wwPDB EM Validation Summary Report (i)

Sep 9, 2026 – 02:55 PM JST

PDB ID	:	5XNL / pdb_00005xnl
EMDB ID	:	EMD-6741
Title	:	Structure of stacked C2S2M2-type PSII-LHCII supercomplex from Pisum sativum
Authors	:	Su, X.D.; Ma, J.; Wei, X.P.; Cao, P.; Zhu, D.J.; Chang, W.R.; Liu, Z.F.; Zhang, X.Z.; Li, M.
Deposited on	:	2017-05-23
Resolution	:	2.70 Å(reported)

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

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

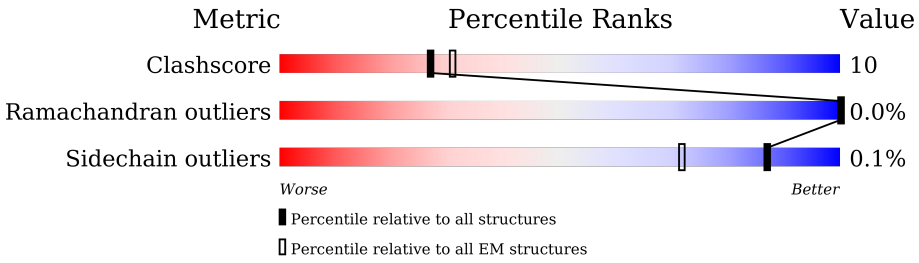
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

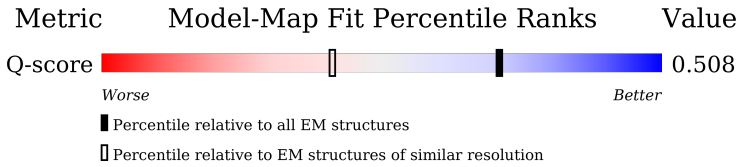
1 Overall quality at a glance

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

The reported resolution of this entry is 2.70 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	10327 (2.20 - 3.20)

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

Mol	Chain	Length	Quality of chain
1	1	232	93% 80% 14% 6%
1	2	232	94% 80% 14% 6%
1	5	232	94% 81% 13% 6%
1	6	232	94% 80% 13% 6%

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Mol	Chain	Length	Quality of chain
1	G	232	27% 76% 18% 6%
1	N	232	18% 80% 14% 6%
1	Y	232	5% 75% 18% 6%
1	g	232	26% 77% 17% 6%
1	n	232	18% 81% 13% 6%
1	y	232	5% 75% 19% 6%
2	3	243	91% 75% 16% 9%
2	7	243	91% 75% 15% 9%
3	4	210	92% 80% 13% 6%
3	8	210	92% 79% 15% 6%
4	A	344	71% 26%
4	a	344	71% 26%
5	B	507	7% 82% 17%
5	b	507	7% 81% 18%
6	C	473	75% 19% 5%
6	c	473	76% 19% 5%
7	D	353	74% 22%
7	d	353	75% 21%
8	E	83	6% 81% 10% 10%
8	e	83	6% 81% 10% 10%
9	F	39	5% 67% 10% 23%
9	f	39	5% 67% 10% 23%
10	H	73	5% 66% 16% 18%
10	h	73	5% 66% 16% 18%
11	I	36	78% 17% 6%

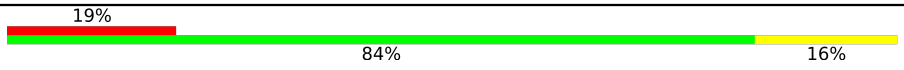
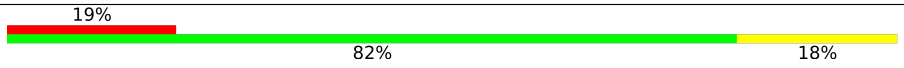
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Mol	Chain	Length	Quality of chain
11	i	36	78% 17% 6%
12	J	40	8% 78% 10% 12%
12	j	40	8% 78% 10% 12%
13	K	61	8% 49% 11% 39%
13	k	61	8% 51% 10% 39%
14	L	38	11% 68% 26%
14	l	38	11% 71% 24%
15	M	34	18% 79% 18%
15	m	34	18% 79% 18%
16	O	248	14% 79% 21%
16	o	248	13% 78% 22%
17	P	186	19% 83% 17%
17	p	186	19% 82% 18%
18	Q	148	85% 73% 14% 13%
18	q	148	84% 72% 15% 13%
19	R	246	21% 75% 20% 5%
19	r	246	21% 76% 20% 5%
20	S	244	32% 74% 15% 11%
20	s	244	32% 73% 16% 11%
21	T	35	6% 74% 17% 9%
21	t	35	6% 74% 17% 9%
22	W	54	11% 89% 11%
22	w	54	11% 89% 11%
23	X	86	10% 35% 10% 55%
23	x	86	10% 35% 10% 55%

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Mol	Chain	Length	Quality of chain
24	Z	62	
24	z	62	

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
25	CHL	1	607	X	-	-	-
25	CHL	1	609	X	-	-	-
25	CHL	2	607	X	-	-	-
25	CHL	2	609	X	-	-	-
25	CHL	3	601	X	-	-	-
25	CHL	3	609	X	-	-	-
25	CHL	5	607	X	-	-	-
25	CHL	5	609	X	-	-	-
25	CHL	6	607	X	-	-	-
25	CHL	6	609	X	-	-	-
25	CHL	7	601	X	-	-	-
25	CHL	7	609	X	-	-	-
25	CHL	G	601	X	-	-	-
25	CHL	G	607	X	-	-	-
25	CHL	G	608	X	-	-	-
25	CHL	G	609	X	-	-	-
25	CHL	N	601	X	-	-	-
25	CHL	N	607	X	-	-	-
25	CHL	N	608	X	-	-	-
25	CHL	N	609	X	-	-	-
25	CHL	R	606	X	-	-	-
25	CHL	R	607	X	-	-	-
25	CHL	R	608	X	-	-	-
25	CHL	S	607	X	-	-	-
25	CHL	Y	601	X	-	-	-
25	CHL	Y	607	X	-	-	-
25	CHL	Y	608	X	-	-	-
25	CHL	Y	609	X	-	-	-
25	CHL	g	601	X	-	-	-
25	CHL	g	607	X	-	-	-
25	CHL	g	608	X	-	-	-
25	CHL	g	609	X	-	-	-
25	CHL	n	601	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CHL	n	607	X	-	-	-
25	CHL	n	608	X	-	-	-
25	CHL	n	609	X	-	-	-
25	CHL	r	606	X	-	-	-
25	CHL	r	607	X	-	-	-
25	CHL	r	608	X	-	-	-
25	CHL	s	607	X	-	-	-
25	CHL	y	601	X	-	-	-
25	CHL	y	607	X	-	-	-
25	CHL	y	608	X	-	-	-
25	CHL	y	609	X	-	-	-

2 Entry composition (i)

There are 42 unique types of molecules in this entry. The entry contains 98986 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 Chlorophyll a-b binding protein 8, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		
1	2	218	Total	C	N	O	S	0	0
			1664	1079	269	311	5		
1	G	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		
1	N	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		
1	Y	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		
1	5	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		
1	6	218	Total	C	N	O	S	0	0
			1664	1079	269	311	5		
1	g	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		
1	n	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		
1	y	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		

- Molecule 2 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	220	Total	C	N	O	S	0	0
			1707	1116	277	309	5		
2	7	220	Total	C	N	O	S	0	0
			1707	1116	277	309	5		

- Molecule 3 is a protein called Light harvesting chlorophyll a/b-binding protein Lhcb6, CP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	197	Total	C	N	O	S	0	0
			1534	1009	247	274	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	8	197	Total 1534	C 1009	N 247	O 274	S 4	0	0

- Molecule 4 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	334	Total 2616	C 1708	N 431	O 464	S 13	0	0
4	a	334	Total 2616	C 1708	N 431	O 464	S 13	0	0

- Molecule 5 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	503	Total 3948	C 2581	N 669	O 686	S 12	0	0
5	b	503	Total 3948	C 2581	N 669	O 686	S 12	0	0

- Molecule 6 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	450	Total 3497	C 2300	N 583	O 604	S 10	0	0
6	c	450	Total 3497	C 2300	N 583	O 604	S 10	0	0

- Molecule 7 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	341	Total 2712	C 1790	N 444	O 466	S 12	0	0
7	d	341	Total 2712	C 1790	N 444	O 466	S 12	0	0

- Molecule 8 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	E	75	Total 612	C 400	N 100	O 112	0	0
8	e	75	Total 612	C 400	N 100	O 112	0	0

- Molecule 9 is a protein called Cytochrome b559 subunit beta, PsbF.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	30	Total	C	N	O	S	0	0
			241	162	41	37	1		
9	f	30	Total	C	N	O	S	0	0
			241	162	41	37	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	60	Total	C	N	O	S	0	0
			452	296	72	81	3		
10	h	60	Total	C	N	O	S	0	0
			452	296	72	81	3		

- Molecule 11 is a protein called Photosystem II reaction center protein I, PsbI.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	34	Total	C	N	O	S	0	0
			278	191	43	43	1		
11	i	34	Total	C	N	O	S	0	0
			278	191	43	43	1		

- Molecule 12 is a protein called Photosystem II reaction center protein J.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	J	35	Total	C	N	O	0	0
			256	174	39	43		
12	j	35	Total	C	N	O	0	0
			256	174	39	43		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	K	37	Total	C	N	O	S	0	0
			306	215	44	46	1		
13	k	37	Total	C	N	O	S	0	0
			306	215	44	46	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
14	L	37	Total 311	C 205	N 49	O 57	0	0
14	l	37	Total 311	C 205	N 49	O 57	0	0

- Molecule 15 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	M	33	Total 256	C 176	N 36	O 43	S 1	0	0
15	m	33	Total 256	C 176	N 36	O 43	S 1	0	0

- Molecule 16 is a protein called Oxygen-evolving enhancer protein 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	248	Total 1870	C 1179	N 306	O 382	S 3	0	0
16	o	248	Total 1870	C 1179	N 306	O 382	S 3	0	0

- Molecule 17 is a protein called Oxygen-evolving enhancer protein 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	186	Total 1434	C 909	N 238	O 286	S 1	0	0
17	p	186	Total 1434	C 909	N 238	O 286	S 1	0	0

- Molecule 18 is a protein called Oxygen-evolving enhancer protein 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	Q	129	Total 1034	C 661	N 177	O 196	0	0
18	q	129	Total 1034	C 661	N 177	O 196	0	0

- Molecule 19 is a protein called Light harvesting chlorophyll a/b-binding protein Lhcb4, CP29.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	R	234	Total 1835	C 1194	N 297	O 341	S 3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
19	r	234	Total	C	N	O	S	0	0
			1835	1194	297	341	3		

- Molecule 20 is a protein called Light harvesting chlorophyll a/b-binding protein Lhcb5, CP26.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	218	Total	C	N	O	S	0	0
			1689	1107	273	305	4		
20	s	218	Total	C	N	O	S	0	0
			1689	1107	273	305	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	T	32	Total	C	N	O	S	0	0
			261	182	37	41	1		
21	t	32	Total	C	N	O	S	0	0
			261	182	37	41	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	54	Total	C	N	O	S	0	0
			419	275	61	82	1		
22	w	54	Total	C	N	O	S	0	0
			419	275	61	82	1		

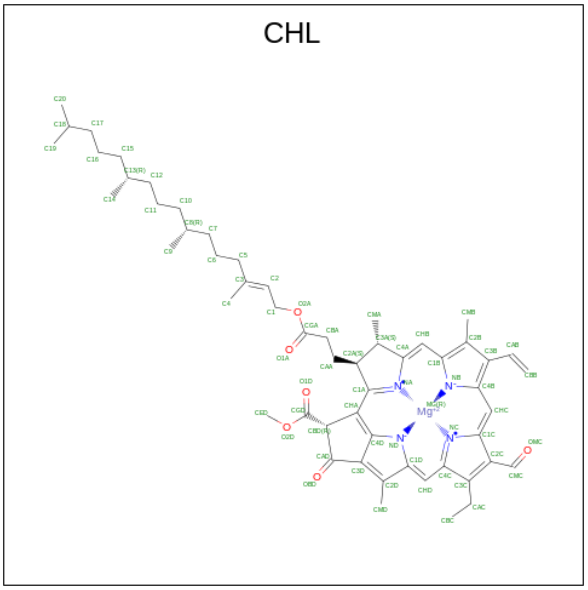
- Molecule 23 is a protein called Photosystem II reaction center protein X.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	X	39	Total	C	N	O	0	0
			276	180	46	50		
23	x	39	Total	C	N	O	0	0
			276	180	46	50		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Z	62	Total	C	N	O	S	0	0
			464	312	69	82	1		
24	z	62	Total	C	N	O	S	0	0
			464	312	69	82	1		

- Molecule 25 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
25	1	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	1	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	1	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	1	1	Total	C	Mg	N	O	0
			63	52	1	4	6	
25	1	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	1	1	Total	C	Mg	N	O	0
			62	51	1	4	6	
25	2	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	2	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	2	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	2	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
25	2	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	2	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
25	3	1	Total	C	Mg	N	O	0
			64	53	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
25	3	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	3	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	3	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
25	3	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	3	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
25	4	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
25	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
25	G	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	G	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
25	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
25	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
25	G	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
25	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
25	N	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
25	N	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
25	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
25	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
25	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
25	R	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
25	R	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
25	R	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
25	R	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
25	S	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	S	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	S	1	Total	C	Mg	N	O	0
			58	47	1	4	6	
25	S	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
25	Y	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
25	Y	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
25	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
25	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
25	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
25	5	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	5	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	5	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	5	1	Total	C	Mg	N	O	0
			63	52	1	4	6	
25	5	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	5	1	Total	C	Mg	N	O	0
			62	51	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
25	6	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	6	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	6	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	6	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
25	6	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	6	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
25	7	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
25	7	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	7	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	7	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
25	7	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	7	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
25	8	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
25	8	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	8	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	8	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	8	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	g	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
25	g	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	g	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
25	g	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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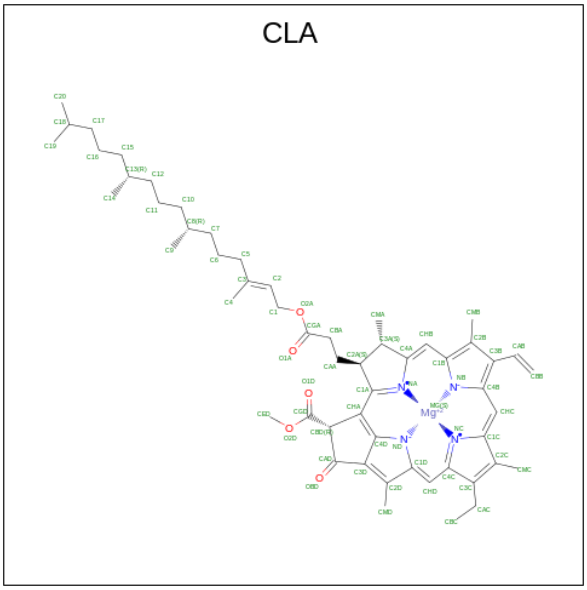
Mol	Chain	Residues	Atoms					AltConf
25	g	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
25	g	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
25	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
25	n	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
25	n	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
25	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
25	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
25	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
25	r	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
25	r	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
25	r	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
25	r	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
25	s	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	s	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	s	1	Total	C	Mg	N	O	0
			58	47	1	4	6	
25	s	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
25	y	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
25	y	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
25	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
25	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
25	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 26 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
26	1	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
26	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
26	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
26	1	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
26	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
26	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	2	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
26	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
26	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
26	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
26	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
26	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	3	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
26	3	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
26	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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

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Mol	Chain	Residues	Atoms					AltConf
26	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
26	G	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
26	G	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	G	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	G	1	Total	C	Mg	N	O	0
			48	38	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
26	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	N	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
26	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	N	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	N	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	N	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	N	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
26	R	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	R	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	R	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	R	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
26	R	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
26	R	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	R	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	R	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	R	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	S	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
26	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	S	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
26	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	S	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
26	S	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
26	S	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	S	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
26	S	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	Y	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
26	Y	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	Y	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	Y	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	Y	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
26	5	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
26	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
26	5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
26	5	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
26	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
26	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	6	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
26	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
26	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	6	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
26	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	7	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	7	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
26	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	7	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	7	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
26	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	7	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
26	7	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
26	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
26	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
26	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
26	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	g	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
26	g	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
26	g	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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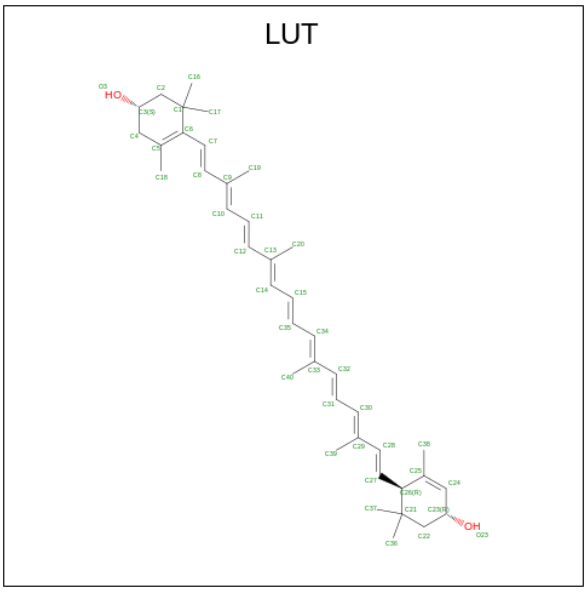
Mol	Chain	Residues	Atoms					AltConf
26	g	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	g	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
26	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	n	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
26	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	n	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	n	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	n	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	n	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
26	r	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	r	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	r	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	r	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
26	r	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
26	r	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	r	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	r	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	r	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	r	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
26	s	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
26	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	s	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
26	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	s	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
26	s	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
26	s	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	s	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
26	s	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	y	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
26	y	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	y	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	y	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	y	1	Total	C	Mg	N	O	0
			48	38	1	4	5	

- Molecule 27 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3 ,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$).



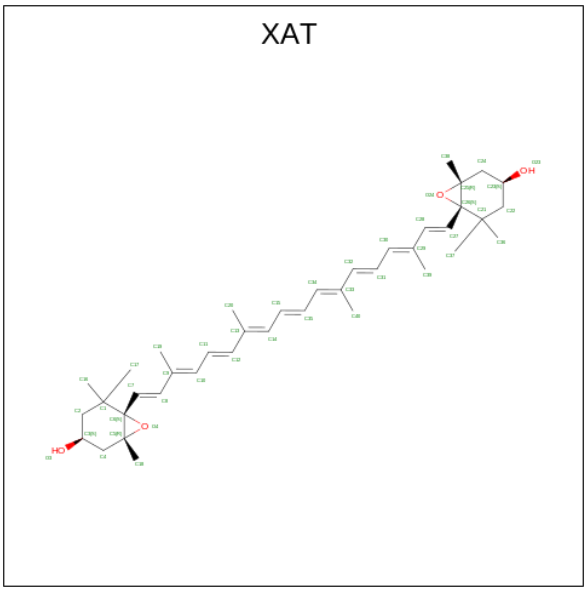
Mol	Chain	Residues	Atoms			AltConf
27	1	1	Total	C	O	0
			42	40	2	
27	1	1	Total	C	O	0
			42	40	2	
27	2	1	Total	C	O	0
			42	40	2	
27	2	1	Total	C	O	0
			42	40	2	
27	3	1	Total	C	O	0
			42	40	2	
27	3	1	Total	C	O	0
			42	40	2	
27	4	1	Total	C	O	0
			42	40	2	
27	G	1	Total	C	O	0
			42	40	2	
27	G	1	Total	C	O	0
			42	40	2	
27	N	1	Total	C	O	0
			42	40	2	
27	N	1	Total	C	O	0
			42	40	2	
27	R	1	Total	C	O	0
			42	40	2	
27	S	1	Total	C	O	0
			42	40	2	
27	S	1	Total	C	O	0
			42	40	2	

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Mol	Chain	Residues	Atoms	AltConf
27	Y	1	Total C O 42 40 2	0
27	Y	1	Total C O 42 40 2	0
27	5	1	Total C O 42 40 2	0
27	5	1	Total C O 42 40 2	0
27	6	1	Total C O 42 40 2	0
27	6	1	Total C O 42 40 2	0
27	7	1	Total C O 42 40 2	0
27	7	1	Total C O 42 40 2	0
27	8	1	Total C O 42 40 2	0
27	g	1	Total C O 42 40 2	0
27	g	1	Total C O 42 40 2	0
27	n	1	Total C O 42 40 2	0
27	n	1	Total C O 42 40 2	0
27	r	1	Total C O 42 40 2	0
27	s	1	Total C O 42 40 2	0
27	s	1	Total C O 42 40 2	0
27	y	1	Total C O 42 40 2	0
27	y	1	Total C O 42 40 2	0

- Molecule 28 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: $C_{40}H_{56}O_4$).



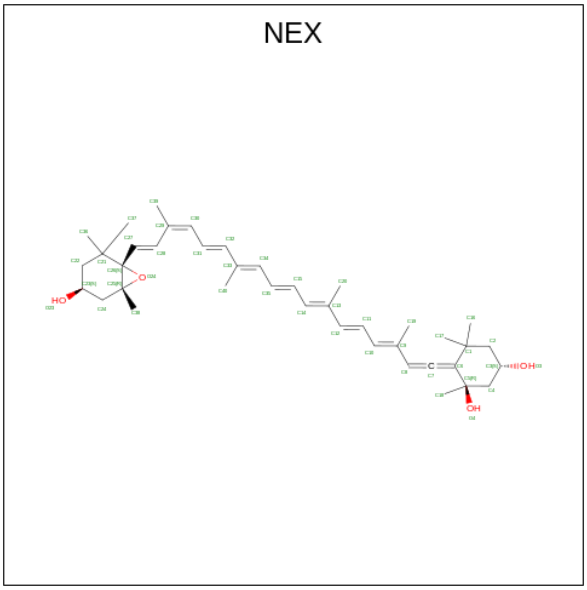
Mol	Chain	Residues	Atoms	AltConf
28	1	1	Total C O 44 40 4	0
28	2	1	Total C O 44 40 4	0
28	3	1	Total C O 44 40 4	0
28	4	1	Total C O 44 40 4	0
28	G	1	Total C O 44 40 4	0
28	N	1	Total C O 44 40 4	0
28	R	1	Total C O 44 40 4	0
28	Y	1	Total C O 44 40 4	0
28	5	1	Total C O 44 40 4	0
28	6	1	Total C O 44 40 4	0
28	7	1	Total C O 44 40 4	0
28	8	1	Total C O 44 40 4	0
28	g	1	Total C O 44 40 4	0
28	n	1	Total C O 44 40 4	0

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Mol	Chain	Residues	Atoms	AltConf
28	r	1	Total C O 44 40 4	0
28	y	1	Total C O 44 40 4	0

- Molecule 29 is (1R,3R)-6-{(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: $C_{40}H_{56}O_4$).



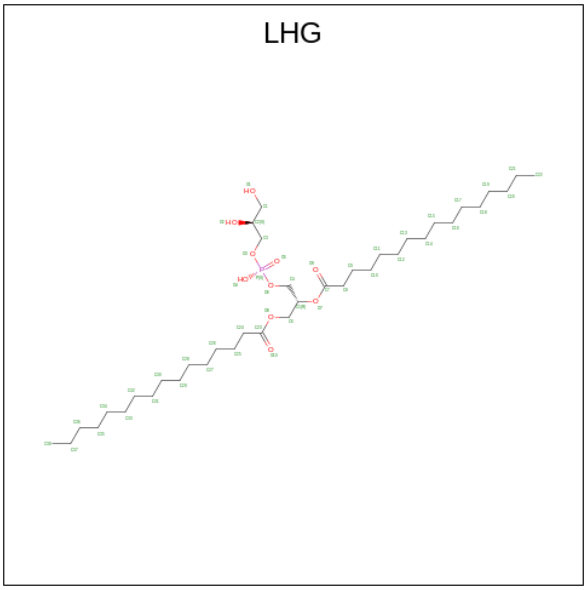
Mol	Chain	Residues	Atoms	AltConf
29	1	1	Total C O 44 40 4	0
29	2	1	Total C O 44 40 4	0
29	3	1	Total C O 44 40 4	0
29	G	1	Total C O 44 40 4	0
29	N	1	Total C O 44 40 4	0
29	R	1	Total C O 44 40 4	0
29	S	1	Total C O 44 40 4	0
29	Y	1	Total C O 44 40 4	0

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Mol	Chain	Residues	Atoms	AltConf
29	5	1	Total C O 44 40 4	0
29	6	1	Total C O 44 40 4	0
29	7	1	Total C O 44 40 4	0
29	g	1	Total C O 44 40 4	0
29	n	1	Total C O 44 40 4	0
29	r	1	Total C O 44 40 4	0
29	s	1	Total C O 44 40 4	0
29	y	1	Total C O 44 40 4	0

- Molecule 30 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms	AltConf
30	1	1	Total C O P 41 30 10 1	0
30	2	1	Total C O P 37 26 10 1	0
30	3	1	Total C O P 47 36 10 1	0

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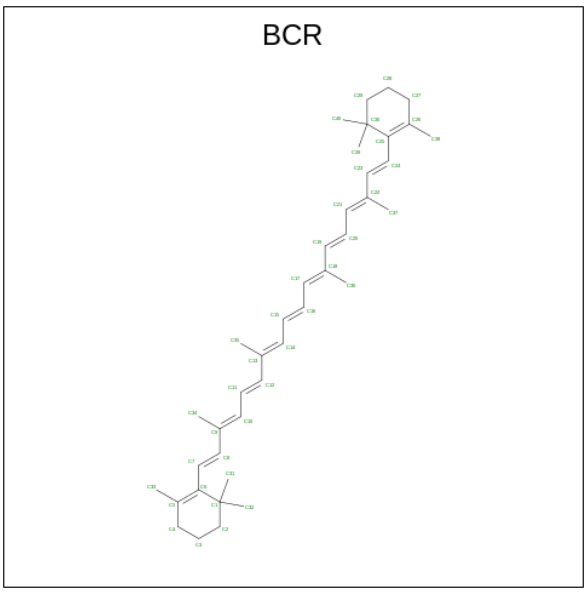
Mol	Chain	Residues	Atoms				AltConf
30	4	1	Total	C	O	P	0
			21	10	10	1	
30	B	1	Total	C	O	P	0
			47	36	10	1	
30	B	1	Total	C	O	P	0
			49	38	10	1	
30	C	1	Total	C	O	P	0
			49	38	10	1	
30	C	1	Total	C	O	P	0
			49	38	10	1	
30	C	1	Total	C	O	P	0
			49	38	10	1	
30	D	1	Total	C	O	P	0
			46	35	10	1	
30	D	1	Total	C	O	P	0
			49	38	10	1	
30	D	1	Total	C	O	P	0
			43	32	10	1	
30	G	1	Total	C	O	P	0
			49	38	10	1	
30	L	1	Total	C	O	P	0
			49	38	10	1	
30	N	1	Total	C	O	P	0
			49	38	10	1	
30	R	1	Total	C	O	P	0
			42	31	10	1	
30	S	1	Total	C	O	P	0
			49	38	10	1	
30	Y	1	Total	C	O	P	0
			49	38	10	1	
30	5	1	Total	C	O	P	0
			41	30	10	1	
30	6	1	Total	C	O	P	0
			37	26	10	1	
30	7	1	Total	C	O	P	0
			47	36	10	1	
30	8	1	Total	C	O	P	0
			21	10	10	1	
30	b	1	Total	C	O	P	0
			47	36	10	1	
30	b	1	Total	C	O	P	0
			49	38	10	1	

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Mol	Chain	Residues	Atoms				AltConf
30	c	1	Total	C	O	P	0
			49	38	10	1	
30	c	1	Total	C	O	P	0
			49	38	10	1	
30	c	1	Total	C	O	P	0
			49	38	10	1	
30	d	1	Total	C	O	P	0
			46	35	10	1	
30	d	1	Total	C	O	P	0
			49	38	10	1	
30	d	1	Total	C	O	P	0
			43	32	10	1	
30	g	1	Total	C	O	P	0
			49	38	10	1	
30	l	1	Total	C	O	P	0
			49	38	10	1	
30	n	1	Total	C	O	P	0
			49	38	10	1	
30	r	1	Total	C	O	P	0
			42	31	10	1	
30	s	1	Total	C	O	P	0
			49	38	10	1	
30	y	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 31 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



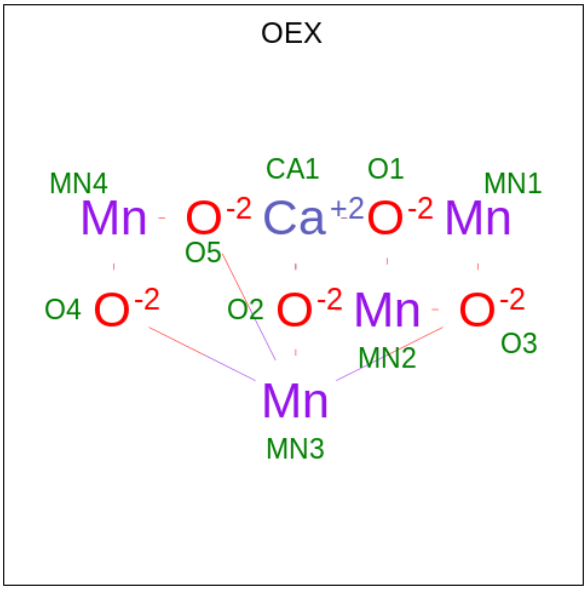
Mol	Chain	Residues	Atoms	AltConf
31	4	1	Total C 40 40	0
31	A	1	Total C 40 40	0
31	B	1	Total C 40 40	0
31	B	1	Total C 40 40	0
31	B	1	Total C 40 40	0
31	C	1	Total C 40 40	0
31	C	1	Total C 40 40	0
31	C	1	Total C 40 40	0
31	C	1	Total C 40 40	0
31	D	1	Total C 40 40	0
31	H	1	Total C 40 40	0
31	T	1	Total C 40 40	0
31	8	1	Total C 40 40	0
31	a	1	Total C 40 40	0
31	b	1	Total C 40 40	0
31	b	1	Total C 40 40	0
31	b	1	Total C 40 40	0
31	c	1	Total C 40 40	0
31	c	1	Total C 40 40	0
31	c	1	Total C 40 40	0
31	c	1	Total C 40 40	0
31	d	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
31	h	1	Total C 40 40	0
31	t	1	Total C 40 40	0

- Molecule 32 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: $CaMn_4O_5$).



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

- Molecule 33 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 34 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

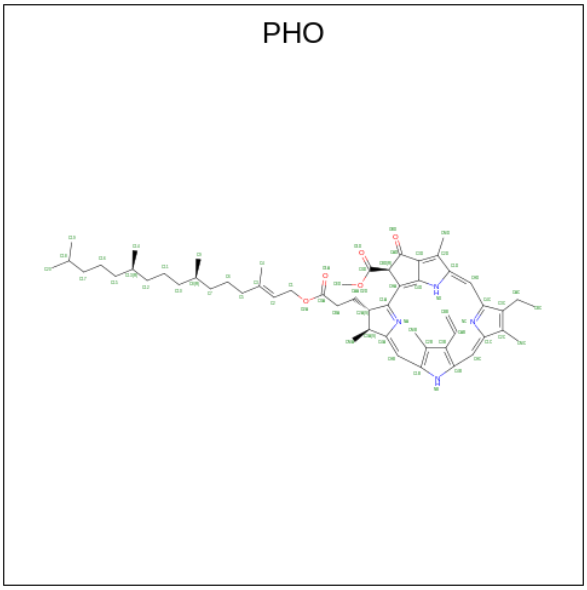
Mol	Chain	Residues	Atoms	AltConf
34	A	2	Total Cl 2 2	0

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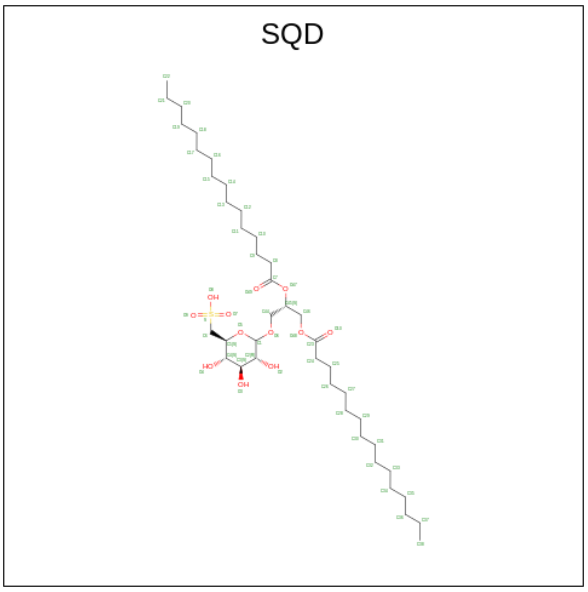
Mol	Chain	Residues	Atoms	AltConf
34	a	2	Total Cl 2 2	0

- Molecule 35 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



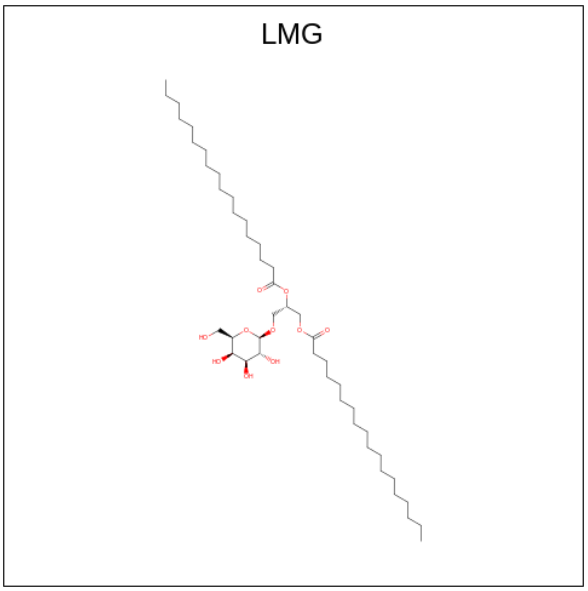
Mol	Chain	Residues	Atoms	AltConf
35	A	1	Total C N O 64 55 4 5	0
35	A	1	Total C N O 64 55 4 5	0
35	a	1	Total C N O 64 55 4 5	0
35	a	1	Total C N O 64 55 4 5	0

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



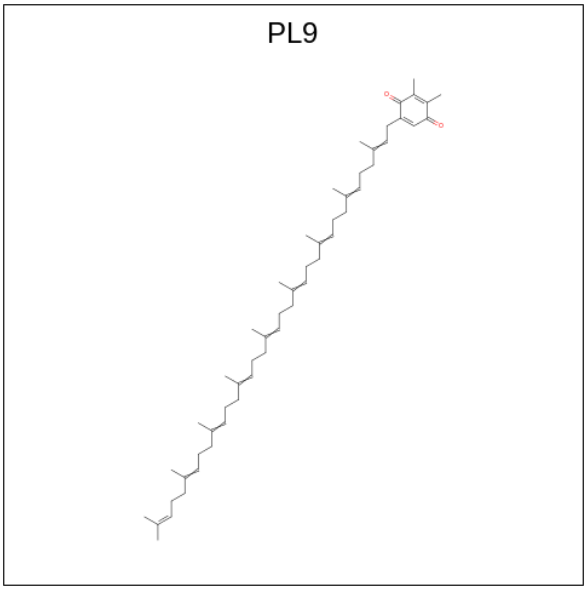
Mol	Chain	Residues	Atoms				AltConf
36	A	1	Total 50	C 37	O 12	S 1	0
36	A	1	Total 54	C 41	O 12	S 1	0
36	B	1	Total 54	C 41	O 12	S 1	0
36	B	1	Total 42	C 29	O 12	S 1	0
36	a	1	Total 50	C 37	O 12	S 1	0
36	a	1	Total 54	C 41	O 12	S 1	0
36	b	1	Total 54	C 41	O 12	S 1	0
36	b	1	Total 42	C 29	O 12	S 1	0

- Molecule 37 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



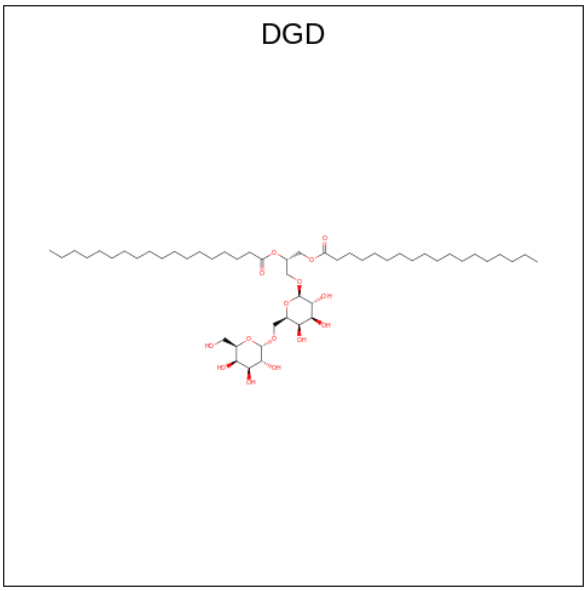
Mol	Chain	Residues	Atoms	AltConf
37	A	1	Total C O 48 38 10	0
37	A	1	Total C O 40 30 10	0
37	B	1	Total C O 51 41 10	0
37	B	1	Total C O 55 45 10	0
37	C	1	Total C O 51 41 10	0
37	D	1	Total C O 46 36 10	0
37	Z	1	Total C O 51 41 10	0
37	a	1	Total C O 48 38 10	0
37	a	1	Total C O 40 30 10	0
37	b	1	Total C O 51 41 10	0
37	b	1	Total C O 55 45 10	0
37	c	1	Total C O 51 41 10	0
37	d	1	Total C O 46 36 10	0
37	z	1	Total C O 51 41 10	0

- Molecule 38 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: $C_{53}H_{80}O_2$).



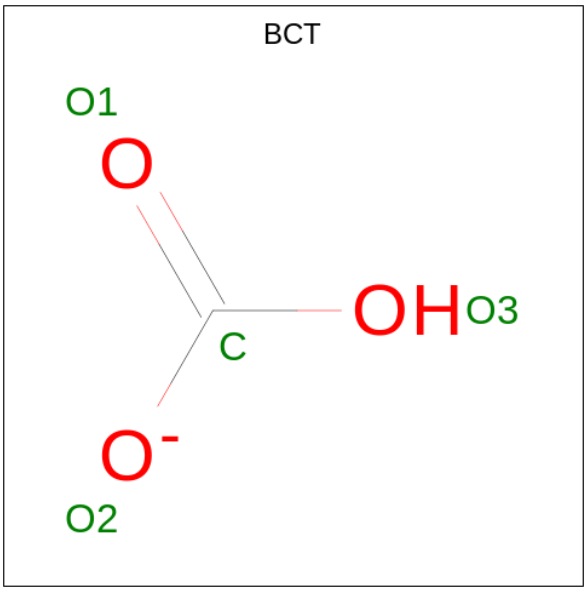
Mol	Chain	Residues	Atoms	AltConf
38	A	1	Total C O 13 11 2	0
38	D	1	Total C O 55 53 2	0
38	a	1	Total C O 13 11 2	0
38	d	1	Total C O 55 53 2	0

- Molecule 39 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



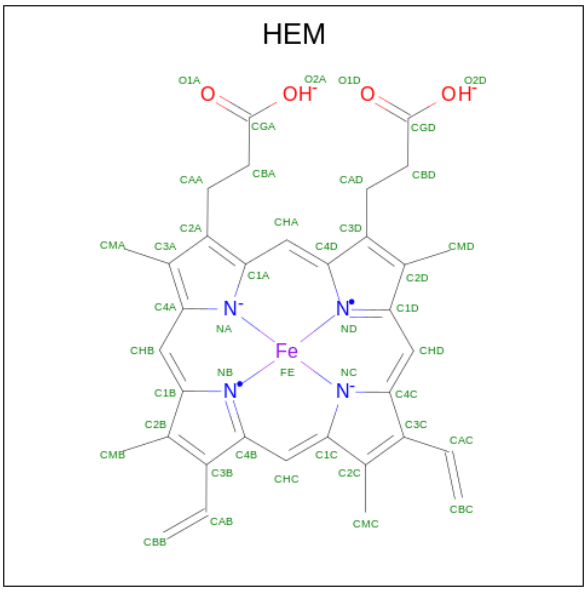
Mol	Chain	Residues	Atoms	AltConf
39	B	1	Total C O 59 44 15	0
39	C	1	Total C O 55 40 15	0
39	C	1	Total C O 62 47 15	0
39	C	1	Total C O 60 45 15	0
39	H	1	Total C O 62 47 15	0
39	b	1	Total C O 59 44 15	0
39	c	1	Total C O 55 40 15	0
39	c	1	Total C O 62 47 15	0
39	c	1	Total C O 60 45 15	0
39	h	1	Total C O 62 47 15	0

- Molecule 40 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms			AltConf
40	D	1	Total	C	O	0
			4	1	3	
40	d	1	Total	C	O	0
			4	1	3	

- Molecule 41 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

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

- Molecule 42 is water.

Mol	Chain	Residues	Atoms		AltConf
42	A	96	Total	O	0
			96	96	
42	B	89	Total	O	0
			89	89	
42	C	68	Total	O	0
			68	68	
42	D	58	Total	O	0
			58	58	
42	E	10	Total	O	0
			10	10	
42	F	2	Total	O	0
			2	2	
42	G	15	Total	O	0
			15	15	
42	H	16	Total	O	0
			16	16	
42	J	3	Total	O	0
			3	3	
42	K	2	Total	O	0
			2	2	
42	L	10	Total	O	0
			10	10	
42	M	4	Total	O	0
			4	4	
42	N	20	Total	O	0
			20	20	
42	O	31	Total	O	0
			31	31	
42	P	16	Total	O	0
			16	16	
42	R	30	Total	O	0
			30	30	
42	S	14	Total	O	0
			14	14	
42	T	2	Total	O	0
			2	2	

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Mol	Chain	Residues	Atoms	AltConf
42	W	4	Total O 4 4	0
42	X	5	Total O 5 5	0
42	Y	39	Total O 39 39	0
42	Z	4	Total O 4 4	0
42	a	96	Total O 96 96	0
42	b	89	Total O 89 89	0
42	c	68	Total O 68 68	0
42	d	58	Total O 58 58	0
42	e	10	Total O 10 10	0
42	f	2	Total O 2 2	0
42	g	15	Total O 15 15	0
42	h	16	Total O 16 16	0
42	j	3	Total O 3 3	0
42	k	2	Total O 2 2	0
42	l	10	Total O 10 10	0
42	m	4	Total O 4 4	0
42	n	20	Total O 20 20	0
42	o	31	Total O 31 31	0
42	p	16	Total O 16 16	0
42	r	30	Total O 30 30	0
42	s	14	Total O 14 14	0

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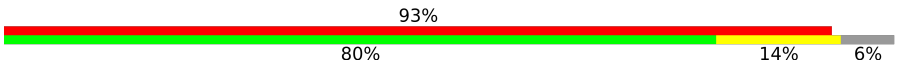
Mol	Chain	Residues	Atoms	AltConf
42	t	2	Total O 2 2	0
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42	x	5	Total O 5 5	0
42	y	39	Total O 39 39	0
42	z	4	Total O 4 4	0

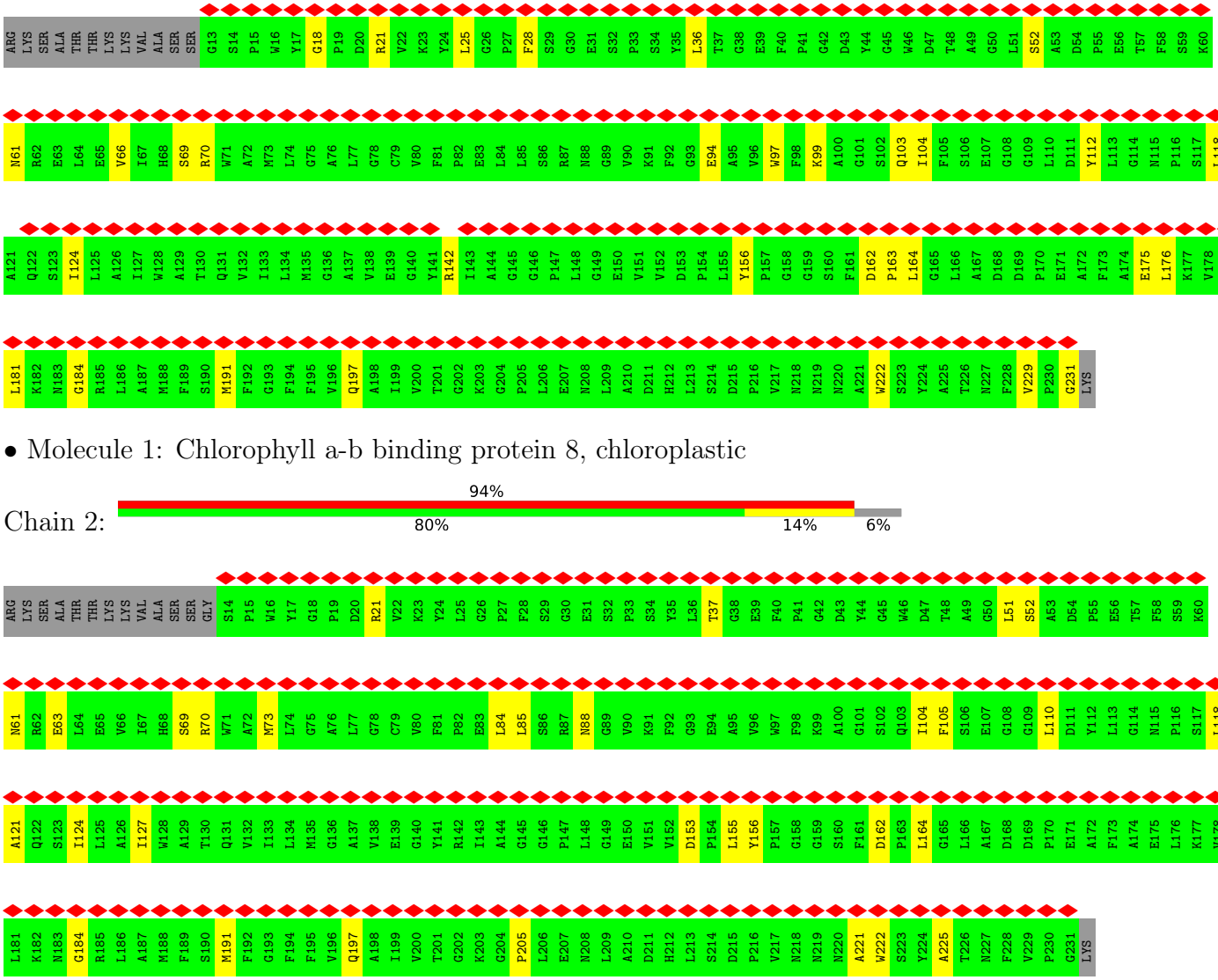
3 Residue-property plots (i)

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: Chlorophyll a-b binding protein 8, chloroplastic

Chain 1:



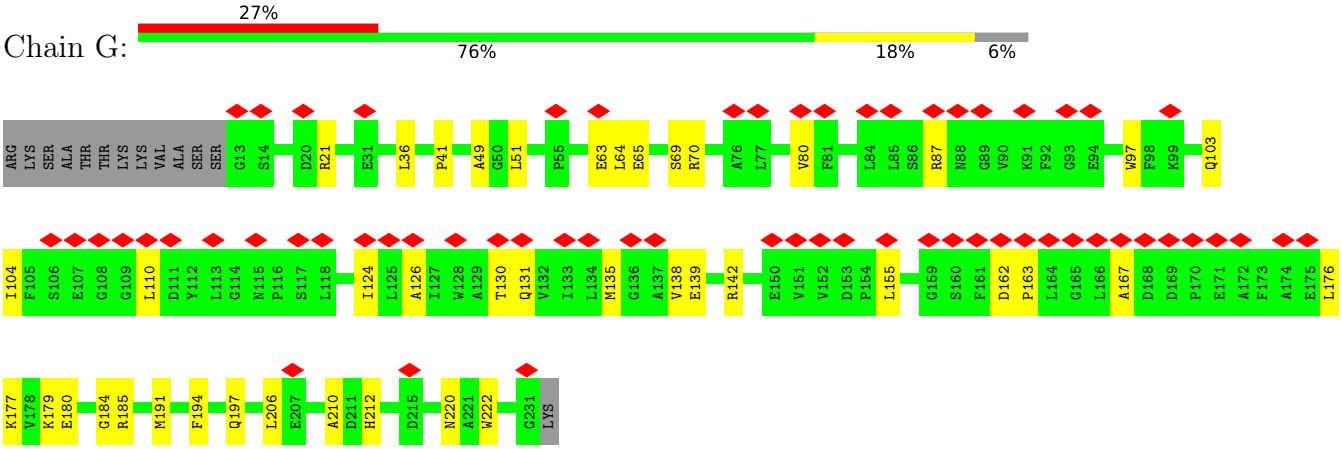


• Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

Chain 2:

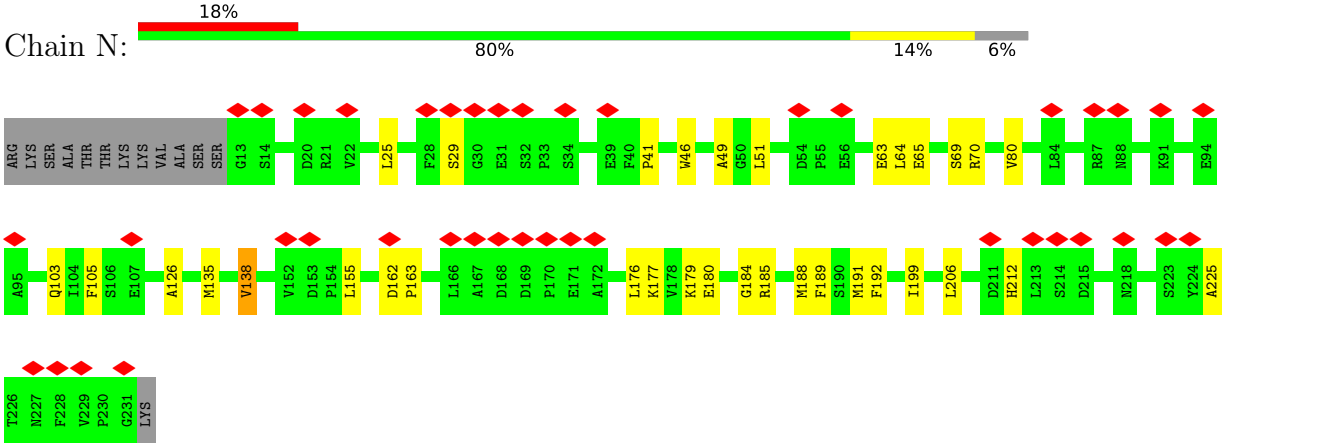
• Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

Chain G:



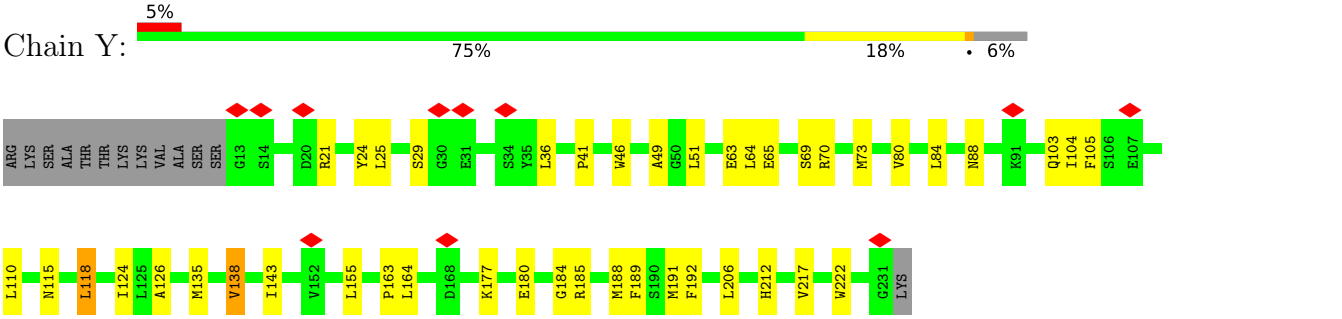
• Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

Chain N:



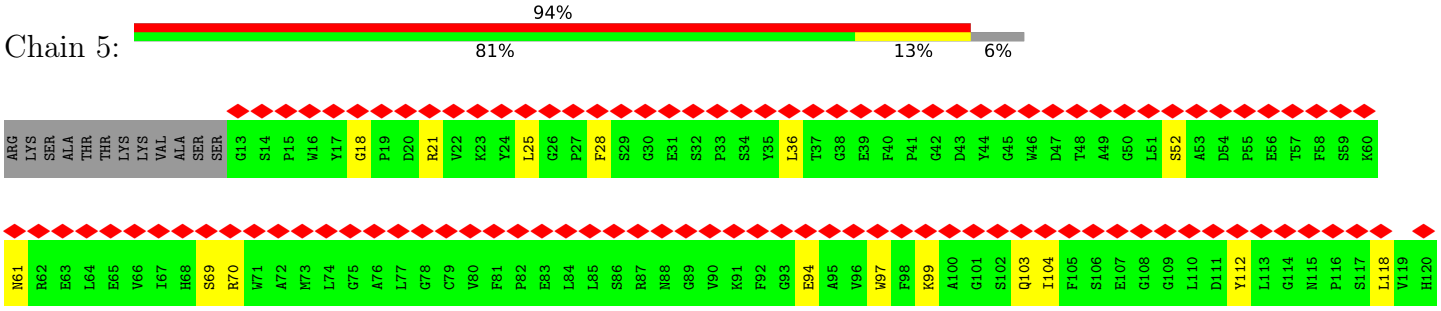
• Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

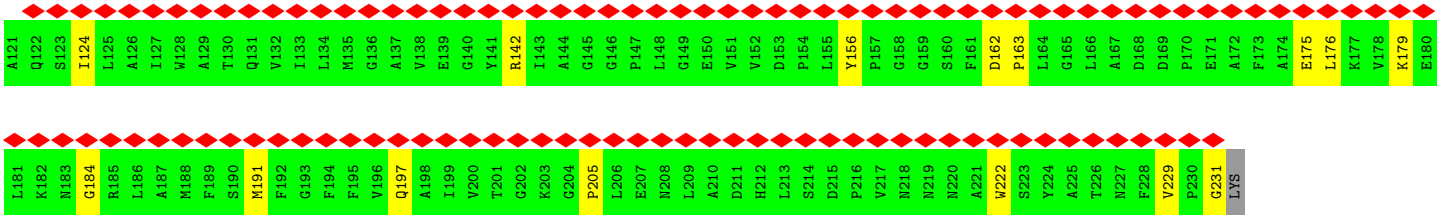
Chain Y:



• Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

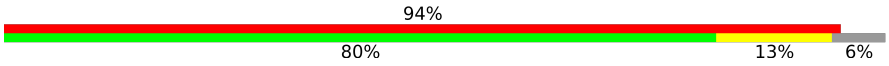
Chain 5:

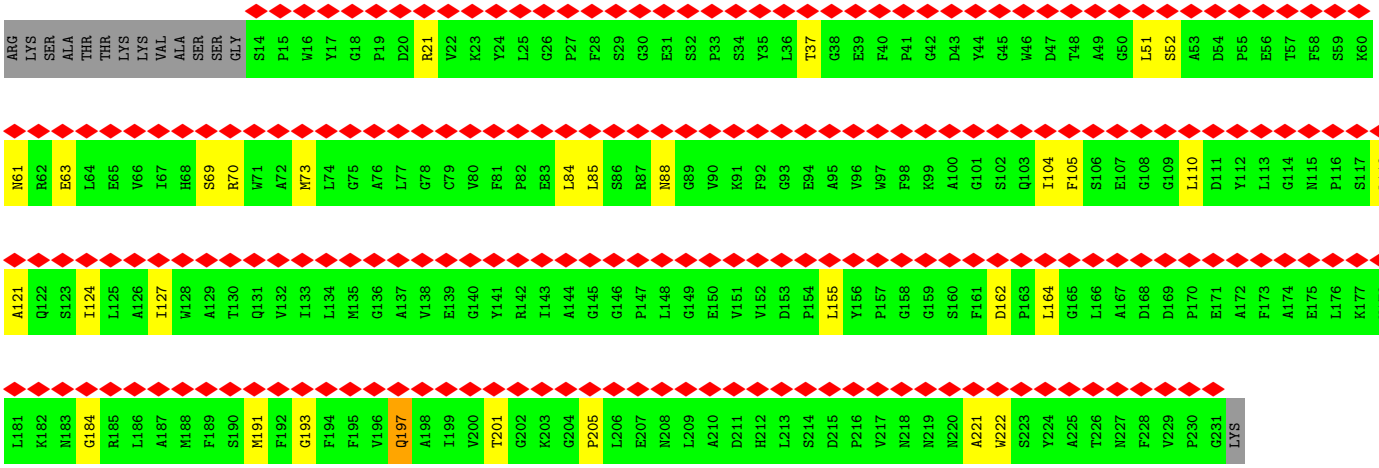




• Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

Chain 6:

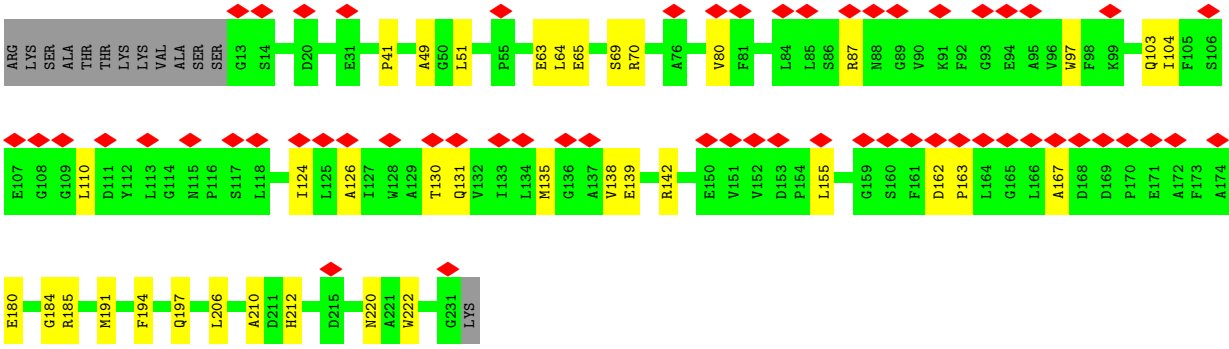




• Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

Chain g:

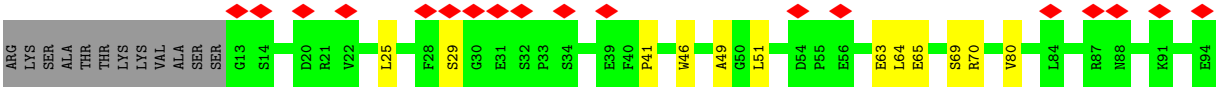


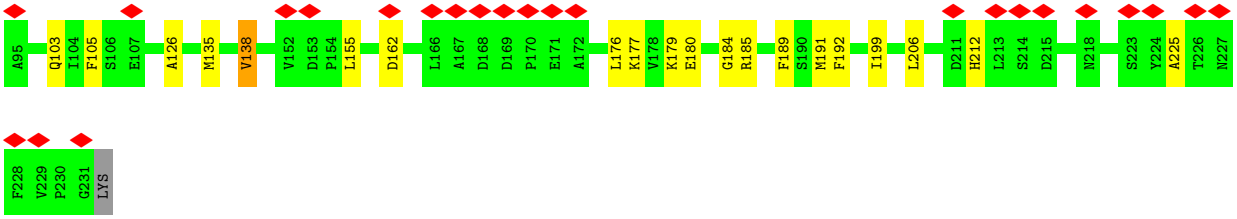


• Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

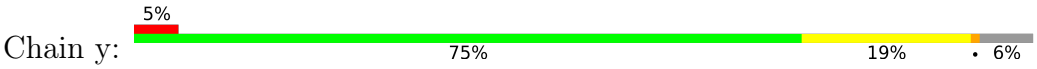
Chain n:

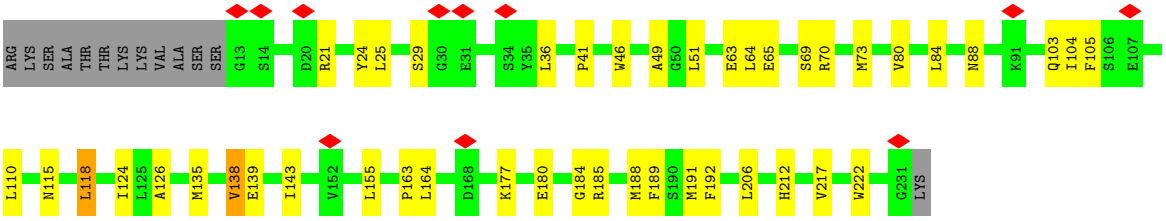




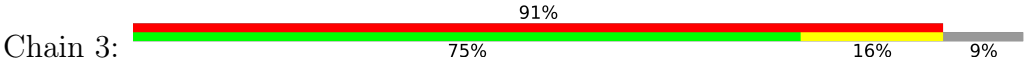


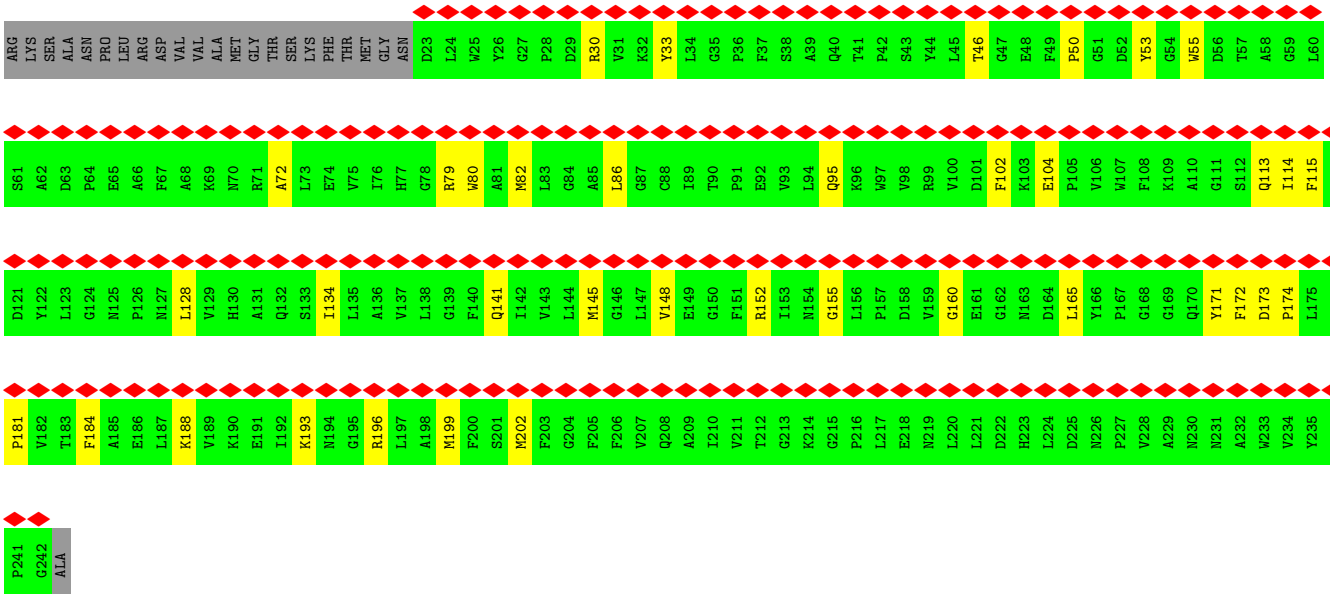
• Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic



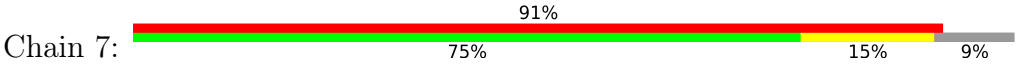


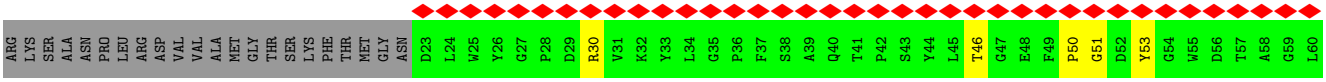
• Molecule 2: Chlorophyll a-b binding protein, chloroplastic





• Molecule 2: Chlorophyll a-b binding protein, chloroplastic

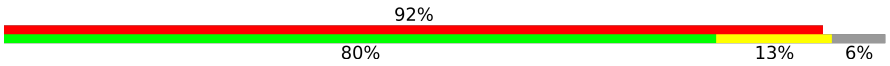


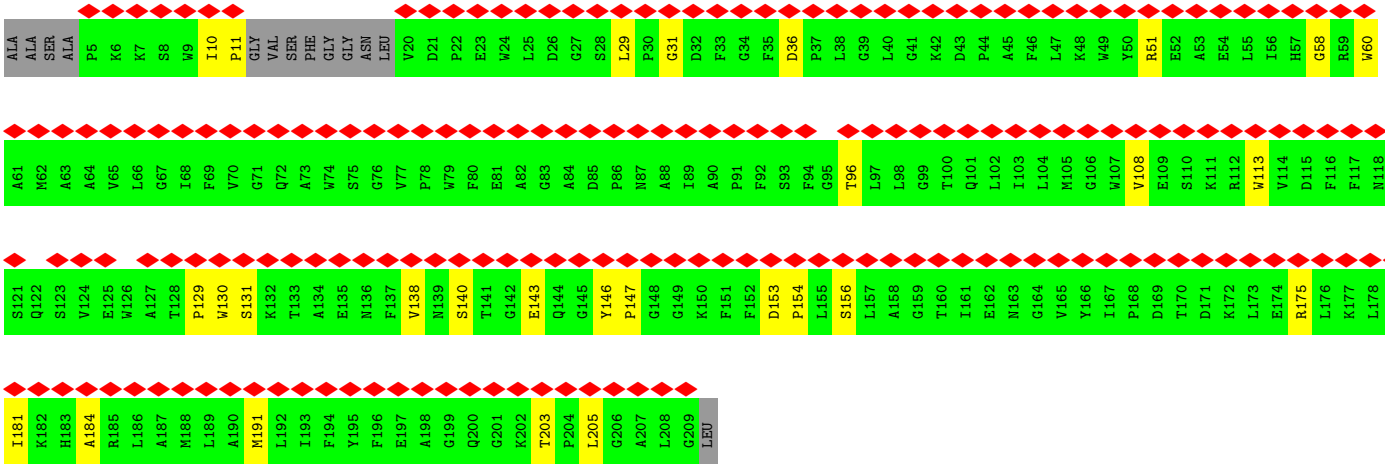




• Molecule 3: Light harvesting chlorophyll a/b-binding protein Lhcb6, CP24

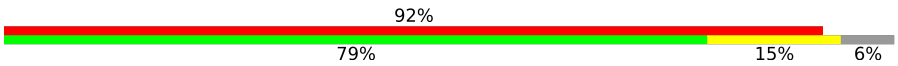
Chain 4:





• Molecule 3: Light harvesting chlorophyll a/b-binding protein Lhcb6, CP24

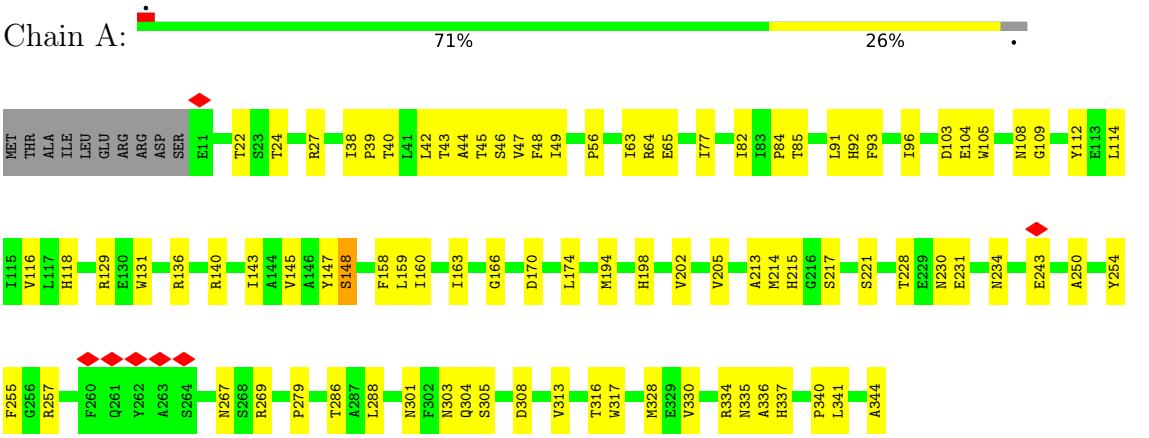
Chain 8:





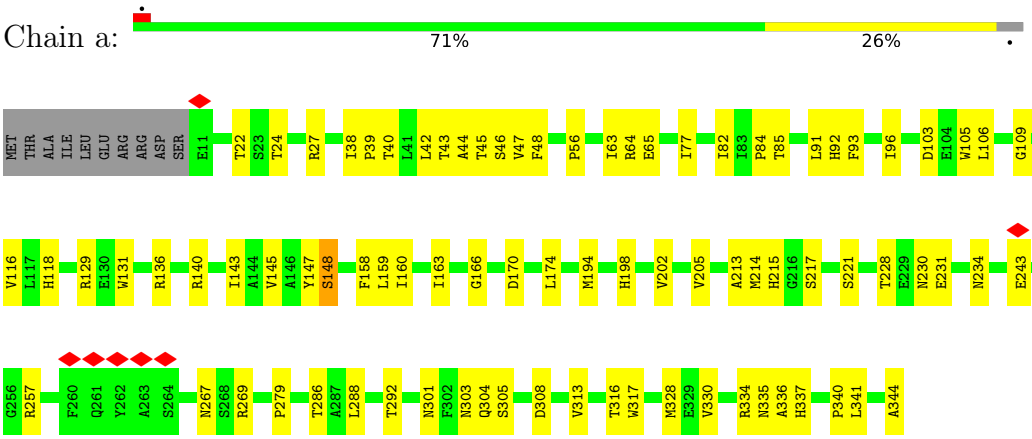
• Molecule 4: Photosystem II protein D1

Chain A:



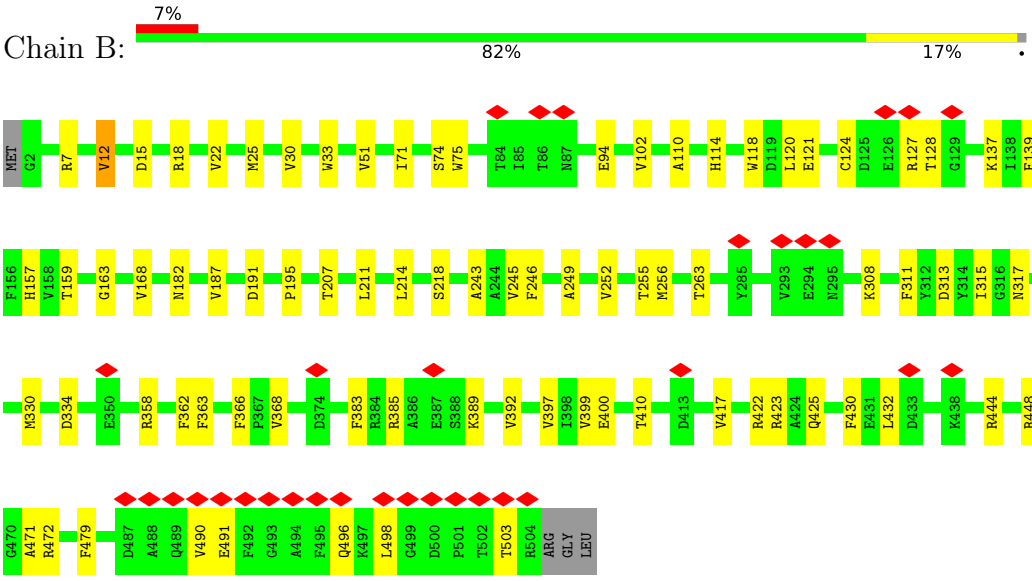
• Molecule 4: Photosystem II protein D1

Chain a:



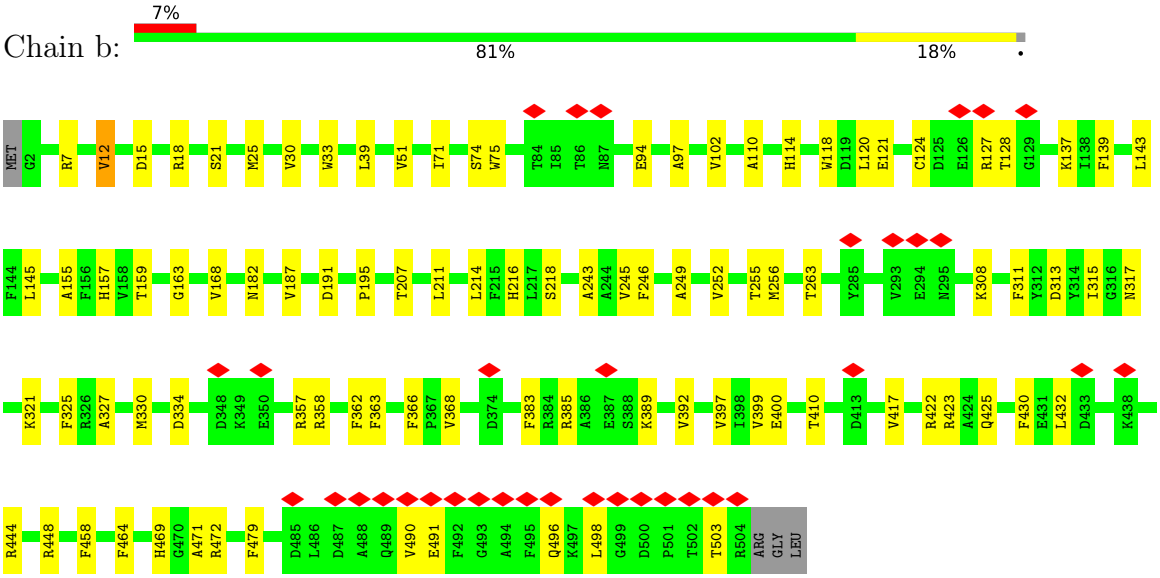
• Molecule 5: Photosystem II CP47 reaction center protein

Chain B:



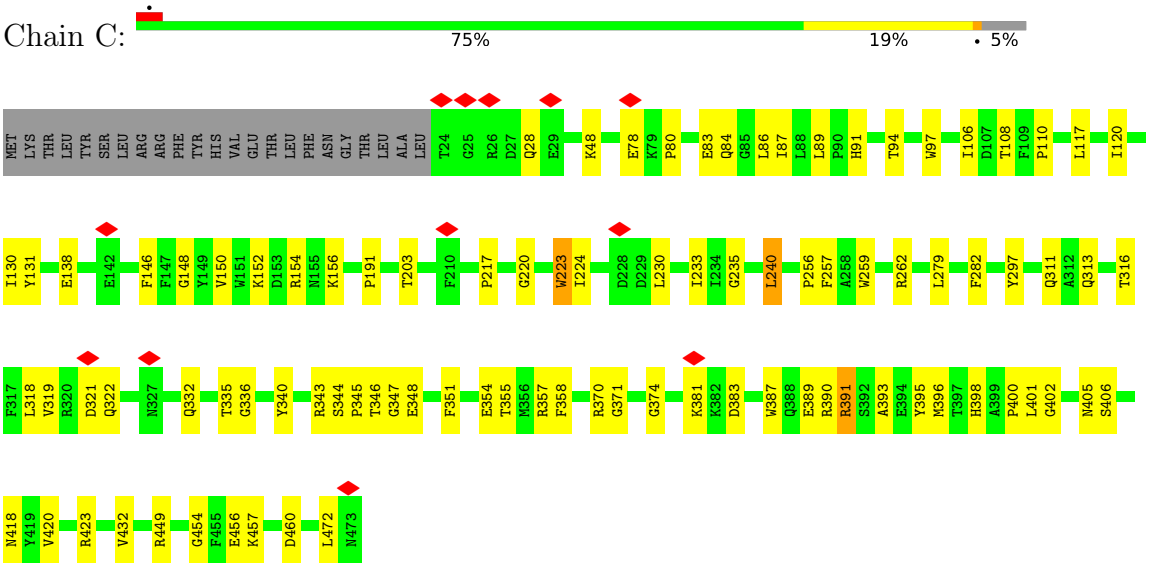
• Molecule 5: Photosystem II CP47 reaction center protein

Chain b:



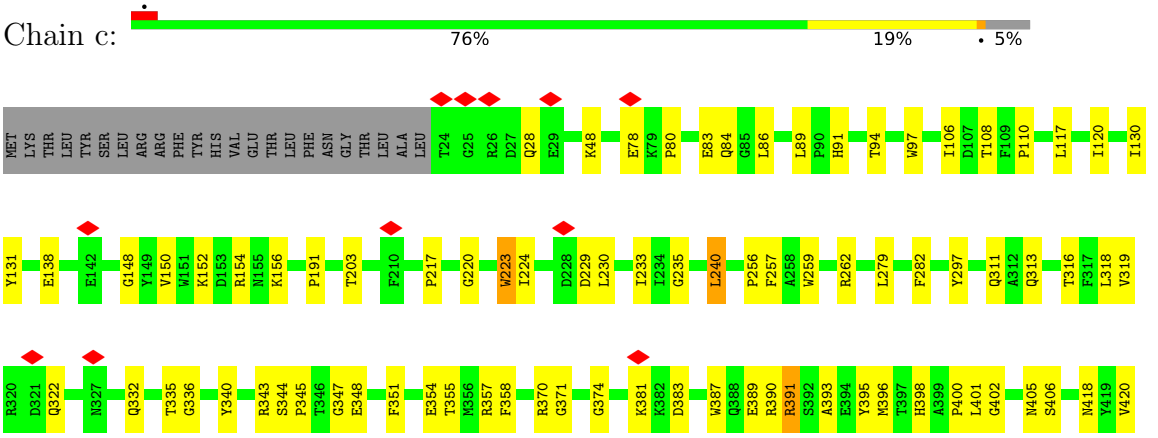
• Molecule 6: Photosystem II CP43 reaction center protein

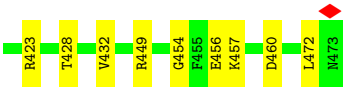
Chain C:



• Molecule 6: Photosystem II CP43 reaction center protein

Chain c:

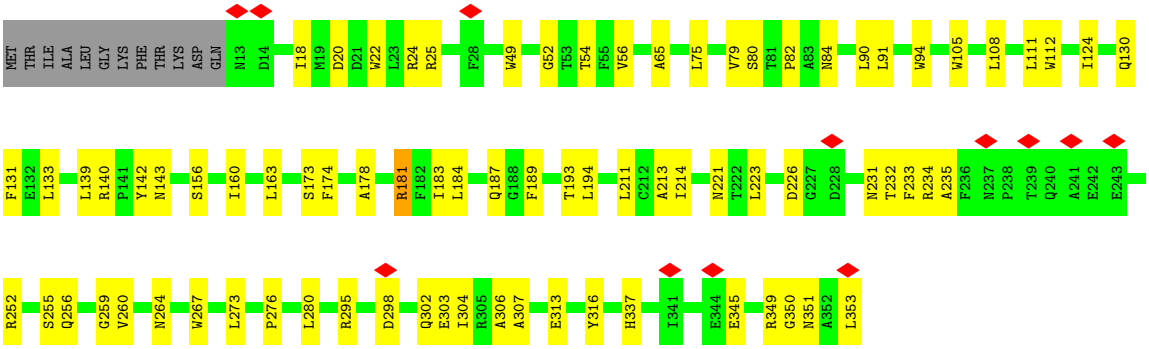




• Molecule 7: Photosystem II D2 protein

Chain D:

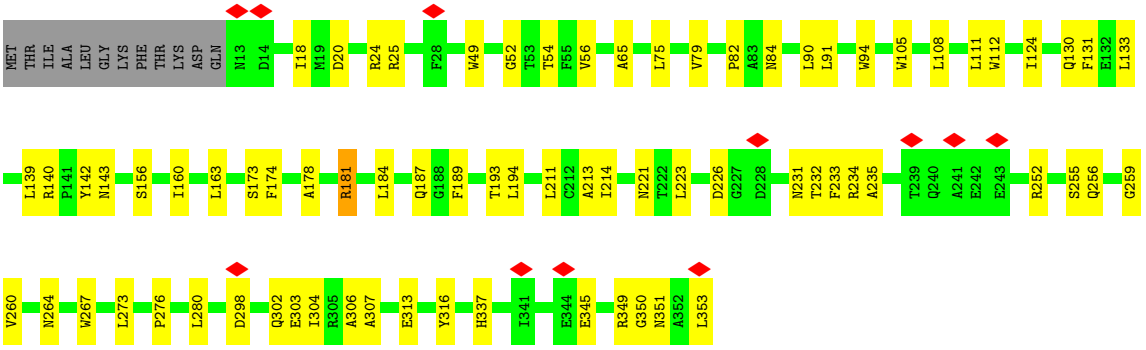




• Molecule 7: Photosystem II D2 protein

Chain d:

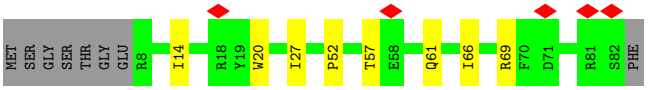




• Molecule 8: Cytochrome b559 subunit alpha

Chain E:

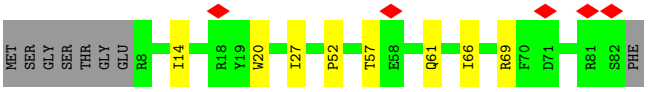




• Molecule 8: Cytochrome b559 subunit alpha

Chain e:

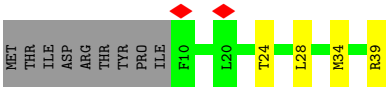




• Molecule 9: Cytochrome b559 subunit beta, PsbF

Chain F:

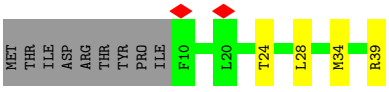




• Molecule 9: Cytochrome b559 subunit beta, PsbF

Chain f:

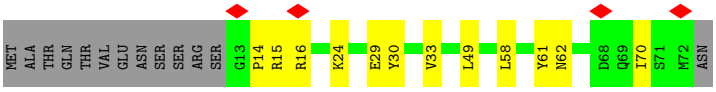




• Molecule 10: Photosystem II reaction center protein H

Chain H:

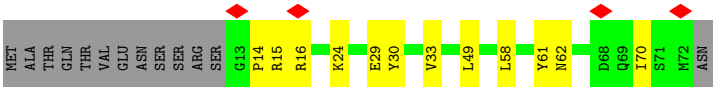




• Molecule 10: Photosystem II reaction center protein H

Chain h:

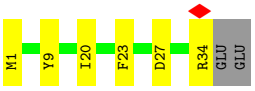




• Molecule 11: Photosystem II reaction center protein I, PsbI

Chain I:

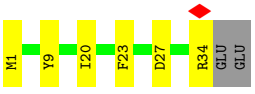




• Molecule 11: Photosystem II reaction center protein I, PsbI

Chain i:

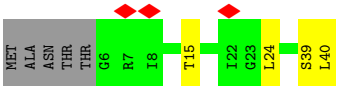




• Molecule 12: Photosystem II reaction center protein J

Chain J:

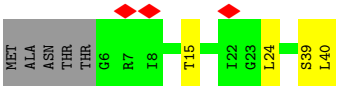




• Molecule 12: Photosystem II reaction center protein J

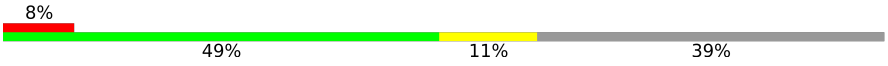
Chain j:

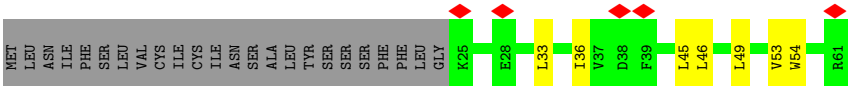




• Molecule 13: Photosystem II reaction center protein K

Chain K:

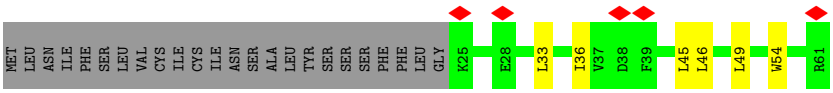




• Molecule 13: Photosystem II reaction center protein K

Chain k:

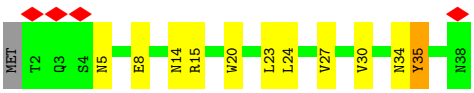




• Molecule 14: Photosystem II reaction center protein L

Chain L:

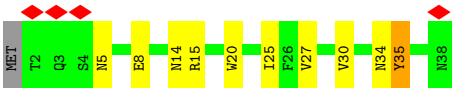




• Molecule 14: Photosystem II reaction center protein L

Chain l:





• Molecule 15: Photosystem II reaction center protein M

Chain M:

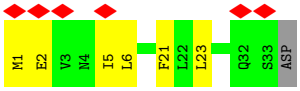




• Molecule 15: Photosystem II reaction center protein M

Chain m:

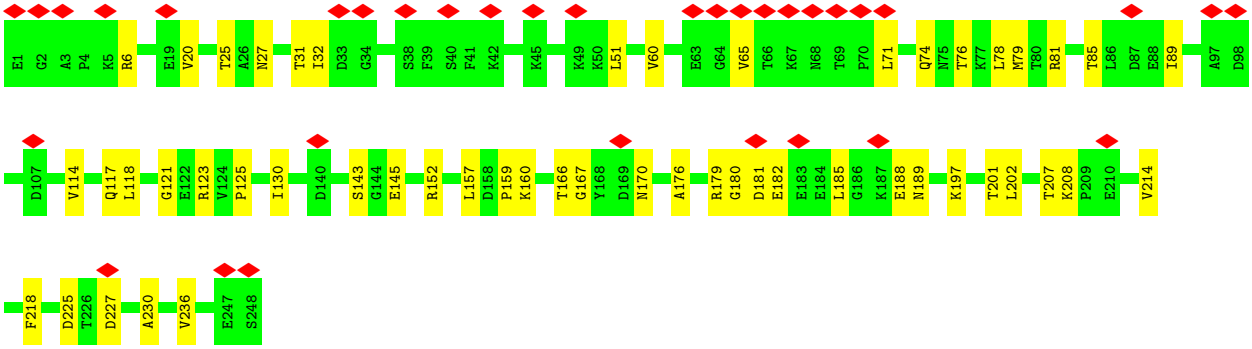




• Molecule 16: Oxygen-evolving enhancer protein 1, chloroplastic

Chain O:

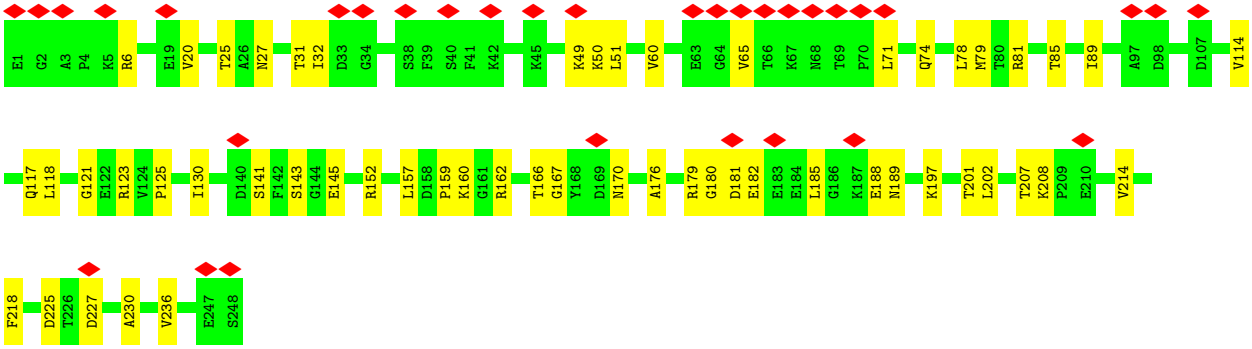




• Molecule 16: Oxygen-evolving enhancer protein 1, chloroplastic

Chain o:

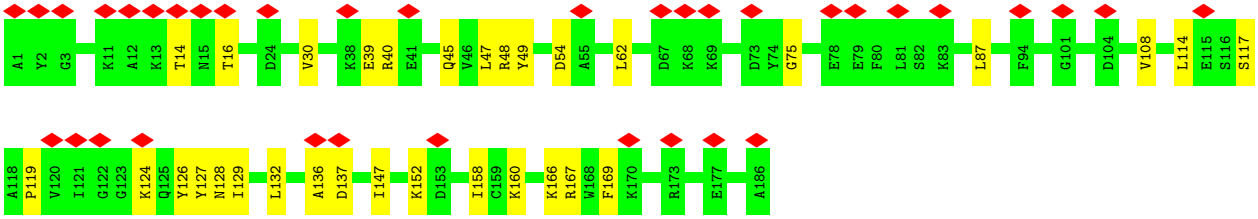




• Molecule 17: Oxygen-evolving enhancer protein 2, chloroplastic

Chain P:

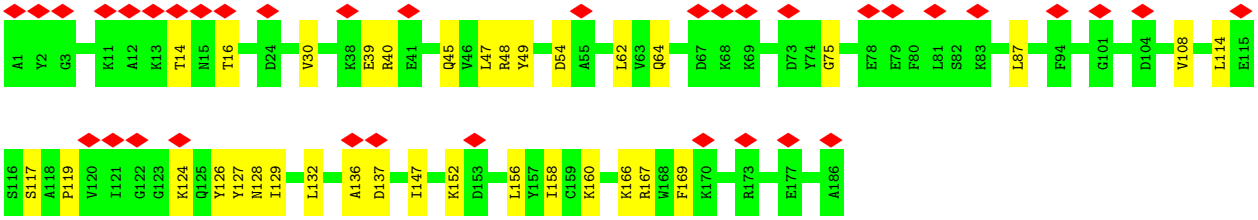




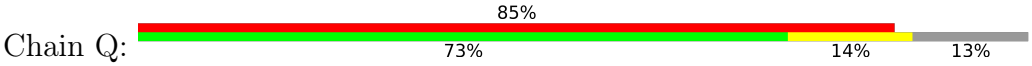
• Molecule 17: Oxygen-evolving enhancer protein 2, chloroplastic

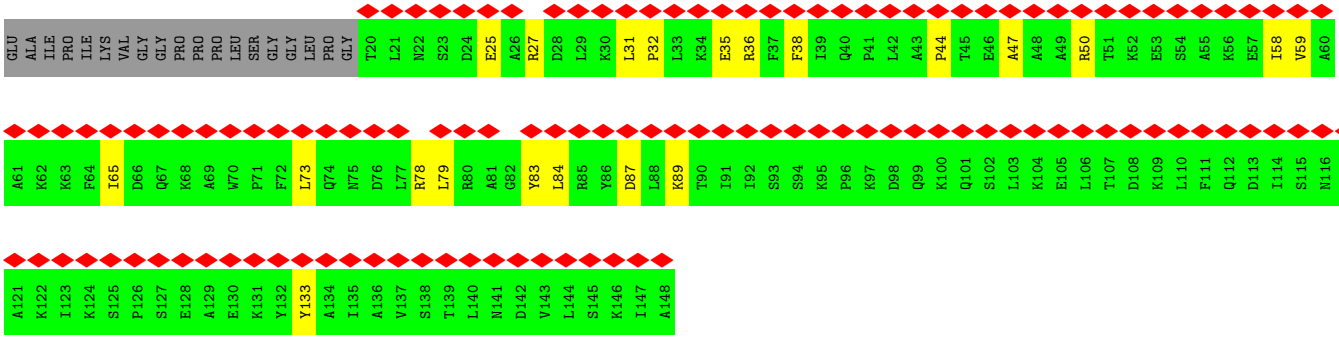
Chain p:



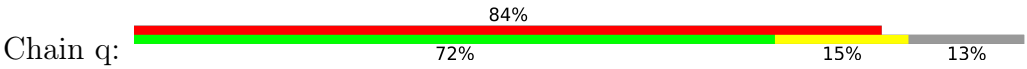


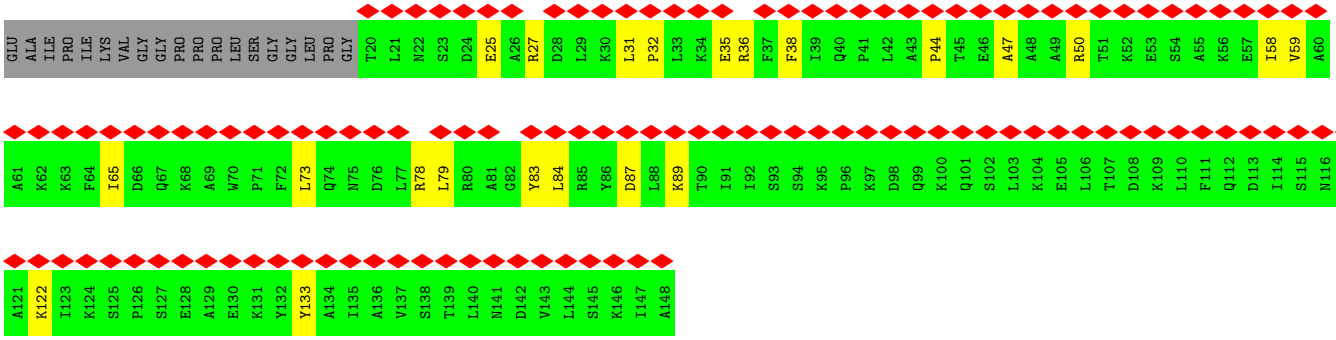
• Molecule 18: Oxygen-evolving enhancer protein 3



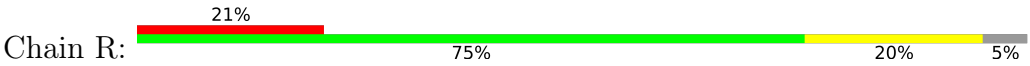


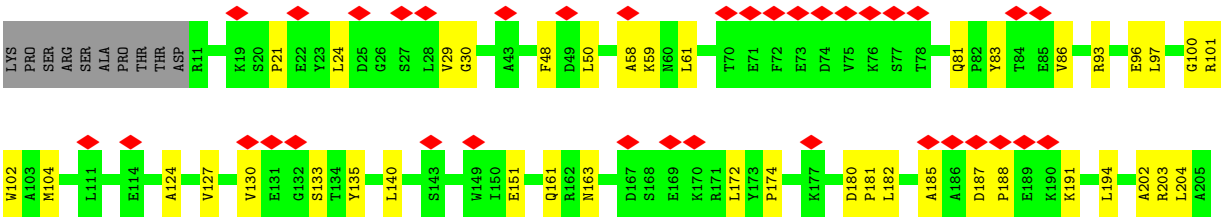
• Molecule 18: Oxygen-evolving enhancer protein 3

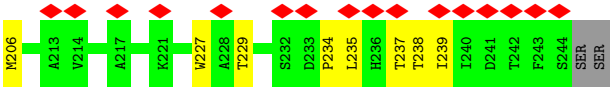




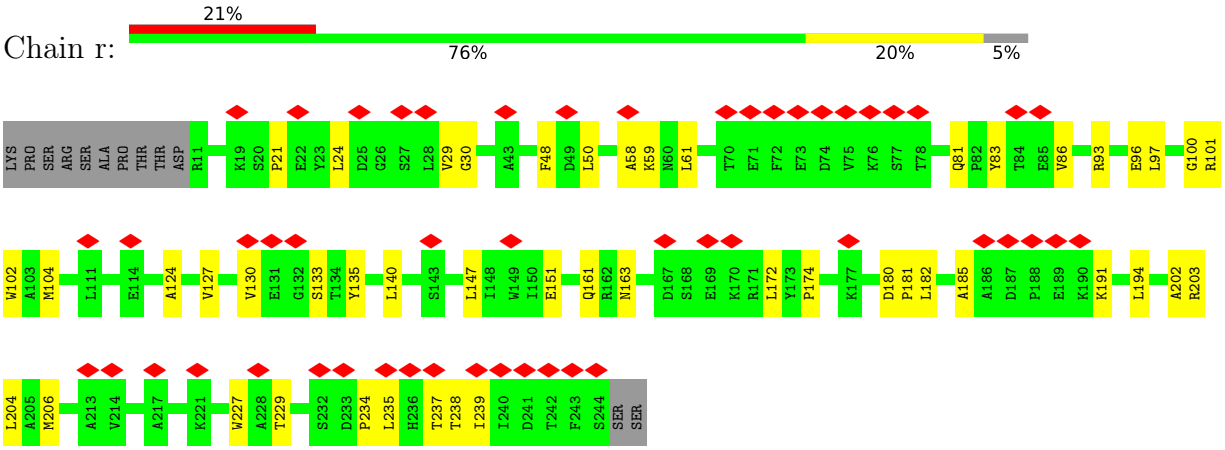
• Molecule 19: Light harvesting chlorophyll a/b-binding protein Lhcb4, CP29



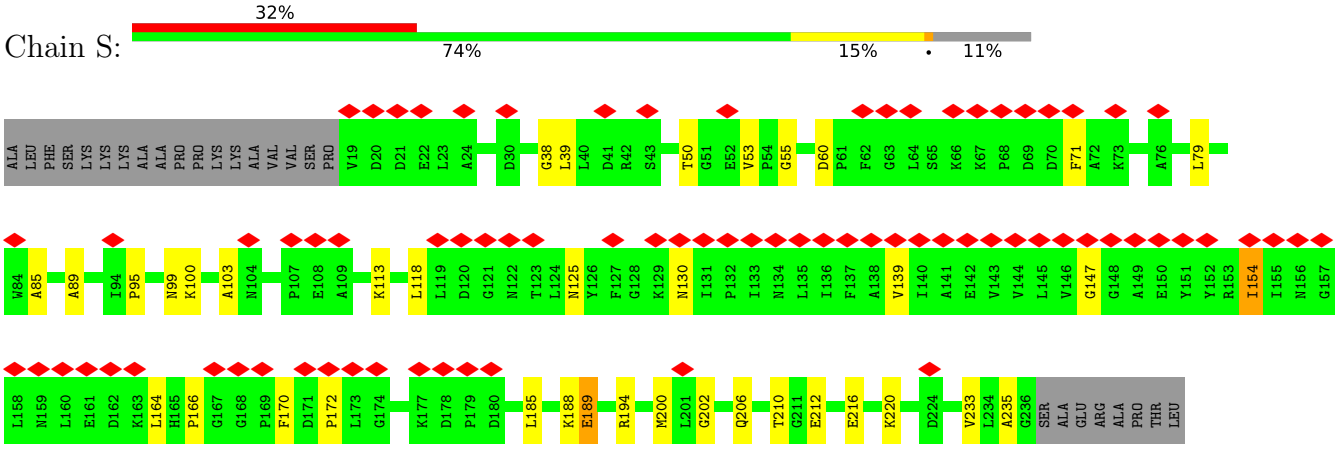




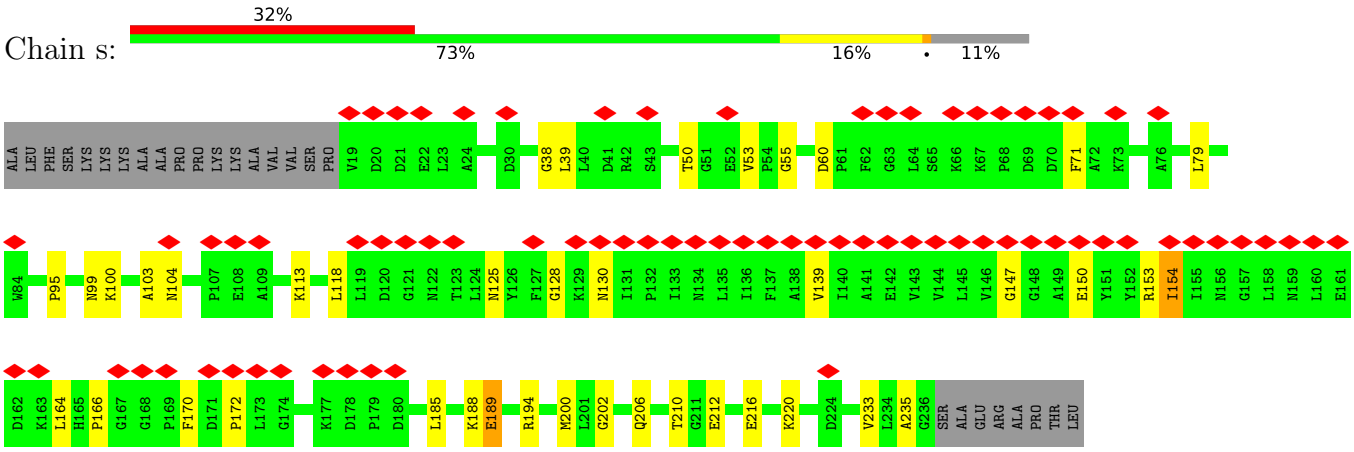
• Molecule 19: Light harvesting chlorophyll a/b-binding protein Lhcb4, CP29



• Molecule 20: Light harvesting chlorophyll a/b-binding protein Lhcb5, CP26

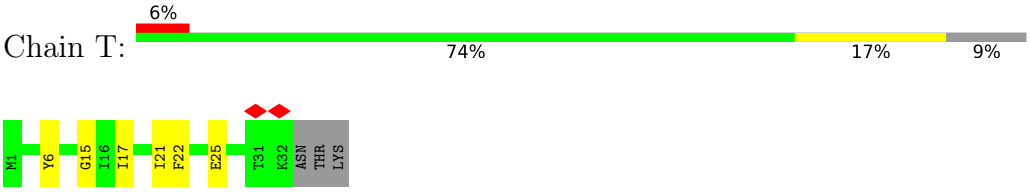


• Molecule 20: Light harvesting chlorophyll a/b-binding protein Lhcb5, CP26



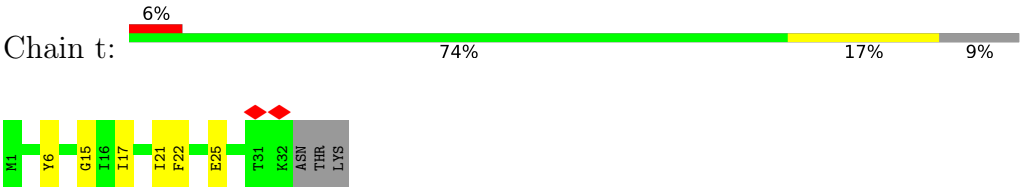
• Molecule 21: Photosystem II reaction center protein T

Chain T:



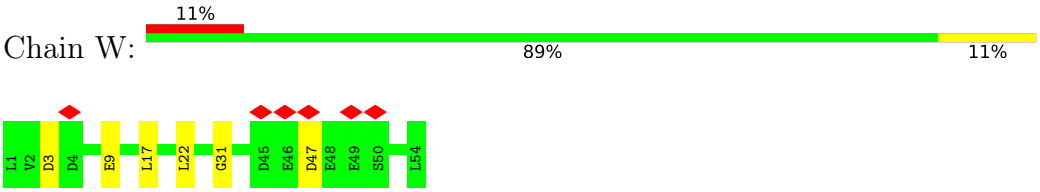
• Molecule 21: Photosystem II reaction center protein T

Chain t:



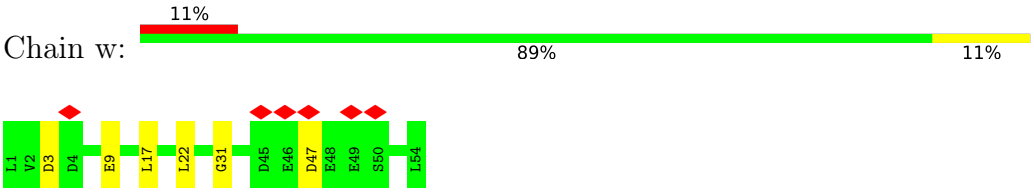
• Molecule 22: Photosystem II reaction center protein W

Chain W:



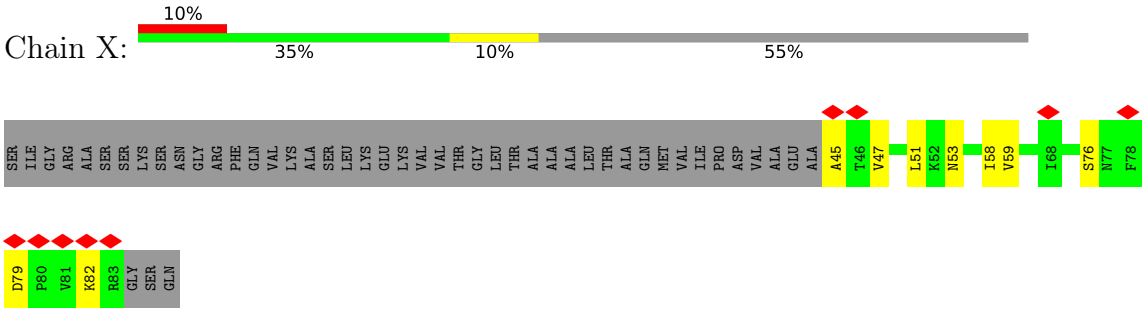
• Molecule 22: Photosystem II reaction center protein W

Chain w:



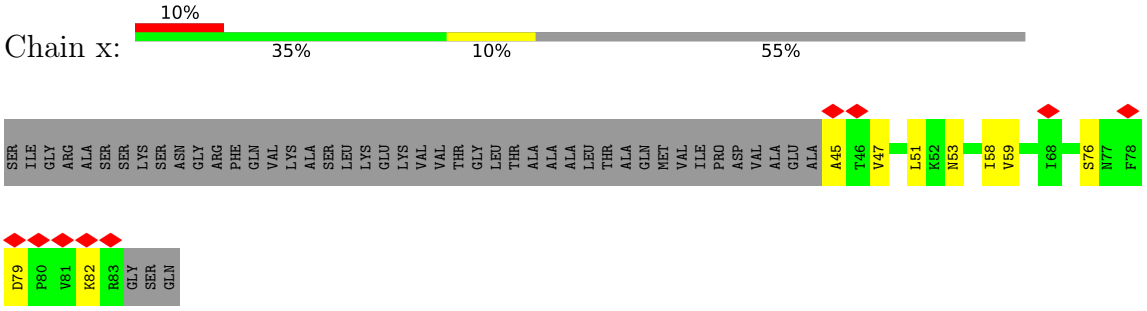
• Molecule 23: Photosystem II reaction center protein X

Chain X:



• Molecule 23: Photosystem II reaction center protein X

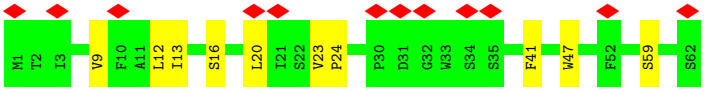
Chain x:



• Molecule 24: Photosystem II reaction center protein Z

Chain Z:

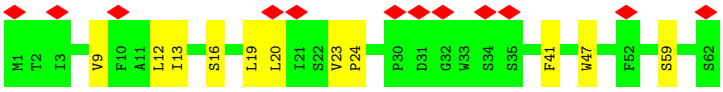




• Molecule 24: Photosystem II reaction center protein Z

Chain z:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	136521	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 ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	168.730	Depositor
Minimum map value	-94.103	Depositor
Average map value	0.061	Depositor
Map value standard deviation	6.582	Depositor
Recommended contour level	17.5	Depositor
Map size (Å)	312.0, 312.0, 312.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NEX, SQD, XAT, DGD, FE2, LUT, CLA, BCR, CL, OEX, BCT, LHG, PL9, PHO, CHL, HEM, LMG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	1	0.27	0/1720	0.46	0/2342
1	2	0.25	0/1716	0.49	1/2337 (0.0%)
1	5	0.28	0/1720	0.46	0/2342
1	6	0.25	0/1716	0.49	1/2337 (0.0%)
1	G	0.39	0/1720	0.52	0/2342
1	N	0.50	0/1720	0.61	1/2342 (0.0%)
1	Y	0.44	0/1720	0.63	3/2342 (0.1%)
1	g	0.39	0/1720	0.52	0/2342
1	n	0.50	0/1720	0.61	1/2342 (0.0%)
1	y	0.44	0/1720	0.63	3/2342 (0.1%)
2	3	0.31	0/1759	0.50	0/2396
2	7	0.31	0/1759	0.50	0/2396
3	4	0.28	0/1586	0.59	0/2158
3	8	0.28	0/1586	0.59	0/2158
4	A	0.53	1/2697 (0.0%)	0.62	0/3677
4	a	0.53	1/2697 (0.0%)	0.62	0/3677
5	B	0.54	0/4081	0.61	0/5556
5	b	0.54	0/4081	0.61	0/5556
6	C	0.57	1/3614 (0.0%)	0.61	1/4922 (0.0%)
6	c	0.57	1/3614 (0.0%)	0.61	1/4922 (0.0%)
7	D	0.46	0/2804	0.62	0/3823
7	d	0.46	0/2804	0.62	0/3823
8	E	0.39	0/630	0.49	0/857
8	e	0.39	0/630	0.49	0/857
9	F	0.77	1/248 (0.4%)	0.78	0/335
9	f	0.78	1/248 (0.4%)	0.78	0/335
10	H	0.49	0/461	0.51	0/626
10	h	0.49	0/461	0.51	0/626
11	I	0.49	0/286	0.69	0/386
11	i	0.49	0/286	0.69	0/386
12	J	0.58	0/262	0.76	0/354

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
12	j	0.58	0/262	0.76	0/354
13	K	0.45	0/318	0.71	0/434
13	k	0.45	0/318	0.71	0/434
14	L	0.59	0/319	0.68	1/434 (0.2%)
14	l	0.59	0/319	0.68	1/434 (0.2%)
15	M	0.44	0/260	0.68	0/355
15	m	0.45	0/260	0.68	0/355
16	O	0.45	1/1906 (0.1%)	0.61	0/2575
16	o	0.45	1/1906 (0.1%)	0.61	0/2575
17	P	0.55	0/1464	0.62	0/1978
17	p	0.55	0/1464	0.62	0/1978
18	Q	0.27	0/1051	0.56	0/1414
18	q	0.27	0/1051	0.56	0/1414
19	R	0.52	0/1886	0.64	1/2569 (0.0%)
19	r	0.52	0/1886	0.65	1/2569 (0.0%)
20	S	0.44	0/1736	0.70	3/2359 (0.1%)
20	s	0.44	0/1736	0.70	3/2359 (0.1%)
21	T	0.37	0/269	0.51	0/365
21	t	0.37	0/269	0.51	0/365
22	W	0.53	0/429	0.57	0/581
22	w	0.53	0/429	0.57	0/581
23	X	0.26	0/279	0.49	0/380
23	x	0.26	0/279	0.49	0/380
24	Z	0.39	0/474	0.61	0/648
24	z	0.40	0/474	0.61	0/648
All	All	0.46	8/74830 (0.0%)	0.60	22/101774 (0.0%)

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	c	223	TRP	C-O	-5.55	1.19	1.24
6	C	223	TRP	C-O	-5.49	1.19	1.24
9	f	24	THR	C-O	-5.35	1.17	1.24
9	F	24	THR	C-O	-5.32	1.18	1.24
16	O	114	VAL	C-O	-5.31	1.18	1.24

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	y	143	ILE	N-CA-C	8.60	120.38	111.00
1	Y	143	ILE	N-CA-C	8.59	120.36	111.00
1	N	138	VAL	N-CA-C	7.78	118.56	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	n	138	VAL	N-CA-C	7.78	118.56	110.62
1	Y	138	VAL	N-CA-C	7.77	118.55	110.62

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1668	0	1596	25	0
1	2	1664	0	1593	24	0
1	5	1668	0	1596	23	0
1	6	1664	0	1593	24	0
1	G	1668	0	1596	33	0
1	N	1668	0	1596	28	0
1	Y	1668	0	1596	34	0
1	g	1668	0	1596	34	0
1	n	1668	0	1596	26	0
1	y	1668	0	1596	35	0
2	3	1707	0	1659	28	0
2	7	1707	0	1659	28	0
3	4	1534	0	1486	22	0
3	8	1534	0	1486	23	0
4	A	2616	0	2522	98	0
4	a	2616	0	2522	94	0
5	B	3948	0	3818	80	0
5	b	3948	0	3818	84	0
6	C	3497	0	3422	87	0
6	c	3497	0	3422	84	0
7	D	2712	0	2604	84	0
7	d	2712	0	2604	79	0
8	E	612	0	595	6	0
8	e	612	0	595	6	0
9	F	241	0	246	3	0
9	f	241	0	246	3	0
10	H	452	0	473	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	h	452	0	473	18	0
11	I	278	0	291	8	0
11	i	278	0	291	8	0
12	J	256	0	269	4	0
12	j	256	0	269	4	0
13	K	306	0	313	7	0
13	k	306	0	313	6	0
14	L	311	0	299	13	0
14	l	311	0	299	12	0
15	M	256	0	284	6	0
15	m	256	0	284	6	0
16	O	1870	0	1851	34	0
16	o	1870	0	1851	36	0
17	P	1434	0	1392	22	0
17	p	1434	0	1392	23	0
18	Q	1034	0	1075	22	0
18	q	1034	0	1075	23	0
19	R	1835	0	1801	43	0
19	r	1835	0	1801	42	0
20	S	1689	0	1670	33	0
20	s	1689	0	1670	35	0
21	T	261	0	280	9	0
21	t	261	0	280	9	0
22	W	419	0	402	5	0
22	w	419	0	402	5	0
23	X	276	0	301	8	0
23	x	276	0	301	8	0
24	Z	464	0	493	9	0
24	z	464	0	493	10	0
25	1	309	0	244	9	0
25	2	306	0	238	5	0
25	3	316	0	254	16	0
25	4	229	0	152	7	0
25	5	309	0	244	9	0
25	6	306	0	238	6	0
25	7	316	0	254	17	0
25	8	229	0	152	7	0
25	G	355	0	335	26	0
25	N	362	0	350	13	0
25	R	225	0	201	8	0
25	S	196	0	144	6	0
25	Y	362	0	350	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	g	355	0	335	26	0
25	n	362	0	350	12	0
25	r	225	0	201	9	0
25	s	196	0	144	5	0
25	y	362	0	350	13	0
26	1	412	0	348	8	0
26	2	391	0	314	7	0
26	3	426	0	373	12	0
26	4	270	0	198	3	0
26	5	412	0	348	8	0
26	6	391	0	314	8	0
26	7	426	0	373	10	0
26	8	270	0	198	2	0
26	A	240	0	242	16	0
26	B	1040	0	1152	53	0
26	C	845	0	936	37	0
26	D	130	0	144	7	0
26	G	477	0	477	19	0
26	N	473	0	468	25	0
26	R	543	0	490	29	0
26	S	465	0	393	14	0
26	Y	473	0	468	22	0
26	a	240	0	242	14	0
26	b	1040	0	1152	53	0
26	c	845	0	936	31	0
26	d	130	0	144	8	0
26	g	477	0	477	20	0
26	n	473	0	468	27	0
26	r	543	0	490	29	0
26	s	465	0	393	17	0
26	y	473	0	468	18	0
27	1	84	0	112	10	0
27	2	84	0	112	9	0
27	3	84	0	112	8	0
27	4	42	0	56	2	0
27	5	84	0	112	10	0
27	6	84	0	112	8	0
27	7	84	0	112	6	0
27	8	42	0	56	3	0
27	G	84	0	112	13	0
27	N	84	0	112	10	0
27	R	42	0	56	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	S	84	0	112	5	0
27	Y	84	0	112	10	0
27	g	84	0	112	15	0
27	n	84	0	112	9	0
27	r	42	0	56	5	0
27	s	84	0	112	6	0
27	y	84	0	112	9	0
28	1	44	0	56	4	0
28	2	44	0	56	6	0
28	3	44	0	56	3	0
28	4	44	0	56	3	0
28	5	44	0	56	3	0
28	6	44	0	56	4	0
28	7	44	0	56	3	0
28	8	44	0	56	4	0
28	G	44	0	56	5	0
28	N	44	0	56	6	0
28	R	44	0	56	4	0
28	Y	44	0	56	6	0
28	g	44	0	56	5	0
28	n	44	0	56	7	0
28	r	44	0	56	5	0
28	y	44	0	56	5	0
29	1	44	0	56	2	0
29	2	44	0	56	1	0
29	3	44	0	56	3	0
29	5	44	0	56	2	0
29	6	44	0	56	0	0
29	7	44	0	56	3	0
29	G	44	0	56	5	0
29	N	44	0	56	1	0
29	R	44	0	56	5	0
29	S	44	0	56	2	0
29	Y	44	0	56	2	0
29	g	44	0	56	2	0
29	n	44	0	56	1	0
29	r	44	0	56	4	0
29	s	44	0	56	3	0
29	y	44	0	56	1	0
30	1	41	0	55	2	0
30	2	37	0	44	1	0
30	3	47	0	67	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	4	21	0	12	1	0
30	5	41	0	55	2	0
30	6	37	0	44	1	0
30	7	47	0	67	2	0
30	8	21	0	12	1	0
30	B	96	0	141	5	0
30	C	147	0	222	12	0
30	D	138	0	195	17	0
30	G	49	0	74	4	0
30	L	49	0	74	3	0
30	N	49	0	74	4	0
30	R	42	0	57	4	0
30	S	49	0	74	4	0
30	Y	49	0	74	4	0
30	b	96	0	141	5	0
30	c	147	0	222	11	0
30	d	138	0	195	15	0
30	g	49	0	74	4	0
30	l	49	0	74	2	0
30	n	49	0	74	3	0
30	r	42	0	57	4	0
30	s	49	0	74	5	0
30	y	49	0	74	4	0
31	4	40	0	56	7	0
31	8	40	0	56	8	0
31	A	40	0	56	4	0
31	B	120	0	168	11	0
31	C	160	0	224	22	0
31	D	40	0	56	3	0
31	H	40	0	56	6	0
31	T	40	0	56	10	0
31	a	40	0	56	5	0
31	b	120	0	168	16	0
31	c	160	0	224	19	0
31	d	40	0	56	3	0
31	h	40	0	56	6	0
31	t	40	0	56	8	0
32	A	10	0	0	0	0
32	a	10	0	0	0	0
33	A	1	0	0	0	0
33	a	1	0	0	0	0
34	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	a	2	0	0	0	0
35	A	128	0	148	10	0
35	a	128	0	148	11	0
36	A	104	0	144	13	0
36	B	96	0	126	8	0
36	a	104	0	144	12	0
36	b	96	0	126	8	0
37	A	88	0	116	3	0
37	B	106	0	158	8	0
37	C	51	0	72	1	0
37	D	46	0	62	2	0
37	Z	51	0	72	5	0
37	a	88	0	116	3	0
37	b	106	0	158	8	0
37	c	51	0	72	1	0
37	d	46	0	62	2	0
37	z	51	0	72	5	0
38	A	13	0	7	1	0
38	D	55	0	80	2	0
38	a	13	0	7	1	0
38	d	55	0	80	1	0
39	B	59	0	76	5	0
39	C	177	0	227	6	0
39	H	62	0	82	3	0
39	b	59	0	76	5	0
39	c	177	0	227	5	0
39	h	62	0	82	4	0
40	D	4	0	0	0	0
40	d	4	0	0	0	0
41	F	43	0	30	1	0
41	f	43	0	30	1	0
42	A	96	0	0	0	0
42	B	89	0	0	0	0
42	C	68	0	0	0	0
42	D	58	0	0	0	0
42	E	10	0	0	0	0
42	F	2	0	0	0	0
42	G	15	0	0	1	0
42	H	16	0	0	0	0
42	J	3	0	0	0	0
42	K	2	0	0	0	0
42	L	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	M	4	0	0	0	0
42	N	20	0	0	0	0
42	O	31	0	0	0	0
42	P	16	0	0	0	0
42	R	30	0	0	0	0
42	S	14	0	0	1	0
42	T	2	0	0	0	0
42	W	4	0	0	0	0
42	X	5	0	0	0	0
42	Y	39	0	0	0	0
42	Z	4	0	0	0	0
42	a	96	0	0	0	0
42	b	89	0	0	0	0
42	c	68	0	0	0	0
42	d	58	0	0	0	0
42	e	10	0	0	0	0
42	f	2	0	0	0	0
42	g	15	0	0	1	0
42	h	16	0	0	0	0
42	j	3	0	0	0	0
42	k	2	0	0	0	0
42	l	10	0	0	0	0
42	m	4	0	0	0	0
42	n	20	0	0	0	0
42	o	31	0	0	0	0
42	p	16	0	0	0	0
42	r	30	0	0	0	0
42	s	14	0	0	1	0
42	t	2	0	0	0	0
42	w	4	0	0	0	0
42	x	5	0	0	0	0
42	y	39	0	0	0	0
42	z	4	0	0	0	0
All	All	98986	0	97642	1942	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 10.

The worst 5 of 1942 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)
3:8:130:TRP:CD1	26:r:611:CLA:HAB	2.08	0.87
3:4:130:TRP:CD1	26:R:611:CLA:HAB	2.08	0.87
31:4:623:BCR:HC42	26:R:601:CLA:HBB1	1.62	0.82
31:8:623:BCR:HC42	26:r:601:CLA:HBB1	1.62	0.79
1:2:191:MET:HE2	27:2:1621:LUT:H10	1.65	0.78

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	217/232 (94%)	209 (96%)	8 (4%)	0	100	100
1	2	216/232 (93%)	210 (97%)	5 (2%)	1 (0%)	24	48
1	5	217/232 (94%)	209 (96%)	8 (4%)	0	100	100
1	6	216/232 (93%)	210 (97%)	5 (2%)	1 (0%)	24	48
1	G	217/232 (94%)	213 (98%)	4 (2%)	0	100	100
1	N	217/232 (94%)	214 (99%)	3 (1%)	0	100	100
1	Y	217/232 (94%)	213 (98%)	4 (2%)	0	100	100
1	g	217/232 (94%)	213 (98%)	4 (2%)	0	100	100
1	n	217/232 (94%)	214 (99%)	3 (1%)	0	100	100
1	y	217/232 (94%)	213 (98%)	4 (2%)	0	100	100
2	3	218/243 (90%)	209 (96%)	9 (4%)	0	100	100
2	7	218/243 (90%)	209 (96%)	9 (4%)	0	100	100
3	4	193/210 (92%)	179 (93%)	14 (7%)	0	100	100
3	8	193/210 (92%)	179 (93%)	14 (7%)	0	100	100
4	A	332/344 (96%)	326 (98%)	6 (2%)	0	100	100
4	a	332/344 (96%)	326 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	B	501/507 (99%)	493 (98%)	8 (2%)	0	100	100
5	b	501/507 (99%)	493 (98%)	8 (2%)	0	100	100
6	C	448/473 (95%)	441 (98%)	7 (2%)	0	100	100
6	c	448/473 (95%)	442 (99%)	6 (1%)	0	100	100
7	D	339/353 (96%)	335 (99%)	4 (1%)	0	100	100
7	d	339/353 (96%)	335 (99%)	4 (1%)	0	100	100
8	E	73/83 (88%)	73 (100%)	0	0	100	100
8	e	73/83 (88%)	73 (100%)	0	0	100	100
9	F	28/39 (72%)	28 (100%)	0	0	100	100
9	f	28/39 (72%)	28 (100%)	0	0	100	100
10	H	58/73 (80%)	58 (100%)	0	0	100	100
10	h	58/73 (80%)	58 (100%)	0	0	100	100
11	I	32/36 (89%)	32 (100%)	0	0	100	100
11	i	32/36 (89%)	32 (100%)	0	0	100	100
12	J	33/40 (82%)	33 (100%)	0	0	100	100
12	j	33/40 (82%)	33 (100%)	0	0	100	100
13	K	35/61 (57%)	35 (100%)	0	0	100	100
13	k	35/61 (57%)	35 (100%)	0	0	100	100
14	L	35/38 (92%)	35 (100%)	0	0	100	100
14	l	35/38 (92%)	35 (100%)	0	0	100	100
15	M	31/34 (91%)	29 (94%)	2 (6%)	0	100	100
15	m	31/34 (91%)	29 (94%)	2 (6%)	0	100	100
16	O	246/248 (99%)	240 (98%)	6 (2%)	0	100	100
16	o	246/248 (99%)	240 (98%)	6 (2%)	0	100	100
17	P	184/186 (99%)	183 (100%)	1 (0%)	0	100	100
17	p	184/186 (99%)	183 (100%)	1 (0%)	0	100	100
18	Q	127/148 (86%)	125 (98%)	2 (2%)	0	100	100
18	q	127/148 (86%)	125 (98%)	2 (2%)	0	100	100
19	R	232/246 (94%)	228 (98%)	4 (2%)	0	100	100
19	r	232/246 (94%)	228 (98%)	4 (2%)	0	100	100
20	S	216/244 (88%)	209 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	s	216/244 (88%)	208 (96%)	8 (4%)	0	100	100
21	T	30/35 (86%)	30 (100%)	0	0	100	100
21	t	30/35 (86%)	30 (100%)	0	0	100	100
22	W	52/54 (96%)	52 (100%)	0	0	100	100
22	w	52/54 (96%)	52 (100%)	0	0	100	100
23	X	37/86 (43%)	36 (97%)	1 (3%)	0	100	100
23	x	37/86 (43%)	36 (97%)	1 (3%)	0	100	100
24	Z	60/62 (97%)	60 (100%)	0	0	100	100
24	z	60/62 (97%)	60 (100%)	0	0	100	100
All	All	9248/10006 (92%)	9056 (98%)	190 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	2	119	VAL
1	6	119	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	171/182 (94%)	171 (100%)	0	100	100
1	2	171/182 (94%)	171 (100%)	0	100	100
1	5	171/182 (94%)	171 (100%)	0	100	100
1	6	171/182 (94%)	171 (100%)	0	100	100
1	G	171/182 (94%)	171 (100%)	0	100	100
1	N	171/182 (94%)	171 (100%)	0	100	100
1	Y	171/182 (94%)	171 (100%)	0	100	100
1	g	171/182 (94%)	171 (100%)	0	100	100
1	n	171/182 (94%)	171 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	y	171/182 (94%)	171 (100%)	0	100	100
2	3	175/193 (91%)	175 (100%)	0	100	100
2	7	175/193 (91%)	175 (100%)	0	100	100
3	4	154/162 (95%)	154 (100%)	0	100	100
3	8	154/162 (95%)	154 (100%)	0	100	100
4	A	270/279 (97%)	270 (100%)	0	100	100
4	a	270/279 (97%)	270 (100%)	0	100	100
5	B	400/403 (99%)	399 (100%)	1 (0%)	86	94
5	b	400/403 (99%)	399 (100%)	1 (0%)	86	94
6	C	352/373 (94%)	351 (100%)	1 (0%)	86	94
6	c	352/373 (94%)	351 (100%)	1 (0%)	86	94
7	D	275/285 (96%)	274 (100%)	1 (0%)	84	93
7	d	275/285 (96%)	274 (100%)	1 (0%)	84	93
8	E	67/73 (92%)	67 (100%)	0	100	100
8	e	67/73 (92%)	67 (100%)	0	100	100
9	F	25/34 (74%)	25 (100%)	0	100	100
9	f	25/34 (74%)	25 (100%)	0	100	100
10	H	49/61 (80%)	49 (100%)	0	100	100
10	h	49/61 (80%)	49 (100%)	0	100	100
11	I	31/33 (94%)	31 (100%)	0	100	100
11	i	31/33 (94%)	31 (100%)	0	100	100
12	J	26/30 (87%)	26 (100%)	0	100	100
12	j	26/30 (87%)	26 (100%)	0	100	100
13	K	32/54 (59%)	32 (100%)	0	100	100
13	k	32/54 (59%)	32 (100%)	0	100	100
14	L	35/36 (97%)	35 (100%)	0	100	100
14	l	35/36 (97%)	35 (100%)	0	100	100
15	M	29/30 (97%)	29 (100%)	0	100	100
15	m	29/30 (97%)	29 (100%)	0	100	100
16	O	204/204 (100%)	204 (100%)	0	100	100
16	o	204/204 (100%)	204 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	P	150/150 (100%)	150 (100%)	0	100	100
17	p	150/150 (100%)	150 (100%)	0	100	100
18	Q	112/125 (90%)	112 (100%)	0	100	100
18	q	112/125 (90%)	112 (100%)	0	100	100
19	R	191/202 (95%)	191 (100%)	0	100	100
19	r	191/202 (95%)	191 (100%)	0	100	100
20	S	170/190 (90%)	170 (100%)	0	100	100
20	s	170/190 (90%)	170 (100%)	0	100	100
21	T	29/32 (91%)	29 (100%)	0	100	100
21	t	29/32 (91%)	29 (100%)	0	100	100
22	W	44/44 (100%)	44 (100%)	0	100	100
22	w	44/44 (100%)	44 (100%)	0	100	100
23	X	32/67 (48%)	32 (100%)	0	100	100
23	x	32/67 (48%)	32 (100%)	0	100	100
24	Z	54/54 (100%)	54 (100%)	0	100	100
24	z	54/54 (100%)	54 (100%)	0	100	100
All	All	7522/8048 (94%)	7516 (100%)	6 (0%)	87	96

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	b	12	VAL
6	c	391	ARG
7	d	181	ARG
6	C	391	ARG
5	B	12	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 72 such sidechains are listed below:

Mol	Chain	Res	Type
1	g	122	GLN
1	y	88	ASN
16	o	74	GLN
19	r	47	GLN
16	O	190	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 490 ligands modelled in this entry, 6 are monoatomic - leaving 484 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	$\#\|Z\| > 2$
26	CLA	1	613	1	59,63,73	1.36	9 (15%)	71,101,113	1.23	5 (7%)
26	CLA	7	611	30	59,63,73	1.38	10 (16%)	71,101,113	1.45	10 (14%)
25	CHL	1	606	-	50,54,74	2.25	17 (34%)	56,90,114	3.16	22 (39%)
26	CLA	S	603	20	49,53,73	1.47	7 (14%)	59,89,113	1.75	10 (16%)
26	CLA	Y	610	1	64,68,73	1.30	9 (14%)	77,107,113	1.19	9 (11%)
26	CLA	s	603	20	49,53,73	1.48	7 (14%)	59,89,113	1.75	10 (16%)
26	CLA	7	610	2	64,68,73	1.29	7 (10%)	77,107,113	1.18	7 (9%)
28	XAT	4	622	-	39,47,47	0.93	1 (2%)	54,74,74	2.62	21 (38%)
26	CLA	6	612	1	49,53,73	1.51	8 (16%)	59,89,113	1.37	6 (10%)
25	CHL	6	606	-	50,54,74	2.26	18 (36%)	56,90,114	3.23	21 (37%)
26	CLA	n	610	1	69,73,73	1.21	9 (13%)	83,113,113	1.28	11 (13%)
39	DGD	c	520	-	61,61,67	1.17	8 (13%)	75,75,81	1.47	12 (16%)
38	PL9	A	414	-	13,13,55	0.87	0	17,17,69	1.68	4 (23%)
25	CHL	7	609	2	65,69,74	2.04	17 (26%)	74,108,114	2.73	23 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
37	LMG	b	2633	-	55,55,55	0.78	3 (5%)	63,63,63	1.32	7 (11%)
31	BCR	b	618	-	41,41,41	0.84	1 (2%)	56,56,56	1.85	14 (25%)
26	CLA	R	610	19	69,73,73	1.23	9 (13%)	83,113,113	1.26	11 (13%)
25	CHL	G	601	1	70,74,74	1.86	17 (24%)	80,114,114	3.11	28 (35%)
26	CLA	1	602	1	65,69,73	1.28	10 (15%)	78,108,113	1.19	8 (10%)
26	CLA	c	503	6	69,73,73	1.31	11 (15%)	83,113,113	1.35	9 (10%)
27	LUT	Y	1621	-	42,43,43	0.88	1 (2%)	51,60,60	1.69	13 (25%)
27	LUT	G	1621	-	42,43,43	0.89	1 (2%)	51,60,60	1.96	17 (33%)
25	CHL	3	605	2	50,54,74	2.27	18 (36%)	56,90,114	3.30	24 (42%)
25	CHL	g	605	1	50,54,74	2.26	17 (34%)	56,90,114	3.47	24 (42%)
25	CHL	1	609	1	66,70,74	1.95	17 (25%)	75,109,114	2.86	22 (29%)
26	CLA	6	603	1	59,63,73	1.35	10 (16%)	71,101,113	1.41	8 (11%)
26	CLA	Y	611	30	64,68,73	1.32	9 (14%)	77,107,113	1.46	8 (10%)
26	CLA	D	403	7	69,73,73	1.23	8 (11%)	83,113,113	1.53	11 (13%)
30	LHG	5	2630	26	40,40,48	0.72	1 (2%)	43,46,54	1.33	6 (13%)
31	BCR	c	514	-	41,41,41	0.90	2 (4%)	56,56,56	1.74	13 (23%)
25	CHL	r	614	19	46,50,74	2.31	18 (39%)	51,85,114	3.57	21 (41%)
25	CHL	6	605	1	50,54,74	2.27	19 (38%)	56,90,114	3.30	22 (39%)
26	CLA	r	609	19	62,66,73	1.31	7 (11%)	74,104,113	1.42	6 (8%)
26	CLA	B	613	5	69,73,73	1.32	10 (14%)	83,113,113	1.67	14 (16%)
30	LHG	s	2630	26	48,48,48	0.74	1 (2%)	51,54,54	1.26	7 (13%)
26	CLA	B	607	5	69,73,73	1.30	11 (15%)	83,113,113	1.47	14 (16%)
29	NEX	5	1623	-	38,46,46	0.98	2 (5%)	50,70,70	2.41	16 (32%)
25	CHL	s	607	42	62,66,74	1.95	18 (29%)	70,104,114	3.11	24 (34%)
26	CLA	3	611	30	59,63,73	1.38	9 (15%)	71,101,113	1.45	10 (14%)
31	BCR	C	516	-	41,41,41	0.74	0	56,56,56	1.98	17 (30%)
26	CLA	s	613	20	59,63,73	1.32	9 (15%)	71,101,113	1.36	7 (9%)
26	CLA	d	402	7	69,73,73	1.38	10 (14%)	83,113,113	1.61	12 (14%)
25	CHL	s	606	42	50,54,74	2.26	17 (34%)	56,90,114	3.45	23 (41%)
26	CLA	Y	604	42	54,58,73	1.45	10 (18%)	65,95,113	1.64	10 (15%)
28	XAT	y	1622	-	39,47,47	1.08	3 (7%)	54,74,74	3.00	21 (38%)
26	CLA	C	505	6	69,73,73	1.30	11 (15%)	83,113,113	1.64	9 (10%)
26	CLA	b	617	5	69,73,73	1.31	11 (15%)	83,113,113	1.47	10 (12%)
27	LUT	S	1620	-	42,43,43	0.79	0	51,60,60	1.76	12 (23%)
26	CLA	n	603	1	69,73,73	1.31	10 (14%)	83,113,113	1.54	16 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	LHG	D	410	-	42,42,48	0.68	1 (2%)	45,48,54	1.22	4 (8%)
40	BCT	d	401	33	2,3,3	1.32	0	2,3,3	4.19	2 (100%)
25	CHL	2	608	-	50,54,74	2.21	18 (36%)	56,90,114	3.36	21 (37%)
26	CLA	8	603	3	49,53,73	1.49	10 (20%)	59,89,113	1.43	6 (10%)
26	CLA	N	602	1	69,73,73	1.27	9 (13%)	83,113,113	1.41	12 (14%)
26	CLA	G	604	42	54,58,73	1.48	10 (18%)	65,95,113	1.58	11 (16%)
27	LUT	5	1620	-	42,43,43	0.80	0	51,60,60	1.66	15 (29%)
25	CHL	6	601	1	50,54,74	2.27	18 (36%)	56,90,114	3.46	26 (46%)
27	LUT	3	1621	-	42,43,43	0.85	1 (2%)	51,60,60	1.60	11 (21%)
27	LUT	4	620	-	42,43,43	0.80	0	51,60,60	1.87	18 (35%)
30	LHG	d	409	-	48,48,48	0.75	1 (2%)	51,54,54	1.31	7 (13%)
26	CLA	3	612	2	49,53,73	1.47	10 (20%)	59,89,113	1.39	9 (15%)
27	LUT	R	620	-	42,43,43	0.86	2 (4%)	51,60,60	1.82	14 (27%)
29	NEX	s	1623	-	38,46,46	0.90	2 (5%)	50,70,70	2.24	15 (30%)
26	CLA	B	611	42	69,73,73	1.26	10 (14%)	83,113,113	1.59	13 (15%)
26	CLA	G	611	30	64,68,73	1.34	10 (15%)	77,107,113	1.48	6 (7%)
30	LHG	B	2631	-	48,48,48	0.68	2 (4%)	51,54,54	1.22	6 (11%)
26	CLA	b	606	5	69,73,73	1.35	11 (15%)	83,113,113	1.56	12 (14%)
26	CLA	7	612	2	49,53,73	1.46	10 (20%)	59,89,113	1.39	9 (15%)
26	CLA	s	611	30	60,64,73	1.30	10 (16%)	72,102,113	1.39	6 (8%)
29	NEX	2	1623	-	38,46,46	0.93	1 (2%)	50,70,70	2.39	15 (30%)
25	CHL	1	608	-	50,54,74	2.18	17 (34%)	56,90,114	3.36	18 (32%)
28	XAT	r	622	-	39,47,47	0.97	1 (2%)	54,74,74	2.77	21 (38%)
26	CLA	S	610	20	59,63,73	1.36	9 (15%)	71,101,113	1.41	11 (15%)
26	CLA	5	611	30	49,53,73	1.48	10 (20%)	59,89,113	1.29	6 (10%)
25	CHL	2	601	1	50,54,74	2.27	18 (36%)	56,90,114	3.46	26 (46%)
25	CHL	g	601	1	70,74,74	1.86	17 (24%)	80,114,114	3.11	28 (35%)
26	CLA	b	616	5	69,73,73	1.22	10 (14%)	83,113,113	1.37	10 (12%)
26	CLA	c	507	42	69,73,73	1.30	12 (17%)	83,113,113	1.61	9 (10%)
30	LHG	C	2630	-	48,48,48	0.66	1 (2%)	51,54,54	1.31	7 (13%)
25	CHL	1	607	-	67,71,74	1.92	19 (28%)	76,110,114	3.11	24 (31%)
26	CLA	r	602	19	64,68,73	1.28	10 (15%)	77,107,113	1.49	11 (14%)
25	CHL	S	608	-	50,54,74	2.24	18 (36%)	56,90,114	3.31	19 (33%)
26	CLA	R	611	30	53,57,73	1.43	10 (18%)	62,93,113	1.60	10 (16%)
30	LHG	C	522	-	48,48,48	0.69	1 (2%)	51,54,54	1.26	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	CLA	r	610	19	69,73,73	1.24	8 (11%)	83,113,113	1.26	11 (13%)
38	PL9	d	405	-	55,55,55	1.83	12 (21%)	68,69,69	1.57	12 (17%)
26	CLA	b	613	5	69,73,73	1.32	10 (14%)	83,113,113	1.68	14 (16%)
30	LHG	8	2630	26	20,20,48	0.91	0	23,26,54	1.29	2 (8%)
26	CLA	C	504	42	69,73,73	1.24	13 (18%)	83,113,113	1.47	7 (8%)
27	LUT	N	1620	-	42,43,43	0.81	0	51,60,60	1.69	12 (23%)
25	CHL	G	605	1	50,54,74	2.27	17 (34%)	56,90,114	3.48	24 (42%)
26	CLA	n	614	1	52,56,73	1.39	6 (11%)	62,92,113	1.48	9 (14%)
27	LUT	2	1620	-	42,43,43	0.81	0	51,60,60	1.81	15 (29%)
25	CHL	8	607	-	50,54,74	2.30	18 (36%)	56,90,114	3.18	21 (37%)
27	LUT	6	1620	-	42,43,43	0.81	0	51,60,60	1.80	15 (29%)
26	CLA	A	406	42	69,73,73	1.26	10 (14%)	83,113,113	1.59	16 (19%)
36	SQD	a	418	-	53,54,54	0.92	5 (9%)	62,65,65	1.67	14 (22%)
26	CLA	Y	603	1	69,73,73	1.32	10 (14%)	83,113,113	1.51	14 (16%)
26	CLA	A	410	4	64,68,73	1.27	10 (15%)	77,107,113	1.53	9 (11%)
26	CLA	S	611	30	60,64,73	1.30	10 (16%)	72,102,113	1.38	6 (8%)
26	CLA	5	610	1	60,64,73	1.30	7 (11%)	72,102,113	1.17	6 (8%)
26	CLA	3	614	2	52,56,73	1.42	8 (15%)	62,92,113	1.16	5 (8%)
26	CLA	C	508	6	69,73,73	1.30	11 (15%)	83,113,113	1.64	11 (13%)
27	LUT	y	1621	-	42,43,43	0.88	1 (2%)	51,60,60	1.69	13 (25%)
25	CHL	N	601	1	70,74,74	1.88	19 (27%)	80,114,114	3.04	27 (33%)
26	CLA	b	602	42	69,73,73	1.26	9 (13%)	83,113,113	1.32	6 (7%)
26	CLA	8	610	3	49,53,73	1.49	9 (18%)	59,89,113	1.19	6 (10%)
27	LUT	S	1621	-	42,43,43	0.85	1 (2%)	51,60,60	1.78	17 (33%)
37	LMG	C	521	-	51,51,55	0.80	3 (5%)	59,59,63	1.38	6 (10%)
25	CHL	7	601	2	68,72,74	1.95	16 (23%)	77,111,114	3.10	27 (35%)
27	LUT	1	1620	-	42,43,43	0.79	0	51,60,60	1.66	14 (27%)
26	CLA	C	513	6	69,73,73	1.20	9 (13%)	83,113,113	1.46	15 (18%)
26	CLA	B	612	5	69,73,73	1.31	9 (13%)	83,113,113	1.52	11 (13%)
27	LUT	N	1621	-	42,43,43	0.89	2 (4%)	51,60,60	1.83	14 (27%)
26	CLA	c	506	6	69,73,73	1.27	10 (14%)	83,113,113	1.44	11 (13%)
28	XAT	3	1622	-	39,47,47	1.03	2 (5%)	54,74,74	2.85	24 (44%)
26	CLA	N	612	1	64,68,73	1.29	7 (10%)	77,107,113	1.32	8 (10%)
26	CLA	8	604	-	49,53,73	1.49	9 (18%)	59,89,113	1.27	5 (8%)
25	CHL	2	607	-	65,69,74	1.97	19 (29%)	74,108,114	2.95	24 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	BCR	8	623	-	41,41,41	0.74	0	56,56,56	2.31	17 (30%)
26	CLA	s	612	20	53,57,73	1.38	8 (15%)	62,93,113	1.46	6 (9%)
26	CLA	6	614	1	49,53,73	1.49	7 (14%)	59,89,113	1.27	3 (5%)
36	SQD	A	418	-	53,54,54	0.92	5 (9%)	62,65,65	1.67	14 (22%)
26	CLA	5	604	-	54,58,73	1.43	10 (18%)	65,95,113	1.37	10 (15%)
26	CLA	b	603	5	69,73,73	1.25	10 (14%)	83,113,113	1.34	8 (9%)
25	CHL	8	608	-	50,54,74	2.16	17 (34%)	56,90,114	3.43	21 (37%)
37	LMG	B	2633	-	55,55,55	0.78	3 (5%)	63,63,63	1.32	7 (11%)
27	LUT	g	1621	-	42,43,43	0.89	1 (2%)	51,60,60	1.95	17 (33%)
26	CLA	4	611	30	49,53,73	1.49	7 (14%)	59,89,113	1.32	4 (6%)
30	LHG	R	2630	26	41,41,48	0.70	1 (2%)	44,47,54	1.27	6 (13%)
26	CLA	r	616	19	49,53,73	1.51	8 (16%)	59,89,113	1.34	4 (6%)
26	CLA	B	610	5	69,73,73	1.25	11 (15%)	83,113,113	1.48	10 (12%)
26	CLA	7	603	2	59,63,73	1.30	10 (16%)	71,101,113	1.47	8 (11%)
25	CHL	6	608	-	50,54,74	2.21	18 (36%)	56,90,114	3.35	21 (37%)
26	CLA	R	616	19	49,53,73	1.51	8 (16%)	59,89,113	1.33	4 (6%)
26	CLA	8	611	30	49,53,73	1.49	7 (14%)	59,89,113	1.32	4 (6%)
26	CLA	r	612	19	53,57,73	1.45	7 (13%)	62,93,113	1.51	6 (9%)
28	XAT	R	622	-	39,47,47	0.97	1 (2%)	54,74,74	2.76	21 (38%)
26	CLA	b	614	5	69,73,73	1.29	9 (13%)	83,113,113	1.33	6 (7%)
27	LUT	1	1621	-	42,43,43	0.90	2 (4%)	51,60,60	1.73	15 (29%)
28	XAT	G	1622	-	39,47,47	0.98	2 (5%)	54,74,74	2.91	23 (42%)
26	CLA	c	502	6	69,73,73	1.27	10 (14%)	83,113,113	1.58	6 (7%)
25	CHL	y	609	1	70,74,74	1.87	18 (25%)	80,114,114	2.85	25 (31%)
26	CLA	c	501	6	69,73,73	1.24	8 (11%)	83,113,113	1.28	9 (10%)
26	CLA	s	610	20	59,63,73	1.35	9 (15%)	71,101,113	1.41	11 (15%)
26	CLA	n	602	1	69,73,73	1.27	9 (13%)	83,113,113	1.41	12 (14%)
25	CHL	5	609	1	66,70,74	1.95	17 (25%)	75,109,114	2.86	22 (29%)
25	CHL	2	609	1	65,69,74	1.99	18 (27%)	74,108,114	2.86	24 (32%)
25	CHL	7	607	-	57,61,74	2.25	20 (35%)	64,98,114	3.12	26 (40%)
30	LHG	c	2630	-	48,48,48	0.66	1 (2%)	51,54,54	1.31	7 (13%)
26	CLA	g	603	1	69,73,73	1.29	11 (15%)	83,113,113	1.50	13 (15%)
25	CHL	n	601	1	70,74,74	1.88	19 (27%)	80,114,114	3.03	27 (33%)
30	LHG	c	522	-	48,48,48	0.69	1 (2%)	51,54,54	1.26	6 (11%)
27	LUT	5	1621	-	42,43,43	0.90	2 (4%)	51,60,60	1.73	15 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	CLA	c	504	42	69,73,73	1.23	13 (18%)	83,113,113	1.46	7 (8%)
26	CLA	4	602	3	49,53,73	1.45	9 (18%)	59,89,113	1.41	6 (10%)
25	CHL	R	607	42	60,64,74	2.04	18 (30%)	68,102,114	3.33	25 (36%)
26	CLA	n	612	1	64,68,73	1.29	7 (10%)	77,107,113	1.32	9 (11%)
25	CHL	s	608	-	50,54,74	2.24	18 (36%)	56,90,114	3.31	19 (33%)
26	CLA	y	611	30	64,68,73	1.32	8 (12%)	77,107,113	1.46	8 (10%)
26	CLA	B	615	5	69,73,73	1.21	10 (14%)	83,113,113	1.38	8 (9%)
26	CLA	y	610	1	64,68,73	1.30	10 (15%)	77,107,113	1.19	9 (11%)
26	CLA	B	603	5	69,73,73	1.25	10 (14%)	83,113,113	1.34	8 (9%)
28	XAT	N	1622	-	39,47,47	0.92	0	54,74,74	3.00	24 (44%)
37	LMG	z	101	-	51,51,55	0.84	1 (1%)	59,59,63	1.32	5 (8%)
26	CLA	c	508	6	69,73,73	1.31	11 (15%)	83,113,113	1.64	12 (14%)
26	CLA	7	604	-	49,53,73	1.48	8 (16%)	59,89,113	1.32	7 (11%)
30	LHG	D	409	-	48,48,48	0.75	1 (2%)	51,54,54	1.31	7 (13%)
26	CLA	y	603	1	69,73,73	1.32	10 (14%)	83,113,113	1.51	14 (16%)
26	CLA	b	609	5	69,73,73	1.20	10 (14%)	83,113,113	1.52	13 (15%)
37	LMG	c	521	-	51,51,55	0.79	3 (5%)	59,59,63	1.37	6 (10%)
26	CLA	1	614	1	49,53,73	1.47	7 (14%)	59,89,113	1.30	6 (10%)
27	LUT	r	620	-	42,43,43	0.87	2 (4%)	51,60,60	1.82	14 (27%)
26	CLA	R	604	42	52,56,73	1.40	11 (21%)	62,92,113	1.55	10 (16%)
36	SQD	A	412	-	49,50,54	0.96	6 (12%)	58,61,65	1.74	11 (18%)
25	CHL	4	606	-	50,54,74	2.29	18 (36%)	56,90,114	3.30	26 (46%)
29	NEX	N	1623	-	38,46,46	0.90	1 (2%)	50,70,70	2.36	15 (30%)
39	DGD	c	518	-	56,56,67	1.17	7 (12%)	70,70,81	1.56	12 (17%)
26	CLA	b	605	5	69,73,73	1.43	11 (15%)	83,113,113	1.94	23 (27%)
26	CLA	1	603	1	59,63,73	1.31	10 (16%)	71,101,113	1.44	7 (9%)
25	CHL	7	605	2	50,54,74	2.27	18 (36%)	56,90,114	3.30	24 (42%)
27	LUT	8	620	-	42,43,43	0.80	0	51,60,60	1.87	18 (35%)
25	CHL	n	607	42	70,74,74	1.81	17 (24%)	80,114,114	3.05	23 (28%)
26	CLA	3	610	2	64,68,73	1.29	8 (12%)	77,107,113	1.18	7 (9%)
25	CHL	y	601	1	70,74,74	1.88	19 (27%)	80,114,114	3.11	27 (33%)
25	CHL	g	606	42	54,58,74	2.19	18 (33%)	59,94,114	3.18	25 (42%)
26	CLA	y	602	1	69,73,73	1.27	10 (14%)	83,113,113	1.38	11 (13%)
25	CHL	G	609	1	65,69,74	1.94	18 (27%)	74,108,114	2.95	25 (33%)
25	CHL	Y	601	1	70,74,74	1.88	19 (27%)	80,114,114	3.10	27 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	CLA	G	613	1	69,73,73	1.25	9 (13%)	83,113,113	1.26	6 (7%)
36	SQD	b	621	-	53,54,54	0.94	4 (7%)	62,65,65	1.64	13 (20%)
26	CLA	4	610	3	49,53,73	1.49	9 (18%)	59,89,113	1.18	6 (10%)
30	LHG	B	2630	-	46,46,48	0.65	1 (2%)	49,52,54	1.28	6 (12%)
25	CHL	5	608	-	50,54,74	2.18	17 (34%)	56,90,114	3.36	18 (32%)
30	LHG	L	101	-	48,48,48	0.90	1 (2%)	51,54,54	1.31	6 (11%)
26	CLA	b	612	5	69,73,73	1.31	9 (13%)	83,113,113	1.52	10 (12%)
25	CHL	R	614	19	46,50,74	2.31	18 (39%)	51,85,114	3.57	21 (41%)
26	CLA	R	601	19	53,57,73	1.39	6 (11%)	62,93,113	1.74	12 (19%)
26	CLA	d	403	7	69,73,73	1.23	8 (11%)	83,113,113	1.53	11 (13%)
29	NEX	6	1623	-	38,46,46	0.93	1 (2%)	50,70,70	2.38	15 (30%)
25	CHL	4	609	3	50,54,74	2.31	19 (38%)	56,90,114	3.26	20 (35%)
26	CLA	Y	612	1	64,68,73	1.33	10 (15%)	77,107,113	1.34	6 (7%)
26	CLA	2	611	30	49,53,73	1.46	6 (12%)	59,89,113	1.38	7 (11%)
41	HEM	f	101	8,9	50,50,50	1.34	7 (14%)	66,82,82	1.18	7 (10%)
26	CLA	r	613	19	64,68,73	1.31	7 (10%)	77,107,113	1.18	7 (9%)
29	NEX	G	1623	-	38,46,46	1.00	2 (5%)	50,70,70	2.39	14 (28%)
26	CLA	r	604	42	52,56,73	1.39	11 (21%)	62,92,113	1.55	10 (16%)
26	CLA	G	602	1	69,73,73	1.27	11 (15%)	83,113,113	1.43	12 (14%)
26	CLA	B	614	5	69,73,73	1.29	9 (13%)	83,113,113	1.33	6 (7%)
30	LHG	C	523	-	48,48,48	0.66	1 (2%)	51,54,54	1.20	5 (9%)
26	CLA	G	603	1	69,73,73	1.29	11 (15%)	83,113,113	1.49	13 (15%)
26	CLA	g	611	30	64,68,73	1.34	10 (15%)	77,107,113	1.49	6 (7%)
26	CLA	a	407	42	54,58,73	1.40	9 (16%)	65,95,113	1.48	8 (12%)
31	BCR	B	619	-	41,41,41	0.80	0	56,56,56	1.81	17 (30%)
29	NEX	R	623	-	38,46,46	1.05	3 (7%)	50,70,70	2.51	19 (38%)
31	BCR	C	517	-	41,41,41	0.89	1 (2%)	56,56,56	2.08	11 (19%)
30	LHG	1	2630	26	40,40,48	0.72	1 (2%)	43,46,54	1.34	6 (13%)
39	DGD	H	102	-	63,63,67	1.08	7 (11%)	77,77,81	1.40	11 (14%)
37	LMG	Z	101	-	51,51,55	0.84	1 (1%)	59,59,63	1.32	5 (8%)
26	CLA	5	614	1	49,53,73	1.47	7 (14%)	59,89,113	1.30	7 (11%)
29	NEX	g	1623	-	38,46,46	1.00	3 (7%)	50,70,70	2.39	14 (28%)
26	CLA	B	604	5	69,73,73	1.33	10 (14%)	83,113,113	1.38	12 (14%)
30	LHG	b	2630	-	46,46,48	0.66	1 (2%)	49,52,54	1.28	6 (12%)
26	CLA	5	603	1	59,63,73	1.31	10 (16%)	71,101,113	1.44	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
37	LMG	a	415	-	40,40,55	0.86	0	48,48,63	1.29	5 (10%)
26	CLA	s	604	42	54,58,73	1.41	10 (18%)	65,95,113	1.76	9 (13%)
26	CLA	3	603	2	59,63,73	1.30	10 (16%)	71,101,113	1.47	8 (11%)
25	CHL	y	607	42	70,74,74	1.84	16 (22%)	80,114,114	2.94	26 (32%)
27	LUT	G	1620	-	42,43,43	0.76	0	51,60,60	1.64	12 (23%)
25	CHL	Y	608	42	70,74,74	1.84	18 (25%)	80,114,114	2.89	27 (33%)
27	LUT	s	1620	-	42,43,43	0.78	0	51,60,60	1.76	12 (23%)
25	CHL	3	609	2	65,69,74	2.04	17 (26%)	74,108,114	2.73	23 (31%)
26	CLA	B	617	5	69,73,73	1.31	11 (15%)	83,113,113	1.47	10 (12%)
30	LHG	l	101	-	48,48,48	0.90	1 (2%)	51,54,54	1.31	7 (13%)
25	CHL	5	601	1	50,54,74	2.32	18 (36%)	56,90,114	3.27	24 (42%)
26	CLA	4	612	3	49,53,73	1.47	7 (14%)	59,89,113	1.34	6 (10%)
39	DGD	b	626	-	60,60,67	1.05	3 (5%)	74,74,81	1.39	12 (16%)
26	CLA	c	512	6	69,73,73	1.24	10 (14%)	83,113,113	1.39	9 (10%)
26	CLA	S	609	20	49,53,73	1.50	6 (12%)	59,89,113	1.26	8 (13%)
41	HEM	F	101	8,9	50,50,50	1.34	7 (14%)	66,82,82	1.18	7 (10%)
26	CLA	a	406	42	69,73,73	1.26	10 (14%)	83,113,113	1.59	16 (19%)
26	CLA	g	602	1	69,73,73	1.27	11 (15%)	83,113,113	1.42	12 (14%)
26	CLA	y	604	42	54,58,73	1.46	10 (18%)	65,95,113	1.64	10 (15%)
31	BCR	H	101	-	41,41,41	0.78	0	56,56,56	1.90	10 (17%)
30	LHG	G	2630	26	48,48,48	0.66	1 (2%)	51,54,54	1.28	6 (11%)
26	CLA	g	610	1	68,72,73	1.24	7 (10%)	81,111,113	1.23	6 (7%)
28	XAT	g	1622	-	39,47,47	0.98	2 (5%)	54,74,74	2.91	22 (40%)
31	BCR	b	620	-	41,41,41	0.80	0	56,56,56	1.99	16 (28%)
26	CLA	S	613	20	59,63,73	1.32	9 (15%)	71,101,113	1.36	8 (11%)
25	CHL	G	607	42	70,74,74	1.93	17 (24%)	80,114,114	2.91	26 (32%)
27	LUT	s	1621	-	42,43,43	0.85	1 (2%)	51,60,60	1.78	17 (33%)
26	CLA	A	407	42	54,58,73	1.39	9 (16%)	65,95,113	1.49	8 (12%)
26	CLA	N	613	1	64,68,73	1.25	8 (12%)	77,107,113	1.44	5 (6%)
25	CHL	G	606	42	54,58,74	2.20	18 (33%)	59,94,114	3.18	25 (42%)
25	CHL	N	606	42	54,58,74	2.14	18 (33%)	59,94,114	3.15	23 (38%)
26	CLA	7	613	2	62,66,73	1.32	9 (14%)	74,104,113	1.28	7 (9%)
28	XAT	6	1622	-	39,47,47	0.91	1 (2%)	54,74,74	2.81	21 (38%)
37	LMG	A	415	-	40,40,55	0.86	0	48,48,63	1.28	5 (10%)
30	LHG	r	2630	26	41,41,48	0.70	1 (2%)	44,47,54	1.27	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	CLA	N	614	1	52,56,73	1.39	6 (11%)	62,92,113	1.47	8 (12%)
25	CHL	G	608	42	70,74,74	1.87	19 (27%)	80,114,114	2.89	25 (31%)
26	CLA	7	614	2	52,56,73	1.42	8 (15%)	62,92,113	1.15	5 (8%)
27	LUT	n	1620	-	42,43,43	0.80	0	51,60,60	1.69	12 (23%)
26	CLA	2	602	1	65,69,73	1.30	10 (15%)	78,108,113	1.19	8 (10%)
26	CLA	N	611	30	64,68,73	1.29	8 (12%)	77,107,113	1.37	6 (7%)
26	CLA	N	610	1	69,73,73	1.21	9 (13%)	83,113,113	1.28	11 (13%)
30	LHG	c	523	-	48,48,48	0.66	1 (2%)	51,54,54	1.20	5 (9%)
26	CLA	c	510	6	69,73,73	1.26	8 (11%)	83,113,113	1.43	10 (12%)
25	CHL	5	607	-	67,71,74	1.92	19 (28%)	76,110,114	3.11	24 (31%)
25	CHL	3	608	-	50,54,74	2.19	18 (36%)	56,90,114	3.42	21 (37%)
30	LHG	7	2630	26	46,46,48	0.70	1 (2%)	49,52,54	1.25	5 (10%)
31	BCR	b	619	-	41,41,41	0.80	0	56,56,56	1.81	17 (30%)
25	CHL	r	606	42	70,74,74	1.90	16 (22%)	80,114,114	2.93	26 (32%)
31	BCR	c	516	-	41,41,41	0.73	0	56,56,56	1.98	17 (30%)
39	DGD	C	518	-	56,56,67	1.17	7 (12%)	70,70,81	1.56	13 (18%)
25	CHL	S	601	20	50,54,74	2.29	18 (36%)	56,90,114	3.38	25 (44%)
25	CHL	7	608	-	50,54,74	2.19	18 (36%)	56,90,114	3.42	22 (39%)
25	CHL	N	609	1	70,74,74	1.90	18 (25%)	80,114,114	2.86	26 (32%)
31	BCR	t	101	-	41,41,41	0.76	0	56,56,56	2.55	19 (33%)
26	CLA	y	612	1	64,68,73	1.33	9 (14%)	77,107,113	1.34	7 (9%)
26	CLA	R	602	19	64,68,73	1.28	9 (14%)	77,107,113	1.48	11 (14%)
25	CHL	r	608	42	65,69,74	1.93	13 (20%)	74,108,114	2.99	26 (35%)
26	CLA	S	612	20	53,57,73	1.38	8 (15%)	62,93,113	1.47	6 (9%)
25	CHL	n	609	1	70,74,74	1.90	18 (25%)	80,114,114	2.86	26 (32%)
25	CHL	R	608	42	65,69,74	1.93	13 (20%)	74,108,114	2.99	27 (36%)
25	CHL	N	605	1	52,56,74	2.20	19 (36%)	58,92,114	3.43	24 (41%)
26	CLA	S	602	20	65,69,73	1.27	11 (16%)	78,108,113	1.35	13 (16%)
26	CLA	n	613	1	64,68,73	1.25	8 (12%)	77,107,113	1.45	5 (6%)
25	CHL	n	605	1	52,56,74	2.21	18 (34%)	58,92,114	3.44	24 (41%)
26	CLA	1	612	1	49,53,73	1.48	9 (18%)	59,89,113	1.45	10 (16%)
26	CLA	4	603	3	49,53,73	1.49	10 (20%)	59,89,113	1.44	6 (10%)
26	CLA	R	603	19	64,68,73	1.24	10 (15%)	77,107,113	1.51	14 (18%)
25	CHL	g	608	42	70,74,74	1.87	18 (25%)	80,114,114	2.89	25 (31%)
25	CHL	n	606	42	54,58,74	2.15	18 (33%)	59,94,114	3.15	23 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	CLA	B	616	5	69,73,73	1.22	10 (14%)	83,113,113	1.37	10 (12%)
26	CLA	7	602	2	64,68,73	1.30	8 (12%)	77,107,113	1.21	8 (10%)
26	CLA	g	612	1	64,68,73	1.28	7 (10%)	77,107,113	1.24	7 (9%)
36	SQD	B	621	-	53,54,54	0.94	4 (7%)	62,65,65	1.64	13 (20%)
31	BCR	d	404	-	41,41,41	0.74	0	56,56,56	1.84	12 (21%)
26	CLA	b	604	5	69,73,73	1.33	10 (14%)	83,113,113	1.37	12 (14%)
31	BCR	a	411	-	41,41,41	0.79	0	56,56,56	1.78	13 (23%)
25	CHL	y	605	1	52,56,74	2.15	17 (32%)	58,92,114	3.43	21 (36%)
26	CLA	3	604	-	49,53,73	1.48	9 (18%)	59,89,113	1.32	6 (10%)
31	BCR	C	515	-	41,41,41	0.93	2 (4%)	56,56,56	2.01	16 (28%)
25	CHL	2	605	1	50,54,74	2.27	19 (38%)	56,90,114	3.31	22 (39%)
26	CLA	C	511	6	69,73,73	1.25	11 (15%)	83,113,113	1.42	9 (10%)
26	CLA	B	605	5	69,73,73	1.42	10 (14%)	83,113,113	1.94	23 (27%)
27	LUT	7	1620	-	42,43,43	0.84	0	51,60,60	1.71	12 (23%)
35	PHO	A	409	-	58,69,69	1.91	9 (15%)	56,99,99	1.68	10 (17%)
26	CLA	b	610	5	69,73,73	1.25	11 (15%)	83,113,113	1.48	10 (12%)
26	CLA	C	507	42	69,73,73	1.29	12 (17%)	83,113,113	1.61	9 (10%)
31	BCR	B	620	-	41,41,41	0.79	0	56,56,56	1.99	16 (28%)
25	CHL	N	608	42	70,74,74	1.87	18 (25%)	80,114,114	2.95	29 (36%)
27	LUT	2	1621	-	42,43,43	0.84	1 (2%)	51,60,60	1.68	15 (29%)
25	CHL	3	601	2	68,72,74	1.95	16 (23%)	77,111,114	3.10	27 (35%)
26	CLA	8	602	3	49,53,73	1.45	8 (16%)	59,89,113	1.42	6 (10%)
26	CLA	2	612	1	49,53,73	1.51	7 (14%)	59,89,113	1.37	6 (10%)
29	NEX	1	1623	-	38,46,46	0.99	2 (5%)	50,70,70	2.42	15 (30%)
39	DGD	h	102	-	63,63,67	1.08	7 (11%)	77,77,81	1.41	11 (14%)
28	XAT	5	1622	-	39,47,47	0.90	0	54,74,74	2.77	22 (40%)
31	BCR	h	101	-	41,41,41	0.78	0	56,56,56	1.89	10 (17%)
27	LUT	g	1620	-	42,43,43	0.77	0	51,60,60	1.63	12 (23%)
26	CLA	y	613	1	69,73,73	1.25	9 (13%)	83,113,113	1.33	10 (12%)
26	CLA	C	512	6	69,73,73	1.24	10 (14%)	83,113,113	1.39	9 (10%)
28	XAT	8	622	-	39,47,47	0.93	1 (2%)	54,74,74	2.62	21 (38%)
25	CHL	Y	605	1	52,56,74	2.15	17 (32%)	58,92,114	3.43	21 (36%)
28	XAT	n	1622	-	39,47,47	0.93	0	54,74,74	3.00	24 (44%)
25	CHL	Y	606	42	54,58,74	2.04	15 (27%)	59,94,114	3.19	21 (35%)
26	CLA	c	513	6	69,73,73	1.20	9 (13%)	83,113,113	1.47	15 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	BCR	4	623	-	41,41,41	0.74	0	56,56,56	2.31	17 (30%)
37	LMG	B	622	-	51,51,55	0.83	1 (1%)	59,59,63	1.30	4 (6%)
26	CLA	b	608	42	69,73,73	1.33	10 (14%)	83,113,113	1.55	10 (12%)
30	LHG	4	2630	26	20,20,48	0.91	1 (5%)	23,26,54	1.30	2 (8%)
26	CLA	4	604	-	49,53,73	1.49	8 (16%)	59,89,113	1.28	5 (8%)
25	CHL	n	608	42	70,74,74	1.86	18 (25%)	80,114,114	2.95	29 (36%)
30	LHG	g	2630	26	48,48,48	0.66	1 (2%)	51,54,54	1.28	6 (11%)
26	CLA	S	614	20	53,57,73	1.37	7 (13%)	62,93,113	1.54	9 (14%)
28	XAT	2	1622	-	39,47,47	0.91	1 (2%)	54,74,74	2.82	21 (38%)
37	LMG	a	413	-	48,48,55	0.79	0	56,56,63	1.31	6 (10%)
25	CHL	4	607	-	50,54,74	2.30	18 (36%)	56,90,114	3.17	21 (37%)
25	CHL	1	601	1	50,54,74	2.33	18 (36%)	56,90,114	3.27	24 (42%)
25	CHL	r	607	42	60,64,74	2.04	17 (28%)	68,102,114	3.33	25 (36%)
29	NEX	S	1623	-	38,46,46	0.91	2 (5%)	50,70,70	2.24	15 (30%)
25	CHL	3	607	-	57,61,74	2.25	20 (35%)	64,98,114	3.12	26 (40%)
26	CLA	G	614	1	52,56,73	1.44	6 (11%)	62,92,113	1.31	9 (14%)
26	CLA	R	612	19	53,57,73	1.45	7 (13%)	62,93,113	1.51	6 (9%)
26	CLA	b	607	5	69,73,73	1.31	11 (15%)	83,113,113	1.48	15 (18%)
30	LHG	6	2630	26	36,36,48	0.74	1 (2%)	39,42,54	1.27	4 (10%)
39	DGD	B	626	-	60,60,67	1.04	3 (5%)	74,74,81	1.39	12 (16%)
26	CLA	6	610	1	54,58,73	1.37	8 (14%)	65,95,113	1.23	8 (12%)
37	LMG	d	411	-	46,46,55	0.92	3 (6%)	54,54,63	1.45	4 (7%)
26	CLA	6	613	1	49,53,73	1.46	9 (18%)	59,89,113	1.28	6 (10%)
35	PHO	a	409	-	58,69,69	1.91	9 (15%)	56,99,99	1.69	10 (17%)
27	LUT	7	1621	-	42,43,43	0.86	1 (2%)	51,60,60	1.60	11 (21%)
26	CLA	a	405	4	69,73,73	1.36	10 (14%)	83,113,113	1.46	11 (13%)
25	CHL	6	609	1	65,69,74	2.00	18 (27%)	74,108,114	2.87	24 (32%)
37	LMG	D	411	-	46,46,55	0.92	3 (6%)	54,54,63	1.46	4 (7%)
26	CLA	1	604	-	54,58,73	1.43	10 (18%)	65,95,113	1.37	10 (15%)
26	CLA	3	602	2	64,68,73	1.30	8 (12%)	77,107,113	1.21	8 (10%)
26	CLA	C	501	6	69,73,73	1.25	8 (11%)	83,113,113	1.28	9 (10%)
30	LHG	d	410	-	42,42,48	0.68	1 (2%)	45,48,54	1.22	4 (8%)
26	CLA	1	611	30	49,53,73	1.48	10 (20%)	59,89,113	1.28	6 (10%)
26	CLA	2	603	1	59,63,73	1.35	9 (15%)	71,101,113	1.40	8 (11%)
30	LHG	D	408	-	45,45,48	0.77	1 (2%)	48,51,54	1.28	5 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	CLA	Y	602	1	69,73,73	1.27	10 (14%)	83,113,113	1.38	11 (13%)
26	CLA	5	613	1	59,63,73	1.36	9 (15%)	71,101,113	1.23	5 (7%)
36	SQD	b	623	-	41,42,54	1.09	5 (12%)	50,53,65	1.77	10 (20%)
25	CHL	5	605	1	50,54,74	2.23	18 (36%)	56,90,114	3.38	24 (42%)
26	CLA	1	610	1	60,64,73	1.30	8 (13%)	72,102,113	1.16	6 (8%)
26	CLA	2	613	1	49,53,73	1.46	9 (18%)	59,89,113	1.28	6 (10%)
25	CHL	5	606	-	50,54,74	2.25	17 (34%)	56,90,114	3.16	22 (39%)
25	CHL	g	609	1	65,69,74	1.94	18 (27%)	74,108,114	2.95	25 (33%)
28	XAT	Y	1622	-	39,47,47	1.08	4 (10%)	54,74,74	3.00	21 (38%)
26	CLA	A	405	4	69,73,73	1.36	10 (14%)	83,113,113	1.47	11 (13%)
26	CLA	g	613	1	69,73,73	1.25	9 (13%)	83,113,113	1.26	6 (7%)
27	LUT	3	1620	-	42,43,43	0.85	0	51,60,60	1.72	13 (25%)
25	CHL	2	606	-	50,54,74	2.26	18 (36%)	56,90,114	3.22	22 (39%)
26	CLA	6	611	30	49,53,73	1.46	8 (16%)	59,89,113	1.38	7 (11%)
40	BCT	D	401	33	2,3,3	1.32	0	2,3,3	4.20	2 (100%)
26	CLA	B	606	5	69,73,73	1.35	11 (15%)	83,113,113	1.56	12 (14%)
27	LUT	n	1621	-	42,43,43	0.89	2 (4%)	51,60,60	1.83	14 (27%)
26	CLA	r	603	19	64,68,73	1.25	10 (15%)	77,107,113	1.51	14 (18%)
27	LUT	y	1620	-	42,43,43	0.88	1 (2%)	51,60,60	1.72	13 (25%)
26	CLA	6	602	1	65,69,73	1.30	10 (15%)	78,108,113	1.20	9 (11%)
35	PHO	A	408	-	58,69,69	1.93	12 (20%)	56,99,99	1.71	15 (26%)
37	LMG	b	622	-	51,51,55	0.83	1 (1%)	59,59,63	1.30	4 (6%)
25	CHL	7	606	-	50,54,74	2.20	17 (34%)	56,90,114	3.24	22 (39%)
28	XAT	7	1622	-	39,47,47	1.03	2 (5%)	54,74,74	2.85	24 (44%)
30	LHG	S	2630	26	48,48,48	0.73	1 (2%)	51,54,54	1.26	7 (13%)
26	CLA	r	601	19	53,57,73	1.39	6 (11%)	62,93,113	1.74	12 (19%)
25	CHL	S	607	42	62,66,74	1.96	18 (29%)	70,104,114	3.10	24 (34%)
25	CHL	1	605	1	50,54,74	2.23	18 (36%)	56,90,114	3.38	24 (42%)
26	CLA	C	509	6	69,73,73	1.27	10 (14%)	83,113,113	1.56	12 (14%)
30	LHG	N	2630	26	48,48,48	0.66	1 (2%)	51,54,54	1.30	6 (11%)
37	LMG	A	413	-	48,48,55	0.79	0	56,56,63	1.31	6 (10%)
25	CHL	N	607	42	70,74,74	1.81	17 (24%)	80,114,114	3.06	23 (28%)
31	BCR	D	404	-	41,41,41	0.75	0	56,56,56	1.83	12 (21%)
26	CLA	D	402	7	69,73,73	1.38	10 (14%)	83,113,113	1.61	12 (14%)
39	DGD	C	519	-	63,63,67	1.11	5 (7%)	77,77,81	1.47	12 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CHL	S	606	42	50,54,74	2.26	17 (34%)	56,90,114	3.46	23 (41%)
30	LHG	n	2630	26	48,48,48	0.66	1 (2%)	51,54,54	1.30	6 (11%)
26	CLA	Y	613	1	69,73,73	1.25	9 (13%)	83,113,113	1.34	10 (12%)
26	CLA	a	410	4	64,68,73	1.27	10 (15%)	77,107,113	1.54	9 (11%)
26	CLA	B	609	5	69,73,73	1.20	10 (14%)	83,113,113	1.51	13 (15%)
26	CLA	s	614	20	53,57,73	1.37	7 (13%)	62,93,113	1.54	9 (14%)
26	CLA	y	614	1	52,56,73	1.41	10 (19%)	62,92,113	1.45	8 (12%)
26	CLA	s	609	20	49,53,73	1.50	5 (10%)	59,89,113	1.26	8 (13%)
29	NEX	r	623	-	38,46,46	1.04	3 (7%)	50,70,70	2.51	19 (38%)
32	OEX	A	401	6,4	0,14,14	-	-	-		
26	CLA	2	614	1	49,53,73	1.49	7 (14%)	59,89,113	1.27	4 (6%)
26	CLA	G	610	1	68,72,73	1.24	7 (10%)	81,111,113	1.23	7 (8%)
26	CLA	Y	614	1	52,56,73	1.41	10 (19%)	62,92,113	1.45	9 (14%)
36	SQD	B	623	-	41,42,54	1.10	5 (12%)	50,53,65	1.77	10 (20%)
31	BCR	A	411	-	41,41,41	0.79	0	56,56,56	1.78	13 (23%)
36	SQD	a	412	-	49,50,54	0.96	6 (12%)	58,61,65	1.75	11 (18%)
26	CLA	5	602	1	65,69,73	1.29	10 (15%)	78,108,113	1.20	8 (10%)
26	CLA	S	604	42	54,58,73	1.41	10 (18%)	65,95,113	1.75	8 (12%)
38	PL9	D	405	-	55,55,55	1.83	12 (21%)	68,69,69	1.57	12 (17%)
26	CLA	B	602	42	69,73,73	1.26	9 (13%)	83,113,113	1.32	6 (7%)
25	CHL	6	607	-	65,69,74	1.96	19 (29%)	74,108,114	2.95	24 (32%)
25	CHL	y	608	42	70,74,74	1.84	18 (25%)	80,114,114	2.89	27 (33%)
26	CLA	N	604	42	54,58,73	1.49	10 (18%)	65,95,113	1.62	9 (13%)
30	LHG	2	2630	26	36,36,48	0.74	1 (2%)	39,42,54	1.27	4 (10%)
25	CHL	8	609	3	50,54,74	2.31	19 (38%)	56,90,114	3.26	20 (35%)
26	CLA	s	602	20	65,69,73	1.27	11 (16%)	78,108,113	1.34	13 (16%)
25	CHL	Y	609	1	70,74,74	1.87	18 (25%)	80,114,114	2.84	25 (31%)
26	CLA	N	603	1	69,73,73	1.31	10 (14%)	83,113,113	1.54	16 (19%)
26	CLA	g	604	42	54,58,73	1.48	10 (18%)	65,95,113	1.58	11 (16%)
25	CHL	8	606	-	50,54,74	2.29	19 (38%)	56,90,114	3.30	25 (44%)
26	CLA	C	506	6	69,73,73	1.27	10 (14%)	83,113,113	1.45	12 (14%)
32	OEX	a	401	6,4	0,14,14	-	-	-		
25	CHL	4	608	-	50,54,74	2.16	17 (34%)	56,90,114	3.42	21 (37%)
26	CLA	2	610	1	54,58,73	1.37	8 (14%)	65,95,113	1.23	8 (12%)
29	NEX	7	1623	-	38,46,46	0.87	1 (2%)	50,70,70	2.39	16 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	BCR	c	515	-	41,41,41	0.93	2 (4%)	56,56,56	2.01	16 (28%)
25	CHL	g	607	42	70,74,74	1.92	17 (24%)	80,114,114	2.91	25 (31%)
26	CLA	c	511	6	69,73,73	1.25	11 (15%)	83,113,113	1.42	9 (10%)
26	CLA	6	604	-	49,53,73	1.47	8 (16%)	59,89,113	1.36	6 (10%)
31	BCR	T	101	-	41,41,41	0.75	0	56,56,56	2.55	19 (33%)
39	DGD	C	520	-	61,61,67	1.17	8 (13%)	75,75,81	1.47	12 (16%)
28	XAT	1	1622	-	39,47,47	0.90	0	54,74,74	2.77	22 (40%)
25	CHL	s	601	20	50,54,74	2.29	18 (36%)	56,90,114	3.38	25 (44%)
26	CLA	b	611	42	69,73,73	1.26	10 (14%)	83,113,113	1.58	13 (15%)
26	CLA	c	505	6	69,73,73	1.30	11 (15%)	83,113,113	1.64	9 (10%)
26	CLA	r	611	30	53,57,73	1.43	10 (18%)	62,93,113	1.59	10 (16%)
26	CLA	G	612	1	64,68,73	1.28	7 (10%)	77,107,113	1.24	7 (9%)
30	LHG	y	2630	26	48,48,48	0.79	2 (4%)	51,54,54	1.23	6 (11%)
26	CLA	C	503	6	69,73,73	1.31	11 (15%)	83,113,113	1.35	10 (12%)
26	CLA	2	604	-	49,53,73	1.47	8 (16%)	59,89,113	1.36	6 (10%)
25	CHL	8	601	3	48,53,74	2.38	19 (39%)	53,89,114	3.18	19 (35%)
26	CLA	c	509	6	69,73,73	1.27	10 (14%)	83,113,113	1.56	12 (14%)
26	CLA	g	614	1	52,56,73	1.44	6 (11%)	62,92,113	1.31	9 (14%)
26	CLA	3	613	2	62,66,73	1.32	9 (14%)	74,104,113	1.28	7 (9%)
39	DGD	c	519	-	63,63,67	1.11	5 (7%)	77,77,81	1.47	12 (15%)
30	LHG	b	2631	-	48,48,48	0.68	2 (4%)	51,54,54	1.22	6 (11%)
31	BCR	C	514	-	41,41,41	0.90	1 (2%)	56,56,56	1.75	13 (23%)
30	LHG	d	408	-	45,45,48	0.78	1 (2%)	48,51,54	1.28	5 (10%)
26	CLA	b	615	5	69,73,73	1.21	10 (14%)	83,113,113	1.38	8 (9%)
26	CLA	8	612	3	49,53,73	1.47	7 (14%)	59,89,113	1.35	6 (10%)
26	CLA	C	510	6	69,73,73	1.27	8 (11%)	83,113,113	1.43	10 (12%)
25	CHL	R	606	42	70,74,74	1.90	16 (22%)	80,114,114	2.93	26 (32%)
26	CLA	C	502	6	69,73,73	1.27	10 (14%)	83,113,113	1.59	7 (8%)
25	CHL	y	606	42	54,58,74	2.04	15 (27%)	59,94,114	3.20	21 (35%)
35	PHO	a	408	-	58,69,69	1.94	12 (20%)	56,99,99	1.71	13 (23%)
26	CLA	5	612	1	49,53,73	1.49	9 (18%)	59,89,113	1.45	10 (16%)
31	BCR	c	517	-	41,41,41	0.89	1 (2%)	56,56,56	2.09	11 (19%)
27	LUT	6	1621	-	42,43,43	0.84	1 (2%)	51,60,60	1.68	15 (29%)
26	CLA	B	608	42	69,73,73	1.32	10 (14%)	83,113,113	1.55	11 (13%)
29	NEX	n	1623	-	38,46,46	0.90	1 (2%)	50,70,70	2.36	15 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	LUT	Y	1620	-	42,43,43	0.87	1 (2%)	51,60,60	1.73	13 (25%)
30	LHG	3	2630	26	46,46,48	0.70	1 (2%)	49,52,54	1.24	5 (10%)
26	CLA	n	611	30	64,68,73	1.29	8 (12%)	77,107,113	1.37	6 (7%)
29	NEX	3	1623	-	38,46,46	0.87	1 (2%)	50,70,70	2.40	16 (32%)
30	LHG	Y	2630	26	48,48,48	0.79	2 (4%)	51,54,54	1.23	6 (11%)
38	PL9	a	414	-	13,13,55	0.87	0	17,17,69	1.68	4 (23%)
25	CHL	3	606	-	50,54,74	2.20	17 (34%)	56,90,114	3.24	23 (41%)
25	CHL	4	601	3	48,53,74	2.38	19 (39%)	53,89,114	3.18	19 (35%)
25	CHL	Y	607	42	70,74,74	1.84	17 (24%)	80,114,114	2.94	26 (32%)
29	NEX	y	1623	-	38,46,46	0.94	2 (5%)	50,70,70	2.59	18 (36%)
31	BCR	B	618	-	41,41,41	0.84	1 (2%)	56,56,56	1.85	14 (25%)
26	CLA	n	604	42	54,58,73	1.48	10 (18%)	65,95,113	1.62	9 (13%)
26	CLA	R	613	19	64,68,73	1.30	7 (10%)	77,107,113	1.17	7 (9%)
29	NEX	Y	1623	-	38,46,46	0.94	2 (5%)	50,70,70	2.59	18 (36%)
26	CLA	R	609	19	62,66,73	1.32	7 (11%)	74,104,113	1.42	6 (8%)

