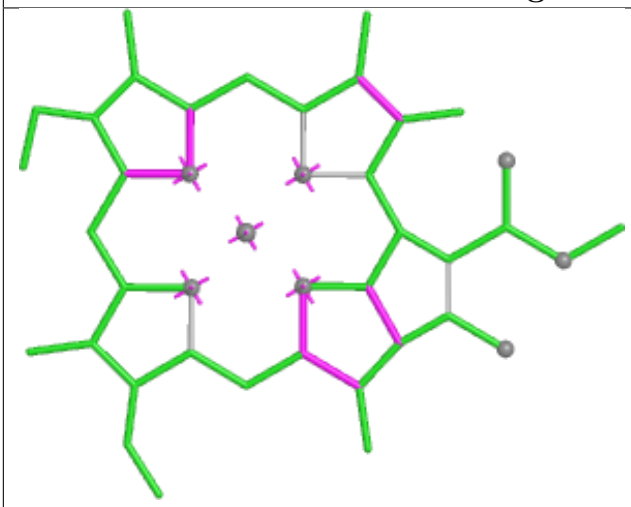


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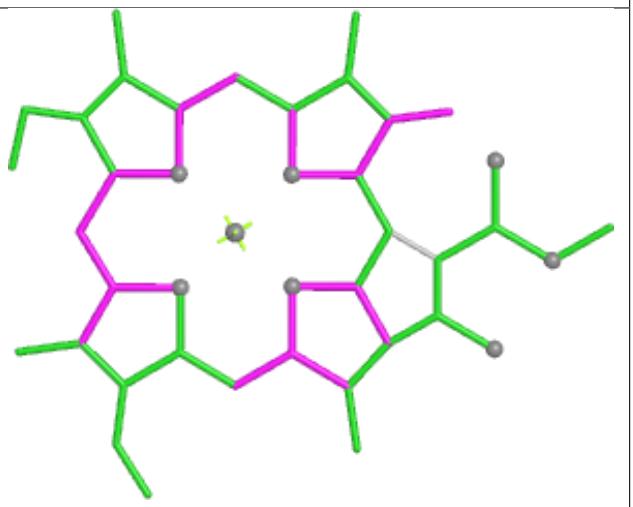


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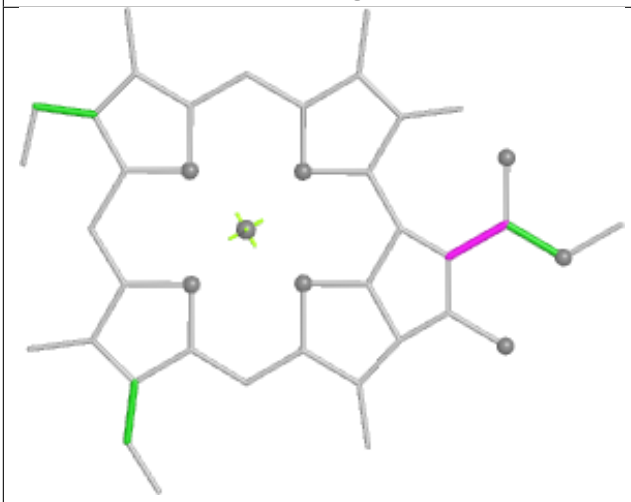
Ligand CLA d 606



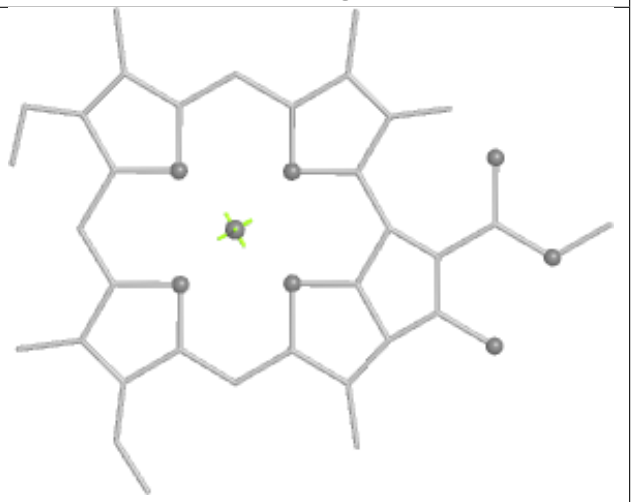
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Bond angles

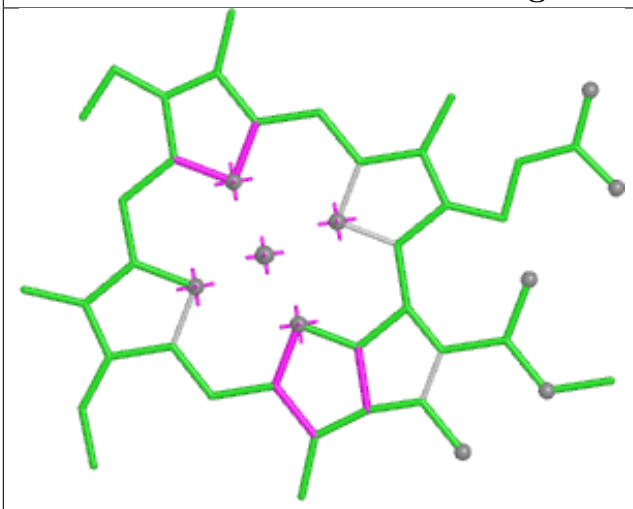


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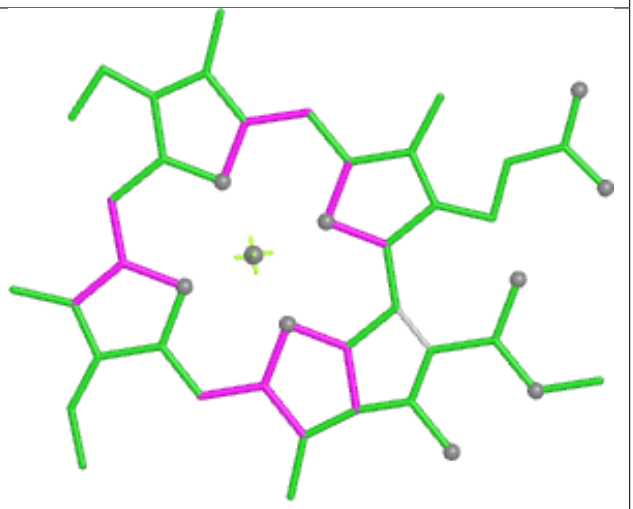


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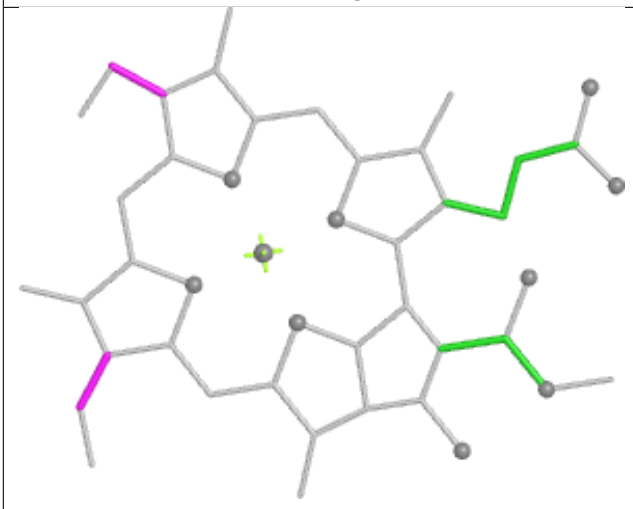
Ligand CLA 6 601



Bond lengths



Bond angles

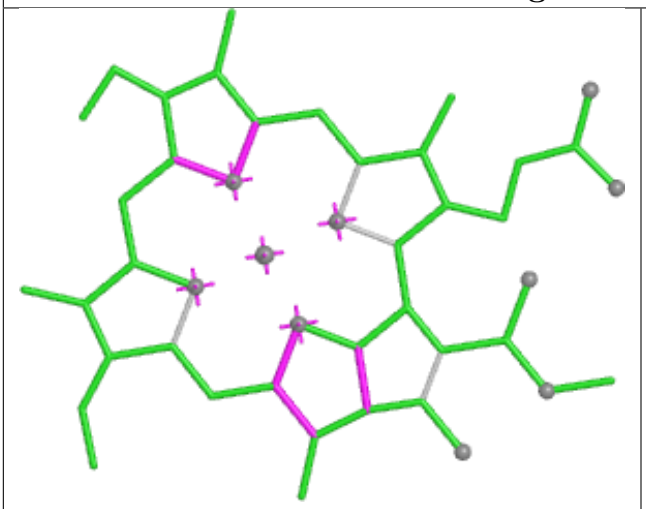


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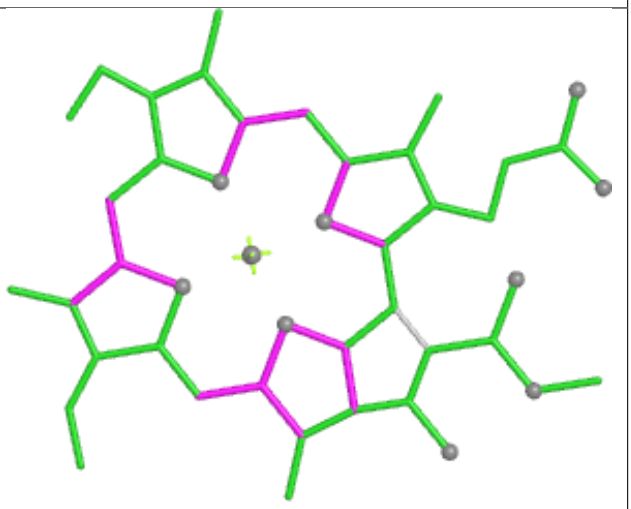


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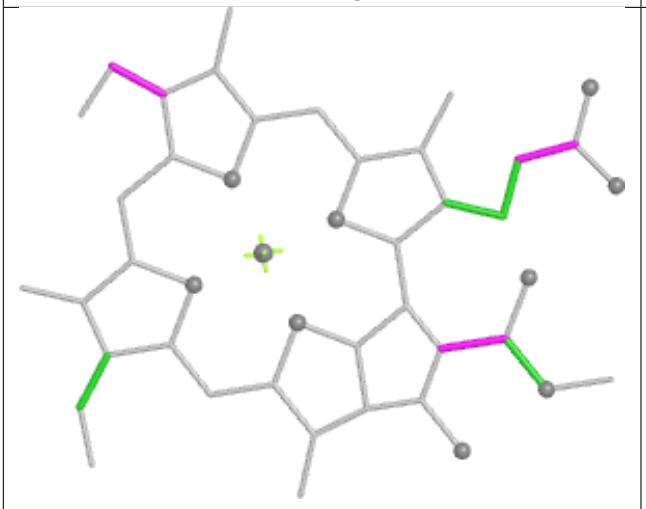
Ligand CLA 3 612



Bond lengths



Bond angles



Torsions

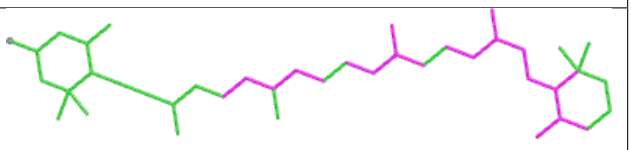


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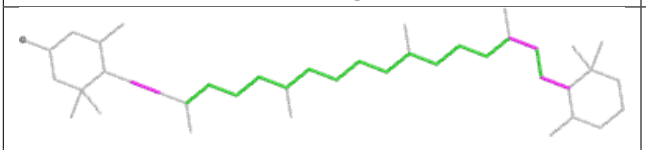
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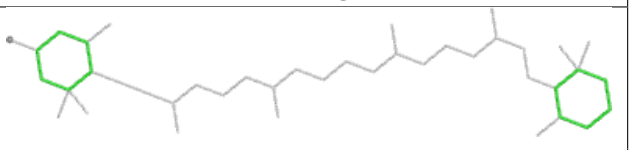
Bond lengths



Bond angles

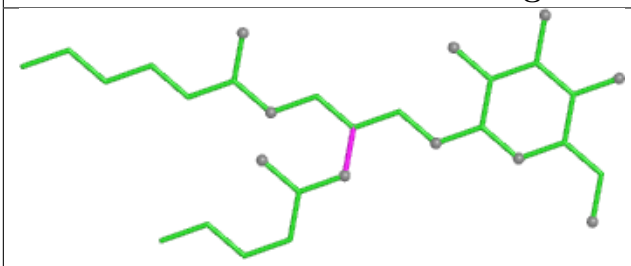


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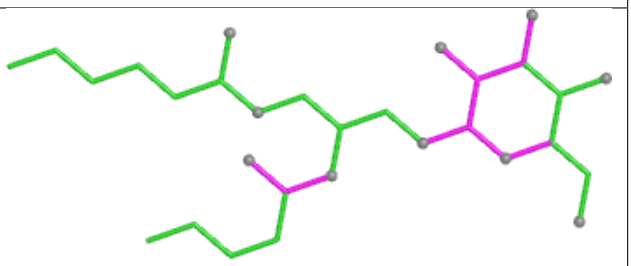


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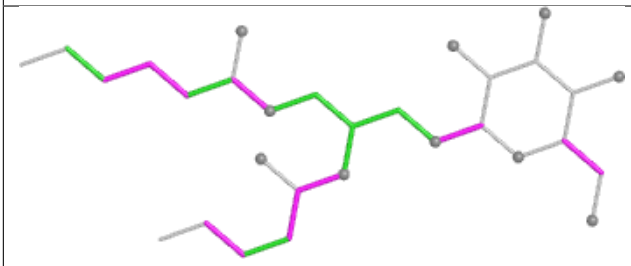
Ligand LMG 3 618



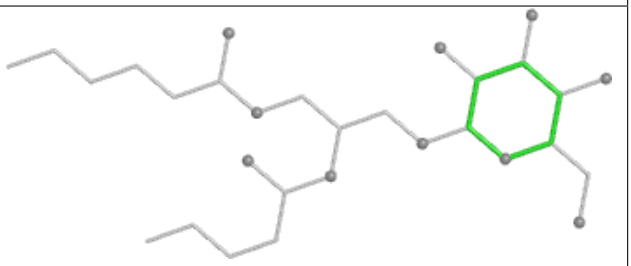
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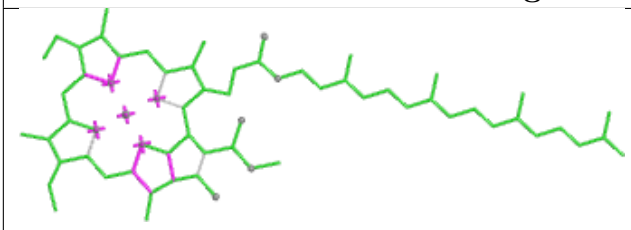


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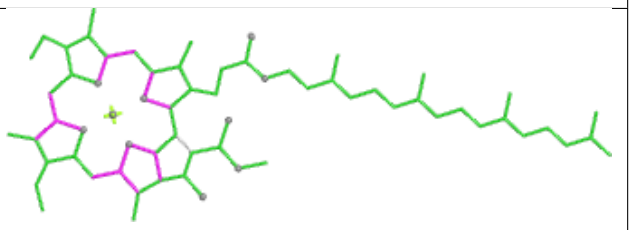


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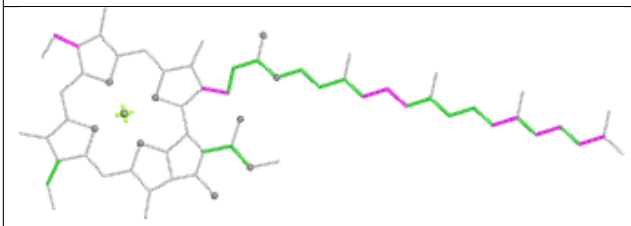
Ligand CLA A 831



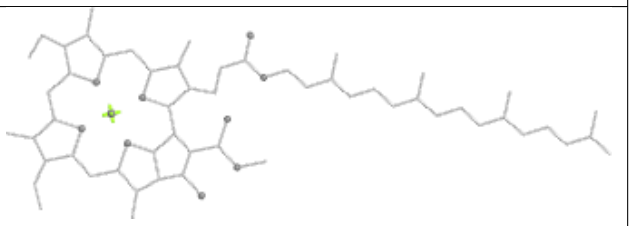
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Bond angles

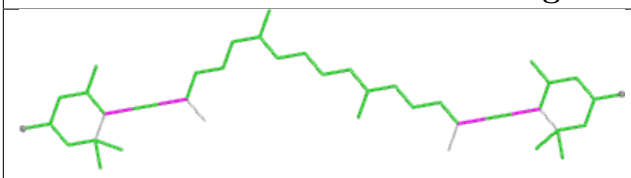


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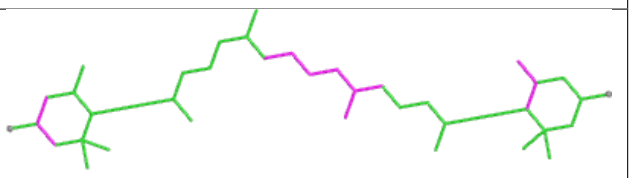


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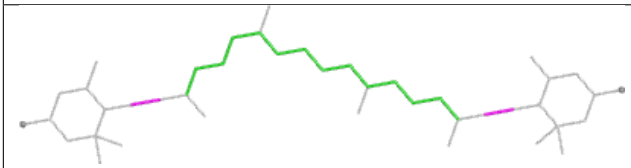
Ligand II0 3 616



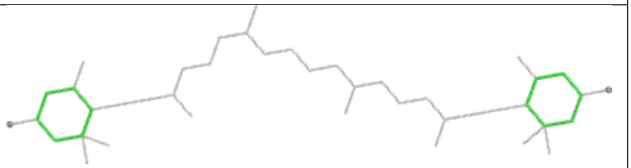
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Bond angles

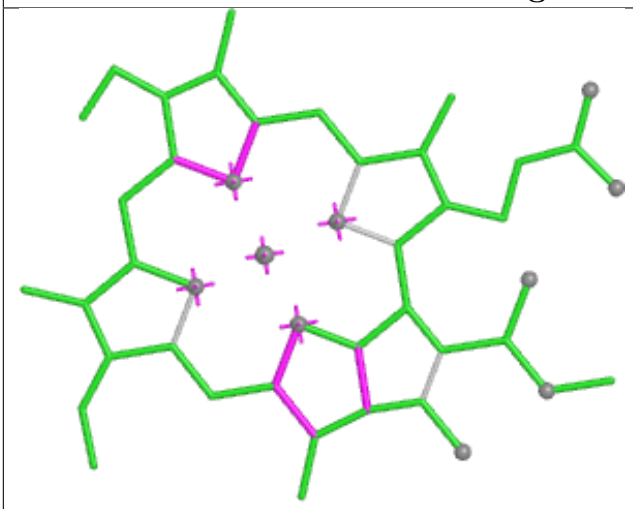


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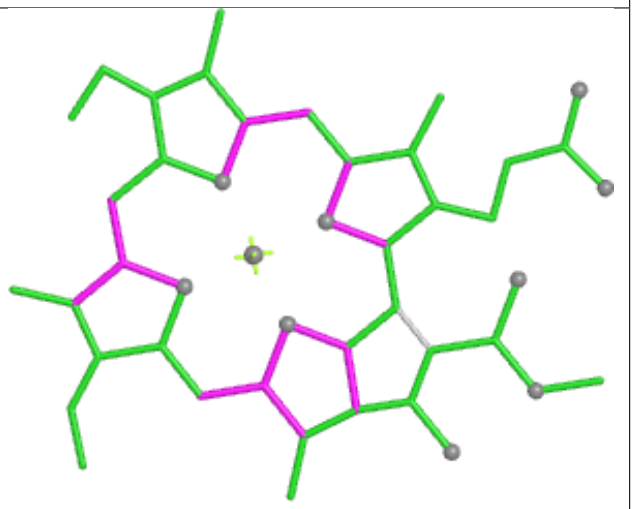


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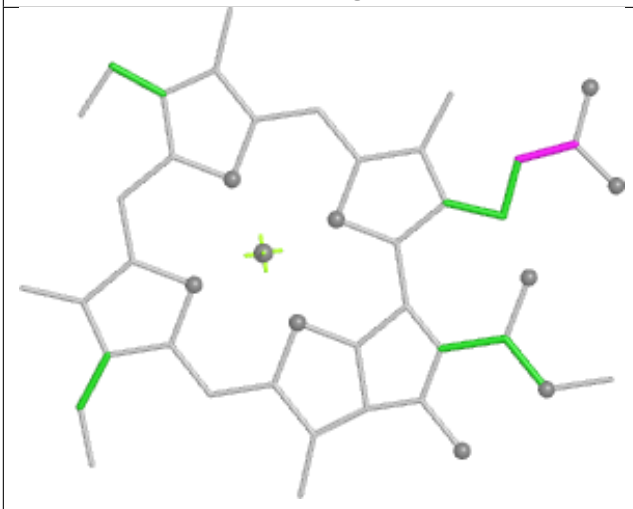
Ligand CLA 8 601



Bond lengths



Bond angles

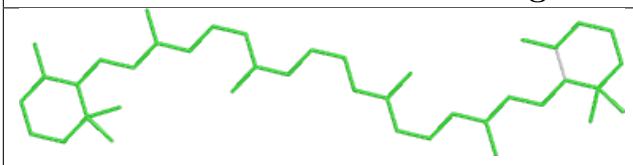


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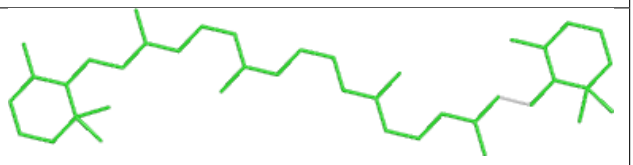


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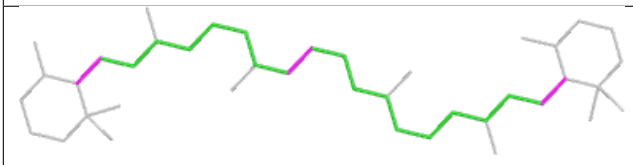
Ligand 8CT Z 308



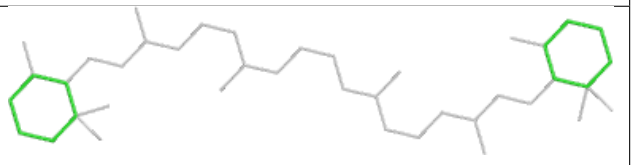
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Bond angles

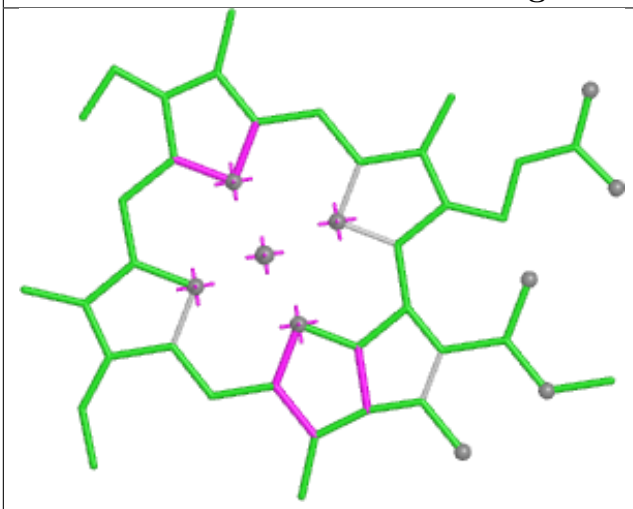


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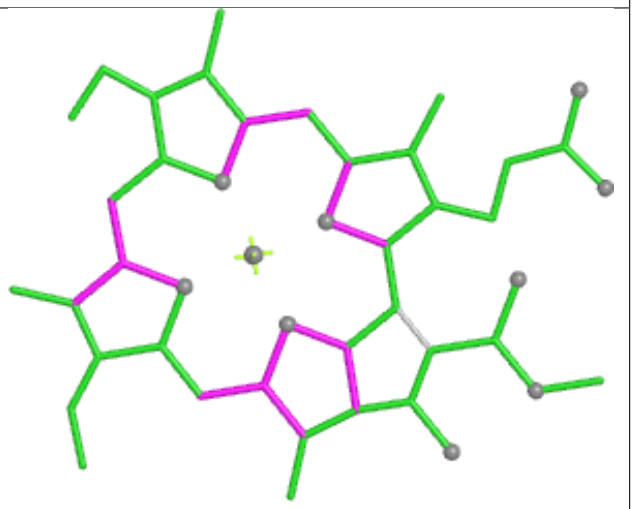


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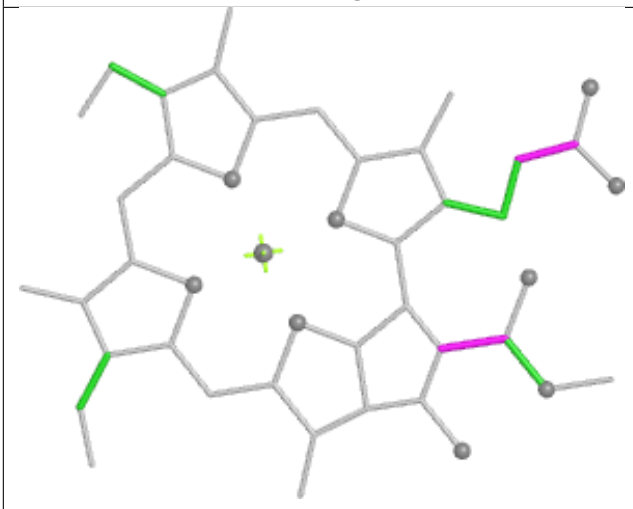
Ligand CLA 1 611



Bond lengths



Bond angles

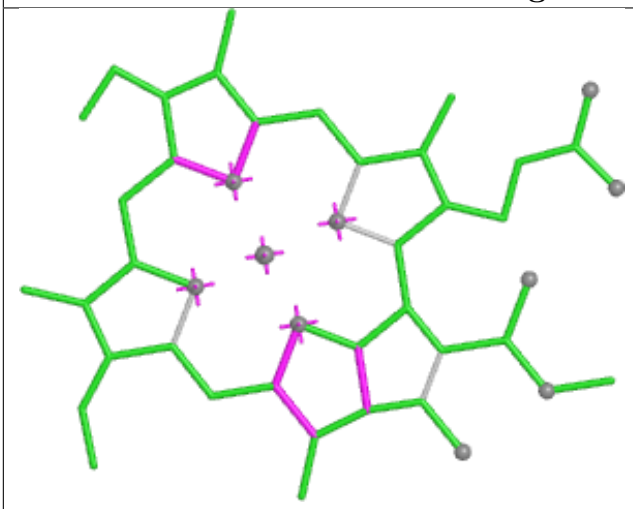


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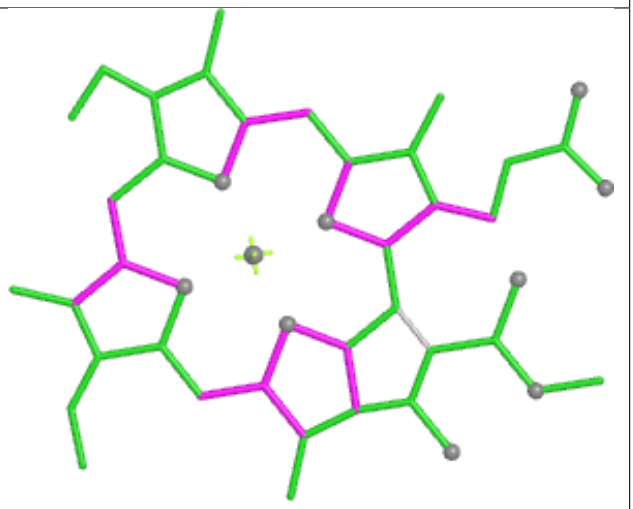


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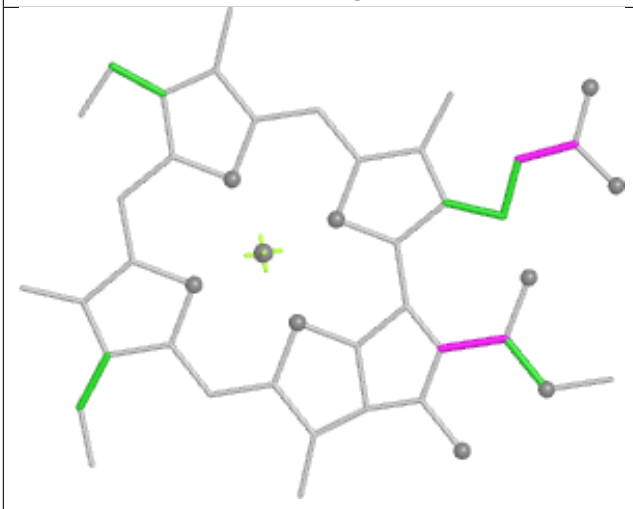
Ligand CLA 5 603



Bond lengths



Bond angles

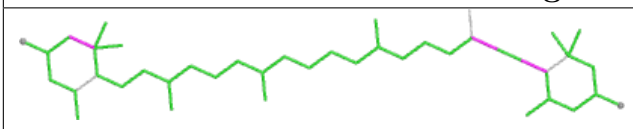


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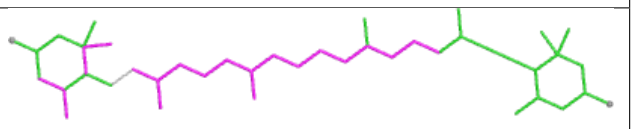


Rings

Ligand II3 e 613



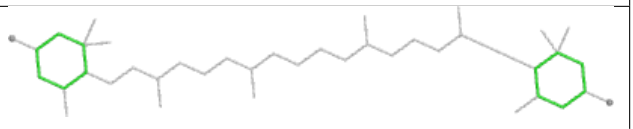
Bond lengths



Bond angles

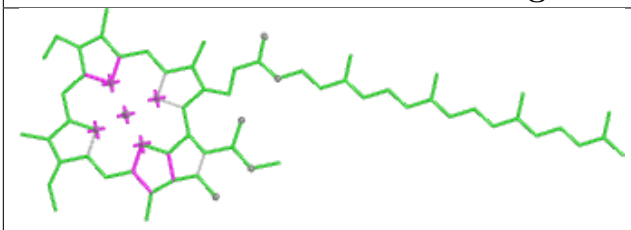


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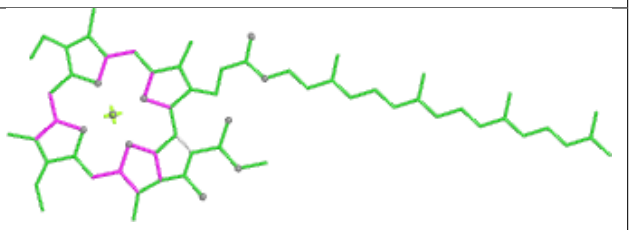


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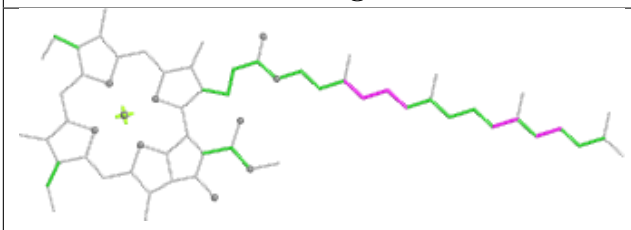
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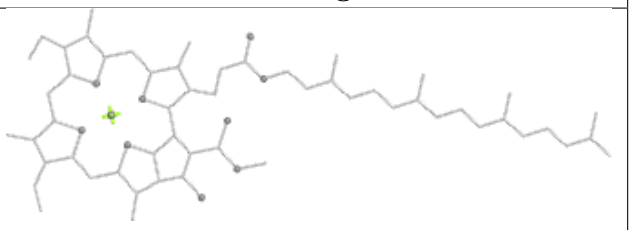
Bond lengths



Bond angles

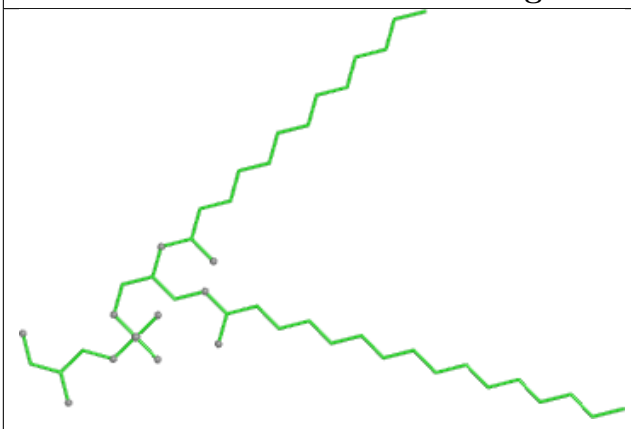


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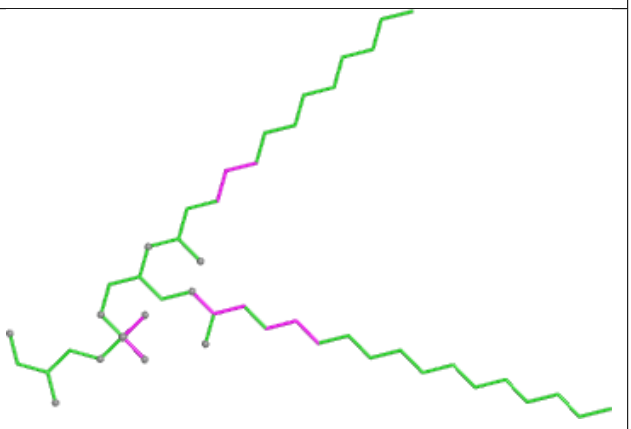


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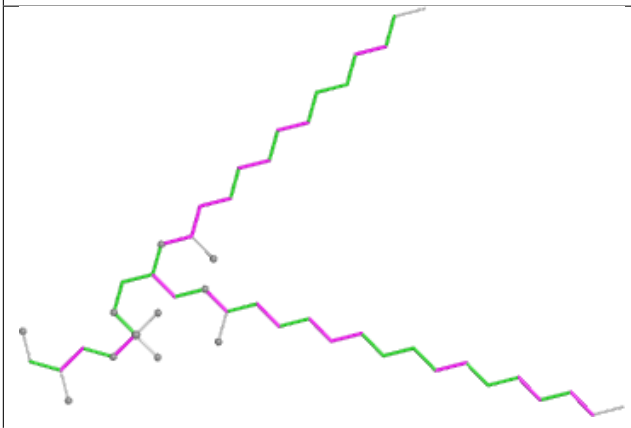
Ligand LHG Z 310



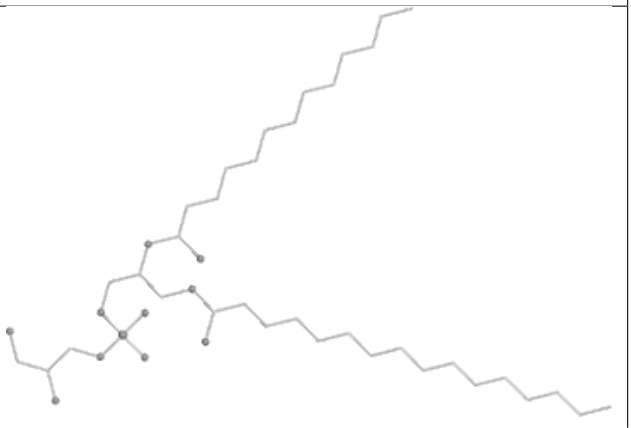
Bond lengths



Bond angles

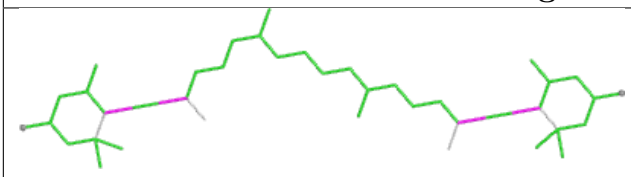


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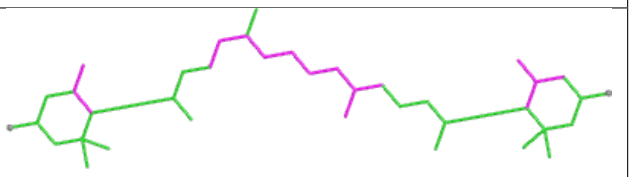


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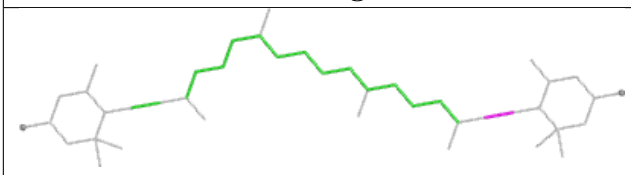
Ligand II0 R 204



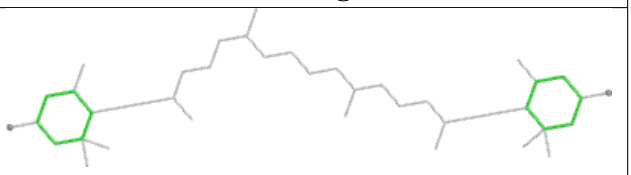
Bond lengths



Bond angles

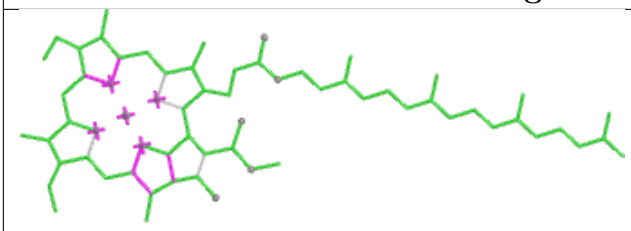


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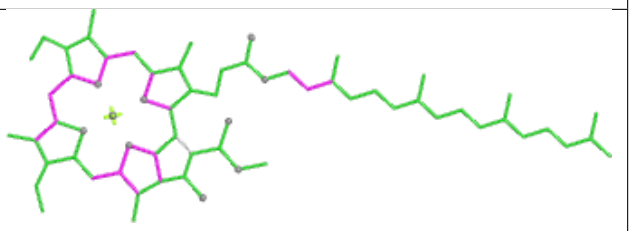


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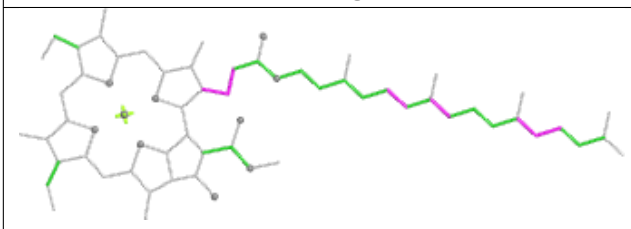
Ligand CLA B 835



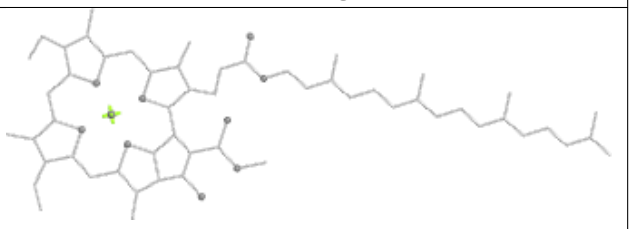
Bond lengths



Bond angles

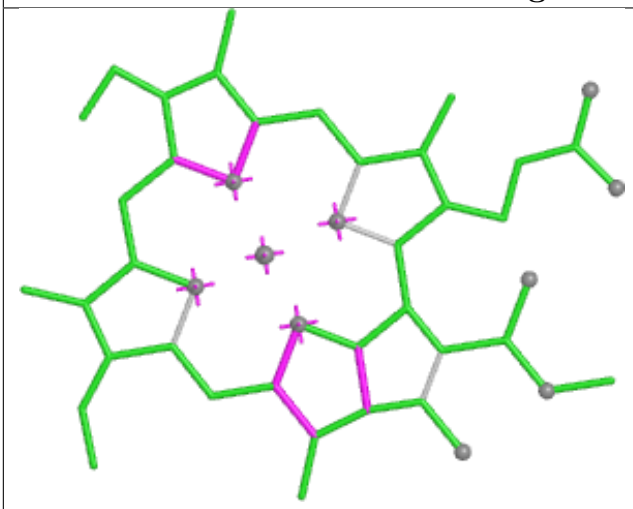


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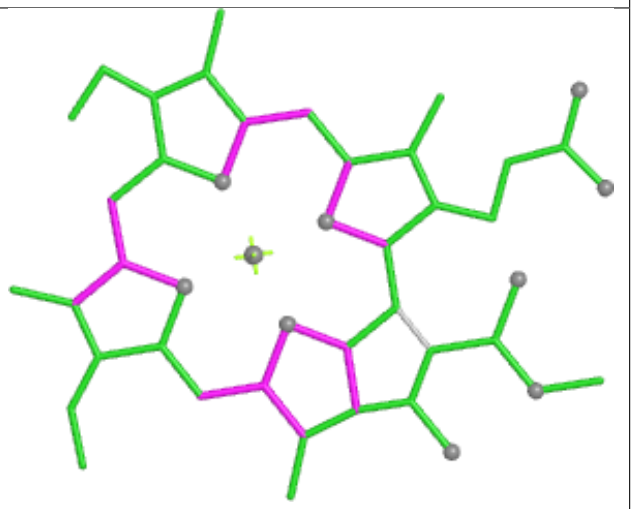


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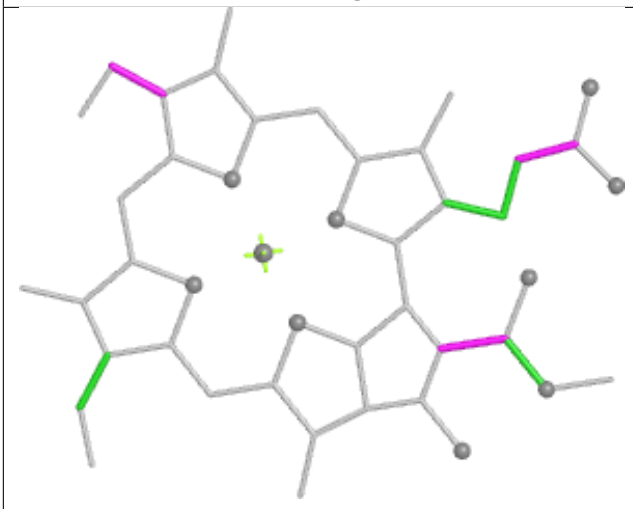
Ligand CLA 3 601



Bond lengths



Bond angles

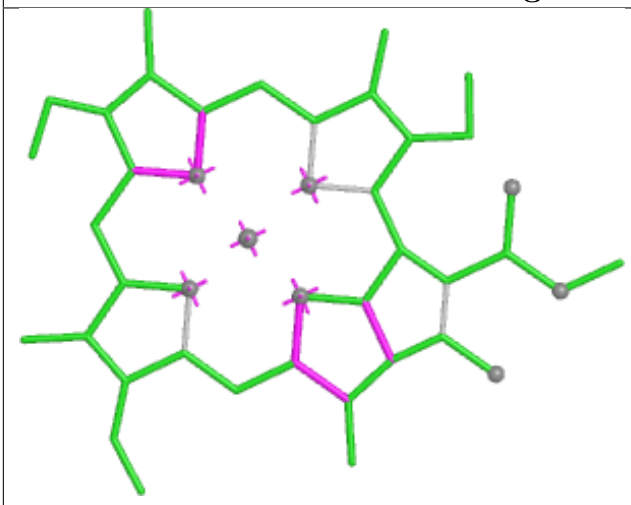


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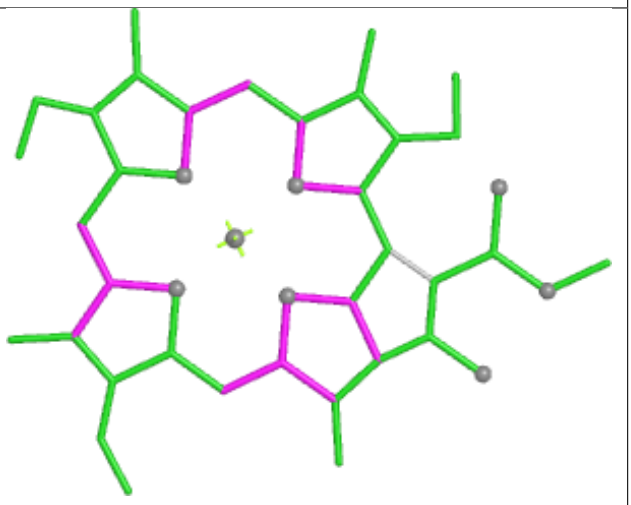


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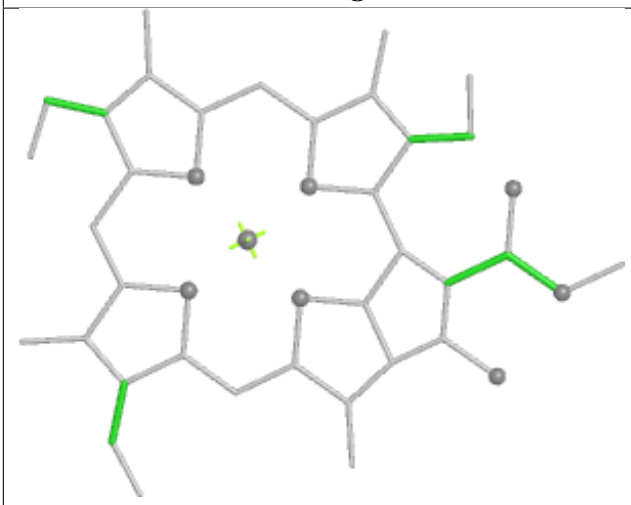
Ligand CLA A 813



Bond lengths



Bond angles

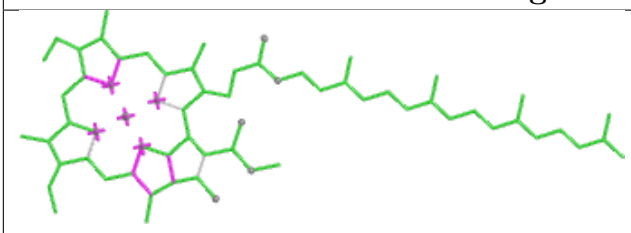


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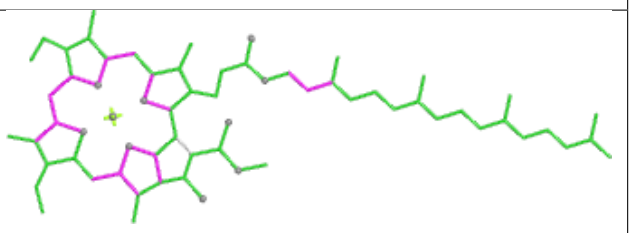


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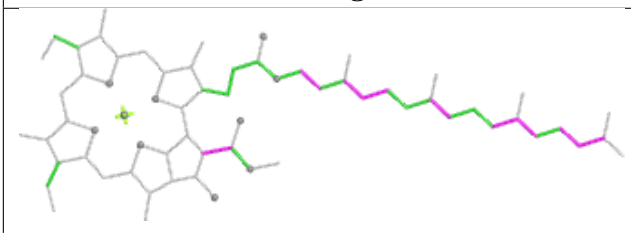
Ligand CLA c 606



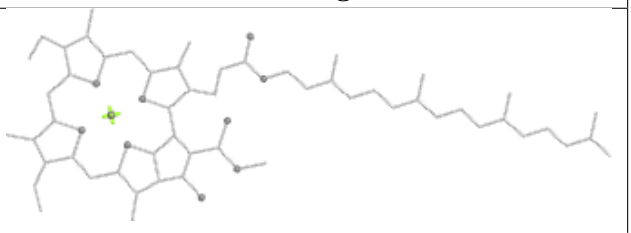
Bond lengths



Bond angles

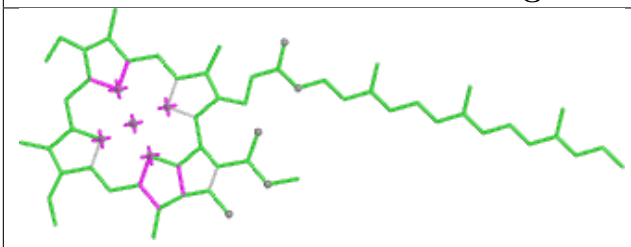


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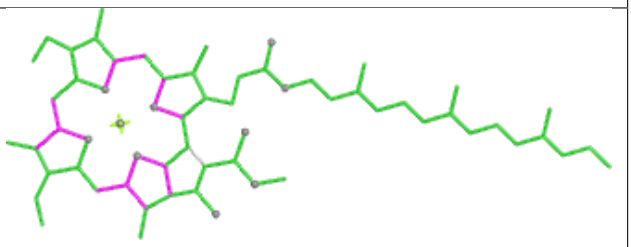


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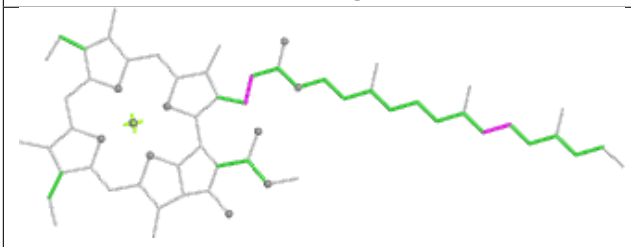
Ligand CLA A 815



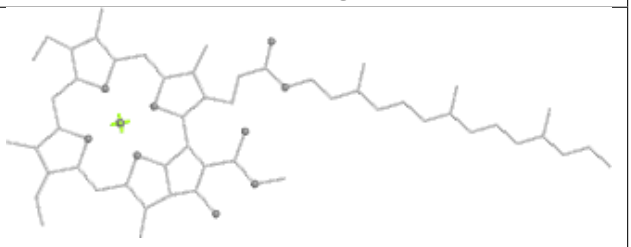
Bond lengths



Bond angles

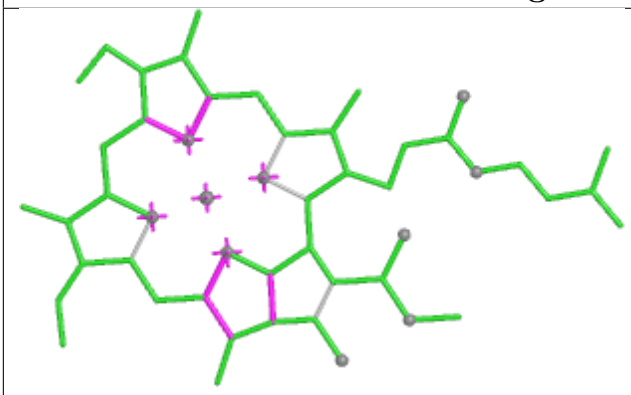


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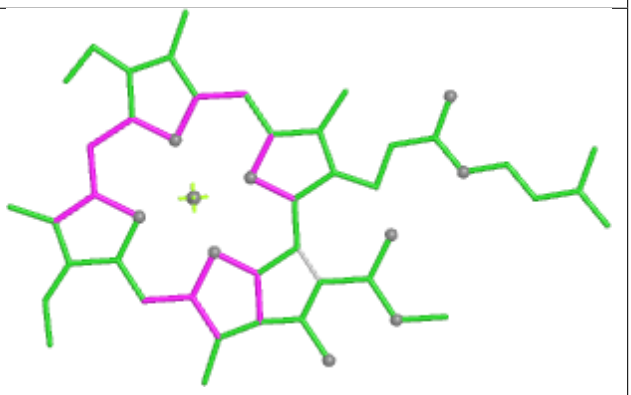


Rings

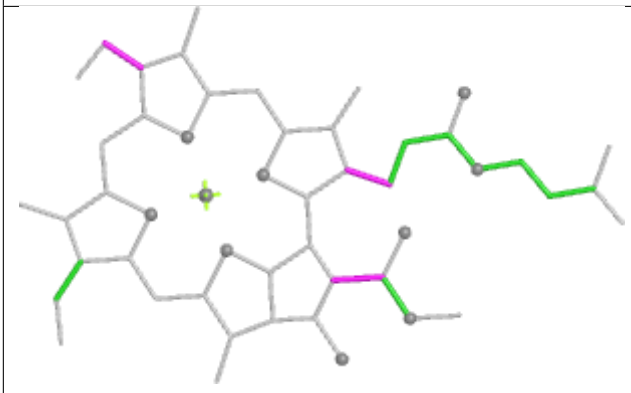
Ligand CLA 3 611



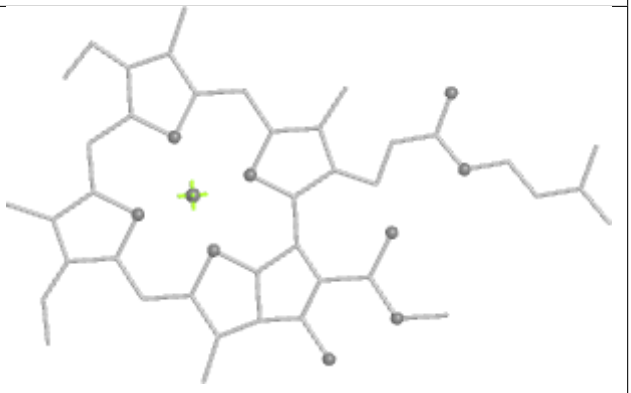
Bond lengths



Bond angles

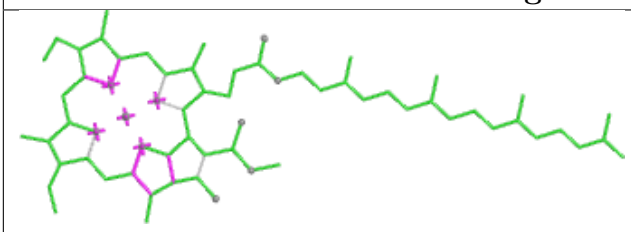


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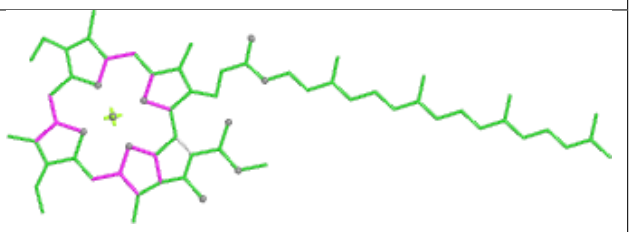


Rings

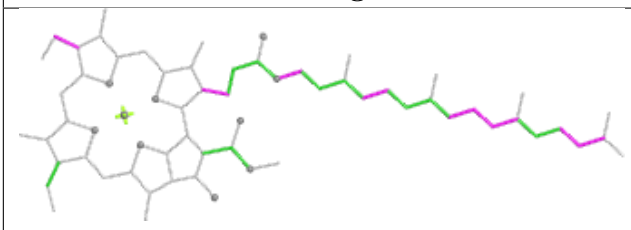
Ligand CLA B 826



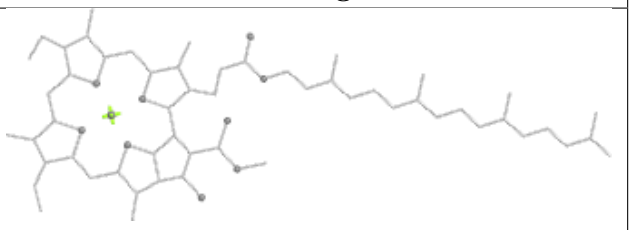
Bond lengths



Bond angles

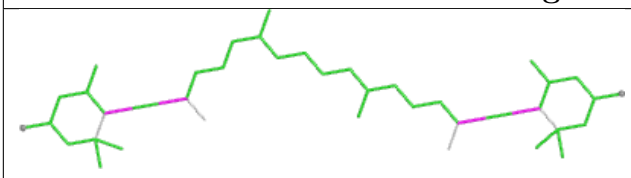


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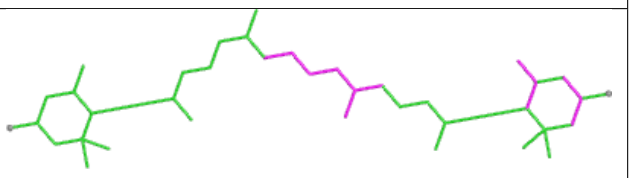


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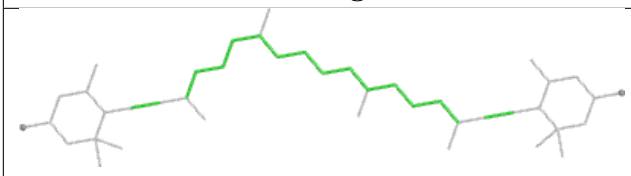
Ligand II0 4 613



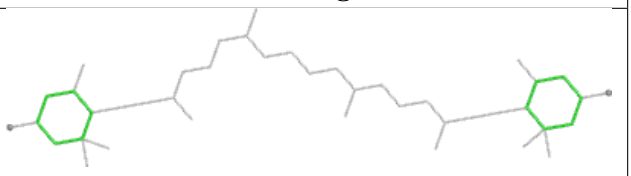
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Bond angles

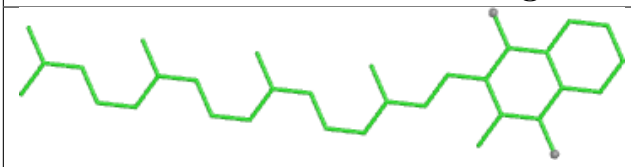


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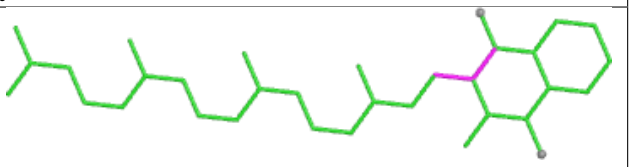


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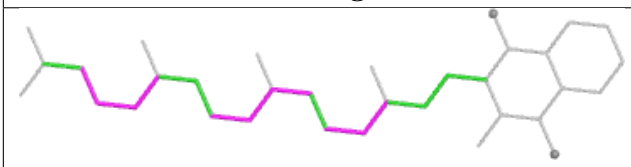
Ligand PQN A 849



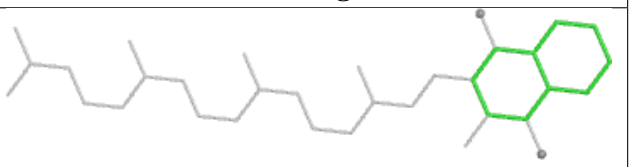
Bond lengths



Bond angles



Torsions

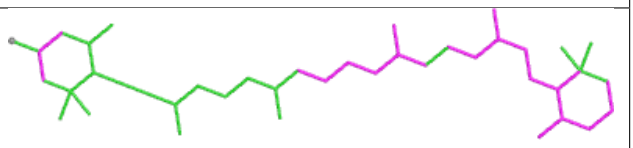


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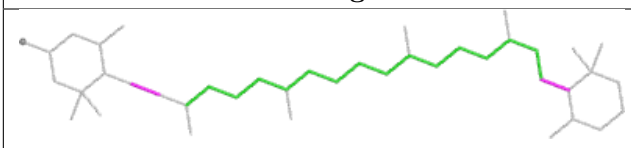
Ligand IHT Z 302



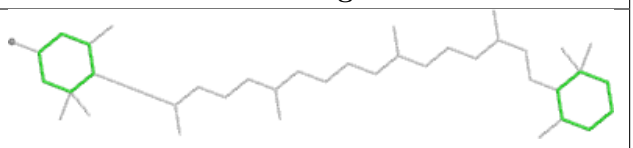
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Bond angles

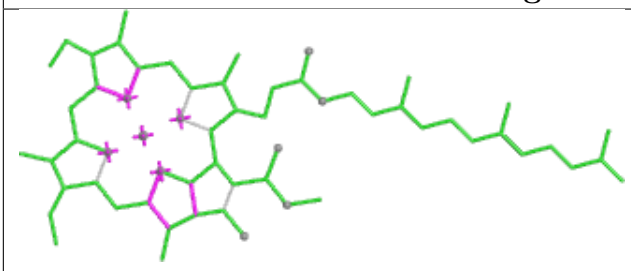


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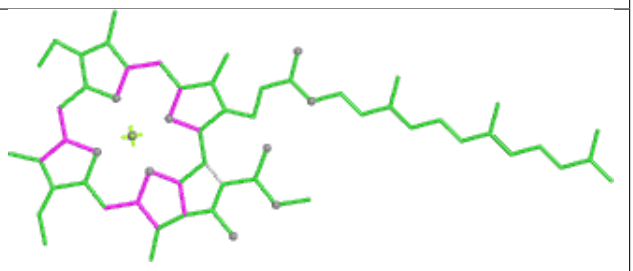


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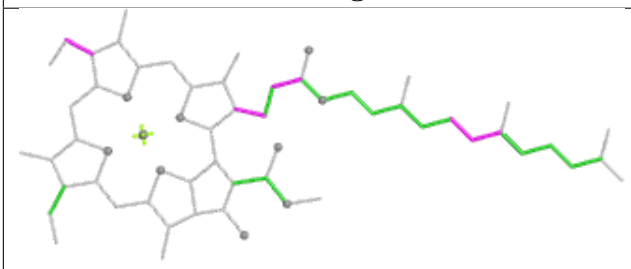
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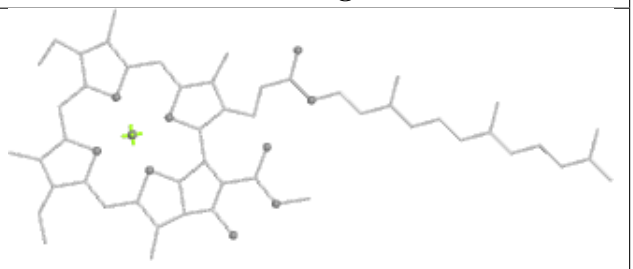
Bond lengths



Bond angles

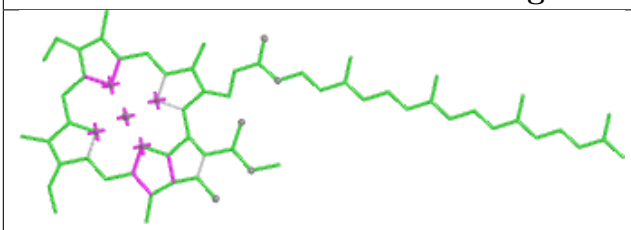


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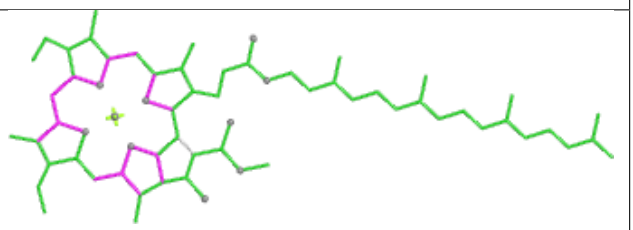


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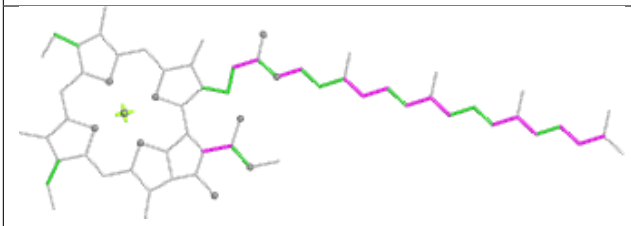
Ligand CLA b 604



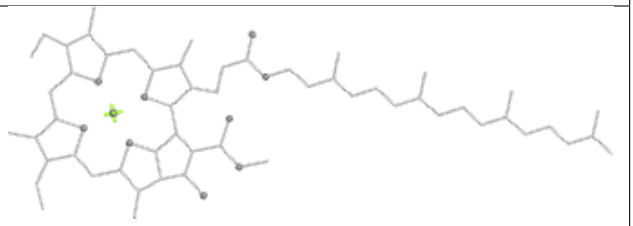
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Bond angles

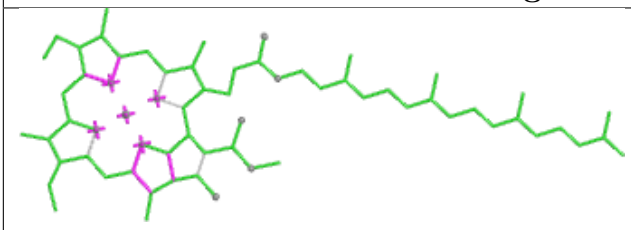


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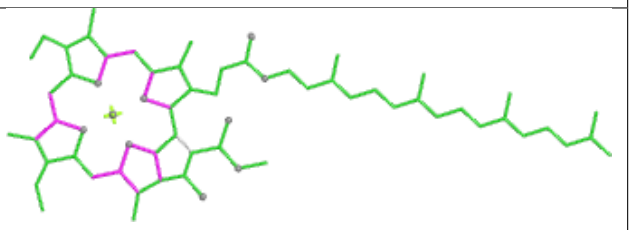


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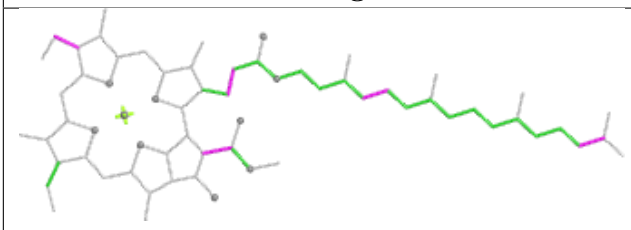
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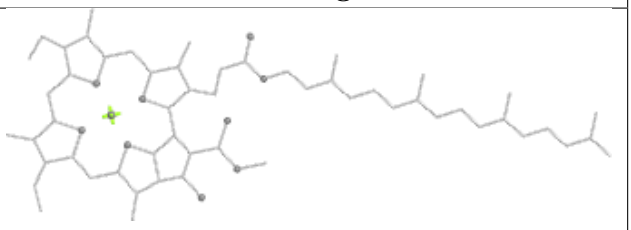
Bond lengths



Bond angles

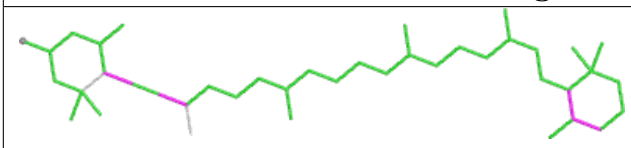


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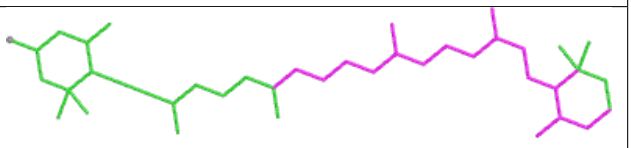


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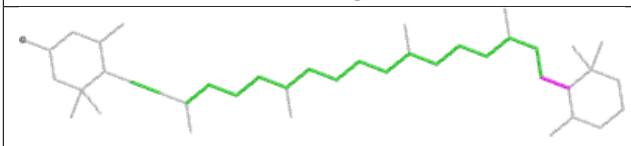
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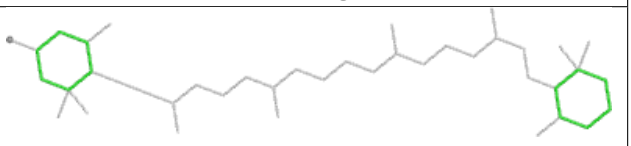
Bond lengths



Bond angles

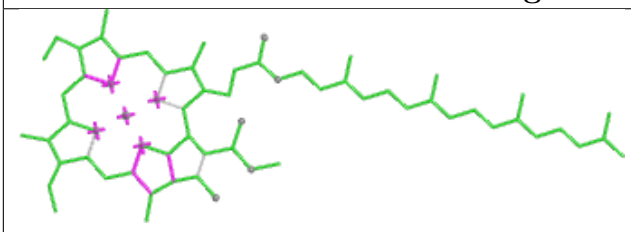


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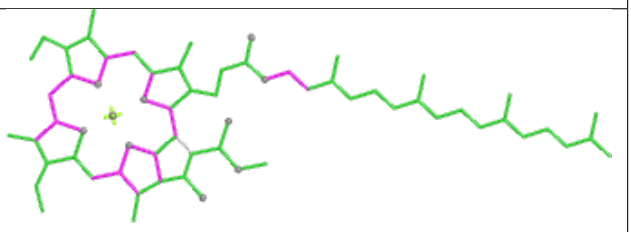


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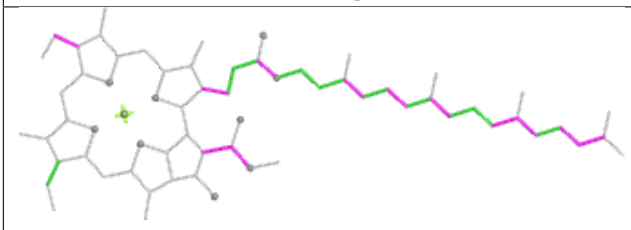
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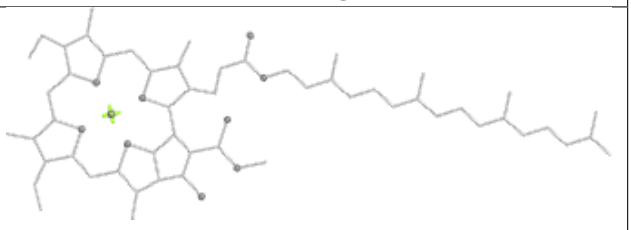
Bond lengths



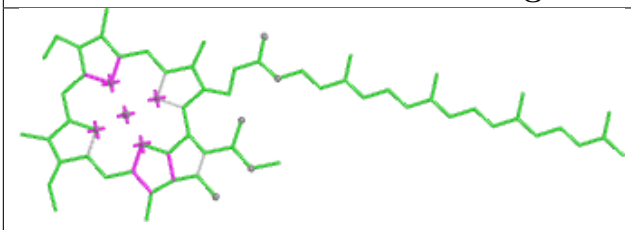
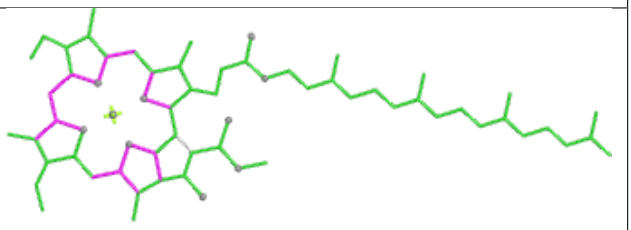
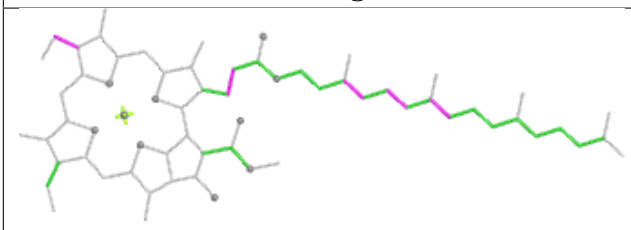
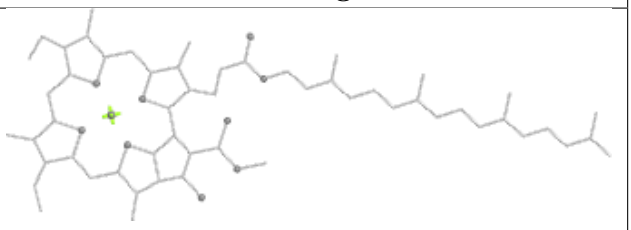
Bond angles

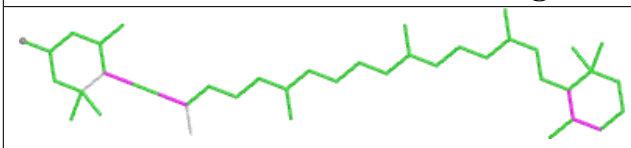
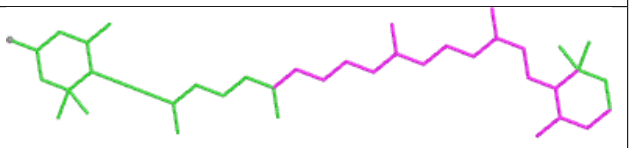
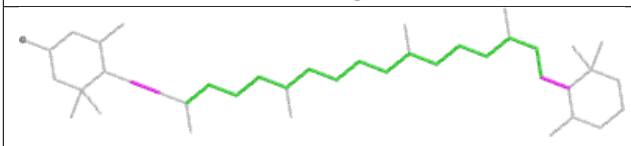
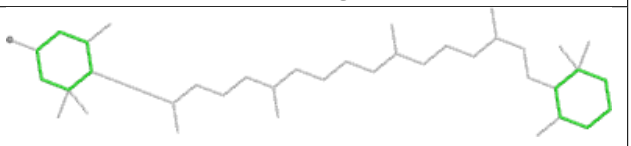


