wwPDB EM Validation Summary Report

Oct 1, 2026 – 12:42 PM JST

PDB ID	:	7VD5 / pdb_00007vd5
EMDB ID	:	EMD-31905
Title	:	Structure of C2S2M2-type PSII-FCPII supercomplex from diatom
Authors	:	Nagao, R.; Kato, K.; Akita, F.; Miyazaki, N.; Shen, J.R.
Deposited on	:	2021-09-06
Resolution	:	2.50 Å(reported)
Based on initial model	:	6J40

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 ⓘ 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 ⓘ) were used in the production of this report:

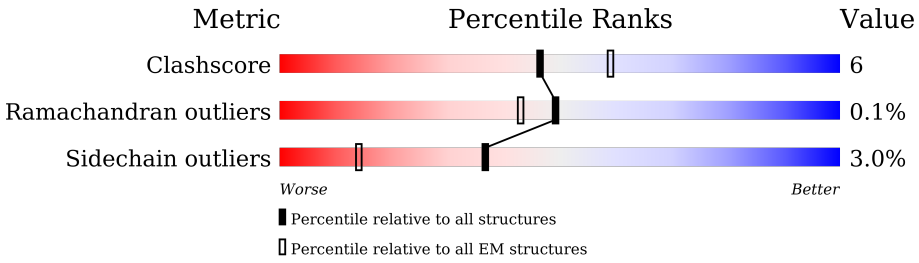
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using 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)	:	2.51

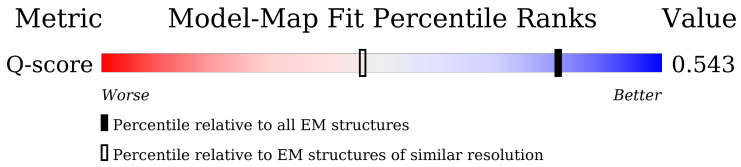
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 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	7115 (2.00 - 3.00)

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	A	334	89% 11%
1	a	334	87% 13%
2	B	484	86% 14%
2	b	484	87% 13%

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Mol	Chain	Length	Quality of chain
3	C	451	88% 11%
3	c	451	89% 11%
4	D	341	87% 13%
4	d	341	87% 13%
5	E	75	91% 9%
5	e	75	91% 9%
6	F	28	89% 11%
6	f	28	86% 14%
7	H	66	91% 9%
7	h	66	88% 12%
8	I	35	91% 9%
8	i	35	94% 6%
9	J	34	94% 6%
9	j	34	91% 9%
10	K	37	81% 19%
10	k	37	89% 11%
11	L	38	97%
11	l	38	95% 5%
12	M	42	5% 95% 5%
12	m	42	5% 95% 5%
13	O	245	82% 16%
13	o	245	80% 18%
14	T	30	97%
14	t	30	87% 13%
15	U	93	81% 19%

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Mol	Chain	Length	Quality of chain
15	u	93	82% 18%
16	V	136	87% 12%
16	v	136	87% 12%
17	Y	34	88% 12%
17	y	34	91% 9%
18	X	37	5% 92% 8%
18	x	37	5% 86% 14%
19	Z	59	92% 8%
19	z	59	97%
20	Q	151	89% 11%
20	q	151	87% 13%
21	W	52	96%
21	w	52	94% 6%
22	0	31	97%
22	5	31	97%
23	1	30	100%
23	6	30	100%
24	11	176	86% 13%
24	31	176	84% 16%
25	12	169	82% 17%
25	32	169	82% 18%
26	13	169	6% 83% 17%
26	33	169	5% 81% 18%
27	14	172	80% 19%
27	34	172	77% 22%

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Mol	Chain	Length	Quality of chain
28	15	170	75% 77% 20%
28	35	170	75% 79% 19%
29	16	179	12% 79% 20%
29	36	179	12% 80% 18%
30	17	176	21% 81% 18%
30	37	176	21% 86% 14%
31	18	168	78% 76% 21%
31	38	168	80% 75% 21%
32	19	227	8% 81% 19%
32	39	227	8% 81% 17%
33	20	155	41% 77% 19%
33	40	155	47% 76% 21%
34	21	162	94% 73% 20%
34	41	162	94% 73% 21%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
47	HEC	V	201	X	-	-	-
47	HEC	v	201	X	-	-	-

2 Entry composition (i)

There are 53 unique types of molecules in this entry. The entry contains 100884 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 Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	334	Total	C	N	O	S	0	0
			2619	1712	429	463	15		
1	a	334	Total	C	N	O	S	0	0
			2619	1712	429	463	15		

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	484	Total	C	N	O	S	0	0
			3812	2494	645	660	13		
2	b	484	Total	C	N	O	S	0	0
			3812	2494	645	660	13		

- Molecule 3 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	451	Total	C	N	O	S	0	0
			3504	2289	589	612	14		
3	c	451	Total	C	N	O	S	0	0
			3504	2289	589	612	14		

- Molecule 4 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	341	Total	C	N	O	S	0	0
			2697	1781	441	465	10		
4	d	341	Total	C	N	O	S	0	0
			2697	1781	441	465	10		

- Molecule 5 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	75	Total 616	C 401	N 102	O 113	0	0
5	e	75	Total 616	C 401	N 102	O 113	0	0

- Molecule 6 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	28	Total 228	C 155	N 39	O 33	S 1	0	0
6	f	28	Total 228	C 155	N 39	O 33	S 1	0	0

- Molecule 7 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	66	Total 513	C 340	N 83	O 88	S 2	0	0
7	h	66	Total 513	C 340	N 83	O 88	S 2	0	0

- Molecule 8 is a protein called Photosystem II reaction center protein I.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	35	Total 287	C 194	N 45	O 47	S 1	0	0
8	i	35	Total 287	C 194	N 45	O 47	S 1	0	0

- Molecule 9 is a protein called Photosystem II reaction center protein J.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	34	Total 254	C 172	N 38	O 43	S 1	0	0
9	j	34	Total 254	C 172	N 38	O 43	S 1	0	0

- Molecule 10 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	K	37	Total 302	C 212	N 45	O 45	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
10	k	37	Total 302	C 212	N 45	O 45	0	0

- Molecule 11 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	38	Total 310	C 208	N 48	O 53	S 1	0	0
11	l	38	Total 310	C 208	N 48	O 53	S 1	0	0

- Molecule 12 is a protein called Photosystem II subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	M	42	Total 316	C 207	N 51	O 58	0	0
12	m	42	Total 316	C 207	N 51	O 58	0	0

- Molecule 13 is a protein called Extrinsic protein in photosystem II.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	245	Total 1845	C 1166	N 306	O 365	S 8	0	0
13	o	245	Total 1845	C 1166	N 306	O 365	S 8	0	0

- Molecule 14 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	T	30	Total 250	C 174	N 36	O 38	S 2	0	0
14	t	30	Total 250	C 174	N 36	O 38	S 2	0	0

- Molecule 15 is a protein called Extrinsic protein in photosystem II.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	U	93	Total 713	C 455	N 119	O 137	S 2	0	0
15	u	93	Total 713	C 455	N 119	O 137	S 2	0	0

- Molecule 16 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	V	136	Total	C	N	O	S	0	0
			1037	647	180	206	4		
16	v	136	Total	C	N	O	S	0	0
			1037	647	180	206	4		

- Molecule 17 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Y	34	Total	C	N	O	S	0	0
			250	166	41	40	3		
17	y	34	Total	C	N	O	S	0	0
			250	166	41	40	3		

- Molecule 18 is a protein called Photosystem II reaction center X protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	X	37	Total	C	N	O	S	0	0
			263	171	45	46	1		
18	x	37	Total	C	N	O	S	0	0
			263	171	45	46	1		

- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Z	59	Total	C	N	O	S	0	0
			447	305	68	73	1		
19	z	59	Total	C	N	O	S	0	0
			447	305	68	73	1		

- Molecule 20 is a protein called Extrinsic protein in photosystem II.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Q	151	Total	C	N	O	S	0	0
			1180	749	196	234	1		
20	q	151	Total	C	N	O	S	0	0
			1180	749	196	234	1		

- Molecule 21 is a protein called Photosystem II reaction center protein W.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	W	52	Total	C	N	O	0	0
			422	273	65	84		
21	w	52	Total	C	N	O	0	0
			422	273	65	84		

- Molecule 22 is a protein called Unknown protein 0.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	0	31	Total	C	N	O	0	0
			155	93	31	31		
22	5	31	Total	C	N	O	0	0
			155	93	31	31		

- Molecule 23 is a protein called Unknown protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	1	30	Total	C	N	O	0	0
			150	90	30	30		
23	6	30	Total	C	N	O	0	0
			150	90	30	30		

- Molecule 24 is a protein called Chlorophyll a/b-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	11	176	Total	C	N	O	S	0	0
			1343	852	228	256	7		
24	31	176	Total	C	N	O	S	0	0
			1343	852	228	256	7		

- Molecule 25 is a protein called Fcpb2, Fucoxanthin chlorophyll a/c-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	12	169	Total	C	N	O	S	0	0
			1302	828	222	244	8		
25	32	169	Total	C	N	O	S	0	0
			1302	828	222	244	8		

- Molecule 26 is a protein called Chlorophyll a/b-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	13	169	Total	C	N	O	S	0	0
			1296	823	220	246	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
26	33	169	Total	C	N	O	S	0	0
			1296	823	220	246	7		

- Molecule 27 is a protein called Chlorophyll a/b-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	14	172	Total	C	N	O	S	0	0
			1319	838	223	251	7		
27	34	172	Total	C	N	O	S	0	0
			1319	838	223	251	7		

- Molecule 28 is a protein called Chlorophyll a/b-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	15	170	Total	C	N	O	S	0	0
			1307	832	221	247	7		
28	35	170	Total	C	N	O	S	0	0
			1307	832	221	247	7		

- Molecule 29 is a protein called Fcpb3, Fucoxanthin chlorophyll a/c-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	16	179	Total	C	N	O	S	0	0
			1386	891	233	256	6		
29	36	179	Total	C	N	O	S	0	0
			1386	891	233	256	6		

- Molecule 30 is a protein called Fcpb4, Fucoxanthin chlorophyll a/c-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	17	176	Total	C	N	O	S	0	0
			1353	862	227	258	6		
30	37	176	Total	C	N	O	S	0	0
			1353	862	227	258	6		

- Molecule 31 is a protein called Chlorophyll a/b-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	18	168	Total	C	N	O	S	0	0
			1289	818	219	245	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
31	38	168	Total	C	N	O	S	0	0
			1289	818	219	245	7		

- Molecule 32 is a protein called Fcpb5, Fucoxanthin chlorophyll a/c-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	19	227	Total	C	N	O	S	0	0
			1746	1128	291	322	5		
32	39	227	Total	C	N	O	S	0	0
			1746	1128	291	322	5		

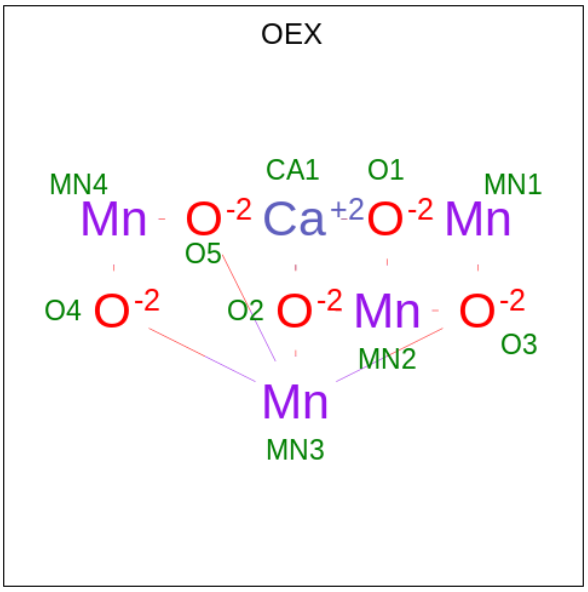
- Molecule 33 is a protein called Fcpb6, Fucoxanthin chlorophyll a/c-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	20	155	Total	C	N	O	S	0	0
			1193	769	201	215	8		
33	40	155	Total	C	N	O	S	0	0
			1193	769	201	215	8		

- Molecule 34 is a protein called Fcpb7, Fucoxanthin chlorophyll a/c-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	21	162	Total	C	N	O	S	0	0
			1262	822	206	229	5		
34	41	162	Total	C	N	O	S	0	0
			1262	822	206	229	5		

- Molecule 35 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: $CaMn_4O_5$).

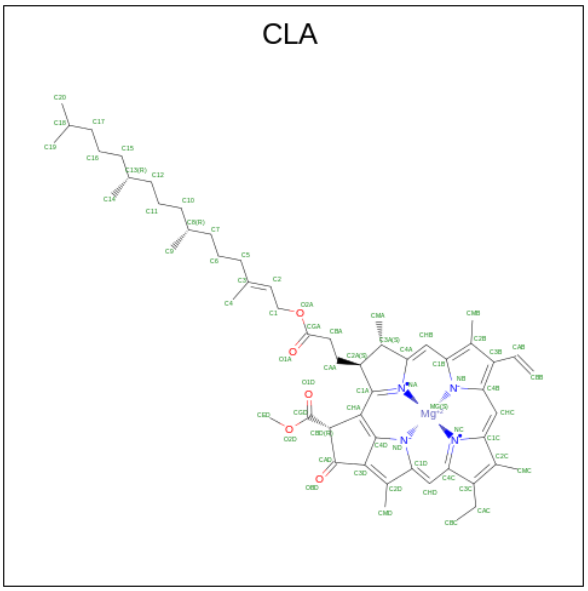


Mol	Chain	Residues	Atoms				AltConf
35	A	1	Total	Ca	Mn	O	0
			10	1	4	5	
35	a	1	Total	Ca	Mn	O	0
			10	1	4	5	

- Molecule 36 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
36	A	1	Total	Fe	0
			1	1	
36	a	1	Total	Fe	0
			1	1	

- Molecule 37 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
37	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
37	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	B	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
37	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
37	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	Z	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	W	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	W	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
37	b	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
37	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
37	z	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	w	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	11	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	11	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	11	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	11	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
37	11	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	11	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
37	12	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	12	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	12	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	12	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
37	12	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
37	12	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	12	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	13	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	13	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
37	13	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	13	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
37	13	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	13	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
37	14	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	14	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	14	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
37	14	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	14	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
37	14	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	14	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	15	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	15	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
37	15	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	15	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
37	15	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	15	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	16	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	16	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
37	16	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	16	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
37	16	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	17	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	17	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
37	17	1	Total	C	Mg	N	O	0
			52	42	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
37	17	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	18	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	18	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	18	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	18	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
37	18	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	18	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
37	18	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	18	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	19	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	19	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	19	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	19	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	19	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
37	19	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	19	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	19	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	19	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	20	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
37	20	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
37	20	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
37	20	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	20	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
37	21	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
37	21	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
37	21	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	21	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	21	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	21	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	21	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	31	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	31	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	31	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	31	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	31	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
37	31	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
37	32	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	32	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	32	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	32	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	32	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
37	32	1	Total	C	Mg	N	O	0
			52	42	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
37	32	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	32	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	33	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	33	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
37	33	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	33	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
37	33	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	33	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	34	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	34	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	34	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
37	34	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	34	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
37	34	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	34	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	35	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	35	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
37	35	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	35	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
37	35	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	35	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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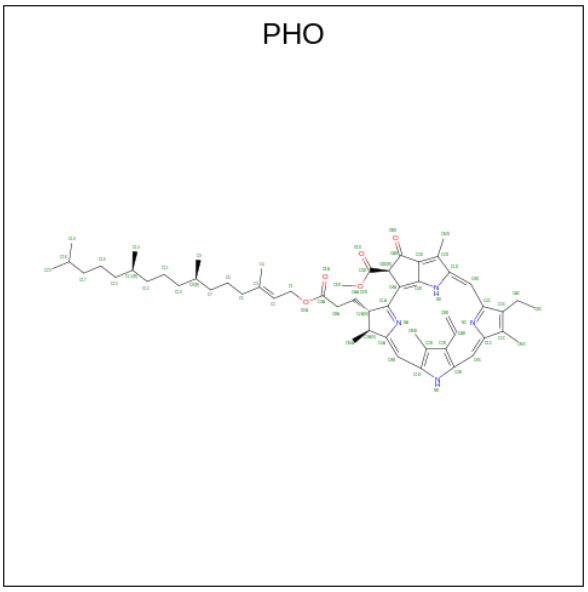
Mol	Chain	Residues	Atoms					AltConf
37	36	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	36	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
37	36	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	36	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
37	36	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	37	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	37	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
37	37	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
37	37	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	38	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	38	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	38	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	38	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
37	38	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	38	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
37	38	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	38	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	39	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	39	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	39	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	39	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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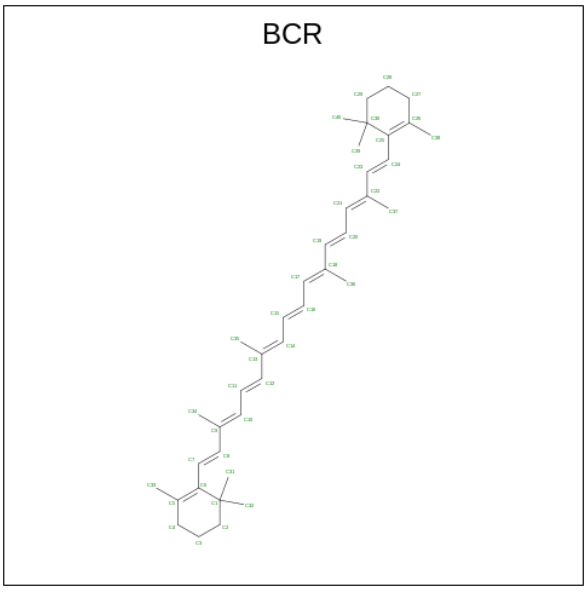
Mol	Chain	Residues	Atoms					AltConf
37	39	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
37	39	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	39	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	39	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	39	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	40	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
37	40	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
37	40	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
37	40	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	40	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
37	41	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
37	41	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
37	41	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	41	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	41	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	41	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	41	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 38 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



Mol	Chain	Residues	Atoms				AltConf
38	A	1	Total	C	N	O	0
			64	55	4	5	
38	D	1	Total	C	N	O	0
			64	55	4	5	
38	a	1	Total	C	N	O	0
			64	55	4	5	
38	a	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 39 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



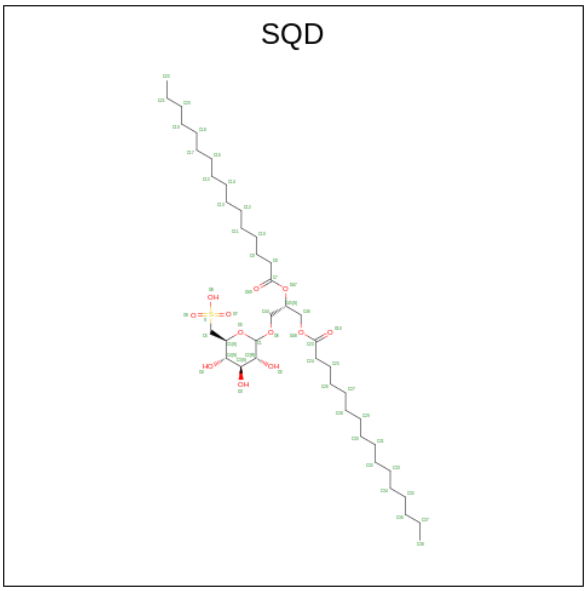
Mol	Chain	Residues	Atoms	AltConf
39	A	1	Total C 40 40	0
39	A	1	Total C 40 40	0
39	B	1	Total C 40 40	0
39	B	1	Total C 40 40	0
39	B	1	Total C 40 40	0
39	C	1	Total C 40 40	0
39	C	1	Total C 40 40	0
39	C	1	Total C 40 40	0
39	D	1	Total C 40 40	0
39	H	1	Total C 40 40	0
39	K	1	Total C 40 40	0
39	0	1	Total C 40 40	0
39	a	1	Total C 40 40	0
39	a	1	Total C 40 40	0
39	b	1	Total C 40 40	0
39	b	1	Total C 40 40	0
39	b	1	Total C 40 40	0
39	c	1	Total C 40 40	0
39	c	1	Total C 40 40	0
39	c	1	Total C 40 40	0
39	d	1	Total C 40 40	0
39	h	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
39	y	1	Total C 40 40	0
39	5	1	Total C 40 40	0

- Molecule 40 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



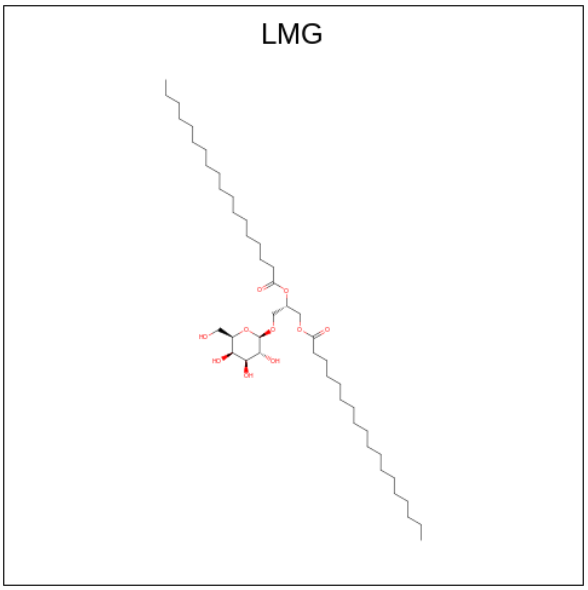
Mol	Chain	Residues	Atoms	AltConf
40	A	1	Total C O S 54 41 12 1	0
40	B	1	Total C O S 54 41 12 1	0
40	B	1	Total C O S 37 24 12 1	0
40	L	1	Total C O S 54 41 12 1	0
40	a	1	Total C O S 54 41 12 1	0
40	b	1	Total C O S 37 24 12 1	0
40	16	1	Total C O S 54 41 12 1	0
40	17	1	Total C O S 49 36 12 1	0
40	36	1	Total C O S 49 36 12 1	0

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Mol	Chain	Residues	Atoms				AltConf
40	40	1	Total	C	O	S	0
			54	41	12	1	

- Molecule 41 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



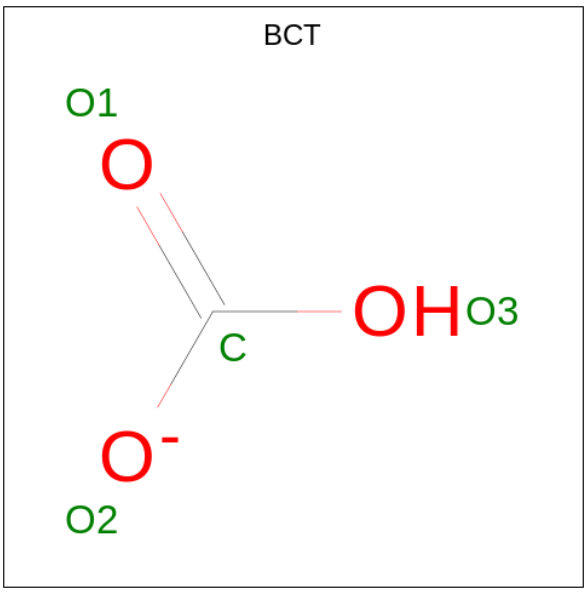
Mol	Chain	Residues	Atoms			AltConf
41	A	1	Total	C	O	0
			51	41	10	
41	B	1	Total	C	O	0
			51	41	10	
41	B	1	Total	C	O	0
			51	41	10	
41	C	1	Total	C	O	0
			51	41	10	
41	D	1	Total	C	O	0
			51	41	10	
41	L	1	Total	C	O	0
			40	30	10	
41	a	1	Total	C	O	0
			51	41	10	
41	b	1	Total	C	O	0
			51	41	10	
41	b	1	Total	C	O	0
			51	41	10	
41	c	1	Total	C	O	0
			51	41	10	

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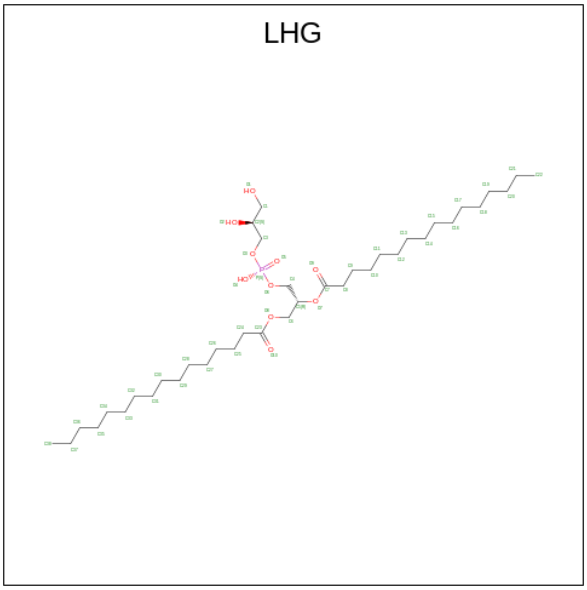
Mol	Chain	Residues	Atoms	AltConf
41	d	1	Total C O 51 41 10	0
41	l	1	Total C O 40 30 10	0
41	11	1	Total C O 42 32 10	0
41	11	1	Total C O 32 22 10	0
41	12	1	Total C O 39 29 10	0
41	16	1	Total C O 36 26 10	0
41	17	1	Total C O 37 27 10	0
41	31	1	Total C O 42 32 10	0
41	31	1	Total C O 32 22 10	0
41	32	1	Total C O 39 29 10	0
41	36	1	Total C O 36 26 10	0
41	37	1	Total C O 37 27 10	0

- Molecule 42 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms	AltConf
42	A	1	Total C O 4 1 3	0
42	a	1	Total C O 4 1 3	0

- Molecule 43 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



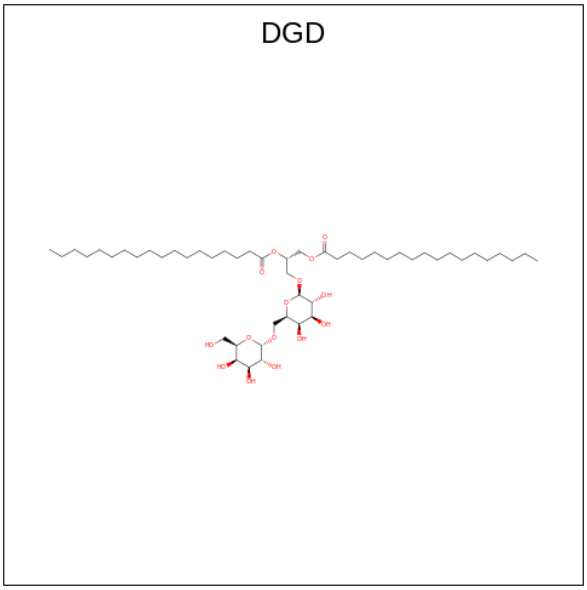
Mol	Chain	Residues	Atoms	AltConf
43	B	1	Total C O P 49 38 10 1	0
43	D	1	Total C O P 49 38 10 1	0
43	D	1	Total C O P 49 38 10 1	0
43	D	1	Total C O P 46 35 10 1	0
43	a	1	Total C O P 46 35 10 1	0
43	b	1	Total C O P 49 38 10 1	0
43	d	1	Total C O P 49 38 10 1	0
43	d	1	Total C O P 49 38 10 1	0
43	17	1	Total C O P 44 33 10 1	0

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Mol	Chain	Residues	Atoms				AltConf
43	19	1	Total	C	O	P	0
			49	38	10	1	
43	21	1	Total	C	O	P	0
			35	25	9	1	
43	21	1	Total	C	O	P	0
			45	34	10	1	
43	37	1	Total	C	O	P	0
			44	33	10	1	
43	37	1	Total	C	O	P	0
			45	34	10	1	
43	39	1	Total	C	O	P	0
			49	38	10	1	
43	41	1	Total	C	O	P	0
			35	25	9	1	

- Molecule 44 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



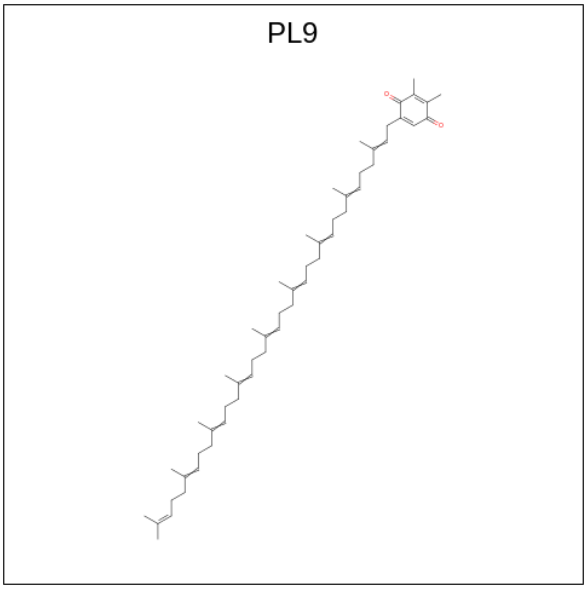
Mol	Chain	Residues	Atoms			AltConf
44	C	1	Total	C	O	0
			62	47	15	
44	C	1	Total	C	O	0
			62	47	15	
44	H	1	Total	C	O	0
			62	47	15	
44	J	1	Total	C	O	0
			62	47	15	

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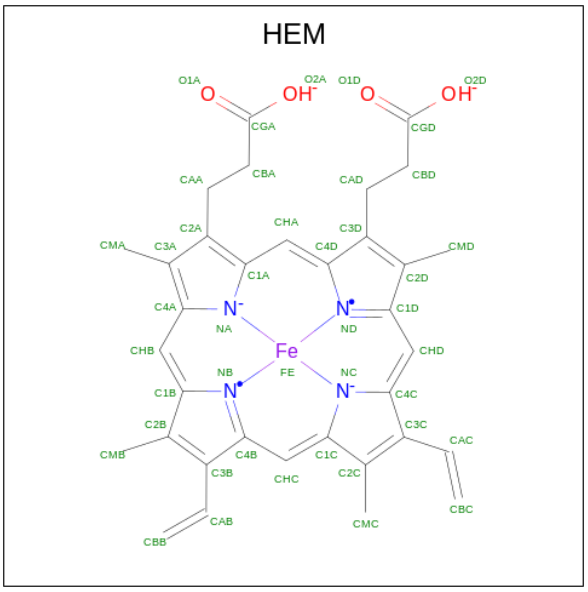
Mol	Chain	Residues	Atoms	AltConf
44	c	1	Total C O 62 47 15	0
44	c	1	Total C O 62 47 15	0
44	h	1	Total C O 62 47 15	0
44	j	1	Total C O 62 47 15	0

- Molecule 45 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$).



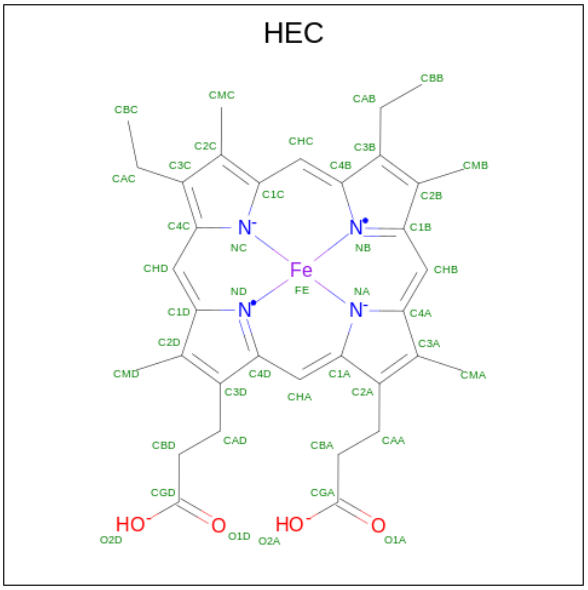
Mol	Chain	Residues	Atoms	AltConf
45	D	1	Total C O 55 53 2	0
45	D	1	Total C O 55 53 2	0
45	d	1	Total C O 55 53 2	0
45	d	1	Total C O 55 53 2	0

- Molecule 46 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



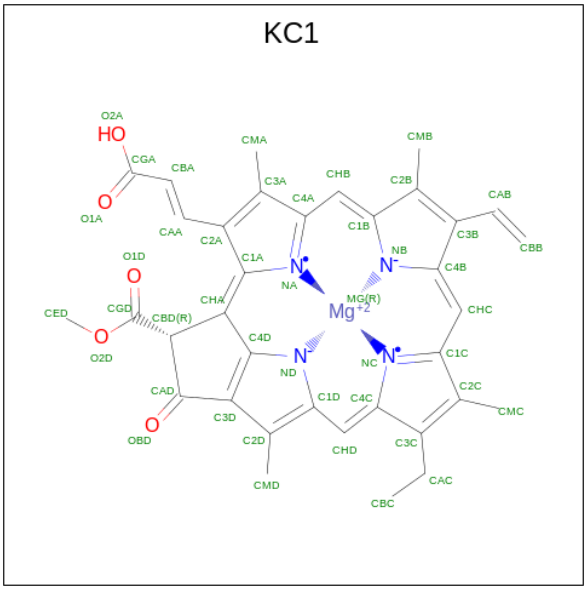
Mol	Chain	Residues	Atoms					AltConf
46	F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
46	f	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 47 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
47	V	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
47	v	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 48 is Chlorophyll c1 (CCD ID: KC1) (formula: $C_{35}H_{30}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
48	11	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
48	11	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
48	11	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
48	11	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
48	12	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
48	12	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
48	12	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
48	13	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
48	13	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
48	13	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
48	13	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
48	14	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
48	14	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
48	14	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
48	15	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
48	15	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
48	15	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
48	15	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
48	16	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
48	16	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
48	16	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
48	16	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
48	17	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
48	17	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
48	17	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
48	17	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
48	18	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
48	18	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
48	18	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
48	19	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
48	20	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
48	20	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
48	20	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
48	21	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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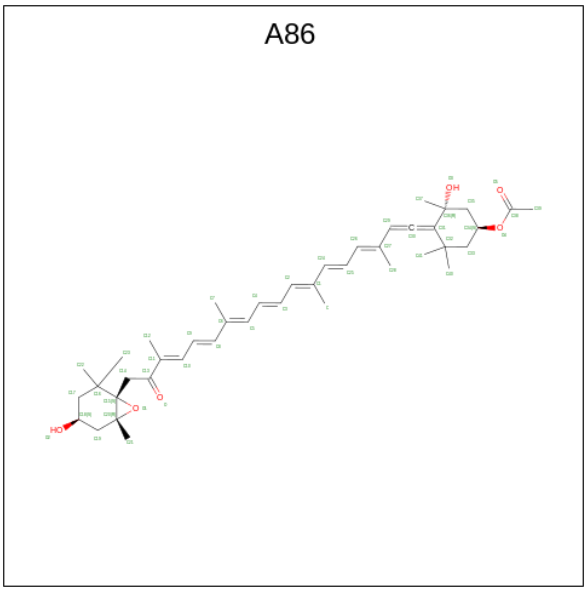
Mol	Chain	Residues	Atoms					AltConf
48	21	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
48	31	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
48	31	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
48	31	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
48	31	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
48	32	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
48	32	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
48	32	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
48	33	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
48	33	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
48	33	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
48	33	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
48	34	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
48	34	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
48	34	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
48	35	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
48	35	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
48	35	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
48	35	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
48	36	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
48	36	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
48	36	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
48	36	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
48	37	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
48	37	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
48	37	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
48	37	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
48	38	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
48	38	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
48	38	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
48	39	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
48	40	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
48	40	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
48	40	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
48	41	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
48	41	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 49 is (3S,3'S,5R,5'R,6S,6'R,8'R)-3,5'-dihydroxy-8-oxo-6',7'-didehydro-5,5',6,6',7,8-hexahydro-5,6-epoxy-beta,beta-caroten-3'- yl acetate (CCD ID: A86) (formula: $C_{42}H_{58}O_6$).



Mol	Chain	Residues	Atoms	AltConf
49	11	1	Total C O 48 42 6	0
49	11	1	Total C O 48 42 6	0
49	11	1	Total C O 48 42 6	0
49	11	1	Total C O 48 42 6	0
49	11	1	Total C O 48 42 6	0
49	11	1	Total C O 48 42 6	0
49	12	1	Total C O 48 42 6	0
49	12	1	Total C O 48 42 6	0
49	12	1	Total C O 48 42 6	0
49	12	1	Total C O 48 42 6	0
49	12	1	Total C O 48 42 6	0
49	12	1	Total C O 48 42 6	0
49	12	1	Total C O 48 42 6	0
49	13	1	Total C O 48 42 6	0

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Mol	Chain	Residues	Atoms	AltConf
49	13	1	Total C O 48 42 6	0
49	13	1	Total C O 48 42 6	0
49	13	1	Total C O 48 42 6	0
49	13	1	Total C O 48 42 6	0
49	14	1	Total C O 48 42 6	0
49	14	1	Total C O 48 42 6	0
49	14	1	Total C O 48 42 6	0
49	14	1	Total C O 48 42 6	0
49	14	1	Total C O 48 42 6	0
49	14	1	Total C O 48 42 6	0
49	15	1	Total C O 48 42 6	0
49	15	1	Total C O 48 42 6	0
49	15	1	Total C O 48 42 6	0
49	15	1	Total C O 48 42 6	0
49	15	1	Total C O 48 42 6	0
49	15	1	Total C O 48 42 6	0
49	16	1	Total C O 48 42 6	0
49	16	1	Total C O 48 42 6	0
49	16	1	Total C O 48 42 6	0
49	16	1	Total C O 48 42 6	0

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Mol	Chain	Residues	Atoms	AltConf
49	17	1	Total C O 48 42 6	0
49	17	1	Total C O 48 42 6	0
49	17	1	Total C O 48 42 6	0
49	17	1	Total C O 48 42 6	0
49	17	1	Total C O 48 42 6	0
49	17	1	Total C O 48 42 6	0
49	17	1	Total C O 48 42 6	0
49	18	1	Total C O 48 42 6	0
49	18	1	Total C O 48 42 6	0
49	18	1	Total C O 48 42 6	0
49	18	1	Total C O 48 42 6	0
49	19	1	Total C O 48 42 6	0
49	19	1	Total C O 48 42 6	0
49	20	1	Total C O 48 42 6	0
49	20	1	Total C O 48 42 6	0
49	21	1	Total C O 48 42 6	0
49	21	1	Total C O 48 42 6	0
49	21	1	Total C O 48 42 6	0
49	21	1	Total C O 48 42 6	0
49	31	1	Total C O 48 42 6	0
49	31	1	Total C O 48 42 6	0

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Mol	Chain	Residues	Atoms	AltConf
49	31	1	Total C O 48 42 6	0
49	31	1	Total C O 48 42 6	0
49	31	1	Total C O 48 42 6	0
49	31	1	Total C O 48 42 6	0
49	32	1	Total C O 48 42 6	0
49	32	1	Total C O 48 42 6	0
49	32	1	Total C O 48 42 6	0
49	32	1	Total C O 48 42 6	0
49	32	1	Total C O 48 42 6	0
49	32	1	Total C O 48 42 6	0
49	32	1	Total C O 48 42 6	0
49	33	1	Total C O 48 42 6	0
49	33	1	Total C O 48 42 6	0
49	33	1	Total C O 48 42 6	0
49	33	1	Total C O 48 42 6	0
49	33	1	Total C O 48 42 6	0
49	34	1	Total C O 48 42 6	0
49	34	1	Total C O 48 42 6	0
49	34	1	Total C O 48 42 6	0
49	34	1	Total C O 48 42 6	0
49	34	1	Total C O 48 42 6	0

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Mol	Chain	Residues	Atoms	AltConf
49	34	1	Total C O 48 42 6	0
49	35	1	Total C O 48 42 6	0
49	35	1	Total C O 48 42 6	0
49	35	1	Total C O 48 42 6	0
49	35	1	Total C O 48 42 6	0
49	35	1	Total C O 48 42 6	0
49	35	1	Total C O 48 42 6	0
49	35	1	Total C O 48 42 6	0
49	36	1	Total C O 48 42 6	0
49	36	1	Total C O 48 42 6	0
49	36	1	Total C O 48 42 6	0
49	37	1	Total C O 48 42 6	0
49	37	1	Total C O 48 42 6	0
49	37	1	Total C O 48 42 6	0
49	37	1	Total C O 48 42 6	0
49	37	1	Total C O 48 42 6	0
49	37	1	Total C O 48 42 6	0
49	37	1	Total C O 48 42 6	0
49	38	1	Total C O 48 42 6	0
49	38	1	Total C O 48 42 6	0
49	38	1	Total C O 48 42 6	0

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Mol	Chain	Residues	Atoms	AltConf
49	38	1	Total C O 48 42 6	0
49	39	1	Total C O 48 42 6	0
49	39	1	Total C O 48 42 6	0
49	40	1	Total C O 48 42 6	0
49	40	1	Total C O 48 42 6	0
49	40	1	Total C O 48 42 6	0
49	41	1	Total C O 48 42 6	0
49	41	1	Total C O 48 42 6	0
49	41	1	Total C O 48 42 6	0
49	41	1	Total C O 48 42 6	0

- Molecule 50 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

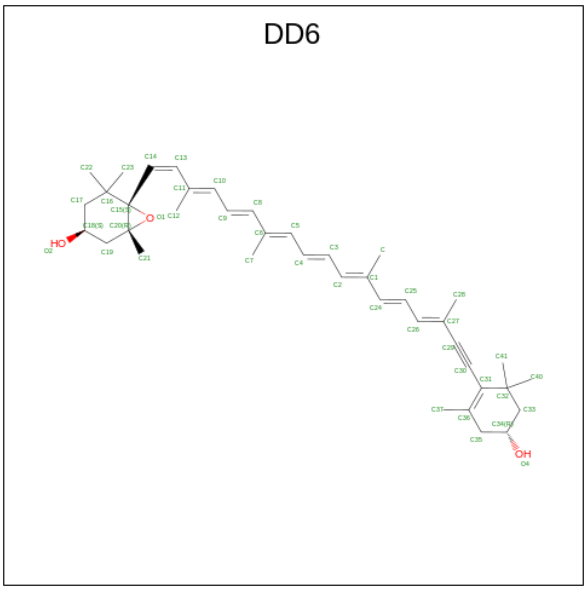
Mol	Chain	Residues	Atoms	AltConf
50	11	1	Total C O 19 17 2	0
50	12	2	Total C O 34 32 2	0
50	13	3	Total C O 49 47 2	0
50	14	1	Total C 16 16	0
50	15	2	Total C 28 28	0
50	16	2	Total C 24 24	0
50	17	3	Total C O 54 48 6	0
50	18	4	Total C 58 58	0
50	19	1	Total C 12 12	0

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Mol	Chain	Residues	Atoms	AltConf
50	31	1	Total C O 19 17 2	0
50	32	2	Total C O 34 32 2	0
50	33	3	Total C O 49 47 2	0
50	34	1	Total C 16 16	0
50	35	2	Total C 28 28	0
50	36	2	Total C 24 24	0
50	37	3	Total C O 54 48 6	0
50	38	4	Total C 58 58	0
50	39	1	Total C 12 12	0

- Molecule 51 is (3S,3'R,5R,6S,7cis)-7',8'-didehydro-5,6-dihydro-5,6-epoxy-beta,beta-carotene -3,3'-diol (CCD ID: DD6) (formula: $C_{40}H_{54}O_3$).



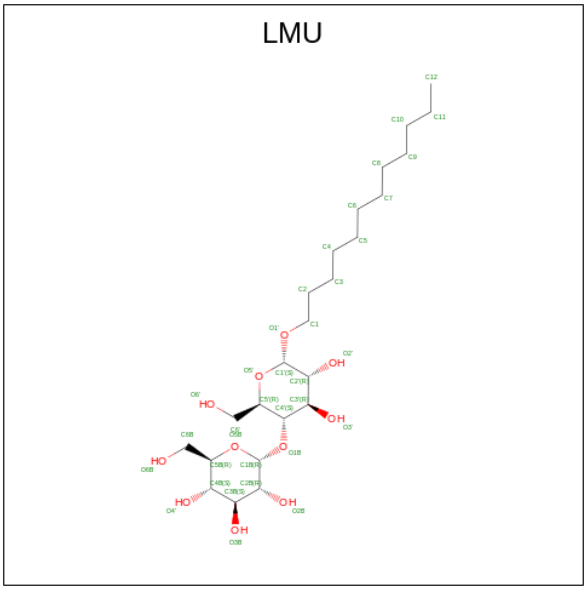
Mol	Chain	Residues	Atoms	AltConf
51	16	1	Total C O 43 40 3	0
51	19	1	Total C O 43 40 3	0

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Mol	Chain	Residues	Atoms	AltConf
51	20	1	Total C O 43 40 3	0
51	20	1	Total C O 43 40 3	0
51	21	1	Total C O 43 40 3	0
51	21	1	Total C O 43 40 3	0
51	36	1	Total C O 43 40 3	0
51	39	1	Total C O 43 40 3	0
51	40	1	Total C O 43 40 3	0
51	40	1	Total C O 43 40 3	0
51	41	1	Total C O 43 40 3	0
51	41	1	Total C O 43 40 3	0

- Molecule 52 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms	AltConf
52	19	1	Total C O 35 24 11	0

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Mol	Chain	Residues	Atoms	AltConf
52	39	1	Total C O 35 24 11	0

- Molecule 53 is water.

Mol	Chain	Residues	Atoms	AltConf
53	B	5	Total O 5 5	0
53	C	3	Total O 3 3	0
53	D	4	Total O 4 4	0
53	Z	1	Total O 1 1	0
53	a	2	Total O 2 2	0
53	b	5	Total O 5 5	0
53	c	3	Total O 3 3	0
53	d	2	Total O 2 2	0
53	z	1	Total O 1 1	0
53	11	3	Total O 3 3	0
53	12	2	Total O 2 2	0
53	13	1	Total O 1 1	0
53	14	1	Total O 1 1	0
53	15	1	Total O 1 1	0
53	16	1	Total O 1 1	0
53	17	2	Total O 2 2	0
53	18	1	Total O 1 1	0
53	19	1	Total O 1 1	0

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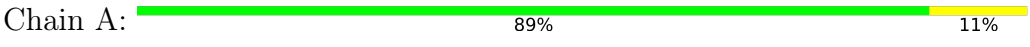
Mol	Chain	Residues	Atoms	AltConf
53	31	3	Total O 3 3	0
53	32	2	Total O 2 2	0
53	33	1	Total O 1 1	0
53	34	1	Total O 1 1	0
53	35	1	Total O 1 1	0
53	36	1	Total O 1 1	0
53	37	2	Total O 2 2	0
53	38	1	Total O 1 1	0
53	39	1	Total O 1 1	0

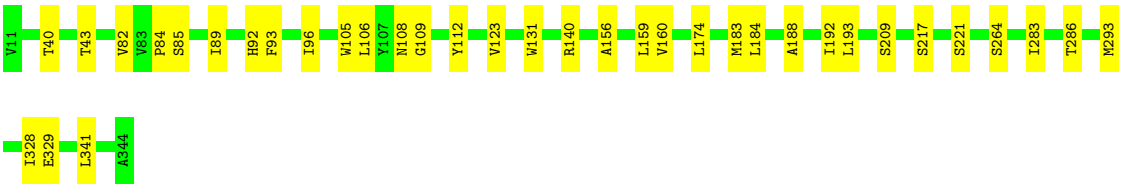
3 Residue-property plots (i)

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: Photosystem II protein D1

Chain A:

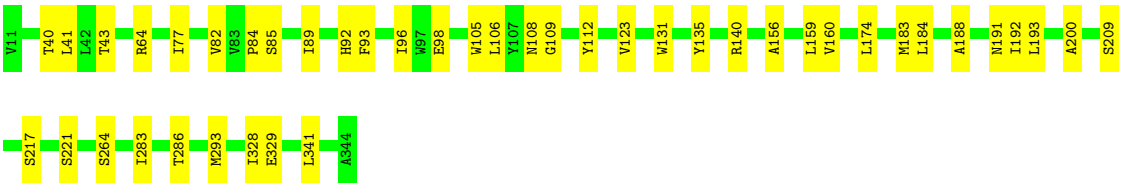




• Molecule 1: Photosystem II protein D1

Chain a:

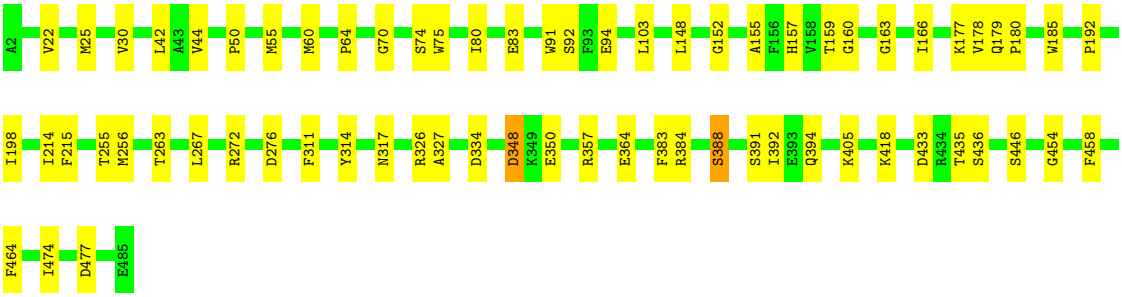




• Molecule 2: Photosystem II CP47 reaction center protein

Chain B:

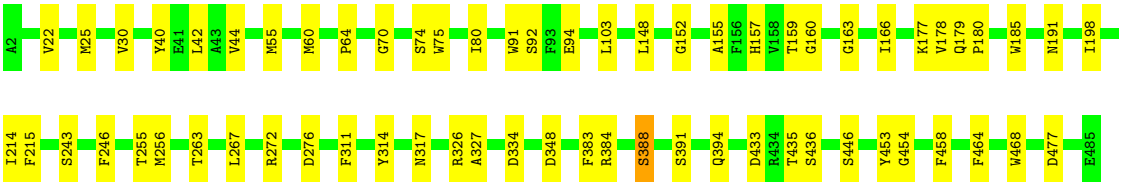




• Molecule 2: Photosystem II CP47 reaction center protein

Chain b:

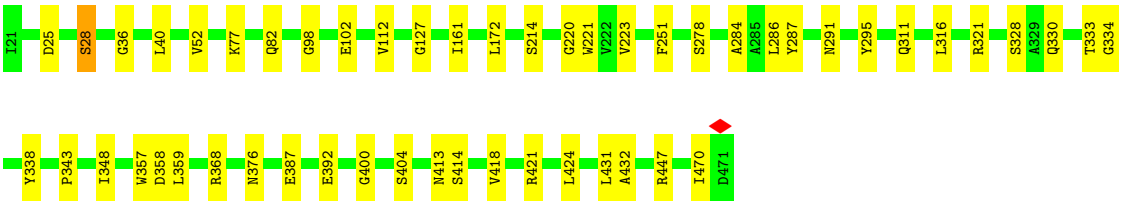




• Molecule 3: Photosystem II CP43 reaction center protein

Chain C:

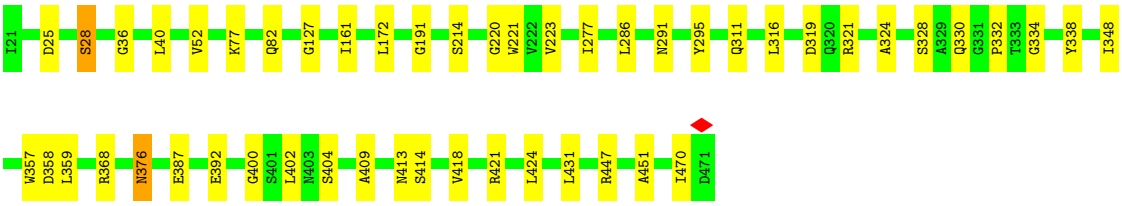




• Molecule 3: Photosystem II CP43 reaction center protein

Chain c:

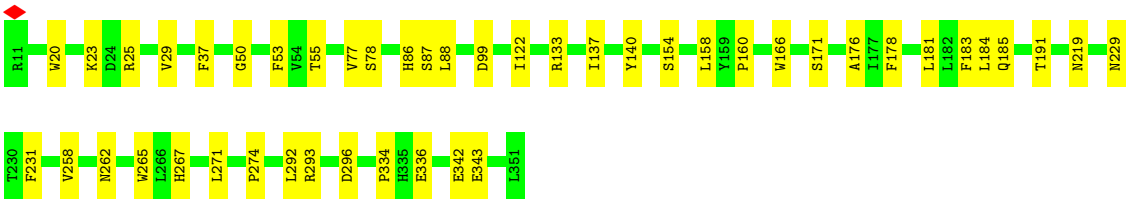




• Molecule 4: Photosystem II D2 protein

Chain D:

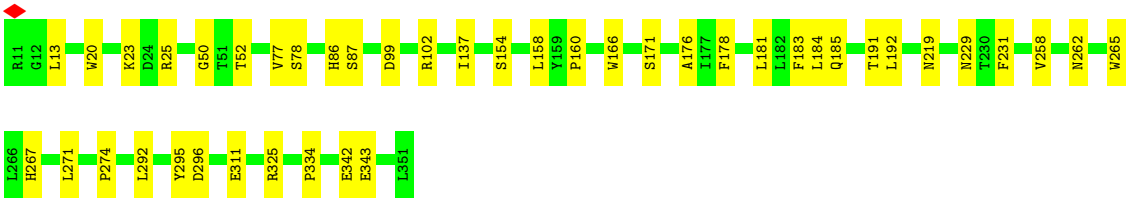




• Molecule 4: Photosystem II D2 protein

Chain d:

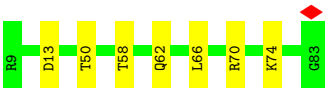




• Molecule 5: Cytochrome b559 subunit alpha

Chain E:

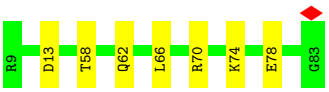




• Molecule 5: Cytochrome b559 subunit alpha

Chain e:





• Molecule 6: Cytochrome b559 subunit beta

Chain F:

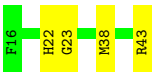




• Molecule 6: Cytochrome b559 subunit beta

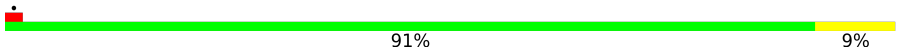
Chain f:

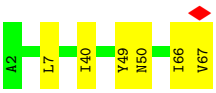




• Molecule 7: Photosystem II reaction center protein H

Chain H:

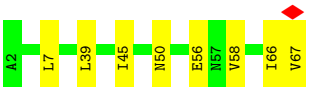




• Molecule 7: Photosystem II reaction center protein H

Chain h:

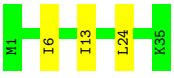




• Molecule 8: Photosystem II reaction center protein I

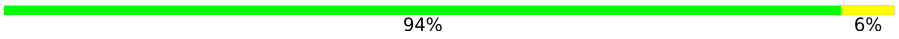
Chain I:





• Molecule 8: Photosystem II reaction center protein I

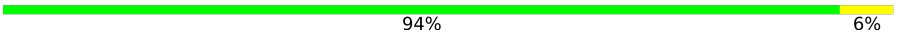
Chain i:





• Molecule 9: Photosystem II reaction center protein J

Chain J:

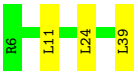




• Molecule 9: Photosystem II reaction center protein J

Chain j:

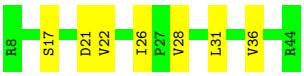




• Molecule 10: Photosystem II reaction center protein K

Chain K:

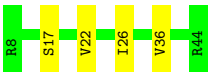




• Molecule 10: Photosystem II reaction center protein K

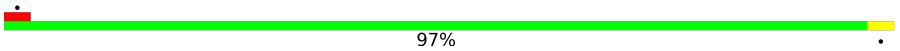
Chain k:

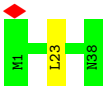




• Molecule 11: Photosystem II reaction center protein L

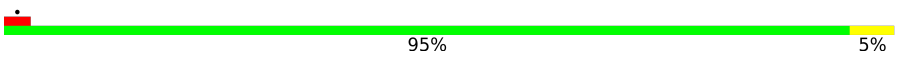
Chain L:

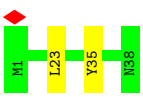




• Molecule 11: Photosystem II reaction center protein L

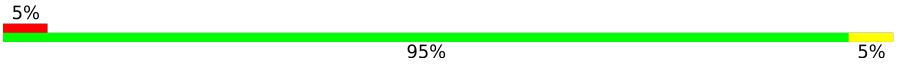
Chain l:

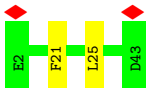




• Molecule 12: Photosystem II subunit

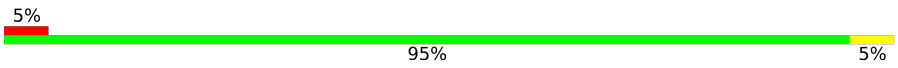
Chain M:





• Molecule 12: Photosystem II subunit

Chain m:

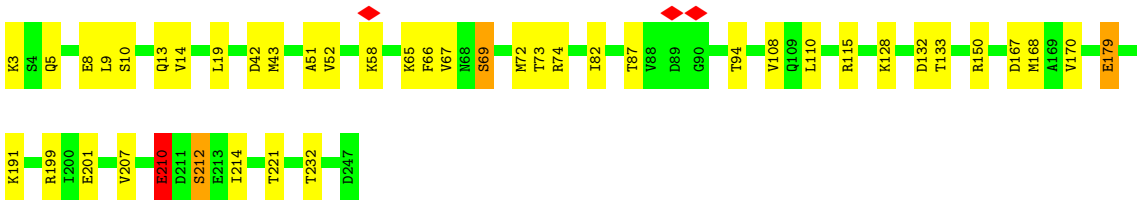




• Molecule 13: Extrinsic protein in photosystem II

Chain O:

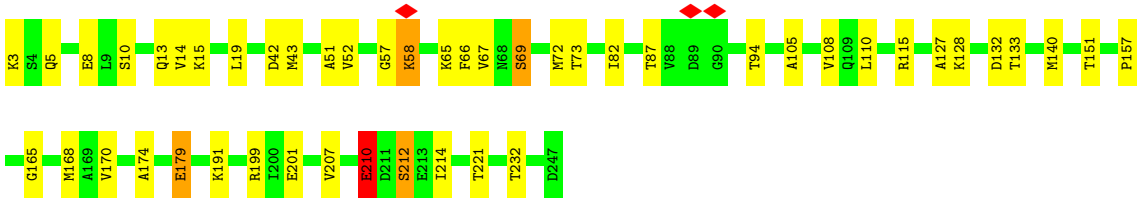




• Molecule 13: Extrinsic protein in photosystem II

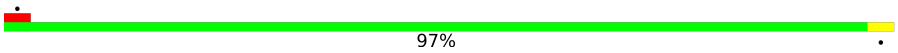
Chain o:

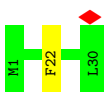




• Molecule 14: Photosystem II reaction center protein T

Chain T:

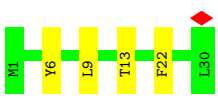




• Molecule 14: Photosystem II reaction center protein T

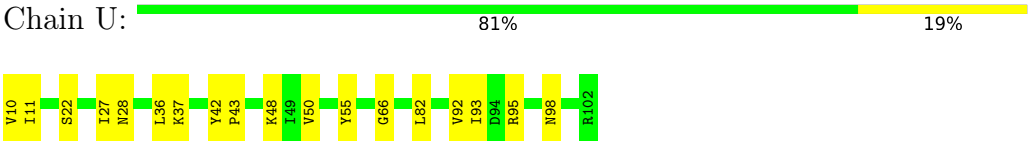
Chain t:





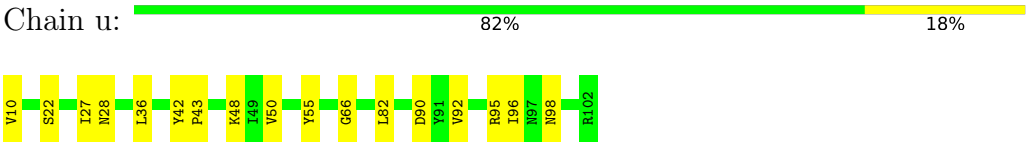
• Molecule 15: Extrinsic protein in photosystem II

Chain U:



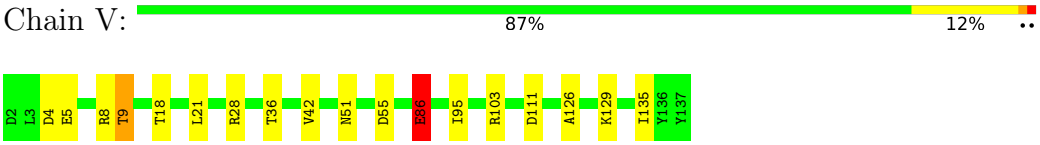
• Molecule 15: Extrinsic protein in photosystem II

Chain u:



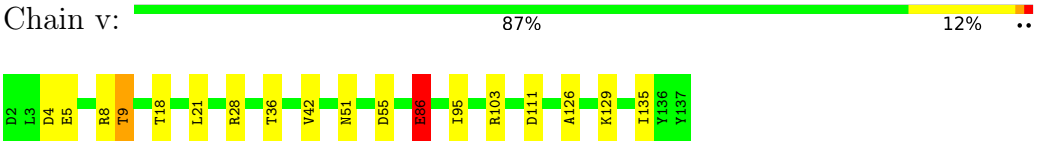
• Molecule 16: Cytochrome c-550

Chain V:



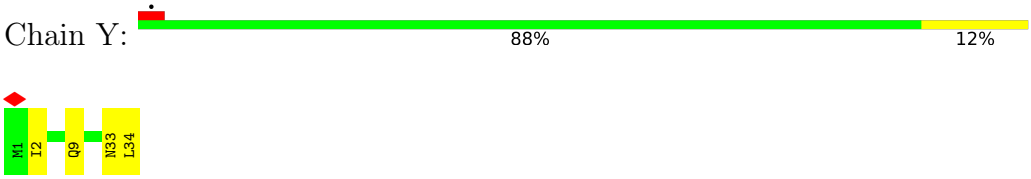
• Molecule 16: Cytochrome c-550

Chain v:



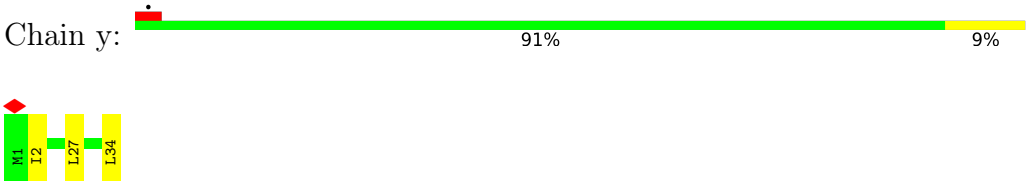
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y:



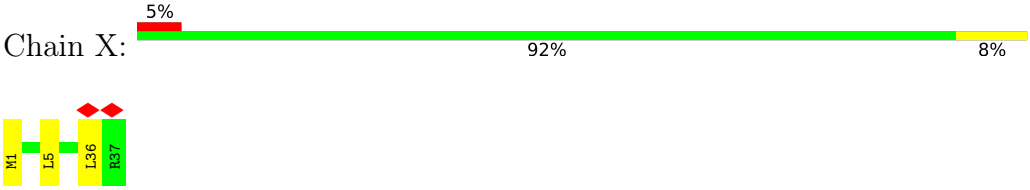
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain y:



• Molecule 18: Photosystem II reaction center X protein

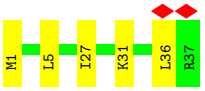
Chain X:



• Molecule 18: Photosystem II reaction center X protein

Chain x:

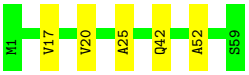




• Molecule 19: Photosystem II reaction center protein Z

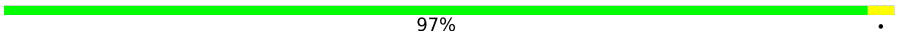
Chain Z:





• Molecule 19: Photosystem II reaction center protein Z

Chain z:





• Molecule 20: Extrinsic protein in photosystem II

Chain Q:





• Molecule 20: Extrinsic protein in photosystem II

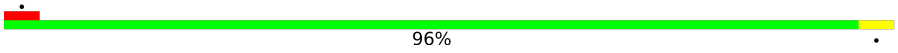
Chain q:

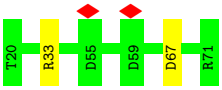




• Molecule 21: Photosystem II reaction center protein W

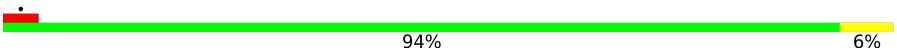
Chain W:

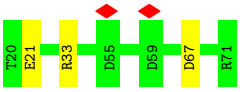




• Molecule 21: Photosystem II reaction center protein W

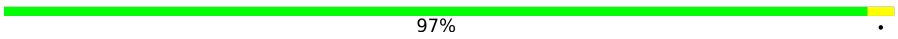
Chain w:





• Molecule 22: Unknown protein 0

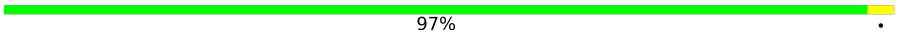
Chain 0:





• Molecule 22: Unknown protein 0

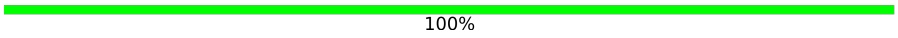
Chain 5:





• Molecule 23: Unknown protein 1

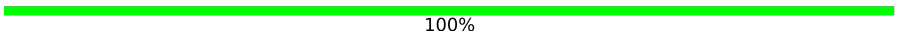
Chain 1:



There are no outlier residues recorded for this chain.

• Molecule 23: Unknown protein 1

Chain 6:



There are no outlier residues recorded for this chain.

• Molecule 24: Chlorophyll a/b-binding protein

Chain 11:

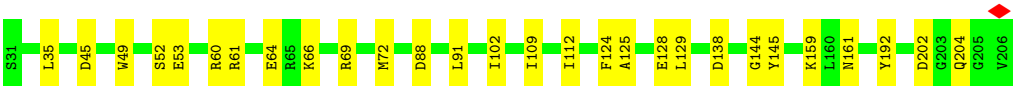




• Molecule 24: Chlorophyll a/b-binding protein

Chain 31:

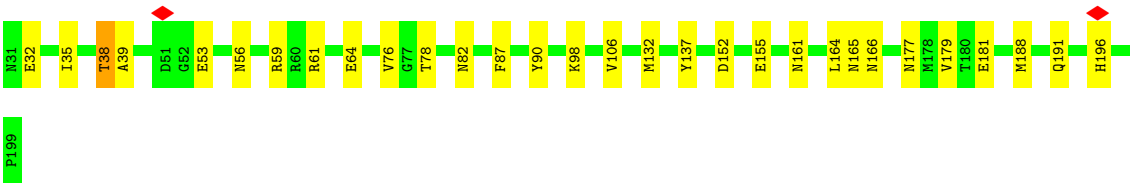




• Molecule 25: Fcpb2, Fucoxanthin chlorophyll a/c-binding protein

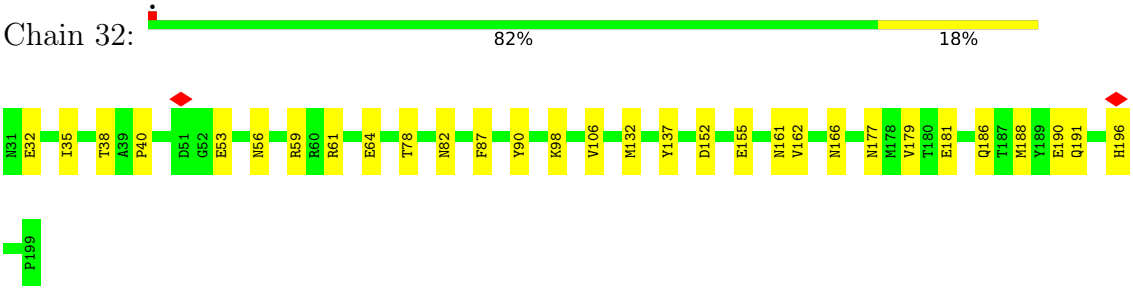
Chain 12:





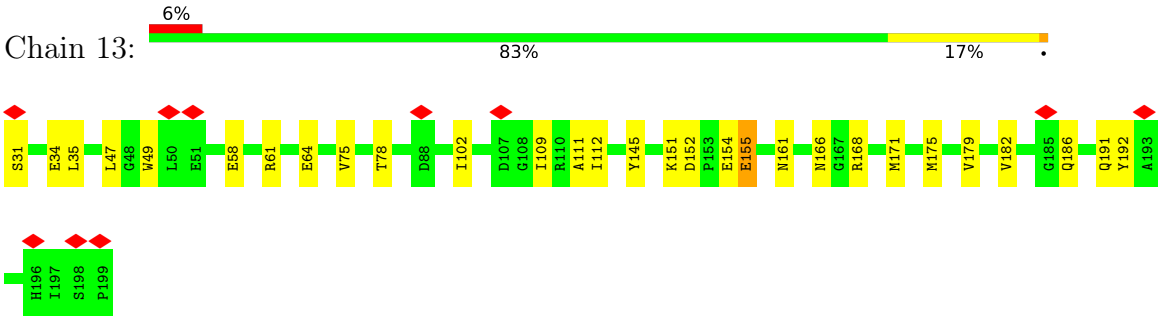
• Molecule 25: Fcpb2, Fucoxanthin chlorophyll a/c-binding protein

Chain 32:



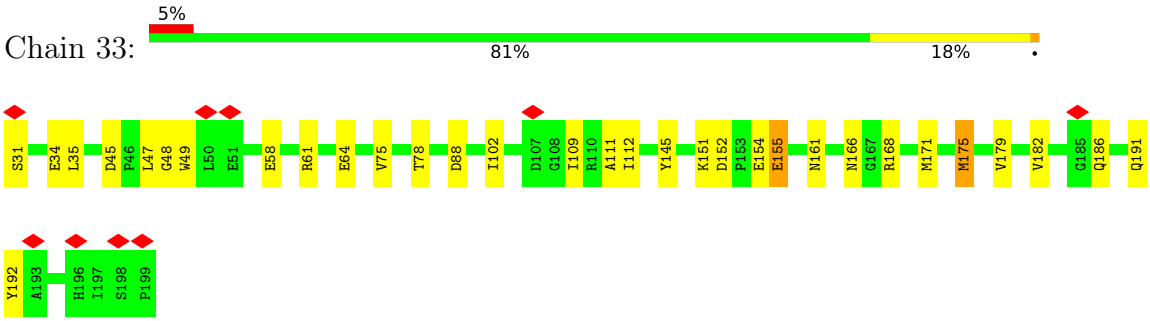
• Molecule 26: Chlorophyll a/b-binding protein

Chain 13:



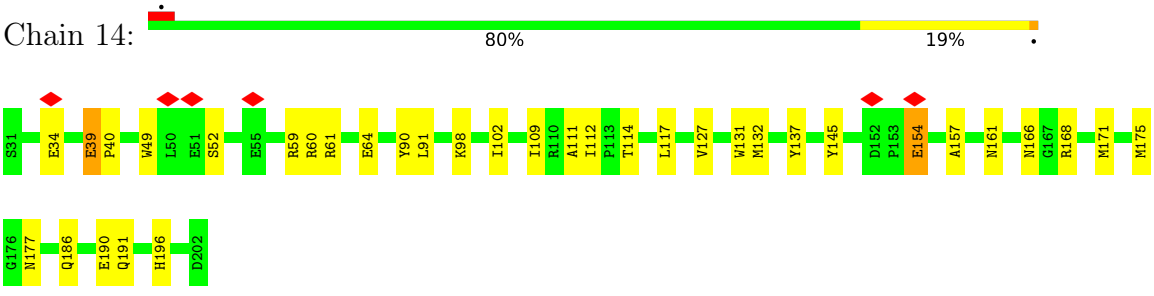
• Molecule 26: Chlorophyll a/b-binding protein

Chain 33:



• Molecule 27: Chlorophyll a/b-binding protein

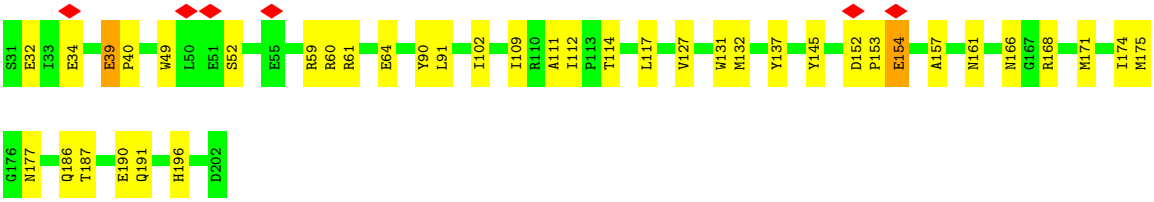
Chain 14:



• Molecule 27: Chlorophyll a/b-binding protein

Chain 34:

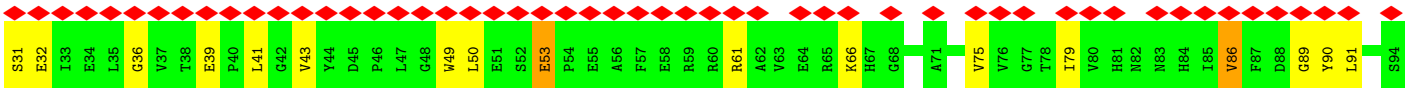




• Molecule 28: Chlorophyll a/b-binding protein

Chain 15:

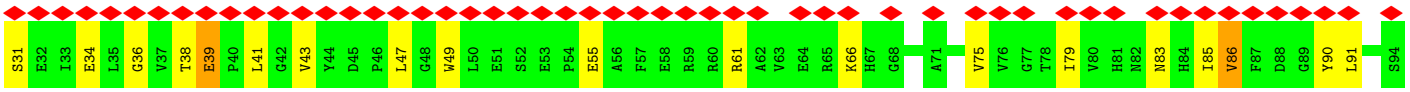




• Molecule 28: Chlorophyll a/b-binding protein

Chain 35:

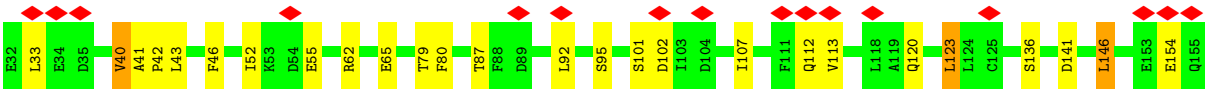




• Molecule 29: Fcpb3, Fucoxanthin chlorophyll a/c-binding protein

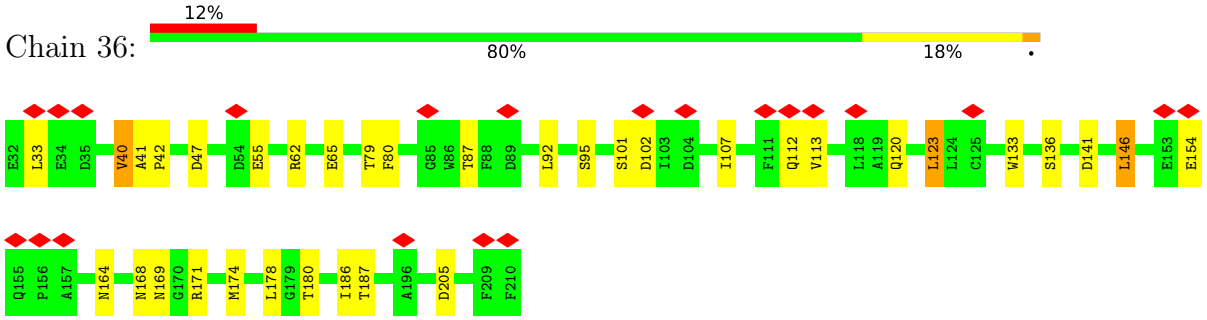
Chain 16:





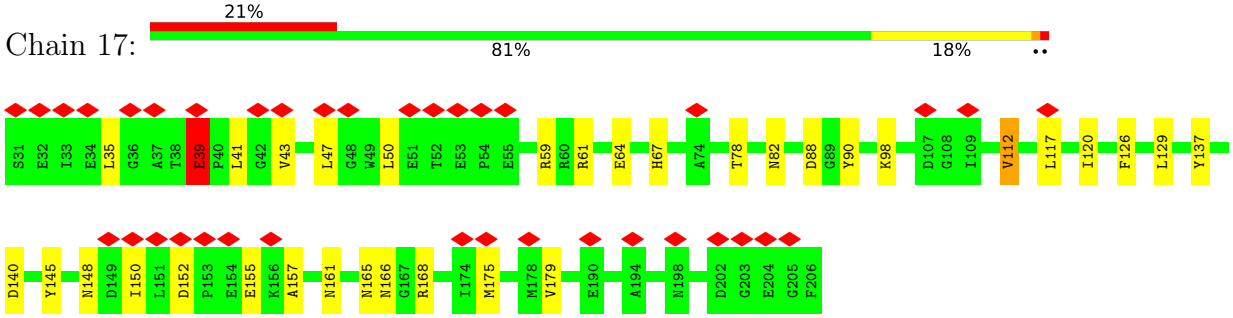
• Molecule 29: Fcpb3, Fucoxanthin chlorophyll a/c-binding protein

Chain 36:



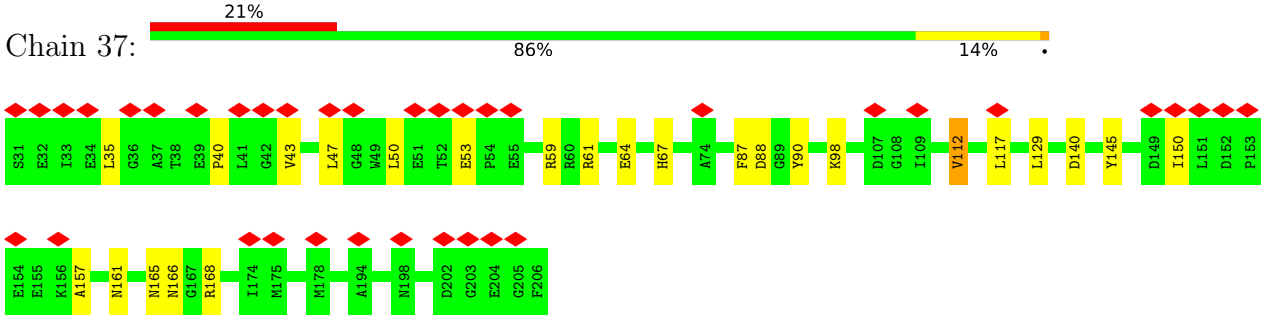
• Molecule 30: Fcpb4, Fucoxanthin chlorophyll a/c-binding protein

Chain 17:



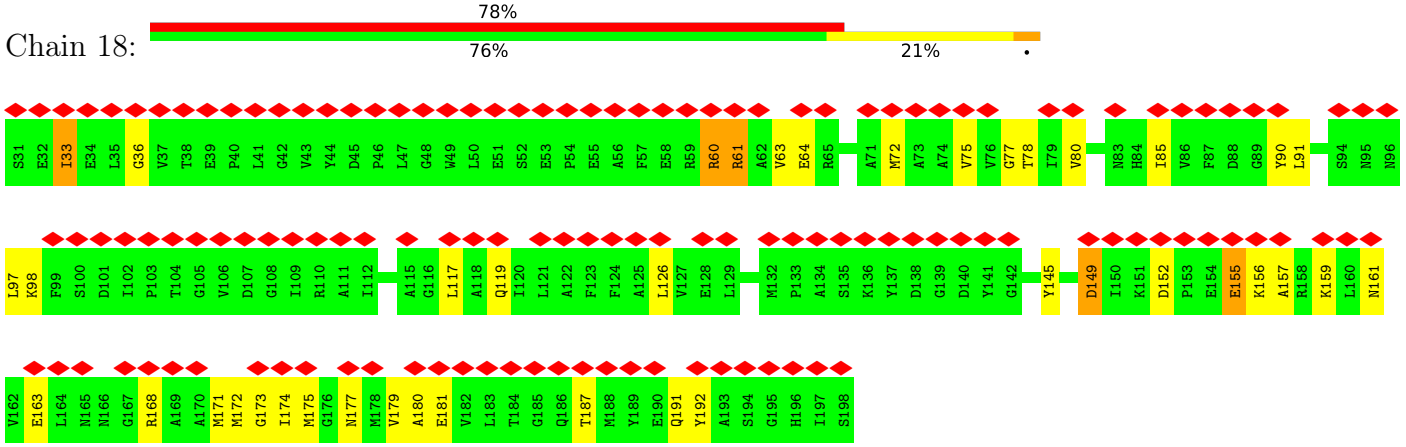
• Molecule 30: Fcpb4, Fucoxanthin chlorophyll a/c-binding protein

Chain 37:



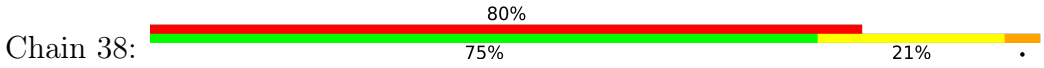
• Molecule 31: Chlorophyll a/b-binding protein

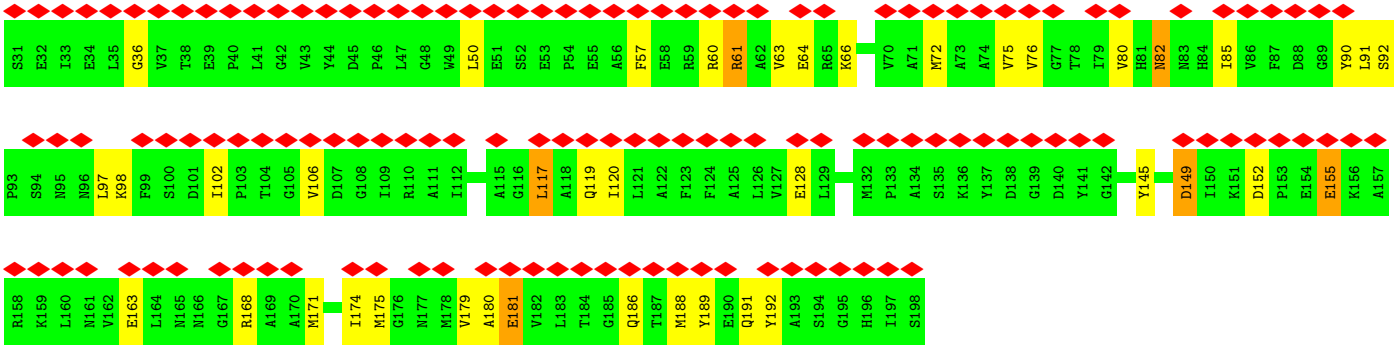
Chain 18:



• Molecule 31: Chlorophyll a/b-binding protein

Chain 38:

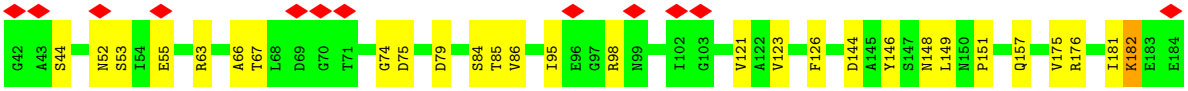




• Molecule 32: Fcpb5, Fucoxanthin chlorophyll a/c-binding protein

Chain 19:

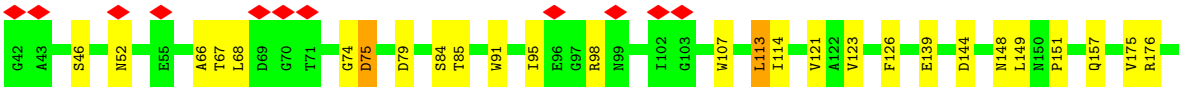




• Molecule 32: Fcpb5, Fucoxanthin chlorophyll a/c-binding protein

Chain 39:

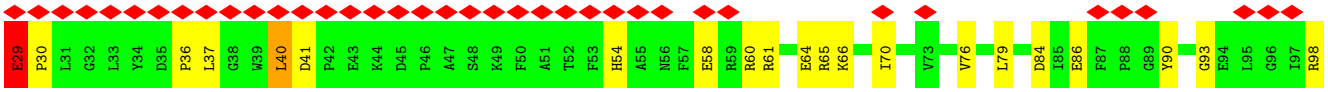




• Molecule 33: Fcpb6, Fucoxanthin chlorophyll a/c-binding protein

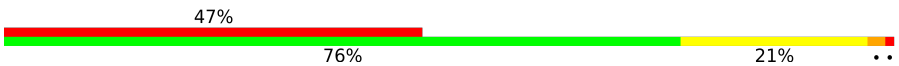
Chain 20:

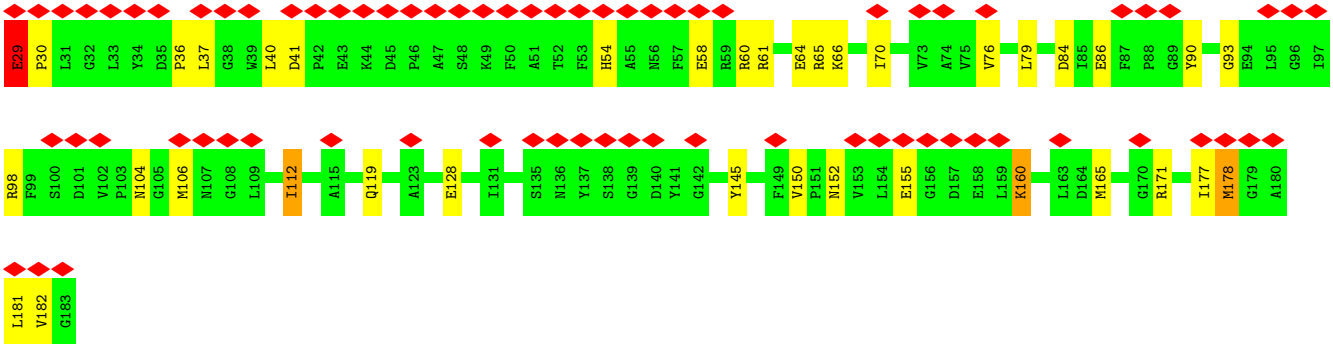




• Molecule 33: Fcpb6, Fucoxanthin chlorophyll a/c-binding protein

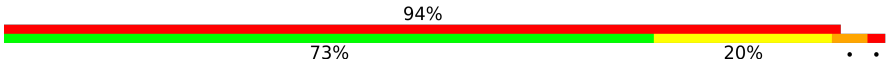
Chain 40:

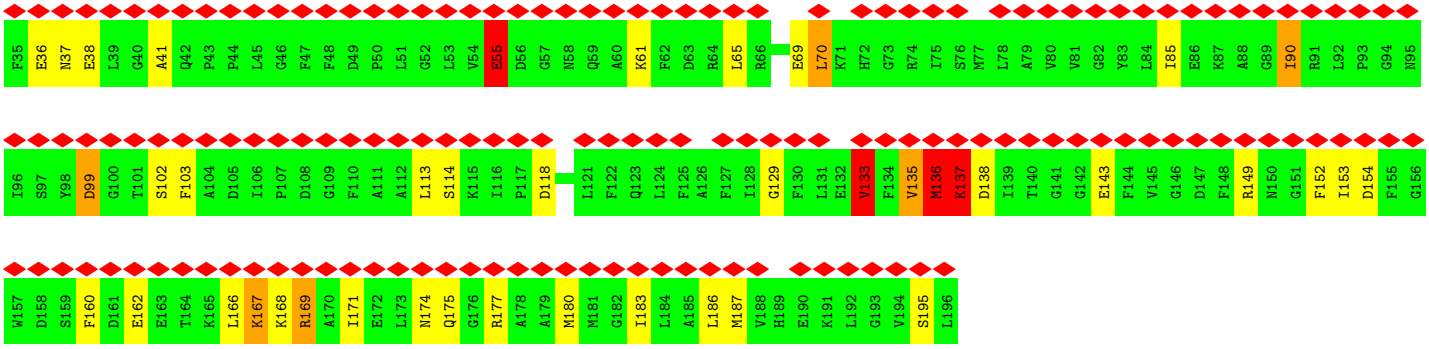




• Molecule 34: Fcpb7, Fucoxanthin chlorophyll a/c-binding protein

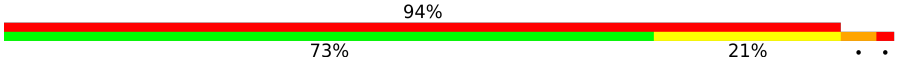
Chain 21:

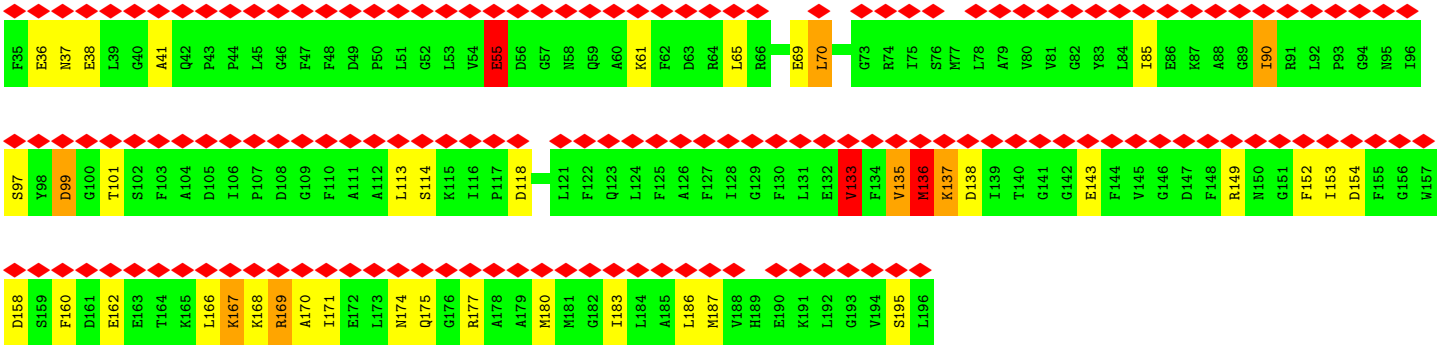




• Molecule 34: Fcpb7, Fucoxanthin chlorophyll a/c-binding protein

Chain 41:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	210825	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 ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.369	Depositor
Minimum map value	-0.142	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.045	Depositor
Map size (Å)	569.856, 569.856, 569.856	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.113, 1.113, 1.113	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LMG, BCT, PL9, PHO, LHG, KC1, CLA, A86, HEC, SQD, LMU, OEX, DGD, HEM, UNL, FE2, BCR, DD6

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	A	0.39	0/2702	0.49	0/3682
1	a	0.39	0/2702	0.49	0/3682
2	B	0.39	0/3942	0.47	0/5362
2	b	0.39	0/3942	0.47	0/5362
3	C	0.40	0/3620	0.50	0/4933
3	c	0.40	0/3620	0.50	0/4933
4	D	0.40	0/2789	0.48	0/3803
4	d	0.40	0/2789	0.48	0/3803
5	E	0.30	0/634	0.46	0/864
5	e	0.30	0/634	0.46	0/864
6	F	0.36	0/235	0.53	0/316
6	f	0.36	0/235	0.53	0/316
7	H	0.36	0/523	0.54	0/714
7	h	0.36	0/523	0.54	0/714
8	I	0.38	0/294	0.64	0/397
8	i	0.38	0/294	0.64	0/397
9	J	0.26	0/260	0.40	0/351
9	j	0.26	0/260	0.40	0/351
10	K	0.38	0/313	0.62	0/429
10	k	0.38	0/313	0.62	0/429
11	L	0.39	0/319	0.45	0/433
11	l	0.39	0/319	0.45	0/433
12	M	0.36	0/321	0.56	0/433
12	m	0.36	0/321	0.55	0/433
13	O	0.32	0/1875	0.56	2/2528 (0.1%)
13	o	0.32	0/1875	0.56	2/2528 (0.1%)
14	T	0.31	0/256	0.41	0/346
14	t	0.31	0/256	0.41	0/346
15	U	0.29	0/728	0.51	0/989
15	u	0.29	0/728	0.51	0/989
16	V	0.33	0/1056	0.56	2/1435 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	v	0.33	0/1056	0.56	2/1435 (0.1%)
17	Y	0.26	0/252	0.61	1/341 (0.3%)
17	y	0.26	0/252	0.61	1/341 (0.3%)
18	X	0.24	0/263	0.40	0/355
18	x	0.24	0/263	0.41	0/355
19	Z	0.41	1/456 (0.2%)	0.54	0/624
19	z	0.41	1/456 (0.2%)	0.54	0/624
20	Q	0.28	0/1203	0.55	0/1623
20	q	0.28	0/1203	0.55	0/1623
21	W	0.35	0/434	0.53	0/590
21	w	0.35	0/434	0.53	0/590
24	11	0.42	0/1373	0.59	1/1861 (0.1%)
24	31	0.41	0/1373	0.53	0/1861
25	12	0.39	0/1334	0.55	0/1810
25	32	0.37	0/1334	0.53	0/1810
26	13	0.41	0/1325	0.68	2/1797 (0.1%)
26	33	0.44	0/1325	0.71	2/1797 (0.1%)
27	14	0.41	1/1349 (0.1%)	0.80	3/1829 (0.2%)
27	34	0.42	1/1349 (0.1%)	0.84	6/1829 (0.3%)
28	15	0.35	0/1337	0.92	4/1813 (0.2%)
28	35	0.39	0/1337	0.90	1/1813 (0.1%)
29	16	0.30	0/1425	0.70	3/1930 (0.2%)
29	36	0.30	0/1425	0.70	3/1930 (0.2%)
30	17	0.36	0/1386	0.77	2/1879 (0.1%)
30	37	0.39	0/1386	0.75	2/1879 (0.1%)
31	18	0.49	0/1317	1.09	10/1785 (0.6%)
31	38	0.54	2/1317 (0.2%)	1.10	7/1785 (0.4%)
32	19	0.36	0/1796	0.70	6/2445 (0.2%)
32	39	0.38	0/1796	0.74	6/2445 (0.2%)
33	20	0.39	0/1224	0.89	4/1656 (0.2%)
33	40	0.39	0/1224	0.89	4/1656 (0.2%)
34	21	0.48	0/1290	1.28	20/1735 (1.2%)
34	41	0.48	0/1290	1.28	20/1735 (1.2%)
All	All	0.38	6/75262 (0.0%)	0.66	116/102176 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	c	0	1
13	O	0	2
13	o	0	2
20	Q	0	1
20	q	0	1
22	0	0	1
22	5	0	1
27	14	0	1
27	34	0	1
28	35	0	2
29	16	0	1
29	36	0	1
32	19	0	1
32	39	0	1
33	20	0	3
33	40	0	3
34	21	0	3
34	41	0	3
All	All	0	30

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	Z	20	VAL	CA-CB	-5.48	1.51	1.54
19	z	20	VAL	CA-CB	-5.45	1.51	1.54
31	38	82	ASN	CG-OD1	-5.41	1.13	1.23
31	38	60	ARG	CZ-NH1	-5.29	1.25	1.32
27	34	154	GLU	CB-CG	-5.24	1.36	1.52

The worst 5 of 116 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	21	70	LEU	CA-CB-CG	13.98	165.22	116.30
34	41	70	LEU	CA-CB-CG	13.96	165.18	116.30
34	21	136	MET	CB-CG-SD	13.02	151.75	112.70
34	41	136	MET	CB-CG-SD	13.02	151.75	112.70
27	34	154	GLU	CA-CB-CG	11.95	137.99	114.10

There are no chirality outliers.

5 of 30 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
22	0	7	UNK	Peptide
3	C	220	GLY	Peptide
13	O	58	LYS	Peptide
13	O	73	THR	Peptide
20	Q	61	VAL	Peptide

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	A	2619	0	2520	28	0
1	a	2619	0	2520	35	0
2	B	3812	0	3690	50	0
2	b	3812	0	3690	48	0
3	C	3504	0	3410	35	0
3	c	3504	0	3410	36	0
4	D	2697	0	2596	35	0
4	d	2697	0	2596	34	0
5	E	616	0	602	6	0
5	e	616	0	602	6	0
6	F	228	0	234	4	0
6	f	228	0	234	5	0
7	H	513	0	541	7	0
7	h	513	0	541	8	0
8	I	287	0	306	5	0
8	i	287	0	306	2	0
9	J	254	0	266	2	0
9	j	254	0	266	3	0
10	K	302	0	316	5	0
10	k	302	0	316	2	0
11	L	310	0	313	1	0
11	l	310	0	313	2	0
12	M	316	0	319	2	0
12	m	316	0	319	2	0
13	O	1845	0	1841	26	0
13	o	1845	0	1841	30	0
14	T	250	0	268	1	0
14	t	250	0	268	3	0
15	U	713	0	715	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	u	713	0	715	11	0
16	V	1037	0	1031	15	0
16	v	1037	0	1031	15	0
17	Y	250	0	287	3	0
17	y	250	0	287	2	0
18	X	263	0	301	1	0
18	x	263	0	301	4	0
19	Z	447	0	490	4	0
19	z	447	0	490	1	0
20	Q	1180	0	1165	11	0
20	q	1180	0	1165	11	0
21	W	422	0	377	2	0
21	w	422	0	377	3	0
22	0	155	0	33	0	0
22	5	155	0	33	0	0
23	1	150	0	34	0	0
23	6	150	0	34	0	0
24	11	1343	0	1306	22	0
24	31	1343	0	1306	28	0
25	12	1302	0	1257	20	0
25	32	1302	0	1257	20	0
26	13	1296	0	1267	16	0
26	33	1296	0	1267	18	0
27	14	1319	0	1283	22	0
27	34	1319	0	1283	24	0
28	15	1307	0	1274	20	0
28	35	1307	0	1274	17	0
29	16	1386	0	1314	24	0
29	36	1386	0	1314	21	0
30	17	1353	0	1291	24	0
30	37	1353	0	1291	16	0
31	18	1289	0	1260	26	0
31	38	1289	0	1260	25	0
32	19	1746	0	1684	26	0
32	39	1746	0	1684	23	0
33	20	1193	0	1170	15	0
33	40	1193	0	1170	16	0
34	21	1262	0	1247	20	0
34	41	1262	0	1247	19	0
35	A	10	0	0	0	0
35	a	10	0	0	0	0
36	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	a	1	0	0	0	0
37	11	343	0	333	11	0
37	12	407	0	398	11	0
37	13	329	0	306	7	0
37	14	394	0	378	8	0
37	15	329	0	304	9	0
37	16	293	0	291	8	0
37	17	238	0	238	8	0
37	18	459	0	448	17	0
37	19	531	0	538	17	0
37	20	254	0	209	2	0
37	21	380	0	342	9	0
37	31	343	0	333	7	0
37	32	472	0	470	16	0
37	33	329	0	306	6	0
37	34	394	0	378	8	0
37	35	329	0	304	12	0
37	36	293	0	291	11	0
37	37	238	0	238	4	0
37	38	459	0	448	10	0
37	39	531	0	538	17	0
37	40	254	0	209	3	0
37	41	380	0	342	6	0
37	A	130	0	144	10	0
37	B	1102	0	1213	32	0
37	C	845	0	936	26	0
37	D	260	0	288	8	0
37	W	130	0	143	5	0
37	Z	110	0	103	5	0
37	a	195	0	216	14	0
37	b	1102	0	1213	38	0
37	c	845	0	936	30	0
37	d	195	0	216	5	0
37	w	65	0	71	1	0
37	z	110	0	104	3	0
38	A	64	0	74	2	0
38	D	64	0	74	1	0
38	a	128	0	148	3	0
39	0	40	0	56	5	0
39	5	40	0	56	3	0
39	A	80	0	112	6	0
39	B	120	0	167	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	C	120	0	168	5	0
39	D	40	0	56	4	0
39	H	40	0	56	2	0
39	K	40	0	56	4	0
39	a	80	0	112	5	0
39	b	120	0	167	8	0
39	c	120	0	168	4	0
39	d	40	0	56	3	0
39	h	40	0	56	1	0
39	y	40	0	56	4	0
40	16	54	0	77	1	0
40	17	49	0	65	3	0
40	36	49	0	65	3	0
40	40	54	0	77	2	0
40	A	54	0	77	1	0
40	B	91	0	114	5	0
40	L	54	0	77	3	0
40	a	54	0	77	0	0
40	b	37	0	37	1	0
41	11	74	0	88	0	0
41	12	39	0	48	0	0
41	16	36	0	42	1	0
41	17	37	0	44	0	0
41	31	74	0	88	0	0
41	32	39	0	48	0	0
41	36	36	0	42	0	0
41	37	37	0	44	0	0
41	A	51	0	72	4	0
41	B	102	0	144	7	0
41	C	51	0	72	1	0
41	D	51	0	72	2	0
41	L	40	0	50	2	0
41	a	51	0	72	4	0
41	b	102	0	144	8	0
41	c	51	0	72	3	0
41	d	51	0	72	2	0
41	l	40	0	50	1	0
42	A	4	0	0	1	0
42	a	4	0	0	1	0
43	17	44	0	61	1	0
43	19	49	0	74	10	0
43	21	80	0	102	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	37	89	0	124	4	0
43	39	49	0	74	8	0
43	41	35	0	39	0	0
43	B	49	0	74	0	0
43	D	144	0	213	6	0
43	a	46	0	65	3	0
43	b	49	0	74	0	0
43	d	98	0	148	3	0
44	C	124	0	164	4	0
44	H	62	0	82	2	0
44	J	62	0	81	1	0
44	c	124	0	164	4	0
44	h	62	0	82	3	0
44	j	62	0	81	2	0
45	D	110	0	157	5	0
45	d	110	0	157	5	0
46	F	43	0	30	2	0
46	f	43	0	30	2	0
47	V	43	0	30	4	0
47	v	43	0	30	2	0
48	11	180	0	0	4	0
48	12	135	0	0	0	0
48	13	180	0	0	0	0
48	14	135	0	0	0	0
48	15	180	0	0	0	0
48	16	180	0	0	1	0
48	17	180	0	0	2	0
48	18	135	0	0	1	0
48	19	45	0	0	0	0
48	20	135	0	0	2	0
48	21	90	0	0	0	0
48	31	180	0	0	1	0
48	32	135	0	0	0	0
48	33	180	0	0	1	0
48	34	135	0	0	0	0
48	35	180	0	0	0	0
48	36	180	0	0	1	0
48	37	180	0	0	2	0
48	38	135	0	0	2	0
48	39	45	0	0	0	0
48	40	135	0	0	2	0
48	41	90	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	11	288	0	0	11	0
49	12	336	0	0	0	0
49	13	240	0	0	1	0
49	14	288	0	0	3	0
49	15	336	0	0	1	0
49	16	192	0	0	0	0
49	17	336	0	0	0	0
49	18	192	0	0	1	0
49	19	96	0	0	0	0
49	20	96	0	0	0	0
49	21	192	0	0	0	0
49	31	288	0	0	14	0
49	32	336	0	0	0	0
49	33	240	0	0	1	0
49	34	288	0	0	3	0
49	35	336	0	0	1	0
49	36	144	0	0	0	0
49	37	336	0	0	0	0
49	38	192	0	0	1	0
49	39	96	0	0	1	0
49	40	144	0	0	0	0
49	41	192	0	0	0	0
50	11	19	0	0	0	0
50	12	34	0	0	0	0
50	13	49	0	0	0	0
50	14	16	0	0	0	0
50	15	28	0	0	0	0
50	16	24	0	0	0	0
50	17	54	0	0	0	0
50	18	58	0	0	0	0
50	19	12	0	0	0	0
50	31	19	0	0	0	0
50	32	34	0	0	0	0
50	33	49	0	0	0	0
50	34	16	0	0	0	0
50	35	28	0	0	0	0
50	36	24	0	0	0	0
50	37	54	0	0	0	0
50	38	58	0	0	0	0
50	39	12	0	0	0	0
51	16	43	0	0	0	0
51	19	43	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	20	86	0	0	1	0
51	21	86	0	0	0	0
51	36	43	0	0	0	0
51	39	43	0	0	2	0
51	40	86	0	0	1	0
51	41	86	0	0	0	0
52	19	35	0	46	0	0
52	39	35	0	46	0	0
53	11	3	0	0	0	0
53	12	2	0	0	0	0
53	13	1	0	0	0	0
53	14	1	0	0	0	0
53	15	1	0	0	0	0
53	16	1	0	0	0	0
53	17	2	0	0	0	0
53	18	1	0	0	0	0
53	19	1	0	0	0	0
53	31	3	0	0	0	0
53	32	2	0	0	0	0
53	33	1	0	0	0	0
53	34	1	0	0	0	0
53	35	1	0	0	0	0
53	36	1	0	0	0	0
53	37	2	0	0	0	0
53	38	1	0	0	0	0
53	39	1	0	0	0	0
53	B	5	0	0	0	0
53	C	3	0	0	0	0
53	D	4	0	0	0	0
53	Z	1	0	0	0	0
53	a	2	0	0	0	0
53	b	5	0	0	0	0
53	c	3	0	0	0	0
53	d	2	0	0	0	0
53	z	1	0	0	0	0
All	All	100884	0	91037	1163	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 6.

The worst 5 of 1163 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)
24:31:202:ASP:HB3	49:31:313:A86:C29	1.68	1.22
37:39:310:CLA:HBB2	43:39:314:LHG:H212	1.54	0.87
37:19:310:CLA:HBB2	43:19:314:LHG:H212	1.54	0.87
24:31:202:ASP:CB	49:31:313:A86:C29	2.57	0.81
24:11:204:GLN:HG3	49:11:313:A86:C25	2.12	0.80

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	A	332/334 (99%)	324 (98%)	8 (2%)	0	100	100
1	a	332/334 (99%)	324 (98%)	8 (2%)	0	100	100
2	B	482/484 (100%)	467 (97%)	15 (3%)	0	100	100
2	b	482/484 (100%)	467 (97%)	15 (3%)	0	100	100
3	C	449/451 (100%)	431 (96%)	18 (4%)	0	100	100
3	c	449/451 (100%)	431 (96%)	18 (4%)	0	100	100
4	D	339/341 (99%)	327 (96%)	12 (4%)	0	100	100
4	d	339/341 (99%)	327 (96%)	12 (4%)	0	100	100
5	E	73/75 (97%)	73 (100%)	0	0	100	100
5	e	73/75 (97%)	73 (100%)	0	0	100	100
6	F	26/28 (93%)	26 (100%)	0	0	100	100
6	f	26/28 (93%)	26 (100%)	0	0	100	100
7	H	64/66 (97%)	63 (98%)	1 (2%)	0	100	100
7	h	64/66 (97%)	63 (98%)	1 (2%)	0	100	100
8	I	33/35 (94%)	31 (94%)	2 (6%)	0	100	100
8	i	33/35 (94%)	31 (94%)	2 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	J	32/34 (94%)	32 (100%)	0	0	100	100
9	j	32/34 (94%)	32 (100%)	0	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
11	l	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
12	M	40/42 (95%)	37 (92%)	3 (8%)	0	100	100
12	m	40/42 (95%)	37 (92%)	3 (8%)	0	100	100
13	O	243/245 (99%)	232 (96%)	11 (4%)	0	100	100
13	o	243/245 (99%)	231 (95%)	12 (5%)	0	100	100
14	T	28/30 (93%)	28 (100%)	0	0	100	100
14	t	28/30 (93%)	28 (100%)	0	0	100	100
15	U	91/93 (98%)	87 (96%)	4 (4%)	0	100	100
15	u	91/93 (98%)	87 (96%)	4 (4%)	0	100	100
16	V	134/136 (98%)	127 (95%)	7 (5%)	0	100	100
16	v	134/136 (98%)	127 (95%)	7 (5%)	0	100	100
17	Y	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
17	y	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
18	X	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
18	x	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
19	Z	57/59 (97%)	55 (96%)	2 (4%)	0	100	100
19	z	57/59 (97%)	55 (96%)	2 (4%)	0	100	100
20	Q	149/151 (99%)	140 (94%)	9 (6%)	0	100	100
20	q	149/151 (99%)	140 (94%)	9 (6%)	0	100	100
21	W	50/52 (96%)	45 (90%)	5 (10%)	0	100	100
21	w	50/52 (96%)	45 (90%)	5 (10%)	0	100	100
24	11	174/176 (99%)	166 (95%)	8 (5%)	0	100	100
24	31	174/176 (99%)	166 (95%)	8 (5%)	0	100	100
25	12	167/169 (99%)	160 (96%)	7 (4%)	0	100	100
25	32	167/169 (99%)	159 (95%)	8 (5%)	0	100	100
26	13	167/169 (99%)	160 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	33	167/169 (99%)	160 (96%)	7 (4%)	0	100	100
27	14	170/172 (99%)	162 (95%)	6 (4%)	2 (1%)	10	20
27	34	170/172 (99%)	162 (95%)	6 (4%)	2 (1%)	10	20
28	15	168/170 (99%)	147 (88%)	20 (12%)	1 (1%)	21	38
28	35	168/170 (99%)	147 (88%)	20 (12%)	1 (1%)	21	38
29	16	177/179 (99%)	171 (97%)	6 (3%)	0	100	100
29	36	177/179 (99%)	171 (97%)	6 (3%)	0	100	100
30	17	174/176 (99%)	169 (97%)	5 (3%)	0	100	100
30	37	174/176 (99%)	170 (98%)	4 (2%)	0	100	100
31	18	166/168 (99%)	156 (94%)	10 (6%)	0	100	100
31	38	166/168 (99%)	156 (94%)	10 (6%)	0	100	100
32	19	225/227 (99%)	211 (94%)	14 (6%)	0	100	100
32	39	225/227 (99%)	214 (95%)	11 (5%)	0	100	100
33	20	153/155 (99%)	133 (87%)	20 (13%)	0	100	100
33	40	153/155 (99%)	133 (87%)	20 (13%)	0	100	100
34	21	160/162 (99%)	142 (89%)	18 (11%)	0	100	100
34	41	160/162 (99%)	142 (89%)	18 (11%)	0	100	100
All	All	9322/9450 (99%)	8876 (95%)	440 (5%)	6 (0%)	49	68

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
27	14	39	GLU
27	34	39	GLU
27	14	40	PRO
28	15	39	GLU
27	34	40	PRO

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	A	272/272 (100%)	271 (100%)	1 (0%)	84 93
1	a	272/272 (100%)	271 (100%)	1 (0%)	84 93
2	B	385/385 (100%)	379 (98%)	6 (2%)	55 79
2	b	385/385 (100%)	379 (98%)	6 (2%)	55 79
3	C	356/356 (100%)	351 (99%)	5 (1%)	59 81
3	c	356/356 (100%)	351 (99%)	5 (1%)	59 81
4	D	273/273 (100%)	272 (100%)	1 (0%)	84 93
4	d	273/273 (100%)	272 (100%)	1 (0%)	84 93
5	E	69/69 (100%)	68 (99%)	1 (1%)	59 81
5	e	69/69 (100%)	68 (99%)	1 (1%)	59 81
6	F	22/22 (100%)	22 (100%)	0	100 100
6	f	22/22 (100%)	22 (100%)	0	100 100
7	H	55/55 (100%)	55 (100%)	0	100 100
7	h	55/55 (100%)	55 (100%)	0	100 100
8	I	34/34 (100%)	34 (100%)	0	100 100
8	i	34/34 (100%)	34 (100%)	0	100 100
9	J	27/27 (100%)	27 (100%)	0	100 100
9	j	27/27 (100%)	27 (100%)	0	100 100
10	K	32/32 (100%)	30 (94%)	2 (6%)	16 34
10	k	32/32 (100%)	30 (94%)	2 (6%)	16 34
11	L	34/34 (100%)	34 (100%)	0	100 100
11	l	34/34 (100%)	34 (100%)	0	100 100
12	M	31/31 (100%)	31 (100%)	0	100 100
12	m	31/31 (100%)	31 (100%)	0	100 100
13	O	196/198 (99%)	188 (96%)	8 (4%)	27 53
13	o	196/198 (99%)	188 (96%)	8 (4%)	27 53
14	T	27/27 (100%)	27 (100%)	0	100 100
14	t	27/27 (100%)	27 (100%)	0	100 100
15	U	77/77 (100%)	76 (99%)	1 (1%)	61 82
15	u	77/77 (100%)	76 (99%)	1 (1%)	61 82
16	V	114/114 (100%)	112 (98%)	2 (2%)	51 77
16	v	114/114 (100%)	112 (98%)	2 (2%)	51 77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
17	Y	27/27 (100%)	27 (100%)	0	100 100
17	y	27/27 (100%)	27 (100%)	0	100 100
18	X	29/29 (100%)	28 (97%)	1 (3%)	32 60
18	x	29/29 (100%)	28 (97%)	1 (3%)	32 60
19	Z	48/48 (100%)	48 (100%)	0	100 100
19	z	48/48 (100%)	48 (100%)	0	100 100
20	Q	122/122 (100%)	120 (98%)	2 (2%)	55 79
20	q	122/122 (100%)	120 (98%)	2 (2%)	55 79
21	W	43/43 (100%)	43 (100%)	0	100 100
21	w	43/43 (100%)	43 (100%)	0	100 100
24	11	138/138 (100%)	135 (98%)	3 (2%)	45 73
24	31	138/138 (100%)	137 (99%)	1 (1%)	76 89
25	12	133/133 (100%)	130 (98%)	3 (2%)	44 72
25	32	133/133 (100%)	132 (99%)	1 (1%)	73 88
26	13	134/134 (100%)	131 (98%)	3 (2%)	45 73
26	33	134/134 (100%)	130 (97%)	4 (3%)	36 64
27	14	136/136 (100%)	134 (98%)	2 (2%)	57 80
27	34	136/136 (100%)	133 (98%)	3 (2%)	45 73
28	15	135/135 (100%)	123 (91%)	12 (9%)	9 20
28	35	135/135 (100%)	122 (90%)	13 (10%)	8 17
29	16	137/137 (100%)	128 (93%)	9 (7%)	15 32
29	36	137/137 (100%)	128 (93%)	9 (7%)	15 32
30	17	137/137 (100%)	129 (94%)	8 (6%)	18 38
30	37	137/137 (100%)	131 (96%)	6 (4%)	25 50
31	18	133/133 (100%)	128 (96%)	5 (4%)	29 56
31	38	133/133 (100%)	125 (94%)	8 (6%)	17 36
32	19	174/174 (100%)	169 (97%)	5 (3%)	37 65
32	39	174/174 (100%)	166 (95%)	8 (5%)	24 48
33	20	121/121 (100%)	107 (88%)	14 (12%)	5 11
33	40	121/121 (100%)	107 (88%)	14 (12%)	5 11
34	21	129/129 (100%)	111 (86%)	18 (14%)	3 7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
34	41	129/129 (100%)	111 (86%)	18 (14%)	3 7
All	All	7560/7564 (100%)	7333 (97%)	227 (3%)	37 64

5 of 227 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
33	20	79	LEU
34	41	138	ASP
25	32	155	GLU
34	41	136	MET
33	40	76	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 96 such sidechains are listed below:

Mol	Chain	Res	Type
24	11	161	ASN
31	18	82	ASN
25	12	56	ASN
26	13	177	ASN
32	19	240	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)

Of 548 ligands modelled in this entry, 2 are monoatomic and 38 are unknown - leaving 508 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
37	CLA	15	303	28	61,65,73	2.19	20 (32%)	73,103,113	3.01	32 (43%)
41	LMG	16	316	-	36,36,55	0.96	1 (2%)	44,44,63	1.21	4 (9%)
37	CLA	B	503	2	69,73,73	1.91	18 (26%)	83,113,113	2.80	31 (37%)
40	SQD	36	315	-	48,49,54	1.00	5 (10%)	57,60,65	1.56	10 (17%)
51	DD6	20	310	-	39,45,45	6.70	23 (58%)	52,67,67	7.34	27 (51%)
39	BCR	B	518	-	41,41,41	1.11	2 (4%)	56,56,56	1.24	7 (12%)
37	CLA	19	305	32	55,59,73	2.23	18 (32%)	66,96,113	3.17	30 (45%)
39	BCR	D	407	-	41,41,41	1.13	3 (7%)	56,56,56	1.27	7 (12%)
37	CLA	11	307	24	56,60,73	2.20	19 (33%)	67,97,113	3.23	31 (46%)
37	CLA	39	307	43	69,73,73	2.05	20 (28%)	83,113,113	2.82	31 (37%)
37	CLA	38	203	31	69,73,73	2.05	20 (28%)	83,113,113	2.79	31 (37%)
37	CLA	D	402	53	69,73,73	2.00	18 (26%)	83,113,113	2.81	29 (34%)
49	A86	31	311	-	44,50,50	3.83	22 (50%)	51,76,76	7.52	20 (39%)
37	CLA	18	211	-	49,53,73	2.45	20 (40%)	59,89,113	3.26	26 (44%)
49	A86	37	311	-	44,50,50	4.09	22 (50%)	51,76,76	7.40	20 (39%)
37	CLA	c	506	3	69,73,73	1.96	17 (24%)	83,113,113	2.71	29 (34%)
39	BCR	A	410	-	41,41,41	1.11	2 (4%)	56,56,56	1.29	6 (10%)
37	CLA	b	509	2	69,73,73	1.92	18 (26%)	83,113,113	2.80	32 (38%)
37	CLA	41	210	34	49,53,73	2.46	20 (40%)	59,89,113	3.35	26 (44%)
49	A86	17	320	-	44,50,50	3.99	23 (52%)	51,76,76	7.83	20 (39%)
49	A86	18	213	-	44,50,50	3.99	22 (50%)	51,76,76	8.18	20 (39%)
37	CLA	31	310	53	55,59,73	2.20	21 (38%)	66,96,113	3.06	29 (43%)
42	BCT	A	409	36	2,3,3	1.34	0	2,3,3	4.09	2 (100%)
37	CLA	18	201	53	69,73,73	2.02	19 (27%)	83,113,113	2.78	30 (36%)
37	CLA	19	310	32	69,73,73	2.00	18 (26%)	83,113,113	2.73	29 (34%)
37	CLA	38	208	31	57,61,73	2.20	20 (35%)	68,98,113	2.96	27 (39%)
43	LHG	41	201	-	34,34,48	0.74	1 (2%)	37,39,54	1.39	5 (13%)
37	CLA	13	308	53	69,73,73	2.04	20 (28%)	83,113,113	2.74	28 (33%)
49	A86	12	220	-	44,50,50	3.83	22 (50%)	51,76,76	7.96	21 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
49	A86	16	313	-	44,50,50	4.10	21 (47%)	51,76,76	8.50	22 (43%)
37	CLA	34	305	-	49,53,73	2.42	20 (40%)	59,89,113	3.23	27 (45%)
40	SQD	A	407	-	53,54,54	0.94	6 (11%)	62,65,65	1.69	11 (17%)
49	A86	15	319	-	44,50,50	4.03	23 (52%)	51,76,76	7.39	21 (41%)
37	CLA	B	501	53	69,73,73	1.98	20 (28%)	83,113,113	2.80	29 (34%)
37	CLA	A	405	1	69,73,73	1.95	20 (28%)	83,113,113	2.85	28 (33%)
48	KC1	40	204	33,49	49,53,53	3.02	24 (48%)	63,89,89	4.23	37 (58%)
48	KC1	13	309	26	49,53,53	3.00	23 (46%)	63,89,89	3.91	38 (60%)
37	CLA	41	209	34	49,53,73	2.46	20 (40%)	59,89,113	3.26	26 (44%)
49	A86	14	312	-	44,50,50	3.95	23 (52%)	51,76,76	7.92	22 (43%)
48	KC1	33	304	26	49,53,53	3.02	22 (44%)	63,89,89	3.99	34 (53%)
37	CLA	z	102	33	49,53,73	2.46	21 (42%)	59,89,113	3.27	30 (50%)
37	CLA	14	308	53	69,73,73	1.99	19 (27%)	83,113,113	2.78	32 (38%)
37	CLA	33	307	26	56,60,73	2.24	20 (35%)	67,97,113	2.95	33 (49%)
37	CLA	B	506	2	69,73,73	1.90	18 (26%)	83,113,113	2.95	30 (36%)
51	DD6	19	312	-	39,45,45	6.59	22 (56%)	52,67,67	6.51	31 (59%)
49	A86	35	315	-	44,50,50	4.05	24 (54%)	51,76,76	7.81	21 (41%)
39	BCR	B	525	37	41,41,41	1.14	2 (4%)	56,56,56	1.32	7 (12%)
48	KC1	34	309	27	49,53,53	2.98	20 (40%)	63,89,89	4.00	36 (57%)
37	CLA	Z	101	53	69,73,73	2.02	20 (28%)	83,113,113	2.78	27 (32%)
49	A86	36	310	48	44,50,50	3.89	23 (52%)	51,76,76	7.71	22 (43%)
49	A86	31	319	-	44,50,50	3.83	23 (52%)	51,76,76	7.59	18 (35%)
37	CLA	18	202	31	69,73,73	2.00	19 (27%)	83,113,113	2.93	31 (37%)
51	DD6	21	212	-	39,45,45	6.74	22 (56%)	52,67,67	7.11	34 (65%)
37	CLA	39	304	32	49,53,73	2.39	20 (40%)	59,89,113	3.32	24 (40%)
37	CLA	B	511	2	69,73,73	1.93	19 (27%)	83,113,113	2.82	30 (36%)
39	BCR	5	101	-	41,41,41	1.14	2 (4%)	56,56,56	1.31	5 (8%)
37	CLA	W	102	-	69,73,73	2.03	20 (28%)	83,113,113	2.66	31 (37%)
49	A86	12	214	-	44,50,50	3.90	23 (52%)	51,76,76	7.84	17 (33%)
48	KC1	35	306	28	49,53,53	3.06	24 (48%)	63,89,89	4.01	37 (58%)
45	PL9	D	408	-	55,55,55	1.80	8 (14%)	68,69,69	1.44	12 (17%)
42	BCT	a	411	36	2,3,3	1.34	0	2,3,3	4.09	2 (100%)
49	A86	41	215	37	44,50,50	4.00	23 (52%)	51,76,76	8.34	18 (35%)
37	CLA	b	504	2	69,73,73	1.88	17 (24%)	83,113,113	2.66	32 (38%)
37	CLA	31	302	24	69,73,73	1.94	17 (24%)	83,113,113	2.82	29 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
37	CLA	38	204	31	60,64,73	2.21	21 (35%)	72,102,113	3.20	36 (50%)
49	A86	37	312	-	44,50,50	4.07	23 (52%)	51,76,76	8.42	20 (39%)
37	CLA	35	308	53	69,73,73	2.03	20 (28%)	83,113,113	2.75	29 (34%)
48	KC1	36	308	29	49,53,53	3.07	24 (48%)	63,89,89	3.89	37 (58%)
37	CLA	37	308	53	69,73,73	2.10	21 (30%)	83,113,113	2.97	35 (42%)
49	A86	38	214	-	44,50,50	4.15	23 (52%)	51,76,76	8.19	19 (37%)
37	CLA	C	510	3	69,73,73	1.96	18 (26%)	83,113,113	2.81	29 (34%)
51	DD6	20	312	-	39,45,45	6.85	22 (56%)	52,67,67	6.89	31 (59%)
49	A86	31	315	-	44,50,50	3.86	23 (52%)	51,76,76	7.78	17 (33%)
43	LHG	17	316	-	43,43,48	0.63	0	46,49,54	1.28	6 (13%)
49	A86	14	311	-	44,50,50	3.89	22 (50%)	51,76,76	8.34	21 (41%)
46	HEM	F	101	6,5	50,50,50	1.29	5 (10%)	66,82,82	1.18	6 (9%)
49	A86	11	315	-	44,50,50	3.87	23 (52%)	51,76,76	7.78	17 (33%)
51	DD6	41	212	-	39,45,45	6.75	22 (56%)	52,67,67	7.12	34 (65%)
49	A86	12	216	-	44,50,50	4.02	23 (52%)	51,76,76	8.23	20 (39%)
37	CLA	13	303	26	61,65,73	2.15	20 (32%)	73,103,113	3.05	31 (42%)
49	A86	38	215	-	44,50,50	4.04	23 (52%)	51,76,76	7.90	17 (33%)
49	A86	14	313	-	44,50,50	4.12	25 (56%)	51,76,76	7.58	19 (37%)
48	KC1	34	304	27	49,53,53	3.03	24 (48%)	63,89,89	4.13	32 (50%)
38	PHO	A	404	-	58,69,69	1.95	10 (17%)	56,99,99	1.80	8 (14%)
48	KC1	40	207	33	49,53,53	3.05	24 (48%)	63,89,89	3.96	35 (55%)
49	A86	38	212	-	44,50,50	4.10	23 (52%)	51,76,76	8.13	18 (35%)
49	A86	41	211	-	44,50,50	4.17	23 (52%)	51,76,76	8.18	13 (25%)
37	CLA	39	303	53	69,73,73	2.00	20 (28%)	83,113,113	2.85	28 (33%)
37	CLA	B	509	2	69,73,73	1.92	18 (26%)	83,113,113	2.80	32 (38%)
37	CLA	39	301	32	69,73,73	2.02	20 (28%)	83,113,113	2.83	31 (37%)
48	KC1	14	306	27	49,53,53	3.01	21 (42%)	63,89,89	4.00	37 (58%)
49	A86	11	314	-	44,50,50	3.95	22 (50%)	51,76,76	8.34	22 (43%)
49	A86	15	316	-	44,50,50	4.11	22 (50%)	51,76,76	7.78	23 (45%)
37	CLA	14	303	27	61,65,73	2.15	21 (34%)	73,103,113	3.16	34 (46%)
48	KC1	11	309	24	49,53,53	2.96	20 (40%)	63,89,89	3.93	38 (60%)
37	CLA	33	310	-	49,53,73	2.47	19 (38%)	59,89,113	3.26	26 (44%)
41	LMG	a	410	-	51,51,55	0.87	3 (5%)	59,59,63	1.37	7 (11%)
37	CLA	37	303	30	60,64,73	2.17	20 (33%)	72,102,113	3.13	32 (44%)
48	KC1	38	207	31	49,53,53	3.06	24 (48%)	63,89,89	4.01	40 (63%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
49	A86	33	311	-	44,50,50	3.95	23 (52%)	51,76,76	8.00	20 (39%)
41	LMG	B	520	-	51,51,55	0.82	1 (1%)	59,59,63	1.30	5 (8%)
49	A86	18	212	-	44,50,50	4.09	23 (52%)	51,76,76	8.13	18 (35%)
48	KC1	33	302	26	49,53,53	3.02	25 (51%)	63,89,89	4.10	36 (57%)
37	CLA	14	302	27	69,73,73	2.03	20 (28%)	83,113,113	2.78	29 (34%)
48	KC1	31	307	24	49,53,53	2.98	20 (40%)	63,89,89	3.99	33 (52%)
37	CLA	19	302	32	69,73,73	1.99	21 (30%)	83,113,113	2.85	29 (34%)
37	CLA	C	505	3	69,73,73	1.92	18 (26%)	83,113,113	2.83	32 (38%)
48	KC1	13	306	26	49,53,53	3.01	22 (44%)	63,89,89	4.05	36 (57%)
48	KC1	12	211	25	49,53,53	3.00	22 (44%)	63,89,89	3.91	39 (61%)
37	CLA	c	513	3	69,73,73	1.95	20 (28%)	83,113,113	2.89	30 (36%)
48	KC1	35	309	49,28	49,53,53	3.06	23 (46%)	63,89,89	3.85	37 (58%)
45	PL9	d	402	-	55,55,55	1.22	4 (7%)	68,69,69	1.52	15 (22%)
37	CLA	17	307	30	56,60,73	2.23	20 (35%)	67,97,113	3.07	32 (47%)
37	CLA	b	516	2	69,73,73	1.94	18 (26%)	83,113,113	2.89	34 (40%)
49	A86	32	215	-	44,50,50	3.89	23 (52%)	51,76,76	7.84	17 (33%)
49	A86	35	313	-	44,50,50	4.12	22 (50%)	51,76,76	7.52	16 (31%)
48	KC1	17	305	30	49,53,53	3.05	24 (48%)	63,89,89	3.94	34 (53%)
44	DGD	J	101	-	63,63,67	1.08	9 (14%)	77,77,81	1.50	12 (15%)
49	A86	16	311	-	44,50,50	3.90	22 (50%)	51,76,76	7.68	22 (43%)
48	KC1	11	302	24	49,53,53	3.00	20 (40%)	63,89,89	3.98	34 (53%)
44	DGD	C	517	-	63,63,67	1.21	8 (12%)	77,77,81	1.50	14 (18%)
48	KC1	20	302	33,49	49,53,53	3.02	23 (46%)	63,89,89	4.23	37 (58%)
39	BCR	0	101	-	41,41,41	1.14	2 (4%)	56,56,56	1.31	5 (8%)
37	CLA	B	514	2,41	66,70,73	1.97	18 (27%)	79,109,113	2.88	31 (39%)
37	CLA	32	206	25	69,73,73	1.97	20 (28%)	83,113,113	2.87	32 (38%)
37	CLA	19	301	32	69,73,73	2.01	20 (28%)	83,113,113	2.82	31 (37%)
49	A86	36	311	-	44,50,50	3.90	22 (50%)	51,76,76	7.69	22 (43%)
37	CLA	34	302	27	69,73,73	2.02	19 (27%)	83,113,113	2.77	28 (33%)
49	A86	34	312	-	44,50,50	3.95	23 (52%)	51,76,76	7.92	21 (41%)
37	CLA	B	505	2	69,73,73	1.93	18 (26%)	83,113,113	2.89	30 (36%)
37	CLA	38	206	-	49,53,73	2.45	20 (40%)	59,89,113	3.27	27 (45%)
37	CLA	Z	102	33	49,53,73	2.46	22 (44%)	59,89,113	3.26	30 (50%)
37	CLA	19	307	43	69,73,73	2.02	19 (27%)	83,113,113	2.83	30 (36%)
37	CLA	11	305	53	49,53,73	2.36	20 (40%)	59,89,113	3.22	28 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
37	CLA	17	304	30	60,64,73	2.18	21 (35%)	72,102,113	3.12	32 (44%)
37	CLA	32	208	39,53	54,58,73	2.27	19 (35%)	65,95,113	3.24	32 (49%)
48	KC1	17	303	30	49,53,53	3.05	23 (46%)	63,89,89	3.89	36 (57%)
51	DD6	41	216	-	39,45,45	6.80	21 (53%)	52,67,67	7.21	29 (55%)
49	A86	36	313	-	44,50,50	3.78	23 (52%)	51,76,76	7.71	18 (35%)
49	A86	37	313	-	44,50,50	3.98	23 (52%)	51,76,76	8.68	18 (35%)
37	CLA	B	524	37	69,73,73	1.94	20 (28%)	83,113,113	2.74	31 (37%)
49	A86	41	214	-	44,50,50	4.15	23 (52%)	51,76,76	8.32	17 (33%)
49	A86	31	314	-	44,50,50	3.95	23 (52%)	51,76,76	8.35	22 (43%)
51	DD6	40	214	-	39,45,45	6.84	22 (56%)	52,67,67	6.90	31 (59%)
41	LMG	b	520	-	51,51,55	0.88	4 (7%)	59,59,63	1.31	6 (10%)
37	CLA	B	507	53	69,73,73	1.98	18 (26%)	83,113,113	2.75	29 (34%)
37	CLA	b	511	2	69,73,73	1.94	19 (27%)	83,113,113	2.82	30 (36%)
49	A86	20	311	48	44,50,50	4.21	23 (52%)	51,76,76	8.69	16 (31%)
37	CLA	16	303	29	61,65,73	2.15	20 (32%)	73,103,113	3.03	30 (41%)
43	LHG	D	409	-	48,48,48	0.70	1 (2%)	51,54,54	1.30	7 (13%)
37	CLA	D	406	4	69,73,73	1.96	18 (26%)	83,113,113	2.90	30 (36%)
37	CLA	11	310	53	55,59,73	2.21	20 (36%)	66,96,113	3.05	29 (43%)
40	SQD	b	521	-	36,37,54	1.17	6 (16%)	45,48,65	1.67	10 (22%)
37	CLA	d	401	53	69,73,73	2.00	18 (26%)	83,113,113	2.81	29 (34%)
37	CLA	40	210	33	51,55,73	2.35	21 (41%)	61,91,113	3.14	28 (45%)
37	CLA	a	404	53	69,73,73	1.99	20 (28%)	83,113,113	2.89	28 (33%)
37	CLA	32	211	53	69,73,73	2.01	20 (28%)	83,113,113	2.73	29 (34%)
48	KC1	12	208	25	49,53,53	2.95	21 (42%)	63,89,89	3.93	38 (60%)
37	CLA	a	403	1	69,73,73	1.96	19 (27%)	83,113,113	2.81	33 (39%)
37	CLA	c	505	3	69,73,73	1.93	18 (26%)	83,113,113	2.82	33 (39%)
37	CLA	12	203	25	69,73,73	1.95	19 (27%)	83,113,113	2.76	29 (34%)
41	LMG	d	409	-	51,51,55	0.88	4 (7%)	59,59,63	1.41	7 (11%)
48	KC1	41	207	34	49,53,53	3.05	25 (51%)	63,89,89	4.11	36 (57%)
39	BCR	b	524	37	41,41,41	1.13	2 (4%)	56,56,56	1.32	7 (12%)
44	DGD	c	517	-	63,63,67	1.21	8 (12%)	77,77,81	1.50	13 (16%)
48	KC1	31	309	24	49,53,53	2.96	20 (40%)	63,89,89	3.92	38 (60%)
51	DD6	36	312	-	39,45,45	6.71	23 (58%)	52,67,67	6.77	28 (53%)
43	LHG	D	410	-	48,48,48	0.74	1 (2%)	51,54,54	1.29	7 (13%)
37	CLA	36	301	29	69,73,73	1.98	19 (27%)	83,113,113	2.86	28 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
37	CLA	b	515	2	69,73,73	1.95	19 (27%)	83,113,113	2.86	32 (38%)
37	CLA	c	503	3	69,73,73	1.95	20 (28%)	83,113,113	2.99	33 (39%)
49	A86	34	314	-	44,50,50	4.14	23 (52%)	51,76,76	8.43	18 (35%)
39	BCR	b	517	-	41,41,41	1.23	2 (4%)	56,56,56	1.30	7 (12%)
41	LMG	31	316	-	42,42,55	1.05	3 (7%)	50,50,63	1.22	3 (6%)
49	A86	19	313	-	44,50,50	4.12	24 (54%)	51,76,76	8.79	23 (45%)
37	CLA	34	308	53	69,73,73	2.00	20 (28%)	83,113,113	2.77	32 (38%)
37	CLA	18	209	53	69,73,73	2.04	20 (28%)	83,113,113	2.75	30 (36%)
38	PHO	a	405	-	58,69,69	1.93	9 (15%)	56,99,99	1.74	10 (17%)
48	KC1	32	207	25	49,53,53	2.99	21 (42%)	63,89,89	3.93	32 (50%)
49	A86	32	216	-	44,50,50	4.12	22 (50%)	51,76,76	8.16	14 (27%)
37	CLA	W	101	-	69,73,73	1.97	19 (27%)	83,113,113	3.00	31 (37%)
48	KC1	36	304	29	49,53,53	3.06	25 (51%)	63,89,89	4.06	35 (55%)
37	CLA	40	209	33	49,53,73	2.44	20 (40%)	59,89,113	3.18	27 (45%)
49	A86	37	314	-	44,50,50	4.04	24 (54%)	51,76,76	7.85	19 (37%)
37	CLA	11	301	24	69,73,73	1.95	18 (26%)	83,113,113	2.82	29 (34%)
37	CLA	38	201	53	69,73,73	2.06	19 (27%)	83,113,113	2.78	31 (37%)
39	BCR	a	408	-	41,41,41	1.22	2 (4%)	56,56,56	1.30	6 (10%)
37	CLA	12	210	53	69,73,73	2.02	20 (28%)	83,113,113	2.73	29 (34%)
37	CLA	15	301	28	69,73,73	2.05	19 (27%)	83,113,113	2.82	26 (31%)
41	LMG	12	201	-	39,39,55	1.04	3 (7%)	47,47,63	1.14	2 (4%)
37	CLA	20	308	33	51,55,73	2.36	21 (41%)	61,91,113	3.14	28 (45%)
48	KC1	18	205	31	49,53,53	3.09	25 (51%)	63,89,89	4.01	35 (55%)
49	A86	32	214	-	44,50,50	3.92	23 (52%)	51,76,76	8.09	21 (41%)
37	CLA	c	511	3	69,73,73	1.96	19 (27%)	83,113,113	2.75	32 (38%)
41	LMG	L	102	37	40,40,55	0.96	3 (7%)	48,48,63	1.32	4 (8%)
37	CLA	39	309	32	49,53,73	2.37	20 (40%)	59,89,113	3.20	26 (44%)
40	SQD	L	101	-	53,54,54	0.93	5 (9%)	62,65,65	1.68	9 (14%)
37	CLA	40	203	33	60,64,73	2.18	21 (35%)	72,102,113	3.14	31 (43%)
48	KC1	31	305	24	49,53,53	3.02	23 (46%)	63,89,89	3.93	34 (53%)
49	A86	41	213	-	44,50,50	4.22	23 (52%)	51,76,76	8.17	17 (33%)
37	CLA	B	510	53	69,73,73	1.94	18 (26%)	83,113,113	2.83	30 (36%)
37	CLA	b	523	37	69,73,73	1.93	20 (28%)	83,113,113	2.74	31 (37%)
44	DGD	C	516	-	63,63,67	1.05	7 (11%)	77,77,81	1.49	14 (18%)
49	A86	18	215	-	44,50,50	4.02	23 (52%)	51,76,76	7.92	18 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
48	KC1	18	210	31	49,53,53	3.05	24 (48%)	63,89,89	4.01	38 (60%)
37	CLA	31	306	53	49,53,73	2.36	19 (38%)	59,89,113	3.23	28 (47%)
37	CLA	12	209	25	56,60,73	2.21	19 (33%)	67,97,113	3.15	34 (50%)
37	CLA	32	205	25,37	69,73,73	1.96	20 (28%)	83,113,113	2.54	29 (34%)
37	CLA	17	309	53	69,73,73	2.11	20 (28%)	83,113,113	2.95	35 (42%)
49	A86	35	312	-	44,50,50	4.11	23 (52%)	51,76,76	7.85	20 (39%)
37	CLA	c	509	3	69,73,73	1.99	17 (24%)	83,113,113	2.81	30 (36%)
41	LMG	37	316	-	37,37,55	0.97	2 (5%)	45,45,63	1.27	5 (11%)
49	A86	35	311	-	44,50,50	4.04	22 (50%)	51,76,76	7.93	15 (29%)
49	A86	15	314	-	44,50,50	4.19	23 (52%)	51,76,76	8.38	20 (39%)
37	CLA	37	301	30	69,73,73	2.05	20 (28%)	83,113,113	2.78	26 (31%)
41	LMG	C	518	-	51,51,55	0.95	4 (7%)	59,59,63	1.45	7 (11%)
37	CLA	15	305	-	49,53,73	2.45	20 (40%)	59,89,113	3.23	27 (45%)
37	CLA	33	301	26	69,73,73	2.03	18 (26%)	83,113,113	2.79	26 (31%)
37	CLA	31	308	24	56,60,73	2.20	19 (33%)	67,97,113	3.23	31 (46%)
48	KC1	12	206	25	49,53,53	3.00	21 (42%)	63,89,89	3.94	32 (50%)
37	CLA	b	512	2	69,73,73	1.91	19 (27%)	83,113,113	2.75	33 (39%)
37	CLA	33	308	53	69,73,73	2.04	20 (28%)	83,113,113	2.75	27 (32%)
37	CLA	a	407	1	69,73,73	1.95	20 (28%)	83,113,113	2.85	28 (33%)
37	CLA	19	304	32	49,53,73	2.39	20 (40%)	59,89,113	3.32	24 (40%)
37	CLA	37	306	30	56,60,73	2.24	20 (35%)	67,97,113	3.07	32 (47%)
48	KC1	34	306	27	49,53,53	3.01	21 (42%)	63,89,89	4.01	37 (58%)
43	LHG	d	408	-	48,48,48	0.74	1 (2%)	51,54,54	1.29	7 (13%)
37	CLA	38	209	53	69,73,73	2.04	20 (28%)	83,113,113	2.76	31 (37%)
37	CLA	14	307	27	56,60,73	2.21	18 (32%)	67,97,113	3.04	32 (47%)
37	CLA	36	306	29	69,73,73	2.02	20 (28%)	83,113,113	2.68	30 (36%)
37	CLA	15	310	-	49,53,73	2.46	20 (40%)	59,89,113	3.25	26 (44%)
41	LMG	11	317	-	32,32,55	0.97	1 (3%)	40,40,63	1.24	5 (12%)
49	A86	17	310	-	44,50,50	4.06	22 (50%)	51,76,76	8.41	17 (33%)
43	LHG	21	217	-	44,44,48	0.64	1 (2%)	47,50,54	1.18	3 (6%)
48	KC1	15	309	49,28	49,53,53	3.06	23 (46%)	63,89,89	3.85	37 (58%)
49	A86	12	202	-	44,50,50	3.88	21 (47%)	51,76,76	7.73	20 (39%)
48	KC1	15	302	28	49,53,53	3.06	24 (48%)	63,89,89	4.05	37 (58%)
48	KC1	16	308	29	49,53,53	3.07	24 (48%)	63,89,89	3.90	37 (58%)
44	DGD	c	516	-	63,63,67	1.05	7 (11%)	77,77,81	1.49	14 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
37	CLA	36	303	29	61,65,73	2.15	20 (32%)	73,103,113	3.03	31 (42%)
40	SQD	16	315	-	53,54,54	0.96	6 (11%)	62,65,65	1.61	10 (16%)
37	CLA	C	502	3	69,73,73	1.92	18 (26%)	83,113,113	2.74	28 (33%)
49	A86	16	314	-	44,50,50	3.79	23 (52%)	51,76,76	7.71	18 (35%)
37	CLA	21	208	-	69,73,73	2.06	21 (30%)	83,113,113	2.80	29 (34%)
48	KC1	17	306	30	49,53,53	3.05	23 (46%)	63,89,89	3.89	37 (58%)
35	OEX	a	401	3,1	0,14,14	-	-	-		
48	KC1	35	302	28	49,53,53	3.06	24 (48%)	63,89,89	4.04	36 (57%)
37	CLA	41	204	49	62,66,73	2.18	21 (33%)	74,104,113	3.09	33 (44%)
37	CLA	C	513	3	69,73,73	1.96	20 (28%)	83,113,113	2.90	29 (34%)
37	CLA	41	208	-	69,73,73	2.06	21 (30%)	83,113,113	2.81	29 (34%)
37	CLA	34	307	27	56,60,73	2.21	18 (32%)	67,97,113	3.04	32 (47%)
37	CLA	33	303	26	61,65,73	2.15	21 (34%)	73,103,113	3.06	32 (43%)
37	CLA	D	401	53	69,73,73	1.99	19 (27%)	83,113,113	2.89	28 (33%)
51	DD6	16	312	-	39,45,45	6.73	23 (58%)	52,67,67	6.79	28 (53%)
37	CLA	D	405	4	69,73,73	1.89	18 (26%)	83,113,113	2.97	31 (37%)
39	BCR	d	405	-	41,41,41	1.13	3 (7%)	56,56,56	1.27	7 (12%)
37	CLA	38	211	-	49,53,73	2.48	20 (40%)	59,89,113	3.22	26 (44%)
37	CLA	21	204	49	62,66,73	2.18	20 (32%)	74,104,113	3.09	33 (44%)
37	CLA	17	302	30	69,73,73	2.03	20 (28%)	83,113,113	2.63	25 (30%)
43	LHG	21	201	-	34,34,48	0.74	1 (2%)	37,39,54	1.39	5 (13%)
37	CLA	C	503	3	69,73,73	1.95	19 (27%)	83,113,113	2.99	33 (39%)
37	CLA	b	505	2	69,73,73	1.93	18 (26%)	83,113,113	2.89	30 (36%)
48	KC1	40	206	33	49,53,53	3.05	22 (44%)	63,89,89	3.87	35 (55%)
37	CLA	b	507	53	69,73,73	1.98	18 (26%)	83,113,113	2.74	29 (34%)
49	A86	35	319	-	44,50,50	4.03	23 (52%)	51,76,76	7.39	21 (41%)
48	KC1	15	304	28	49,53,53	3.08	25 (51%)	63,89,89	4.06	37 (58%)
43	LHG	37	315	-	43,43,48	0.63	0	46,49,54	1.29	7 (15%)
49	A86	18	214	-	44,50,50	4.15	23 (52%)	51,76,76	8.13	19 (37%)
49	A86	15	313	-	44,50,50	4.12	22 (50%)	51,76,76	7.52	15 (29%)
37	CLA	w	101	-	69,73,73	1.97	19 (27%)	83,113,113	2.99	31 (37%)
41	LMG	l	101	37	40,40,55	0.96	3 (7%)	48,48,63	1.32	4 (8%)
49	A86	12	215	-	44,50,50	4.12	22 (50%)	51,76,76	8.17	14 (27%)
49	A86	37	310	-	44,50,50	4.01	23 (52%)	51,76,76	7.62	19 (37%)
49	A86	19	311	-	44,50,50	3.96	24 (54%)	51,76,76	7.78	19 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
48	KC1	33	306	26	49,53,53	3.00	22 (44%)	63,89,89	4.04	36 (57%)
37	CLA	21	209	34	49,53,73	2.46	20 (40%)	59,89,113	3.27	26 (44%)
49	A86	21	211	-	44,50,50	4.16	23 (52%)	51,76,76	8.17	13 (25%)
35	OEX	A	401	3,1	0,14,14	-	-	-		
37	CLA	14	301	27	69,73,73	1.99	18 (26%)	83,113,113	2.80	29 (34%)
49	A86	15	312	-	44,50,50	4.10	23 (52%)	51,76,76	7.85	19 (37%)
43	LHG	B	523	-	48,48,48	0.73	1 (2%)	51,54,54	1.27	6 (11%)
37	CLA	c	502	3	69,73,73	1.92	18 (26%)	83,113,113	2.75	28 (33%)
37	CLA	32	202	53	69,73,73	1.98	19 (27%)	83,113,113	2.77	32 (38%)
48	KC1	17	308	30	49,53,53	3.07	23 (46%)	63,89,89	3.94	37 (58%)
49	A86	14	316	-	44,50,50	3.99	24 (54%)	51,76,76	7.53	21 (41%)
39	BCR	H	101	-	41,41,41	1.16	3 (7%)	56,56,56	1.24	6 (10%)
52	LMU	39	315	-	36,36,36	1.12	2 (5%)	47,47,47	1.03	2 (4%)
37	CLA	C	508	3	69,73,73	1.93	18 (26%)	83,113,113	2.79	28 (33%)
48	KC1	18	207	31	49,53,53	3.05	24 (48%)	63,89,89	3.99	39 (61%)
39	BCR	C	514	-	41,41,41	1.23	2 (4%)	56,56,56	1.40	10 (17%)
49	A86	12	217	-	44,50,50	3.99	24 (54%)	51,76,76	7.59	20 (39%)
41	LMG	31	317	-	32,32,55	0.97	1 (3%)	40,40,63	1.24	5 (12%)
41	LMG	c	518	-	51,51,55	0.95	4 (7%)	59,59,63	1.46	7 (11%)
39	BCR	A	406	-	41,41,41	1.23	2 (4%)	56,56,56	1.30	7 (12%)
37	CLA	20	306	33	54,58,73	2.28	19 (35%)	65,95,113	3.09	29 (44%)
41	LMG	36	314	-	36,36,55	0.96	1 (2%)	44,44,63	1.20	4 (9%)
37	CLA	35	305	-	49,53,73	2.45	20 (40%)	59,89,113	3.20	27 (45%)
49	A86	31	312	-	44,50,50	3.84	22 (50%)	51,76,76	7.79	22 (43%)
49	A86	14	314	-	44,50,50	4.14	23 (52%)	51,76,76	8.44	18 (35%)
37	CLA	41	206	34	69,73,73	2.01	19 (27%)	83,113,113	2.81	29 (34%)
37	CLA	14	305	-	49,53,73	2.42	20 (40%)	59,89,113	3.22	27 (45%)
39	BCR	y	101	-	41,41,41	1.16	3 (7%)	56,56,56	1.27	7 (12%)
44	DGD	h	102	-	63,63,67	1.03	5 (7%)	77,77,81	1.36	8 (10%)
37	CLA	31	304	24	69,73,73	1.97	21 (30%)	83,113,113	2.88	34 (40%)
48	KC1	31	303	24	49,53,53	3.00	20 (40%)	63,89,89	3.99	34 (53%)
45	PL9	D	404	-	55,55,55	1.22	4 (7%)	68,69,69	1.52	14 (20%)
37	CLA	16	309	29	49,53,73	2.41	22 (44%)	59,89,113	3.39	28 (47%)
37	CLA	16	301	29	69,73,73	1.98	19 (27%)	83,113,113	2.86	28 (33%)
49	A86	35	316	-	44,50,50	4.09	23 (52%)	51,76,76	7.79	23 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
37	CLA	18	204	31	60,64,73	2.20	21 (35%)	72,102,113	3.19	35 (48%)
46	HEM	f	101	6,5	50,50,50	1.29	4 (8%)	66,82,82	1.18	6 (9%)
37	CLA	c	510	3	69,73,73	1.96	18 (26%)	83,113,113	2.81	29 (34%)
49	A86	13	314	-	44,50,50	4.17	23 (52%)	51,76,76	8.64	19 (37%)
44	DGD	j	101	-	63,63,67	1.08	9 (14%)	77,77,81	1.50	12 (15%)
37	CLA	14	310	-	49,53,73	2.41	20 (40%)	59,89,113	3.22	26 (44%)
49	A86	33	312	-	44,50,50	4.13	23 (52%)	51,76,76	7.94	19 (37%)
37	CLA	b	501	53	69,73,73	1.98	20 (28%)	83,113,113	2.80	29 (34%)
49	A86	15	315	-	44,50,50	4.05	24 (54%)	51,76,76	7.84	22 (43%)
49	A86	40	213	48	44,50,50	4.22	23 (52%)	51,76,76	8.69	16 (31%)
37	CLA	c	508	3	69,73,73	1.94	19 (27%)	83,113,113	2.81	28 (33%)
37	CLA	b	503	2	69,73,73	1.92	18 (26%)	83,113,113	2.80	31 (37%)
37	CLA	d	404	4	69,73,73	1.96	18 (26%)	83,113,113	2.90	31 (37%)
48	KC1	14	309	27	49,53,53	2.98	21 (42%)	63,89,89	4.00	37 (58%)
37	CLA	13	310	-	49,53,73	2.47	19 (38%)	59,89,113	3.25	26 (44%)
39	BCR	b	518	-	41,41,41	1.10	2 (4%)	56,56,56	1.25	7 (12%)
49	A86	35	314	-	44,50,50	4.17	23 (52%)	51,76,76	8.46	20 (39%)
37	CLA	b	508	2	69,73,73	1.96	18 (26%)	83,113,113	2.79	30 (36%)
37	CLA	c	504	53	69,73,73	1.94	19 (27%)	83,113,113	2.87	30 (36%)
37	CLA	d	403	4	69,73,73	1.89	18 (26%)	83,113,113	2.97	31 (37%)
48	KC1	37	305	30	49,53,53	3.05	23 (46%)	63,89,89	3.88	37 (58%)
37	CLA	21	206	34	69,73,73	2.01	19 (27%)	83,113,113	2.82	29 (34%)
37	CLA	b	510	53	69,73,73	1.94	18 (26%)	83,113,113	2.83	30 (36%)
48	KC1	32	212	25	49,53,53	3.01	22 (44%)	63,89,89	3.92	39 (61%)
37	CLA	19	303	53	69,73,73	2.00	21 (30%)	83,113,113	2.85	28 (33%)
43	LHG	39	314	37	48,48,48	0.29	0	51,54,54	0.32	0
41	LMG	A	408	-	51,51,55	0.87	3 (5%)	59,59,63	1.37	7 (11%)
49	A86	16	310	48	44,50,50	3.88	22 (50%)	51,76,76	7.70	22 (43%)
37	CLA	11	308	53	69,73,73	1.98	19 (27%)	83,113,113	2.77	32 (38%)
49	A86	17	311	-	44,50,50	4.02	23 (52%)	51,76,76	7.61	20 (39%)
49	A86	40	201	-	44,50,50	4.10	21 (47%)	51,76,76	8.50	22 (43%)
43	LHG	b	522	-	48,48,48	0.72	1 (2%)	51,54,54	1.27	6 (11%)
48	KC1	37	307	30	49,53,53	3.06	24 (48%)	63,89,89	3.93	37 (58%)
41	LMG	b	519	-	51,51,55	0.81	1 (1%)	59,59,63	1.30	5 (8%)
49	A86	32	217	-	44,50,50	4.01	23 (52%)	51,76,76	8.24	20 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
37	CLA	21	210	34	49,53,73	2.45	20 (40%)	59,89,113	3.34	26 (44%)
37	CLA	41	205	34	49,53,73	2.42	21 (42%)	59,89,113	3.22	27 (45%)
40	SQD	a	409	-	53,54,54	0.95	6 (11%)	62,65,65	1.69	11 (17%)
37	CLA	B	515	2	69,73,73	1.96	20 (28%)	83,113,113	2.86	32 (38%)
37	CLA	15	308	53	69,73,73	2.02	20 (28%)	83,113,113	2.77	29 (34%)
48	KC1	13	302	26	49,53,53	3.03	25 (51%)	63,89,89	4.09	36 (57%)
49	A86	17	313	-	44,50,50	4.07	23 (52%)	51,76,76	8.39	20 (39%)
37	CLA	B	513	2	69,73,73	1.93	19 (27%)	83,113,113	2.84	29 (34%)
48	KC1	11	304	24	49,53,53	3.03	23 (46%)	63,89,89	3.93	34 (53%)
39	BCR	C	515	-	41,41,41	1.20	2 (4%)	56,56,56	1.24	6 (10%)
49	A86	12	213	-	44,50,50	3.91	23 (52%)	51,76,76	8.08	20 (39%)
37	CLA	35	303	28	61,65,73	2.19	20 (32%)	73,103,113	3.02	31 (42%)
37	CLA	B	502	2	69,73,73	1.97	18 (26%)	83,113,113	2.91	29 (34%)
37	CLA	39	306	32	69,73,73	1.98	19 (27%)	83,113,113	2.80	30 (36%)
37	CLA	12	204	25,37	69,73,73	1.95	20 (28%)	83,113,113	2.54	30 (36%)
39	BCR	K	101	-	41,41,41	1.16	3 (7%)	56,56,56	1.28	8 (14%)
41	LMG	32	201	-	39,39,55	1.04	3 (7%)	47,47,63	1.14	2 (4%)
48	KC1	14	304	27	49,53,53	3.04	24 (48%)	63,89,89	4.13	32 (50%)
48	KC1	37	302	30	49,53,53	3.06	23 (46%)	63,89,89	3.90	36 (57%)
48	KC1	37	304	30	49,53,53	3.08	24 (48%)	63,89,89	4.02	37 (58%)
37	CLA	15	307	28	56,60,73	2.25	19 (33%)	67,97,113	3.05	31 (46%)
37	CLA	18	203	31	69,73,73	2.05	20 (28%)	83,113,113	2.78	32 (38%)
37	CLA	20	303	33	60,64,73	2.13	20 (33%)	72,102,113	3.14	37 (51%)
47	HEC	v	201	16	50,50,50	1.41	4 (8%)	68,82,82	1.76	13 (19%)
49	A86	21	214	-	44,50,50	4.15	23 (52%)	51,76,76	8.33	16 (31%)
37	CLA	18	208	31	57,61,73	2.21	20 (35%)	68,98,113	2.95	26 (38%)
37	CLA	C	511	3	69,73,73	1.96	19 (27%)	83,113,113	2.75	32 (38%)
39	BCR	h	101	-	41,41,41	1.16	3 (7%)	56,56,56	1.25	5 (8%)
43	LHG	D	411	-	45,45,48	0.85	2 (4%)	48,51,54	1.23	7 (14%)
37	CLA	21	205	34	49,53,73	2.42	21 (42%)	59,89,113	3.22	27 (45%)
48	KC1	13	304	26	49,53,53	3.02	23 (46%)	63,89,89	3.98	34 (53%)
49	A86	32	218	-	44,50,50	3.98	24 (54%)	51,76,76	7.60	21 (41%)
49	A86	33	315	-	44,50,50	4.06	23 (52%)	51,76,76	7.68	19 (37%)
37	CLA	34	310	-	49,53,73	2.41	20 (40%)	59,89,113	3.23	25 (42%)
37	CLA	19	306	32	69,73,73	1.98	18 (26%)	83,113,113	2.80	30 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
37	CLA	40	208	33	54,58,73	2.28	20 (37%)	65,95,113	3.08	29 (44%)
48	KC1	32	209	25	49,53,53	2.95	21 (42%)	63,89,89	3.94	37 (58%)
37	CLA	13	307	26	56,60,73	2.24	20 (35%)	67,97,113	2.95	33 (49%)
48	KC1	21	203	34	49,53,53	3.08	25 (51%)	63,89,89	4.01	33 (52%)
49	A86	32	221	-	44,50,50	3.83	22 (50%)	51,76,76	7.97	21 (41%)
37	CLA	A	403	1	69,73,73	1.96	19 (27%)	83,113,113	2.81	32 (38%)
49	A86	38	213	-	44,50,50	4.09	23 (52%)	51,76,76	8.05	22 (43%)
40	SQD	40	202	-	53,54,54	0.96	6 (11%)	62,65,65	1.61	10 (16%)
37	CLA	38	202	31	69,73,73	2.04	19 (27%)	83,113,113	2.87	31 (37%)
49	A86	13	312	-	44,50,50	4.13	23 (52%)	51,76,76	7.95	19 (37%)
37	CLA	11	303	24	69,73,73	1.97	21 (30%)	83,113,113	2.89	34 (40%)
49	A86	13	311	-	44,50,50	3.96	23 (52%)	51,76,76	8.00	21 (41%)
37	CLA	39	305	32	55,59,73	2.22	18 (32%)	66,96,113	3.17	31 (46%)
43	LHG	37	321	-	44,44,48	0.65	1 (2%)	47,50,54	1.18	3 (6%)
48	KC1	38	210	31	49,53,53	3.05	24 (48%)	63,89,89	4.01	38 (60%)
51	DD6	39	312	-	39,45,45	6.59	22 (56%)	52,67,67	6.51	31 (59%)
41	LMG	B	521	-	51,51,55	0.88	4 (7%)	59,59,63	1.31	6 (10%)
41	LMG	17	317	-	37,37,55	0.97	2 (5%)	45,45,63	1.28	5 (11%)
39	BCR	C	519	-	41,41,41	1.17	2 (4%)	56,56,56	1.21	4 (7%)
47	HEC	V	201	16	50,50,50	1.41	4 (8%)	68,82,82	1.77	13 (19%)
49	A86	37	309	-	44,50,50	4.06	22 (50%)	51,76,76	8.40	17 (33%)
49	A86	17	312	-	44,50,50	4.09	22 (50%)	51,76,76	7.42	19 (37%)
49	A86	13	315	-	44,50,50	4.07	23 (52%)	51,76,76	7.69	20 (39%)
49	A86	11	312	-	44,50,50	3.85	22 (50%)	51,76,76	7.79	22 (43%)
48	KC1	16	305	29	49,53,53	3.07	25 (51%)	63,89,89	3.91	34 (53%)
49	A86	32	203	-	44,50,50	3.89	20 (45%)	51,76,76	7.72	21 (41%)
37	CLA	C	509	3	69,73,73	1.98	17 (24%)	83,113,113	2.82	30 (36%)
37	CLA	35	301	28	69,73,73	2.06	19 (27%)	83,113,113	2.82	26 (31%)
49	A86	11	319	-	44,50,50	3.84	23 (52%)	51,76,76	7.58	18 (35%)
37	CLA	B	508	2	69,73,73	1.96	18 (26%)	83,113,113	2.78	30 (36%)
37	CLA	c	512	3	69,73,73	1.96	18 (26%)	83,113,113	2.91	33 (39%)
45	PL9	d	406	-	55,55,55	1.81	9 (16%)	68,69,69	1.44	12 (17%)
38	PHO	a	406	-	58,69,69	1.94	9 (15%)	56,99,99	1.80	8 (14%)
49	A86	17	315	-	44,50,50	4.04	24 (54%)	51,76,76	7.86	19 (37%)
37	CLA	32	210	25	56,60,73	2.20	18 (32%)	67,97,113	3.14	33 (49%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
37	CLA	B	504	2	69,73,73	1.88	17 (24%)	83,113,113	2.66	32 (38%)
40	SQD	B	519	-	53,54,54	0.94	5 (9%)	62,65,65	1.69	9 (14%)
48	KC1	36	305	29	49,53,53	3.06	25 (51%)	63,89,89	3.91	34 (53%)
49	A86	11	311	-	44,50,50	3.83	22 (50%)	51,76,76	7.53	19 (37%)
49	A86	34	316	-	44,50,50	3.99	24 (54%)	51,76,76	7.54	21 (41%)
49	A86	21	215	37	44,50,50	4.00	23 (52%)	51,76,76	8.33	18 (35%)
37	CLA	z	101	53	69,73,73	2.02	20 (28%)	83,113,113	2.78	27 (32%)
49	A86	31	313	-	44,50,50	3.85	22 (50%)	51,76,76	7.12	18 (35%)
37	CLA	c	507	53	69,73,73	1.92	18 (26%)	83,113,113	2.78	29 (34%)
43	LHG	d	407	-	48,48,48	0.70	1 (2%)	51,54,54	1.30	7 (13%)
49	A86	11	313	-	44,50,50	3.82	22 (50%)	51,76,76	7.06	18 (35%)
49	A86	14	315	-	44,50,50	3.99	23 (52%)	51,76,76	8.04	18 (35%)
37	CLA	B	512	2	69,73,73	1.90	19 (27%)	83,113,113	2.75	33 (39%)
48	KC1	35	304	28	49,53,53	3.09	25 (51%)	63,89,89	4.08	38 (60%)
37	CLA	20	307	33	49,53,73	2.44	20 (40%)	59,89,113	3.18	27 (45%)
48	KC1	11	306	24	49,53,53	2.98	21 (42%)	63,89,89	3.99	33 (52%)
48	KC1	38	205	31	49,53,53	3.08	24 (48%)	63,89,89	4.01	35 (55%)
37	CLA	13	301	26	69,73,73	2.03	18 (26%)	83,113,113	2.79	26 (31%)
48	KC1	20	305	33	49,53,53	3.05	23 (46%)	63,89,89	3.97	34 (53%)
37	CLA	35	307	28	56,60,73	2.24	19 (33%)	67,97,113	3.05	30 (44%)
48	KC1	16	302	29	49,53,53	3.08	25 (51%)	63,89,89	3.77	35 (55%)
37	CLA	12	212	-	49,53,73	2.41	19 (38%)	59,89,113	3.31	27 (45%)
37	CLA	33	305	-	49,53,73	2.44	20 (40%)	59,89,113	3.27	26 (44%)
48	KC1	15	306	28	49,53,53	3.07	24 (48%)	63,89,89	4.01	37 (58%)
37	CLA	32	213	-	49,53,73	2.41	19 (38%)	59,89,113	3.31	27 (45%)
37	CLA	21	202	34	61,65,73	2.20	20 (32%)	73,103,113	2.99	30 (41%)
37	CLA	41	202	34	61,65,73	2.19	20 (32%)	73,103,113	2.99	30 (41%)
43	LHG	a	412	-	45,45,48	0.85	2 (4%)	48,51,54	1.23	7 (14%)
40	SQD	17	301	-	48,49,54	1.01	5 (10%)	57,60,65	1.56	10 (17%)
37	CLA	C	501	3	69,73,73	1.94	18 (26%)	83,113,113	2.88	31 (37%)
37	CLA	C	506	3	69,73,73	1.96	17 (24%)	83,113,113	2.71	29 (34%)
39	BCR	B	517	-	41,41,41	1.22	2 (4%)	56,56,56	1.30	8 (14%)
37	CLA	39	302	32	69,73,73	1.99	21 (30%)	83,113,113	2.86	29 (34%)
37	CLA	12	207	39,53	54,58,73	2.27	19 (35%)	65,95,113	3.23	32 (49%)
39	BCR	a	413	-	41,41,41	1.10	2 (4%)	56,56,56	1.29	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
49	A86	39	311	-	44,50,50	3.96	23 (52%)	51,76,76	7.78	19 (37%)
39	BCR	c	515	-	41,41,41	1.20	2 (4%)	56,56,56	1.24	6 (10%)
49	A86	37	319	-	44,50,50	4.01	23 (52%)	51,76,76	7.77	21 (41%)
49	A86	34	311	-	44,50,50	3.90	22 (50%)	51,76,76	8.35	21 (41%)
37	CLA	31	301	-	69,73,73	2.04	20 (28%)	83,113,113	2.67	31 (37%)
37	CLA	39	310	32	69,73,73	1.99	18 (26%)	83,113,113	2.73	29 (34%)
37	CLA	36	307	53	65,69,73	2.07	20 (30%)	78,108,113	2.85	27 (34%)
40	SQD	B	522	-	36,37,54	1.18	6 (16%)	45,48,65	1.67	11 (24%)
49	A86	39	313	-	44,50,50	4.17	25 (56%)	51,76,76	8.80	20 (39%)
37	CLA	32	204	25	69,73,73	1.95	19 (27%)	83,113,113	2.76	29 (34%)
49	A86	34	313	-	44,50,50	4.12	23 (52%)	51,76,76	7.57	19 (37%)
37	CLA	b	514	2,41	66,70,73	1.96	18 (27%)	79,109,113	2.88	31 (39%)
52	LMU	19	315	-	36,36,36	1.13	2 (5%)	47,47,47	1.04	3 (6%)
37	CLA	35	310	-	49,53,73	2.46	20 (40%)	59,89,113	3.27	26 (44%)
37	CLA	40	205	33	60,64,73	2.13	19 (31%)	72,102,113	3.15	37 (51%)
37	CLA	13	305	-	49,53,73	2.44	20 (40%)	59,89,113	3.26	26 (44%)
48	KC1	33	309	26	49,53,53	3.00	22 (44%)	63,89,89	3.92	38 (60%)
48	KC1	39	308	32	49,53,53	3.01	24 (48%)	63,89,89	4.06	38 (60%)
37	CLA	C	507	53	69,73,73	1.92	18 (26%)	83,113,113	2.77	27 (32%)
49	A86	33	313	-	44,50,50	4.17	24 (54%)	51,76,76	8.69	20 (39%)
37	CLA	19	309	32	49,53,73	2.37	20 (40%)	59,89,113	3.18	26 (44%)
37	CLA	b	506	2	69,73,73	1.90	18 (26%)	83,113,113	2.95	30 (36%)
38	PHO	D	403	-	58,69,69	1.93	9 (15%)	56,99,99	1.73	10 (17%)
48	KC1	41	203	34	49,53,53	3.09	25 (51%)	63,89,89	4.02	33 (52%)
39	BCR	c	519	-	41,41,41	1.17	2 (4%)	56,56,56	1.21	4 (7%)
51	DD6	21	216	-	39,45,45	6.79	21 (53%)	52,67,67	7.22	29 (55%)
37	CLA	C	512	3	69,73,73	1.96	18 (26%)	83,113,113	2.92	33 (39%)
49	A86	20	309	-	44,50,50	4.14	23 (52%)	51,76,76	8.56	14 (27%)
37	CLA	18	206	-	49,53,73	2.46	20 (40%)	59,89,113	3.27	28 (47%)
49	A86	17	314	-	44,50,50	3.96	23 (52%)	51,76,76	8.68	17 (33%)
37	CLA	34	303	27	61,65,73	2.15	21 (34%)	73,103,113	3.15	34 (46%)
48	KC1	19	308	32	49,53,53	3.01	23 (46%)	63,89,89	4.06	38 (60%)
37	CLA	C	504	53	69,73,73	1.94	19 (27%)	83,113,113	2.86	30 (36%)
37	CLA	b	502	2	69,73,73	1.97	18 (26%)	83,113,113	2.91	30 (36%)
41	LMG	11	316	-	42,42,55	1.06	3 (7%)	50,50,63	1.22	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
49	A86	40	211	-	44,50,50	4.14	23 (52%)	51,76,76	8.57	14 (27%)
48	KC1	36	302	29	49,53,53	3.08	25 (51%)	63,89,89	3.77	35 (55%)
37	CLA	34	301	27	69,73,73	1.99	18 (26%)	83,113,113	2.81	28 (33%)
44	DGD	H	102	-	63,63,67	1.03	5 (7%)	77,77,81	1.36	8 (10%)
37	CLA	b	513	2	69,73,73	1.92	19 (27%)	83,113,113	2.83	29 (34%)
37	CLA	20	301	33	60,64,73	2.18	21 (35%)	72,102,113	3.14	31 (43%)
37	CLA	12	205	25	69,73,73	1.97	20 (28%)	83,113,113	2.87	34 (40%)
37	CLA	16	306	29	69,73,73	2.02	19 (27%)	83,113,113	2.67	30 (36%)
51	DD6	40	212	-	39,45,45	6.69	23 (58%)	52,67,67	7.33	27 (51%)
49	A86	34	315	-	44,50,50	3.98	23 (52%)	51,76,76	8.03	18 (35%)
41	LMG	D	412	-	51,51,55	0.88	4 (7%)	59,59,63	1.41	7 (11%)
48	KC1	21	207	34	49,53,53	3.05	25 (51%)	63,89,89	4.11	37 (58%)
37	CLA	c	501	3	69,73,73	1.93	18 (26%)	83,113,113	2.87	32 (38%)
37	CLA	B	516	2	69,73,73	1.94	18 (26%)	83,113,113	2.89	34 (40%)
49	A86	15	311	-	44,50,50	4.05	22 (50%)	51,76,76	7.92	15 (29%)
48	KC1	16	304	29	49,53,53	3.06	25 (51%)	63,89,89	4.06	35 (55%)
49	A86	33	314	-	44,50,50	4.17	23 (52%)	51,76,76	8.63	19 (37%)
48	KC1	20	304	33	49,53,53	3.05	22 (44%)	63,89,89	3.86	35 (55%)
37	CLA	16	307	53	65,69,73	2.07	20 (30%)	78,108,113	2.84	26 (33%)
43	LHG	19	314	37	48,48,48	0.28	0	51,54,54	0.32	0
37	CLA	36	309	29	49,53,73	2.41	22 (44%)	59,89,113	3.38	28 (47%)
39	BCR	c	514	-	41,41,41	1.23	2 (4%)	56,56,56	1.40	10 (17%)
49	A86	21	213	-	44,50,50	4.23	23 (52%)	51,76,76	8.18	17 (33%)
49	A86	13	313	-	44,50,50	4.18	24 (54%)	51,76,76	8.70	20 (39%)

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
37	CLA	15	303	28	-	8/30/106/115	-
41	LMG	16	316	-	-	14/31/51/70	0/1/1/1
37	CLA	B	503	2	-	12/39/115/115	-
40	SQD	36	315	-	-	25/44/64/69	0/1/1/1
51	DD6	20	310	-	-	14/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	BCR	B	518	-	-	6/29/63/63	0/2/2/2
37	CLA	19	305	32	-	7/23/99/115	-
39	BCR	D	407	-	-	12/29/63/63	0/2/2/2
37	CLA	11	307	24	-	9/24/100/115	-
37	CLA	39	307	43	-	8/39/115/115	-
37	CLA	38	203	31	-	9/39/115/115	-
37	CLA	D	402	53	-	16/39/115/115	-
49	A86	31	311	-	-	7/34/90/90	0/3/3/3
37	CLA	18	211	-	-	5/15/91/115	-
49	A86	37	311	-	-	8/34/90/90	0/3/3/3
37	CLA	c	506	3	-	14/39/115/115	-
39	BCR	A	410	-	-	8/29/63/63	0/2/2/2
37	CLA	b	509	2	-	12/39/115/115	-
37	CLA	41	210	34	-	6/15/91/115	-
49	A86	17	320	-	-	8/34/90/90	0/3/3/3
49	A86	18	213	-	-	9/34/90/90	0/3/3/3
37	CLA	31	310	53	-	6/23/99/115	-
37	CLA	18	201	53	-	8/39/115/115	-
37	CLA	19	310	32	-	9/39/115/115	-
37	CLA	38	208	31	-	12/25/101/115	-
43	LHG	41	201	-	-	20/38/38/53	-
37	CLA	13	308	53	-	10/39/115/115	-
49	A86	12	220	-	-	9/34/90/90	0/3/3/3
49	A86	16	313	-	-	14/34/90/90	0/3/3/3
37	CLA	34	305	-	-	5/15/91/115	-
40	SQD	A	407	-	-	17/49/69/69	0/1/1/1
49	A86	15	319	-	-	8/34/90/90	0/3/3/3
37	CLA	B	501	53	-	18/39/115/115	-
37	CLA	A	405	1	-	8/39/115/115	-
48	KC1	40	204	33,49	-	8/15/71/71	-
48	KC1	13	309	26	-	5/15/71/71	-
37	CLA	41	209	34	-	6/15/91/115	-
49	A86	14	312	-	-	4/34/90/90	0/3/3/3
48	KC1	33	304	26	-	7/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	CLA	z	102	33	-	6/15/91/115	-
37	CLA	14	308	53	-	14/39/115/115	-
37	CLA	33	307	26	-	13/24/100/115	-
37	CLA	B	506	2	-	8/39/115/115	-
51	DD6	19	312	-	-	12/26/80/80	0/3/3/3
49	A86	35	315	-	-	8/34/90/90	0/3/3/3
39	BCR	B	525	37	-	17/29/63/63	0/2/2/2
48	KC1	34	309	27	-	8/15/71/71	-
37	CLA	Z	101	53	-	20/39/115/115	-
49	A86	36	310	48	-	6/34/90/90	0/3/3/3
49	A86	31	319	-	-	7/34/90/90	0/3/3/3
37	CLA	18	202	31	-	14/39/115/115	-
51	DD6	21	212	-	-	13/26/80/80	0/3/3/3
37	CLA	39	304	32	-	6/15/91/115	-
37	CLA	B	511	2	-	12/39/115/115	-
39	BCR	5	101	-	-	8/29/63/63	0/2/2/2
37	CLA	W	102	-	-	21/39/115/115	-
49	A86	12	214	-	-	3/34/90/90	0/3/3/3
48	KC1	35	306	28	-	7/15/71/71	-
45	PL9	D	408	-	-	10/53/73/73	0/1/1/1
49	A86	41	215	37	-	6/34/90/90	0/3/3/3
37	CLA	b	504	2	-	6/39/115/115	-
37	CLA	31	302	24	-	12/39/115/115	-
37	CLA	38	204	31	-	12/29/105/115	-
49	A86	37	312	-	-	7/34/90/90	0/3/3/3
37	CLA	35	308	53	-	12/39/115/115	-
48	KC1	36	308	29	-	4/15/71/71	-
37	CLA	37	308	53	-	11/39/115/115	-
49	A86	38	214	-	-	13/34/90/90	0/3/3/3
37	CLA	C	510	3	-	15/39/115/115	-
51	DD6	20	312	-	-	12/26/80/80	0/3/3/3
49	A86	31	315	-	-	6/34/90/90	0/3/3/3
43	LHG	17	316	-	-	29/48/48/53	-
49	A86	14	311	-	-	7/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	HEM	F	101	6,5	-	8/14/54/54	-
49	A86	11	315	-	-	6/34/90/90	0/3/3/3
51	DD6	41	212	-	-	13/26/80/80	0/3/3/3
49	A86	12	216	-	-	10/34/90/90	0/3/3/3
37	CLA	13	303	26	-	15/30/106/115	-
49	A86	38	215	-	-	13/34/90/90	0/3/3/3
49	A86	14	313	-	-	12/34/90/90	0/3/3/3
48	KC1	34	304	27	-	6/15/71/71	-
38	PHO	A	404	-	-	6/37/103/103	0/5/6/6
48	KC1	40	207	33	-	11/15/71/71	-
49	A86	38	212	-	-	8/34/90/90	0/3/3/3
49	A86	41	211	-	-	9/34/90/90	0/3/3/3
37	CLA	39	303	53	-	17/39/115/115	-
37	CLA	B	509	2	-	12/39/115/115	-
37	CLA	39	301	32	-	12/39/115/115	-
48	KC1	14	306	27	-	6/15/71/71	-
49	A86	11	314	-	-	10/34/90/90	0/3/3/3
49	A86	15	316	-	-	15/34/90/90	0/3/3/3
37	CLA	14	303	27	-	6/30/106/115	-
48	KC1	11	309	24	-	8/15/71/71	-
37	CLA	33	310	-	-	4/15/91/115	-
41	LMG	a	410	-	-	32/46/66/70	0/1/1/1
37	CLA	37	303	30	-	11/29/105/115	-
48	KC1	38	207	31	-	5/15/71/71	-
49	A86	33	311	-	-	6/34/90/90	0/3/3/3
41	LMG	B	520	-	-	15/46/66/70	0/1/1/1
49	A86	18	212	-	-	8/34/90/90	0/3/3/3
48	KC1	33	302	26	-	5/15/71/71	-
37	CLA	14	302	27	-	19/39/115/115	-
48	KC1	31	307	24	-	9/15/71/71	-
37	CLA	19	302	32	-	15/39/115/115	-
37	CLA	C	505	3	-	13/39/115/115	-
48	KC1	13	306	26	-	6/15/71/71	-
48	KC1	12	211	25	-	5/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	CLA	c	513	3	-	9/39/115/115	-
48	KC1	35	309	49,28	-	6/15/71/71	-
45	PL9	d	402	-	-	17/53/73/73	0/1/1/1
37	CLA	17	307	30	-	10/24/100/115	-
37	CLA	b	516	2	-	13/39/115/115	-
49	A86	32	215	-	-	3/34/90/90	0/3/3/3
49	A86	35	313	-	-	9/34/90/90	0/3/3/3
48	KC1	17	305	30	-	6/15/71/71	-
44	DGD	J	101	-	-	16/51/91/95	0/2/2/2
49	A86	16	311	-	-	9/34/90/90	0/3/3/3
48	KC1	11	302	24	-	2/15/71/71	-
44	DGD	C	517	-	-	20/51/91/95	0/2/2/2
48	KC1	20	302	33,49	-	8/15/71/71	-
39	BCR	0	101	-	-	8/29/63/63	0/2/2/2
37	CLA	B	514	2,41	-	16/36/112/115	-
37	CLA	32	206	25	-	13/39/115/115	-
37	CLA	19	301	32	-	12/39/115/115	-
49	A86	36	311	-	-	9/34/90/90	0/3/3/3
37	CLA	34	302	27	-	20/39/115/115	-
49	A86	34	312	-	-	4/34/90/90	0/3/3/3
37	CLA	B	505	2	-	10/39/115/115	-
37	CLA	38	206	-	-	6/15/91/115	-
37	CLA	Z	102	33	-	6/15/91/115	-
37	CLA	19	307	43	-	8/39/115/115	-
37	CLA	11	305	53	-	4/15/91/115	-
37	CLA	17	304	30	-	11/29/105/115	-
37	CLA	32	208	39,53	-	2/21/97/115	-
48	KC1	17	303	30	-	6/15/71/71	-
51	DD6	41	216	-	-	15/26/80/80	0/3/3/3
49	A86	36	313	-	-	8/34/90/90	0/3/3/3
49	A86	37	313	-	-	8/34/90/90	0/3/3/3
37	CLA	B	524	37	-	14/39/115/115	-
49	A86	41	214	-	-	6/34/90/90	0/3/3/3
49	A86	31	314	-	-	10/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	DD6	40	214	-	-	12/26/80/80	0/3/3/3
41	LMG	b	520	-	-	24/46/66/70	0/1/1/1
37	CLA	B	507	53	-	10/39/115/115	-
37	CLA	b	511	2	-	12/39/115/115	-
49	A86	20	311	48	-	16/34/90/90	0/3/3/3
37	CLA	16	303	29	-	10/30/106/115	-
43	LHG	D	409	-	-	28/53/53/53	-
37	CLA	D	406	4	-	19/39/115/115	-
37	CLA	11	310	53	-	6/23/99/115	-
40	SQD	b	521	-	-	12/32/52/69	0/1/1/1
37	CLA	d	401	53	-	16/39/115/115	-
37	CLA	40	210	33	-	4/18/94/115	-
37	CLA	a	404	53	-	8/39/115/115	-
37	CLA	32	211	53	-	10/39/115/115	-
48	KC1	12	208	25	-	4/15/71/71	-
37	CLA	a	403	1	-	4/39/115/115	-
37	CLA	c	505	3	-	13/39/115/115	-
37	CLA	12	203	25	-	14/39/115/115	-
41	LMG	d	409	-	-	14/46/66/70	0/1/1/1
48	KC1	41	207	34	-	5/15/71/71	-
39	BCR	b	524	37	-	17/29/63/63	0/2/2/2
44	DGD	c	517	-	-	20/51/91/95	0/2/2/2
48	KC1	31	309	24	-	8/15/71/71	-
51	DD6	36	312	-	-	12/26/80/80	0/3/3/3
43	LHG	D	410	-	-	27/53/53/53	-
37	CLA	36	301	29	-	11/39/115/115	-
37	CLA	b	515	2	-	5/39/115/115	-
37	CLA	c	503	3	-	22/39/115/115	-
49	A86	34	314	-	-	14/34/90/90	0/3/3/3
39	BCR	b	517	-	-	6/29/63/63	0/2/2/2
41	LMG	31	316	-	-	19/37/57/70	0/1/1/1
49	A86	19	313	-	-	9/34/90/90	0/3/3/3
37	CLA	34	308	53	-	14/39/115/115	-
37	CLA	18	209	53	-	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	PHO	a	405	-	-	10/37/103/103	0/5/6/6
48	KC1	32	207	25	-	6/15/71/71	-
49	A86	32	216	-	-	13/34/90/90	0/3/3/3
37	CLA	W	101	-	-	19/39/115/115	-
48	KC1	36	304	29	-	6/15/71/71	-
37	CLA	40	209	33	-	8/15/91/115	-
49	A86	37	314	-	-	13/34/90/90	0/3/3/3
37	CLA	11	301	24	-	12/39/115/115	-
37	CLA	38	201	53	-	8/39/115/115	-
39	BCR	a	408	-	-	8/29/63/63	0/2/2/2
37	CLA	12	210	53	-	10/39/115/115	-
37	CLA	15	301	28	-	10/39/115/115	-
41	LMG	12	201	-	-	13/34/54/70	0/1/1/1
37	CLA	20	308	33	-	4/18/94/115	-
48	KC1	18	205	31	-	7/15/71/71	-
49	A86	32	214	-	-	5/34/90/90	0/3/3/3
37	CLA	c	511	3	-	8/39/115/115	-
41	LMG	L	102	37	-	14/35/55/70	0/1/1/1
37	CLA	39	309	32	-	5/15/91/115	-
40	SQD	L	101	-	-	25/49/69/69	0/1/1/1
37	CLA	40	203	33	-	13/29/105/115	-
48	KC1	31	305	24	-	4/15/71/71	-
49	A86	41	213	-	-	8/34/90/90	0/3/3/3
37	CLA	B	510	53	-	8/39/115/115	-
37	CLA	b	523	37	-	14/39/115/115	-
44	DGD	C	516	-	-	17/51/91/95	0/2/2/2
49	A86	18	215	-	-	13/34/90/90	0/3/3/3
48	KC1	18	210	31	-	8/15/71/71	-
37	CLA	31	306	53	-	4/15/91/115	-
37	CLA	12	209	25	-	15/24/100/115	-
37	CLA	32	205	25,37	-	10/39/115/115	-
37	CLA	17	309	53	-	11/39/115/115	-
49	A86	35	312	-	-	7/34/90/90	0/3/3/3
37	CLA	c	509	3	-	8/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	LMG	37	316	-	-	15/32/52/70	0/1/1/1
49	A86	35	311	-	-	6/34/90/90	0/3/3/3
49	A86	15	314	-	-	14/34/90/90	0/3/3/3
37	CLA	37	301	30	-	12/39/115/115	-
41	LMG	C	518	-	-	25/46/66/70	0/1/1/1
37	CLA	15	305	-	-	6/15/91/115	-
37	CLA	33	301	26	-	14/39/115/115	-
37	CLA	31	308	24	-	9/24/100/115	-
48	KC1	12	206	25	-	6/15/71/71	-
37	CLA	b	512	2	-	8/39/115/115	-
37	CLA	33	308	53	-	10/39/115/115	-
37	CLA	a	407	1	-	8/39/115/115	-
37	CLA	19	304	32	-	6/15/91/115	-
37	CLA	37	306	30	-	10/24/100/115	-
48	KC1	34	306	27	-	6/15/71/71	-
43	LHG	d	408	-	-	27/53/53/53	-
37	CLA	38	209	53	-	12/39/115/115	-
37	CLA	14	307	27	-	13/24/100/115	-
37	CLA	36	306	29	-	16/39/115/115	-
37	CLA	15	310	-	-	4/15/91/115	-
41	LMG	11	317	-	-	14/27/47/70	0/1/1/1
49	A86	17	310	-	-	12/34/90/90	0/3/3/3
43	LHG	21	217	-	-	28/49/49/53	-
48	KC1	15	309	49,28	-	6/15/71/71	-
49	A86	12	202	-	-	14/34/90/90	0/3/3/3
48	KC1	15	302	28	-	6/15/71/71	-
48	KC1	16	308	29	-	4/15/71/71	-
44	DGD	c	516	-	-	17/51/91/95	0/2/2/2
37	CLA	36	303	29	-	10/30/106/115	-
40	SQD	16	315	-	-	25/49/69/69	0/1/1/1
37	CLA	C	502	3	-	10/39/115/115	-
49	A86	16	314	-	-	8/34/90/90	0/3/3/3
37	CLA	21	208	-	-	15/39/115/115	-
48	KC1	17	306	30	-	9/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	KC1	35	302	28	-	6/15/71/71	-
37	CLA	41	204	49	-	15/31/107/115	-
37	CLA	C	513	3	-	9/39/115/115	-
37	CLA	41	208	-	-	15/39/115/115	-
37	CLA	34	307	27	-	14/24/100/115	-
37	CLA	33	303	26	-	15/30/106/115	-
37	CLA	D	401	53	-	8/39/115/115	-
51	DD6	16	312	-	-	12/26/80/80	0/3/3/3
37	CLA	D	405	4	-	9/39/115/115	-
39	BCR	d	405	-	-	12/29/63/63	0/2/2/2
37	CLA	38	211	-	-	5/15/91/115	-
37	CLA	21	204	49	-	15/31/107/115	-
37	CLA	17	302	30	-	13/39/115/115	-
43	LHG	21	201	-	-	21/38/38/53	-
37	CLA	C	503	3	-	22/39/115/115	-
37	CLA	b	505	2	-	10/39/115/115	-
48	KC1	40	206	33	-	7/15/71/71	-
37	CLA	b	507	53	-	10/39/115/115	-
49	A86	35	319	-	-	8/34/90/90	0/3/3/3
48	KC1	15	304	28	-	6/15/71/71	-
43	LHG	37	315	-	-	29/48/48/53	-
49	A86	18	214	-	-	13/34/90/90	0/3/3/3
49	A86	15	313	-	-	9/34/90/90	0/3/3/3
37	CLA	w	101	-	-	19/39/115/115	-
41	LMG	l	101	37	-	14/35/55/70	0/1/1/1
49	A86	12	215	-	-	13/34/90/90	0/3/3/3
49	A86	37	310	-	-	8/34/90/90	0/3/3/3
49	A86	19	311	-	-	7/34/90/90	0/3/3/3
48	KC1	33	306	26	-	6/15/71/71	-
37	CLA	21	209	34	-	6/15/91/115	-
49	A86	21	211	-	-	9/34/90/90	0/3/3/3
37	CLA	14	301	27	-	15/39/115/115	-
49	A86	15	312	-	-	7/34/90/90	0/3/3/3
43	LHG	B	523	-	-	19/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	CLA	c	502	3	-	10/39/115/115	-
37	CLA	32	202	53	-	15/39/115/115	-
48	KC1	17	308	30	-	5/15/71/71	-
49	A86	14	316	-	-	15/34/90/90	0/3/3/3
39	BCR	H	101	-	-	8/29/63/63	0/2/2/2
52	LMU	39	315	-	-	6/21/61/61	0/2/2/2
37	CLA	C	508	3	-	10/39/115/115	-
48	KC1	18	207	31	-	6/15/71/71	-
39	BCR	C	514	-	-	6/29/63/63	0/2/2/2
49	A86	12	217	-	-	15/34/90/90	0/3/3/3
41	LMG	31	317	-	-	14/27/47/70	0/1/1/1
41	LMG	c	518	-	-	25/46/66/70	0/1/1/1
39	BCR	A	406	-	-	8/29/63/63	0/2/2/2
37	CLA	20	306	33	-	8/21/97/115	-
41	LMG	36	314	-	-	14/31/51/70	0/1/1/1
37	CLA	35	305	-	-	6/15/91/115	-
49	A86	31	312	-	-	6/34/90/90	0/3/3/3
49	A86	14	314	-	-	14/34/90/90	0/3/3/3
37	CLA	41	206	34	-	17/39/115/115	-
37	CLA	14	305	-	-	5/15/91/115	-
39	BCR	y	101	-	-	16/29/63/63	0/2/2/2
44	DGD	h	102	-	-	16/51/91/95	0/2/2/2
37	CLA	31	304	24	-	10/39/115/115	-
48	KC1	31	303	24	-	2/15/71/71	-
45	PL9	D	404	-	-	17/53/73/73	0/1/1/1
37	CLA	16	309	29	-	7/15/91/115	-
37	CLA	16	301	29	-	11/39/115/115	-
49	A86	35	316	-	-	15/34/90/90	0/3/3/3
37	CLA	18	204	31	-	14/29/105/115	-
46	HEM	f	101	6,5	-	8/14/54/54	-
37	CLA	c	510	3	-	15/39/115/115	-
49	A86	13	314	-	-	9/34/90/90	0/3/3/3
44	DGD	j	101	-	-	16/51/91/95	0/2/2/2
37	CLA	14	310	-	-	4/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	A86	33	312	-	-	8/34/90/90	0/3/3/3
37	CLA	b	501	53	-	18/39/115/115	-
49	A86	15	315	-	-	8/34/90/90	0/3/3/3
49	A86	40	213	48	-	16/34/90/90	0/3/3/3
37	CLA	c	508	3	-	10/39/115/115	-
37	CLA	b	503	2	-	12/39/115/115	-
37	CLA	d	404	4	-	19/39/115/115	-
48	KC1	14	309	27	-	8/15/71/71	-
37	CLA	13	310	-	-	4/15/91/115	-
39	BCR	b	518	-	-	6/29/63/63	0/2/2/2
49	A86	35	314	-	-	14/34/90/90	0/3/3/3
37	CLA	b	508	2	-	5/39/115/115	-
37	CLA	c	504	53	-	11/39/115/115	-
37	CLA	d	403	4	-	9/39/115/115	-
48	KC1	37	305	30	-	9/15/71/71	-
37	CLA	21	206	34	-	17/39/115/115	-
37	CLA	b	510	53	-	8/39/115/115	-
48	KC1	32	212	25	-	5/15/71/71	-
37	CLA	19	303	53	-	17/39/115/115	-
43	LHG	39	314	37	-	28/53/53/53	-
41	LMG	A	408	-	-	32/46/66/70	0/1/1/1
49	A86	16	310	48	-	6/34/90/90	0/3/3/3
37	CLA	11	308	53	-	15/39/115/115	-
49	A86	17	311	-	-	8/34/90/90	0/3/3/3
49	A86	40	201	-	-	14/34/90/90	0/3/3/3
43	LHG	b	522	-	-	19/53/53/53	-
48	KC1	37	307	30	-	5/15/71/71	-
41	LMG	b	519	-	-	15/46/66/70	0/1/1/1
49	A86	32	217	-	-	10/34/90/90	0/3/3/3
37	CLA	21	210	34	-	6/15/91/115	-
37	CLA	41	205	34	-	9/15/91/115	-
40	SQD	a	409	-	-	16/49/69/69	0/1/1/1
37	CLA	B	515	2	-	5/39/115/115	-
37	CLA	15	308	53	-	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	KC1	13	302	26	-	5/15/71/71	-
49	A86	17	313	-	-	8/34/90/90	0/3/3/3
37	CLA	B	513	2	-	9/39/115/115	-
48	KC1	11	304	24	-	4/15/71/71	-
39	BCR	C	515	-	-	7/29/63/63	0/2/2/2
49	A86	12	213	-	-	5/34/90/90	0/3/3/3
37	CLA	35	303	28	-	7/30/106/115	-
37	CLA	B	502	2	-	10/39/115/115	-
37	CLA	39	306	32	-	8/39/115/115	-
37	CLA	12	204	25,37	-	10/39/115/115	-
39	BCR	K	101	-	-	16/29/63/63	0/2/2/2
41	LMG	32	201	-	-	13/34/54/70	0/1/1/1
48	KC1	14	304	27	-	6/15/71/71	-
48	KC1	37	302	30	-	6/15/71/71	-
48	KC1	37	304	30	-	6/15/71/71	-
37	CLA	15	307	28	-	14/24/100/115	-
37	CLA	18	203	31	-	9/39/115/115	-
47	HEC	v	201	16	1/1/3/7	2/14/54/54	-
37	CLA	20	303	33	-	12/29/105/115	-
49	A86	21	214	-	-	6/34/90/90	0/3/3/3
37	CLA	18	208	31	-	13/25/101/115	-
37	CLA	C	511	3	-	8/39/115/115	-
39	BCR	h	101	-	-	8/29/63/63	0/2/2/2
43	LHG	D	411	-	-	26/50/50/53	-
37	CLA	21	205	34	-	9/15/91/115	-
48	KC1	13	304	26	-	7/15/71/71	-
49	A86	32	218	-	-	15/34/90/90	0/3/3/3
49	A86	33	315	-	-	10/34/90/90	0/3/3/3
37	CLA	34	310	-	-	4/15/91/115	-
37	CLA	19	306	32	-	7/39/115/115	-
37	CLA	40	208	33	-	8/21/97/115	-
48	KC1	32	209	25	-	4/15/71/71	-
37	CLA	13	307	26	-	13/24/100/115	-
48	KC1	21	203	34	-	4/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	A86	32	221	-	-	9/34/90/90	0/3/3/3
37	CLA	A	403	1	-	4/39/115/115	-
49	A86	38	213	-	-	9/34/90/90	0/3/3/3
40	SQD	40	202	-	-	25/49/69/69	0/1/1/1
37	CLA	38	202	31	-	14/39/115/115	-
49	A86	13	312	-	-	8/34/90/90	0/3/3/3
37	CLA	11	303	24	-	10/39/115/115	-
49	A86	13	311	-	-	6/34/90/90	0/3/3/3
37	CLA	39	305	32	-	7/23/99/115	-
43	LHG	37	321	-	-	28/49/49/53	-
48	KC1	38	210	31	-	8/15/71/71	-
51	DD6	39	312	-	-	12/26/80/80	0/3/3/3
41	LMG	B	521	-	-	24/46/66/70	0/1/1/1
41	LMG	17	317	-	-	15/32/52/70	0/1/1/1
47	HEC	V	201	16	1/1/3/7	4/14/54/54	-
39	BCR	C	519	-	-	7/29/63/63	0/2/2/2
49	A86	37	309	-	-	12/34/90/90	0/3/3/3
49	A86	17	312	-	-	8/34/90/90	0/3/3/3
49	A86	13	315	-	-	10/34/90/90	0/3/3/3
49	A86	11	312	-	-	6/34/90/90	0/3/3/3
48	KC1	16	305	29	-	6/15/71/71	-
49	A86	32	203	-	-	14/34/90/90	0/3/3/3
37	CLA	C	509	3	-	8/39/115/115	-
37	CLA	35	301	28	-	10/39/115/115	-
49	A86	11	319	-	-	7/34/90/90	0/3/3/3
37	CLA	B	508	2	-	5/39/115/115	-
37	CLA	c	512	3	-	8/39/115/115	-
45	PL9	d	406	-	-	10/53/73/73	0/1/1/1
38	PHO	a	406	-	-	6/37/103/103	0/5/6/6
49	A86	17	315	-	-	13/34/90/90	0/3/3/3
37	CLA	32	210	25	-	15/24/100/115	-
37	CLA	B	504	2	-	6/39/115/115	-
40	SQD	B	519	-	-	25/49/69/69	0/1/1/1
48	KC1	36	305	29	-	6/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	A86	11	311	-	-	7/34/90/90	0/3/3/3
49	A86	34	316	-	-	15/34/90/90	0/3/3/3
49	A86	21	215	37	-	6/34/90/90	0/3/3/3
37	CLA	z	101	53	-	20/39/115/115	-
49	A86	31	313	-	-	6/34/90/90	1/3/3/3
37	CLA	c	507	53	-	7/39/115/115	-
43	LHG	d	407	-	-	28/53/53/53	-
49	A86	11	313	-	-	7/34/90/90	1/3/3/3
49	A86	14	315	-	-	6/34/90/90	0/3/3/3
37	CLA	B	512	2	-	8/39/115/115	-
48	KC1	35	304	28	-	6/15/71/71	-
37	CLA	20	307	33	-	8/15/91/115	-
48	KC1	11	306	24	-	9/15/71/71	-
48	KC1	38	205	31	-	7/15/71/71	-
37	CLA	13	301	26	-	14/39/115/115	-
48	KC1	20	305	33	-	11/15/71/71	-
37	CLA	35	307	28	-	14/24/100/115	-
48	KC1	16	302	29	-	2/15/71/71	-
37	CLA	12	212	-	-	8/15/91/115	-
37	CLA	33	305	-	-	4/15/91/115	-
48	KC1	15	306	28	-	7/15/71/71	-
37	CLA	32	213	-	-	8/15/91/115	-
37	CLA	21	202	34	-	9/30/106/115	-
37	CLA	41	202	34	-	9/30/106/115	-
43	LHG	a	412	-	-	26/50/50/53	-
40	SQD	17	301	-	-	25/44/64/69	0/1/1/1
37	CLA	C	501	3	-	13/39/115/115	-
37	CLA	C	506	3	-	14/39/115/115	-
39	BCR	B	517	-	-	6/29/63/63	0/2/2/2
37	CLA	39	302	32	-	15/39/115/115	-
37	CLA	12	207	39,53	-	2/21/97/115	-
39	BCR	a	413	-	-	8/29/63/63	0/2/2/2
49	A86	39	311	-	-	7/34/90/90	0/3/3/3
39	BCR	c	515	-	-	7/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	A86	37	319	-	-	8/34/90/90	0/3/3/3
49	A86	34	311	-	-	7/34/90/90	0/3/3/3
37	CLA	31	301	-	-	21/39/115/115	-
37	CLA	39	310	32	-	9/39/115/115	-
37	CLA	36	307	53	-	12/35/111/115	-
40	SQD	B	522	-	-	12/32/52/69	0/1/1/1
49	A86	39	313	-	-	7/34/90/90	0/3/3/3
37	CLA	32	204	25	-	14/39/115/115	-
49	A86	34	313	-	-	12/34/90/90	0/3/3/3
37	CLA	b	514	2,41	-	16/36/112/115	-
52	LMU	19	315	-	-	6/21/61/61	0/2/2/2
37	CLA	35	310	-	-	4/15/91/115	-
37	CLA	40	205	33	-	12/29/105/115	-
37	CLA	13	305	-	-	4/15/91/115	-
48	KC1	33	309	26	-	5/15/71/71	-
48	KC1	39	308	32	-	3/15/71/71	-
37	CLA	C	507	53	-	7/39/115/115	-
49	A86	33	313	-	-	17/34/90/90	0/3/3/3
37	CLA	19	309	32	-	5/15/91/115	-
37	CLA	b	506	2	-	8/39/115/115	-
38	PHO	D	403	-	-	10/37/103/103	0/5/6/6
48	KC1	41	203	34	-	4/15/71/71	-
39	BCR	c	519	-	-	7/29/63/63	0/2/2/2
51	DD6	21	216	-	-	15/26/80/80	0/3/3/3
37	CLA	C	512	3	-	8/39/115/115	-
49	A86	20	309	-	-	6/34/90/90	0/3/3/3
37	CLA	18	206	-	-	6/15/91/115	-
49	A86	17	314	-	-	8/34/90/90	0/3/3/3
37	CLA	34	303	27	-	6/30/106/115	-
48	KC1	19	308	32	-	3/15/71/71	-
37	CLA	C	504	53	-	11/39/115/115	-
37	CLA	b	502	2	-	10/39/115/115	-
41	LMG	11	316	-	-	19/37/57/70	0/1/1/1
49	A86	40	211	-	-	6/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	KC1	36	302	29	-	2/15/71/71	-
37	CLA	34	301	27	-	15/39/115/115	-
44	DGD	H	102	-	-	16/51/91/95	0/2/2/2
37	CLA	b	513	2	-	9/39/115/115	-
37	CLA	20	301	33	-	13/29/105/115	-
37	CLA	12	205	25	-	13/39/115/115	-
37	CLA	16	306	29	-	16/39/115/115	-
51	DD6	40	212	-	-	14/26/80/80	0/3/3/3
49	A86	34	315	-	-	6/34/90/90	0/3/3/3
41	LMG	D	412	-	-	14/46/66/70	0/1/1/1
48	KC1	21	207	34	-	5/15/71/71	-
37	CLA	c	501	3	-	13/39/115/115	-
37	CLA	B	516	2	-	13/39/115/115	-
49	A86	15	311	-	-	6/34/90/90	0/3/3/3
48	KC1	16	304	29	-	6/15/71/71	-
49	A86	33	314	-	-	9/34/90/90	0/3/3/3
48	KC1	20	304	33	-	7/15/71/71	-
37	CLA	16	307	53	-	12/35/111/115	-
43	LHG	19	314	37	-	28/53/53/53	-
37	CLA	36	309	29	-	8/15/91/115	-
39	BCR	c	514	-	-	6/29/63/63	0/2/2/2
49	A86	21	213	-	-	8/34/90/90	0/3/3/3
49	A86	13	313	-	-	17/34/90/90	0/3/3/3

The worst 5 of 8924 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	20	312	DD6	C10-C11	25.78	1.70	1.35
51	40	214	DD6	C10-C11	25.69	1.69	1.35
51	41	212	DD6	C10-C11	25.53	1.69	1.35
51	39	312	DD6	C10-C11	25.49	1.69	1.35
51	41	216	DD6	C10-C11	25.49	1.69	1.35

The worst 5 of 12166 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	17	314	A86	O1-C20-C19	57.83	156.82	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	37	313	A86	O1-C20-C19	57.77	156.78	113.38
49	39	313	A86	O1-C20-C19	57.61	156.66	113.38
49	40	213	A86	O1-C20-C19	57.29	156.42	113.38
49	20	311	A86	O1-C20-C19	57.26	156.40	113.38

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
47	V	201	HEC	NA
47	v	201	HEC	NA

5 of 5382 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
37	B	501	CLA	CHA-CBD-CGD-O1D
37	B	501	CLA	CHA-CBD-CGD-O2D
37	B	503	CLA	C2B-C3B-CAB-CBB
37	B	503	CLA	C4B-C3B-CAB-CBB
37	B	504	CLA	C2B-C3B-CAB-CBB

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
49	31	313	A86	C31-C32-C33-C34-C35-C36
49	11	313	A86	C31-C32-C33-C34-C35-C36

281 monomers are involved in 582 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	15	303	CLA	1	0
41	16	316	LMG	1	0
37	B	503	CLA	2	0
40	36	315	SQD	3	0
39	B	518	BCR	2	0
37	19	305	CLA	2	0
39	D	407	BCR	4	0
37	11	307	CLA	4	0
37	39	307	CLA	3	0
37	38	203	CLA	2	0
49	31	311	A86	2	0
37	18	211	CLA	1	0
37	c	506	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	A	410	BCR	2	0
37	b	509	CLA	2	0
42	A	409	BCT	1	0
37	18	201	CLA	6	0
37	19	310	CLA	5	0
37	38	208	CLA	3	0
37	13	308	CLA	4	0
40	A	407	SQD	1	0
37	B	501	CLA	1	0
37	A	405	CLA	6	0
48	40	204	KC1	1	0
37	41	209	CLA	1	0
37	z	102	CLA	1	0
37	14	308	CLA	1	0
37	33	307	CLA	1	0
37	B	506	CLA	3	0
51	19	312	DD6	2	0
39	B	525	BCR	2	0
37	Z	101	CLA	3	0
49	31	319	A86	1	0
37	18	202	CLA	2	0
37	B	511	CLA	1	0
39	5	101	BCR	3	0
37	W	102	CLA	2	0
45	D	408	PL9	1	0
42	a	411	BCT	1	0
37	b	504	CLA	5	0
37	31	302	CLA	1	0
37	35	308	CLA	6	0
37	37	308	CLA	1	0
37	C	510	CLA	4	0
51	20	312	DD6	1	0
43	17	316	LHG	1	0
49	14	311	A86	1	0
46	F	101	HEM	2	0
38	A	404	PHO	2	0
49	38	212	A86	1	0
37	39	303	CLA	1	0
37	B	509	CLA	2	0
37	39	301	CLA	2	0
37	14	303	CLA	1	0
37	33	310	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
41	a	410	LMG	4	0
49	33	311	A86	1	0
41	B	520	LMG	3	0
49	18	212	A86	1	0
48	33	302	KC1	1	0
37	14	302	CLA	3	0
37	19	302	CLA	3	0
37	C	505	CLA	1	0
37	c	513	CLA	2	0
45	d	402	PL9	2	0
37	17	307	CLA	1	0
37	b	516	CLA	1	0
44	J	101	DGD	1	0
48	20	302	KC1	1	0
39	0	101	BCR	5	0
37	B	514	CLA	3	0
37	32	206	CLA	3	0
37	19	301	CLA	1	0
37	34	302	CLA	3	0
37	B	505	CLA	2	0
37	Z	102	CLA	2	0
37	19	307	CLA	2	0
48	17	303	KC1	2	0
37	B	524	CLA	3	0
51	40	214	DD6	1	0
41	b	520	LMG	4	0
37	B	507	CLA	2	0
37	b	511	CLA	1	0
43	D	409	LHG	1	0
37	D	406	CLA	2	0
40	b	521	SQD	1	0
37	a	404	CLA	2	0
37	32	211	CLA	2	0
37	a	403	CLA	6	0
37	c	505	CLA	2	0
37	12	203	CLA	2	0
41	d	409	LMG	2	0
39	b	524	BCR	2	0
48	31	309	KC1	1	0
43	D	410	LHG	2	0
37	36	301	CLA	4	0
37	b	515	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	c	503	CLA	4	0
49	34	314	A86	1	0
39	b	517	BCR	4	0
37	34	308	CLA	1	0
37	18	209	CLA	1	0
38	a	405	PHO	2	0
37	W	101	CLA	3	0
48	36	304	KC1	1	0
37	11	301	CLA	1	0
37	38	201	CLA	4	0
39	a	408	BCR	5	0
37	12	210	CLA	2	0
37	15	301	CLA	5	0
48	18	205	KC1	1	0
37	c	511	CLA	5	0
41	L	102	LMG	2	0
40	L	101	SQD	3	0
37	40	203	CLA	1	0
37	b	523	CLA	4	0
44	C	516	DGD	4	0
37	32	205	CLA	2	0
37	17	309	CLA	4	0
37	c	509	CLA	1	0
49	35	311	A86	1	0
37	37	301	CLA	2	0
41	C	518	LMG	1	0
37	31	308	CLA	3	0
37	b	512	CLA	3	0
37	33	308	CLA	4	0
37	a	407	CLA	6	0
37	19	304	CLA	2	0
37	37	306	CLA	1	0
43	d	408	LHG	2	0
37	14	307	CLA	1	0
37	36	306	CLA	2	0
43	21	217	LHG	3	0
44	c	516	DGD	4	0
40	16	315	SQD	1	0
37	C	502	CLA	4	0
37	21	208	CLA	1	0
37	C	513	CLA	2	0
37	41	208	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	34	307	CLA	1	0
37	D	401	CLA	2	0
37	D	405	CLA	4	0
39	d	405	BCR	3	0
37	38	211	CLA	1	0
37	17	302	CLA	3	0
37	C	503	CLA	3	0
37	b	505	CLA	3	0
48	40	206	KC1	1	0
37	b	507	CLA	2	0
43	37	315	LHG	1	0
37	w	101	CLA	1	0
41	l	101	LMG	1	0
37	21	209	CLA	1	0
37	14	301	CLA	2	0
37	c	502	CLA	5	0
37	32	202	CLA	4	0
39	H	101	BCR	2	0
37	C	508	CLA	2	0
39	C	514	BCR	2	0
41	c	518	LMG	3	0
39	A	406	BCR	4	0
37	20	306	CLA	1	0
49	14	314	A86	1	0
37	41	206	CLA	2	0
39	y	101	BCR	4	0
44	h	102	DGD	3	0
37	31	304	CLA	1	0
45	D	404	PL9	4	0
37	16	309	CLA	1	0
37	16	301	CLA	4	0
46	f	101	HEM	2	0
37	c	510	CLA	4	0
44	j	101	DGD	2	0
37	b	501	CLA	3	0
37	c	508	CLA	1	0
37	b	503	CLA	3	0
37	d	404	CLA	1	0
37	13	310	CLA	2	0
39	b	518	BCR	2	0
37	b	508	CLA	1	0
37	c	504	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	d	403	CLA	4	0
37	21	206	CLA	5	0
37	19	303	CLA	1	0
43	39	314	LHG	8	0
41	A	408	LMG	4	0
37	11	308	CLA	5	0
41	b	519	LMG	4	0
37	B	515	CLA	1	0
37	15	308	CLA	2	0
37	B	513	CLA	2	0
39	C	515	BCR	2	0
37	B	502	CLA	4	0
37	39	306	CLA	1	0
37	12	204	CLA	2	0
39	K	101	BCR	4	0
48	37	302	KC1	2	0
37	15	307	CLA	1	0
37	18	203	CLA	3	0
47	v	201	HEC	2	0
37	18	208	CLA	4	0
37	C	511	CLA	4	0
39	h	101	BCR	1	0
43	D	411	LHG	3	0
37	19	306	CLA	1	0
37	40	208	CLA	1	0
37	13	307	CLA	1	0
37	A	403	CLA	4	0
40	40	202	SQD	2	0
37	11	303	CLA	1	0
49	13	311	A86	1	0
37	39	305	CLA	2	0
43	37	321	LHG	3	0
51	39	312	DD6	2	0
41	B	521	LMG	4	0
39	C	519	BCR	1	0
47	V	201	HEC	4	0
37	C	509	CLA	1	0
37	35	301	CLA	4	0
49	11	319	A86	1	0
37	B	508	CLA	2	0
37	c	512	CLA	3	0
45	d	406	PL9	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	a	406	PHO	1	0
37	32	210	CLA	1	0
37	B	504	CLA	5	0
40	B	519	SQD	3	0
49	11	311	A86	1	0
37	z	101	CLA	2	0
49	31	313	A86	11	0
43	d	407	LHG	1	0
49	11	313	A86	9	0
49	14	315	A86	1	0
37	B	512	CLA	3	0
48	11	306	KC1	4	0
48	38	205	KC1	2	0
37	35	307	CLA	1	0
37	12	212	CLA	1	0
37	32	213	CLA	1	0
37	21	202	CLA	2	0
37	41	202	CLA	2	0
43	a	412	LHG	3	0
40	17	301	SQD	3	0
37	C	501	CLA	3	0
37	C	506	CLA	2	0
39	B	517	BCR	3	0
37	39	302	CLA	3	0
37	12	207	CLA	1	0
39	c	515	BCR	2	0
49	34	311	A86	1	0
37	31	301	CLA	2	0
37	39	310	CLA	5	0
37	36	307	CLA	4	0
40	B	522	SQD	2	0
49	39	313	A86	1	0
37	32	204	CLA	3	0
37	b	514	CLA	3	0
37	35	310	CLA	1	0
37	40	205	CLA	1	0
37	b	506	CLA	3	0
38	D	403	PHO	1	0
37	C	512	CLA	4	0
37	34	303	CLA	1	0
37	C	504	CLA	2	0
37	b	502	CLA	7	0

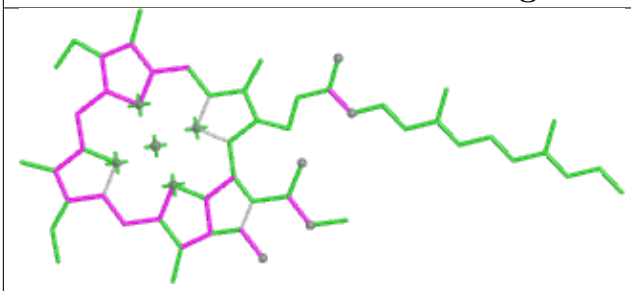
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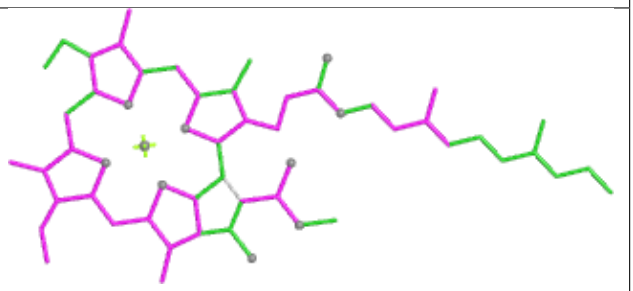
Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	34	301	CLA	2	0
44	H	102	DGD	2	0
37	b	513	CLA	2	0
37	20	301	CLA	1	0
37	12	205	CLA	3	0
49	34	315	A86	1	0
41	D	412	LMG	2	0
37	c	501	CLA	4	0
37	B	516	CLA	2	0
49	15	311	A86	1	0
48	16	304	KC1	1	0
48	20	304	KC1	1	0
37	16	307	CLA	3	0
43	19	314	LHG	10	0
37	36	309	CLA	1	0
39	c	514	BCR	2	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.