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
26	CLA	1	613	1	-	10/27/103/115	-
26	CLA	7	611	30	-	9/27/103/115	-
25	CHL	1	606	-	-	10/17/93/117	-
26	CLA	S	603	20	-	7/15/91/115	-
26	CLA	Y	610	1	-	9/33/109/115	-
26	CLA	s	603	20	-	7/15/91/115	-
26	CLA	7	610	2	-	9/33/109/115	-
28	XAT	4	622	-	-	2/31/93/93	0/4/4/4
26	CLA	6	612	1	-	5/15/91/115	-
25	CHL	6	606	-	-	6/17/93/117	-
26	CLA	n	610	1	-	12/39/115/115	-
39	DGD	c	520	-	-	21/49/89/95	0/2/2/2
38	PL9	A	414	-	-	1/5/18/73	0/1/1/1
25	CHL	7	609	2	1/1/14/21	15/35/111/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	LMG	b	2633	-	-	24/50/70/70	0/1/1/1
31	BCR	b	618	-	-	2/29/63/63	0/2/2/2
26	CLA	R	610	19	-	15/39/115/115	-
25	CHL	G	601	1	1/1/15/21	16/41/117/117	-
26	CLA	1	602	1	-	14/35/111/115	-
26	CLA	c	503	6	-	16/39/115/115	-
27	LUT	Y	1621	-	-	1/29/67/67	0/2/2/2
27	LUT	G	1621	-	-	3/29/67/67	0/2/2/2
25	CHL	3	605	2	-	11/17/93/117	-
25	CHL	g	605	1	-	9/17/93/117	-
25	CHL	1	609	1	1/1/14/21	18/37/113/117	-
26	CLA	6	603	1	-	13/27/103/115	-
26	CLA	Y	611	30	-	8/33/109/115	-
26	CLA	D	403	7	-	12/39/115/115	-
30	LHG	5	2630	26	-	15/45/45/53	-
31	BCR	c	514	-	-	4/29/63/63	0/2/2/2
25	CHL	r	614	19	-	8/12/88/117	-
25	CHL	6	605	1	-	11/17/93/117	-
26	CLA	r	609	19	-	3/31/107/115	-
26	CLA	B	613	5	-	16/39/115/115	-
30	LHG	s	2630	26	-	27/53/53/53	-
26	CLA	B	607	5	-	9/39/115/115	-
29	NEX	5	1623	-	-	6/27/83/83	0/3/3/3
25	CHL	s	607	42	1/1/13/21	19/32/108/117	-
26	CLA	3	611	30	-	9/27/103/115	-
31	BCR	C	516	-	-	7/29/63/63	0/2/2/2
26	CLA	s	613	20	-	6/27/103/115	-
26	CLA	d	402	7	-	4/39/115/115	-
25	CHL	s	606	42	-	10/17/93/117	-
26	CLA	Y	604	42	-	3/21/97/115	-
28	XAT	y	1622	-	-	2/31/93/93	0/4/4/4
26	CLA	C	505	6	-	17/39/115/115	-
26	CLA	b	617	5	-	18/39/115/115	-
27	LUT	S	1620	-	-	2/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	n	603	1	-	15/39/115/115	-
30	LHG	D	410	-	-	29/47/47/53	-
25	CHL	2	608	-	-	7/17/93/117	-
26	CLA	8	603	3	-	6/15/91/115	-
26	CLA	N	602	1	-	12/39/115/115	-
26	CLA	G	604	42	-	5/21/97/115	-
27	LUT	5	1620	-	-	2/29/67/67	0/2/2/2
25	CHL	6	601	1	-	6/17/93/117	-
27	LUT	3	1621	-	-	3/29/67/67	0/2/2/2
27	LUT	4	620	-	-	4/29/67/67	0/2/2/2
30	LHG	d	409	-	-	27/53/53/53	-
26	CLA	3	612	2	-	10/15/91/115	-
27	LUT	R	620	-	-	4/29/67/67	0/2/2/2
29	NEX	s	1623	-	-	5/27/83/83	0/3/3/3
26	CLA	B	611	42	-	12/39/115/115	-
26	CLA	G	611	30	-	13/33/109/115	-
30	LHG	B	2631	-	-	23/53/53/53	-
26	CLA	b	606	5	-	16/39/115/115	-
26	CLA	7	612	2	-	10/15/91/115	-
26	CLA	s	611	30	-	11/29/105/115	-
29	NEX	2	1623	-	-	7/27/83/83	0/3/3/3
25	CHL	1	608	-	-	7/17/93/117	-
28	XAT	r	622	-	-	3/31/93/93	0/4/4/4
26	CLA	S	610	20	-	6/27/103/115	-
26	CLA	5	611	30	-	8/15/91/115	-
25	CHL	2	601	1	-	6/17/93/117	-
25	CHL	g	601	1	1/1/15/21	16/41/117/117	-
26	CLA	b	616	5	-	15/39/115/115	-
26	CLA	c	507	42	-	23/39/115/115	-
30	LHG	C	2630	-	-	27/53/53/53	-
25	CHL	1	607	-	1/1/14/21	22/38/114/117	-
26	CLA	r	602	19	-	8/33/109/115	-
25	CHL	S	608	-	-	4/17/93/117	-
26	CLA	R	611	30	-	9/20/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	LHG	C	522	-	-	20/53/53/53	-
26	CLA	r	610	19	-	15/39/115/115	-
38	PL9	d	405	-	-	10/53/73/73	0/1/1/1
26	CLA	b	613	5	-	16/39/115/115	-
30	LHG	8	2630	26	-	8/23/23/53	-
26	CLA	C	504	42	-	18/39/115/115	-
27	LUT	N	1620	-	-	2/29/67/67	0/2/2/2
25	CHL	G	605	1	-	9/17/93/117	-
26	CLA	n	614	1	-	6/19/95/115	-
27	LUT	2	1620	-	-	2/29/67/67	0/2/2/2
25	CHL	8	607	-	-	10/17/93/117	-
27	LUT	6	1620	-	-	2/29/67/67	0/2/2/2
26	CLA	A	406	42	-	12/39/115/115	-
36	SQD	a	418	-	-	22/49/69/69	0/1/1/1
26	CLA	Y	603	1	-	13/39/115/115	-
26	CLA	A	410	4	-	7/33/109/115	-
26	CLA	S	611	30	-	11/29/105/115	-
26	CLA	5	610	1	-	7/29/105/115	-
26	CLA	3	614	2	-	11/19/95/115	-
26	CLA	C	508	6	-	11/39/115/115	-
27	LUT	y	1621	-	-	1/29/67/67	0/2/2/2
25	CHL	N	601	1	1/1/15/21	16/41/117/117	-
26	CLA	b	602	42	-	17/39/115/115	-
26	CLA	8	610	3	-	6/15/91/115	-
27	LUT	S	1621	-	-	2/29/67/67	0/2/2/2
37	LMG	C	521	-	-	22/46/66/70	0/1/1/1
25	CHL	7	601	2	1/1/14/21	18/39/115/117	-
27	LUT	1	1620	-	-	2/29/67/67	0/2/2/2
26	CLA	C	513	6	-	10/39/115/115	-
26	CLA	B	612	5	-	13/39/115/115	-
27	LUT	N	1621	-	-	3/29/67/67	0/2/2/2
26	CLA	c	506	6	-	22/39/115/115	-
28	XAT	3	1622	-	-	2/31/93/93	0/4/4/4
26	CLA	N	612	1	-	10/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	8	604	-	-	10/15/91/115	-
25	CHL	2	607	-	1/1/14/21	16/35/111/117	-
31	BCR	8	623	-	-	9/29/63/63	0/2/2/2
26	CLA	s	612	20	-	5/20/96/115	-
26	CLA	6	614	1	-	7/15/91/115	-
36	SQD	A	418	-	-	22/49/69/69	0/1/1/1
26	CLA	5	604	-	-	12/21/97/115	-
26	CLA	b	603	5	-	9/39/115/115	-
25	CHL	8	608	-	-	7/17/93/117	-
37	LMG	B	2633	-	-	24/50/70/70	0/1/1/1
27	LUT	g	1621	-	-	3/29/67/67	0/2/2/2
26	CLA	4	611	30	-	6/15/91/115	-
30	LHG	R	2630	26	-	19/46/46/53	-
26	CLA	r	616	19	-	8/15/91/115	-
26	CLA	B	610	5	-	11/39/115/115	-
26	CLA	7	603	2	-	15/27/103/115	-
25	CHL	6	608	-	-	7/17/93/117	-
26	CLA	R	616	19	-	8/15/91/115	-
26	CLA	8	611	30	-	6/15/91/115	-
26	CLA	r	612	19	-	6/20/96/115	-
28	XAT	R	622	-	-	3/31/93/93	0/4/4/4
26	CLA	b	614	5	-	13/39/115/115	-
27	LUT	1	1621	-	-	3/29/67/67	0/2/2/2
28	XAT	G	1622	-	-	2/31/93/93	0/4/4/4
26	CLA	c	502	6	-	20/39/115/115	-
25	CHL	y	609	1	1/1/15/21	13/41/117/117	-
26	CLA	c	501	6	-	17/39/115/115	-
26	CLA	s	610	20	-	6/27/103/115	-
26	CLA	n	602	1	-	11/39/115/115	-
25	CHL	5	609	1	1/1/14/21	18/37/113/117	-
25	CHL	2	609	1	1/1/14/21	13/35/111/117	-
25	CHL	7	607	-	-	8/26/102/117	-
30	LHG	c	2630	-	-	27/53/53/53	-
26	CLA	g	603	1	-	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CHL	n	601	1	1/1/15/21	16/41/117/117	-
30	LHG	c	522	-	-	20/53/53/53	-
27	LUT	5	1621	-	-	3/29/67/67	0/2/2/2
26	CLA	c	504	42	-	18/39/115/115	-
26	CLA	4	602	3	-	9/15/91/115	-
25	CHL	R	607	42	1/1/13/21	9/29/105/117	-
26	CLA	n	612	1	-	10/33/109/115	-
25	CHL	s	608	-	-	4/17/93/117	-
26	CLA	y	611	30	-	8/33/109/115	-
26	CLA	B	615	5	-	13/39/115/115	-
26	CLA	y	610	1	-	9/33/109/115	-
26	CLA	B	603	5	-	9/39/115/115	-
28	XAT	N	1622	-	-	3/31/93/93	0/4/4/4
37	LMG	z	101	-	-	24/46/66/70	0/1/1/1
26	CLA	c	508	6	-	11/39/115/115	-
26	CLA	7	604	-	-	11/15/91/115	-
30	LHG	D	409	-	-	27/53/53/53	-
26	CLA	y	603	1	-	13/39/115/115	-
26	CLA	b	609	5	-	9/39/115/115	-
37	LMG	c	521	-	-	22/46/66/70	0/1/1/1
26	CLA	1	614	1	-	4/15/91/115	-
27	LUT	r	620	-	-	3/29/67/67	0/2/2/2
26	CLA	R	604	42	-	6/19/95/115	-
36	SQD	A	412	-	-	13/45/65/69	0/1/1/1
25	CHL	4	606	-	-	8/17/93/117	-
29	NEX	N	1623	-	-	4/27/83/83	0/3/3/3
39	DGD	c	518	-	-	15/44/84/95	0/2/2/2
26	CLA	b	605	5	-	14/39/115/115	-
26	CLA	1	603	1	-	14/27/103/115	-
25	CHL	7	605	2	-	11/17/93/117	-
27	LUT	8	620	-	-	4/29/67/67	0/2/2/2
25	CHL	n	607	42	1/1/15/21	16/41/117/117	-
26	CLA	3	610	2	-	9/33/109/115	-
25	CHL	y	601	1	1/1/15/21	16/41/117/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CHL	g	606	42	-	11/22/98/117	-
26	CLA	y	602	1	-	10/39/115/115	-
25	CHL	G	609	1	1/1/14/21	10/35/111/117	-
25	CHL	Y	601	1	1/1/15/21	16/41/117/117	-
26	CLA	G	613	1	-	14/39/115/115	-
36	SQD	b	621	-	-	32/49/69/69	0/1/1/1
26	CLA	4	610	3	-	6/15/91/115	-
30	LHG	B	2630	-	-	31/51/51/53	-
25	CHL	5	608	-	-	7/17/93/117	-
30	LHG	L	101	-	-	20/53/53/53	-
26	CLA	b	612	5	-	13/39/115/115	-
25	CHL	R	614	19	-	8/12/88/117	-
26	CLA	R	601	19	-	16/20/96/115	-
26	CLA	d	403	7	-	12/39/115/115	-
29	NEX	6	1623	-	-	7/27/83/83	0/3/3/3
25	CHL	4	609	3	-	6/17/93/117	-
26	CLA	Y	612	1	-	15/33/109/115	-
26	CLA	2	611	30	-	5/15/91/115	-
41	HEM	f	101	8,9	-	1/14/54/54	-
26	CLA	r	613	19	-	12/33/109/115	-
29	NEX	G	1623	-	-	5/27/83/83	0/3/3/3
26	CLA	r	604	42	-	6/19/95/115	-
26	CLA	G	602	1	-	12/39/115/115	-
26	CLA	B	614	5	-	13/39/115/115	-
30	LHG	C	523	-	-	21/53/53/53	-
26	CLA	G	603	1	-	11/39/115/115	-
26	CLA	g	611	30	-	13/33/109/115	-
26	CLA	a	407	42	-	5/21/97/115	-
31	BCR	B	619	-	-	2/29/63/63	0/2/2/2
29	NEX	R	623	-	-	4/27/83/83	0/3/3/3
31	BCR	C	517	-	-	4/29/63/63	0/2/2/2
30	LHG	1	2630	26	-	15/45/45/53	-
39	DGD	H	102	-	-	21/51/91/95	0/2/2/2
37	LMG	Z	101	-	-	24/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	5	614	1	-	4/15/91/115	-
29	NEX	g	1623	-	-	5/27/83/83	0/3/3/3
26	CLA	B	604	5	-	12/39/115/115	-
30	LHG	b	2630	-	-	31/51/51/53	-
26	CLA	5	603	1	-	14/27/103/115	-
37	LMG	a	415	-	-	14/35/55/70	0/1/1/1
26	CLA	s	604	42	-	6/21/97/115	-
26	CLA	3	603	2	-	15/27/103/115	-
25	CHL	y	607	42	1/1/15/21	18/41/117/117	-
27	LUT	G	1620	-	-	2/29/67/67	0/2/2/2
25	CHL	Y	608	42	1/1/15/21	15/41/117/117	-
27	LUT	s	1620	-	-	2/29/67/67	0/2/2/2
25	CHL	3	609	2	1/1/14/21	15/35/111/117	-
26	CLA	B	617	5	-	18/39/115/115	-
30	LHG	l	101	-	-	20/53/53/53	-
25	CHL	5	601	1	-	6/17/93/117	-
26	CLA	4	612	3	-	7/15/91/115	-
39	DGD	b	626	-	-	24/48/88/95	0/2/2/2
26	CLA	c	512	6	-	11/39/115/115	-
26	CLA	S	609	20	-	7/15/91/115	-
41	HEM	F	101	8,9	-	1/14/54/54	-
26	CLA	a	406	42	-	12/39/115/115	-
26	CLA	g	602	1	-	12/39/115/115	-
26	CLA	y	604	42	-	3/21/97/115	-
31	BCR	H	101	-	-	4/29/63/63	0/2/2/2
30	LHG	G	2630	26	-	26/53/53/53	-
26	CLA	g	610	1	-	15/38/114/115	-
28	XAT	g	1622	-	-	2/31/93/93	0/4/4/4
31	BCR	b	620	-	-	6/29/63/63	0/2/2/2
26	CLA	S	613	20	-	6/27/103/115	-
25	CHL	G	607	42	1/1/15/21	18/41/117/117	-
27	LUT	s	1621	-	-	2/29/67/67	0/2/2/2
26	CLA	A	407	42	-	5/21/97/115	-
26	CLA	N	613	1	-	8/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CHL	G	606	42	-	11/22/98/117	-
25	CHL	N	606	42	-	8/22/98/117	-
26	CLA	7	613	2	-	11/31/107/115	-
28	XAT	6	1622	-	-	3/31/93/93	0/4/4/4
37	LMG	A	415	-	-	14/35/55/70	0/1/1/1
30	LHG	r	2630	26	-	19/46/46/53	-
26	CLA	N	614	1	-	6/19/95/115	-
25	CHL	G	608	42	1/1/15/21	15/41/117/117	-
26	CLA	7	614	2	-	11/19/95/115	-
27	LUT	n	1620	-	-	2/29/67/67	0/2/2/2
26	CLA	2	602	1	-	12/35/111/115	-
26	CLA	N	611	30	-	6/33/109/115	-
26	CLA	N	610	1	-	12/39/115/115	-
30	LHG	c	523	-	-	21/53/53/53	-
26	CLA	c	510	6	-	14/39/115/115	-
25	CHL	5	607	-	1/1/14/21	22/38/114/117	-
25	CHL	3	608	-	-	5/17/93/117	-
30	LHG	7	2630	26	-	24/51/51/53	-
31	BCR	b	619	-	-	2/29/63/63	0/2/2/2
25	CHL	r	606	42	1/1/15/21	19/41/117/117	-
31	BCR	c	516	-	-	7/29/63/63	0/2/2/2
39	DGD	C	518	-	-	15/44/84/95	0/2/2/2
25	CHL	S	601	20	-	9/17/93/117	-
25	CHL	7	608	-	-	5/17/93/117	-
25	CHL	N	609	1	1/1/15/21	13/41/117/117	-
31	BCR	t	101	-	-	13/29/63/63	0/2/2/2
26	CLA	y	612	1	-	15/33/109/115	-
26	CLA	R	602	19	-	8/33/109/115	-
25	CHL	r	608	42	1/1/14/21	17/35/111/117	-
26	CLA	S	612	20	-	5/20/96/115	-
25	CHL	n	609	1	1/1/15/21	14/41/117/117	-
25	CHL	R	608	42	1/1/14/21	17/35/111/117	-
25	CHL	N	605	1	-	9/20/96/117	-
26	CLA	S	602	20	-	14/35/111/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	n	613	1	-	8/33/109/115	-
25	CHL	n	605	1	-	9/20/96/117	-
26	CLA	1	612	1	-	5/15/91/115	-
26	CLA	4	603	3	-	6/15/91/115	-
26	CLA	R	603	19	-	14/33/109/115	-
25	CHL	g	608	42	1/1/15/21	15/41/117/117	-
25	CHL	n	606	42	-	8/22/98/117	-
26	CLA	B	616	5	-	15/39/115/115	-
26	CLA	7	602	2	-	16/33/109/115	-
26	CLA	g	612	1	-	12/33/109/115	-
36	SQD	B	621	-	-	32/49/69/69	0/1/1/1
31	BCR	d	404	-	-	7/29/63/63	0/2/2/2
26	CLA	b	604	5	-	12/39/115/115	-
31	BCR	a	411	-	-	6/29/63/63	0/2/2/2
25	CHL	y	605	1	-	8/20/96/117	-
26	CLA	3	604	-	-	11/15/91/115	-
31	BCR	C	515	-	-	6/29/63/63	0/2/2/2
25	CHL	2	605	1	-	11/17/93/117	-
26	CLA	C	511	6	-	14/39/115/115	-
26	CLA	B	605	5	-	14/39/115/115	-
27	LUT	7	1620	-	-	2/29/67/67	0/2/2/2
35	PHO	A	409	-	-	7/37/103/103	0/5/6/6
26	CLA	b	610	5	-	11/39/115/115	-
26	CLA	C	507	42	-	23/39/115/115	-
31	BCR	B	620	-	-	6/29/63/63	0/2/2/2
25	CHL	N	608	42	1/1/15/21	13/41/117/117	-
27	LUT	2	1621	-	-	3/29/67/67	0/2/2/2
25	CHL	3	601	2	1/1/14/21	18/39/115/117	-
26	CLA	8	602	3	-	9/15/91/115	-
26	CLA	2	612	1	-	5/15/91/115	-
29	NEX	1	1623	-	-	6/27/83/83	0/3/3/3
39	DGD	h	102	-	-	21/51/91/95	0/2/2/2
28	XAT	5	1622	-	-	2/31/93/93	0/4/4/4
31	BCR	h	101	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LUT	g	1620	-	-	2/29/67/67	0/2/2/2
26	CLA	y	613	1	-	10/39/115/115	-
26	CLA	C	512	6	-	11/39/115/115	-
28	XAT	8	622	-	-	2/31/93/93	0/4/4/4
25	CHL	Y	605	1	-	8/20/96/117	-
28	XAT	n	1622	-	-	3/31/93/93	0/4/4/4
25	CHL	Y	606	42	-	8/22/98/117	-
26	CLA	c	513	6	-	10/39/115/115	-
31	BCR	4	623	-	-	9/29/63/63	0/2/2/2
37	LMG	B	622	-	-	23/46/66/70	0/1/1/1
26	CLA	b	608	42	-	11/39/115/115	-
30	LHG	4	2630	26	-	8/23/23/53	-
26	CLA	4	604	-	-	10/15/91/115	-
25	CHL	n	608	42	1/1/15/21	13/41/117/117	-
30	LHG	g	2630	26	-	26/53/53/53	-
26	CLA	S	614	20	-	4/20/96/115	-
28	XAT	2	1622	-	-	3/31/93/93	0/4/4/4
37	LMG	a	413	-	-	28/43/63/70	0/1/1/1
25	CHL	4	607	-	-	10/17/93/117	-
25	CHL	1	601	1	-	6/17/93/117	-
25	CHL	r	607	42	1/1/13/21	9/29/105/117	-
29	NEX	S	1623	-	-	5/27/83/83	0/3/3/3
25	CHL	3	607	-	-	8/26/102/117	-
26	CLA	G	614	1	-	3/19/95/115	-
26	CLA	R	612	19	-	6/20/96/115	-
26	CLA	b	607	5	-	9/39/115/115	-
30	LHG	6	2630	26	-	16/41/41/53	-
39	DGD	B	626	-	-	24/48/88/95	0/2/2/2
26	CLA	6	610	1	-	6/21/97/115	-
37	LMG	d	411	-	-	15/41/61/70	0/1/1/1
26	CLA	6	613	1	-	7/15/91/115	-
35	PHO	a	409	-	-	7/37/103/103	0/5/6/6
27	LUT	7	1621	-	-	3/29/67/67	0/2/2/2
26	CLA	a	405	4	-	7/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CHL	6	609	1	1/1/14/21	13/35/111/117	-
37	LMG	D	411	-	-	15/41/61/70	0/1/1/1
26	CLA	1	604	-	-	12/21/97/115	-
26	CLA	3	602	2	-	16/33/109/115	-
26	CLA	C	501	6	-	17/39/115/115	-
30	LHG	d	410	-	-	30/47/47/53	-
26	CLA	1	611	30	-	8/15/91/115	-
26	CLA	2	603	1	-	13/27/103/115	-
30	LHG	D	408	-	-	19/50/50/53	-
26	CLA	Y	602	1	-	10/39/115/115	-
26	CLA	5	613	1	-	10/27/103/115	-
36	SQD	b	623	-	-	17/37/57/69	0/1/1/1
25	CHL	5	605	1	-	10/17/93/117	-
26	CLA	1	610	1	-	7/29/105/115	-
26	CLA	2	613	1	-	7/15/91/115	-
25	CHL	5	606	-	-	10/17/93/117	-
25	CHL	g	609	1	1/1/14/21	10/35/111/117	-
28	XAT	Y	1622	-	-	2/31/93/93	0/4/4/4
26	CLA	A	405	4	-	7/39/115/115	-
26	CLA	g	613	1	-	14/39/115/115	-
27	LUT	3	1620	-	-	2/29/67/67	0/2/2/2
25	CHL	2	606	-	-	6/17/93/117	-
26	CLA	6	611	30	-	5/15/91/115	-
26	CLA	B	606	5	-	16/39/115/115	-
27	LUT	n	1621	-	-	3/29/67/67	0/2/2/2
26	CLA	r	603	19	-	14/33/109/115	-
27	LUT	y	1620	-	-	2/29/67/67	0/2/2/2
26	CLA	6	602	1	-	12/35/111/115	-
35	PHO	A	408	-	-	12/37/103/103	0/5/6/6
37	LMG	b	622	-	-	23/46/66/70	0/1/1/1
25	CHL	7	606	-	-	9/17/93/117	-
28	XAT	7	1622	-	-	2/31/93/93	0/4/4/4
30	LHG	S	2630	26	-	27/53/53/53	-
26	CLA	r	601	19	-	16/20/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CHL	S	607	42	1/1/13/21	19/32/108/117	-
25	CHL	1	605	1	-	10/17/93/117	-
26	CLA	C	509	6	-	8/39/115/115	-
30	LHG	N	2630	26	-	24/53/53/53	-
37	LMG	A	413	-	-	28/43/63/70	0/1/1/1
25	CHL	N	607	42	1/1/15/21	16/41/117/117	-
31	BCR	D	404	-	-	7/29/63/63	0/2/2/2
26	CLA	D	402	7	-	4/39/115/115	-
39	DGD	C	519	-	-	26/51/91/95	0/2/2/2
25	CHL	S	606	42	-	10/17/93/117	-
30	LHG	n	2630	26	-	24/53/53/53	-
26	CLA	Y	613	1	-	10/39/115/115	-
26	CLA	a	410	4	-	7/33/109/115	-
26	CLA	B	609	5	-	9/39/115/115	-
26	CLA	s	614	20	-	4/20/96/115	-
26	CLA	y	614	1	-	5/19/95/115	-
26	CLA	s	609	20	-	7/15/91/115	-
29	NEX	r	623	-	-	4/27/83/83	0/3/3/3
26	CLA	2	614	1	-	7/15/91/115	-
26	CLA	G	610	1	-	15/38/114/115	-
26	CLA	Y	614	1	-	5/19/95/115	-
36	SQD	B	623	-	-	17/37/57/69	0/1/1/1
31	BCR	A	411	-	-	6/29/63/63	0/2/2/2
36	SQD	a	412	-	-	13/45/65/69	0/1/1/1
26	CLA	5	602	1	-	14/35/111/115	-
26	CLA	S	604	42	-	6/21/97/115	-
38	PL9	D	405	-	-	10/53/73/73	0/1/1/1
26	CLA	B	602	42	-	17/39/115/115	-
25	CHL	6	607	-	1/1/14/21	16/35/111/117	-
25	CHL	y	608	42	1/1/15/21	15/41/117/117	-
26	CLA	N	604	42	-	5/21/97/115	-
30	LHG	2	2630	26	-	16/41/41/53	-
25	CHL	8	609	3	-	6/17/93/117	-
26	CLA	s	602	20	-	14/35/111/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CHL	Y	609	1	1/1/15/21	13/41/117/117	-
26	CLA	N	603	1	-	15/39/115/115	-
26	CLA	g	604	42	-	5/21/97/115	-
25	CHL	8	606	-	-	8/17/93/117	-
26	CLA	C	506	6	-	22/39/115/115	-
25	CHL	4	608	-	-	7/17/93/117	-
26	CLA	2	610	1	-	6/21/97/115	-
29	NEX	7	1623	-	-	4/27/83/83	0/3/3/3
31	BCR	c	515	-	-	6/29/63/63	0/2/2/2
25	CHL	g	607	42	1/1/15/21	18/41/117/117	-
26	CLA	c	511	6	-	14/39/115/115	-
26	CLA	6	604	-	-	10/15/91/115	-
31	BCR	T	101	-	-	13/29/63/63	0/2/2/2
39	DGD	C	520	-	-	21/49/89/95	0/2/2/2
28	XAT	1	1622	-	-	2/31/93/93	0/4/4/4
25	CHL	s	601	20	-	9/17/93/117	-
26	CLA	b	611	42	-	12/39/115/115	-
26	CLA	c	505	6	-	17/39/115/115	-
26	CLA	r	611	30	-	9/20/96/115	-
26	CLA	G	612	1	-	12/33/109/115	-
30	LHG	y	2630	26	-	24/53/53/53	-
26	CLA	C	503	6	-	16/39/115/115	-
26	CLA	2	604	-	-	10/15/91/115	-
25	CHL	8	601	3	-	9/15/91/117	-
26	CLA	c	509	6	-	8/39/115/115	-
26	CLA	g	614	1	-	3/19/95/115	-
26	CLA	3	613	2	-	11/31/107/115	-
39	DGD	c	519	-	-	26/51/91/95	0/2/2/2
30	LHG	b	2631	-	-	22/53/53/53	-
31	BCR	C	514	-	-	4/29/63/63	0/2/2/2
30	LHG	d	408	-	-	19/50/50/53	-
26	CLA	b	615	5	-	12/39/115/115	-
26	CLA	8	612	3	-	7/15/91/115	-
26	CLA	C	510	6	-	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CHL	R	606	42	1/1/15/21	19/41/117/117	-
26	CLA	C	502	6	-	20/39/115/115	-
25	CHL	y	606	42	-	8/22/98/117	-
35	PHO	a	408	-	-	12/37/103/103	0/5/6/6
26	CLA	5	612	1	-	5/15/91/115	-
31	BCR	c	517	-	-	4/29/63/63	0/2/2/2
27	LUT	6	1621	-	-	3/29/67/67	0/2/2/2
26	CLA	B	608	42	-	11/39/115/115	-
29	NEX	n	1623	-	-	4/27/83/83	0/3/3/3
27	LUT	Y	1620	-	-	2/29/67/67	0/2/2/2
30	LHG	3	2630	26	-	24/51/51/53	-
26	CLA	n	611	30	-	6/33/109/115	-
29	NEX	3	1623	-	-	4/27/83/83	0/3/3/3
30	LHG	Y	2630	26	-	24/53/53/53	-
38	PL9	a	414	-	-	1/5/18/73	0/1/1/1
25	CHL	3	606	-	-	9/17/93/117	-
25	CHL	Y	607	42	1/1/15/21	18/41/117/117	-
25	CHL	4	601	3	-	9/15/91/117	-
29	NEX	y	1623	-	-	6/27/83/83	0/3/3/3
31	BCR	B	618	-	-	2/29/63/63	0/2/2/2
26	CLA	n	604	42	-	5/21/97/115	-
26	CLA	R	613	19	-	12/33/109/115	-
29	NEX	Y	1623	-	-	6/27/83/83	0/3/3/3
26	CLA	R	609	19	-	3/31/107/115	-

The worst 5 of 4032 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	a	408	PHO	C1B-C2B	8.41	1.48	1.39
35	A	408	PHO	C1B-C2B	8.38	1.48	1.39
35	a	409	PHO	C3B-C4B	7.70	1.50	1.41
35	A	409	PHO	C3B-C4B	7.64	1.50	1.41
35	A	409	PHO	C1B-C2B	7.57	1.48	1.39

The worst 5 of 6272 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	N	607	CHL	C2C-C3C-C4C	-10.86	98.75	106.49
25	n	607	CHL	C2C-C3C-C4C	-10.86	98.75	106.49
25	y	601	CHL	CMD-C2D-C1D	10.85	143.84	124.71
25	Y	601	CHL	CMD-C2D-C1D	10.83	143.81	124.71
25	S	601	CHL	C2B-C1B-NB	10.80	117.47	110.23

5 of 44 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
25	1	607	CHL	C8
25	1	609	CHL	C8
25	2	607	CHL	C8
25	2	609	CHL	C8
25	3	601	CHL	C8

5 of 5265 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	1	601	CHL	C1C-C2C-CMC-OMC
25	1	601	CHL	C3C-C2C-CMC-OMC
25	1	601	CHL	CHA-CBD-CGD-O1D
25	1	601	CHL	CHA-CBD-CGD-O2D
25	1	605	CHL	C1C-C2C-CMC-OMC

There are no ring outliers.

434 monomers are involved in 1103 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	1	613	CLA	1	0
26	7	611	CLA	2	0
26	S	603	CLA	1	0
26	Y	610	CLA	1	0
26	s	603	CLA	1	0
28	4	622	XAT	3	0
26	6	612	CLA	2	0
25	6	606	CHL	1	0
26	n	610	CLA	7	0
39	c	520	DGD	1	0
38	A	414	PL9	1	0
25	7	609	CHL	6	0
37	b	2633	LMG	3	0
31	b	618	BCR	5	0
26	R	610	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	G	601	CHL	6	0
26	1	602	CLA	3	0
26	c	503	CLA	3	0
27	Y	1621	LUT	5	0
27	G	1621	LUT	7	0
25	3	605	CHL	1	0
25	g	605	CHL	1	0
25	1	609	CHL	4	0
26	6	603	CLA	1	0
26	Y	611	CLA	1	0
26	D	403	CLA	3	0
30	5	2630	LHG	2	0
31	c	514	BCR	4	0
25	r	614	CHL	2	0
25	6	605	CHL	1	0
26	r	609	CLA	2	0
26	B	613	CLA	8	0
30	s	2630	LHG	5	0
26	B	607	CLA	5	0
29	5	1623	NEX	2	0
25	s	607	CHL	3	0
26	3	611	CLA	3	0
31	C	516	BCR	6	0
26	s	613	CLA	1	0
26	d	402	CLA	6	0
25	s	606	CHL	2	0
26	Y	604	CLA	1	0
28	y	1622	XAT	5	0
26	C	505	CLA	4	0
26	b	617	CLA	3	0
27	S	1620	LUT	3	0
26	n	603	CLA	5	0
30	D	410	LHG	3	0
26	N	602	CLA	6	0
26	G	604	CLA	2	0
27	5	1620	LUT	4	0
27	3	1621	LUT	4	0
27	4	620	LUT	2	0
30	d	409	LHG	12	0
26	3	612	CLA	1	0
27	R	620	LUT	4	0
29	s	1623	NEX	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	B	611	CLA	2	0
26	G	611	CLA	1	0
30	B	2631	LHG	3	0
26	b	606	CLA	4	0
26	7	612	CLA	1	0
26	s	611	CLA	1	0
29	2	1623	NEX	1	0
25	1	608	CHL	1	0
28	r	622	XAT	5	0
26	S	610	CLA	2	0
25	g	601	CHL	6	0
26	b	616	CLA	1	0
26	c	507	CLA	4	0
30	C	2630	LHG	6	0
25	1	607	CHL	4	0
26	r	602	CLA	4	0
25	S	608	CHL	1	0
26	R	611	CLA	4	0
30	C	522	LHG	4	0
26	r	610	CLA	1	0
38	d	405	PL9	1	0
26	b	613	CLA	7	0
30	8	2630	LHG	1	0
26	C	504	CLA	2	0
27	N	1620	LUT	4	0
25	G	605	CHL	2	0
27	2	1620	LUT	5	0
27	6	1620	LUT	4	0
26	A	406	CLA	3	0
36	a	418	SQD	11	0
26	Y	603	CLA	7	0
26	A	410	CLA	5	0
26	S	611	CLA	1	0
26	5	610	CLA	1	0
26	3	614	CLA	1	0
26	C	508	CLA	3	0
27	y	1621	LUT	5	0
25	N	601	CHL	3	0
26	b	602	CLA	4	0
26	8	610	CLA	1	0
27	S	1621	LUT	2	0
37	C	521	LMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	7	601	CHL	2	0
27	1	1620	LUT	4	0
26	C	513	CLA	4	0
26	B	612	CLA	4	0
27	N	1621	LUT	6	0
26	c	506	CLA	2	0
28	3	1622	XAT	3	0
26	N	612	CLA	4	0
25	2	607	CHL	2	0
31	8	623	BCR	8	0
26	s	612	CLA	1	0
26	6	614	CLA	1	0
36	A	418	SQD	11	0
26	5	604	CLA	1	0
26	b	603	CLA	8	0
25	8	608	CHL	2	0
37	B	2633	LMG	3	0
27	g	1621	LUT	7	0
30	R	2630	LHG	4	0
26	r	616	CLA	3	0
26	7	603	CLA	3	0
26	R	616	CLA	3	0
26	r	612	CLA	2	0
28	R	622	XAT	4	0
26	b	614	CLA	7	0
27	1	1621	LUT	6	0
28	G	1622	XAT	5	0
26	c	502	CLA	4	0
25	y	609	CHL	3	0
26	c	501	CLA	4	0
26	s	610	CLA	3	0
26	n	602	CLA	8	0
25	5	609	CHL	3	0
25	2	609	CHL	2	0
25	7	607	CHL	4	0
30	c	2630	LHG	5	0
26	g	603	CLA	3	0
25	n	601	CHL	3	0
30	c	522	LHG	4	0
27	5	1621	LUT	6	0
26	c	504	CLA	1	0
25	R	607	CHL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	n	612	CLA	4	0
25	s	608	CHL	1	0
26	y	611	CLA	1	0
26	B	615	CLA	2	0
26	y	610	CLA	1	0
26	B	603	CLA	6	0
28	N	1622	XAT	6	0
37	z	101	LMG	5	0
26	c	508	CLA	3	0
26	7	604	CLA	1	0
30	D	409	LHG	13	0
26	y	603	CLA	5	0
26	b	609	CLA	2	0
37	c	521	LMG	1	0
27	r	620	LUT	5	0
26	R	604	CLA	3	0
36	A	412	SQD	2	0
25	4	606	CHL	2	0
29	N	1623	NEX	1	0
39	c	518	DGD	2	0
26	b	605	CLA	6	0
26	1	603	CLA	2	0
27	8	620	LUT	3	0
25	n	607	CHL	3	0
25	y	601	CHL	3	0
25	g	606	CHL	6	0
26	y	602	CLA	6	0
25	G	609	CHL	7	0
25	Y	601	CHL	2	0
26	G	613	CLA	6	0
36	b	621	SQD	5	0
26	4	610	CLA	1	0
30	B	2630	LHG	2	0
25	5	608	CHL	1	0
30	L	101	LHG	3	0
26	b	612	CLA	4	0
25	R	614	CHL	2	0
26	R	601	CLA	3	0
26	d	403	CLA	2	0
25	4	609	CHL	1	0
26	Y	612	CLA	2	0
26	2	611	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
41	f	101	HEM	1	0
26	r	613	CLA	5	0
29	G	1623	NEX	5	0
26	r	604	CLA	2	0
26	G	602	CLA	2	0
26	B	614	CLA	6	0
30	C	523	LHG	2	0
26	G	603	CLA	3	0
26	g	611	CLA	2	0
26	a	407	CLA	1	0
31	B	619	BCR	3	0
29	R	623	NEX	5	0
31	C	517	BCR	8	0
30	1	2630	LHG	2	0
39	H	102	DGD	3	0
37	Z	101	LMG	5	0
26	5	614	CLA	1	0
29	g	1623	NEX	2	0
26	B	604	CLA	3	0
30	b	2630	LHG	2	0
26	5	603	CLA	2	0
37	a	415	LMG	1	0
26	s	604	CLA	3	0
26	3	603	CLA	4	0
25	y	607	CHL	3	0
27	G	1620	LUT	6	0
25	Y	608	CHL	2	0
27	s	1620	LUT	3	0
25	3	609	CHL	5	0
26	B	617	CLA	3	0
30	l	101	LHG	2	0
25	5	601	CHL	1	0
26	4	612	CLA	2	0
39	b	626	DGD	5	0
26	c	512	CLA	3	0
26	S	609	CLA	5	0
41	F	101	HEM	1	0
26	a	406	CLA	4	0
26	g	602	CLA	2	0
26	y	604	CLA	1	0
31	H	101	BCR	6	0
30	G	2630	LHG	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	g	610	CLA	4	0
28	g	1622	XAT	5	0
31	b	620	BCR	5	0
26	S	613	CLA	1	0
25	G	607	CHL	8	0
27	s	1621	LUT	3	0
26	A	407	CLA	1	0
26	N	613	CLA	3	0
25	G	606	CHL	6	0
25	N	606	CHL	1	0
28	6	1622	XAT	4	0
37	A	415	LMG	1	0
30	r	2630	LHG	4	0
25	G	608	CHL	2	0
26	7	614	CLA	1	0
27	n	1620	LUT	4	0
26	2	602	CLA	2	0
26	N	611	CLA	2	0
26	N	610	CLA	8	0
30	c	523	LHG	2	0
26	c	510	CLA	5	0
25	5	607	CHL	5	0
25	3	608	CHL	4	0
30	7	2630	LHG	2	0
31	b	619	BCR	6	0
25	r	606	CHL	3	0
31	c	516	BCR	5	0
39	C	518	DGD	2	0
25	7	608	CHL	4	0
25	N	609	CHL	4	0
31	t	101	BCR	8	0
26	y	612	CLA	1	0
26	R	602	CLA	4	0
25	r	608	CHL	3	0
26	S	612	CLA	1	0
25	n	609	CHL	4	0
25	R	608	CHL	3	0
25	N	605	CHL	1	0
26	n	613	CLA	4	0
25	n	605	CHL	1	0
26	R	603	CLA	3	0
25	g	608	CHL	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	n	606	CHL	1	0
26	B	616	CLA	2	0
26	7	602	CLA	3	0
36	B	621	SQD	5	0
31	d	404	BCR	3	0
26	b	604	CLA	2	0
31	a	411	BCR	5	0
25	y	605	CHL	3	0
26	3	604	CLA	1	0
31	C	515	BCR	4	0
25	2	605	CHL	1	0
26	C	511	CLA	2	0
26	B	605	CLA	7	0
27	7	1620	LUT	3	0
35	A	409	PHO	4	0
26	b	610	CLA	2	0
26	C	507	CLA	5	0
31	B	620	BCR	4	0
25	N	608	CHL	1	0
27	2	1621	LUT	4	0
25	3	601	CHL	1	0
26	2	612	CLA	2	0
29	1	1623	NEX	2	0
39	h	102	DGD	4	0
28	5	1622	XAT	3	0
31	h	101	BCR	6	0
27	g	1620	LUT	8	0
26	y	613	CLA	3	0
26	C	512	CLA	3	0
28	8	622	XAT	4	0
25	Y	605	CHL	3	0
28	n	1622	XAT	7	0
26	c	513	CLA	4	0
31	4	623	BCR	7	0
37	B	622	LMG	5	0
26	b	608	CLA	1	0
30	4	2630	LHG	1	0
25	n	608	CHL	1	0
30	g	2630	LHG	4	0
26	S	614	CLA	2	0
28	2	1622	XAT	6	0
37	a	413	LMG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	1	601	CHL	1	0
25	r	607	CHL	1	0
29	S	1623	NEX	2	0
25	3	607	CHL	4	0
26	G	614	CLA	2	0
26	R	612	CLA	2	0
26	b	607	CLA	4	0
30	6	2630	LHG	1	0
39	B	626	DGD	5	0
37	d	411	LMG	2	0
26	6	613	CLA	1	0
35	a	409	PHO	4	0
27	7	1621	LUT	3	0
26	a	405	CLA	6	0
25	6	609	CHL	3	0
37	D	411	LMG	2	0
26	1	604	CLA	1	0
26	3	602	CLA	2	0
26	C	501	CLA	5	0
30	d	410	LHG	2	0
26	2	603	CLA	1	0
30	D	408	LHG	1	0
26	Y	602	CLA	6	0
26	5	613	CLA	2	0
36	b	623	SQD	4	0
26	1	610	CLA	1	0
26	2	613	CLA	1	0
25	g	609	CHL	7	0
28	Y	1622	XAT	6	0
26	A	405	CLA	9	0
26	g	613	CLA	6	0
27	3	1620	LUT	4	0
25	2	606	CHL	1	0
26	6	611	CLA	1	0
26	B	606	CLA	4	0
27	n	1621	LUT	5	0
26	r	603	CLA	3	0
27	y	1620	LUT	4	0
26	6	602	CLA	2	0
35	A	408	PHO	6	0
37	b	622	LMG	5	0
25	7	606	CHL	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	7	1622	XAT	3	0
30	S	2630	LHG	4	0
26	r	601	CLA	3	0
25	S	607	CHL	4	0
30	N	2630	LHG	4	0
37	A	413	LMG	2	0
25	N	607	CHL	4	0
31	D	404	BCR	3	0
26	D	402	CLA	4	0
39	C	519	DGD	3	0
25	S	606	CHL	2	0
30	n	2630	LHG	3	0
26	Y	613	CLA	4	0
26	a	410	CLA	5	0
26	B	609	CLA	2	0
26	s	614	CLA	2	0
26	s	609	CLA	6	0
29	r	623	NEX	4	0
26	G	610	CLA	4	0
36	B	623	SQD	4	0
31	A	411	BCR	4	0
36	a	412	SQD	1	0
26	5	602	CLA	2	0
26	S	604	CLA	2	0
38	D	405	PL9	2	0
26	B	602	CLA	5	0
25	6	607	CHL	2	0
25	y	608	CHL	2	0
26	N	604	CLA	1	0
30	2	2630	LHG	1	0
25	8	609	CHL	1	0
25	Y	609	CHL	2	0
26	N	603	CLA	5	0
26	g	604	CLA	2	0
25	8	606	CHL	2	0
26	C	506	CLA	3	0
25	4	608	CHL	2	0
29	7	1623	NEX	3	0
31	c	515	BCR	3	0
25	g	607	CHL	9	0
26	c	511	CLA	2	0
26	6	604	CLA	1	0

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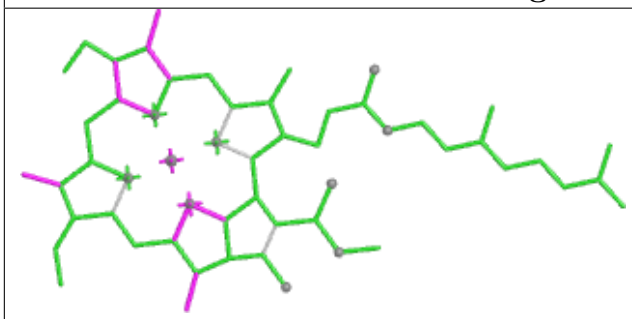
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	T	101	BCR	10	0
39	C	520	DGD	1	0
28	1	1622	XAT	4	0
26	b	611	CLA	3	0
26	c	505	CLA	3	0
26	r	611	CLA	4	0
30	y	2630	LHG	4	0
26	C	503	CLA	3	0
26	2	604	CLA	1	0
25	8	601	CHL	2	0
26	g	614	CLA	2	0
26	3	613	CLA	1	0
39	c	519	DGD	2	0
30	b	2631	LHG	3	0
31	C	514	BCR	4	0
30	d	408	LHG	1	0
26	b	615	CLA	3	0
26	8	612	CLA	1	0
26	C	510	CLA	5	0
25	R	606	CHL	2	0
26	C	502	CLA	5	0
35	a	408	PHO	7	0
31	c	517	BCR	7	0
27	6	1621	LUT	4	0
26	B	608	CLA	2	0
29	n	1623	NEX	1	0
27	Y	1620	LUT	5	0
30	3	2630	LHG	3	0
26	n	611	CLA	2	0
29	3	1623	NEX	3	0
30	Y	2630	LHG	4	0
38	a	414	PL9	1	0
25	3	606	CHL	3	0
25	4	601	CHL	2	0
25	Y	607	CHL	3	0
29	y	1623	NEX	1	0
31	B	618	BCR	4	0
26	n	604	CLA	1	0
26	R	613	CLA	4	0
29	Y	1623	NEX	2	0
26	R	609	CLA	2	0

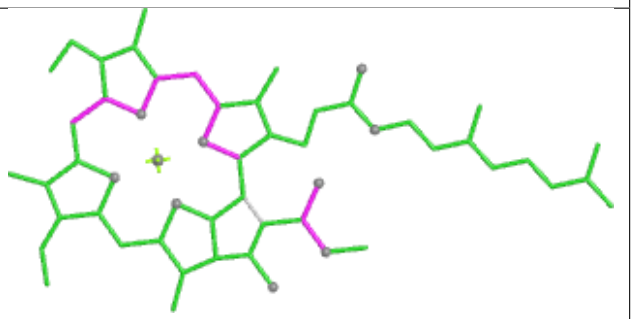
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.

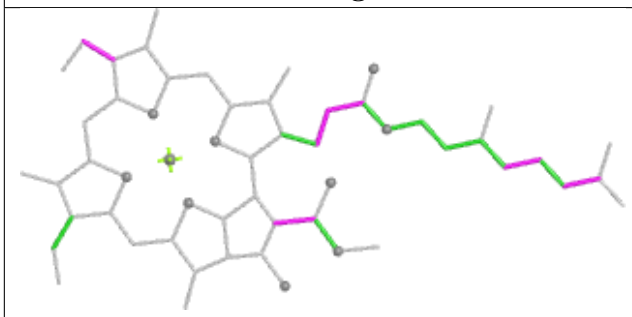
Ligand CLA 1 613



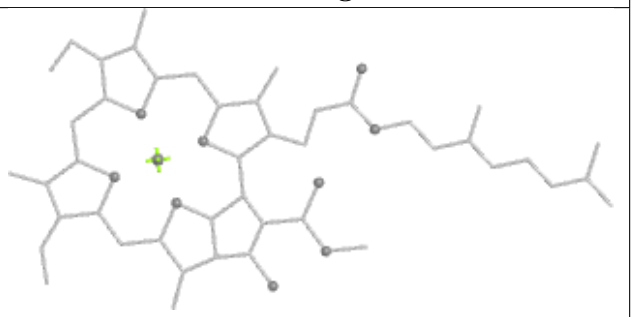
Bond lengths



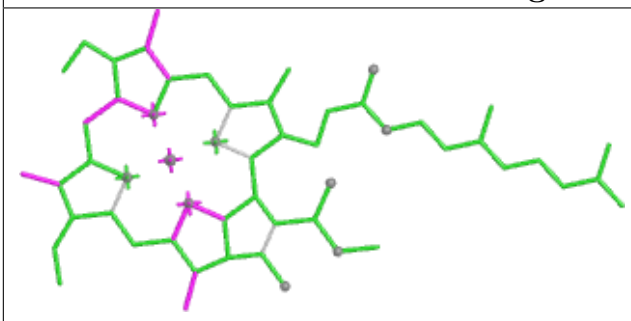
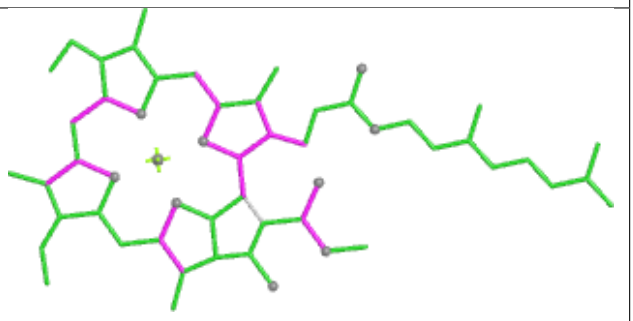
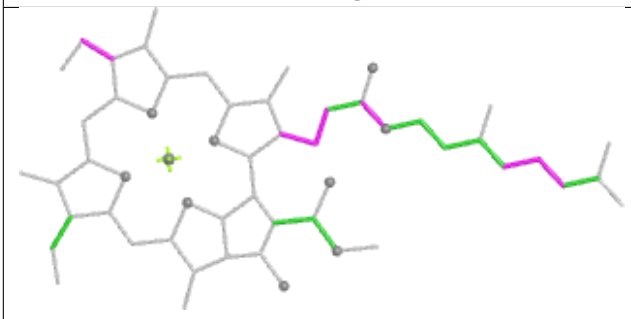
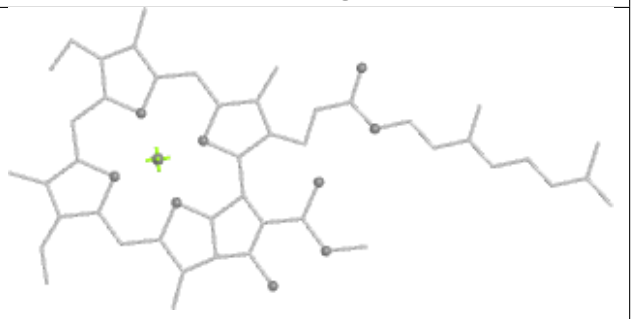
Bond angles



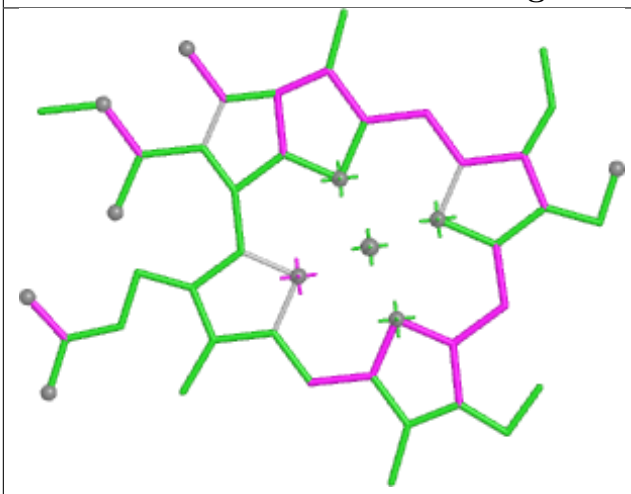
Torsions



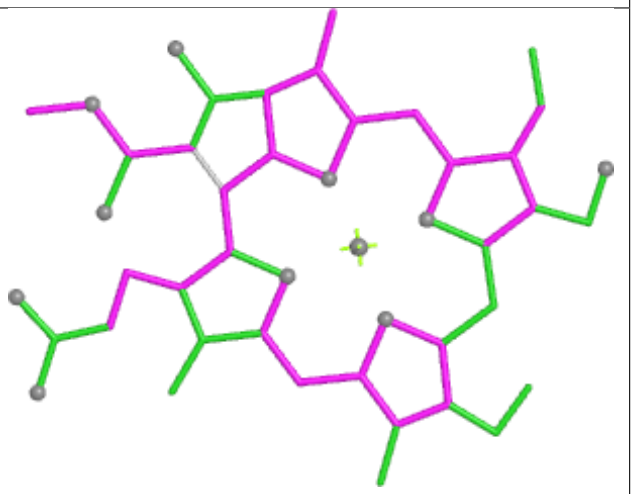
Rings

Ligand CLA 7 611	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

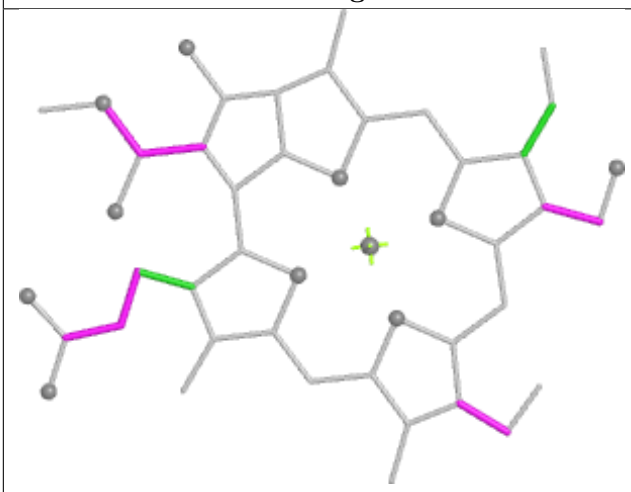
Ligand CHL 1 606



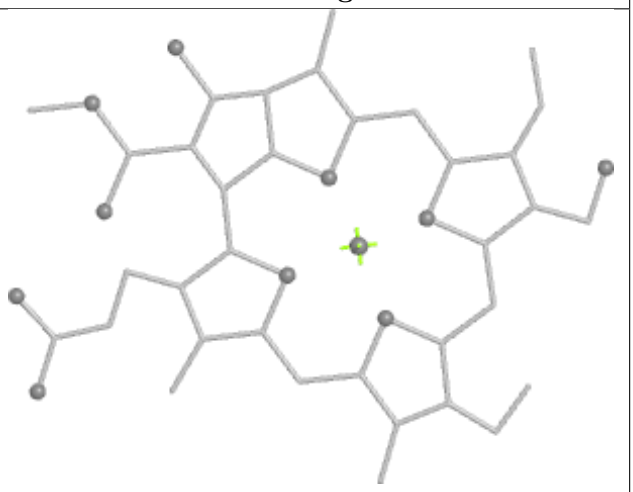
Bond lengths



Bond angles

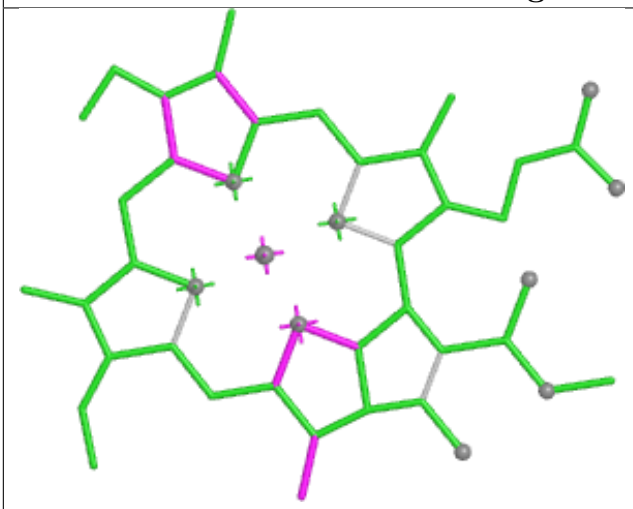


Torsions

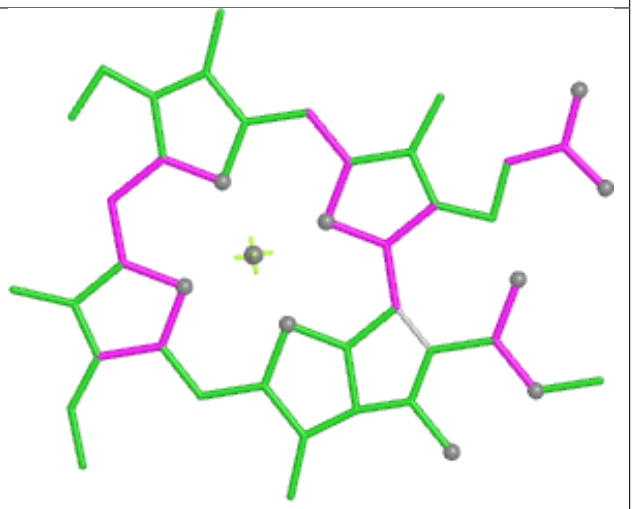


Rings

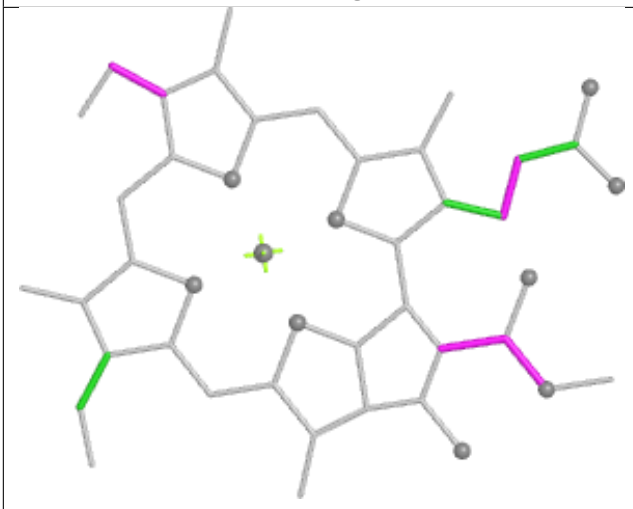
Ligand CLA S 603



Bond lengths



Bond angles

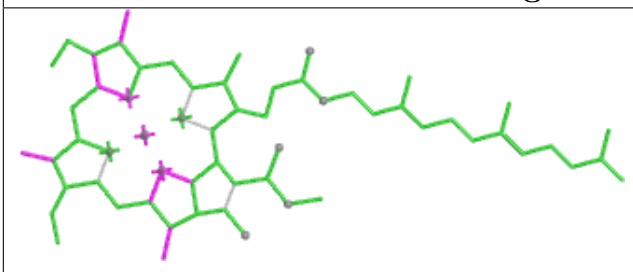


Torsions

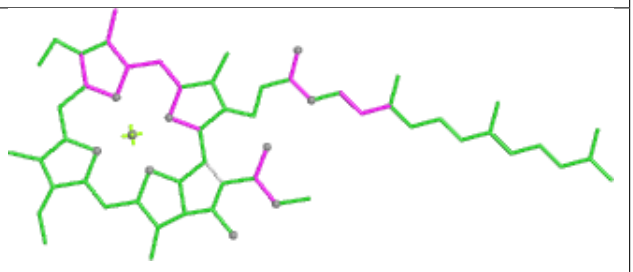


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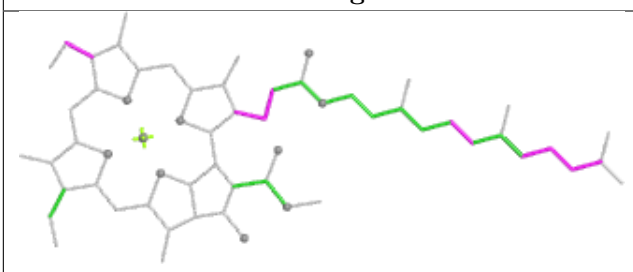
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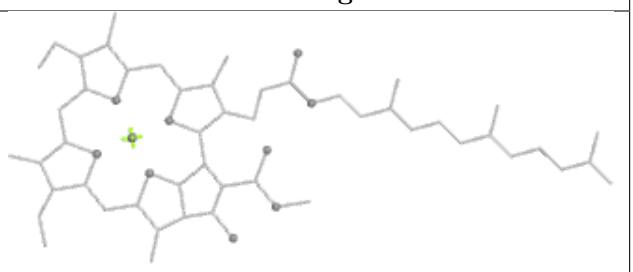
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Bond angles

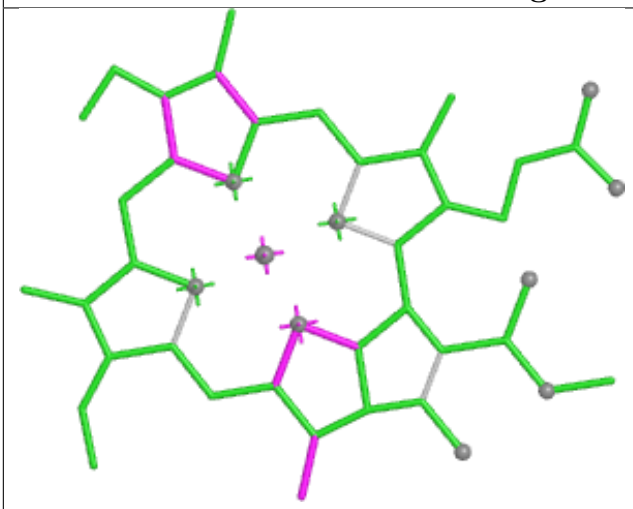


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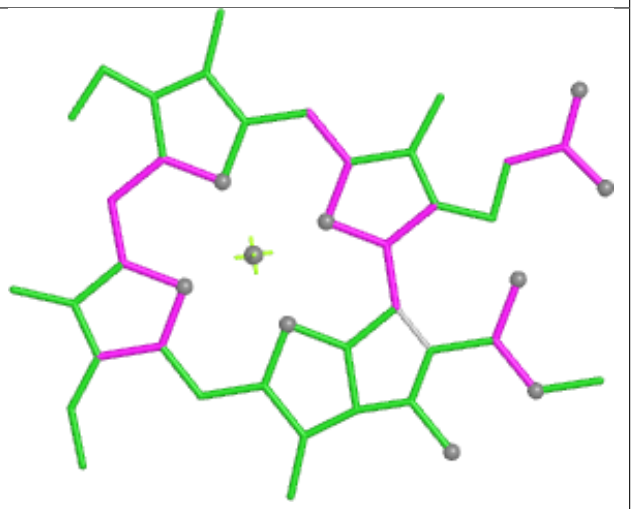


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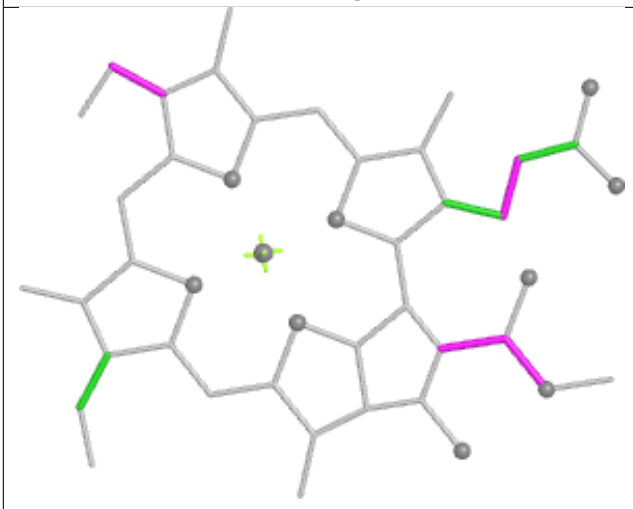
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Bond lengths



Bond angles

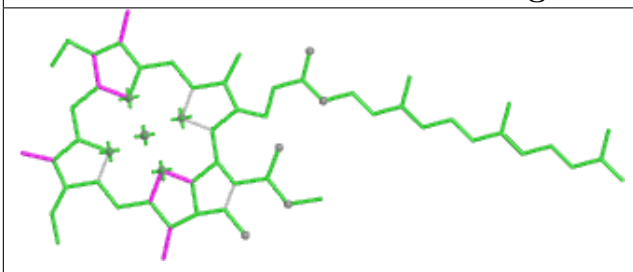


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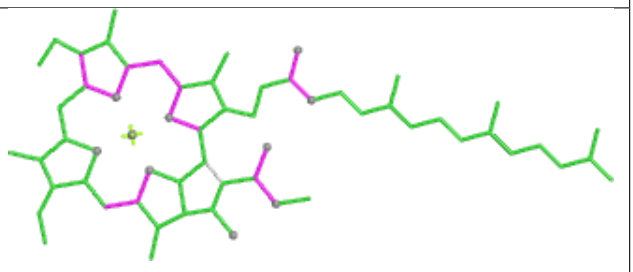


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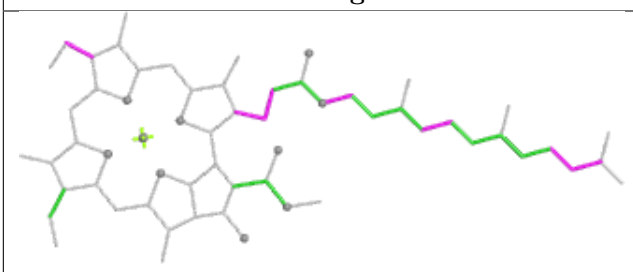
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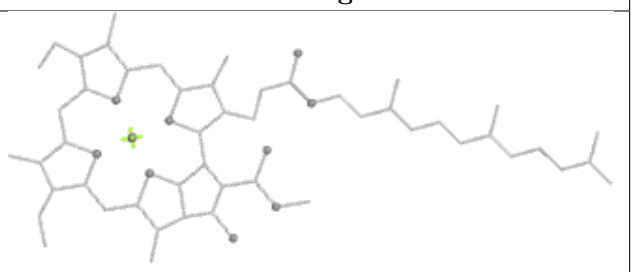
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Bond angles

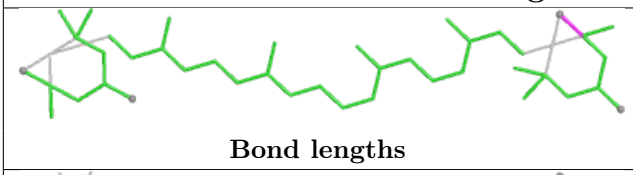


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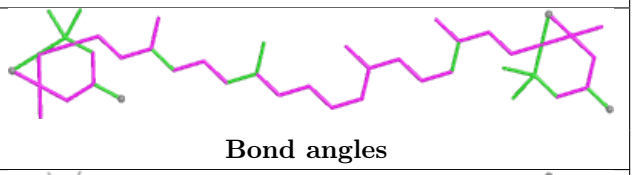


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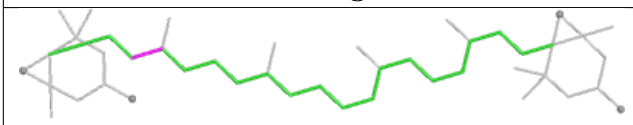
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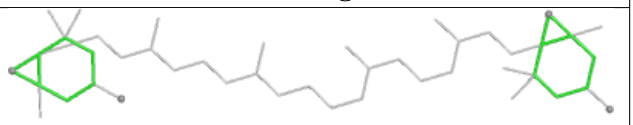
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Bond angles

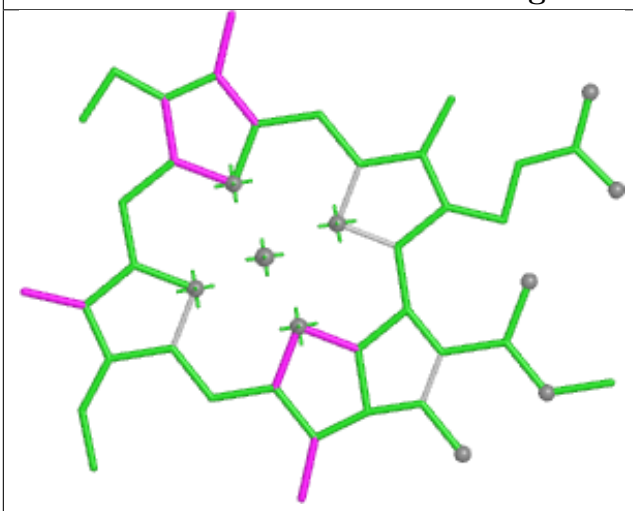


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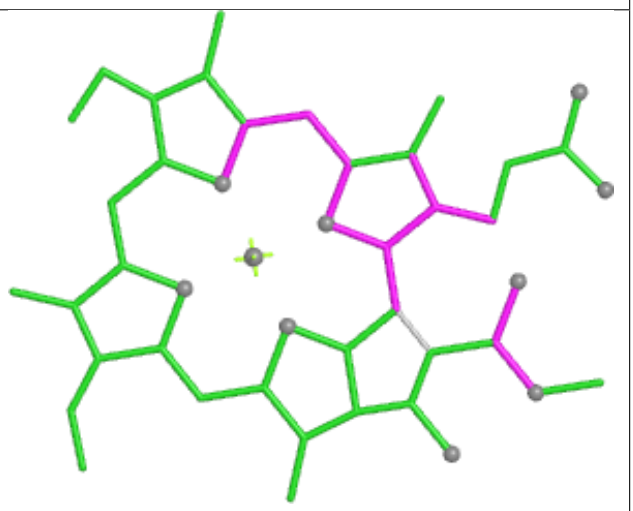


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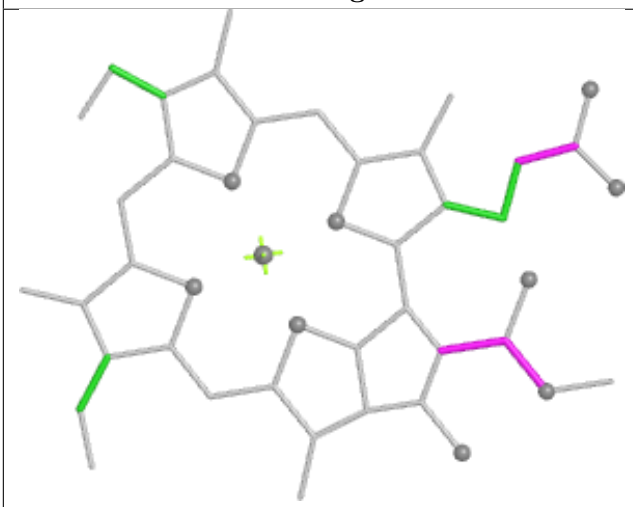
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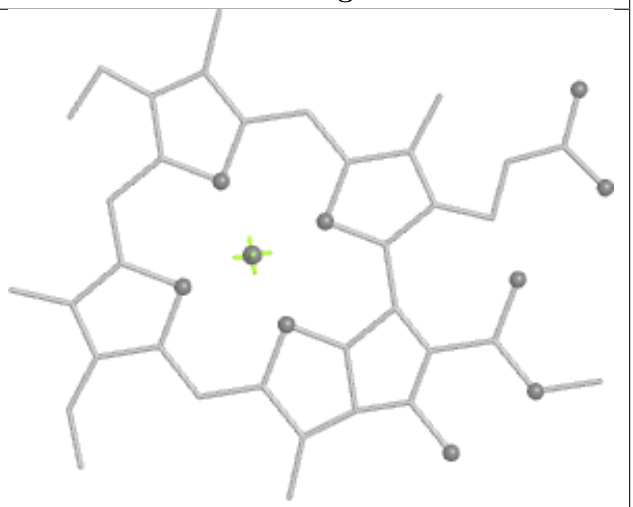
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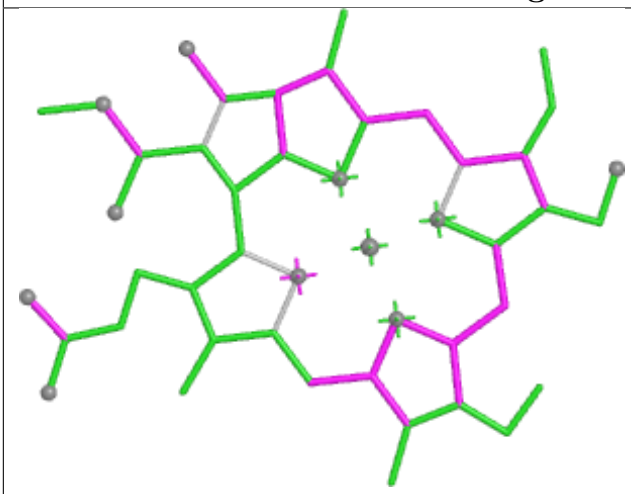


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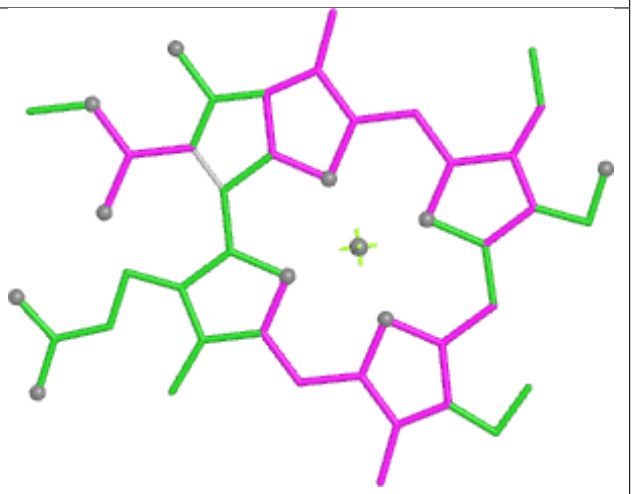


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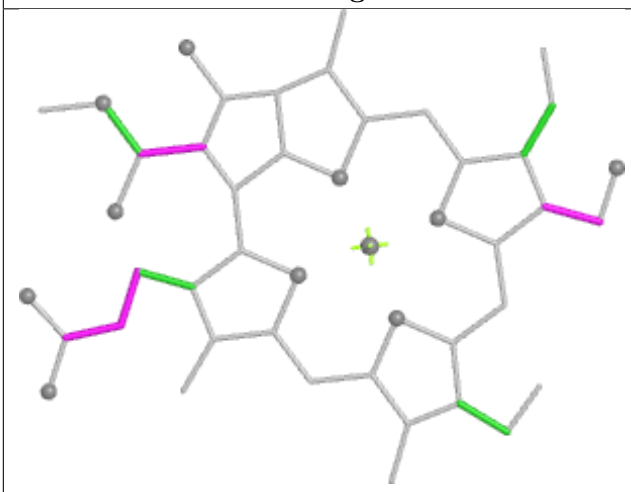
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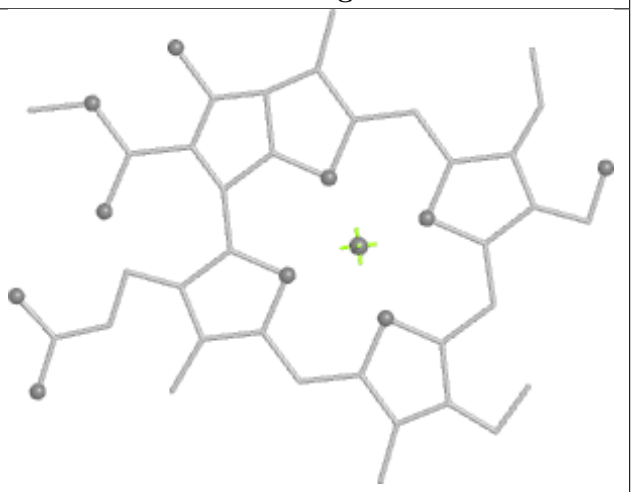
Bond lengths



Bond angles

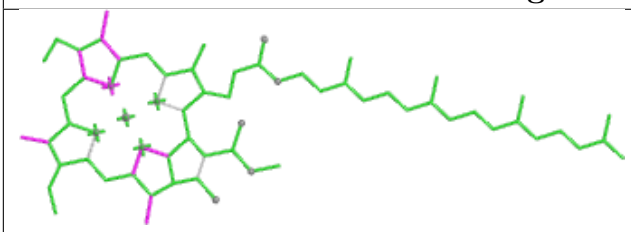


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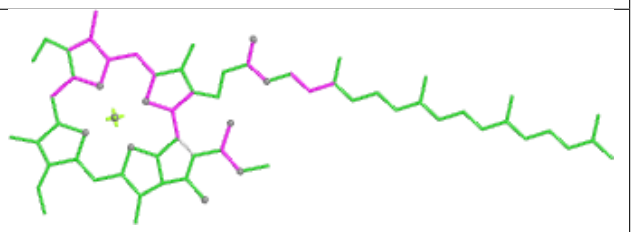


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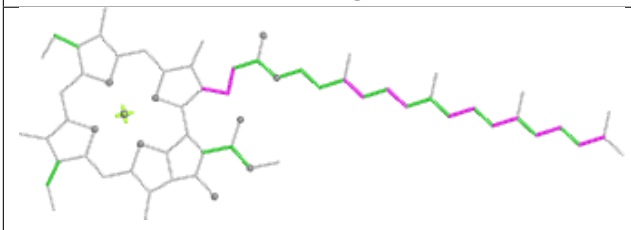
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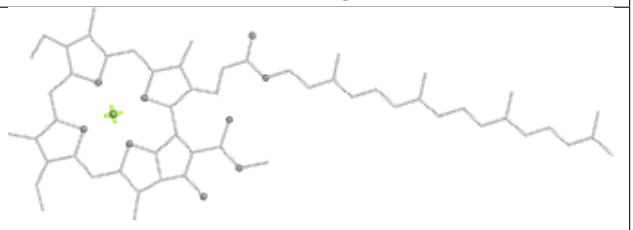
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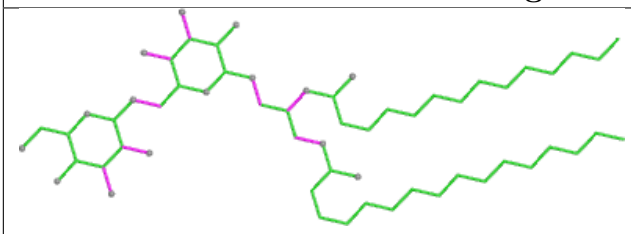


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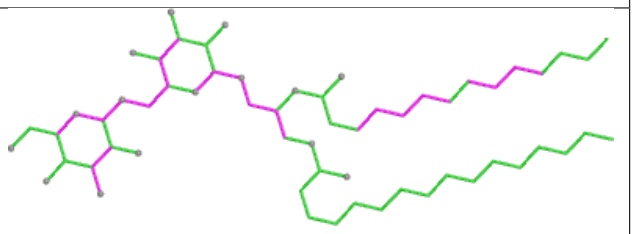


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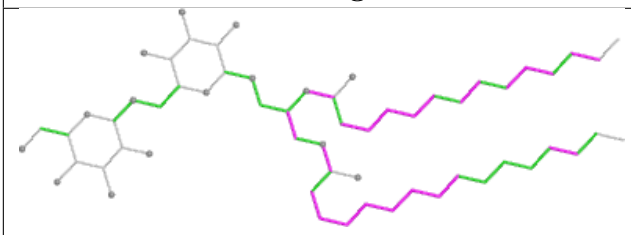
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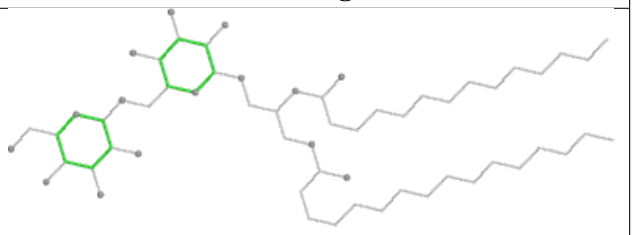
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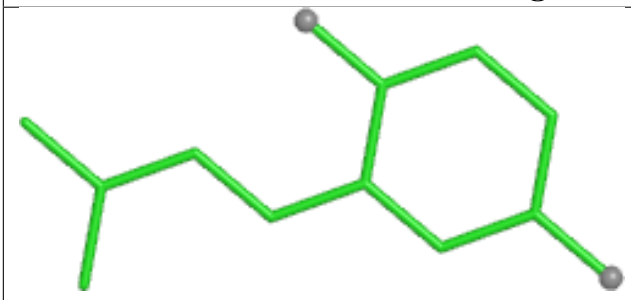


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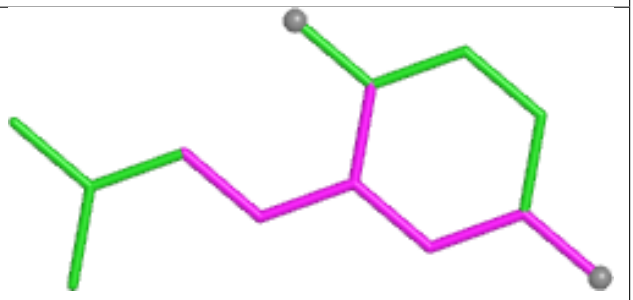


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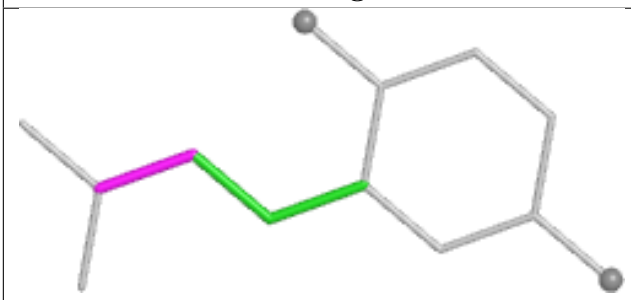
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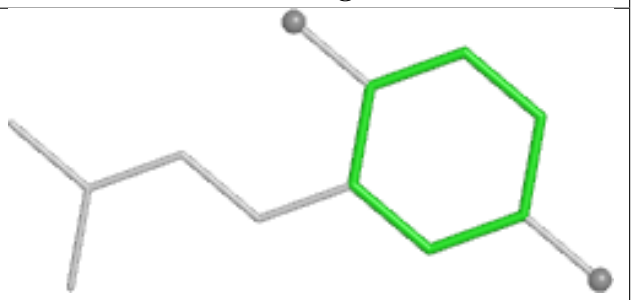
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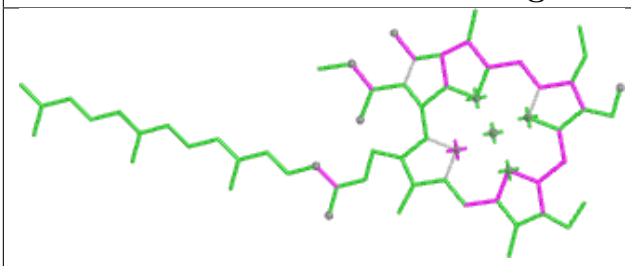


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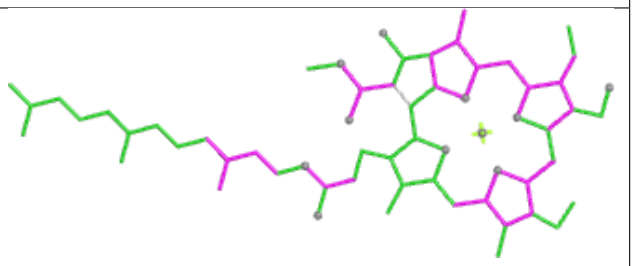


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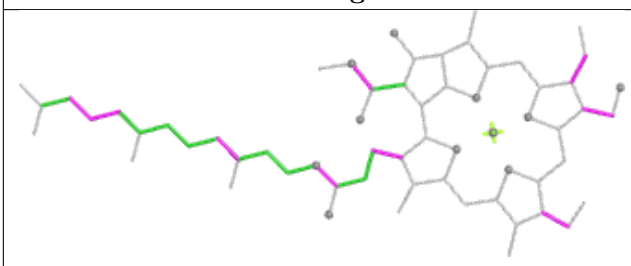
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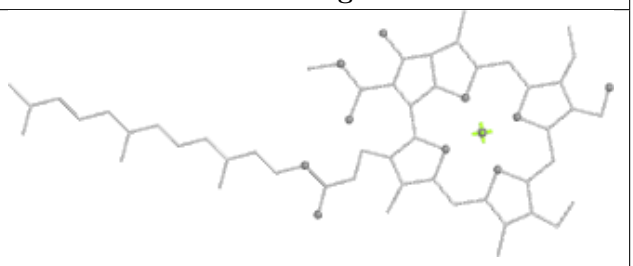
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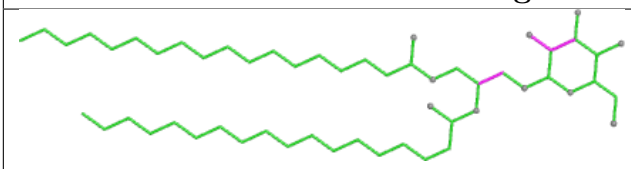


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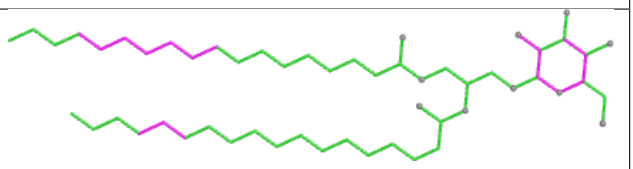


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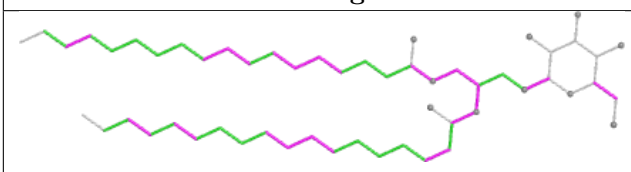
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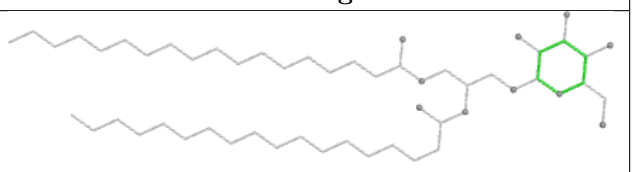
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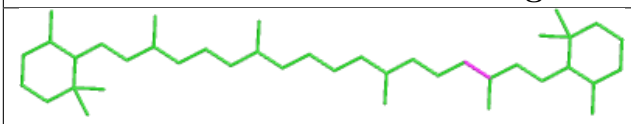


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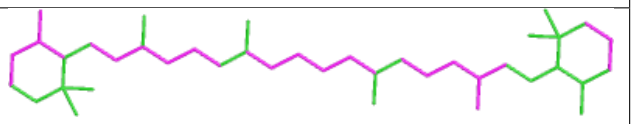


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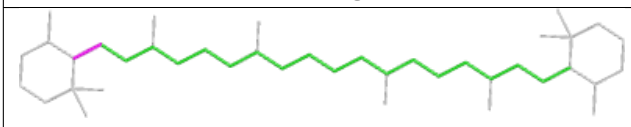
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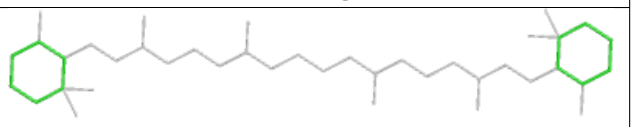
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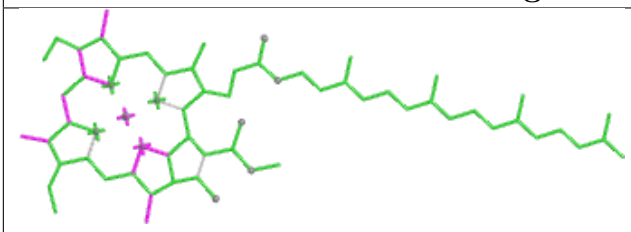


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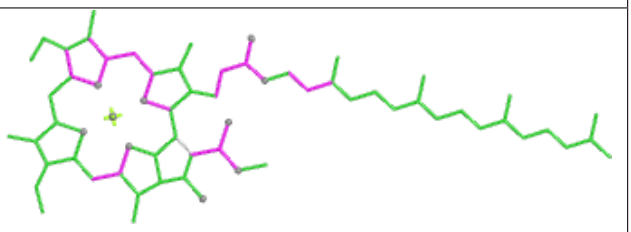


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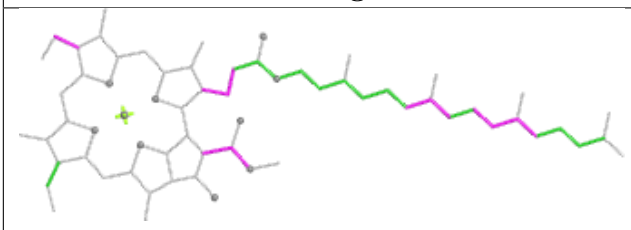
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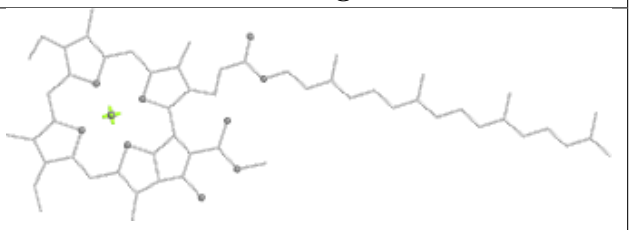
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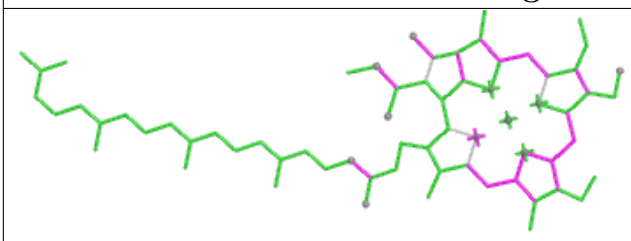


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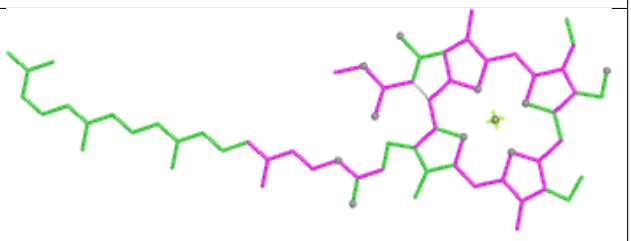


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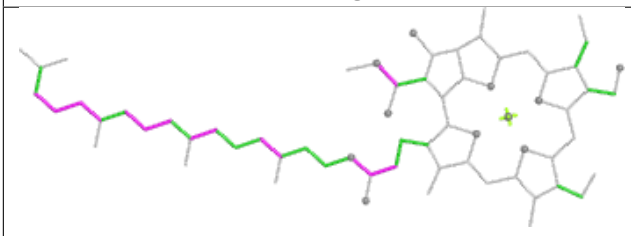
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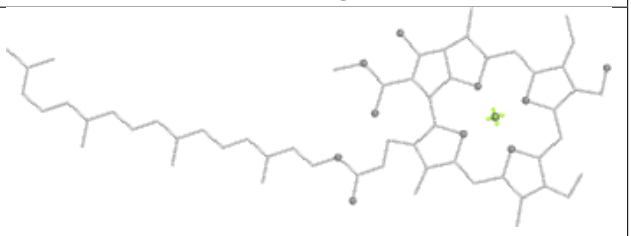
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Bond angles

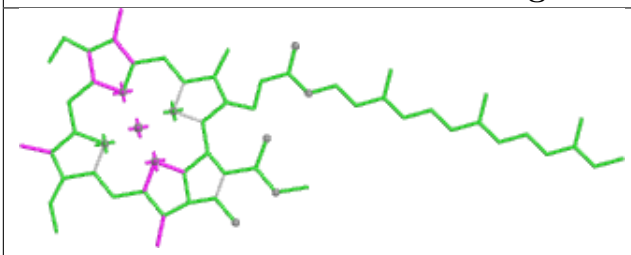


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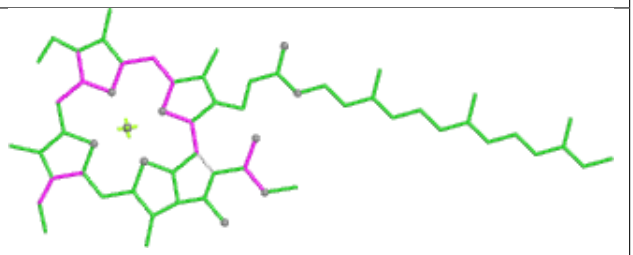


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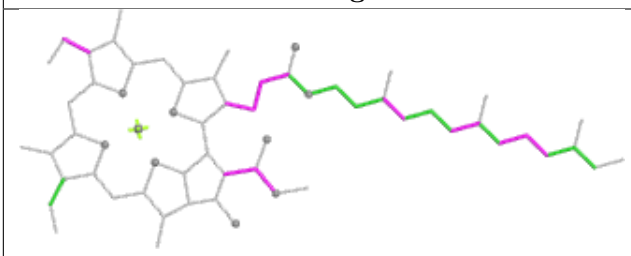
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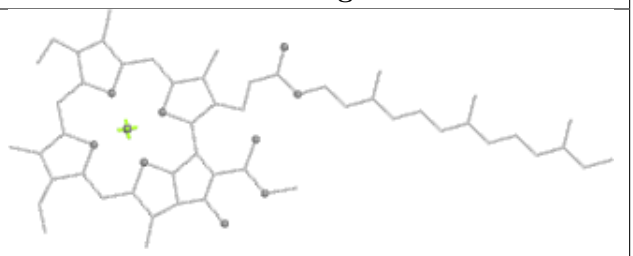
Bond lengths



Bond angles

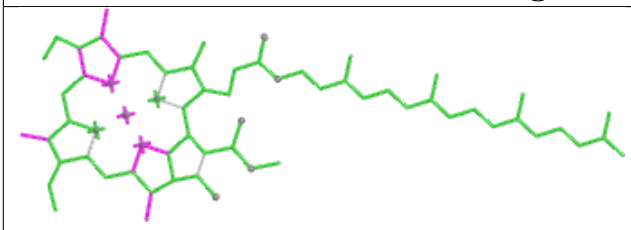


Torsions

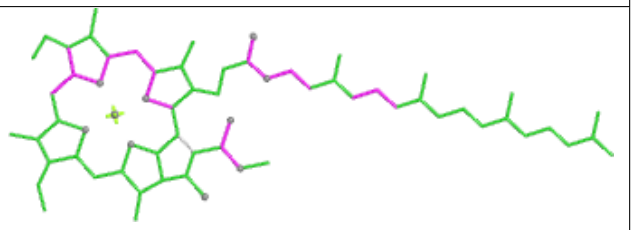


Rings

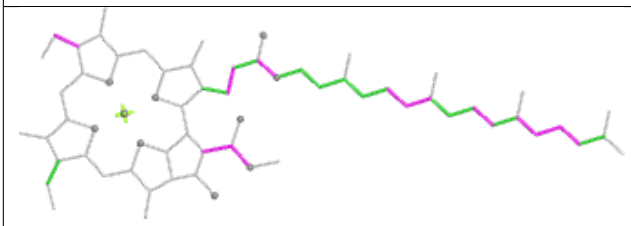
Ligand CLA c 503



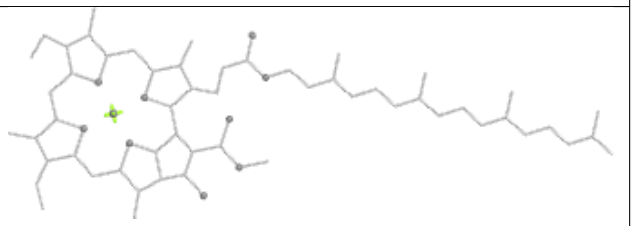
Bond lengths



Bond angles



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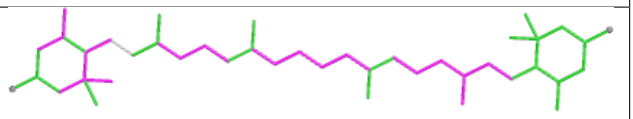


Rings

Ligand LUT Y 1621



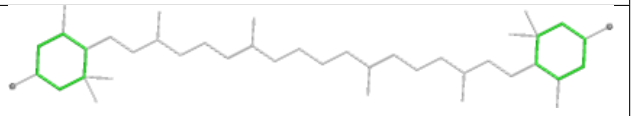
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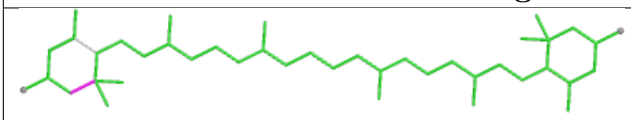


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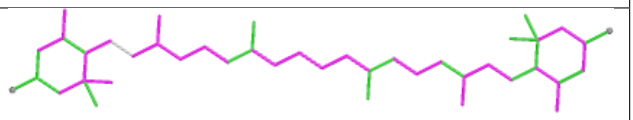


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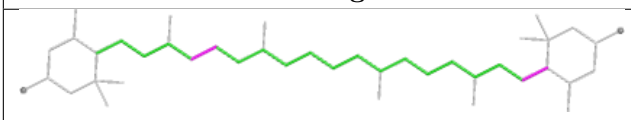
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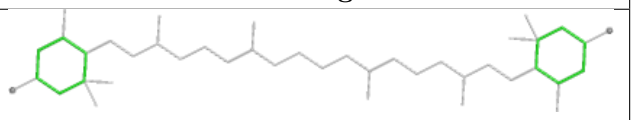
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Bond angles

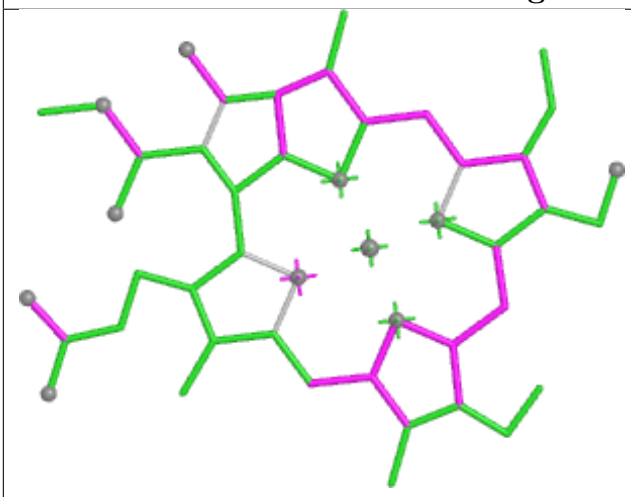


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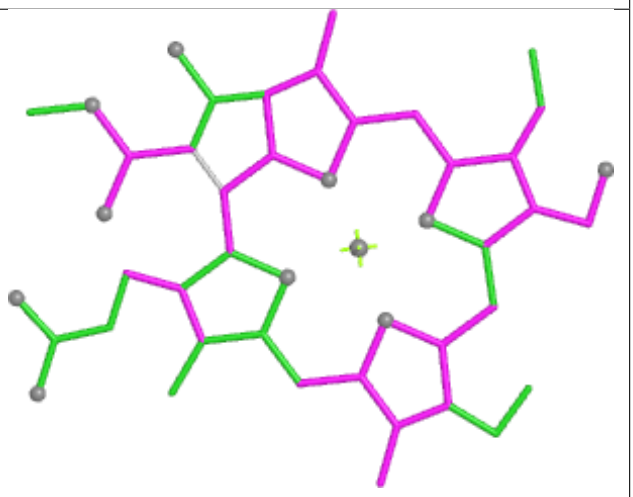


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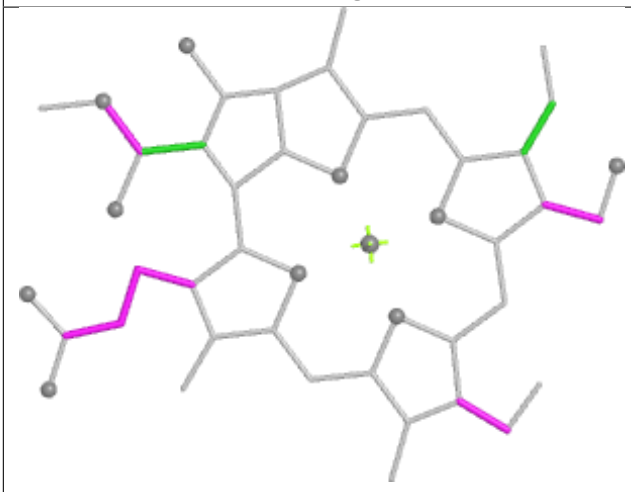
Ligand CHL 3 605



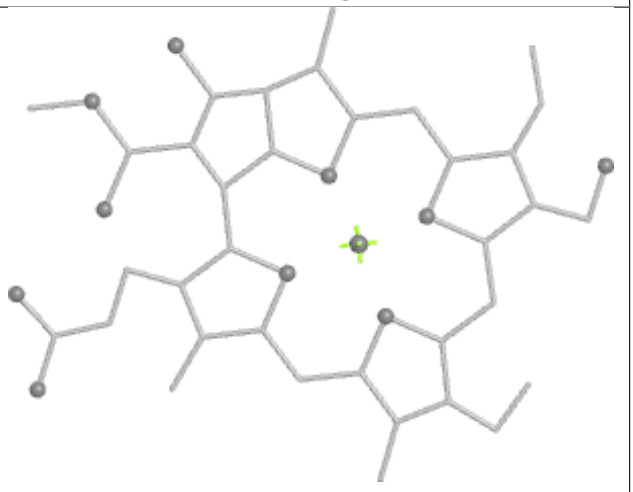
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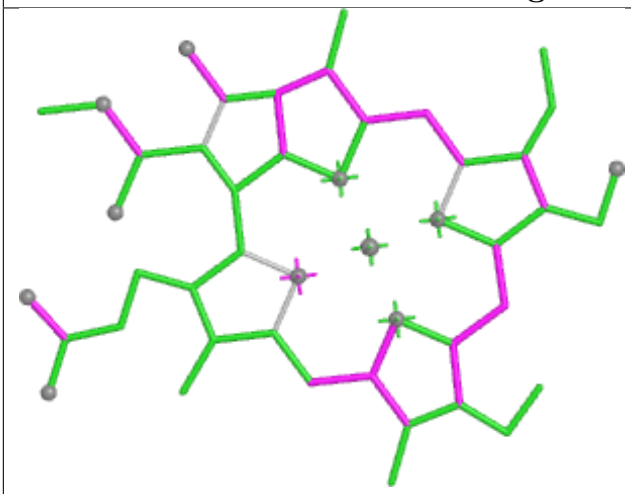


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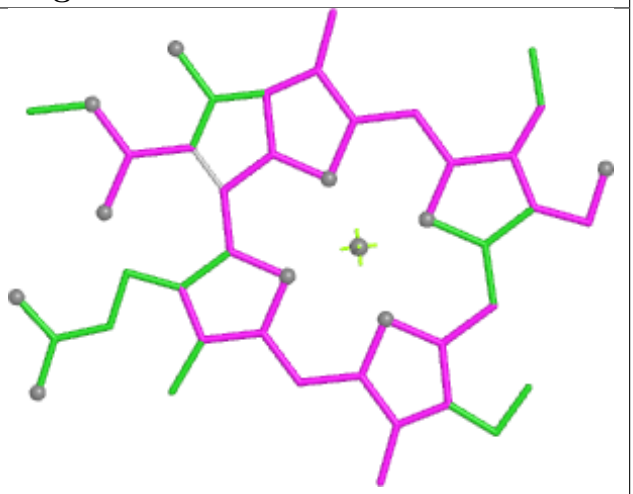


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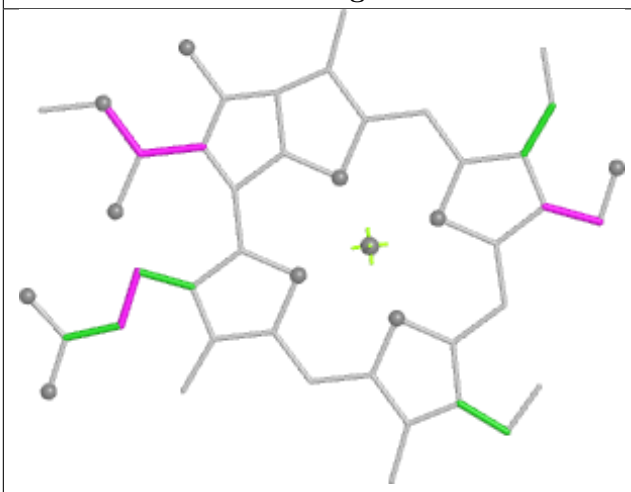
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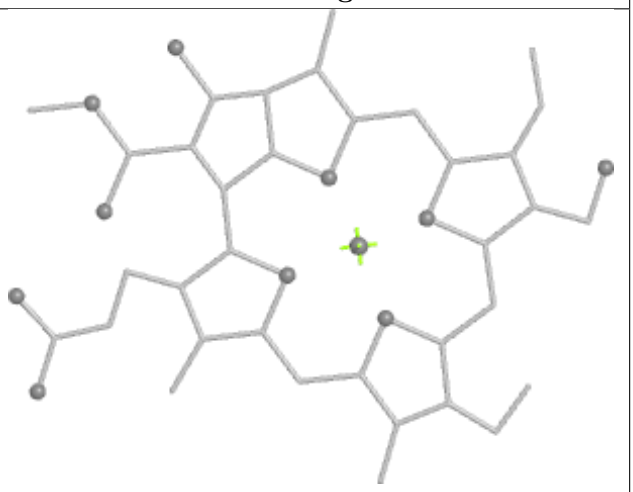
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Bond angles

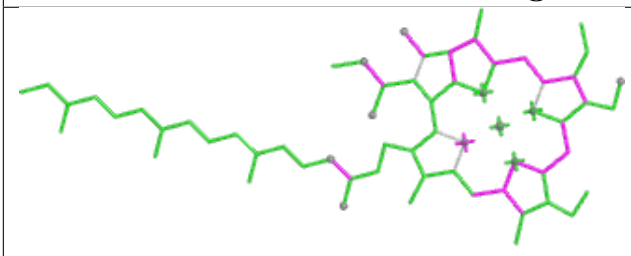


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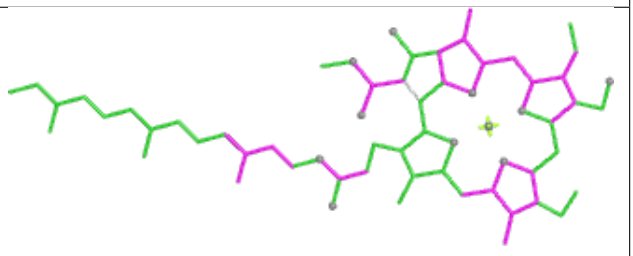


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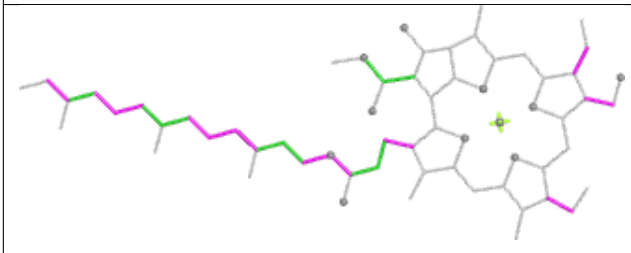
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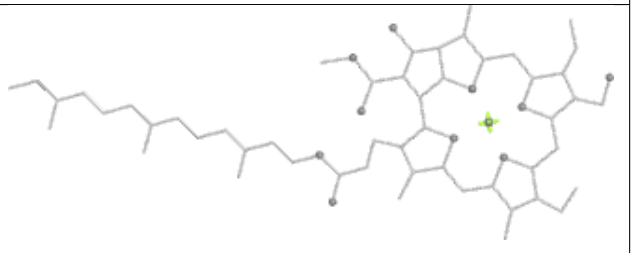
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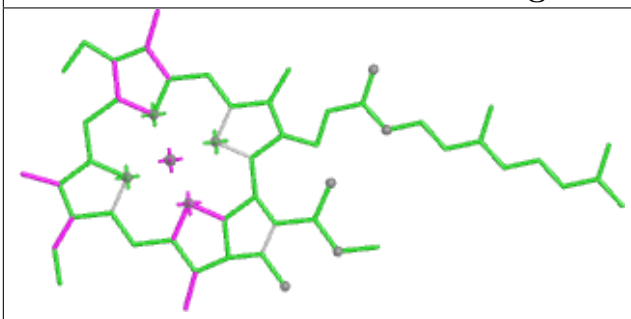


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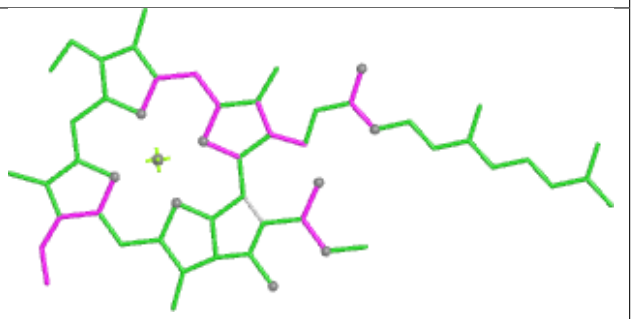


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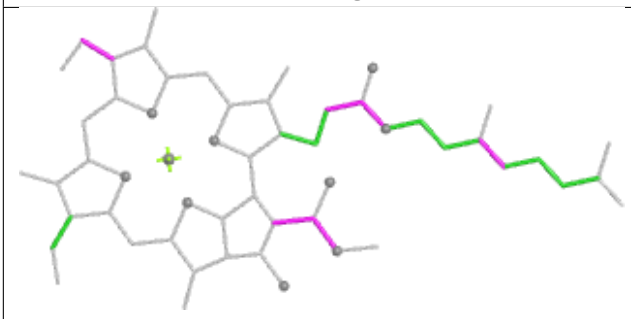
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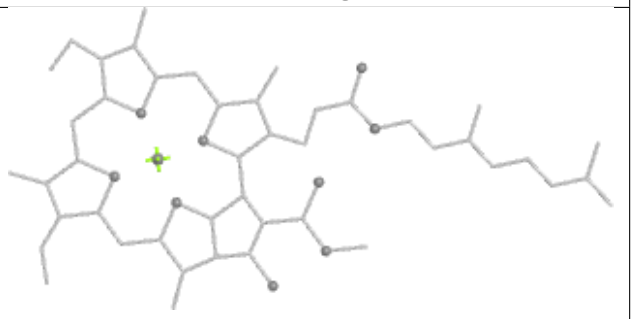
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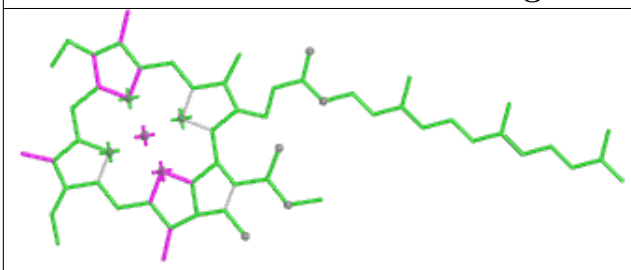


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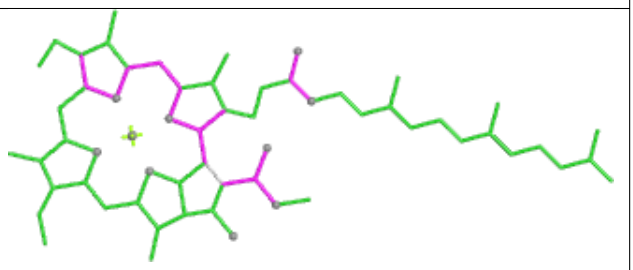


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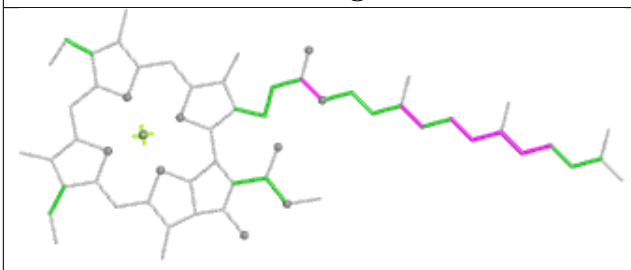
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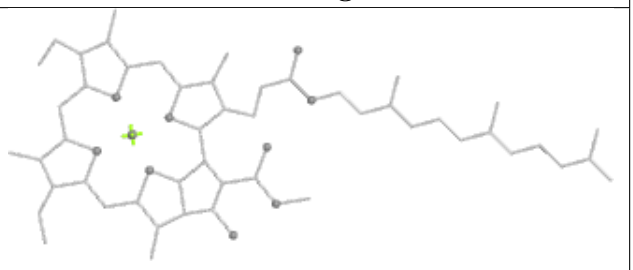
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Bond angles

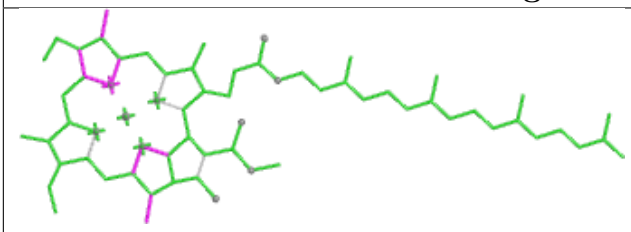


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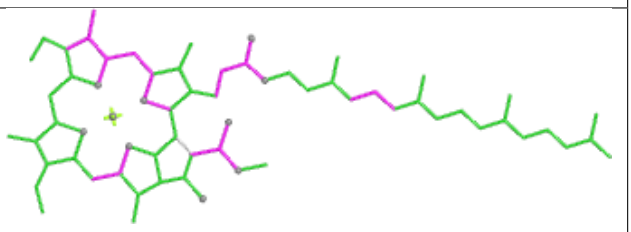


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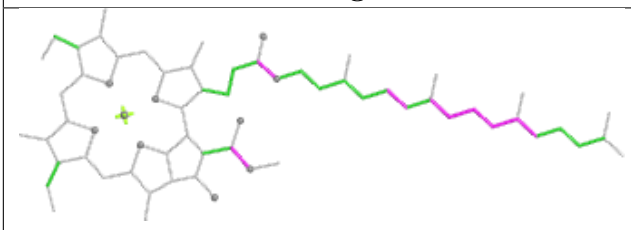
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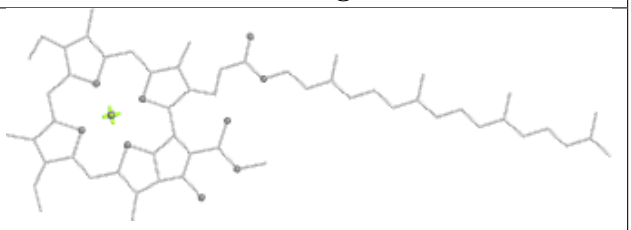
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Bond angles

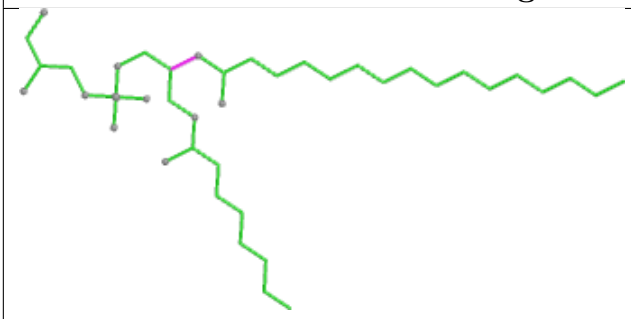


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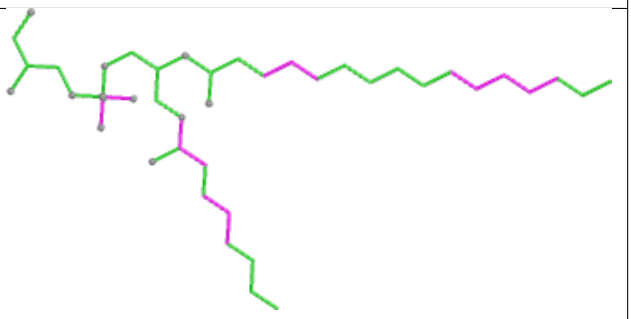


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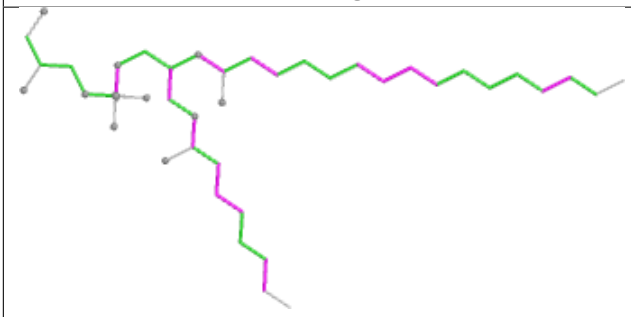
Ligand LHG 5 2630



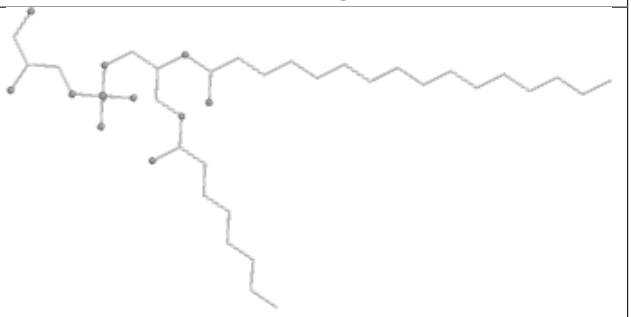
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Bond angles



Torsions



Rings

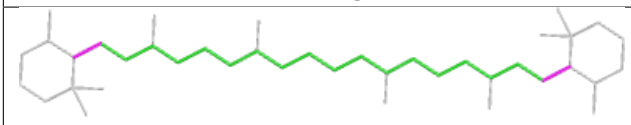
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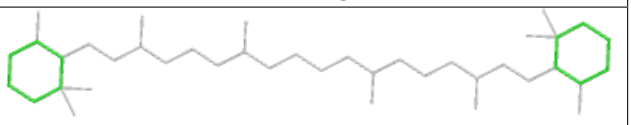
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Bond angles

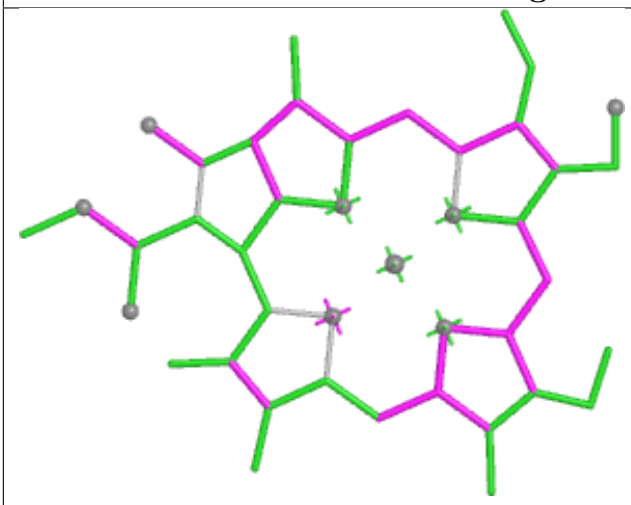


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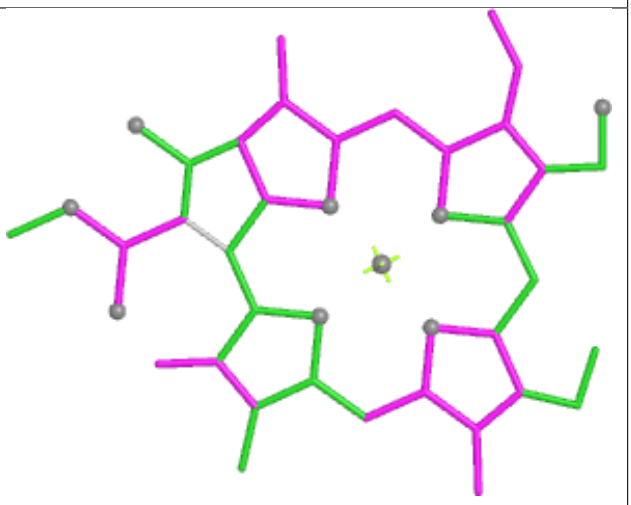


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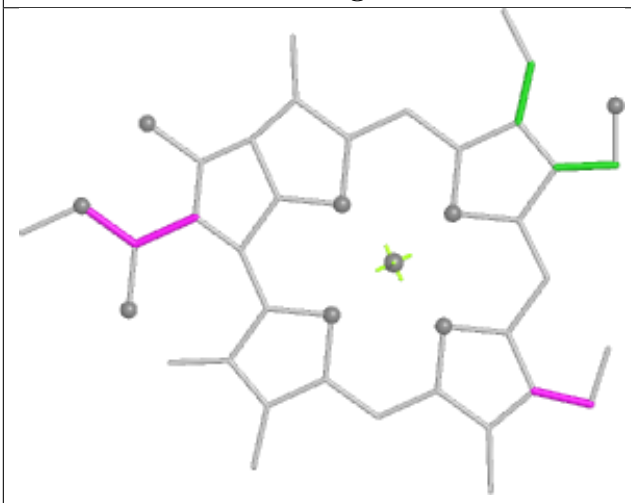
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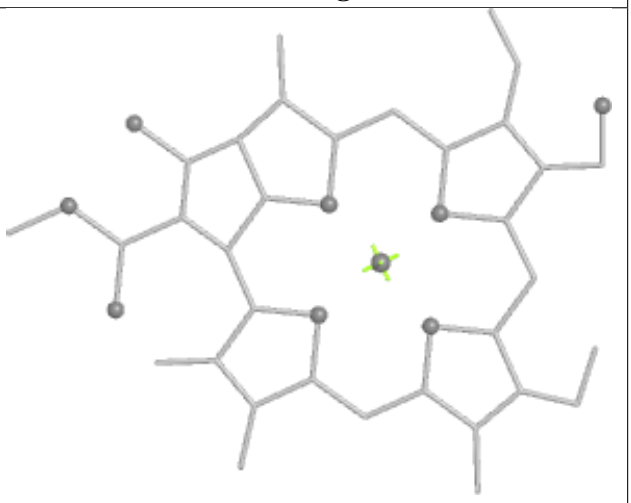
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Bond angles

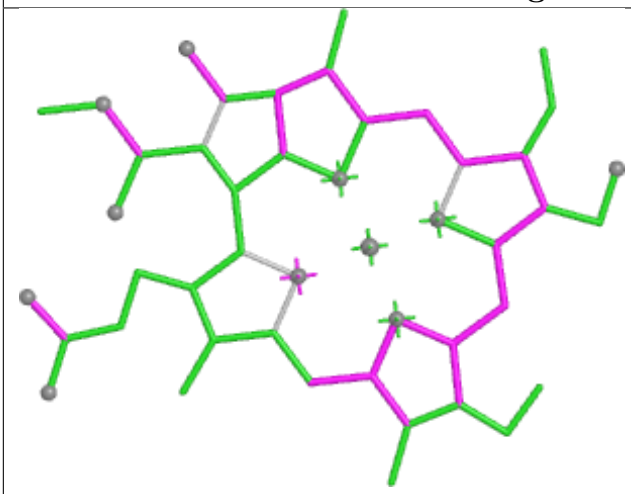


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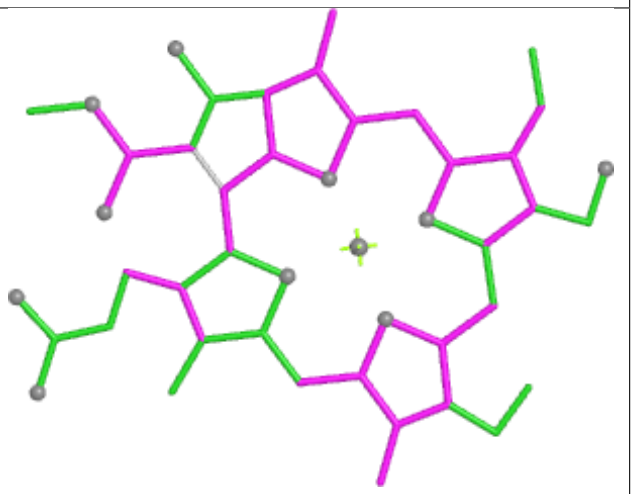


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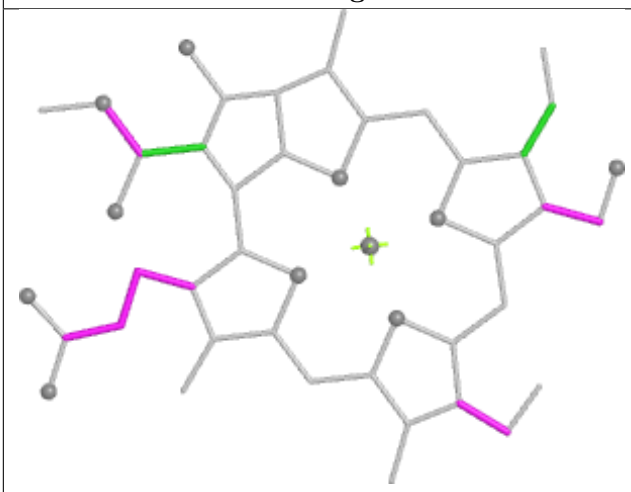
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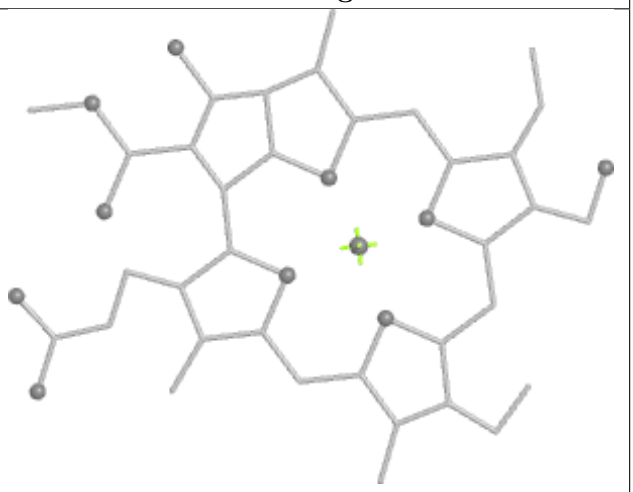
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Bond angles

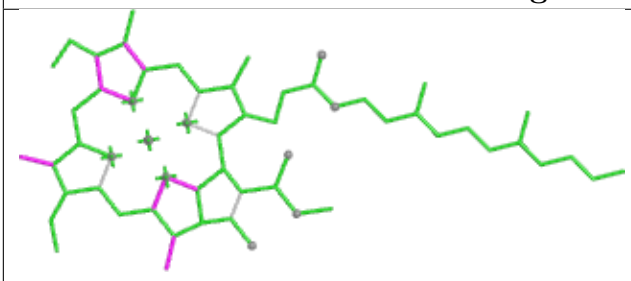


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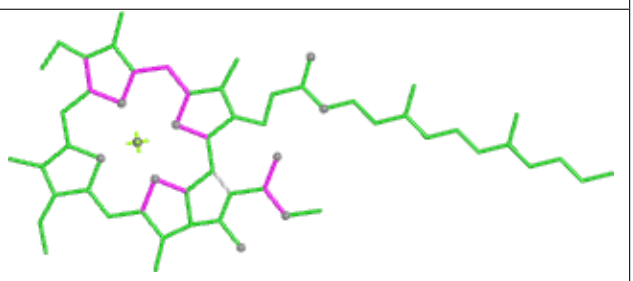


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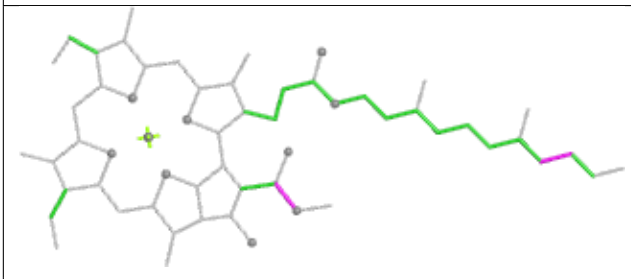
Ligand CLA r 609



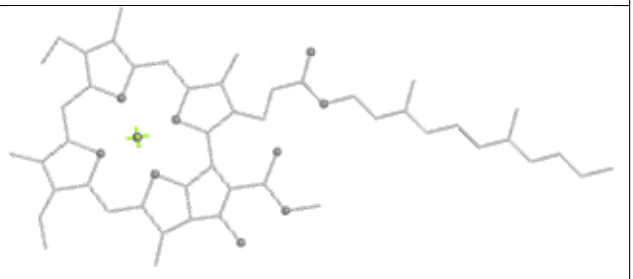
Bond lengths



Bond angles

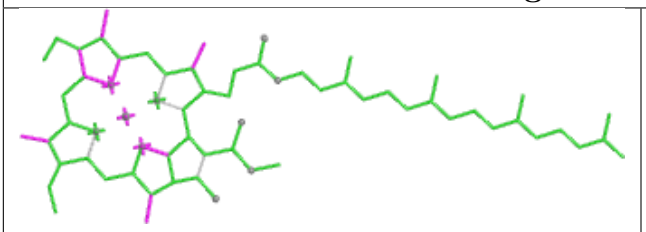


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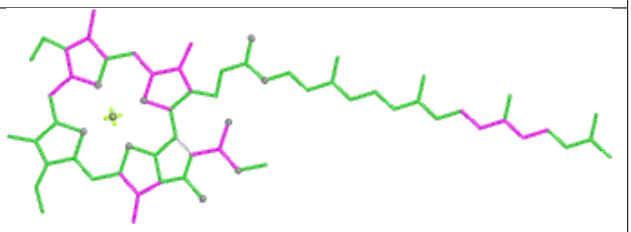


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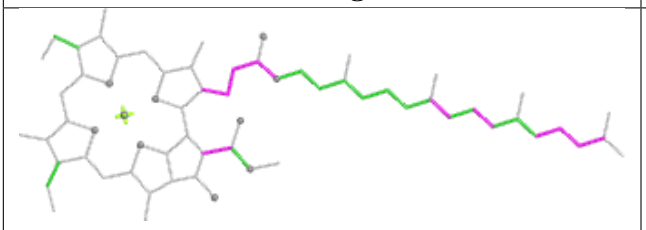
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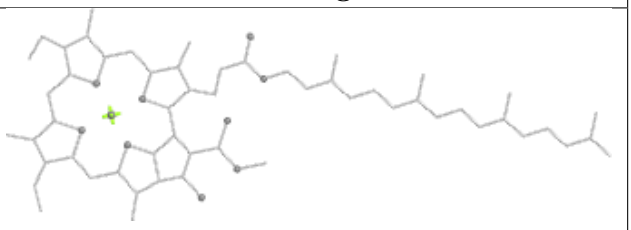
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Bond angles

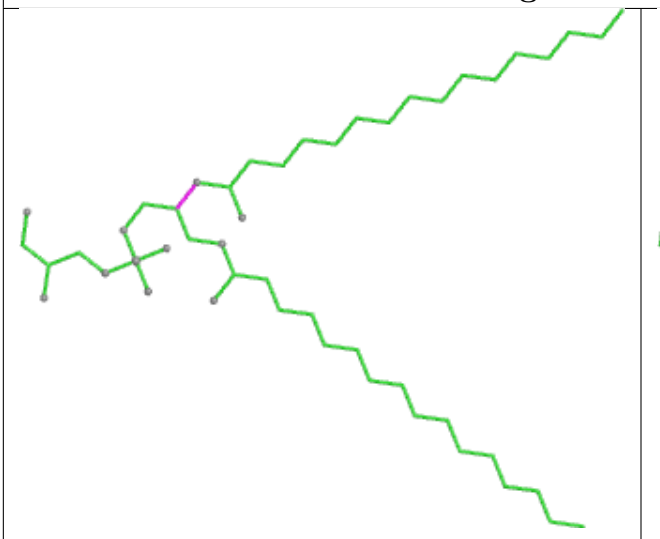


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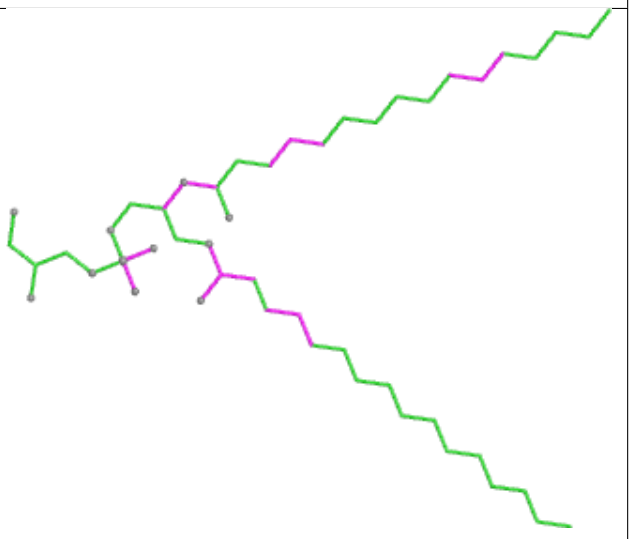


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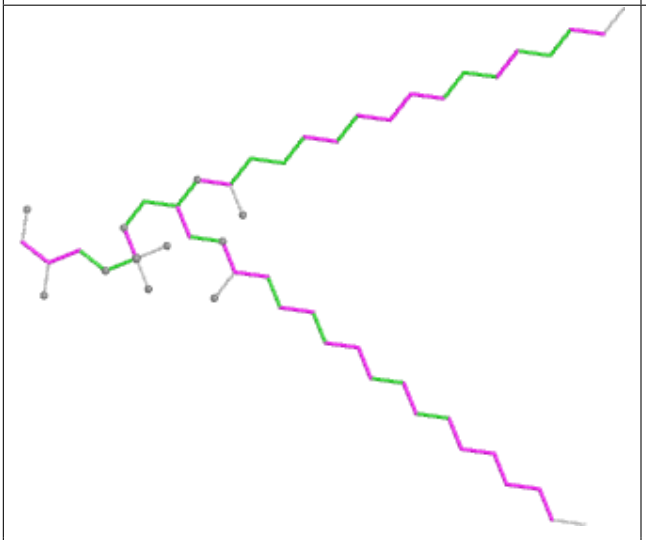
Ligand LHG s 2630



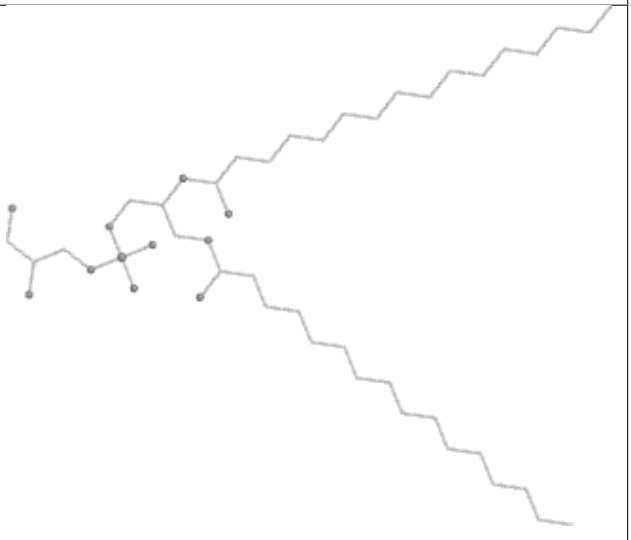
Bond lengths



Bond angles

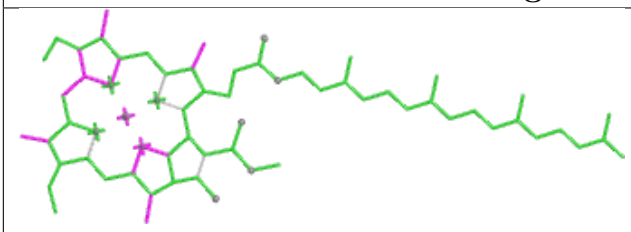


Torsions

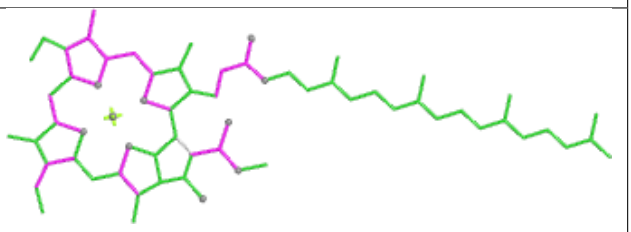


Rings

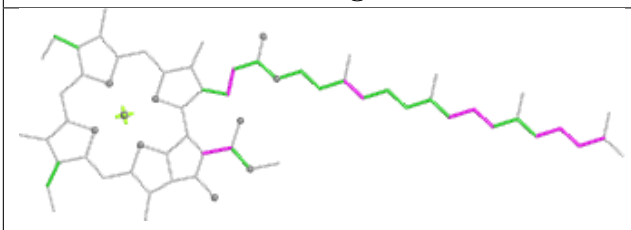
Ligand CLA B 607



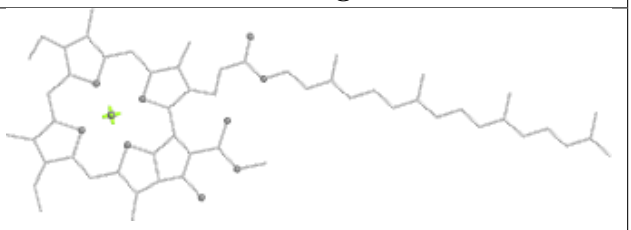
Bond lengths



Bond angles



Torsions

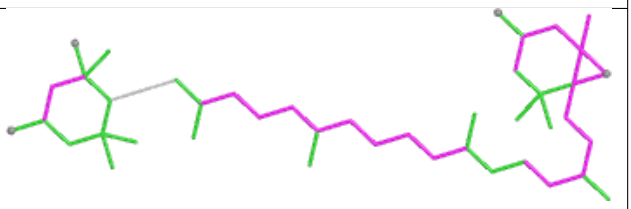


Rings

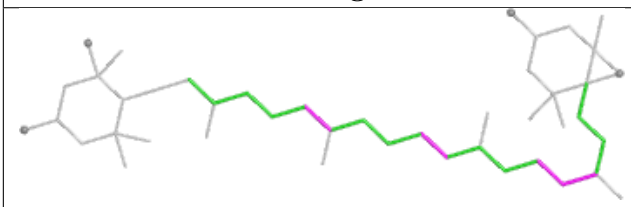
Ligand NEX 5 1623



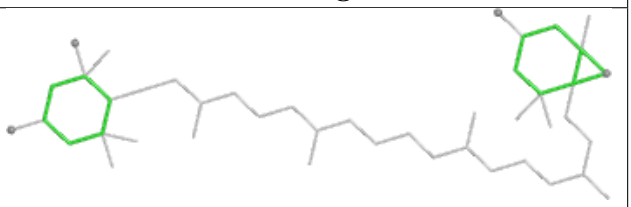
Bond lengths



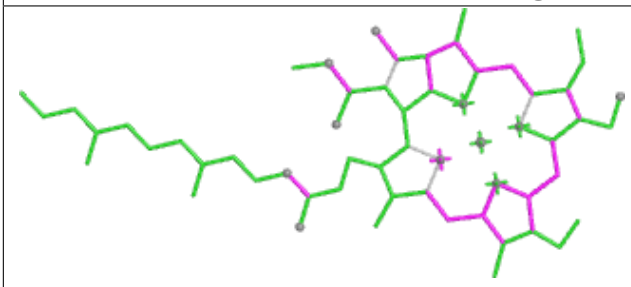
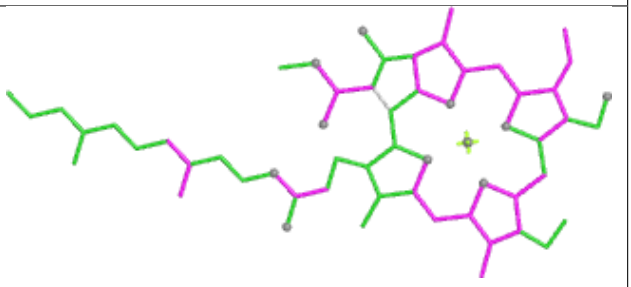
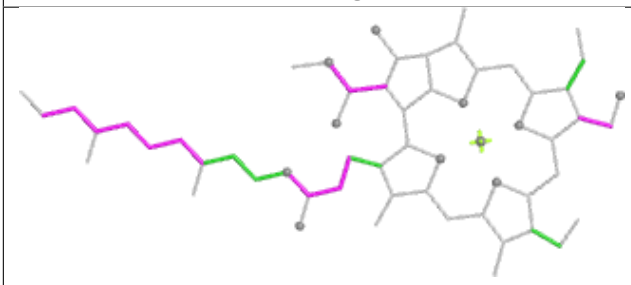
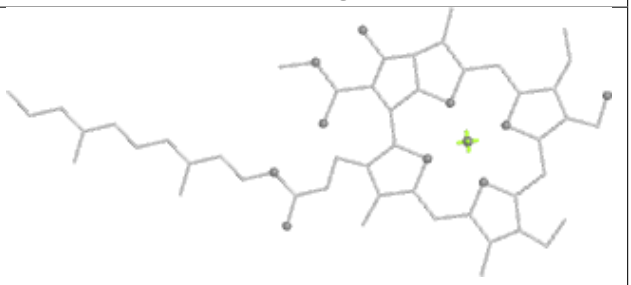
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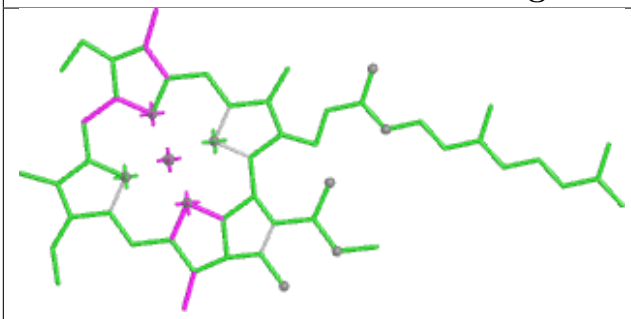
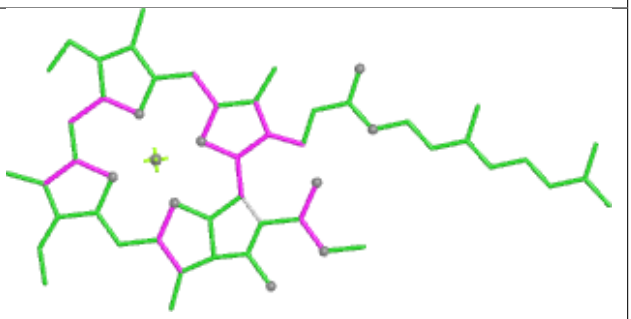
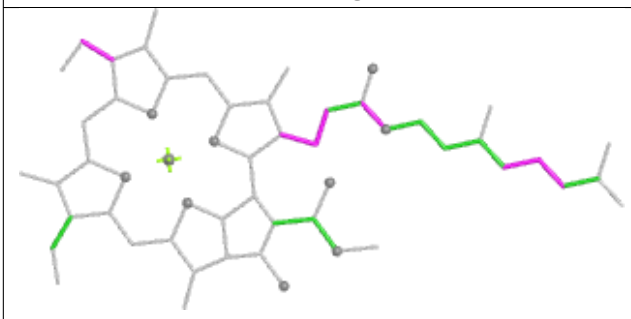
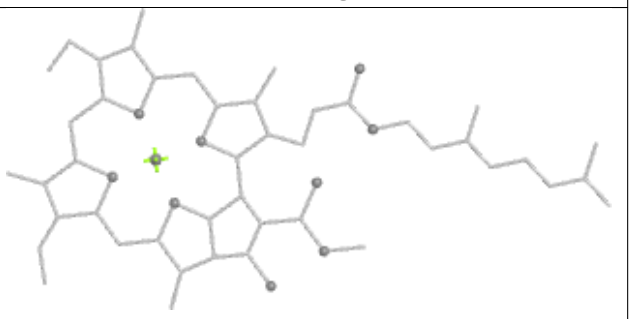


Torsions

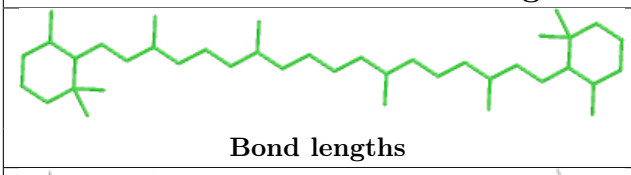


Rings

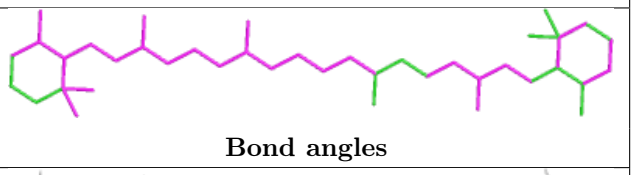
Ligand CHL s 607	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 3 611	
 Bond lengths	 Bond angles
 Torsions	 Rings

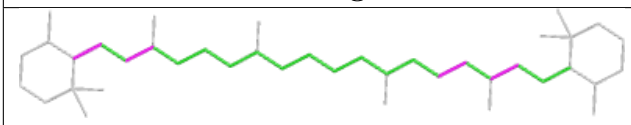
Ligand BCR C 516



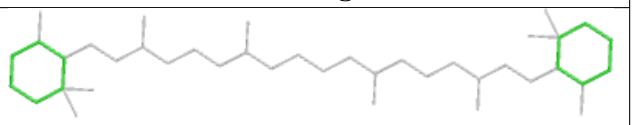
Bond lengths



Bond angles

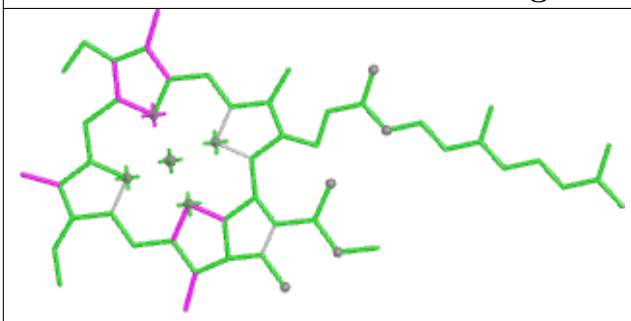


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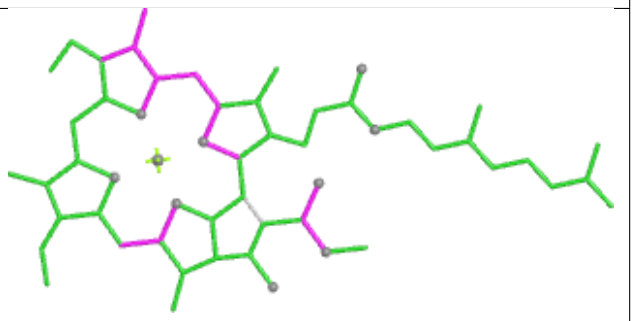


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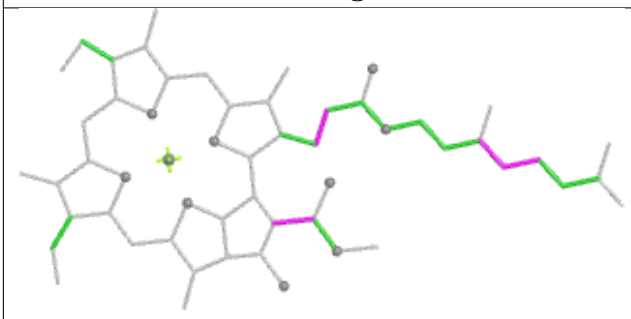
Ligand CLA s 613



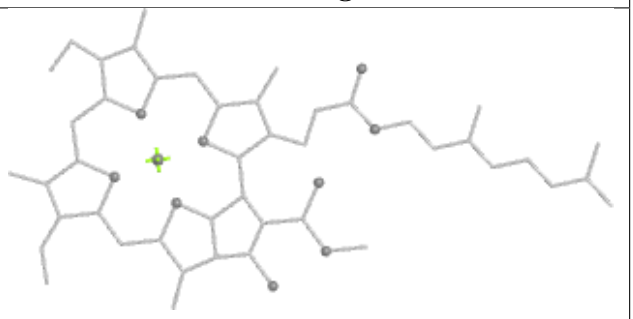
Bond lengths



Bond angles

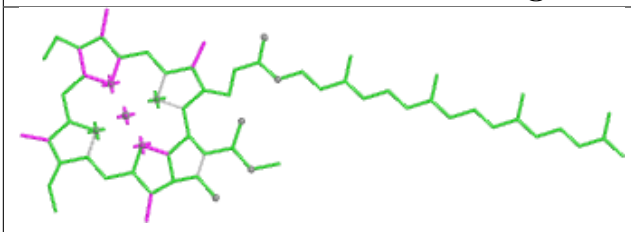


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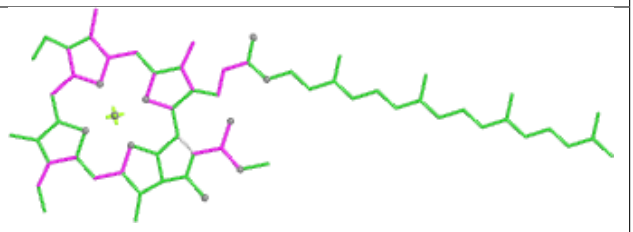


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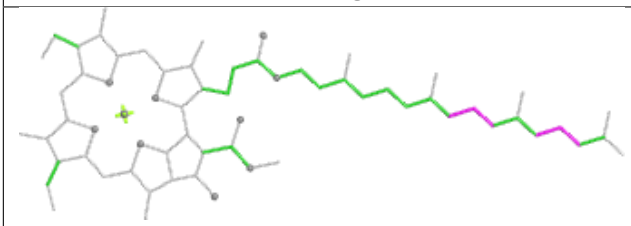
Ligand CLA d 402



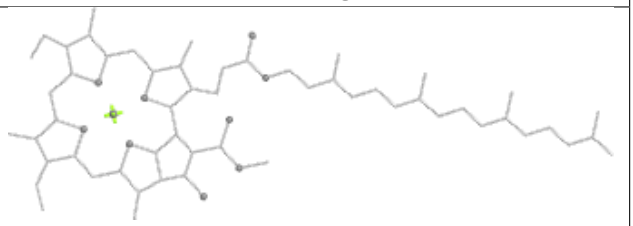
Bond lengths



Bond angles

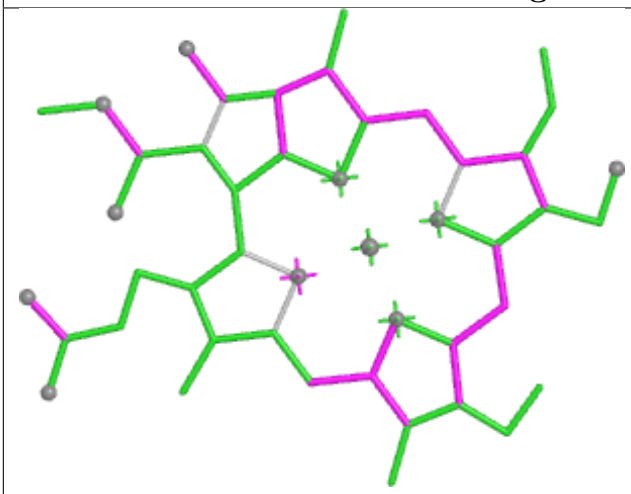


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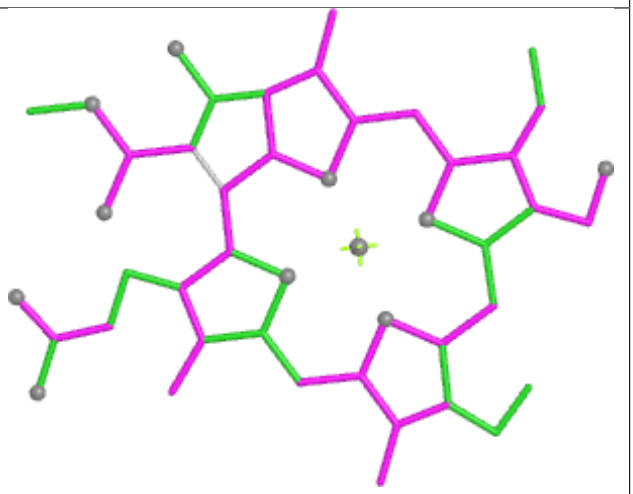


Rings

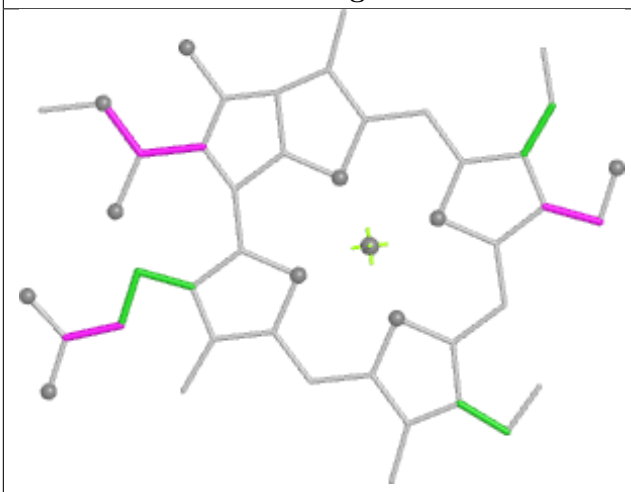
Ligand CHL s 606



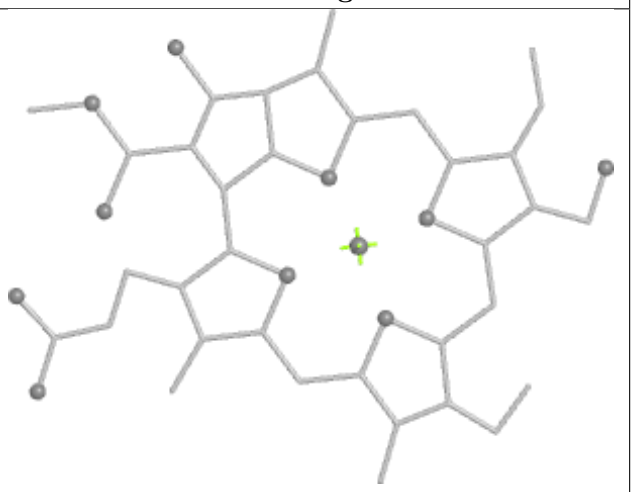
Bond lengths



Bond angles

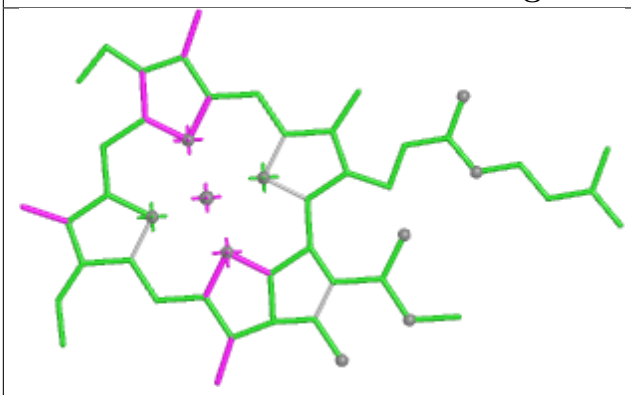


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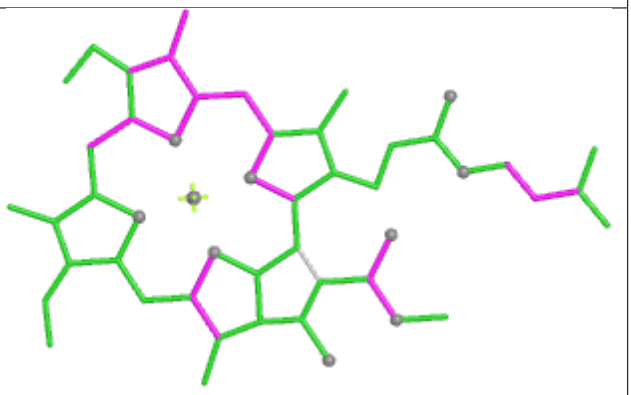


Rings

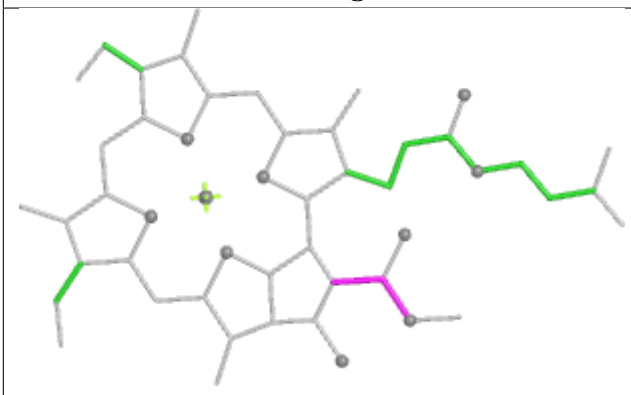
Ligand CLA Y 604



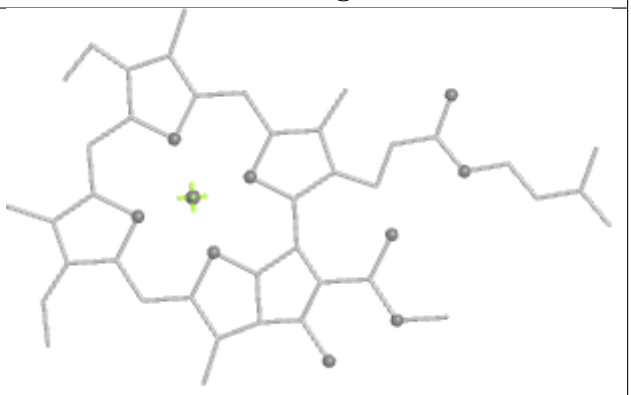
Bond lengths



Bond angles

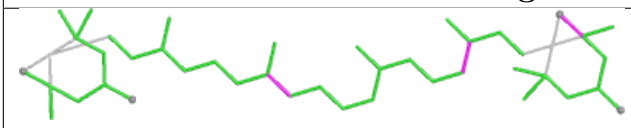


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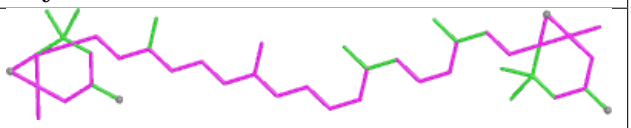


Rings

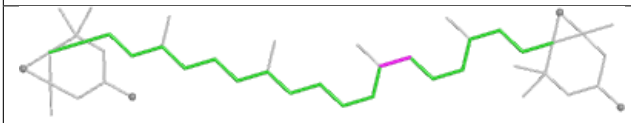
Ligand XAT y 1622



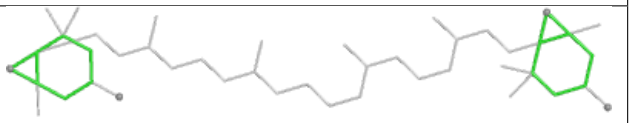
Bond lengths



Bond angles

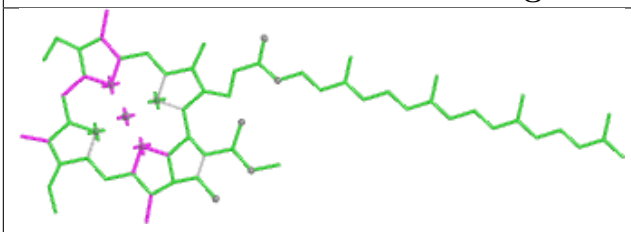


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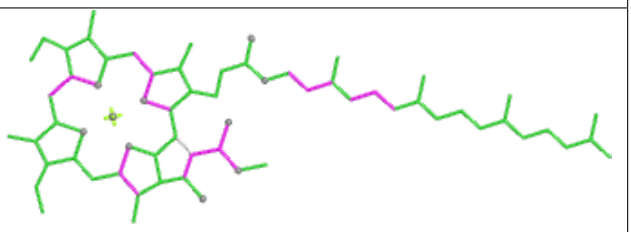


Rings

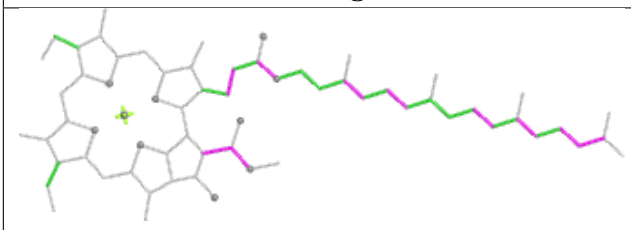
Ligand CLA C 505



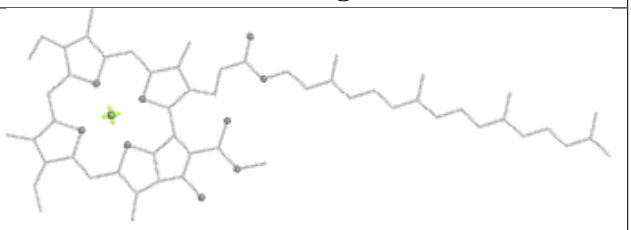
Bond lengths



Bond angles

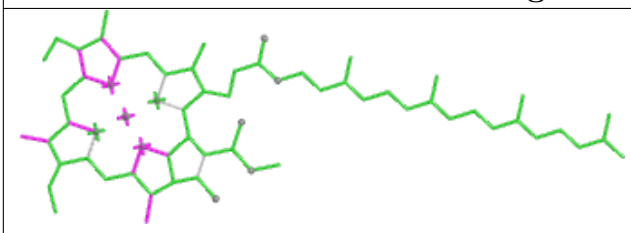


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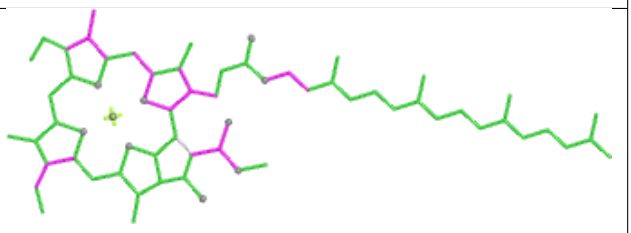


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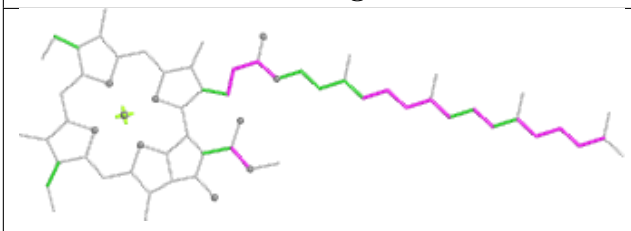
Ligand CLA b 617



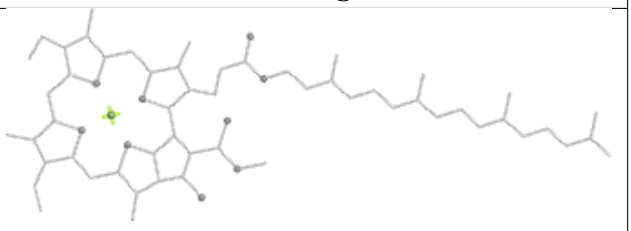
Bond lengths



Bond angles

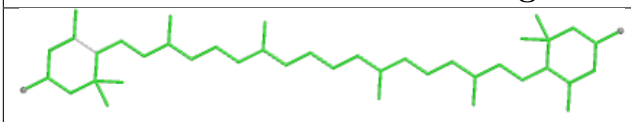


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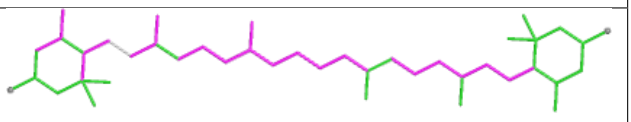


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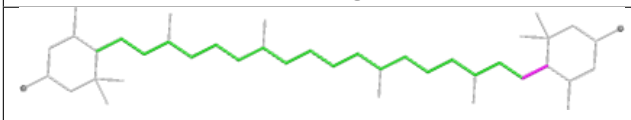
Ligand LUT S 1620



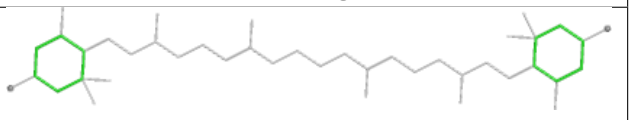
Bond lengths



Bond angles

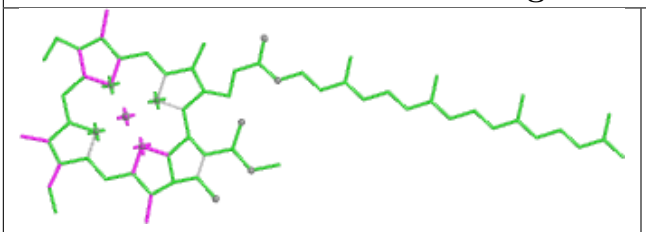


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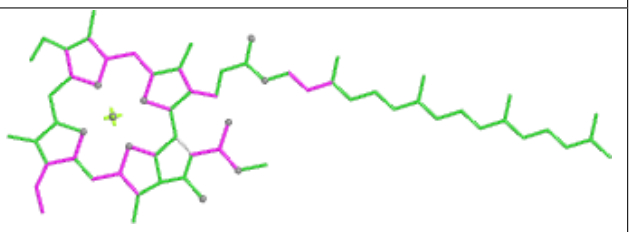


Rings

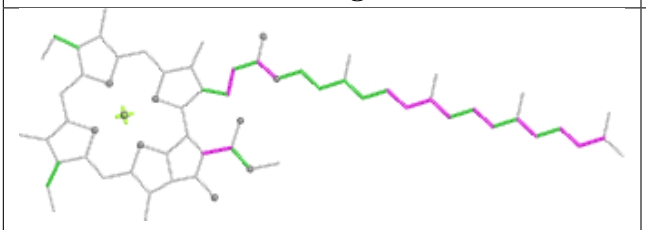
Ligand CLA n 603



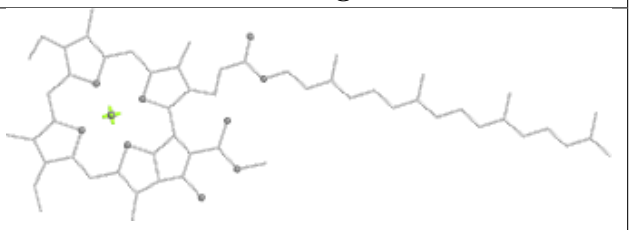
Bond lengths



Bond angles

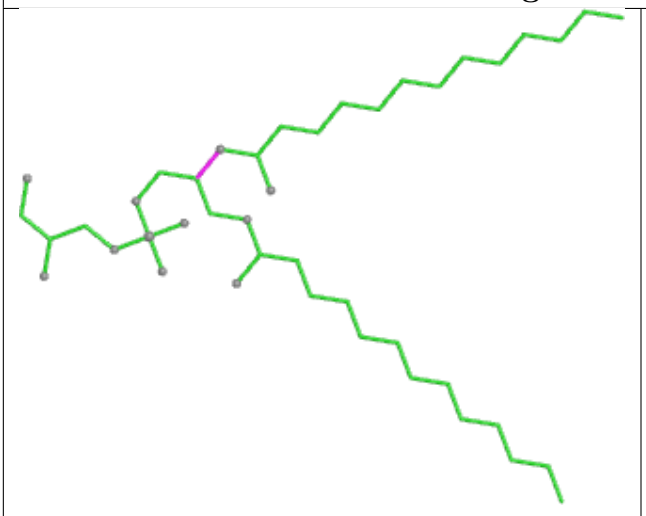


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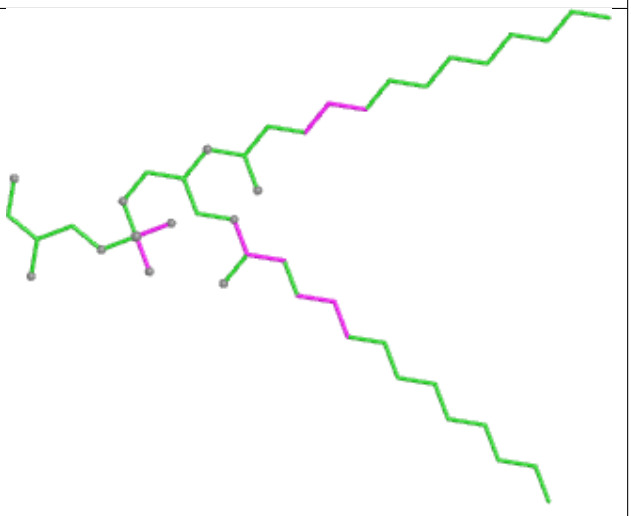


Rings

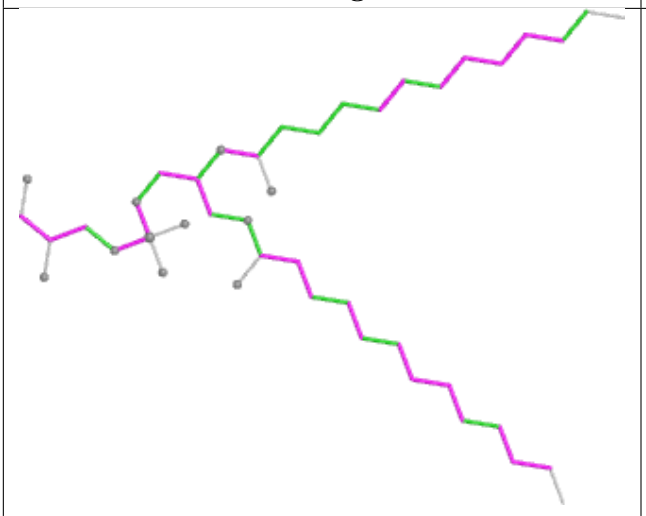
Ligand LHG D 410



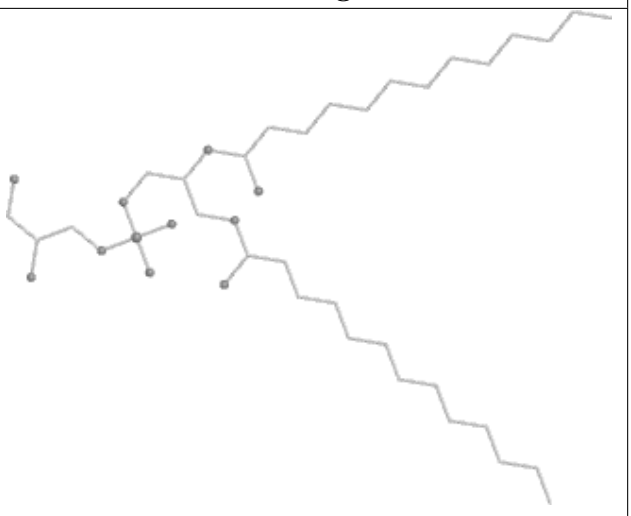
Bond lengths



Bond angles

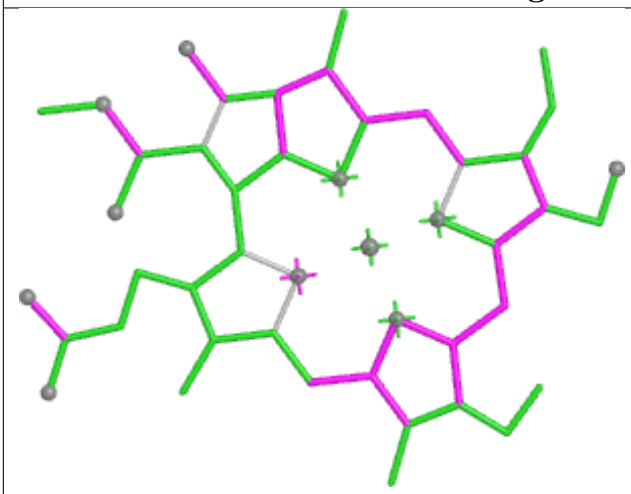


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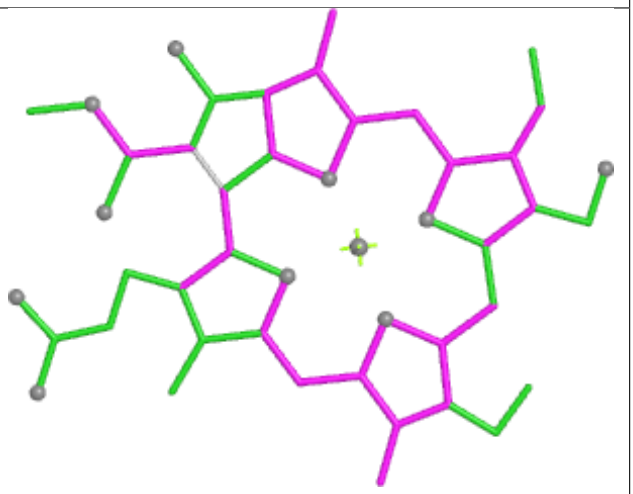


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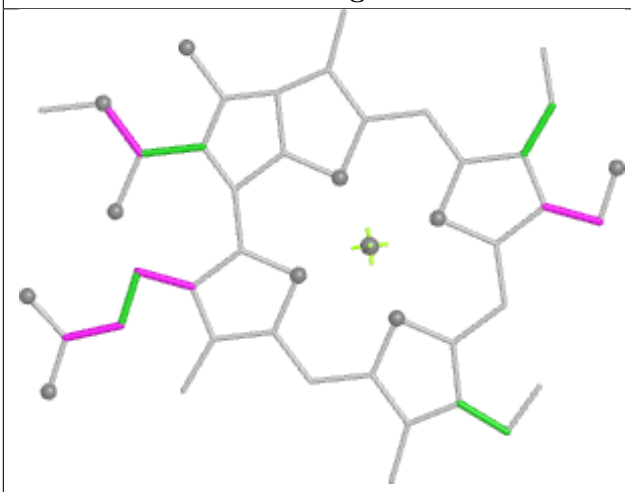
Ligand CHL 2 608



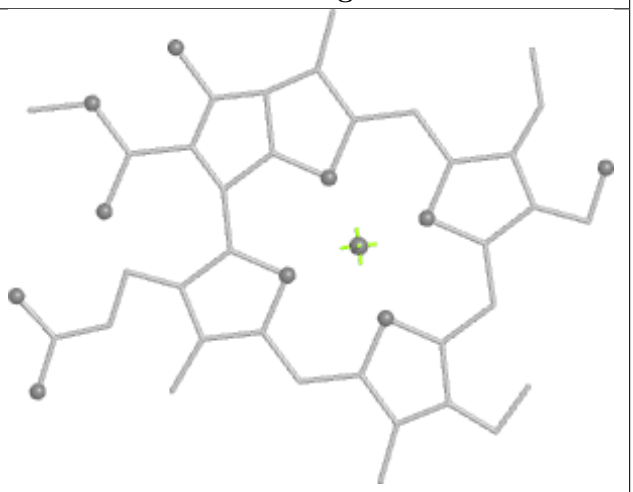
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Bond angles

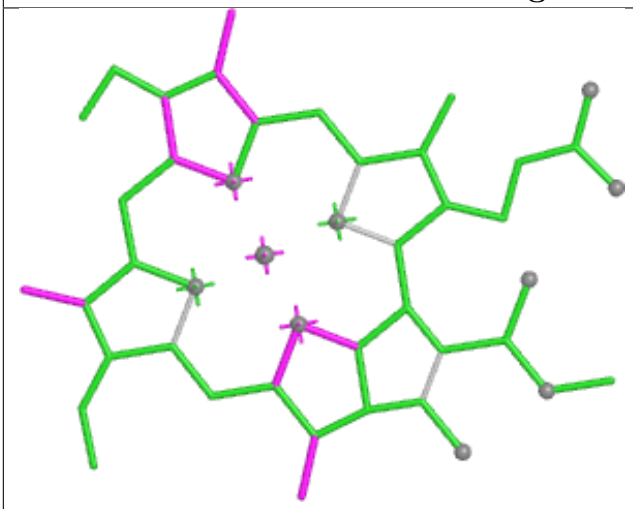


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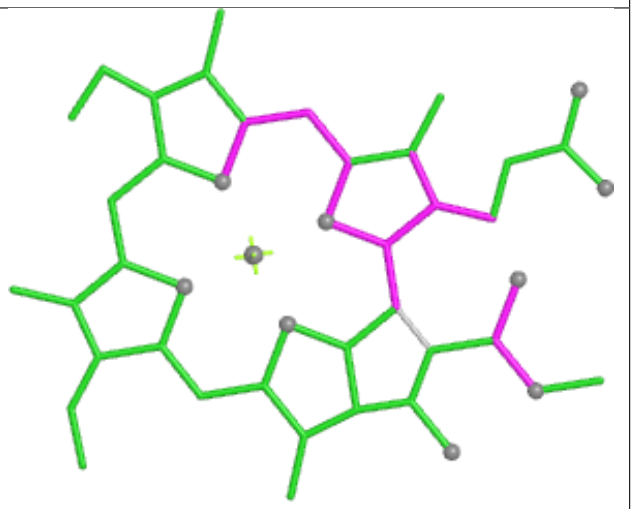


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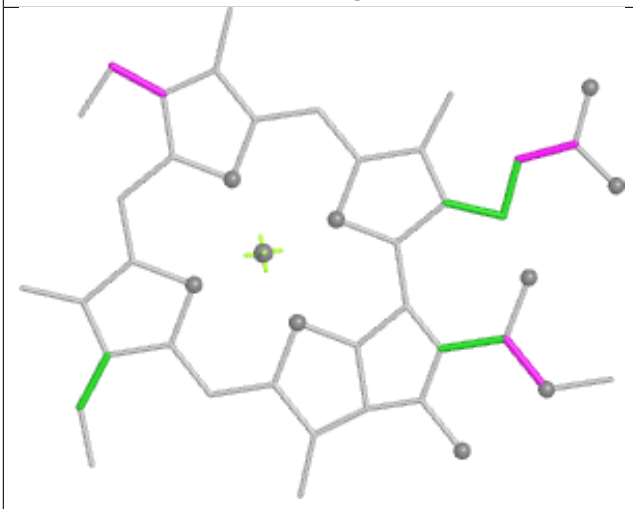
Ligand CLA 8 603



Bond lengths



Bond angles

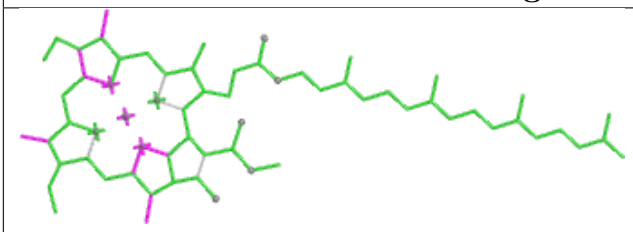


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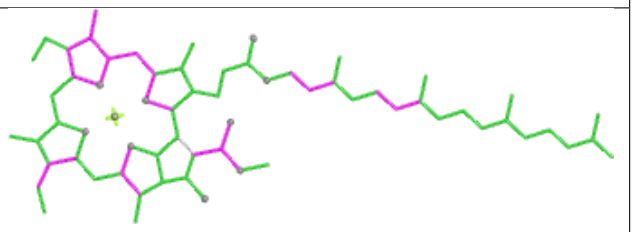


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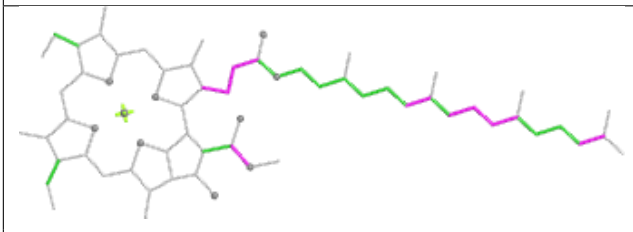
Ligand CLA N 602



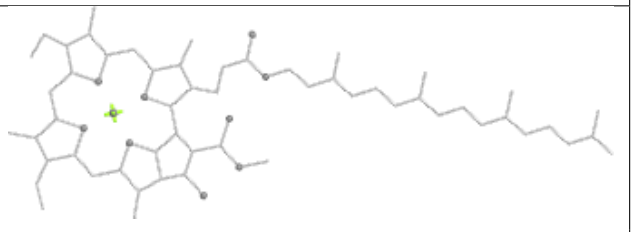
Bond lengths



Bond angles

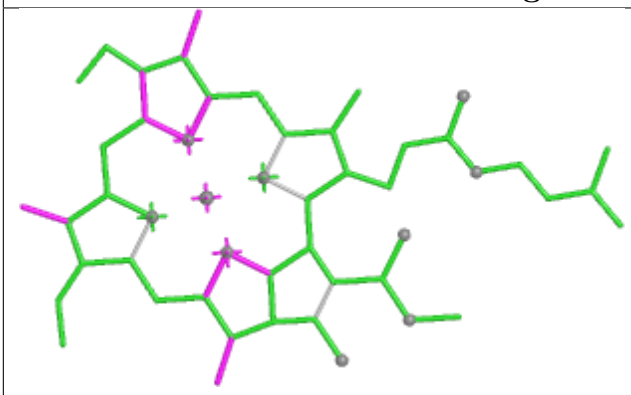


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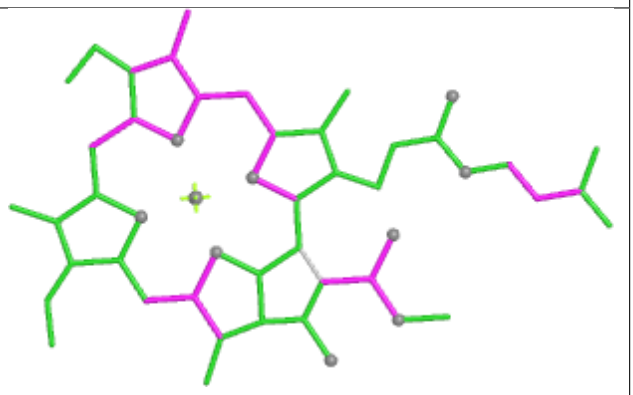


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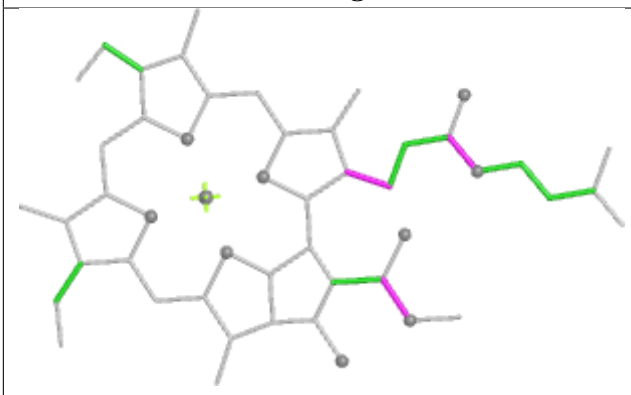
Ligand CLA G 604



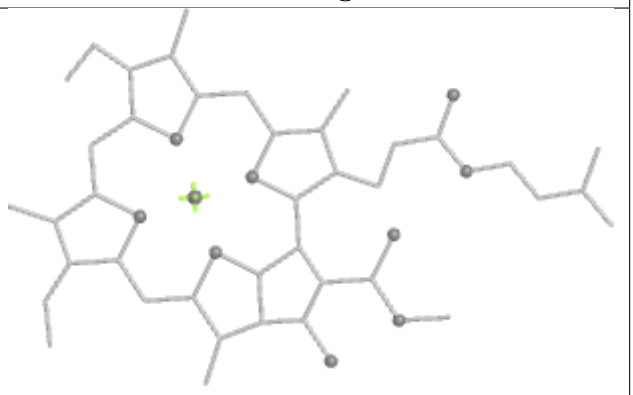
Bond lengths



Bond angles



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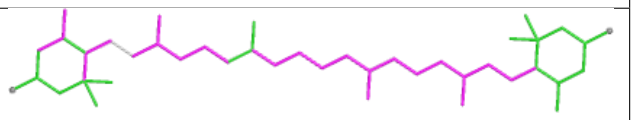