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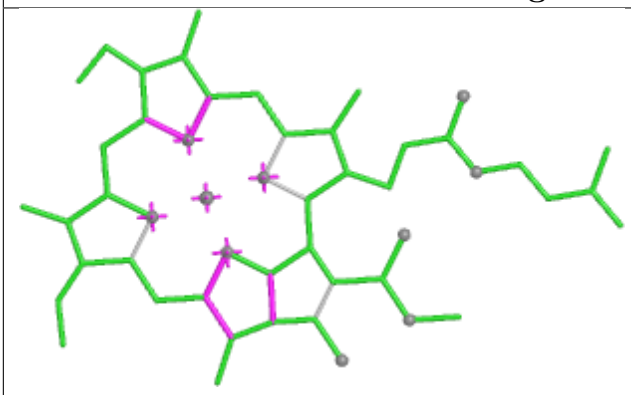


Rings

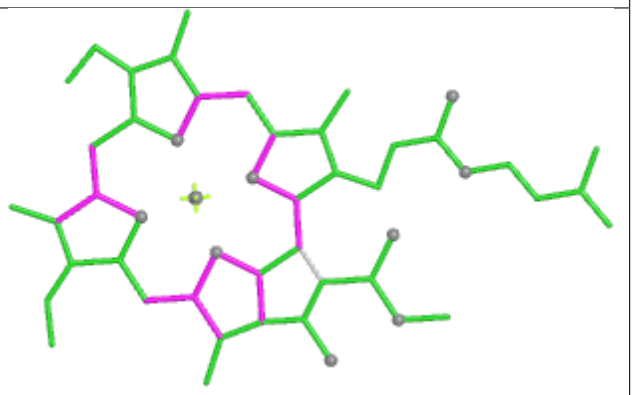
Ligand CLA B 837	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand IHT L 205	
	
Bond lengths	Bond angles
	
Torsions	Rings

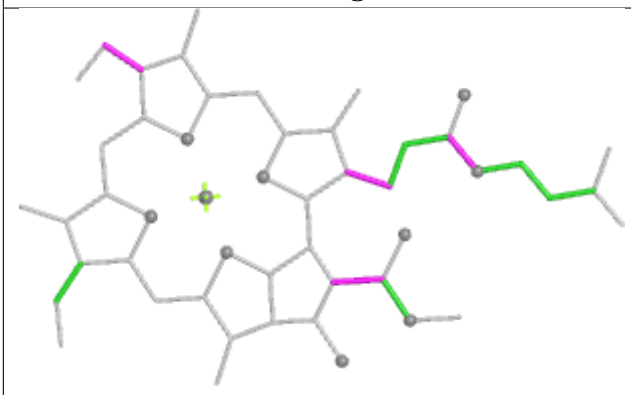
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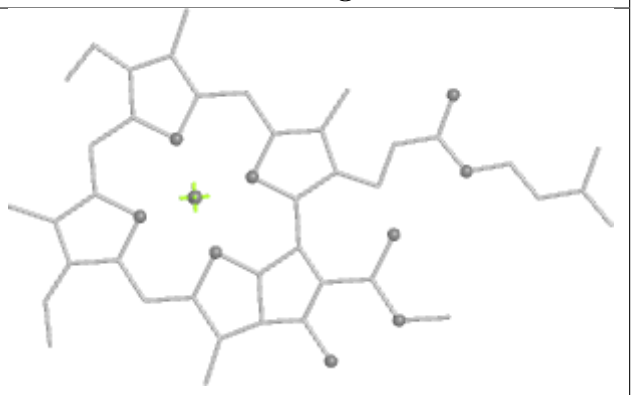
Bond lengths



Bond angles

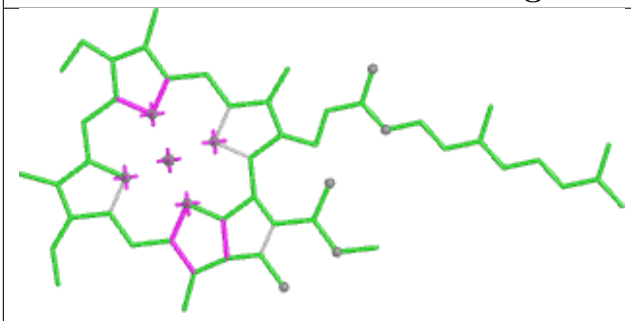


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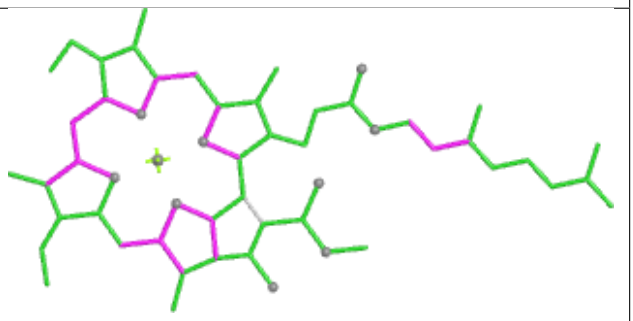


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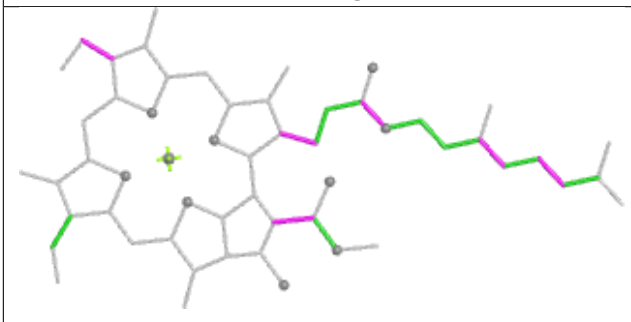
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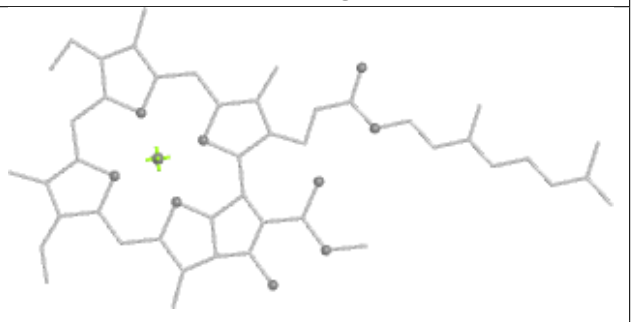
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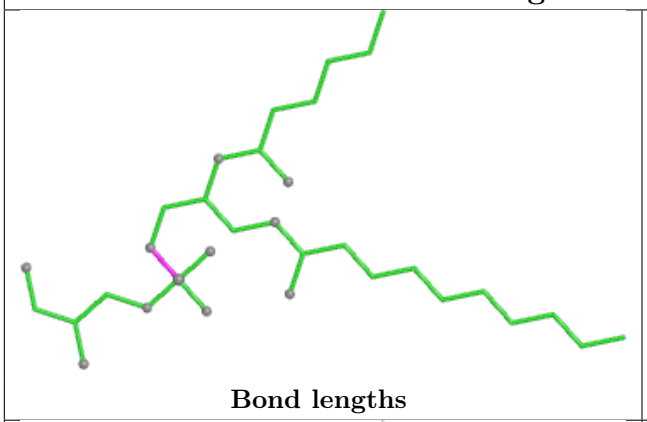


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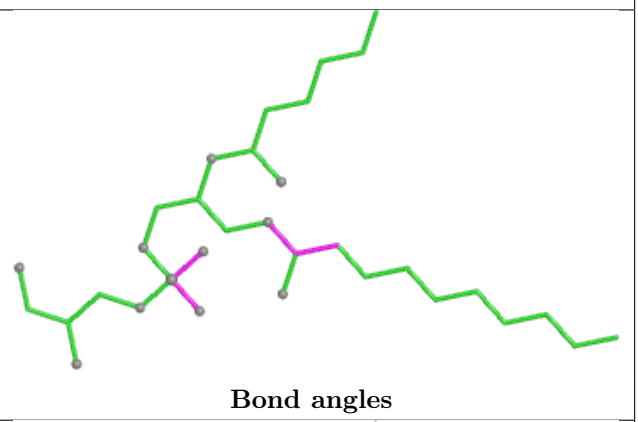


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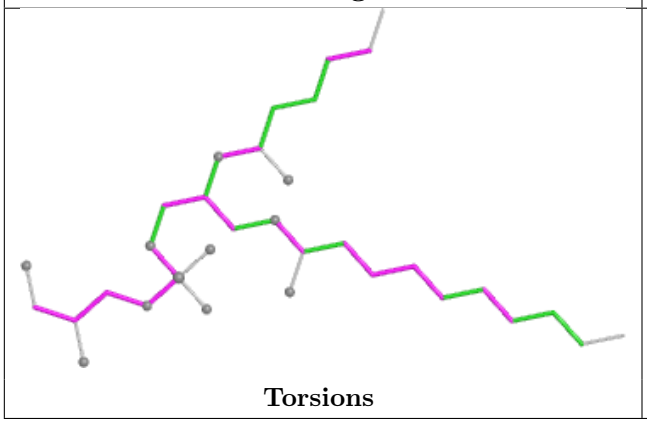
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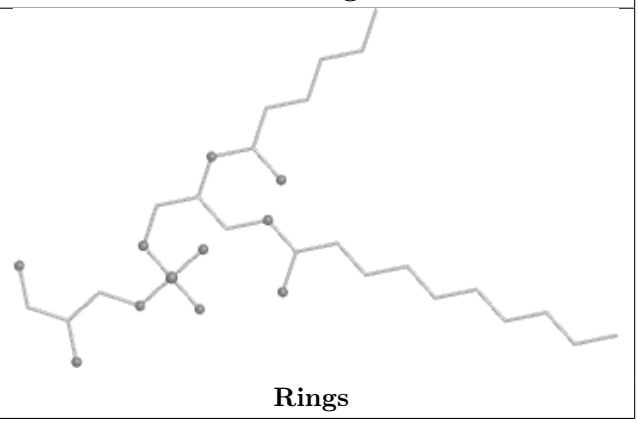
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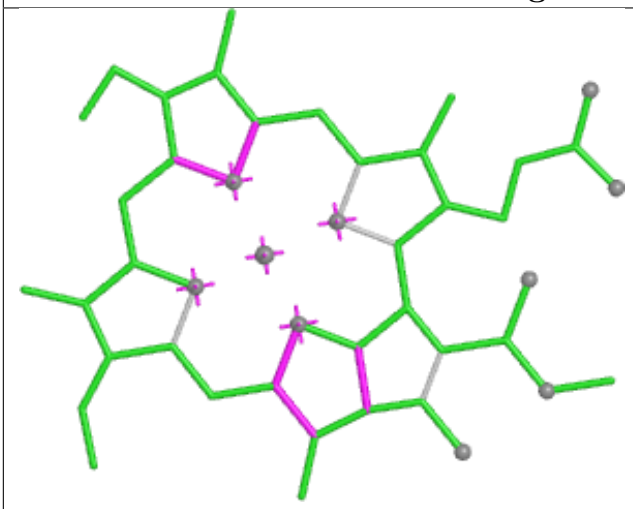


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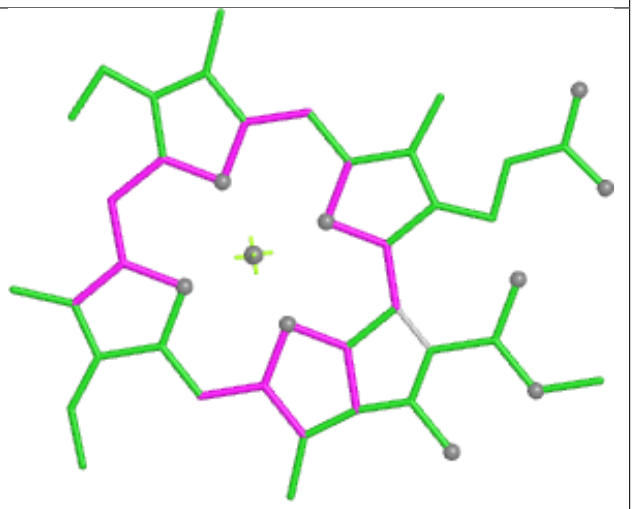


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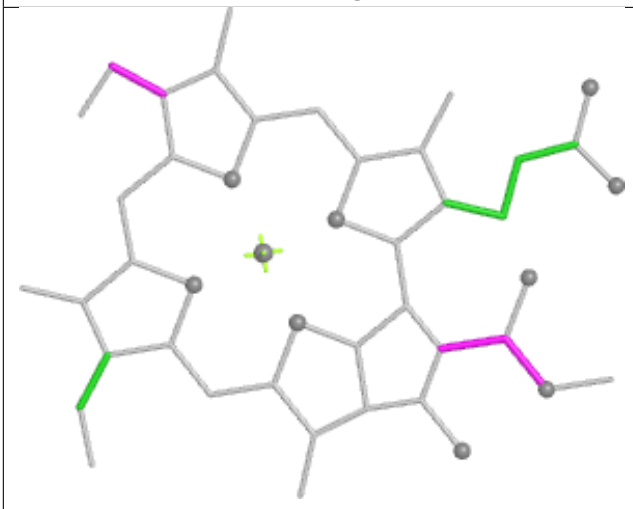
Ligand CLA 1 613



Bond lengths



Bond angles

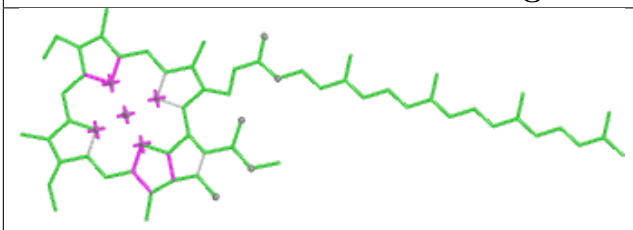


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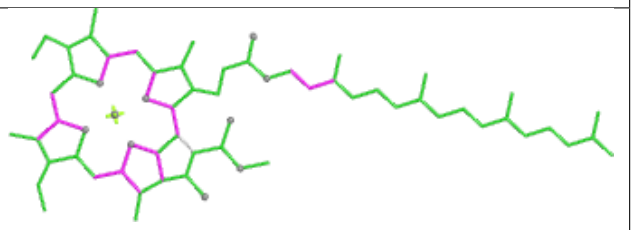


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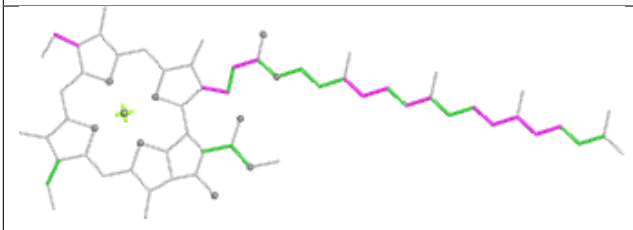
Ligand CLA A 804



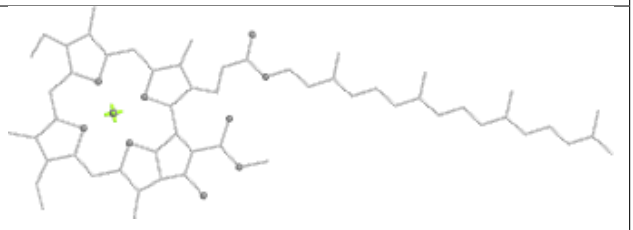
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Bond angles

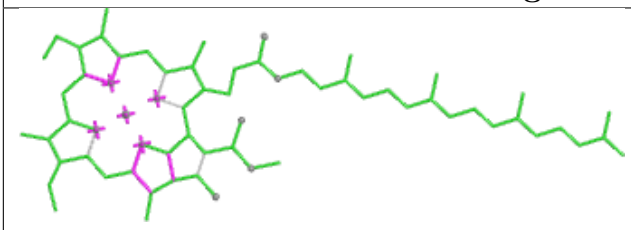


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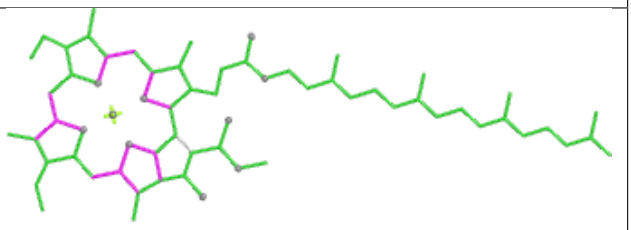


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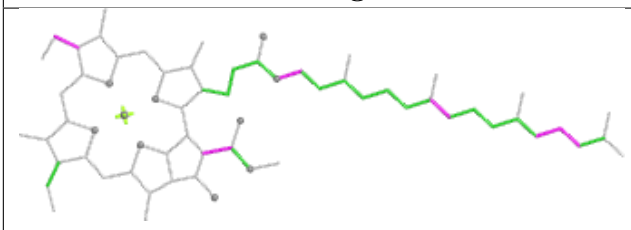
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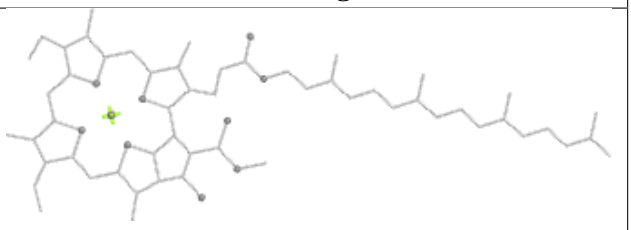
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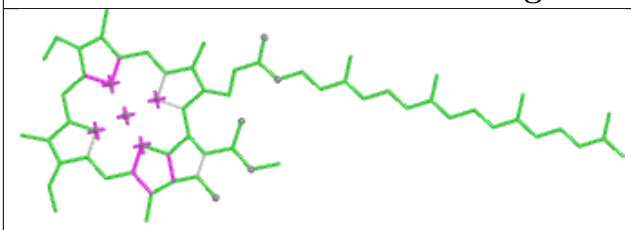


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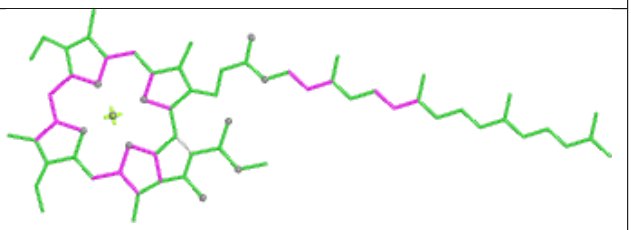


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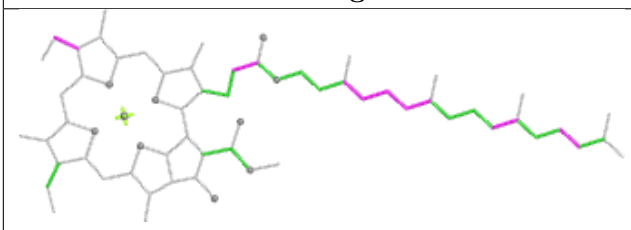
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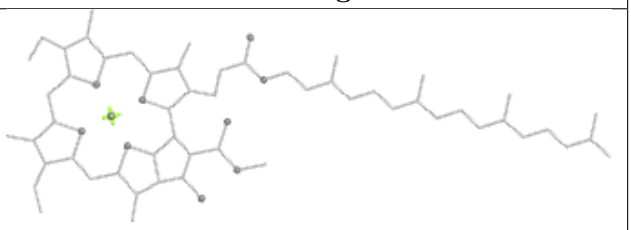
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Bond angles

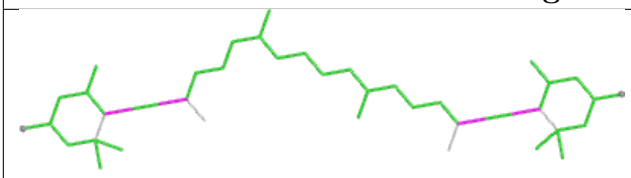


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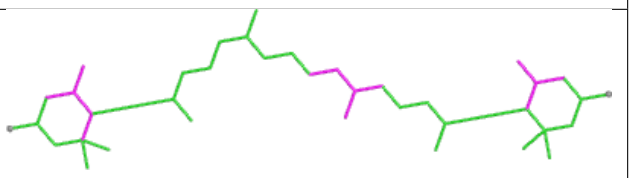


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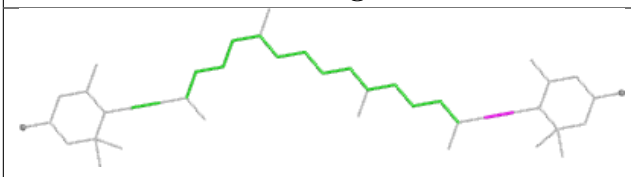
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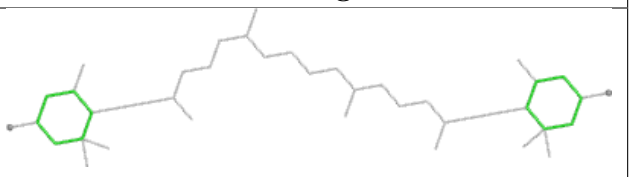
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Bond angles

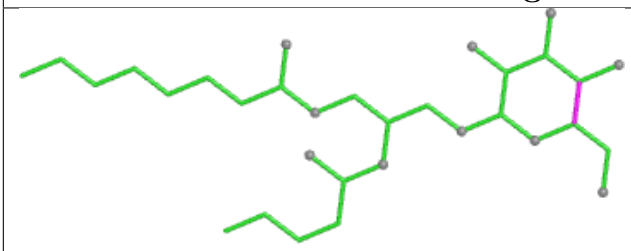


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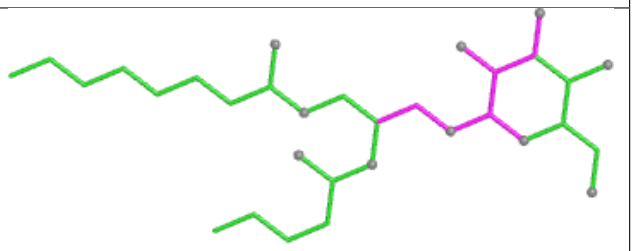


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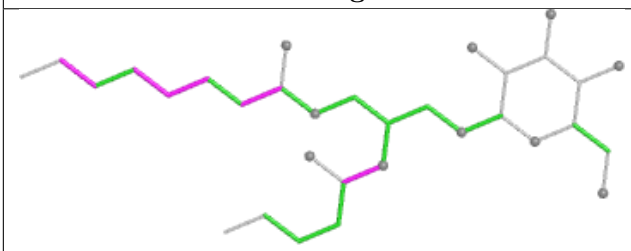
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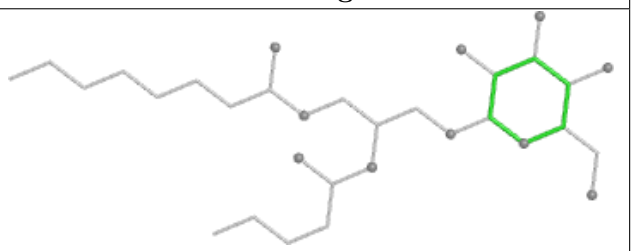
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Bond angles

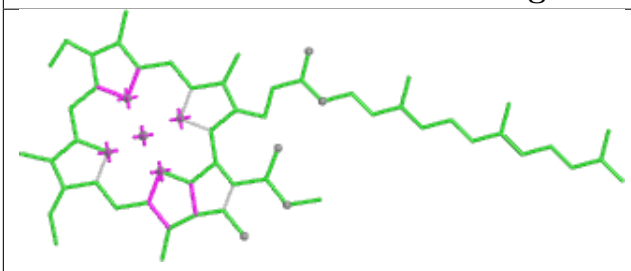


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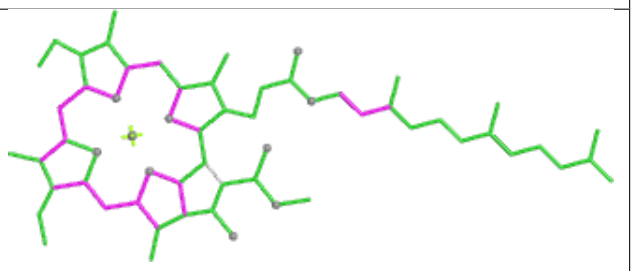


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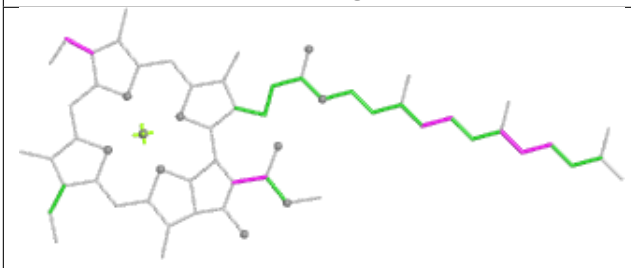
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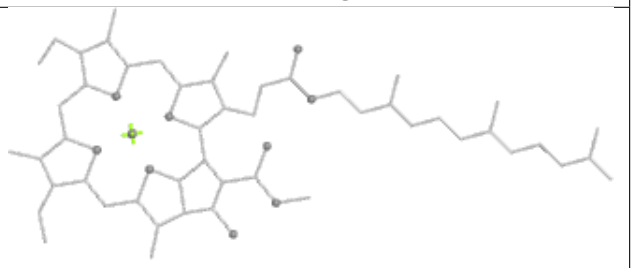
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Bond angles

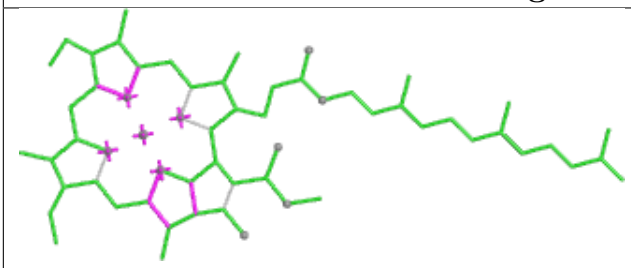


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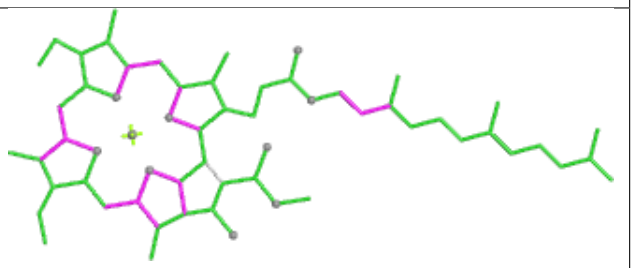


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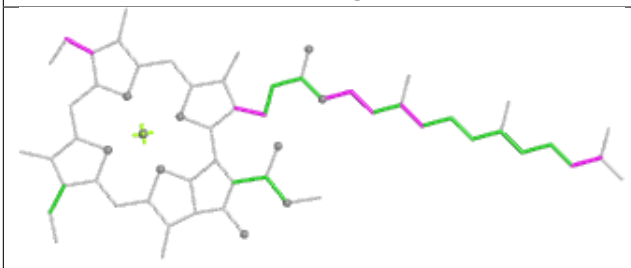
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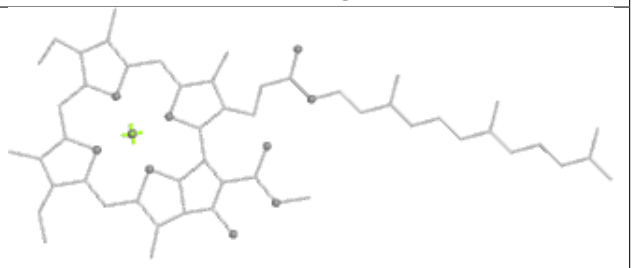
Bond lengths



Bond angles

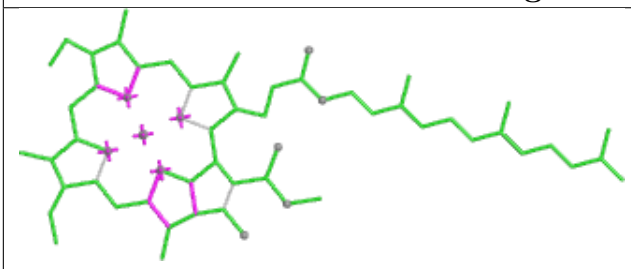


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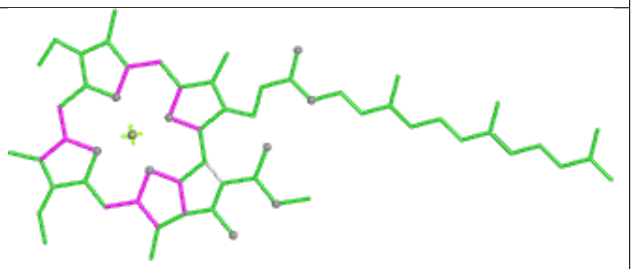


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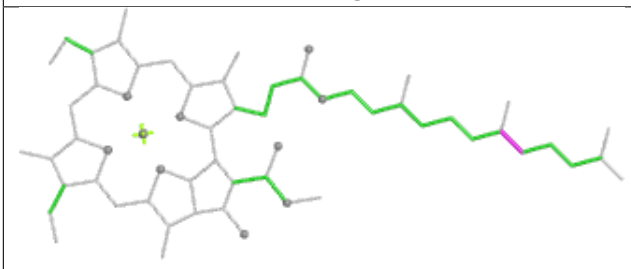
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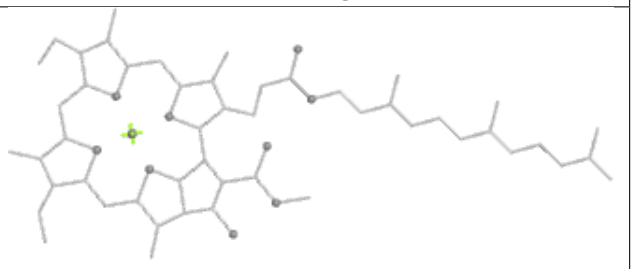
Bond lengths



Bond angles

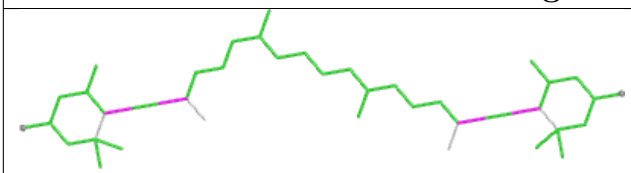


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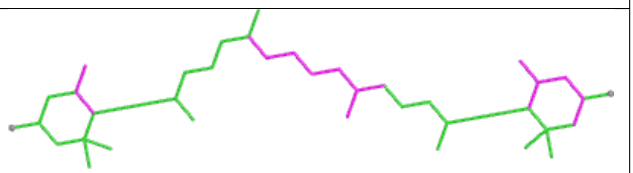


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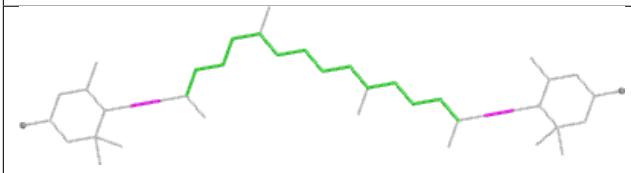
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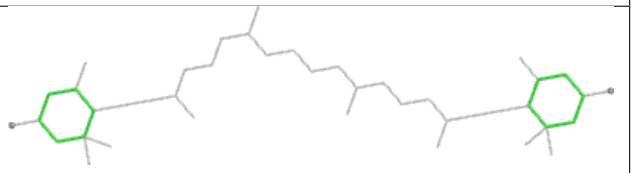
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Bond angles

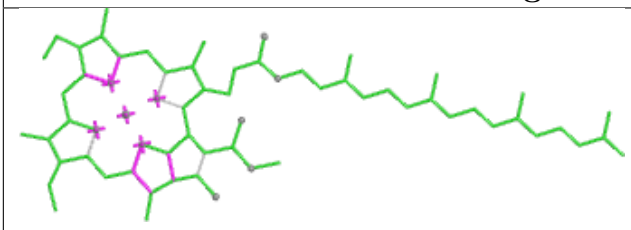


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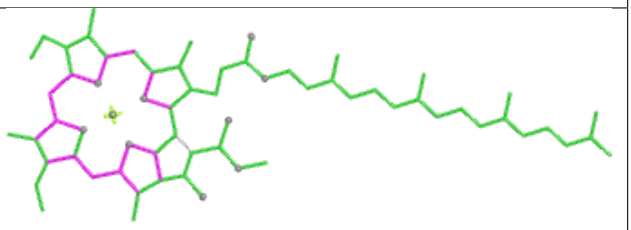


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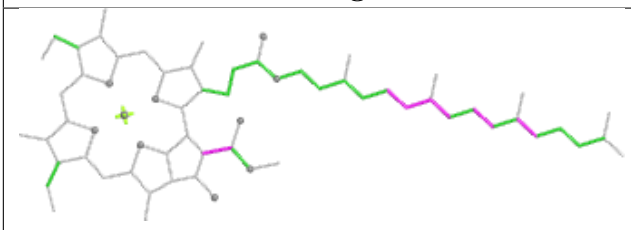
Ligand CLA A 825



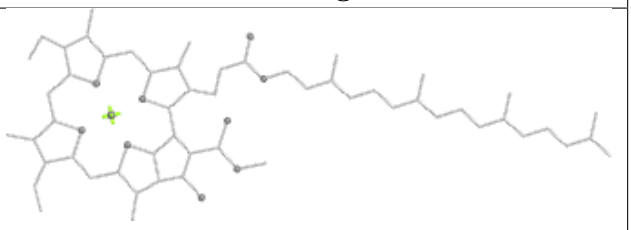
Bond lengths



Bond angles

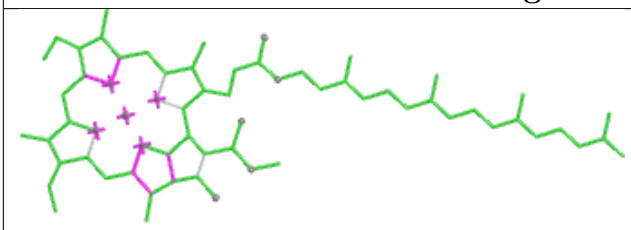


Torsions

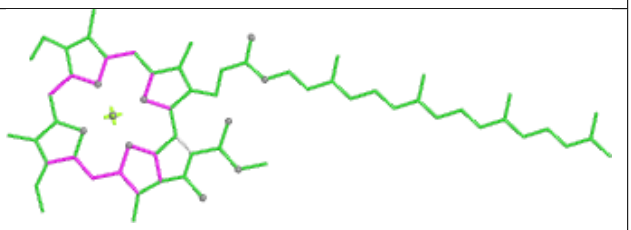


Rings

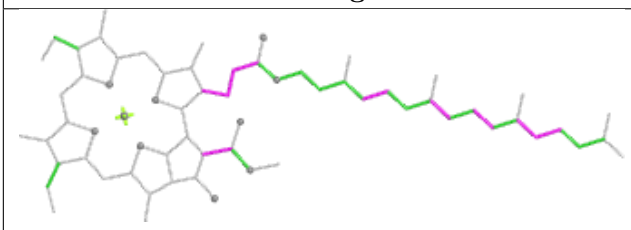
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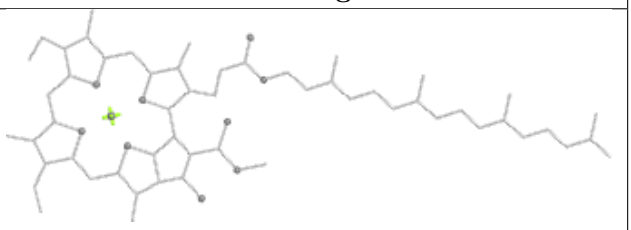
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Bond angles

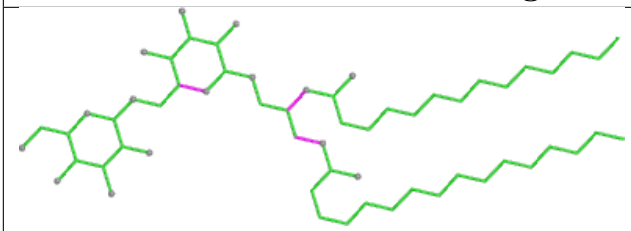


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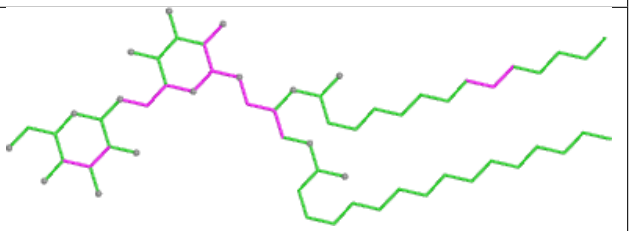


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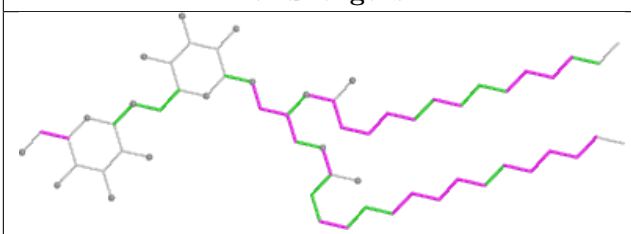
Ligand DGD Z 303



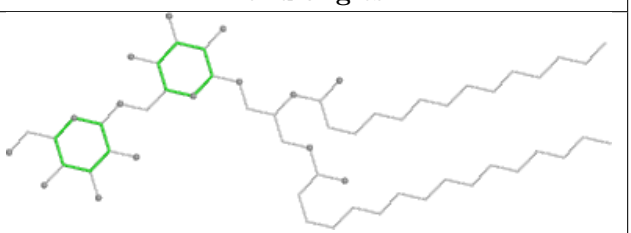
Bond lengths



Bond angles



Torsions

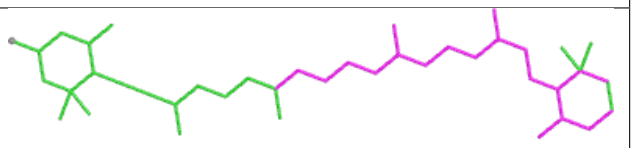


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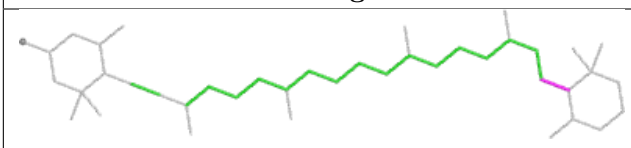
Ligand IHT d 617



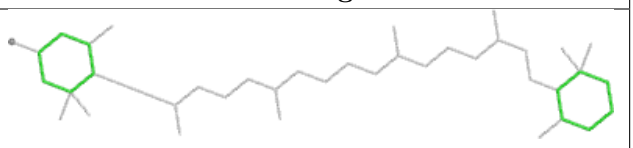
Bond lengths



Bond angles

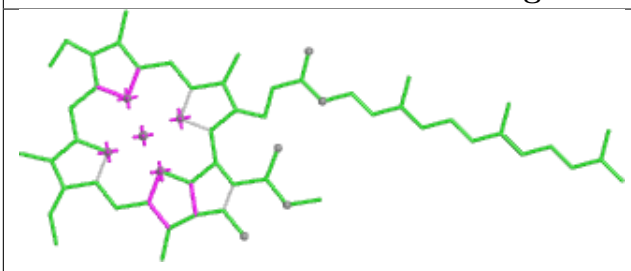


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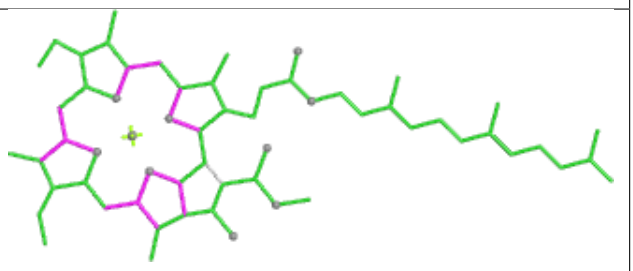


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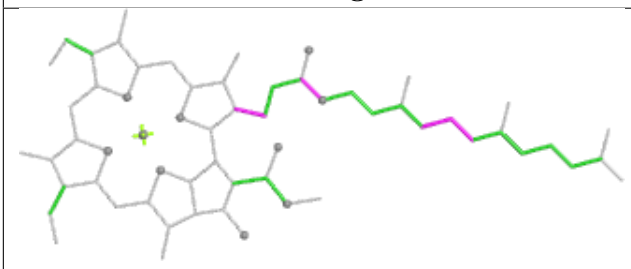
Ligand CLA A 830



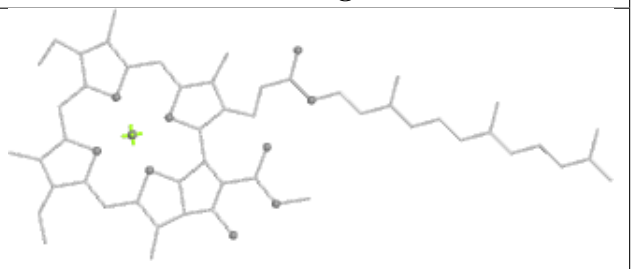
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Bond angles

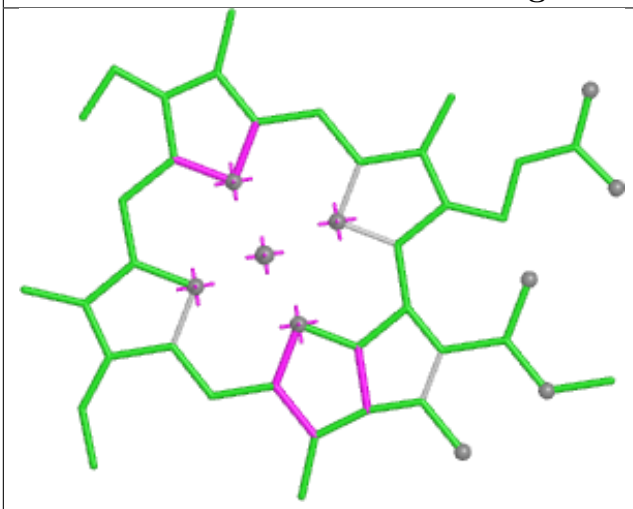


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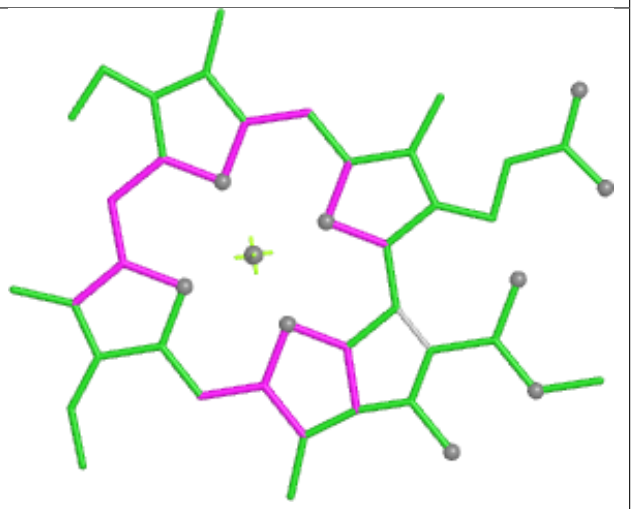


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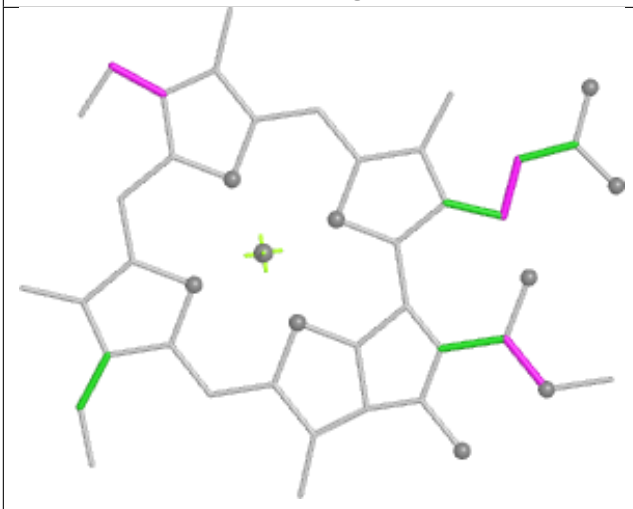
Ligand CLA 9 613



Bond lengths



Bond angles

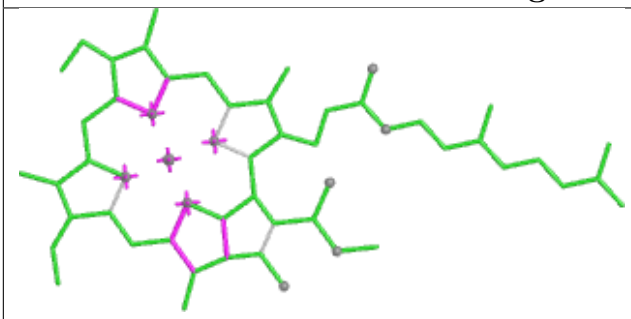


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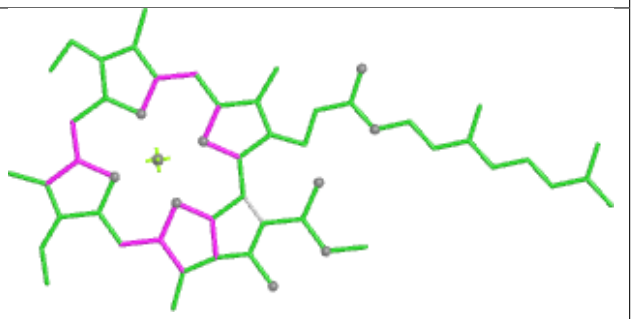


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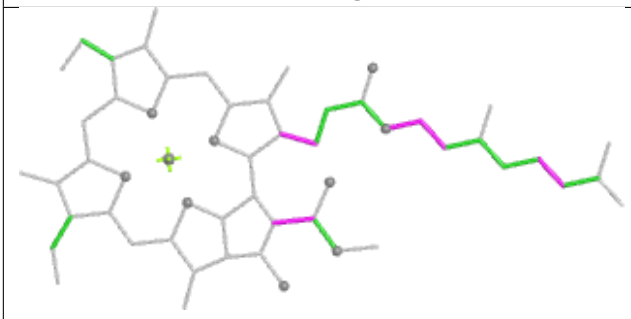
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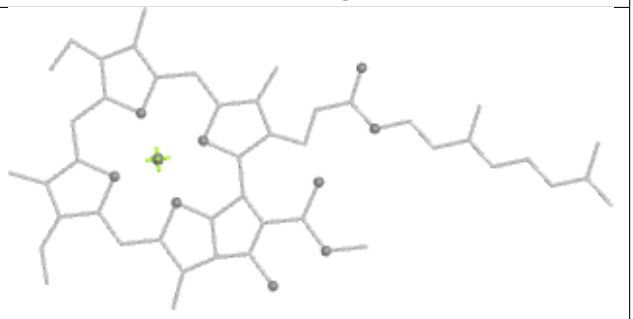
Bond lengths



Bond angles

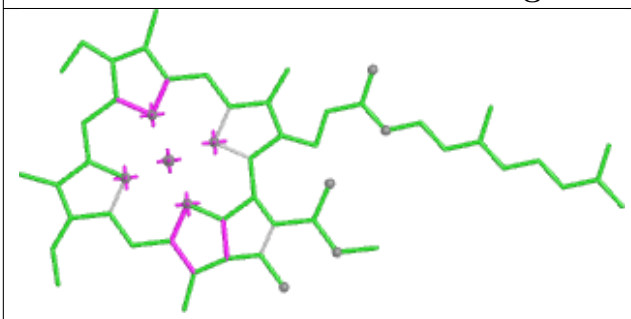


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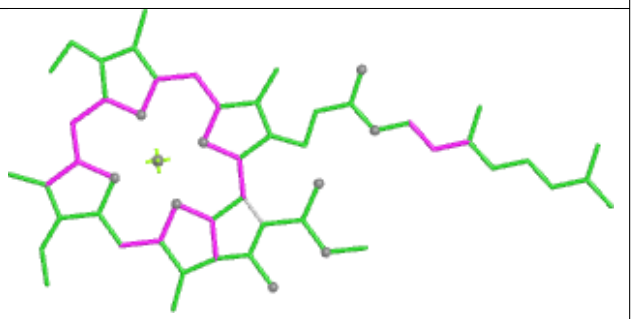


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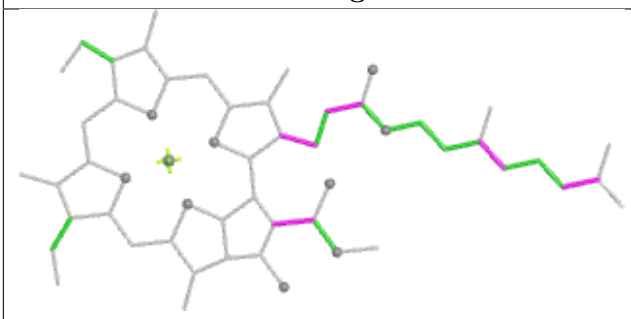
Ligand CLA R 202



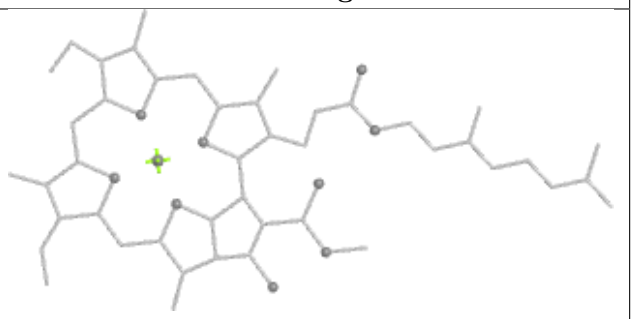
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Bond angles

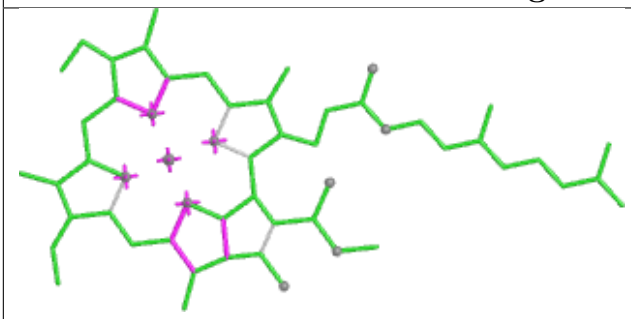


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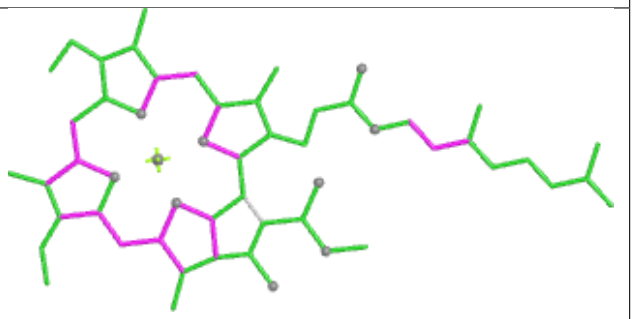


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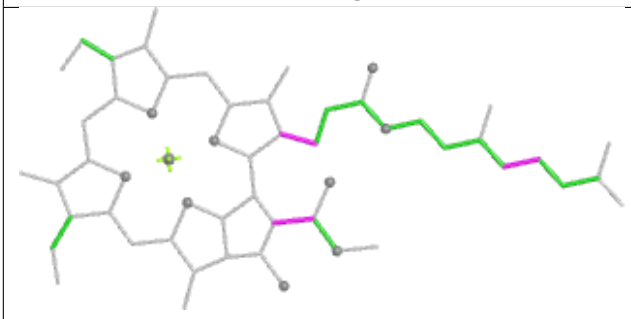
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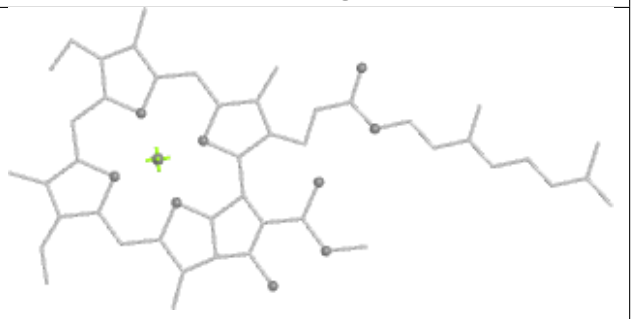
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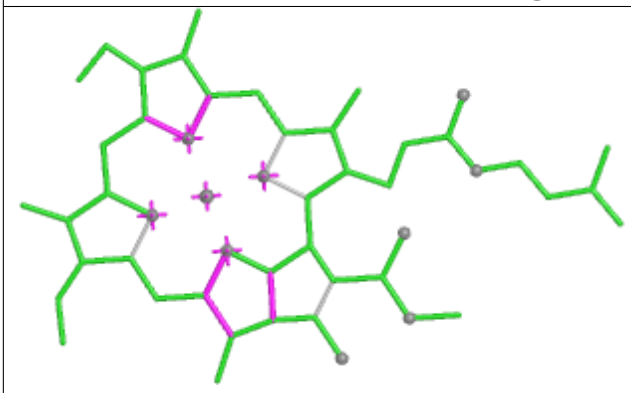


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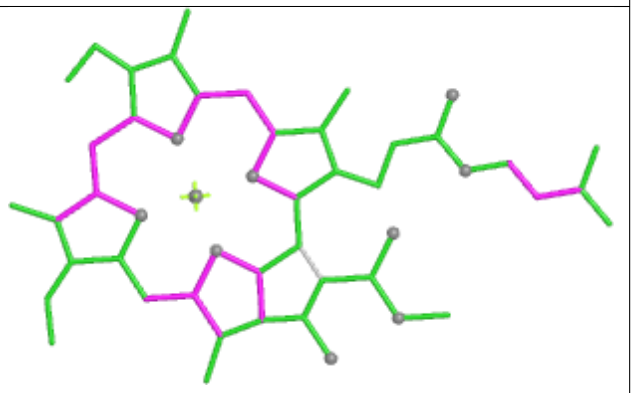


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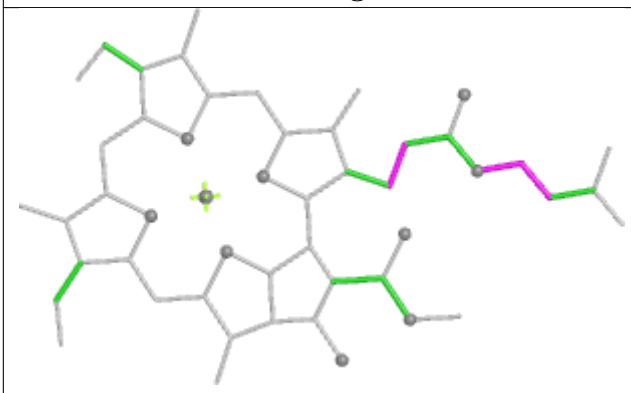
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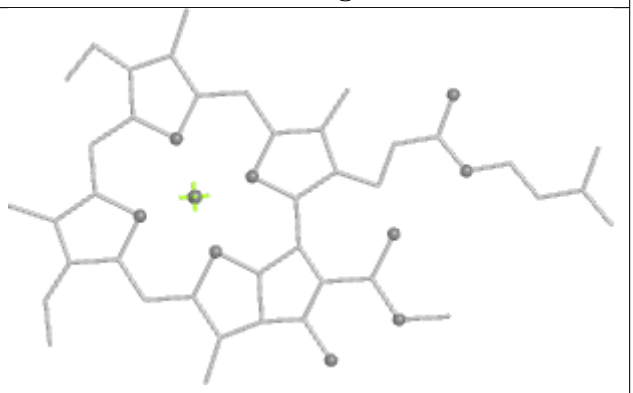
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Bond angles

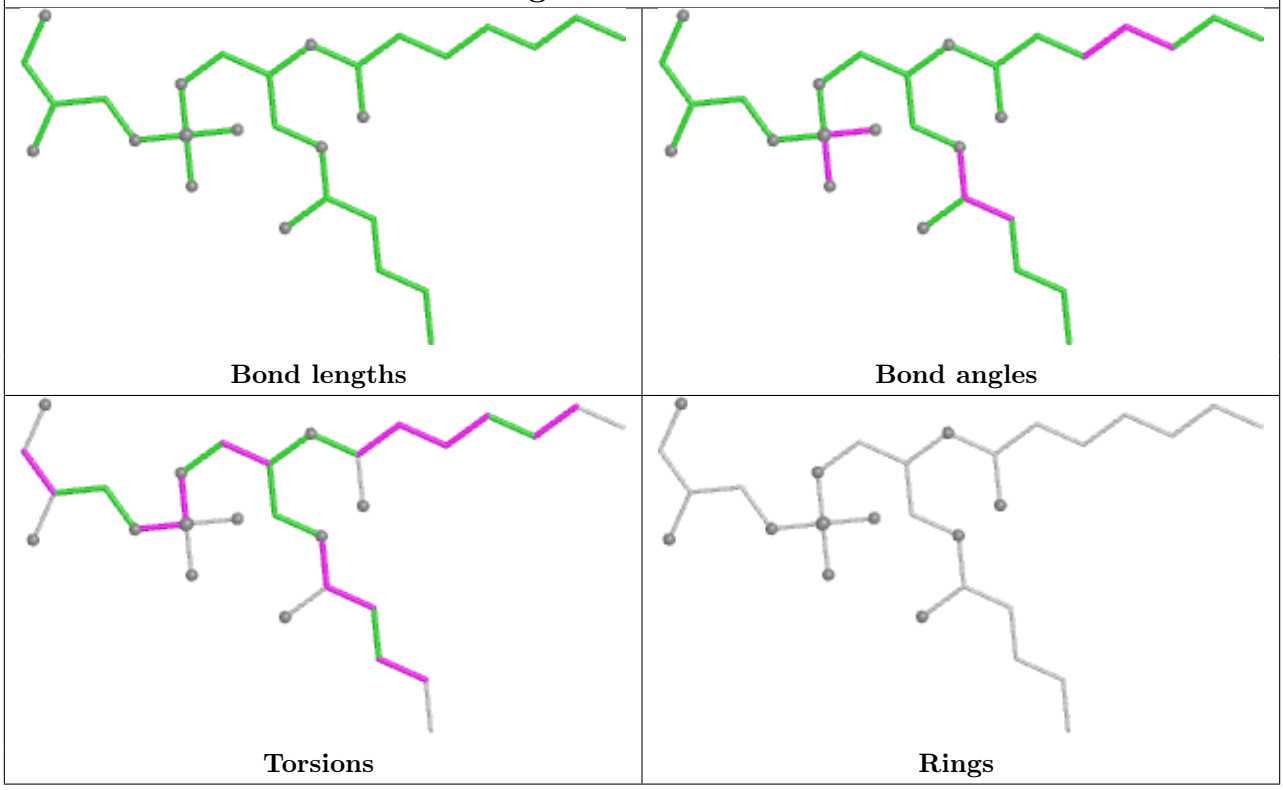


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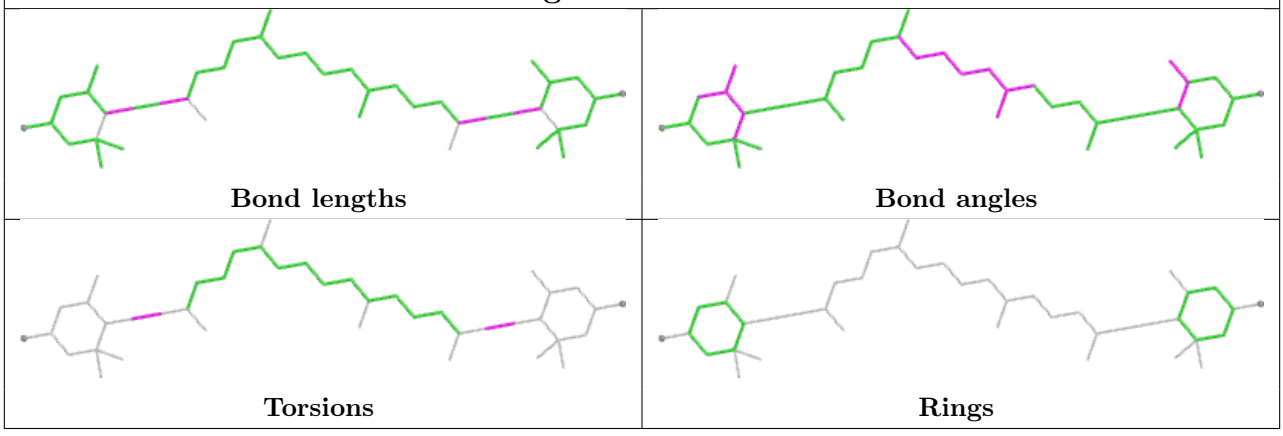


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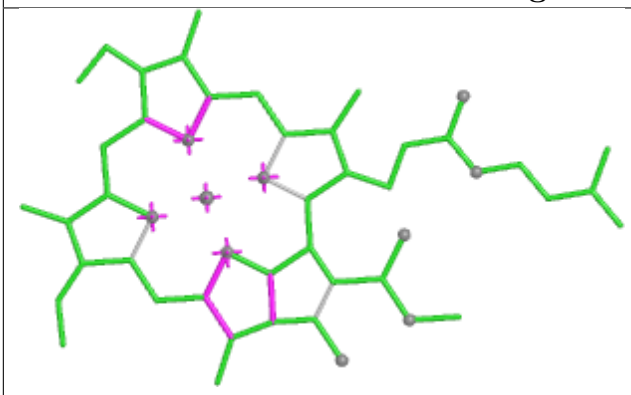
Ligand LHG c 621



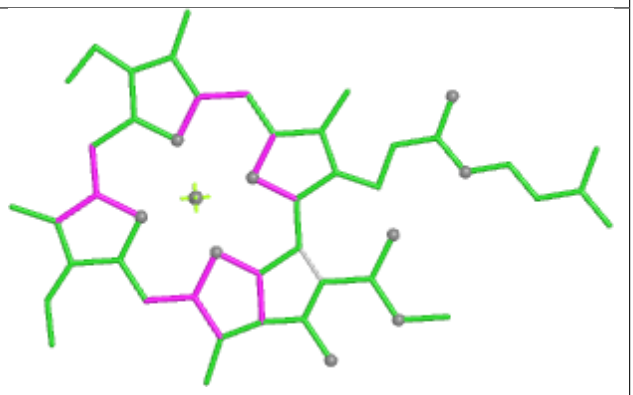
Ligand II0 4 612



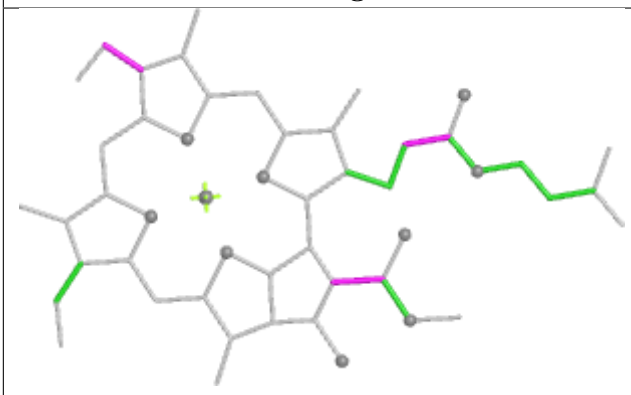
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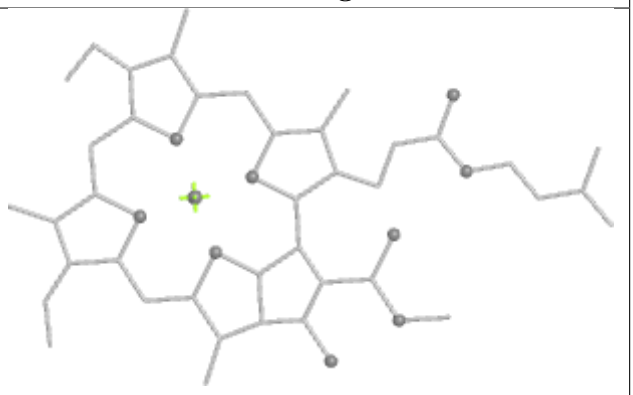
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Bond angles

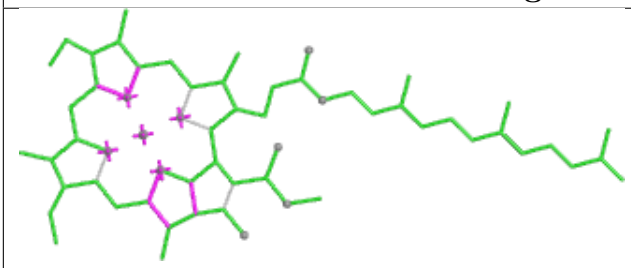


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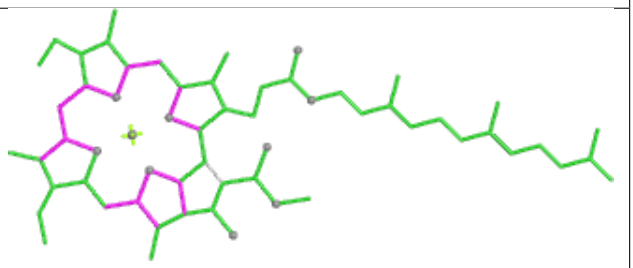


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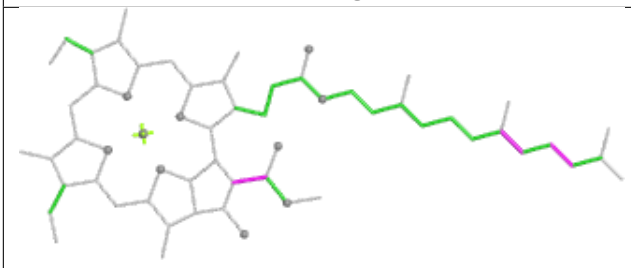
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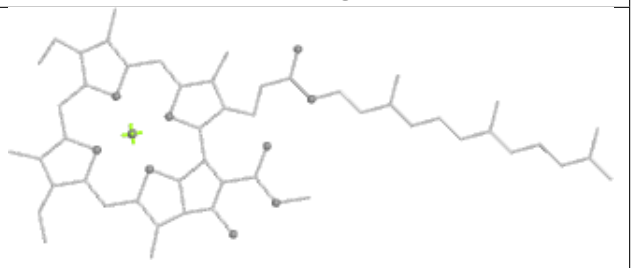
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Bond angles

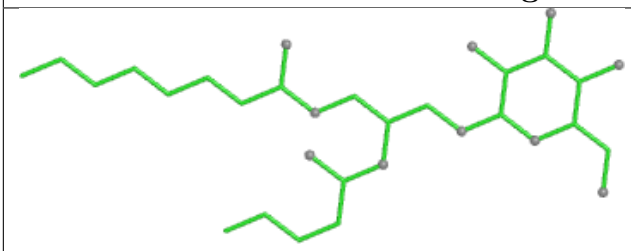


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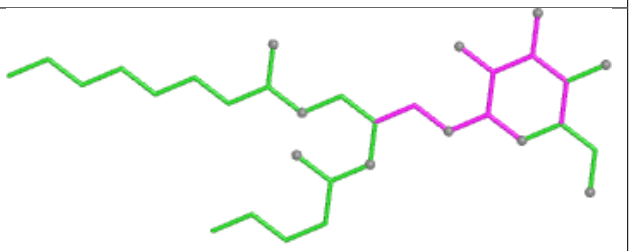


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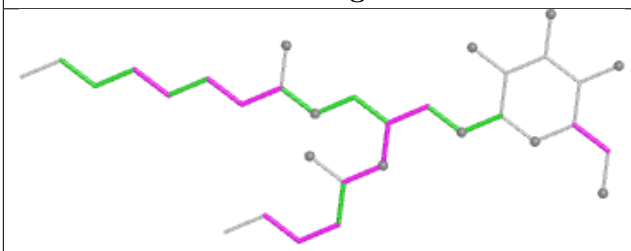
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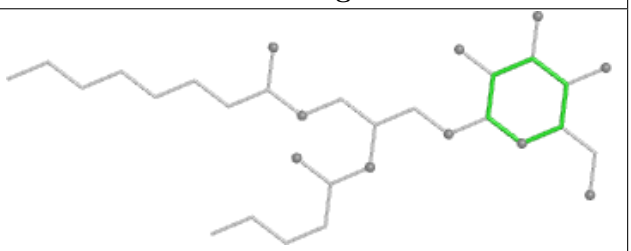
Bond lengths



Bond angles

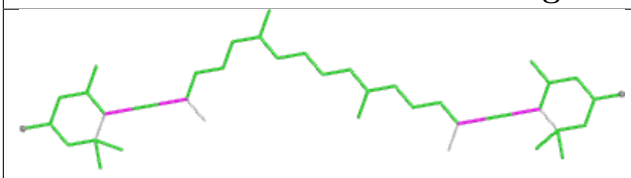


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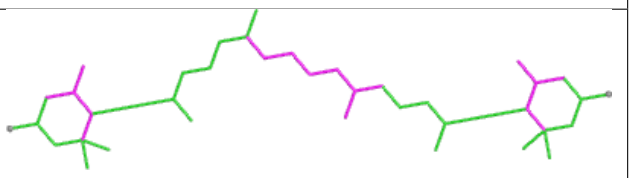


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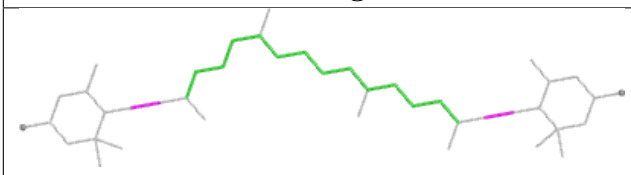
Ligand II0 2 615



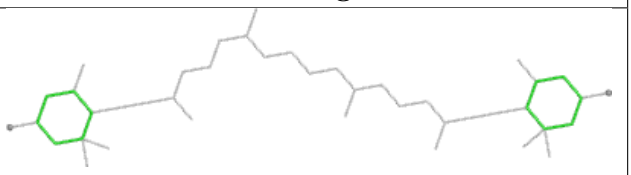
Bond lengths



Bond angles

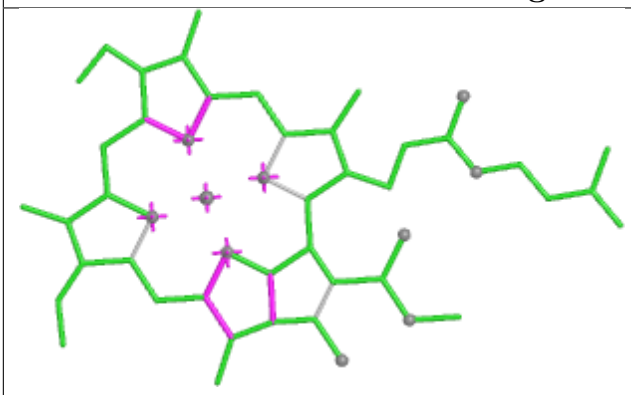


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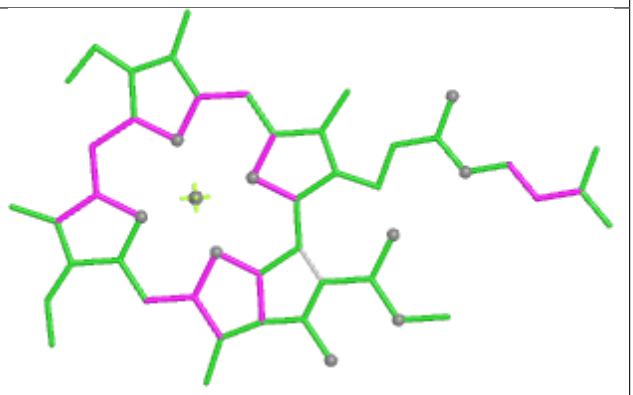


