wwPDB EM Validation Summary Report

Sep 14, 2026 – 12:56 PM JST

PDB ID	:	7DZ7 / pdb_00007dz7
EMDB ID	:	EMD-30925
Title	:	State transition supercomplex PSI-LHCI-LHCII from double phosphatase mutant pph1;pbcp of green alga Chlamydomonas reinhardtii
Authors	:	Pan, X.W.; Li, A.J.; Liu, Z.F.; Li, M.
Deposited on	:	2021-01-23
Resolution	:	2.84 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 ⓘ symbol.

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

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

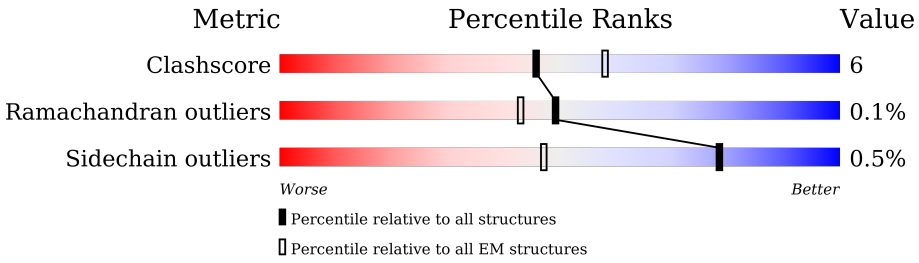
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using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

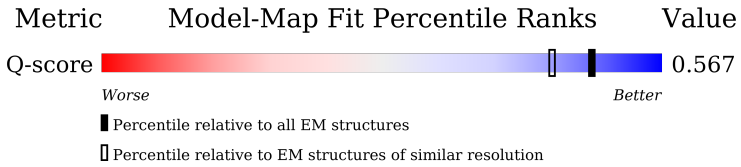
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.84 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	11884 (2.34 - 3.34)

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

Mol	Chain	Length	Quality of chain
1	A	751	87% 12% •
2	B	735	88% 11%
3	C	81	5% 86% 12% •
4	D	196	68% 5% 27%

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Mol	Chain	Length	Quality of chain
5	E	97	60% 35%
6	F	227	64% 9% 27%
7	G	126	67% 8% 25%
8	H	130	65% 12% 23%
9	I	106	34% 6% 60%
10	J	41	83% 17%
11	K	113	67% 9% 24%
12	L	196	72% 9% 19%
13	O	126	68% 9% 23%
14	1	228	78% 7% 15%
14	a	228	75% 10% 15%
15	2	246	82% 6% 12%
16	3	298	66% 7% 26%
17	4	264	74% 5% 20%
18	5	257	80% 8% 12%
19	6	257	81% 9% 11%
20	7	241	80% 8% 12%
21	8	243	77% 12% 11%
22	9	213	76% 10% 14%
23	W	249	24% 78% 10% 12%
23	X	249	44% 76% 12% 12%
24	U	257	14% 72% 12% 15%
24	Y	257	33% 75% 9% 14%
25	Z	256	6% 85% 5% 9%
26	V	268	82% 7% 11%

2 Entry composition (i)

There are 38 unique types of molecules in this entry. The entry contains 69647 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	741	5819	3805	993	999	22	0	0

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	733	5824	3825	977	1004	18	0	0

- Molecule 3 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	80	600	369	103	116	12	0	0

- Molecule 4 is a protein called Photosystem I reaction center subunit II, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	143	1124	719	199	199	7	0	0

- Molecule 5 is a protein called Photosystem I reaction center subunit IV, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	E	63	496	316	87	93	0	0

- Molecule 6 is a protein called Photosystem I reaction center subunit III, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	165	1265	817	213	232	3	0	0

- Molecule 7 is a protein called Photosystem I reaction center subunit V, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	94	Total	C	N	O	0	0
			699	449	118	132		

- Molecule 8 is a protein called Photosystem I reaction center subunit VI, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	100	Total	C	N	O	S	0	0
			776	482	138	154	2		

- Molecule 9 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	42	Total	C	N	O	S	0	0
			316	217	45	53	1		

- Molecule 10 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	41	Total	C	N	O	S	0	0
			337	231	47	58	1		

- Molecule 11 is a protein called Photosystem I reaction center subunit psaK, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	86	Total	C	N	O	S	0	0
			582	370	100	110	2		

- Molecule 12 is a protein called PSI subunit V.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	159	Total	C	N	O	S	0	0
			1161	757	189	212	3		

- Molecule 13 is a protein called Photosystem I subunit O.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	O	97	Total	C	N	O	0	0
			758	503	123	132		

- Molecule 14 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	a	194	Total	C	N	O	S	0	0
			1444	941	240	260	3		
14	1	194	Total	C	N	O	S	0	0
			1444	941	240	260	3		