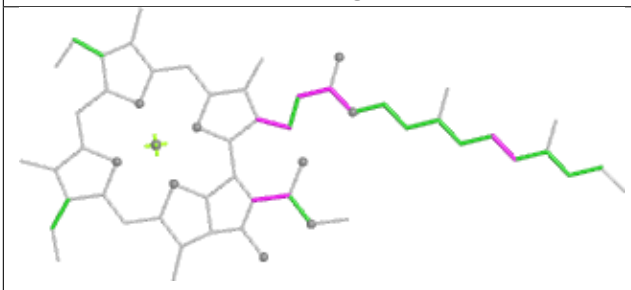
Ligand CLA 15 303



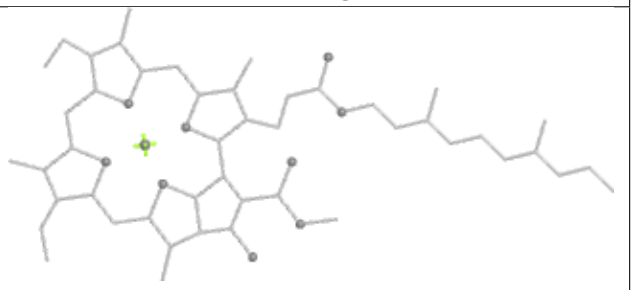
Bond lengths



Bond angles

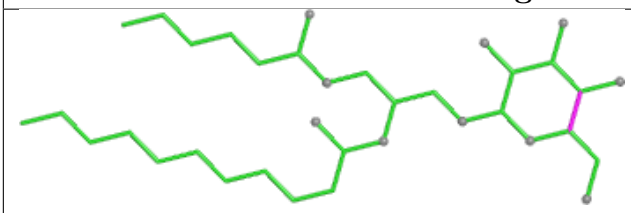


Torsions

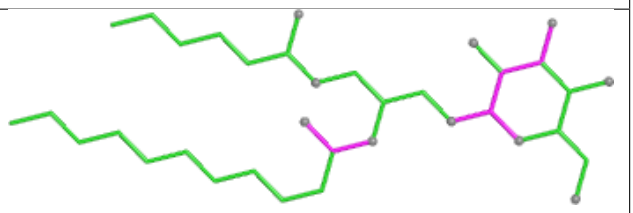


Rings

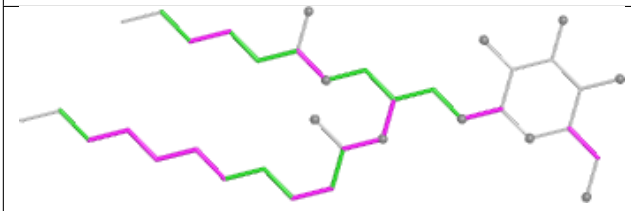
Ligand LMG 16 316



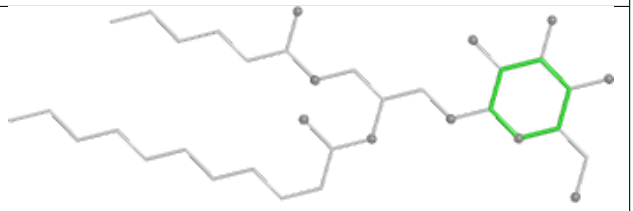
Bond lengths



Bond angles

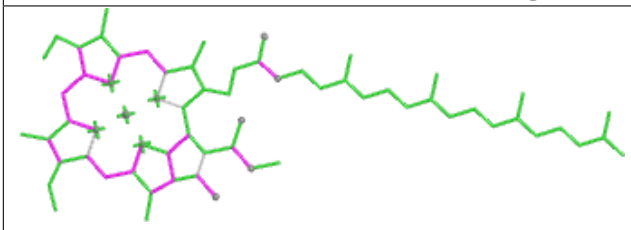


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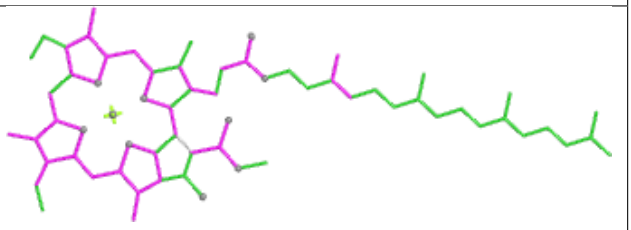


Rings

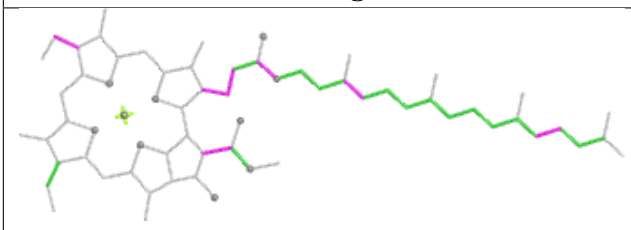
Ligand CLA B 503



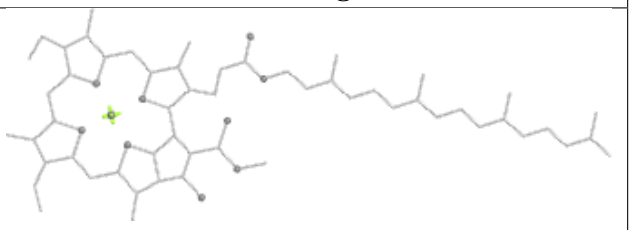
Bond lengths



Bond angles

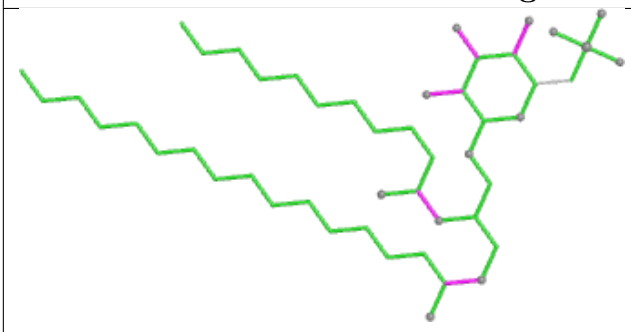


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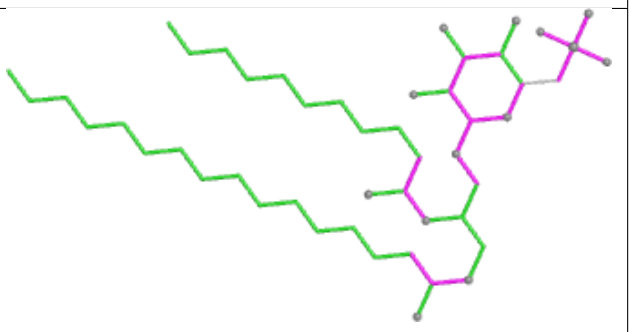


Rings

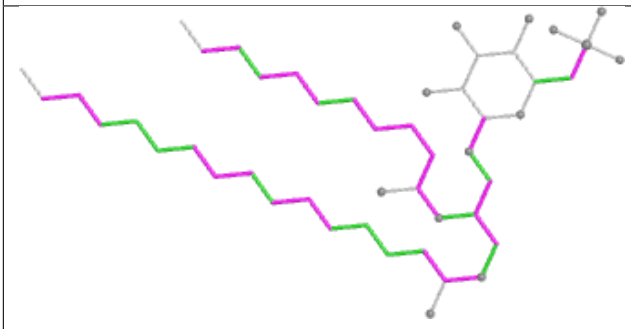
Ligand SQD 36 315



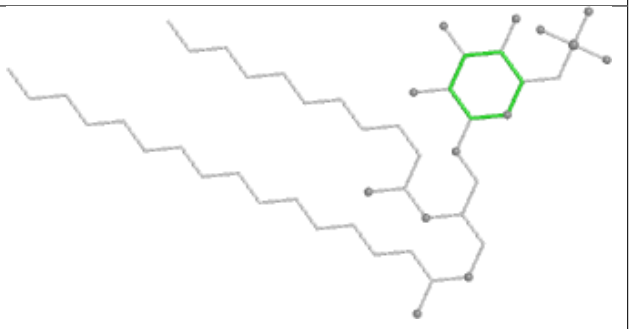
Bond lengths



Bond angles

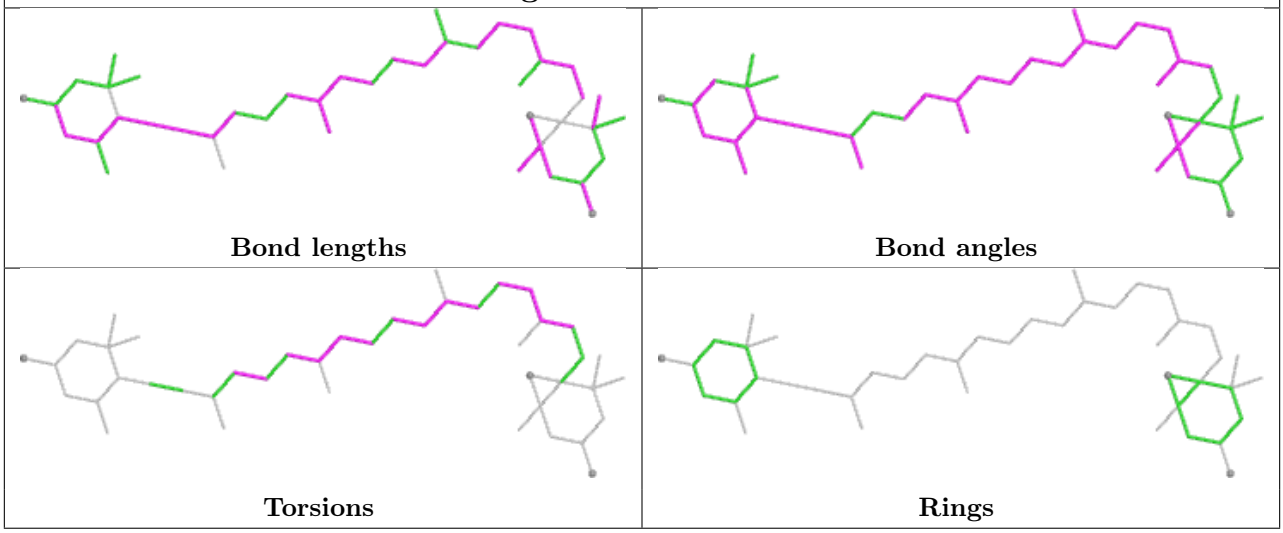


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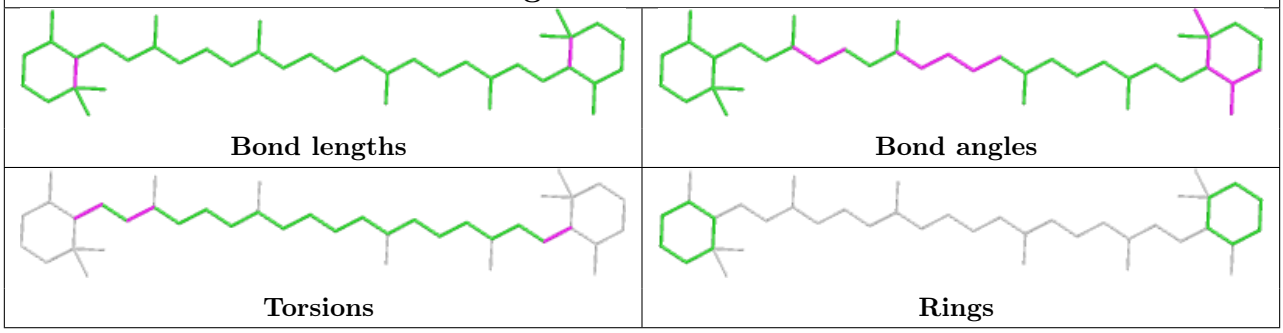


Rings

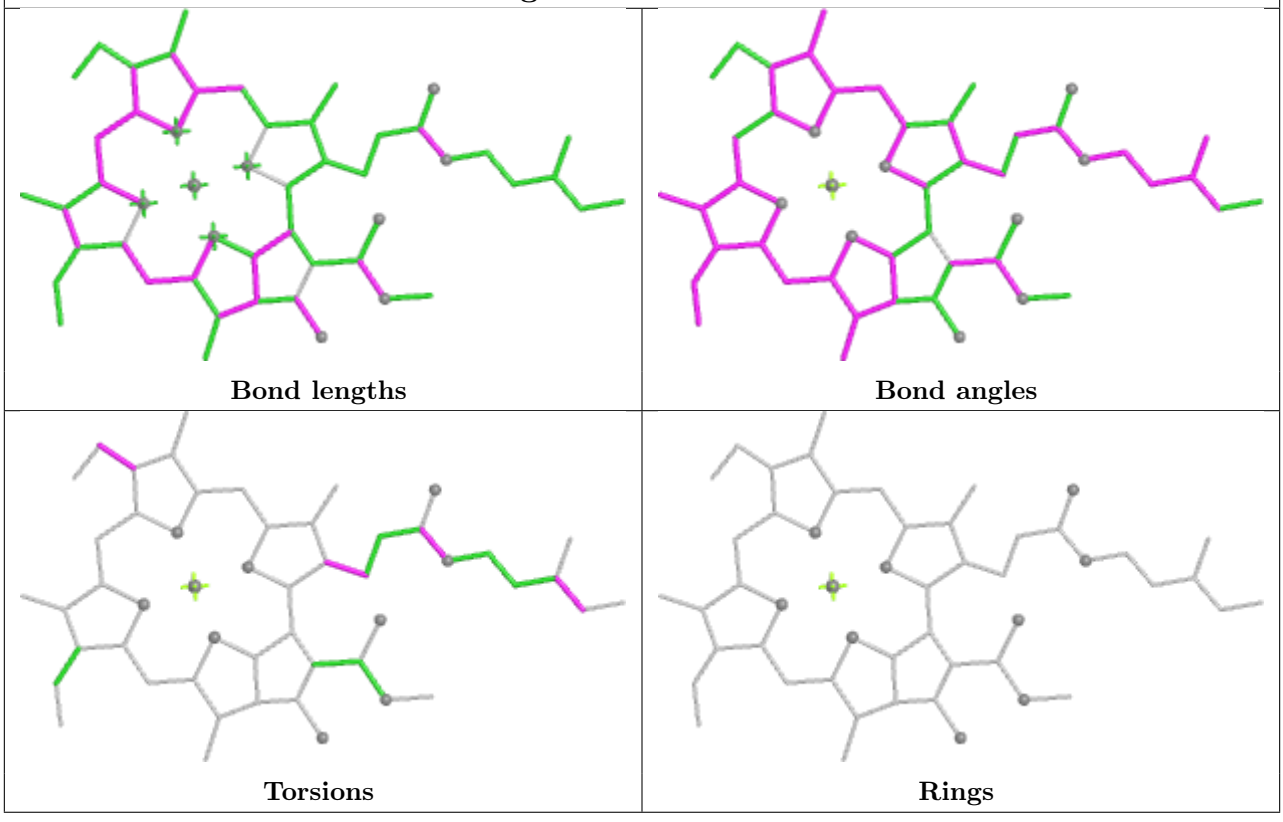
Ligand DD6 20 310



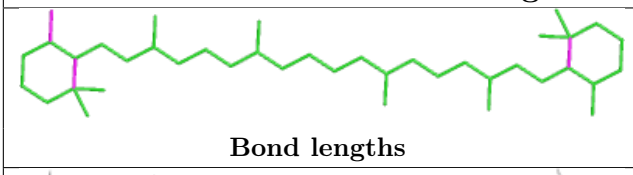
Ligand BCR B 518



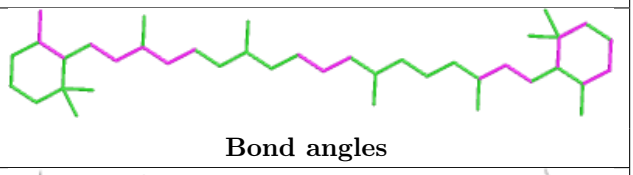
Ligand CLA 19 305



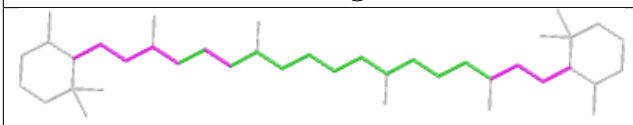
Ligand BCR D 407



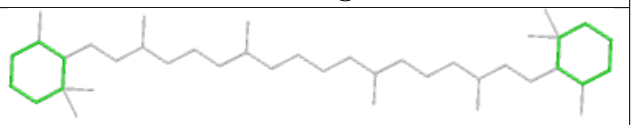
Bond lengths



Bond angles

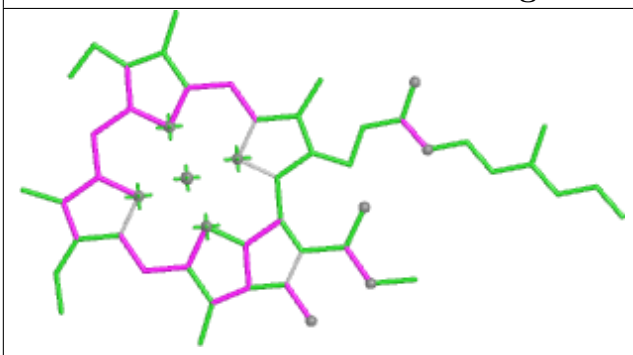


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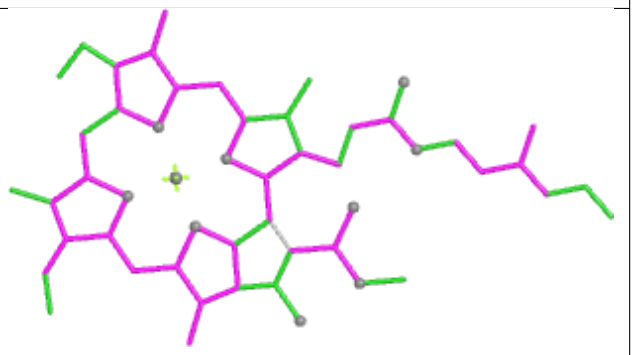


Rings

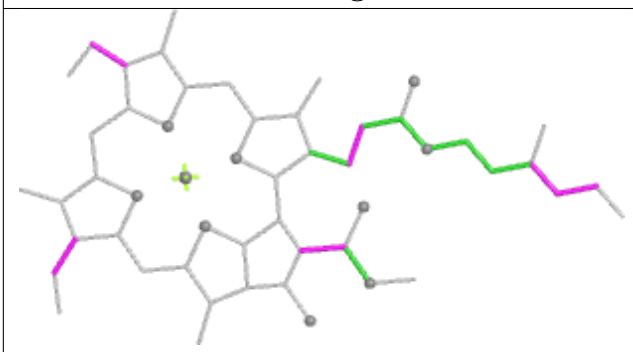
Ligand CLA 11 307



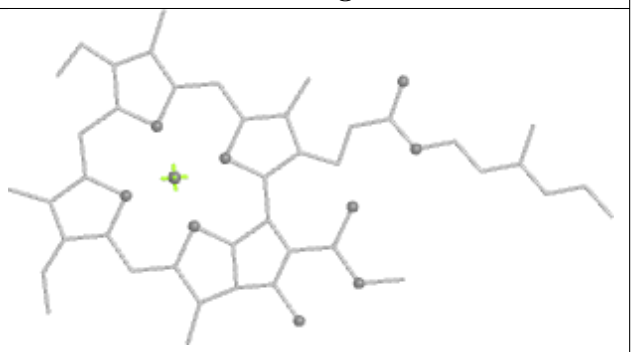
Bond lengths



Bond angles

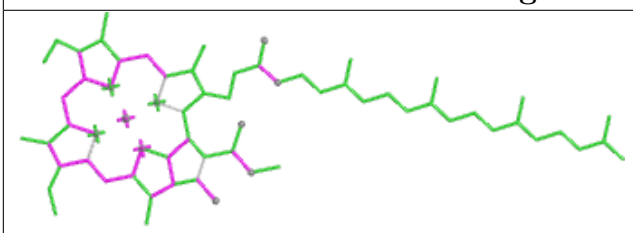


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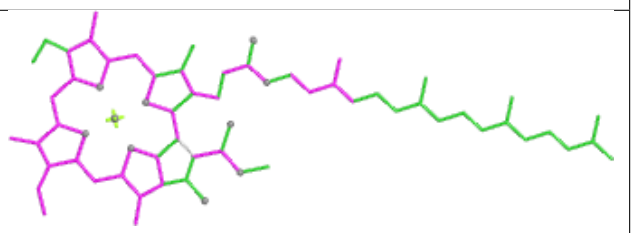


Rings

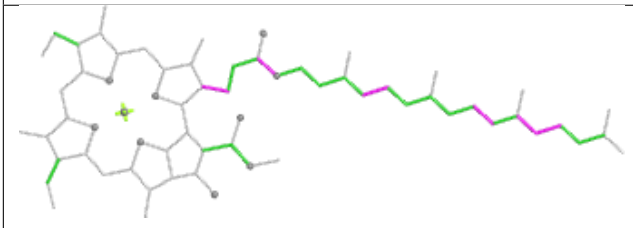
Ligand CLA 39 307



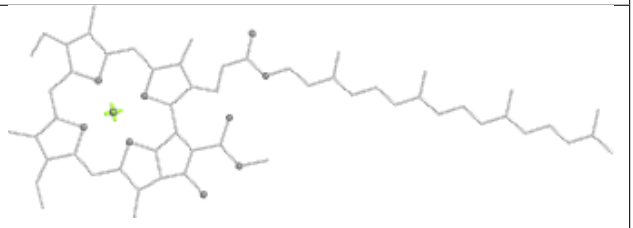
Bond lengths



Bond angles

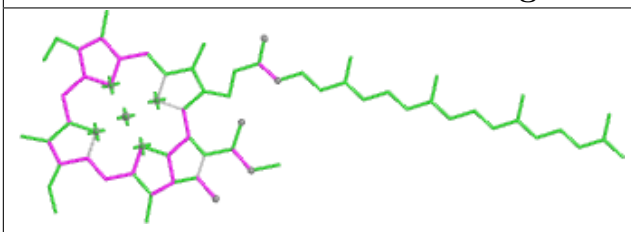


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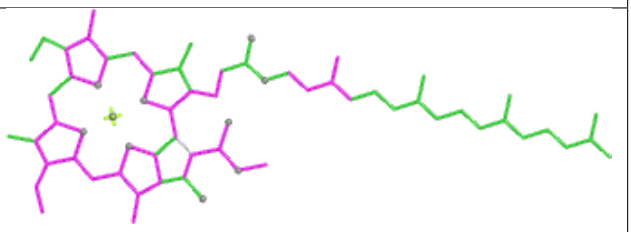


Rings

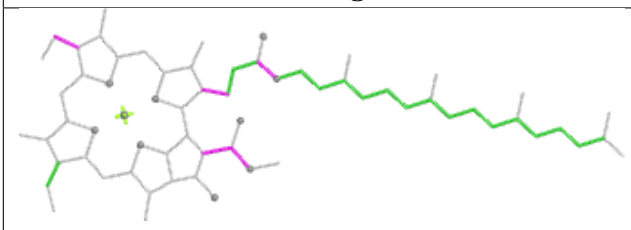
Ligand CLA 38 203



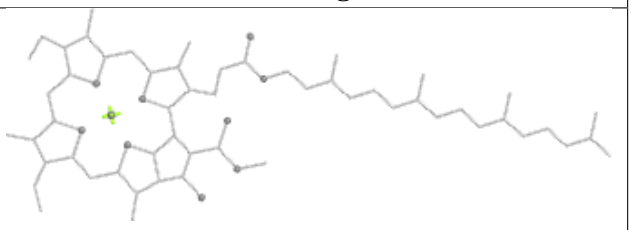
Bond lengths



Bond angles

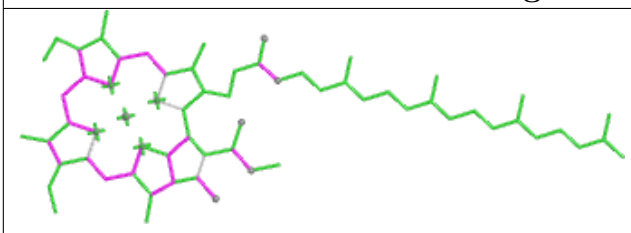


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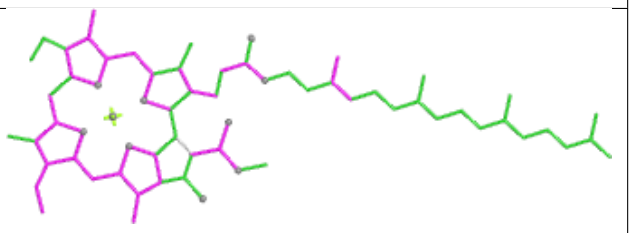


Rings

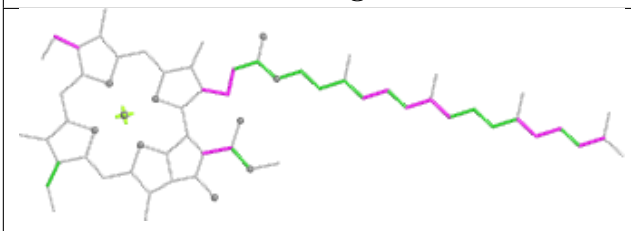
Ligand CLA D 402



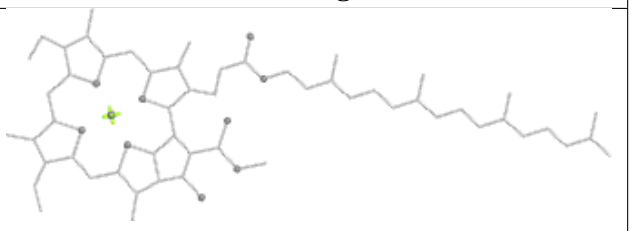
Bond lengths



Bond angles

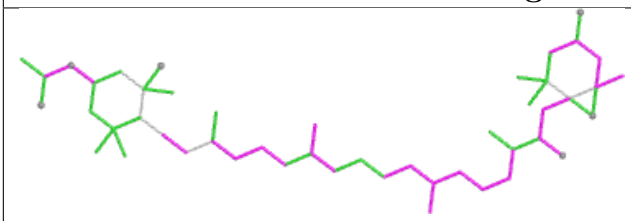


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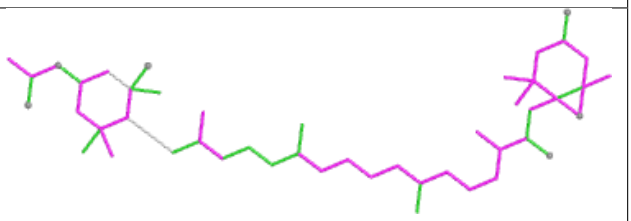


Rings

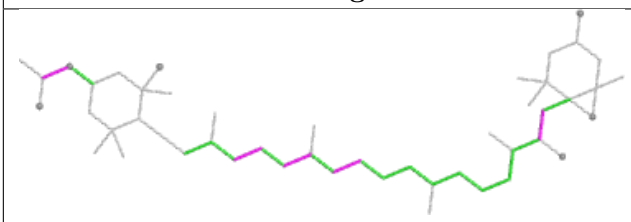
Ligand A86 31 311



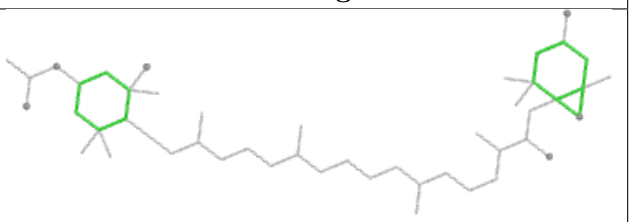
Bond lengths



Bond angles

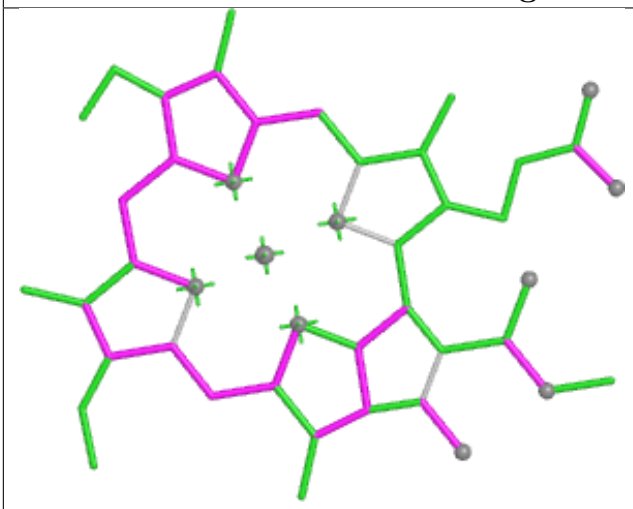


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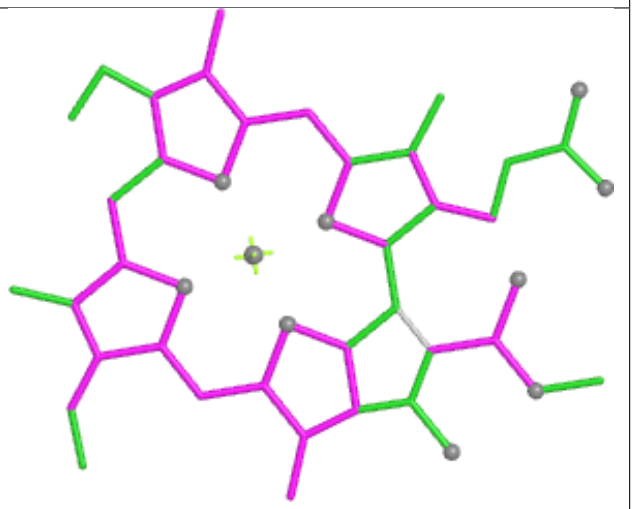


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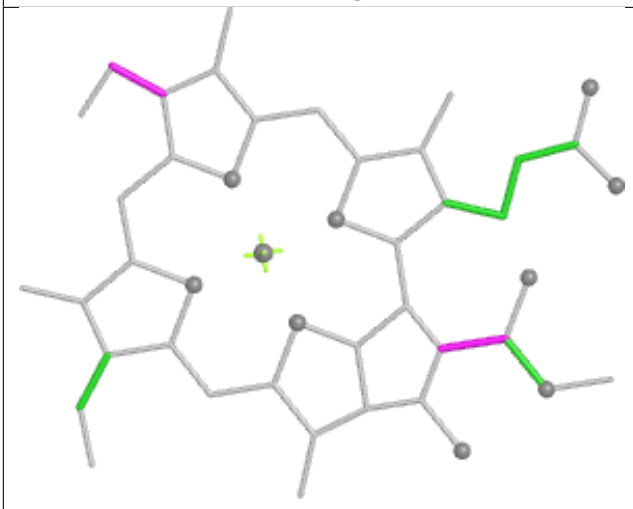
Ligand CLA 18 211



Bond lengths



Bond angles

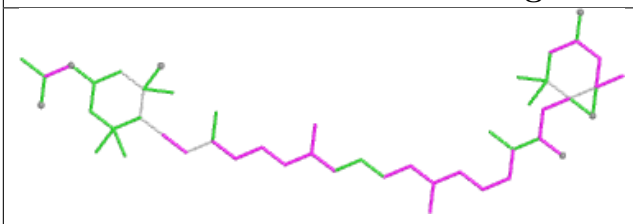


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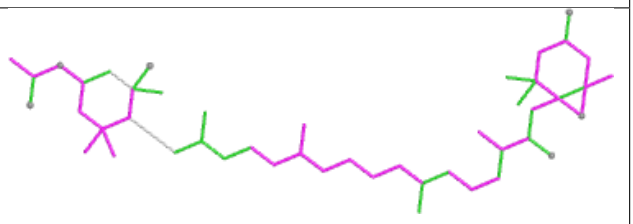


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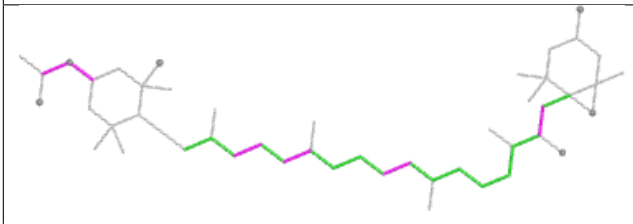
Ligand A86 37 311



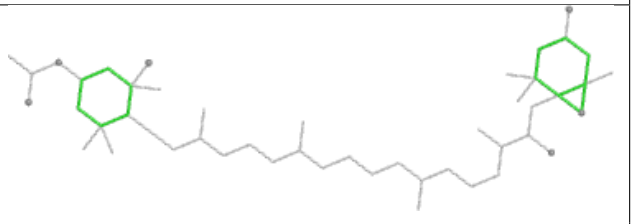
Bond lengths



Bond angles

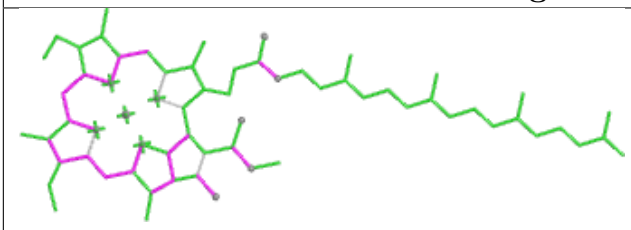


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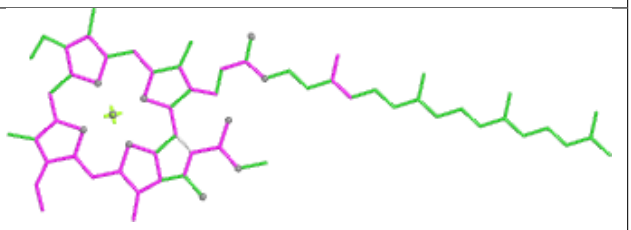


Rings

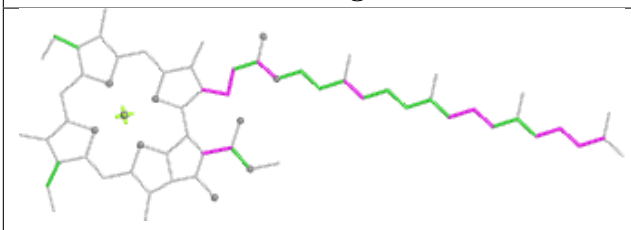
Ligand CLA c 506



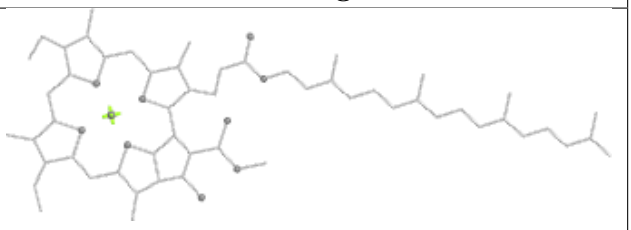
Bond lengths



Bond angles

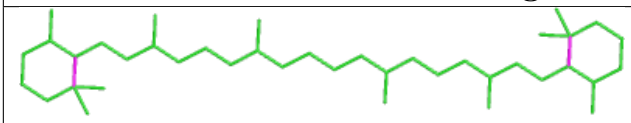


Torsions

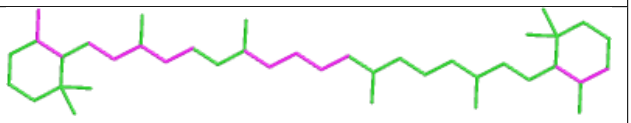


Rings

Ligand BCR A 410



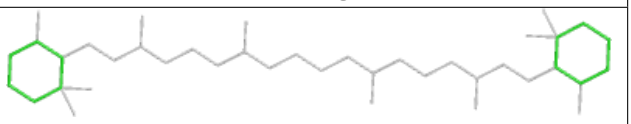
Bond lengths



Bond angles

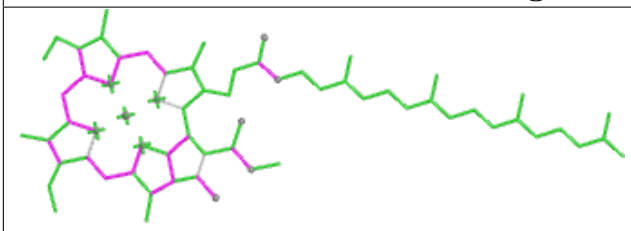


Torsions

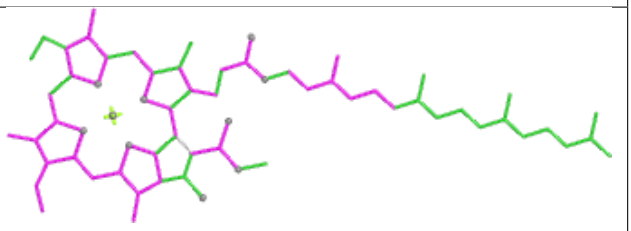


Rings

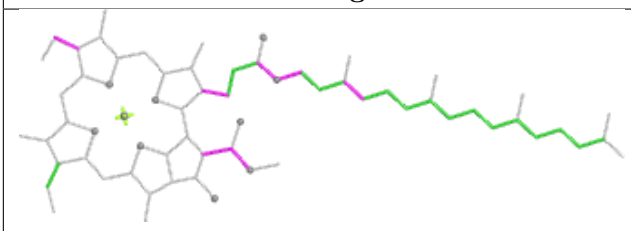
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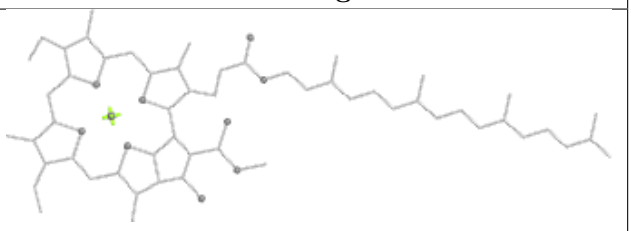
Bond lengths



Bond angles

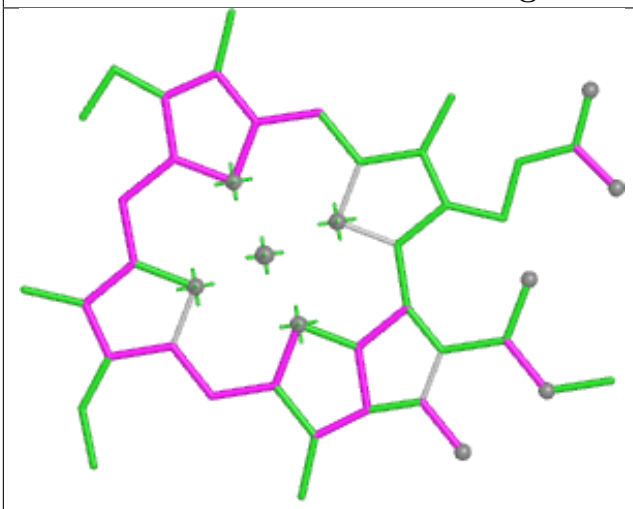


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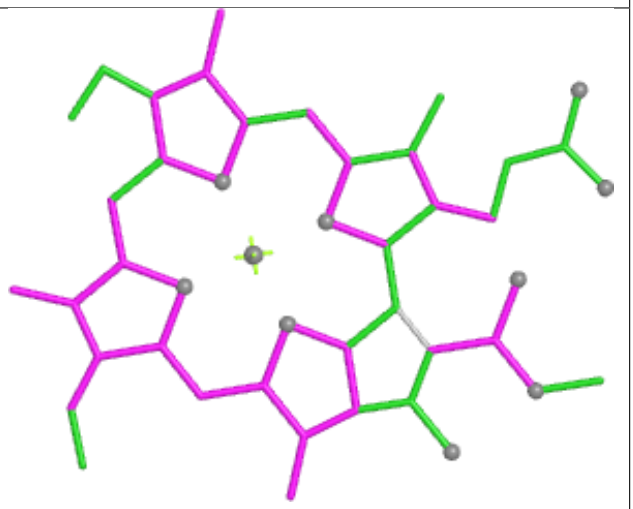


Rings

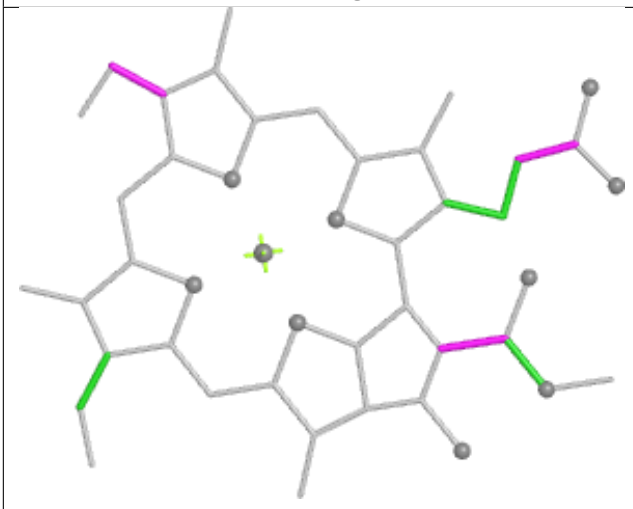
Ligand CLA 41 210



Bond lengths



Bond angles

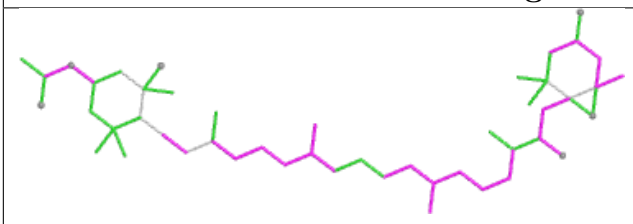


Torsions

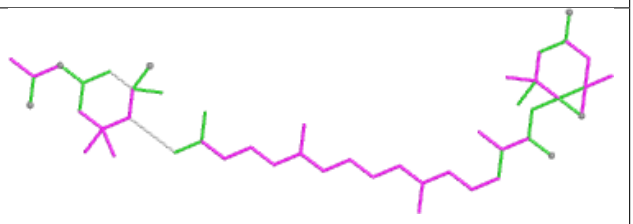


Rings

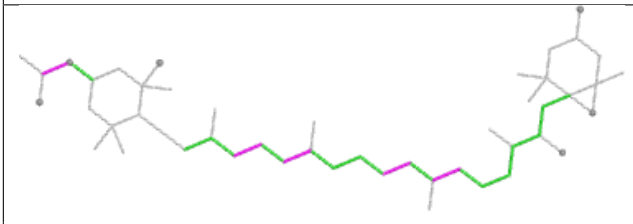
Ligand A86 17 320



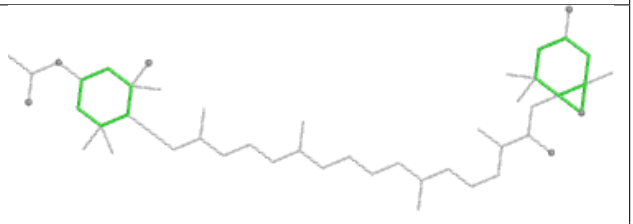
Bond lengths



Bond angles

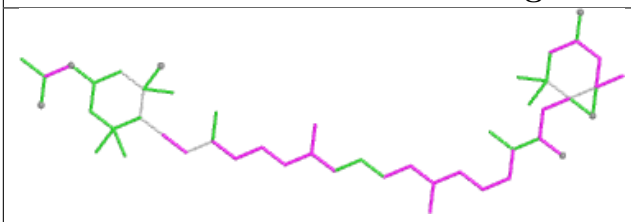


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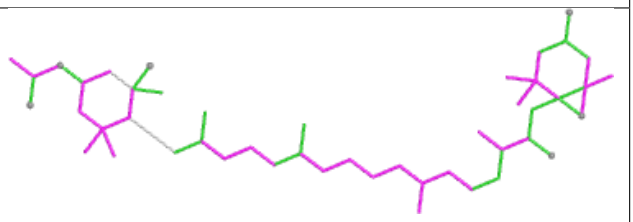


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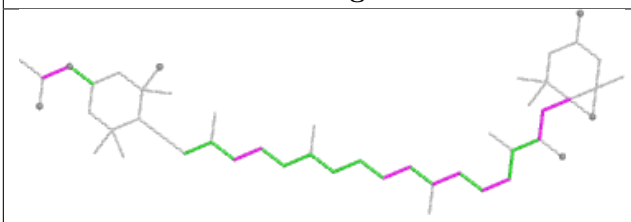
Ligand A86 18 213



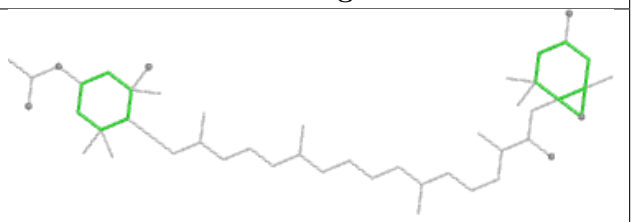
Bond lengths



Bond angles

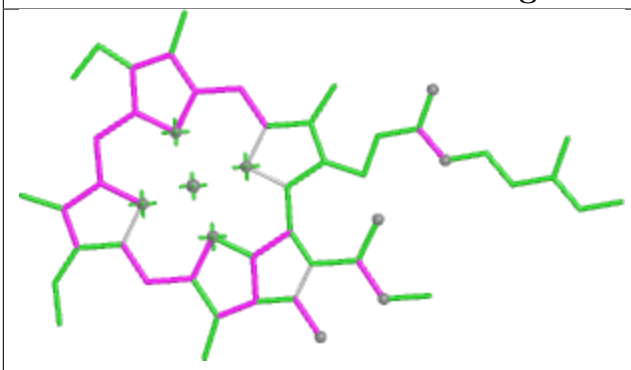


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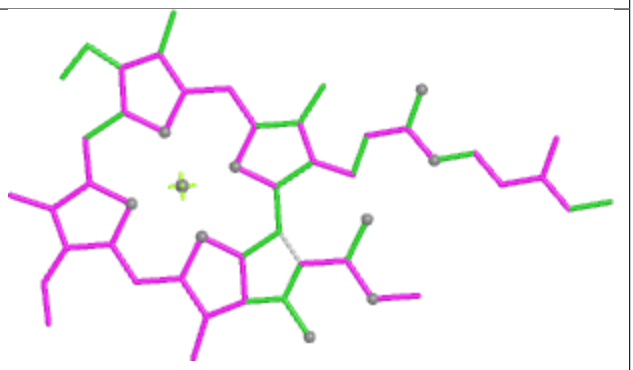


Rings

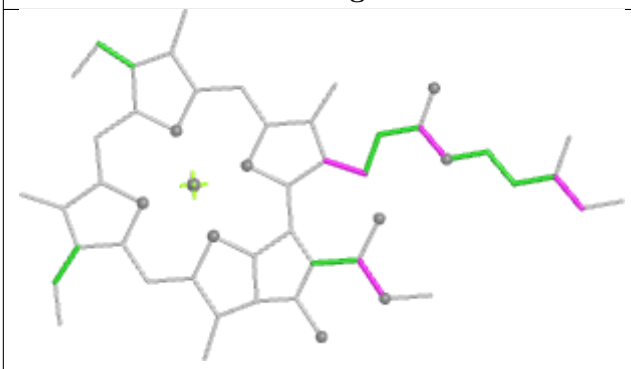
Ligand CLA 31 310



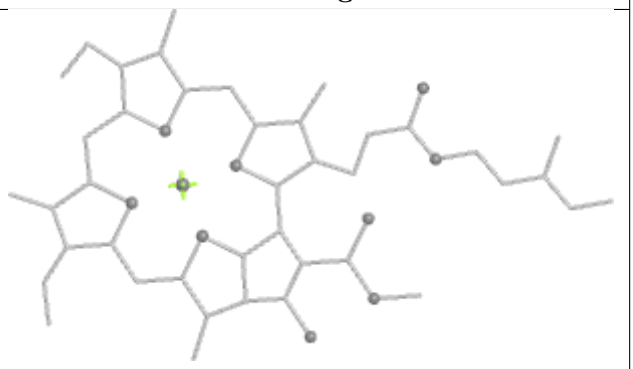
Bond lengths



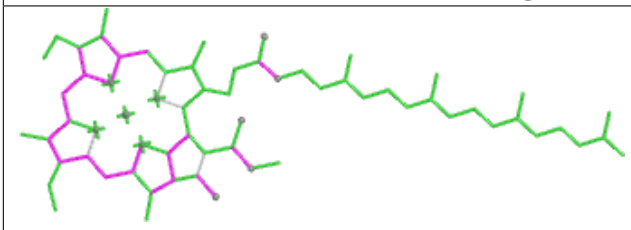
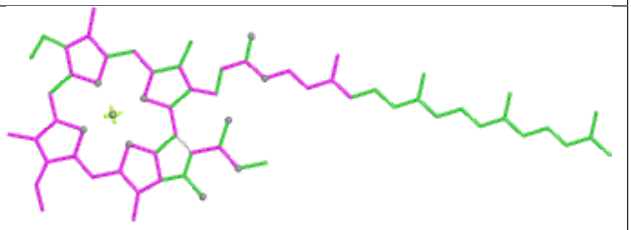
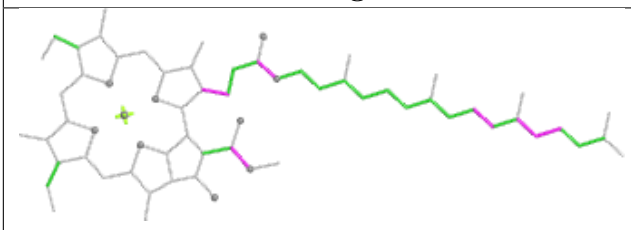
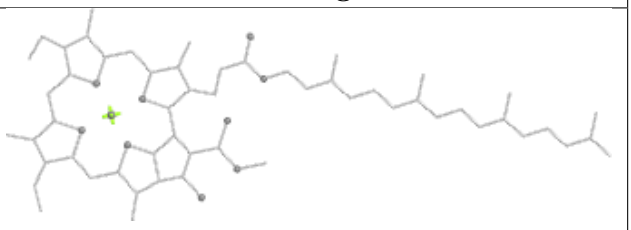
Bond angles

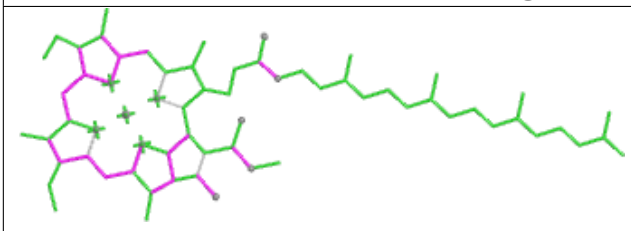
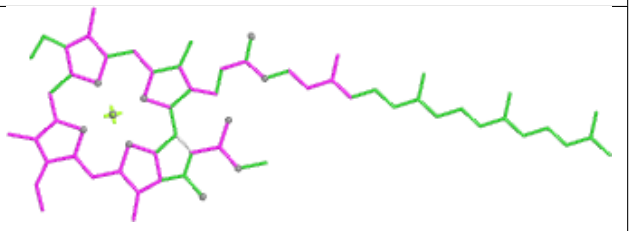
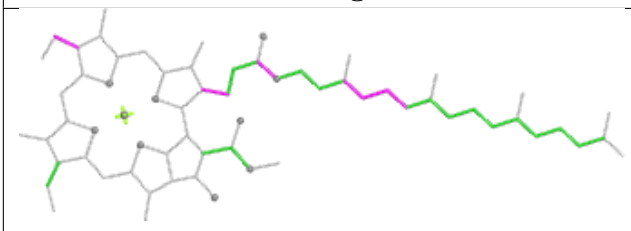
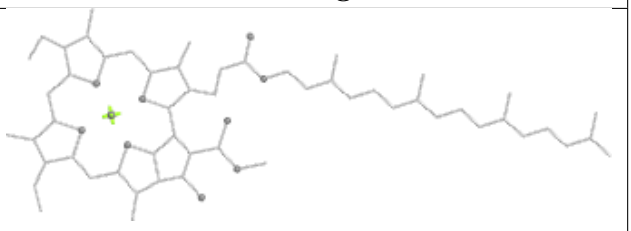


Torsions

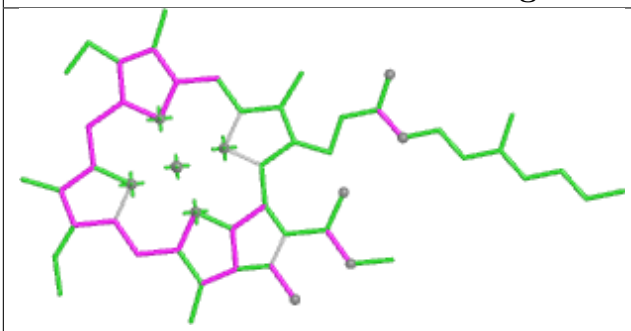


Rings

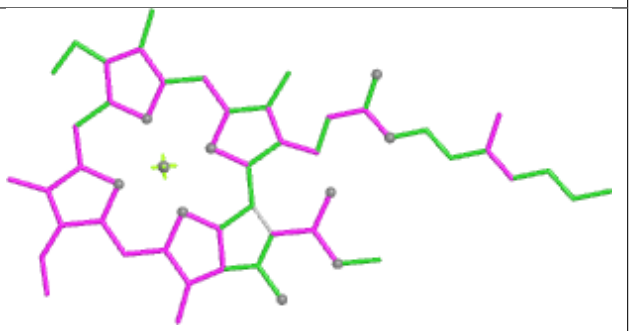
Ligand CLA 18 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 19 310	
 Bond lengths	 Bond angles
 Torsions	 Rings

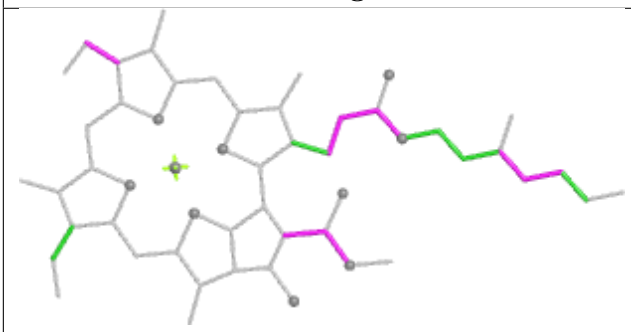
Ligand CLA 38 208



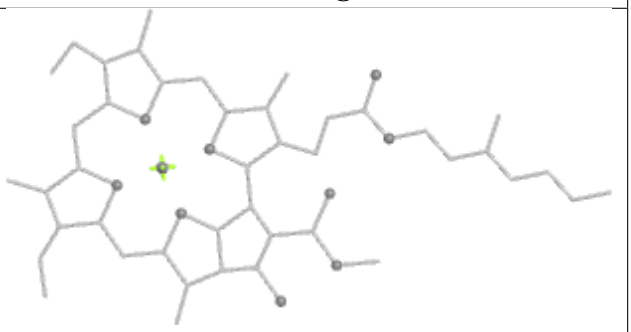
Bond lengths



Bond angles

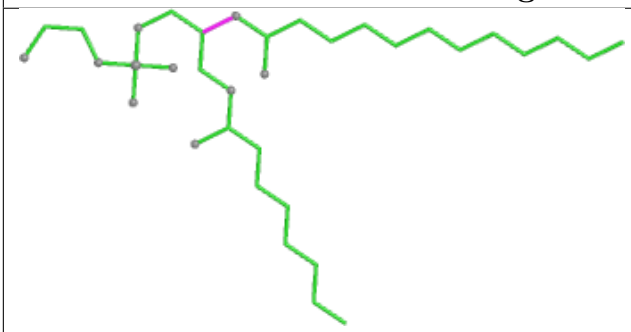


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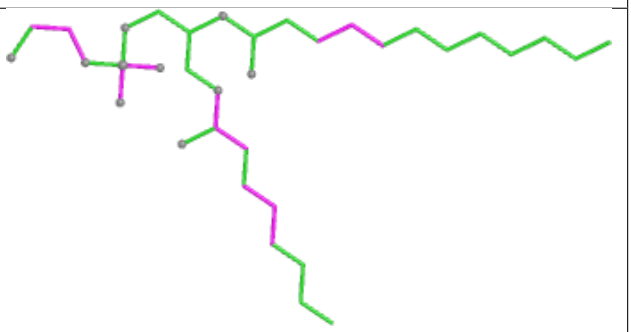


Rings

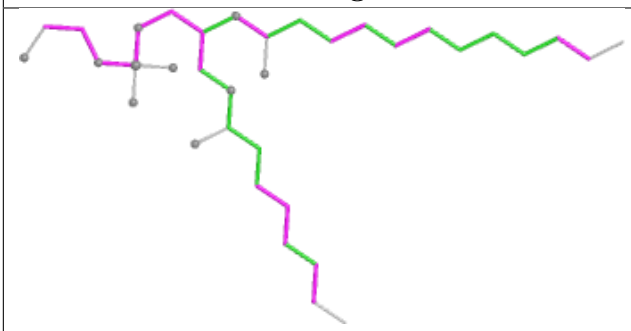
Ligand LHG 41 201



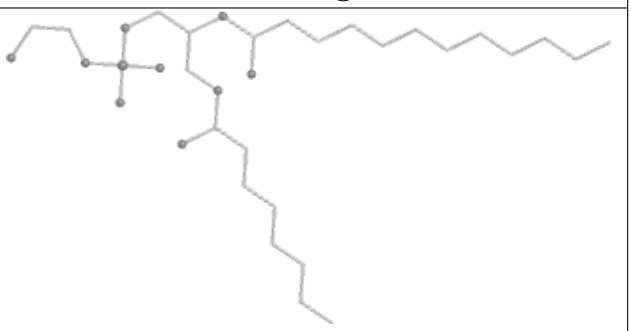
Bond lengths



Bond angles

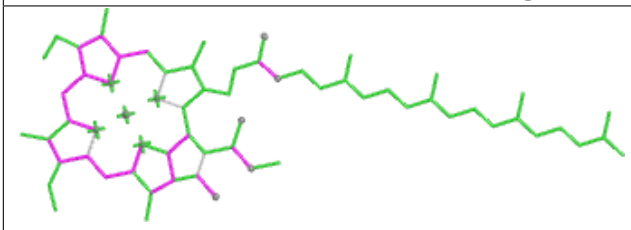


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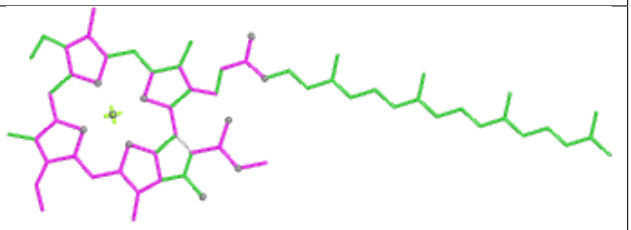


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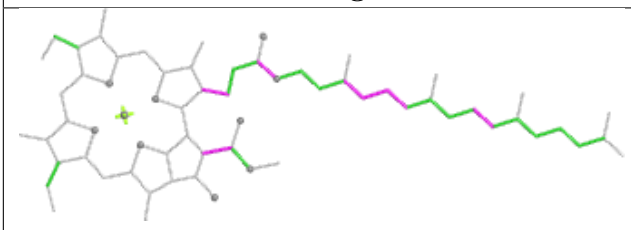
Ligand CLA 13 308



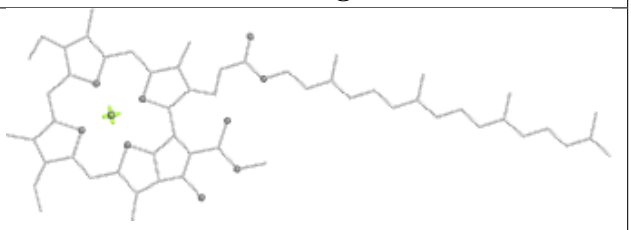
Bond lengths



Bond angles

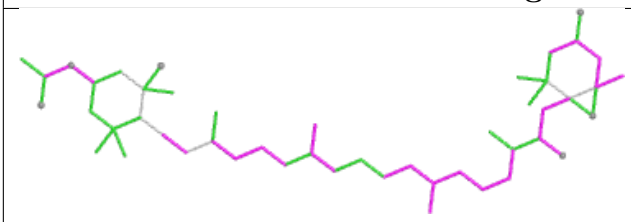


Torsions



Rings

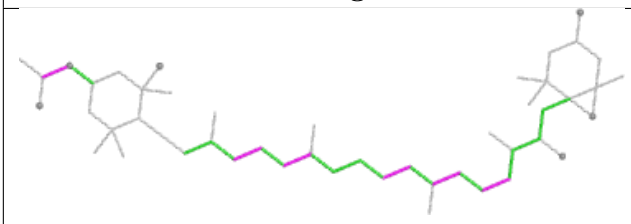
Ligand A86 12 220



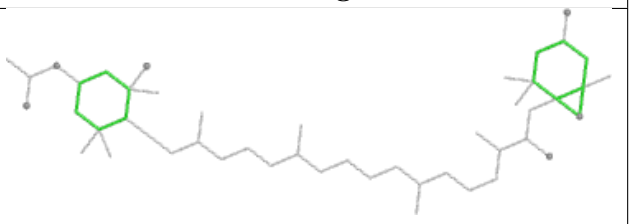
Bond lengths



Bond angles

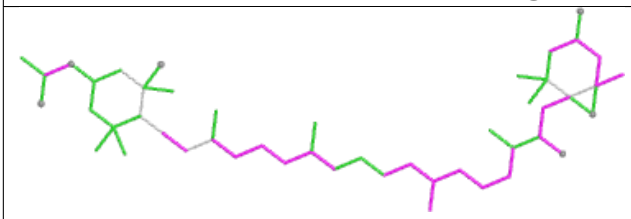


Torsions



Rings

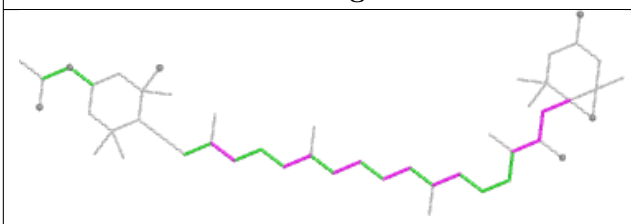
Ligand A86 16 313



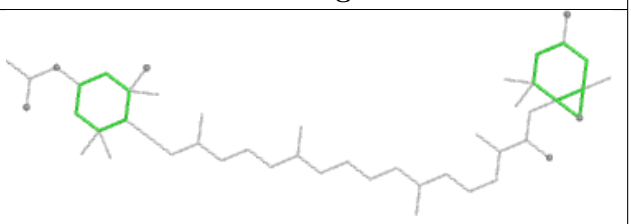
Bond lengths



Bond angles

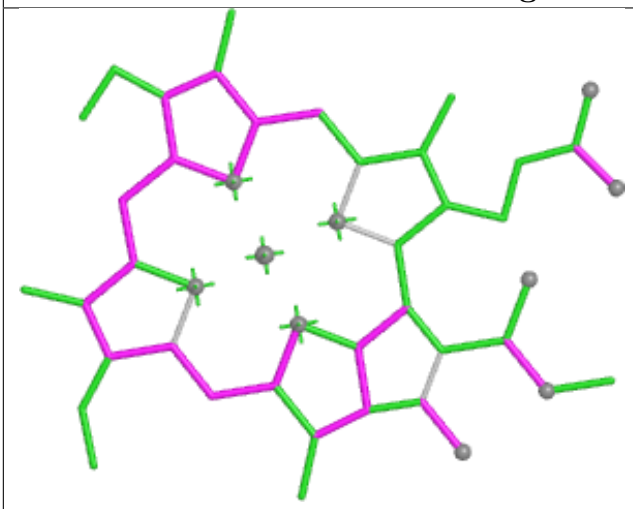


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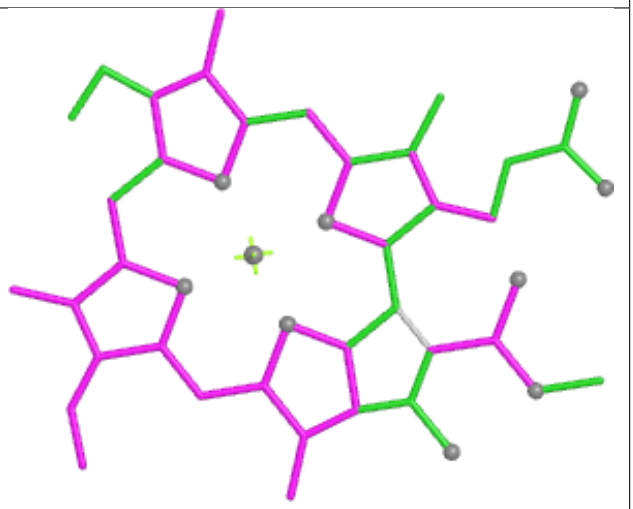


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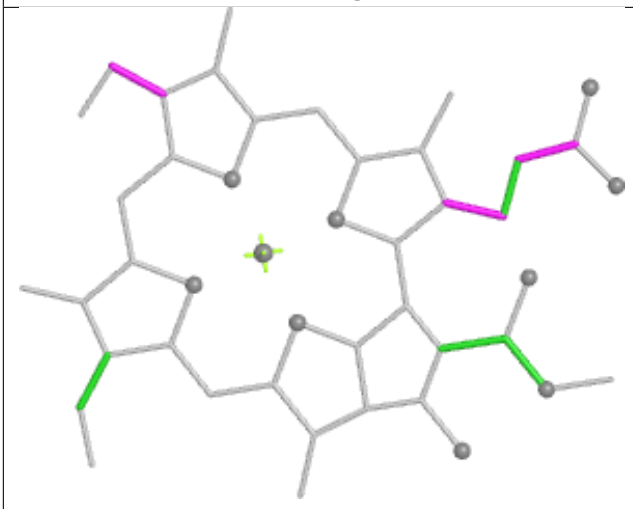
Ligand CLA 34 305



Bond lengths



Bond angles

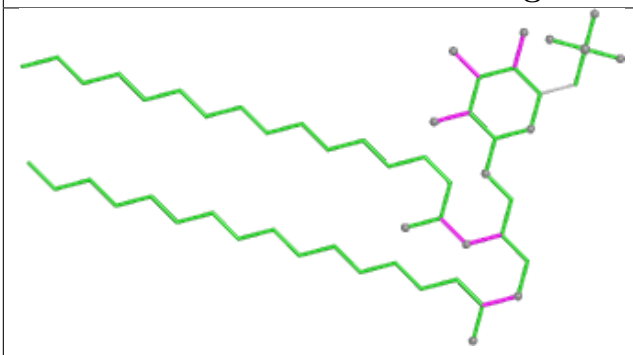


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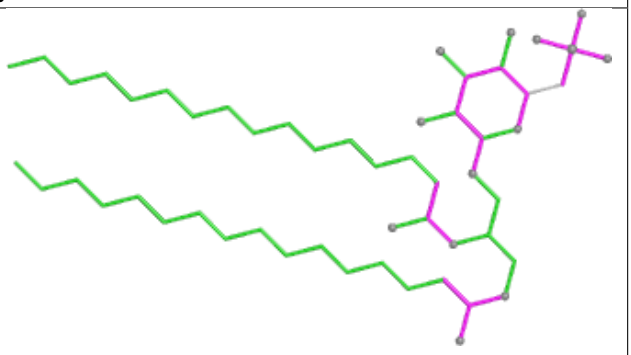


Rings

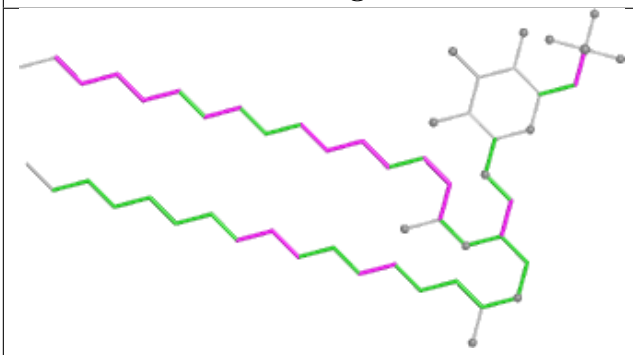
Ligand SQD A 407



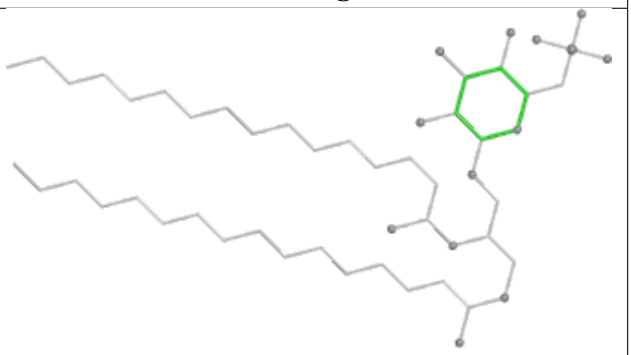
Bond lengths



Bond angles

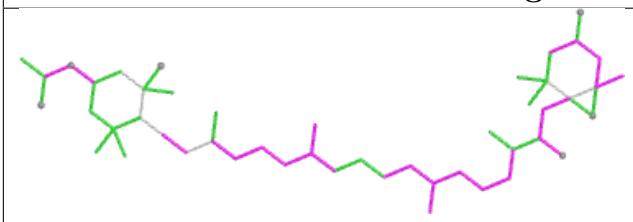


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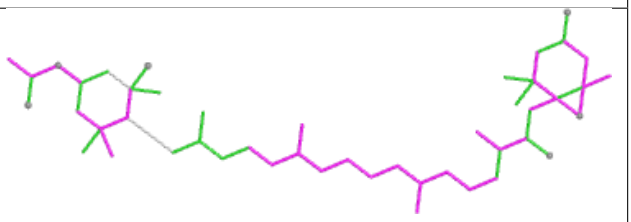


Rings

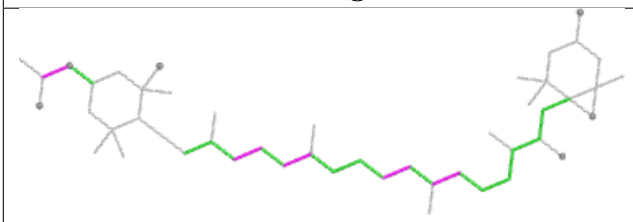
Ligand A86 15 319



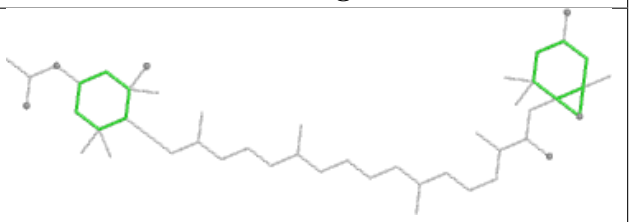
Bond lengths



Bond angles

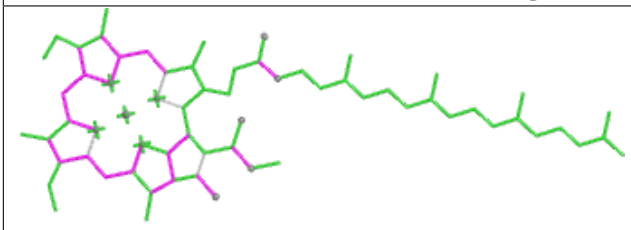


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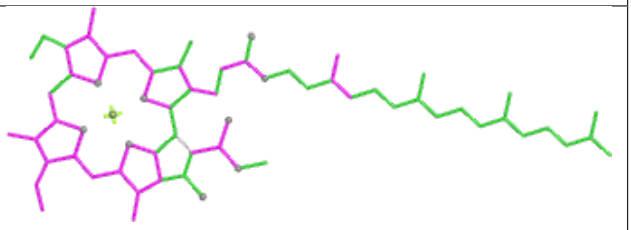


Rings

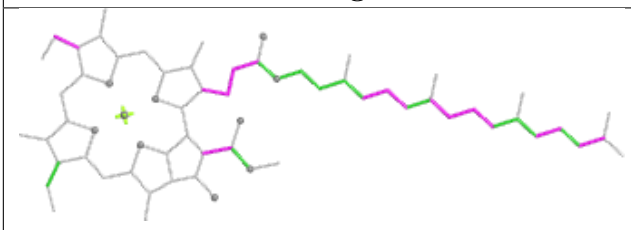
Ligand CLA B 501



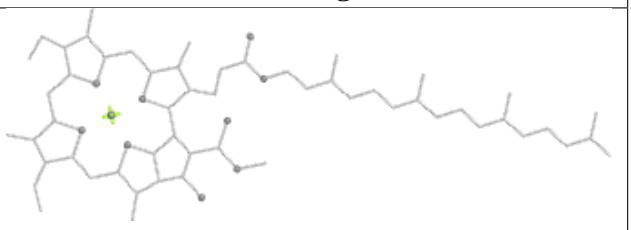
Bond lengths



Bond angles

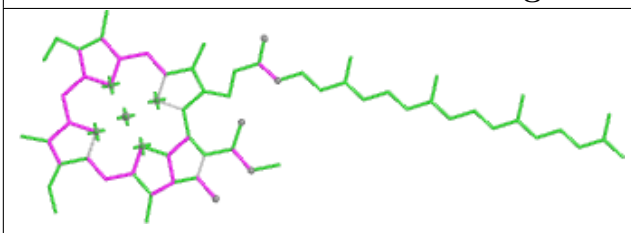


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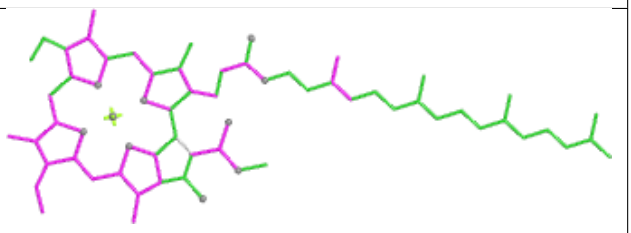


Rings

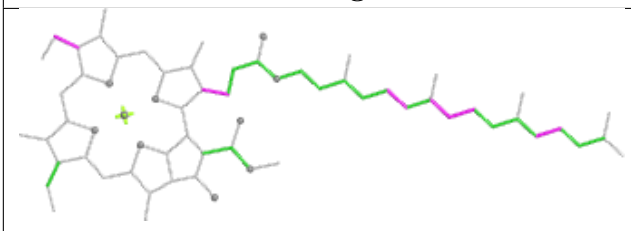
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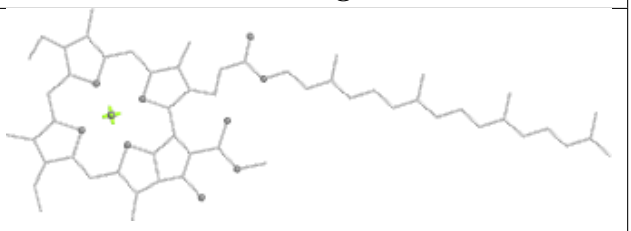
Bond lengths



Bond angles

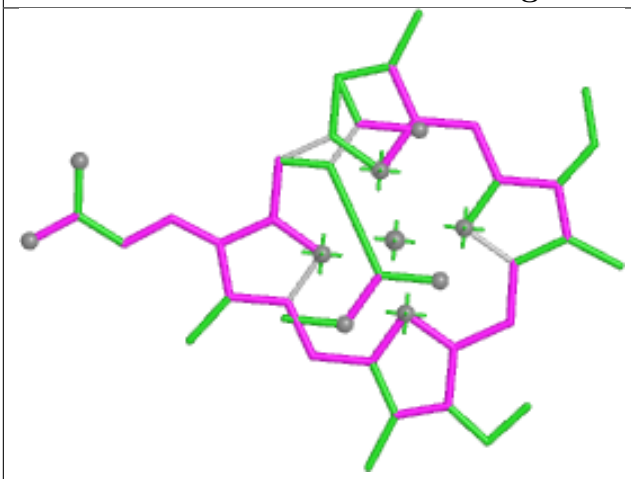


Torsions

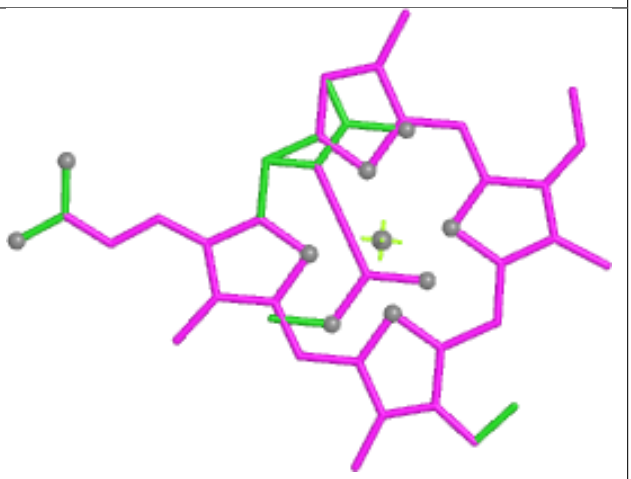


Rings

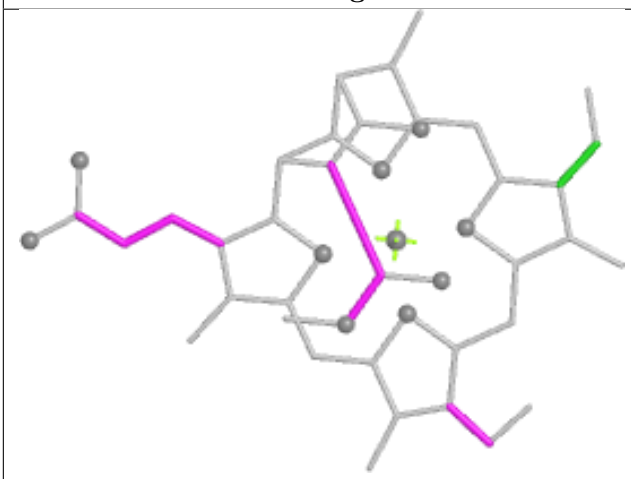
Ligand KC1 40 204



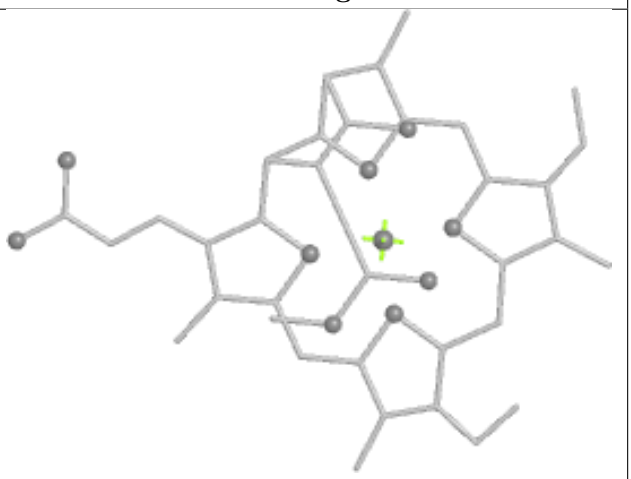
Bond lengths



Bond angles

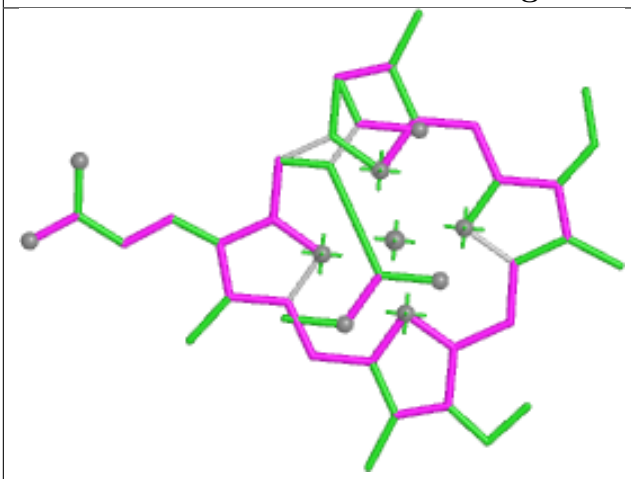


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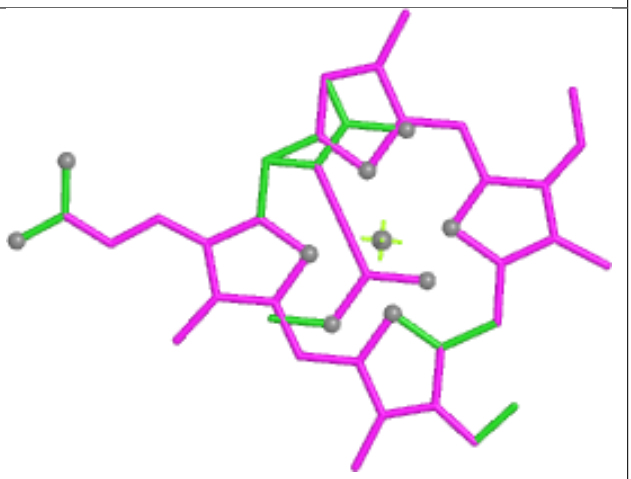


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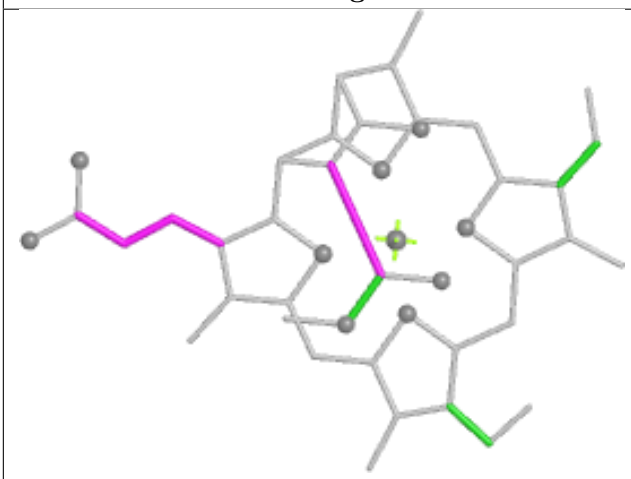
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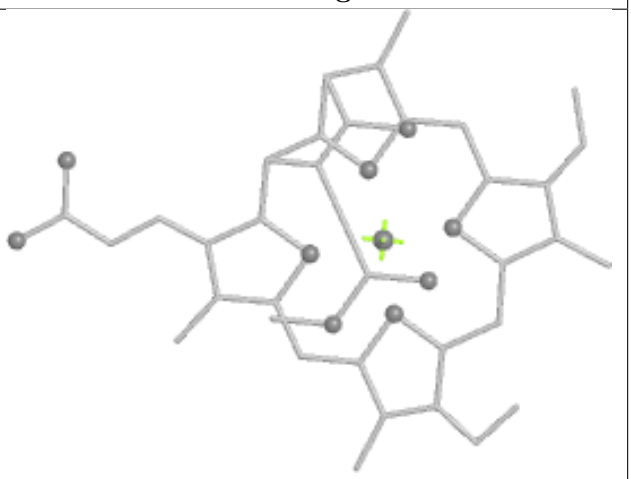
Bond lengths



Bond angles

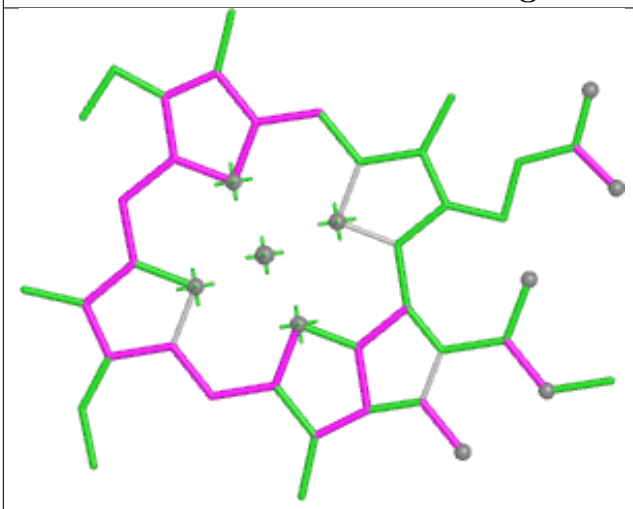


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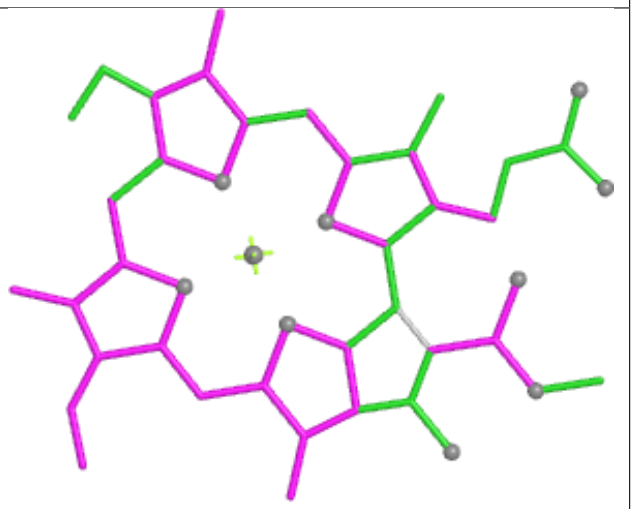


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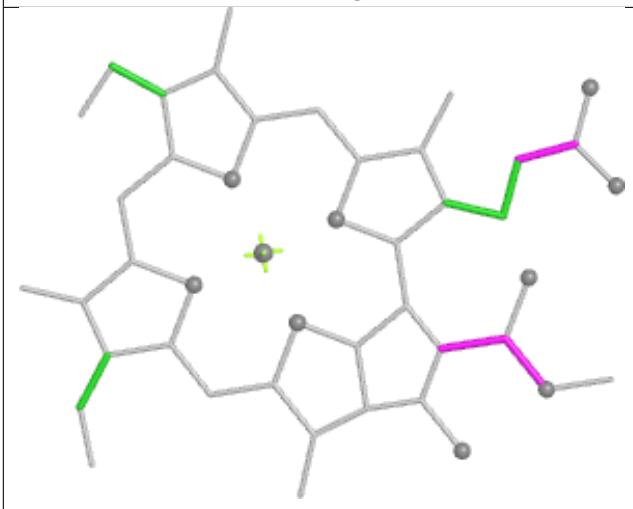
Ligand CLA 41 209



Bond lengths



Bond angles

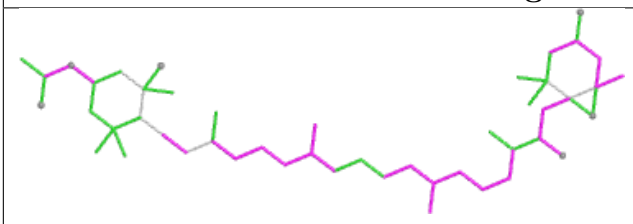


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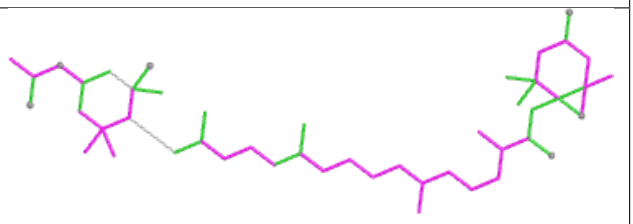


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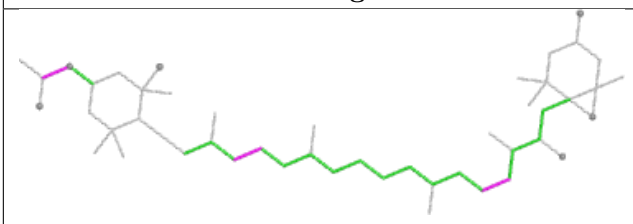
Ligand A86 14 312



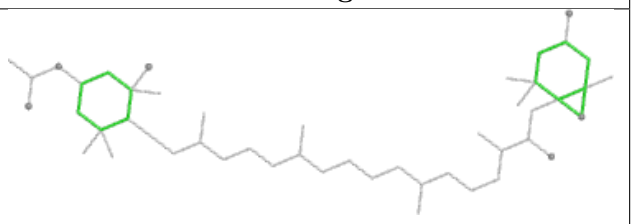
Bond lengths



Bond angles

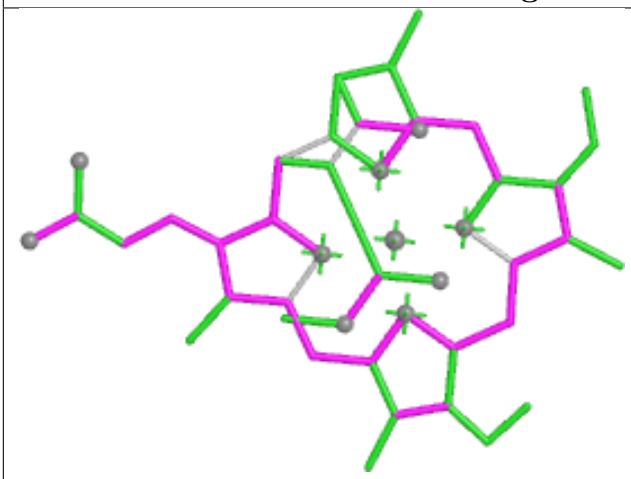


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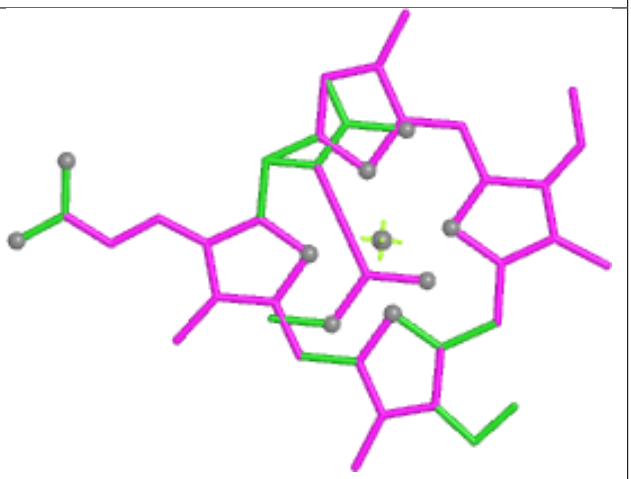


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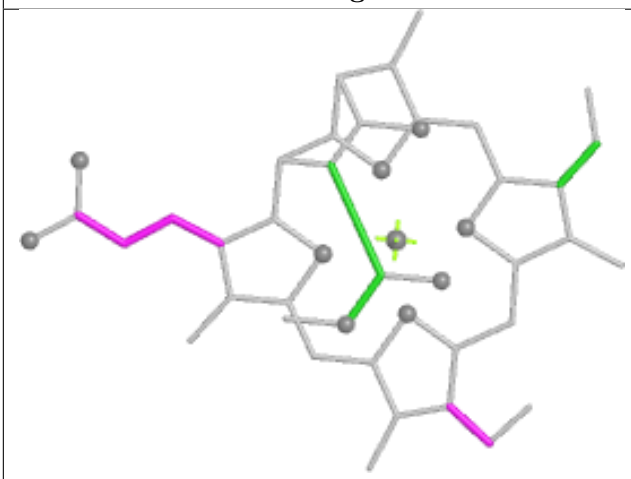
Ligand KC1 33 304



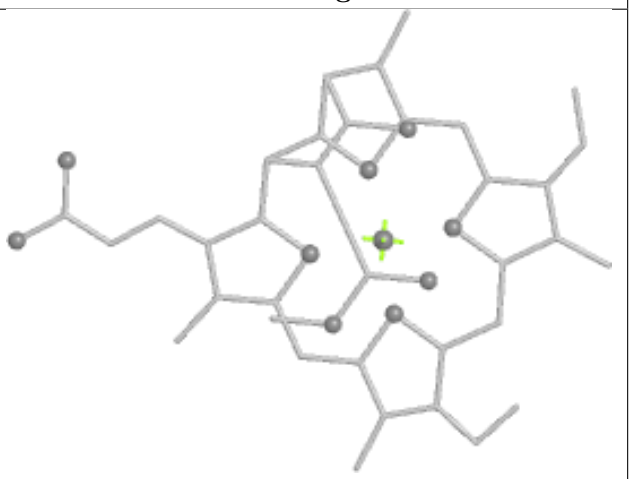
Bond lengths



Bond angles

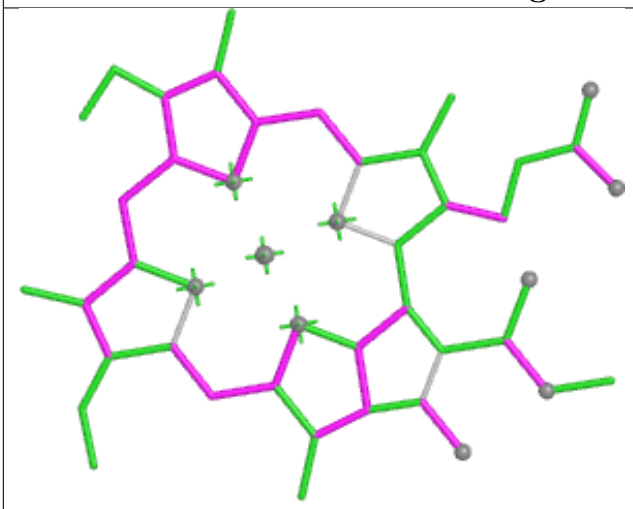


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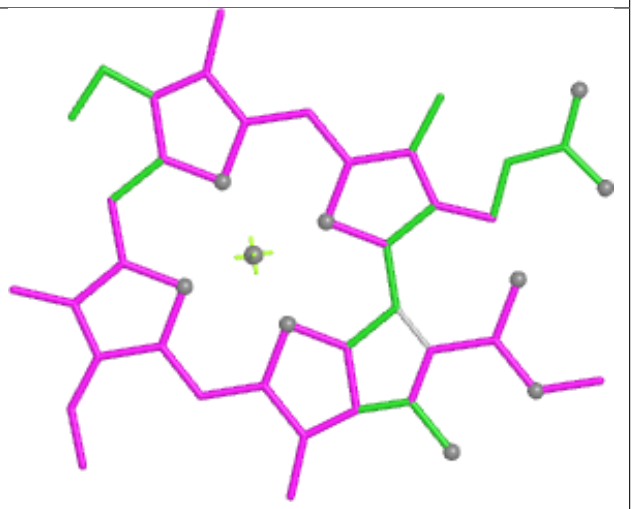


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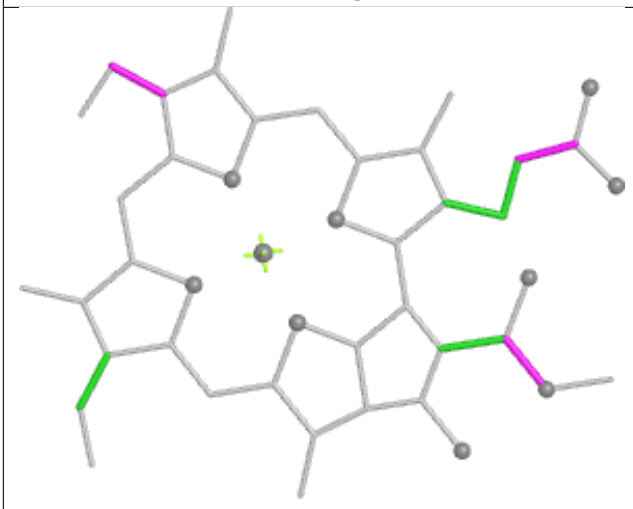
Ligand CLA z 102



Bond lengths



Bond angles

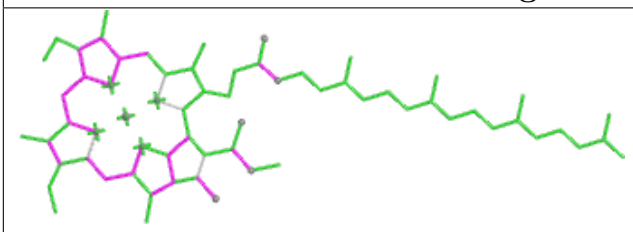


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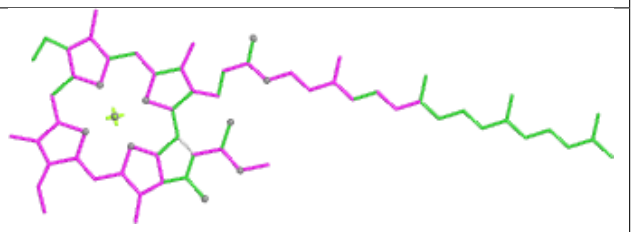


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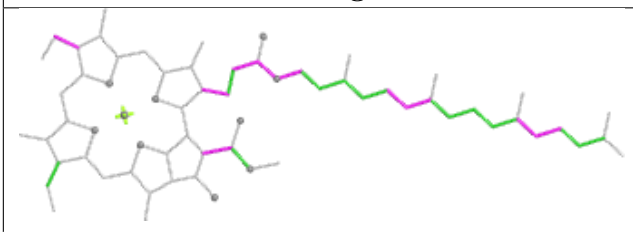
Ligand CLA 14 308



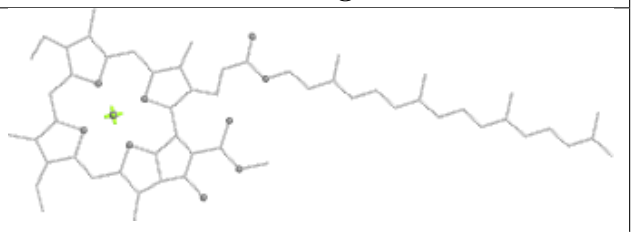
Bond lengths



Bond angles

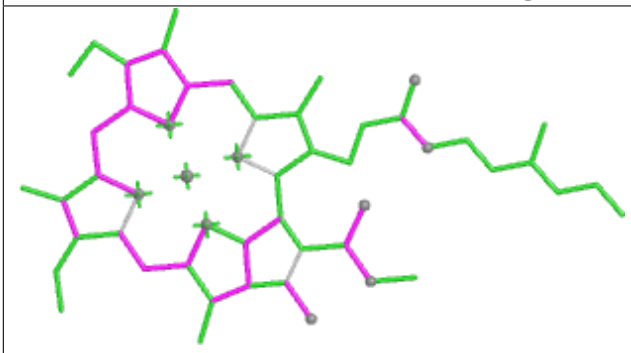


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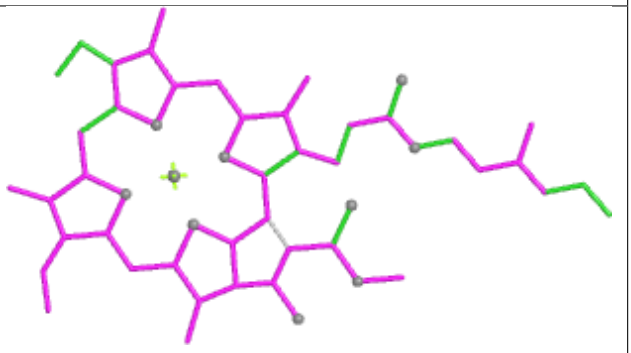


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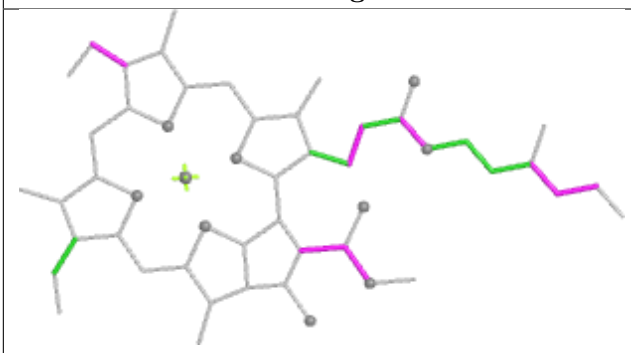
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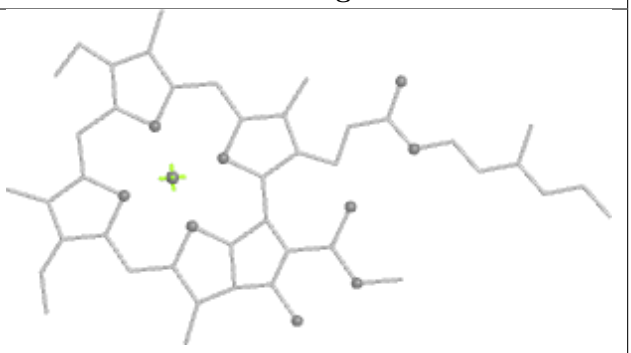
Bond lengths



Bond angles

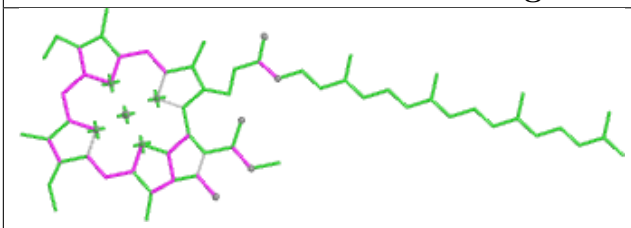


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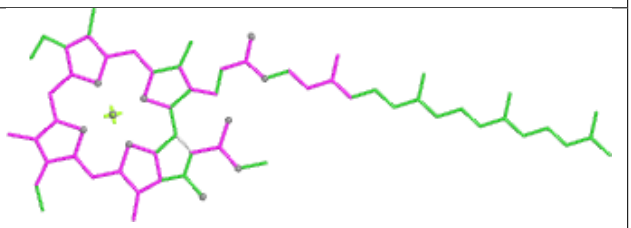


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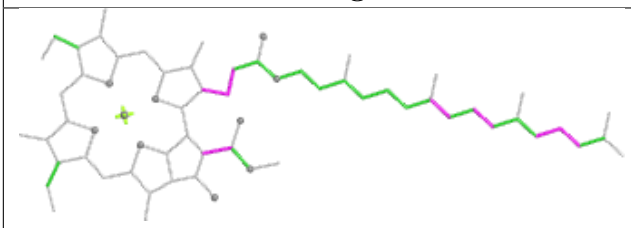
Ligand CLA B 506



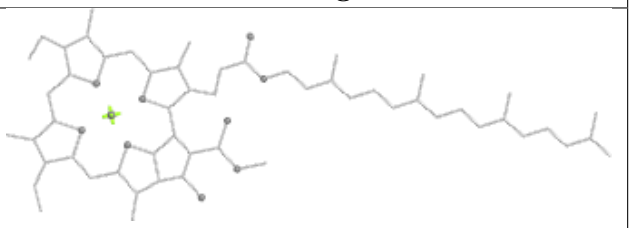
Bond lengths



Bond angles

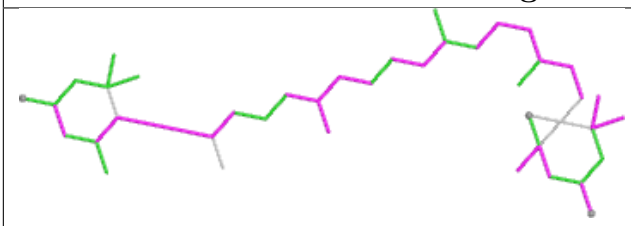


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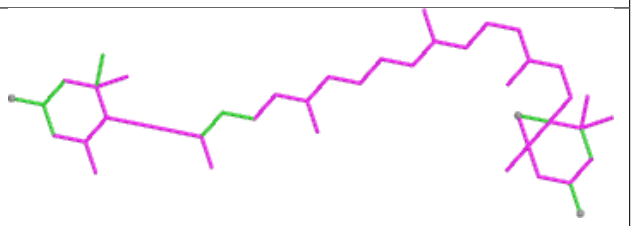


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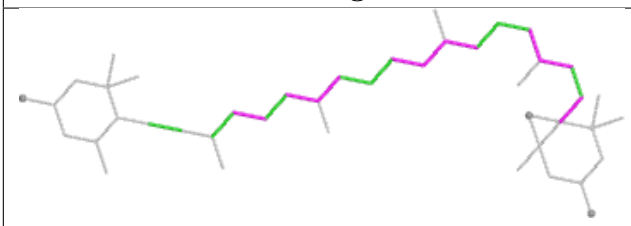
Ligand DD6 19 312



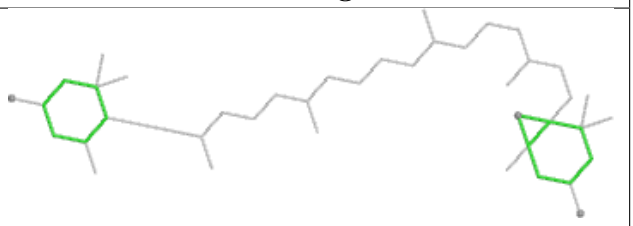
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Bond angles

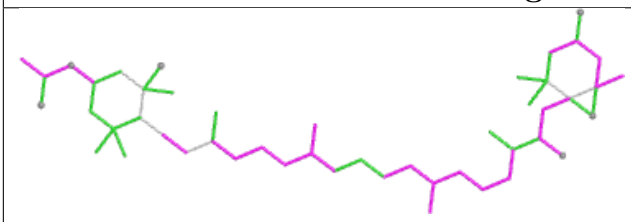


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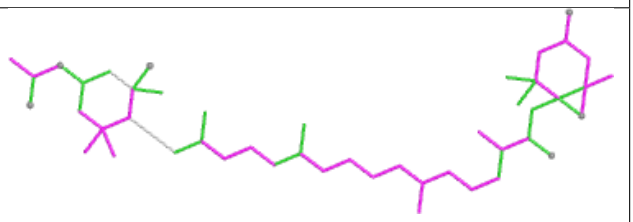


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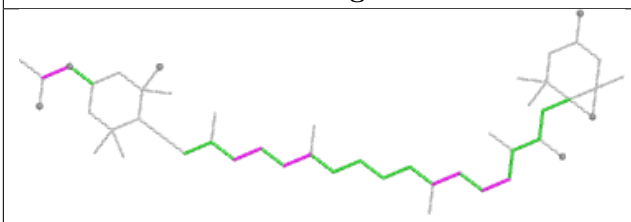
Ligand A86 35 315



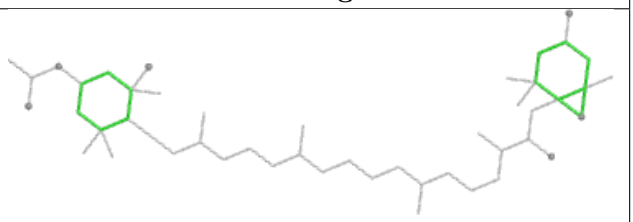
Bond lengths



Bond angles

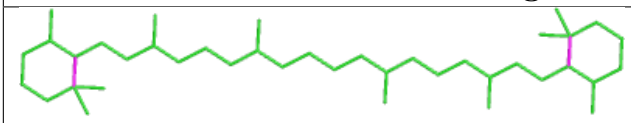


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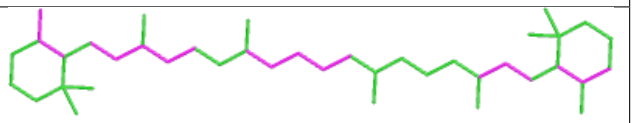


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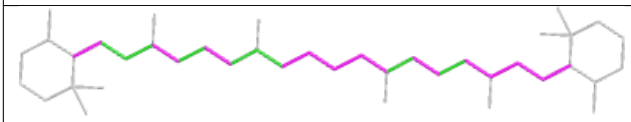
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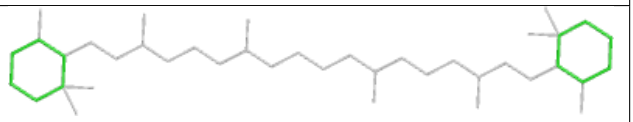
Bond lengths



Bond angles

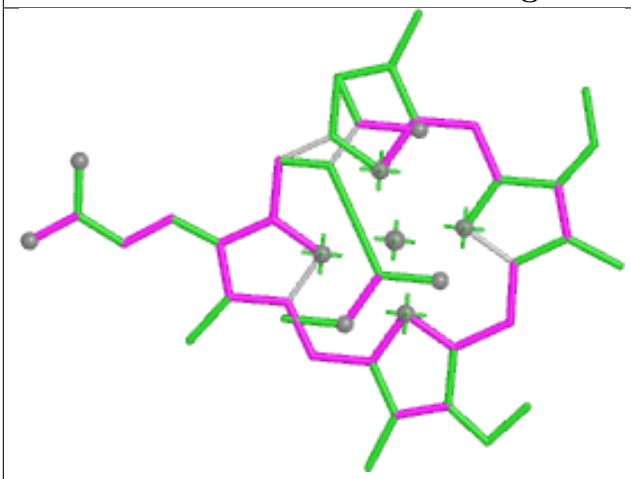


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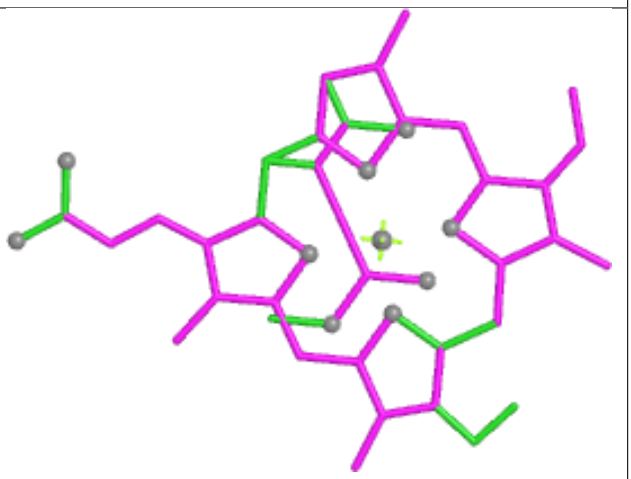


Rings

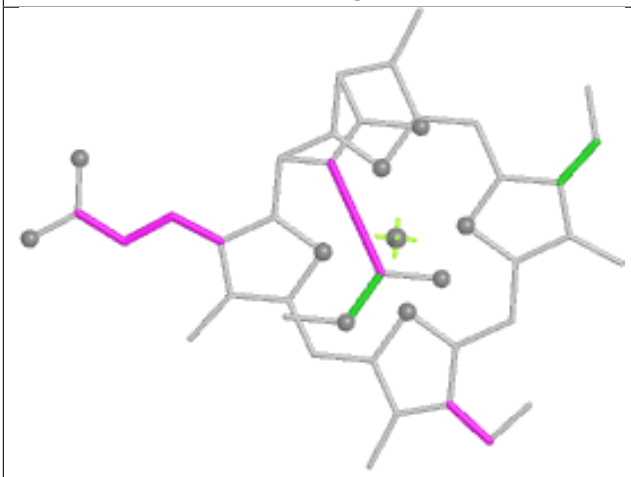
Ligand KC1 34 309



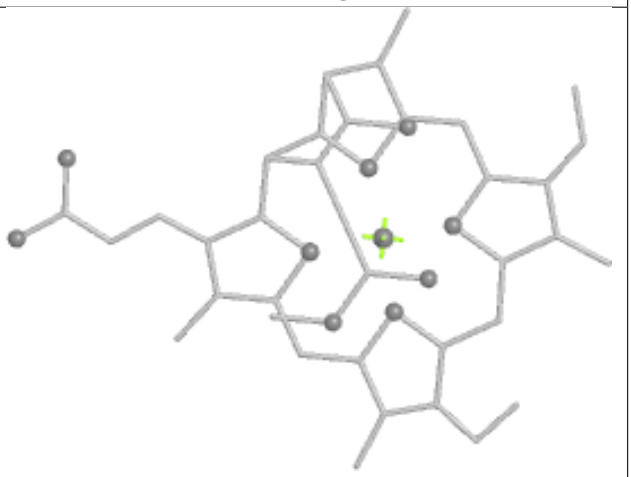
Bond lengths



Bond angles

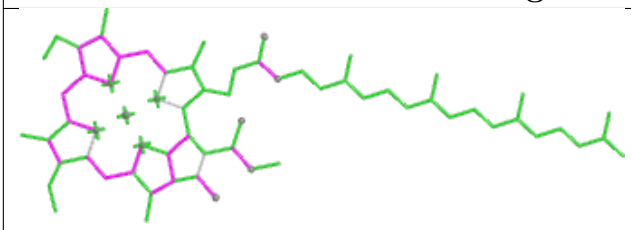


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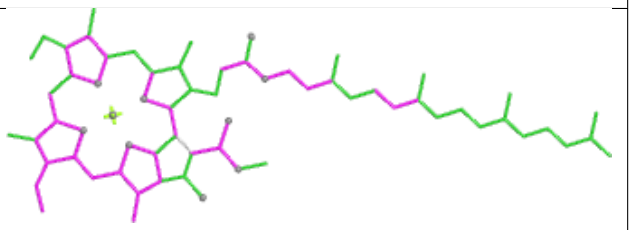


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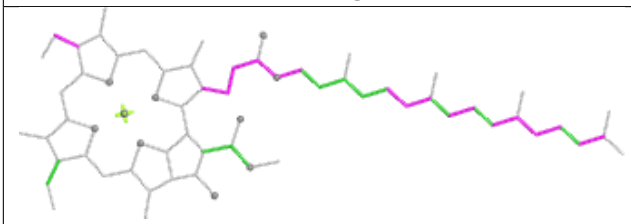
Ligand CLA Z 101



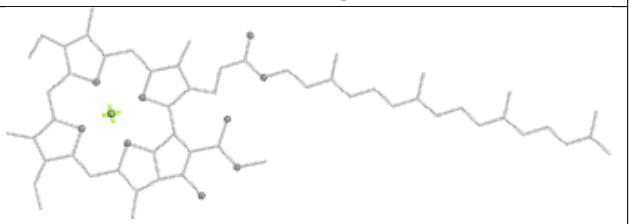
Bond lengths



Bond angles

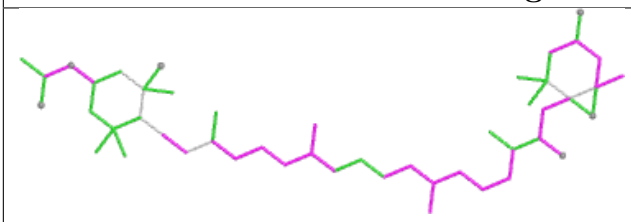


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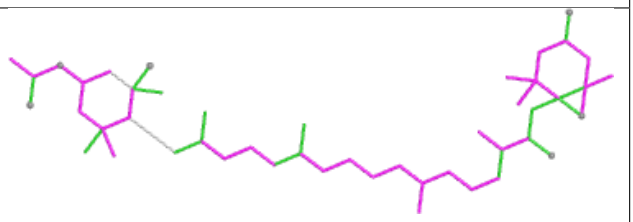


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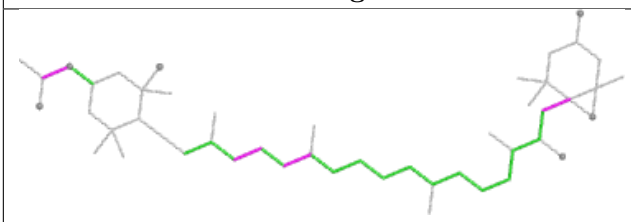
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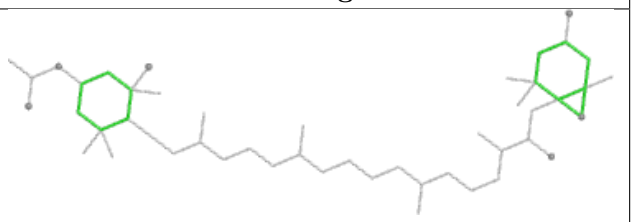
Bond lengths



Bond angles

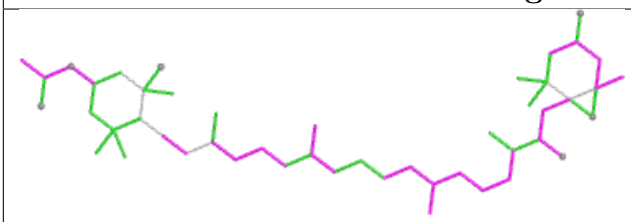


Torsions

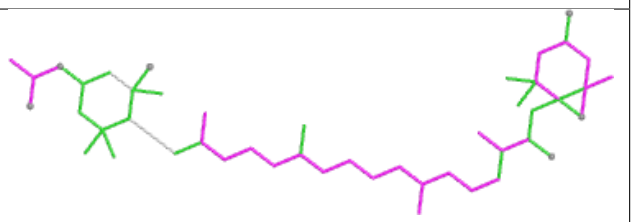


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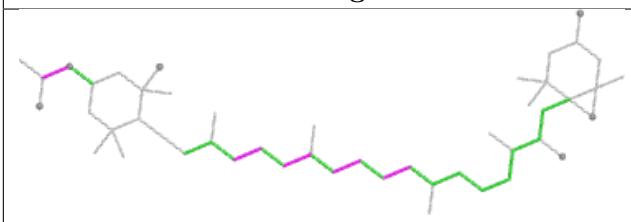
Ligand A86 31 319



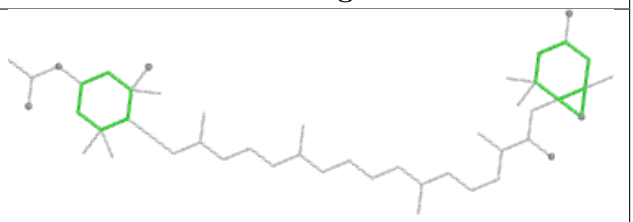
Bond lengths



Bond angles

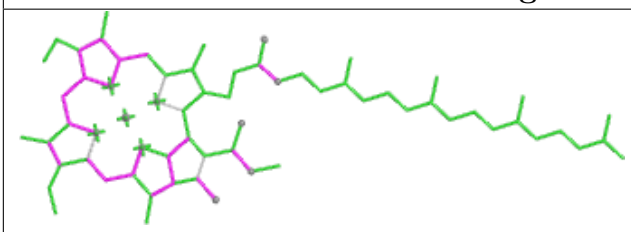


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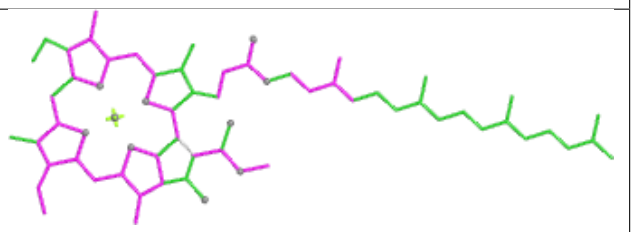


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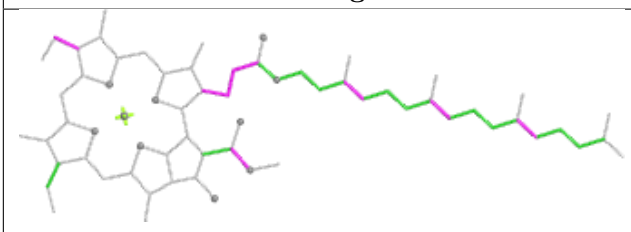
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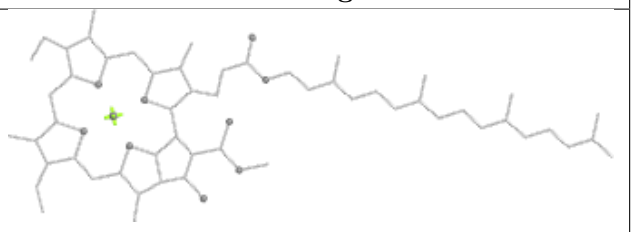
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Bond angles

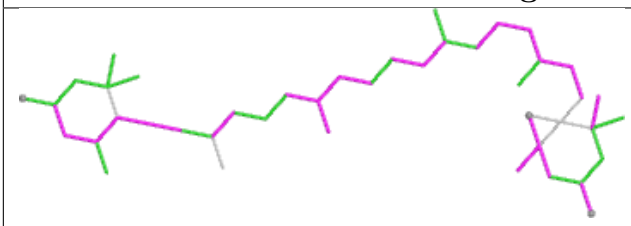


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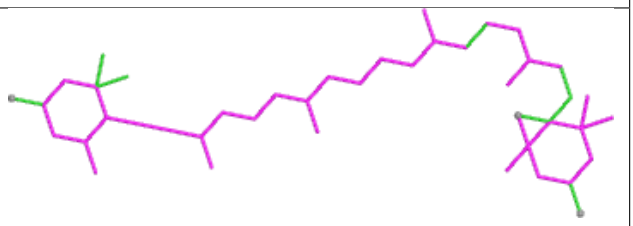


Rings

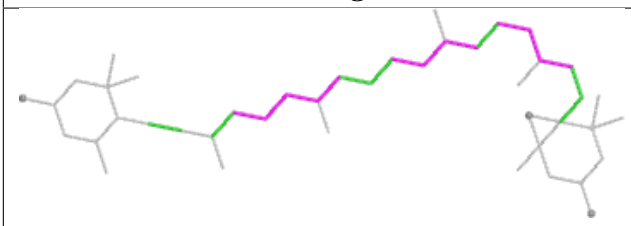
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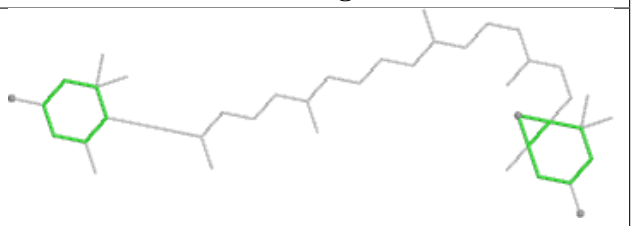
Bond lengths



Bond angles

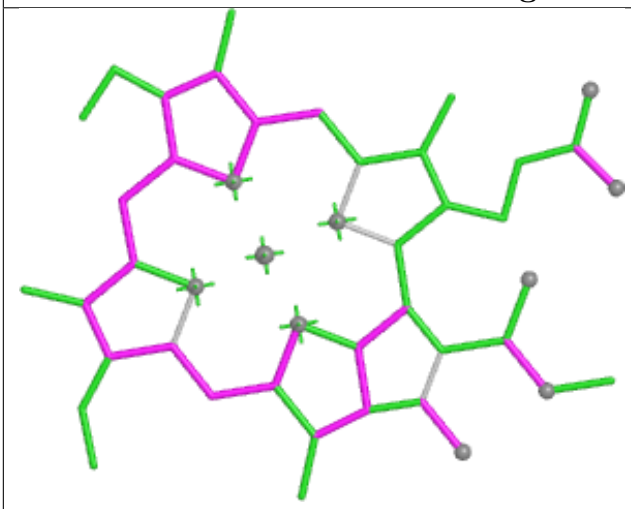


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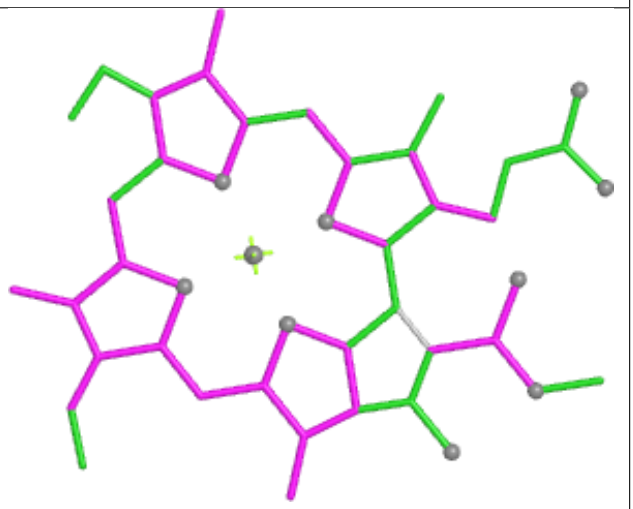


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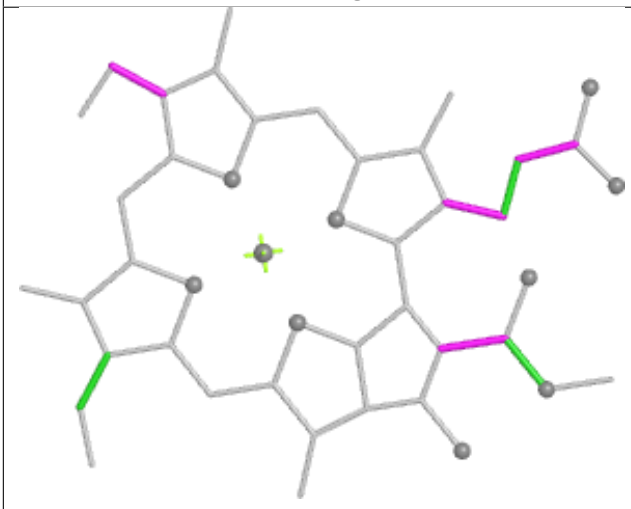
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Bond lengths



Bond angles

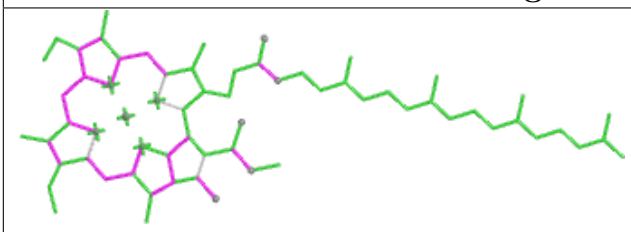


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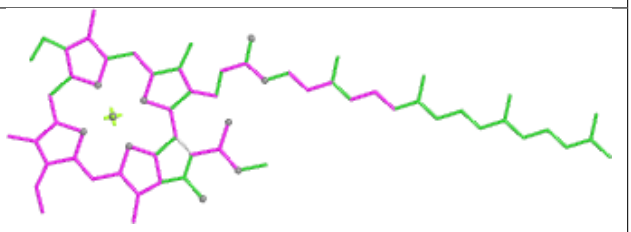


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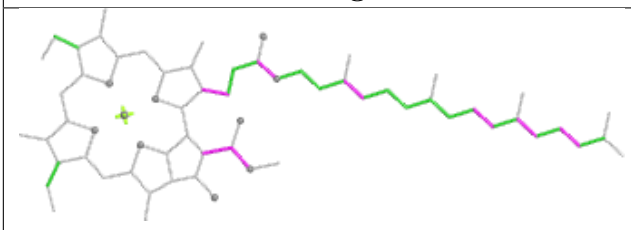
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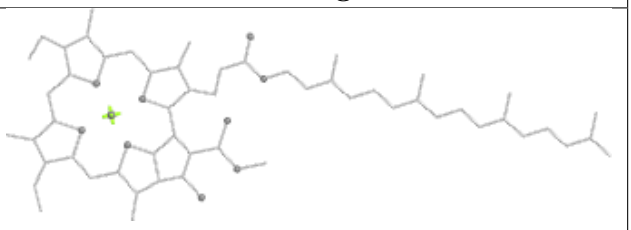
Bond lengths



Bond angles



Torsions

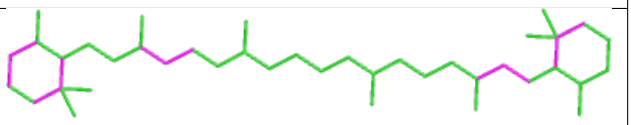


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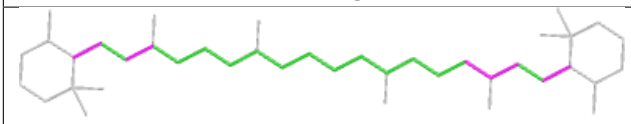
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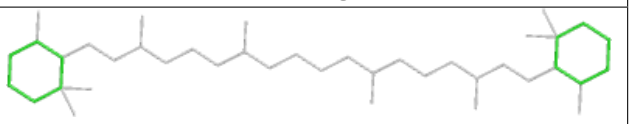
Bond lengths



Bond angles

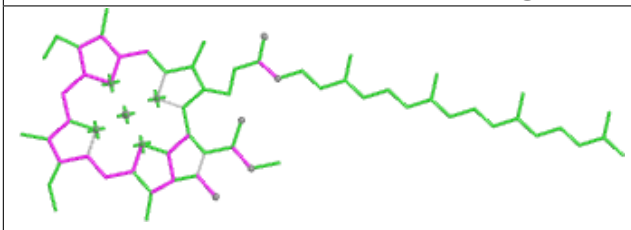


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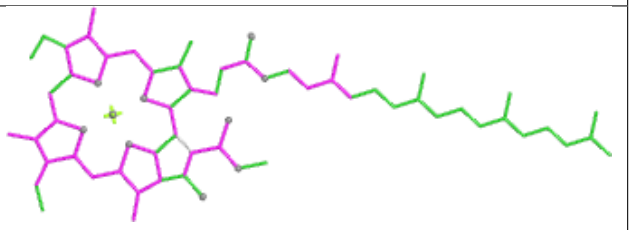


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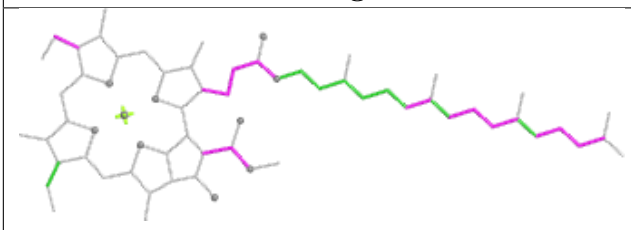
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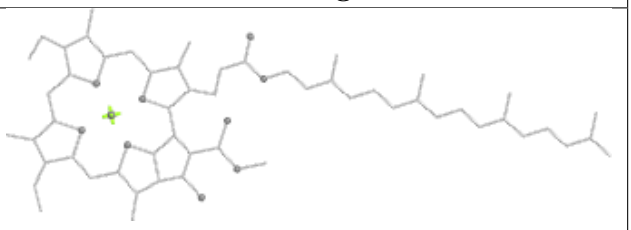
Bond lengths



Bond angles

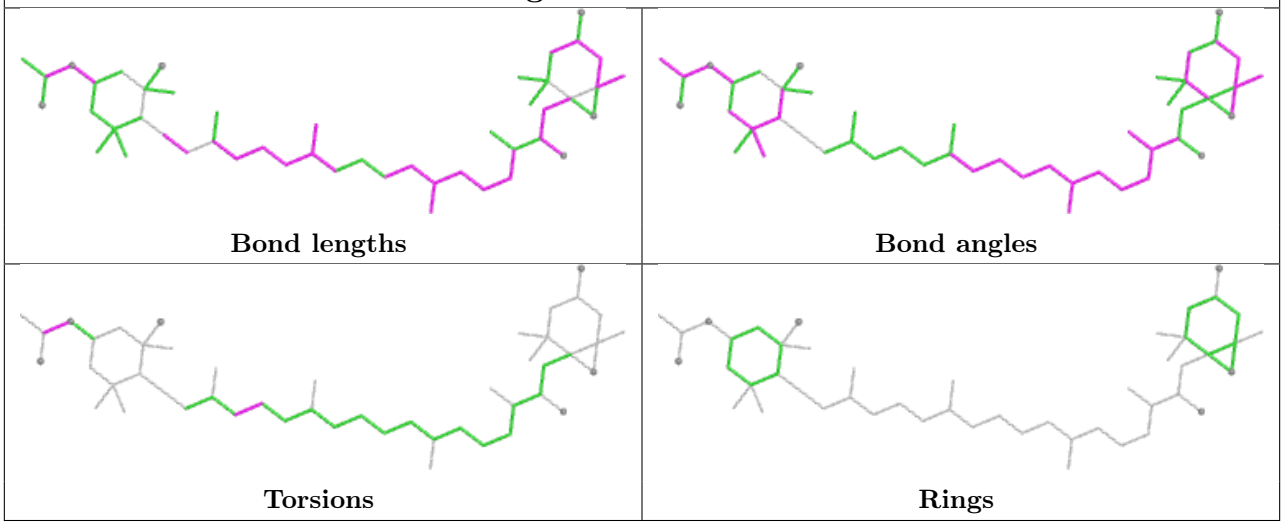


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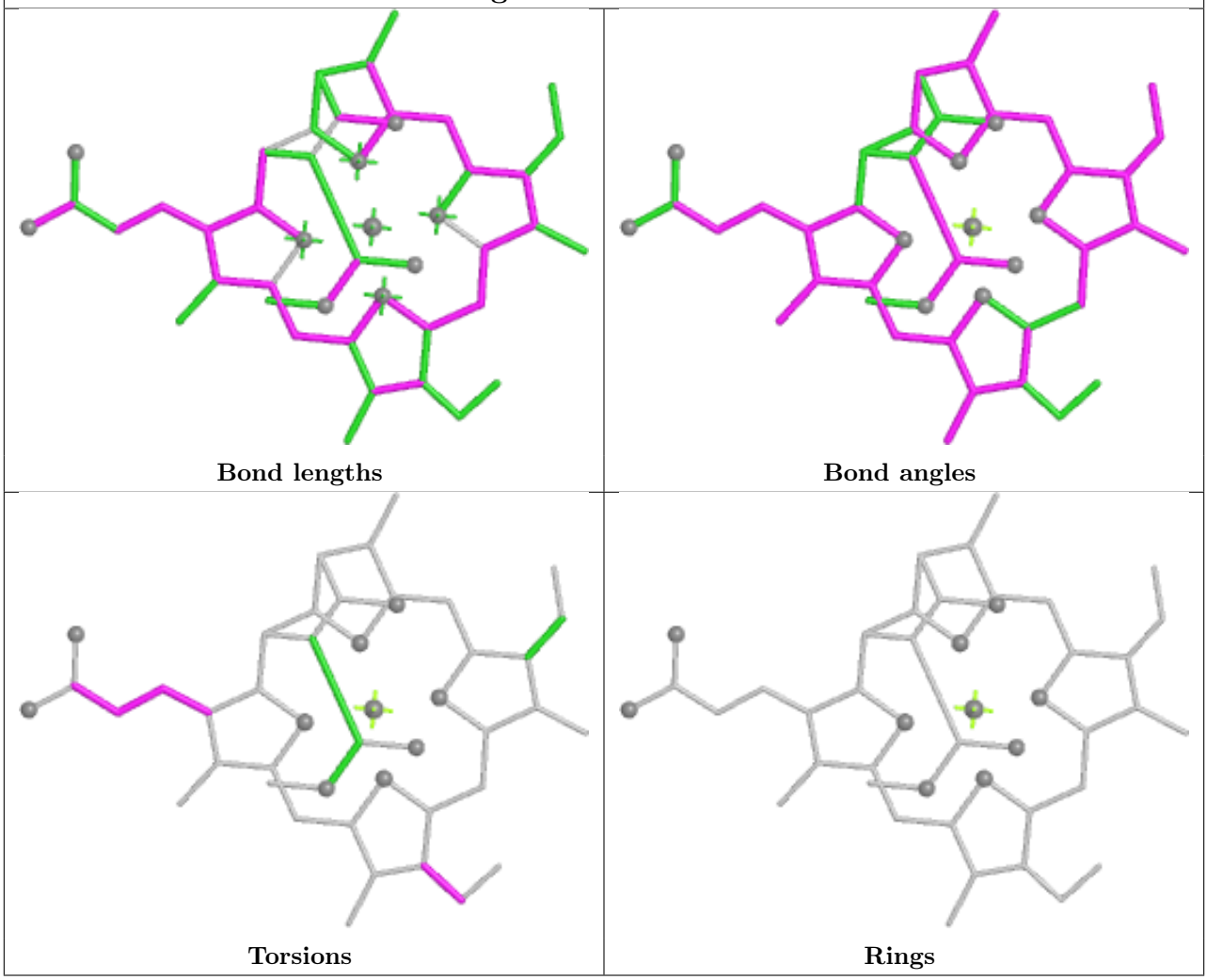


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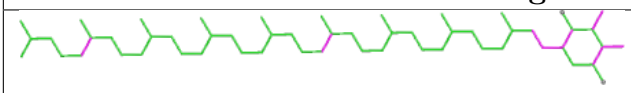
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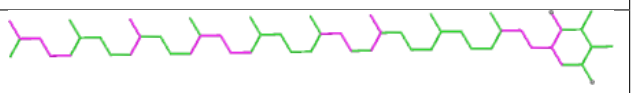
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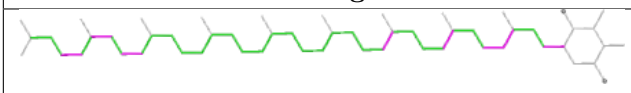
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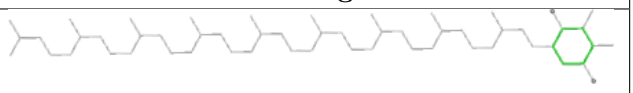
Bond lengths



Bond angles

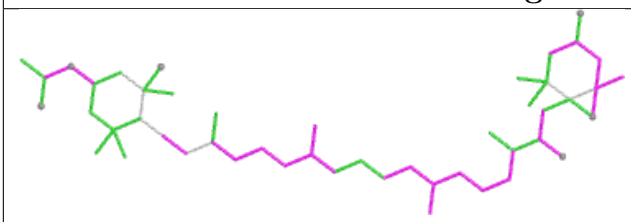


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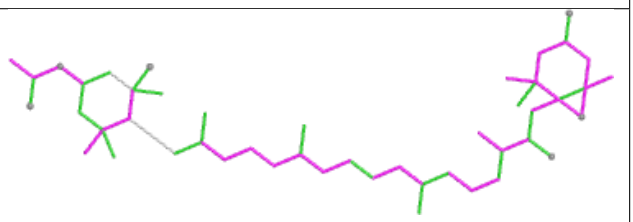


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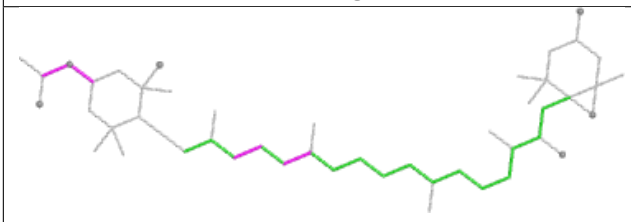
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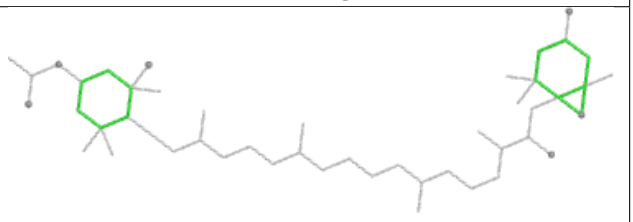
Bond lengths



Bond angles

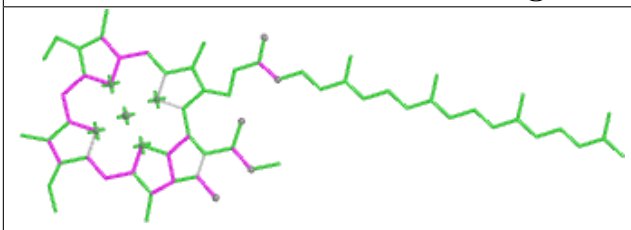


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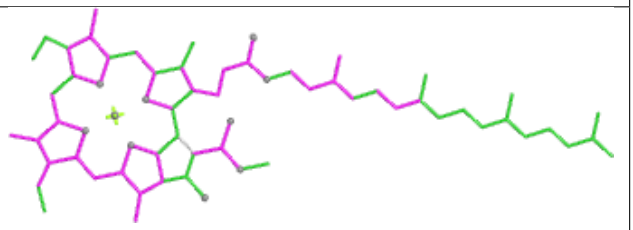


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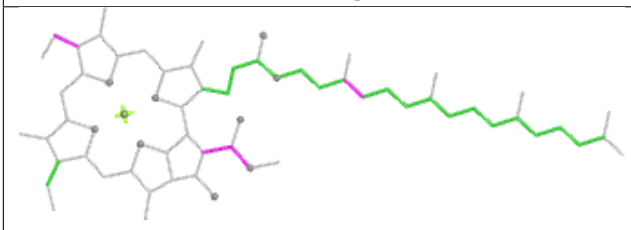
Ligand CLA b 504



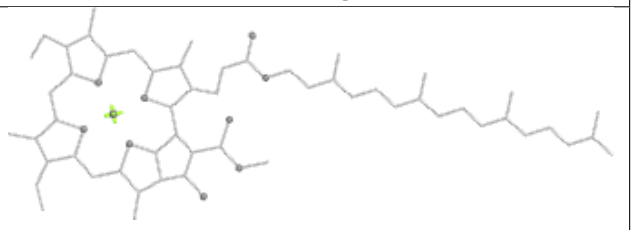
Bond lengths



Bond angles

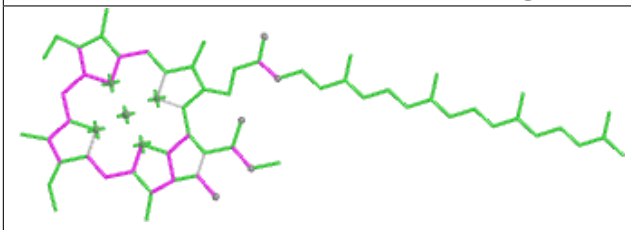


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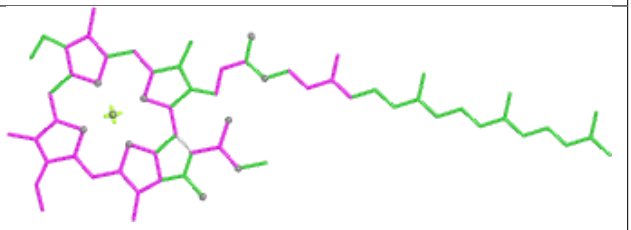


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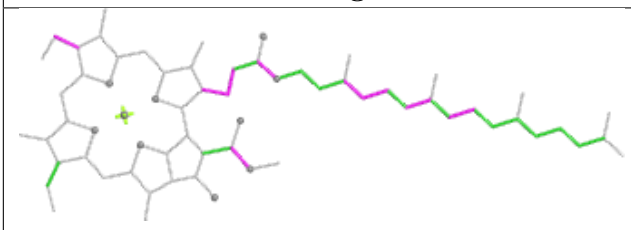
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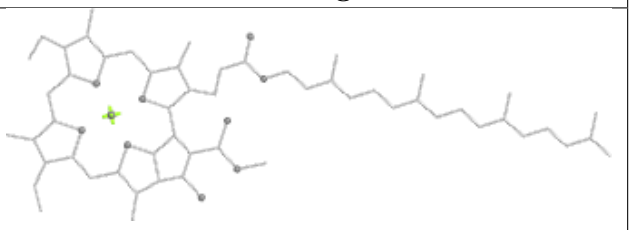
Bond lengths



Bond angles

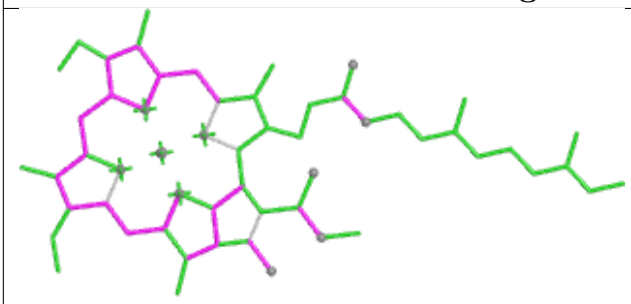


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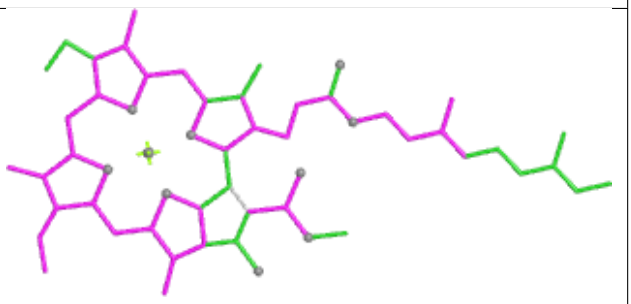


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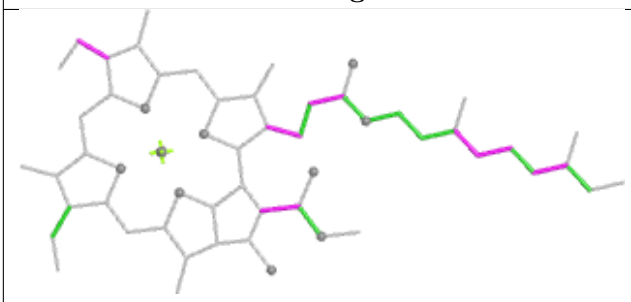
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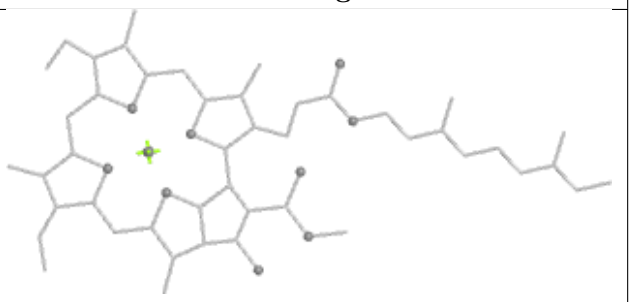
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Bond angles

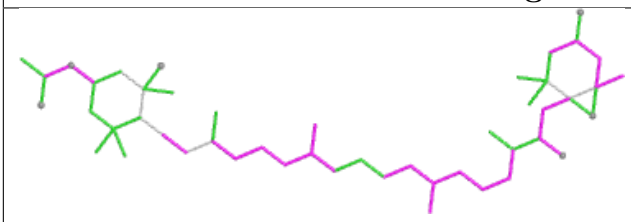


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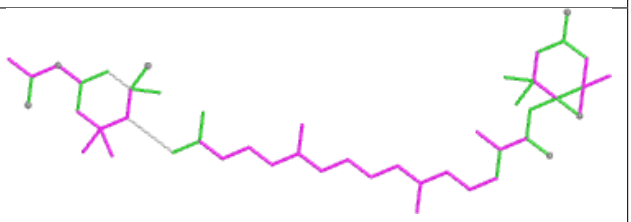


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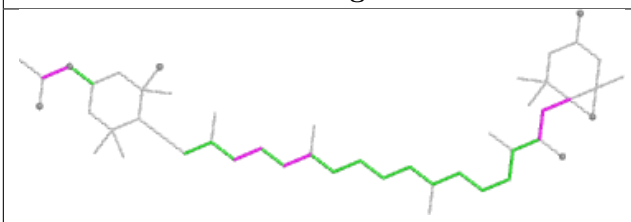
Ligand A86 37 312



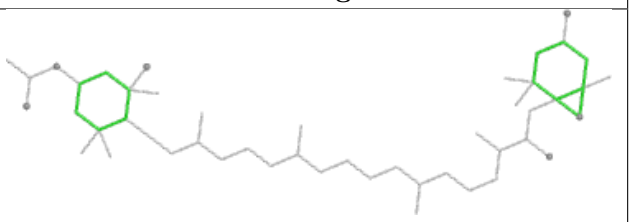
Bond lengths



Bond angles

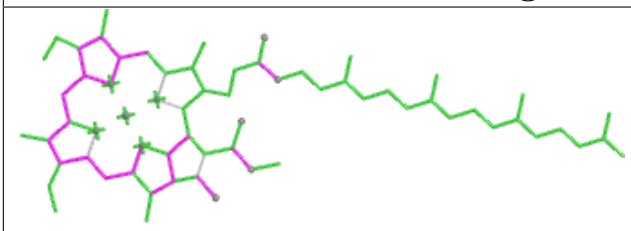


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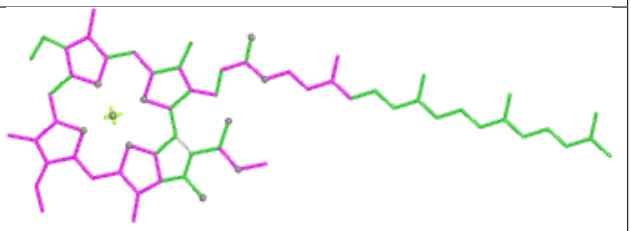


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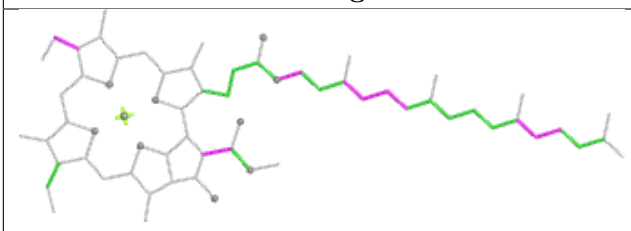
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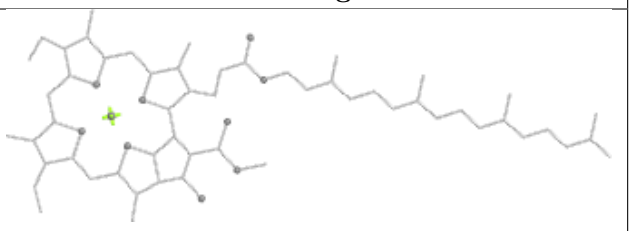
Bond lengths



Bond angles

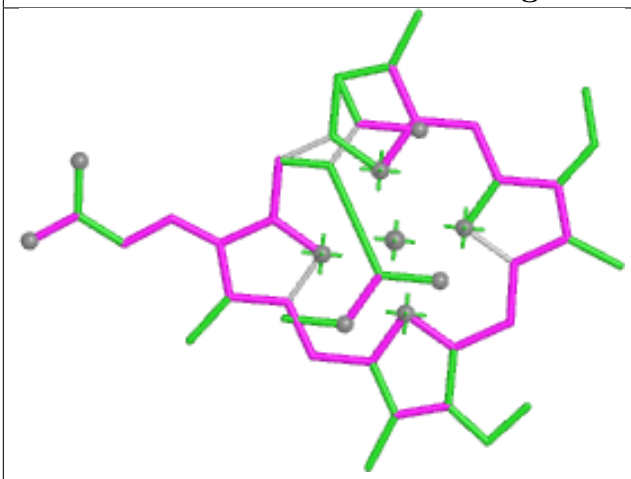


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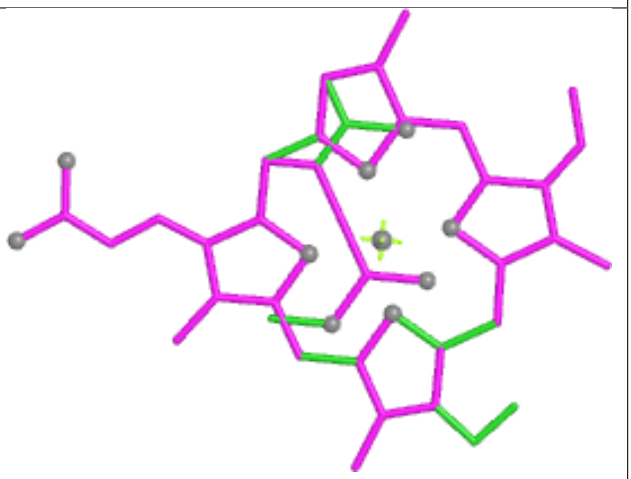


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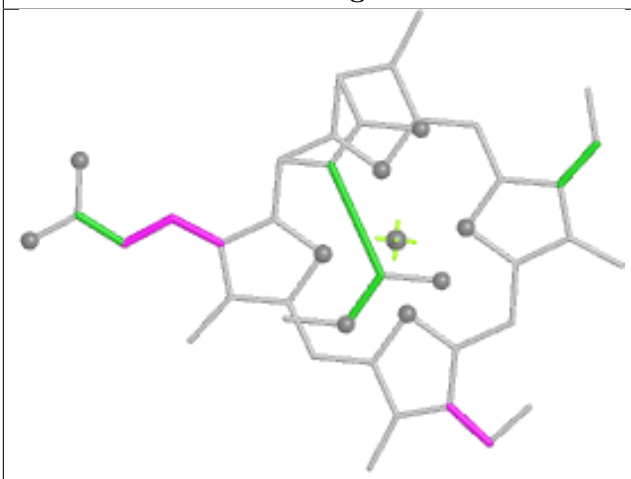
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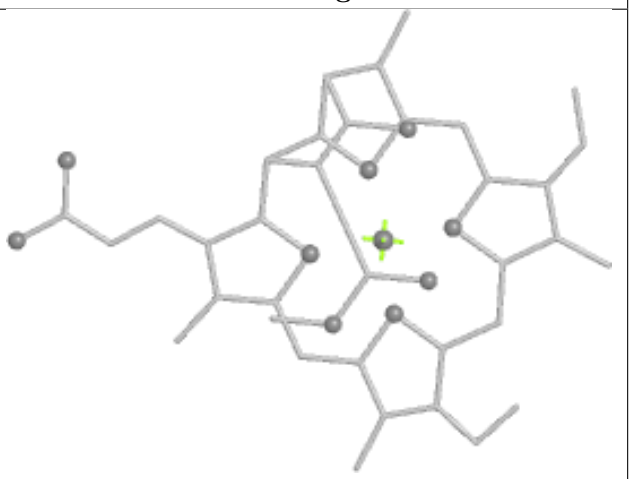
Bond lengths



Bond angles

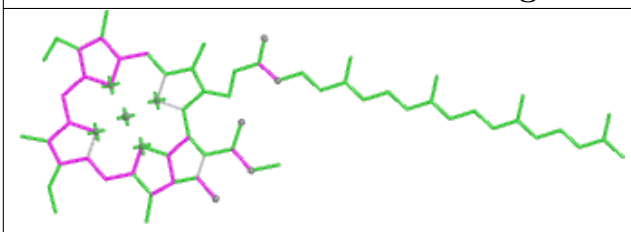


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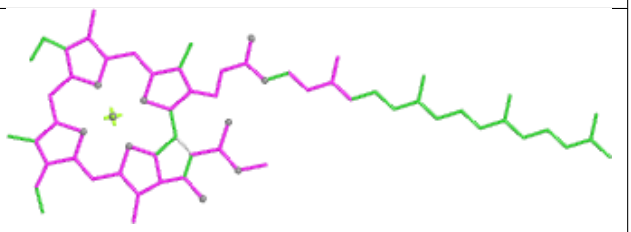


Rings

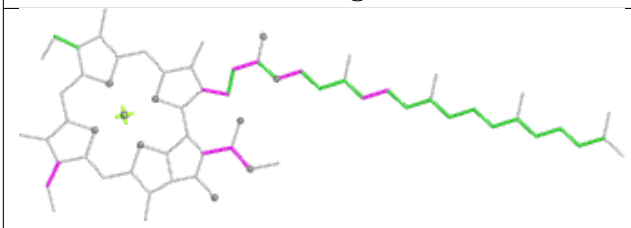
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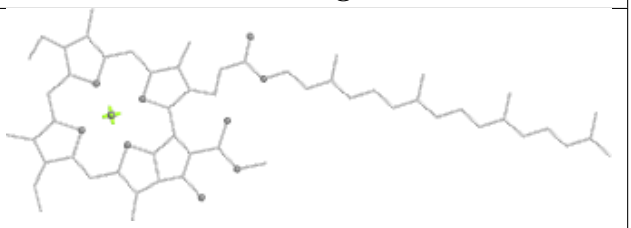
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Bond angles

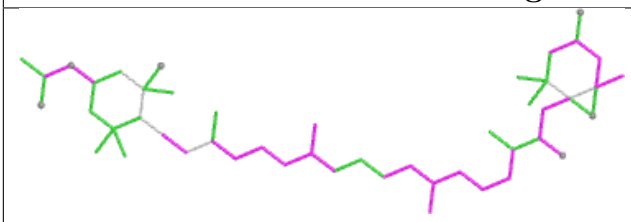


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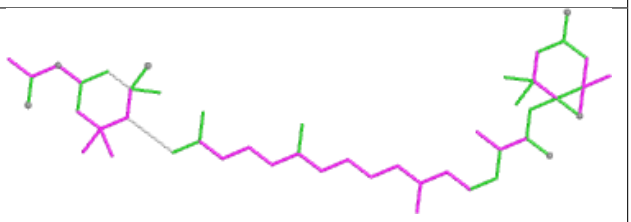


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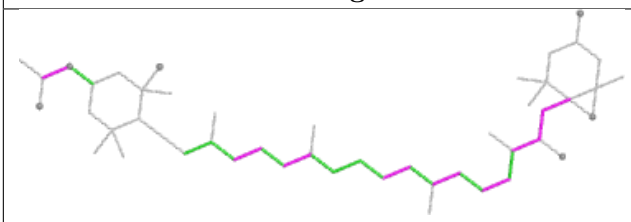
Ligand A86 38 214



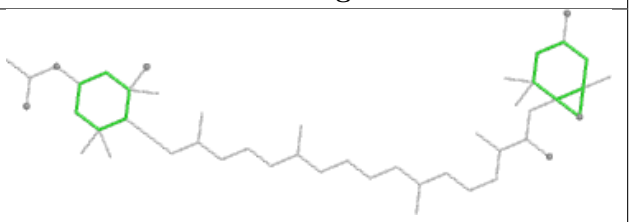
Bond lengths



Bond angles

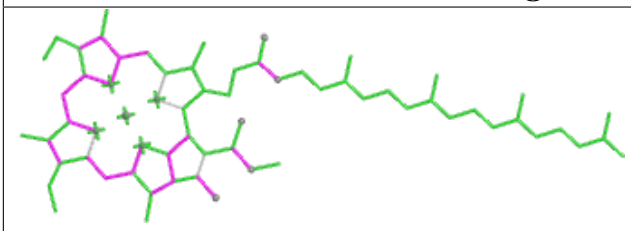


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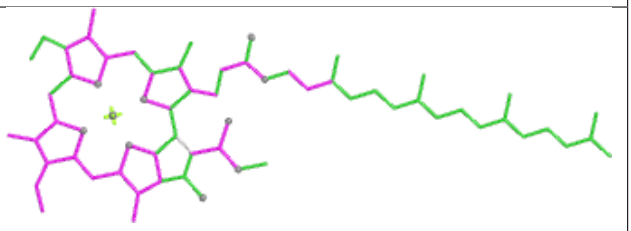


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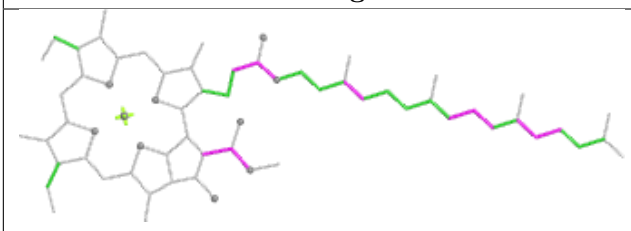
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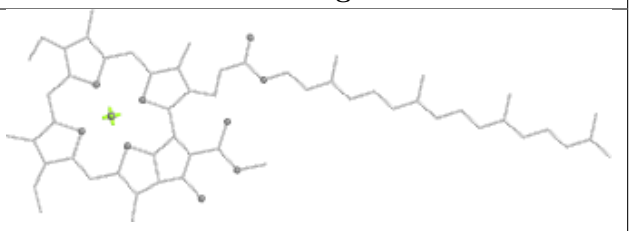
Bond lengths



Bond angles

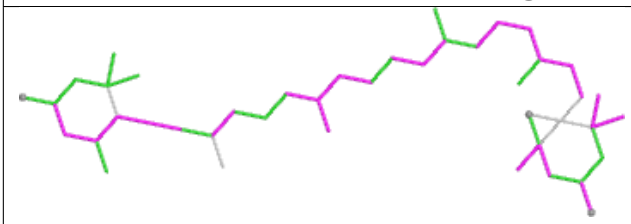


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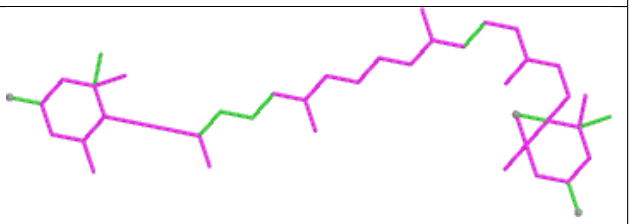


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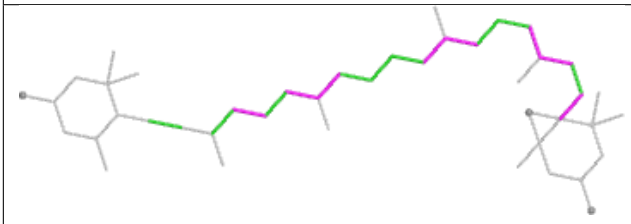
Ligand DD6 20 312