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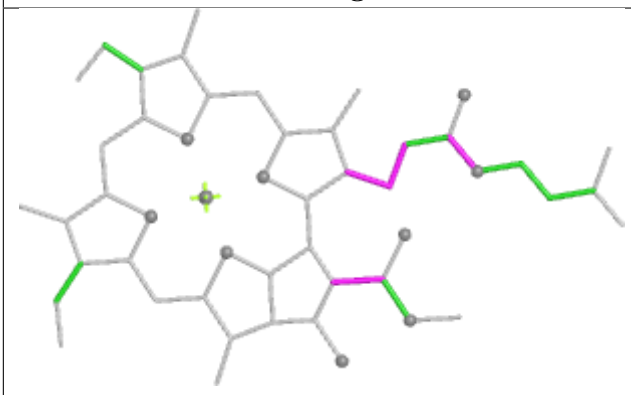
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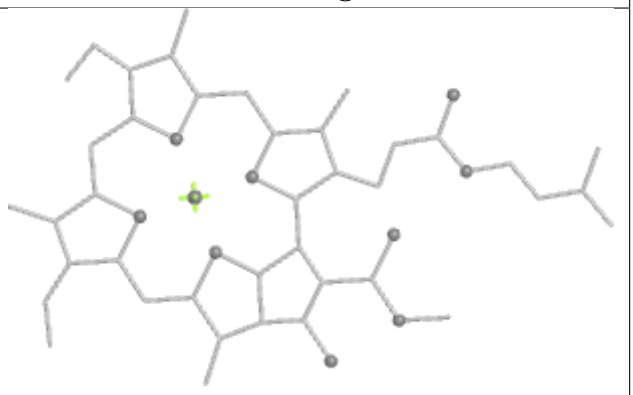
Bond lengths



Bond angles

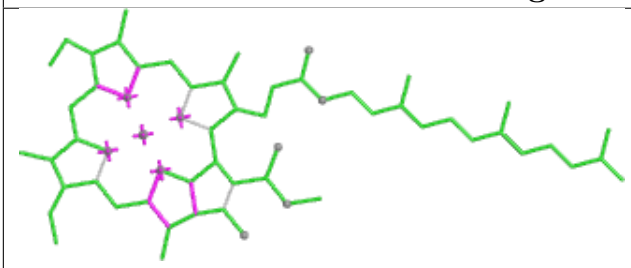


Torsions

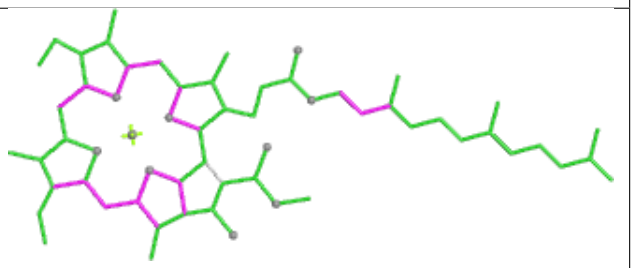


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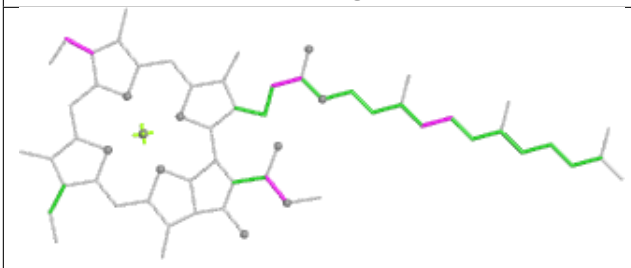
Ligand CLA 1 608



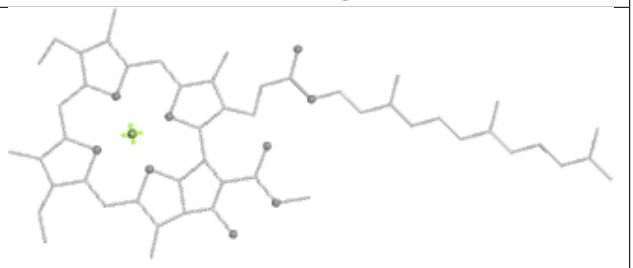
Bond lengths



Bond angles

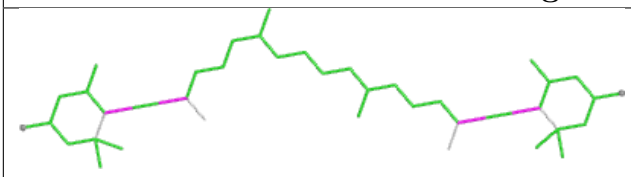


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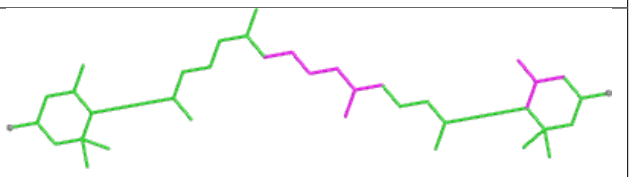


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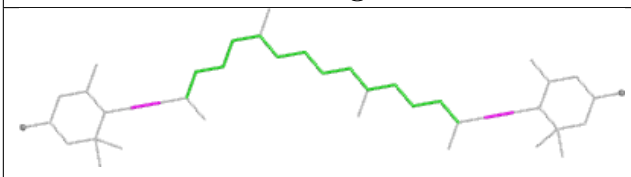
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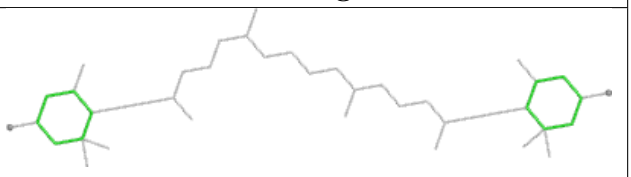
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Bond angles

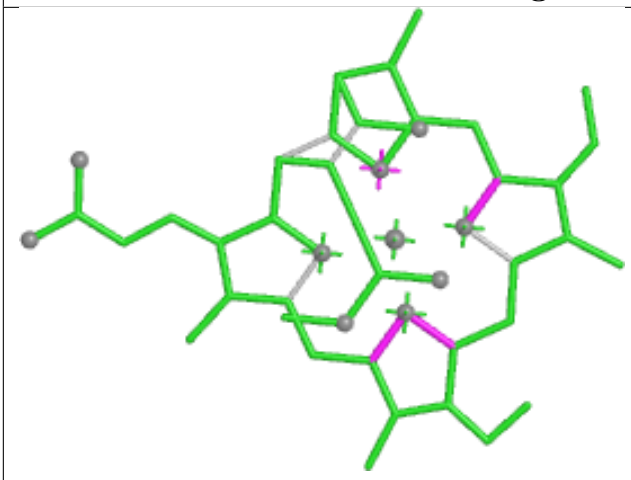


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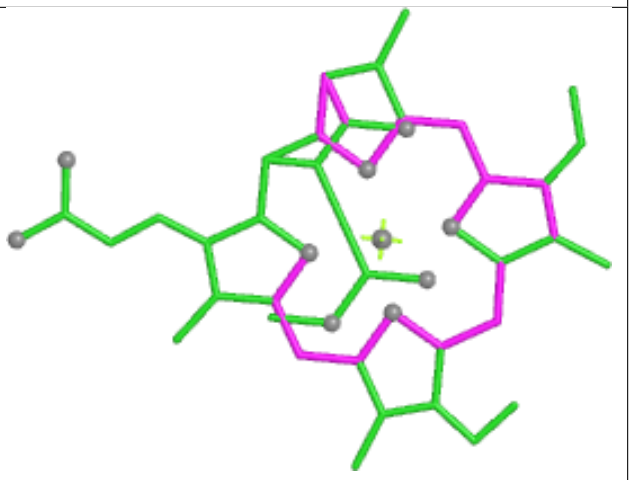


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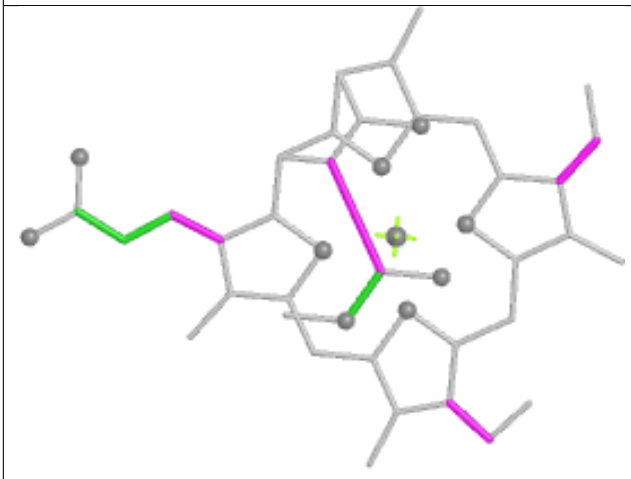
Ligand KC2 3 606



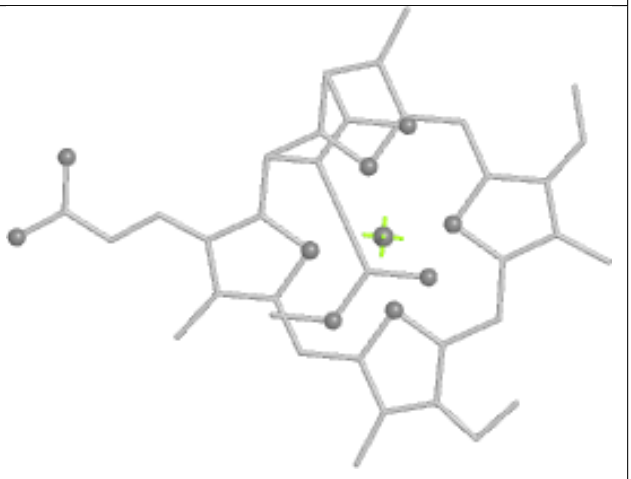
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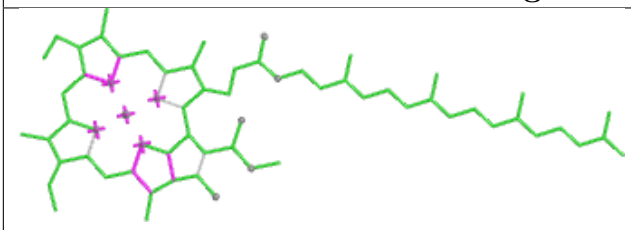
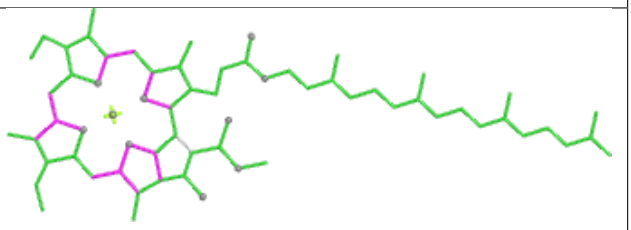
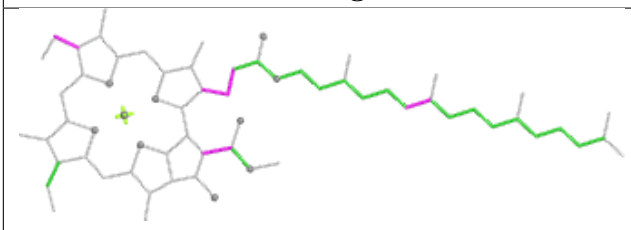
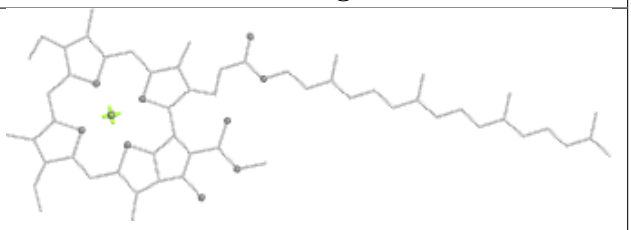
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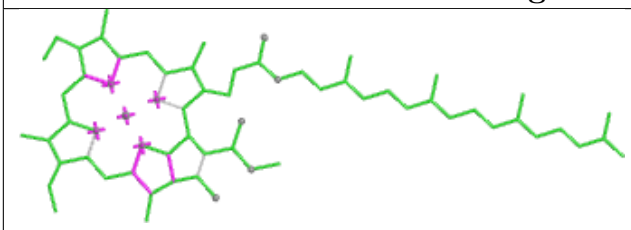
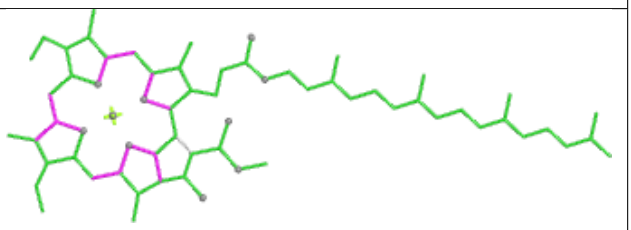
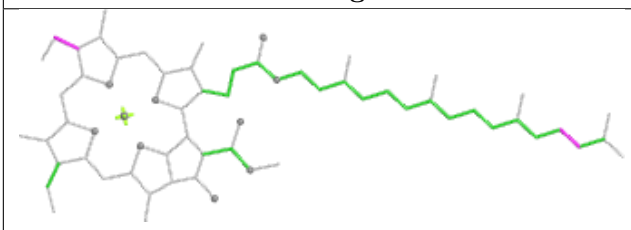
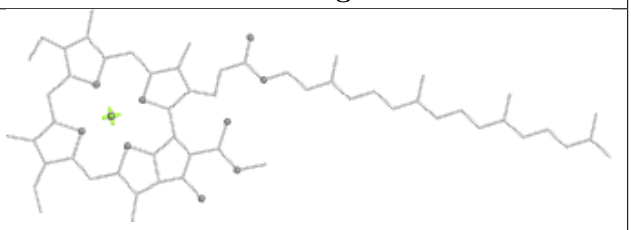


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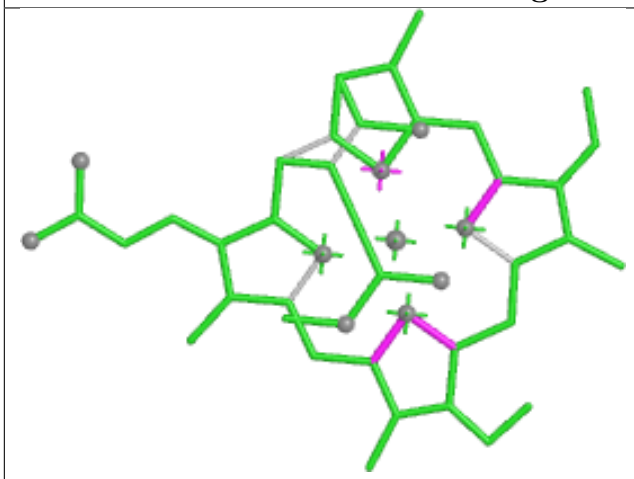


Rings

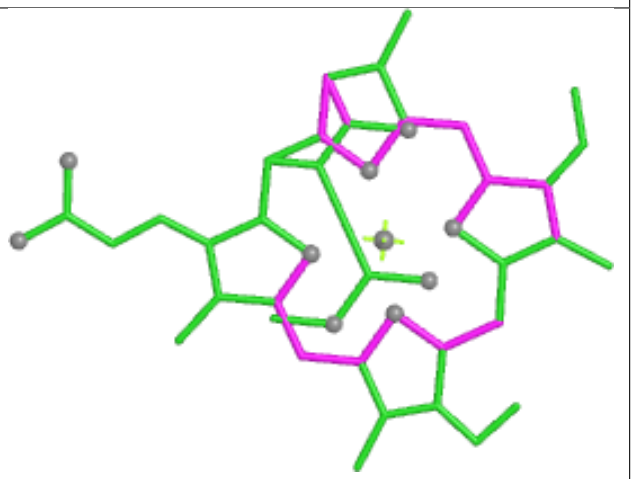
Ligand CLA A 824	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 3 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

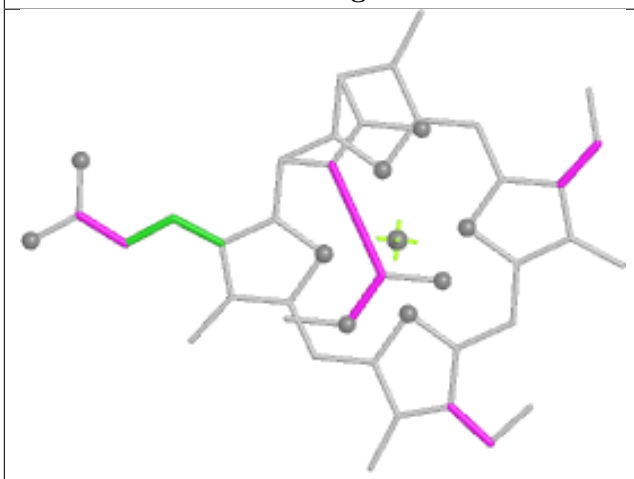
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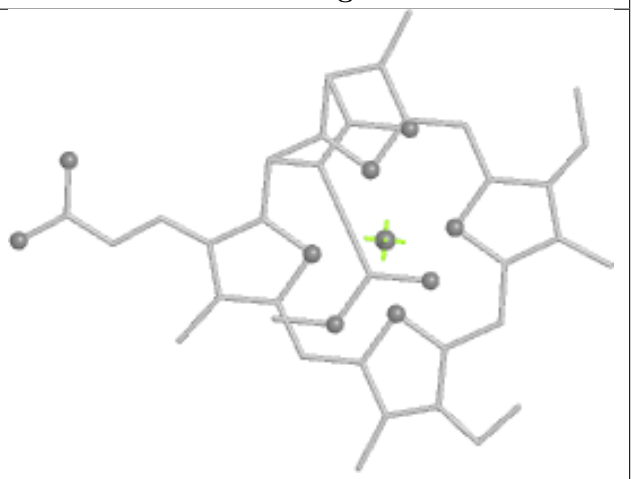
Bond lengths



Bond angles

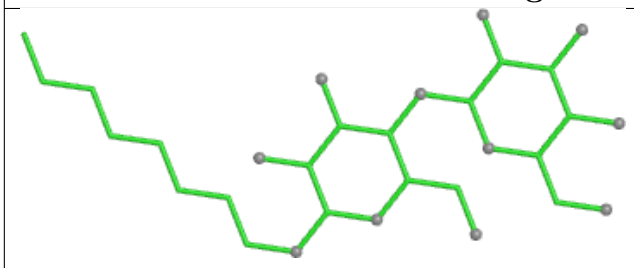


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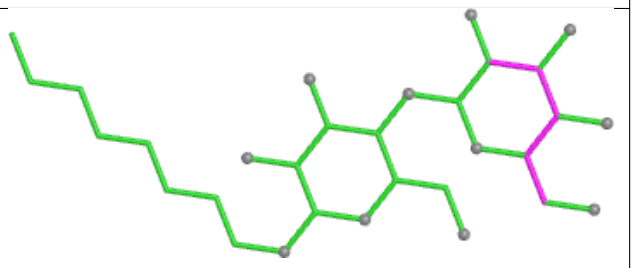


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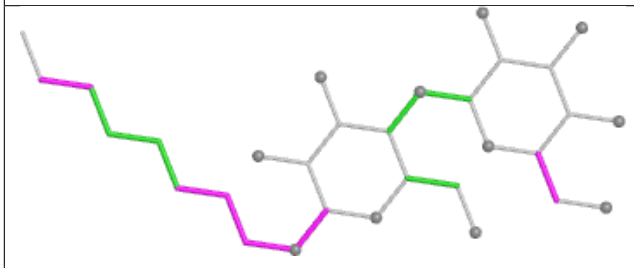
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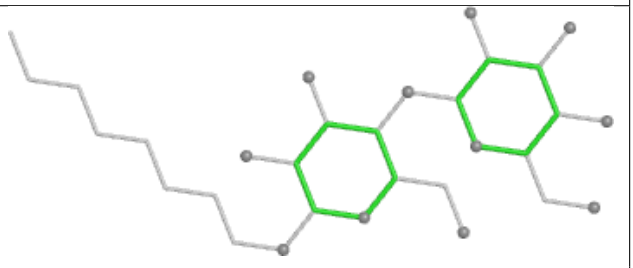
Bond lengths



Bond angles

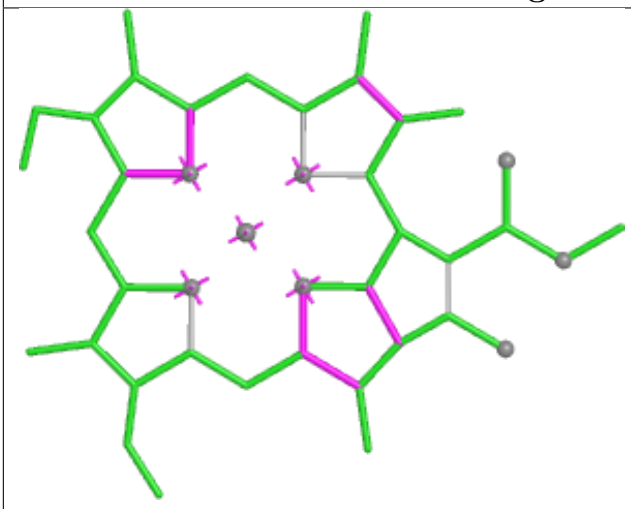


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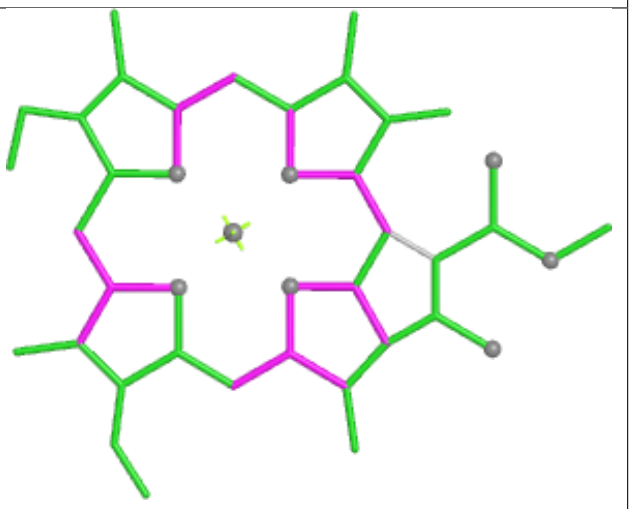


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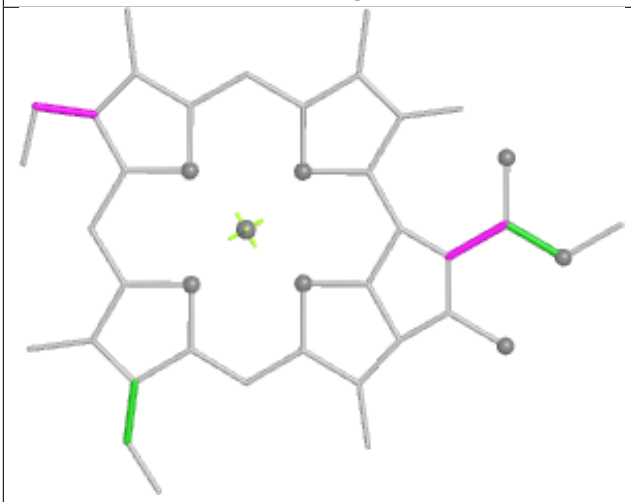
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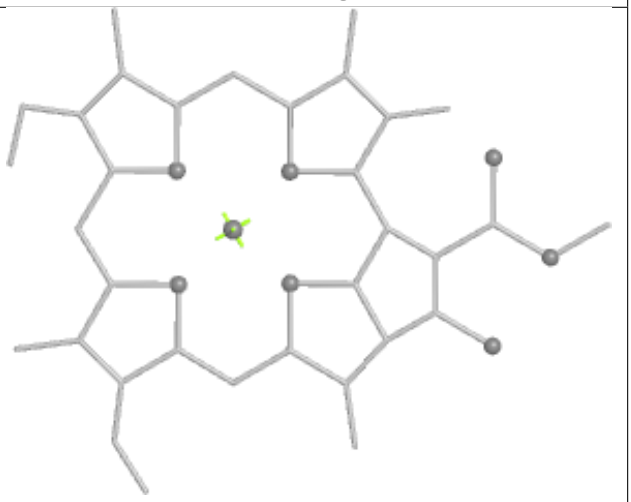
Bond lengths



Bond angles

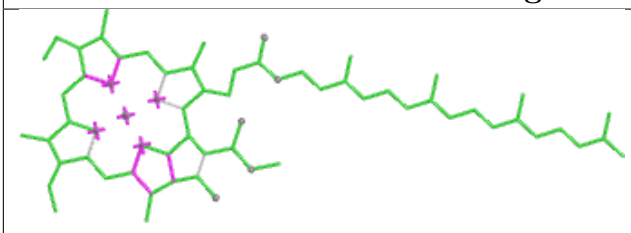


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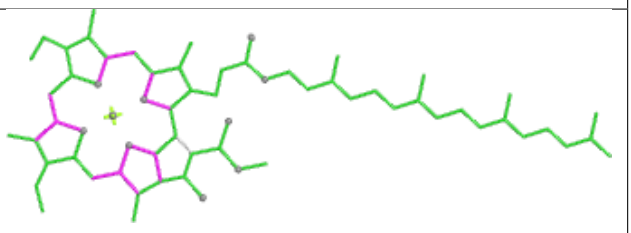


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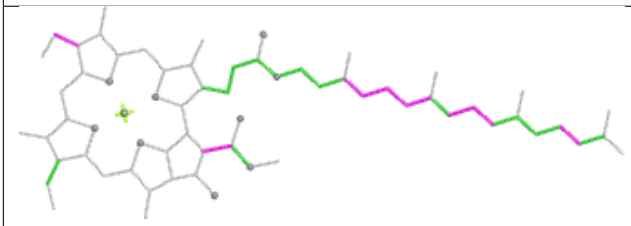
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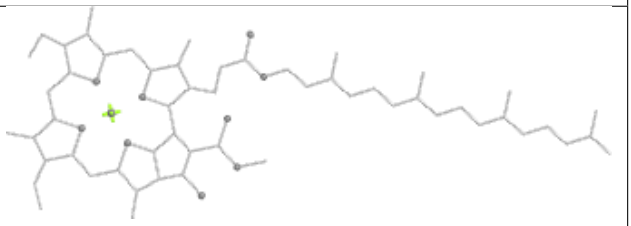
Bond lengths



Bond angles

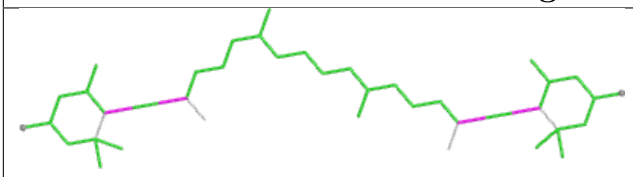


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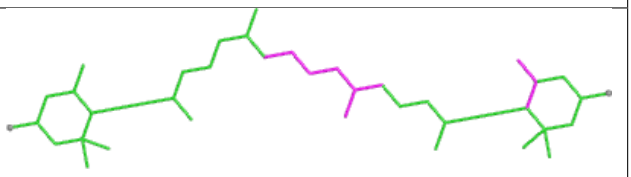


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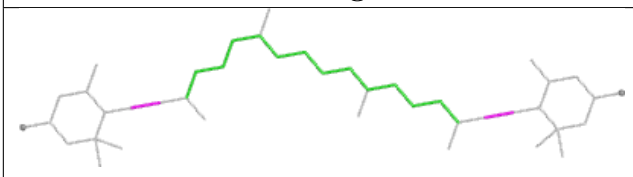
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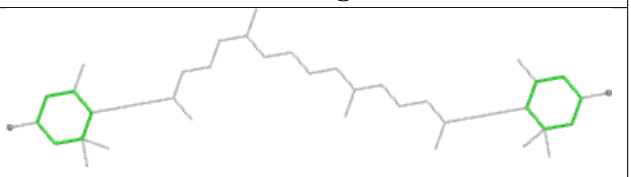
Bond lengths



Bond angles

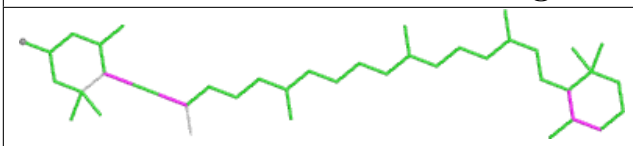


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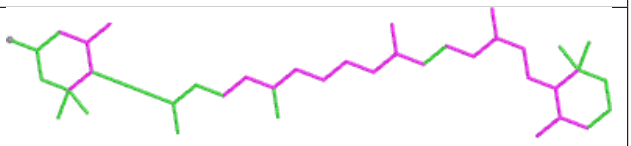


Rings

Ligand IHT 2 616



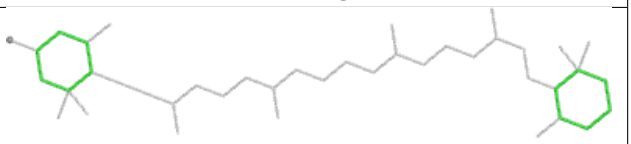
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Bond angles

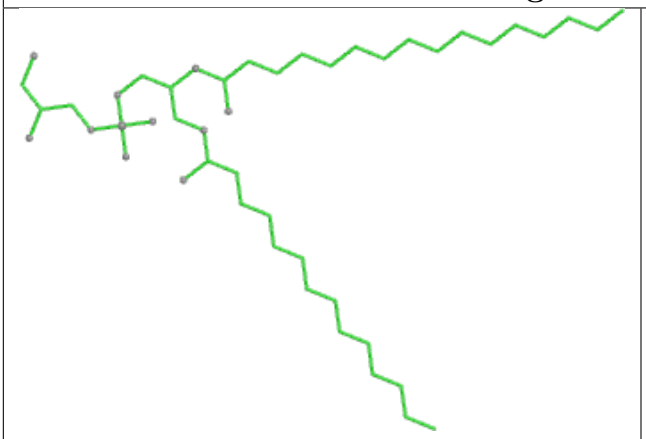


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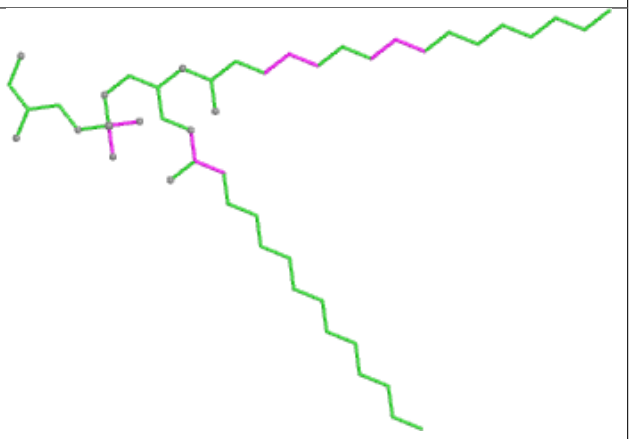


Rings

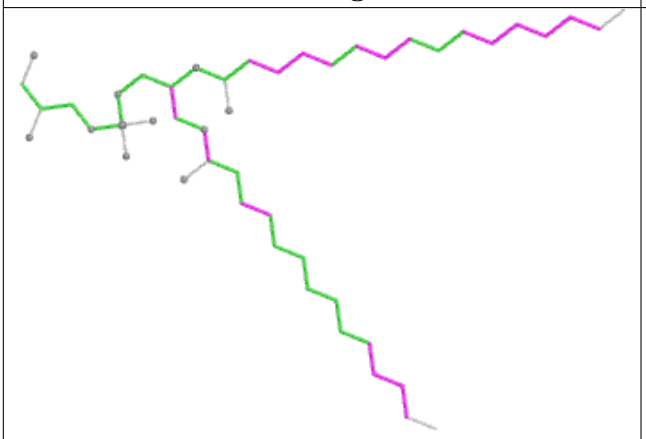
Ligand LHG 4 617



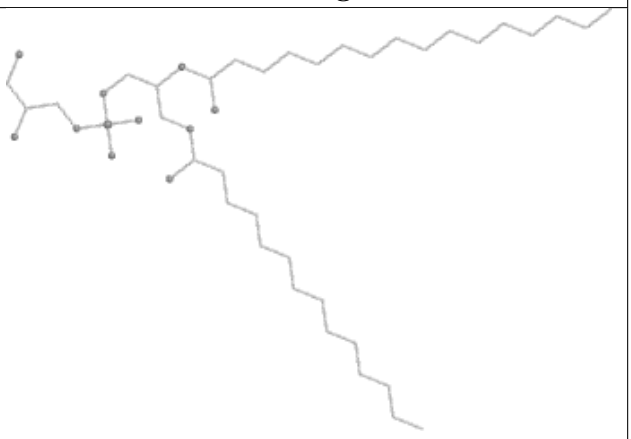
Bond lengths



Bond angles

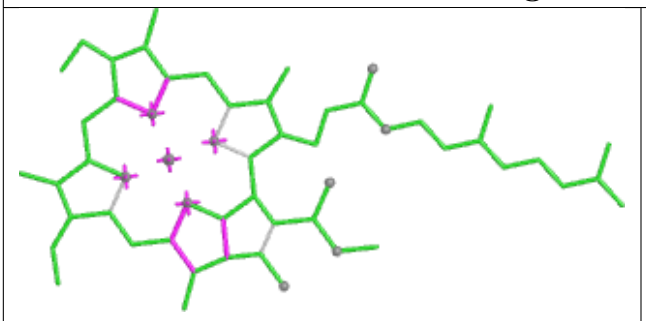


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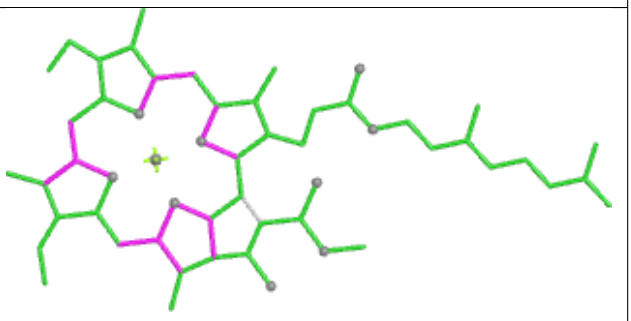


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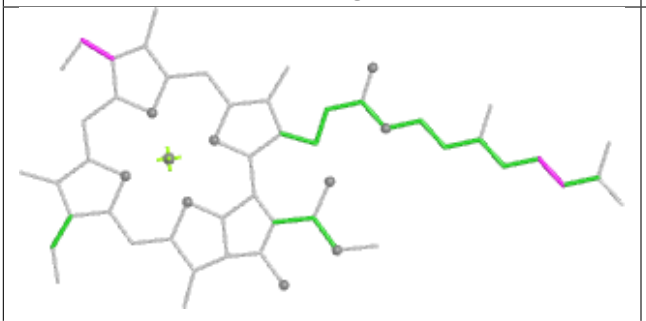
Ligand CLA A 836



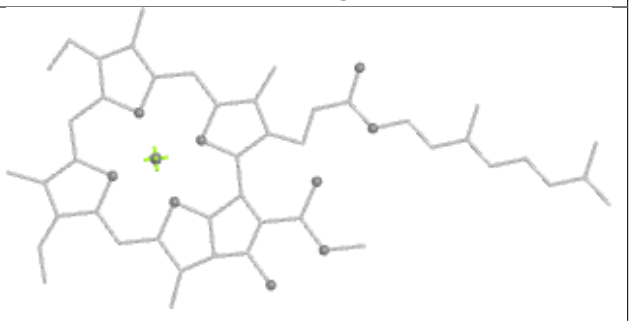
Bond lengths



Bond angles

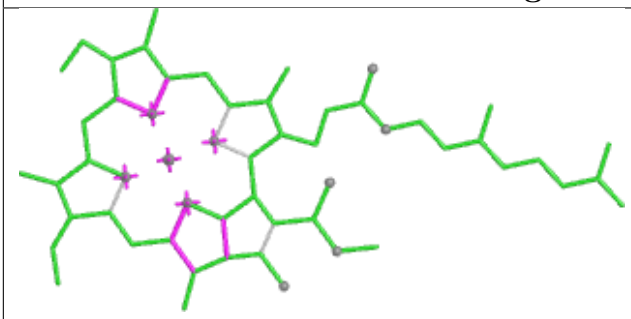


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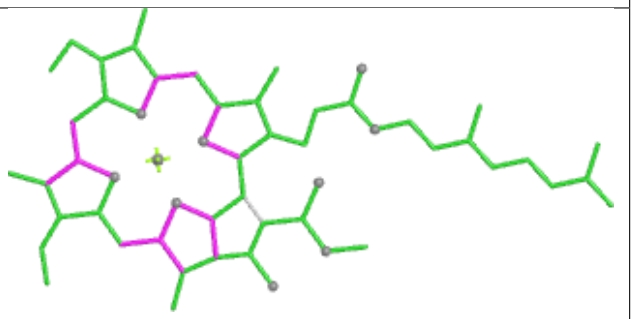


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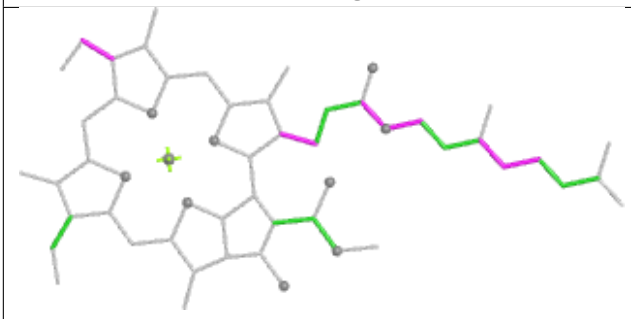
Ligand CLA B 811



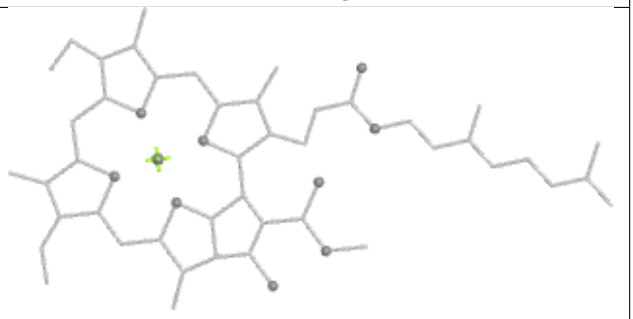
Bond lengths



Bond angles

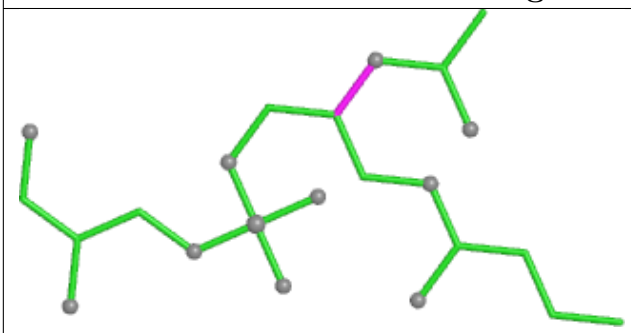


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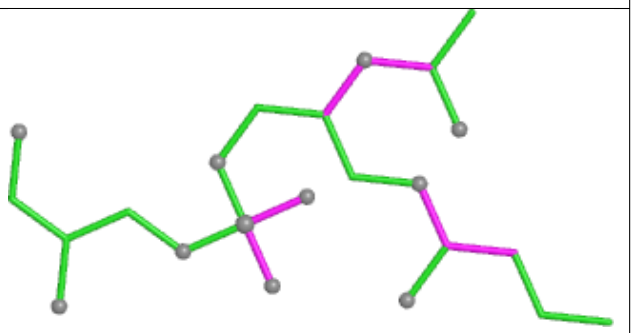


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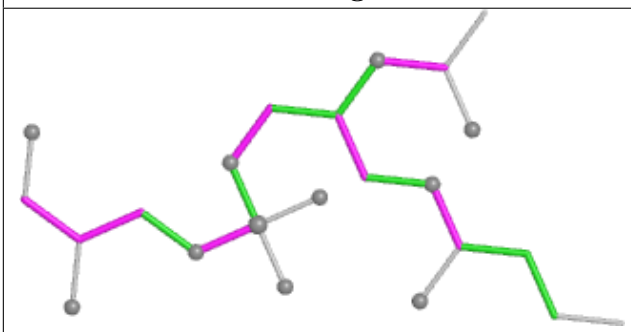
Ligand LHG 5 619



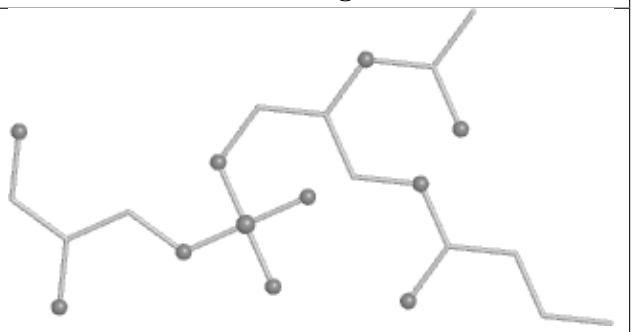
Bond lengths



Bond angles

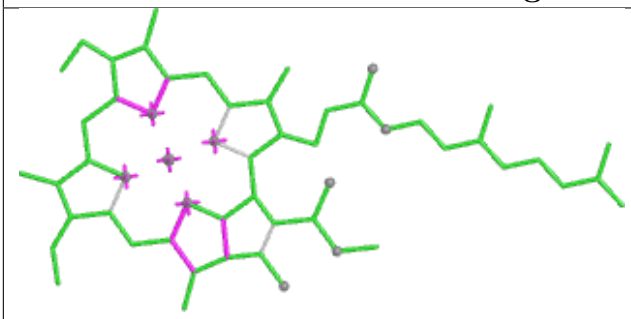


Torsions

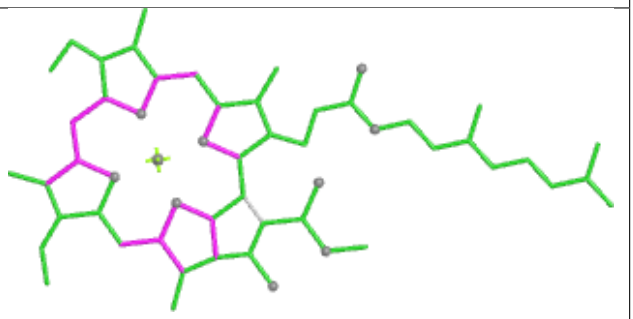


Rings

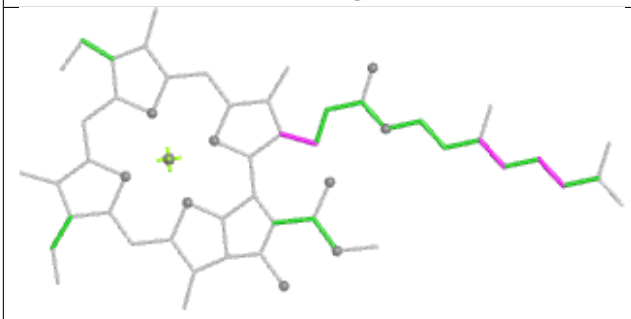
Ligand CLA A 821



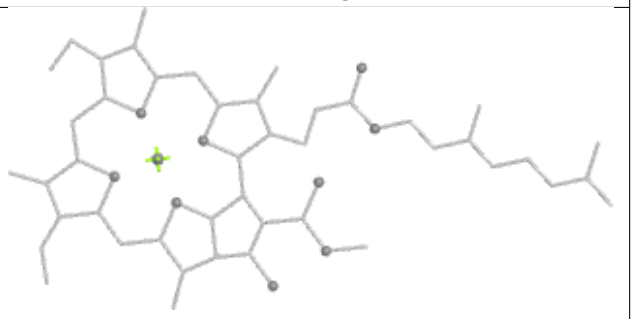
Bond lengths



Bond angles

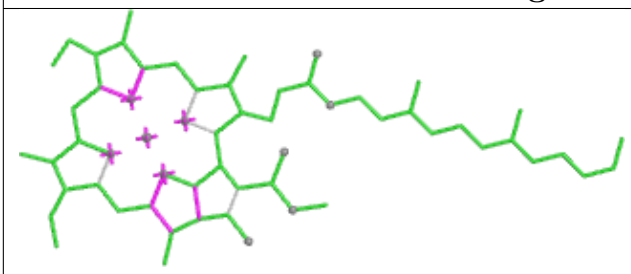


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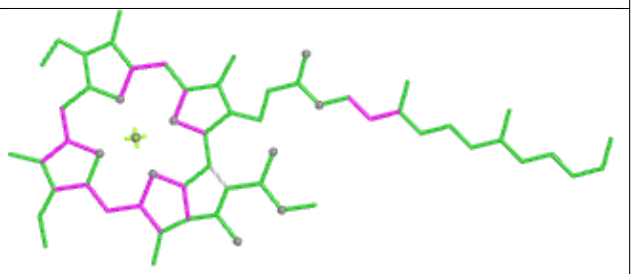


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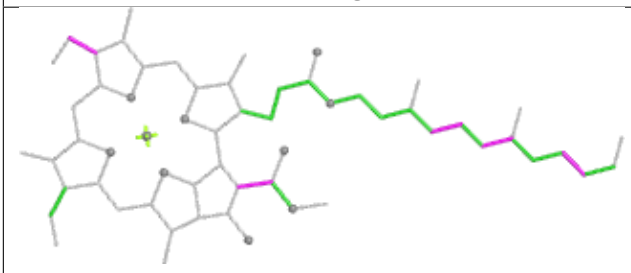
Ligand CLA 1 602



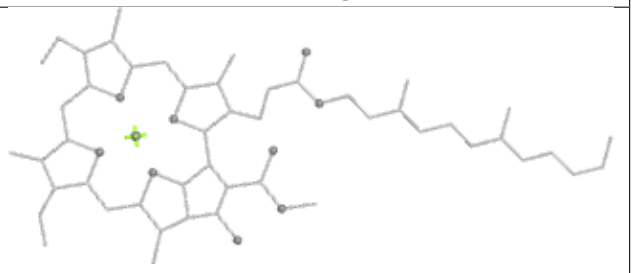
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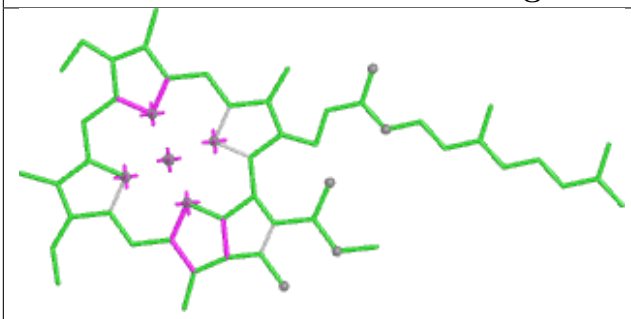
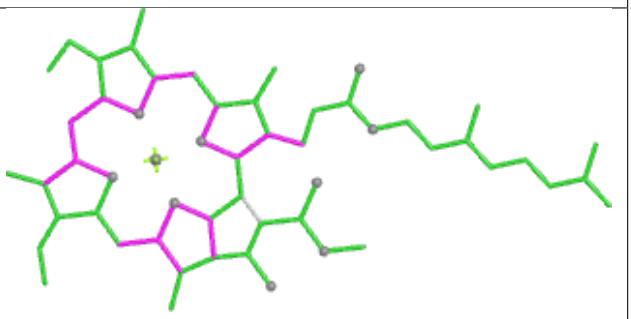
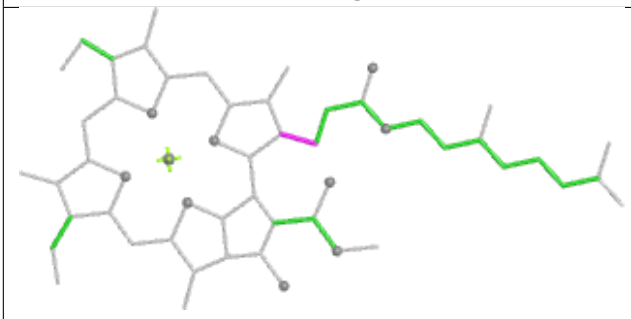
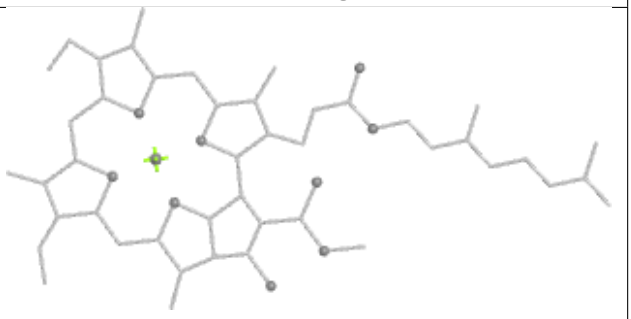
Bond angles

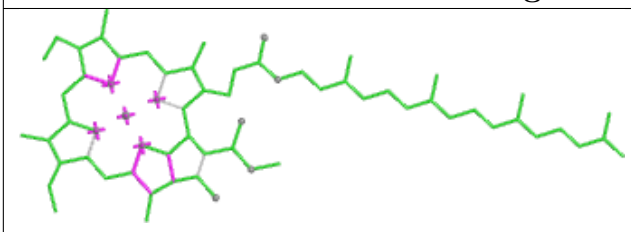
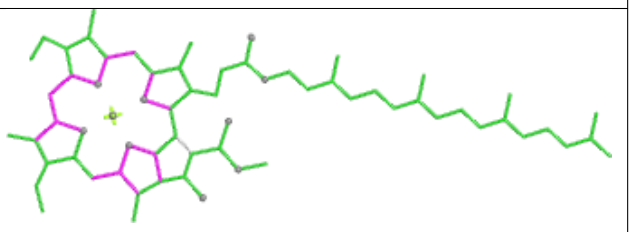
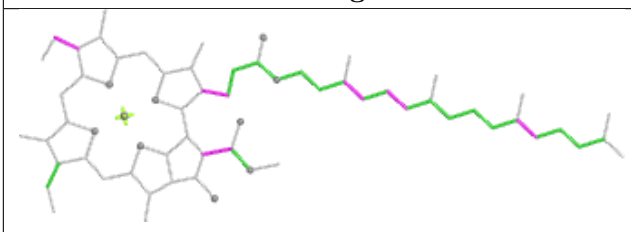
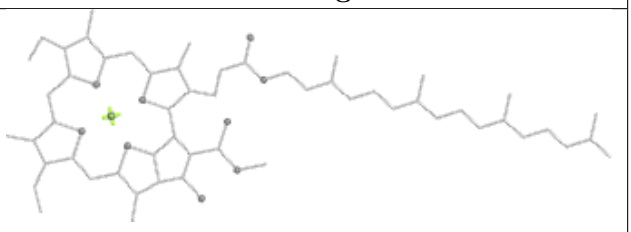


Torsions

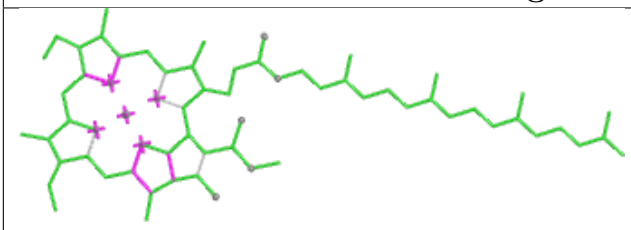


Rings

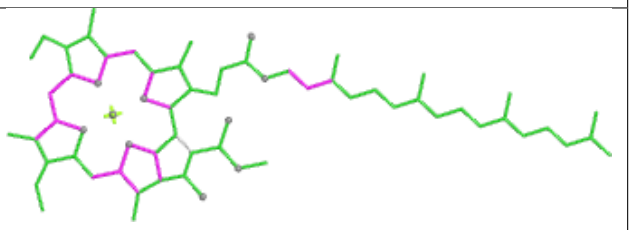
Ligand CLA A 808	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 822	
	
Bond lengths	Bond angles
	
Torsions	Rings

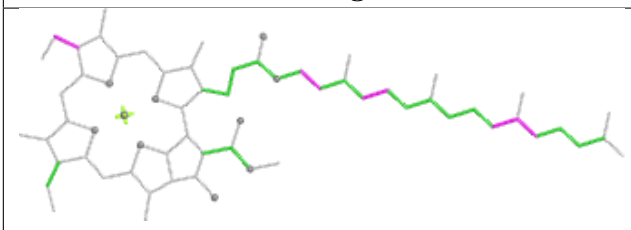
Ligand CLA d 607



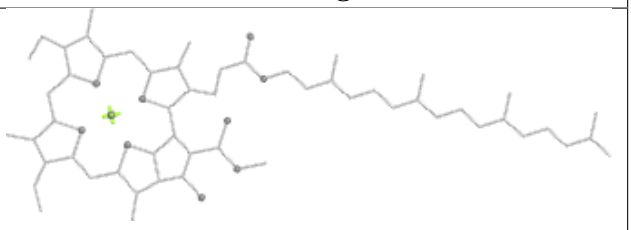
Bond lengths



Bond angles

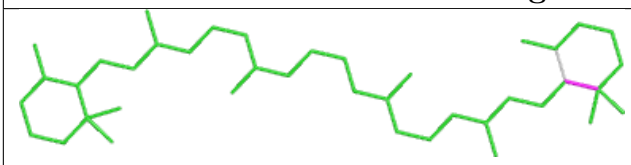


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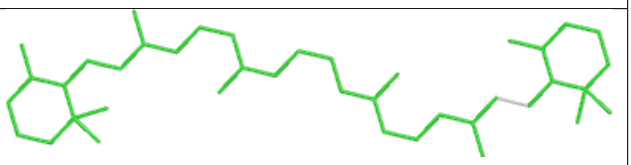


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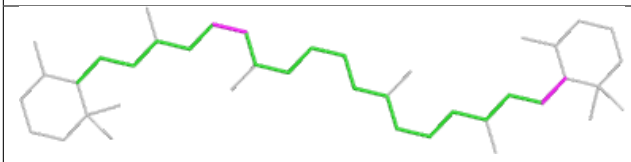
Ligand 8CT F 201



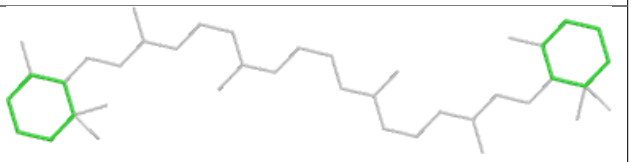
Bond lengths



Bond angles

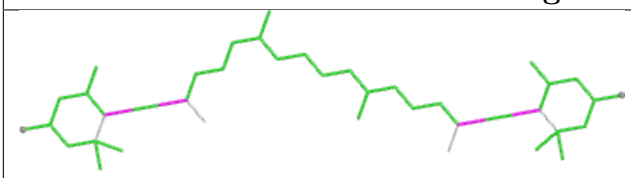


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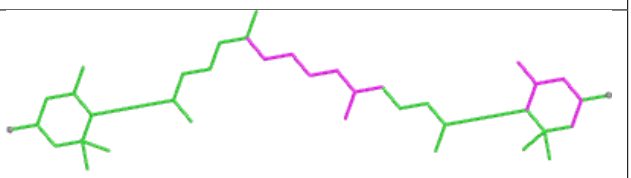


Rings

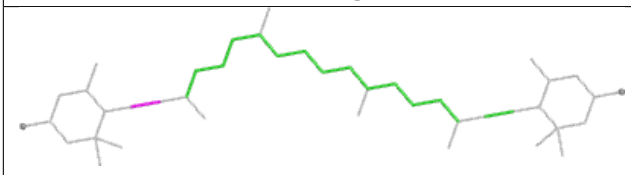
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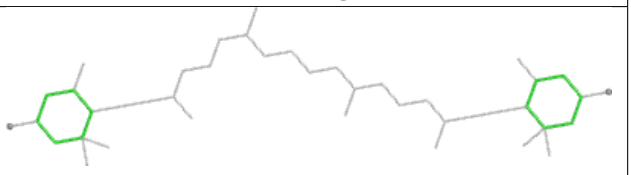
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Bond angles

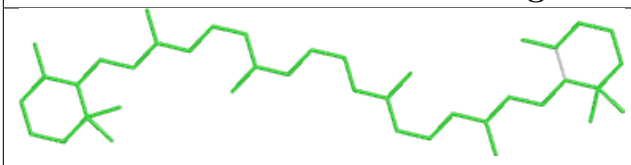


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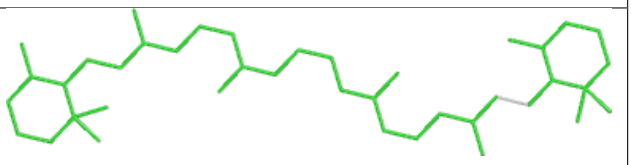


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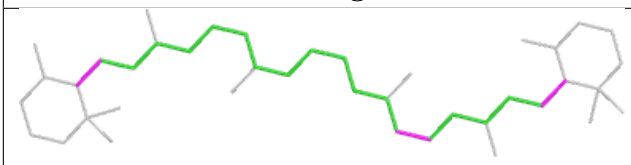
Ligand 8CT B 847



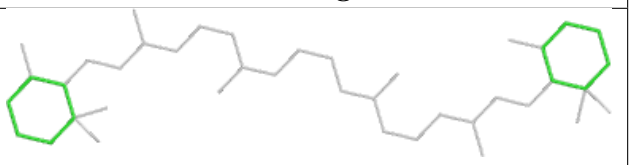
Bond lengths



Bond angles

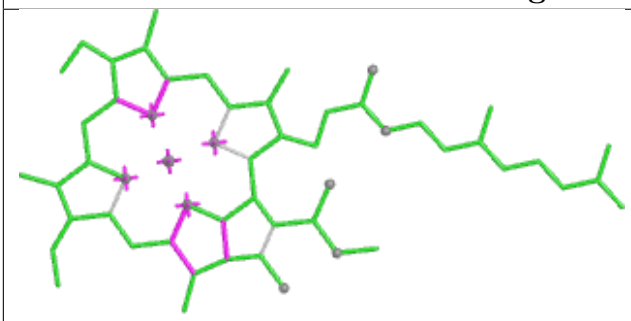


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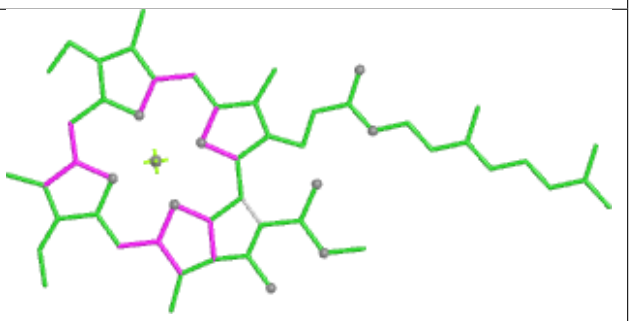


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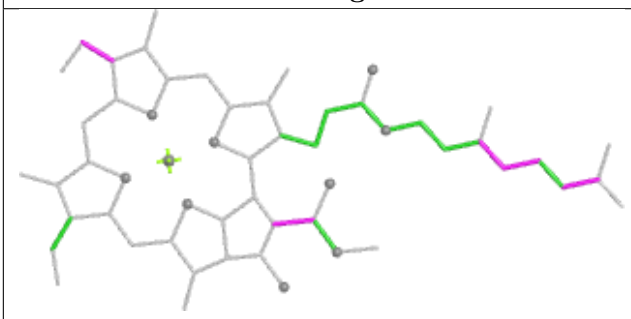
Ligand CLA 4 604



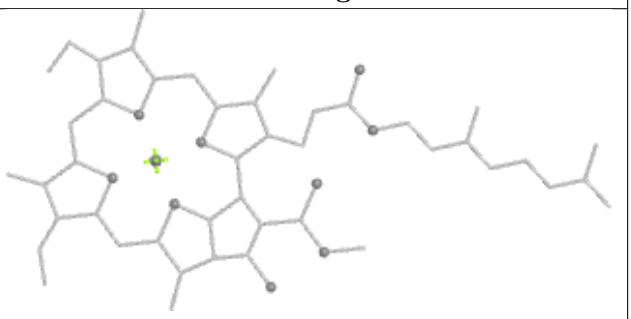
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Bond angles

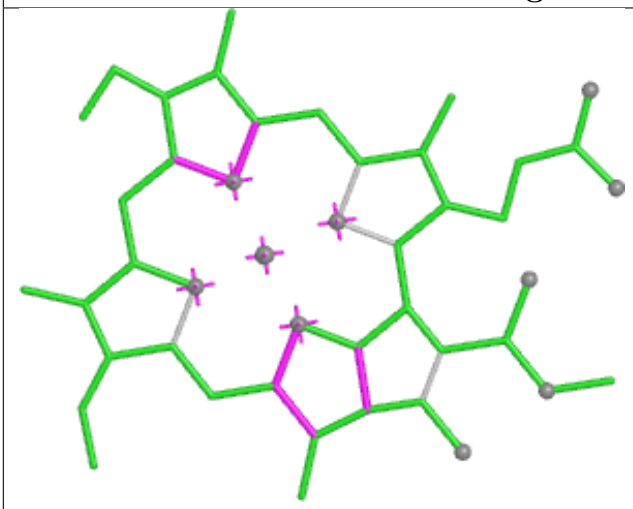


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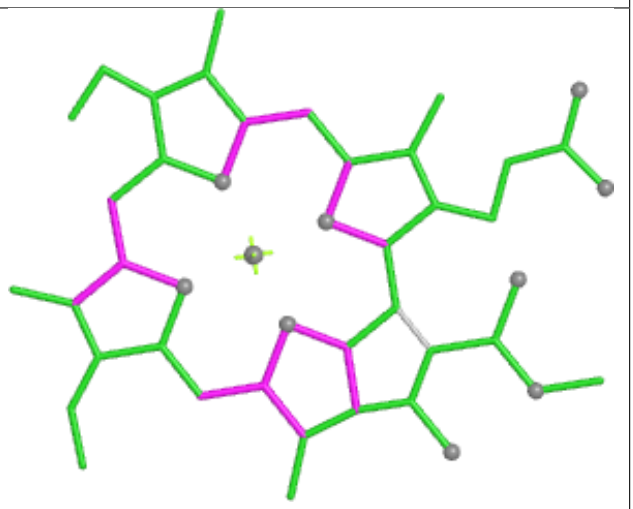


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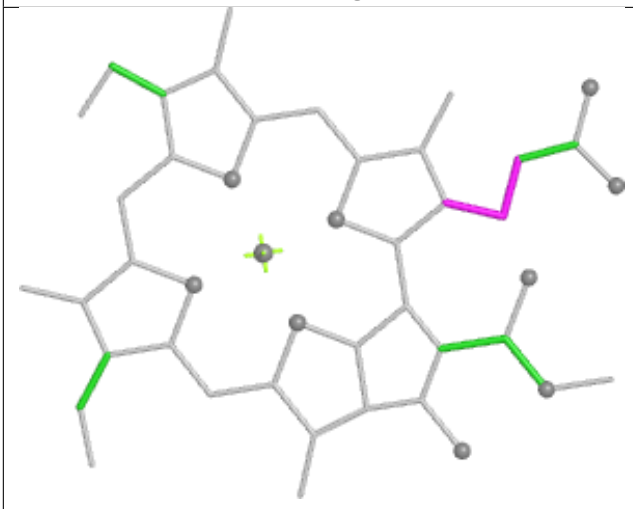
Ligand CLA F 203



Bond lengths



Bond angles

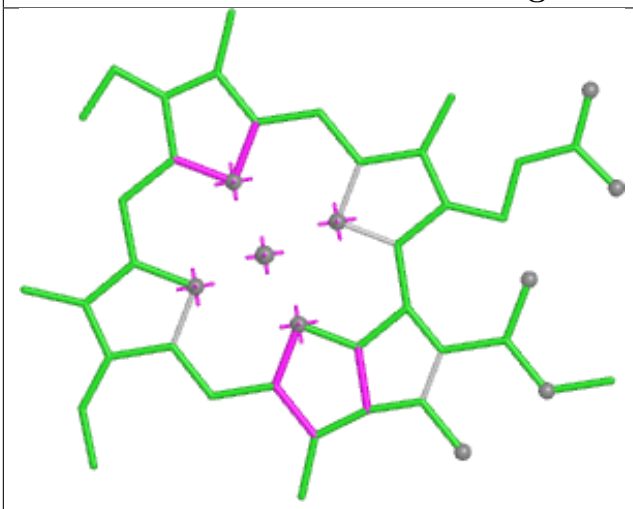


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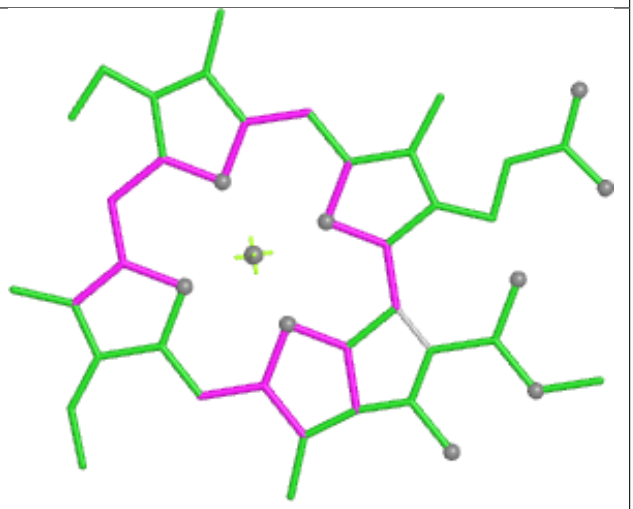


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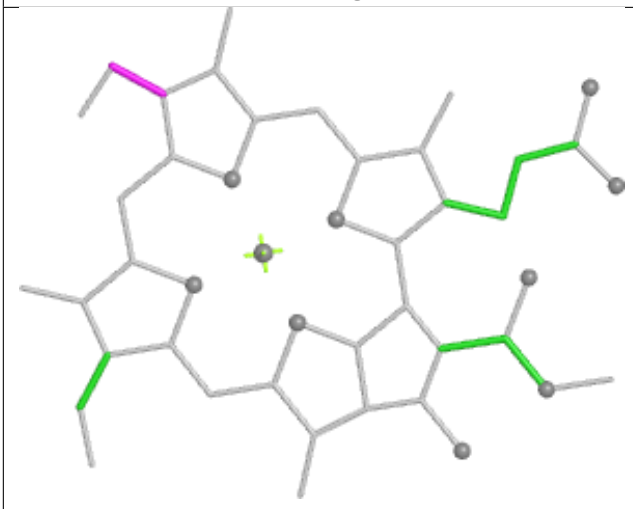
Ligand CLA 2 607



Bond lengths



Bond angles

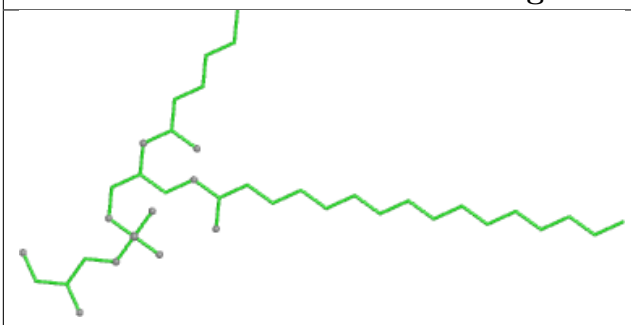


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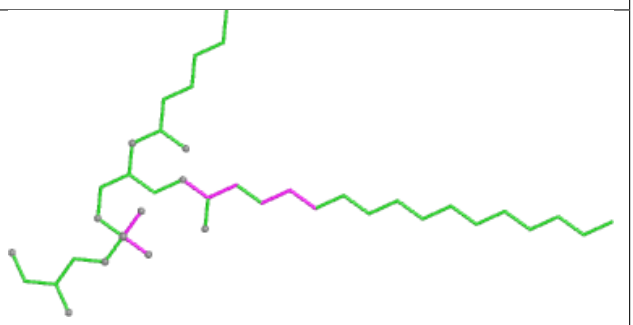


Rings

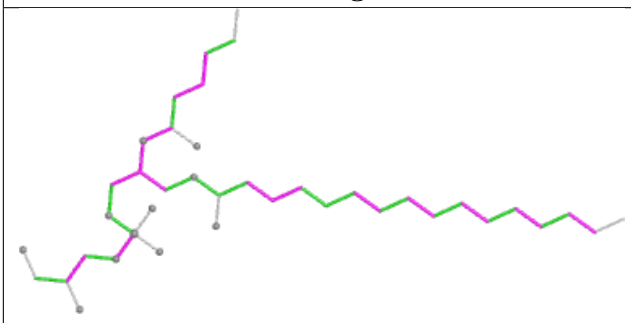
Ligand LHG 7 619



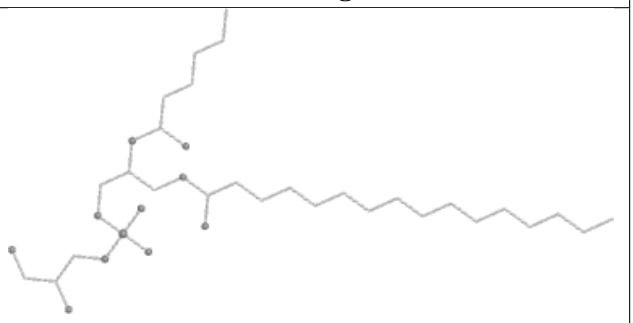
Bond lengths



Bond angles

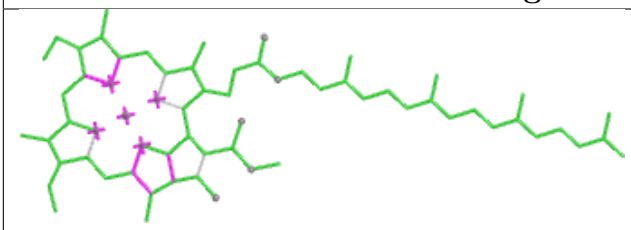


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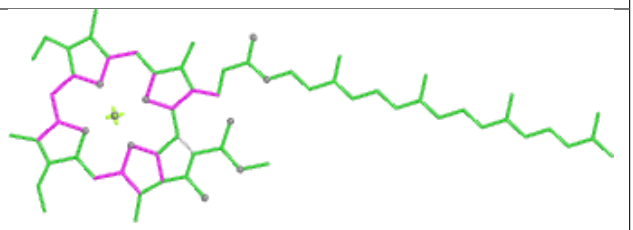


Rings

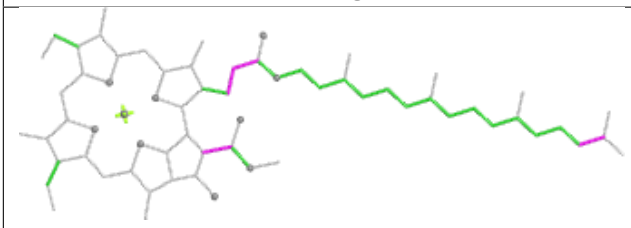
Ligand CLA A 803



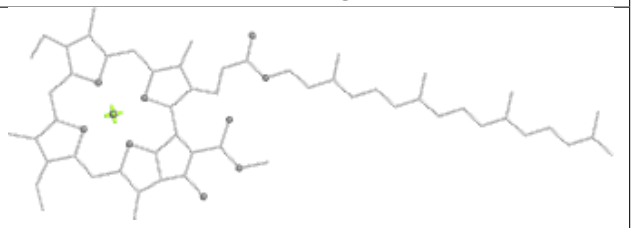
Bond lengths



Bond angles

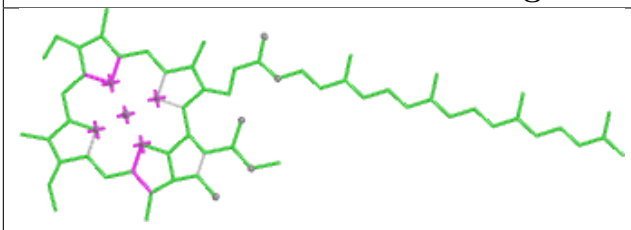


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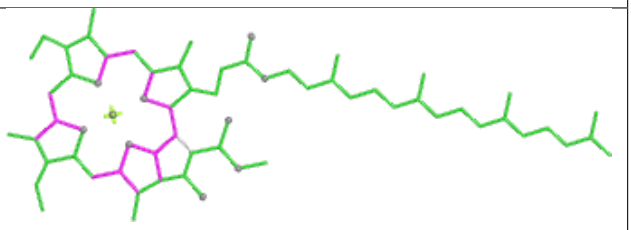


Rings

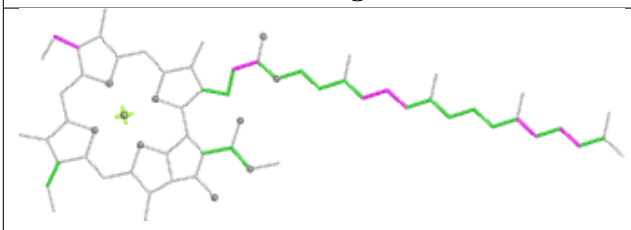
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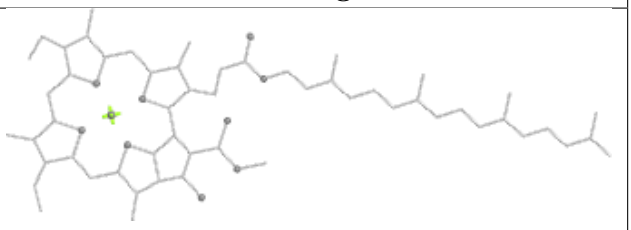
Bond lengths