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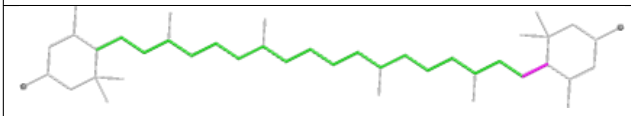
Ligand LUT 5 1620



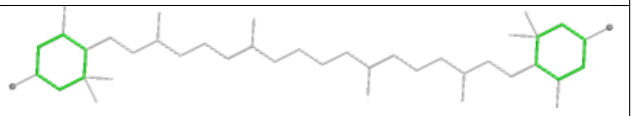
Bond lengths



Bond angles

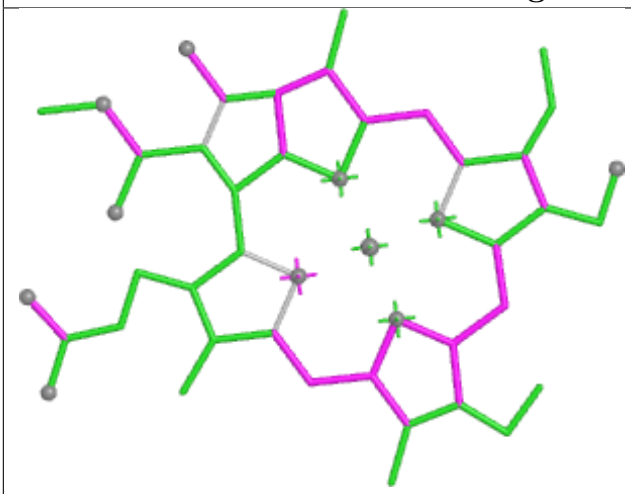


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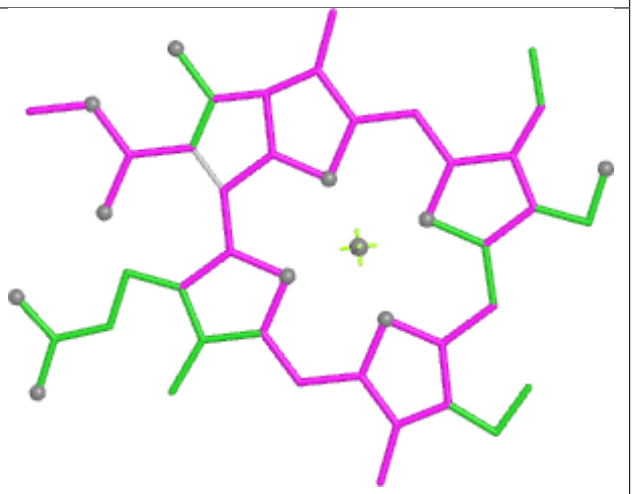


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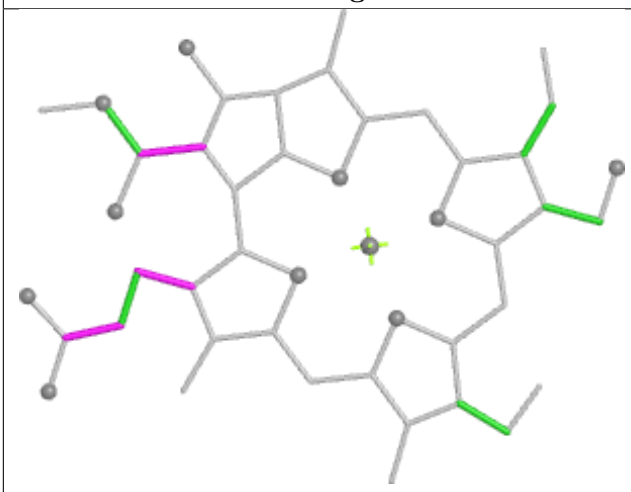
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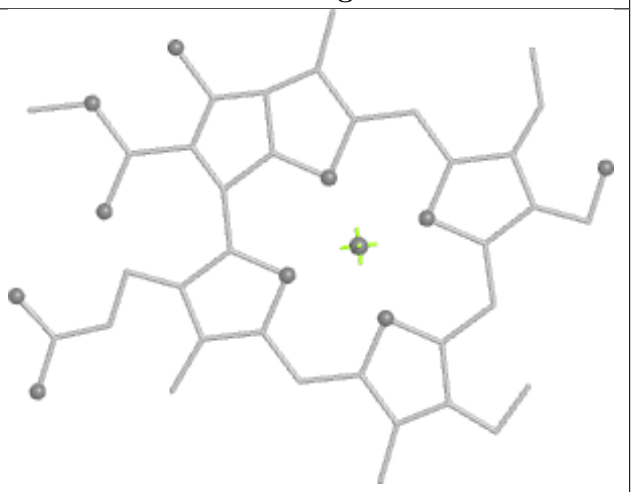
Bond lengths



Bond angles



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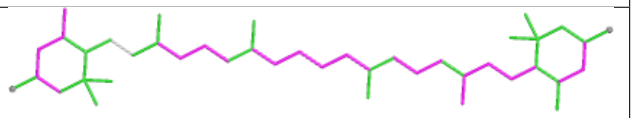


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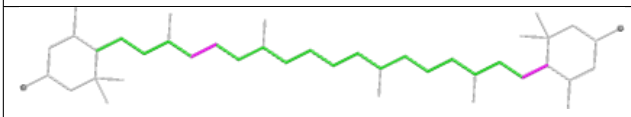
Ligand LUT 3 1621



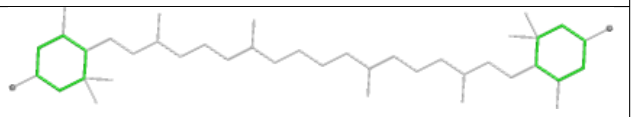
Bond lengths



Bond angles

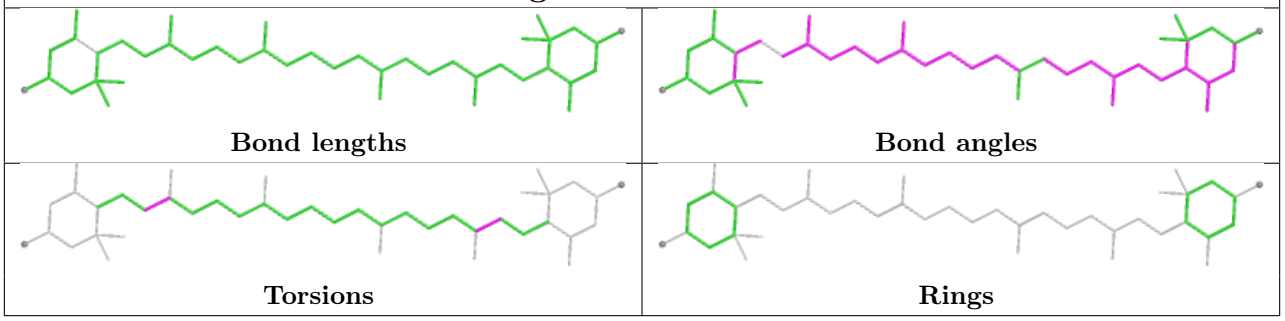


Torsions



Rings

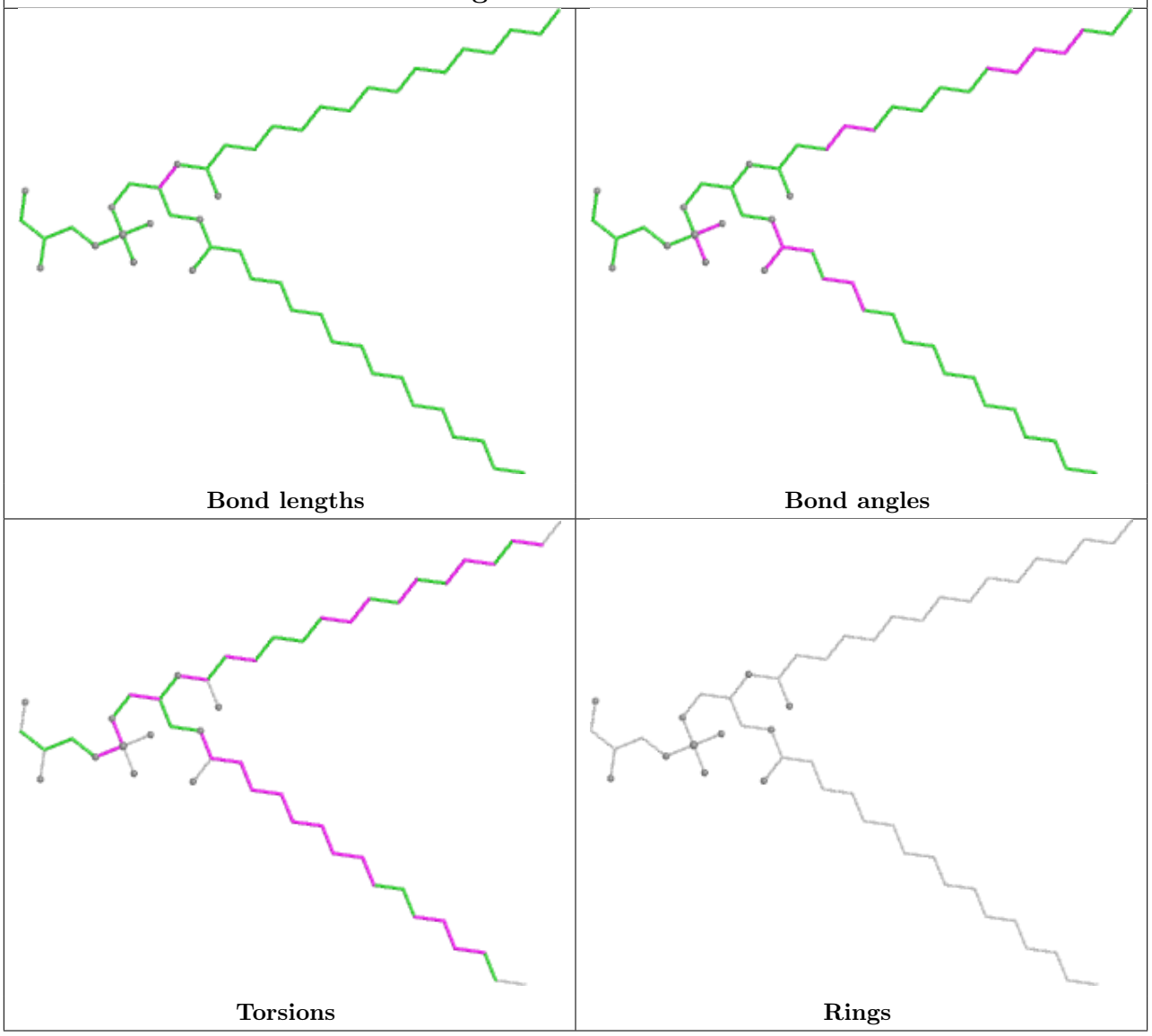
Ligand LUT 4 620



Bond lengths | Bond angles

Torsions | Rings

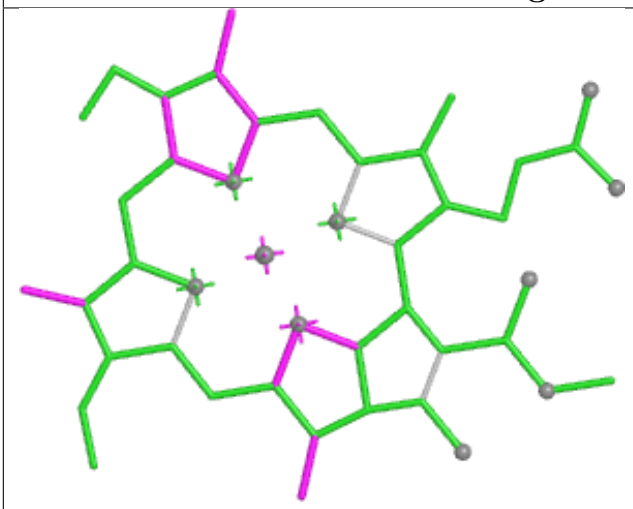
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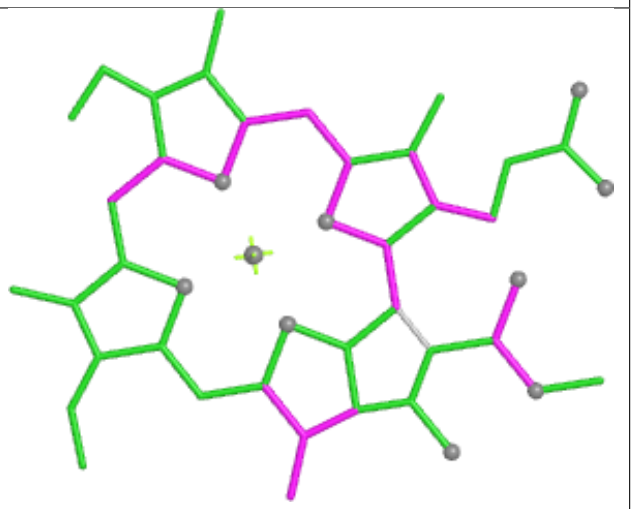
Bond lengths | Bond angles

Torsions | Rings

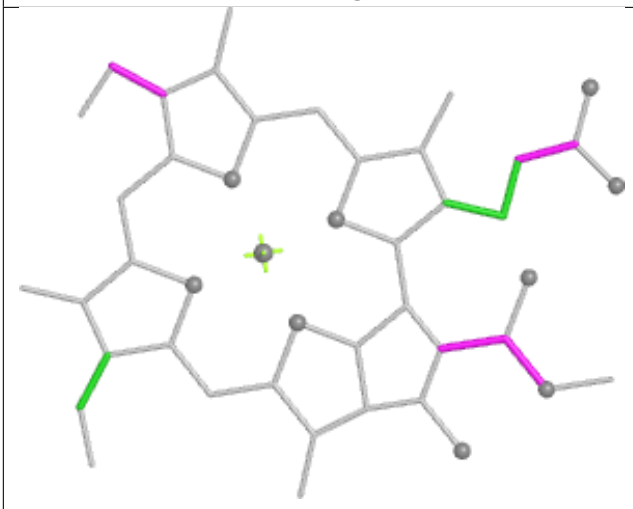
Ligand CLA 3 612



Bond lengths



Bond angles

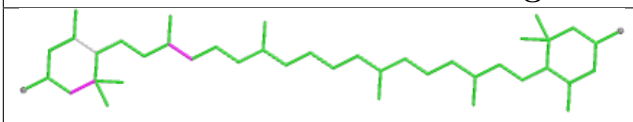


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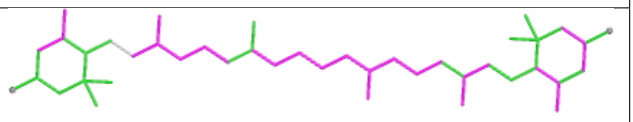


Rings

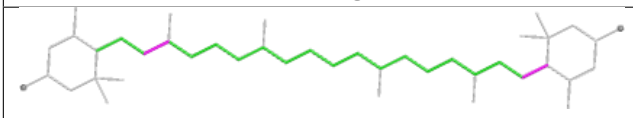
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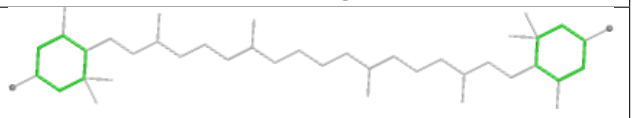
Bond lengths



Bond angles

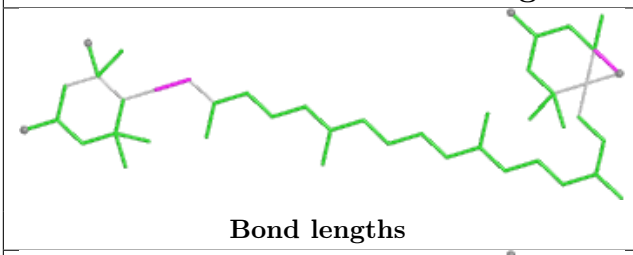


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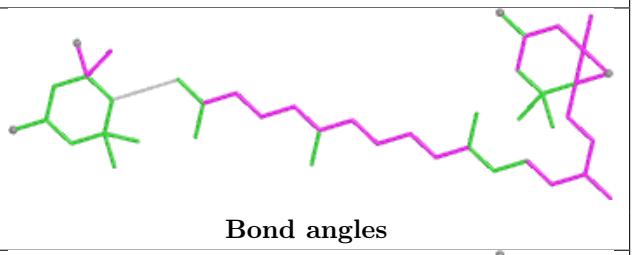


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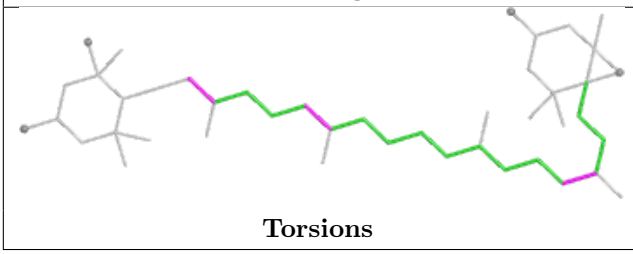
Ligand NEX s 1623



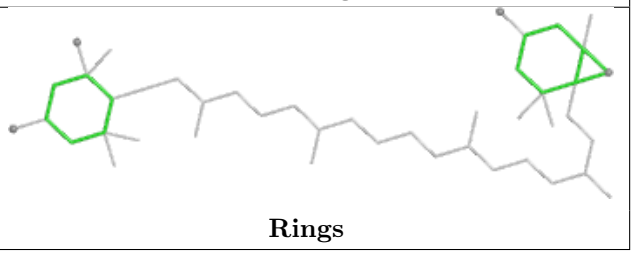
Bond lengths



Bond angles

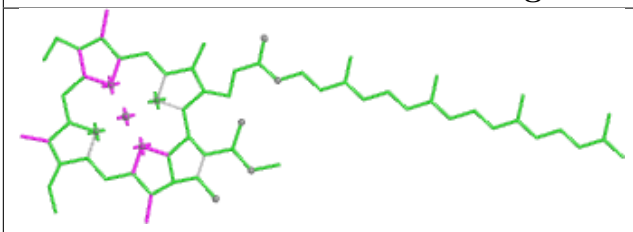


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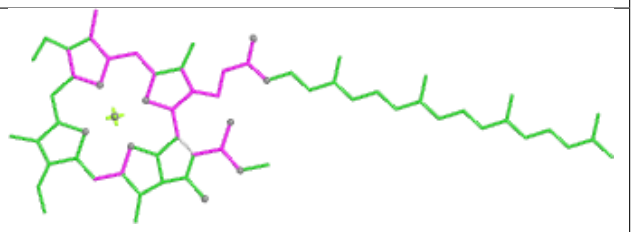


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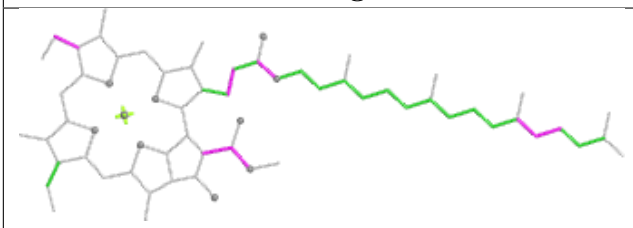
Ligand CLA B 611



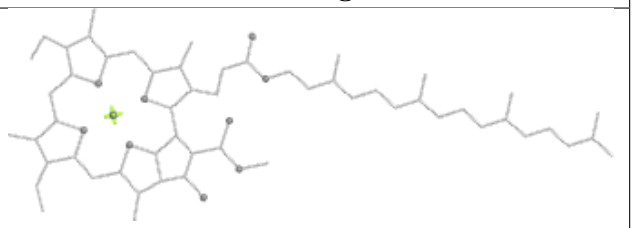
Bond lengths



Bond angles

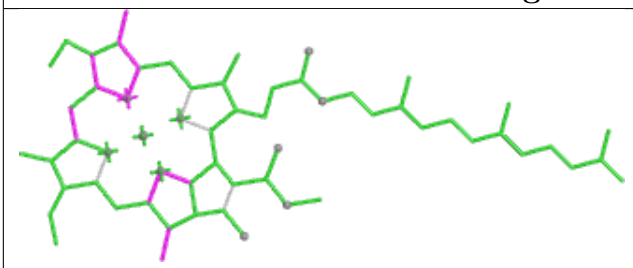


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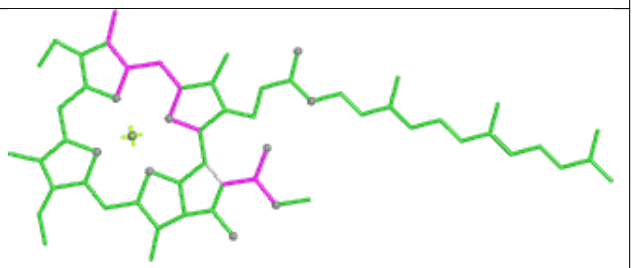


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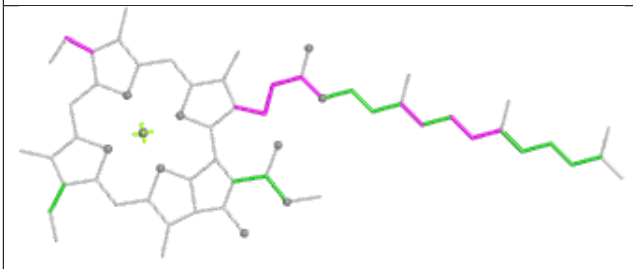
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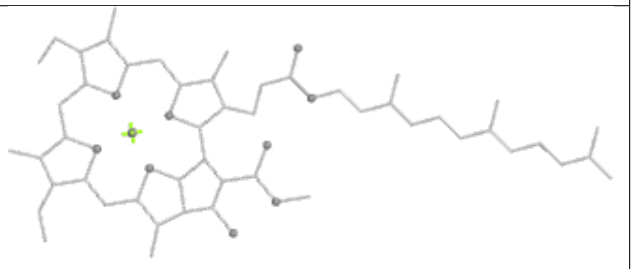
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Bond angles

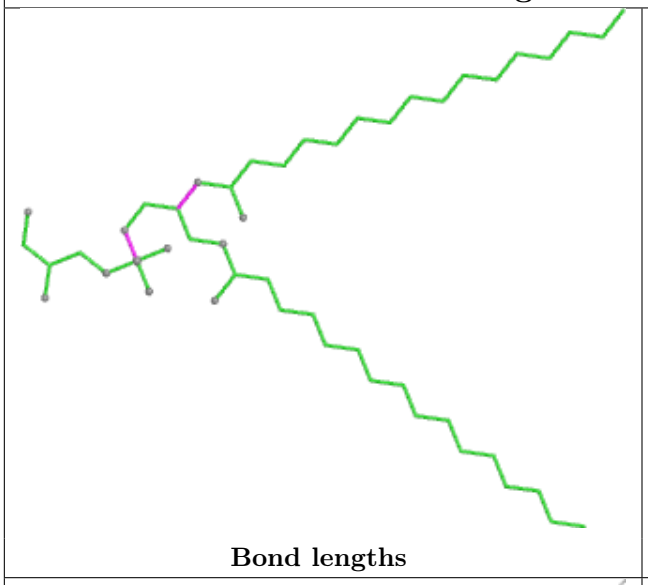


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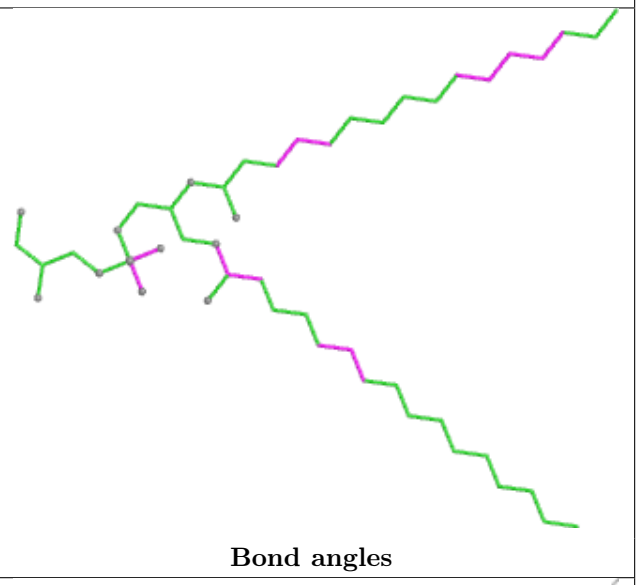


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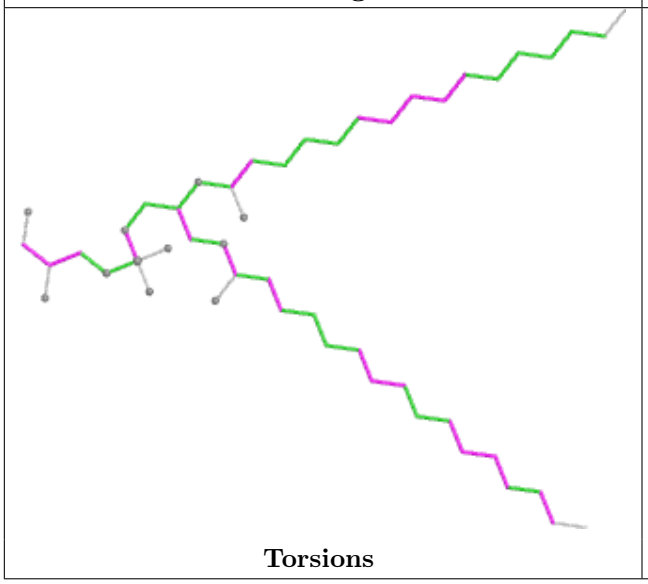
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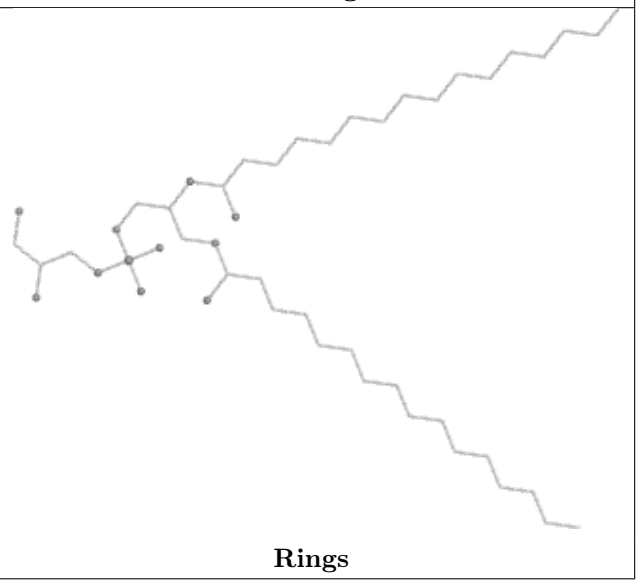
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Bond angles

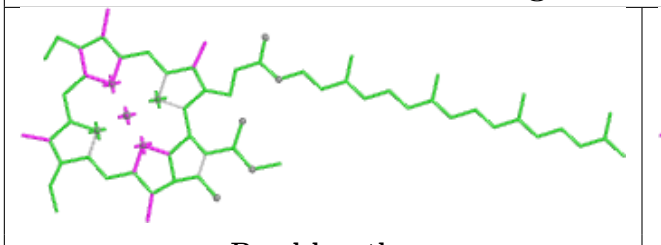


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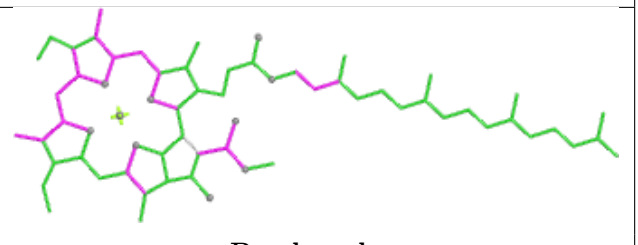


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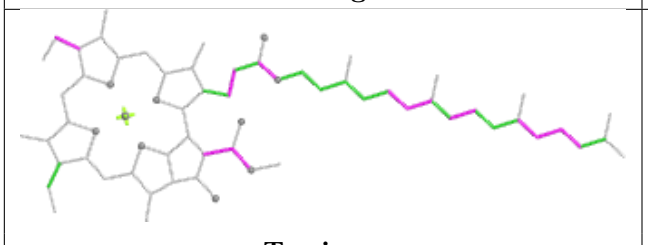
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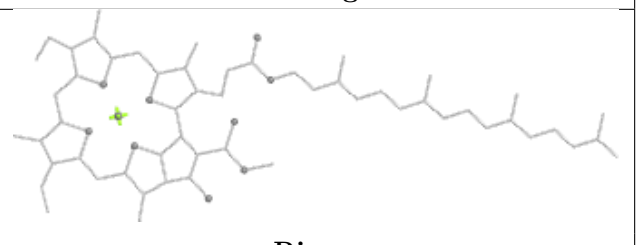
Bond lengths



Bond angles

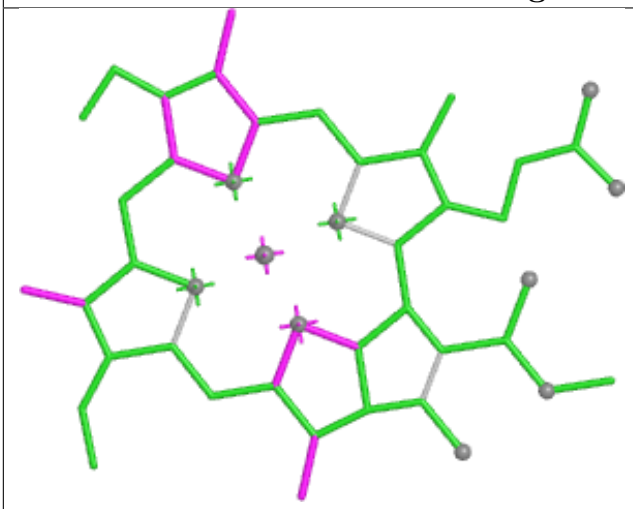


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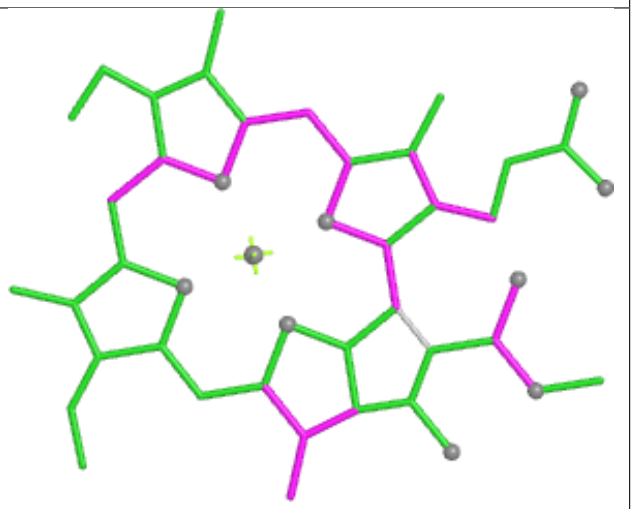


Rings

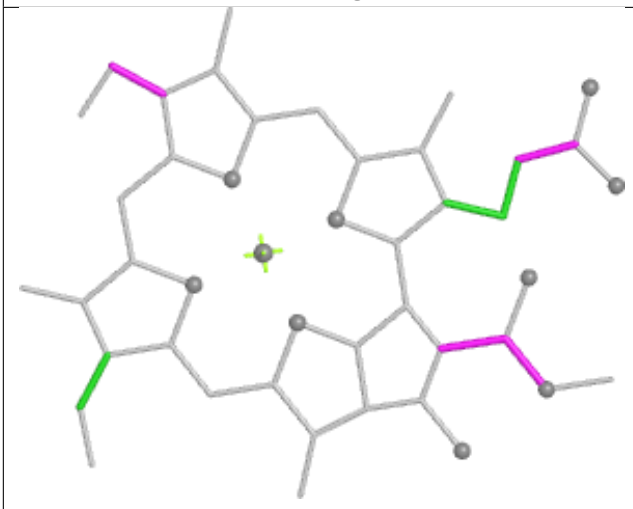
Ligand CLA 7 612



Bond lengths



Bond angles

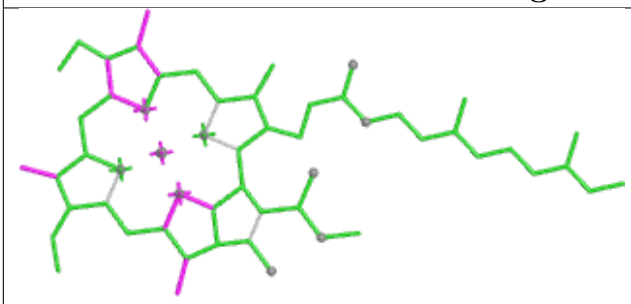


Torsions

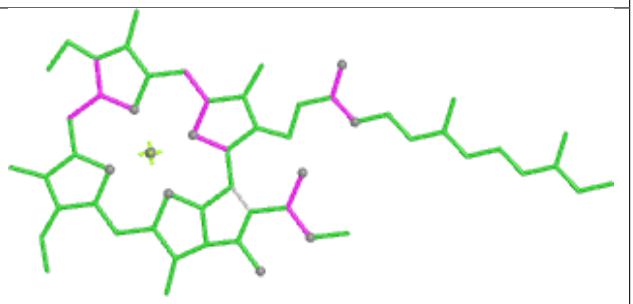


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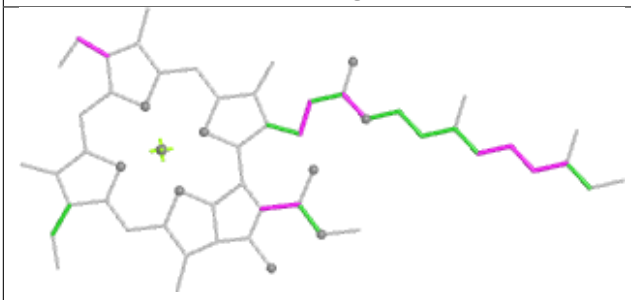
Ligand CLA s 611



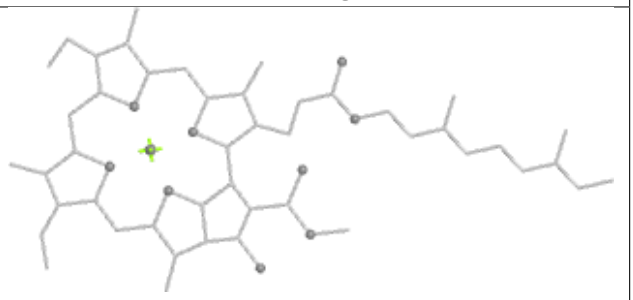
Bond lengths



Bond angles

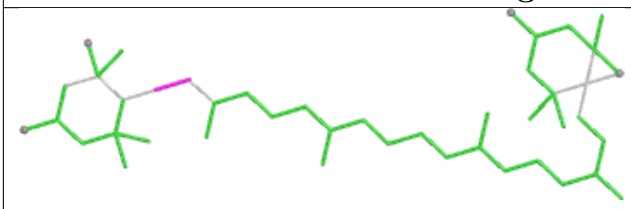


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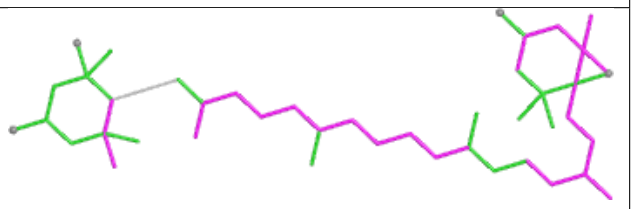


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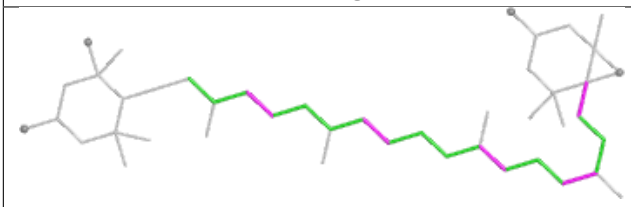
Ligand NEX 2 1623



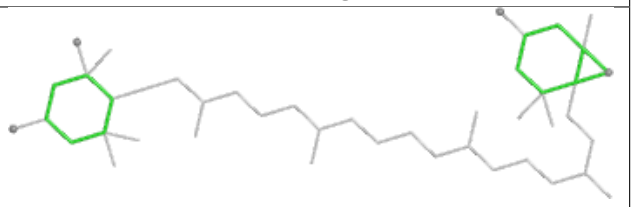
Bond lengths



Bond angles

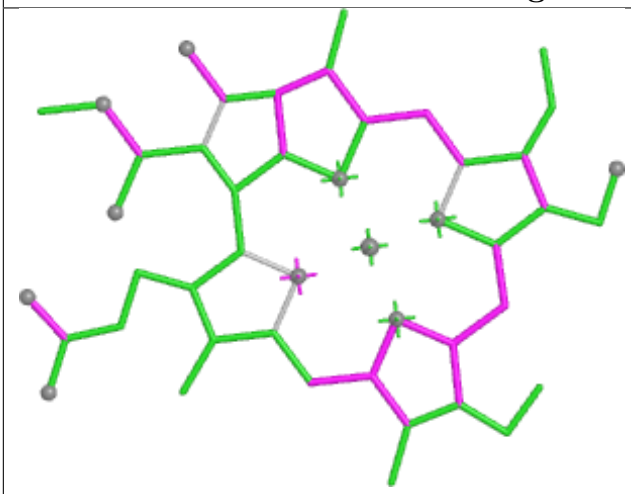


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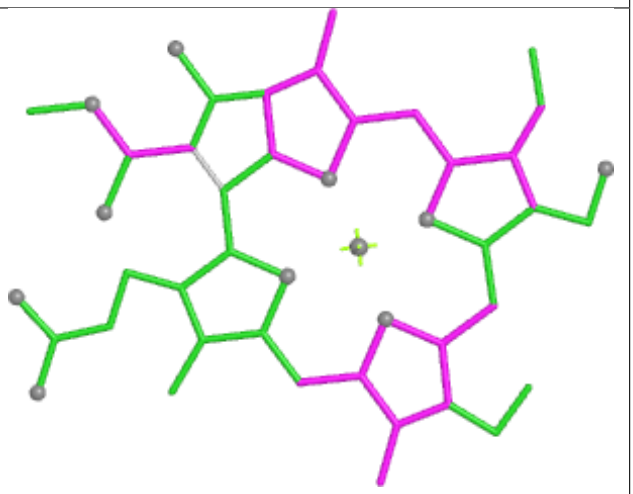


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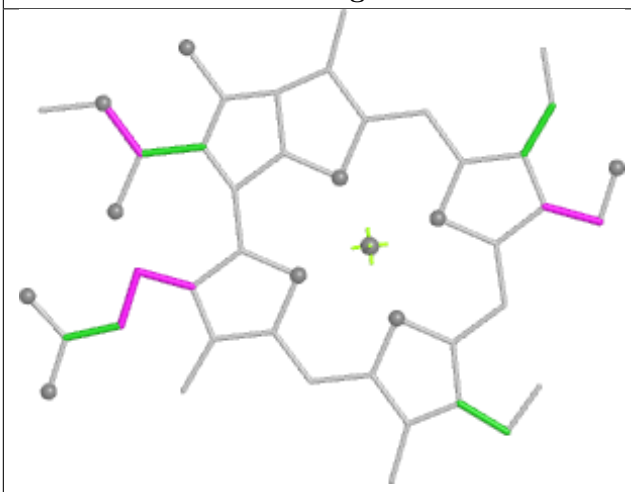
Ligand CHL 1 608



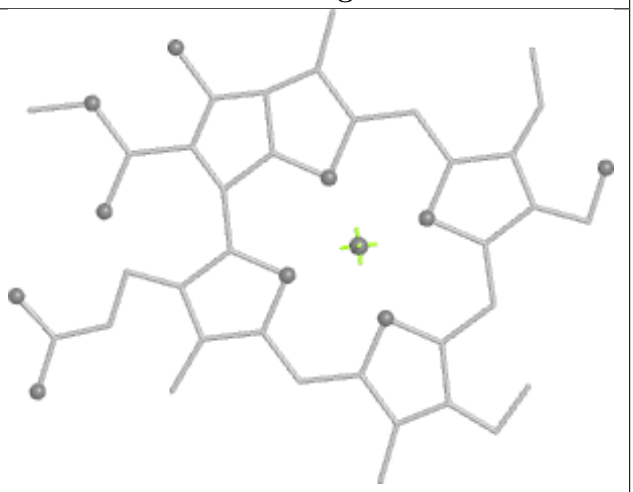
Bond lengths



Bond angles

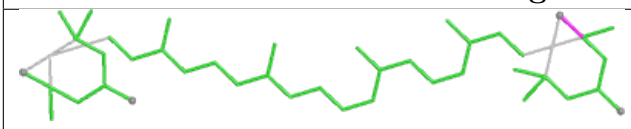


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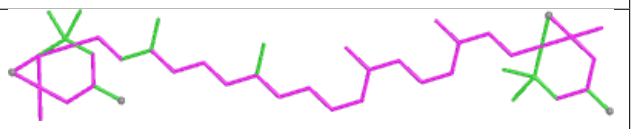


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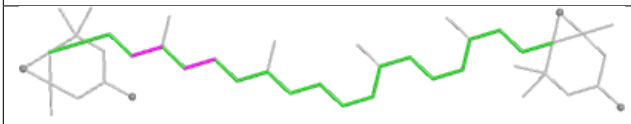
Ligand XAT r 622



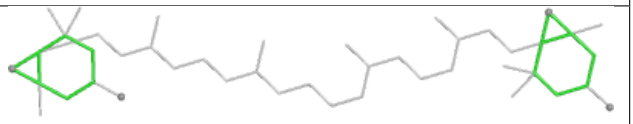
Bond lengths



Bond angles

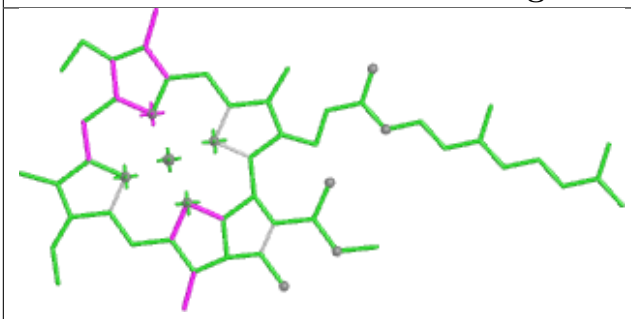


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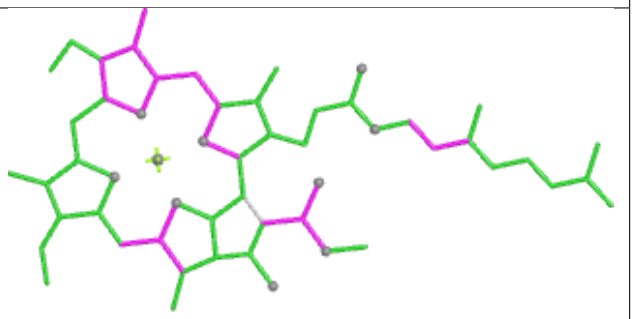


Rings

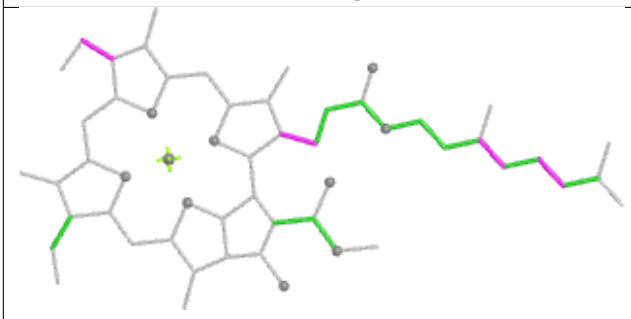
Ligand CLA S 610



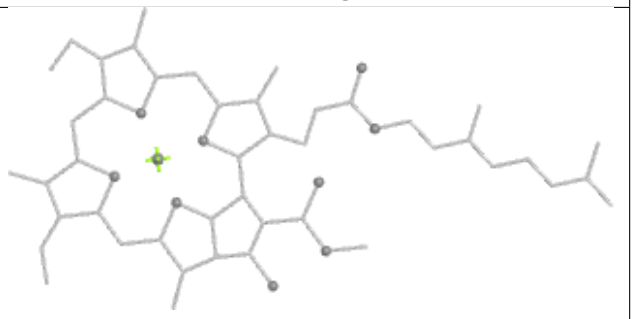
Bond lengths



Bond angles

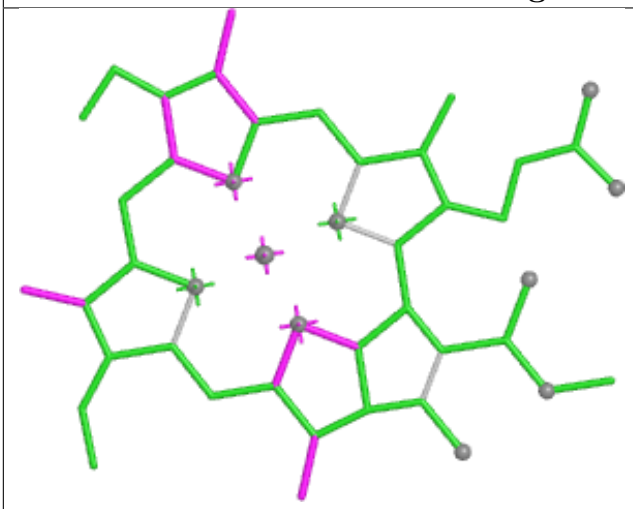


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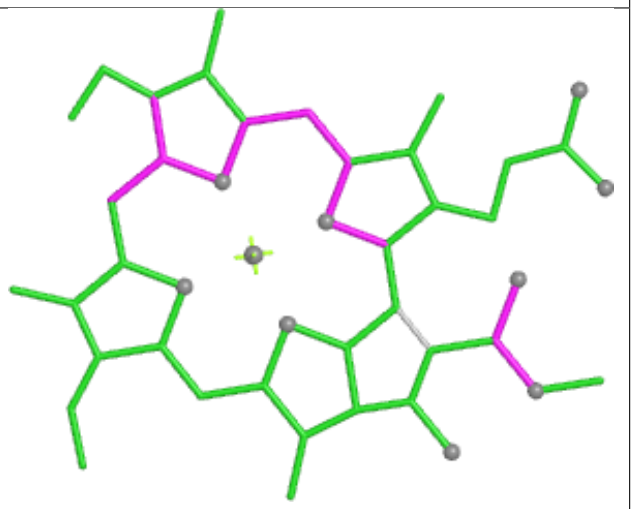


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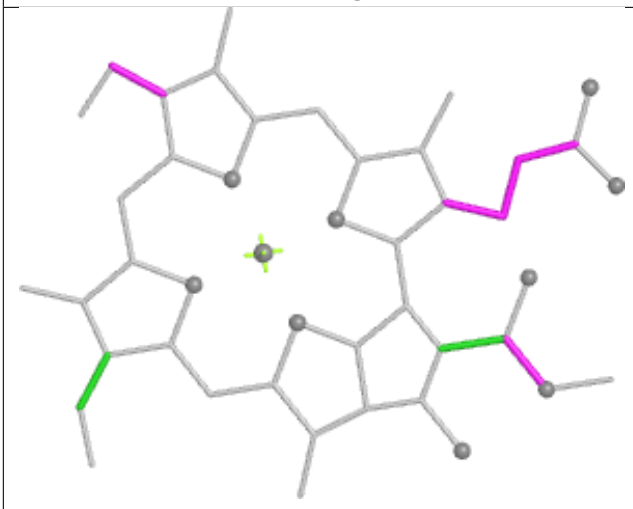
Ligand CLA 5 611



Bond lengths



Bond angles

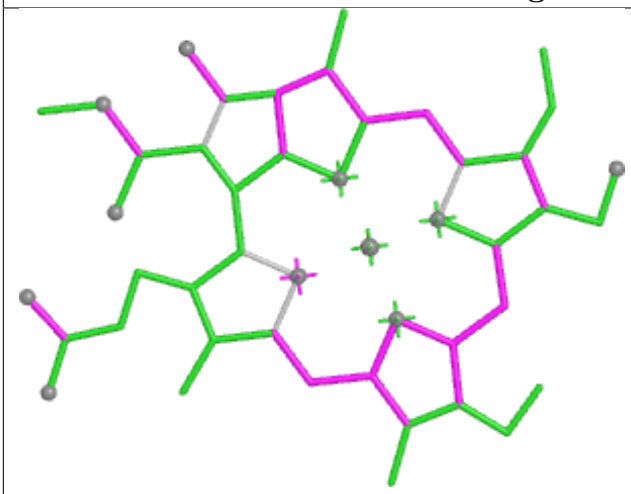


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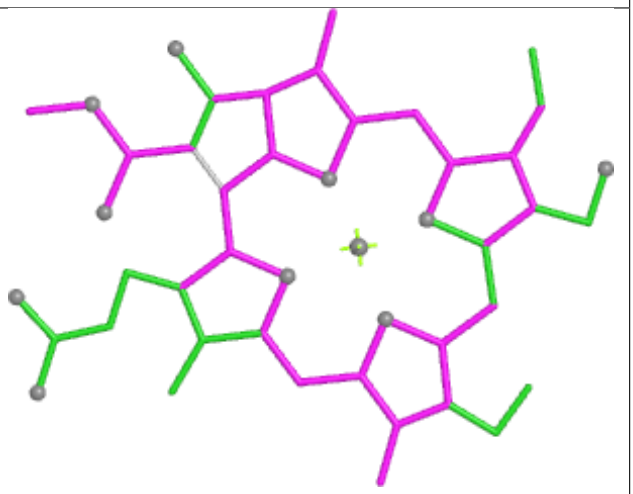


Rings

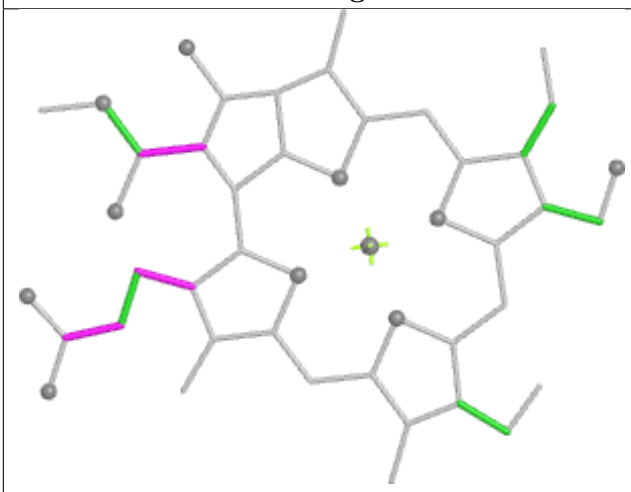
Ligand CHL 2 601



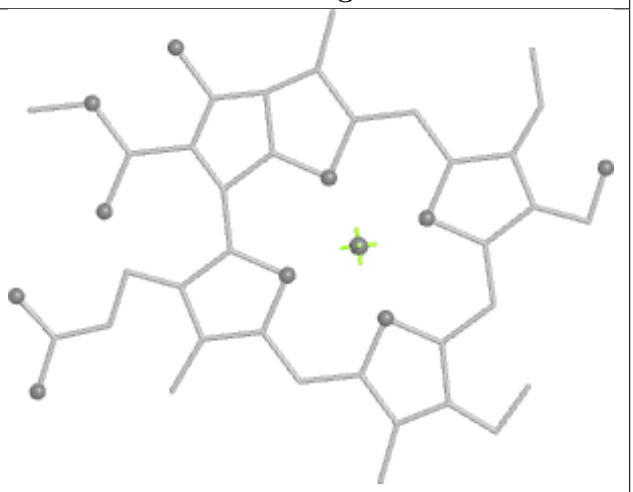
Bond lengths



Bond angles

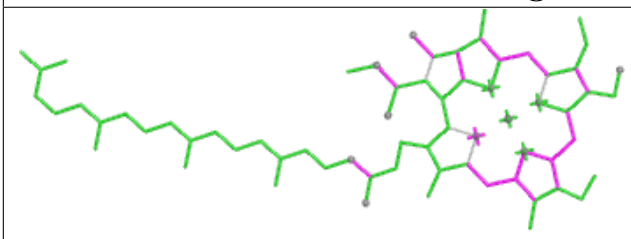


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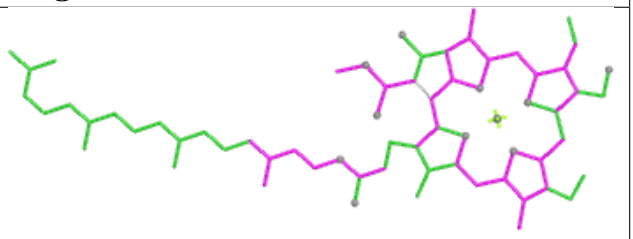


Rings

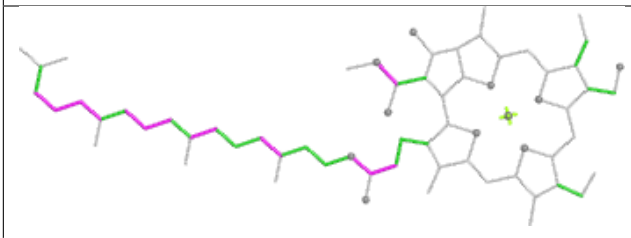
Ligand CHL g 601



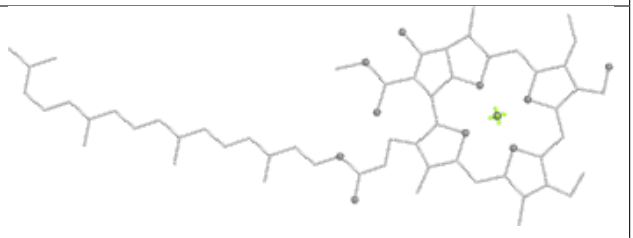
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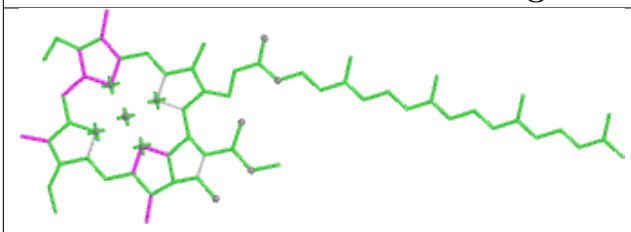
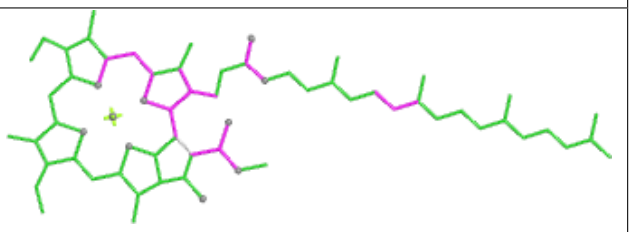
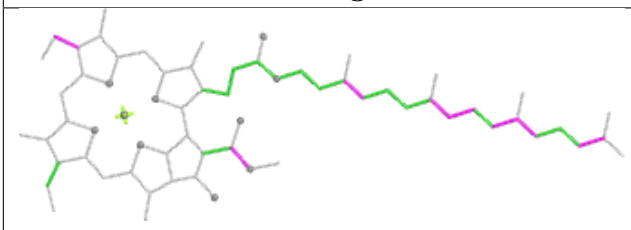
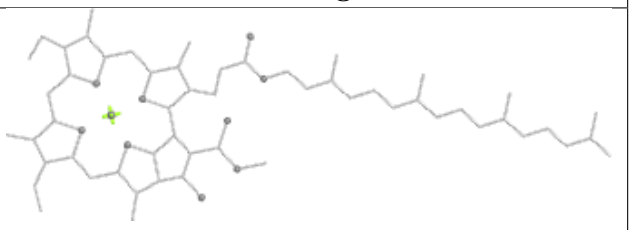
Bond angles

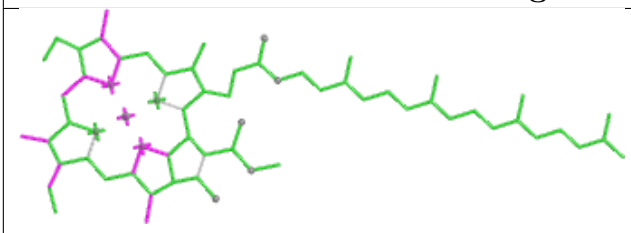
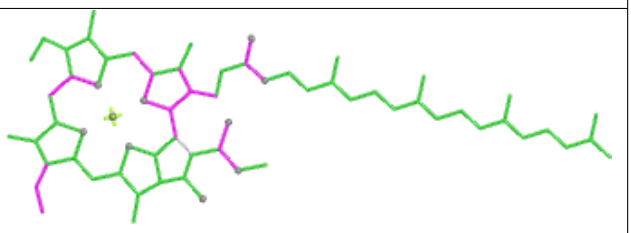
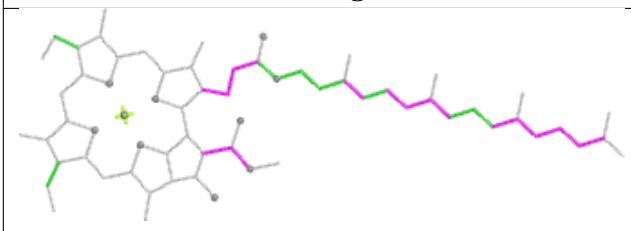
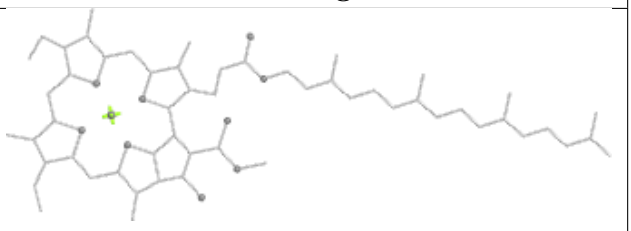


Torsions

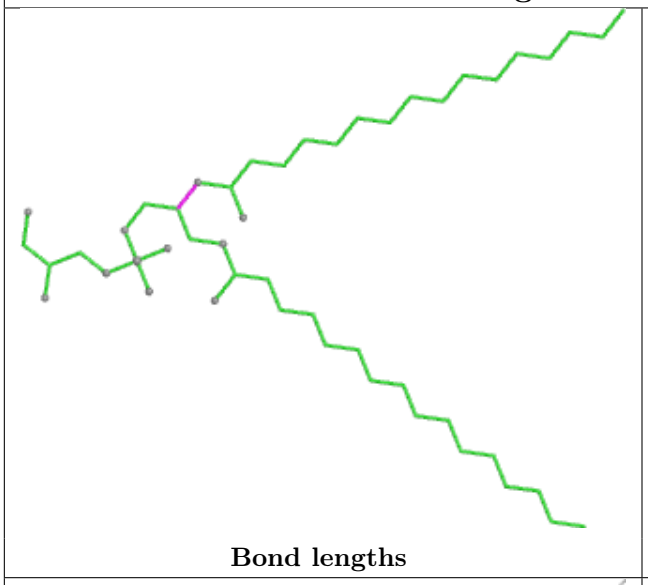


Rings

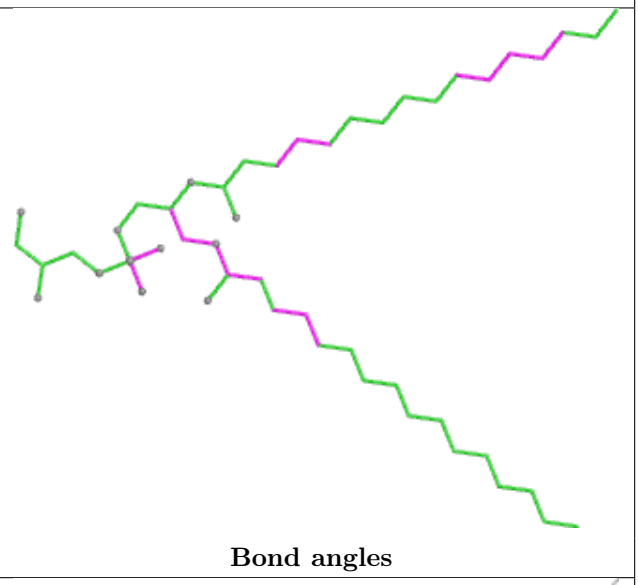
Ligand CLA b 616	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA c 507	
 Bond lengths	 Bond angles
 Torsions	 Rings

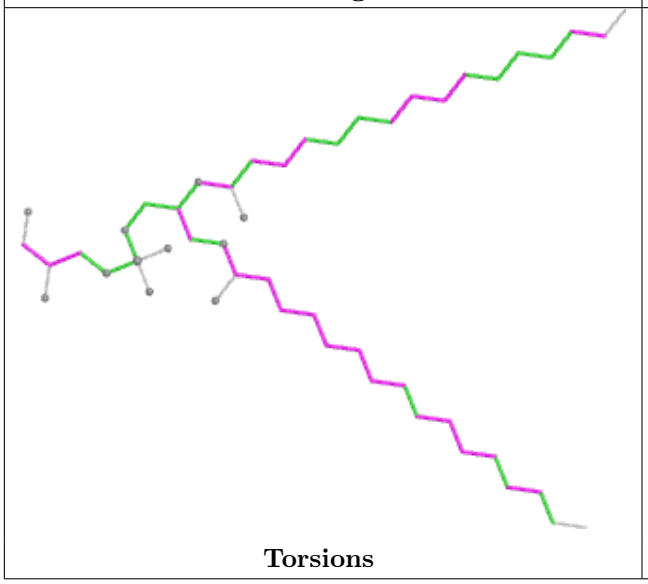
Ligand LHG C 2630



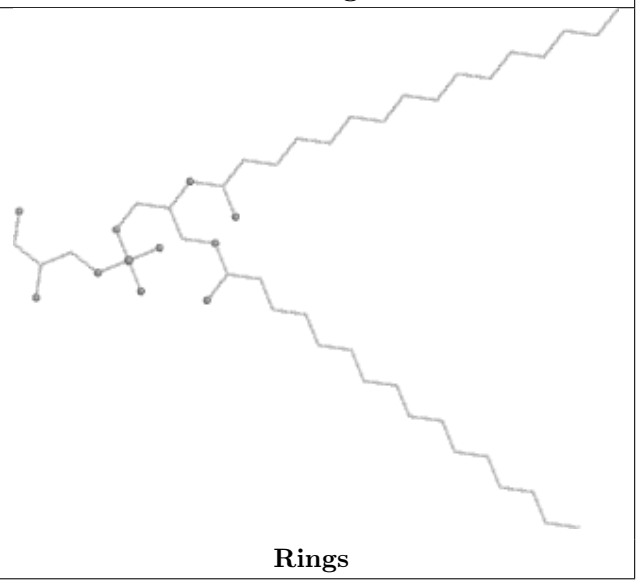
Bond lengths



Bond angles

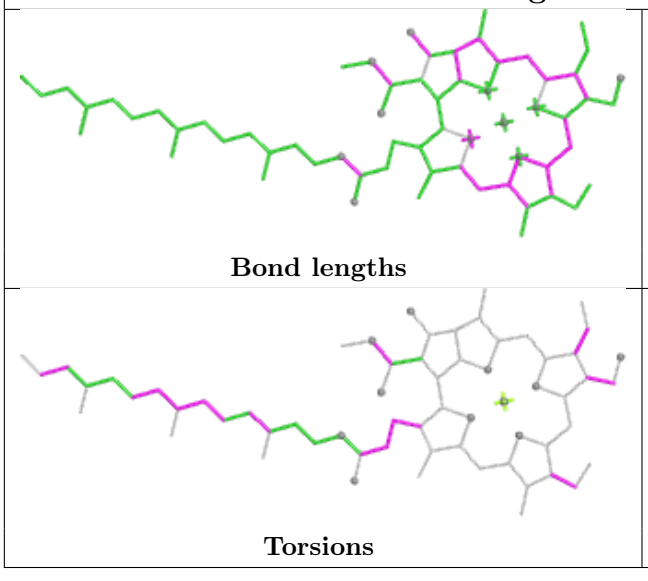


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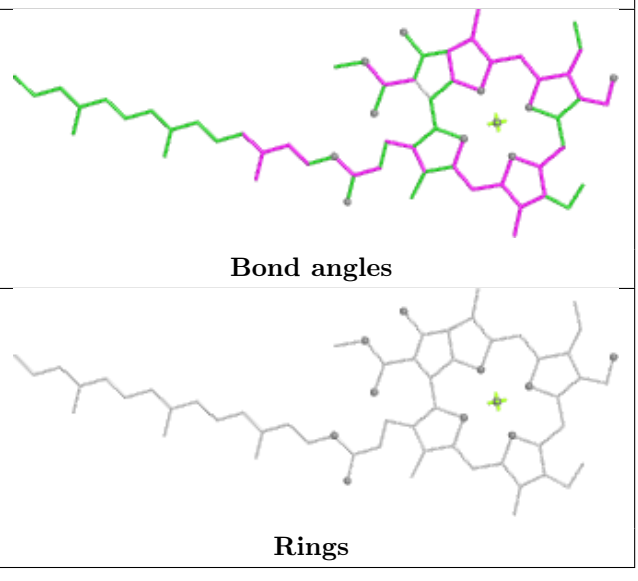


Rings

Ligand CHL 1 607



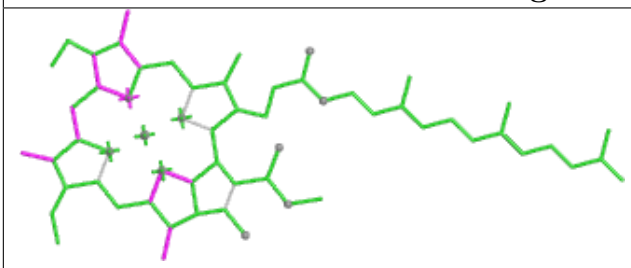
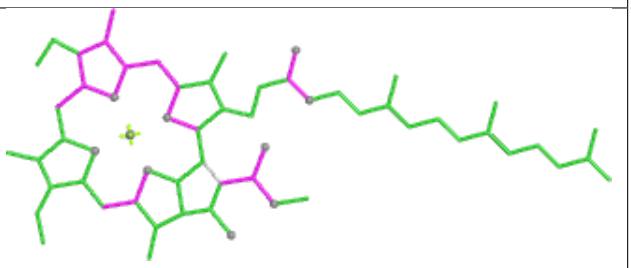
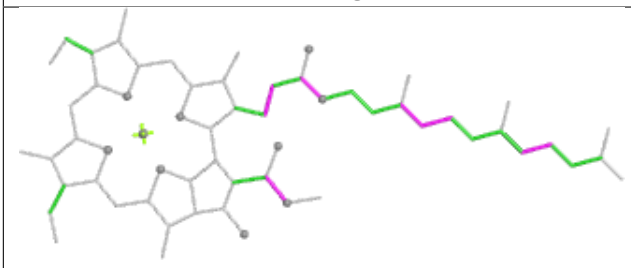
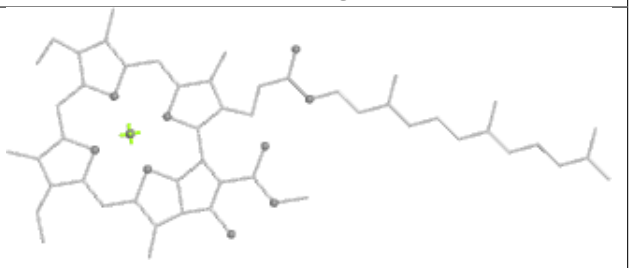
Bond lengths

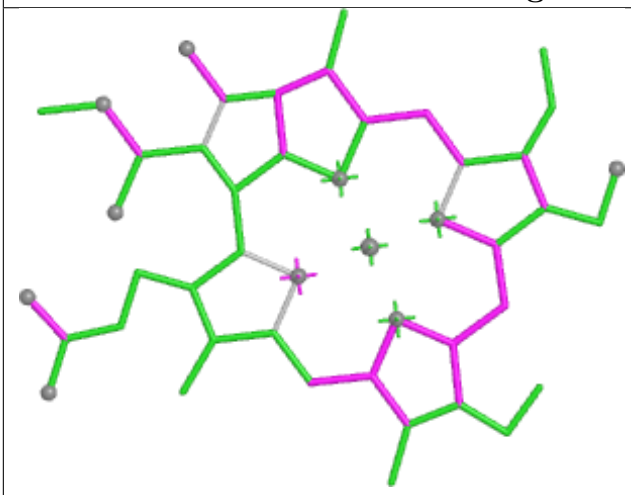
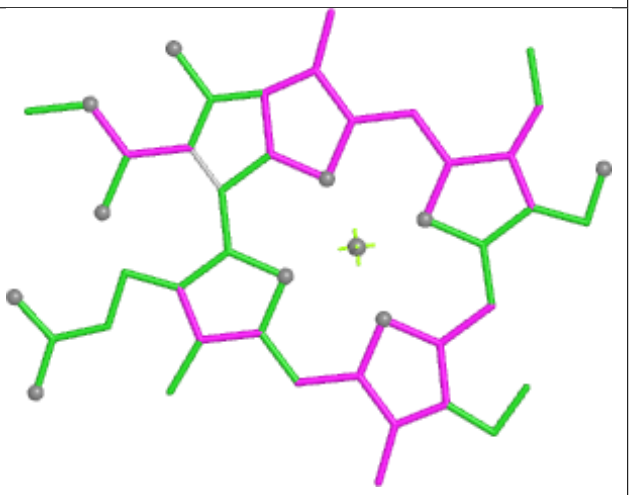
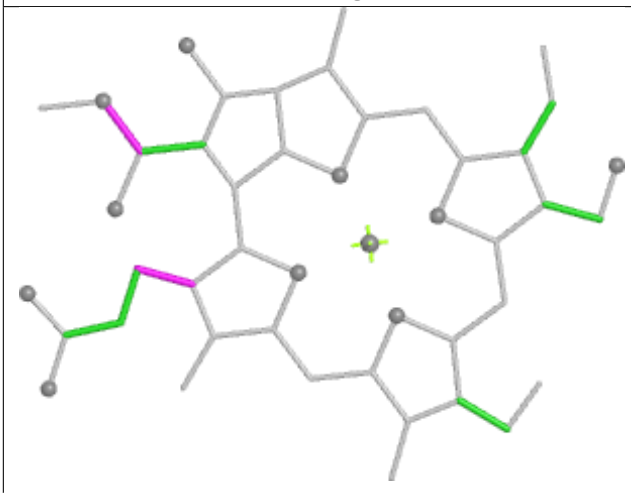
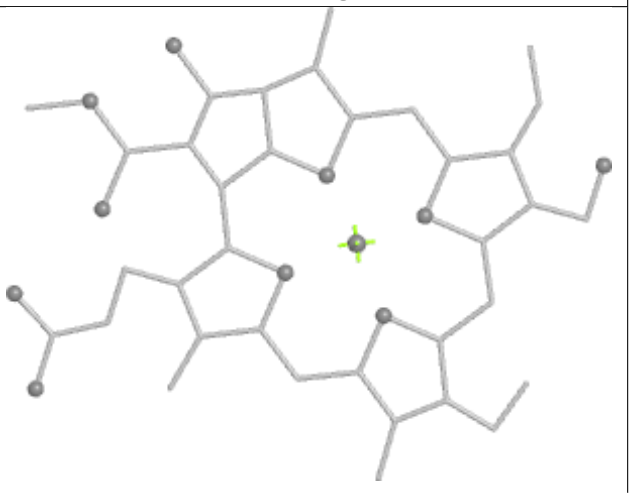


Bond angles

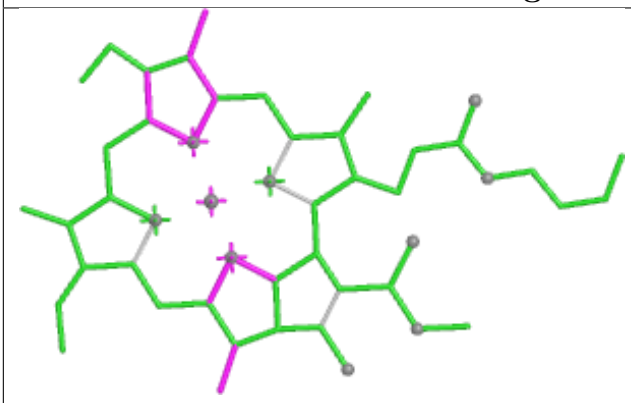
Torsions

Rings

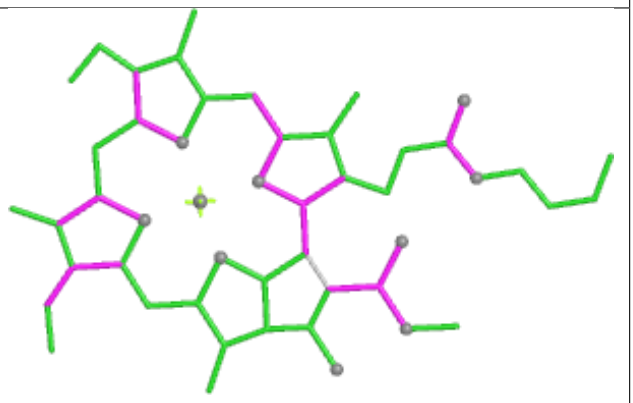
Ligand CLA r 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL S 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

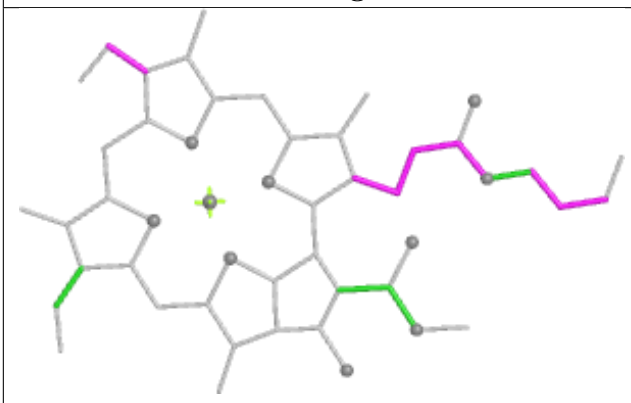
Ligand CLA R 611



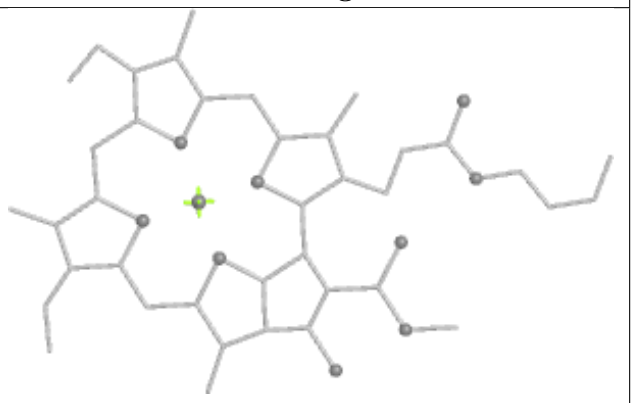
Bond lengths



Bond angles

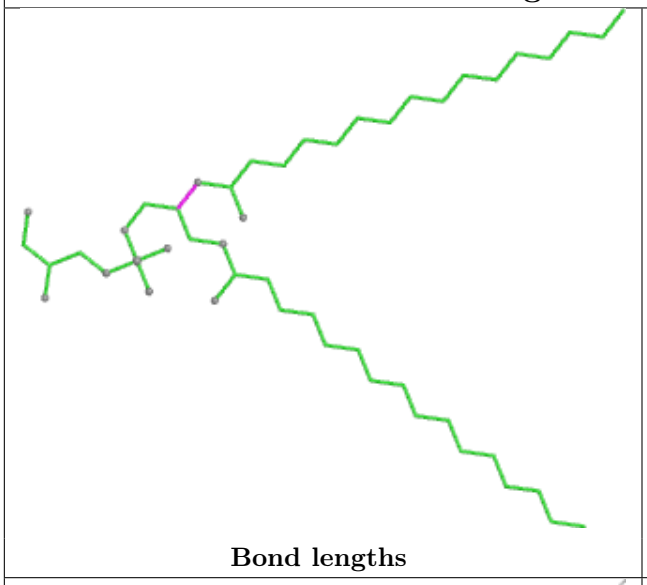


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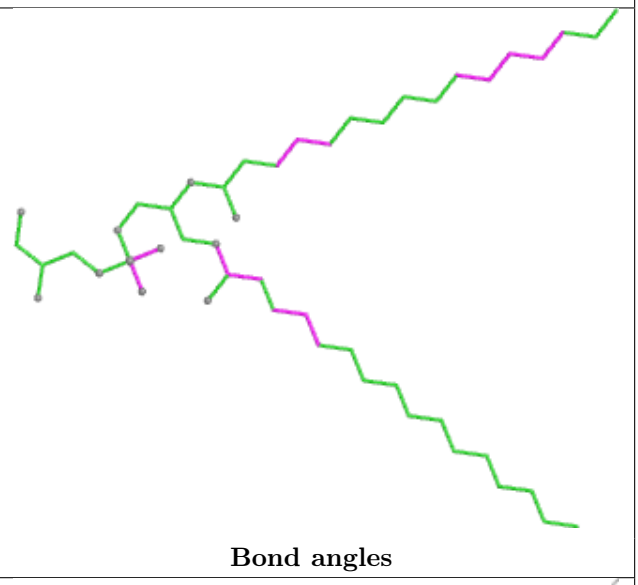


Rings

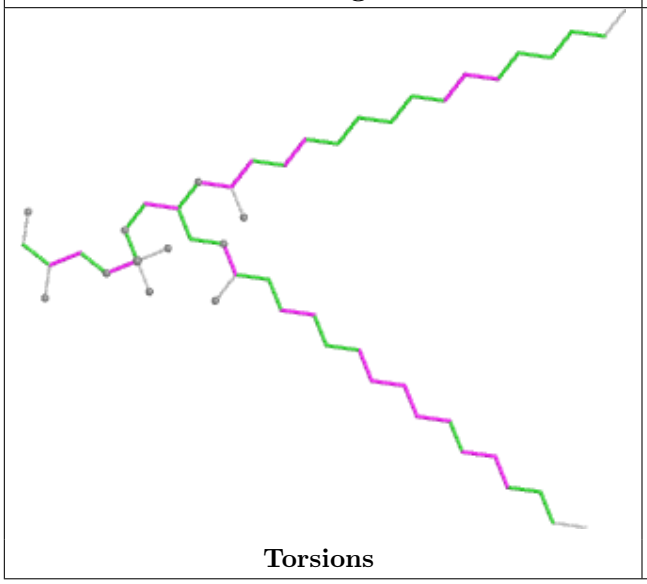
Ligand LHG C 522



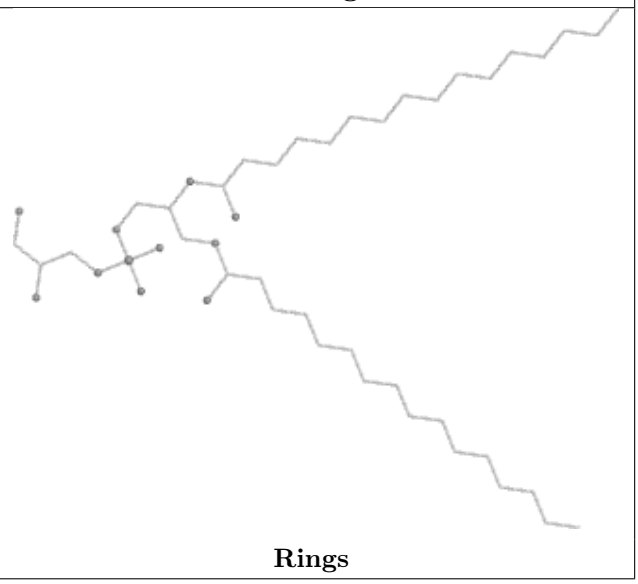
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Bond angles

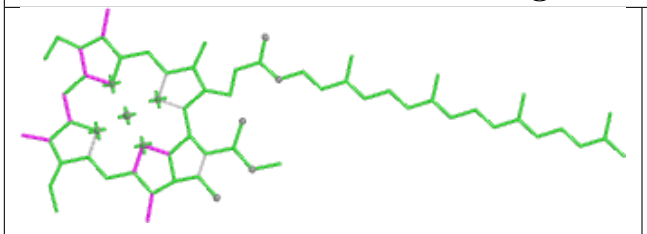


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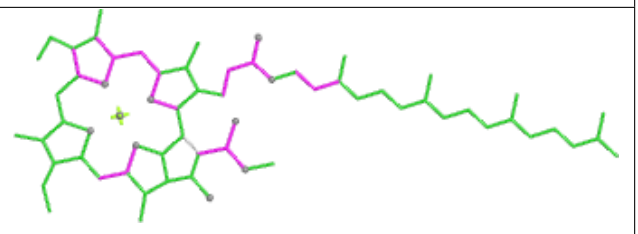


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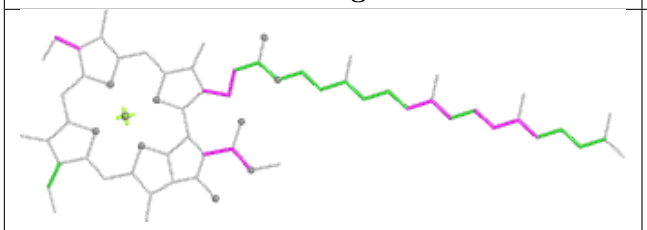
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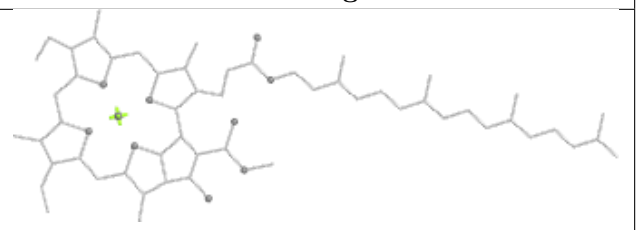
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Bond angles

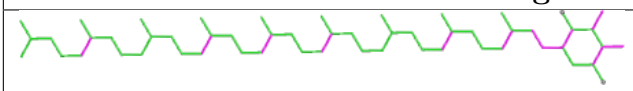


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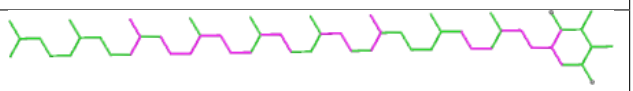


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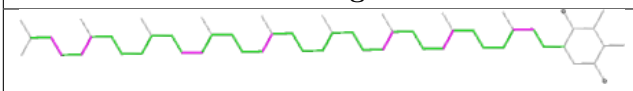
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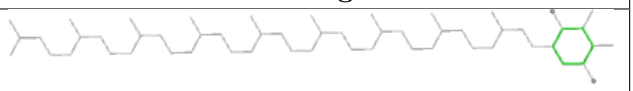
Bond lengths



Bond angles

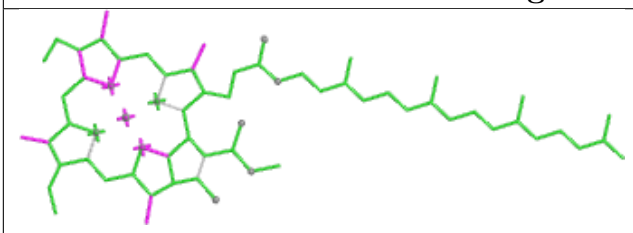


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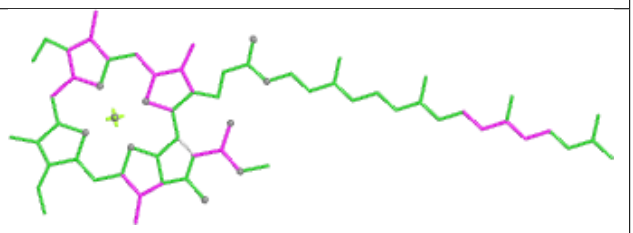


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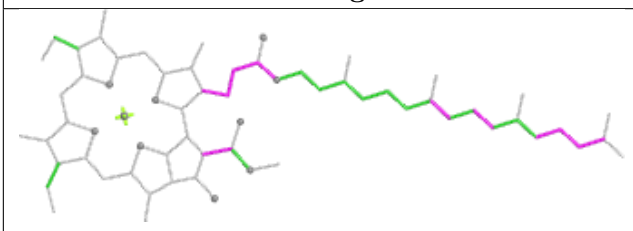
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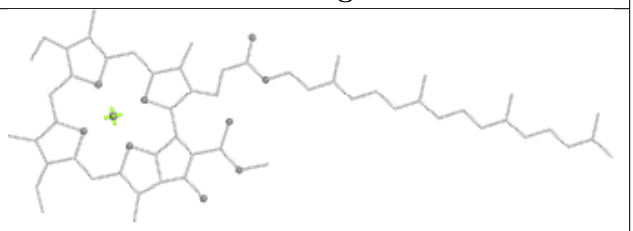
Bond lengths



Bond angles

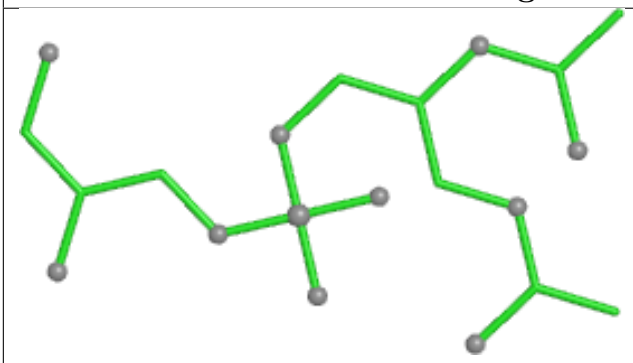


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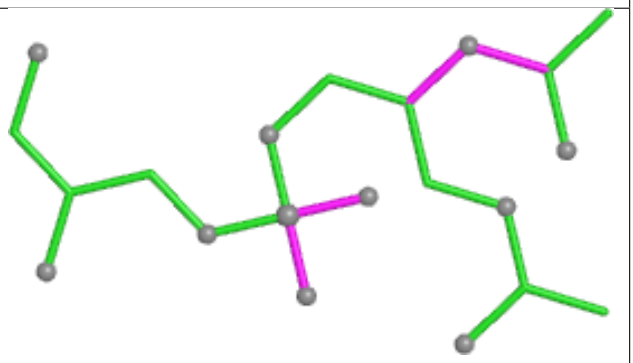


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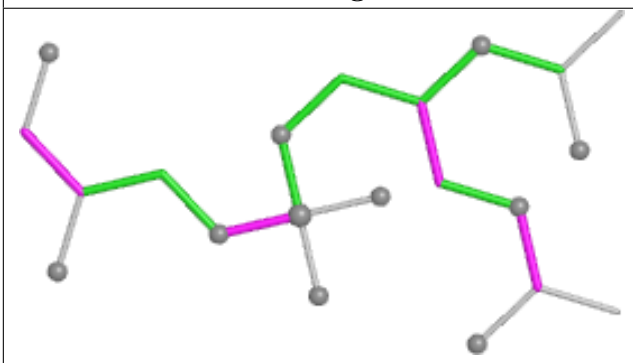
Ligand LHG 8 2630



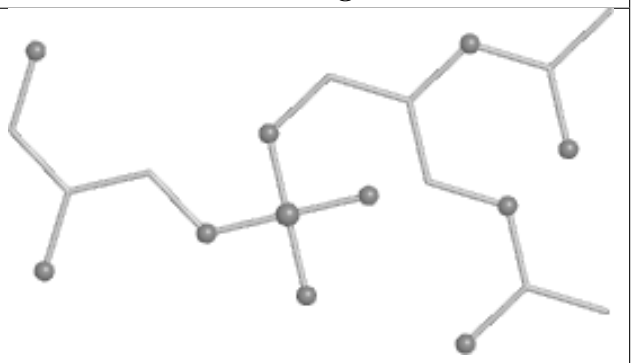
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Bond angles

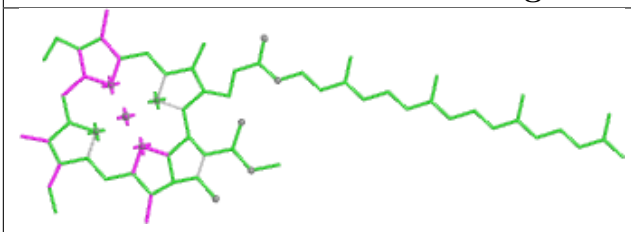


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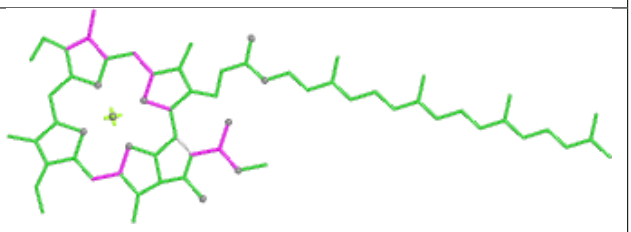


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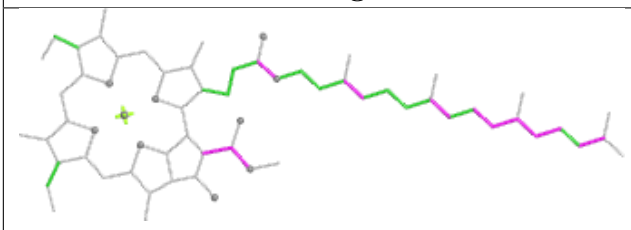
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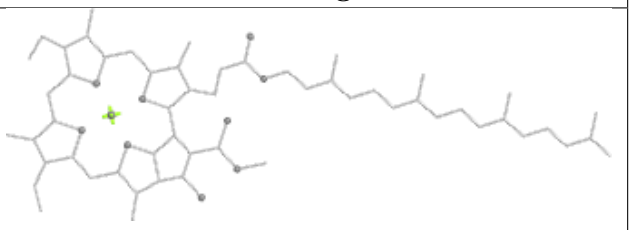
Bond lengths



Bond angles



Torsions

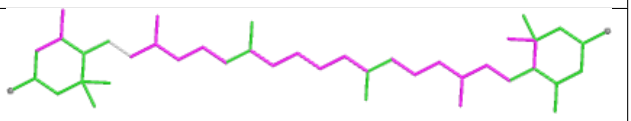


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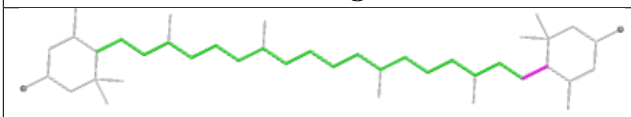
Ligand LUT N 1620



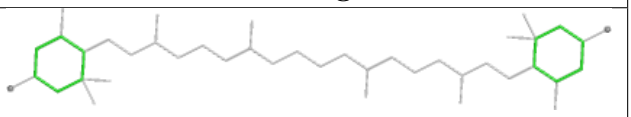
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Bond angles

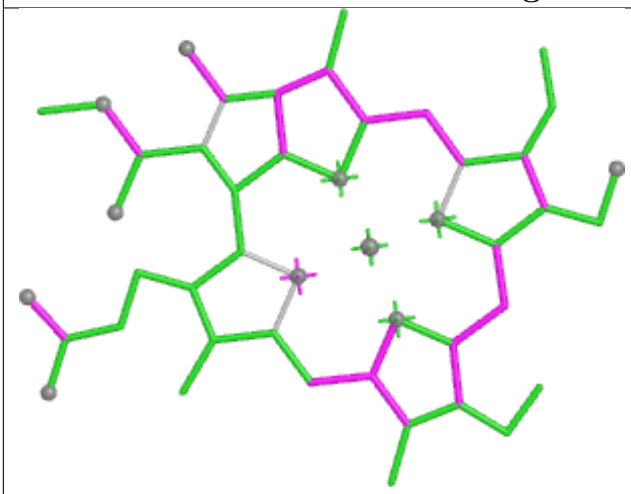


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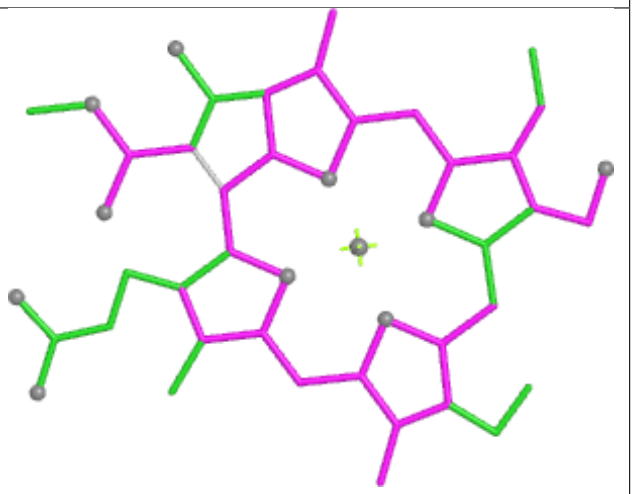


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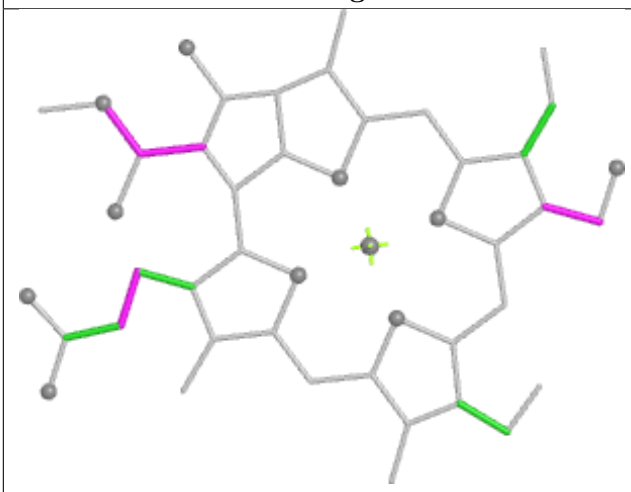
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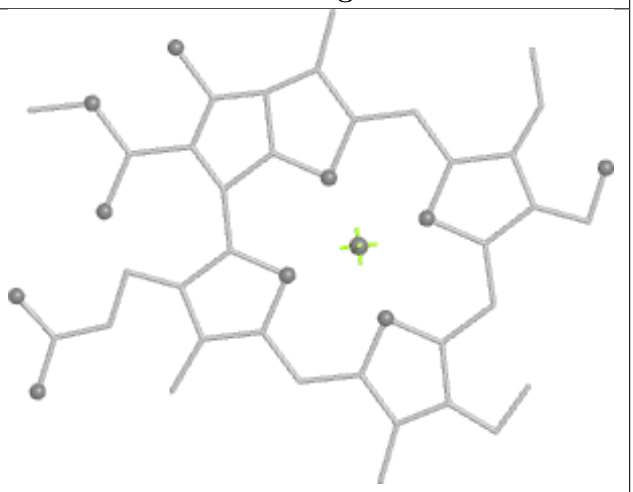
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Bond angles

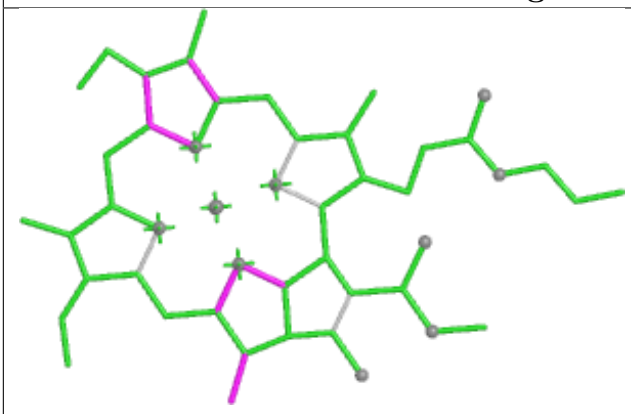


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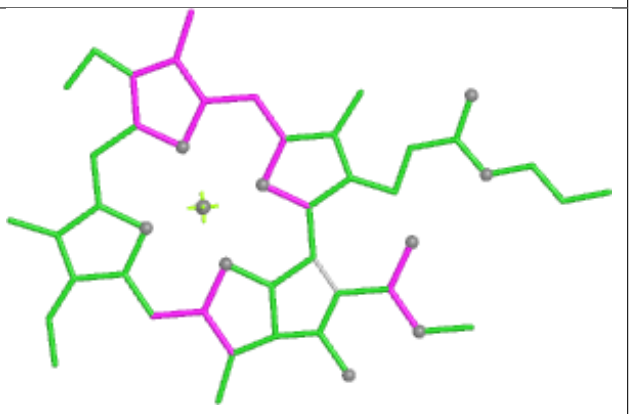


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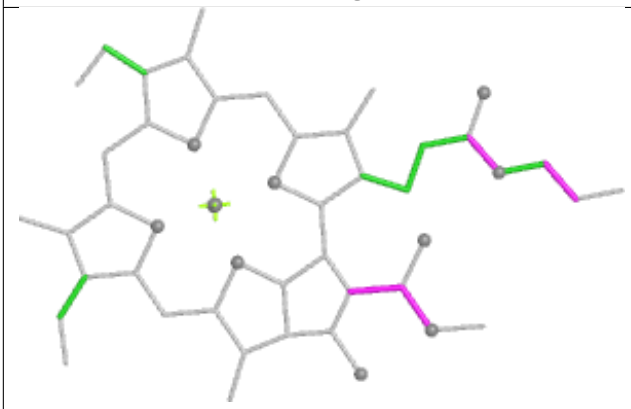
Ligand CLA n 614



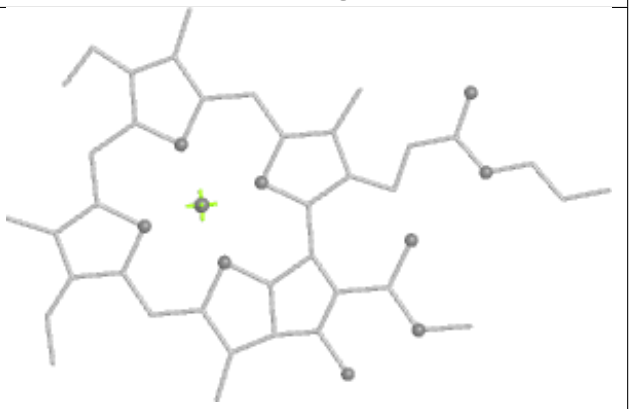
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Bond angles

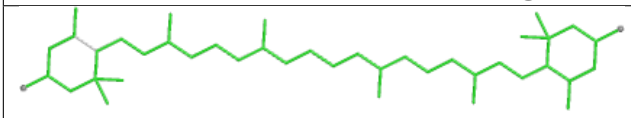


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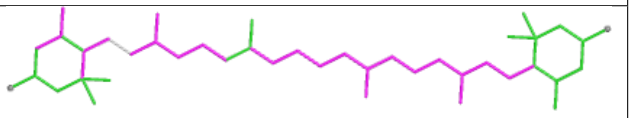


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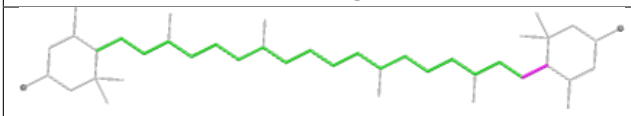
Ligand LUT 2 1620



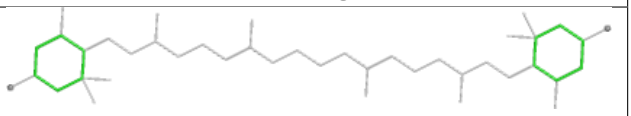
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Bond angles

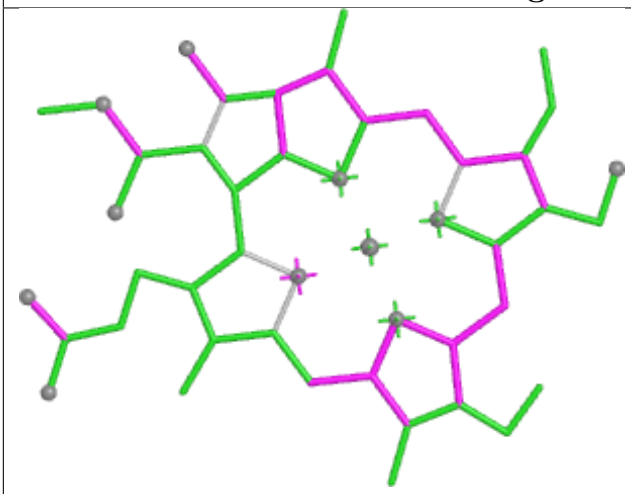


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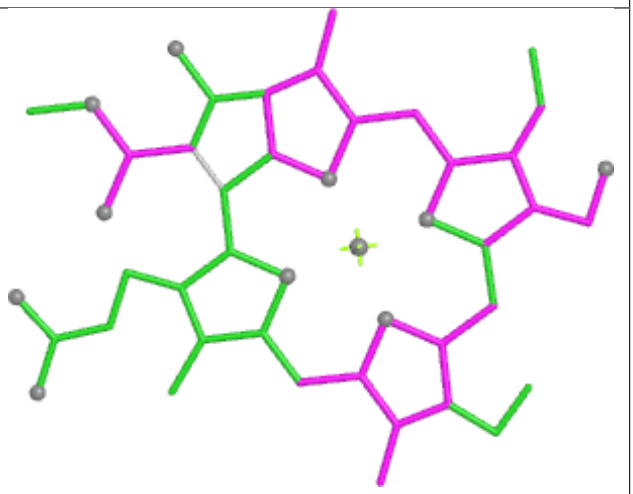


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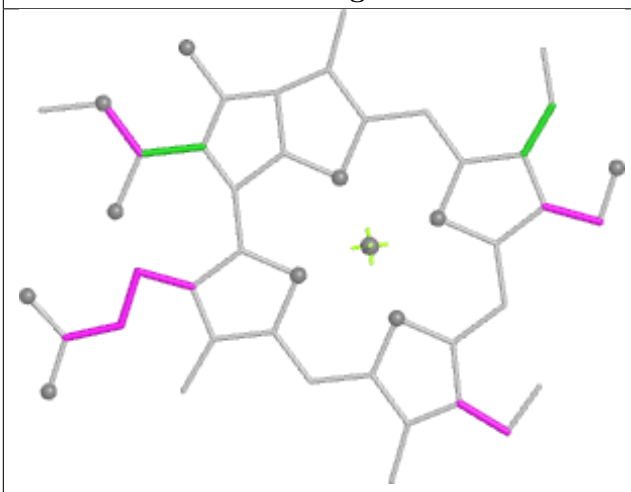
Ligand CHL 8 607



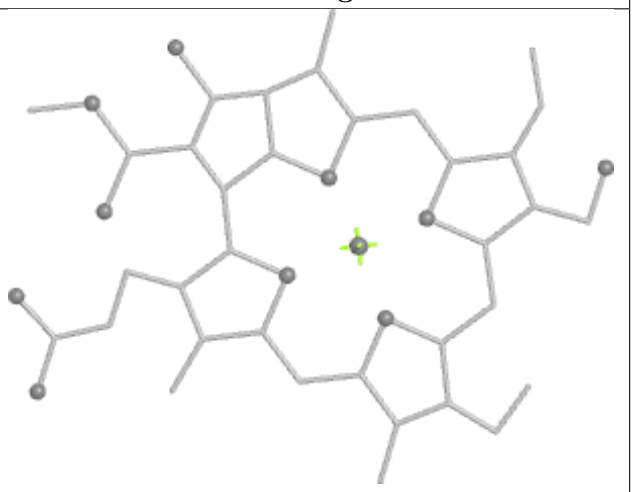
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Bond angles



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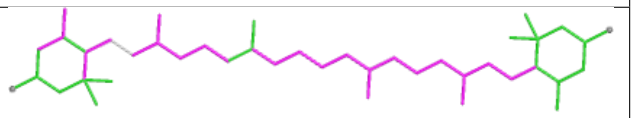


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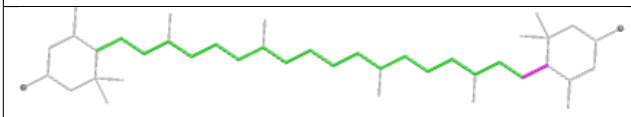
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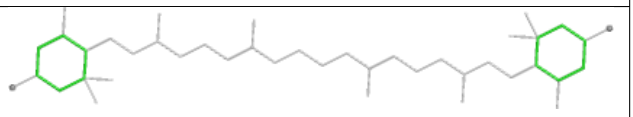
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Bond angles

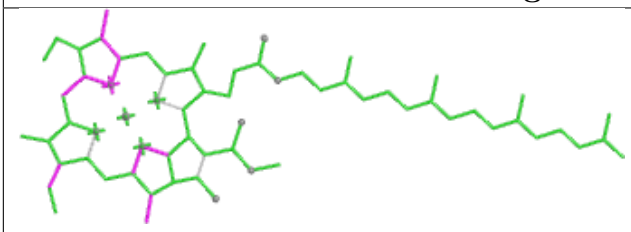


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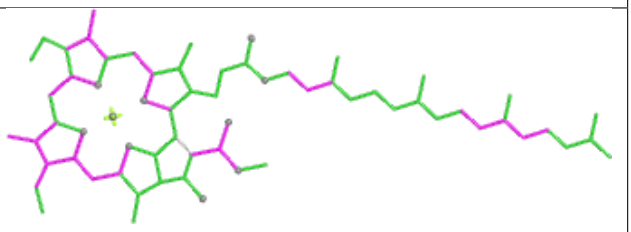


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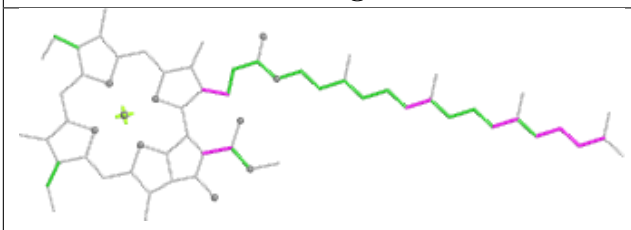
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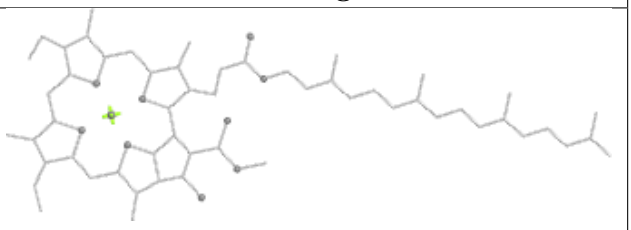
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Bond angles

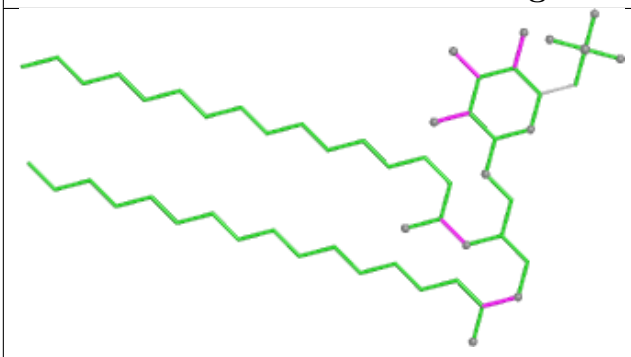


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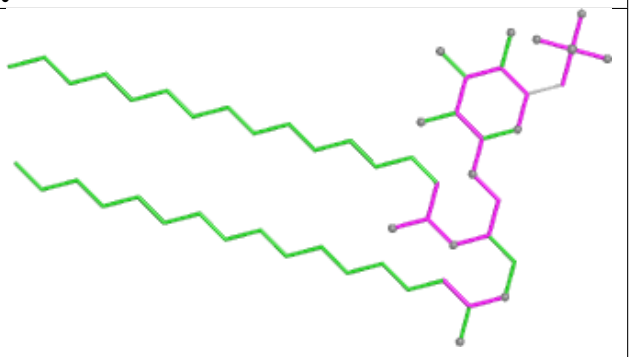


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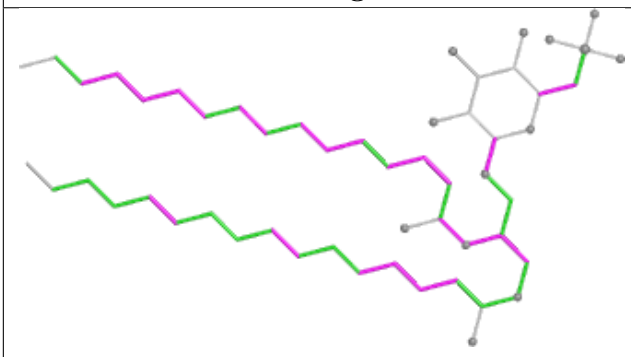
Ligand SQD a 418



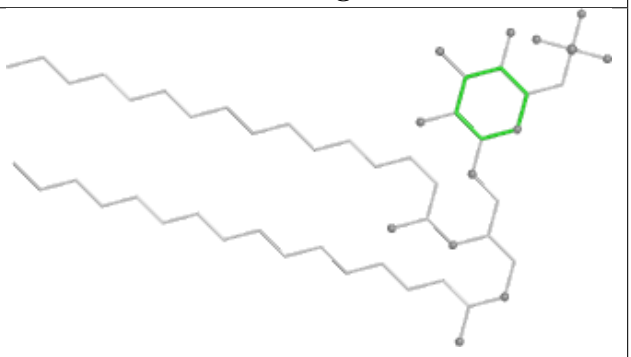
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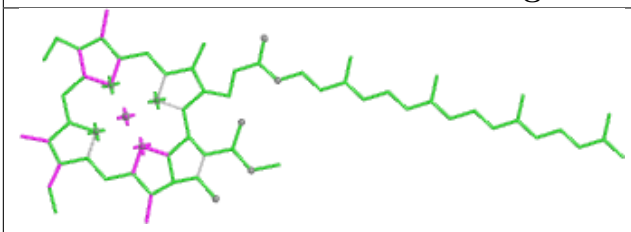
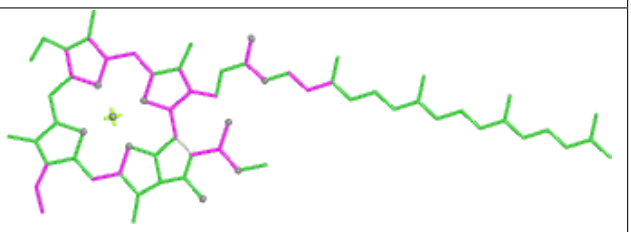
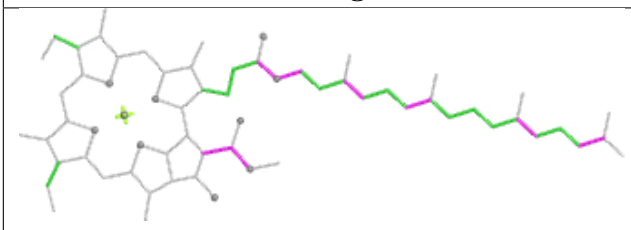
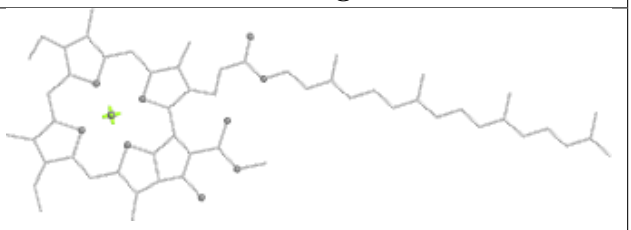
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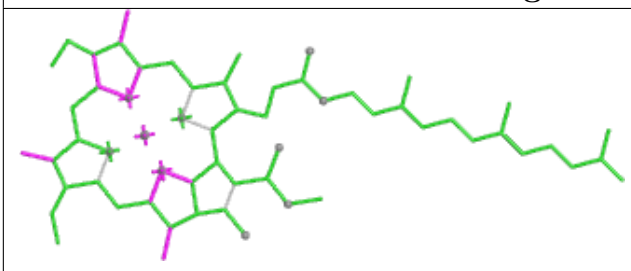
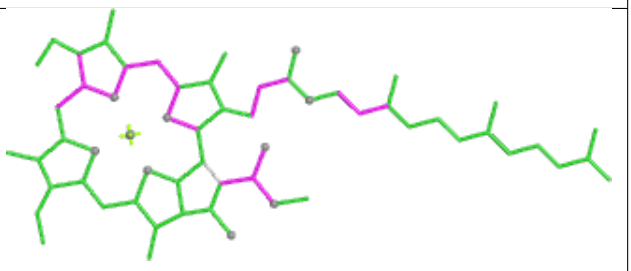
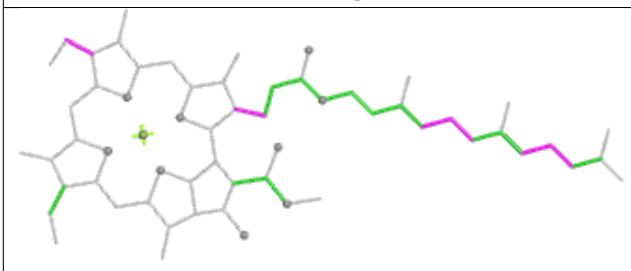
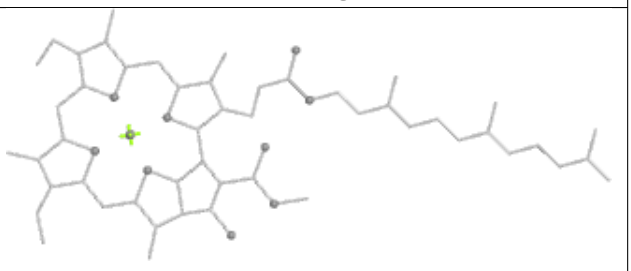


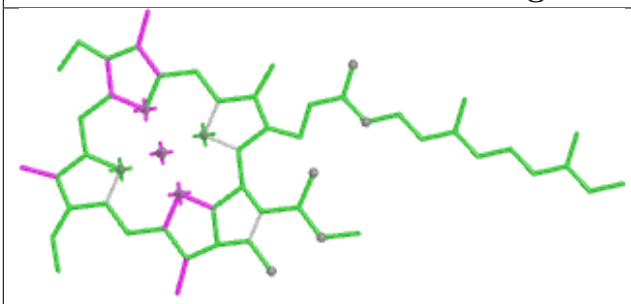
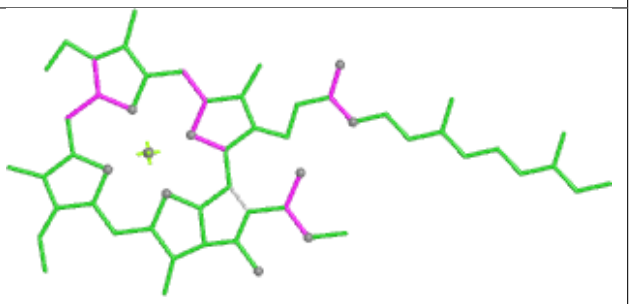
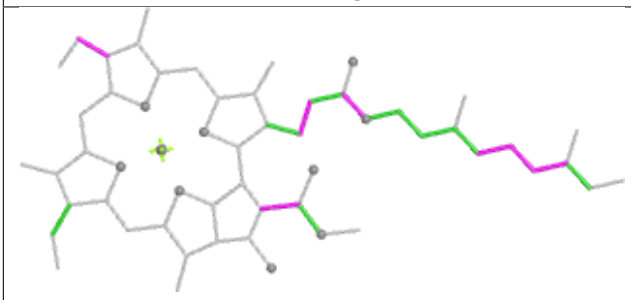
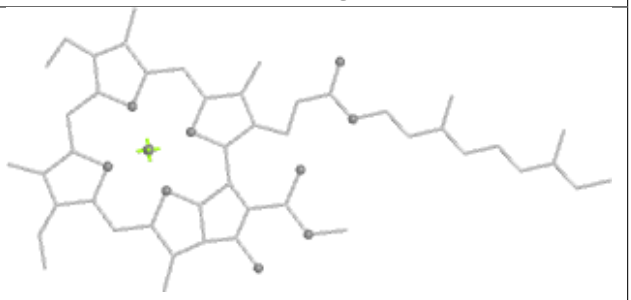
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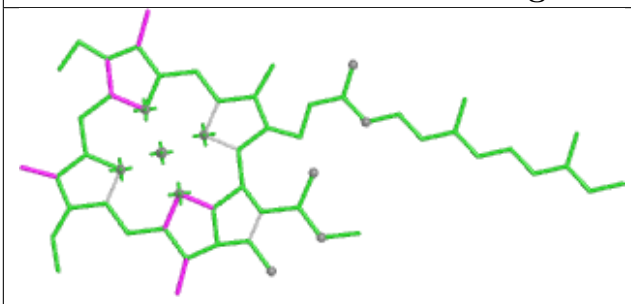
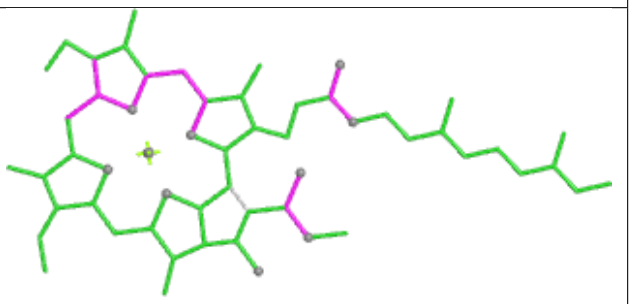
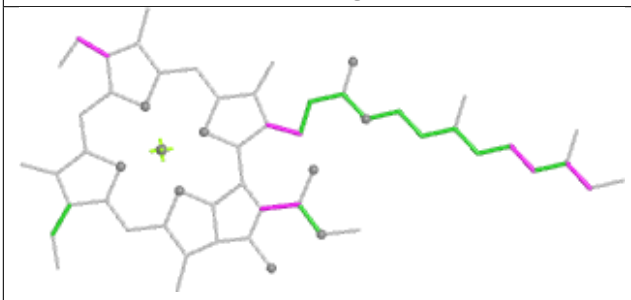
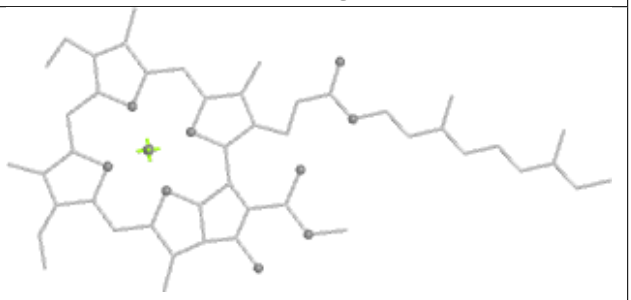


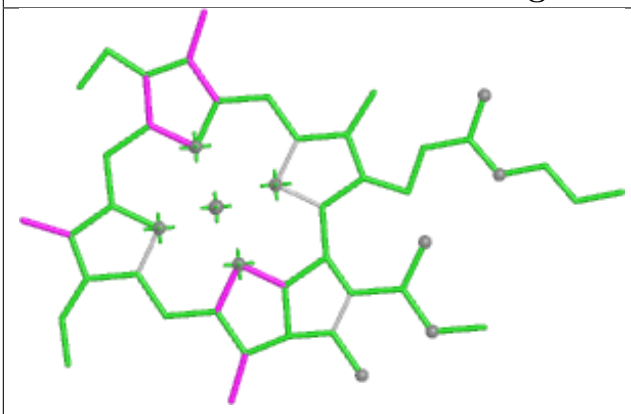
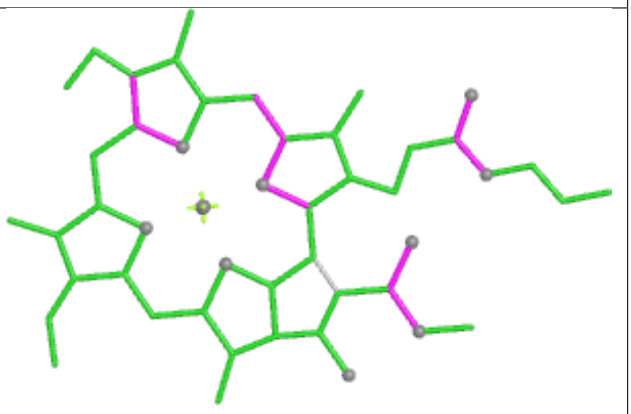
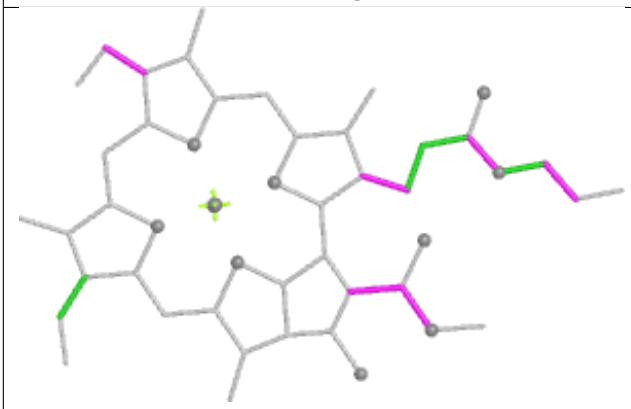
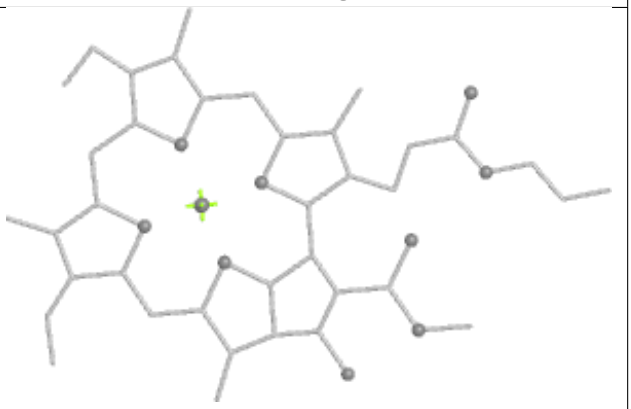
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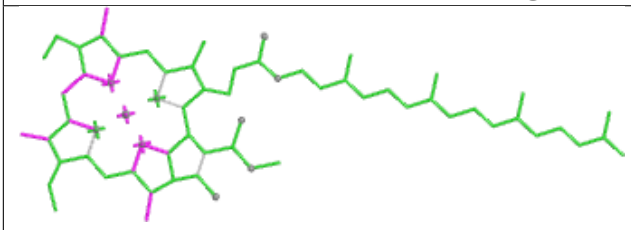
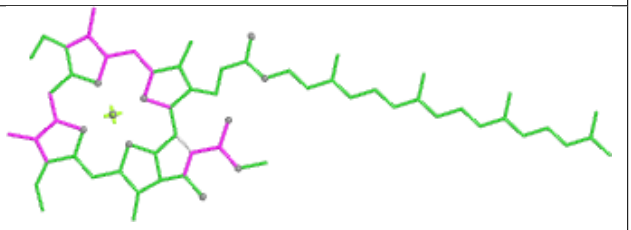
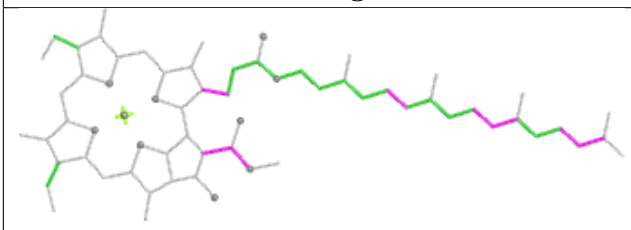
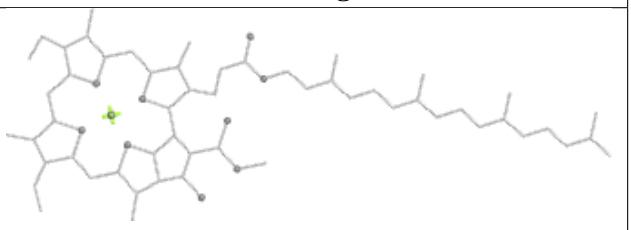
Ligand CLA Y 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 410	
 Bond lengths	 Bond angles
 Torsions	 Rings

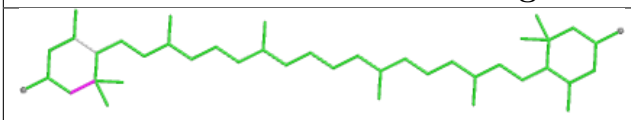
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Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 5 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

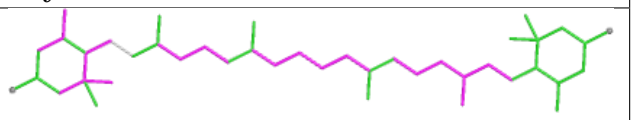
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Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA C 508	
	
Bond lengths	Bond angles
	
Torsions	Rings

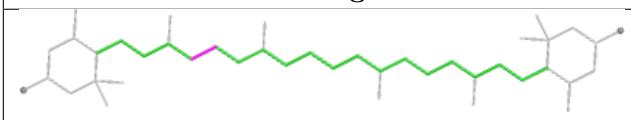
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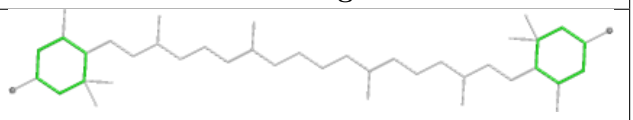
Bond lengths



Bond angles

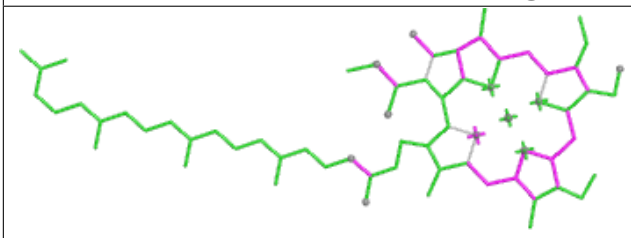


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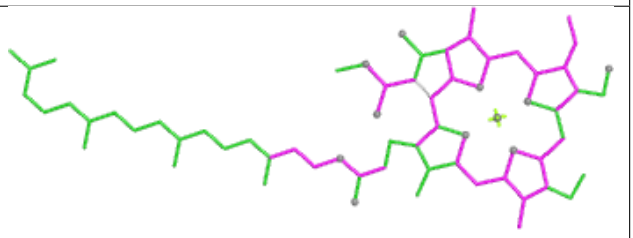


Rings

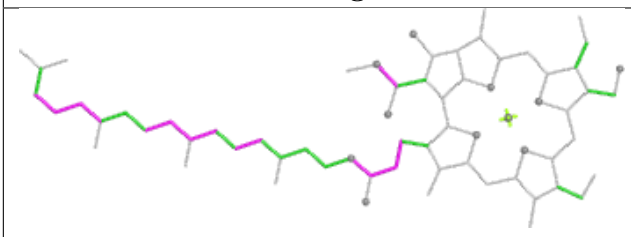
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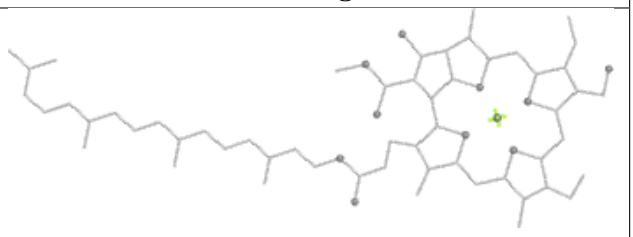
Bond lengths



Bond angles

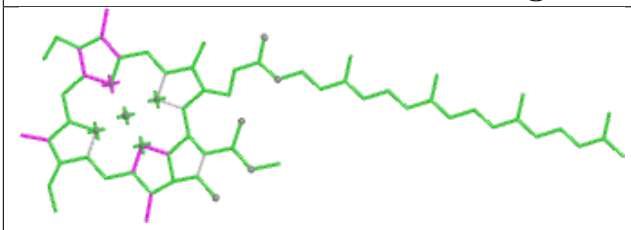


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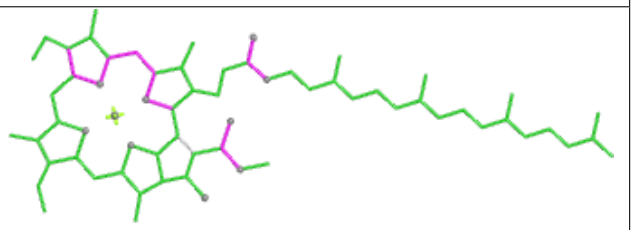


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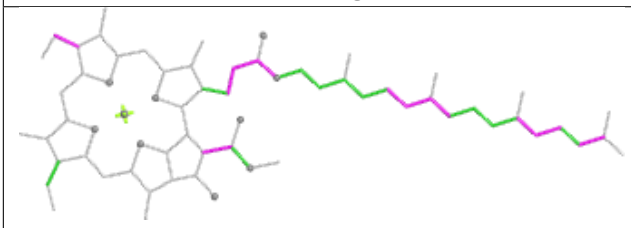
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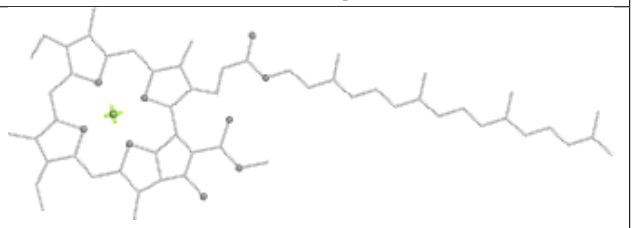
Bond lengths



Bond angles

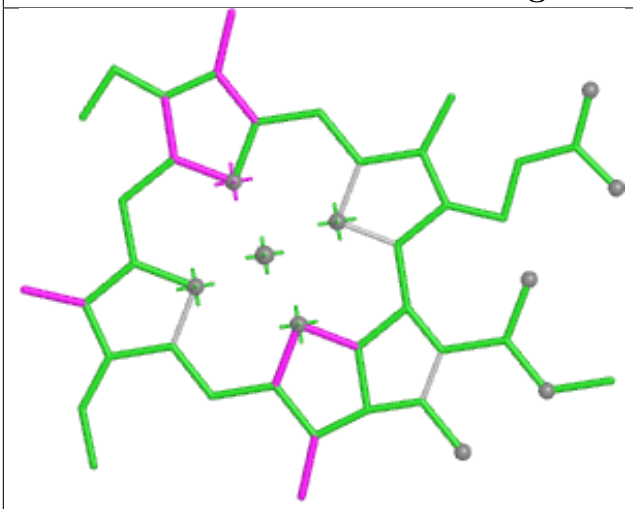


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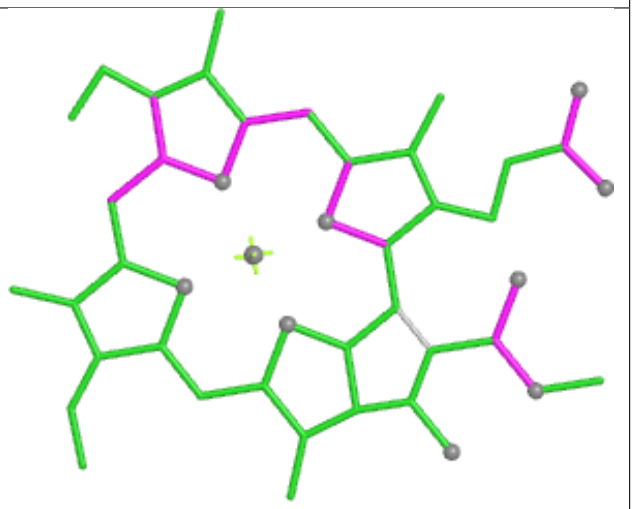


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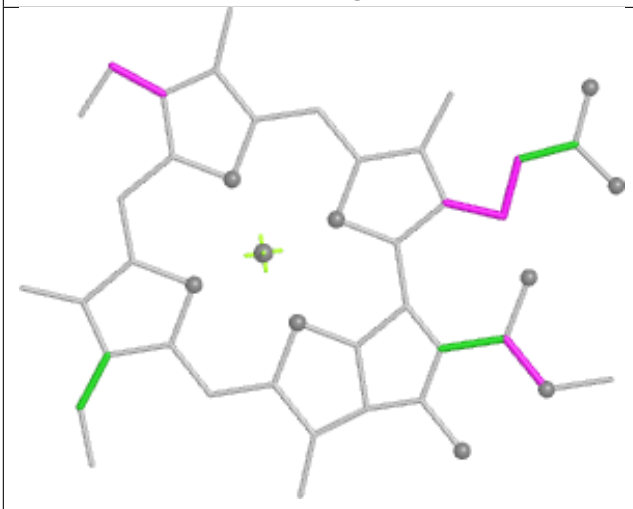
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Bond lengths



Bond angles

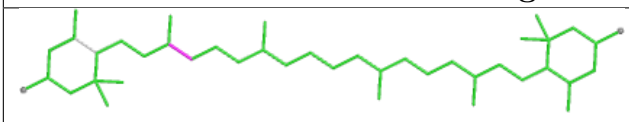


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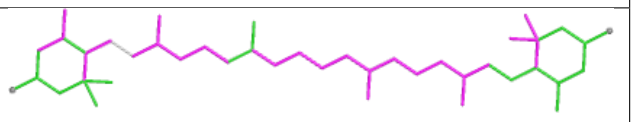


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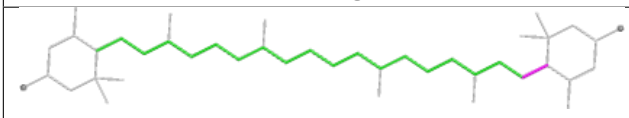
Ligand LUT S 1621



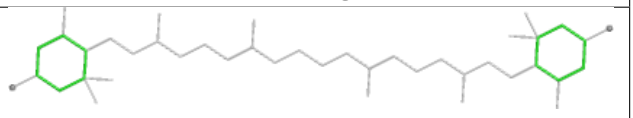
Bond lengths



Bond angles

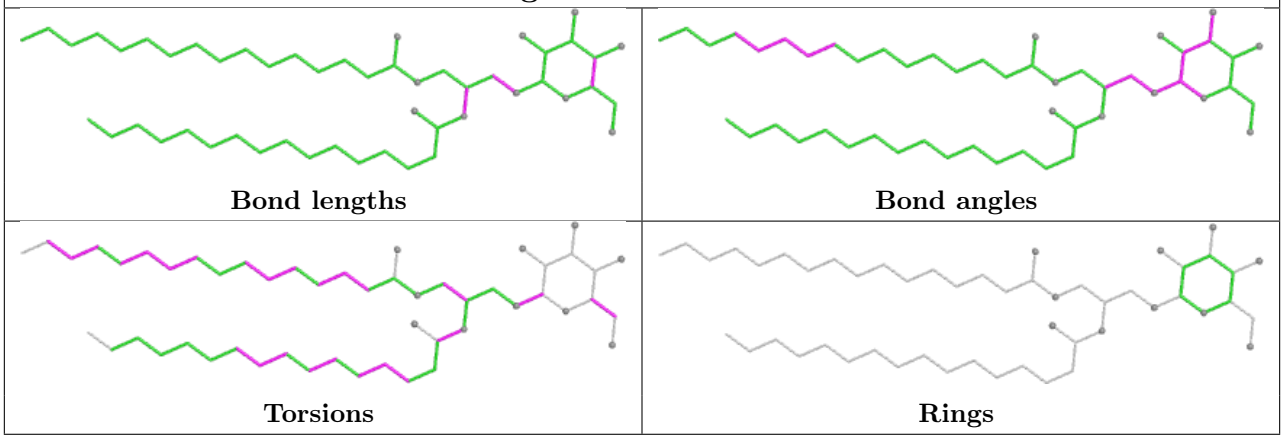


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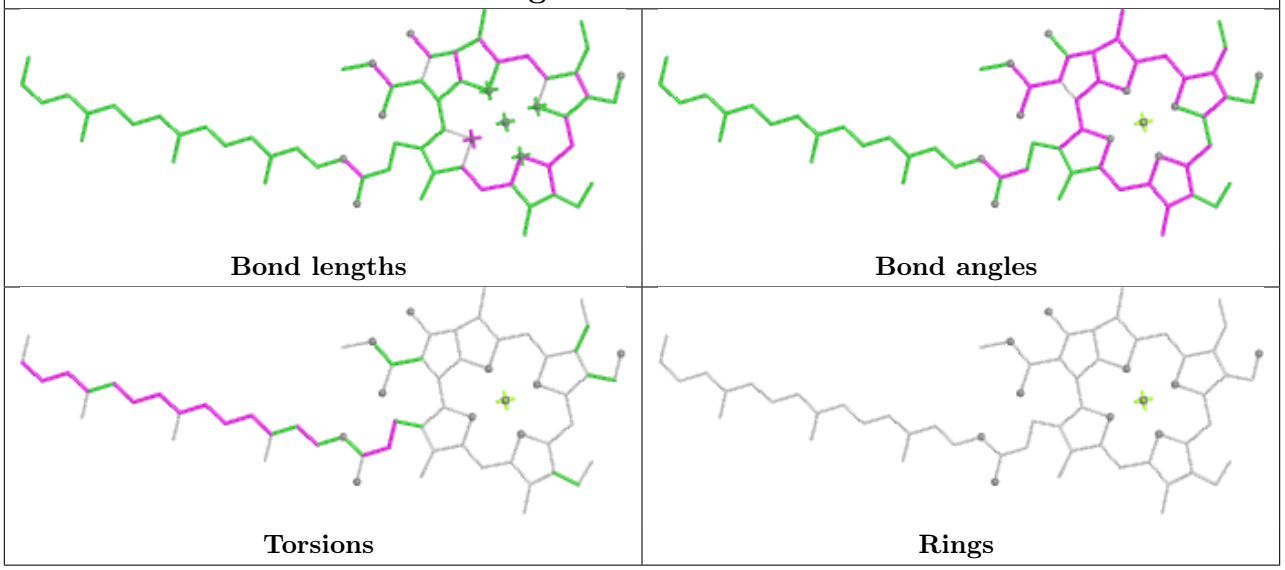


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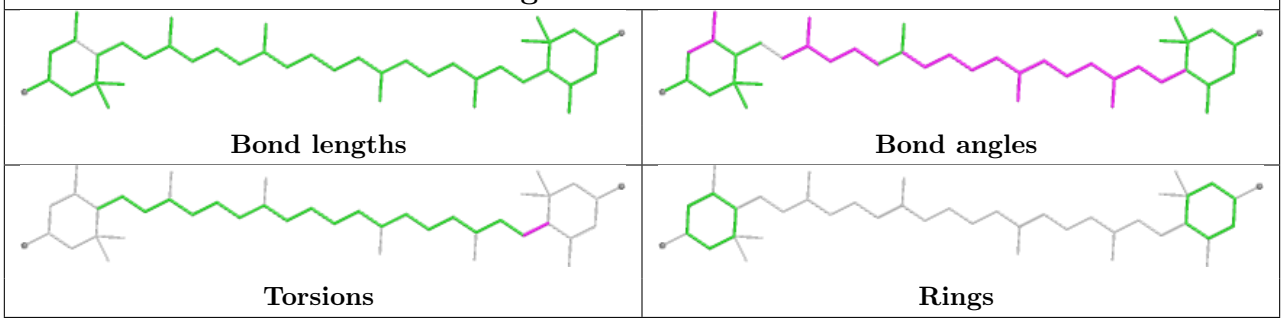
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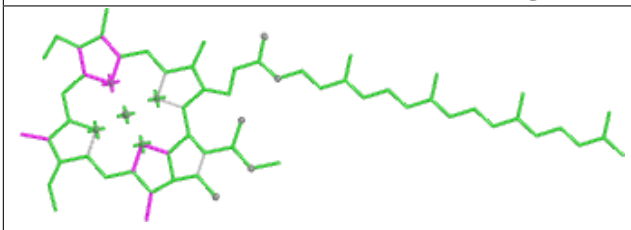
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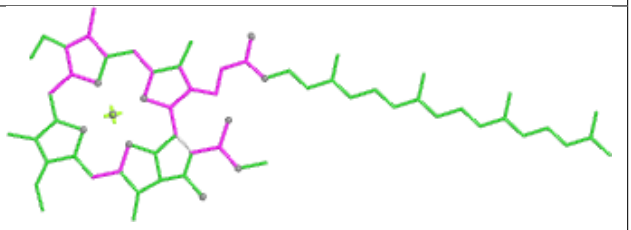
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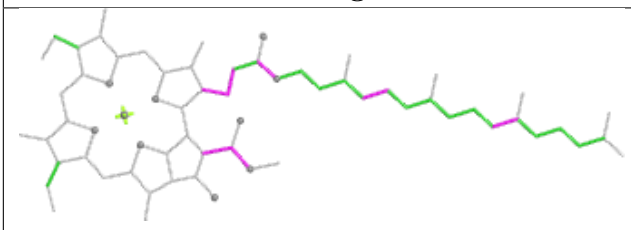
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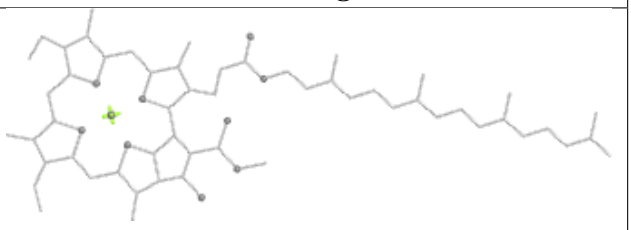
Bond lengths



Bond angles

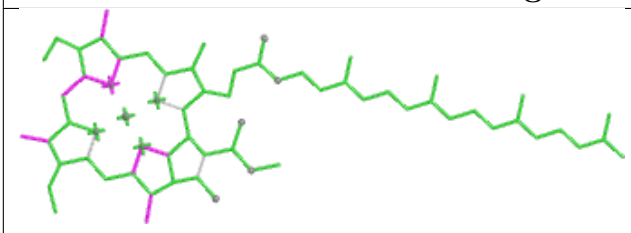


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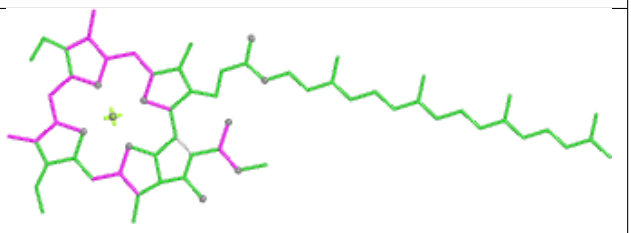


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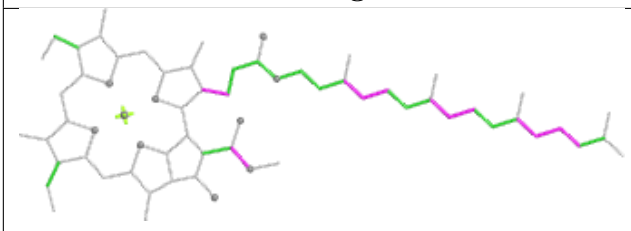
Ligand CLA B 612



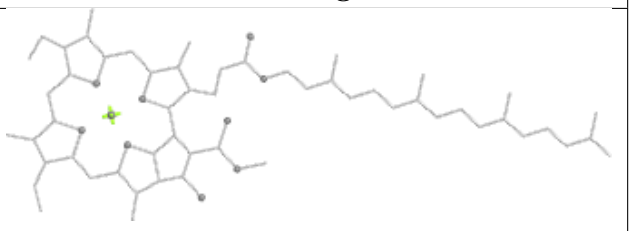
Bond lengths



Bond angles

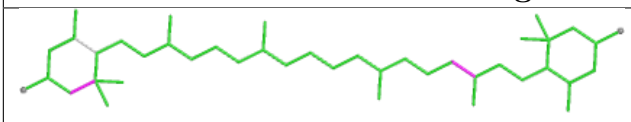


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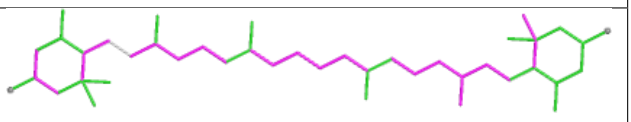


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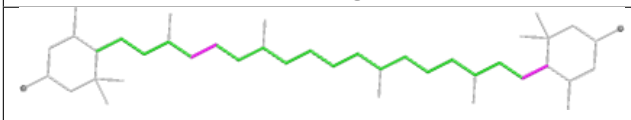
Ligand LUT N 1621



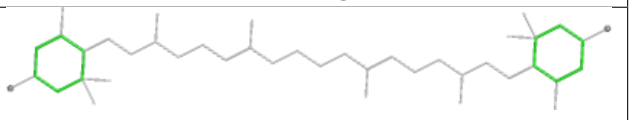
Bond lengths



Bond angles

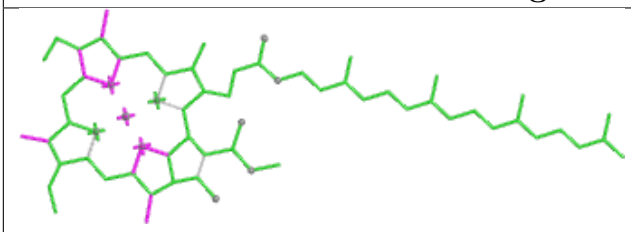


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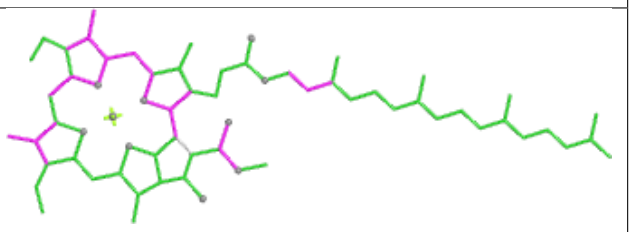


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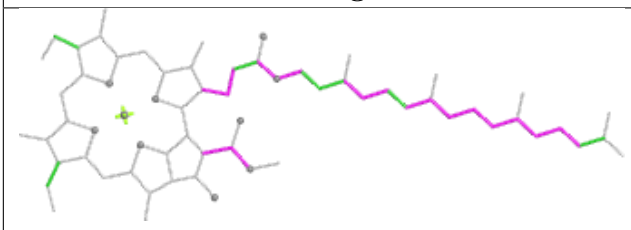
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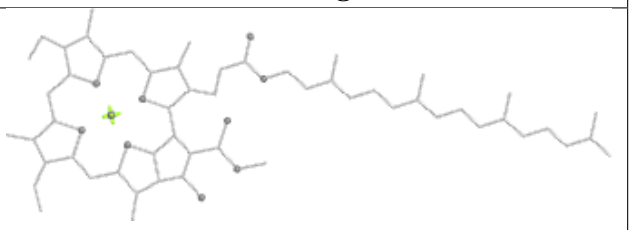
Bond lengths



Bond angles

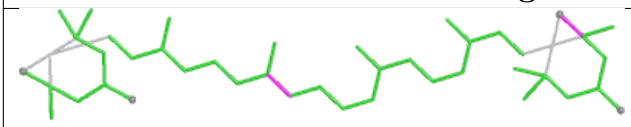


Torsions

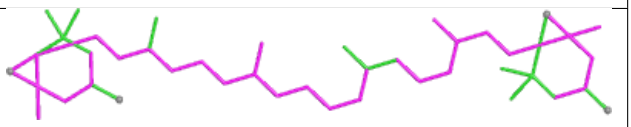


Rings

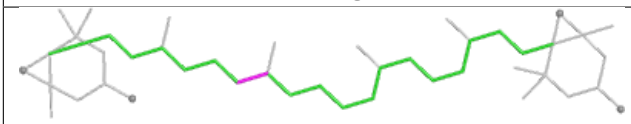
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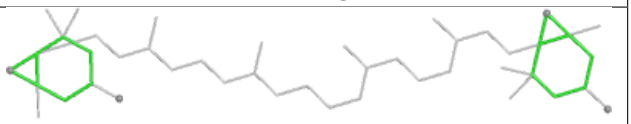
Bond lengths



Bond angles

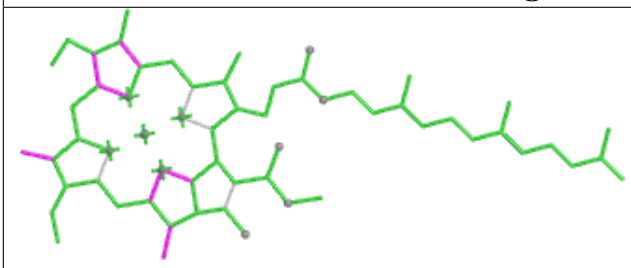


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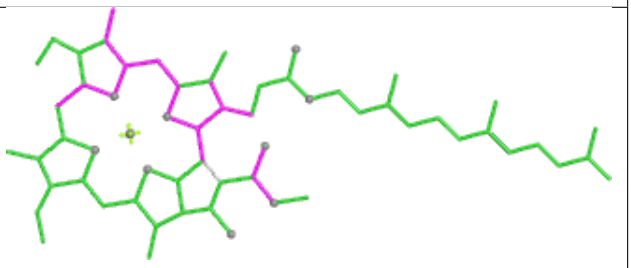


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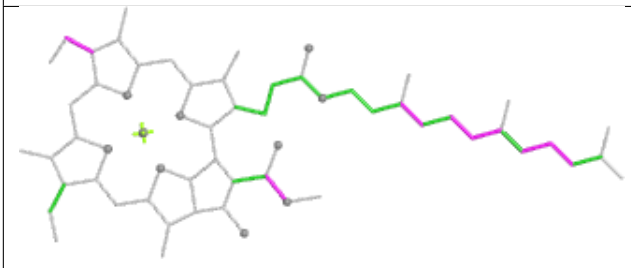
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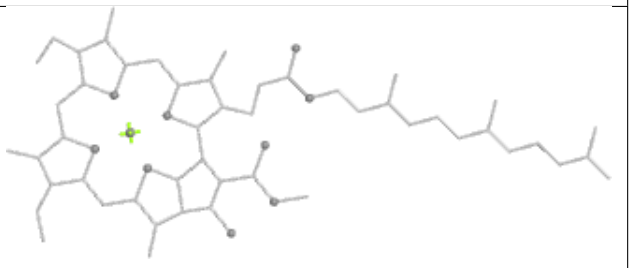
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Bond angles

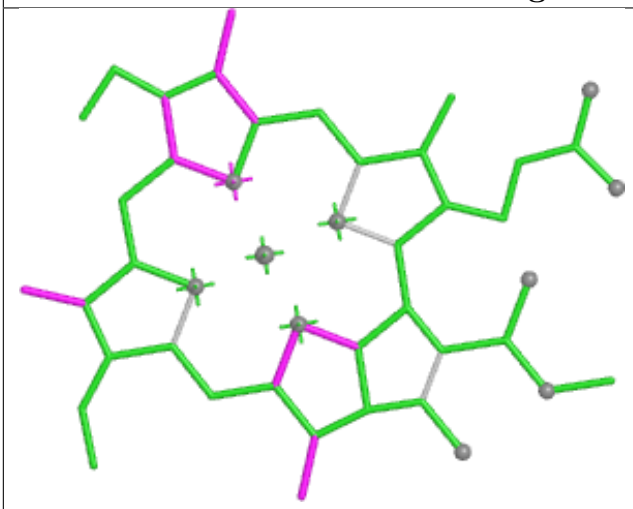


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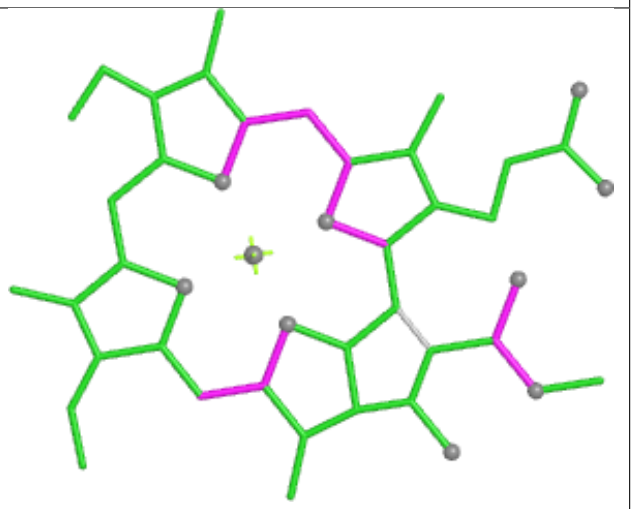


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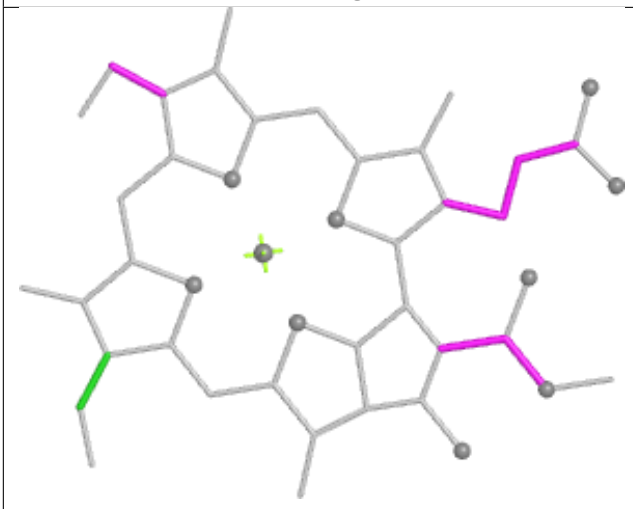
Ligand CLA 8 604



Bond lengths



Bond angles

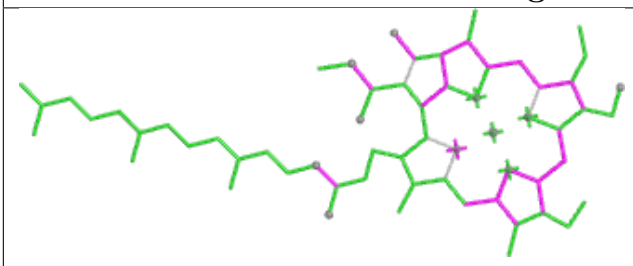


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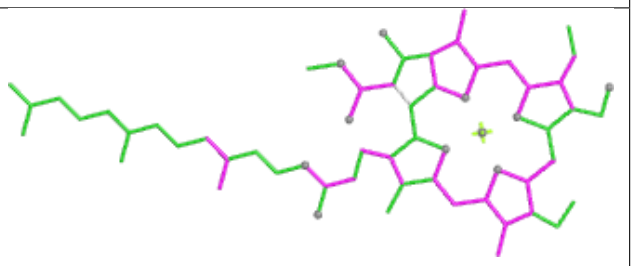


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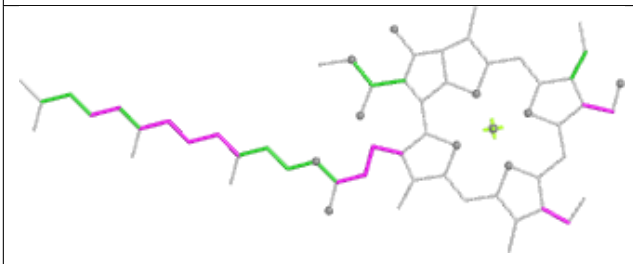
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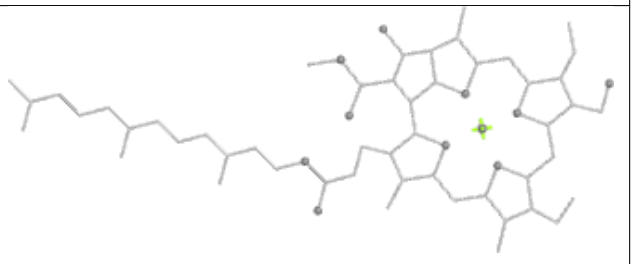
Bond lengths



Bond angles

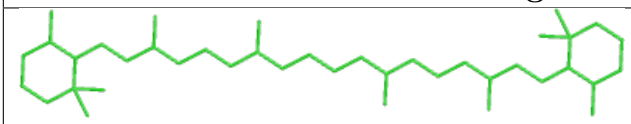


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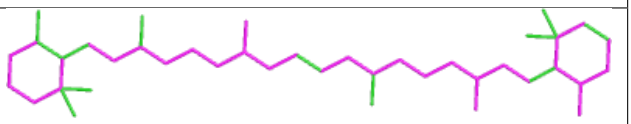


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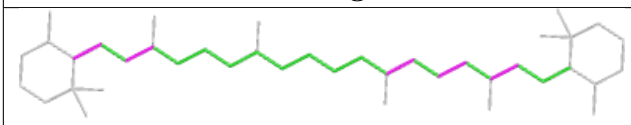
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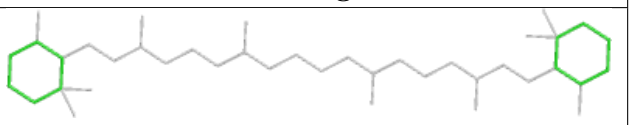
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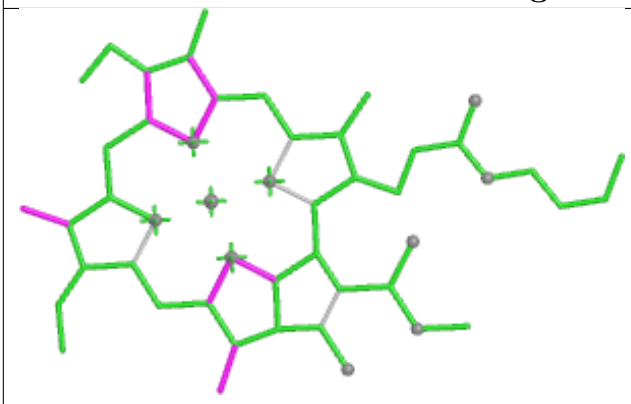


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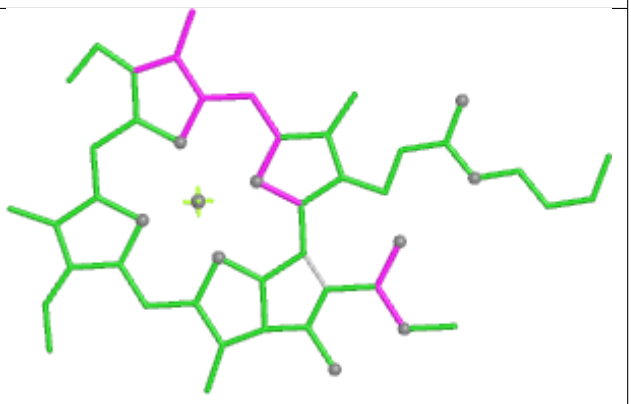


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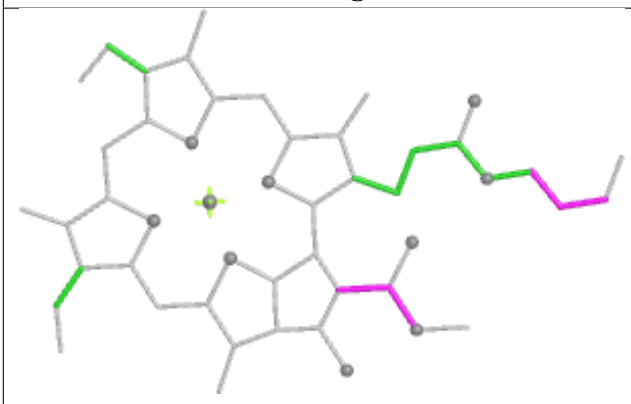
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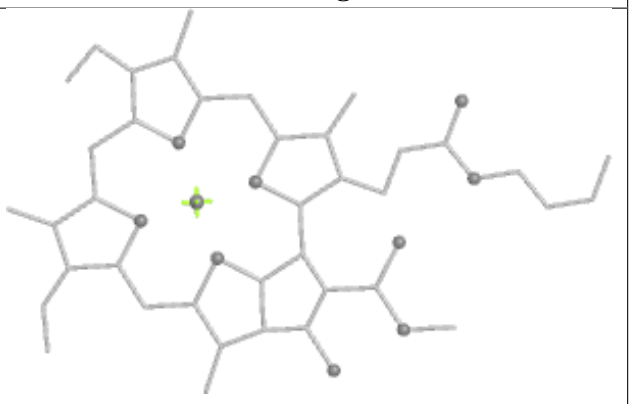
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Bond angles

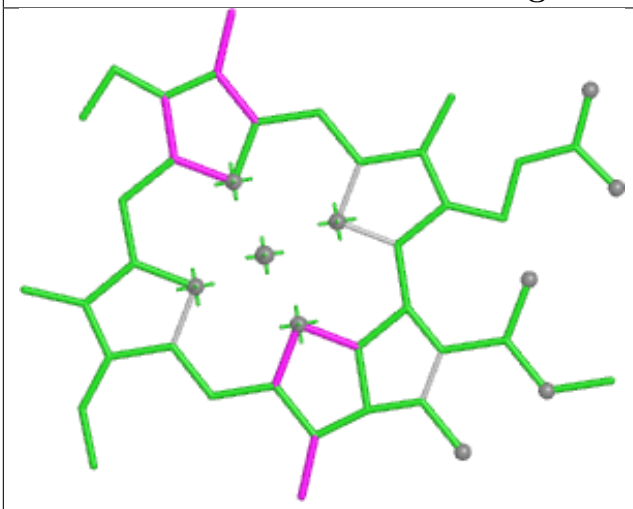


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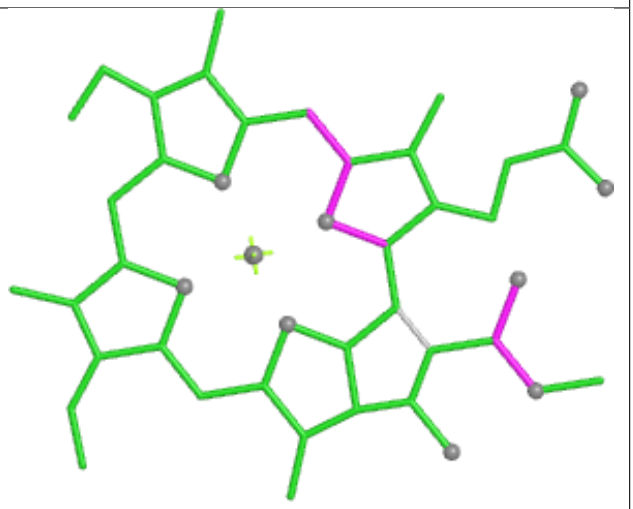


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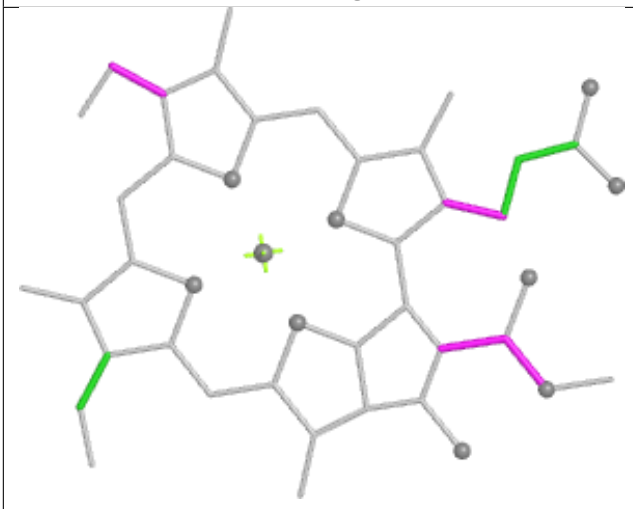
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Bond lengths



Bond angles

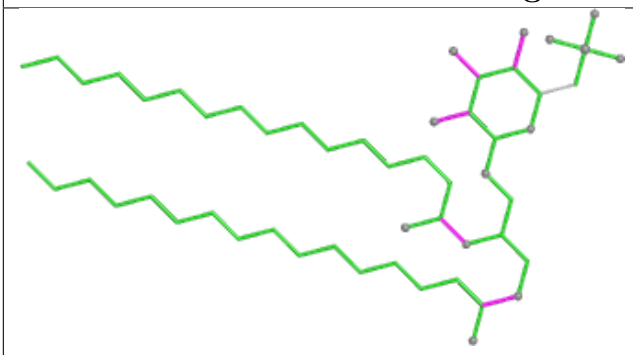


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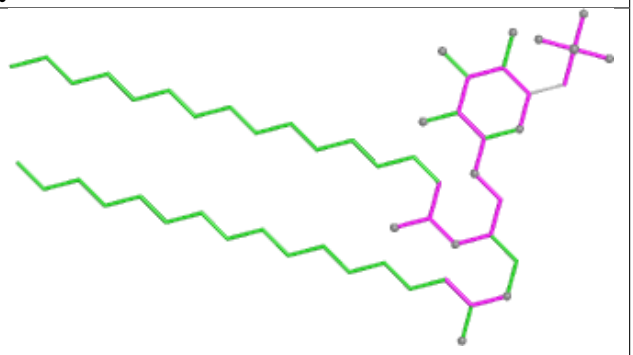


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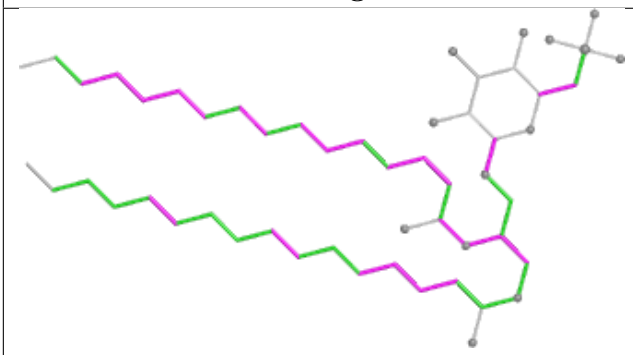
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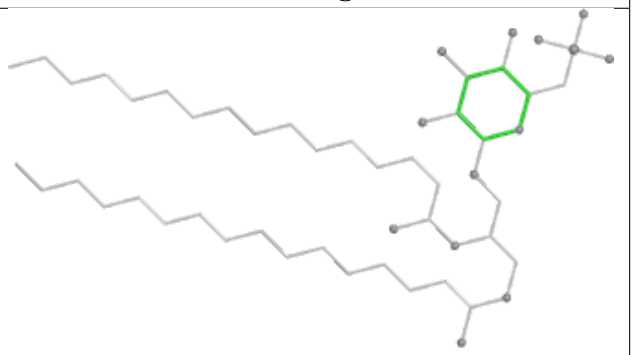
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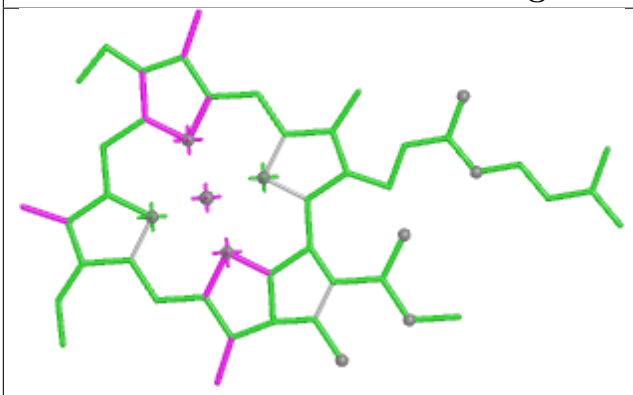


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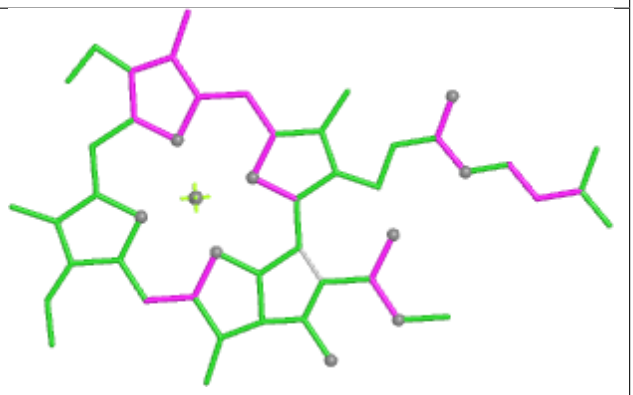


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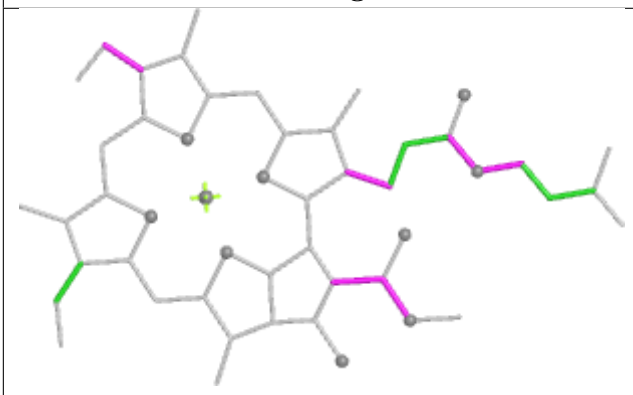
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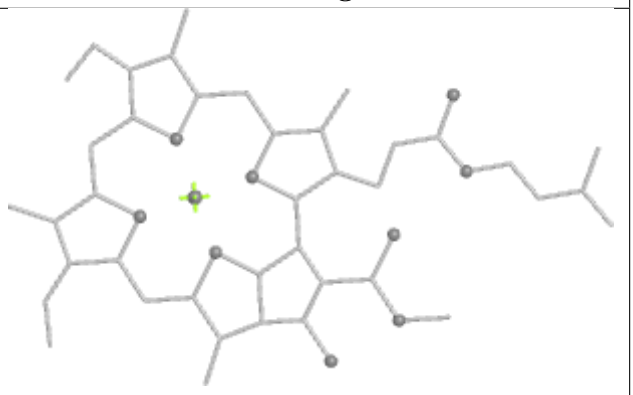
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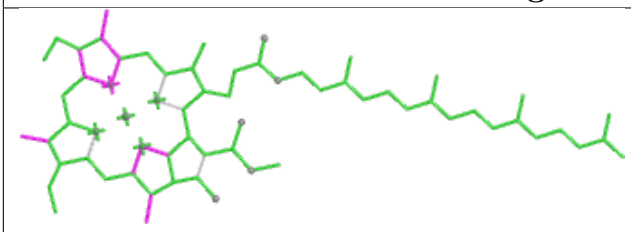


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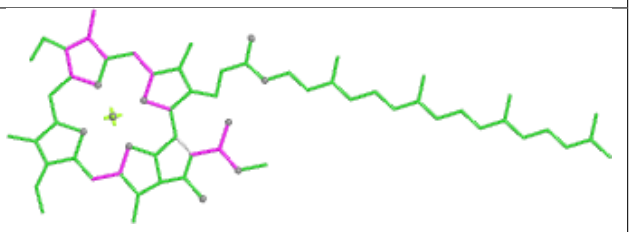


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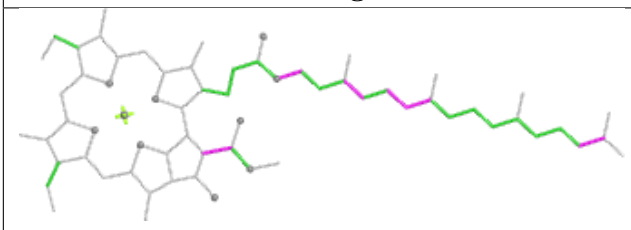
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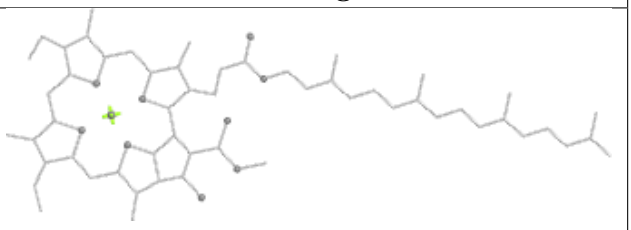
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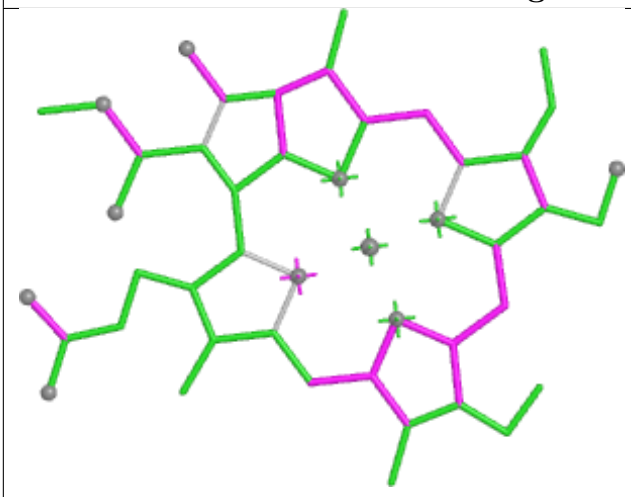


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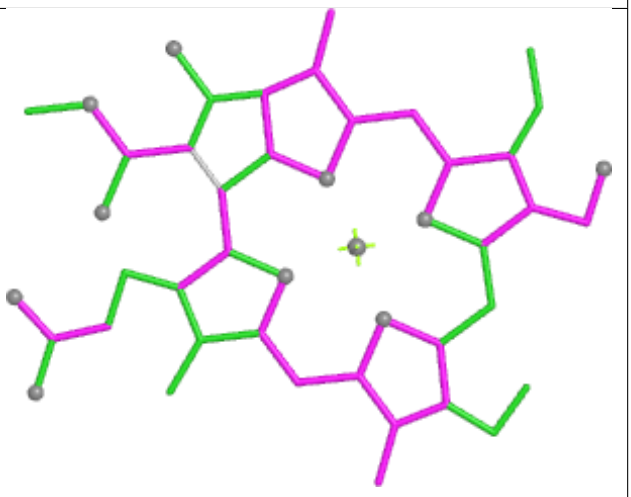


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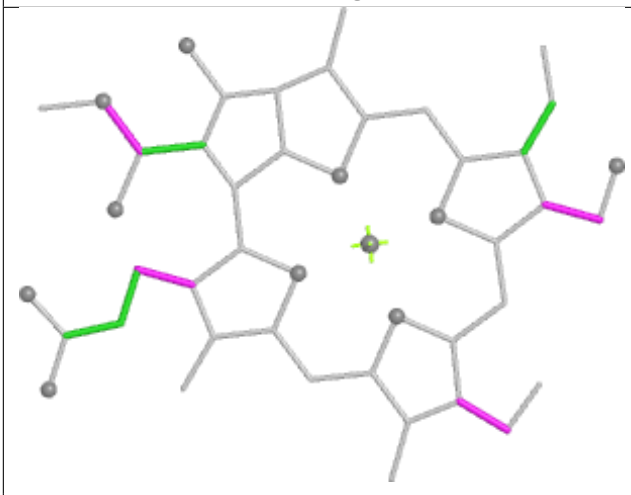
Ligand CHL 8 608



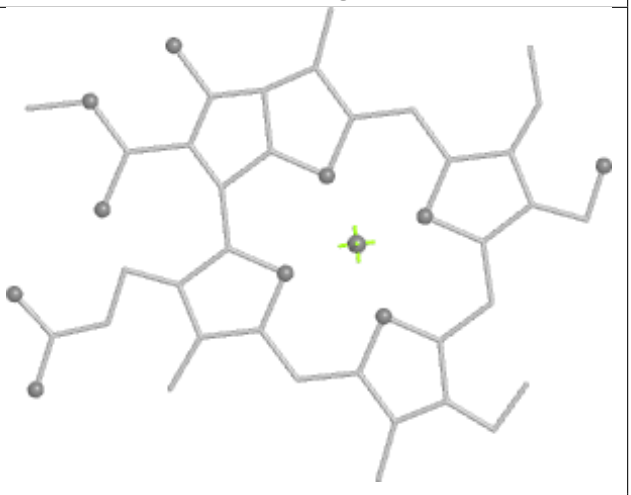
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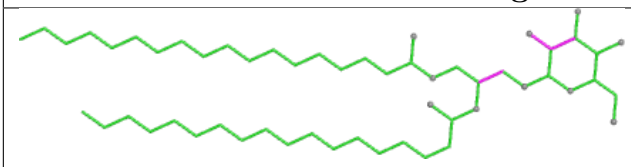


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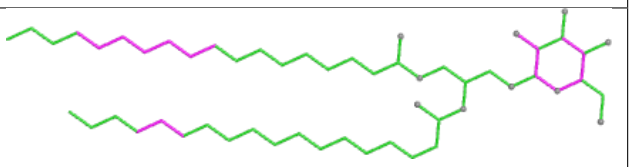


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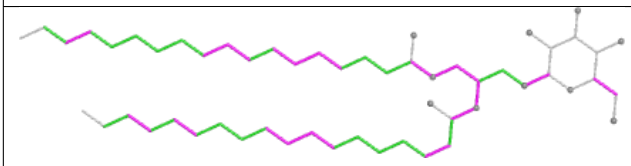
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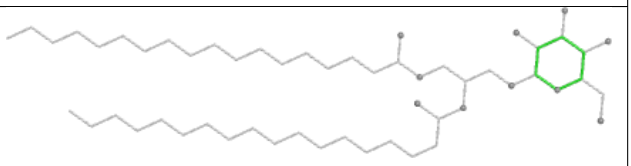
Bond lengths



Bond angles

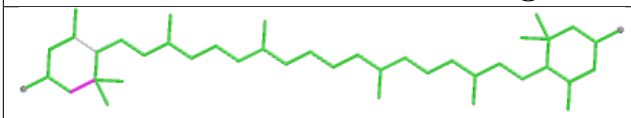


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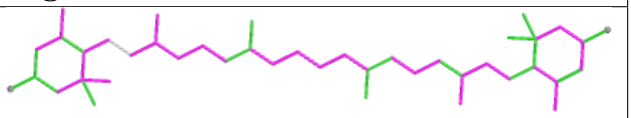


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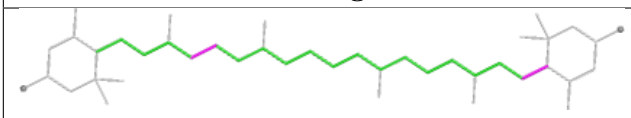
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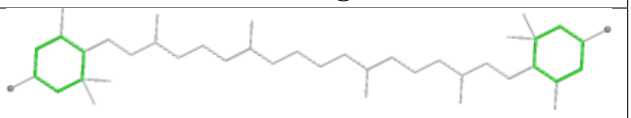
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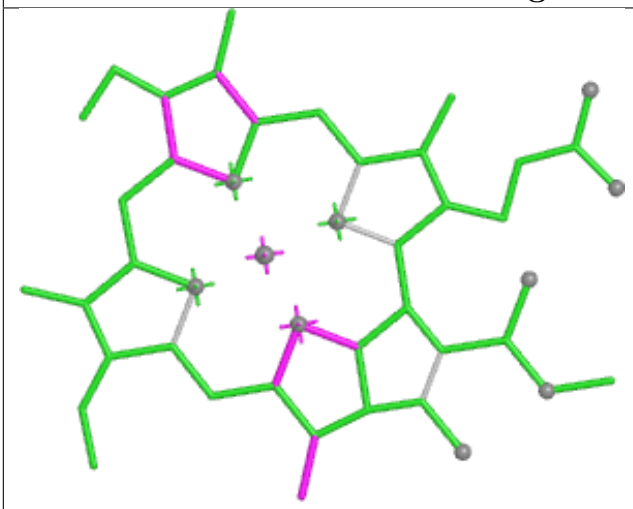


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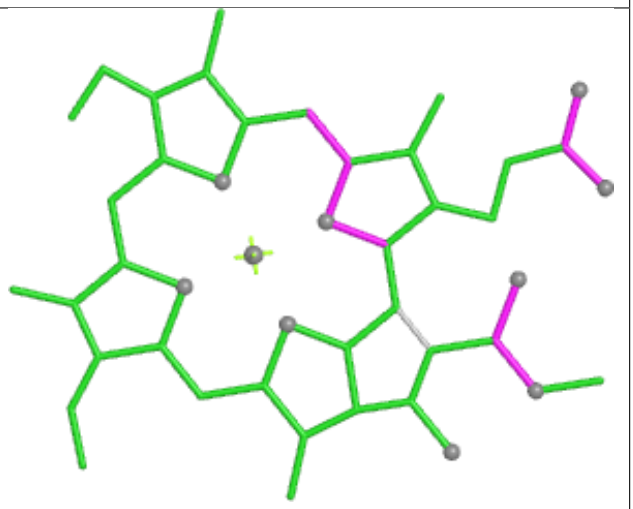


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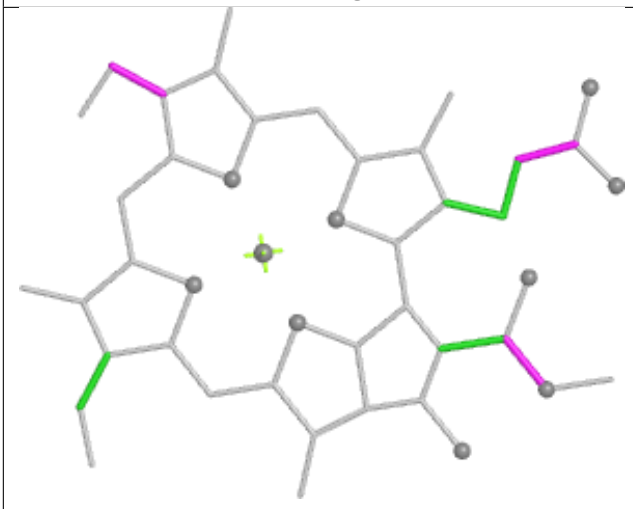
Ligand CLA 4 611



Bond lengths



Bond angles

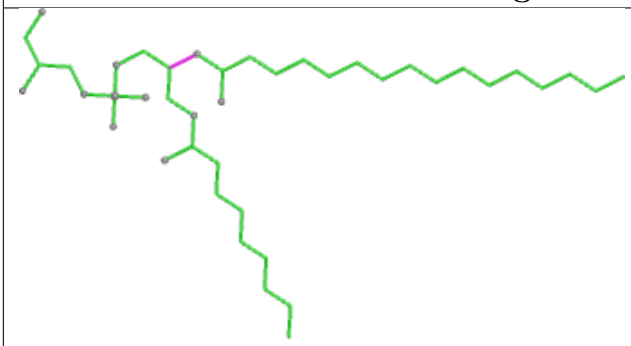


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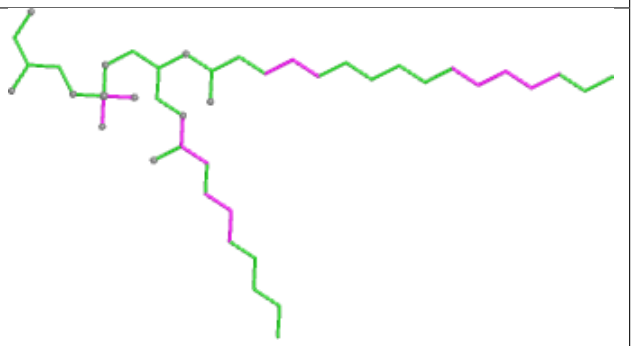


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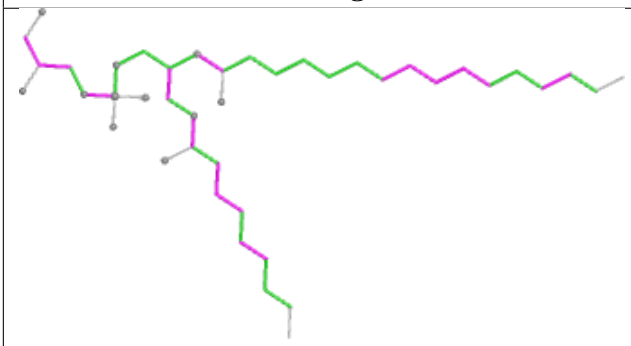
Ligand LHG R 2630