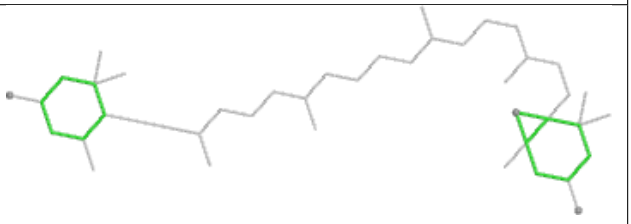
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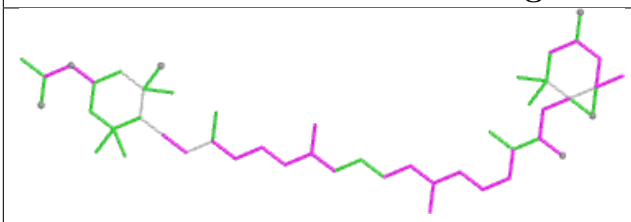


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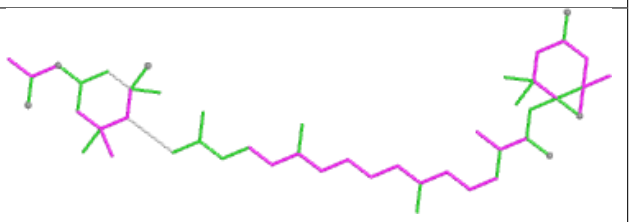


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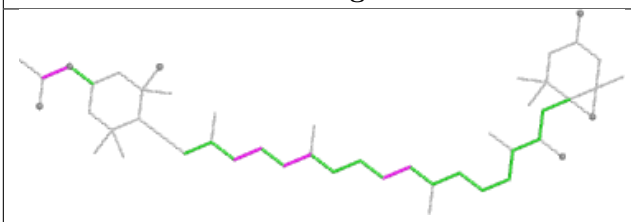
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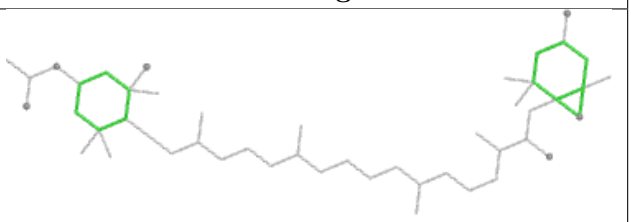
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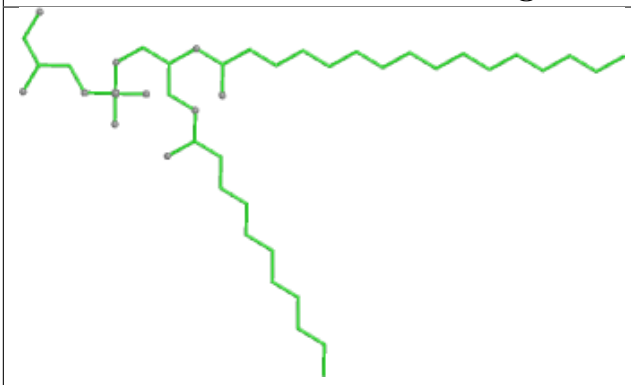


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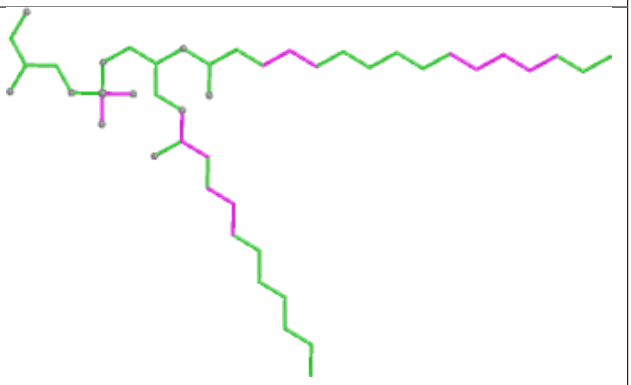


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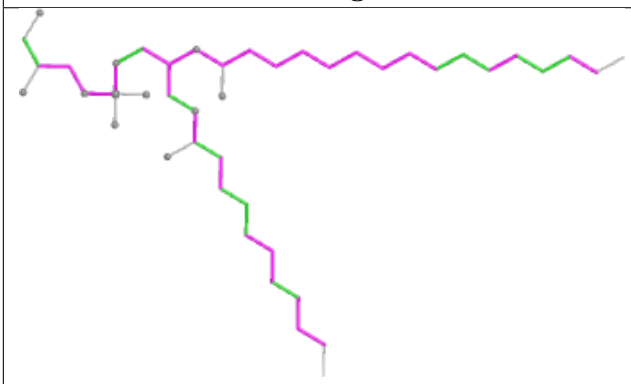
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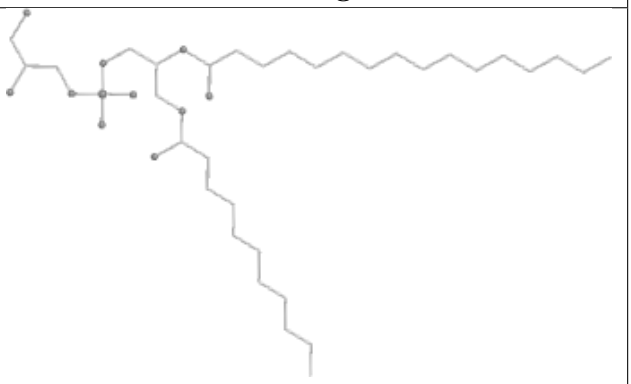
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Bond angles

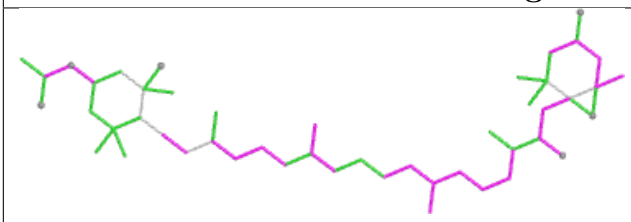


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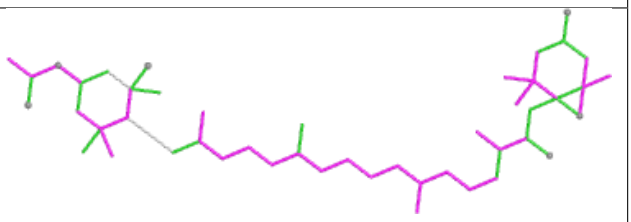


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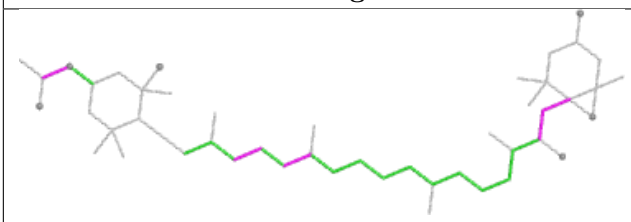
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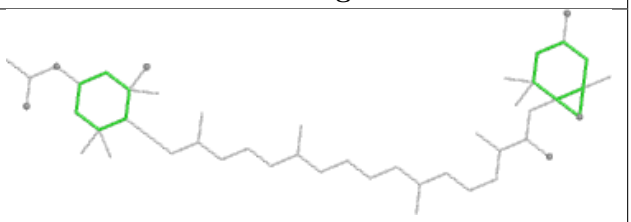
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Bond angles

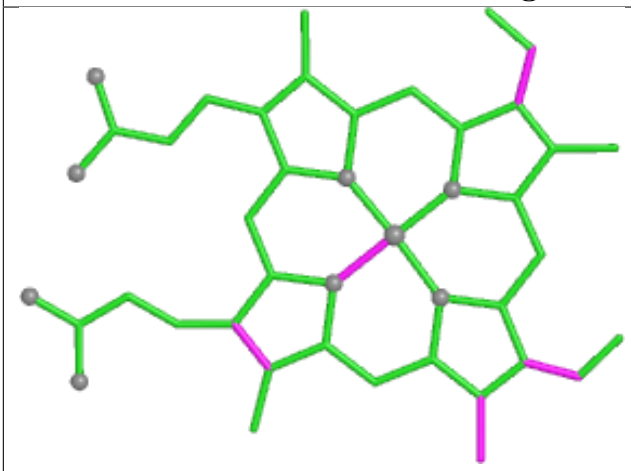


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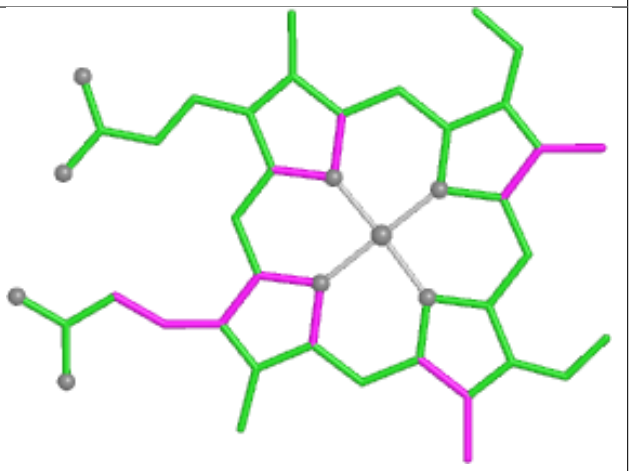


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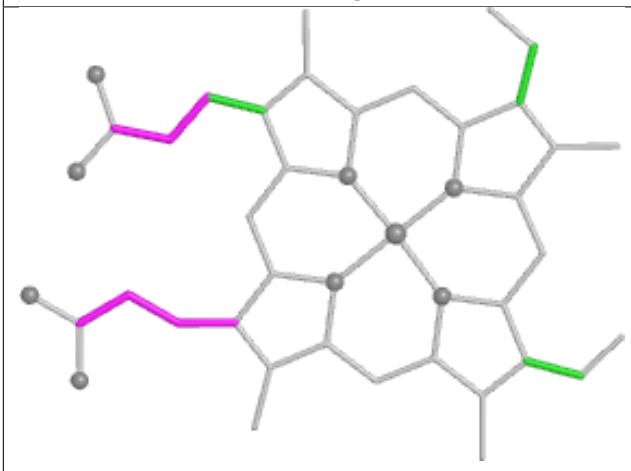
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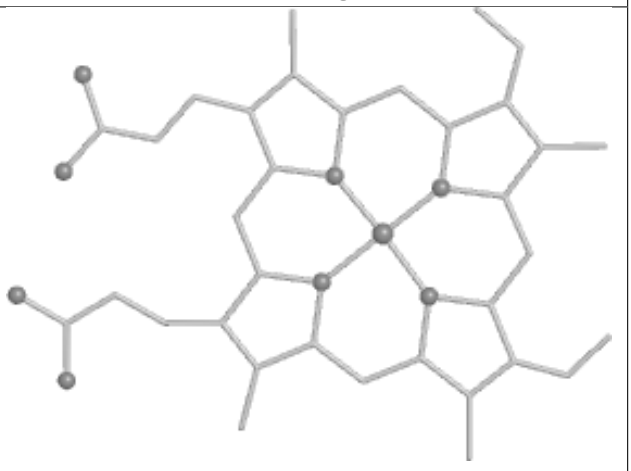
Bond lengths



Bond angles

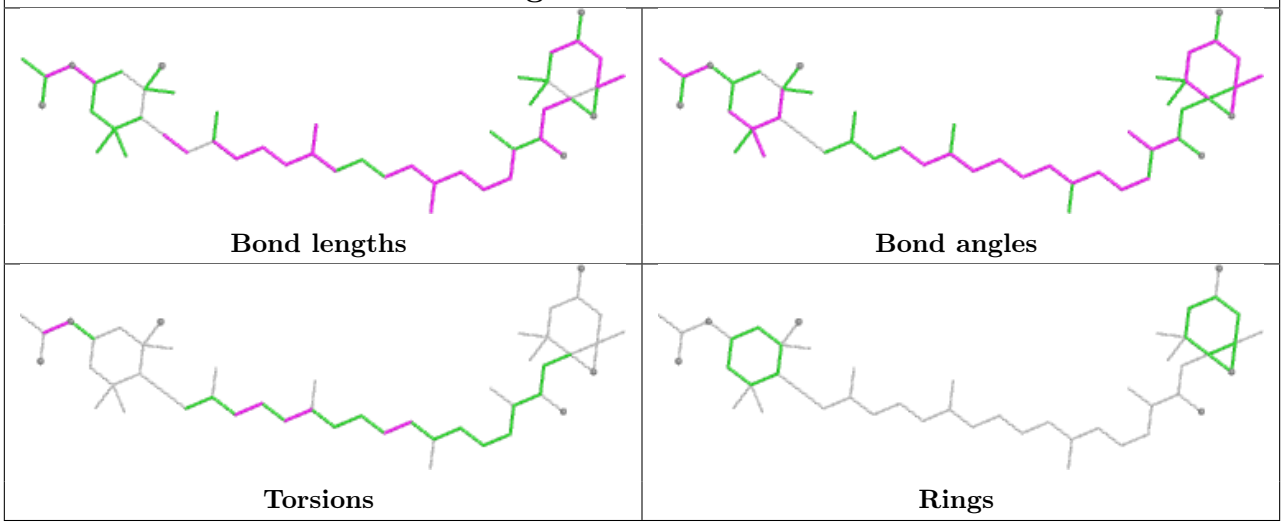


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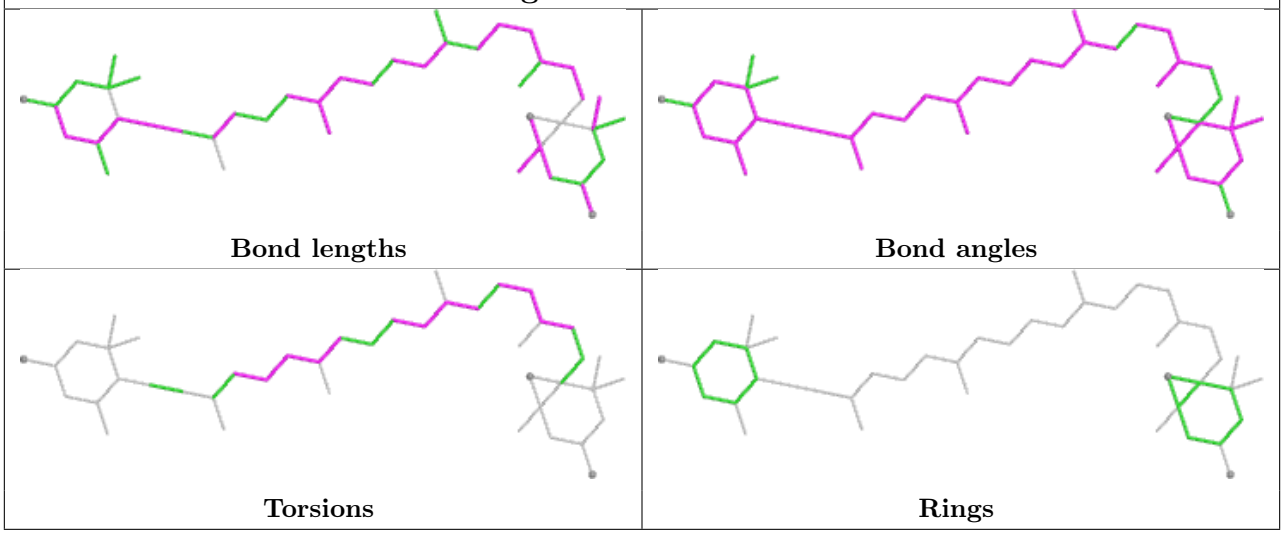


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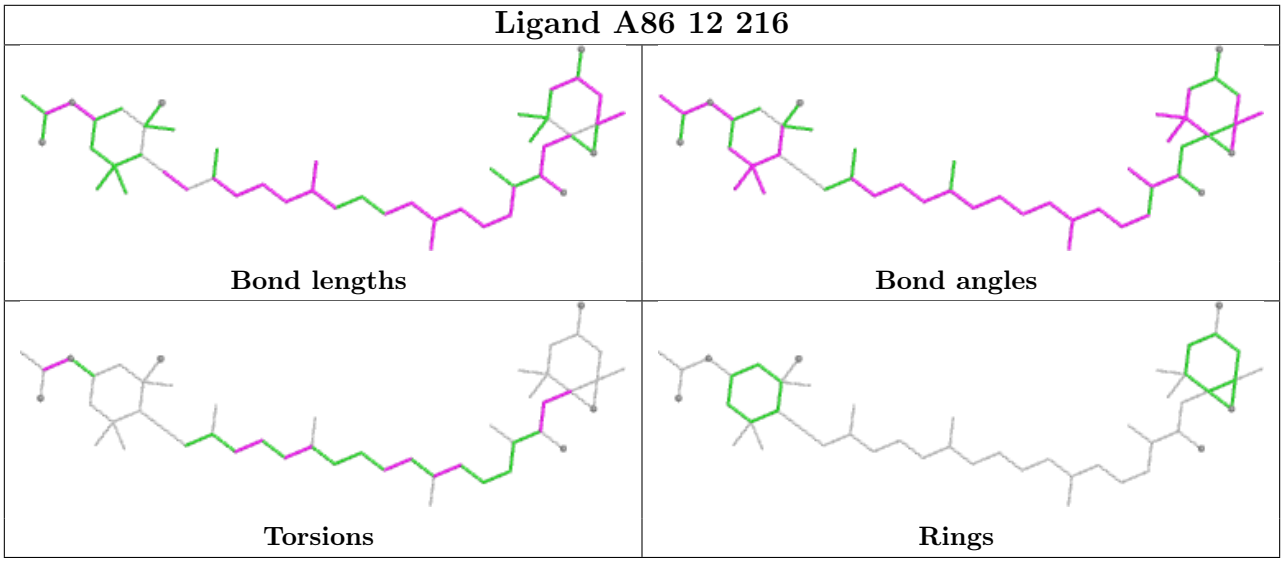
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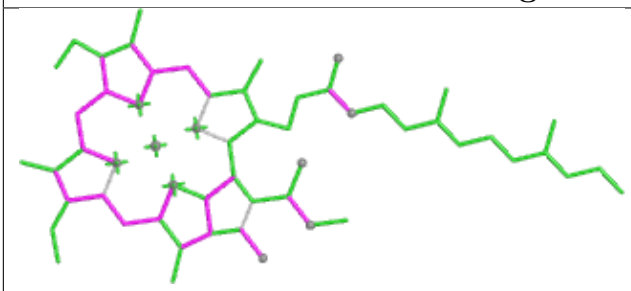
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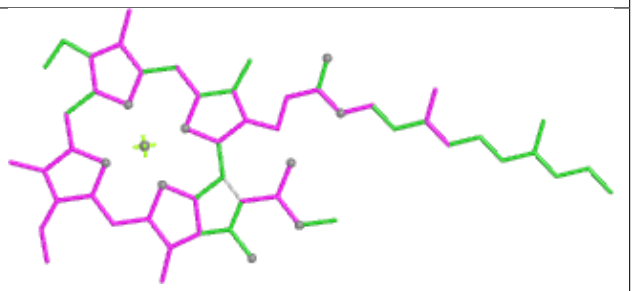
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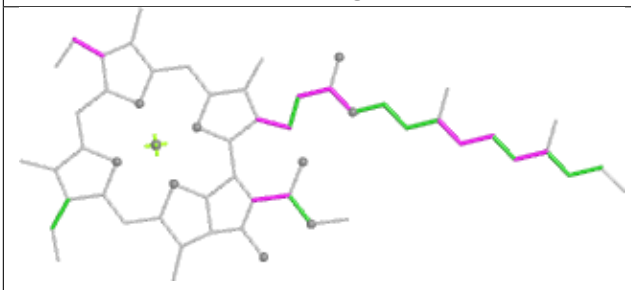
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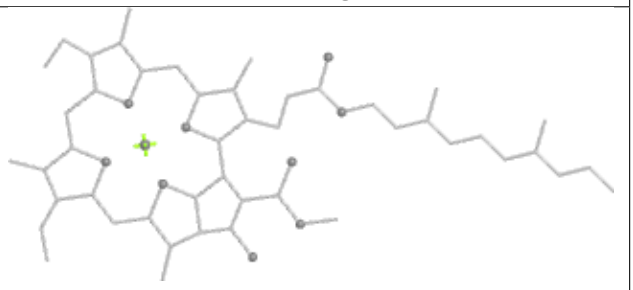
Bond lengths



Bond angles

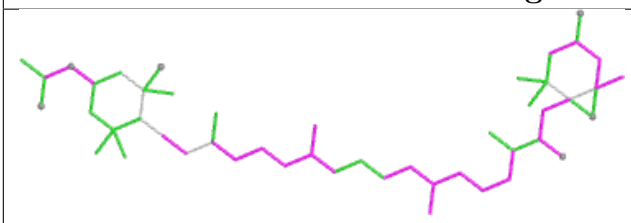


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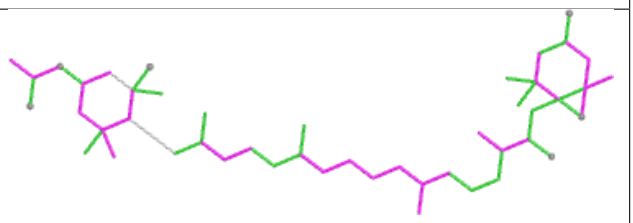


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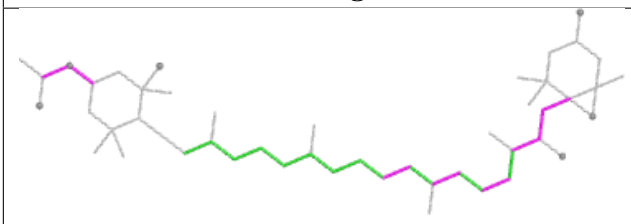
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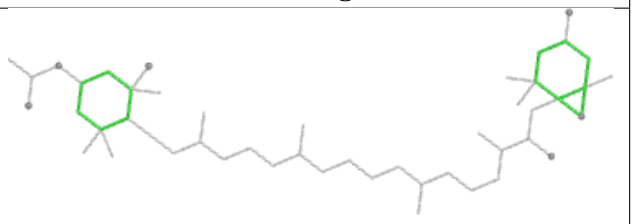
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Bond angles

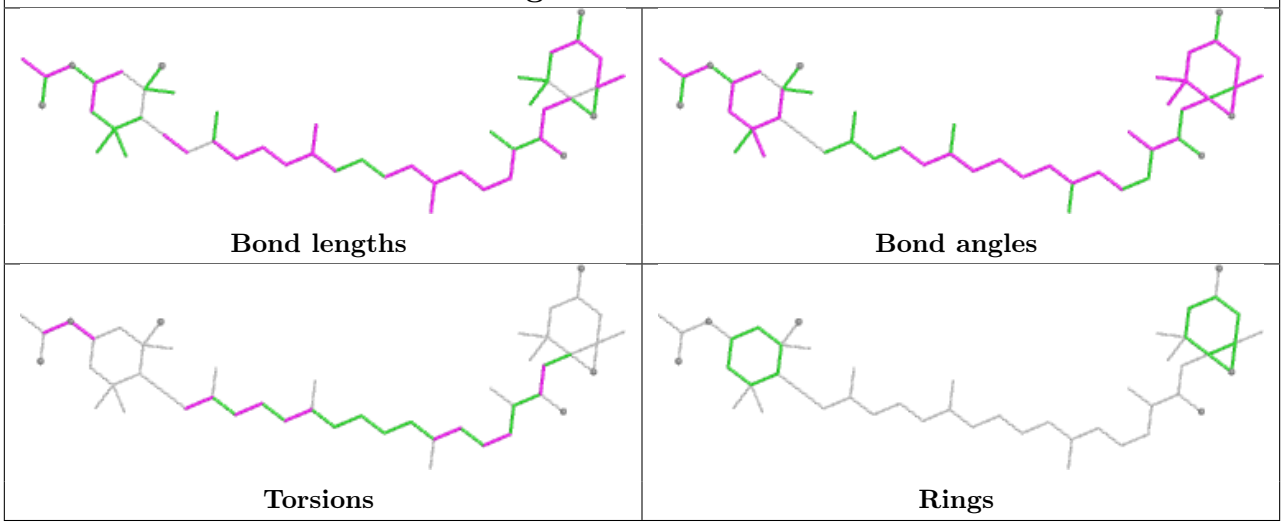


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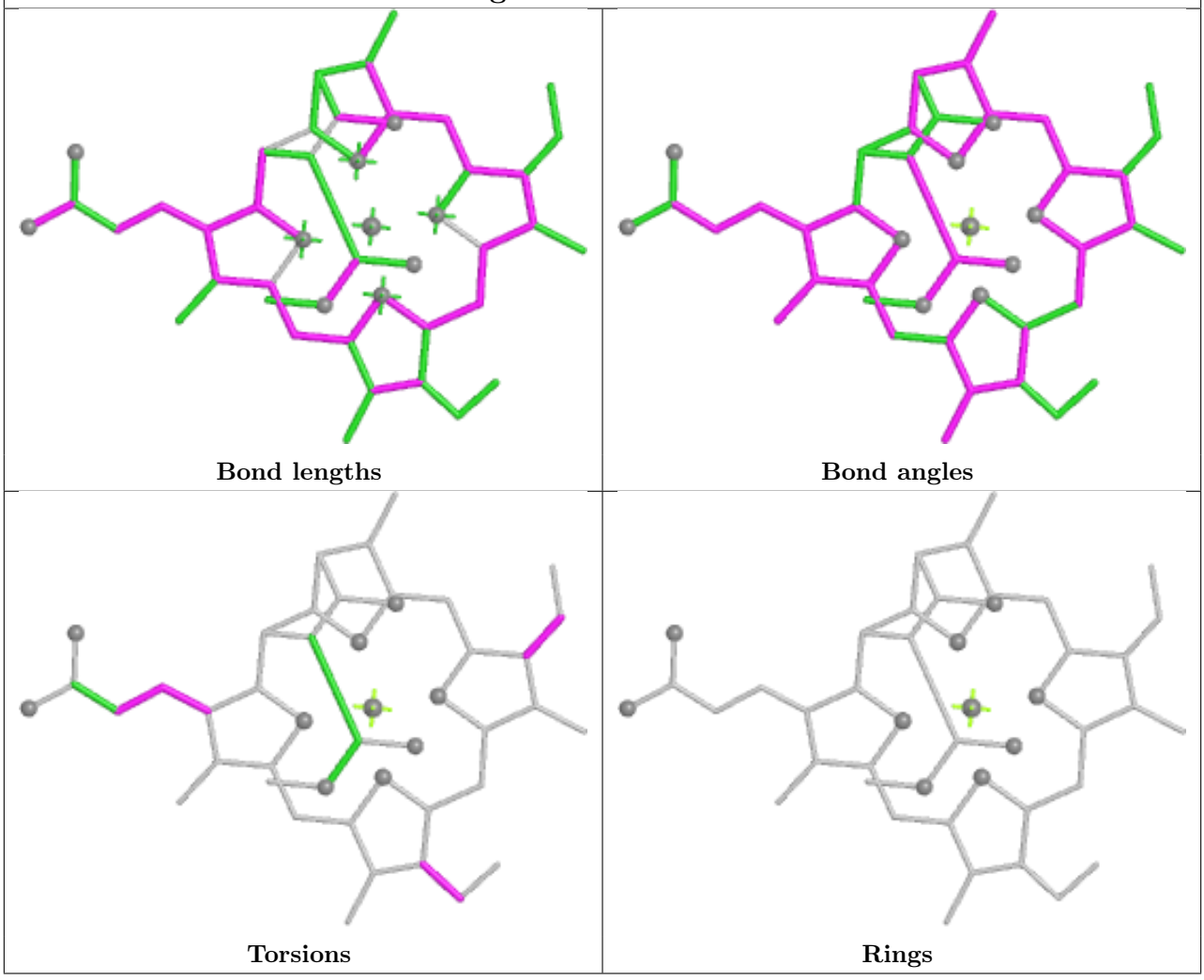


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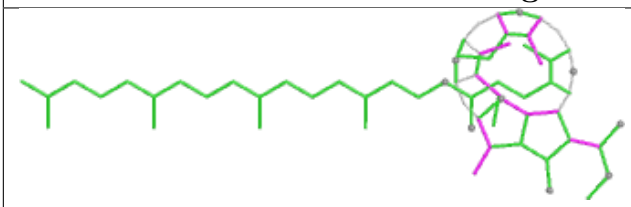
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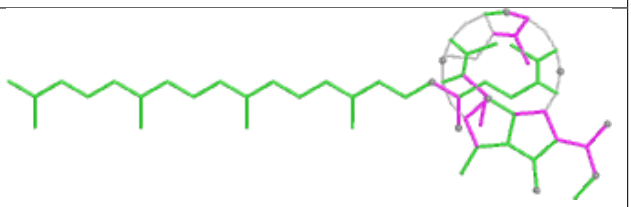
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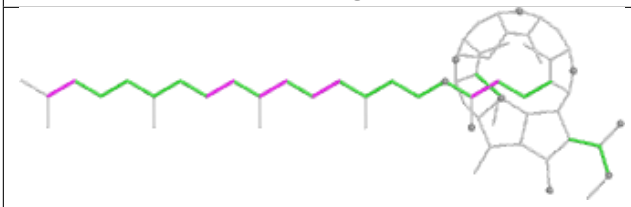
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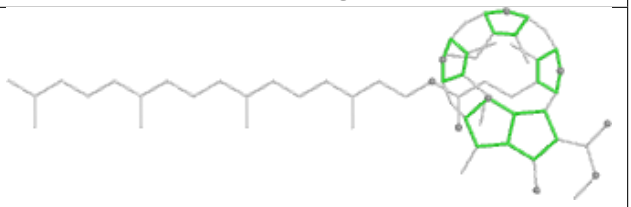
Bond lengths



Bond angles

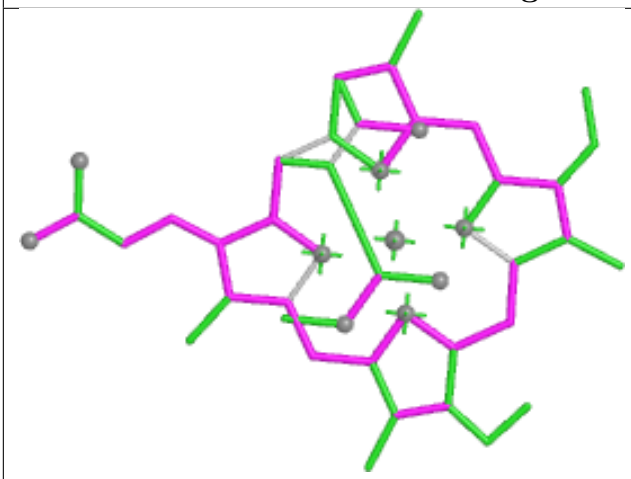


Torsions



Rings

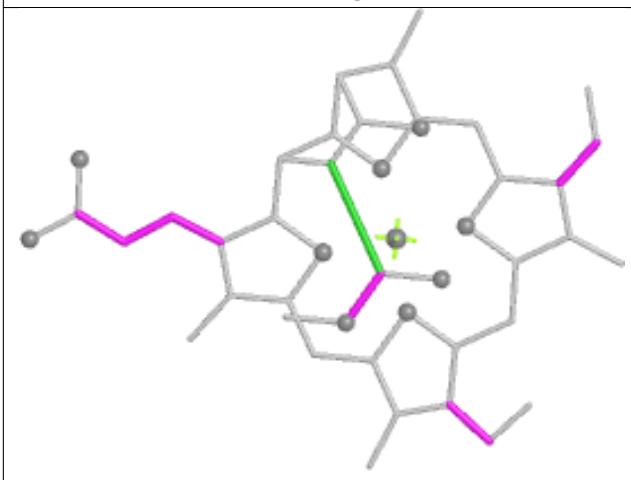
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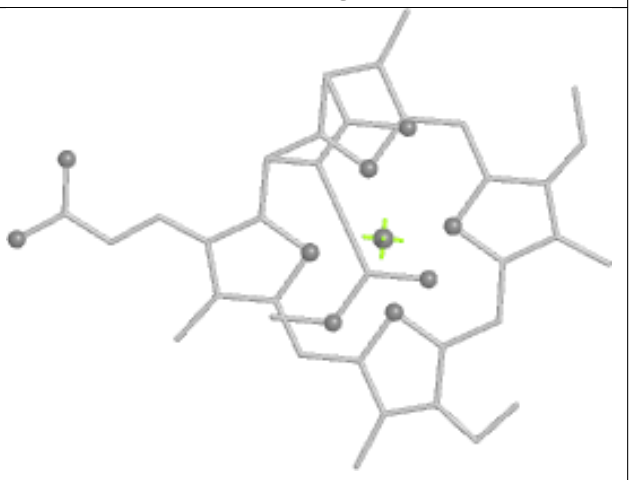
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Bond angles

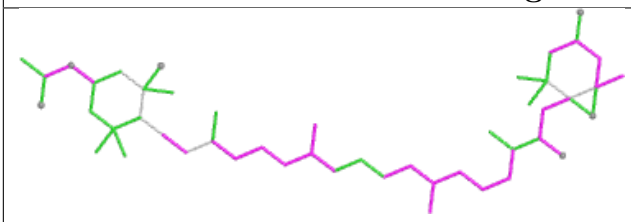


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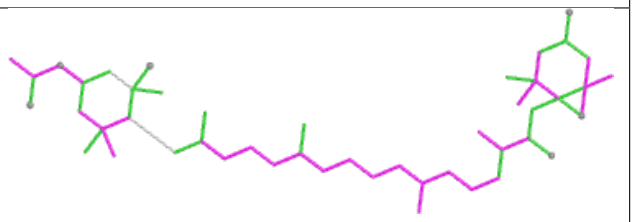


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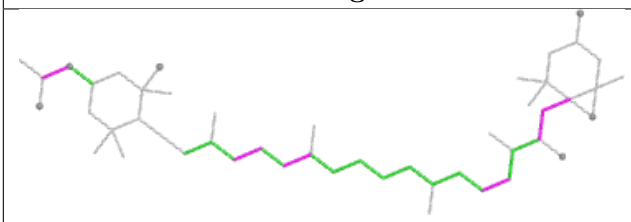
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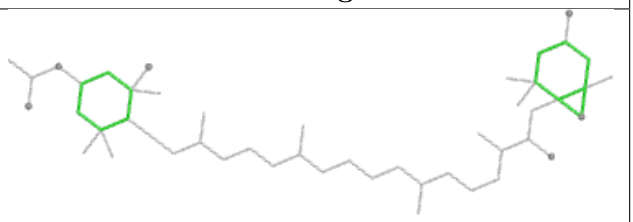
Bond lengths



Bond angles

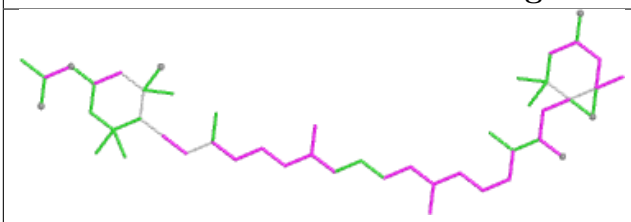


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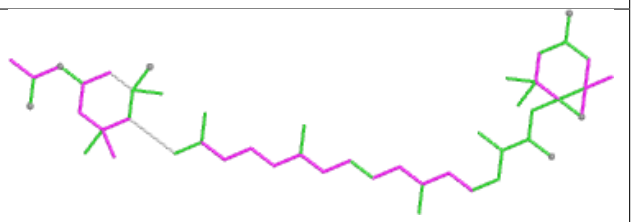


Rings

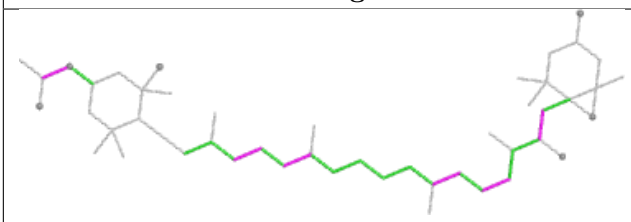
Ligand A86 41 211



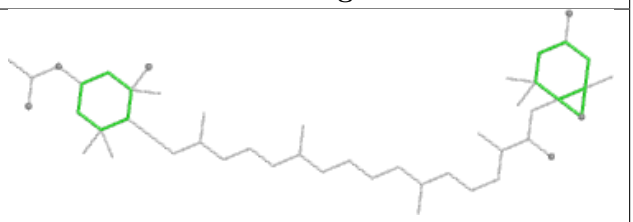
Bond lengths



Bond angles

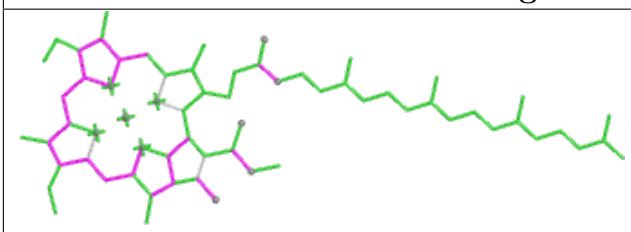


Torsions

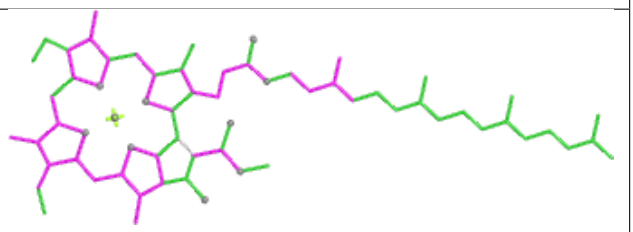


Rings

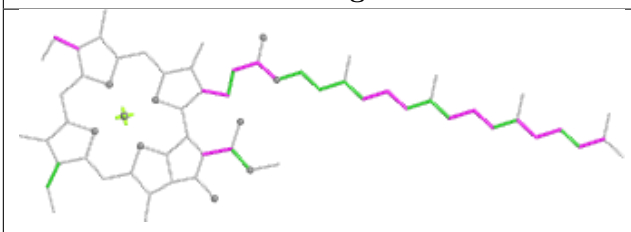
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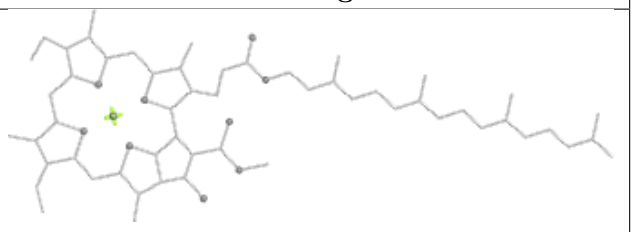
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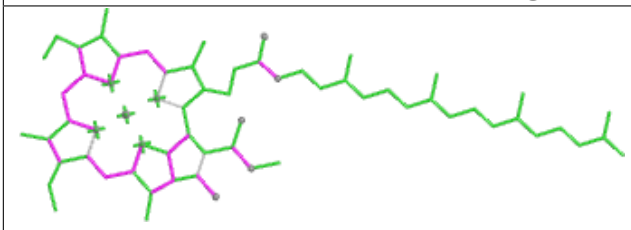
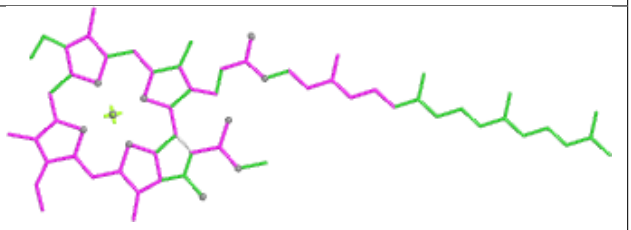
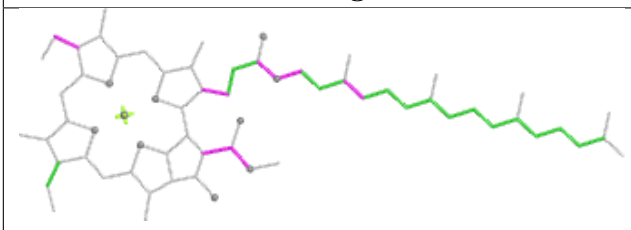
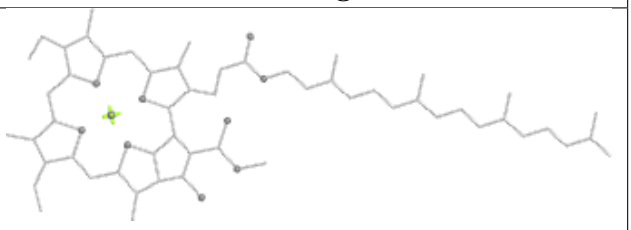
Bond angles

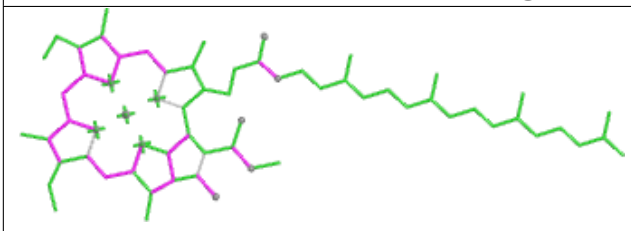
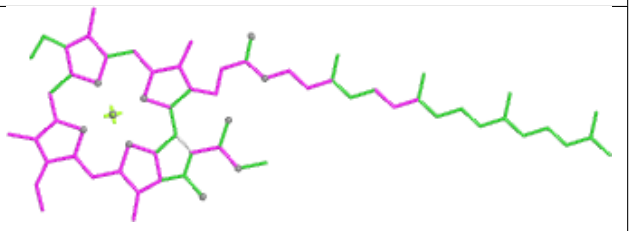
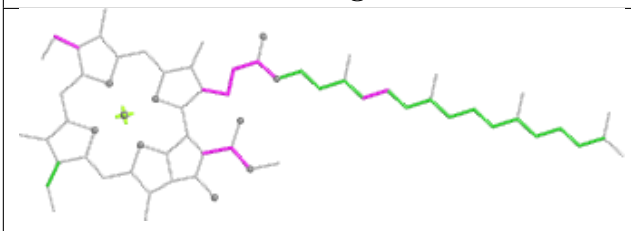
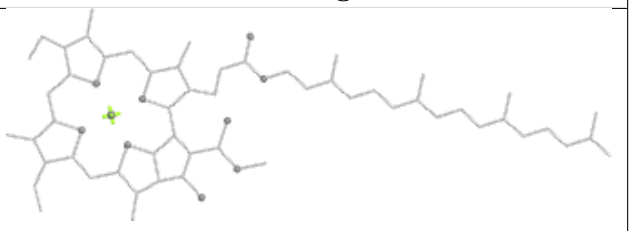


Torsions

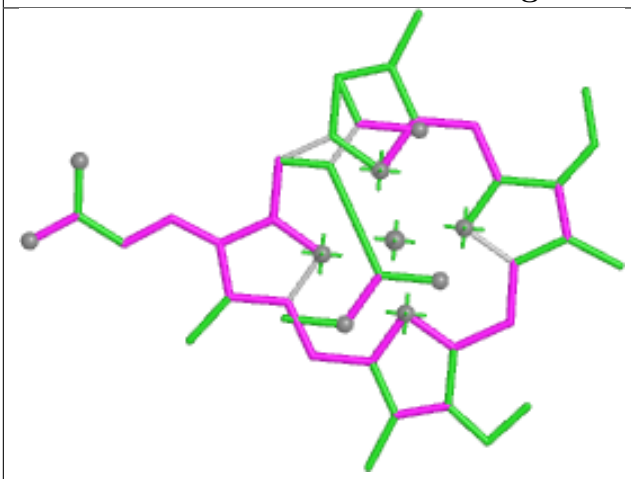


Rings

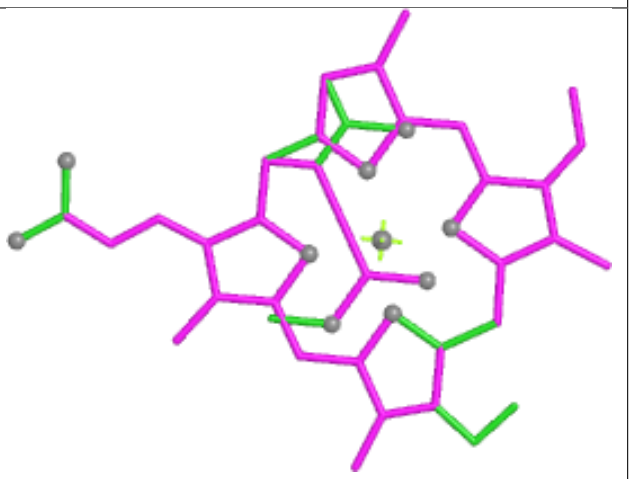
Ligand CLA B 509	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 39 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

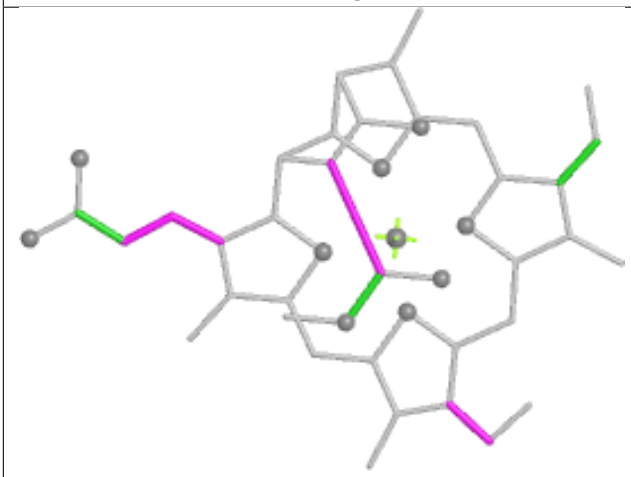
Ligand KC1 14 306



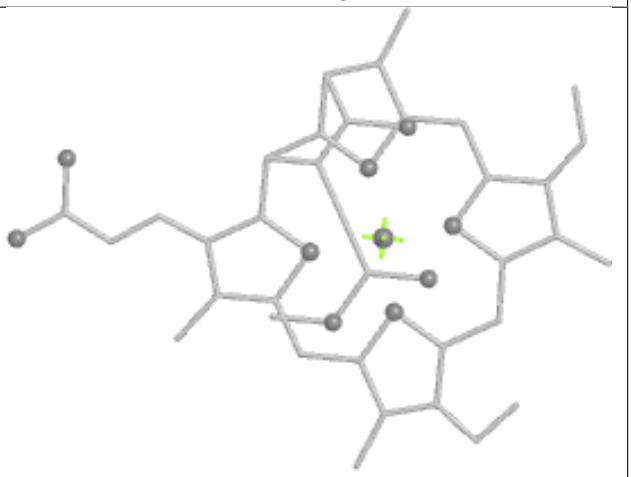
Bond lengths



Bond angles

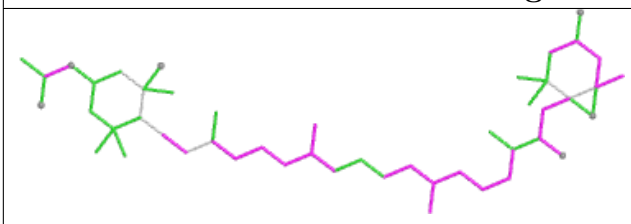


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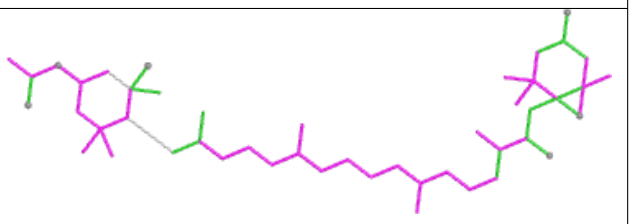


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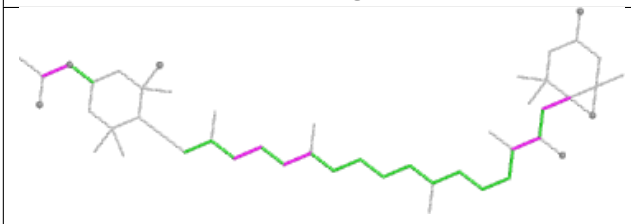
Ligand A86 11 314



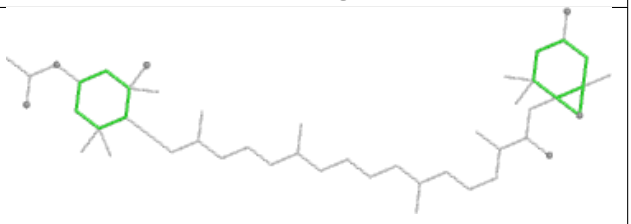
Bond lengths



Bond angles

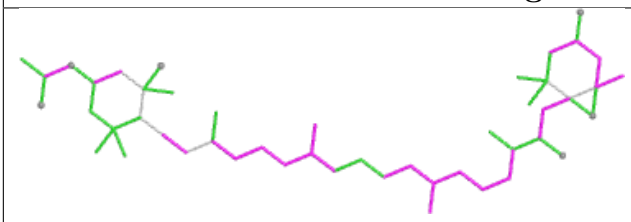


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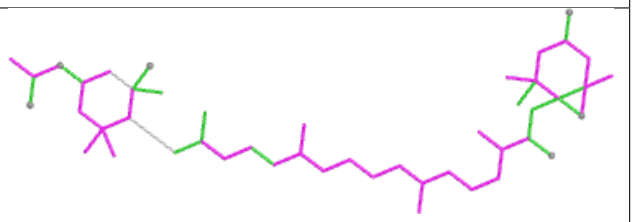


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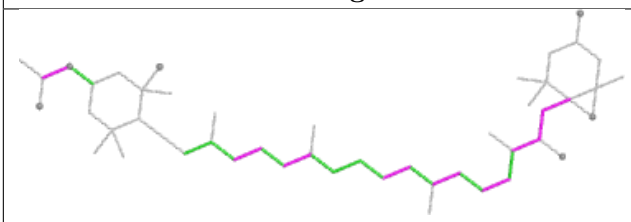
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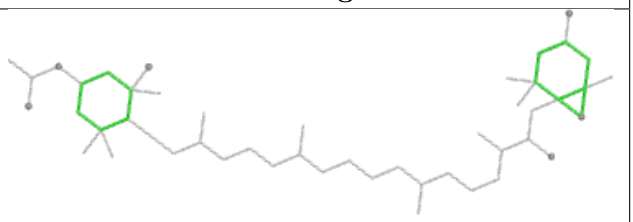
Bond lengths



Bond angles

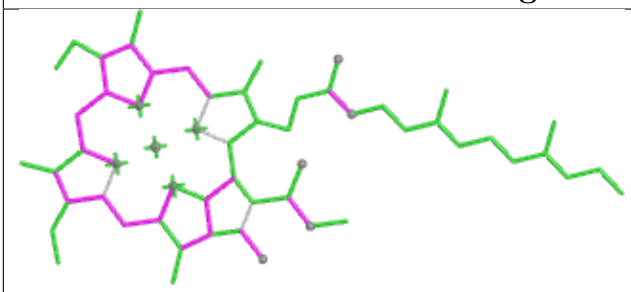


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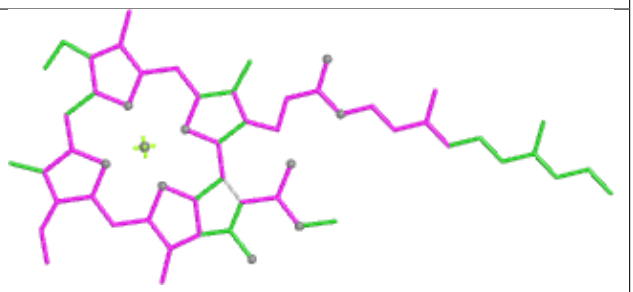


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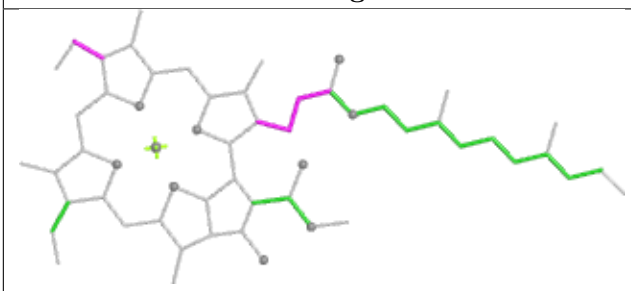
Ligand CLA 14 303



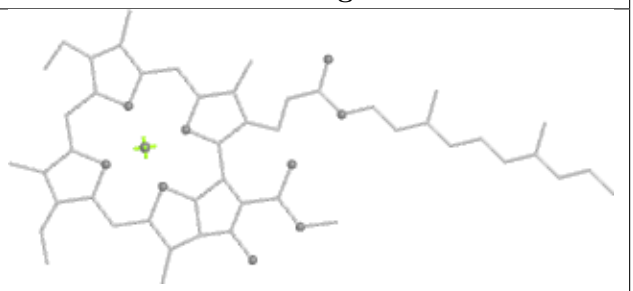
Bond lengths



Bond angles

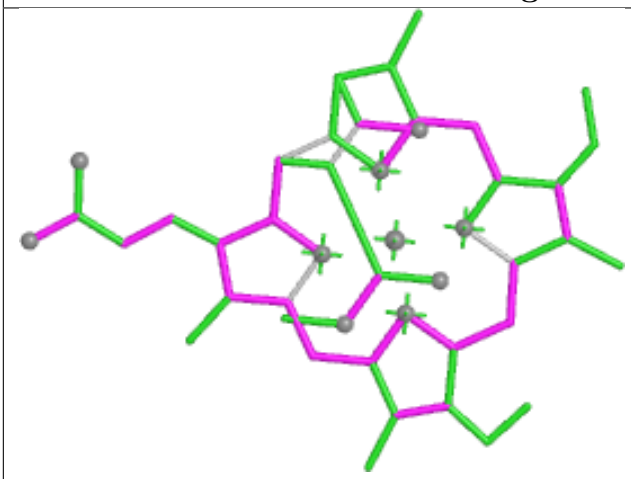


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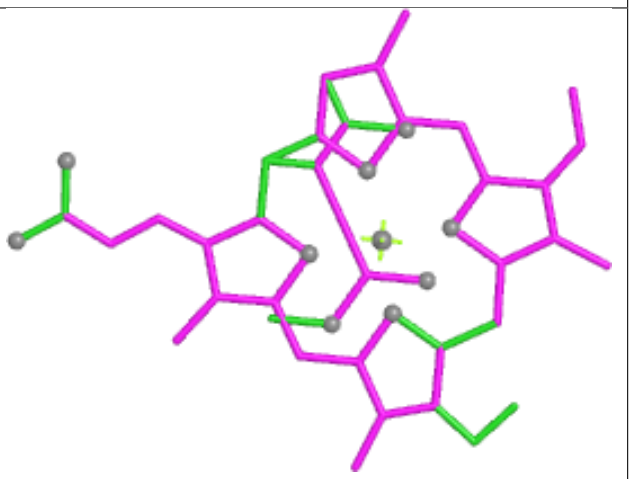


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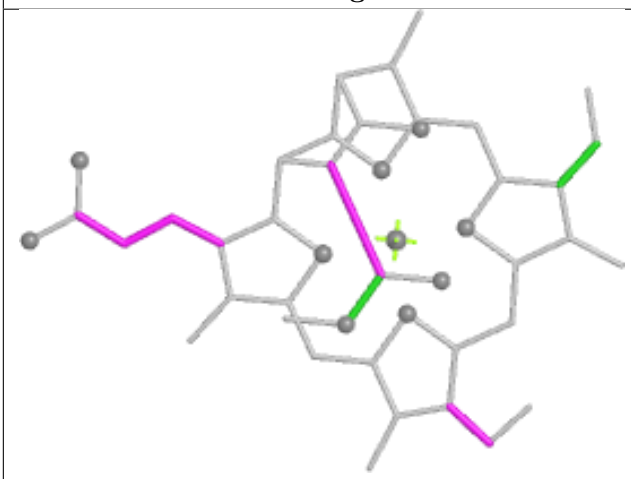
Ligand KC1 11 309



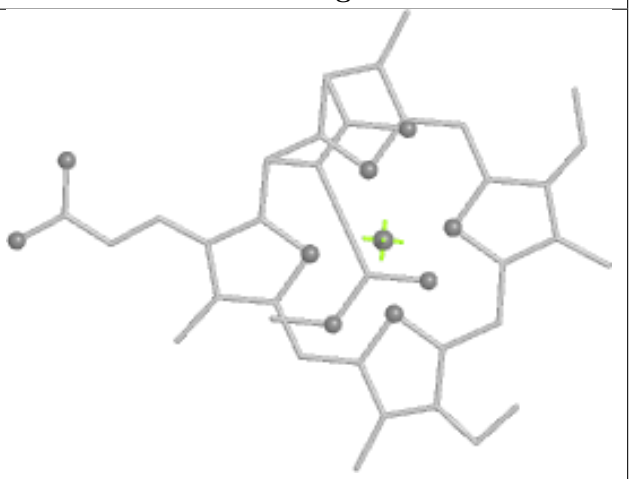
Bond lengths



Bond angles

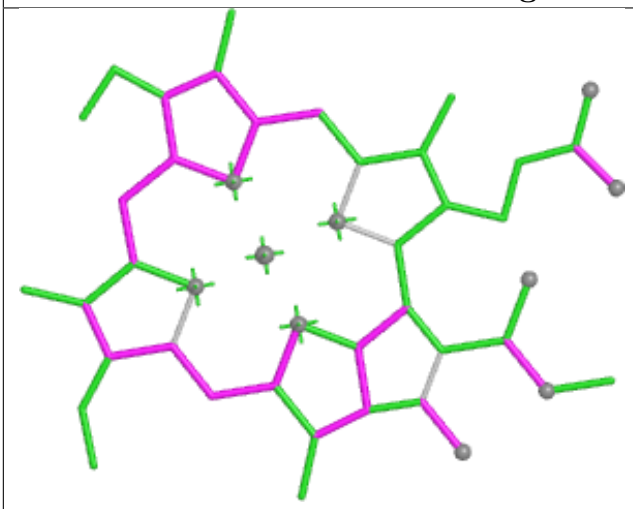


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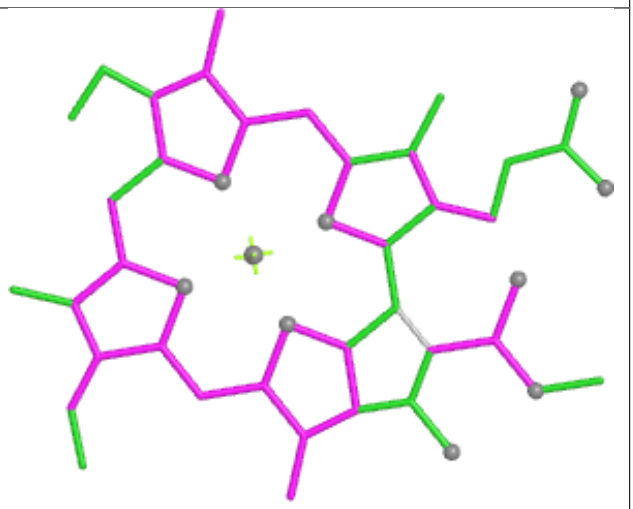


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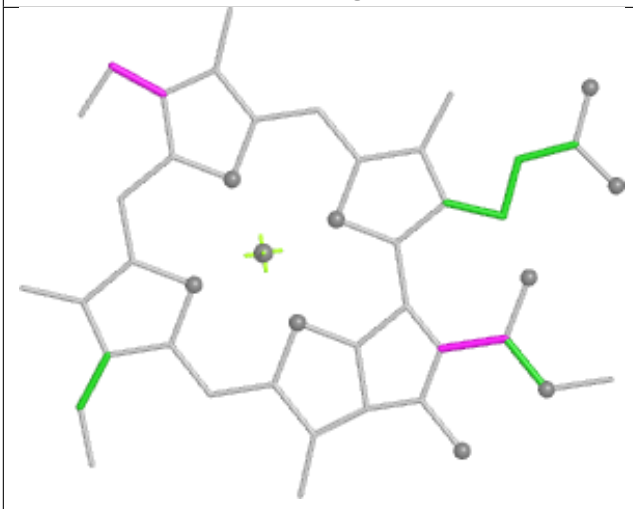
Ligand CLA 33 310



Bond lengths



Bond angles

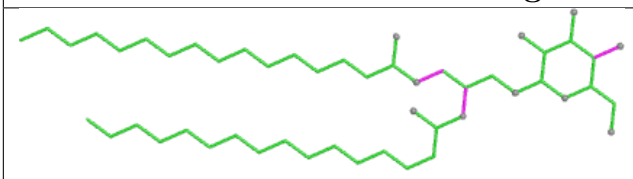


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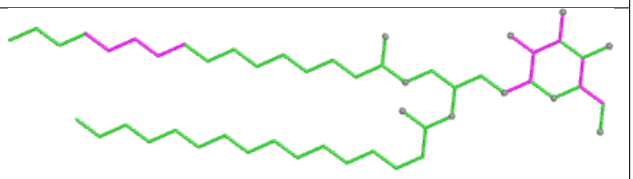


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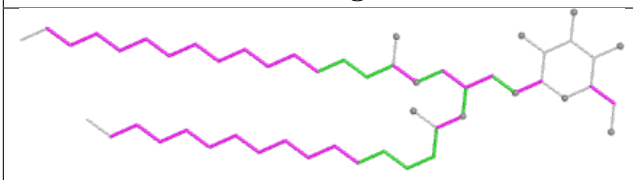
Ligand LMG a 410



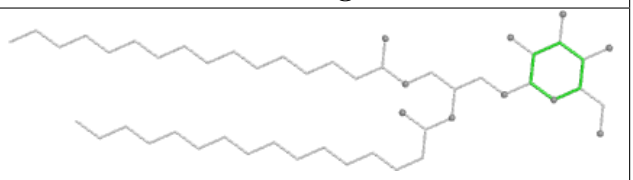
Bond lengths



Bond angles

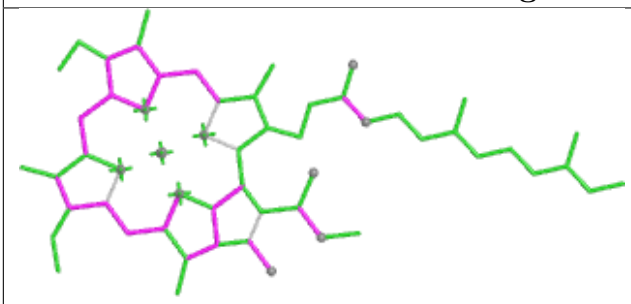


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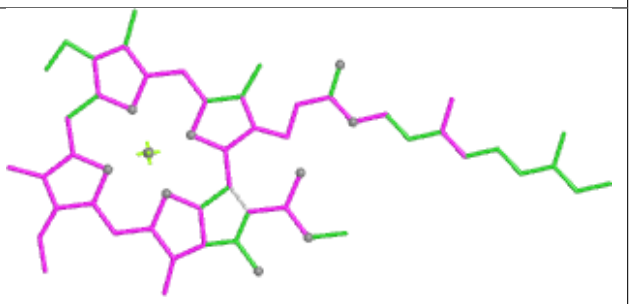


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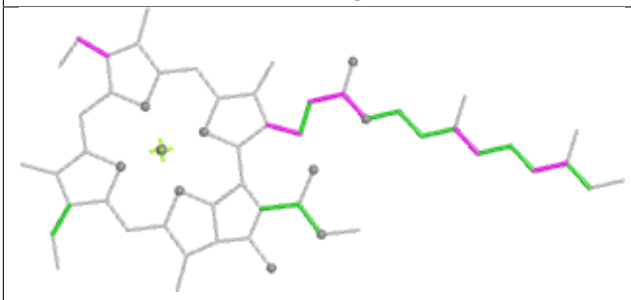
Ligand CLA 37 303



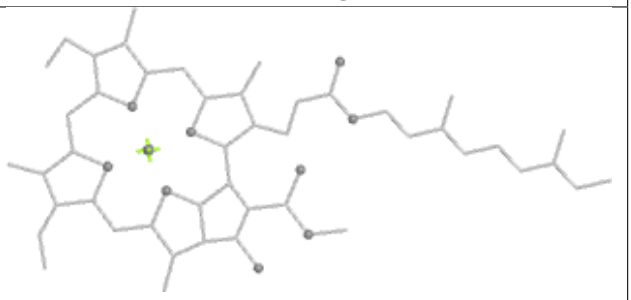
Bond lengths



Bond angles

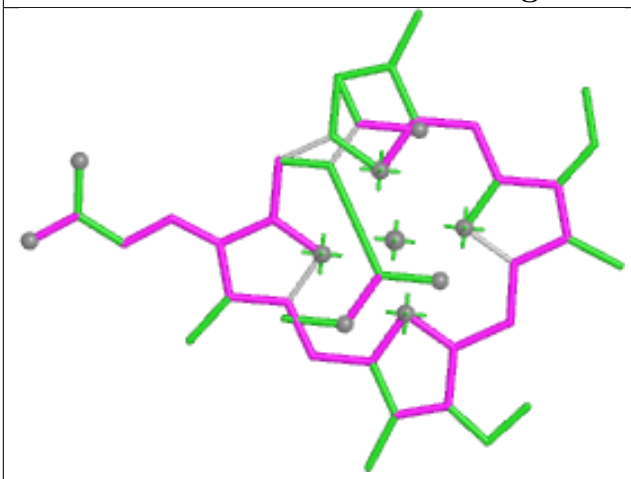


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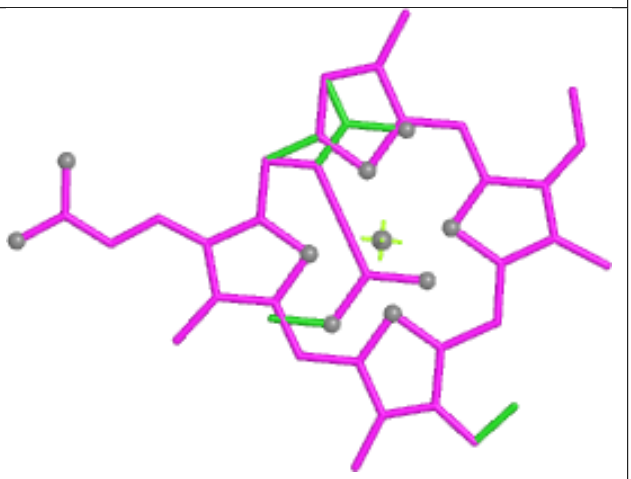


Rings

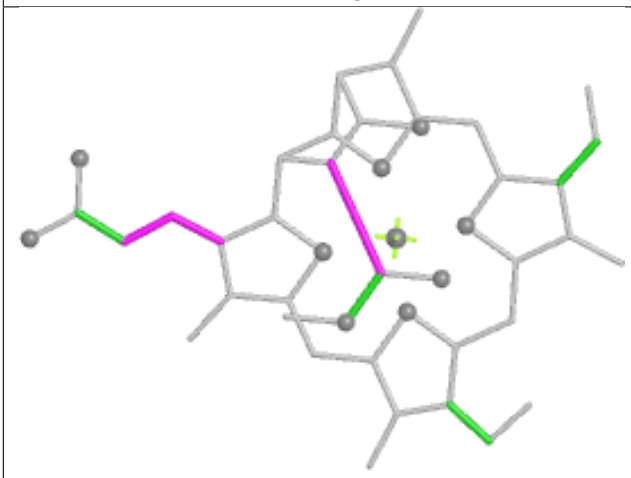
Ligand KC1 38 207



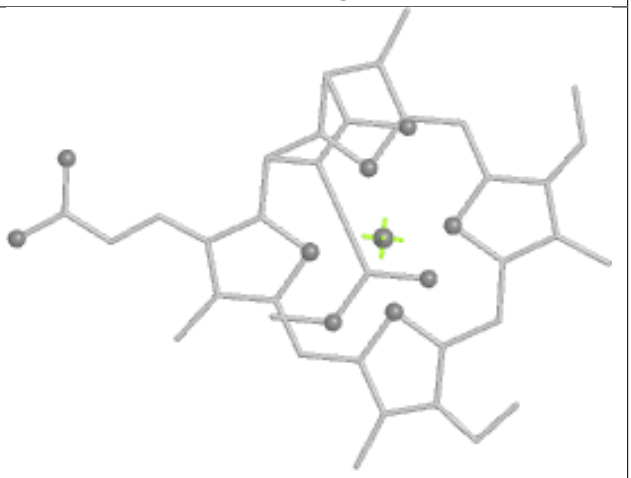
Bond lengths



Bond angles

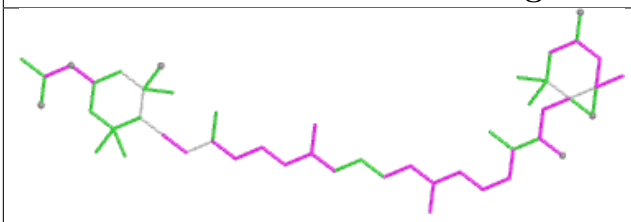


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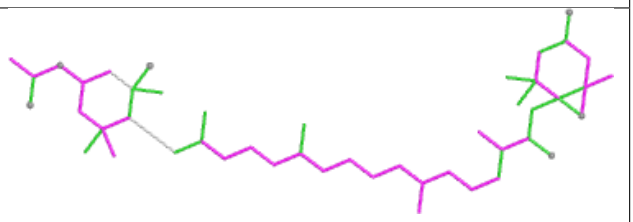


Rings

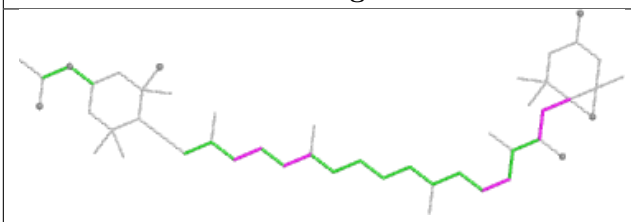
Ligand A86 33 311



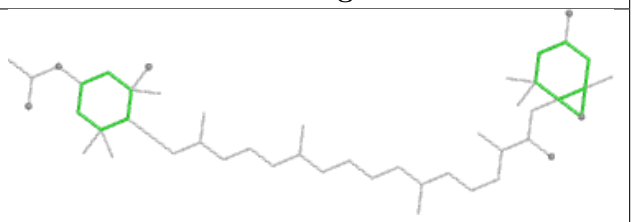
Bond lengths



Bond angles

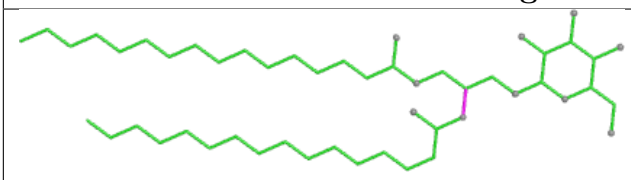


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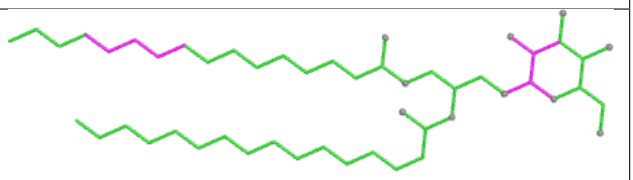


Rings

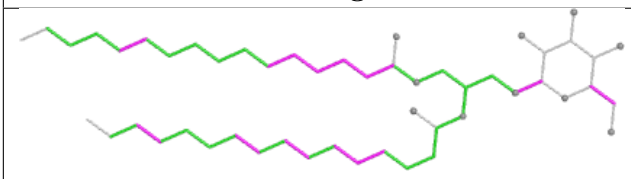
Ligand LMG B 520



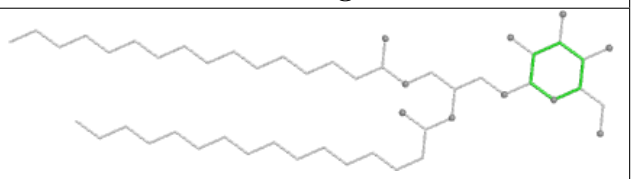
Bond lengths



Bond angles

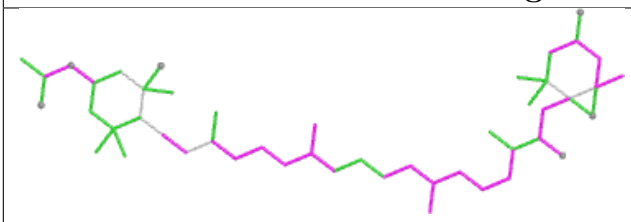


Torsions

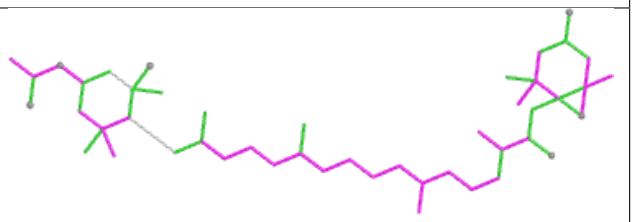


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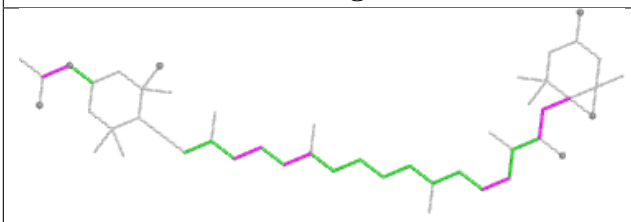
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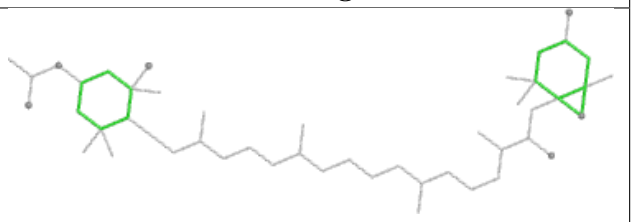
Bond lengths



Bond angles

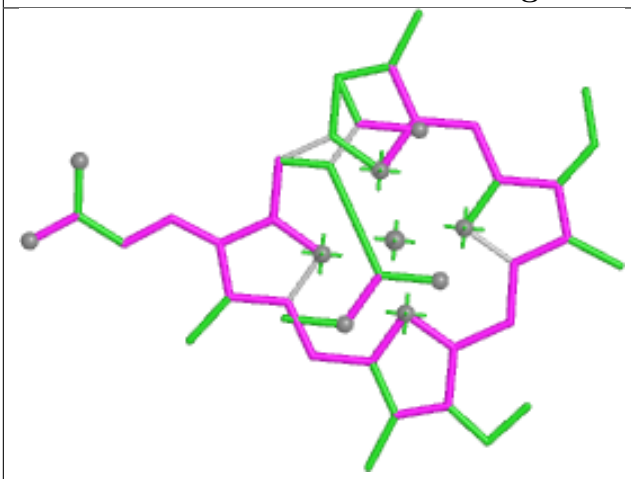


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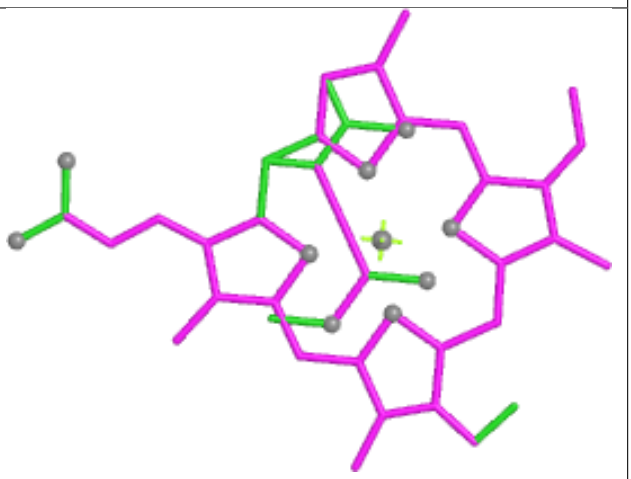


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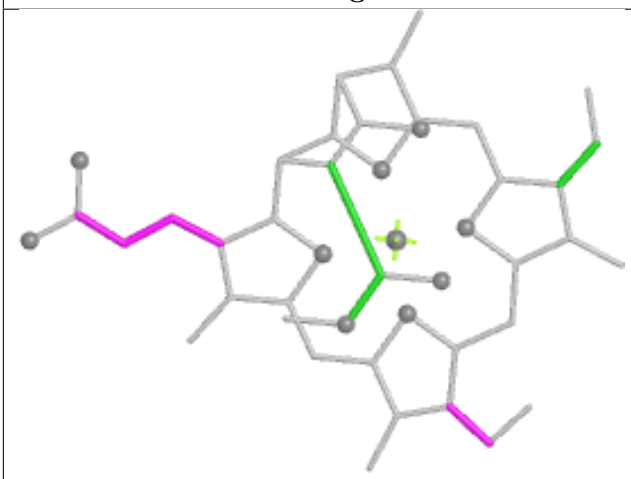
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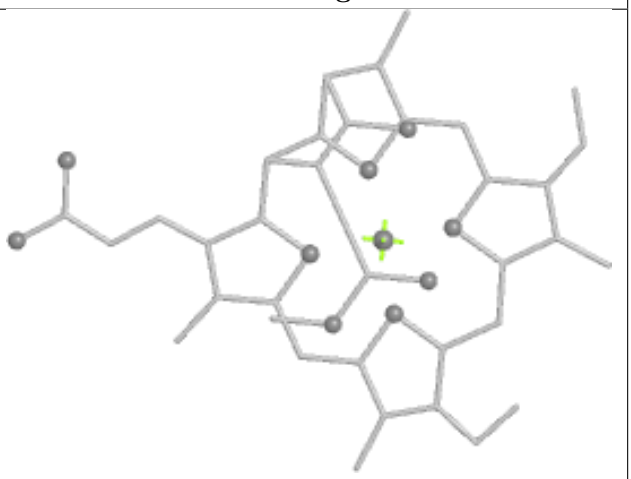
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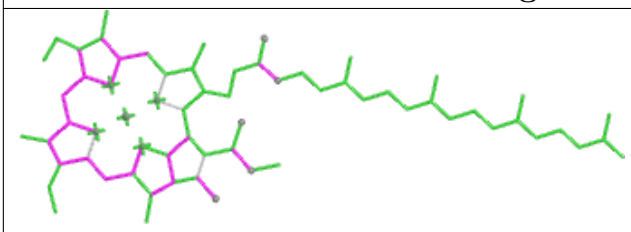


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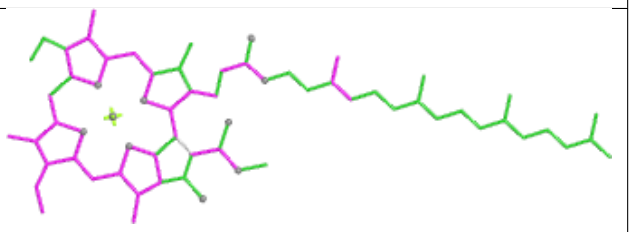


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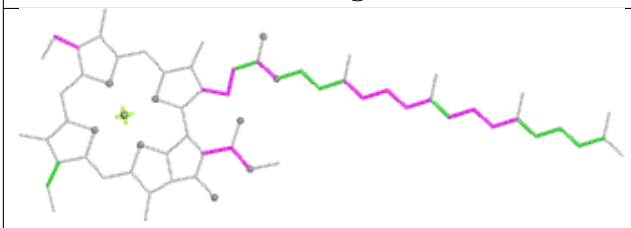
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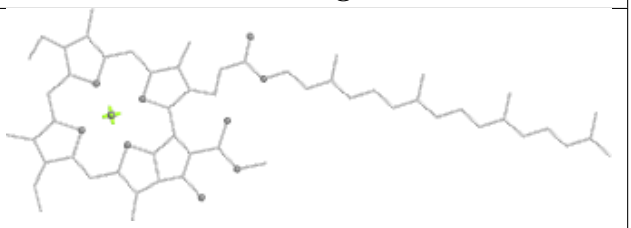
Bond lengths



Bond angles

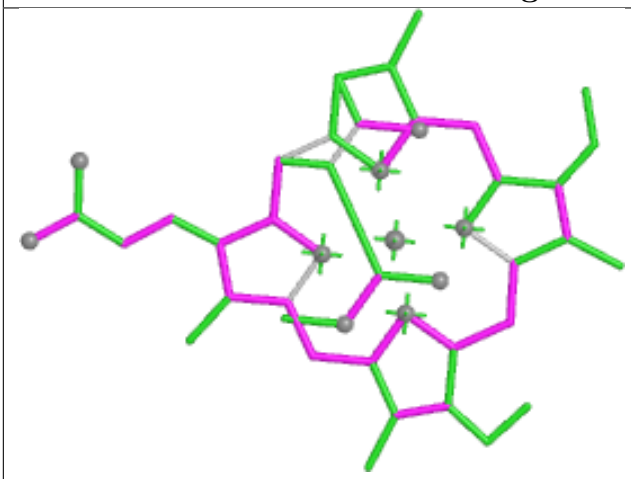


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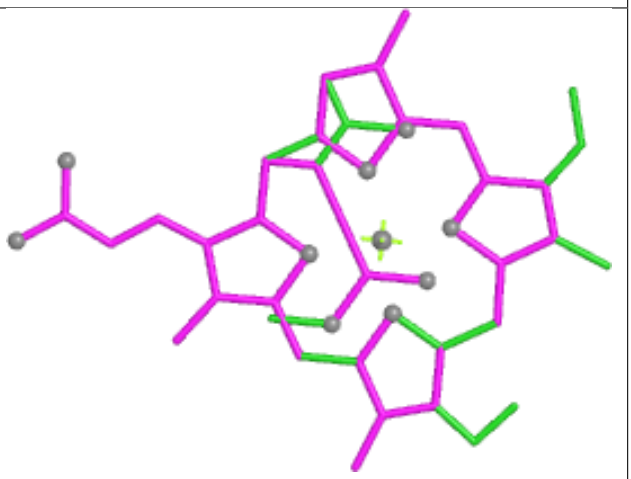


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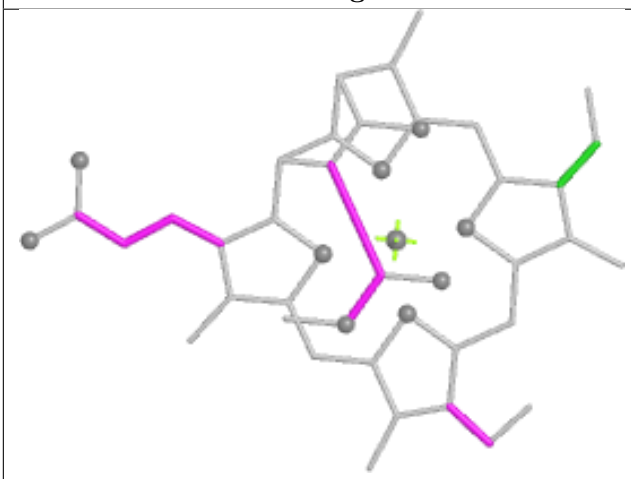
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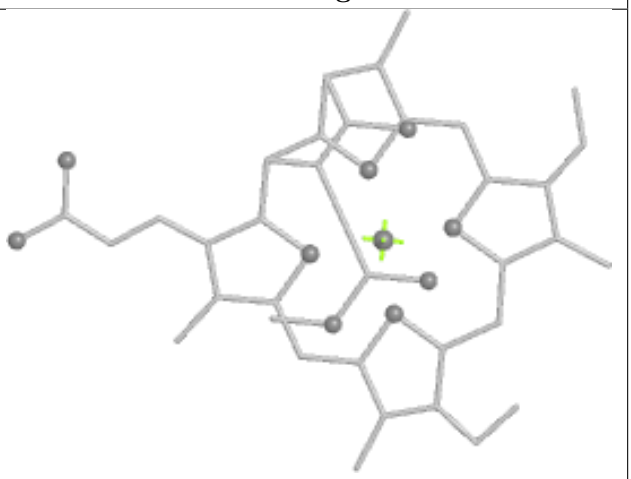
Bond lengths



Bond angles

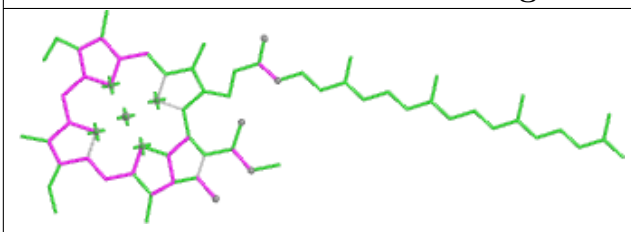


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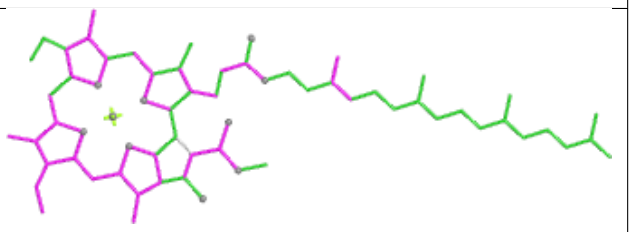


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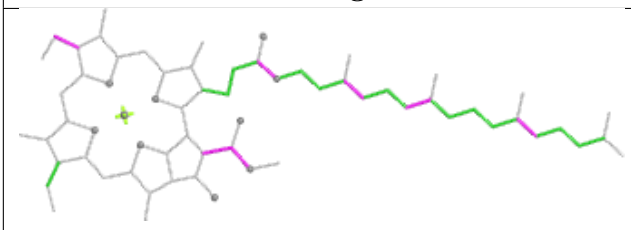
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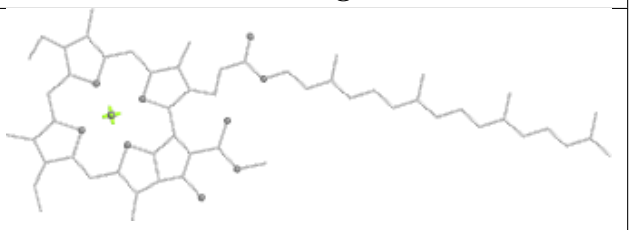
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Bond angles

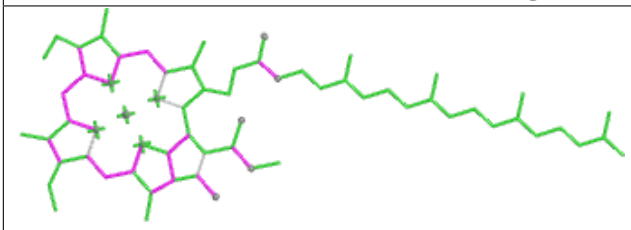


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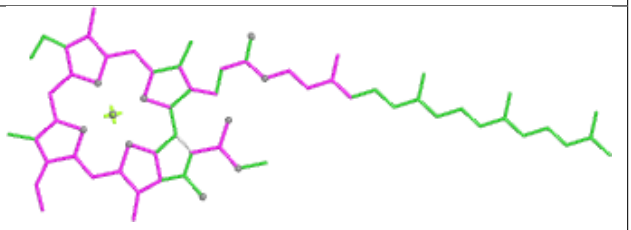


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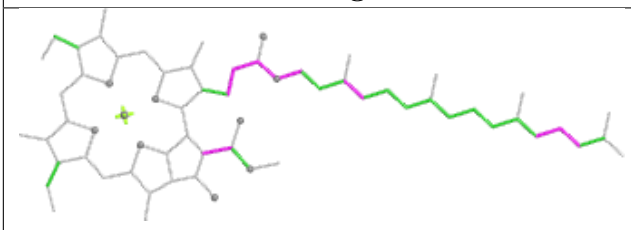
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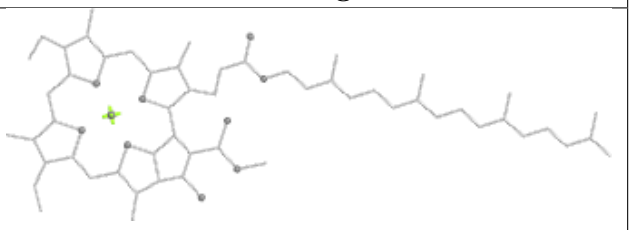
Bond lengths



Bond angles

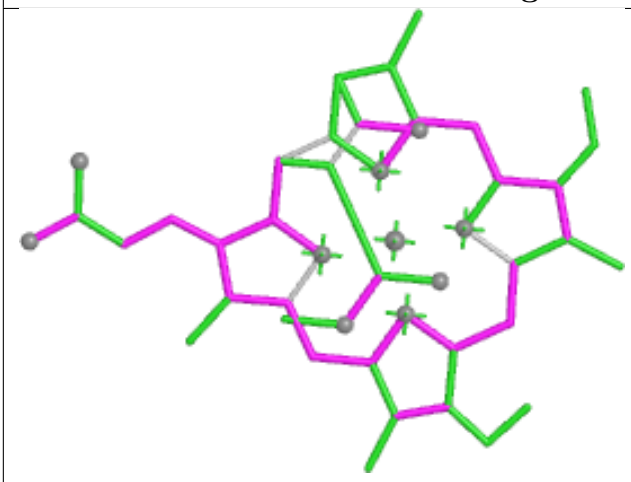


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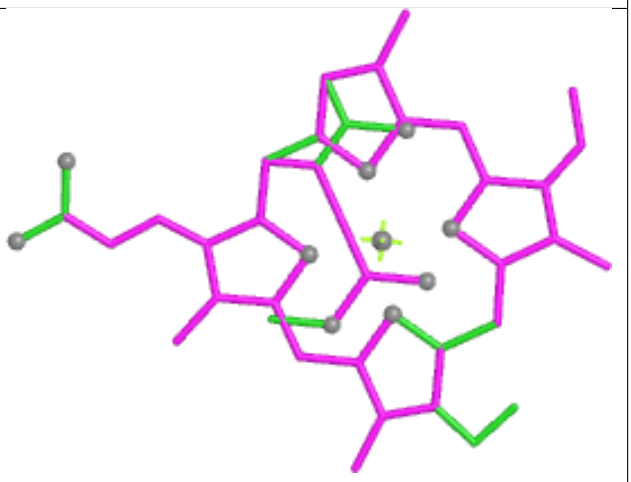


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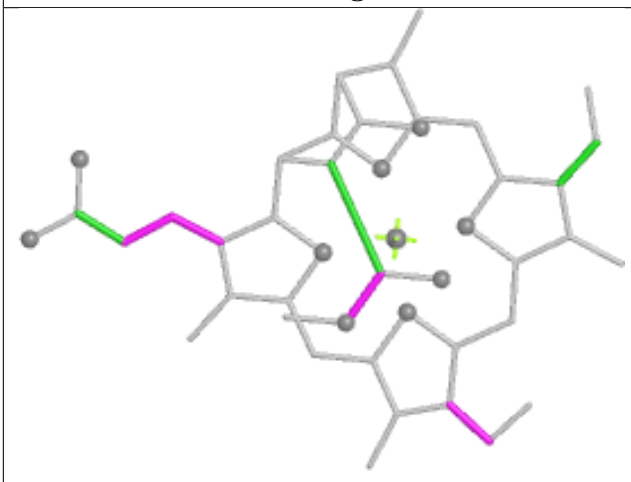
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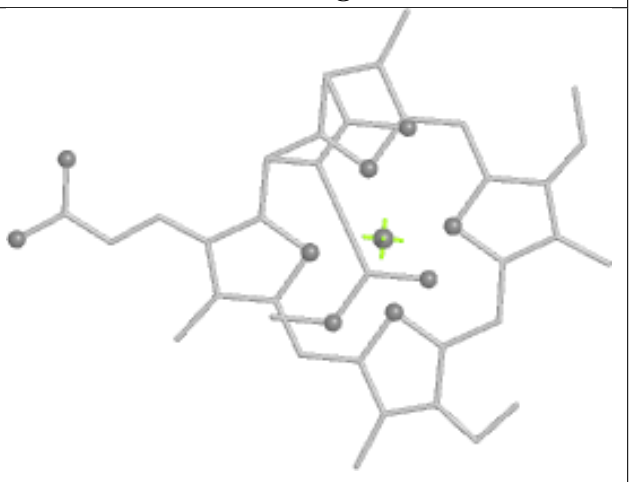
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Bond angles

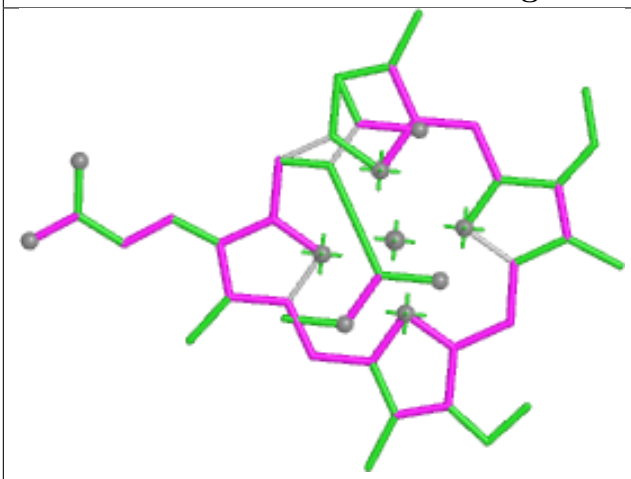


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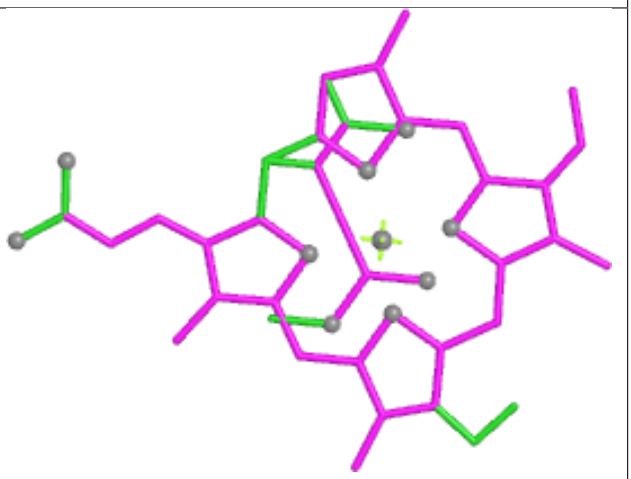


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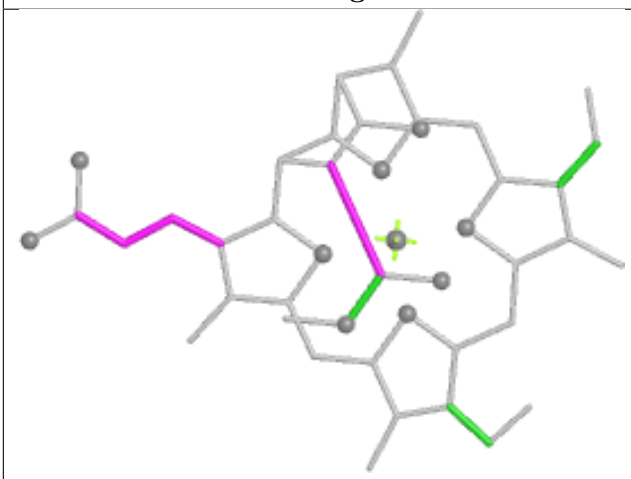
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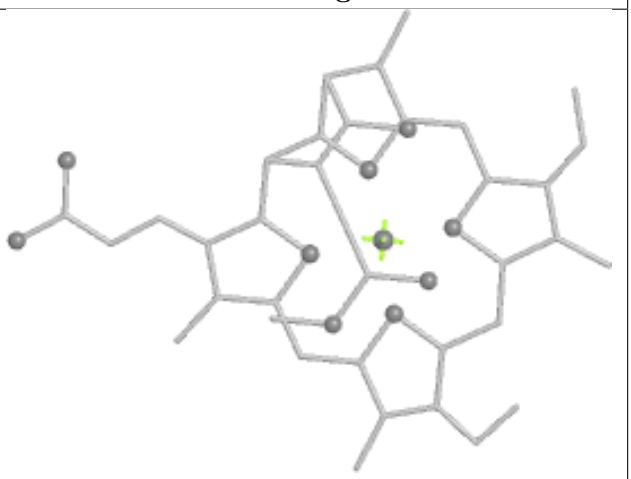
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Bond angles

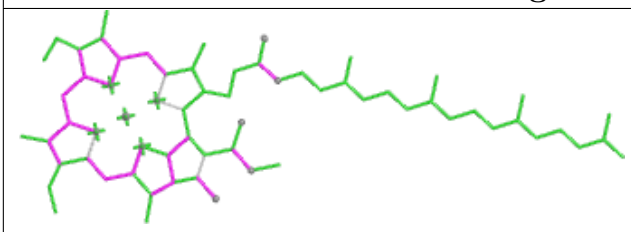


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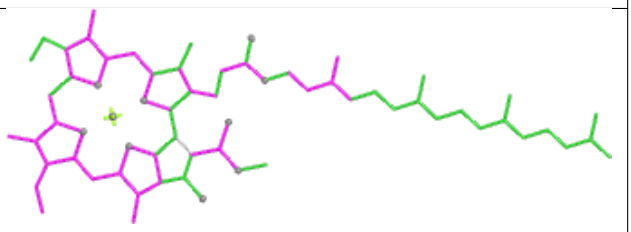


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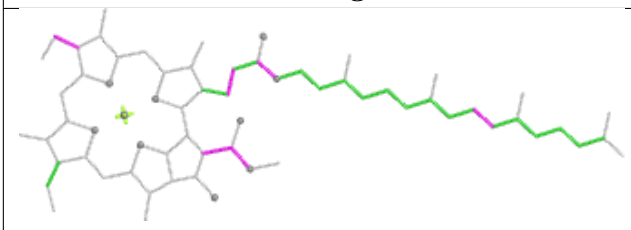
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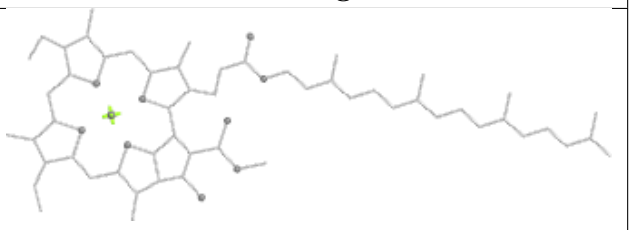
Bond lengths



Bond angles

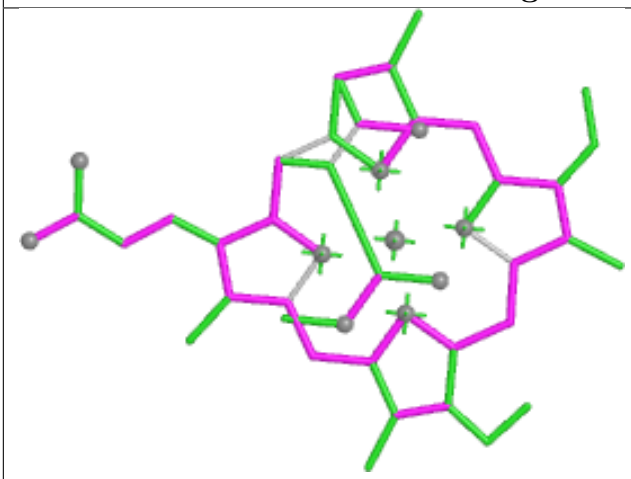


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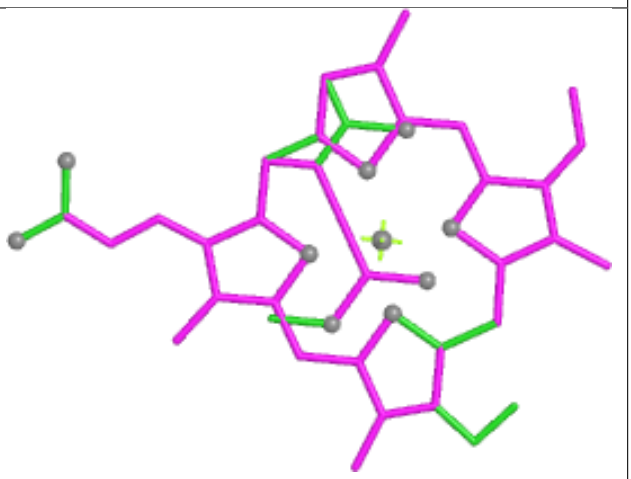


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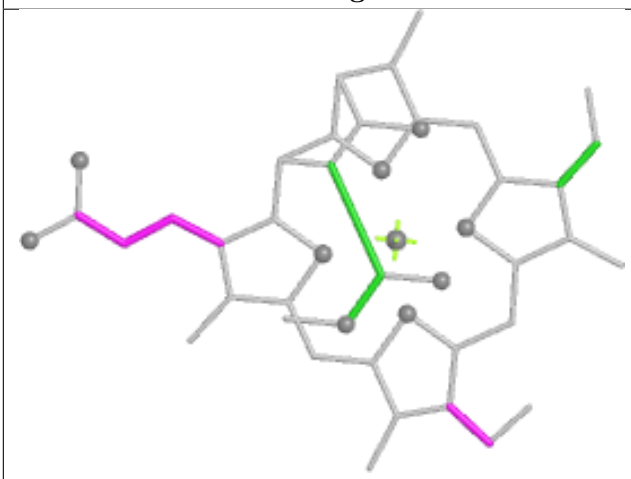
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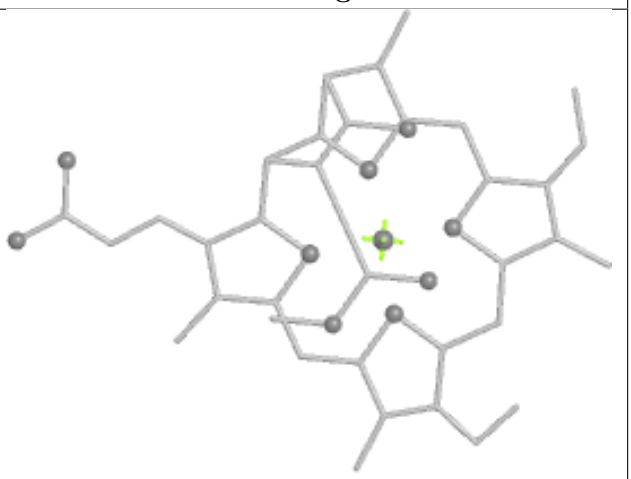
Bond lengths



Bond angles



Torsions



Rings

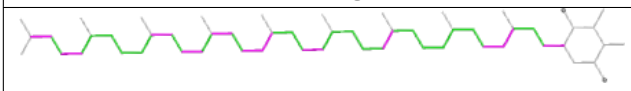
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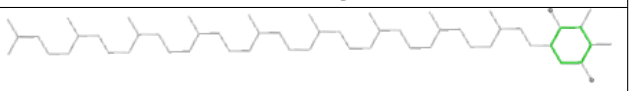
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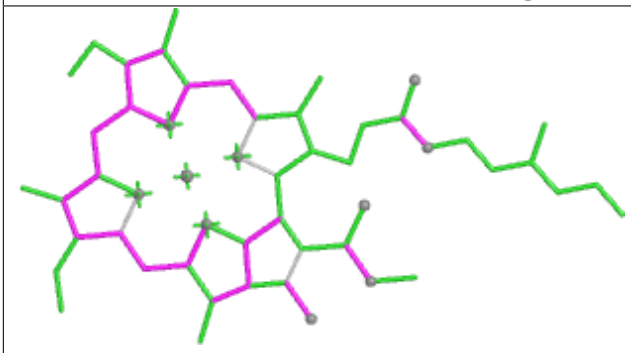
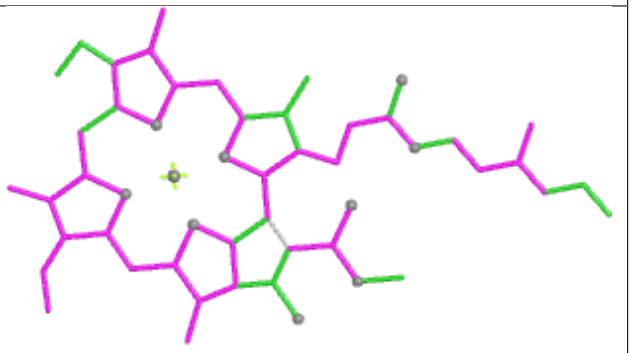
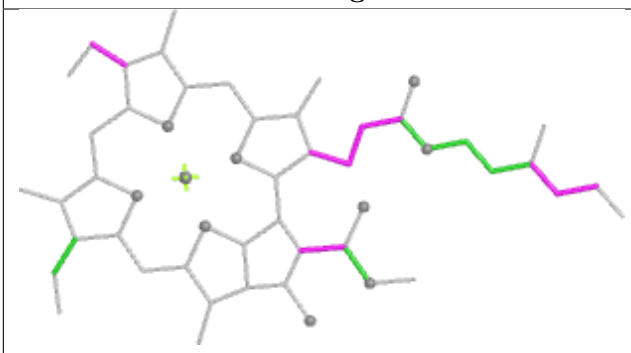
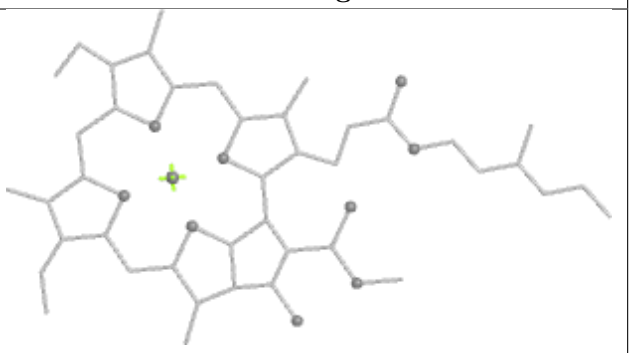
Bond angles

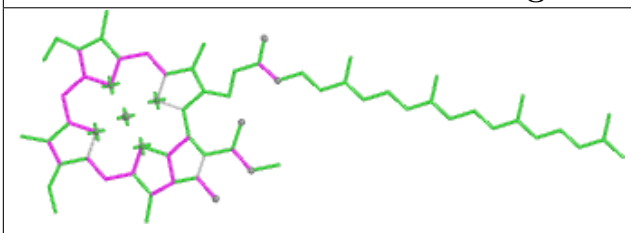
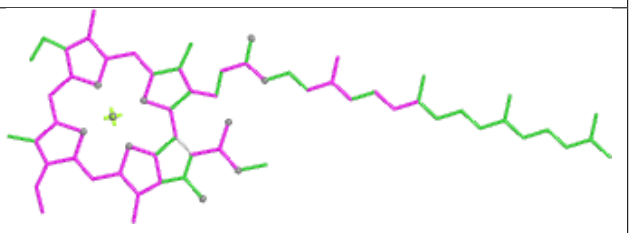
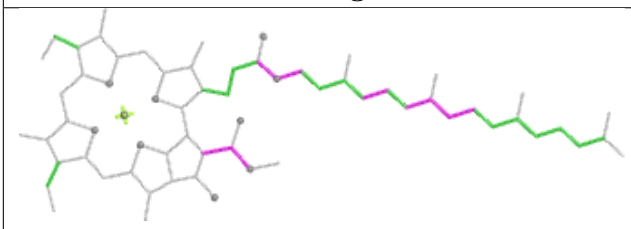
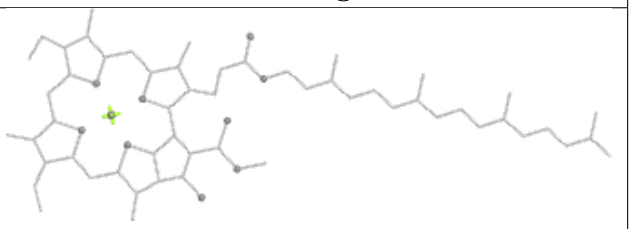


Torsions

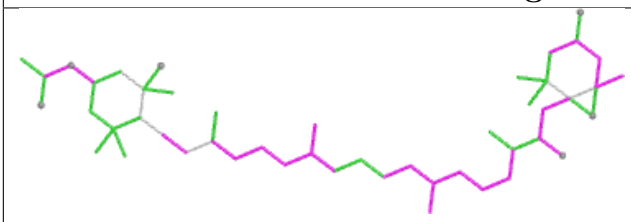


Rings

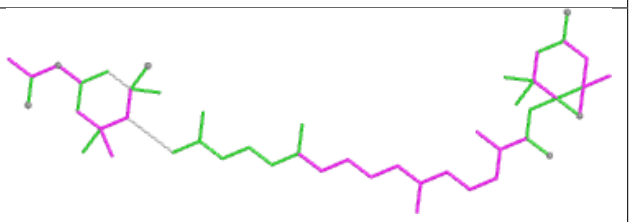
Ligand CLA 17 307	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 516	
	
Bond lengths	Bond angles
	
Torsions	Rings

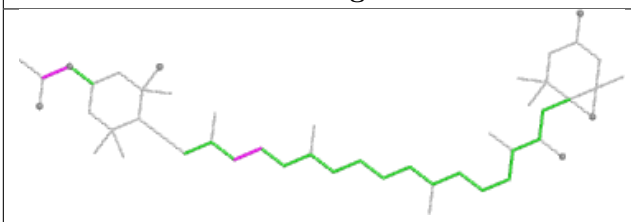
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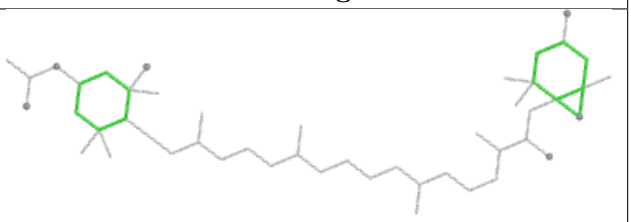
Bond lengths



Bond angles

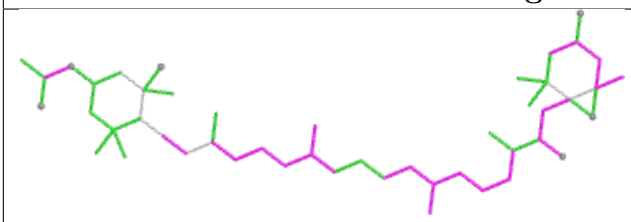


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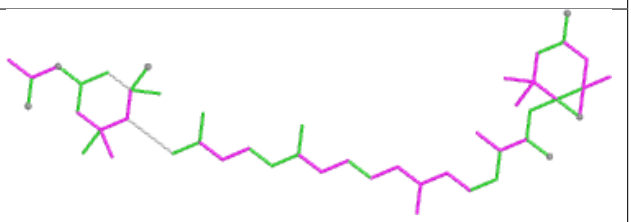


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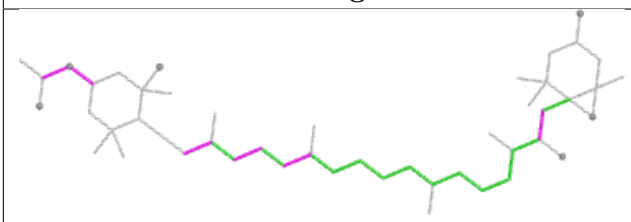
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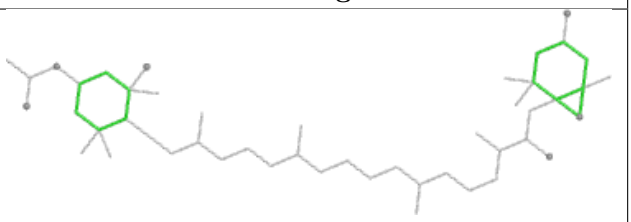
Bond lengths



Bond angles

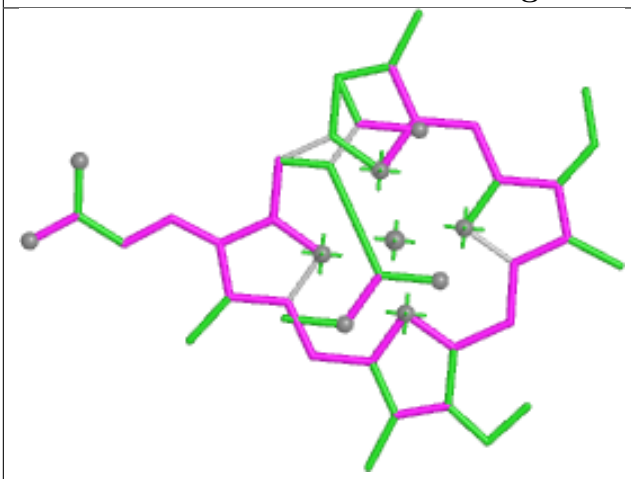


Torsions

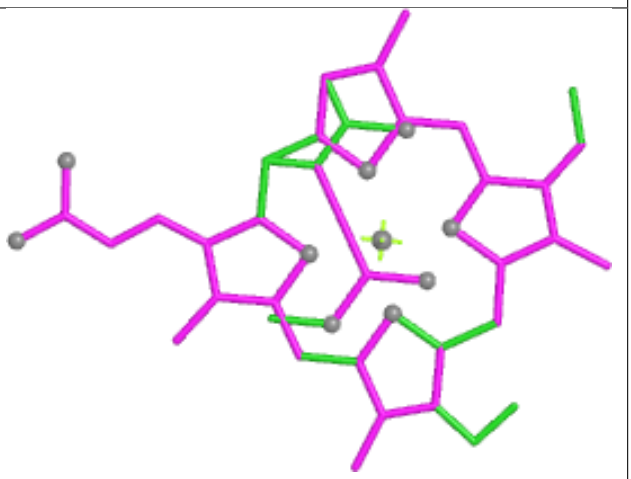


Rings

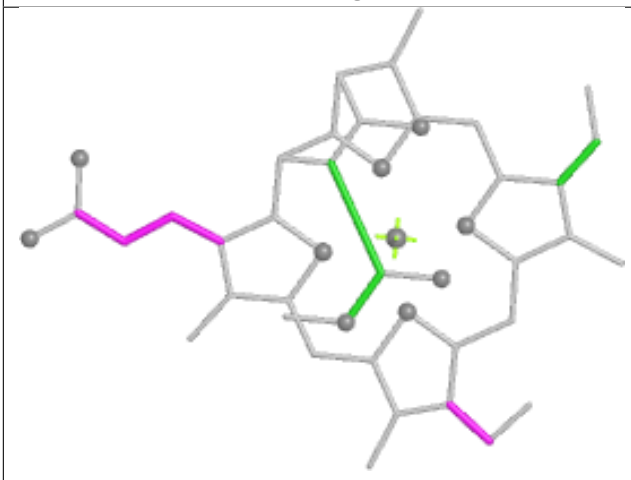
Ligand KC1 17 305



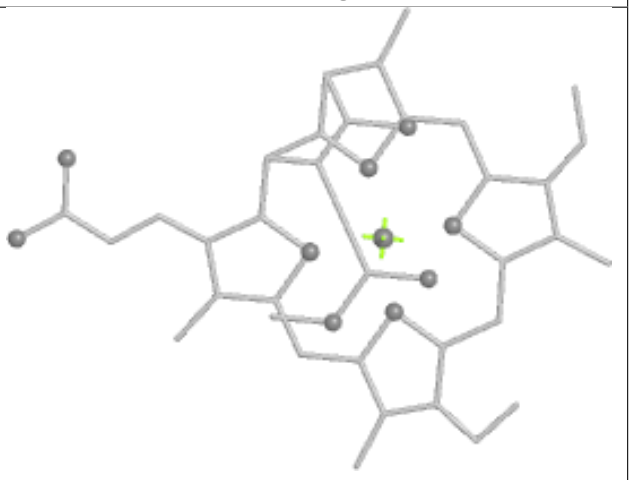
Bond lengths



Bond angles

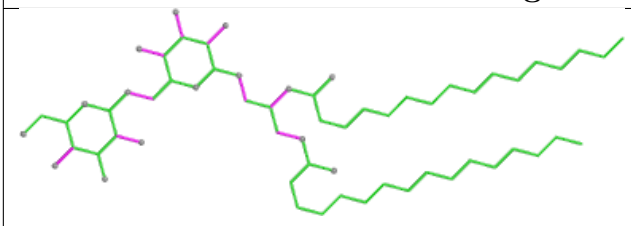


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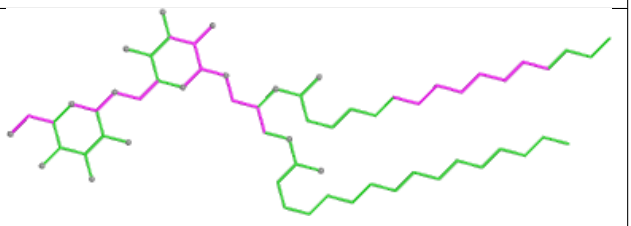


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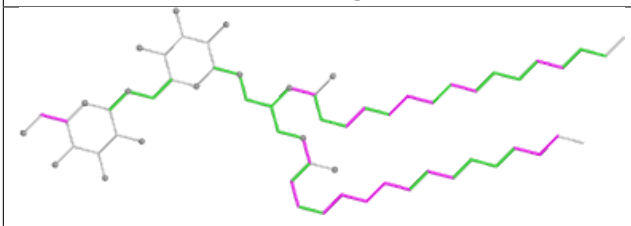
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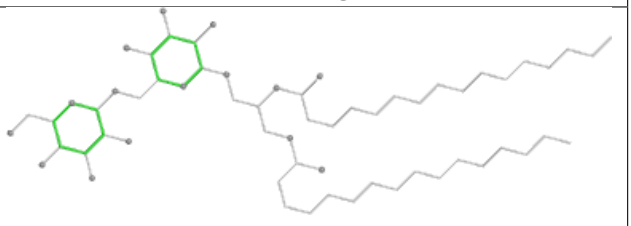
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Bond angles

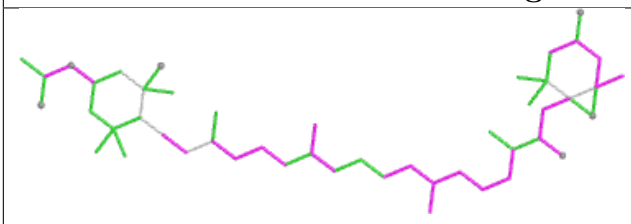


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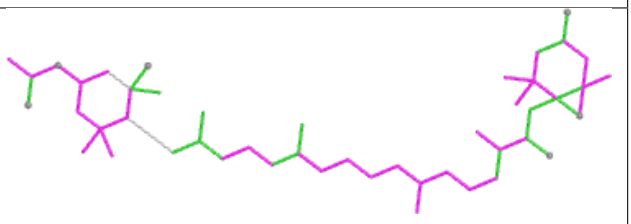


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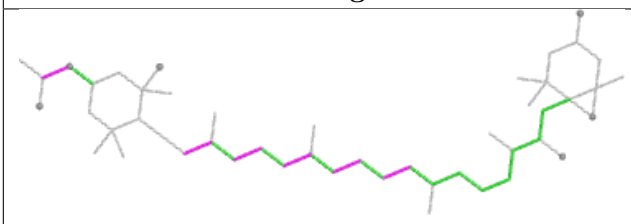
Ligand A86 16 311



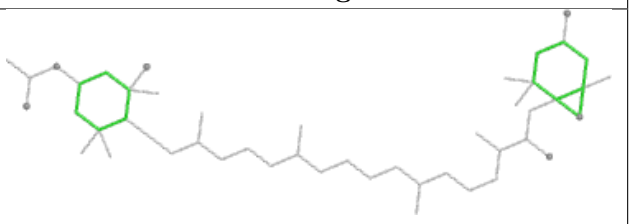
Bond lengths



Bond angles

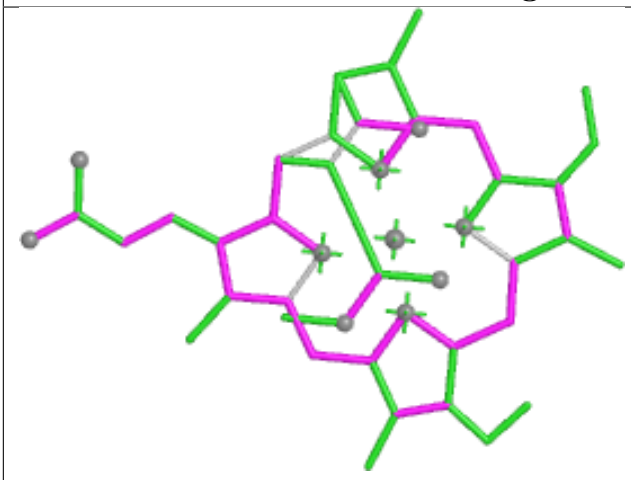


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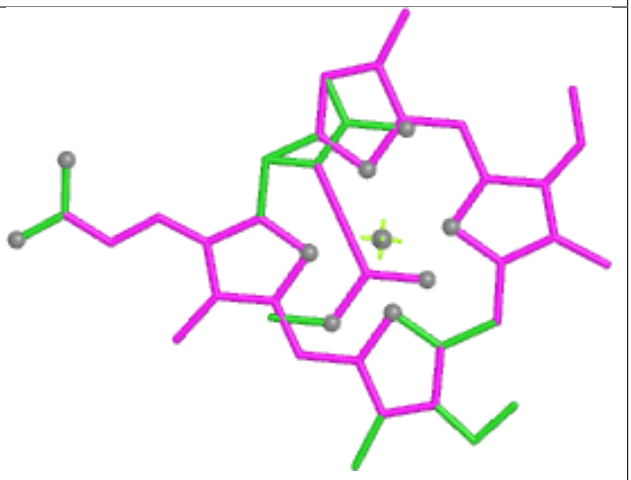


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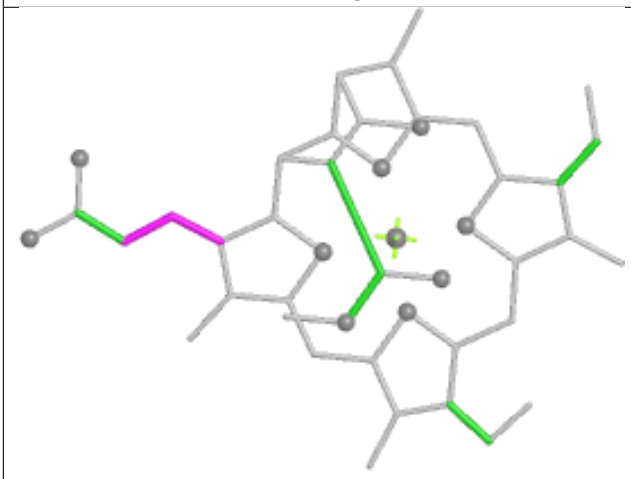
Ligand KC1 11 302



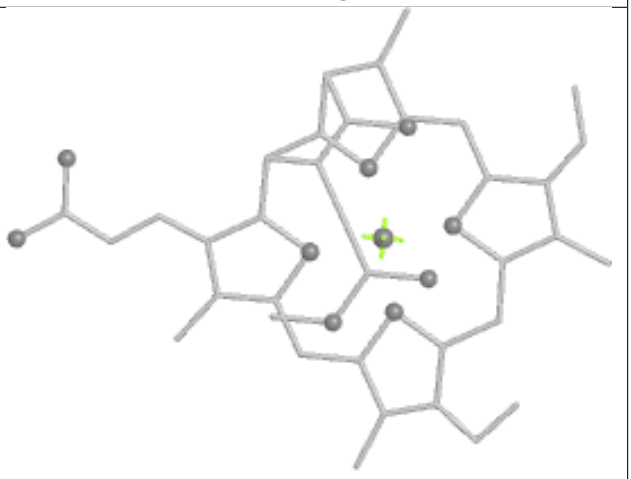
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Bond angles

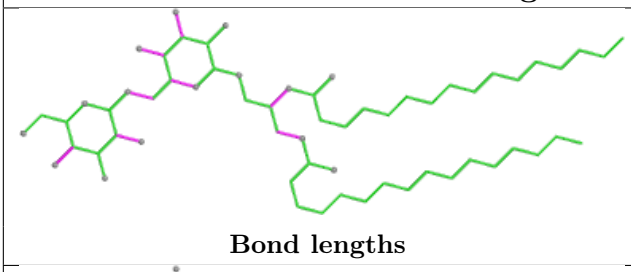


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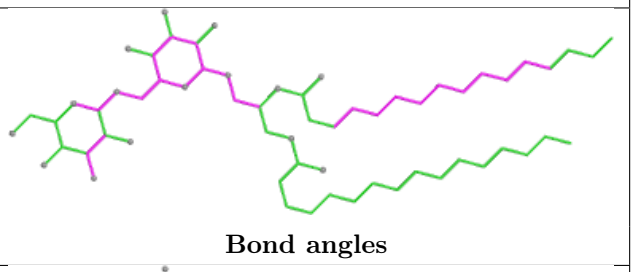


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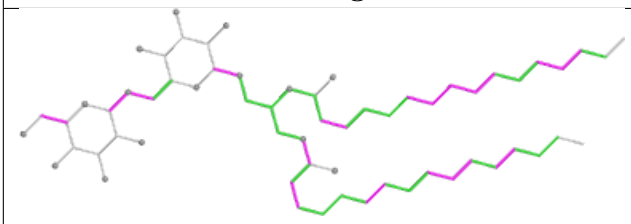
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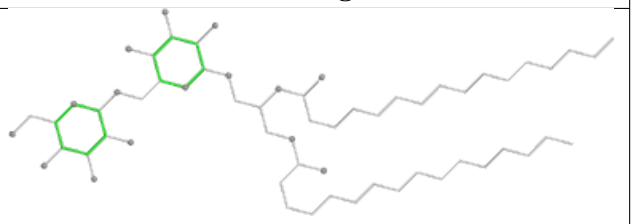
Bond lengths



Bond angles

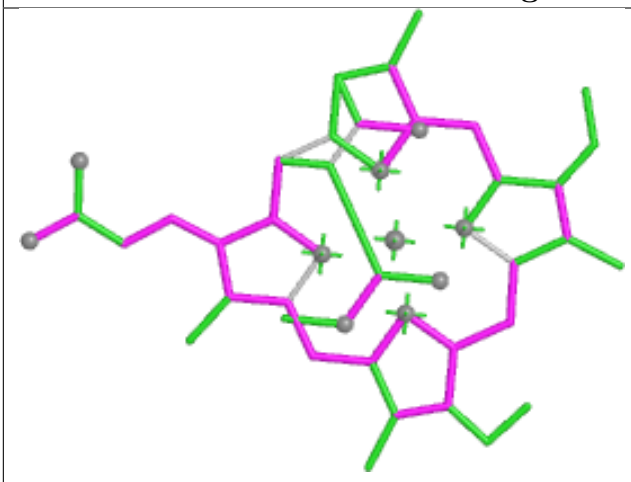


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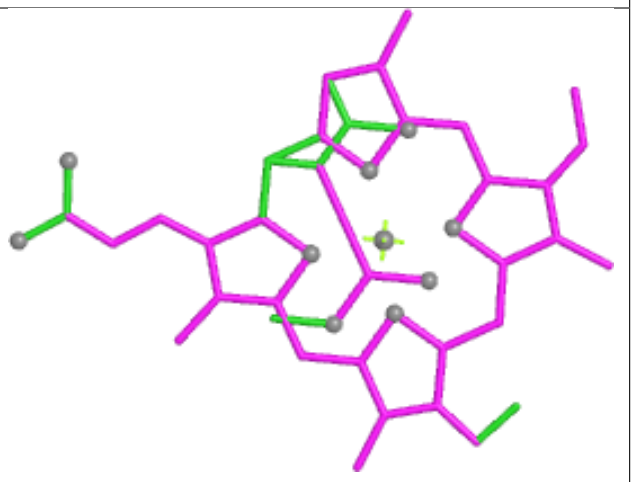


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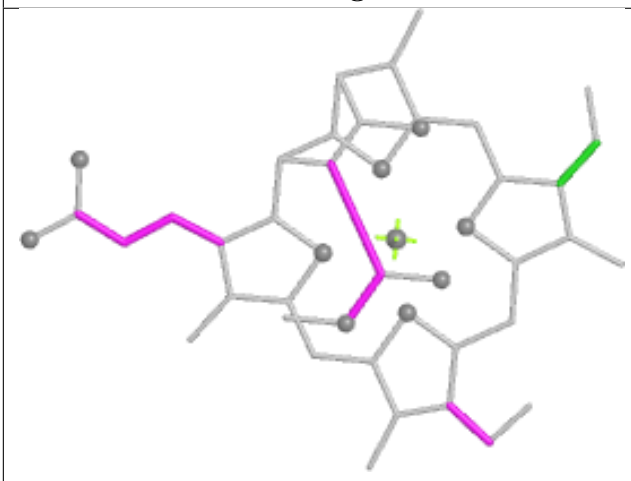
Ligand KC1 20 302



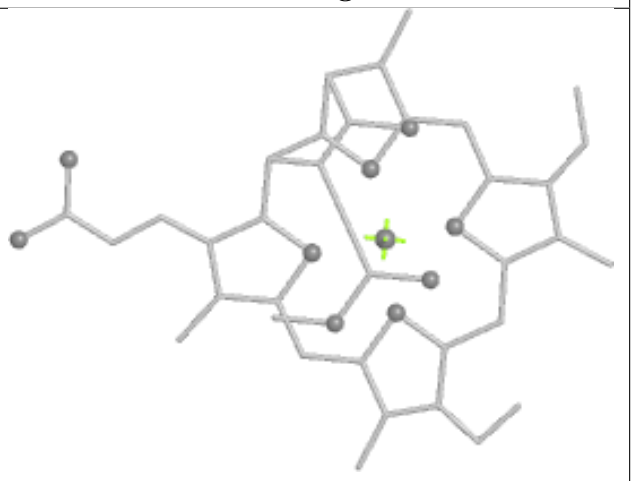
Bond lengths



Bond angles

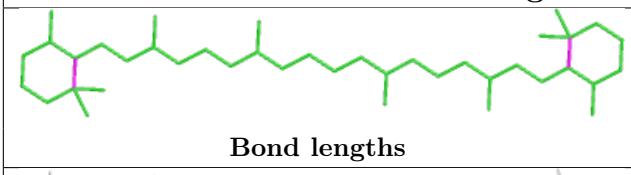


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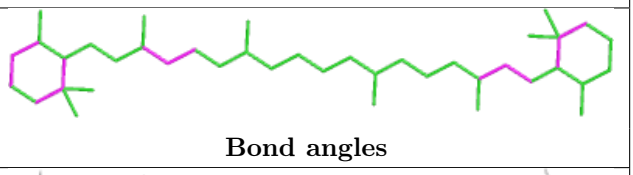


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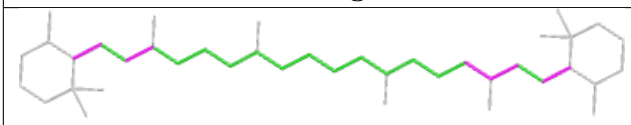
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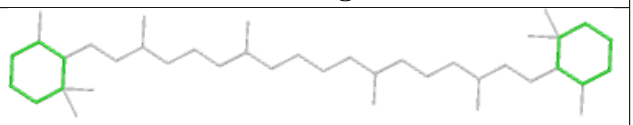
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Bond angles

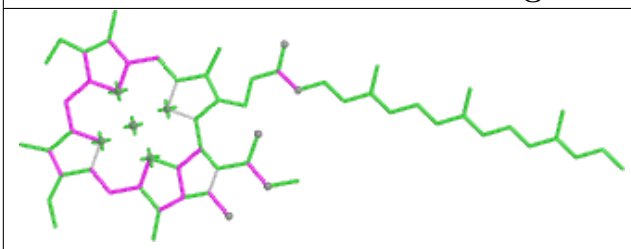


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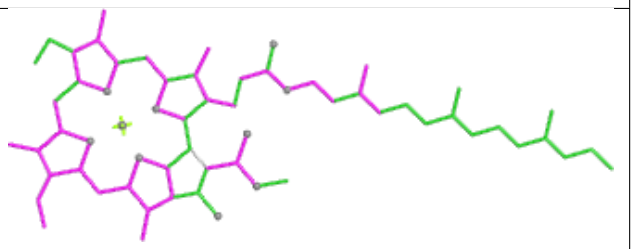


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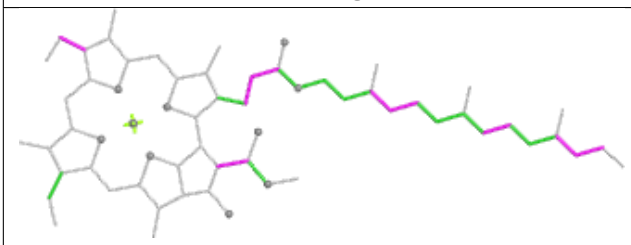
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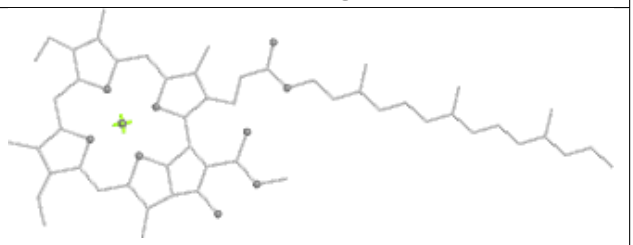
Bond lengths



Bond angles

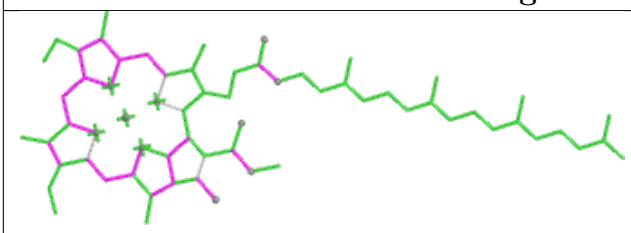


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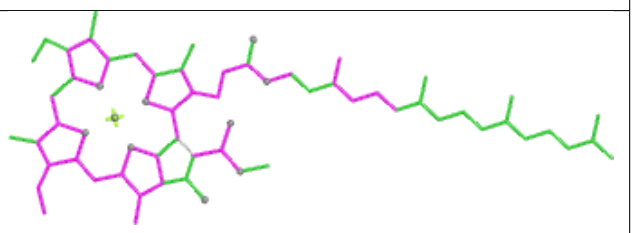


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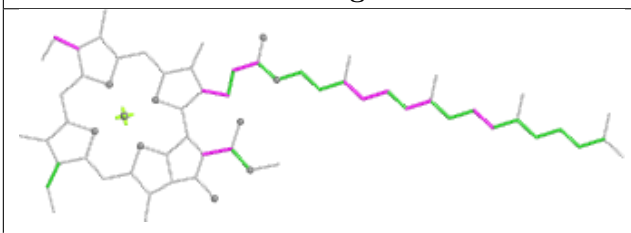
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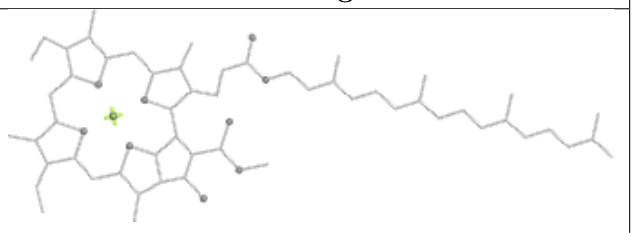
Bond lengths



Bond angles

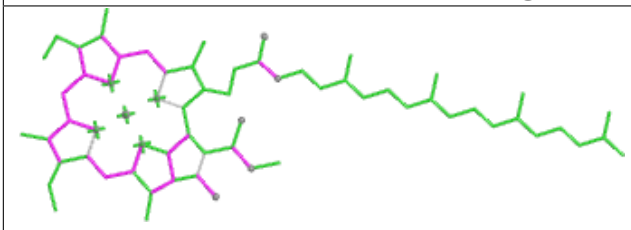


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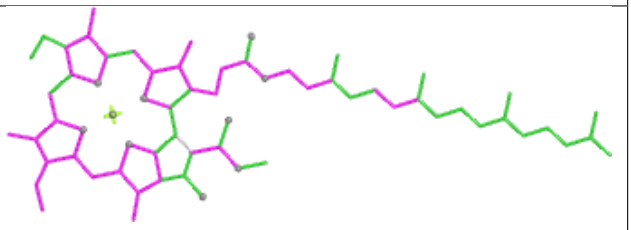


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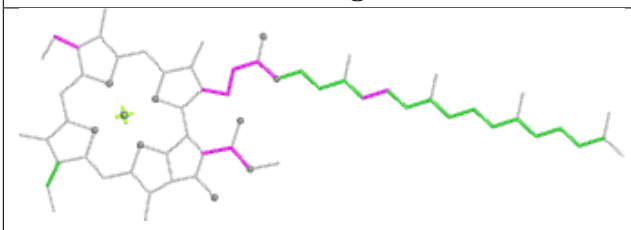
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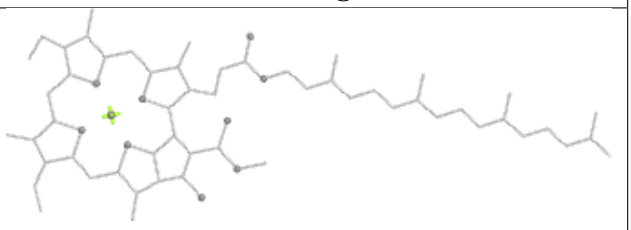
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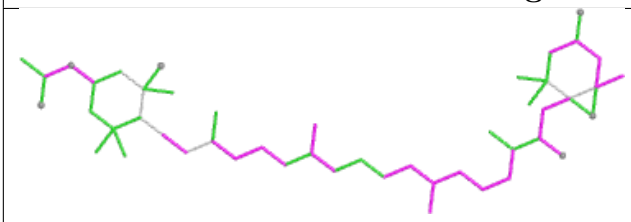


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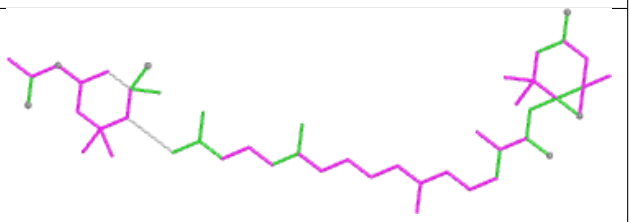


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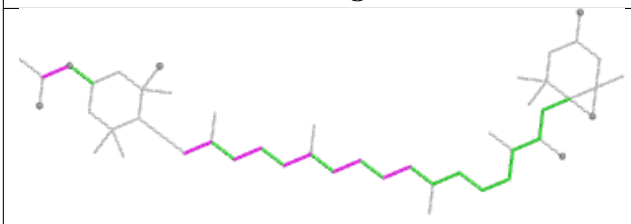
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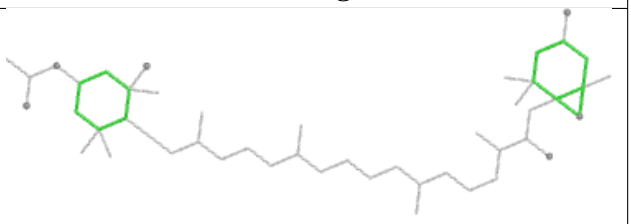
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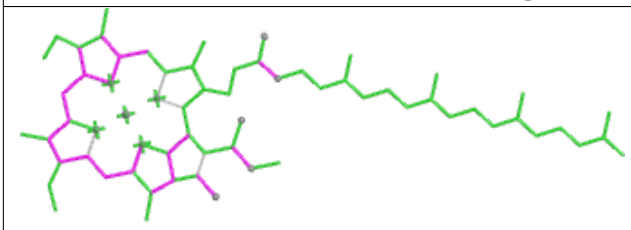


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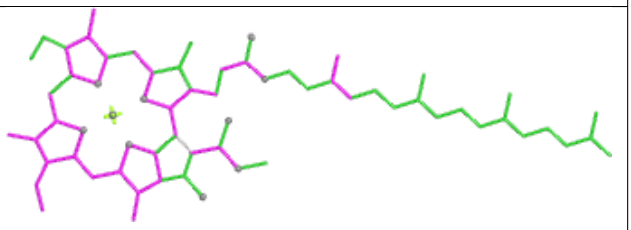


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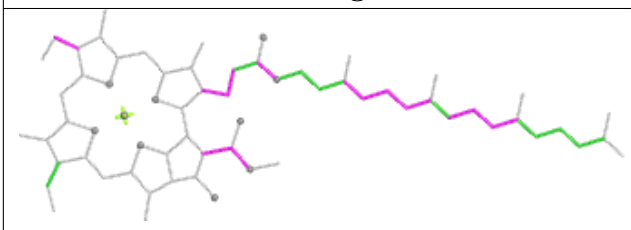
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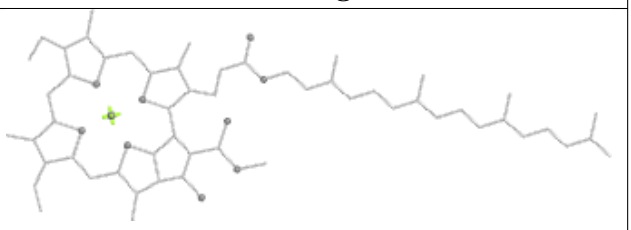
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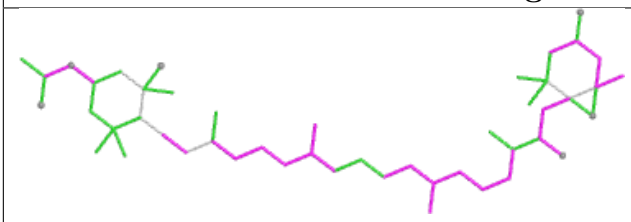


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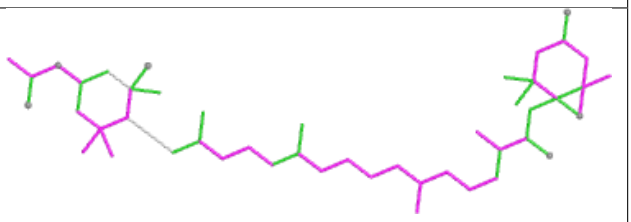


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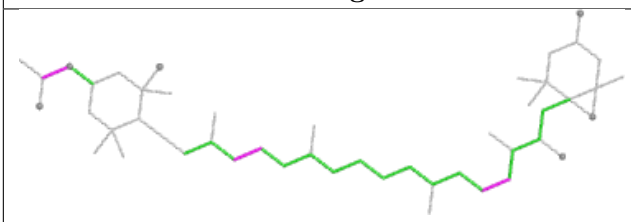
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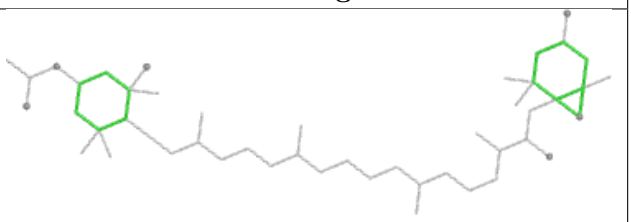
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Bond angles

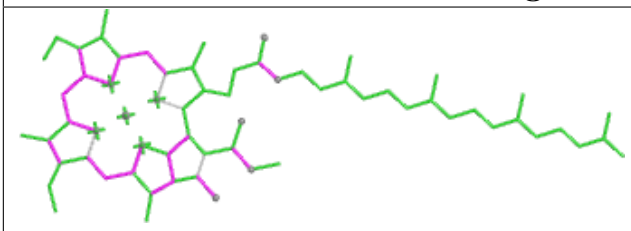


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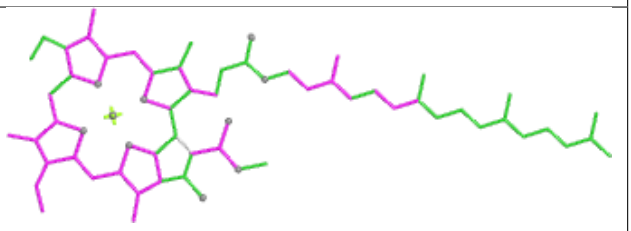


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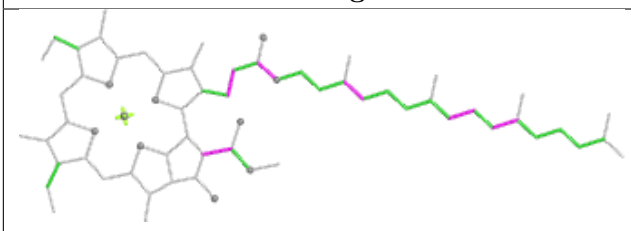
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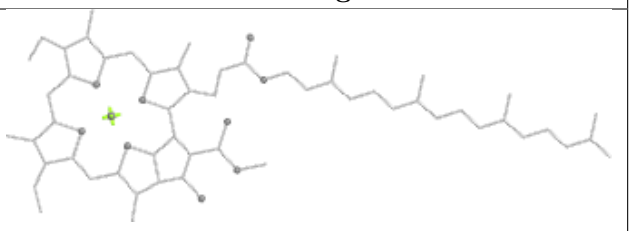
Bond lengths



Bond angles

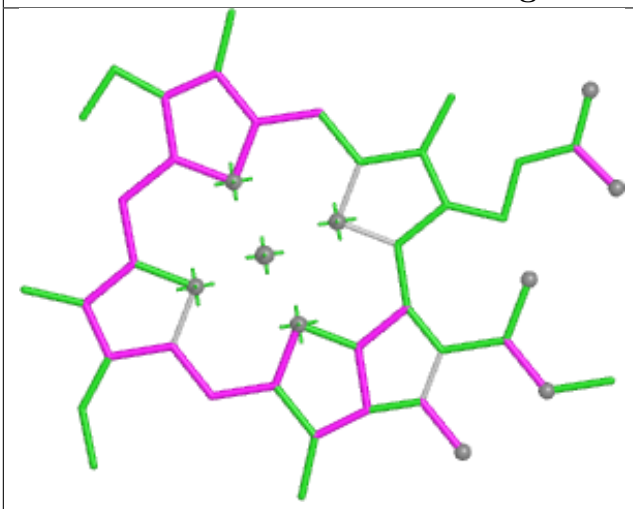


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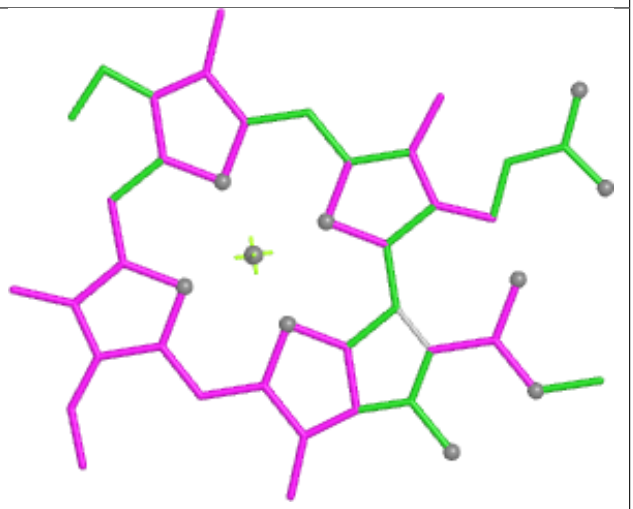


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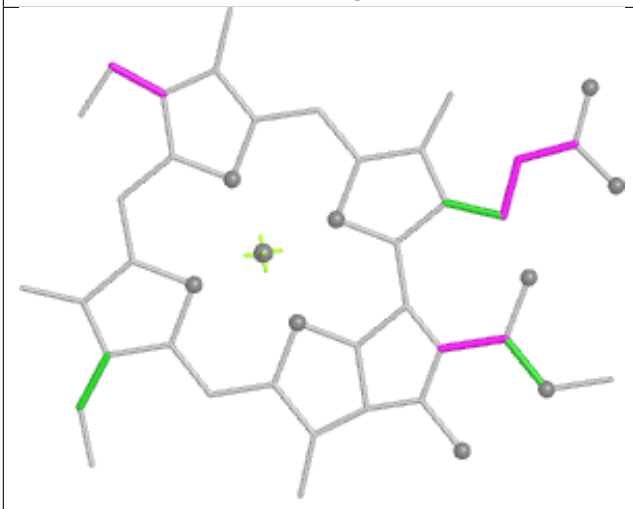
Ligand CLA 38 206



Bond lengths



Bond angles

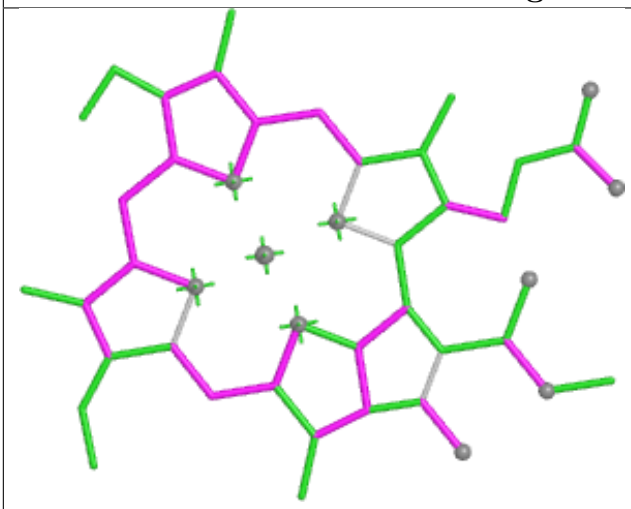


Torsions

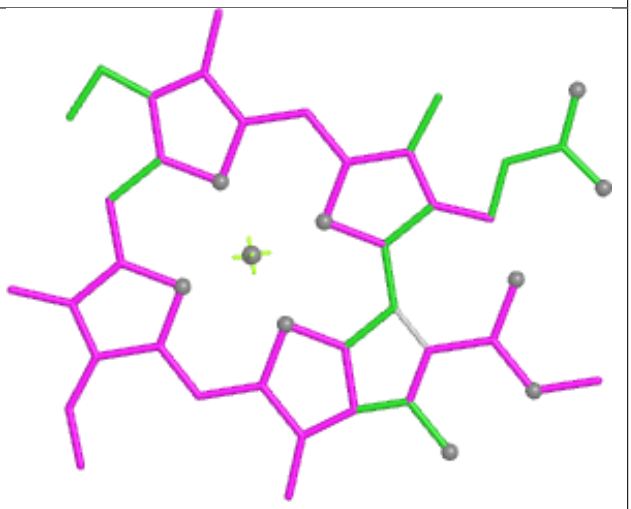


Rings

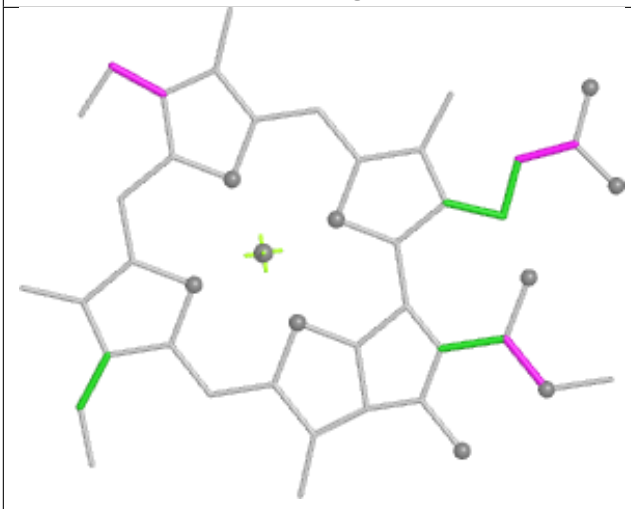
Ligand CLA Z 102



Bond lengths



Bond angles

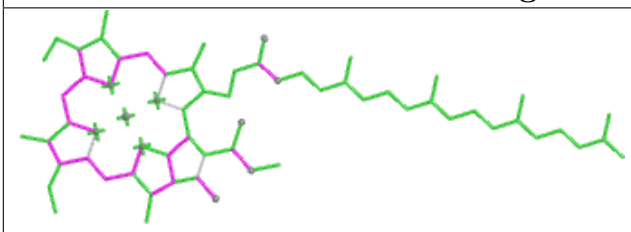


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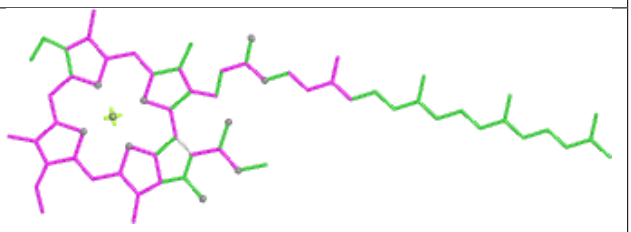


Rings

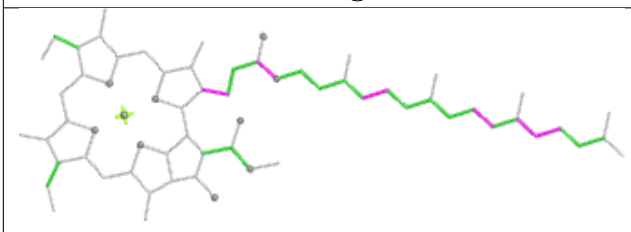
Ligand CLA 19 307



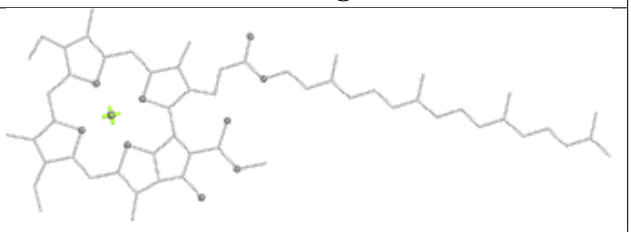
Bond lengths



Bond angles

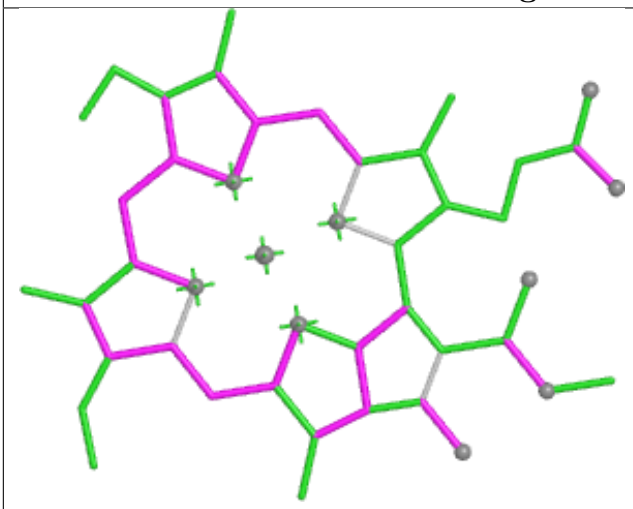


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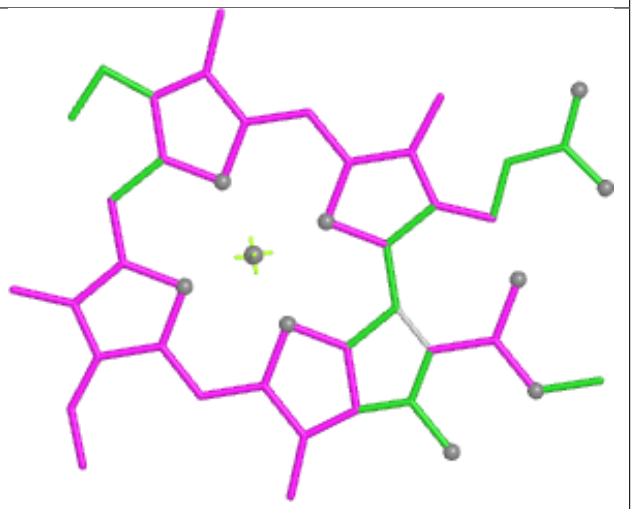


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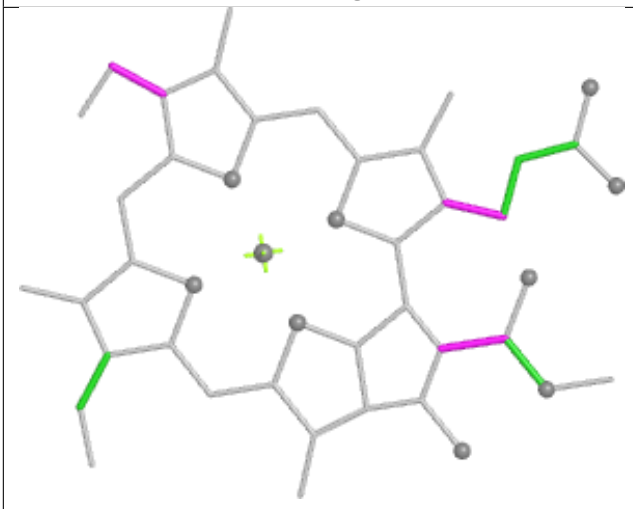
Ligand CLA 11 305



Bond lengths



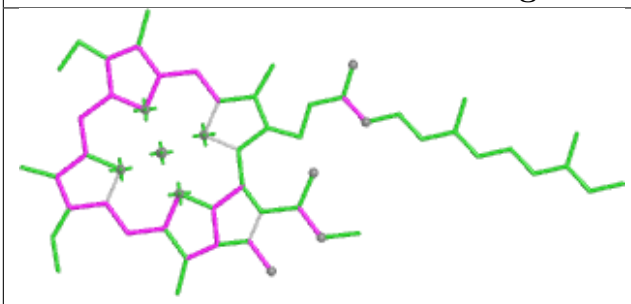
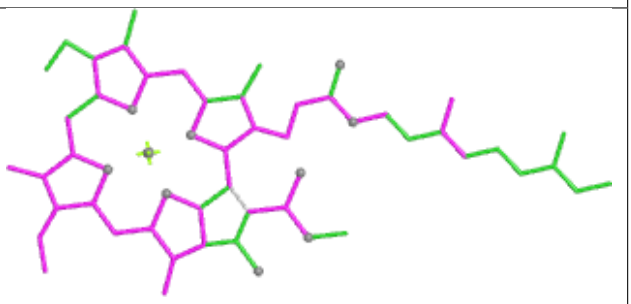
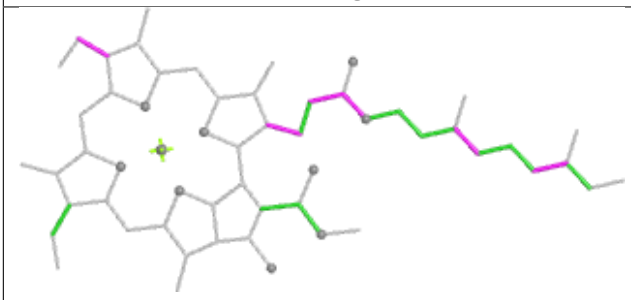
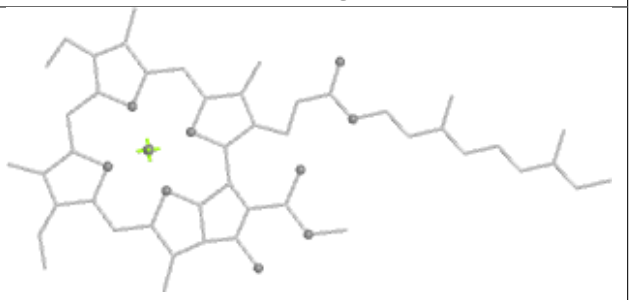
Bond angles

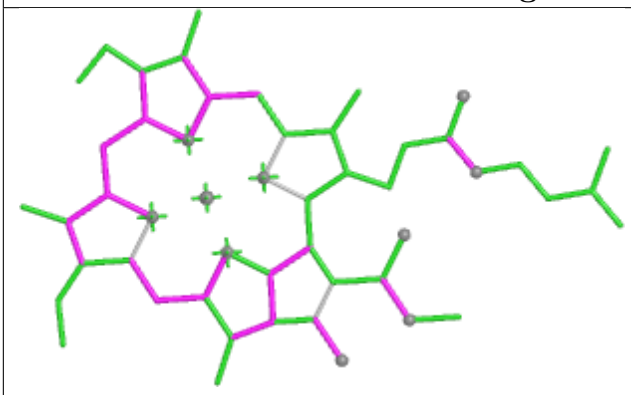
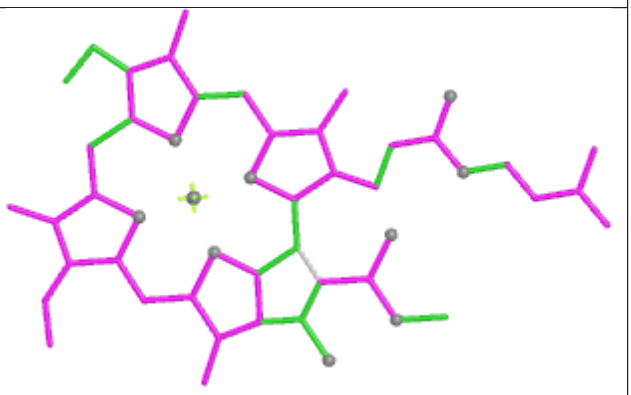
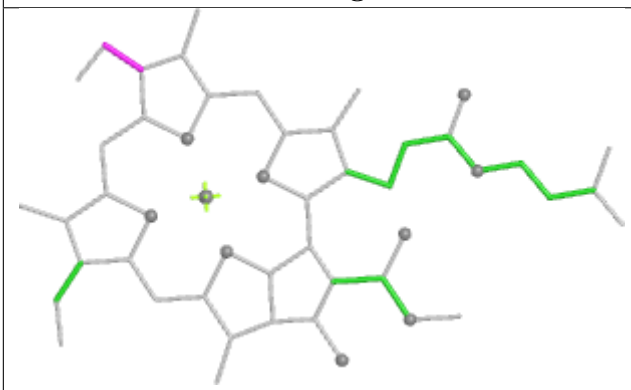
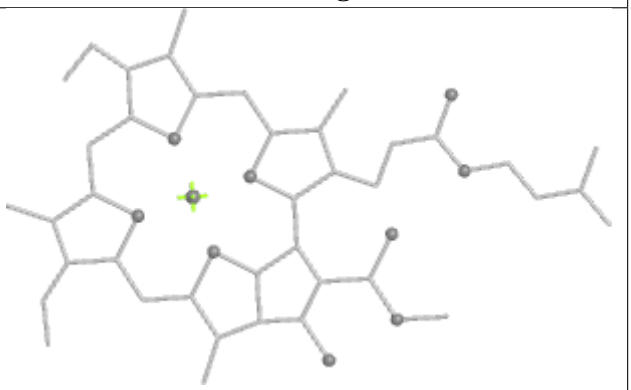


Torsions

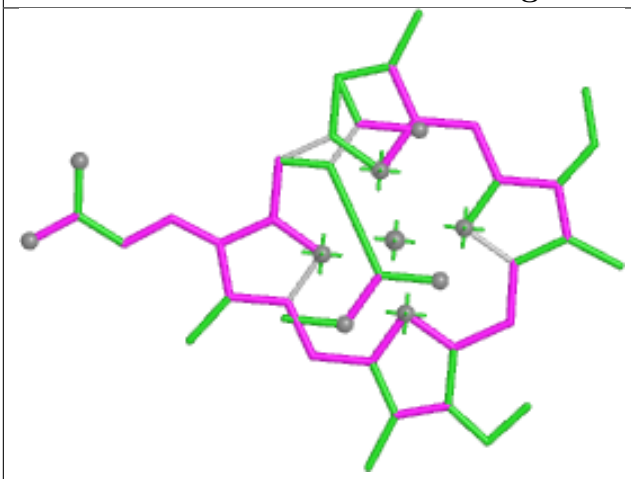


Rings

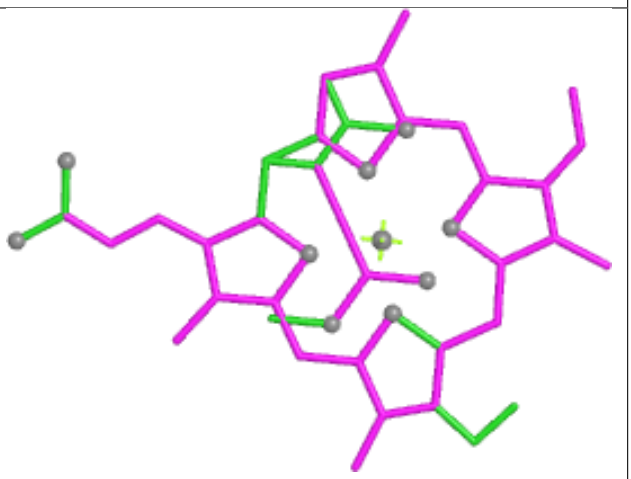
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Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 32 208	
	
Bond lengths	Bond angles
	
Torsions	Rings

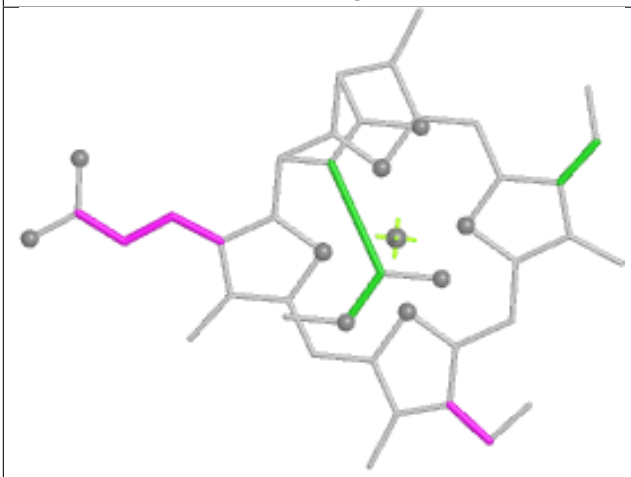
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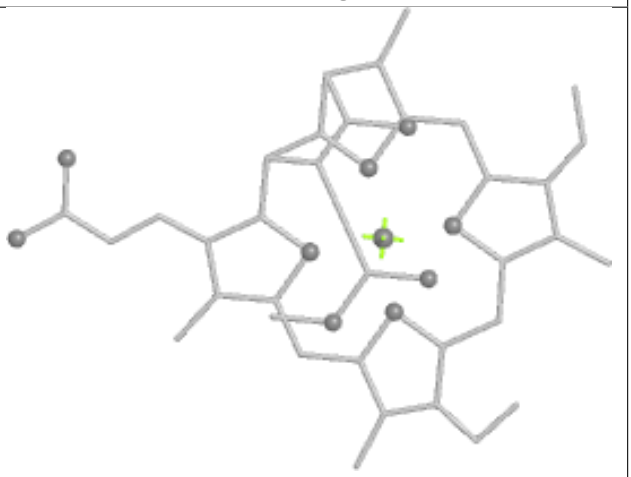
Bond lengths



Bond angles

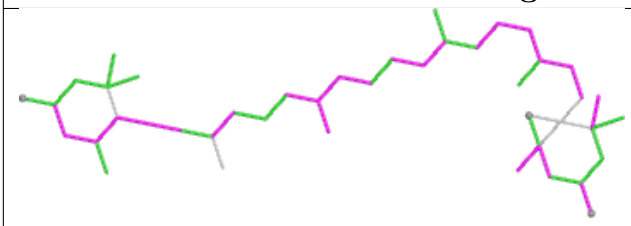


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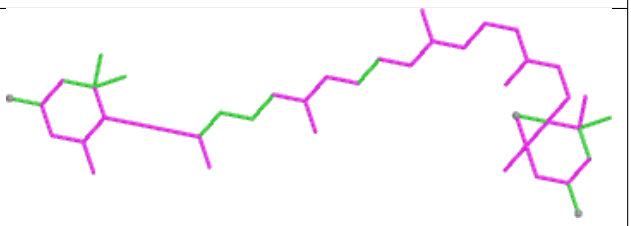


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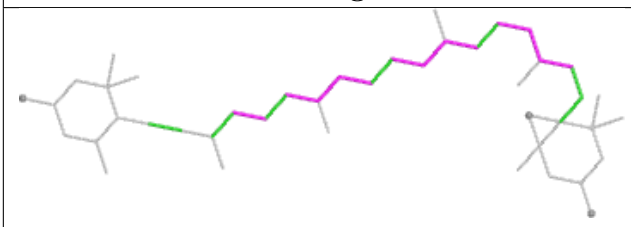
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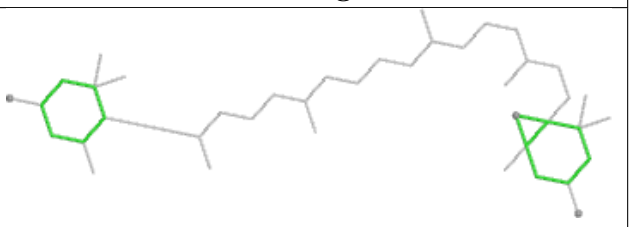
Bond lengths



Bond angles

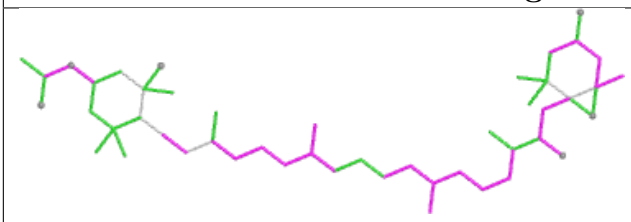


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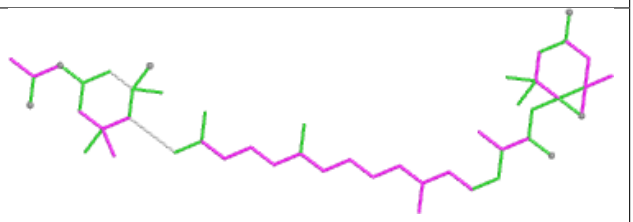


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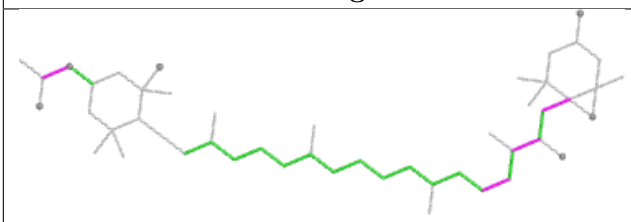
Ligand A86 36 313



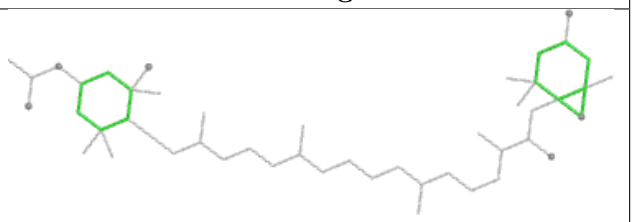
Bond lengths



Bond angles

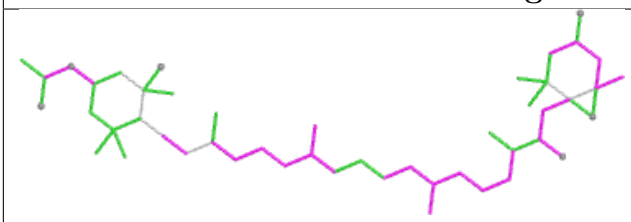


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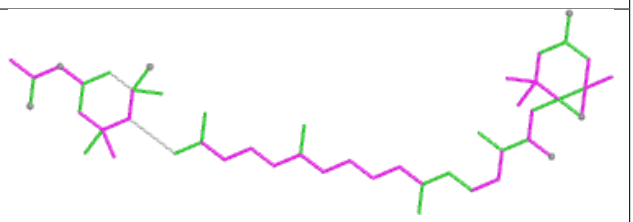


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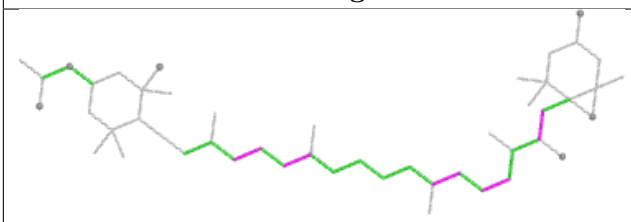
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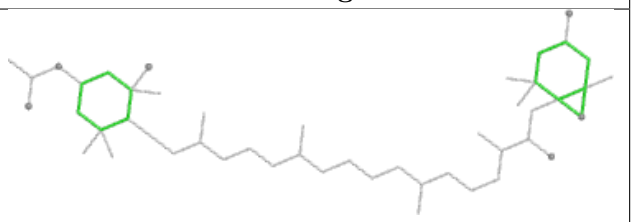
Bond lengths



Bond angles

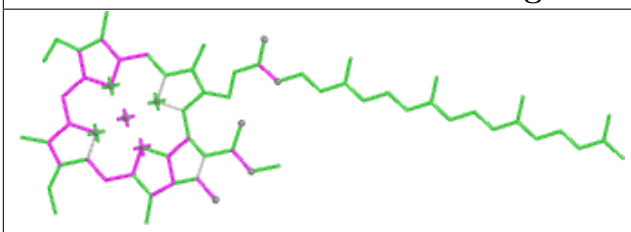


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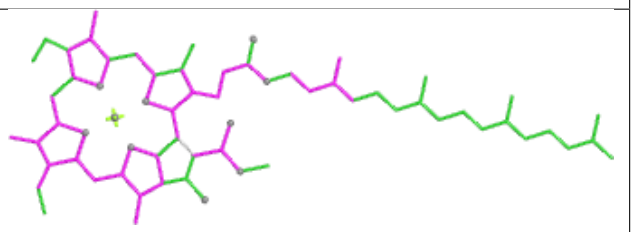


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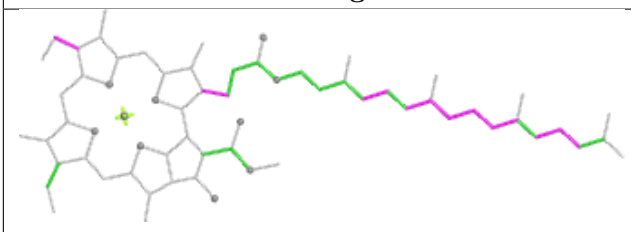
Ligand CLA B 524



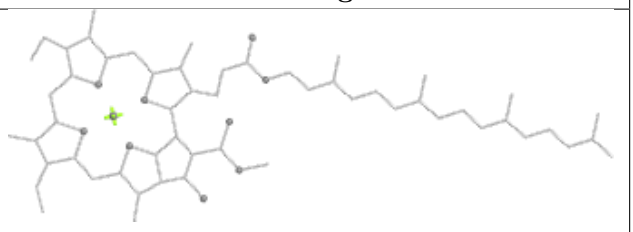
Bond lengths



Bond angles

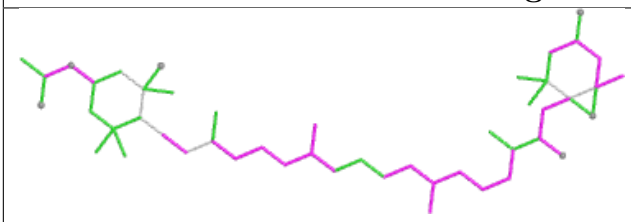


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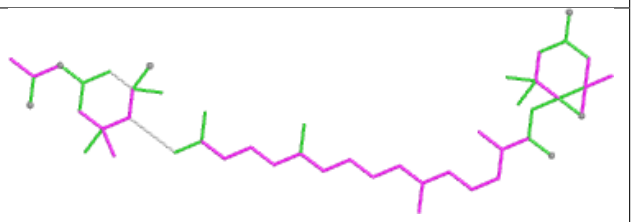


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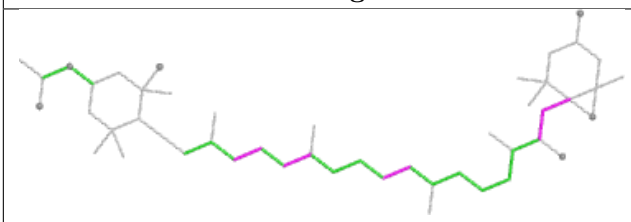
Ligand A86 41 214



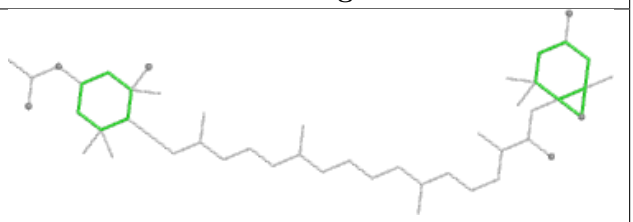
Bond lengths



Bond angles

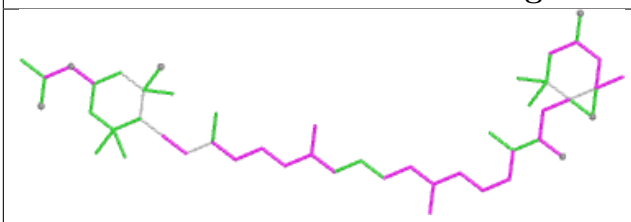


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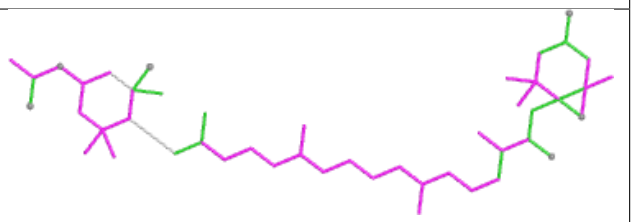


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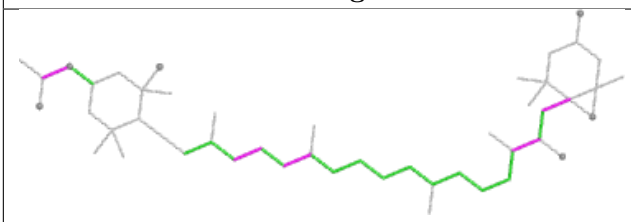
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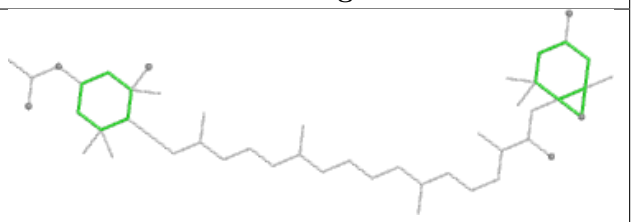
Bond lengths



Bond angles

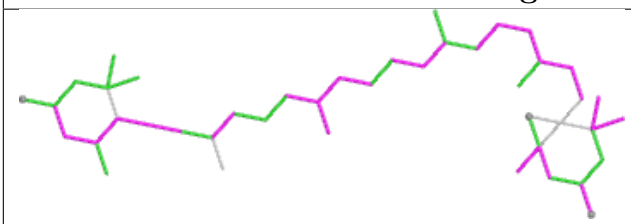


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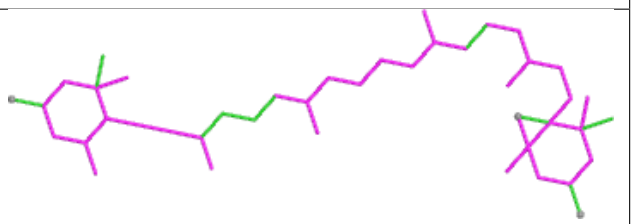


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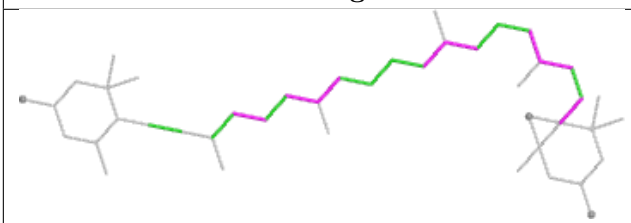
Ligand DD6 40 214



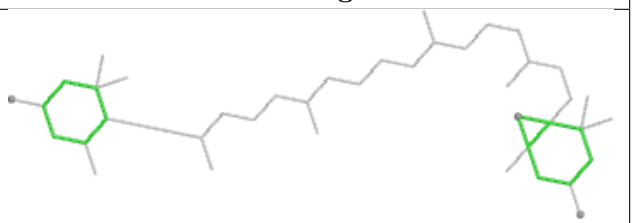
Bond lengths



Bond angles

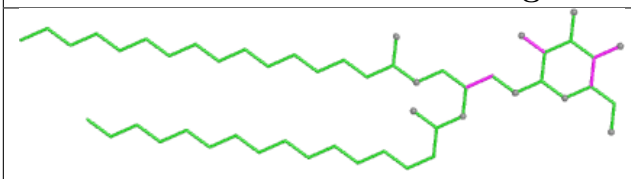


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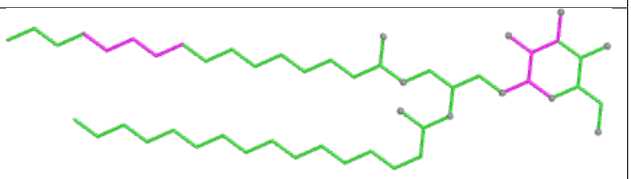


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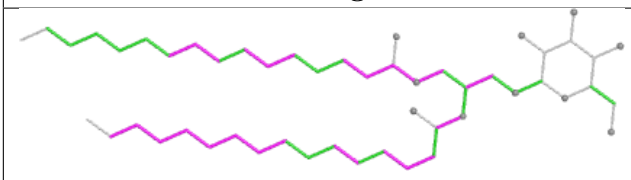
Ligand LMG b 520



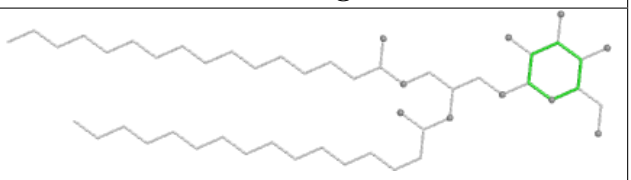
Bond lengths



Bond angles

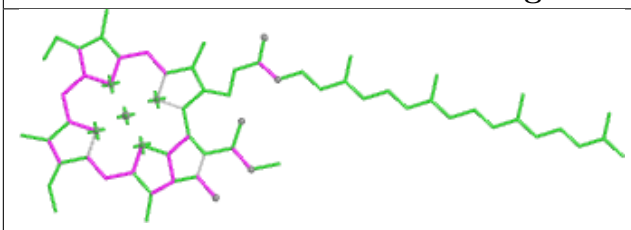


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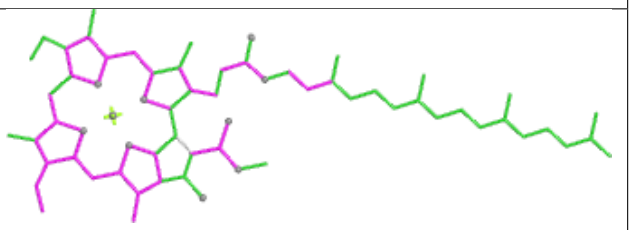


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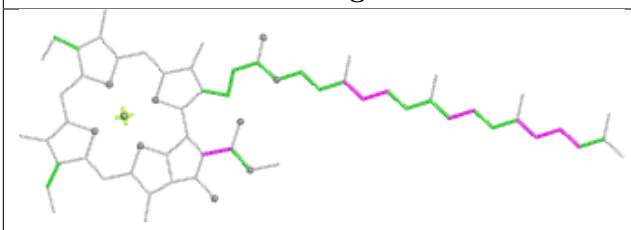
Ligand CLA B 507



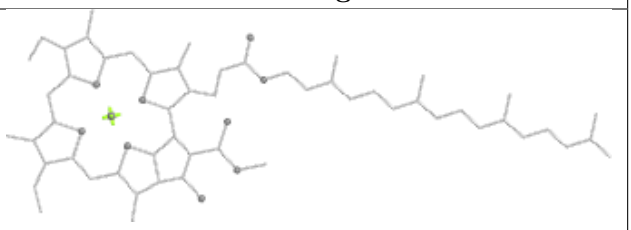
Bond lengths



Bond angles

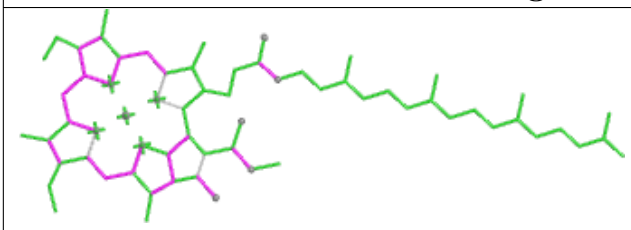


Torsions

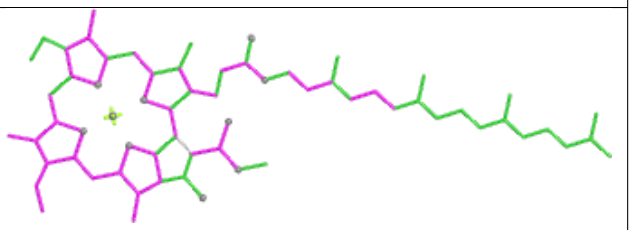


Rings

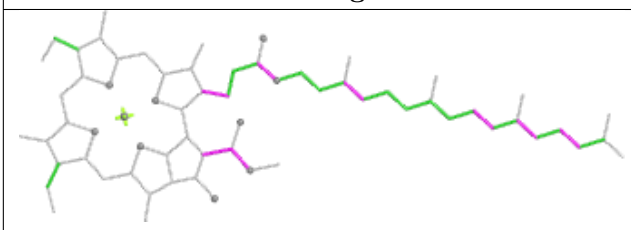
Ligand CLA b 511



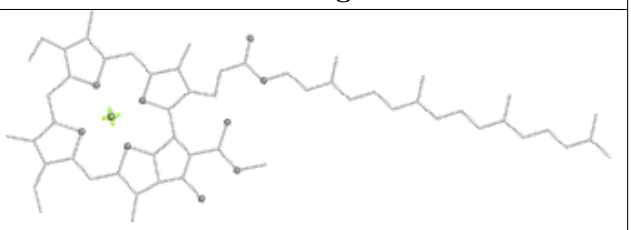
Bond lengths



Bond angles

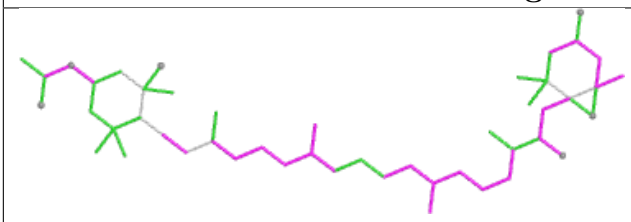


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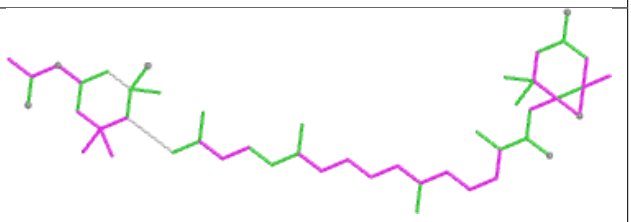


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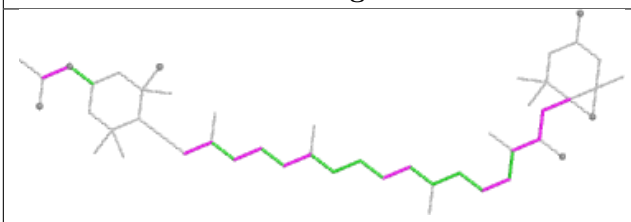
Ligand A86 20 311