Bond angles

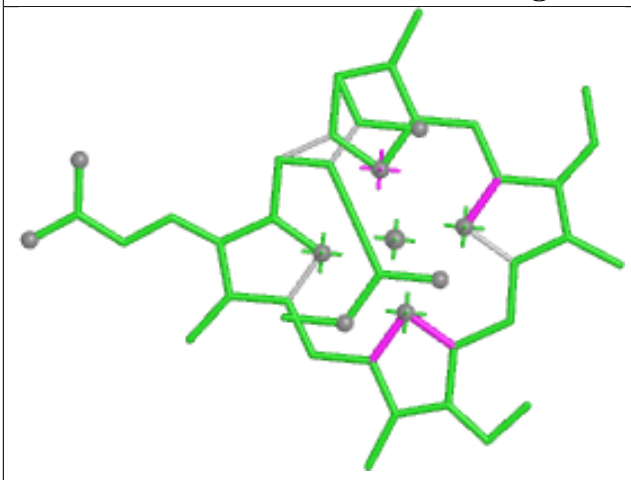


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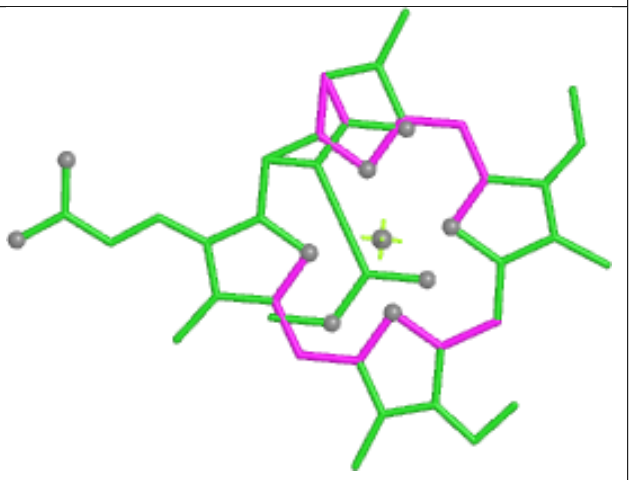


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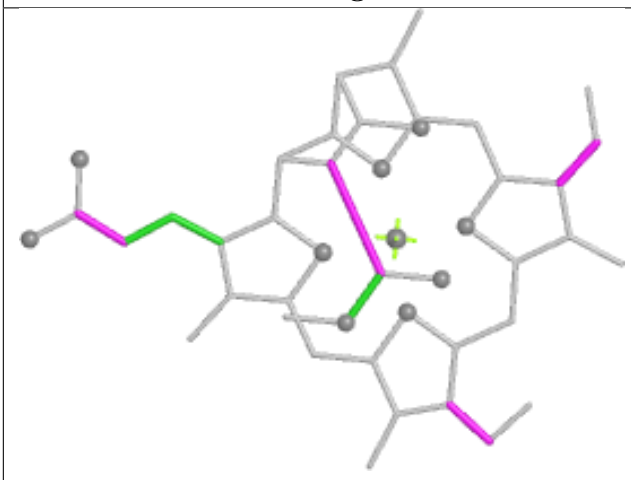
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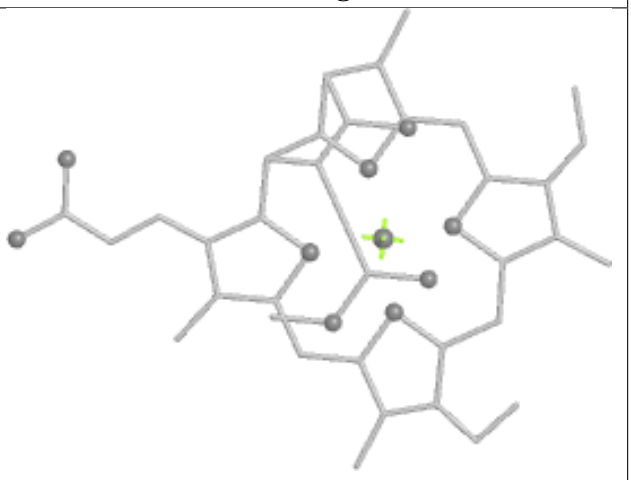
Bond lengths



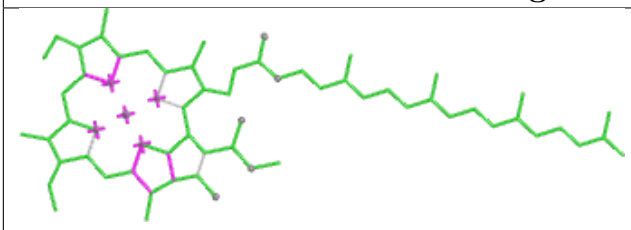
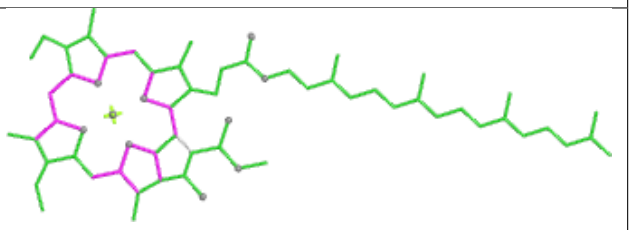
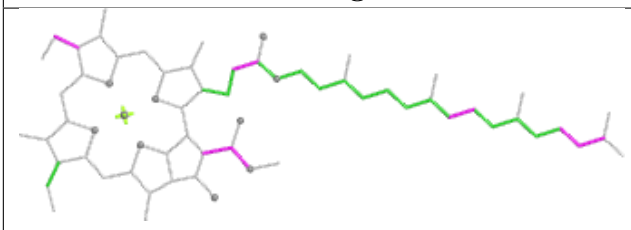
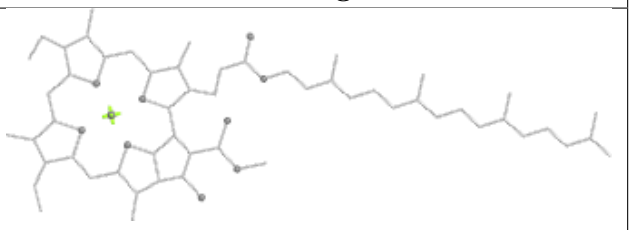
Bond angles

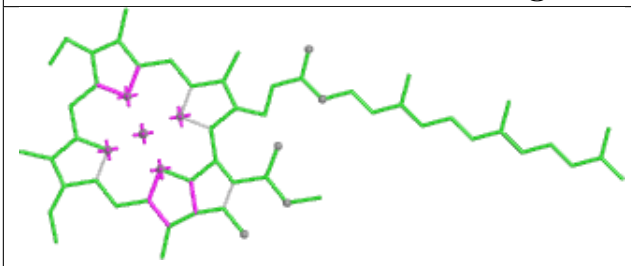
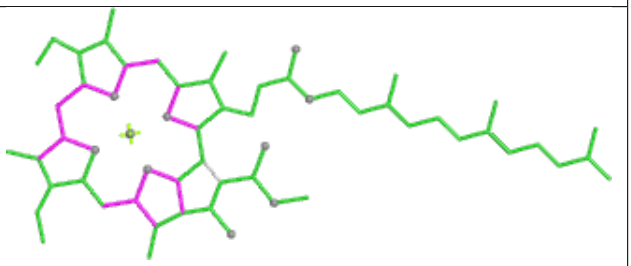
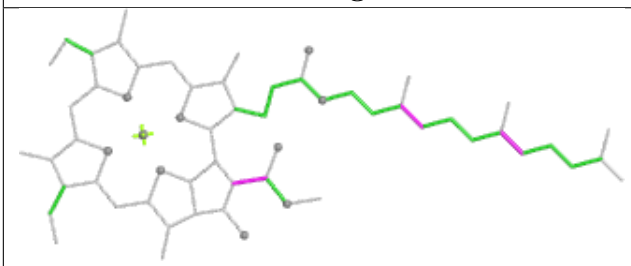
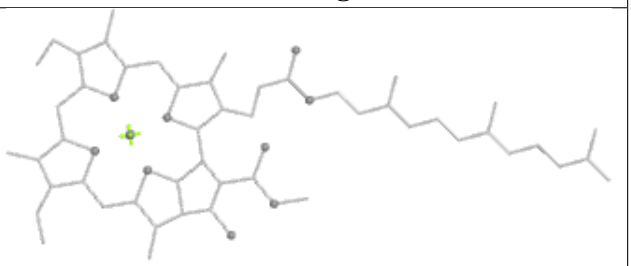


Torsions

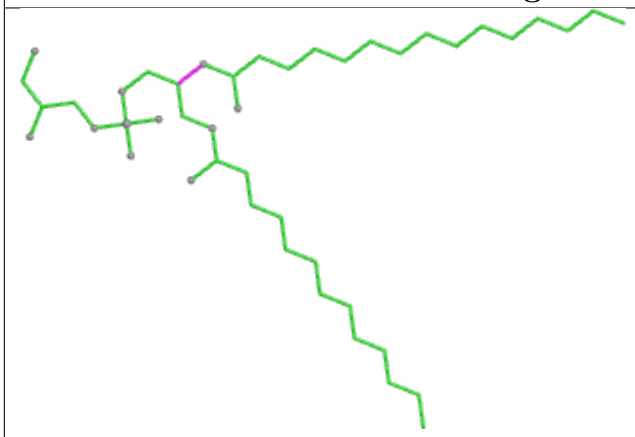


Rings

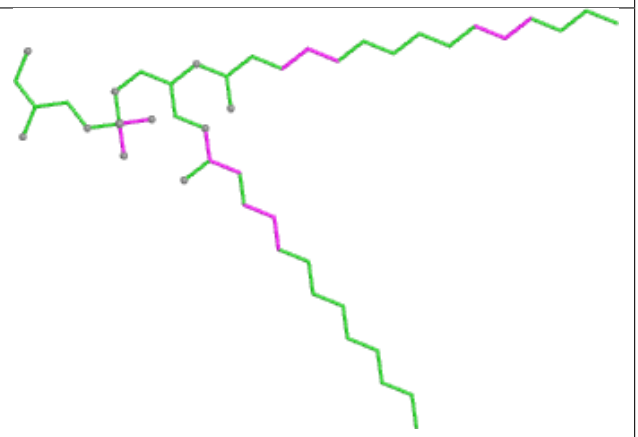
Ligand CLA e 611	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA 6 604	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

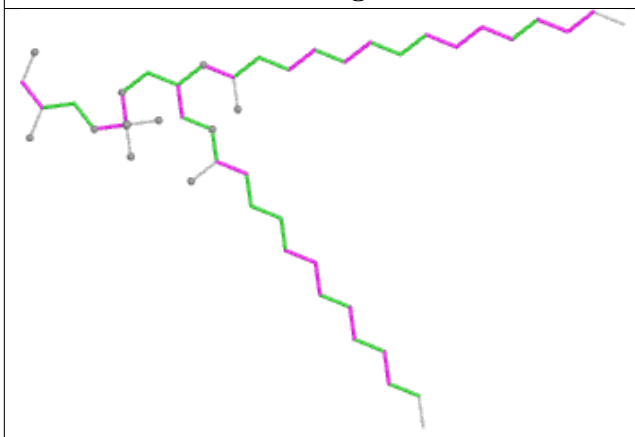
Ligand LHG B 849



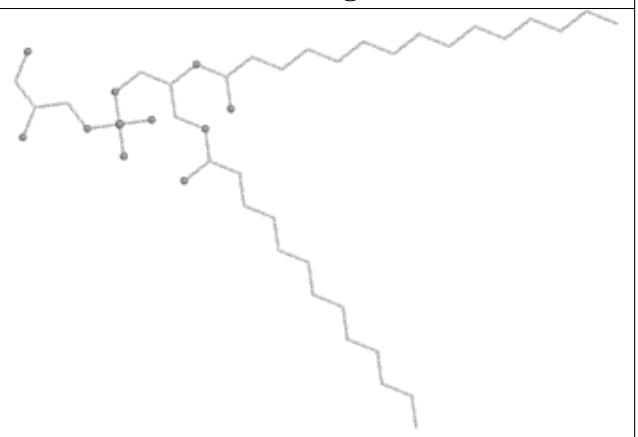
Bond lengths



Bond angles

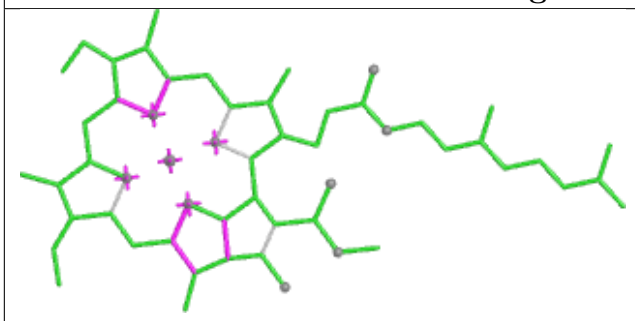


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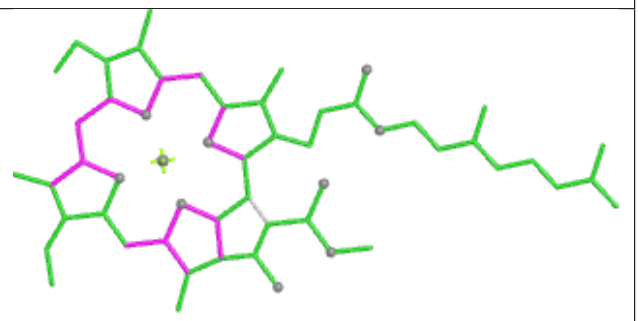


Rings

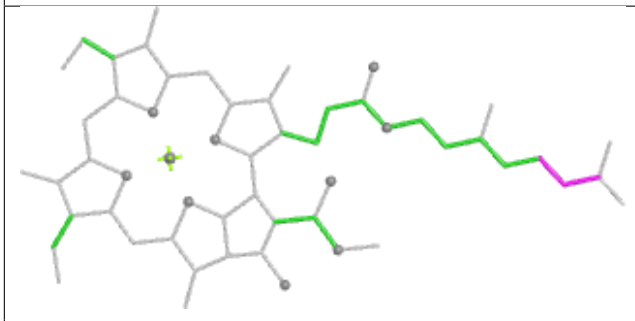
Ligand CLA 7 603



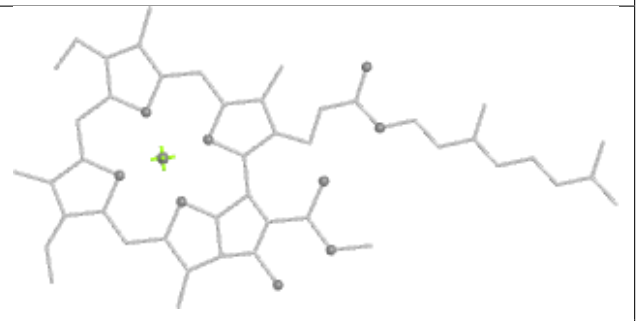
Bond lengths



Bond angles

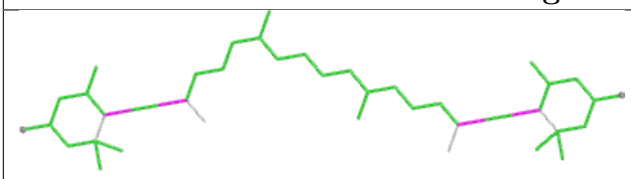


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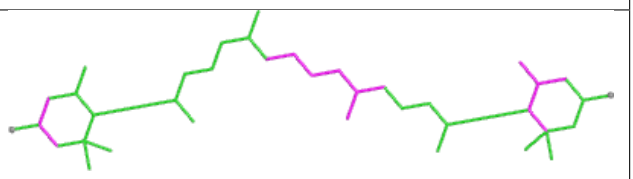


Rings

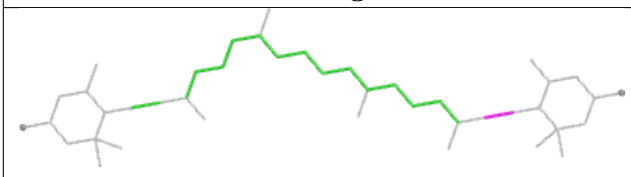
Ligand II0 7 613



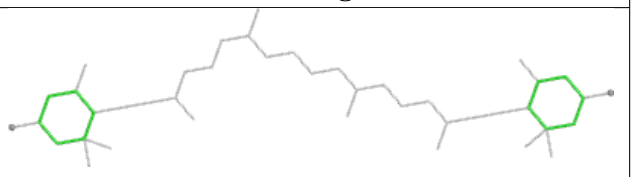
Bond lengths



Bond angles

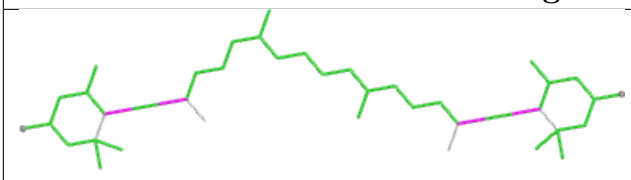


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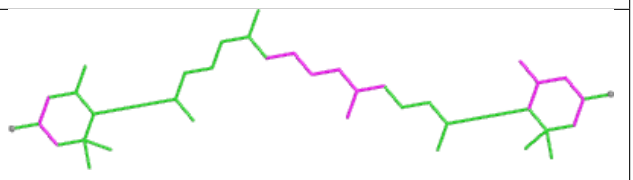


Rings

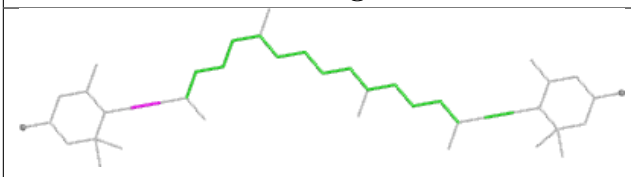
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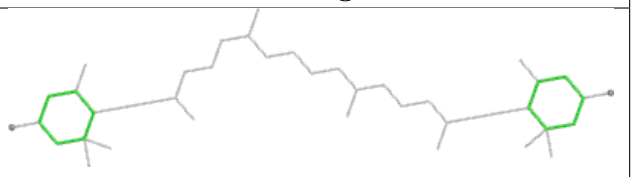
Bond lengths



Bond angles

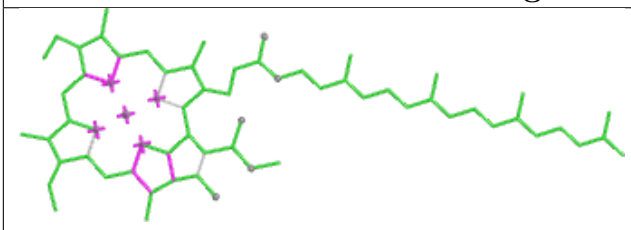


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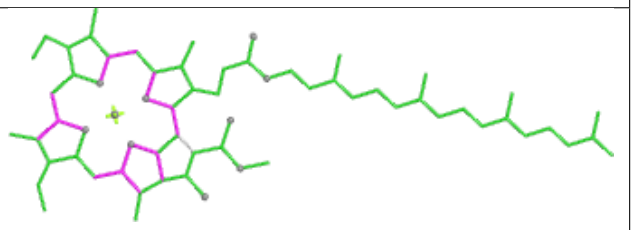


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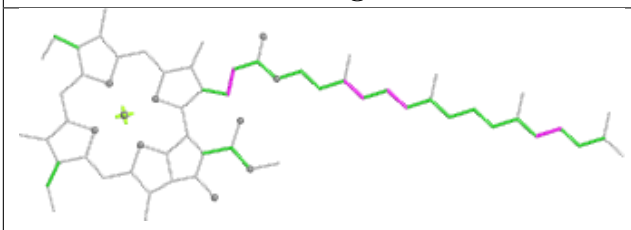
Ligand CLA A 827



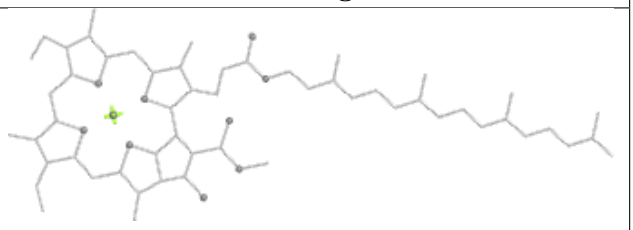
Bond lengths



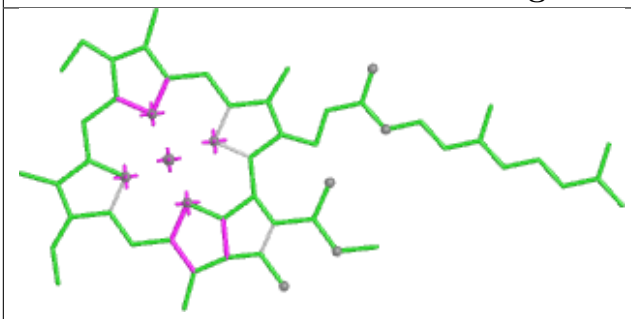
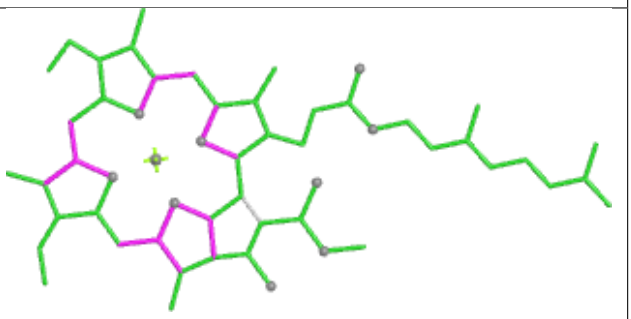
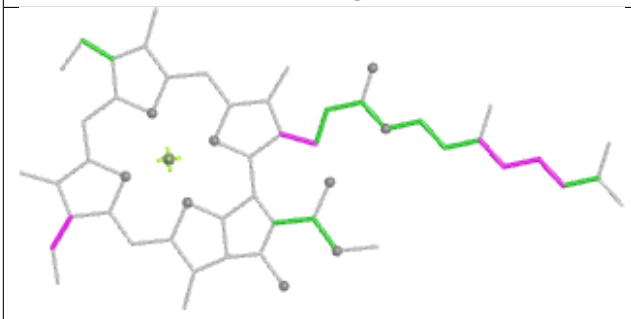
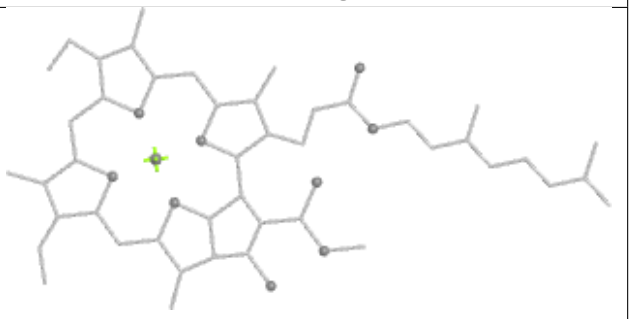
Bond angles

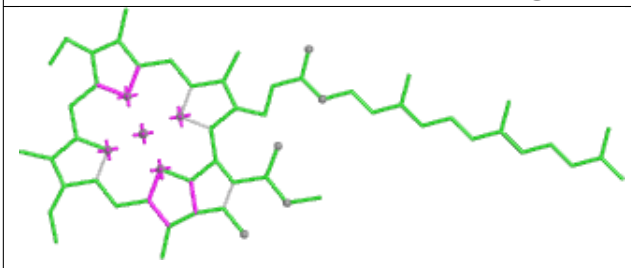
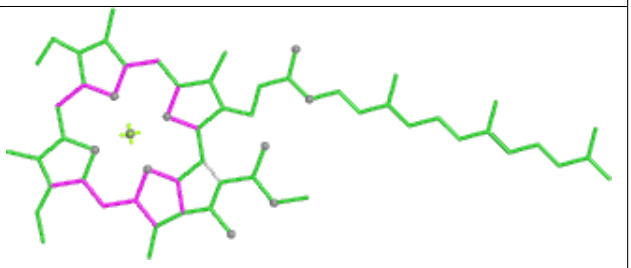
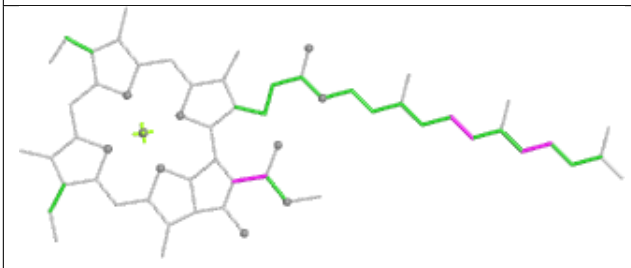
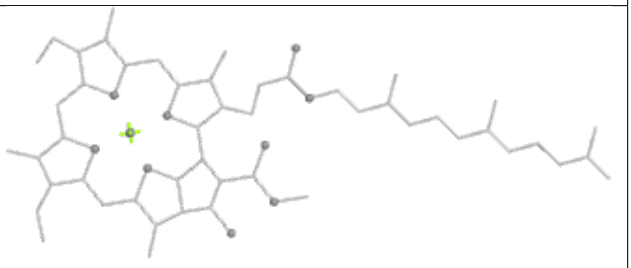


Torsions

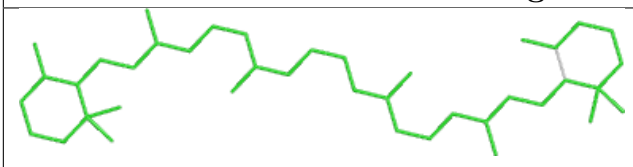


Rings

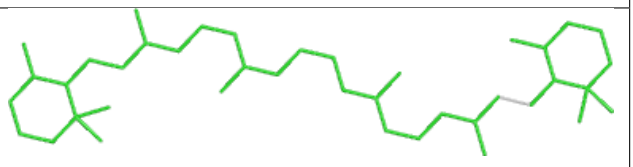
Ligand CLA 4 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA a 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

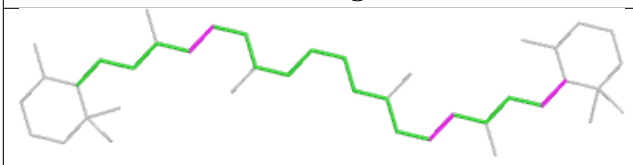
Ligand 8CT B 844



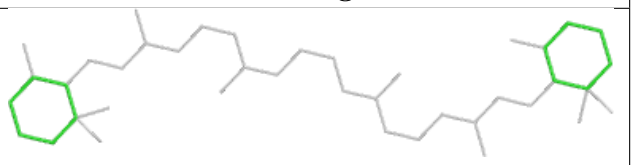
Bond lengths



Bond angles

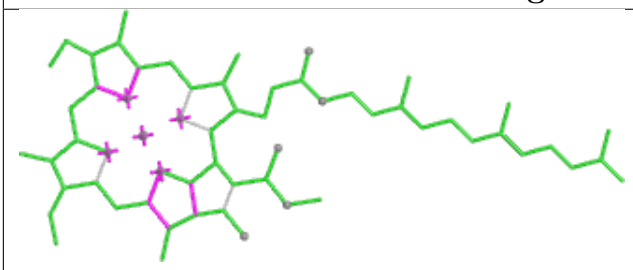


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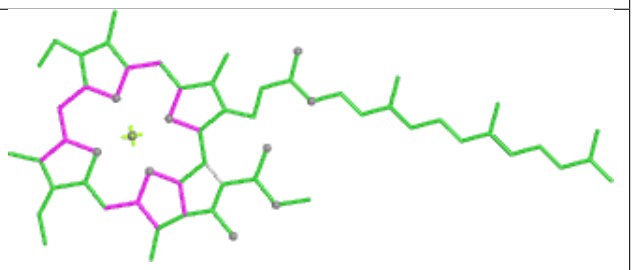


Rings

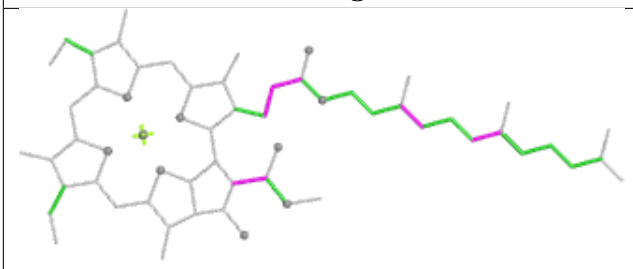
Ligand CLA b 603



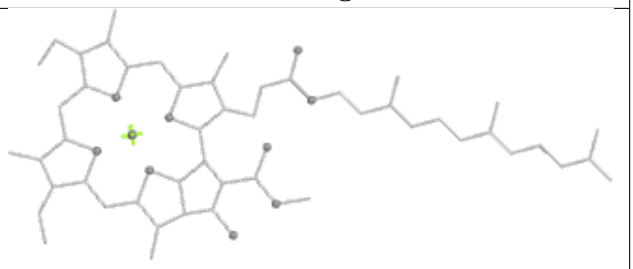
Bond lengths



Bond angles

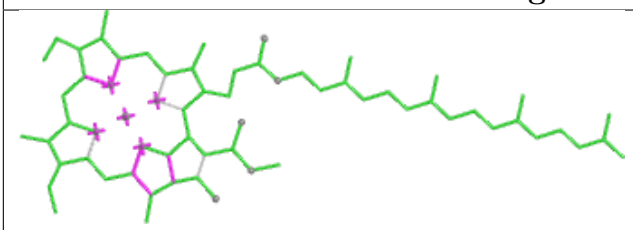


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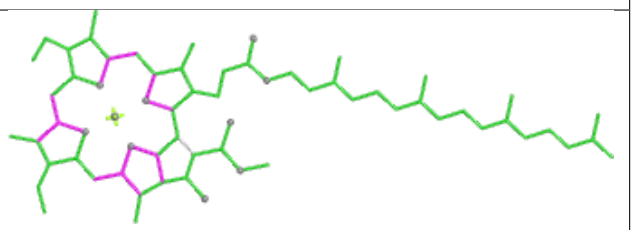


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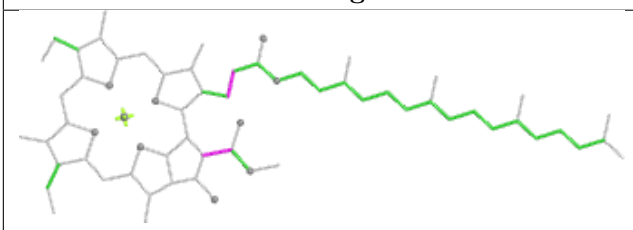
Ligand CLA 3 604



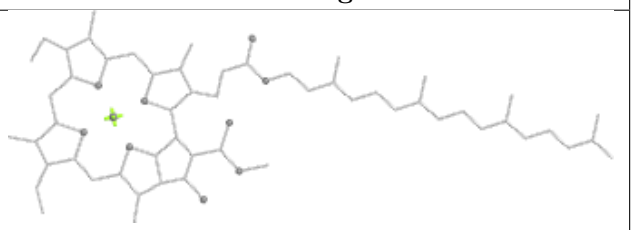
Bond lengths



Bond angles

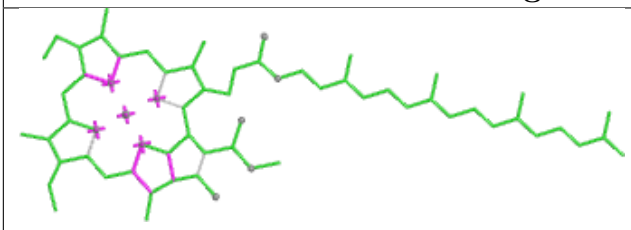


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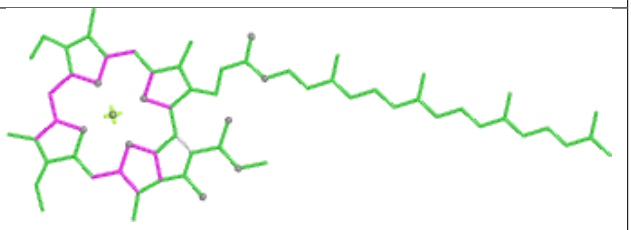


Rings

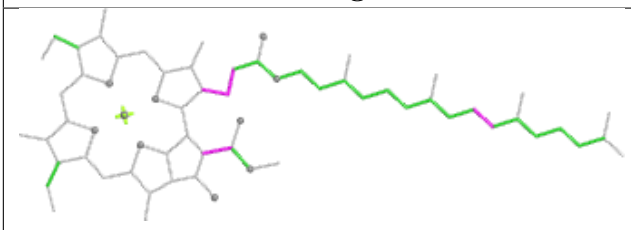
Ligand CLA A 842



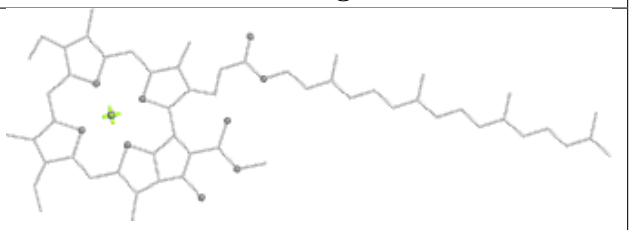
Bond lengths



Bond angles

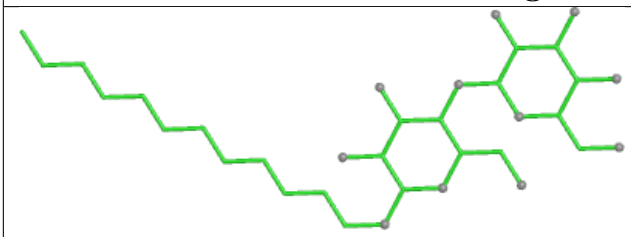


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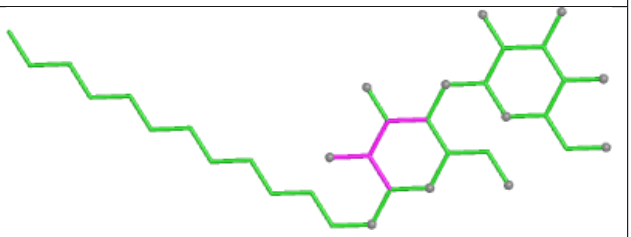


Rings

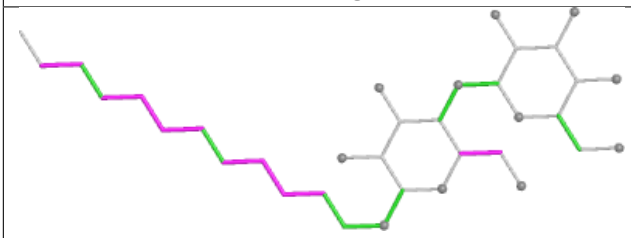
Ligand LMU 7 620



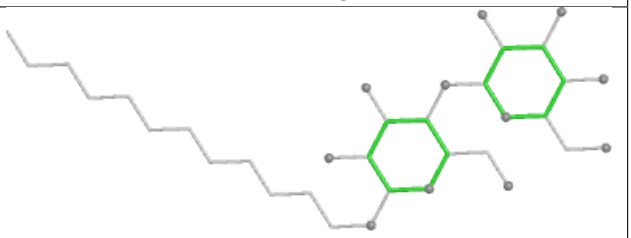
Bond lengths



Bond angles

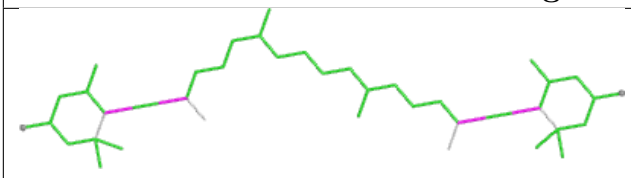


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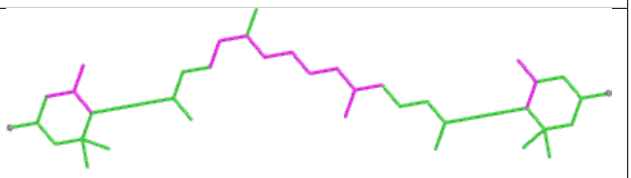


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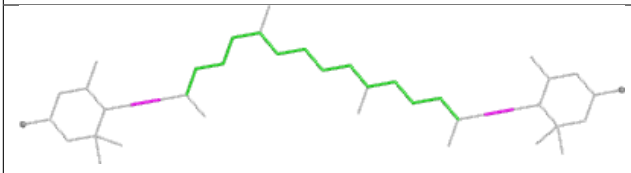
Ligand II0 8 610



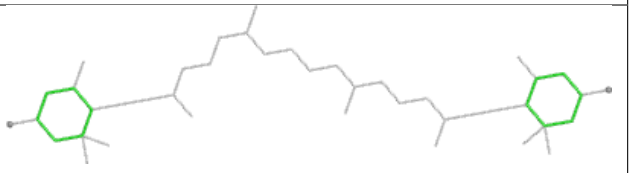
Bond lengths



Bond angles

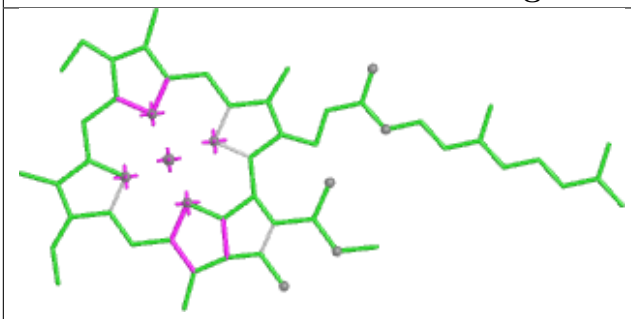


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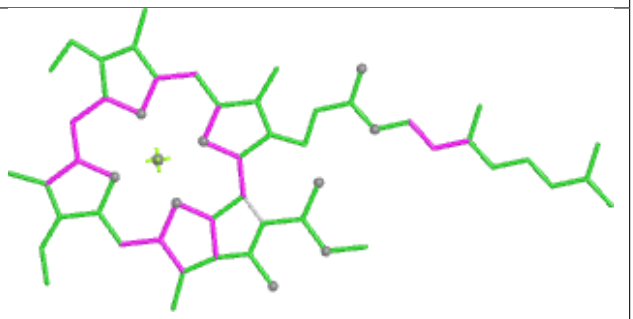


Rings

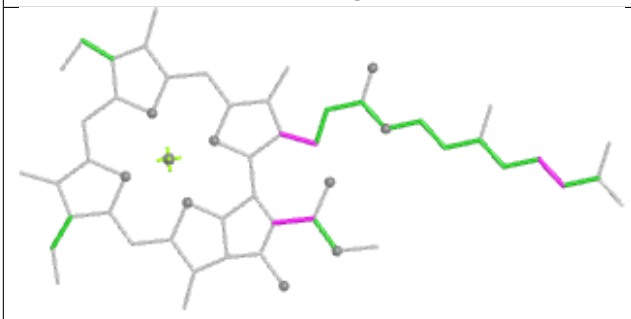
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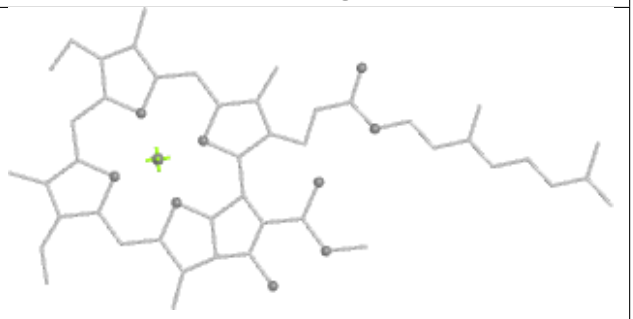
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Bond angles

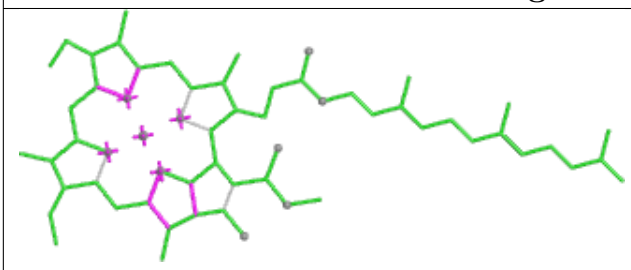


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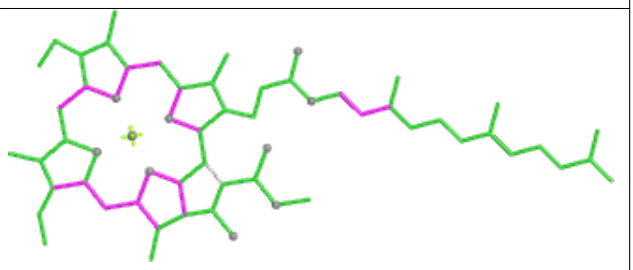


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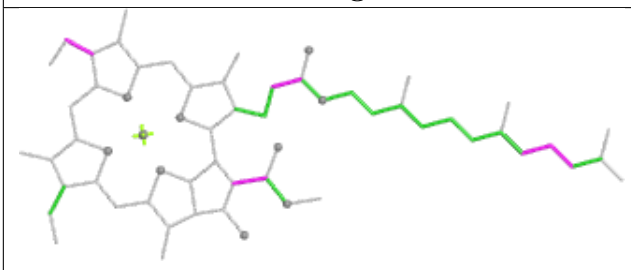
Ligand CLA 2 608



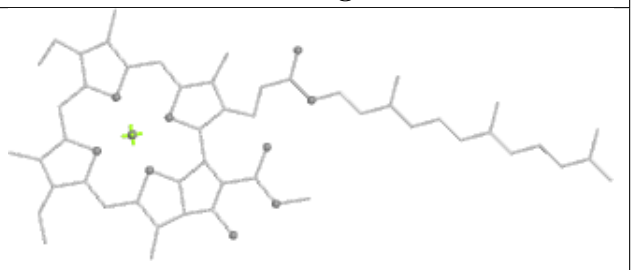
Bond lengths



Bond angles

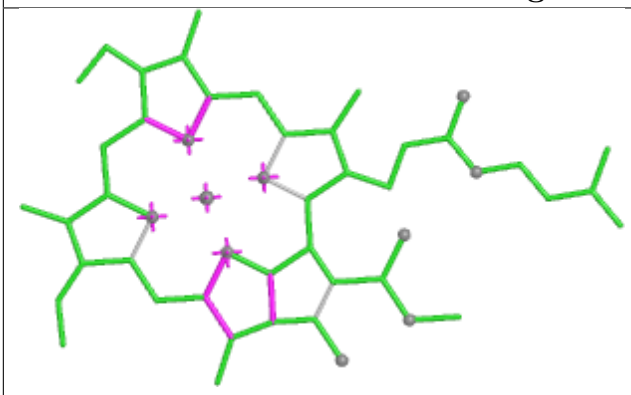


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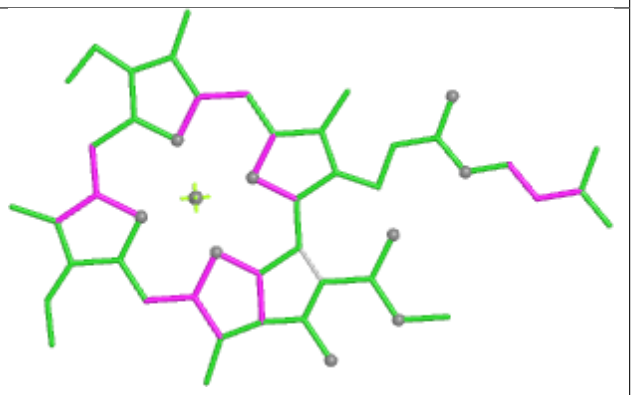


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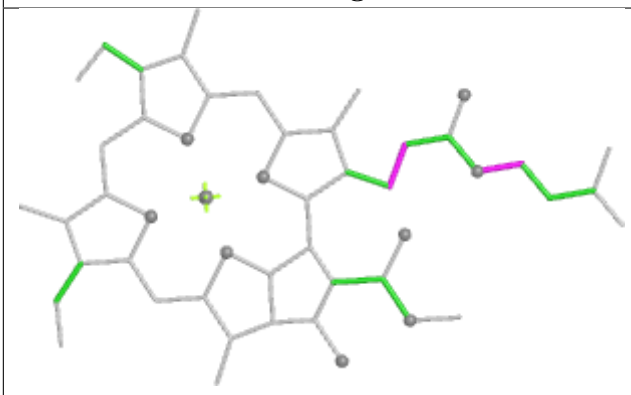
Ligand CLA d 603



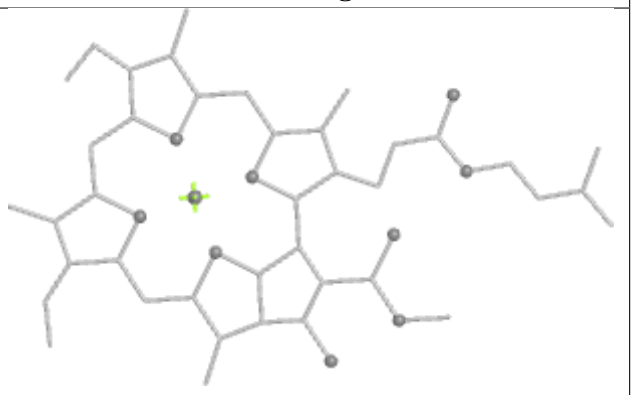
Bond lengths



Bond angles

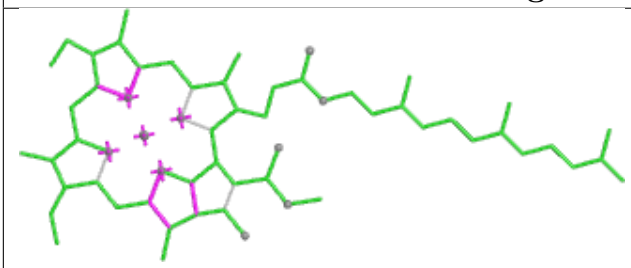


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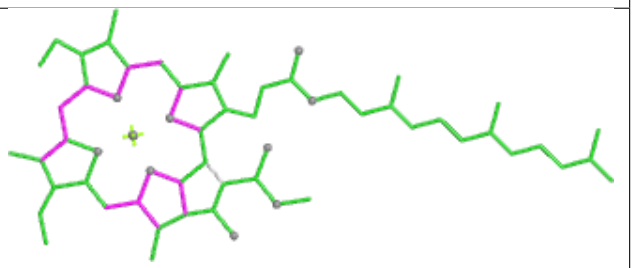


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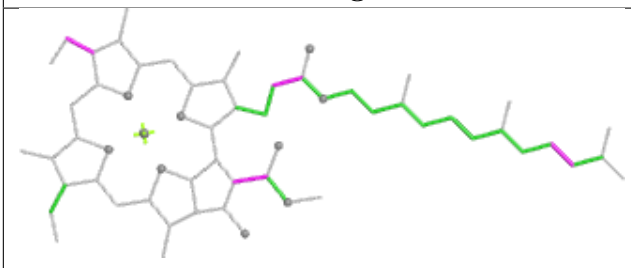
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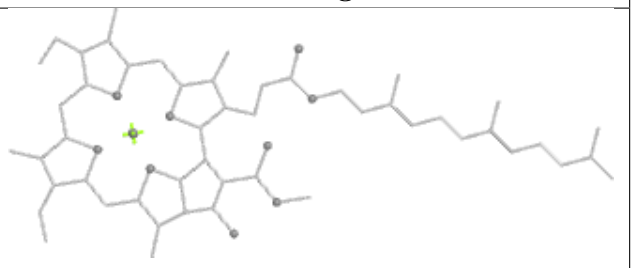
Bond lengths



Bond angles

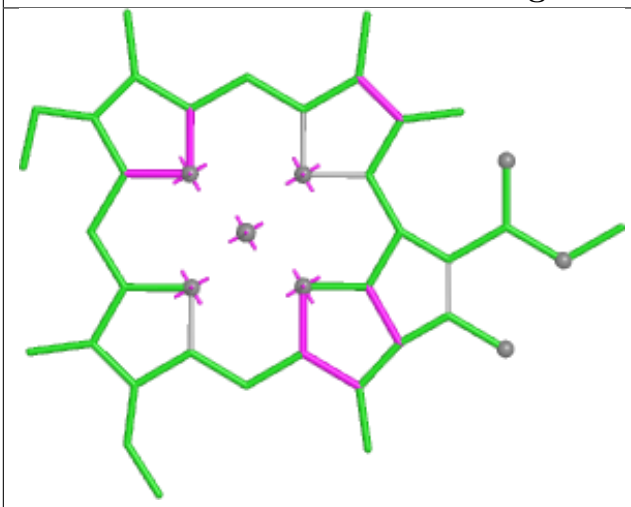


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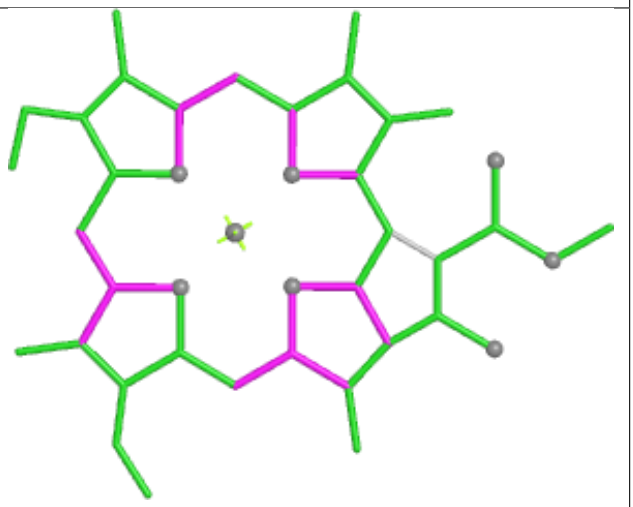


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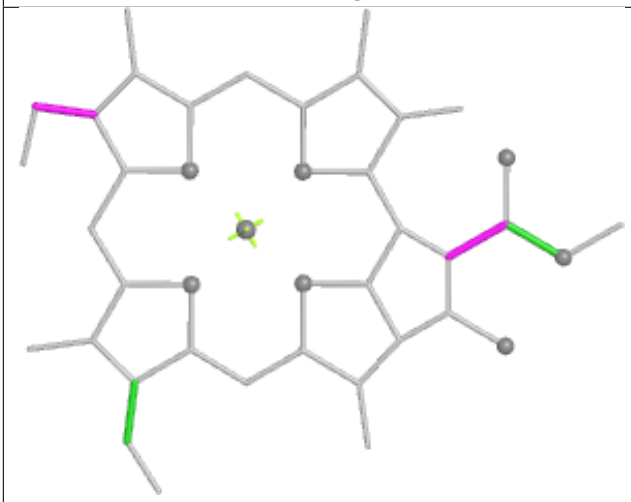
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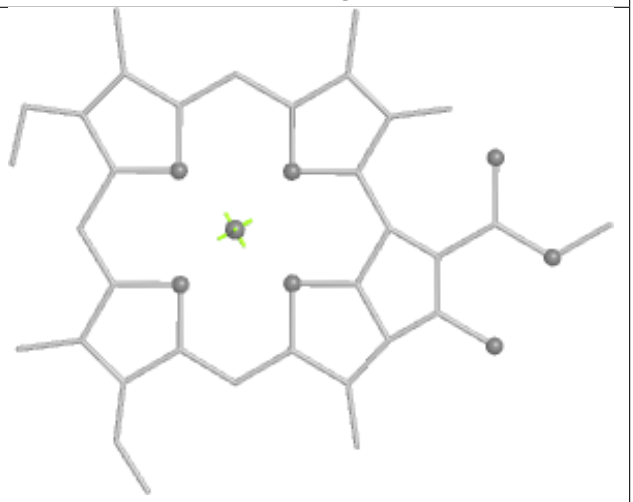
Bond lengths



Bond angles

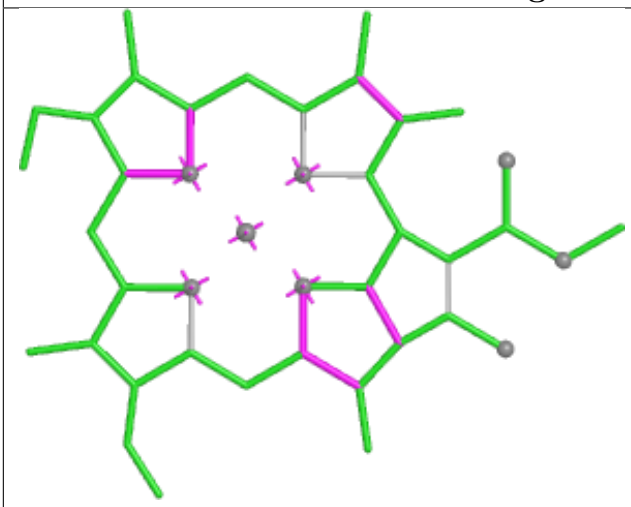


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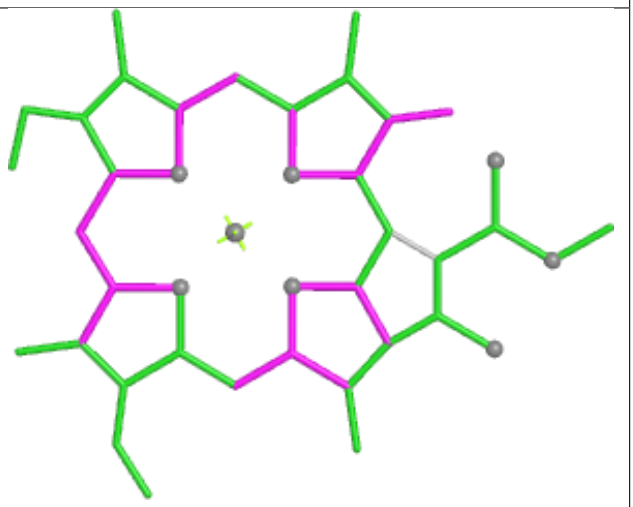


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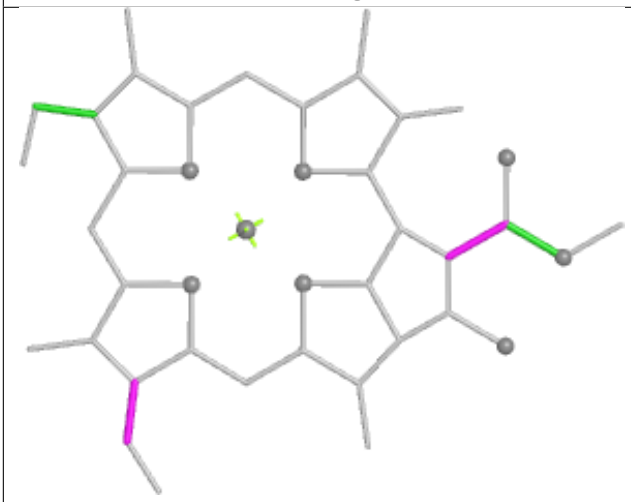
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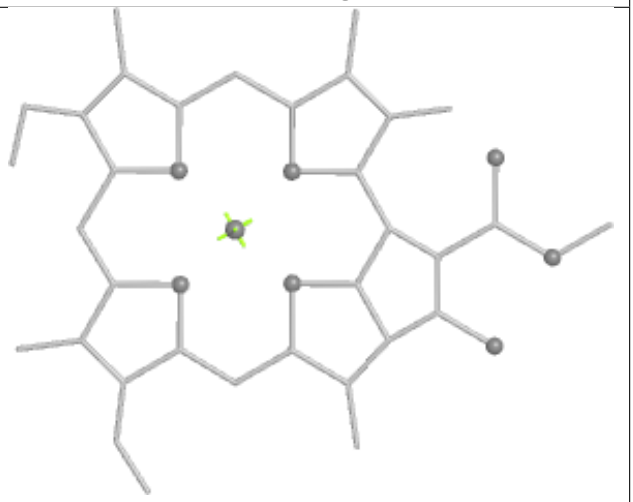
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Bond angles

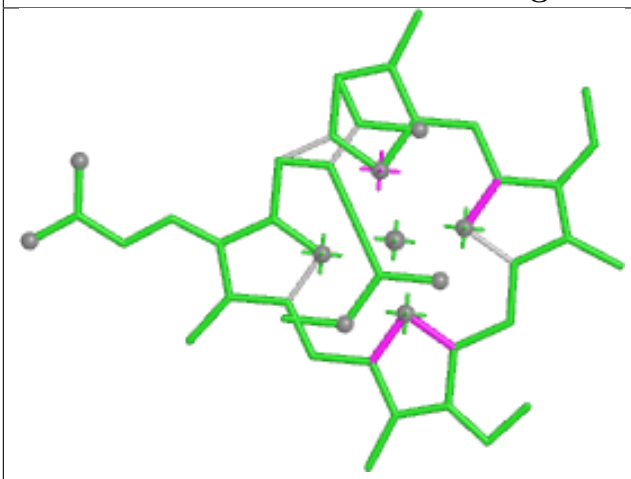


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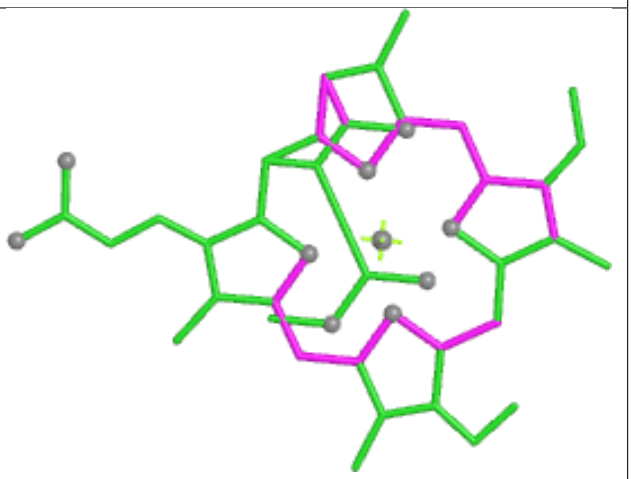


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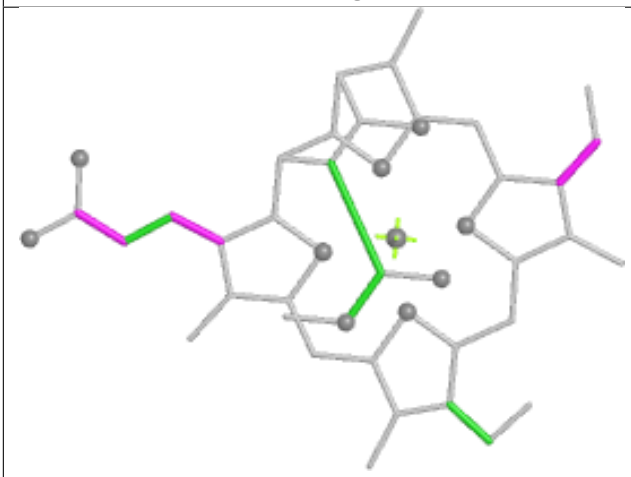
Ligand KC2 e 605



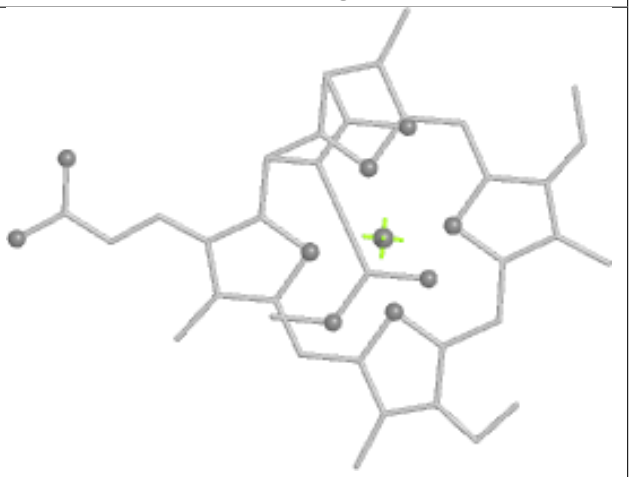
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Bond angles

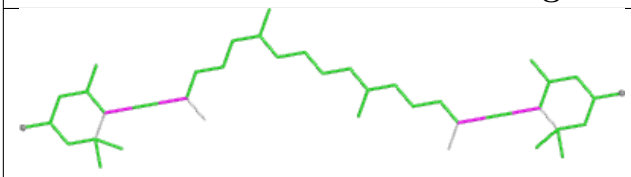


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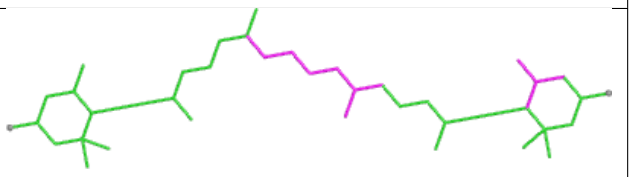


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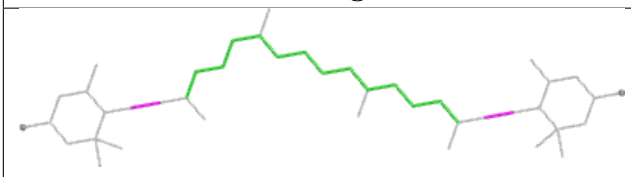
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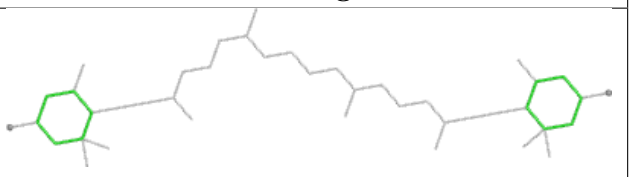
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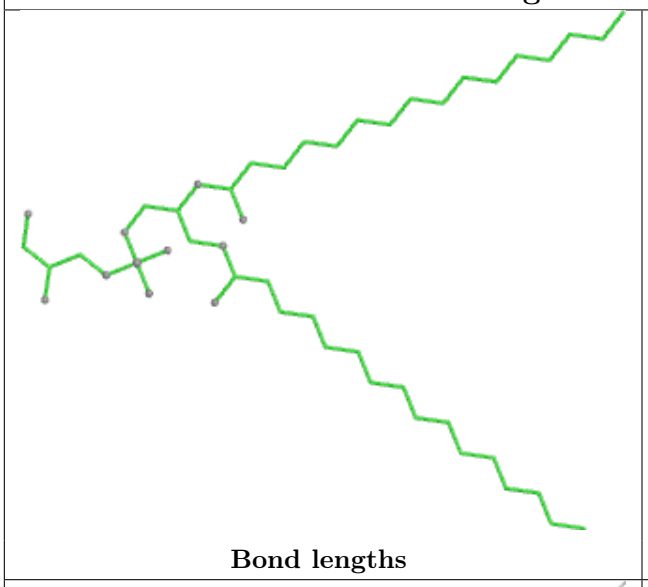


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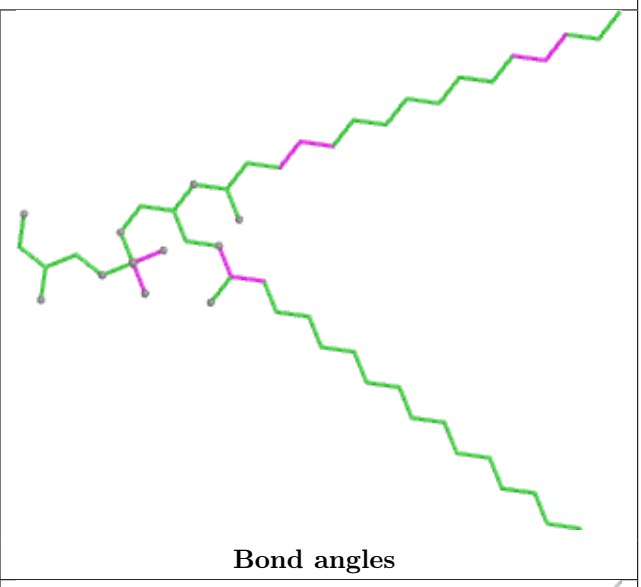


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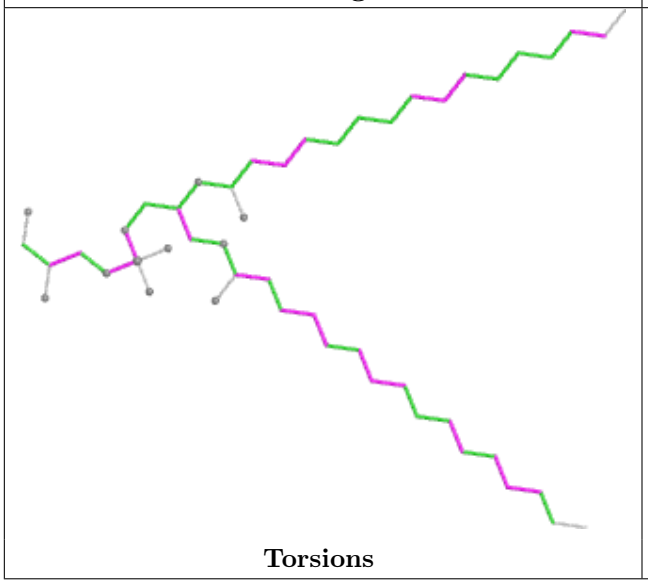
Ligand LHG A 850



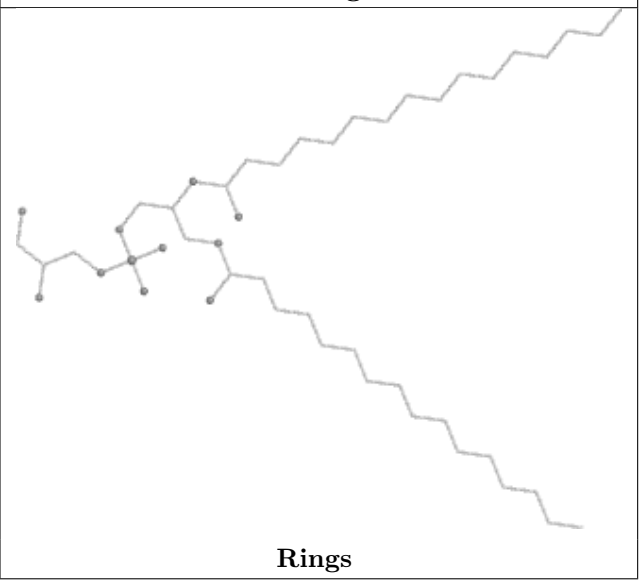
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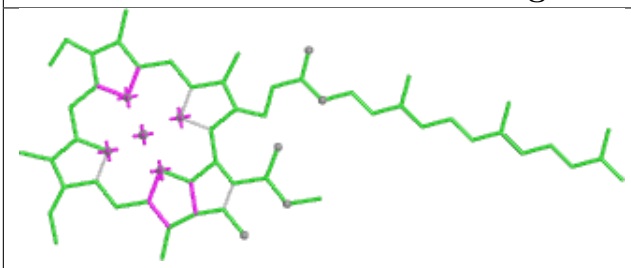
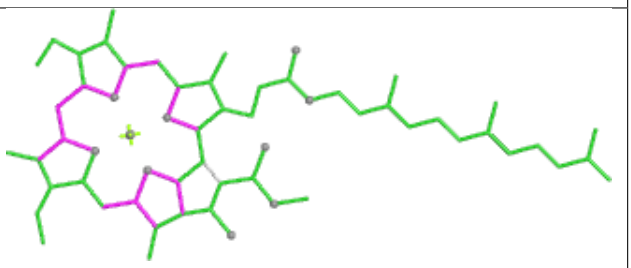
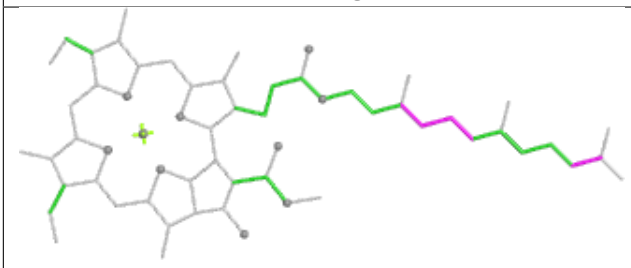
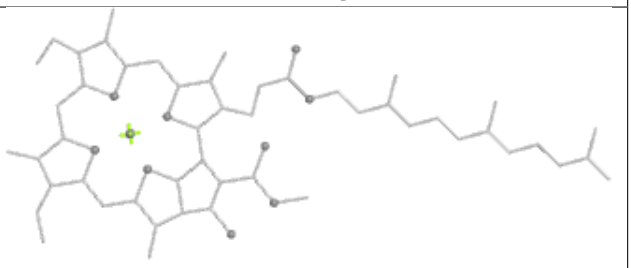
Bond angles

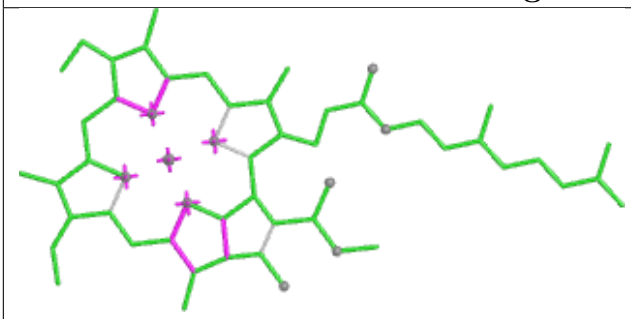
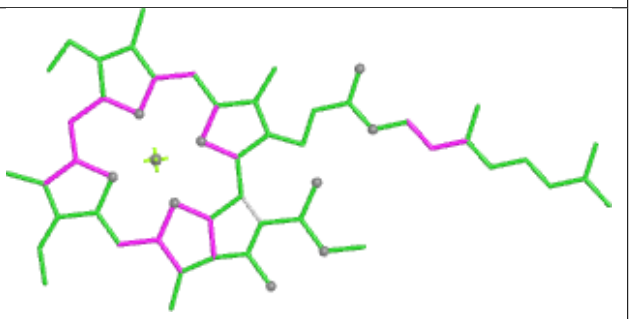
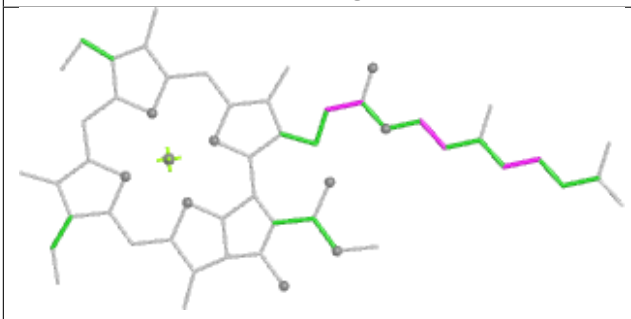
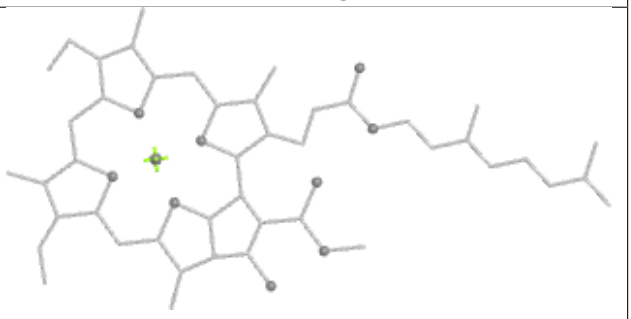


Torsions

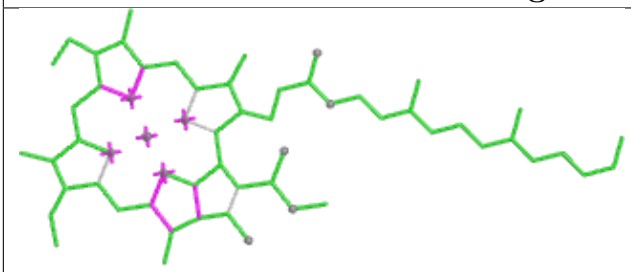


Rings

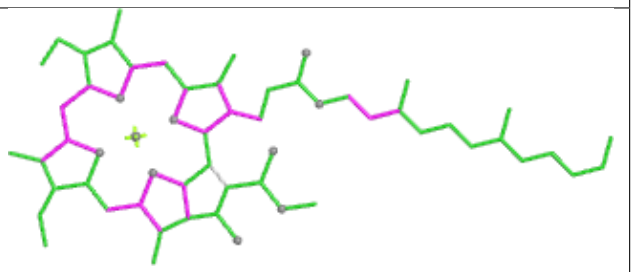
Ligand CLA 3 607	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA O 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