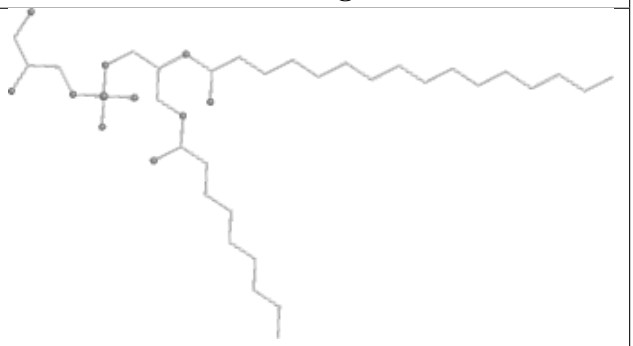
Bond lengths



Bond angles

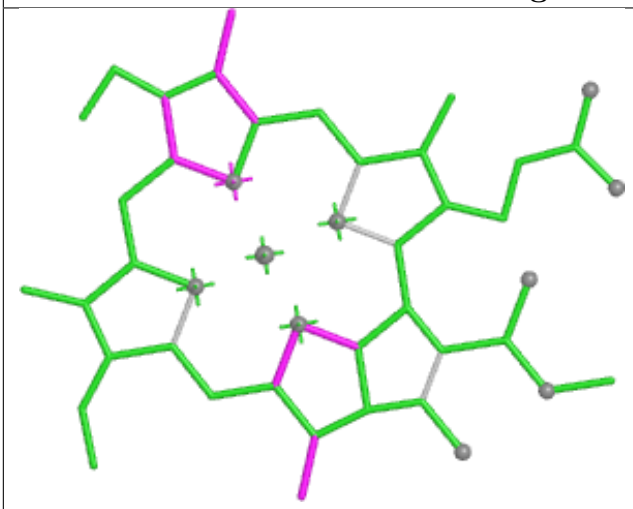


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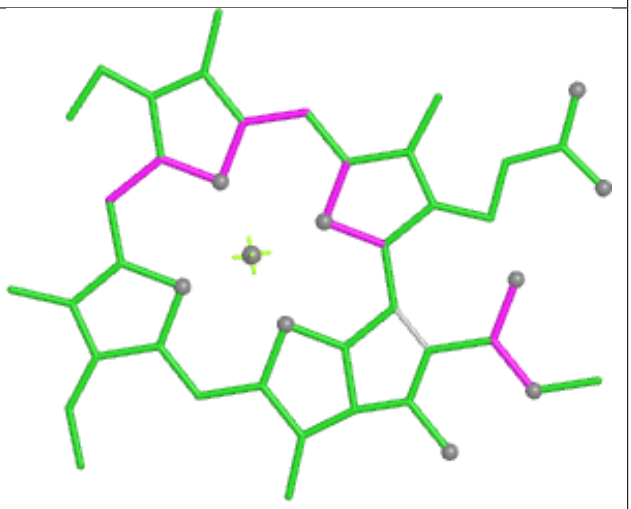


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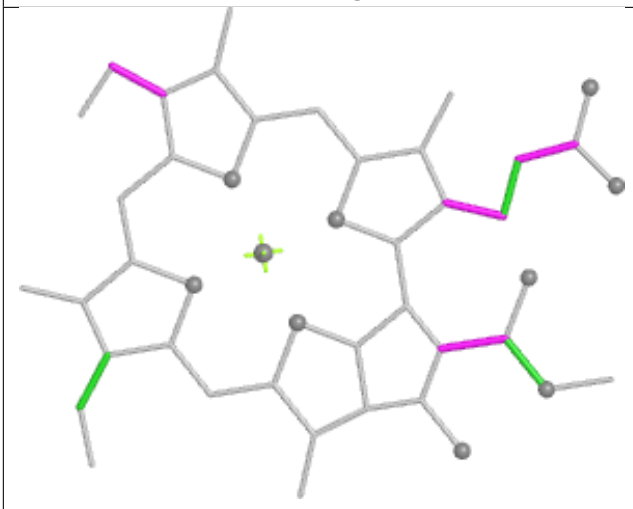
Ligand CLA r 616



Bond lengths



Bond angles

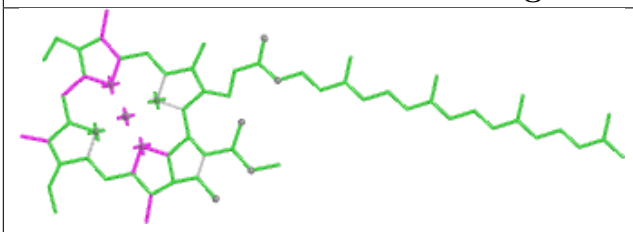


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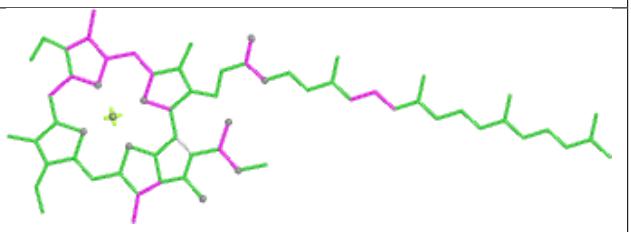


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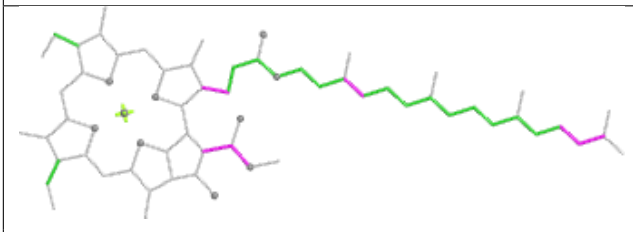
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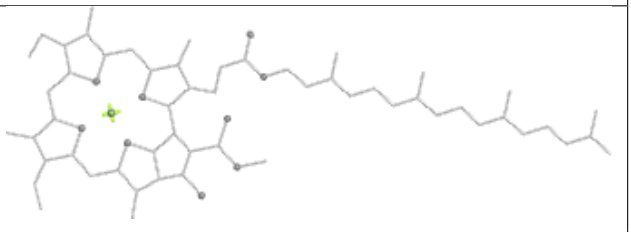
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Bond angles

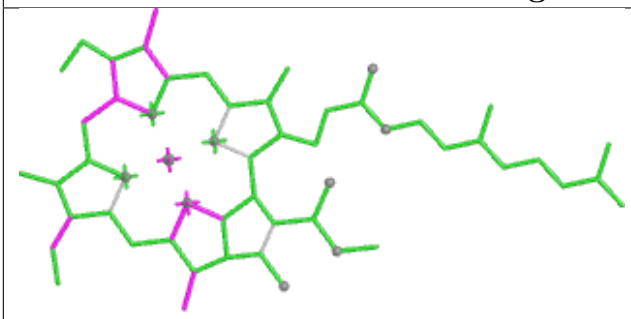


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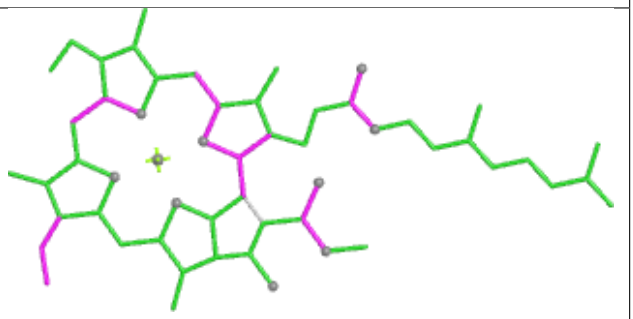


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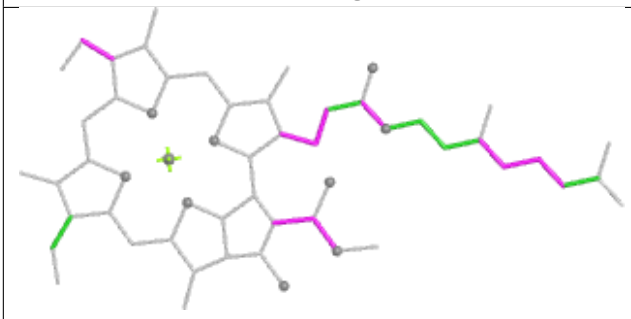
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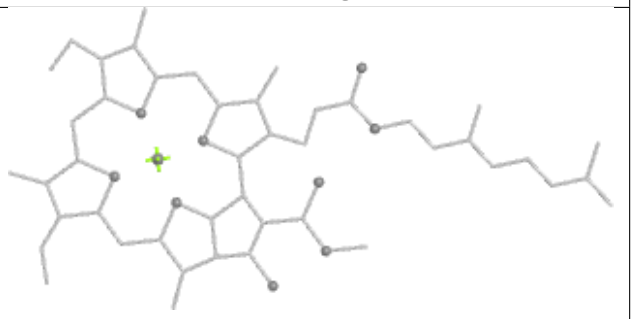
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Bond angles

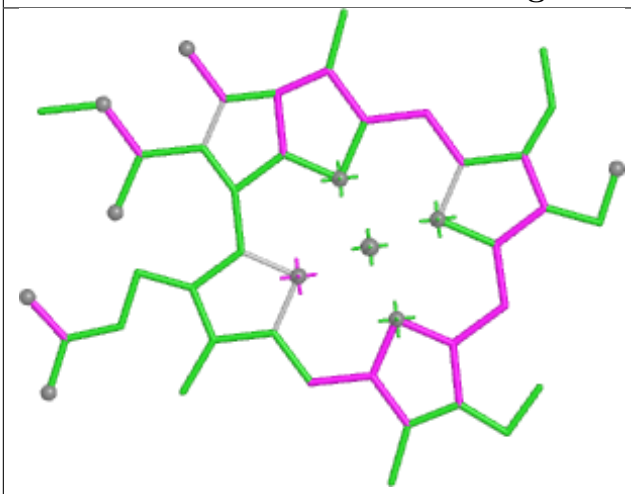


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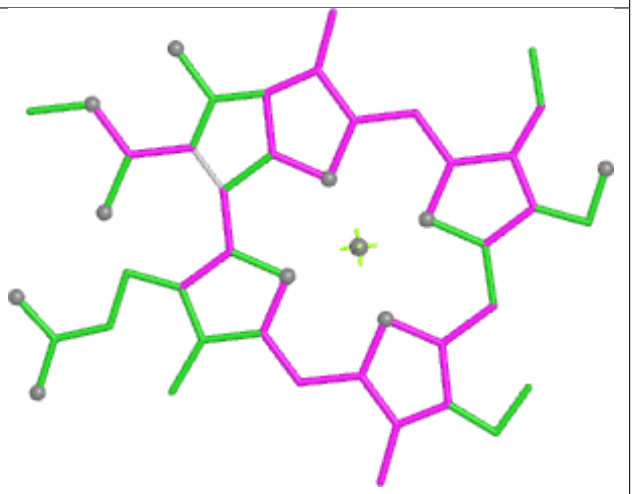


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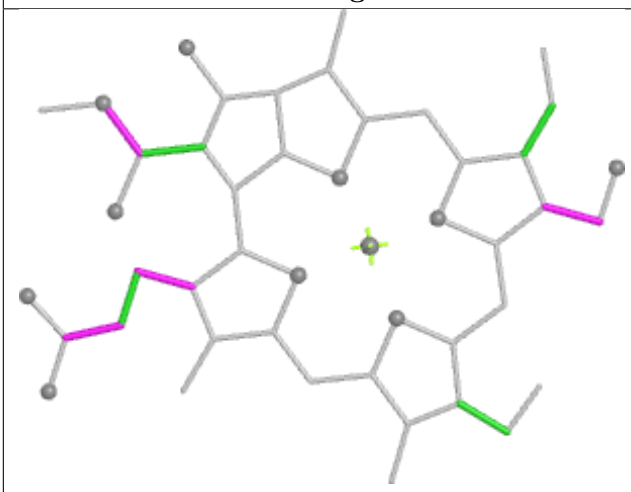
Ligand CHL 6 608



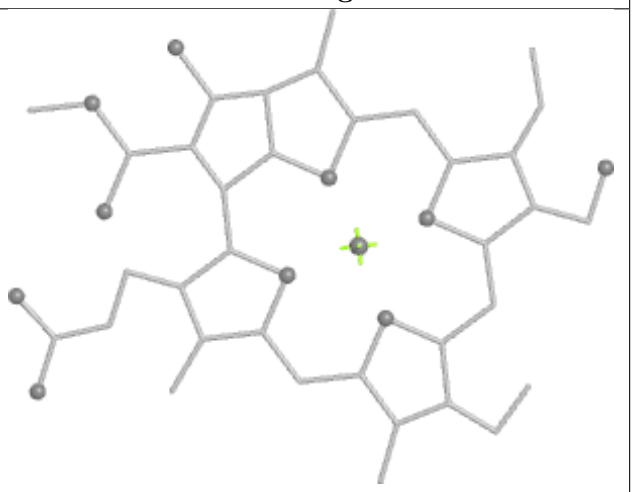
Bond lengths



Bond angles

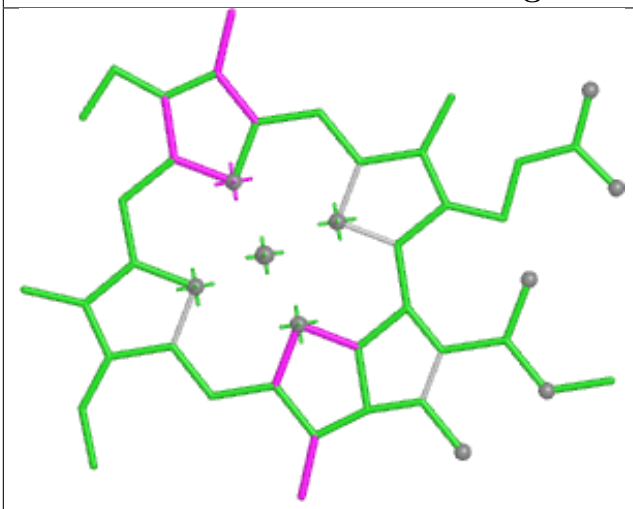


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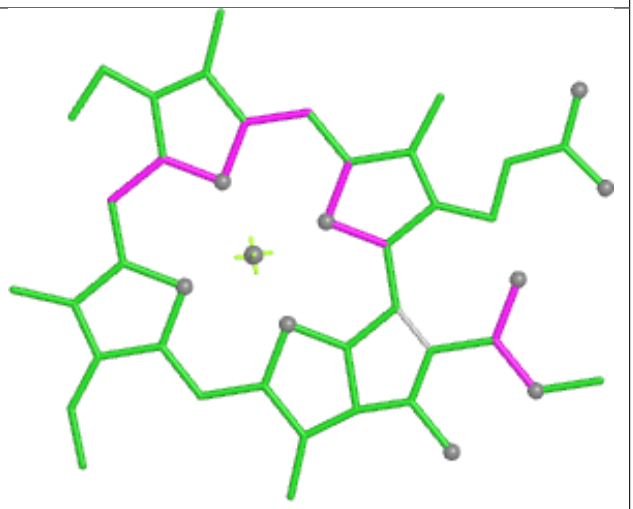


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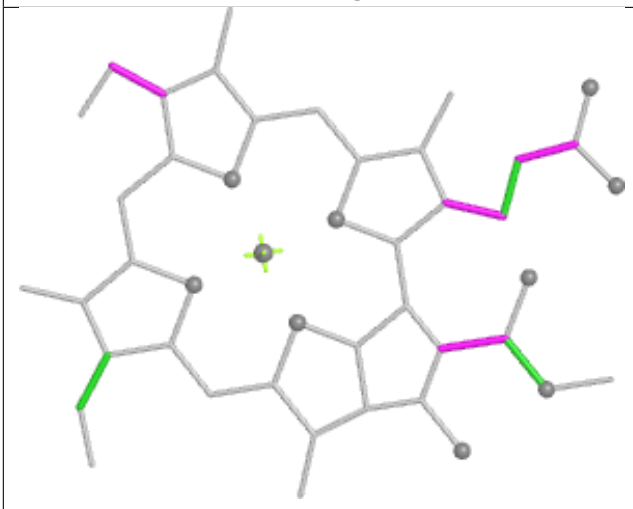
Ligand CLA R 616



Bond lengths



Bond angles

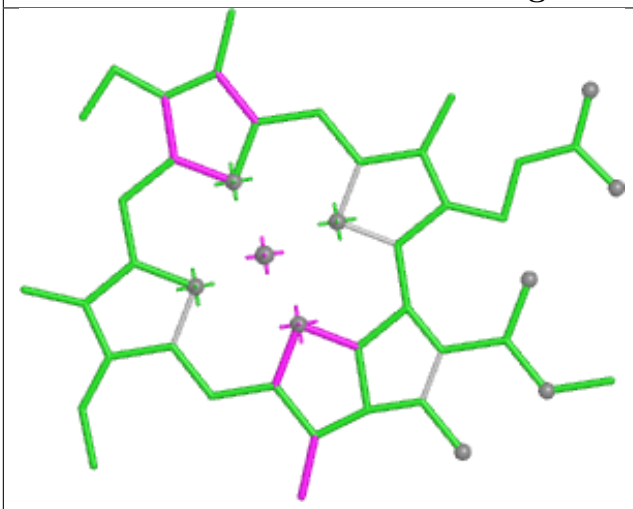


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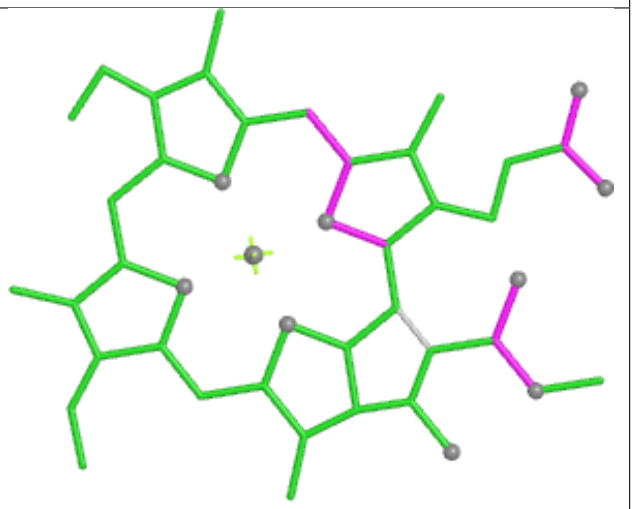


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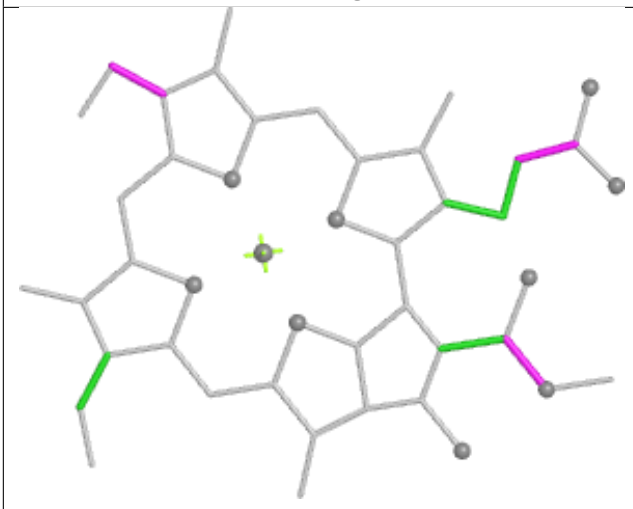
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Bond lengths



Bond angles

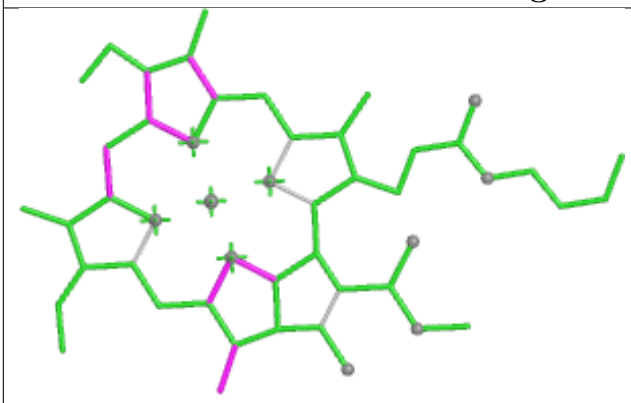


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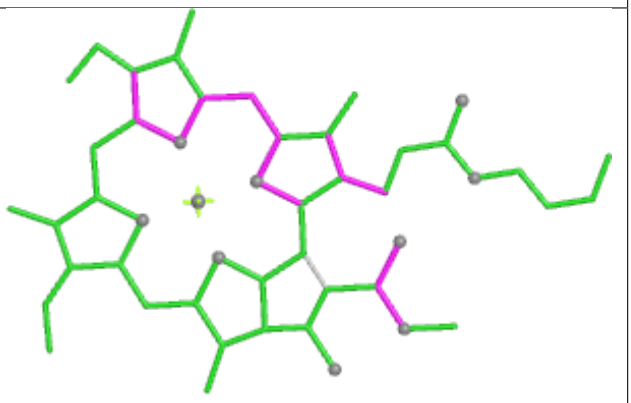


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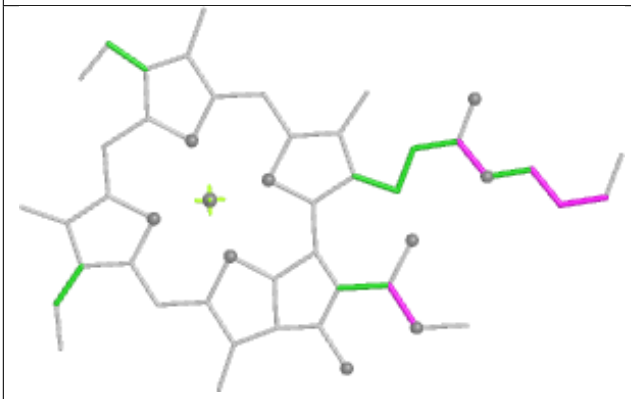
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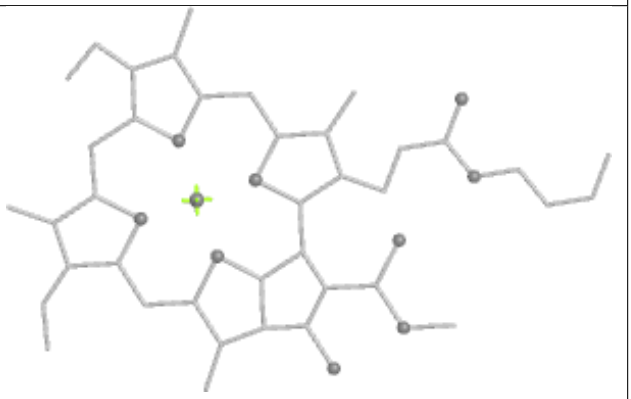
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Bond angles

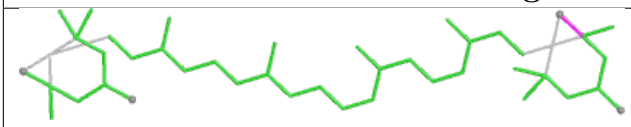


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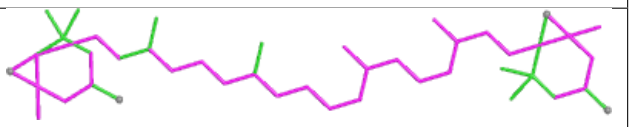


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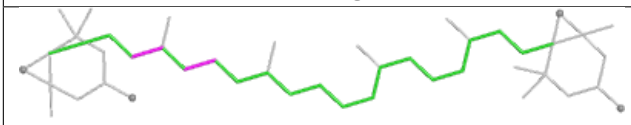
Ligand XAT R 622



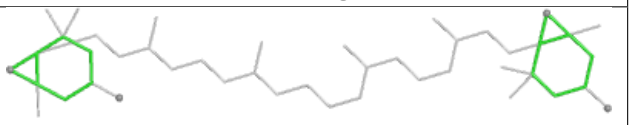
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Bond angles

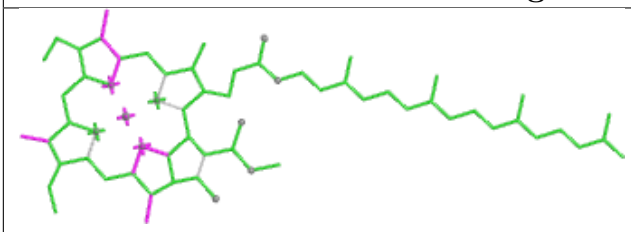


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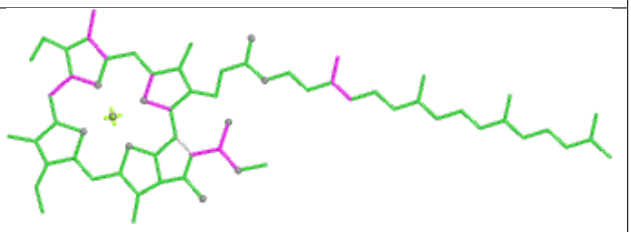


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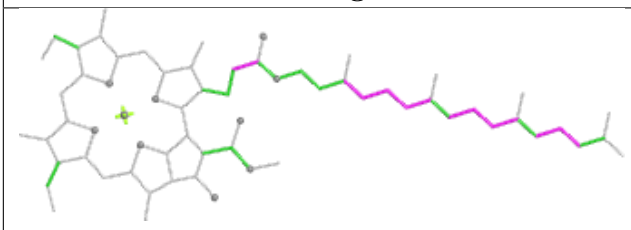
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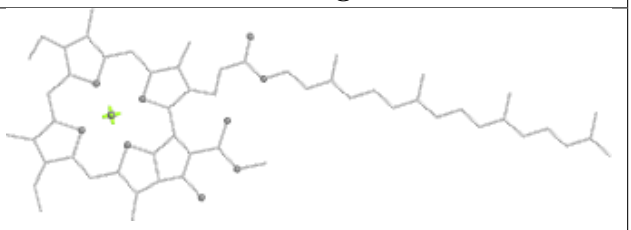
Bond lengths



Bond angles



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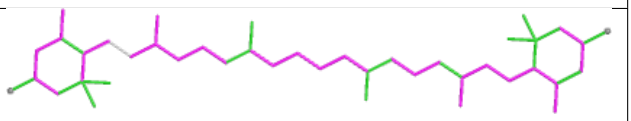


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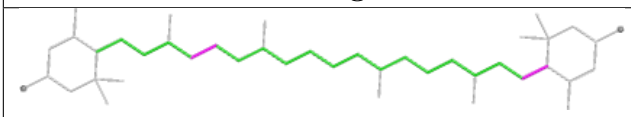
Ligand LUT 1 1621



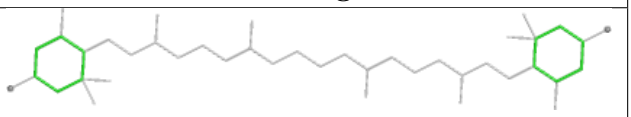
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Bond angles

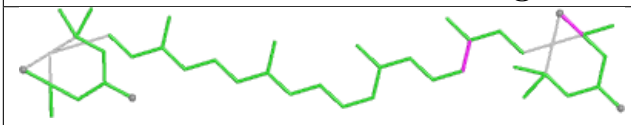


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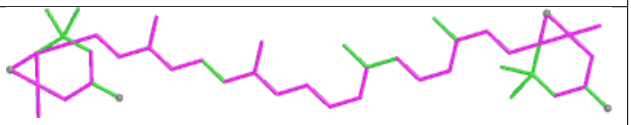


Rings

Ligand XAT G 1622



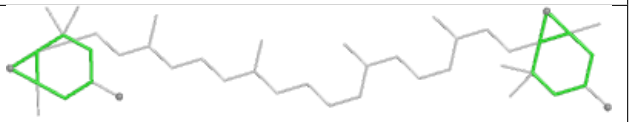
Bond lengths



Bond angles

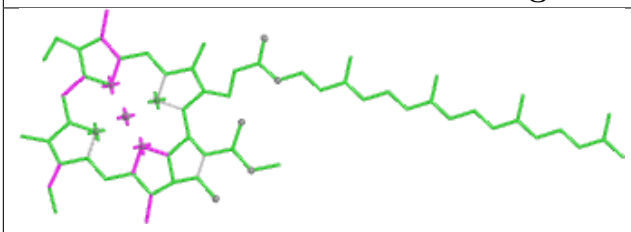


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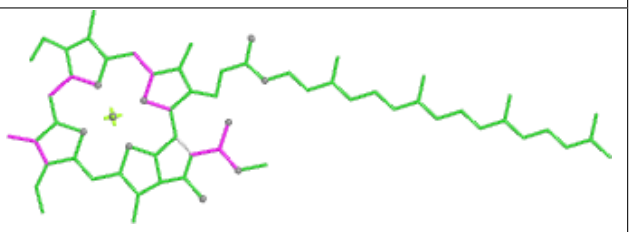


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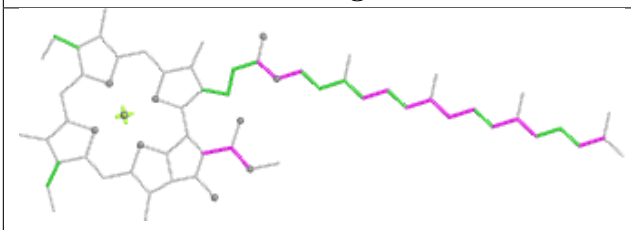
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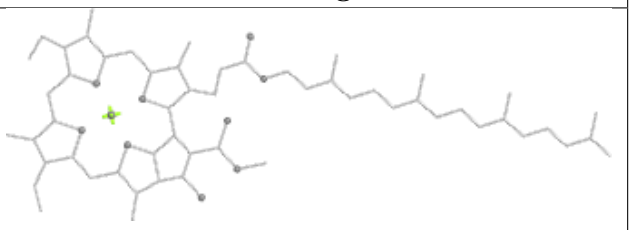
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Bond angles

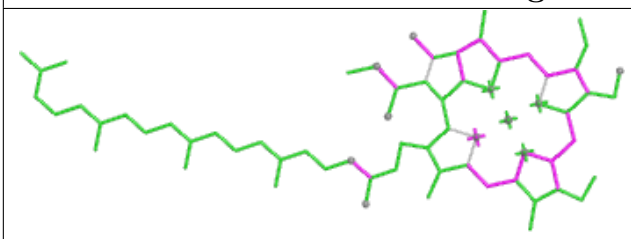


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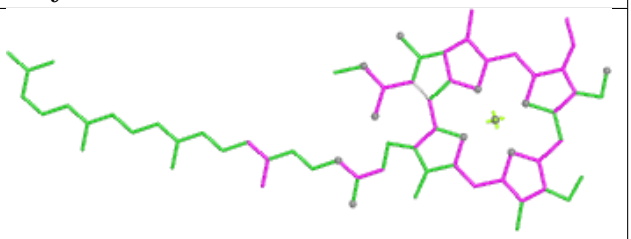


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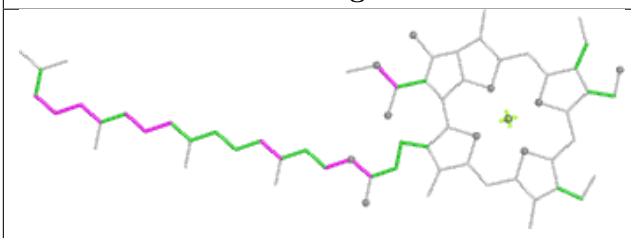
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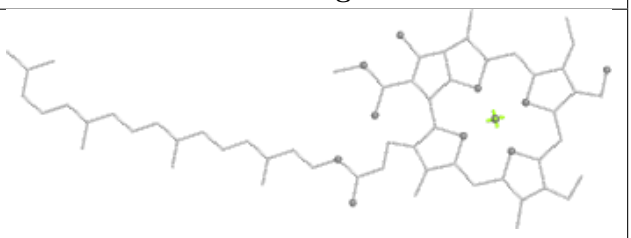
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Bond angles

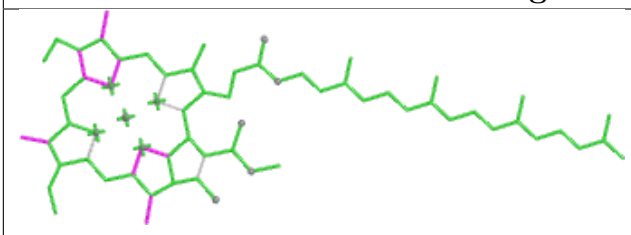


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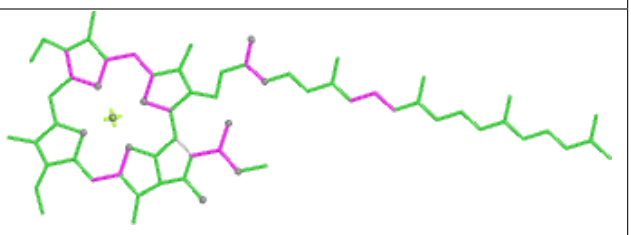


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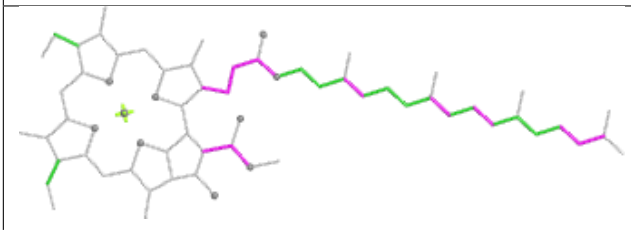
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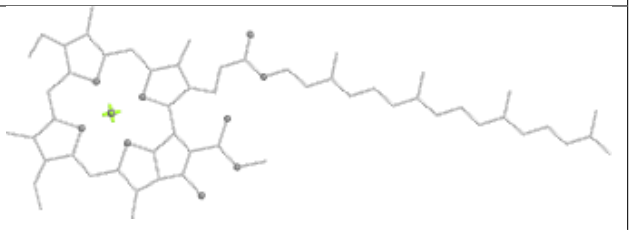
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Bond angles

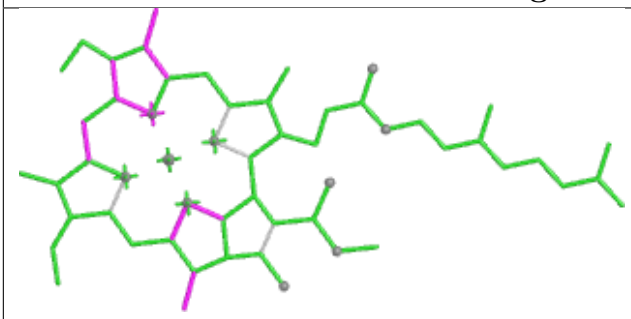


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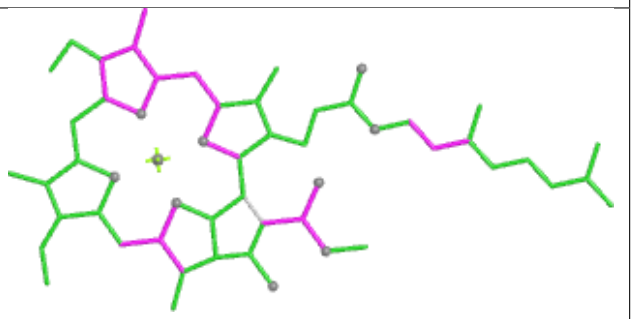


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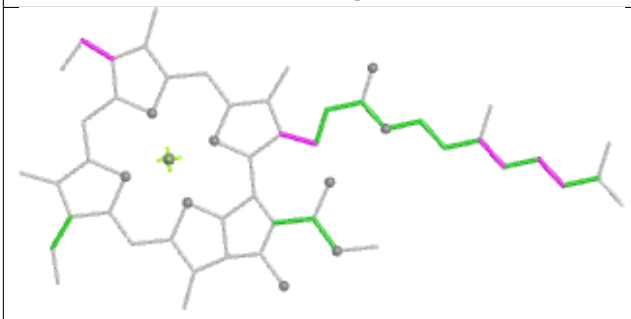
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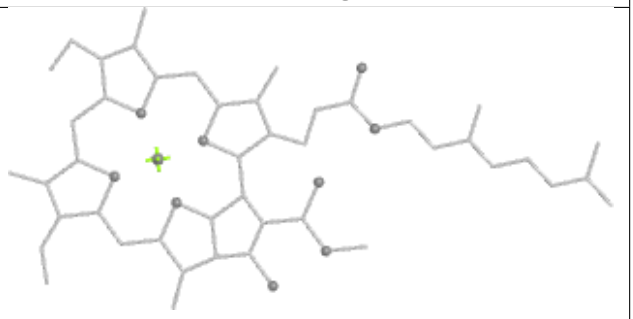
Bond lengths



Bond angles

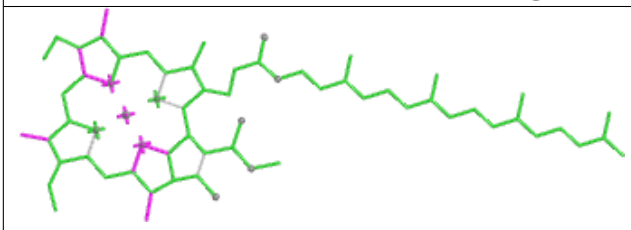


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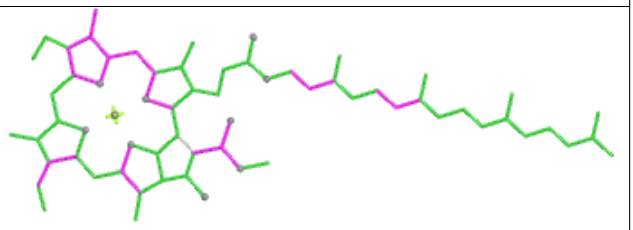


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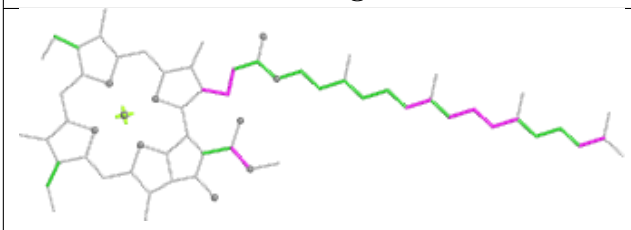
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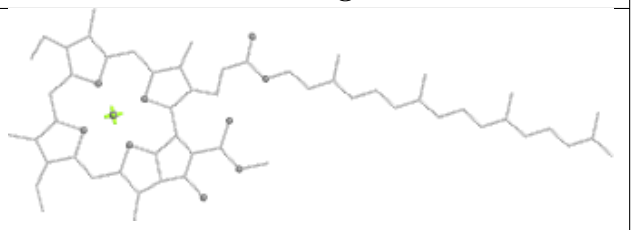
Bond lengths



Bond angles

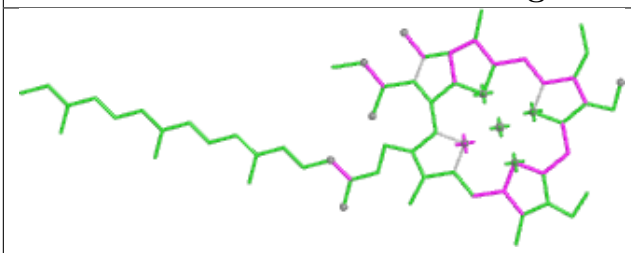


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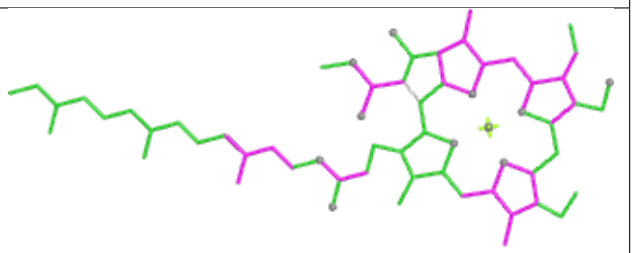


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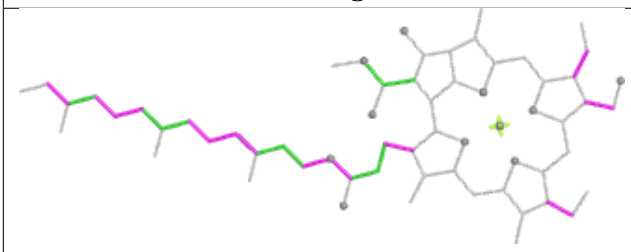
Ligand CHL 5 609



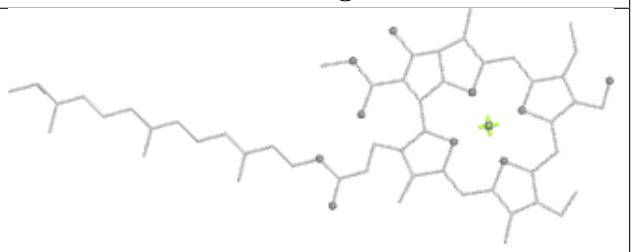
Bond lengths



Bond angles

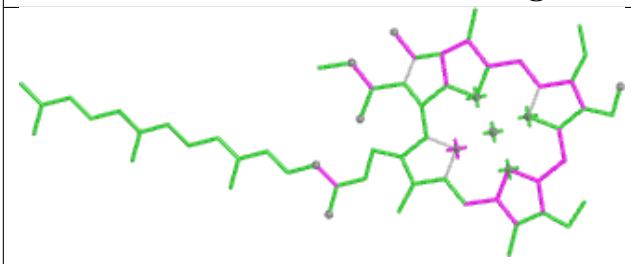


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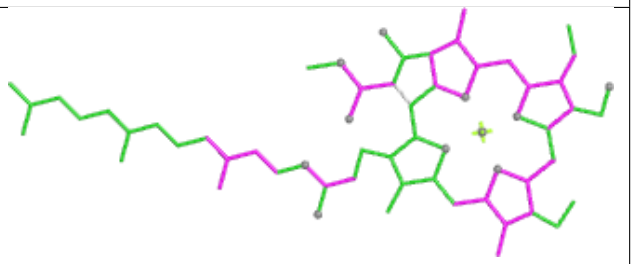


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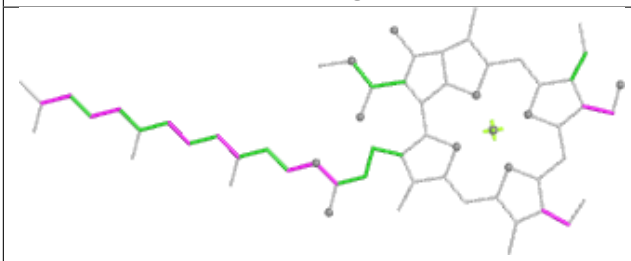
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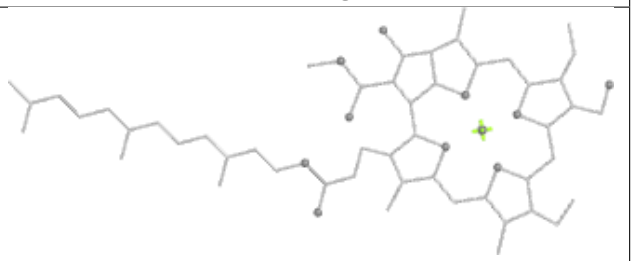
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Bond angles

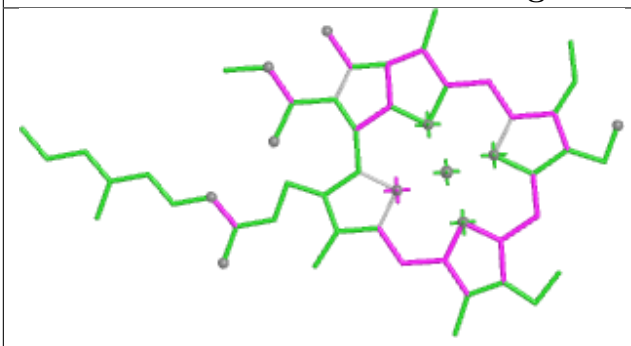


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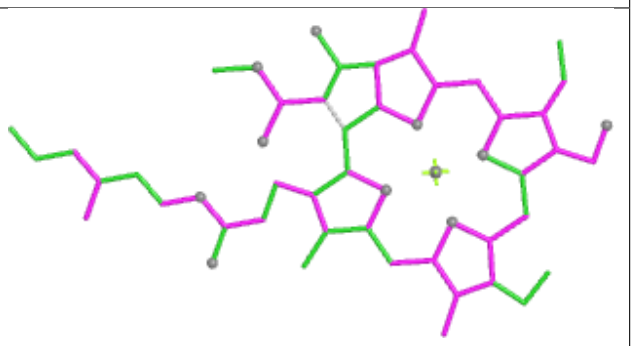


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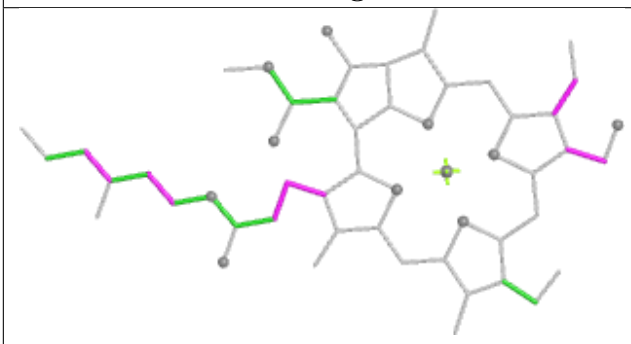
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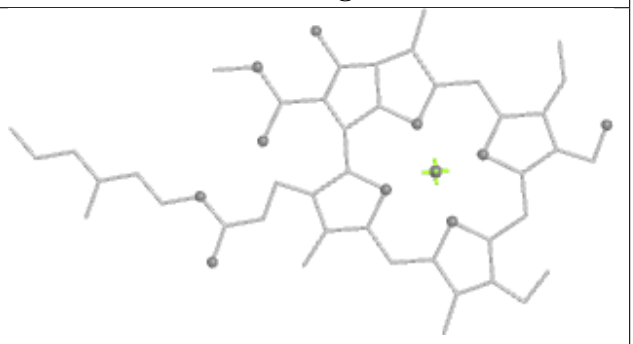
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Bond angles

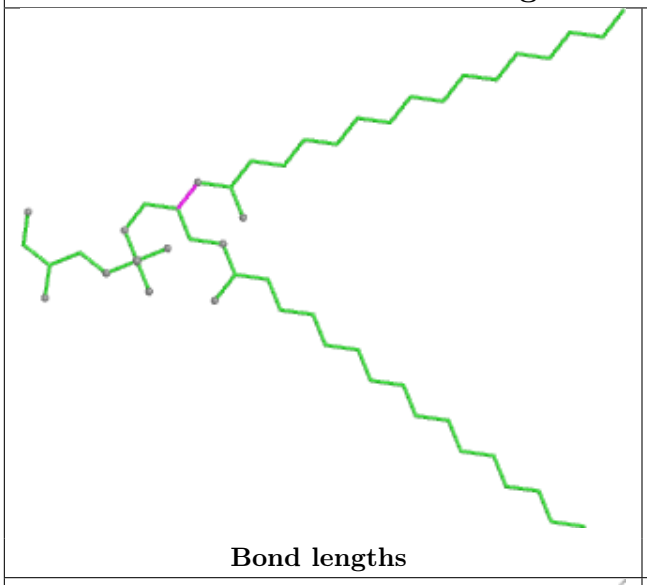


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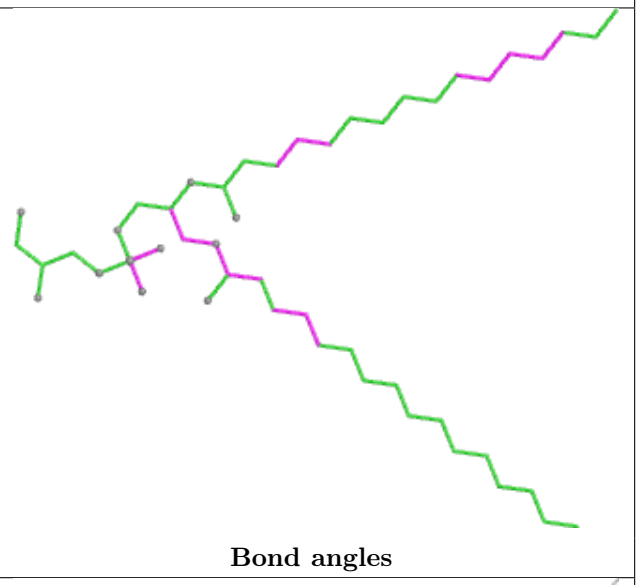


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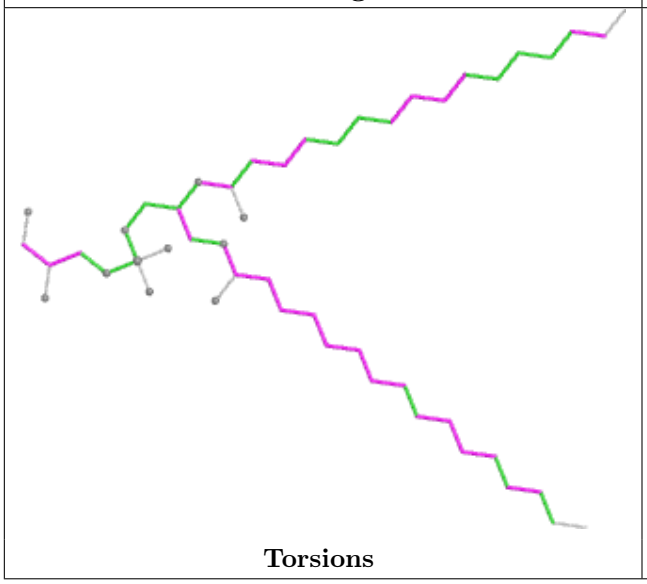
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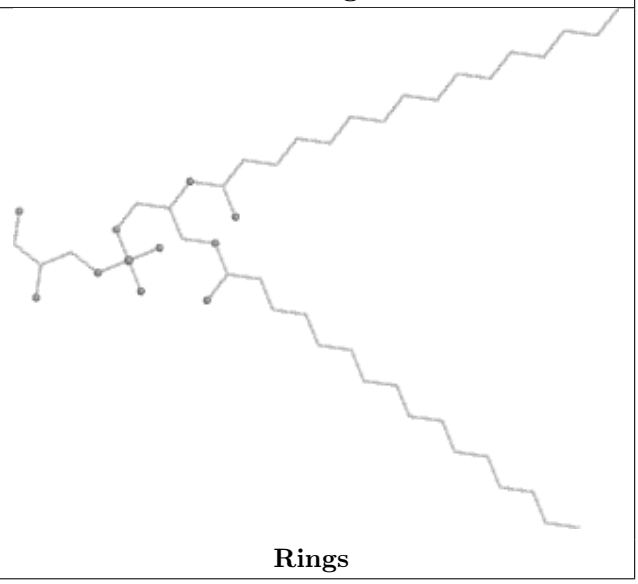
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Bond angles

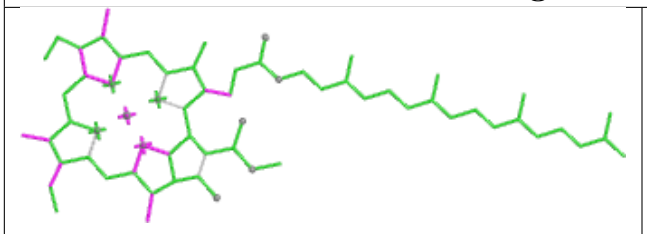


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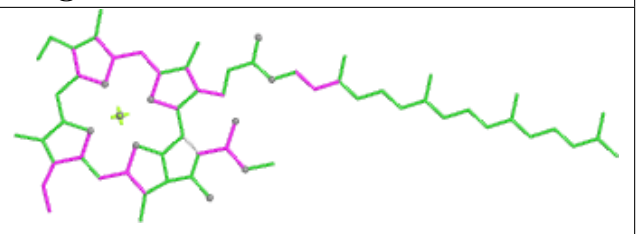


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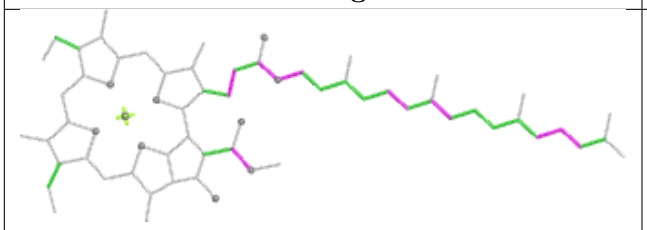
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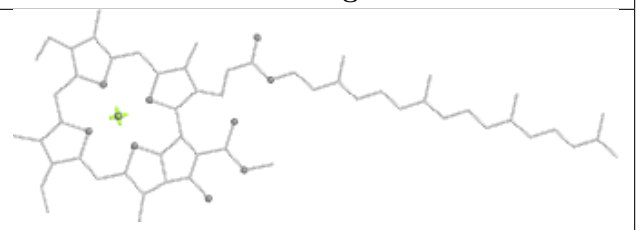
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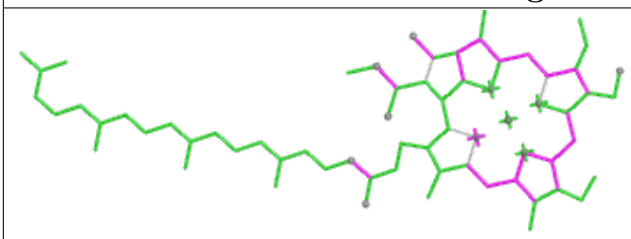


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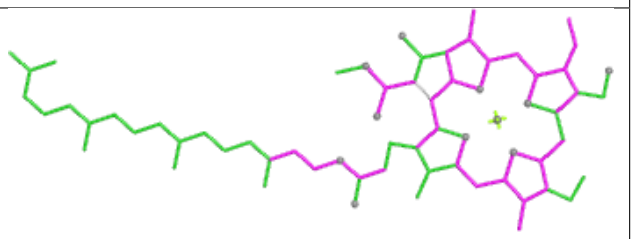


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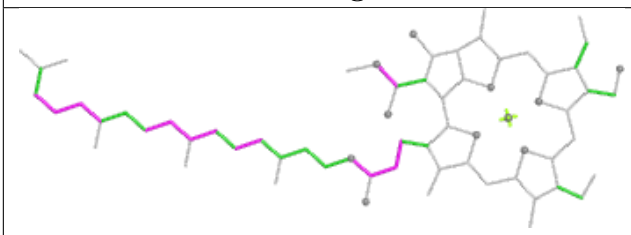
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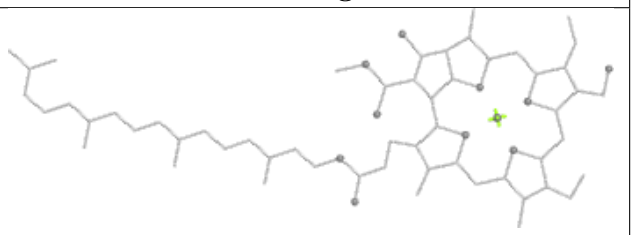
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Bond angles

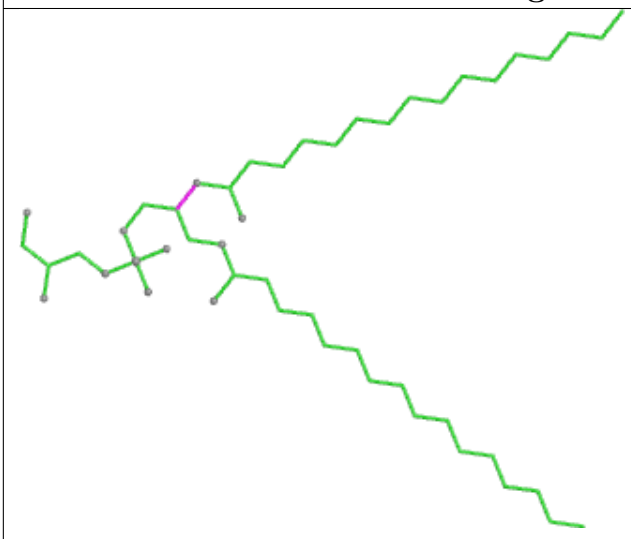


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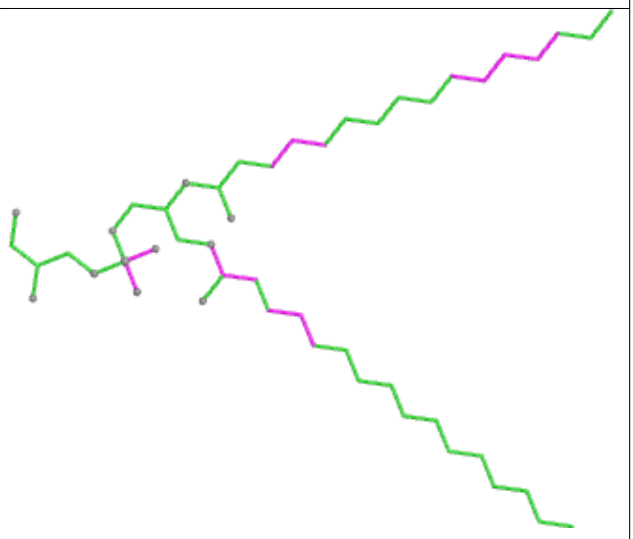


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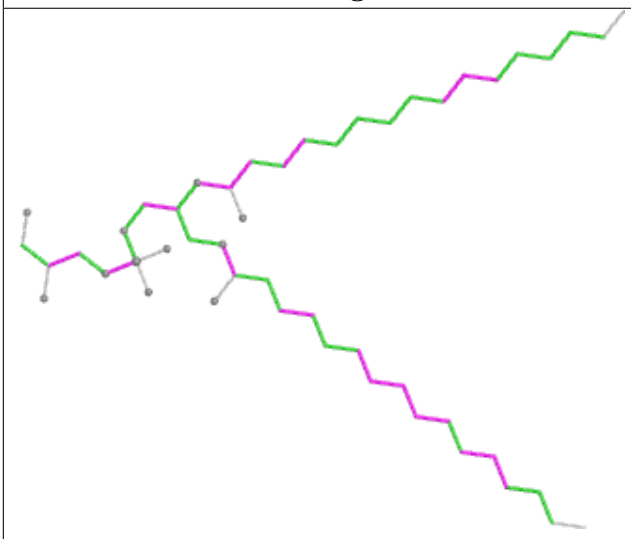
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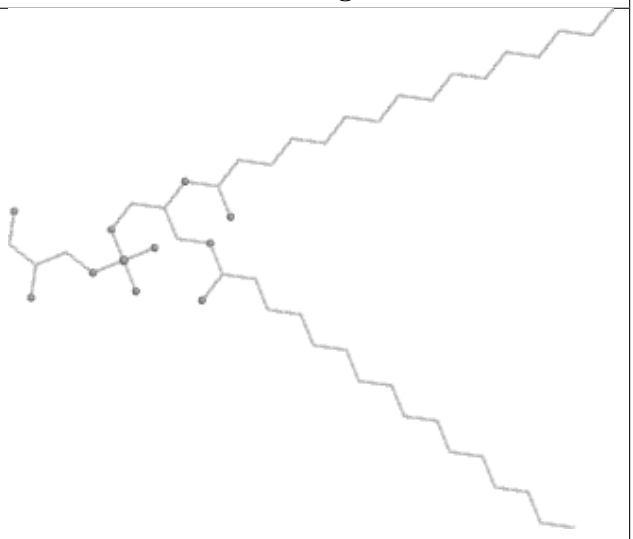
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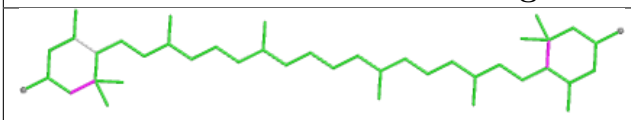


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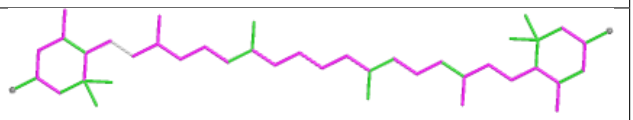


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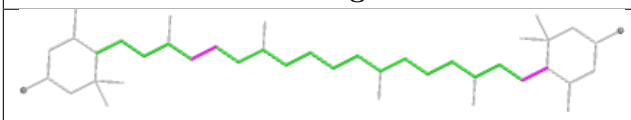
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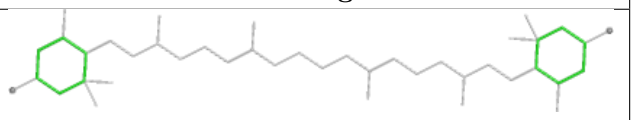
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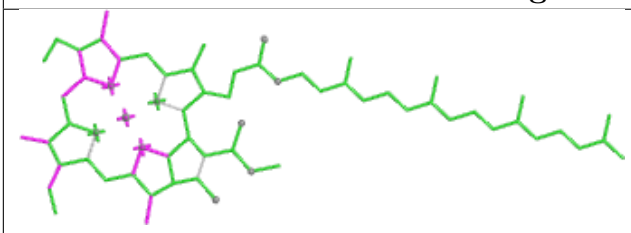


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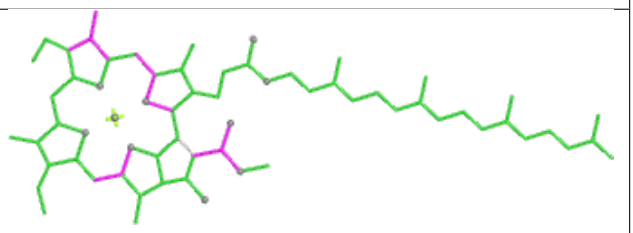


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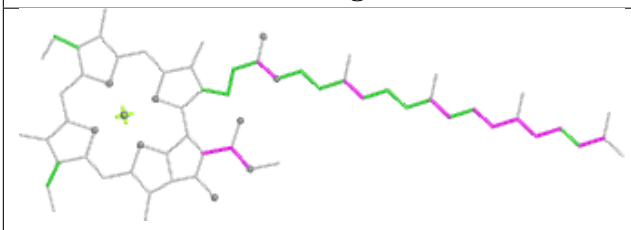
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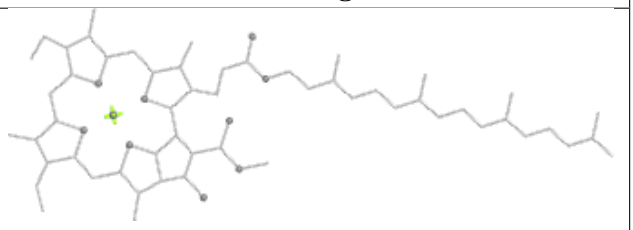
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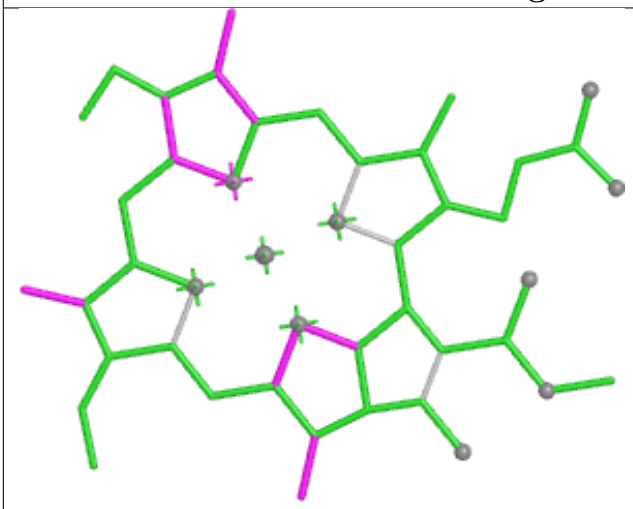


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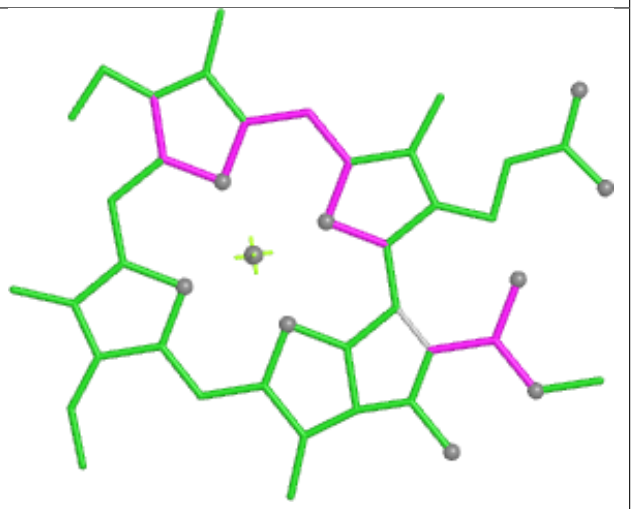


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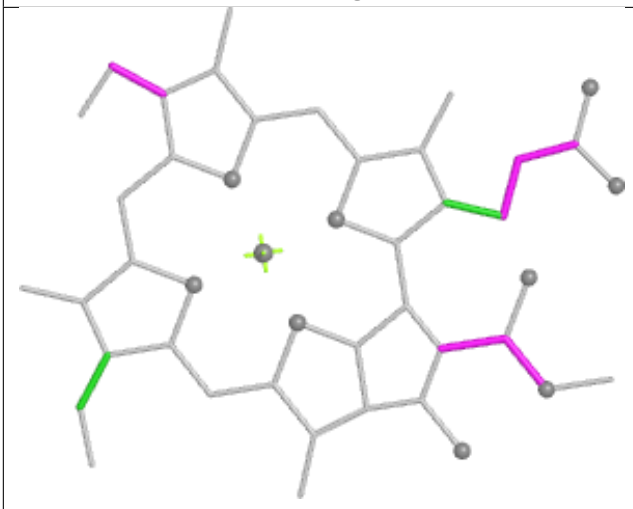
Ligand CLA 4 602



Bond lengths



Bond angles

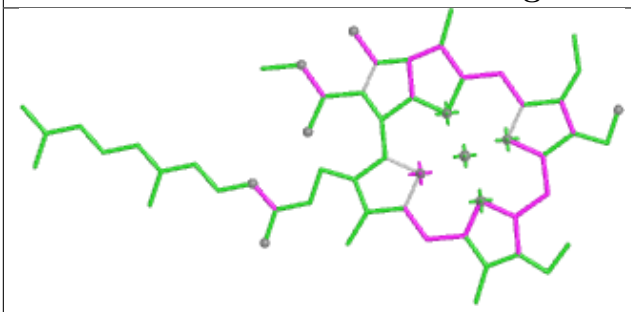


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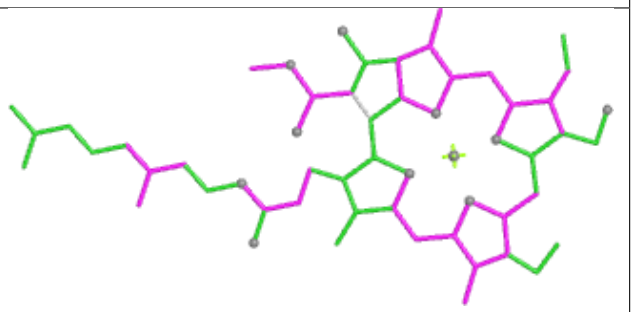


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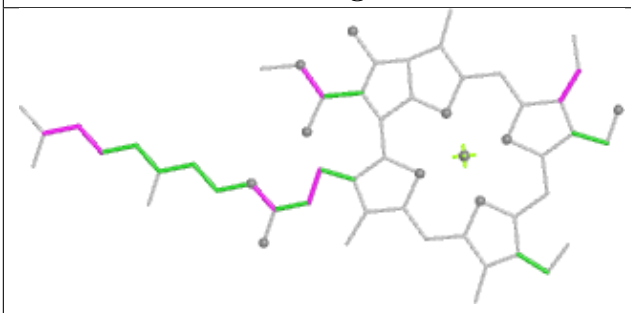
Ligand CHL R 607



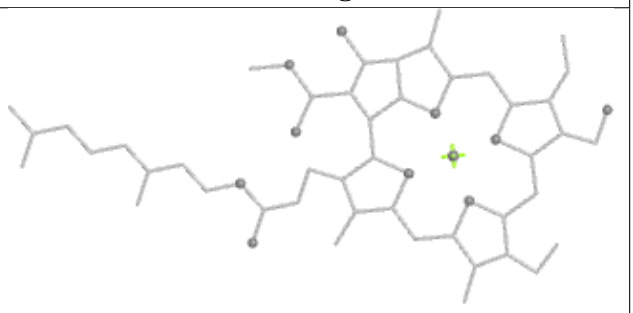
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Bond angles

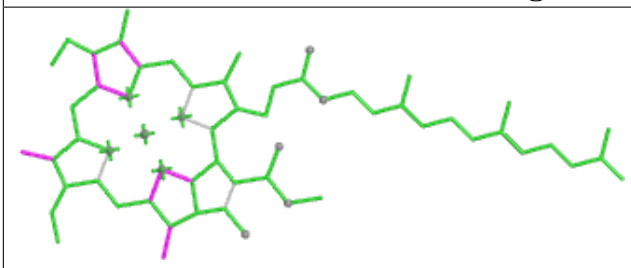


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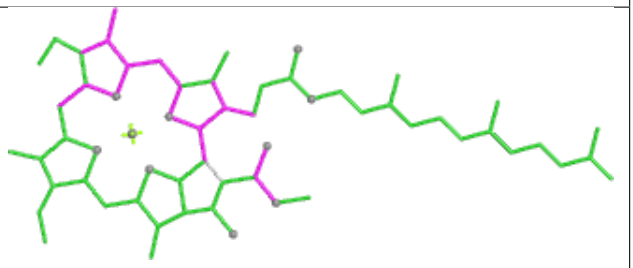


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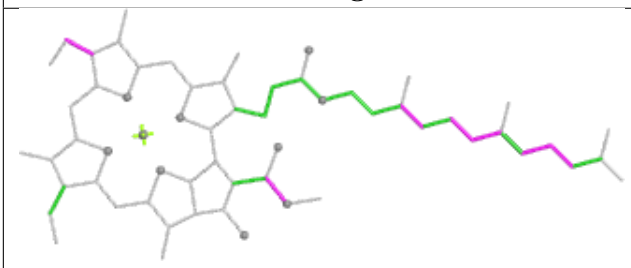
Ligand CLA n 612



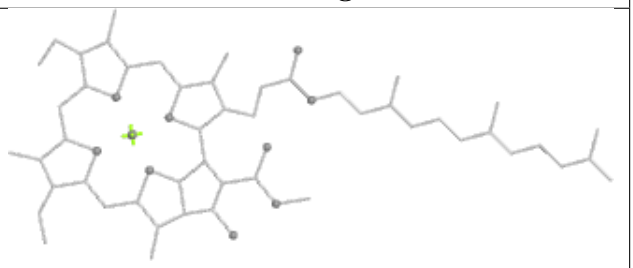
Bond lengths



Bond angles

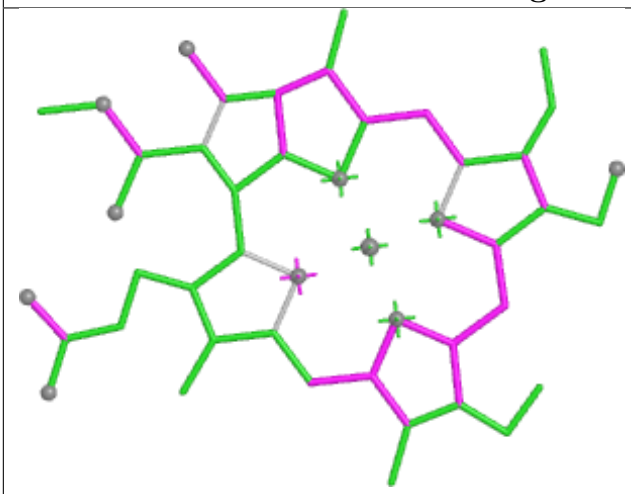


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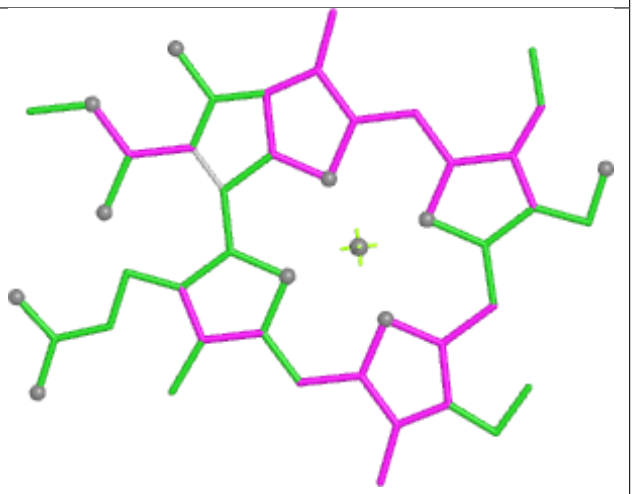


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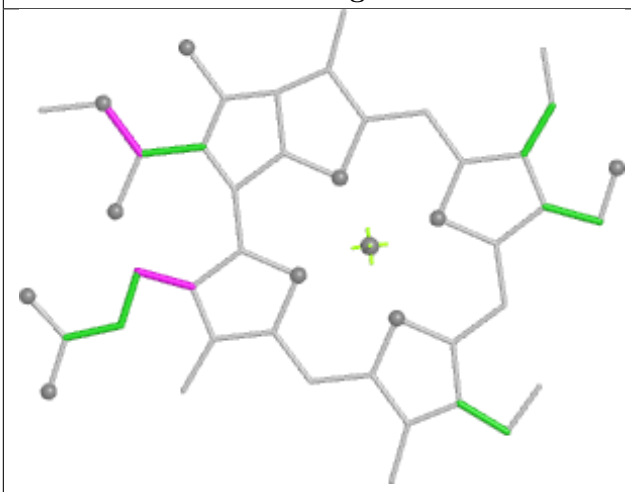
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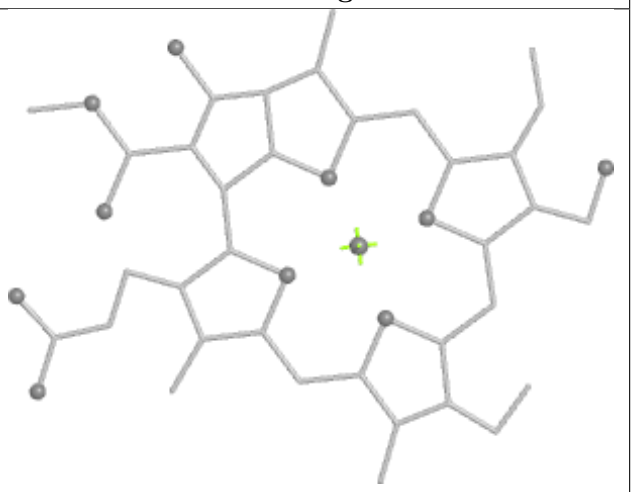
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Bond angles

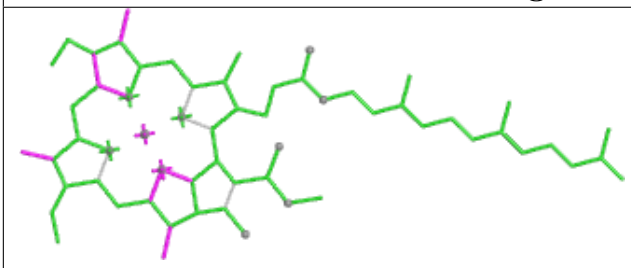


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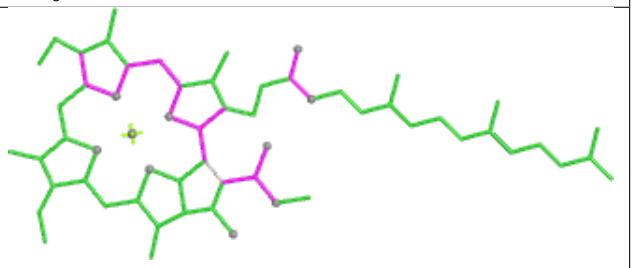


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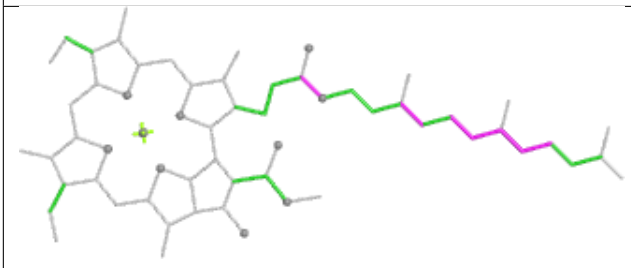
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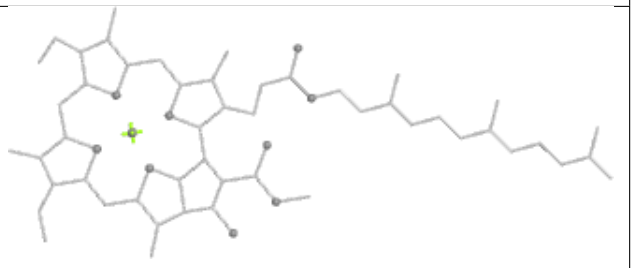
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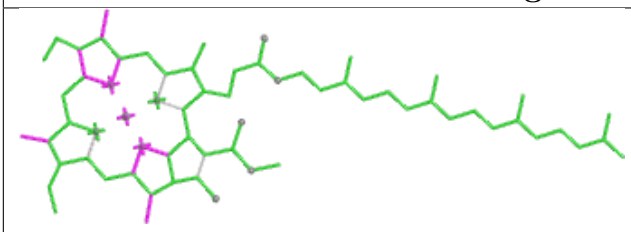
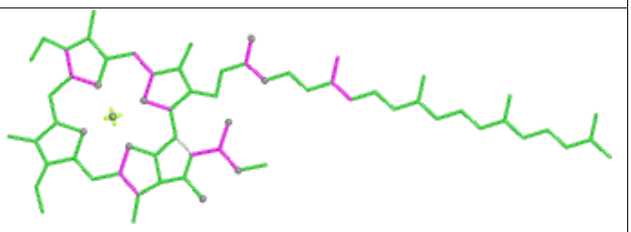
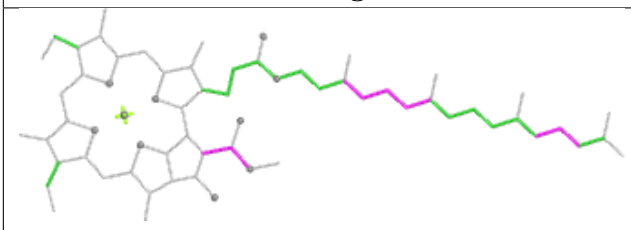
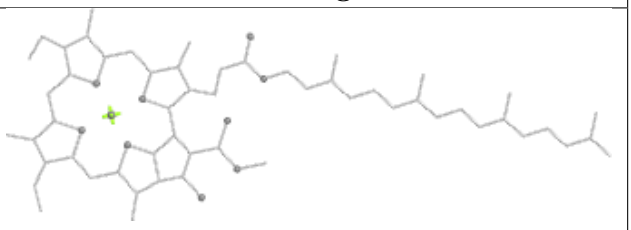
Bond angles

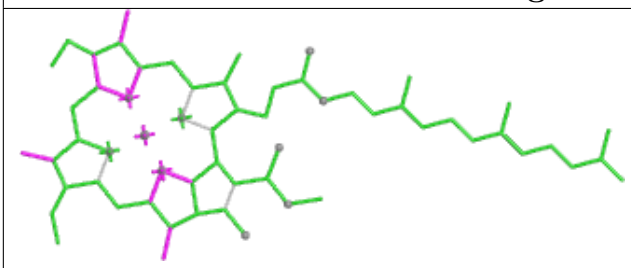
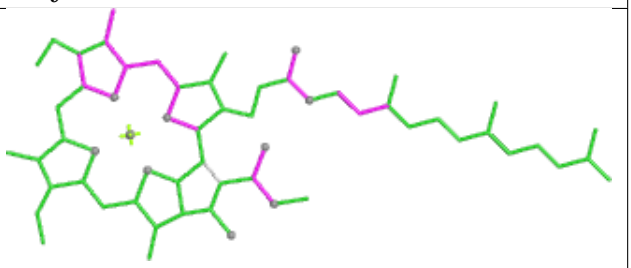
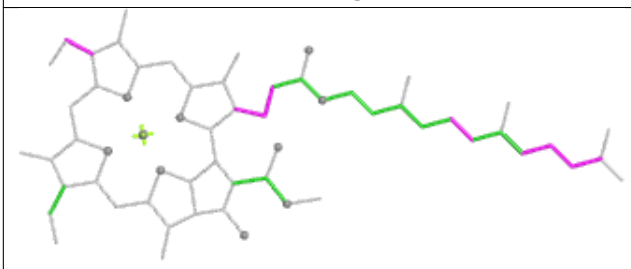
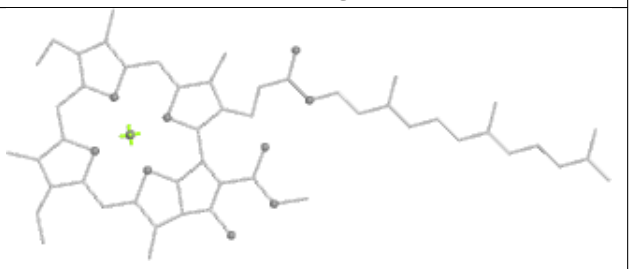


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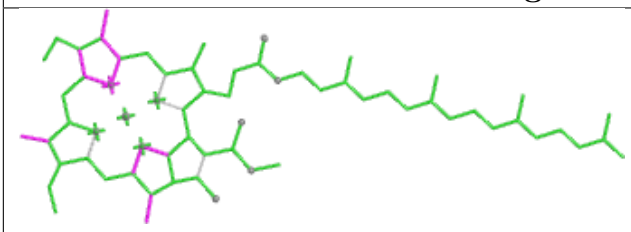


Rings

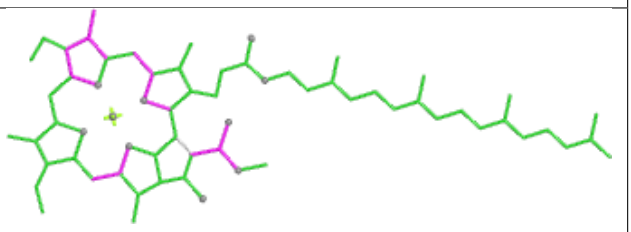
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 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA y 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

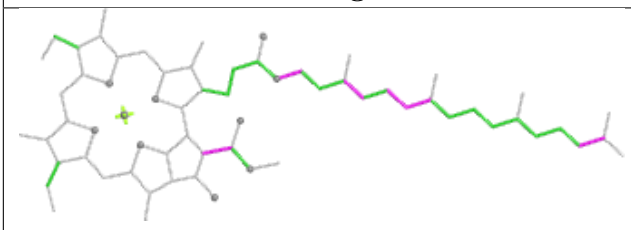
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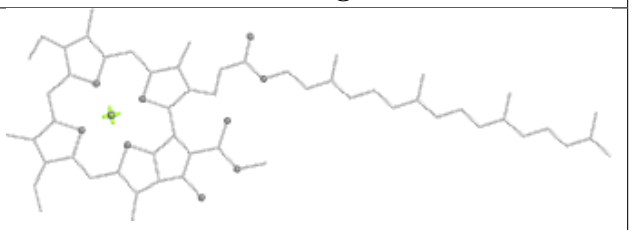
Bond lengths



Bond angles



Torsions

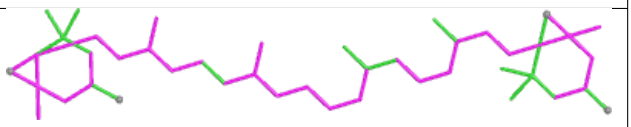


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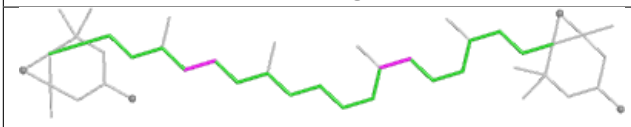
Ligand XAT N 1622



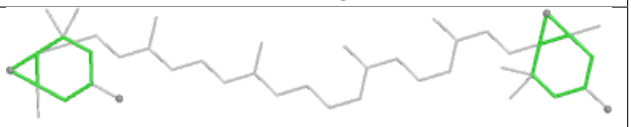
Bond lengths



Bond angles

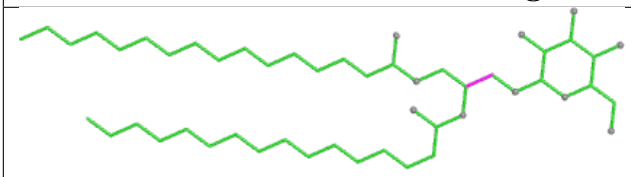


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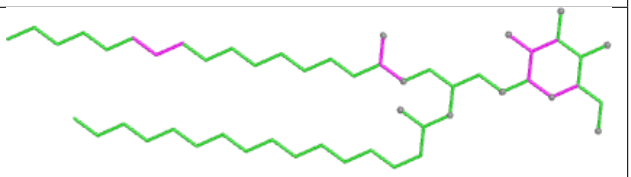


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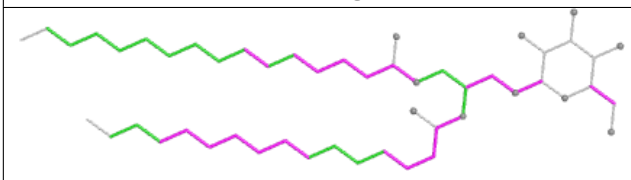
Ligand LMG z 101



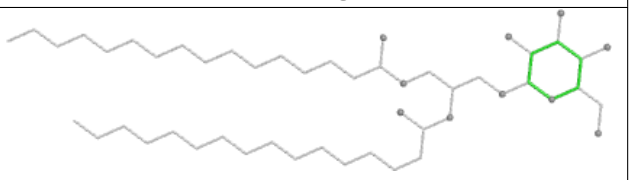
Bond lengths



Bond angles

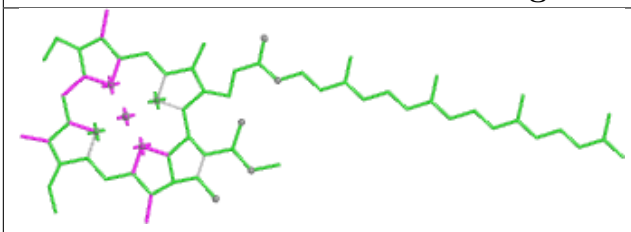


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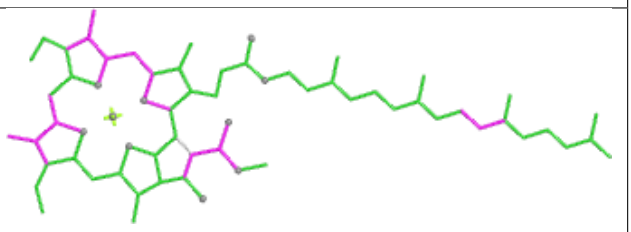


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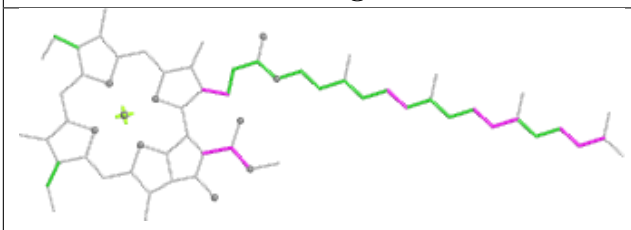
Ligand CLA c 508



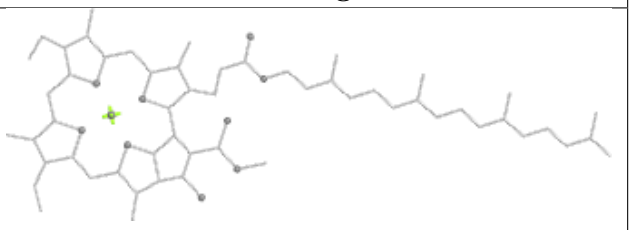
Bond lengths



Bond angles

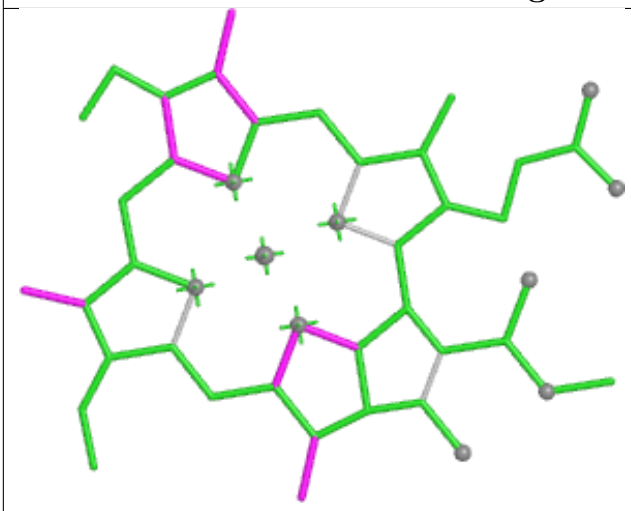


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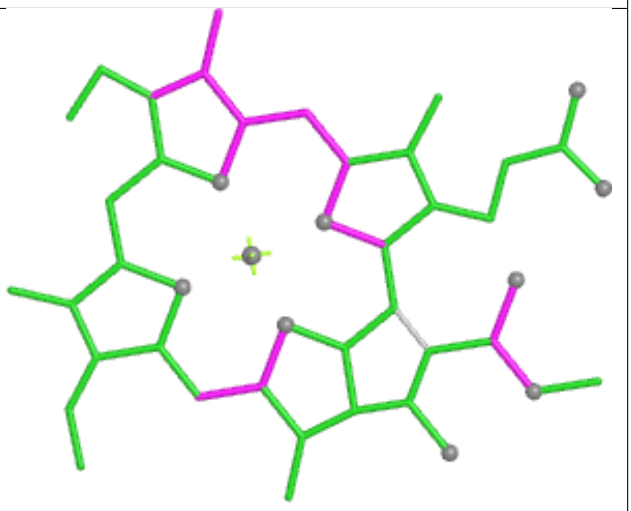


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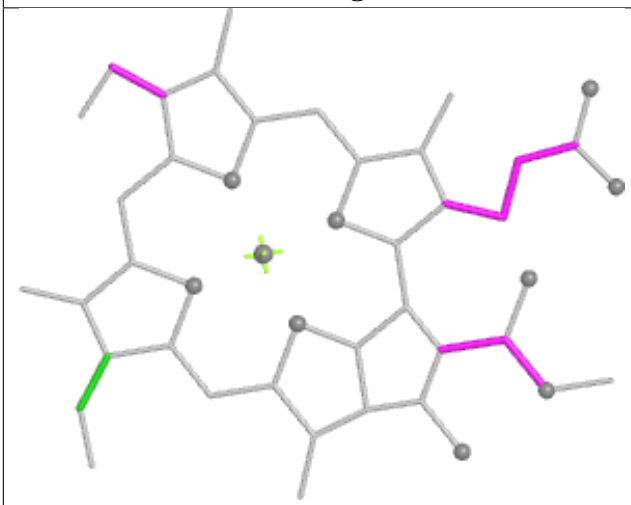
Ligand CLA 7 604



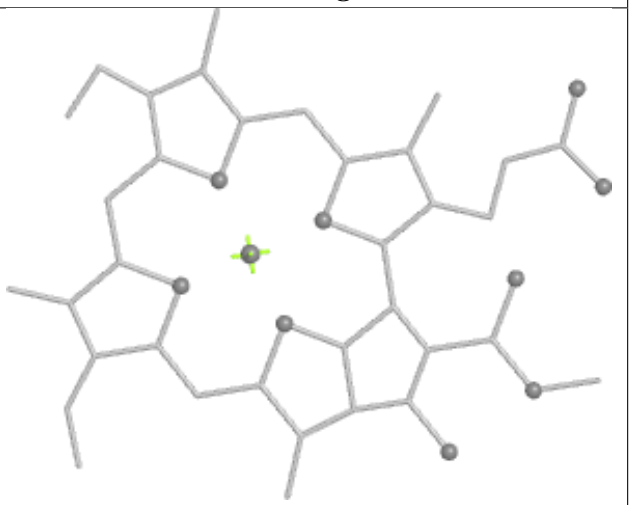
Bond lengths



Bond angles

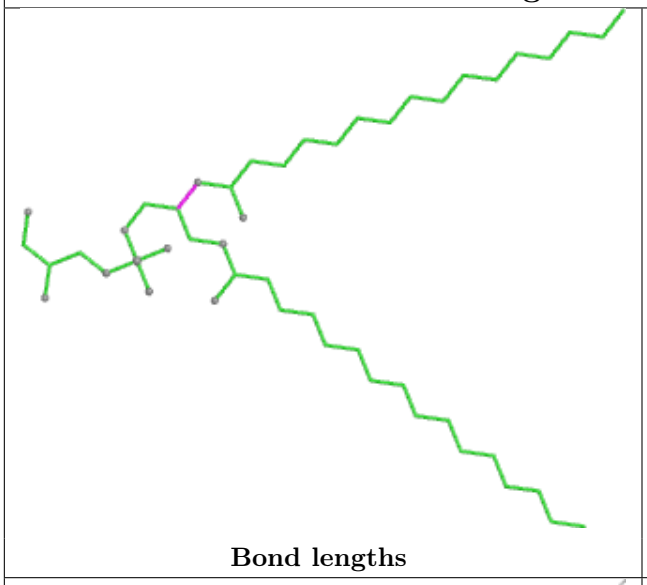


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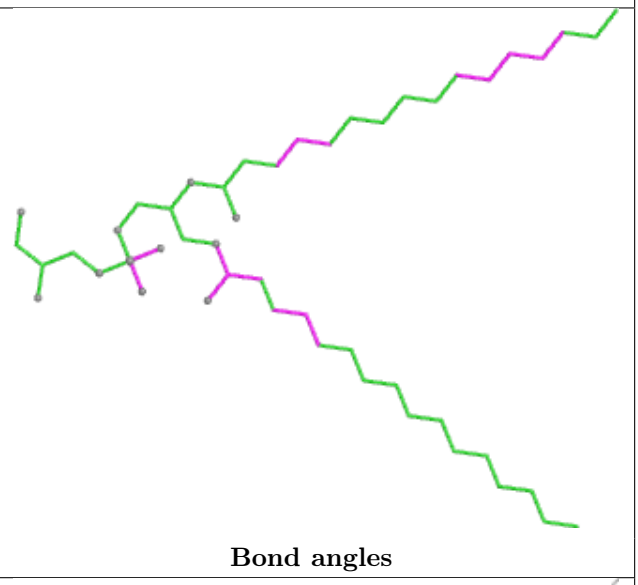


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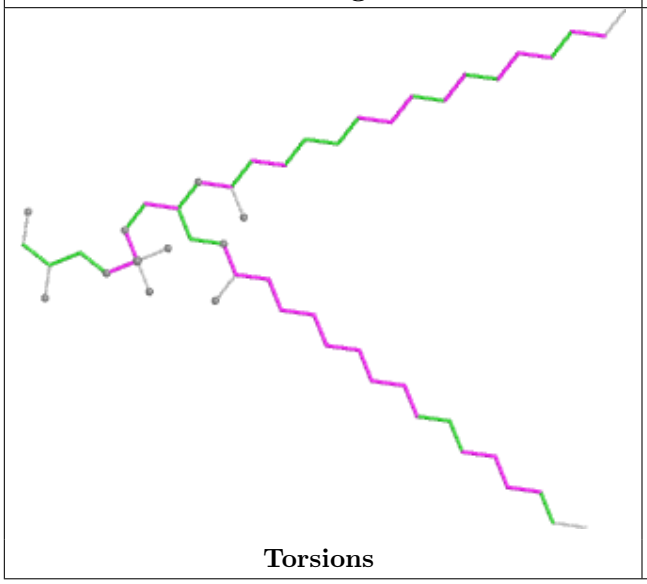
Ligand LHG D 409



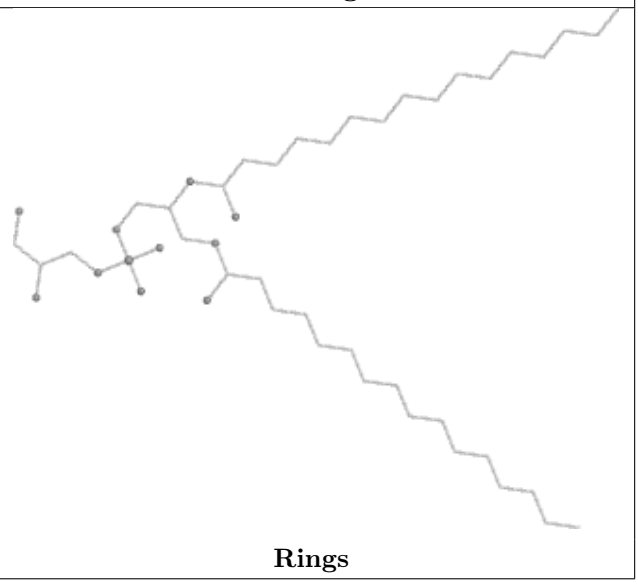
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Bond angles

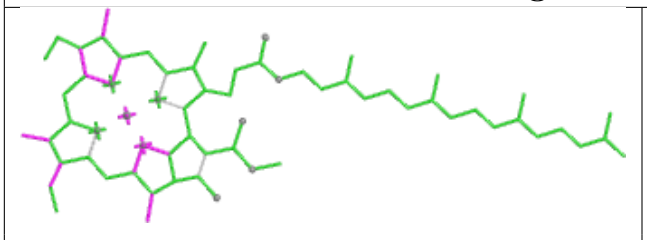


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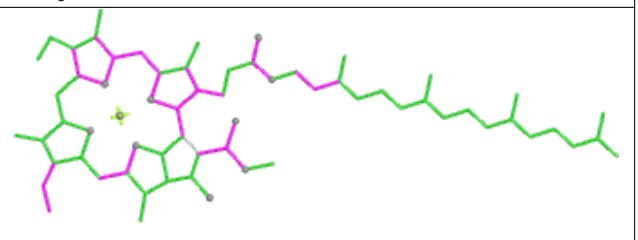


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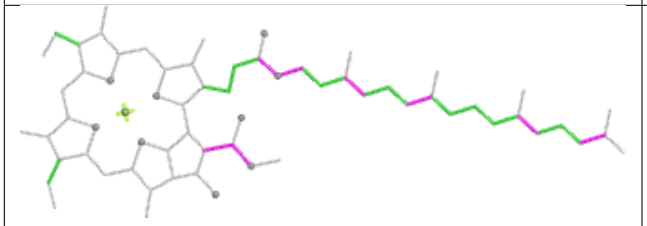
Ligand CLA y 603



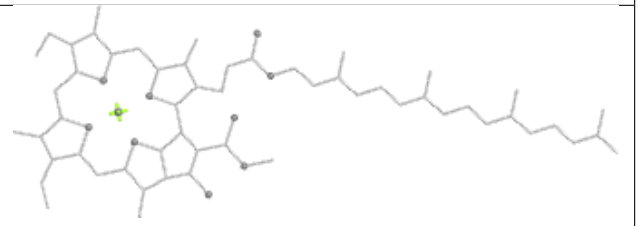
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Bond angles

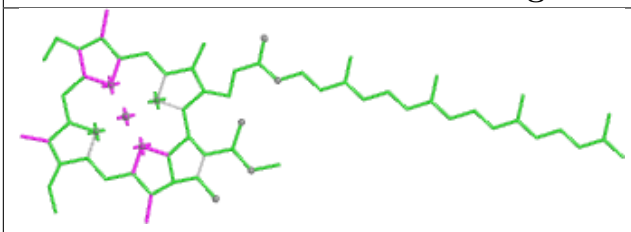


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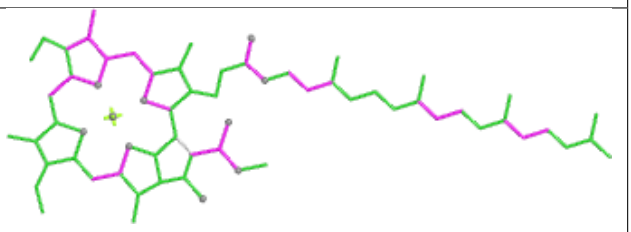


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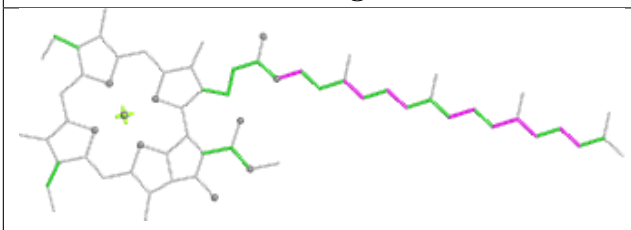
Ligand CLA b 609



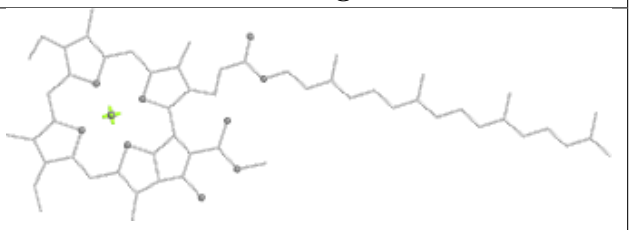
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Bond angles

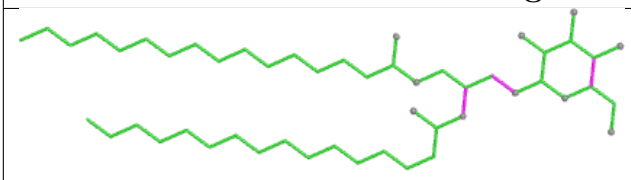


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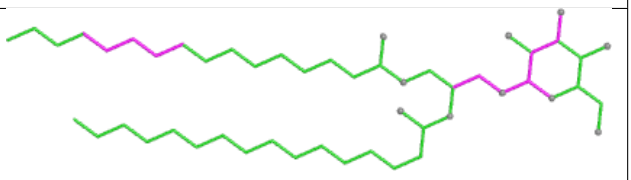


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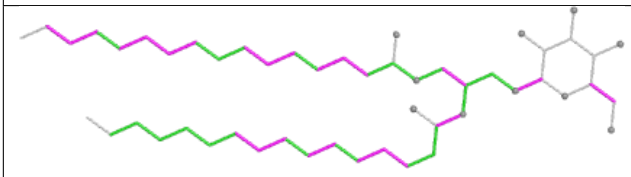
Ligand LMG c 521



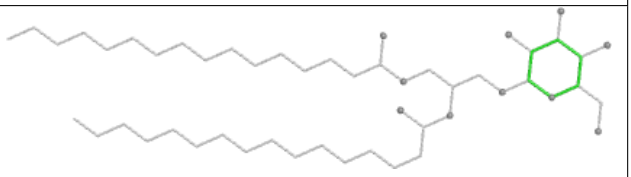
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Bond angles

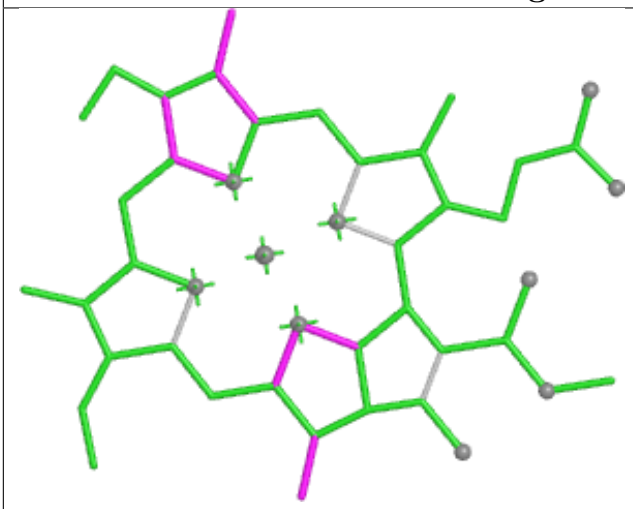


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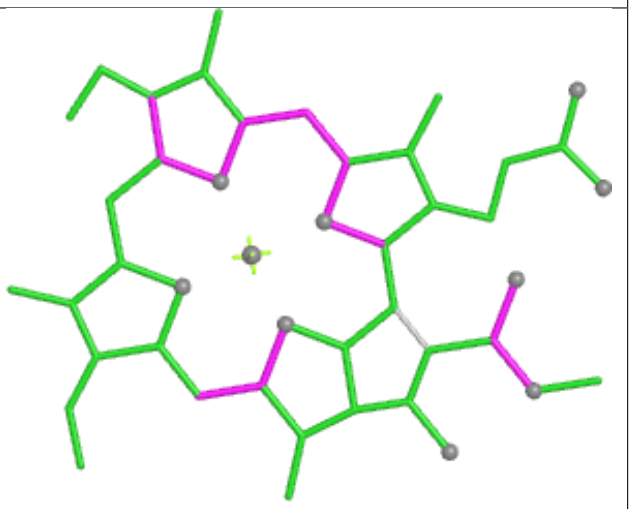


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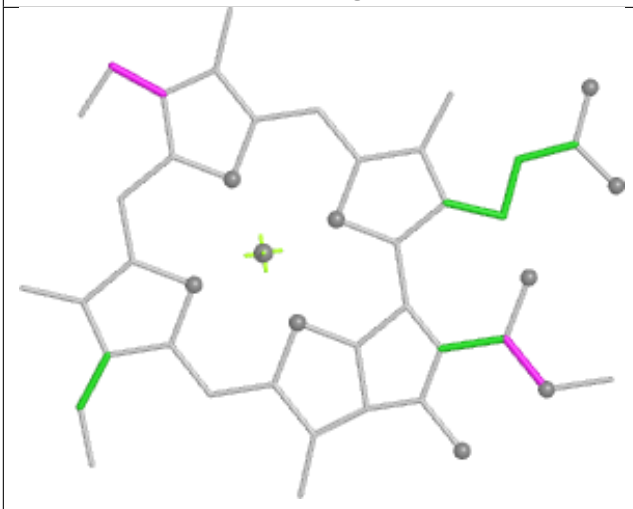
Ligand CLA 1 614



Bond lengths



Bond angles

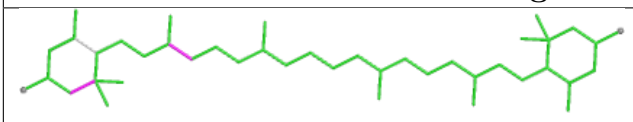


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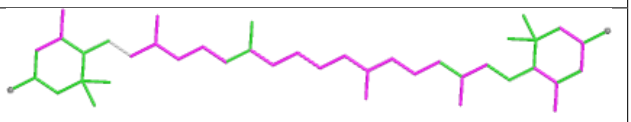


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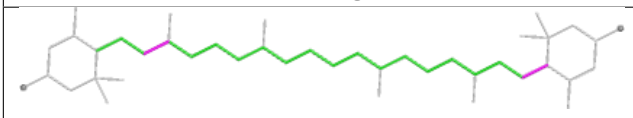
Ligand LUT r 620



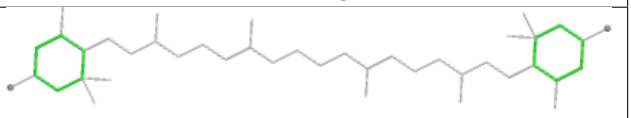
Bond lengths



Bond angles

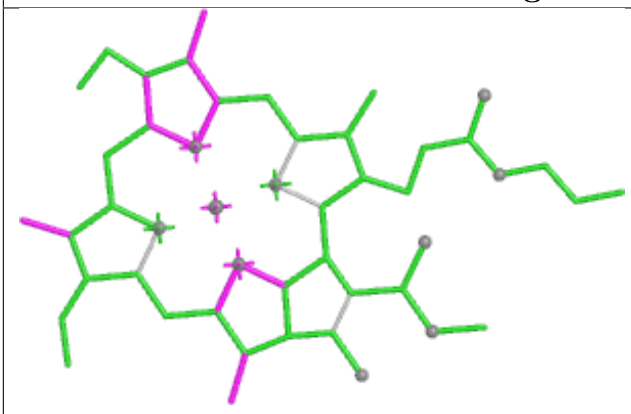


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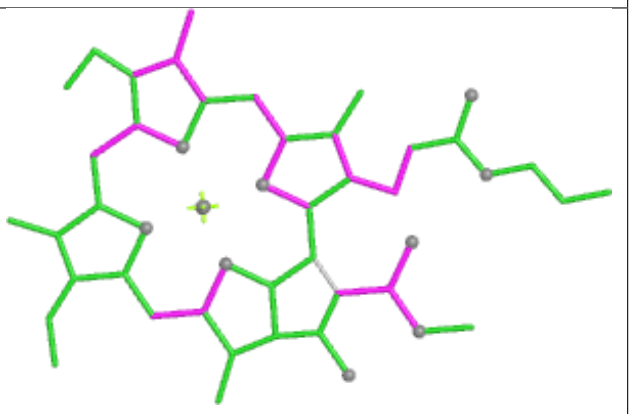


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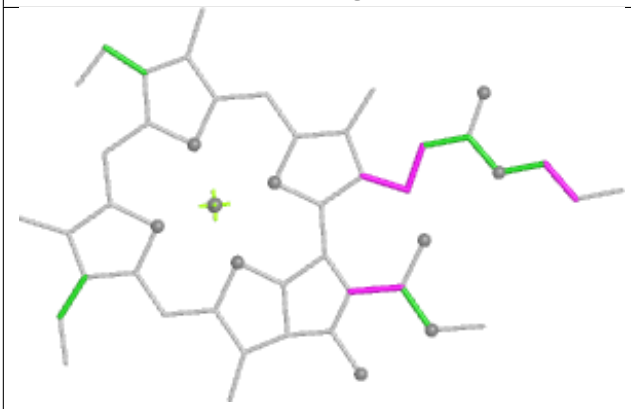
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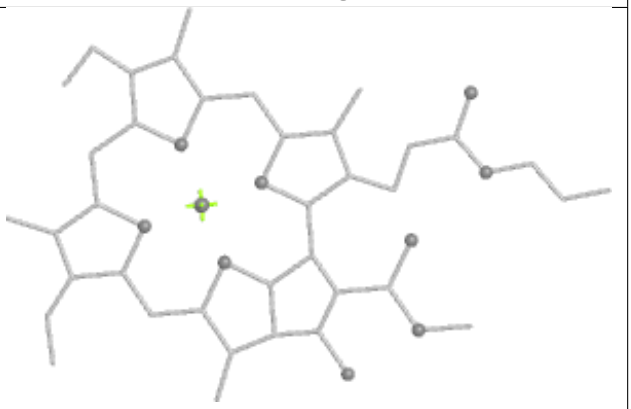
Bond lengths



Bond angles

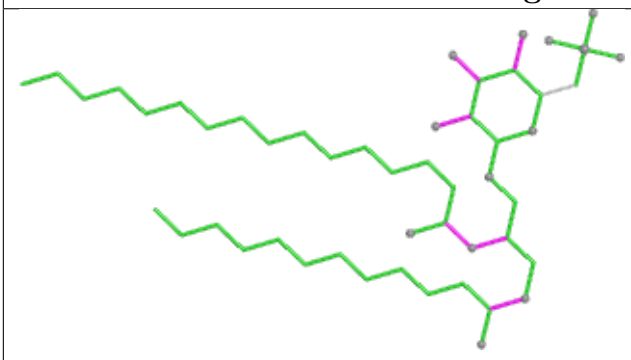


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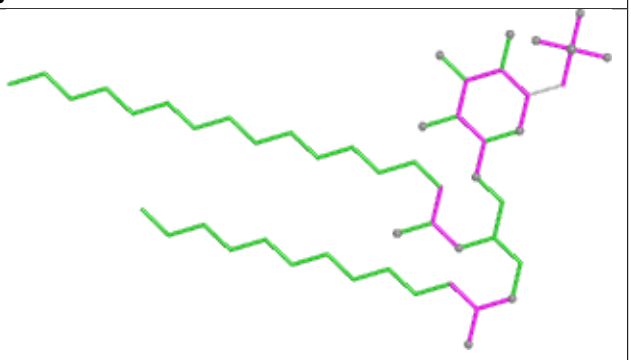


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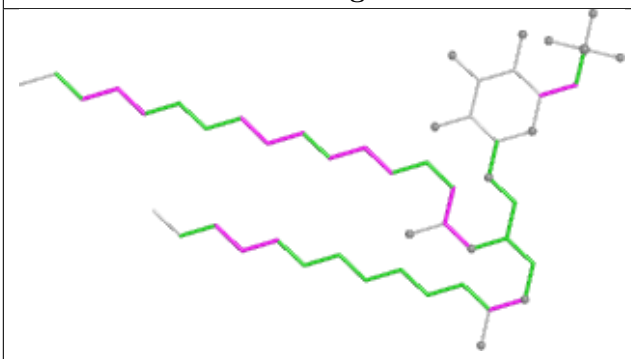
Ligand SQD A 412



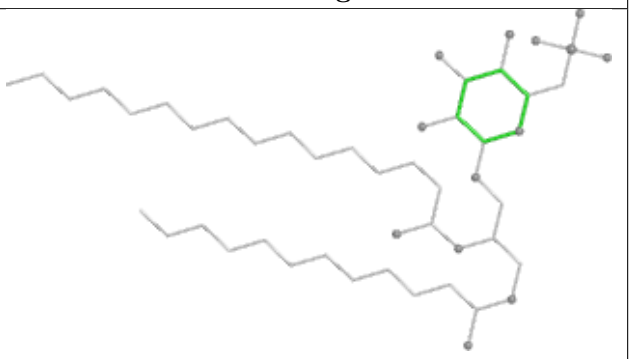
Bond lengths



Bond angles

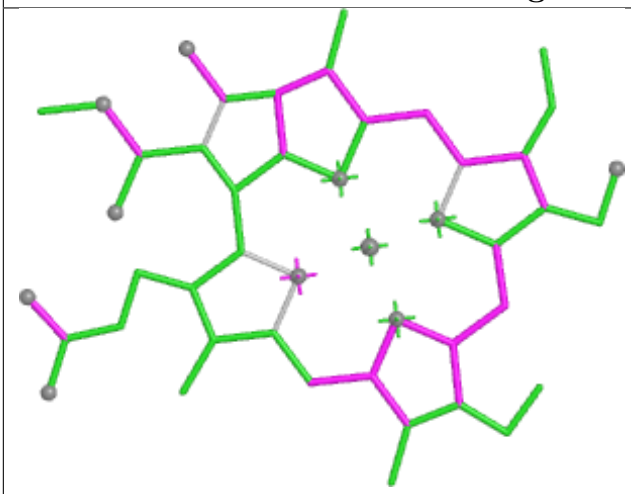


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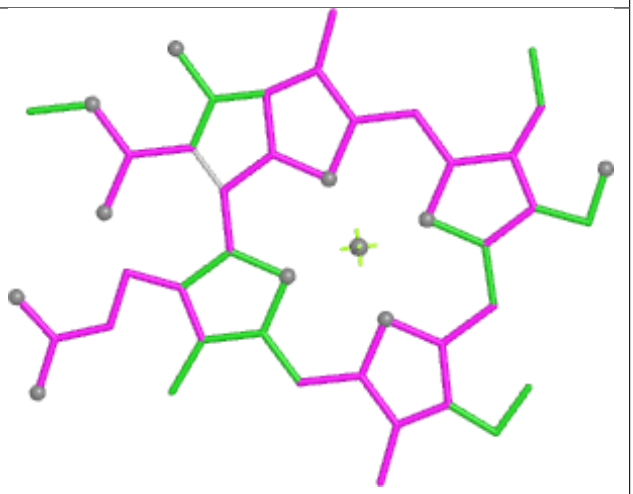


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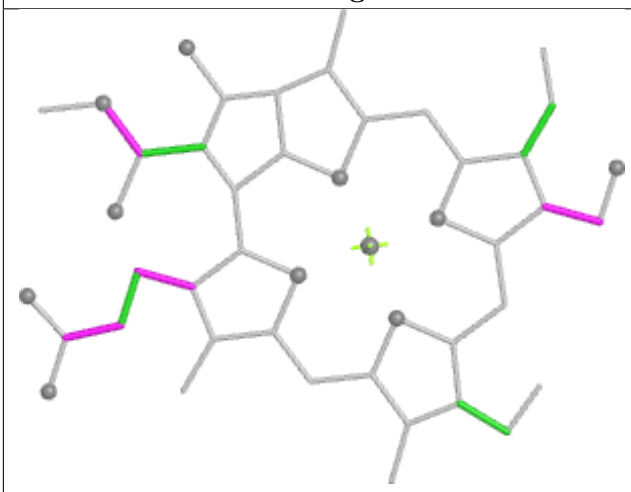
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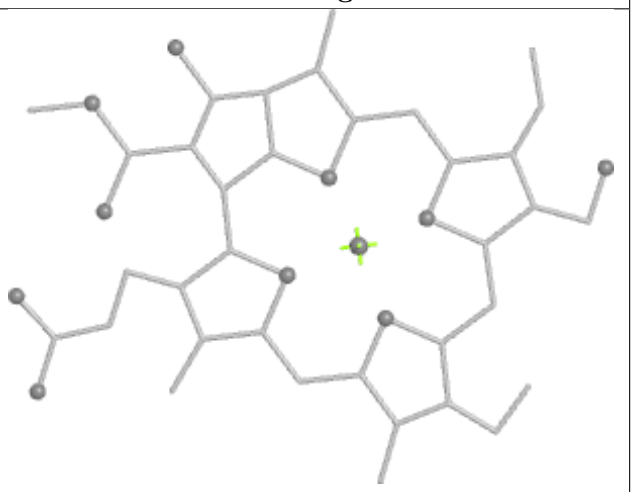
Bond lengths



Bond angles

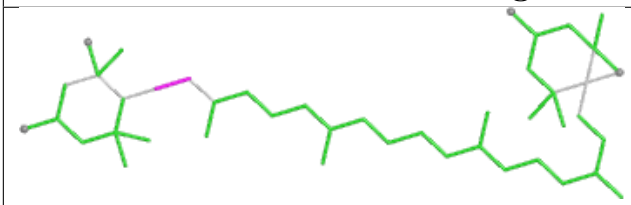


Torsions

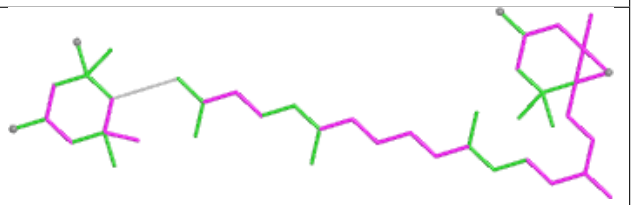


Rings

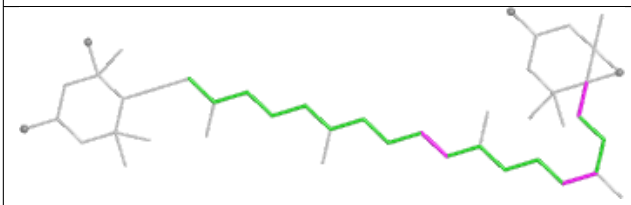
Ligand NEX N 1623



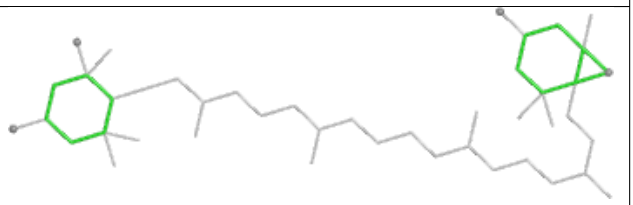
Bond lengths



Bond angles

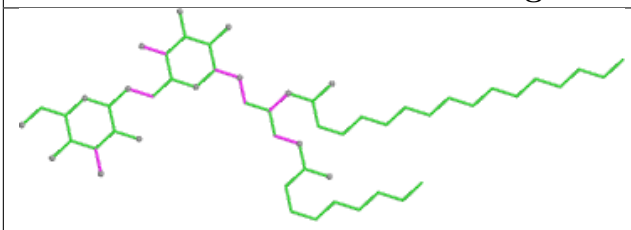


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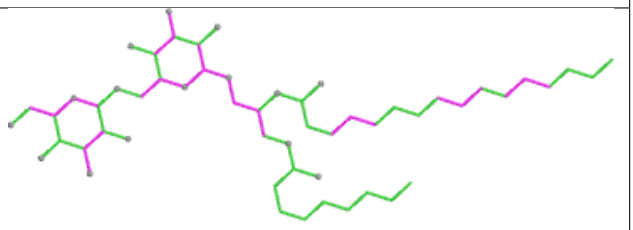


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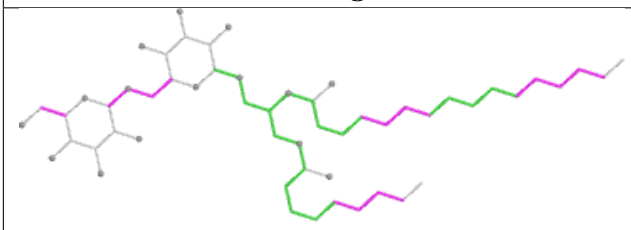
Ligand DGD c 518



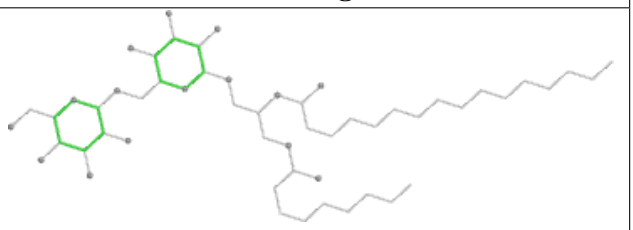
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Bond angles

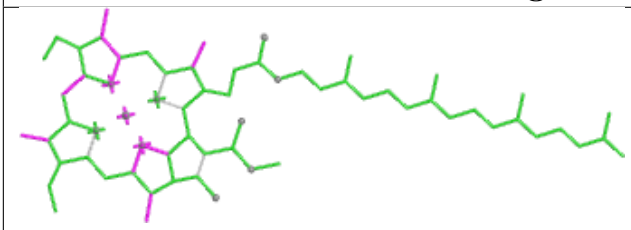


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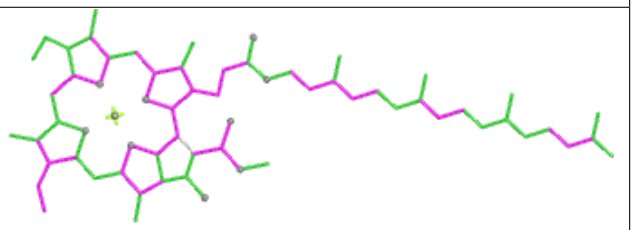


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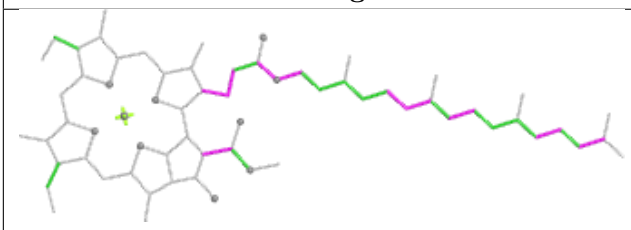
Ligand CLA b 605



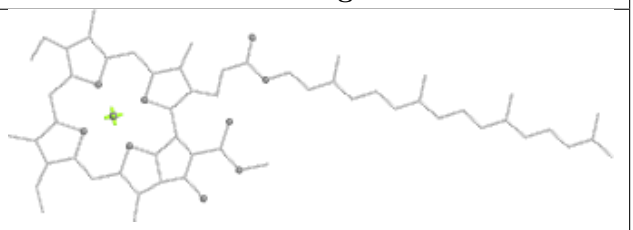
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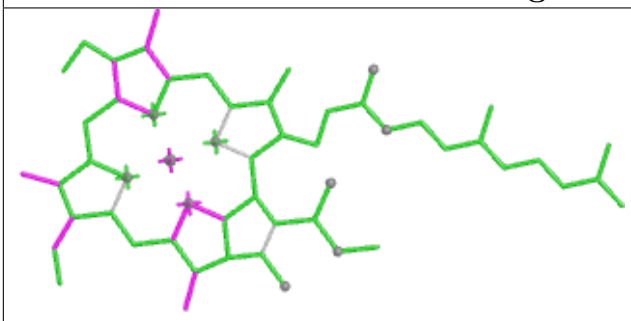
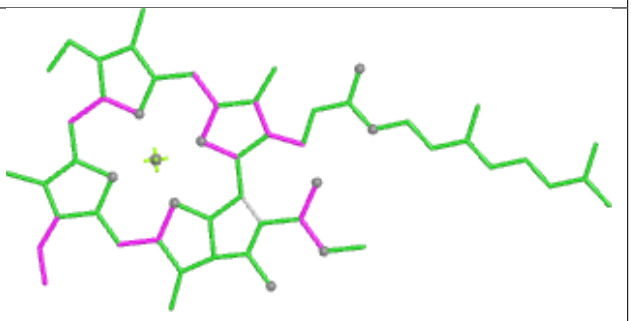
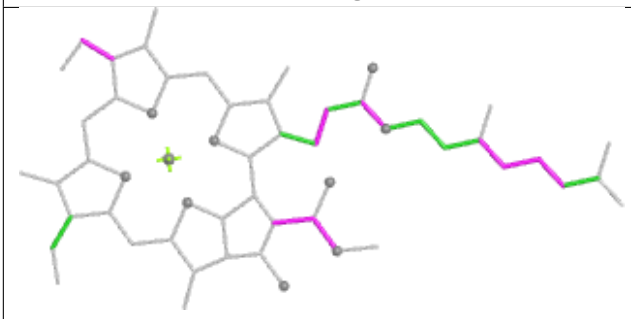
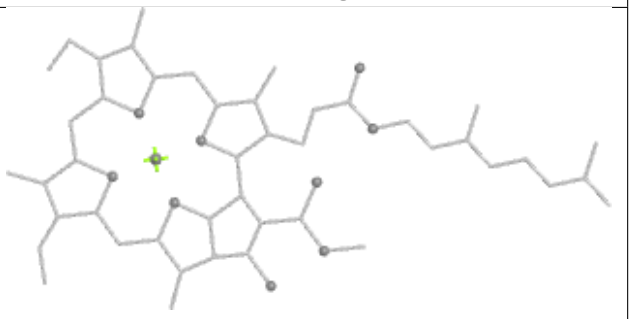
Bond angles



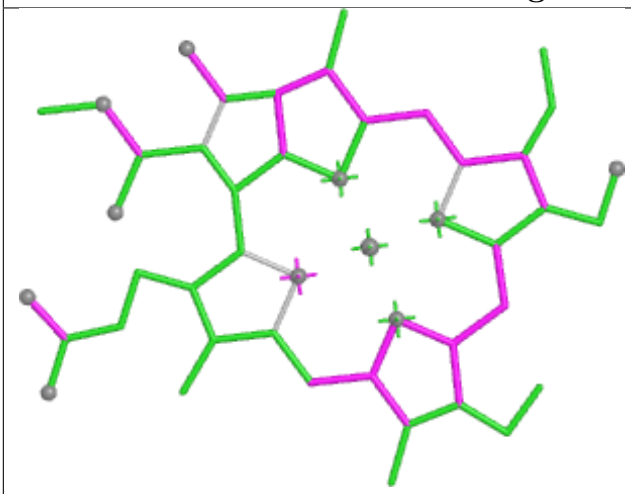
Torsions



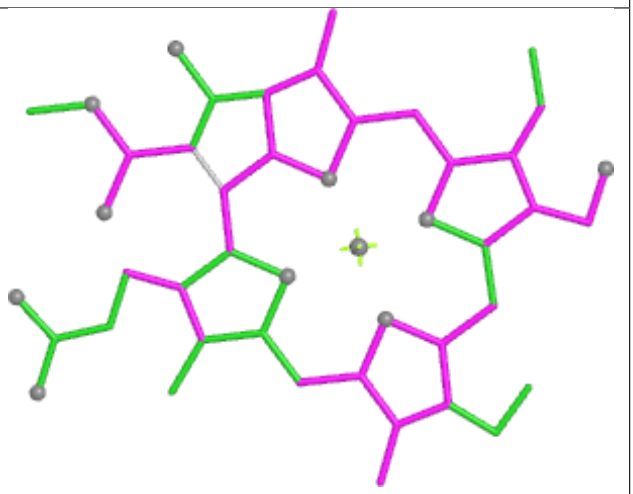
Rings

Ligand CLA 1 603	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

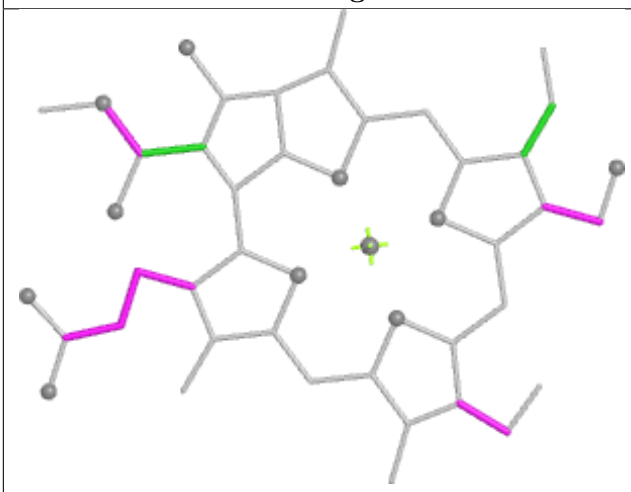
Ligand CHL 7 605



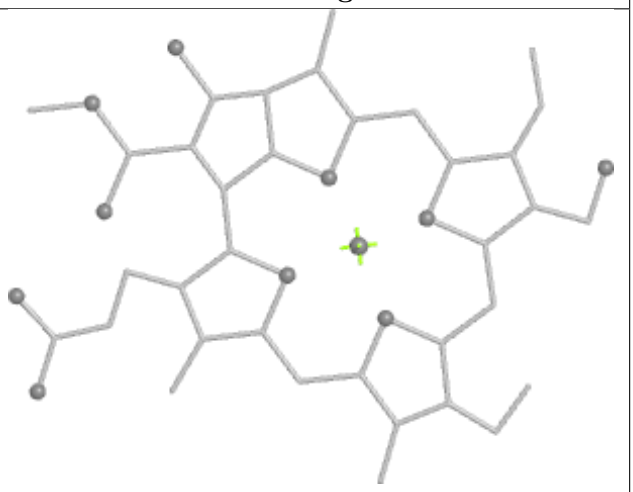
Bond lengths



Bond angles



Torsions

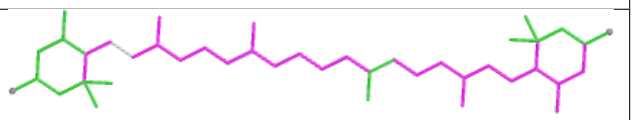


Rings

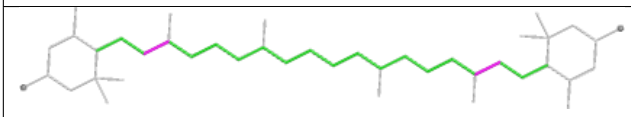
Ligand LUT 8 620



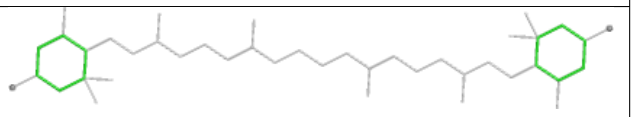
Bond lengths



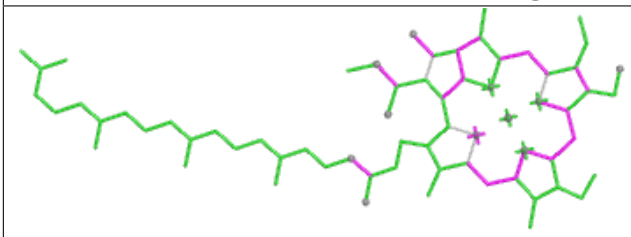
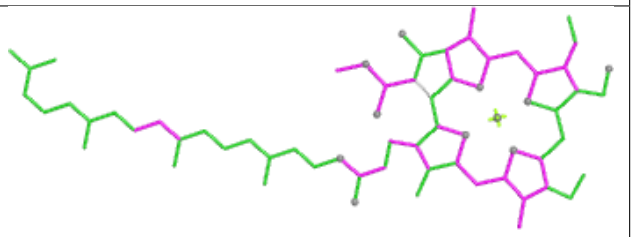
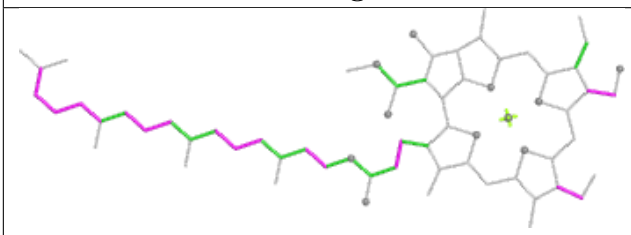
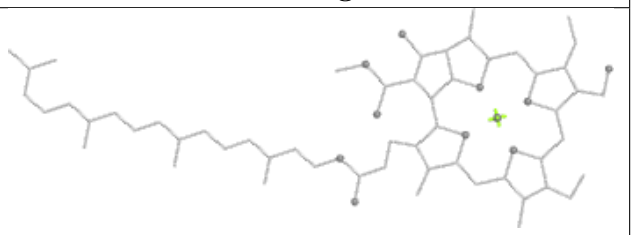
Bond angles

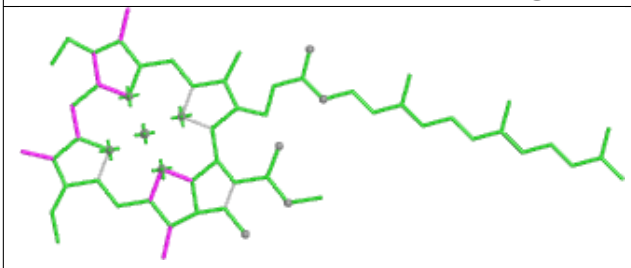
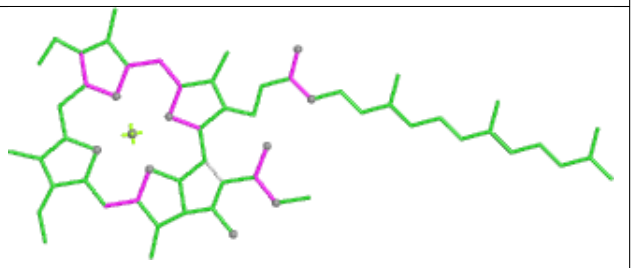
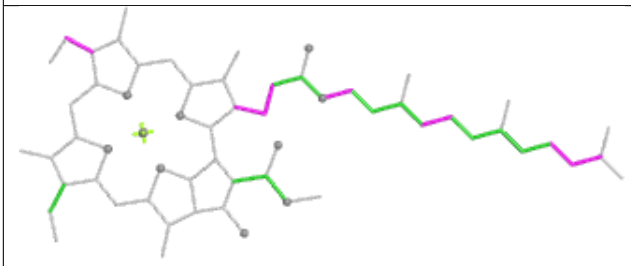
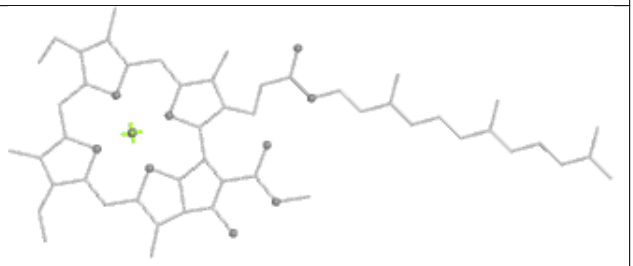


Torsions

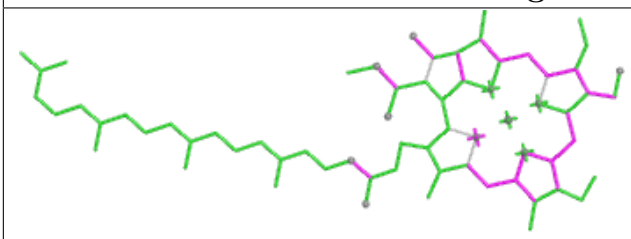


Rings

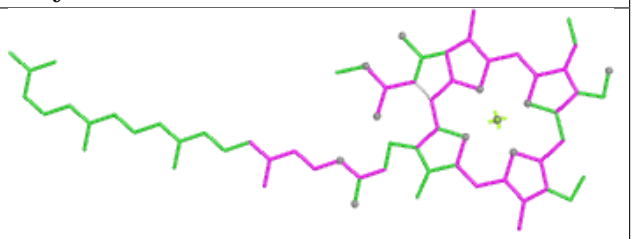
Ligand CHL n 607	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 3 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

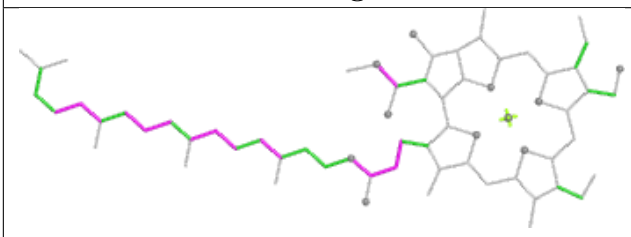
Ligand CHL y 601



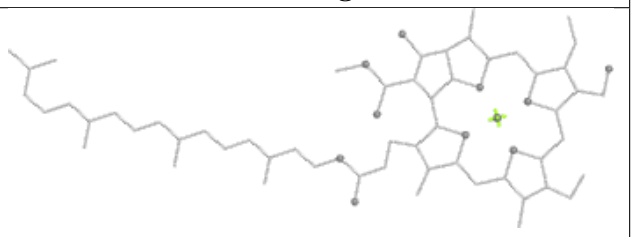
Bond lengths



Bond angles

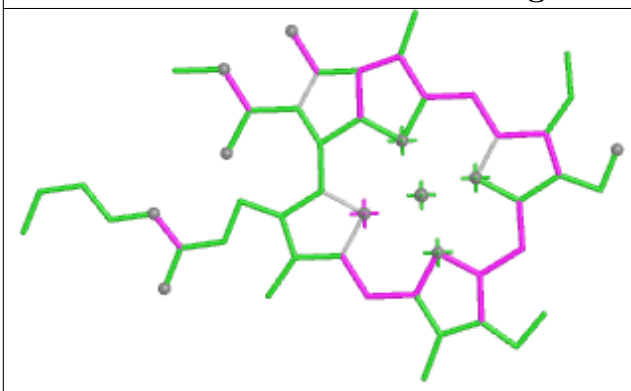


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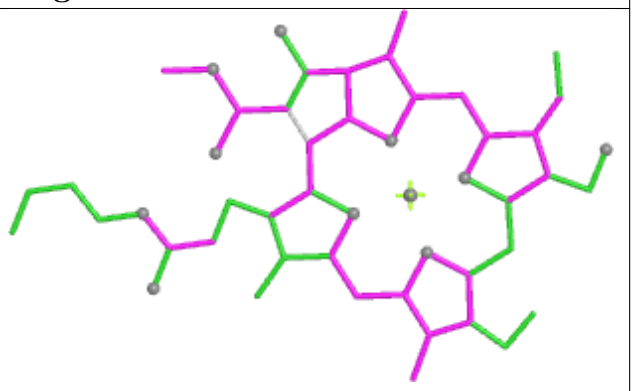


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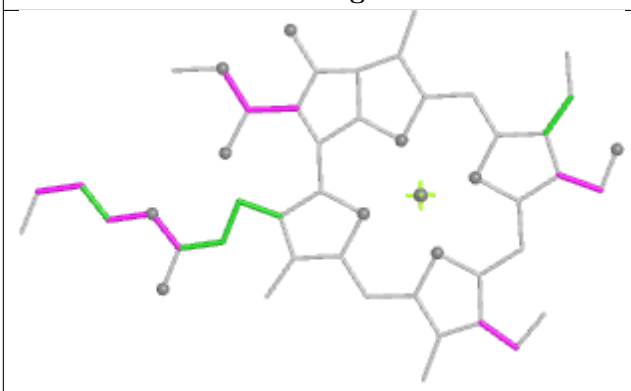
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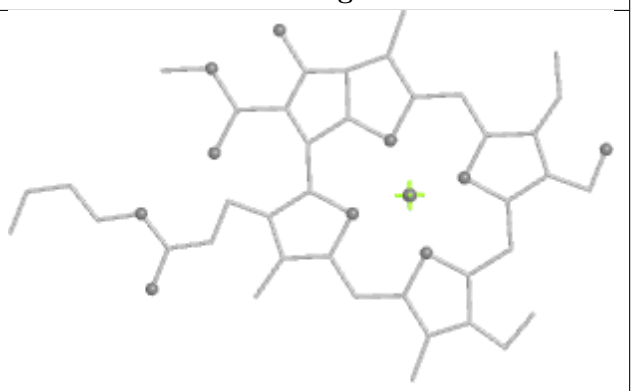
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Bond angles

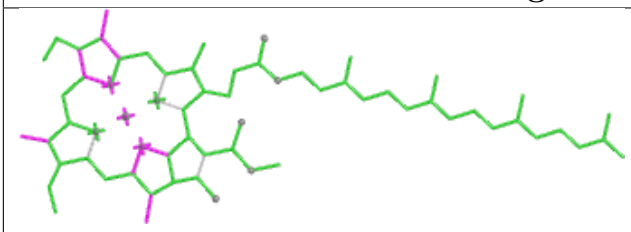


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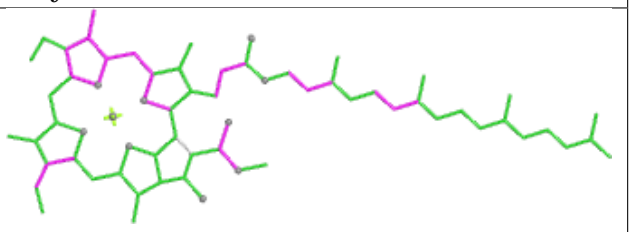


Rings

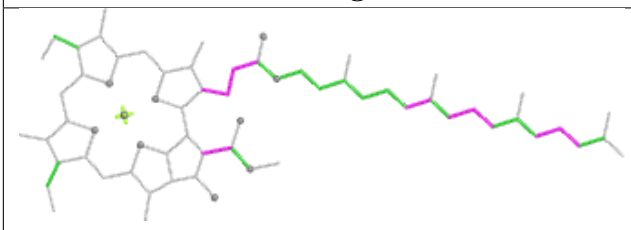
Ligand CLA y 602



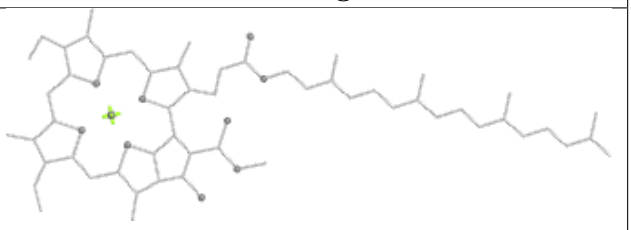
Bond lengths



Bond angles

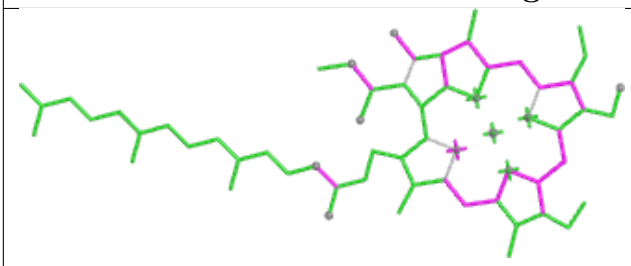


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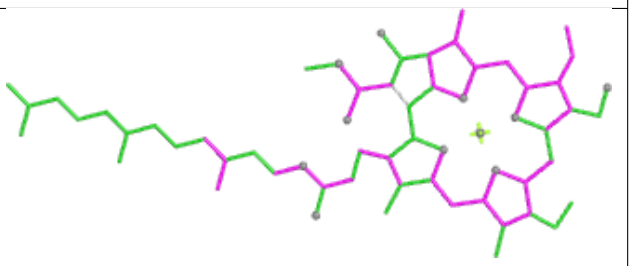


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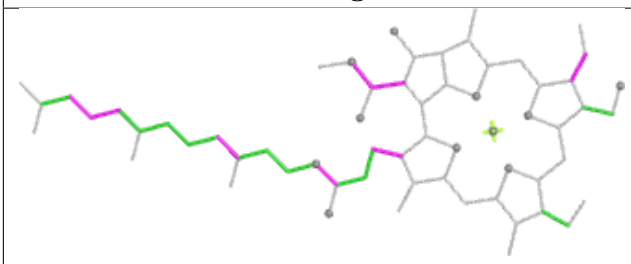
Ligand CHL G 609



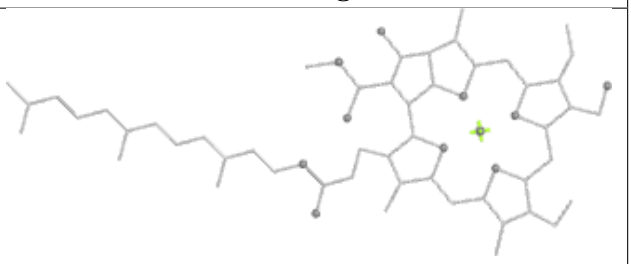
Bond lengths



Bond angles

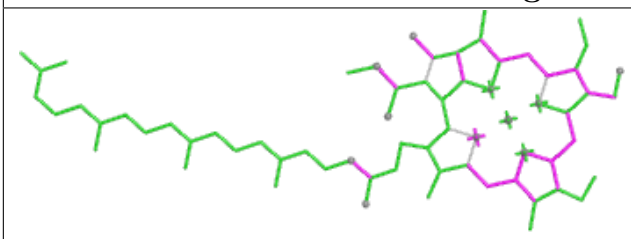


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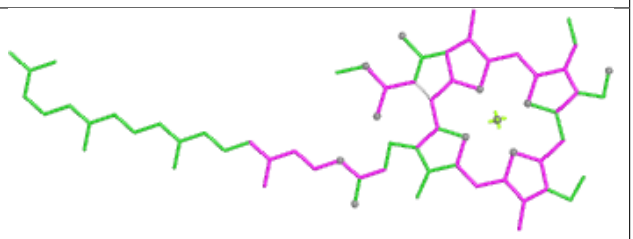


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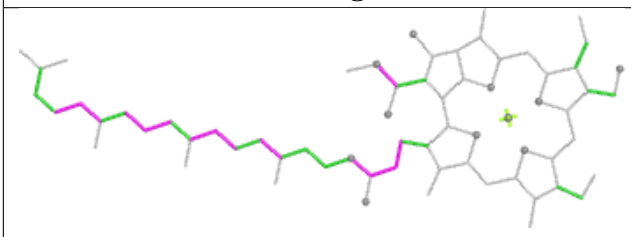
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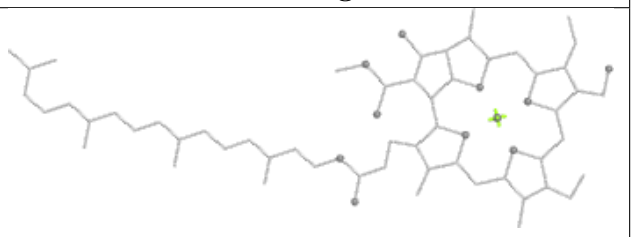
Bond lengths



Bond angles

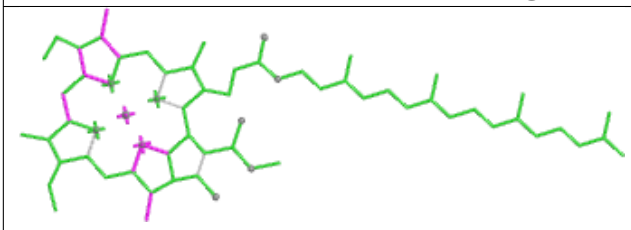


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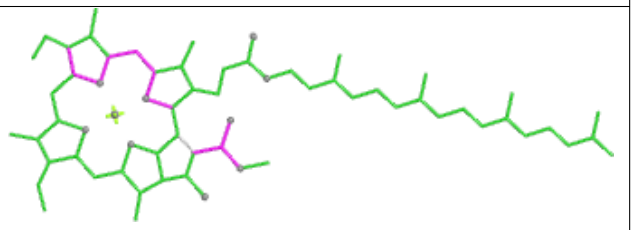


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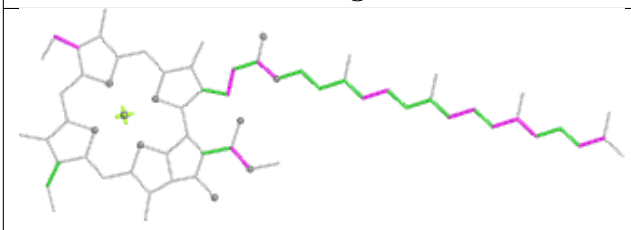
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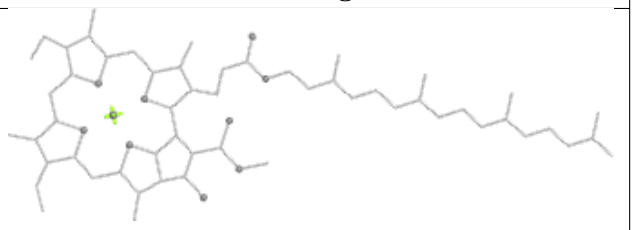
Bond lengths



Bond angles

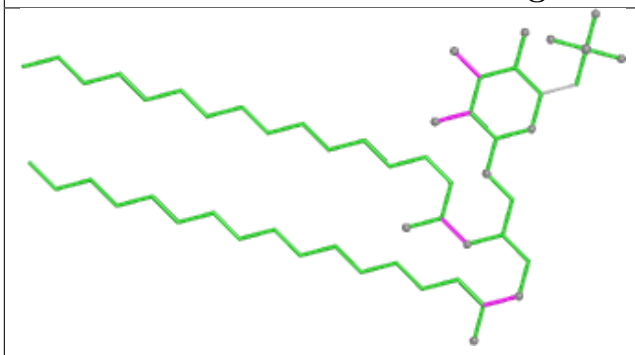


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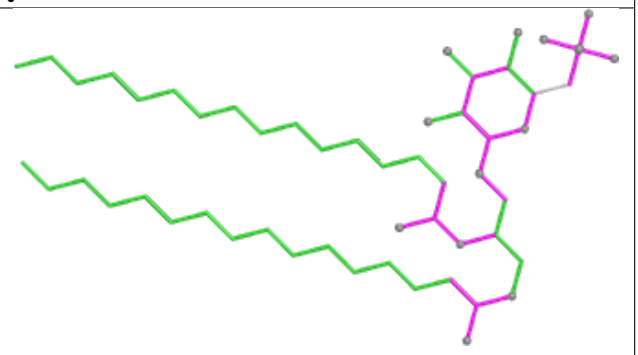


Rings

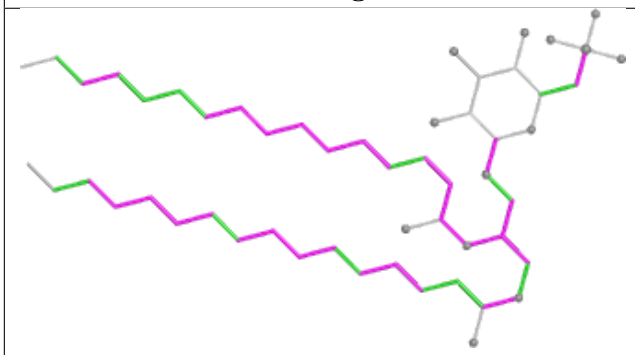
Ligand SQD b 621



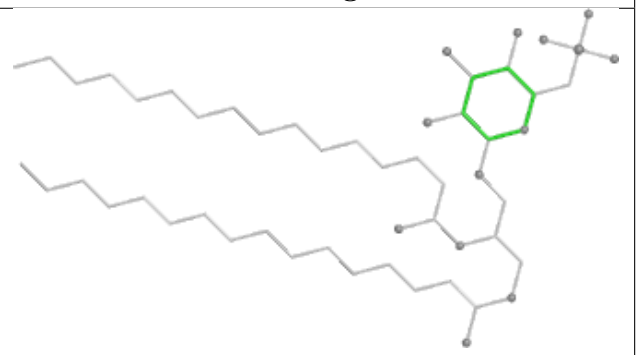
Bond lengths



Bond angles

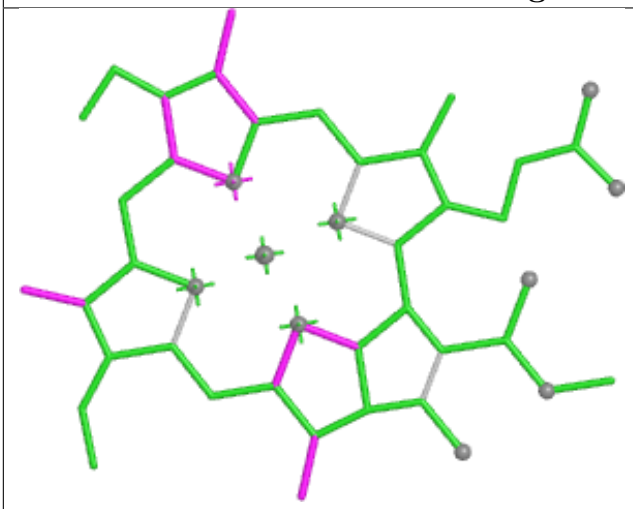


Torsions

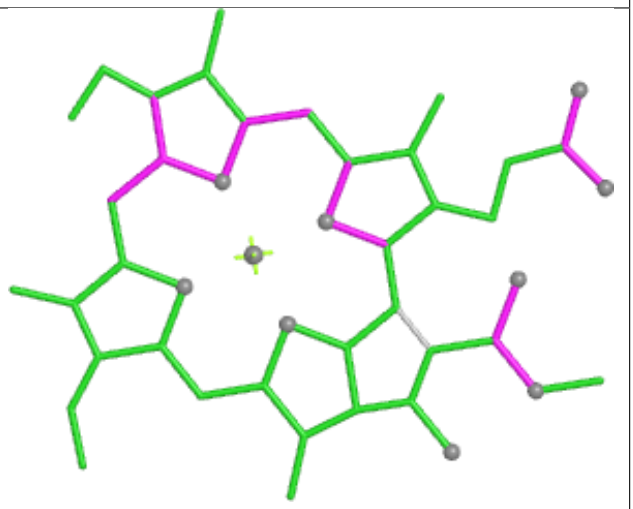


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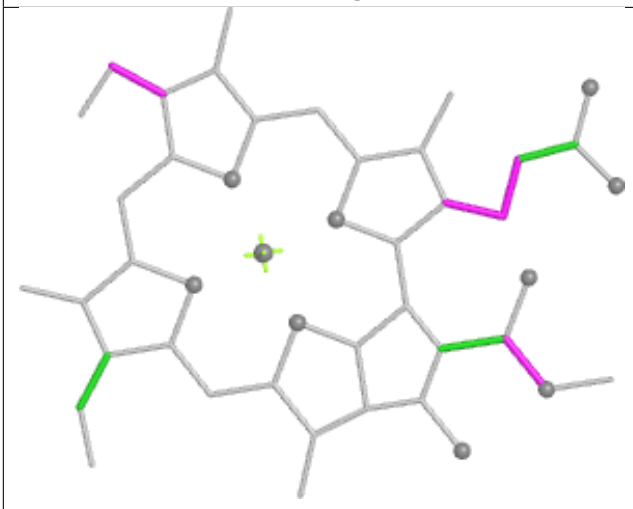
Ligand CLA 4 610



Bond lengths



Bond angles

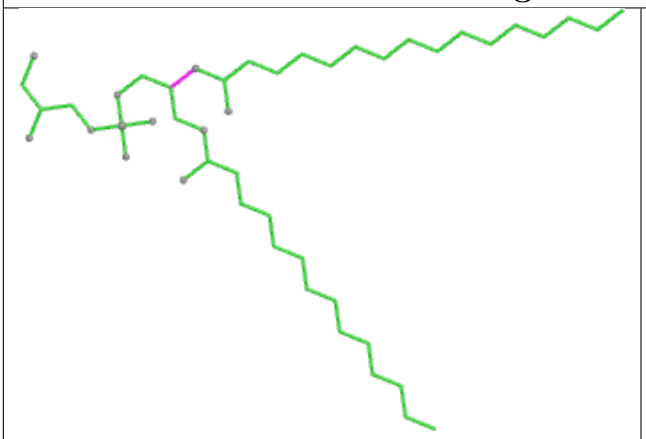


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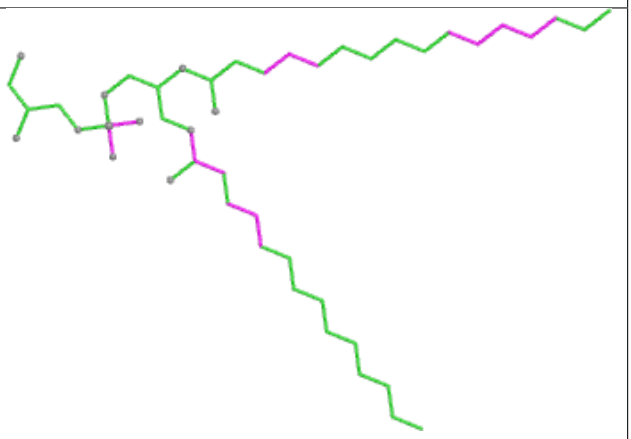


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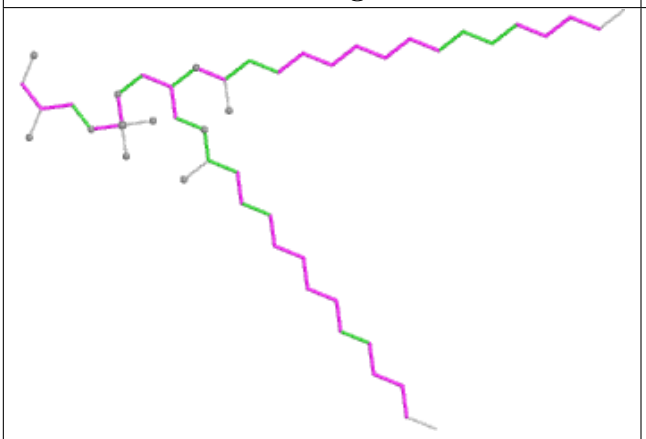
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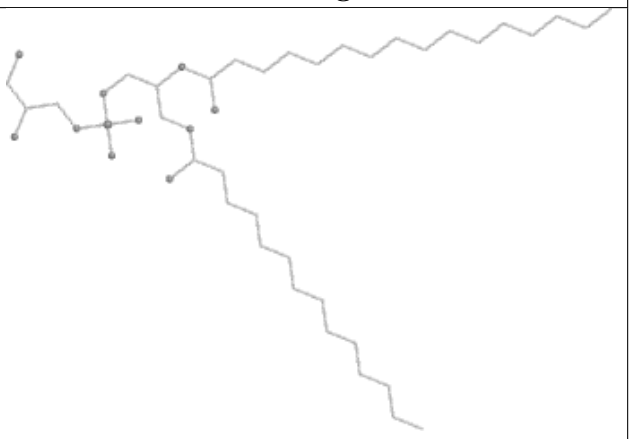
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Bond angles

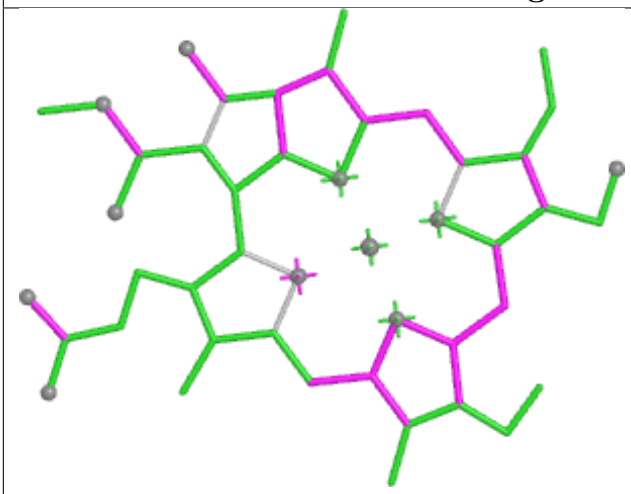


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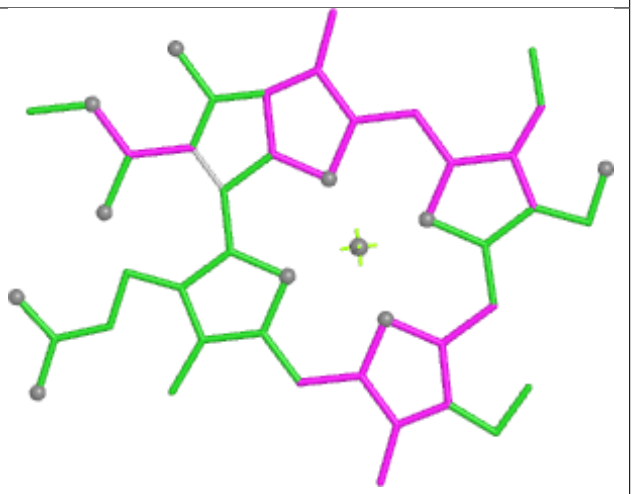


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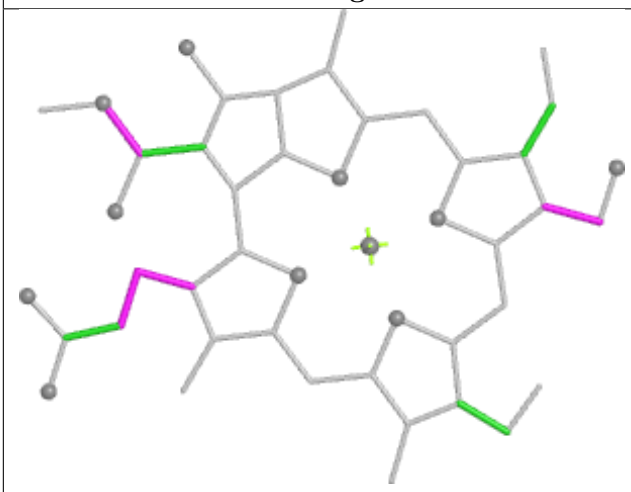
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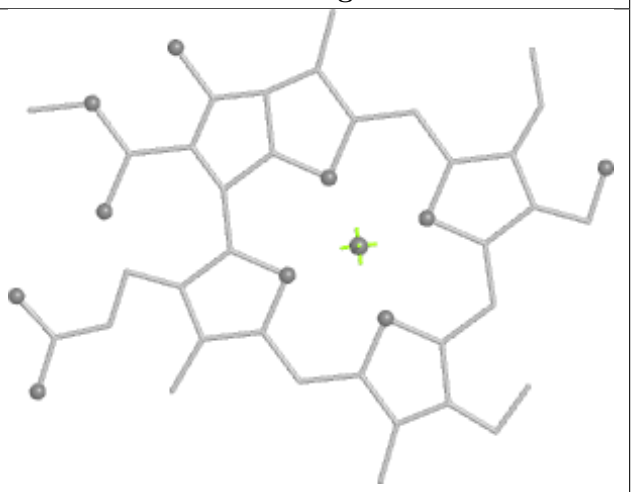
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Bond angles

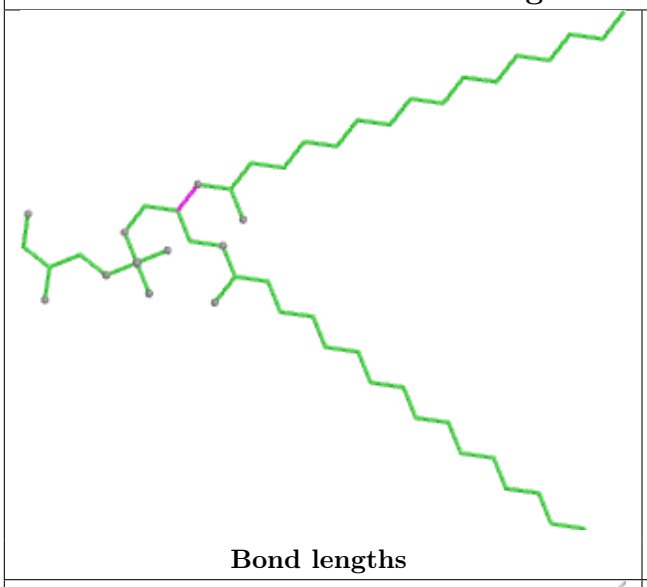


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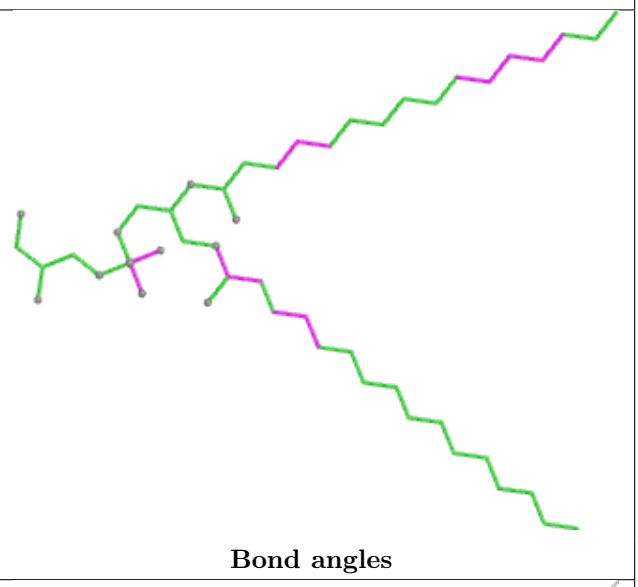


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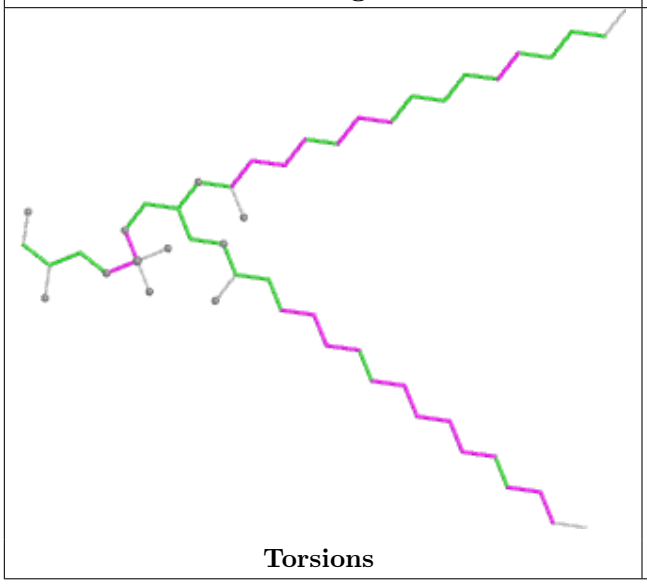
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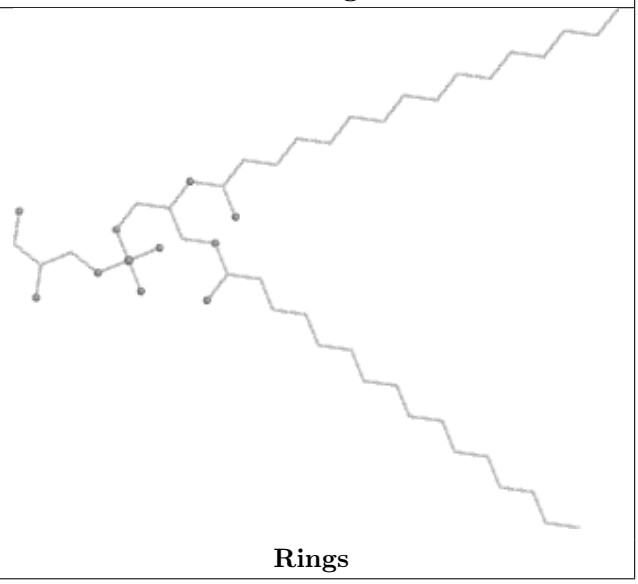
Bond lengths



Bond angles

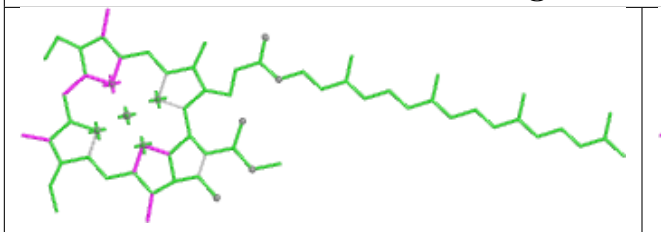


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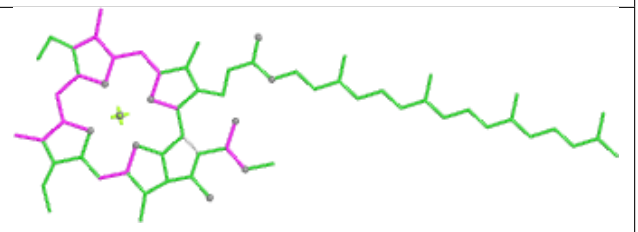


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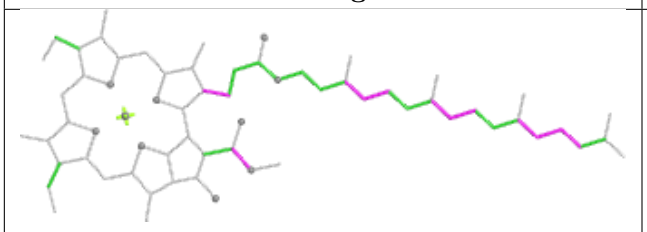
Ligand CLA b 612



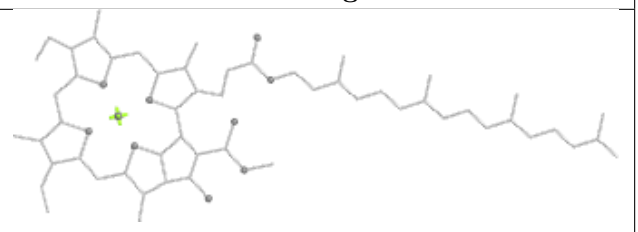
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Bond angles

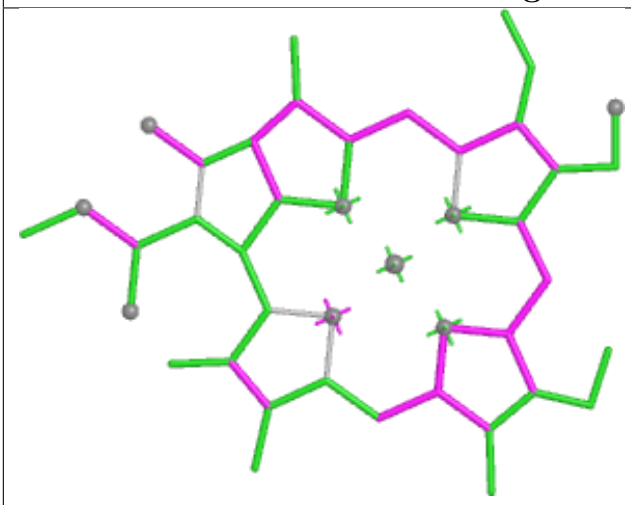


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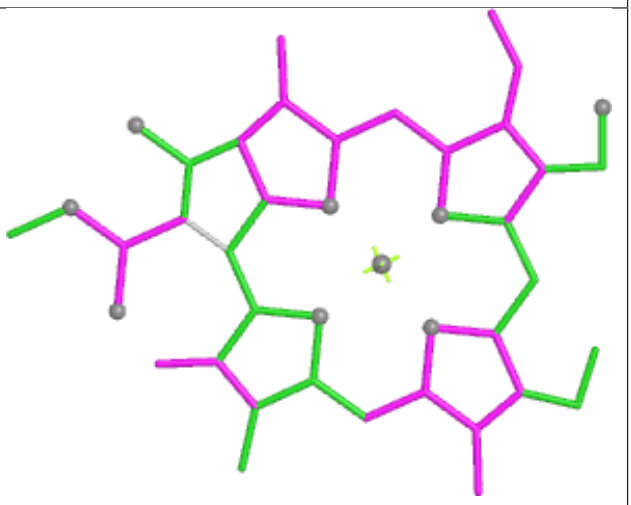


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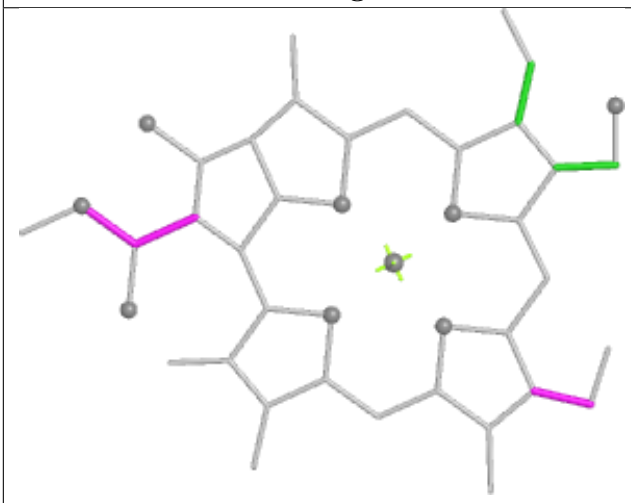
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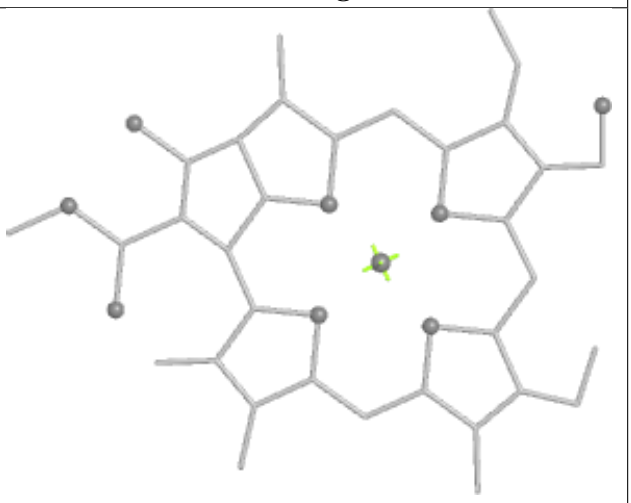
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Bond angles

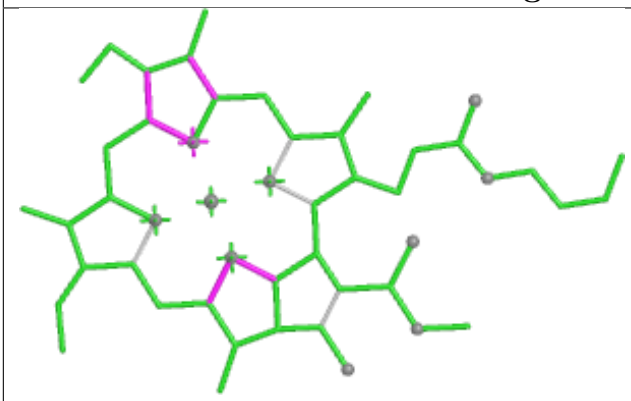


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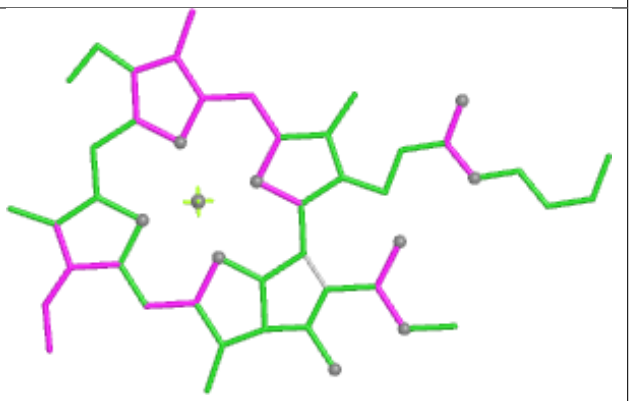


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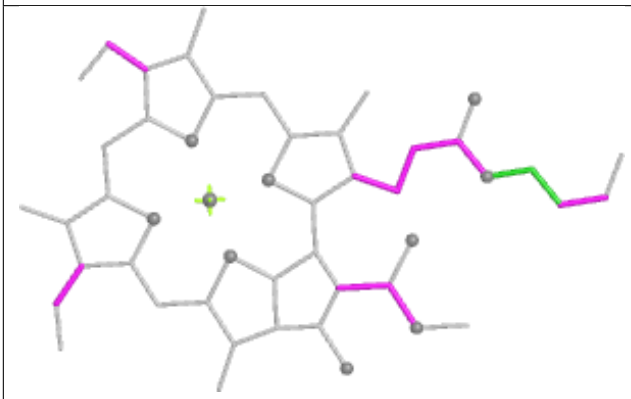
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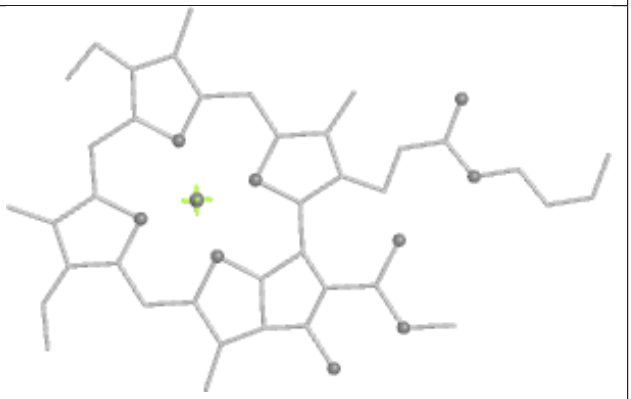
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Bond angles

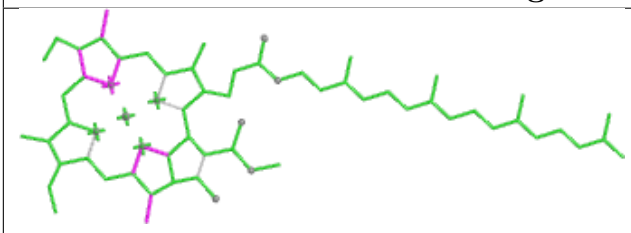


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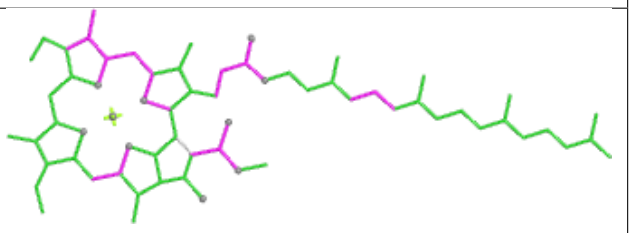


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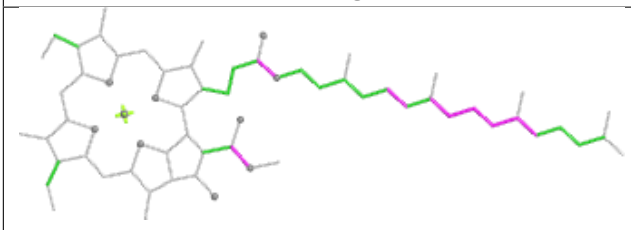
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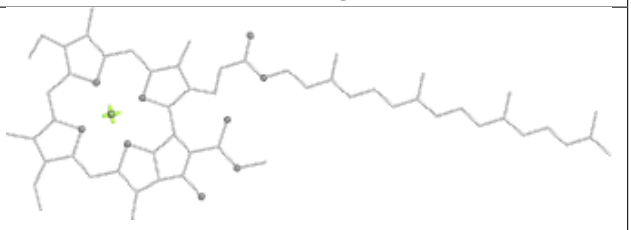
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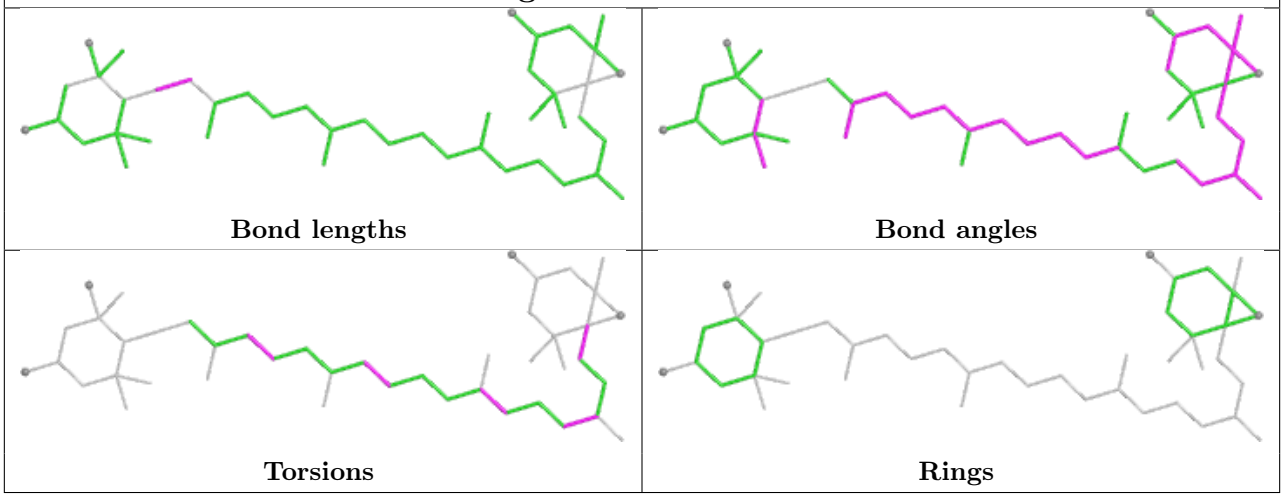


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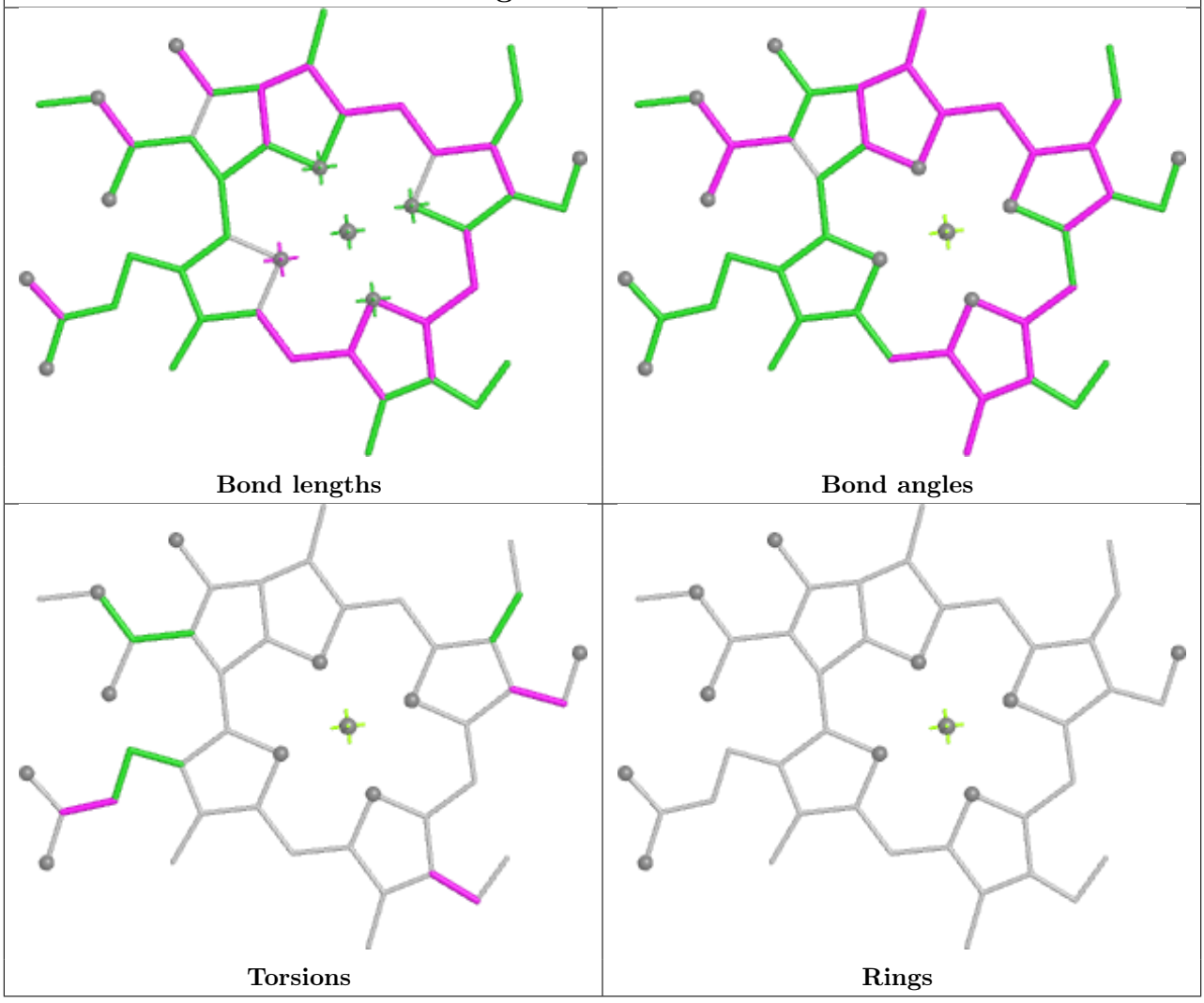