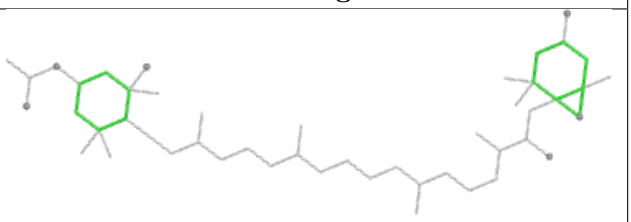
Bond lengths



Bond angles

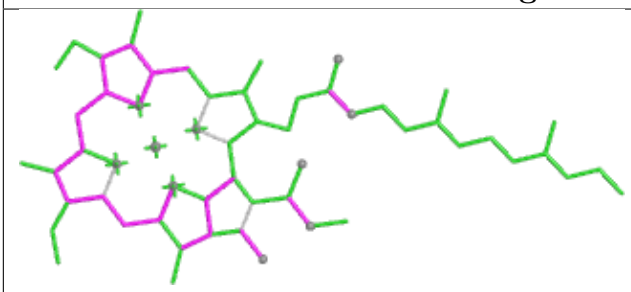


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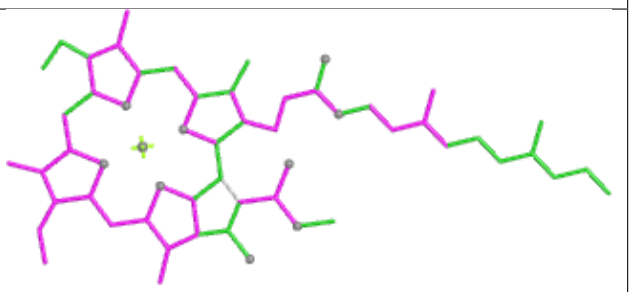


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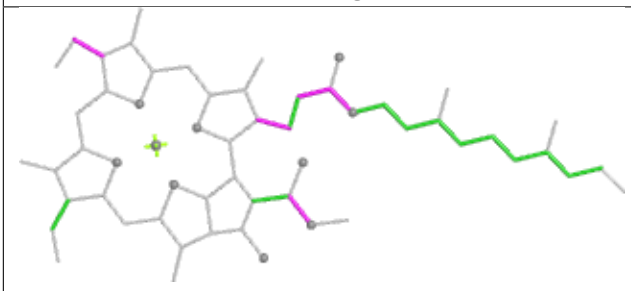
Ligand CLA 16 303



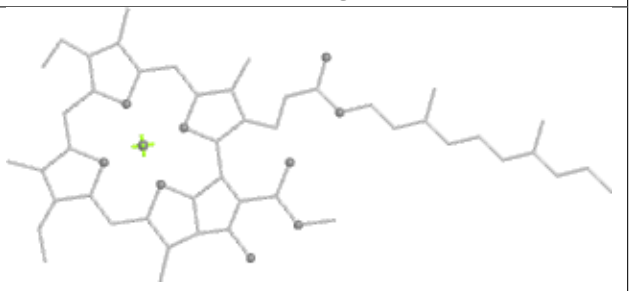
Bond lengths



Bond angles

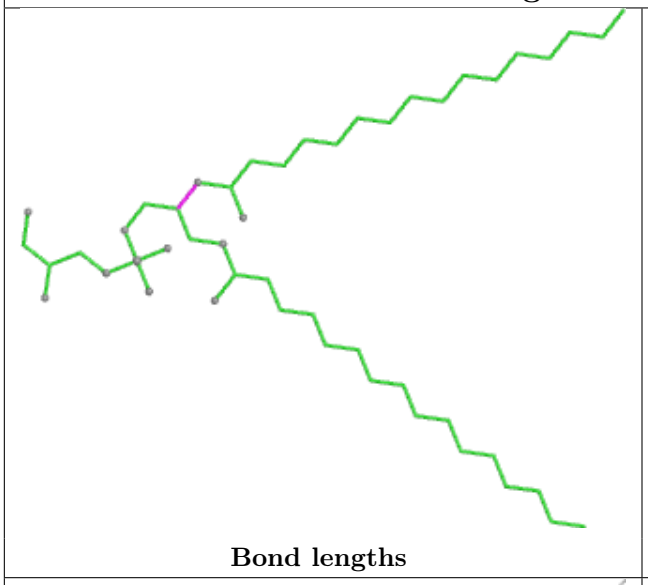


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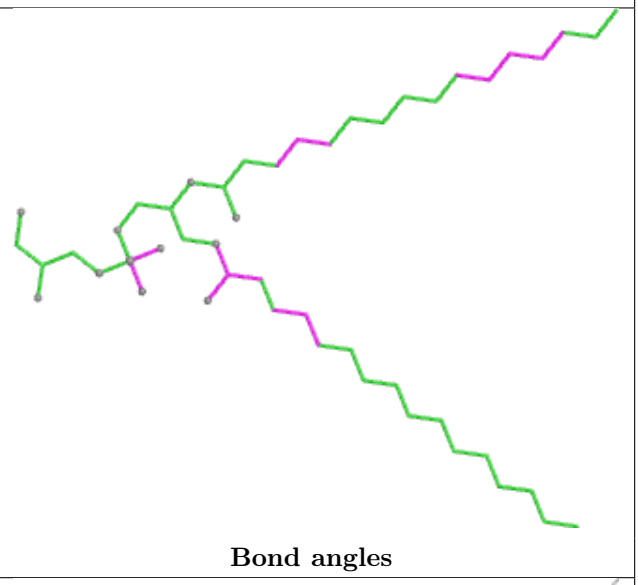


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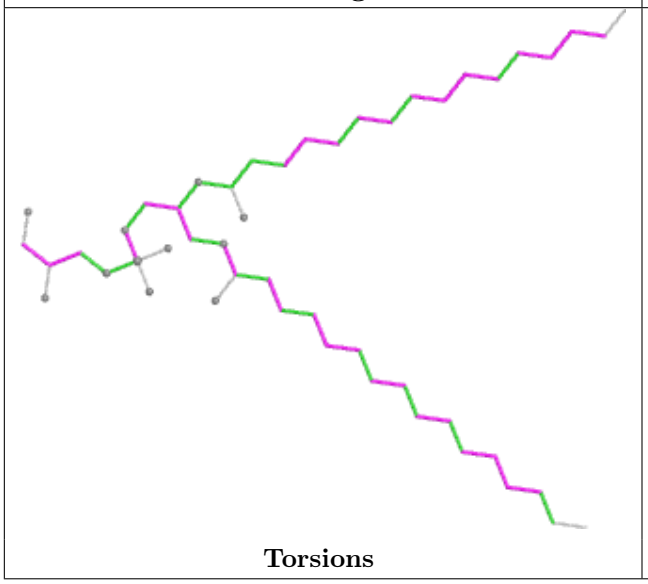
Ligand LHG D 409



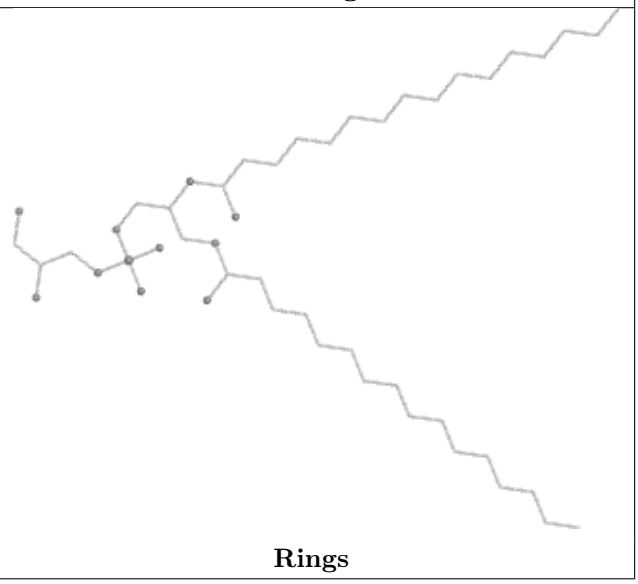
Bond lengths



Bond angles

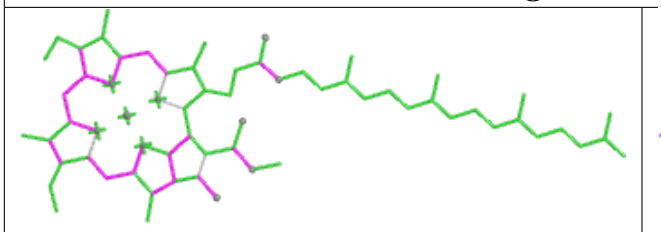


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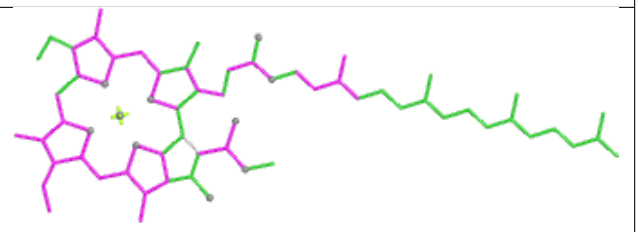


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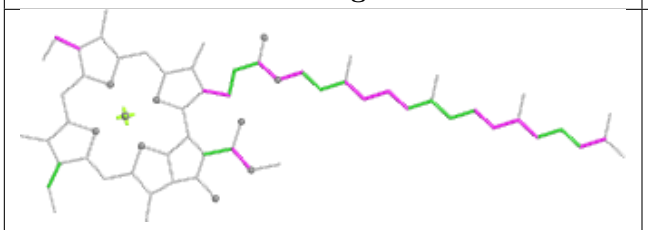
Ligand CLA D 406



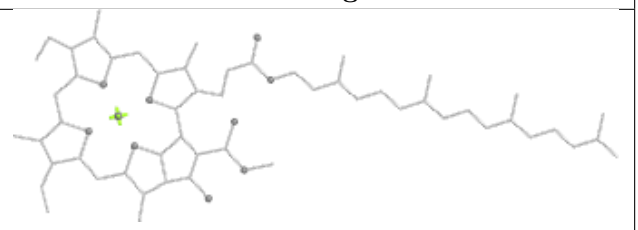
Bond lengths



Bond angles

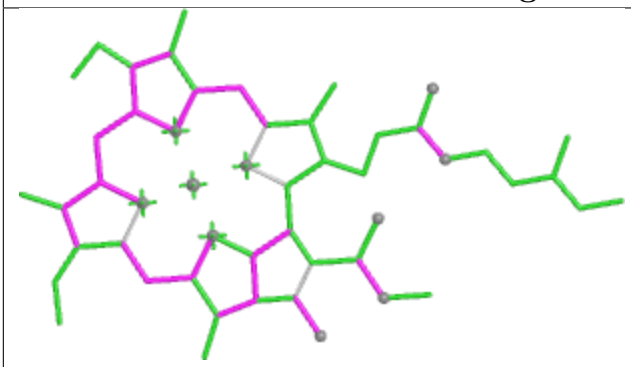


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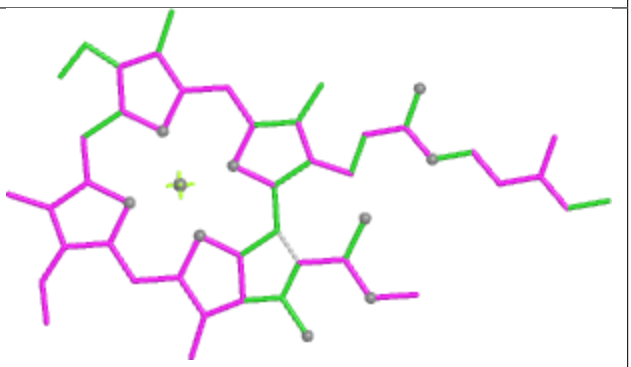


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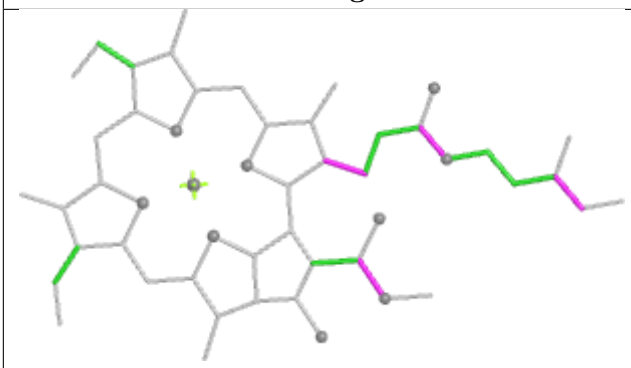
Ligand CLA 11 310



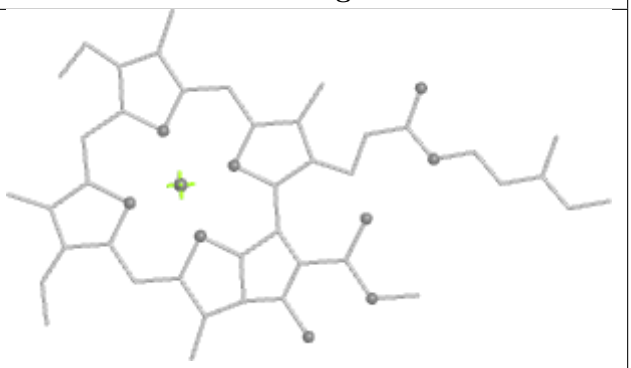
Bond lengths



Bond angles

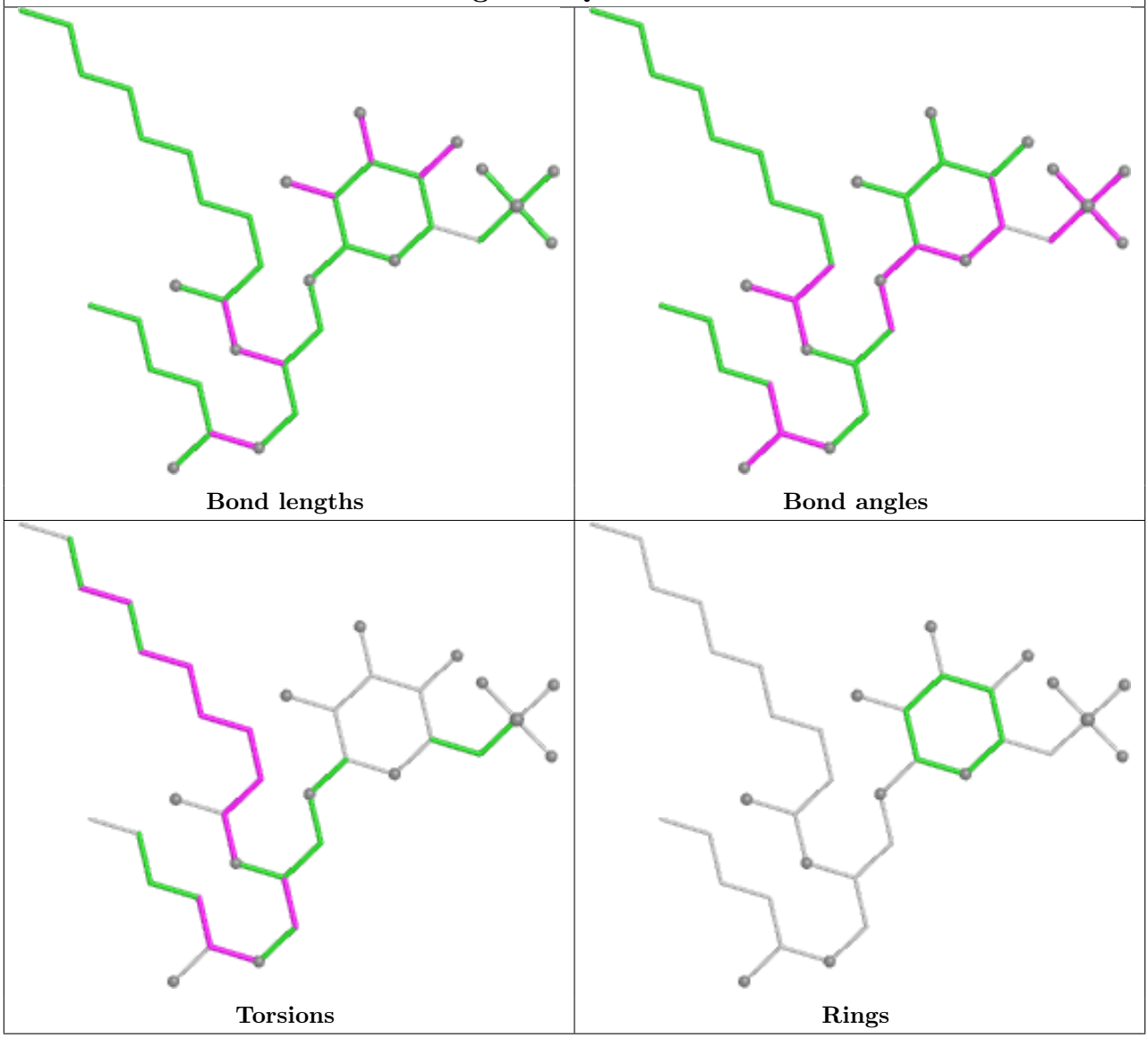


Torsions



Rings

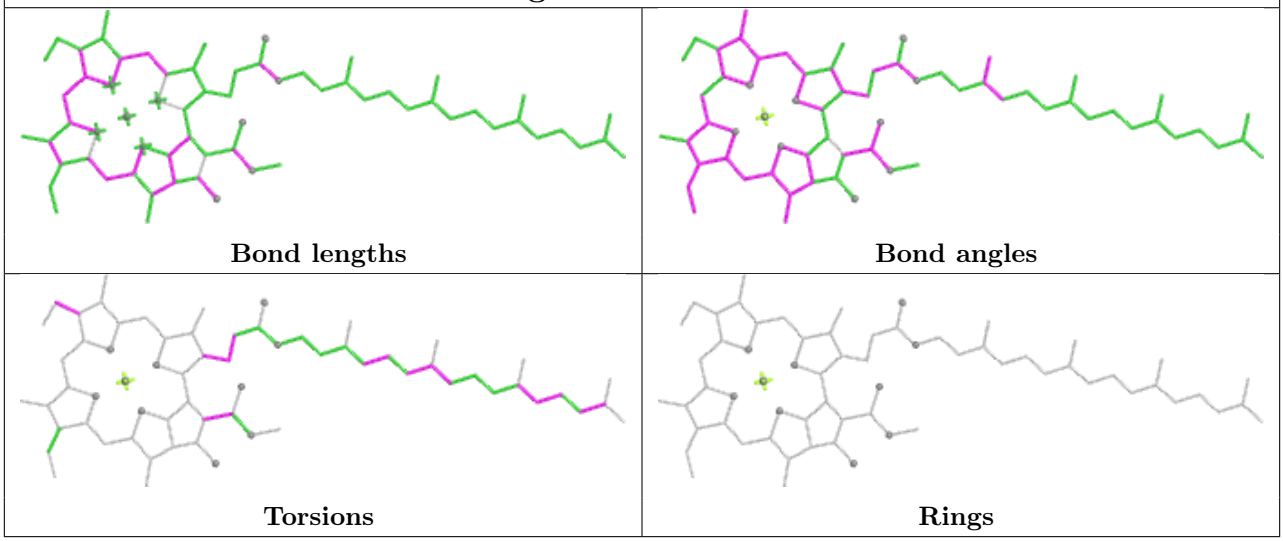
Ligand SQD b 521



Bond lengths | Bond angles

Torsions | Rings

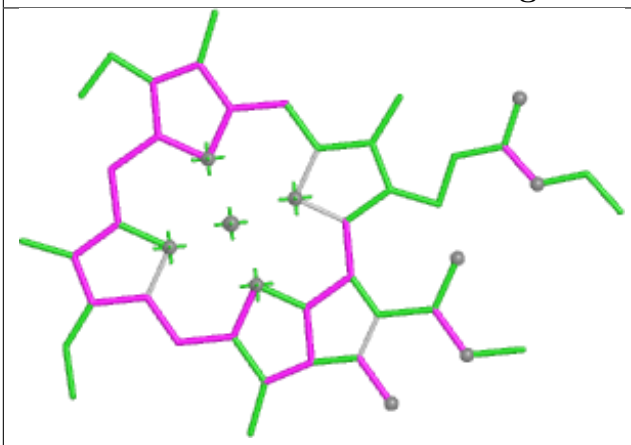
Ligand CLA d 401



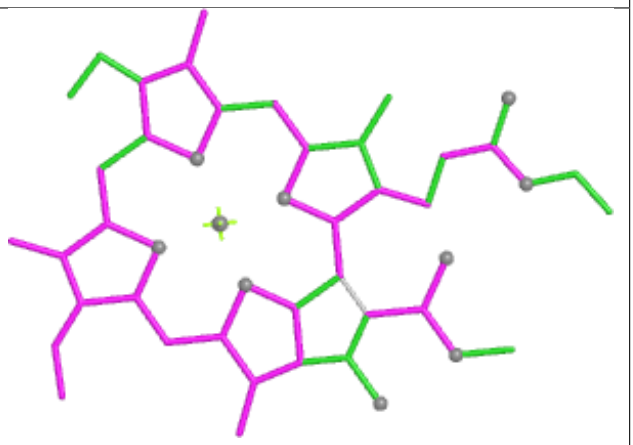
Bond lengths | Bond angles

Torsions | Rings

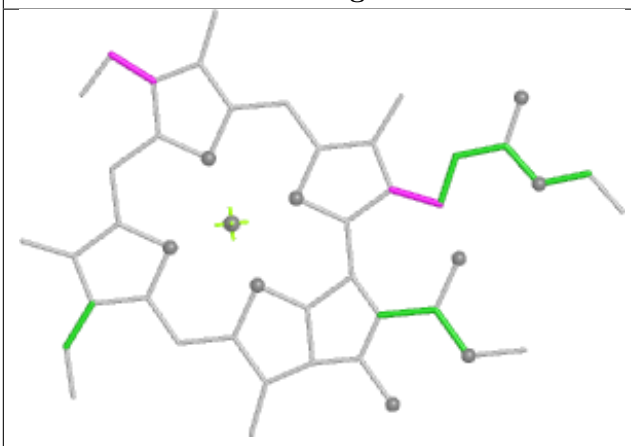
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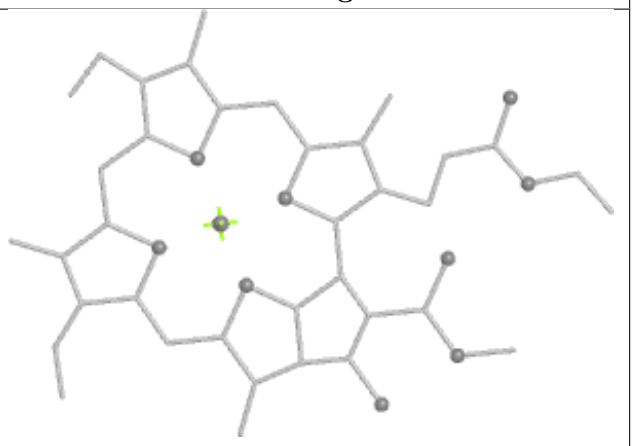
Bond lengths



Bond angles

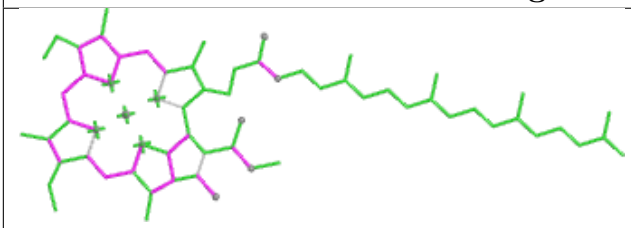


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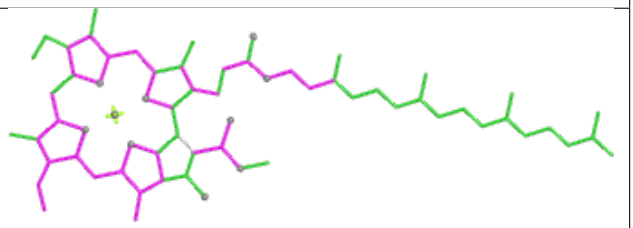


Rings

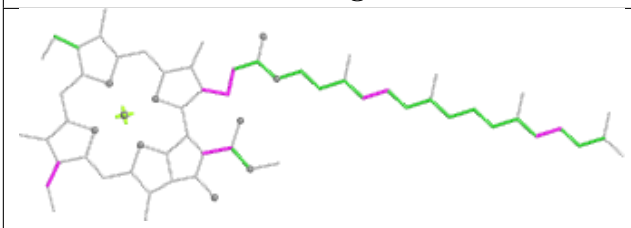
Ligand CLA a 404



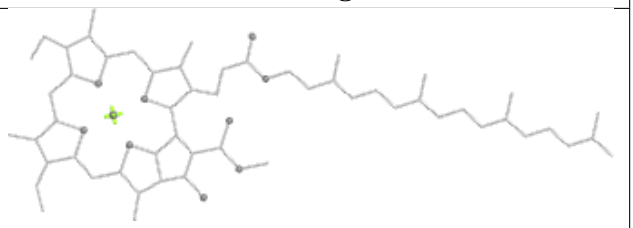
Bond lengths



Bond angles

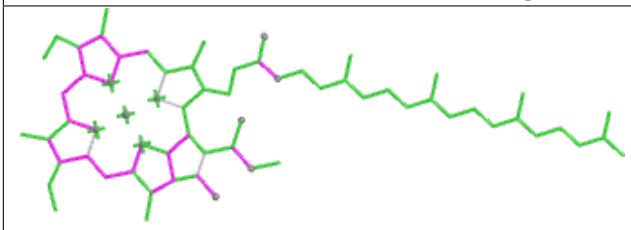


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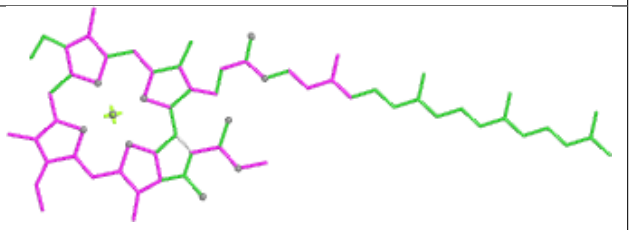


Rings

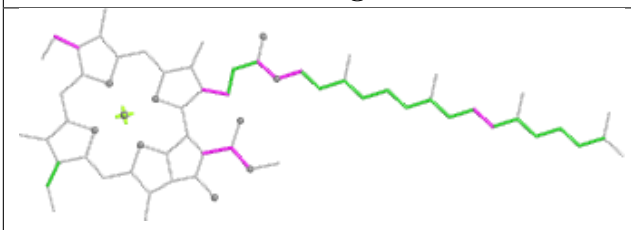
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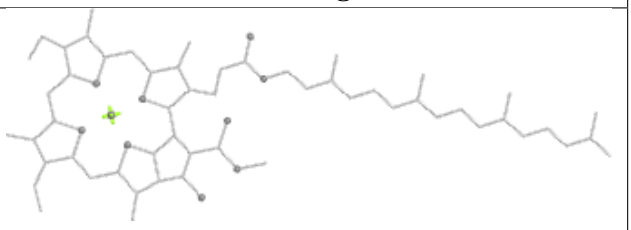
Bond lengths



Bond angles

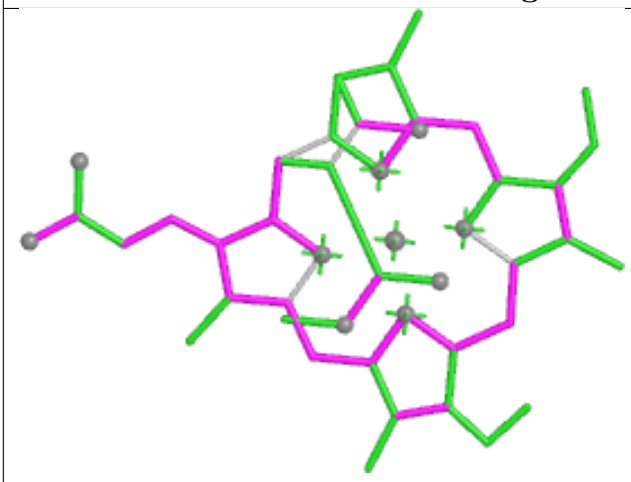


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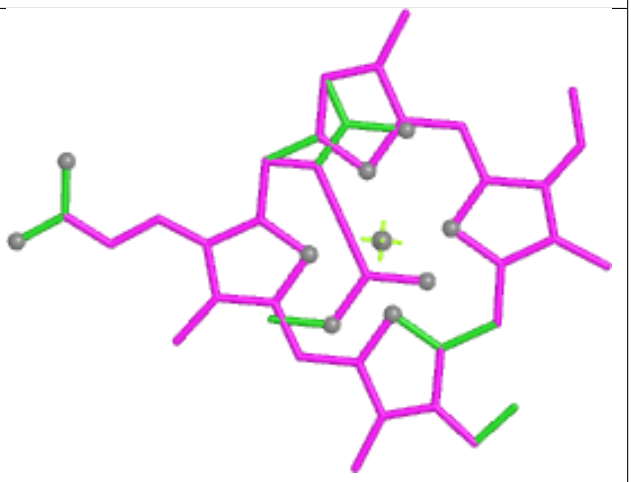


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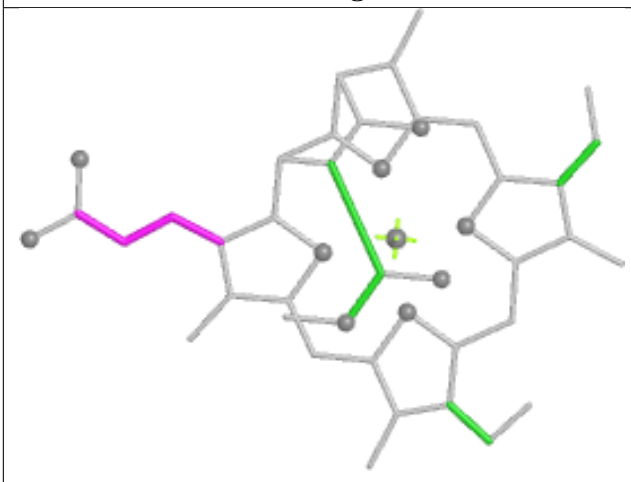
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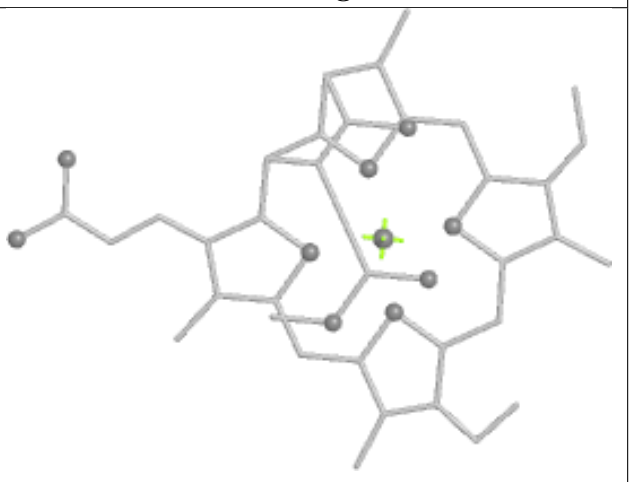
Bond lengths



Bond angles

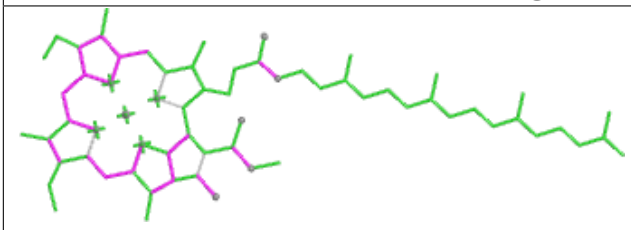


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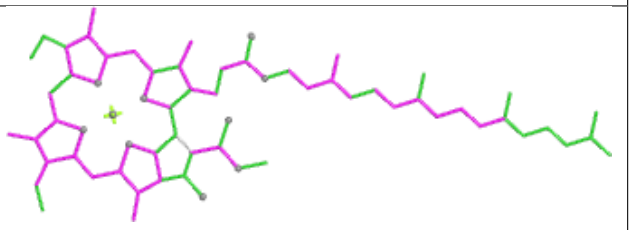


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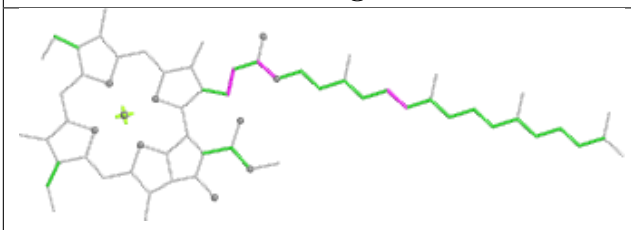
Ligand CLA a 403



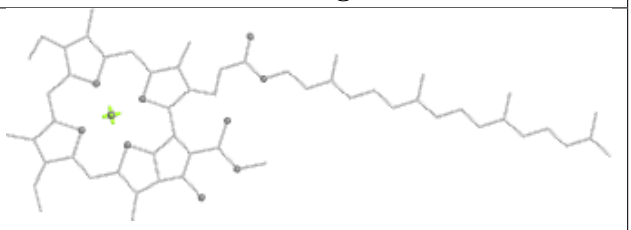
Bond lengths



Bond angles

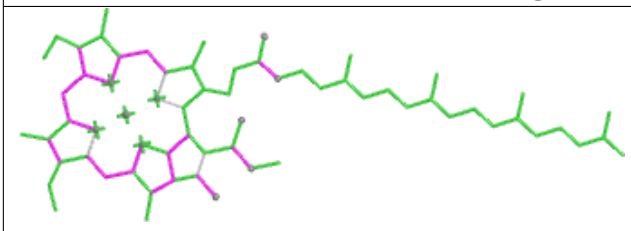


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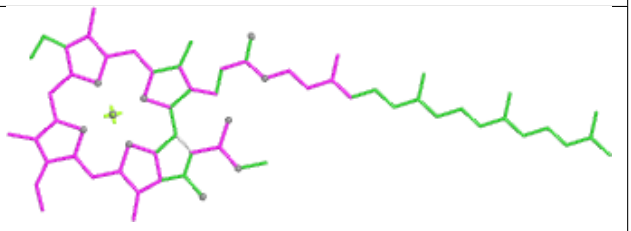


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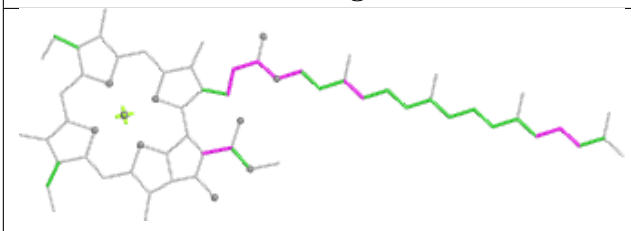
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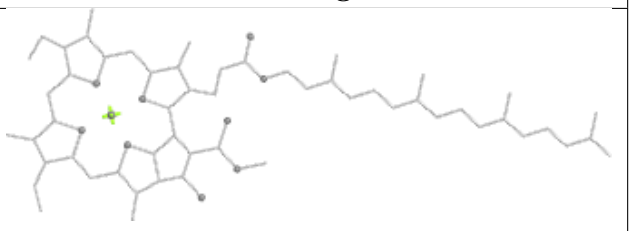
Bond lengths



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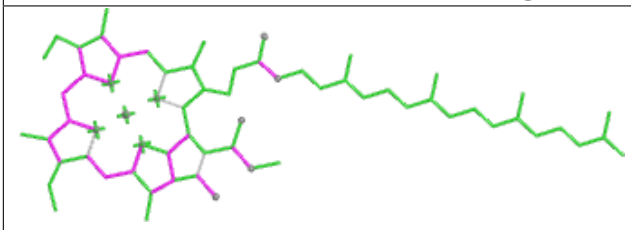


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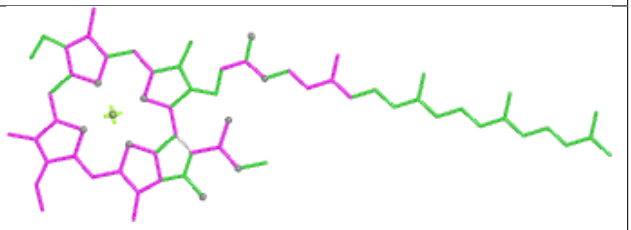


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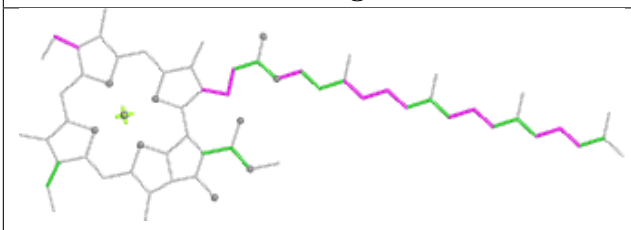
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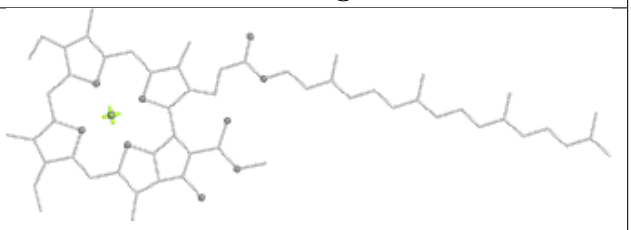
Bond lengths



Bond angles

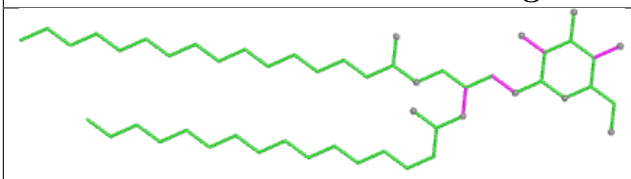


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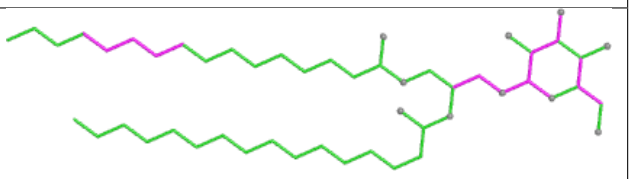


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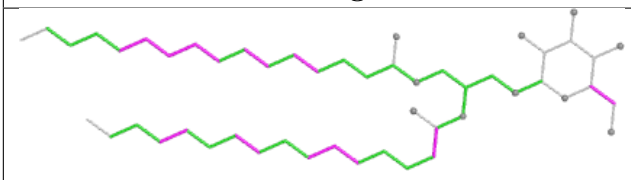
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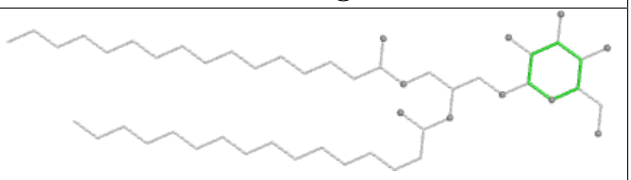
Bond lengths



Bond angles

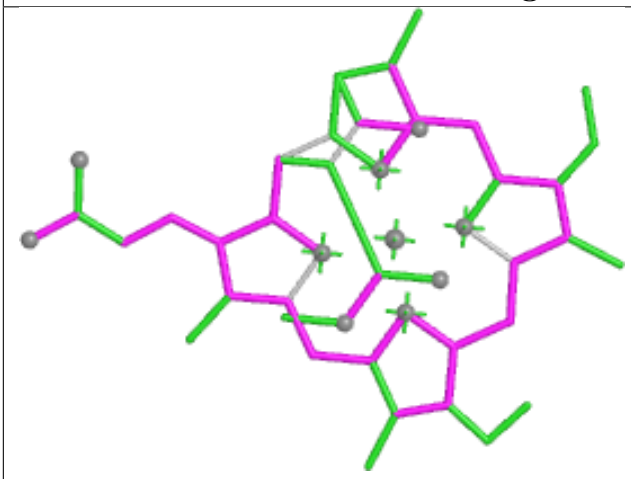


Torsions



Rings

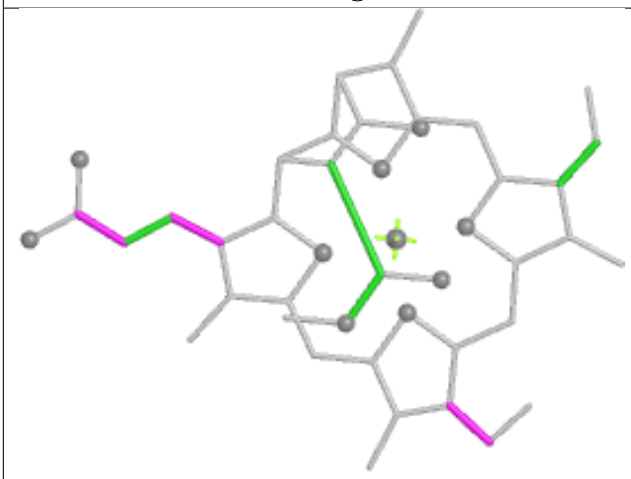
Ligand KC1 41 207



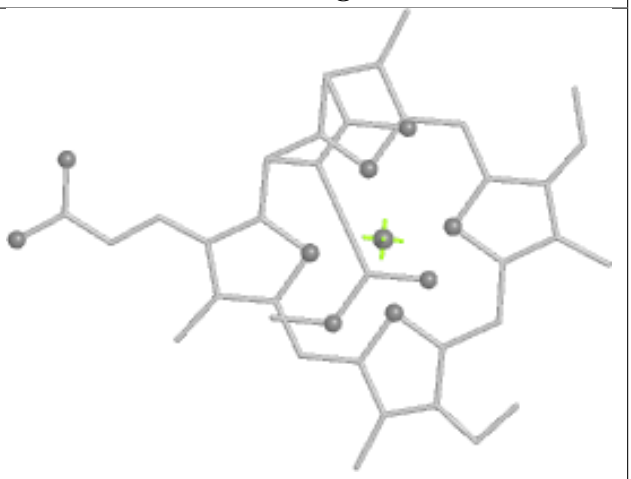
Bond lengths



Bond angles

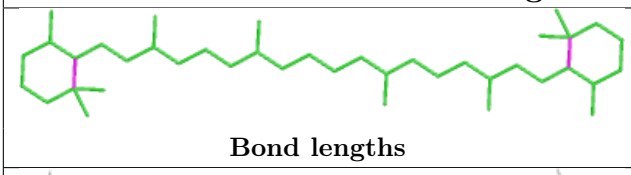


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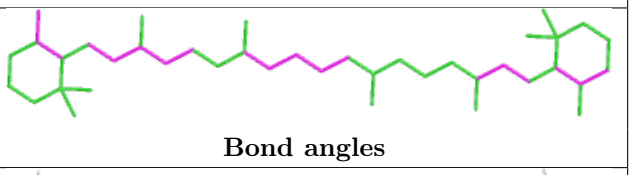


Rings

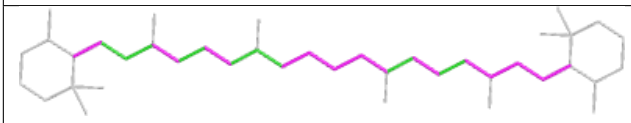
Ligand BCR b 524



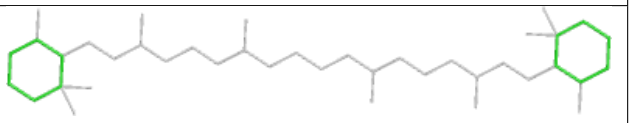
Bond lengths



Bond angles

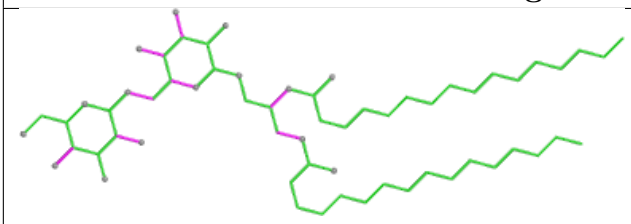


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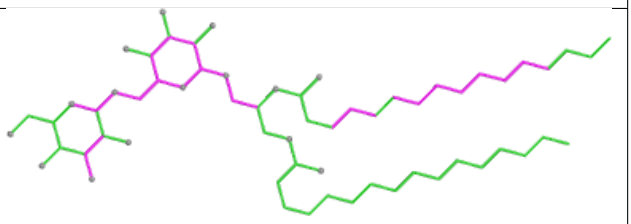


Rings

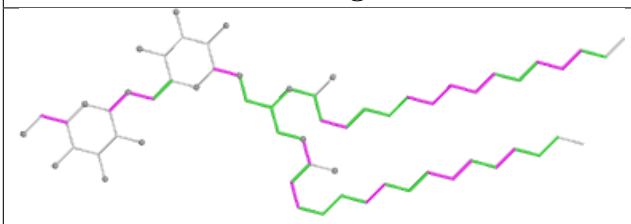
Ligand DGD c 517



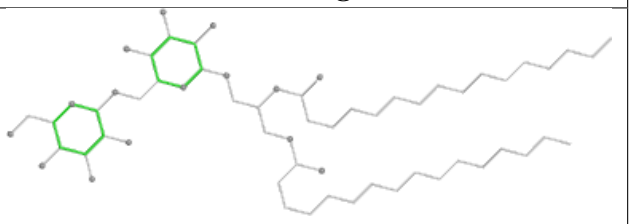
Bond lengths



Bond angles

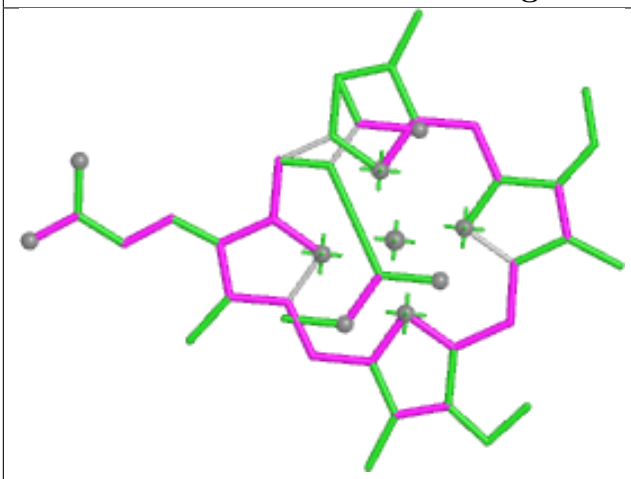


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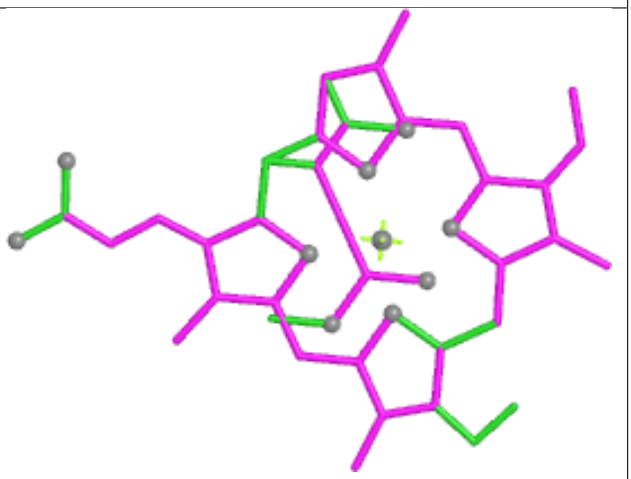


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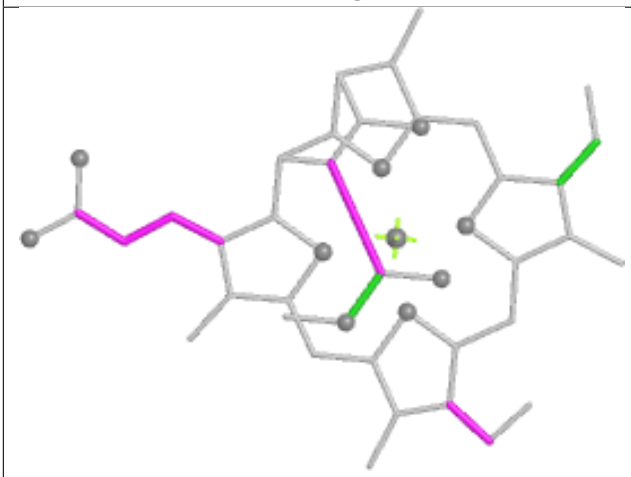
Ligand KC1 31 309



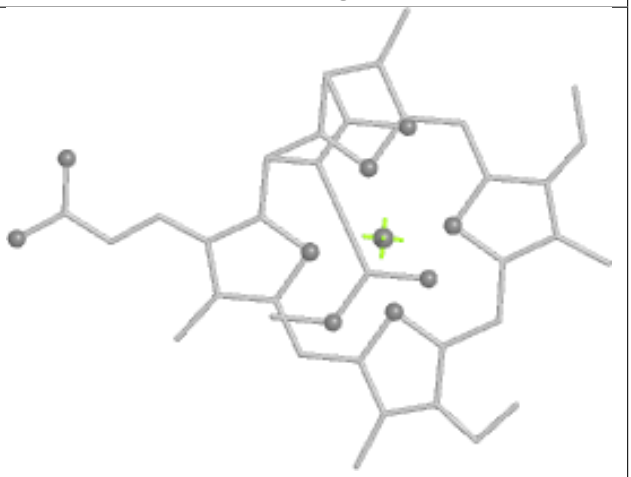
Bond lengths



Bond angles

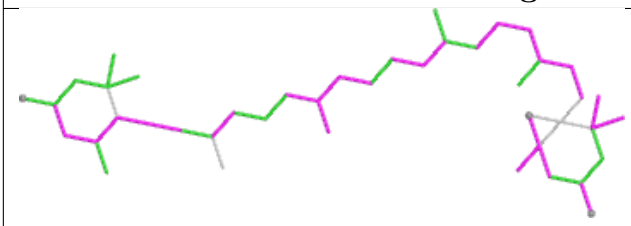


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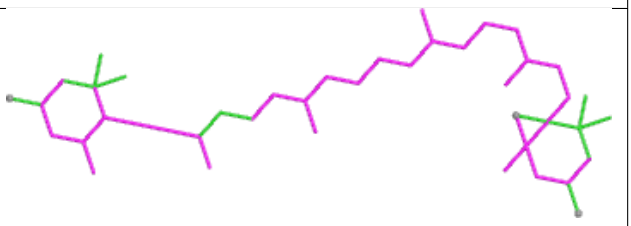


Rings

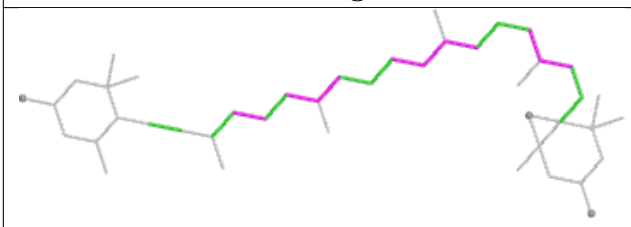
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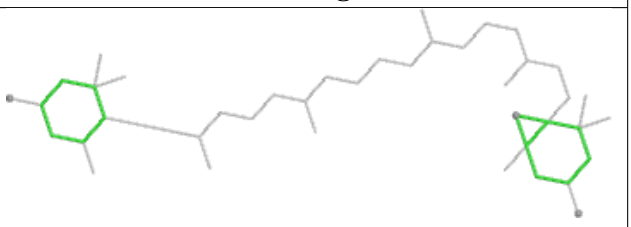
Bond lengths



Bond angles

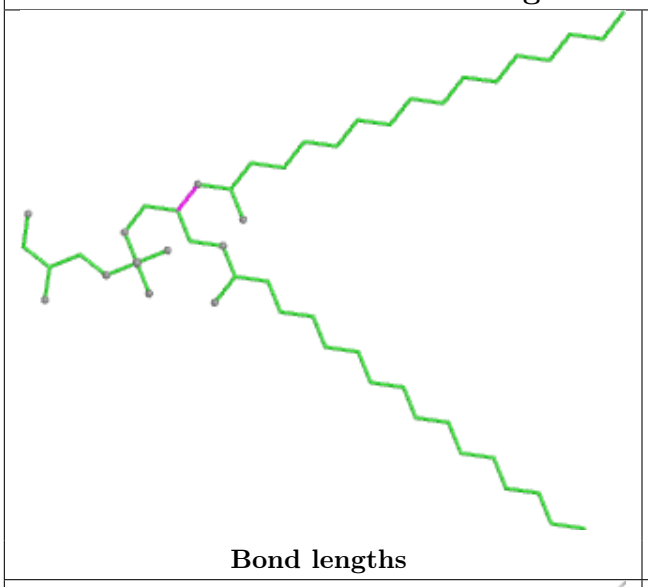


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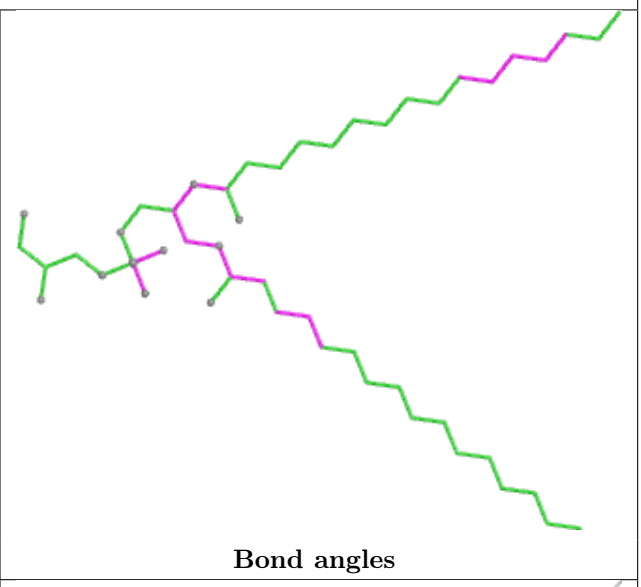


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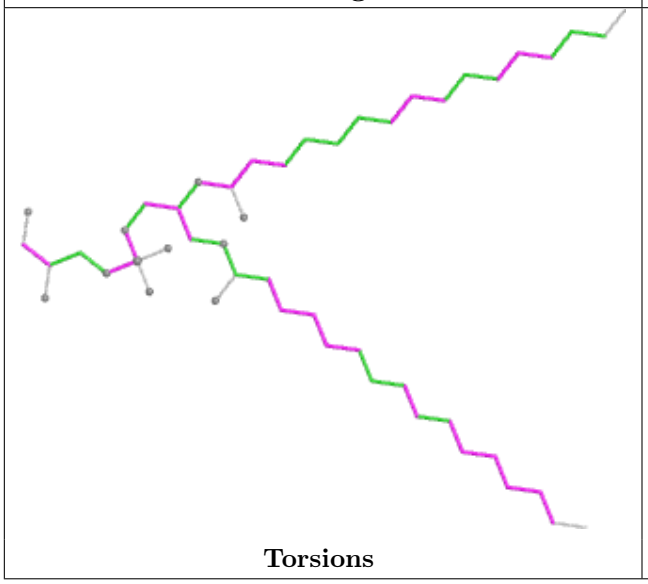
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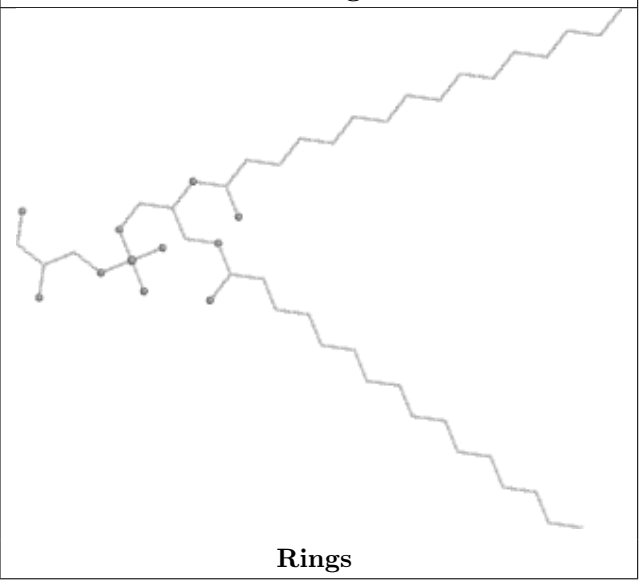
Bond lengths



Bond angles

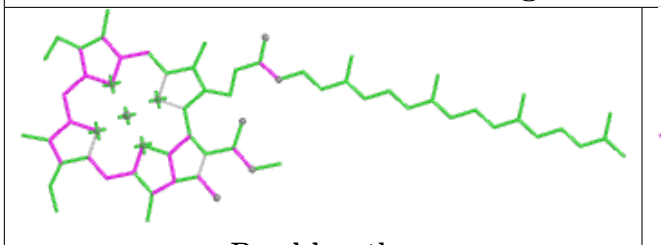


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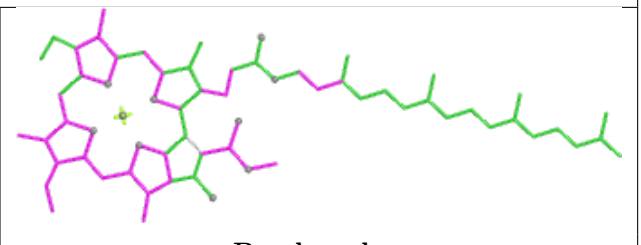


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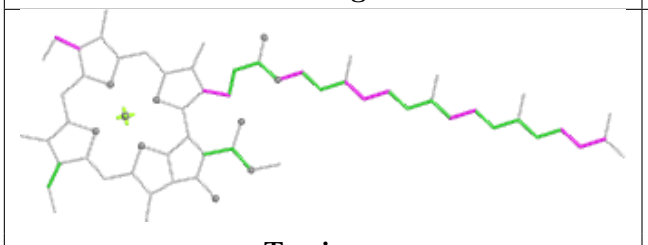
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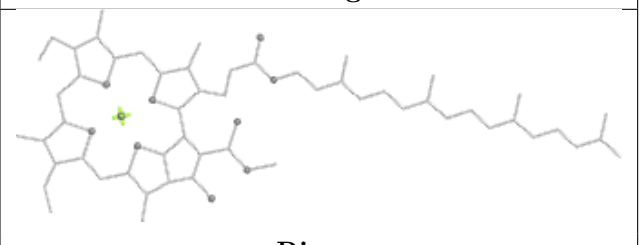
Bond lengths



Bond angles

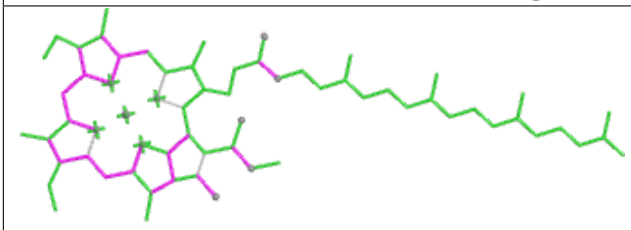


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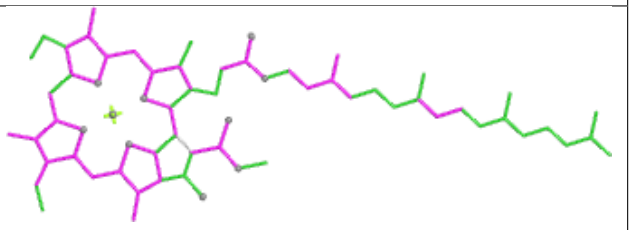


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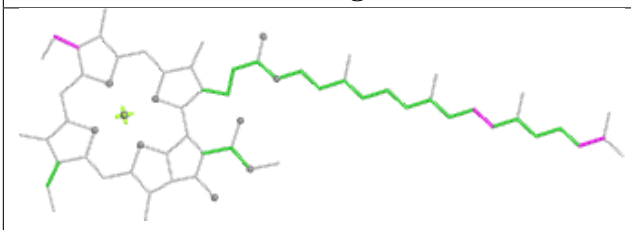
Ligand CLA b 515



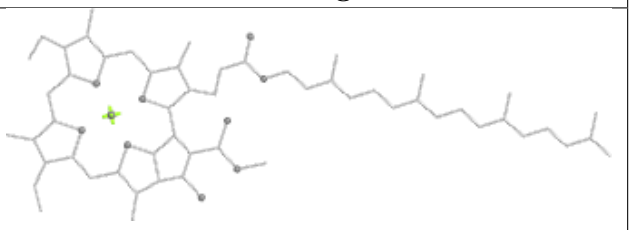
Bond lengths



Bond angles

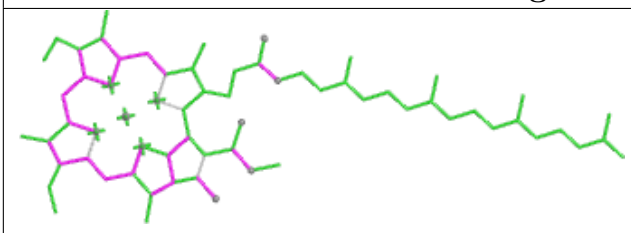


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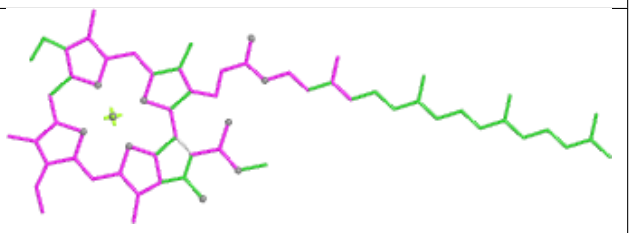


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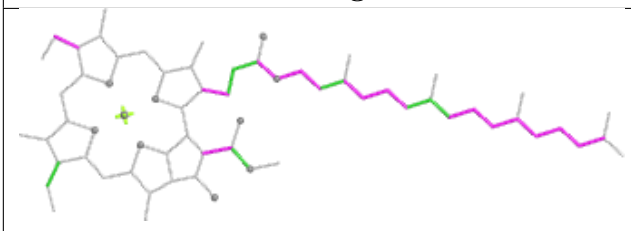
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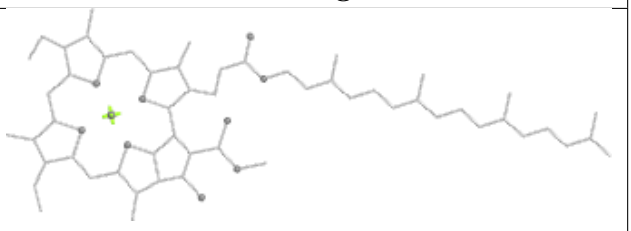
Bond lengths



Bond angles

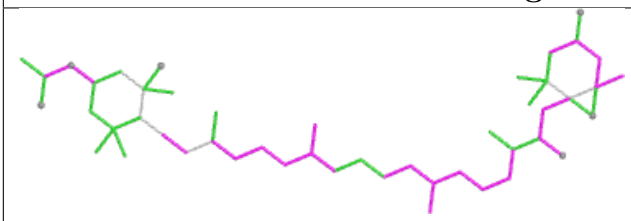


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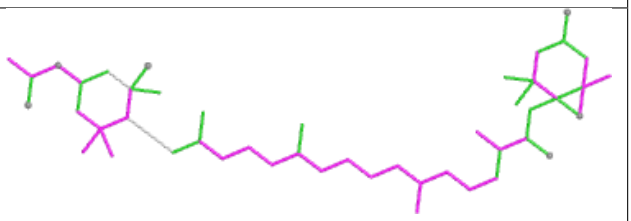


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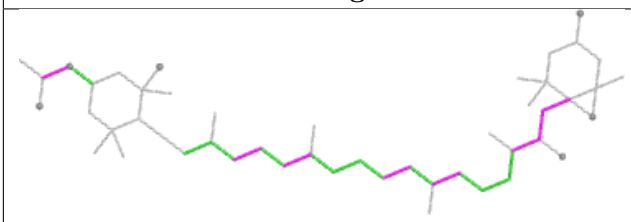
Ligand A86 34 314



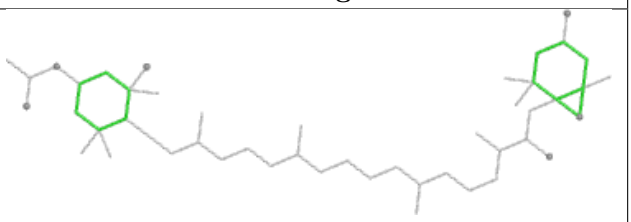
Bond lengths



Bond angles

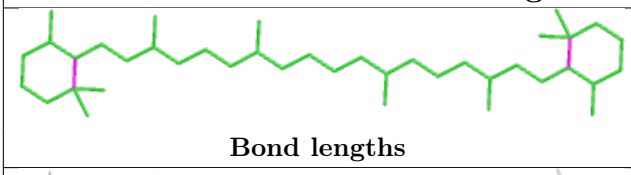


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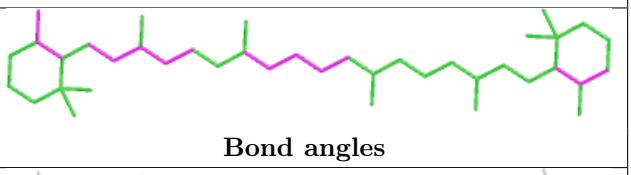


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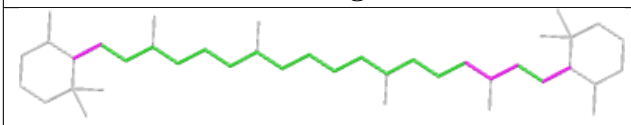
Ligand BCR b 517



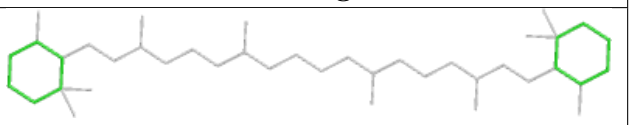
Bond lengths



Bond angles



Torsions

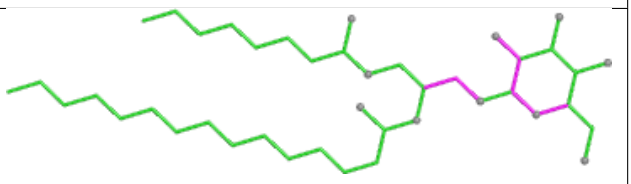


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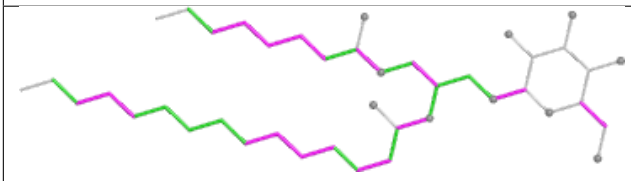
Ligand LMG 31 316



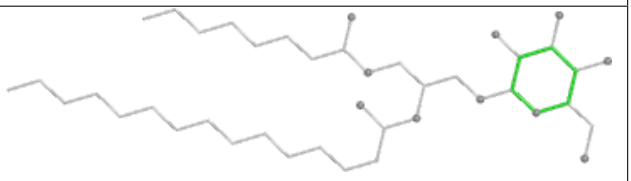
Bond lengths



Bond angles

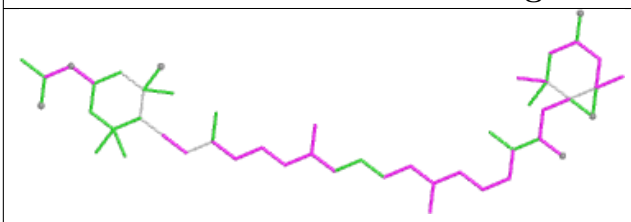


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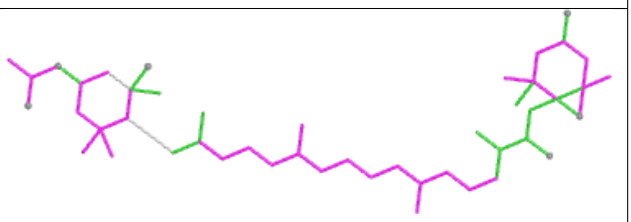


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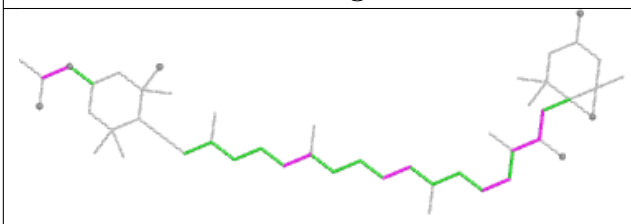
Ligand A86 19 313



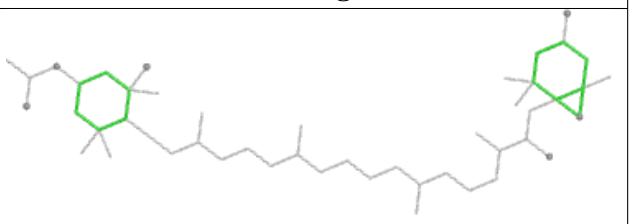
Bond lengths



Bond angles

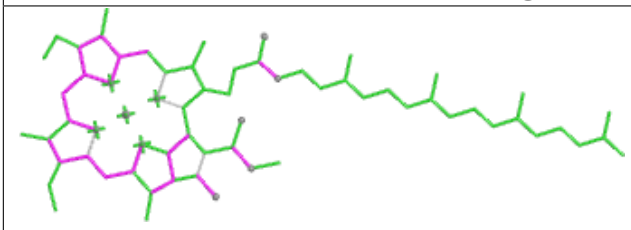


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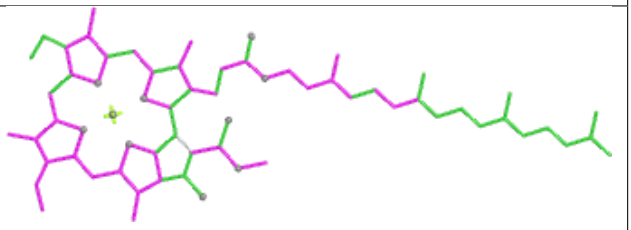


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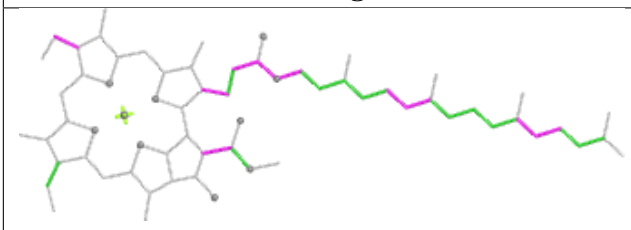
Ligand CLA 34 308



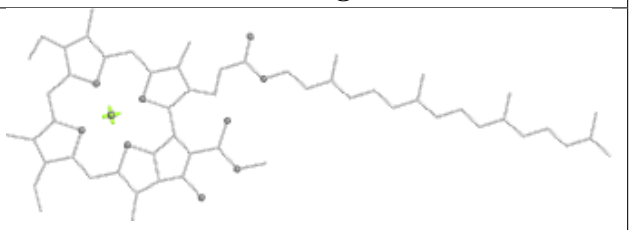
Bond lengths



Bond angles

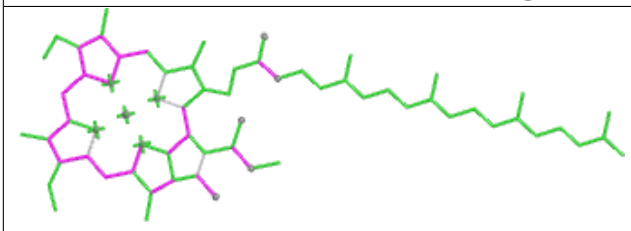


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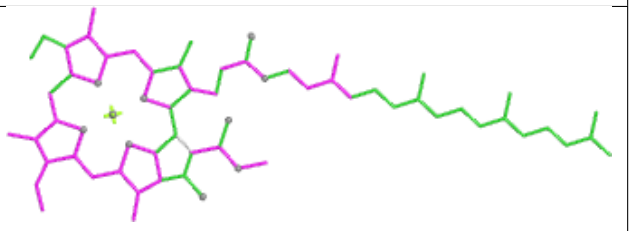


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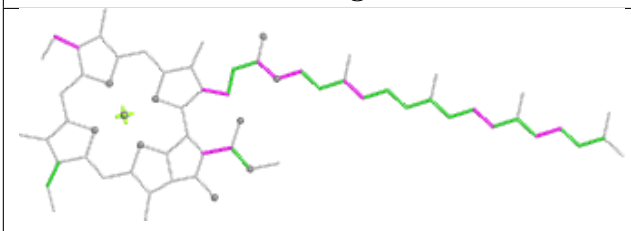
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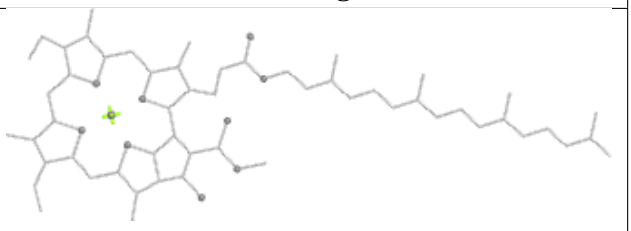
Bond lengths



Bond angles

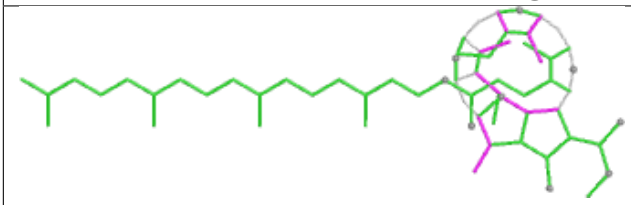


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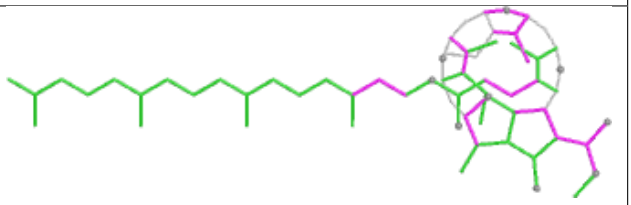


Rings

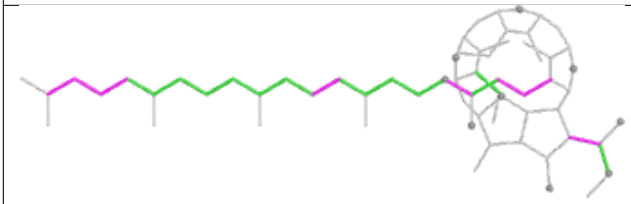
Ligand PHO a 405



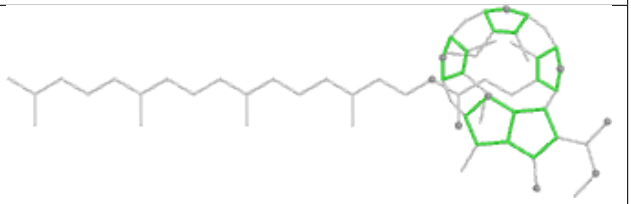
Bond lengths



Bond angles

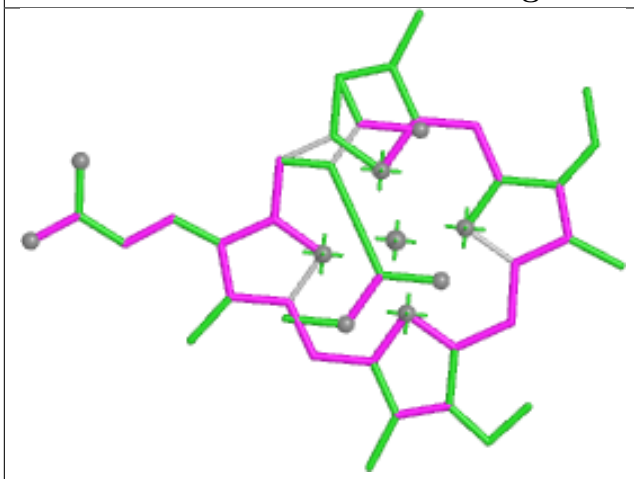


Torsions

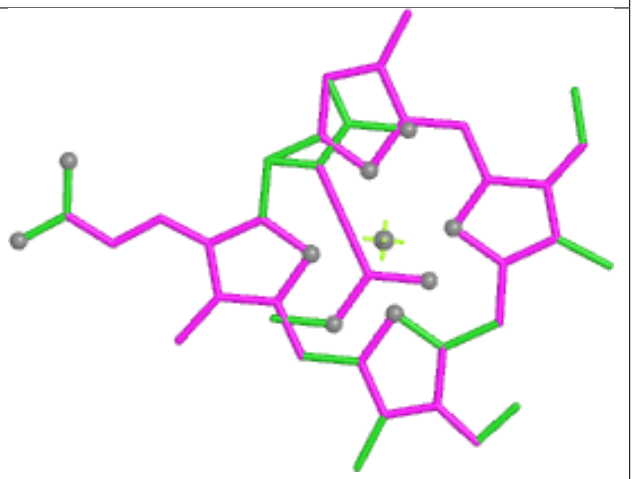


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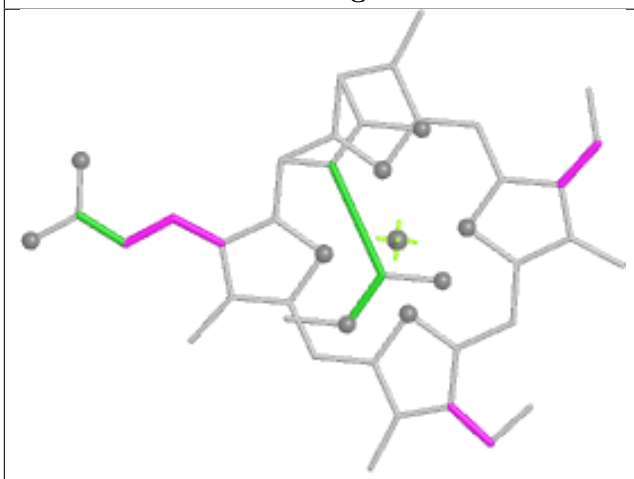
Ligand KC1 32 207



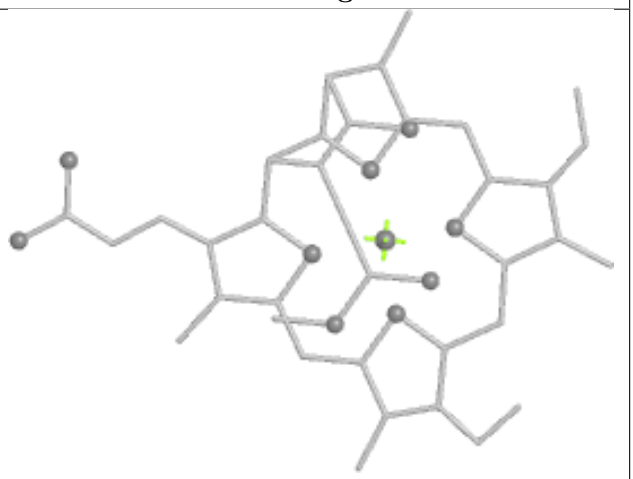
Bond lengths



Bond angles

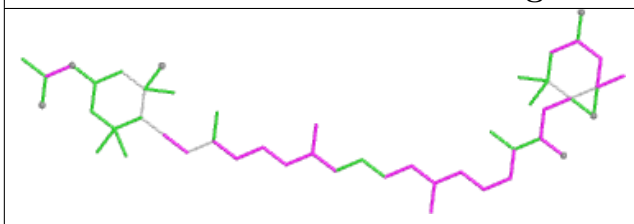


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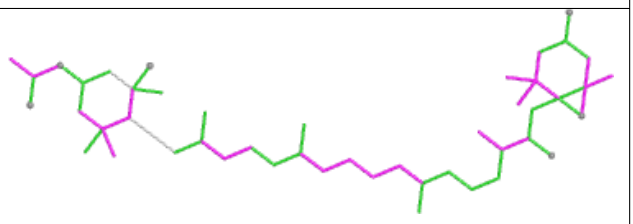


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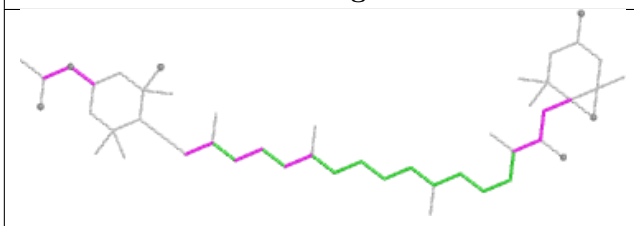
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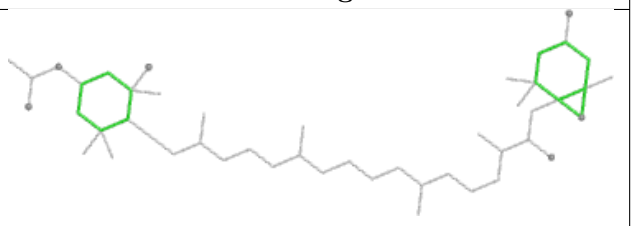
Bond lengths



Bond angles

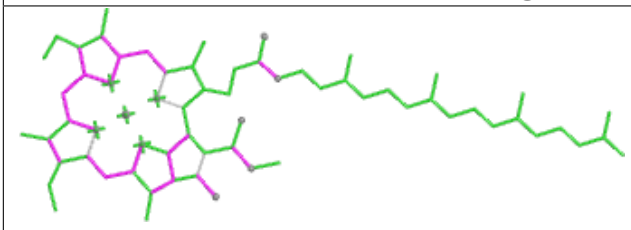


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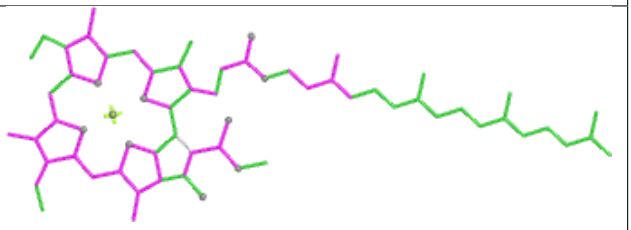


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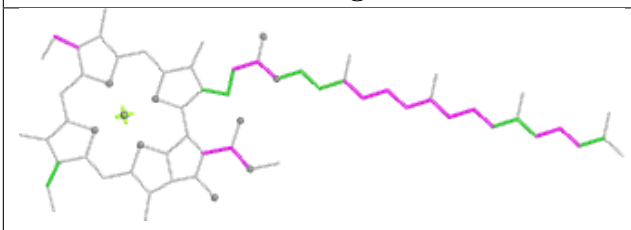
Ligand CLA W 101



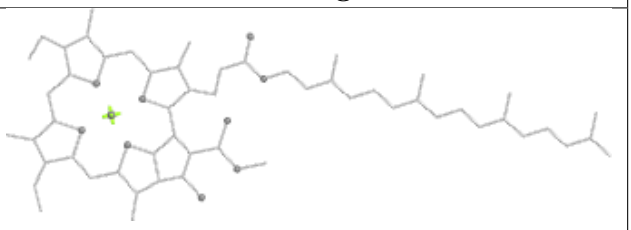
Bond lengths



Bond angles

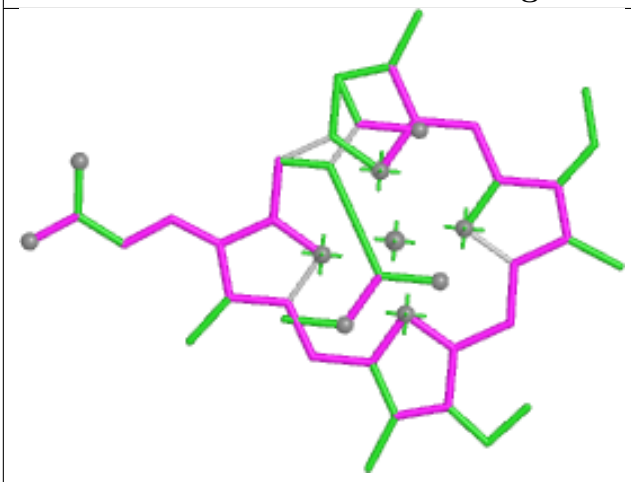


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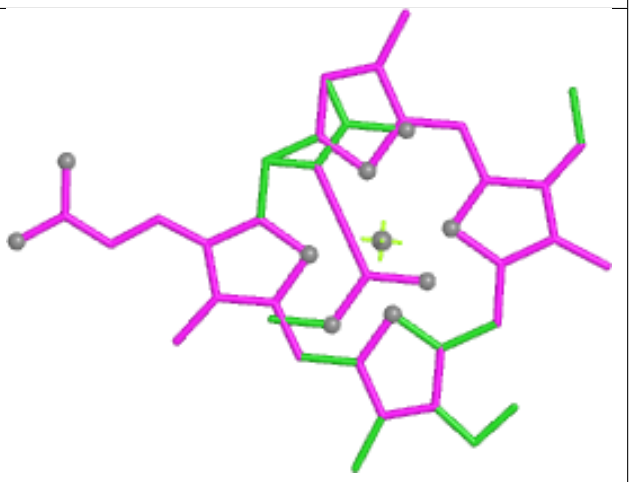


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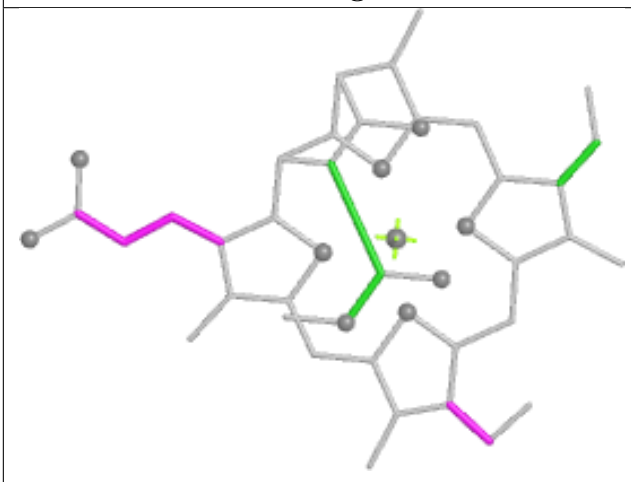
Ligand KC1 36 304



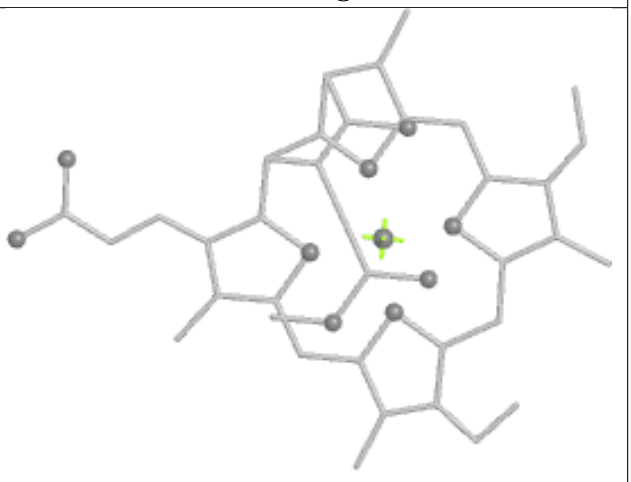
Bond lengths



Bond angles

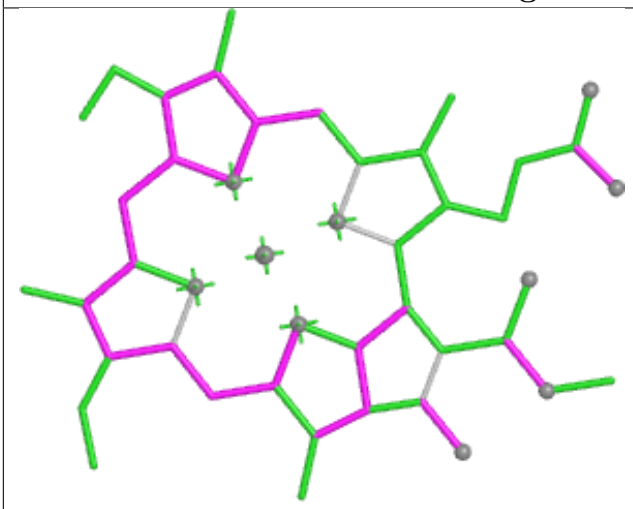


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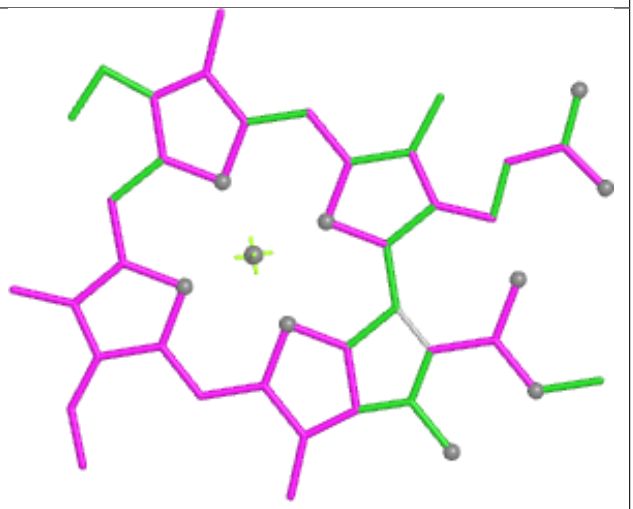


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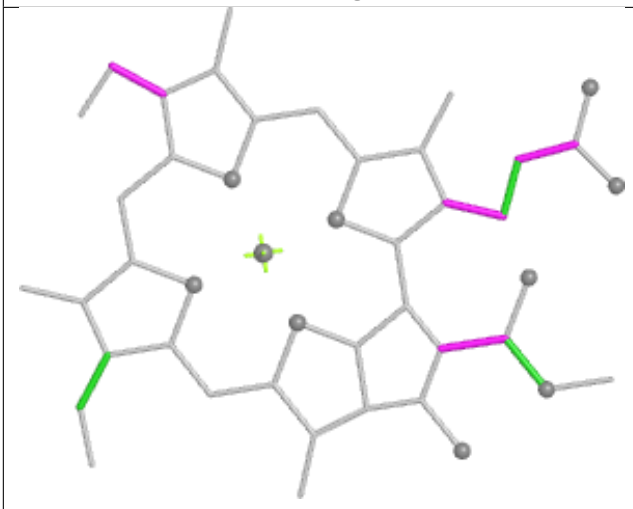
Ligand CLA 40 209



Bond lengths



Bond angles

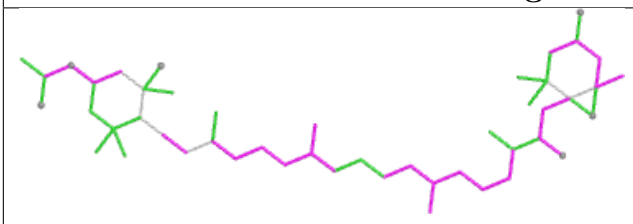


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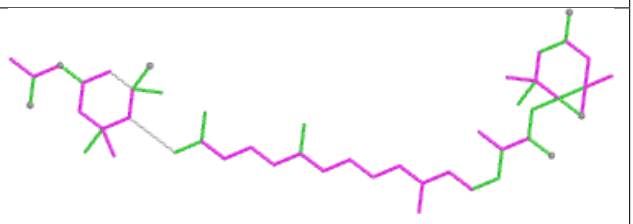


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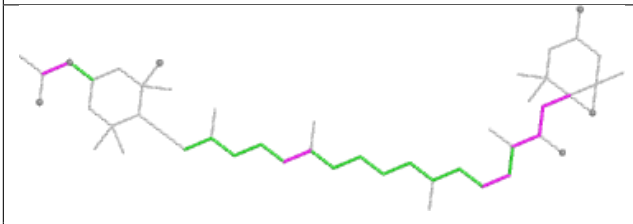
Ligand A86 37 314



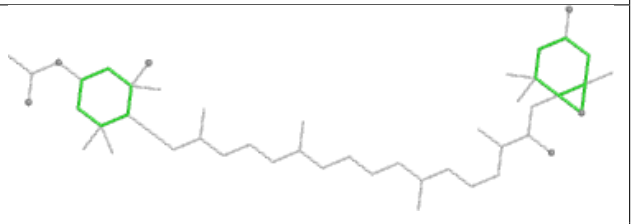
Bond lengths



Bond angles

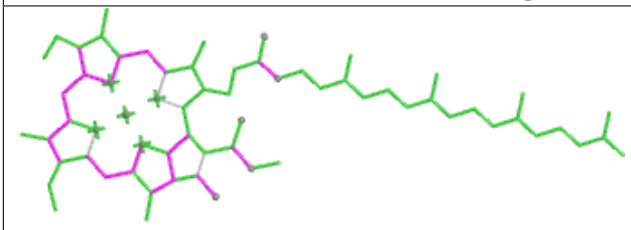


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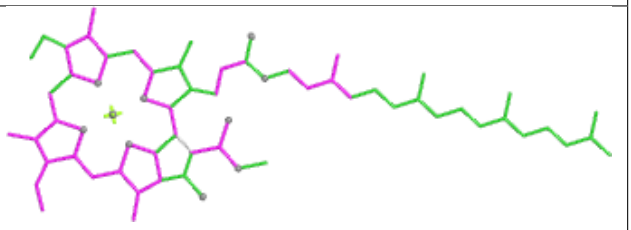


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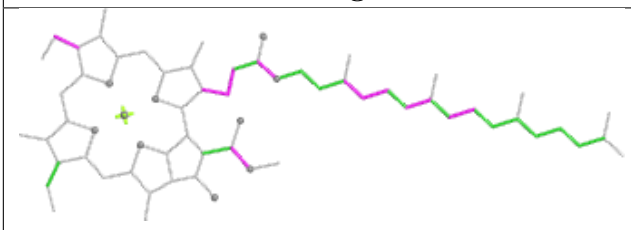
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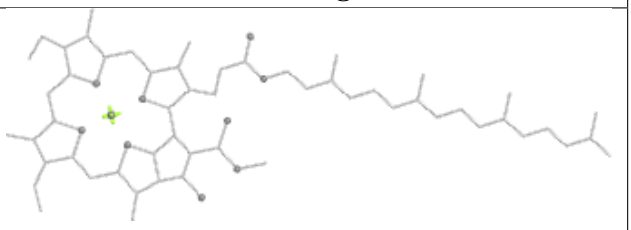
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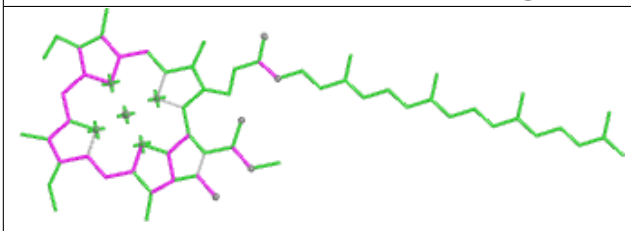


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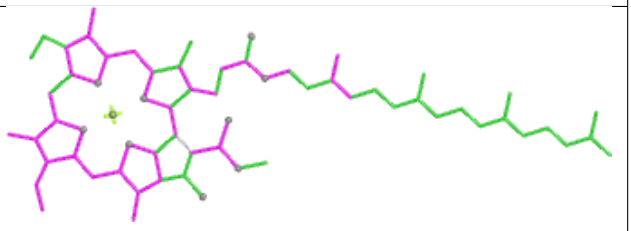


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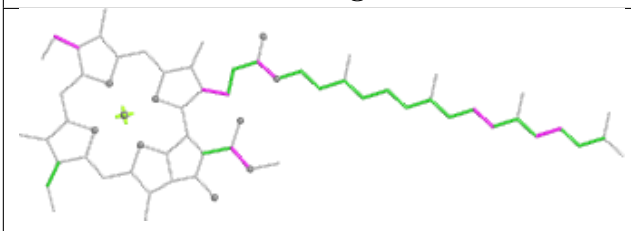
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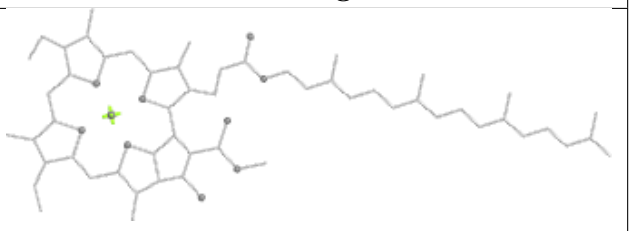
Bond lengths



Bond angles

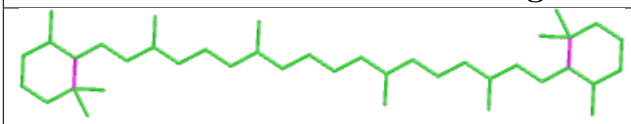


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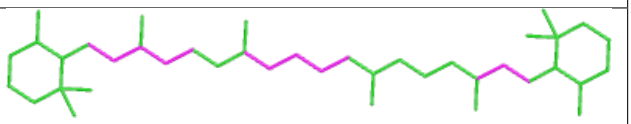


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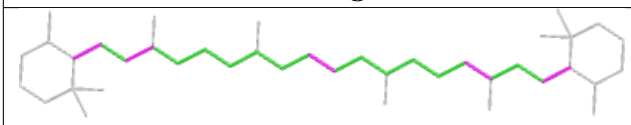
Ligand BCR a 408



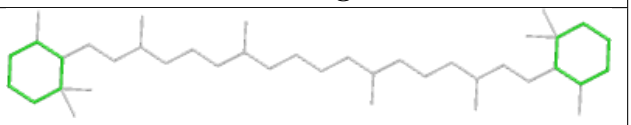
Bond lengths



Bond angles

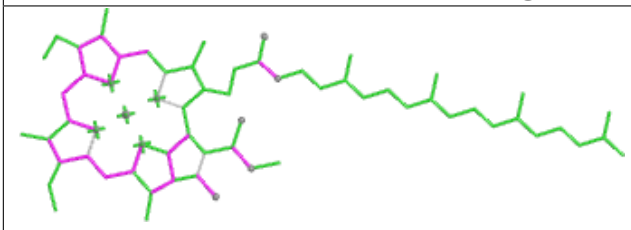


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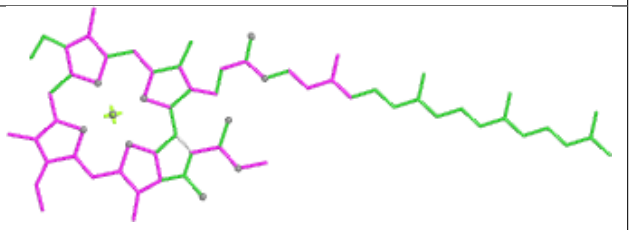


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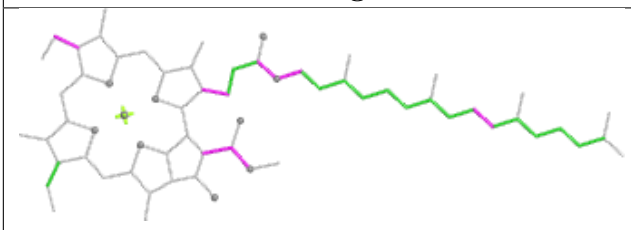
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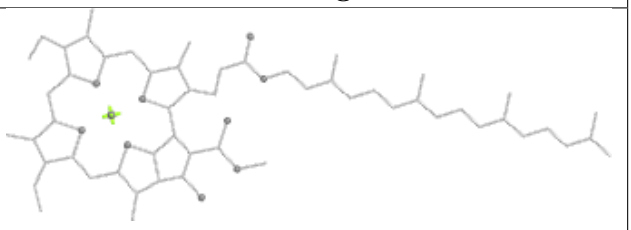
Bond lengths



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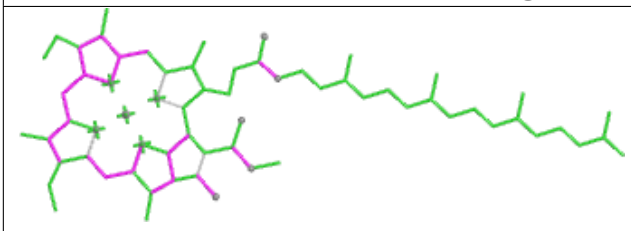


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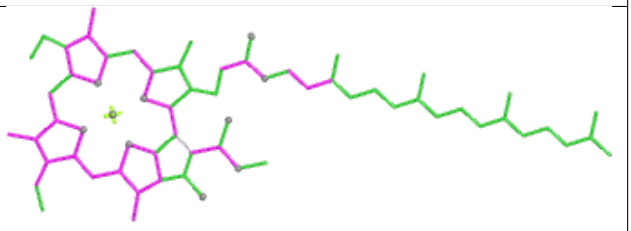


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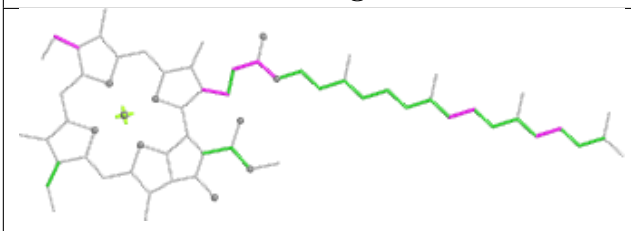
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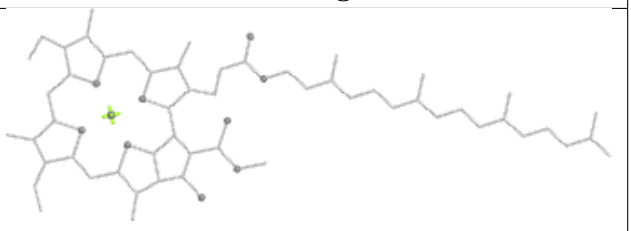
Bond lengths



Bond angles

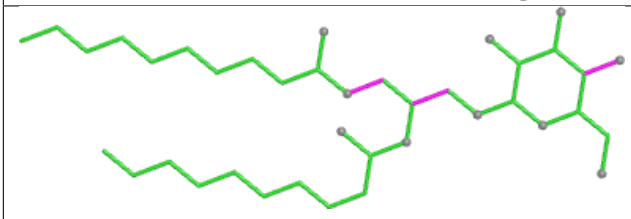


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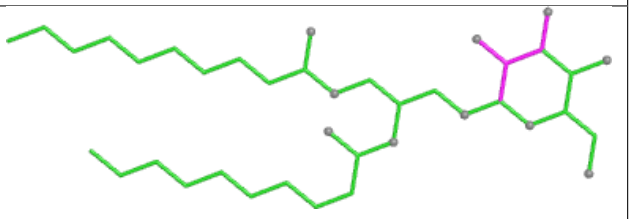


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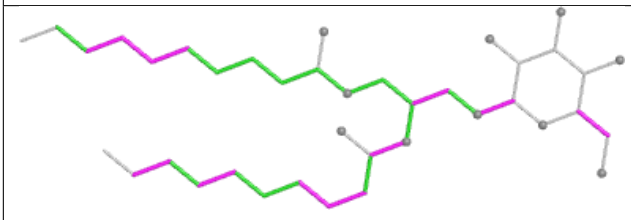
Ligand LMG 12 201



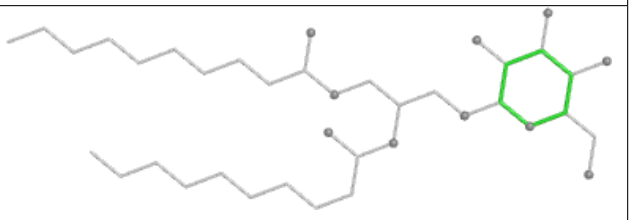
Bond lengths



Bond angles

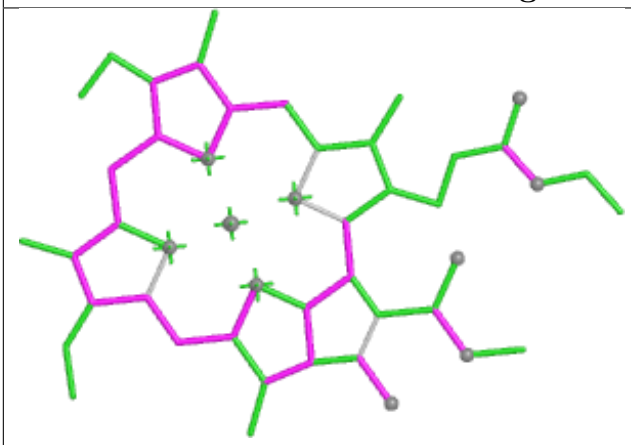


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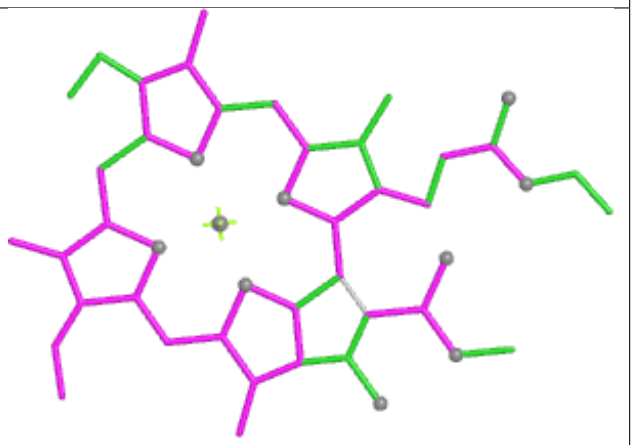


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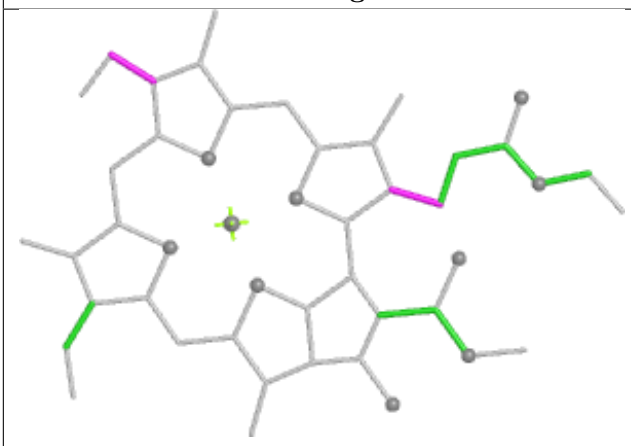
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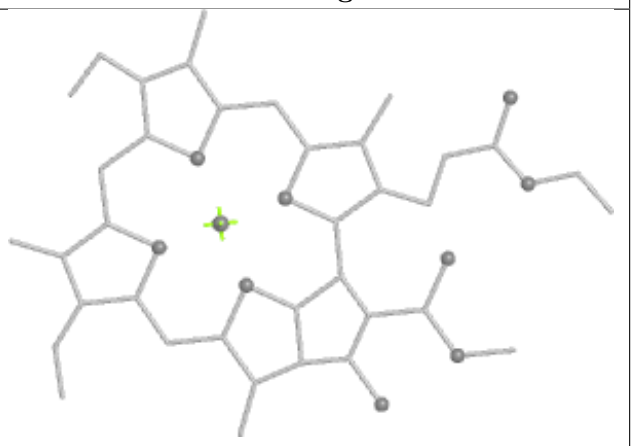
Bond lengths



Bond angles

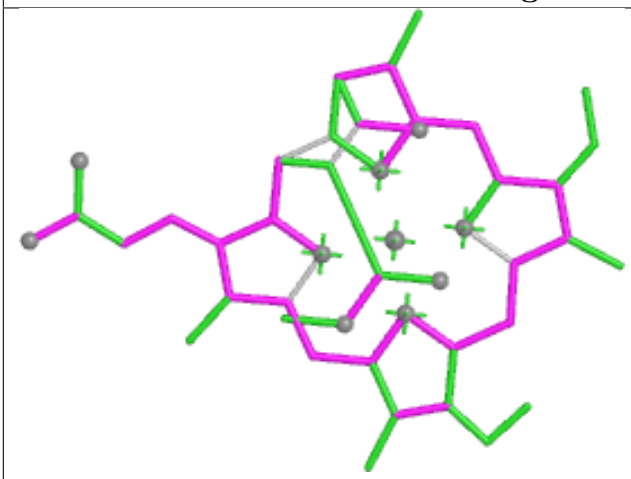


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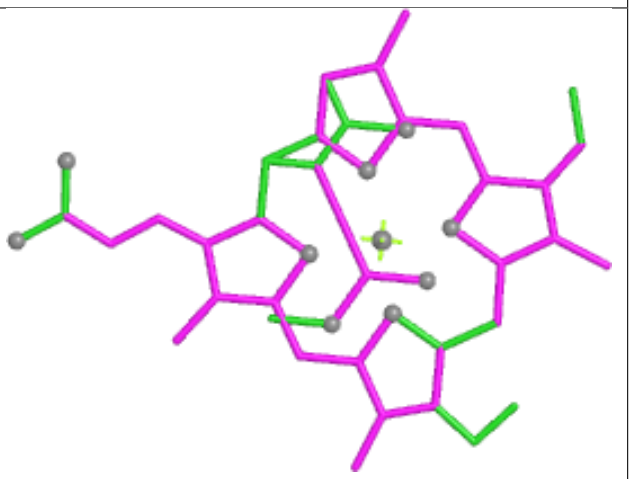


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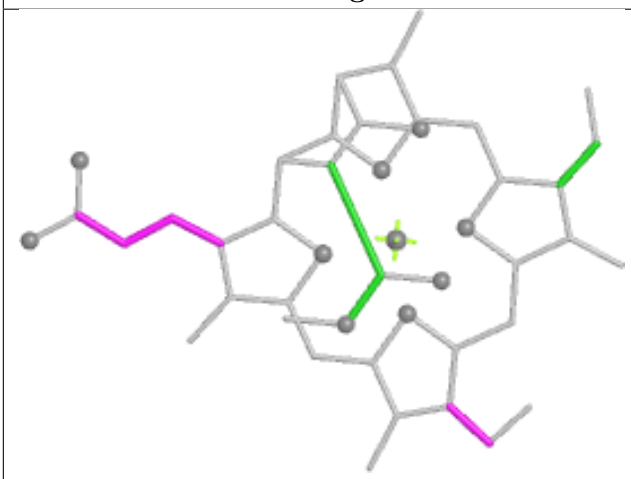
Ligand KC1 18 205



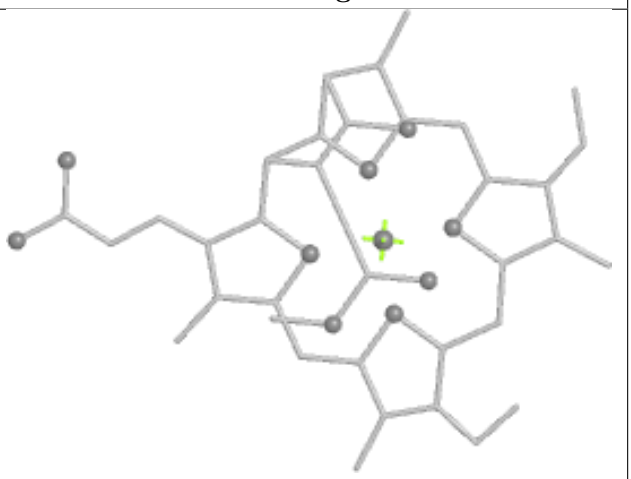
Bond lengths



Bond angles

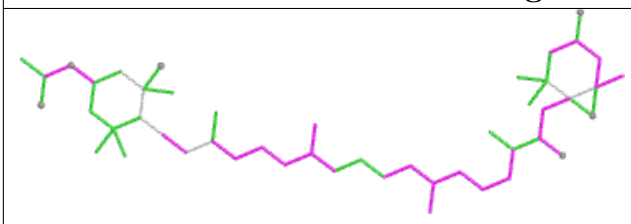


Torsions

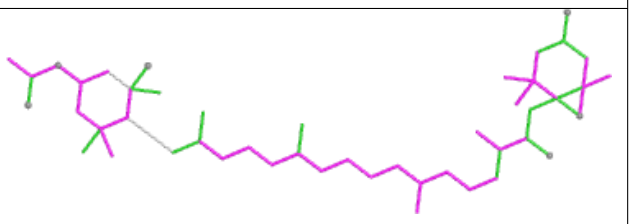


Rings

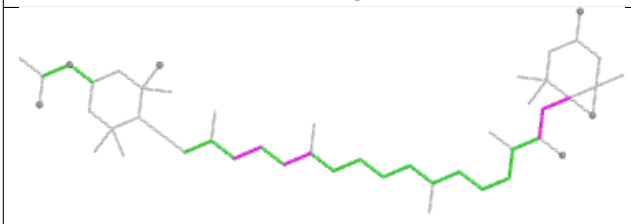
Ligand A86 32 214



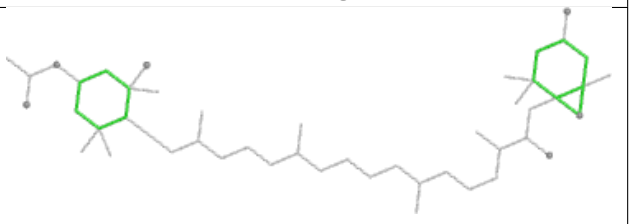
Bond lengths



Bond angles

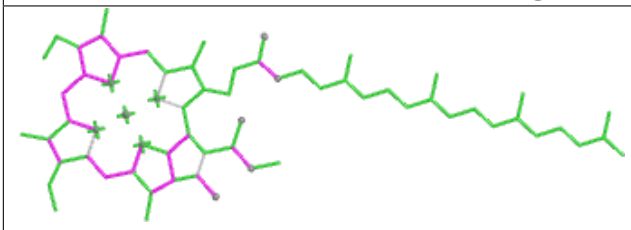


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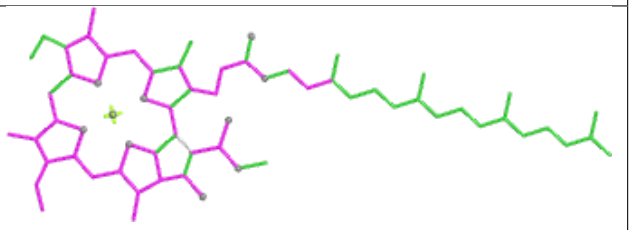


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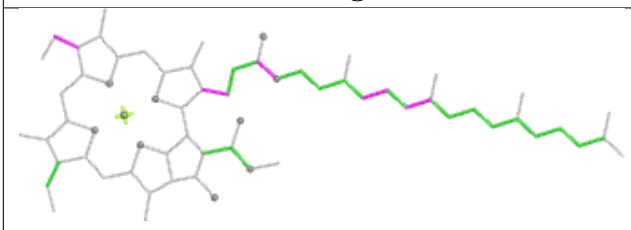
Ligand CLA c 511



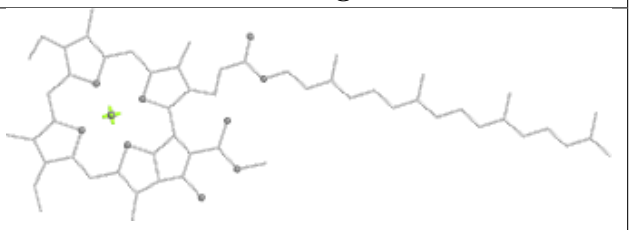
Bond lengths



Bond angles

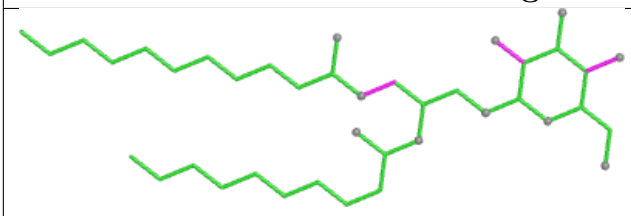


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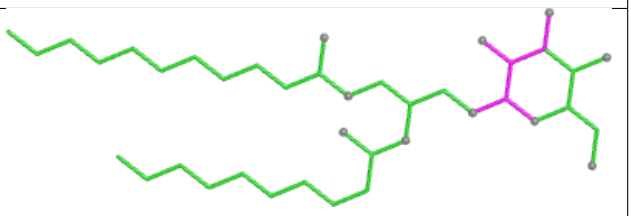


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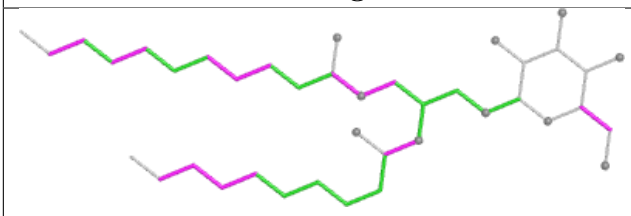
Ligand LMG L 102



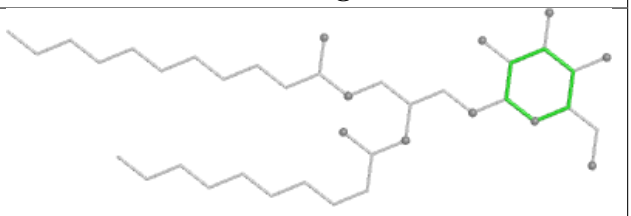
Bond lengths



Bond angles

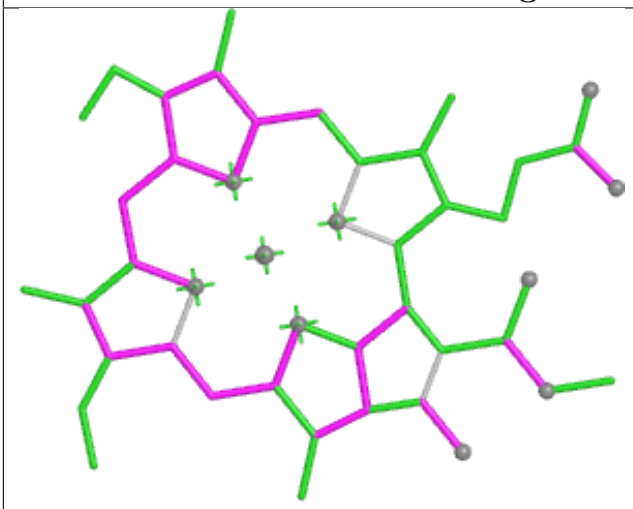


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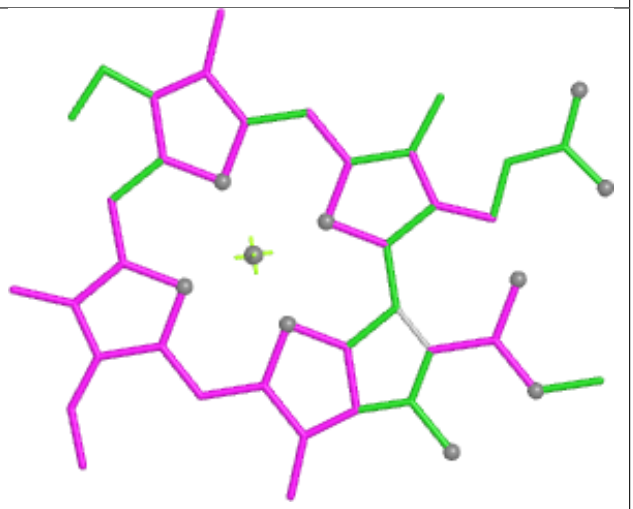


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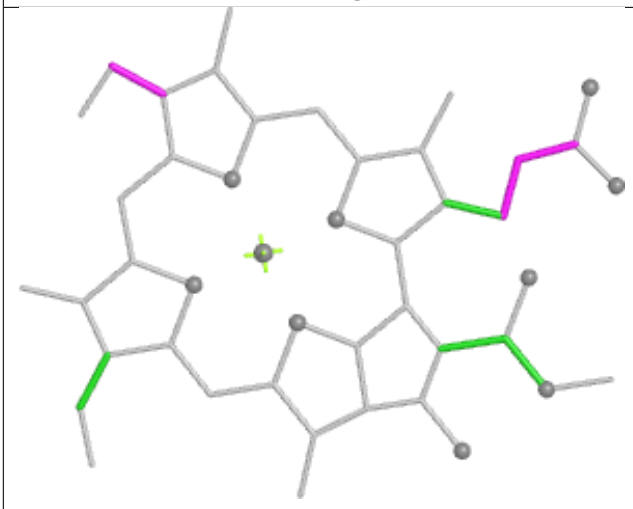
Ligand CLA 39 309



Bond lengths



Bond angles

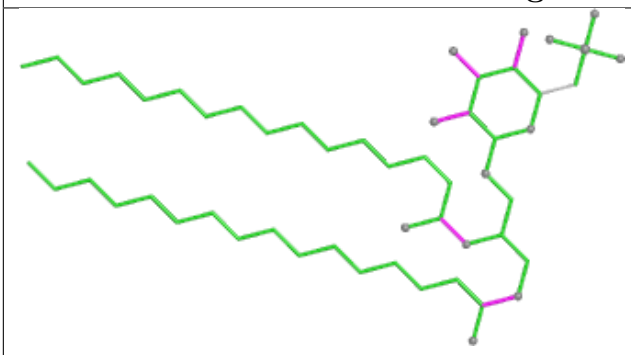


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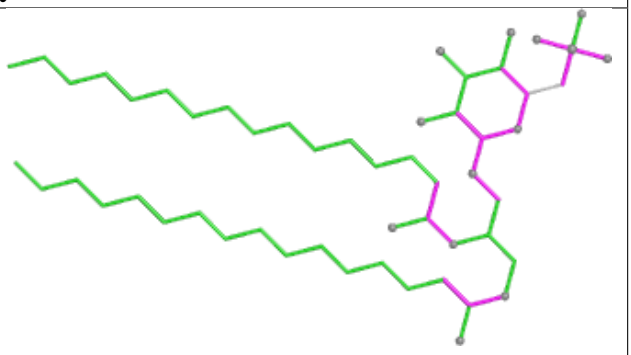


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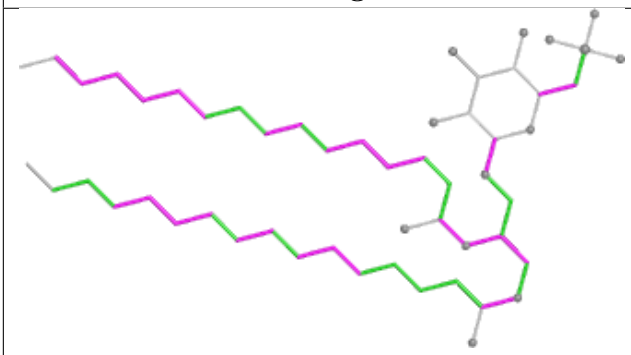
Ligand SQD L 101



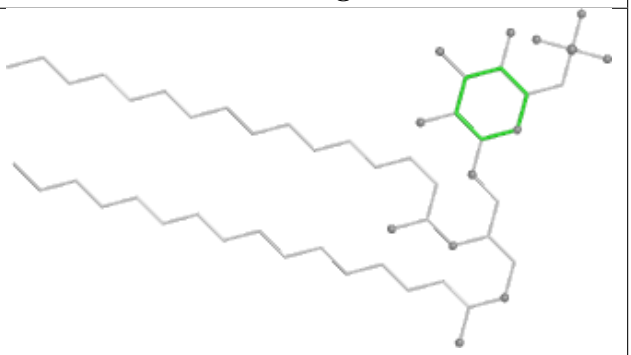
Bond lengths



Bond angles

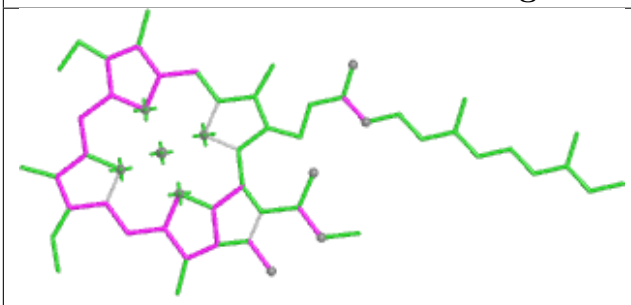


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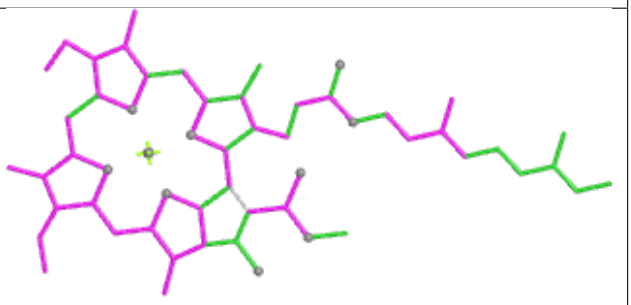


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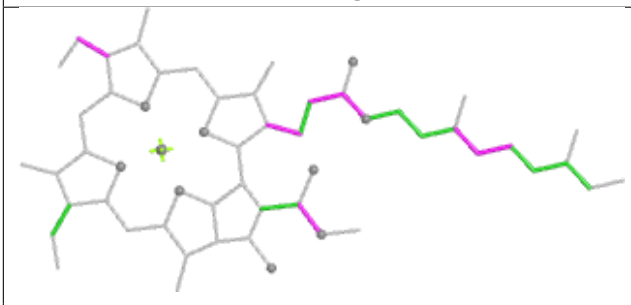
Ligand CLA 40 203



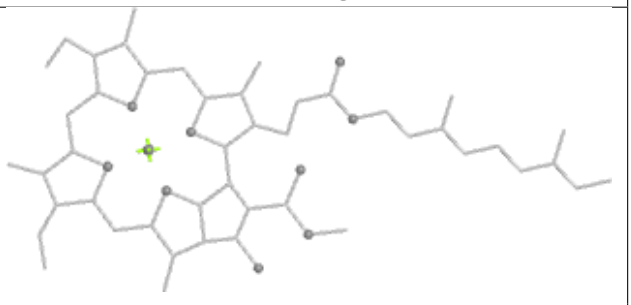
Bond lengths



Bond angles

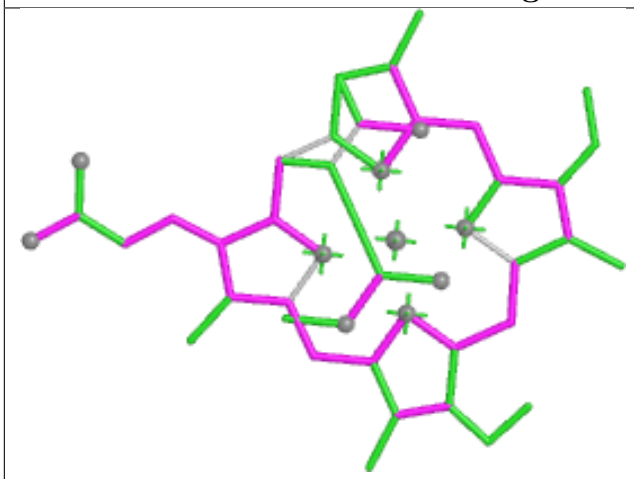


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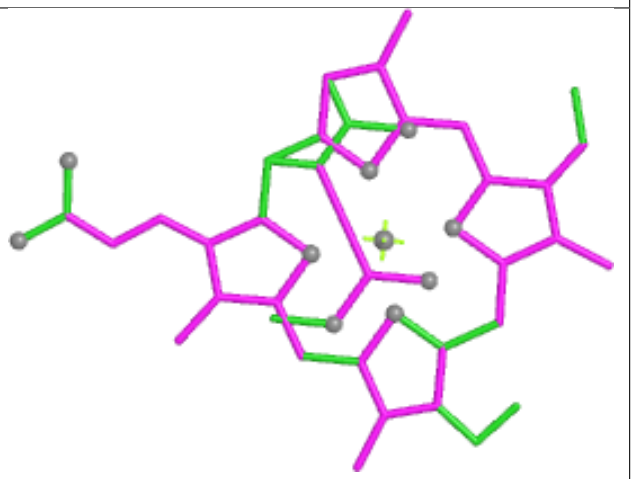


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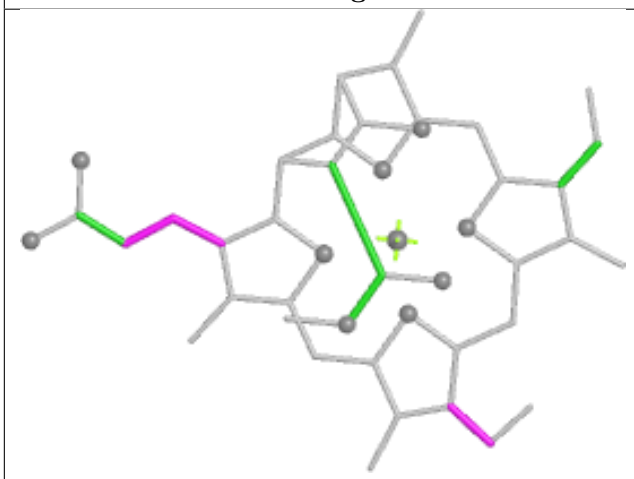
Ligand KC1 31 305



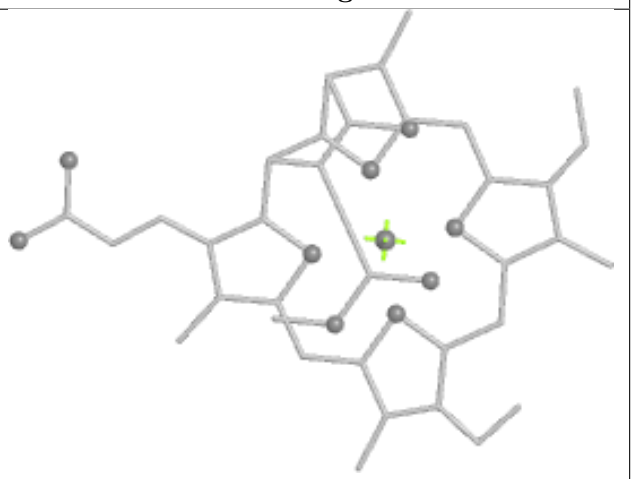
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Bond angles

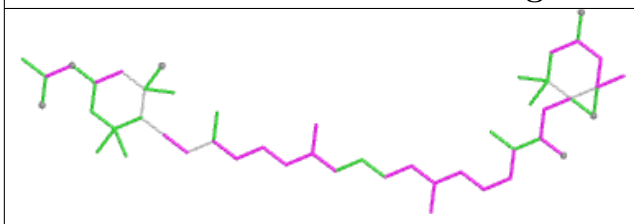


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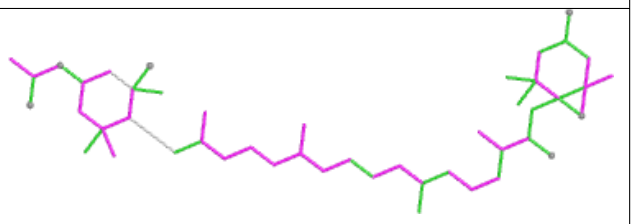


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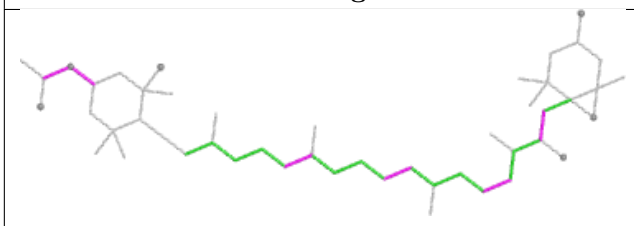
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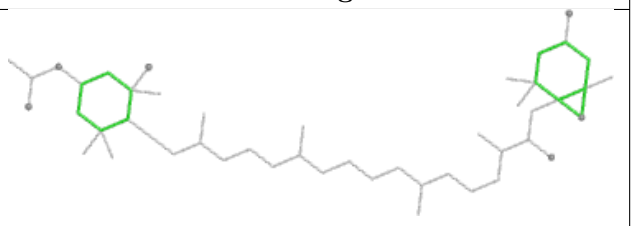
Bond lengths



Bond angles

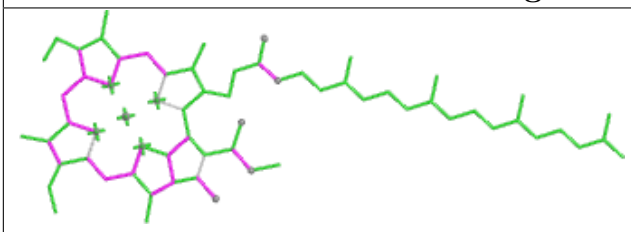


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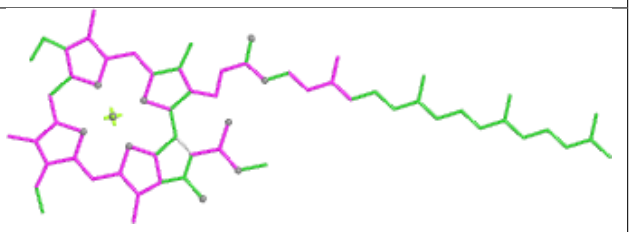


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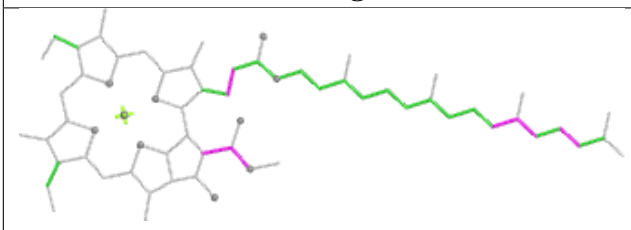
Ligand CLA B 510



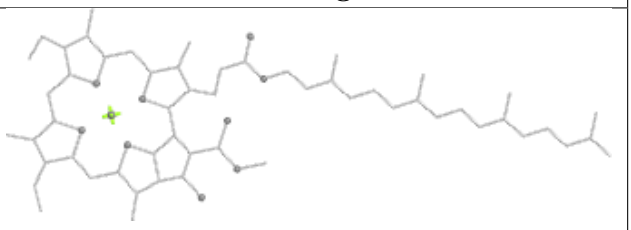
Bond lengths



Bond angles

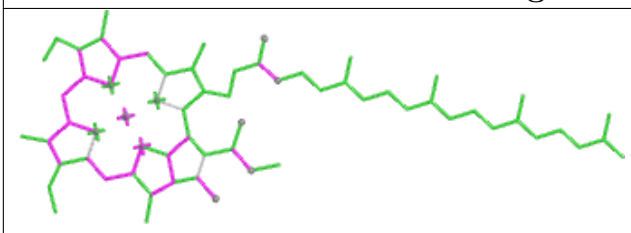


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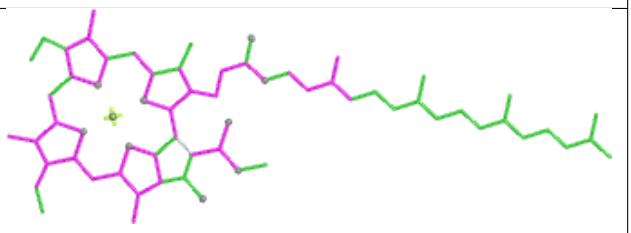


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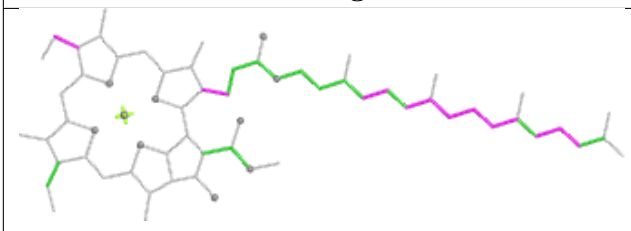
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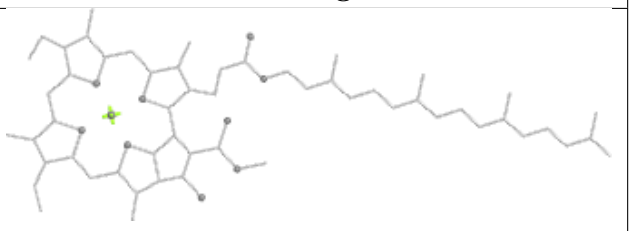
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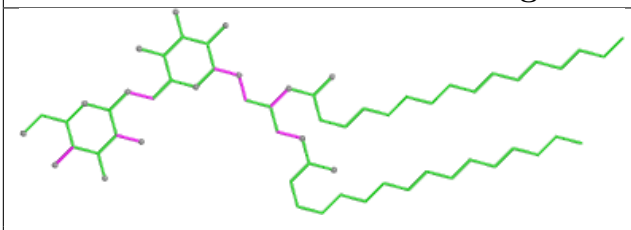


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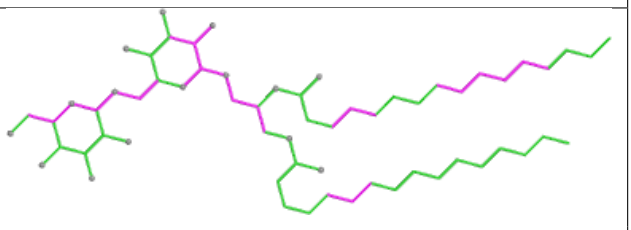


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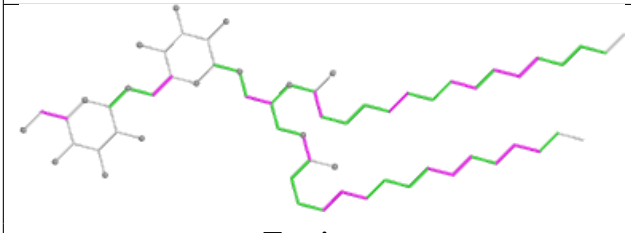
Ligand DGD C 516



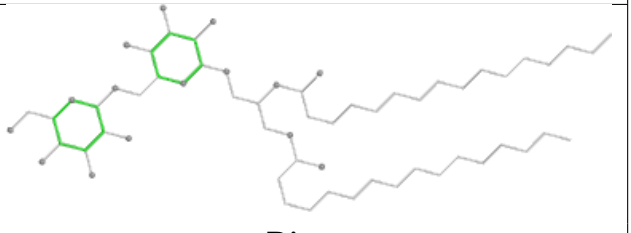
Bond lengths



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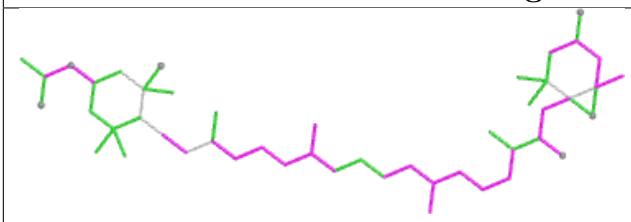


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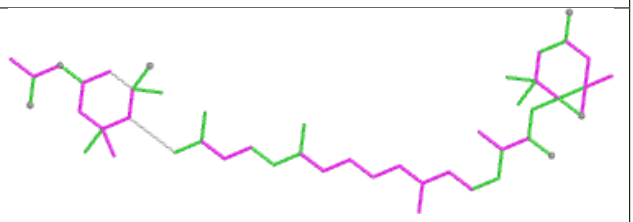


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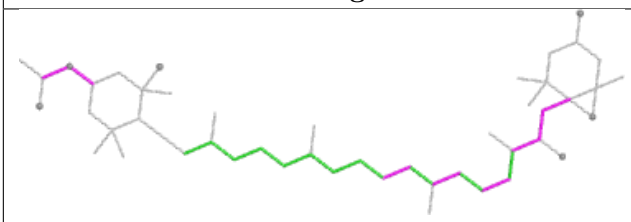
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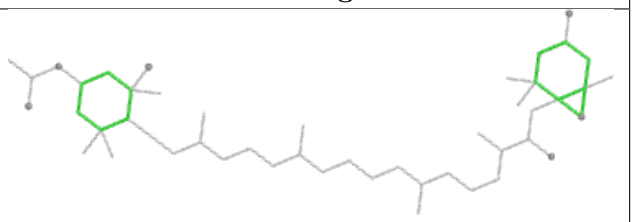
Bond lengths



Bond angles

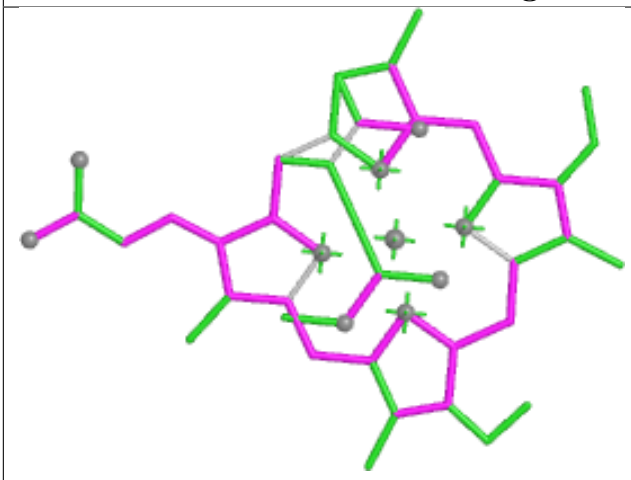


Torsions



Rings

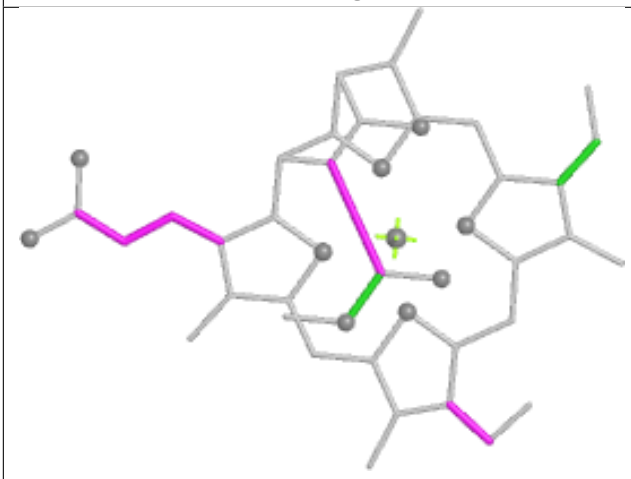
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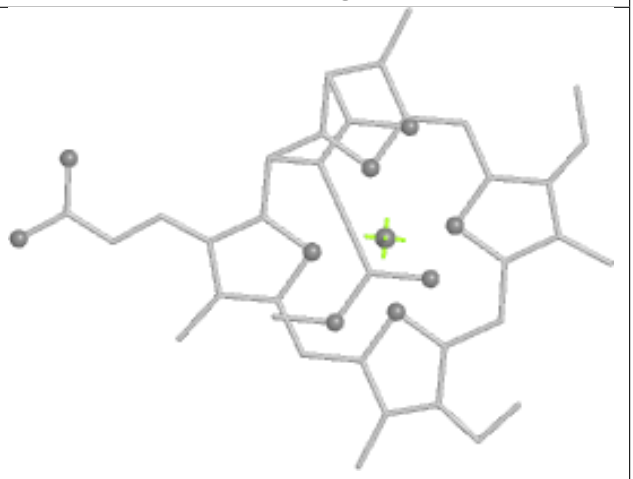
Bond lengths



Bond angles

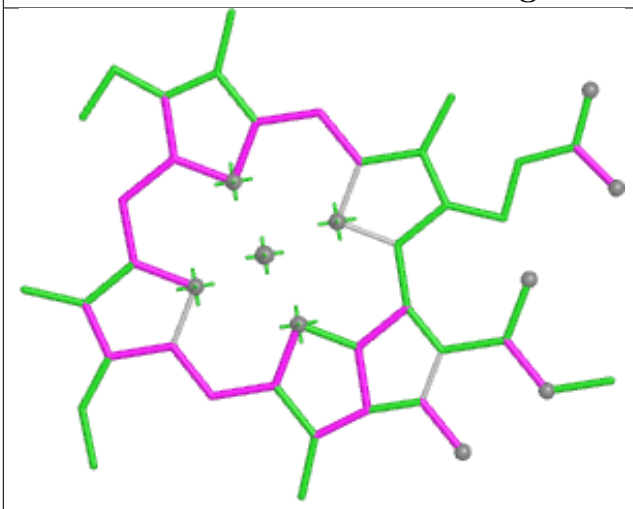


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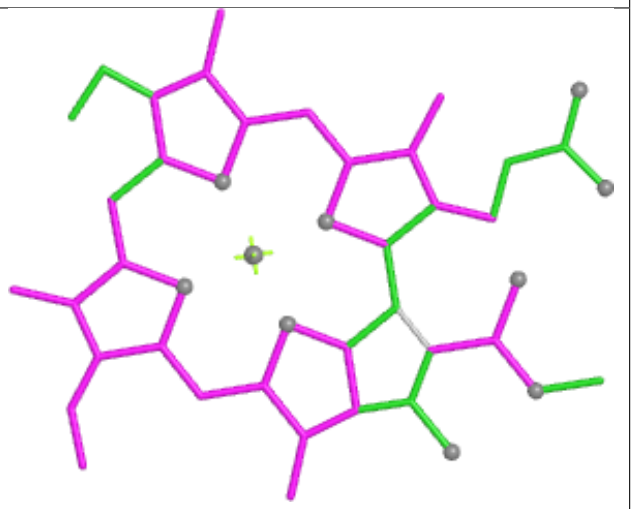


Rings

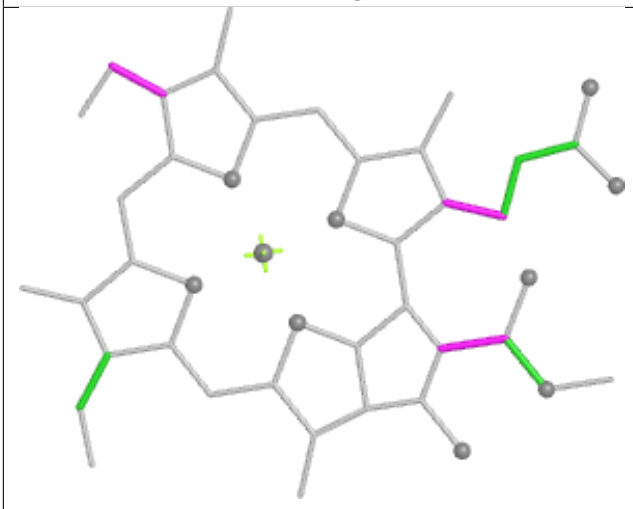
Ligand CLA 31 306



Bond lengths



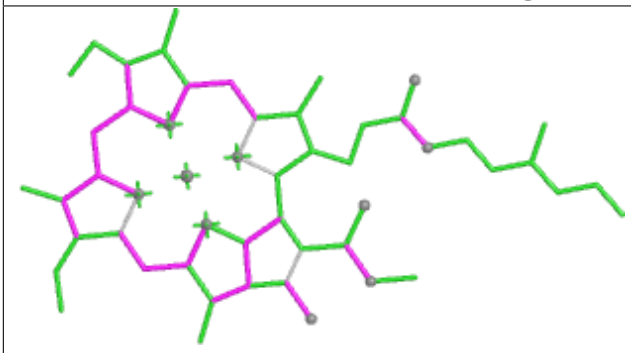
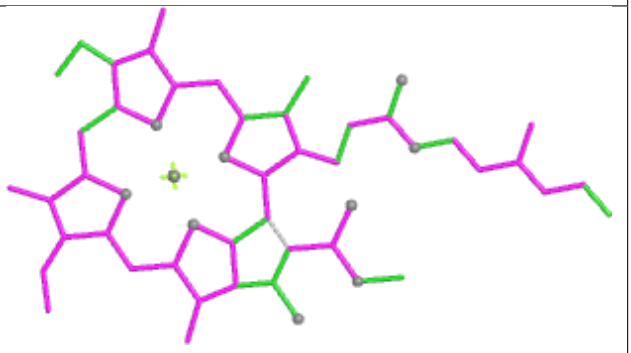
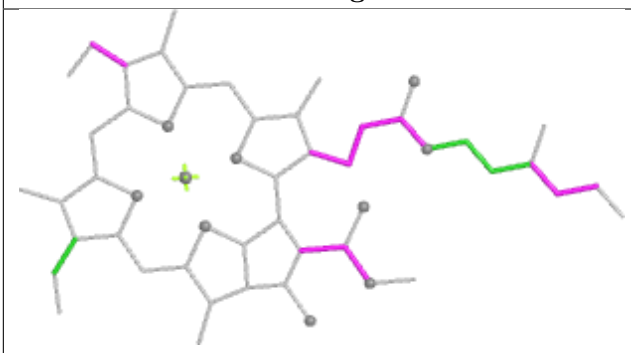
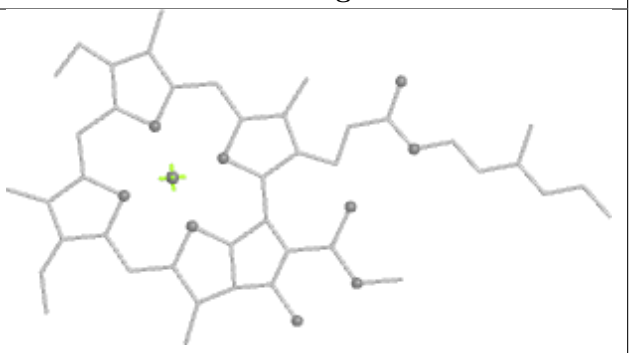
Bond angles

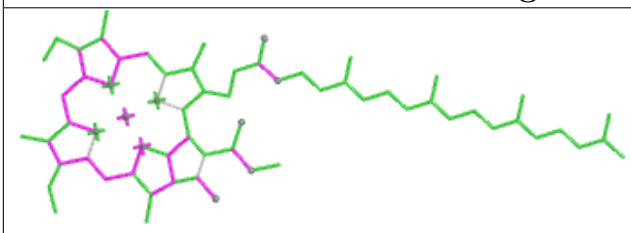
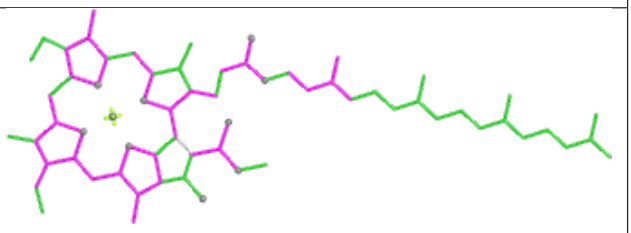
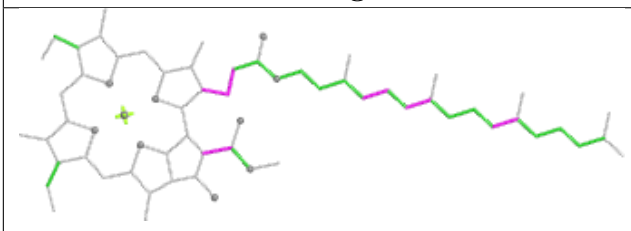
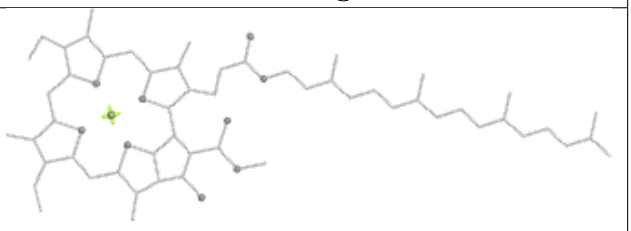


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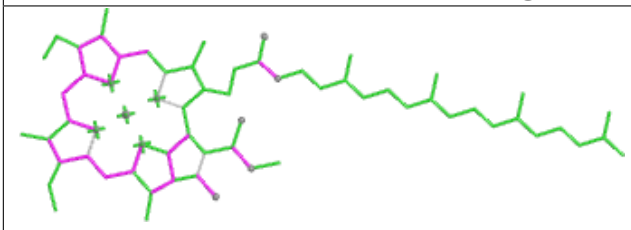


Rings

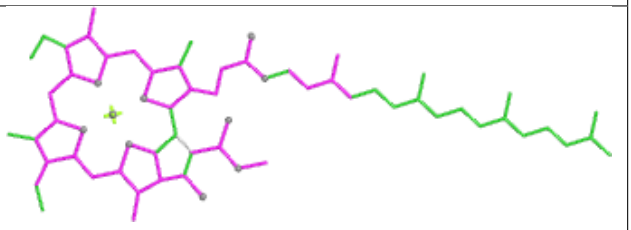
Ligand CLA 12 209	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 32 205	
	
Bond lengths	Bond angles
	
Torsions	Rings

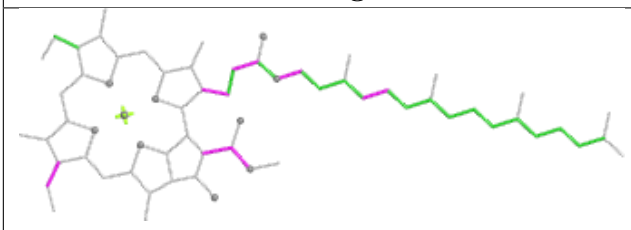
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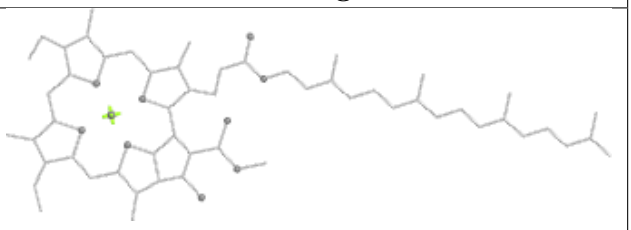
Bond lengths



Bond angles

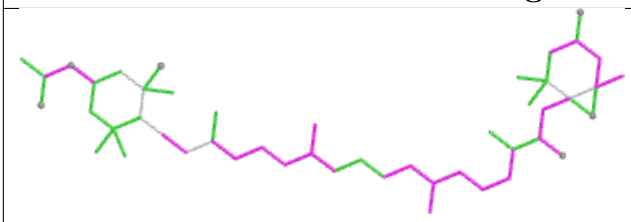


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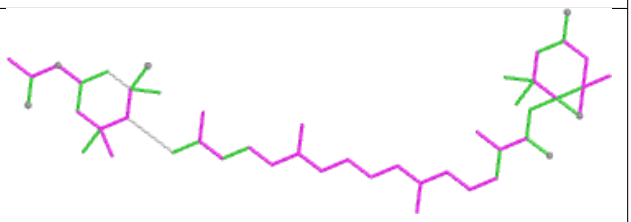


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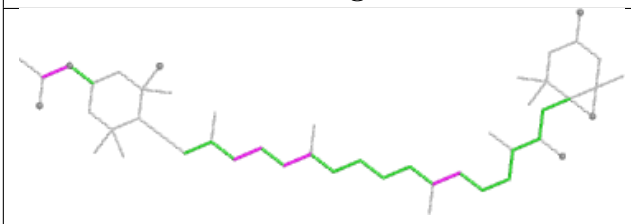
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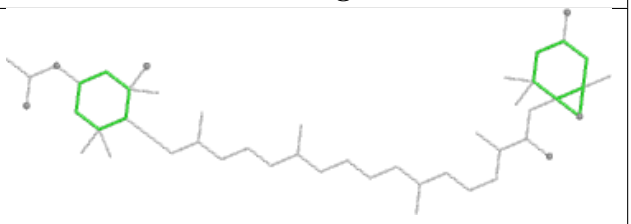
Bond lengths



Bond angles

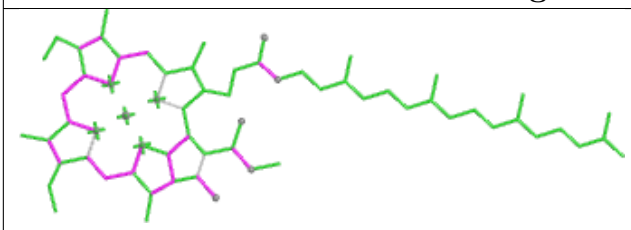


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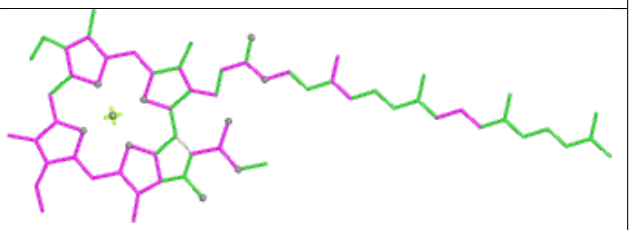


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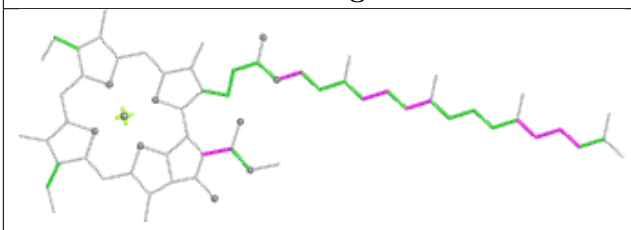
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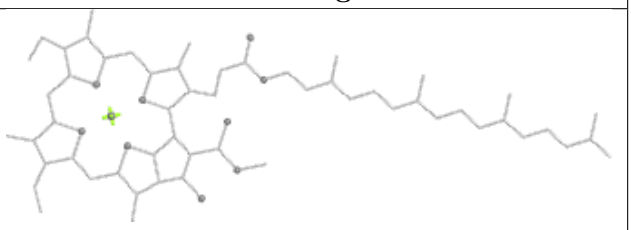
Bond lengths



Bond angles

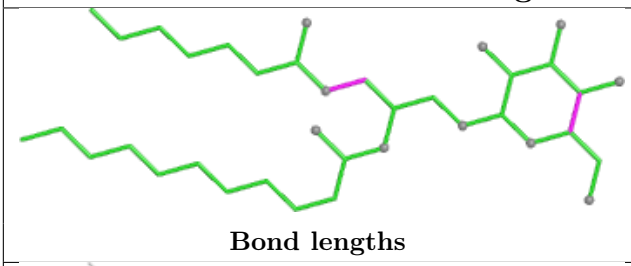


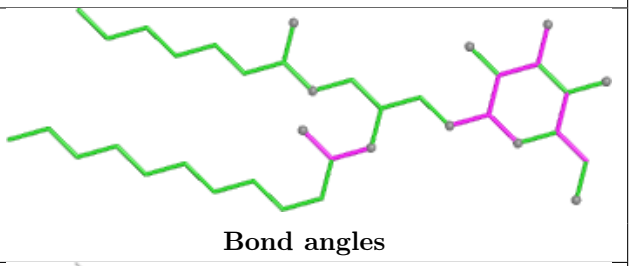
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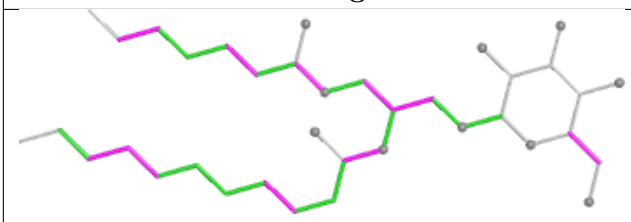


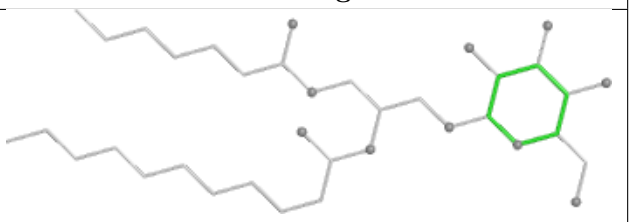
Rings

Ligand LMG 37 316

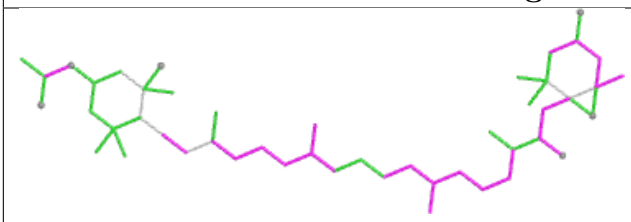

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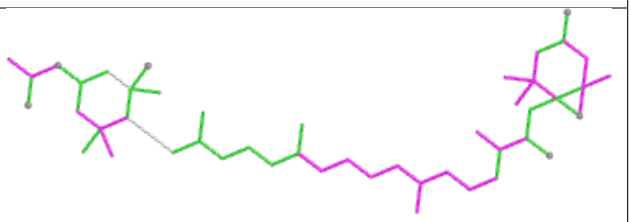

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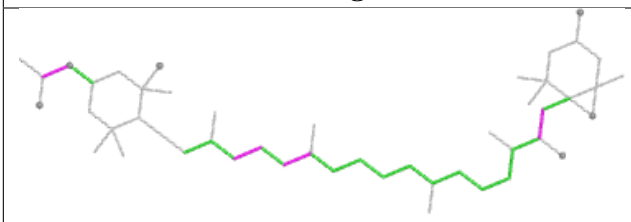

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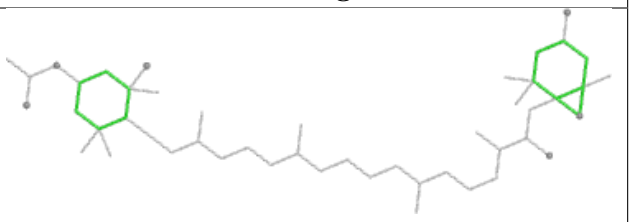

Rings

Ligand A86 35 311

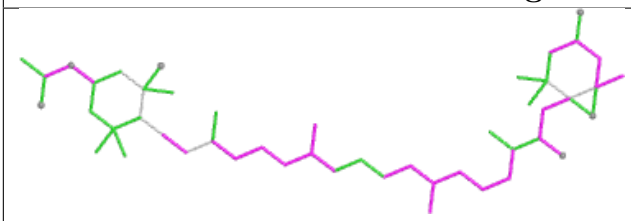

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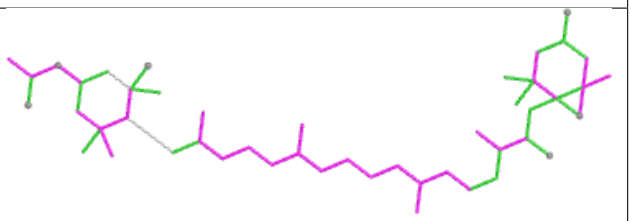

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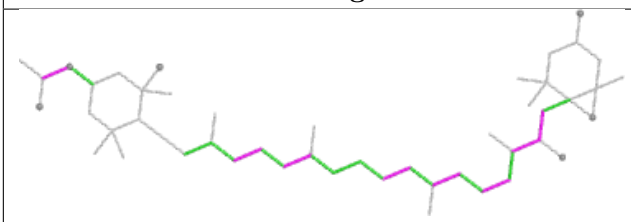

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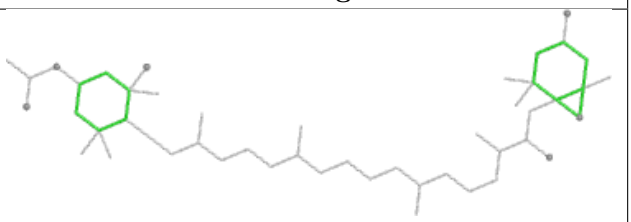

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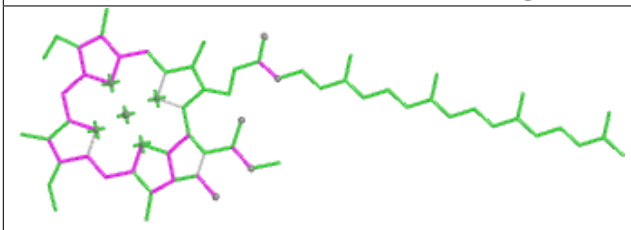

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Bond angles

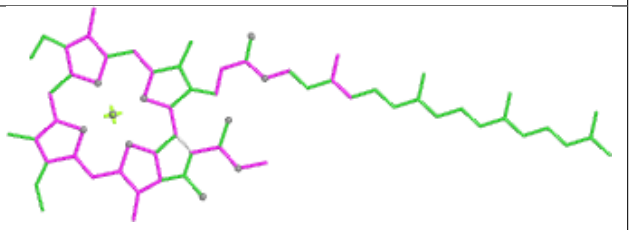

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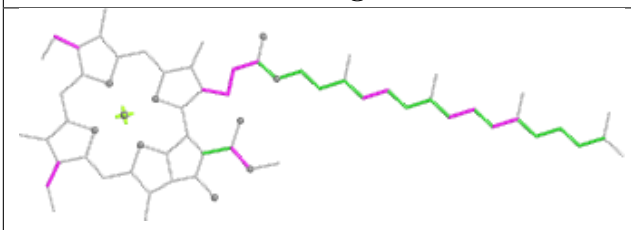
Ligand CLA 37 301



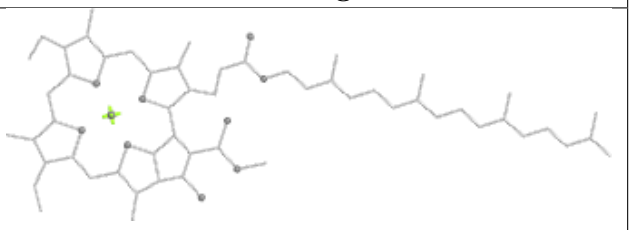
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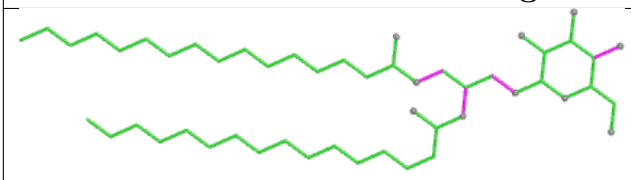


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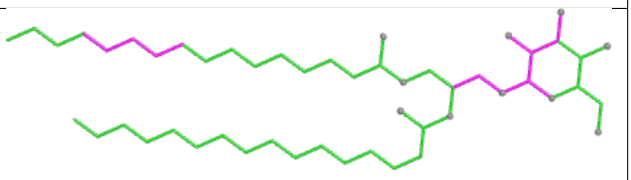


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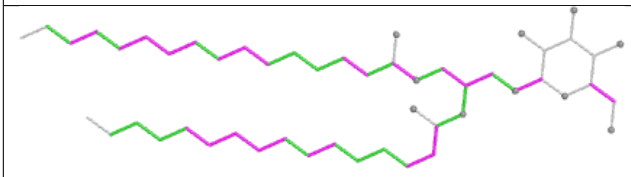
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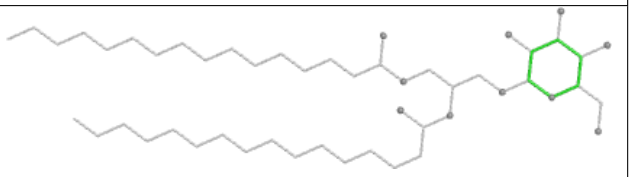
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Bond angles

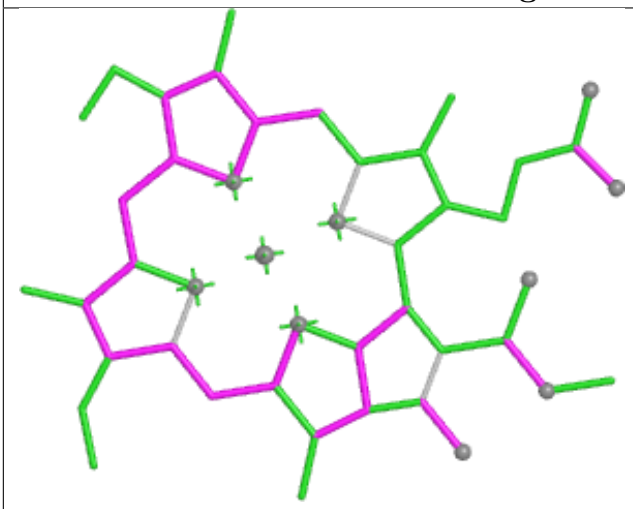


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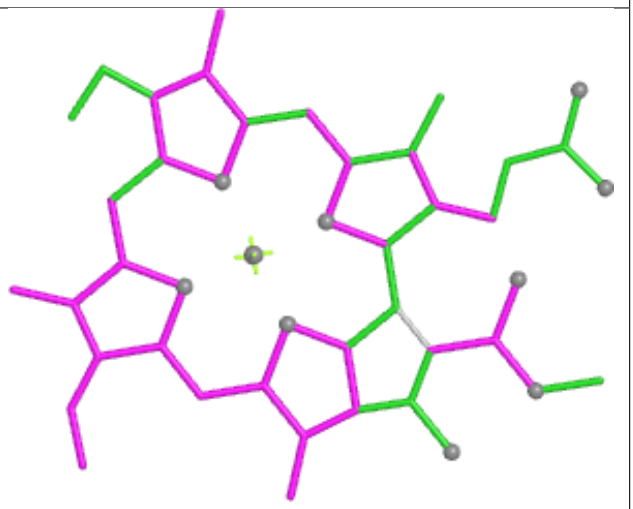


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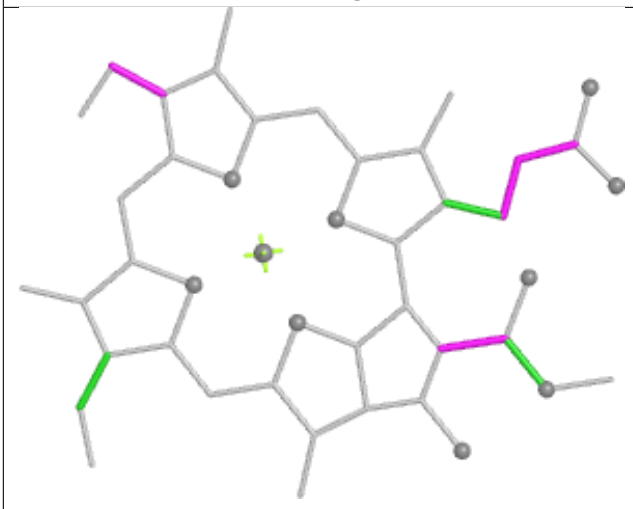
Ligand CLA 15 305



Bond lengths



Bond angles

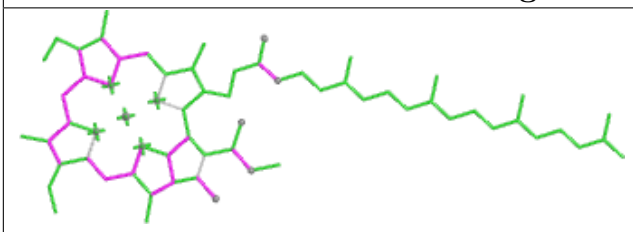


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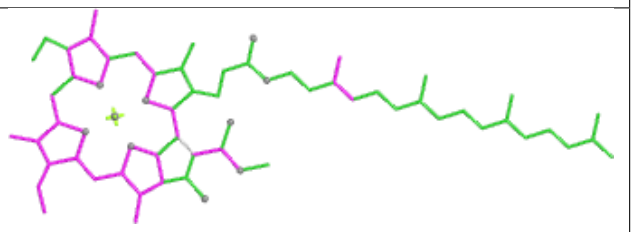


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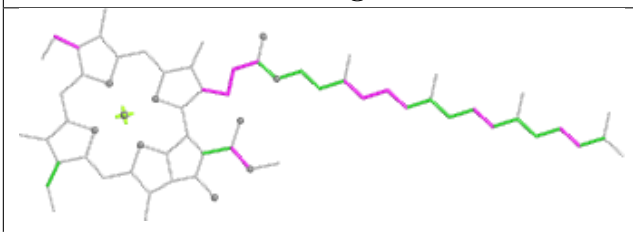
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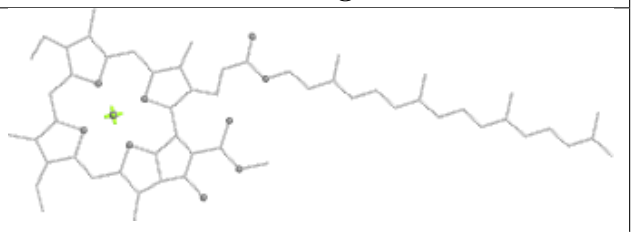
Bond lengths



Bond angles

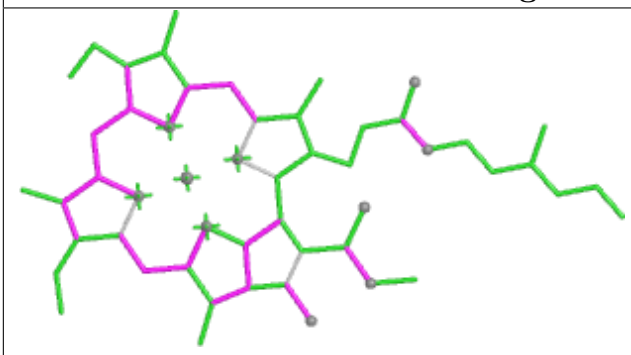


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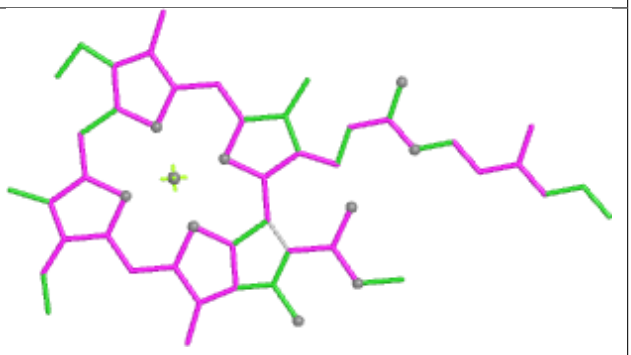


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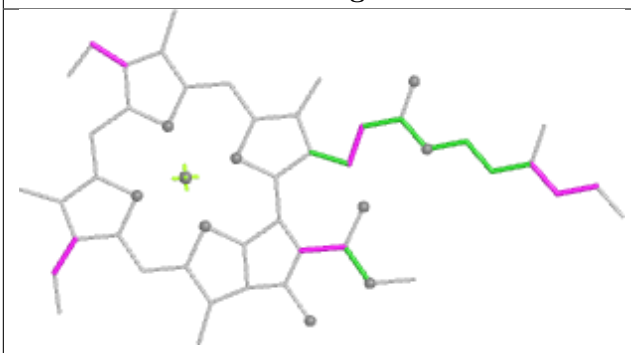
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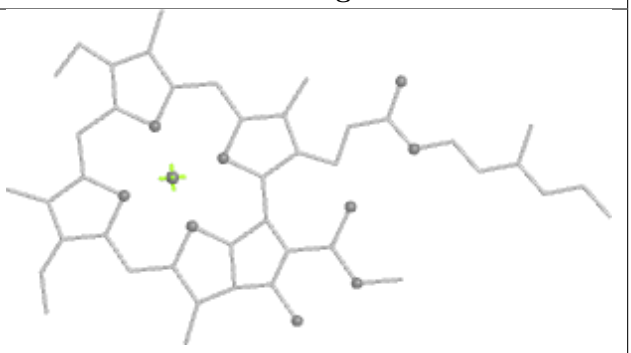
Bond lengths



Bond angles

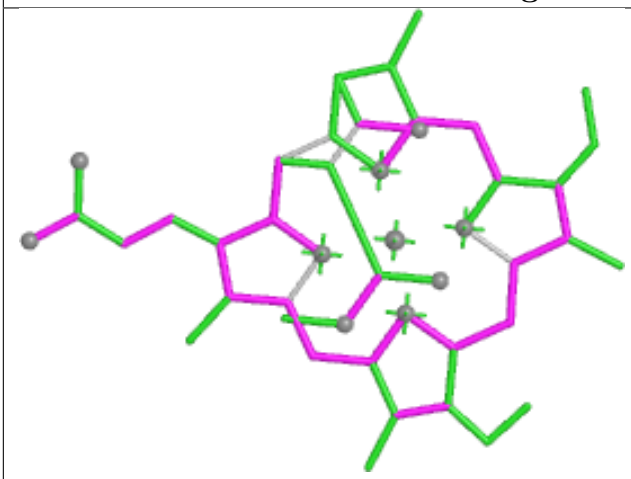


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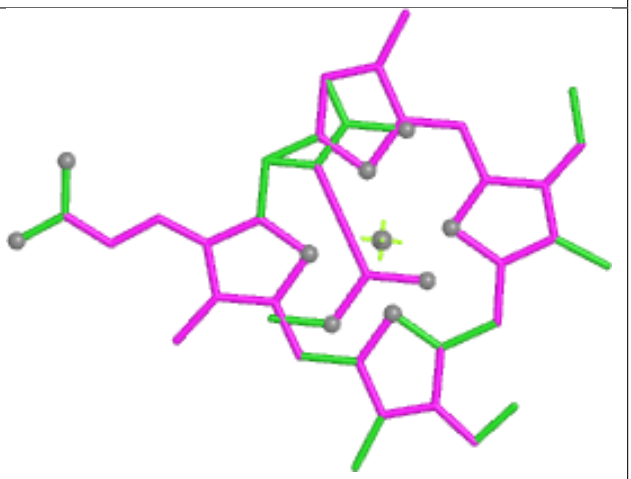


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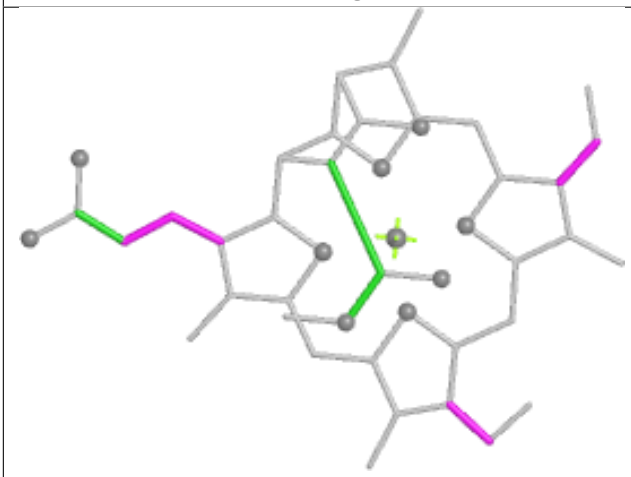
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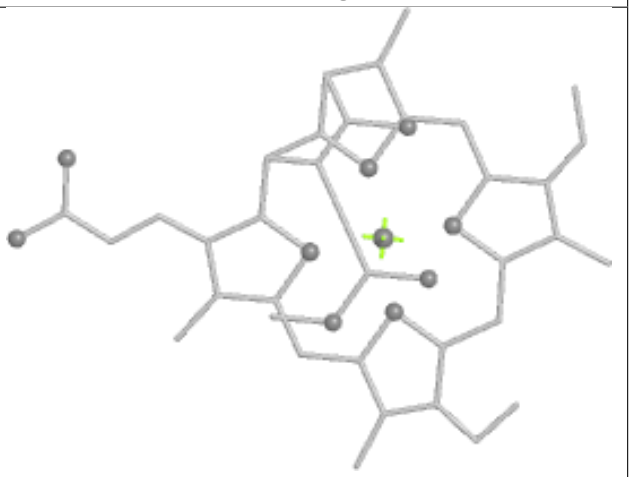
Bond lengths



Bond angles

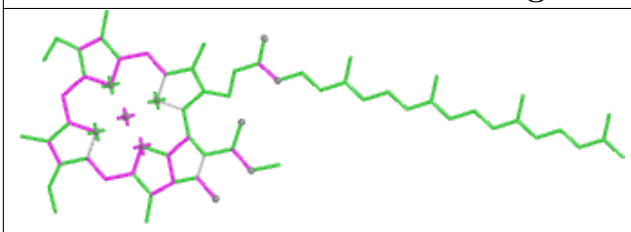


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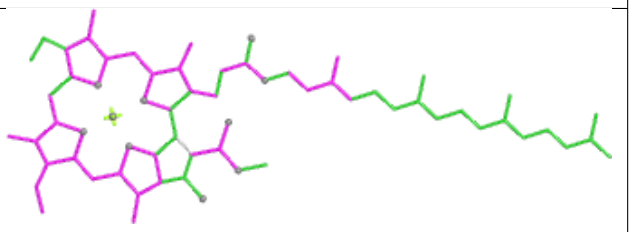


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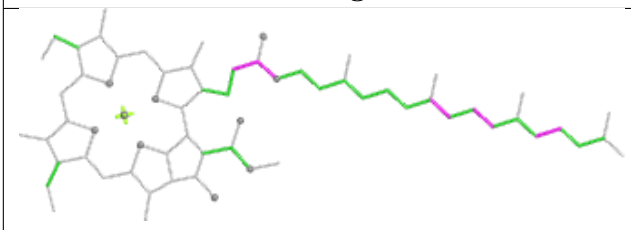
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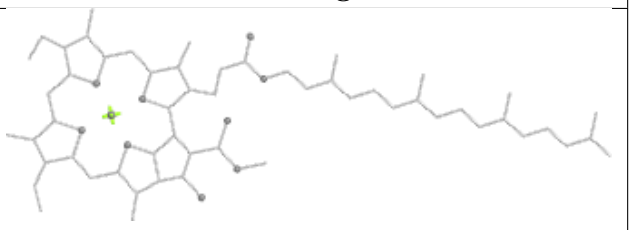
Bond lengths



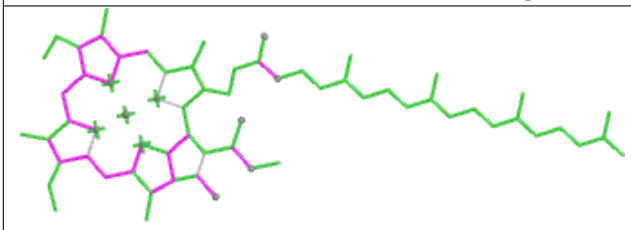
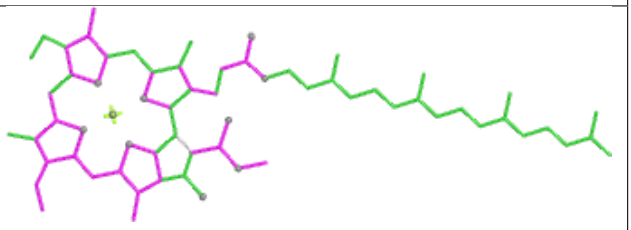
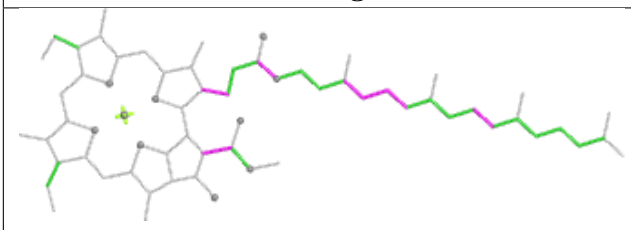
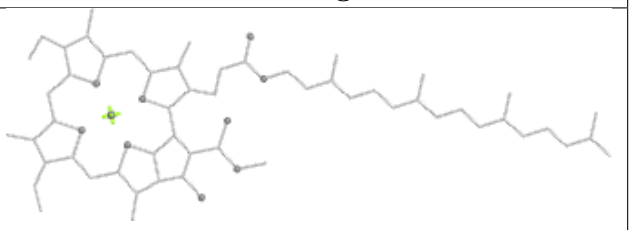
Bond angles

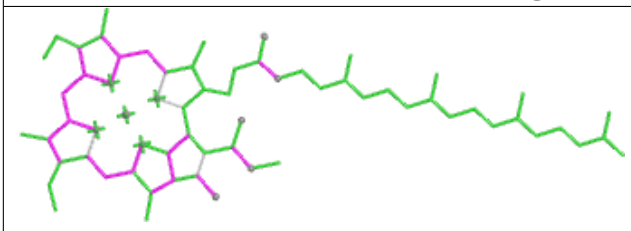
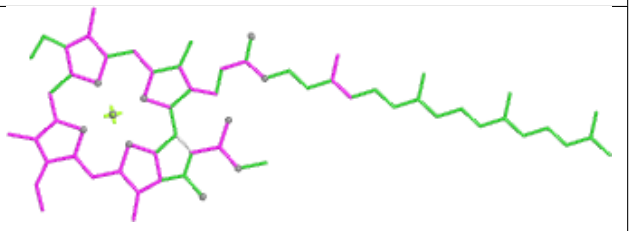
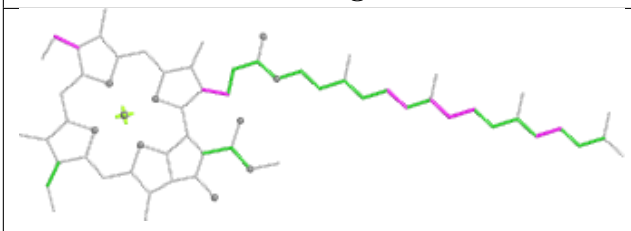
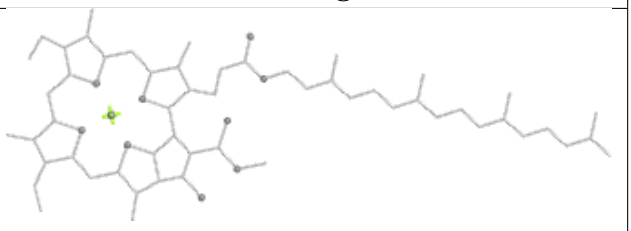


Torsions

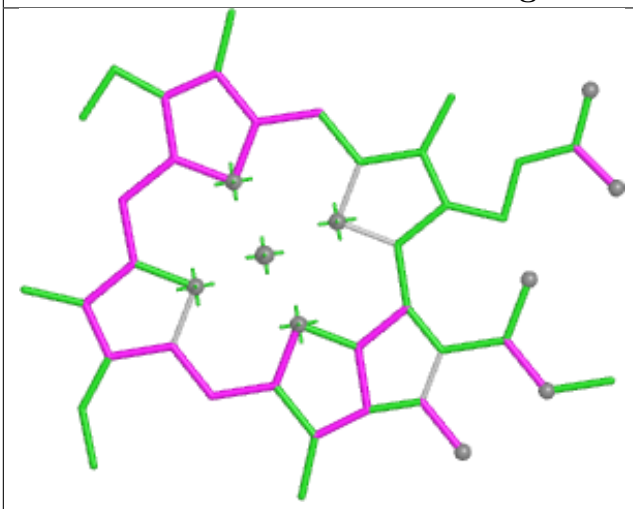


Rings

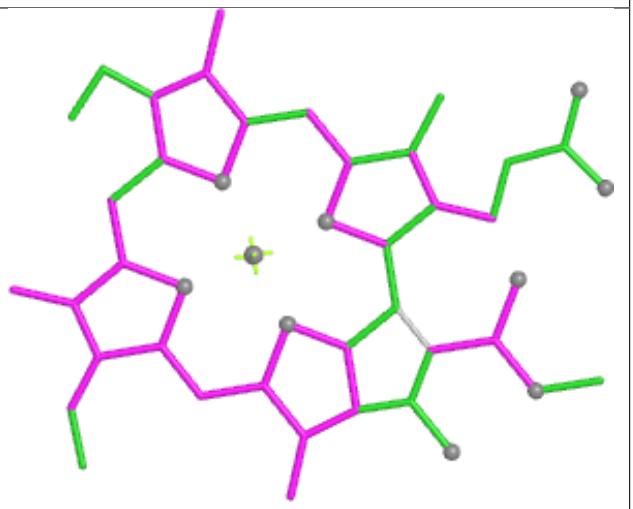
Ligand CLA 33 308	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA a 407	
 Bond lengths	 Bond angles
 Torsions	 Rings