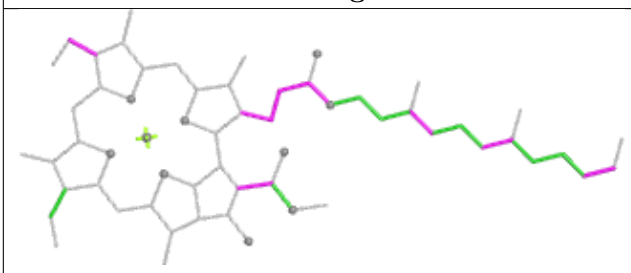
Ligand CLA 2 602



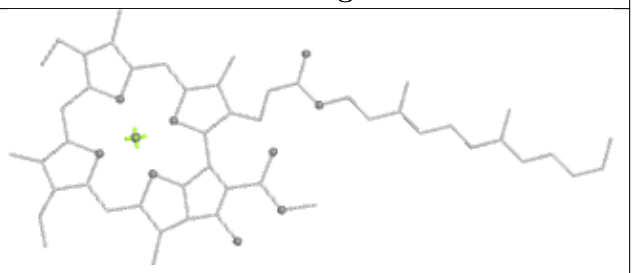
Bond lengths



Bond angles

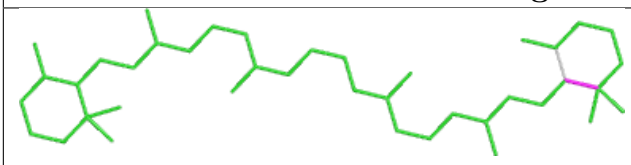


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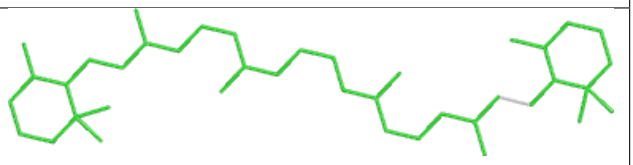


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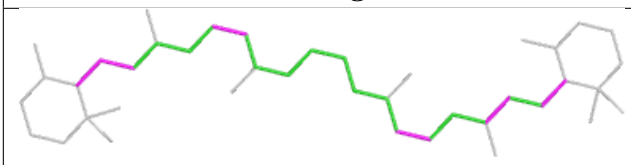
Ligand 8CT 7 617



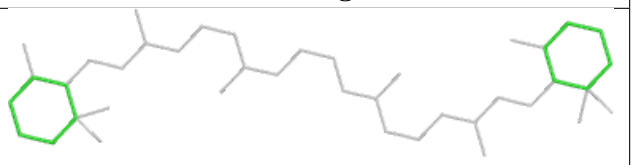
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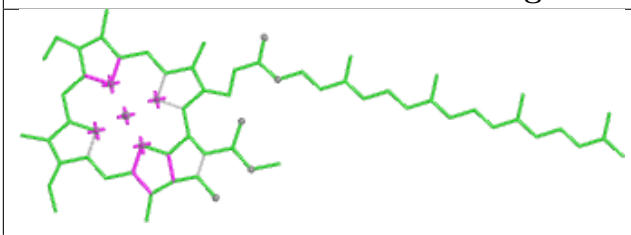


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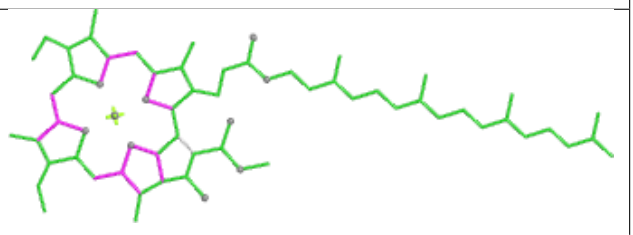


Rings

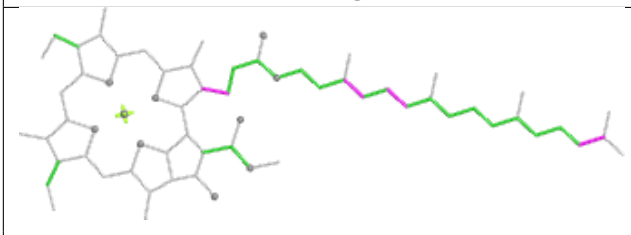
Ligand CLA B 827



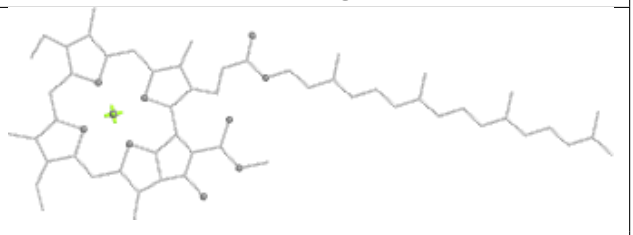
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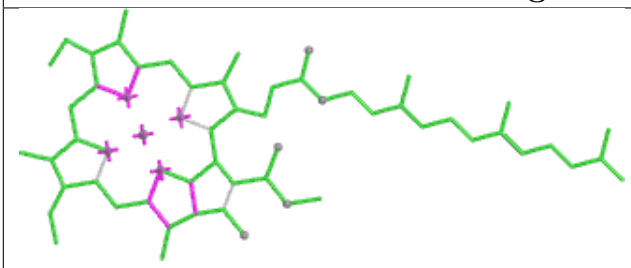
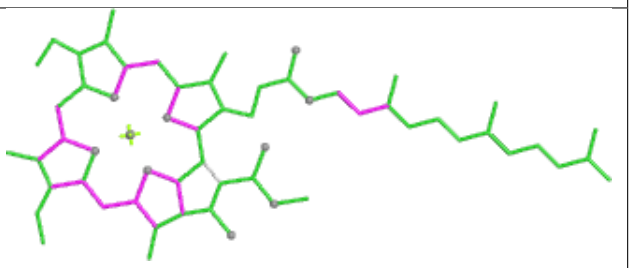
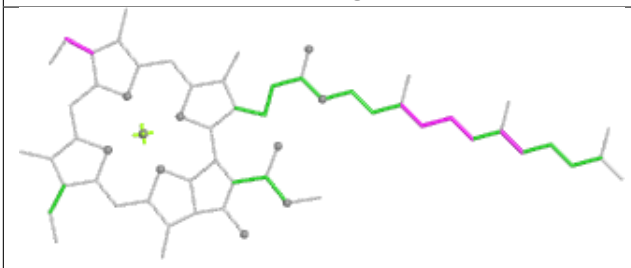
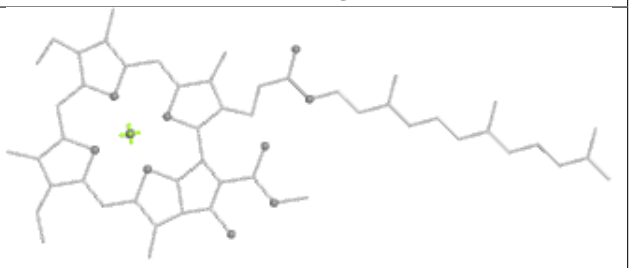
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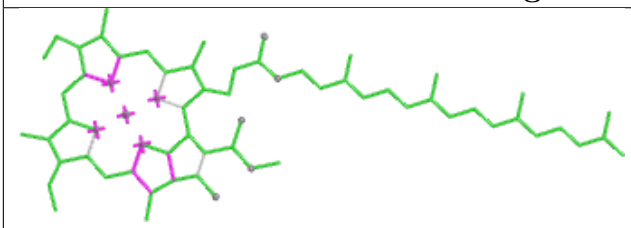
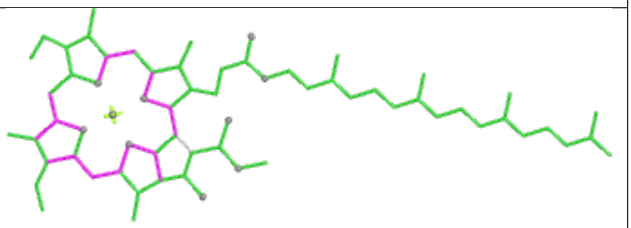
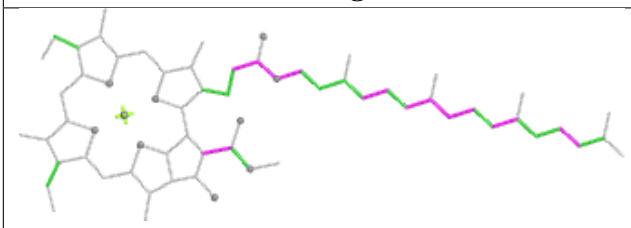
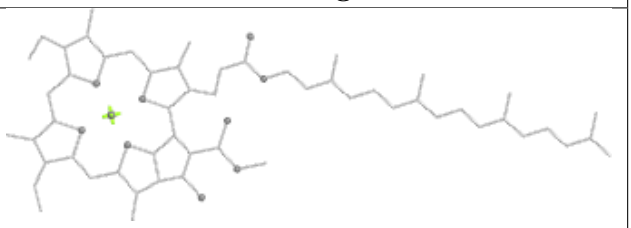


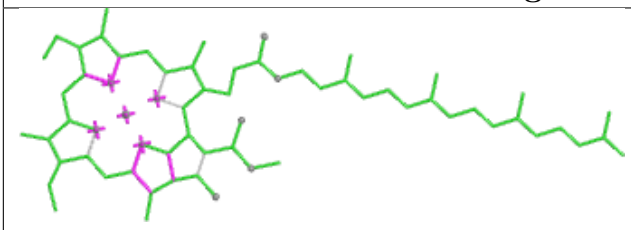
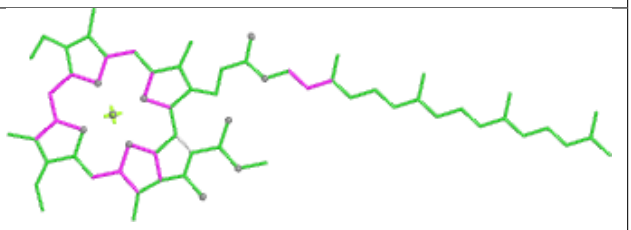
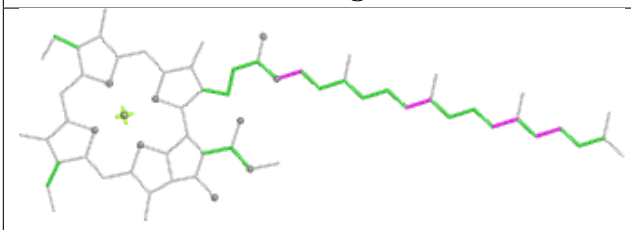
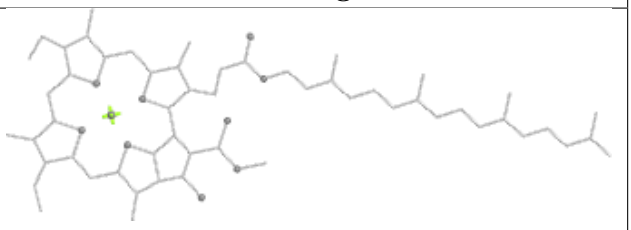
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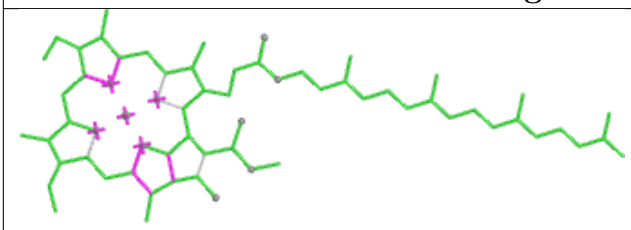
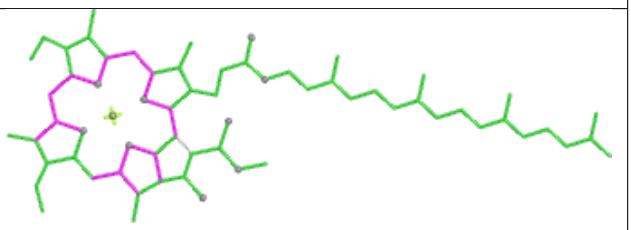
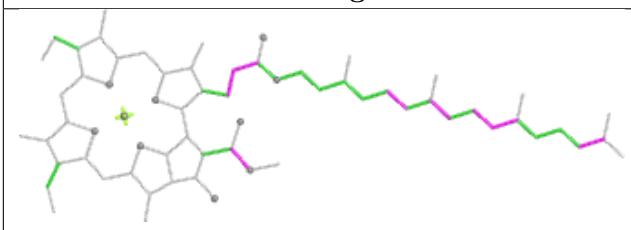
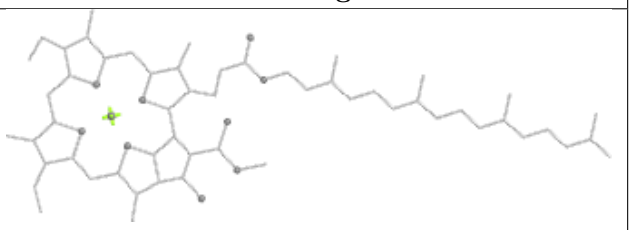


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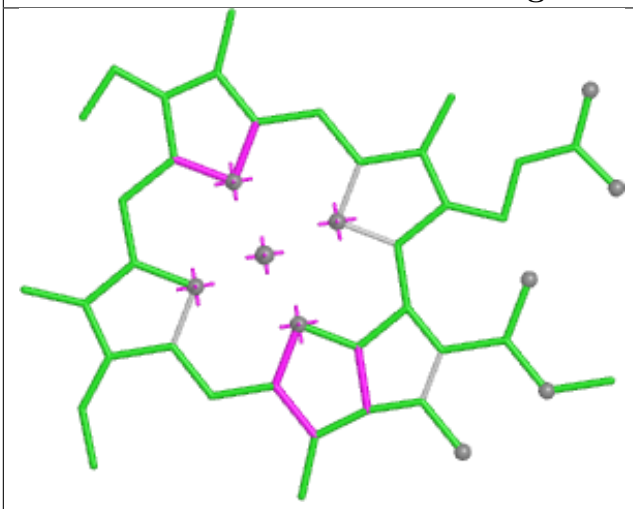
Ligand CLA 4 607	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA A 823	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

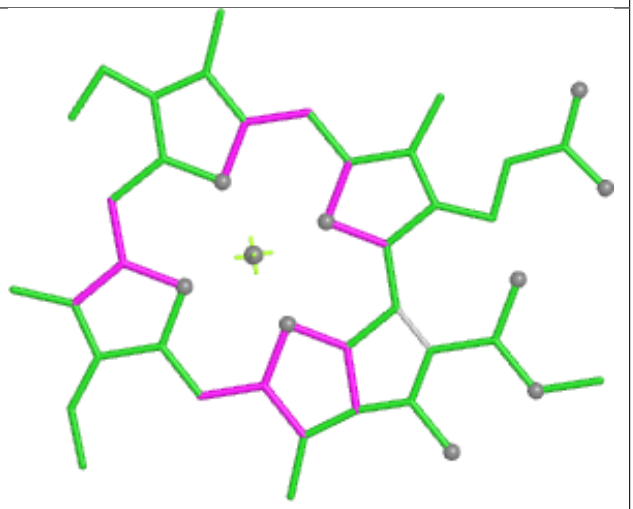
Ligand CLA B 838	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA B 803	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

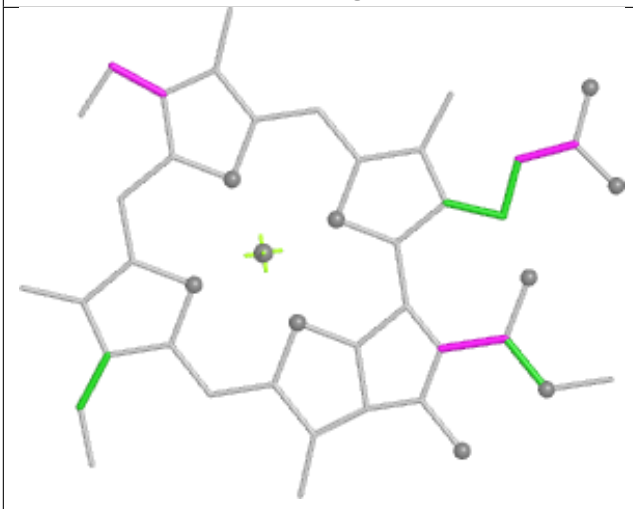
Ligand CLA d 601



Bond lengths



Bond angles

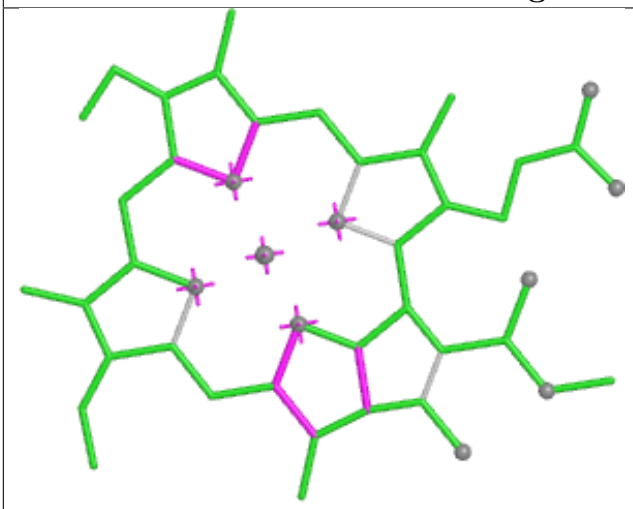


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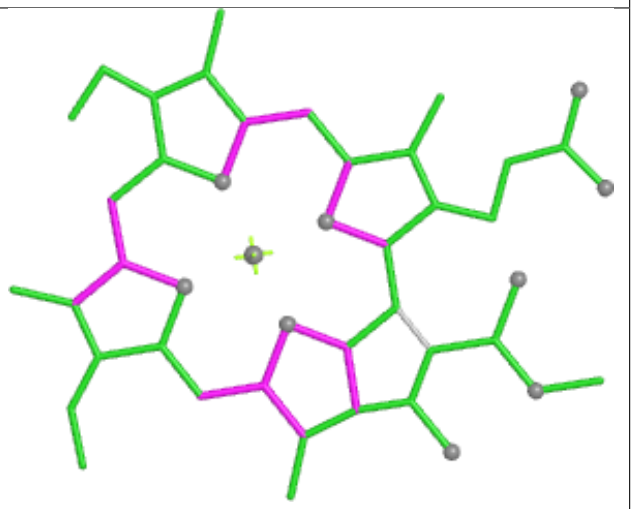


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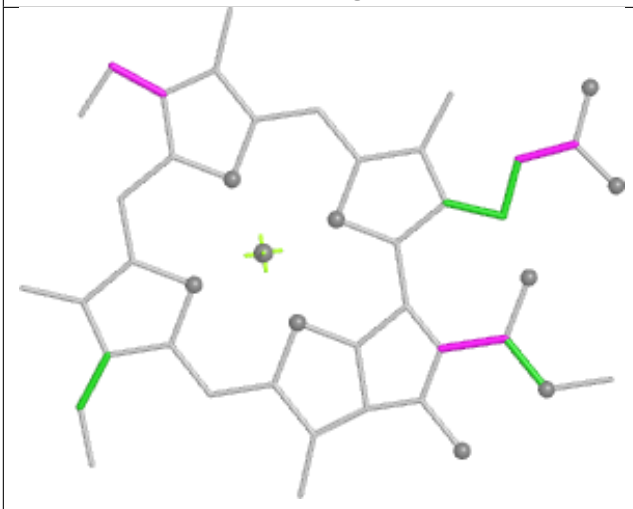
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Bond lengths



Bond angles

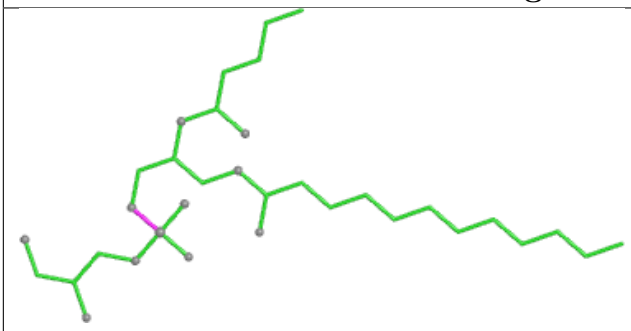


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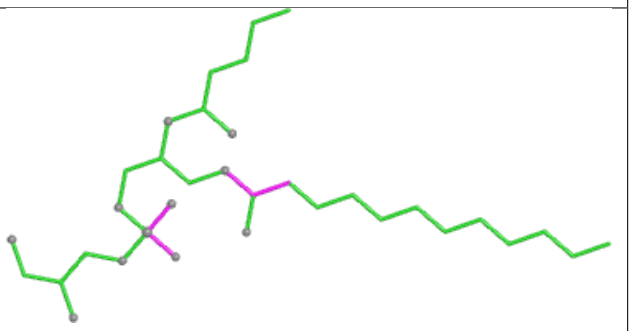


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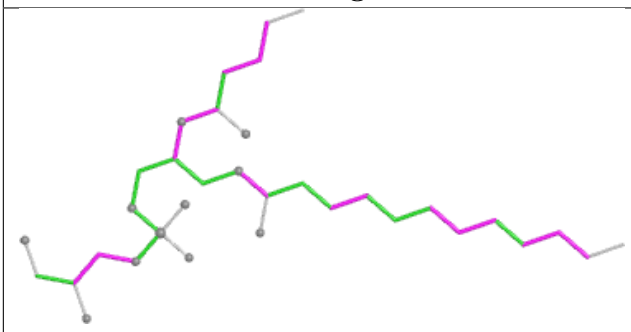
Ligand LHG L 208



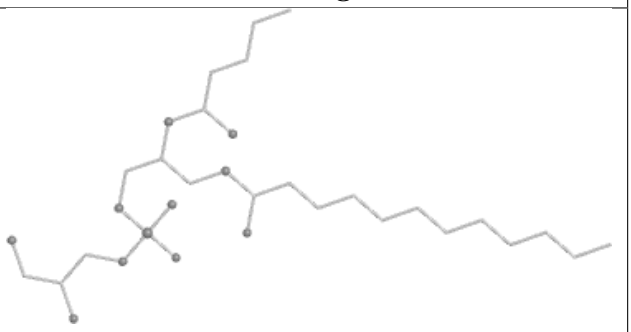
Bond lengths



Bond angles

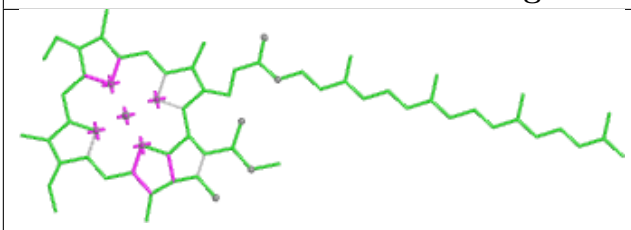


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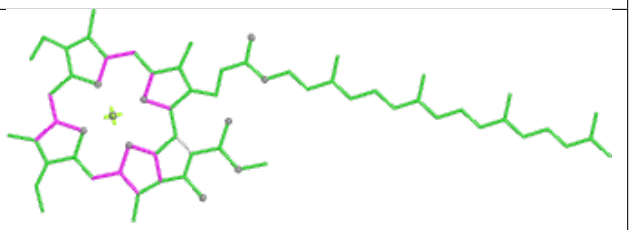


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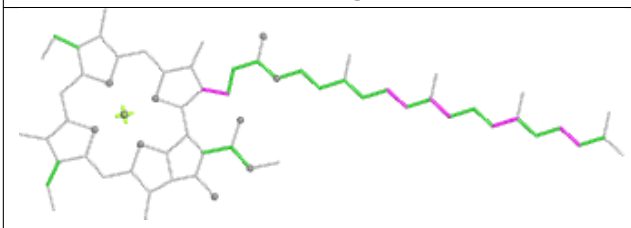
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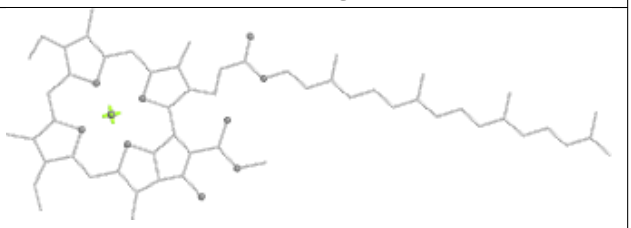
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Bond angles

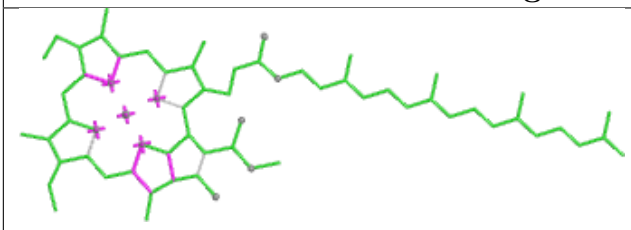


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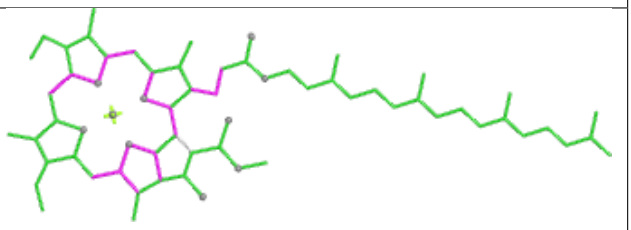


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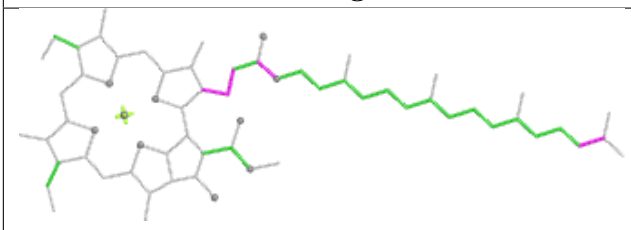
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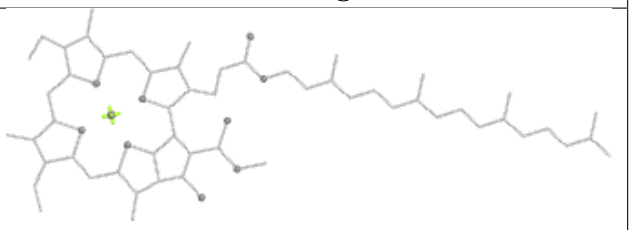
Bond lengths



Bond angles

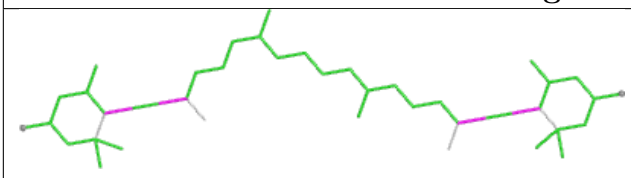


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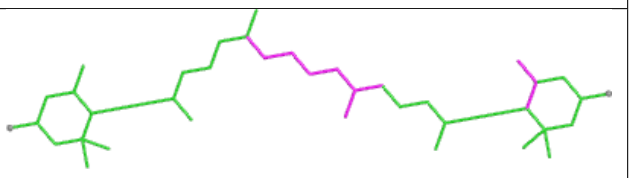


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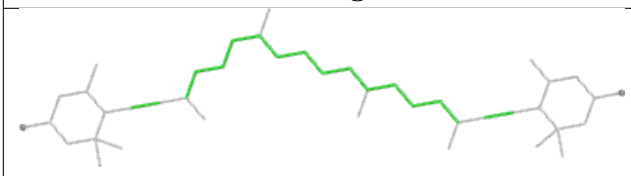
Ligand II0 e 615



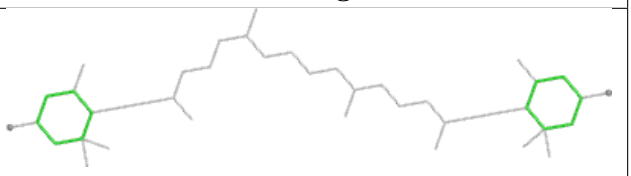
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Bond angles

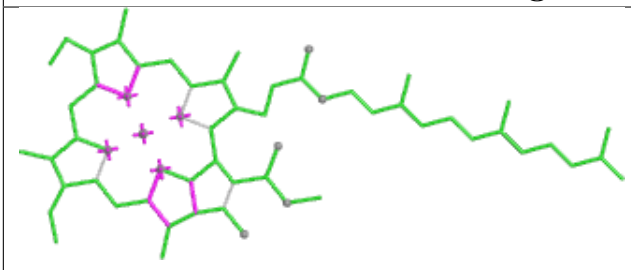


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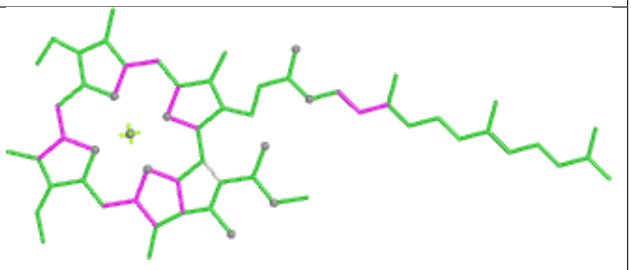


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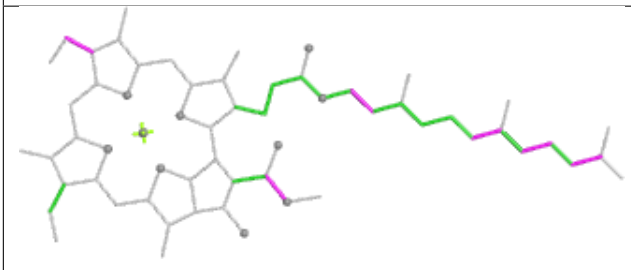
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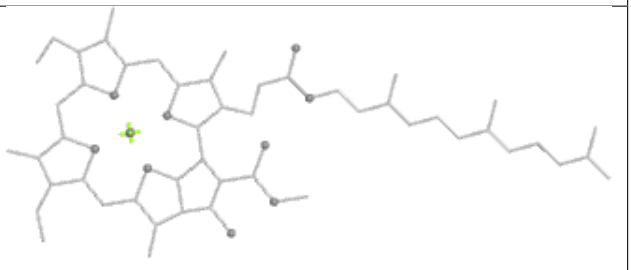
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Bond angles

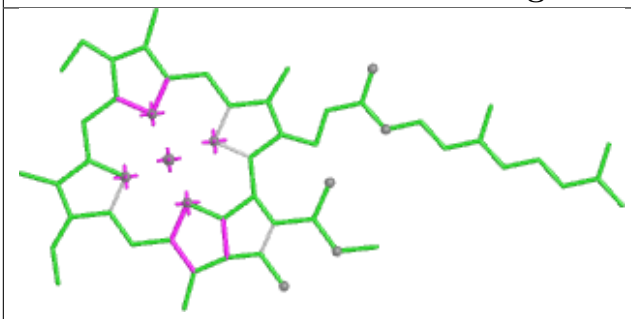


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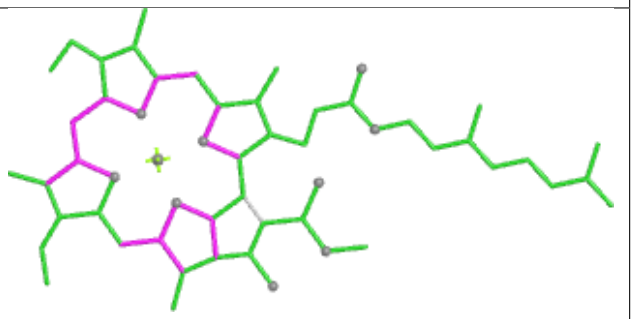


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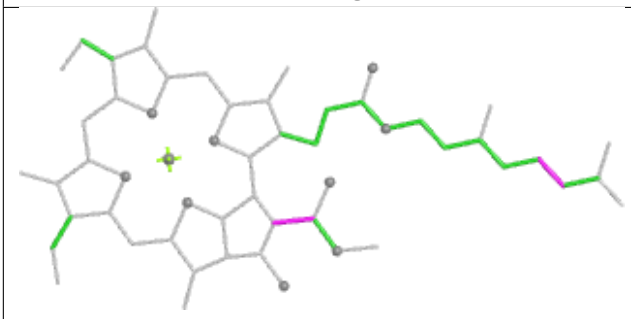
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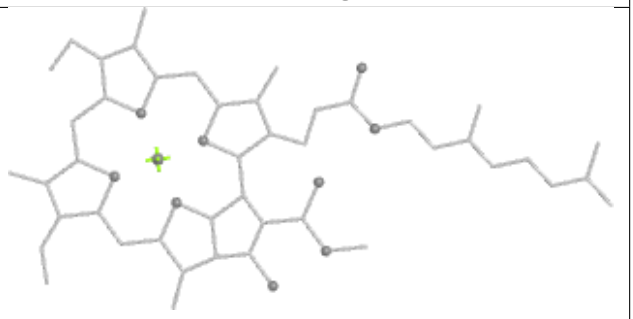
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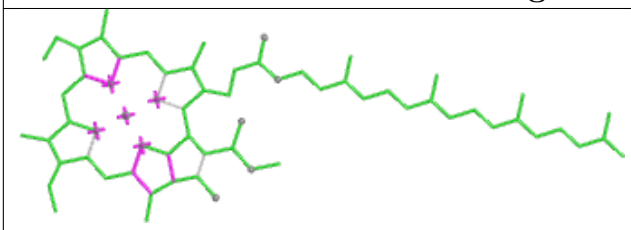


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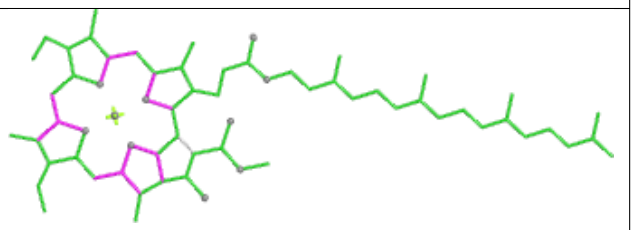


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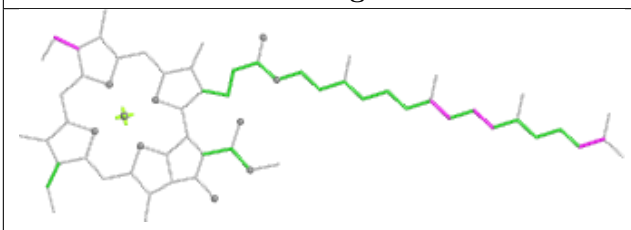
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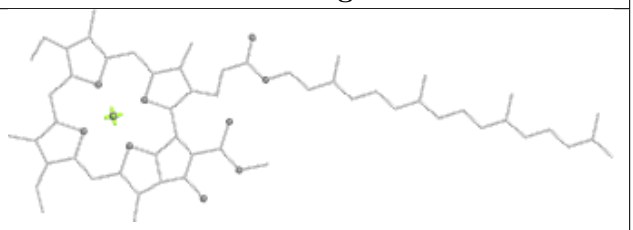
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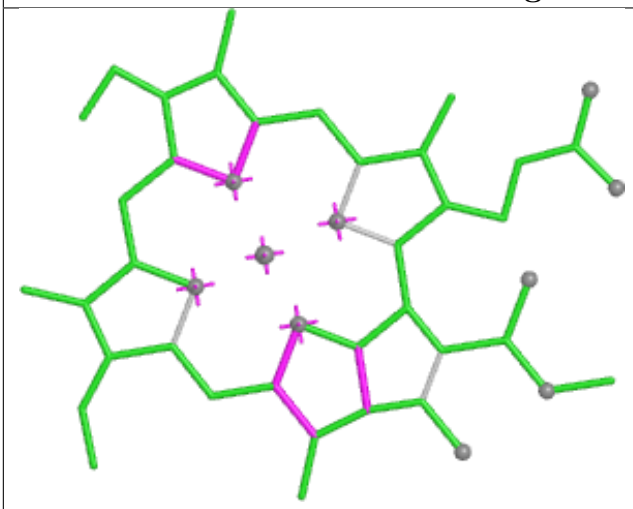


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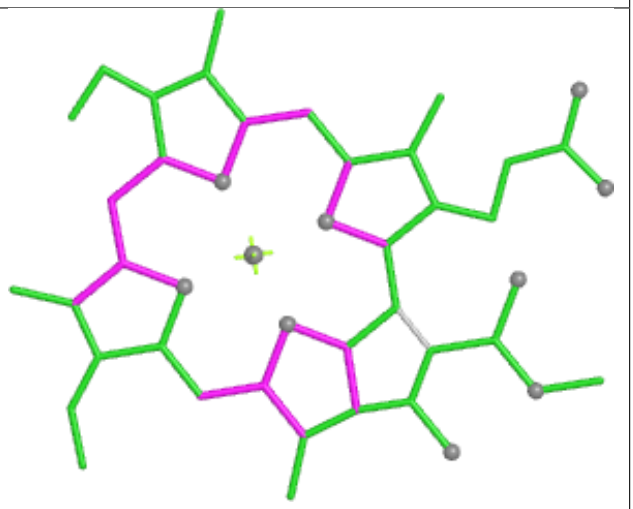


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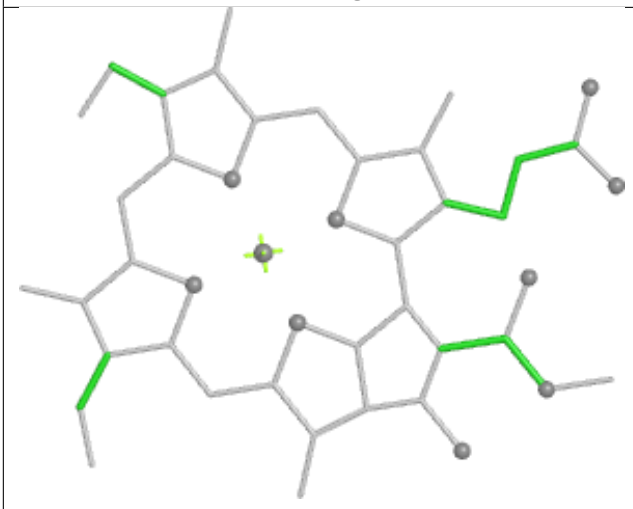
Ligand CLA B 829



Bond lengths



Bond angles

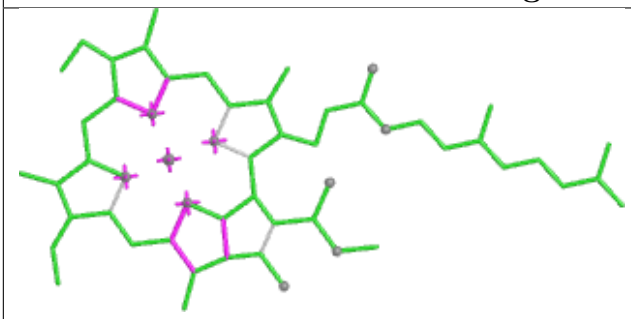


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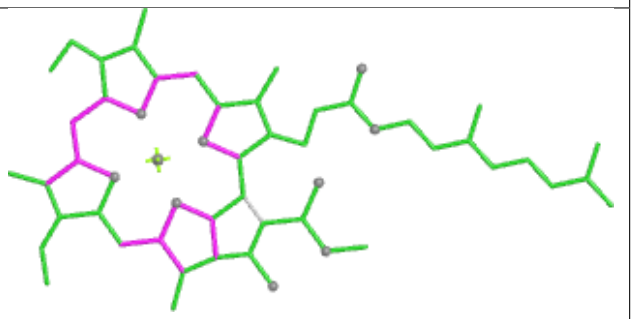


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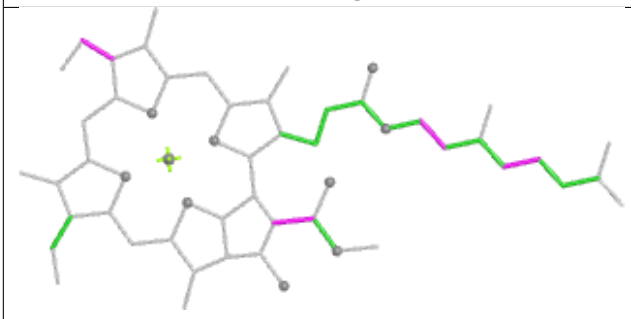
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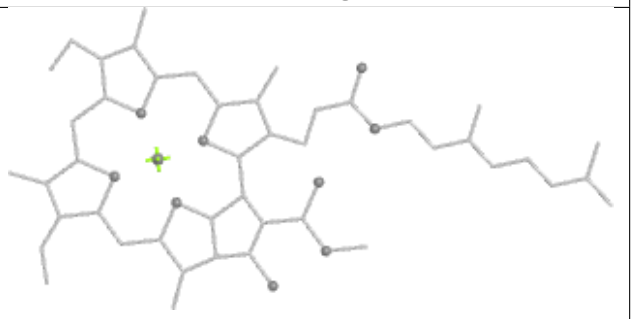
Bond lengths



Bond angles

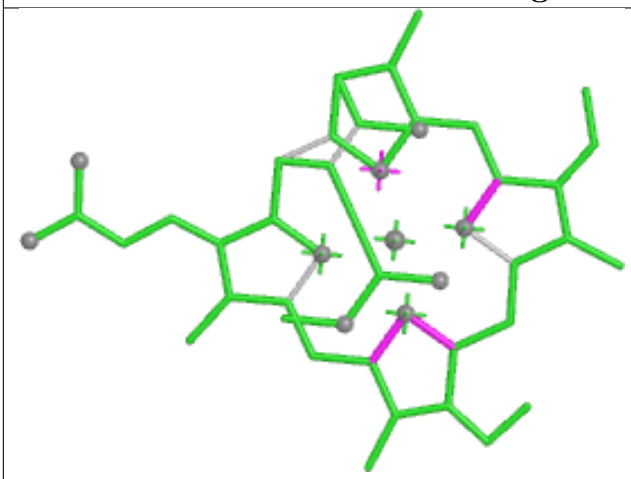


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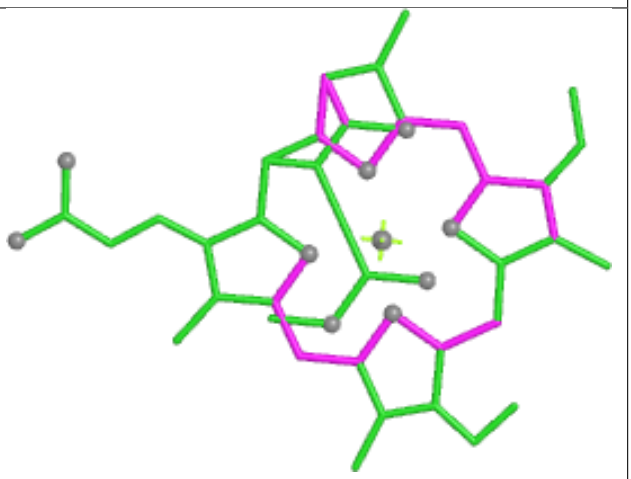


Rings

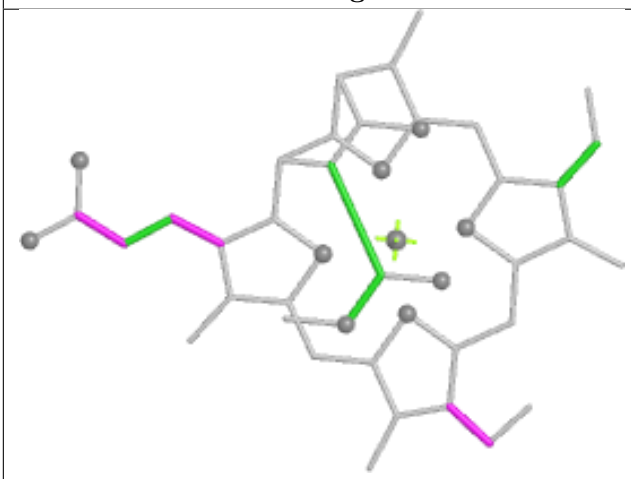
Ligand KC2 c 615



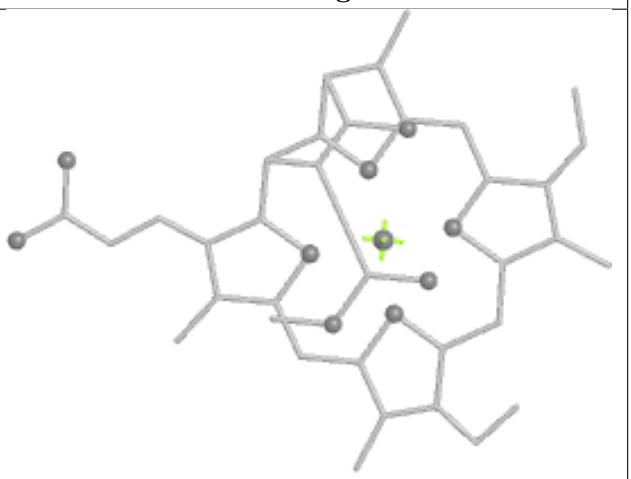
Bond lengths



Bond angles

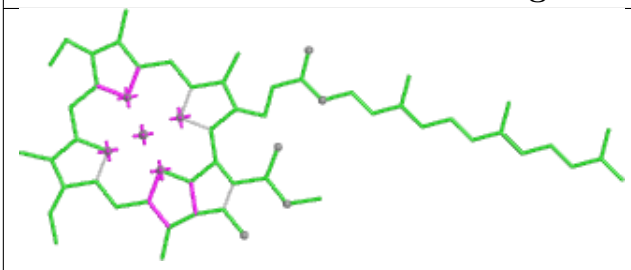


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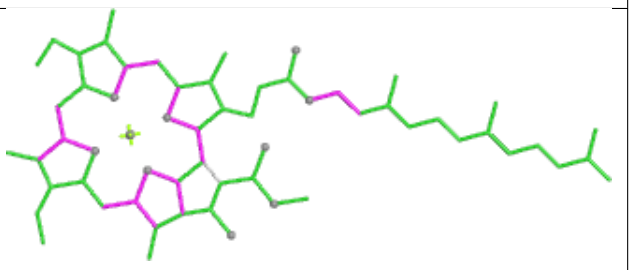


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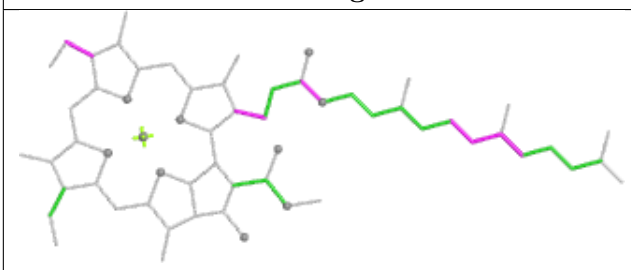
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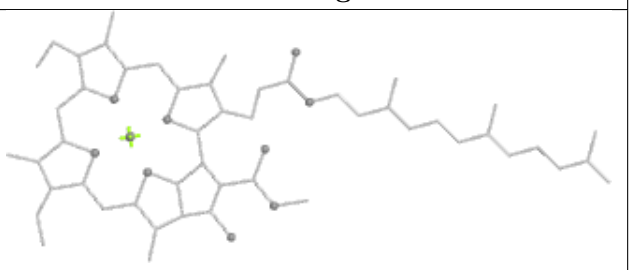
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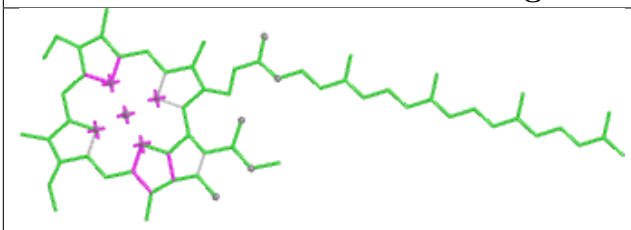


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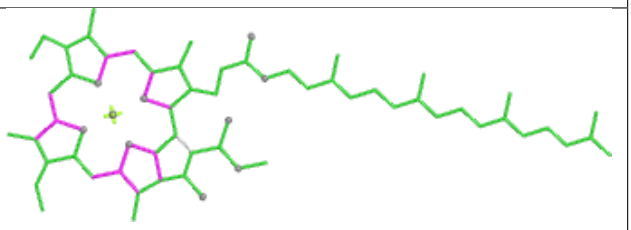


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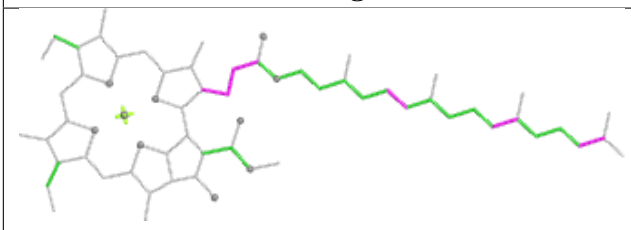
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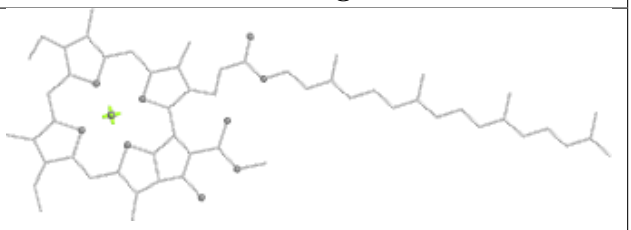
Bond lengths



Bond angles

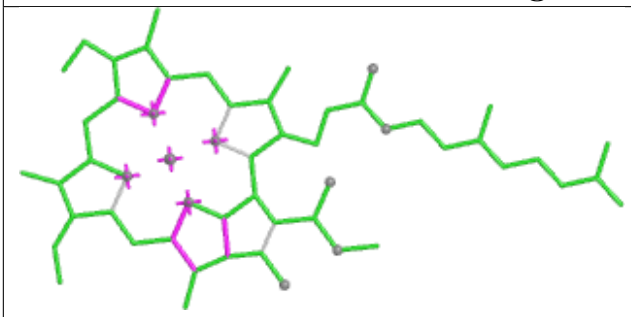


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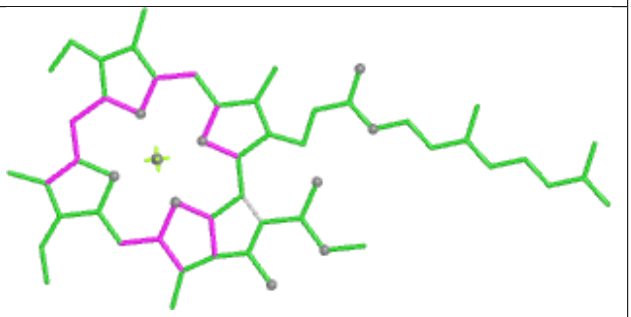


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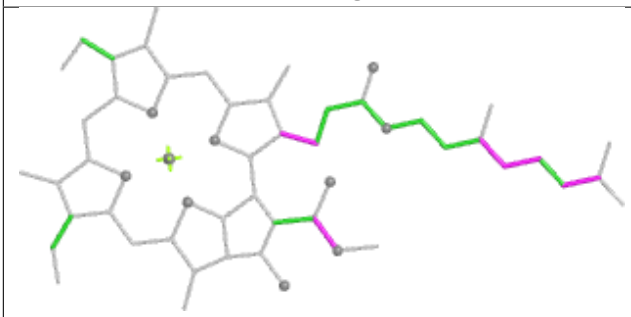
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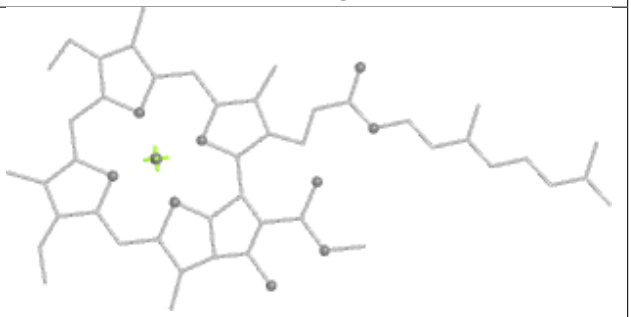
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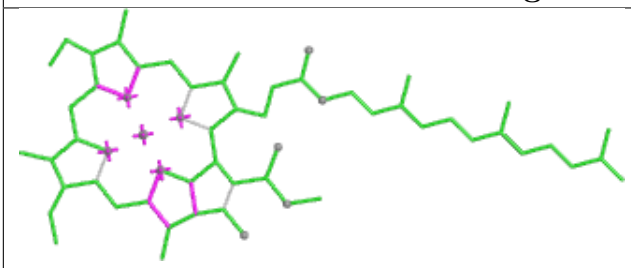


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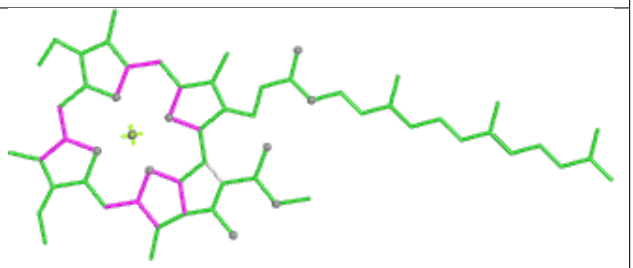


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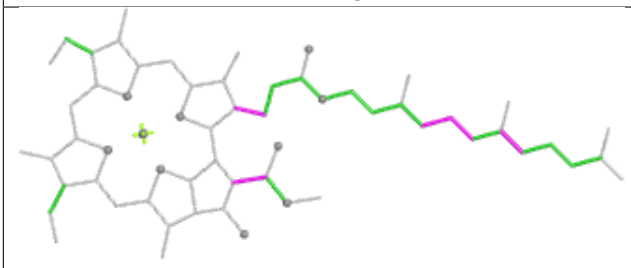
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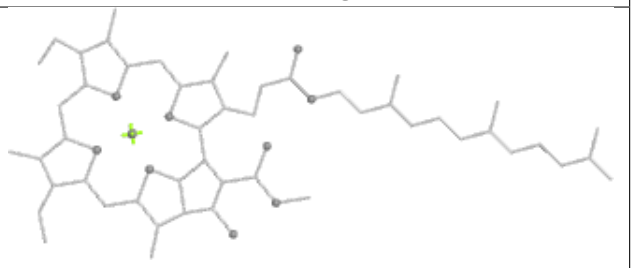
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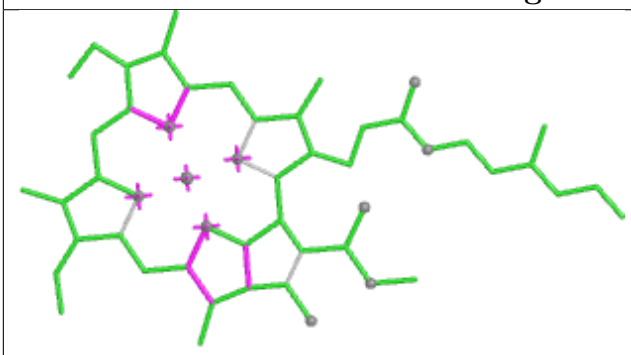


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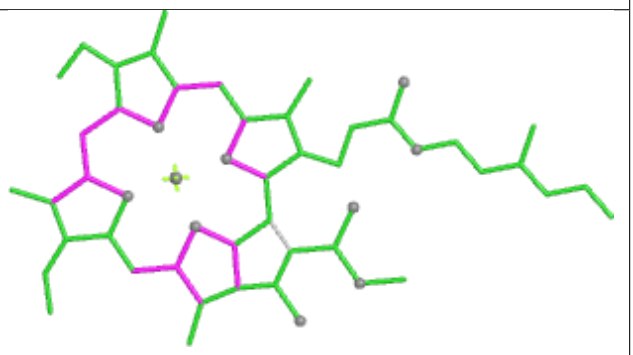


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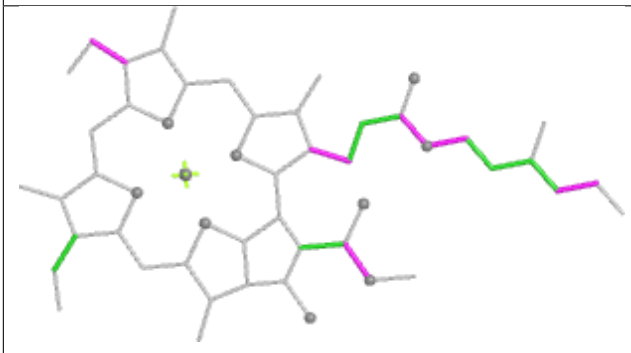
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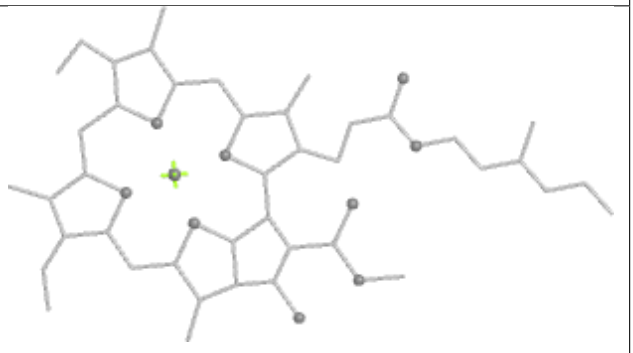
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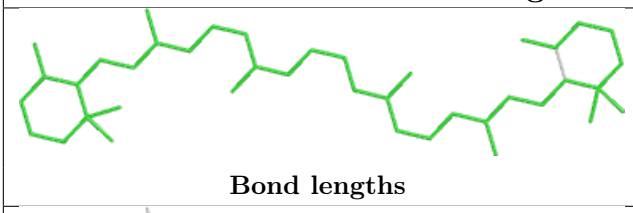


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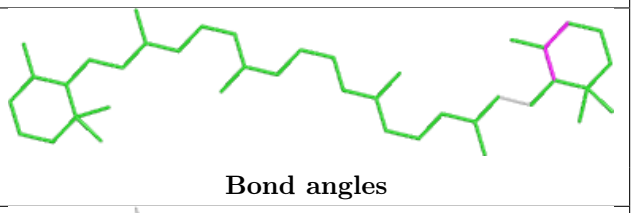


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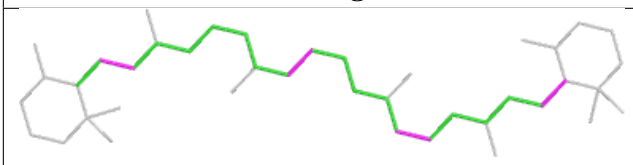
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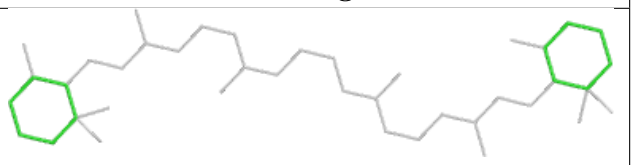
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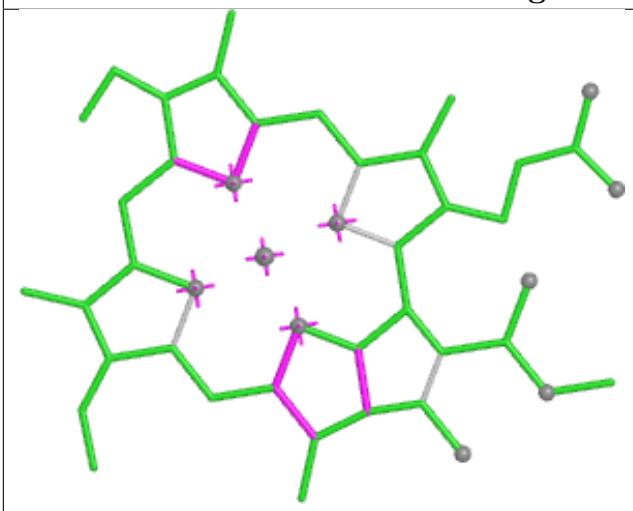


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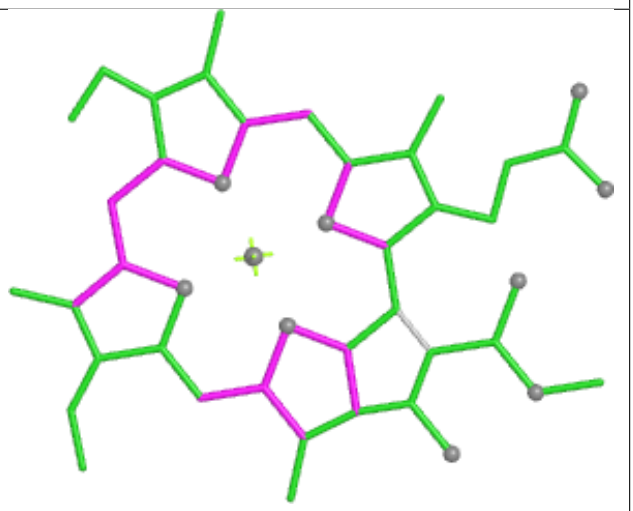


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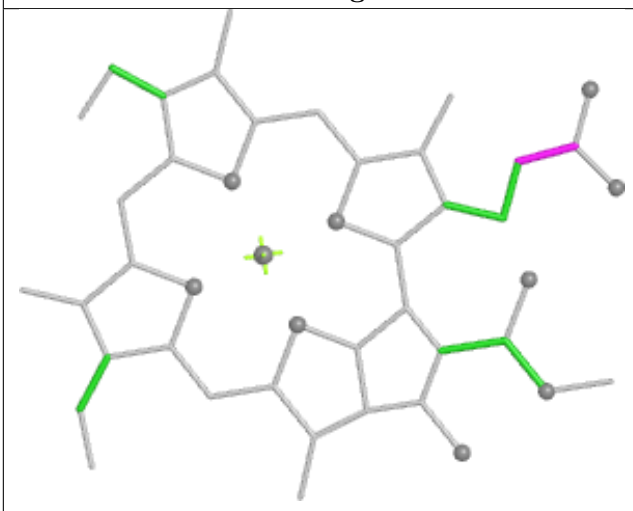
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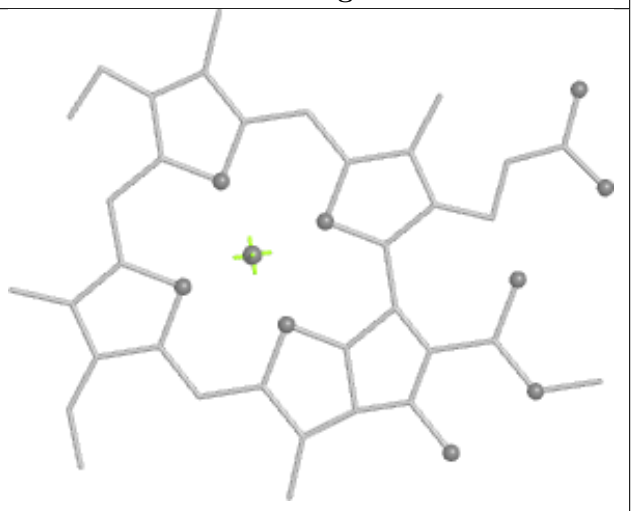
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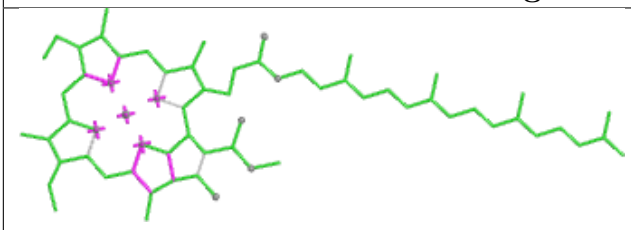


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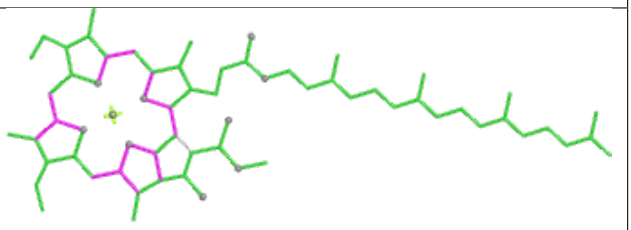


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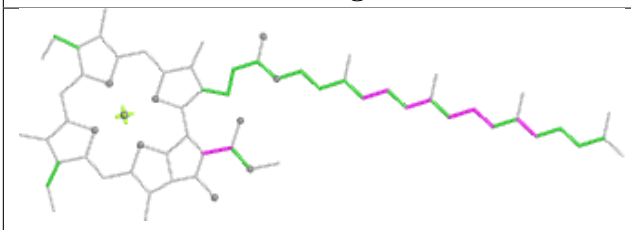
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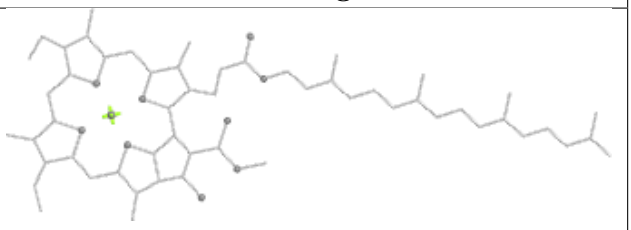
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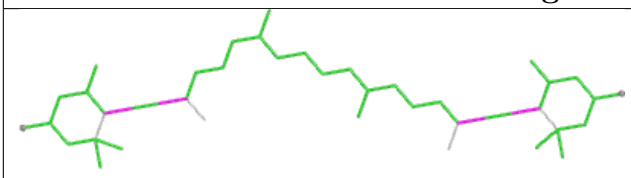


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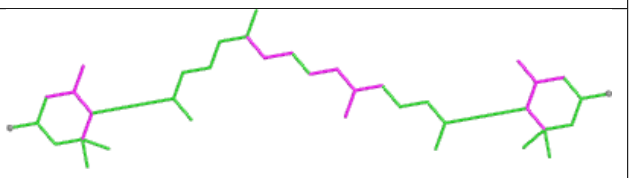


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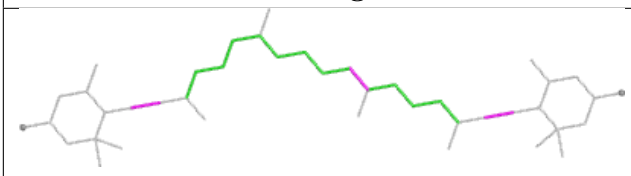
Ligand II0 d 616



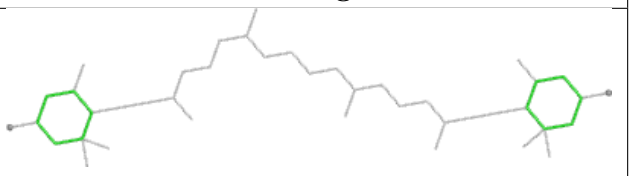
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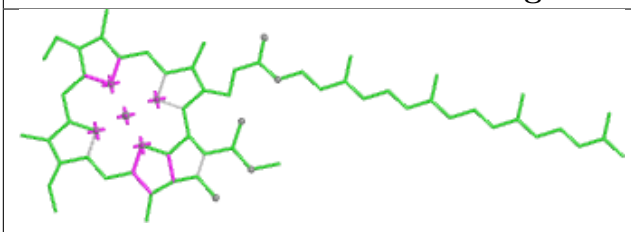


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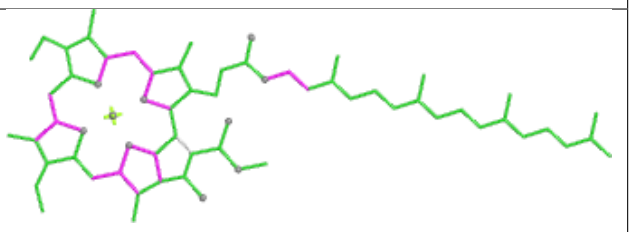


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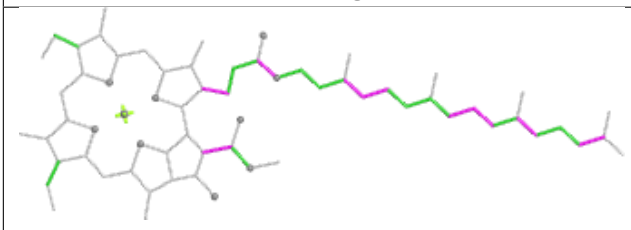
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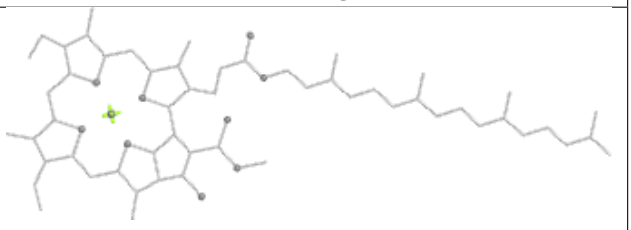
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Bond angles

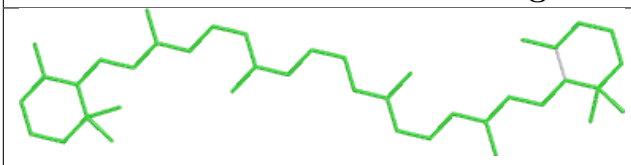


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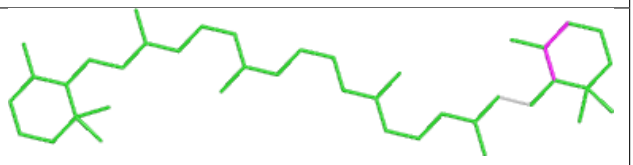


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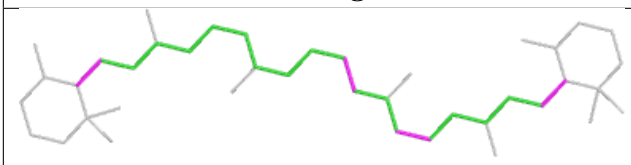
Ligand 8CT Z 309



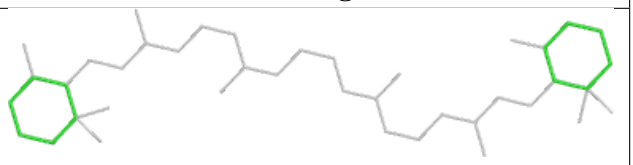
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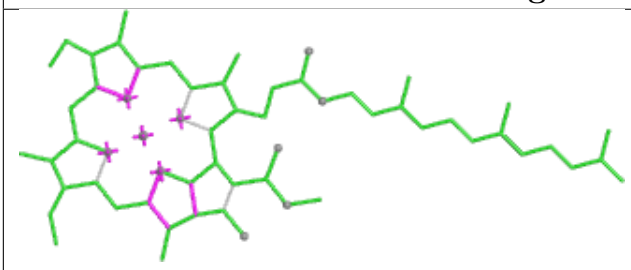


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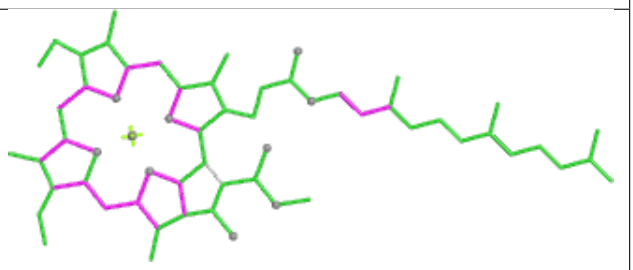


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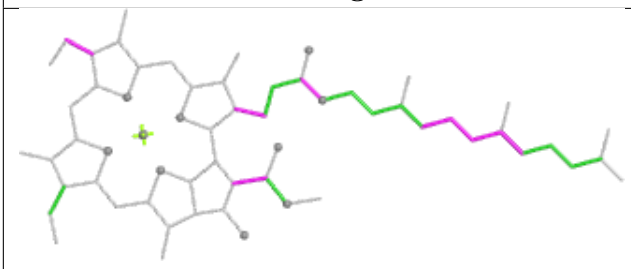
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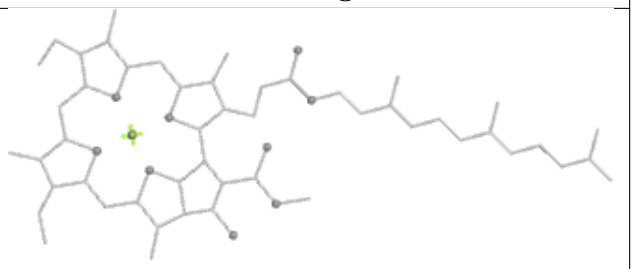
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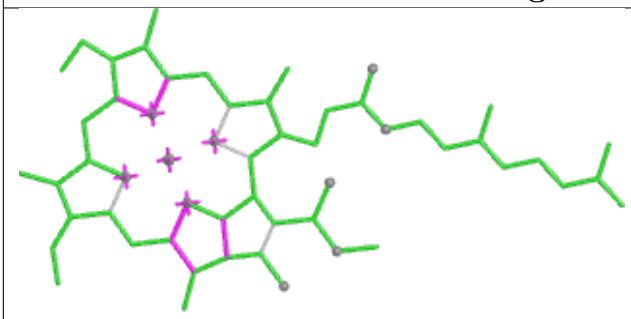