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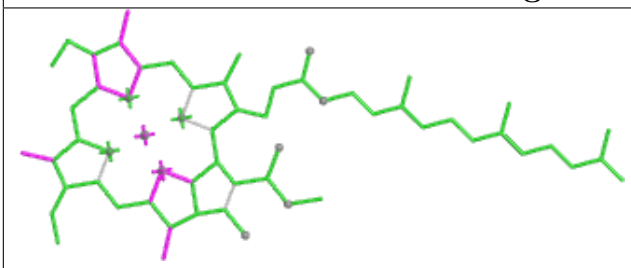
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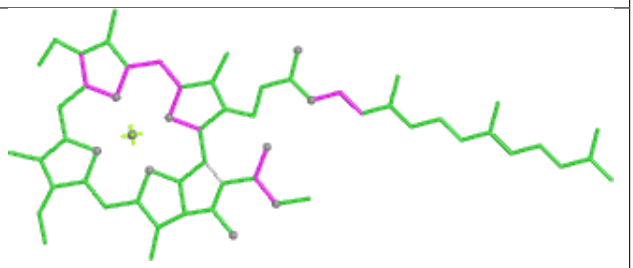
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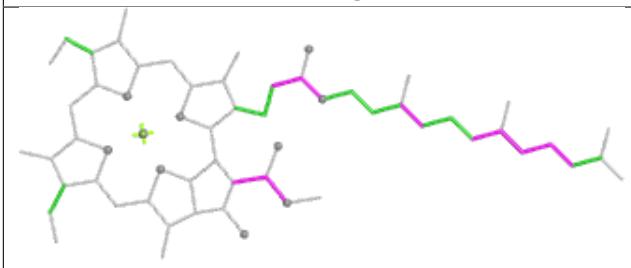
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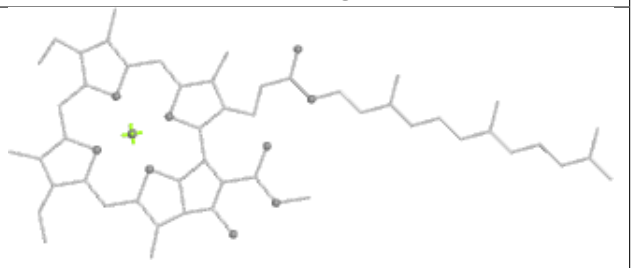
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Bond angles

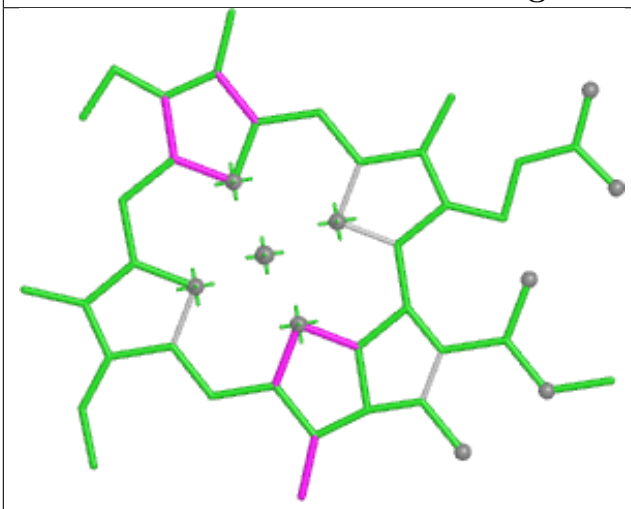


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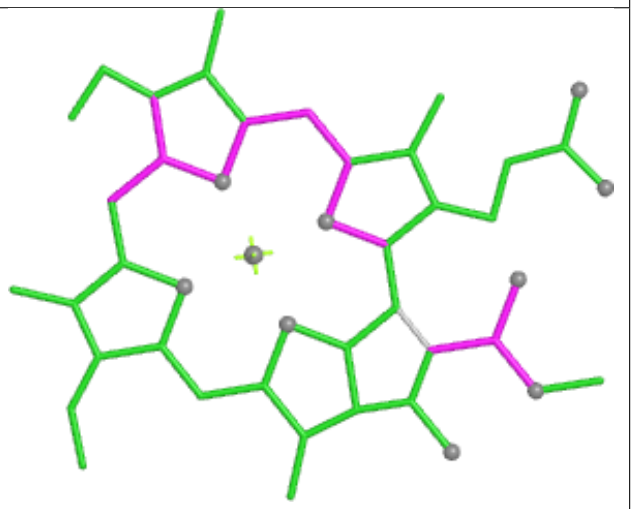


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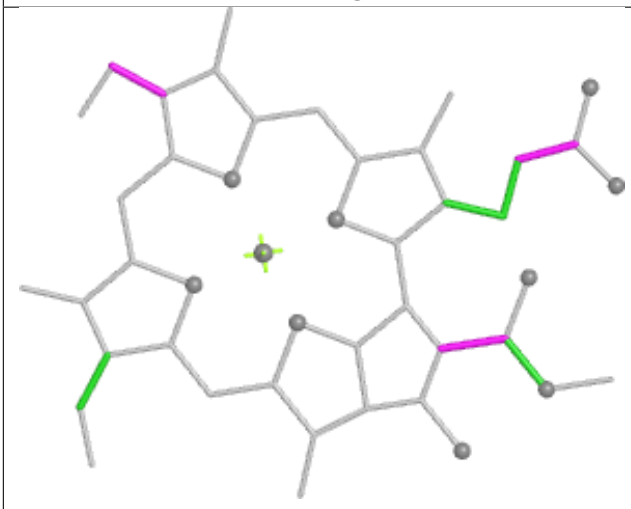
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Bond lengths



Bond angles

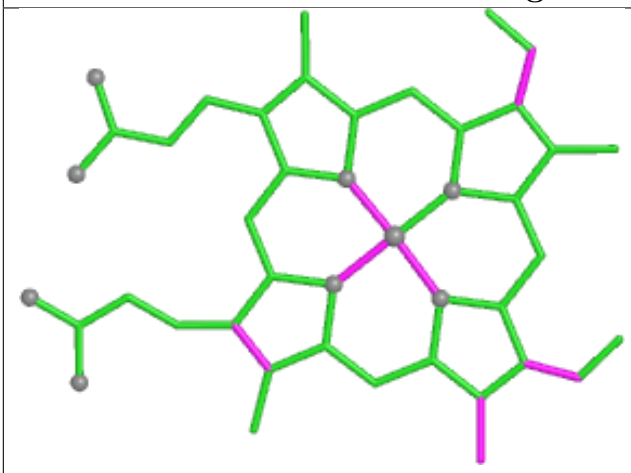


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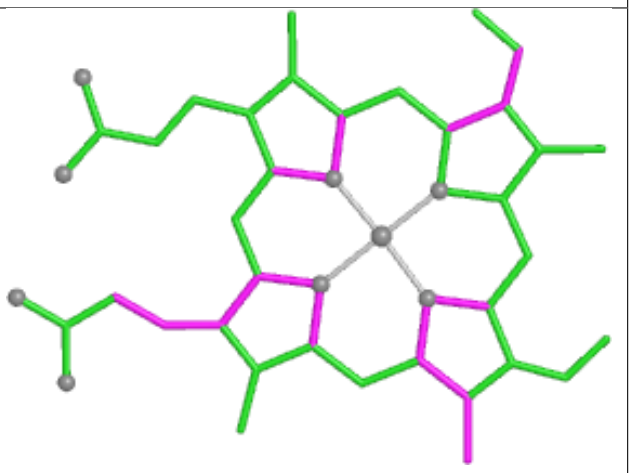


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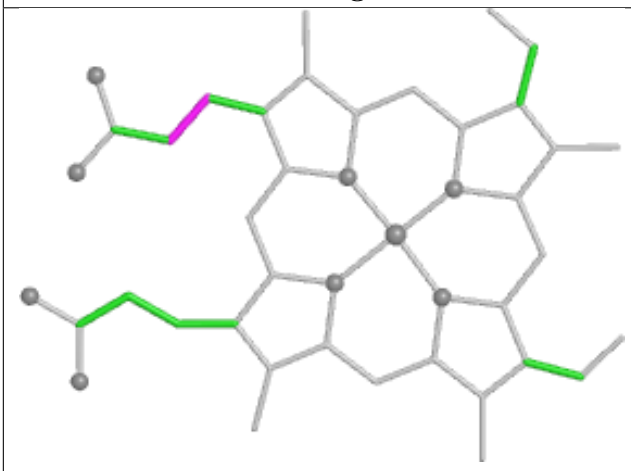
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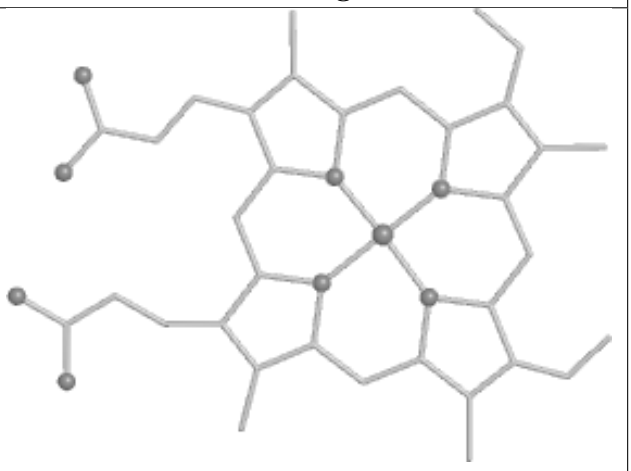
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Bond angles

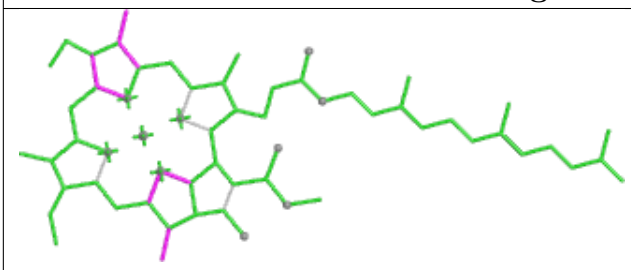


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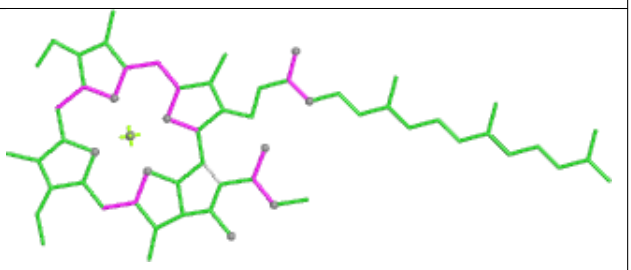


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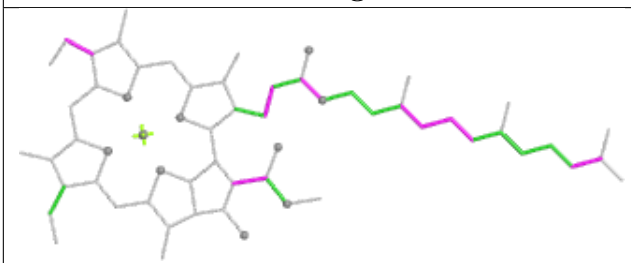
Ligand CLA r 613



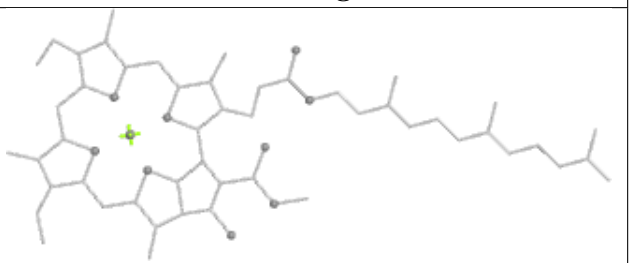
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Bond angles

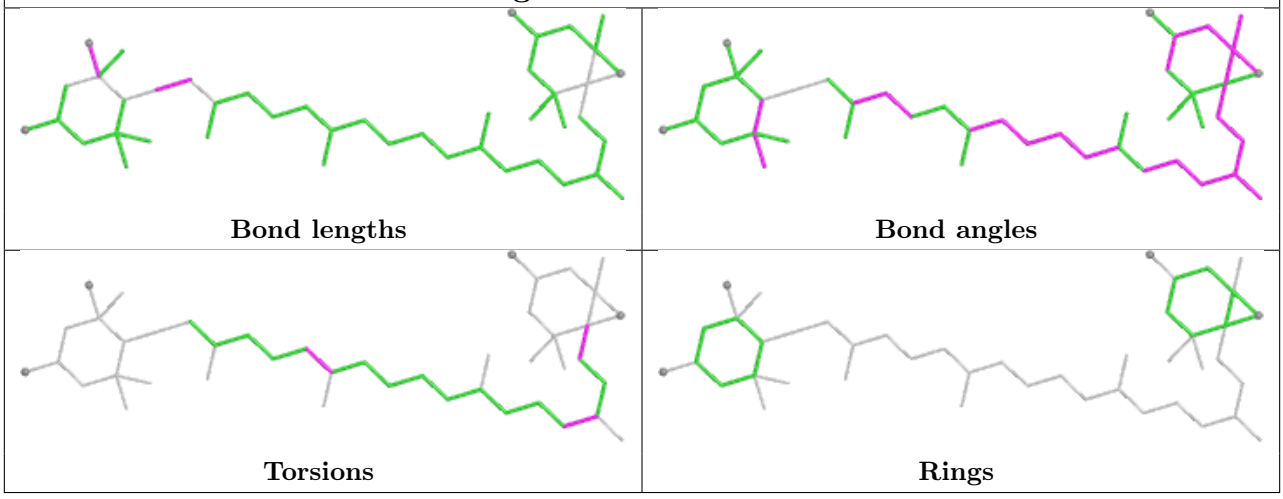


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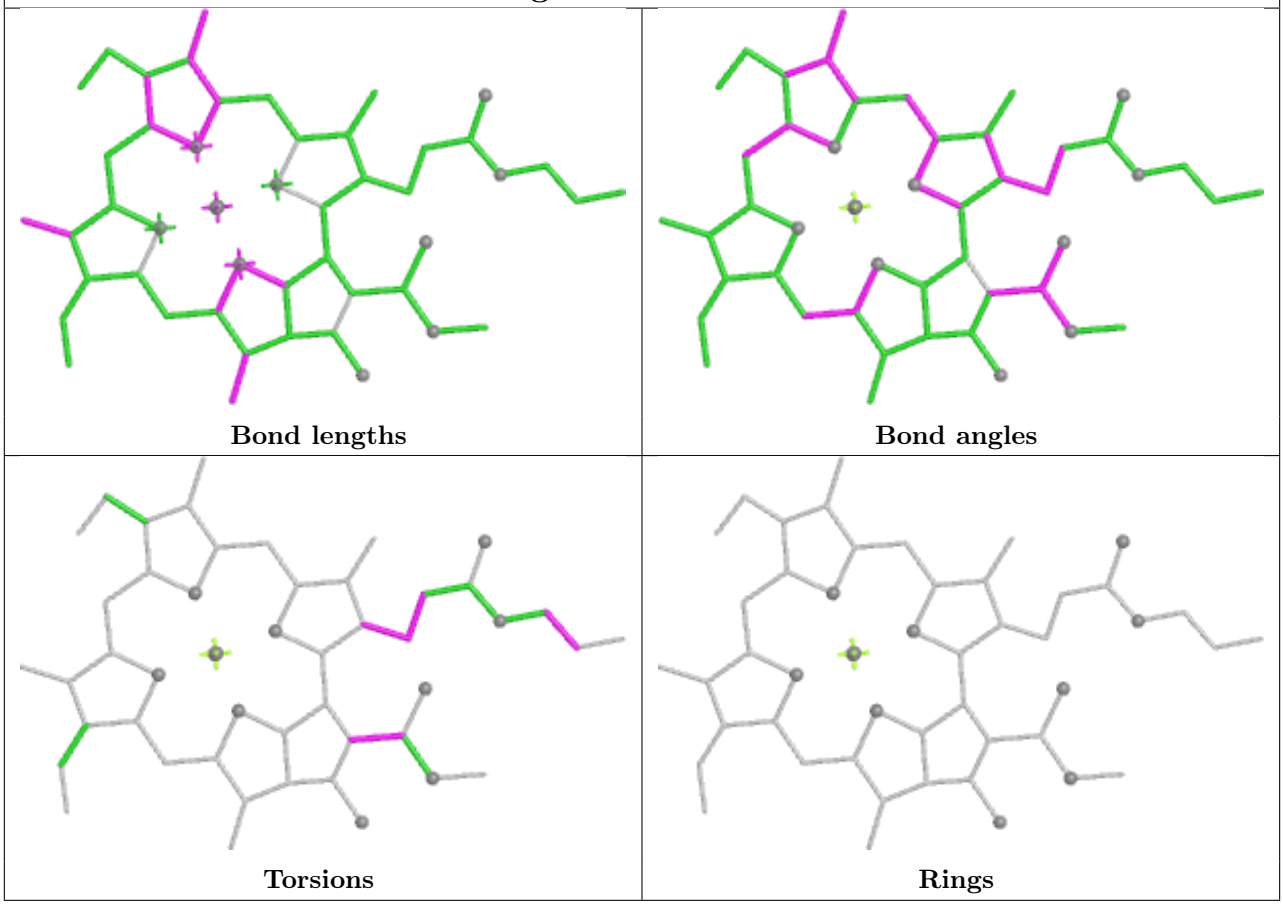


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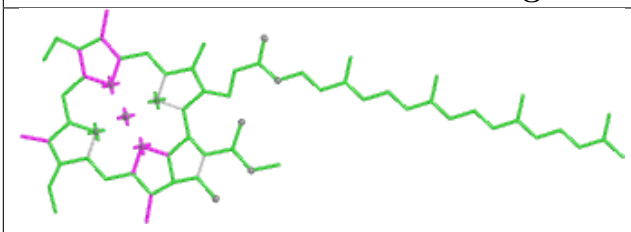
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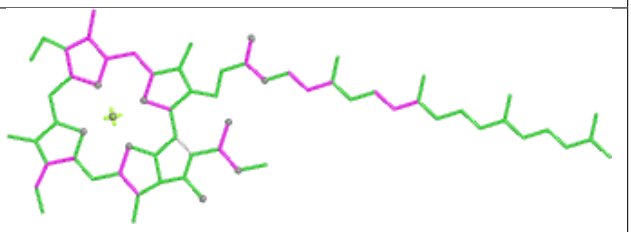
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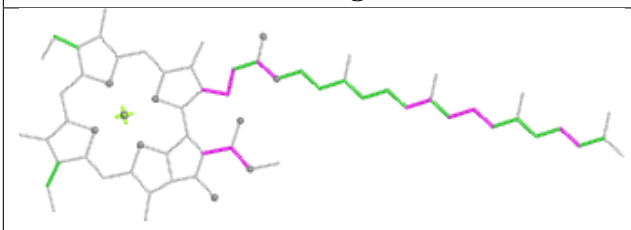
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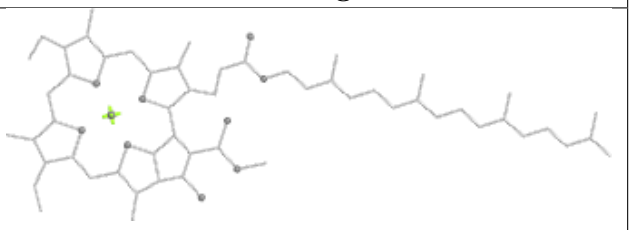
Bond lengths



Bond angles

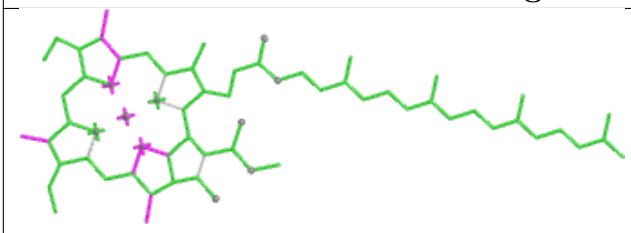


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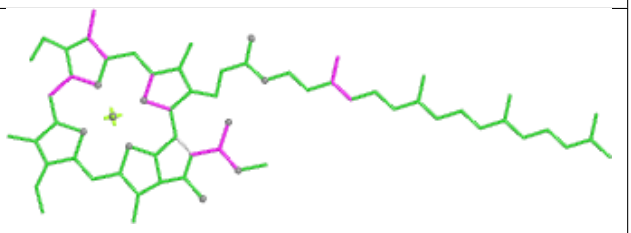


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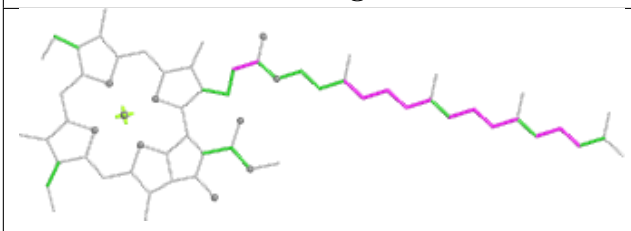
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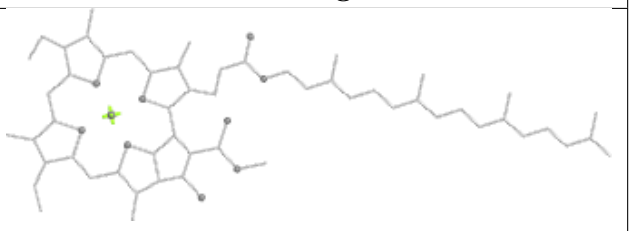
Bond lengths



Bond angles

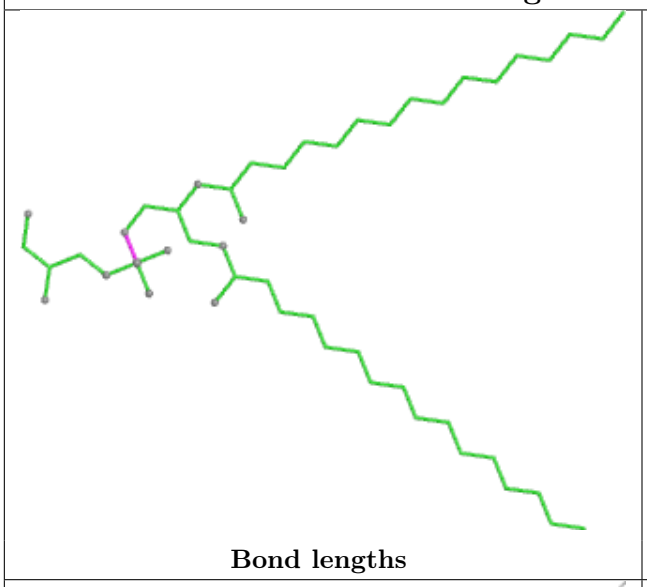


Torsions

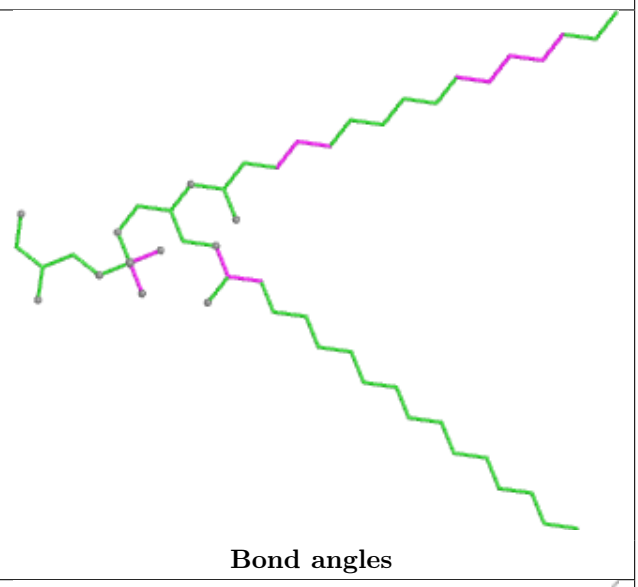


Rings

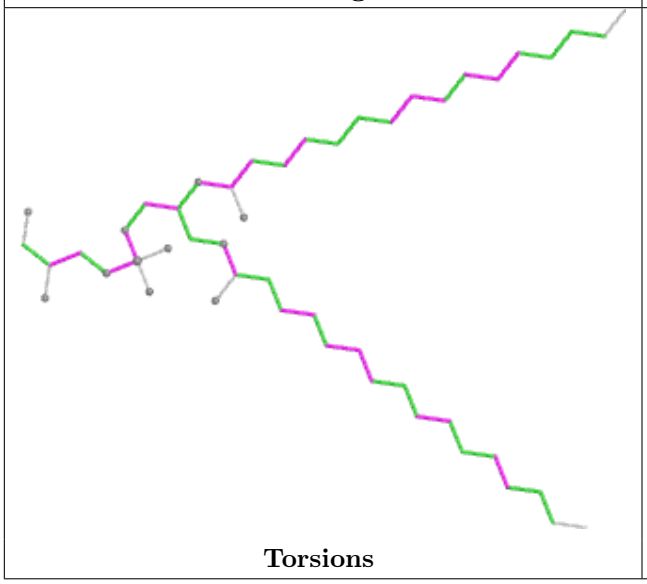
Ligand LHG C 523



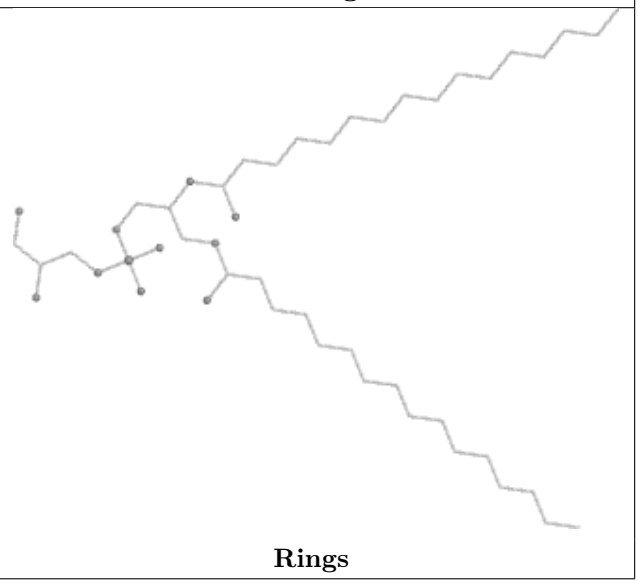
Bond lengths



Bond angles

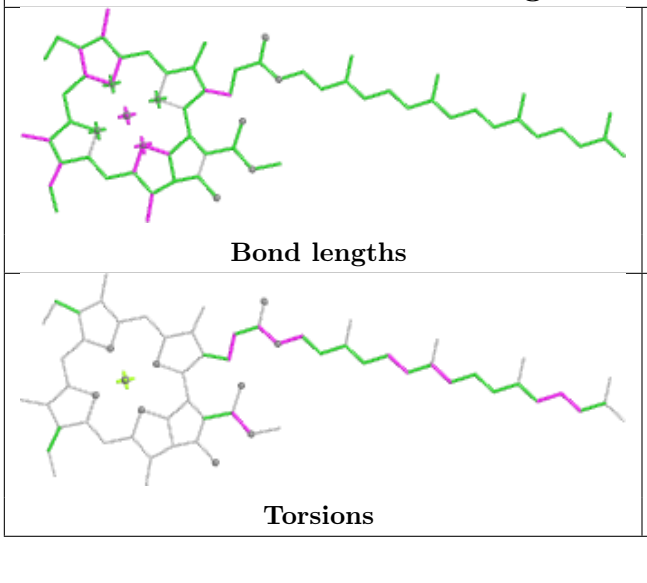


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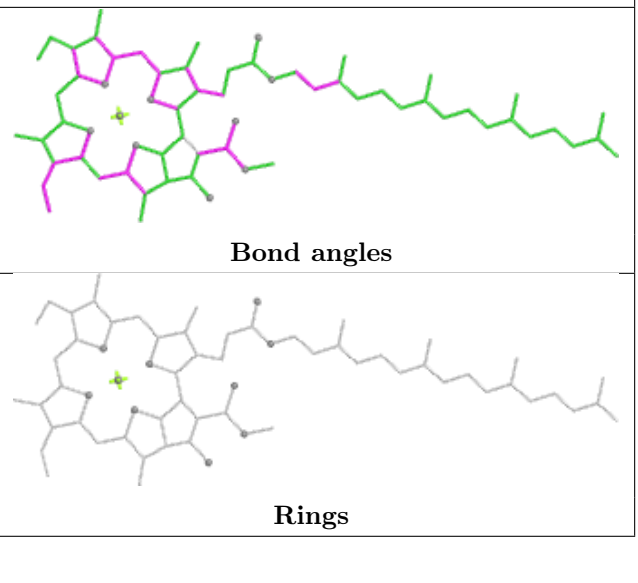


Rings

Ligand CLA G 603



Bond lengths

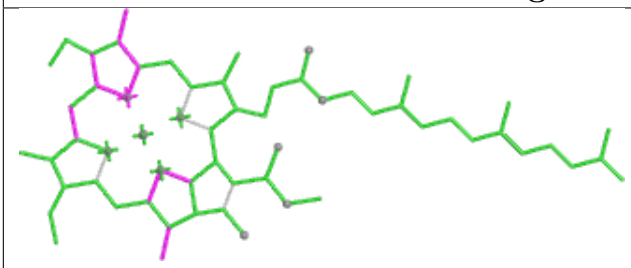


Bond angles

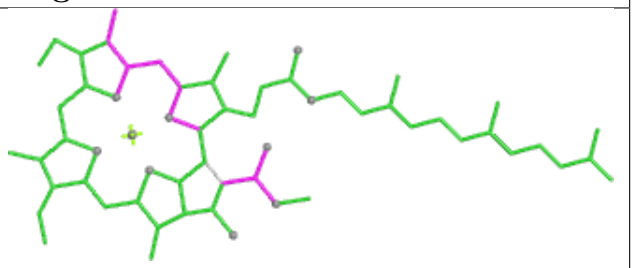
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Rings

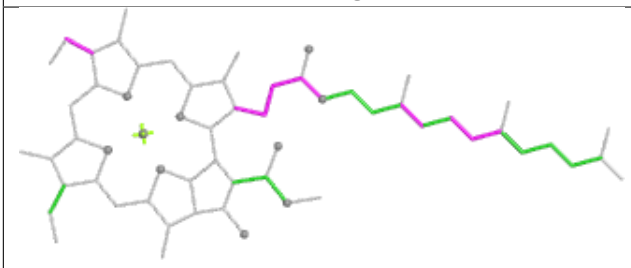
Ligand CLA g 611



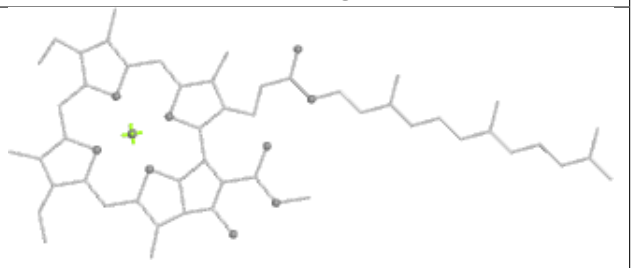
Bond lengths



Bond angles

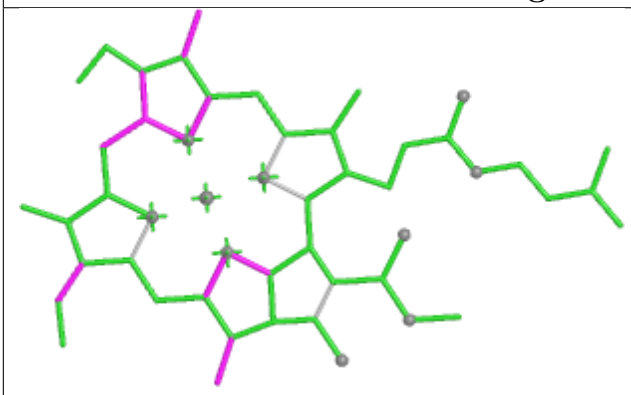


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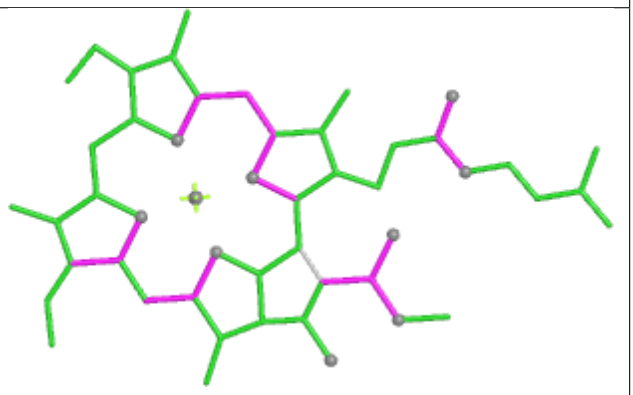


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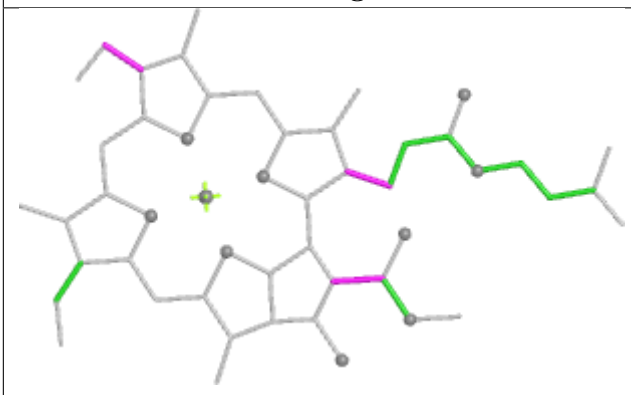
Ligand CLA a 407



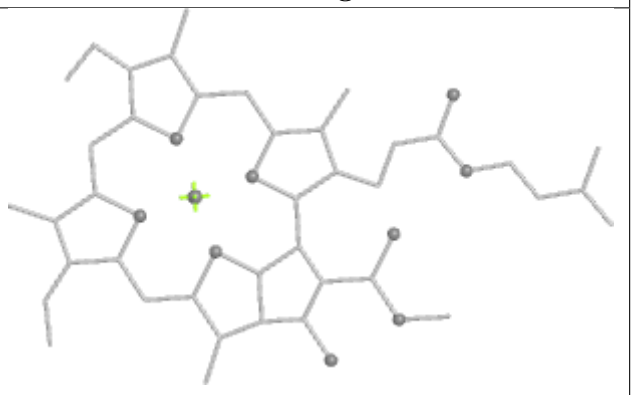
Bond lengths



Bond angles

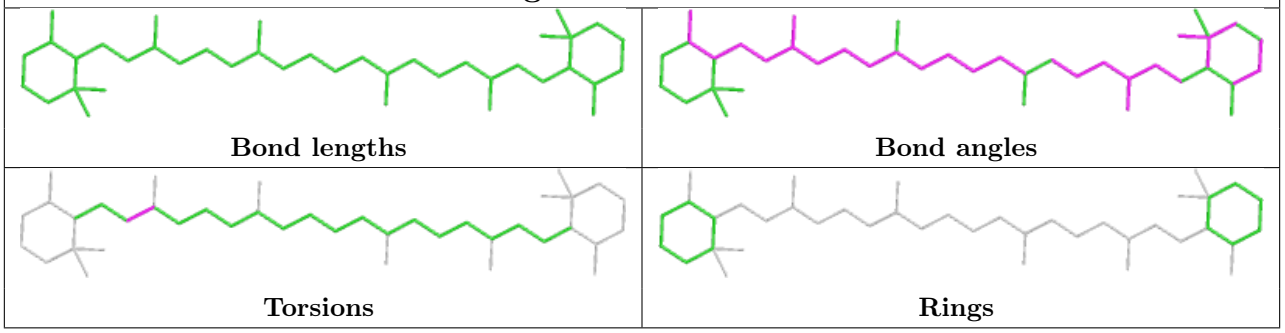


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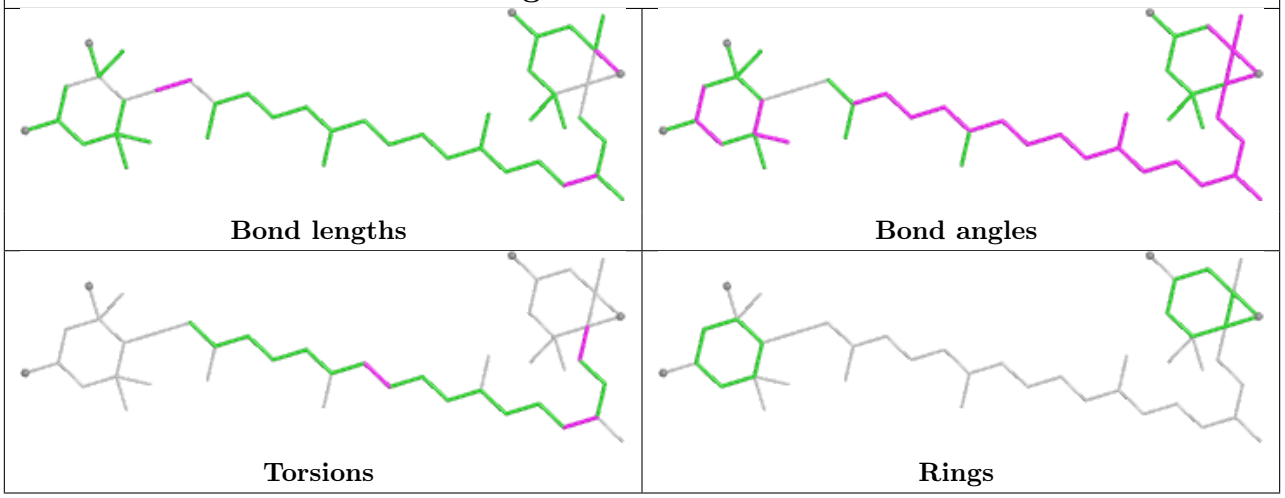


Rings

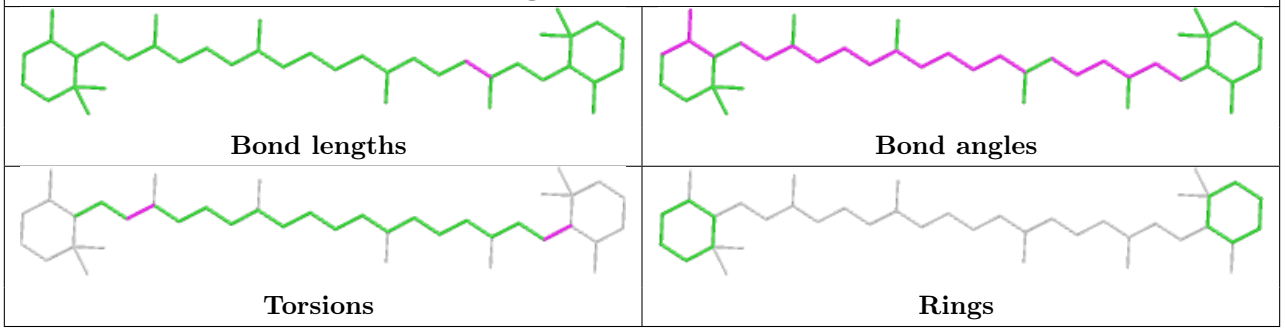
Ligand BCR B 619



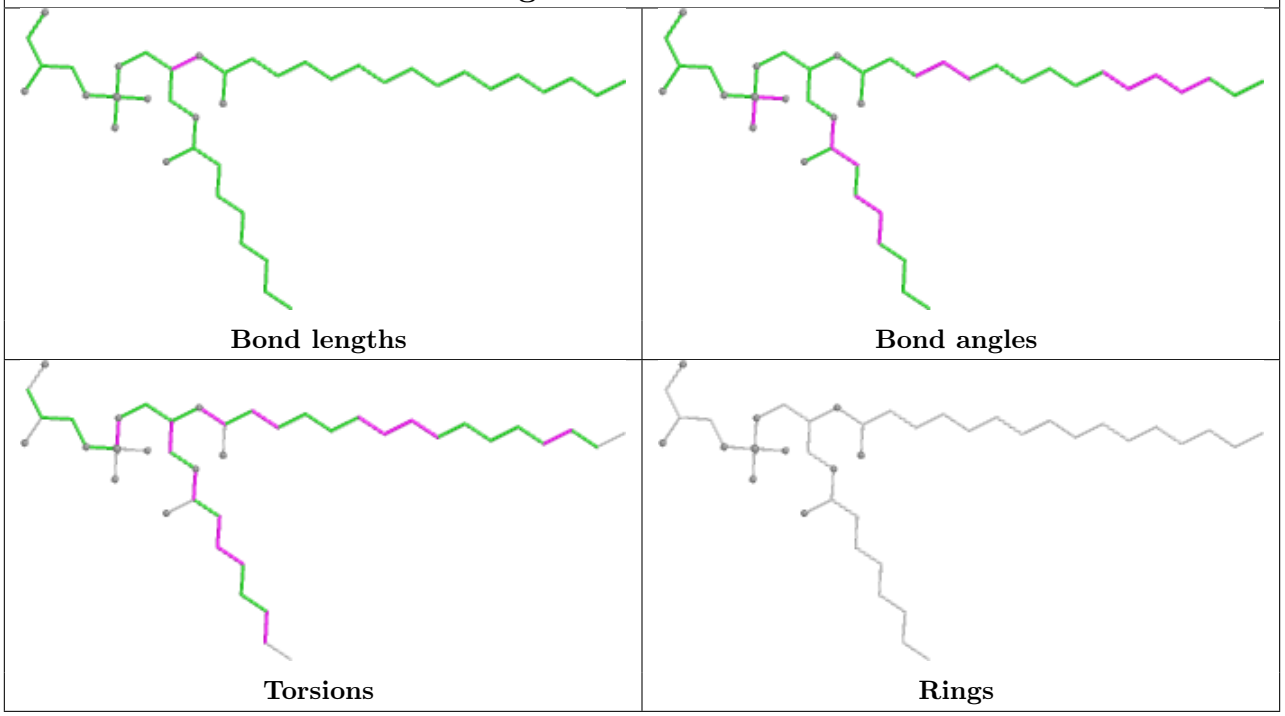
Ligand NEX R 623



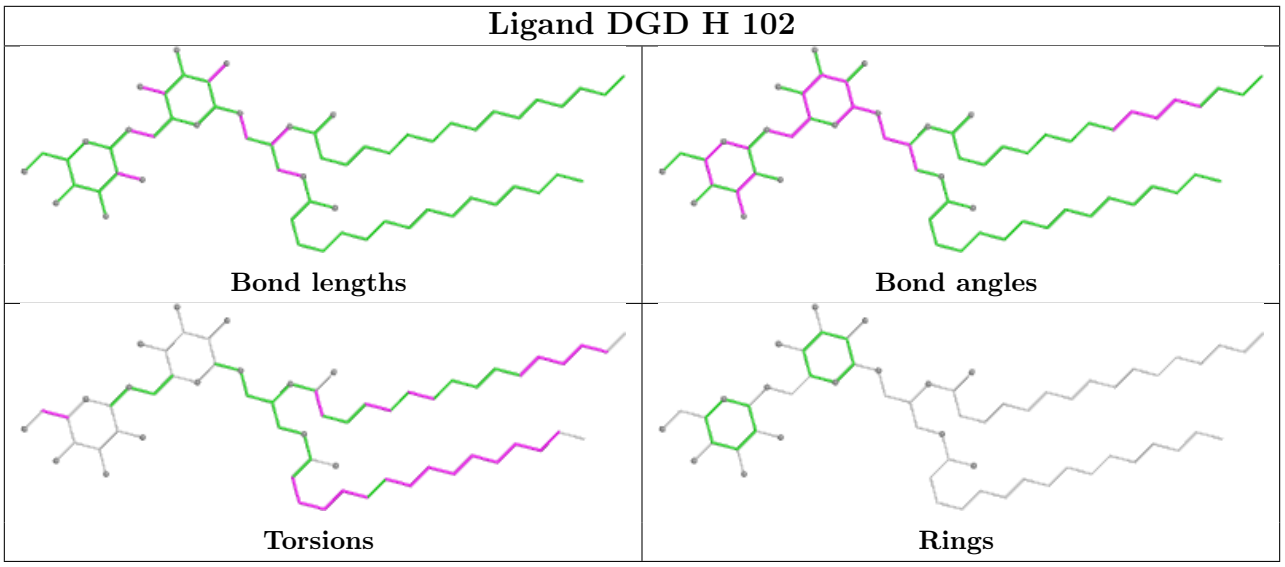
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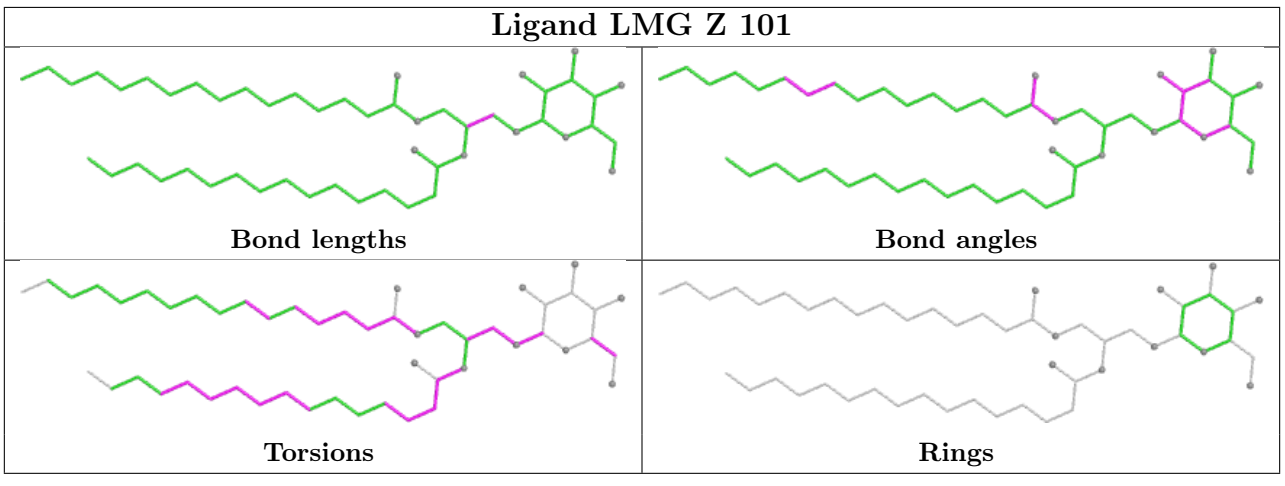
Ligand LHG 1 2630



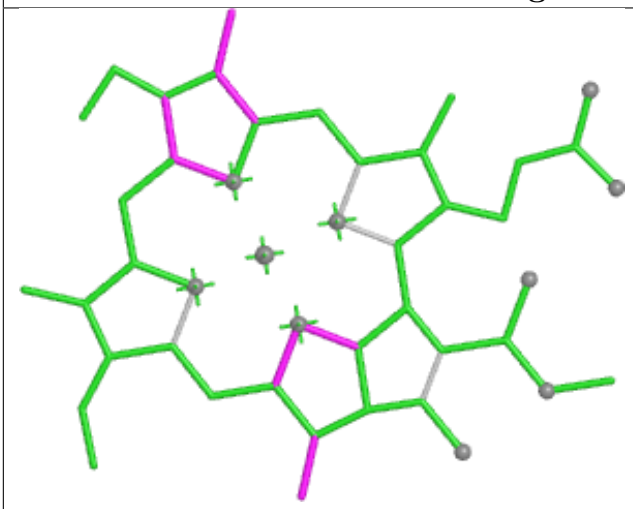
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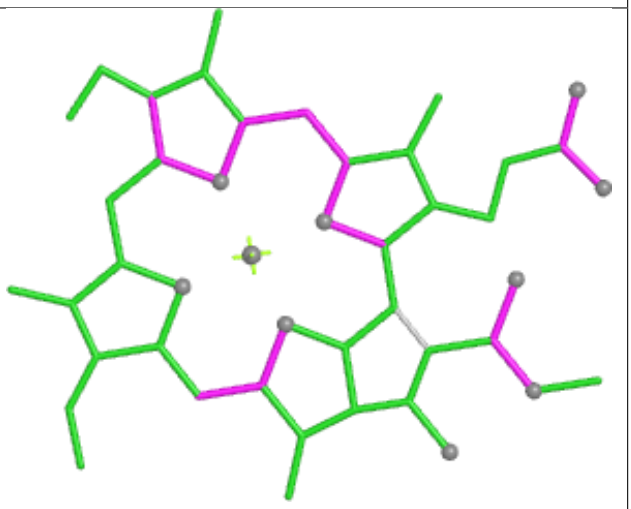
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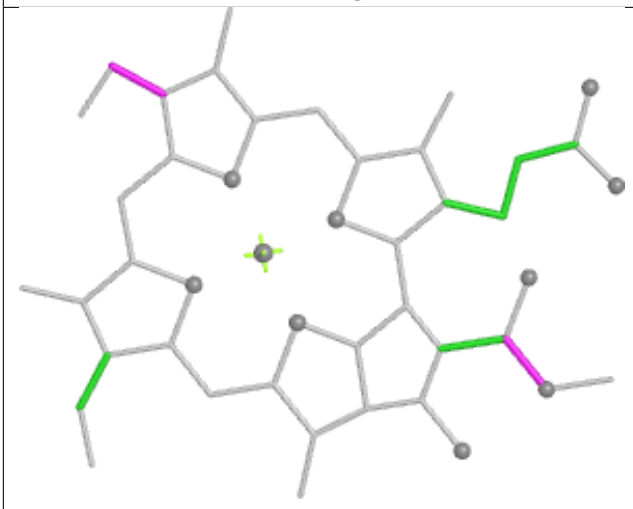
Ligand CLA 5 614



Bond lengths



Bond angles

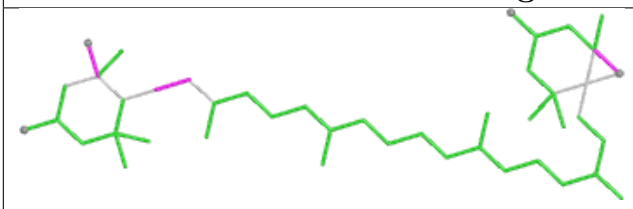


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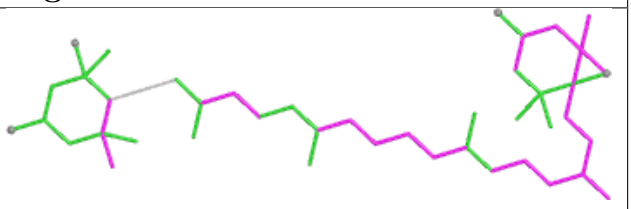


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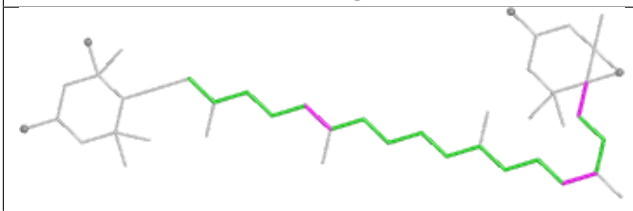
Ligand NEX g 1623



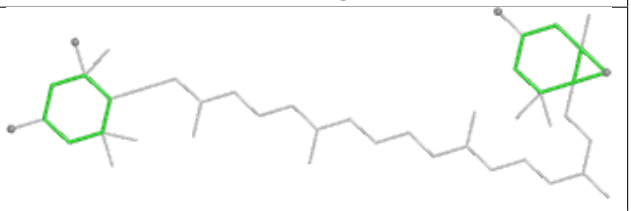
Bond lengths



Bond angles

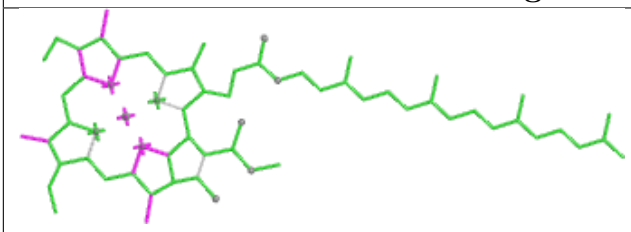


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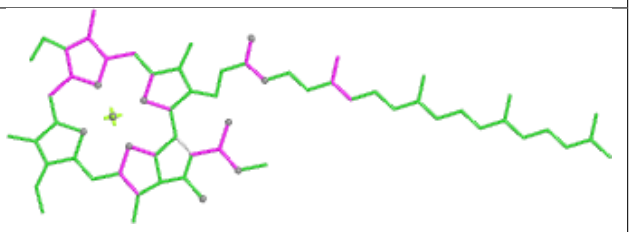


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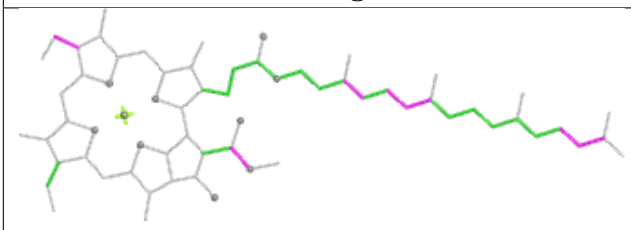
Ligand CLA B 604



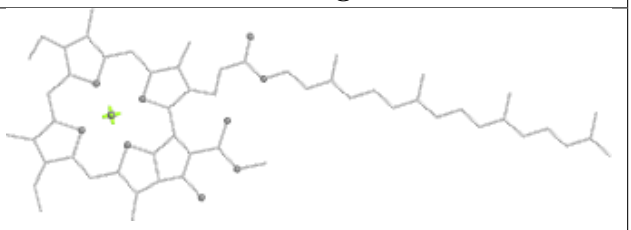
Bond lengths



Bond angles

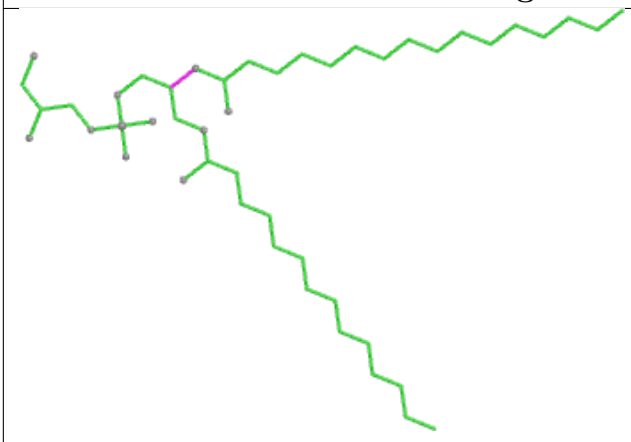


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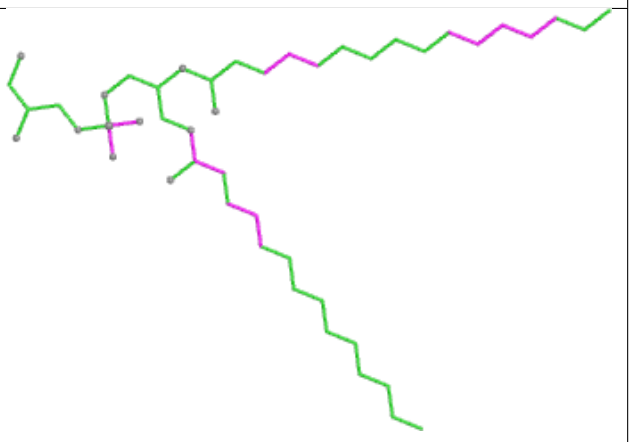


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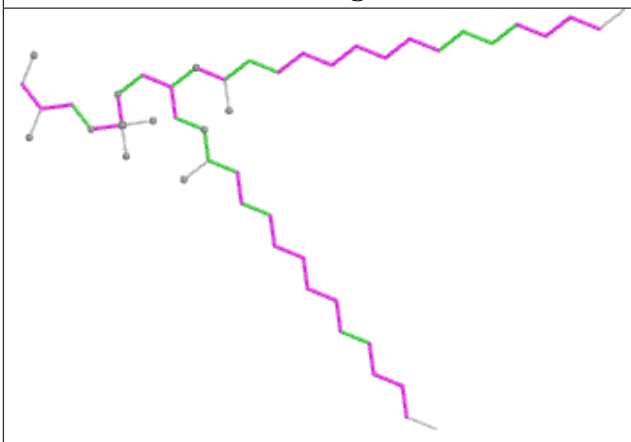
Ligand LHG b 2630



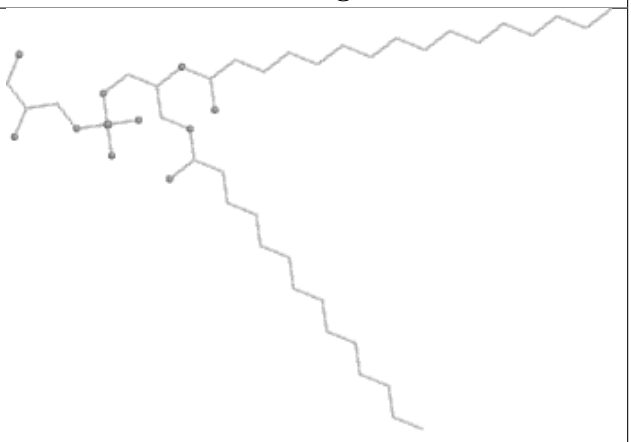
Bond lengths



Bond angles

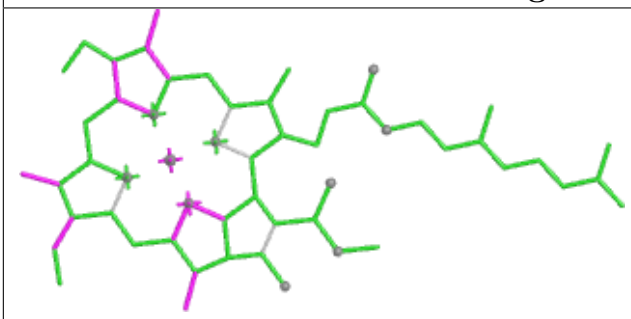


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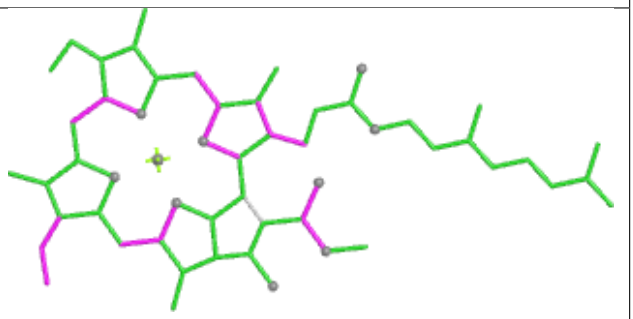


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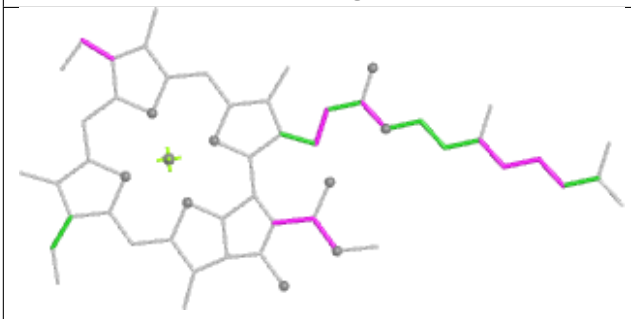
Ligand CLA 5 603



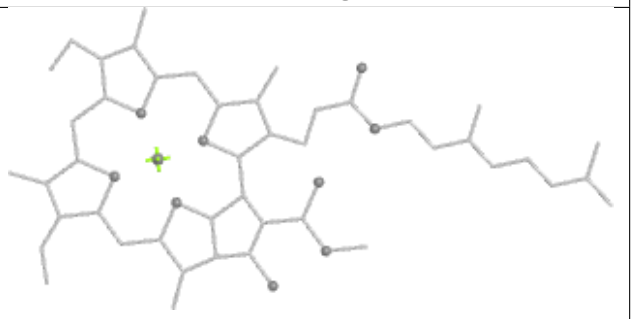
Bond lengths



Bond angles

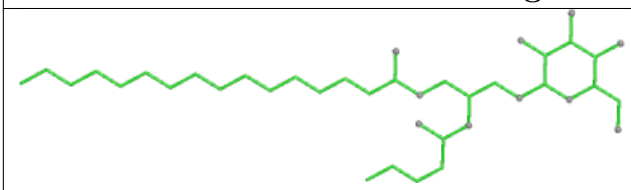


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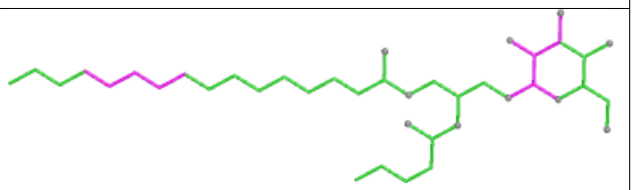


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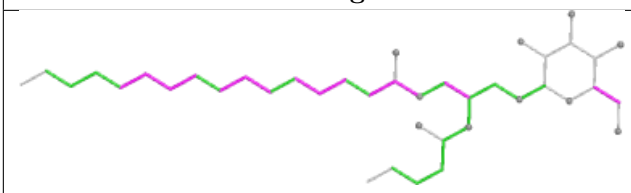
Ligand LMG a 415



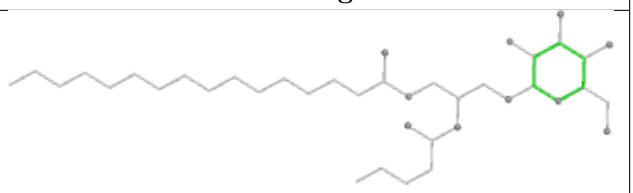
Bond lengths



Bond angles

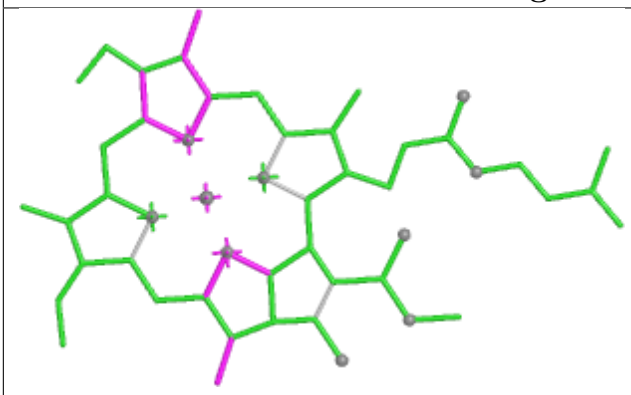


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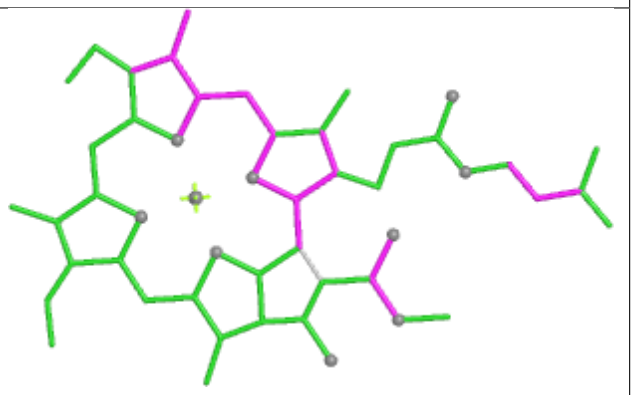


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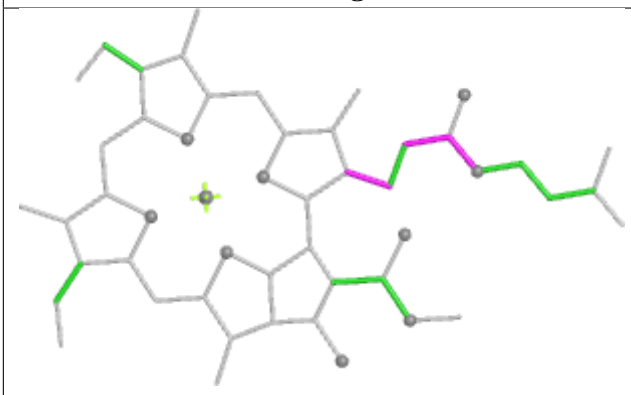
Ligand CLA s 604



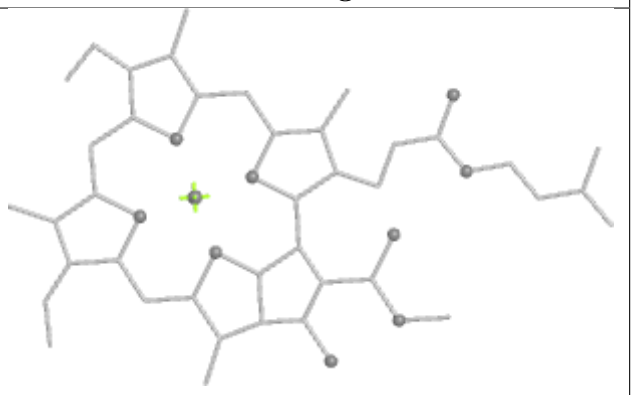
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Bond angles

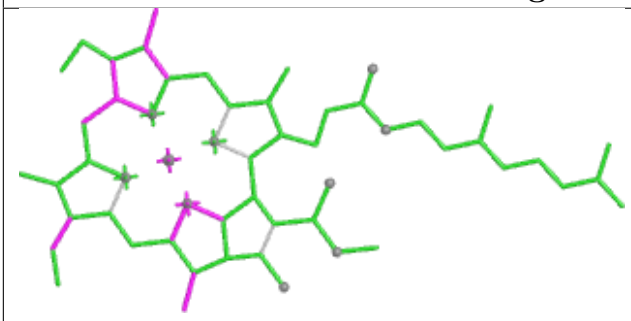


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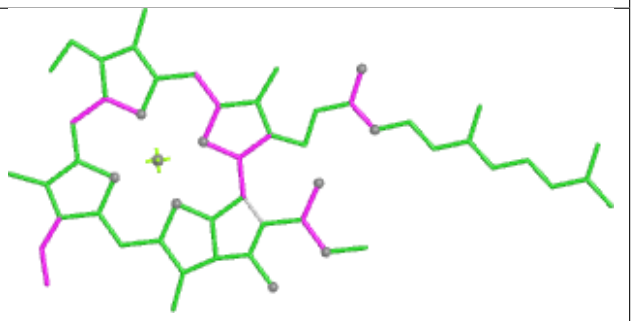


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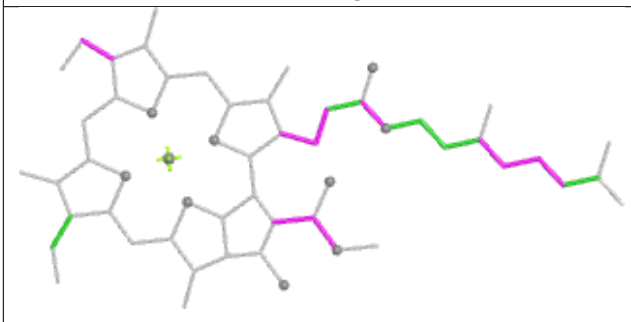
Ligand CLA 3 603



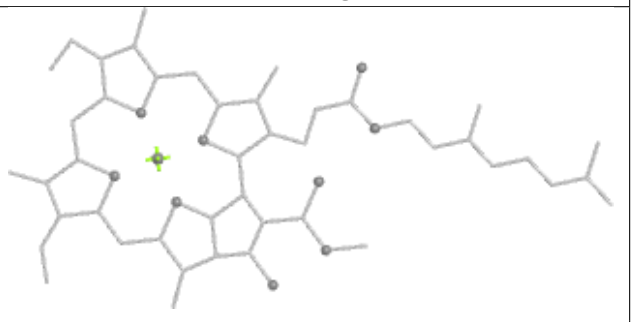
Bond lengths



Bond angles

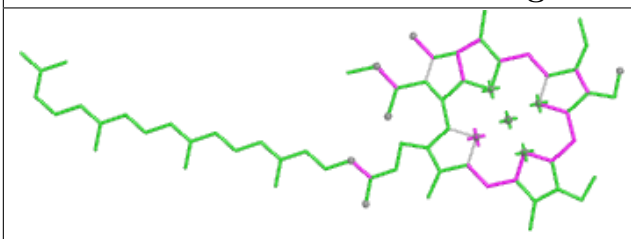


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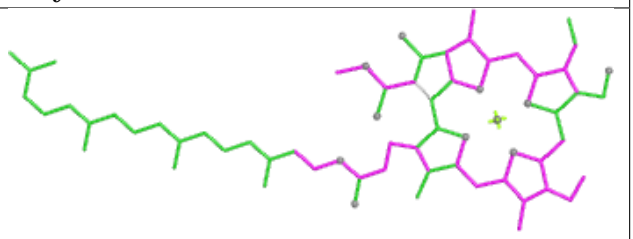


Rings

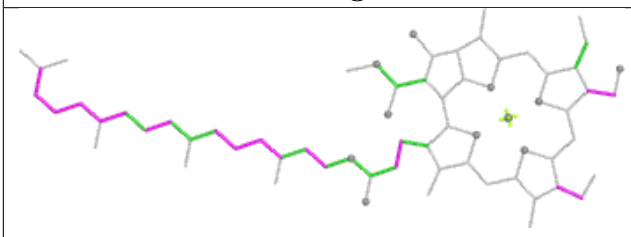
Ligand CHL y 607



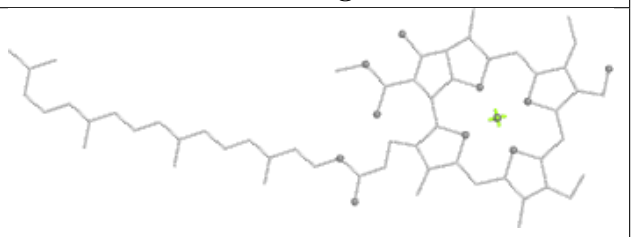
Bond lengths



Bond angles

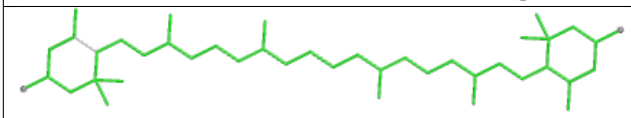


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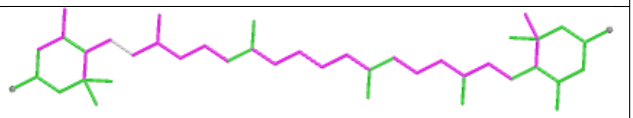


Rings

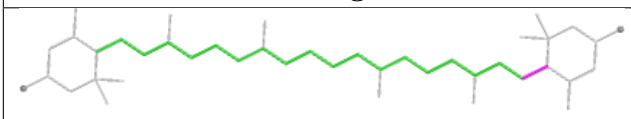
Ligand LUT G 1620



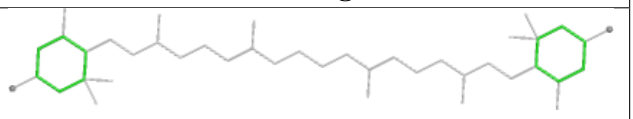
Bond lengths



Bond angles

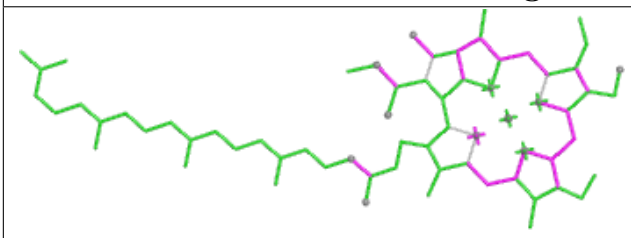


Torsions

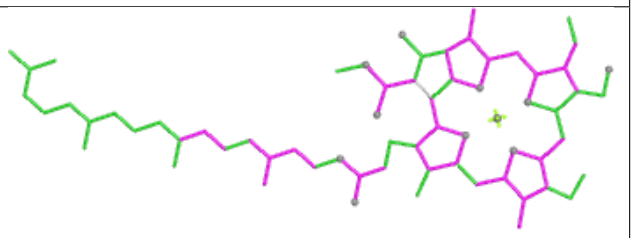


Rings

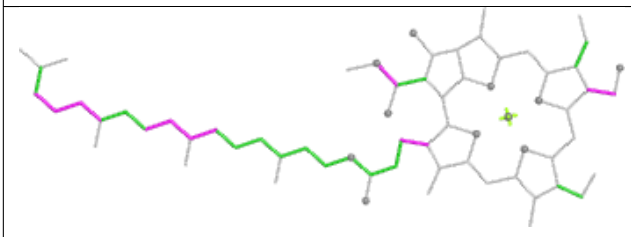
Ligand CHL Y 608



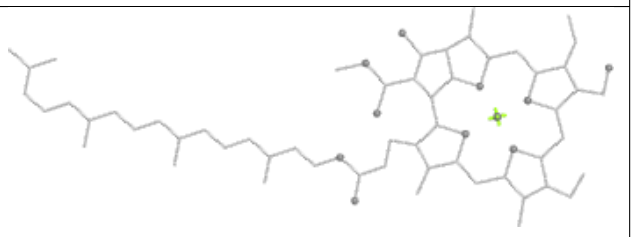
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Bond angles

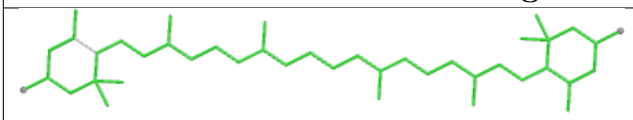


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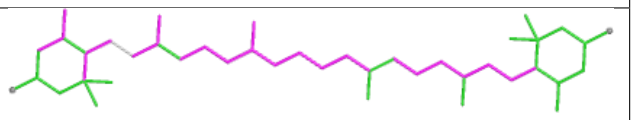


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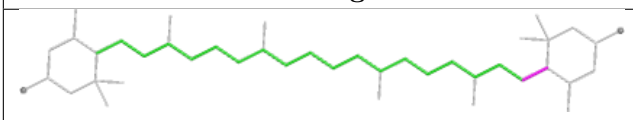
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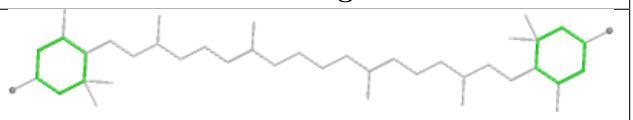
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Bond angles

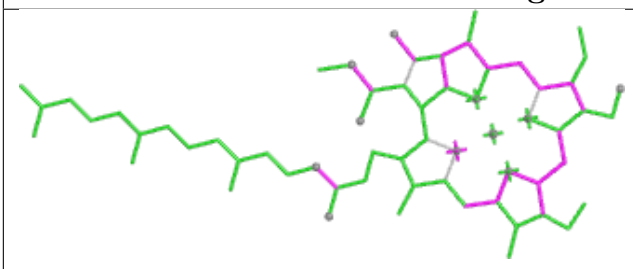


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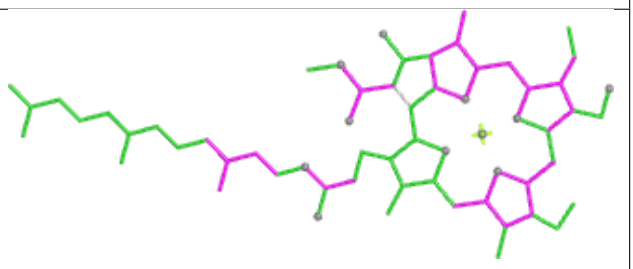


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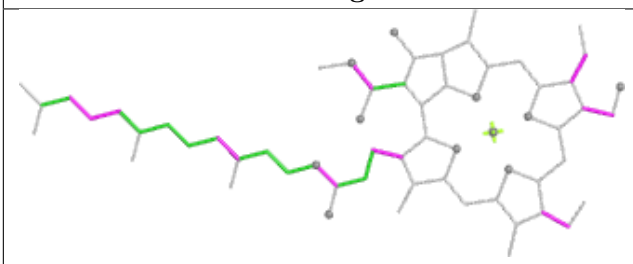
Ligand CHL 3 609



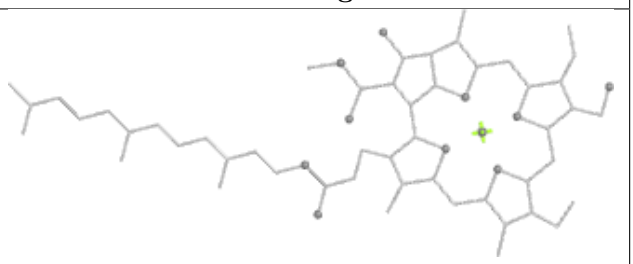
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Bond angles

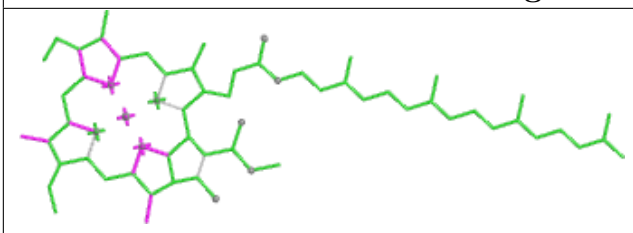


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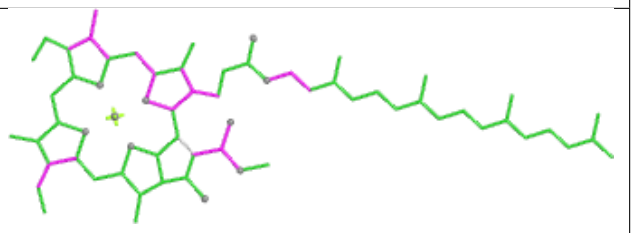


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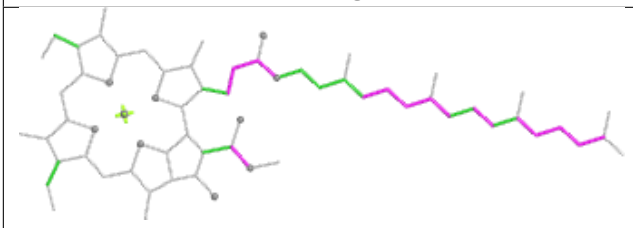
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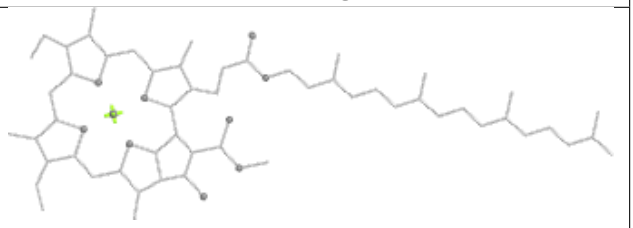
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Bond angles

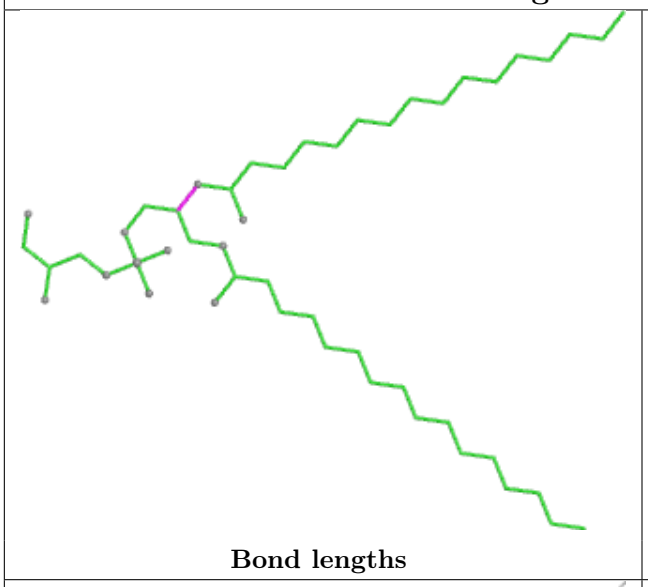


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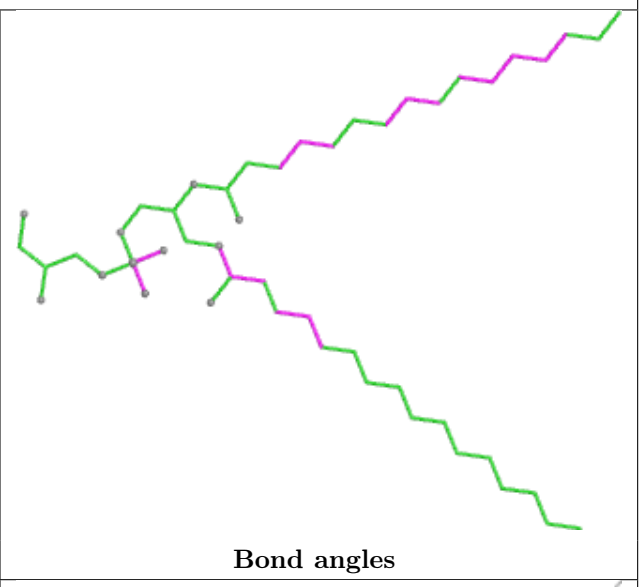


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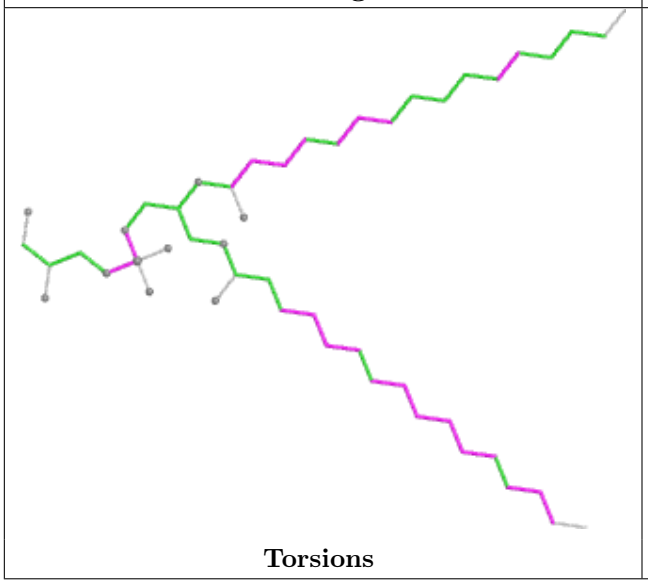
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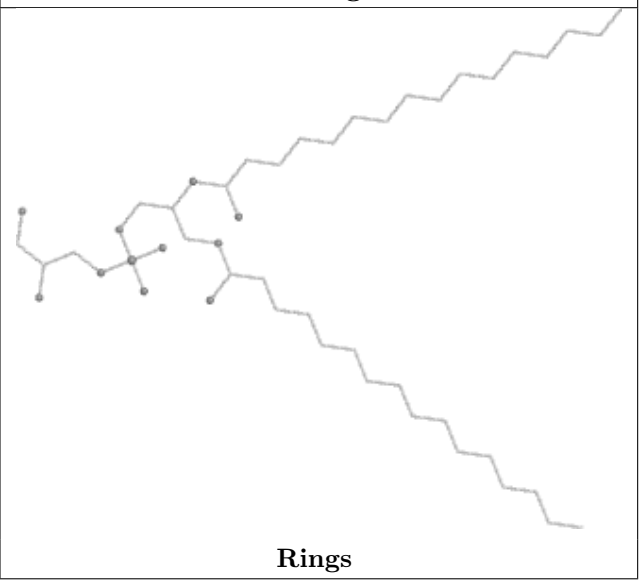
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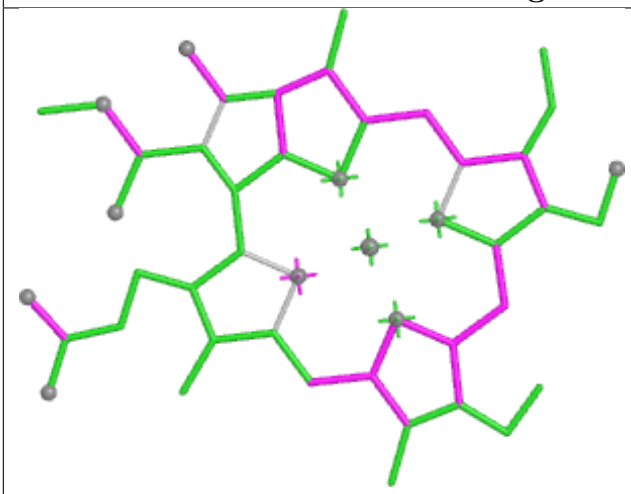


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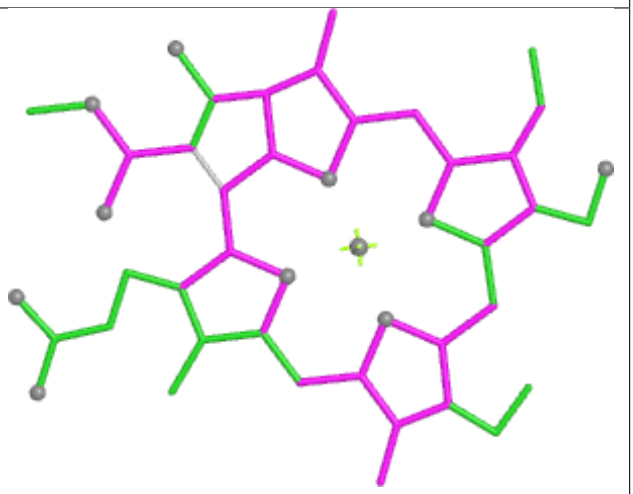


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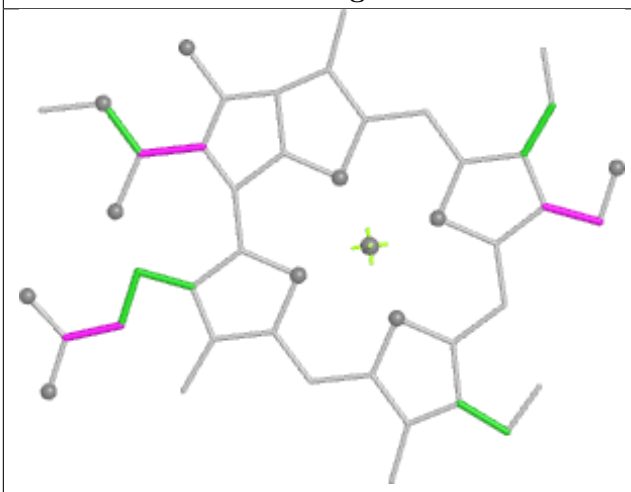
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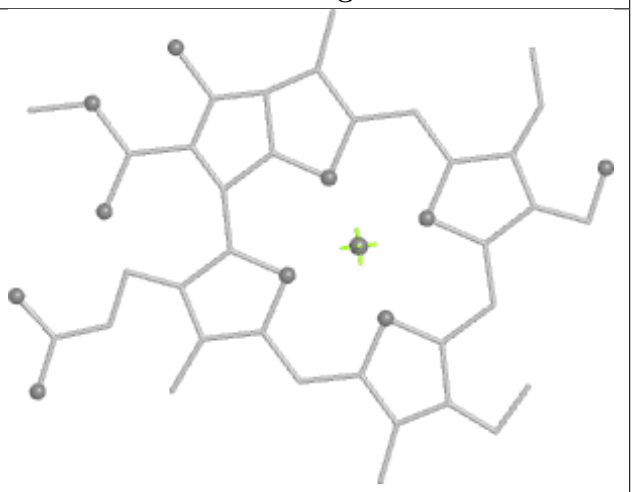
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Bond angles

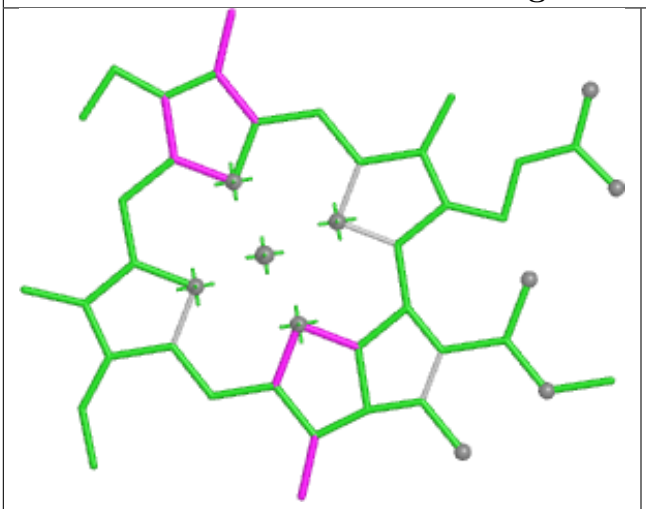


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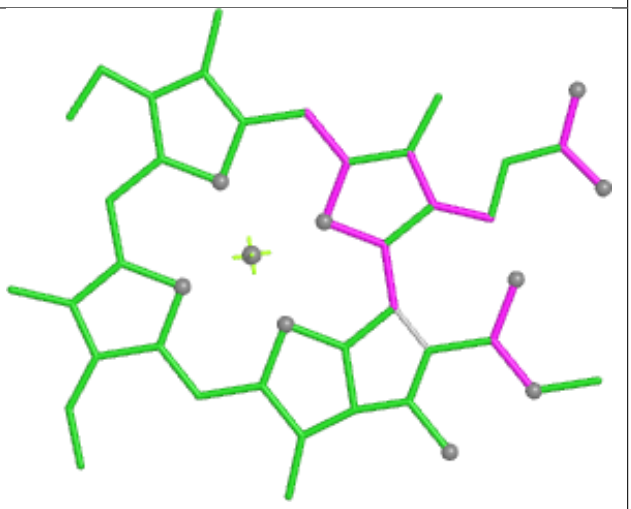


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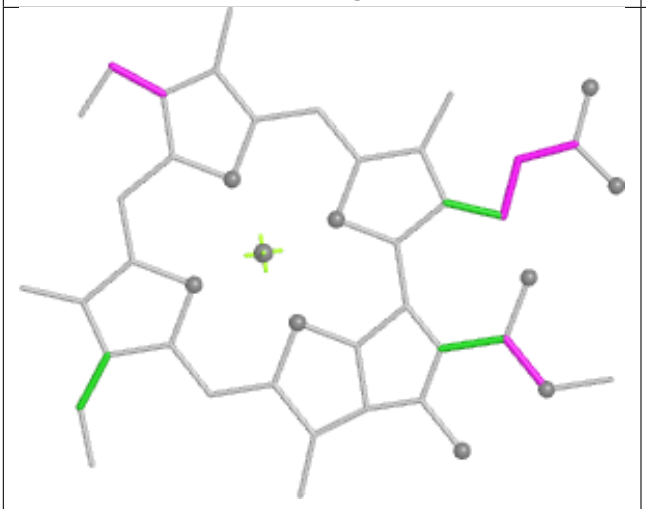
Ligand CLA 4 612



Bond lengths



Bond angles

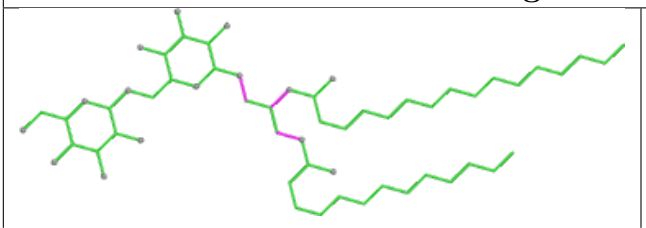


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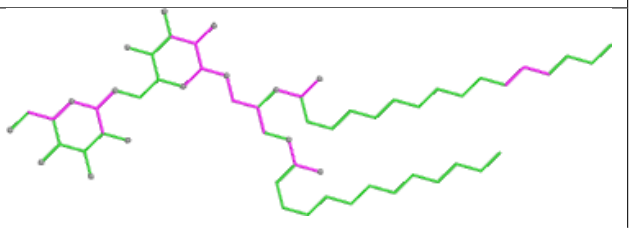


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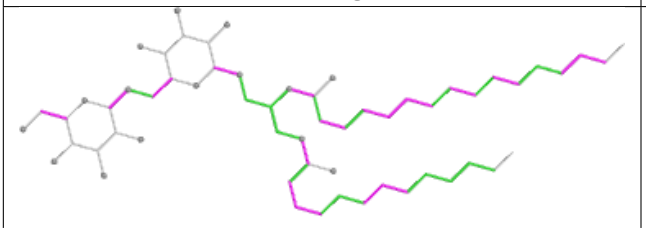
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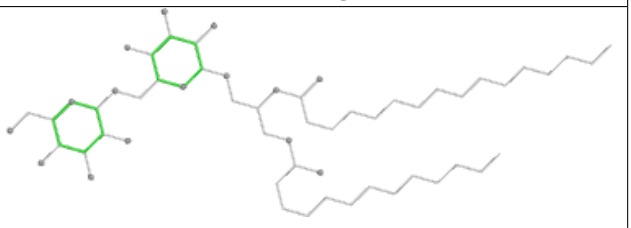
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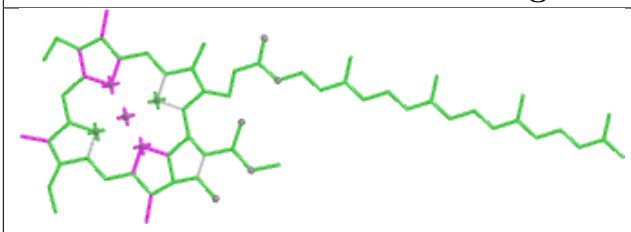


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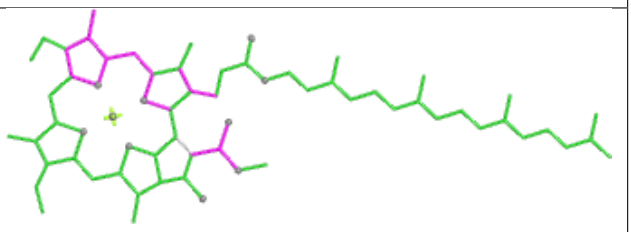


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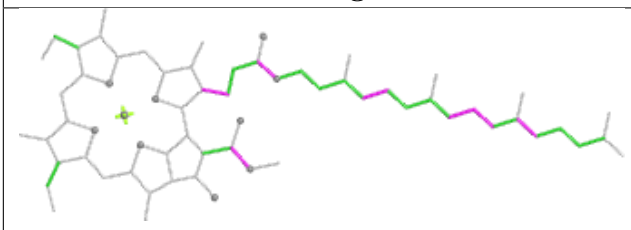
Ligand CLA c 512



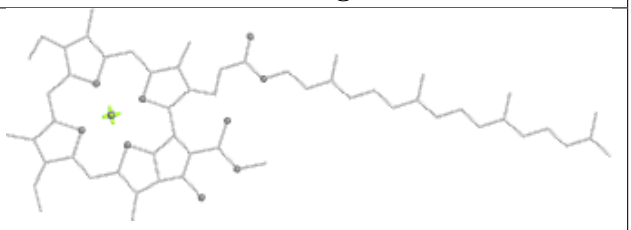
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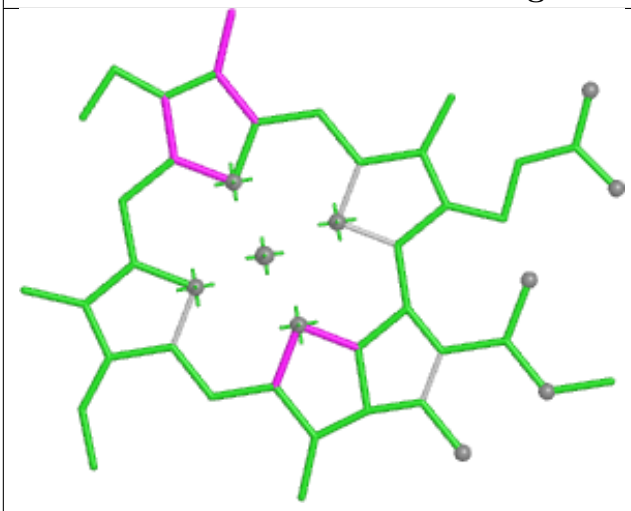


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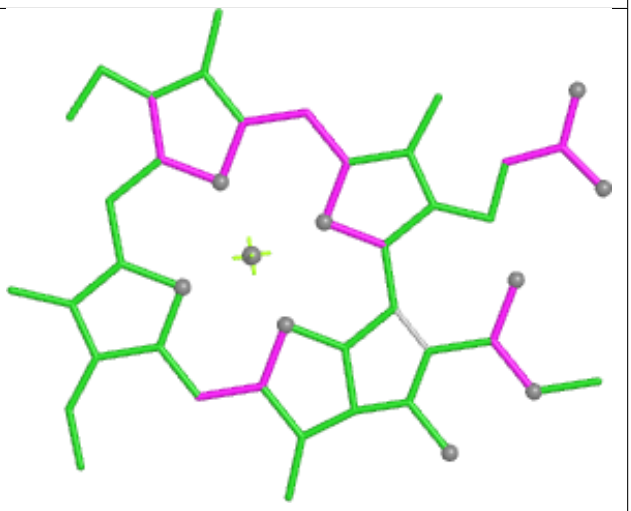


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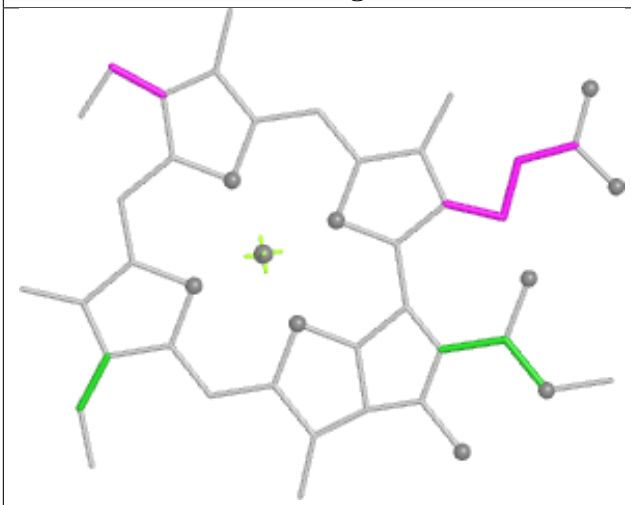
Ligand CLA S 609



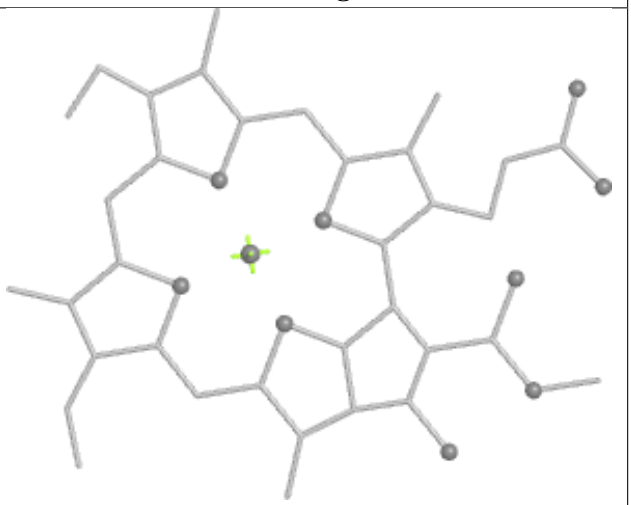
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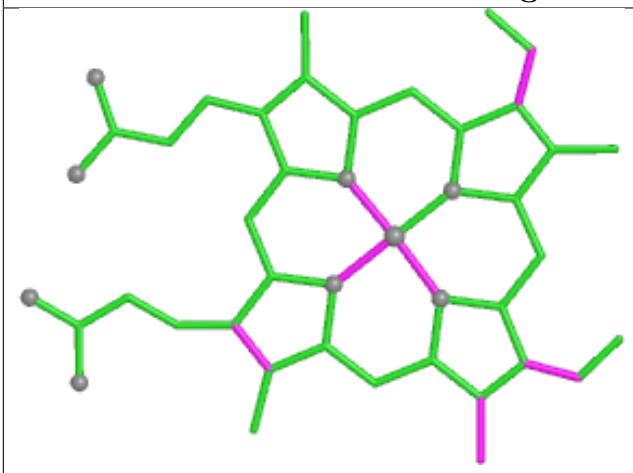


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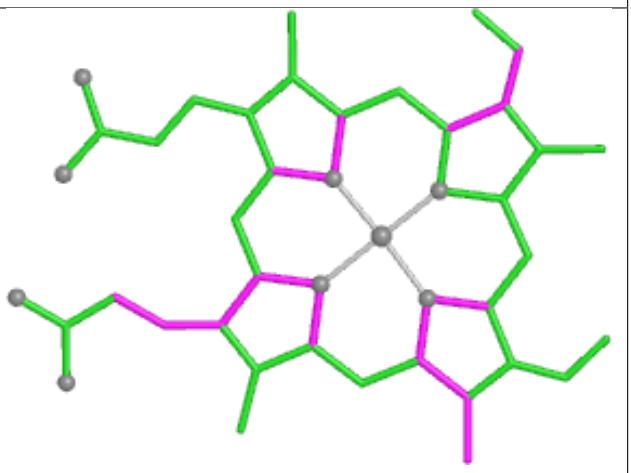


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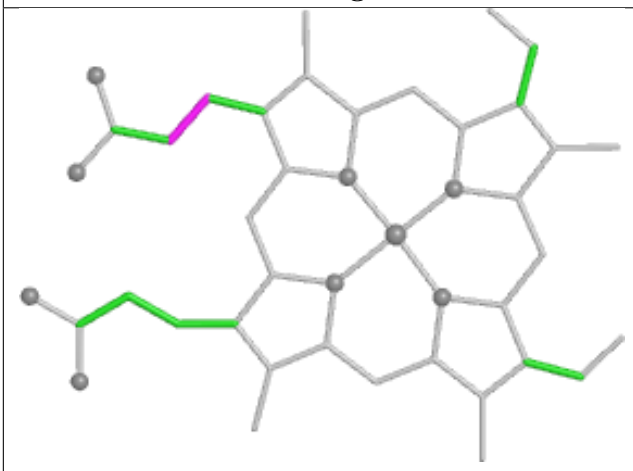
Ligand HEM F 101



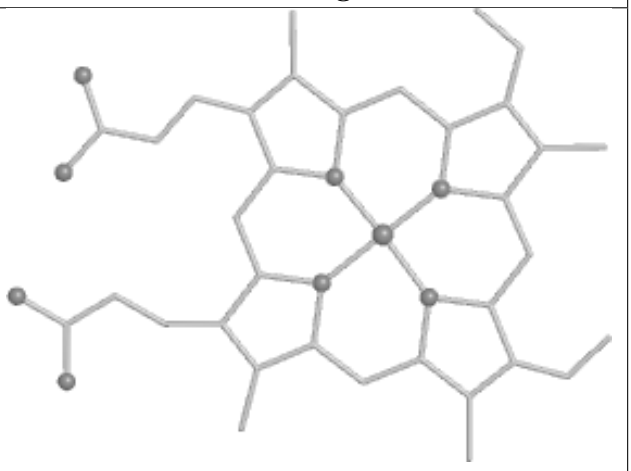
Bond lengths



Bond angles

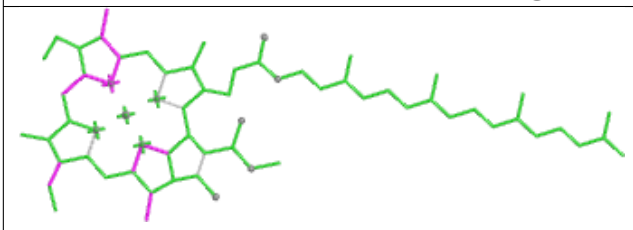


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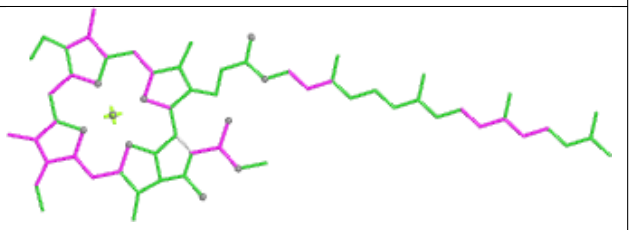


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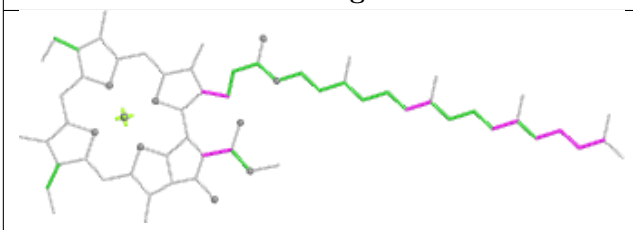
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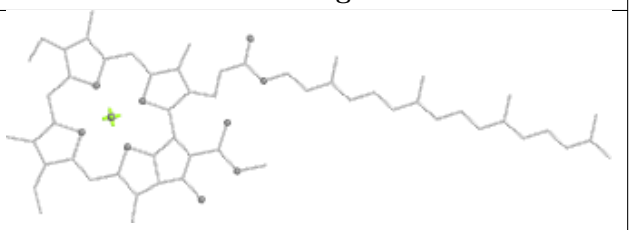
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Bond angles

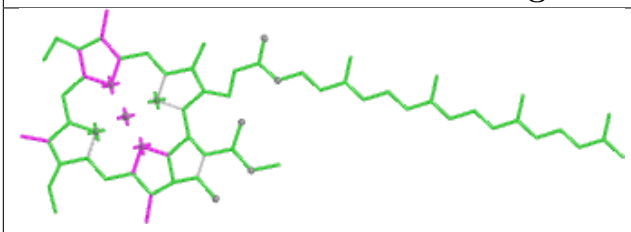


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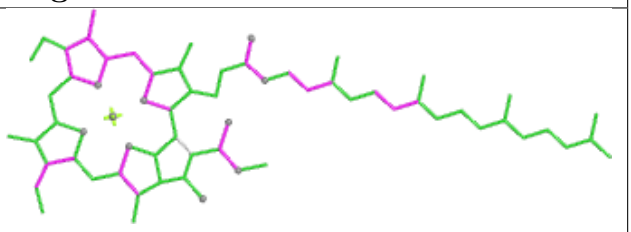


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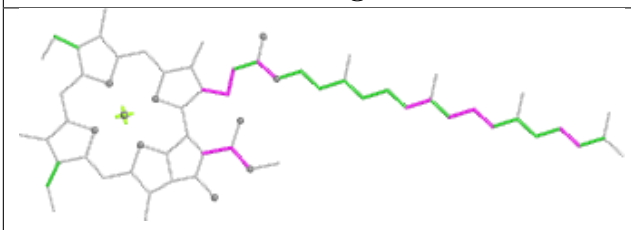
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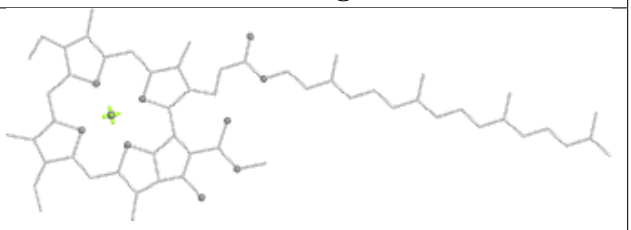
Bond lengths



Bond angles

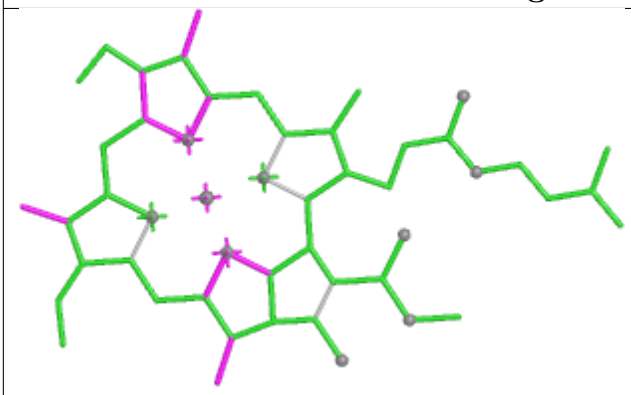


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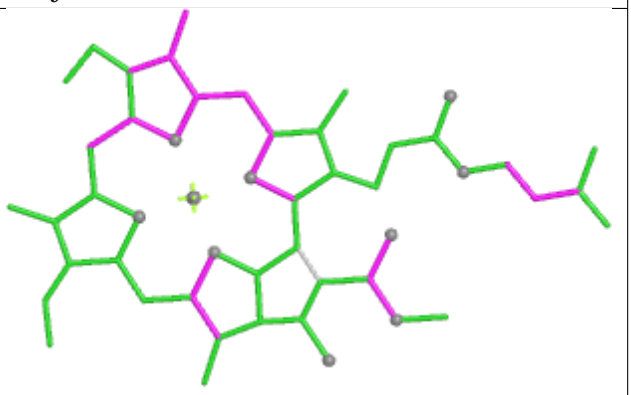


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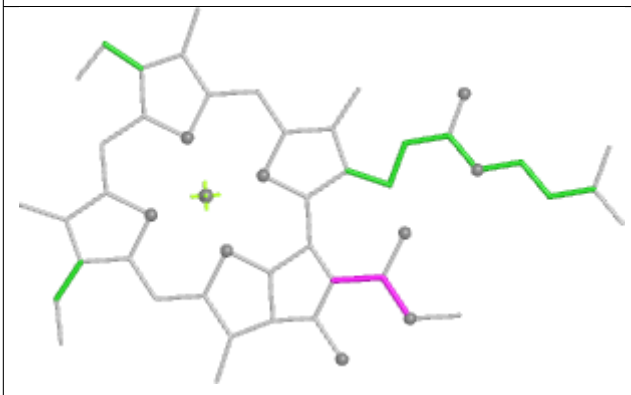
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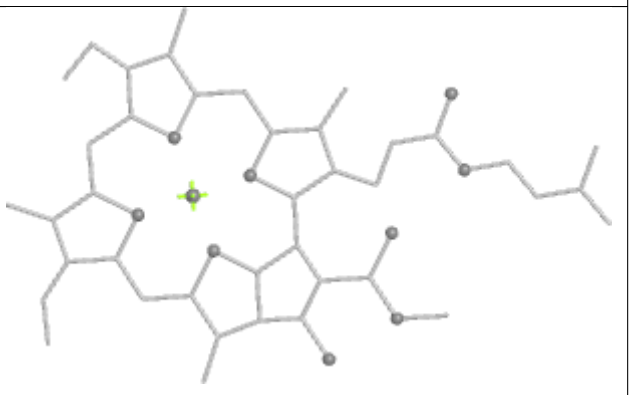
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Bond angles

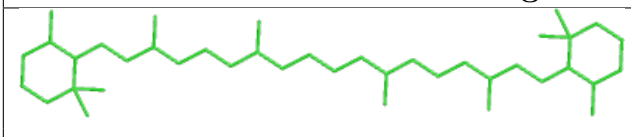


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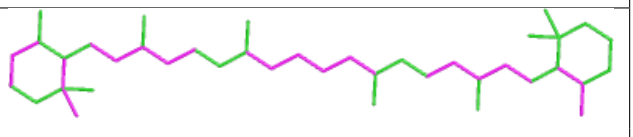


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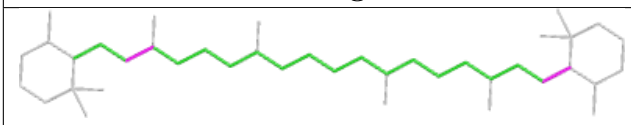
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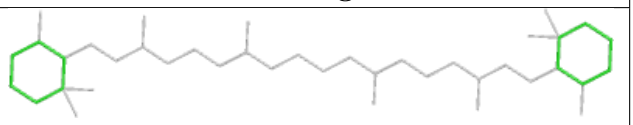
Bond lengths



Bond angles

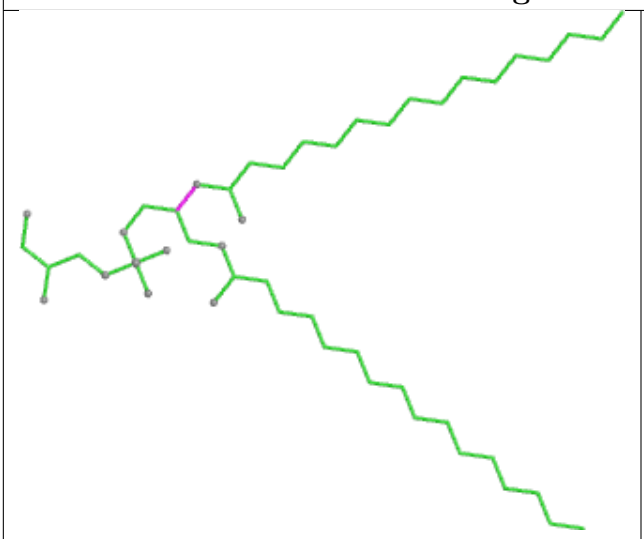


Torsions

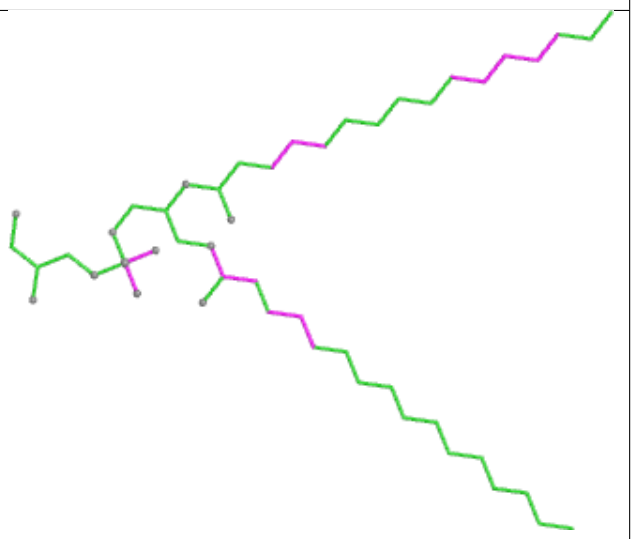


Rings

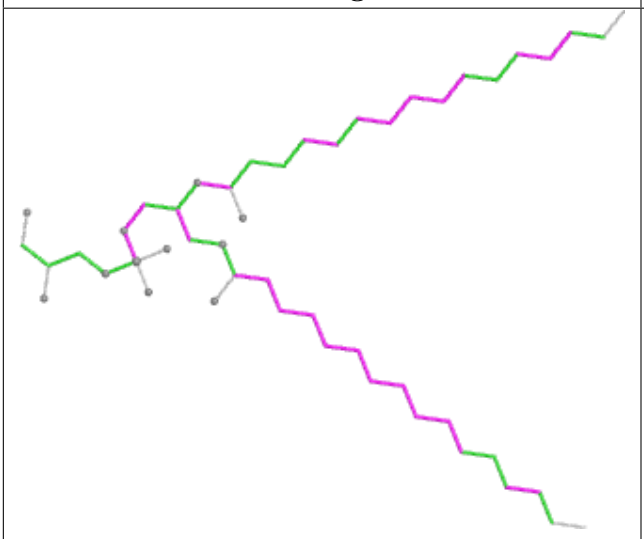
Ligand LHG G 2630



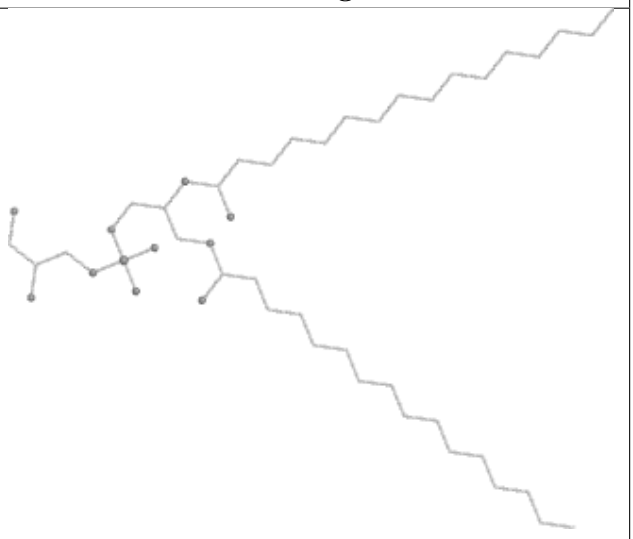
Bond lengths



Bond angles

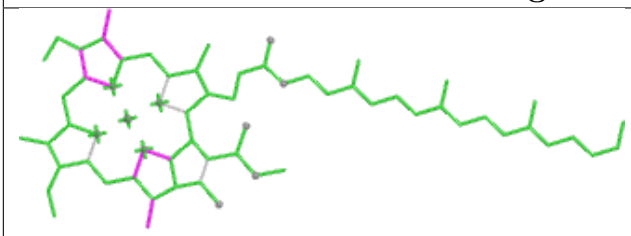


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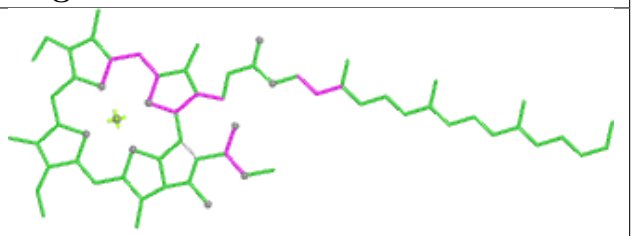


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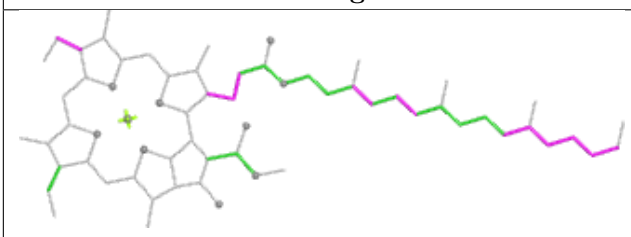
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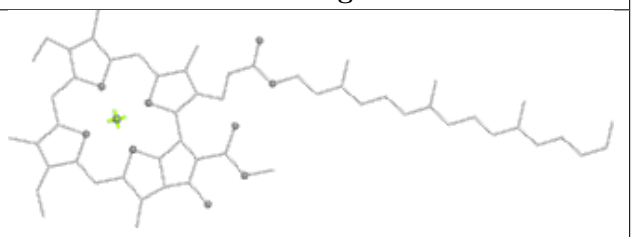
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Bond angles

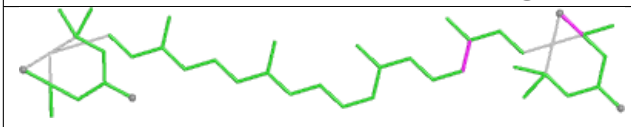


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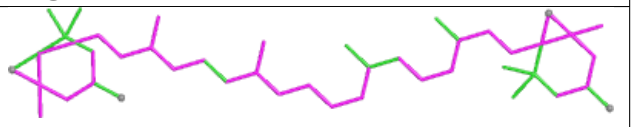


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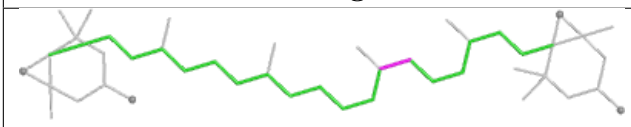
Ligand XAT g 1622



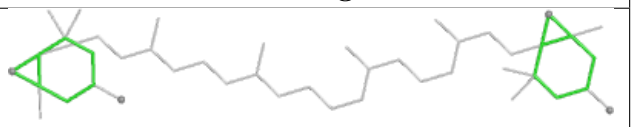
Bond lengths



Bond angles



Torsions

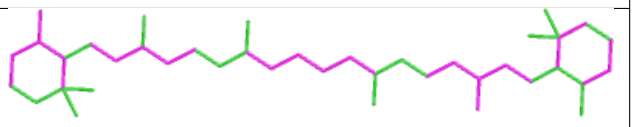


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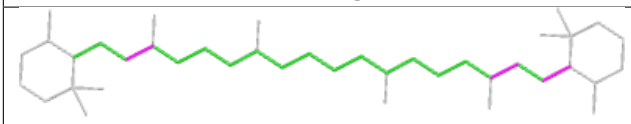
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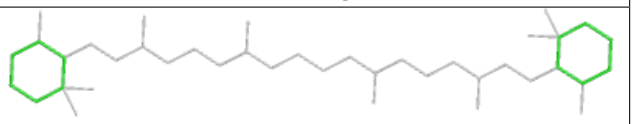
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Bond angles

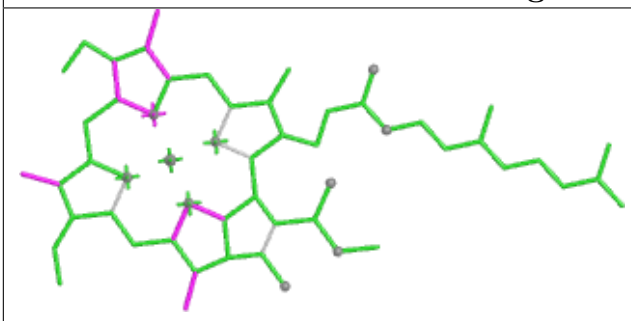


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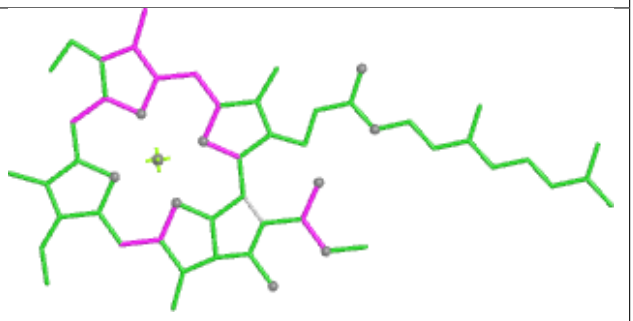


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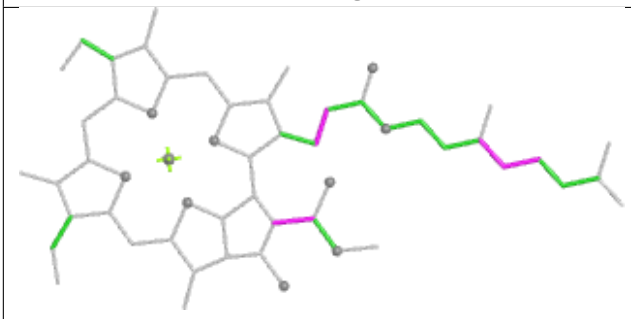
Ligand CLA S 613



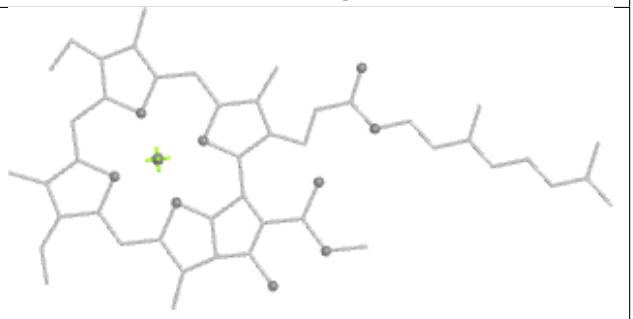
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Bond angles

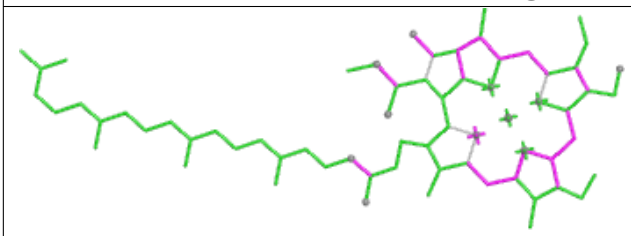


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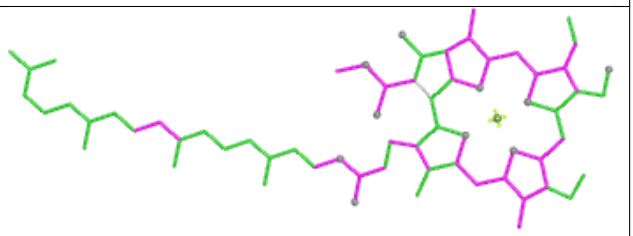


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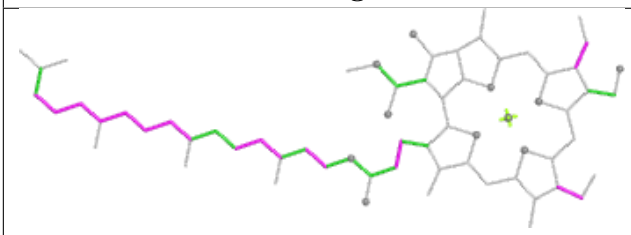
Ligand CHL G 607



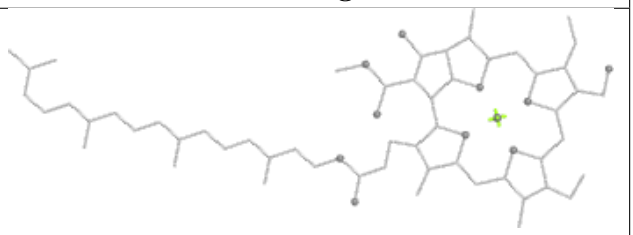
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Bond angles

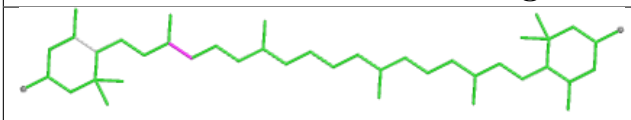


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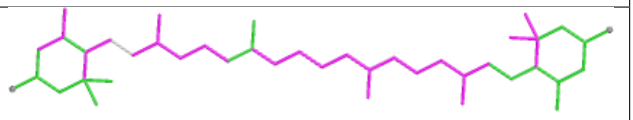


Rings

Ligand LUT s 1621



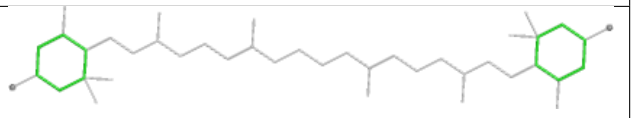
Bond lengths



Bond angles

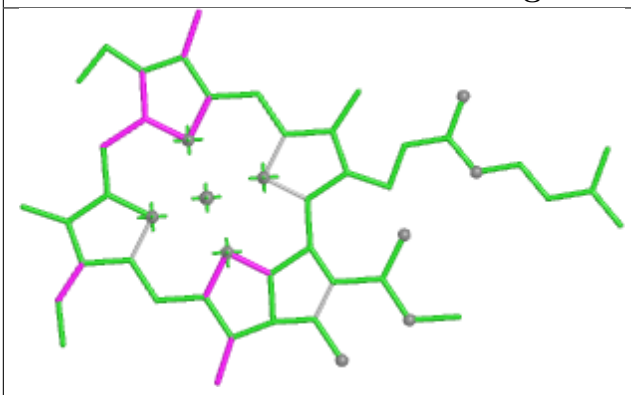


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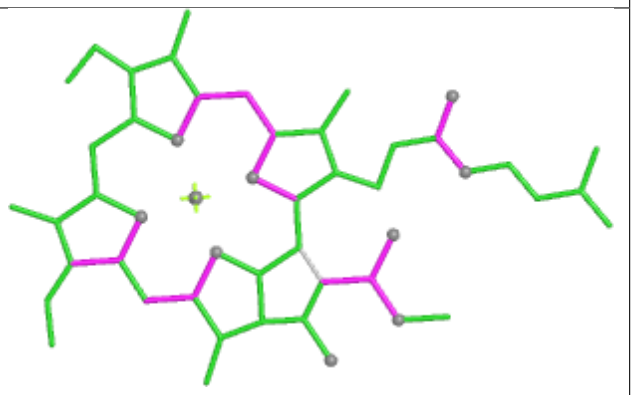


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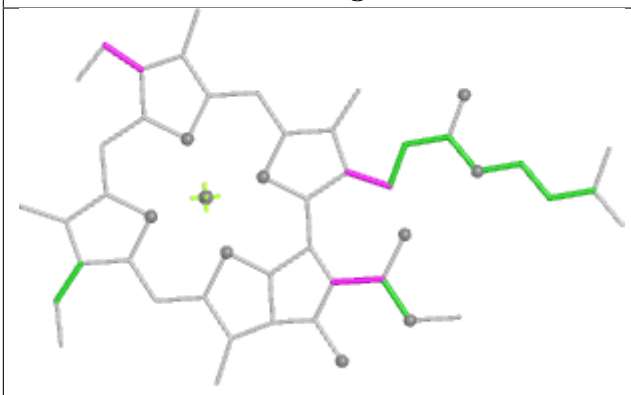
Ligand CLA A 407



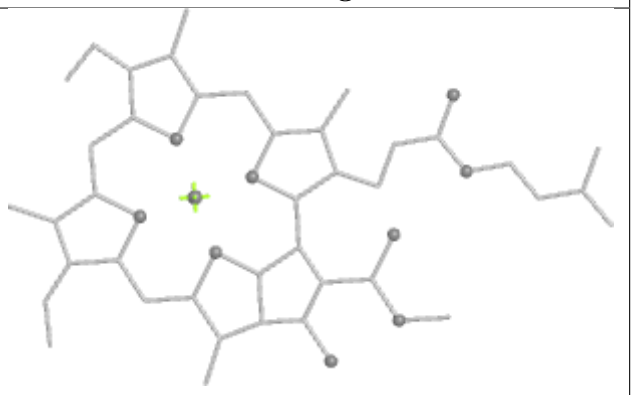
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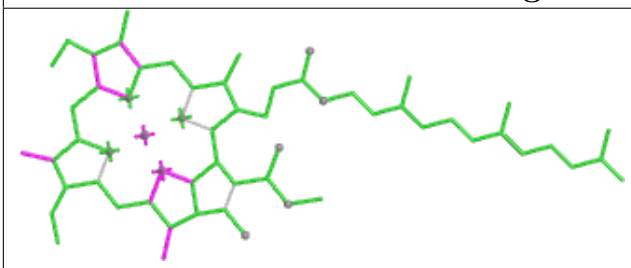


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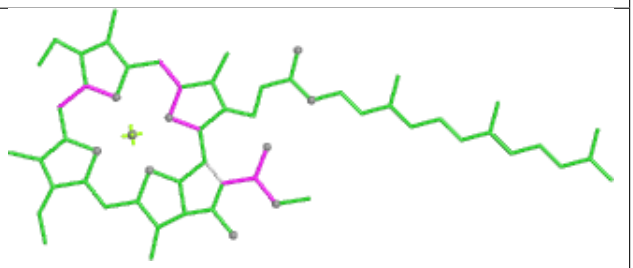


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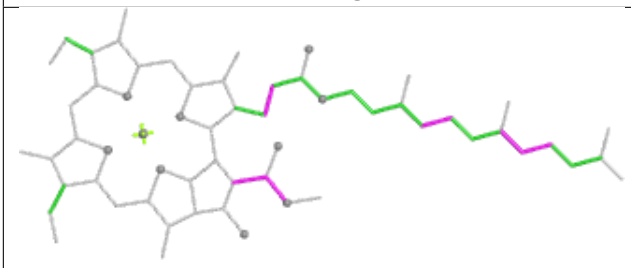
Ligand CLA N 613



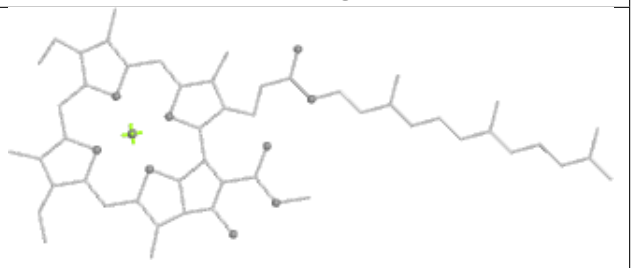
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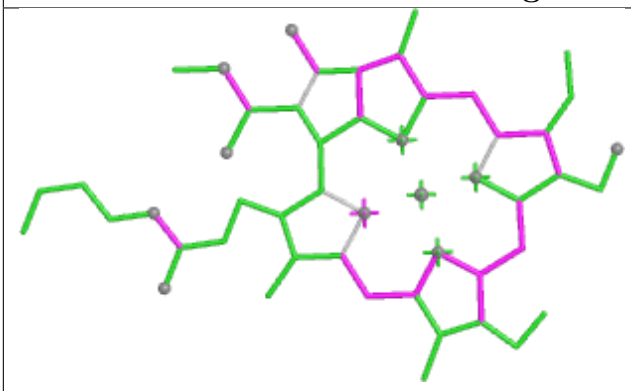


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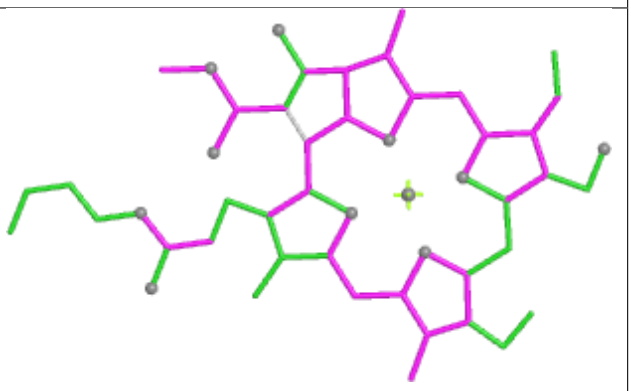


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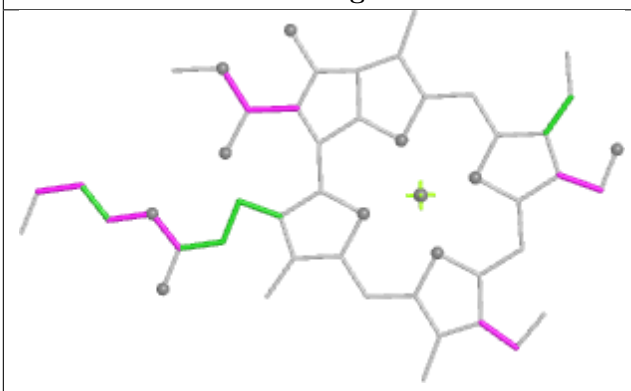
Ligand CHL G 606



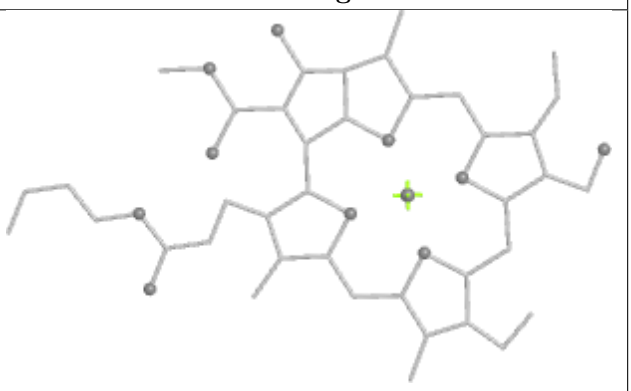
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Bond angles

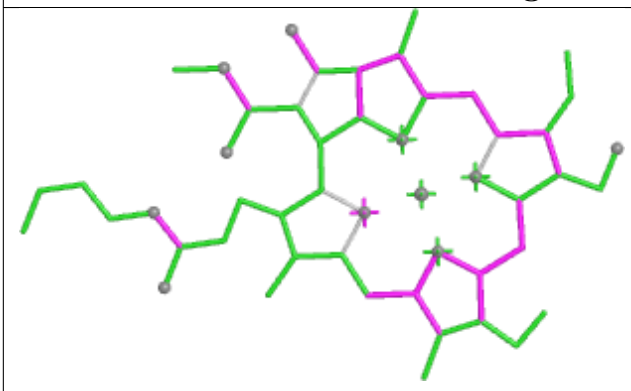


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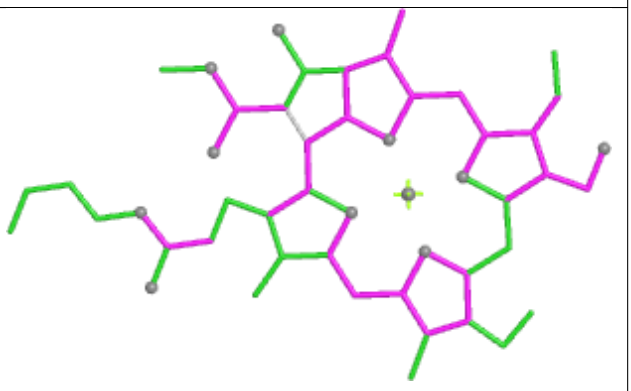


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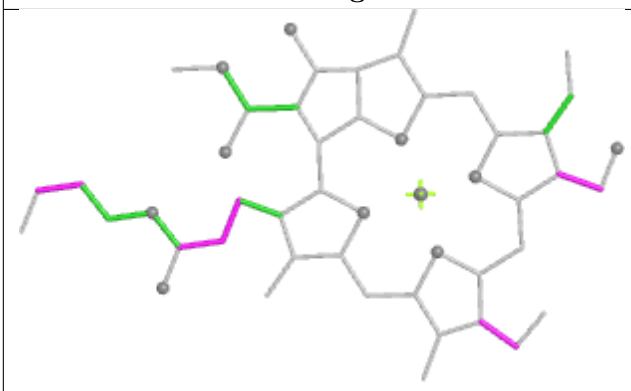
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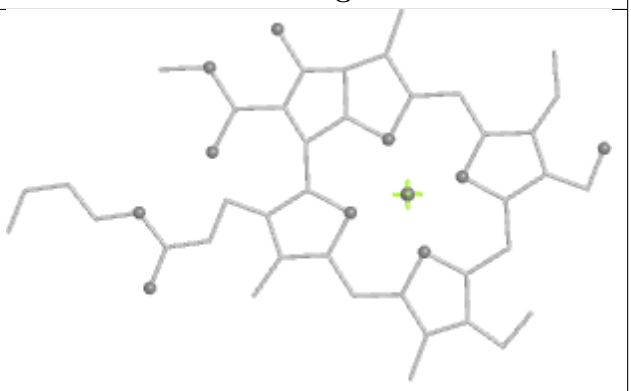
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Bond angles

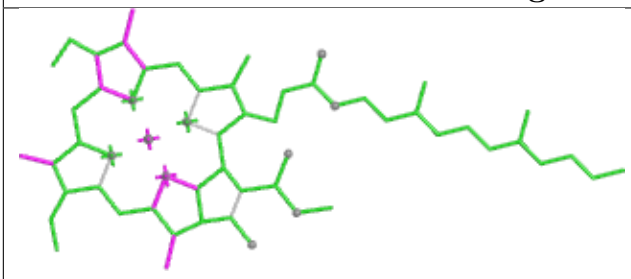


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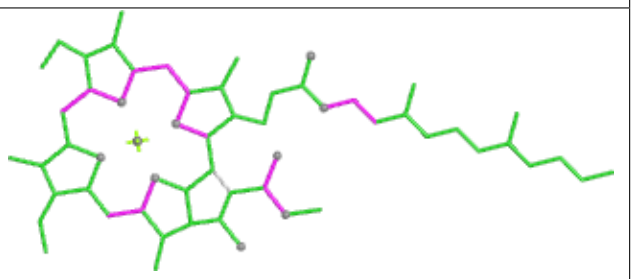


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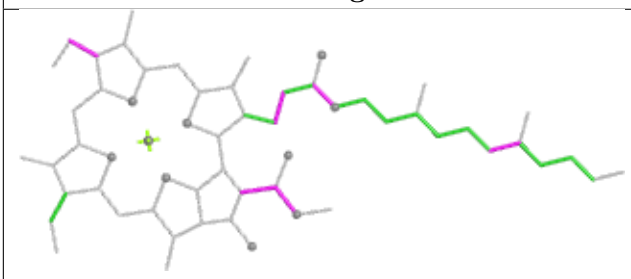
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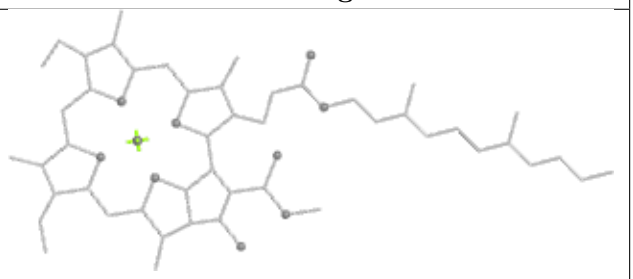
Bond lengths



Bond angles

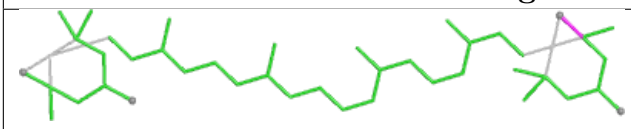


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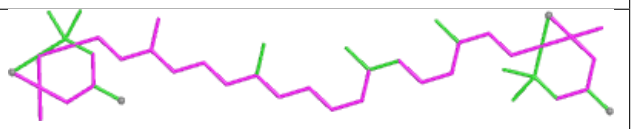


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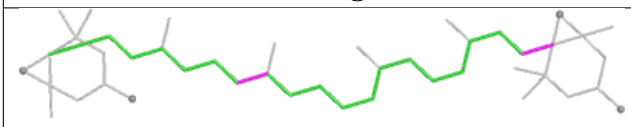
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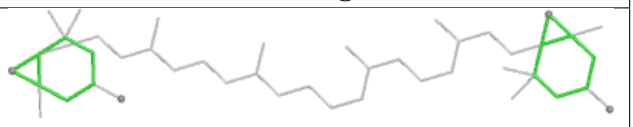
Bond lengths



Bond angles

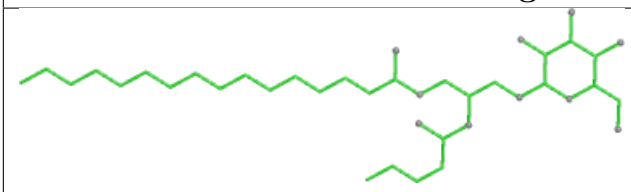


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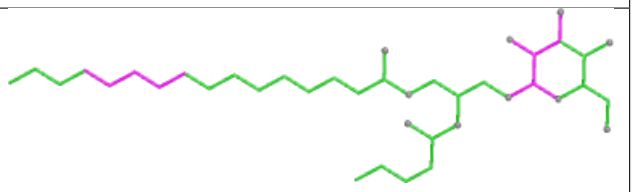


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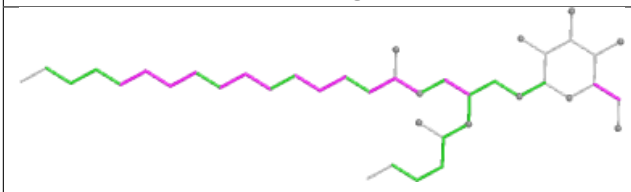
Ligand LMG A 415



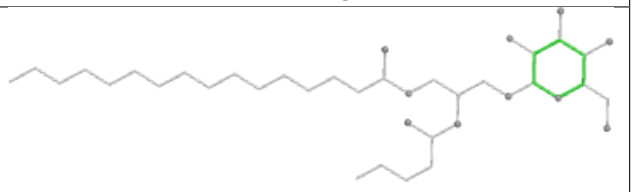
Bond lengths



Bond angles

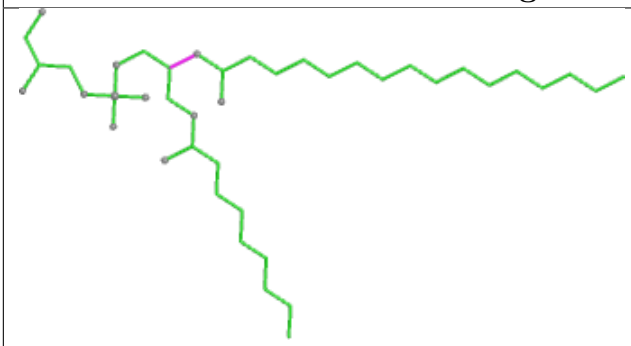


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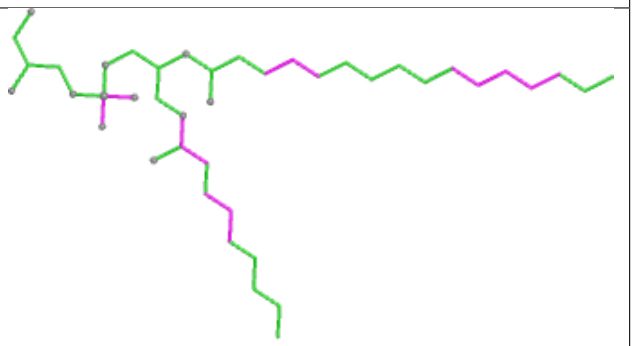


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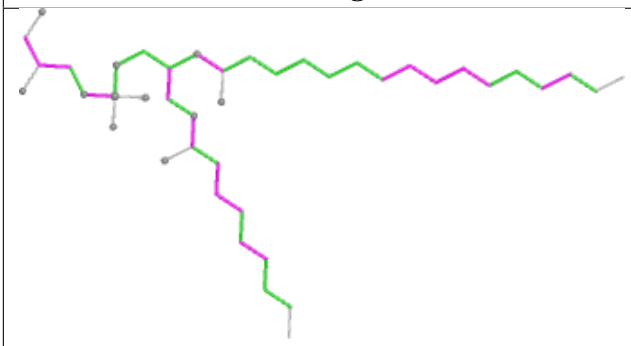
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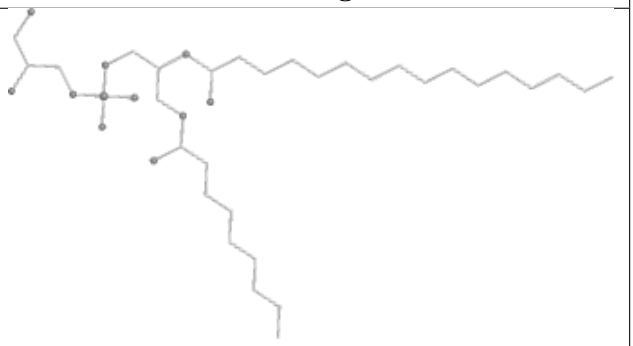
Bond lengths



Bond angles

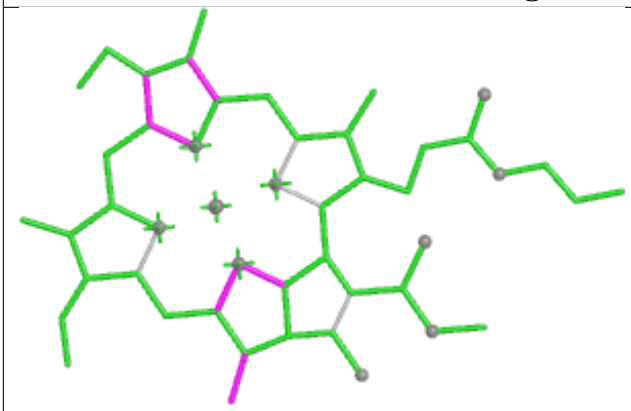


Torsions

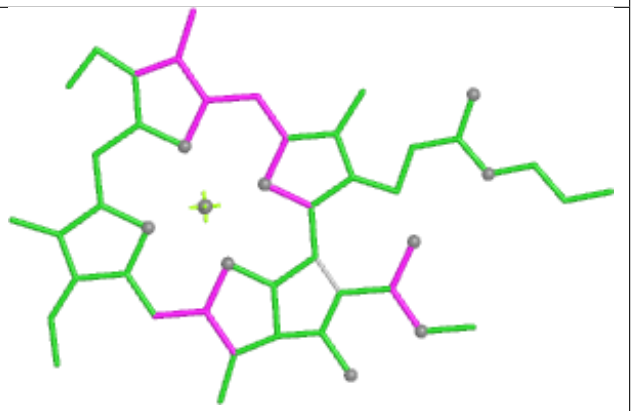


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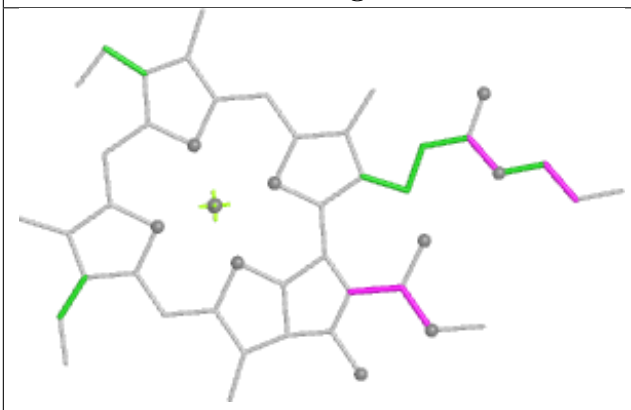
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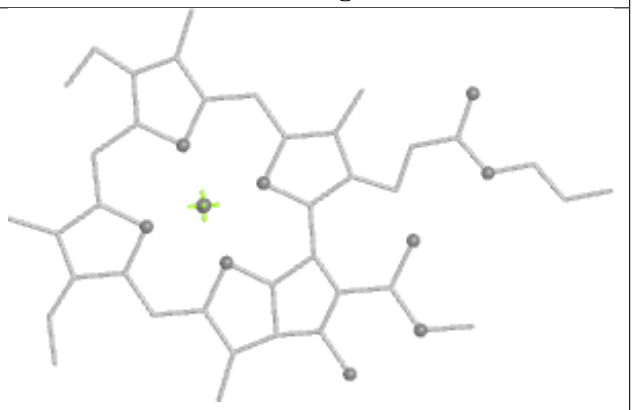
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Bond angles

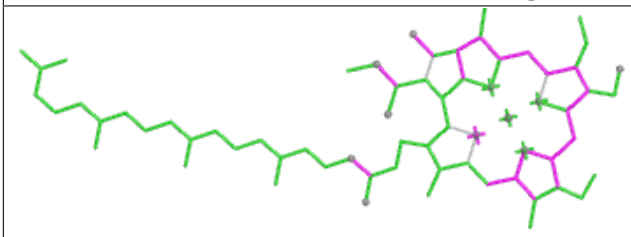


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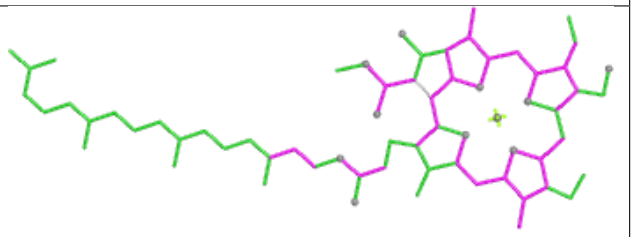


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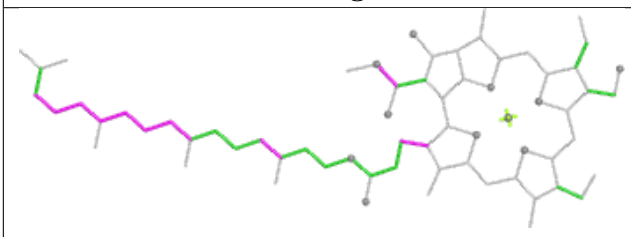
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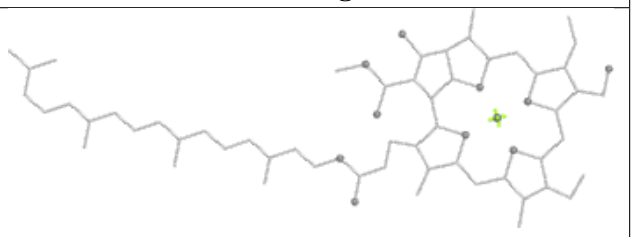
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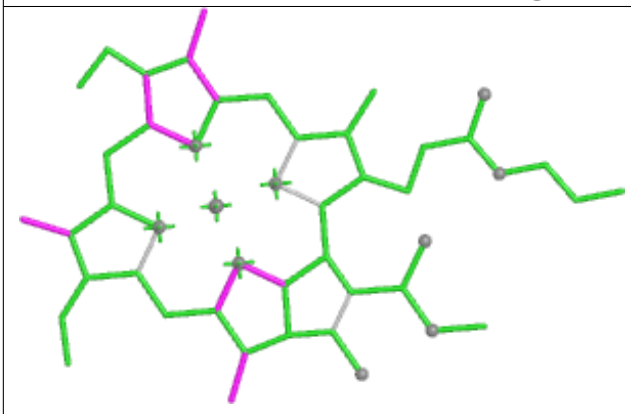


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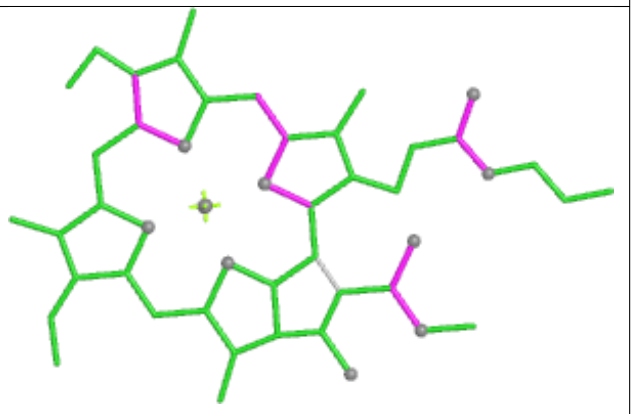


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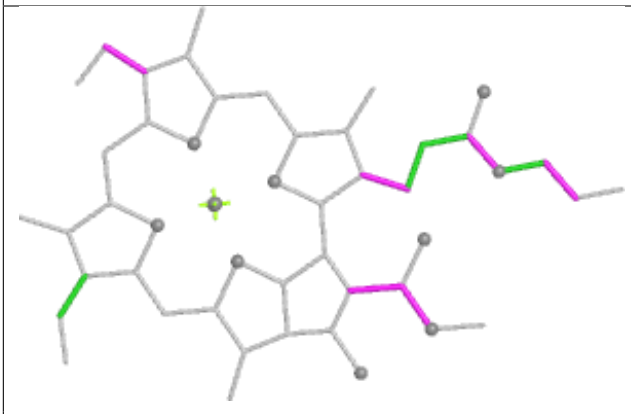
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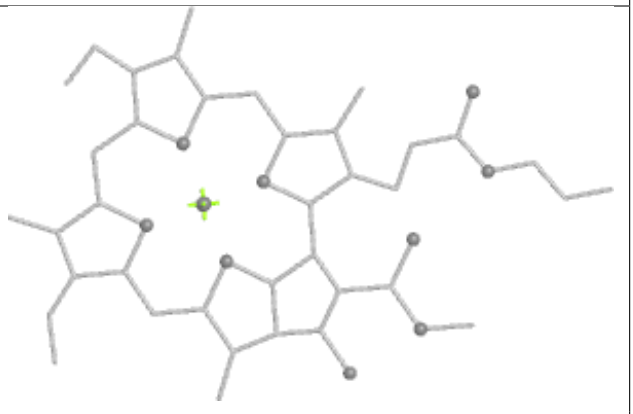
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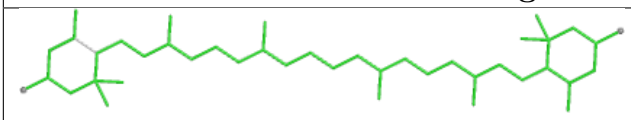


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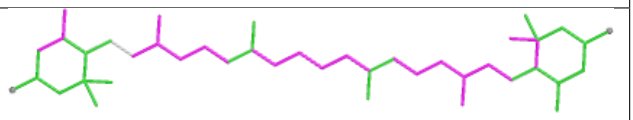


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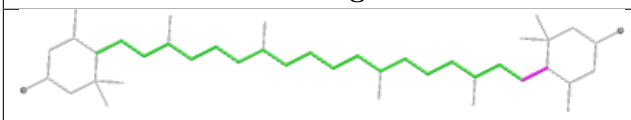
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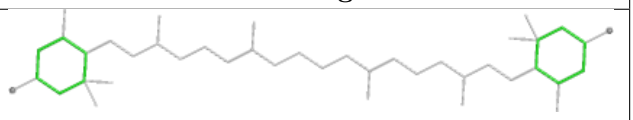
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Bond angles

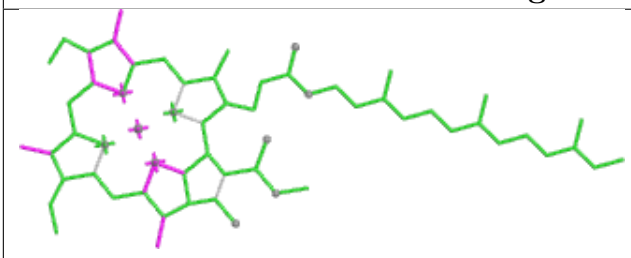


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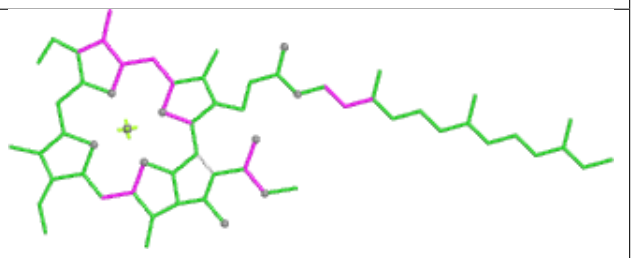


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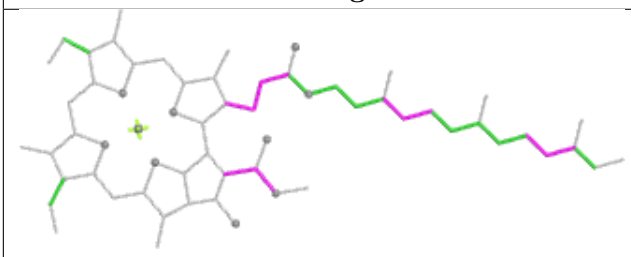
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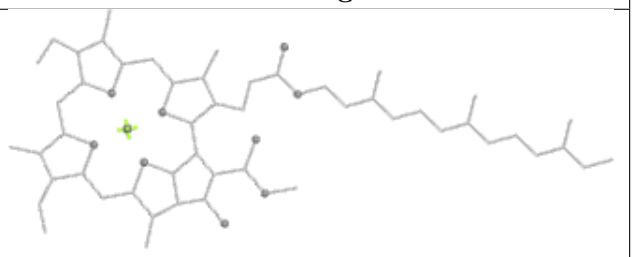
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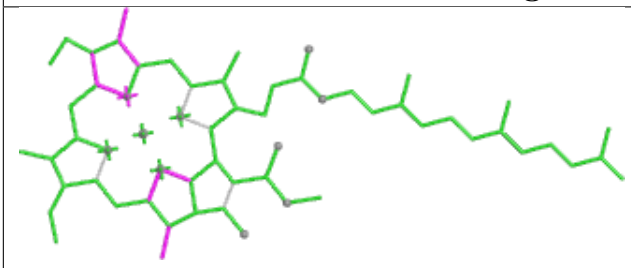


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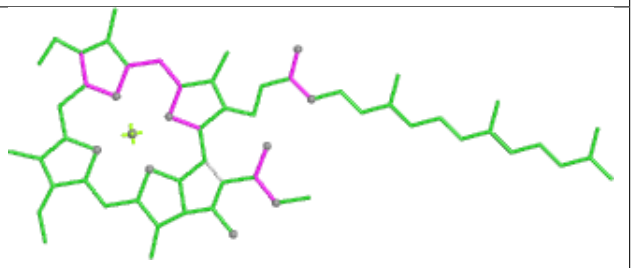


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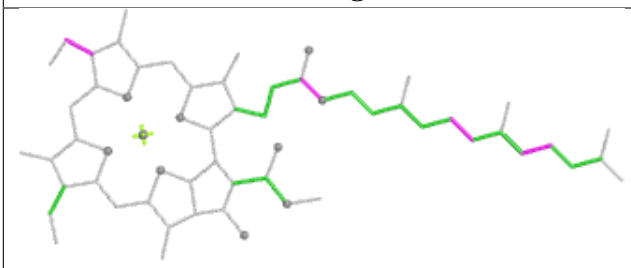
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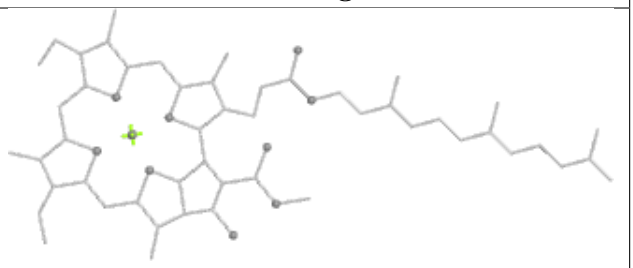
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Bond angles

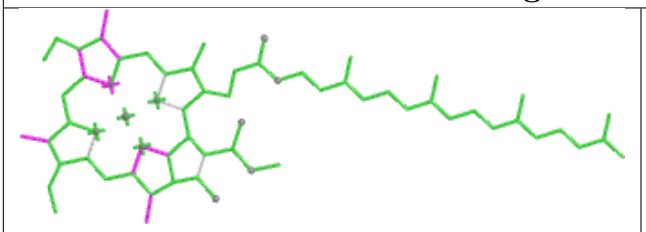


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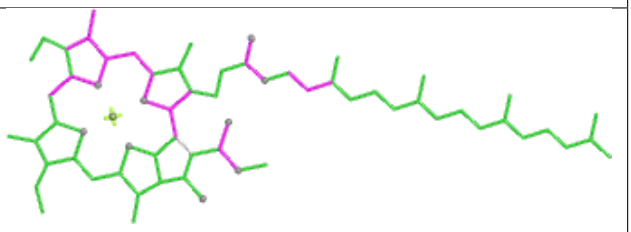


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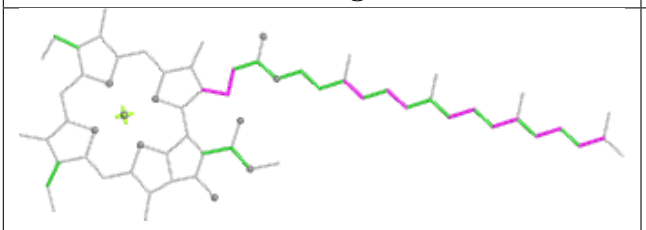
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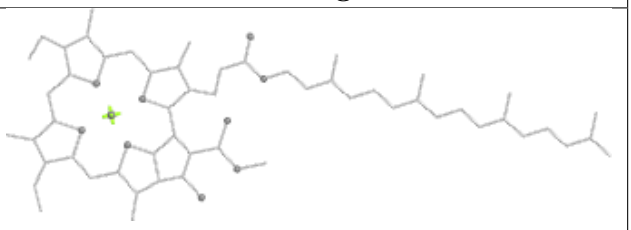
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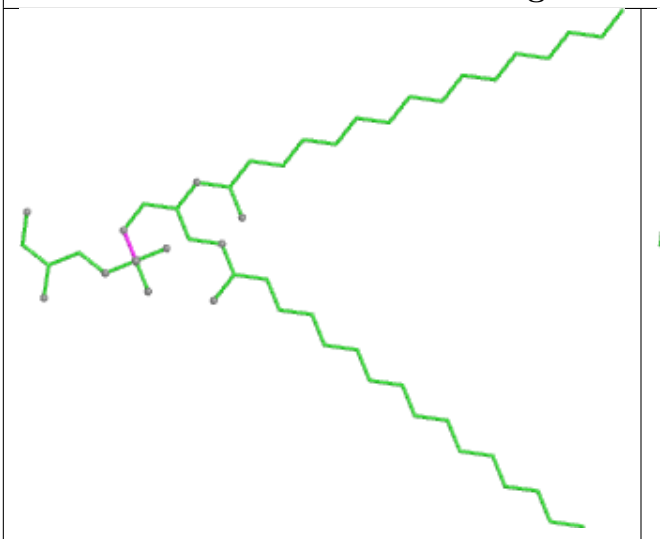


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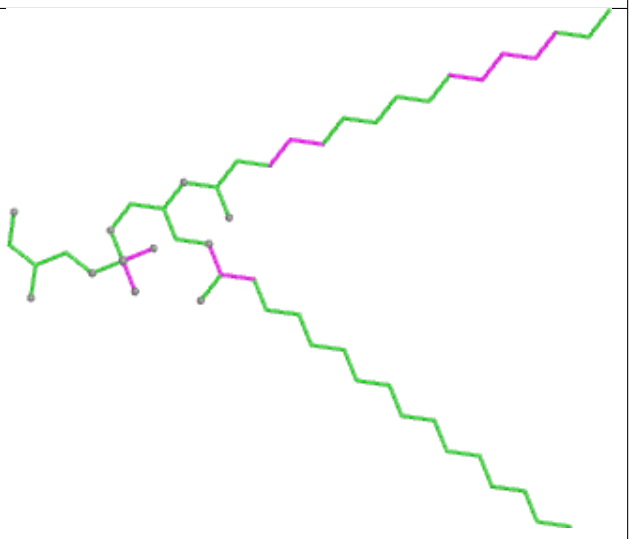


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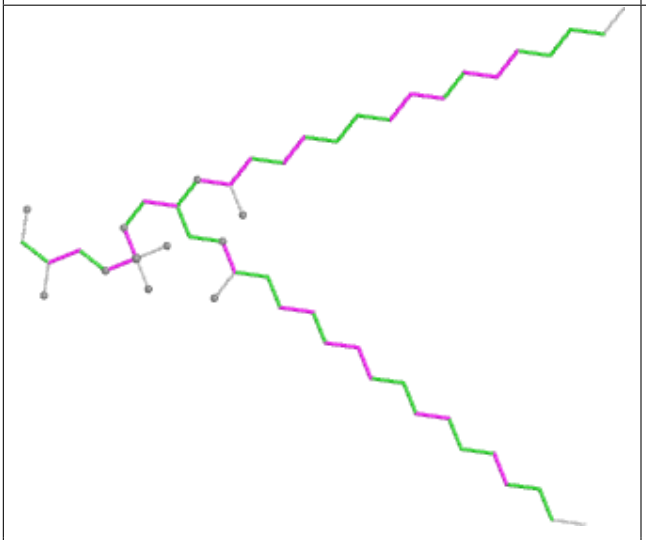
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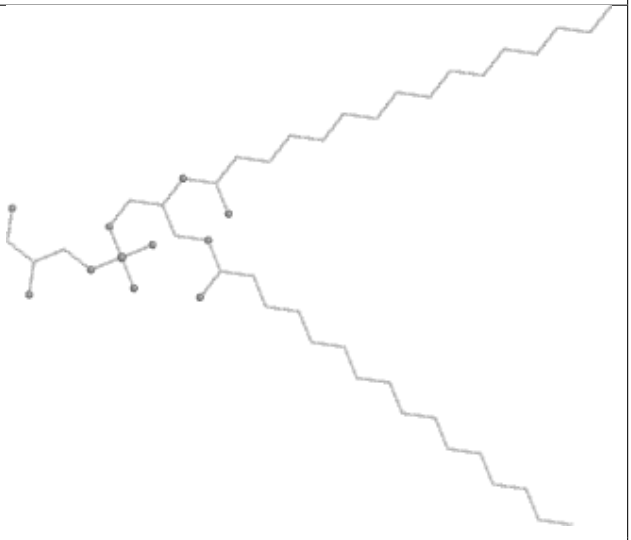
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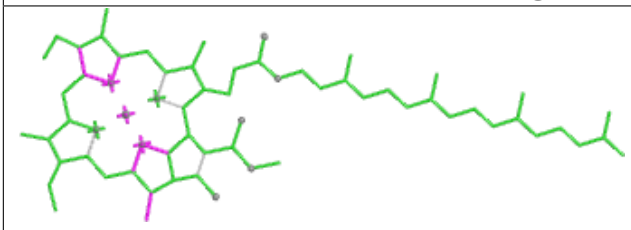


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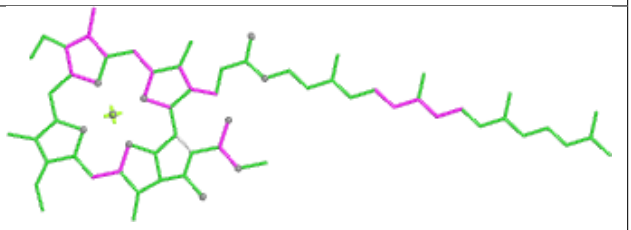


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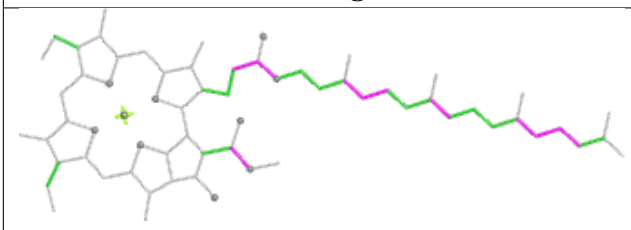
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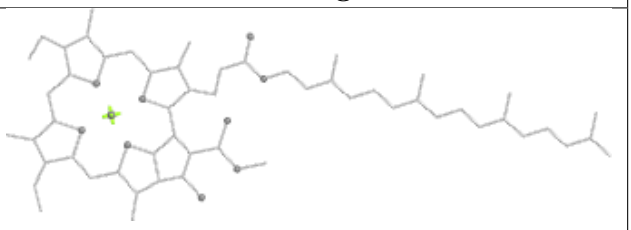
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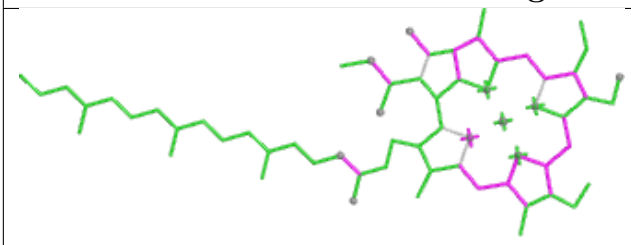


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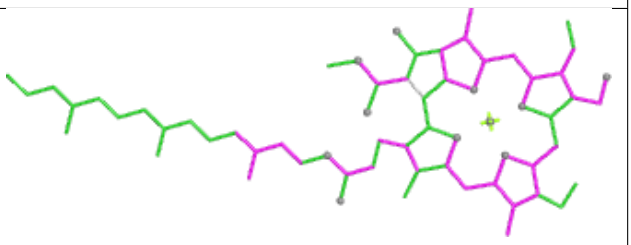


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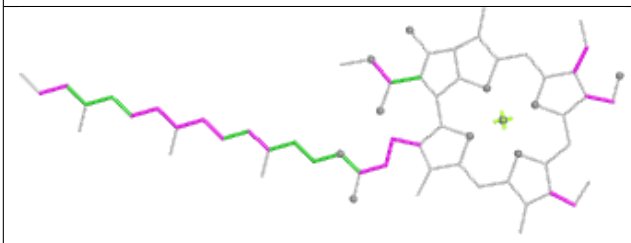
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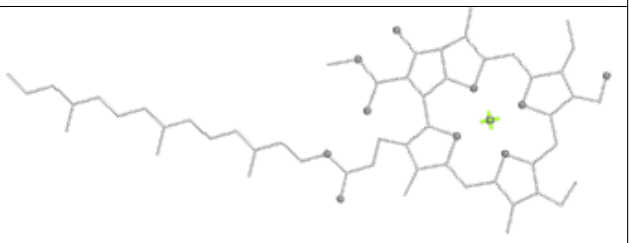
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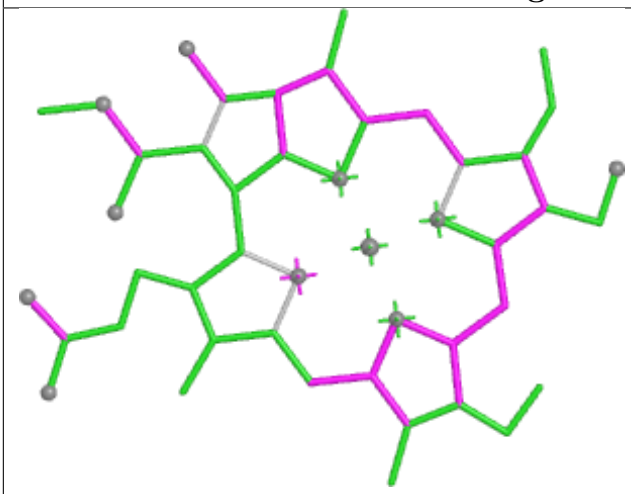


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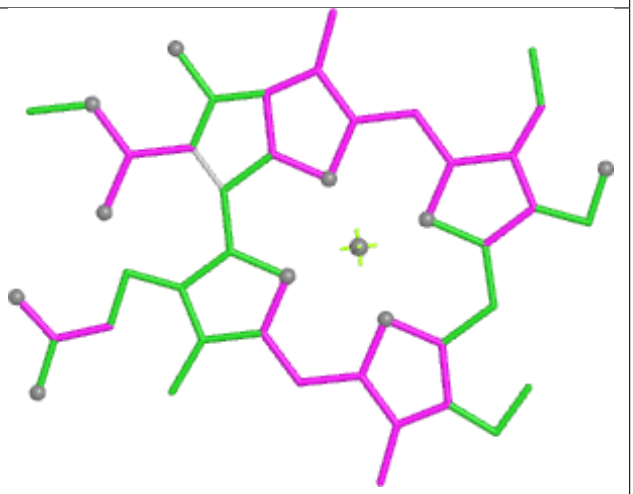


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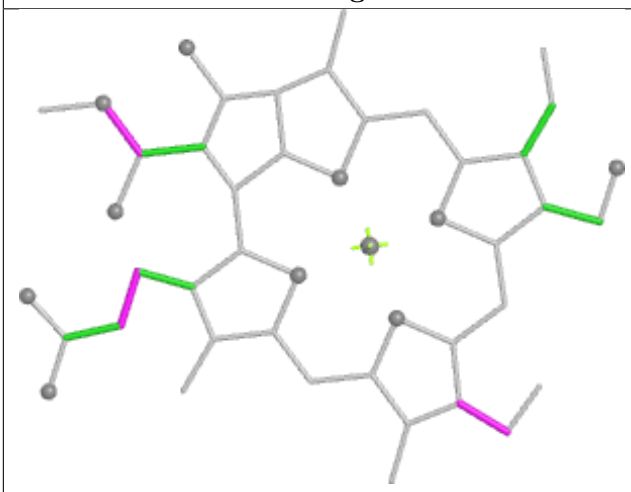
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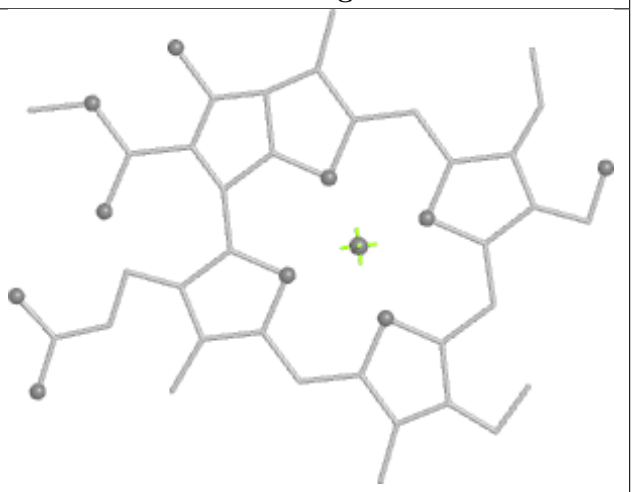
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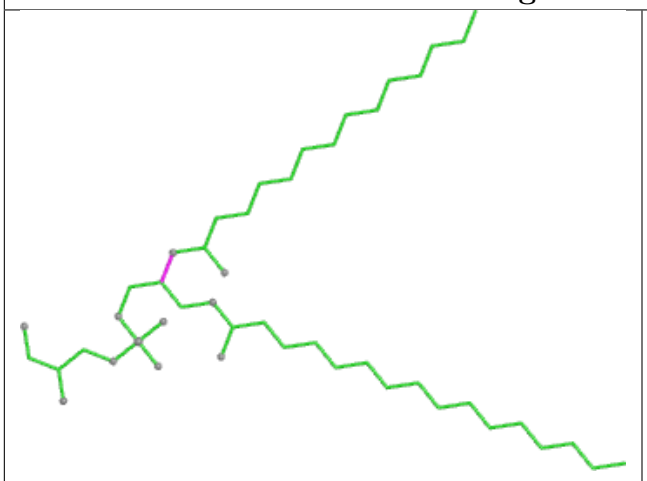


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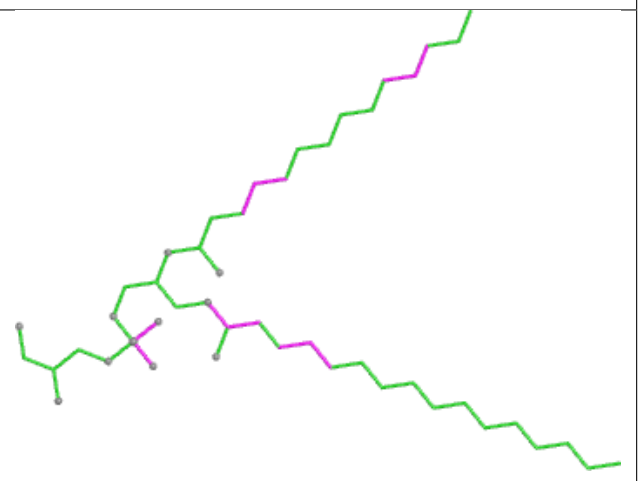


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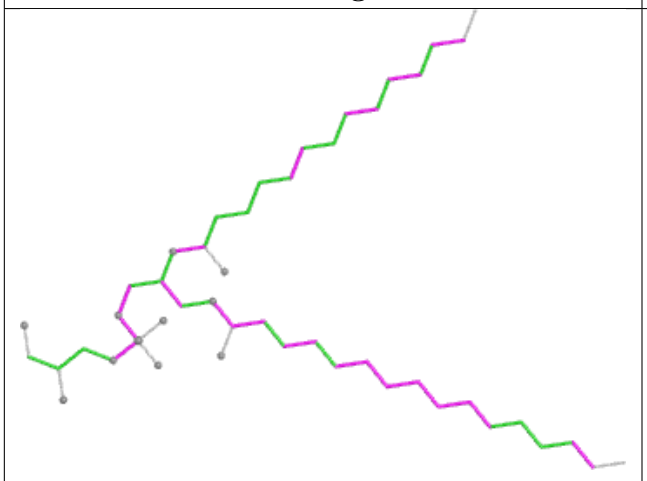
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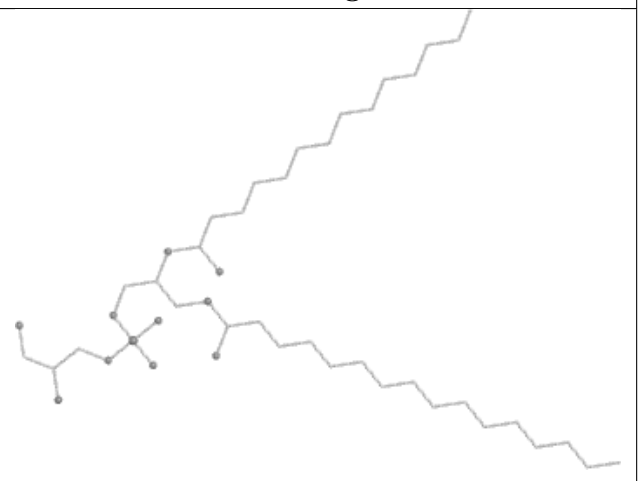
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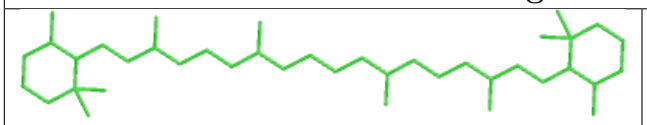


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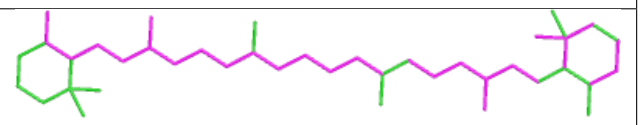


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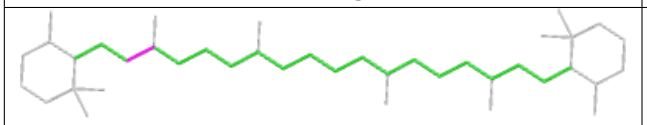
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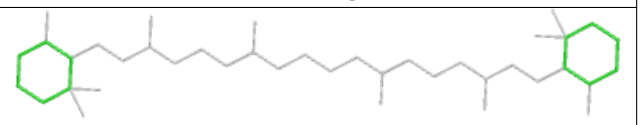
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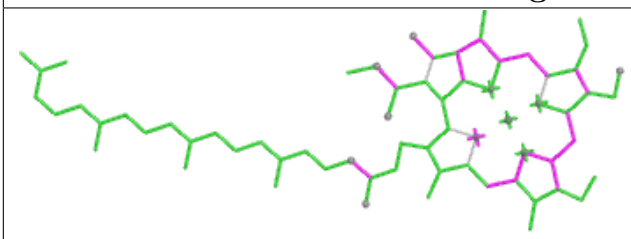


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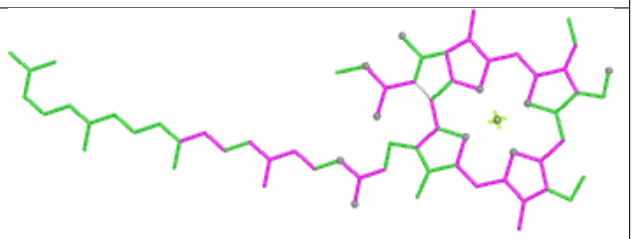


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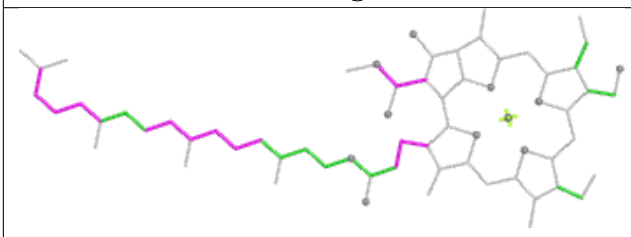
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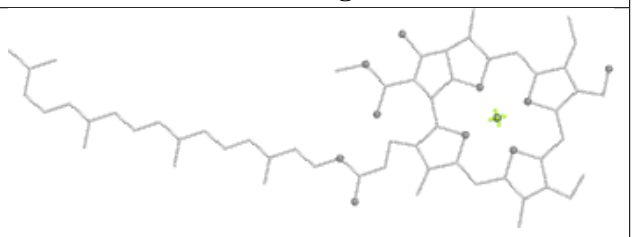
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Bond angles