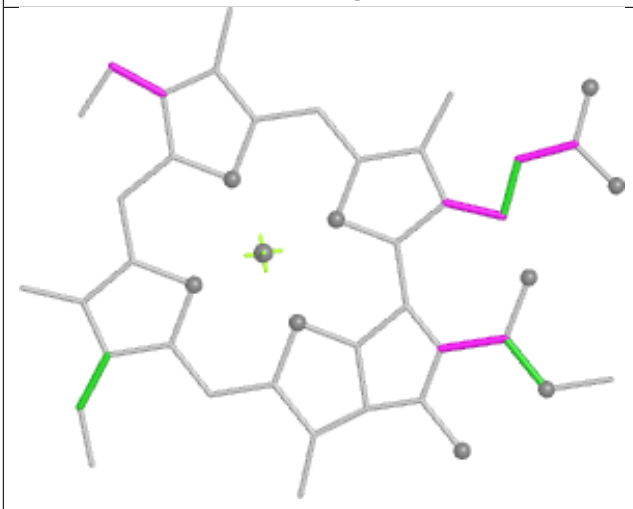
Ligand CLA 19 304



Bond lengths



Bond angles

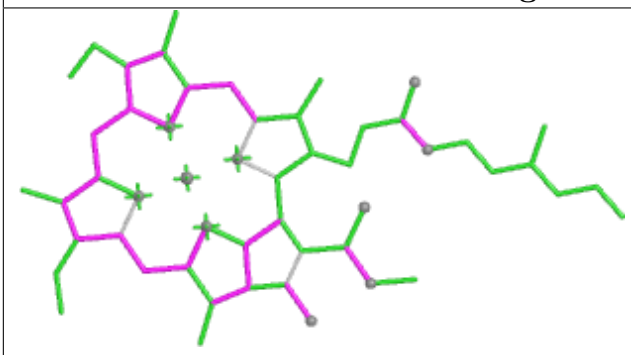


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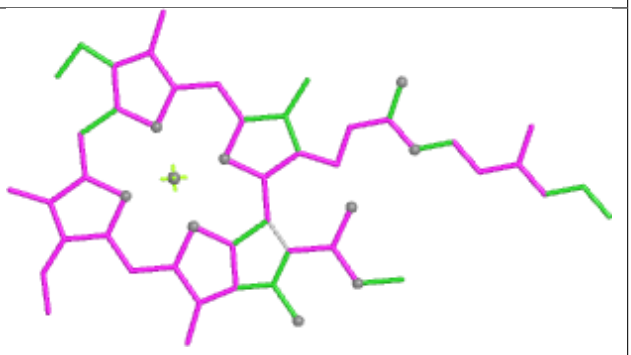


Rings

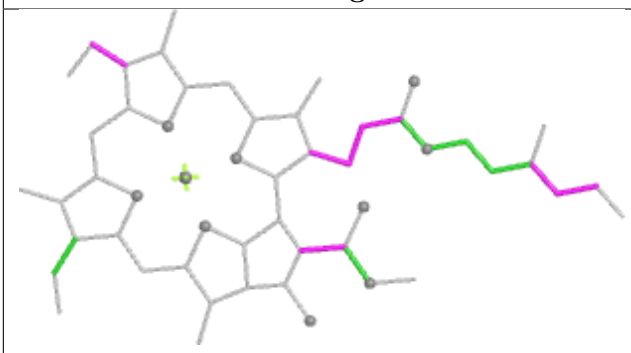
Ligand CLA 37 306



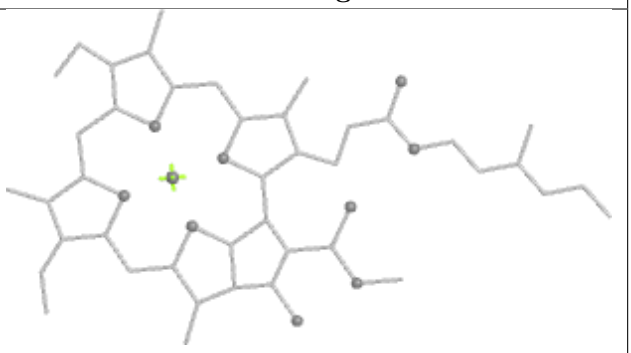
Bond lengths



Bond angles

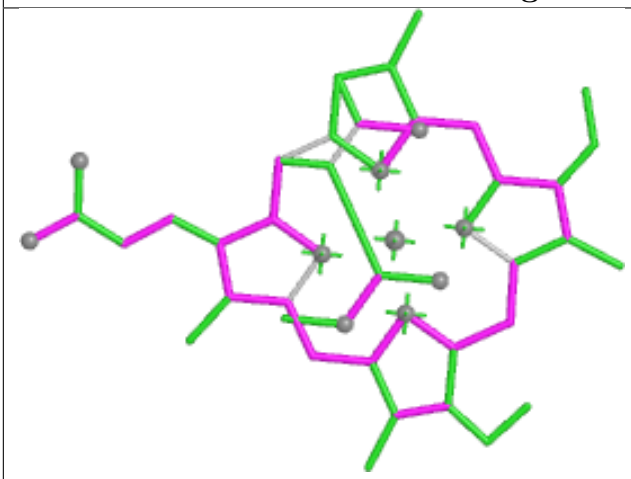


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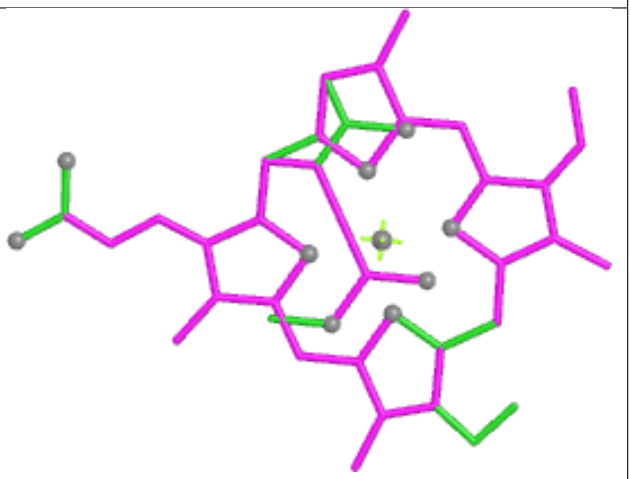


Rings

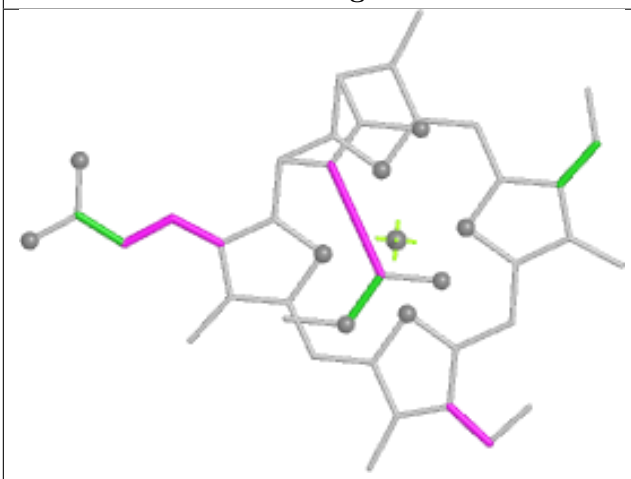
Ligand KC1 34 306



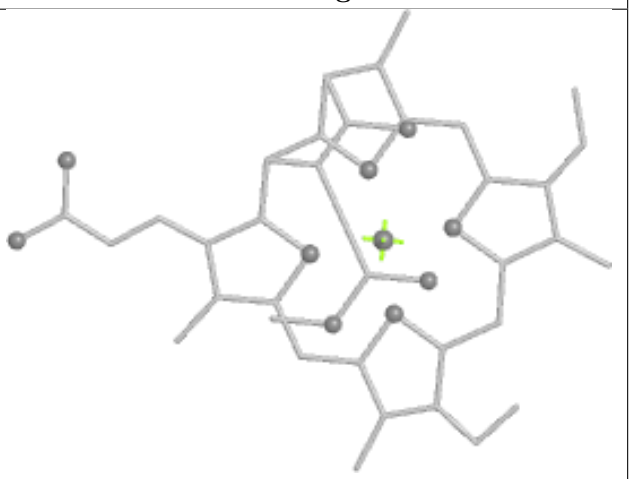
Bond lengths



Bond angles

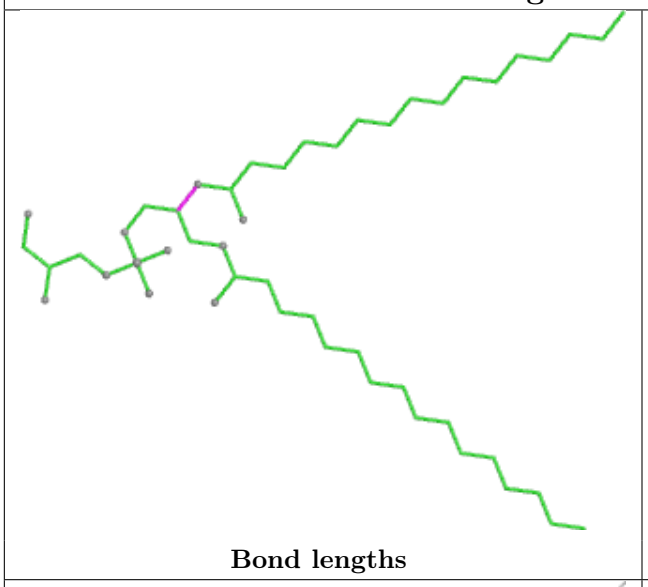


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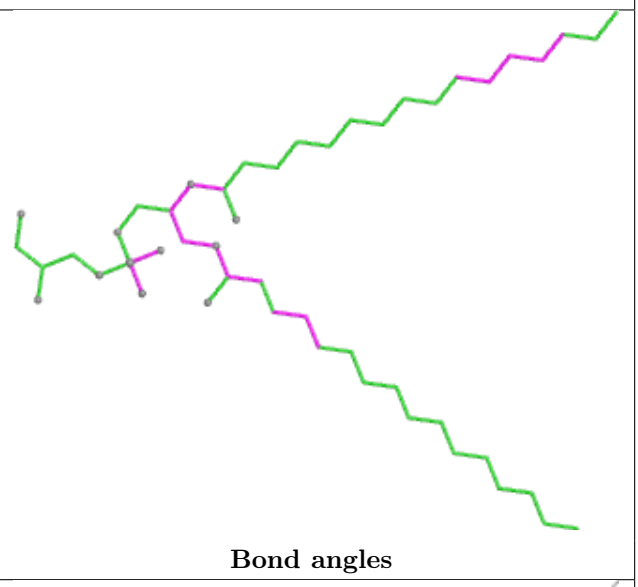


Rings

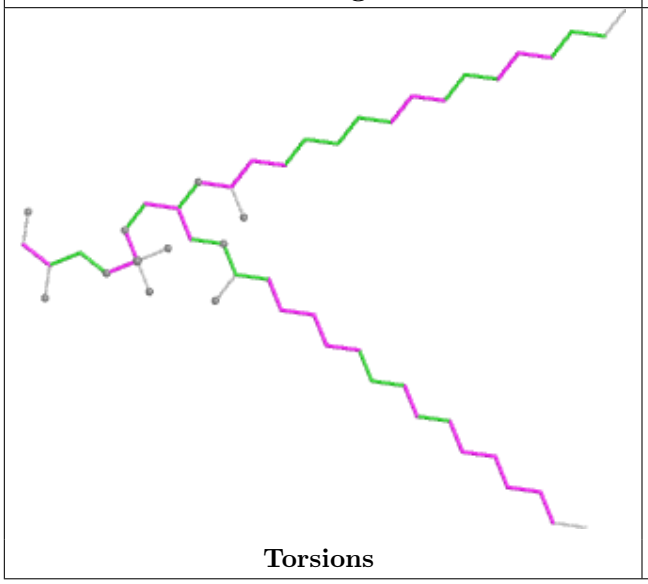
Ligand LHG d 408



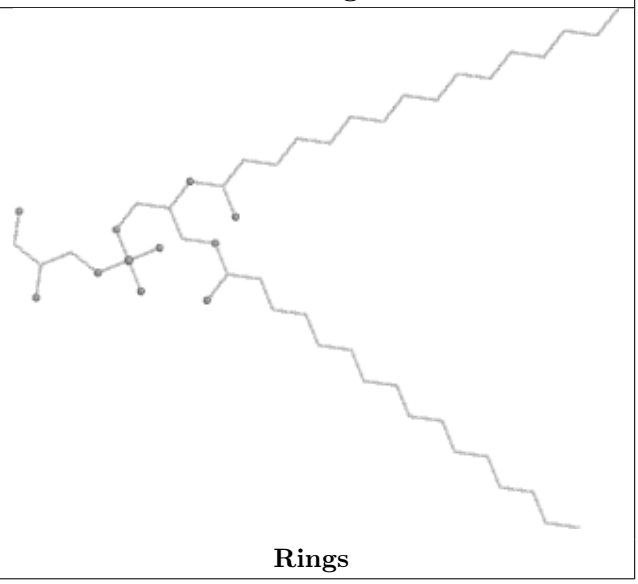
Bond lengths



Bond angles

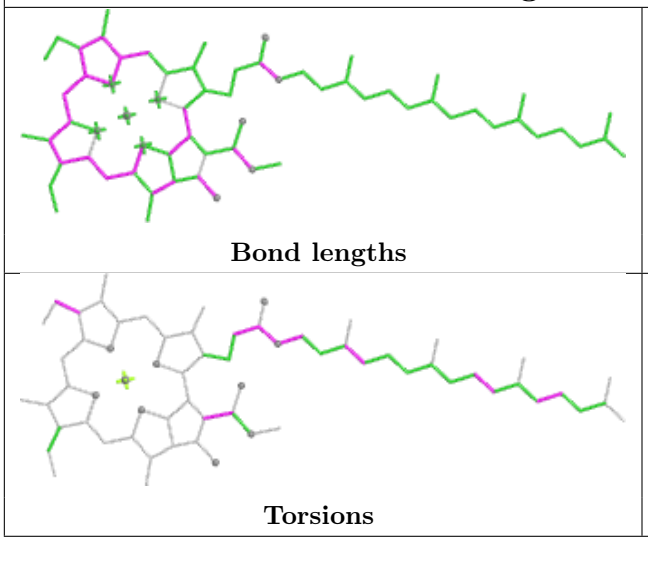


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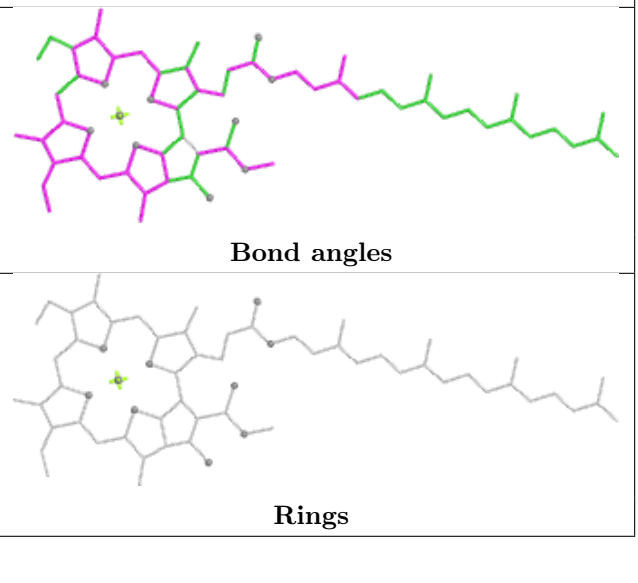


Rings

Ligand CLA 38 209



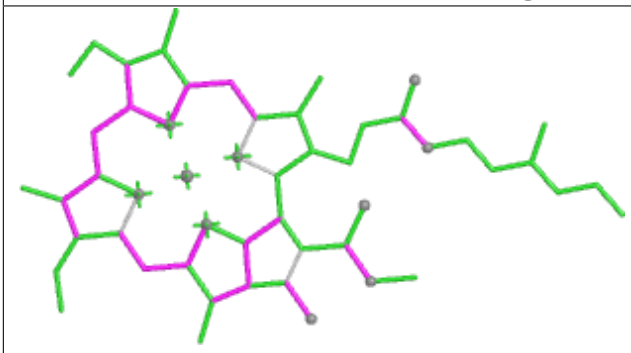
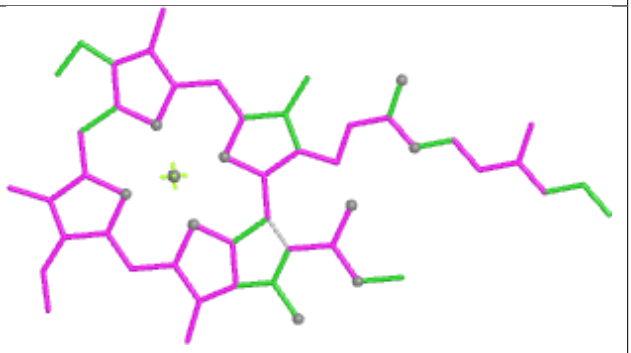
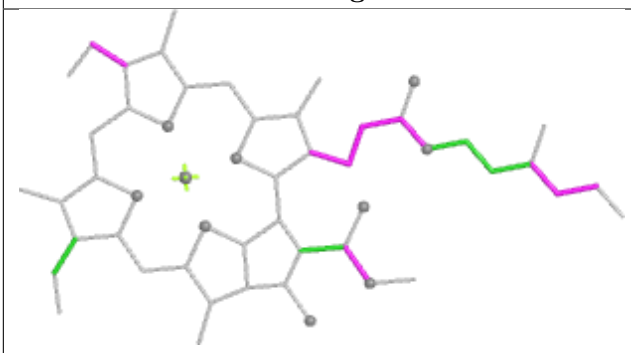
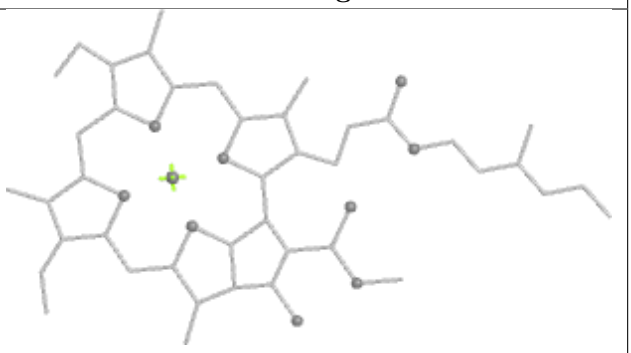
Bond lengths

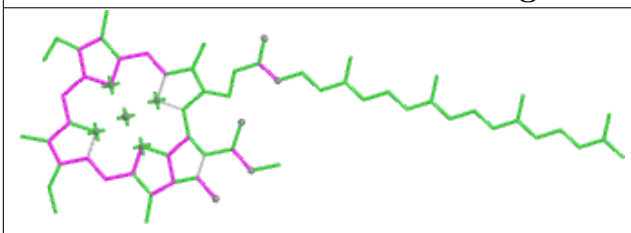
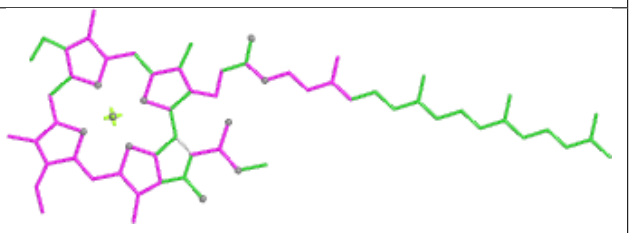
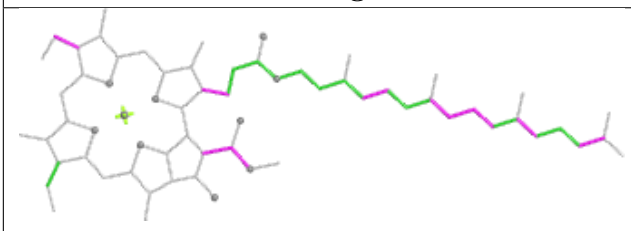
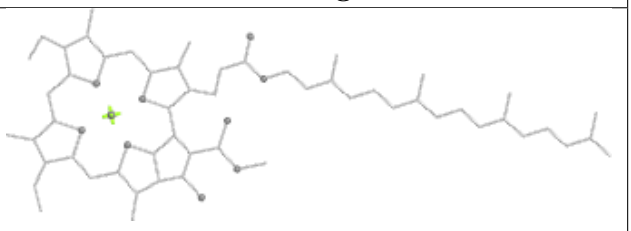


Bond angles

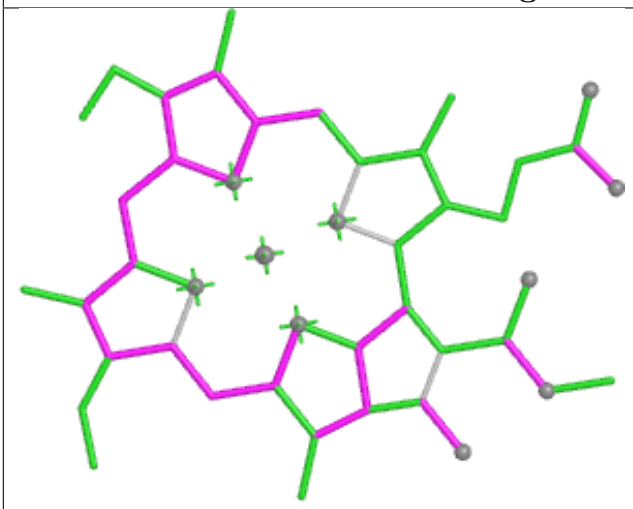
Torsions

Rings

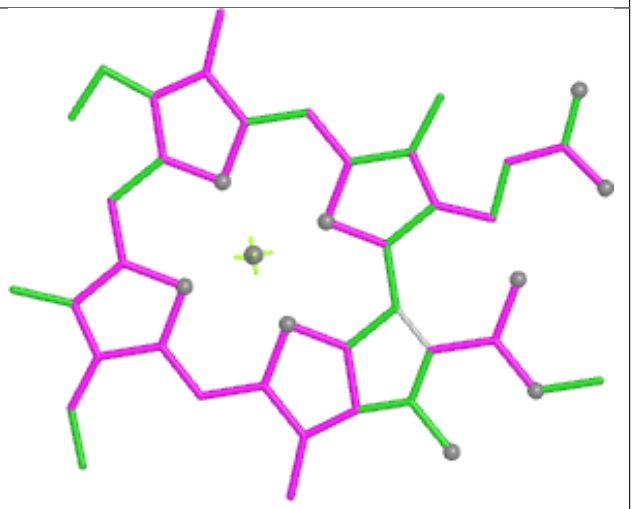
Ligand CLA 14 307	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 36 306	
	
Bond lengths	Bond angles
	
Torsions	Rings

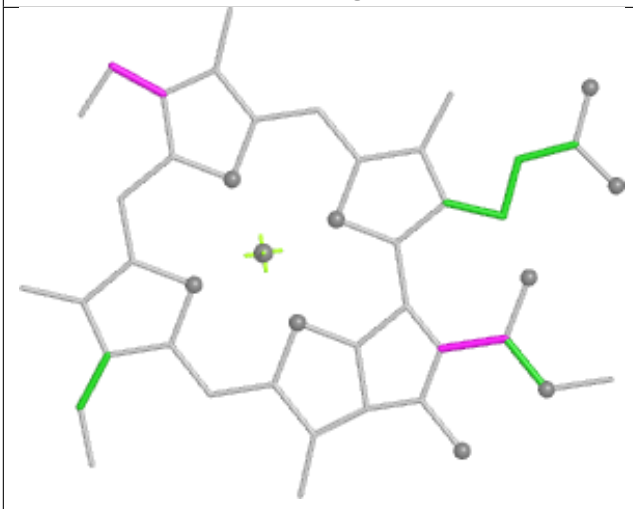
Ligand CLA 15 310



Bond lengths



Bond angles

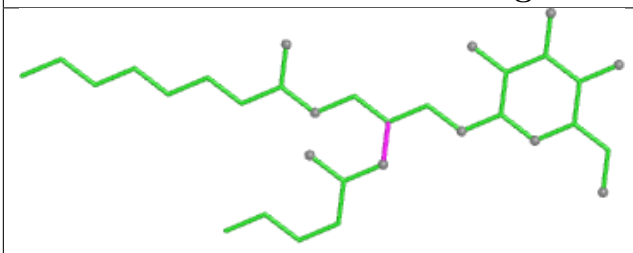


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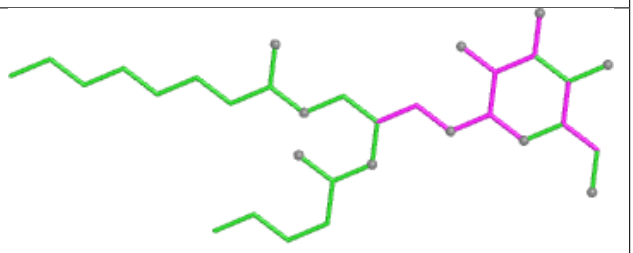


Rings

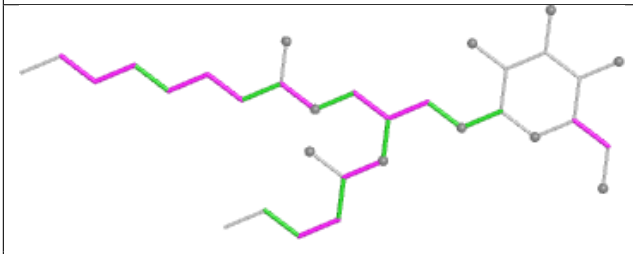
Ligand LMG 11 317



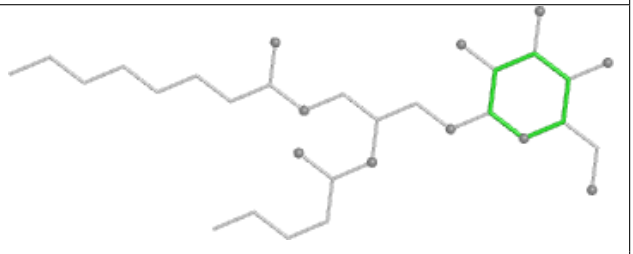
Bond lengths



Bond angles

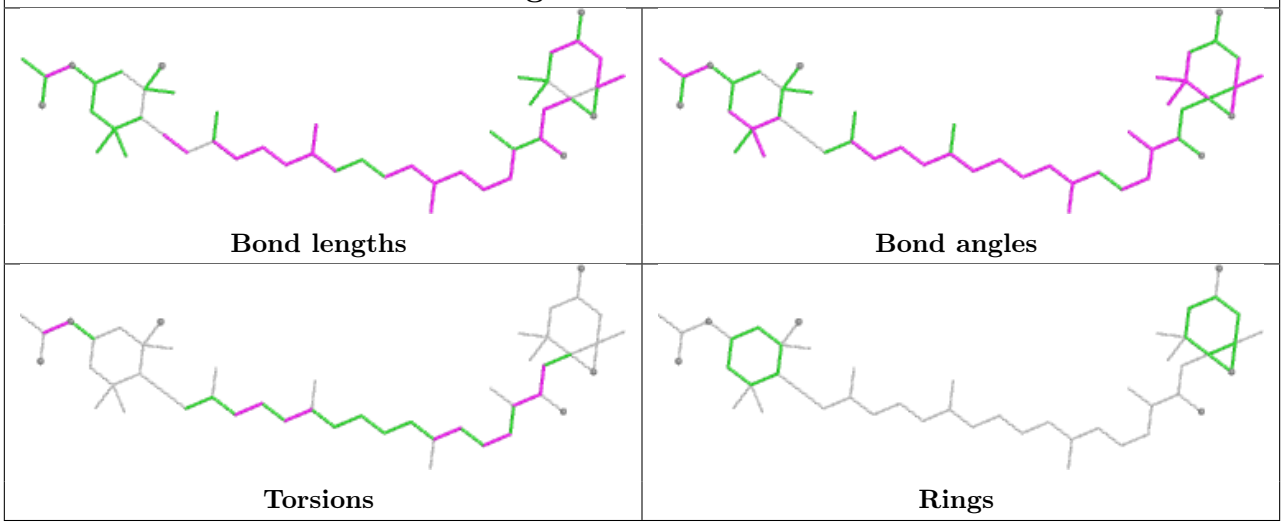


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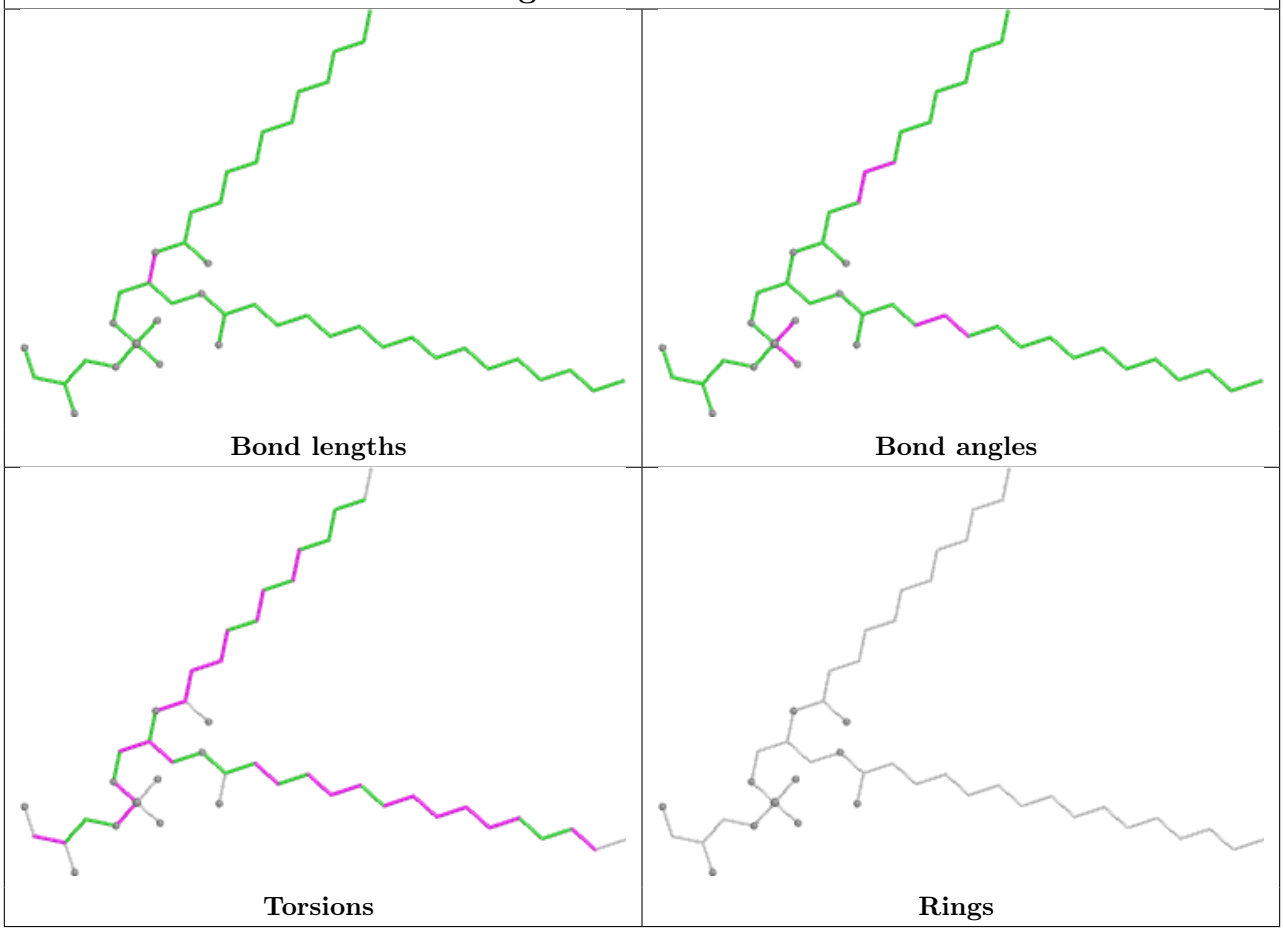


Rings

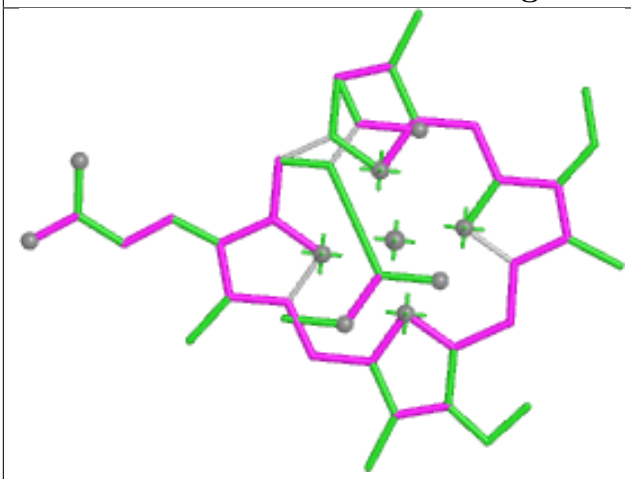
Ligand A86 17 310



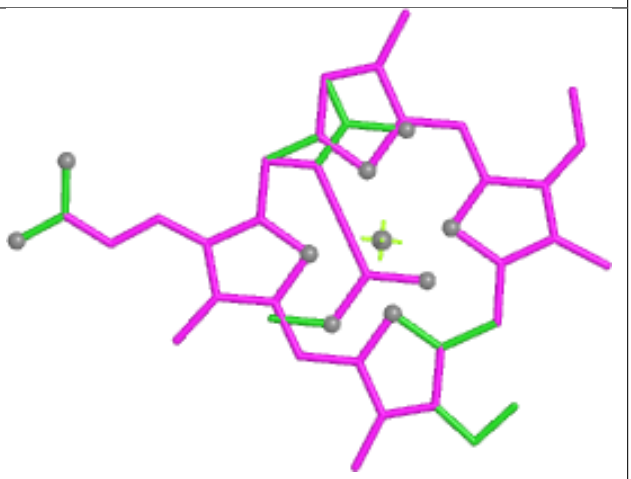
Ligand LHG 21 217



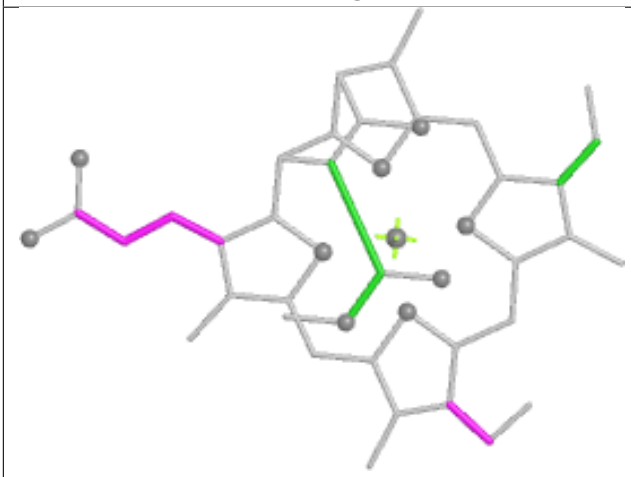
Ligand KC1 15 309



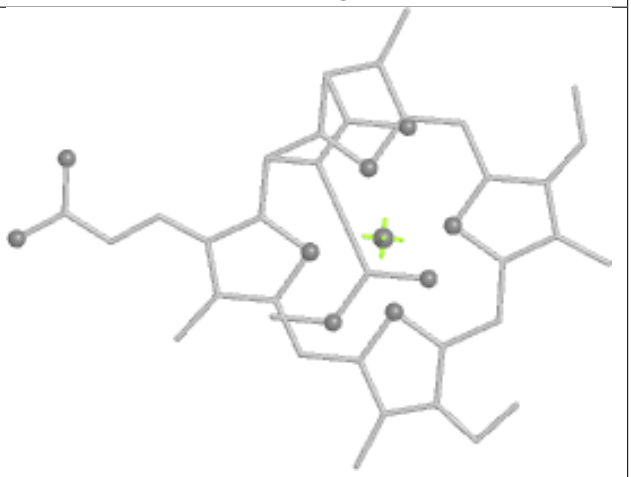
Bond lengths



Bond angles

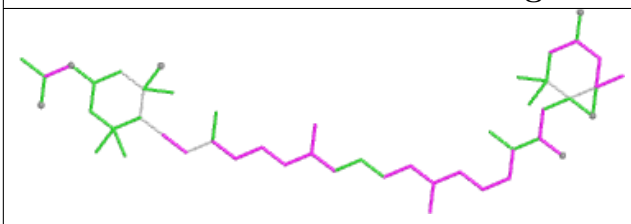


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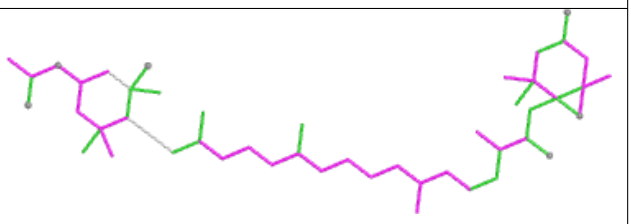


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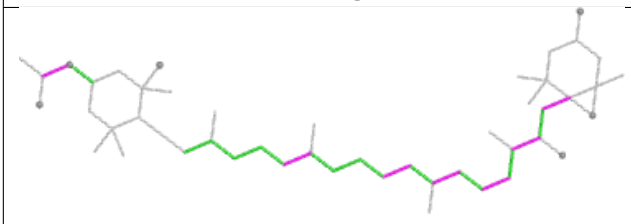
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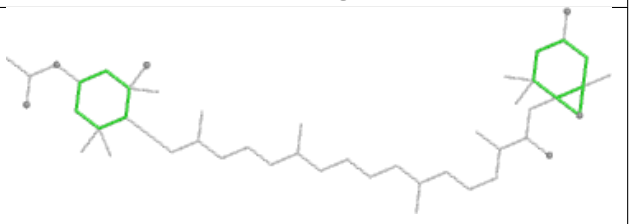
Bond lengths



Bond angles

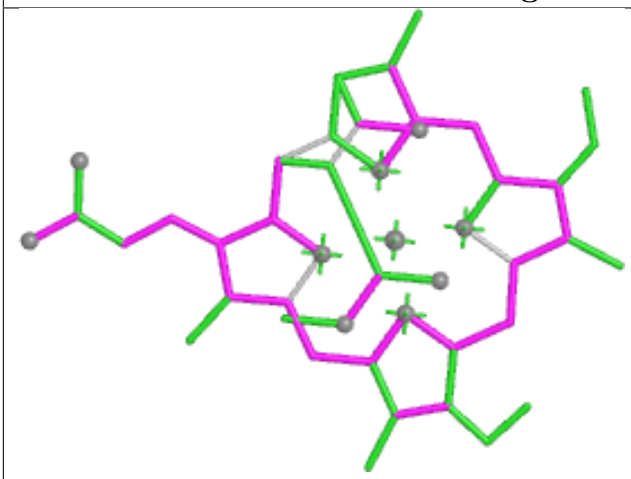


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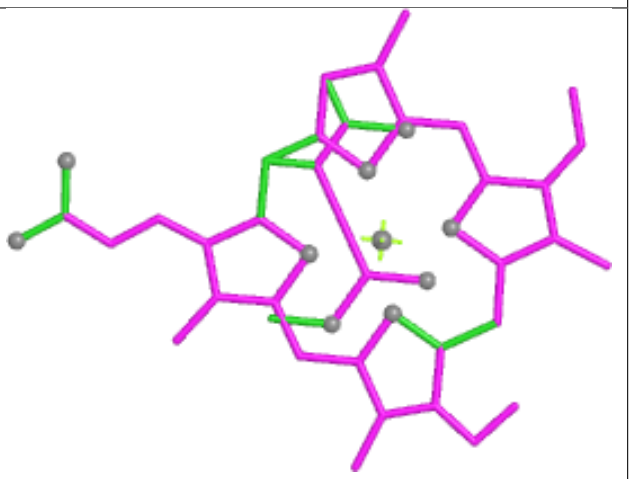


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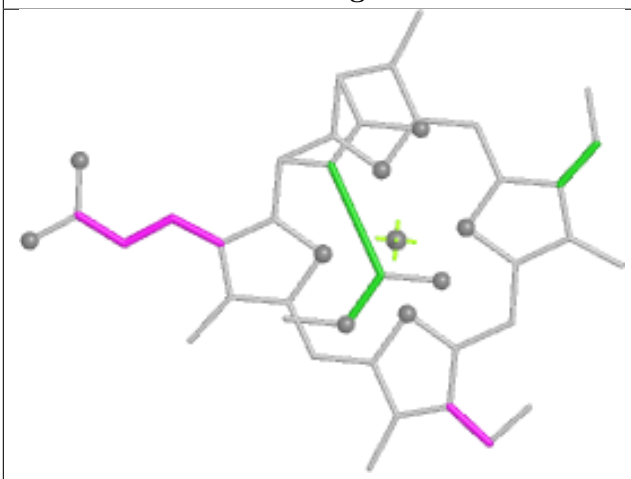
Ligand KC1 15 302



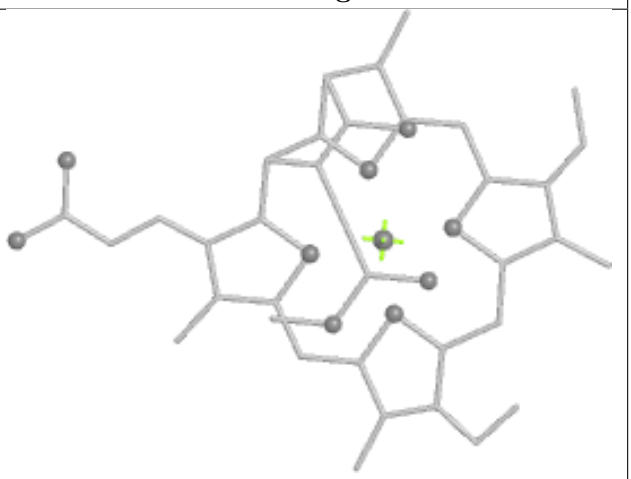
Bond lengths



Bond angles

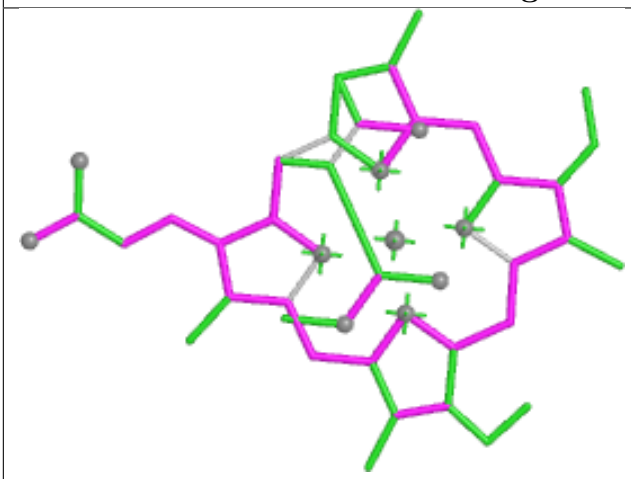


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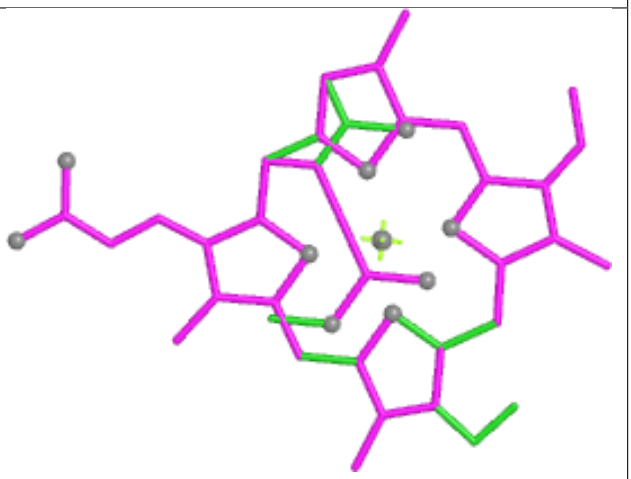


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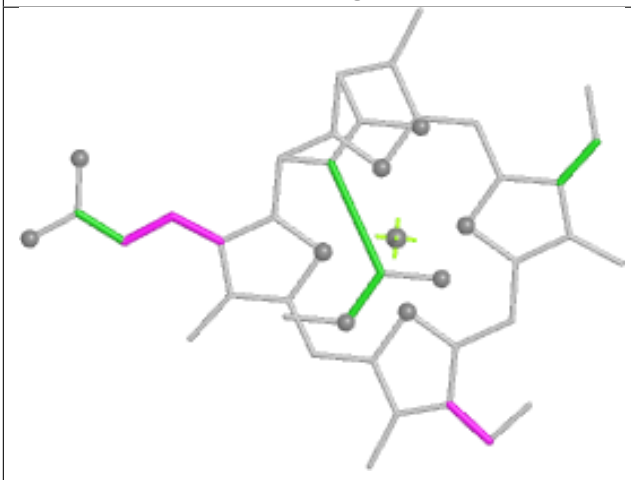
Ligand KC1 16 308



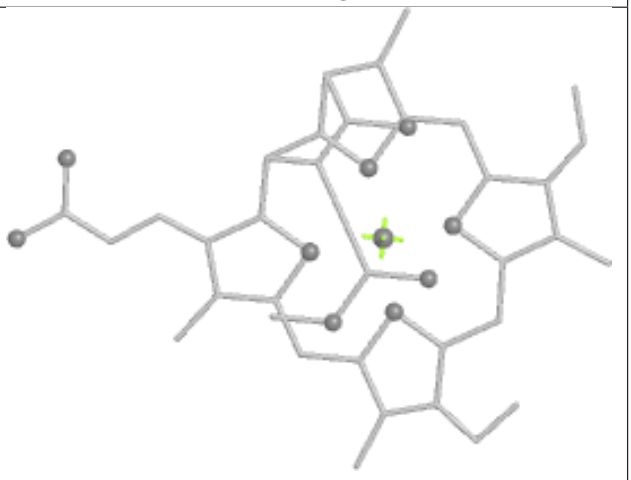
Bond lengths



Bond angles

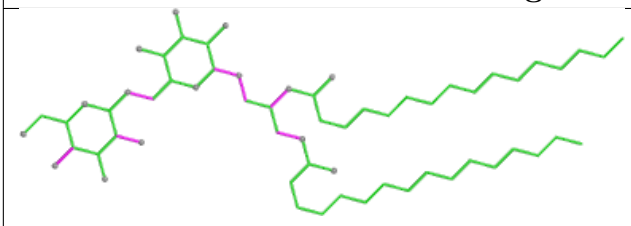


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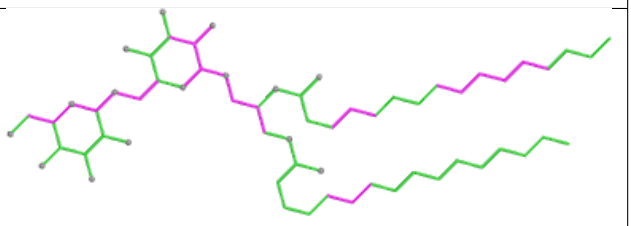


Rings

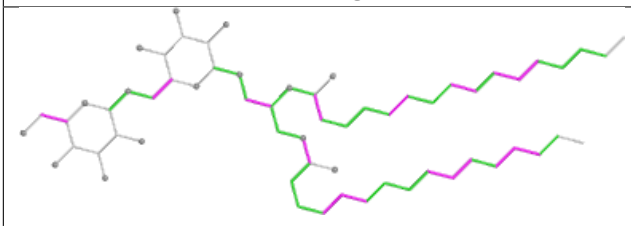
Ligand DGD c 516



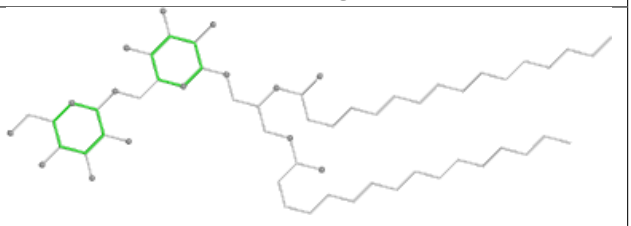
Bond lengths



Bond angles

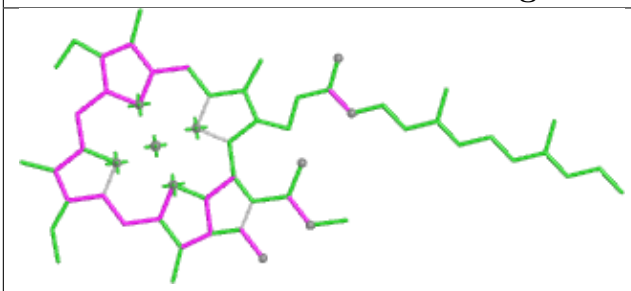


Torsions

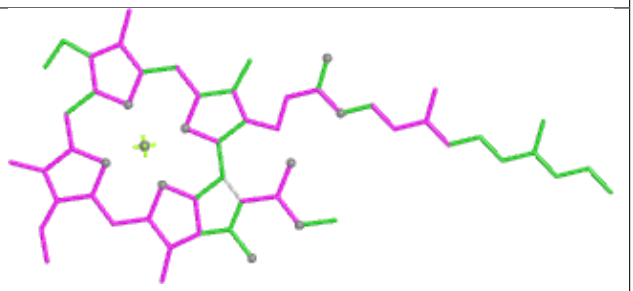


Rings

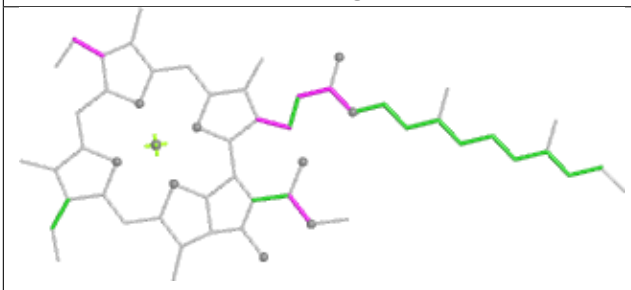
Ligand CLA 36 303



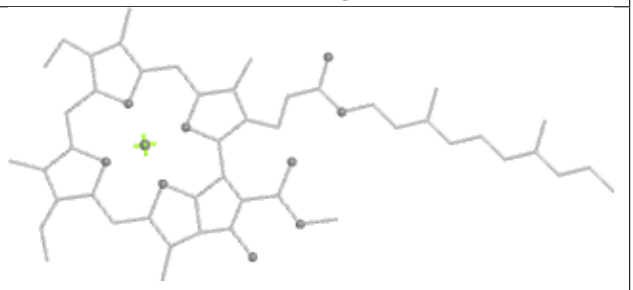
Bond lengths



Bond angles

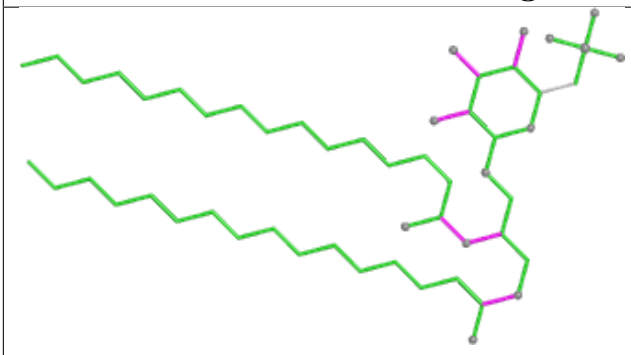


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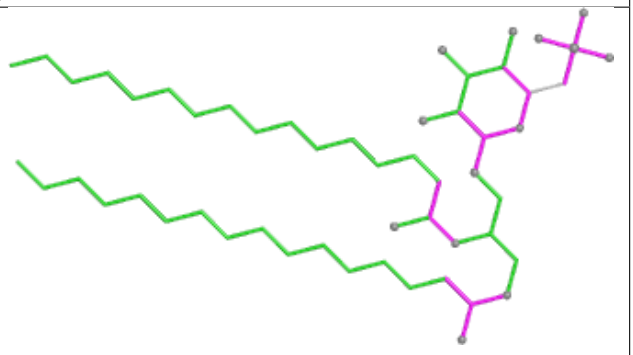


Rings

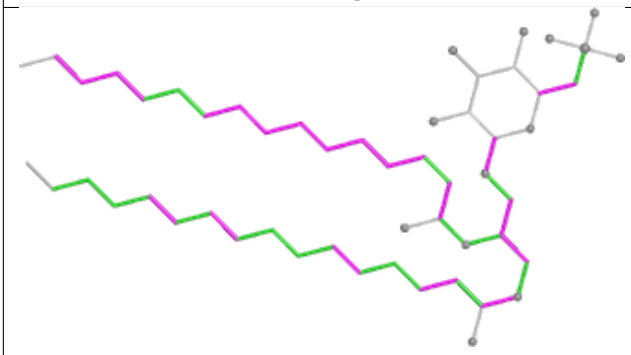
Ligand SQD 16 315



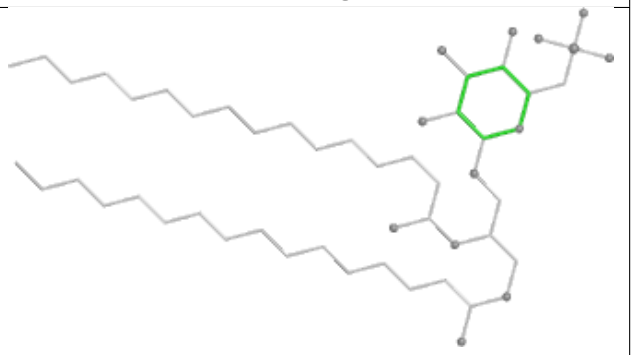
Bond lengths



Bond angles

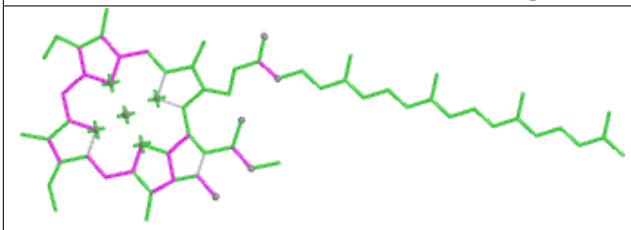


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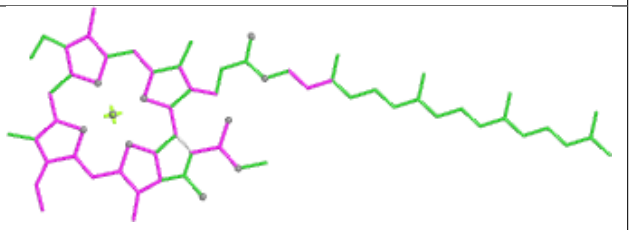


Rings

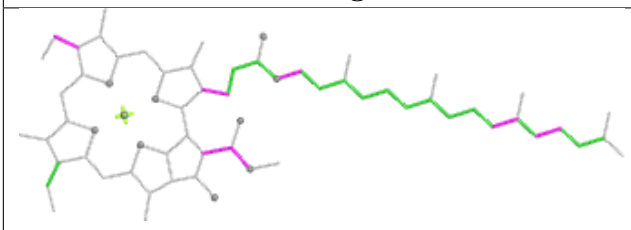
Ligand CLA C 502



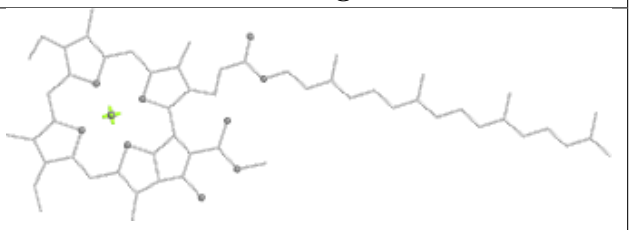
Bond lengths



Bond angles

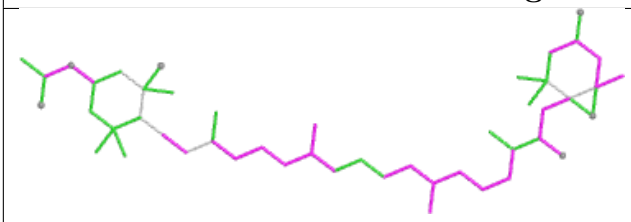


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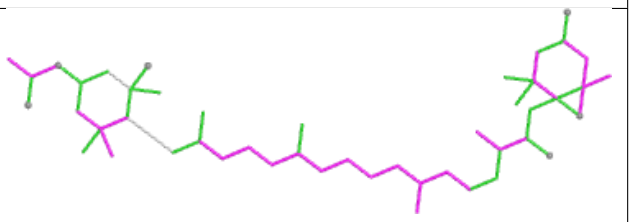


Rings

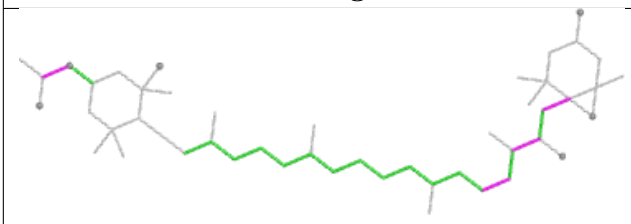
Ligand A86 16 314



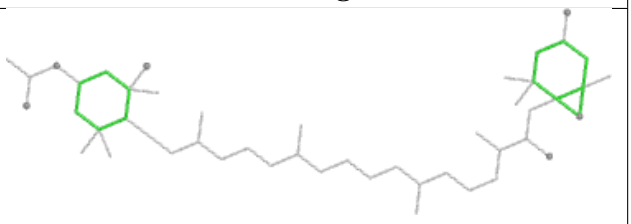
Bond lengths



Bond angles

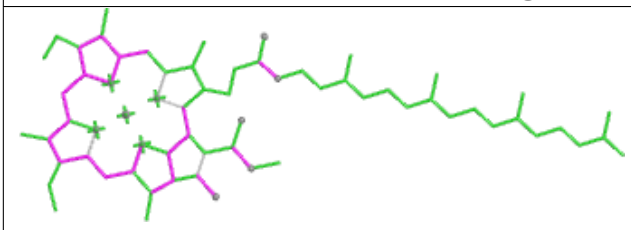


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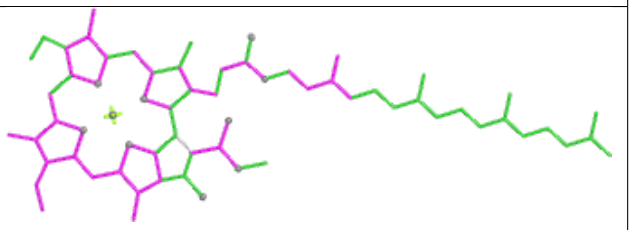


Rings

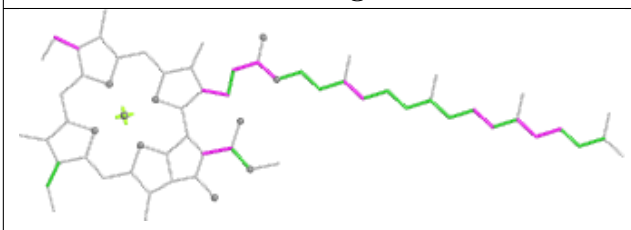
Ligand CLA 21 208



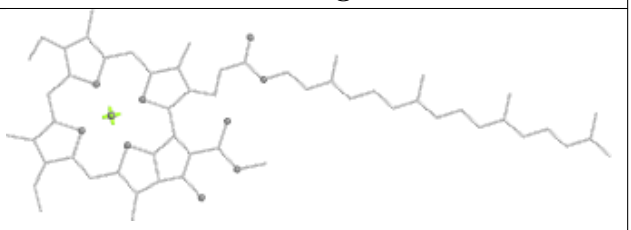
Bond lengths



Bond angles

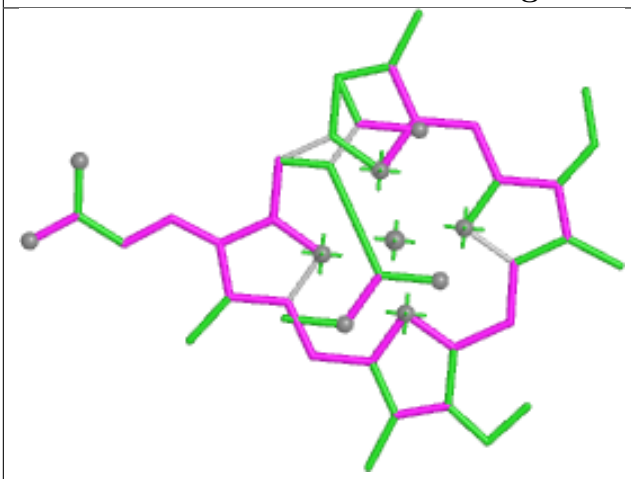


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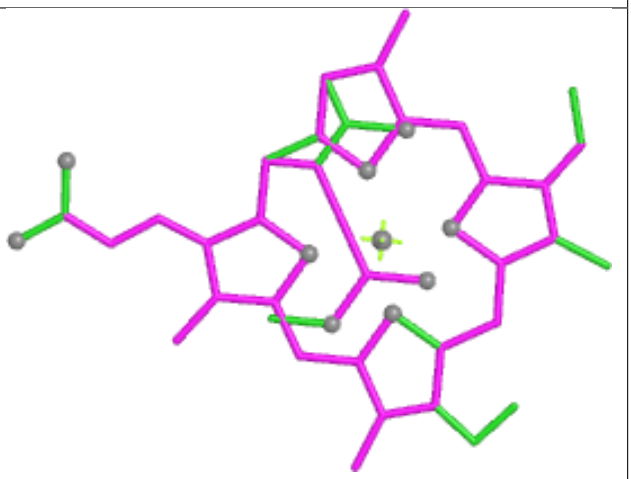


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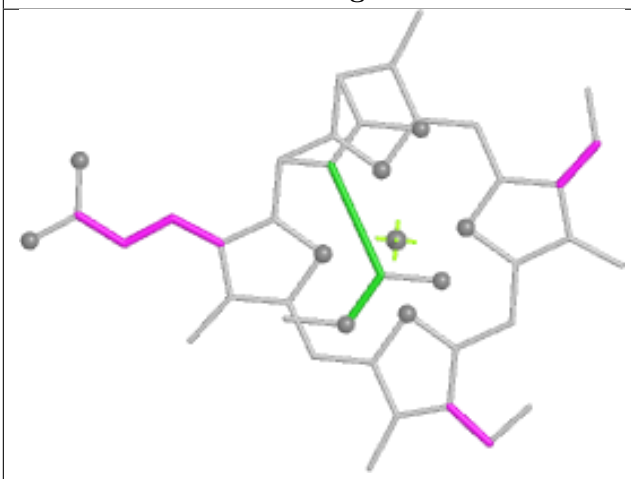
Ligand KC1 17 306



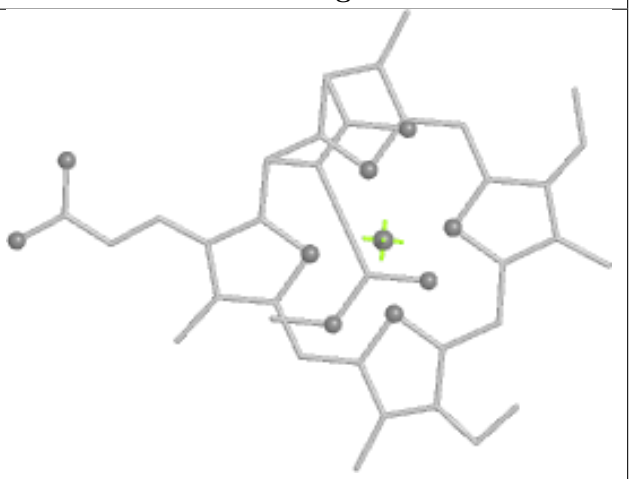
Bond lengths



Bond angles

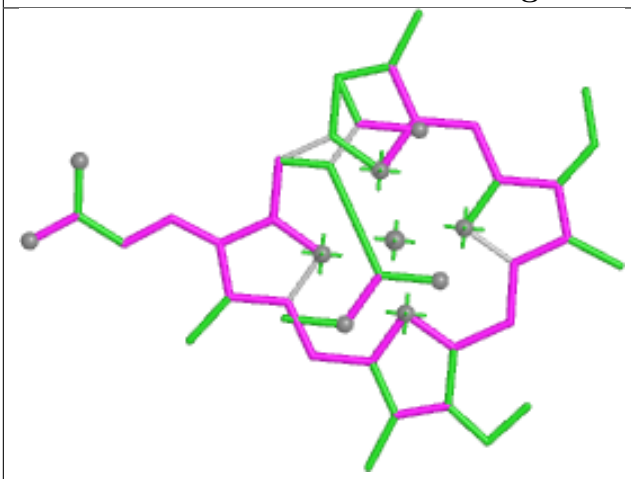


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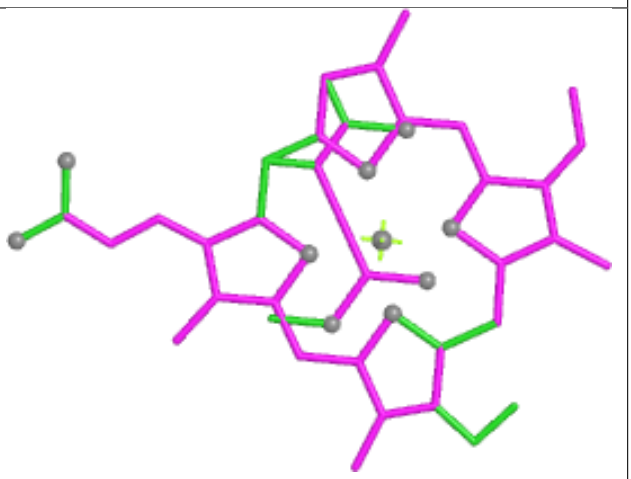


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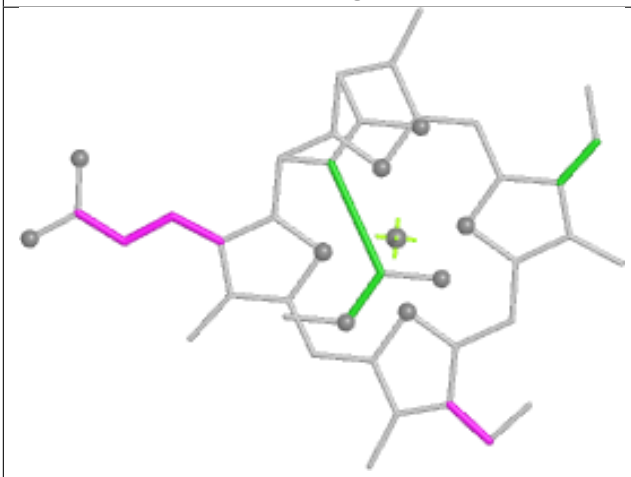
Ligand KC1 35 302



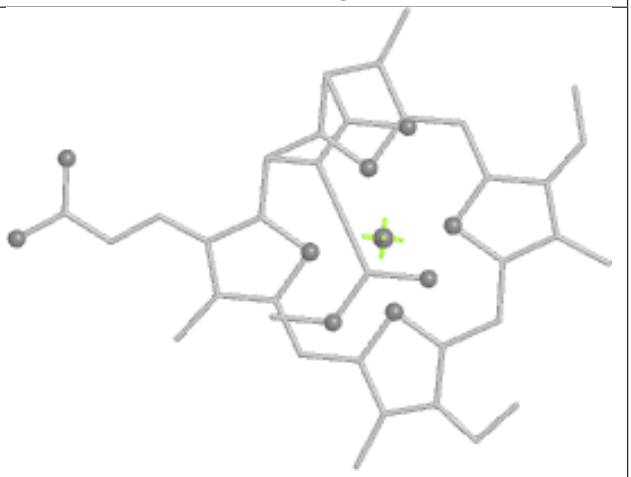
Bond lengths



Bond angles

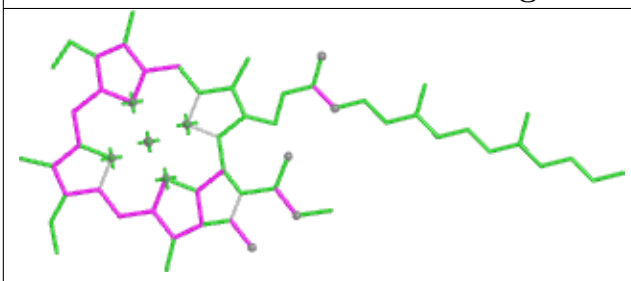


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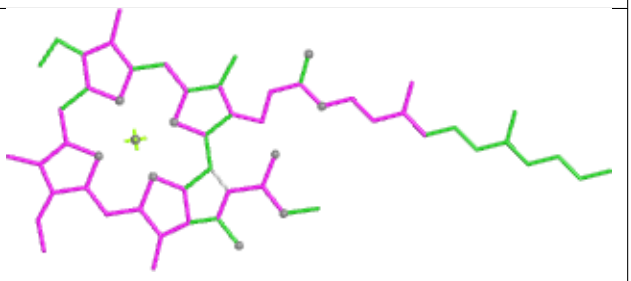


Rings

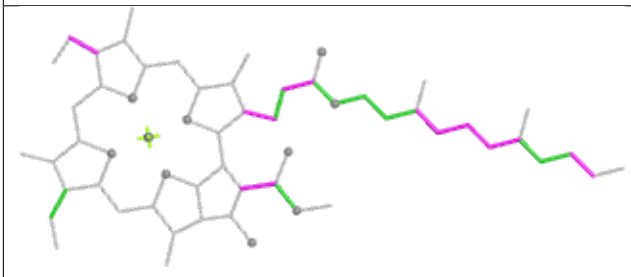
Ligand CLA 41 204



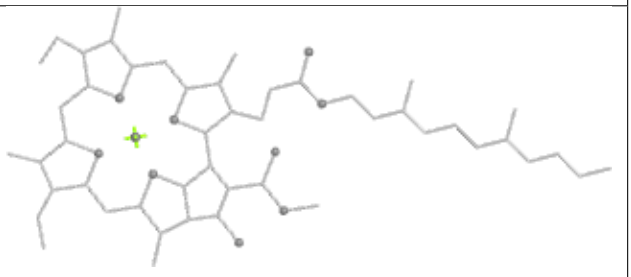
Bond lengths



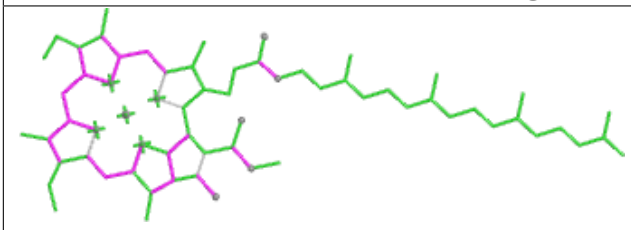
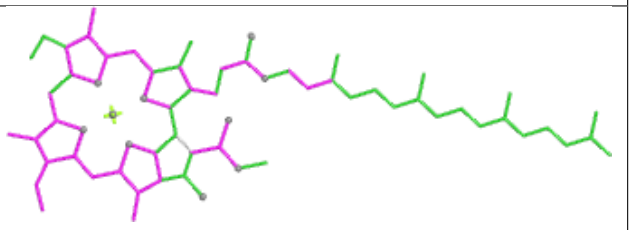
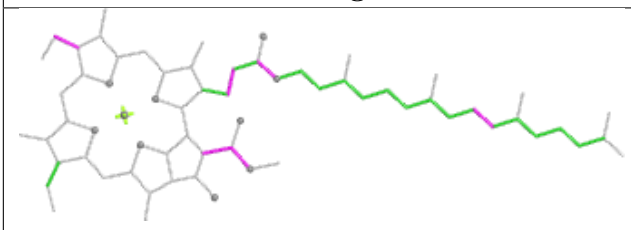
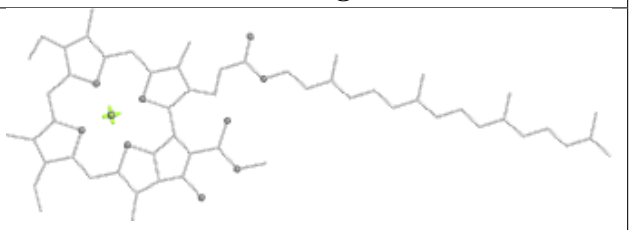
Bond angles

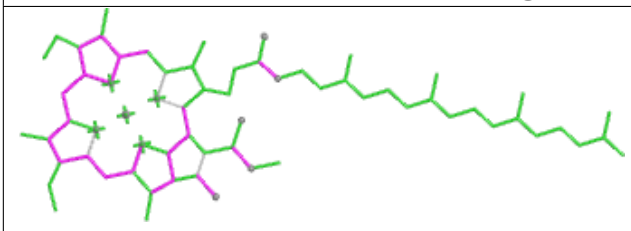
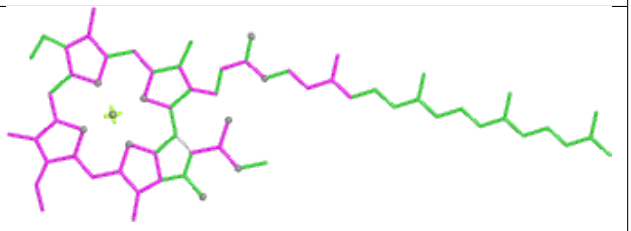
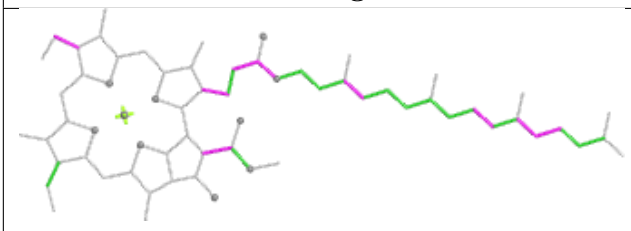
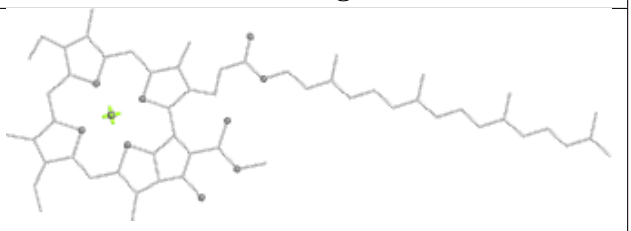


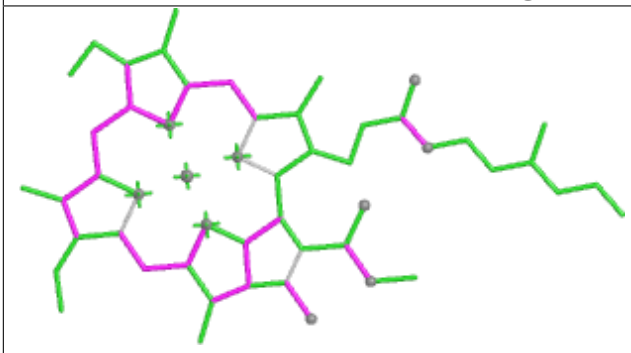
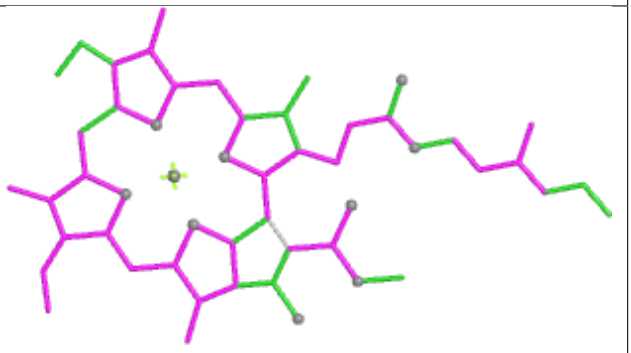
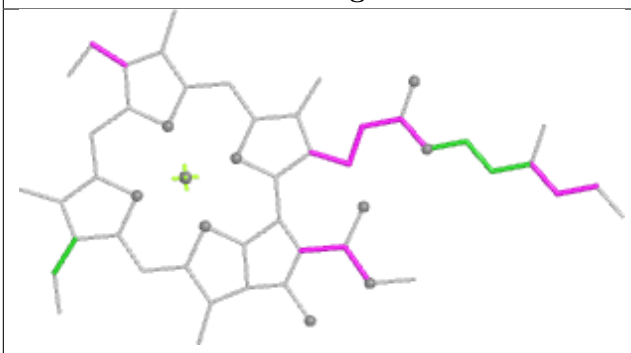
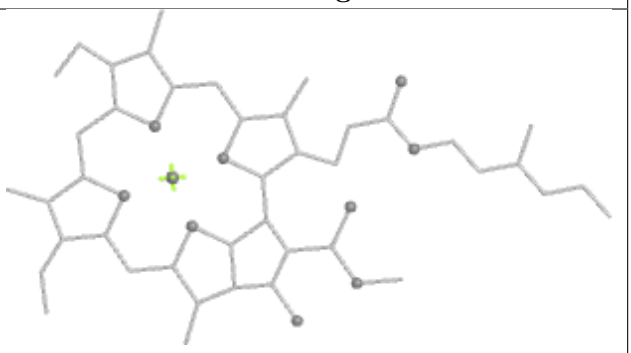
Torsions

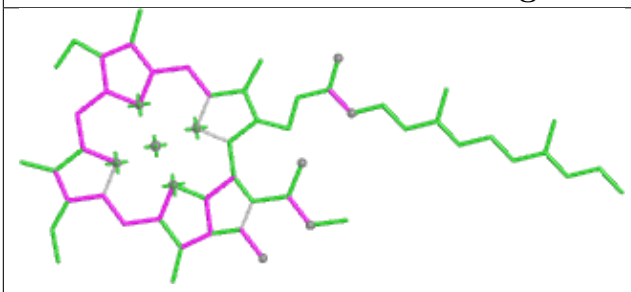
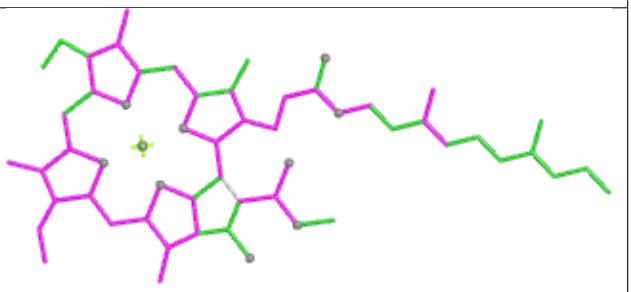
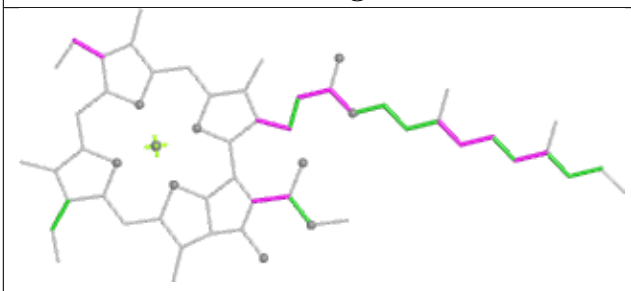
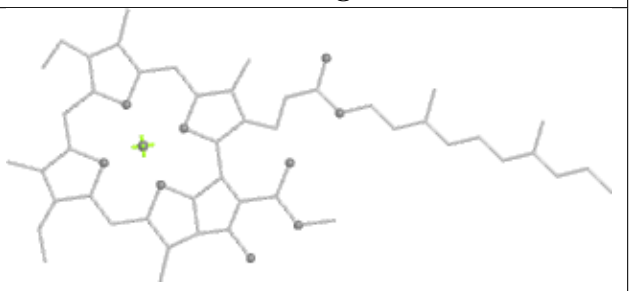


Rings

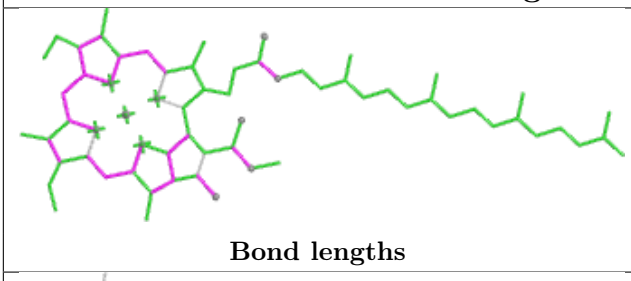
Ligand CLA C 513	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 41 208	
 Bond lengths	 Bond angles
 Torsions	 Rings

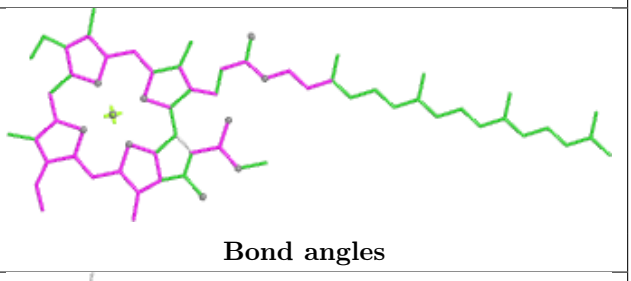
Ligand CLA 34 307	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 33 303	
	
Bond lengths	Bond angles
	
Torsions	Rings

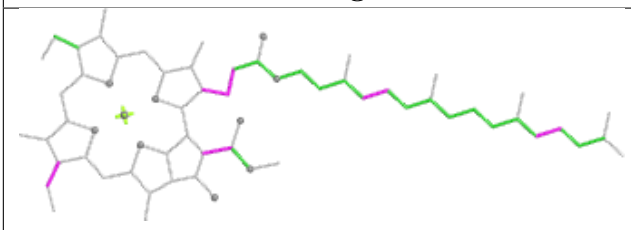
Ligand CLA D 401



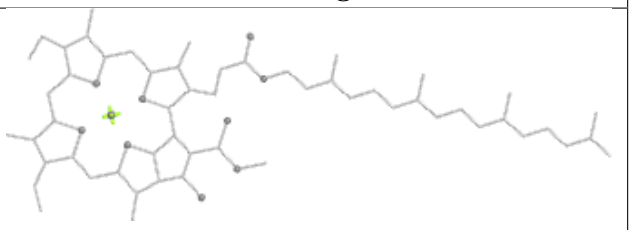
Bond lengths



Bond angles

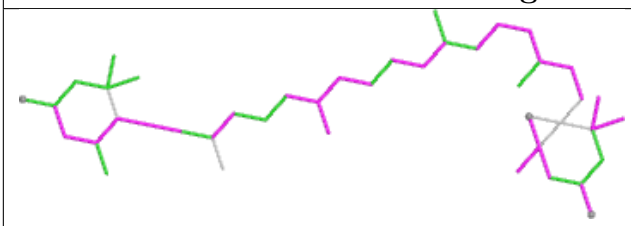


Torsions

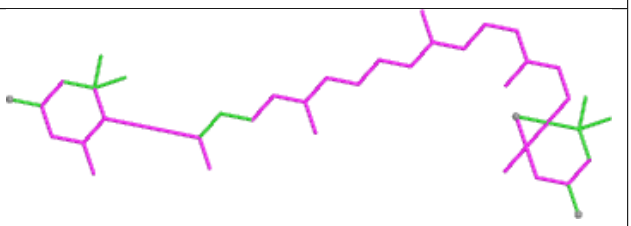


Rings

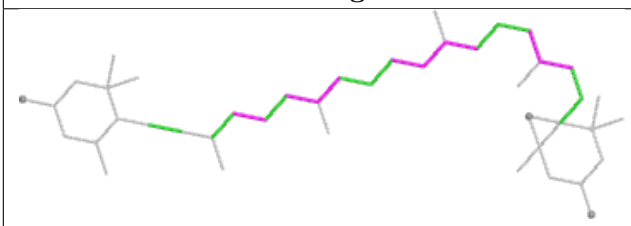
Ligand DD6 16 312



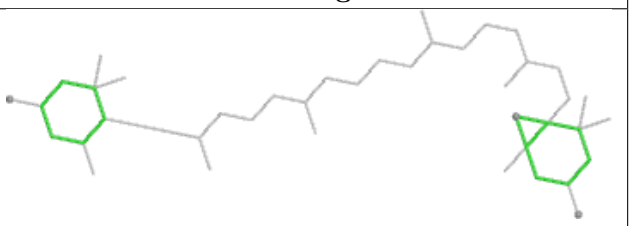
Bond lengths



Bond angles

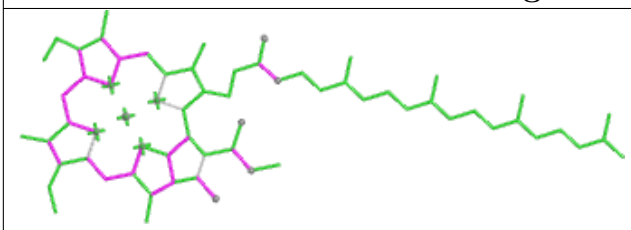


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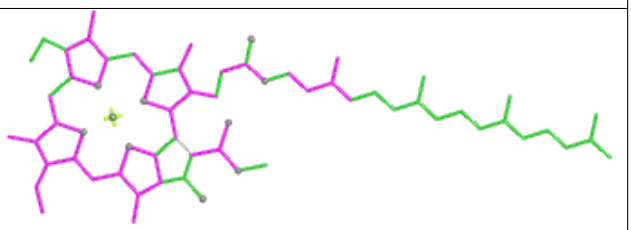


Rings

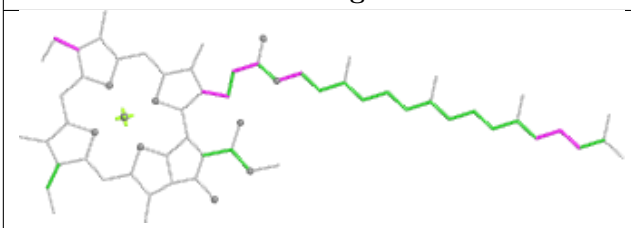
Ligand CLA D 405



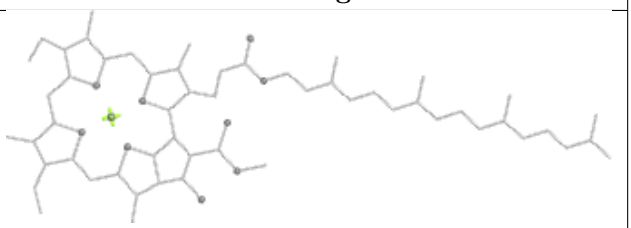
Bond lengths



Bond angles

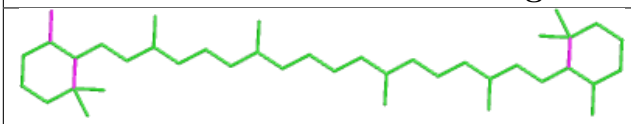


Torsions

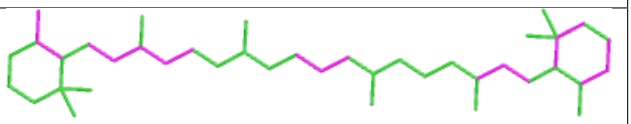


Rings

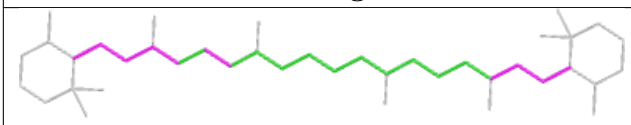
Ligand BCR d 405



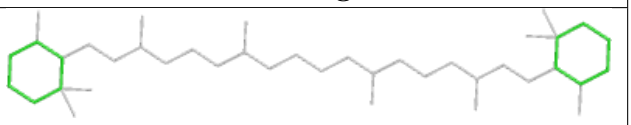
Bond lengths



Bond angles

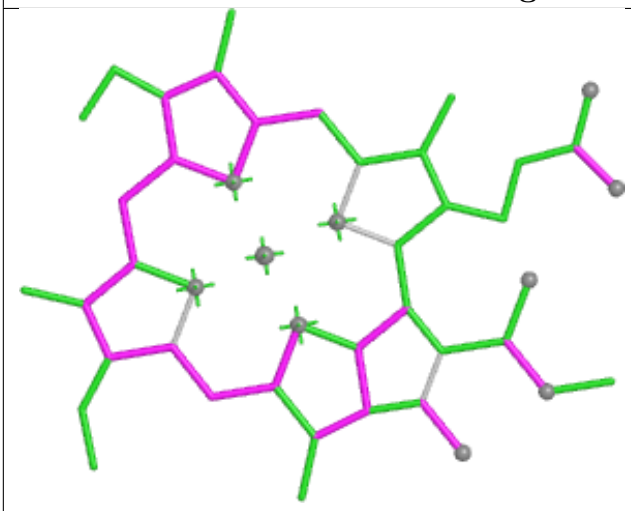


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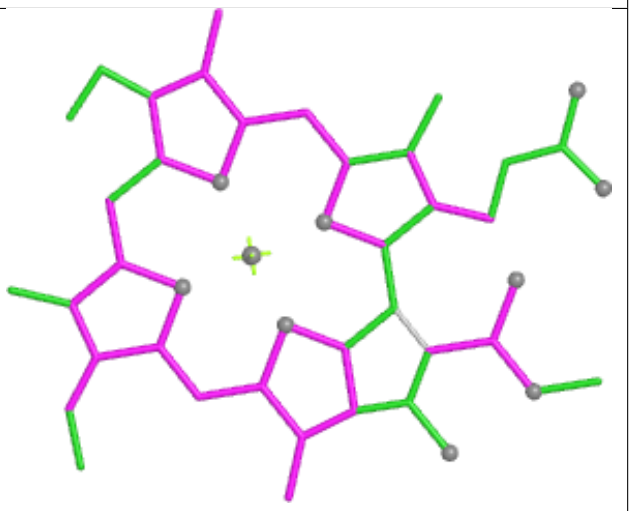


Rings

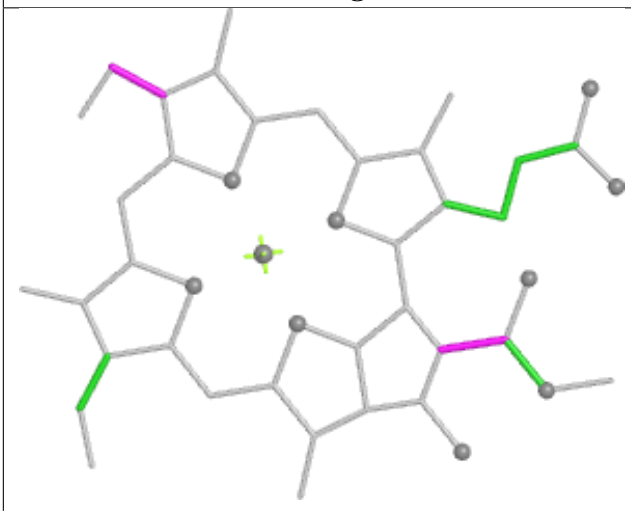
Ligand CLA 38 211



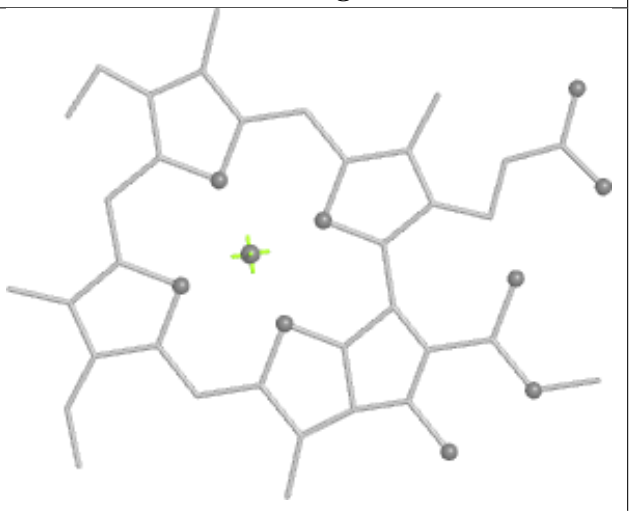
Bond lengths



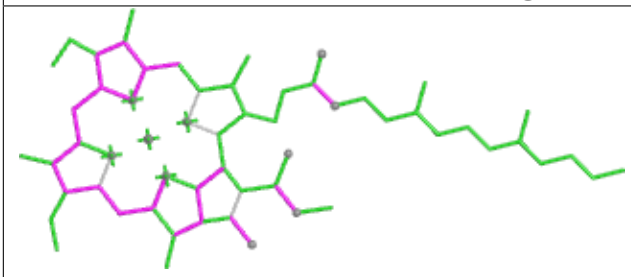
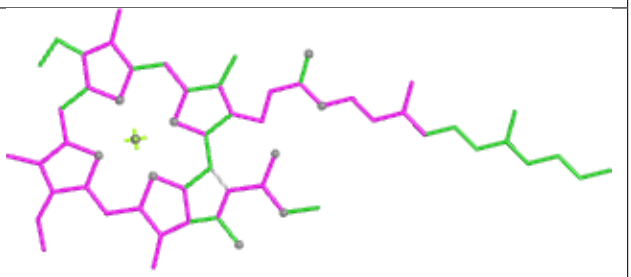
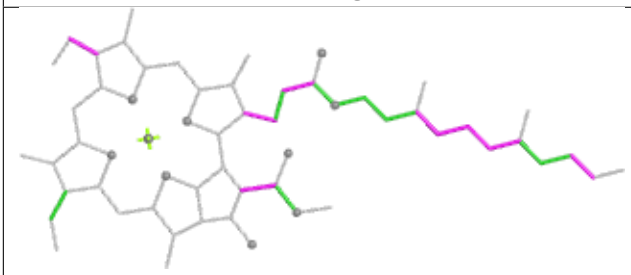
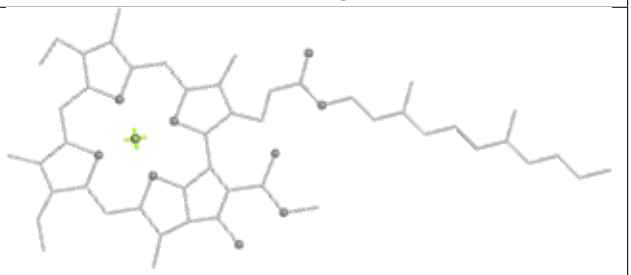
Bond angles

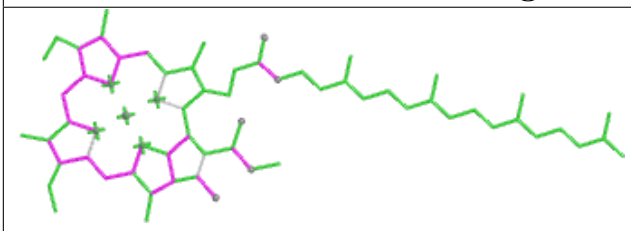
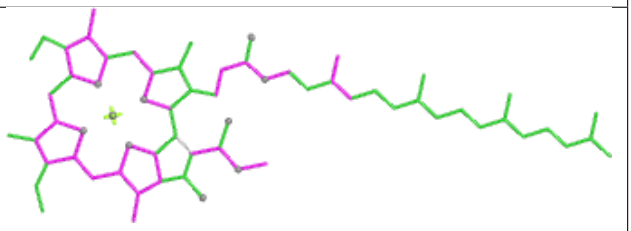
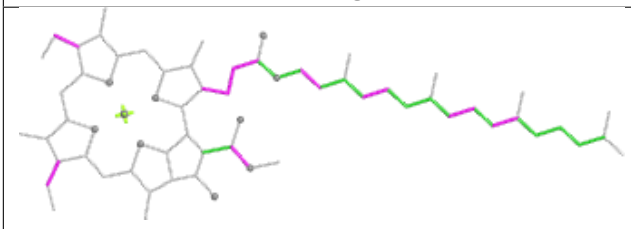
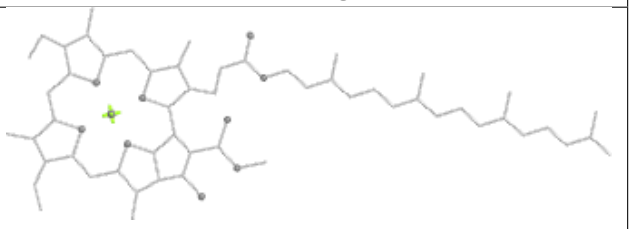


Torsions

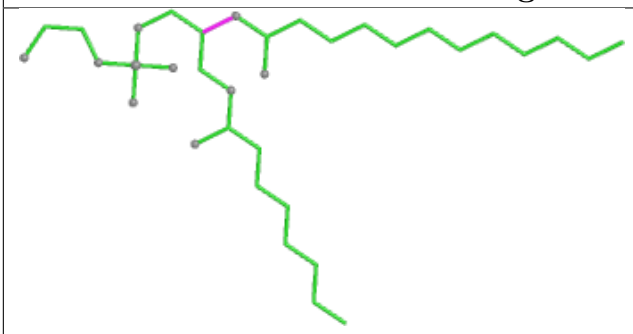


Rings

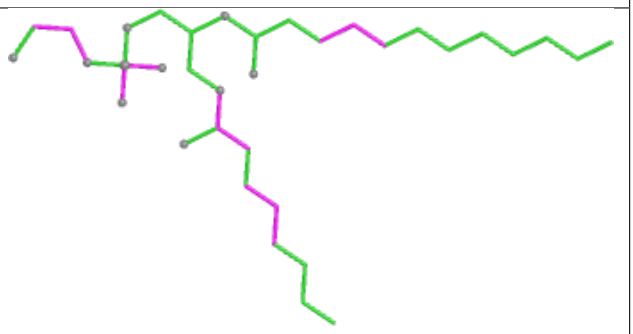
Ligand CLA 21 204	
 Bond lengths	 Bond angles
 Torsions	 Rings

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 Bond lengths	 Bond angles
 Torsions	 Rings

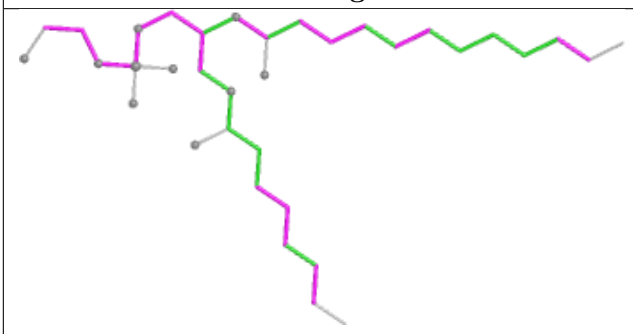
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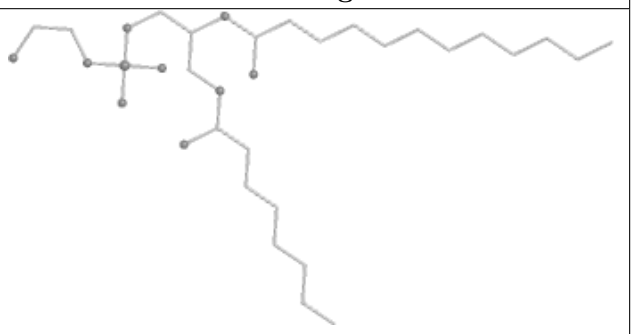
Bond lengths



Bond angles

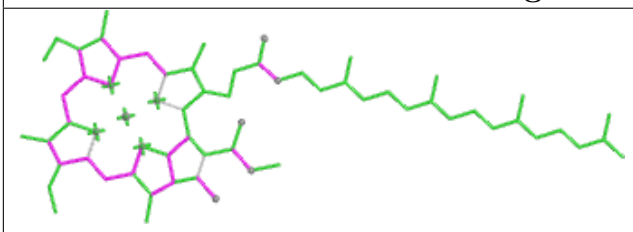


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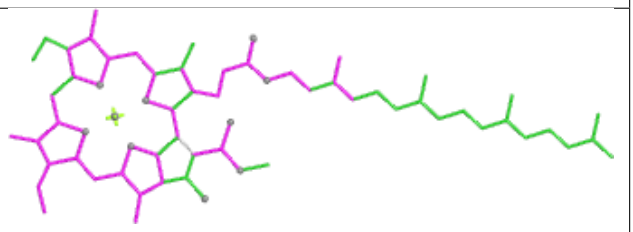


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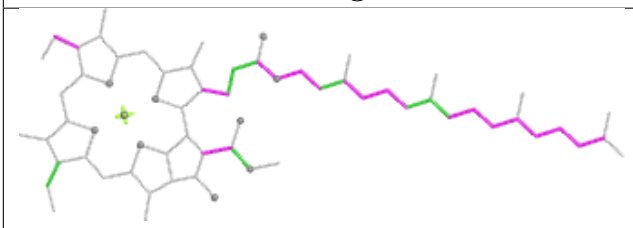
Ligand CLA C 503



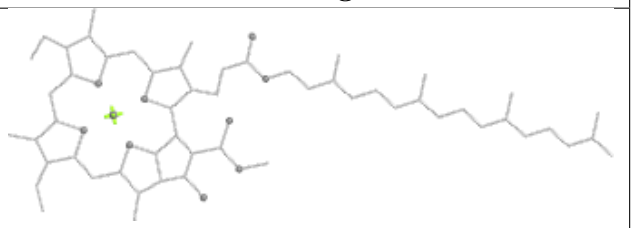
Bond lengths



Bond angles

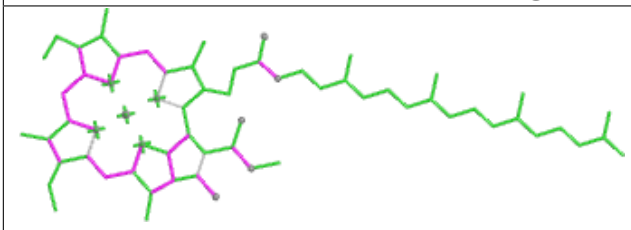


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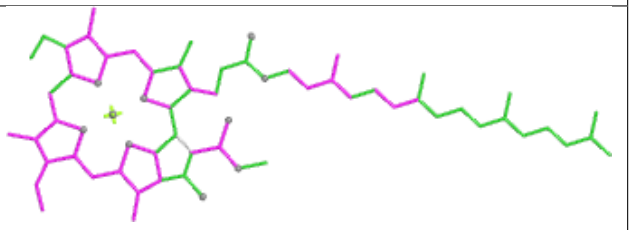


Rings

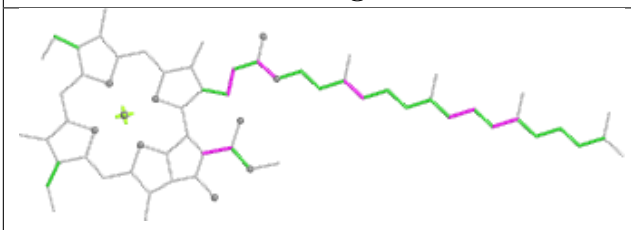
Ligand CLA b 505



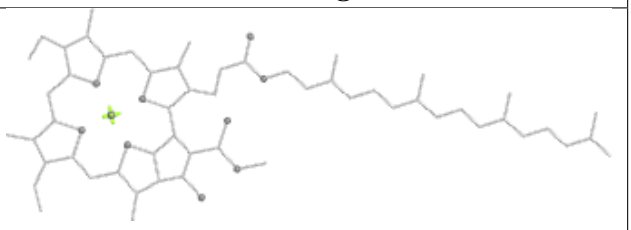
Bond lengths



Bond angles

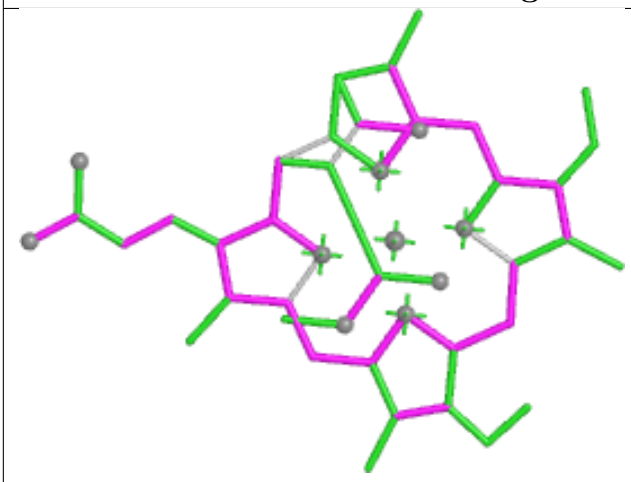


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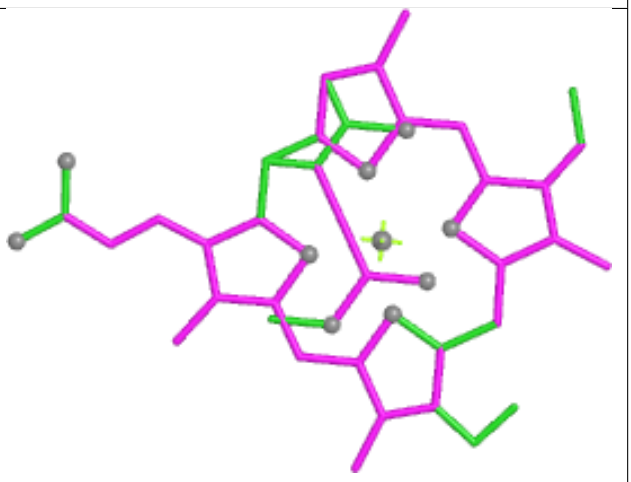


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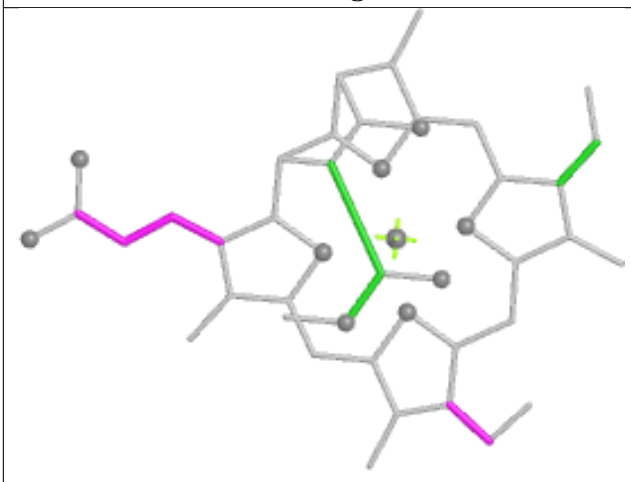
Ligand KC1 40 206



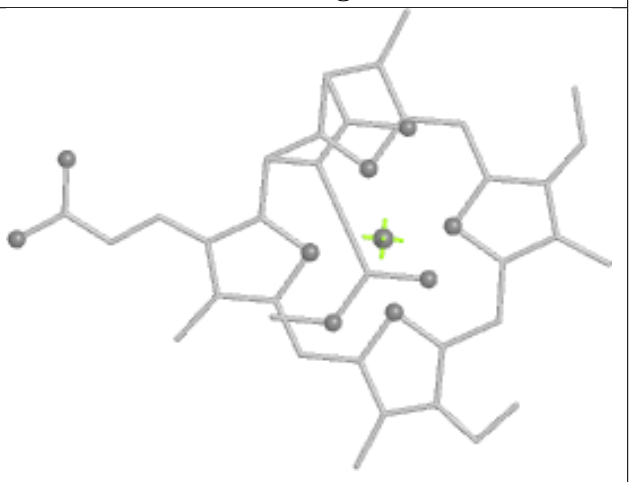
Bond lengths



Bond angles

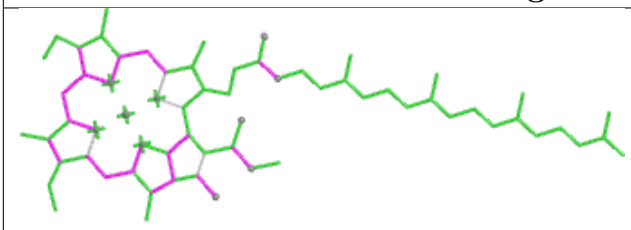


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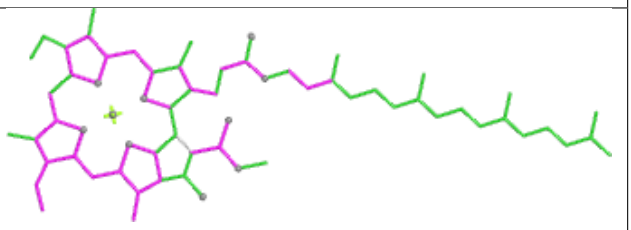


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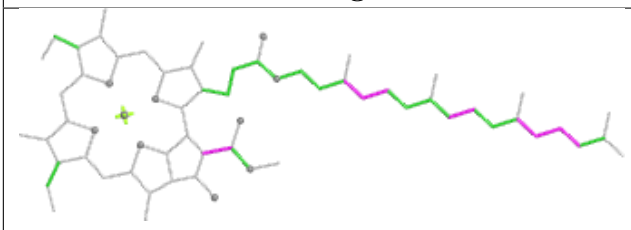
Ligand CLA b 507



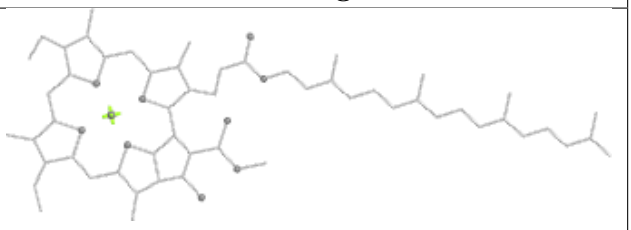
Bond lengths



Bond angles

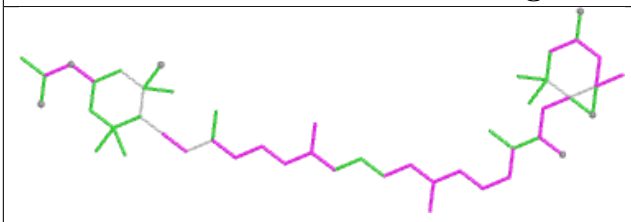


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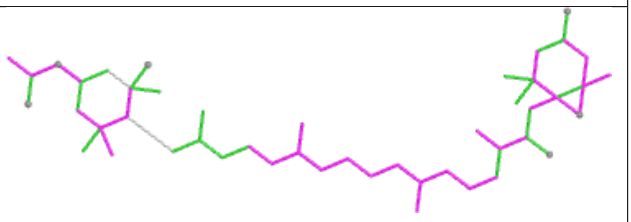


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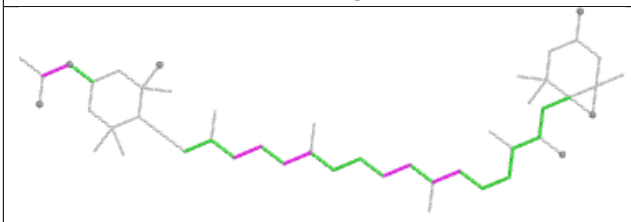
Ligand A86 35 319



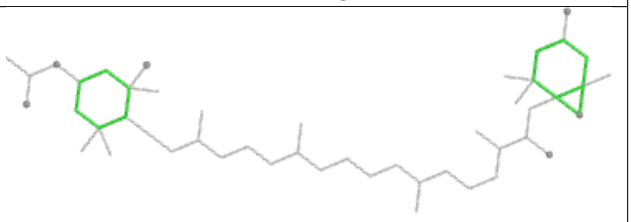
Bond lengths



Bond angles

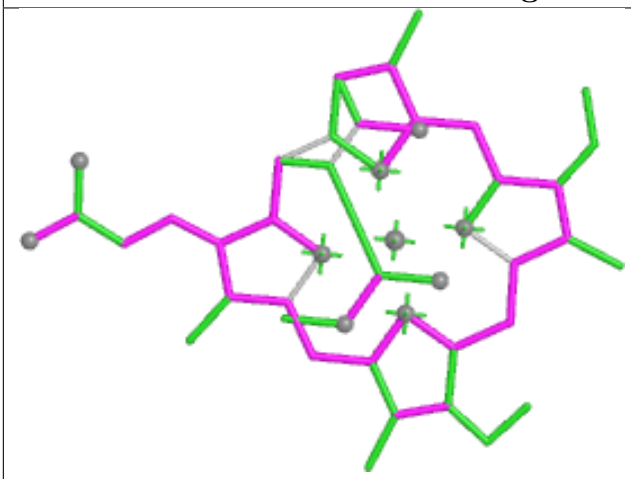


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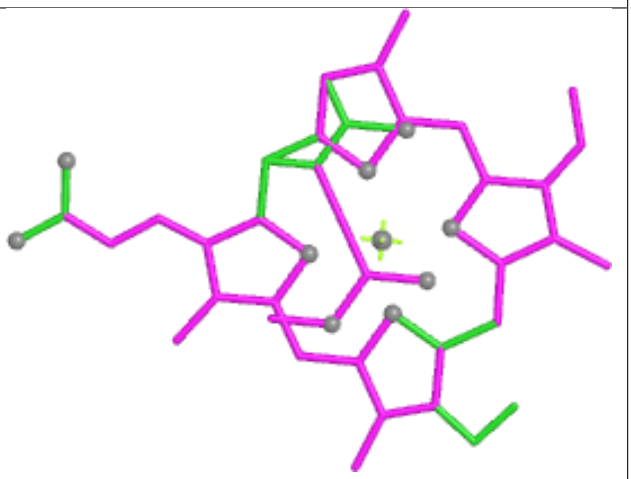


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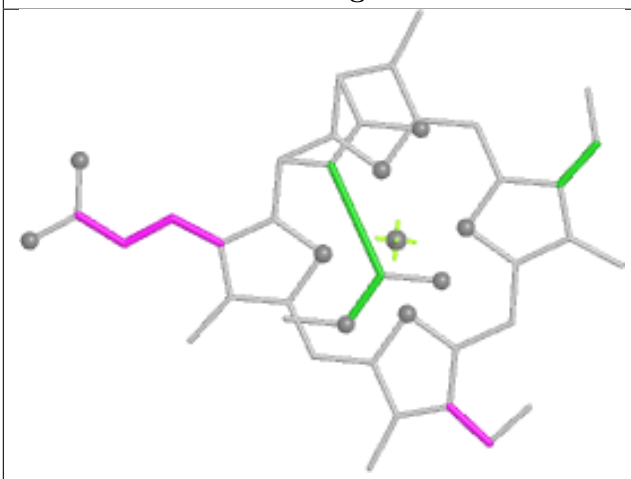
Ligand KC1 15 304



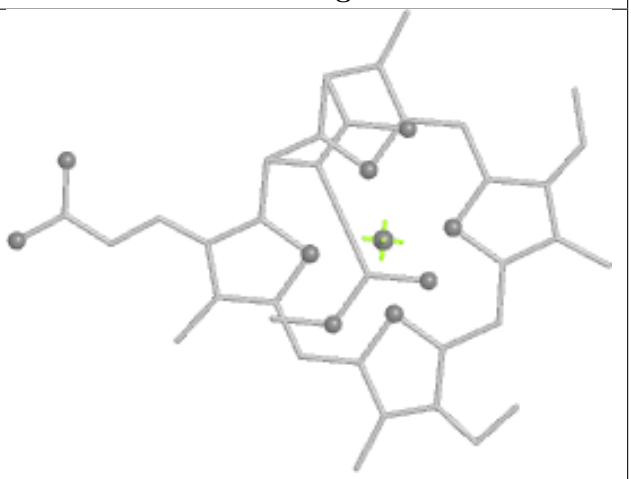
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Bond angles

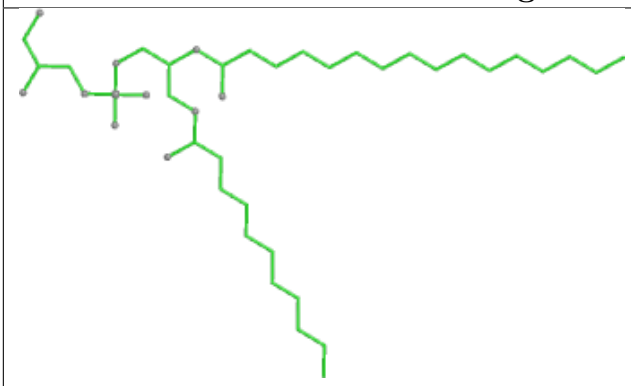


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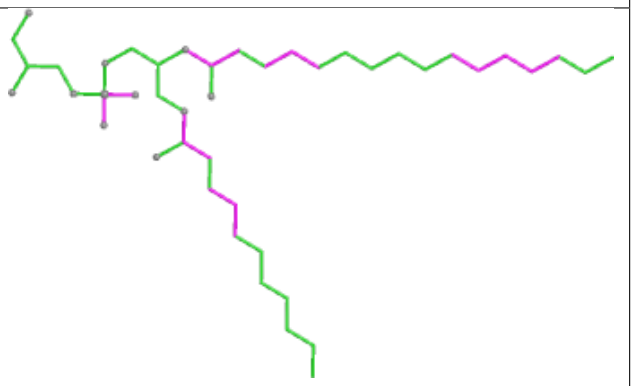


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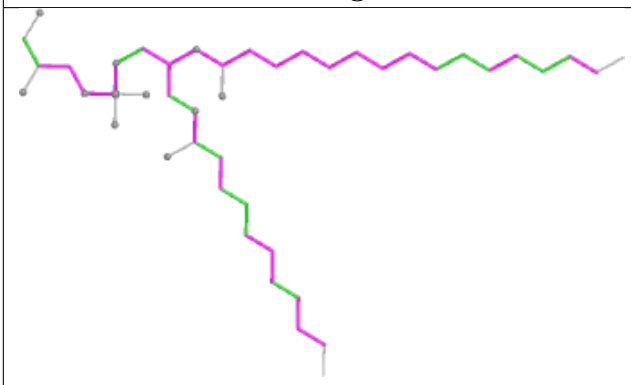
Ligand LHG 37 315



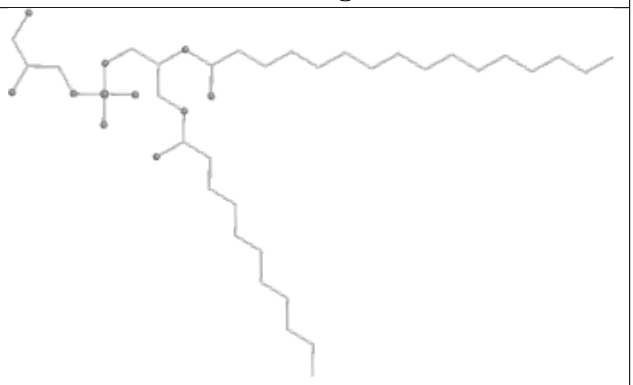
Bond lengths



Bond angles

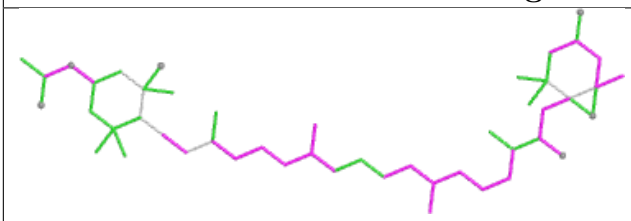


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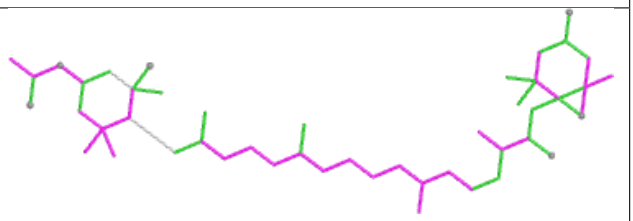


Rings

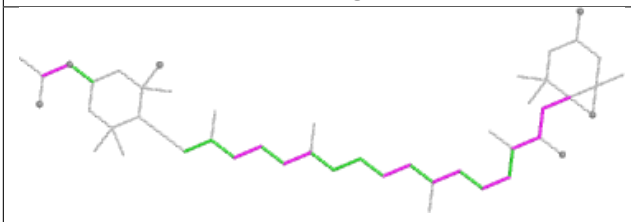
Ligand A86 18 214



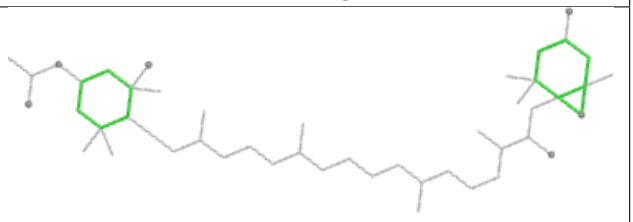
Bond lengths



Bond angles

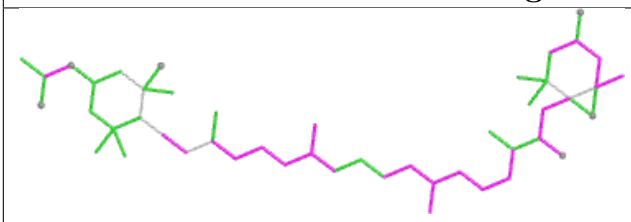


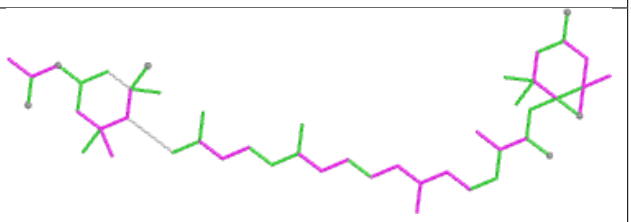
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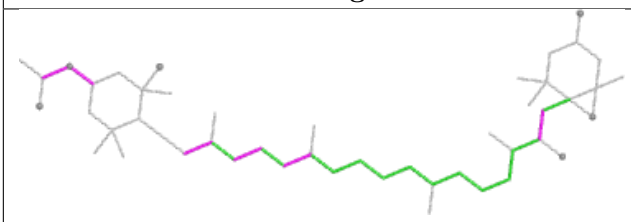


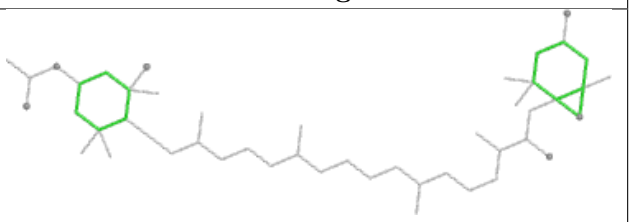
Rings

Ligand A86 15 313

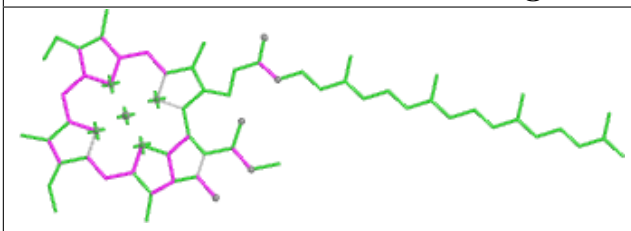

Bond lengths

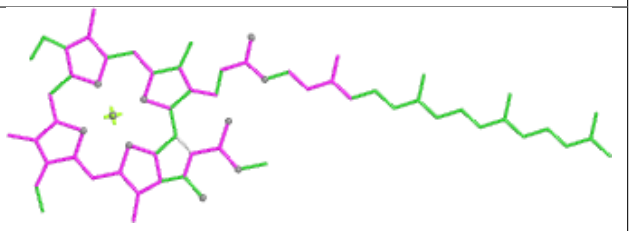

Bond angles

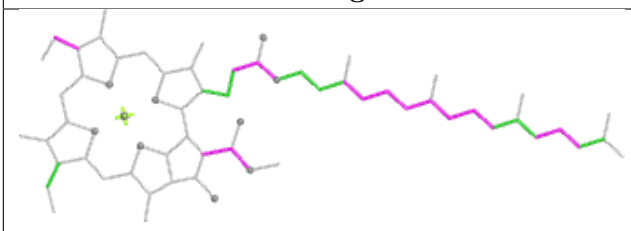

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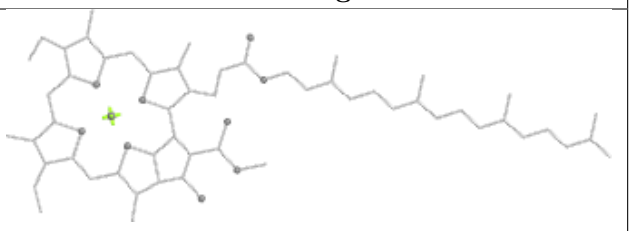

Rings

Ligand CLA w 101

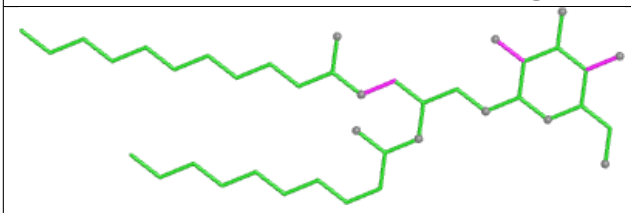

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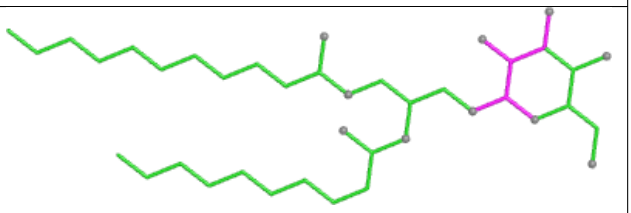

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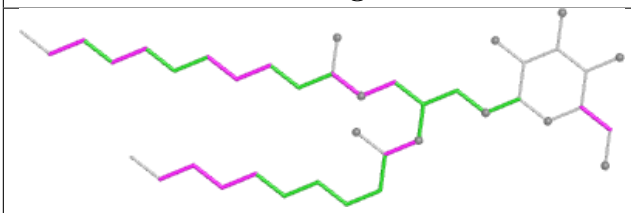

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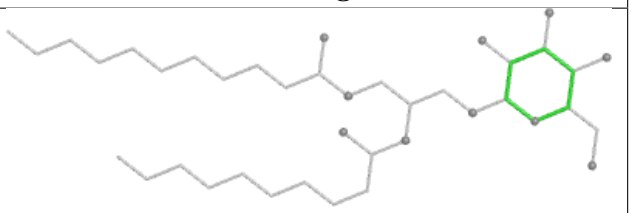

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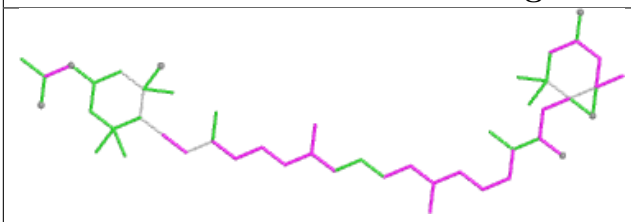

Bond lengths


Bond angles

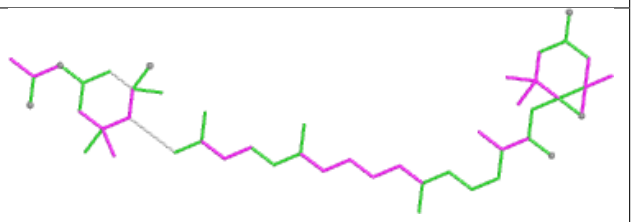

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Rings

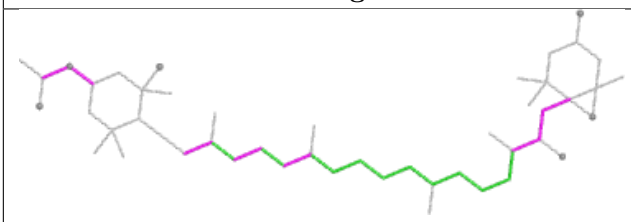
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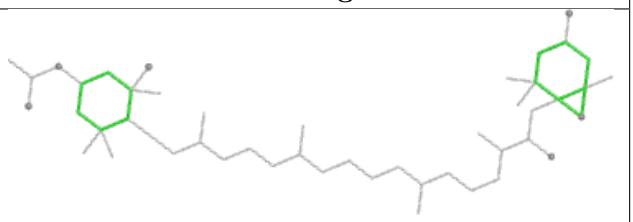
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Bond angles

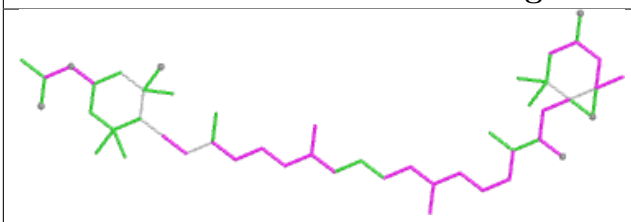


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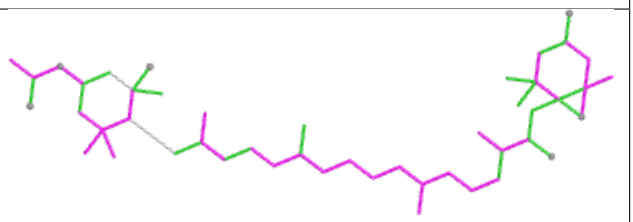


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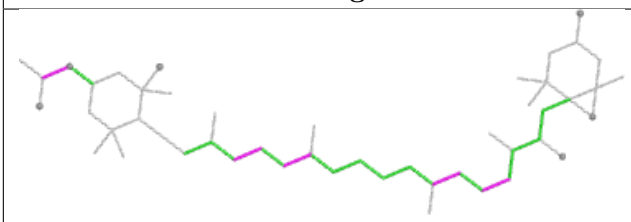
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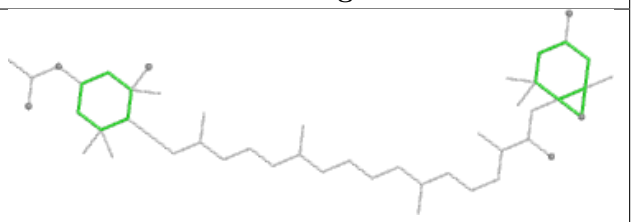
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Bond angles

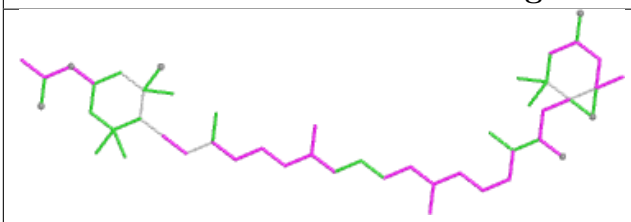


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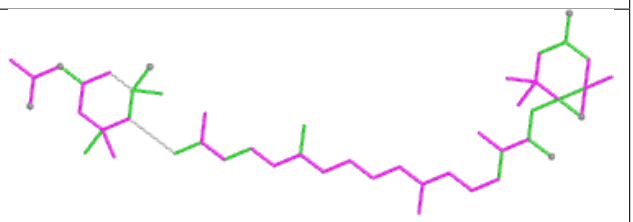


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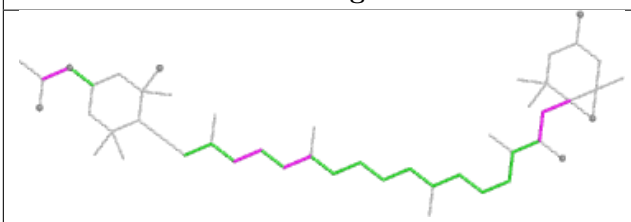
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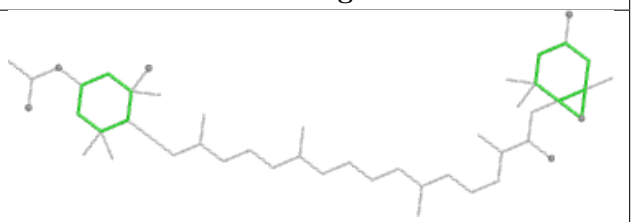
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Bond angles

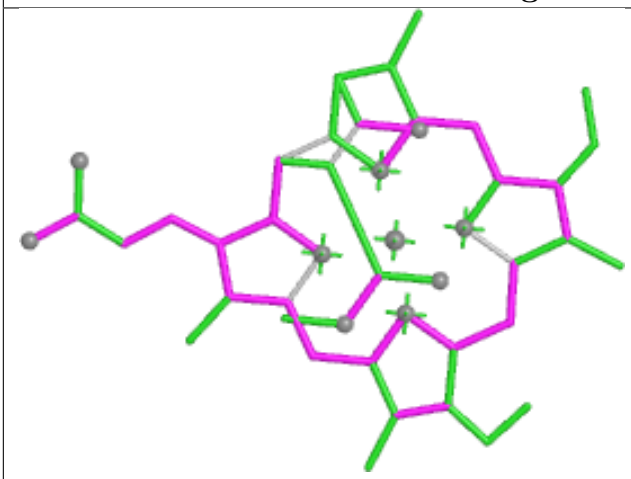


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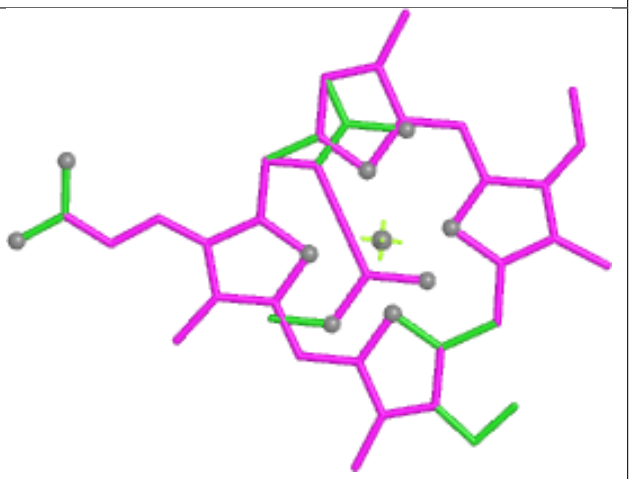


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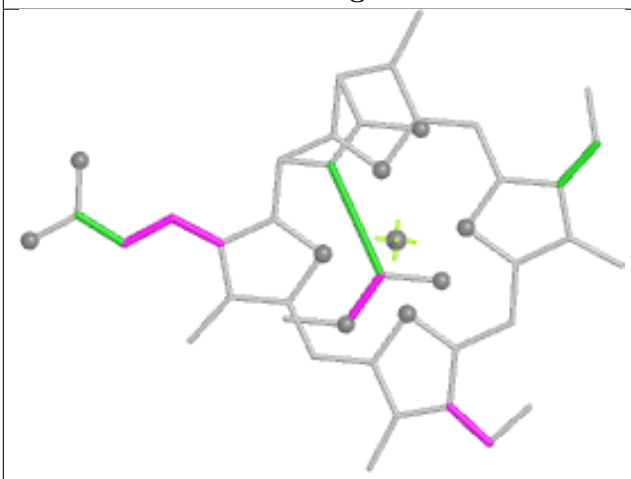
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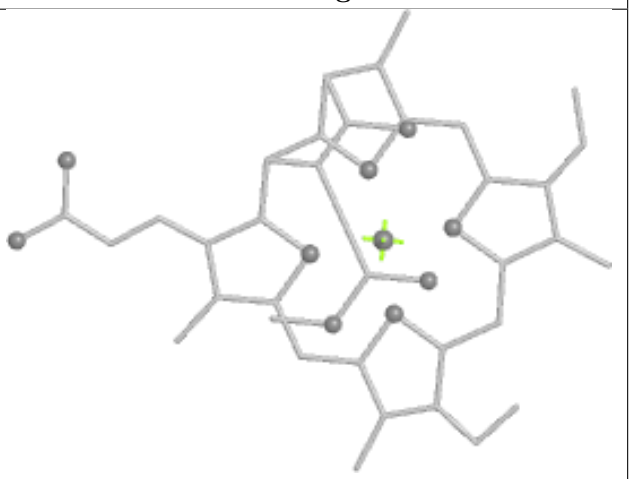
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Bond angles

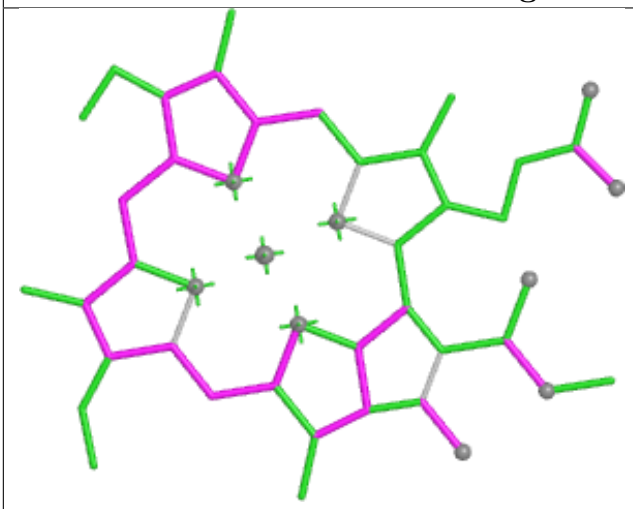


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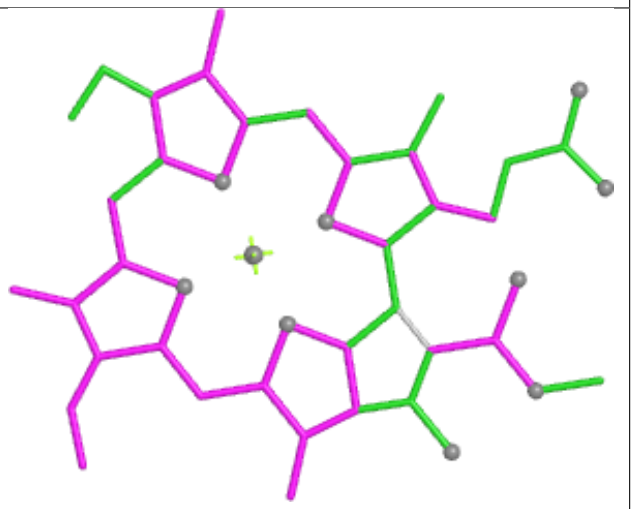


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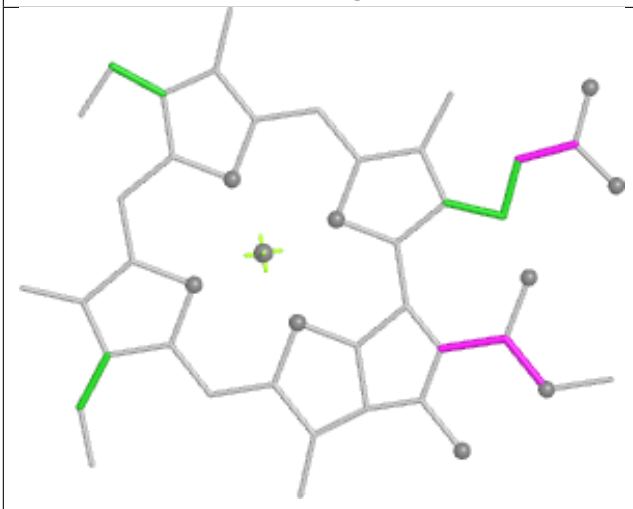
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Bond lengths



Bond angles

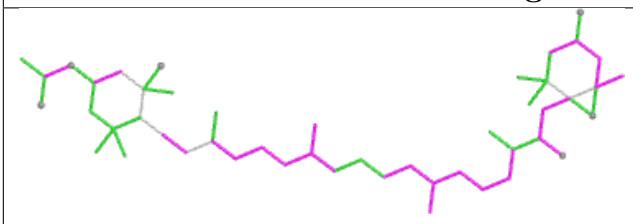


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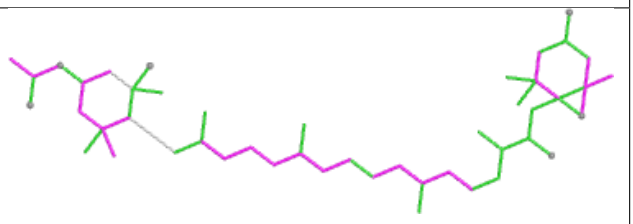


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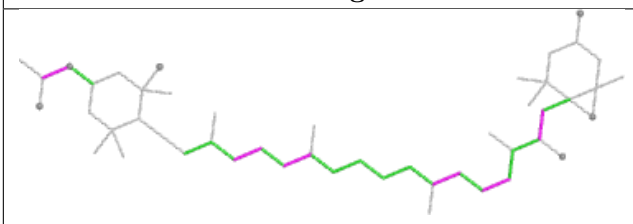
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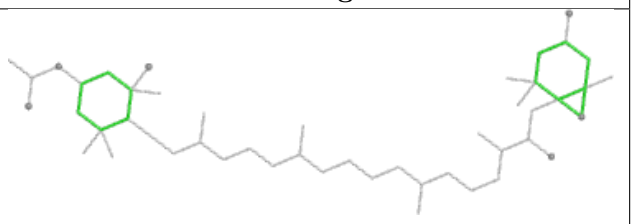
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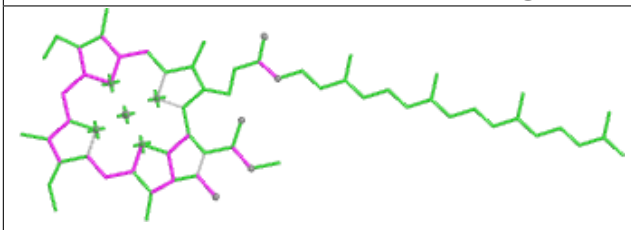


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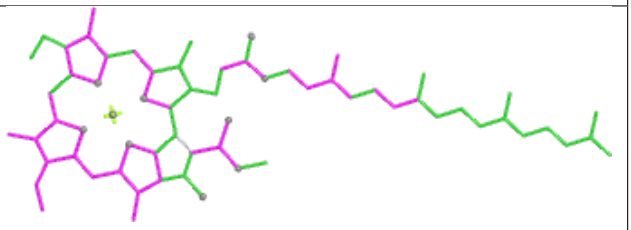


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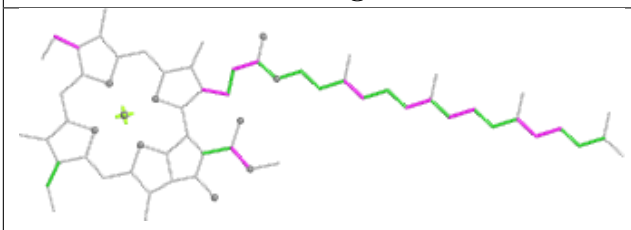
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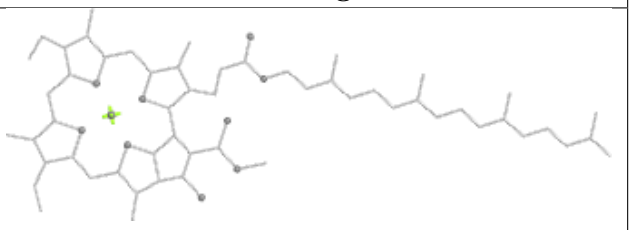
Bond lengths



Bond angles

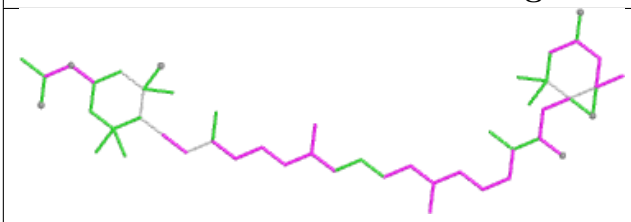


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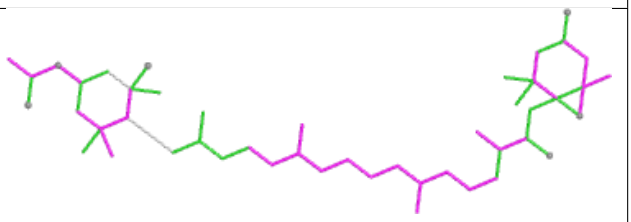


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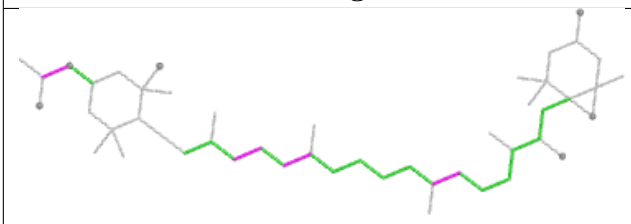
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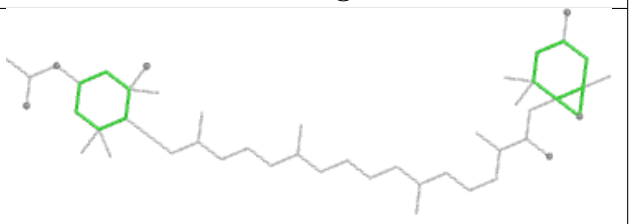
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Bond angles

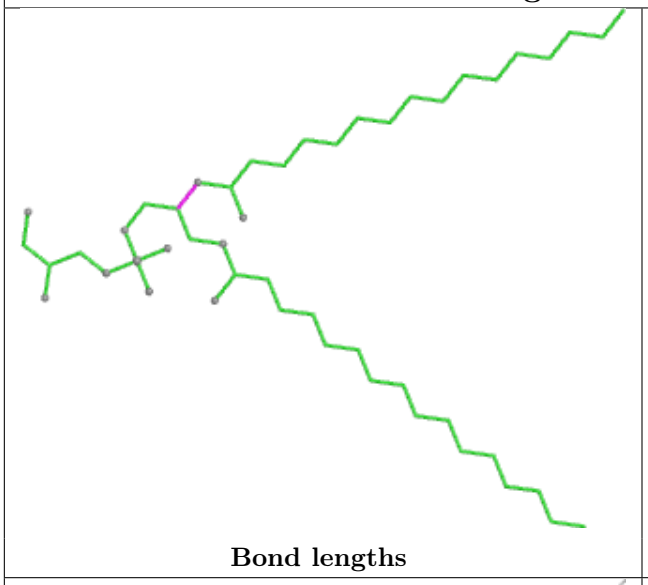


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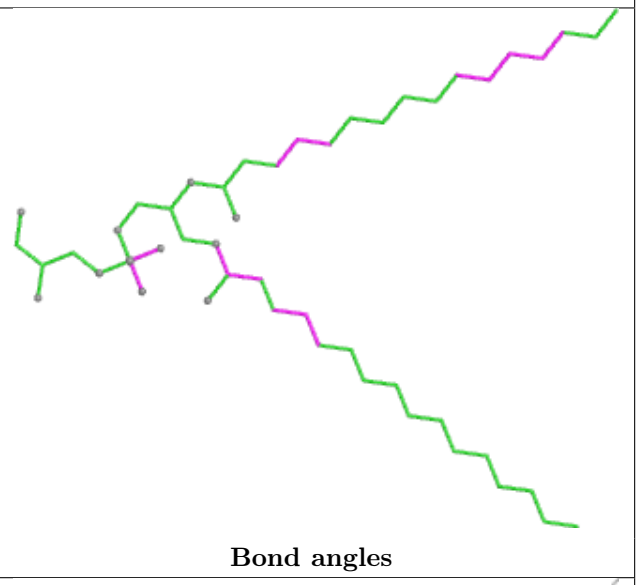


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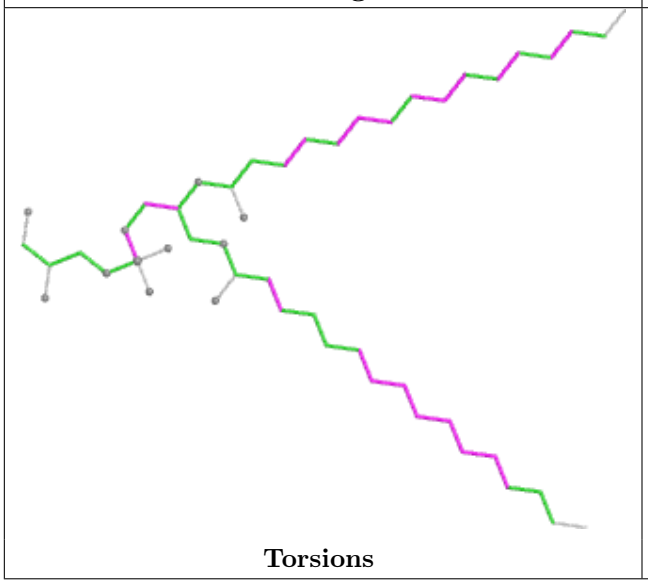
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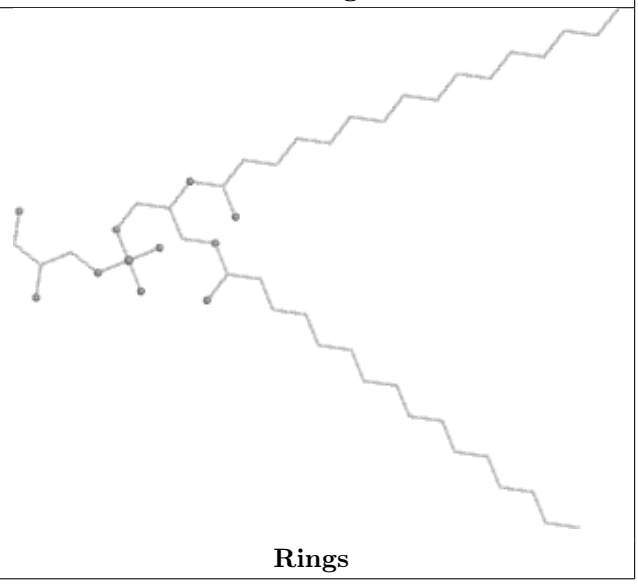
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Bond angles

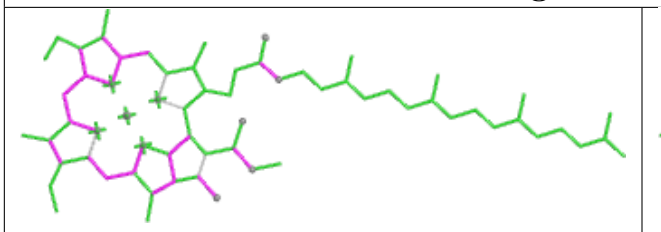


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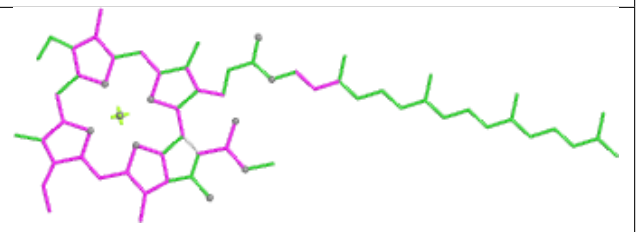


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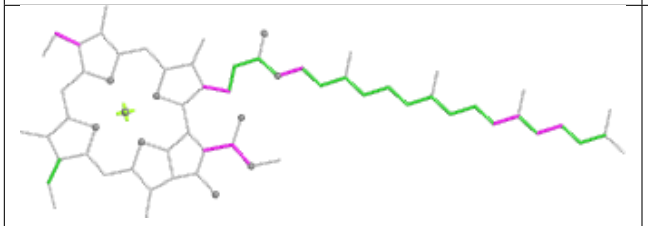
Ligand CLA c 502



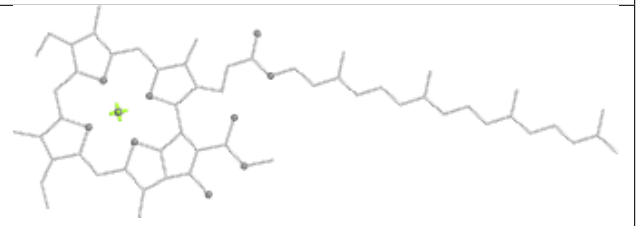
Bond lengths



Bond angles

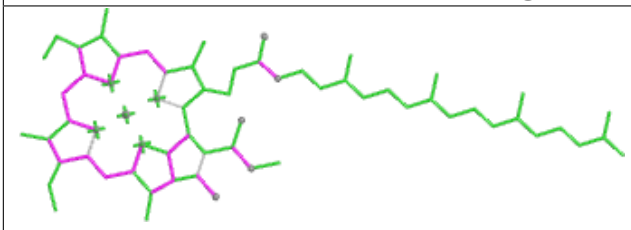


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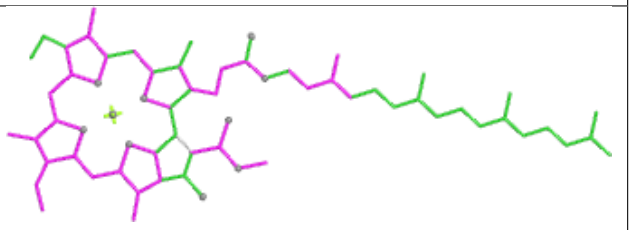


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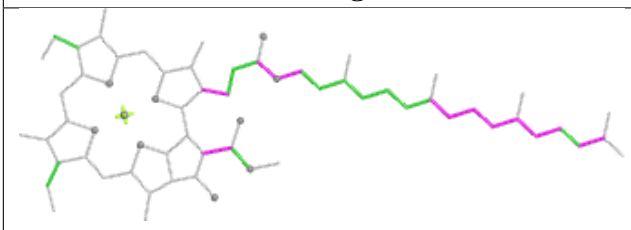
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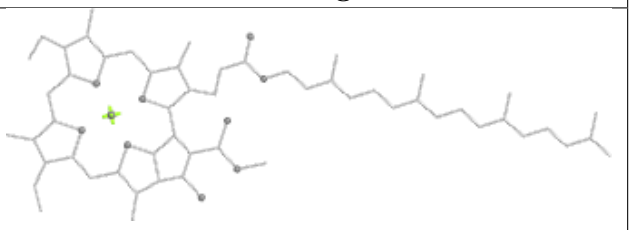
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Bond angles

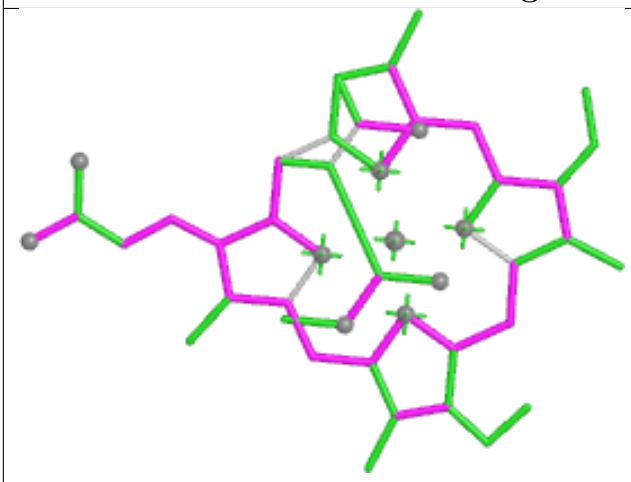


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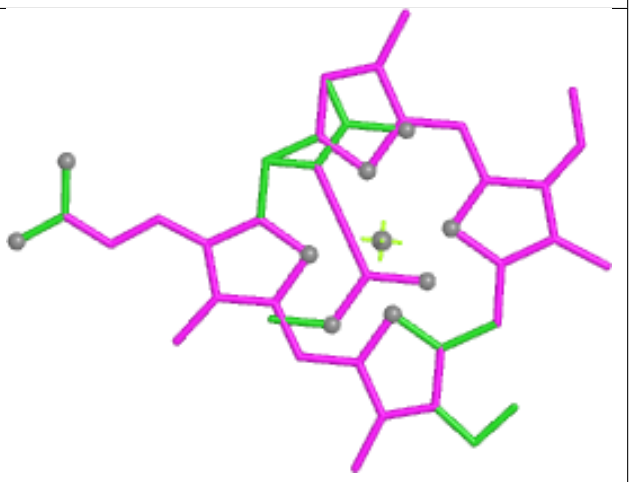


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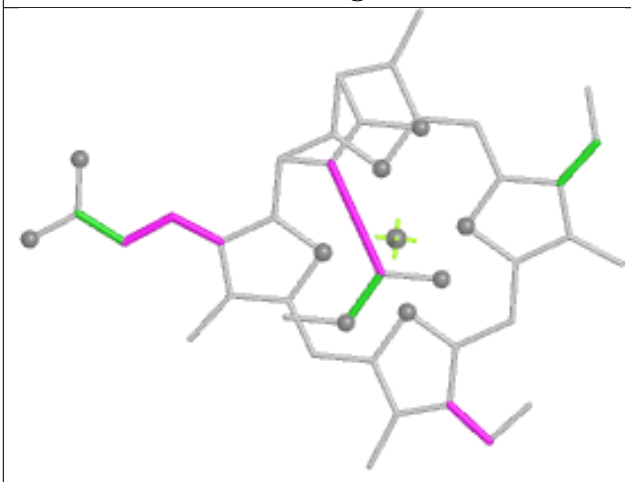
Ligand KC1 17 308



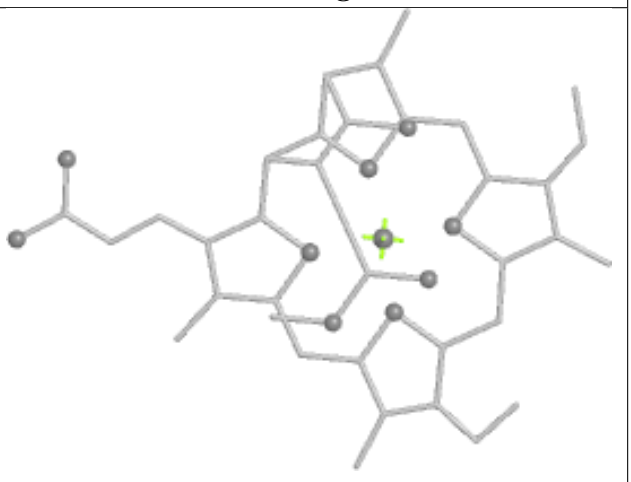
Bond lengths



Bond angles

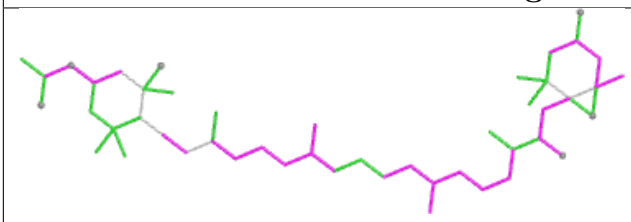


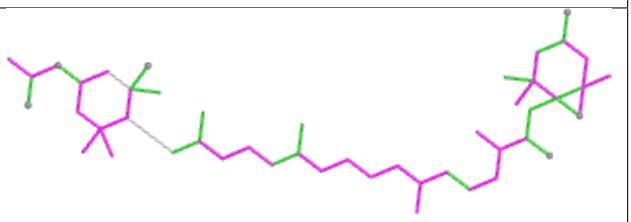
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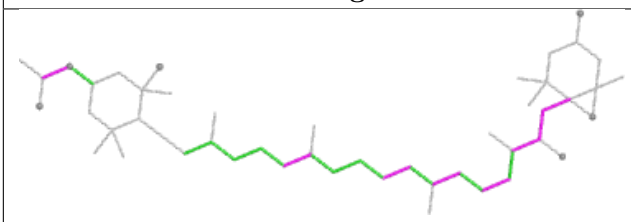


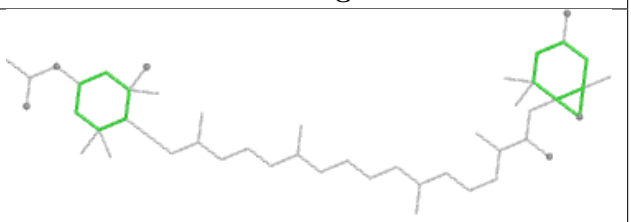
Rings

Ligand A86 14 316


Bond lengths

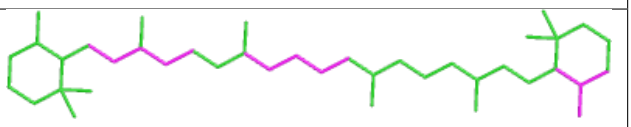

Bond angles

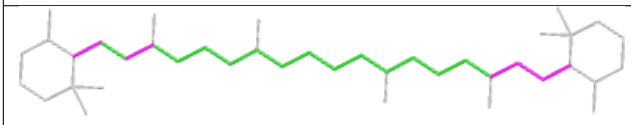

Torsions

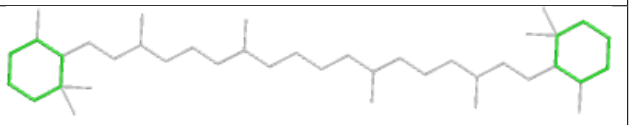

Rings

Ligand BCR H 101

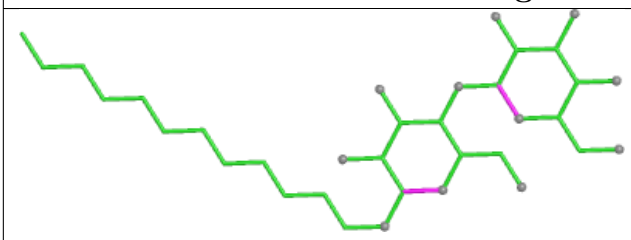

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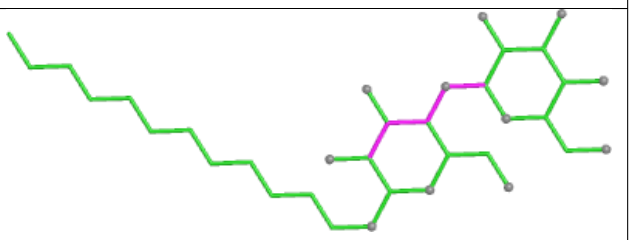

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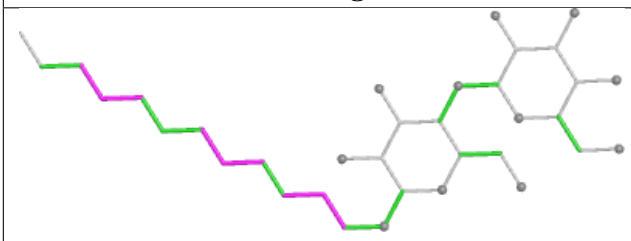

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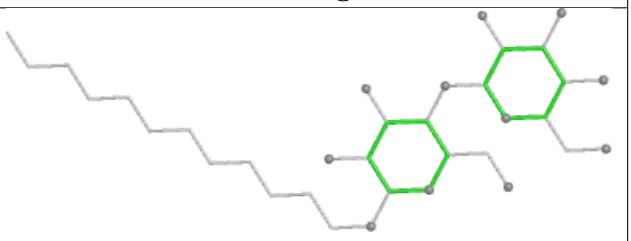

Rings

Ligand LMU 39 315

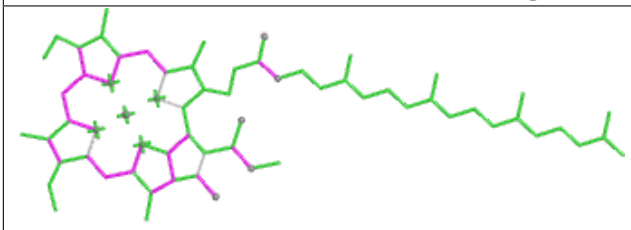

Bond lengths


Bond angles

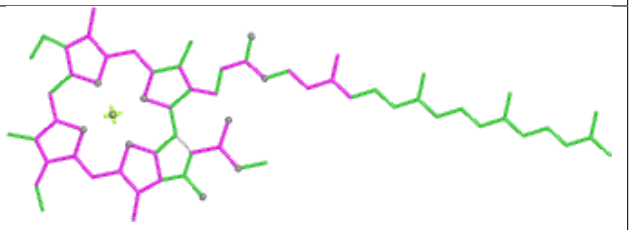

Torsions


Rings

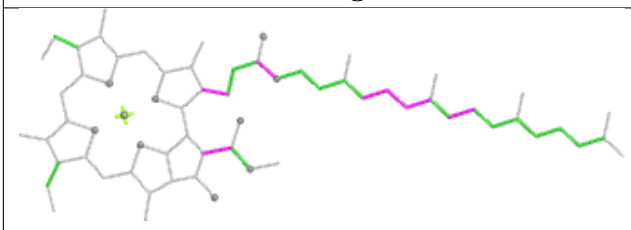
Ligand CLA C 508



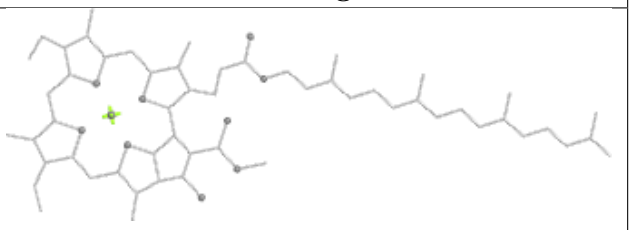
Bond lengths



Bond angles

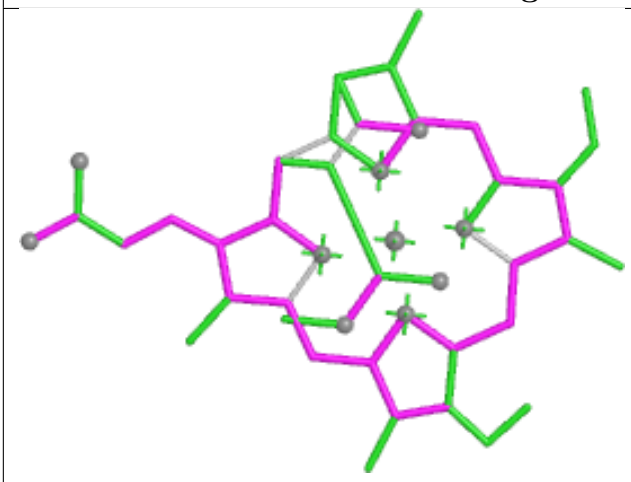


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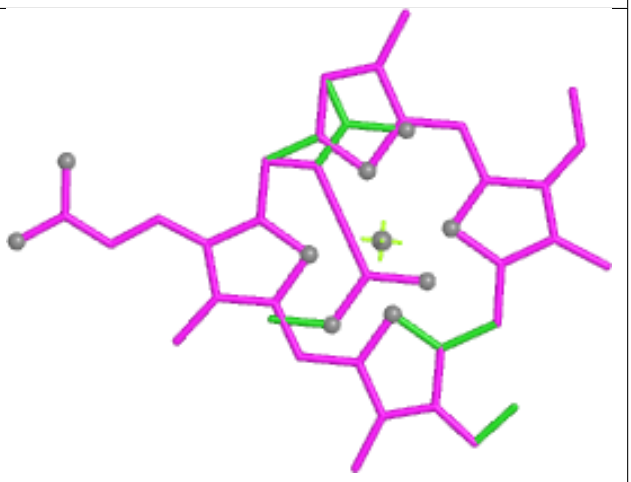


Rings

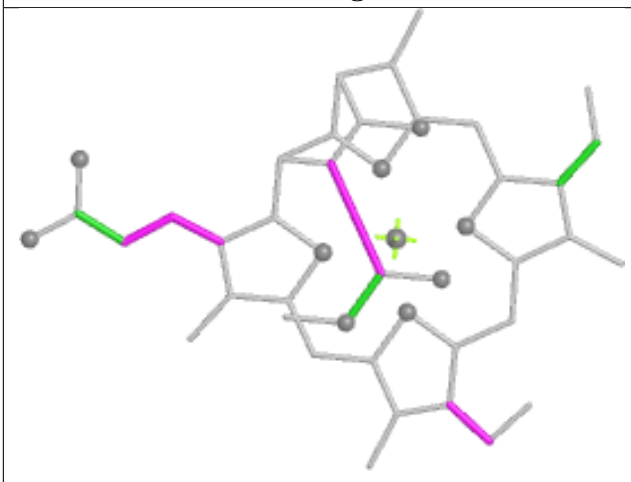
Ligand KC1 18 207



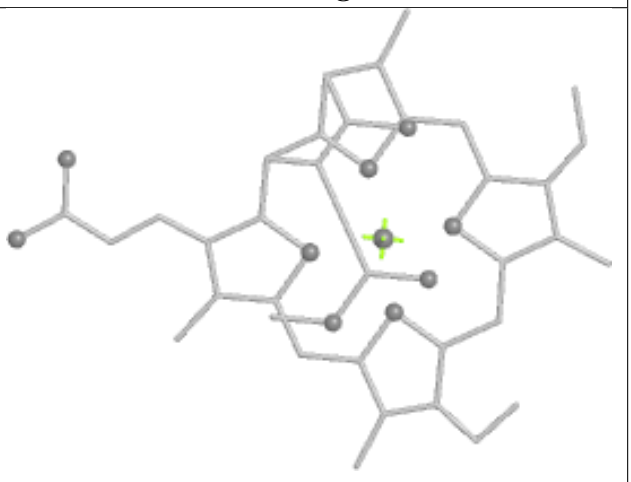
Bond lengths



Bond angles

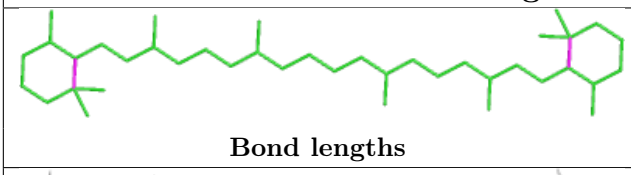


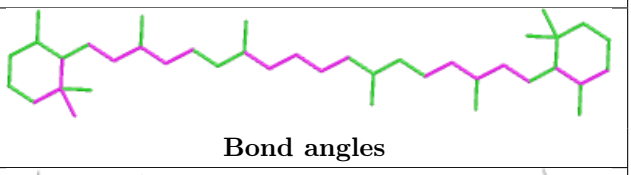
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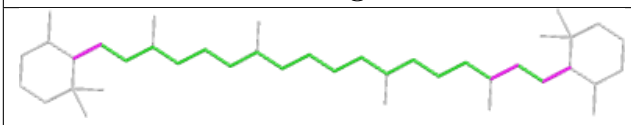


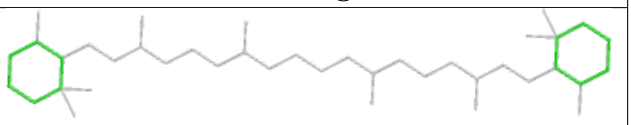
Rings

Ligand BCR C 514

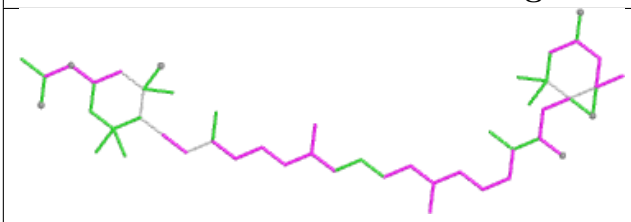

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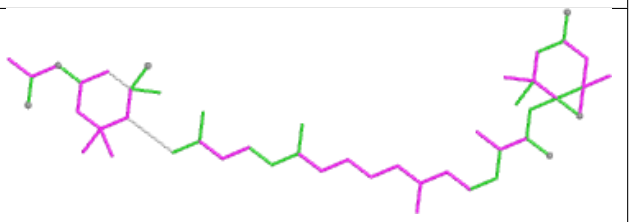

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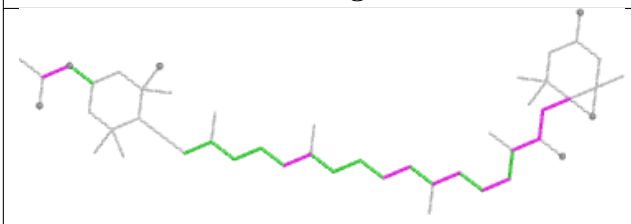

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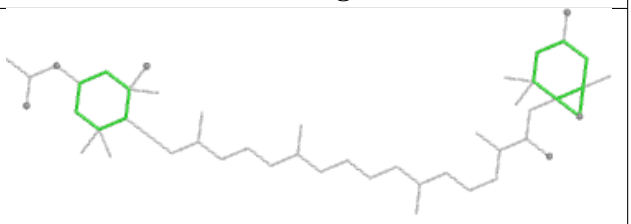

Rings

Ligand A86 12 217

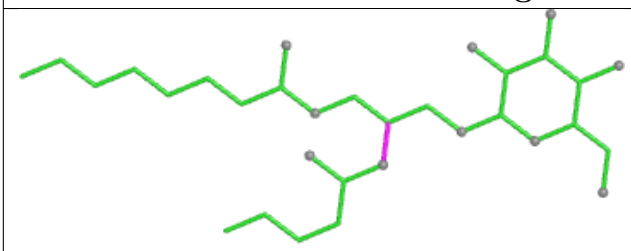

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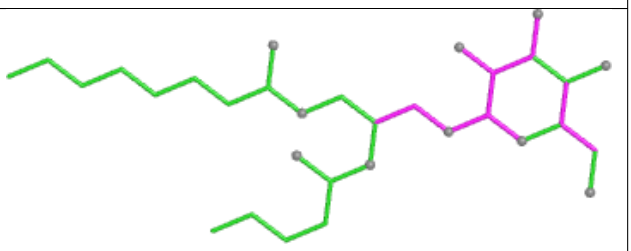

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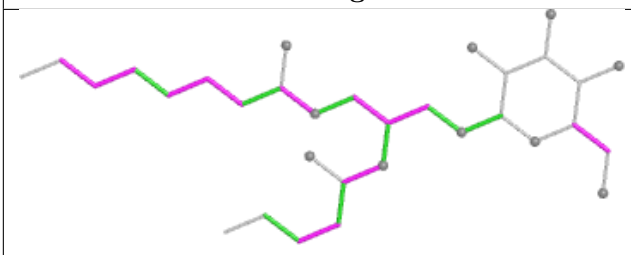

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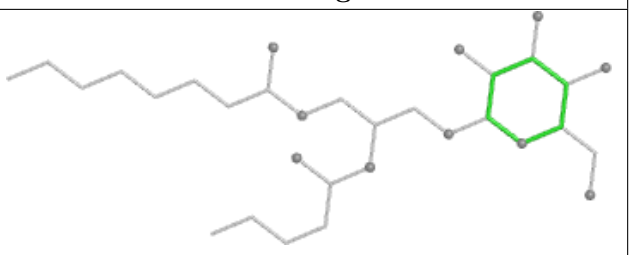

Rings

Ligand LMG 31 317

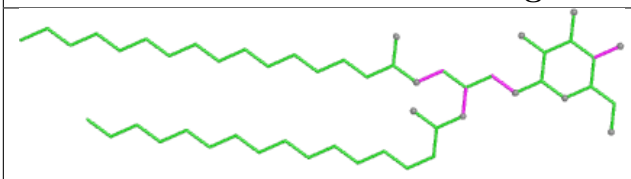

Bond lengths


Bond angles

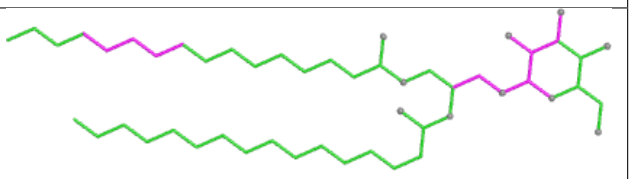

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Rings

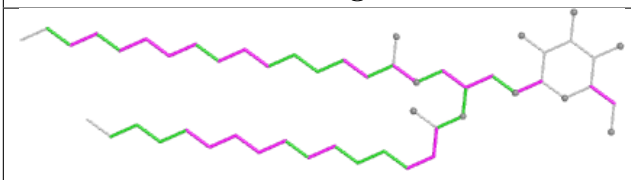
Ligand LMG c 518



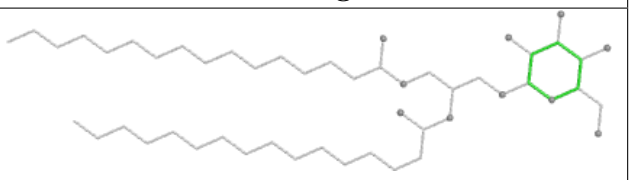
Bond lengths



Bond angles

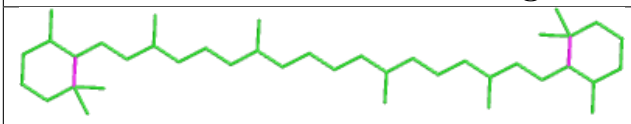


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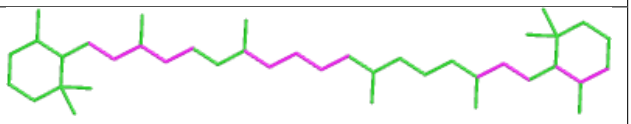


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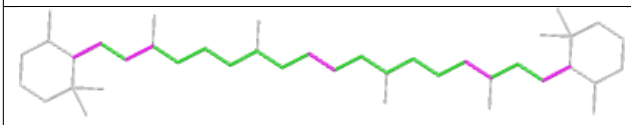
Ligand BCR A 406



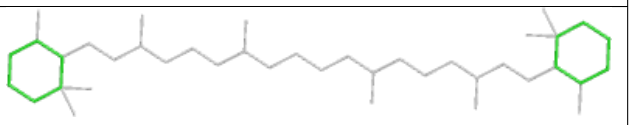
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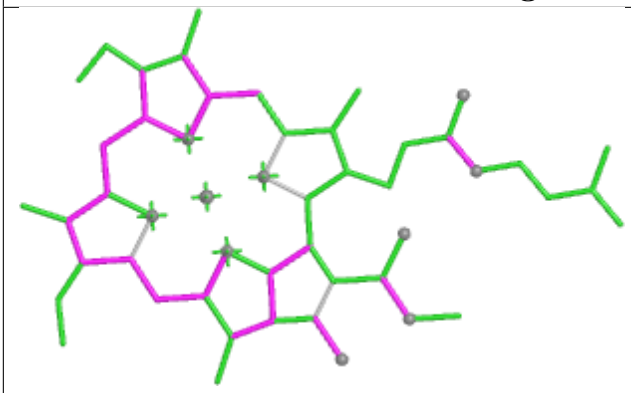


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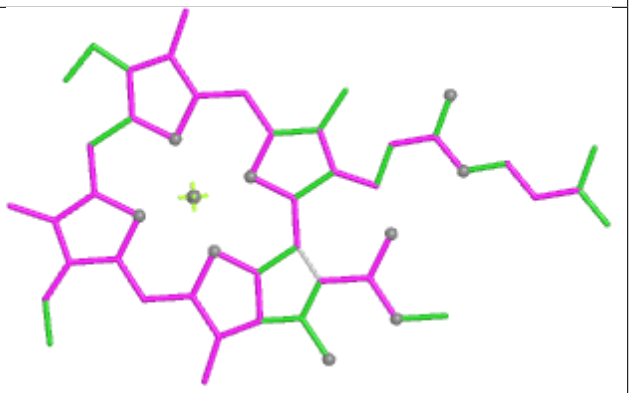


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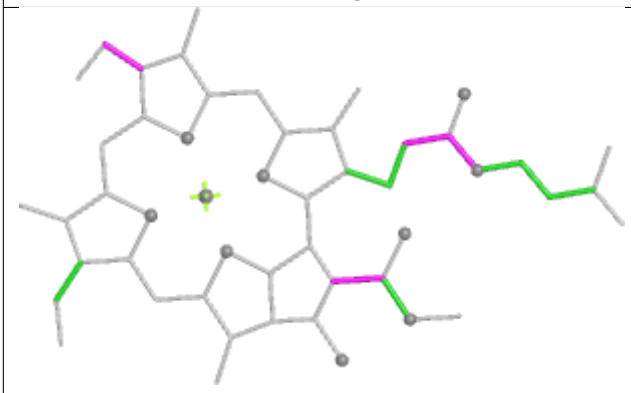
Ligand CLA 20 306



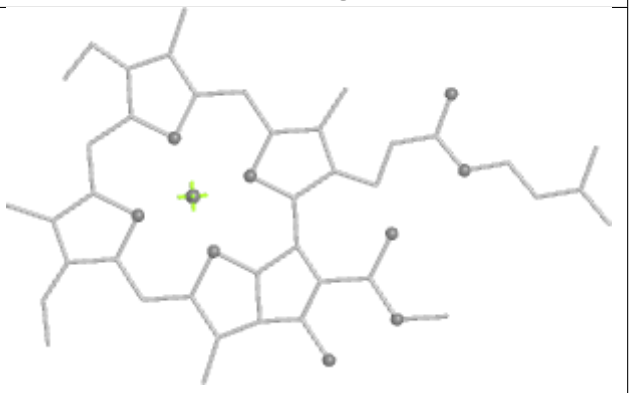
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Bond angles

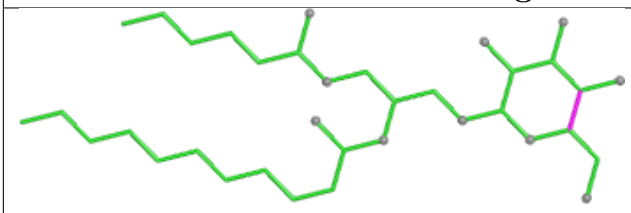


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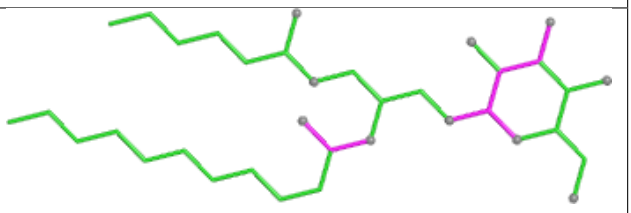


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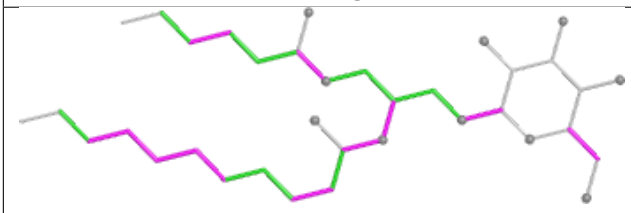
Ligand LMG 36 314



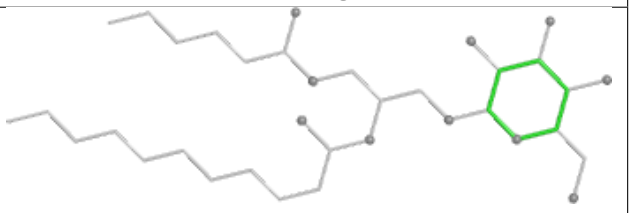
Bond lengths



Bond angles

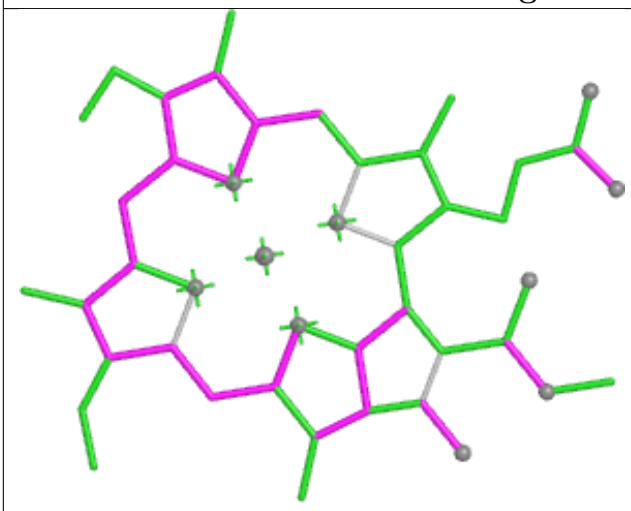


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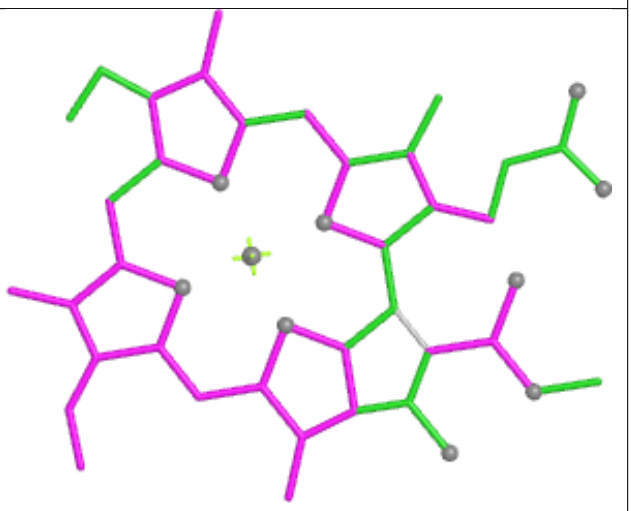


Rings

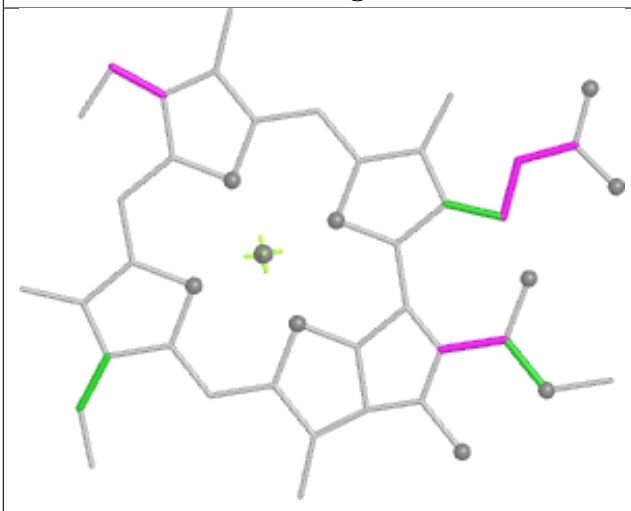
Ligand CLA 35 305



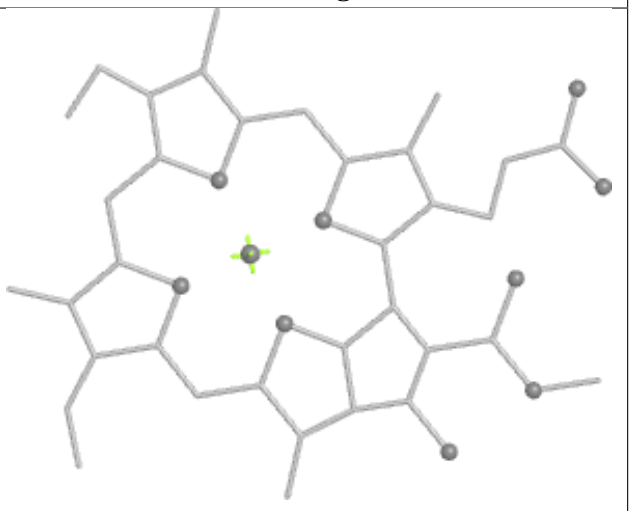
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Bond angles

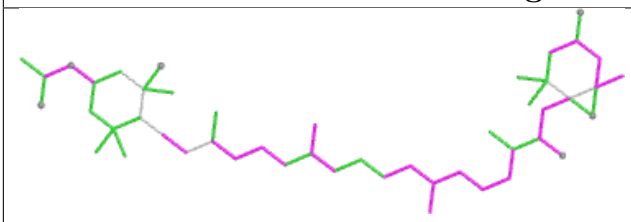


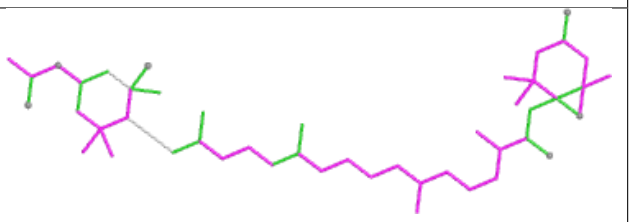
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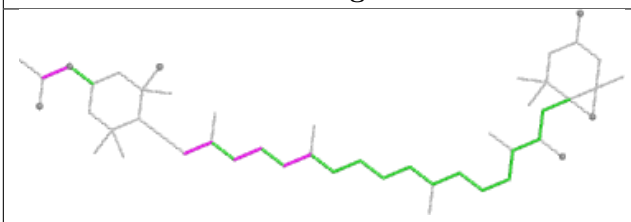