- Molecule 15 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	2	217	Total	C	N	O	S	0	0
			1682	1094	274	304	10		

- Molecule 16 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	3	220	Total	C	N	O	S	0	0
			1678	1097	270	303	8		

- Molecule 17 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	4	210	Total	C	N	O	S	0	0
			1631	1071	263	292	5		

- Molecule 18 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	5	227	Total	C	N	O	S	0	0
			1774	1154	297	315	8		

- Molecule 19 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	6	230	Total	C	N	O	S	0	0
			1771	1167	293	305	6		

- Molecule 20 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	7	213	Total	C	N	O	S	0	0
			1649	1072	274	297	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	8	217	Total	C	N	O	S	0	0
			1649	1073	280	292	4		

- Molecule 22 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	9	183	Total	C	N	O	S	0	0
			1403	909	235	252	7		

- Molecule 23 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	220	Total	C	N	O	S	0	0
			1675	1088	273	309	5		
23	W	220	Total	C	N	O	S	0	0
			1671	1085	273	308	5		

- Molecule 24 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	220	Total	C	N	O	S	0	0
			1679	1086	273	315	5		
24	U	219	Total	C	N	O	S	0	0
			1670	1080	272	313	5		

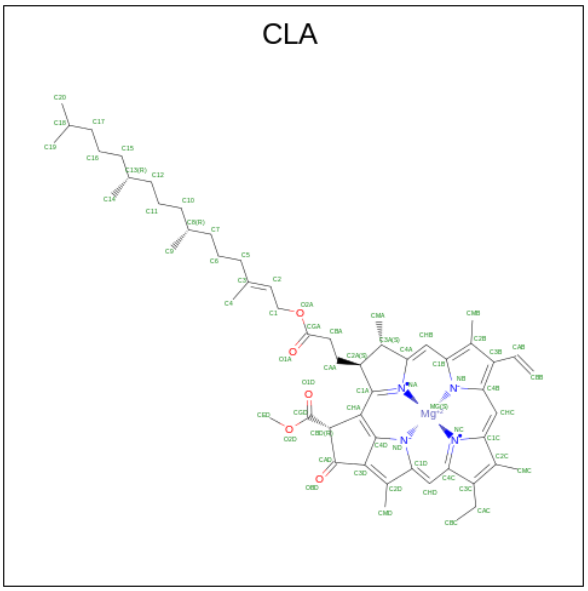
- Molecule 25 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	Z	232	Total	C	N	O	P	S	0	0
			1780	1154	291	329	1	5		

- Molecule 26 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	V	238	Total	C	N	O	P	S	0	0
			1815	1176	300	333	1	5		

- Molecule 27 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
27	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	A	1	Total 52	C 42	Mg 1	N 4	O 5	0
27	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
27	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
27	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	A	1	Total 54	C 44	Mg 1	N 4	O 5	0
27	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
27	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			64	55	1	4	4	
27	A	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			61	51	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			64	55	1	4	4	
27	B	1	Total	C	Mg	N	O	0
			52	43	1	4	4	
27	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
27	B	1	Total	C	Mg	N	O	0
			54	45	1	4	4	
27	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			43	33	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
27	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
27	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	F	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
27	F	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
27	F	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
27	G	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
27	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	H	1	Total	C	Mg	N	O	0
			39	31	1	4	3	
27	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	J	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
27	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	K	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
27	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
27	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	L	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
27	L	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
27	O	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
27	O	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
27	O	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
27	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			54	45	1	4	4	
27	a	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
27	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
27	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
27	1	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
27	1	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
27	1	1	Total	C	Mg	N	O	0
			53	44	1	4	4	
27	1	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
27	1	1	Total	C	Mg	N	O	0
			39	32	1	4	2	
27	1	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
27	1	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
27	1	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
27	1	1	Total	C	Mg	N	O	0
			39	31	1	4	3	
27	1	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
27	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	1	1	Total	C	Mg	N	O	0
			37	29	1	4	3	
27	1	1	Total	C	Mg	N	O	0
			43	33	1	4	5	
27	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	2	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
27	2	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
27	2	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
27	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
27	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	2	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
27	2	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
27	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	2	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
27	2	1	Total	C	Mg	N	O	0
			43	33	1	4	5	
27	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	3	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
27	3	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
27	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	3	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
27	3	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
27	3	1	Total	C	Mg	N	O	0
			53	44	1	4	4	
27	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
27	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
27	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
27	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
27	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
27	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
27	4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
27	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			43	33	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
27	5	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
27	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
27	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
27	5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
27	5	1	Total	C	Mg	N	O	0
			64	55	1	4	4	
27	5	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
27	5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
27	5	1	Total	C	Mg	N	O	0
			43	33	1	4	5	
27	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	6	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
27	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	6	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
27	6	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
27	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	6	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
27	6	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
27	6	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
27	6	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	6	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
27	6	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
27	7	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	7	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
27	7	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	7	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
27	7	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
27	7	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	7	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
27	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	7	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
27	7	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
27	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	7	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
27	7	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
27	7	1	Total	C	Mg	N	O	0
			43	33	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
27	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	8	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	8	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
27	8	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	8	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
27	8	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
27	8	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
27	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	8	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	8	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
27	8	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
27	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	8	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
27	8	1	Total	C	Mg	N	O	0
			43	33	1	4	5	
27	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	9	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	9	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
27	9	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	9	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
27	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	9	1	Total	C	Mg	N	O	0
			61	51	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
27	9	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
27	9	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
27	9	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
27	9	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	X	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	X	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
27	X	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
27	X	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	X	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	X	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
27	X	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	X	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
27	Y	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
27	Y	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	Y	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	Y	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
27	Y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	Y	1	Total	C	Mg	N	O	0
			48	38	1	4	5	