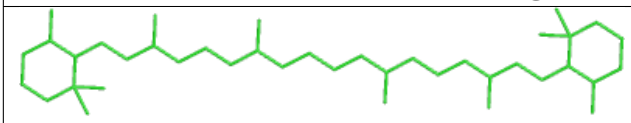


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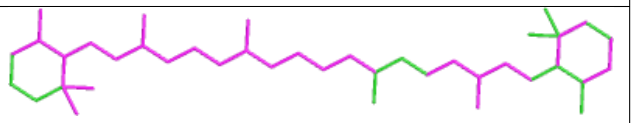


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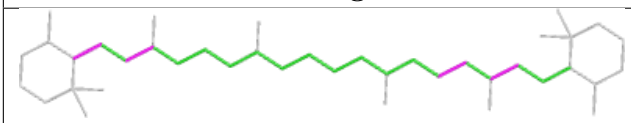
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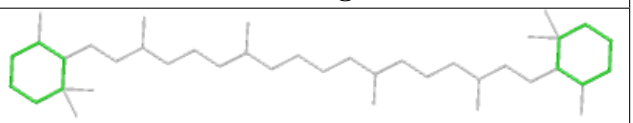
Bond lengths



Bond angles

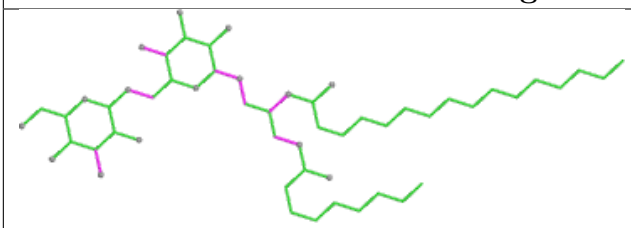


Torsions

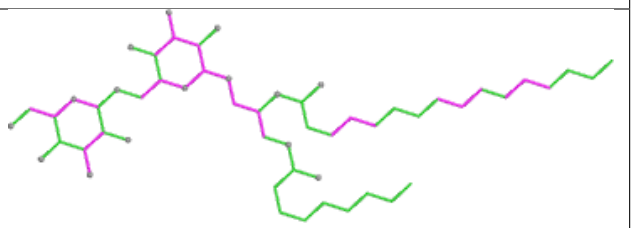


Rings

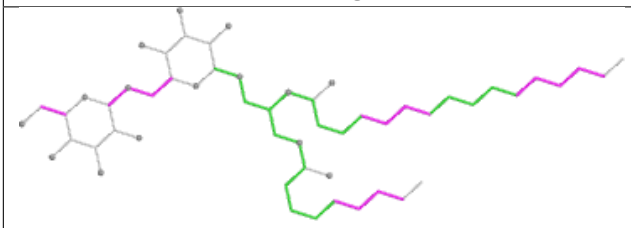
Ligand DGD C 518



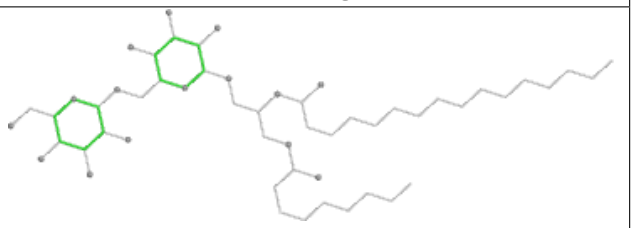
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Bond angles

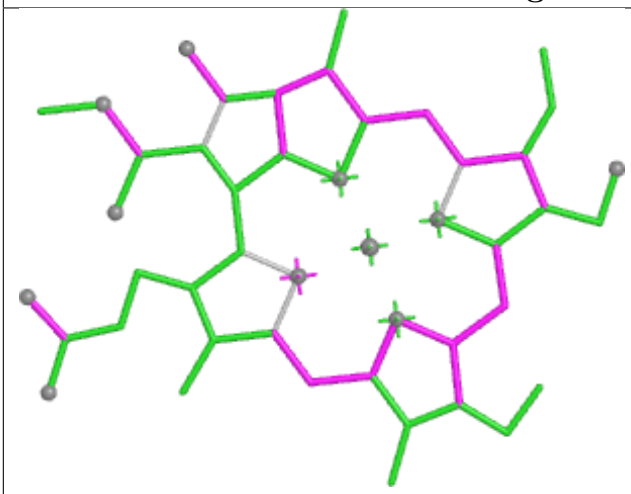


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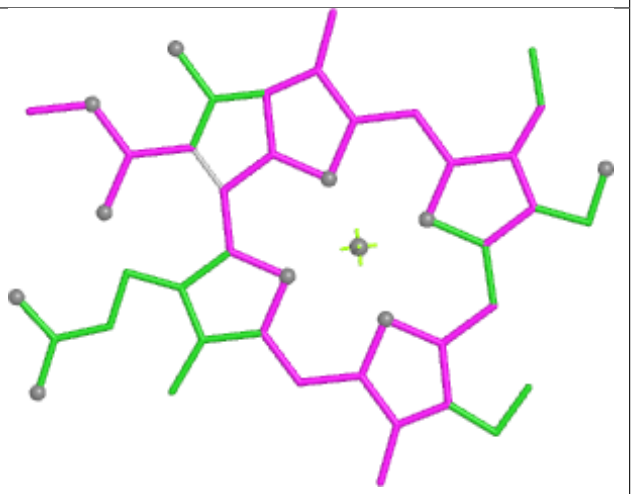


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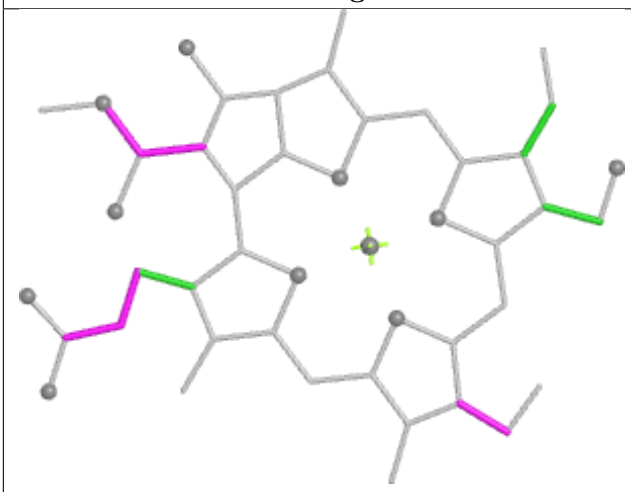
Ligand CHL S 601



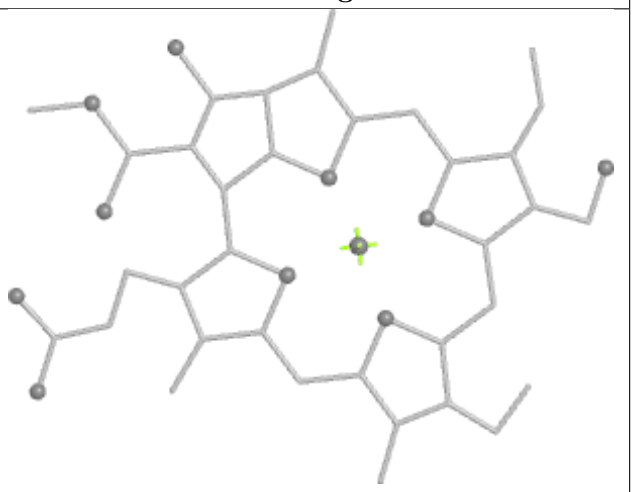
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Bond angles

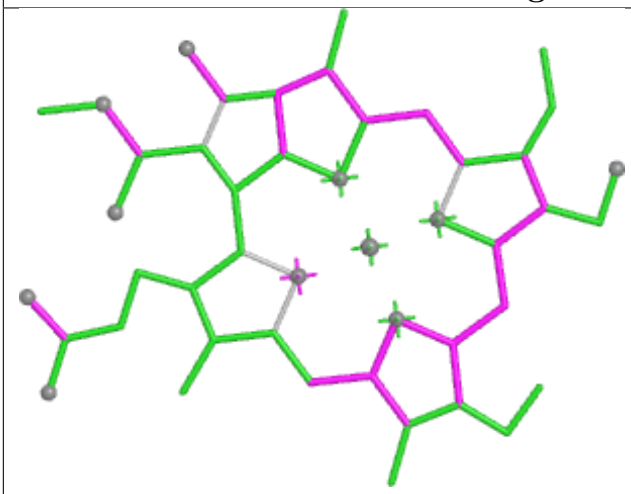


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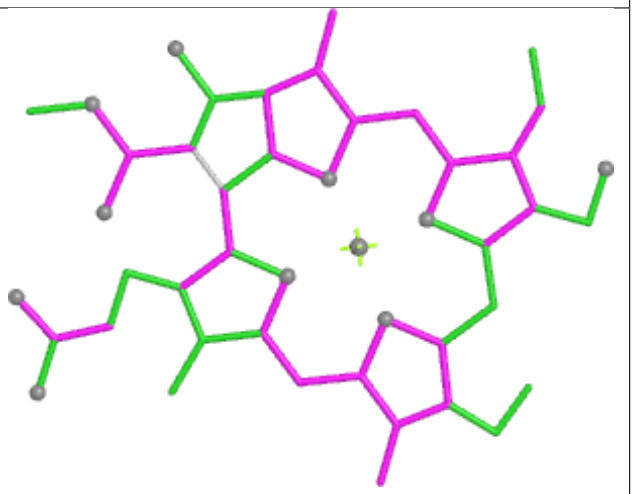


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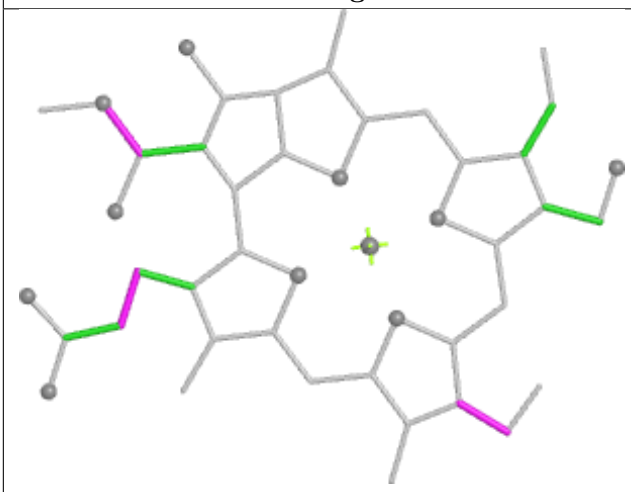
Ligand CHL 7 608



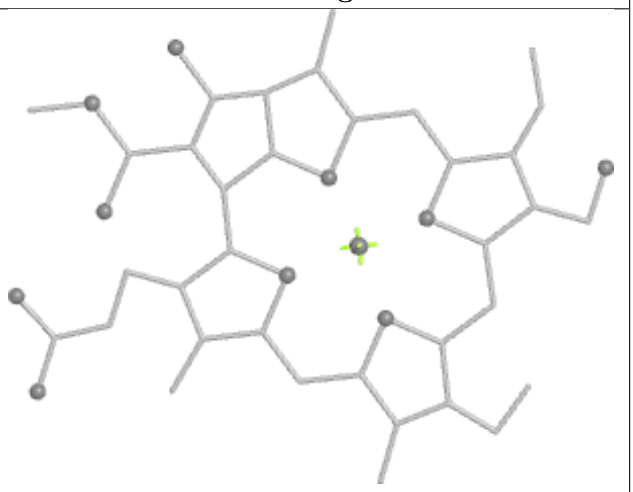
Bond lengths



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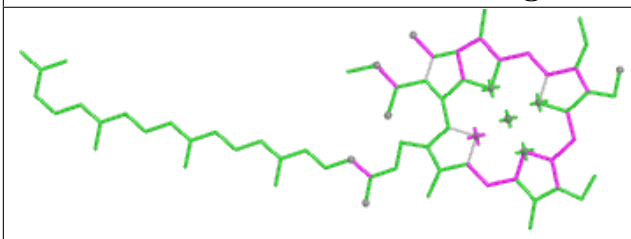


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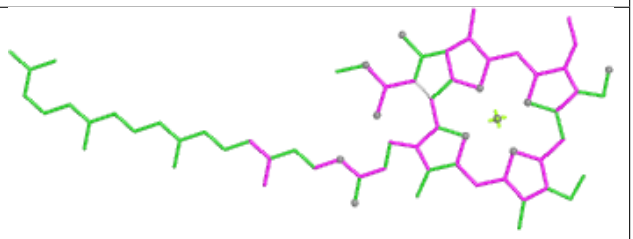


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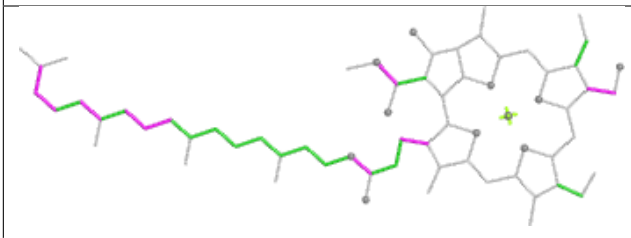
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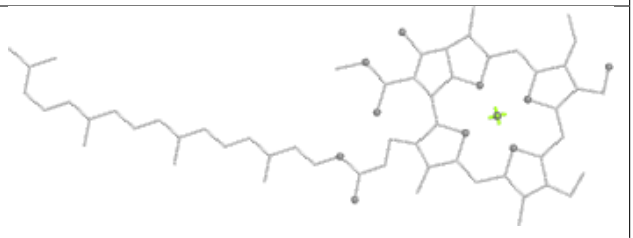
Bond lengths



Bond angles

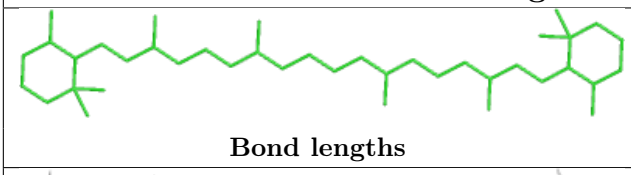


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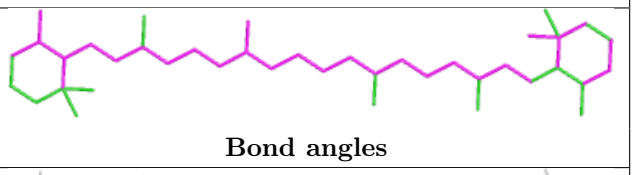


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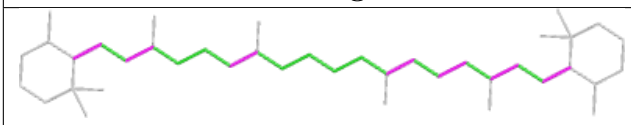
Ligand BCR t 101



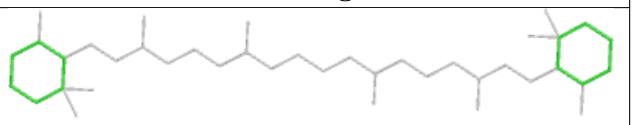
Bond lengths



Bond angles

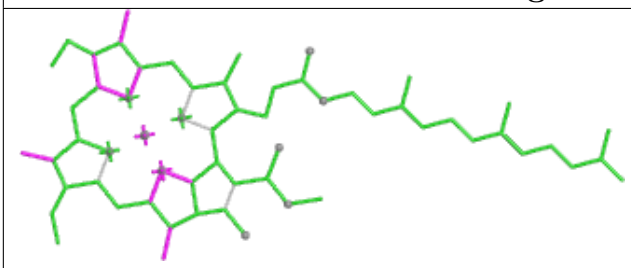


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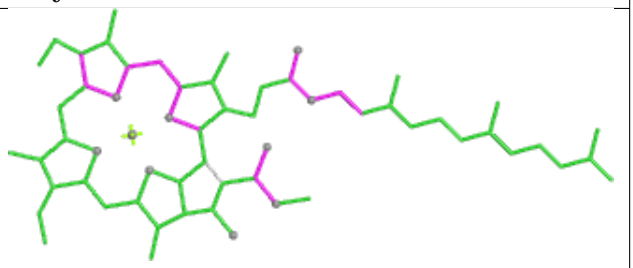


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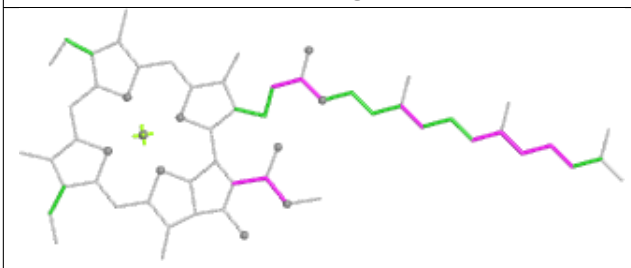
Ligand CLA y 612



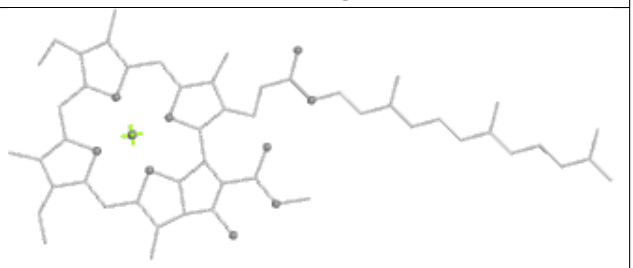
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Bond angles

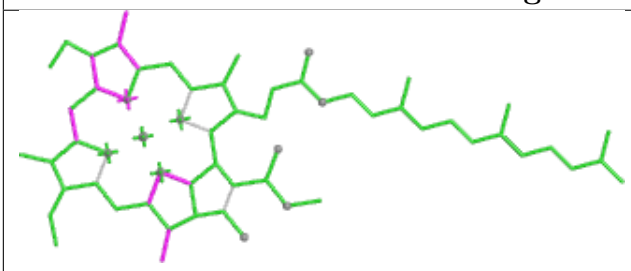


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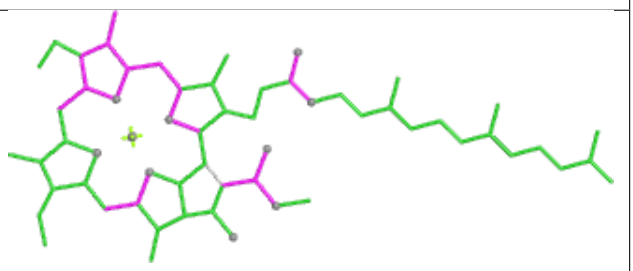


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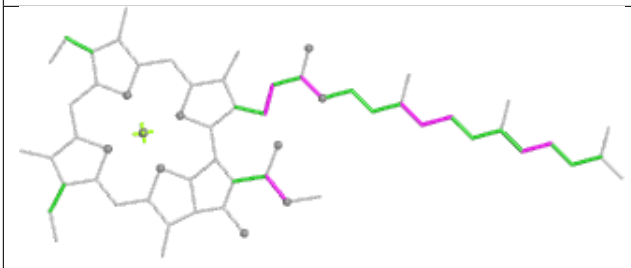
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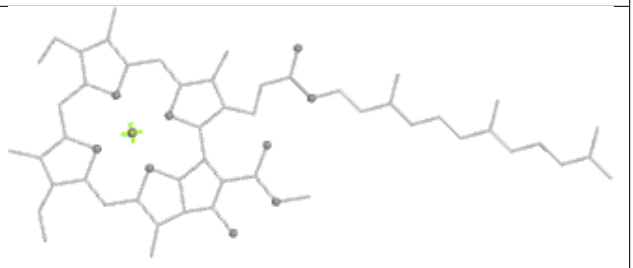
Bond lengths



Bond angles

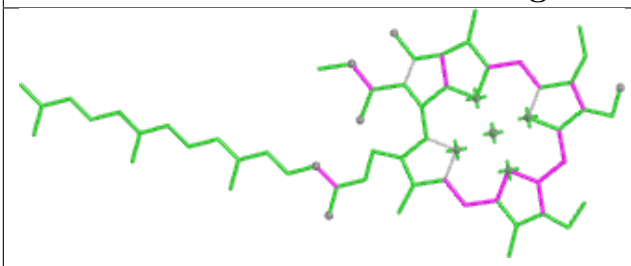


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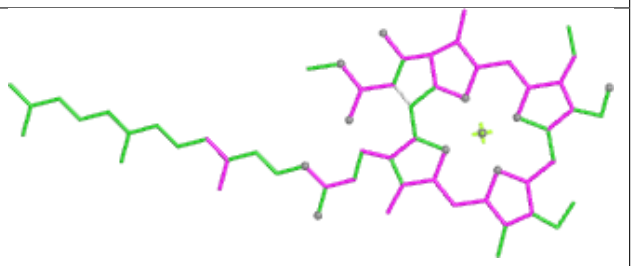


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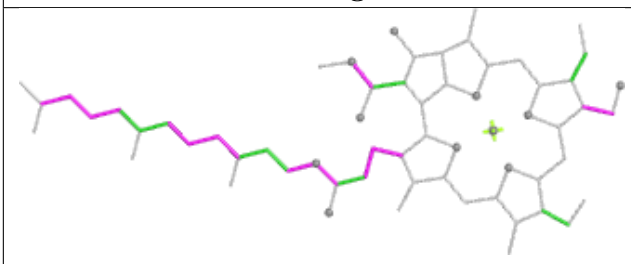
Ligand CHL r 608



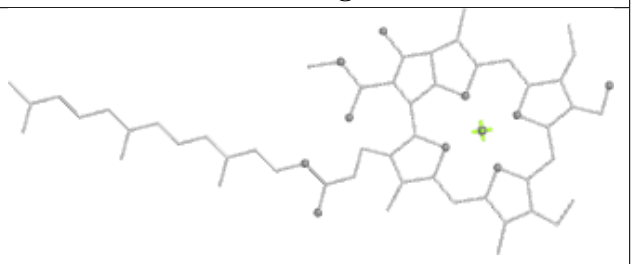
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Bond angles

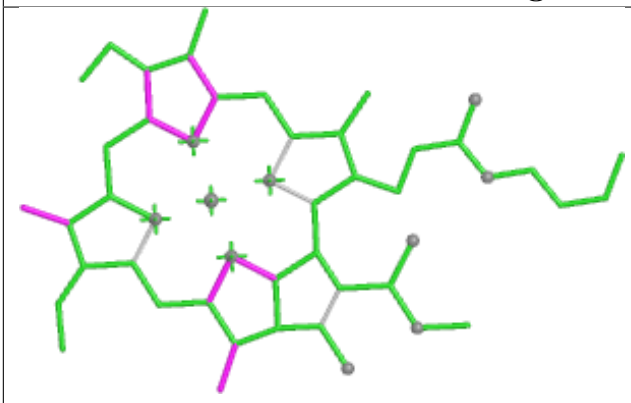


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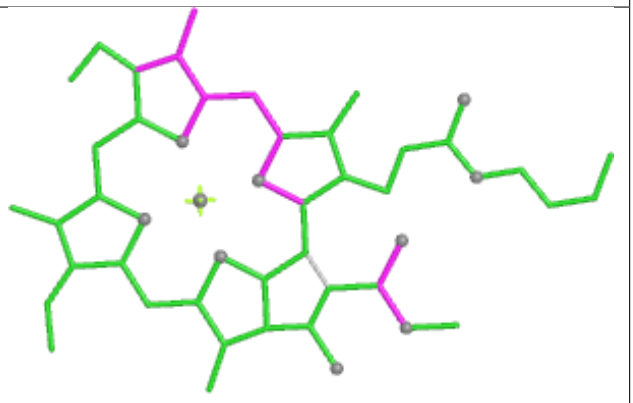


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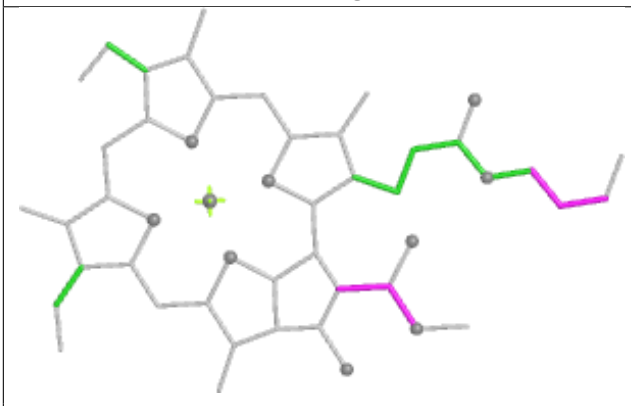
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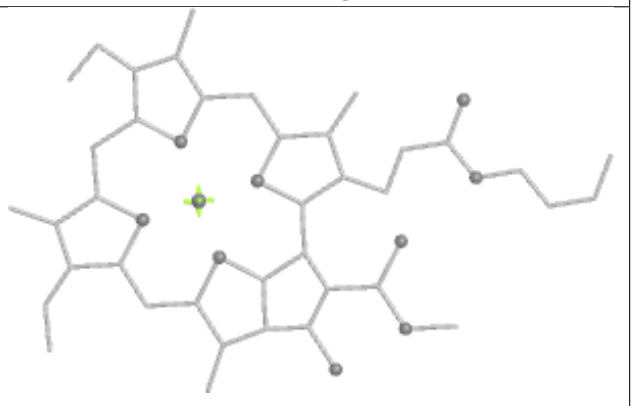
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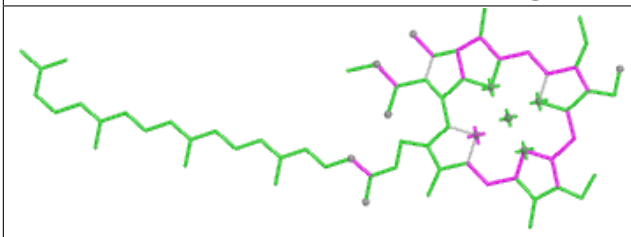
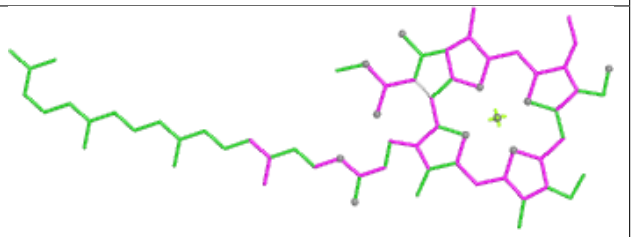
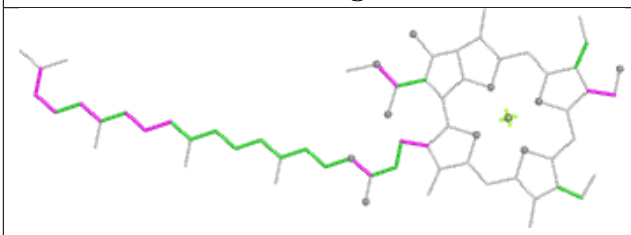
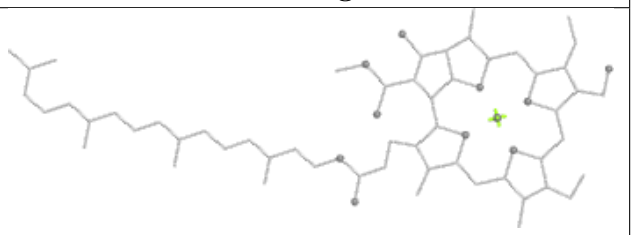
Bond angles

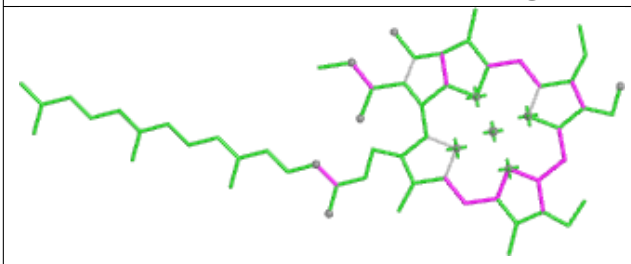
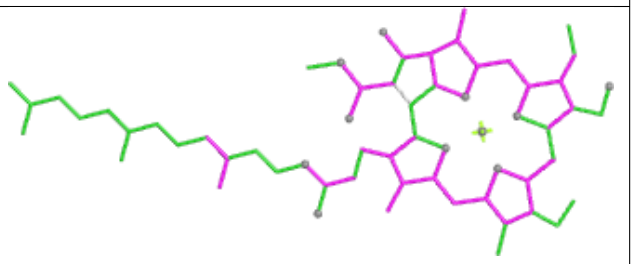
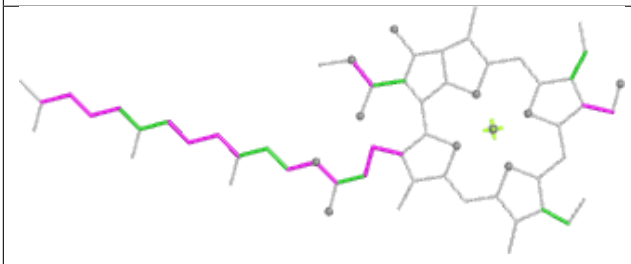
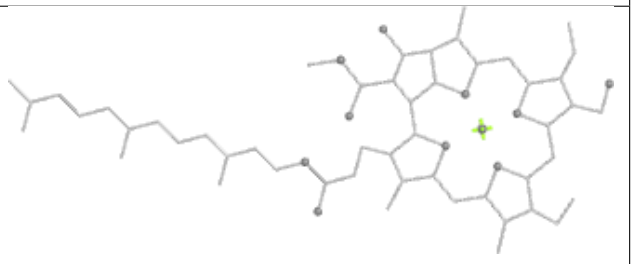


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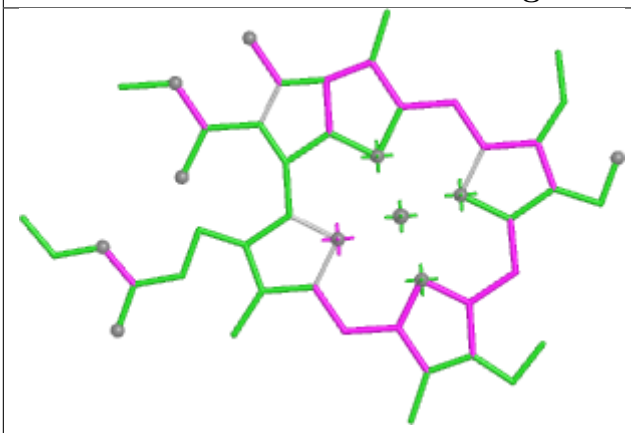


Rings

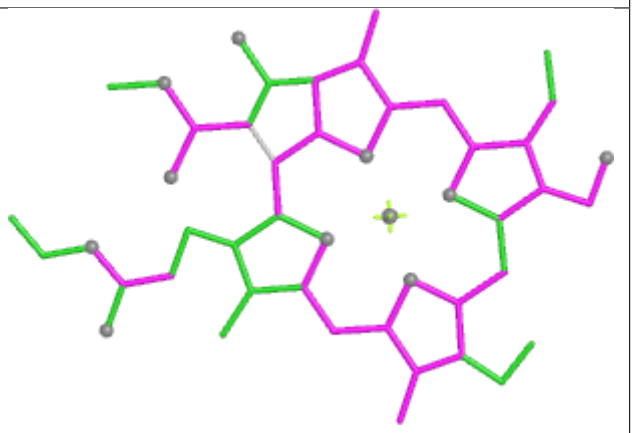
Ligand CHL n 609	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL R 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

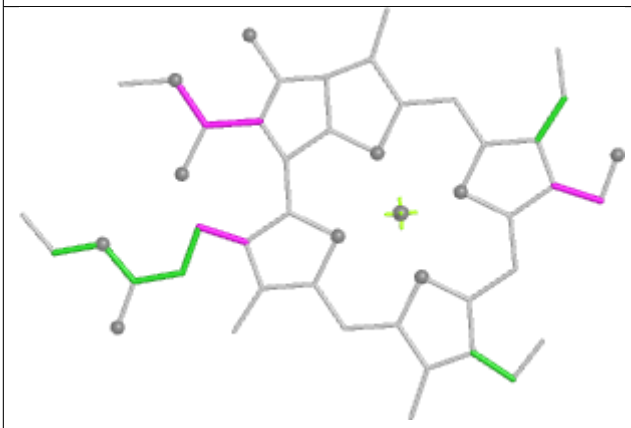
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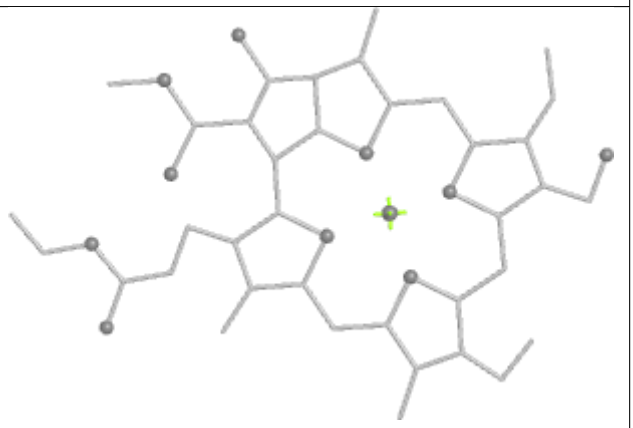
Bond lengths



Bond angles

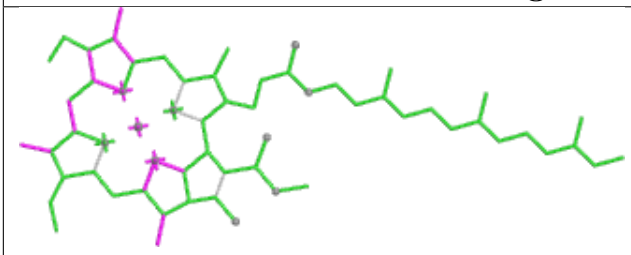


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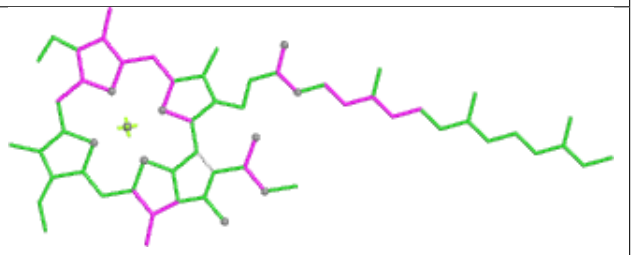


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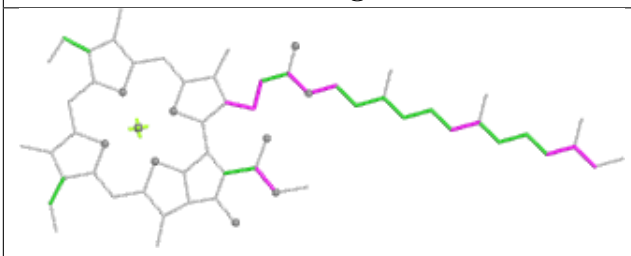
Ligand CLA S 602



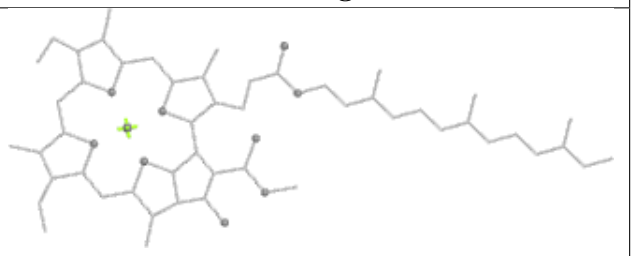
Bond lengths



Bond angles

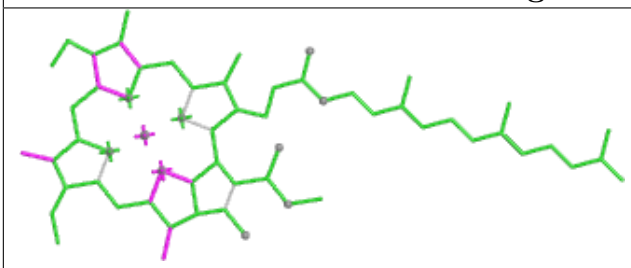


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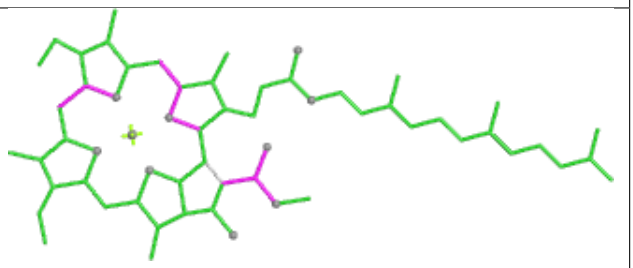


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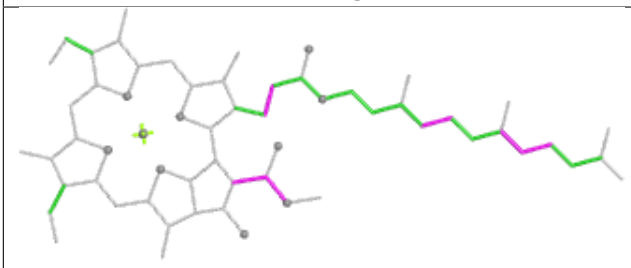
Ligand CLA n 613



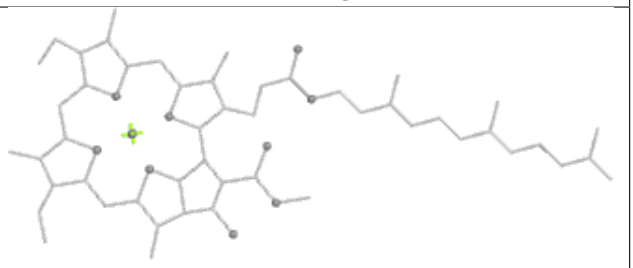
Bond lengths



Bond angles

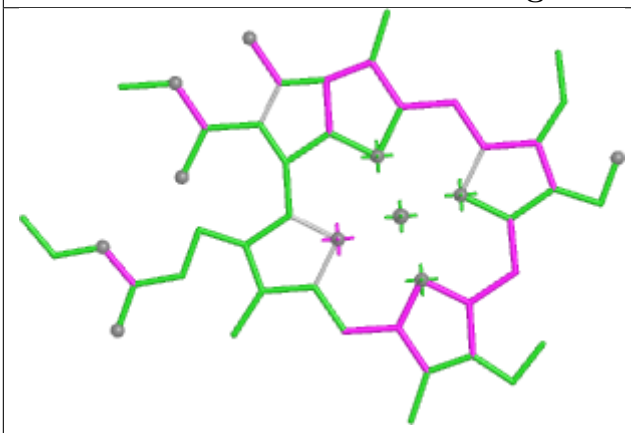


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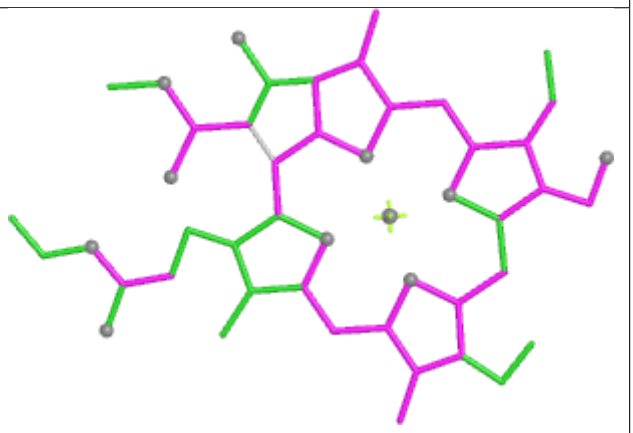


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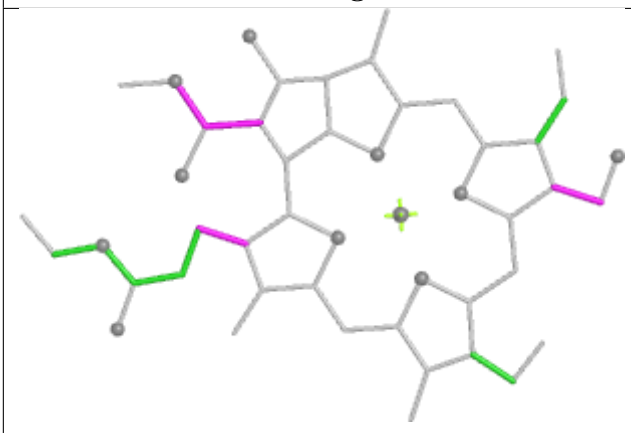
Ligand CHL n 605



Bond lengths



Bond angles

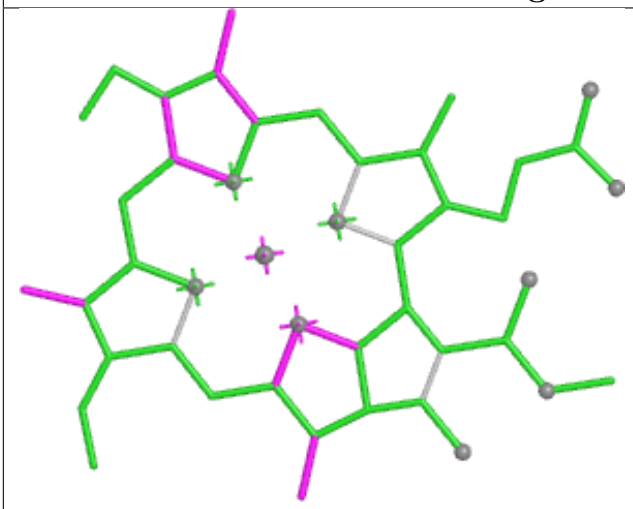


Torsions

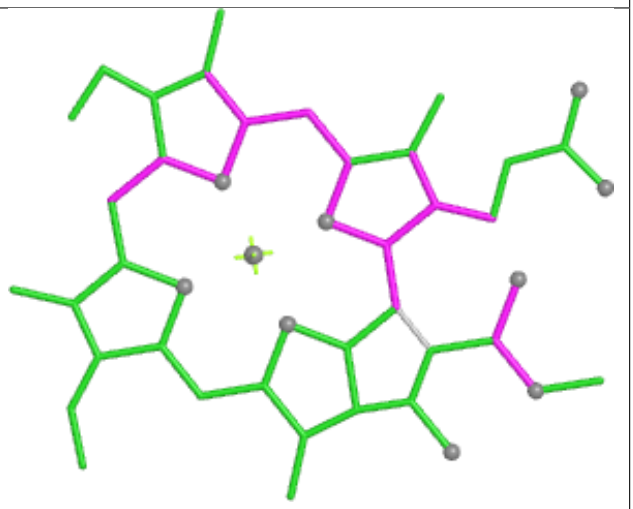


Rings

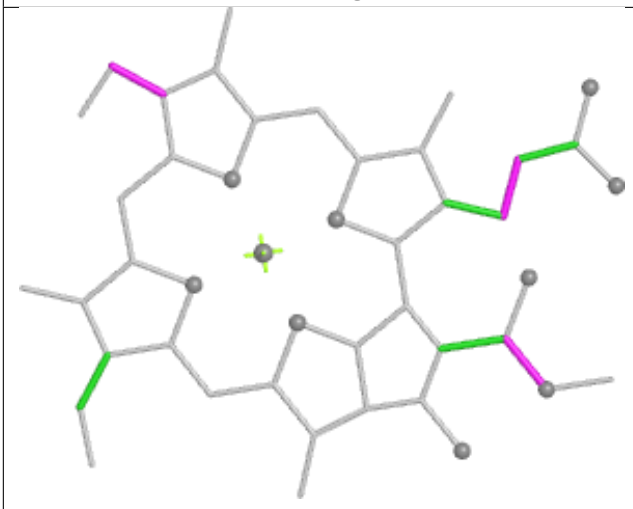
Ligand CLA 1 612



Bond lengths



Bond angles

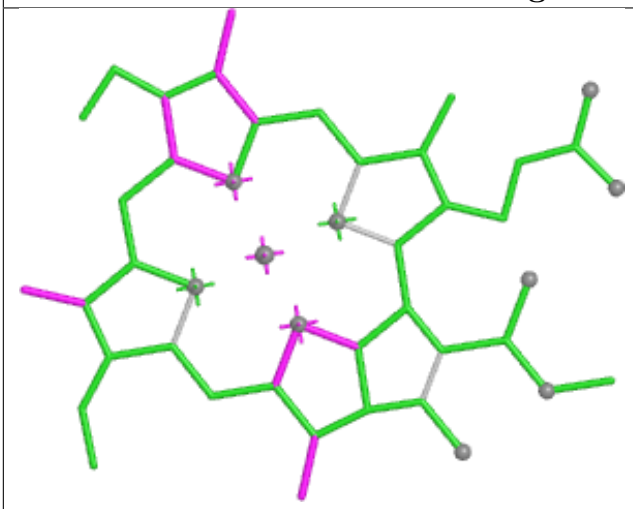


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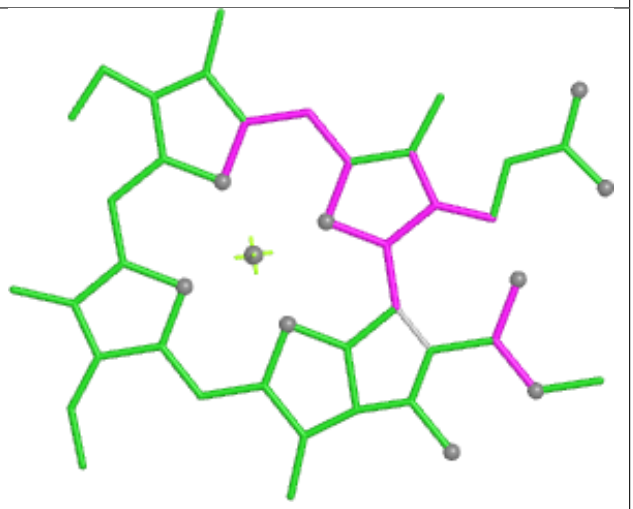


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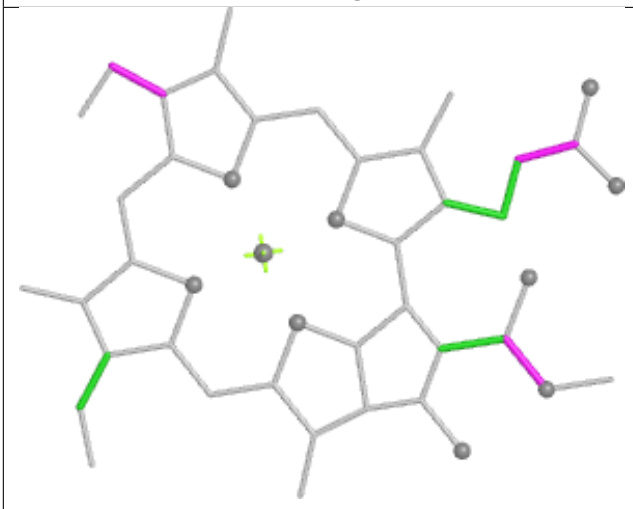
Ligand CLA 4 603



Bond lengths



Bond angles

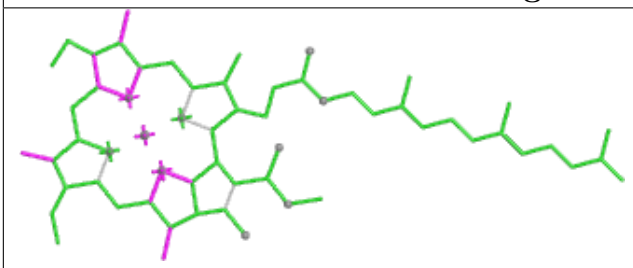


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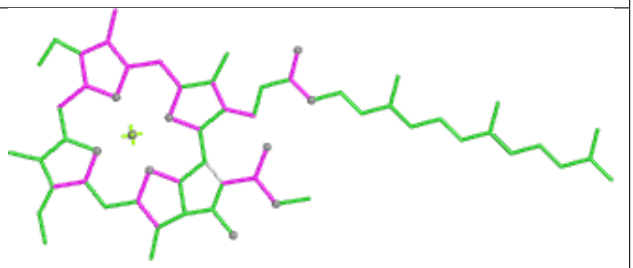


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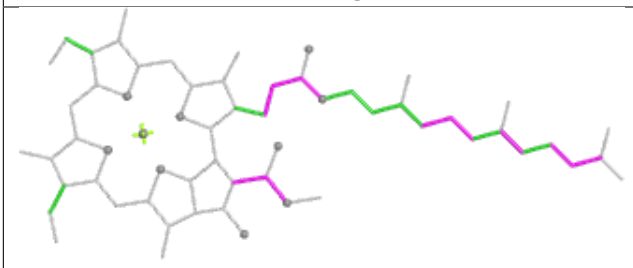
Ligand CLA R 603



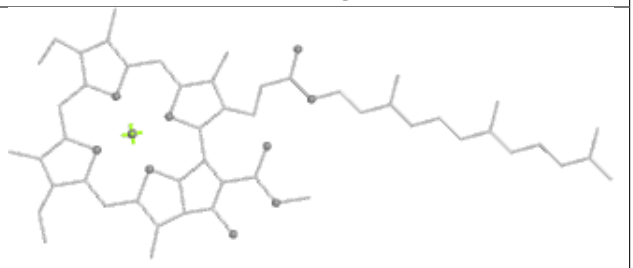
Bond lengths



Bond angles

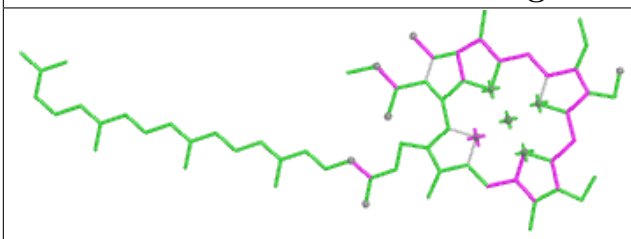


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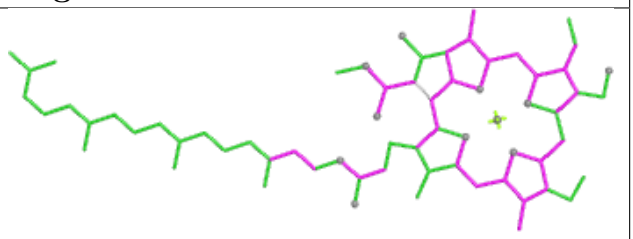


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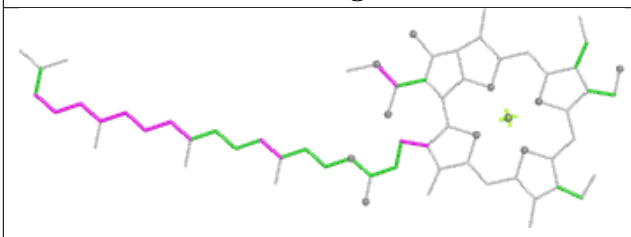
Ligand CHL g 608



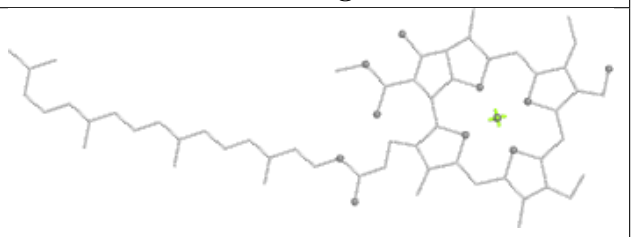
Bond lengths



Bond angles

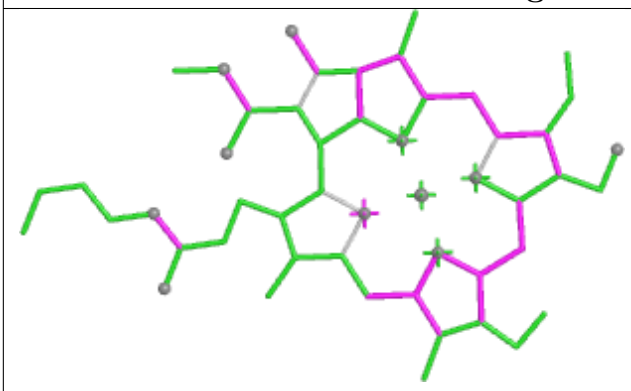


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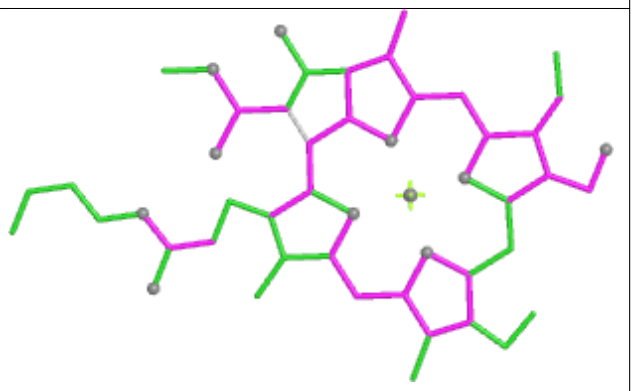


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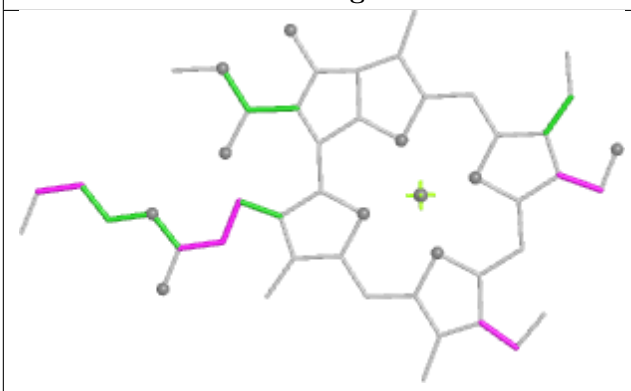
Ligand CHL n 606



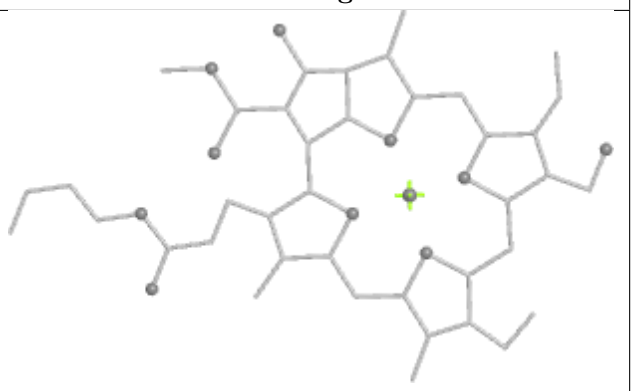
Bond lengths



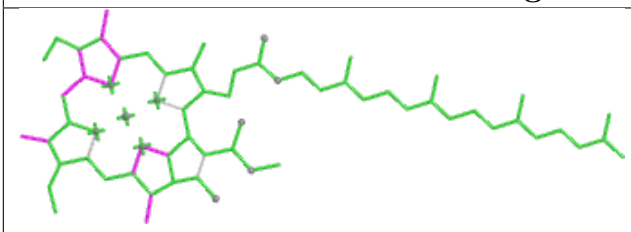
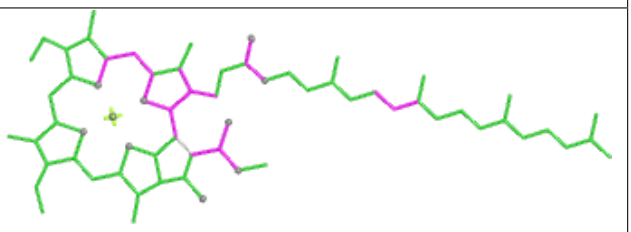
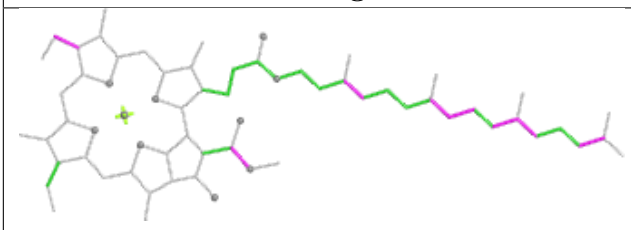
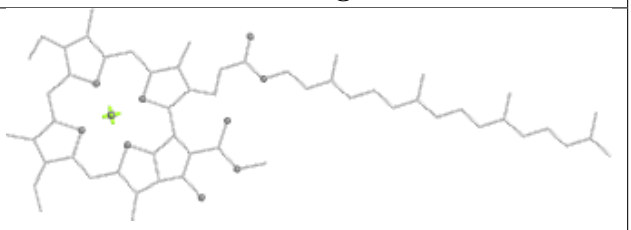
Bond angles

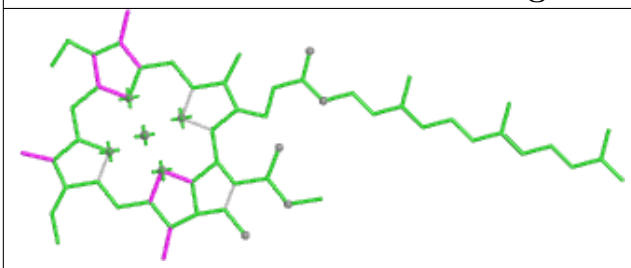
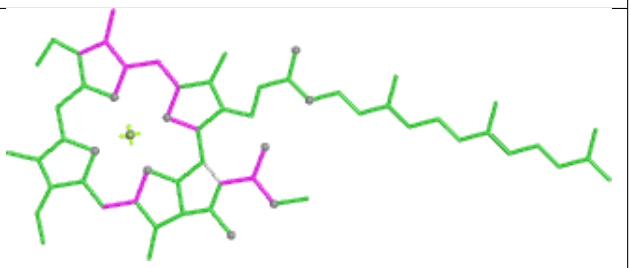
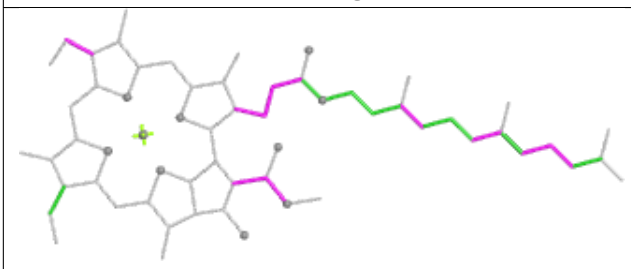
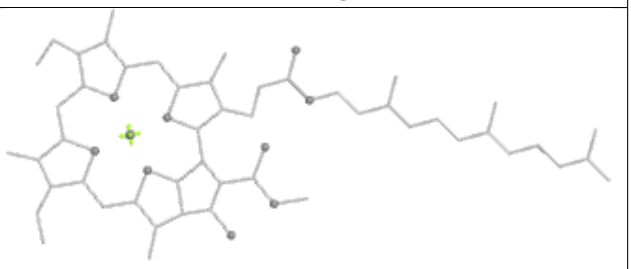


Torsions

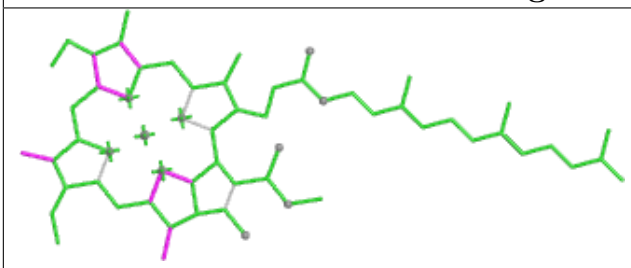


Rings

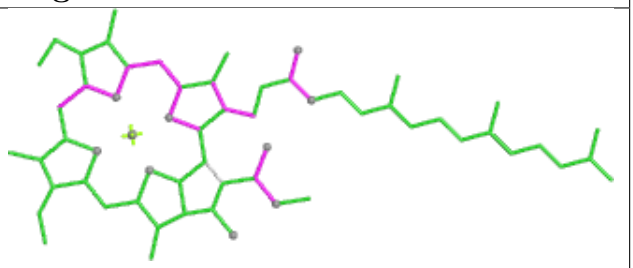
Ligand CLA B 616	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 7 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

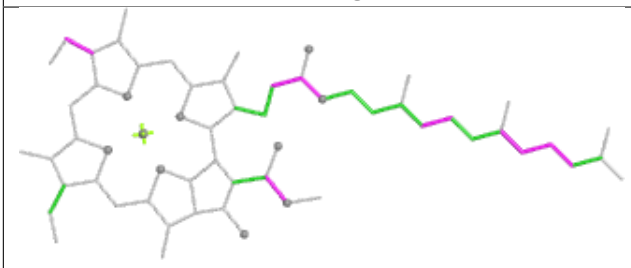
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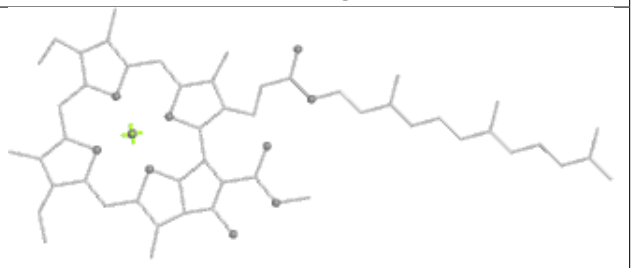
Bond lengths



Bond angles

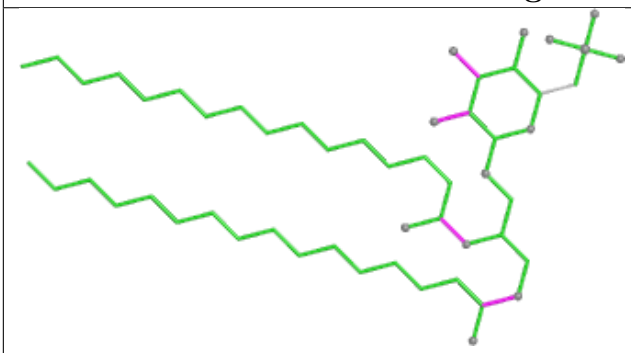


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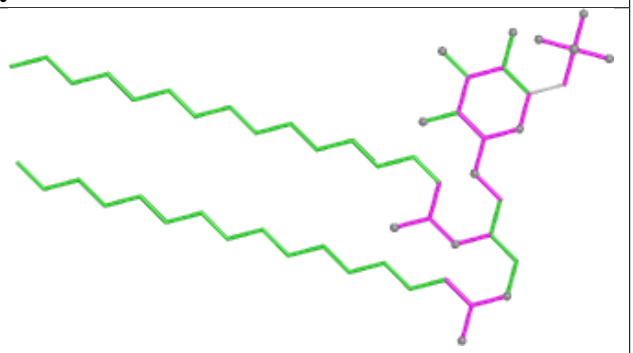


Rings

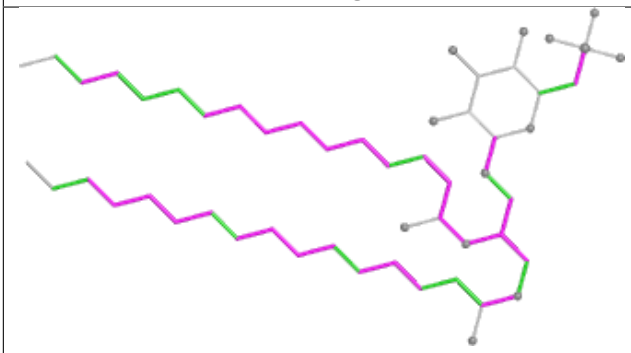
Ligand SQD B 621



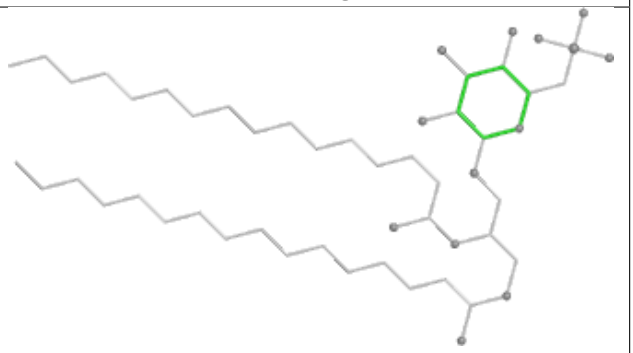
Bond lengths



Bond angles

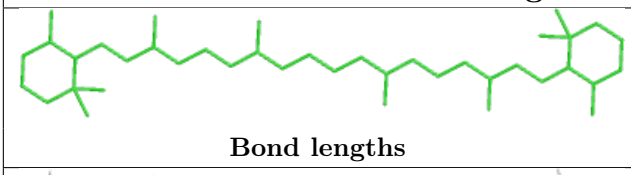


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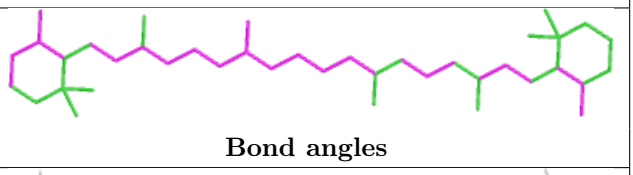


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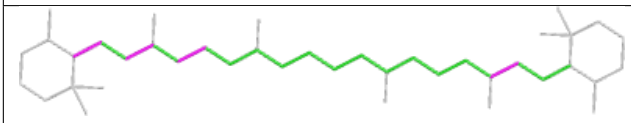
Ligand BCR d 404



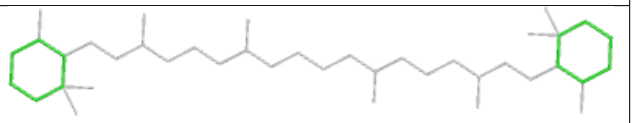
Bond lengths



Bond angles

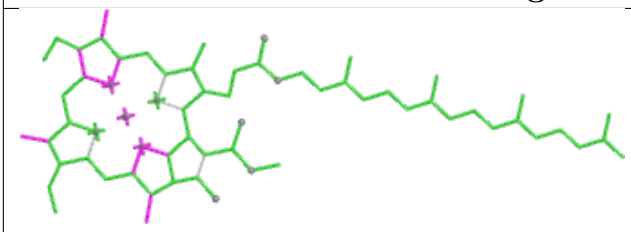


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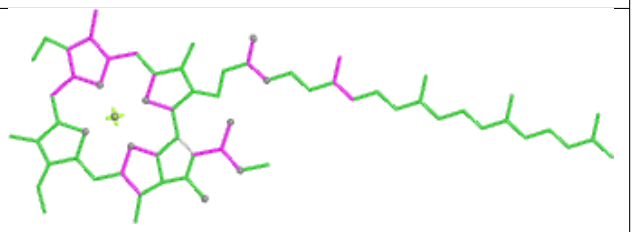


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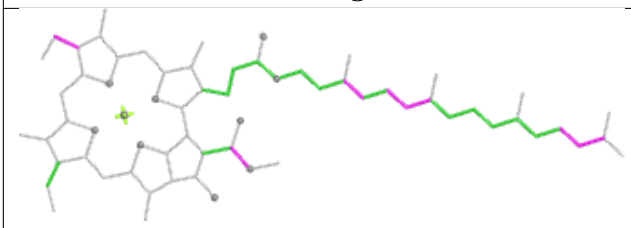
Ligand CLA b 604



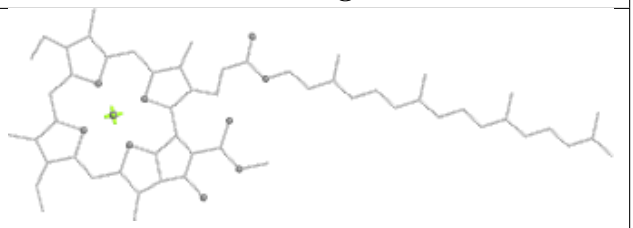
Bond lengths



Bond angles

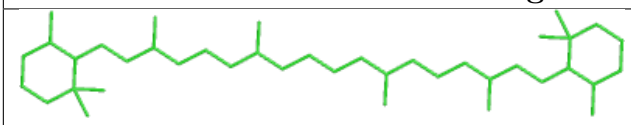


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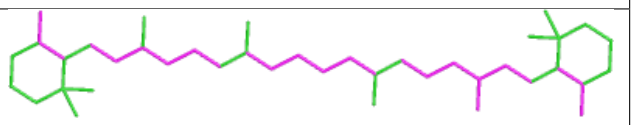


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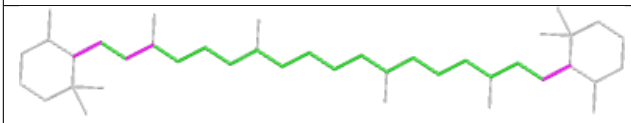
Ligand BCR a 411



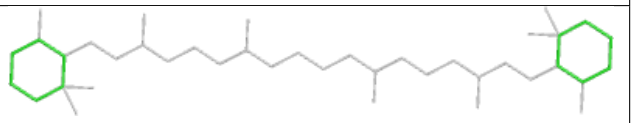
Bond lengths



Bond angles

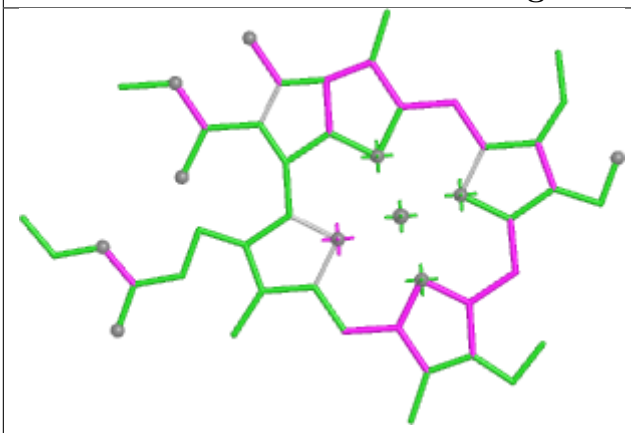


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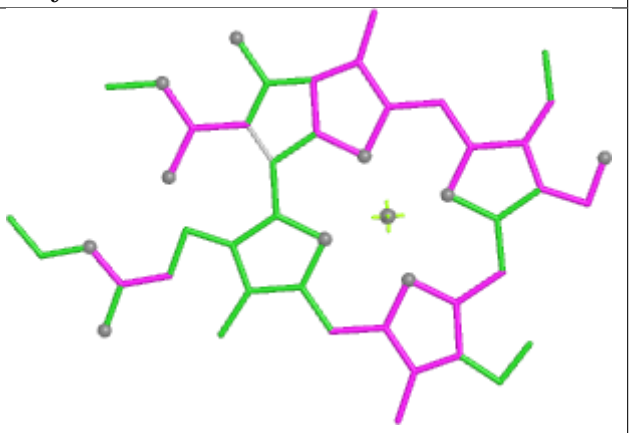


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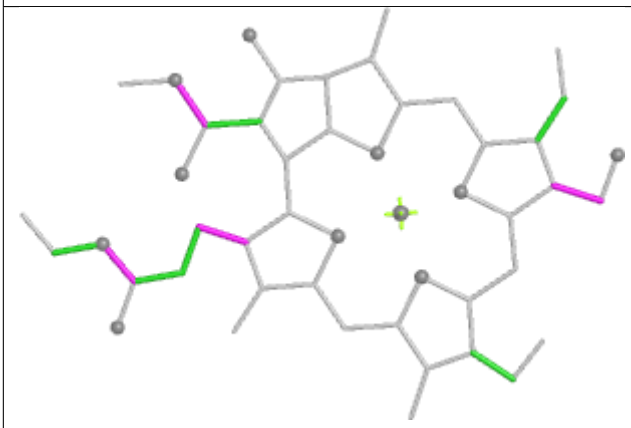
Ligand CHL y 605



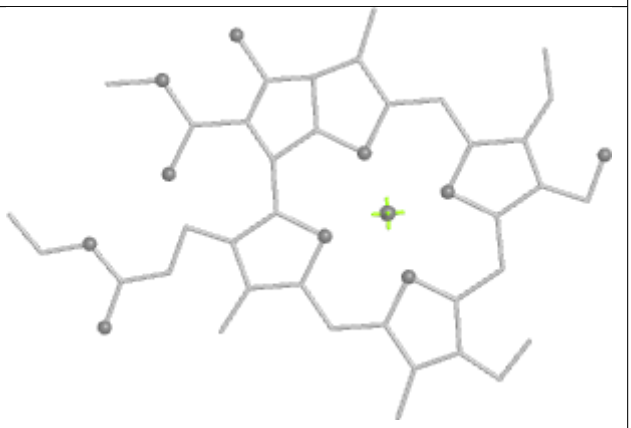
Bond lengths



Bond angles

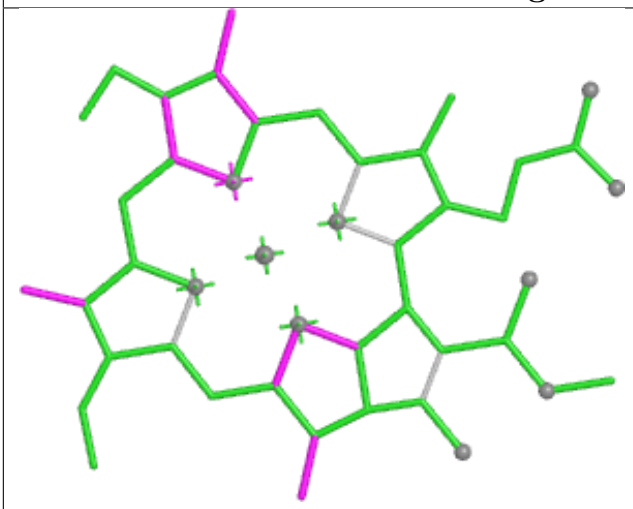


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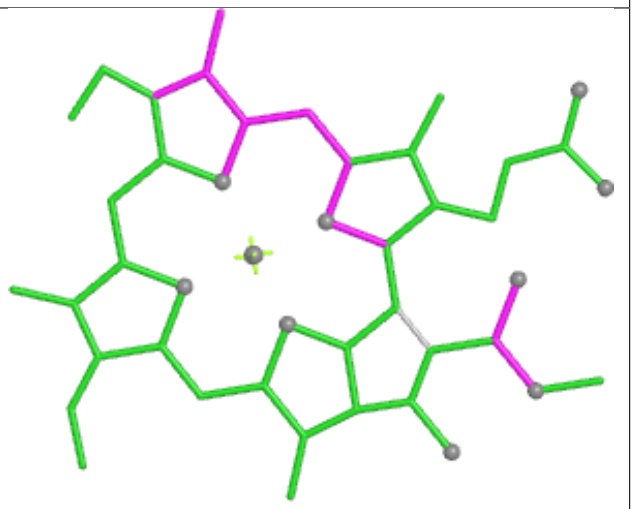


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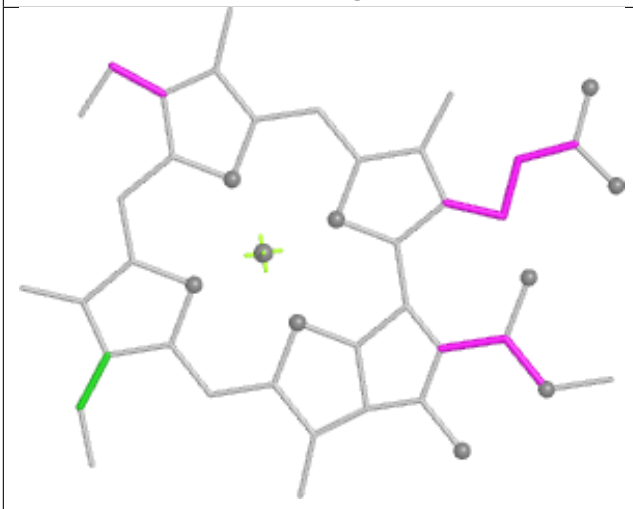
Ligand CLA 3 604



Bond lengths



Bond angles

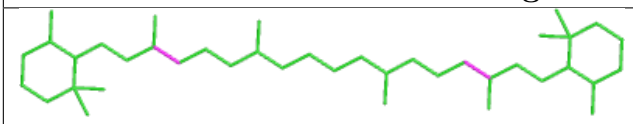


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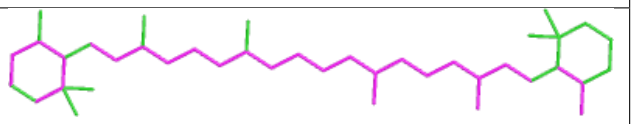


Rings

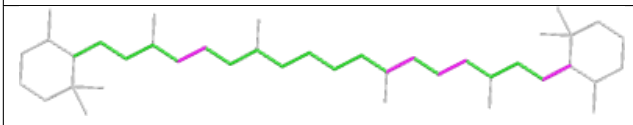
Ligand BCR C 515



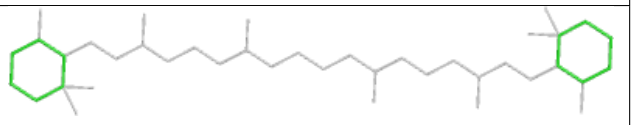
Bond lengths



Bond angles

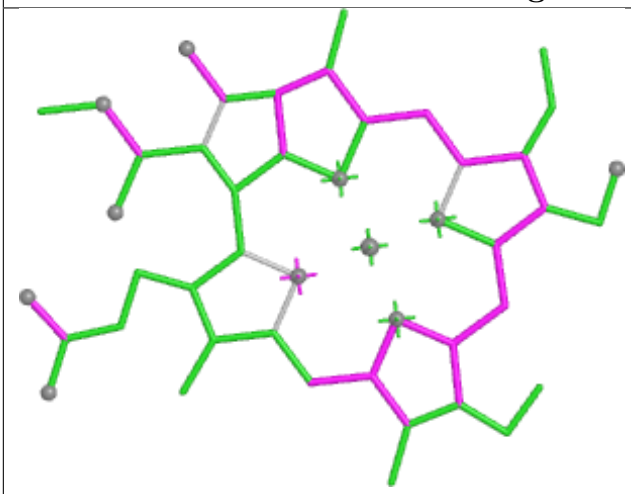


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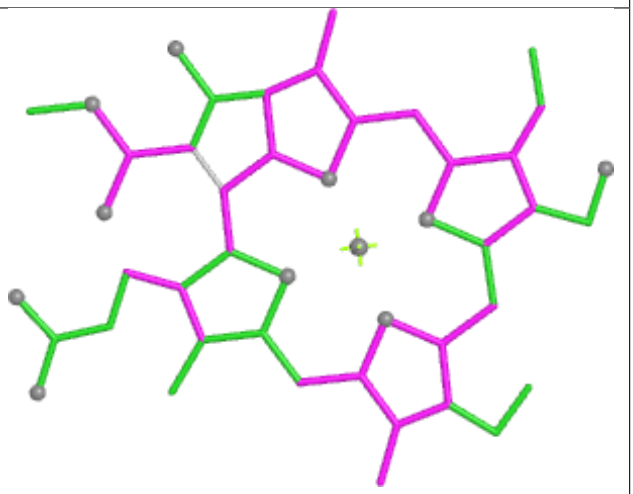


Rings

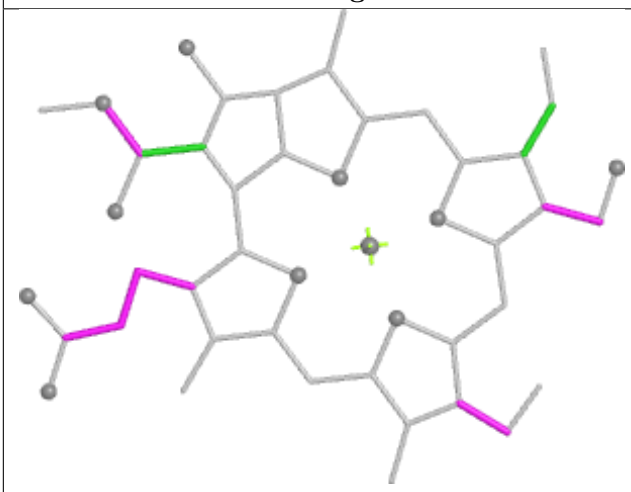
Ligand CHL 2 605



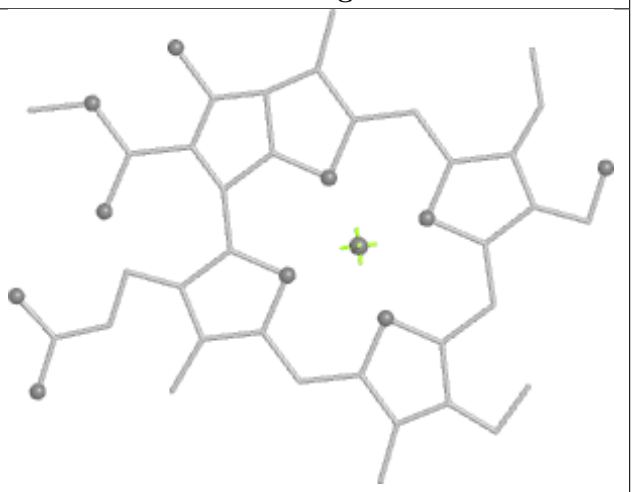
Bond lengths



Bond angles

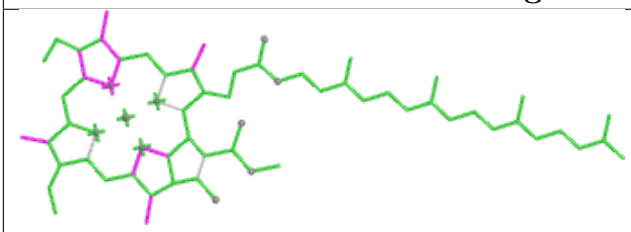


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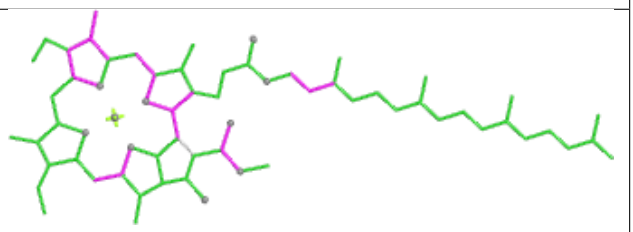


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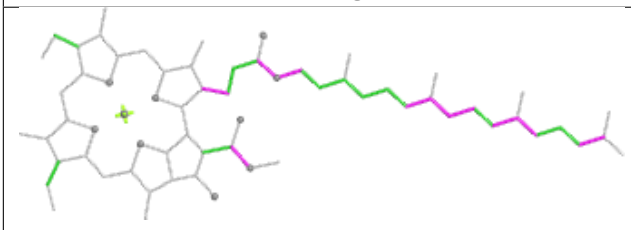
Ligand CLA C 511



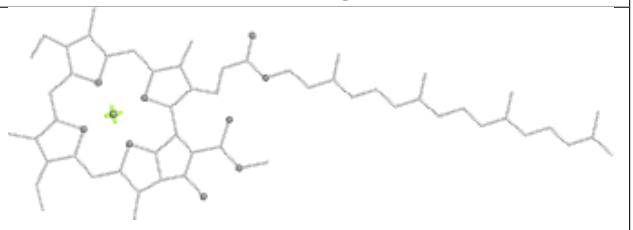
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Bond angles

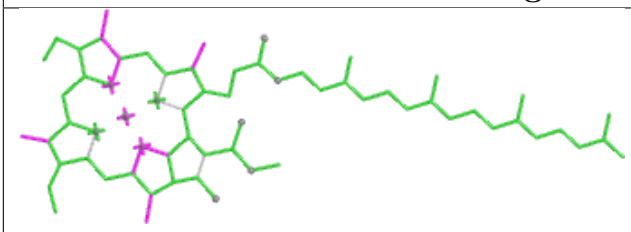


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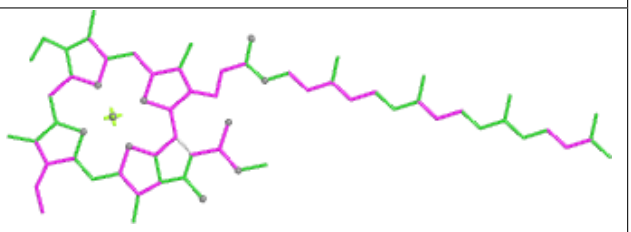


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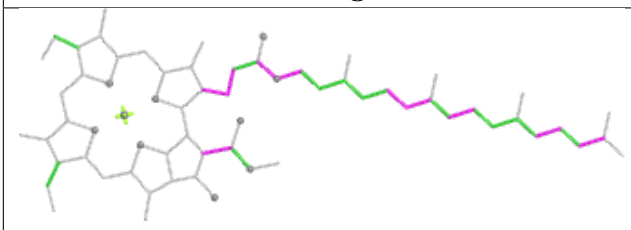
Ligand CLA B 605



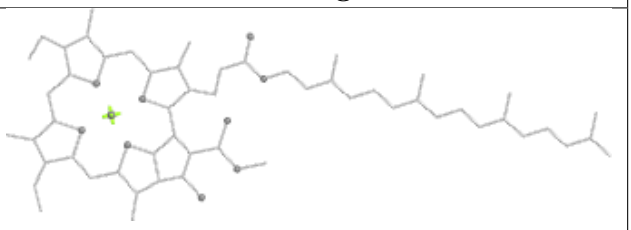
Bond lengths



Bond angles



Torsions



Rings

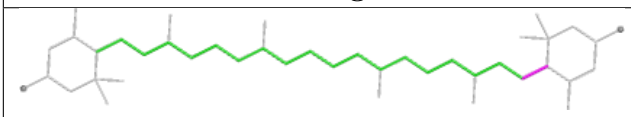
Ligand LUT 7 1620



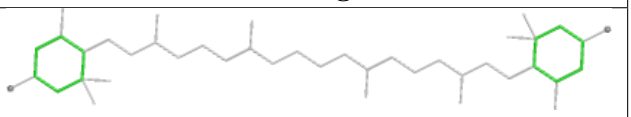
Bond lengths



Bond angles

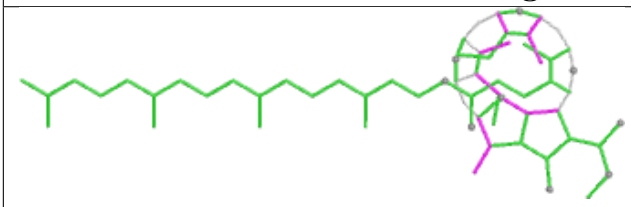


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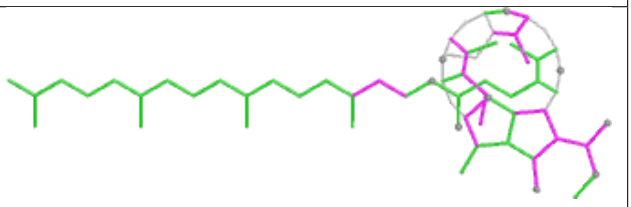


Rings

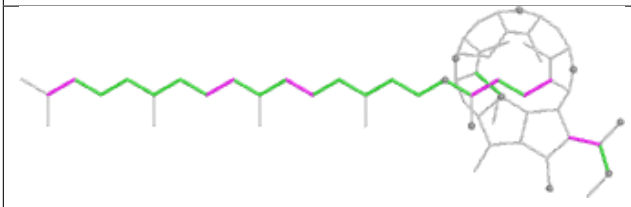
Ligand PHO A 409



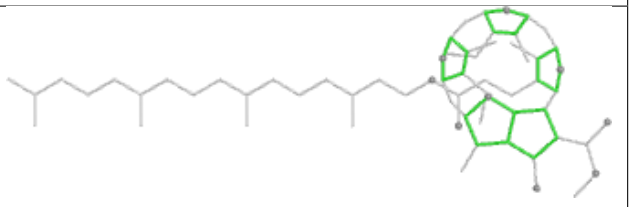
Bond lengths



Bond angles

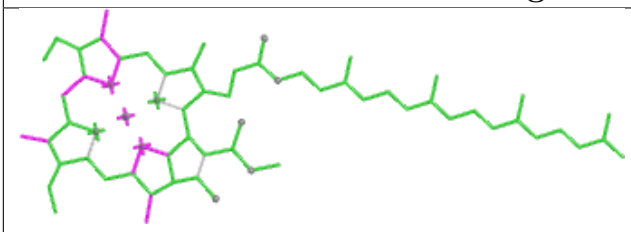


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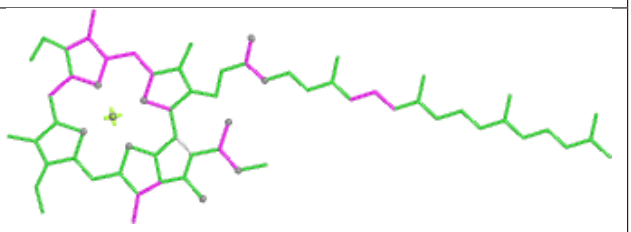


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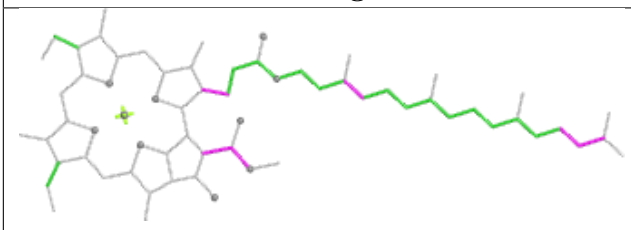
Ligand CLA b 610



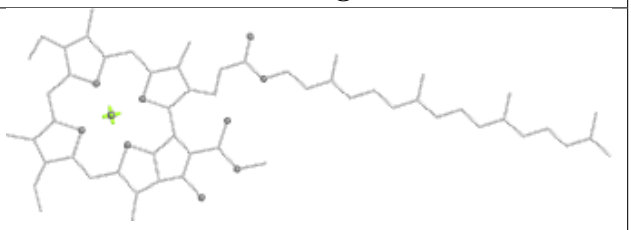
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Bond angles

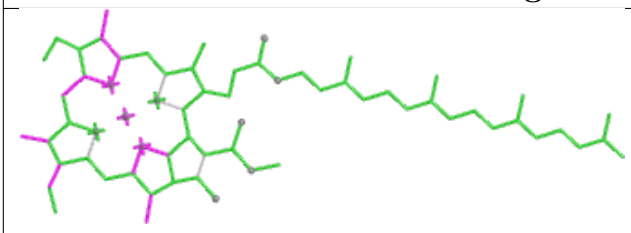


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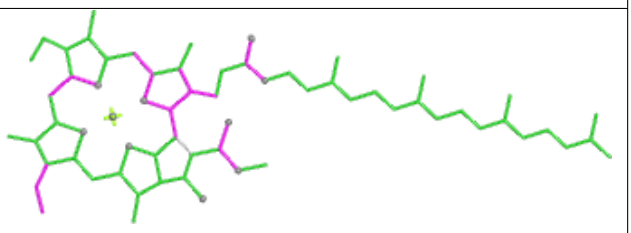


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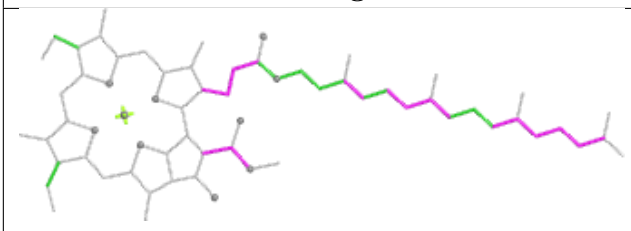
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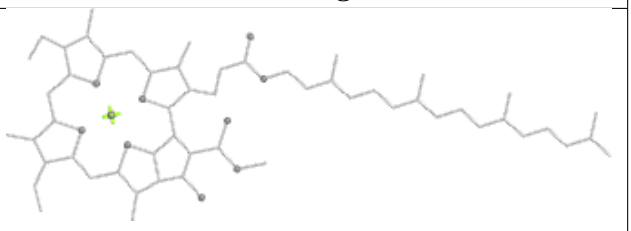
Bond lengths



Bond angles

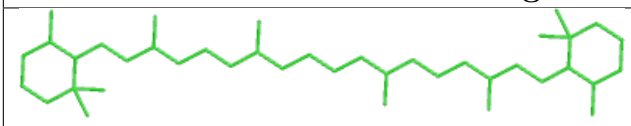


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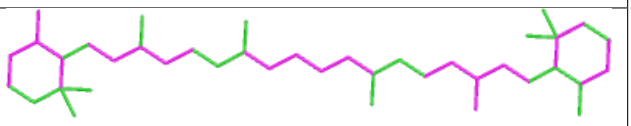


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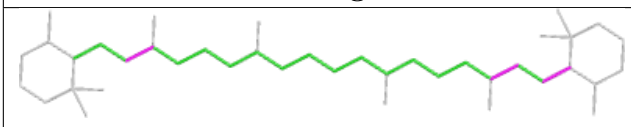
Ligand BCR B 620



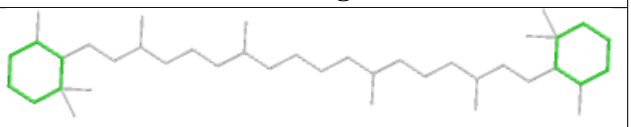
Bond lengths



Bond angles

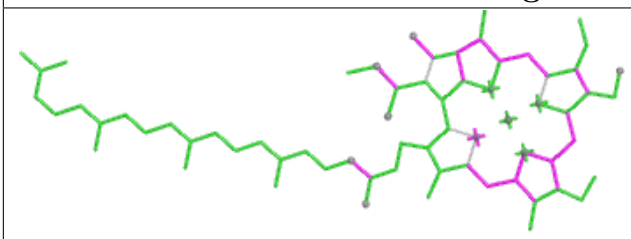


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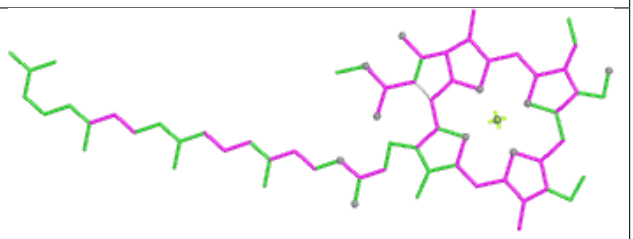


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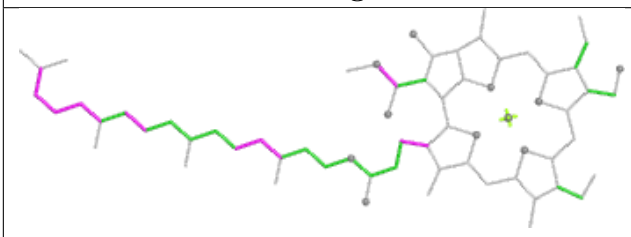
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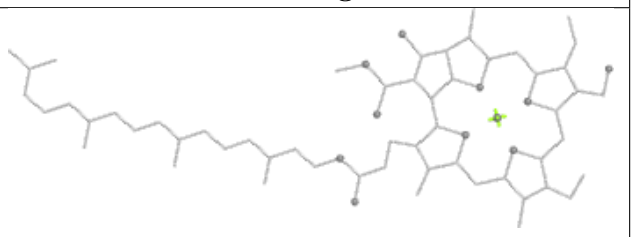
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Bond angles

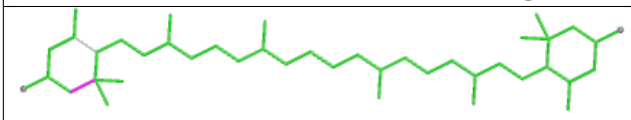


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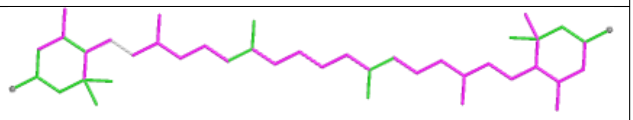


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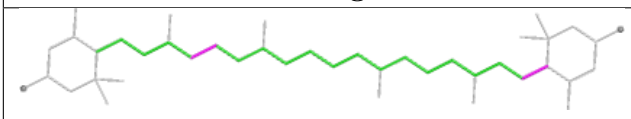
Ligand LUT 2 1621



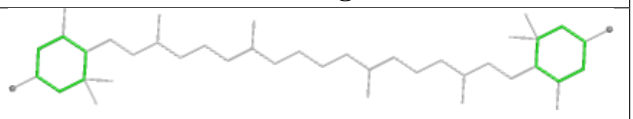
Bond lengths



Bond angles

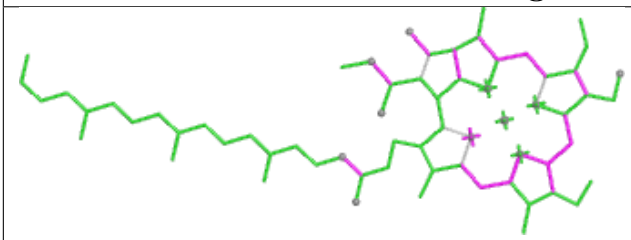


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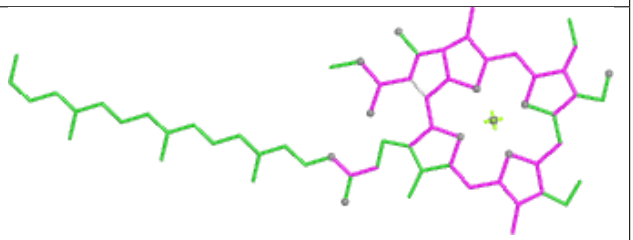


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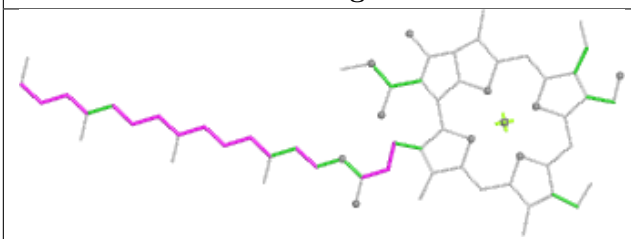
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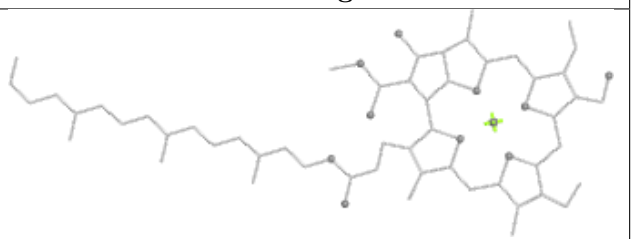
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Bond angles

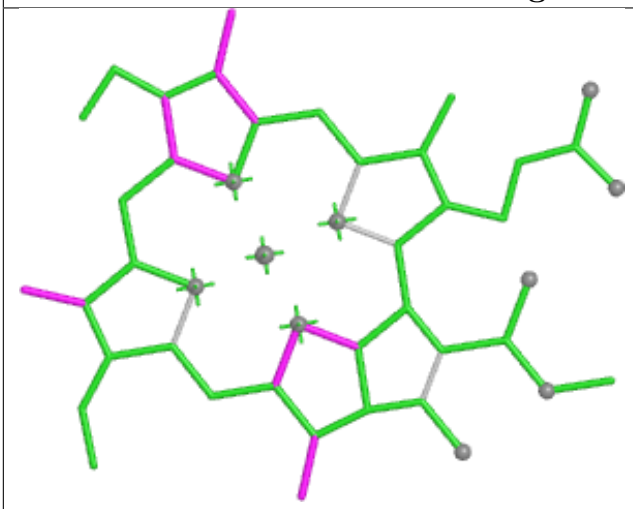


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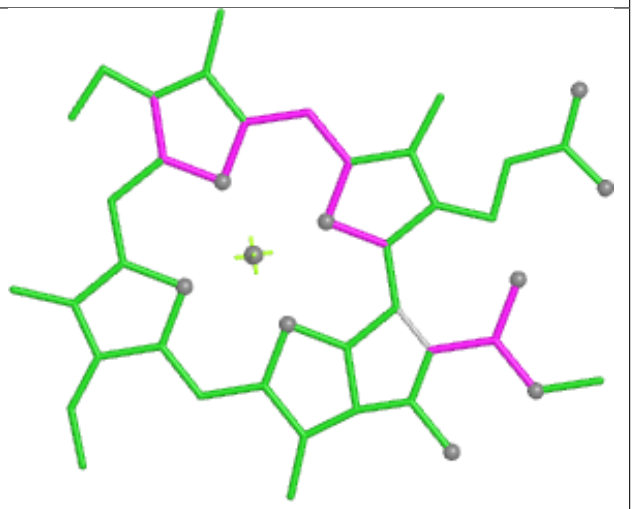


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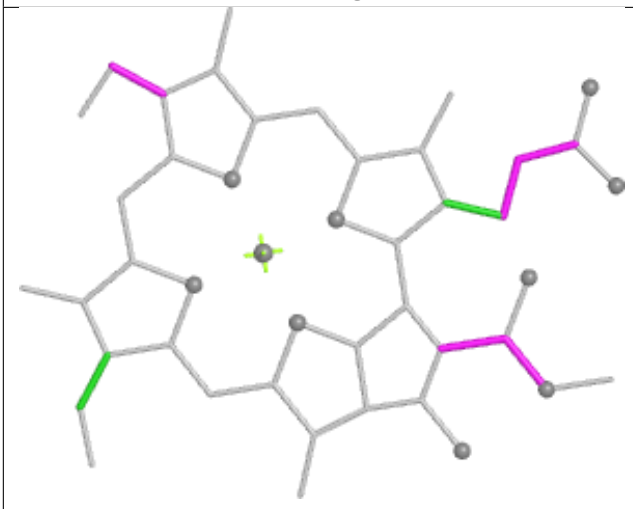
Ligand CLA 8 602



Bond lengths



Bond angles

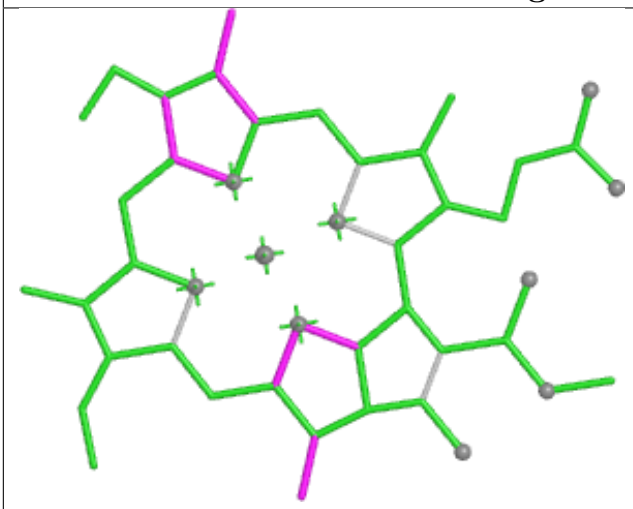


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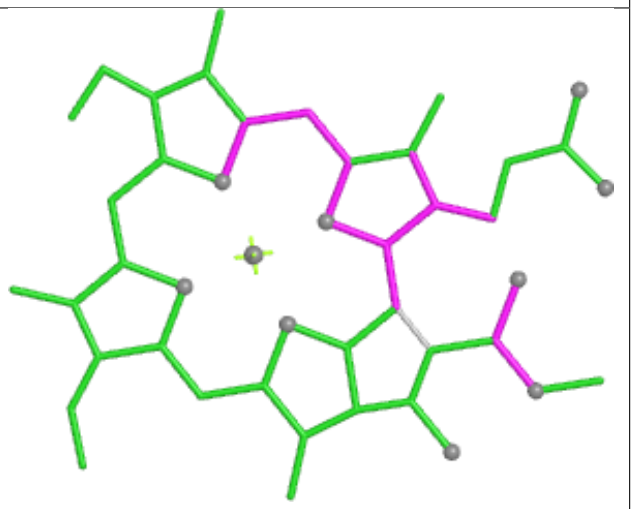


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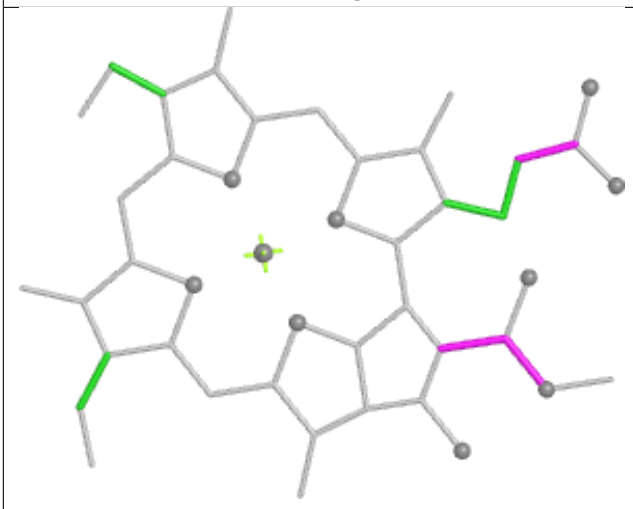
Ligand CLA 2 612



Bond lengths



Bond angles

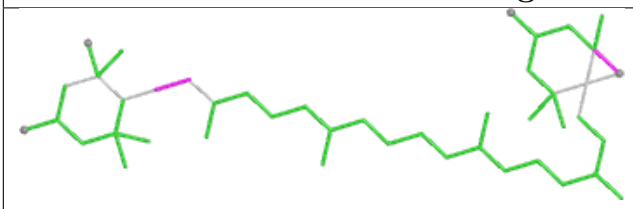


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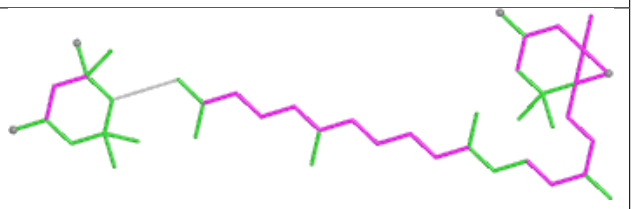


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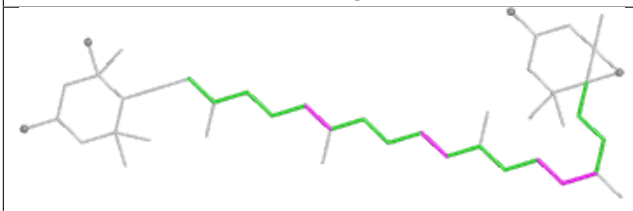
Ligand NEX 1 1623



Bond lengths



Bond angles

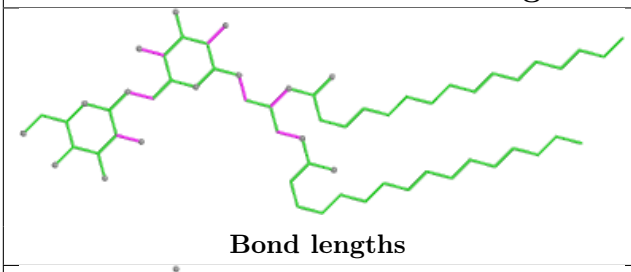


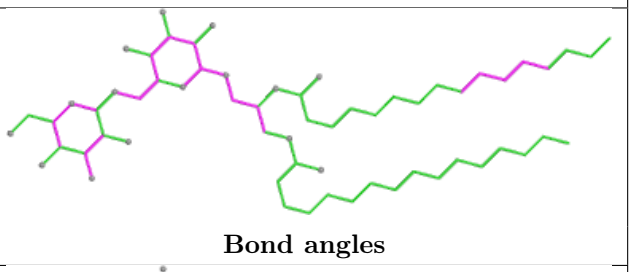
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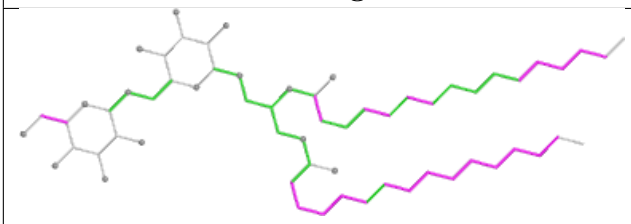


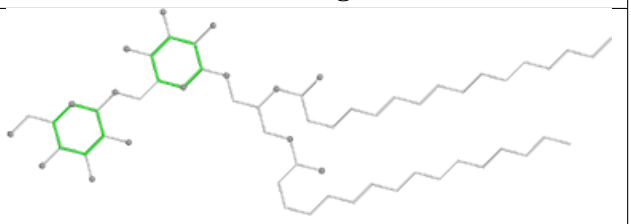
Rings

Ligand DGD h 102

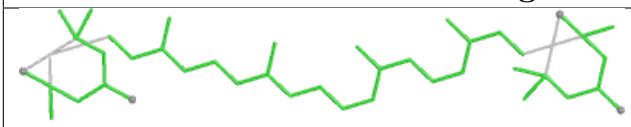

Bond lengths

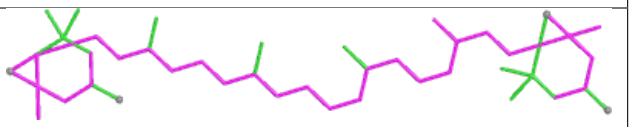

Bond angles

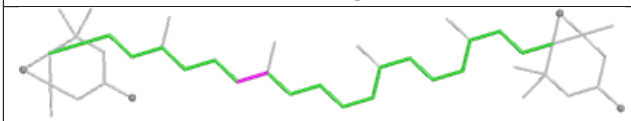

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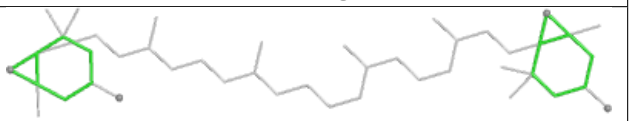

Rings

Ligand XAT 5 1622

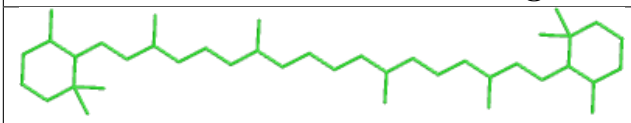

Bond lengths

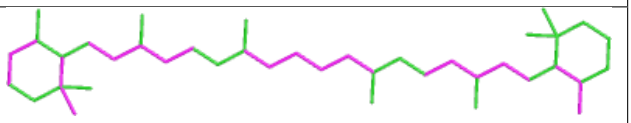

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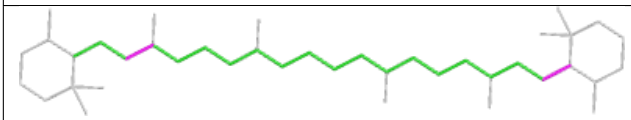

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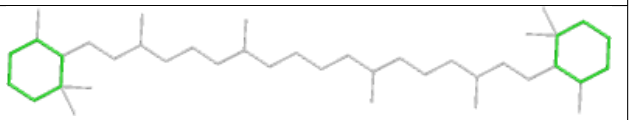

Rings

Ligand BCR h 101


Bond lengths

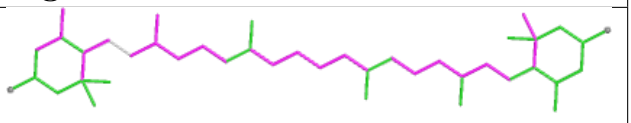

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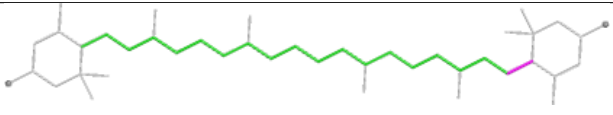

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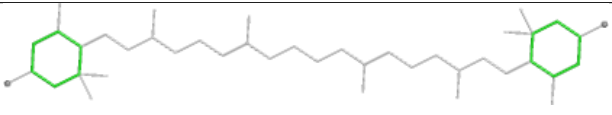

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Ligand LUT g 1620

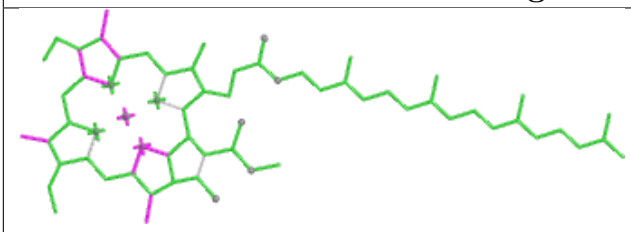

Bond lengths


Bond angles

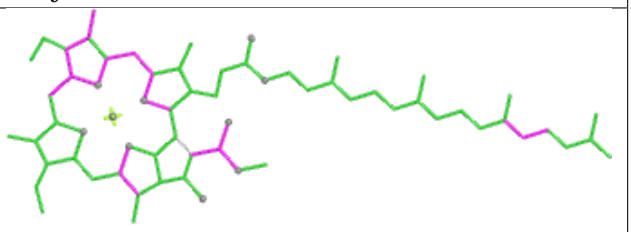

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Rings

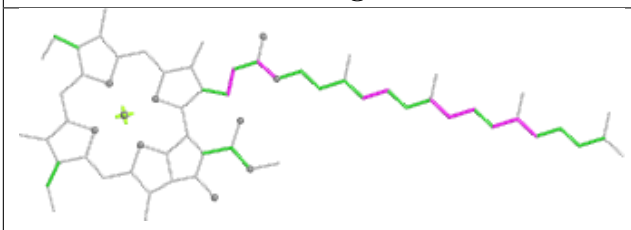
Ligand CLA y 613



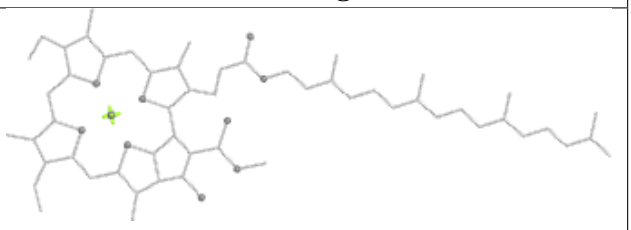
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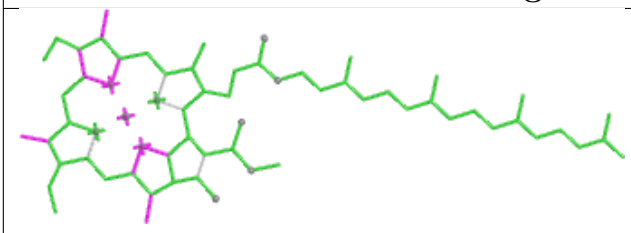


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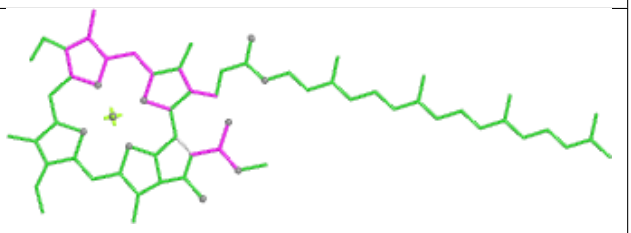


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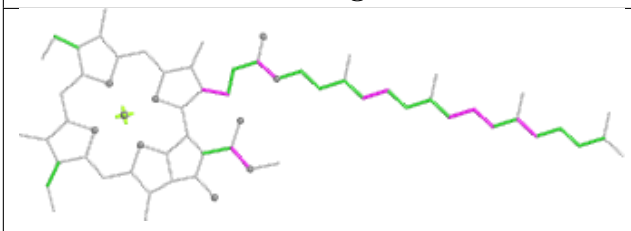
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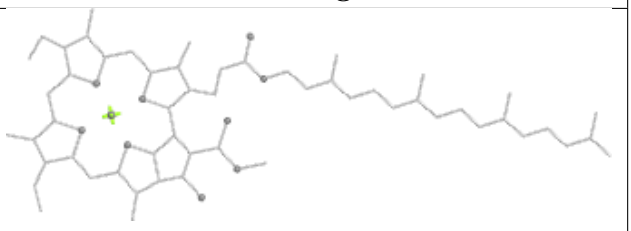
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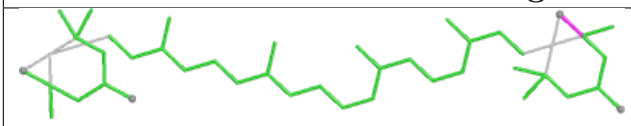


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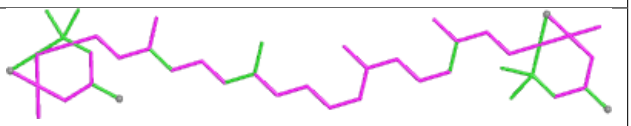


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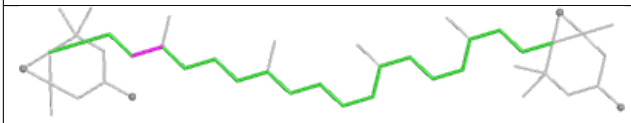
Ligand XAT 8 622



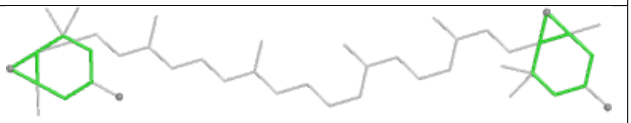
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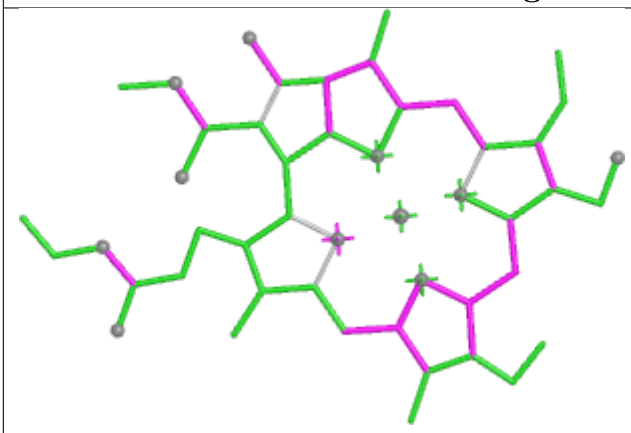


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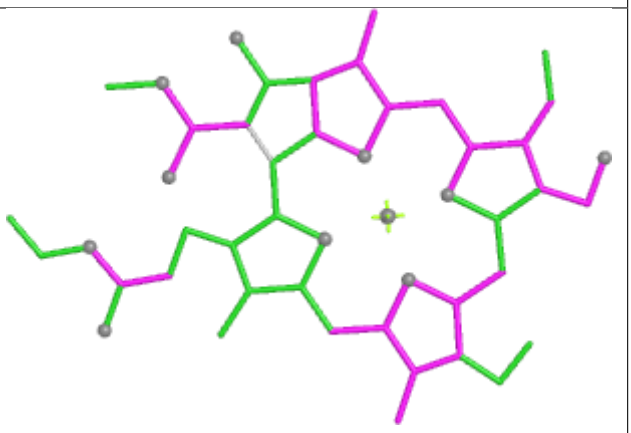


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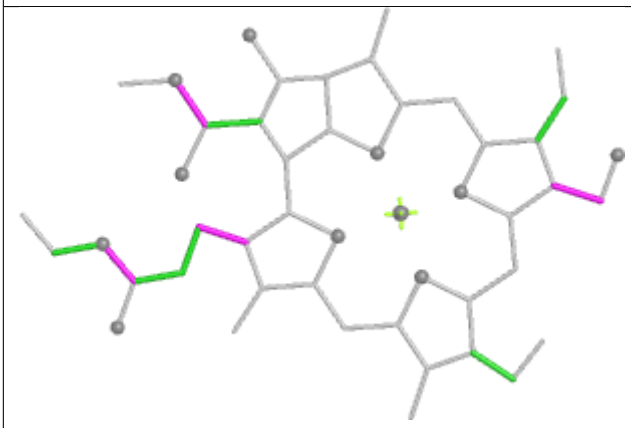
Ligand CHL Y 605



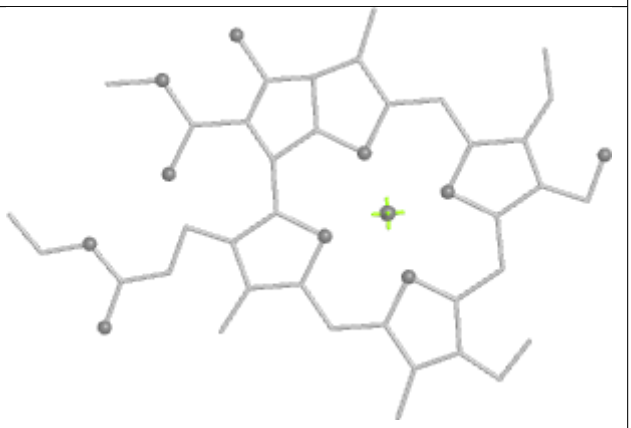
Bond lengths



Bond angles

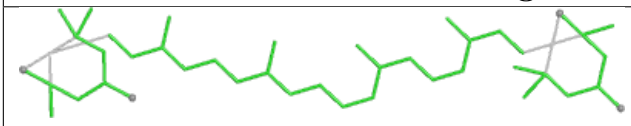


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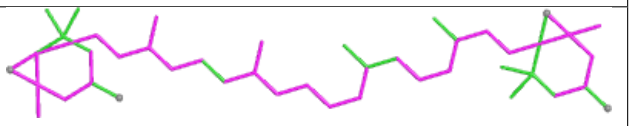


Rings

Ligand XAT n 1622



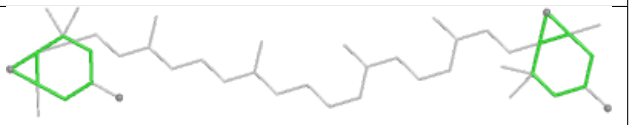
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Bond angles

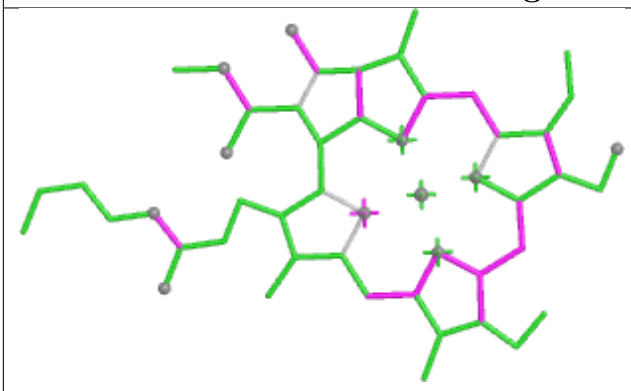


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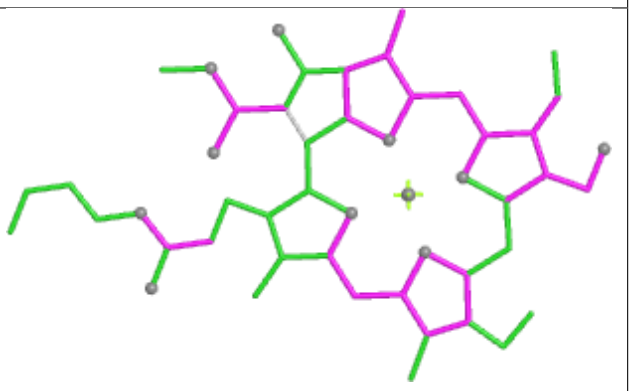


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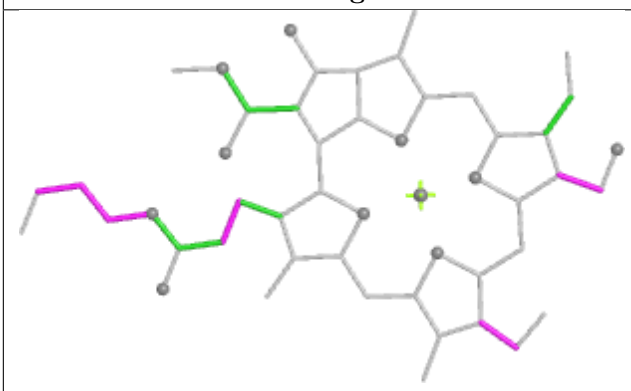
Ligand CHL Y 606



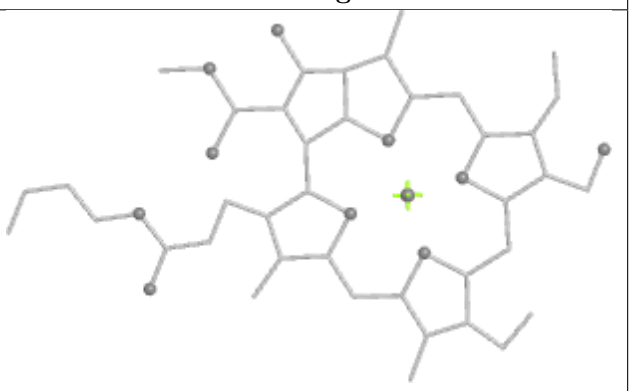
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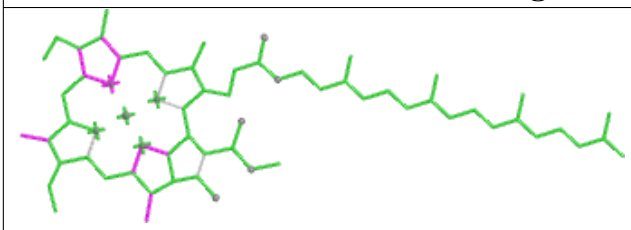


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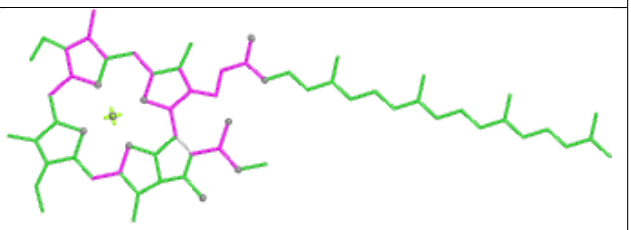


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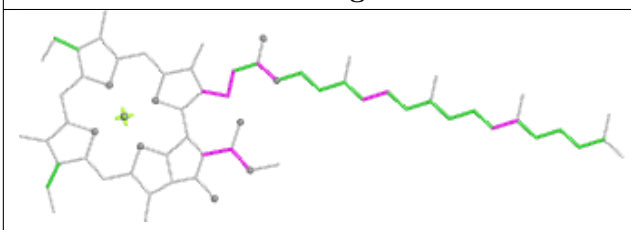
Ligand CLA c 513



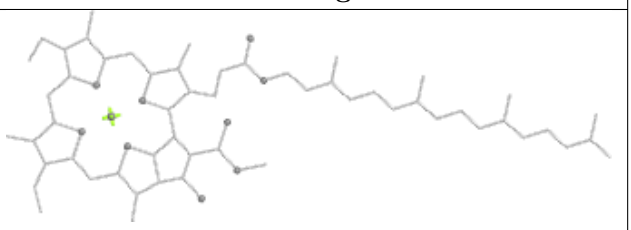
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Bond angles

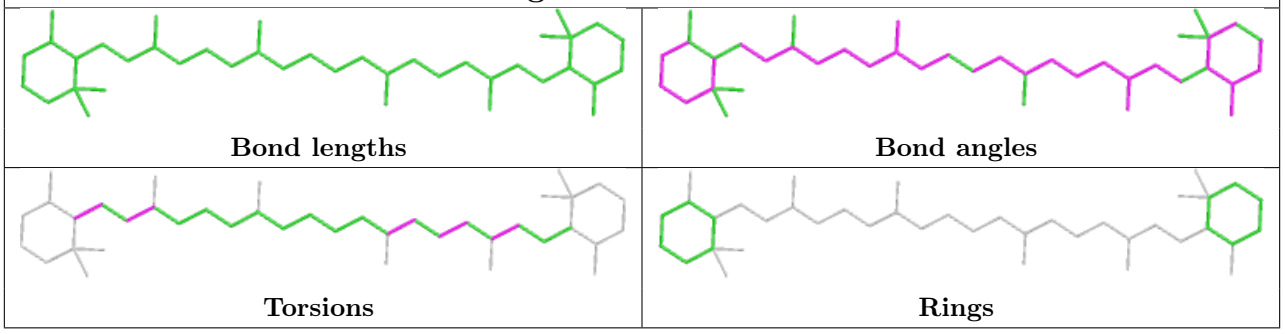


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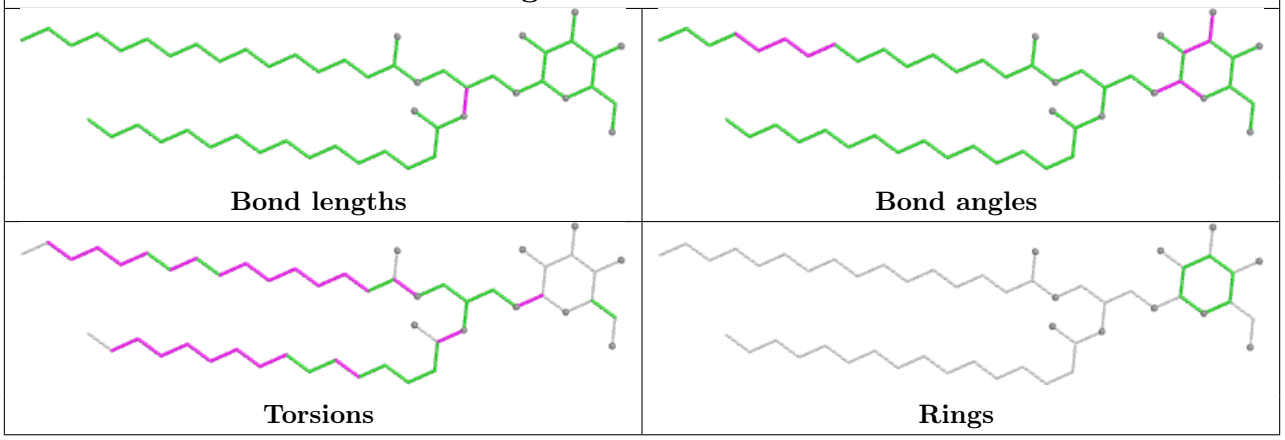


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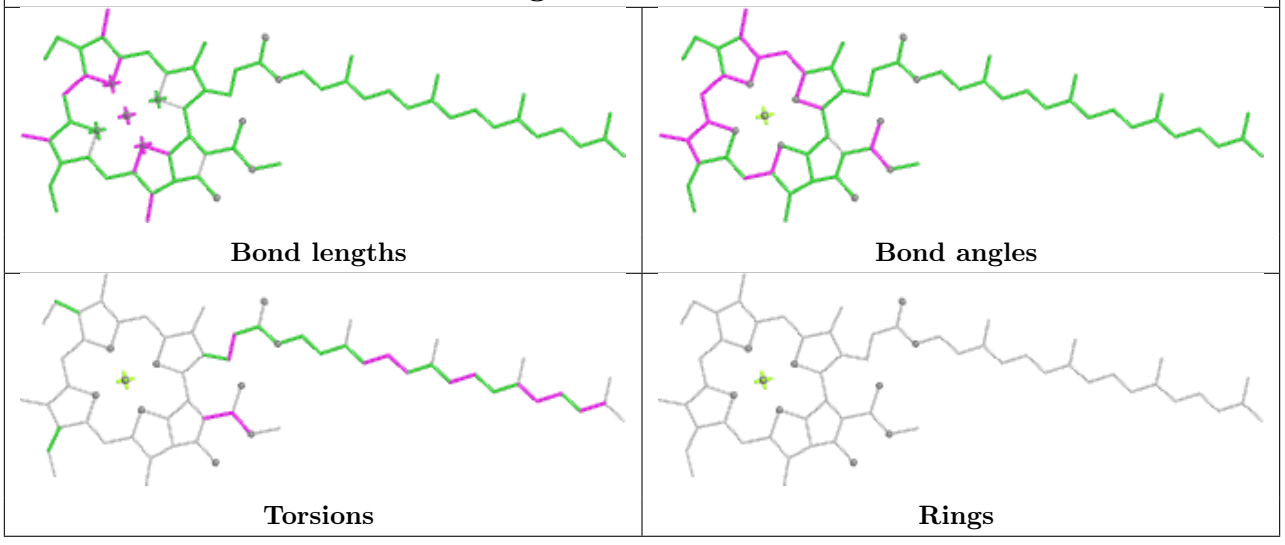
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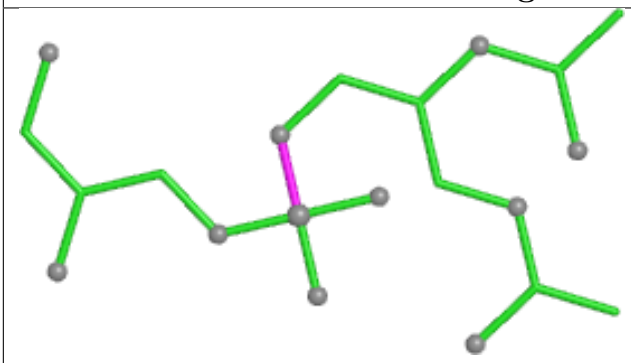
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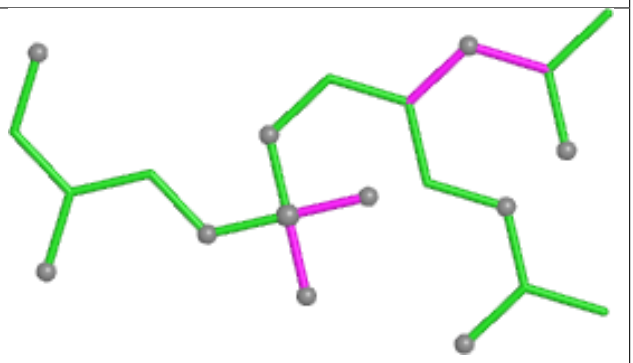
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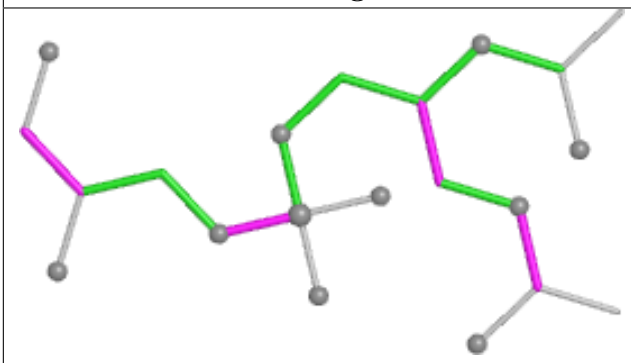
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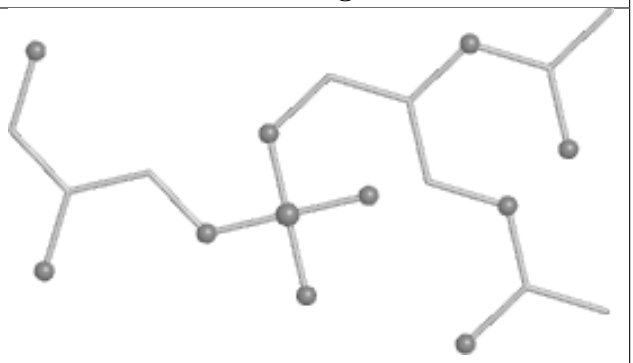
Bond lengths



Bond angles

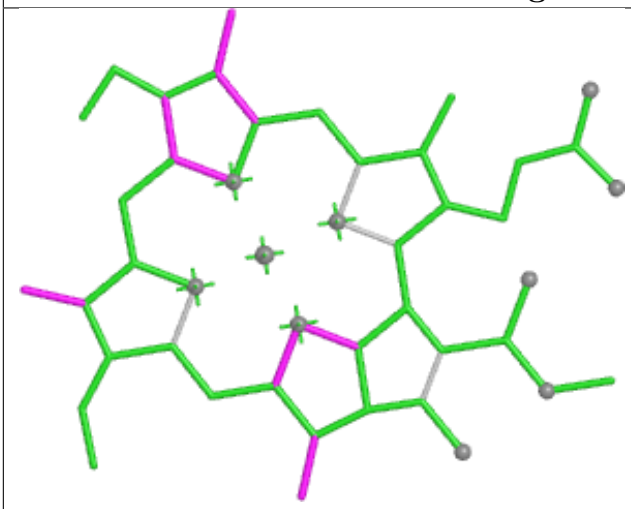


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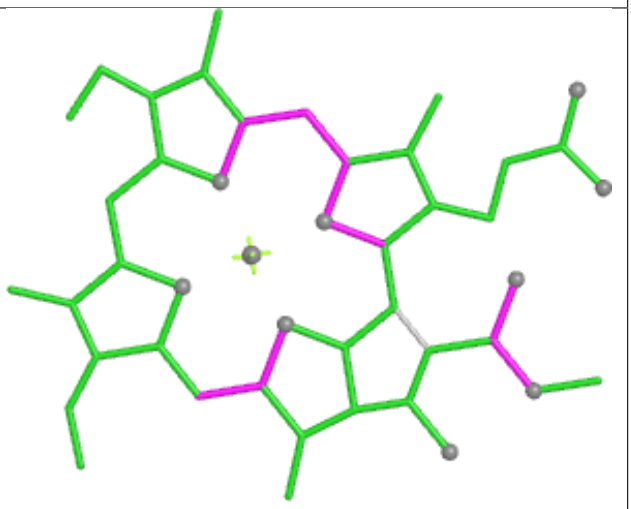


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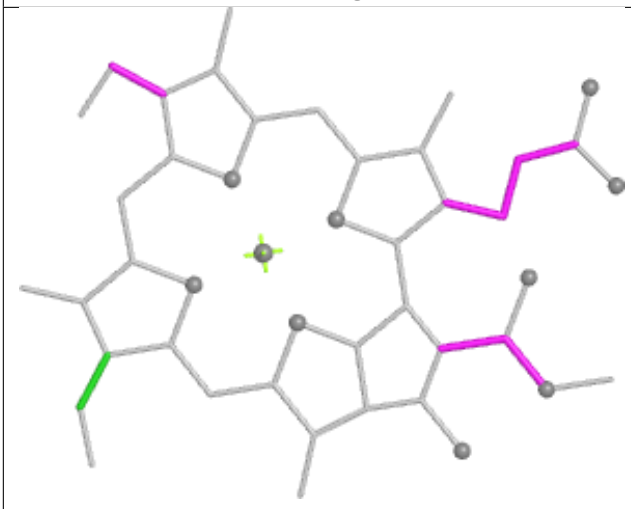
Ligand CLA 4 604



Bond lengths



Bond angles

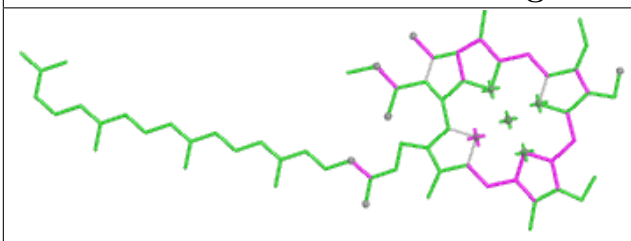


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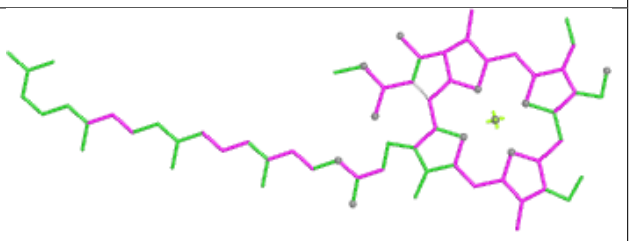


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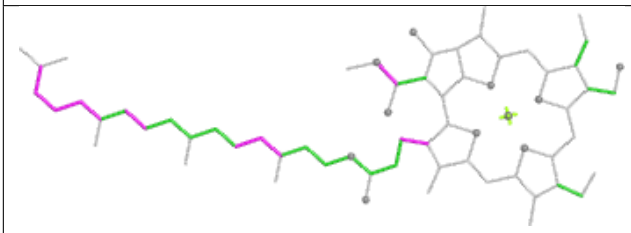
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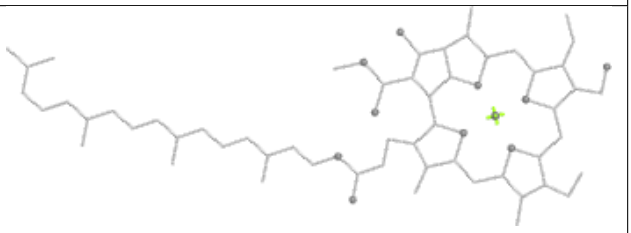
Bond lengths



Bond angles

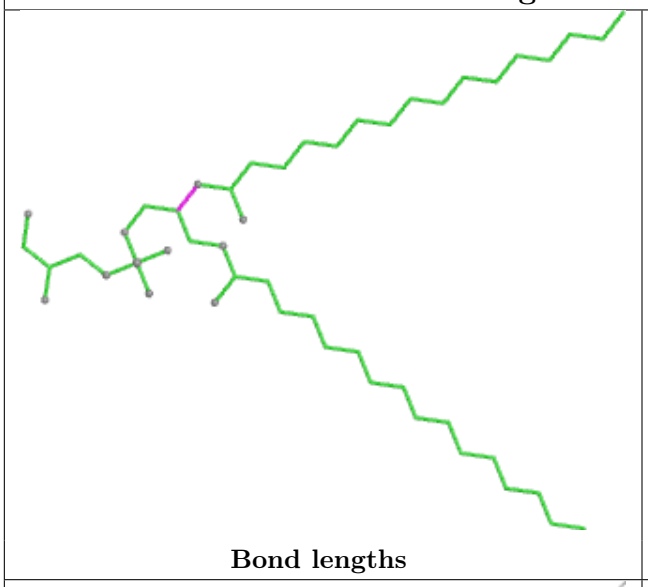


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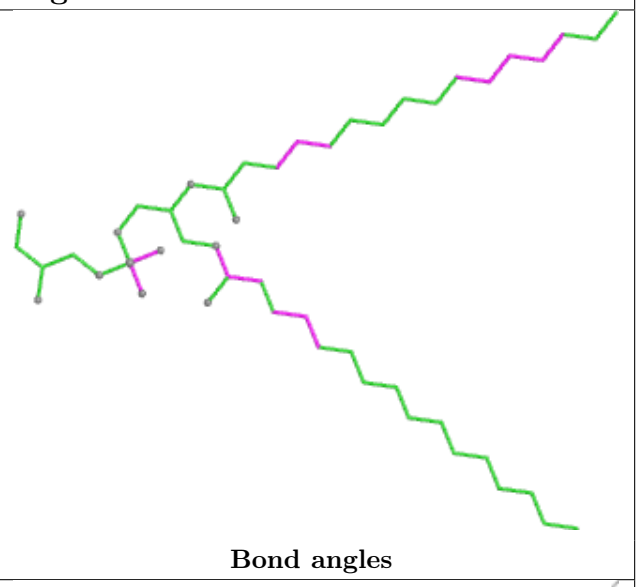


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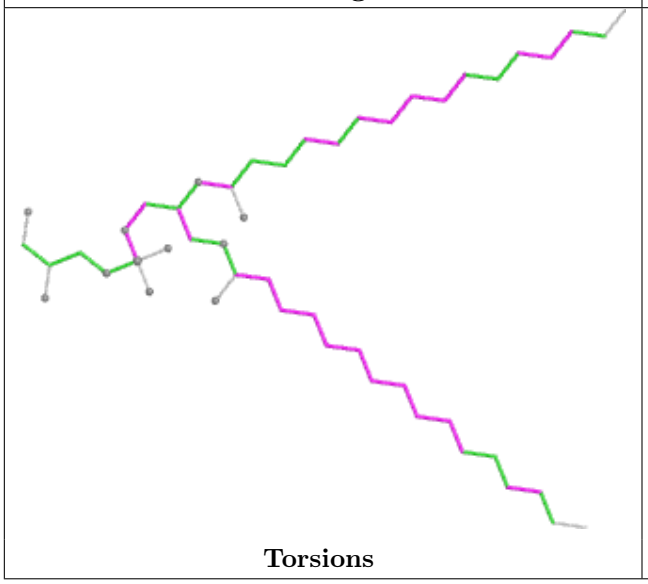
Ligand LHG g 2630



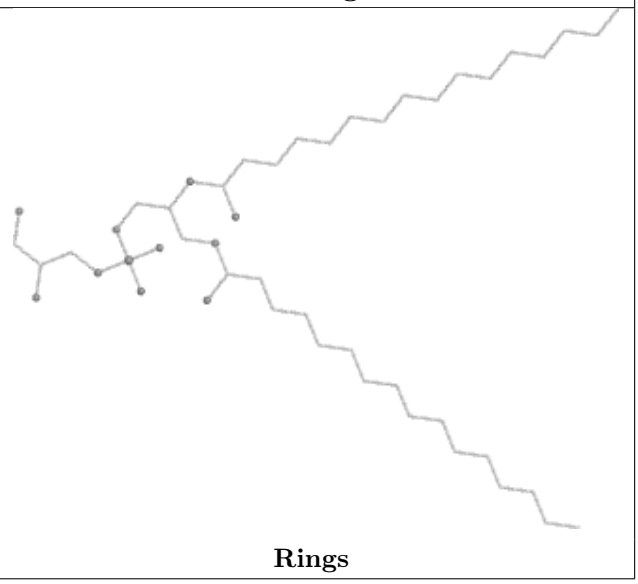
Bond lengths



Bond angles

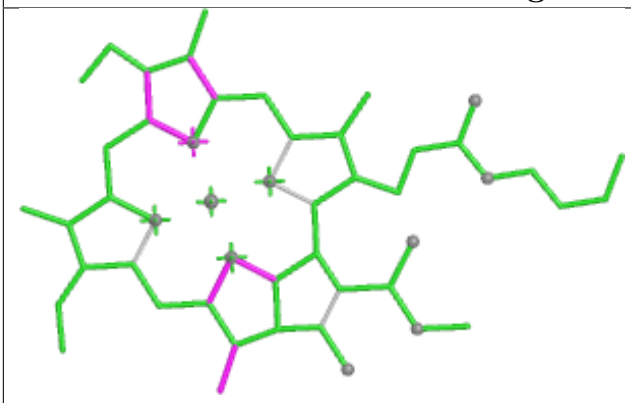


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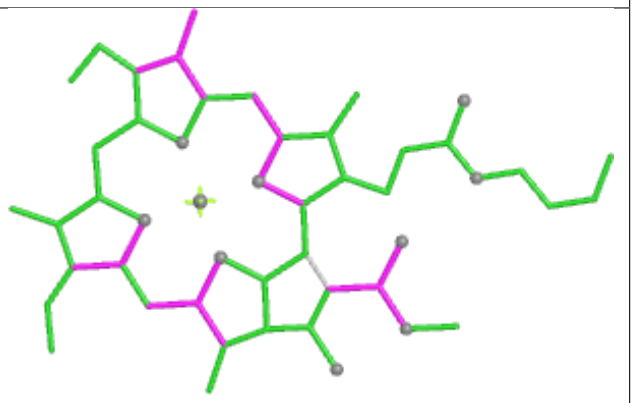


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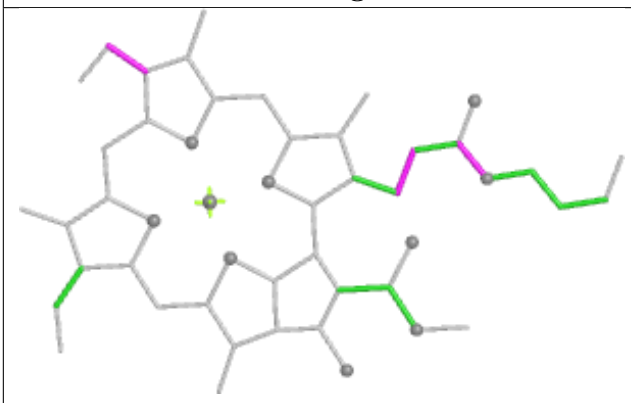
Ligand CLA S 614



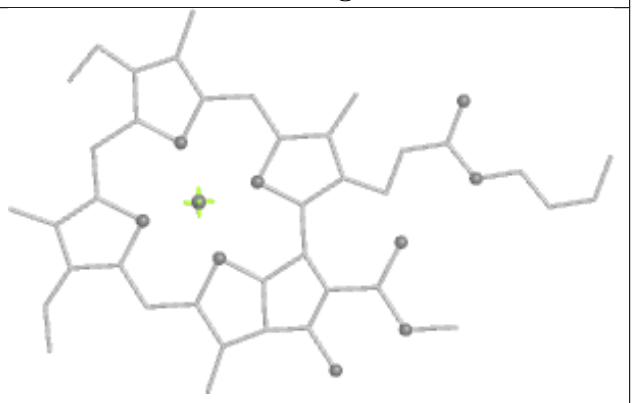
Bond lengths



Bond angles

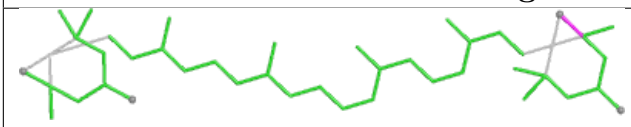


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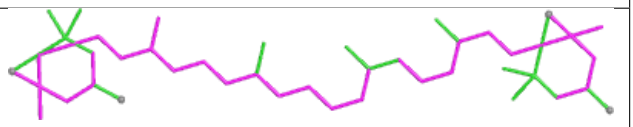


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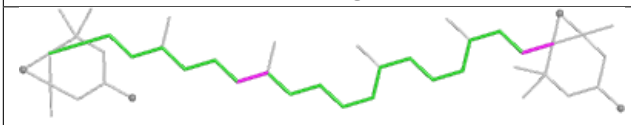
Ligand XAT 2 1622



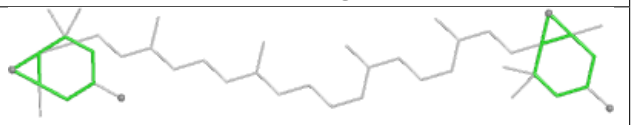
Bond lengths



Bond angles

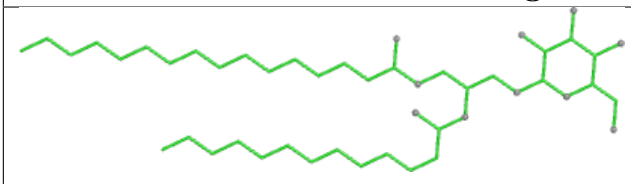


Torsions

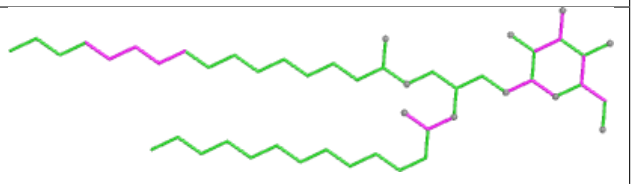


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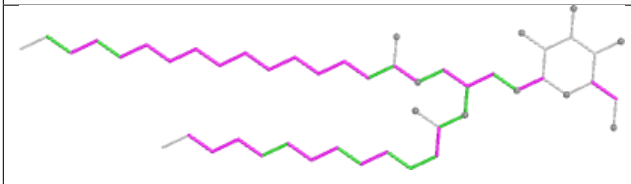
Ligand LMG a 413



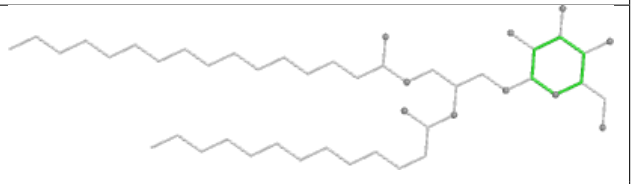
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Bond angles

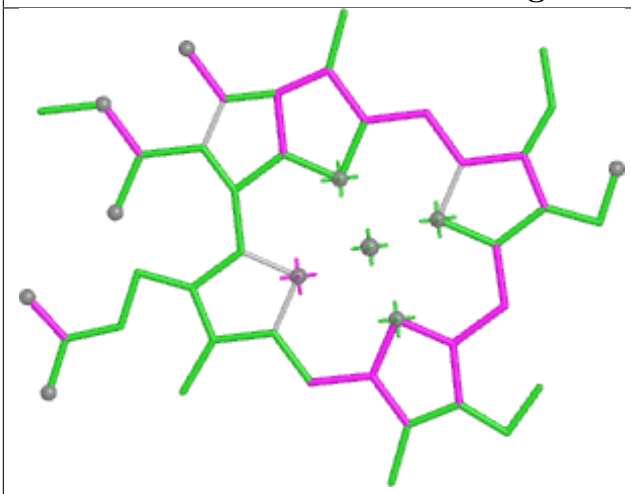


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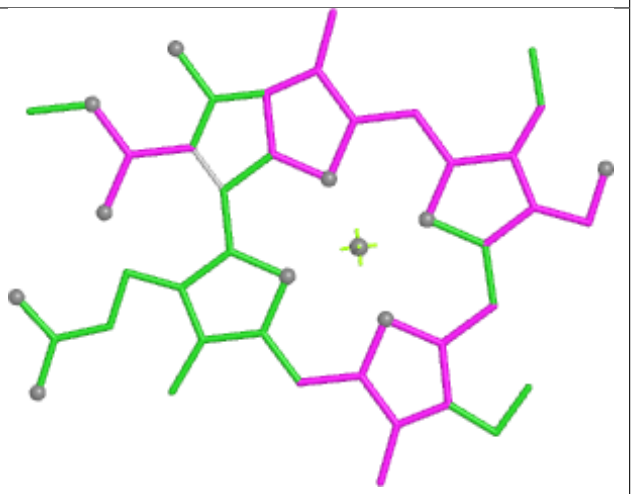


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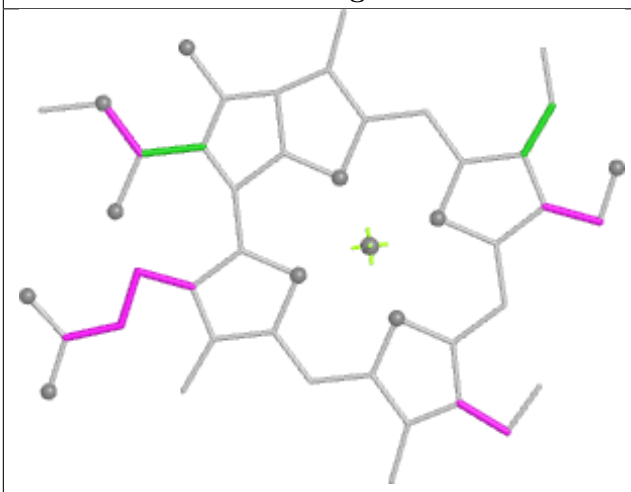
Ligand CHL 4 607



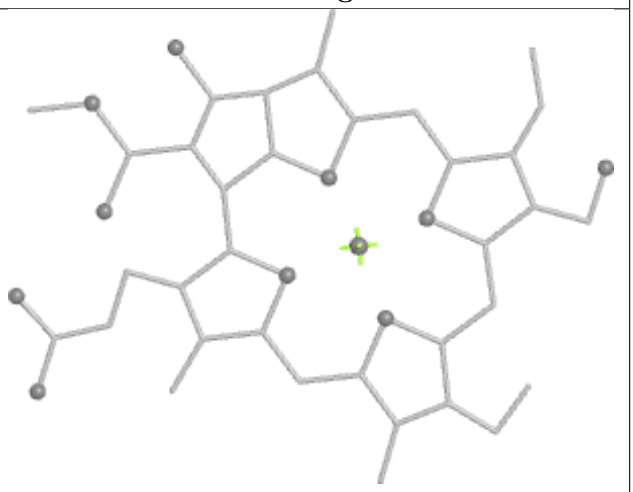
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Bond angles

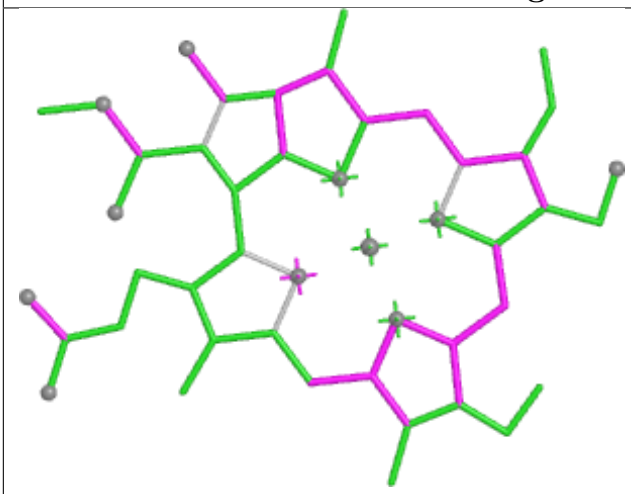


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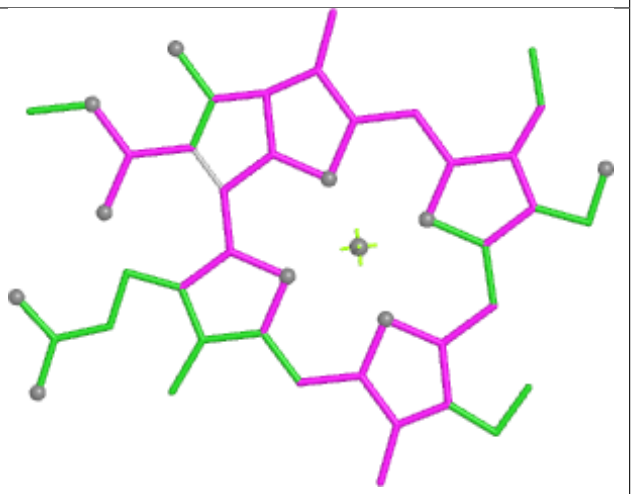


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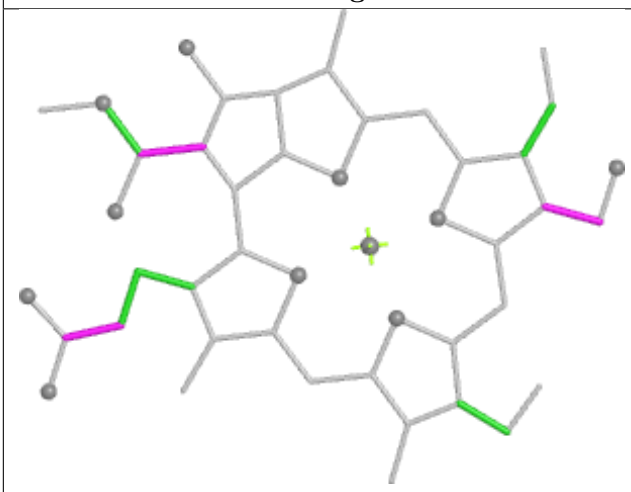
Ligand CHL 1 601



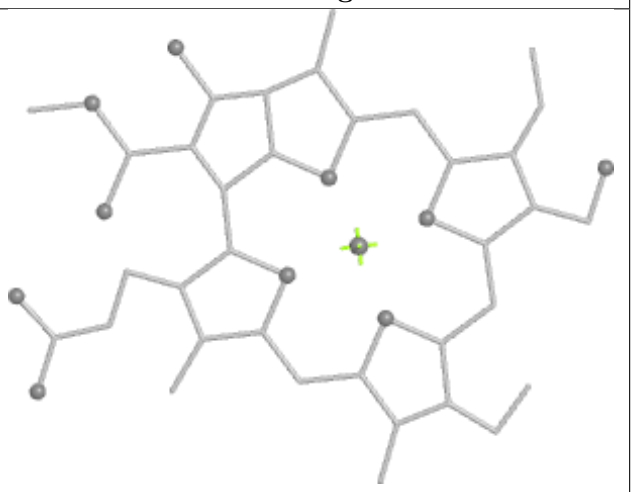
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Bond angles

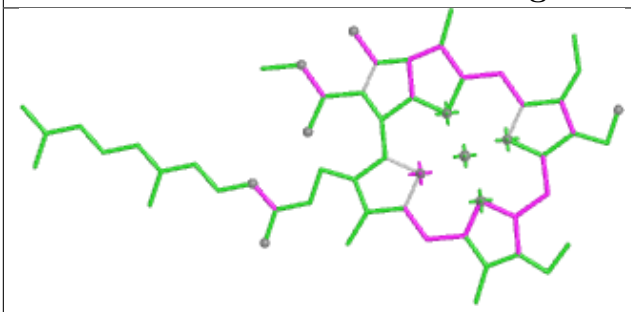


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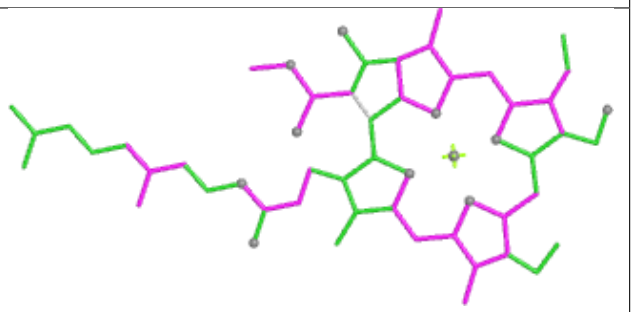


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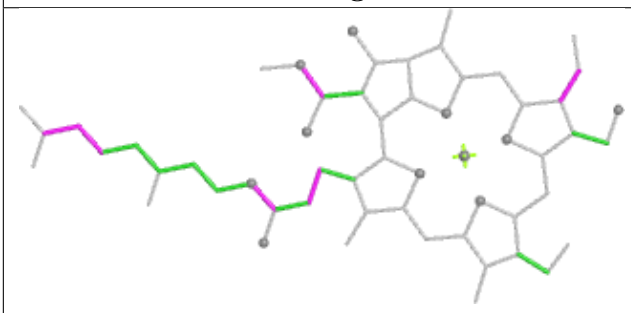
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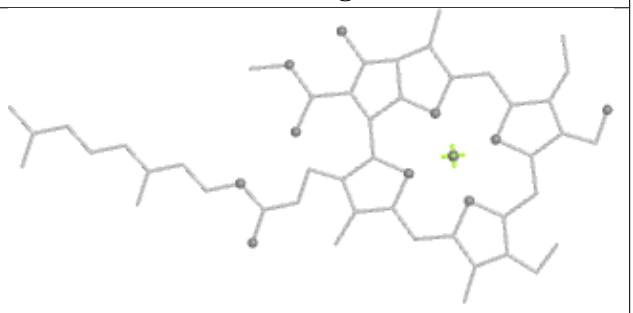
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Bond angles

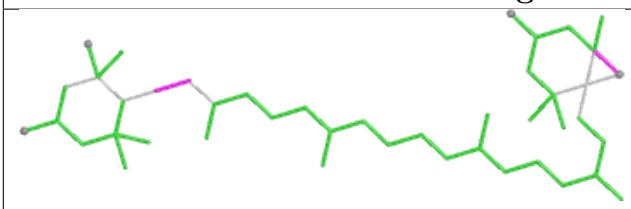


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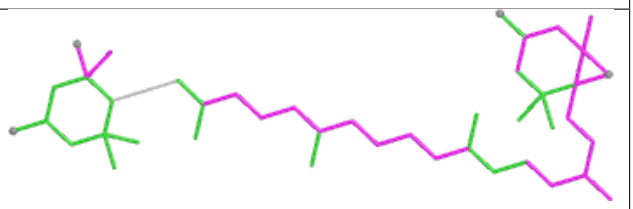


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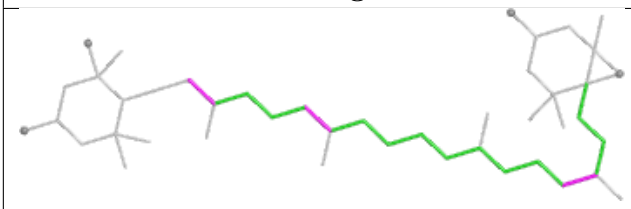
Ligand NEX S 1623



Bond lengths



Bond angles

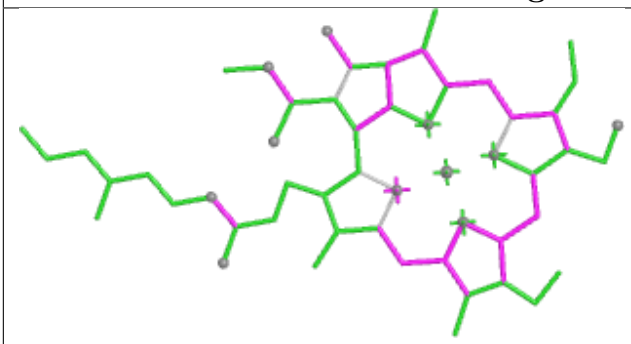


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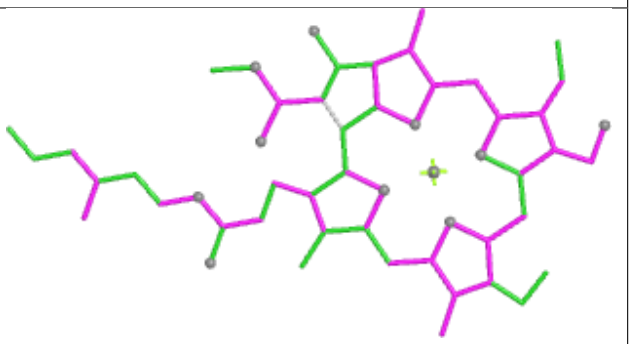


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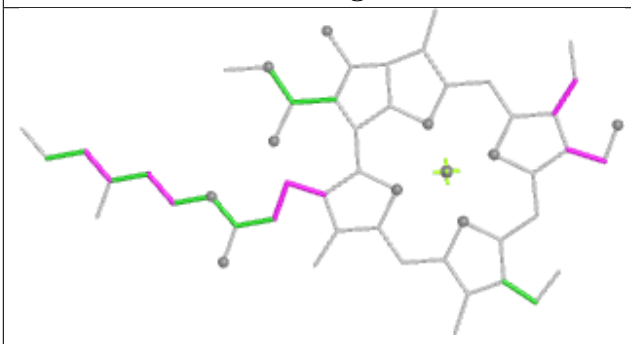
Ligand CHL 3 607



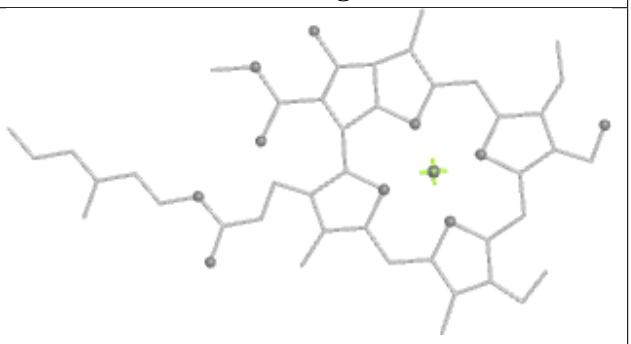
Bond lengths



Bond angles

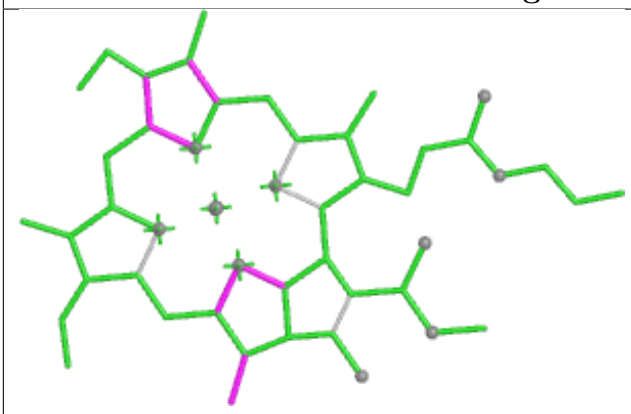


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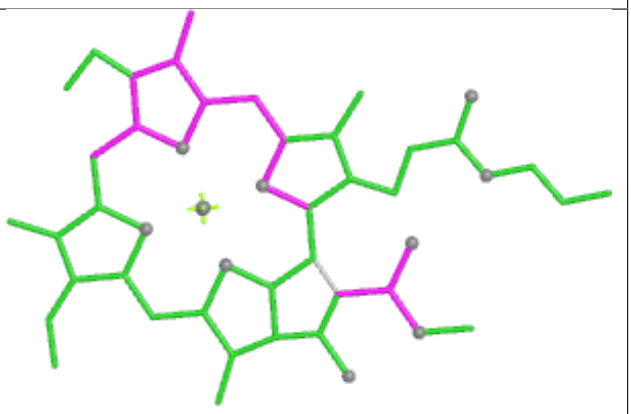


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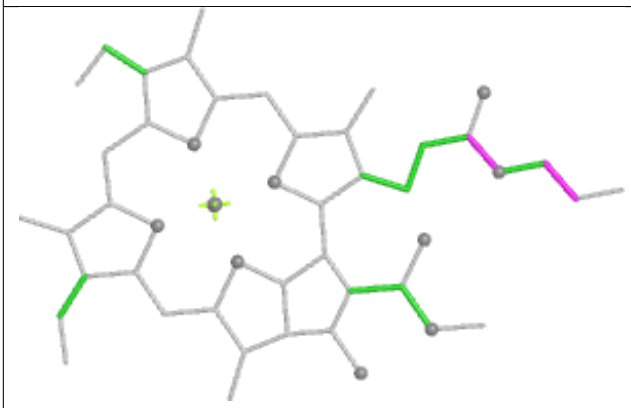
Ligand CLA G 614



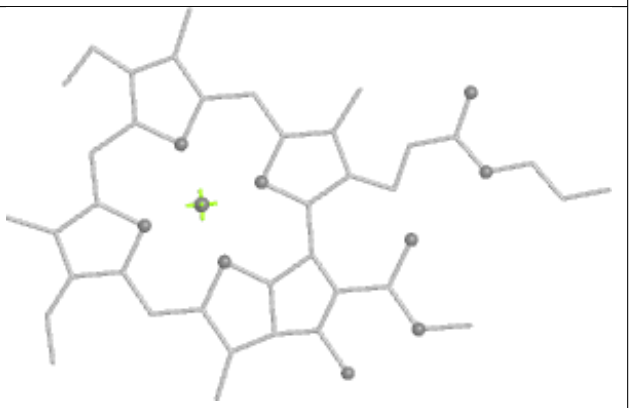
Bond lengths



Bond angles

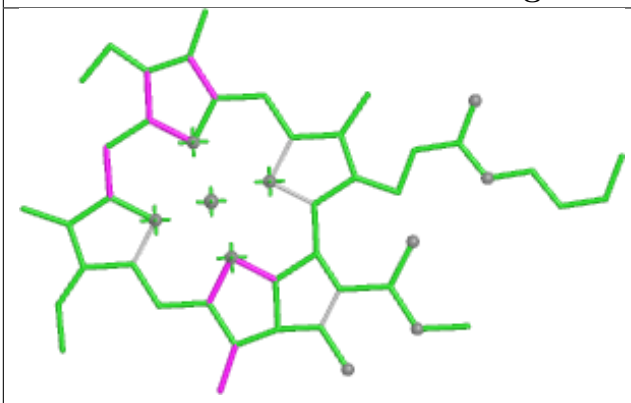


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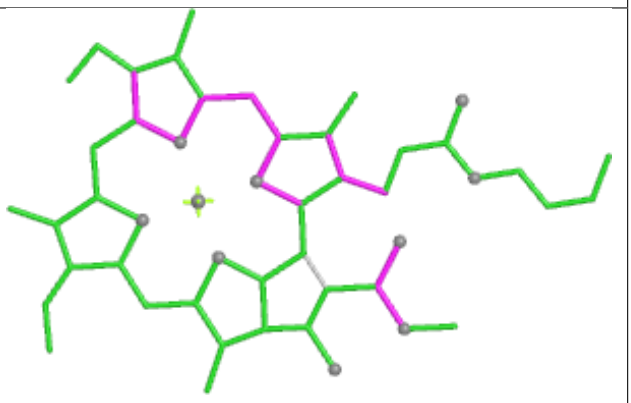


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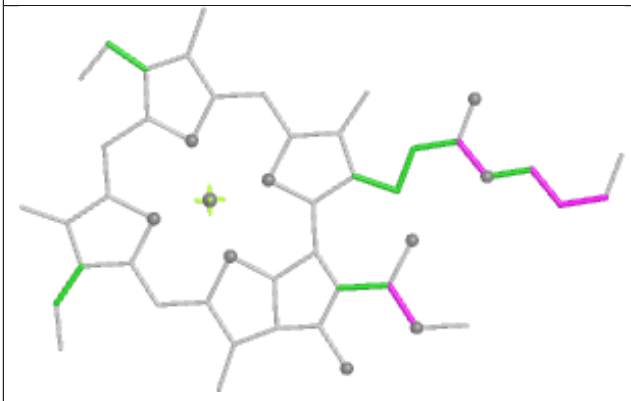
Ligand CLA R 612



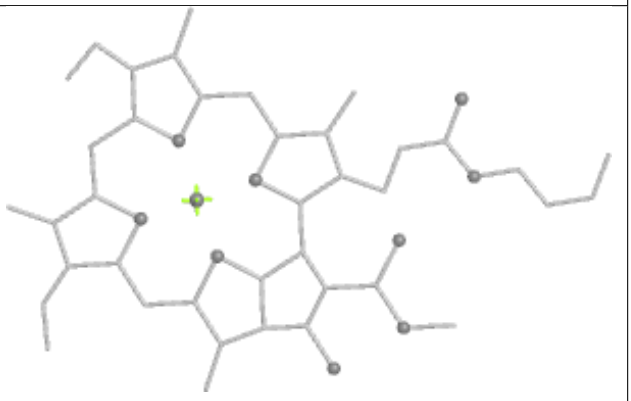
Bond lengths



Bond angles

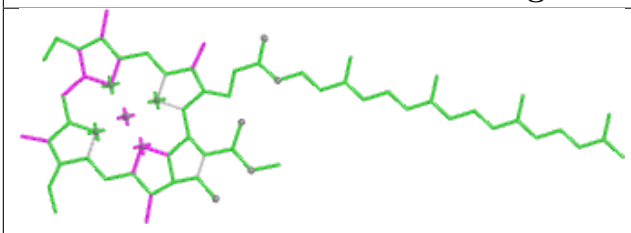


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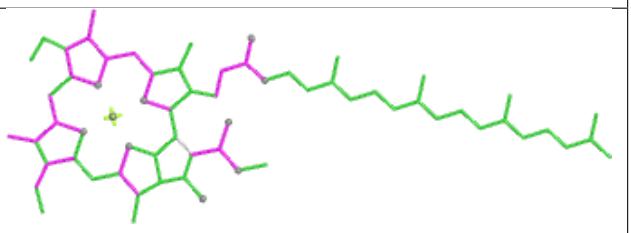


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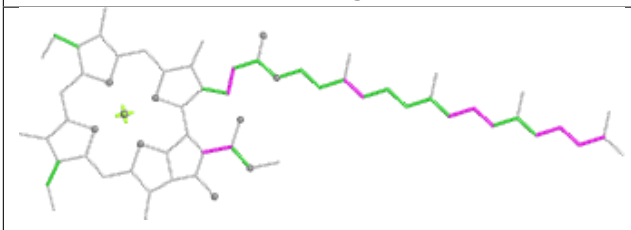
Ligand CLA b 607



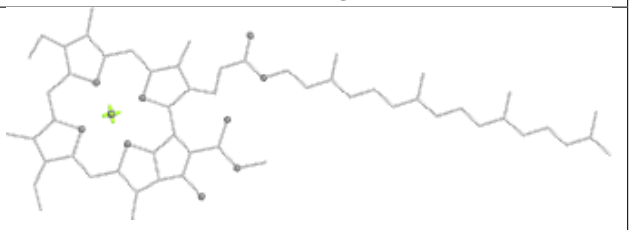
Bond lengths



Bond angles

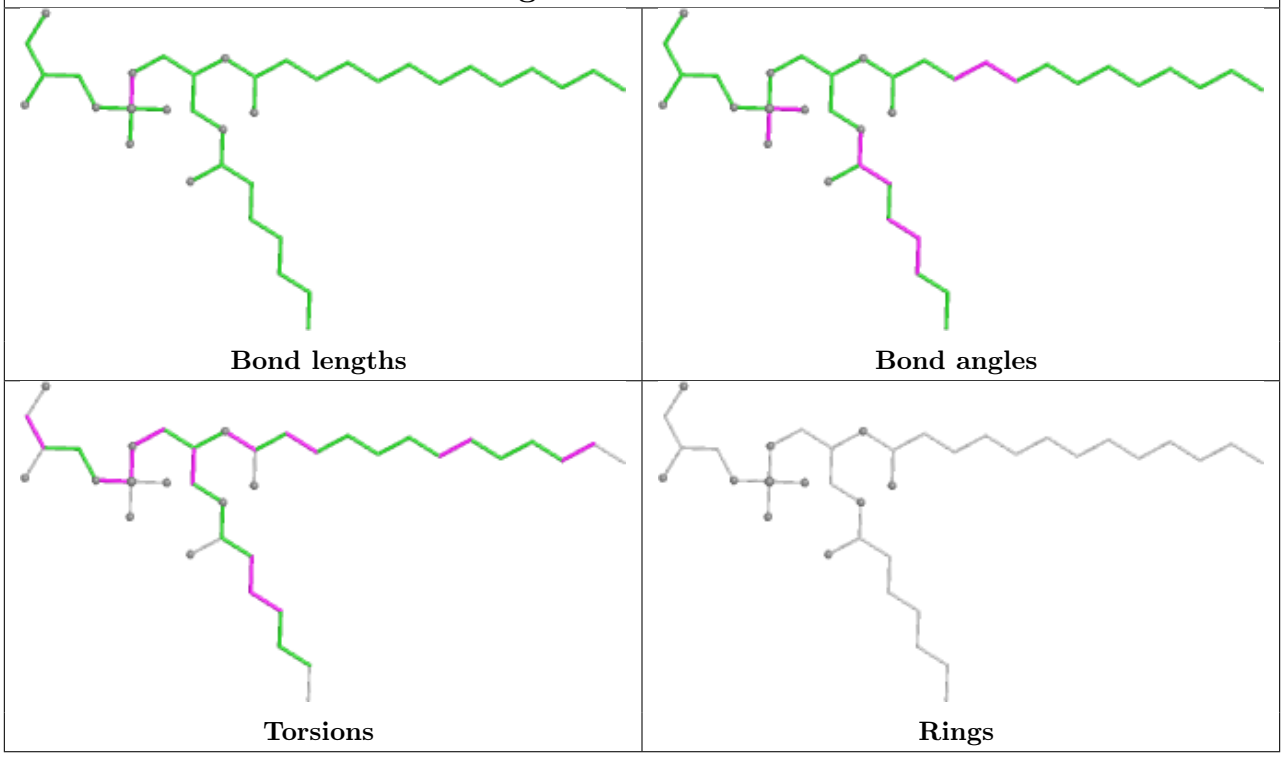


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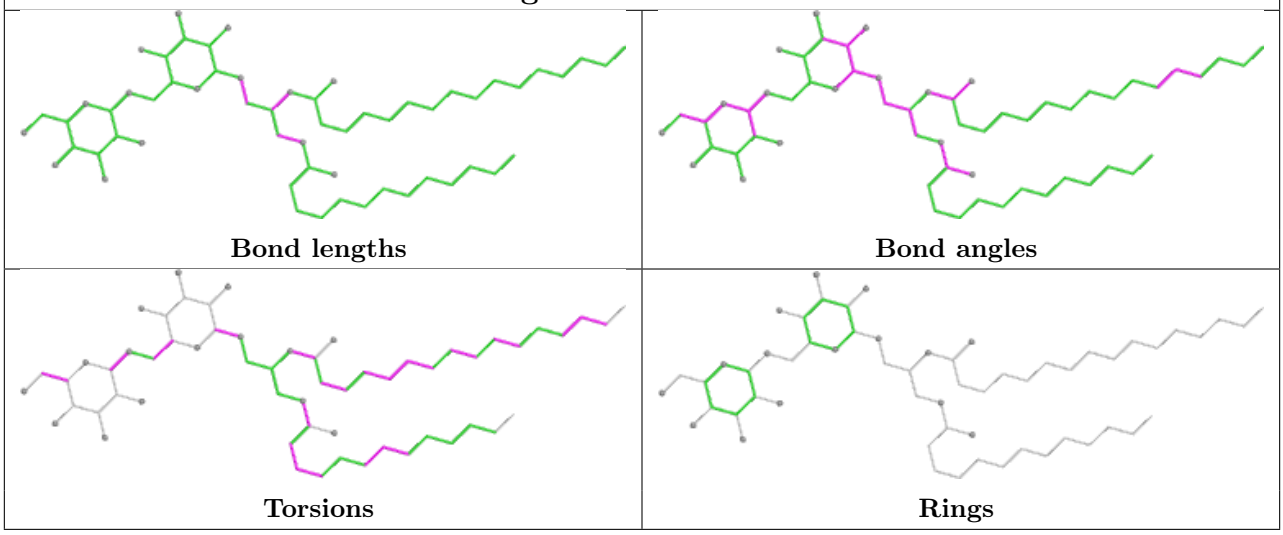


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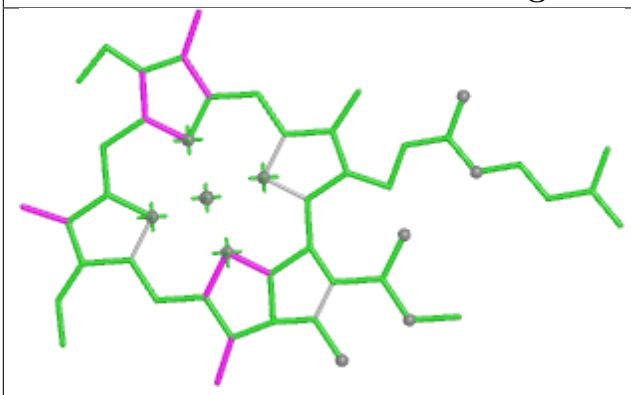
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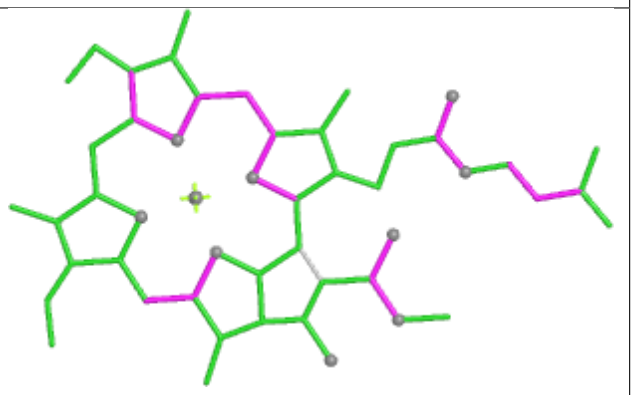
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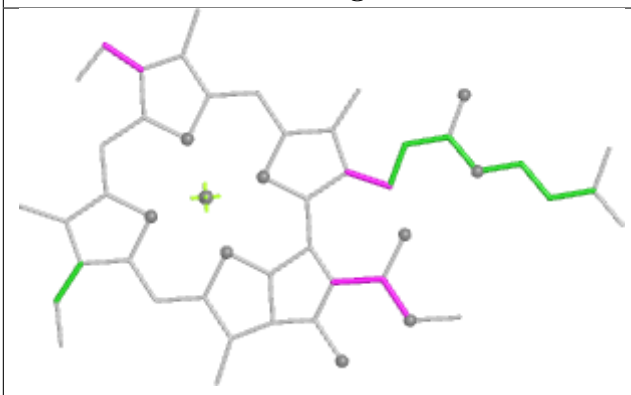
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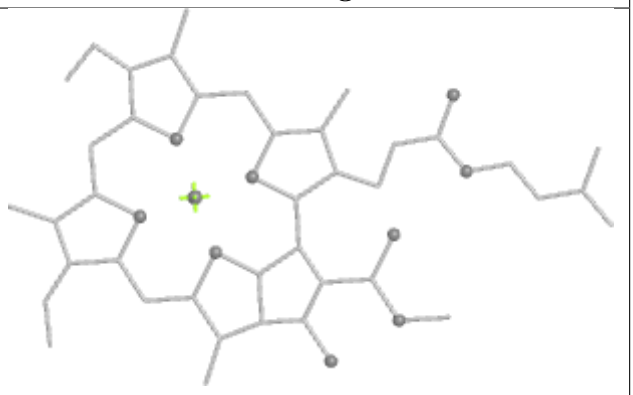
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Bond angles