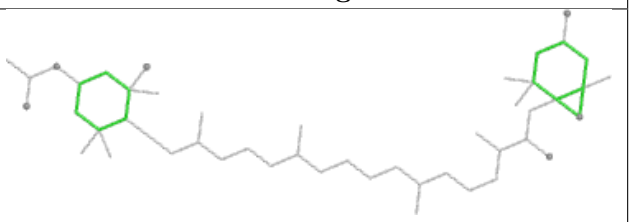
Rings

Ligand A86 31 312

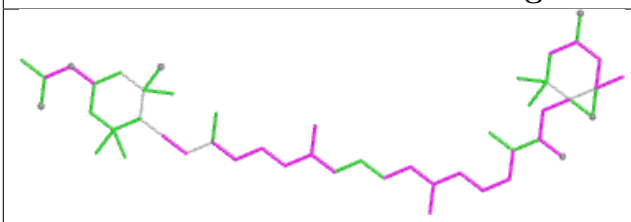

Bond lengths

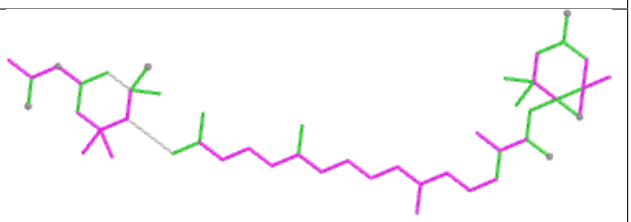

Bond angles

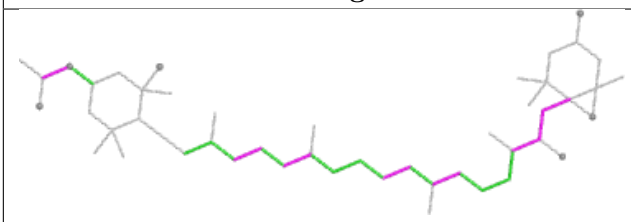

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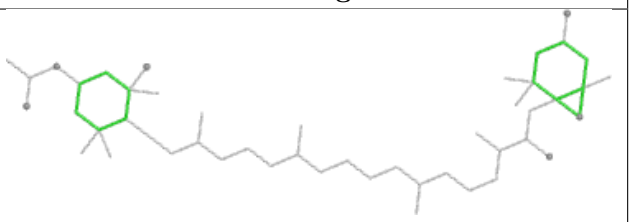

Rings

Ligand A86 14 314

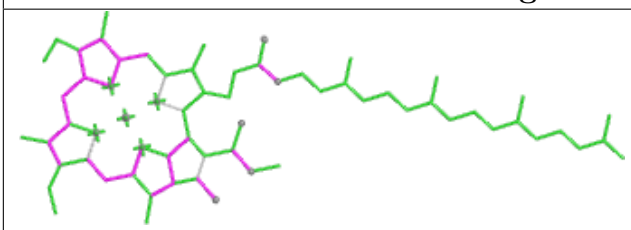

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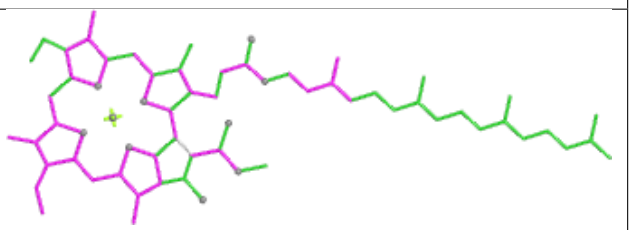

Bond angles

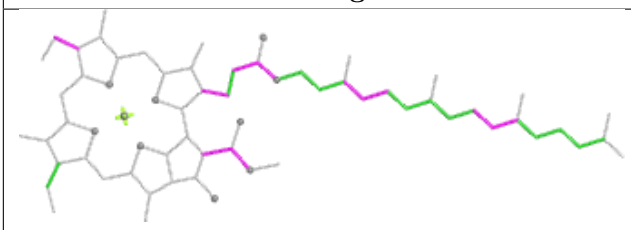

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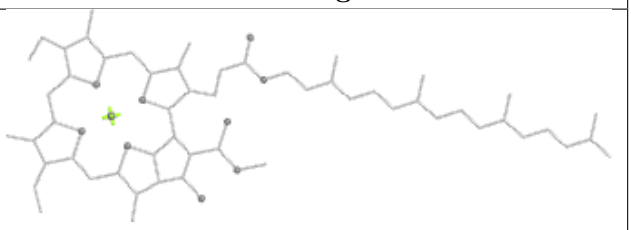

Rings

Ligand CLA 41 206

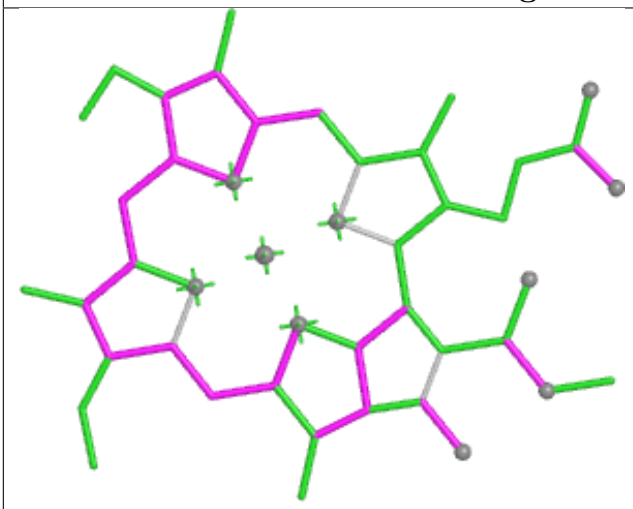

Bond lengths


Bond angles

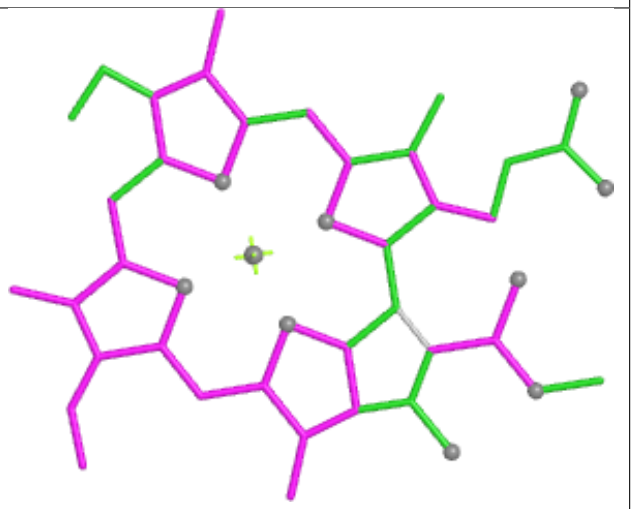

Torsions


Rings

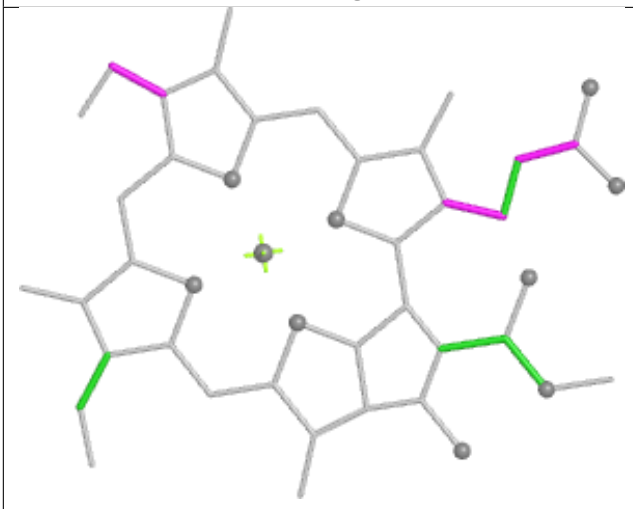
Ligand CLA 14 305



Bond lengths



Bond angles

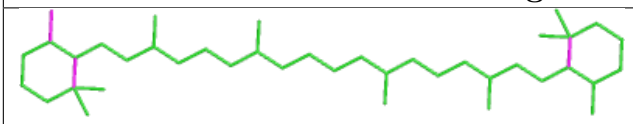


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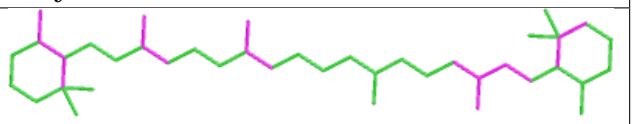


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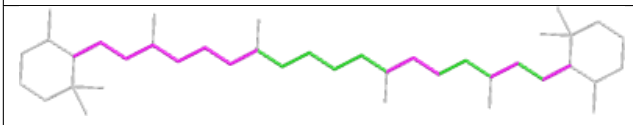
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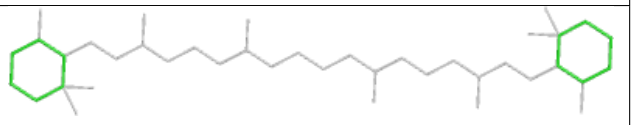
Bond lengths



Bond angles

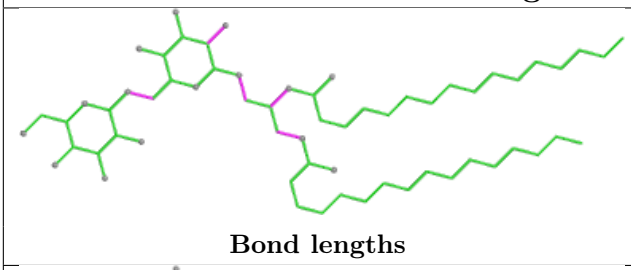


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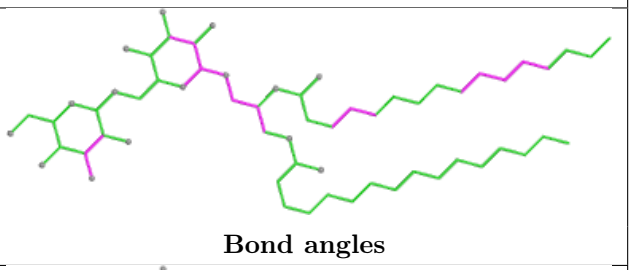


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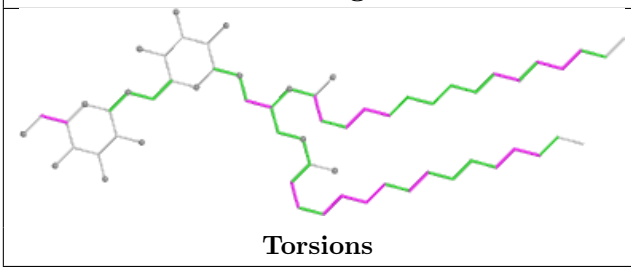
Ligand DGD h 102



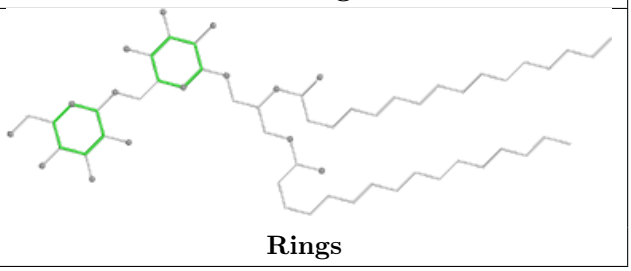
Bond lengths



Bond angles

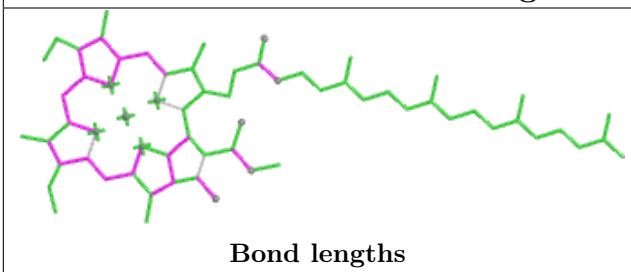


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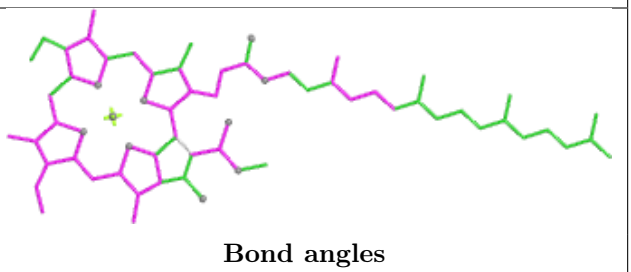


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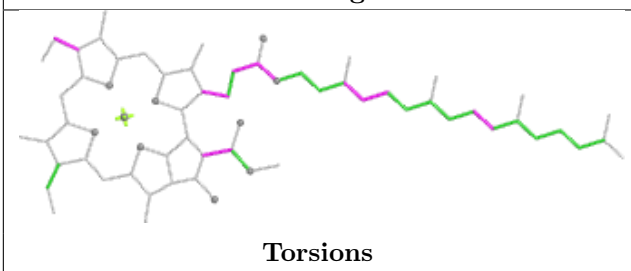
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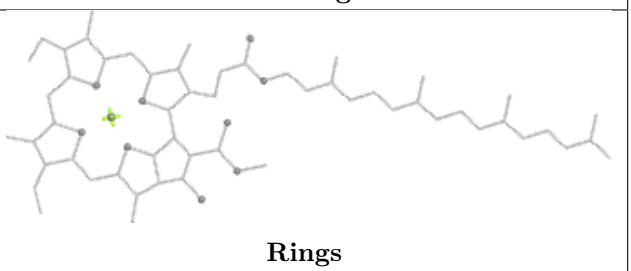
Bond lengths



Bond angles

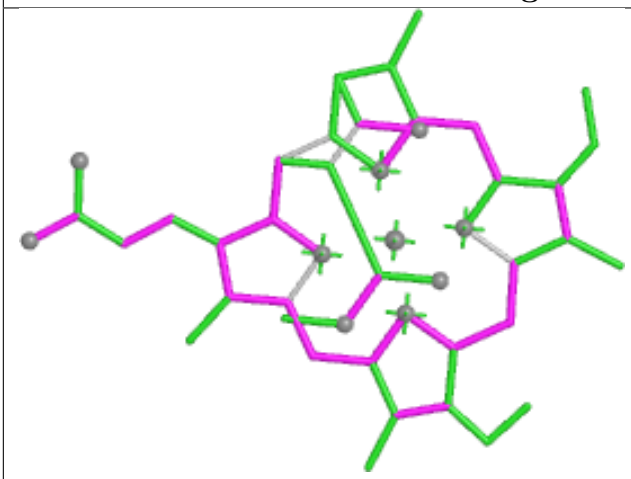


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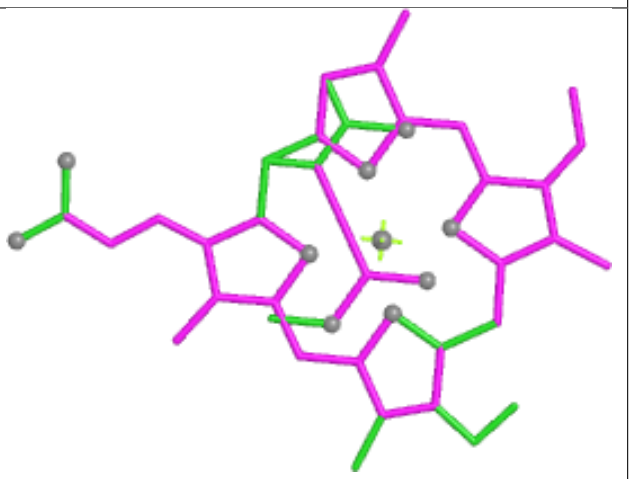


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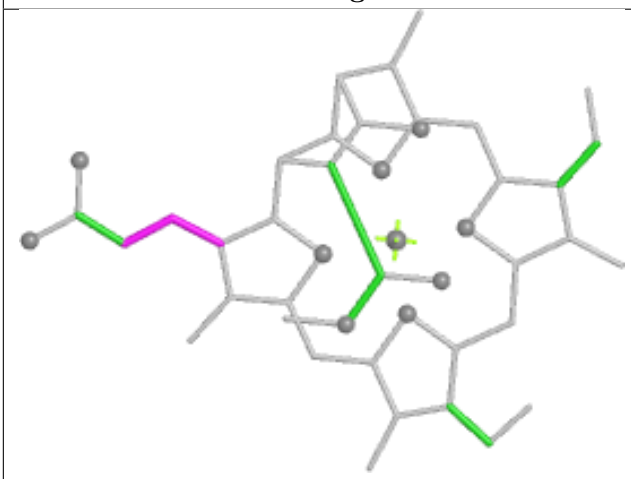
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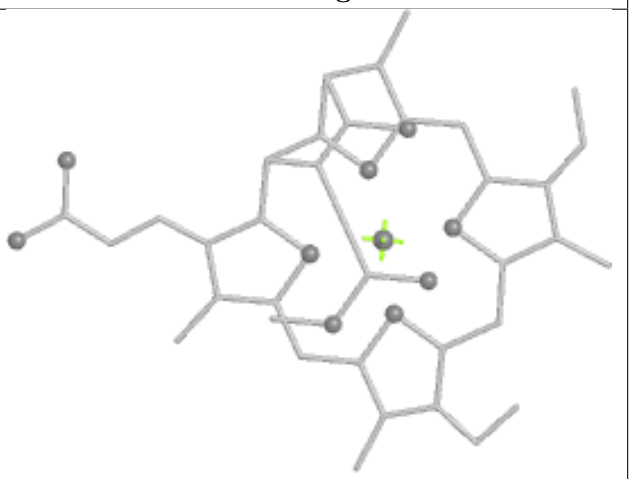
Bond lengths



Bond angles



Torsions



Rings

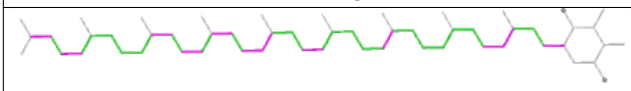
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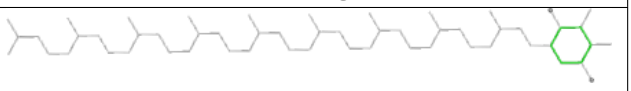
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Bond angles

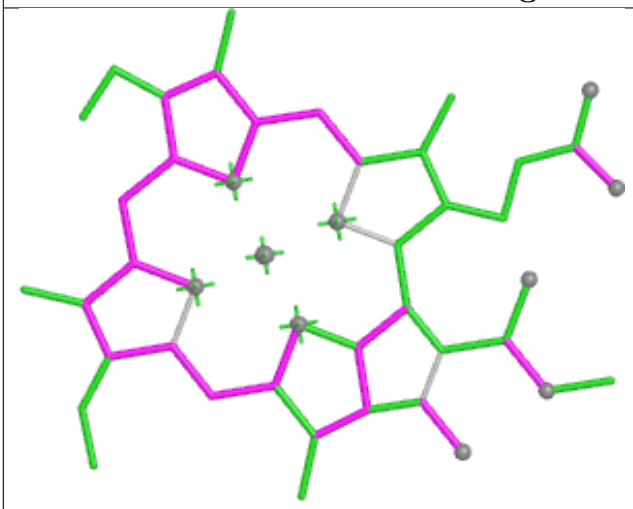


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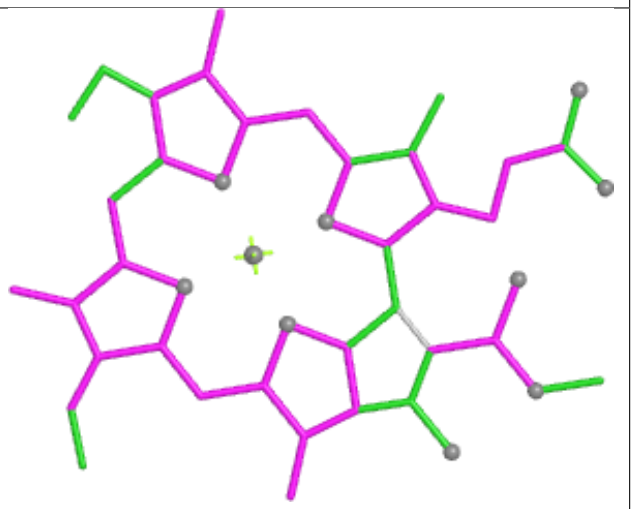


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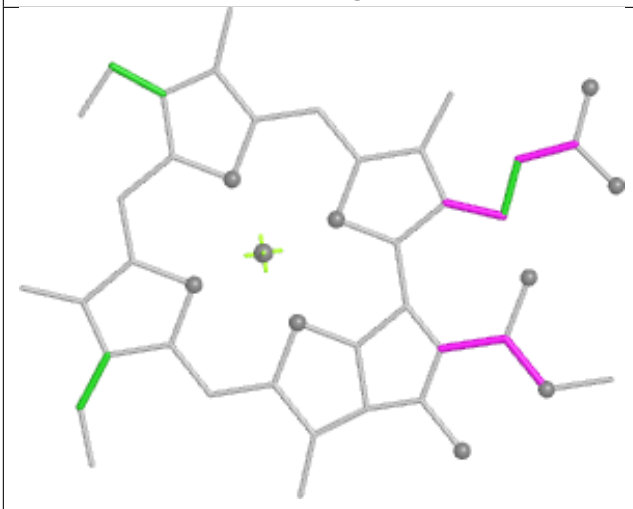
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Bond lengths



Bond angles

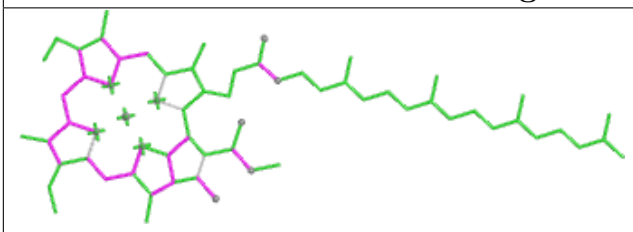


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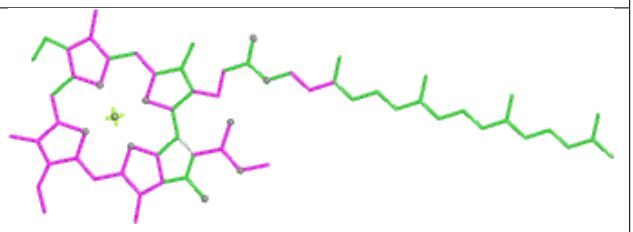


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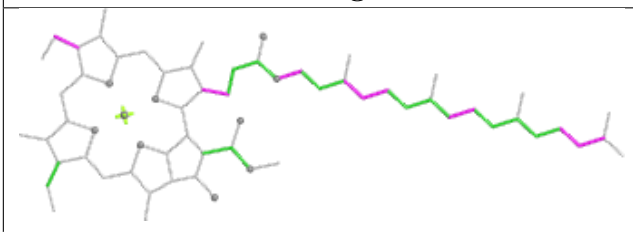
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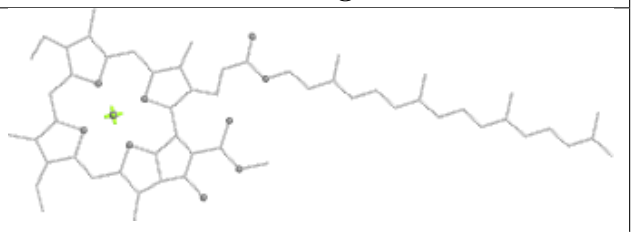
Bond lengths



Bond angles

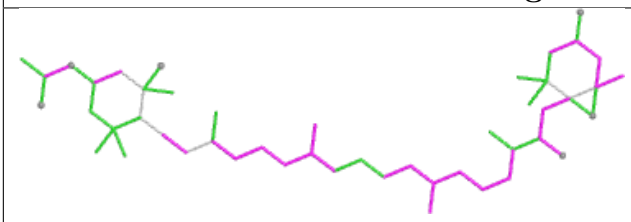


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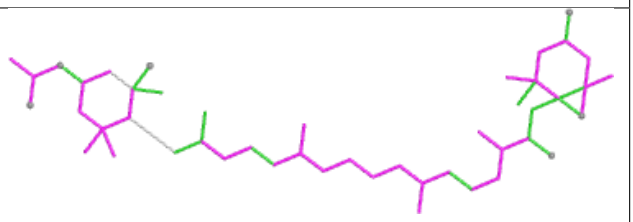


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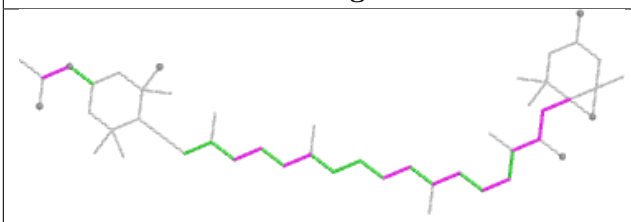
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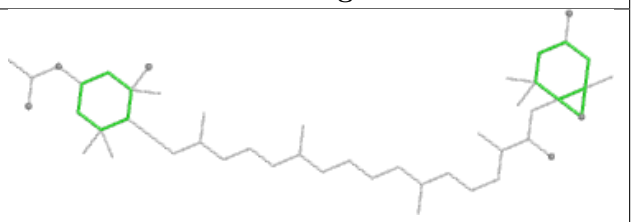
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Bond angles

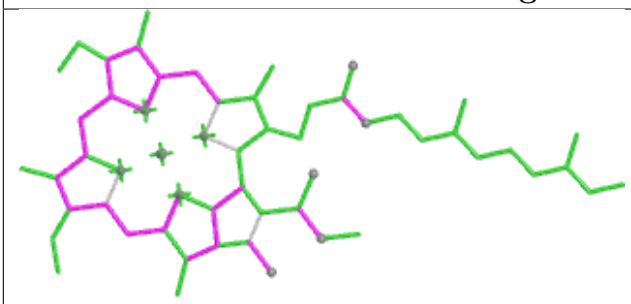


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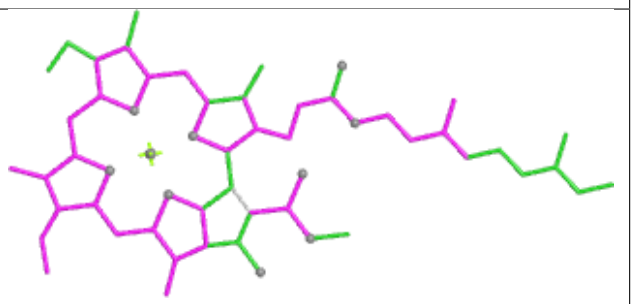


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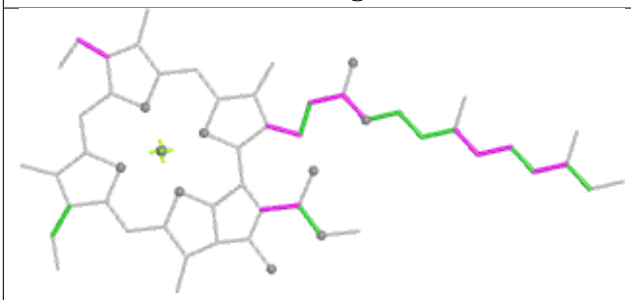
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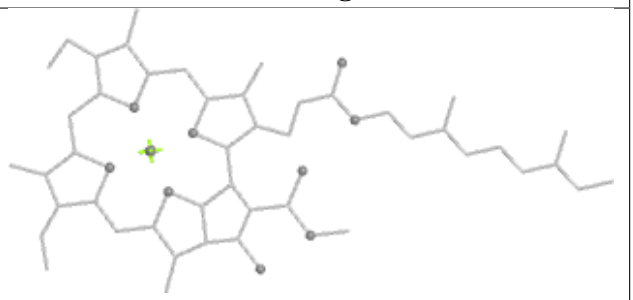
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Bond angles

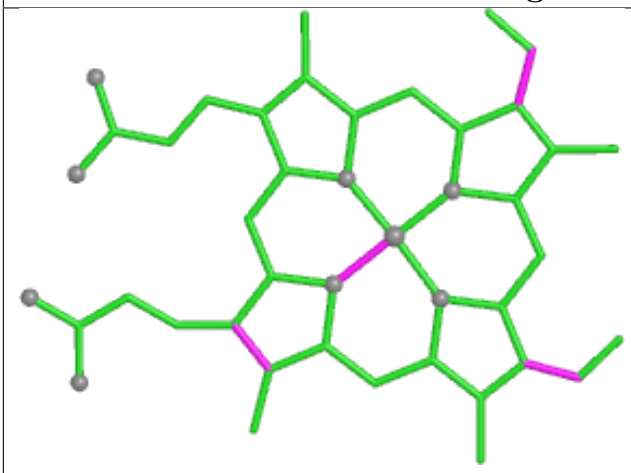


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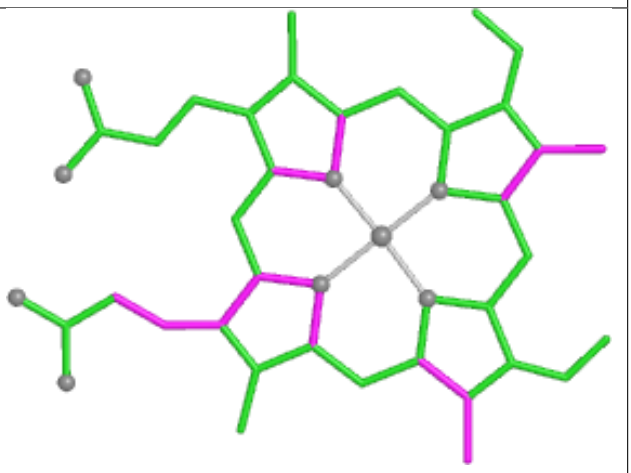


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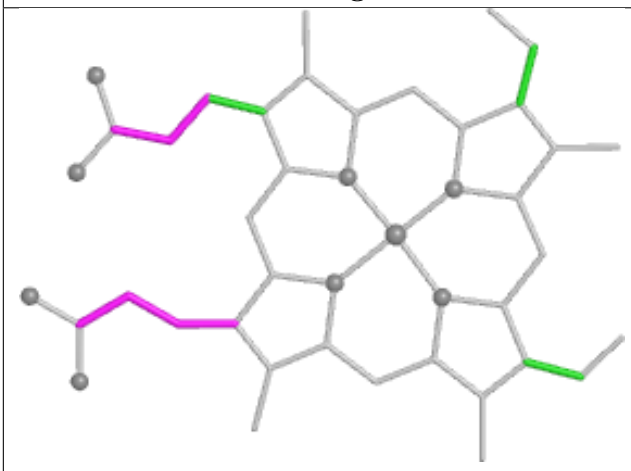
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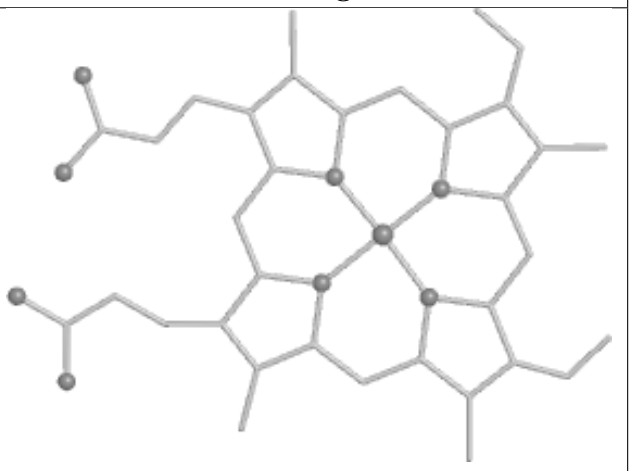
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Bond angles

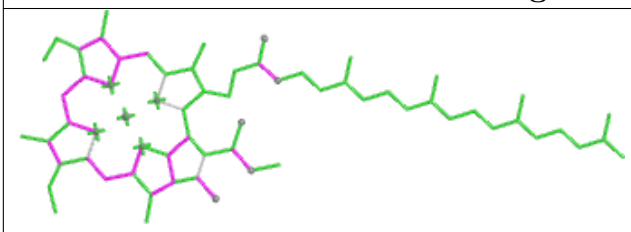


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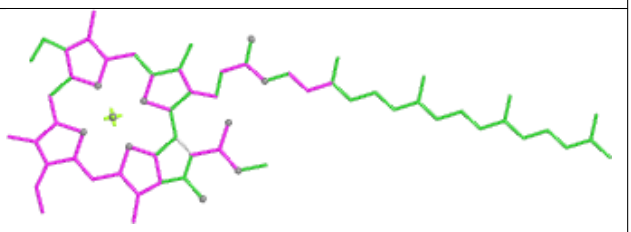


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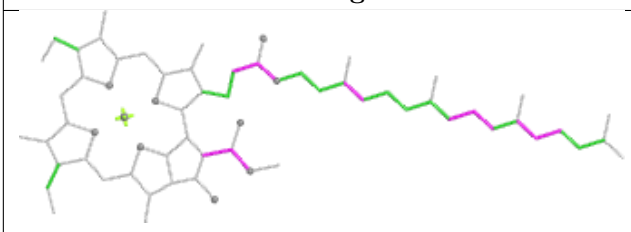
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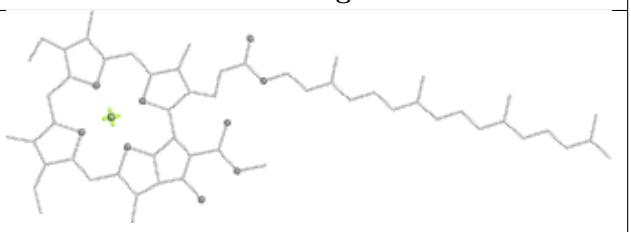
Bond lengths



Bond angles

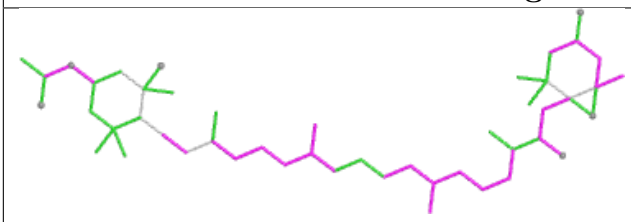


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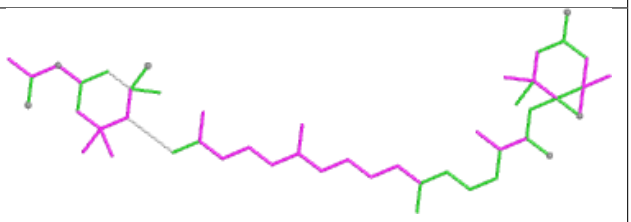


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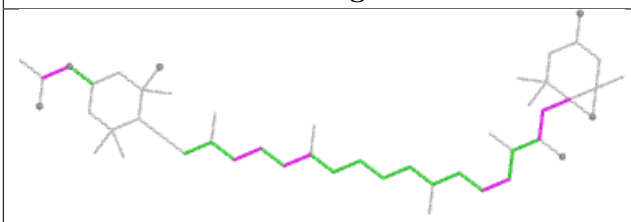
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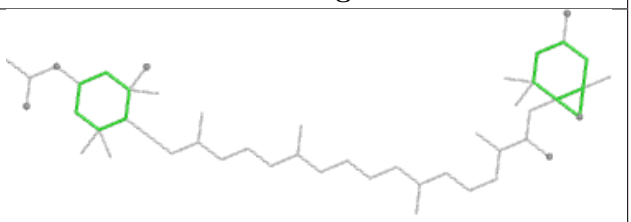
Bond lengths



Bond angles

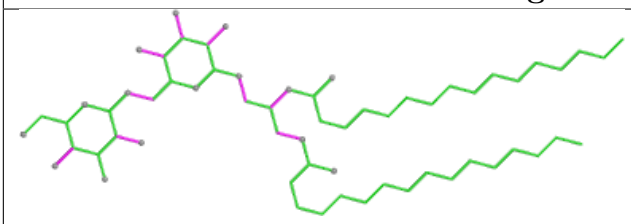


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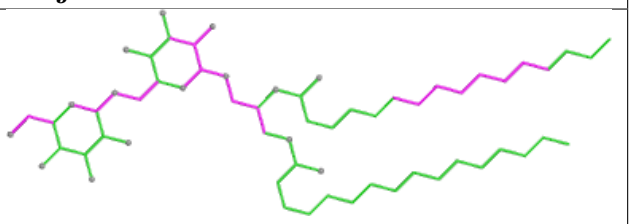


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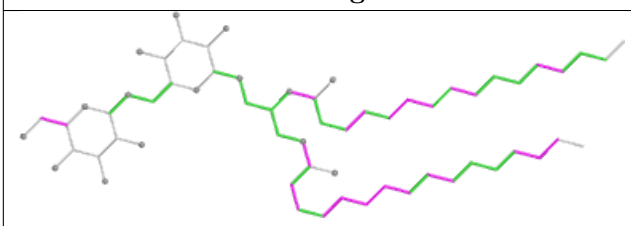
Ligand DGD j 101



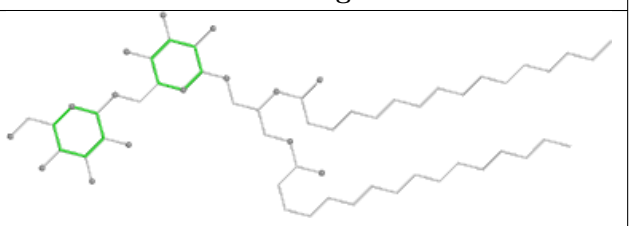
Bond lengths



Bond angles

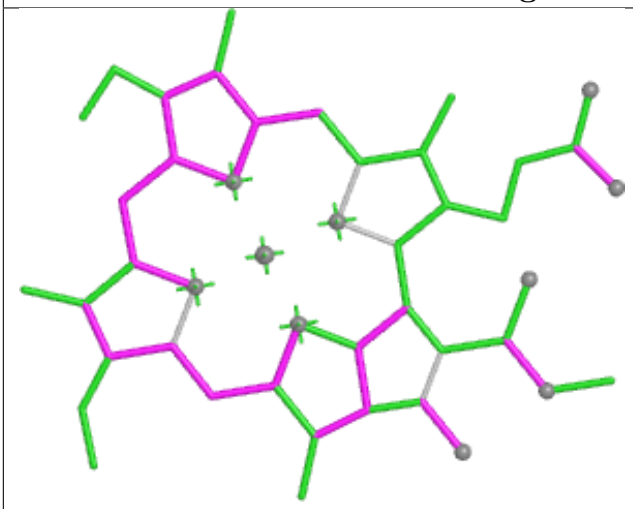


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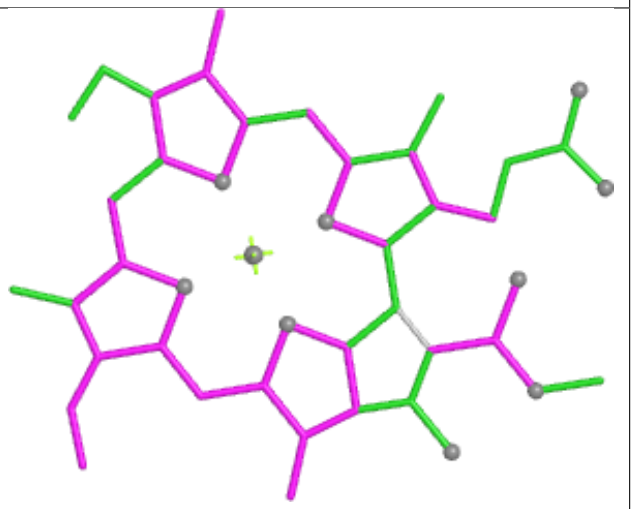


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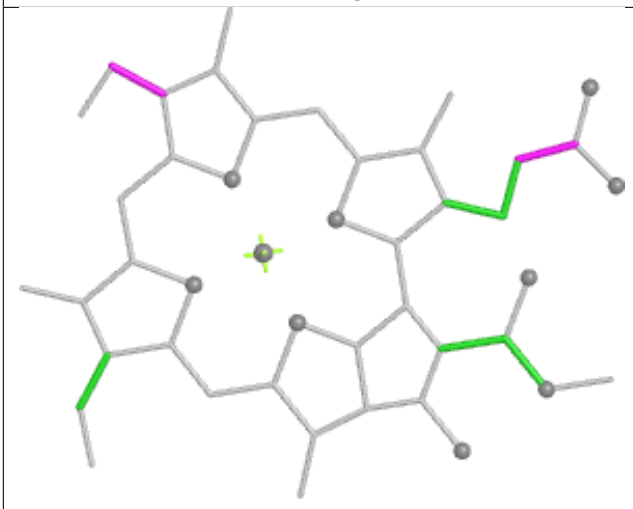
Ligand CLA 14 310



Bond lengths



Bond angles

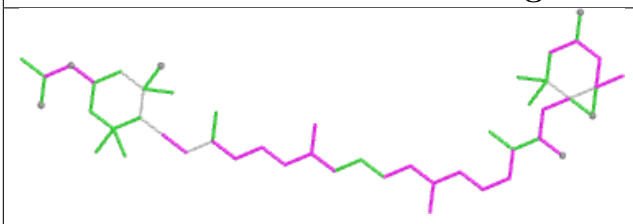


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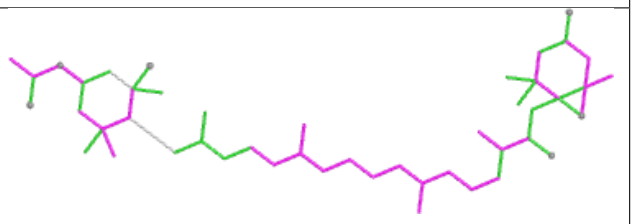


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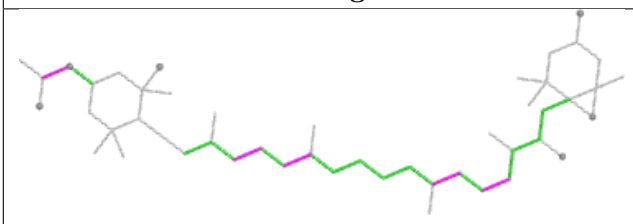
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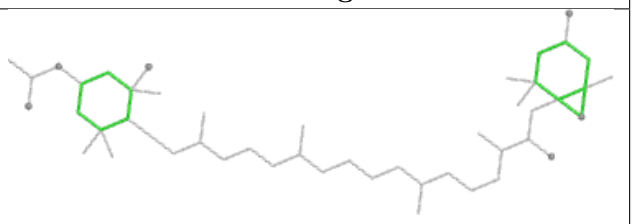
Bond lengths



Bond angles

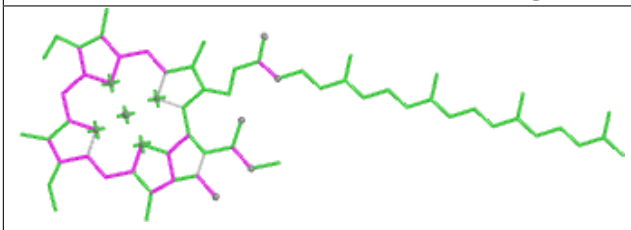


Torsions

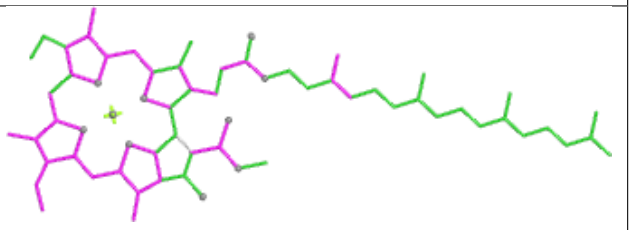


Rings

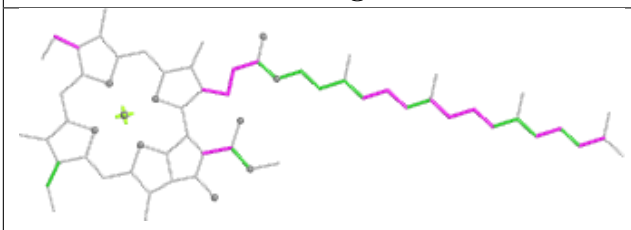
Ligand CLA b 501



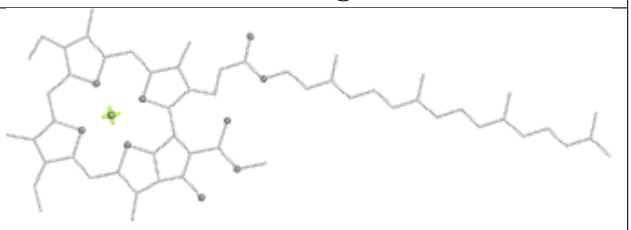
Bond lengths



Bond angles

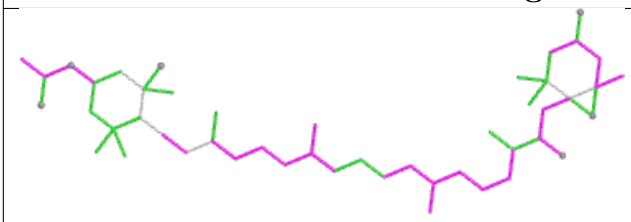


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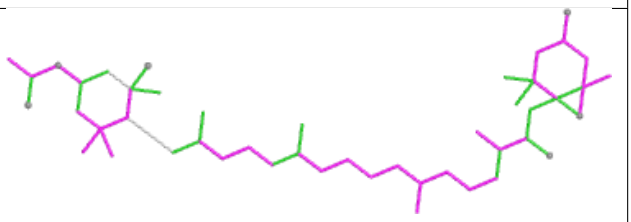


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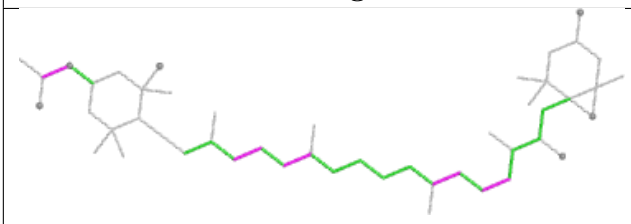
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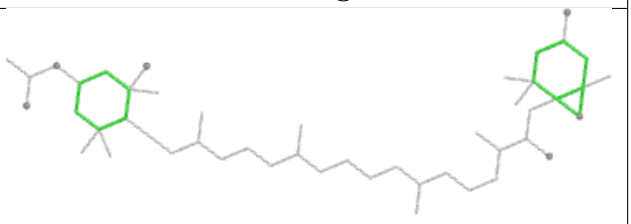
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Bond angles

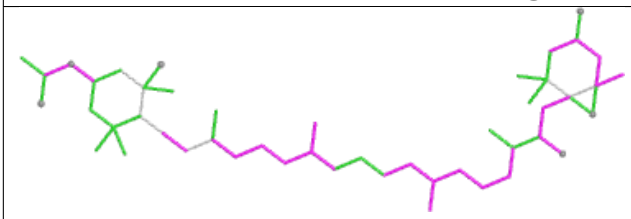


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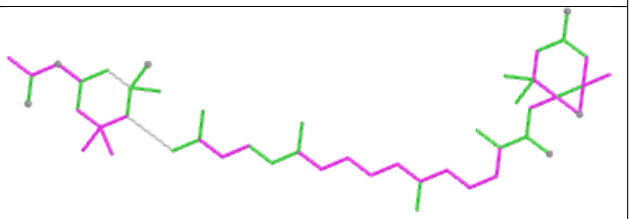


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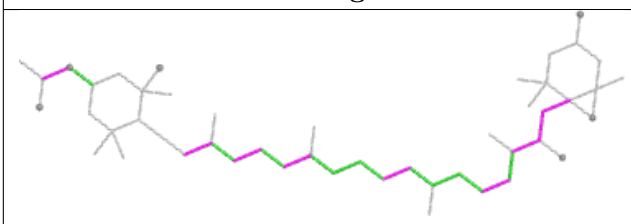
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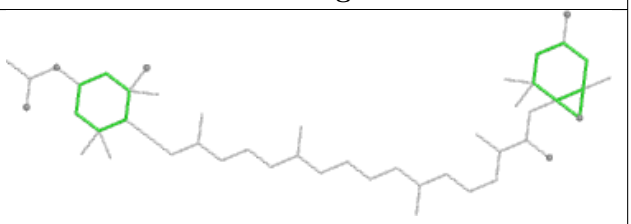
Bond lengths



Bond angles

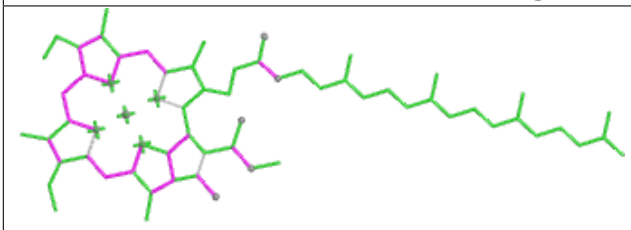


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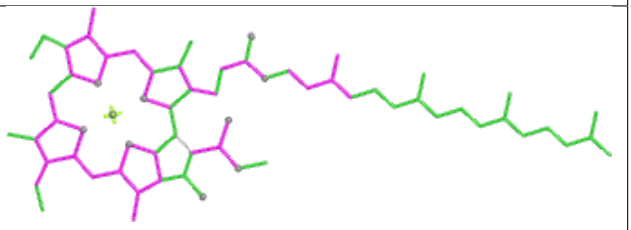


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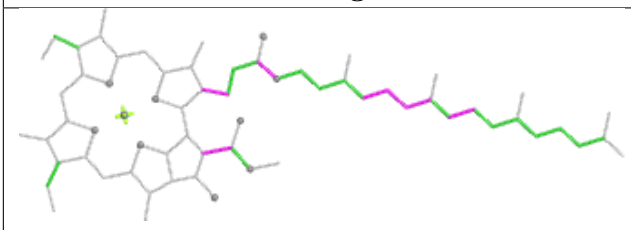
Ligand CLA c 508



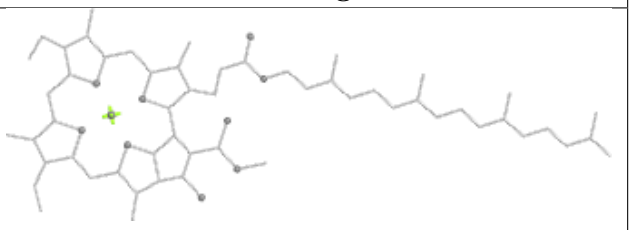
Bond lengths



Bond angles

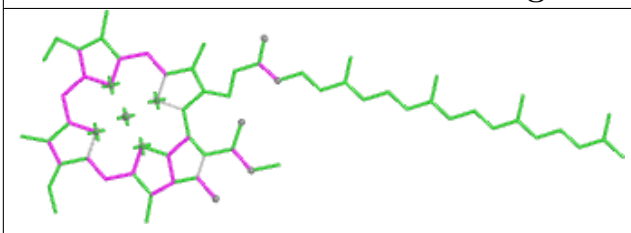


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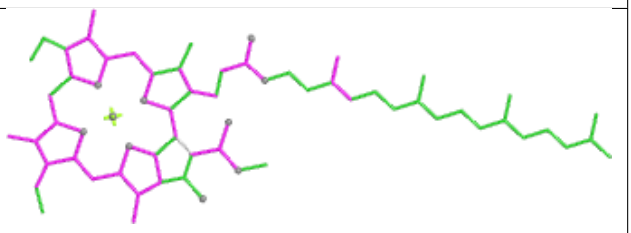


Rings

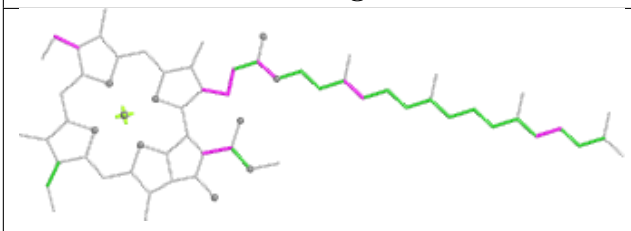
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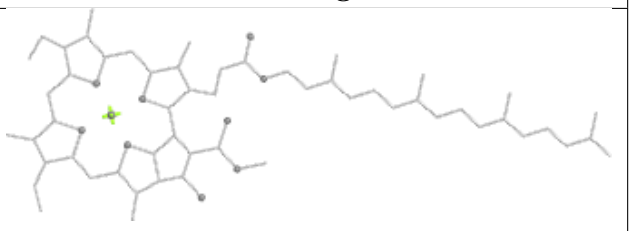
Bond lengths



Bond angles

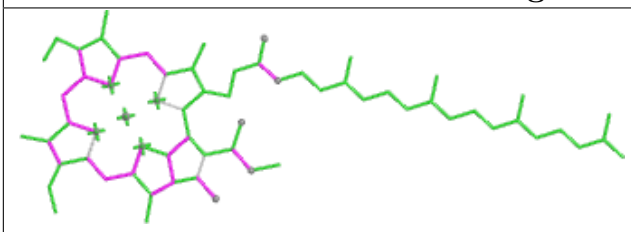


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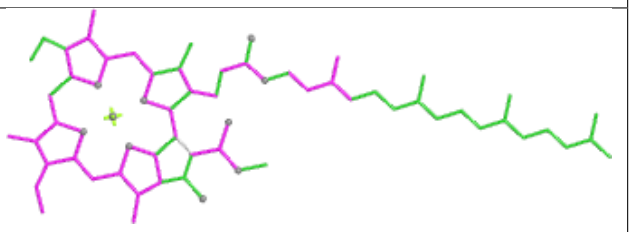


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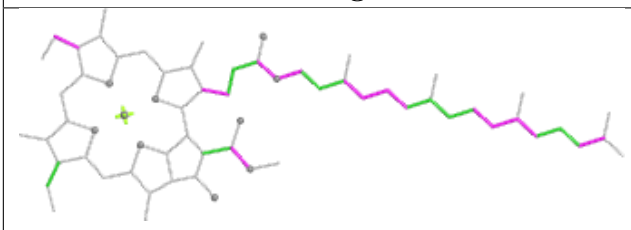
Ligand CLA d 404



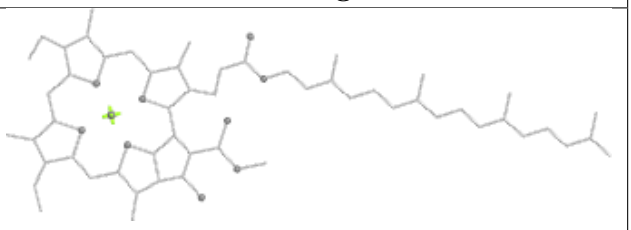
Bond lengths



Bond angles

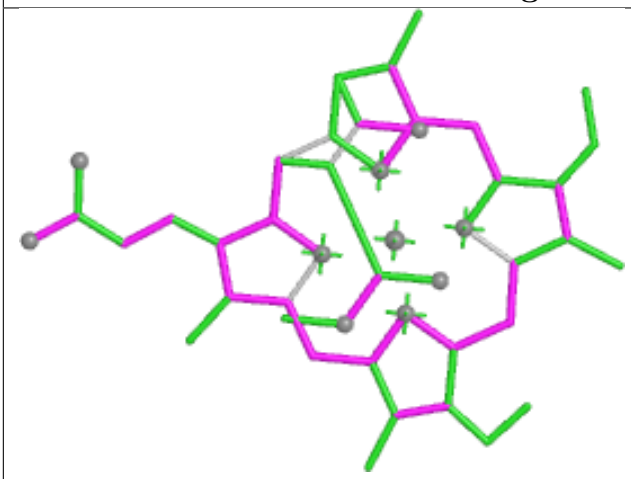


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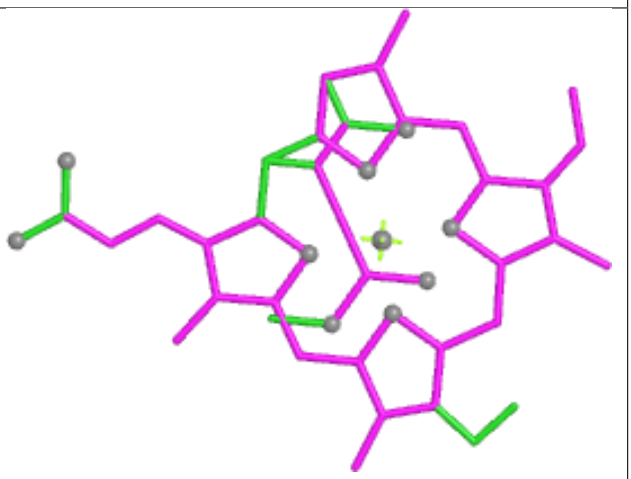


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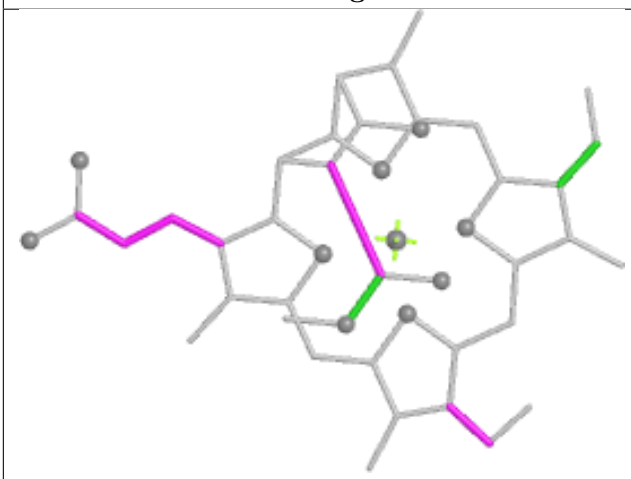
Ligand KC1 14 309



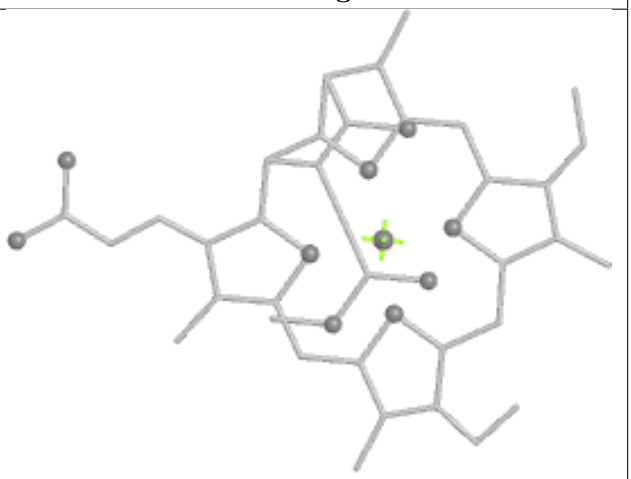
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Bond angles

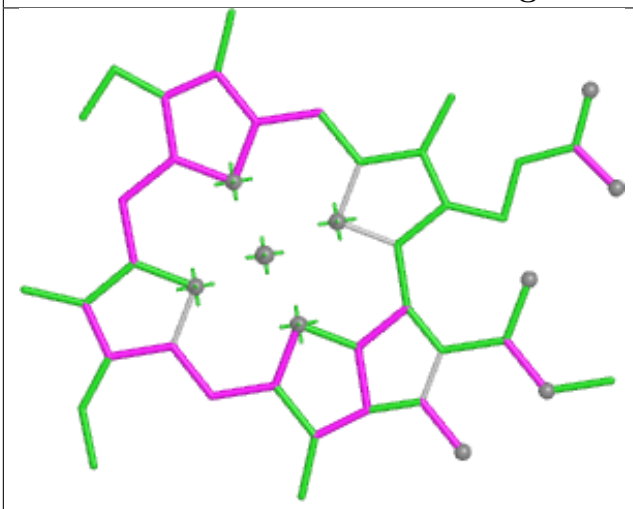


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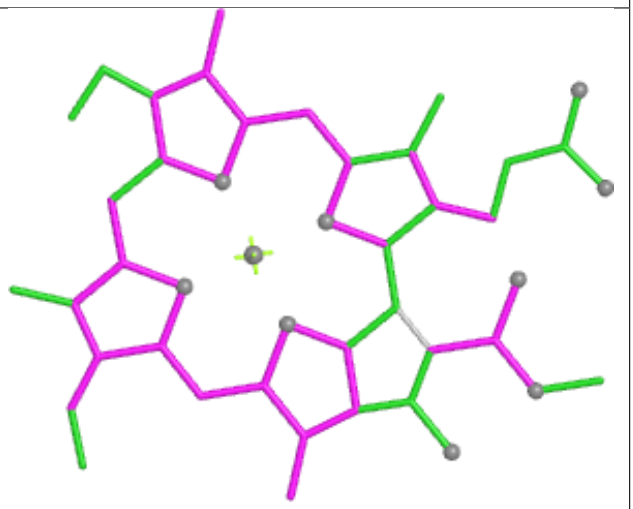


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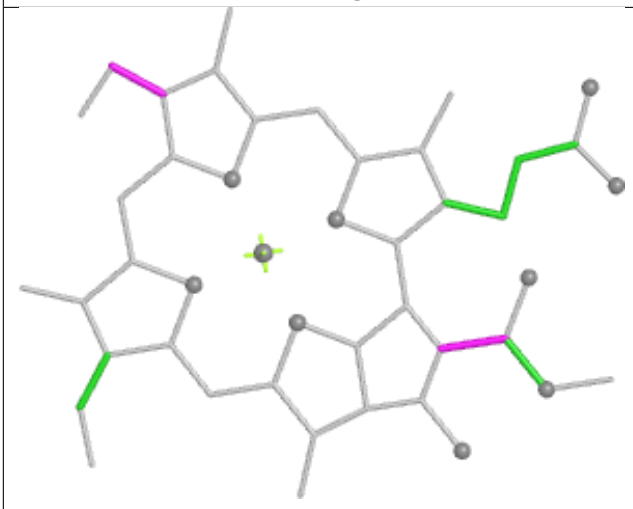
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Bond lengths



Bond angles

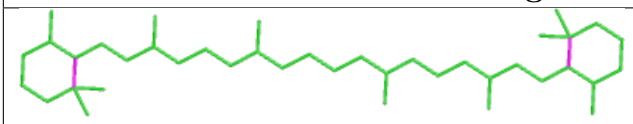


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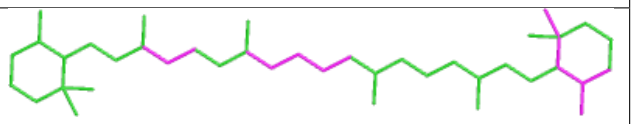


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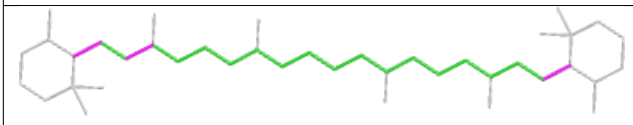
Ligand BCR b 518



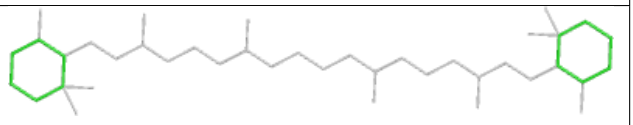
Bond lengths



Bond angles

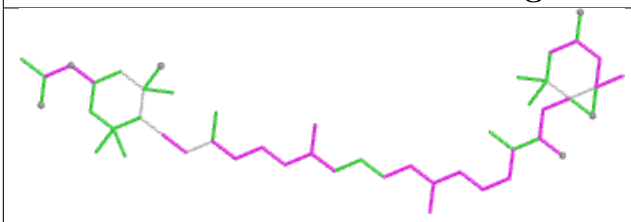


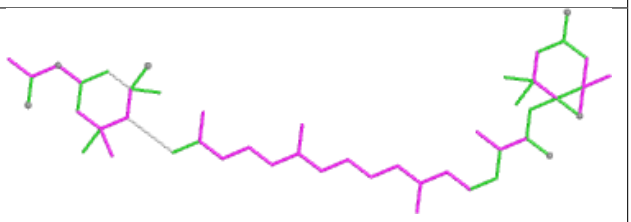
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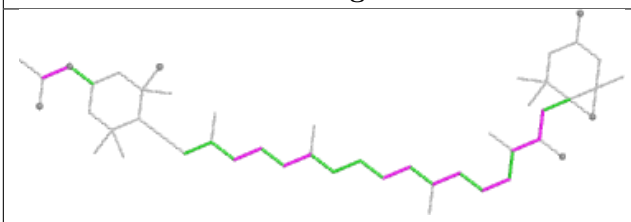


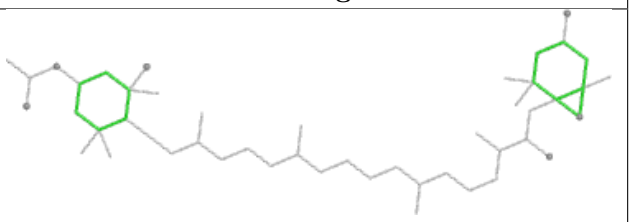
Rings

Ligand A86 35 314

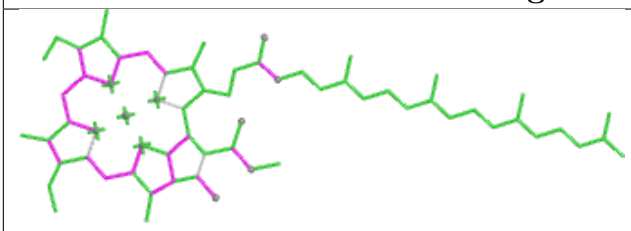

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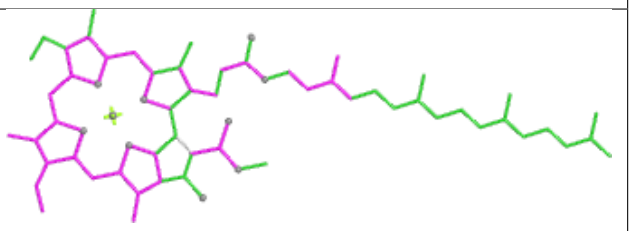

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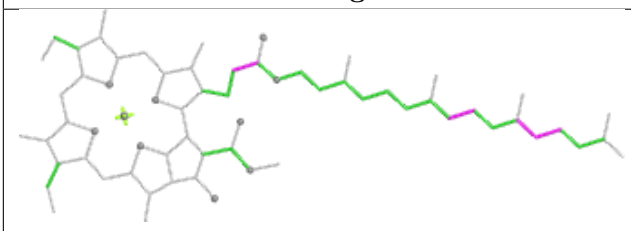

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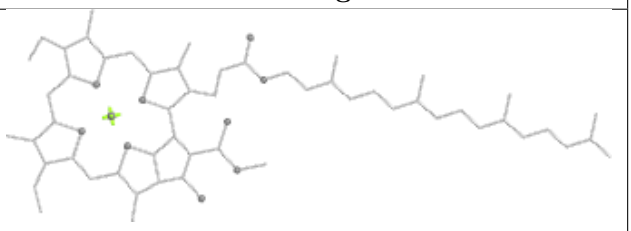

Rings

Ligand CLA b 508

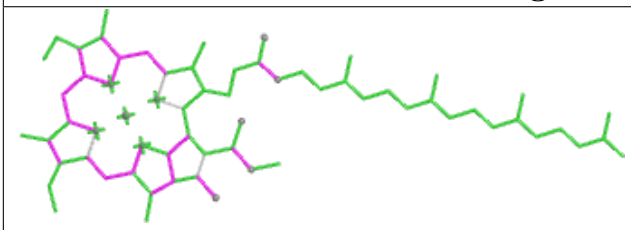

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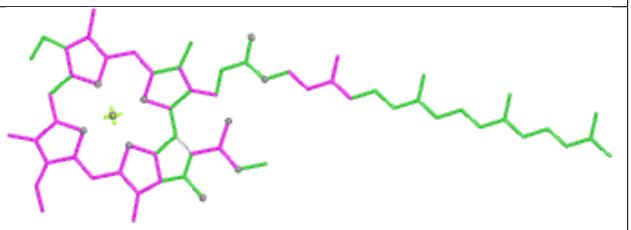

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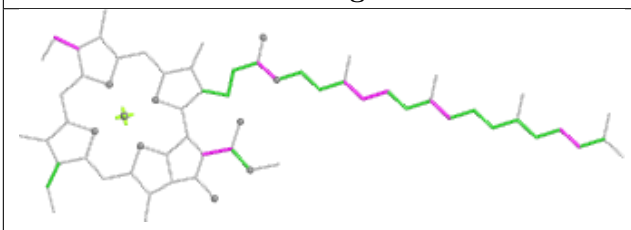

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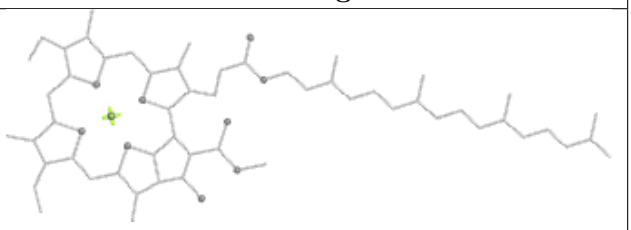

Rings

Ligand CLA c 504

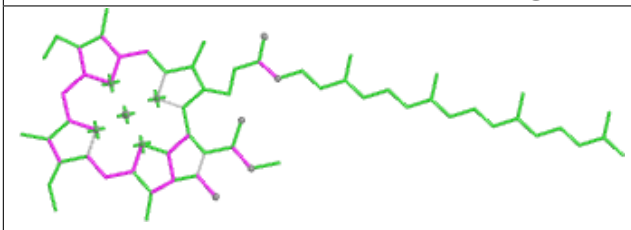

Bond lengths


Bond angles

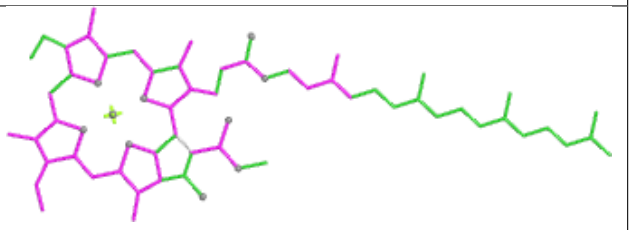

Torsions


Rings

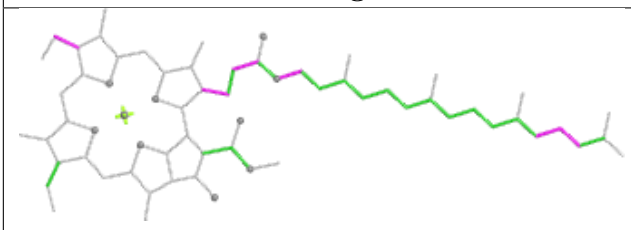
Ligand CLA d 403



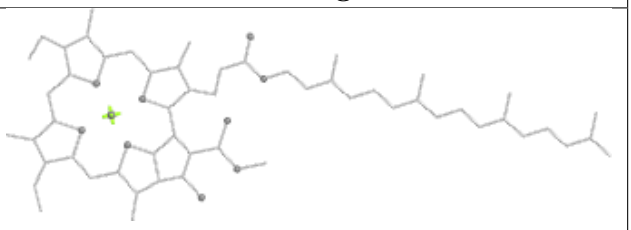
Bond lengths



Bond angles

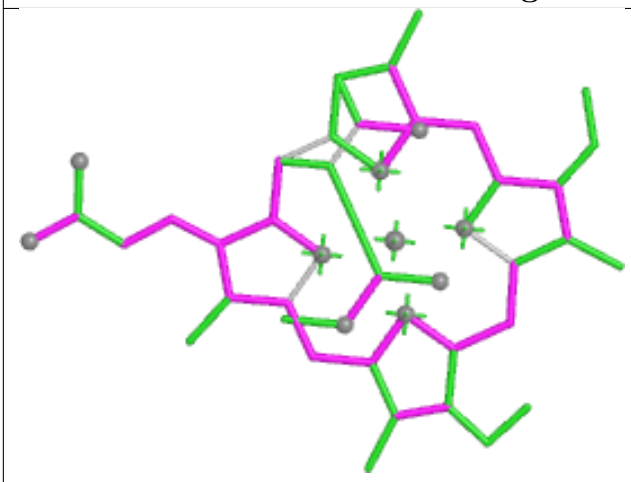


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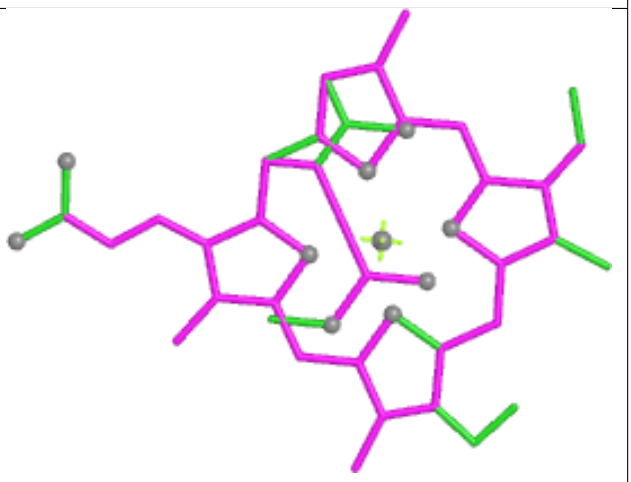


Rings

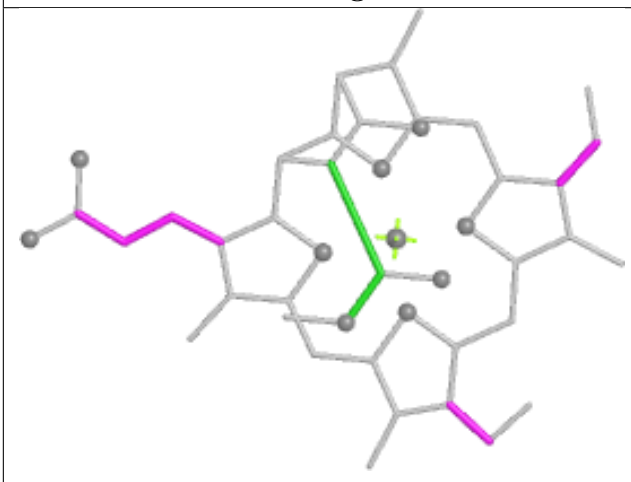
Ligand KC1 37 305



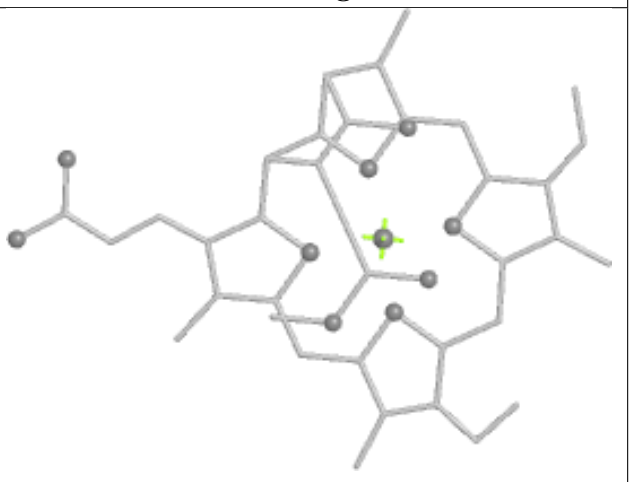
Bond lengths



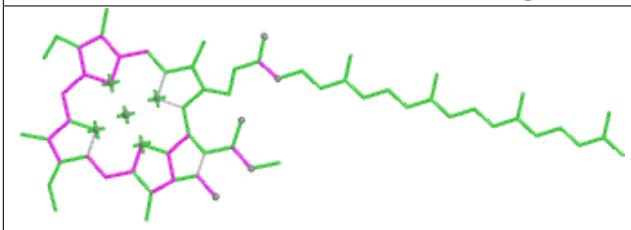
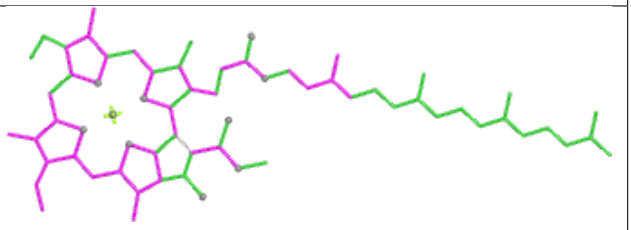
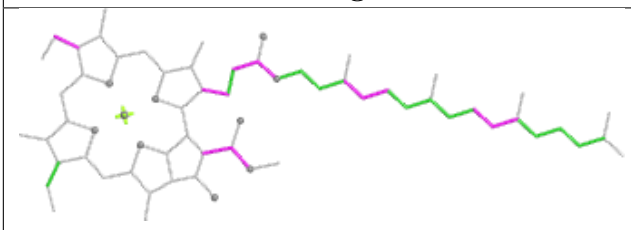
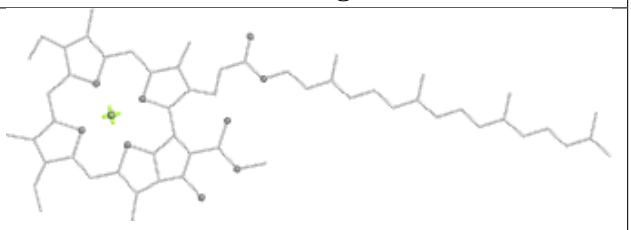
Bond angles

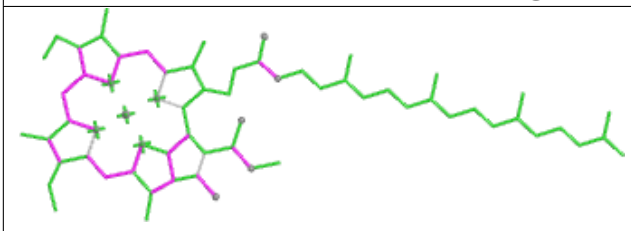
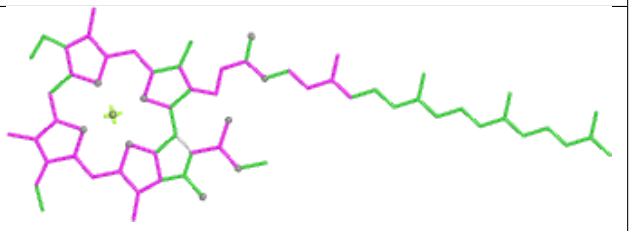
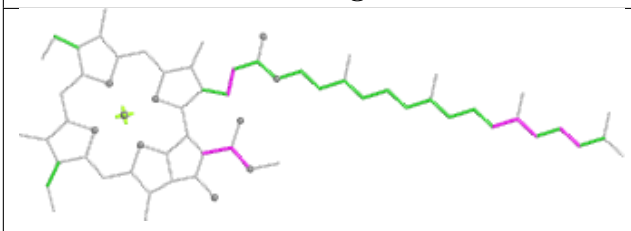
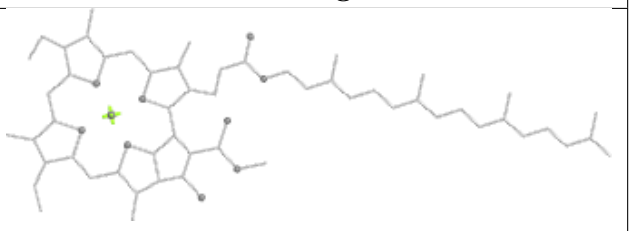


Torsions

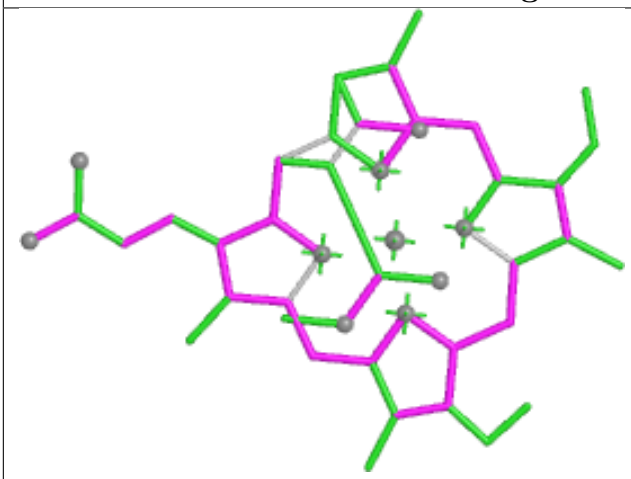


Rings

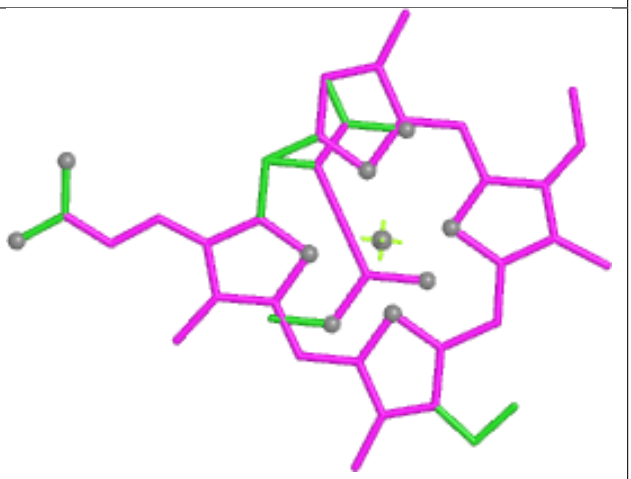
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 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 510	
 Bond lengths	 Bond angles
 Torsions	 Rings

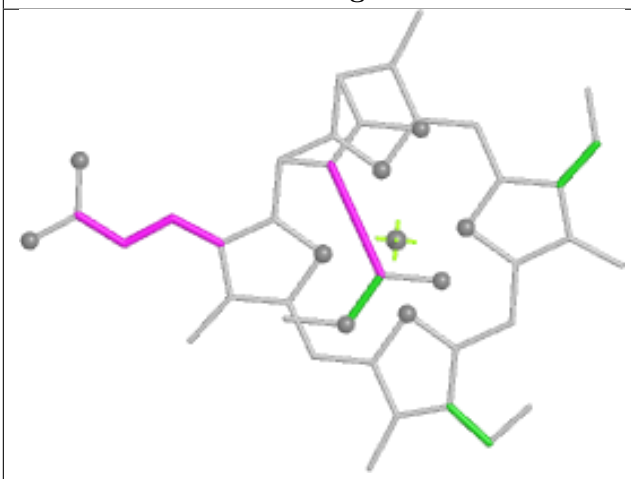
Ligand KC1 32 212



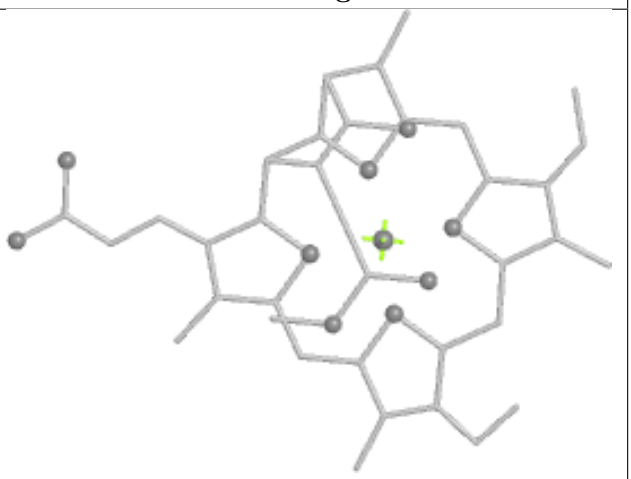
Bond lengths



Bond angles

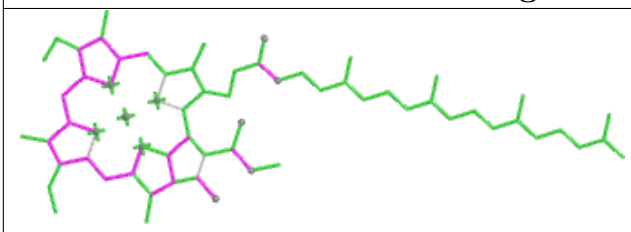


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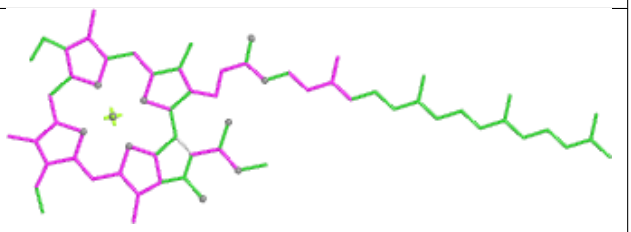


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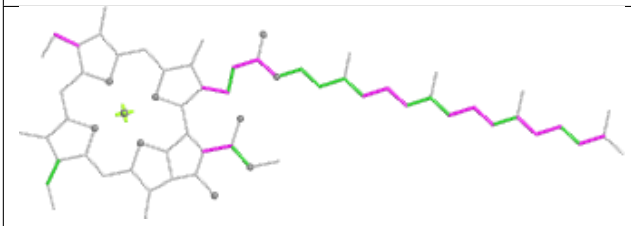
Ligand CLA 19 303



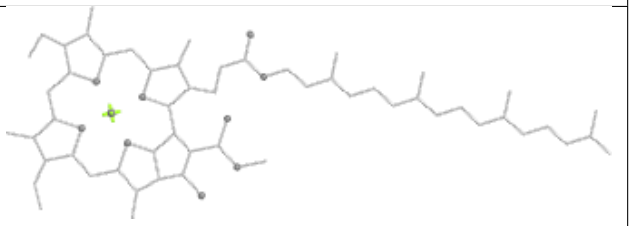
Bond lengths



Bond angles

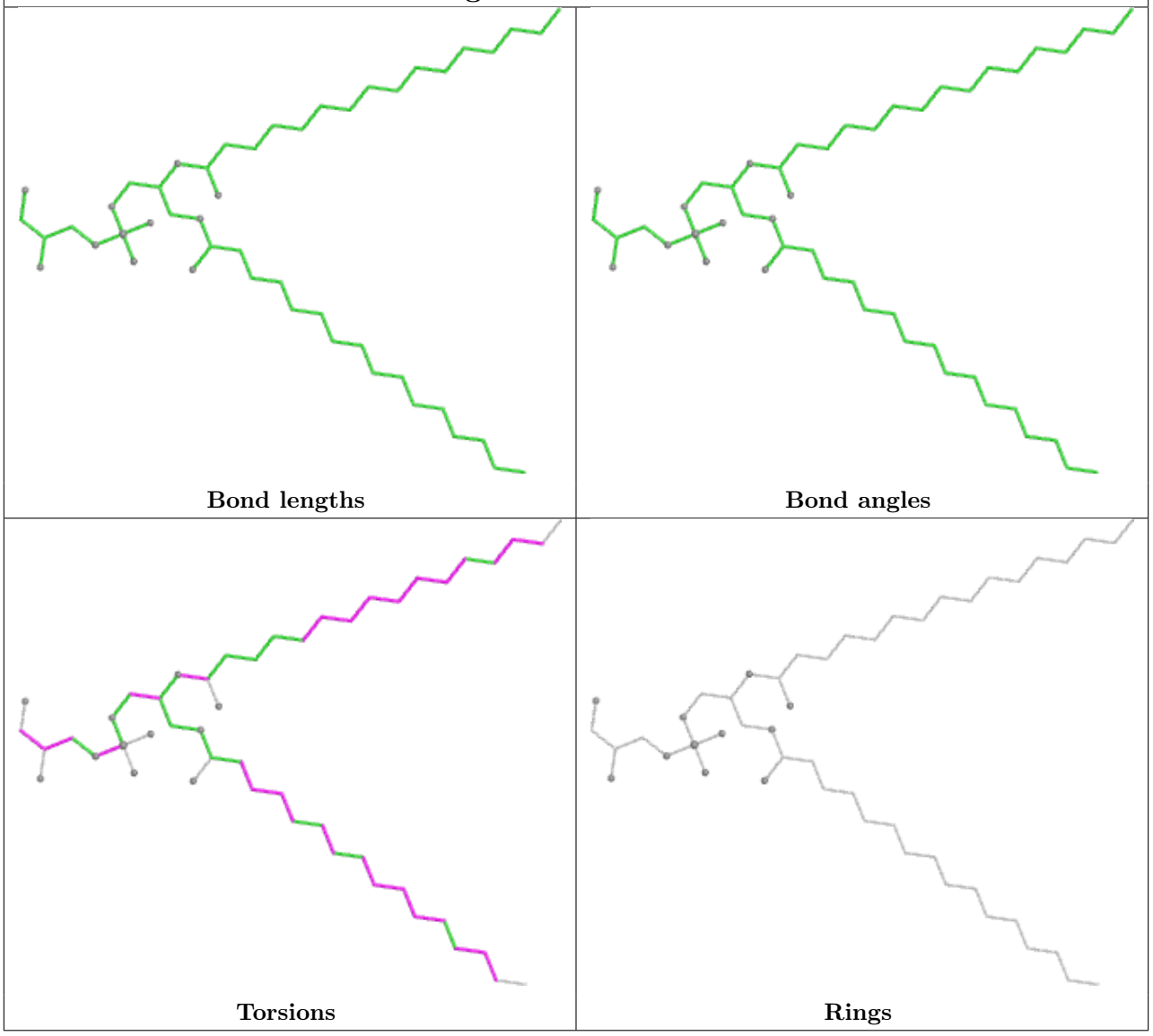


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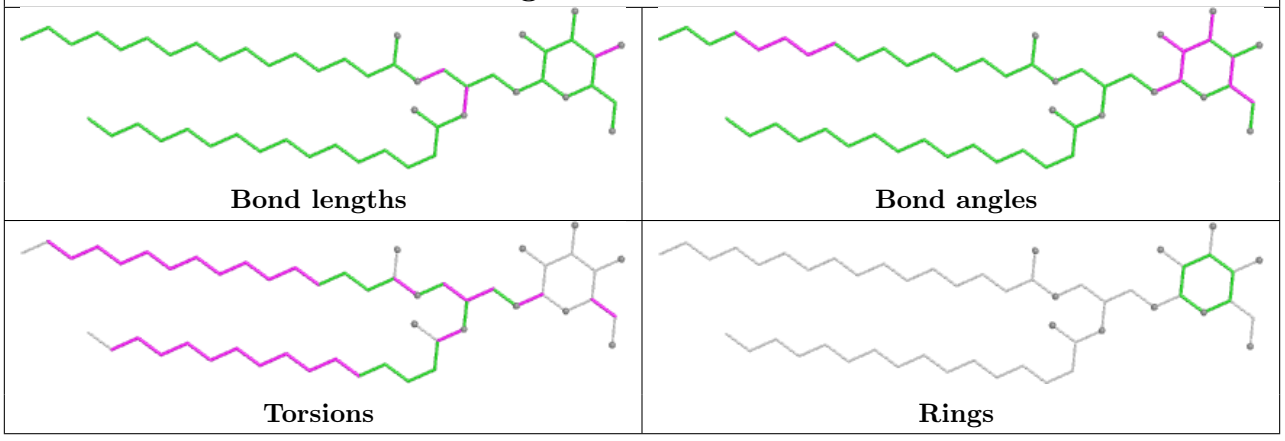


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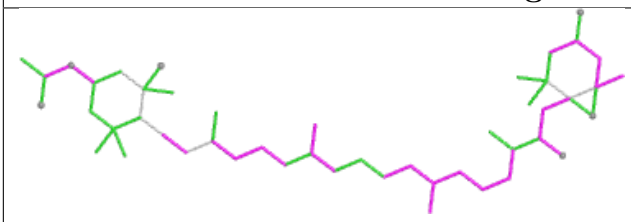
Ligand LHG 39 314



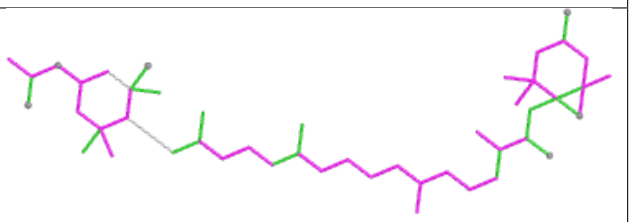
Ligand LMG A 408



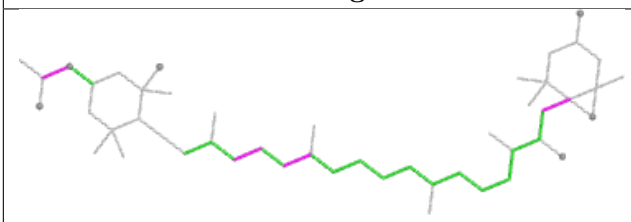
Ligand A86 16 310



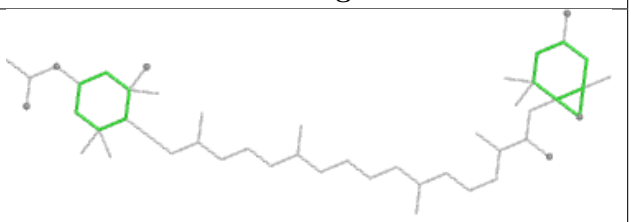
Bond lengths



Bond angles

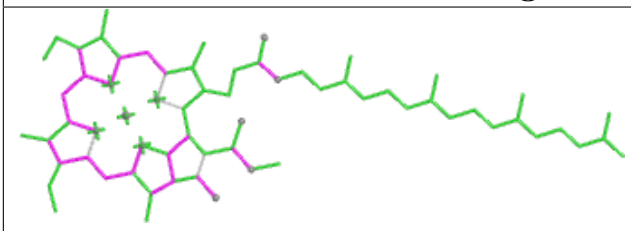


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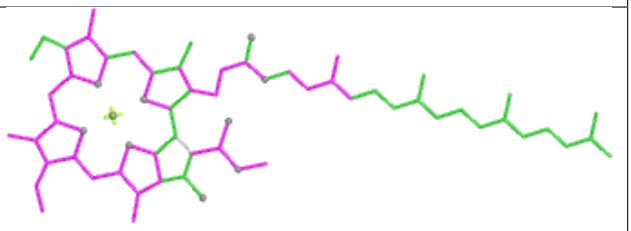


Rings

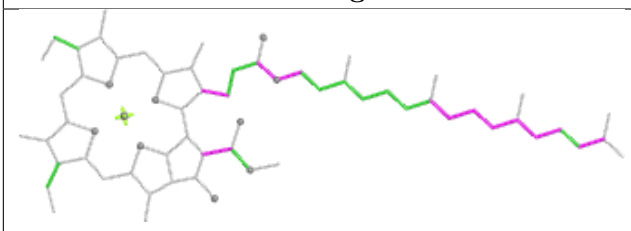
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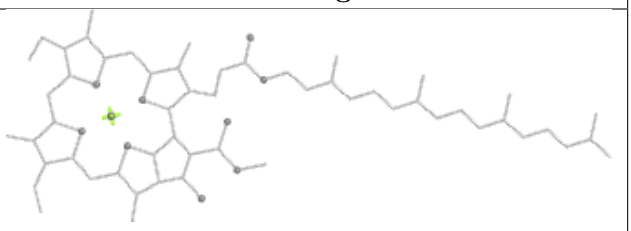
Bond lengths



Bond angles

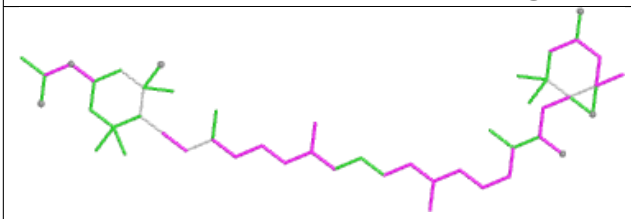


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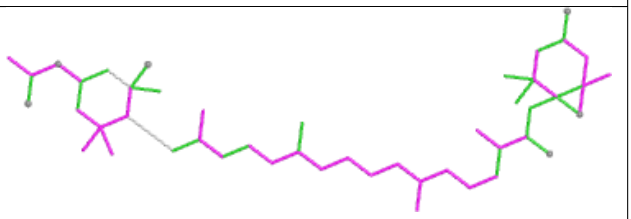


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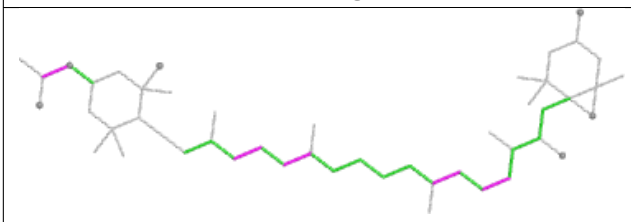
Ligand A86 17 311



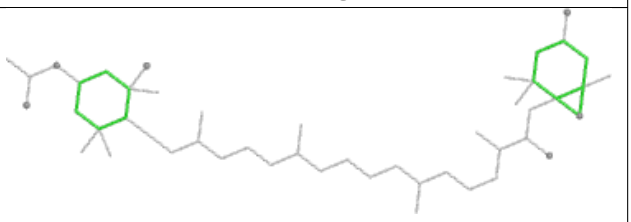
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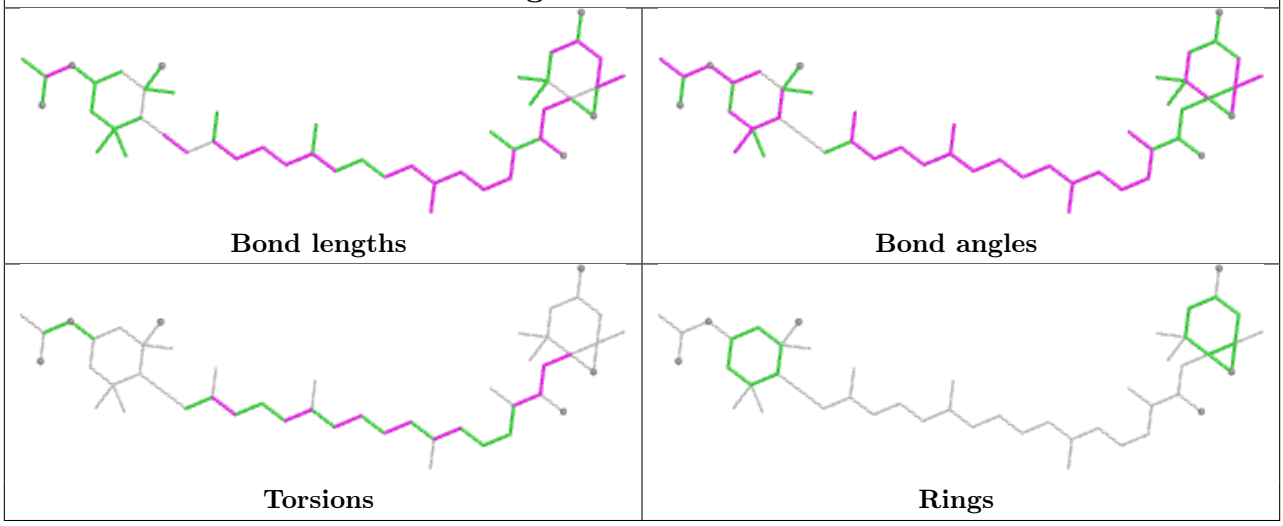


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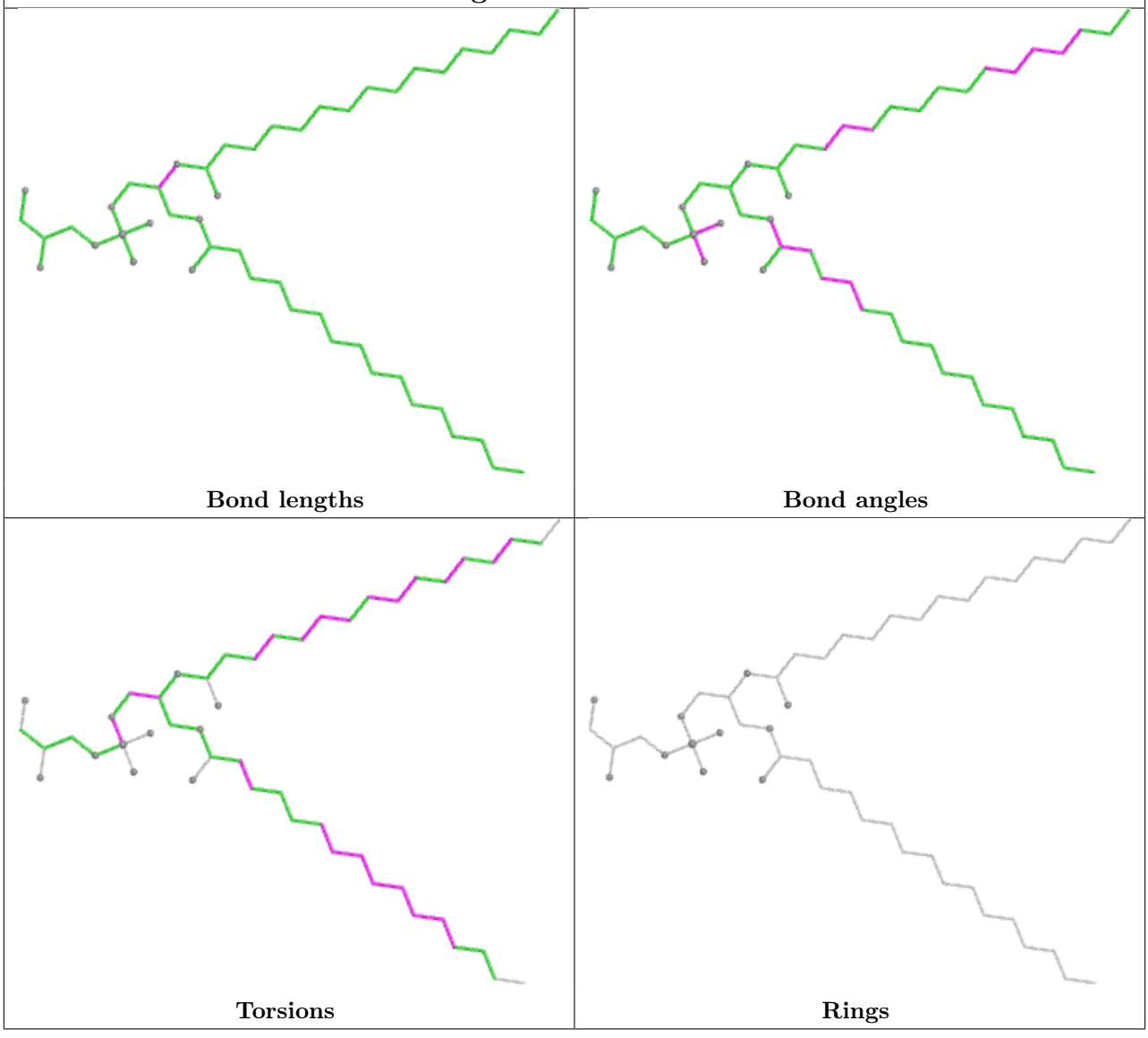


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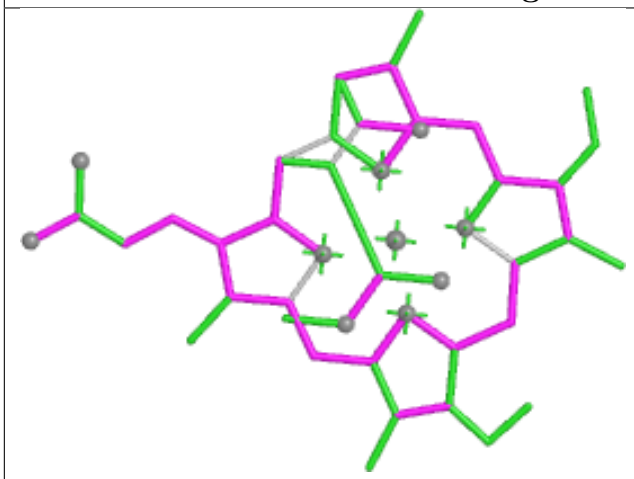
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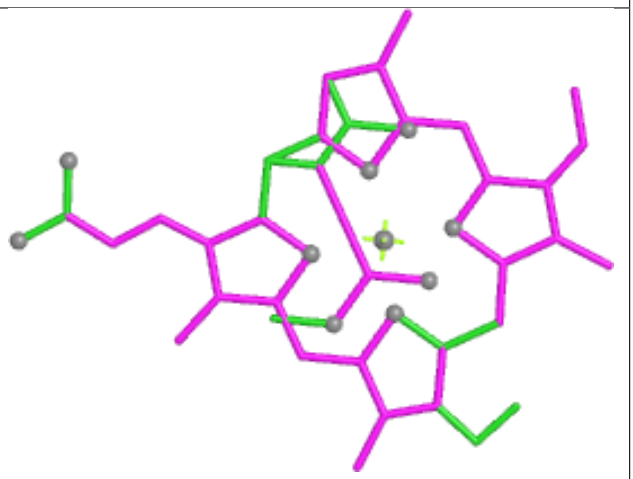
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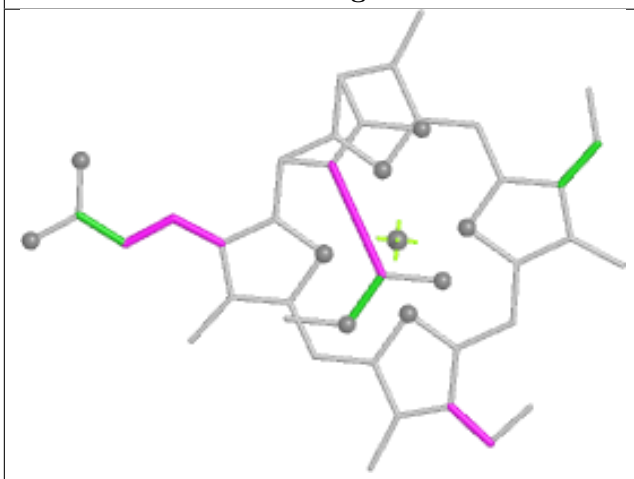
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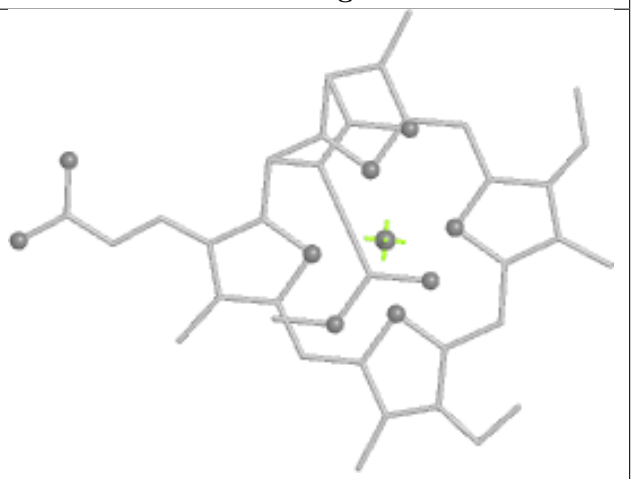
Bond lengths



Bond angles

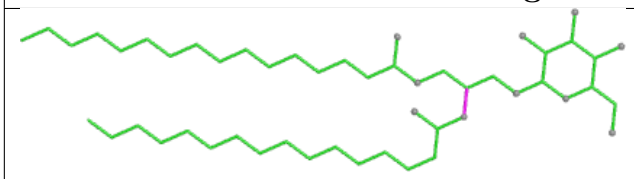


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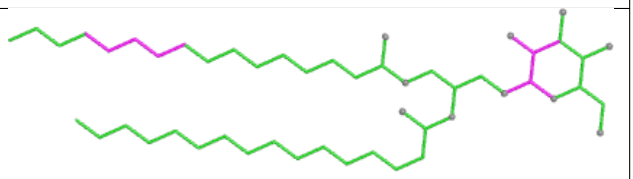


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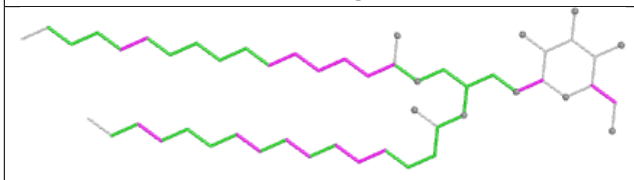
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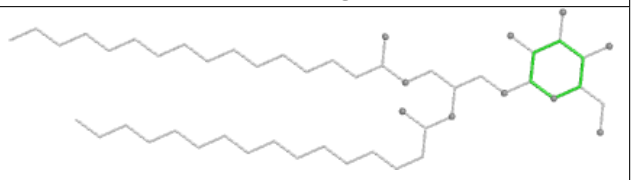
Bond lengths



Bond angles

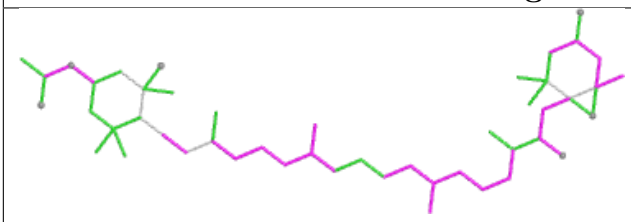


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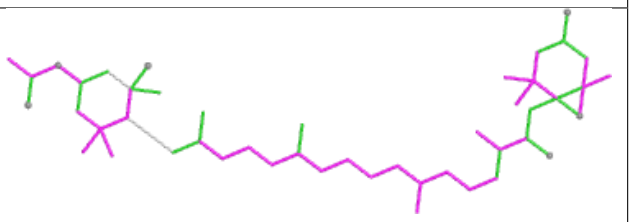


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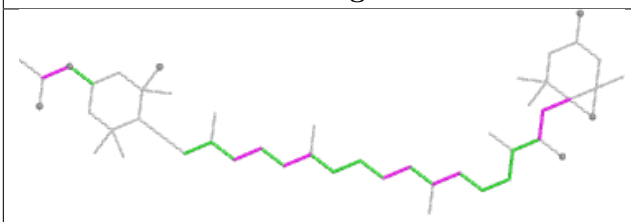
Ligand A86 32 217



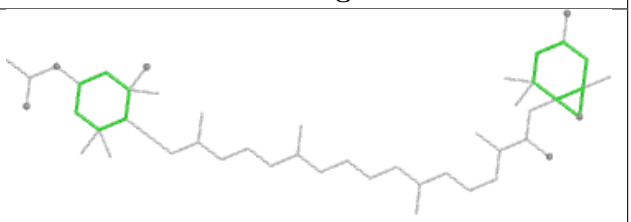
Bond lengths



Bond angles

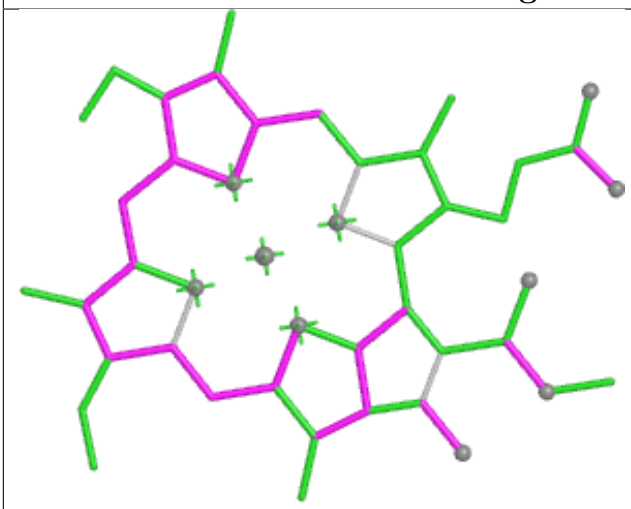


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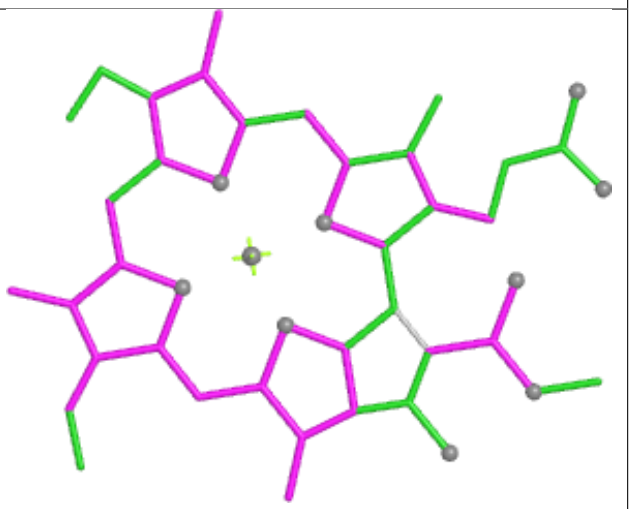


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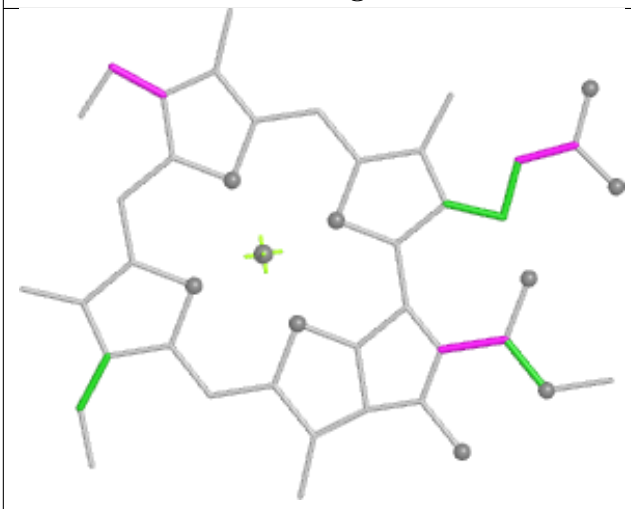
Ligand CLA 21 210



Bond lengths



Bond angles

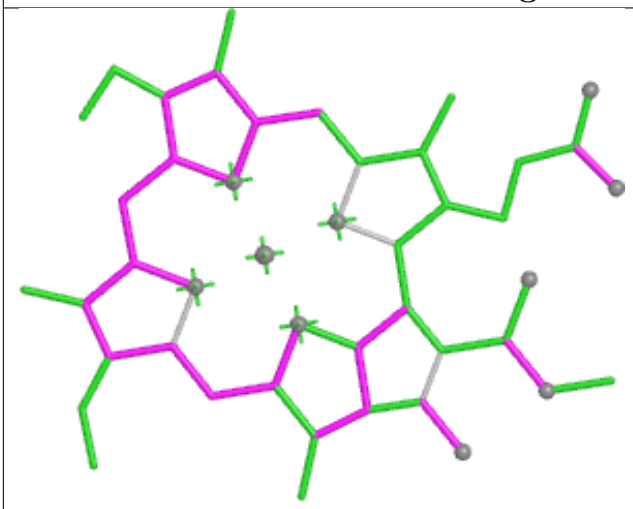


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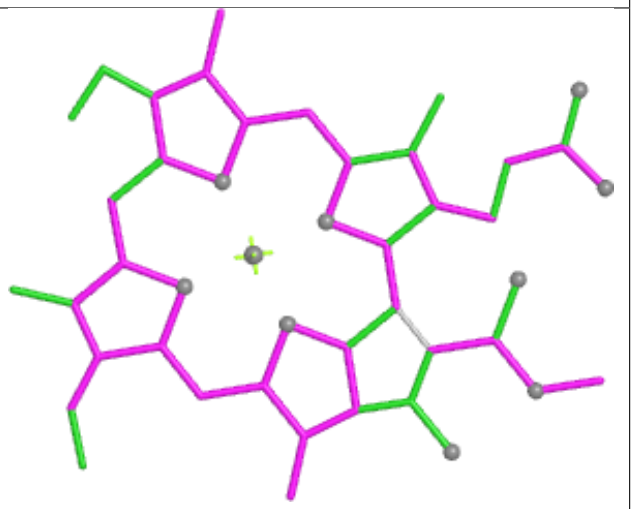


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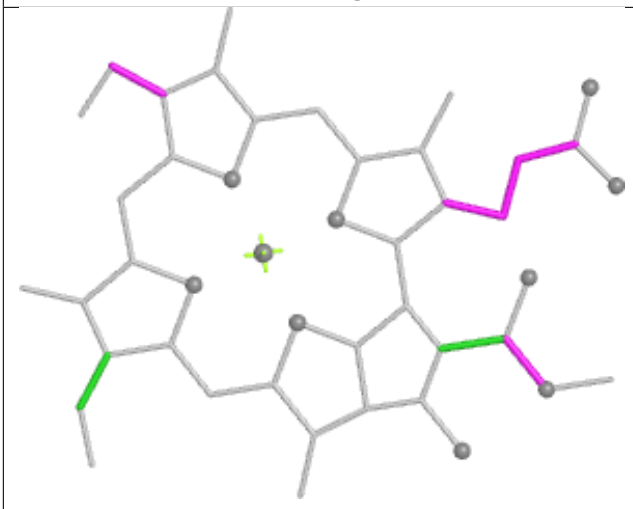
Ligand CLA 41 205



Bond lengths



Bond angles

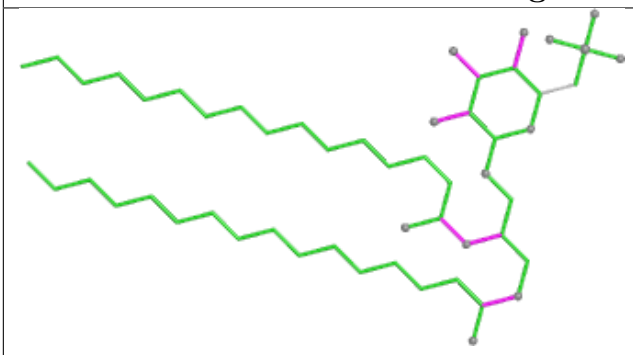


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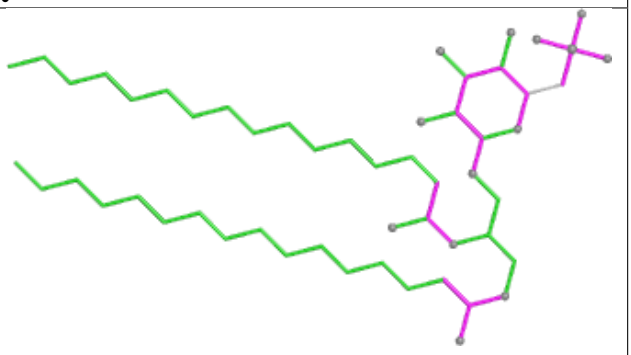


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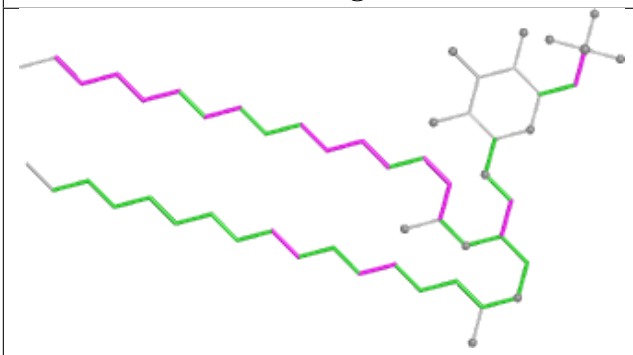
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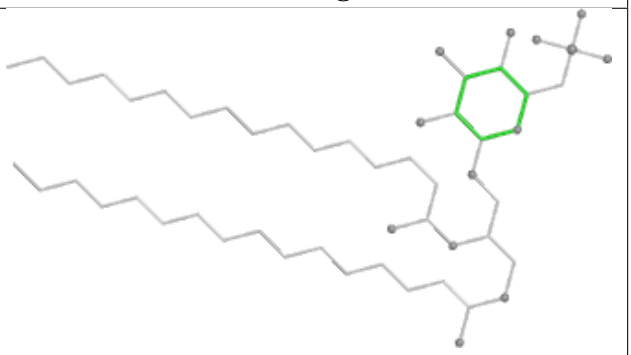
Bond lengths



Bond angles

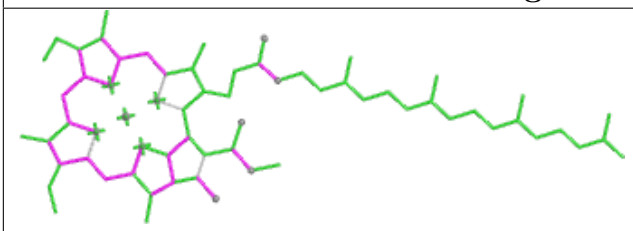


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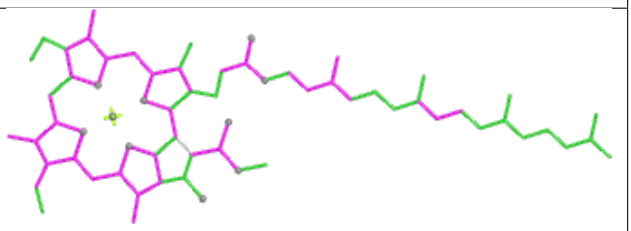


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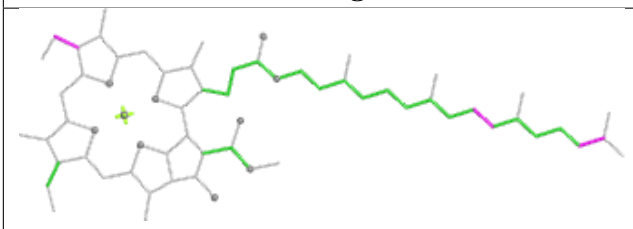
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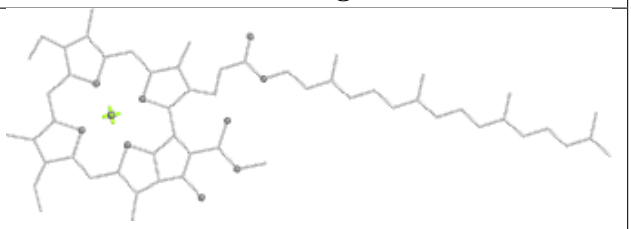
Bond lengths



Bond angles

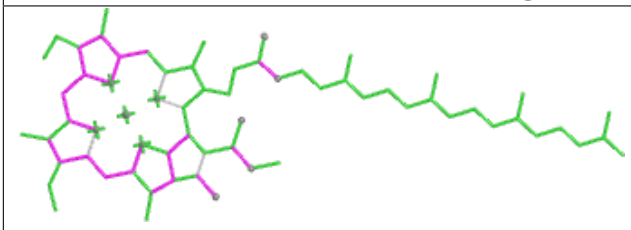


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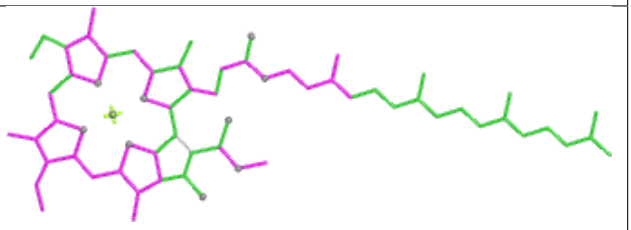


Rings

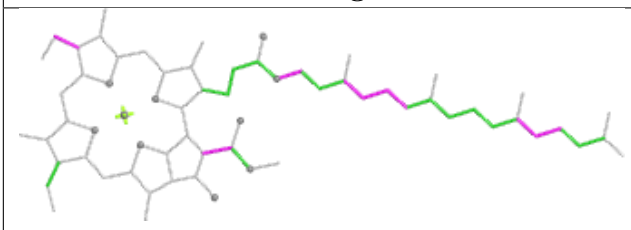
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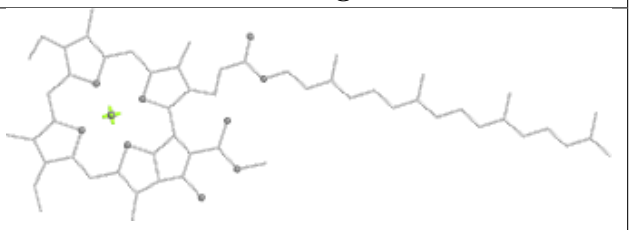
Bond lengths



Bond angles

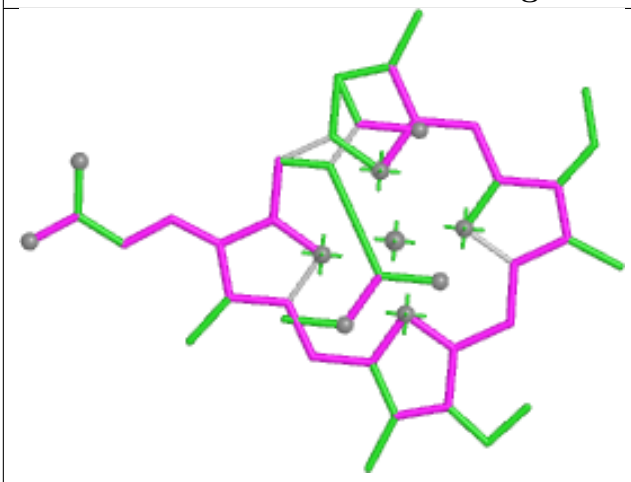


Torsions

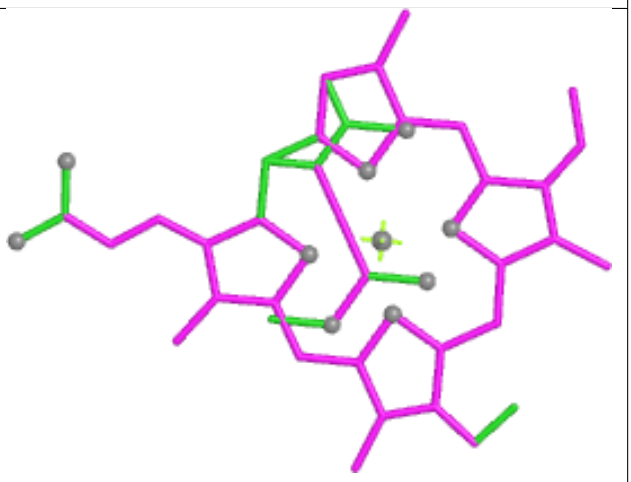


Rings

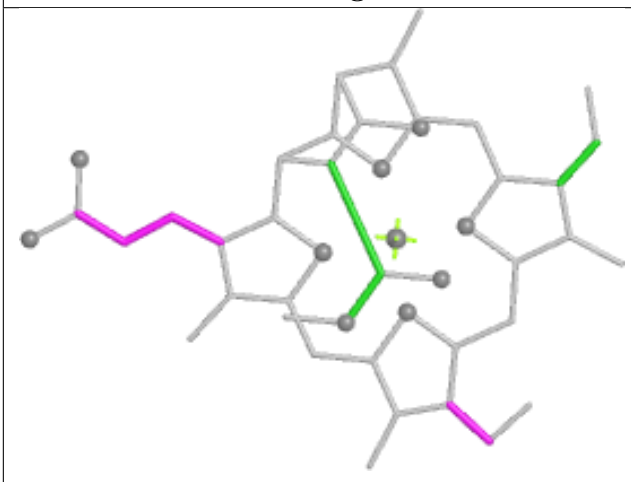
Ligand KC1 13 302



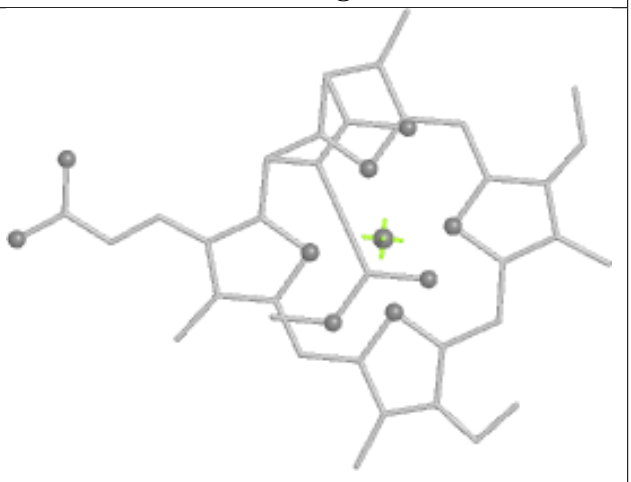
Bond lengths



Bond angles

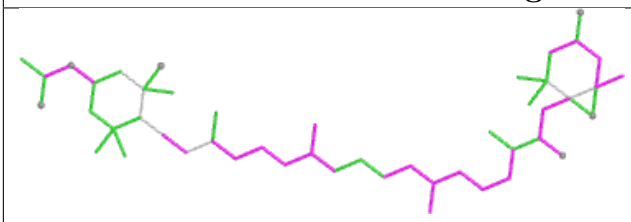


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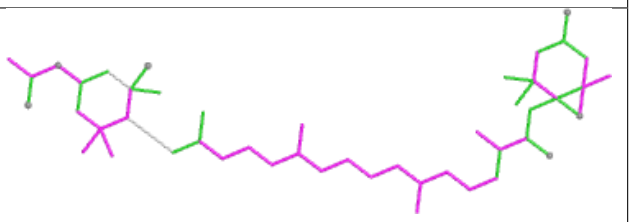


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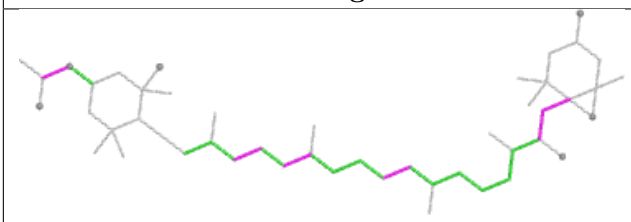
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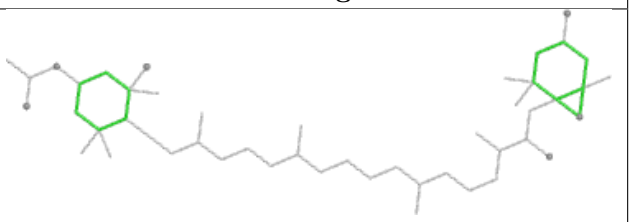
Bond lengths



Bond angles

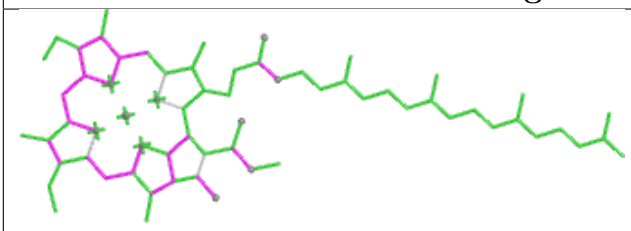


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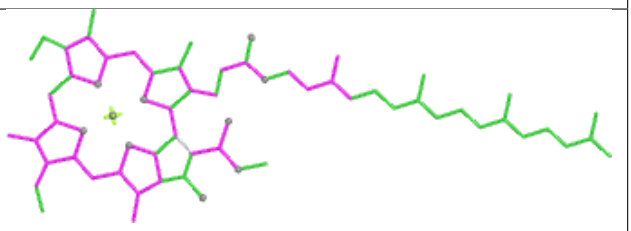


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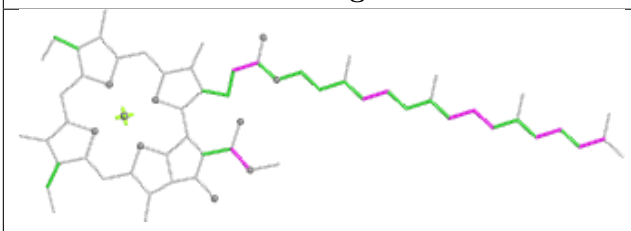
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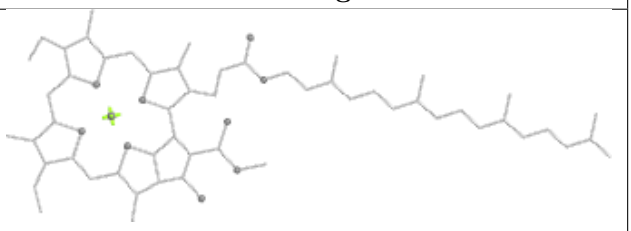
Bond lengths



Bond angles

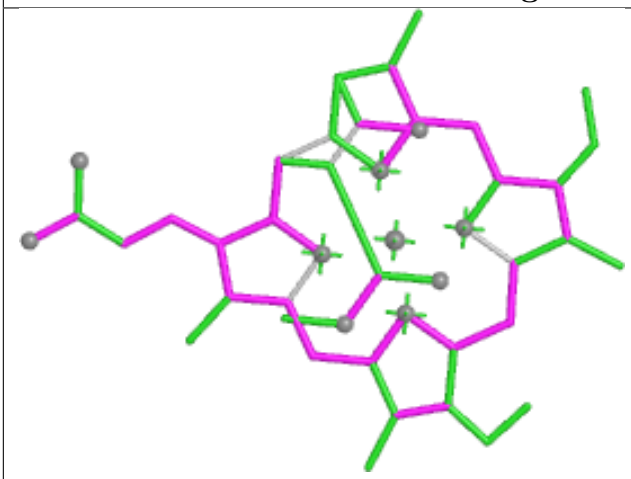


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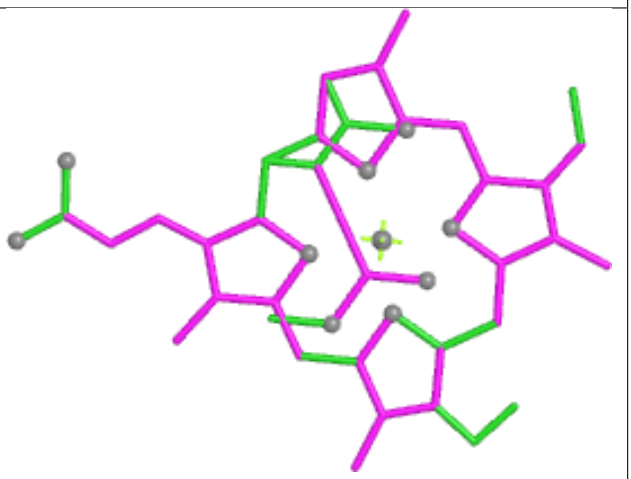


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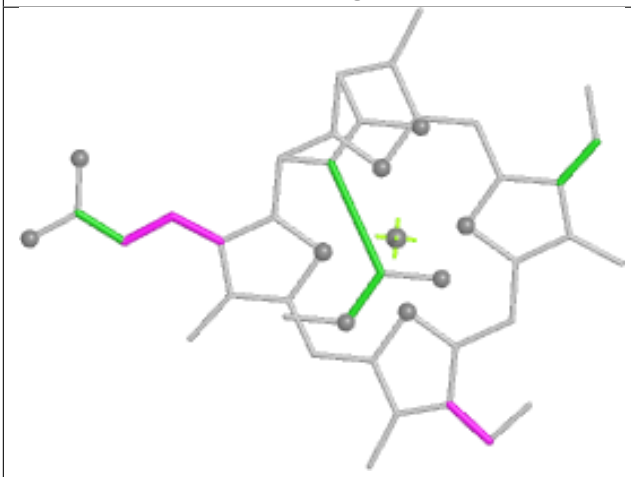
Ligand KC1 11 304



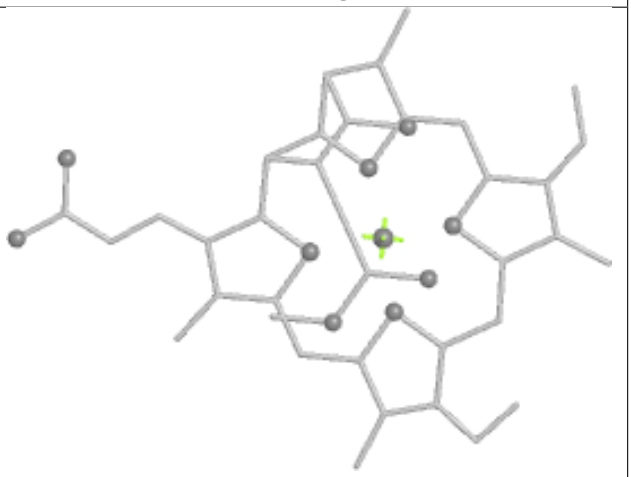
Bond lengths



Bond angles



Torsions

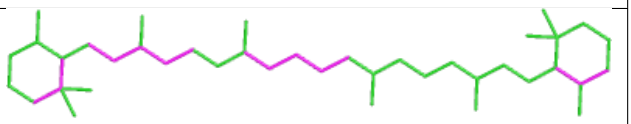


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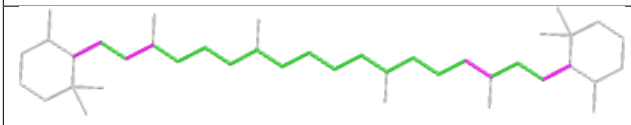
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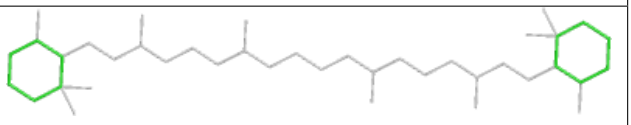
Bond lengths



Bond angles

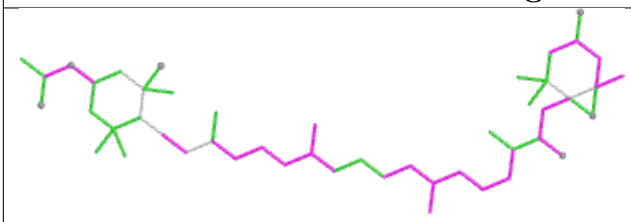


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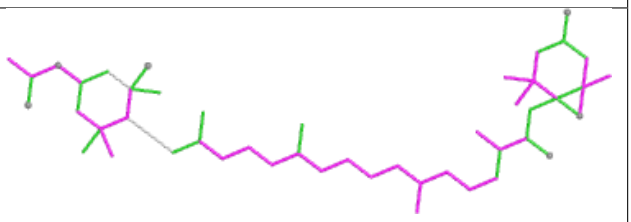


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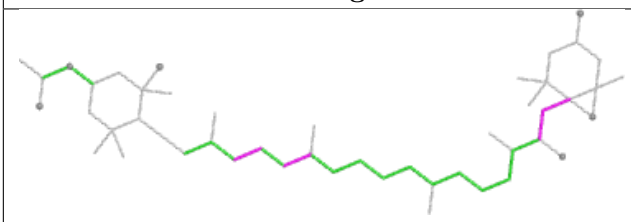
Ligand A86 12 213



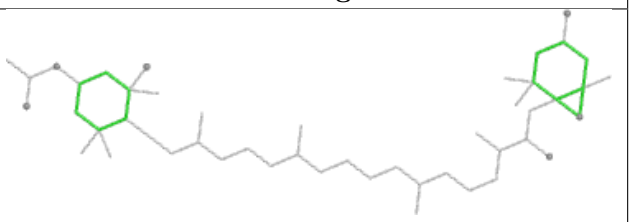
Bond lengths



Bond angles

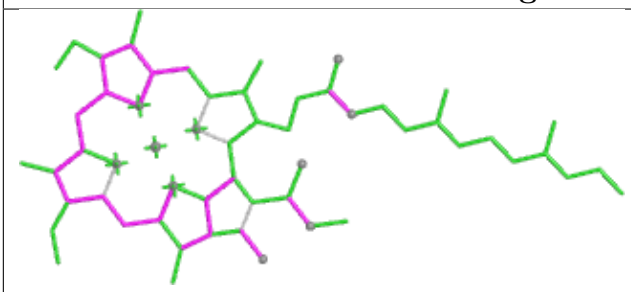


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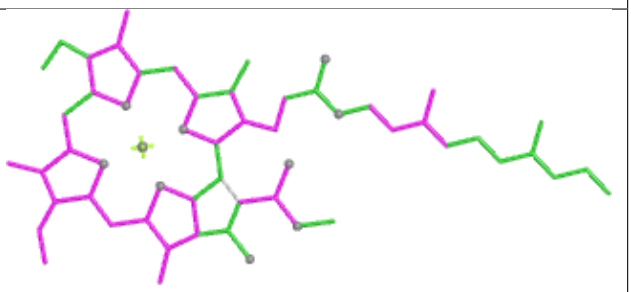


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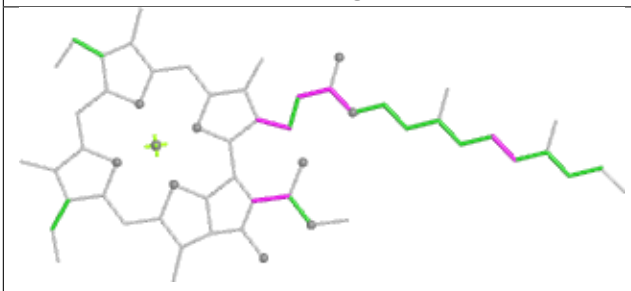
Ligand CLA 35 303



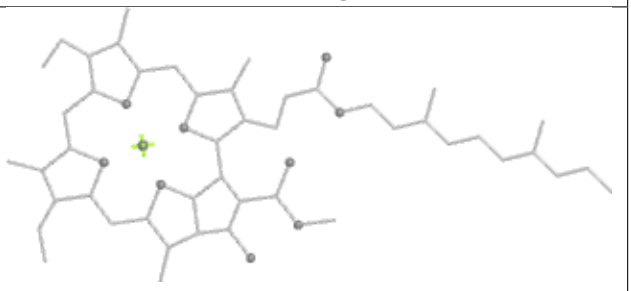
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Bond angles

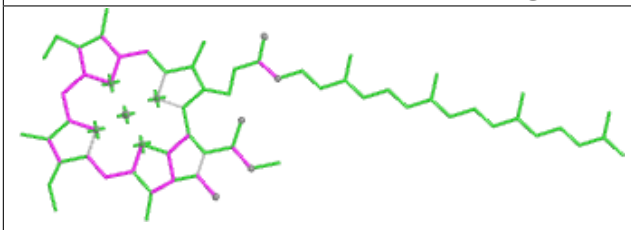


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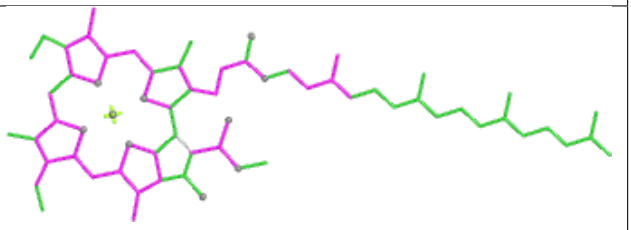


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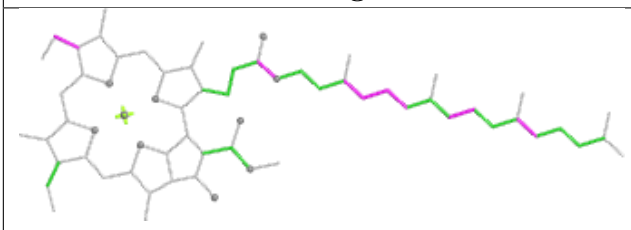
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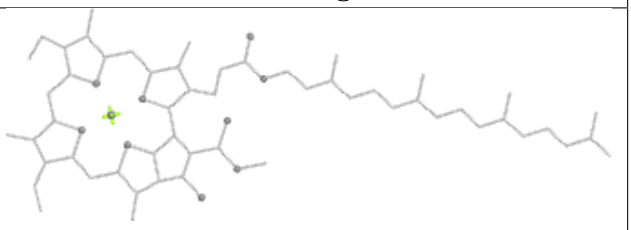
Bond lengths



Bond angles

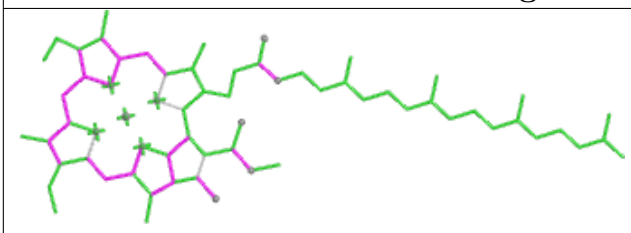


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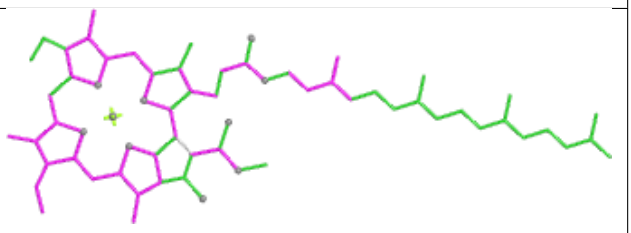


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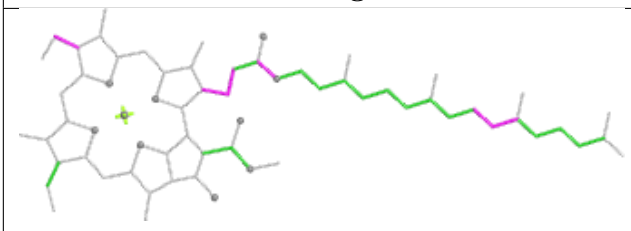
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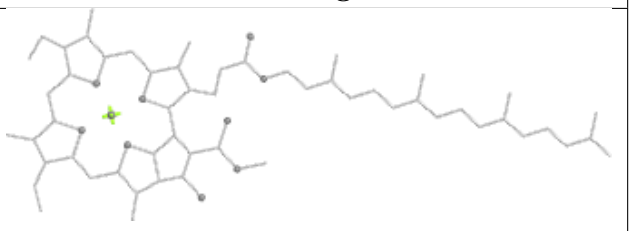
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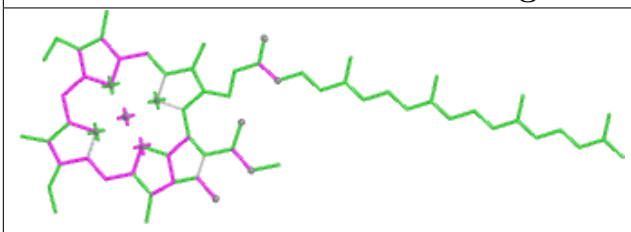


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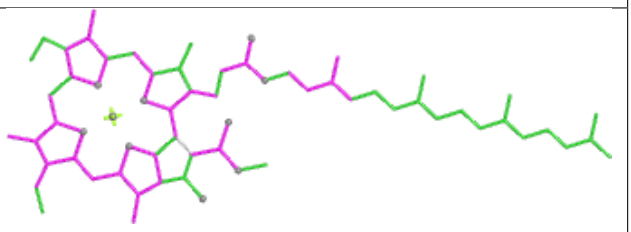


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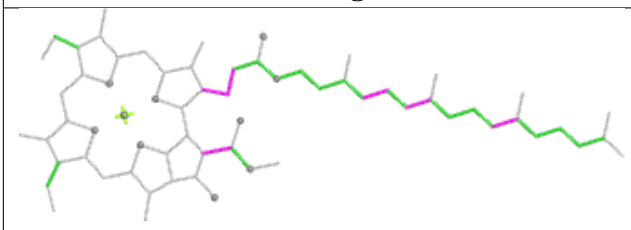
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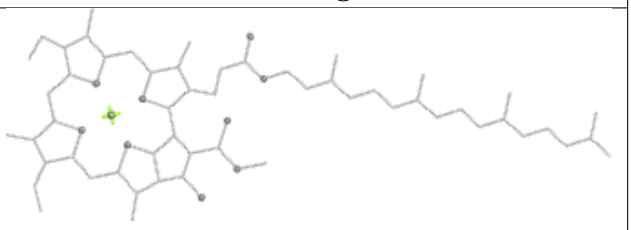
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Bond angles

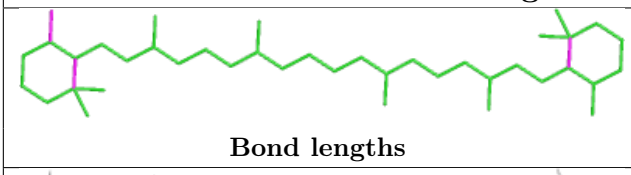


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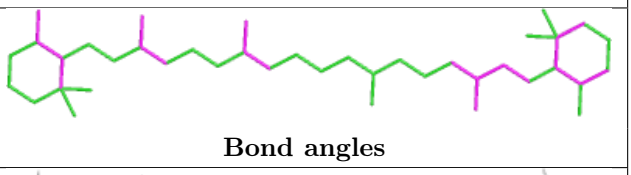


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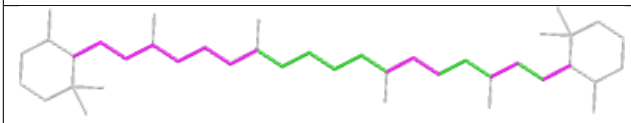
Ligand BCR K 101



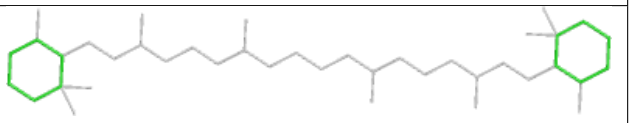
Bond lengths



Bond angles

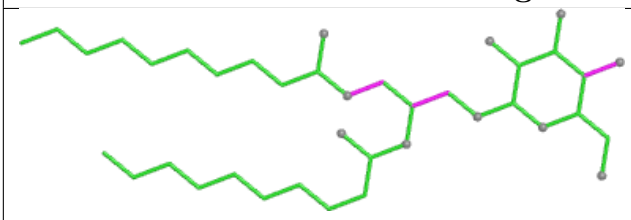


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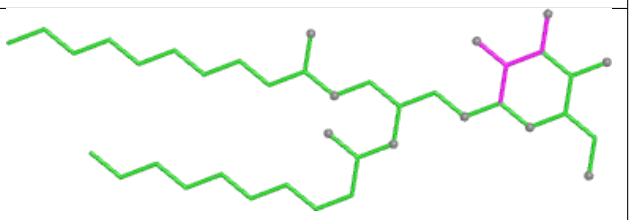


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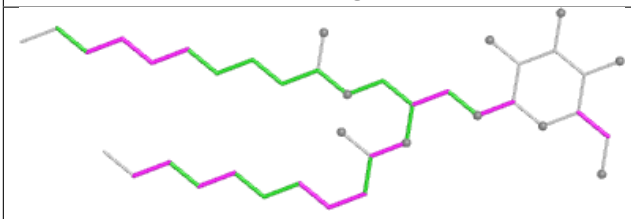
Ligand LMG 32 201



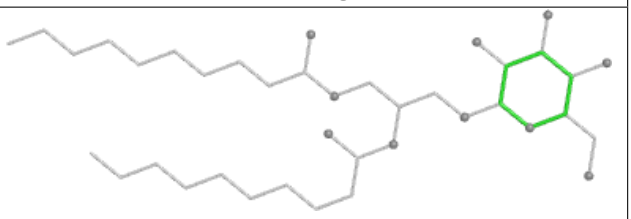
Bond lengths



Bond angles

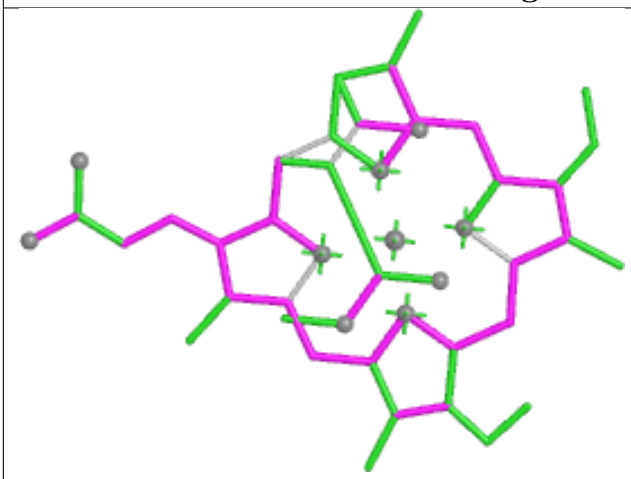


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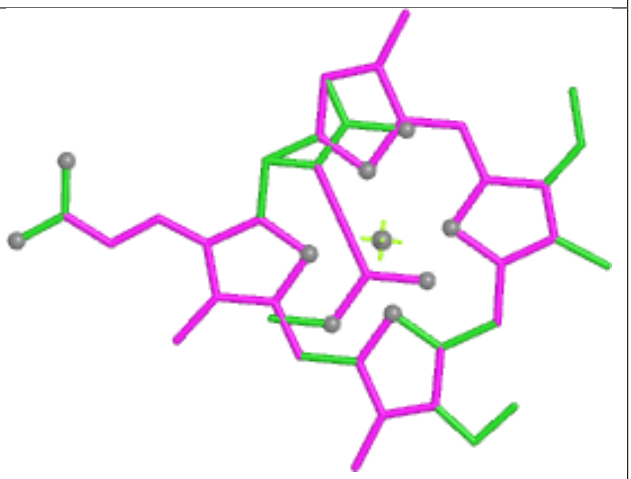


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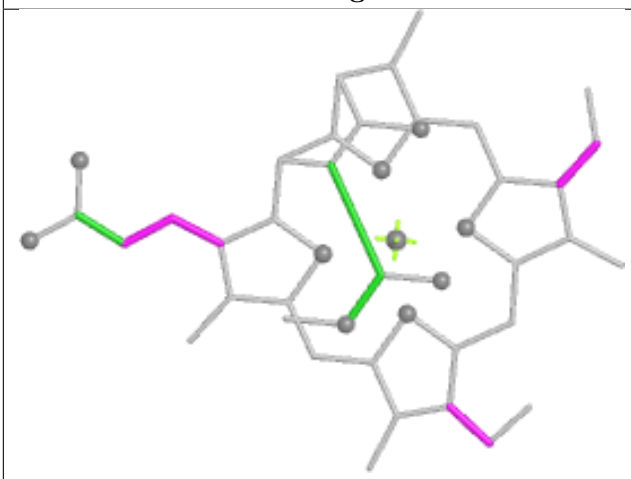
Ligand KC1 14 304



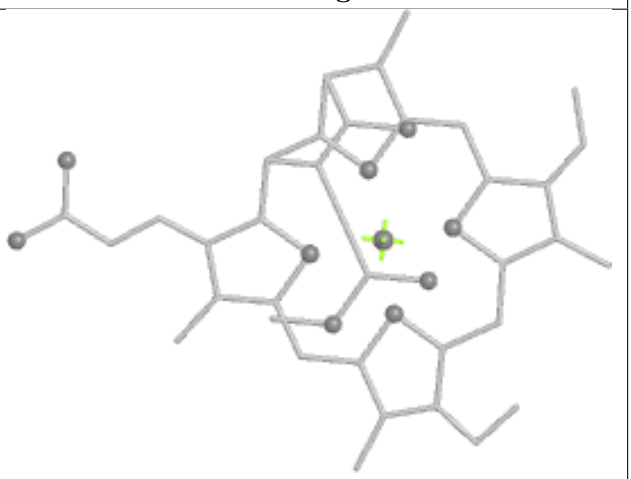
Bond lengths



Bond angles

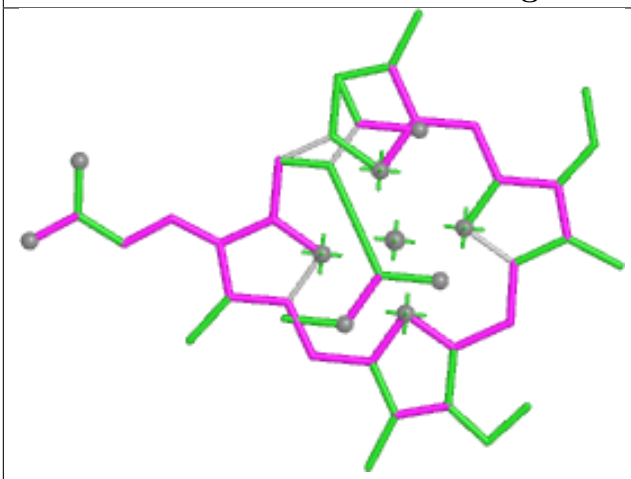


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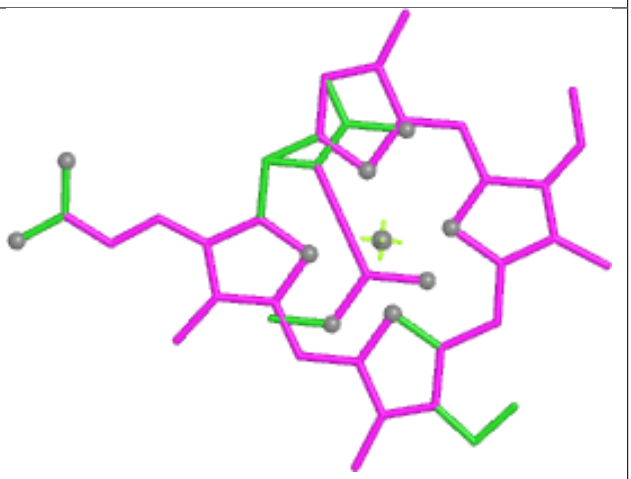


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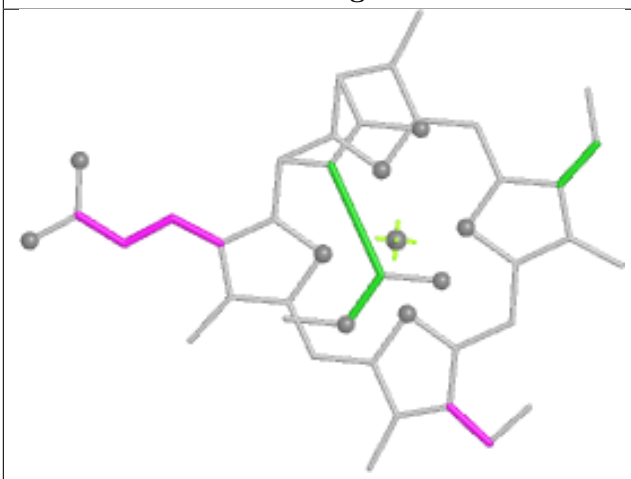
Ligand KC1 37 302



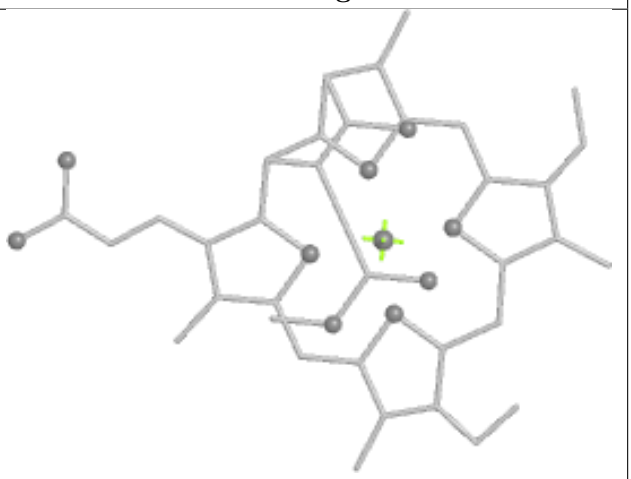
Bond lengths



Bond angles

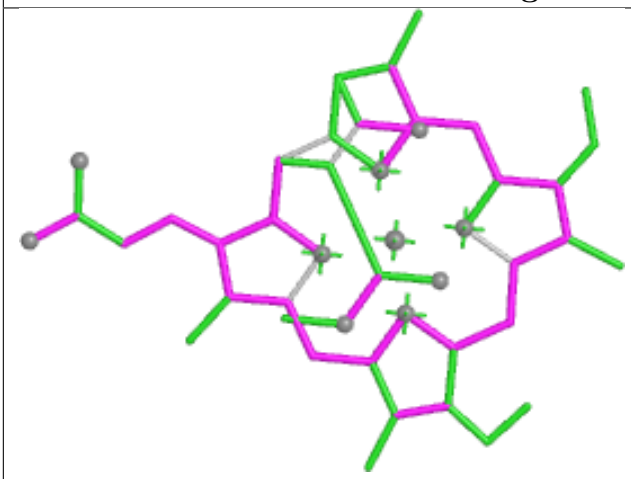


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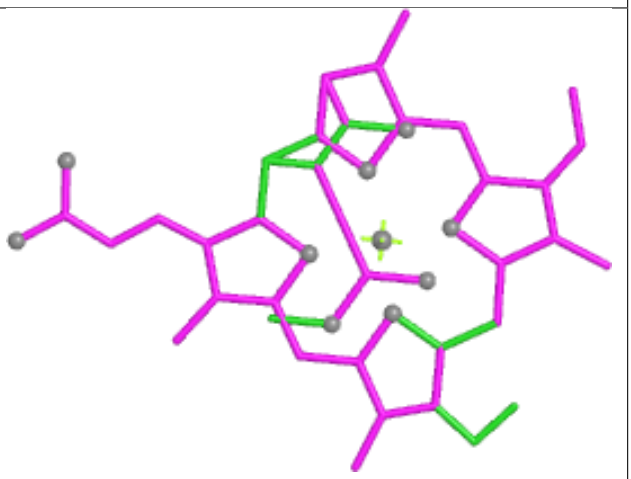


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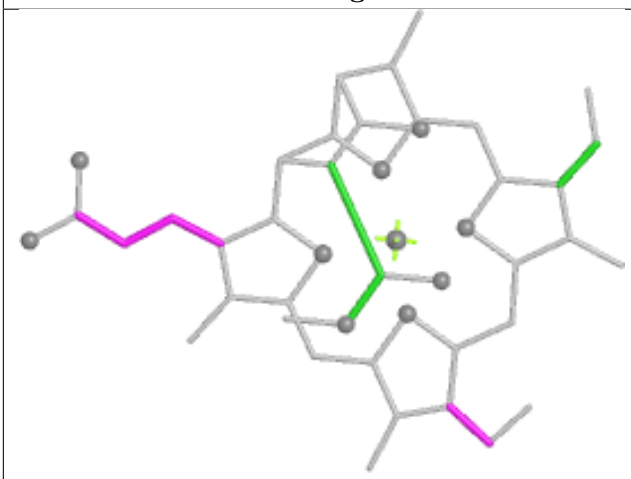
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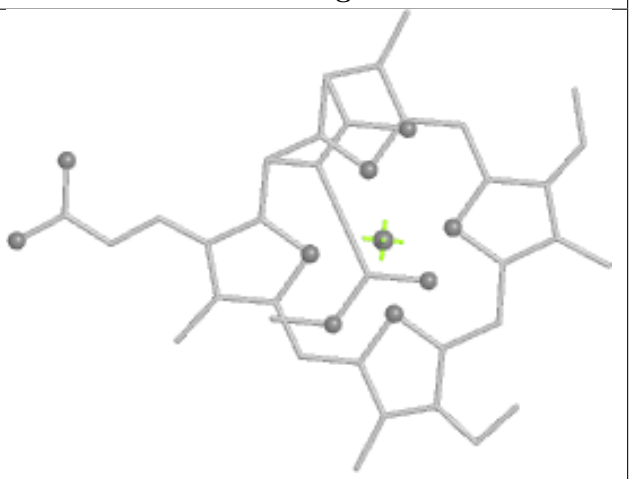
Bond lengths



Bond angles

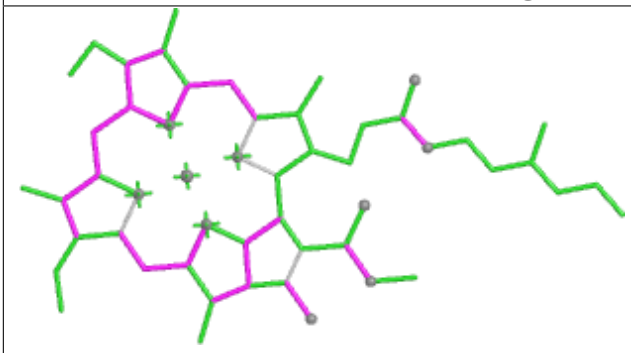


Torsions

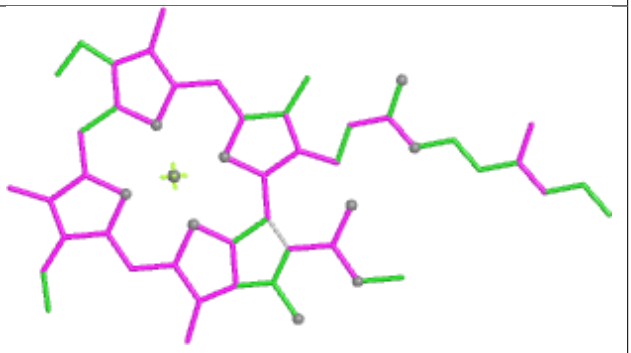


Rings

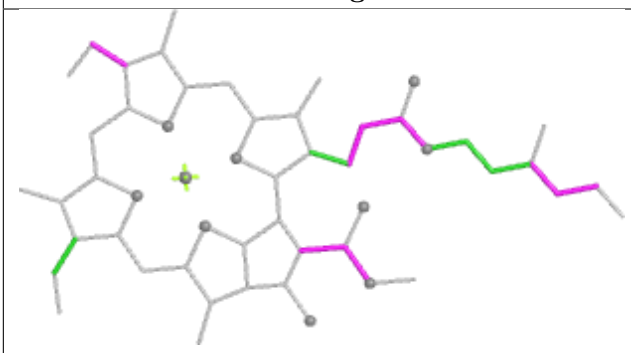
Ligand CLA 15 307



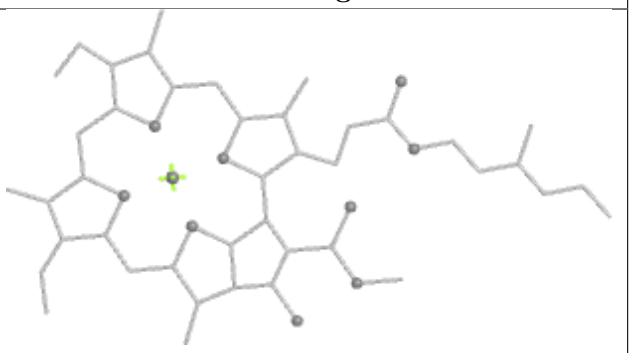
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Bond angles

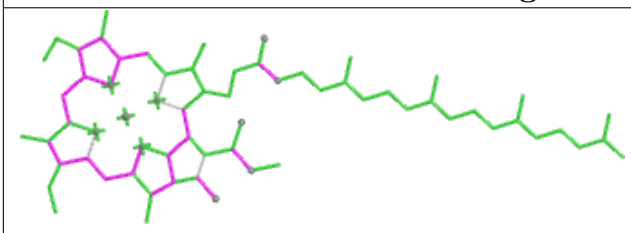


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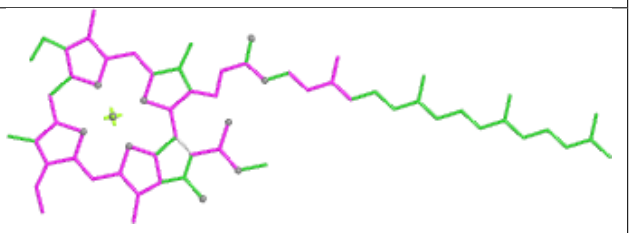


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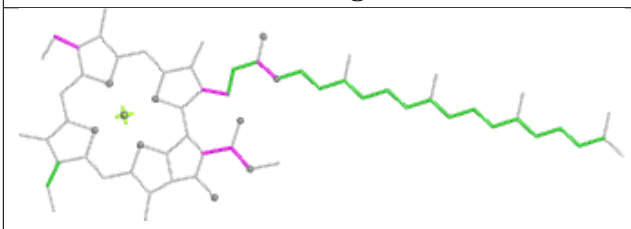
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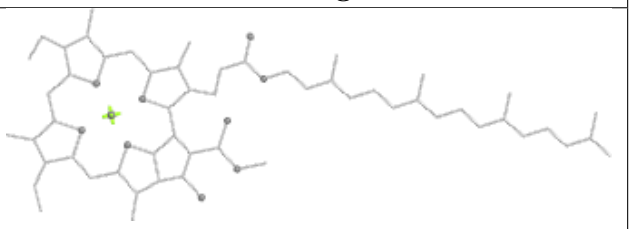
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Bond angles

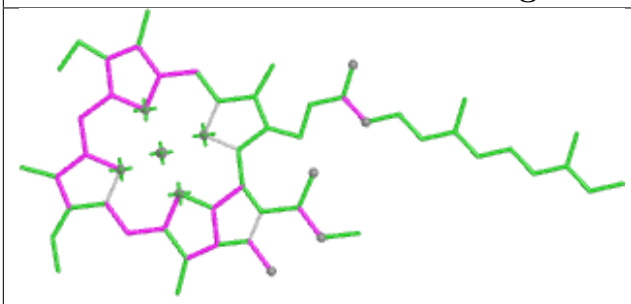


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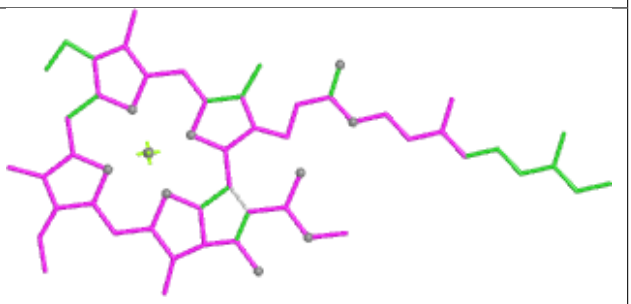


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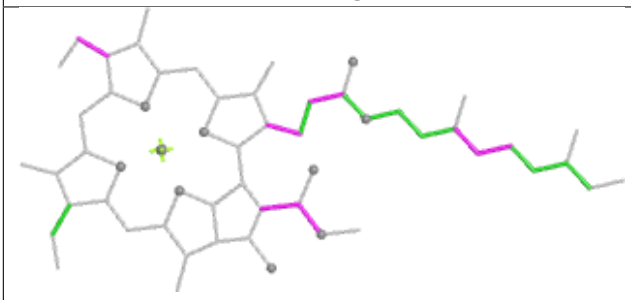
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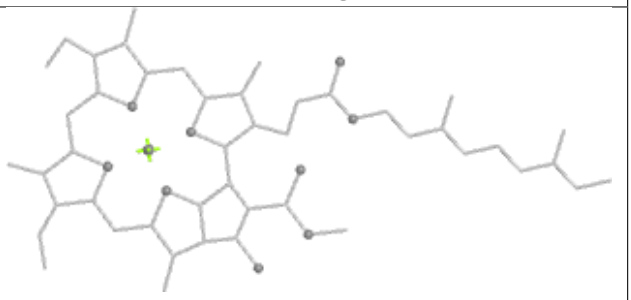
Bond lengths



Bond angles

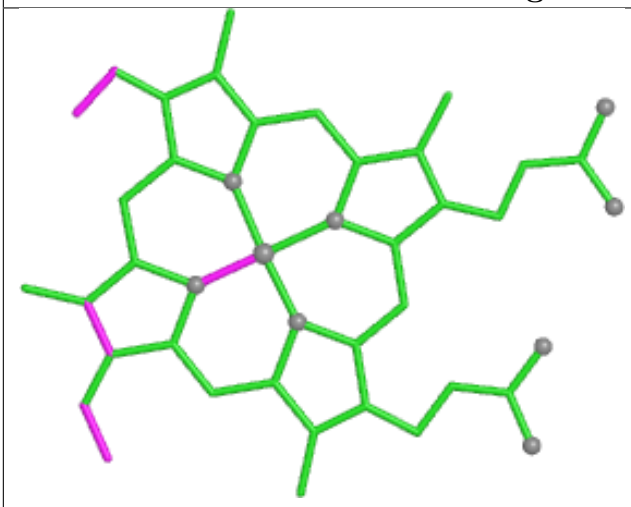


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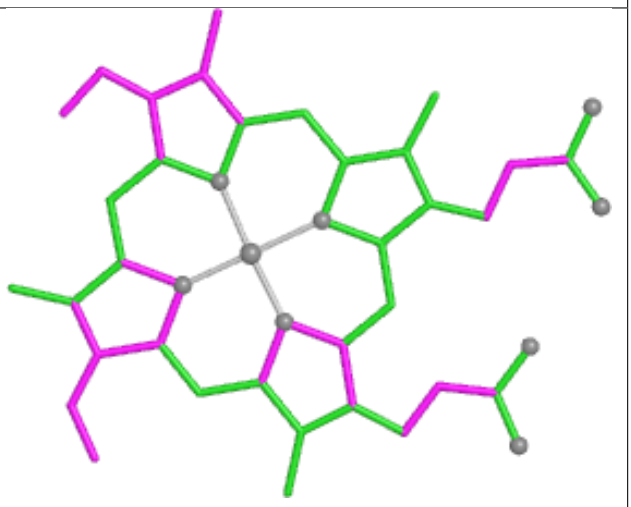


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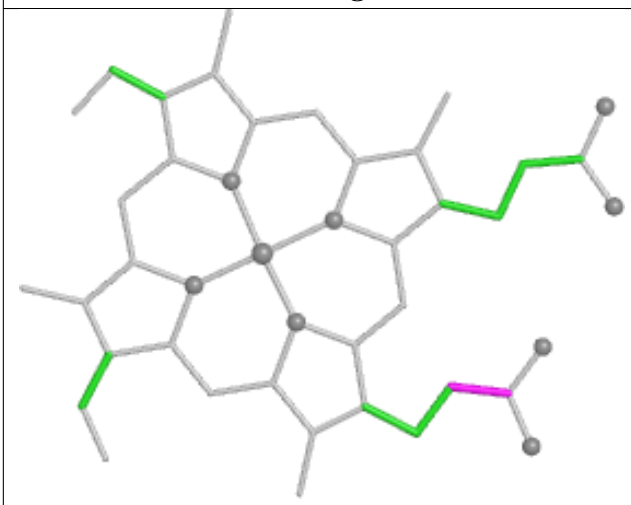
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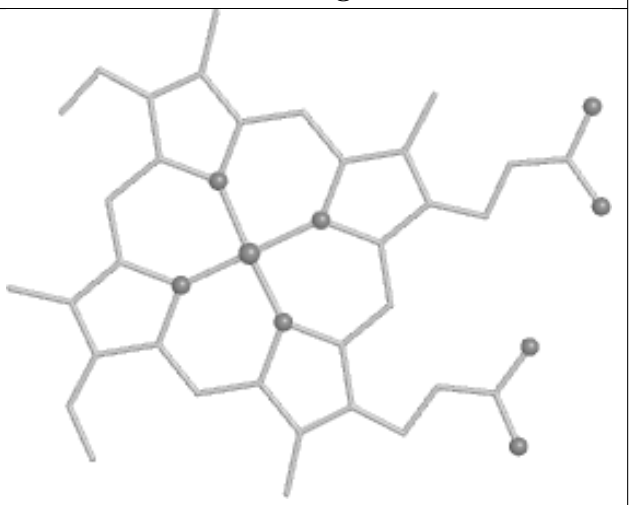
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Bond angles

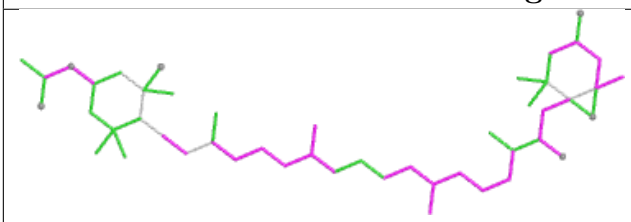


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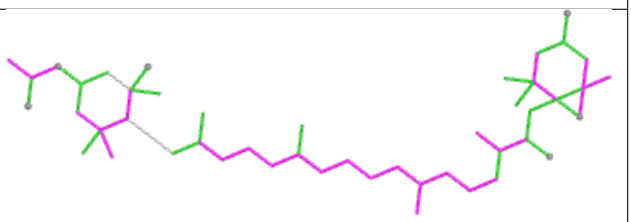


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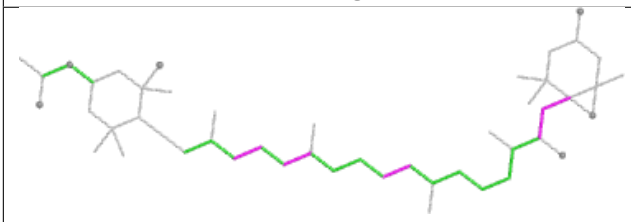
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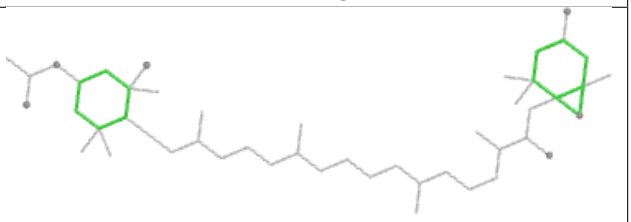
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Bond angles

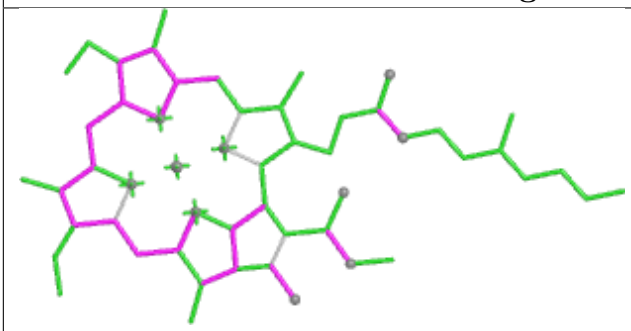


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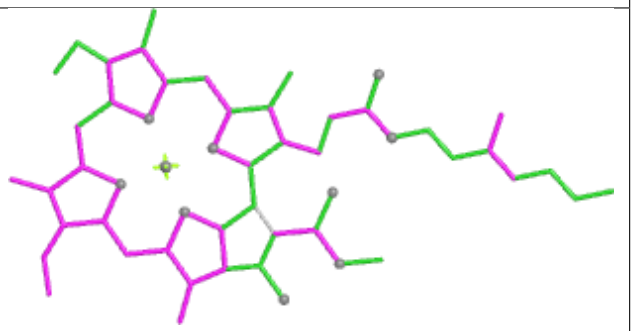


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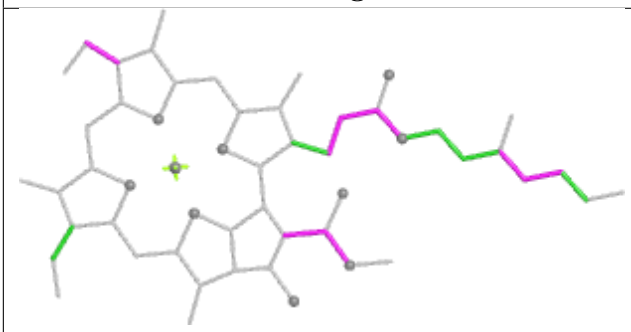
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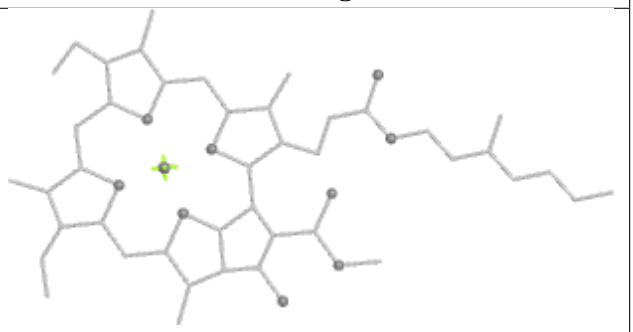
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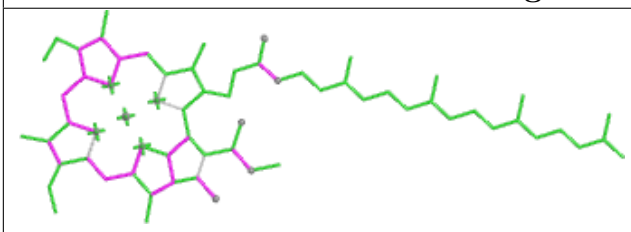


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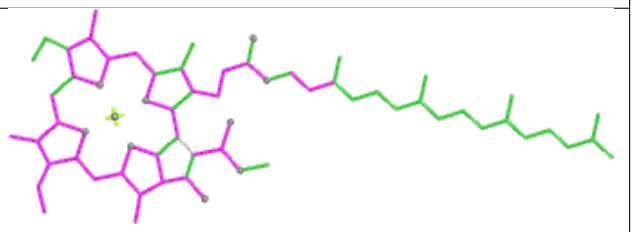


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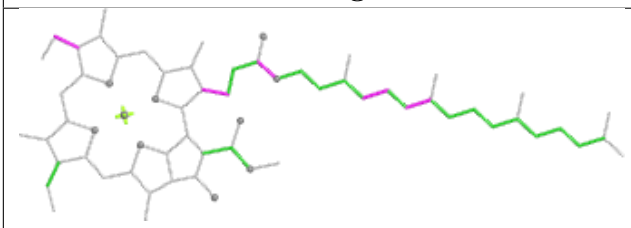
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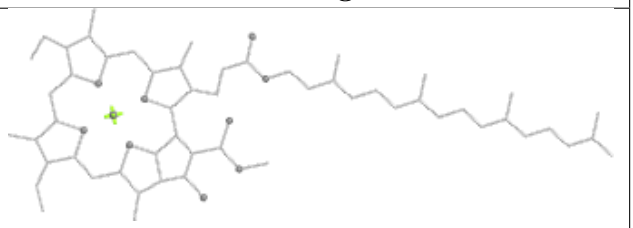
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Bond angles

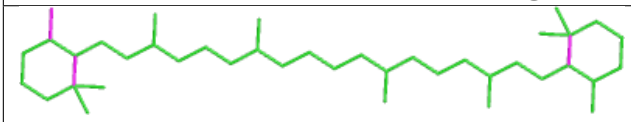


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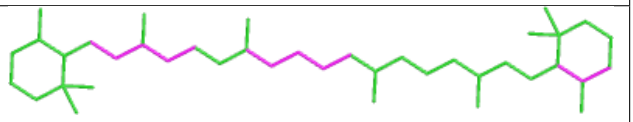


Rings

Ligand BCR h 101



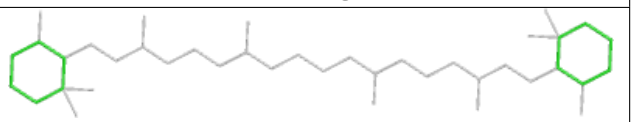
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Bond angles

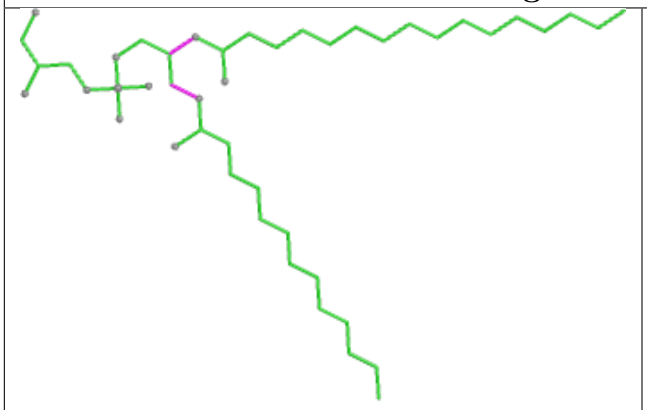


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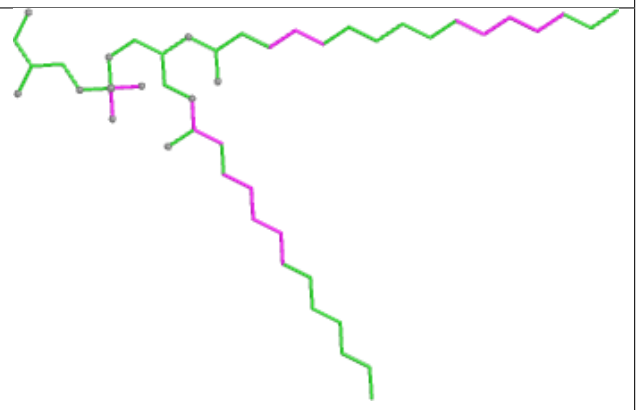


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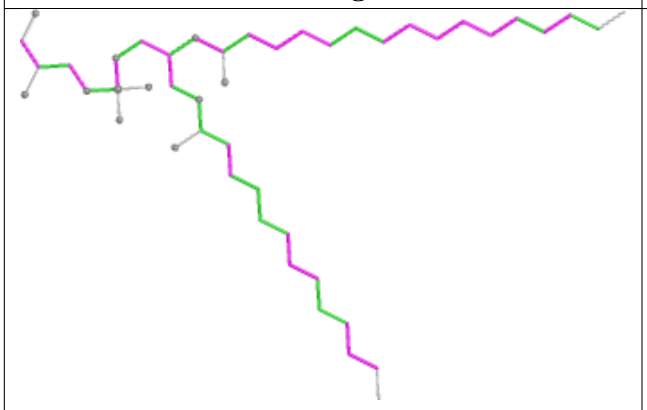
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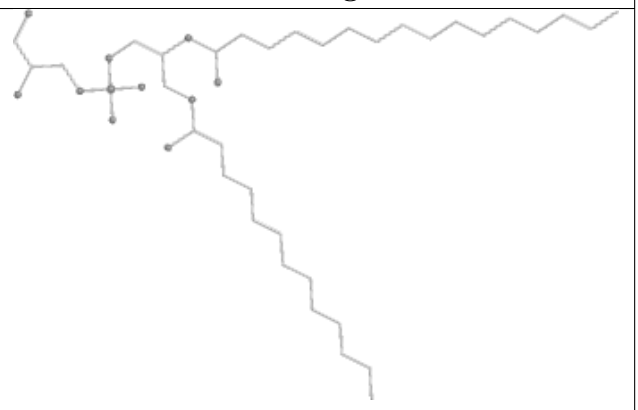
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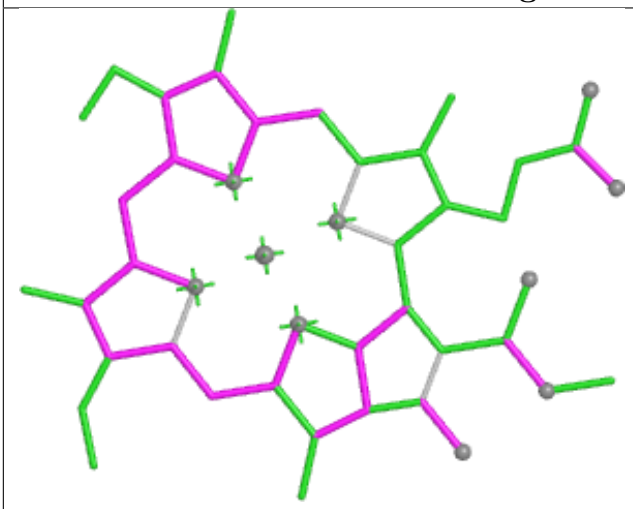


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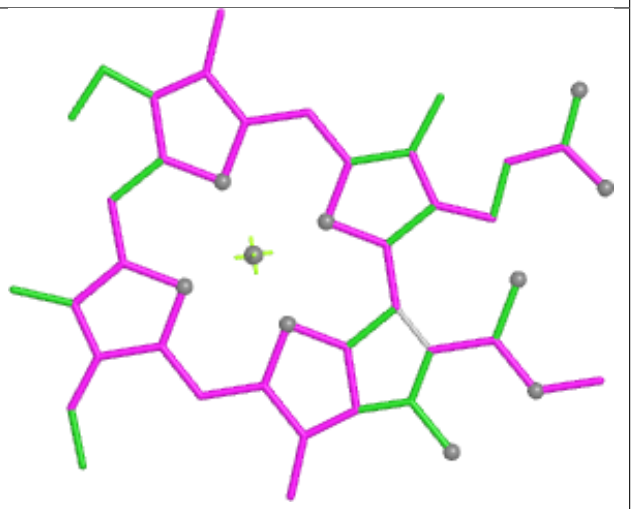