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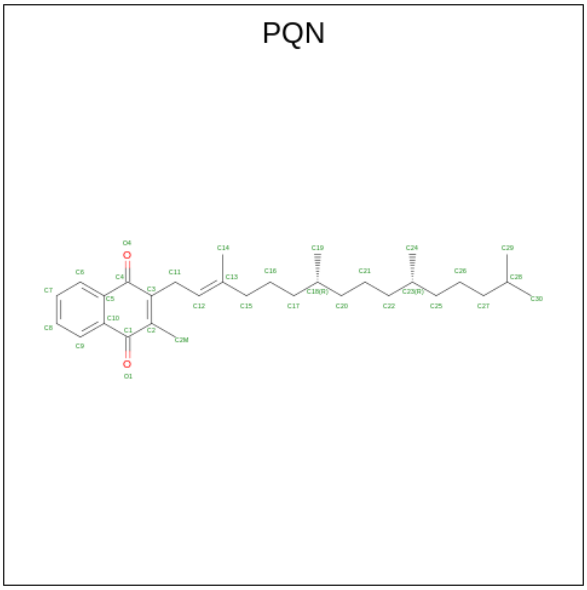
Mol	Chain	Residues	Atoms					AltConf
27	Z	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	Z	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
27	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	Z	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
27	U	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
27	U	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
27	U	1	Total	C	Mg	N	O	0
			48	39	1	4	4	
27	U	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
27	U	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
27	U	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
27	U	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
27	U	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
27	V	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	V	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	V	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	V	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
27	V	1	Total	C	Mg	N	O	0
			43	35	1	4	3	

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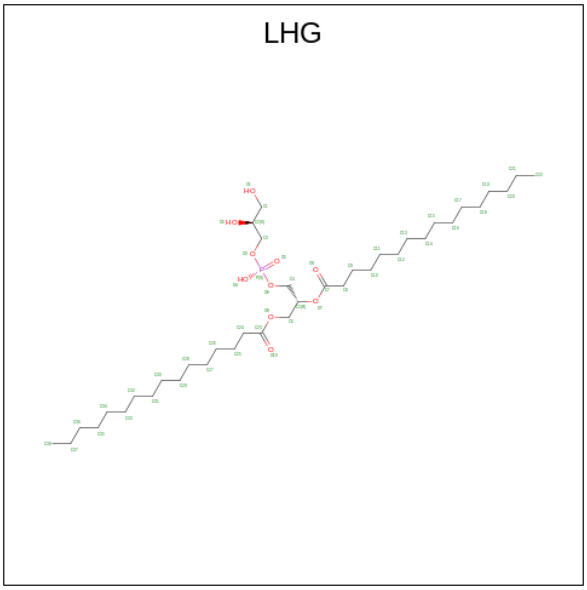
Mol	Chain	Residues	Atoms					AltConf
27	V	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	V	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	V	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	W	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	W	1	Total 52	C 42	Mg 1	N 4	O 5	0
27	W	1	Total 47	C 37	Mg 1	N 4	O 5	0
27	W	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	W	1	Total 57	C 47	Mg 1	N 4	O 5	0
27	W	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	W	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	W	1	Total 45	C 35	Mg 1	N 4	O 5	0