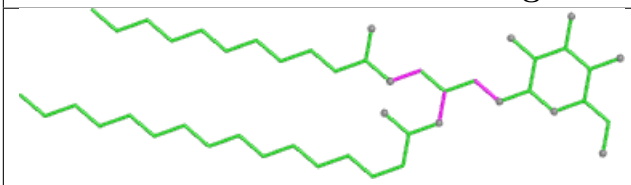


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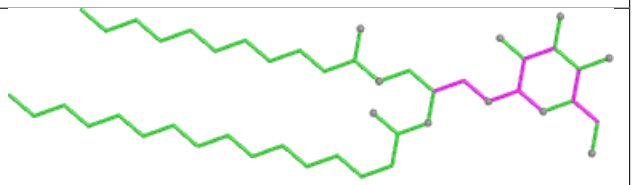


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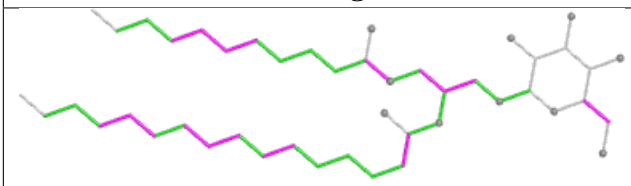
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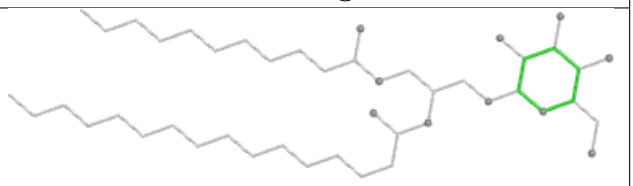
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Bond angles

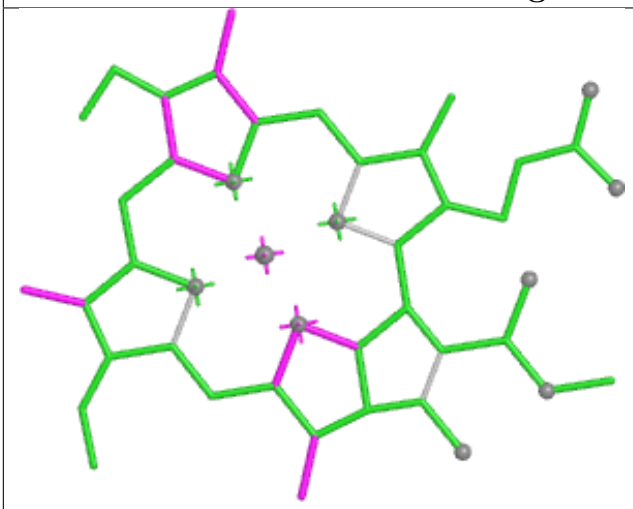


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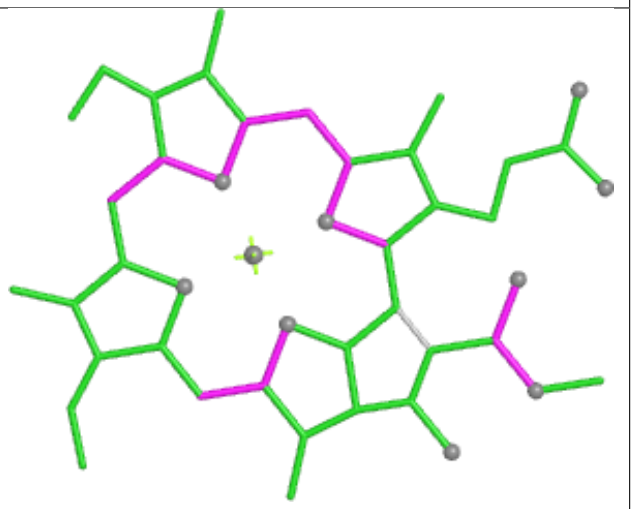


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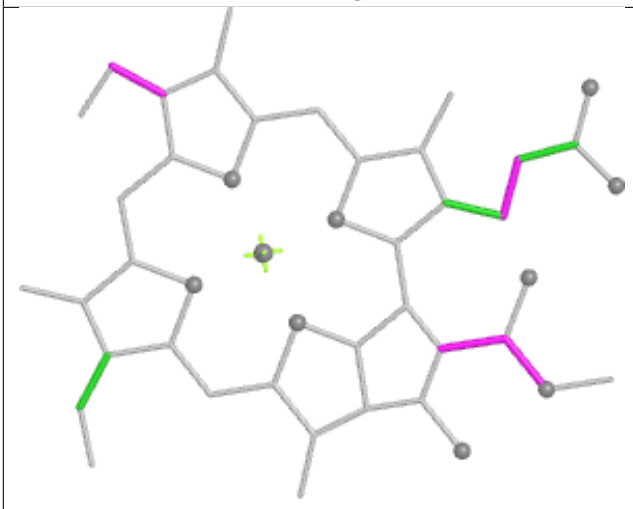
Ligand CLA 6 613



Bond lengths



Bond angles

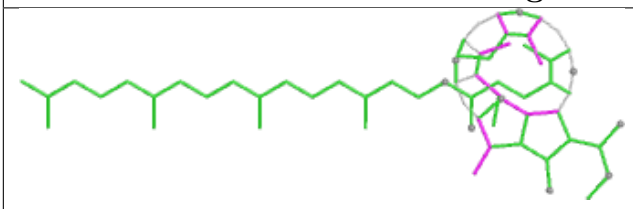


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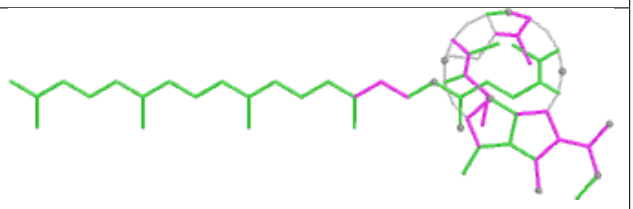


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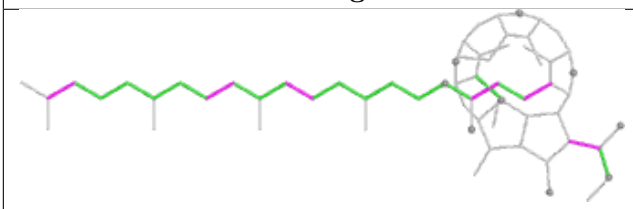
Ligand PHO a 409



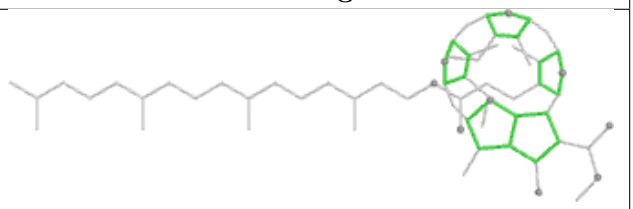
Bond lengths



Bond angles

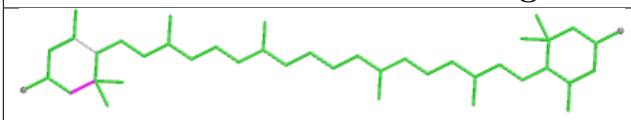


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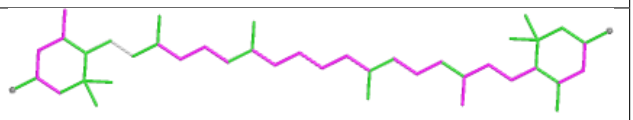


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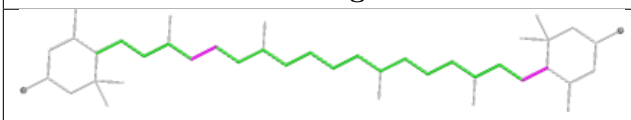
Ligand LUT 7 1621



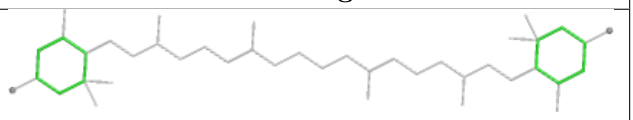
Bond lengths



Bond angles

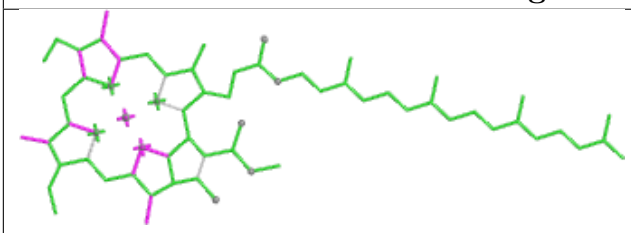


Torsions

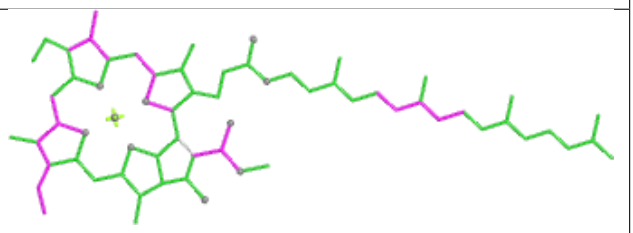


Rings

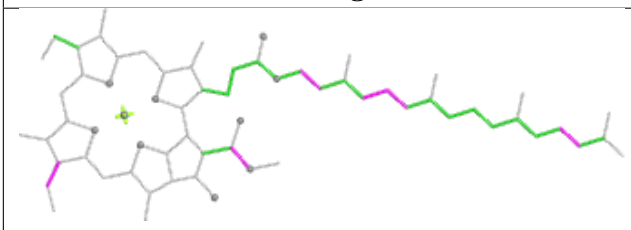
Ligand CLA a 405



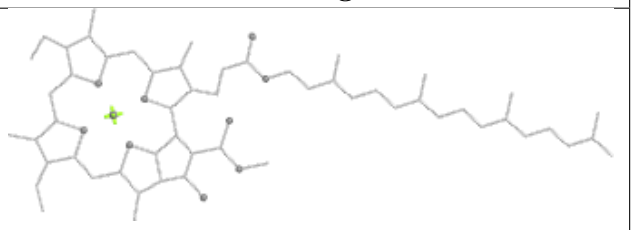
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Bond angles

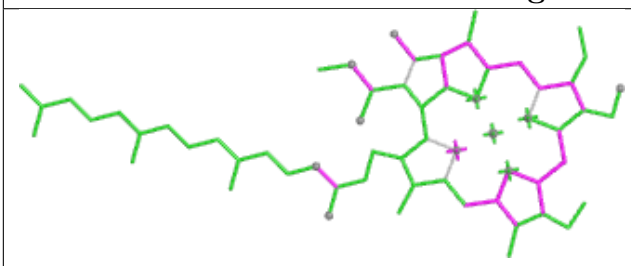


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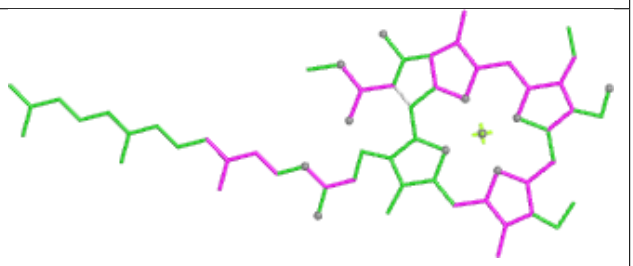


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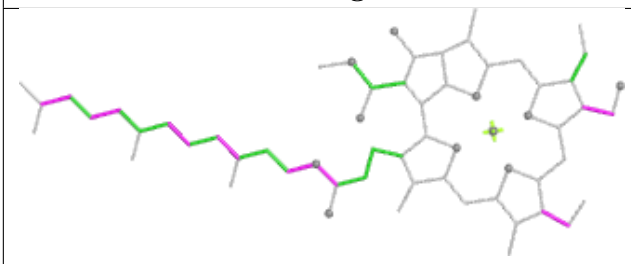
Ligand CHL 6 609



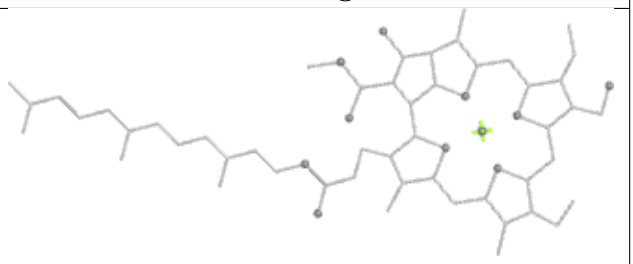
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Bond angles

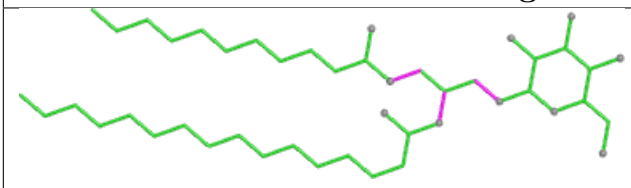


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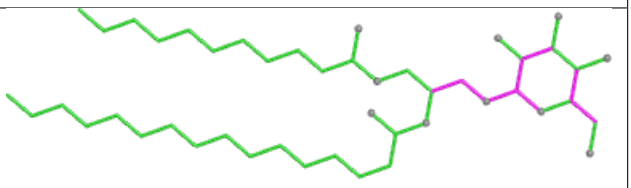


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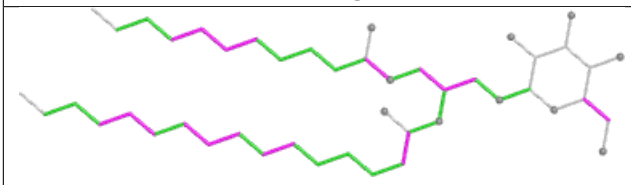
Ligand LMG D 411



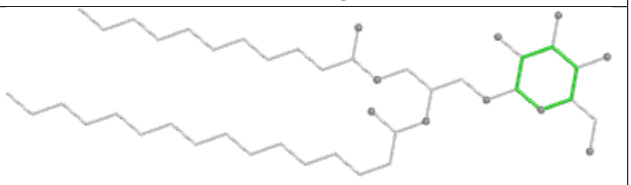
Bond lengths



Bond angles

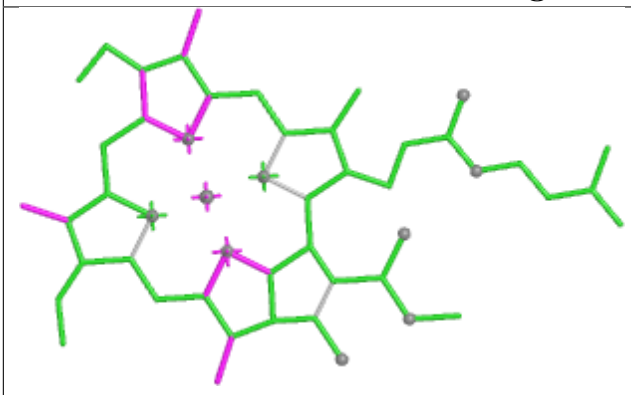


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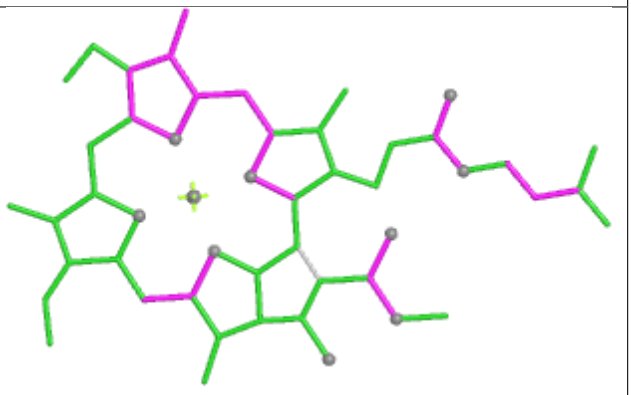


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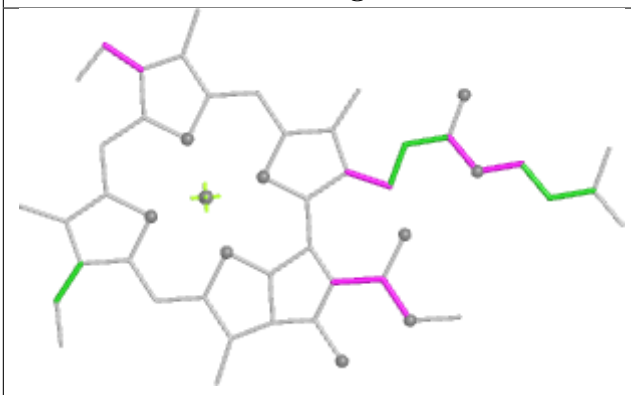
Ligand CLA 1 604



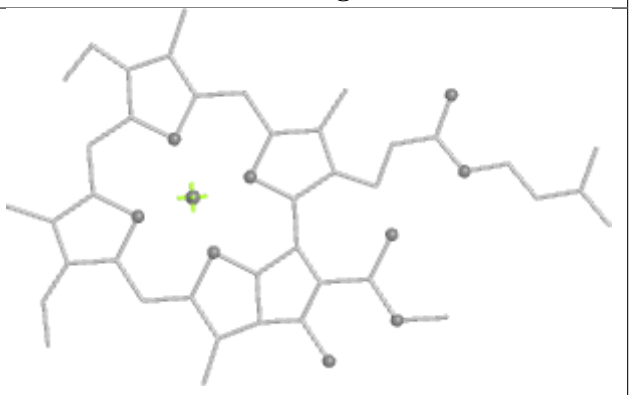
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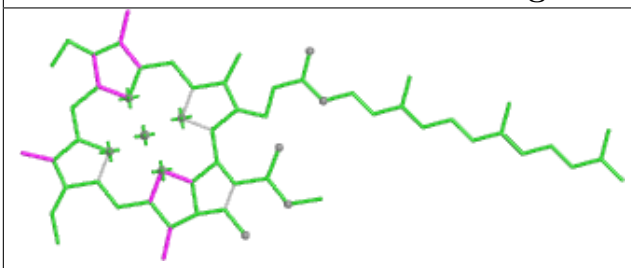
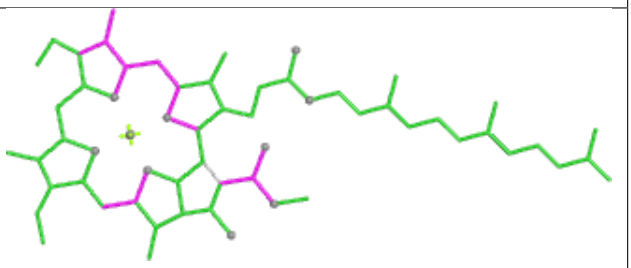
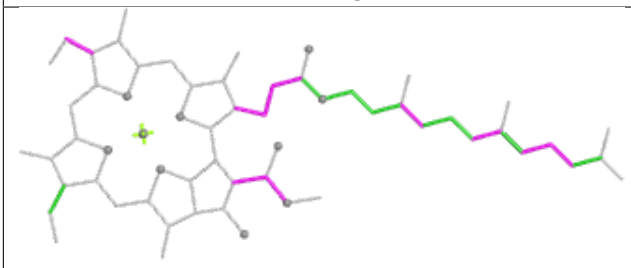
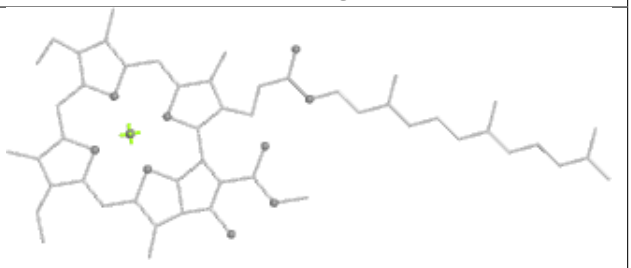
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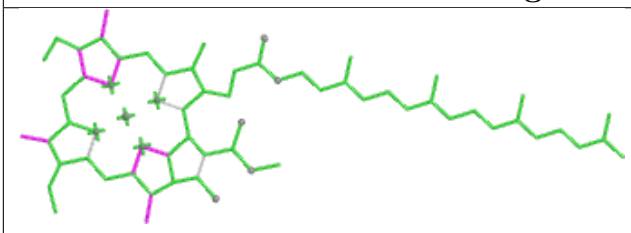
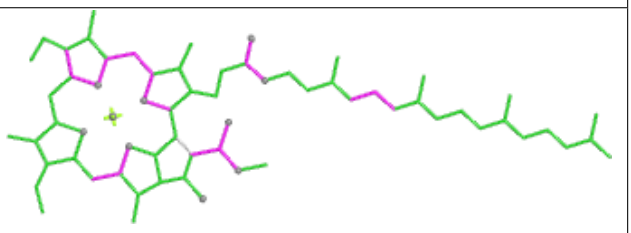
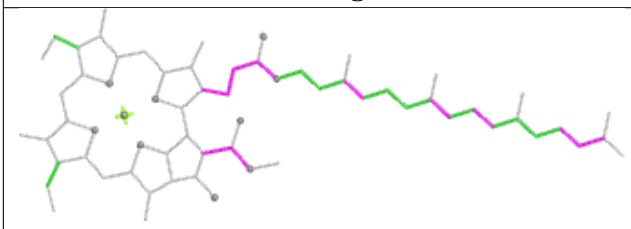
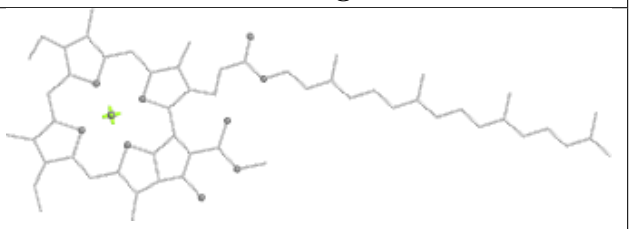


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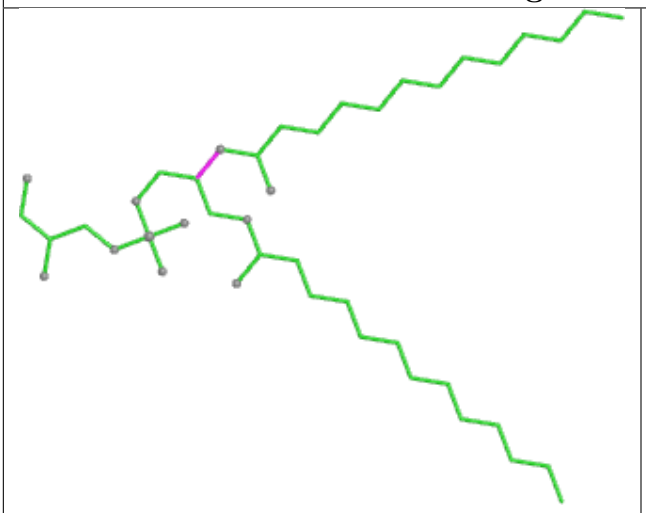


Rings

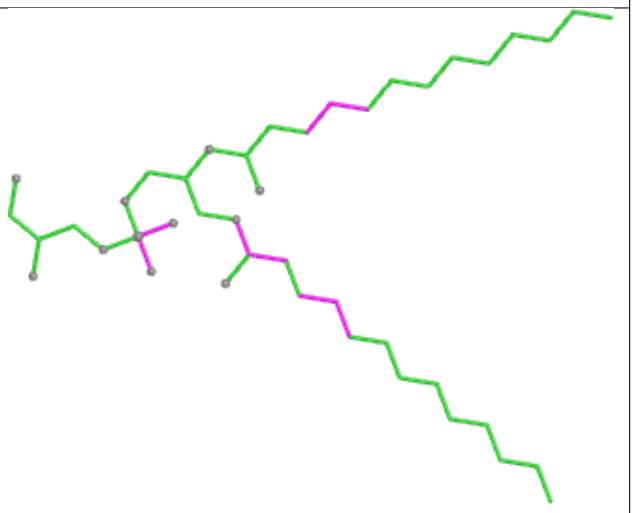
Ligand CLA 3 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA C 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

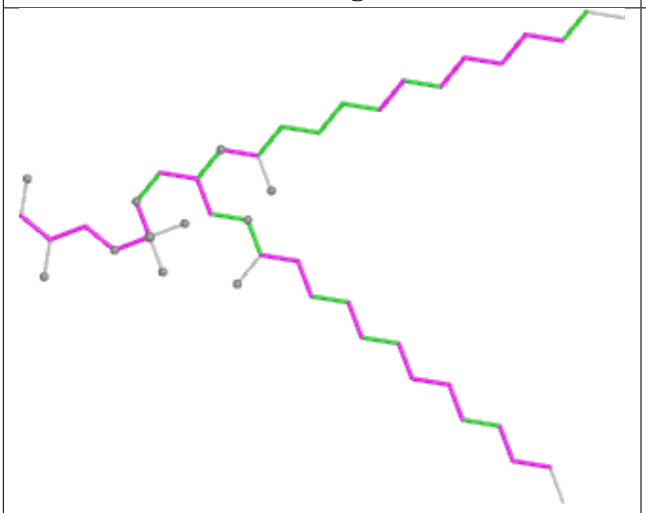
Ligand LHG d 410



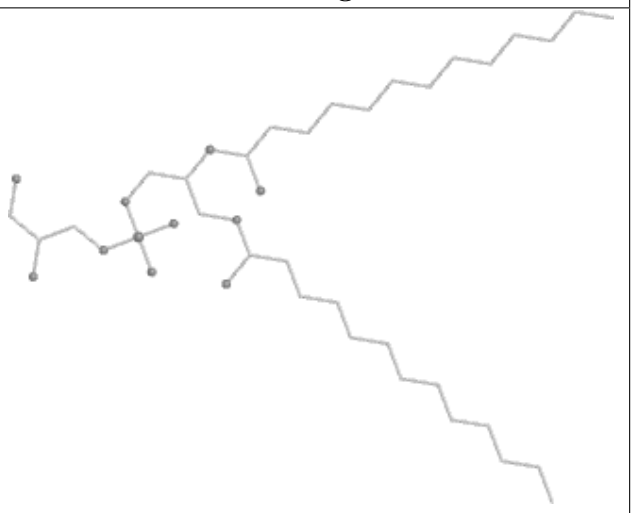
Bond lengths



Bond angles

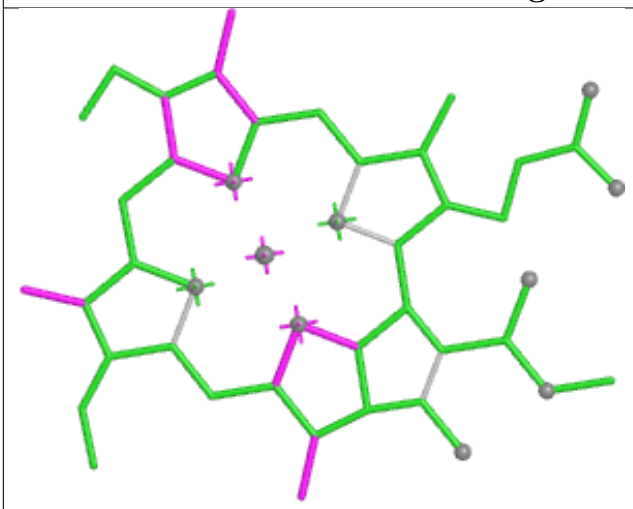


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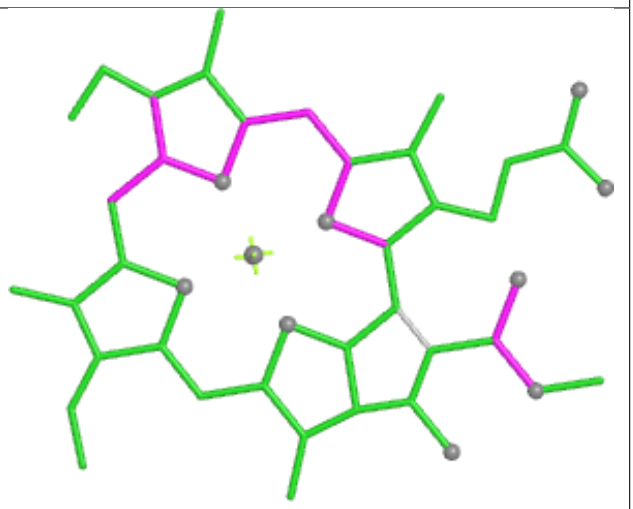


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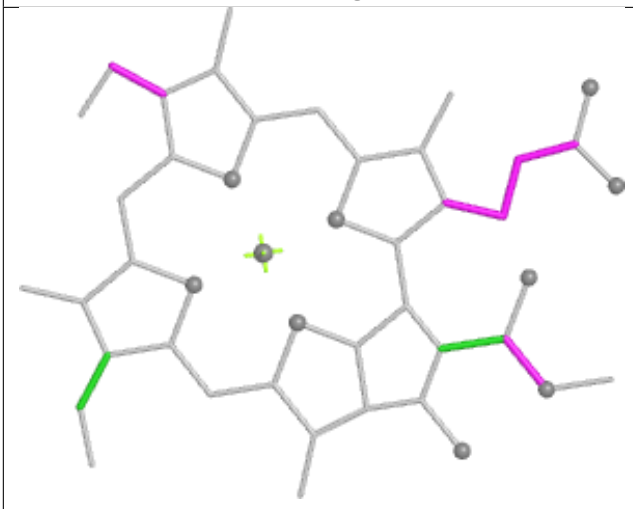
Ligand CLA 1 611



Bond lengths



Bond angles

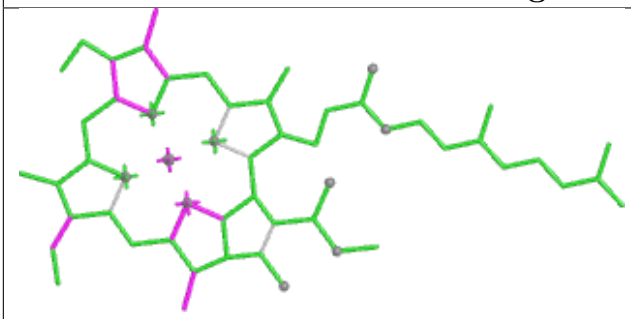


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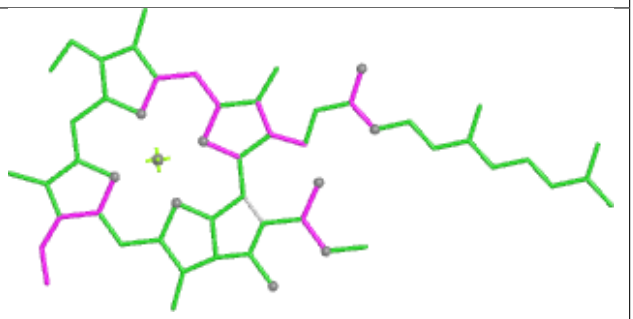


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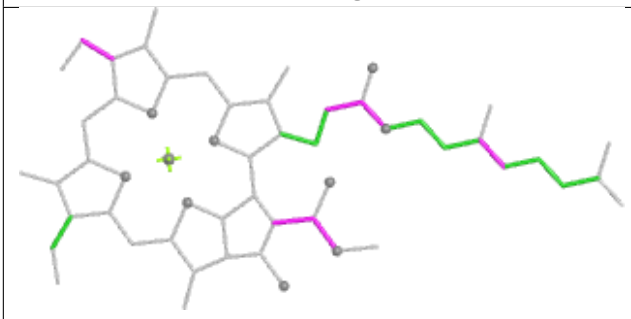
Ligand CLA 2 603



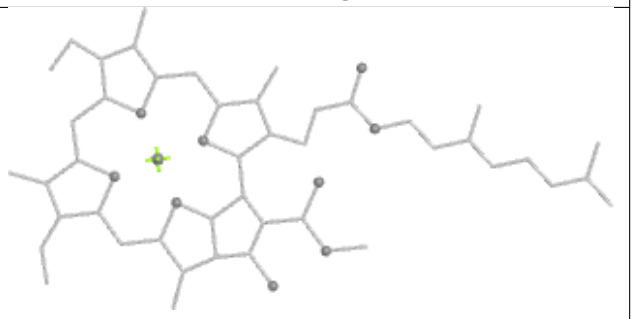
Bond lengths



Bond angles

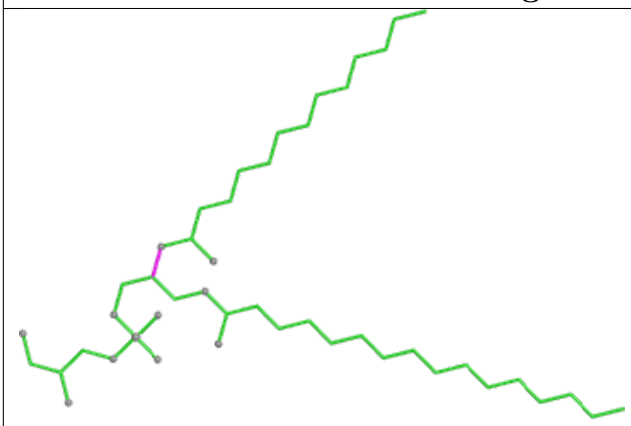


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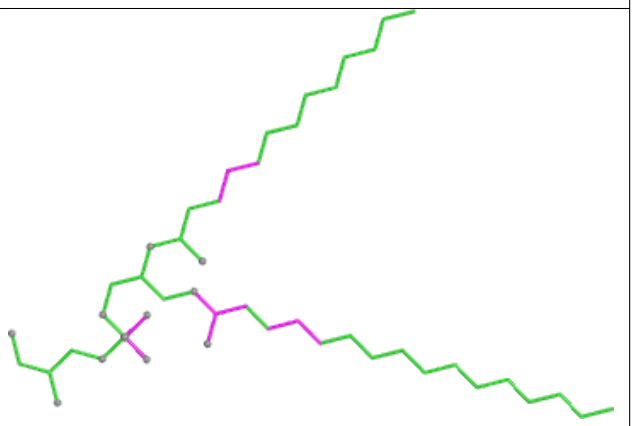


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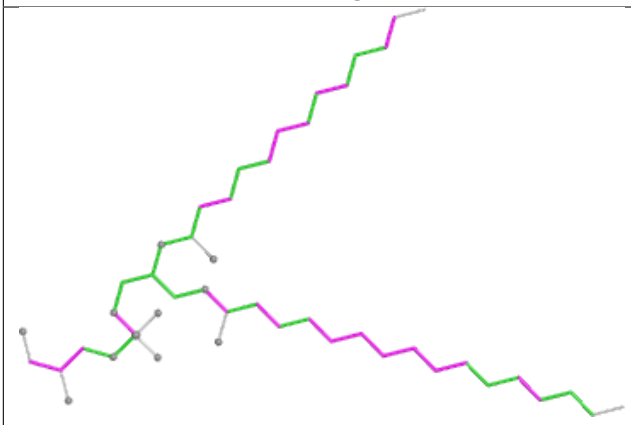
Ligand LHG D 408



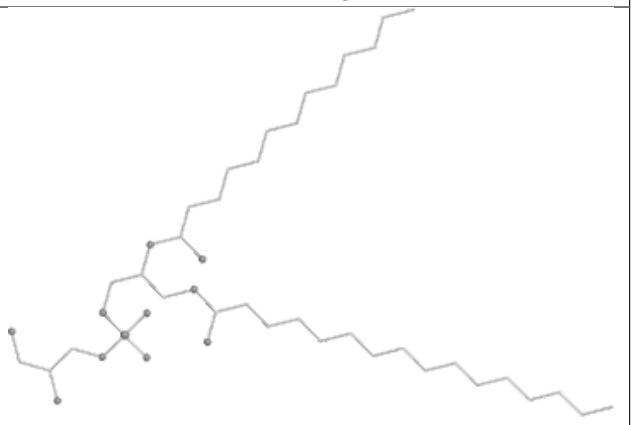
Bond lengths



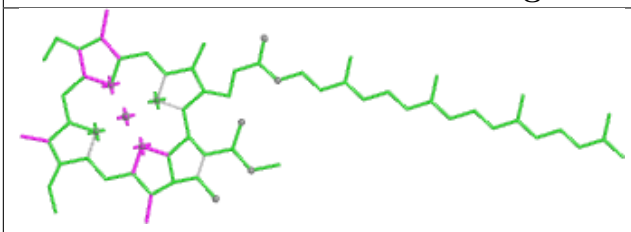
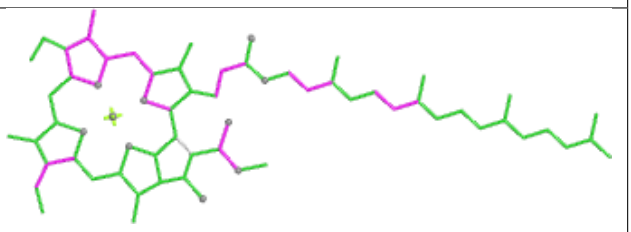
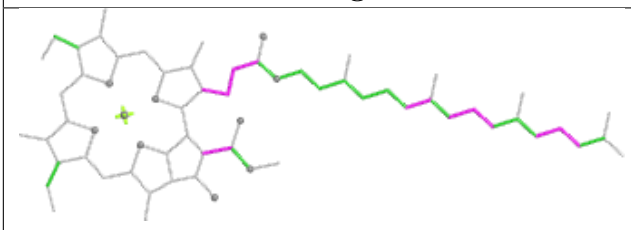
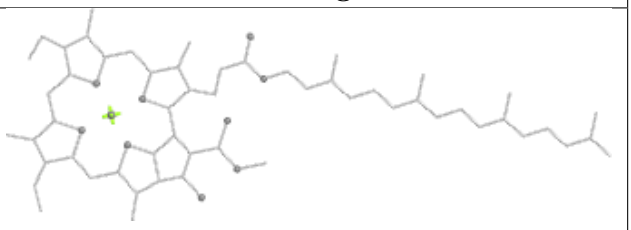
Bond angles

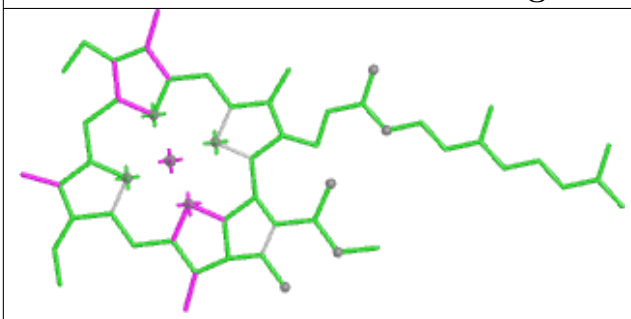
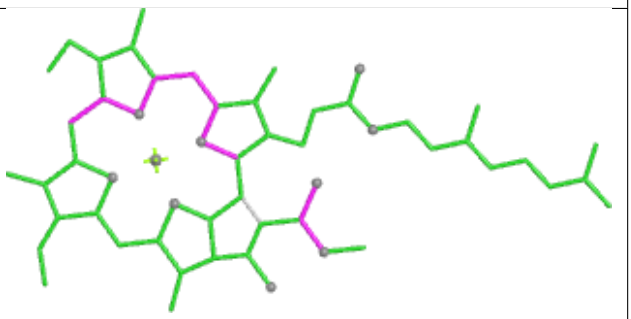
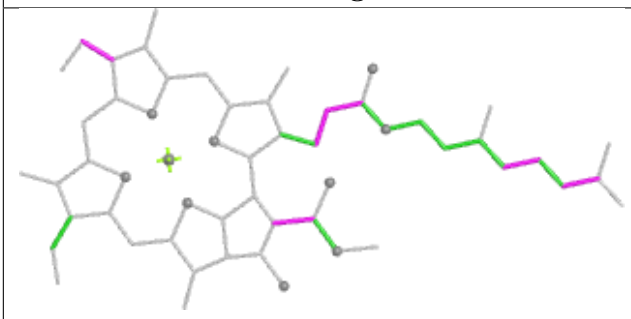
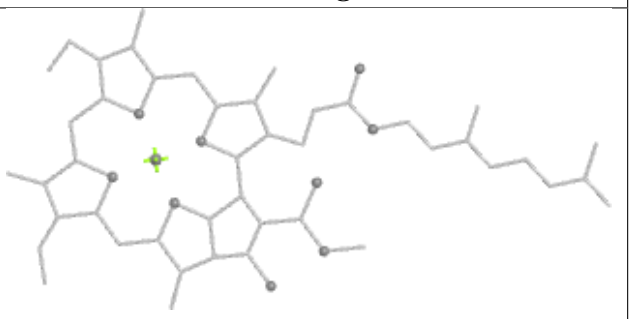


Torsions

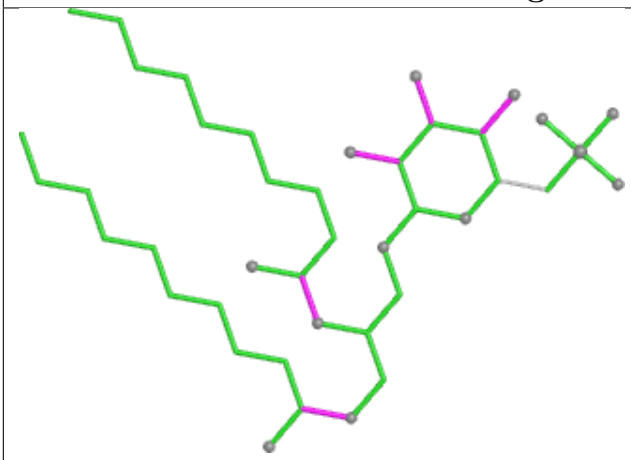


Rings

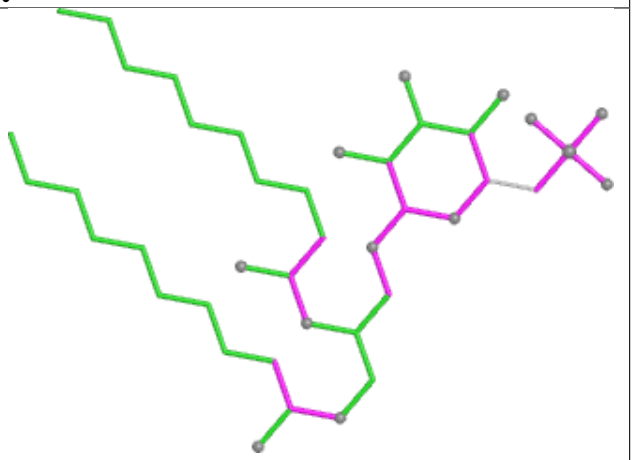
Ligand CLA Y 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 5 613	
 Bond lengths	 Bond angles
 Torsions	 Rings

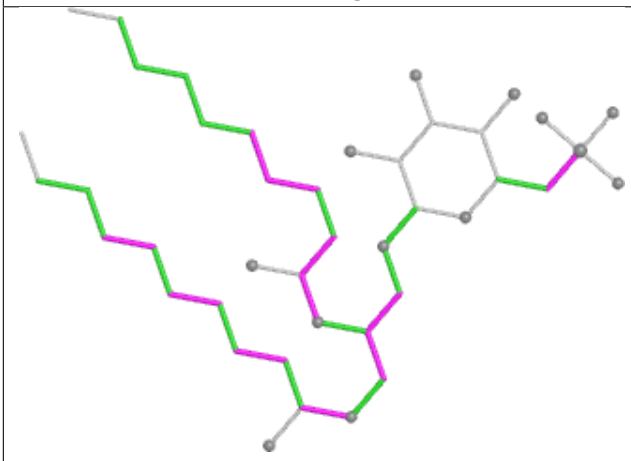
Ligand SQD b 623



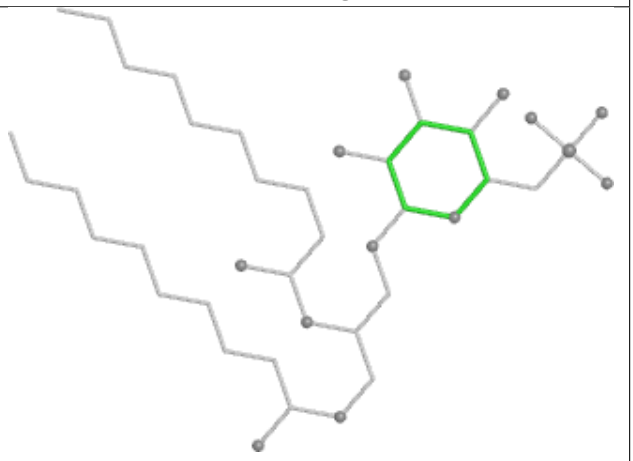
Bond lengths



Bond angles

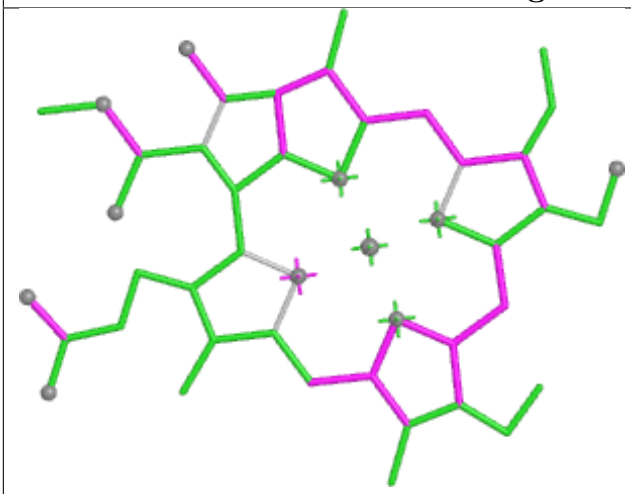


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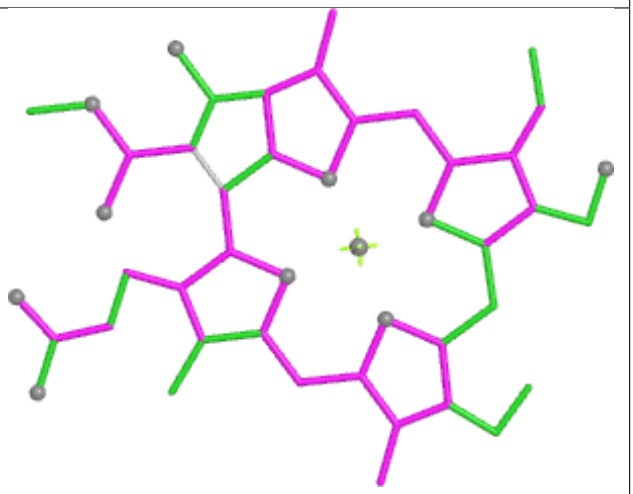


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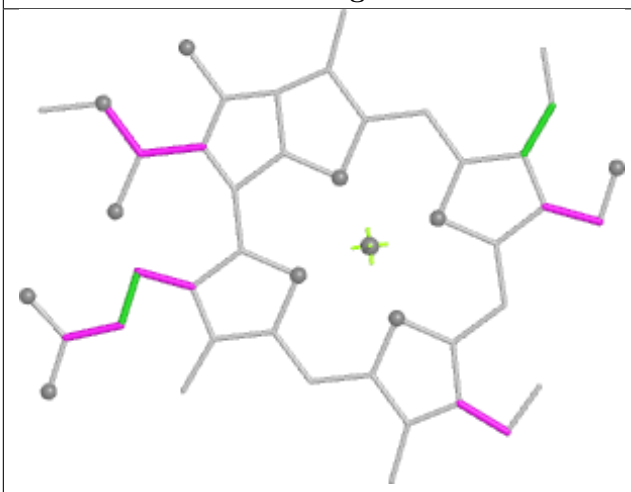
Ligand CHL 5 605



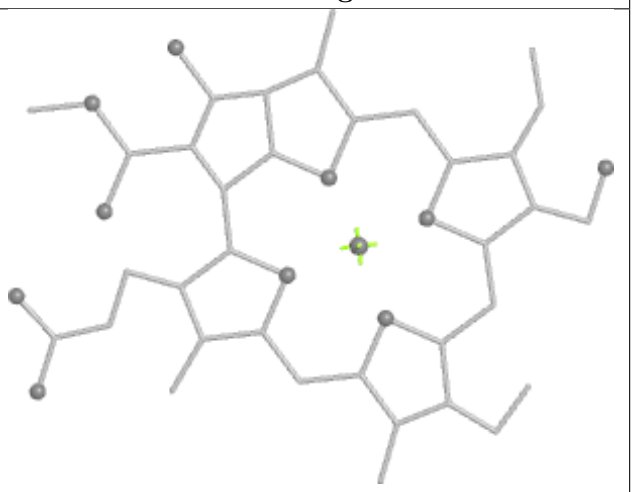
Bond lengths



Bond angles

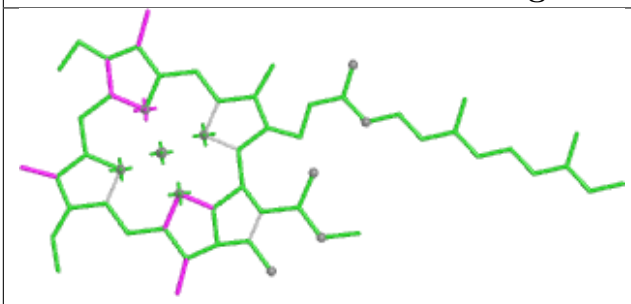


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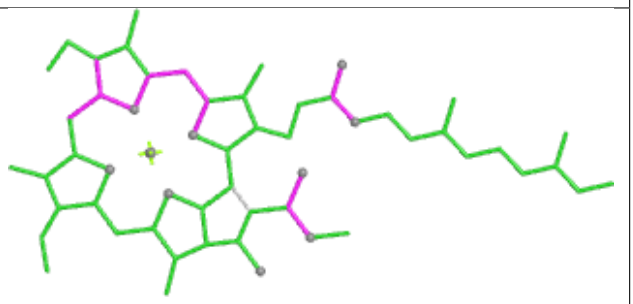


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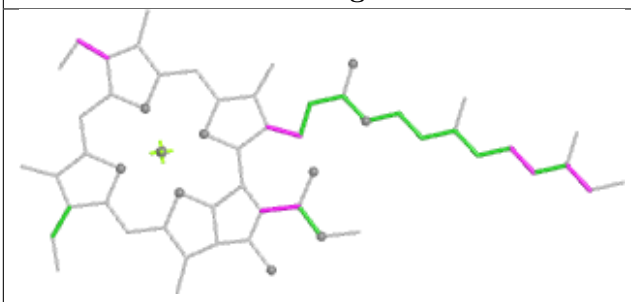
Ligand CLA 1 610



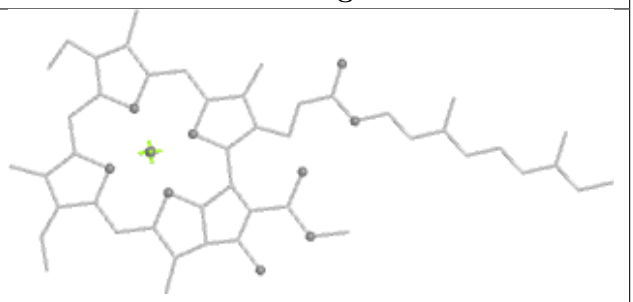
Bond lengths



Bond angles

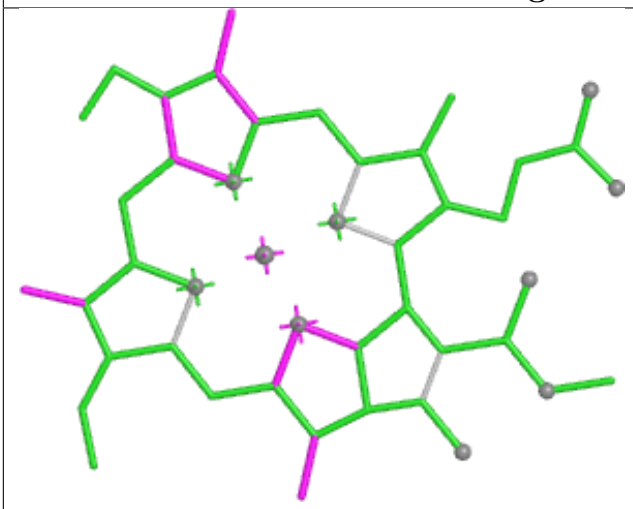


Torsions

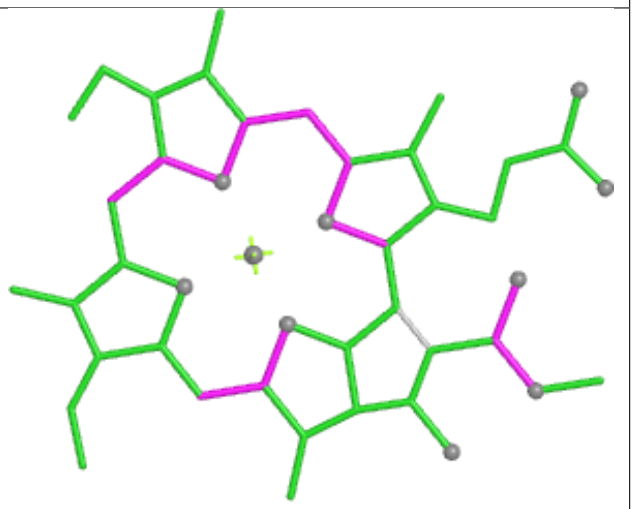


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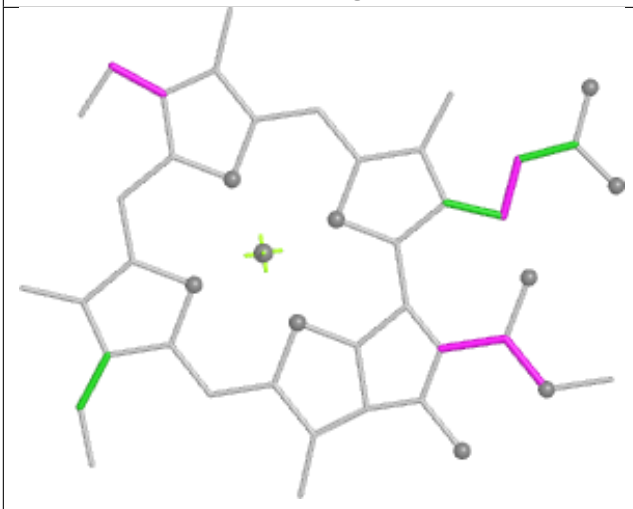
Ligand CLA 2 613



Bond lengths



Bond angles

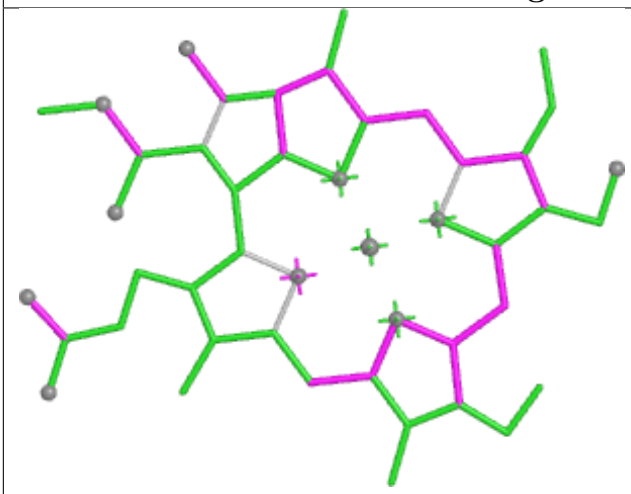


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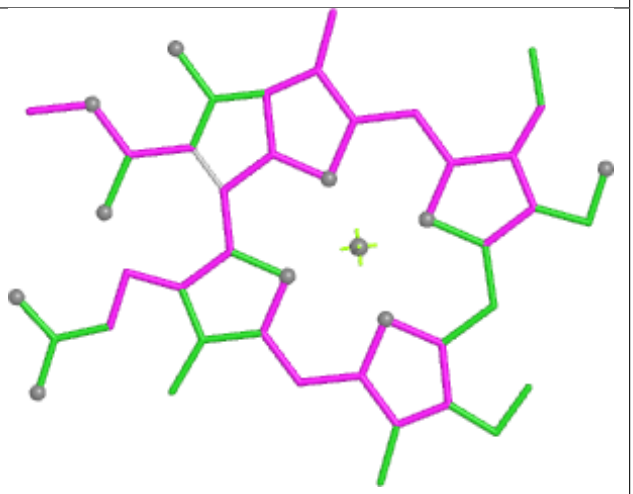


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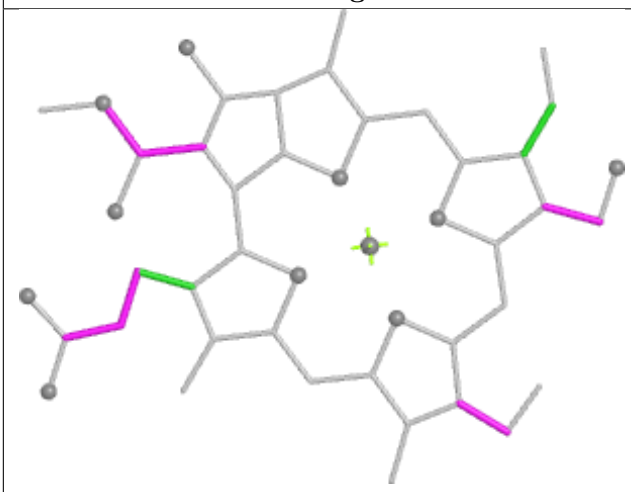
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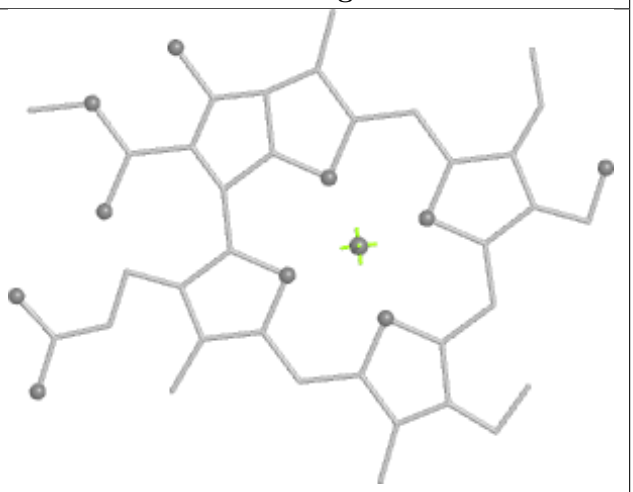
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Bond angles

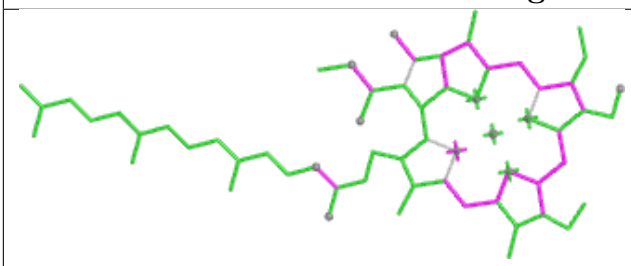


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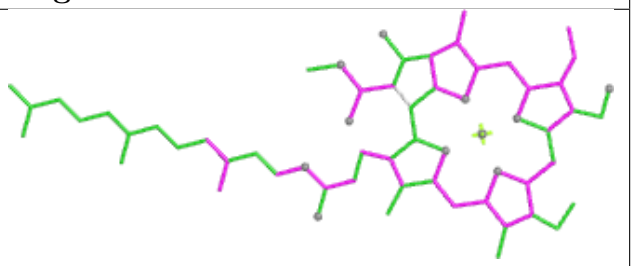


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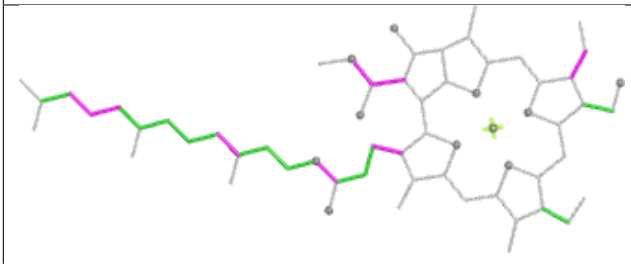
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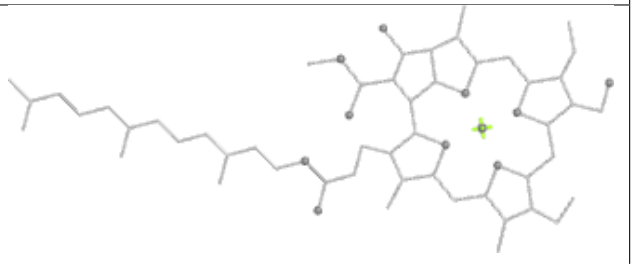
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Bond angles

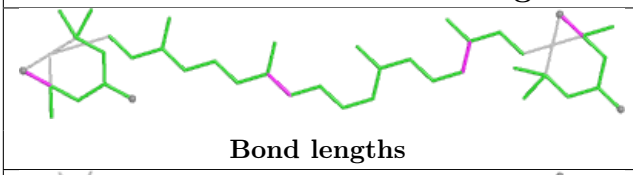


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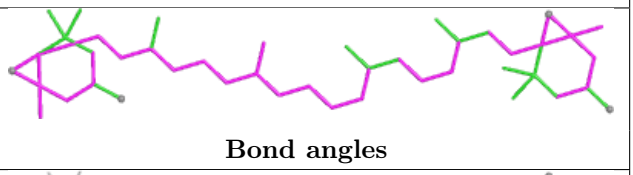


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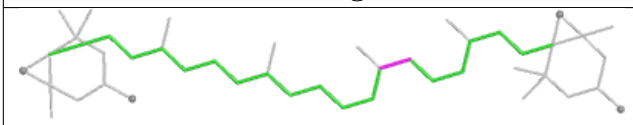
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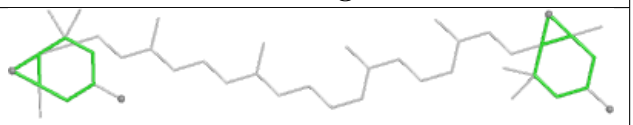
Bond lengths



Bond angles

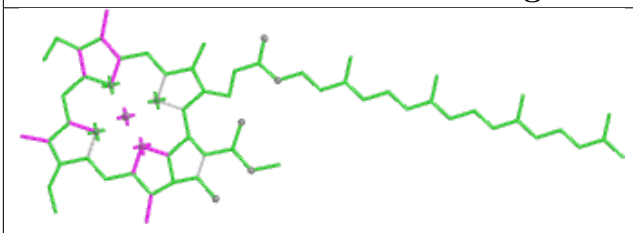


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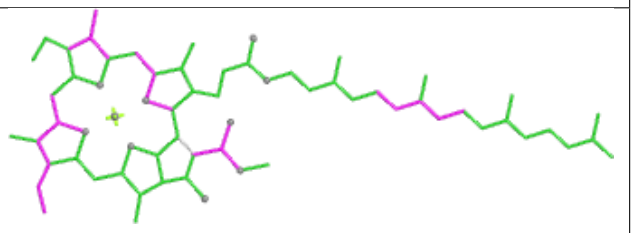


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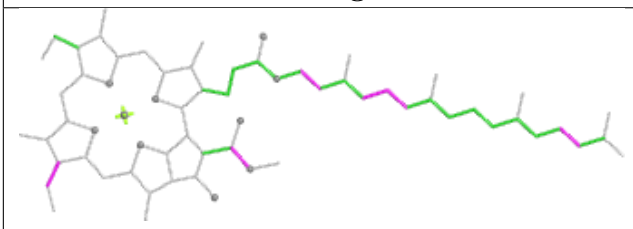
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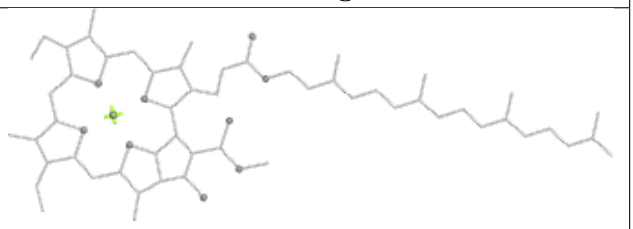
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Bond angles

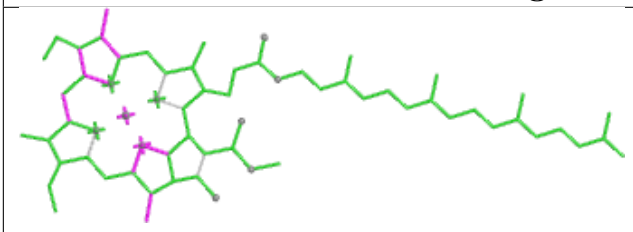


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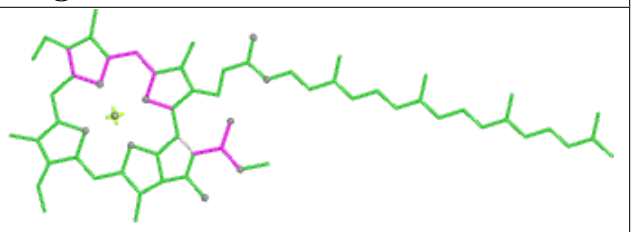


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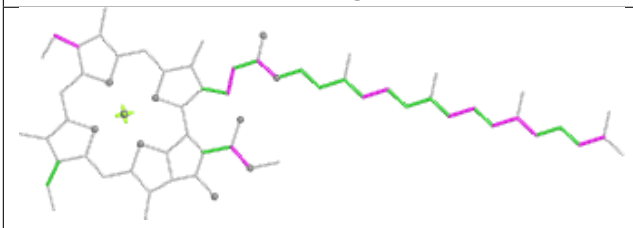
Ligand CLA g 613



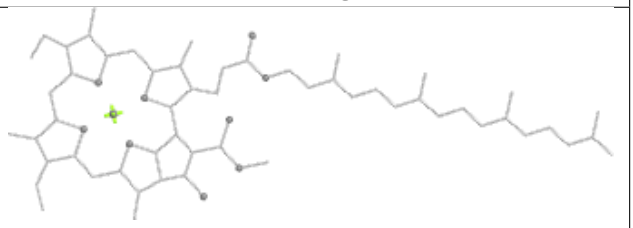
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Bond angles

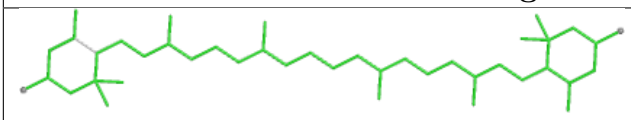


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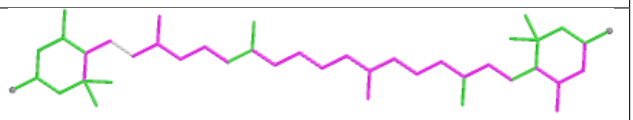


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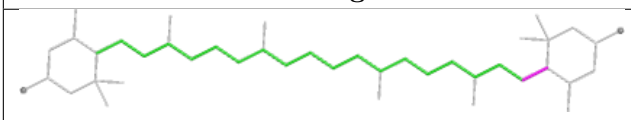
Ligand LUT 3 1620



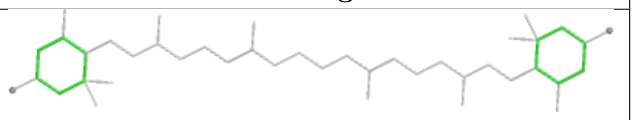
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Bond angles

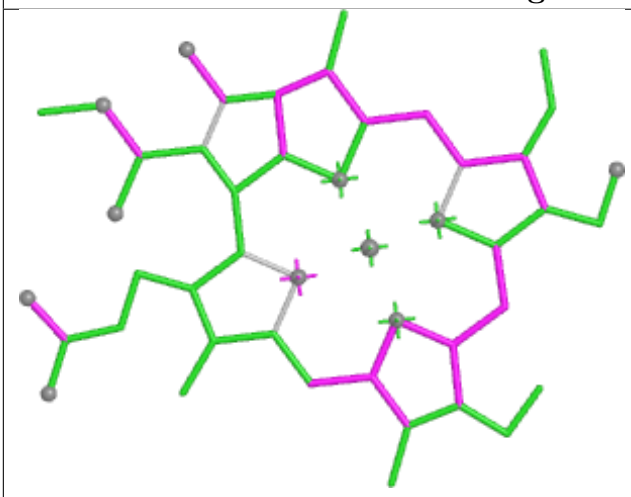


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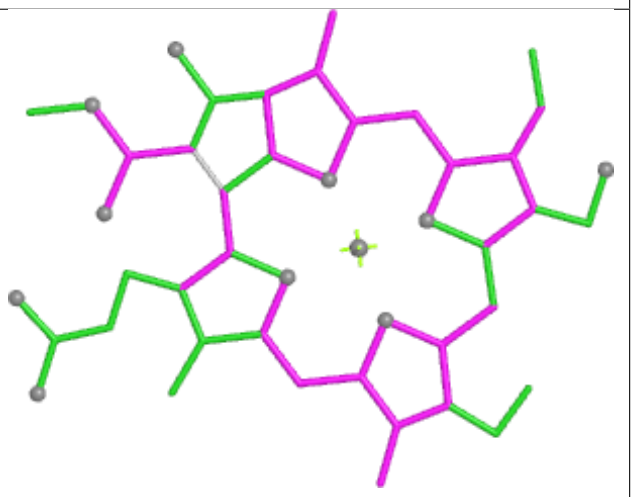


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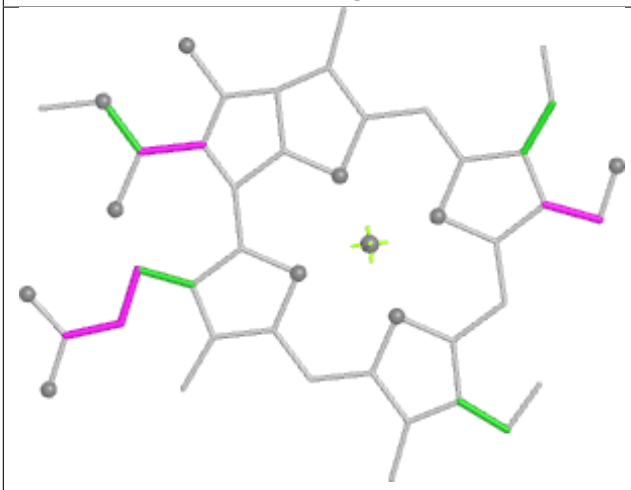
Ligand CHL 2 606



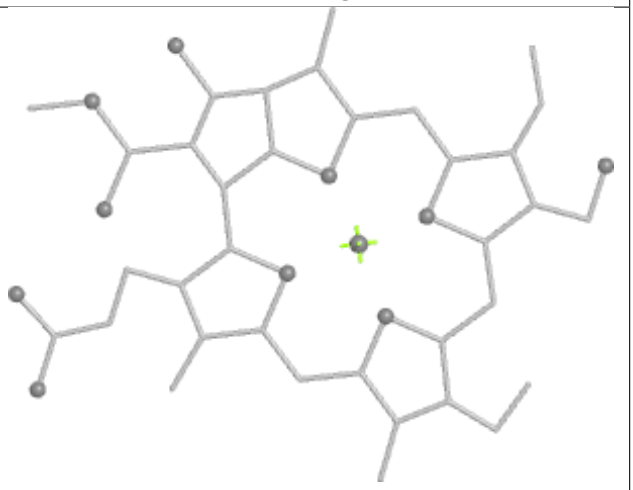
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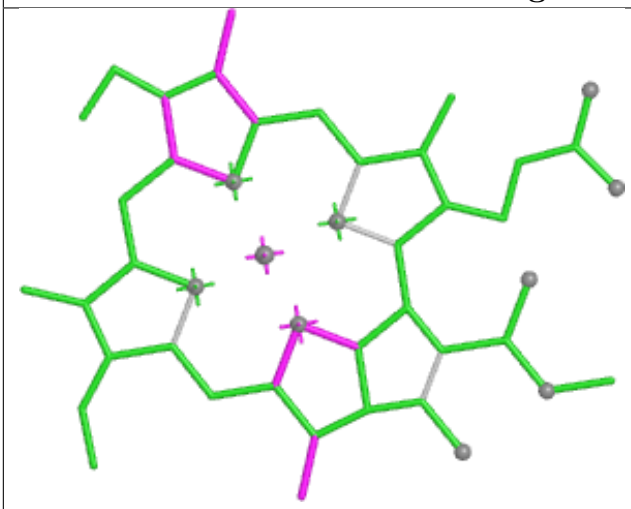


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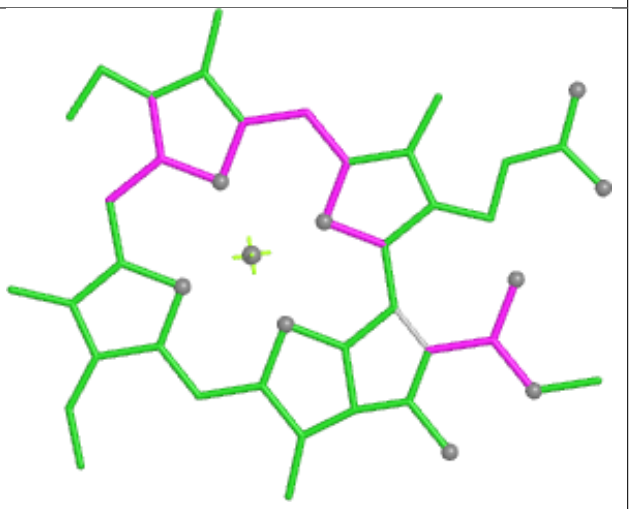


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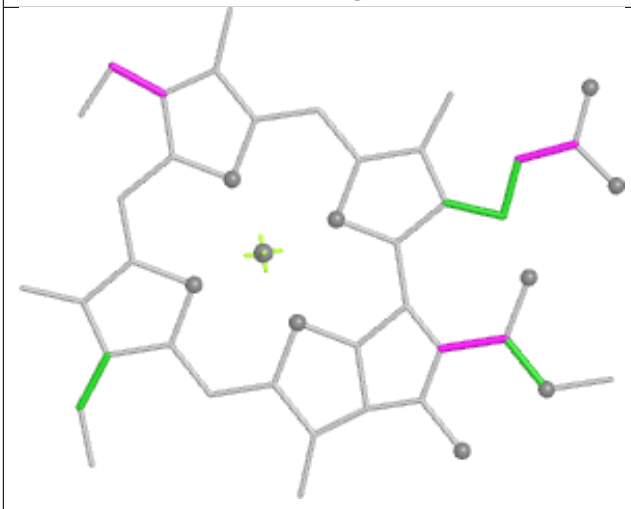
Ligand CLA 6 611



Bond lengths



Bond angles

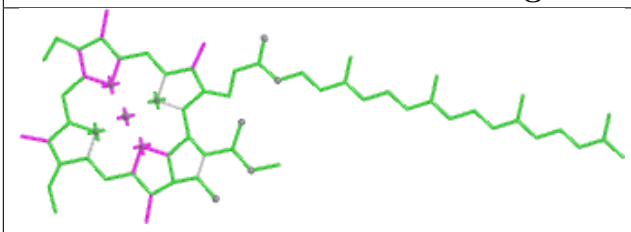


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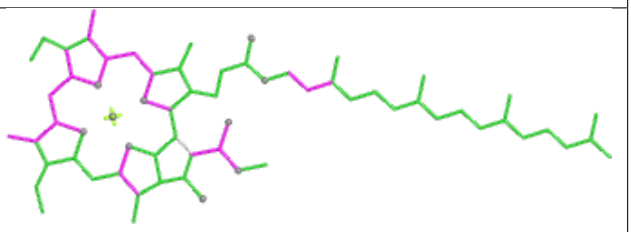


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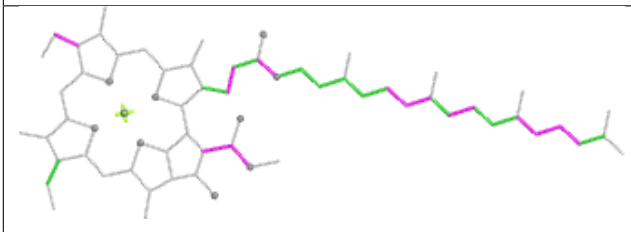
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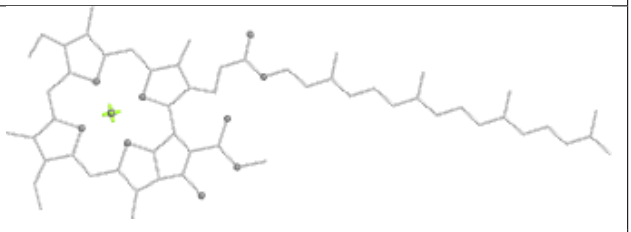
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Bond angles

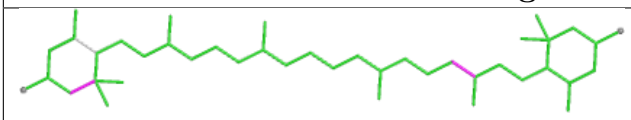


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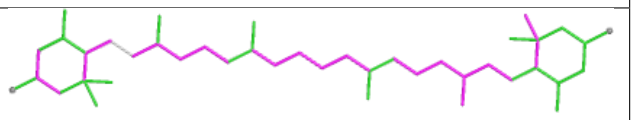


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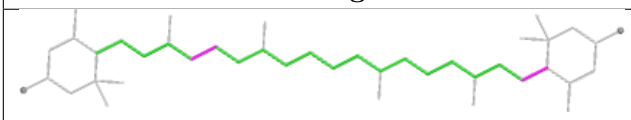
Ligand LUT n 1621



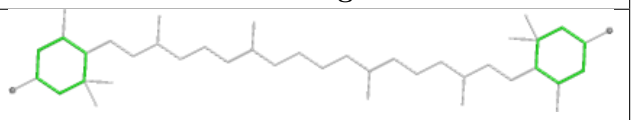
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Bond angles

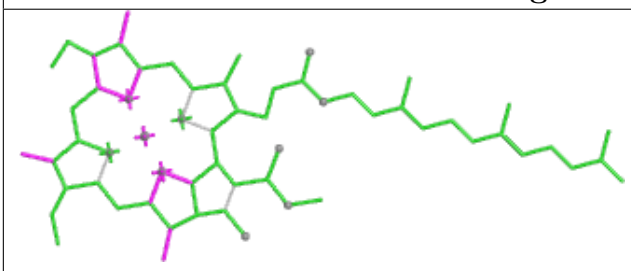


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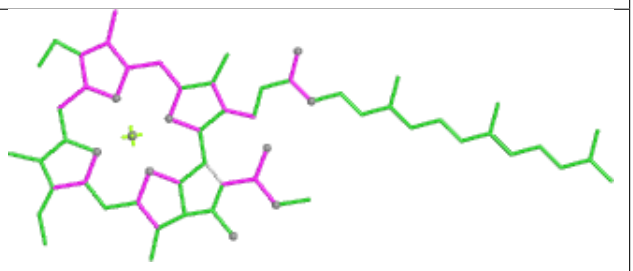


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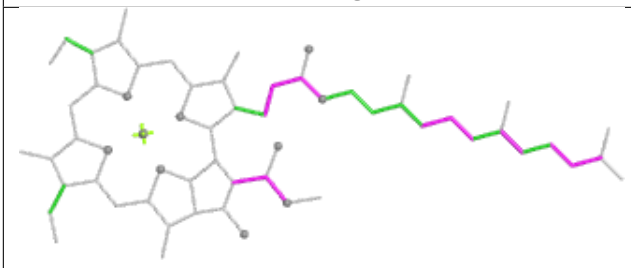
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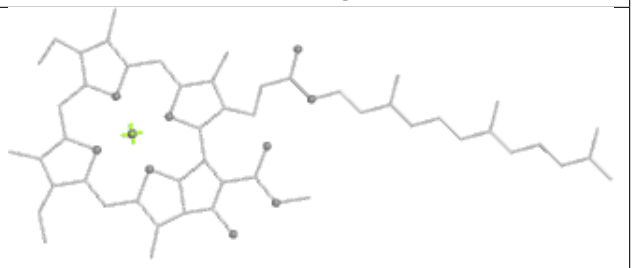
Bond lengths



Bond angles



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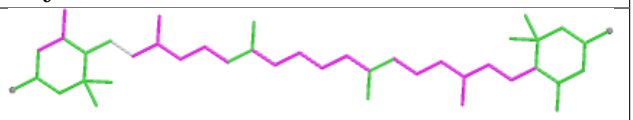


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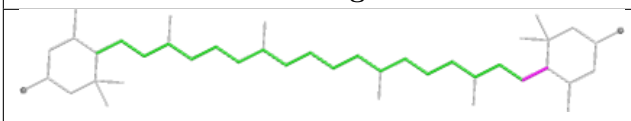
Ligand LUT y 1620



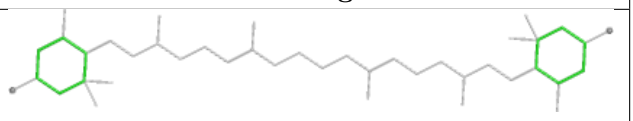
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Bond angles

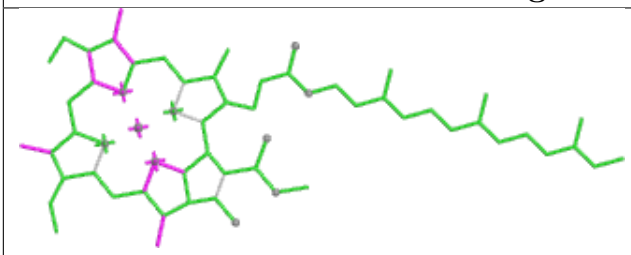


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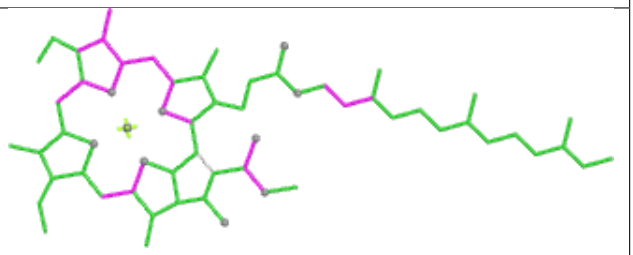


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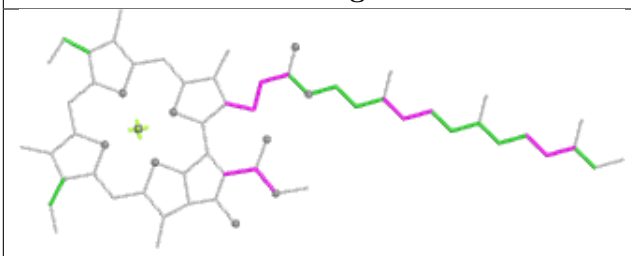
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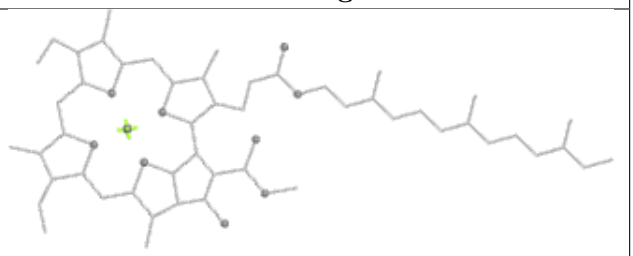
Bond lengths



Bond angles

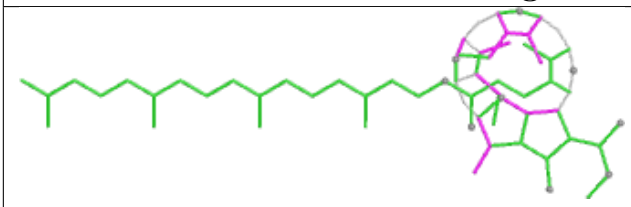


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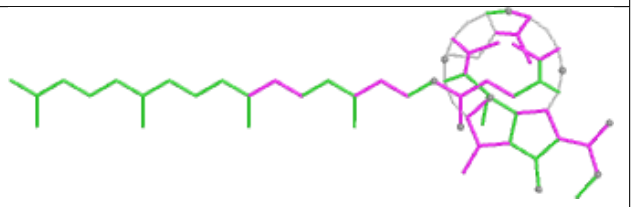


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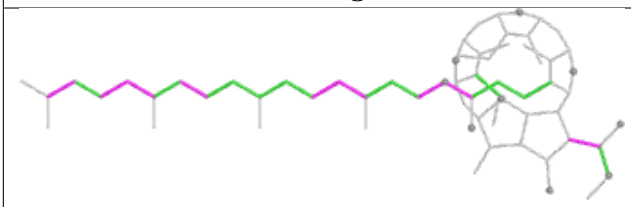
Ligand PHO A 408



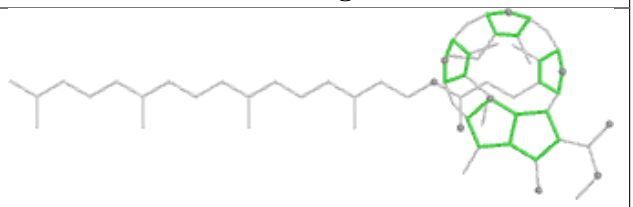
Bond lengths



Bond angles

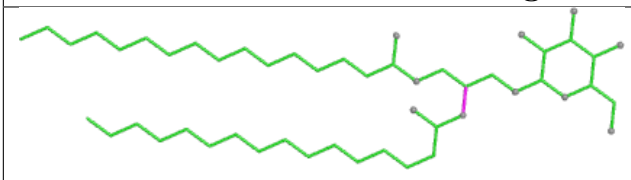


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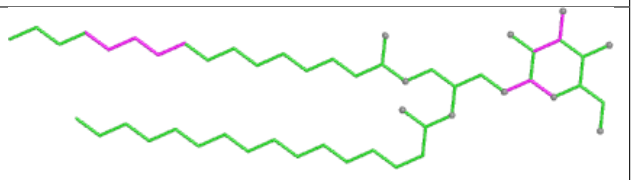


Rings

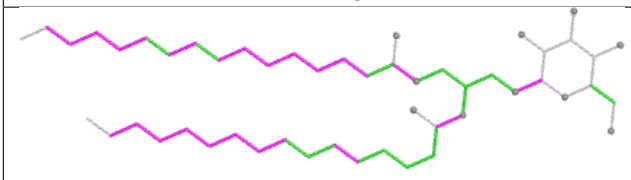
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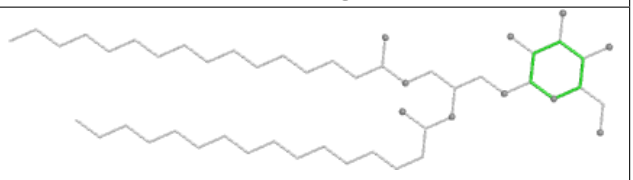
Bond lengths



Bond angles

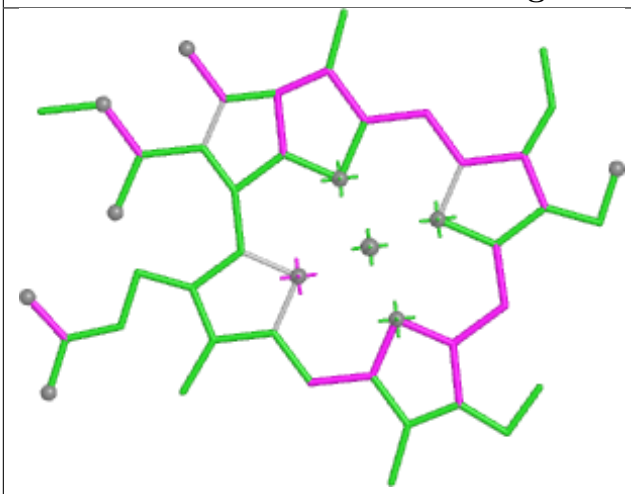


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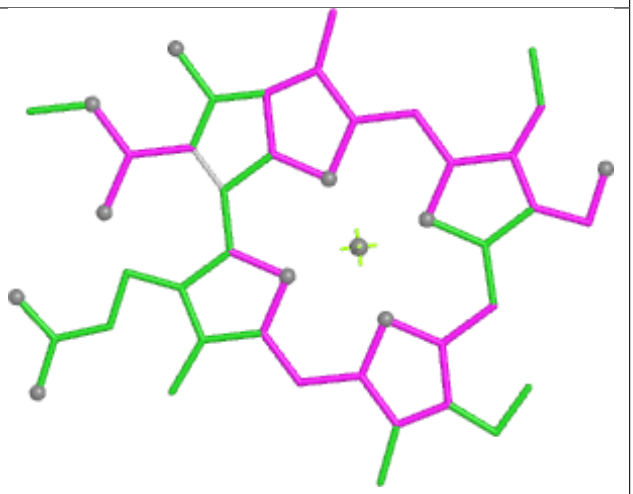


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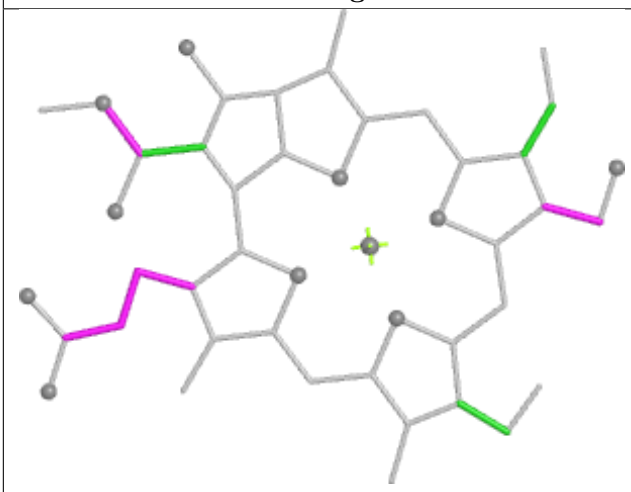
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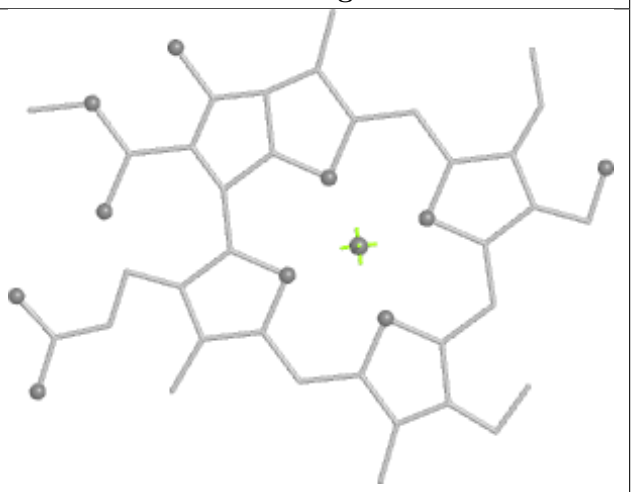
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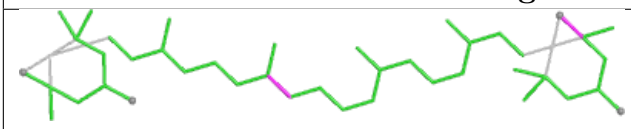


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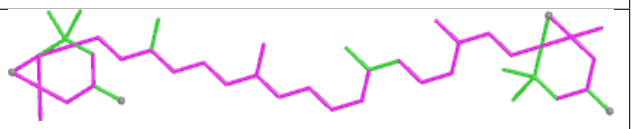


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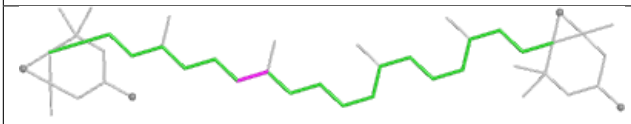
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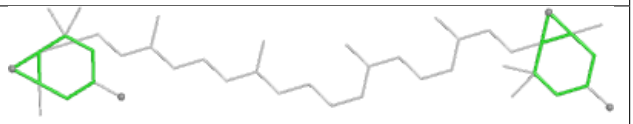
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Bond angles

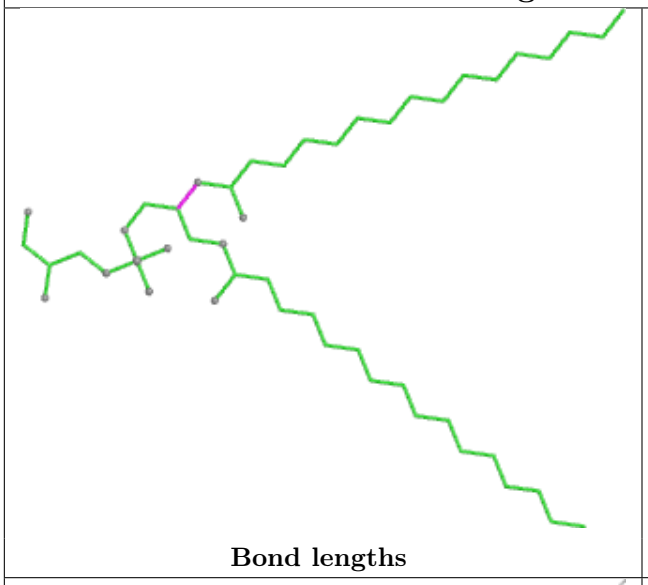


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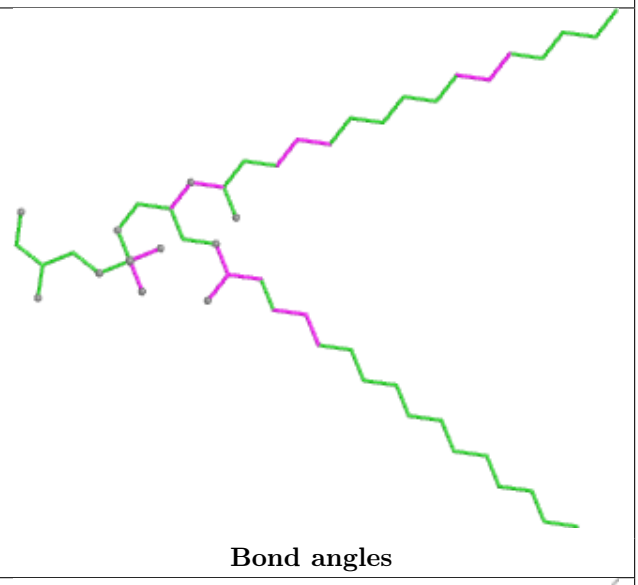


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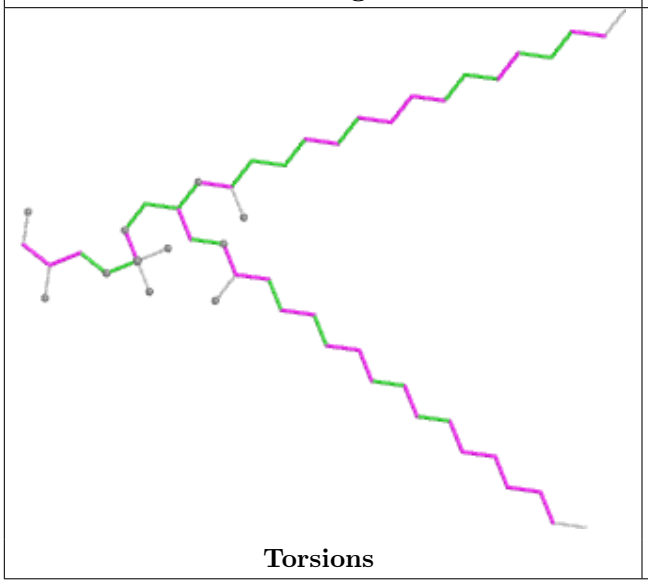
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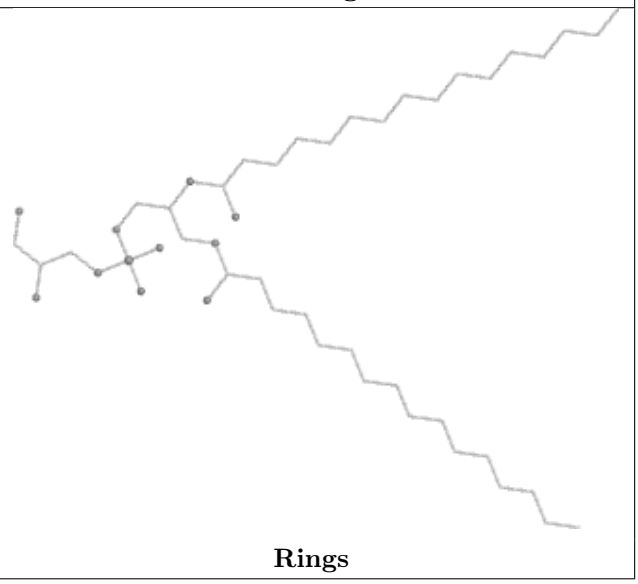
Bond lengths



Bond angles

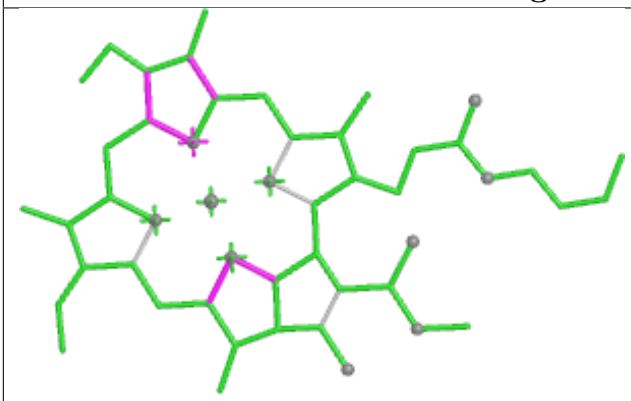


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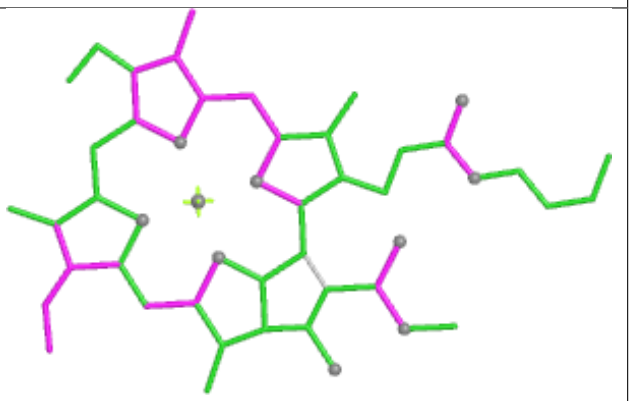


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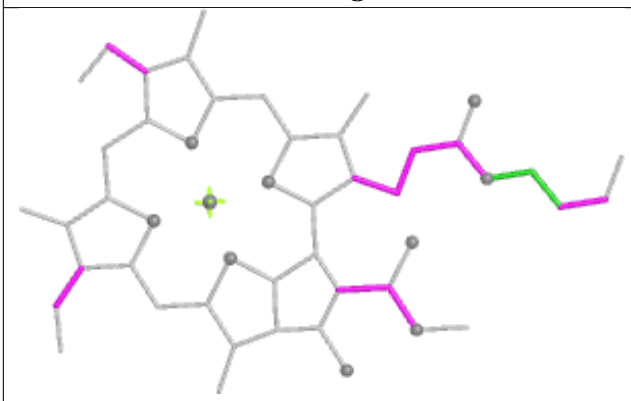
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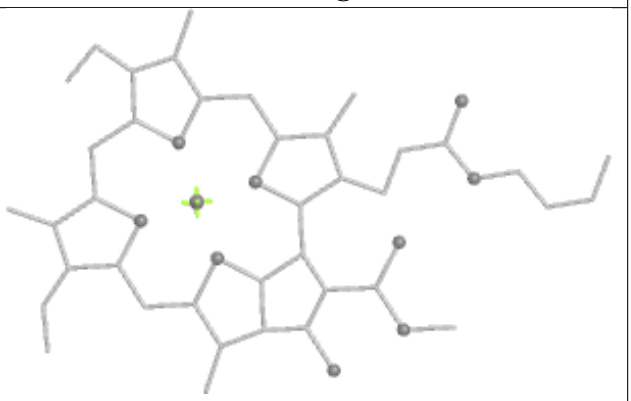
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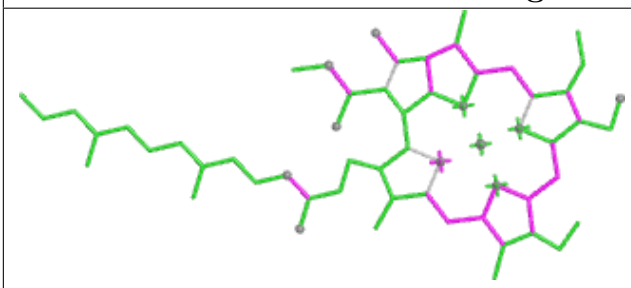


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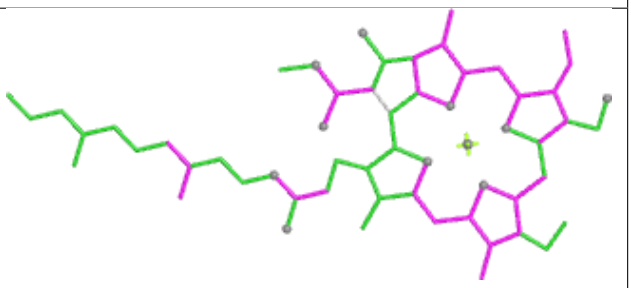


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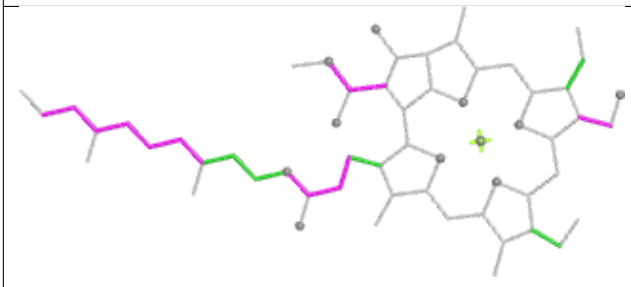
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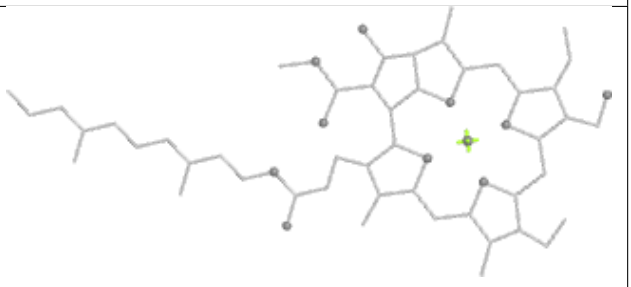
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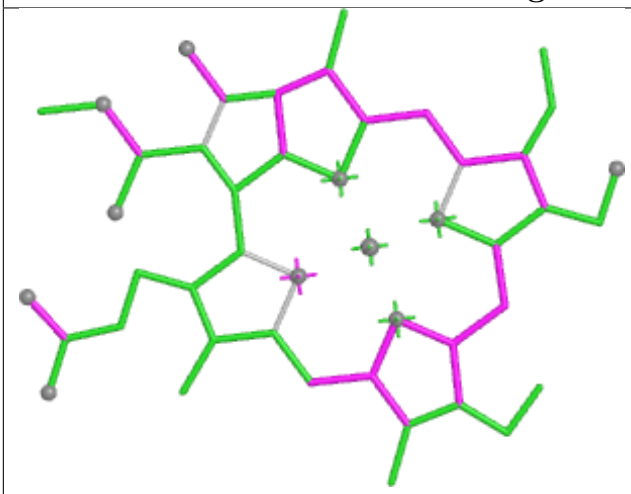


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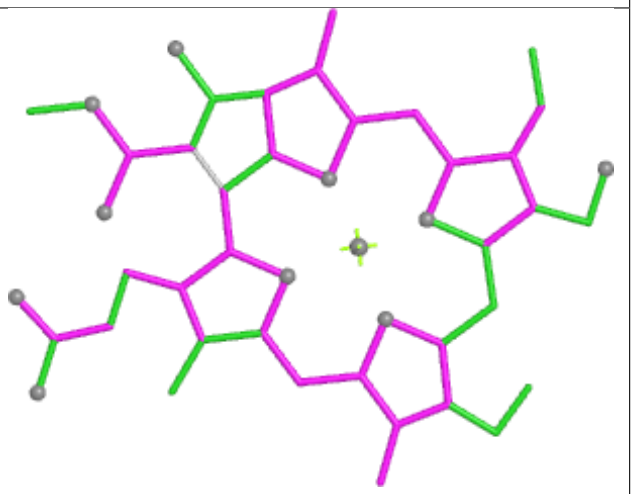


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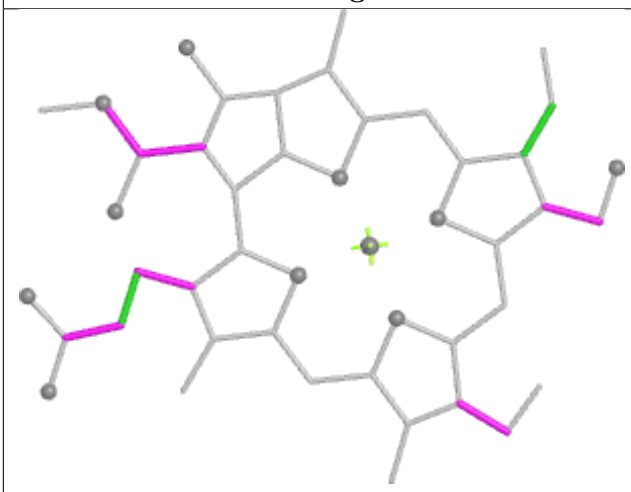
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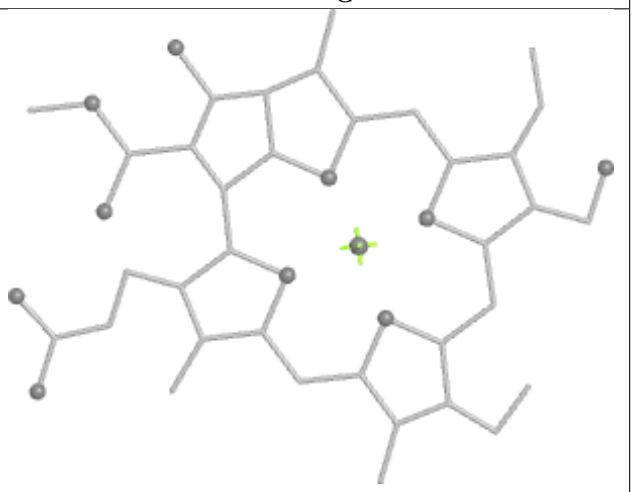
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Bond angles

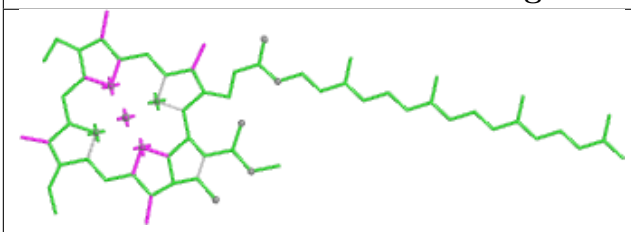


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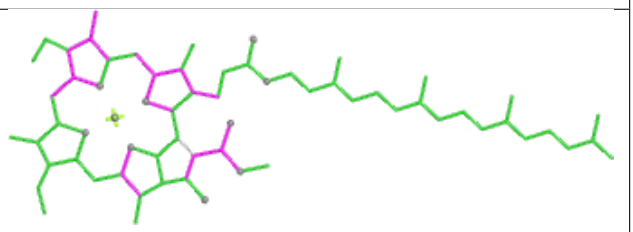


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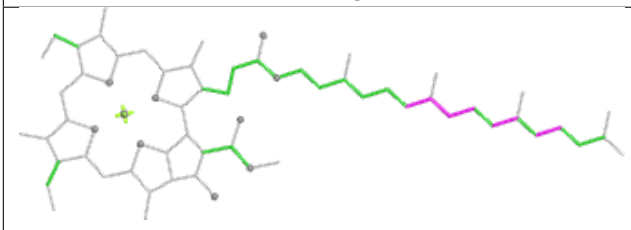
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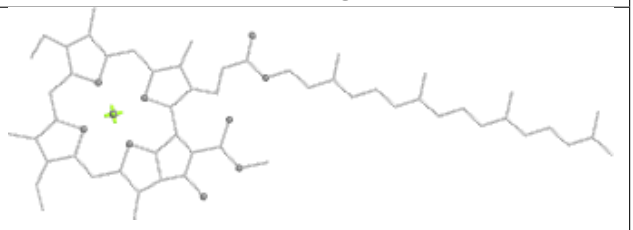
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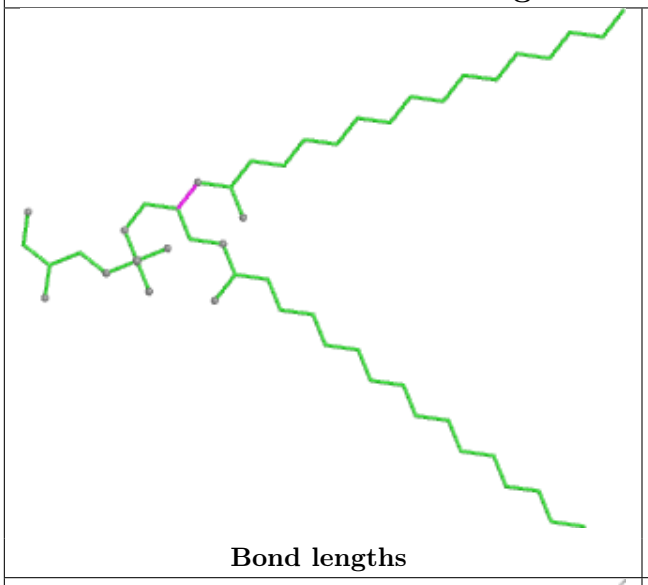


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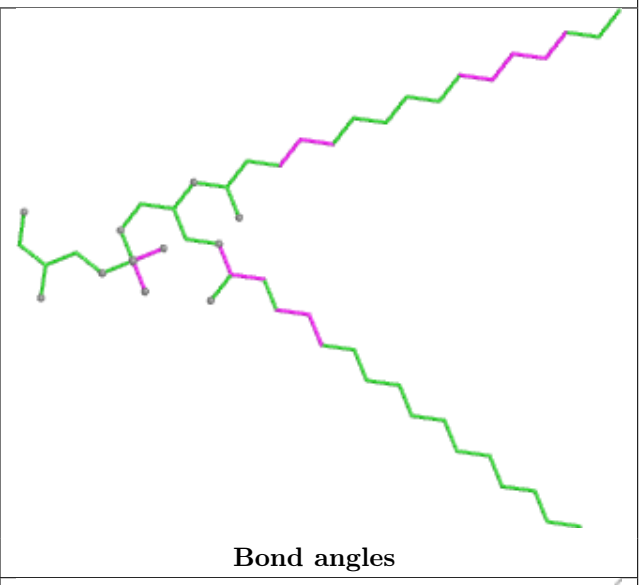


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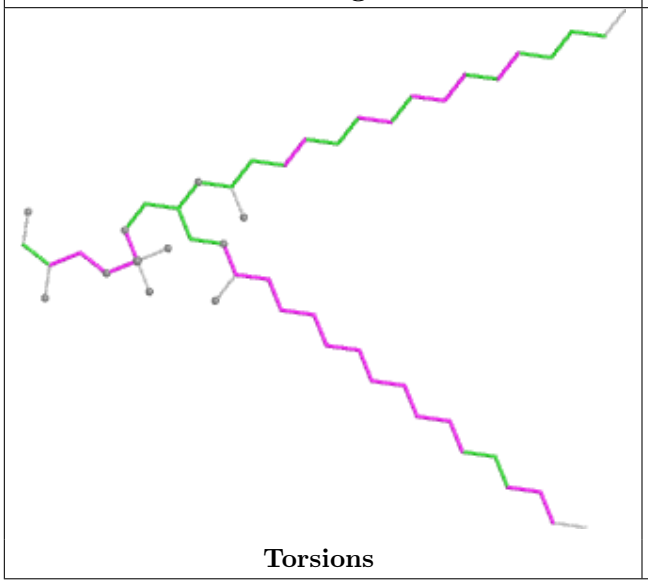
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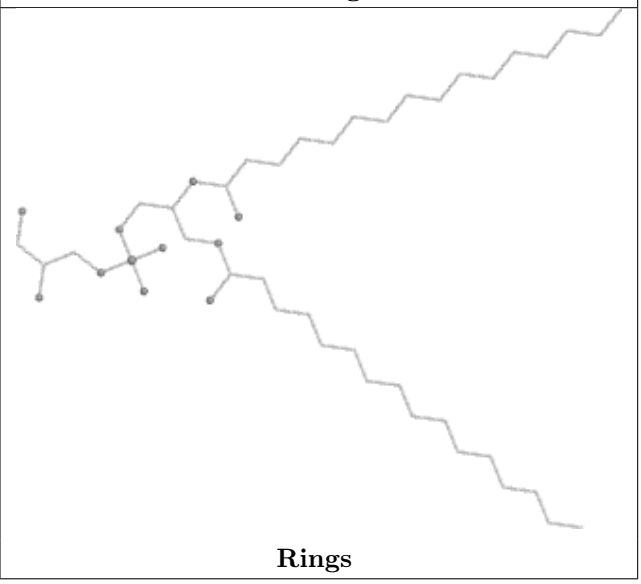
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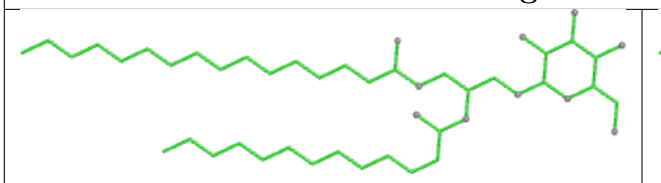


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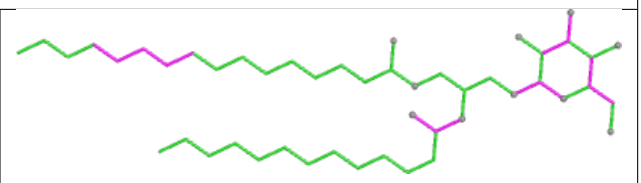


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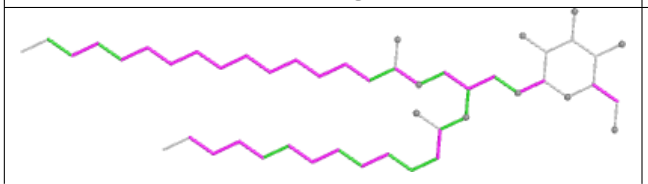
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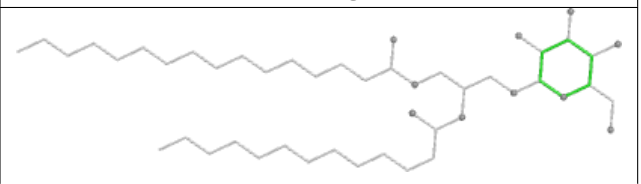
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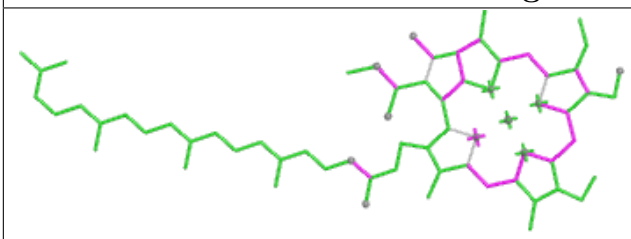


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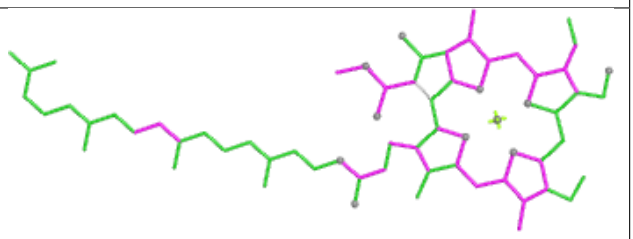


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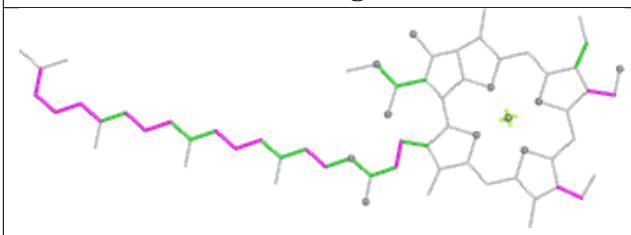
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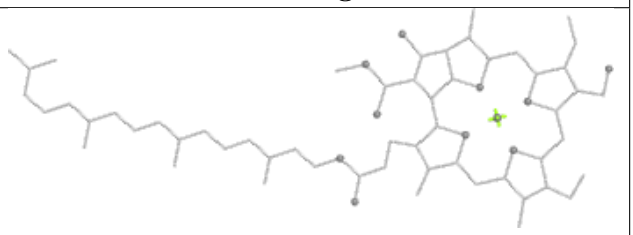
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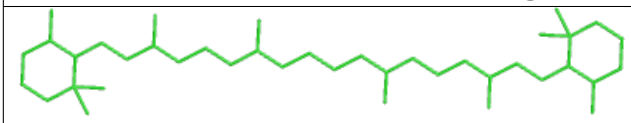


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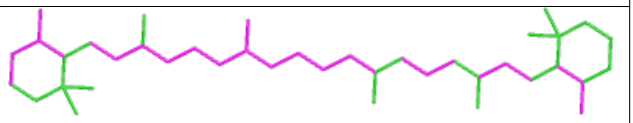


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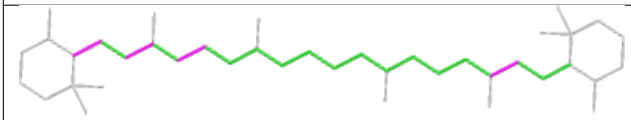
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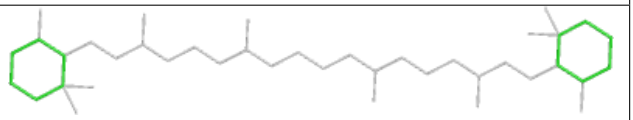
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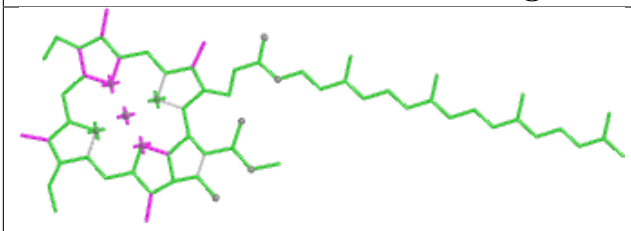


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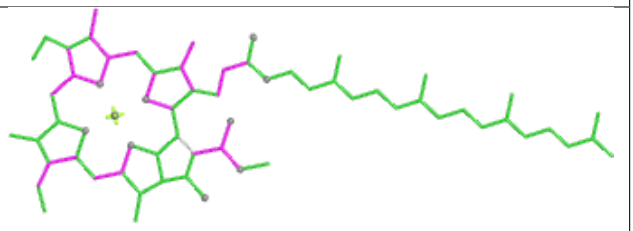


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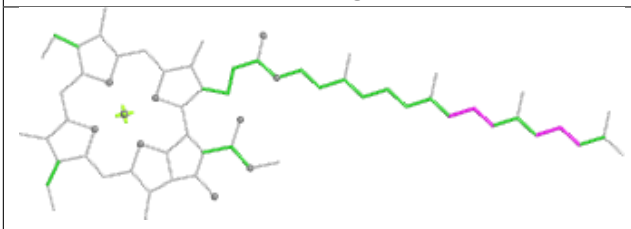
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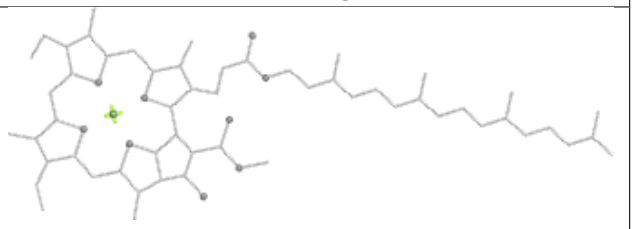
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Bond angles

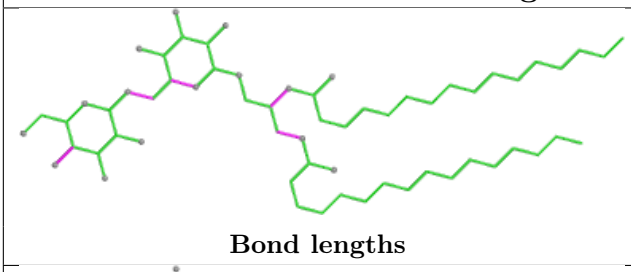


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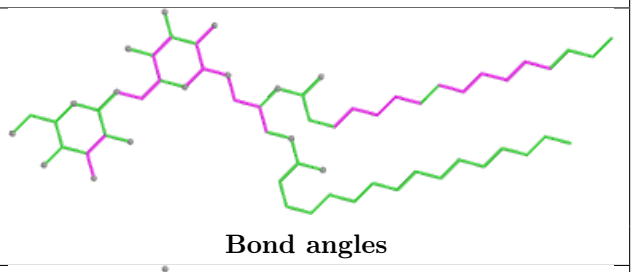


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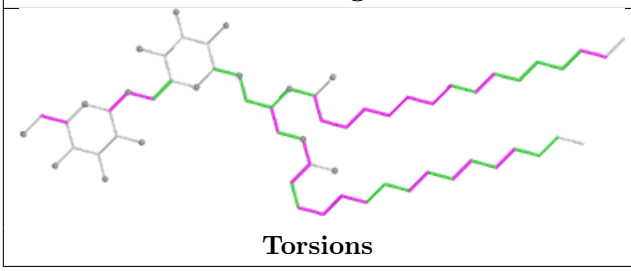
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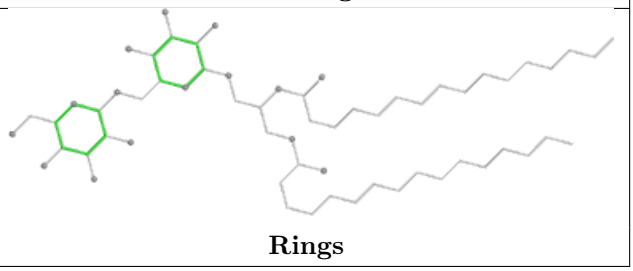
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Bond angles

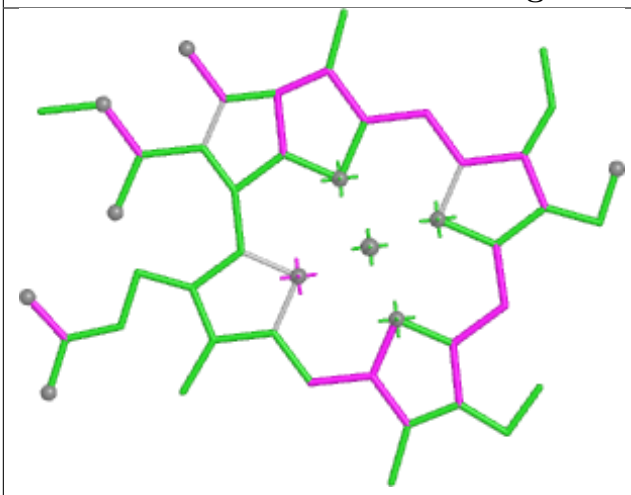


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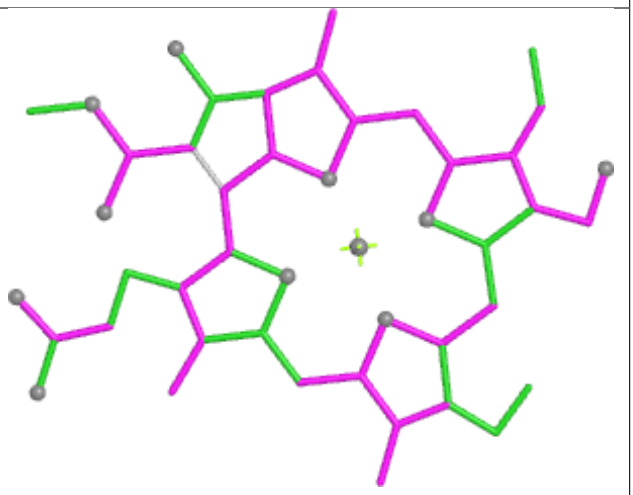


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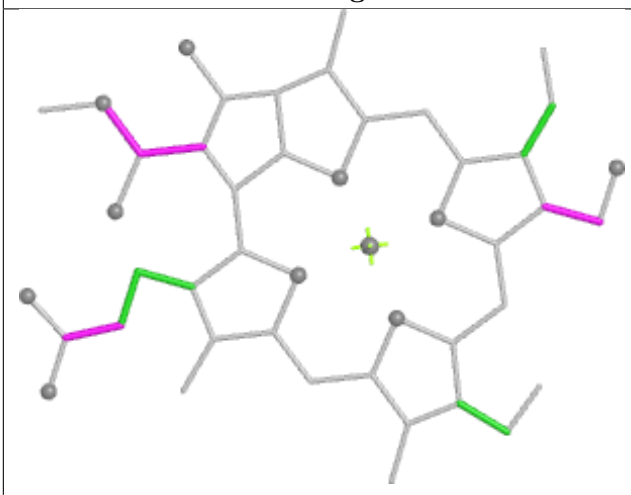
Ligand CHL S 606



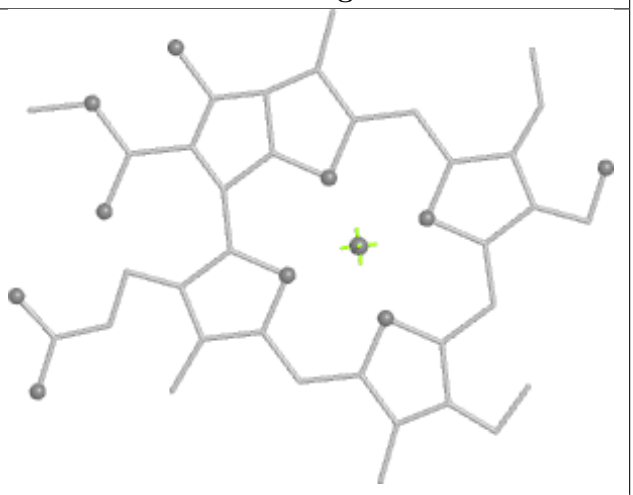
Bond lengths



Bond angles

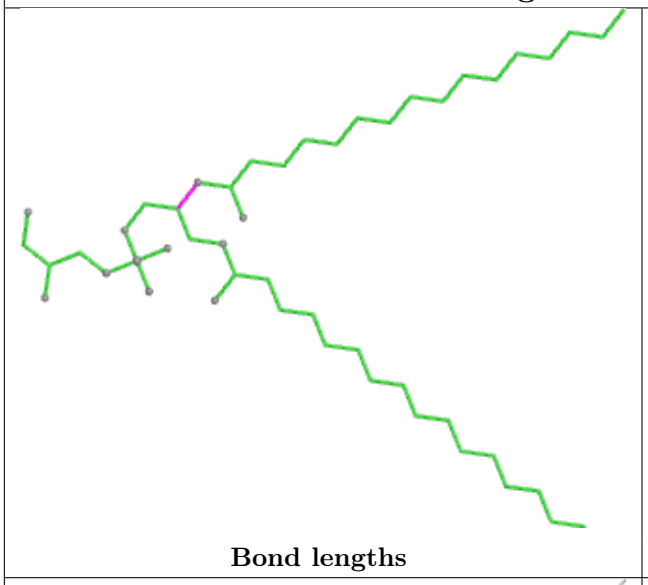


Torsions

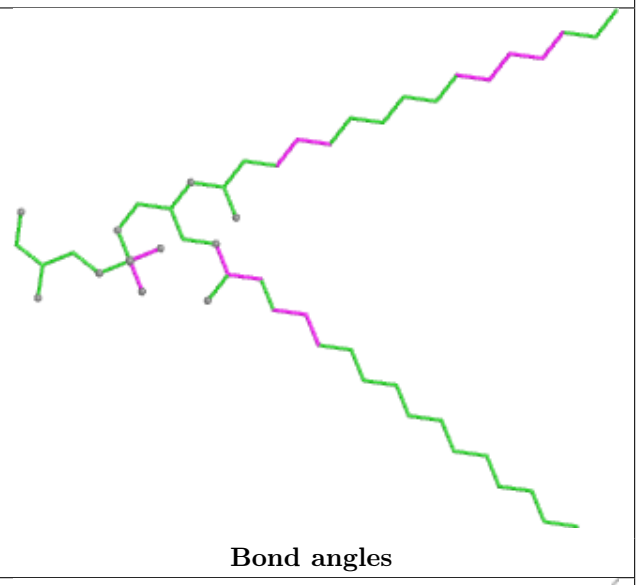


Rings

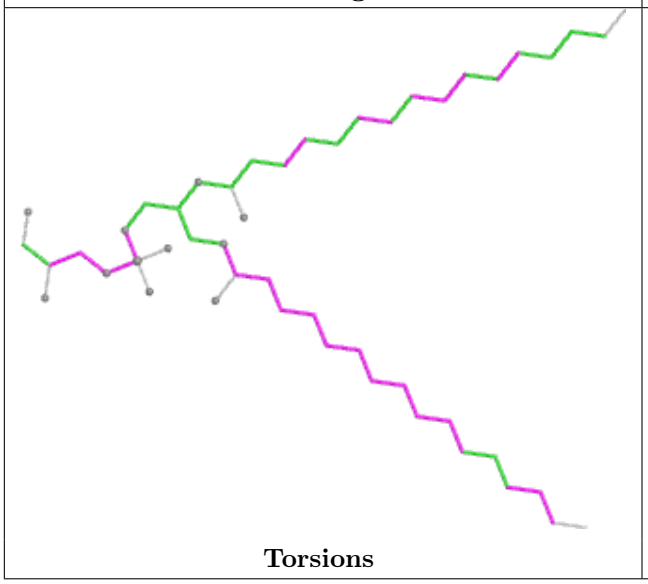
Ligand LHG n 2630



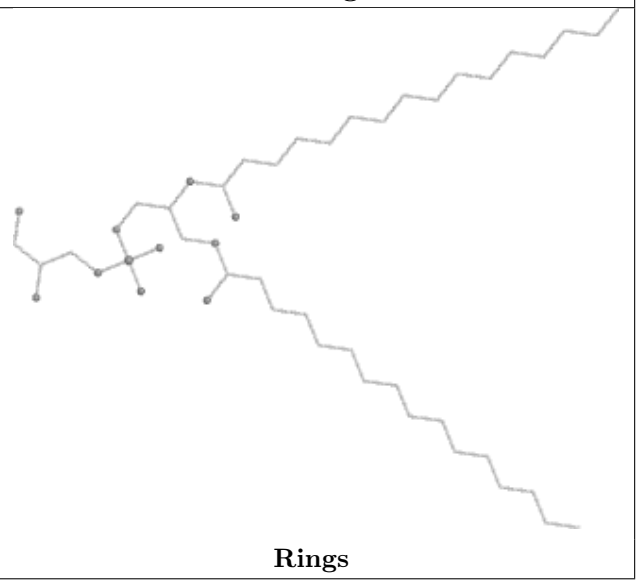
Bond lengths



Bond angles

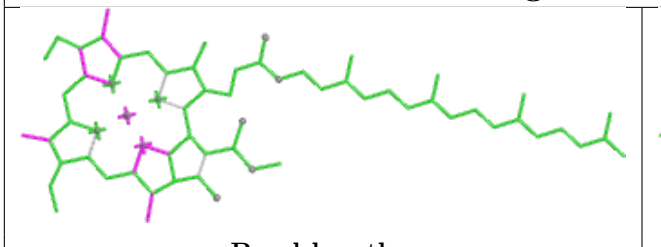


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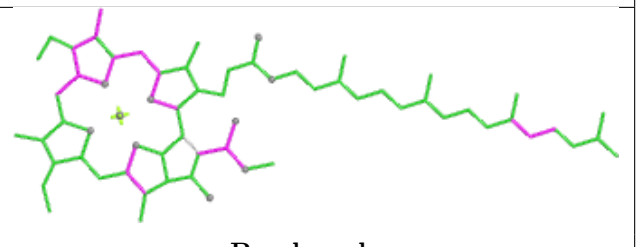


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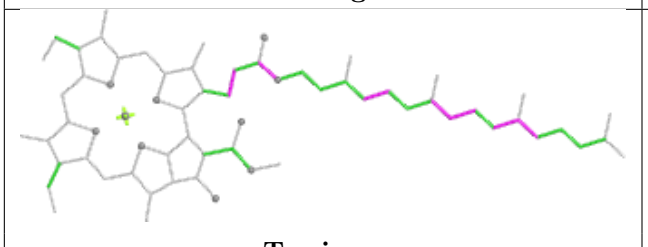
Ligand CLA Y 613



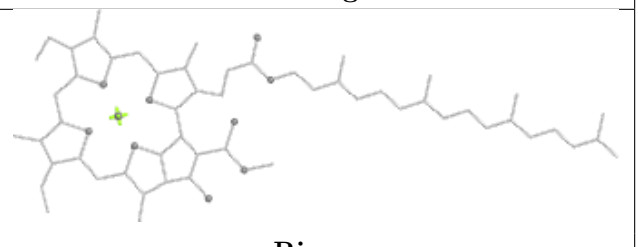
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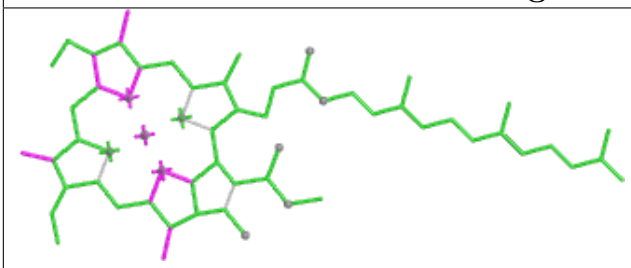
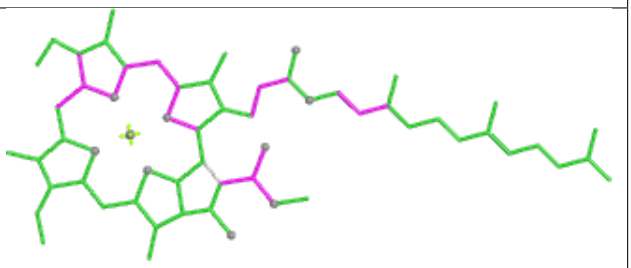
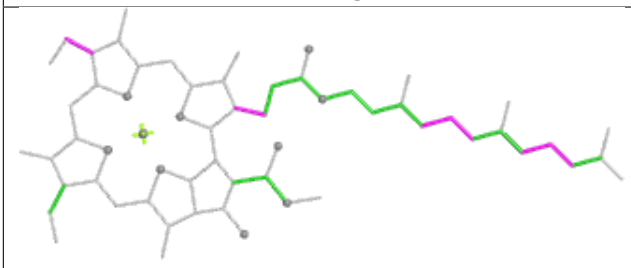
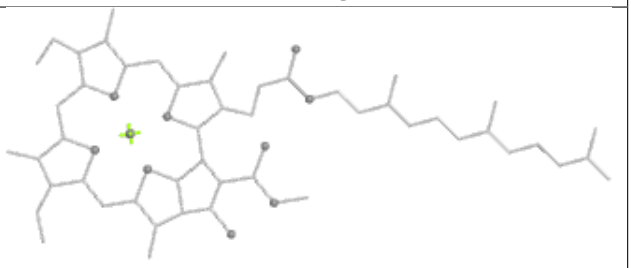
Bond angles

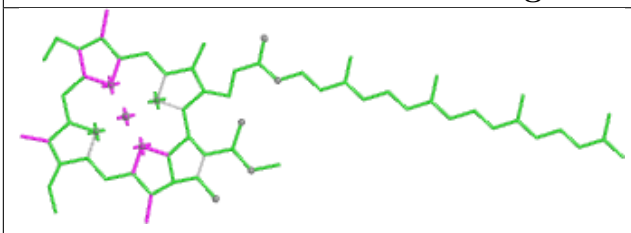
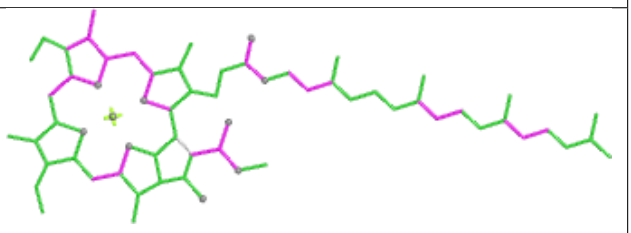
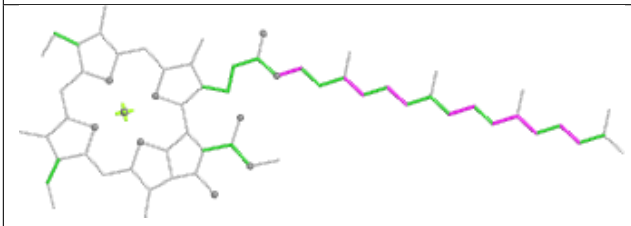
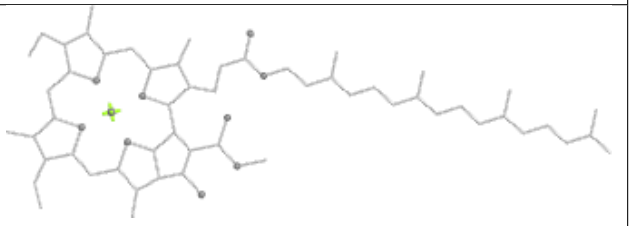


Torsions

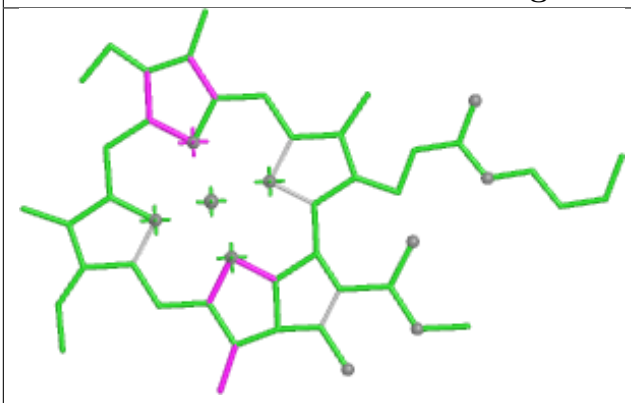


Rings

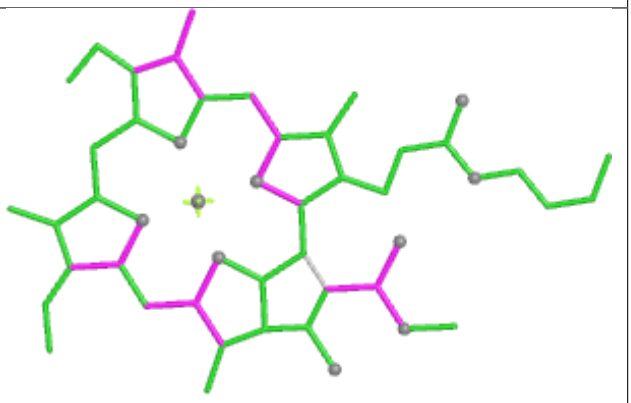
Ligand CLA a 410	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 609	
 Bond lengths	 Bond angles
 Torsions	 Rings

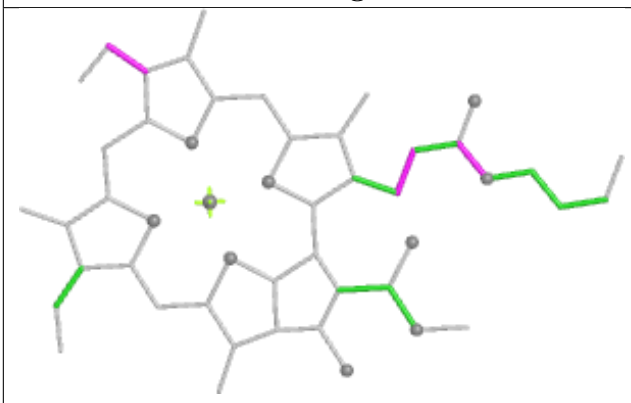
Ligand CLA s 614



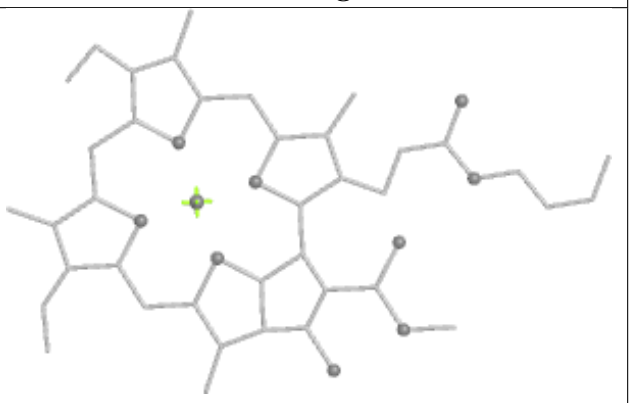
Bond lengths



Bond angles

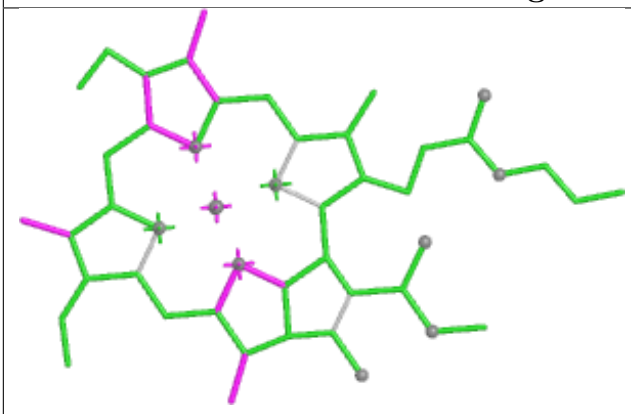


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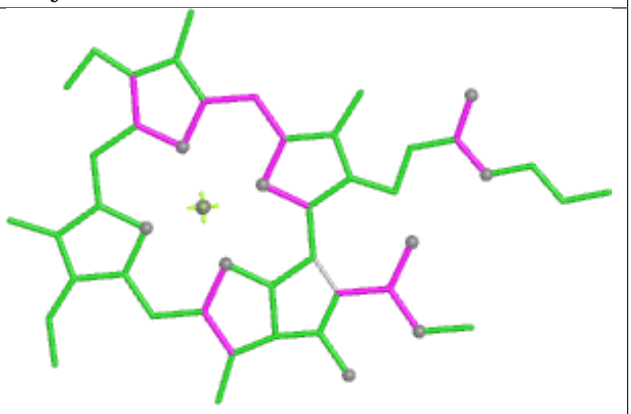


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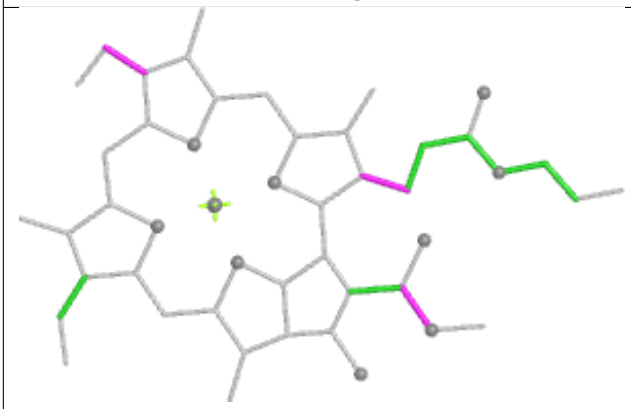
Ligand CLA y 614



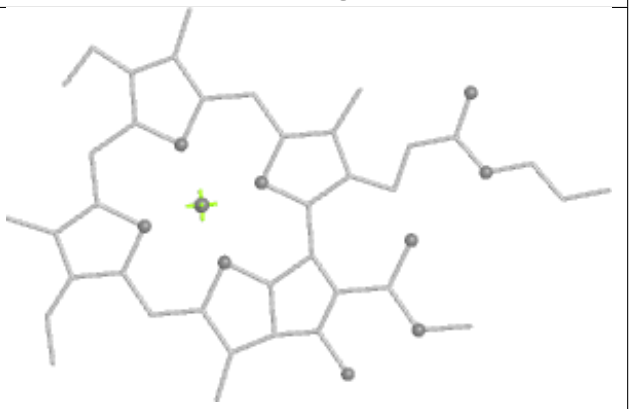
Bond lengths



Bond angles

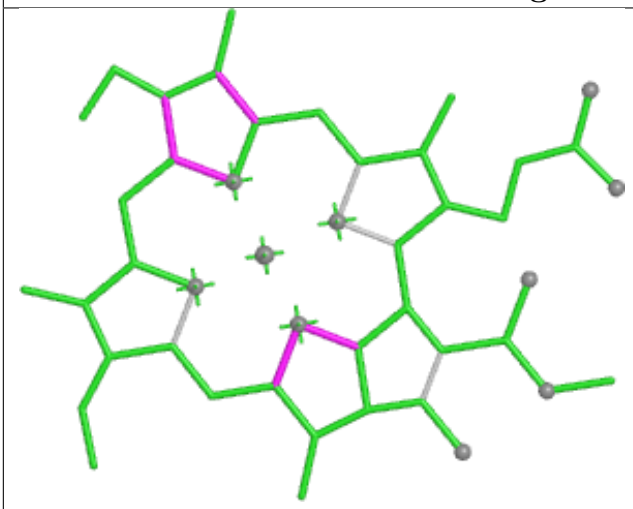


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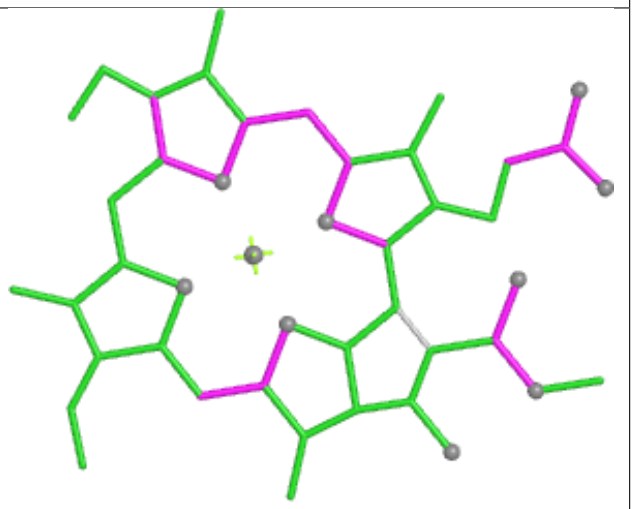


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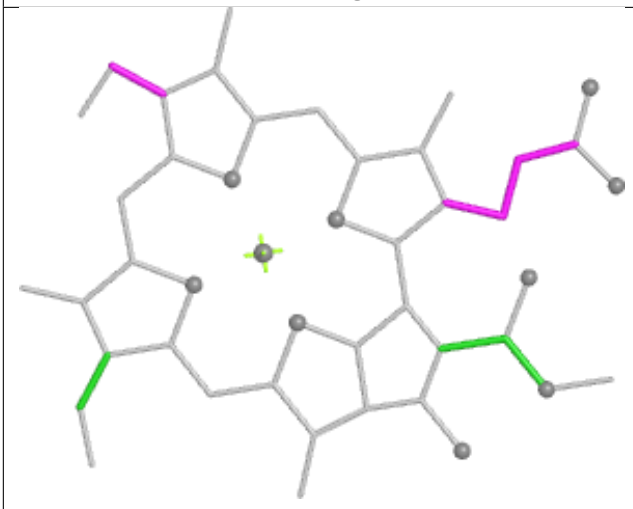
Ligand CLA s 609



Bond lengths



Bond angles

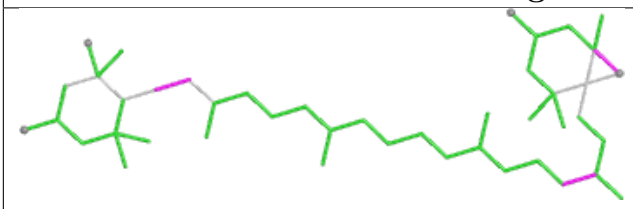


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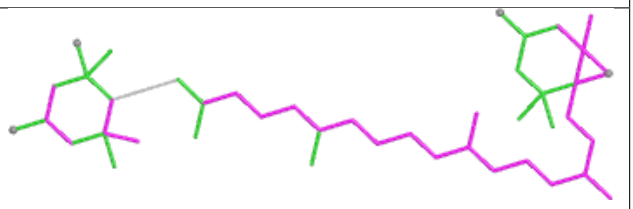


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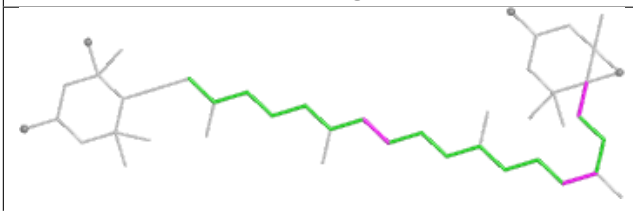
Ligand NEX r 623



Bond lengths



Bond angles

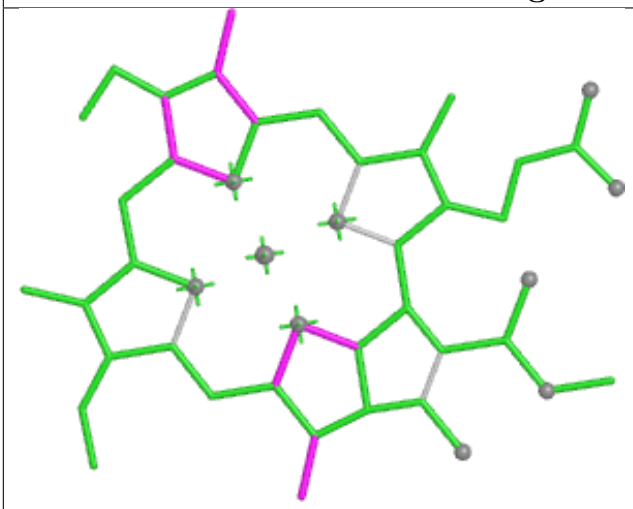


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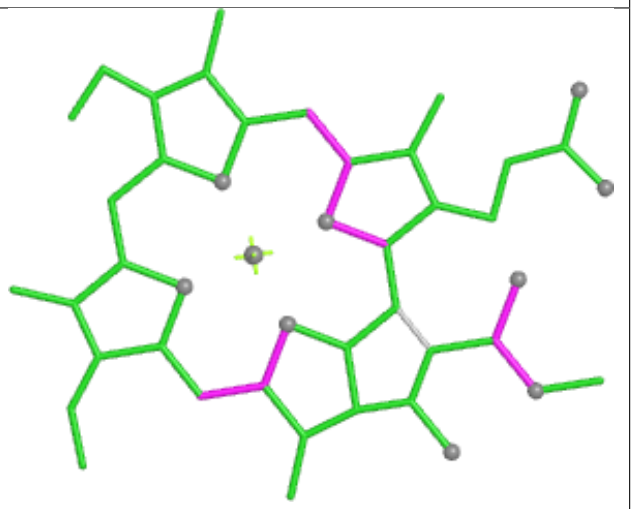


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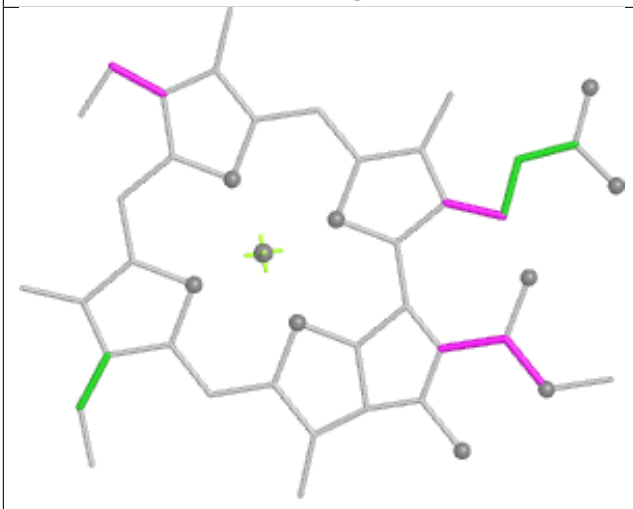
Ligand CLA 2 614



Bond lengths



Bond angles

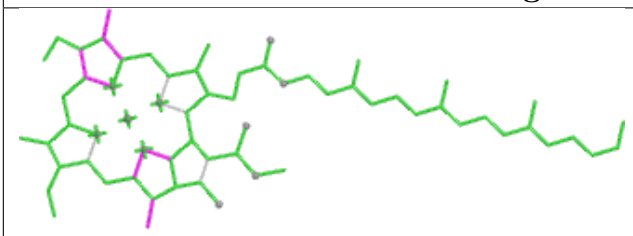


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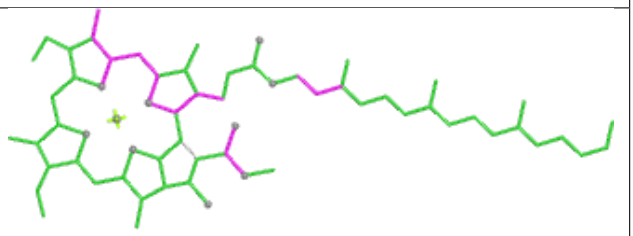


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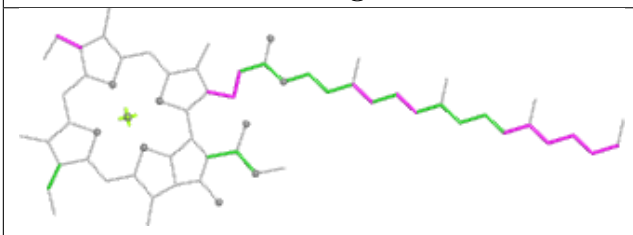
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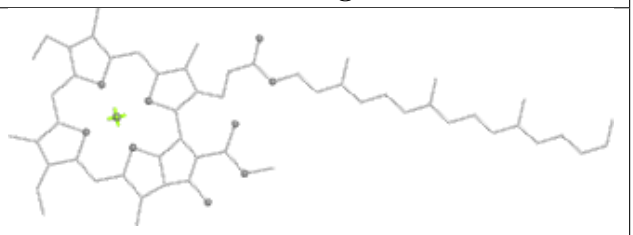
Bond lengths



Bond angles

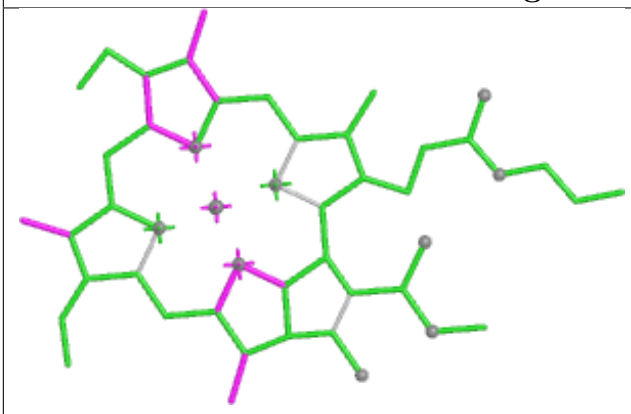


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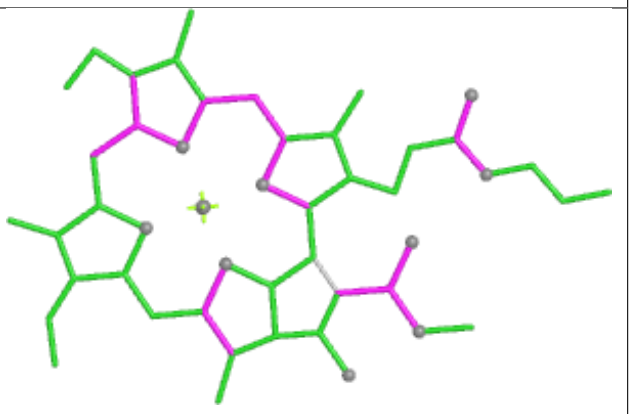


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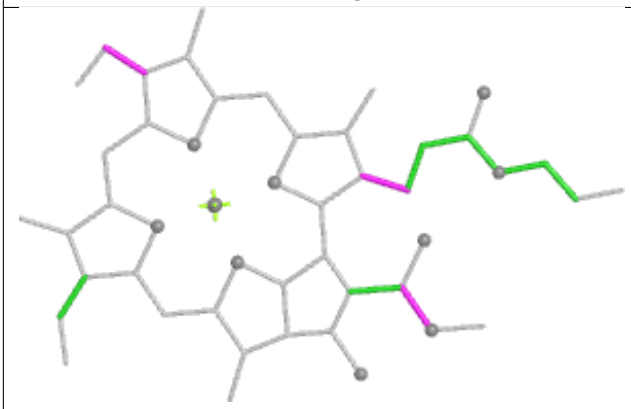
Ligand CLA Y 614



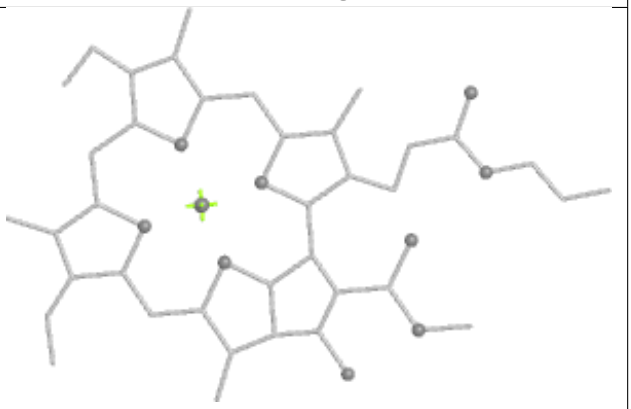
Bond lengths



Bond angles

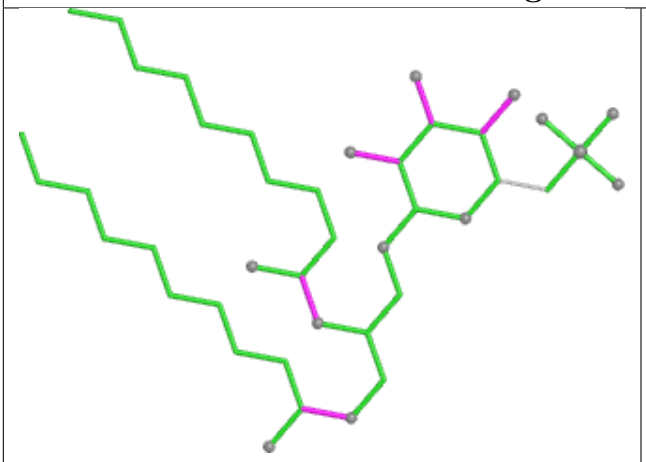


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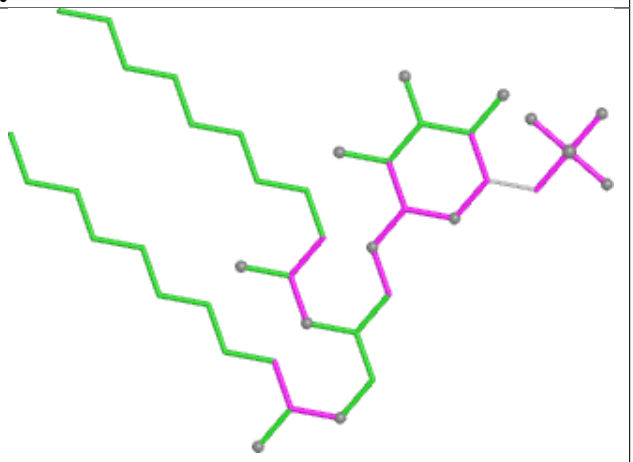


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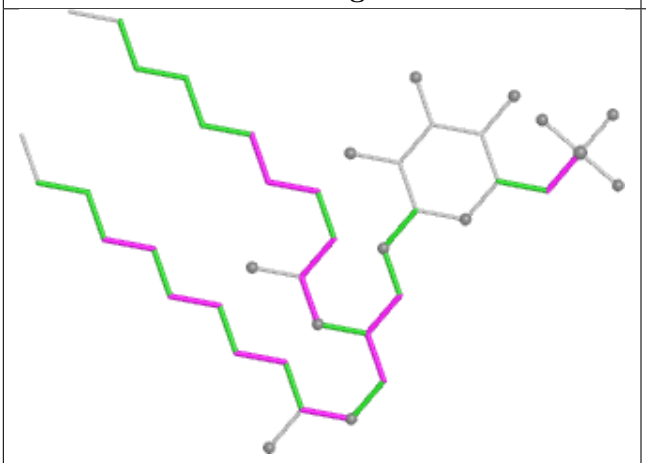
Ligand SQD B 623



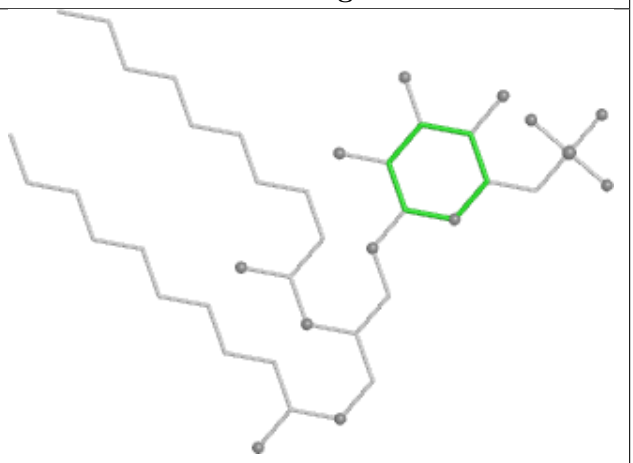
Bond lengths



Bond angles



Torsions

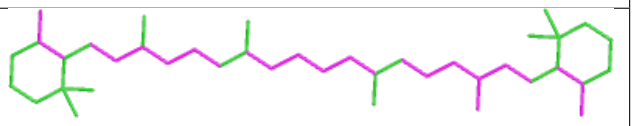


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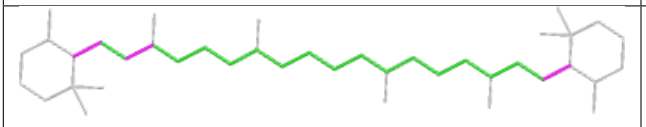
Ligand BCR A 411



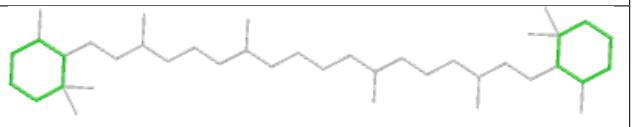
Bond lengths



Bond angles

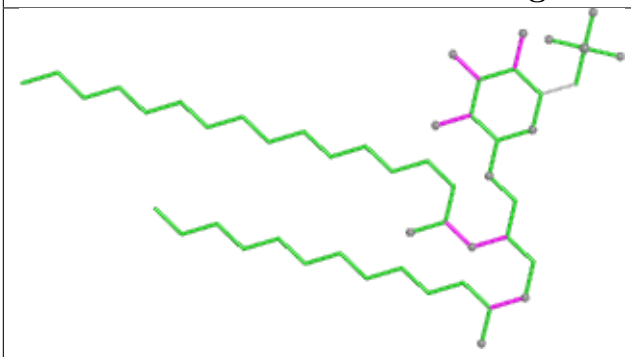


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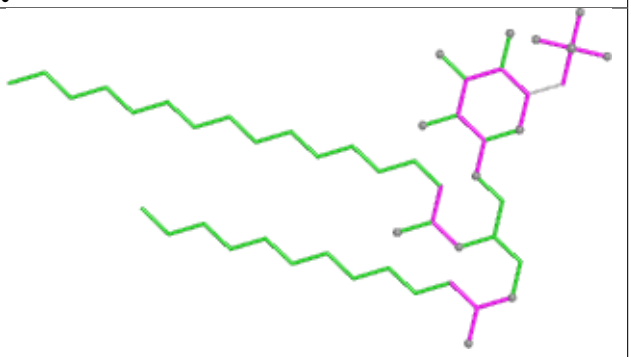


Rings

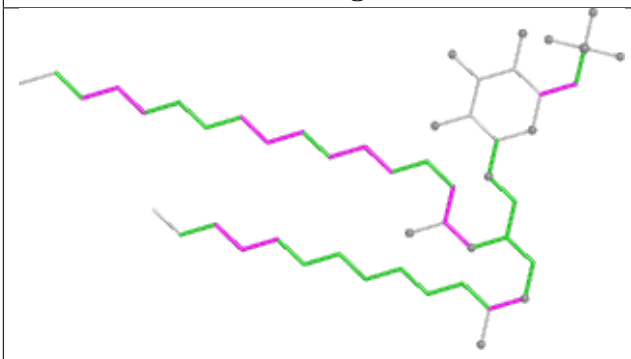
Ligand SQD a 412



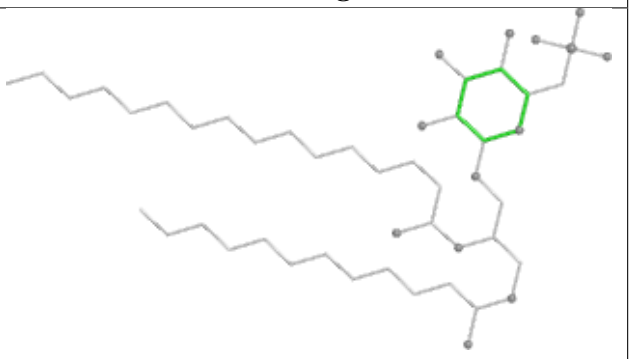
Bond lengths



Bond angles

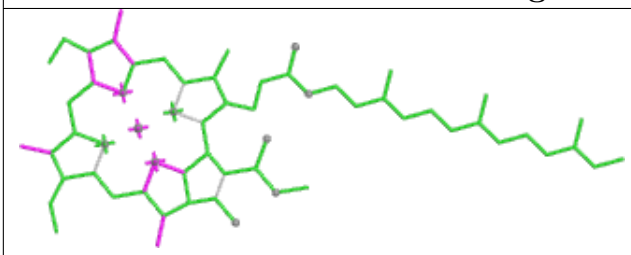


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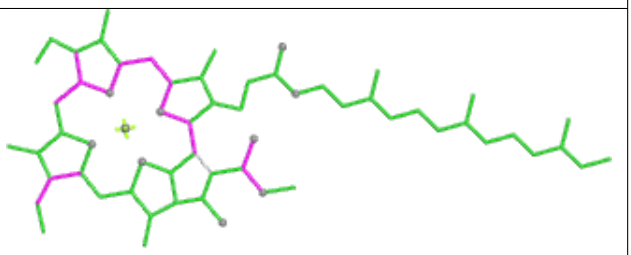


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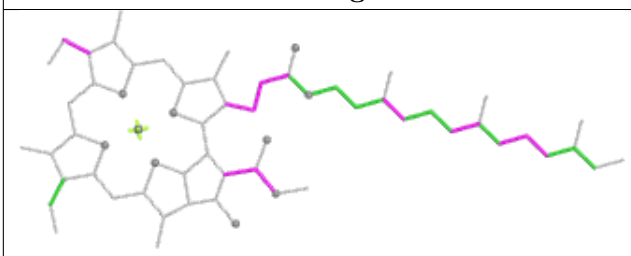
Ligand CLA 5 602



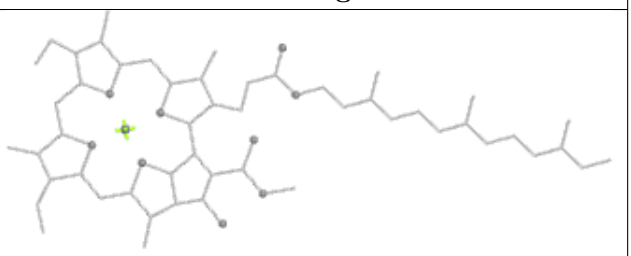
Bond lengths



Bond angles

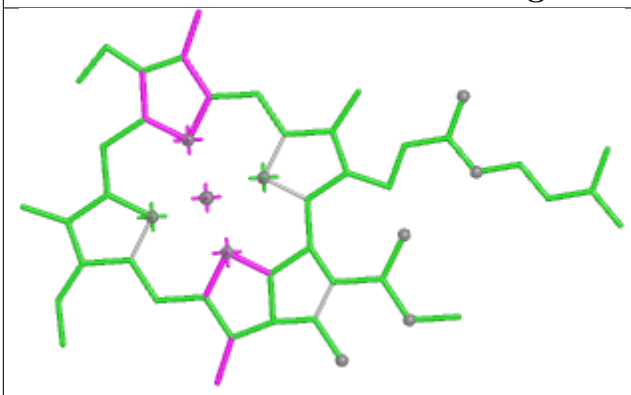


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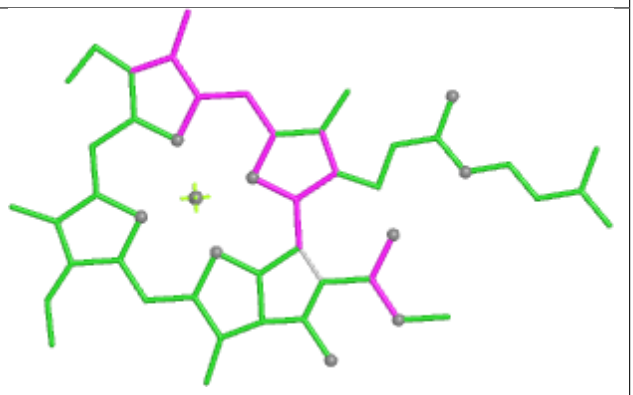


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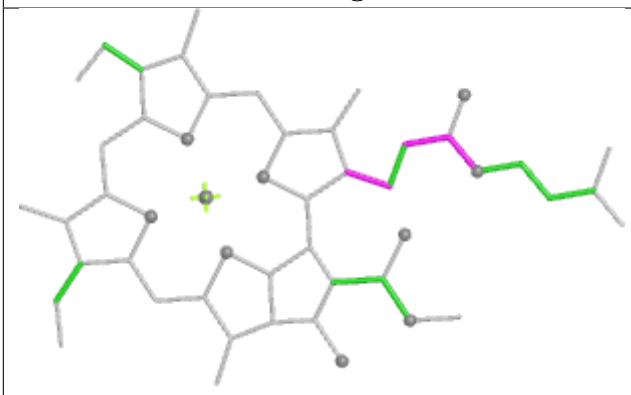
Ligand CLA S 604



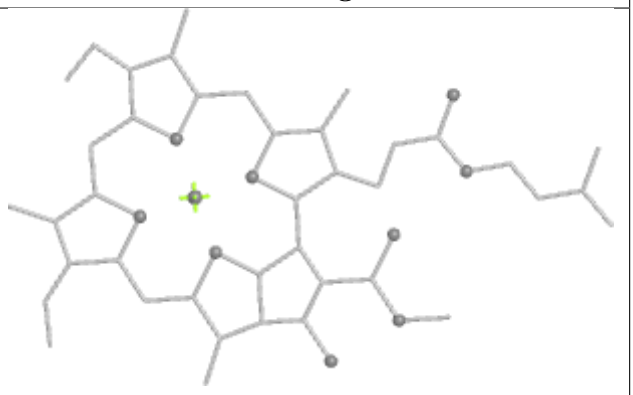
Bond lengths



Bond angles

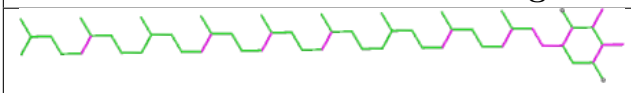


Torsions



Rings

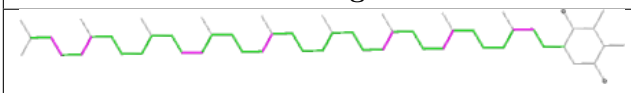
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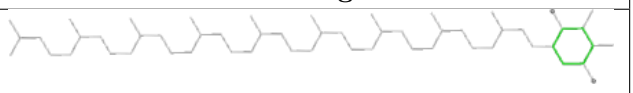
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Bond angles

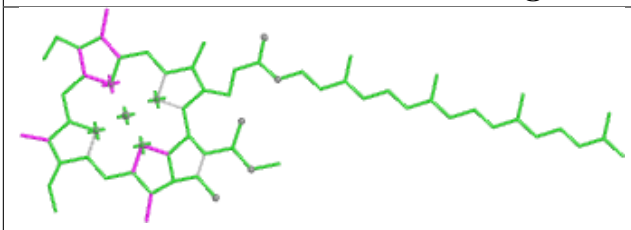


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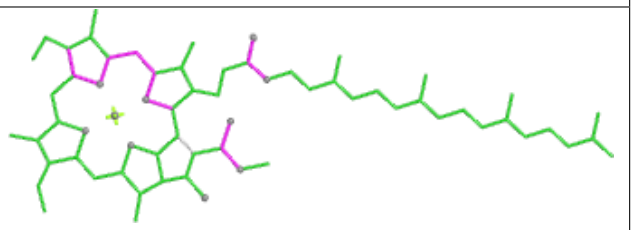


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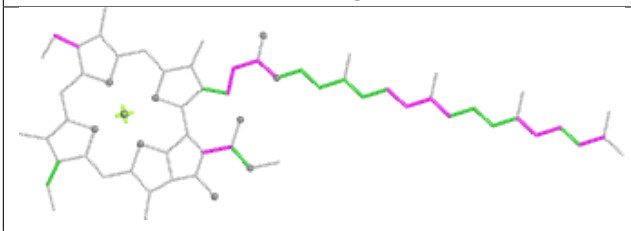
Ligand CLA B 602



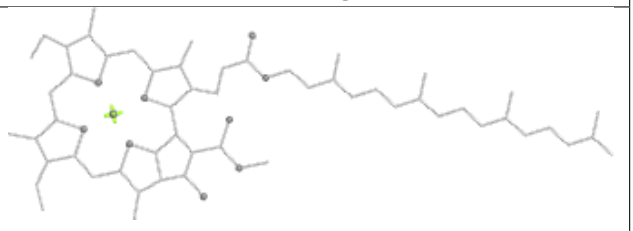
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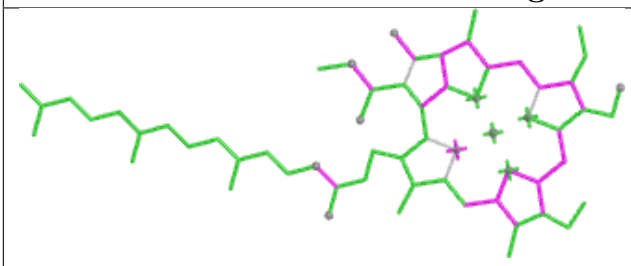
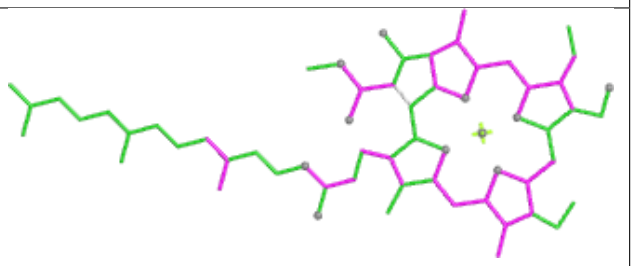
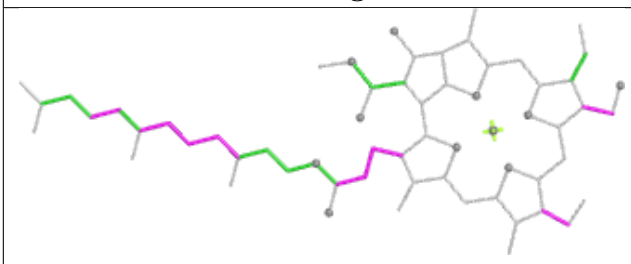
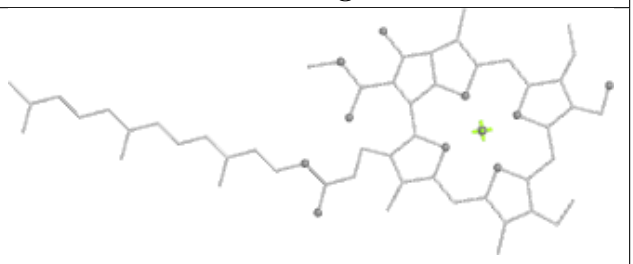
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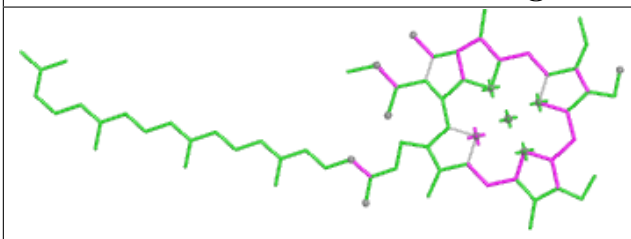
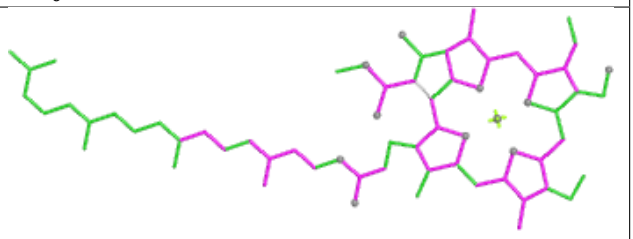
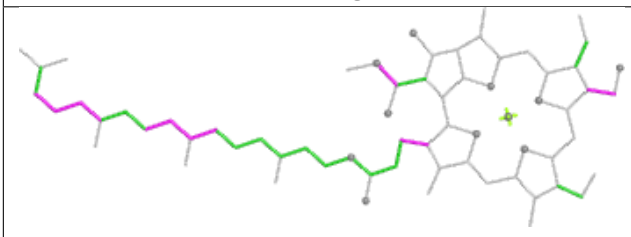
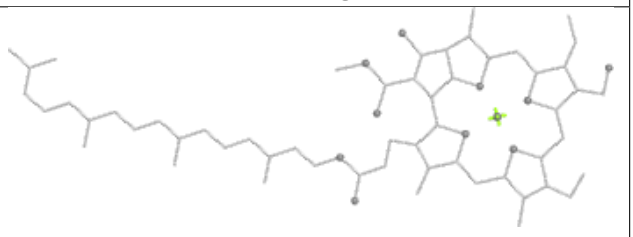


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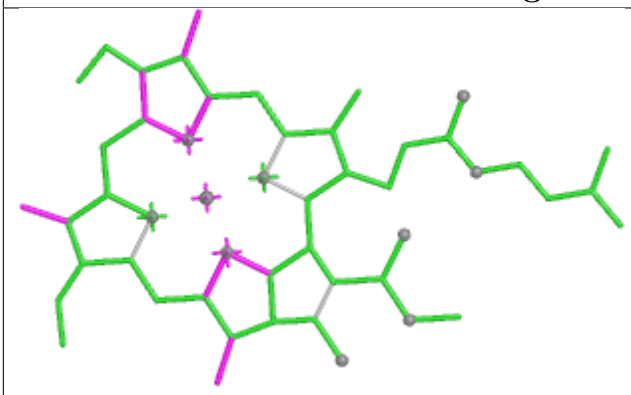


Rings

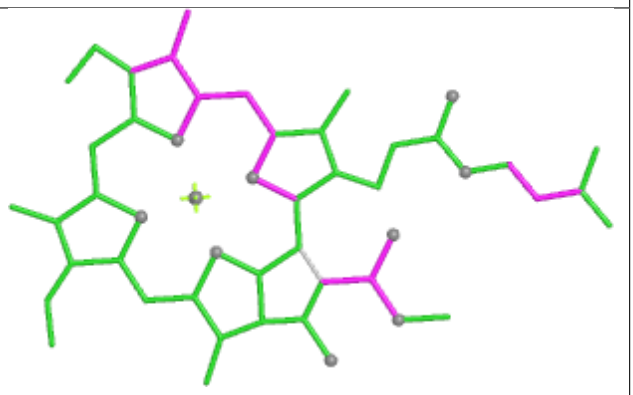
Ligand CHL 6 607	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL y 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

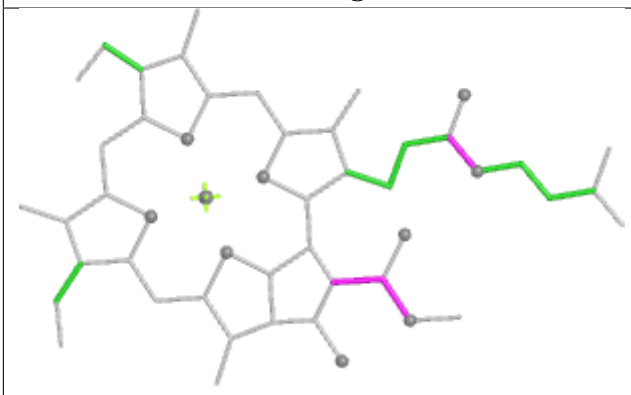
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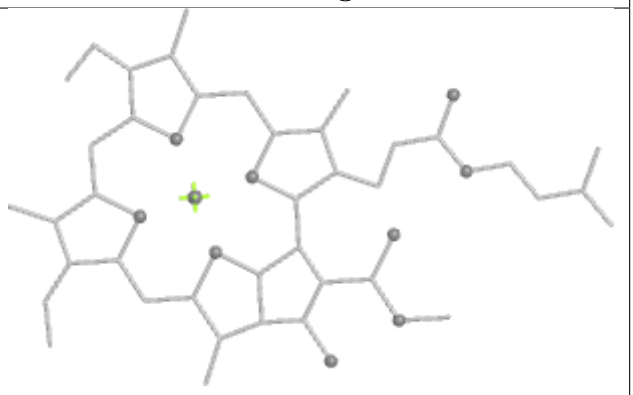
Bond lengths



Bond angles

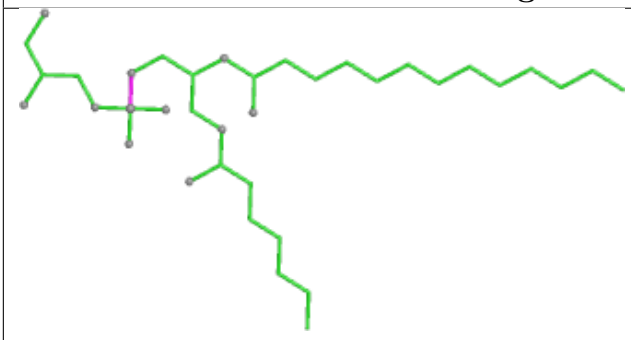


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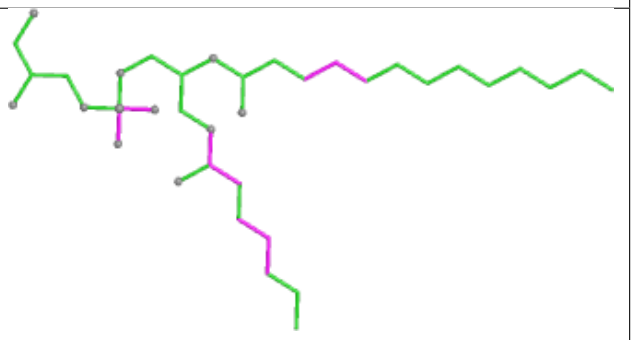


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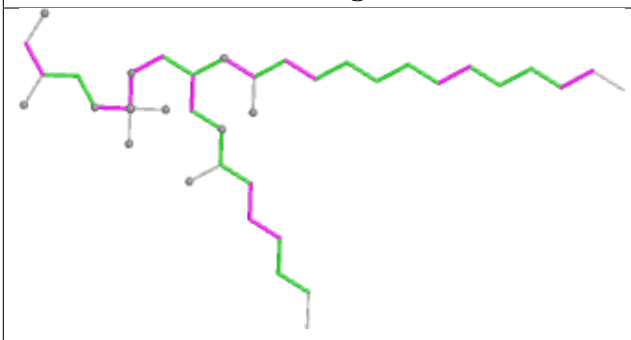
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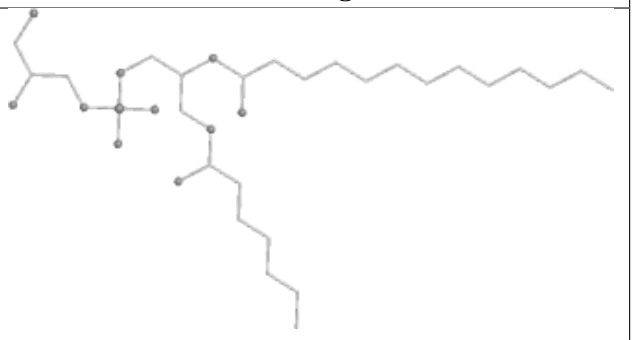
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Bond angles