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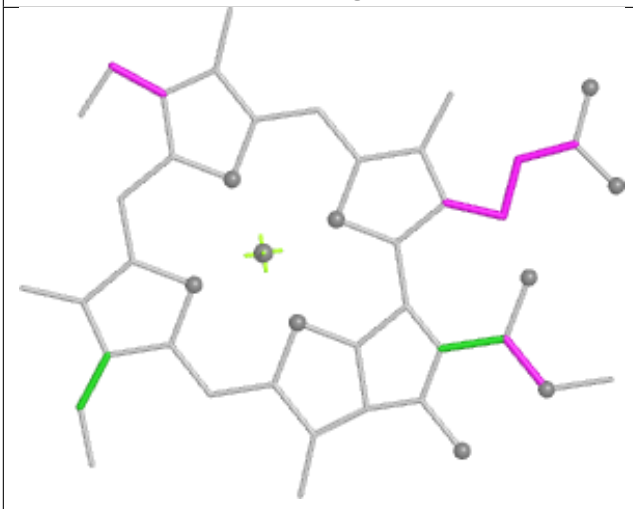
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Bond lengths



Bond angles

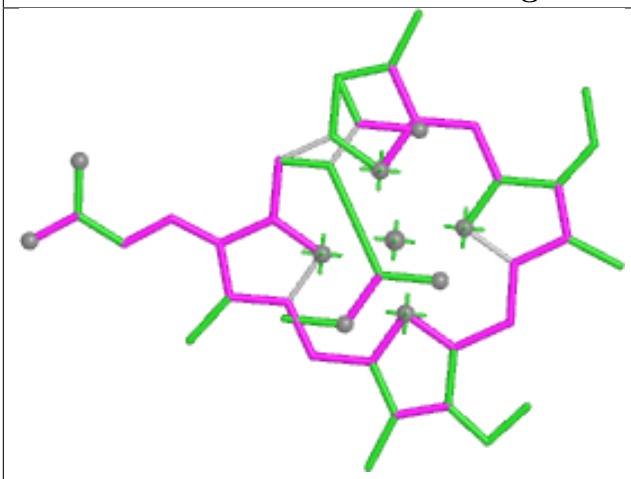


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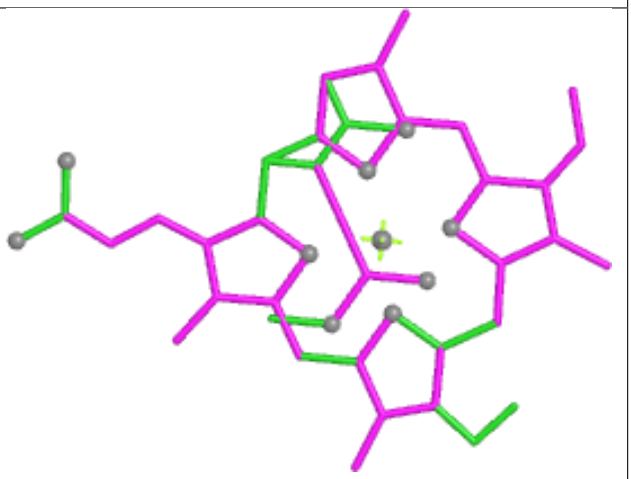


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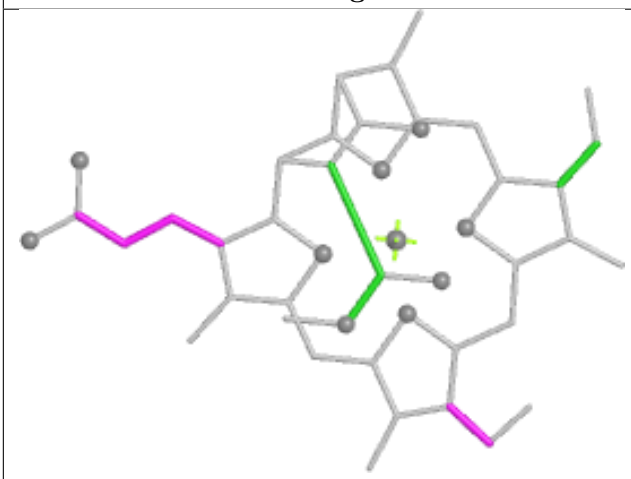
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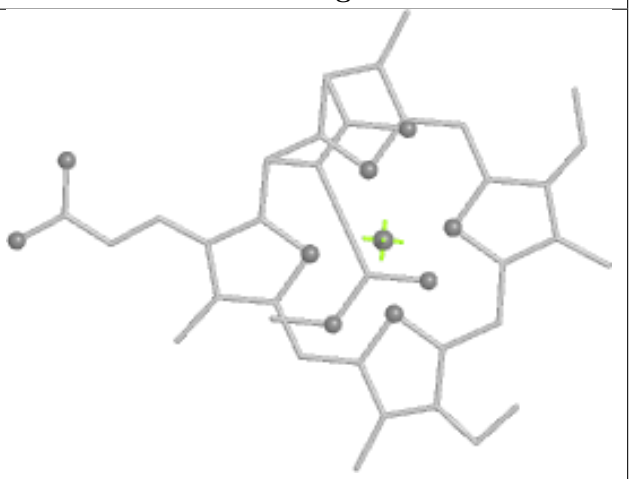
Bond lengths



Bond angles

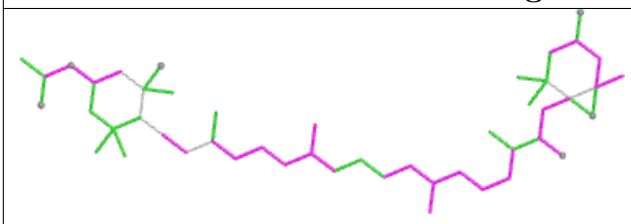


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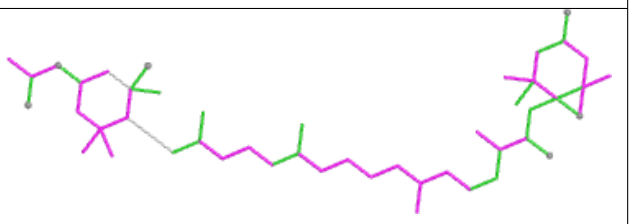


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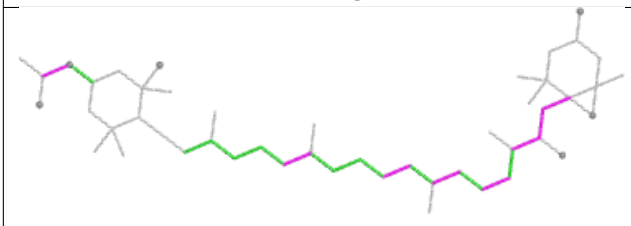
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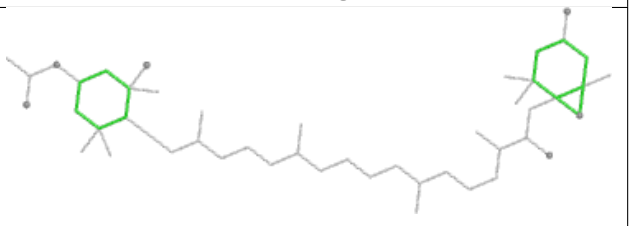
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Bond angles

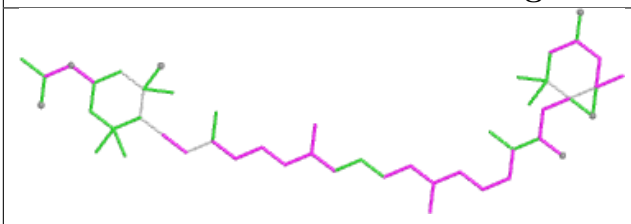


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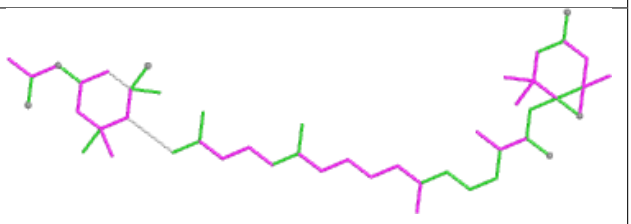


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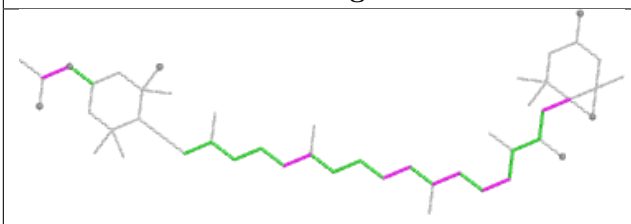
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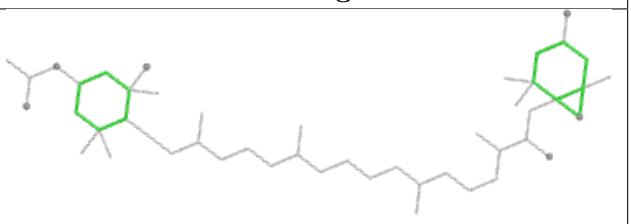
Bond lengths



Bond angles

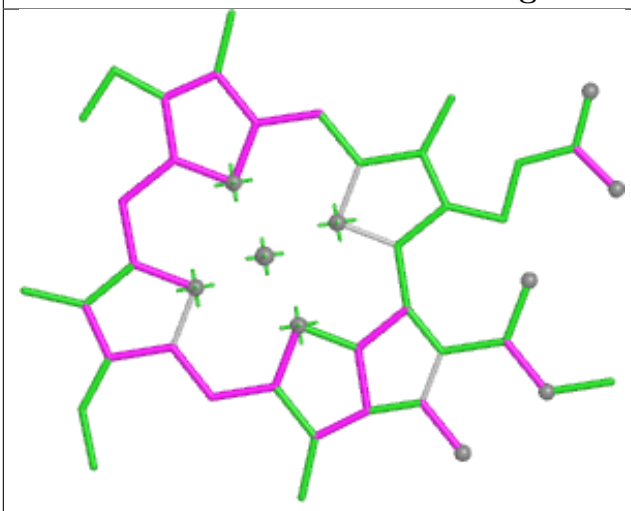


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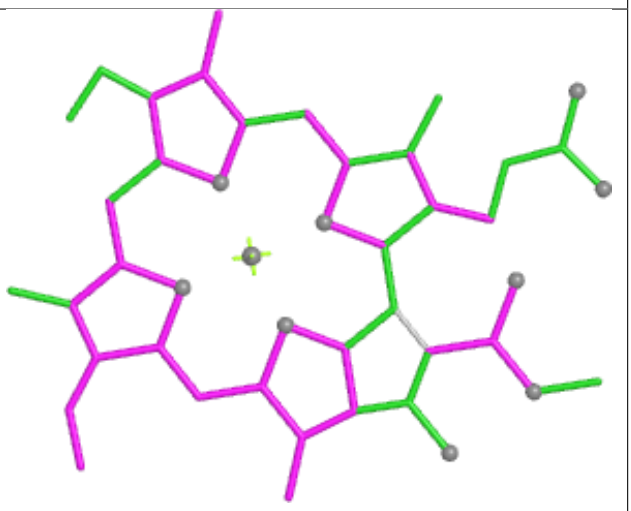


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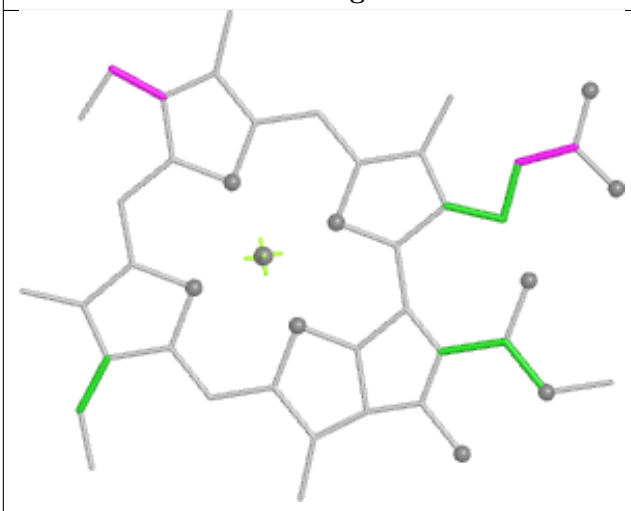
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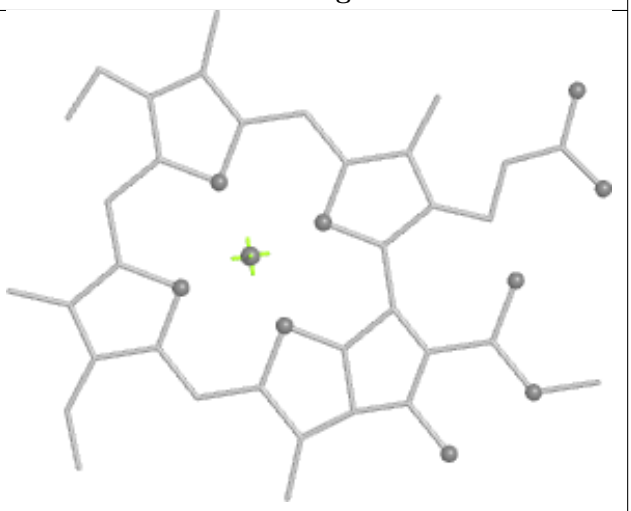
Bond lengths



Bond angles

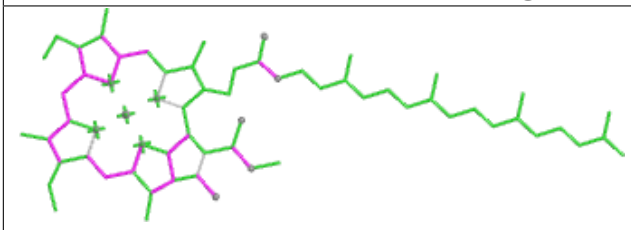


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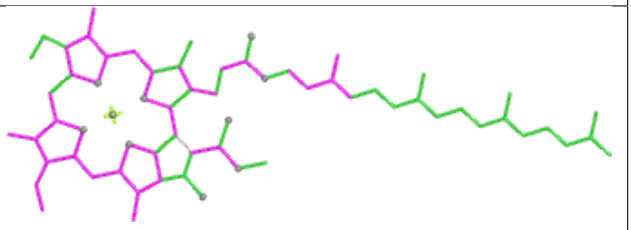


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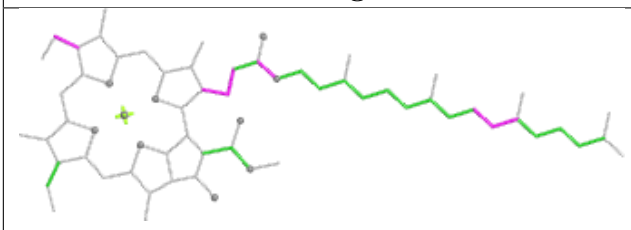
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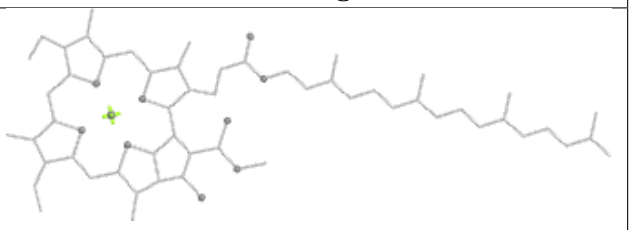
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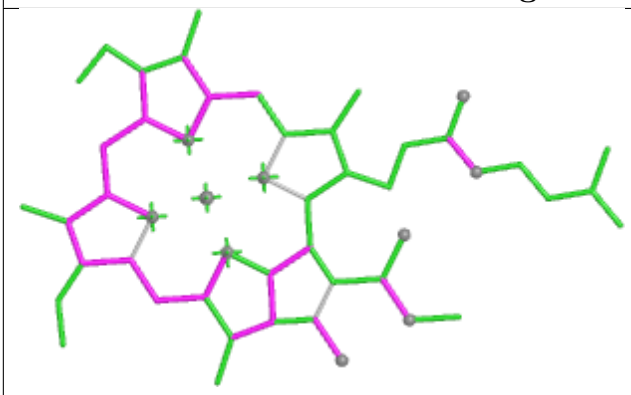


Torsions

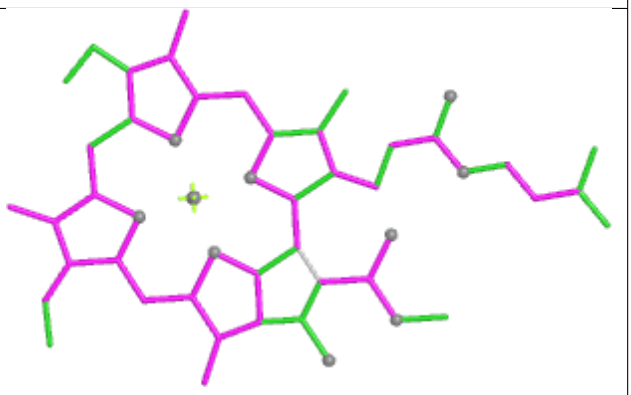


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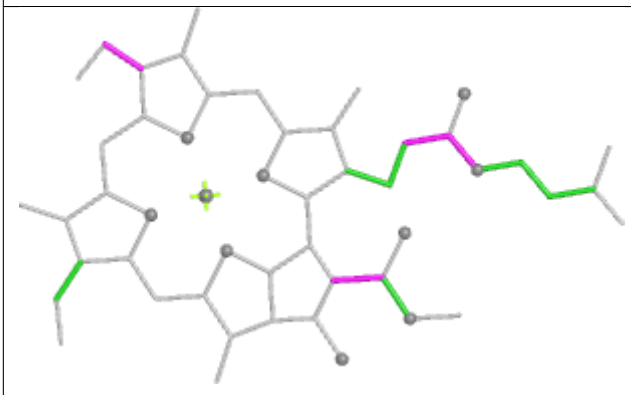
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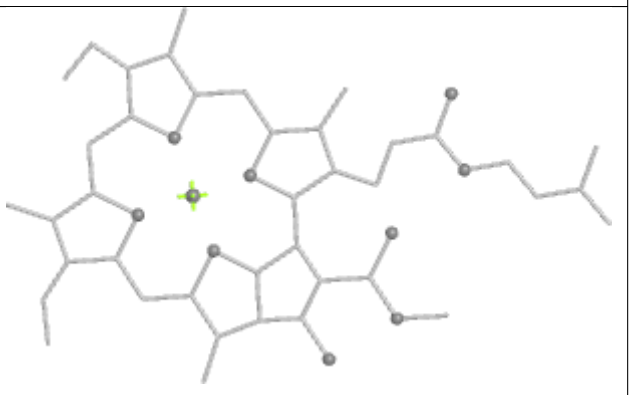
Bond lengths



Bond angles

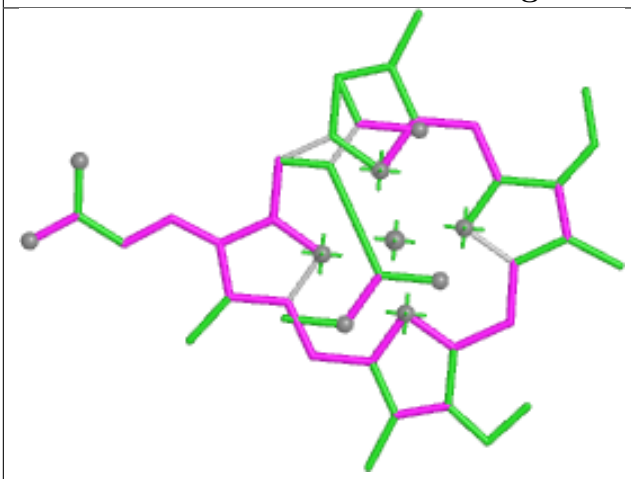


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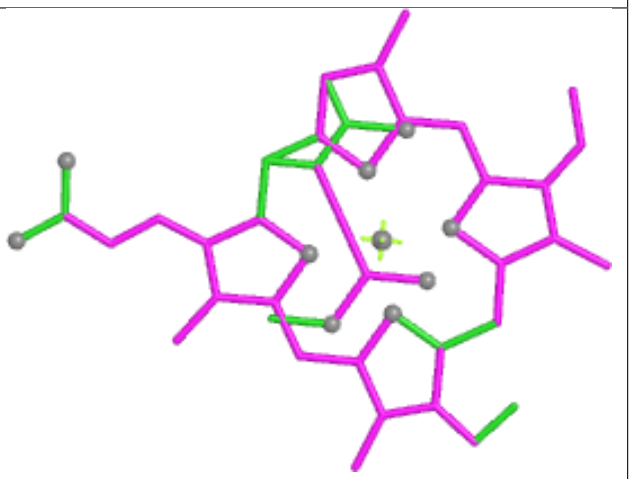


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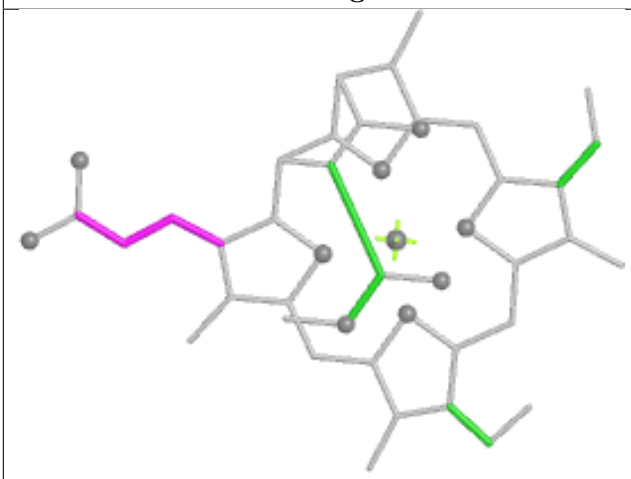
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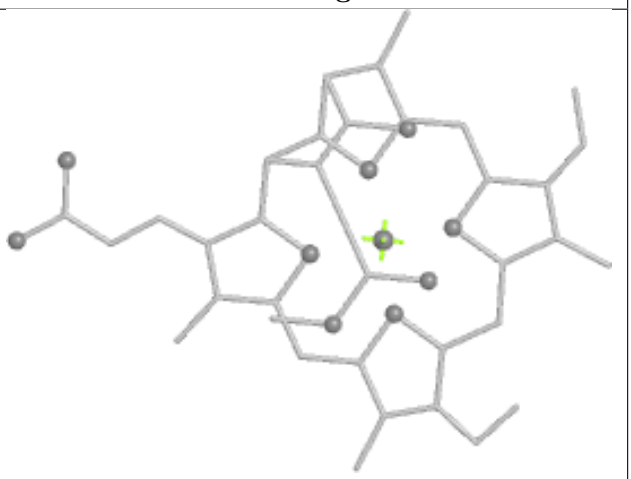
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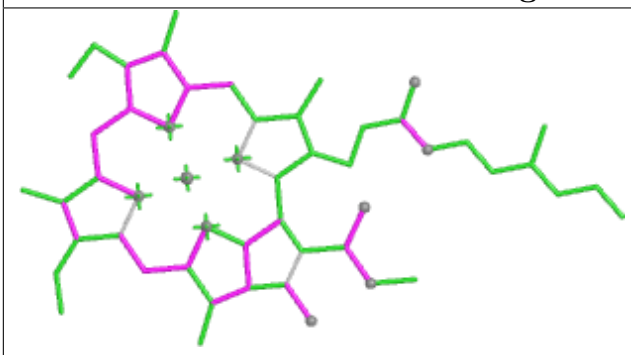


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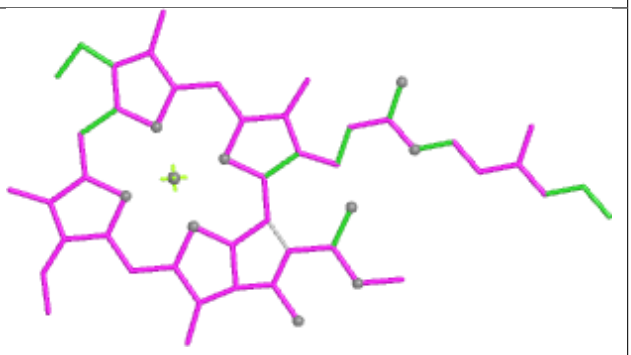


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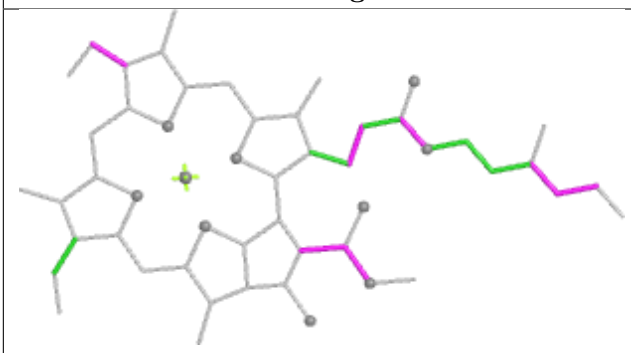
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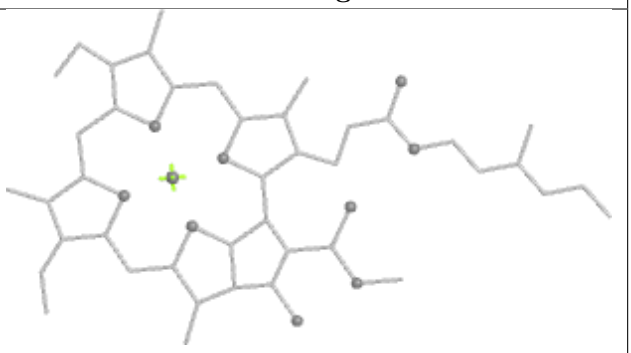
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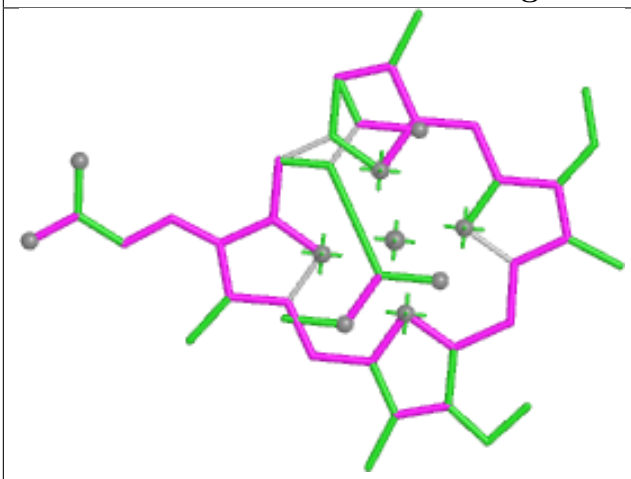


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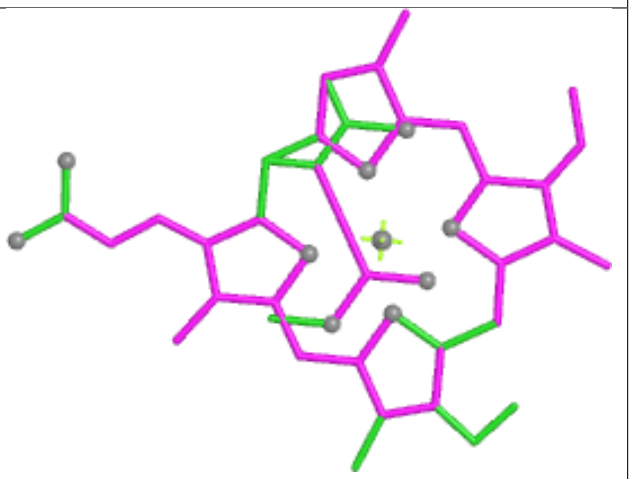


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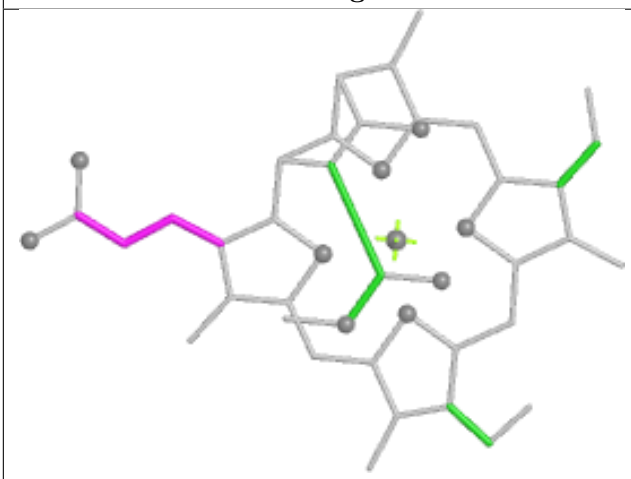
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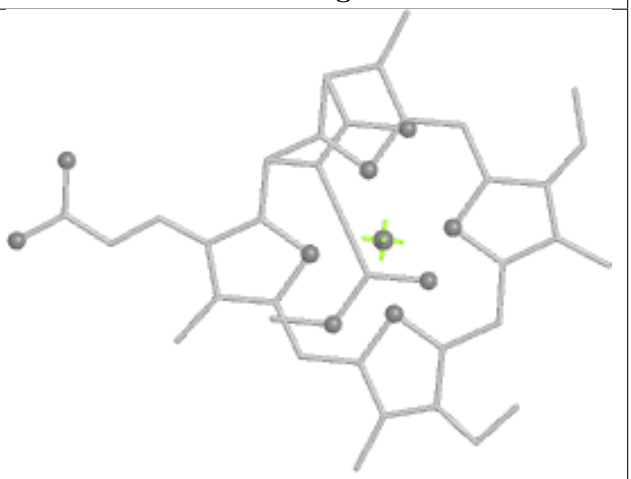
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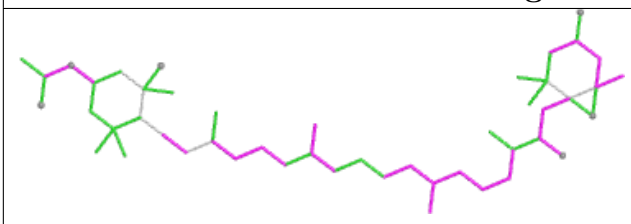


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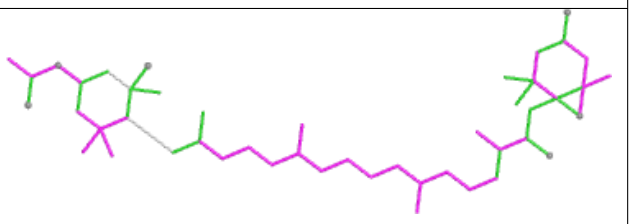


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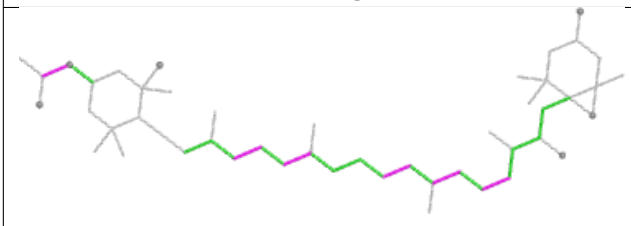
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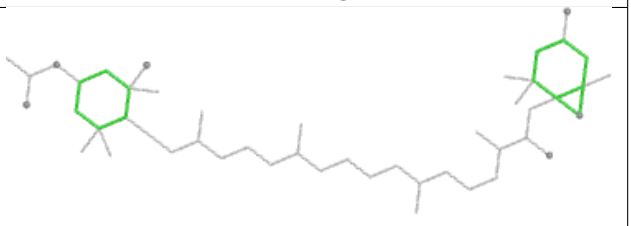
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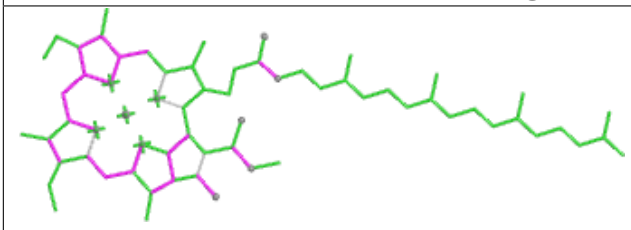


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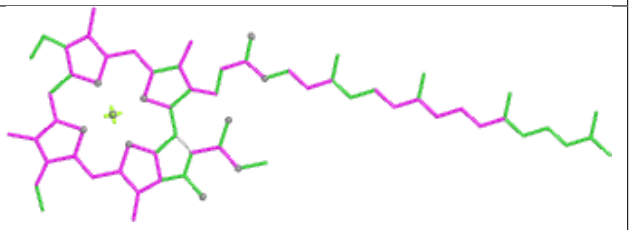


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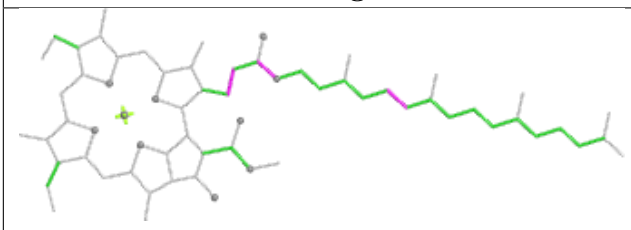
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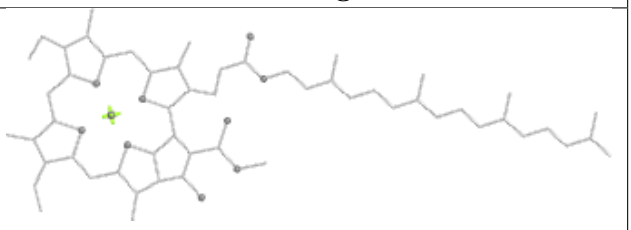
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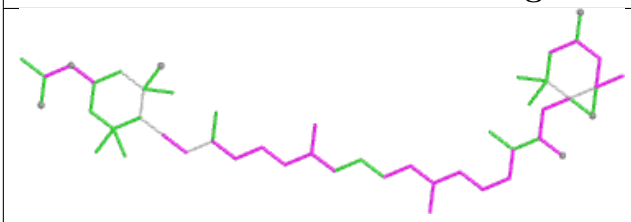


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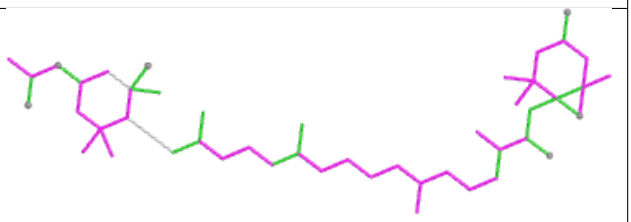


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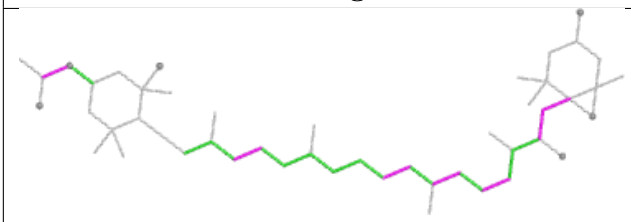
Ligand A86 38 213



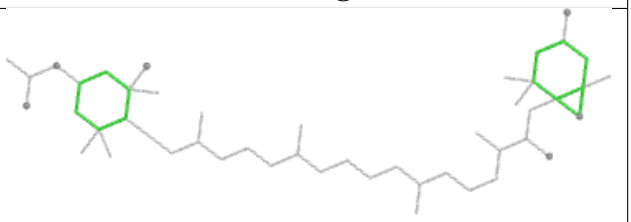
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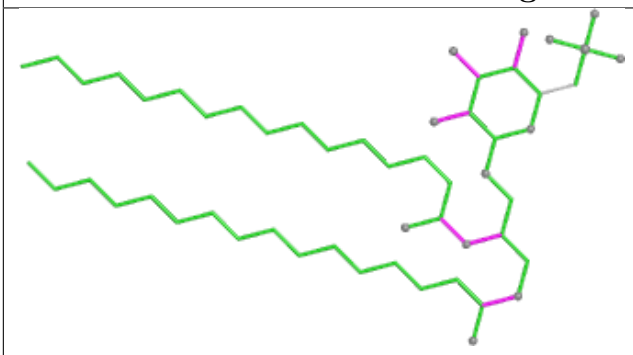


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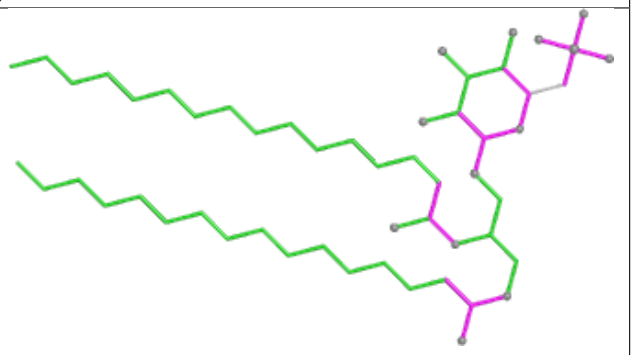


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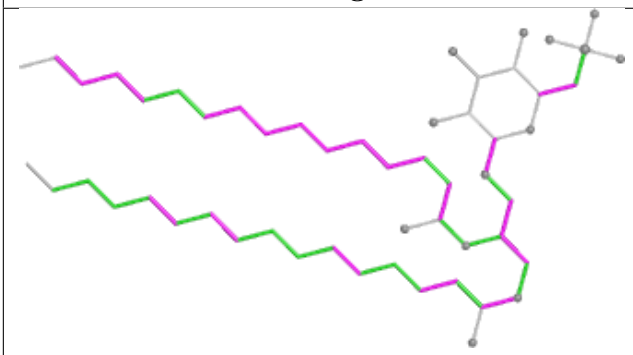
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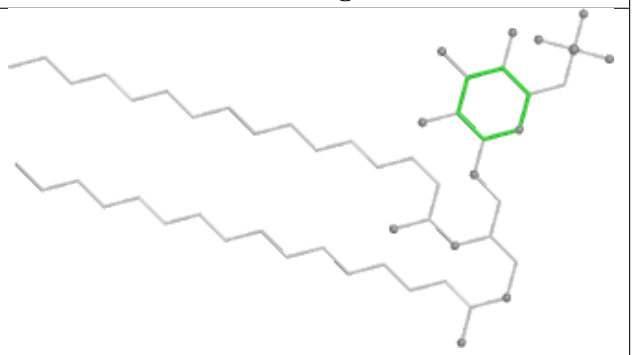
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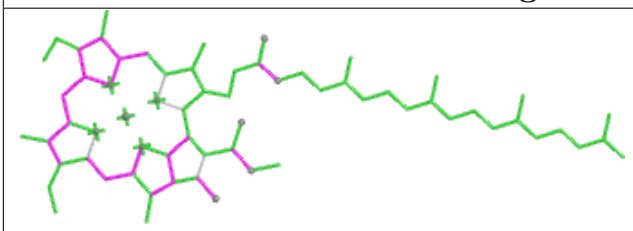


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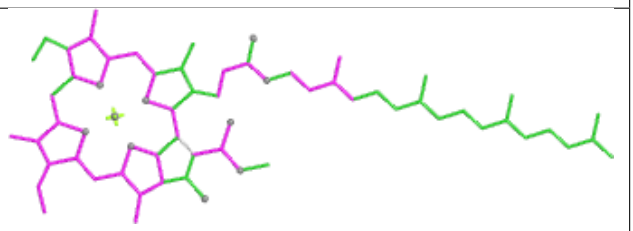


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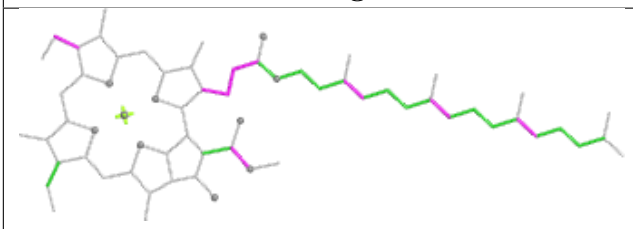
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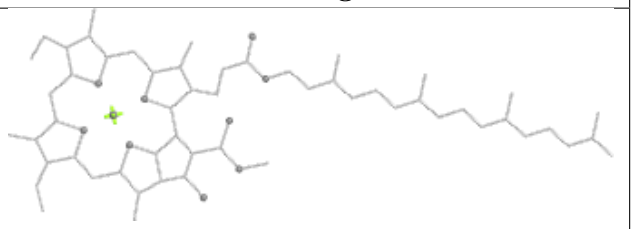
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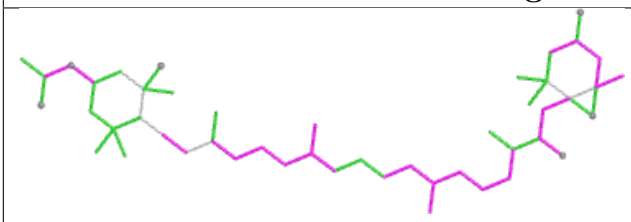


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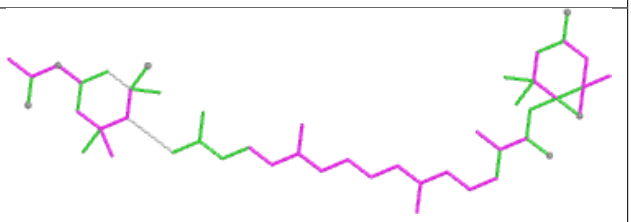


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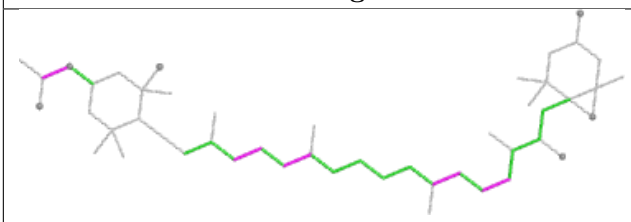
Ligand A86 13 312



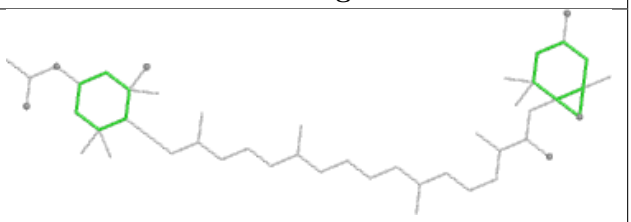
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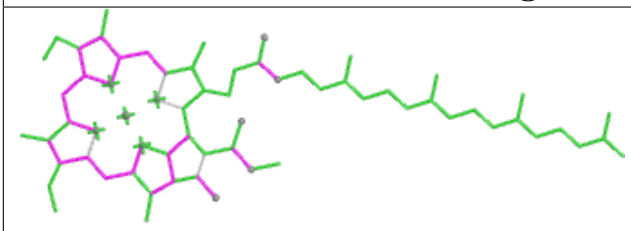


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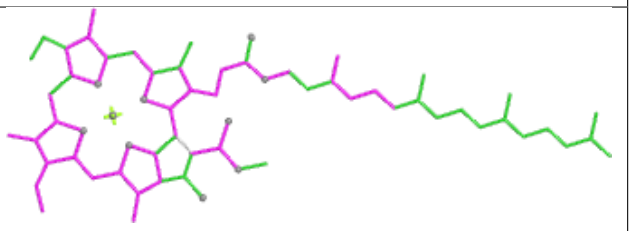


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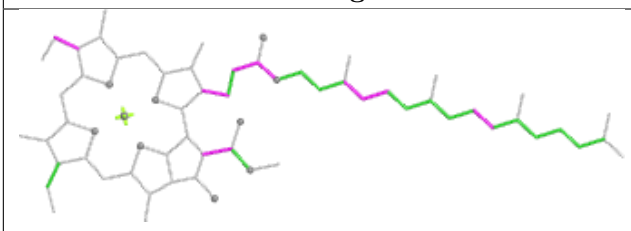
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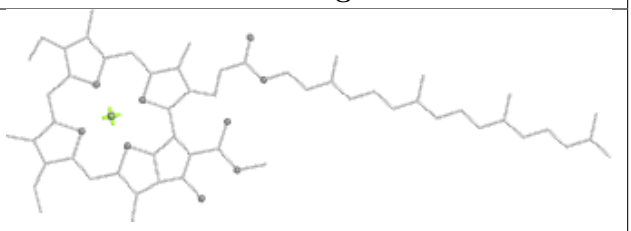
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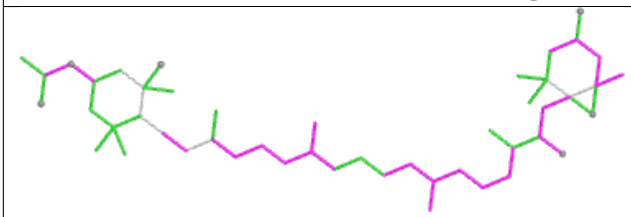


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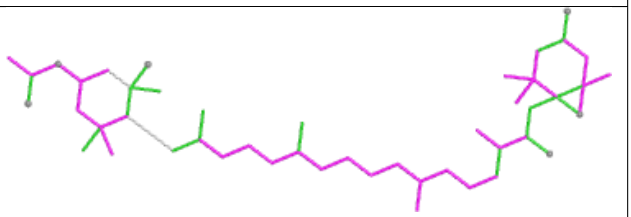


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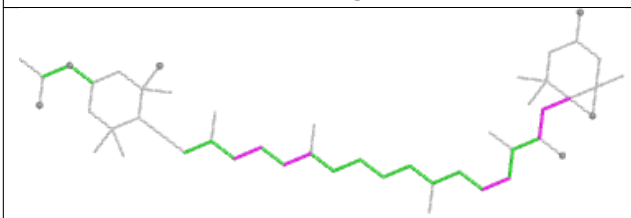
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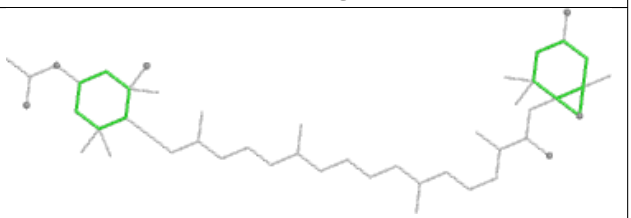
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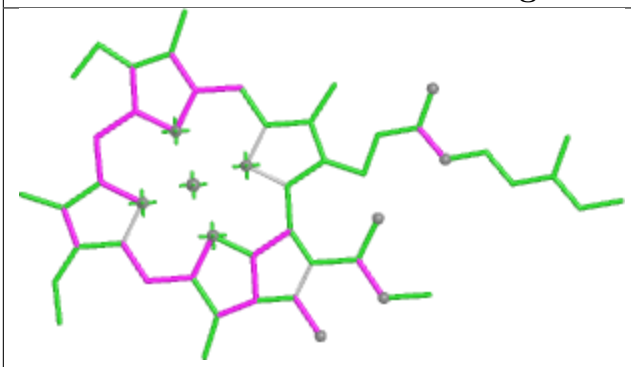


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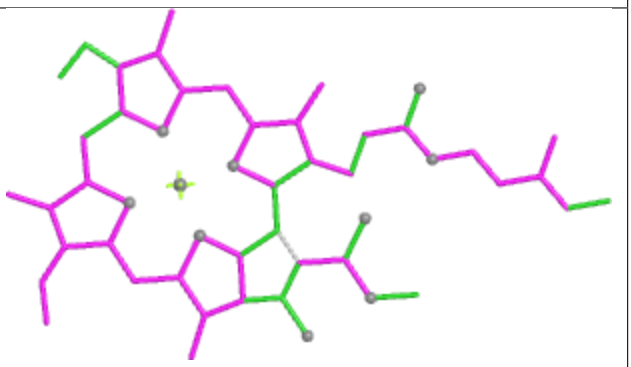


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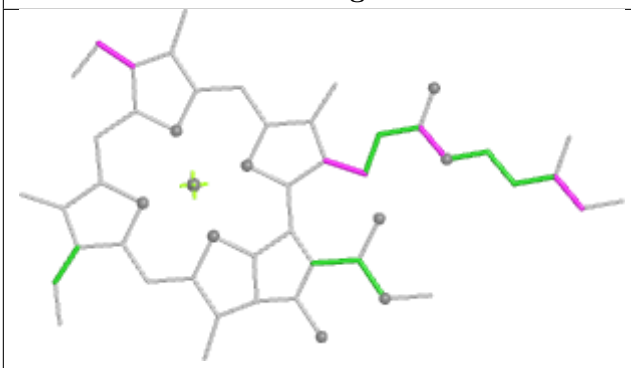
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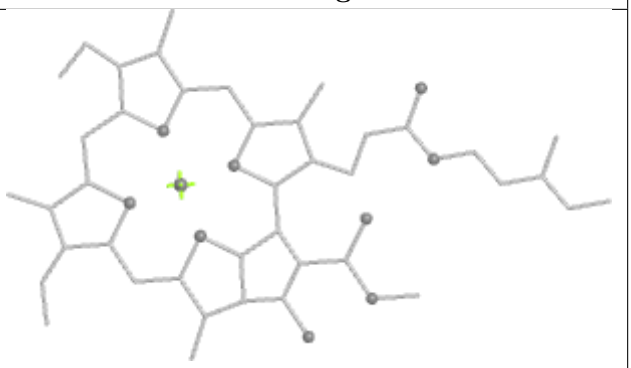
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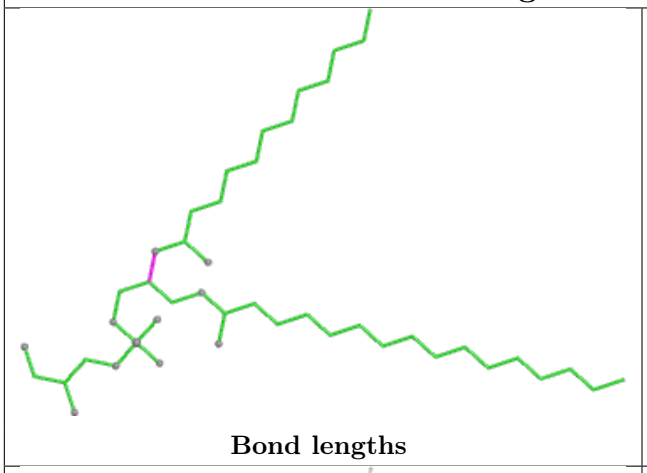


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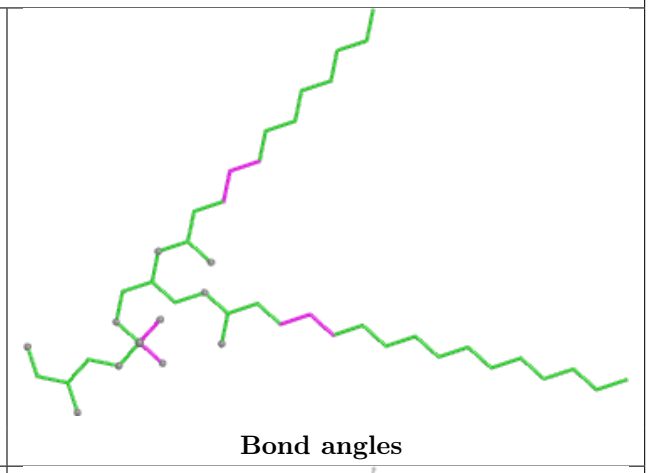


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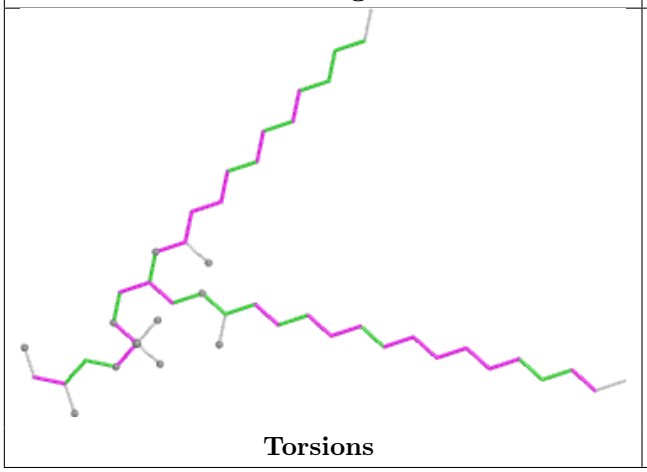
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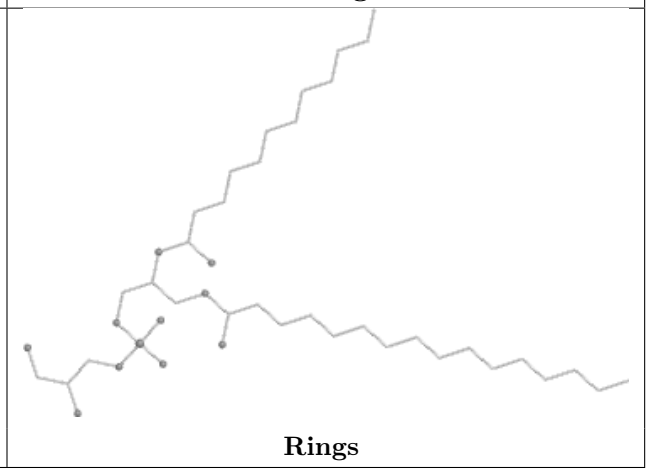
Bond lengths



Bond angles

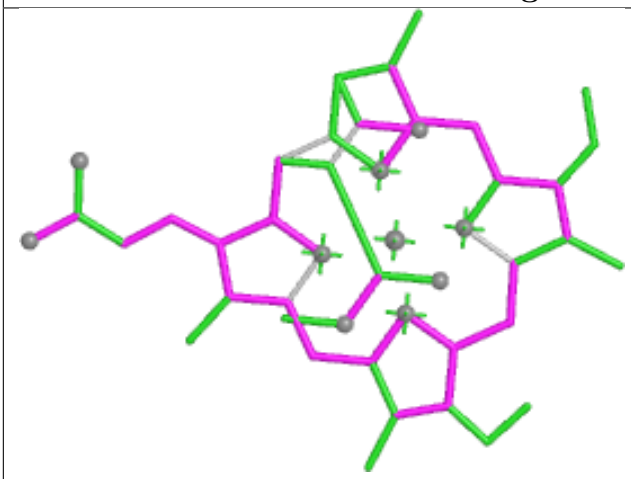


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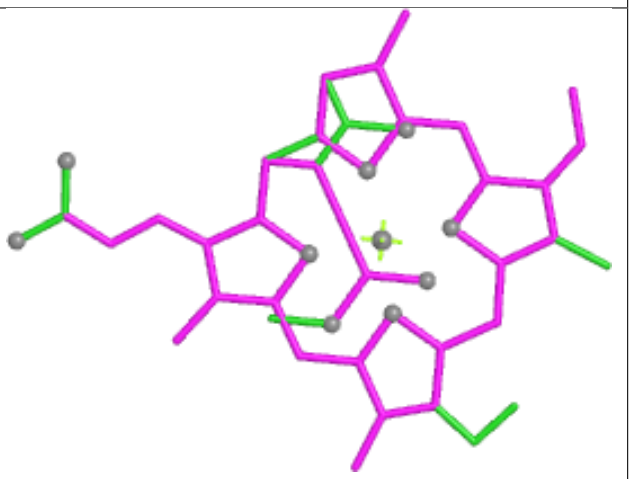


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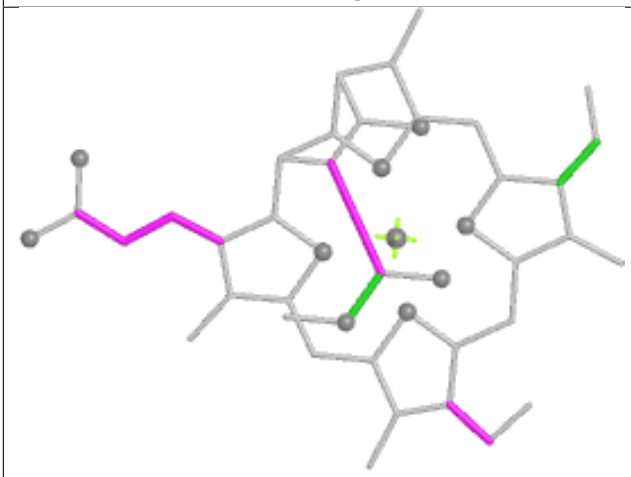
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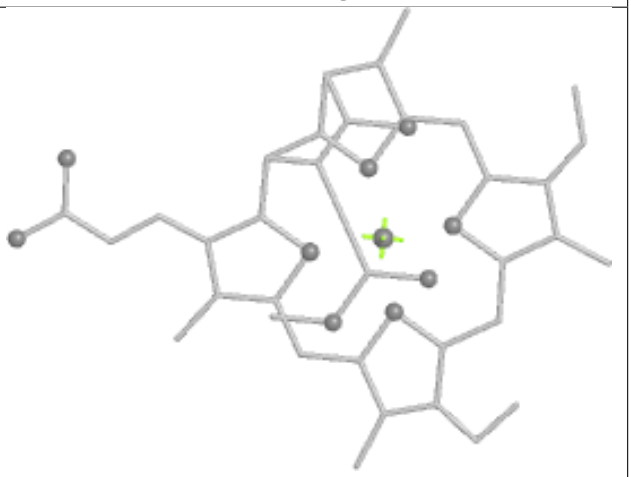
Bond lengths



Bond angles

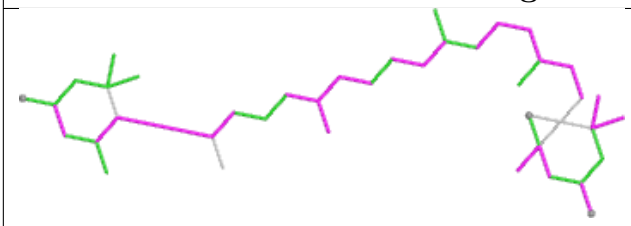


Torsions

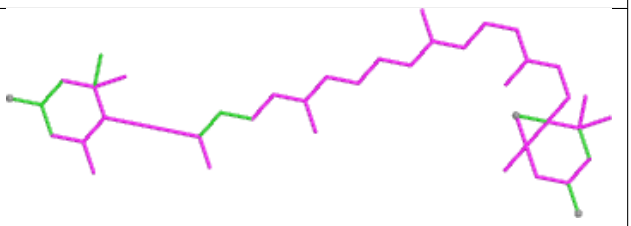


Rings

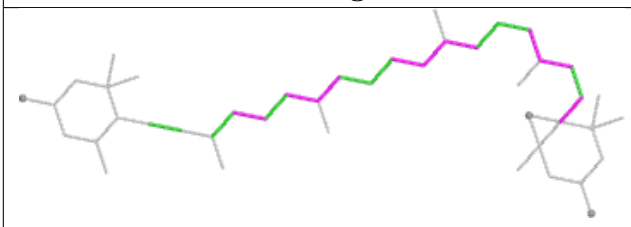
Ligand DD6 39 312



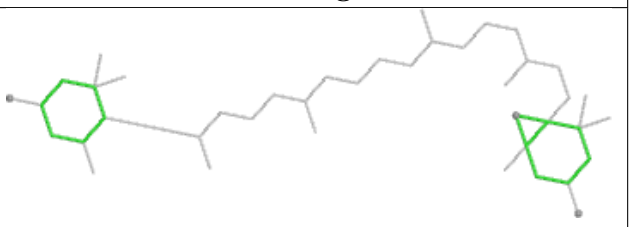
Bond lengths



Bond angles

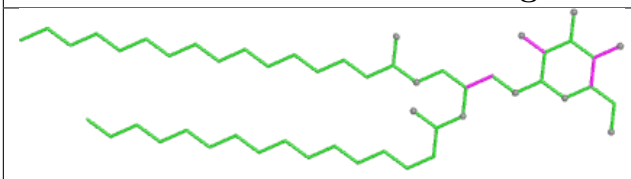


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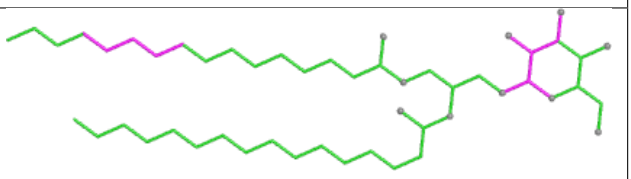


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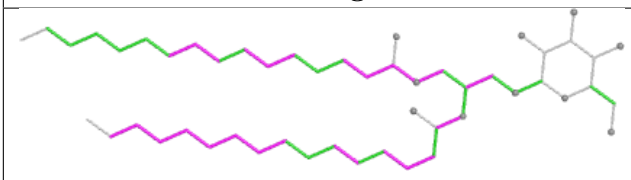
Ligand LMG B 521



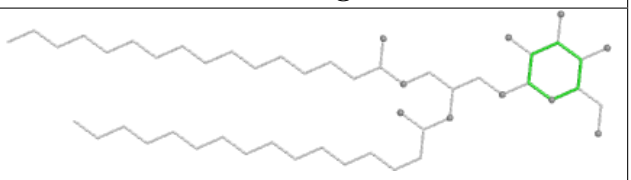
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Bond angles

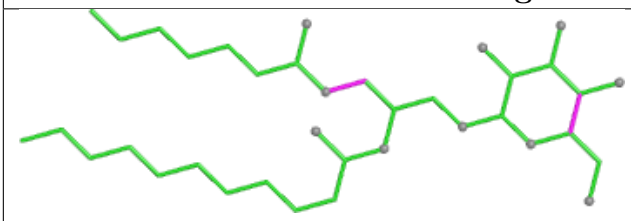


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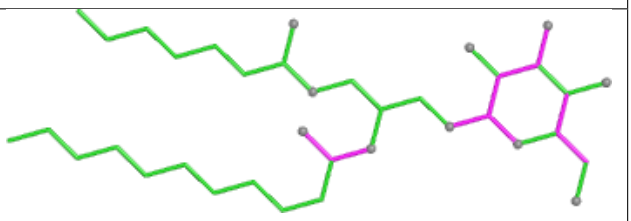


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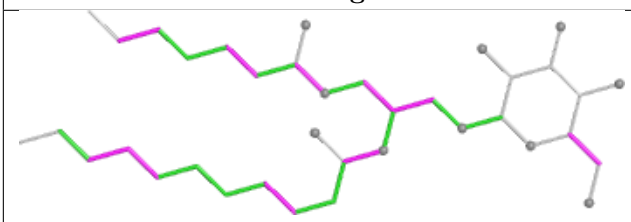
Ligand LMG 17 317



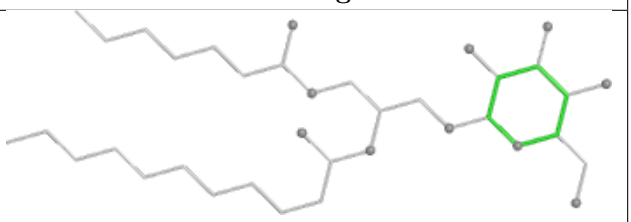
Bond lengths



Bond angles

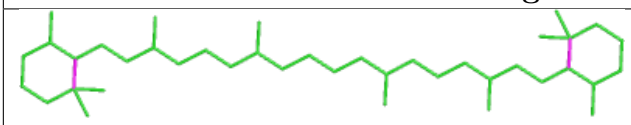


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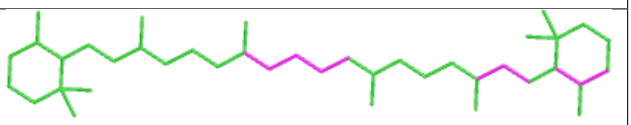


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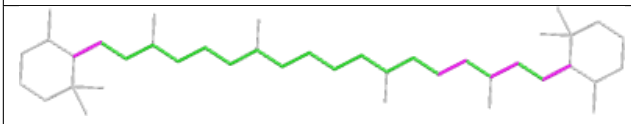
Ligand BCR C 519



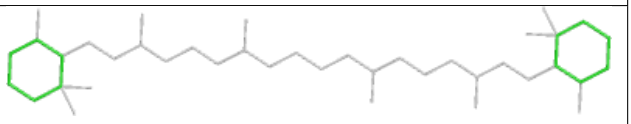
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Bond angles

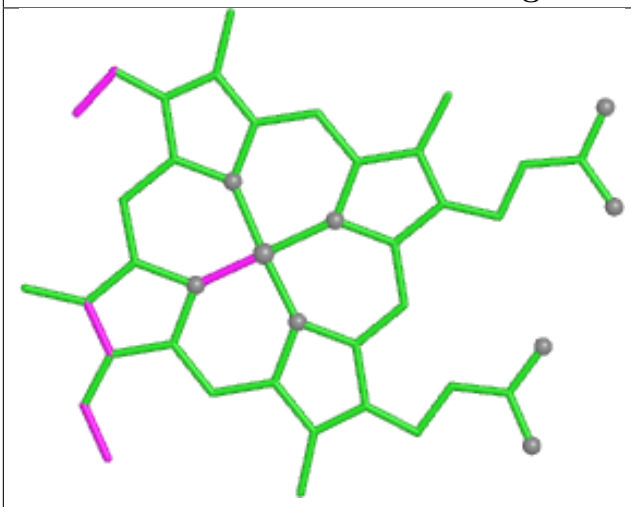


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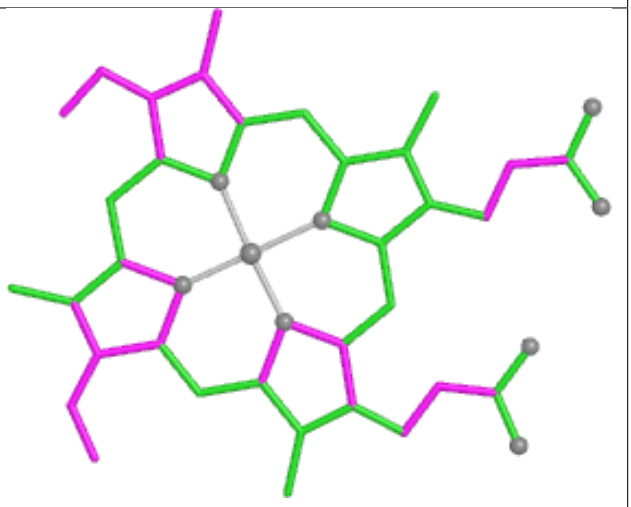


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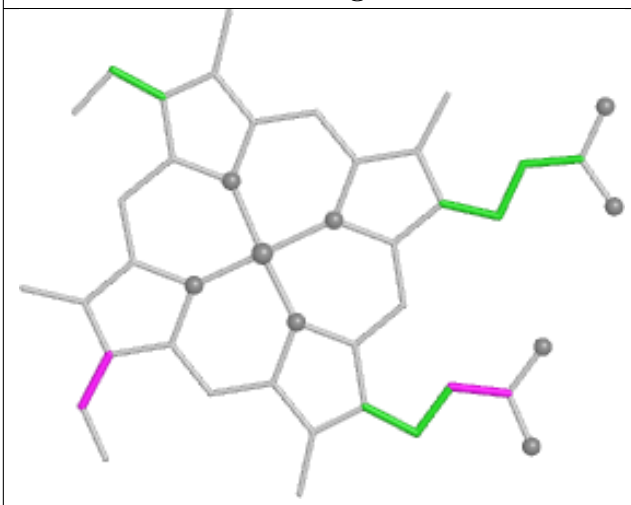
Ligand HEC V 201



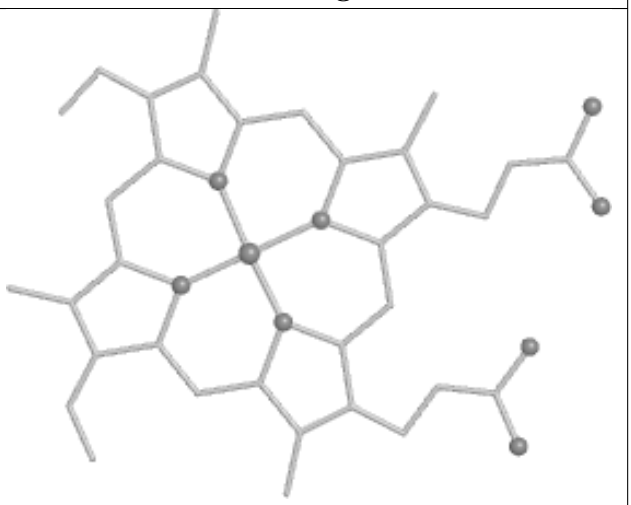
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Bond angles

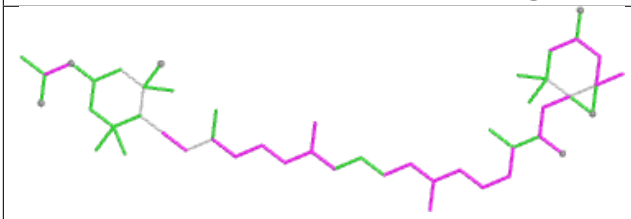


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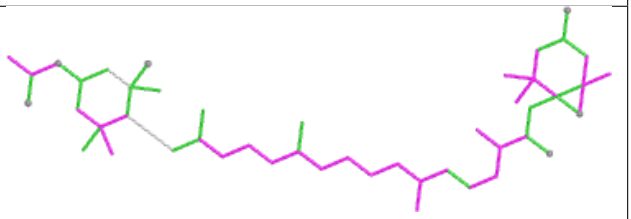


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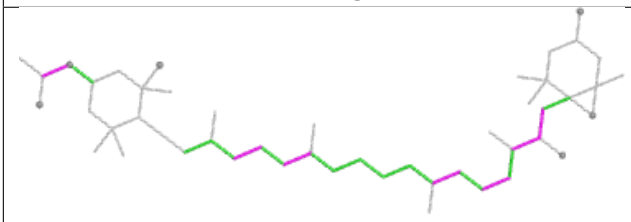
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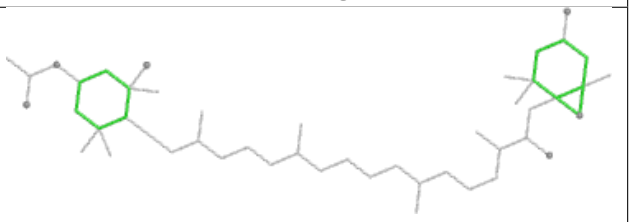
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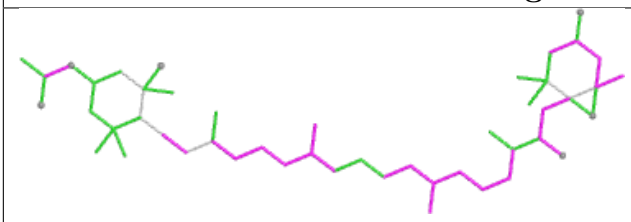


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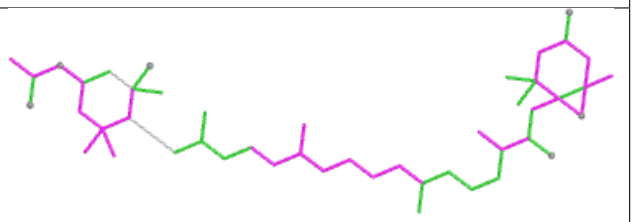


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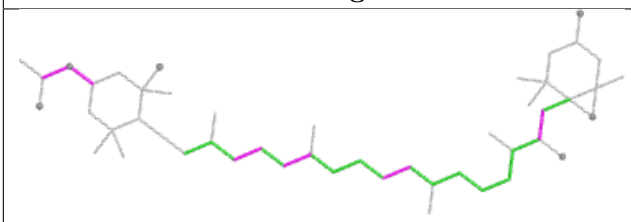
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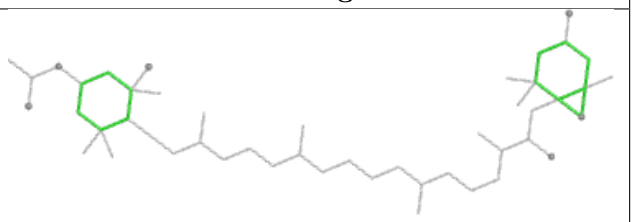
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Bond angles

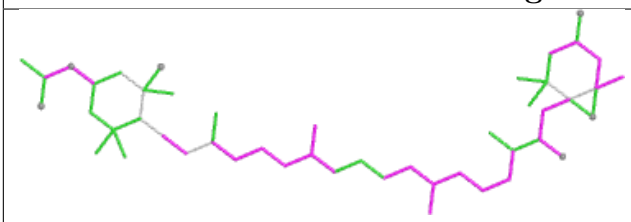


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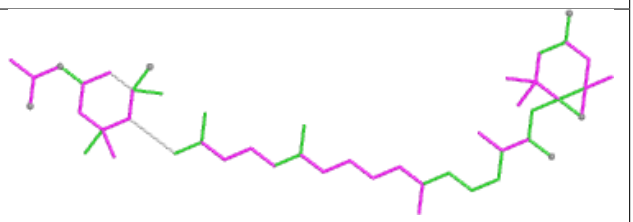


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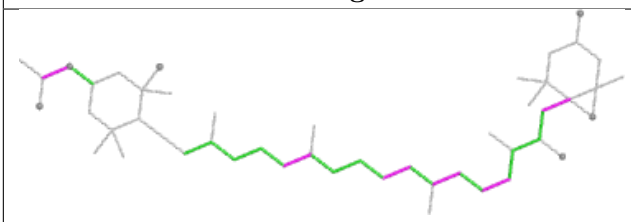
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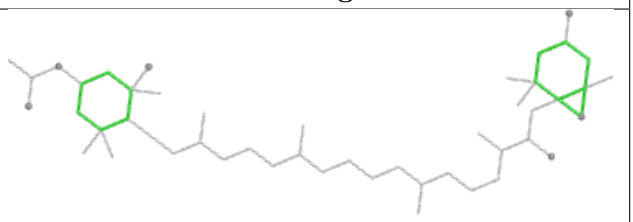
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Bond angles

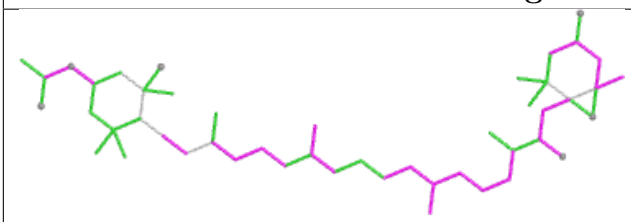


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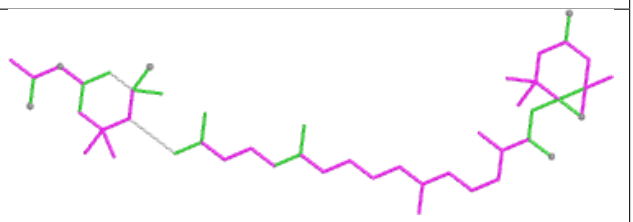


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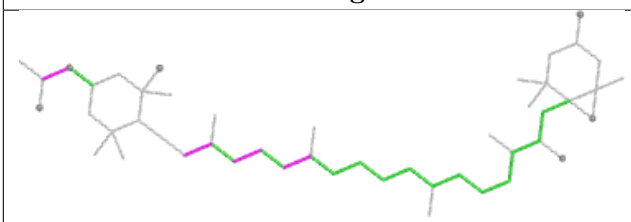
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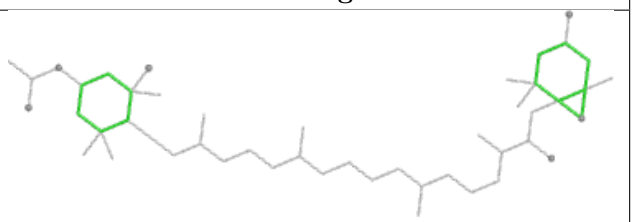
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Bond angles

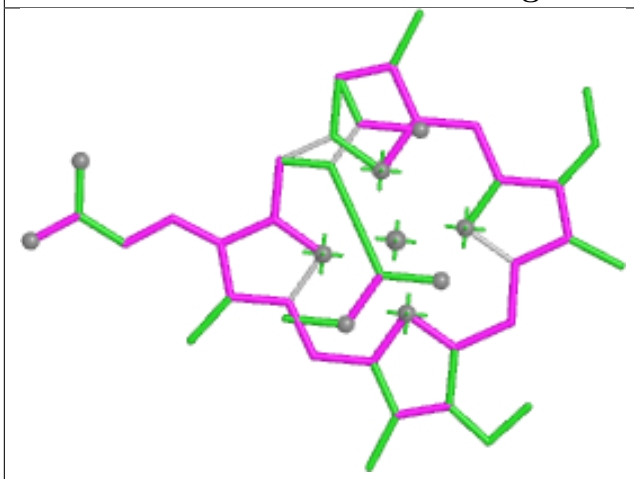


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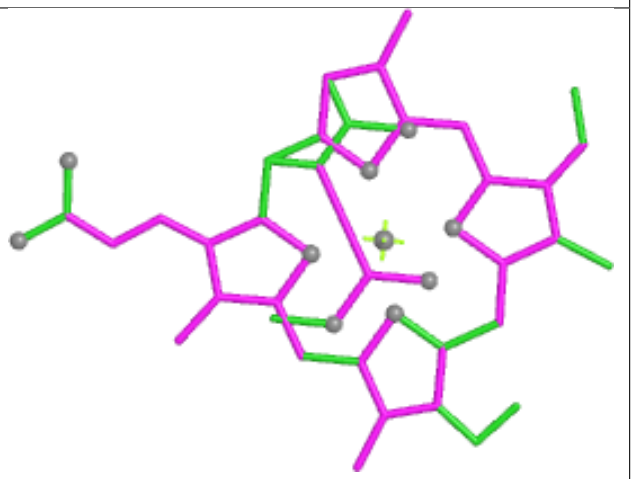


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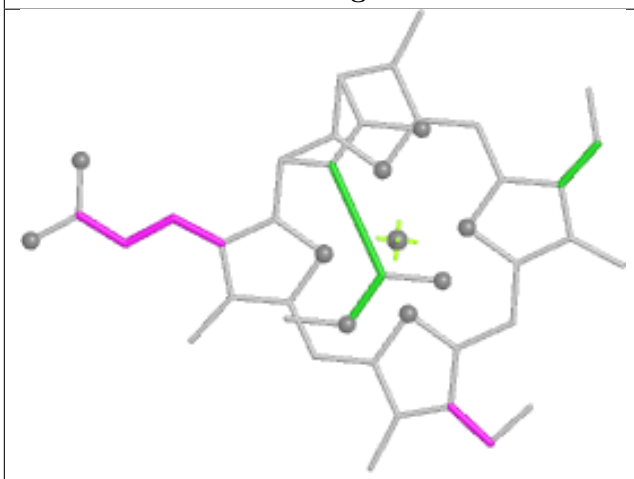
Ligand KC1 16 305



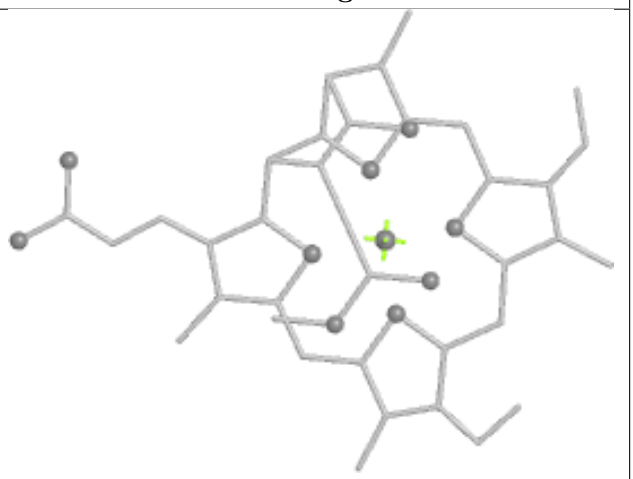
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Bond angles

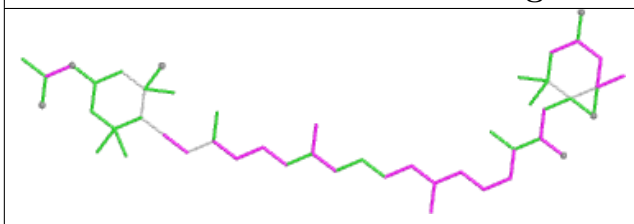


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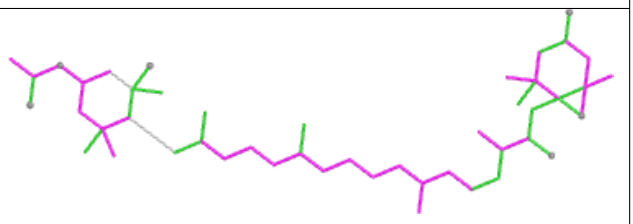


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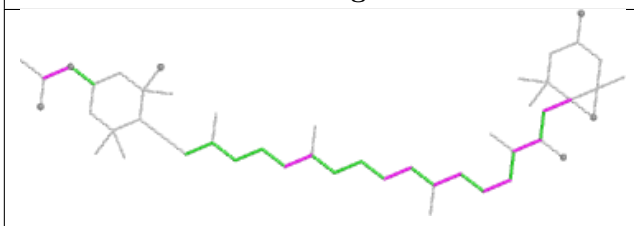
Ligand A86 32 203



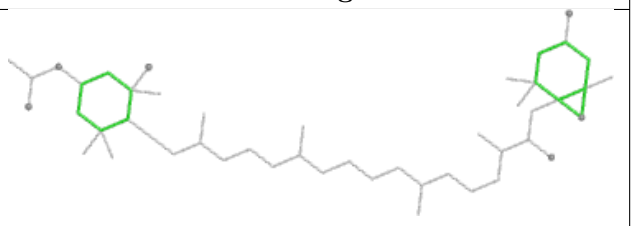
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Bond angles

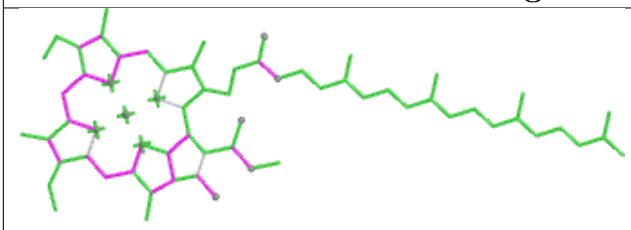


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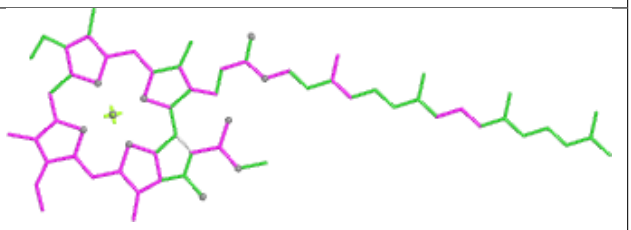


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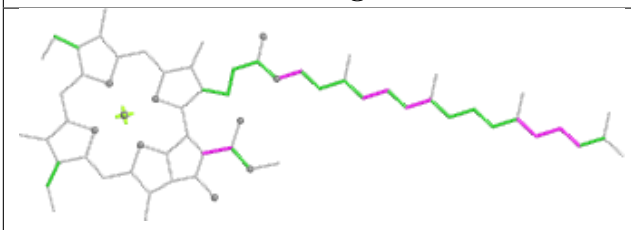
Ligand CLA C 509



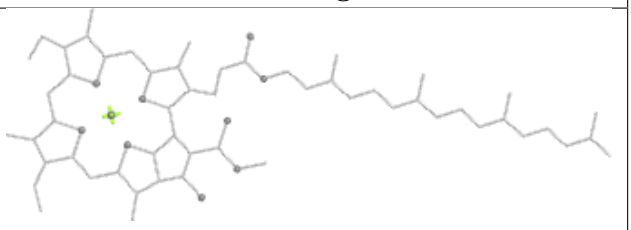
Bond lengths



Bond angles

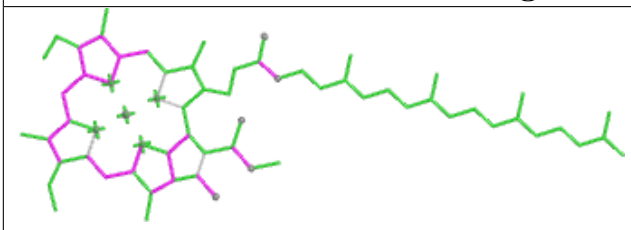


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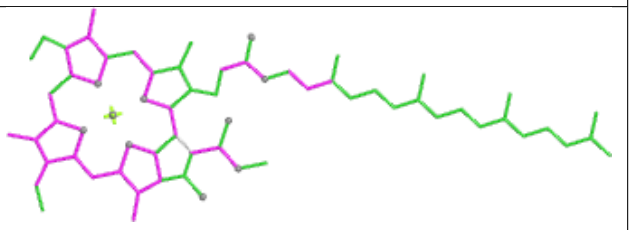


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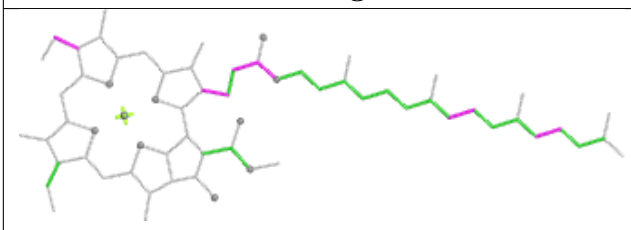
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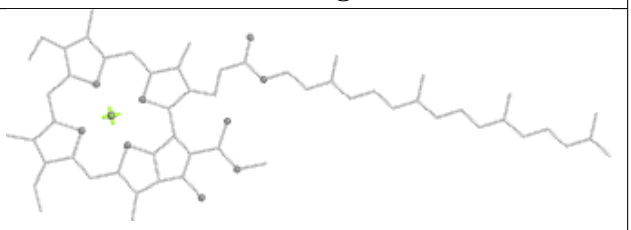
Bond lengths



Bond angles

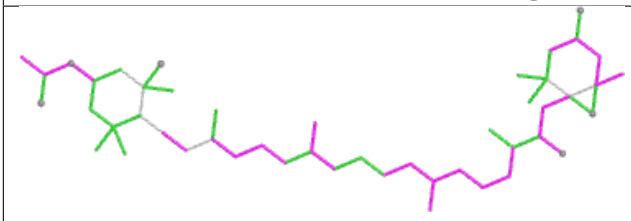


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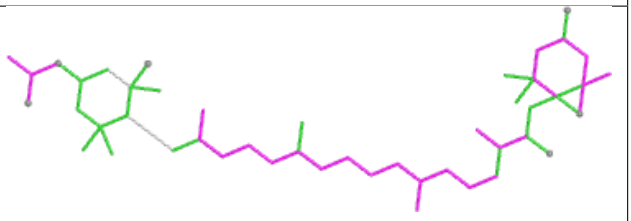


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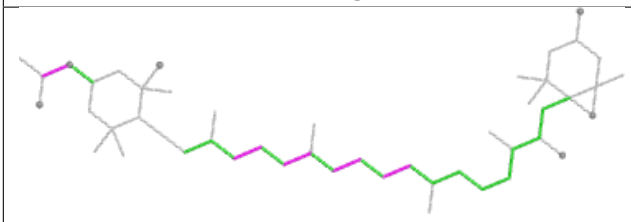
Ligand A86 11 319



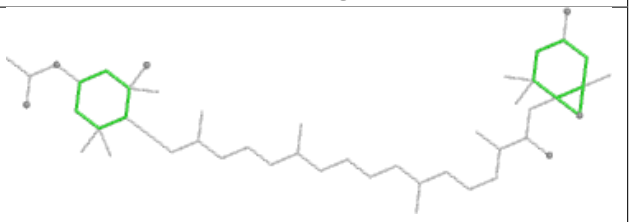
Bond lengths



Bond angles

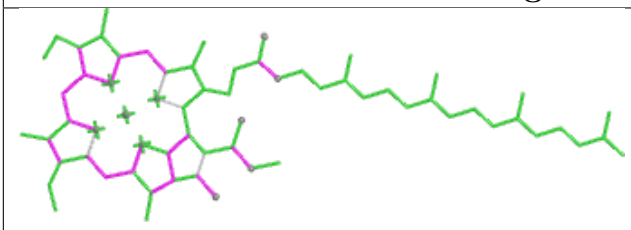


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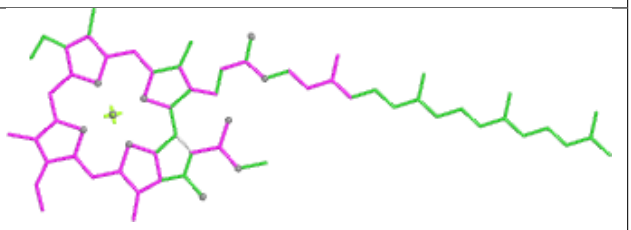


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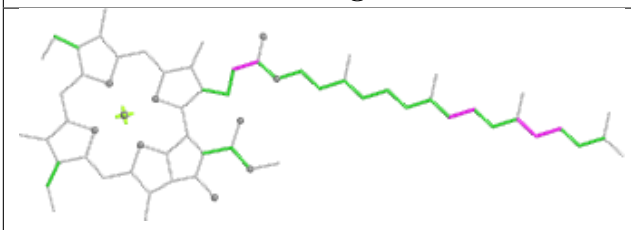
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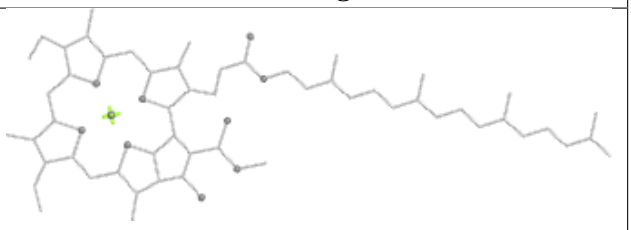
Bond lengths



Bond angles

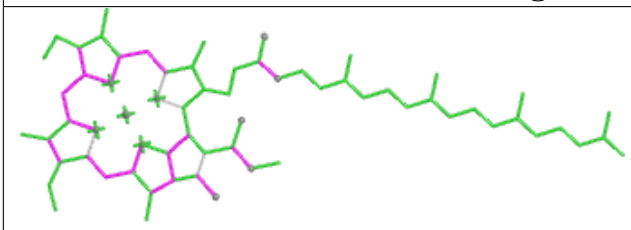


Torsions

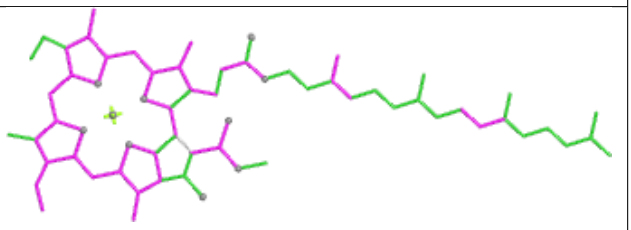


Rings

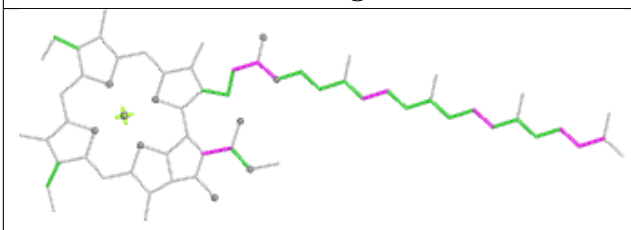
Ligand CLA c 512



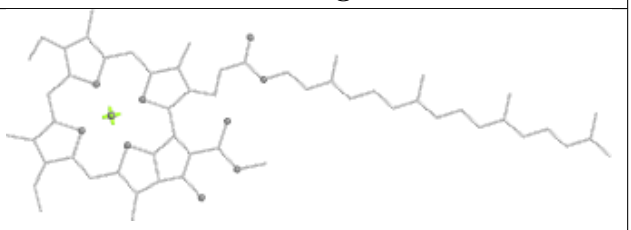
Bond lengths



Bond angles

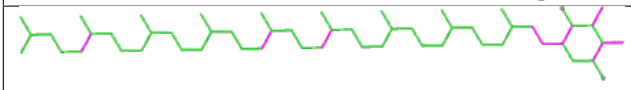


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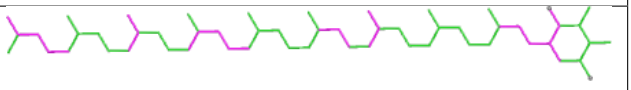


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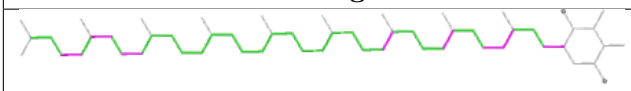
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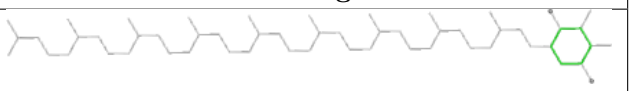
Bond lengths



Bond angles

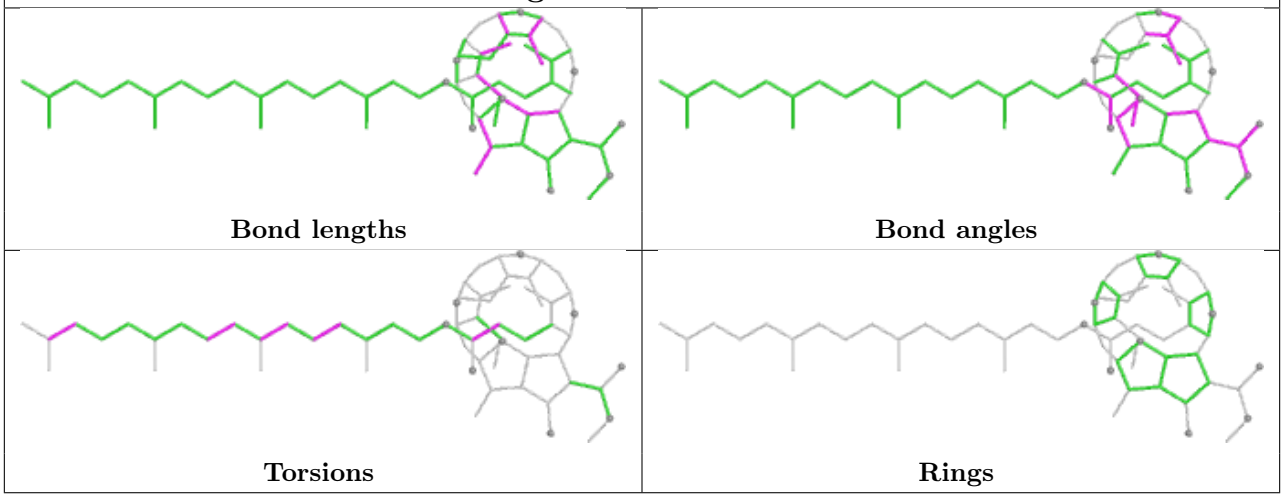


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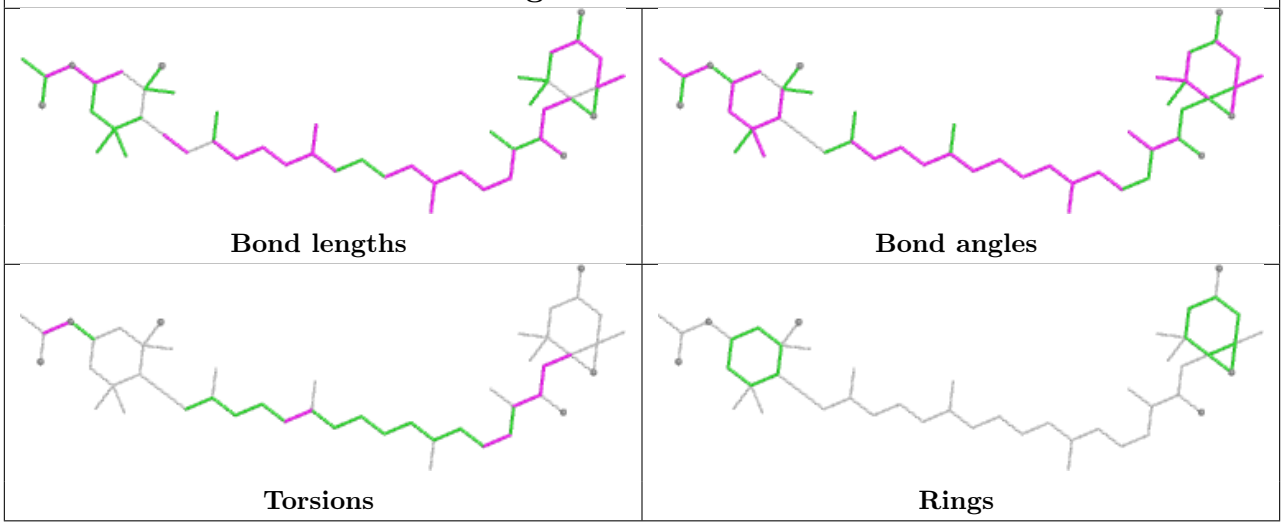


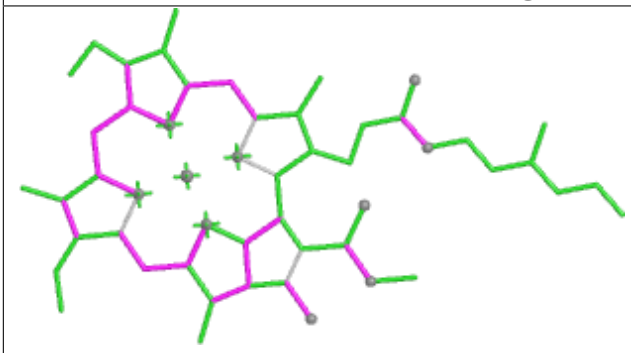
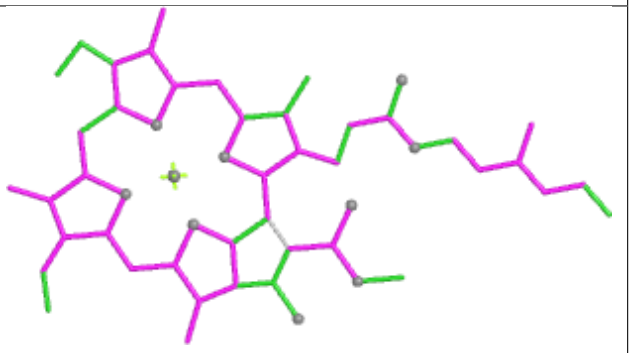
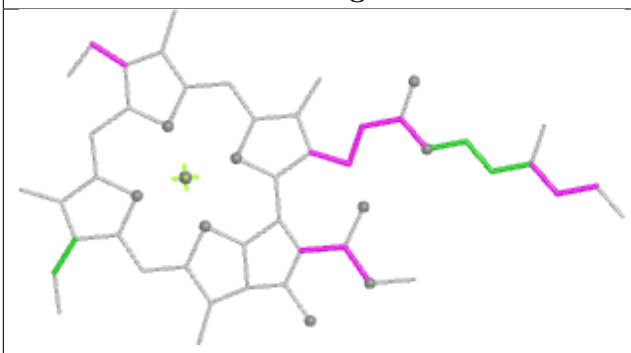
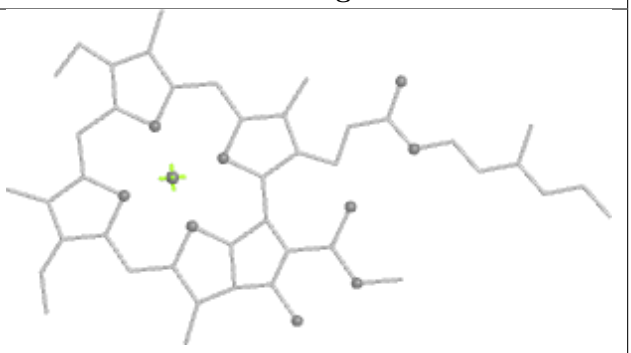
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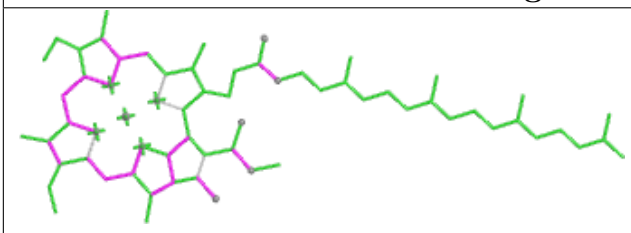
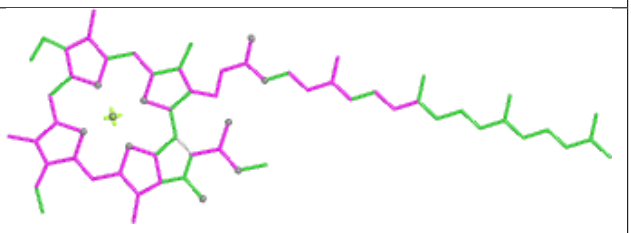
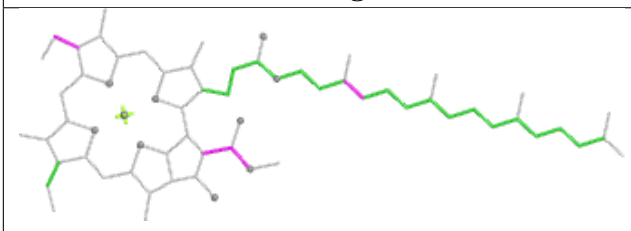
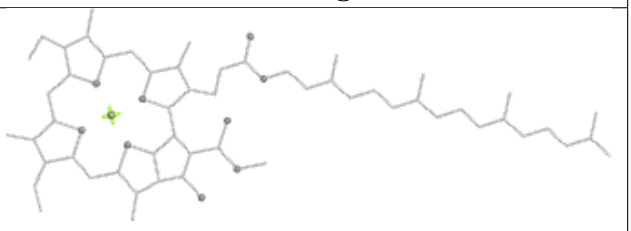
Ligand PHO a 406



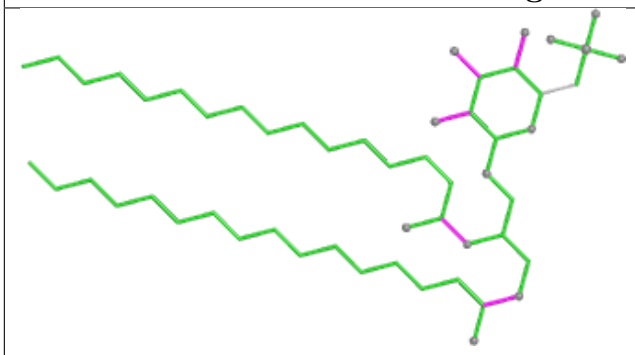
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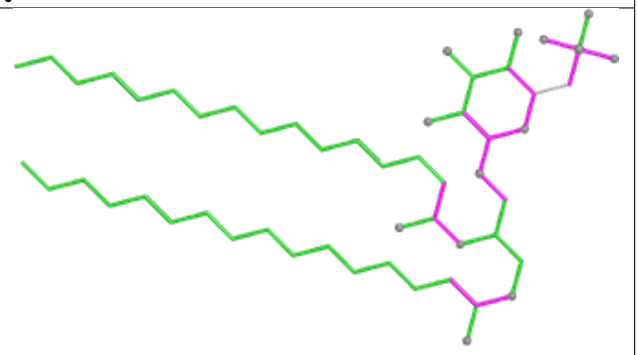
Ligand CLA 32 210	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 504	
	
Bond lengths	Bond angles
	
Torsions	Rings

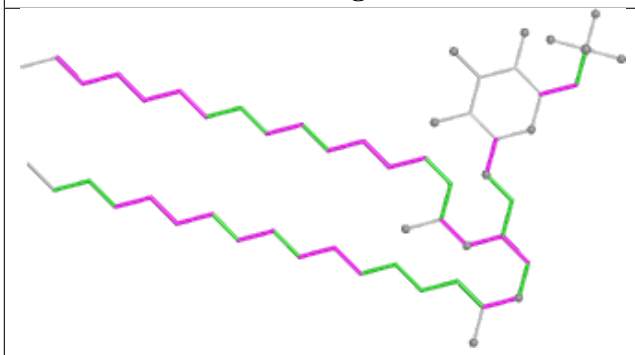
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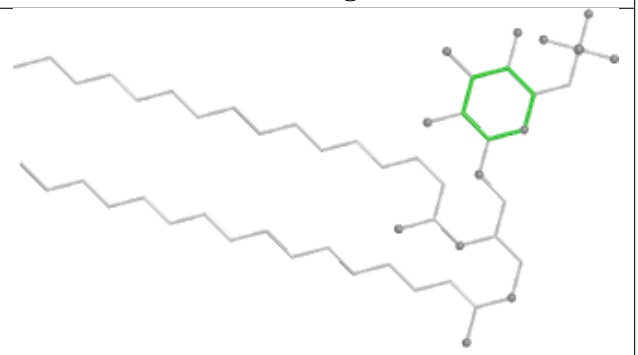
Bond lengths



Bond angles

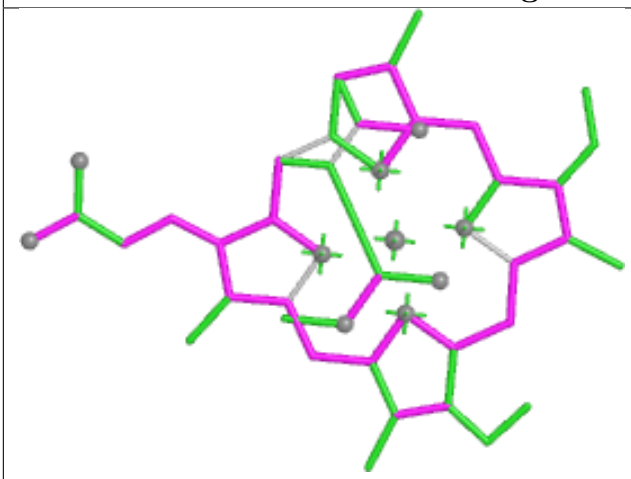


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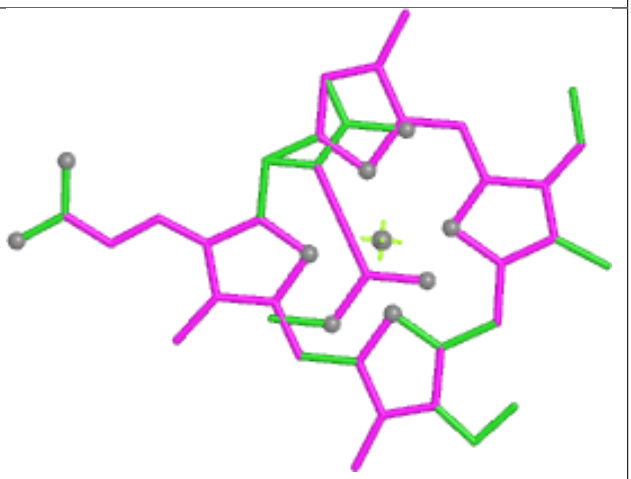


Rings

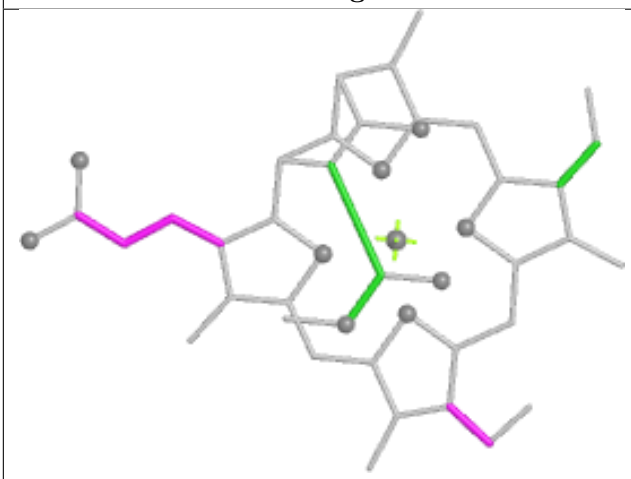
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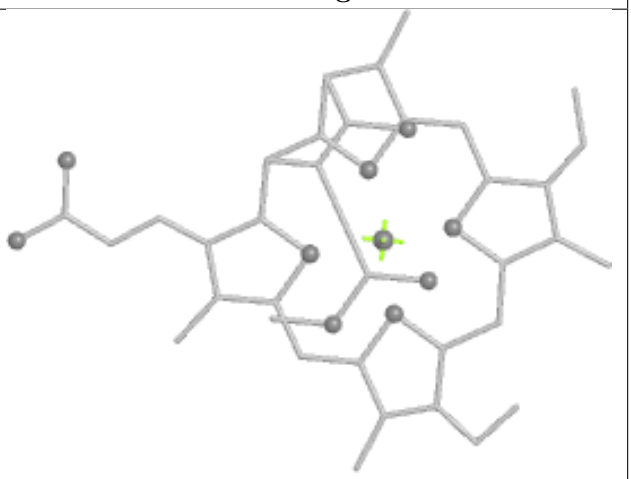
Bond lengths



Bond angles

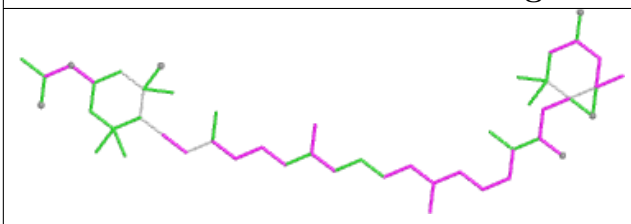


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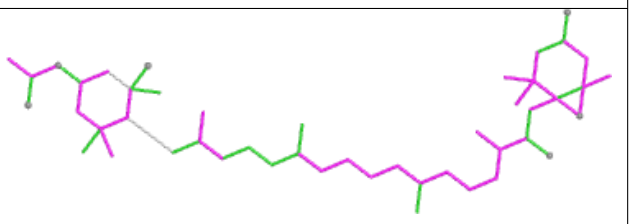


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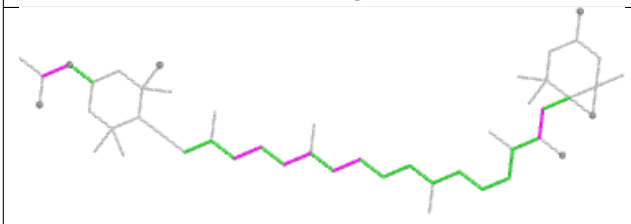
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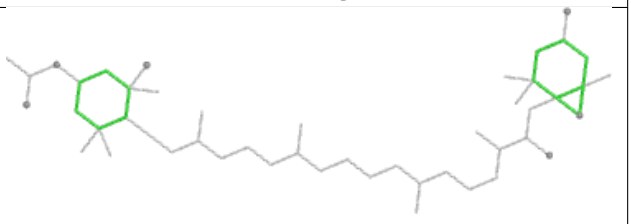
Bond lengths



Bond angles

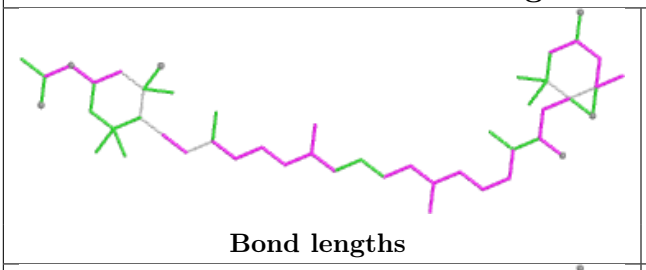


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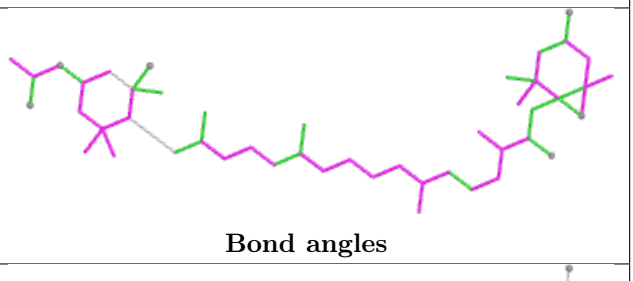


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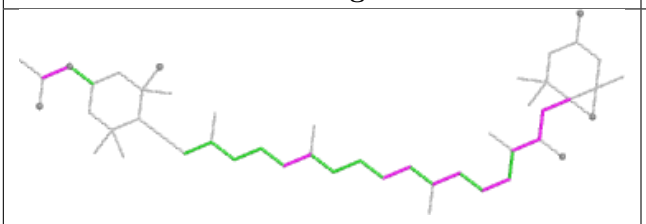
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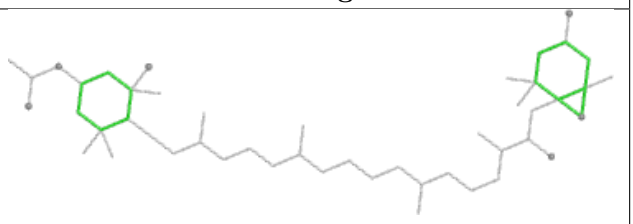
Bond lengths



Bond angles

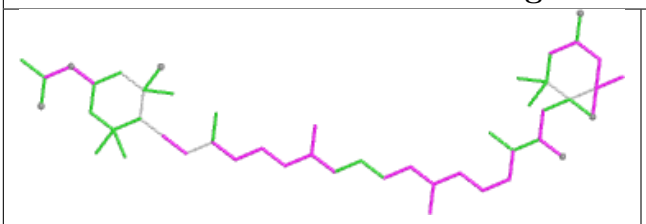


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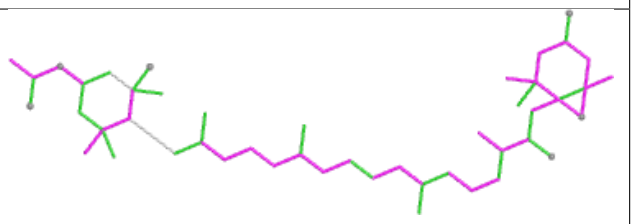


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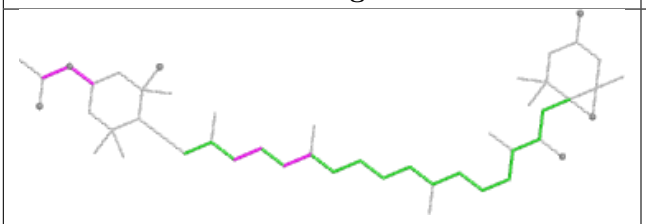
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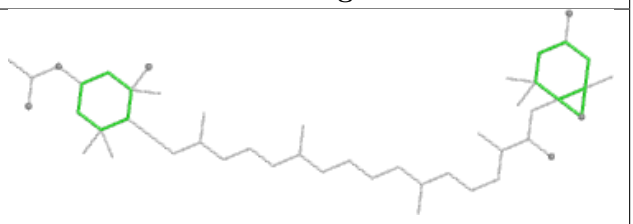
Bond lengths



Bond angles

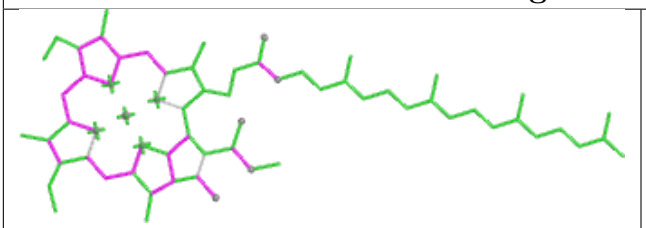


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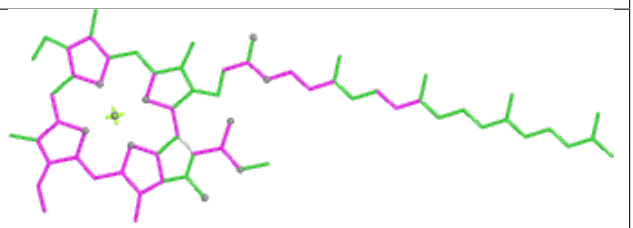


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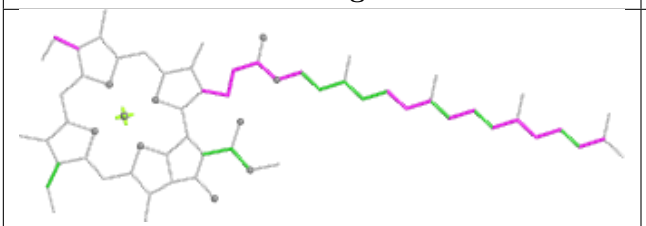
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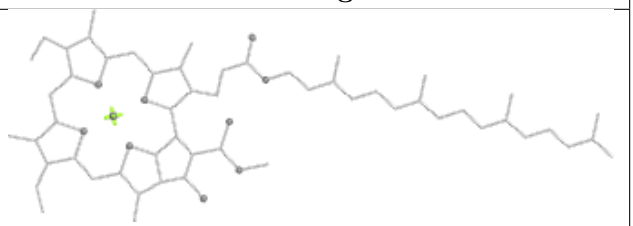
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Bond angles

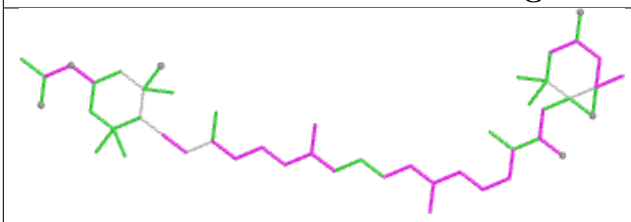


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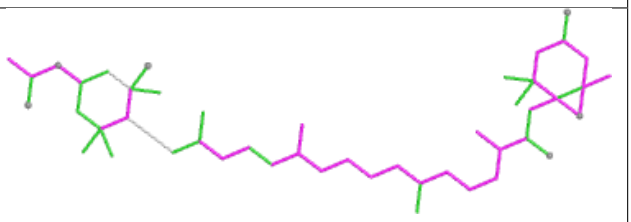


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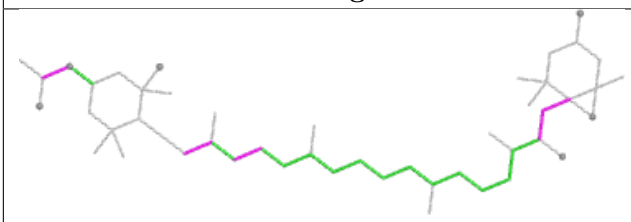
Ligand A86 31 313



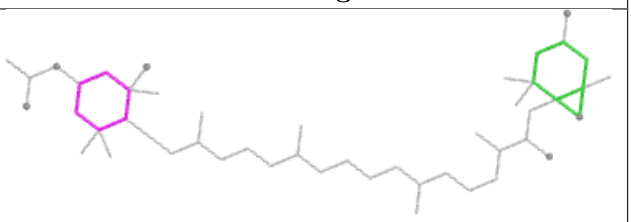
Bond lengths



Bond angles

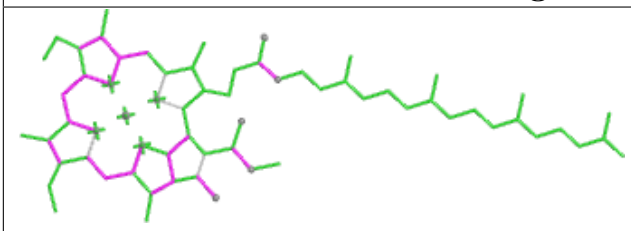


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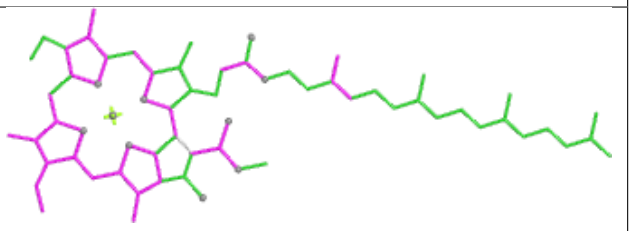


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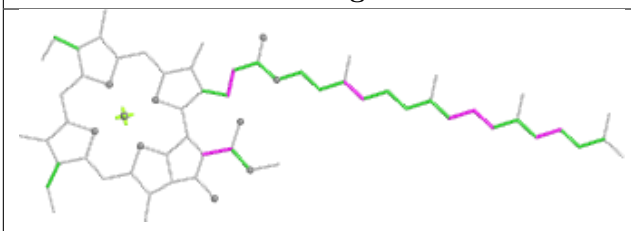
Ligand CLA c 507



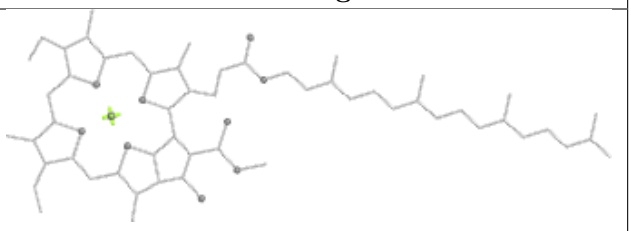
Bond lengths



Bond angles

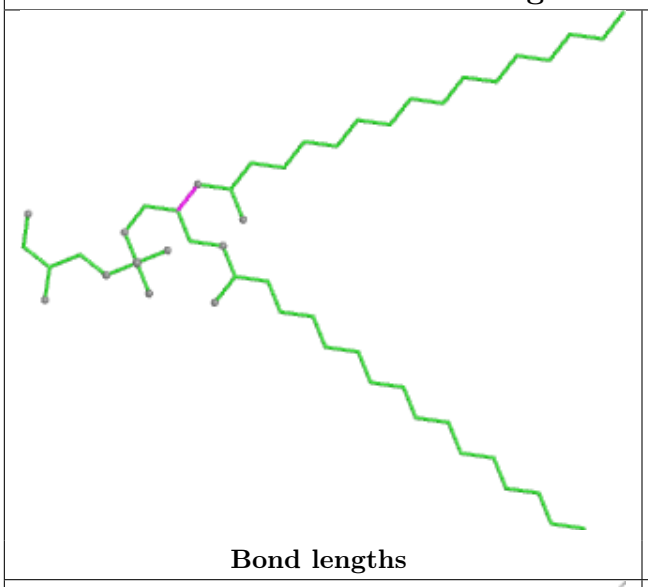


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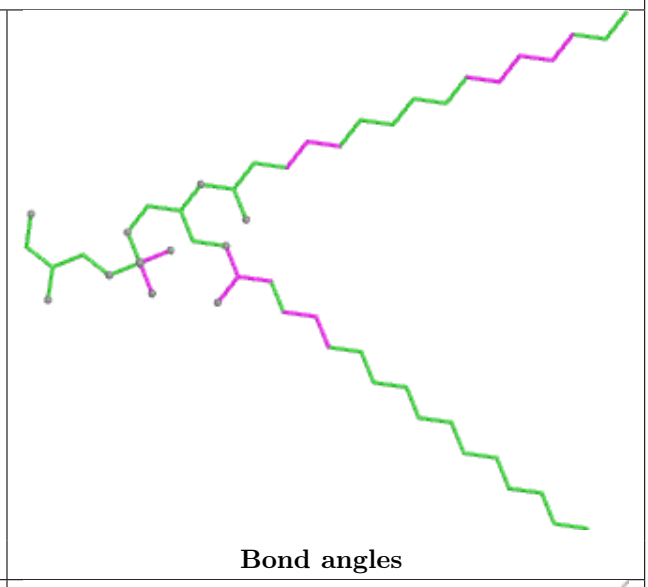


Rings

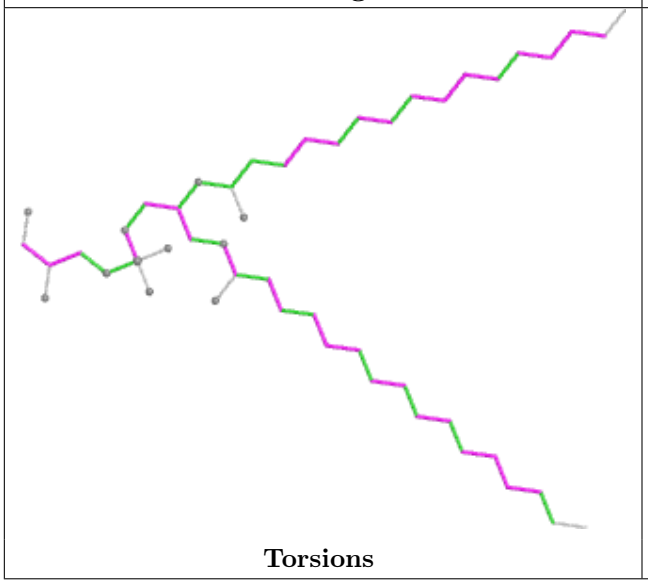
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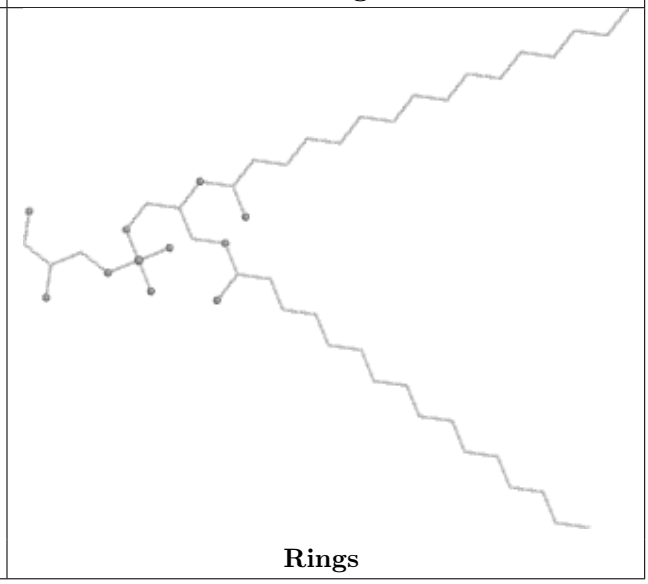
Bond lengths



Bond angles

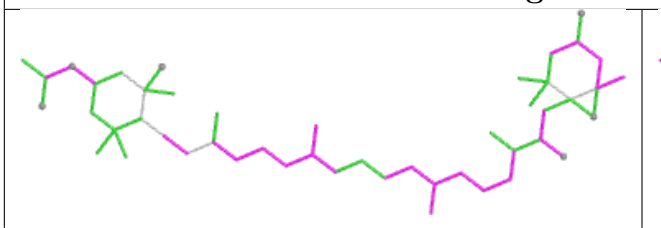


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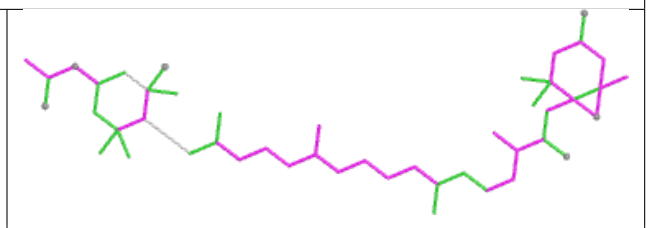


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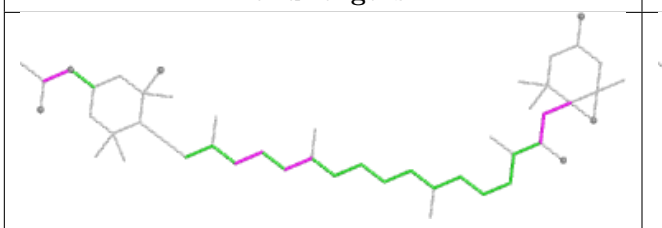
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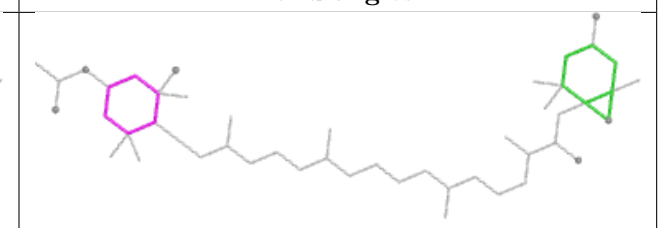
Bond lengths



Bond angles

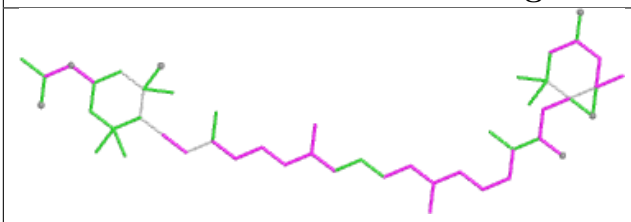


Torsions

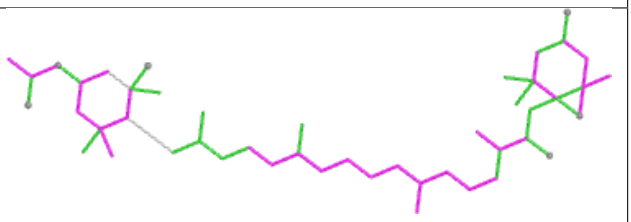


Rings

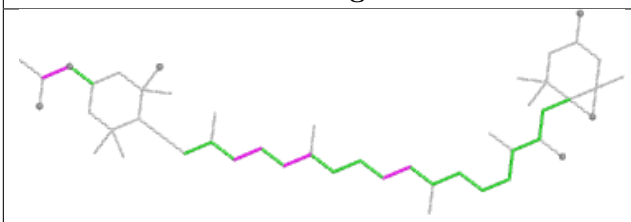
Ligand A86 14 315



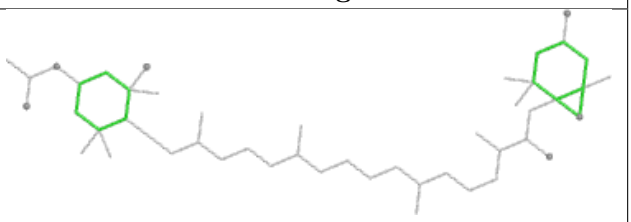
Bond lengths



Bond angles

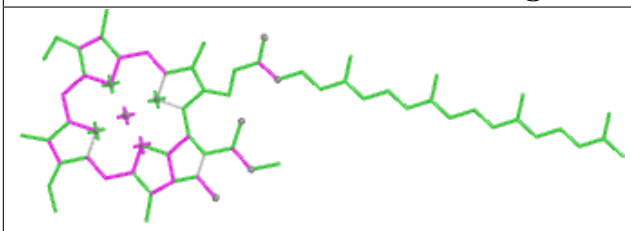


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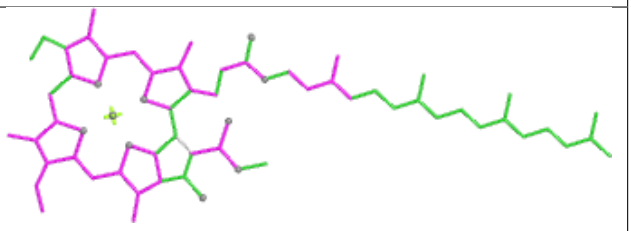


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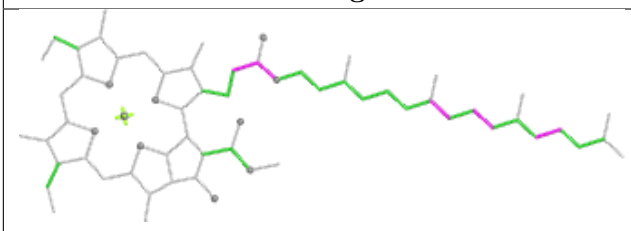
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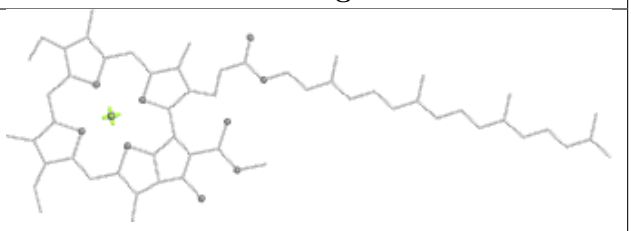
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Bond angles

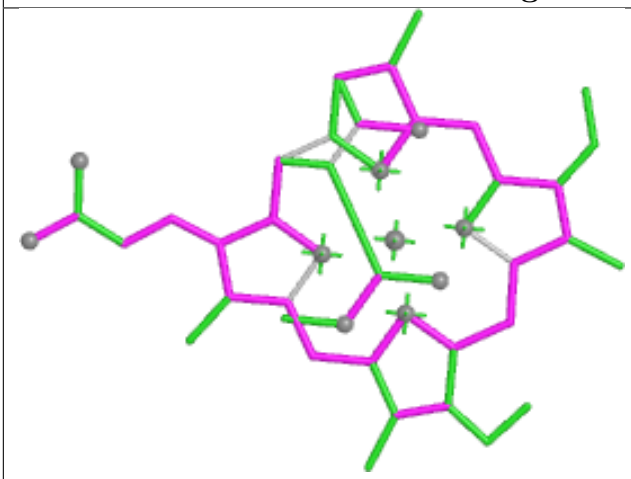


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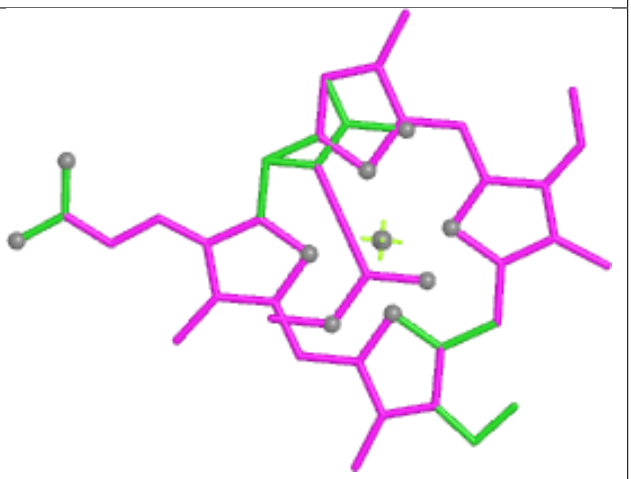


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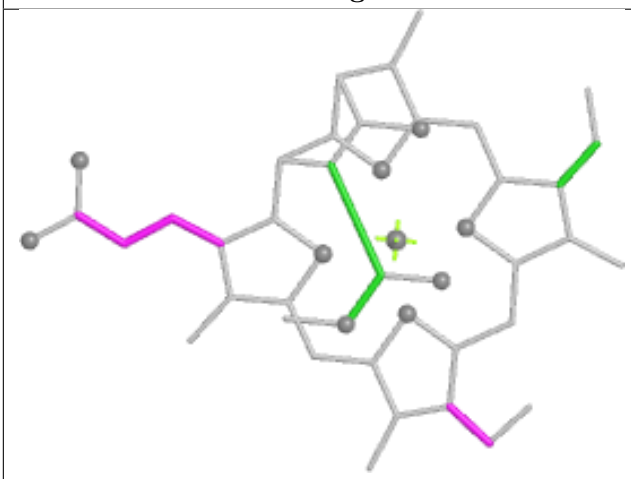
Ligand KC1 35 304



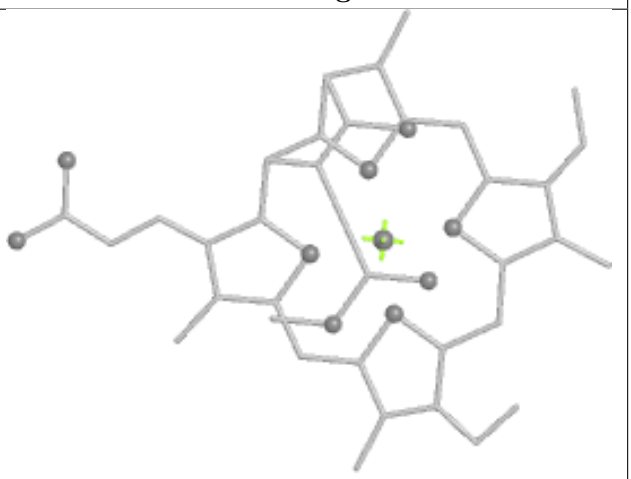
Bond lengths



Bond angles

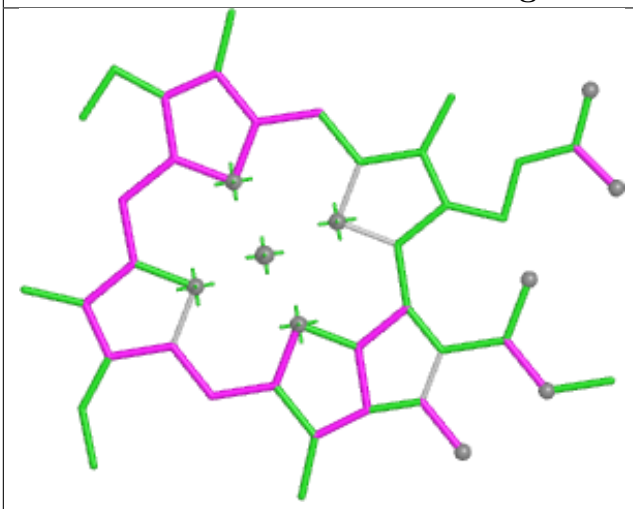


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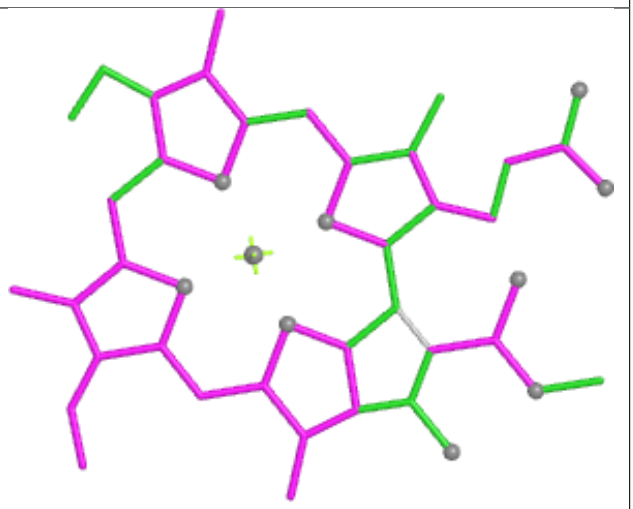


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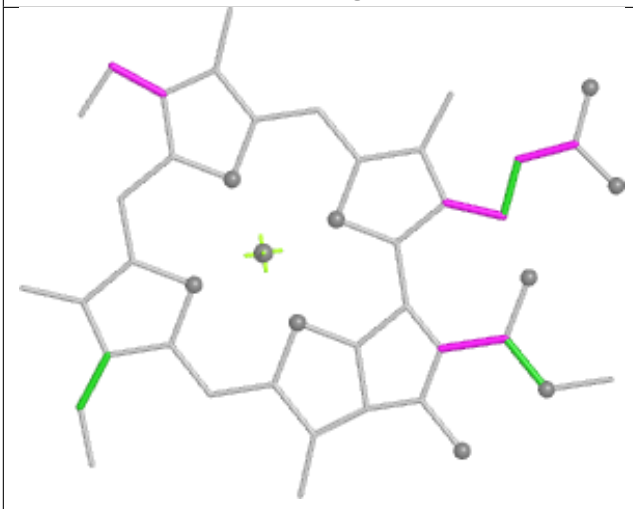
Ligand CLA 20 307



Bond lengths



Bond angles

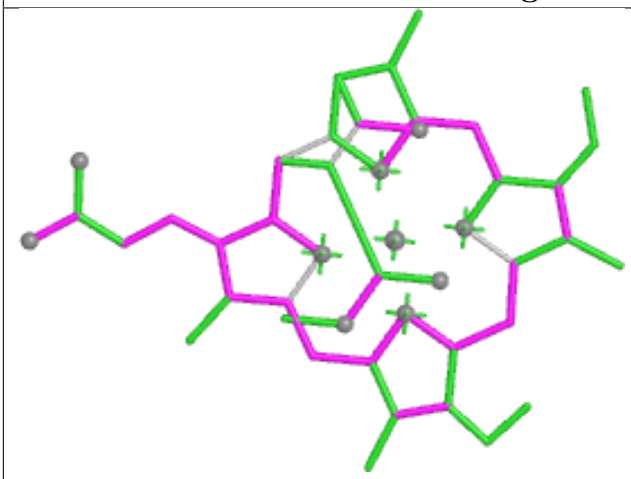


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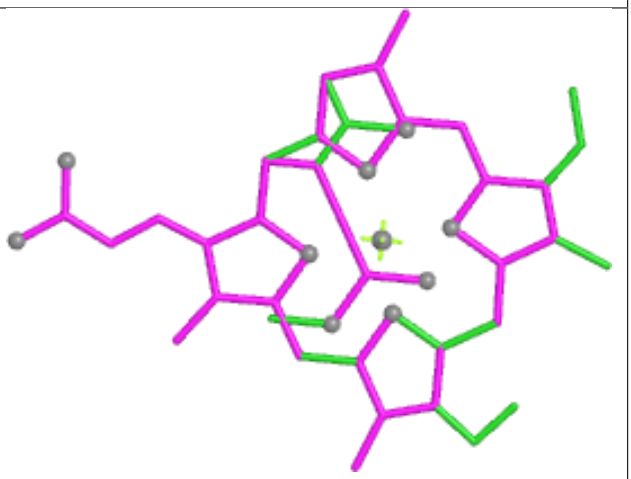


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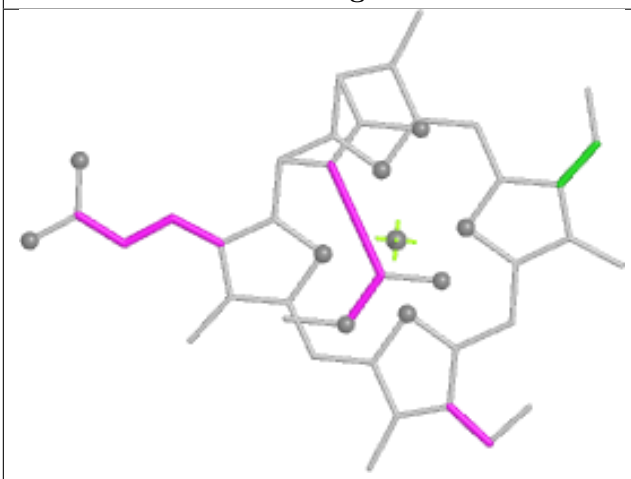
Ligand KC1 11 306



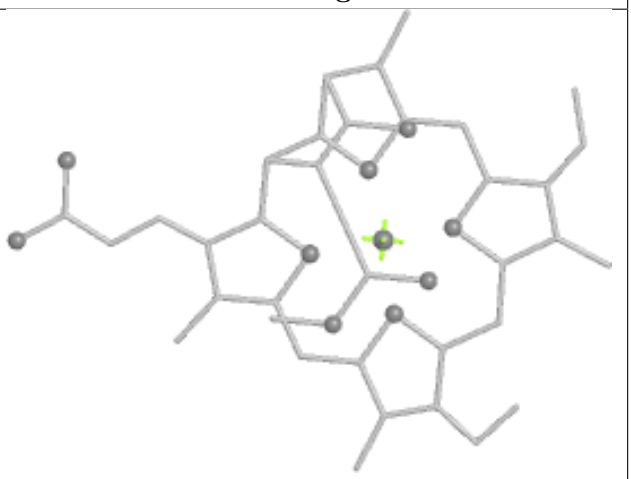
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Bond angles

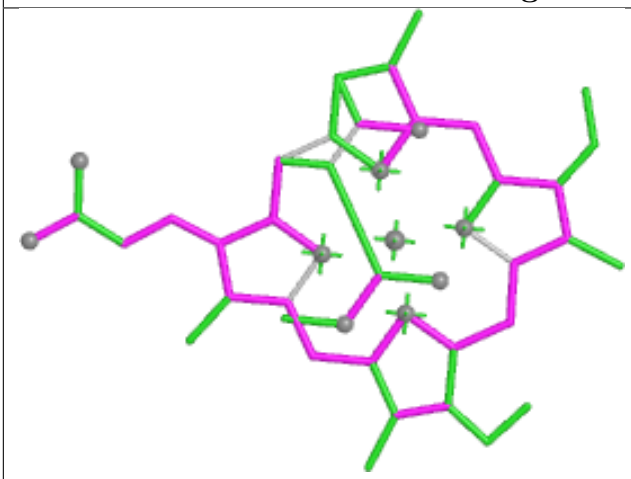


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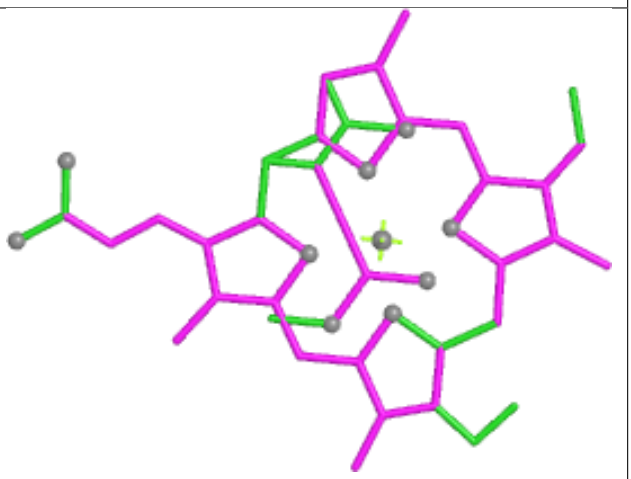


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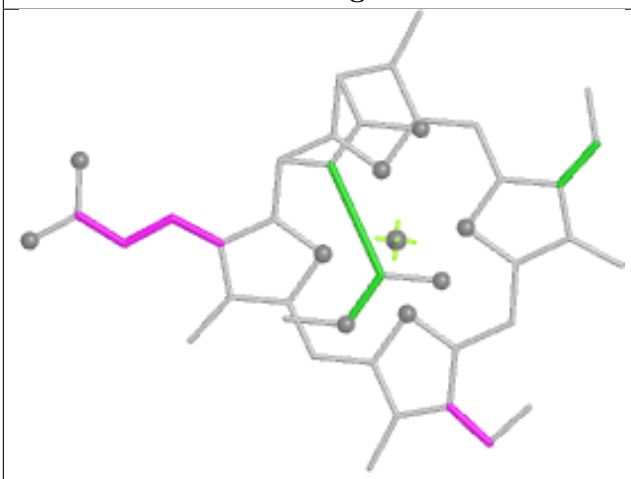
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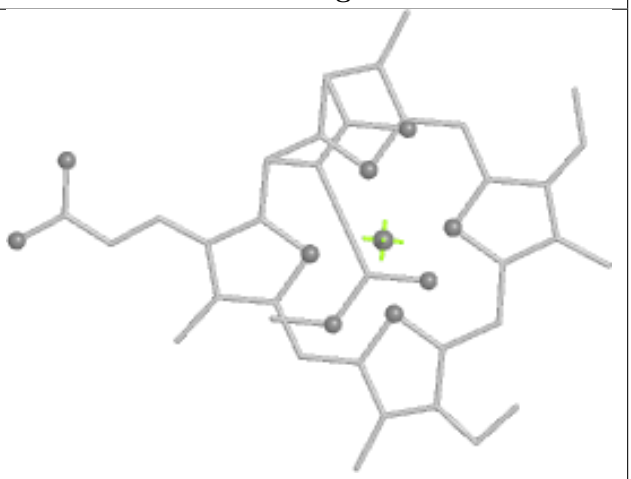
Bond lengths



Bond angles

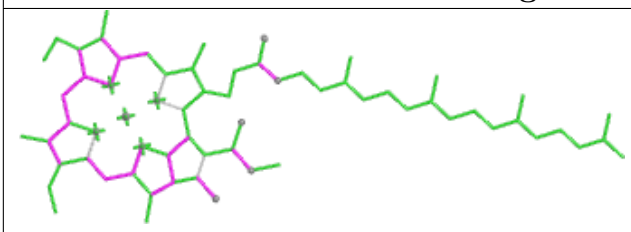


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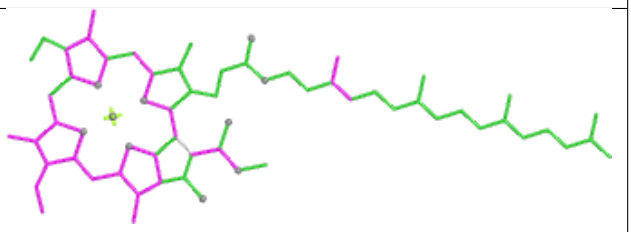


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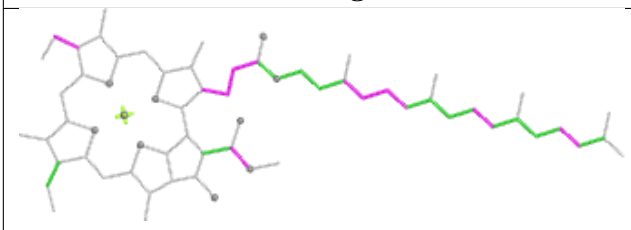
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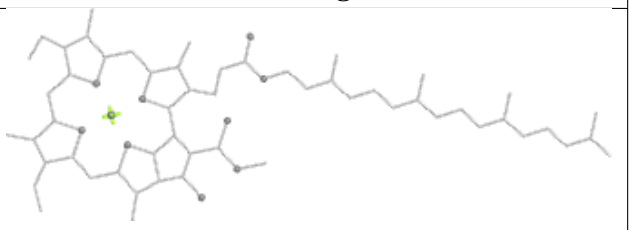
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Bond angles

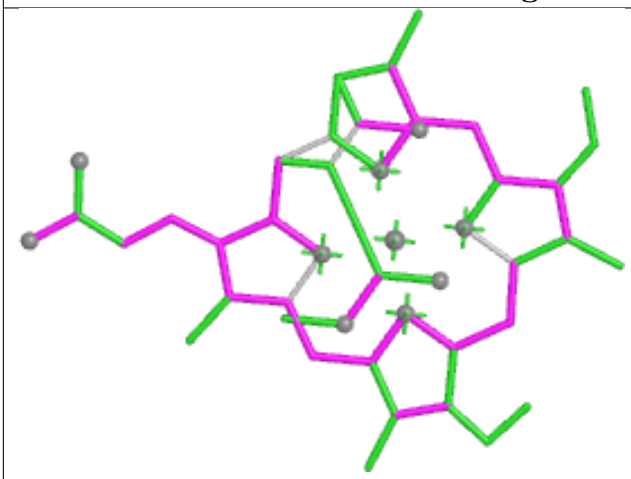


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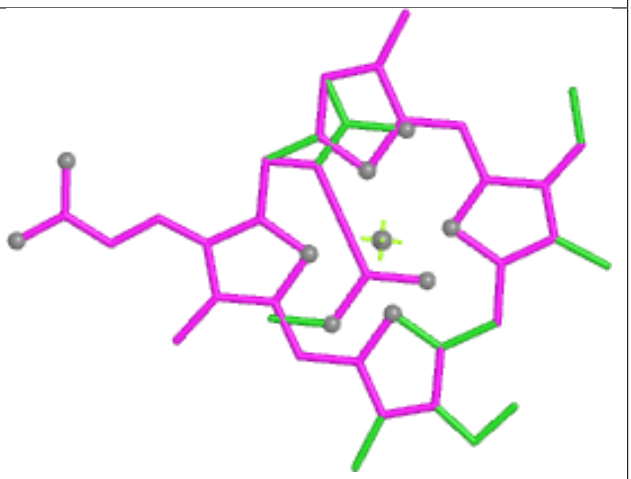


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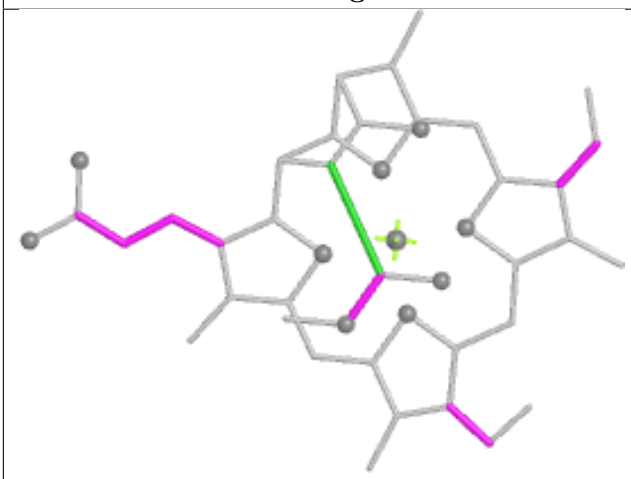
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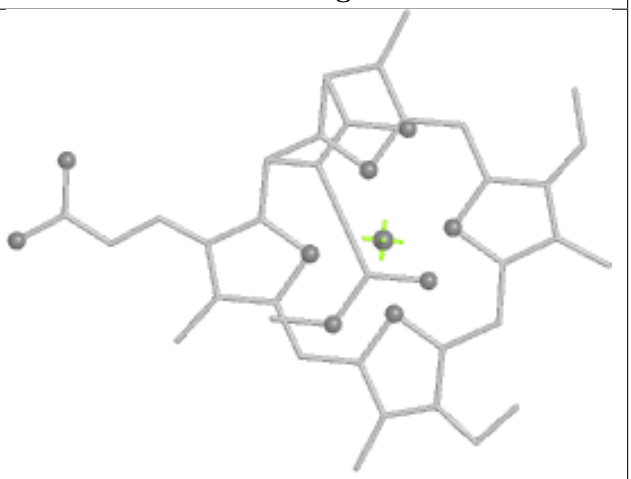
Bond lengths



Bond angles

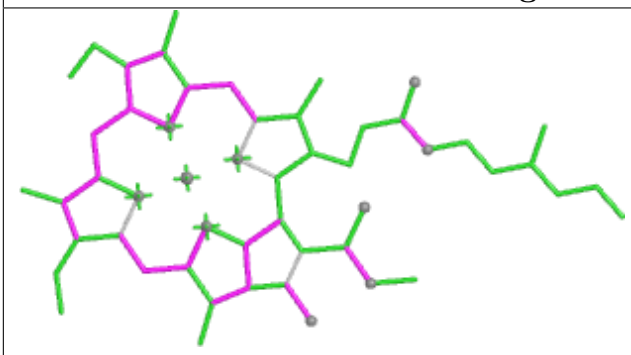


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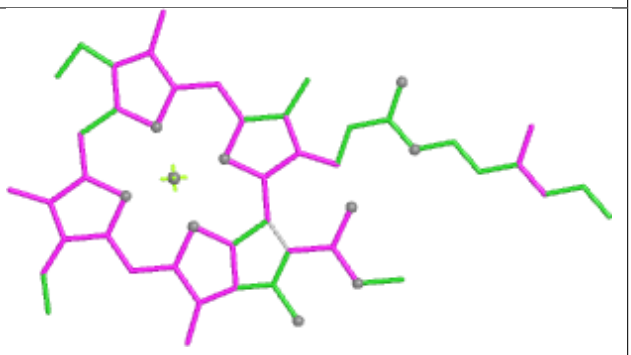


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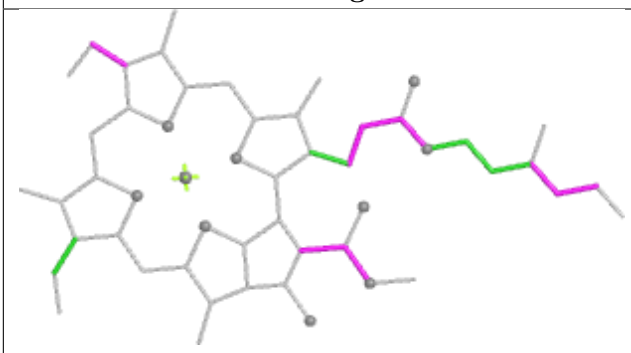
Ligand CLA 35 307



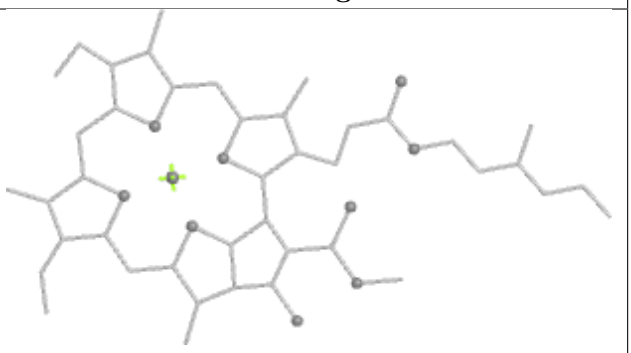
Bond lengths



Bond angles

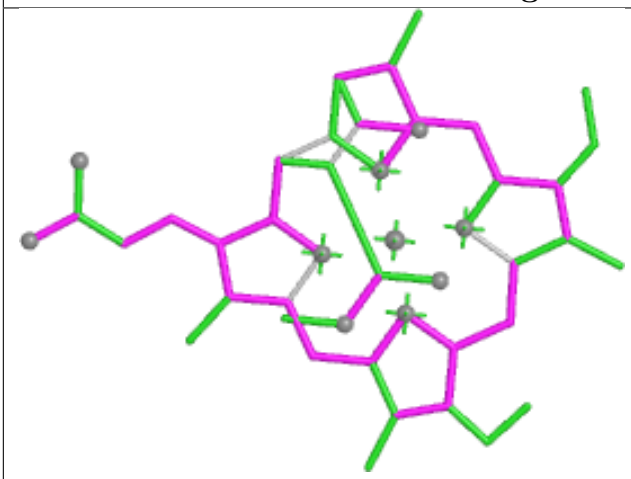


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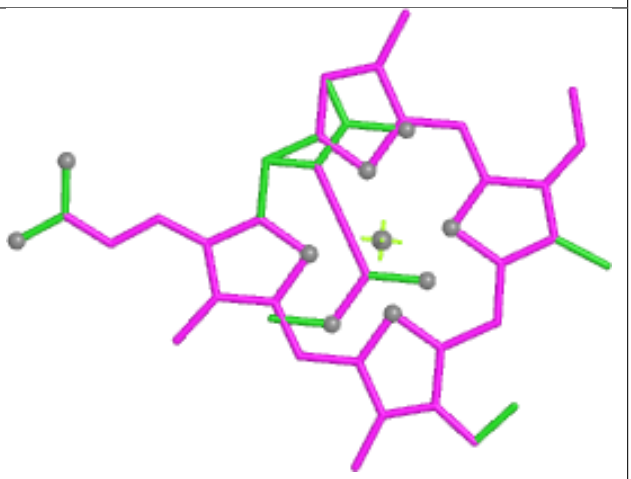


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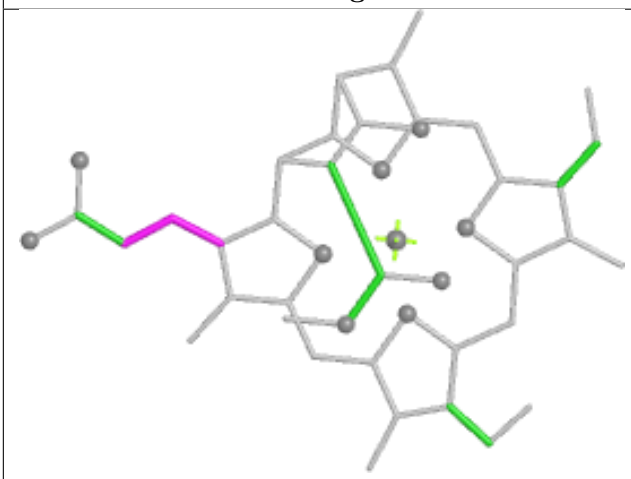
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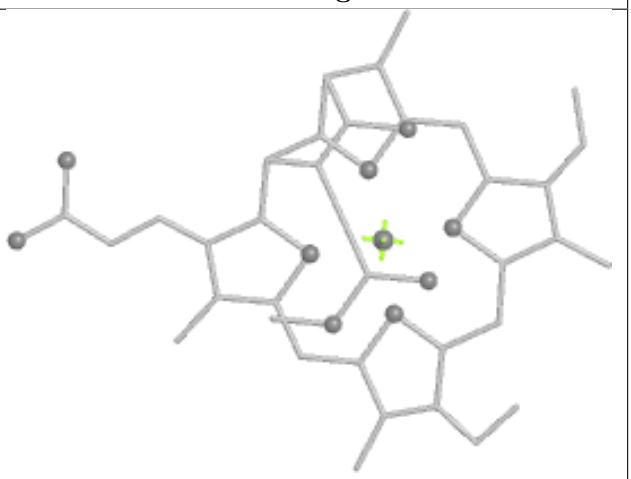
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Bond angles

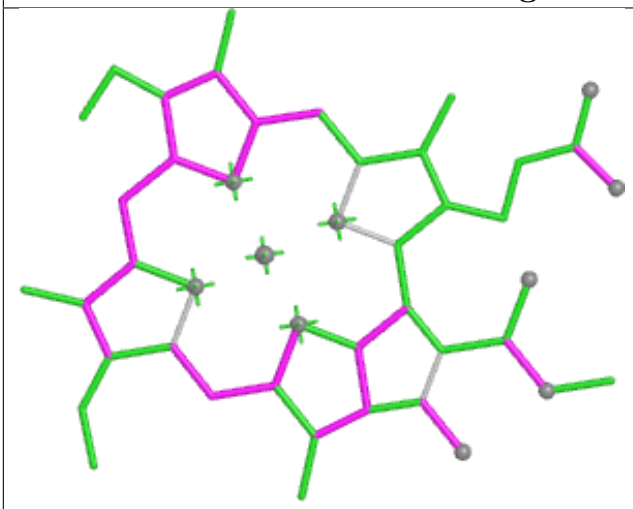


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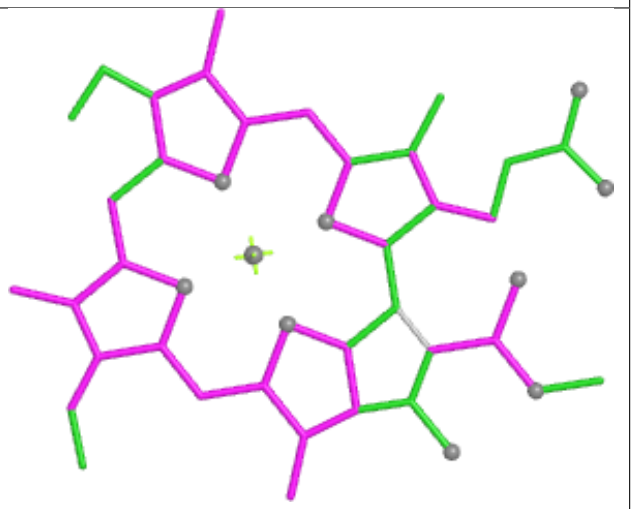


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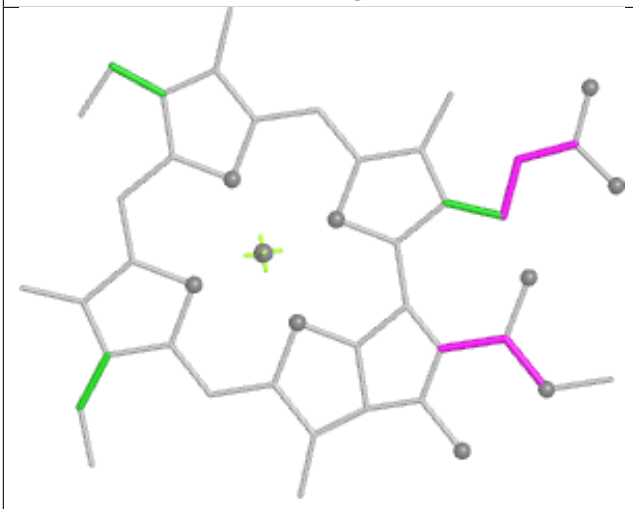
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Bond lengths



Bond angles

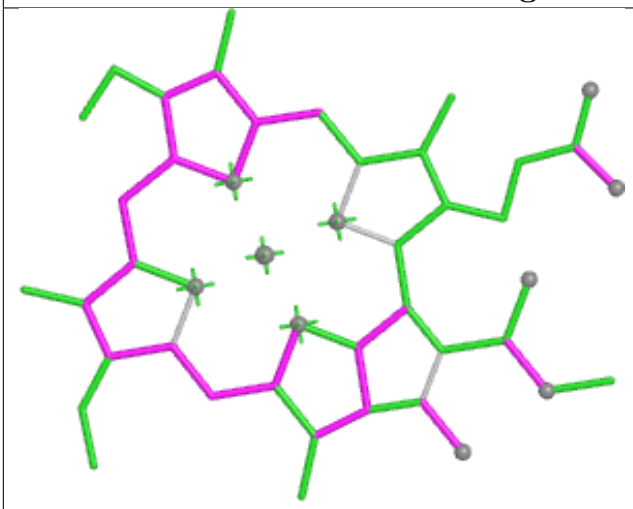


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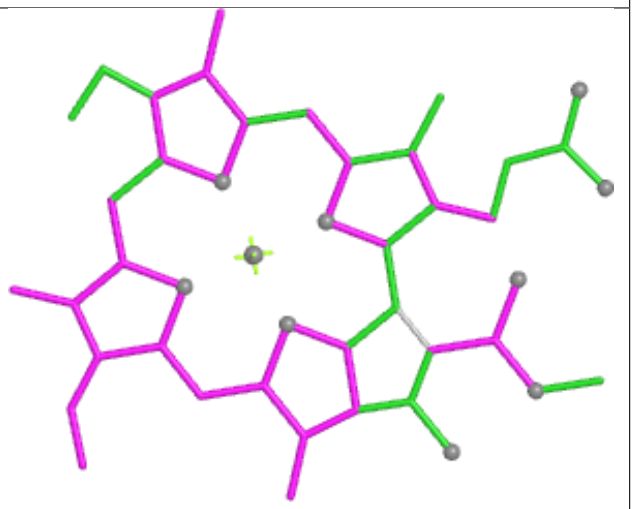


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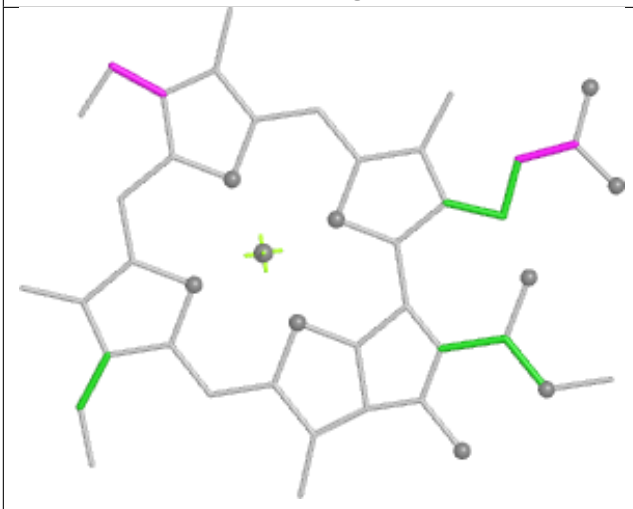
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Bond lengths



Bond angles

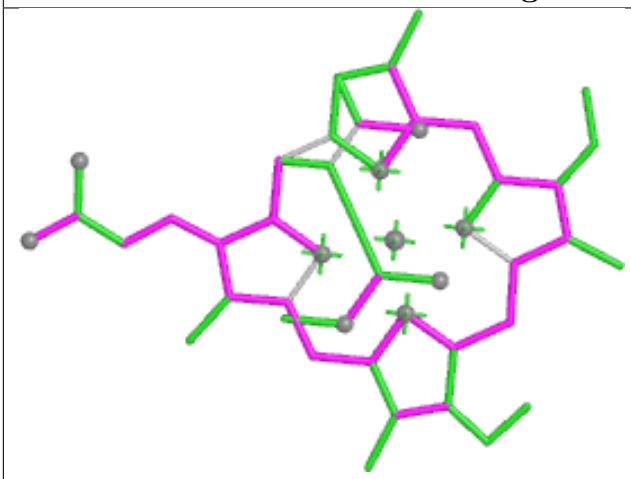


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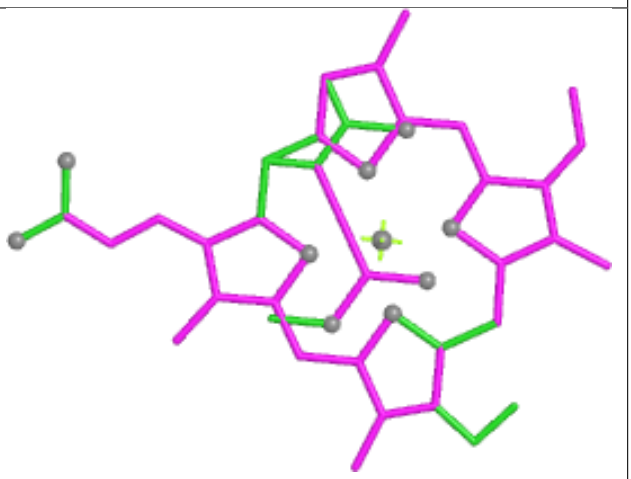


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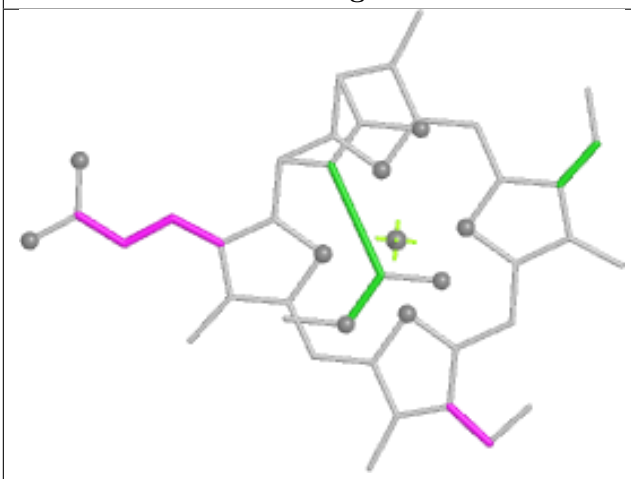
Ligand KC1 15 306



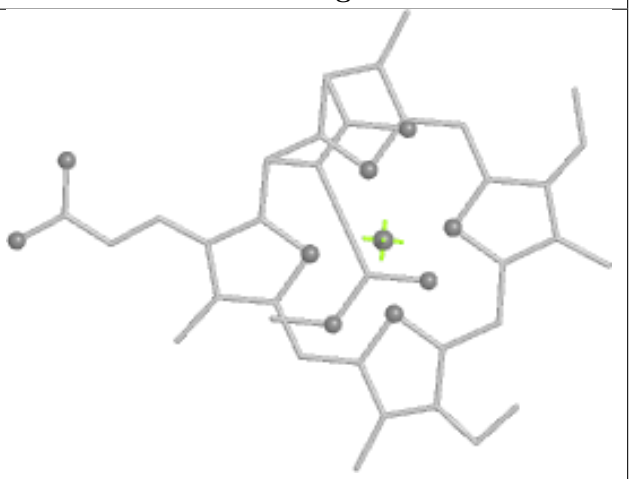
Bond lengths



Bond angles

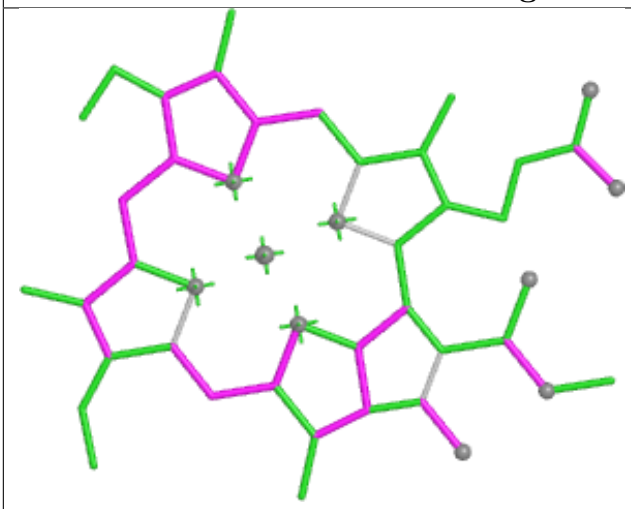


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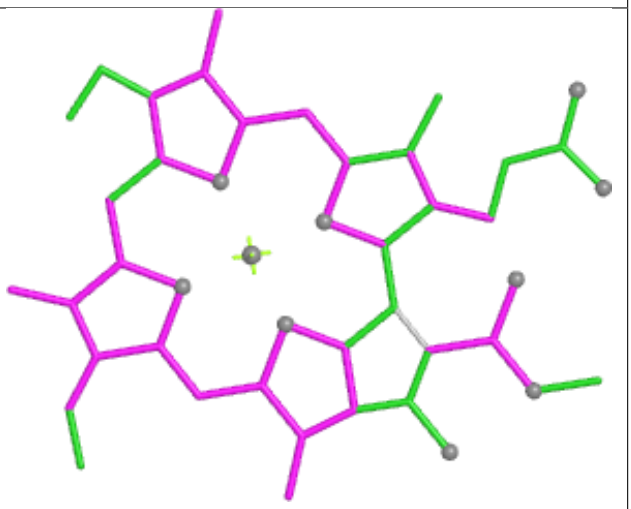


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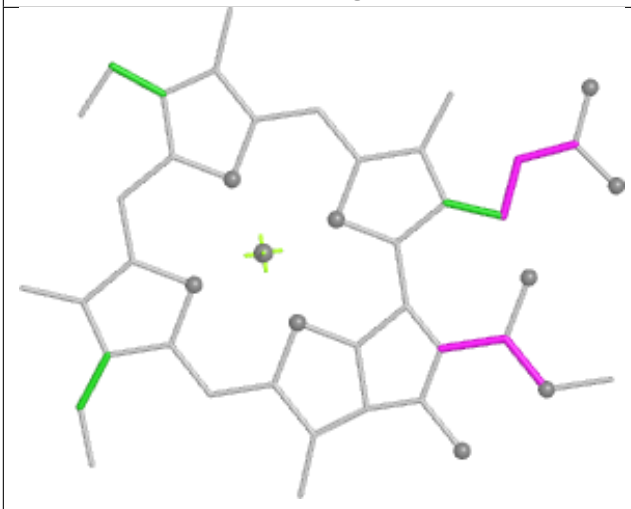
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Bond lengths



Bond angles

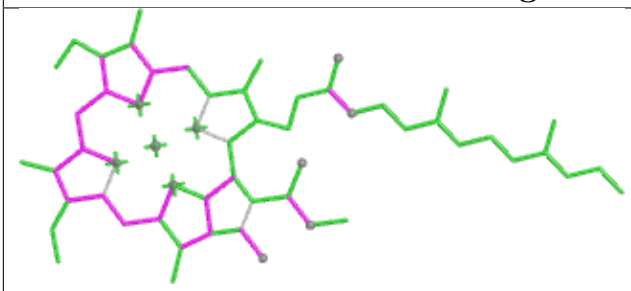


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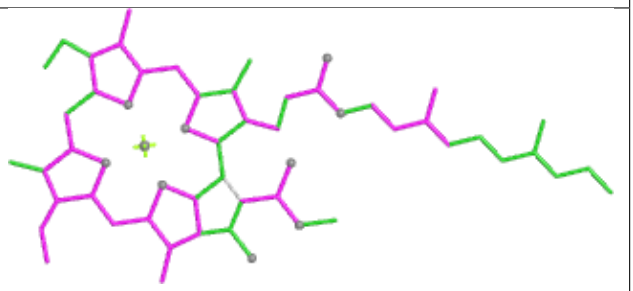


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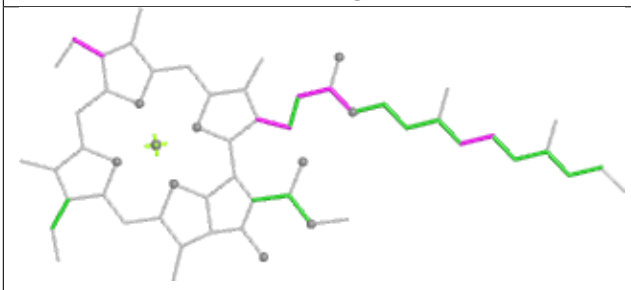
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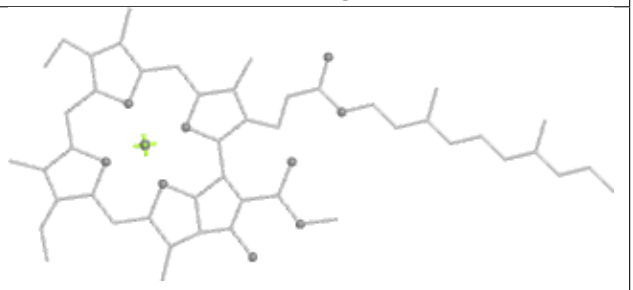
Bond lengths



Bond angles

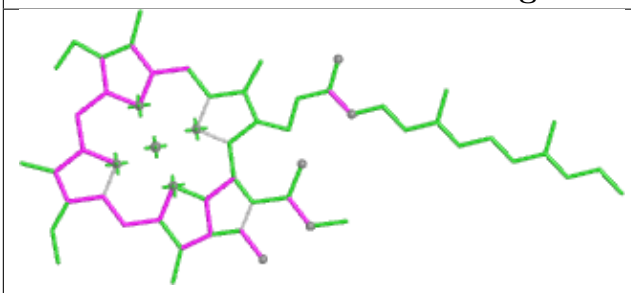


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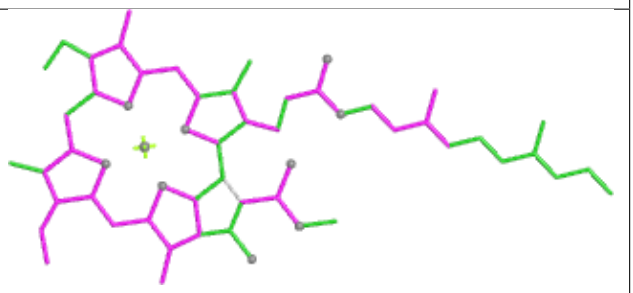


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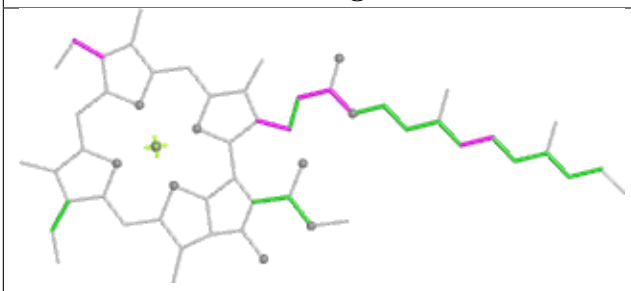
Ligand CLA 41 202



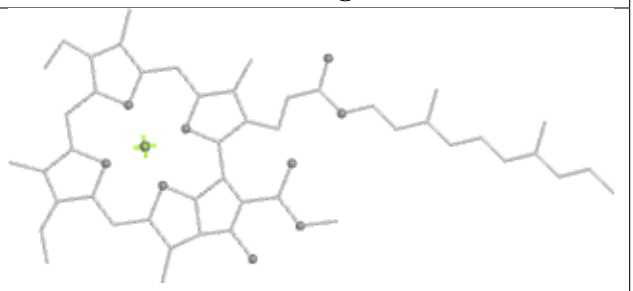
Bond lengths



Bond angles

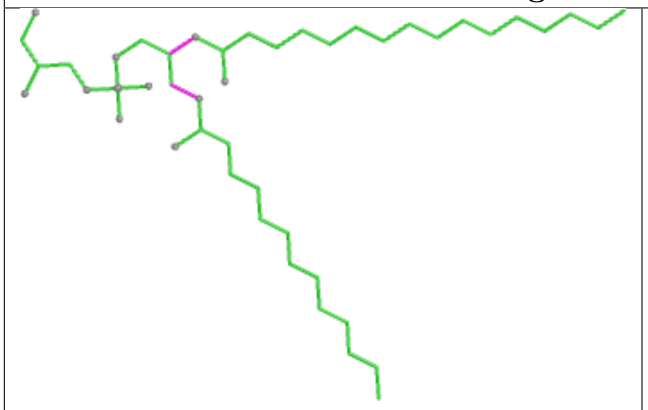


Torsions

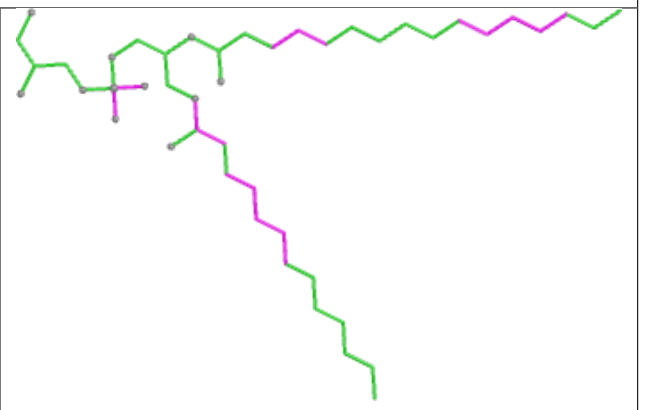


Rings

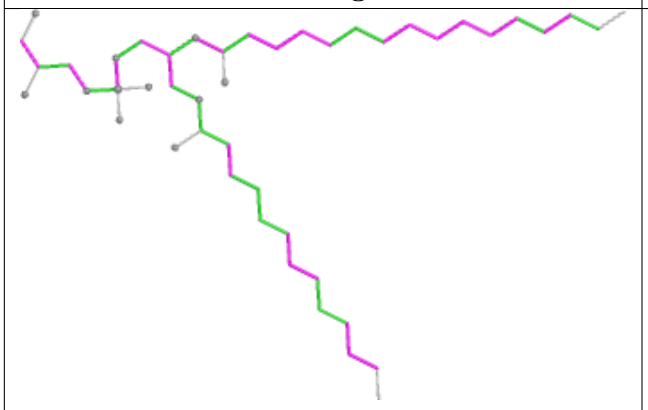
Ligand LHG a 412



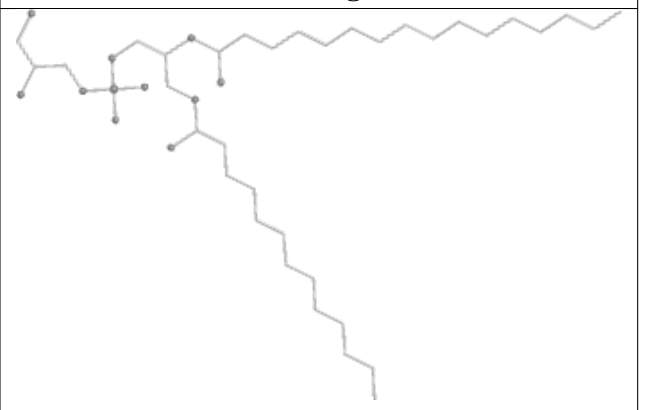
Bond lengths



Bond angles

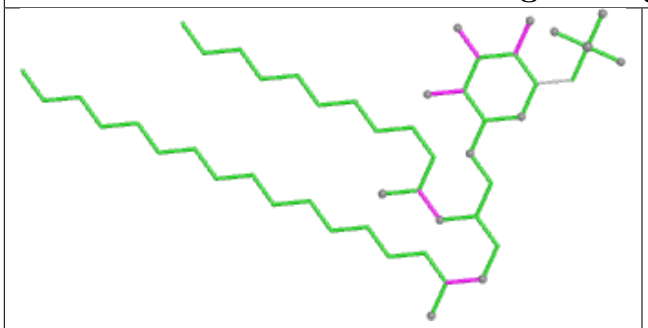


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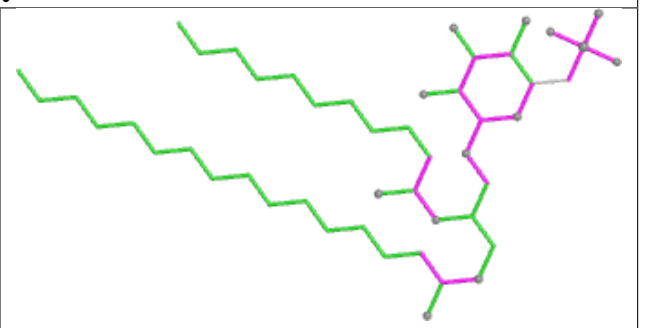


Rings

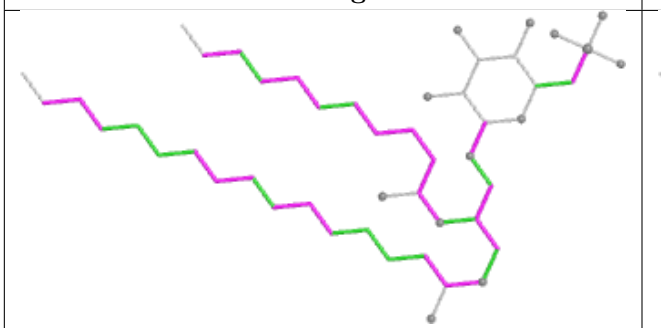
Ligand SQD 17 301



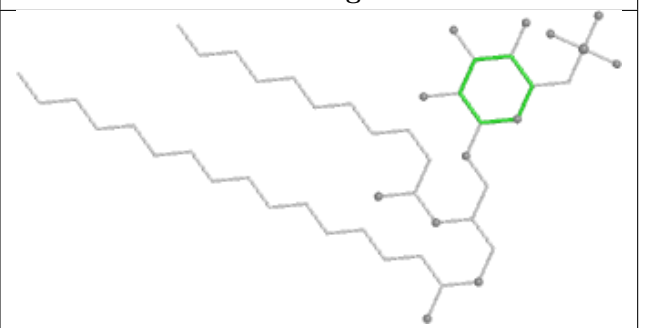
Bond lengths



Bond angles

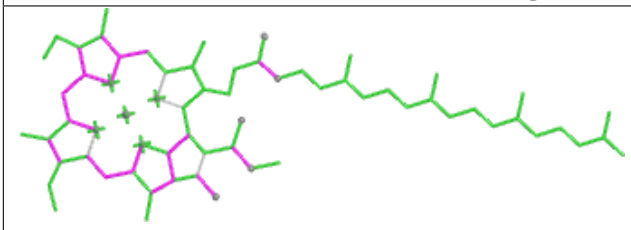


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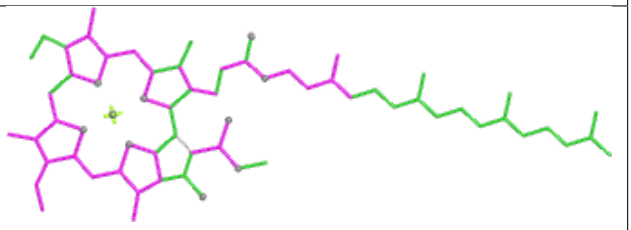


Rings

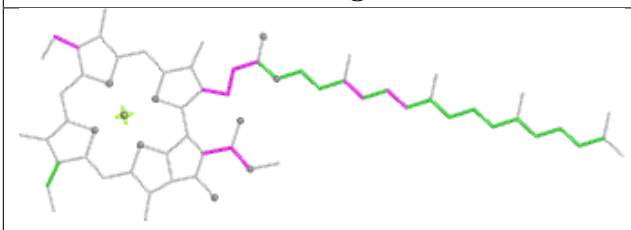
Ligand CLA C 501



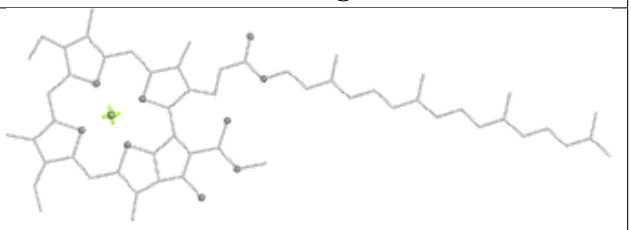
Bond lengths



Bond angles

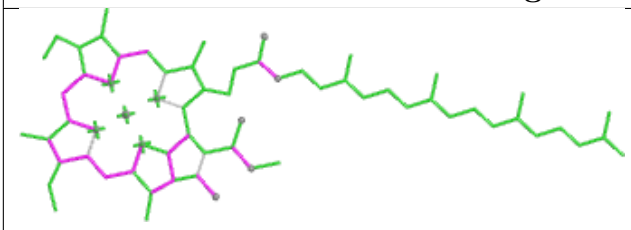


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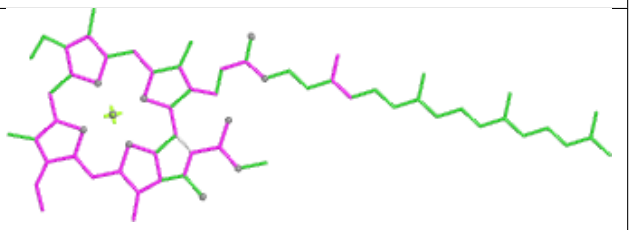