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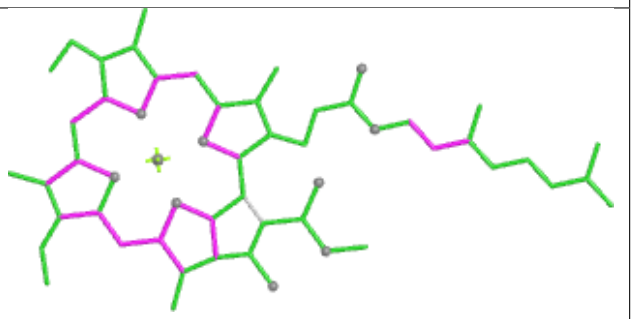


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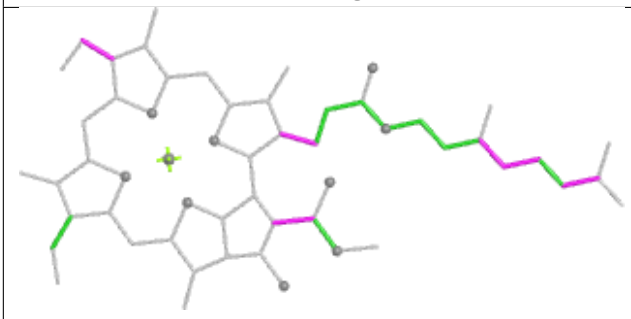
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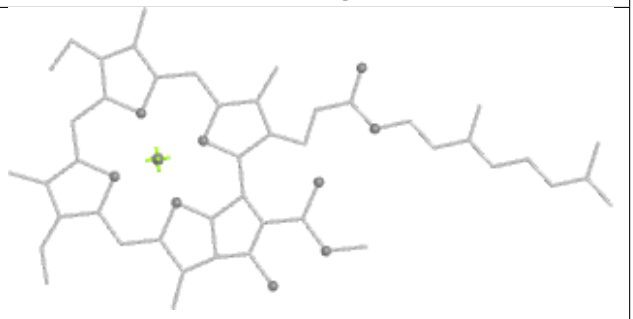
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Bond angles

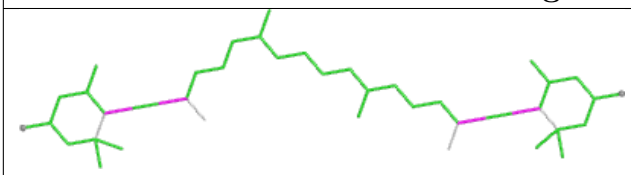


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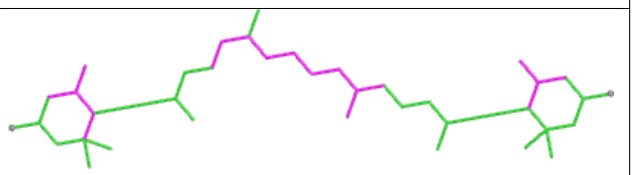


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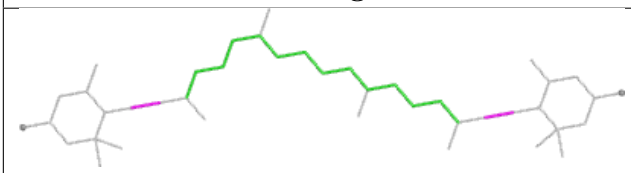
Ligand II0 7 615



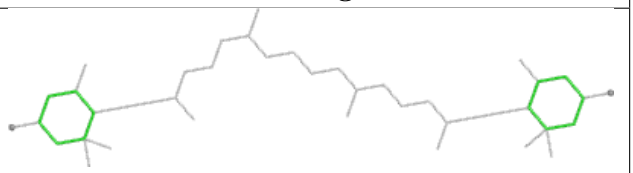
Bond lengths



Bond angles

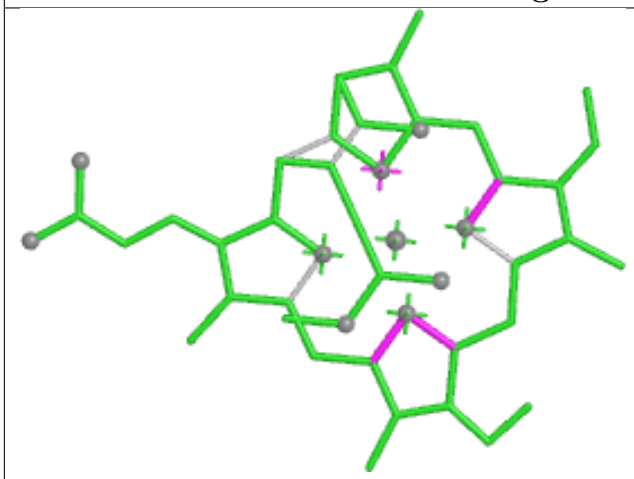


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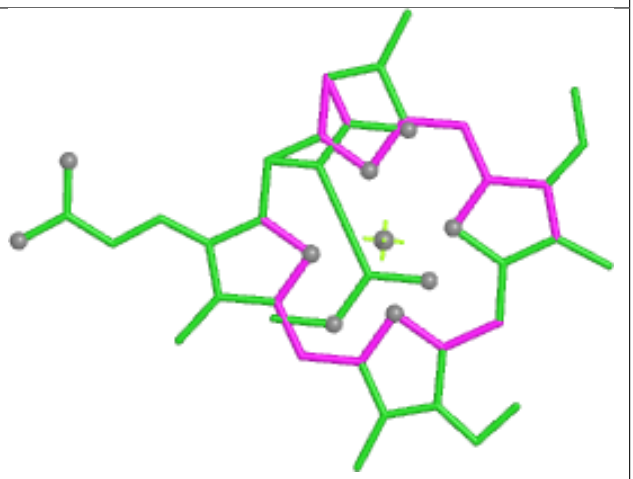


Rings

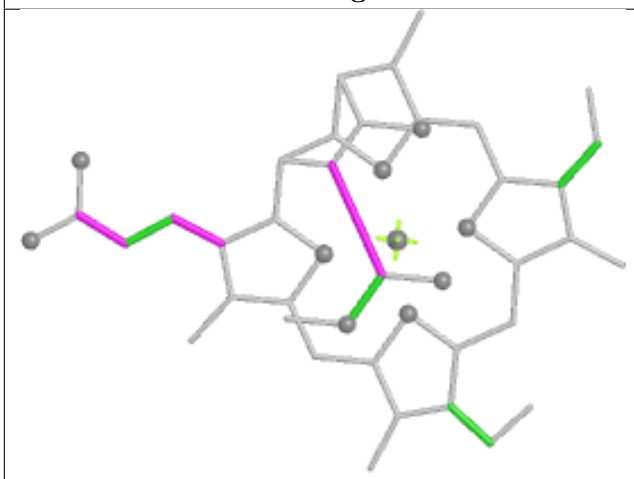
Ligand KC2 c 610



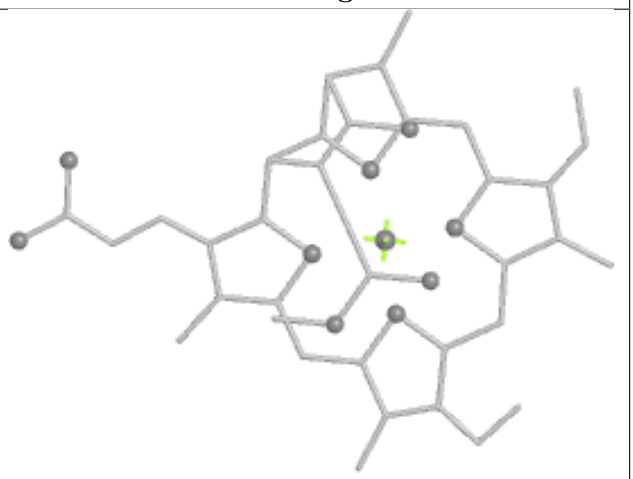
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Bond angles

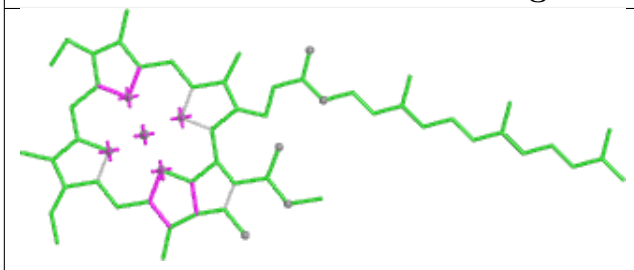


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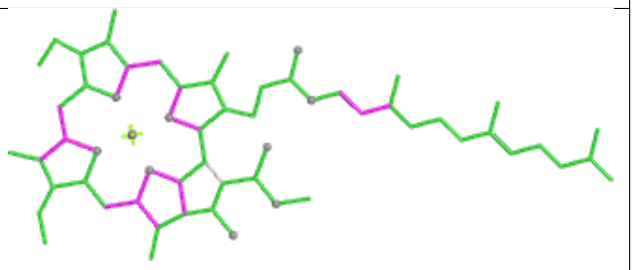


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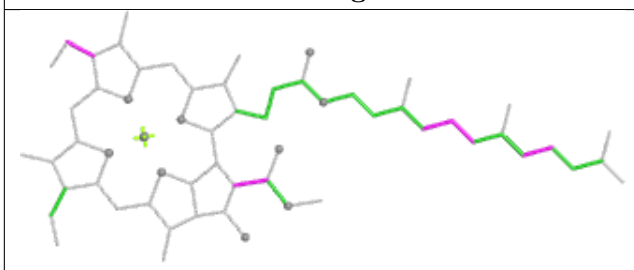
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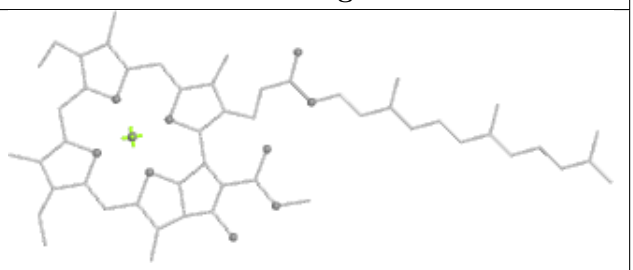
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Bond angles

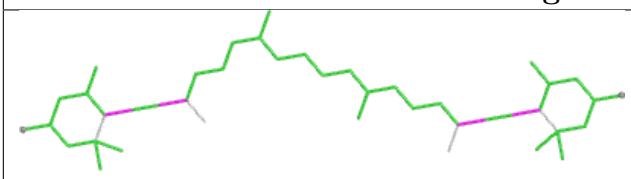


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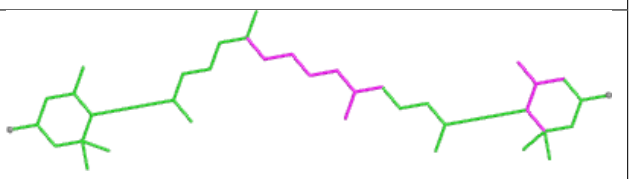


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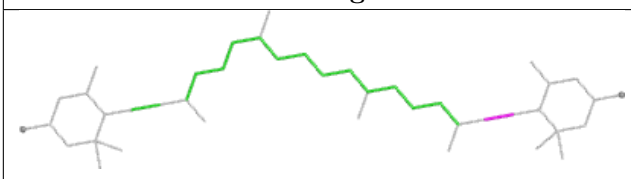
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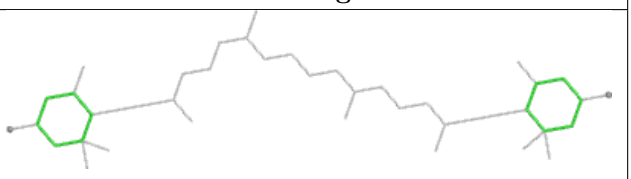
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Bond angles

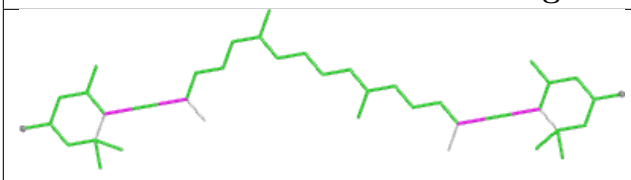


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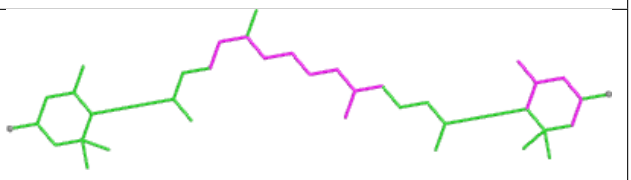


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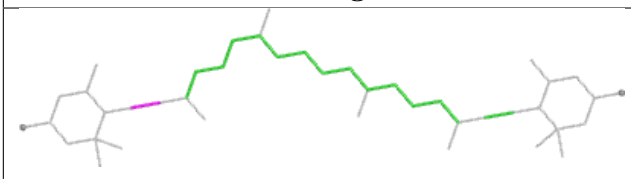
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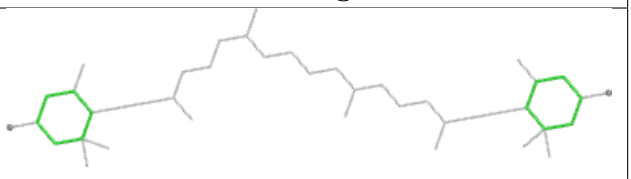
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Bond angles

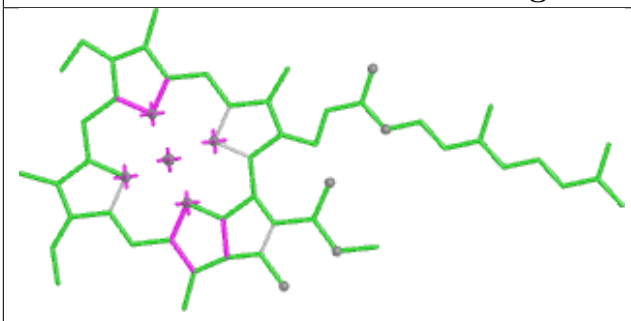


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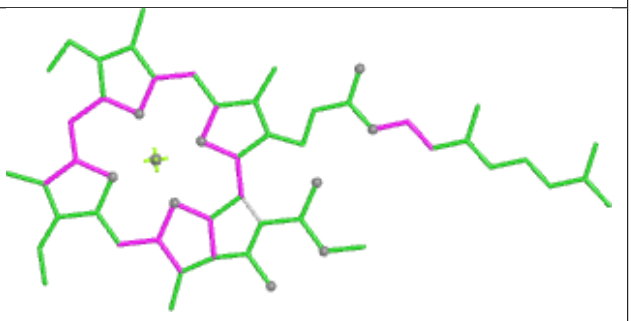


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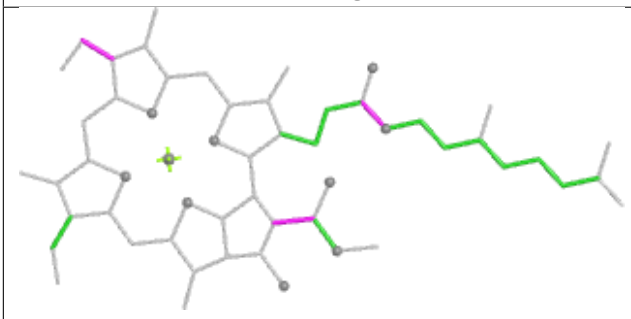
Ligand CLA c 612



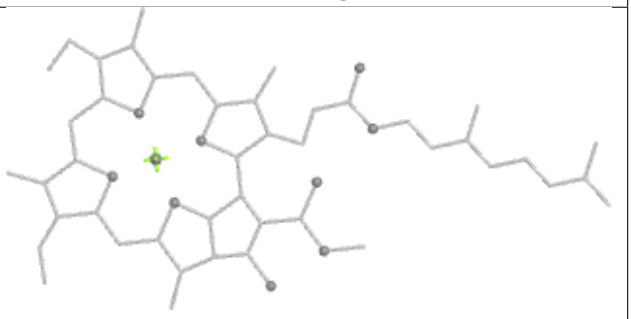
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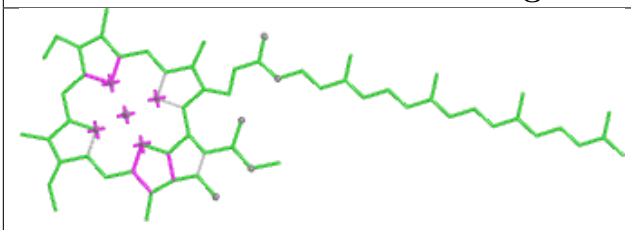


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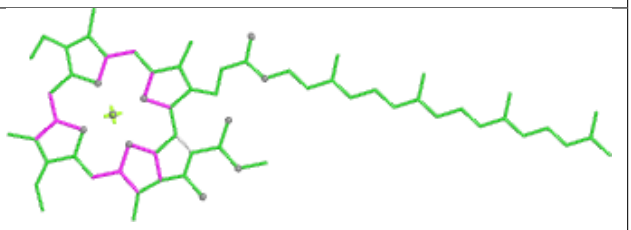


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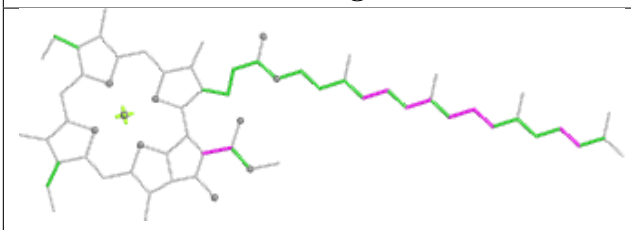
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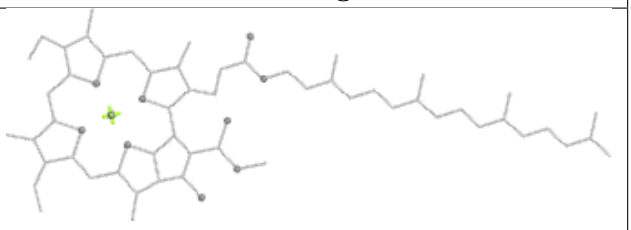
Bond lengths



Bond angles

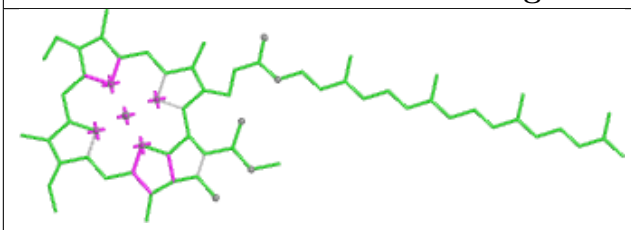


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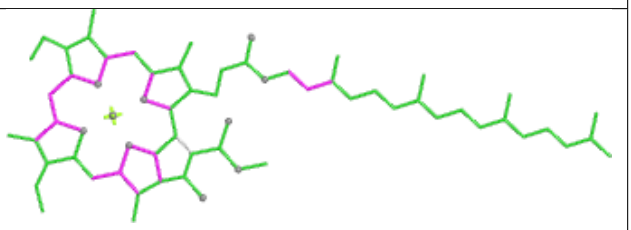


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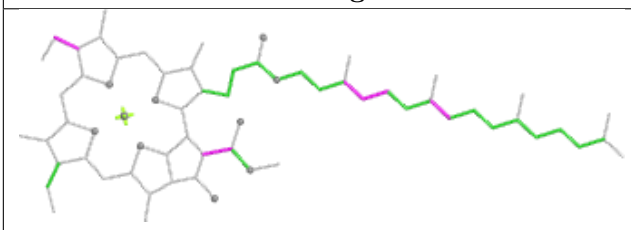
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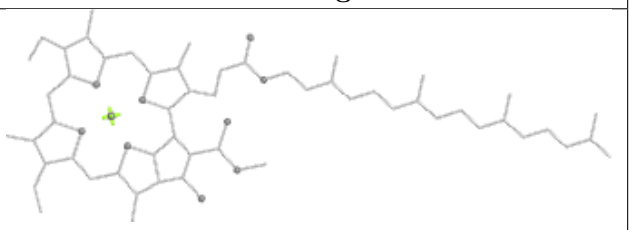
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Bond angles

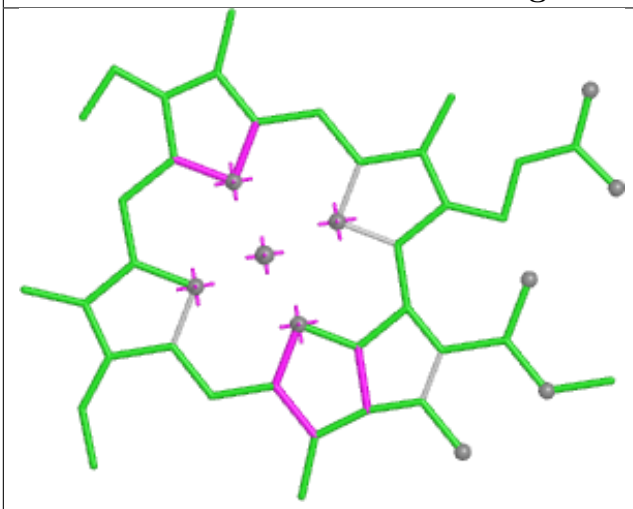


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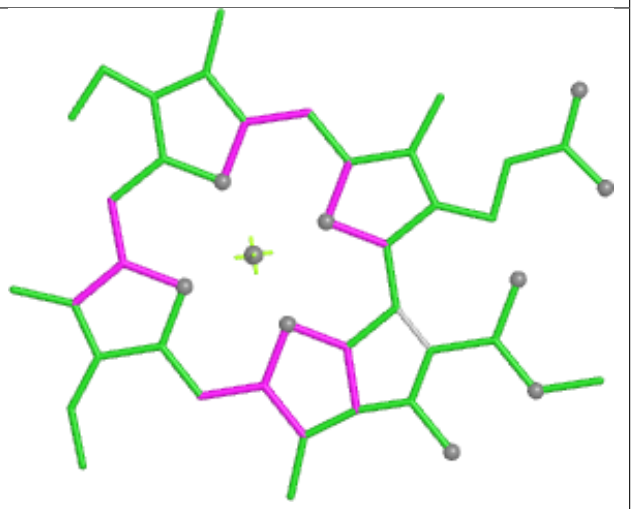


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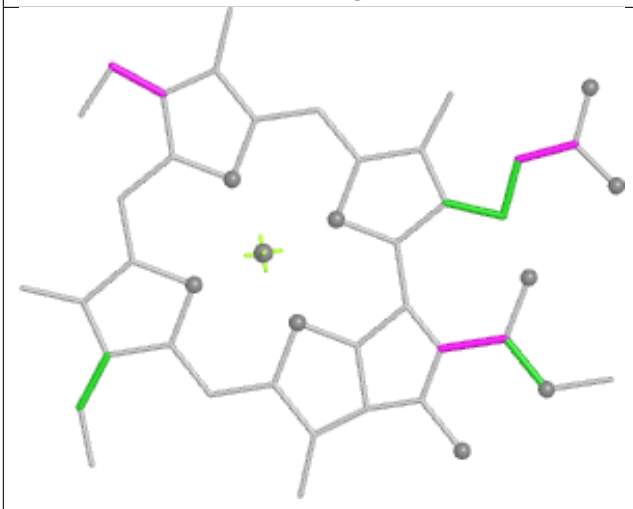
Ligand CLA e 601



Bond lengths



Bond angles

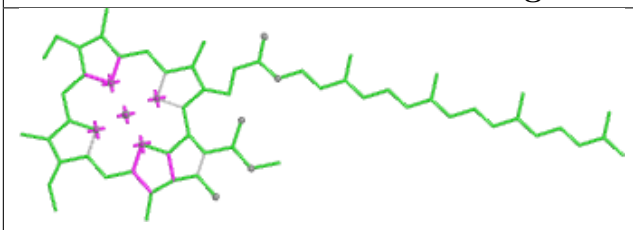


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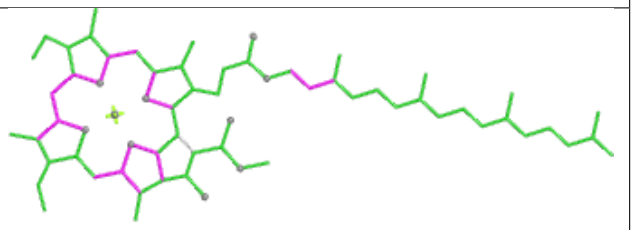


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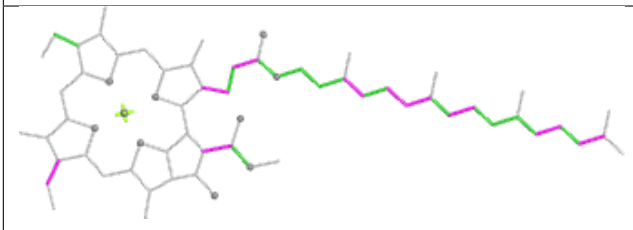
Ligand CLA B 812



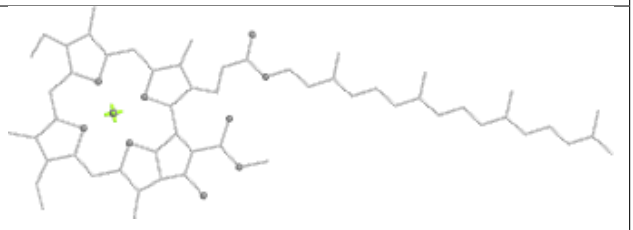
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Bond angles

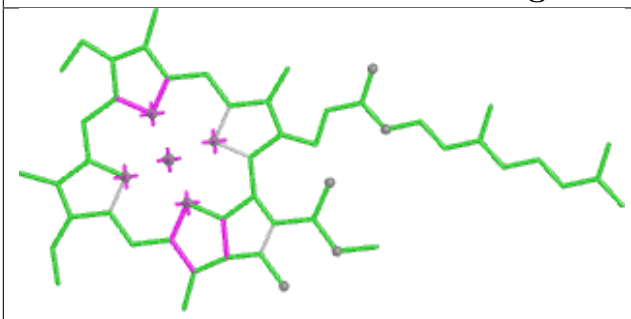


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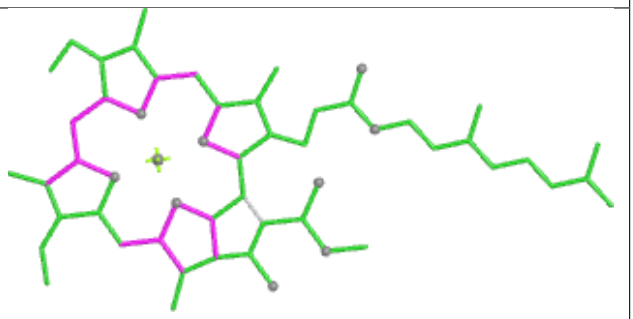


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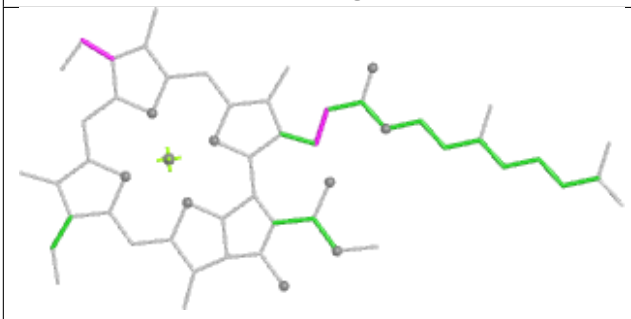
Ligand CLA 2 604



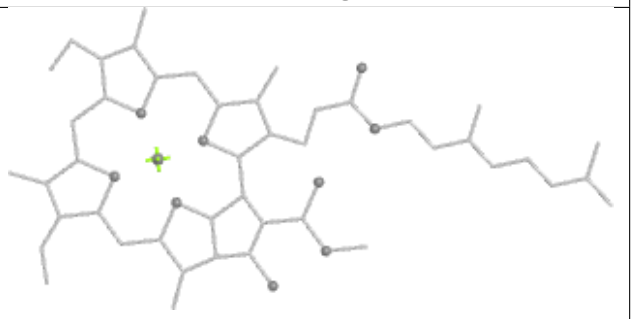
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Bond angles

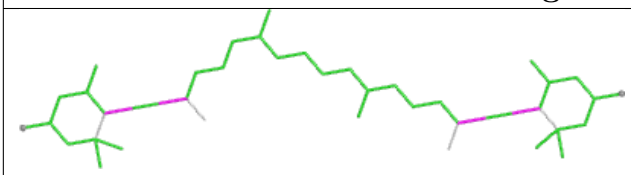


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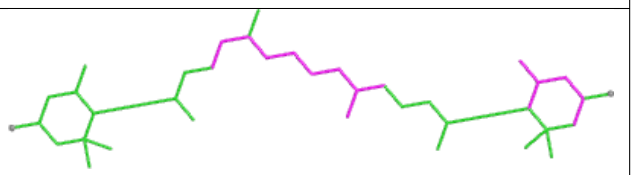


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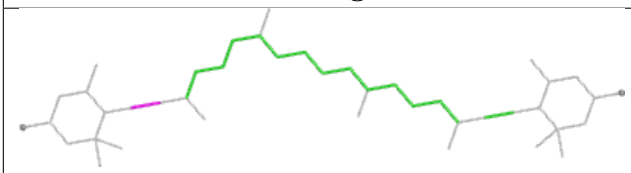
Ligand II0 J 101



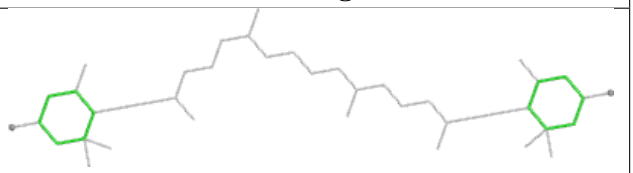
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Bond angles

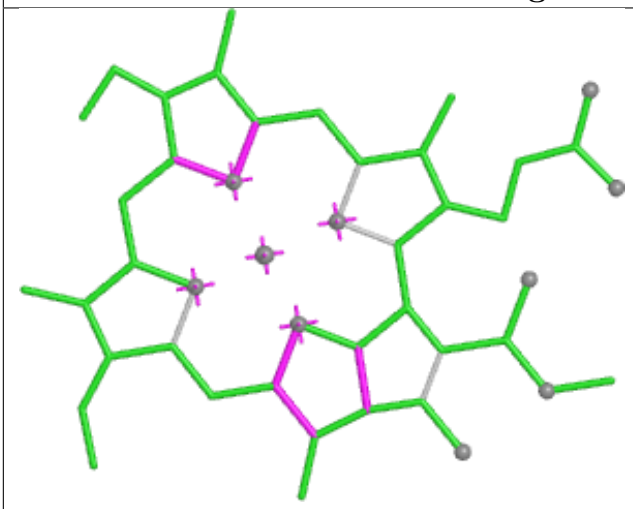


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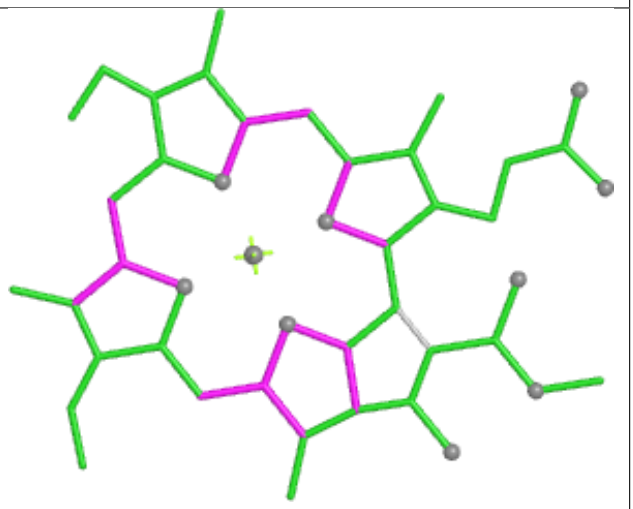


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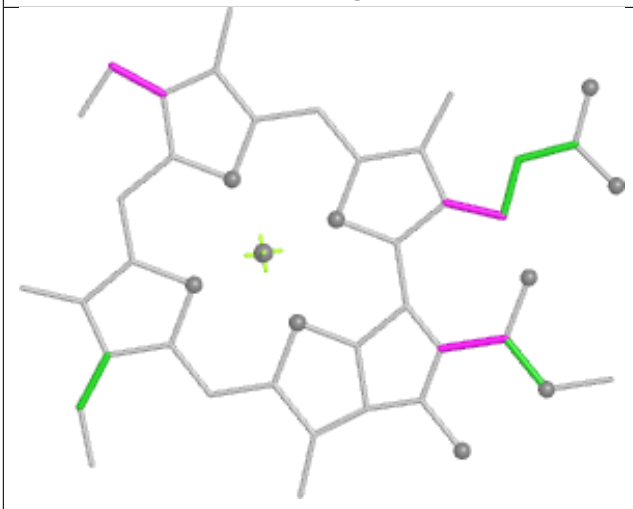
Ligand CLA 2 612



Bond lengths



Bond angles

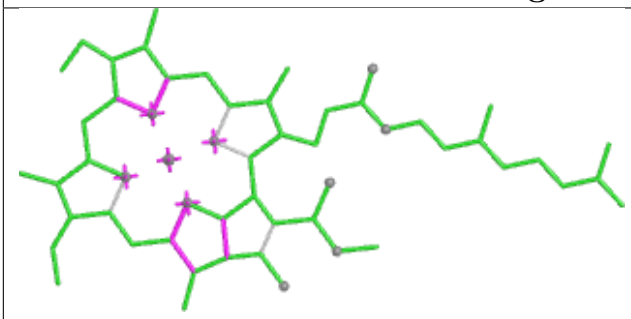


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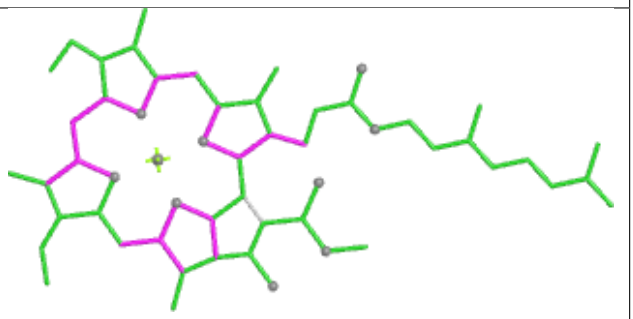


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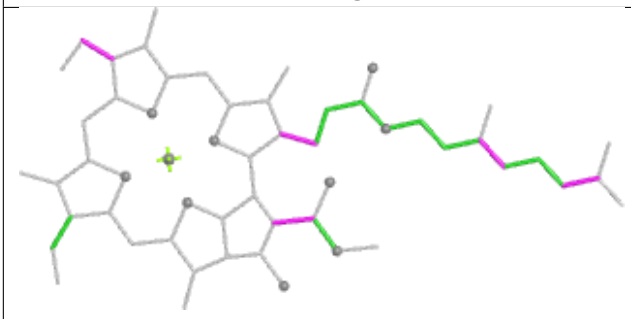
Ligand CLA 9 602



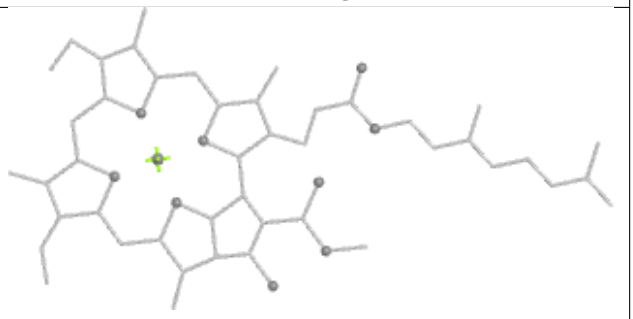
Bond lengths



Bond angles

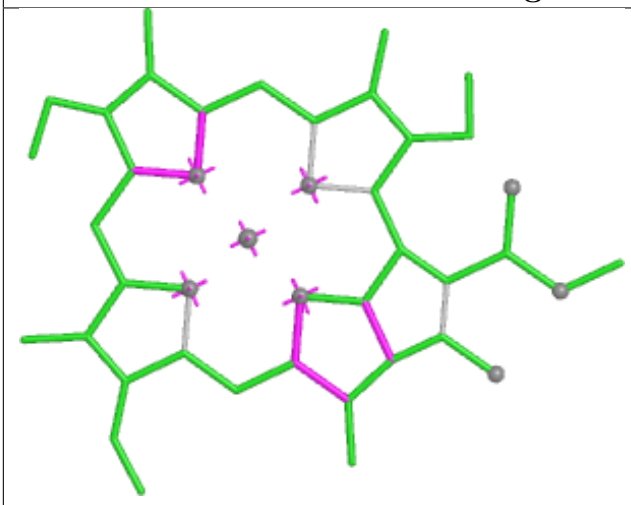


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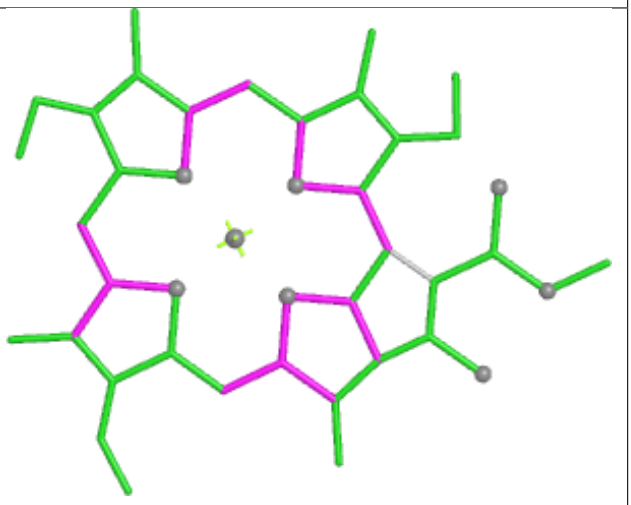


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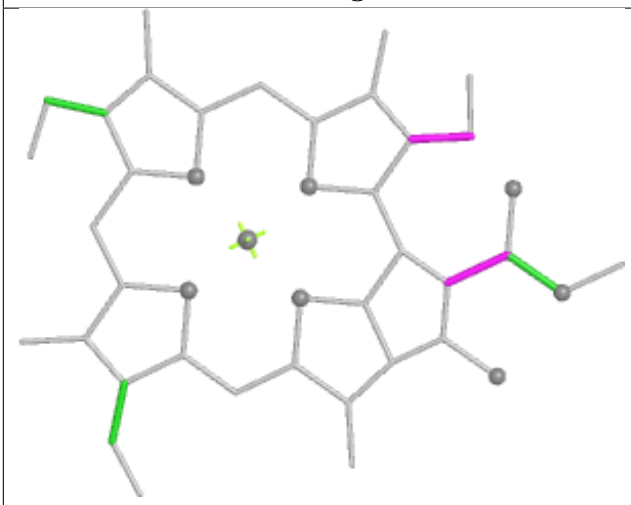
Ligand CLA B 814



Bond lengths



Bond angles

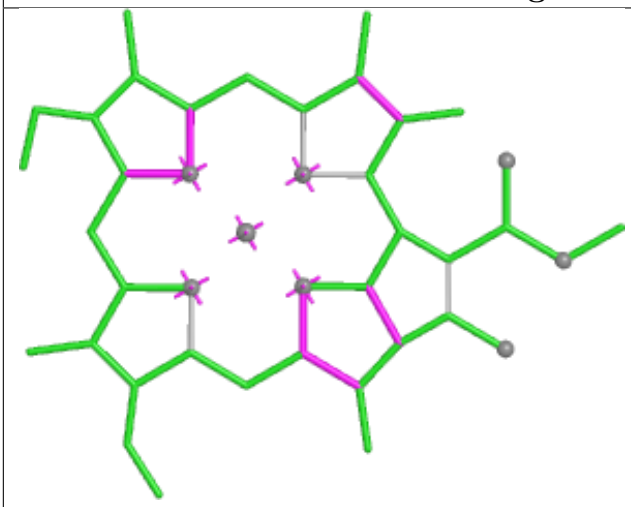


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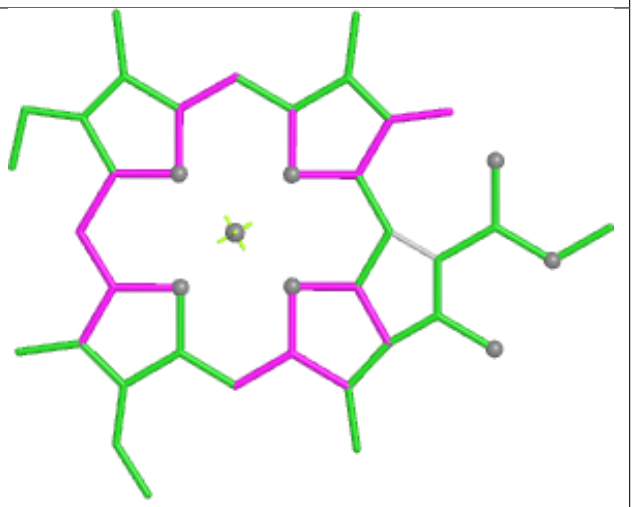


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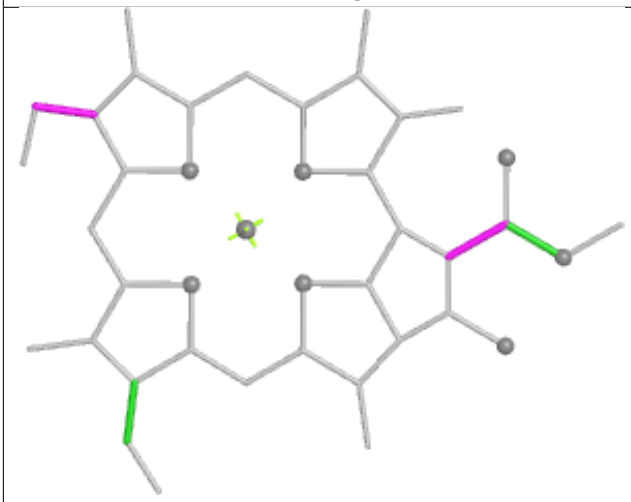
Ligand CLA J 102



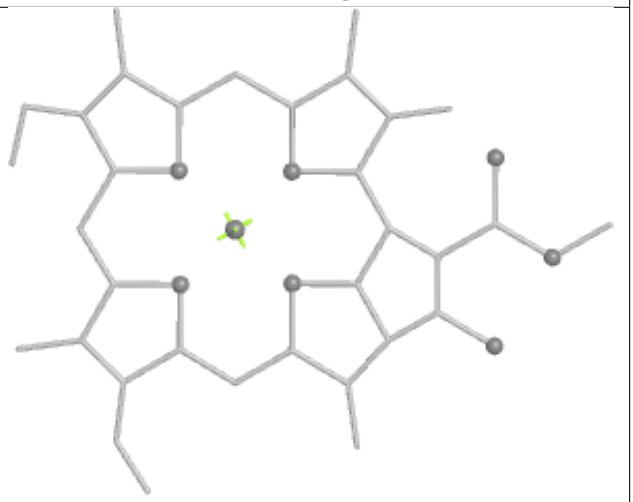
Bond lengths



Bond angles

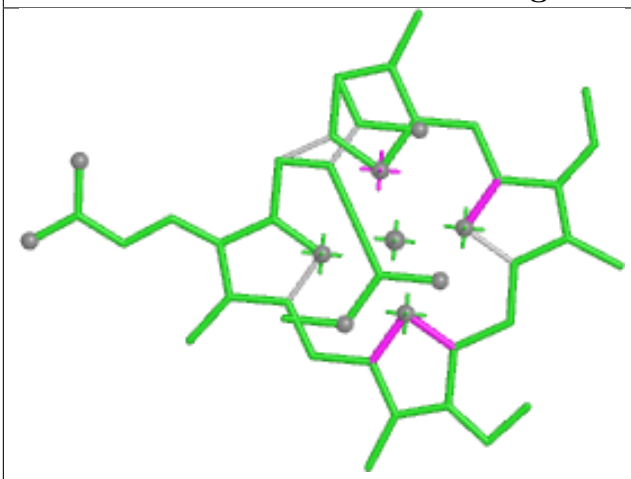


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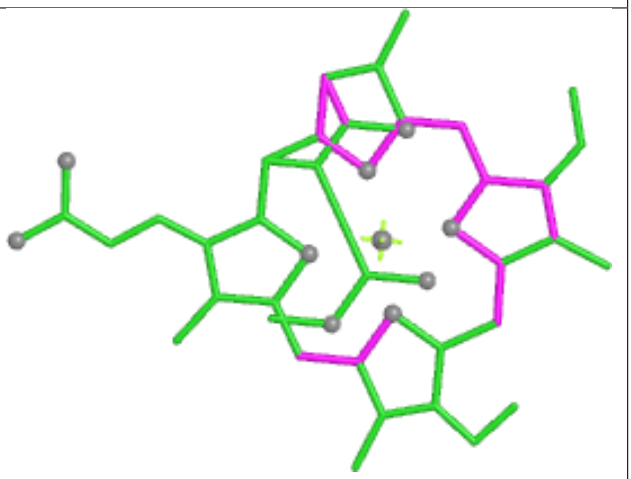


Rings

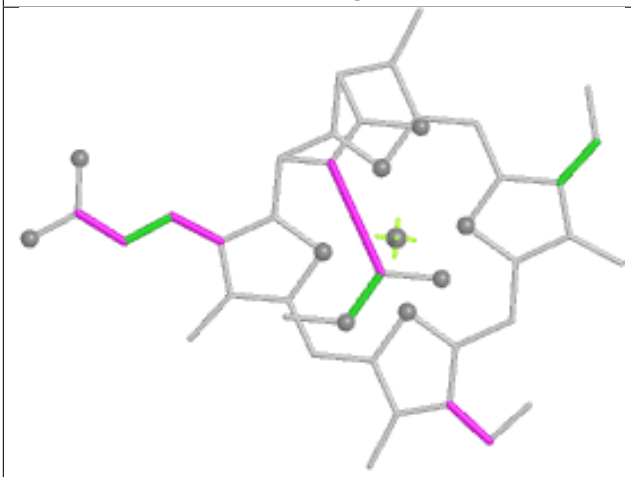
Ligand KC2 1 610



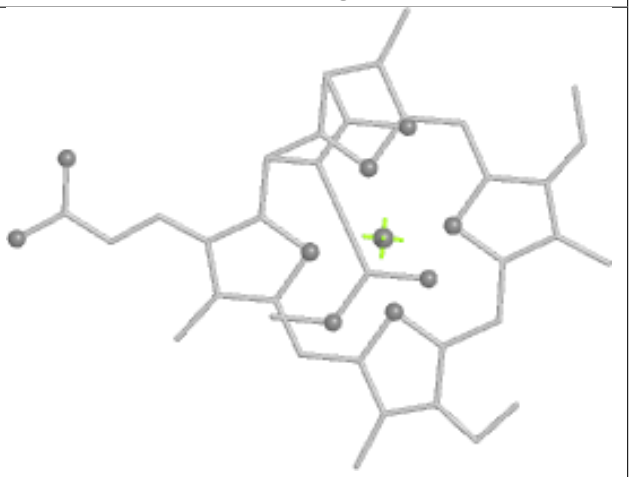
Bond lengths



Bond angles

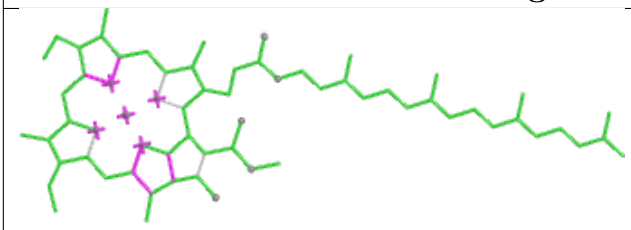


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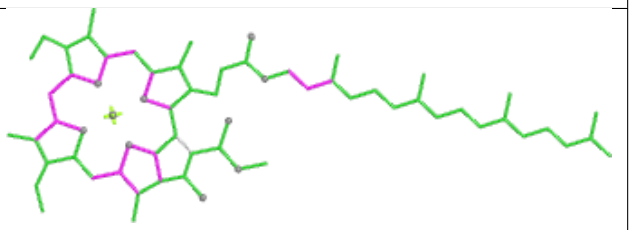


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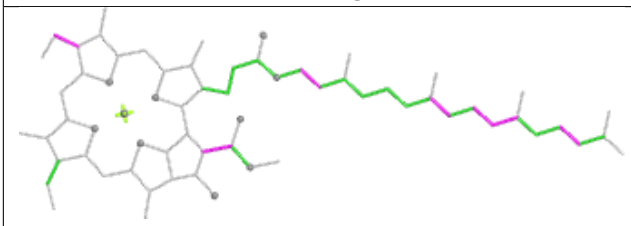
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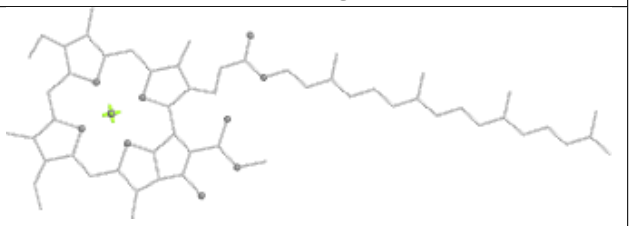
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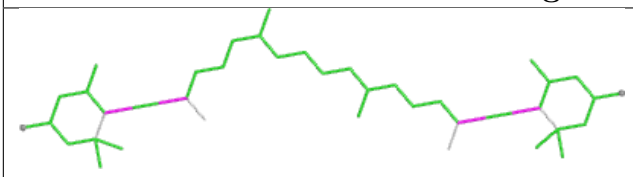


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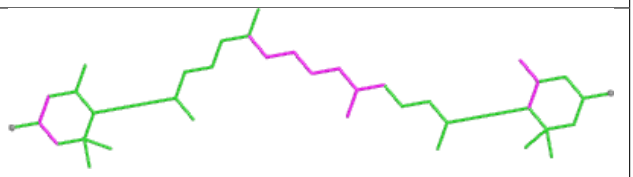


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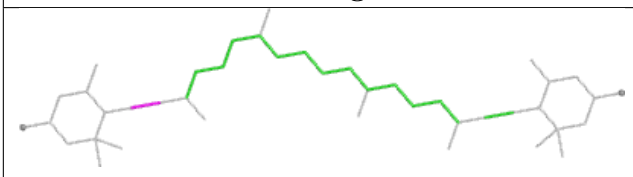
Ligand II0 1 614



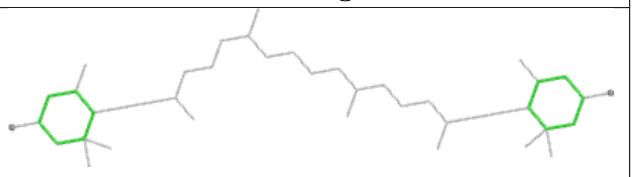
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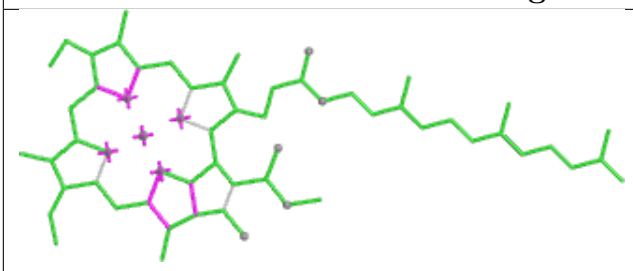


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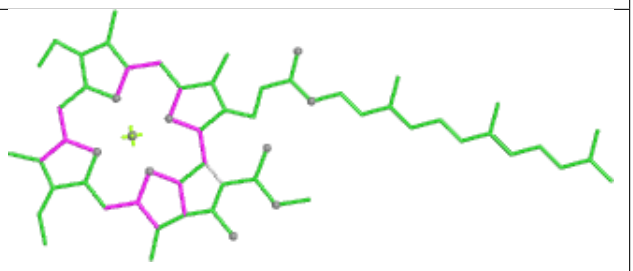


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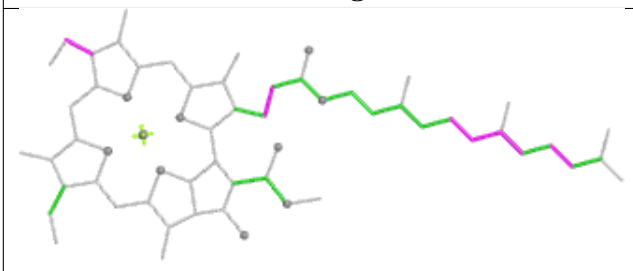
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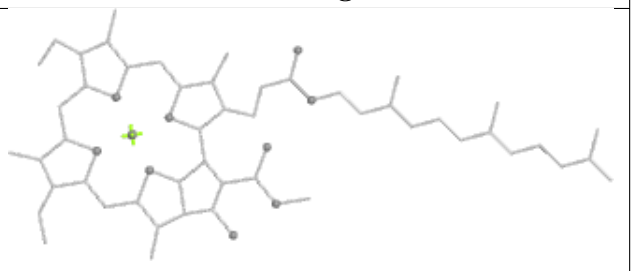
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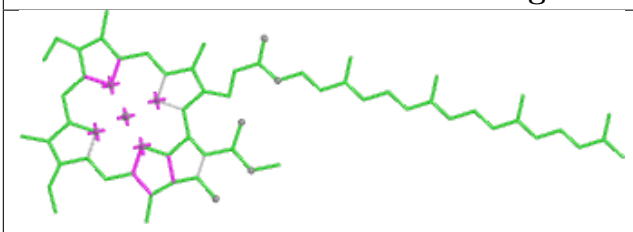


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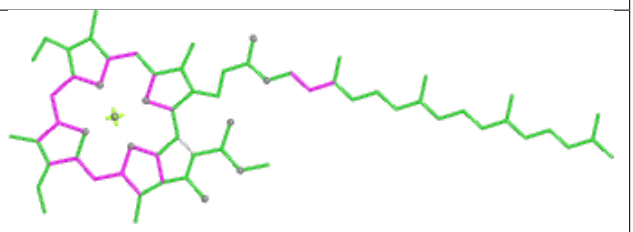


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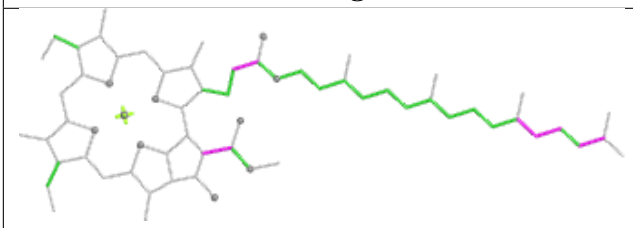
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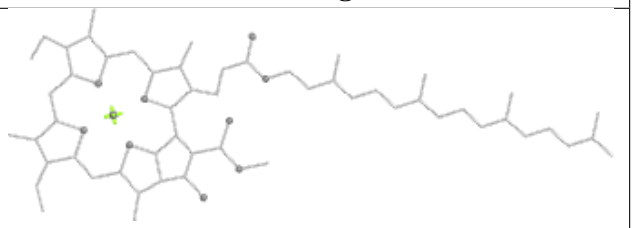
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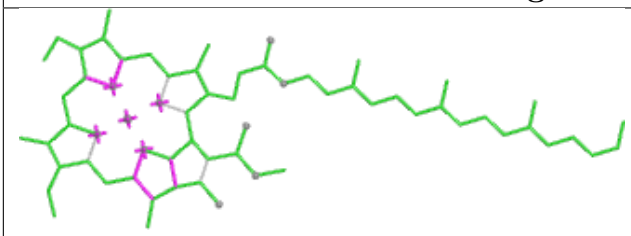


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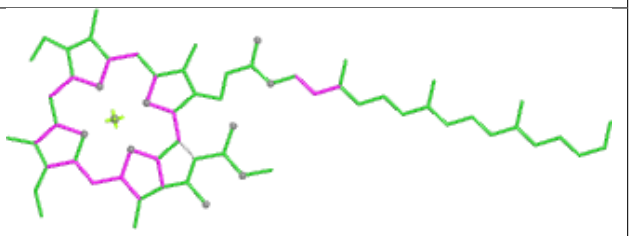


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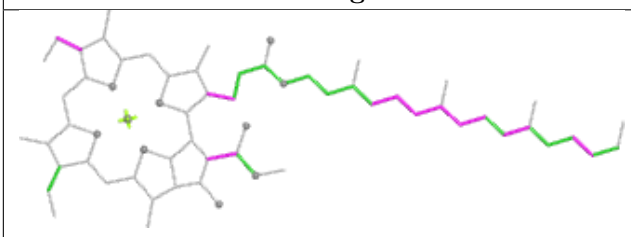
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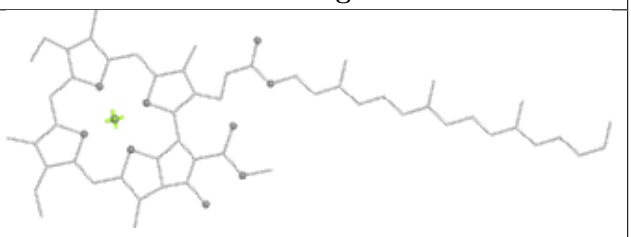
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Bond angles

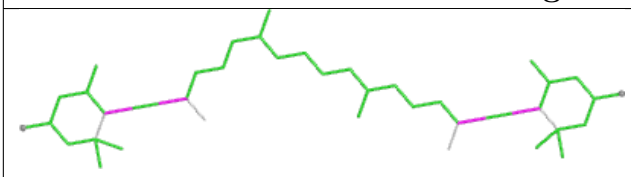


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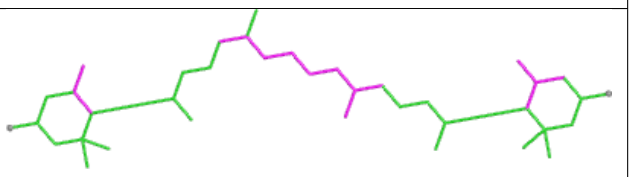


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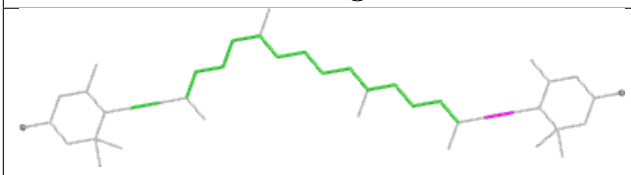
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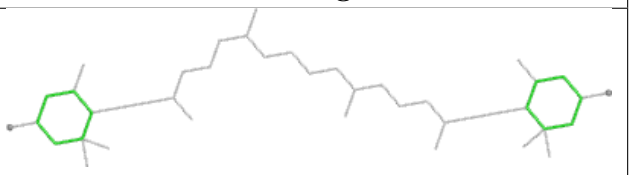
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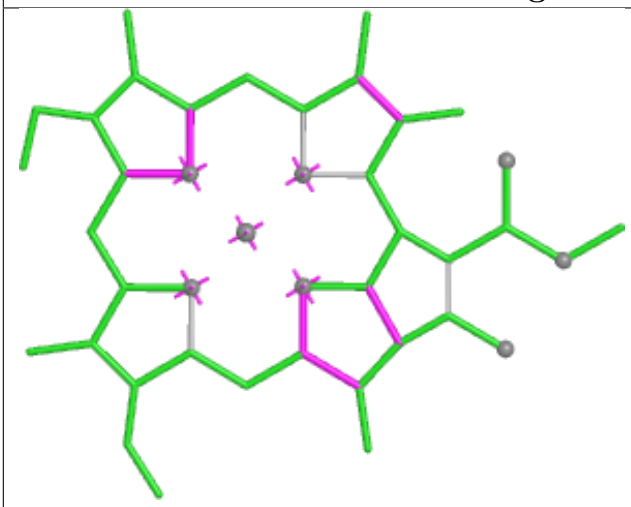


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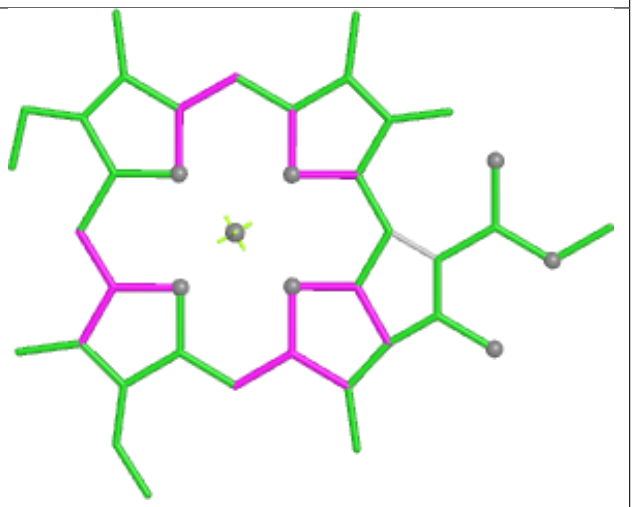


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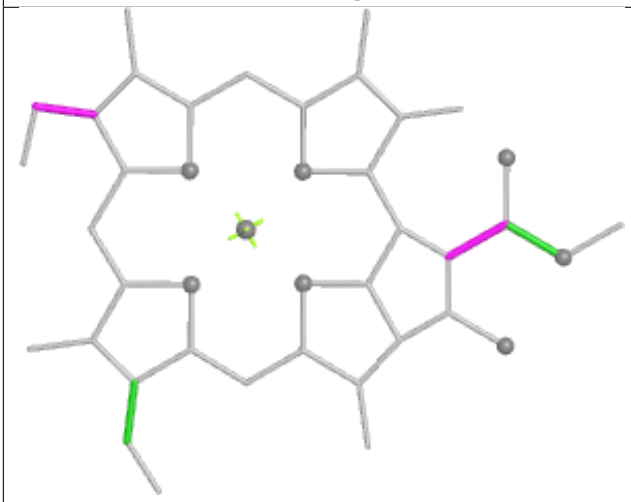
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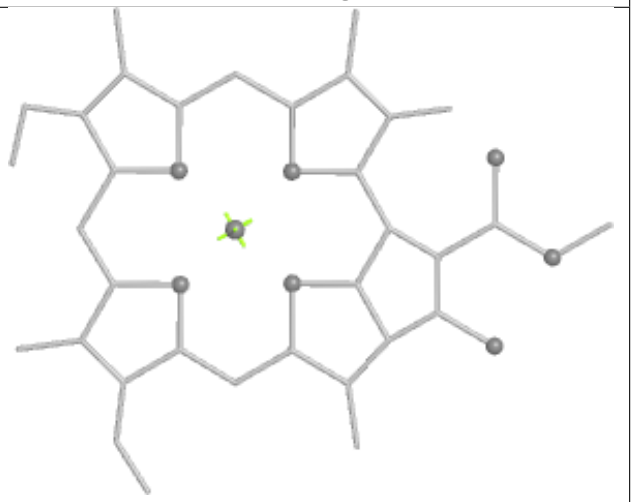
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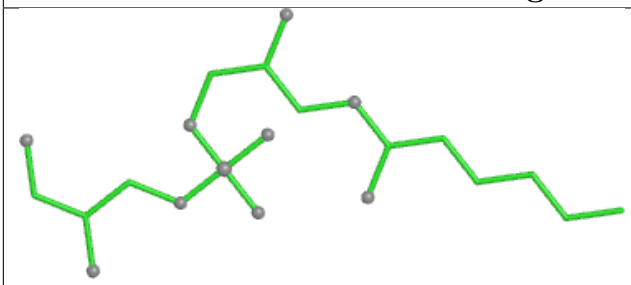


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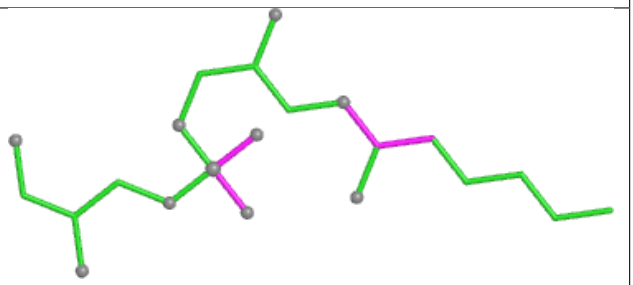


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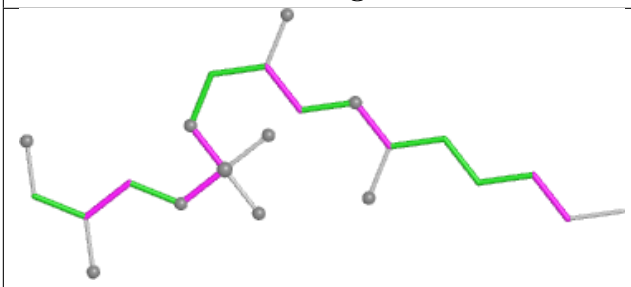
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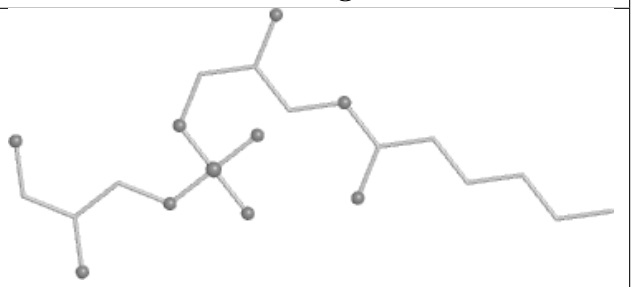
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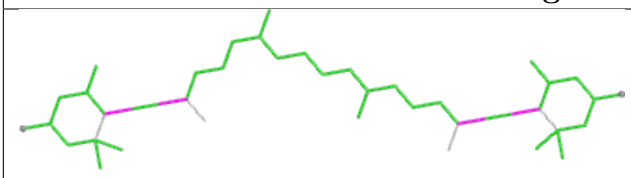


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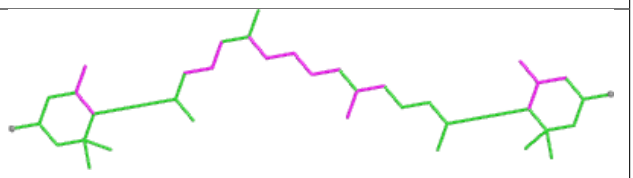


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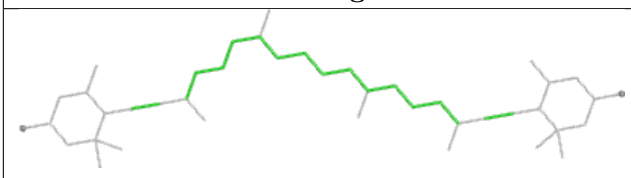
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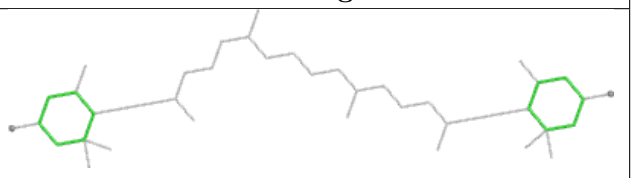
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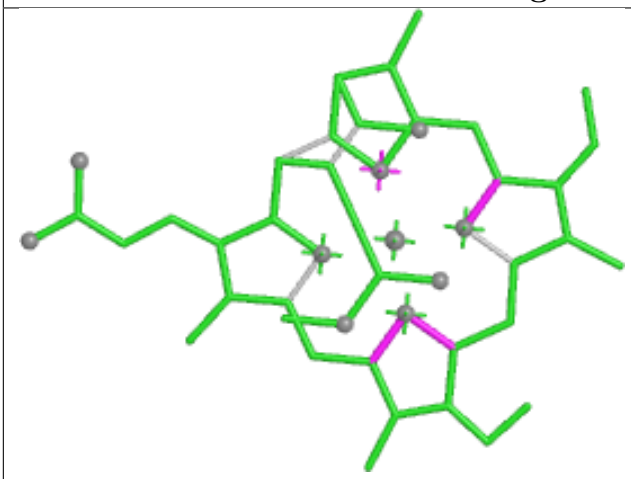


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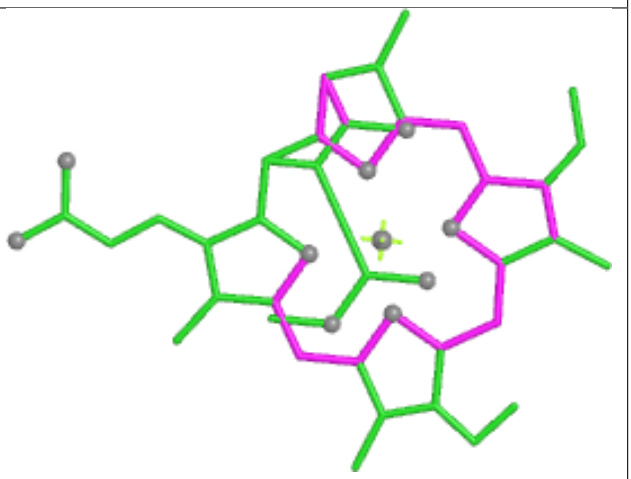


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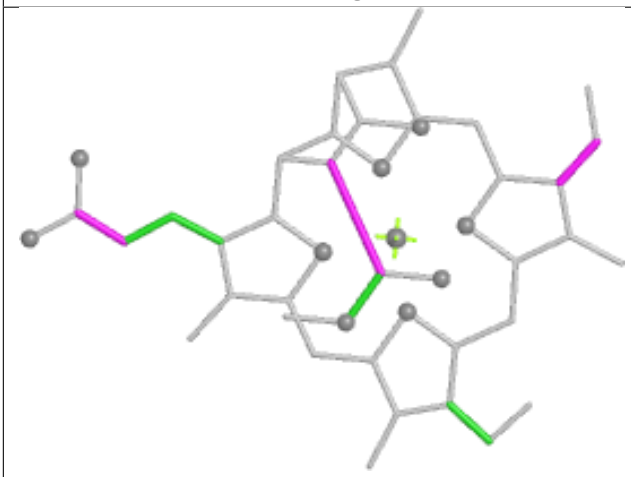
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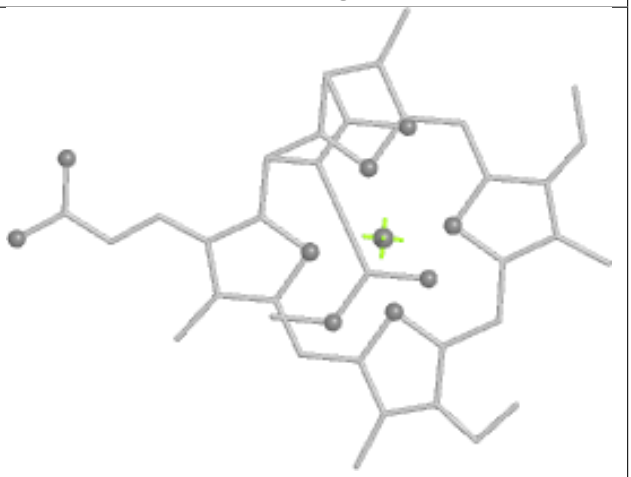
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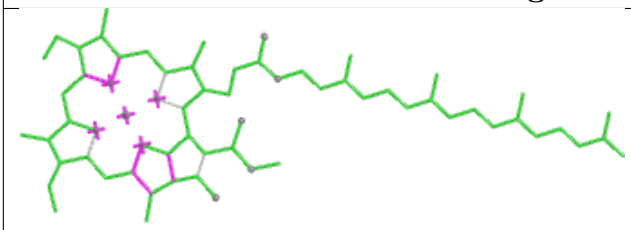


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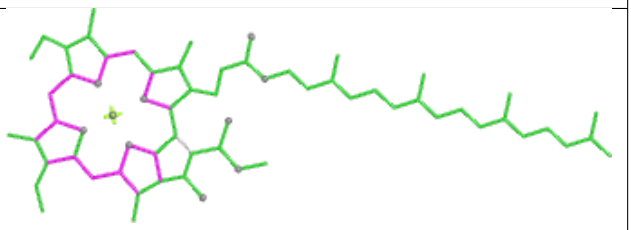