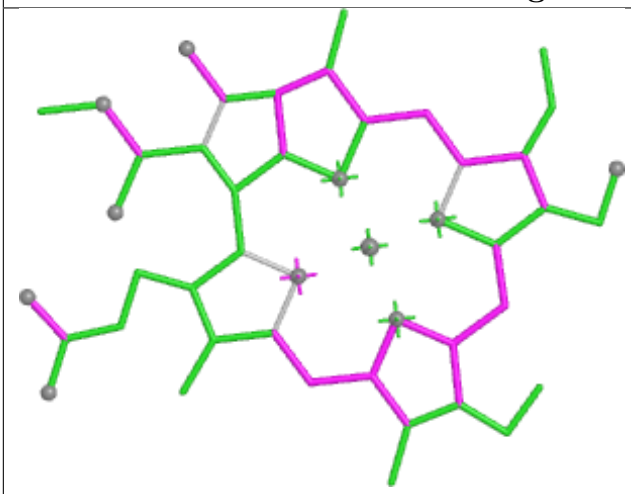


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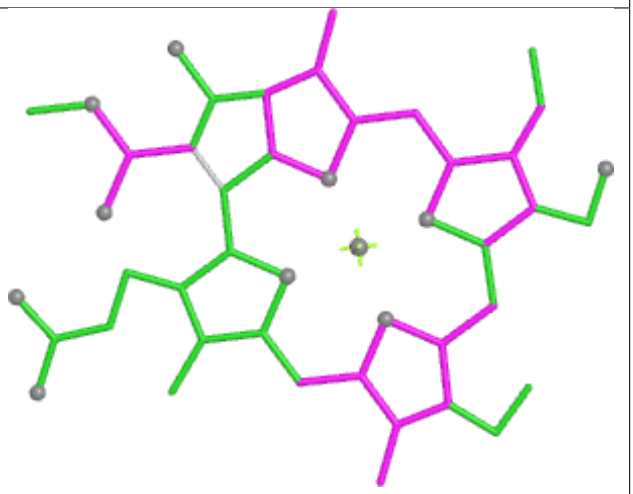


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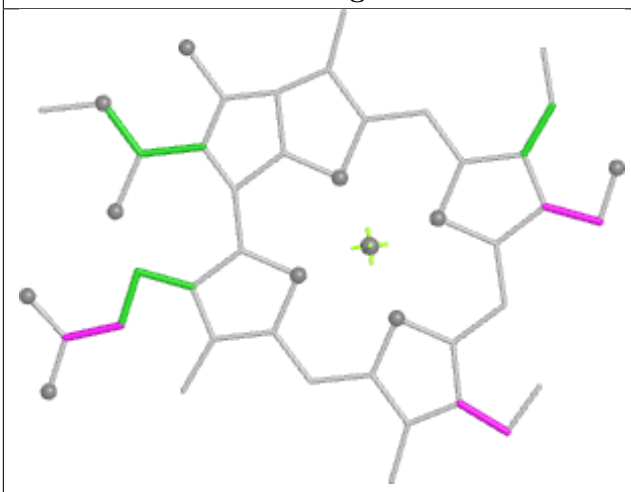
Ligand CHL 8 609



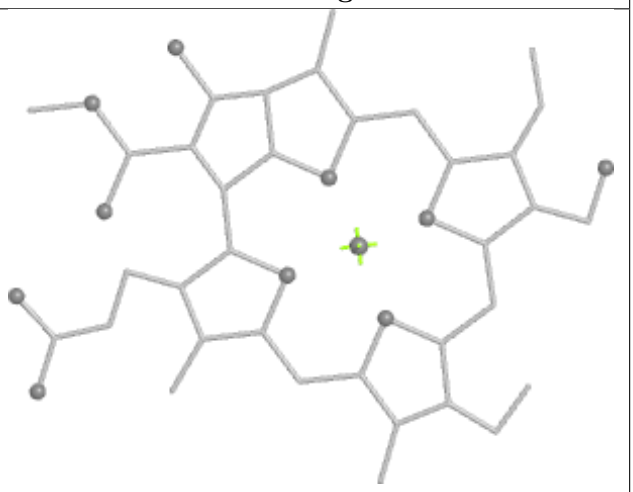
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Bond angles

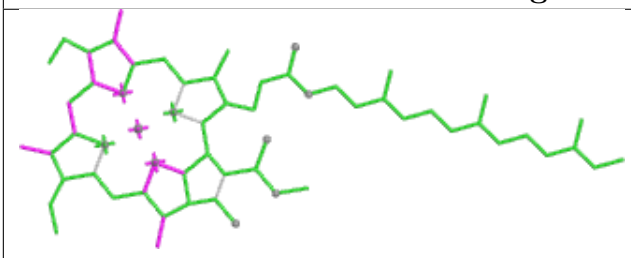


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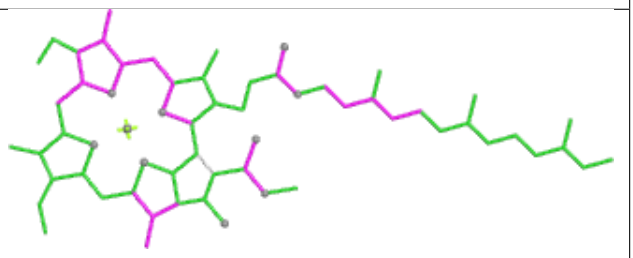


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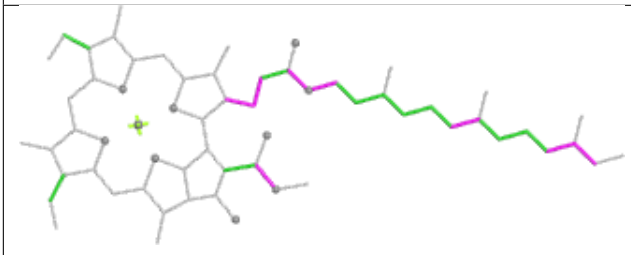
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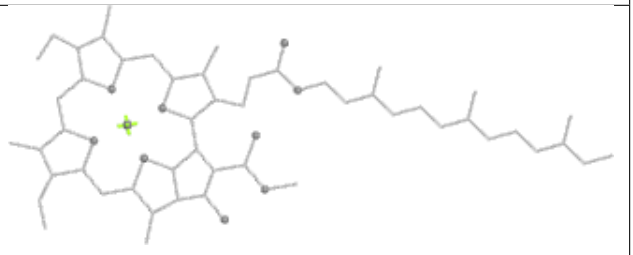
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Bond angles

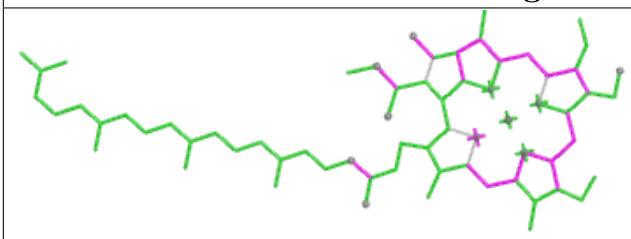


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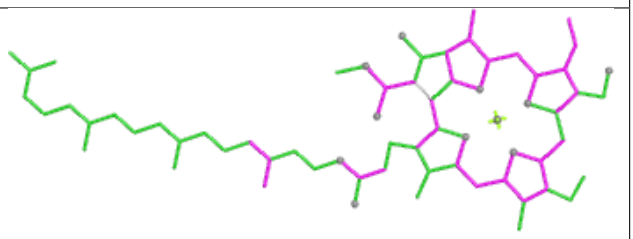


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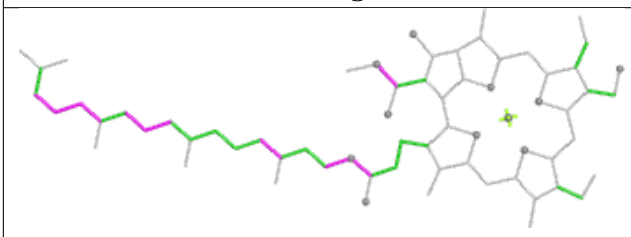
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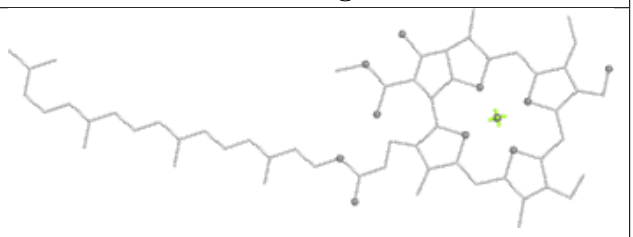
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Bond angles

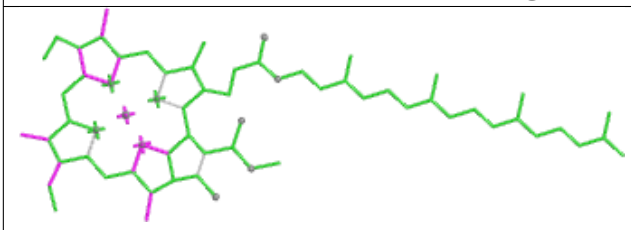


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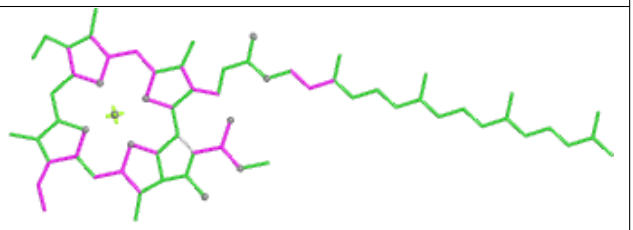


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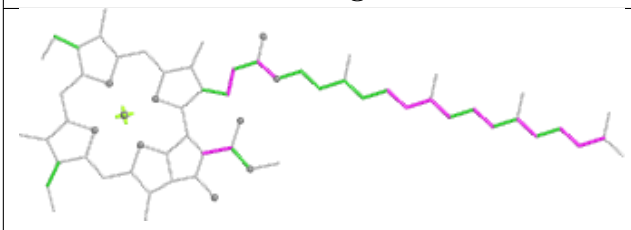
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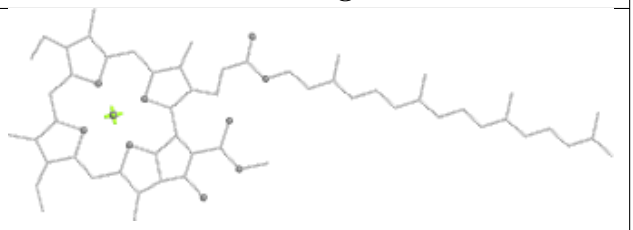
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Bond angles

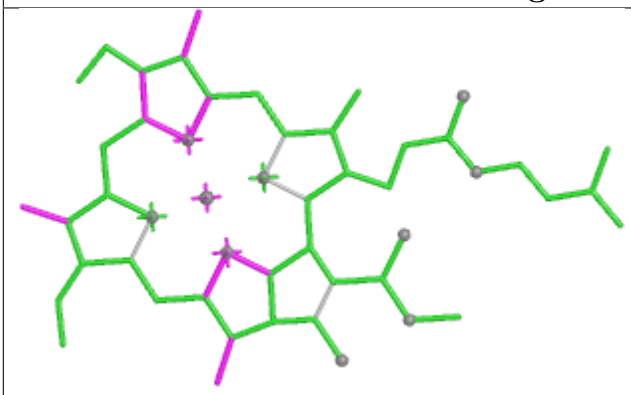


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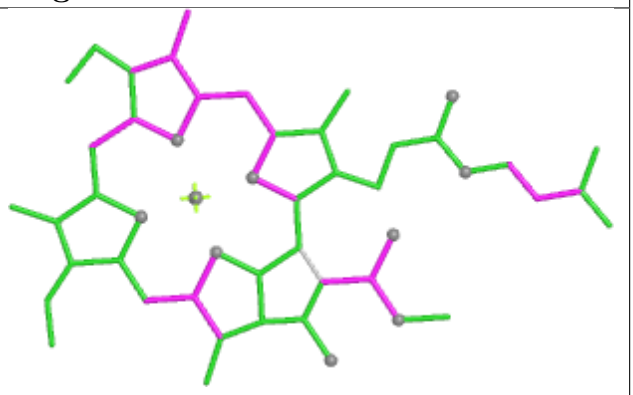


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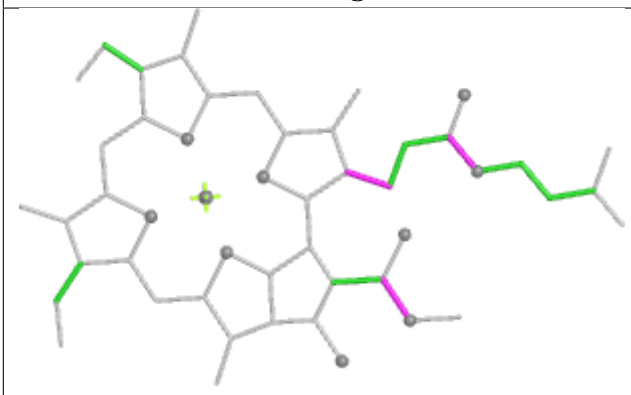
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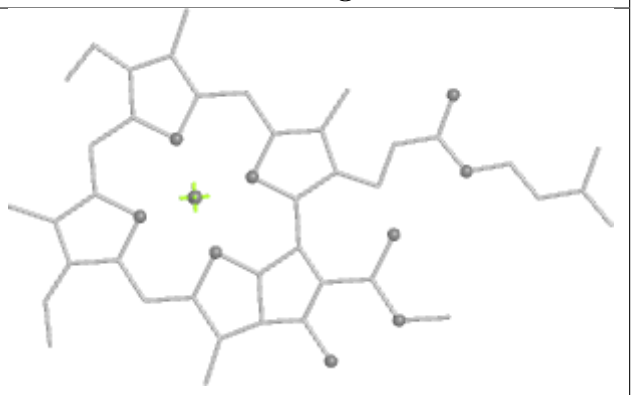
Bond lengths



Bond angles

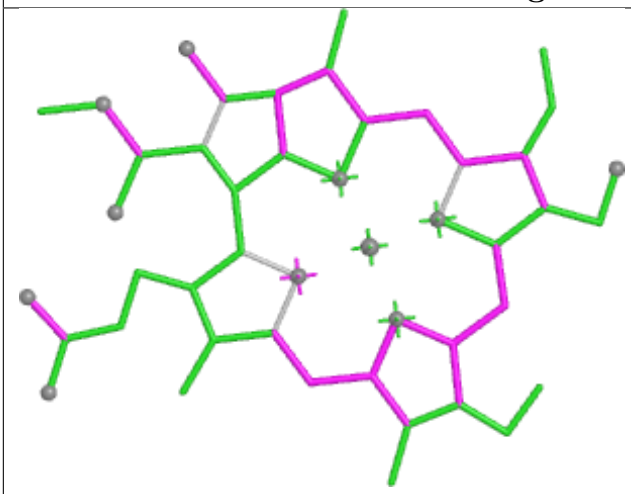


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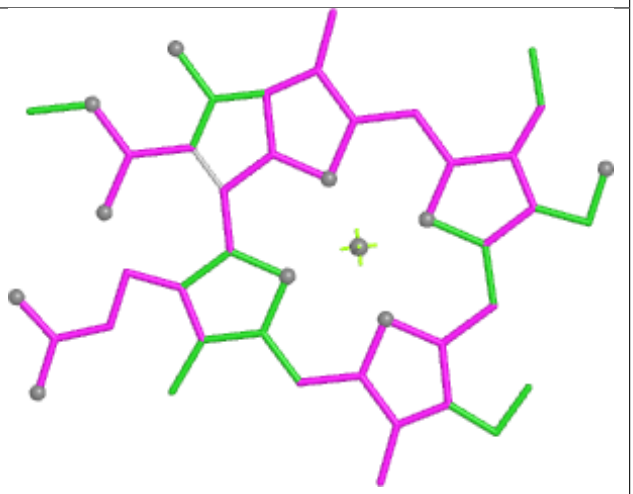


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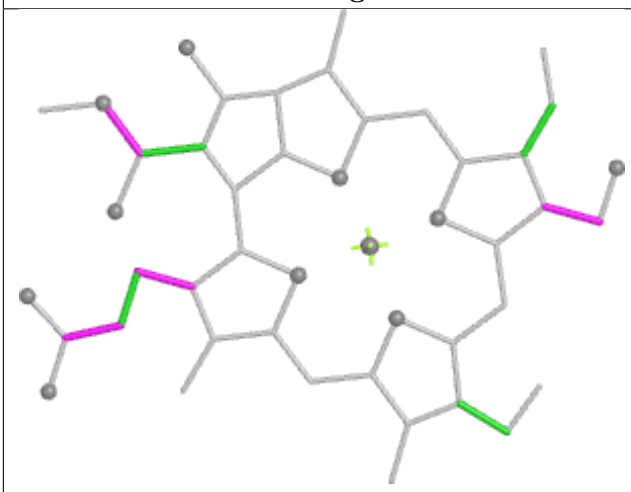
Ligand CHL 8 606



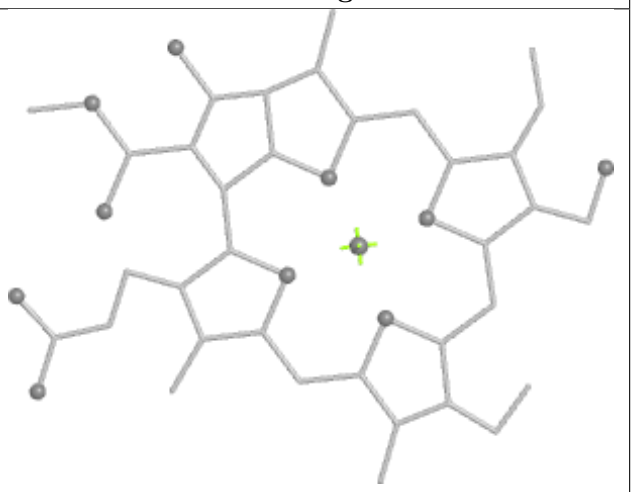
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Bond angles

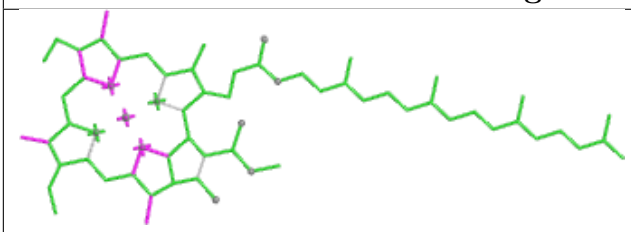


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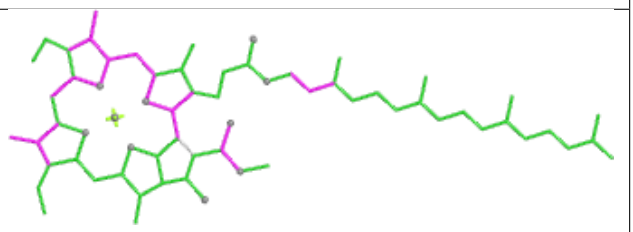


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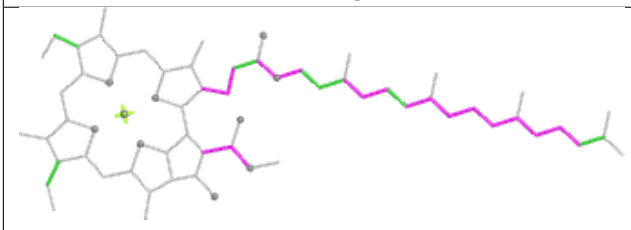
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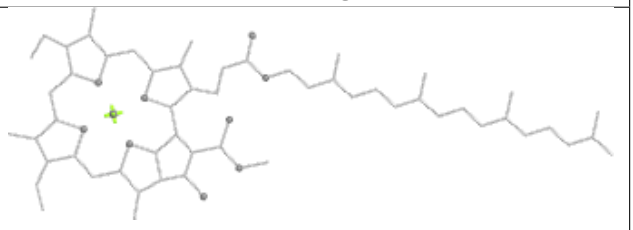
Bond lengths



Bond angles

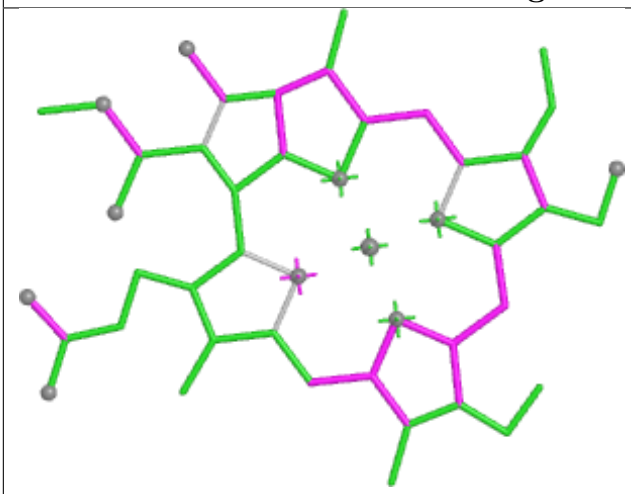


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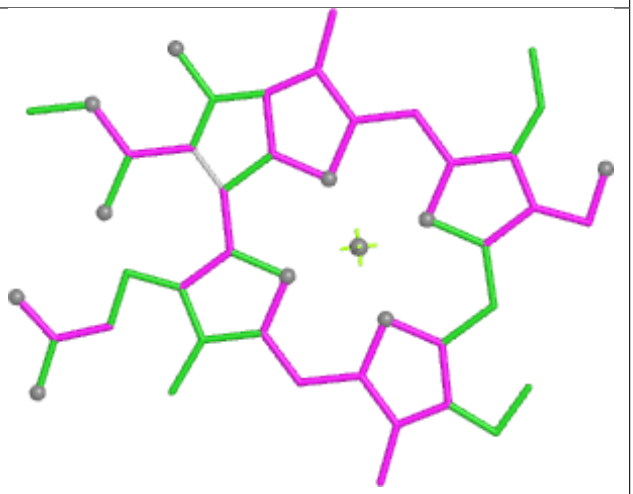


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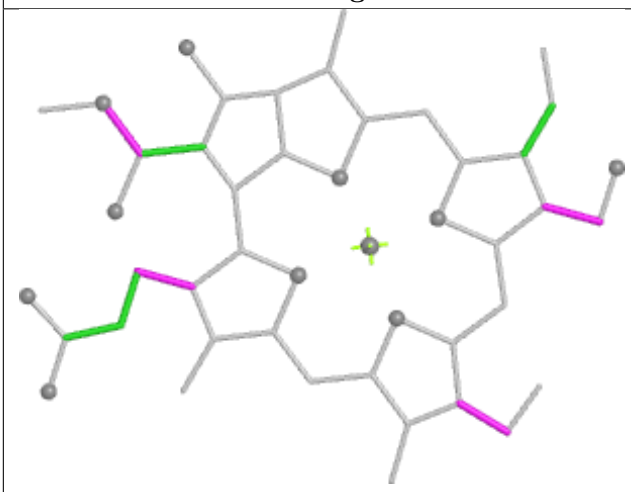
Ligand CHL 4 608



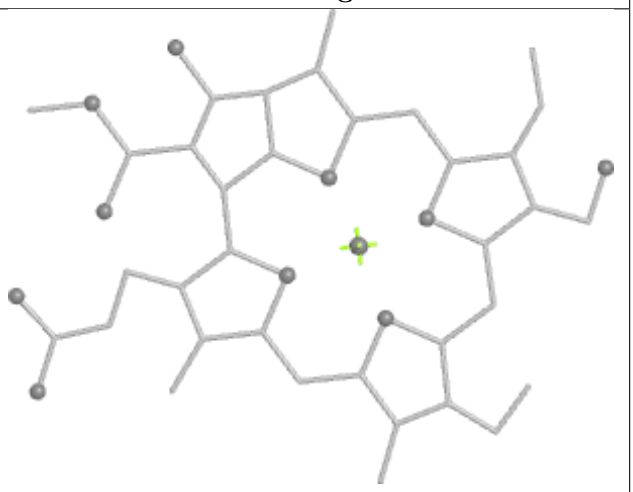
Bond lengths



Bond angles

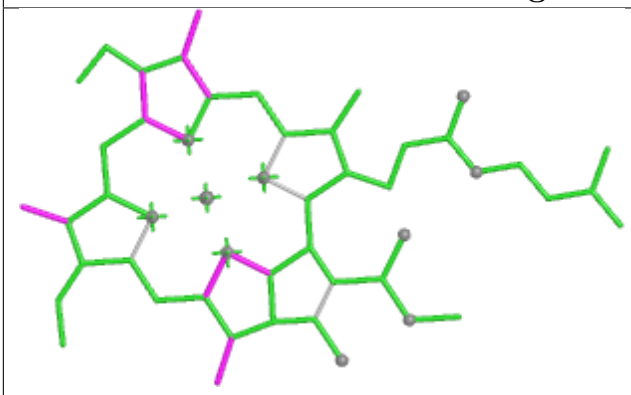


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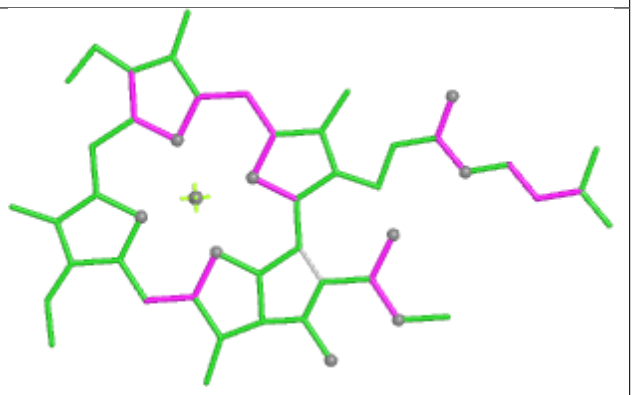


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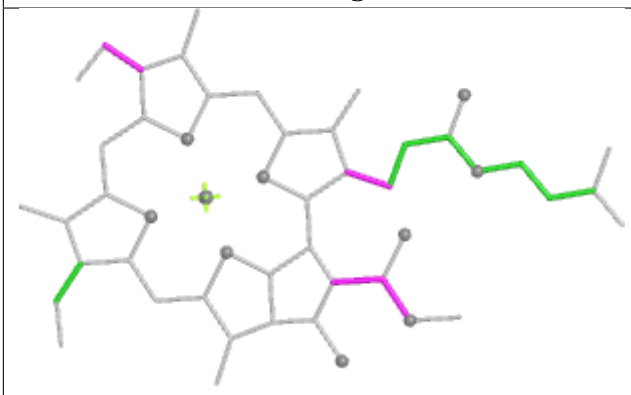
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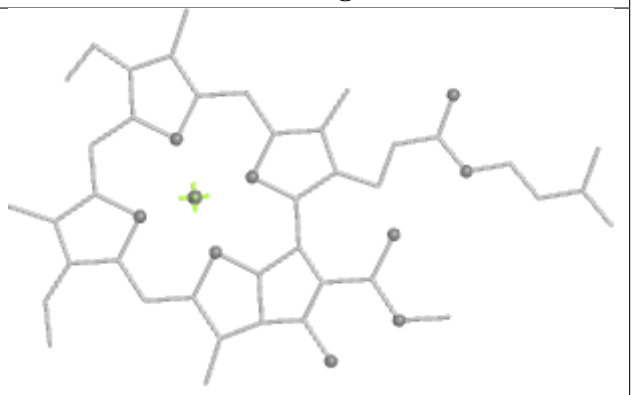
Bond lengths



Bond angles



Torsions



Rings

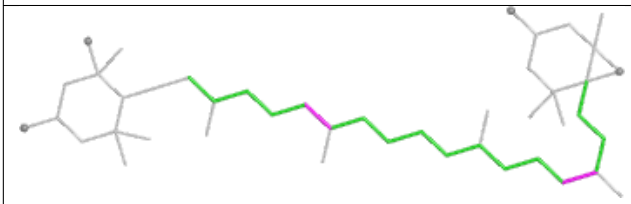
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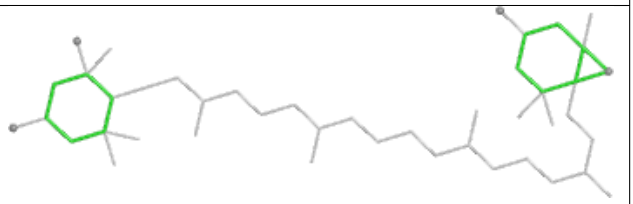
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Bond angles

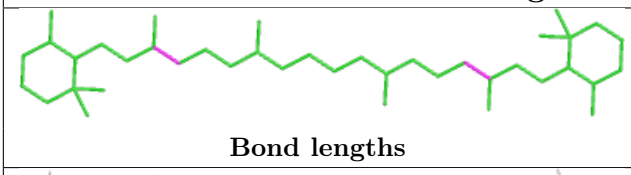


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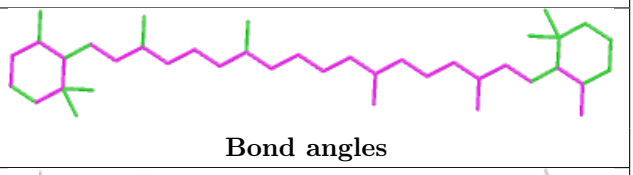


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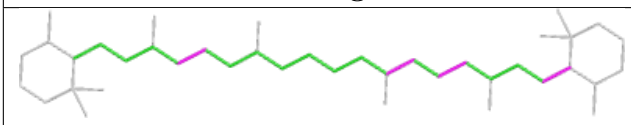
Ligand BCR c 515



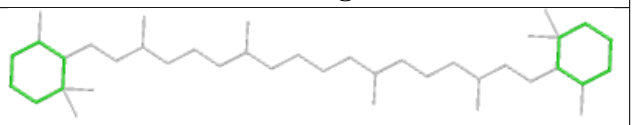
Bond lengths



Bond angles

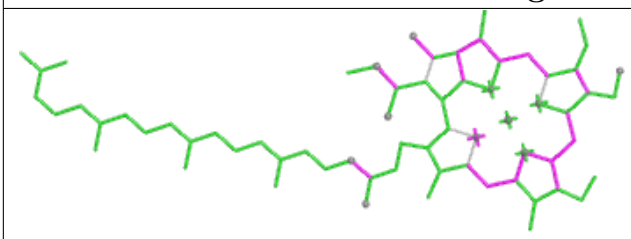


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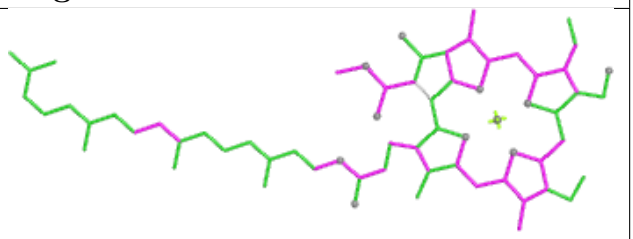


Rings

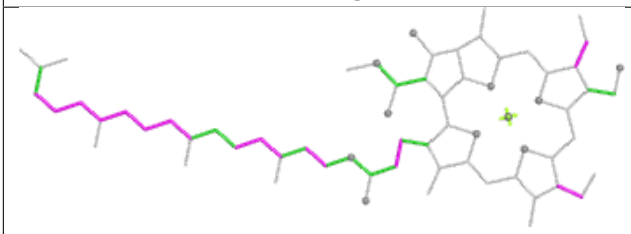
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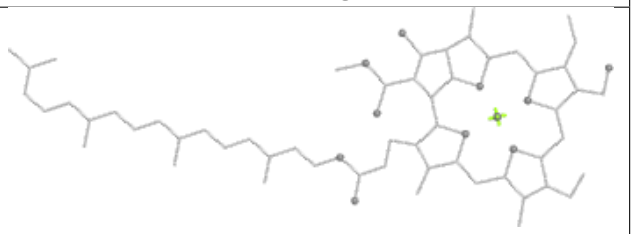
Bond lengths



Bond angles

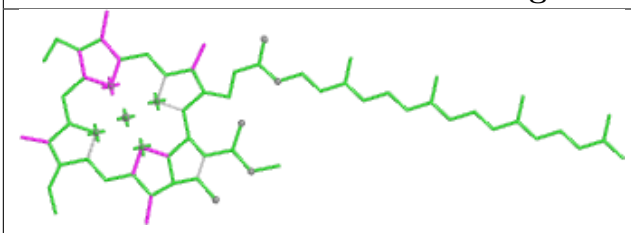


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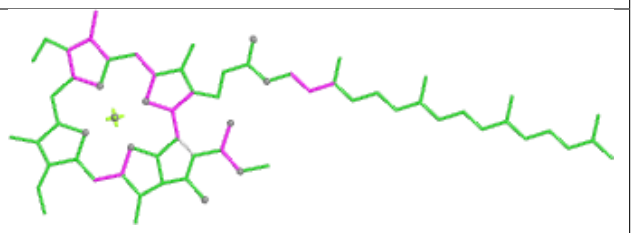


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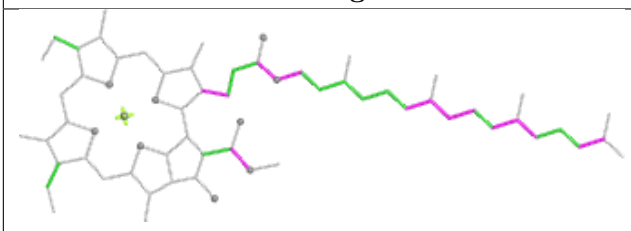
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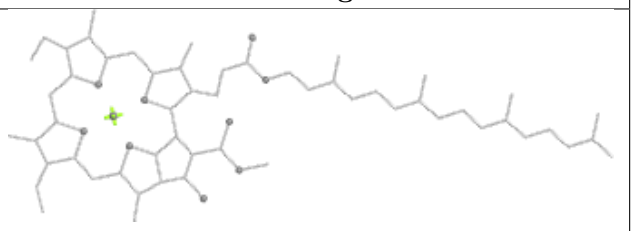
Bond lengths



Bond angles

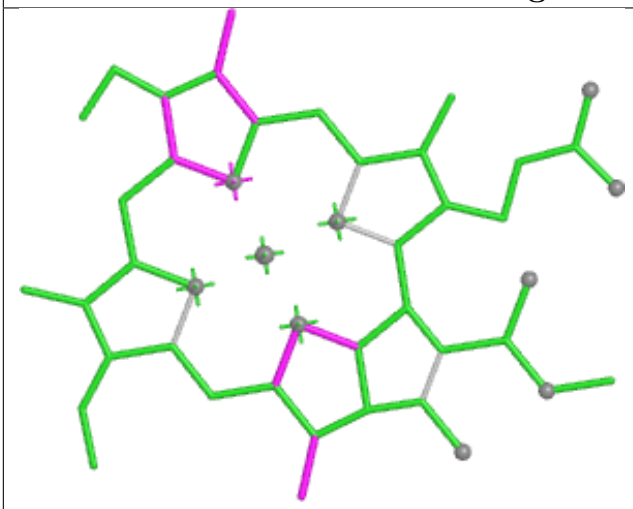


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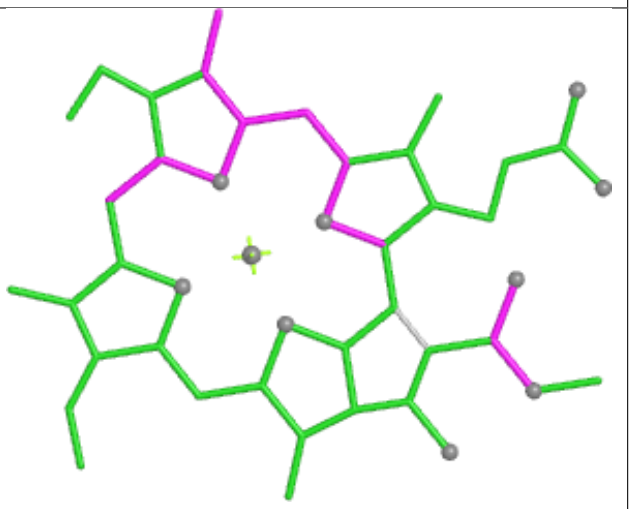


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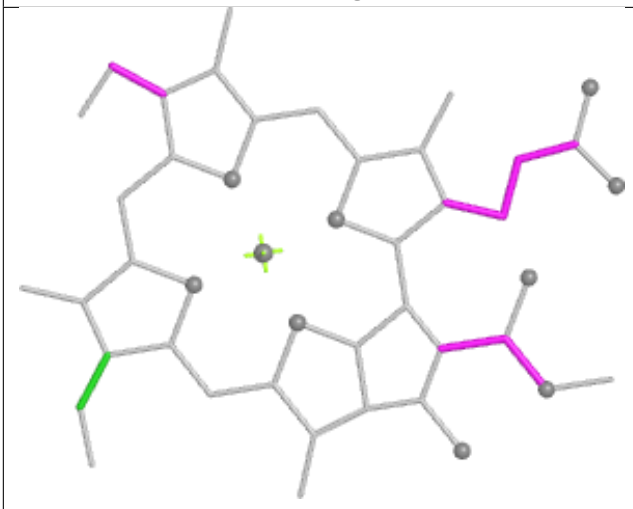
Ligand CLA 6 604



Bond lengths



Bond angles

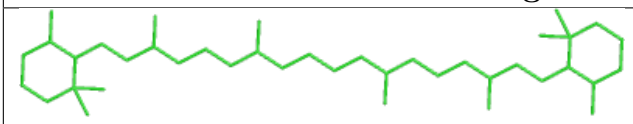


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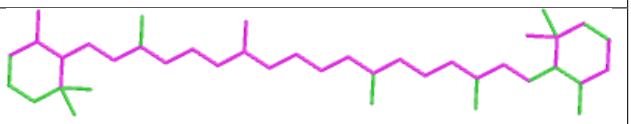


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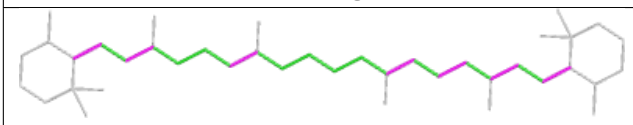
Ligand BCR T 101



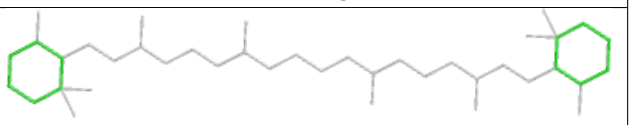
Bond lengths



Bond angles

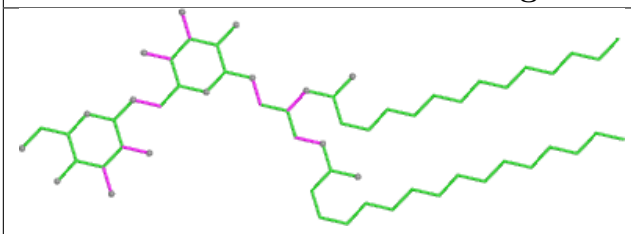


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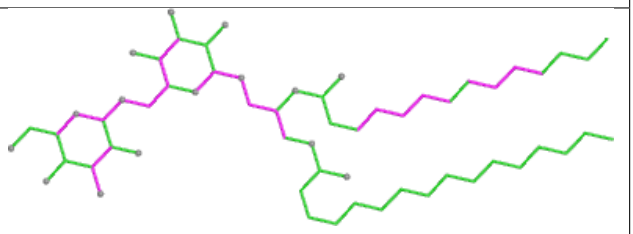


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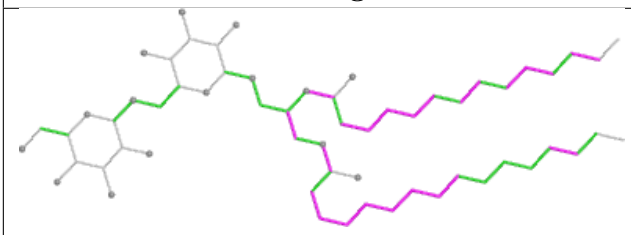
Ligand DGD C 520



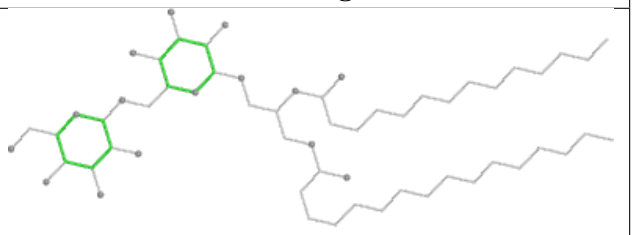
Bond lengths



Bond angles

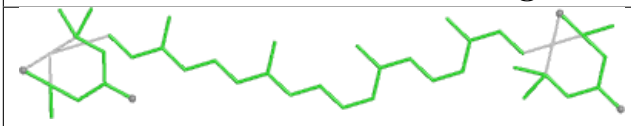


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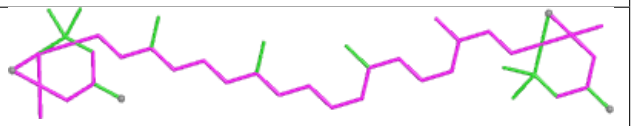


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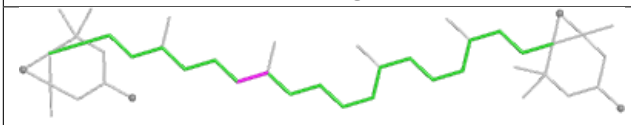
Ligand XAT 1 1622



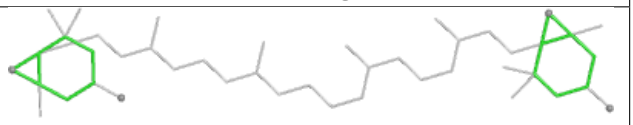
Bond lengths



Bond angles

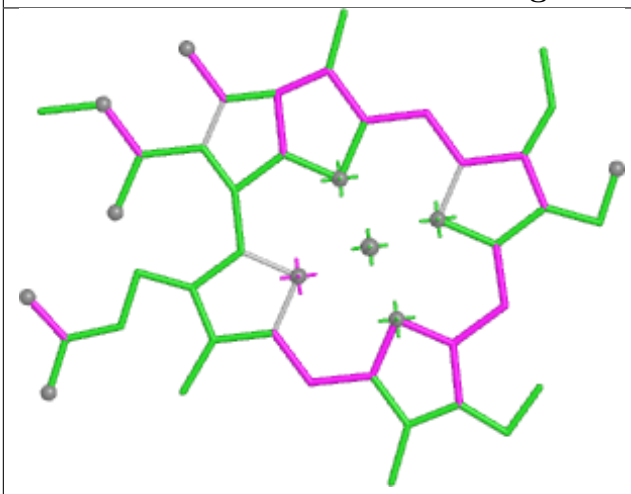


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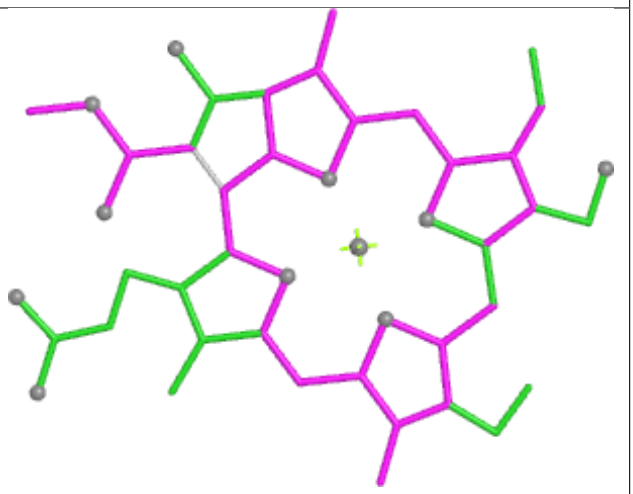


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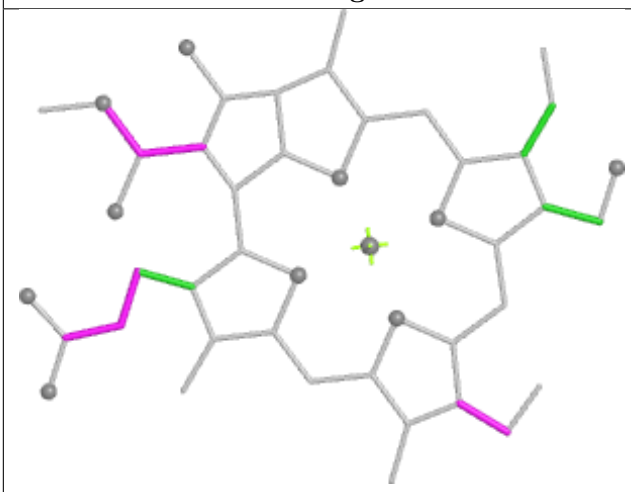
Ligand CHL s 601



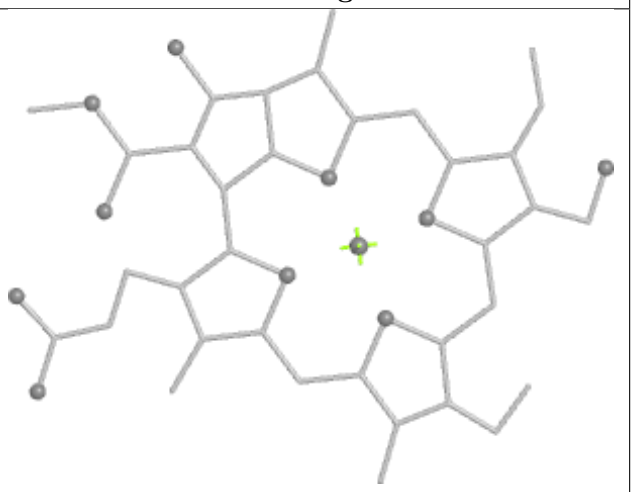
Bond lengths



Bond angles

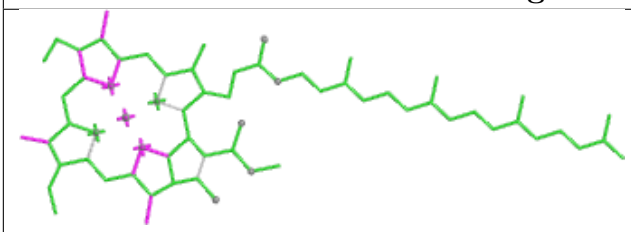


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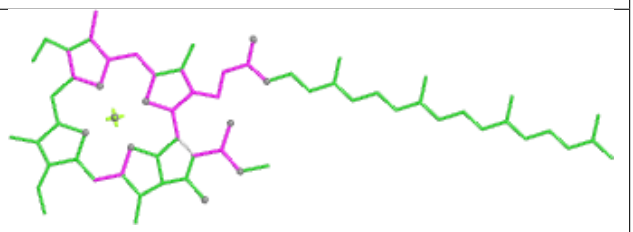


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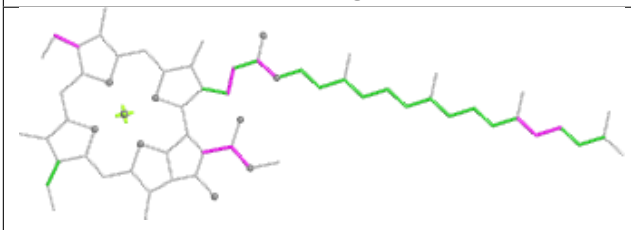
Ligand CLA b 611



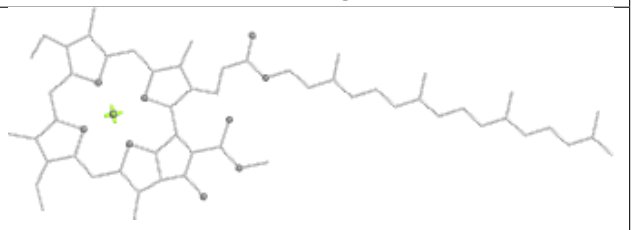
Bond lengths



Bond angles

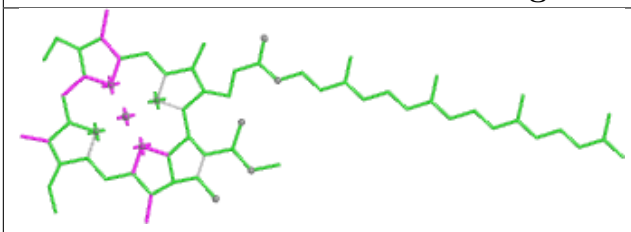


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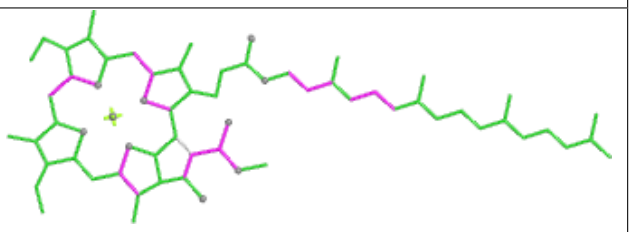


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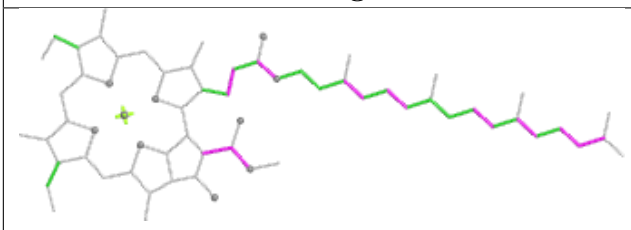
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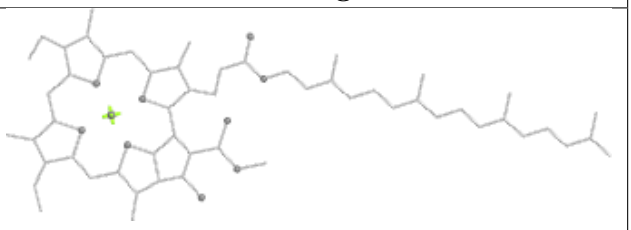
Bond lengths



Bond angles

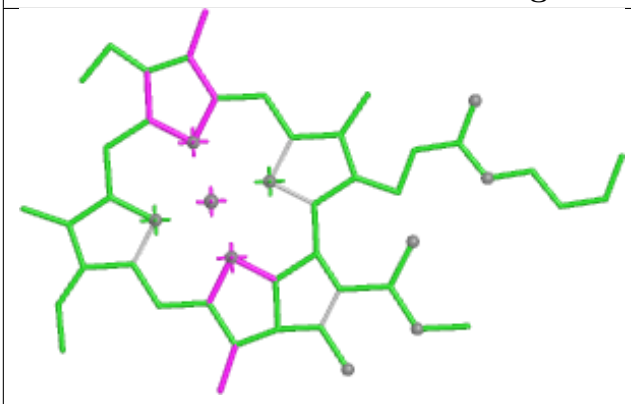


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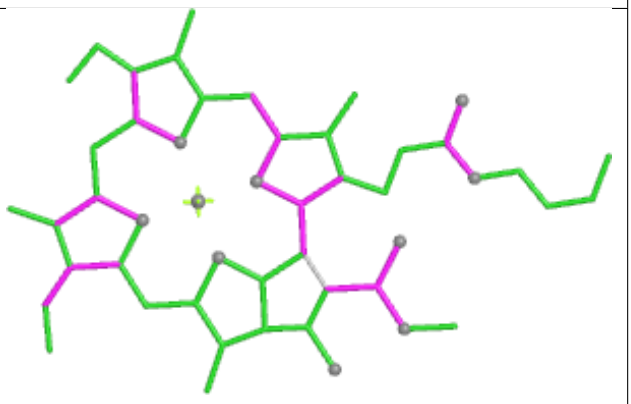


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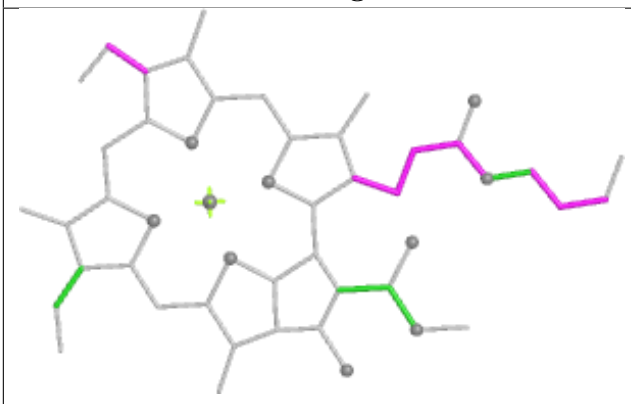
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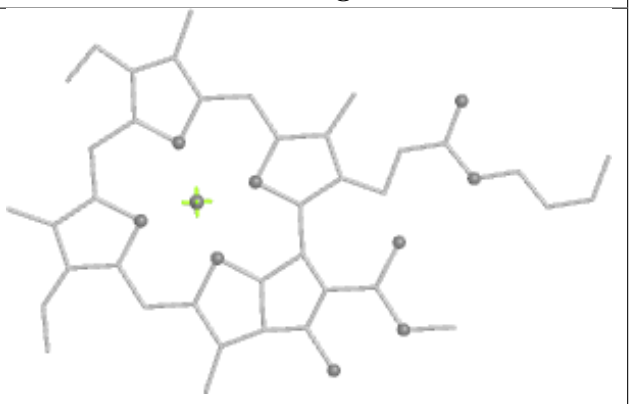
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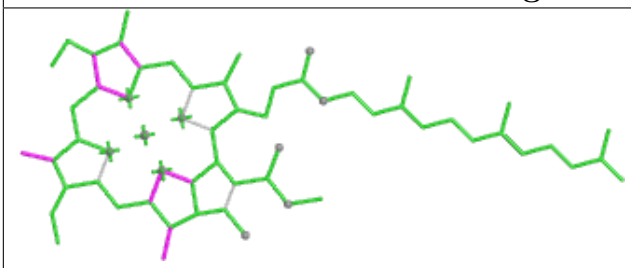
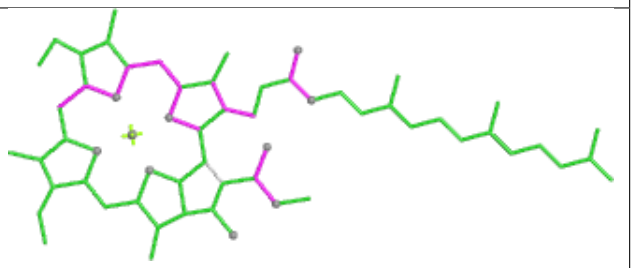
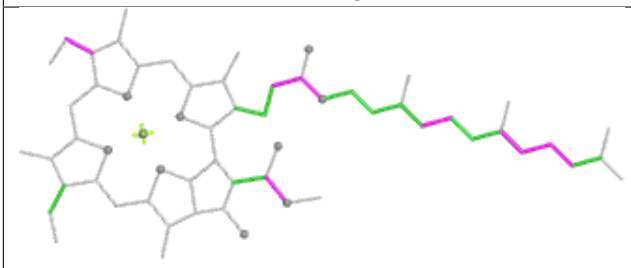
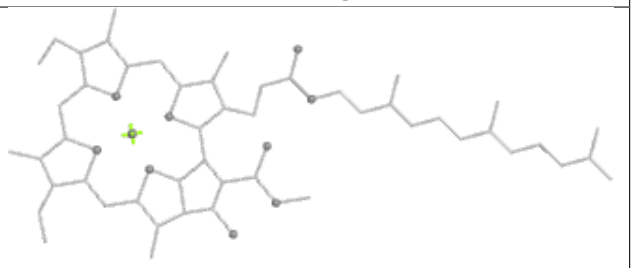
Bond angles



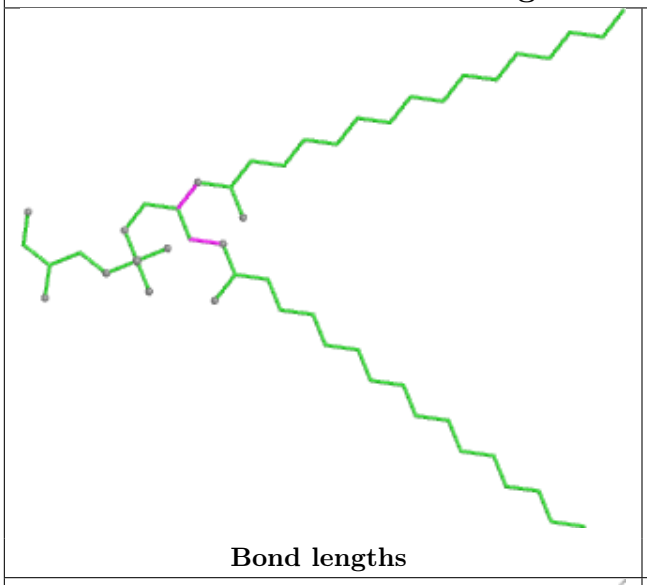
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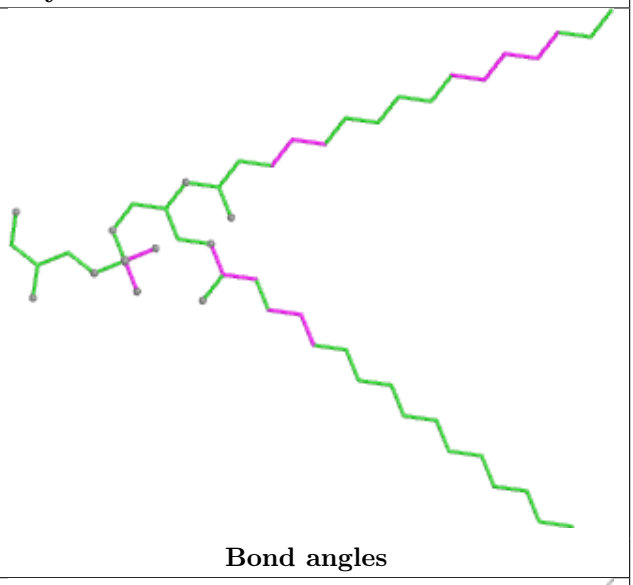
Rings

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

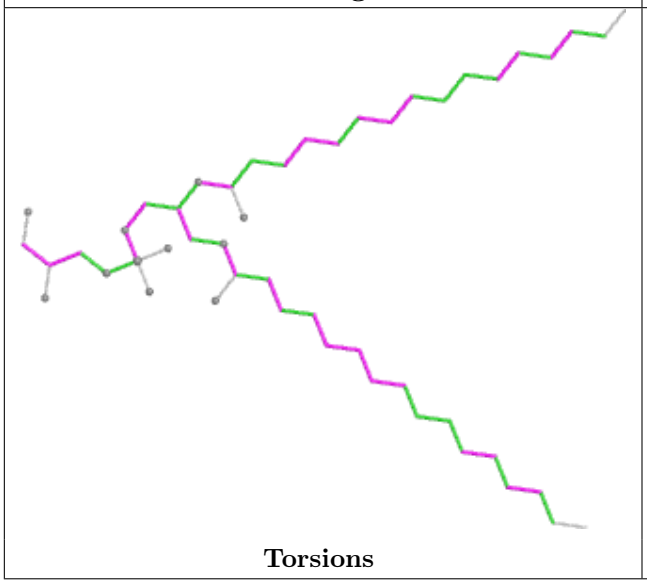
Ligand LHG y 2630



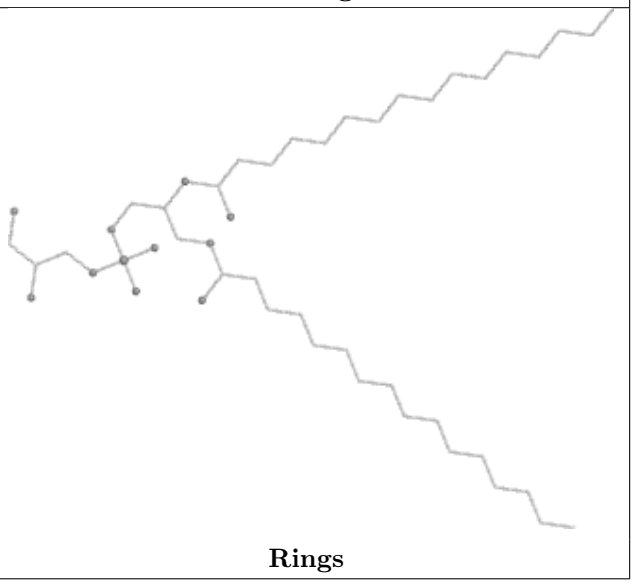
Bond lengths



Bond angles

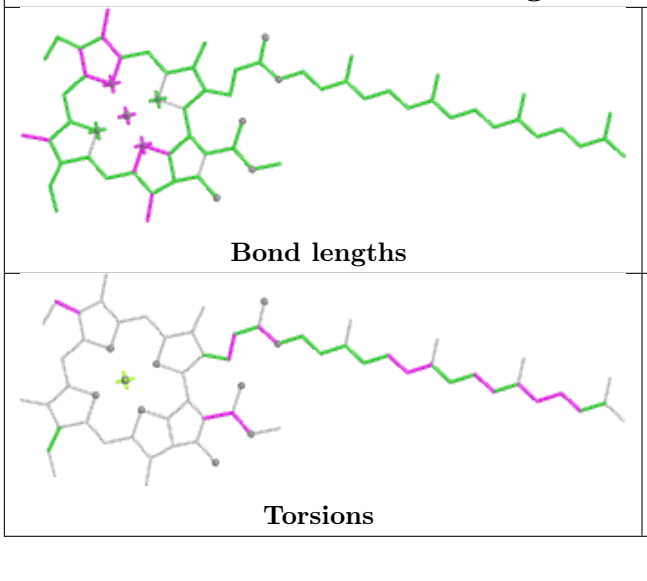


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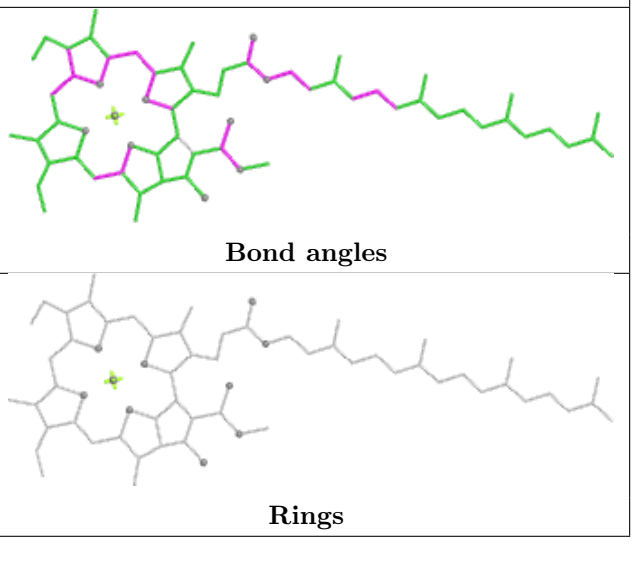


Rings

Ligand CLA C 503



Bond lengths

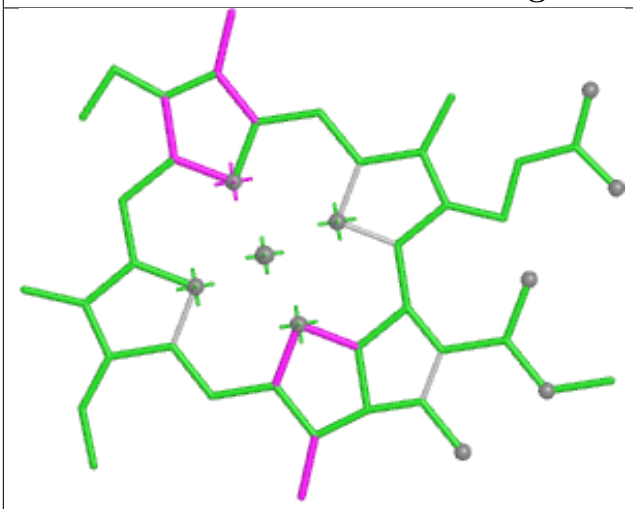


Bond angles

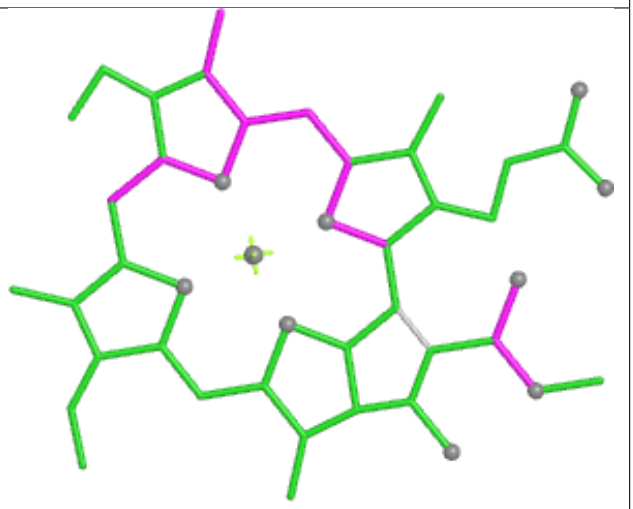
Torsions

Rings

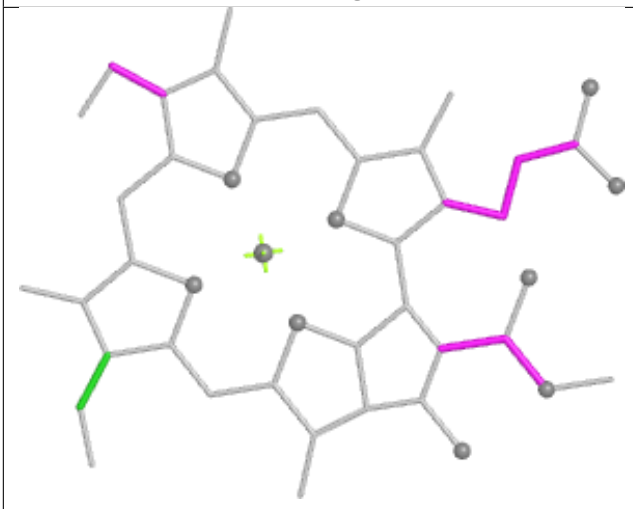
Ligand CLA 2 604



Bond lengths



Bond angles

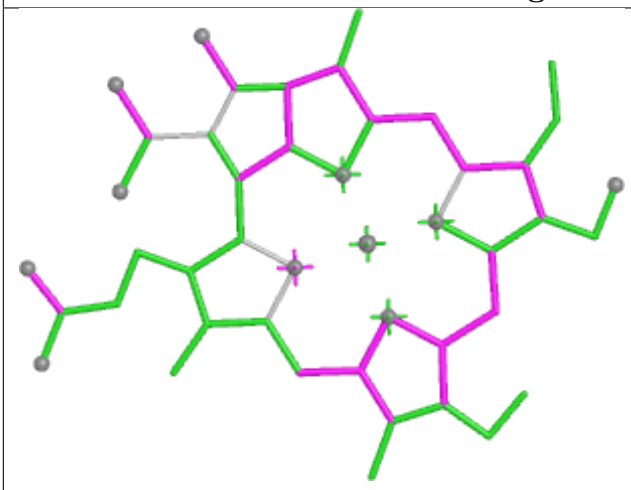


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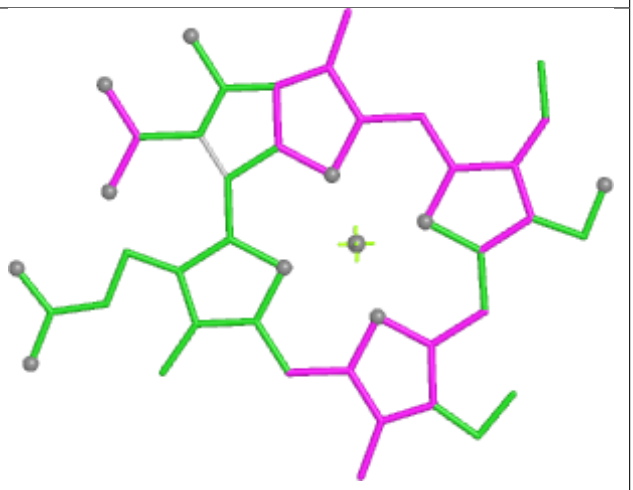


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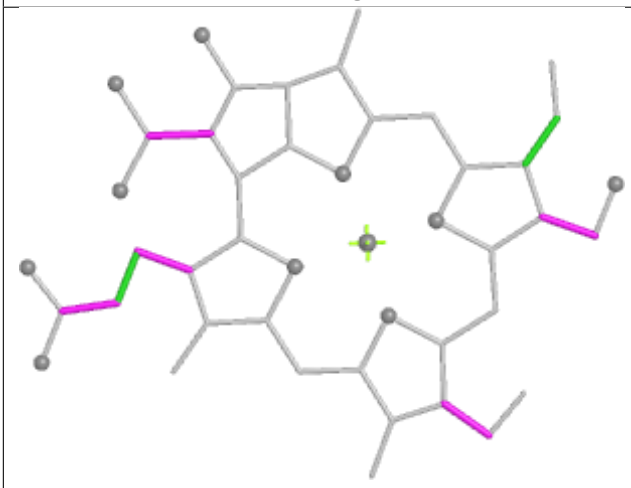
Ligand CHL 8 601



Bond lengths



Bond angles

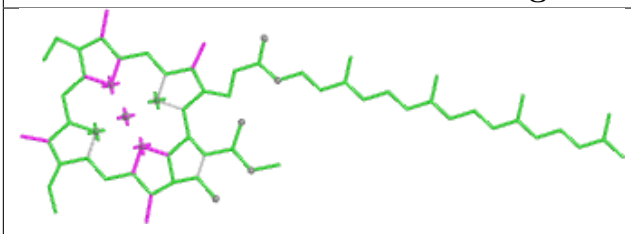


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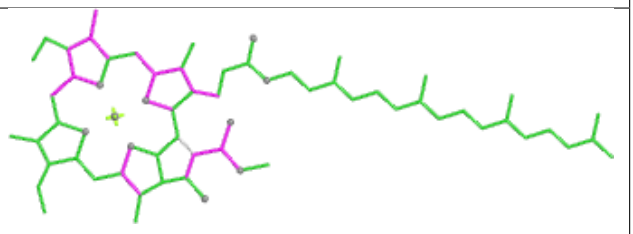


Rings

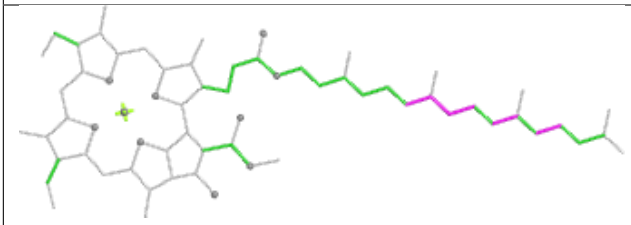
Ligand CLA c 509



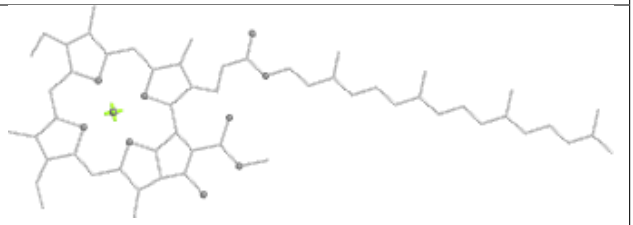
Bond lengths



Bond angles

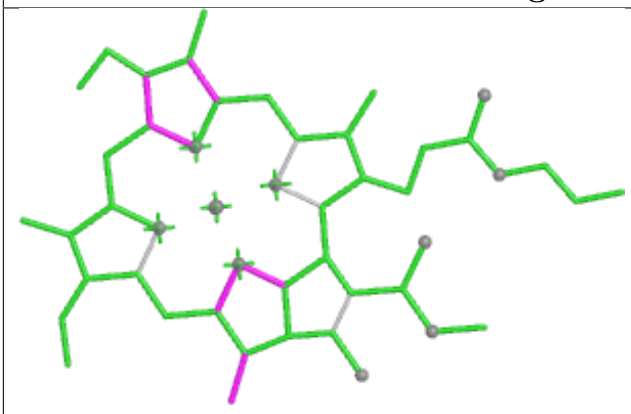


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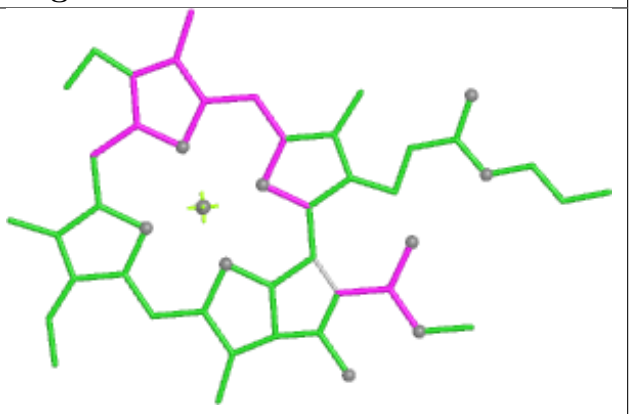


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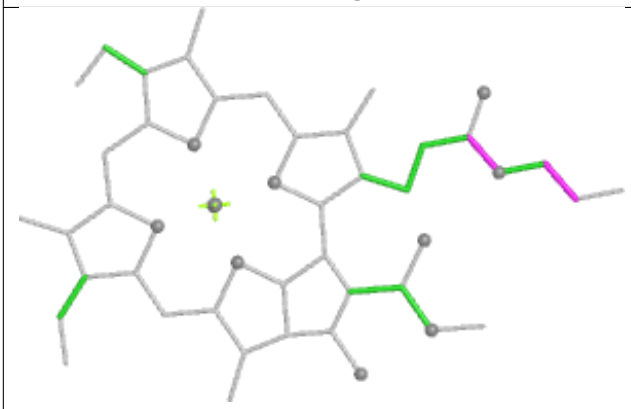
Ligand CLA g 614



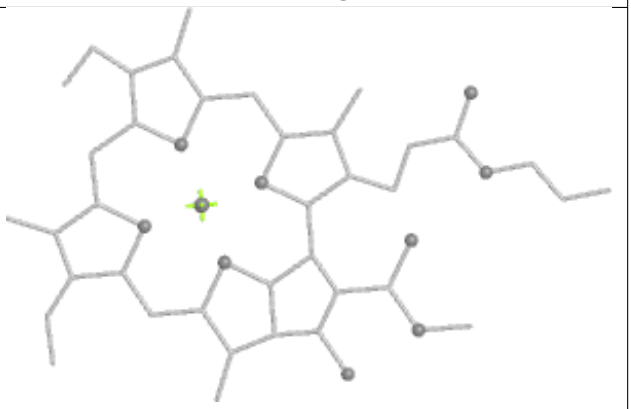
Bond lengths



Bond angles

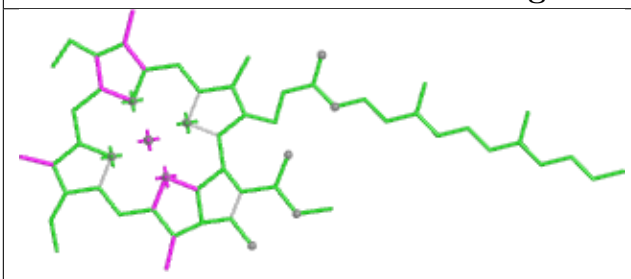


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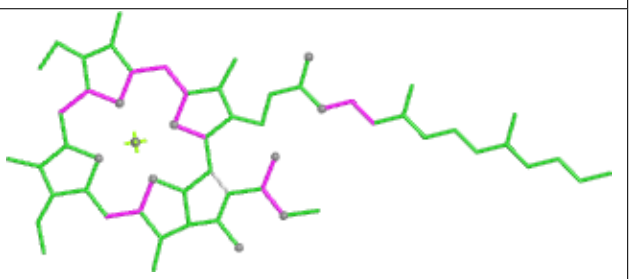


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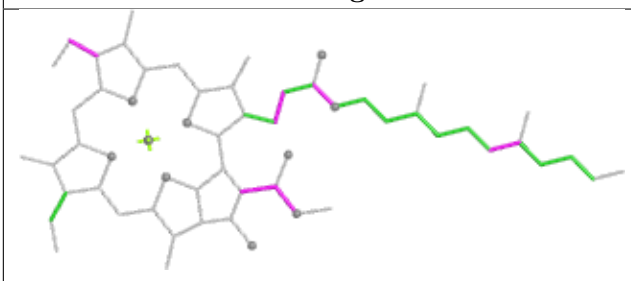
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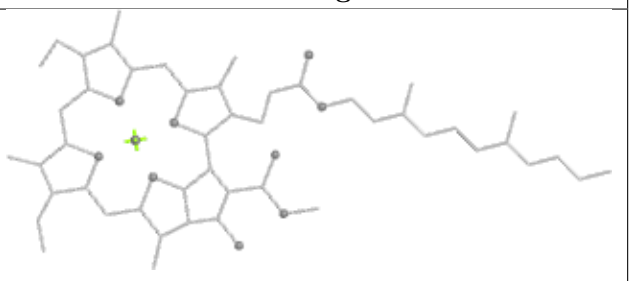
Bond lengths



Bond angles

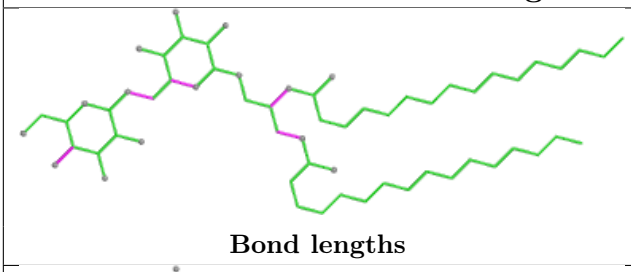


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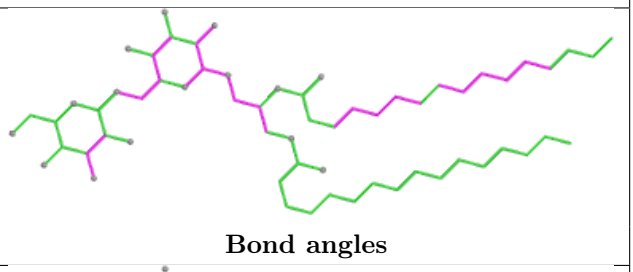


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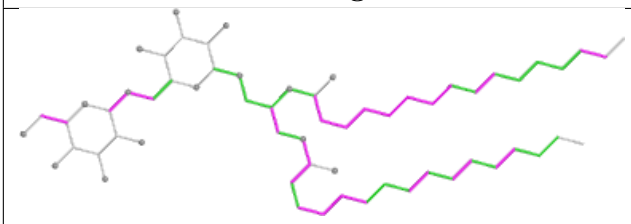
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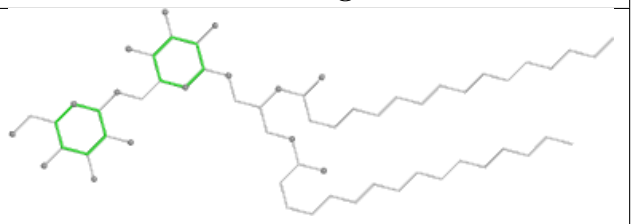
Bond lengths



Bond angles

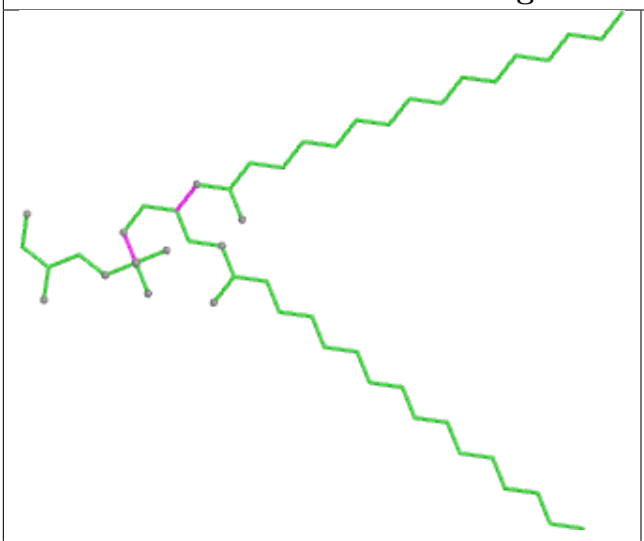


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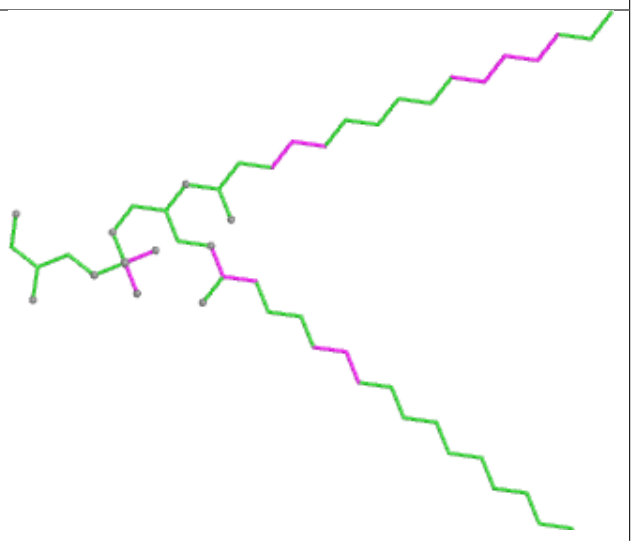


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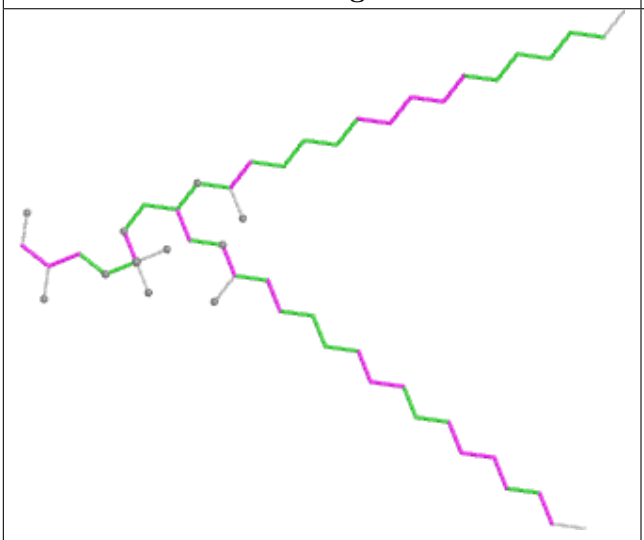
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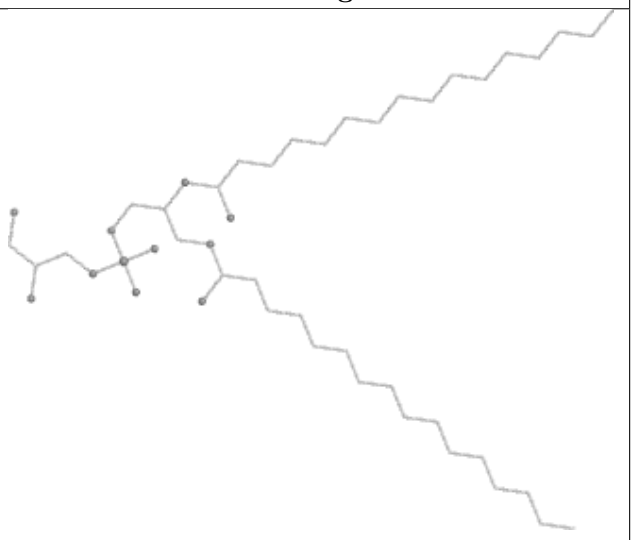
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Bond angles

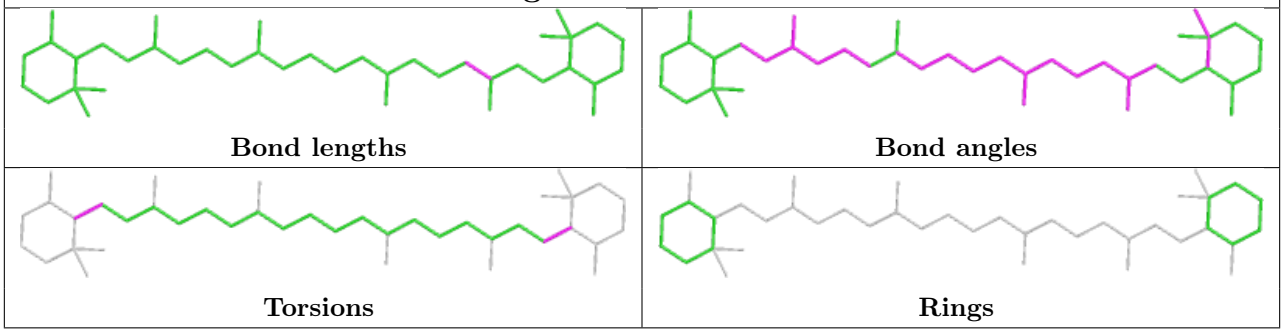


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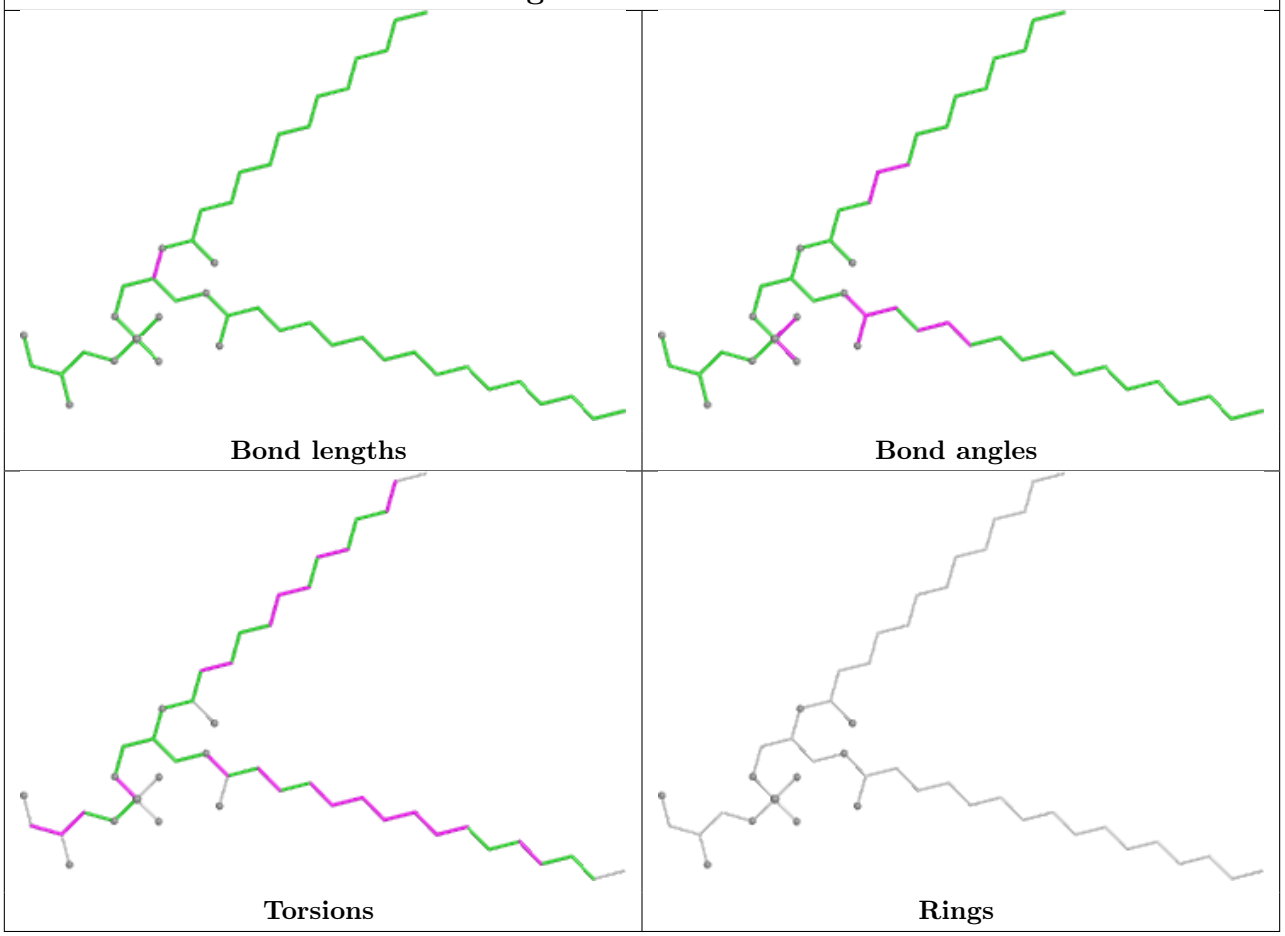


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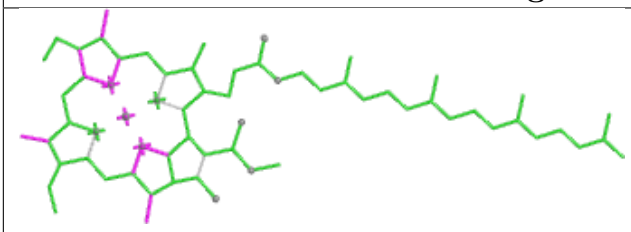
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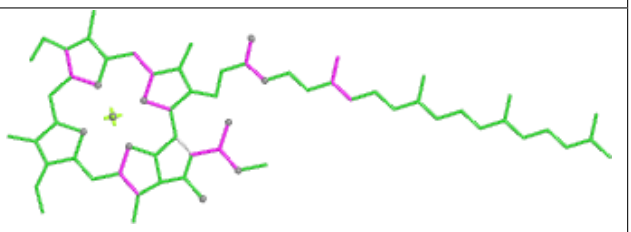
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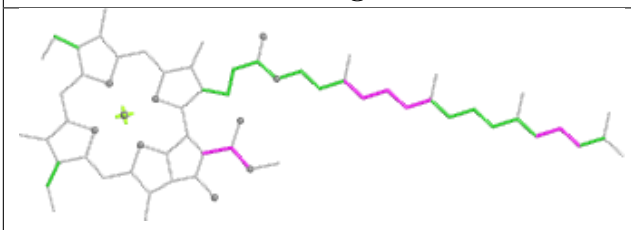
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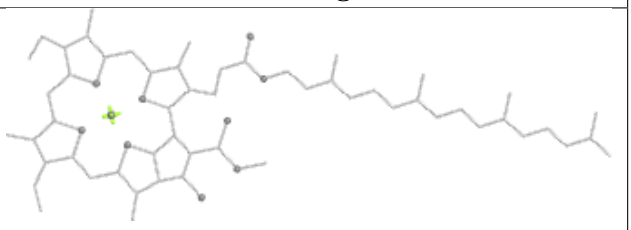
Bond lengths



Bond angles

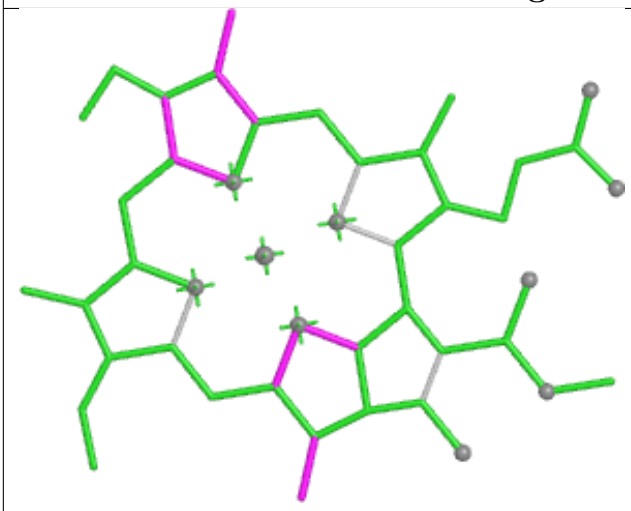


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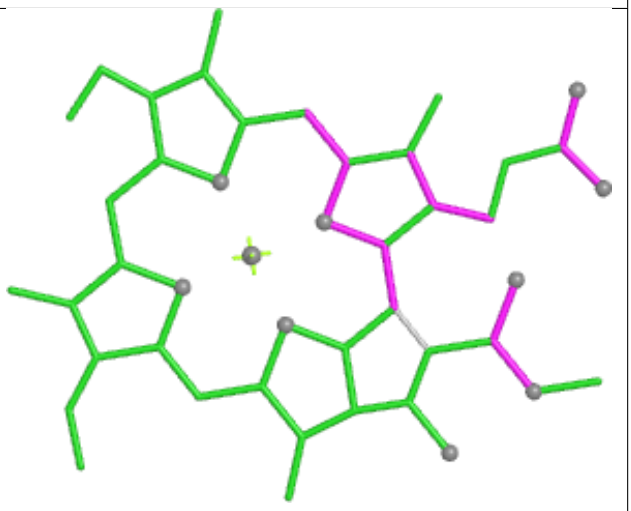


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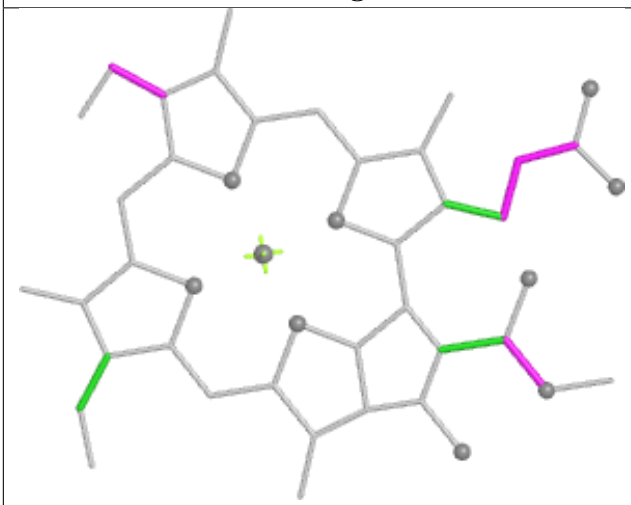
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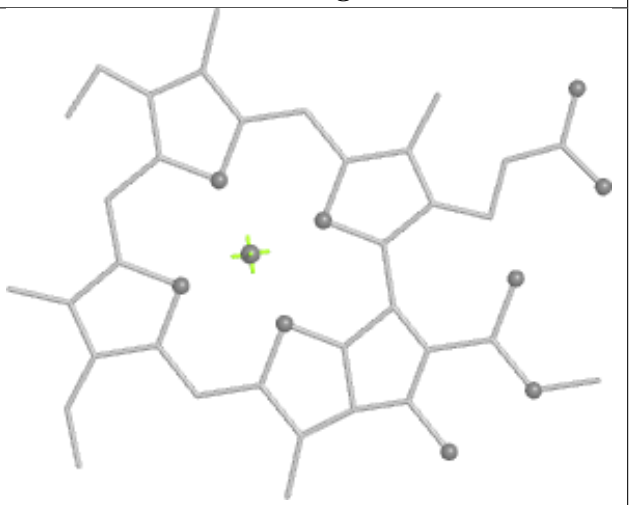
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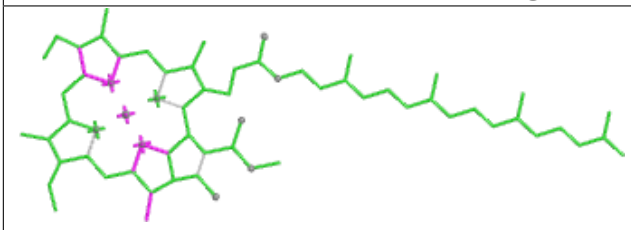


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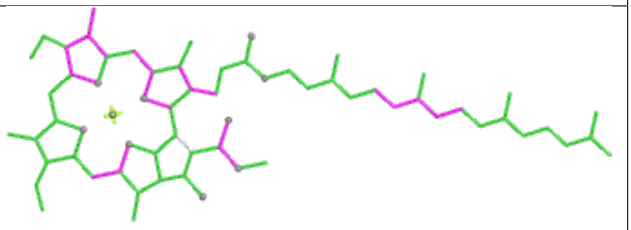


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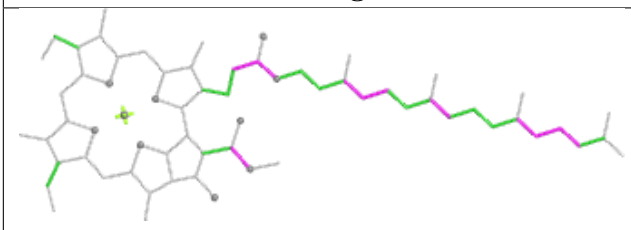
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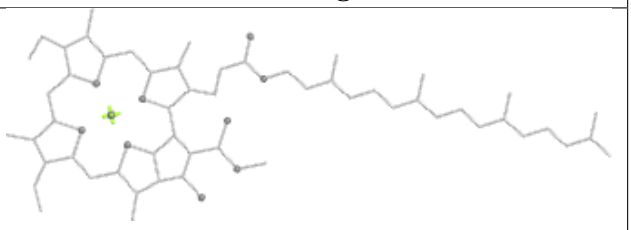
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Bond angles

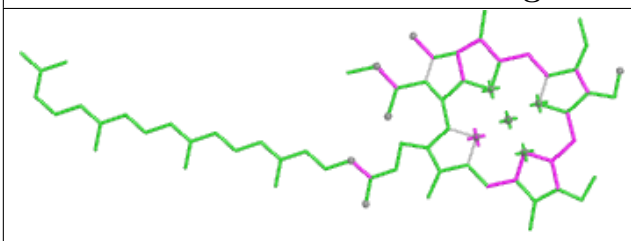


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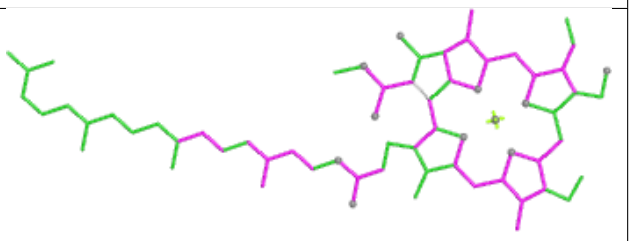


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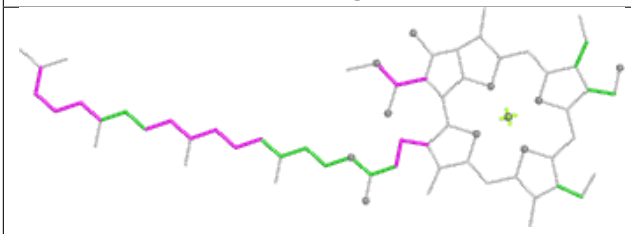
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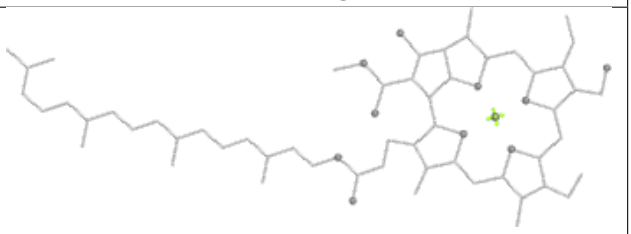
Bond lengths



Bond angles

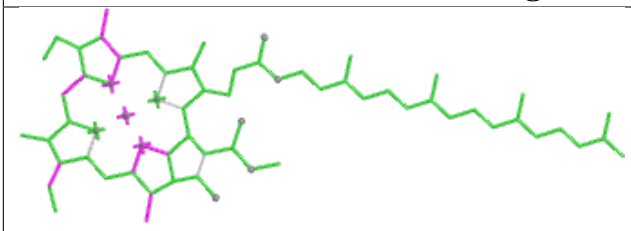


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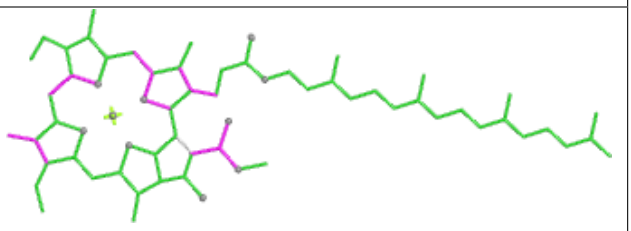


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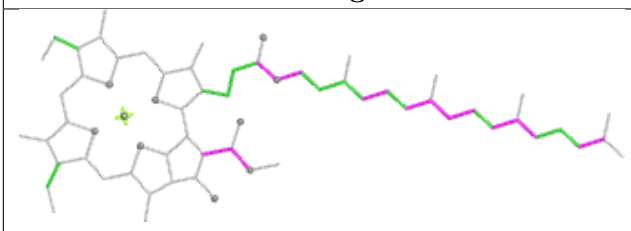
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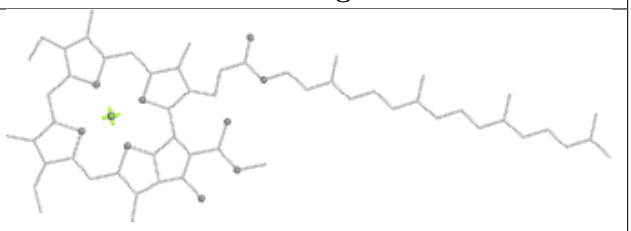
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Bond angles

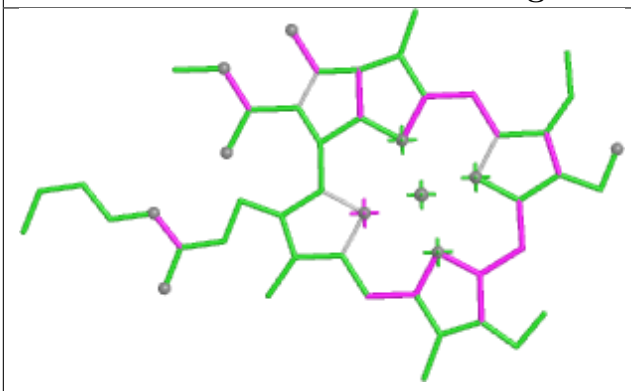


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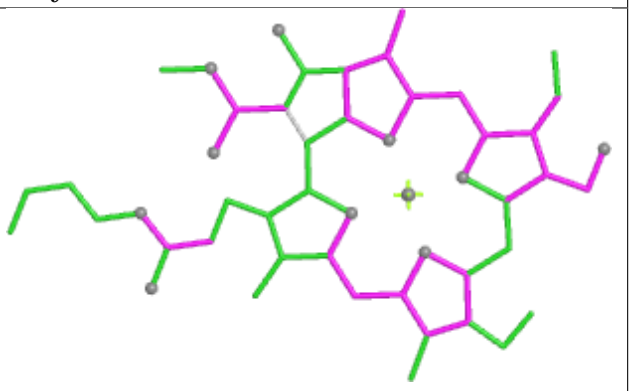


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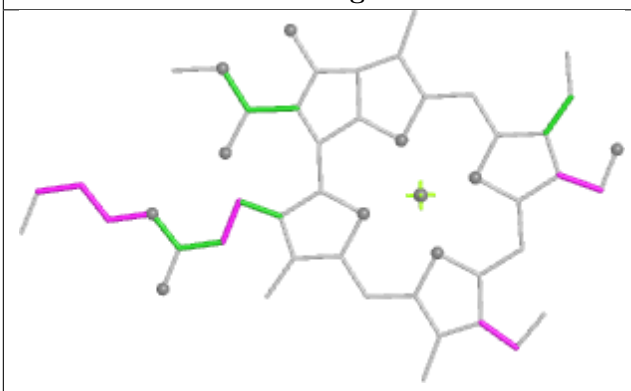
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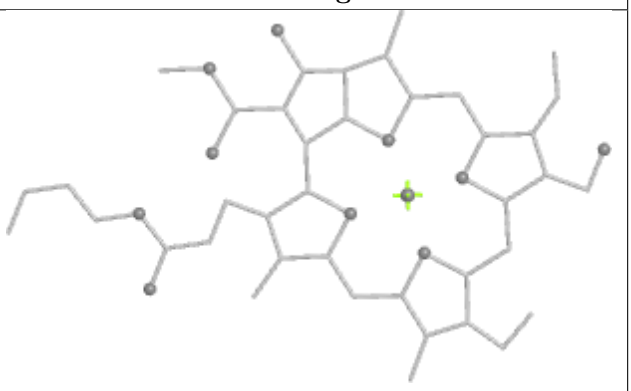
Bond lengths



Bond angles

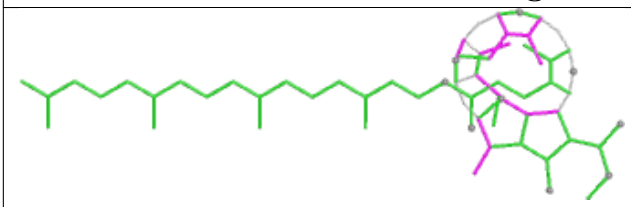


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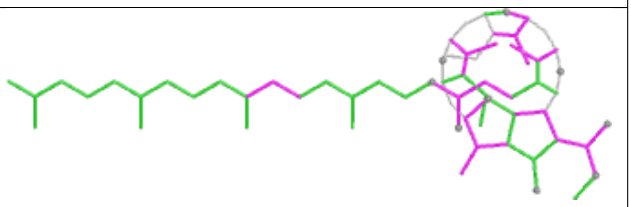


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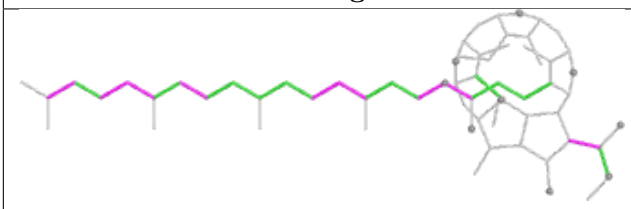
Ligand PHO a 408



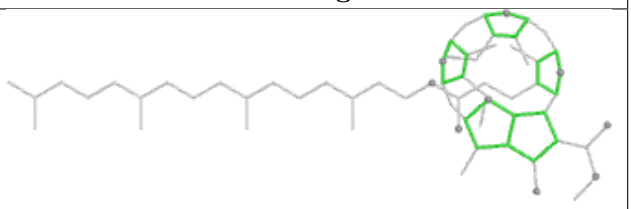
Bond lengths



Bond angles

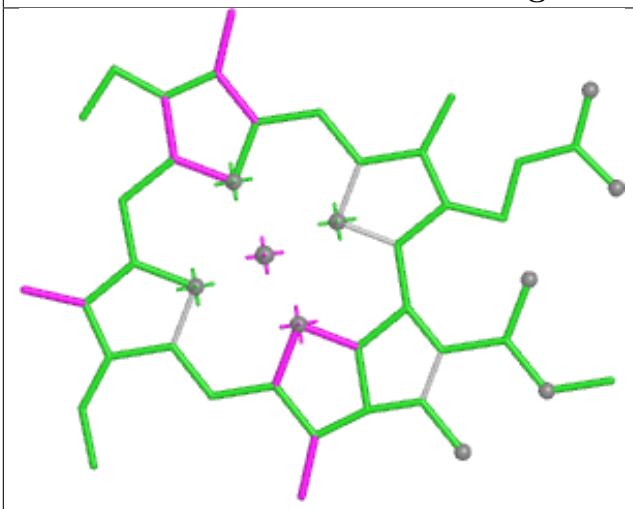


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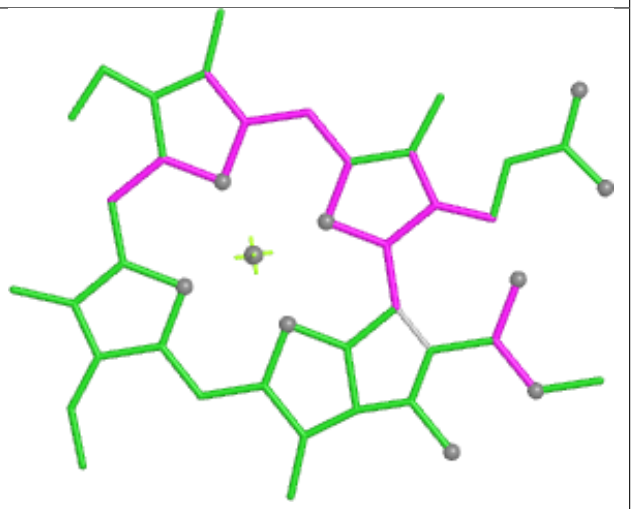


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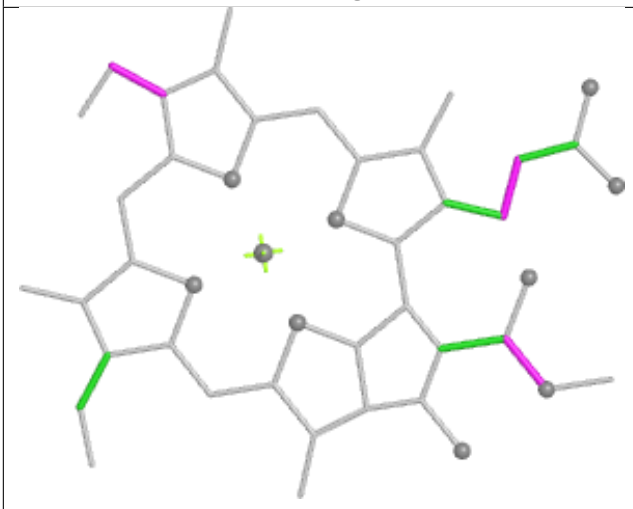
Ligand CLA 5 612



Bond lengths



Bond angles

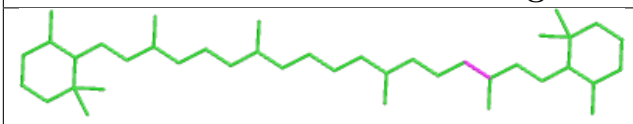


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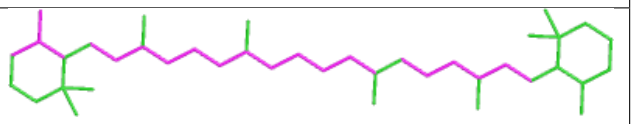


Rings

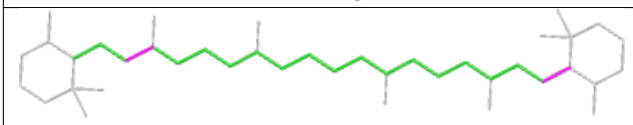
Ligand BCR c 517



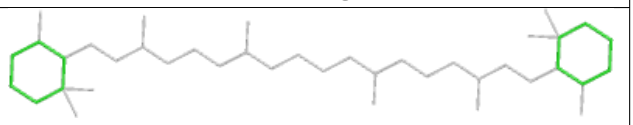
Bond lengths



Bond angles

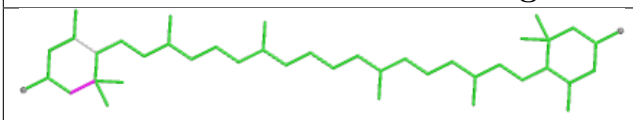


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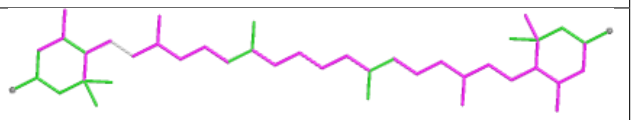


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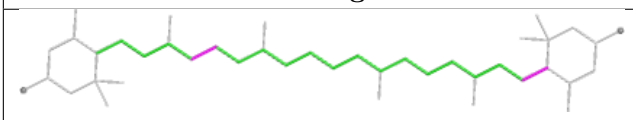
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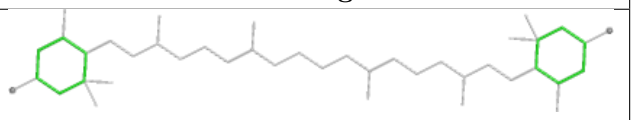
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Bond angles

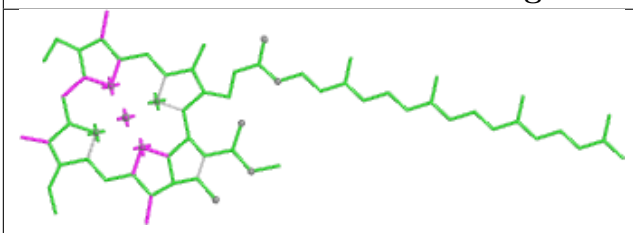


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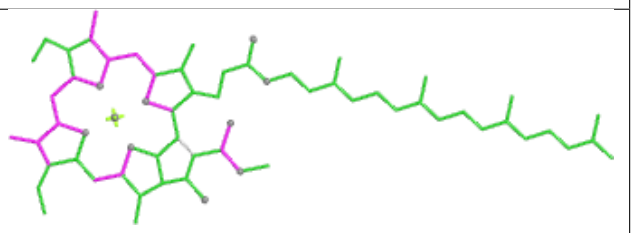


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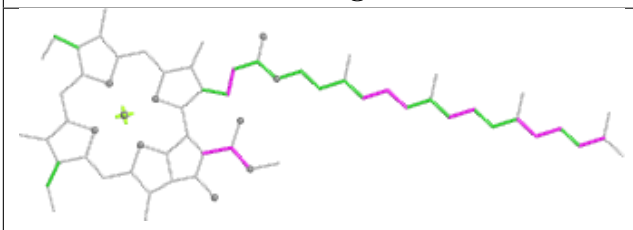
Ligand CLA B 608



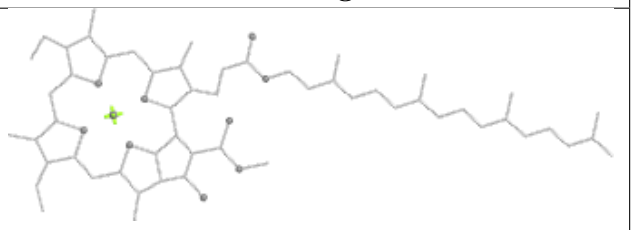
Bond lengths



Bond angles

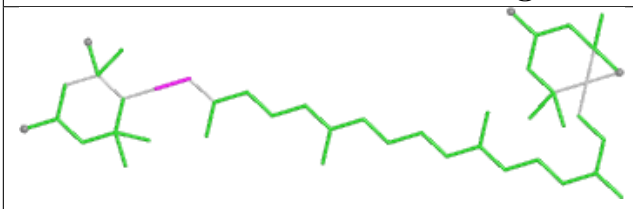


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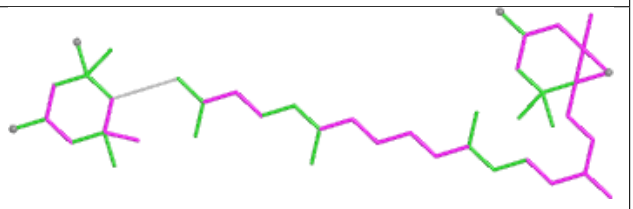


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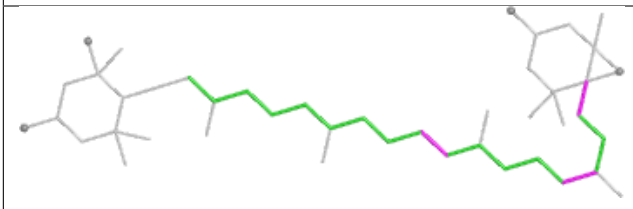
Ligand NEX n 1623



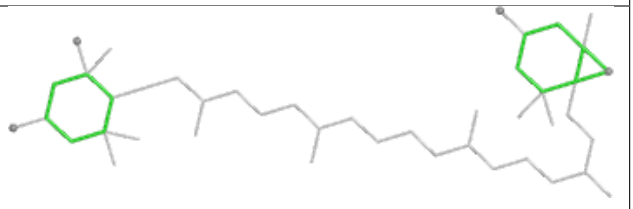
Bond lengths



Bond angles

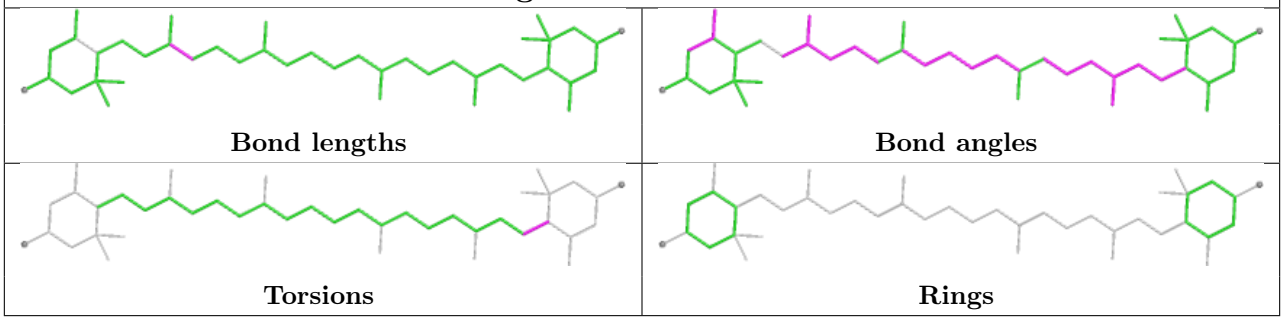


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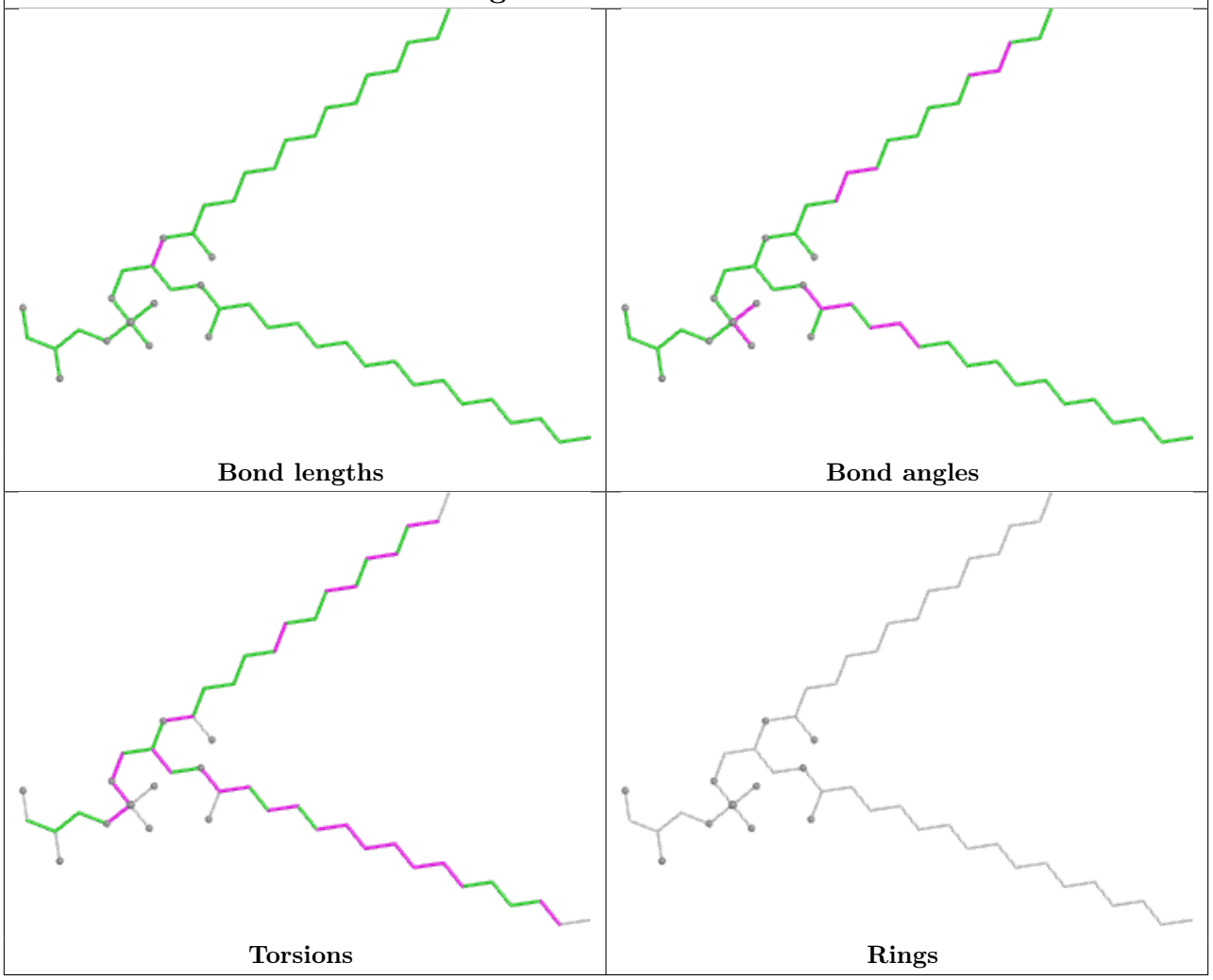


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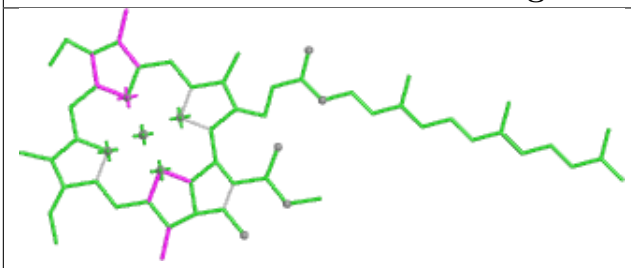
Ligand LUT Y 1620



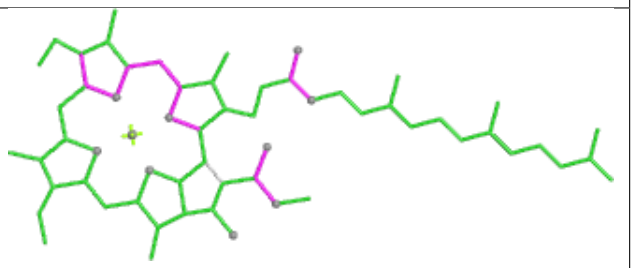
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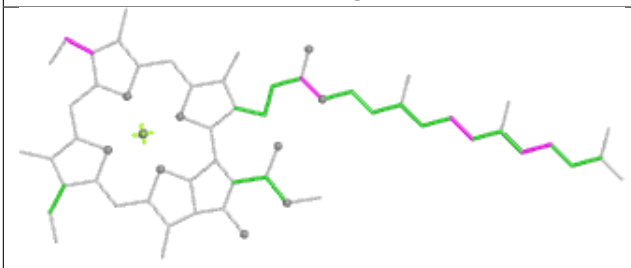
Ligand CLA n 611



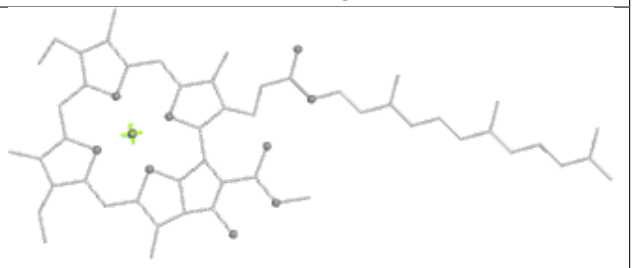
Bond lengths



Bond angles

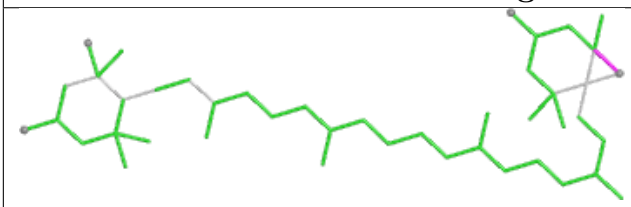


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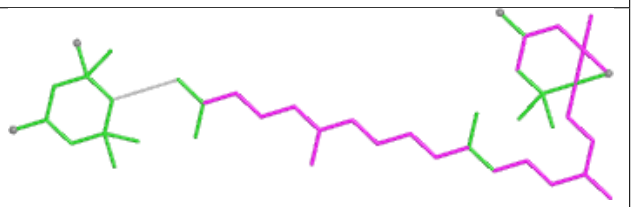


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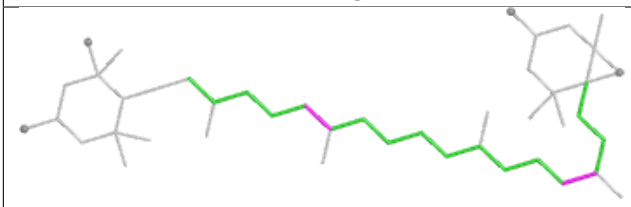
Ligand NEX 3 1623



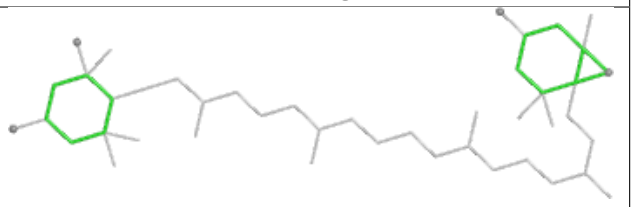
Bond lengths



Bond angles

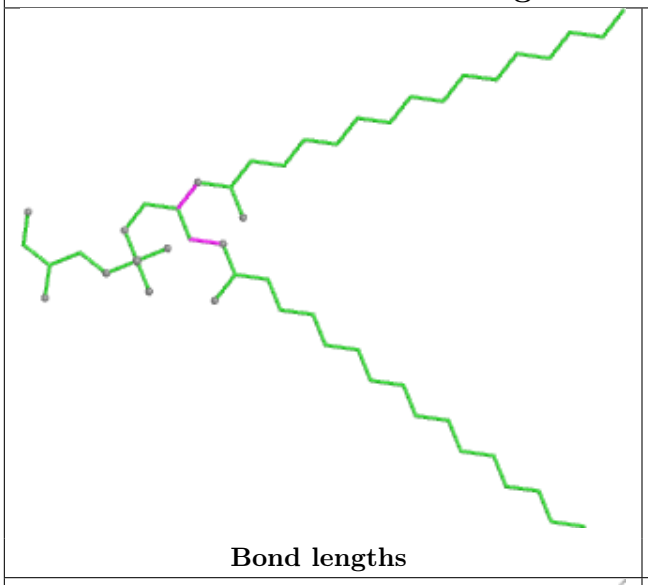


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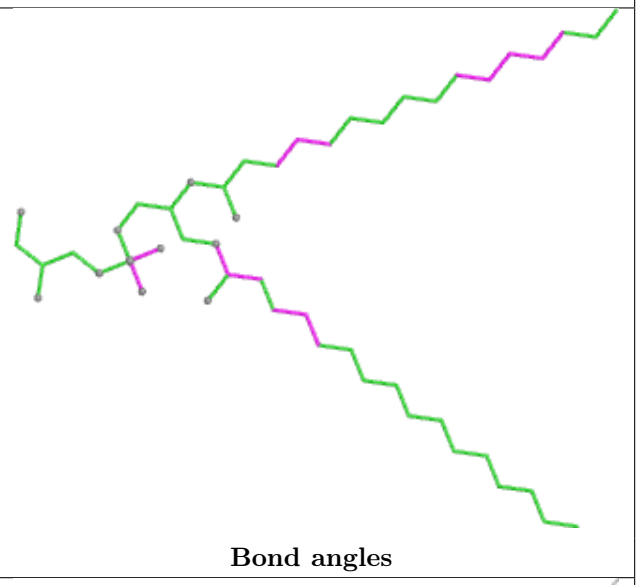


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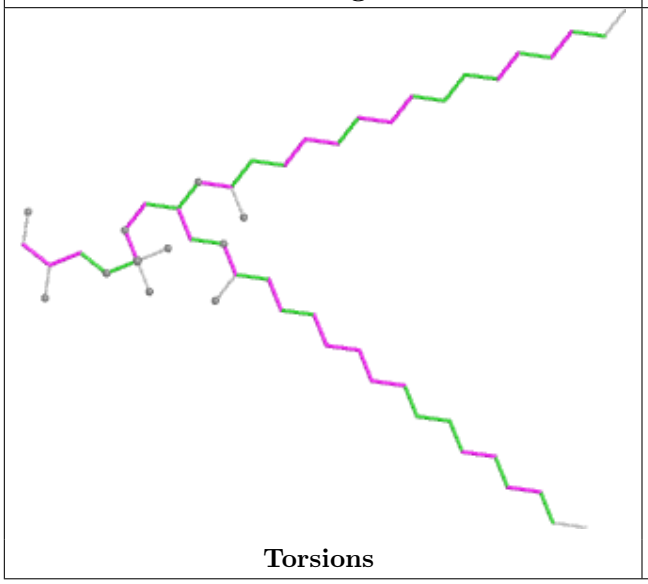
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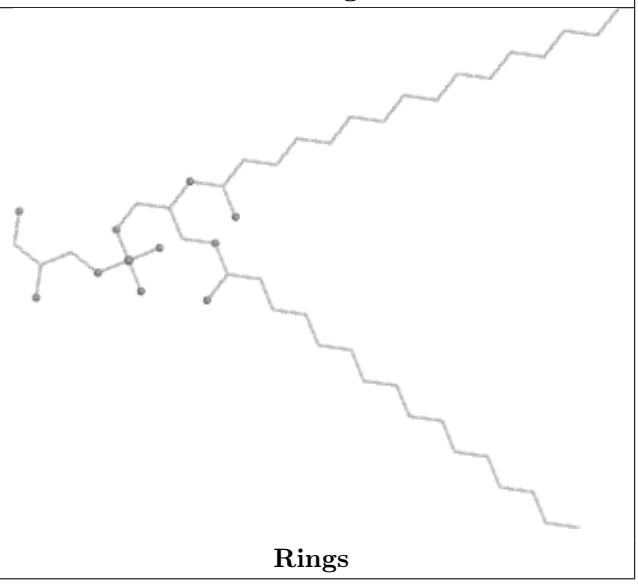
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Bond angles

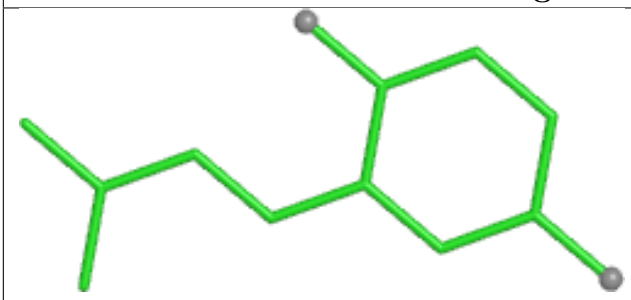


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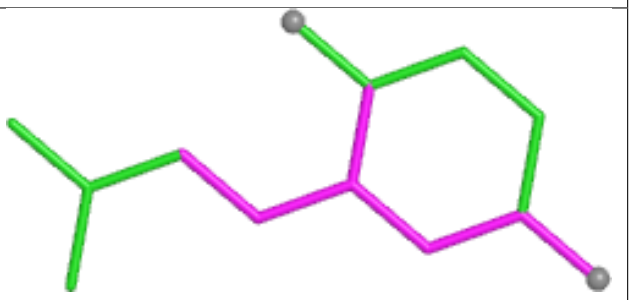


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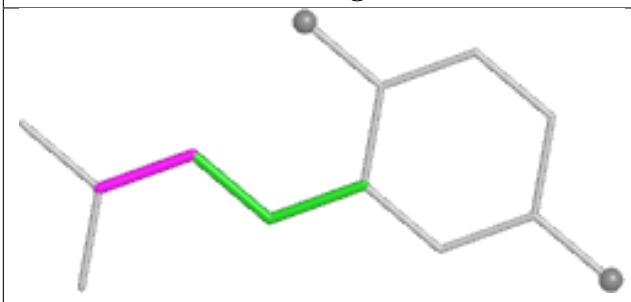
Ligand PL9 a 414



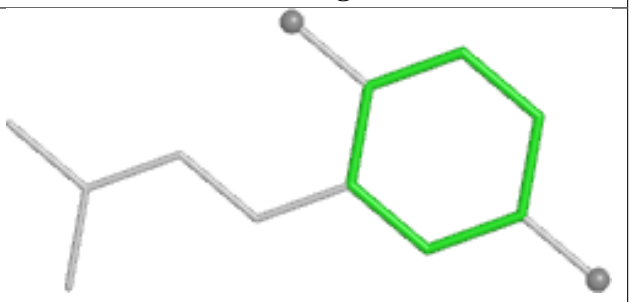
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Bond angles

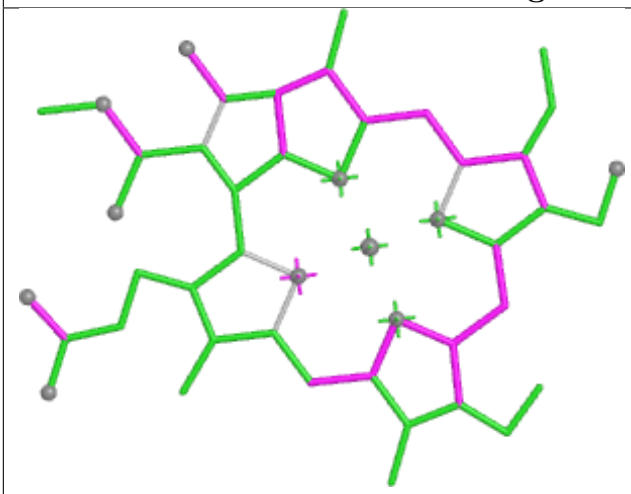


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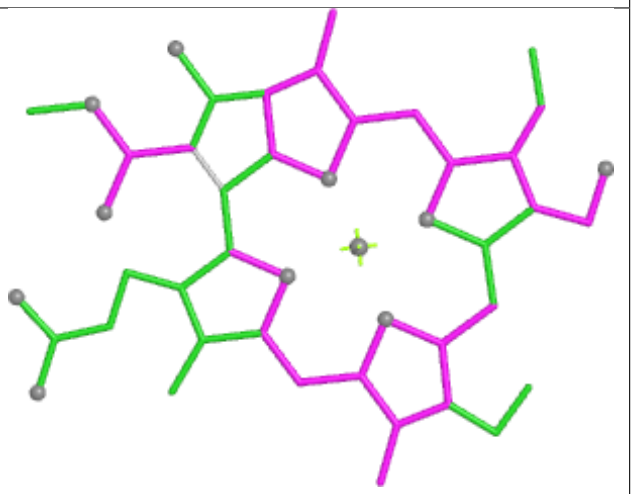


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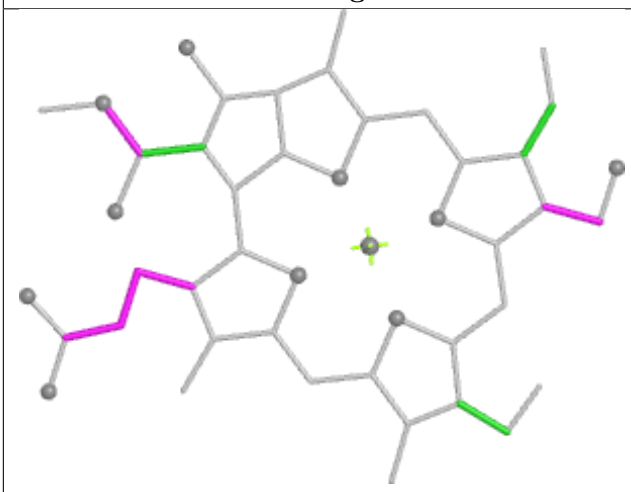
Ligand CHL 3 606



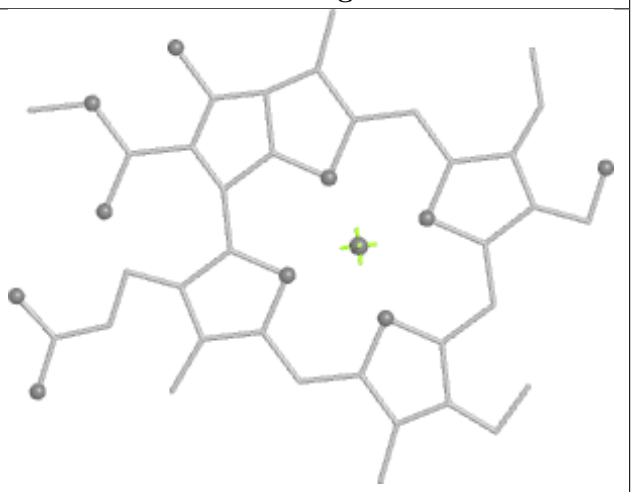
Bond lengths



Bond angles

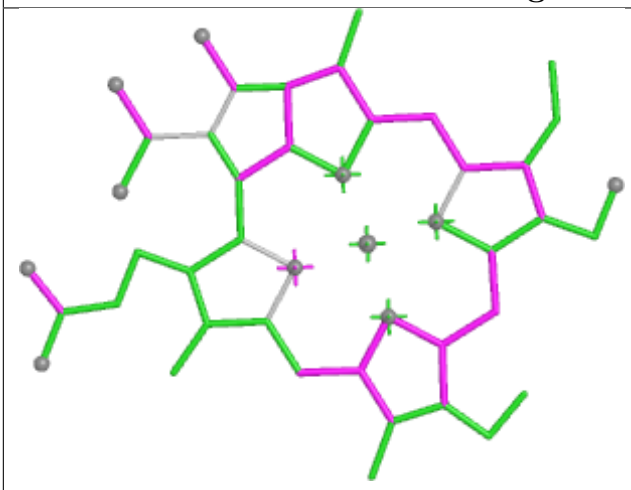


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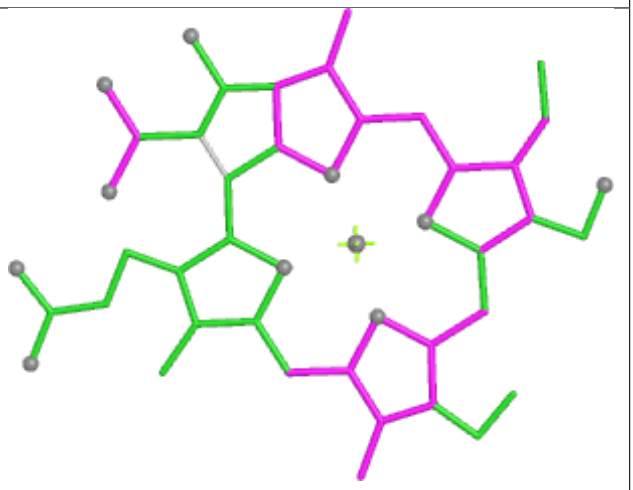


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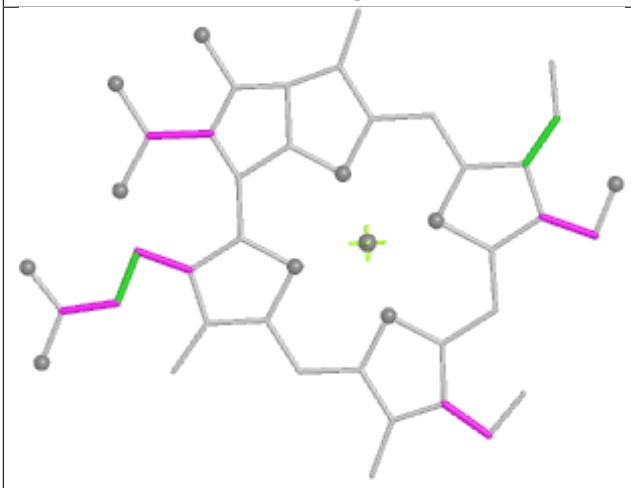
Ligand CHL 4 601



Bond lengths



Bond angles

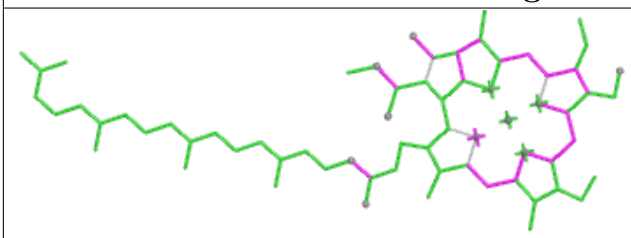


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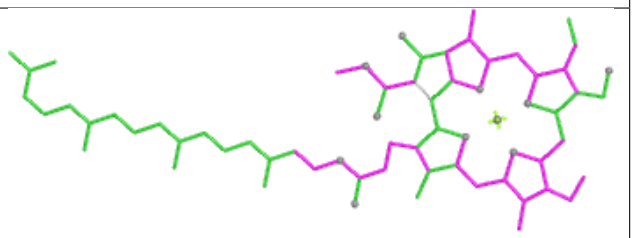


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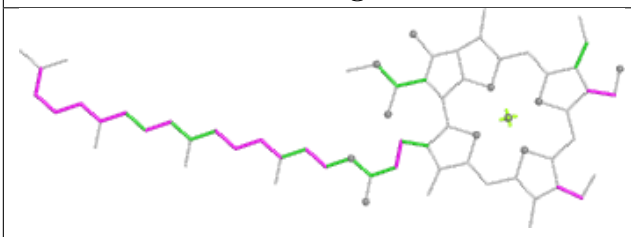
Ligand CHL Y 607



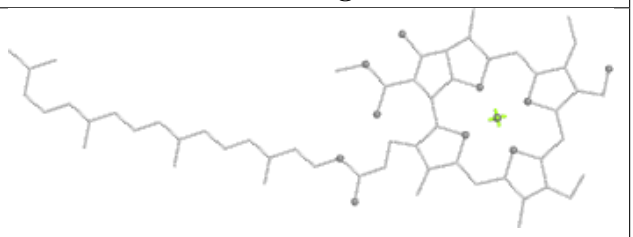
Bond lengths



Bond angles

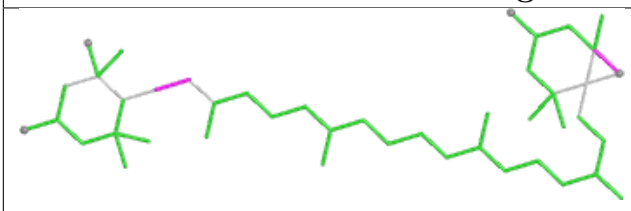


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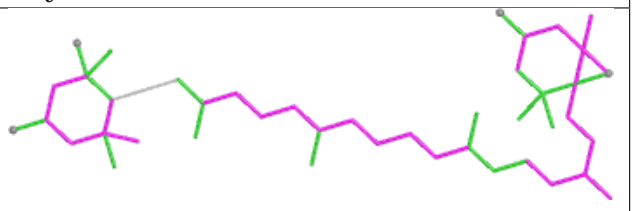


Rings

Ligand NEX y 1623



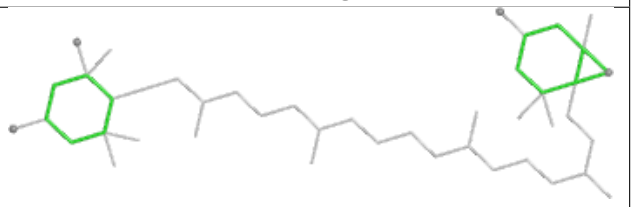
Bond lengths



Bond angles

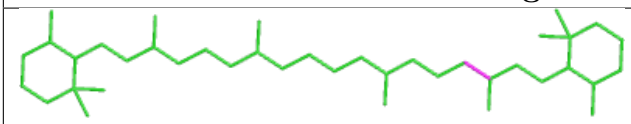


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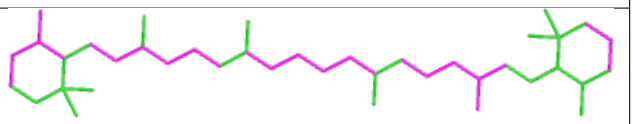


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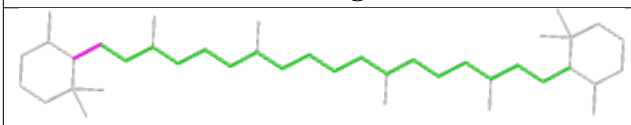
Ligand BCR B 618



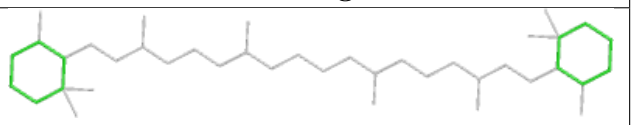
Bond lengths



Bond angles

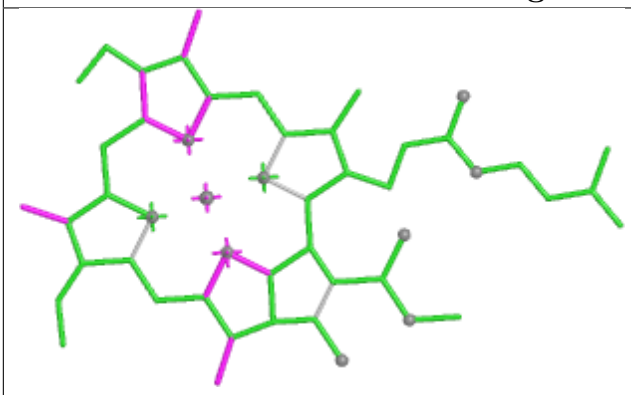


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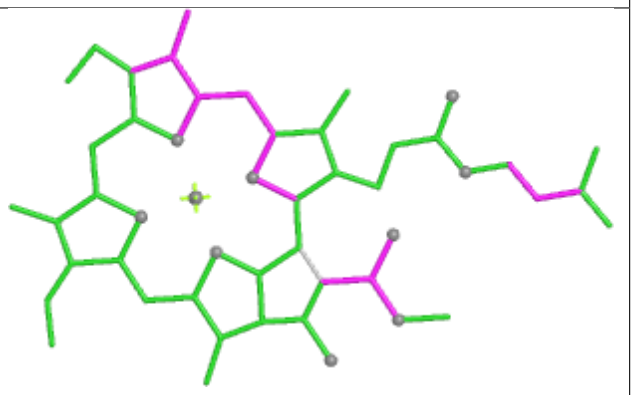


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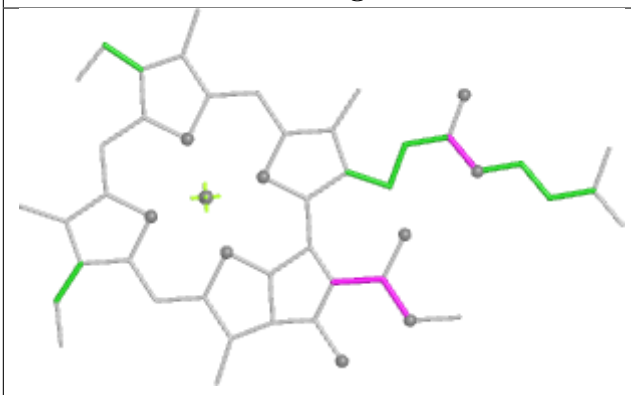
Ligand CLA n 604



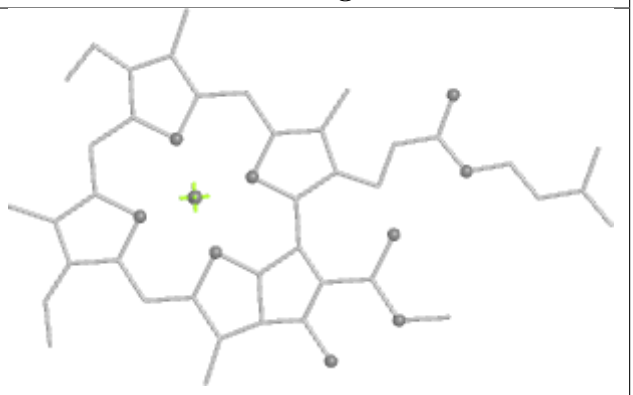
Bond lengths



Bond angles

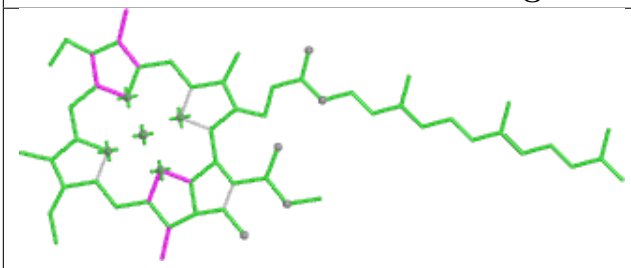


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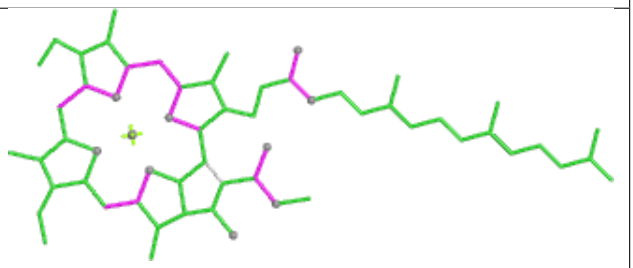


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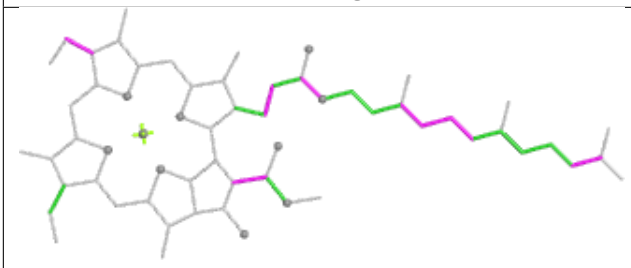
Ligand CLA R 613



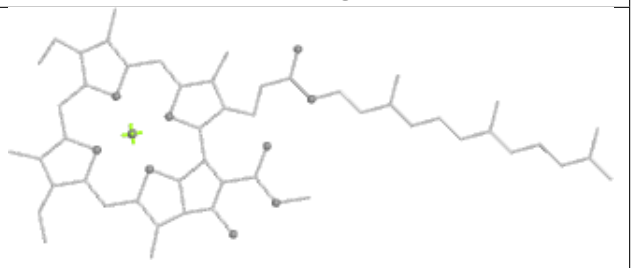
Bond lengths



Bond angles

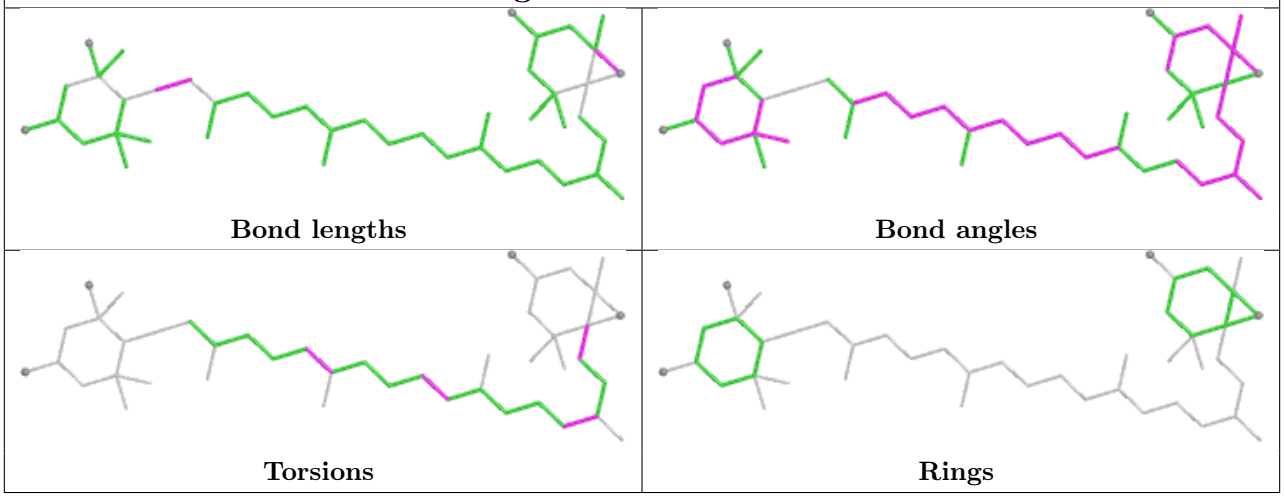


Torsions

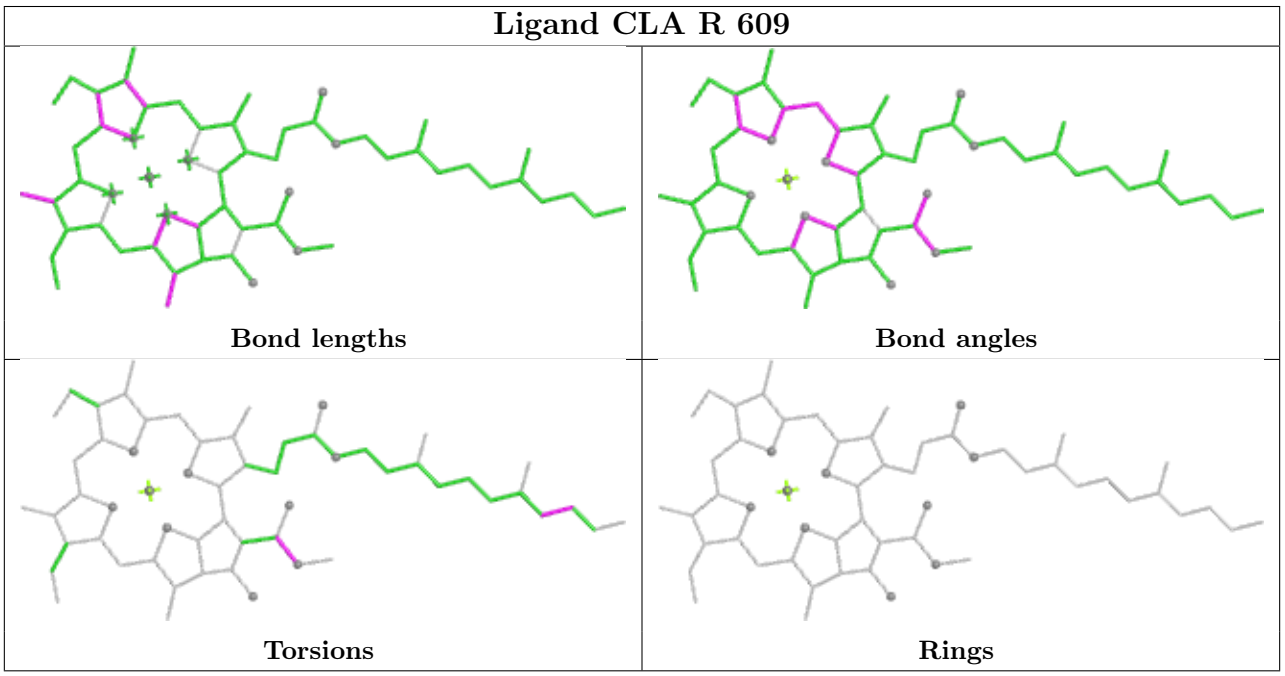


Rings

Ligand NEX Y 1623



Ligand CLA R 609



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.

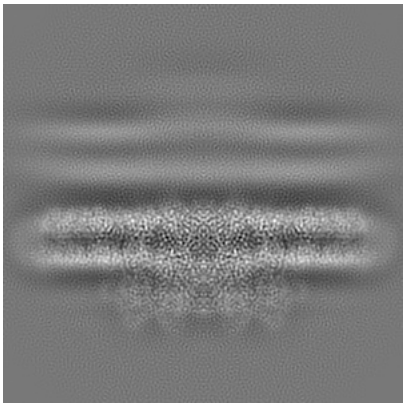
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-6741. These allow visual inspection of the internal detail of the map and identification of artifacts.

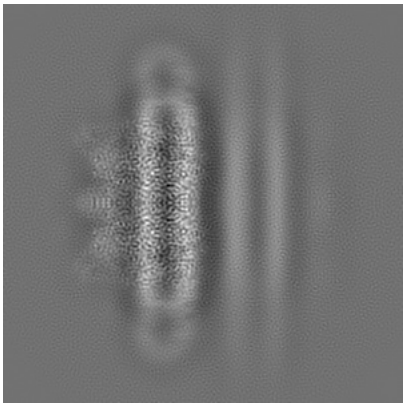
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

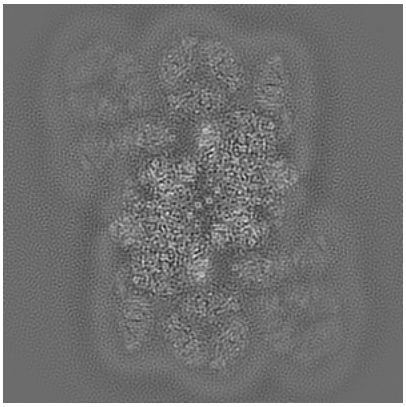
6.1.1 Primary map



X



Y

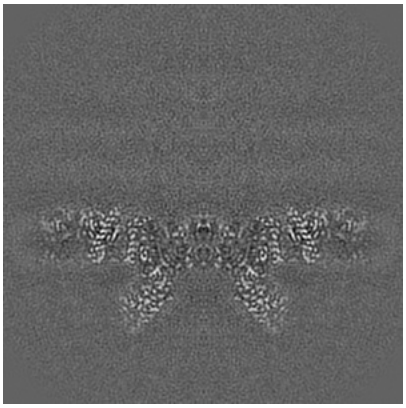


Z

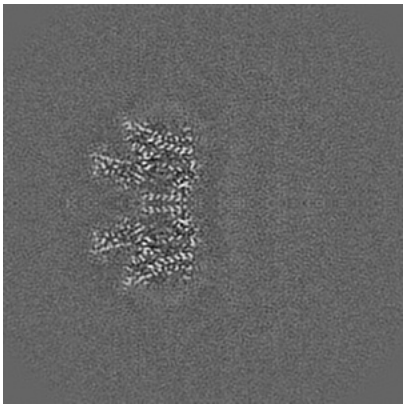
The images above show the map projected in three orthogonal directions.

6.2 Central slices

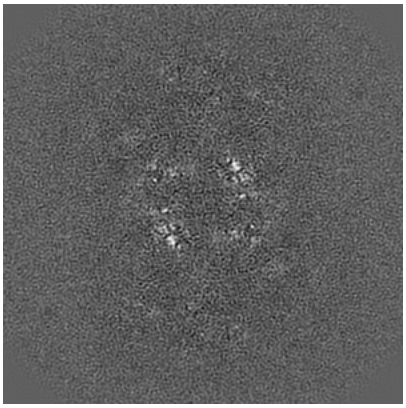
6.2.1 Primary map



X Index: 150



Y Index: 150

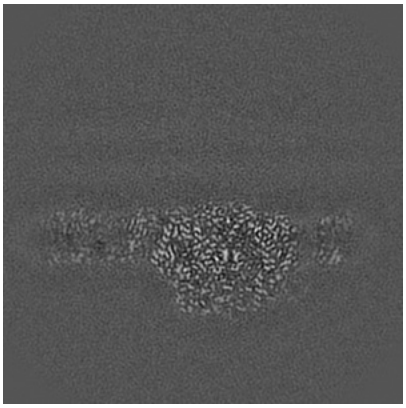


Z Index: 150

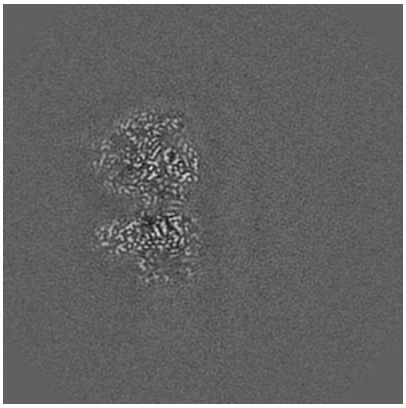
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

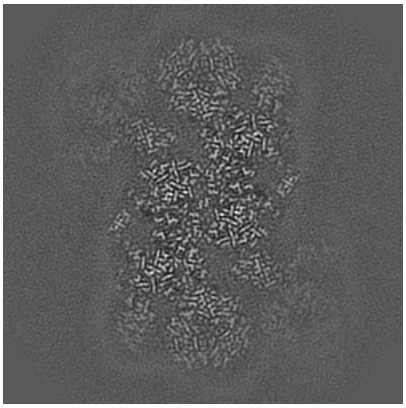
6.3.1 Primary map



X Index: 178



Y Index: 162

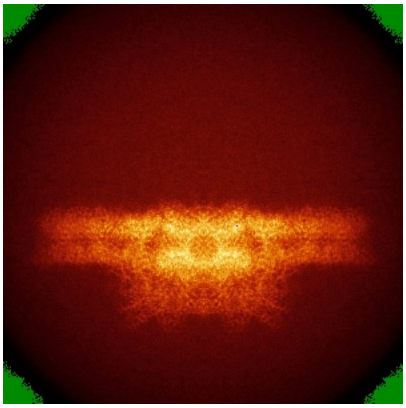


Z Index: 130

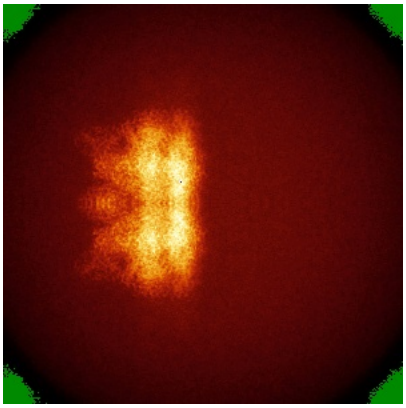
The images above show the largest variance slices of the map in three orthogonal directions.

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

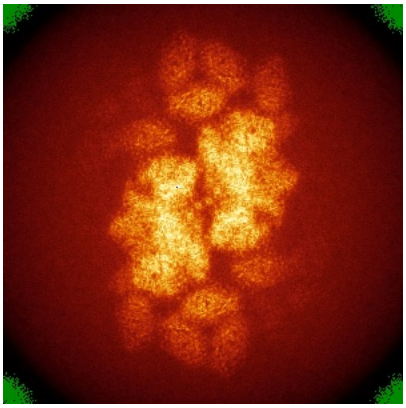
6.4.1 Primary map



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

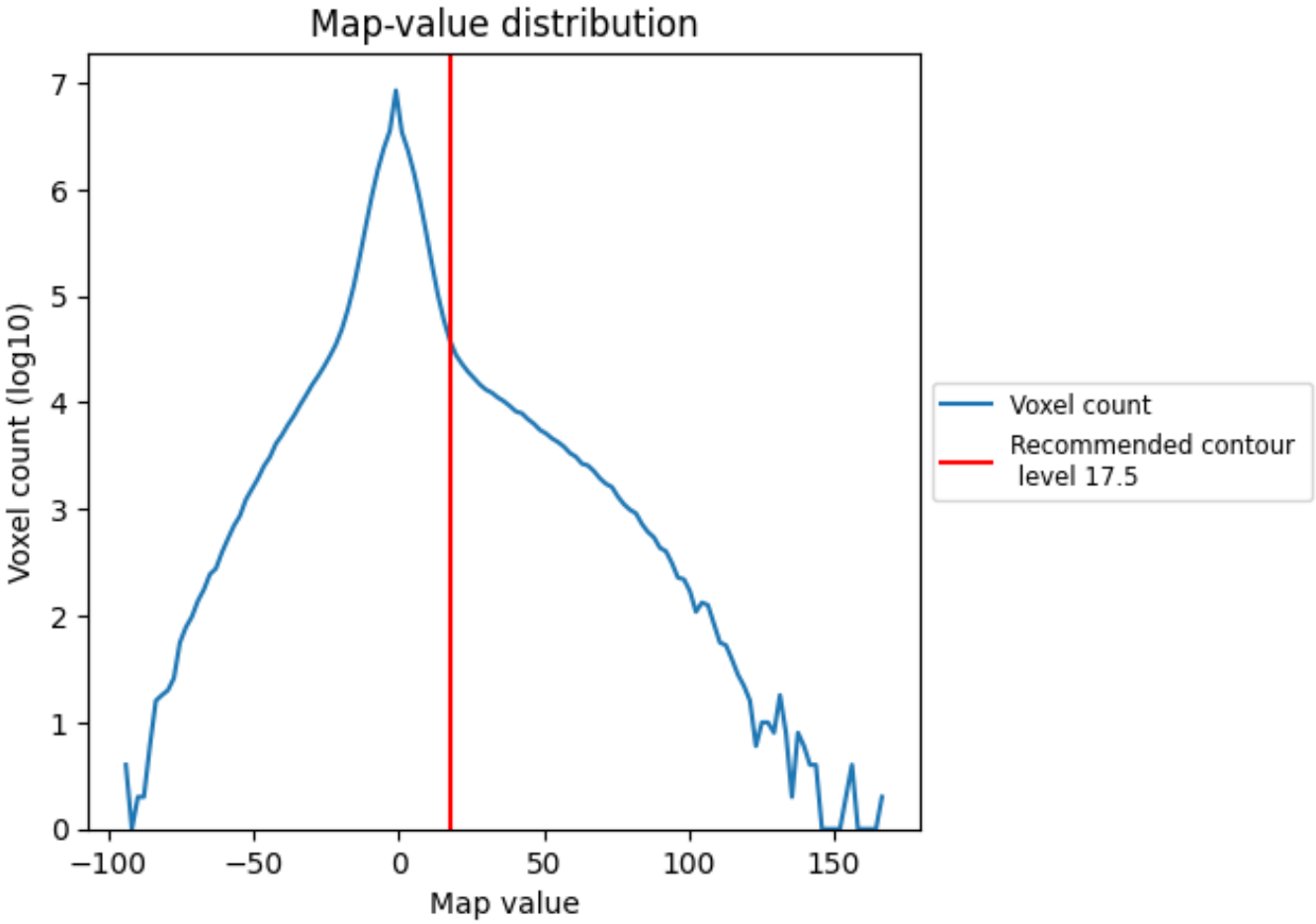
6.6 Mask visualisation (i)

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

7 Map analysis

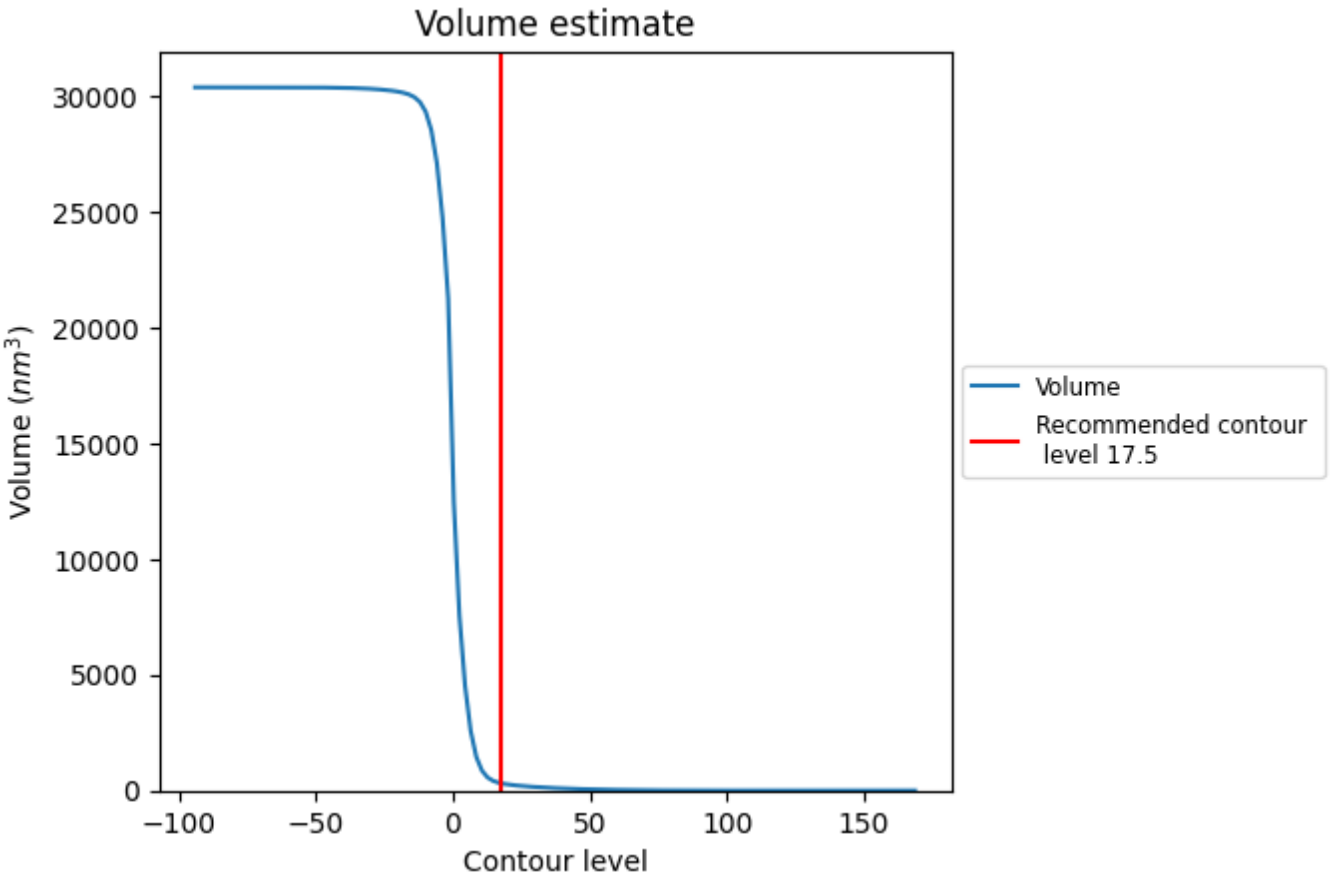
This section contains the results of statistical analysis of the map.

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.

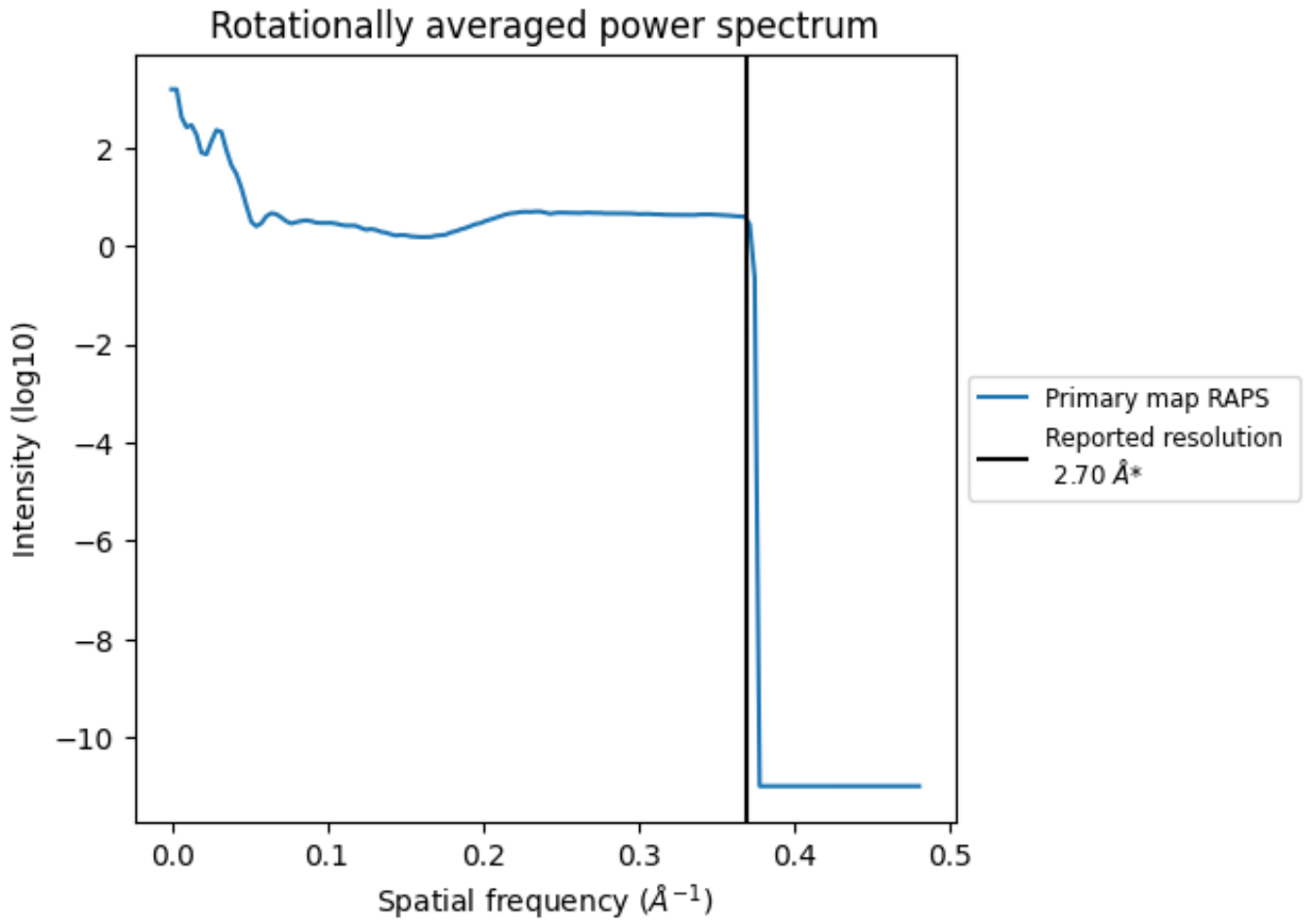
7.2 Volume estimate (i)



The volume at the recommended contour level is 319 nm^3; this corresponds to an approximate mass of 288 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 0.370 Å^{-1}

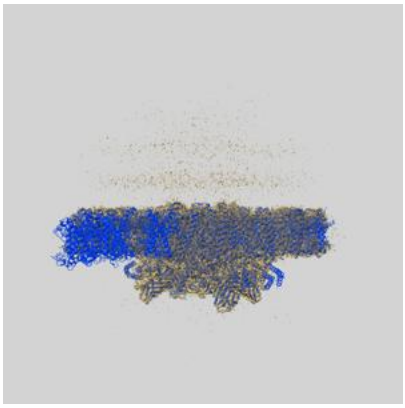
8 Fourier-Shell correlation (i)

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

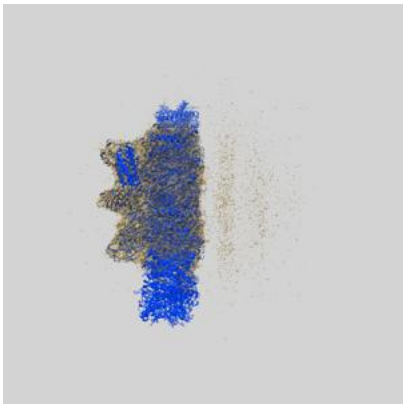
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-6741 and PDB model 5XNL. Per-residue inclusion information can be found in section 3 on page 46.

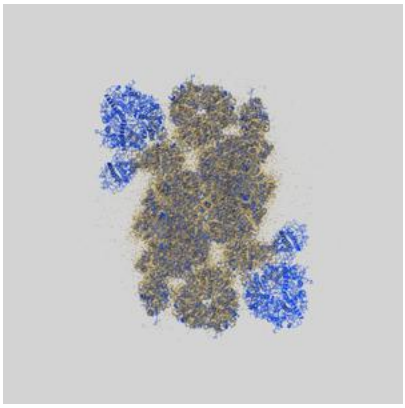
9.1 Map-model overlay



X



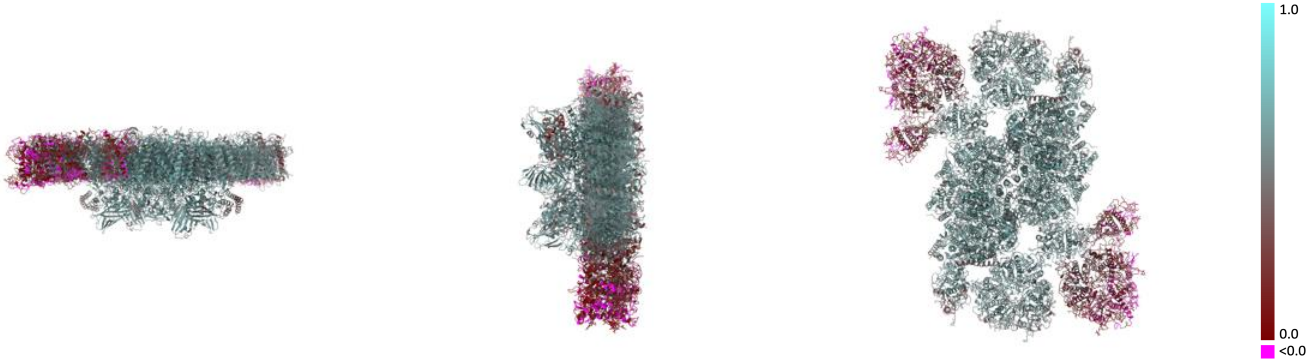
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 17.5 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.

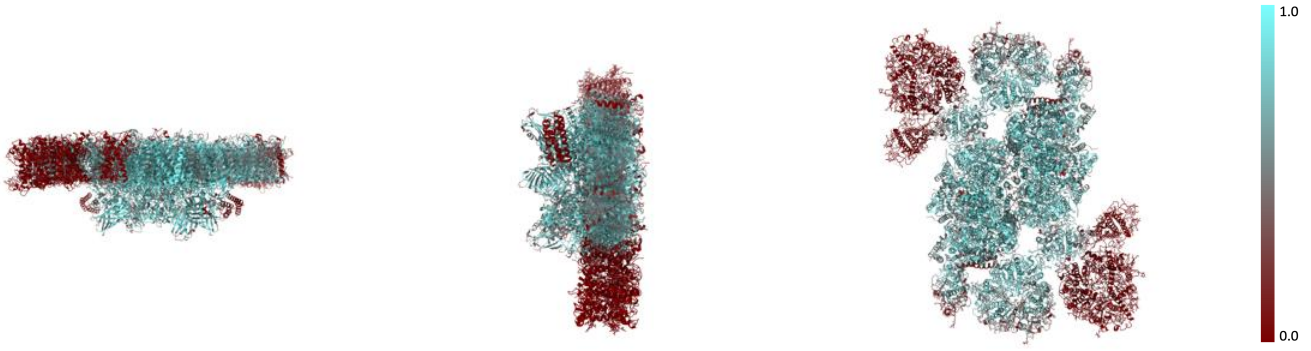
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

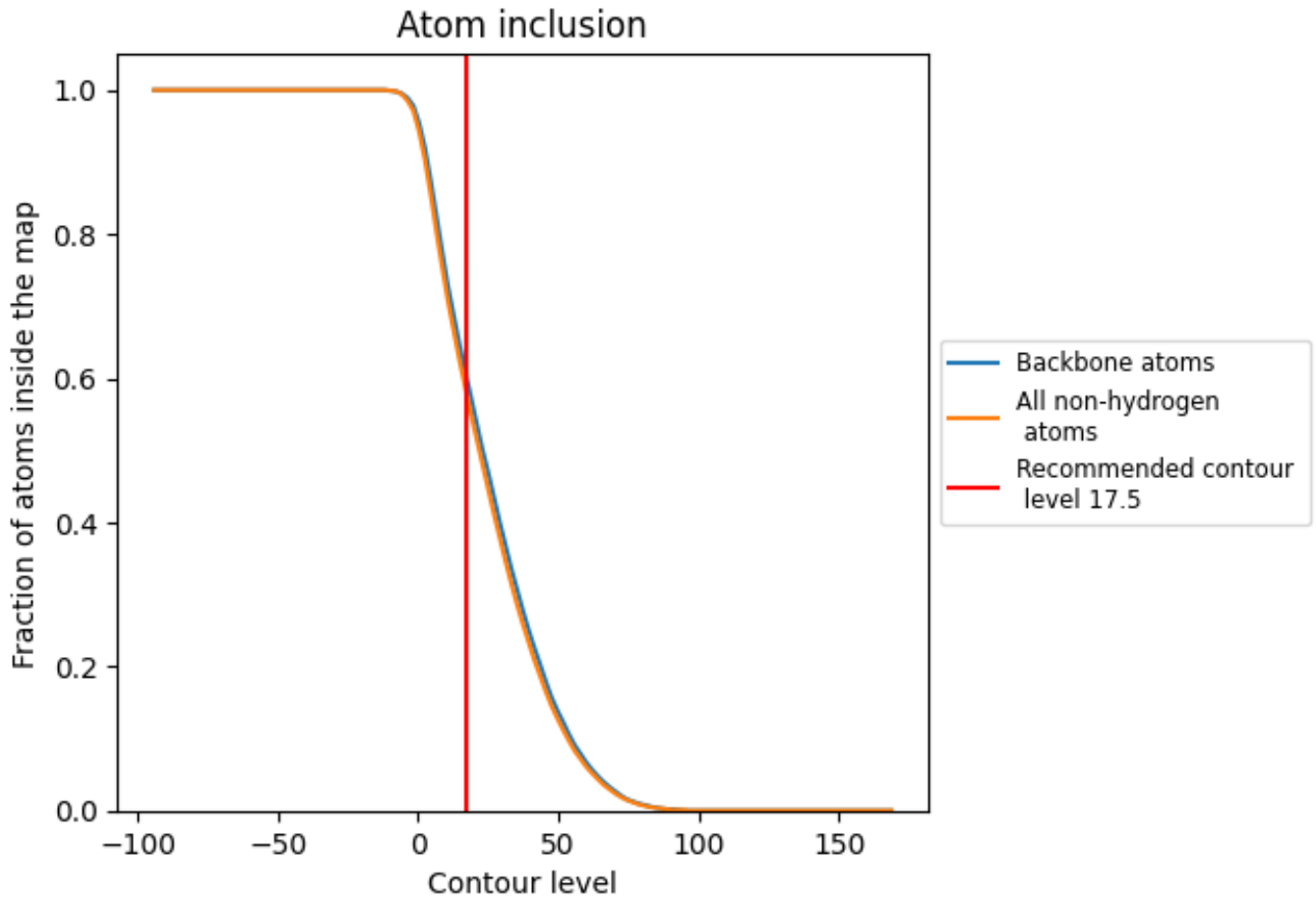
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (17.5).

9.4 Atom inclusion (i)



At the recommended contour level, 60% of all backbone atoms, 57% 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 (17.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5740	0.5080
1	0.0440	0.2350
2	0.0000	0.0900
3	0.0190	0.2140
4	0.0370	0.1910
5	0.0440	0.2370
6	0.0000	0.0880
7	0.0190	0.2130
8	0.0370	0.1890
A	0.8730	0.6430
B	0.8090	0.6200
C	0.8210	0.6290
D	0.8650	0.6370
E	0.7800	0.6010
F	0.7890	0.6140
G	0.5390	0.5460
H	0.8030	0.6150
I	0.8750	0.6340
J	0.6810	0.5830
K	0.7320	0.5880
L	0.8080	0.6190
M	0.6740	0.5720
N	0.6000	0.5620
O	0.7230	0.5810
P	0.6240	0.5760
Q	0.0760	0.4090
R	0.6350	0.5630
S	0.5200	0.5220
T	0.7010	0.6000
W	0.6930	0.5860
X	0.5880	0.5550
Y	0.7970	0.6100
Z	0.5570	0.5360
a	0.8720	0.6420
b	0.8080	0.6200



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Chain	Atom inclusion	Q-score
c	0.8200	0.6300
d	0.8640	0.6370
e	0.7800	0.6010
f	0.7930	0.6130
g	0.5410	0.5450
h	0.8010	0.6110
i	0.8750	0.6330
j	0.6770	0.5810
k	0.7320	0.5800
l	0.8060	0.6240
m	0.6670	0.5710
n	0.5990	0.5610
o	0.7210	0.5820
p	0.6260	0.5770
q	0.0770	0.4070
r	0.6360	0.5650
s	0.5220	0.5210
t	0.6880	0.6000
w	0.6930	0.5880
x	0.5880	0.5590
y	0.7970	0.6110
z	0.5540	0.5340