Rings

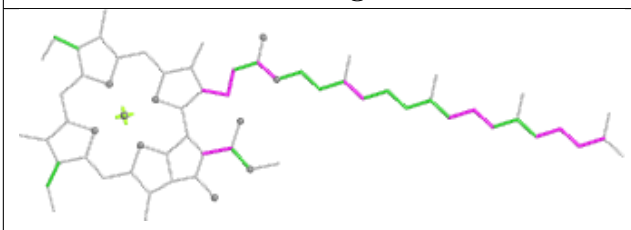
Ligand CLA C 506



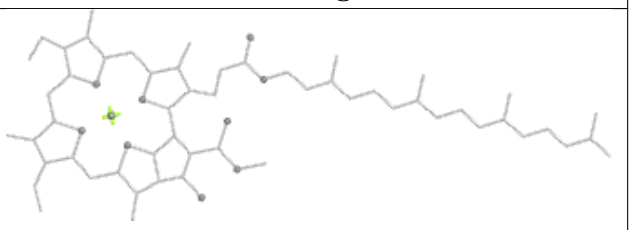
Bond lengths



Bond angles



Torsions

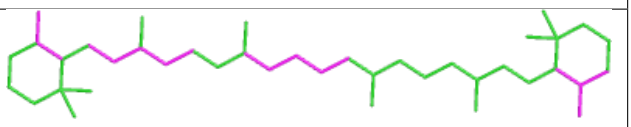


Rings

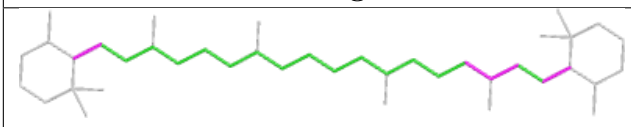
Ligand BCR B 517



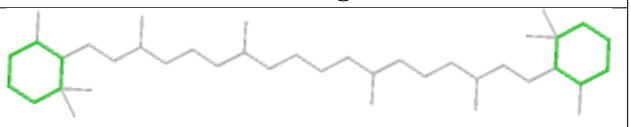
Bond lengths



Bond angles

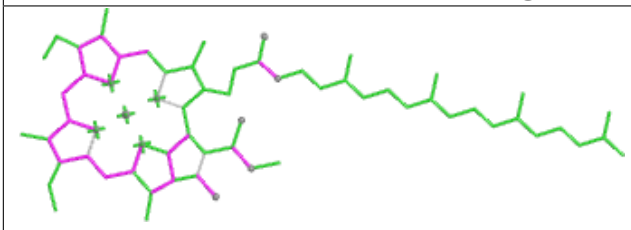


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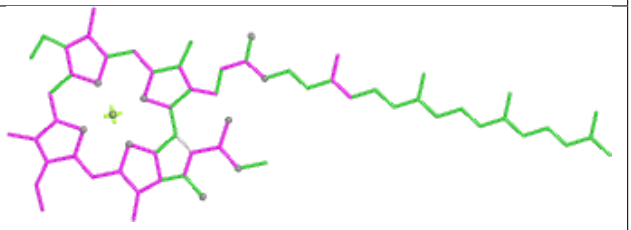


Rings

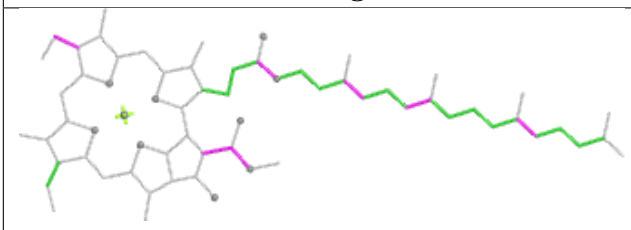
Ligand CLA 39 302



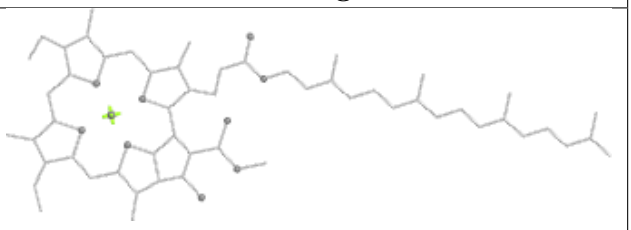
Bond lengths



Bond angles

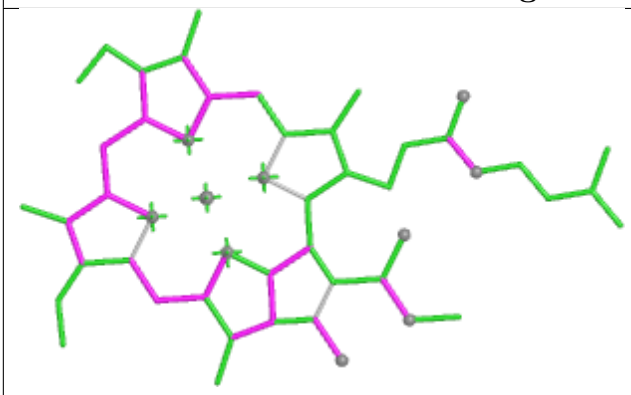


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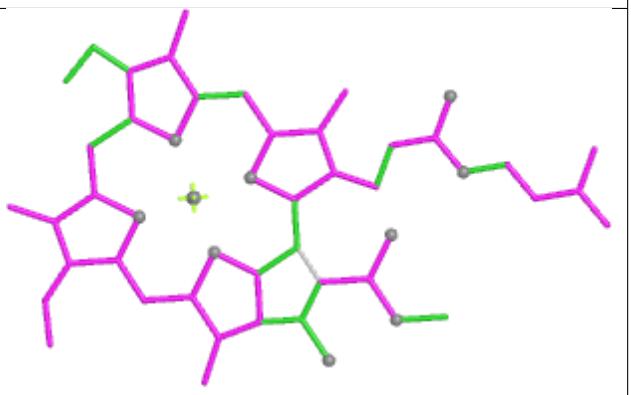


Rings

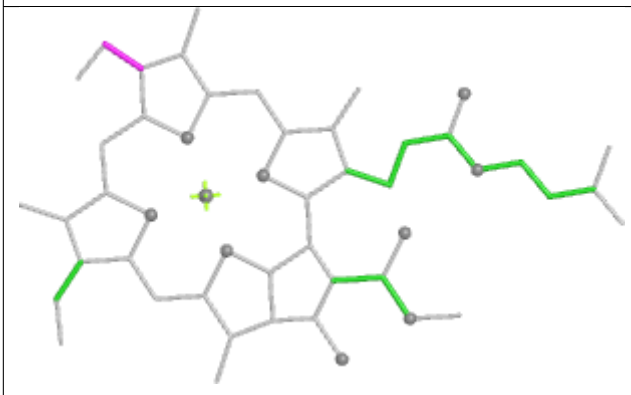
Ligand CLA 12 207



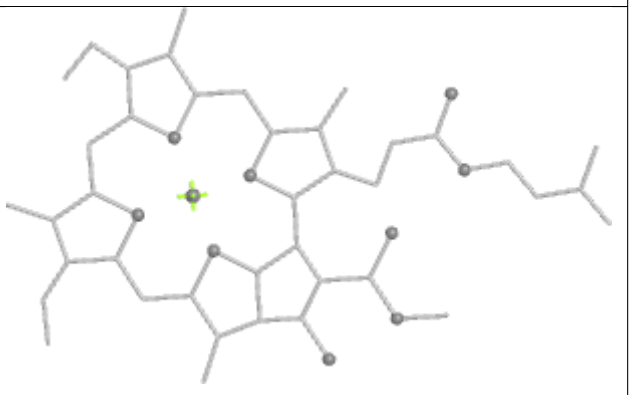
Bond lengths



Bond angles

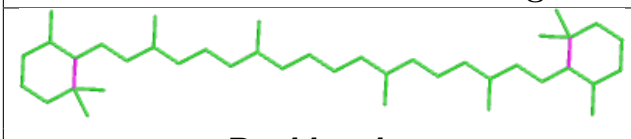


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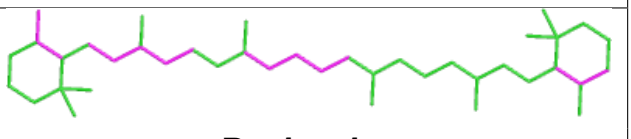


Rings

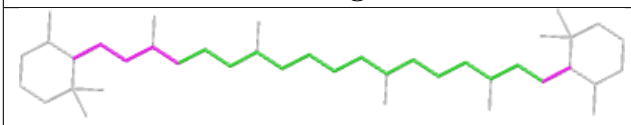
Ligand BCR a 413



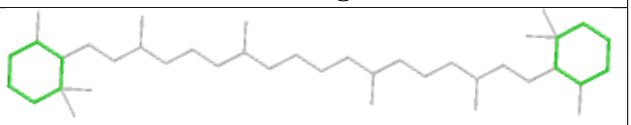
Bond lengths



Bond angles

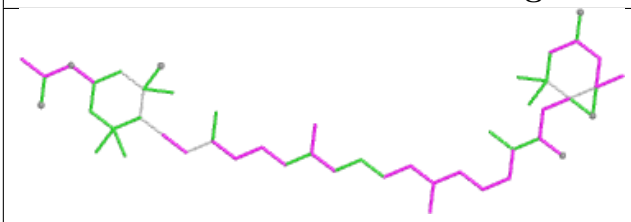


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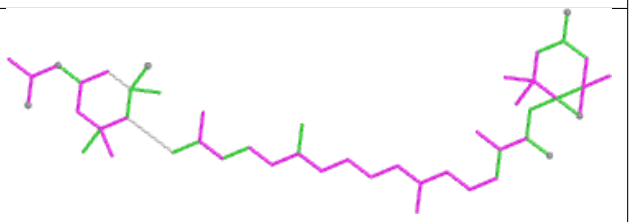


Rings

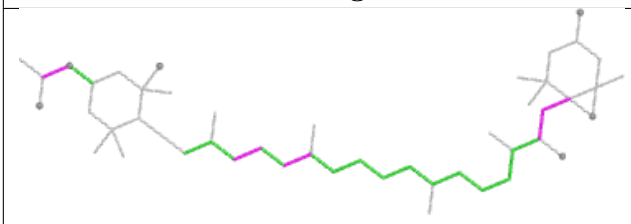
Ligand A86 39 311



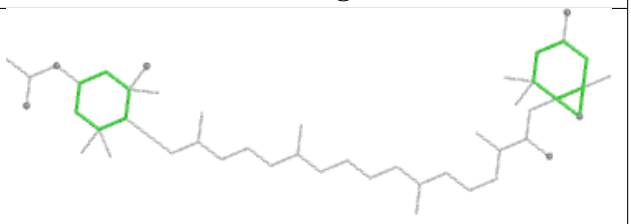
Bond lengths



Bond angles

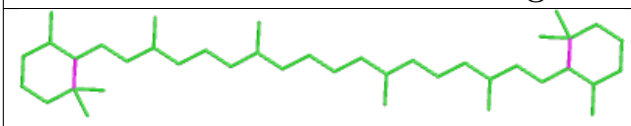


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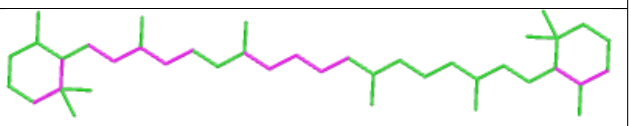


Rings

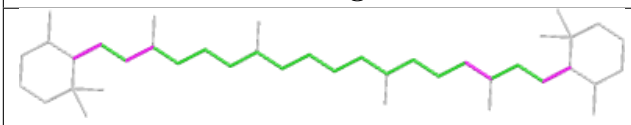
Ligand BCR c 515



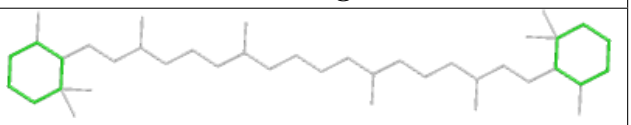
Bond lengths



Bond angles

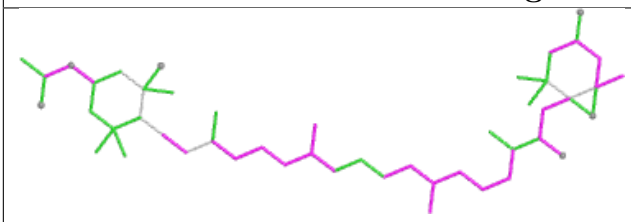


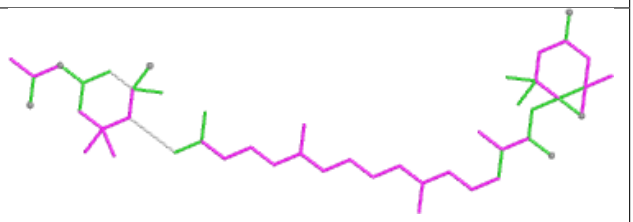
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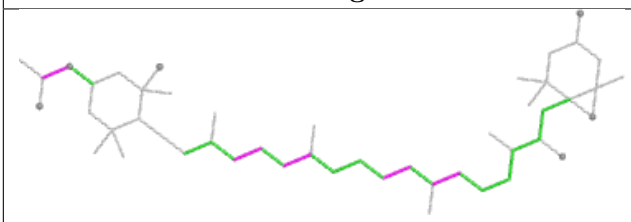


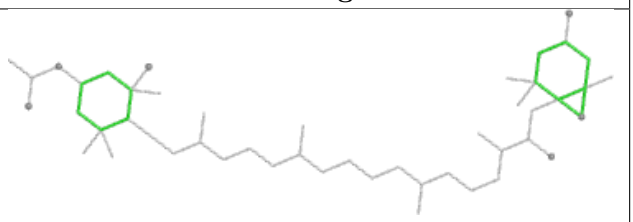
Rings

Ligand A86 37 319

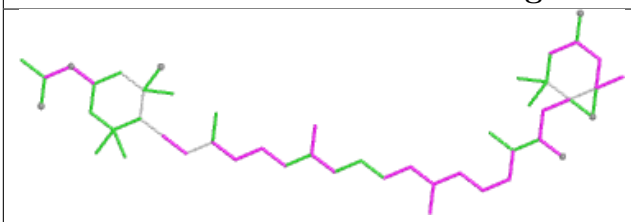

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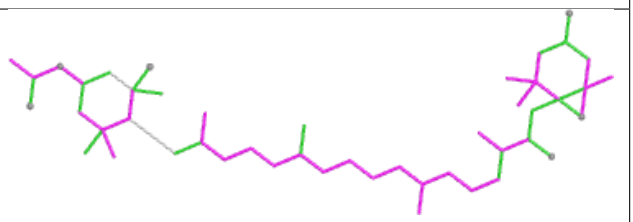

Bond angles

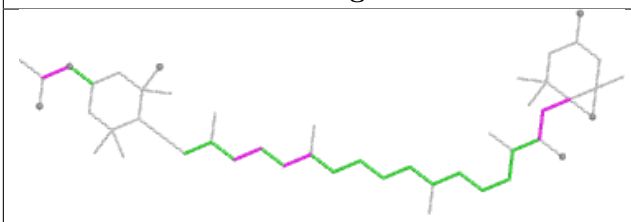

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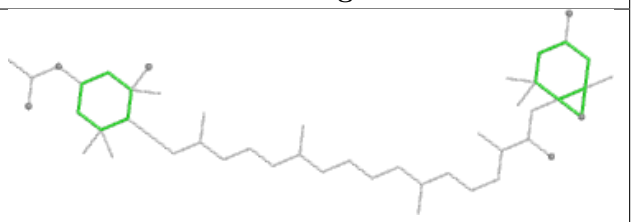

Rings

Ligand A86 34 311

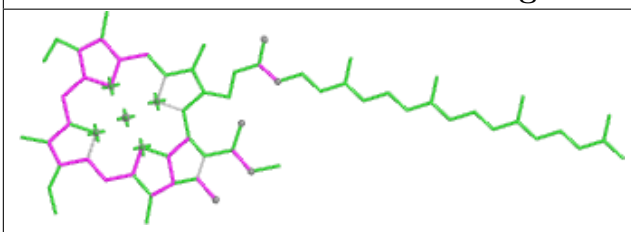

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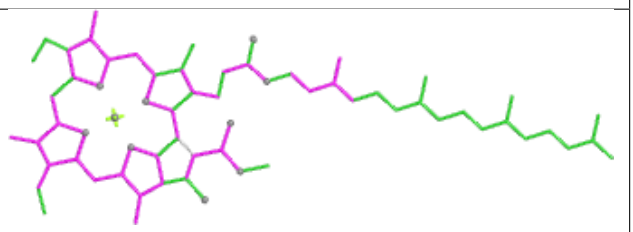

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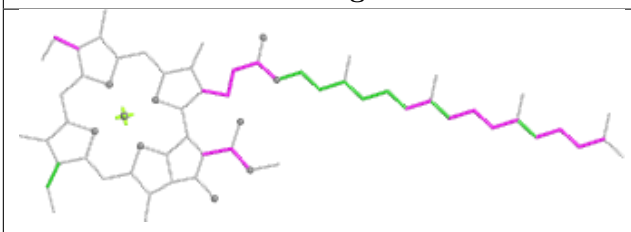

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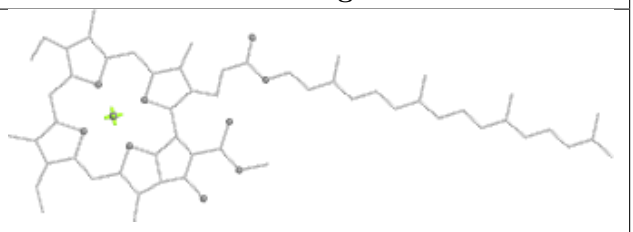

Rings

Ligand CLA 31 301

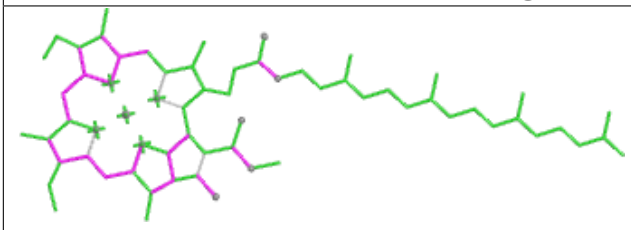

Bond lengths


Bond angles

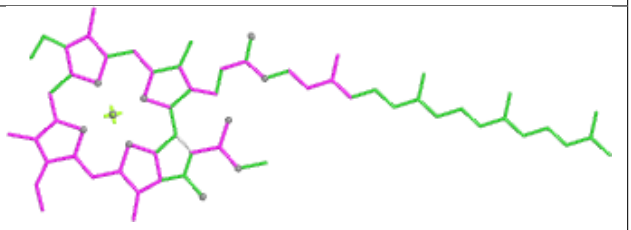

Torsions


Rings

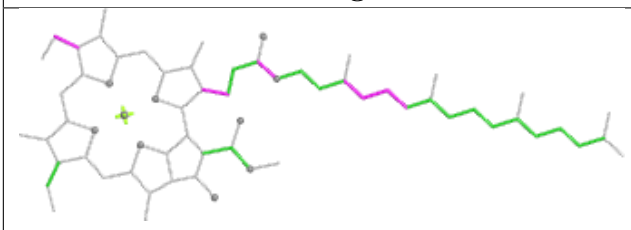
Ligand CLA 39 310



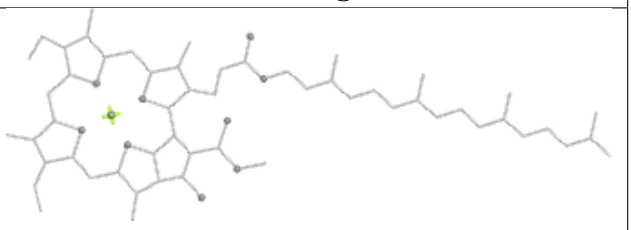
Bond lengths



Bond angles

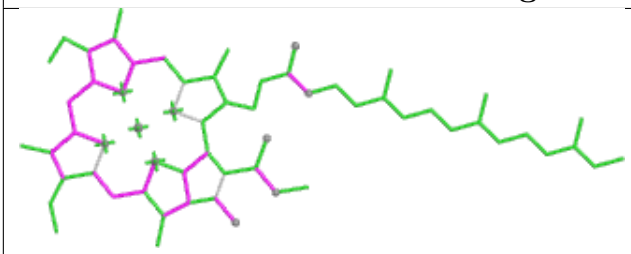


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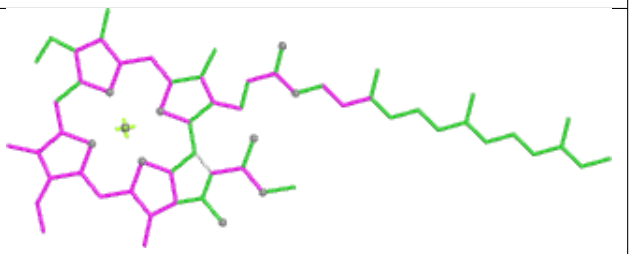


Rings

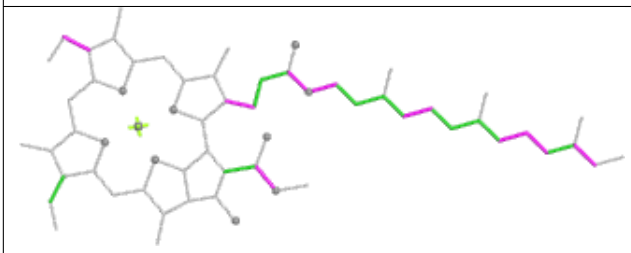
Ligand CLA 36 307



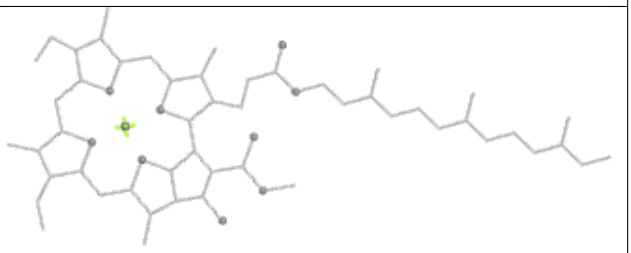
Bond lengths



Bond angles

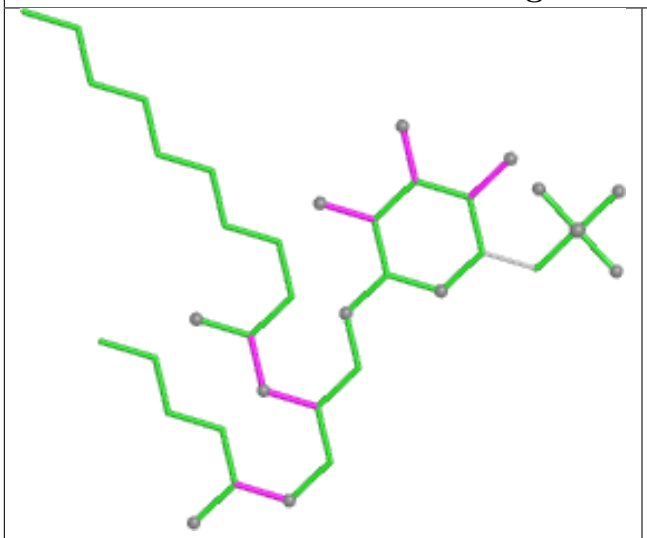


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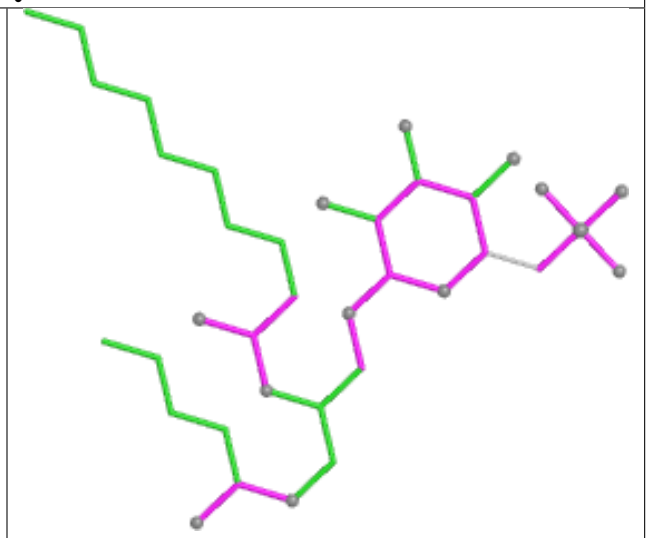


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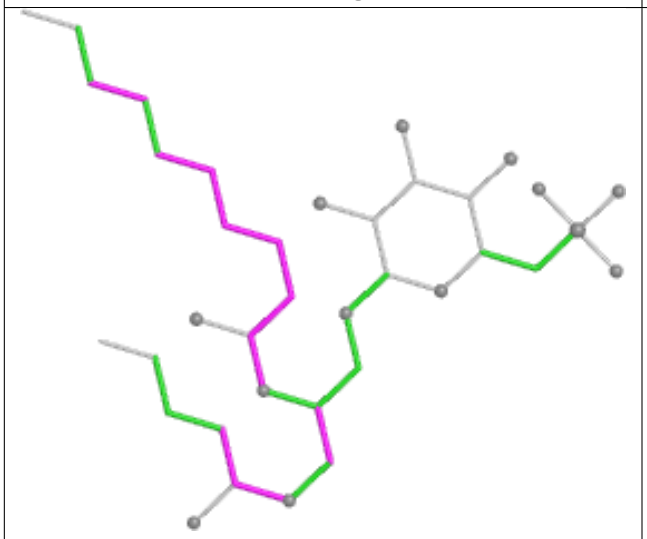
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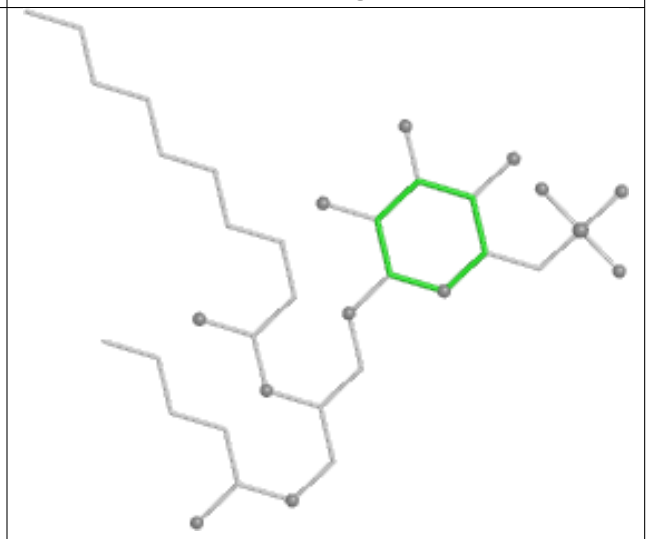
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Bond angles

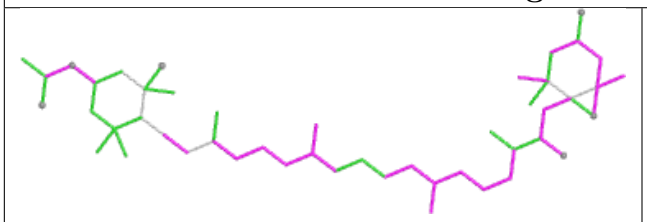


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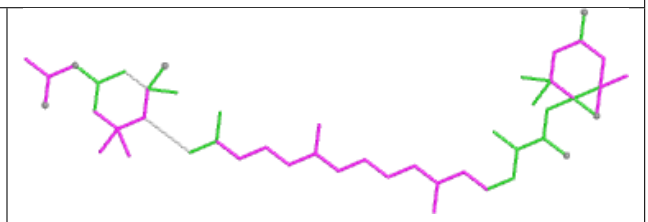


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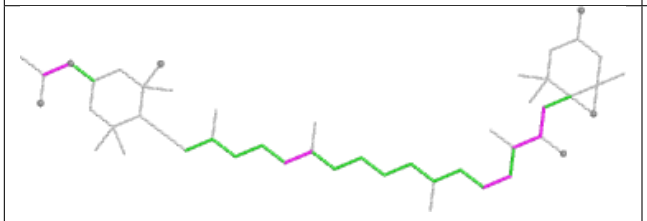
Ligand A86 39 313



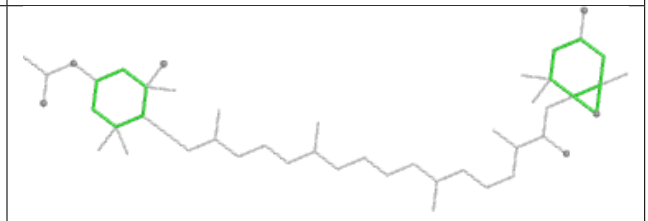
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Bond angles

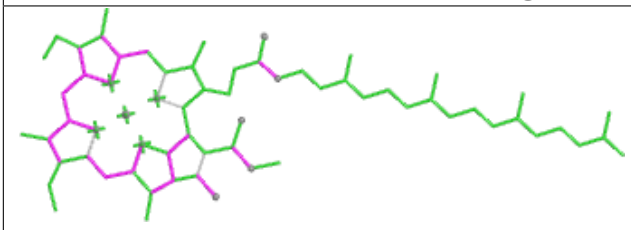


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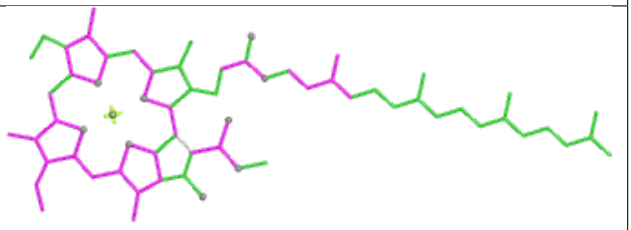


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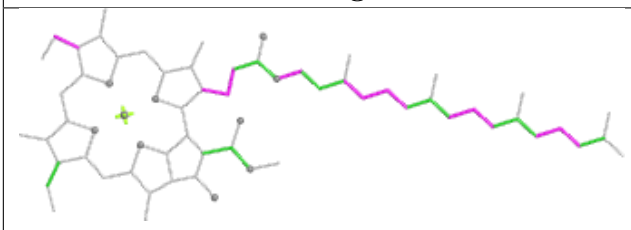
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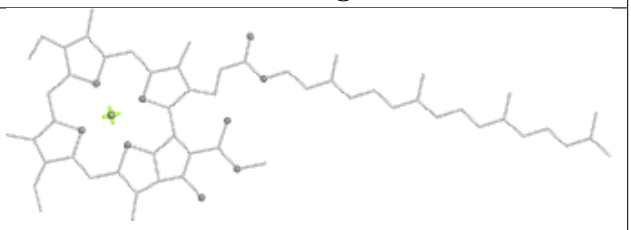
Bond lengths



Bond angles

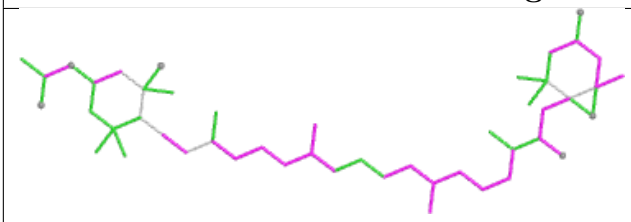


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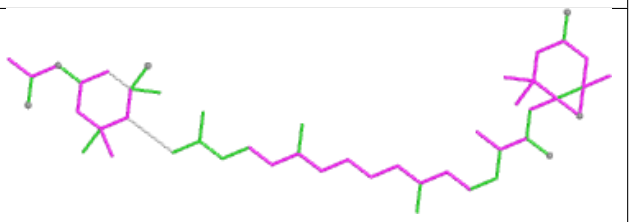


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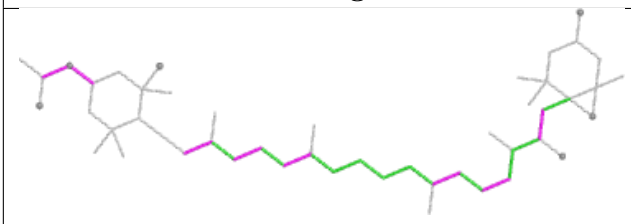
Ligand A86 34 313



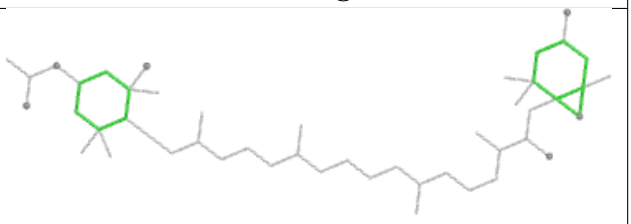
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Bond angles

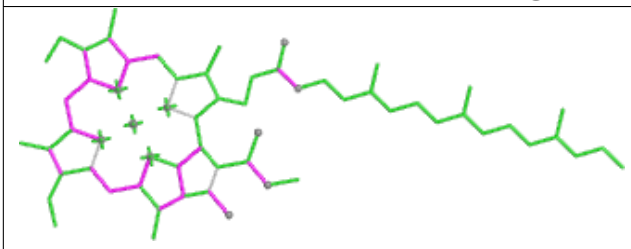


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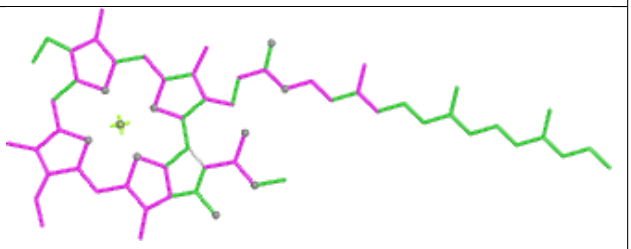


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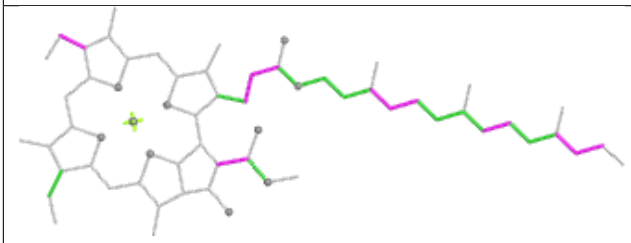
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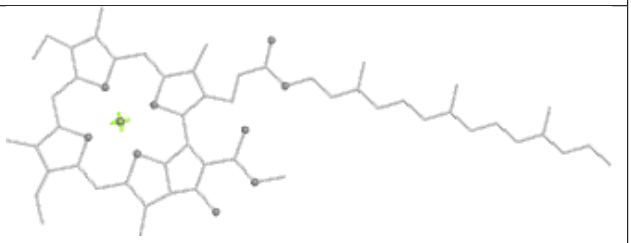
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Bond angles

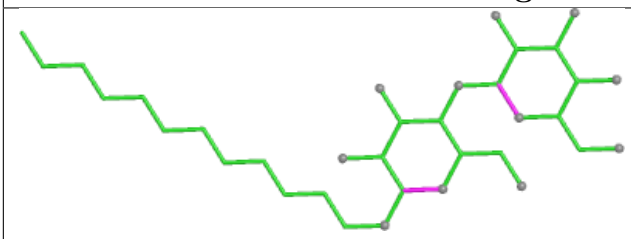


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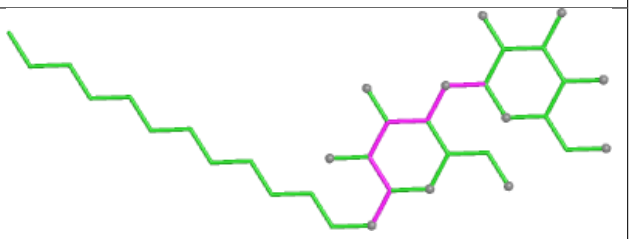


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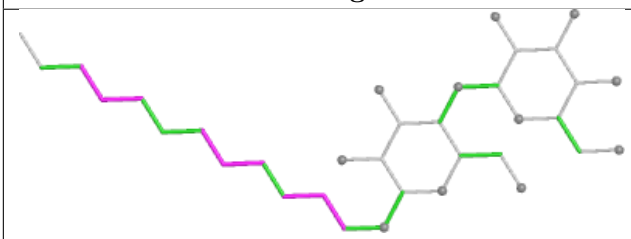
Ligand LMU 19 315



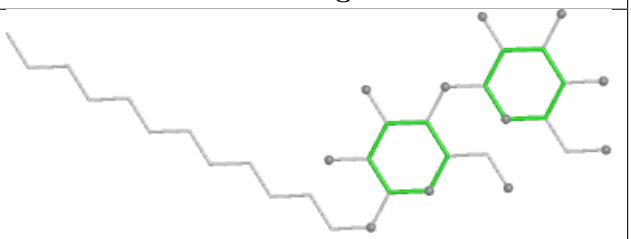
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Bond angles

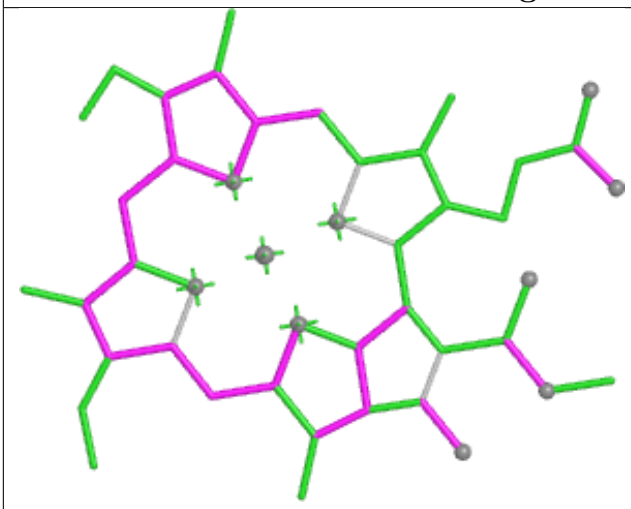


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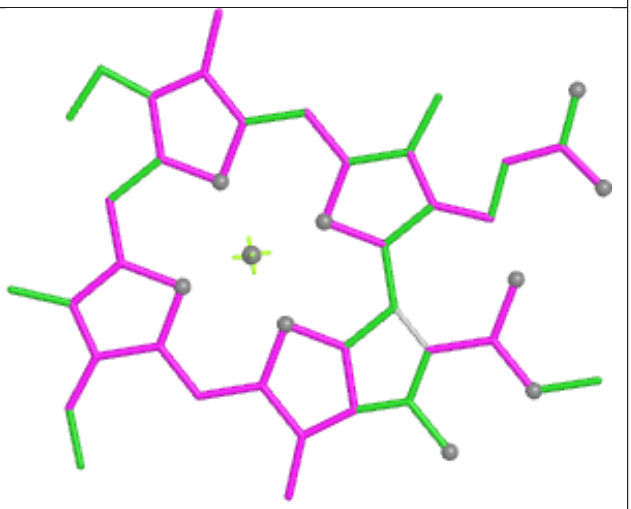


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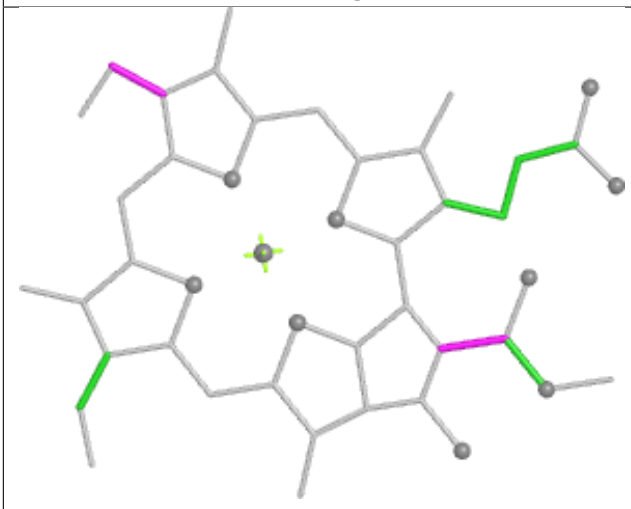
Ligand CLA 35 310



Bond lengths



Bond angles

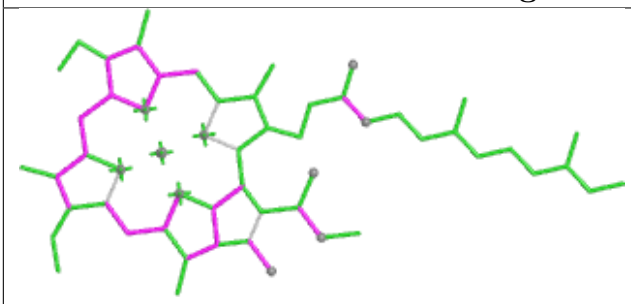


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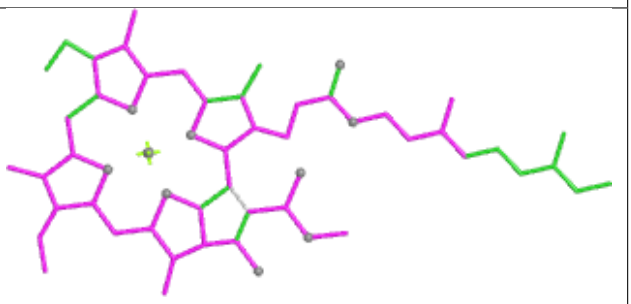


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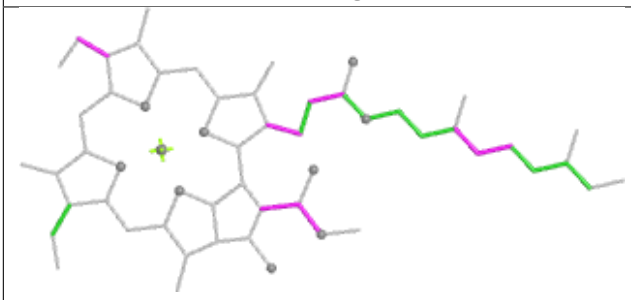
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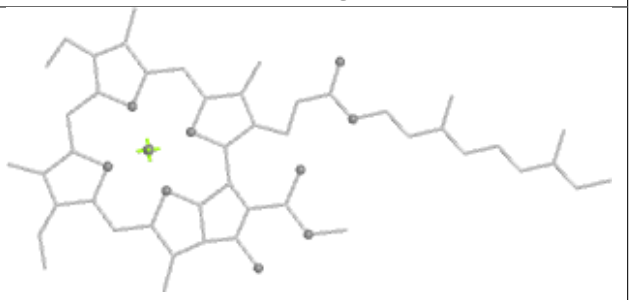
Bond lengths



Bond angles

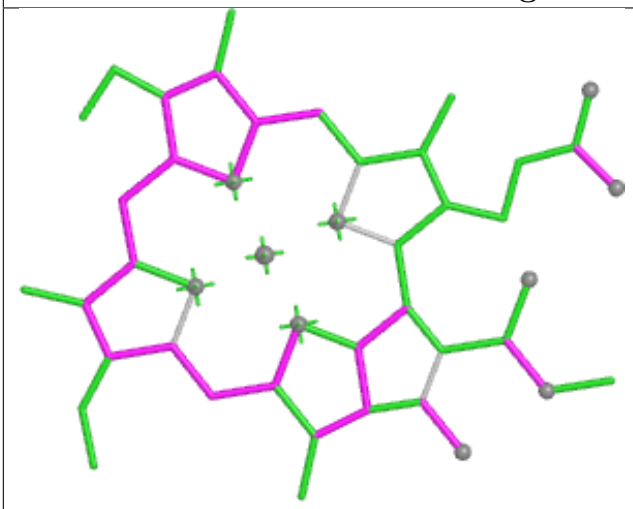


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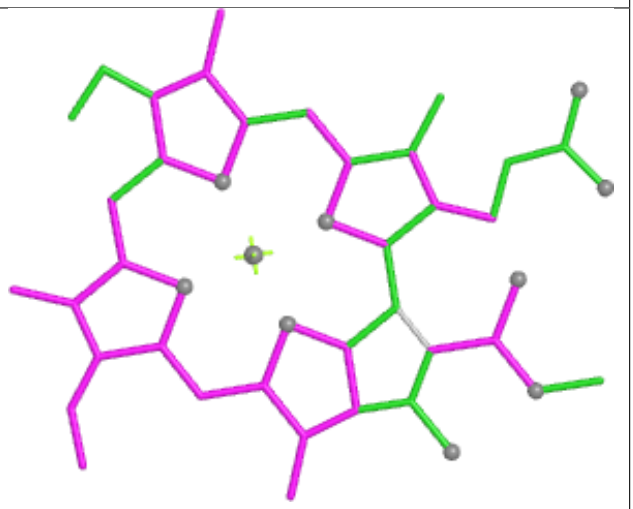


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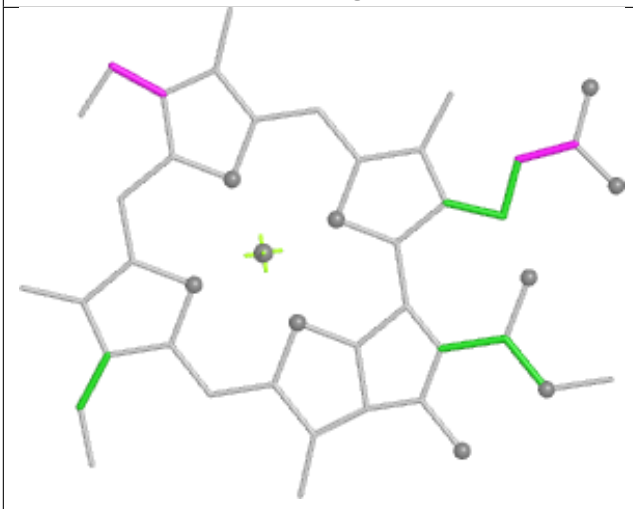
Ligand CLA 13 305



Bond lengths



Bond angles

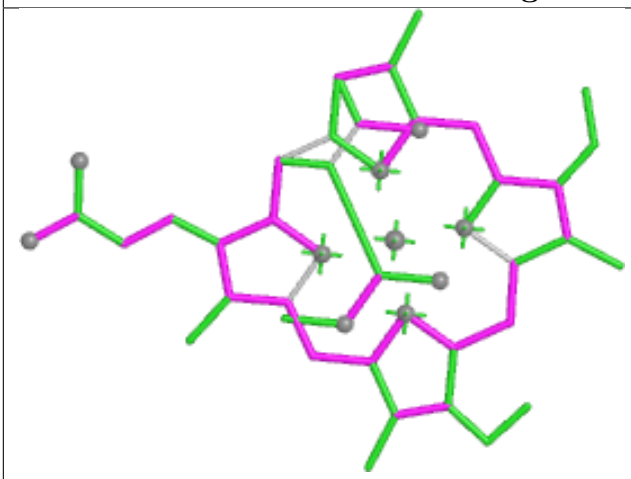


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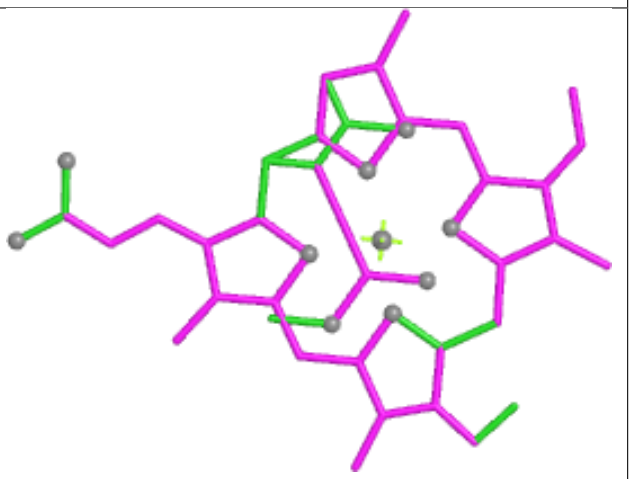


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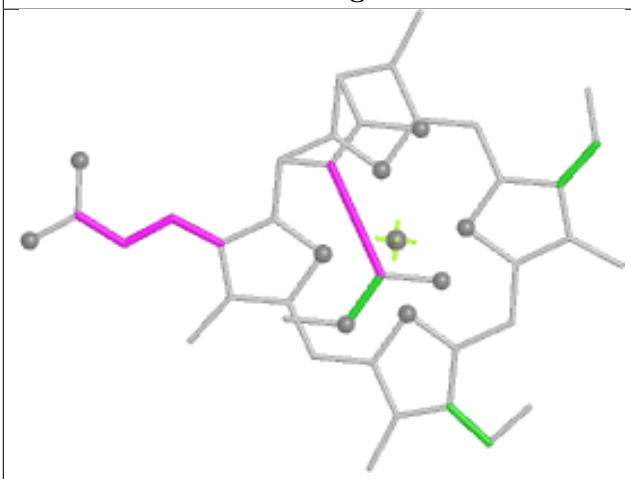
Ligand KC1 33 309



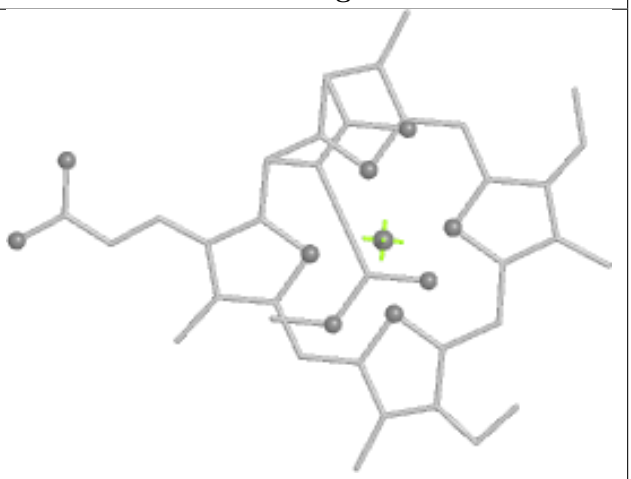
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Bond angles

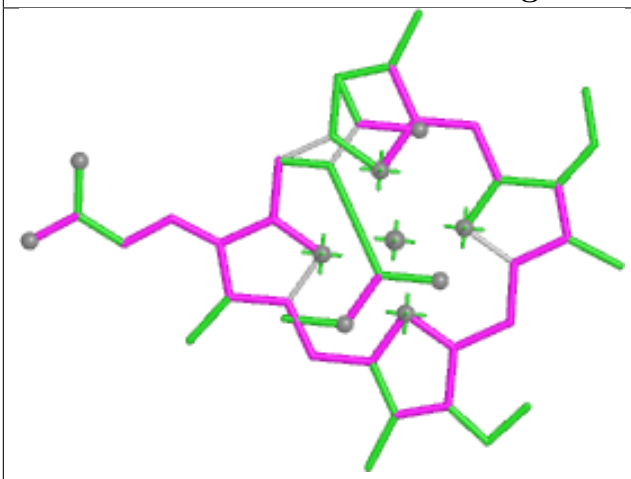


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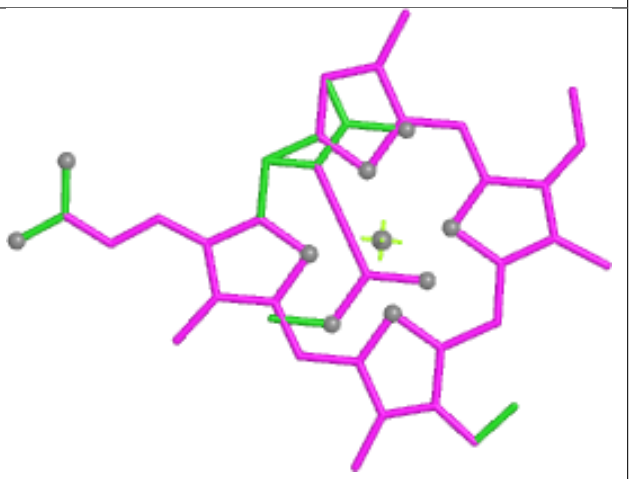


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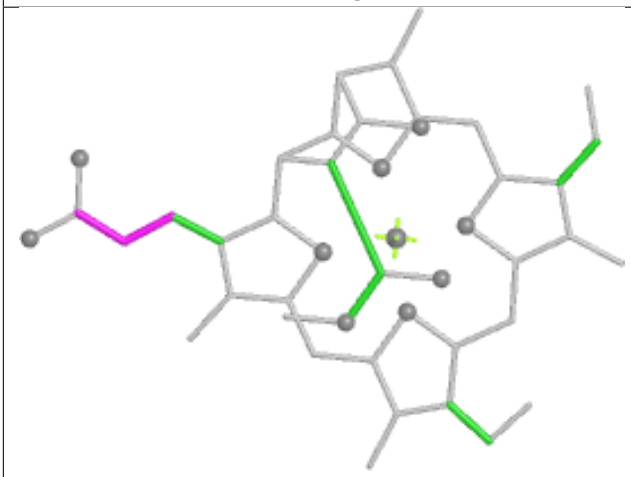
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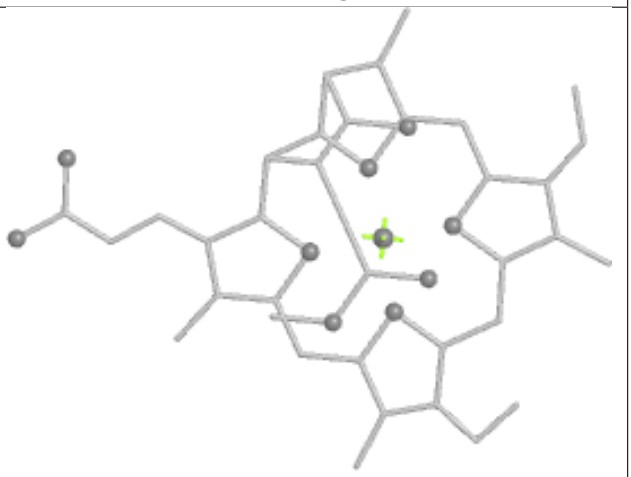
Bond lengths



Bond angles

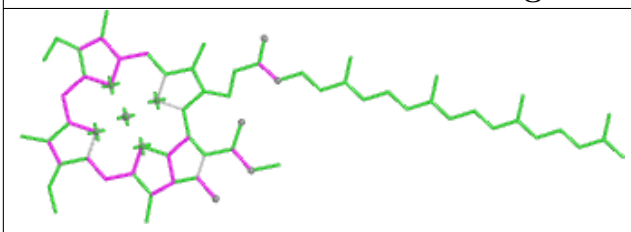


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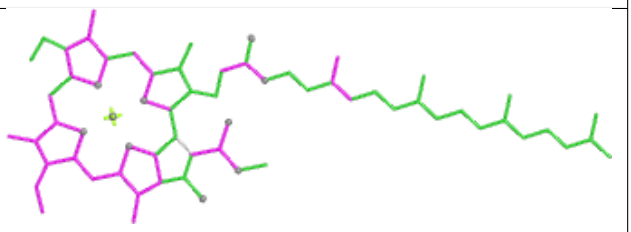


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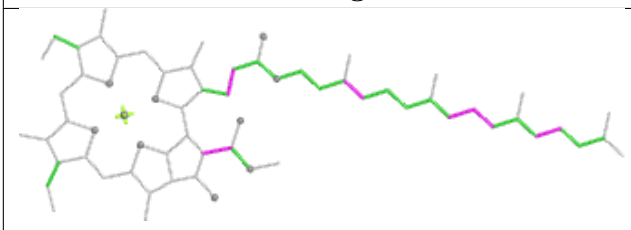
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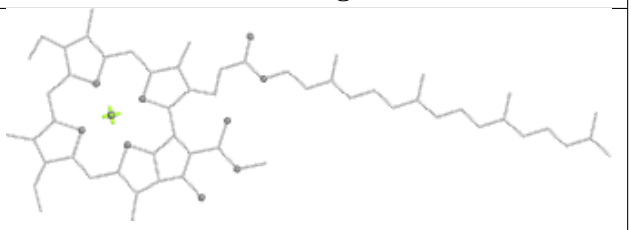
Bond lengths



Bond angles

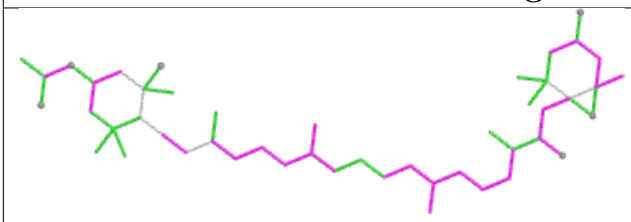


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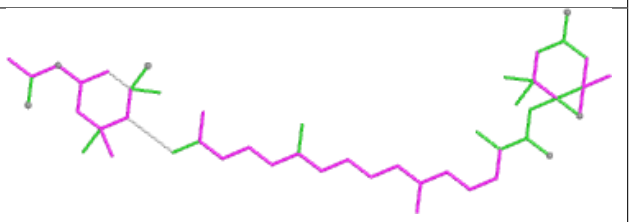


Rings

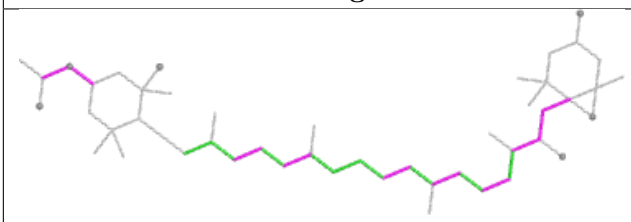
Ligand A86 33 313



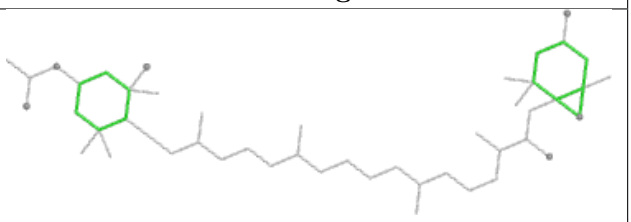
Bond lengths



Bond angles

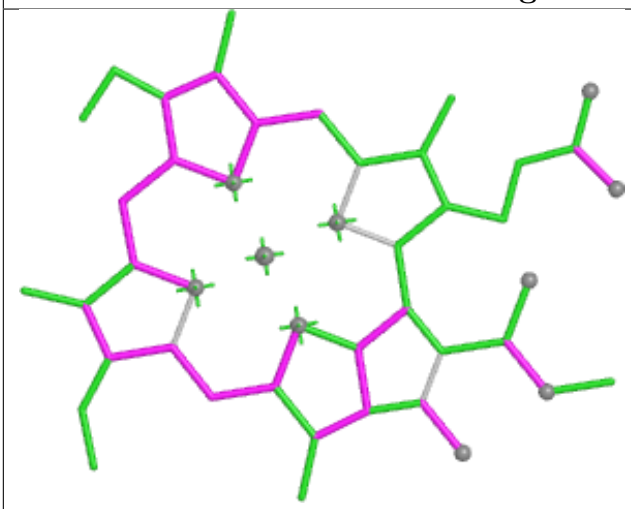


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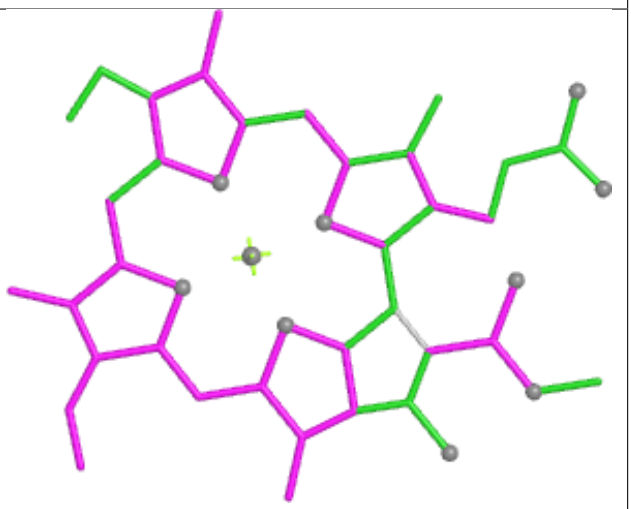


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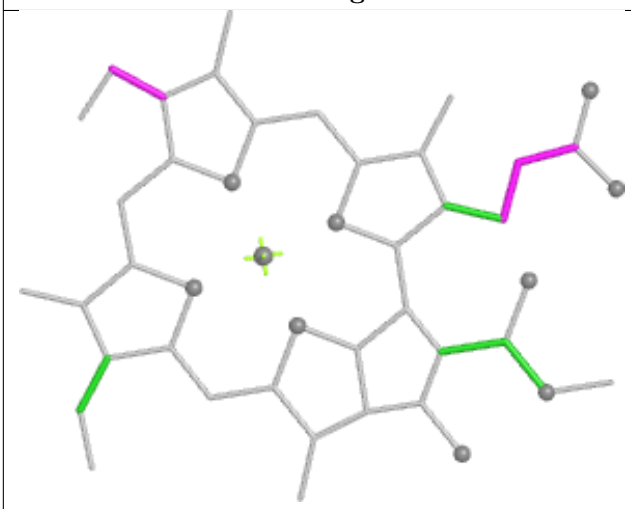
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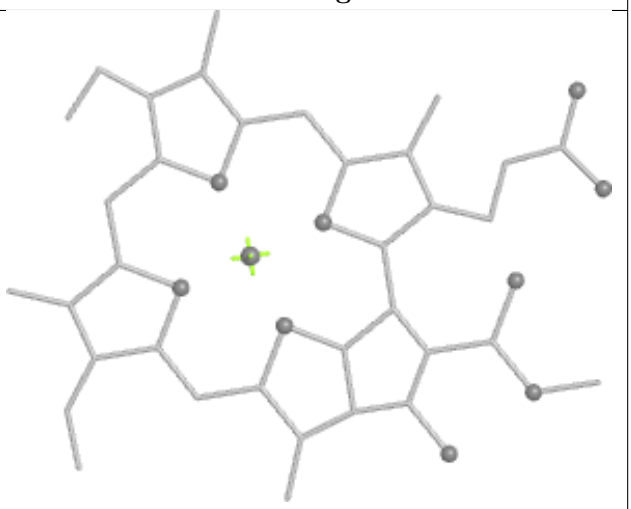
Bond lengths



Bond angles

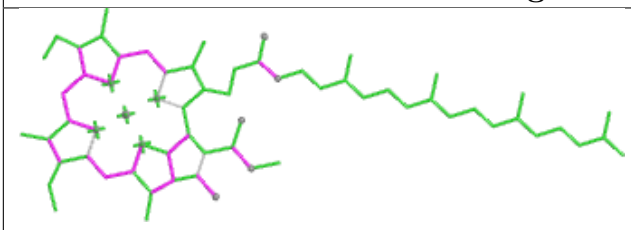


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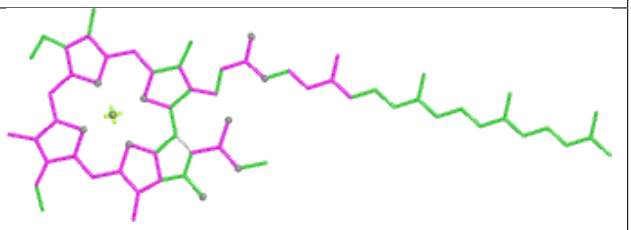


Rings

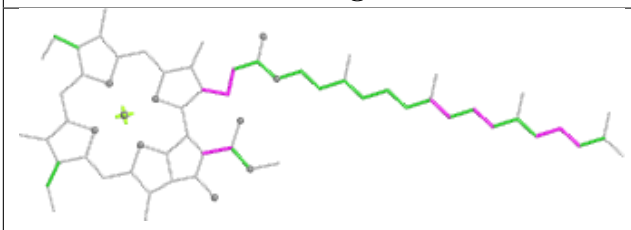
Ligand CLA b 506



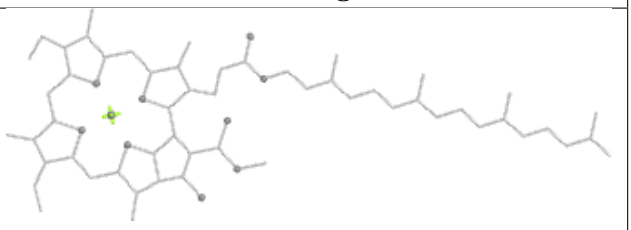
Bond lengths



Bond angles

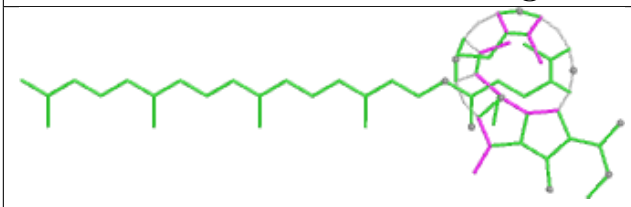


Torsions

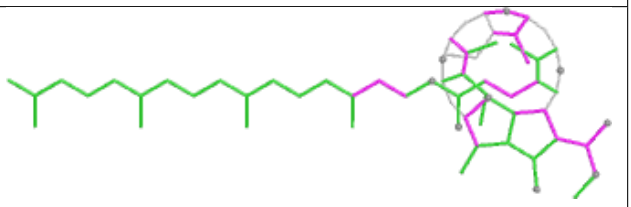


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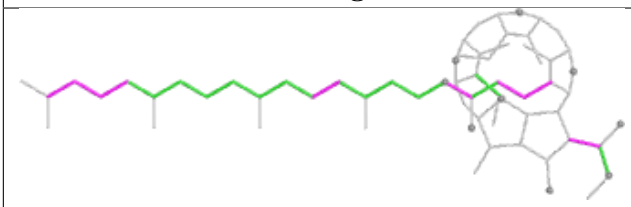
Ligand PHO D 403



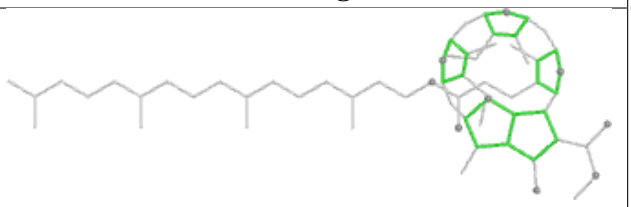
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Bond angles

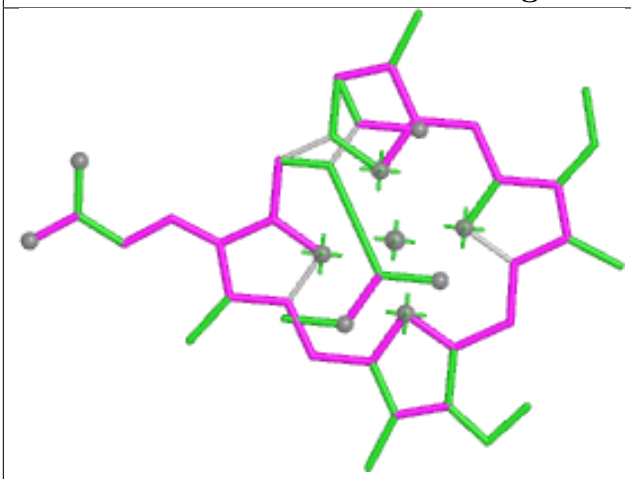


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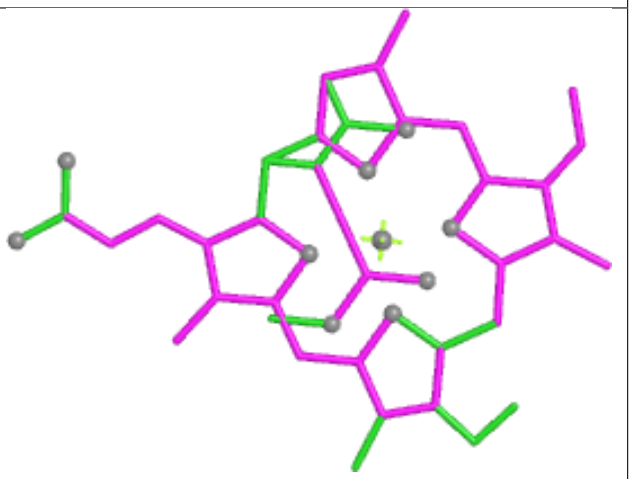


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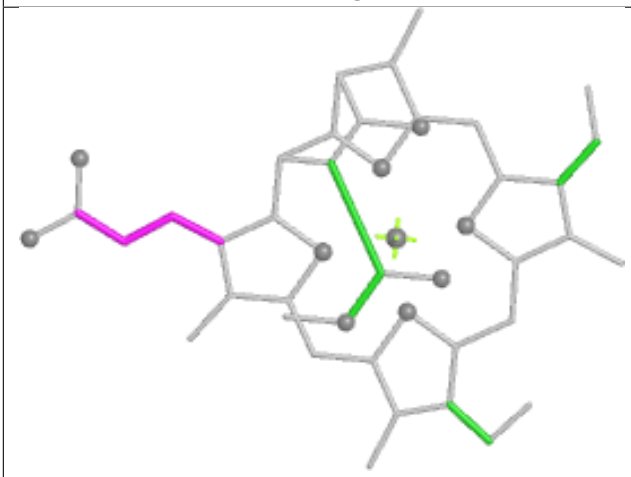
Ligand KC1 41 203



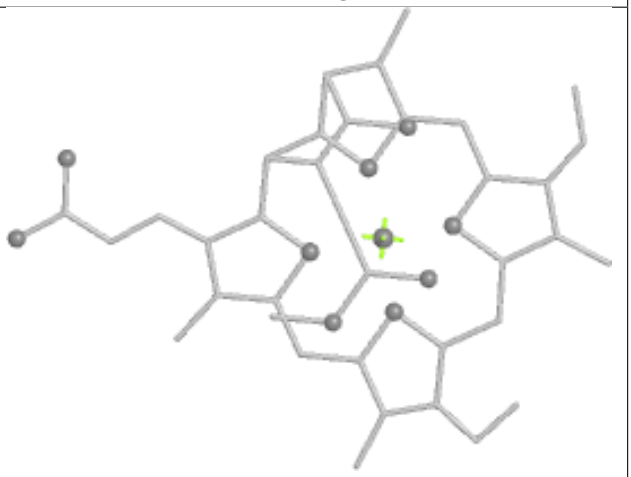
Bond lengths



Bond angles



Torsions

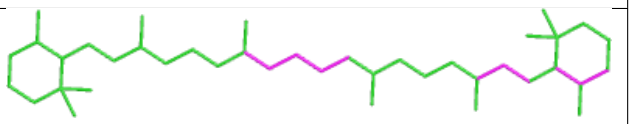


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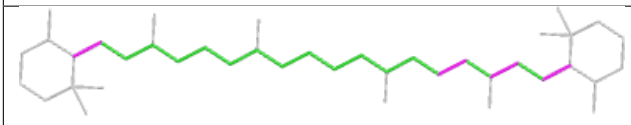
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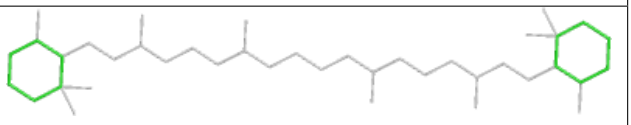
Bond lengths



Bond angles

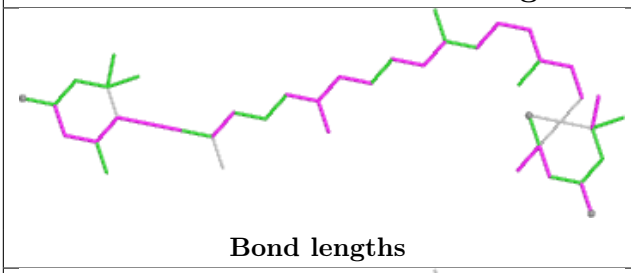


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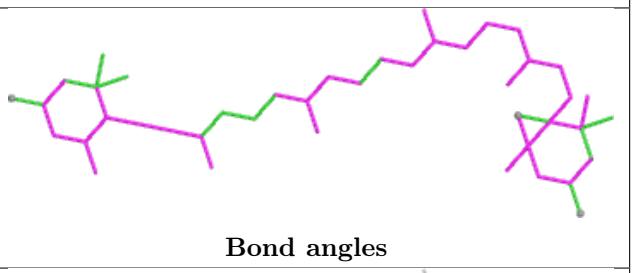


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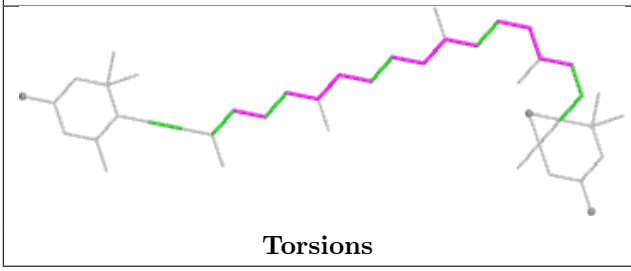
Ligand DD6 21 216



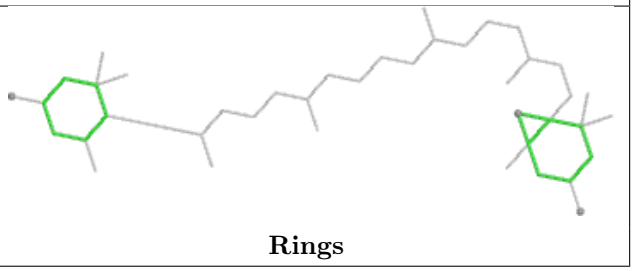
Bond lengths



Bond angles

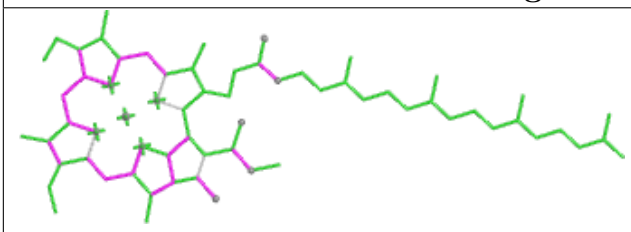


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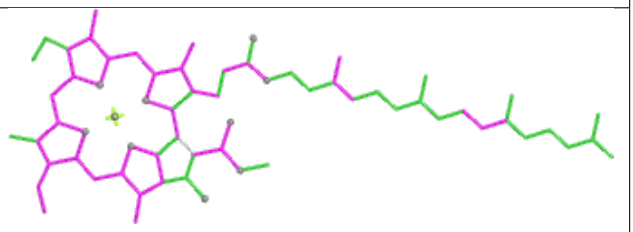


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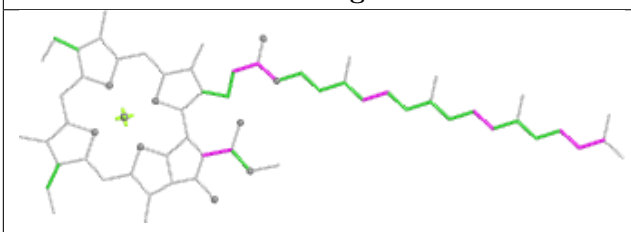
Ligand CLA C 512



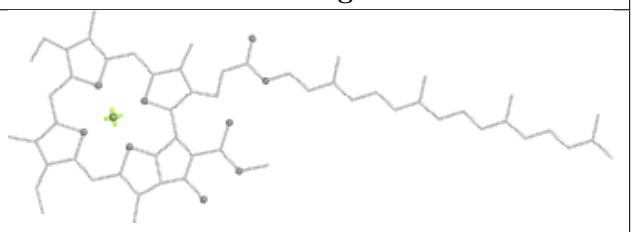
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Bond angles

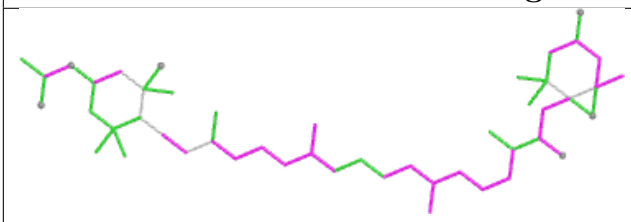


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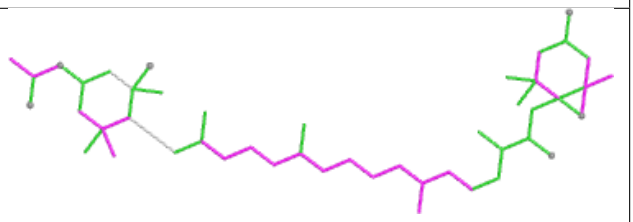


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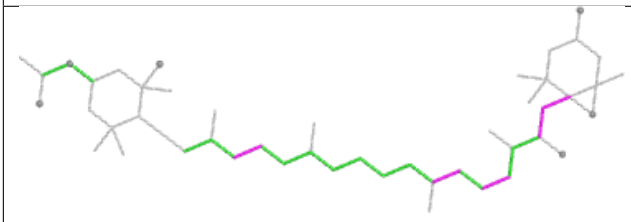
Ligand A86 20 309



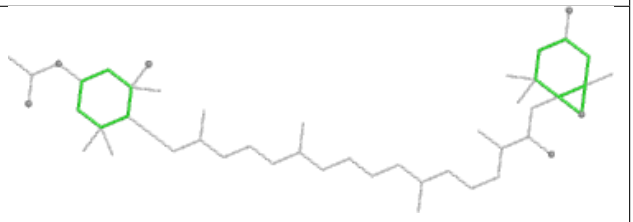
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Bond angles

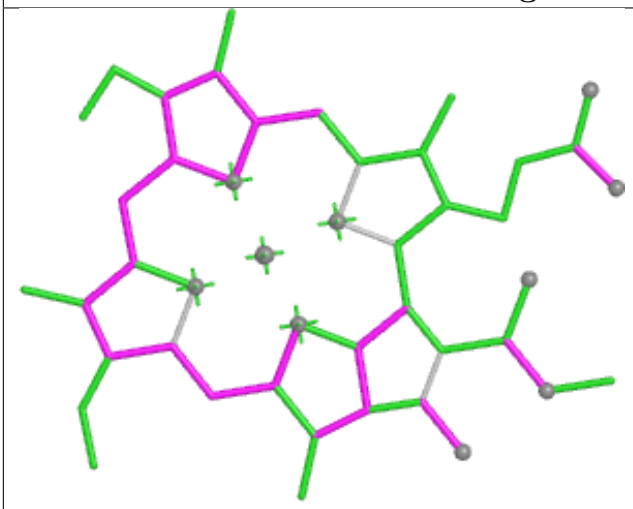


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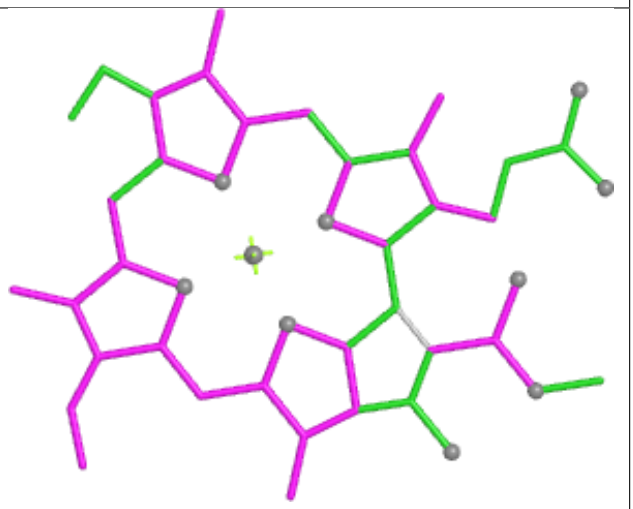


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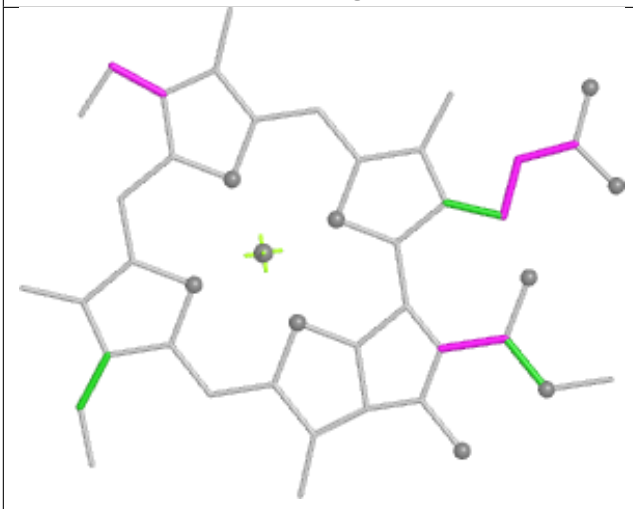
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Bond lengths



Bond angles

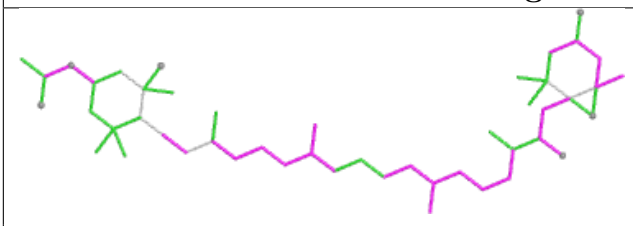


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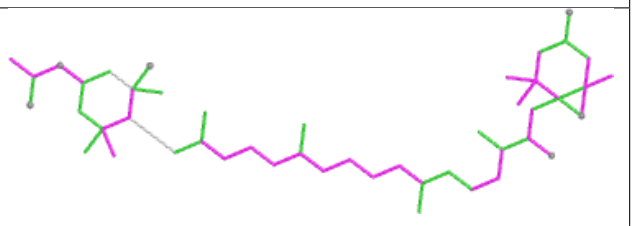


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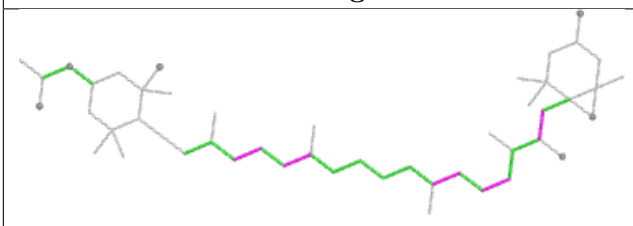
Ligand A86 17 314



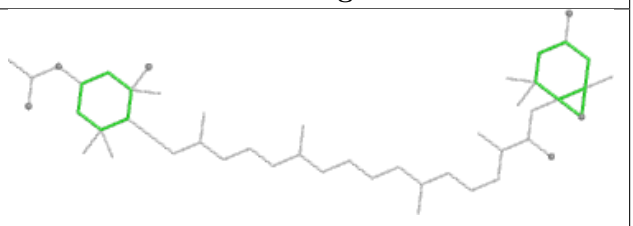
Bond lengths



Bond angles

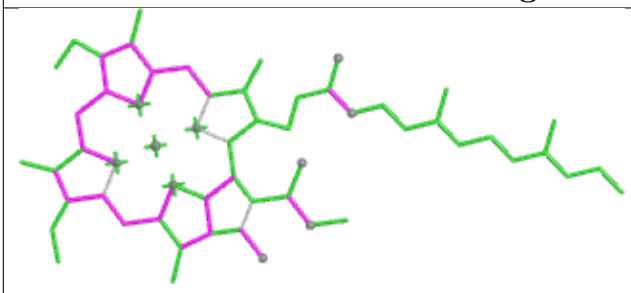


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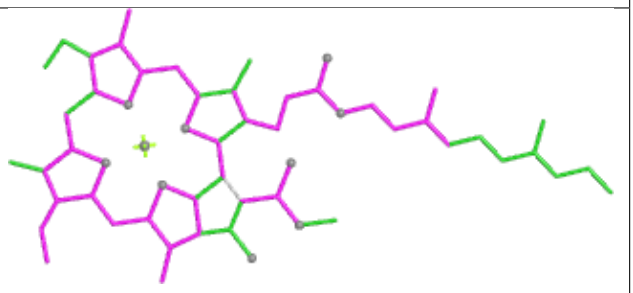


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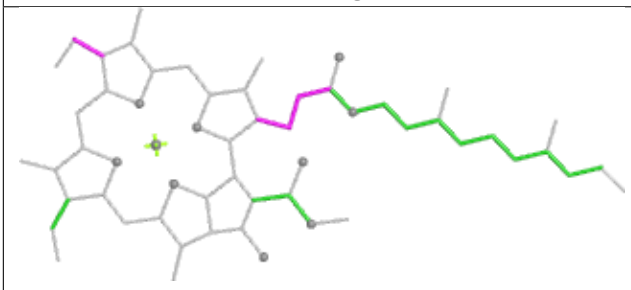
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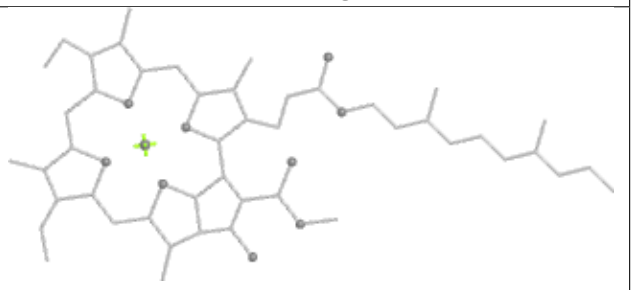
Bond lengths



Bond angles

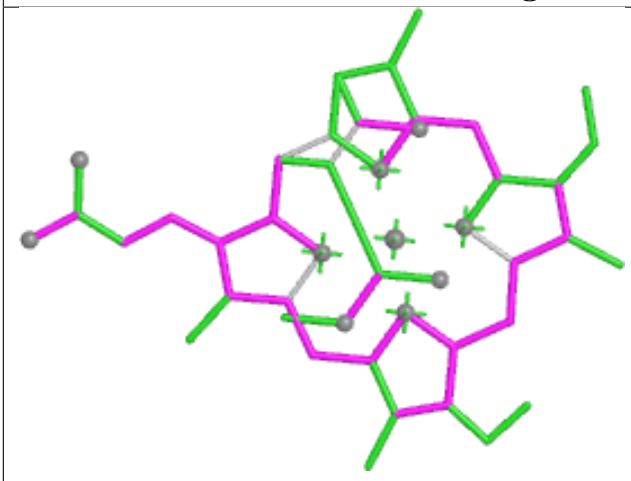


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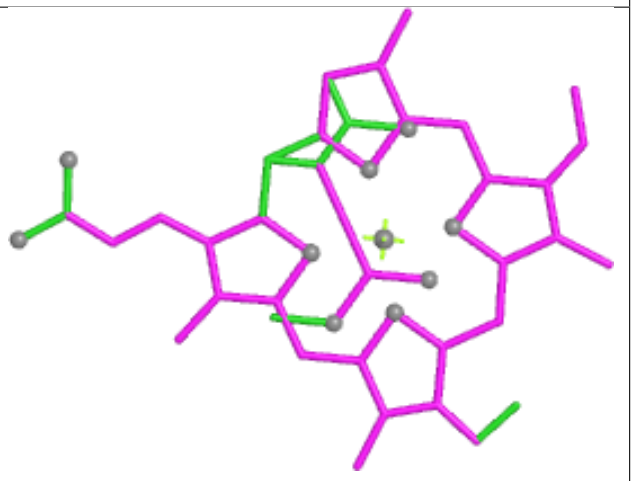


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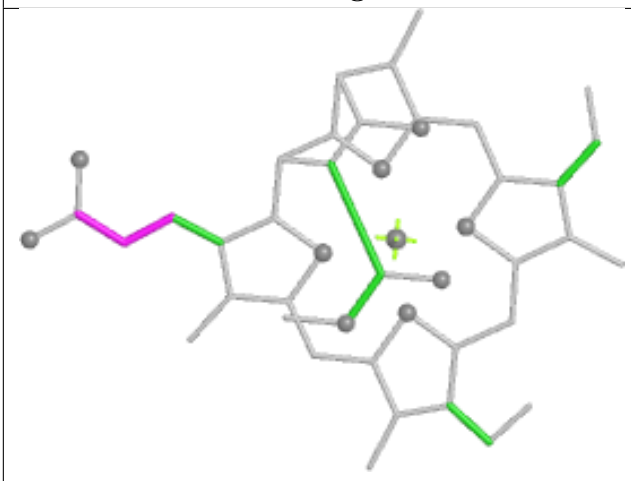
Ligand KC1 19 308



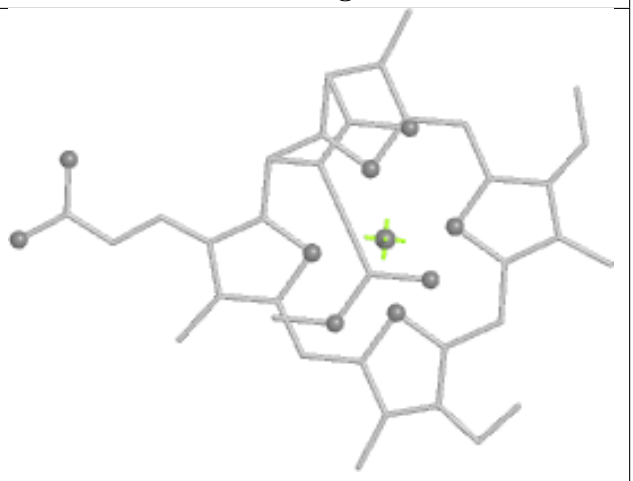
Bond lengths



Bond angles

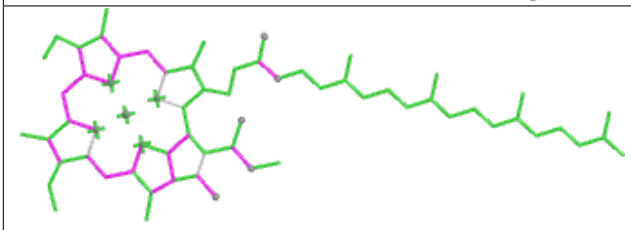


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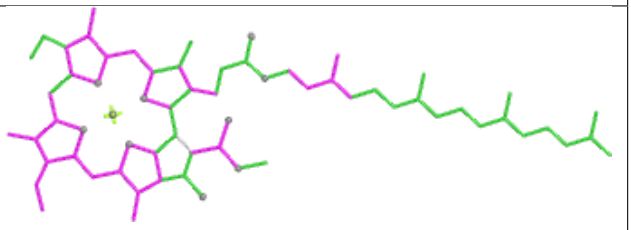


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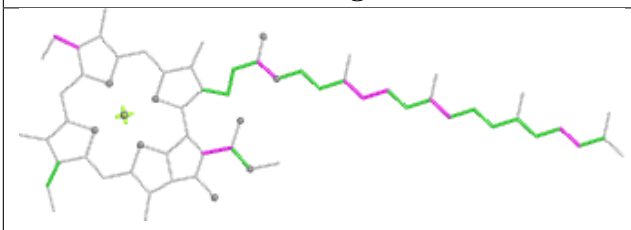
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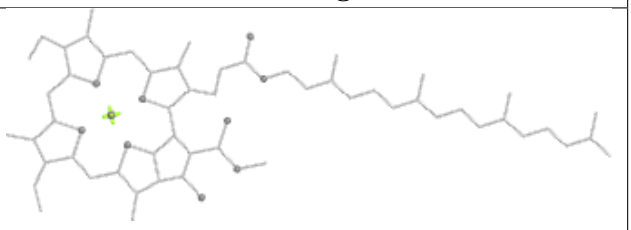
Bond lengths



Bond angles

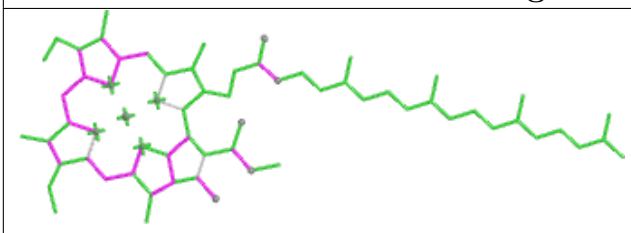


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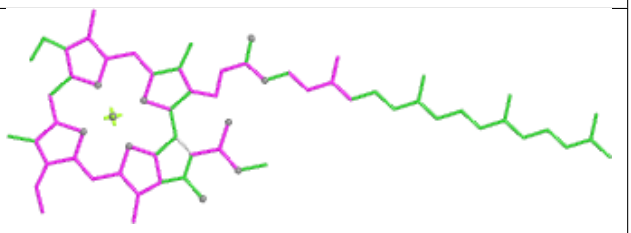


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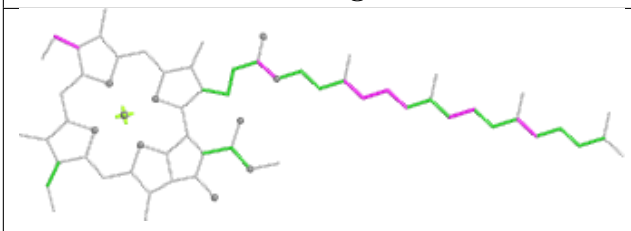
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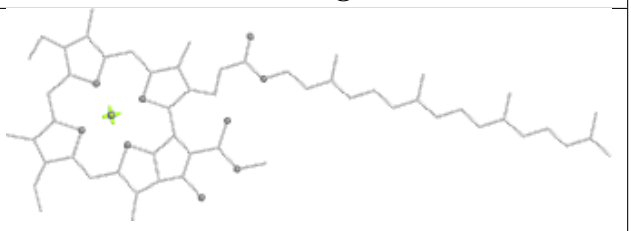
Bond lengths



Bond angles

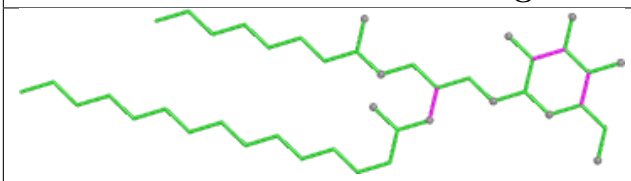


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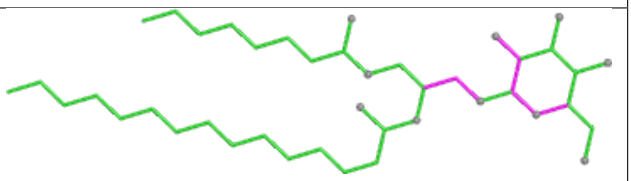


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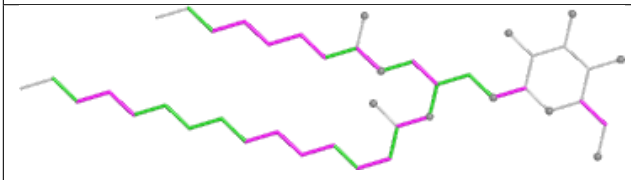
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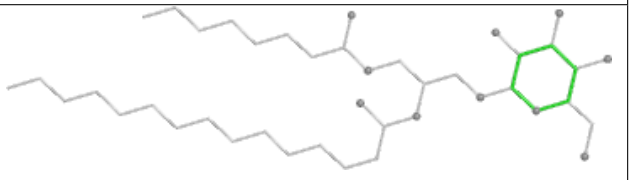
Bond lengths



Bond angles

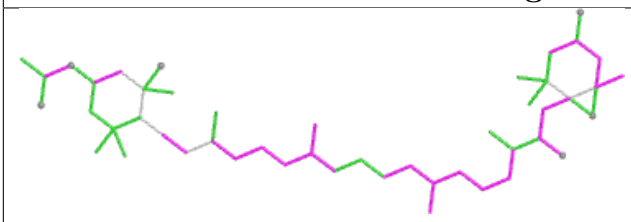


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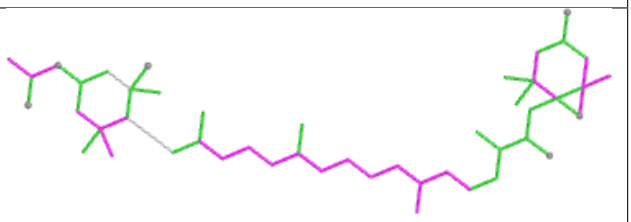


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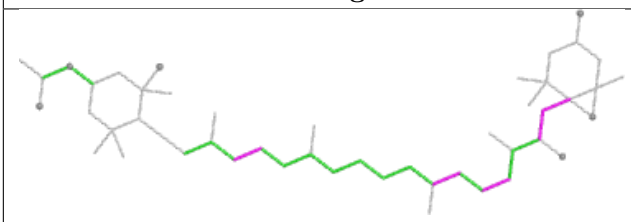
Ligand A86 40 211



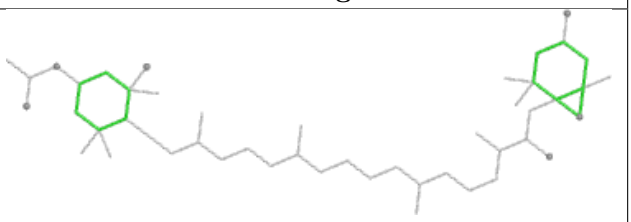
Bond lengths



Bond angles

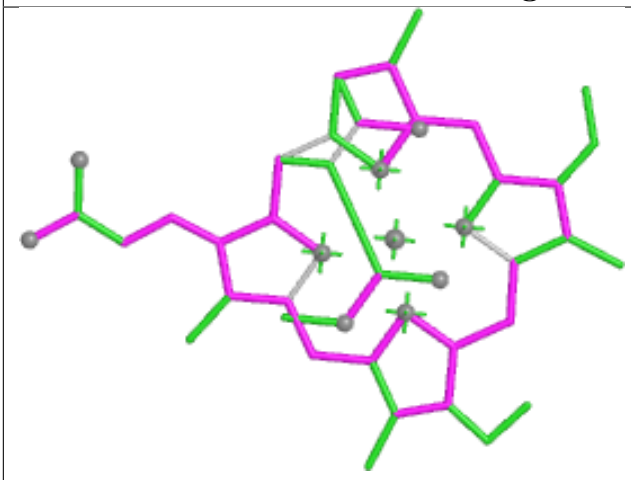


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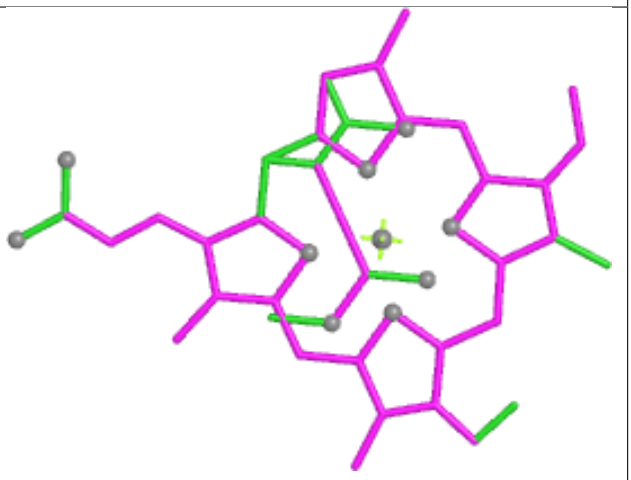


Rings

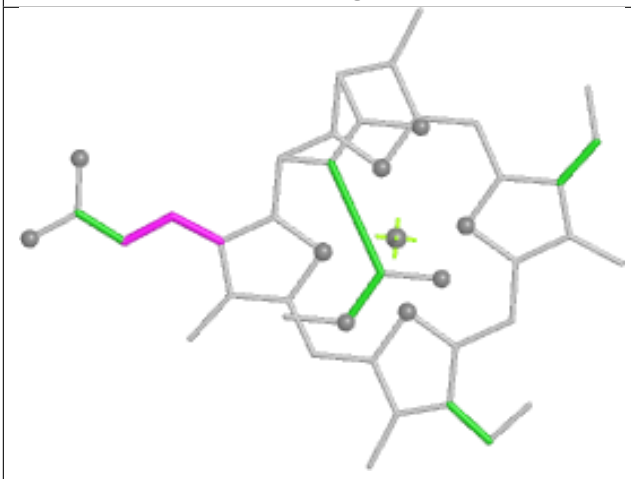
Ligand KC1 36 302



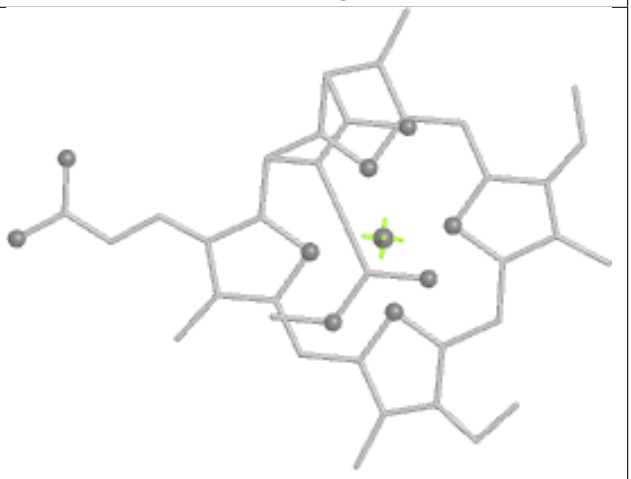
Bond lengths



Bond angles

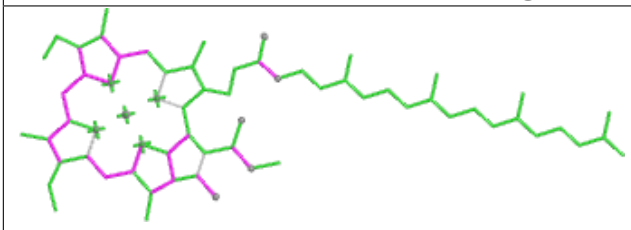


Torsions

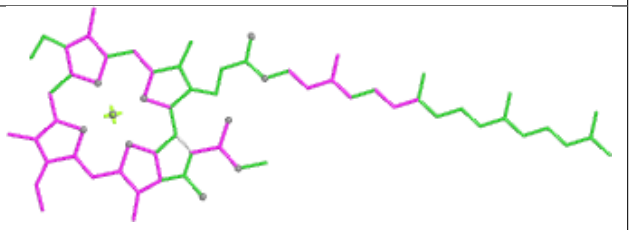


Rings

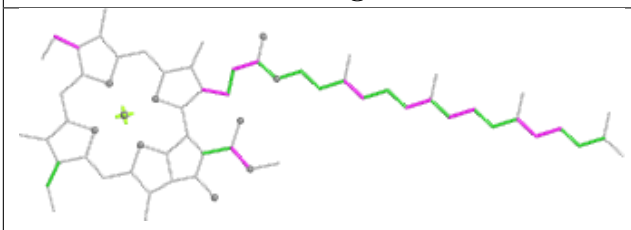
Ligand CLA 34 301



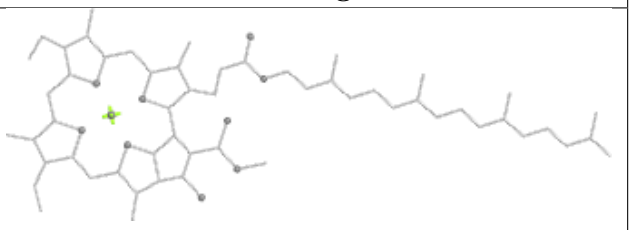
Bond lengths



Bond angles

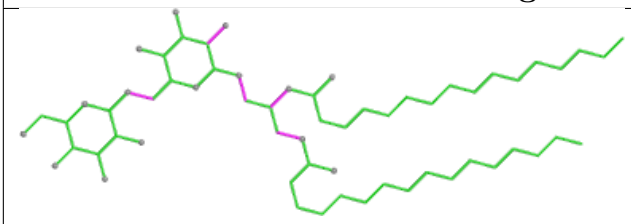


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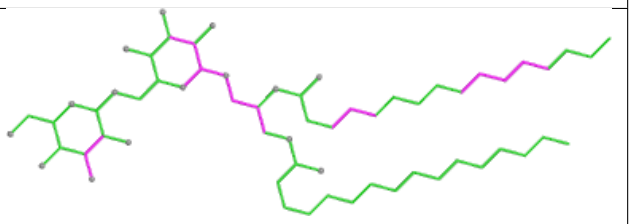


Rings

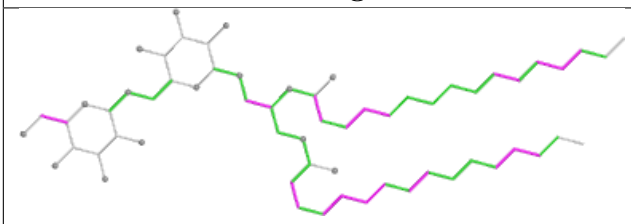
Ligand DGD H 102



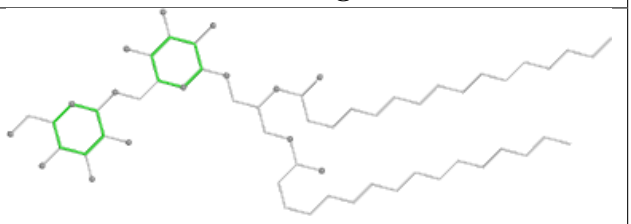
Bond lengths



Bond angles

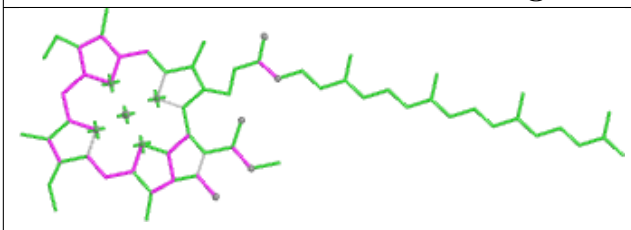


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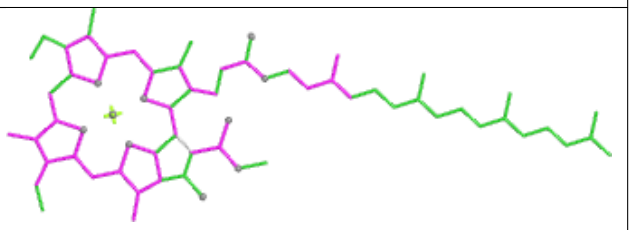


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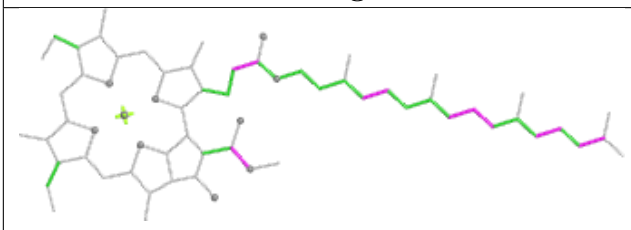
Ligand CLA b 513



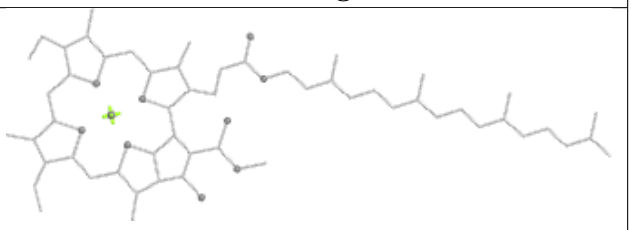
Bond lengths



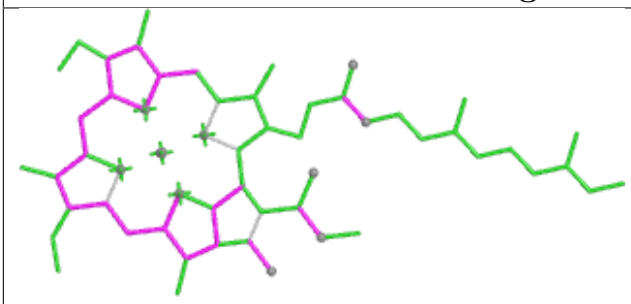
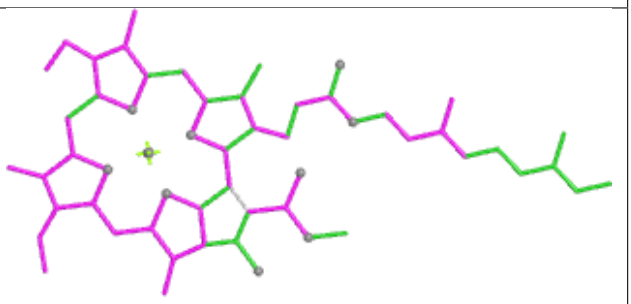
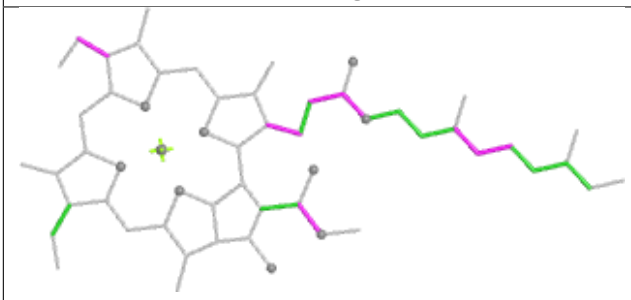
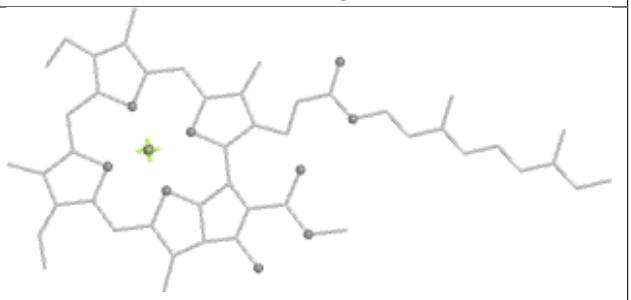
Bond angles

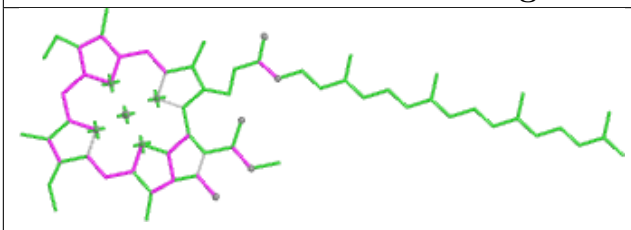
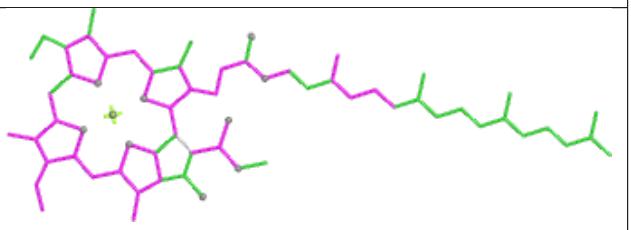
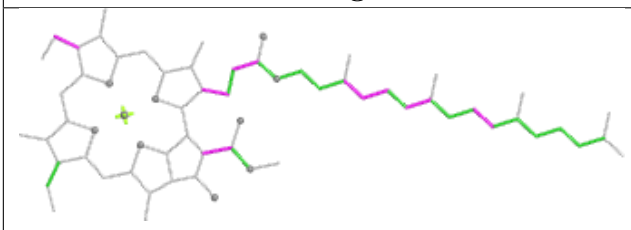
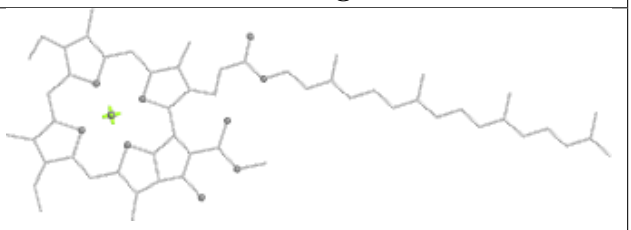


Torsions

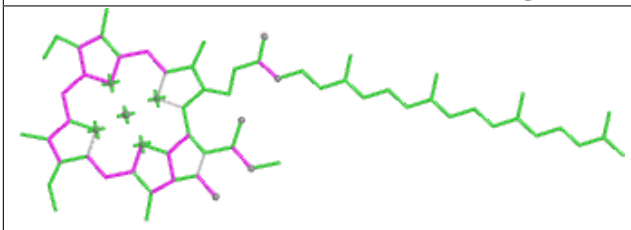


Rings

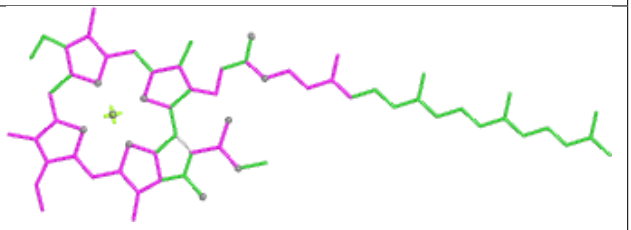
Ligand CLA 20 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 12 205	
	
Bond lengths	Bond angles
	
Torsions	Rings

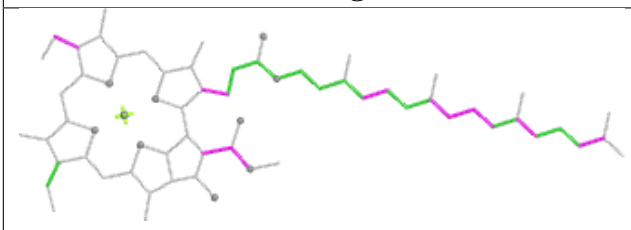
Ligand CLA 16 306



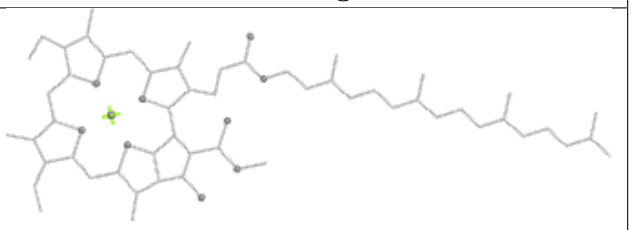
Bond lengths



Bond angles

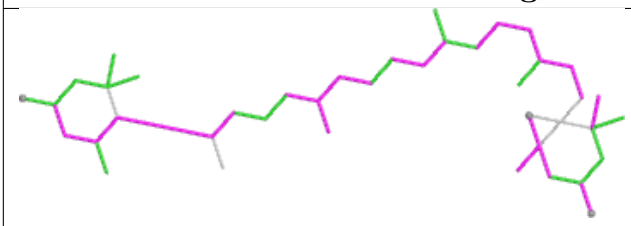


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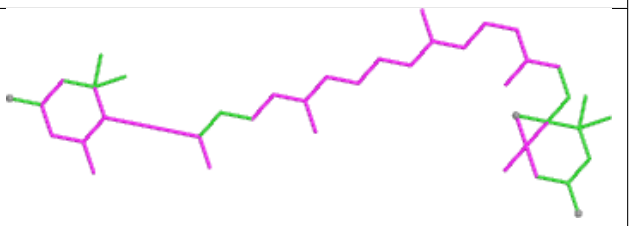


Rings

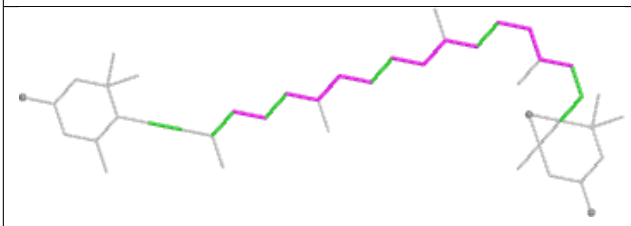
Ligand DD6 40 212



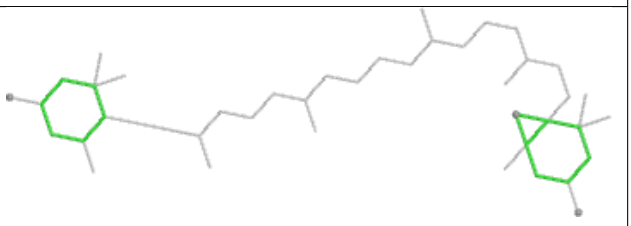
Bond lengths



Bond angles

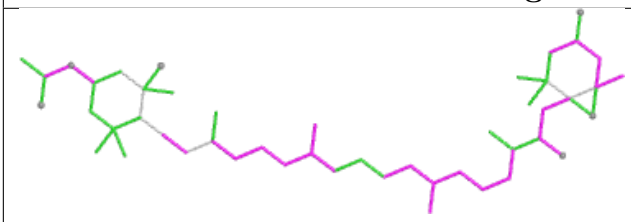


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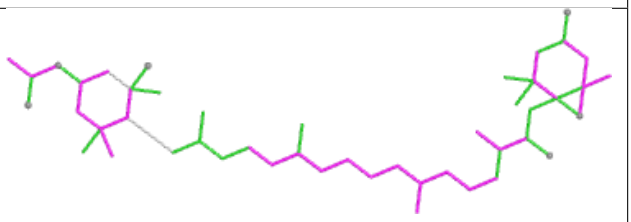


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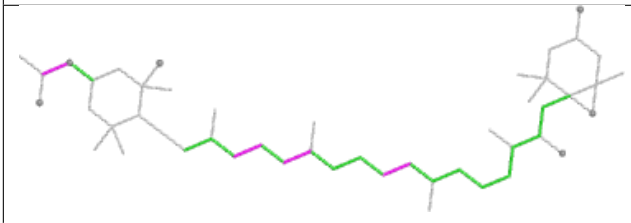
Ligand A86 34 315



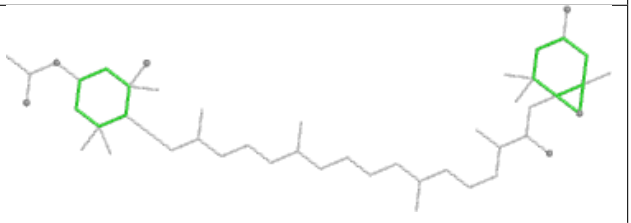
Bond lengths



Bond angles

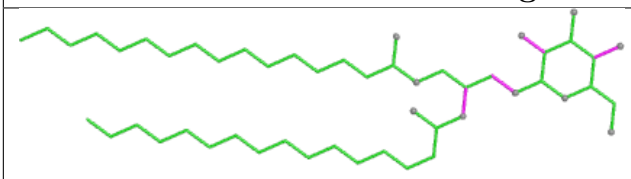


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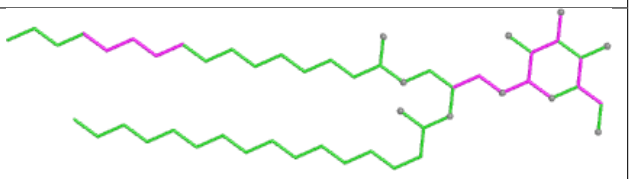


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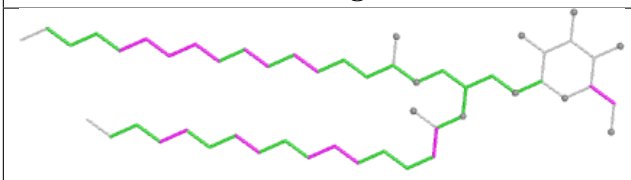
Ligand LMG D 412



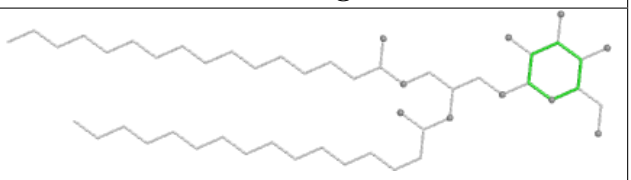
Bond lengths



Bond angles

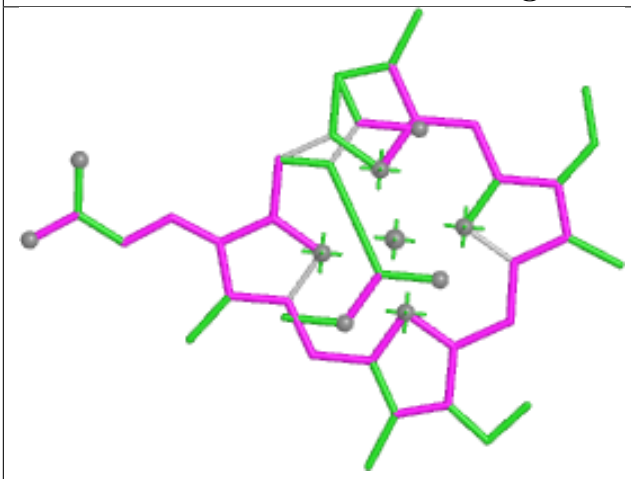


Torsions



Rings

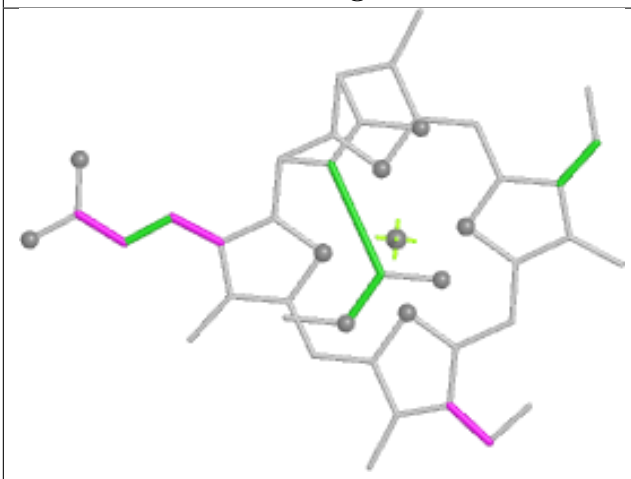
Ligand KC1 21 207



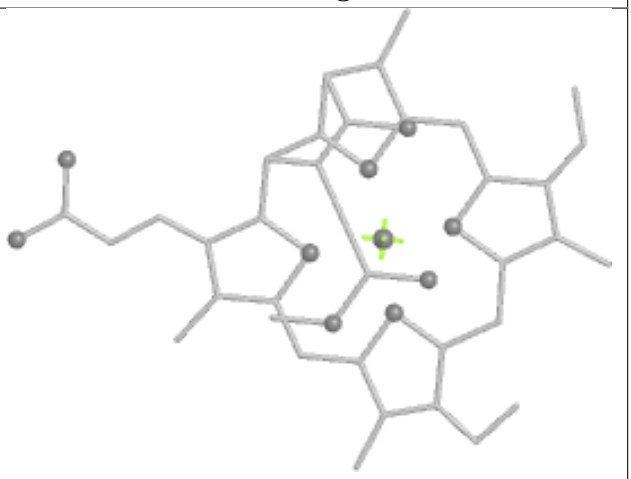
Bond lengths



Bond angles

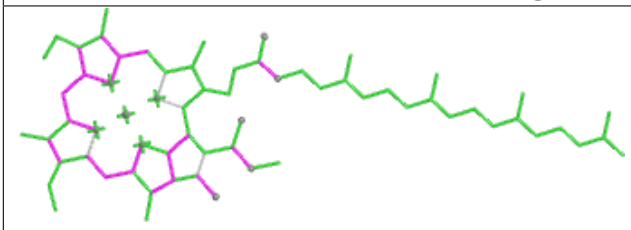


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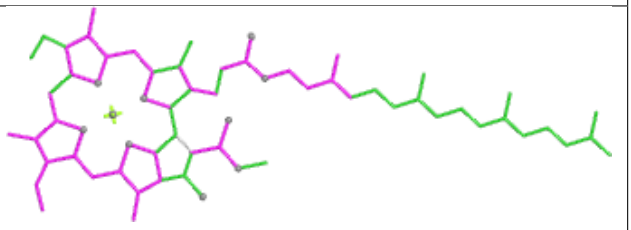


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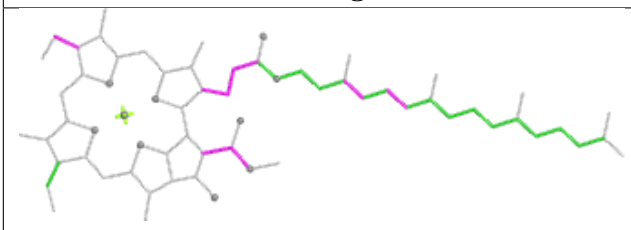
Ligand CLA c 501



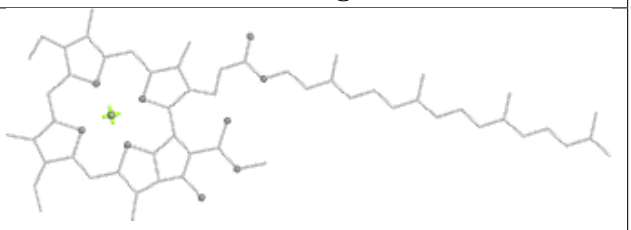
Bond lengths



Bond angles

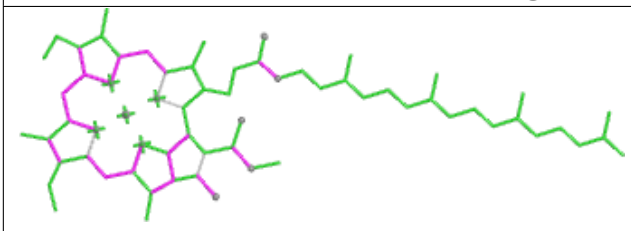


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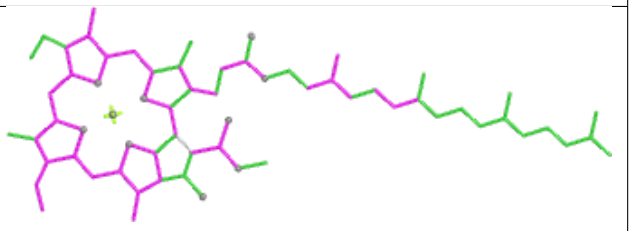


Rings

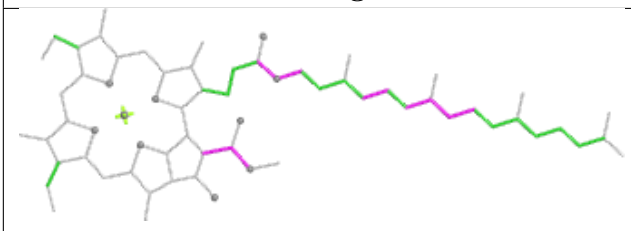
Ligand CLA B 516



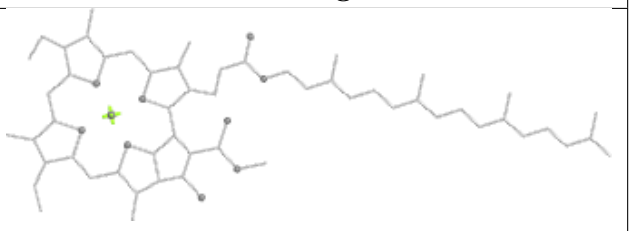
Bond lengths



Bond angles

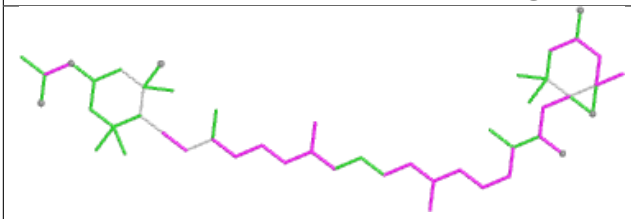


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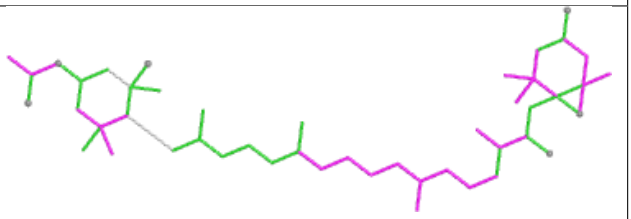


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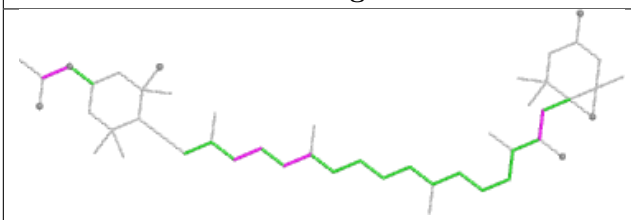
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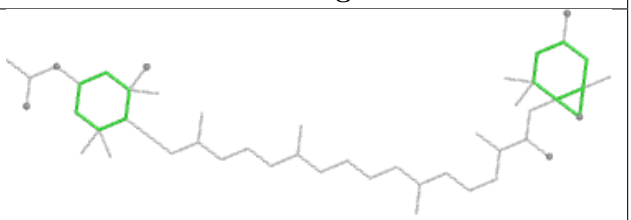
Bond lengths



Bond angles

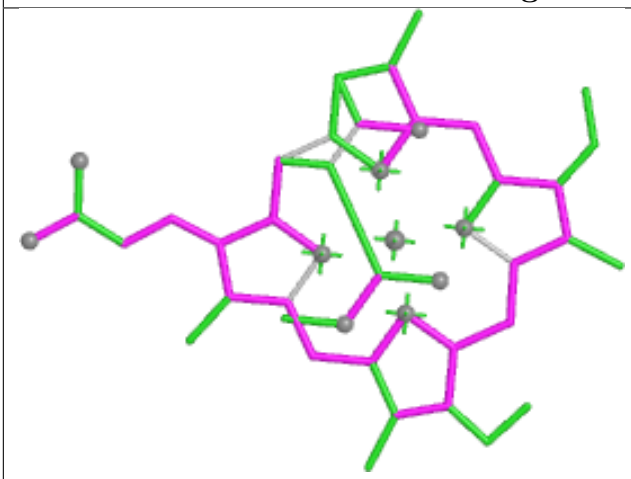


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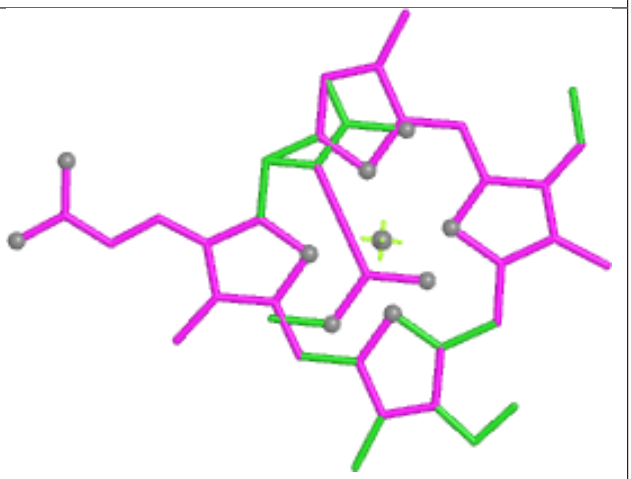


Rings

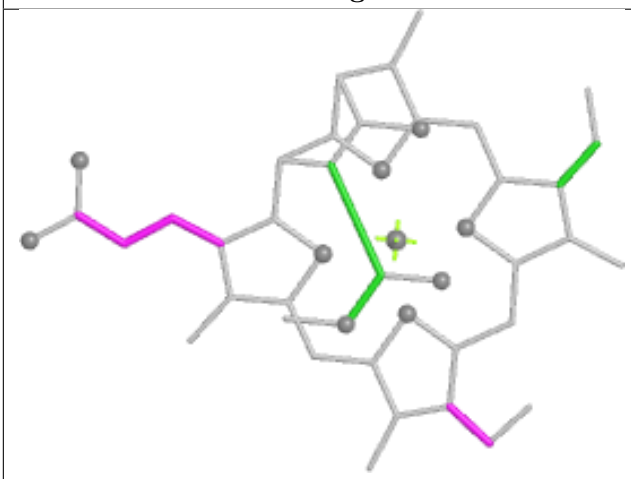
Ligand KC1 16 304



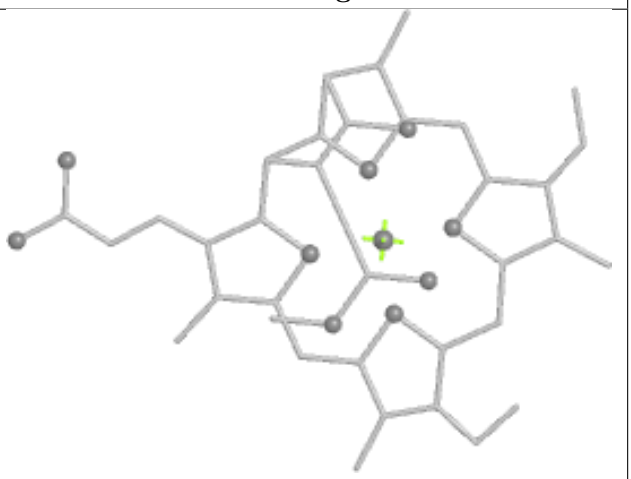
Bond lengths



Bond angles

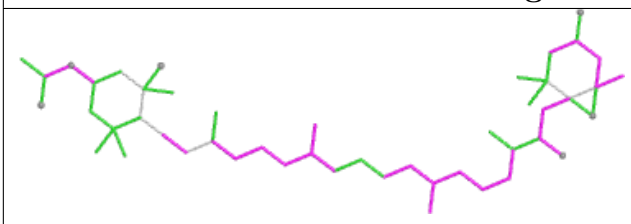


Torsions

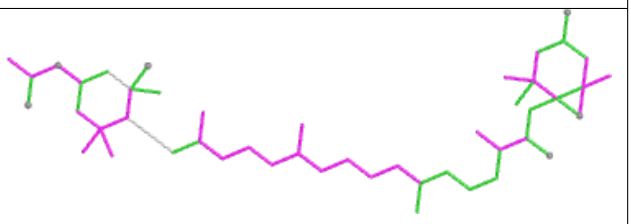


Rings

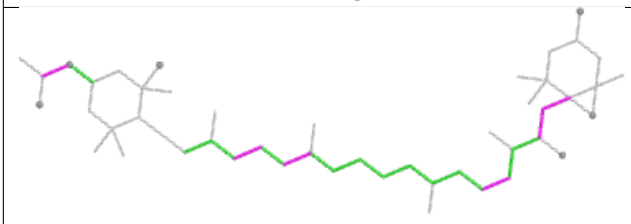
Ligand A86 33 314



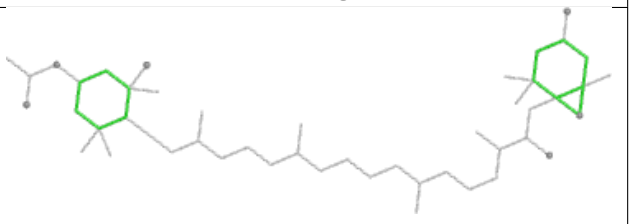
Bond lengths



Bond angles

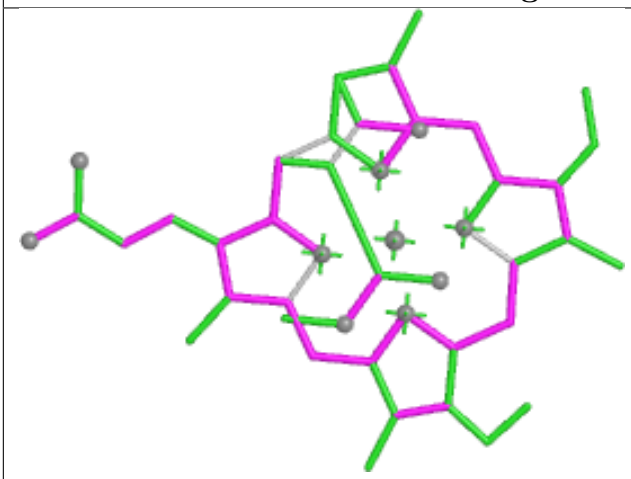


Torsions

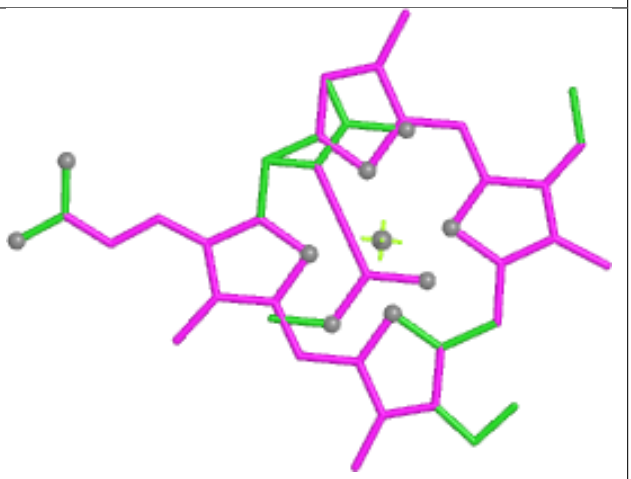


Rings

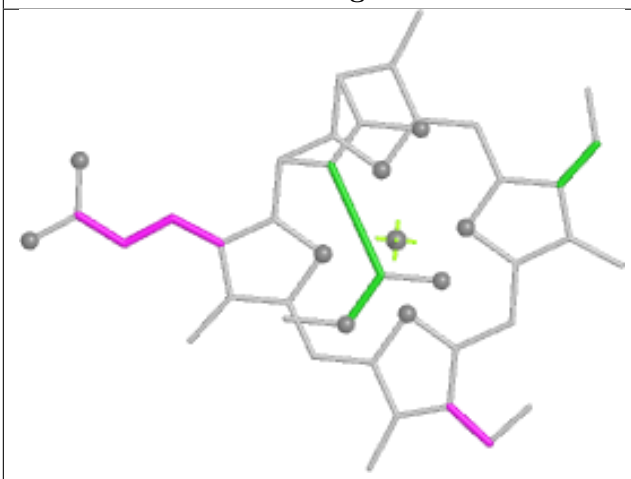
Ligand KC1 20 304



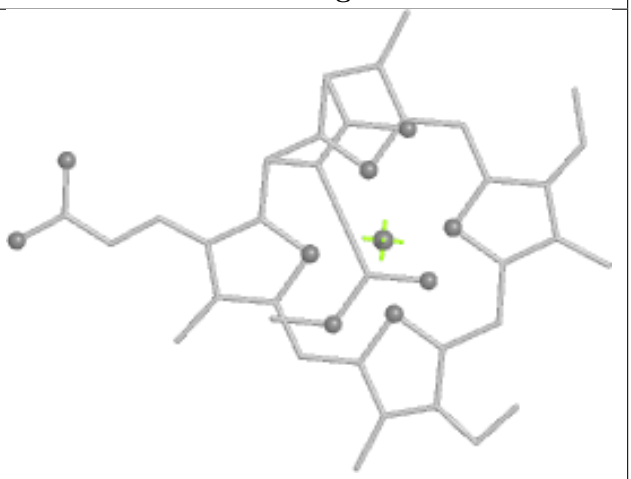
Bond lengths



Bond angles

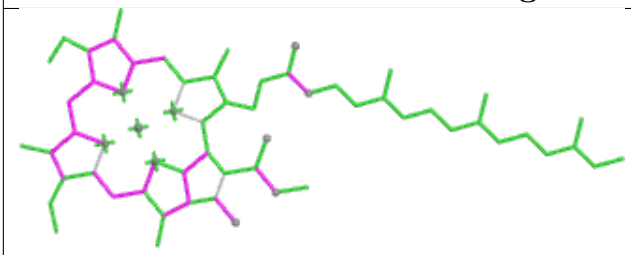


Torsions

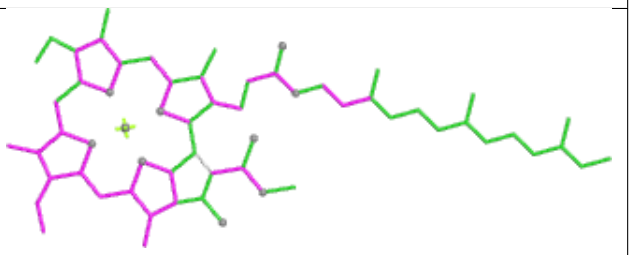


Rings

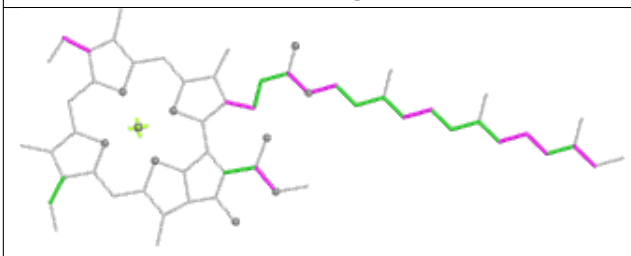
Ligand CLA 16 307



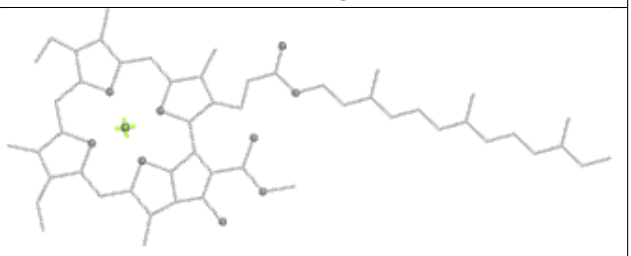
Bond lengths



Bond angles

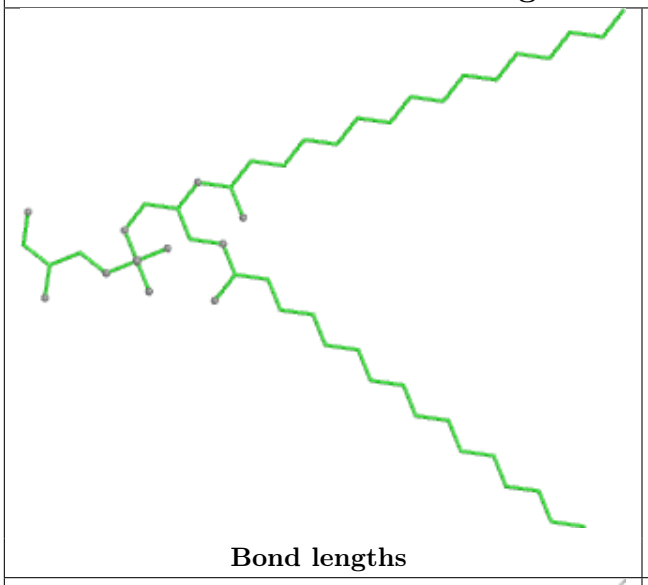


Torsions

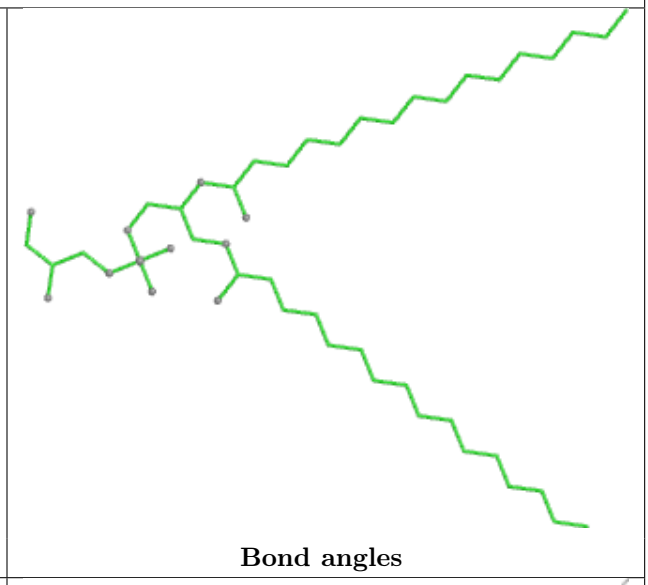


Rings

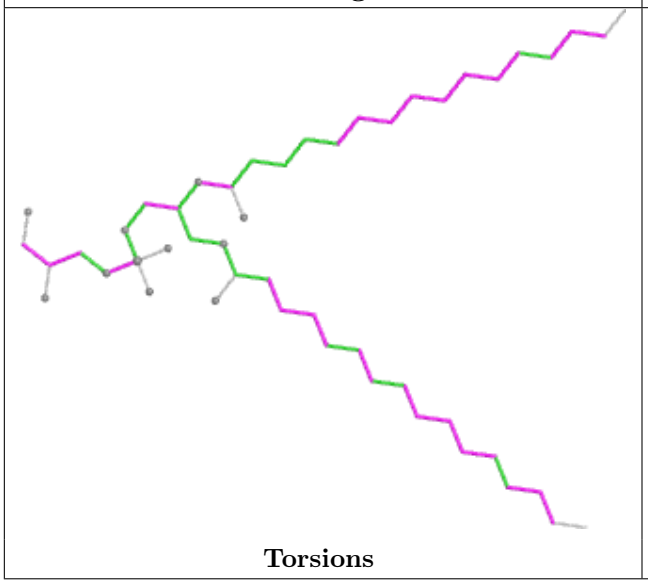
Ligand LHG 19 314



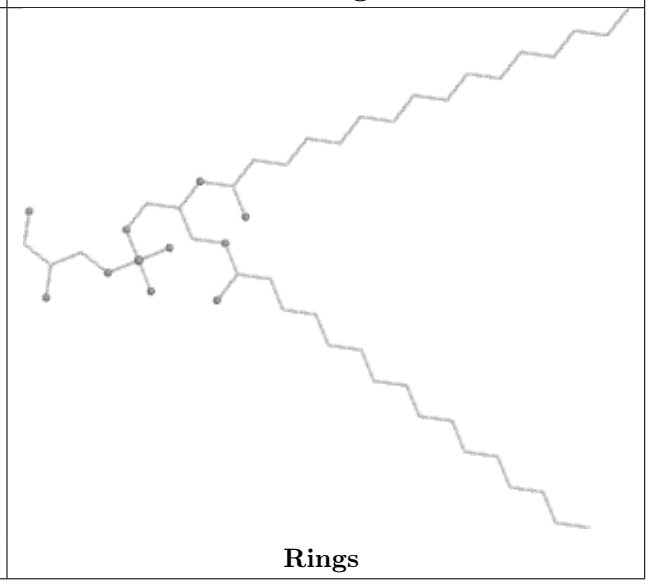
Bond lengths



Bond angles

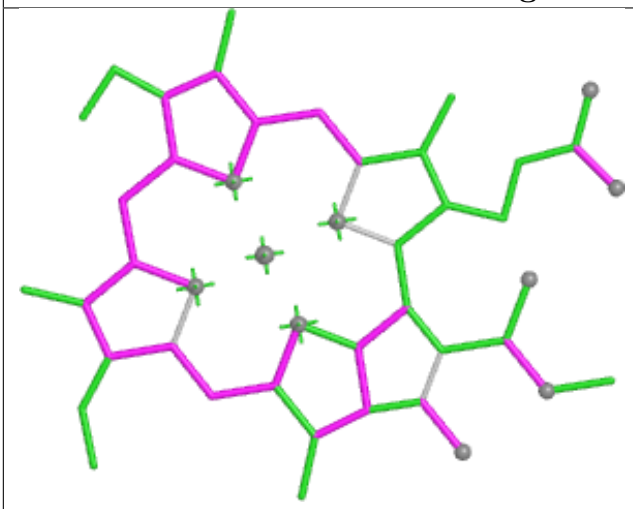


Torsions

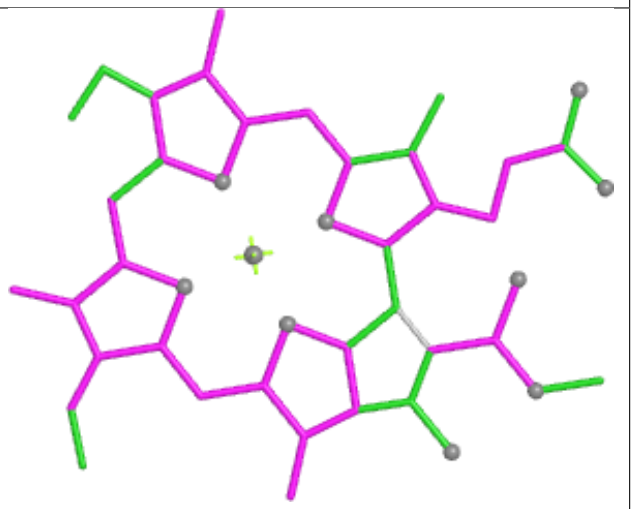


Rings

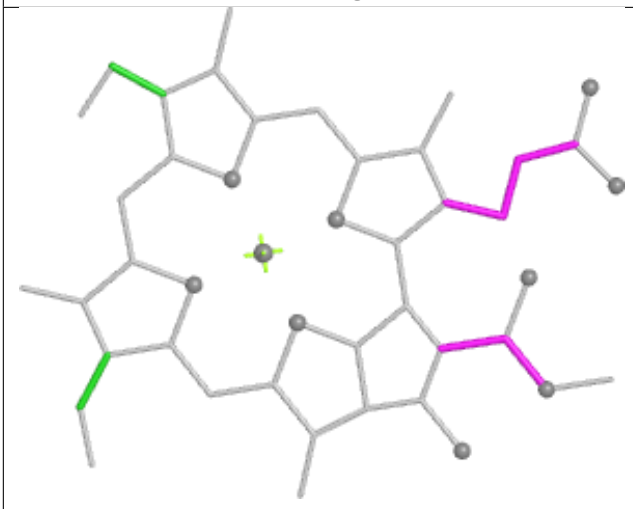
Ligand CLA 36 309



Bond lengths



Bond angles

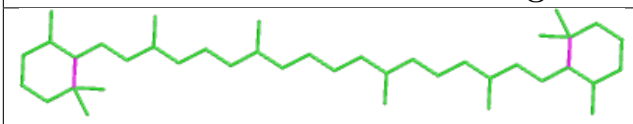


Torsions

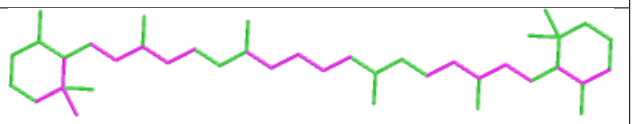


Rings

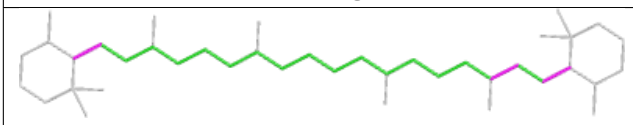
Ligand BCR c 514



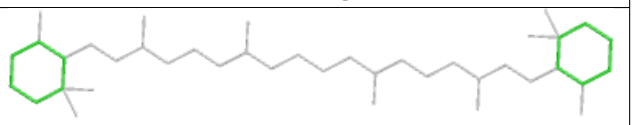
Bond lengths



Bond angles

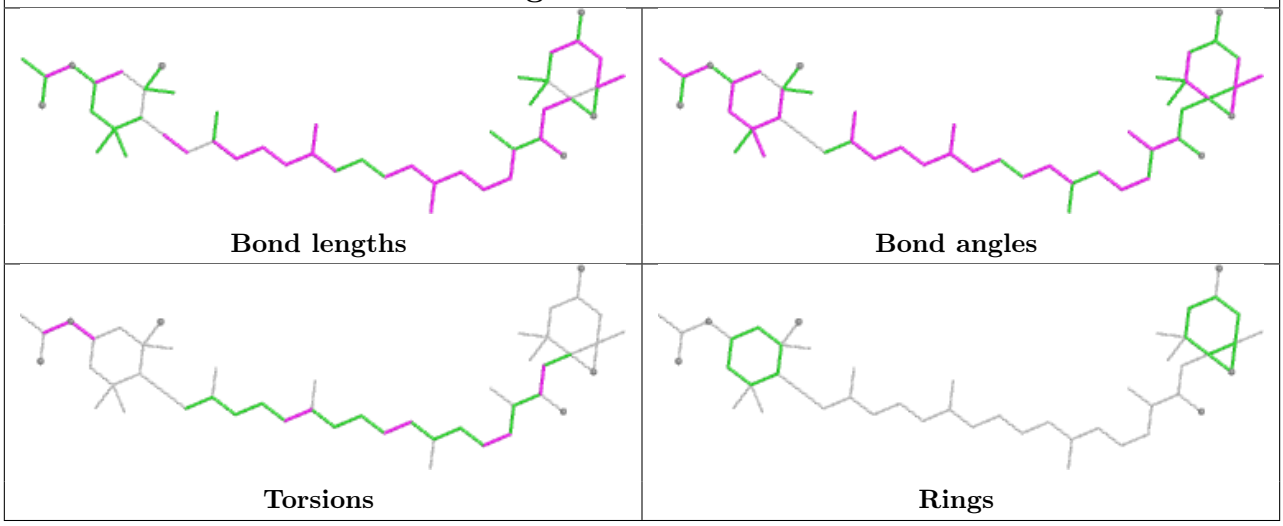


Torsions

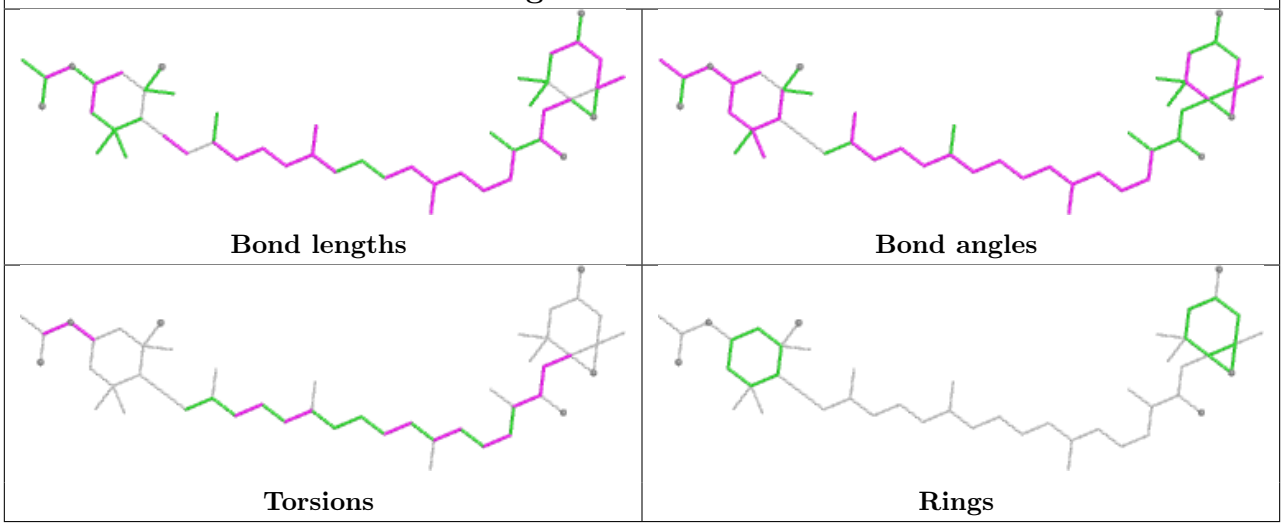


Rings

Ligand A86 21 213



Ligand A86 13 313



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

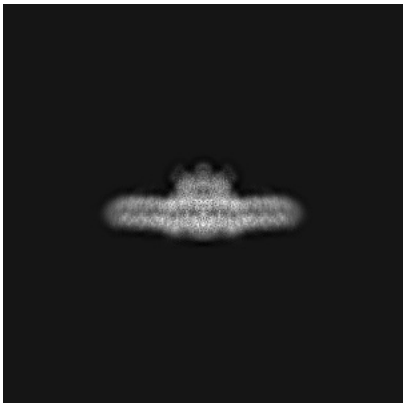
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-31905. These allow visual inspection of the internal detail of the map and identification of artifacts.

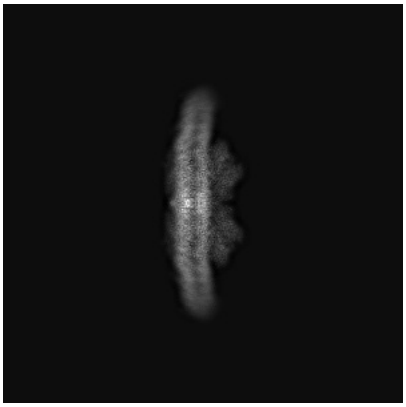
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

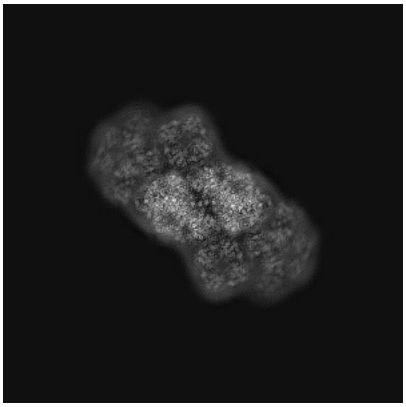
6.1.1 Primary map



X



Y

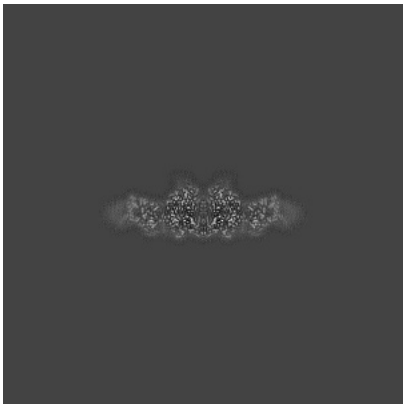


Z

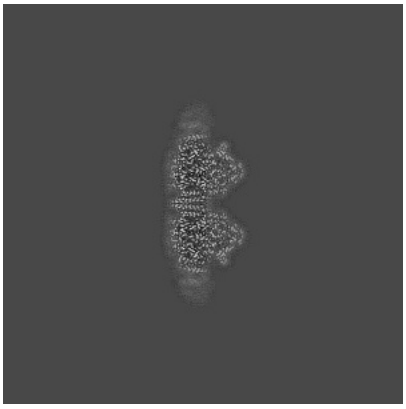
The images above show the map projected in three orthogonal directions.

6.2 Central slices

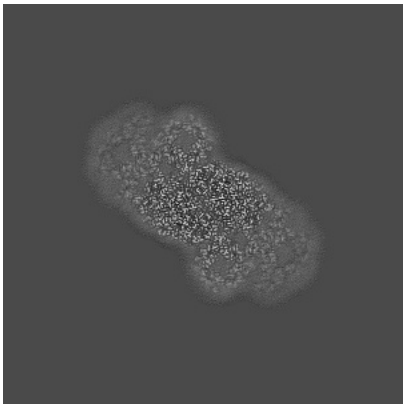
6.2.1 Primary map



X Index: 256



Y Index: 256



Z Index: 256

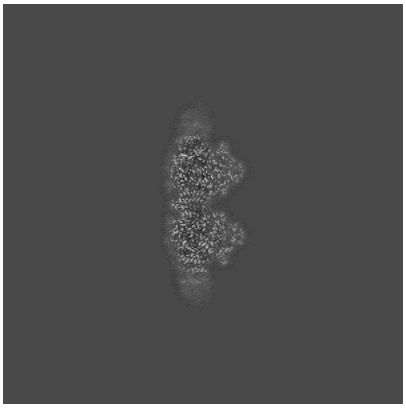
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

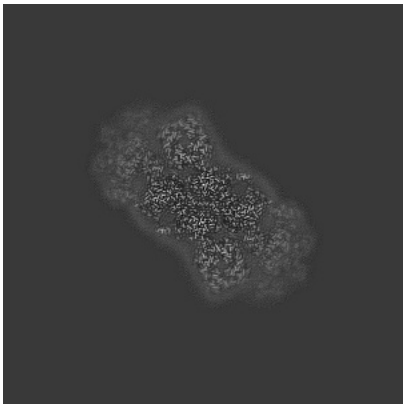
6.3.1 Primary map



X Index: 252



Y Index: 257

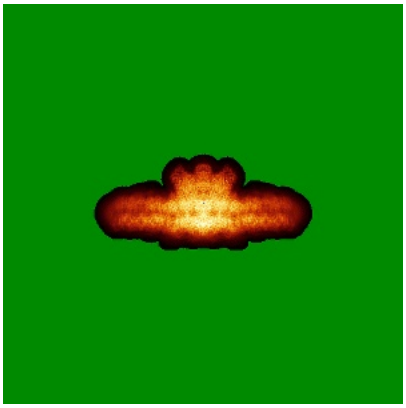


Z Index: 234

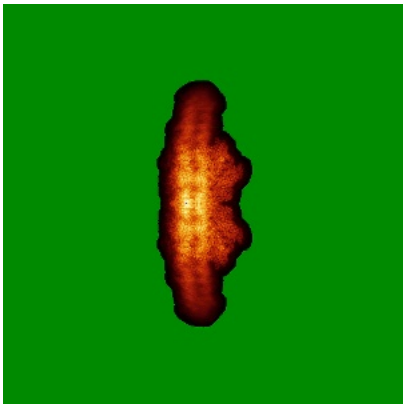
The images above show the largest variance slices of the map in three orthogonal directions.

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

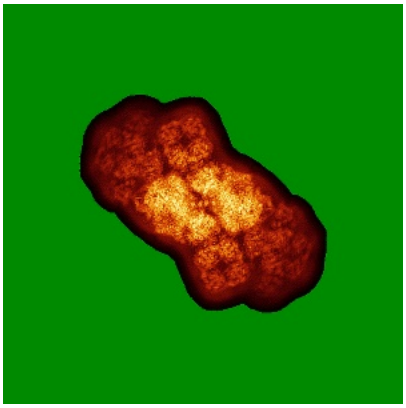
6.4.1 Primary map



X



Y



Z

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 0.045. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

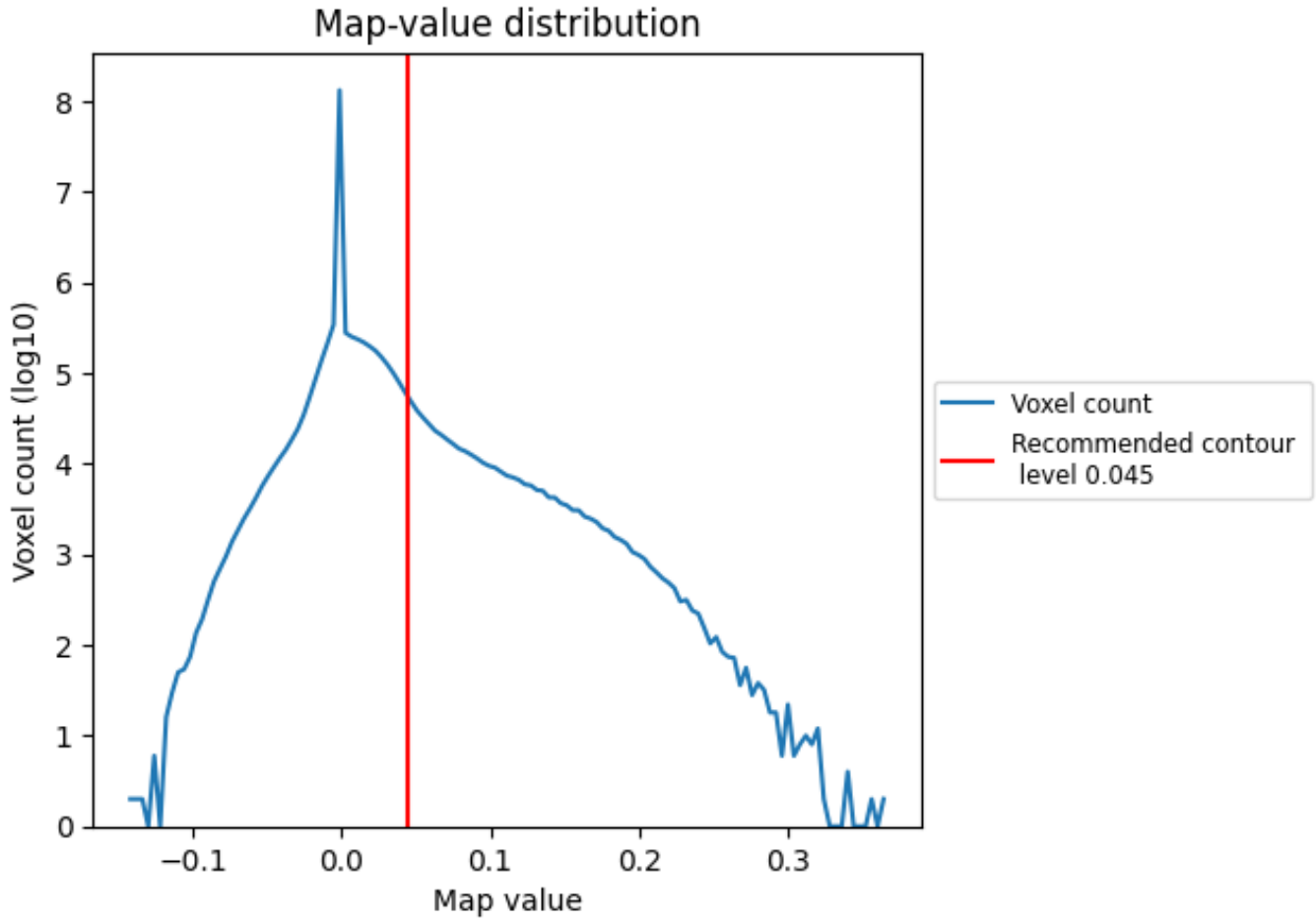
6.6 Mask visualisation (i)

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

7 Map analysis

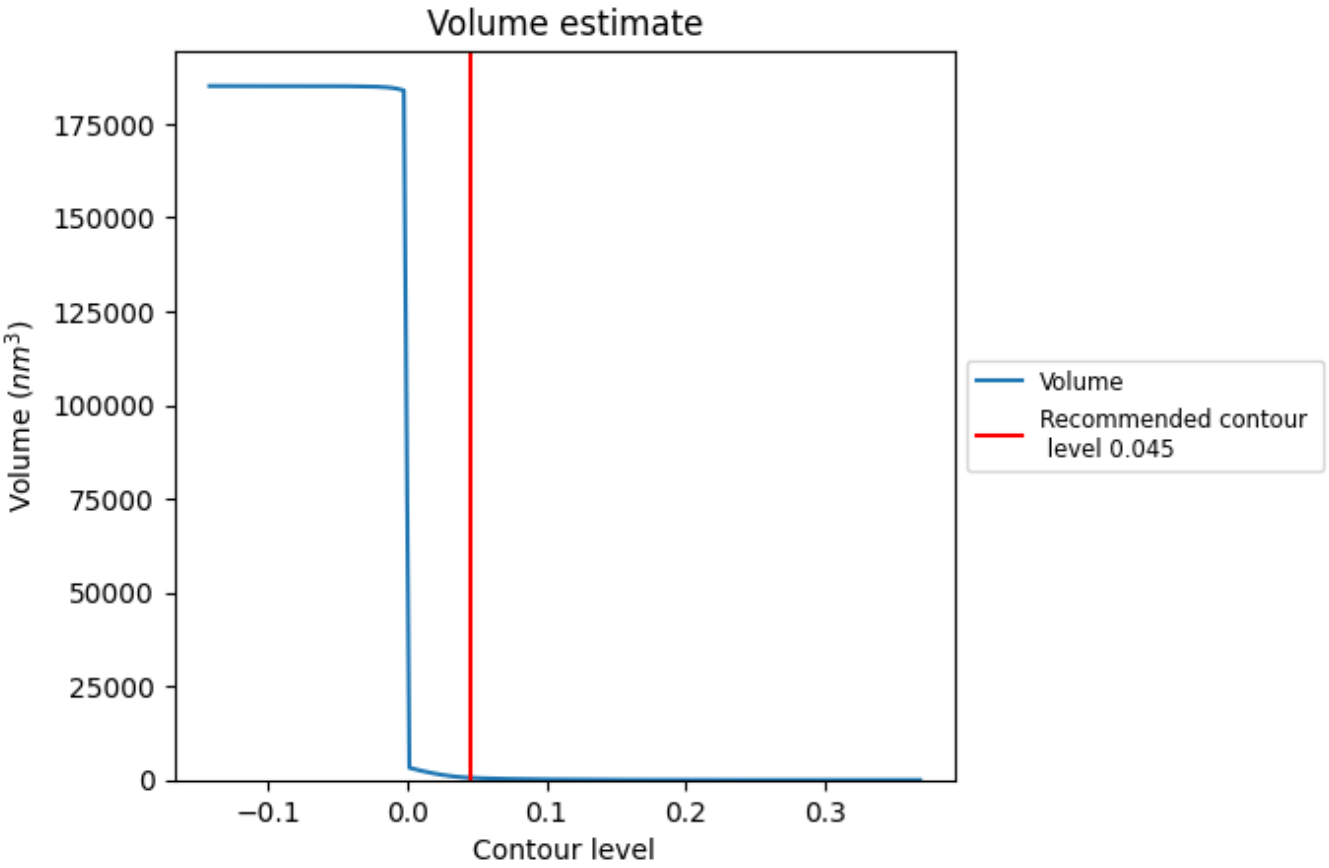
This section contains the results of statistical analysis of the map.

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.

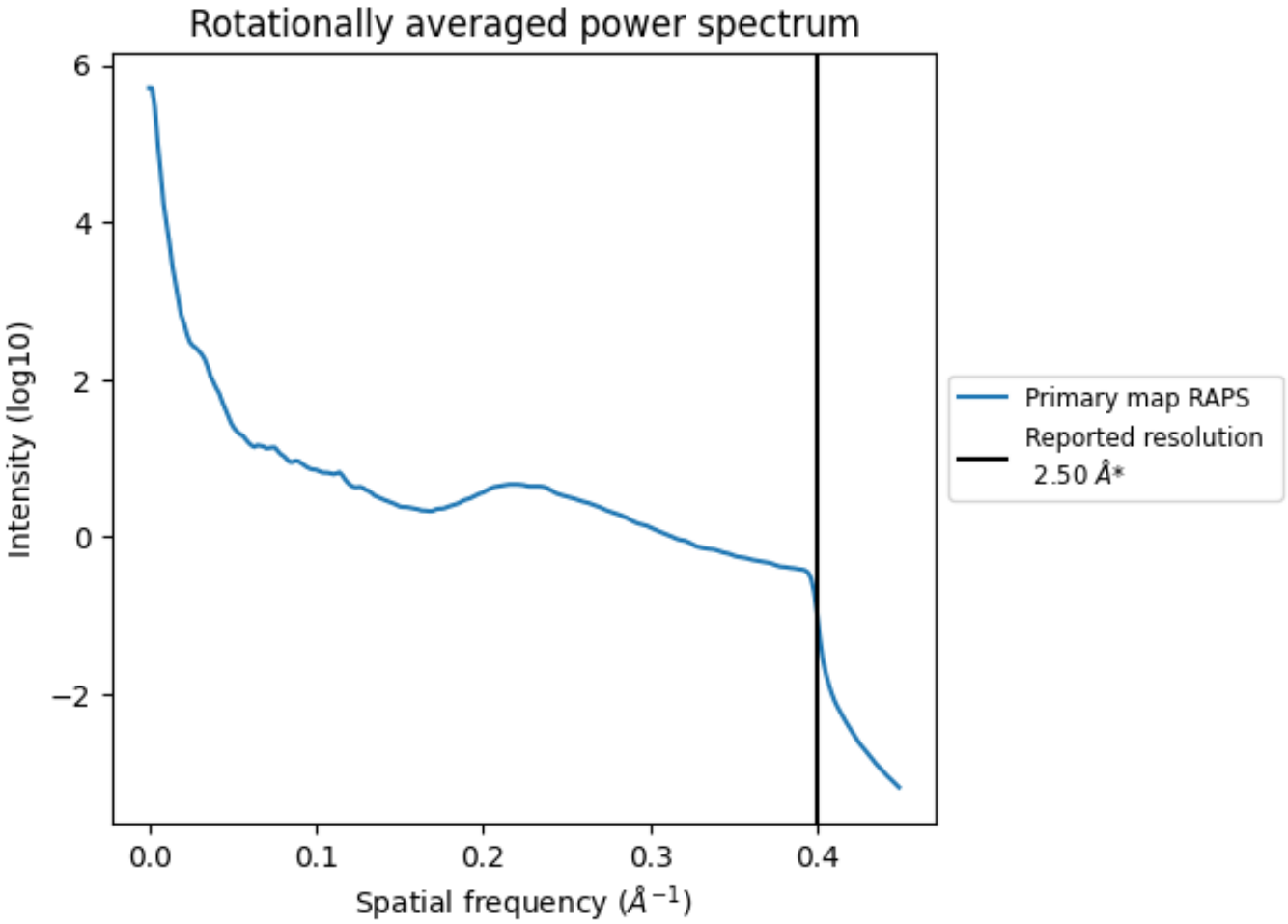
7.2 Volume estimate



The volume at the recommended contour level is 588 nm^3; this corresponds to an approximate mass of 532 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)

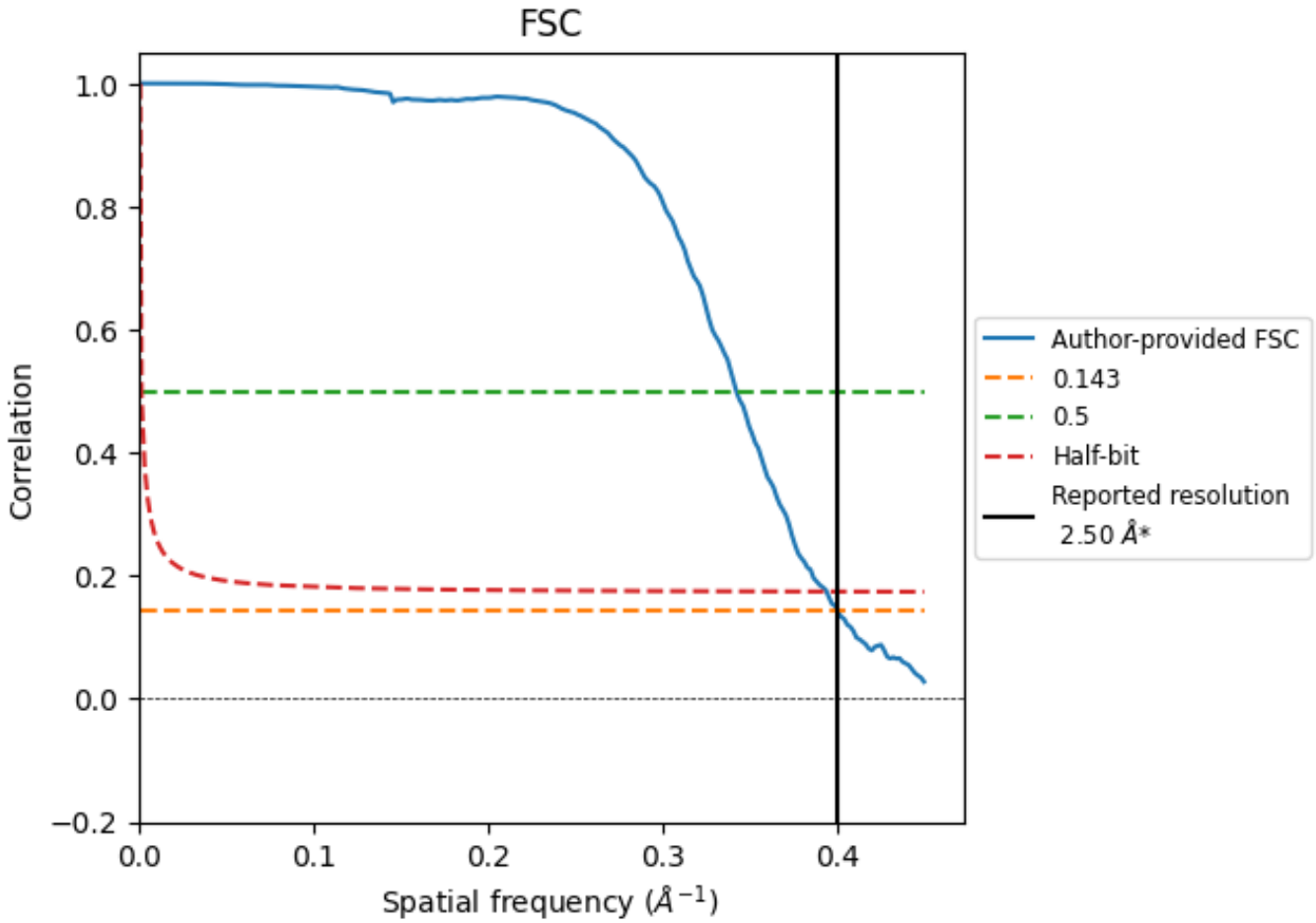


*Reported resolution corresponds to spatial frequency of 0.400 Å^{-1}

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 0.400 Å^{-1}

8.2 Resolution estimates (i)

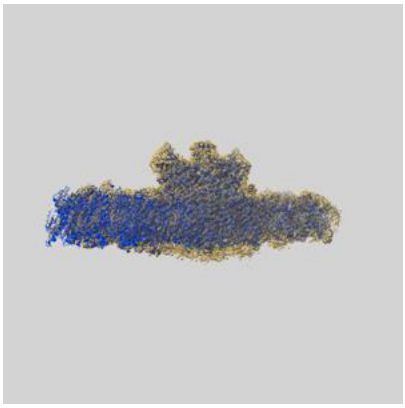
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.50	2.92	2.54
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

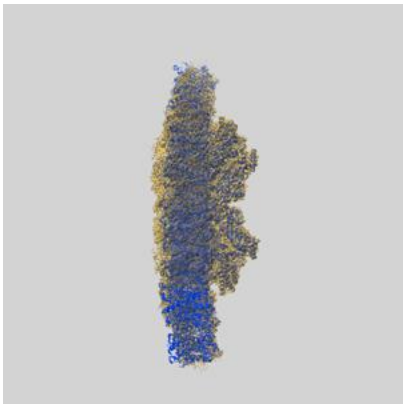
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-31905 and PDB model 7VD5. Per-residue inclusion information can be found in section 3 on page 48.

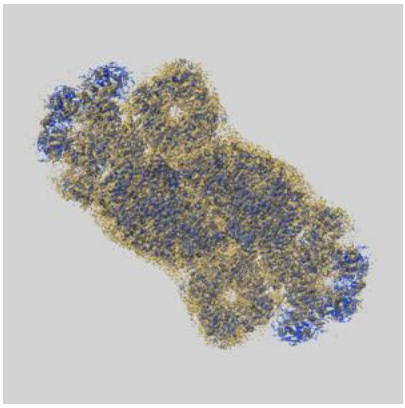
9.1 Map-model overlay



X



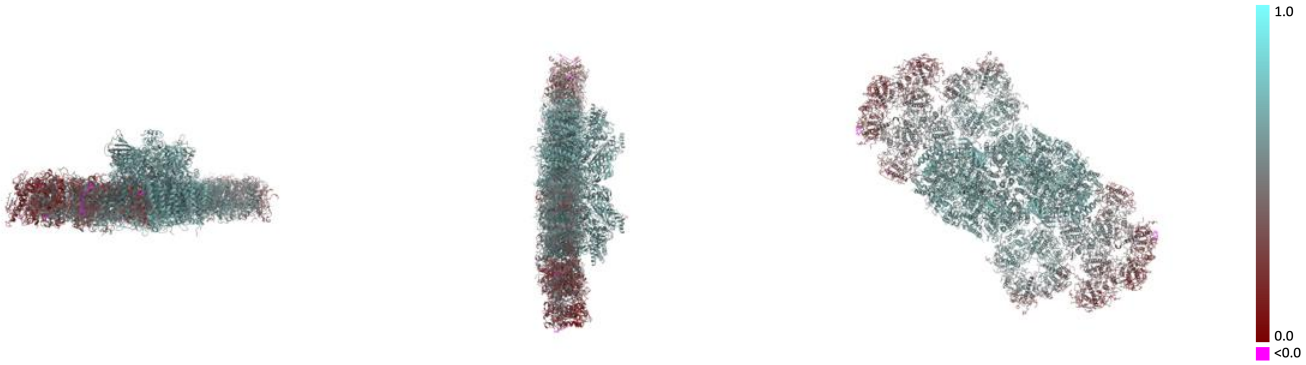
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.045 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.

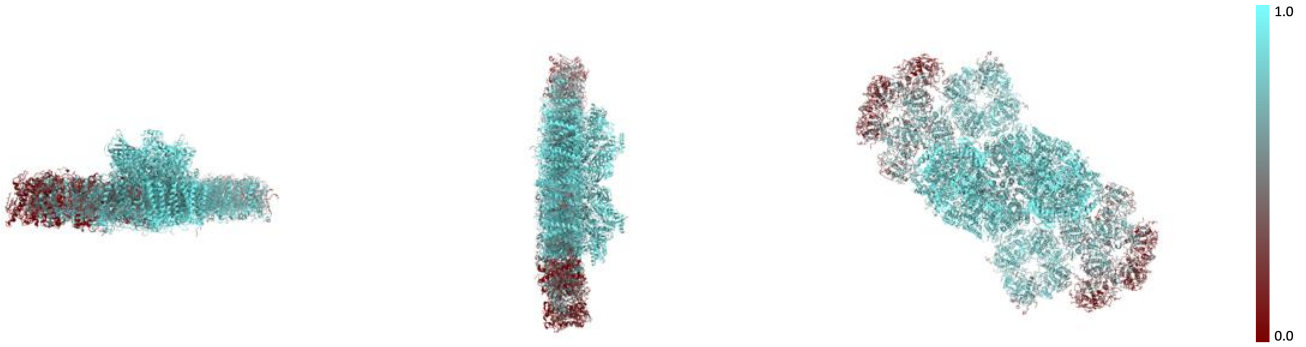
9.2 Q-score mapped to coordinate model



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.

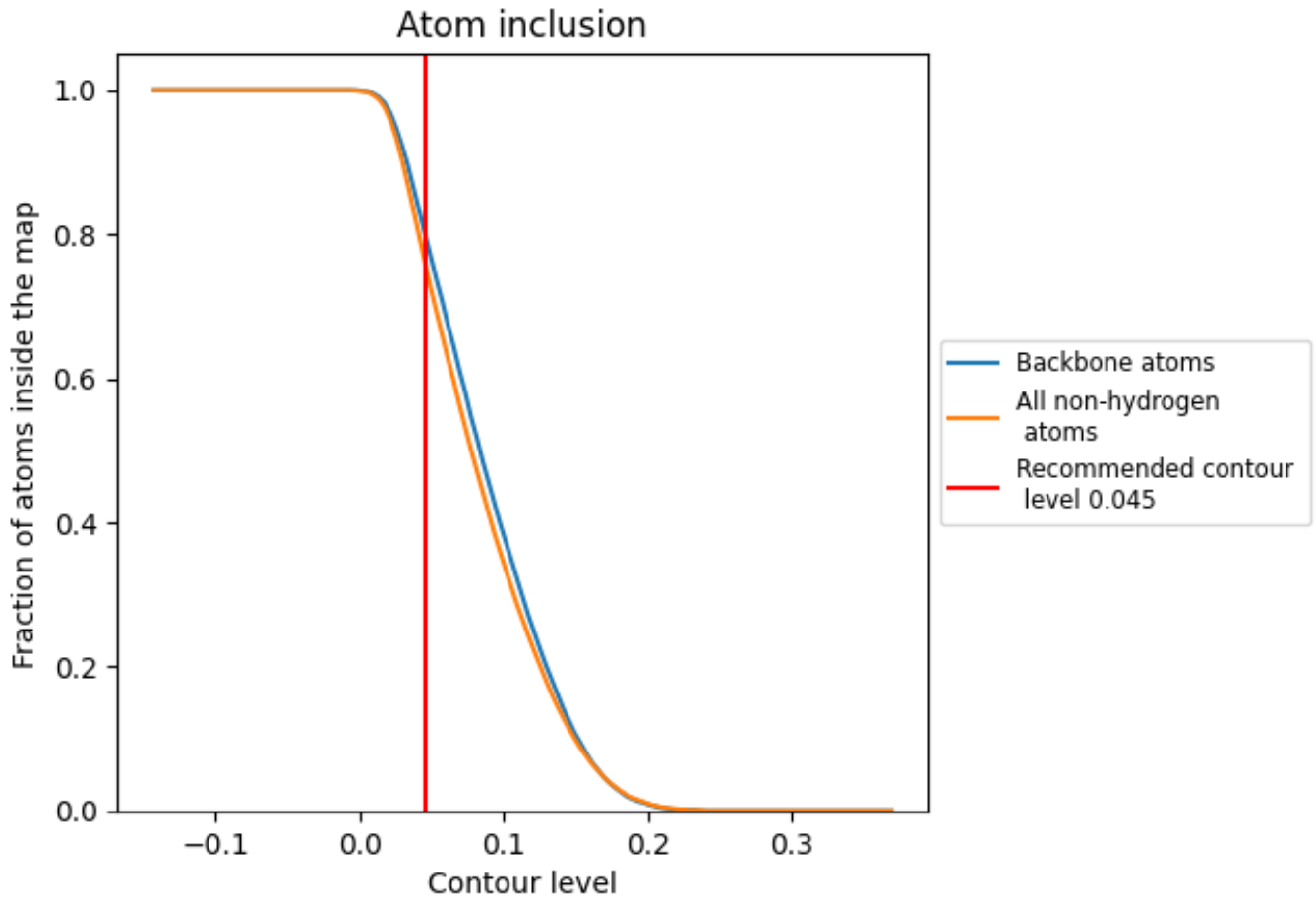
9.3 Atom inclusion mapped to coordinate model



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 (0.045).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 76% 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 (0.045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7640	0.5430
0	0.9590	0.6360
1	0.9330	0.6130
11	0.8820	0.6000
12	0.8680	0.5780
13	0.7230	0.4570
14	0.7450	0.4800
15	0.2430	0.2840
16	0.6780	0.4740
17	0.5850	0.4350
18	0.2380	0.2830
19	0.7830	0.5510
20	0.5020	0.3420
21	0.1260	0.2530
31	0.8690	0.5900
32	0.8710	0.5790
33	0.7220	0.4550
34	0.7460	0.4770
35	0.2400	0.2850
36	0.6890	0.4790
37	0.5830	0.4360
38	0.2400	0.2860
39	0.7830	0.5490
40	0.4820	0.3370
41	0.1300	0.2520
5	0.9590	0.6400
6	0.9330	0.6080
A	0.9630	0.6690
B	0.9350	0.6540
C	0.9440	0.6550
D	0.9420	0.6620
E	0.9020	0.6110
F	0.9200	0.5950
H	0.9340	0.6390
I	0.9540	0.6560



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
J	0.8940	0.6380
K	0.9200	0.6260
L	0.8900	0.6400
M	0.8590	0.6400
O	0.8830	0.6120
Q	0.8670	0.5980
T	0.9100	0.6520
U	0.9070	0.6120
V	0.9320	0.6200
W	0.8070	0.5830
X	0.8380	0.5580
Y	0.8270	0.5920
Z	0.8640	0.5670
a	0.9630	0.6680
b	0.9370	0.6550
c	0.9430	0.6530
d	0.9390	0.6610
e	0.8920	0.6110
f	0.9200	0.5950
h	0.9390	0.6350
i	0.9540	0.6570
j	0.8870	0.6360
k	0.9360	0.6190
l	0.9480	0.6530
m	0.8630	0.6410
o	0.8870	0.6120
q	0.8730	0.6000
t	0.9100	0.6570
u	0.9070	0.6140
v	0.9300	0.6220
w	0.8520	0.6140
x	0.8220	0.5620
y	0.8410	0.6050
z	0.8720	0.5650