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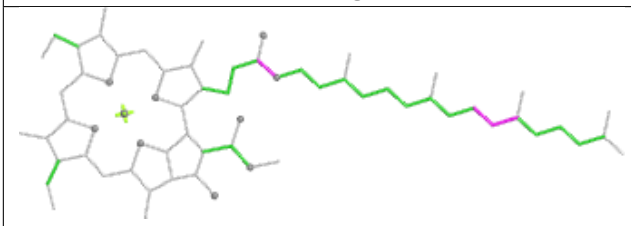
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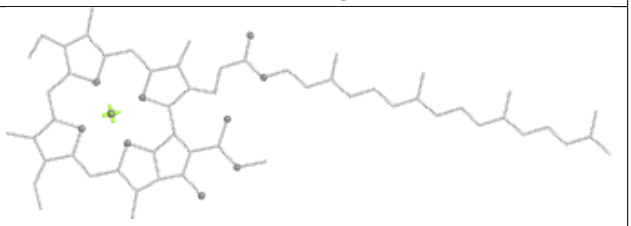
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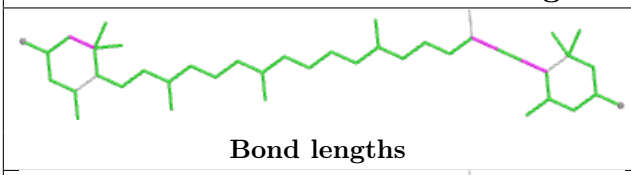


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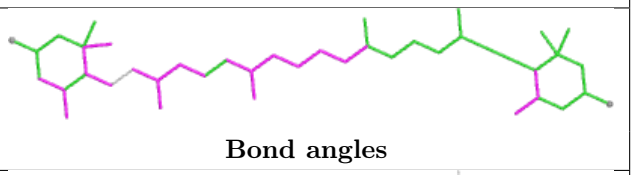


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Ligand II3 1 615



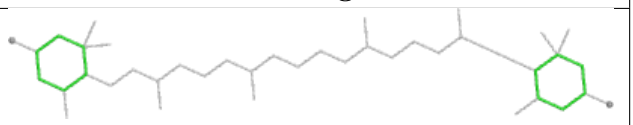
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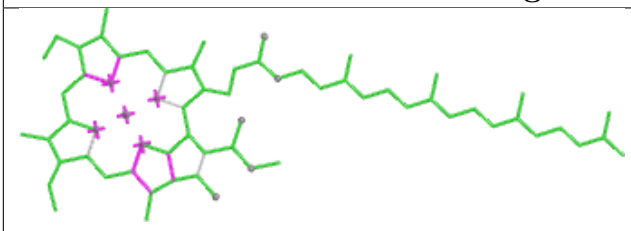


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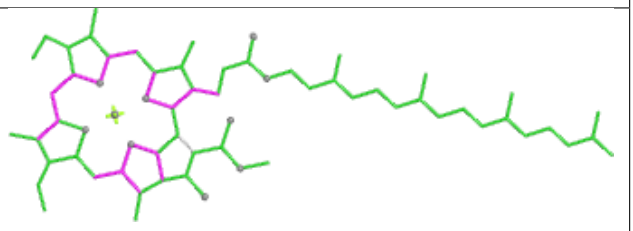


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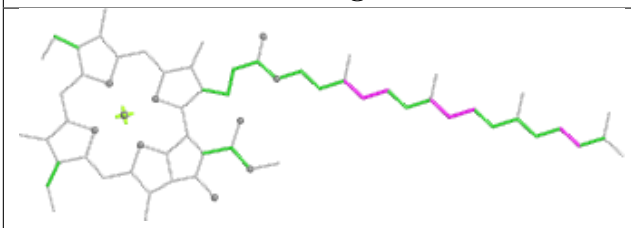
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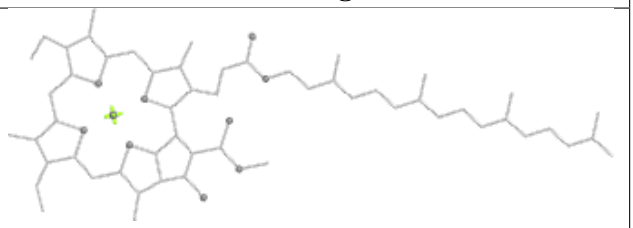
Bond lengths



Bond angles

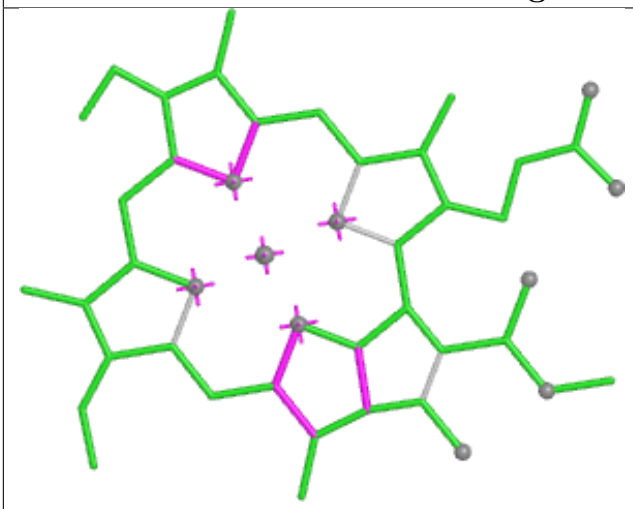


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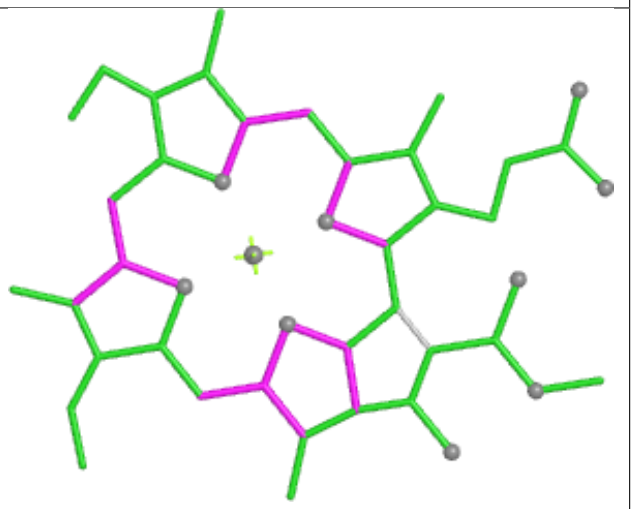


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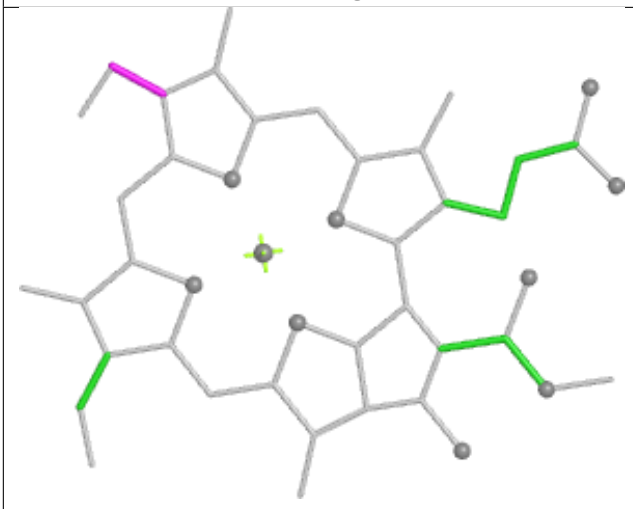
Ligand CLA 7 601



Bond lengths



Bond angles

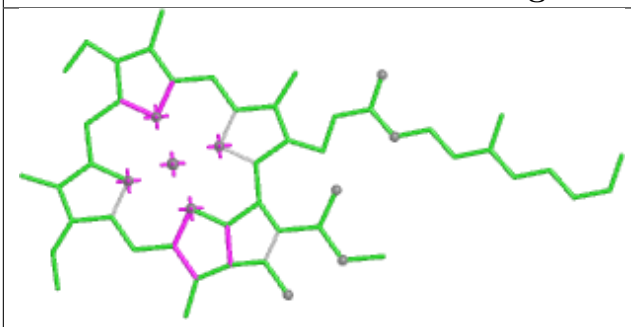


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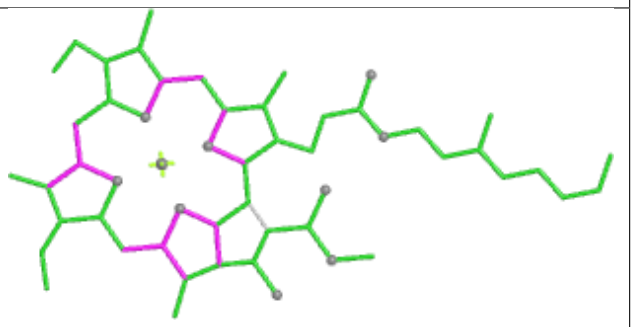


Rings

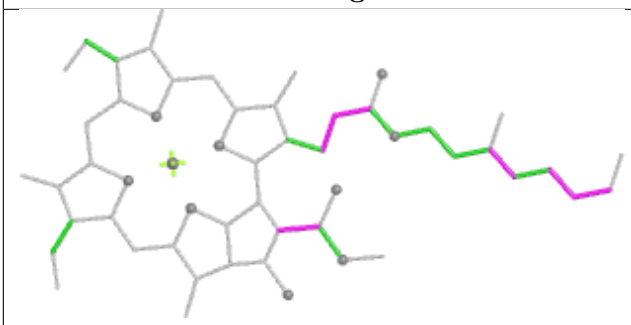
Ligand CLA 4 603



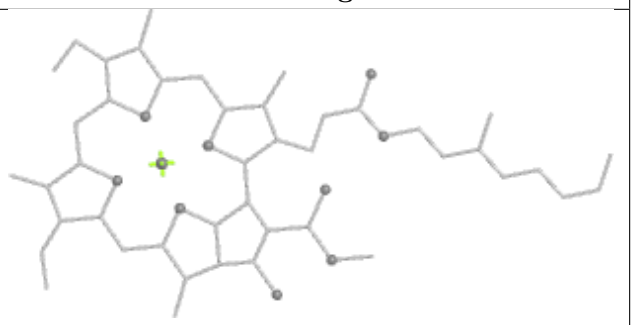
Bond lengths



Bond angles



Torsions

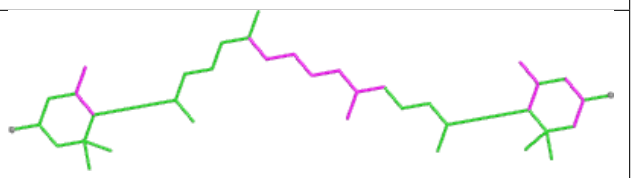


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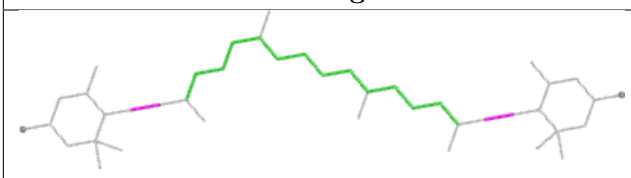
Ligand II0 9 618



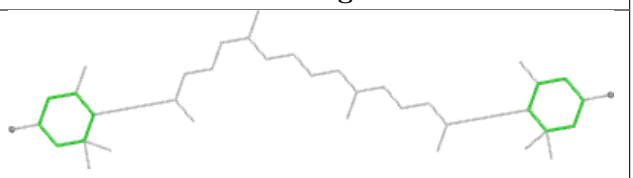
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Bond angles

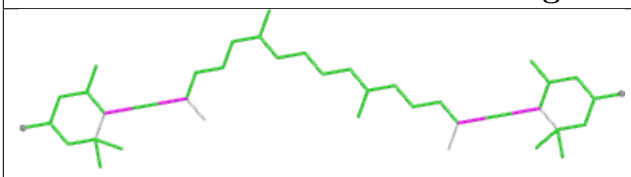


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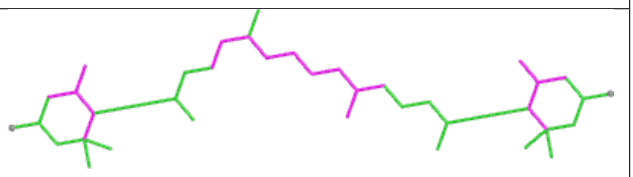


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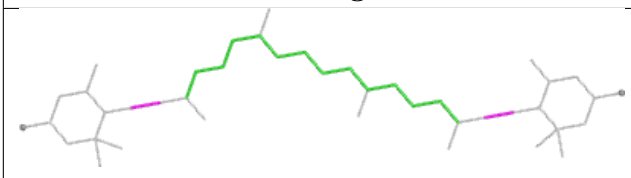
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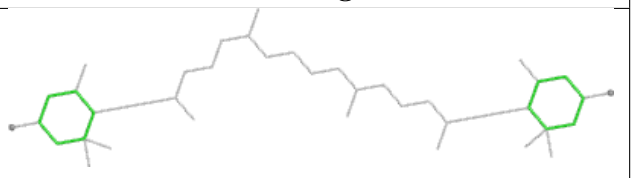
Bond lengths



Bond angles

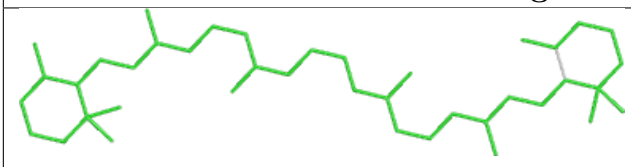


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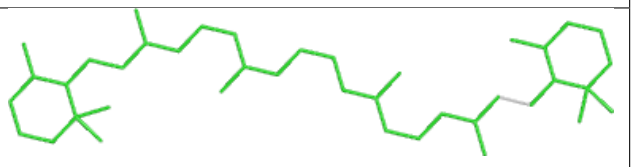


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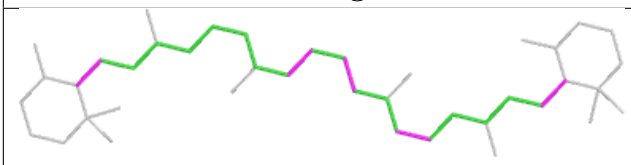
Ligand 8CT J 103



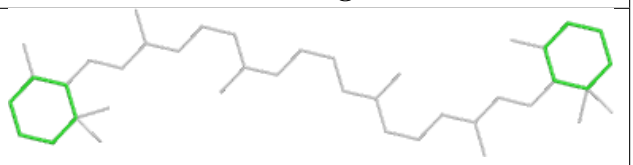
Bond lengths



Bond angles

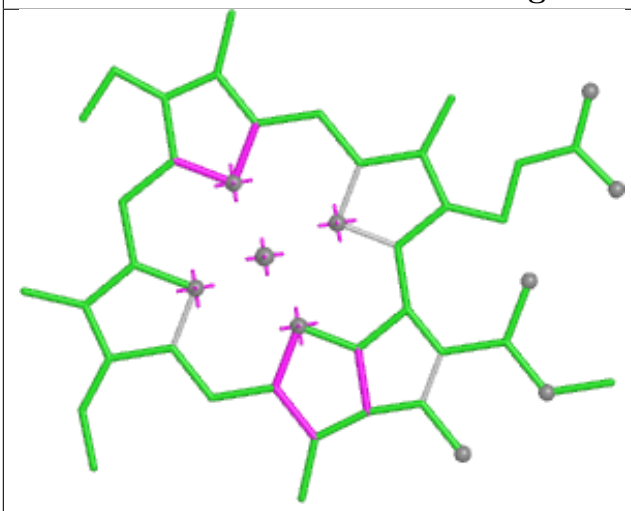


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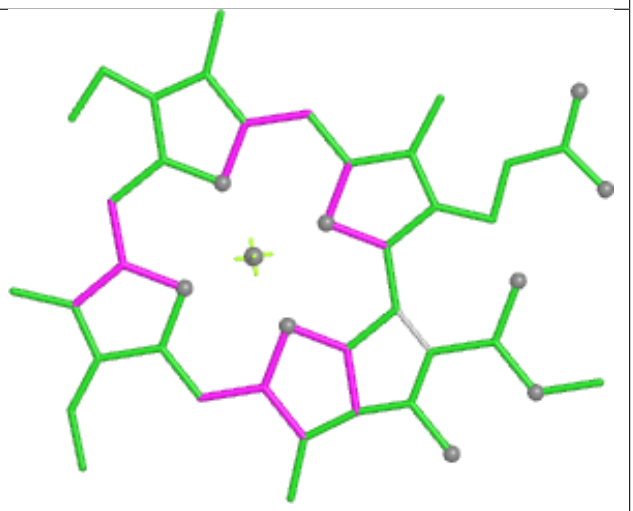


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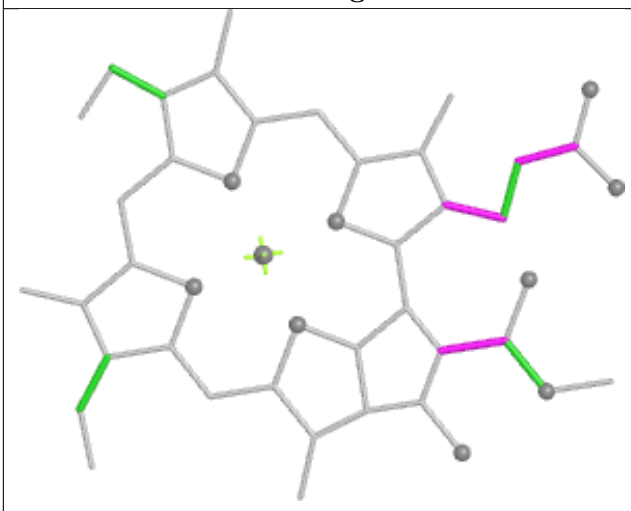
Ligand CLA a 601



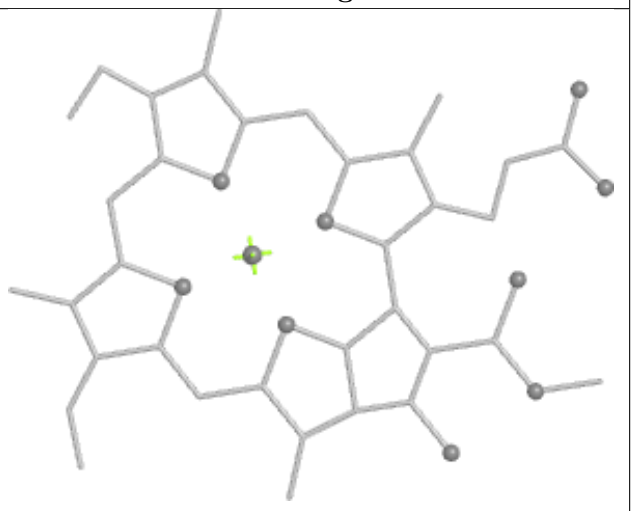
Bond lengths



Bond angles

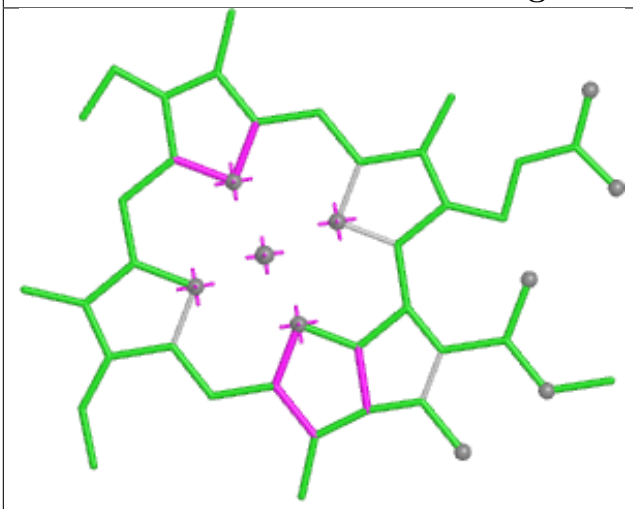


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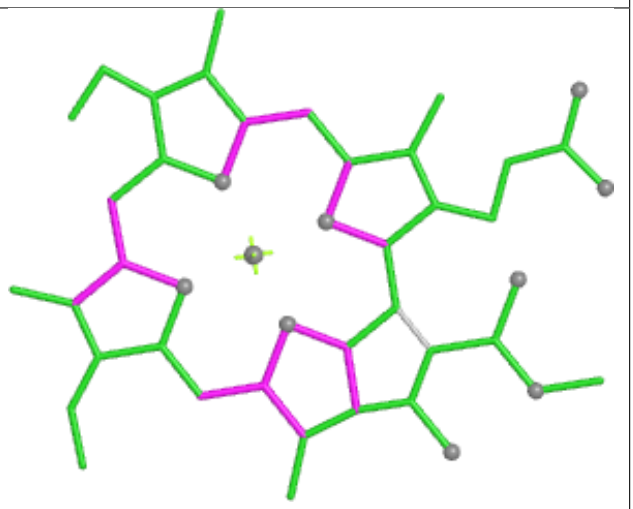


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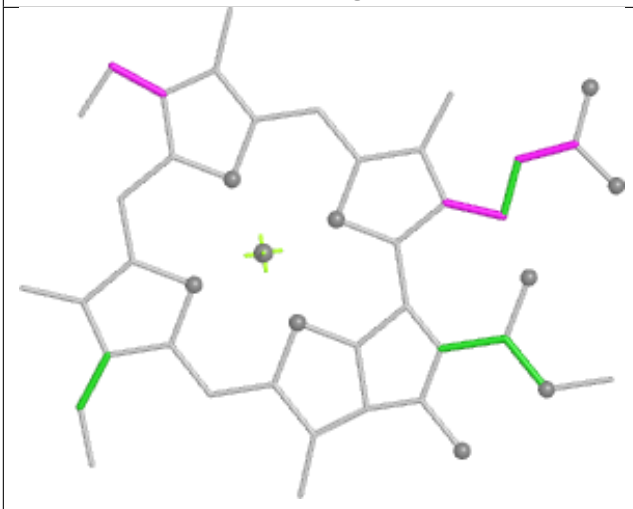
Ligand CLA 6 612



Bond lengths



Bond angles

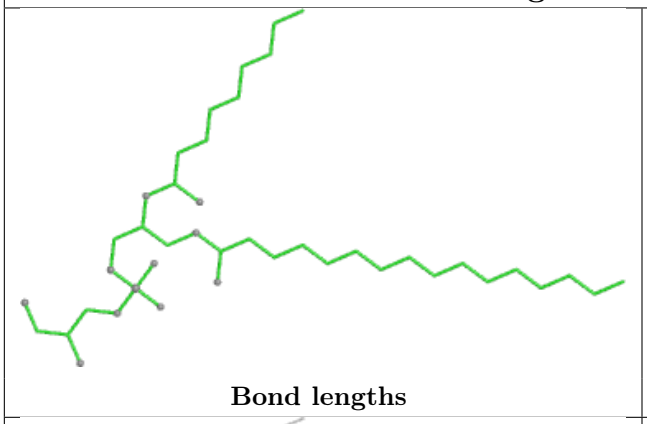


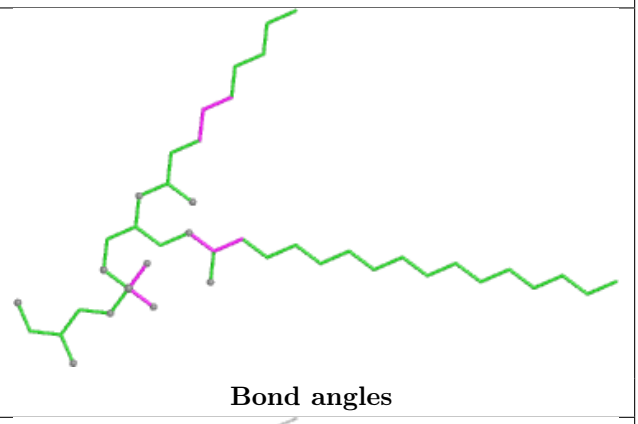
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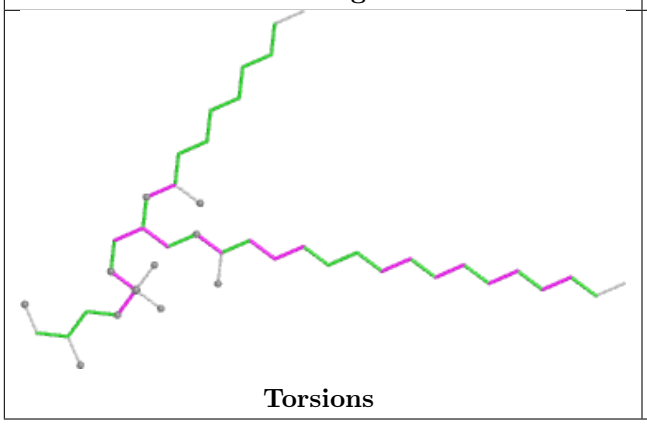


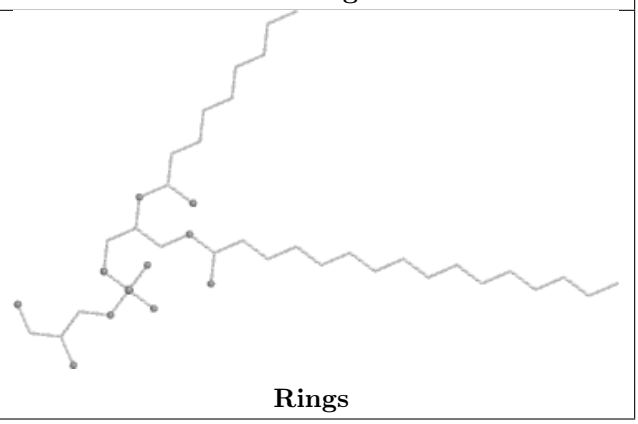
Rings

Ligand LHG 2 620

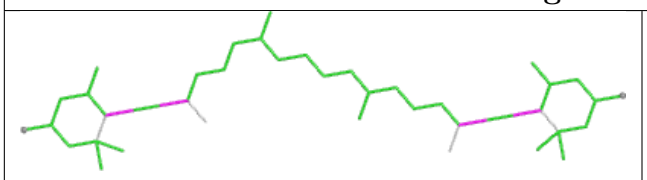

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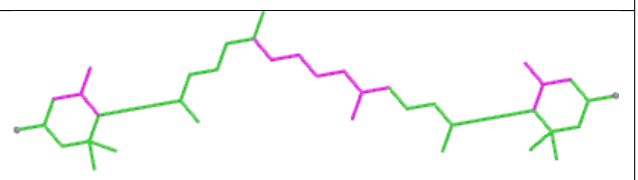

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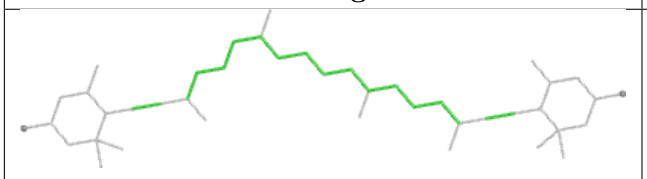

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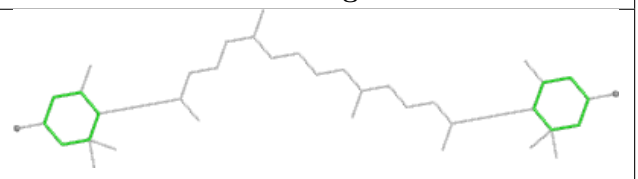

Rings

Ligand II0 5 616

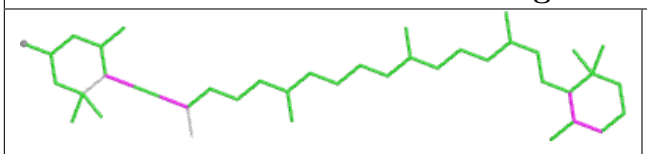

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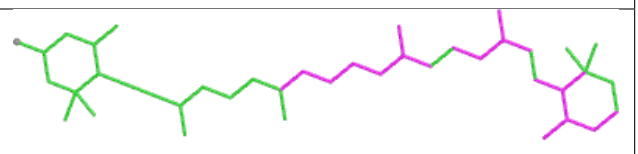

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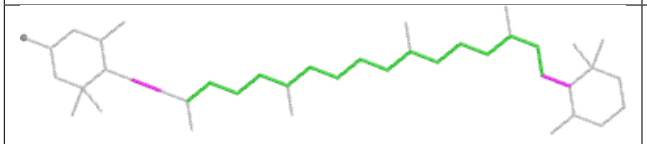

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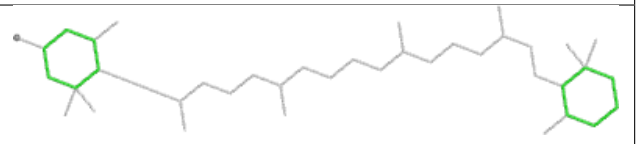

Rings

Ligand IHT 1 618

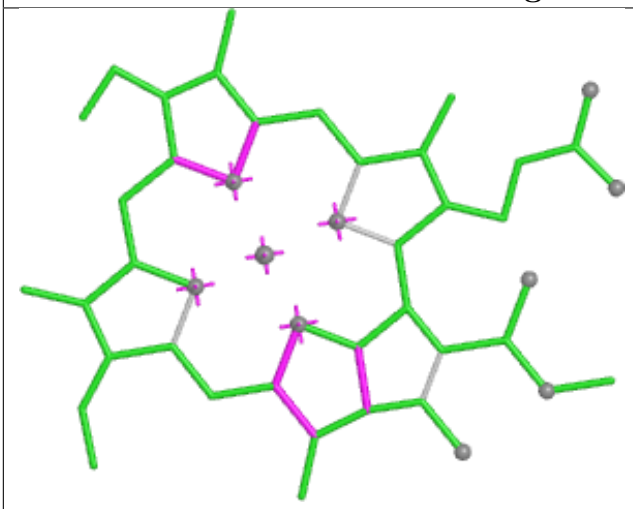

Bond lengths


Bond angles

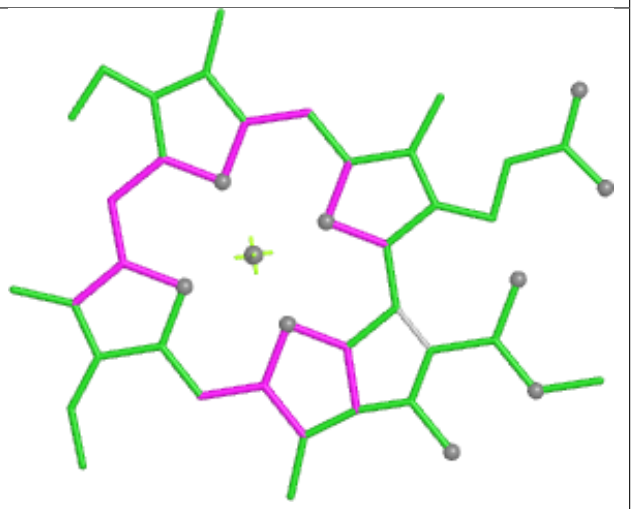

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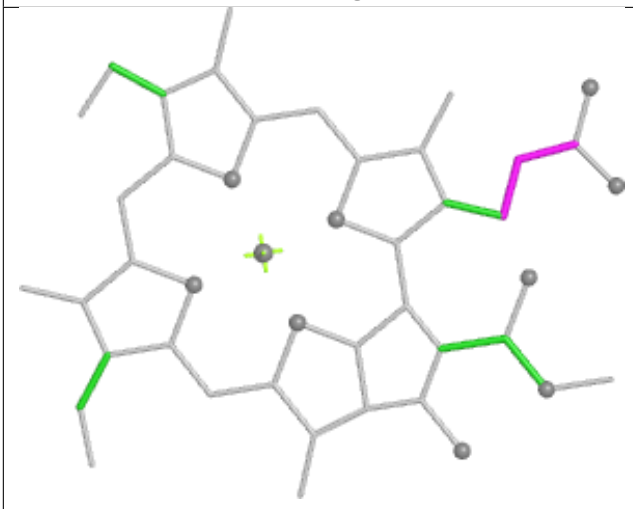
Ligand CLA B 804



Bond lengths



Bond angles

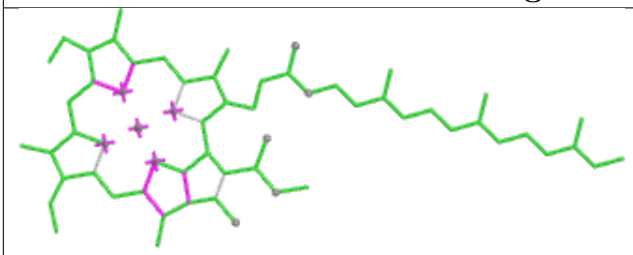


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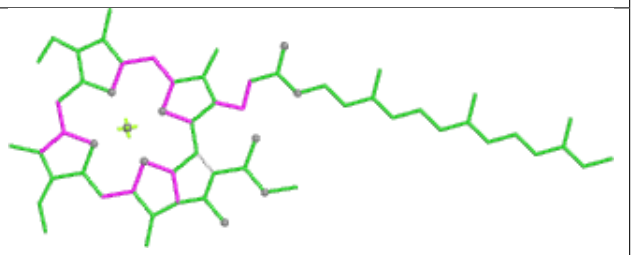


Rings

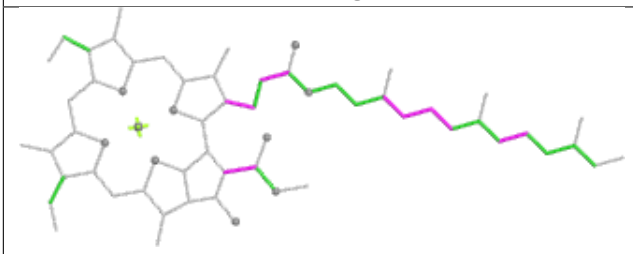
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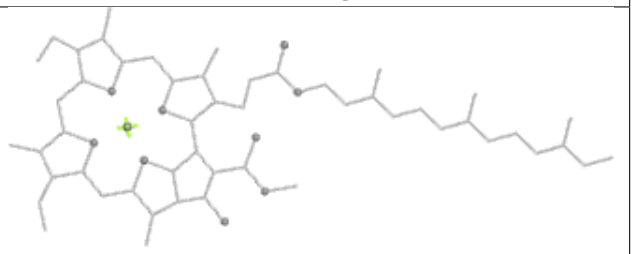
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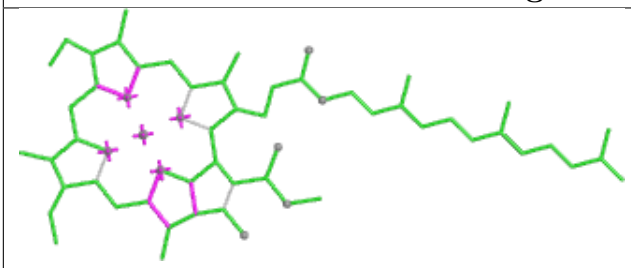
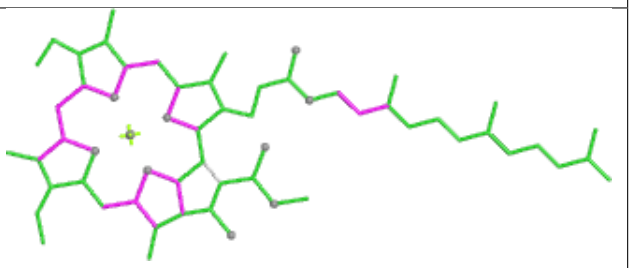
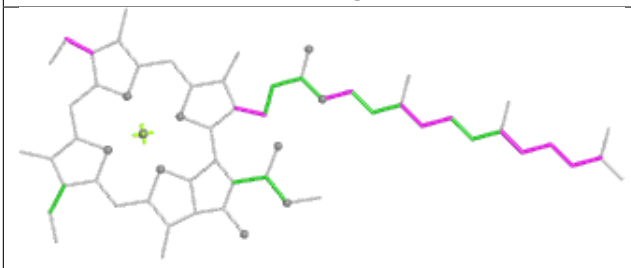
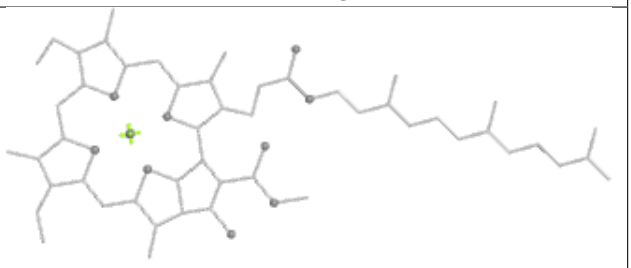
Bond angles

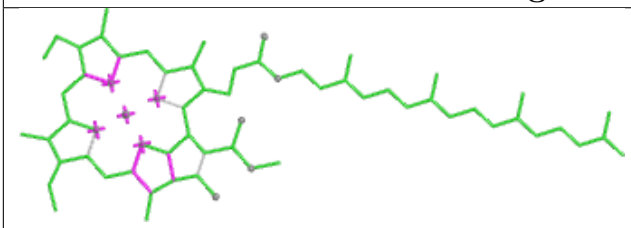
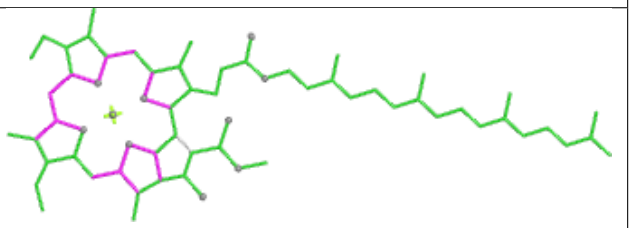
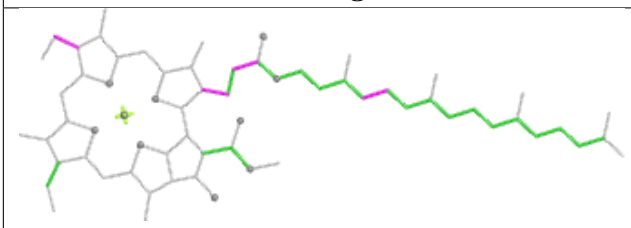
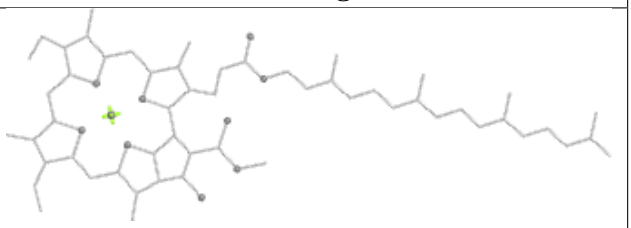


Torsions

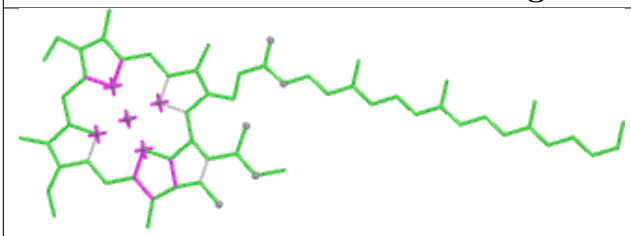


Rings

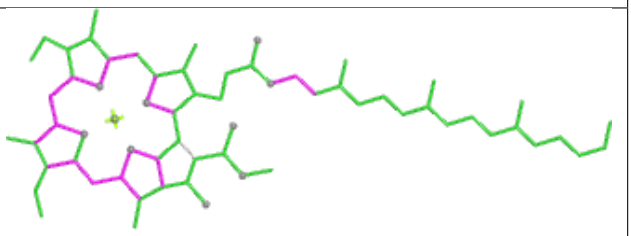
Ligand CLA F 202	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA a 612	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

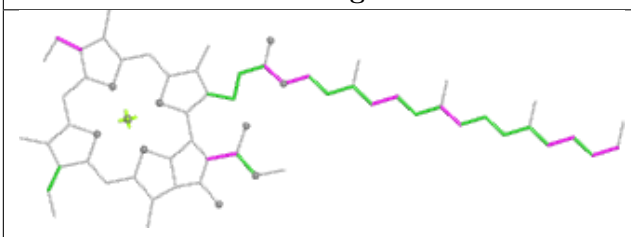
Ligand CLA d 602



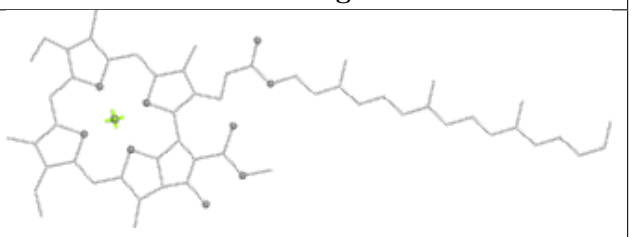
Bond lengths



Bond angles

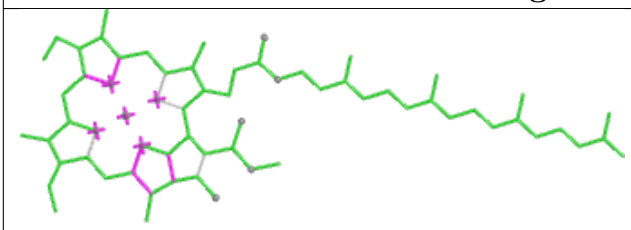


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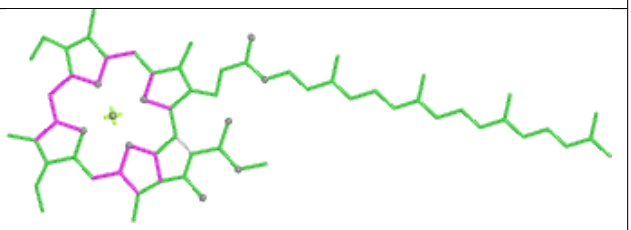


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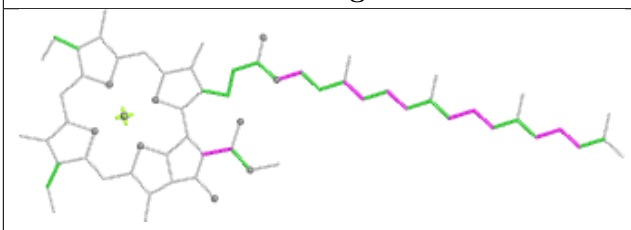
Ligand CLA c 602



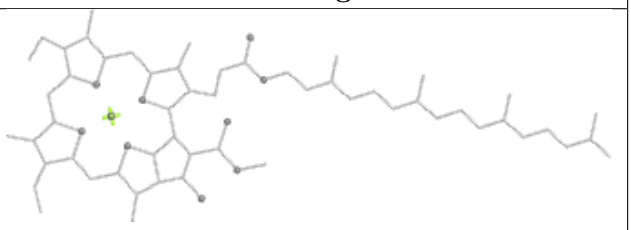
Bond lengths



Bond angles

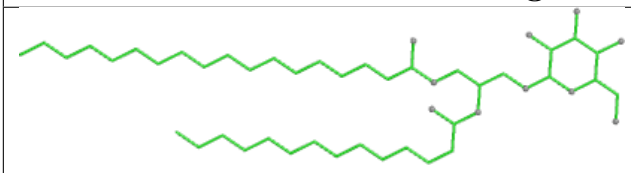


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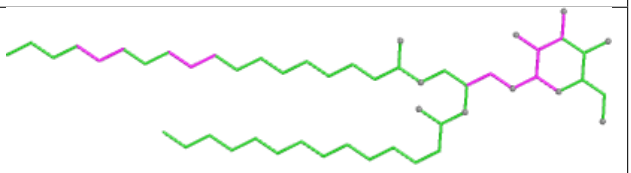


Rings

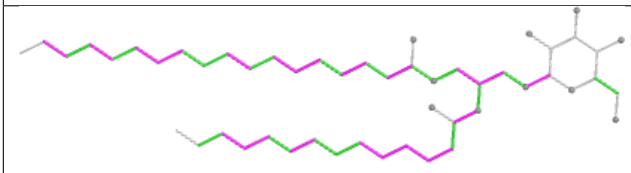
Ligand LMG I 102



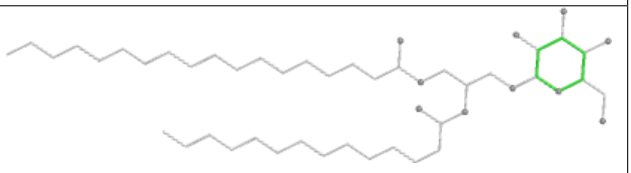
Bond lengths



Bond angles

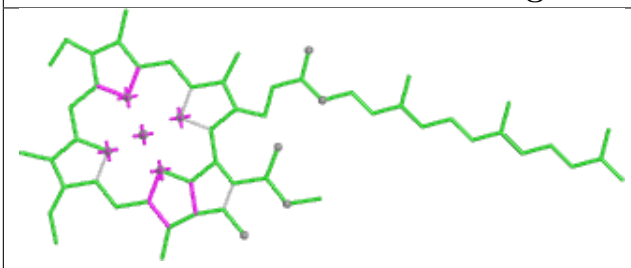


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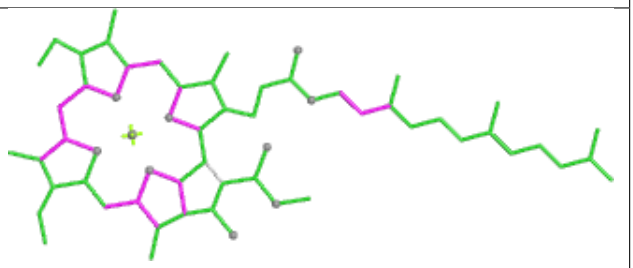


Rings

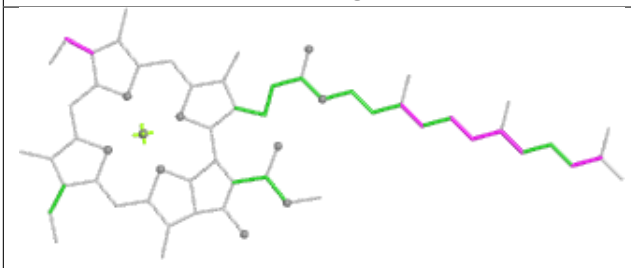
Ligand CLA L 203



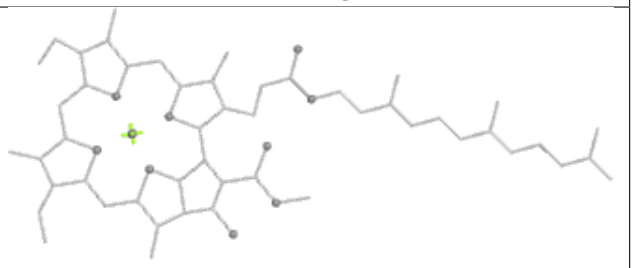
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Bond angles

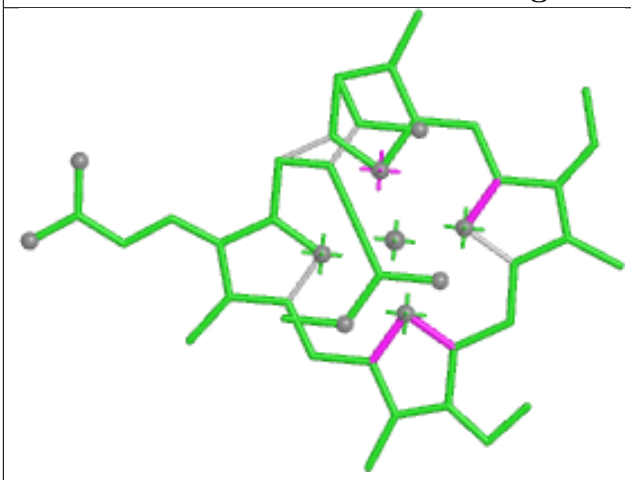


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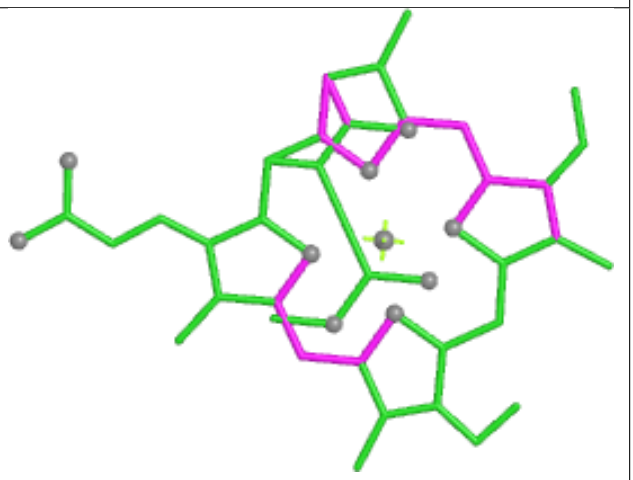


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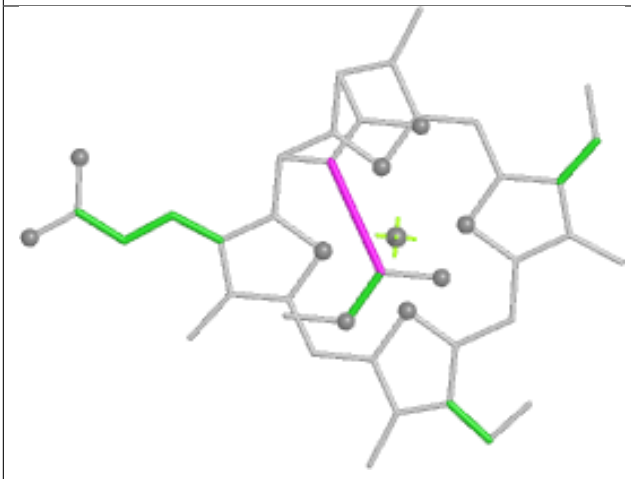
Ligand KC2 a 610



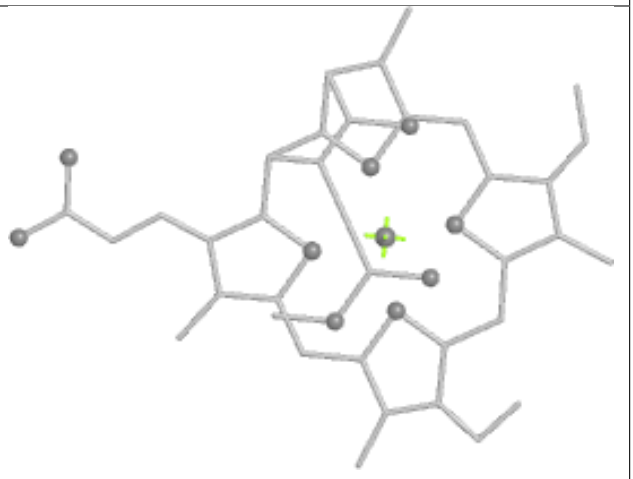
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Bond angles

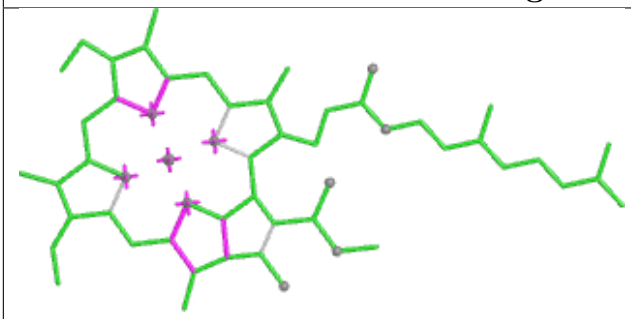


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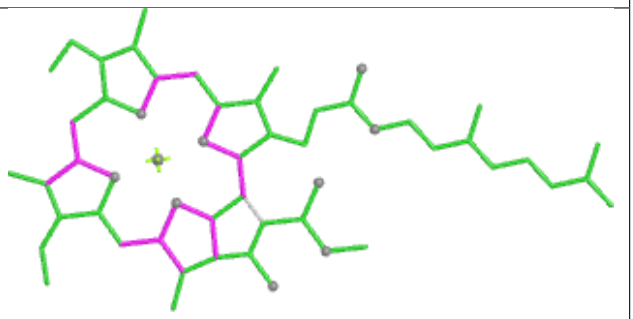


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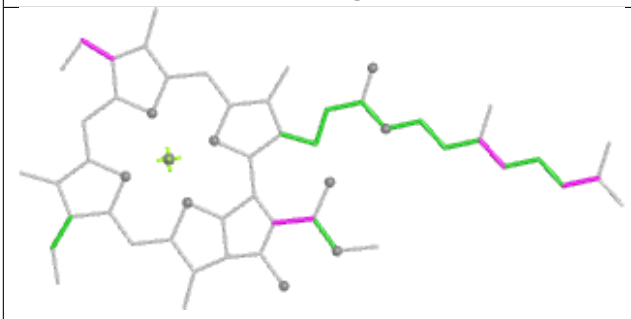
Ligand CLA F 204



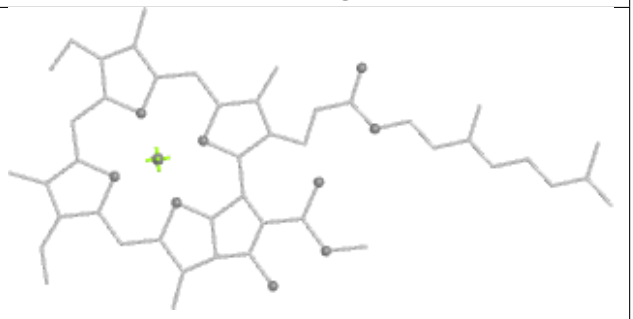
Bond lengths



Bond angles

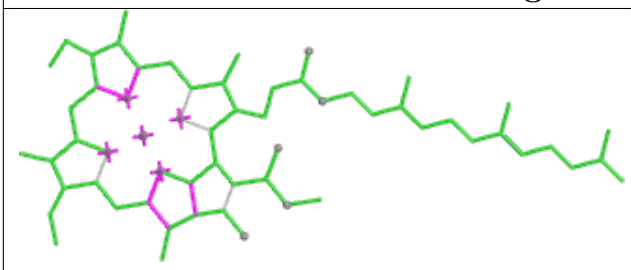


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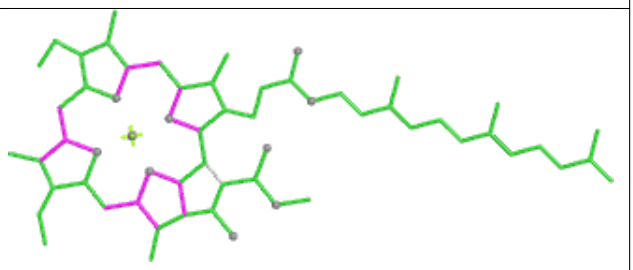


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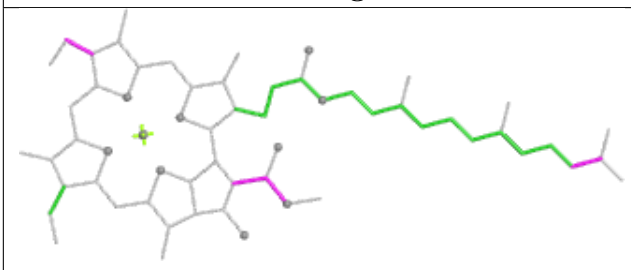
Ligand CLA B 818



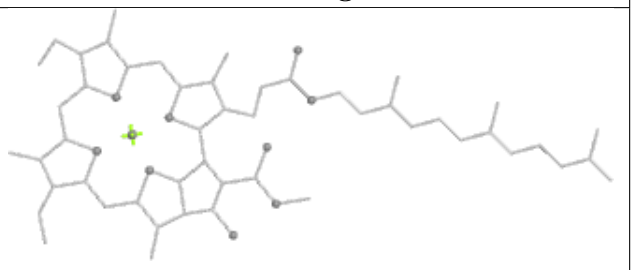
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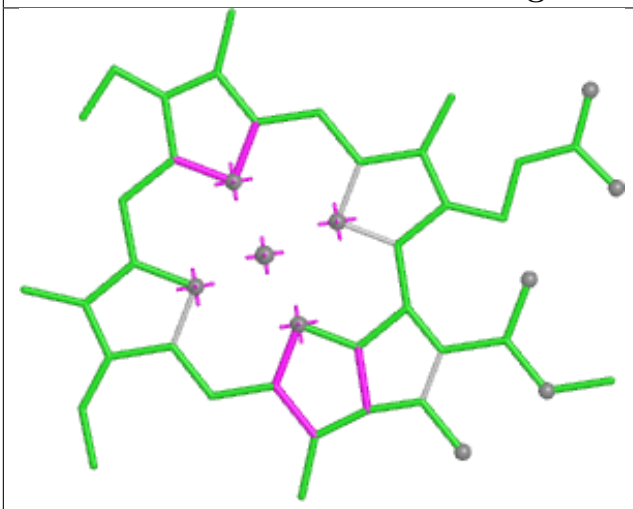


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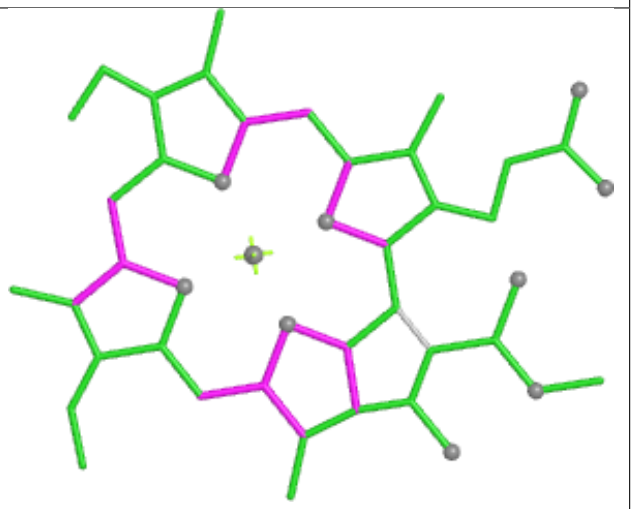


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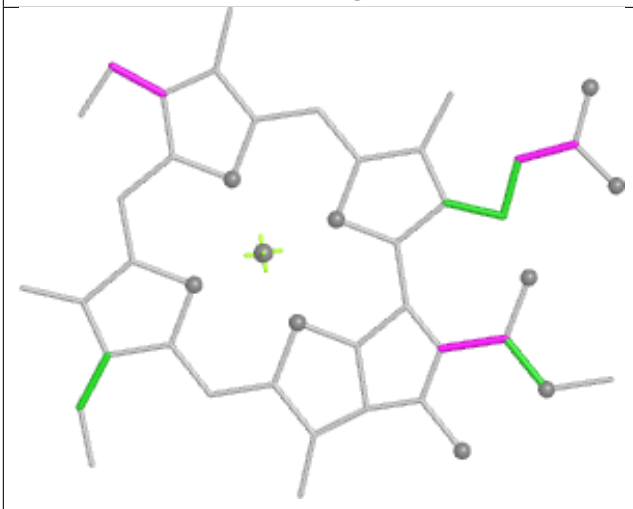
Ligand CLA b 601



Bond lengths



Bond angles

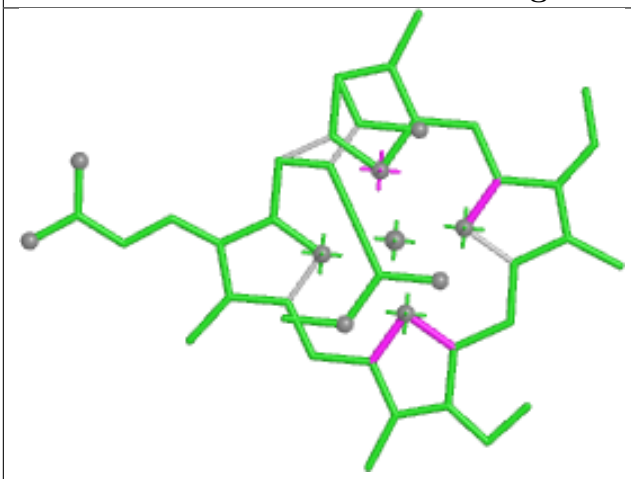


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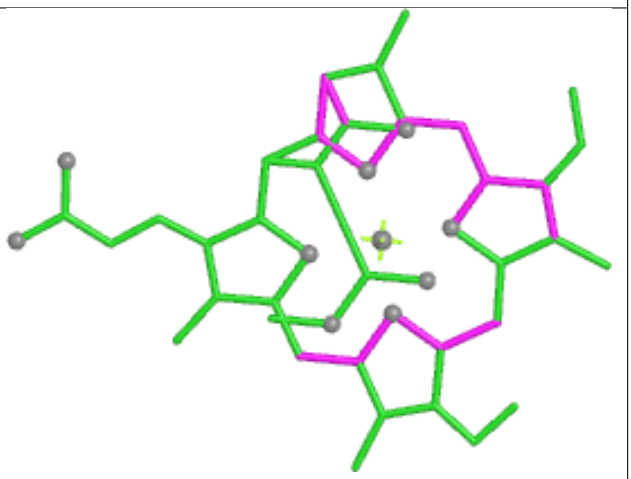


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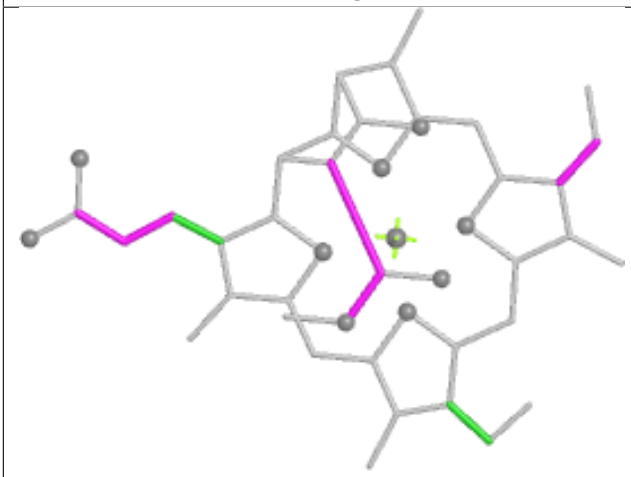
Ligand KC2 2 610



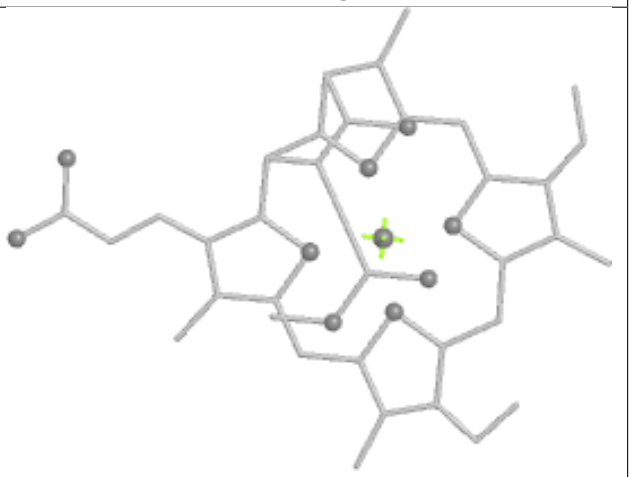
Bond lengths



Bond angles

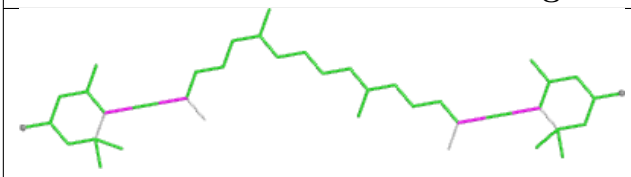


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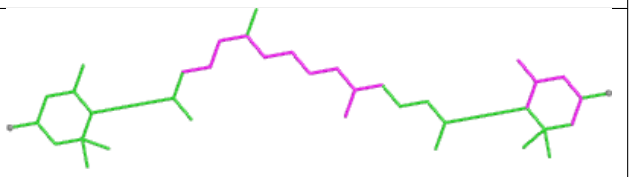


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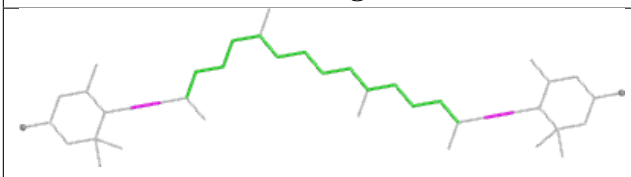
Ligand II0 7 616



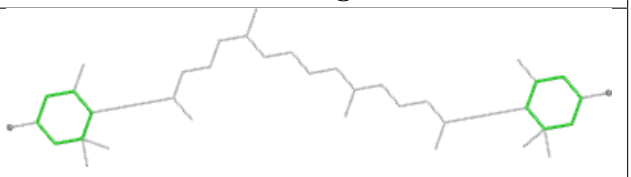
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Bond angles

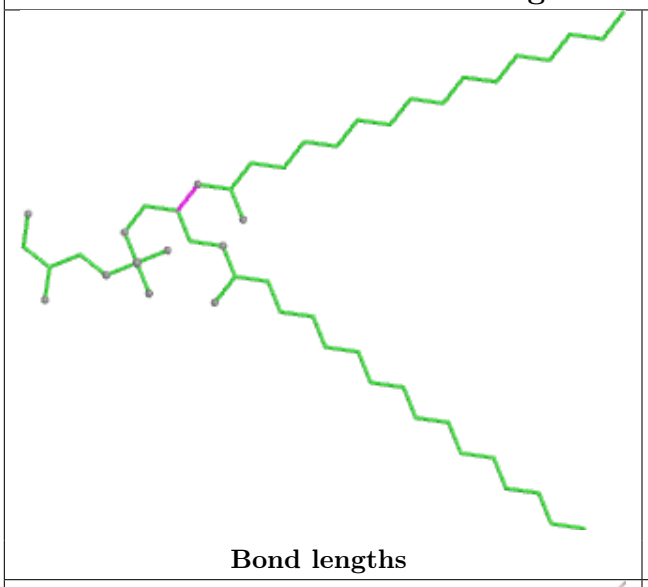


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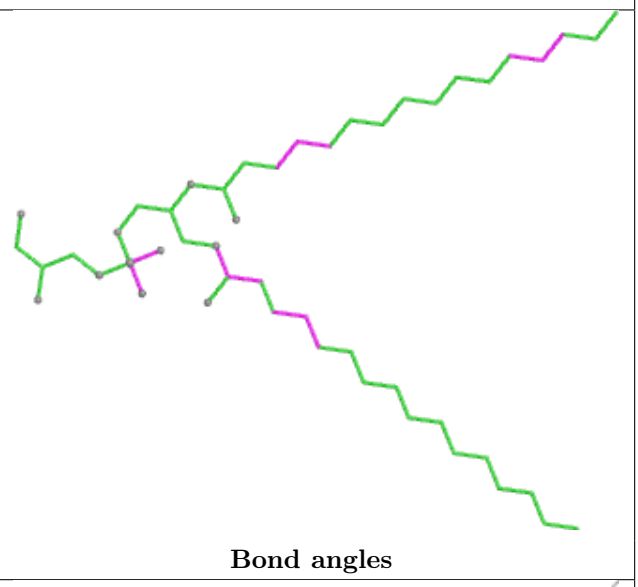


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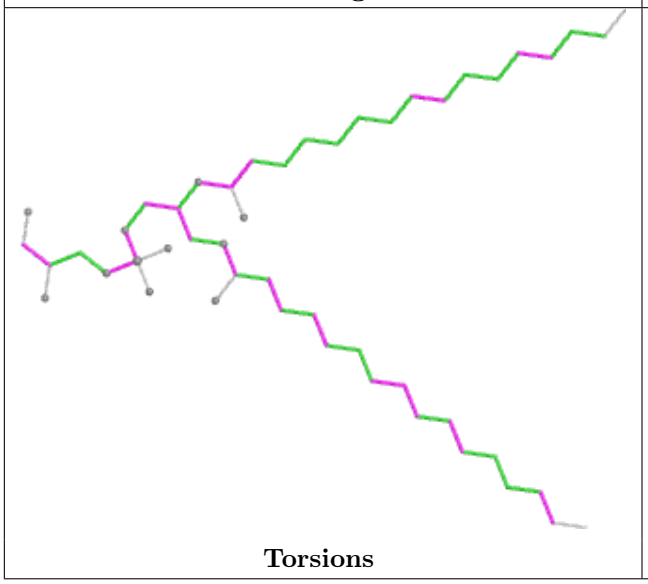
Ligand LHG 3 623



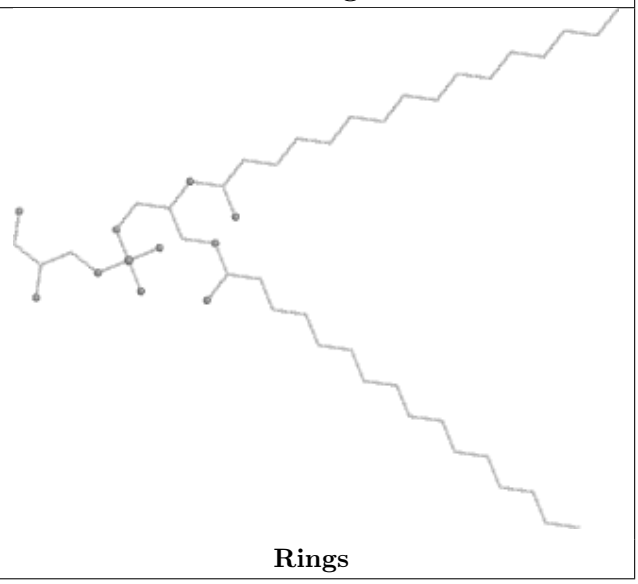
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Bond angles

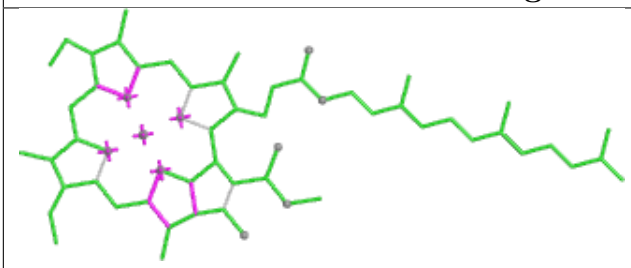


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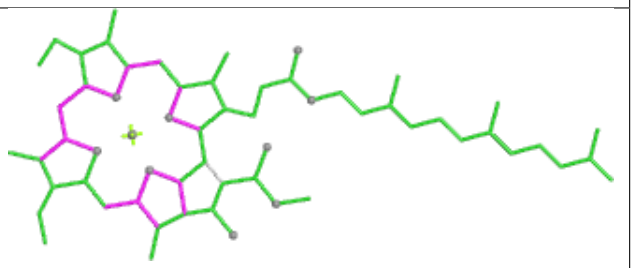


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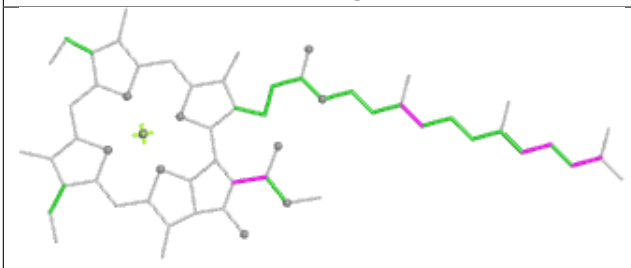
Ligand CLA B 810



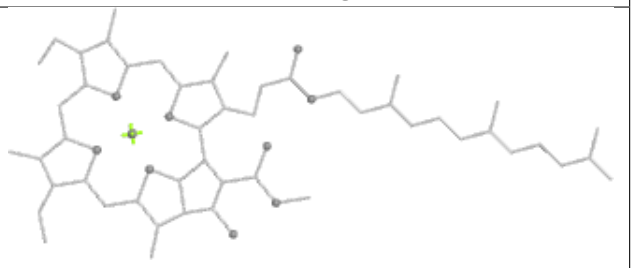
Bond lengths



Bond angles

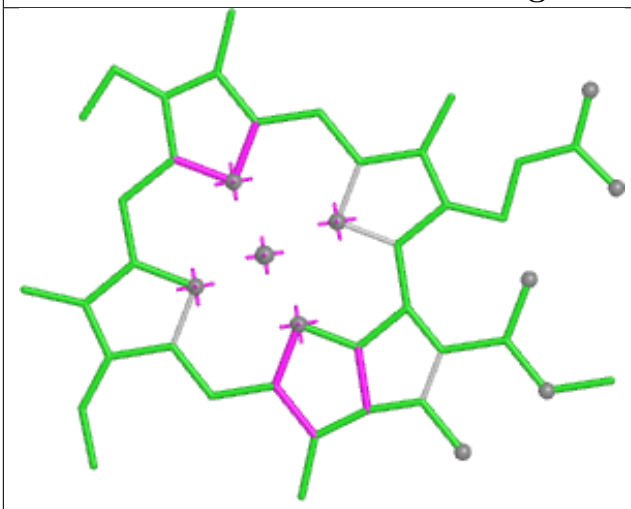


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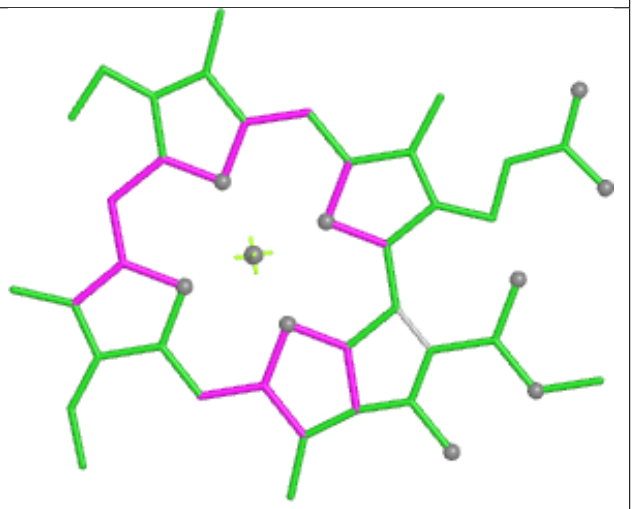


Rings

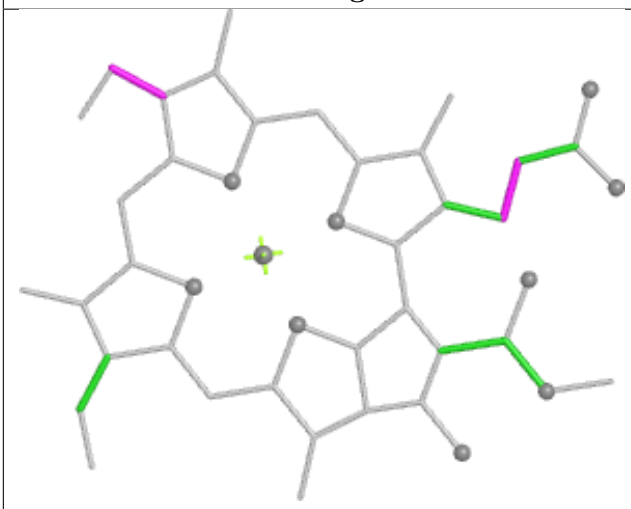
Ligand CLA 1 604



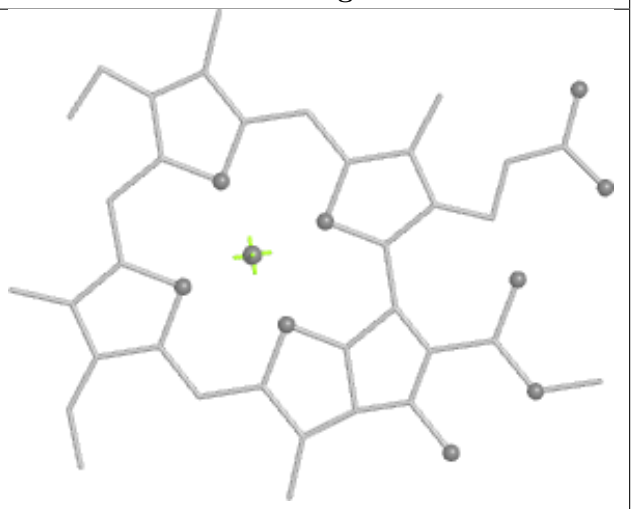
Bond lengths



Bond angles

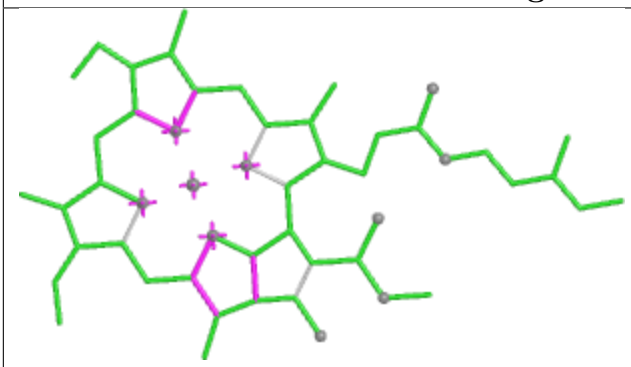


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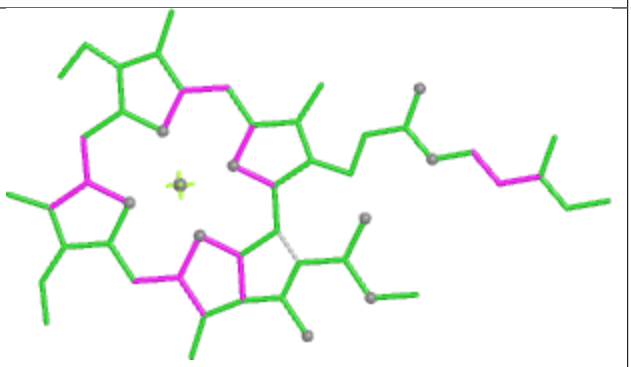


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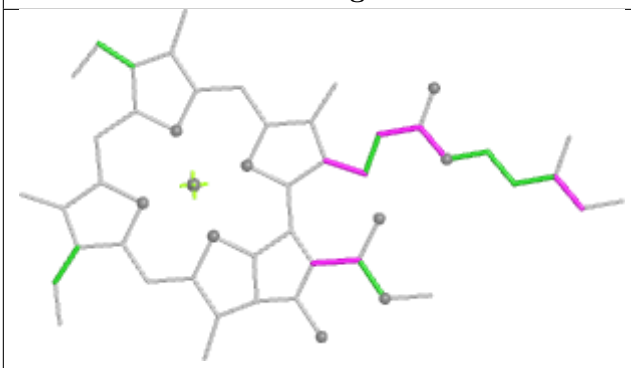
Ligand CLA b 610



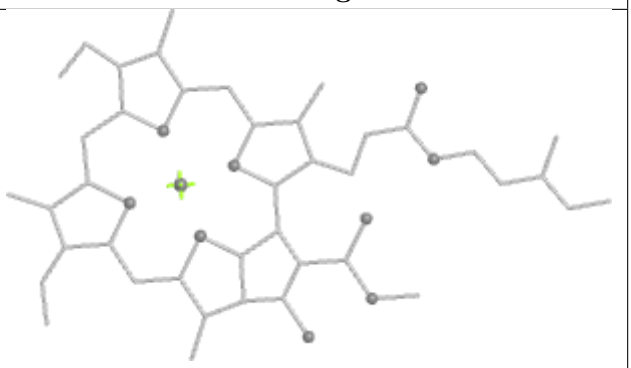
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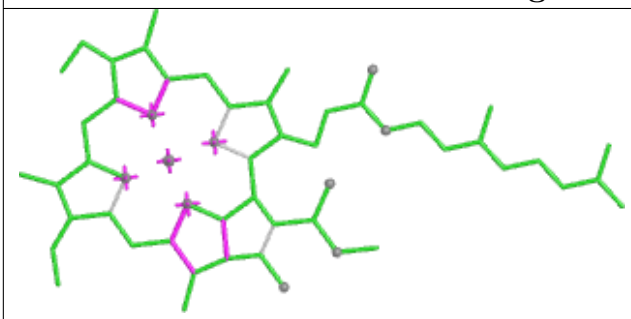


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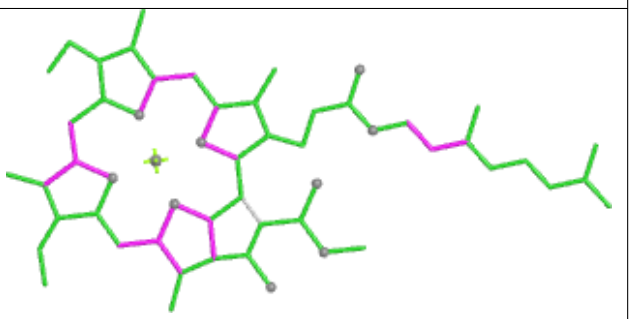


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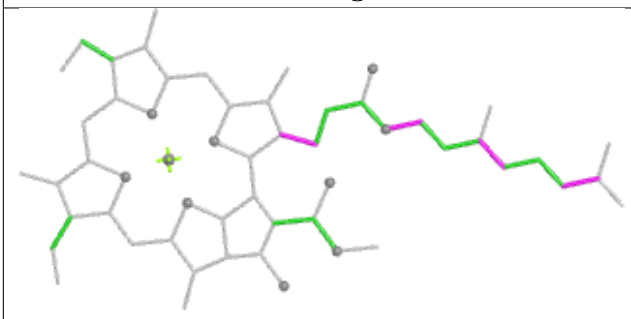
Ligand CLA a 611



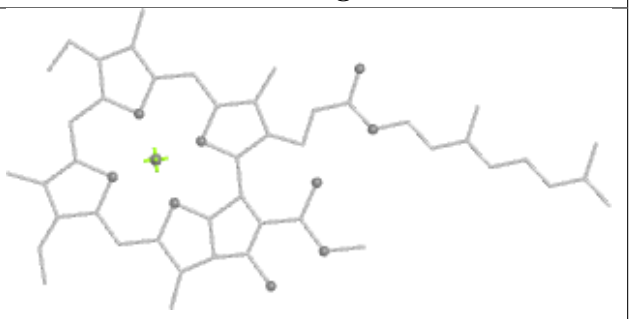
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Bond angles

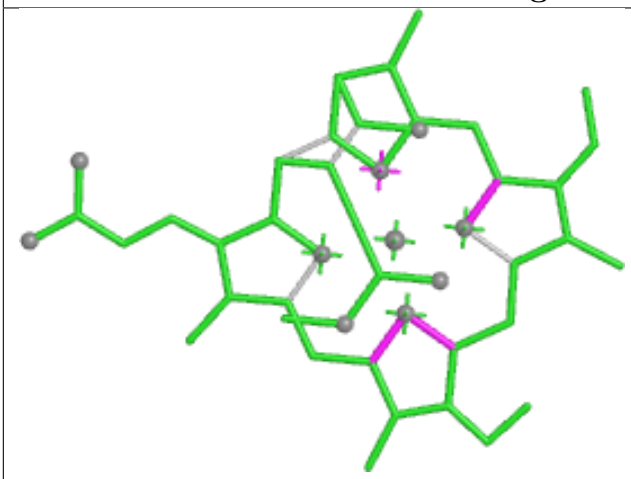


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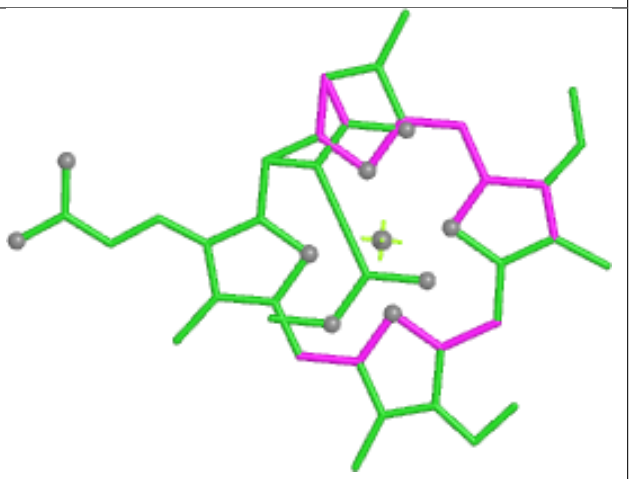


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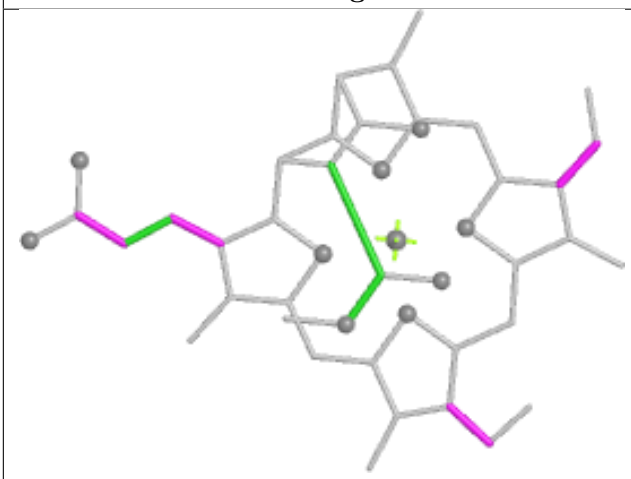
Ligand KC2 4 605



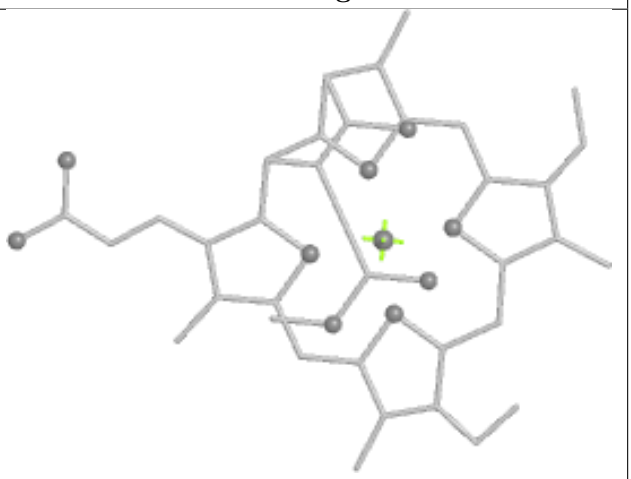
Bond lengths



Bond angles

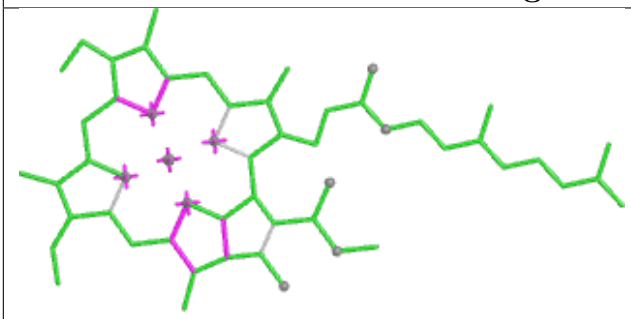


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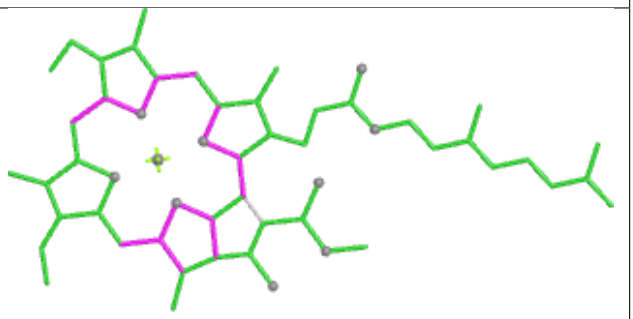


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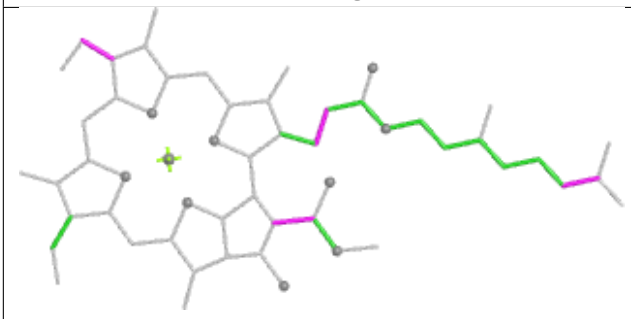
Ligand CLA A 840



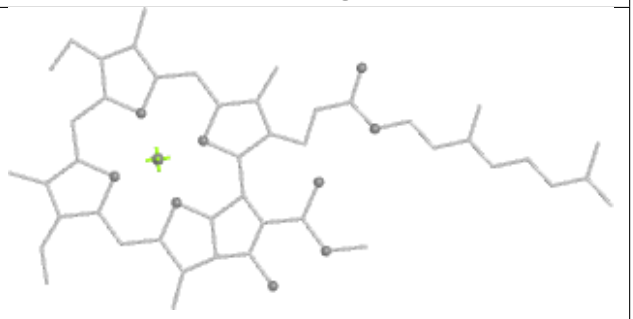
Bond lengths



Bond angles

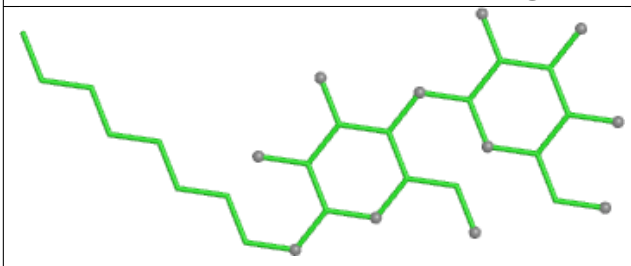


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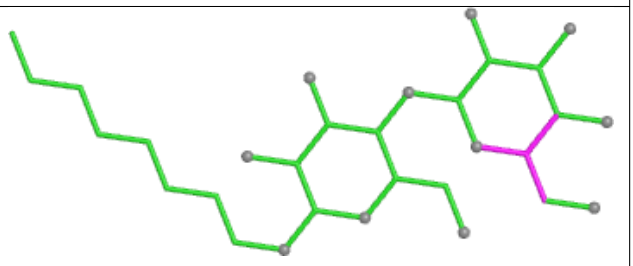


Rings

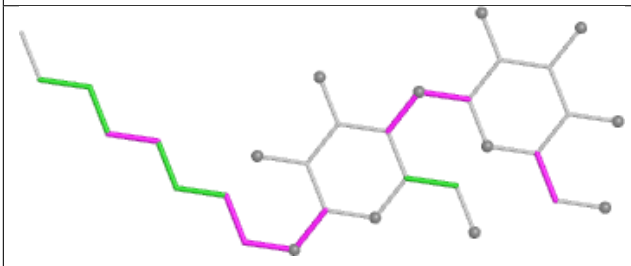
Ligand LMU J 104



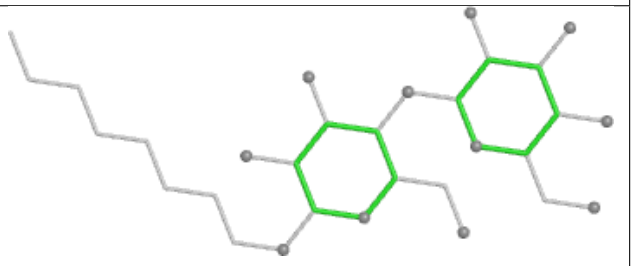
Bond lengths



Bond angles

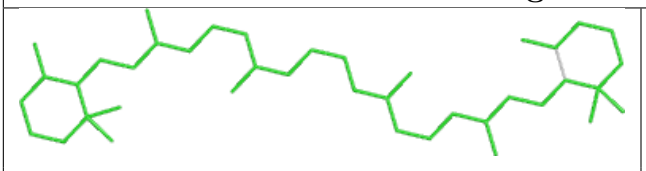


Torsions

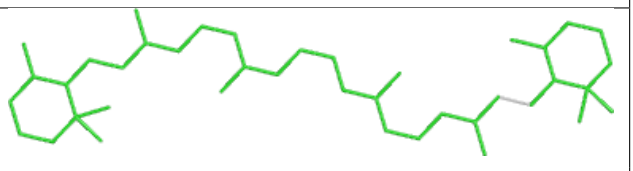


Rings

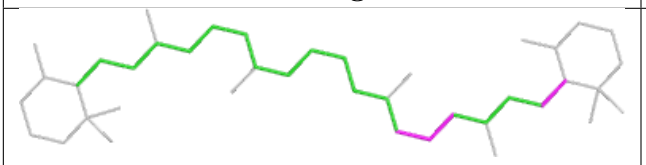
Ligand 8CT A 846



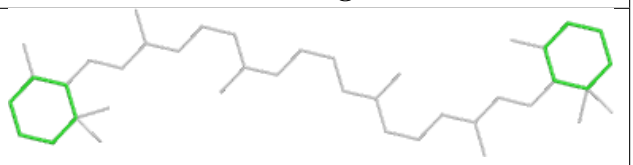
Bond lengths



Bond angles

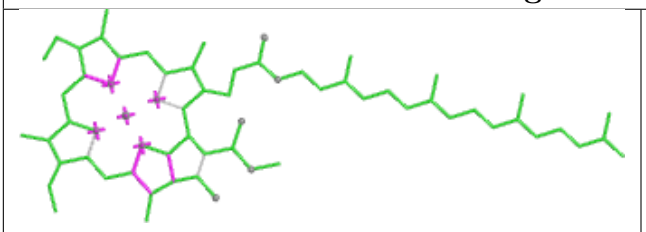


Torsions

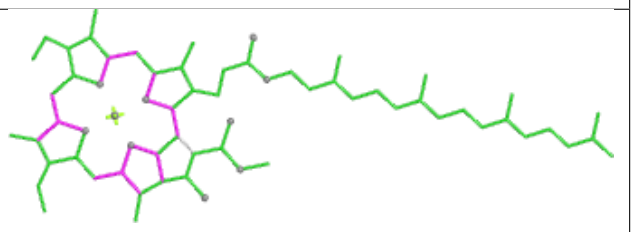


Rings

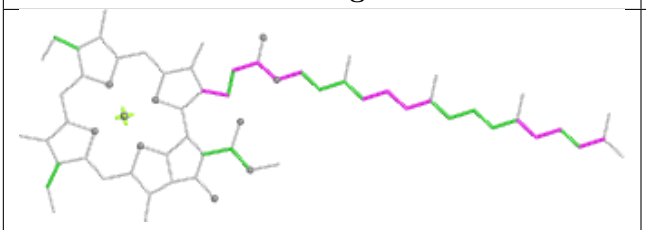
Ligand CLA B 832



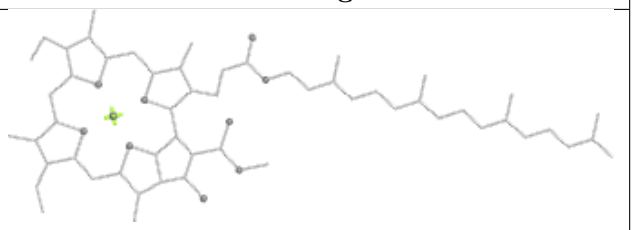
Bond lengths



Bond angles

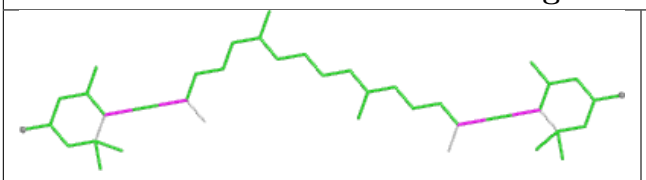


Torsions

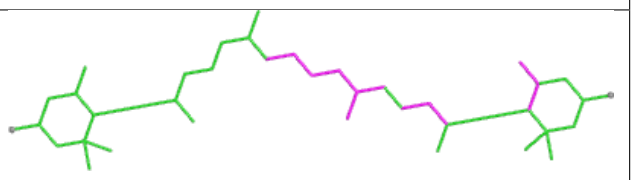


Rings

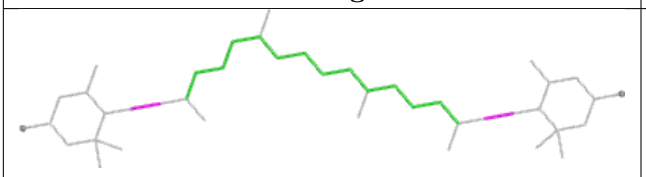
Ligand II0 3 613



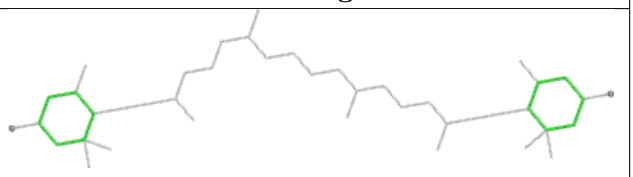
Bond lengths



Bond angles

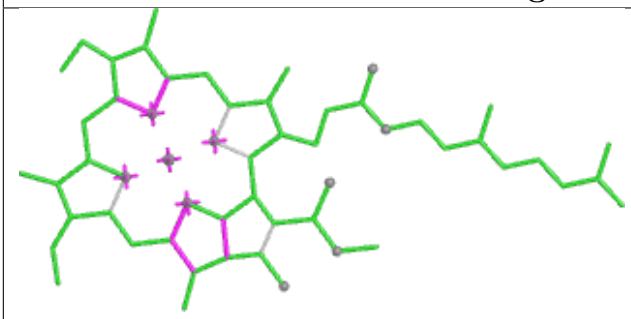


Torsions

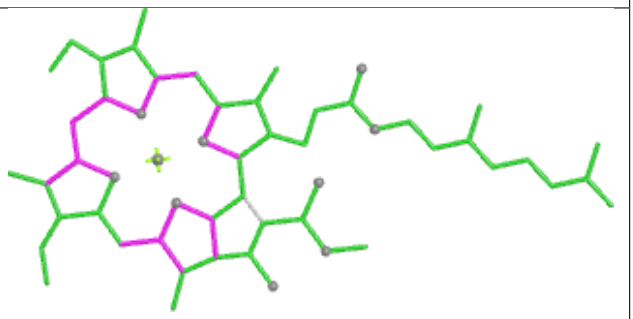


Rings

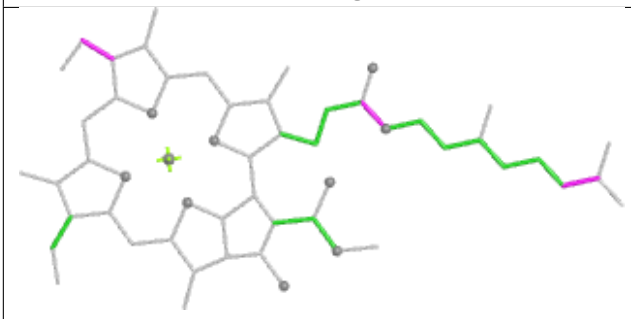
Ligand CLA 6 607



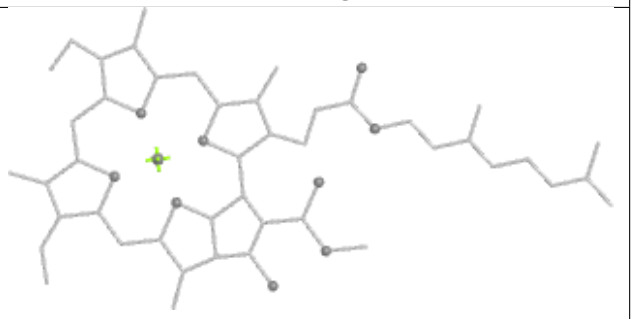
Bond lengths



Bond angles

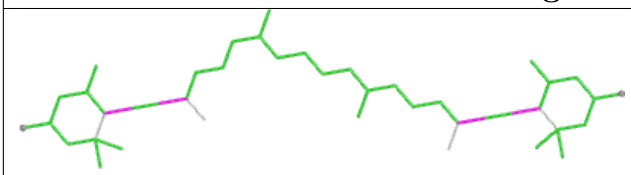


Torsions

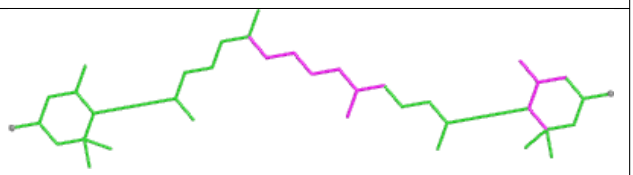


Rings

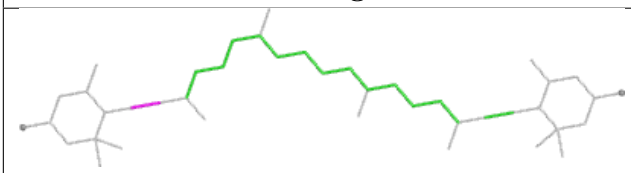
Ligand II0 6 614



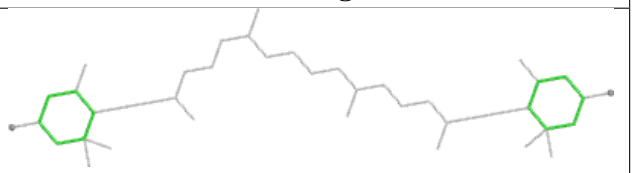
Bond lengths



Bond angles

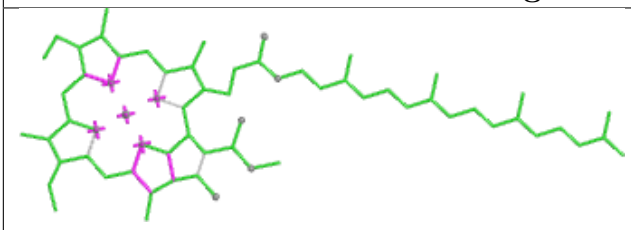


Torsions

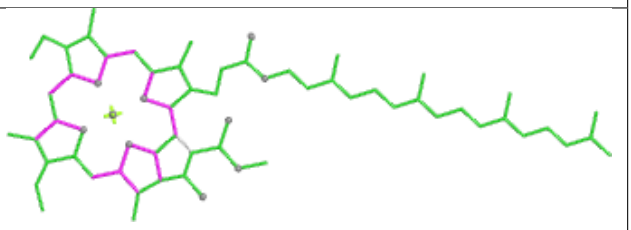


Rings

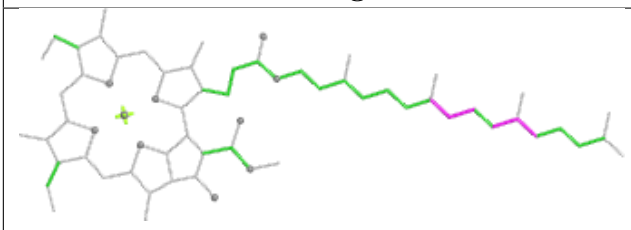
Ligand CLA A 826



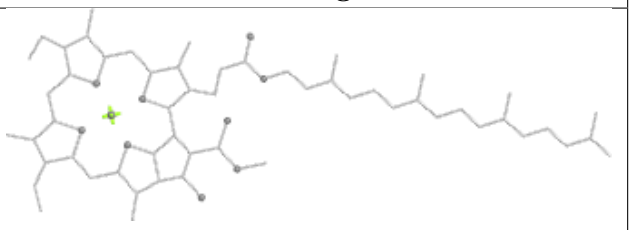
Bond lengths



Bond angles

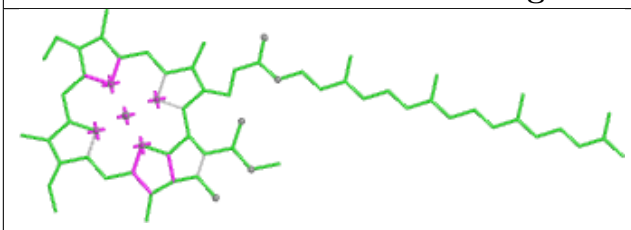


Torsions

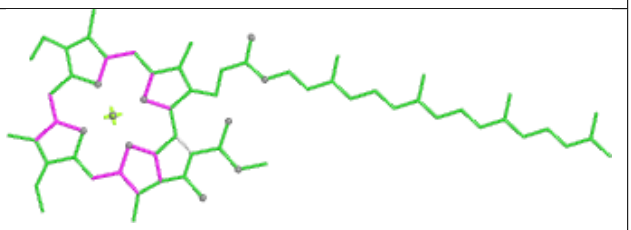


Rings

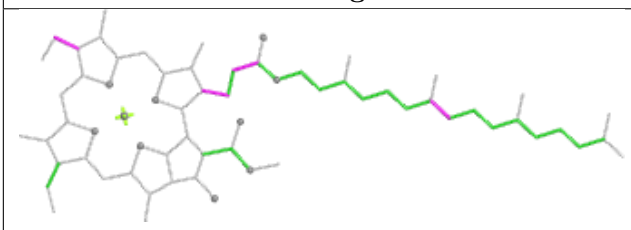
Ligand CLA b 606



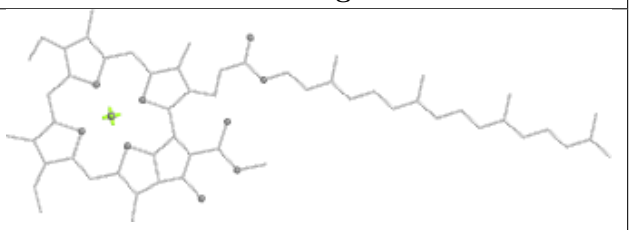
Bond lengths



Bond angles



Torsions



Rings

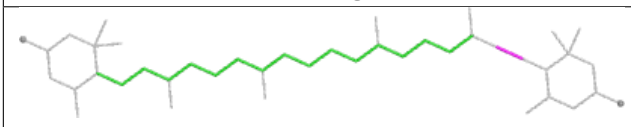
Ligand II3 b 613



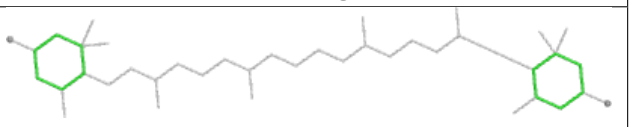
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

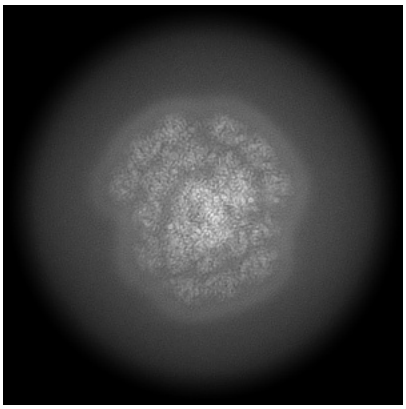
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-33659. These allow visual inspection of the internal detail of the map and identification of artifacts.

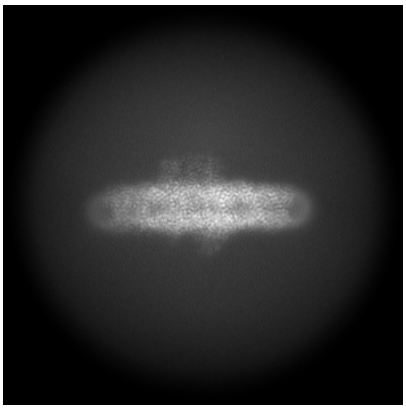
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

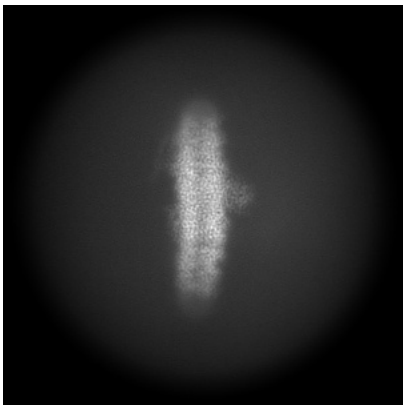
6.1.1 Primary map



X

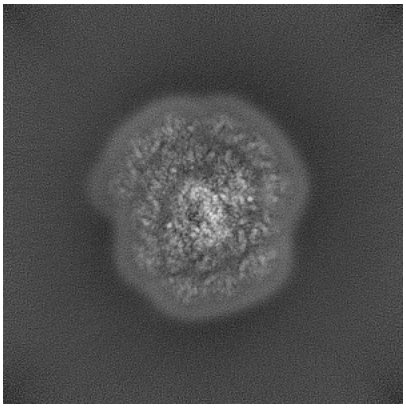


Y

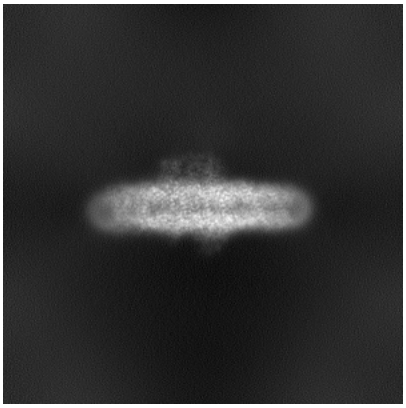


Z

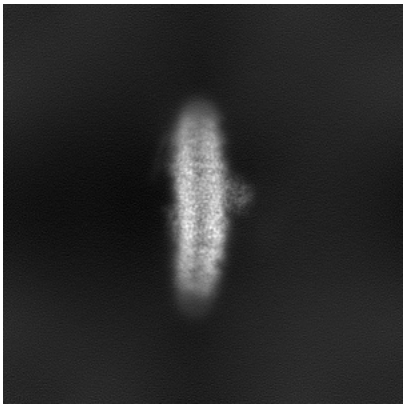
6.1.2 Raw map



X



Y

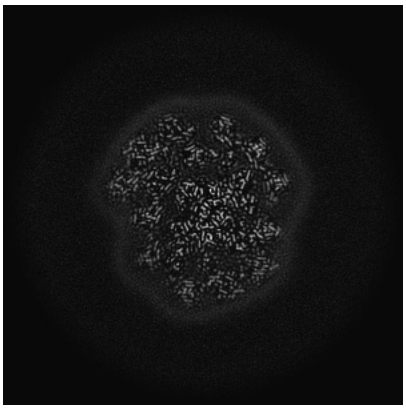


Z

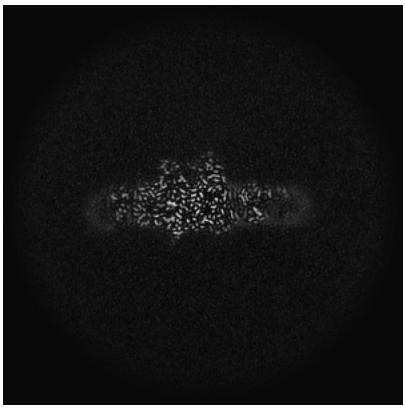
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



X Index: 200

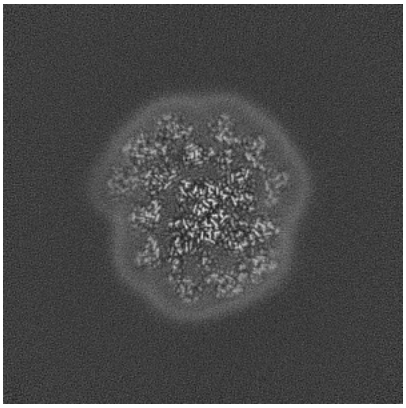


Y Index: 200

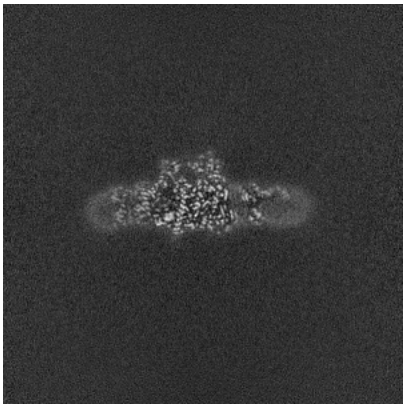


Z Index: 200

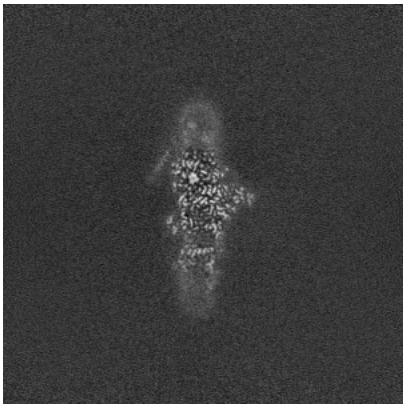
6.2.2 Raw map



X Index: 200



Y Index: 200

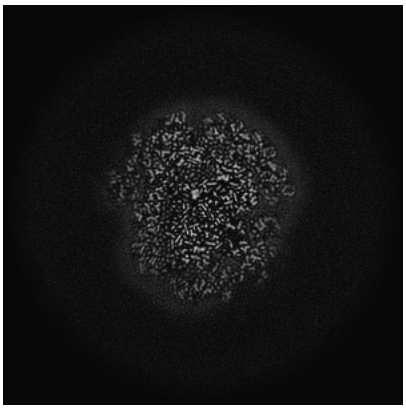


Z Index: 200

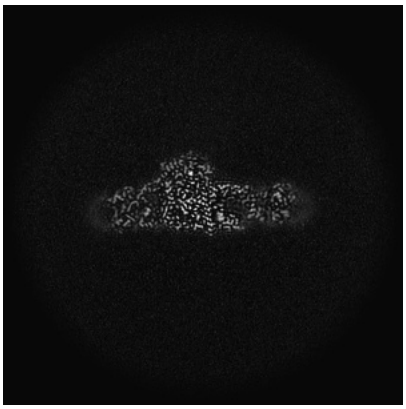
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

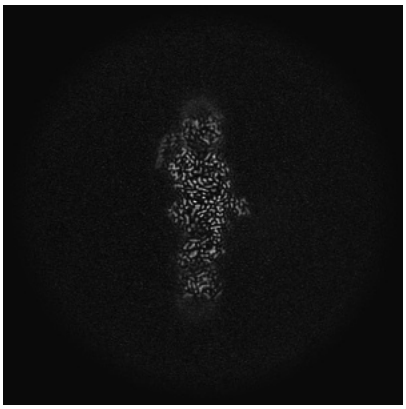
6.3.1 Primary map



X Index: 210

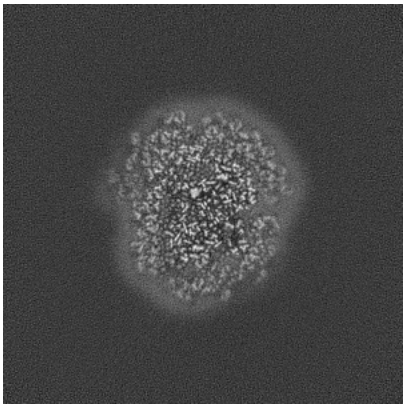


Y Index: 212

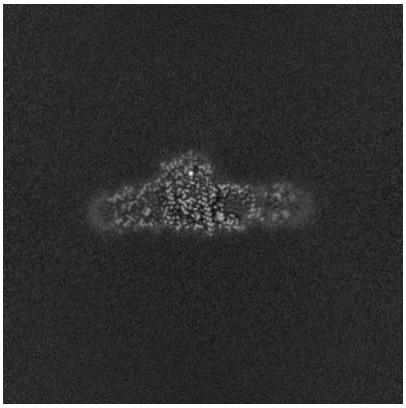


Z Index: 215

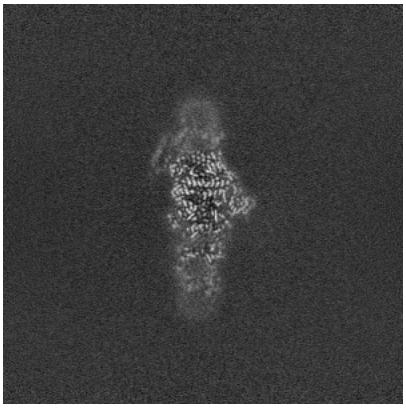
6.3.2 Raw map



X Index: 209



Y Index: 211

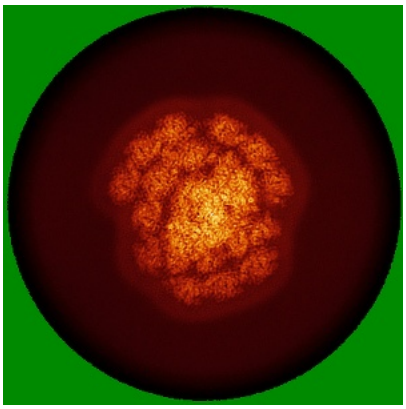


Z Index: 207

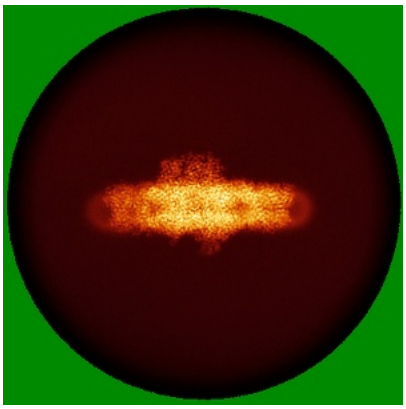
The images above show the largest variance slices of the map in three orthogonal directions.

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

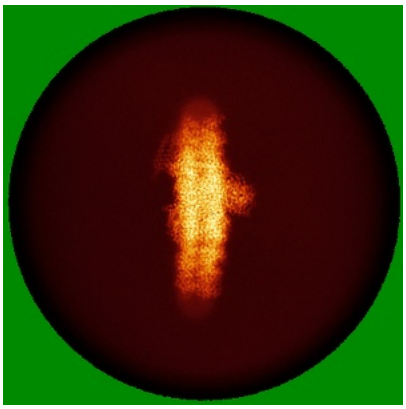
6.4.1 Primary map



X

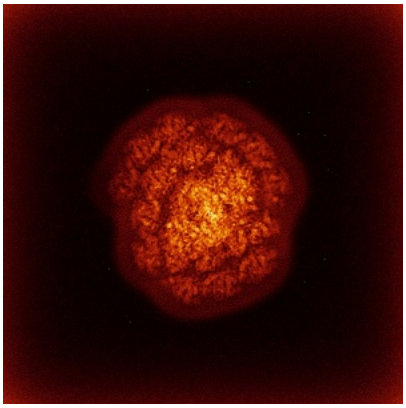


Y

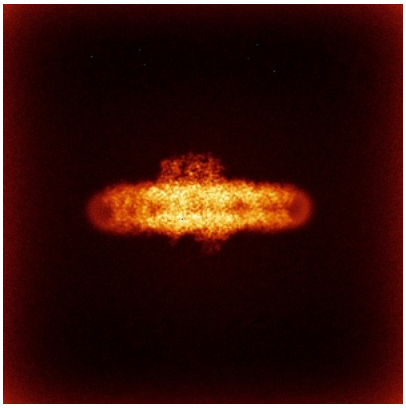


Z

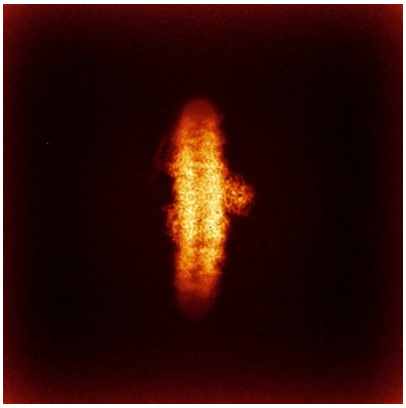
6.4.2 Raw map



X



Y

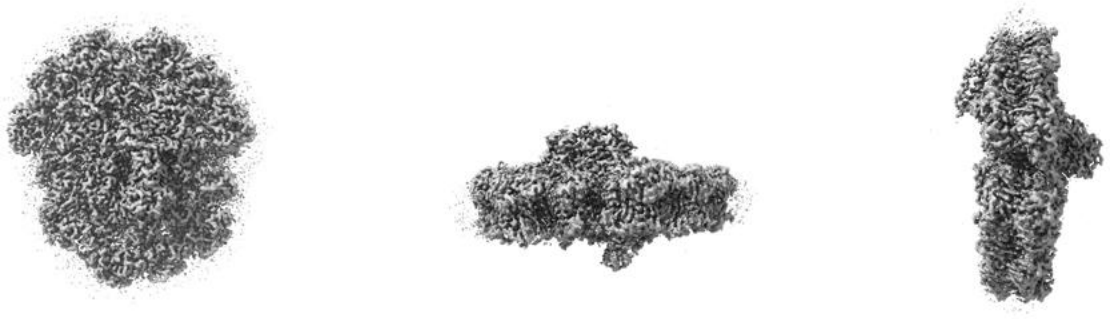


Z

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.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.35. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

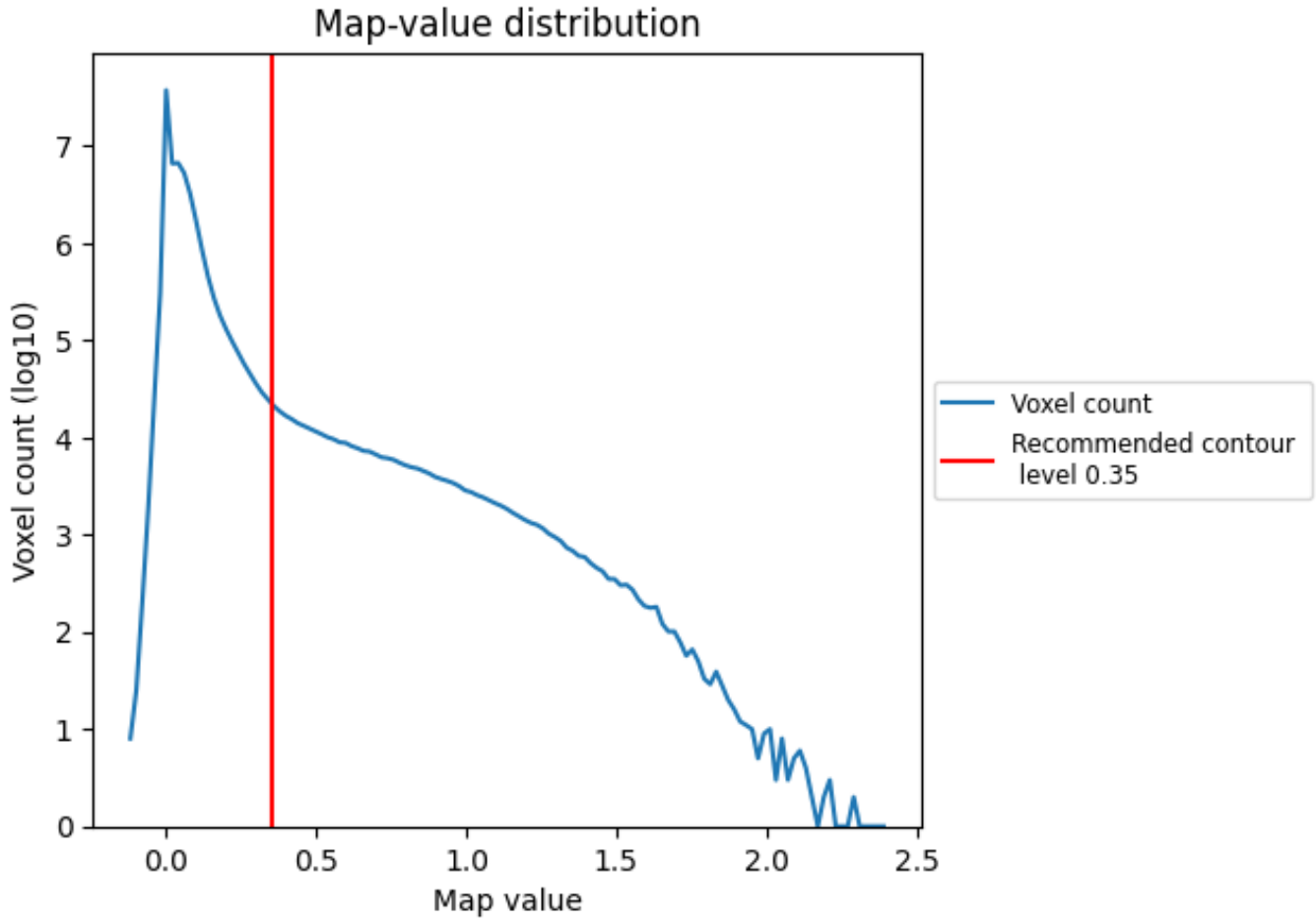
6.6 Mask visualisation (i)

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

7 Map analysis

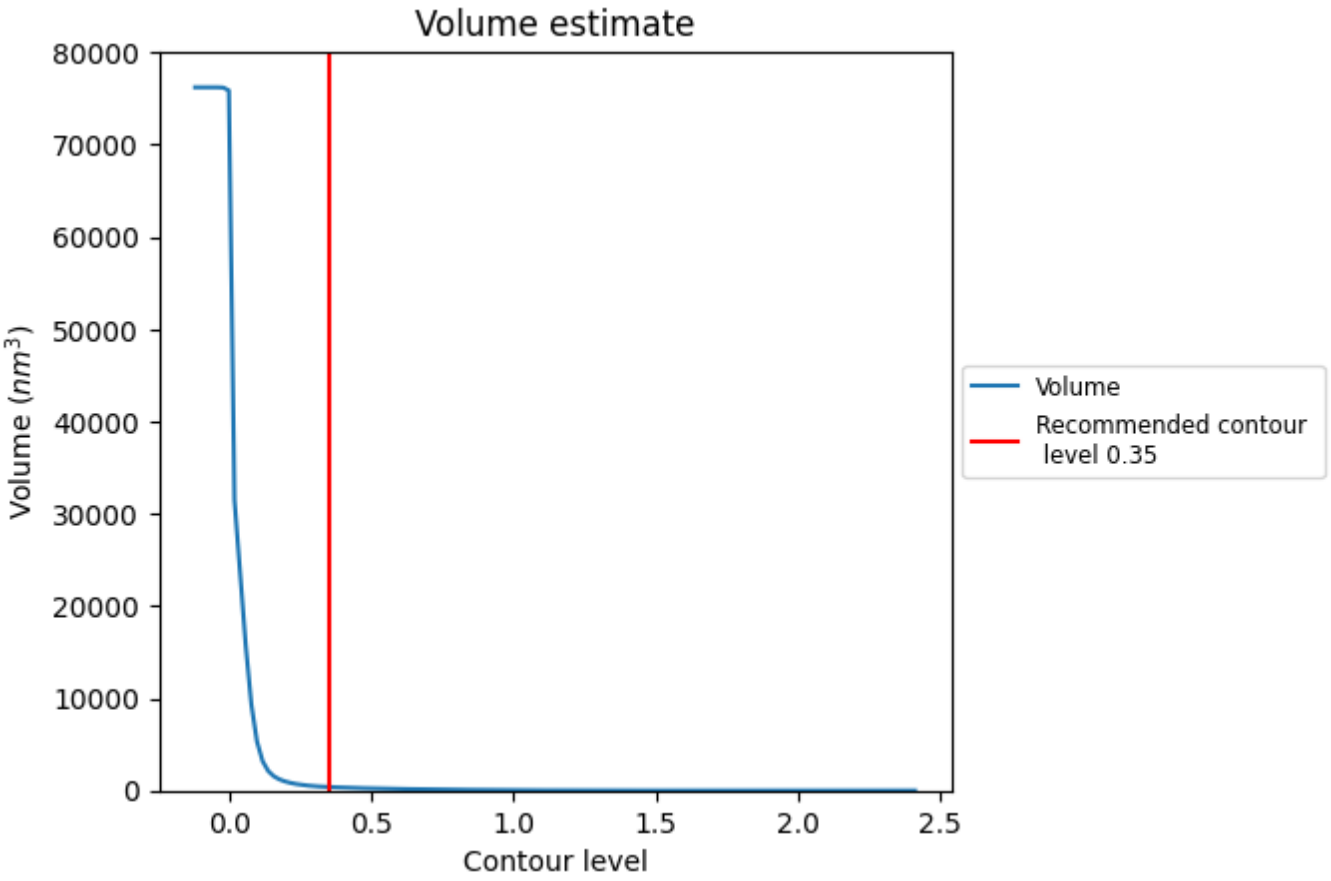
This section contains the results of statistical analysis of the map.

7.1 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.

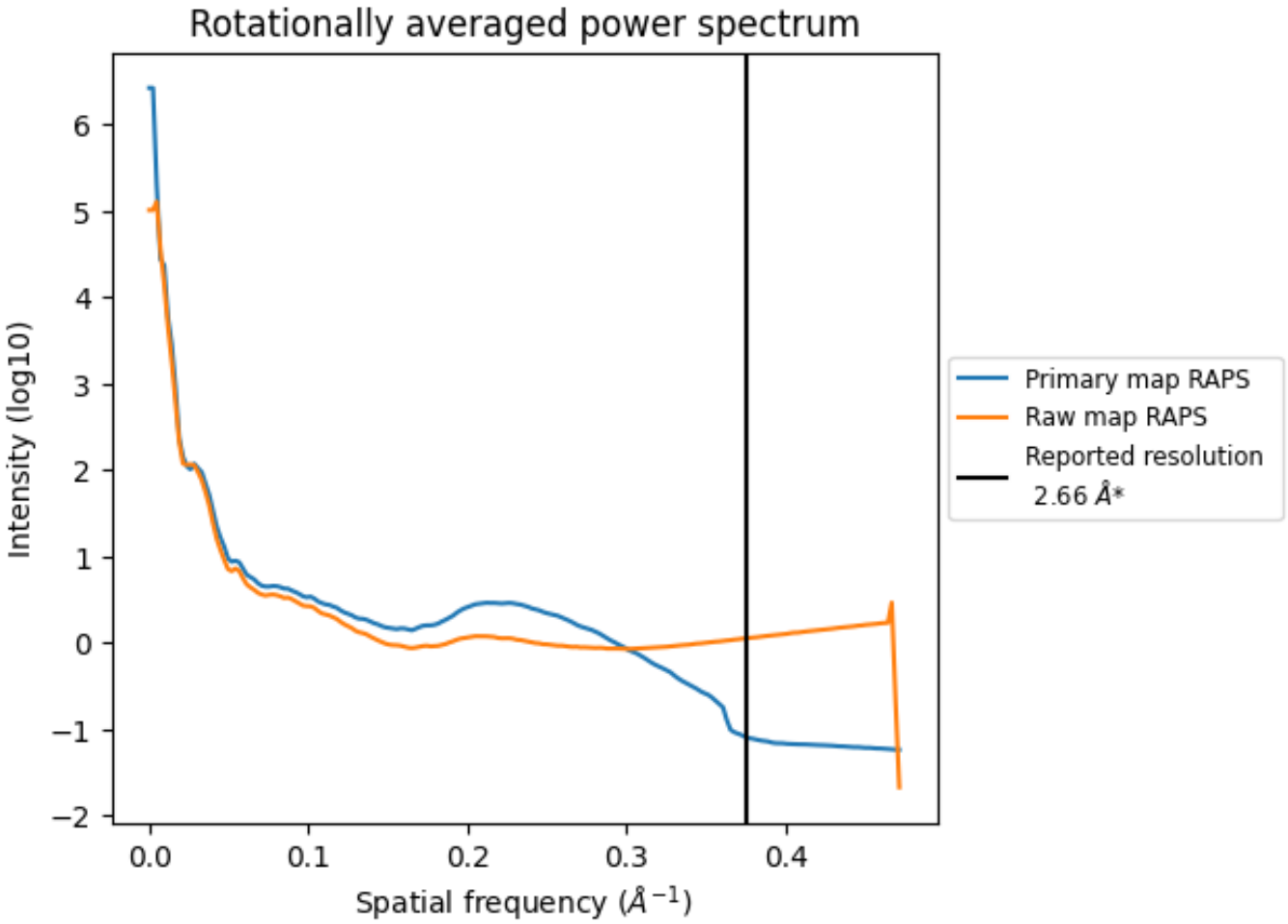
7.2 Volume estimate



The volume at the recommended contour level is 384 nm^3; this corresponds to an approximate mass of 347 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.

7.3 Rotationally averaged power spectrum (i)

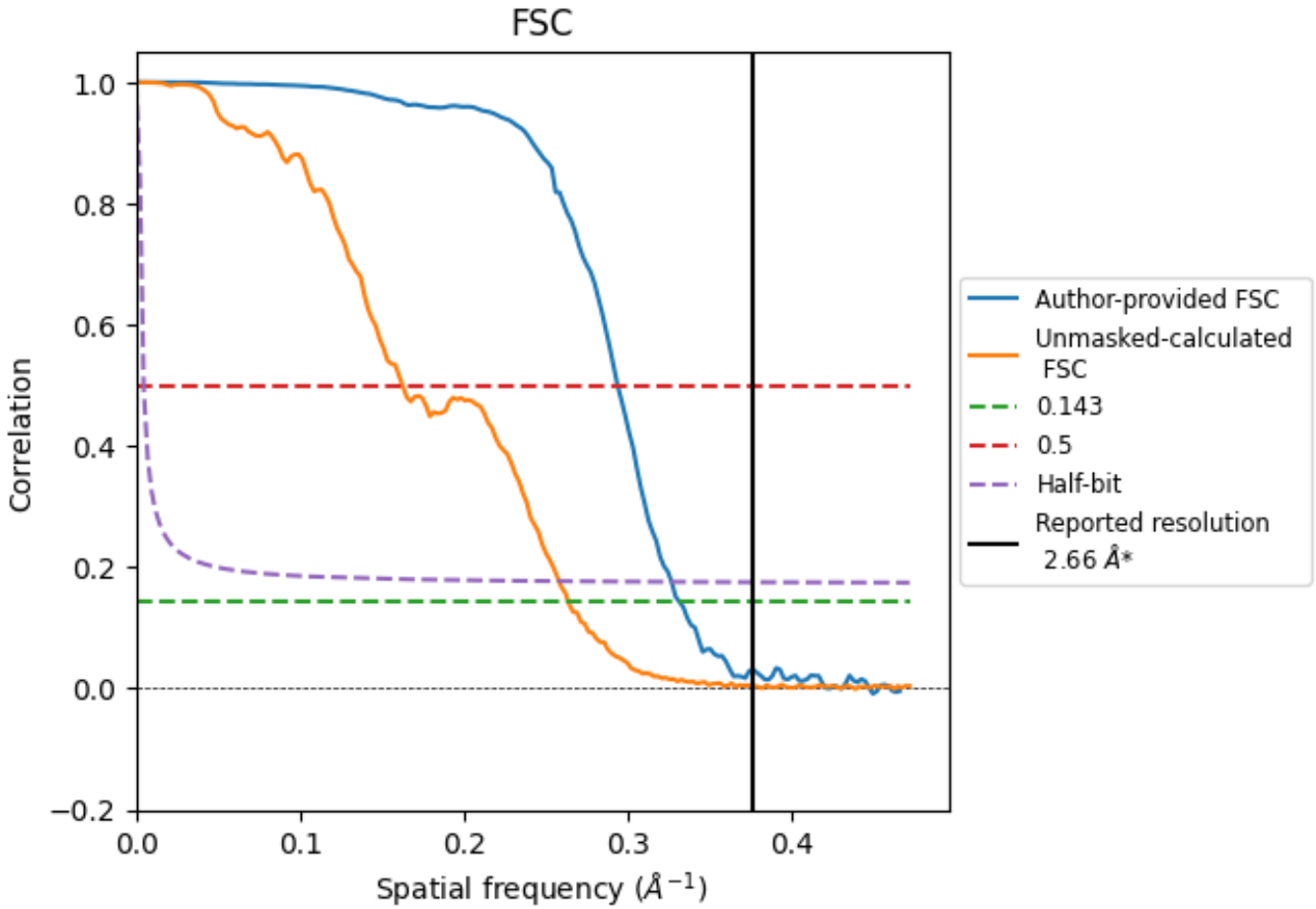


*Reported resolution corresponds to spatial frequency of 0.376 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.376 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.66	-	-
Author-provided FSC curve	3.02	3.41	3.06
Unmasked-calculated*	3.80	6.16	3.88

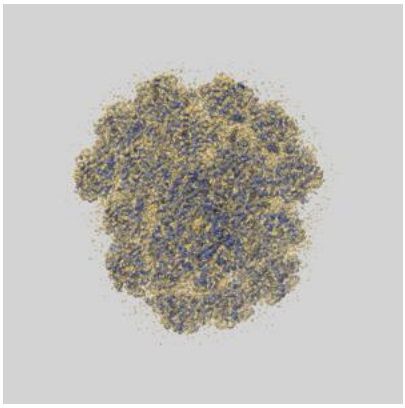
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.02 differs from the reported value 2.66 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.80 differs from the reported value 2.66 by more than 10 %

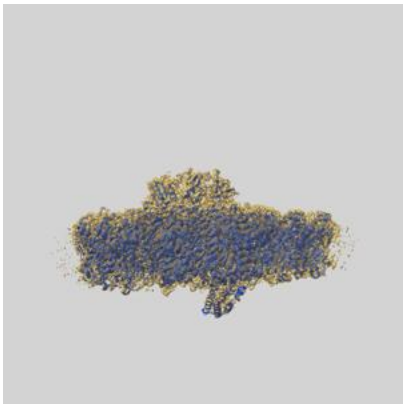
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-33659 and PDB model 7Y7B. Per-residue inclusion information can be found in section 3 on page 35.

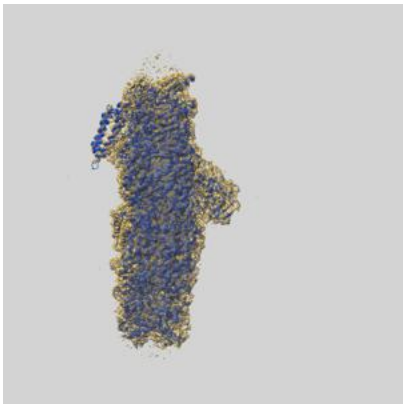
9.1 Map-model overlay



X



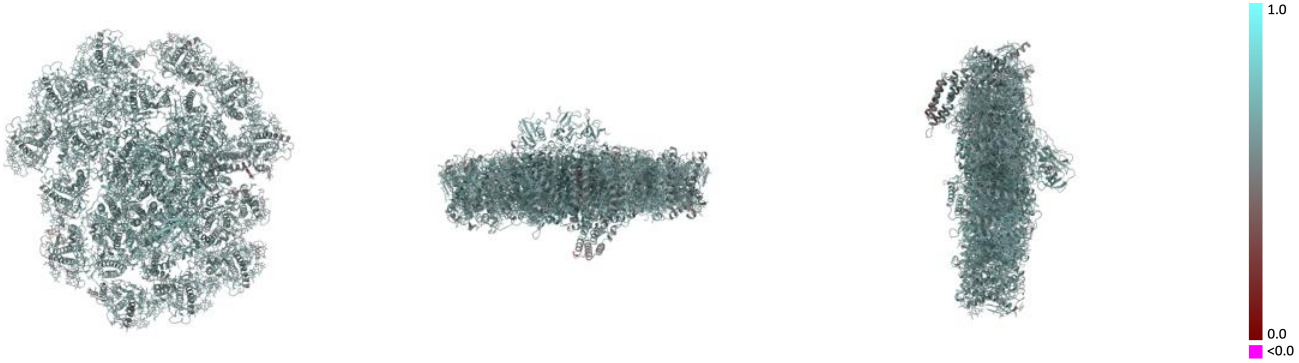
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.35 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.

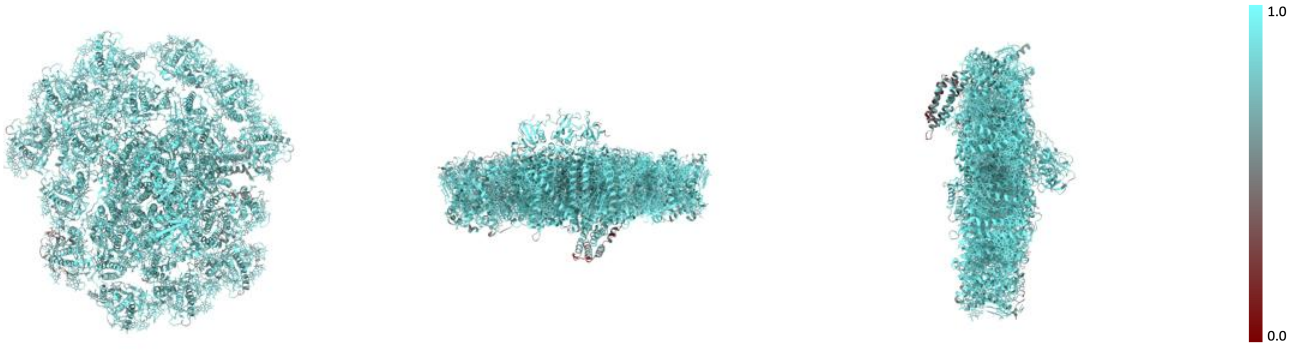
9.2 Q-score mapped to coordinate model



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.

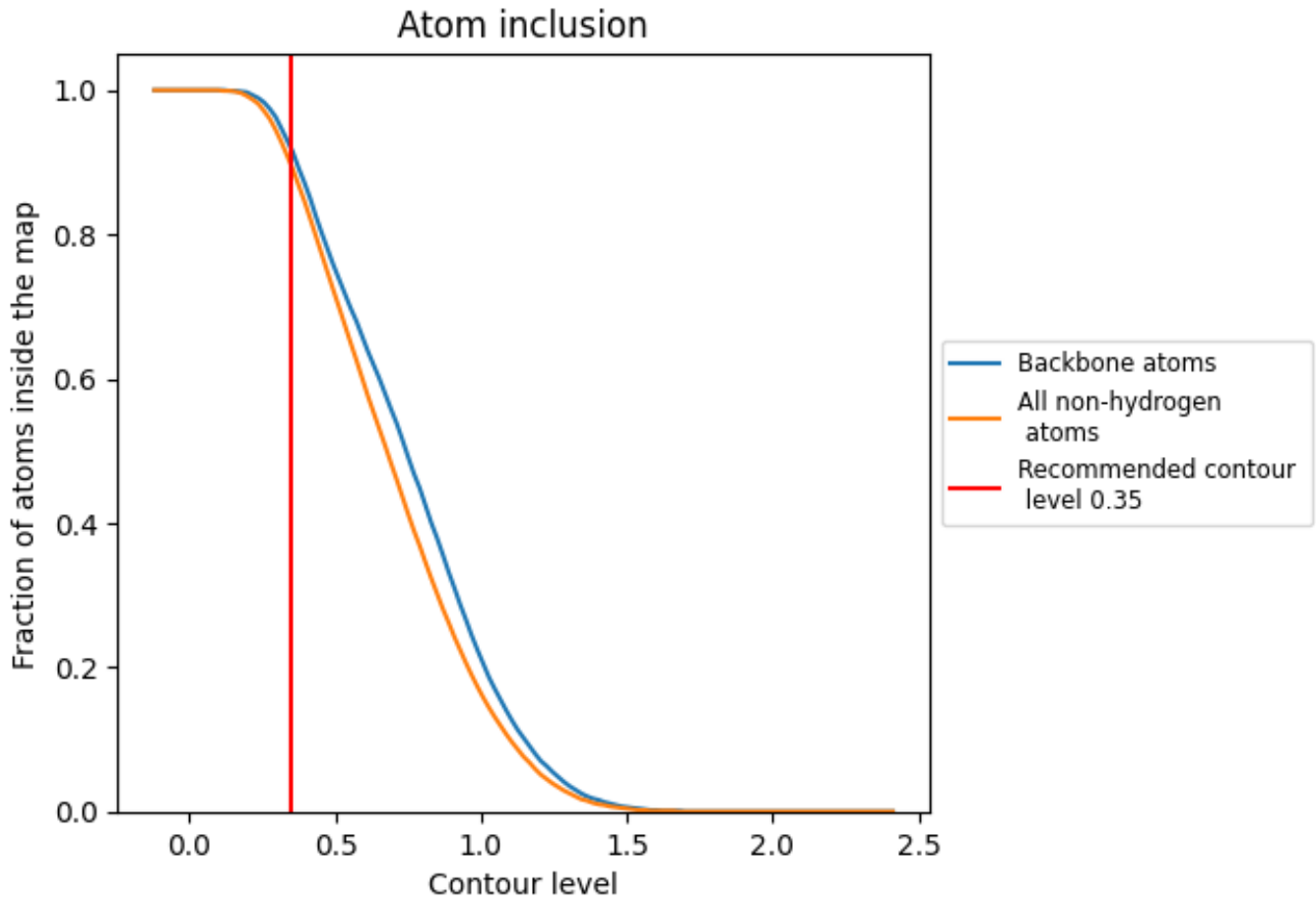
9.3 Atom inclusion mapped to coordinate model



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 (0.35).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8950	0.6070
1	0.7250	0.5490
2	0.9010	0.6030
3	0.9390	0.6270
4	0.9380	0.6130
5	0.8570	0.5600
6	0.8970	0.5810
7	0.8520	0.5580
8	0.8610	0.5920
9	0.7980	0.5750
A	0.9650	0.6450
B	0.9720	0.6440
C	0.9490	0.6110
D	0.8930	0.6030
E	0.8550	0.6070
F	0.9160	0.6230
I	0.9370	0.6280
J	0.9430	0.6340
K	0.8640	0.6050
L	0.9120	0.6160
M	0.9510	0.6260
O	0.8750	0.6090
R	0.9350	0.6080
X	0.6110	0.5150
Z	0.8810	0.6030
a	0.8970	0.5970
b	0.9060	0.5930
c	0.8000	0.5840
d	0.8270	0.5950
e	0.8160	0.5770