- Molecule 28 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



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

- Molecule 29 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



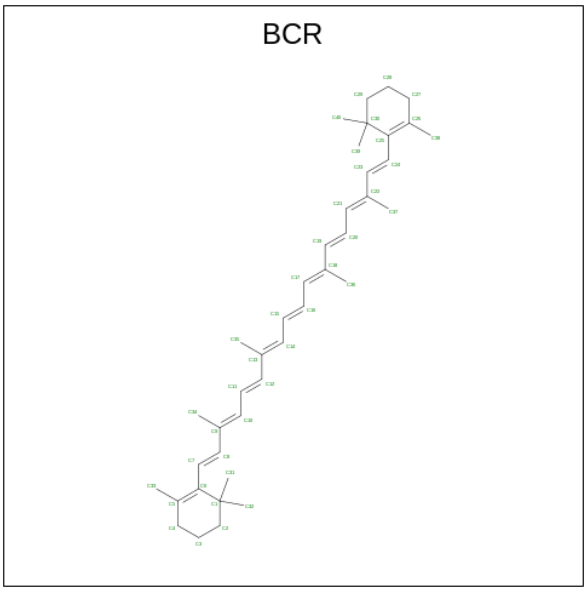
Mol	Chain	Residues	Atoms				AltConf
29	A	1	Total 49	C 38	O 10	P 1	0
29	A	1	Total 30	C 19	O 10	P 1	0
29	B	1	Total 38	C 27	O 10	P 1	0
29	B	1	Total 49	C 38	O 10	P 1	0
29	H	1	Total 49	C 38	O 10	P 1	0
29	O	1	Total 36	C 25	O 10	P 1	0
29	a	1	Total 43	C 32	O 10	P 1	0
29	1	1	Total 49	C 38	O 10	P 1	0
29	2	1	Total 36	C 25	O 10	P 1	0

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Mol	Chain	Residues	Atoms				AltConf
29	3	1	Total	C	O	P	0
			45	34	10	1	
29	3	1	Total	C	O	P	0
			49	38	10	1	
29	4	1	Total	C	O	P	0
			49	38	10	1	
29	5	1	Total	C	O	P	0
			49	38	10	1	
29	5	1	Total	C	O	P	0
			49	38	10	1	
29	6	1	Total	C	O	P	0
			48	37	10	1	
29	7	1	Total	C	O	P	0
			37	26	10	1	
29	8	1	Total	C	O	P	0
			49	38	10	1	
29	8	1	Total	C	O	P	0
			40	29	10	1	
29	9	1	Total	C	O	P	0
			30	19	10	1	
29	9	1	Total	C	O	P	0
			49	38	10	1	
29	9	1	Total	C	O	P	0
			49	38	10	1	
29	X	1	Total	C	O	P	0
			49	38	10	1	
29	Y	1	Total	C	O	P	0
			49	38	10	1	
29	Z	1	Total	C	O	P	0
			49	38	10	1	
29	U	1	Total	C	O	P	0
			49	38	10	1	
29	V	1	Total	C	O	P	0
			48	37	10	1	
29	W	1	Total	C	O	P	0
			44	33	10	1	

- Molecule 30 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	AltConf
30	A	1	Total C 40 40	0
30	A	1	Total C 40 40	0
30	A	1	Total C 40 40	0
30	A	1	Total C 40 40	0
30	A	1	Total C 40 40	0
30	A	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	B	1	Total C 40 40	0

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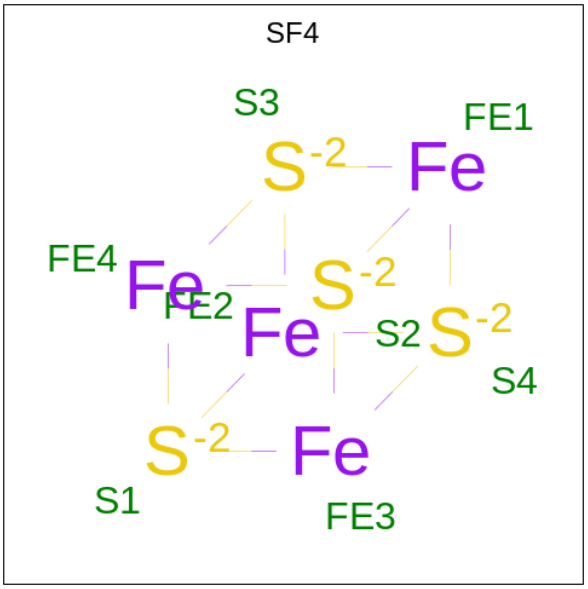
Mol	Chain	Residues	Atoms	AltConf
30	B	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	F	1	Total C 40 40	0
30	G	1	Total C 40 40	0
30	J	1	Total C 40 40	0
30	K	1	Total C 40 40	0
30	K	1	Total C 40 40	0
30	L	1	Total C 40 40	0
30	L	1	Total C 40 40	0
30	L	1	Total C 40 40	0
30	L	1	Total C 40 40	0
30	O	1	Total C 40 40	0
30	O	1	Total C 40 40	0
30	a	1	Total C 40 40	0
30	1	1	Total C 40 40	0
30	2	1	Total C 40 40	0
30	3	1	Total C 40 40	0
30	3	1	Total C 40 40	0
30	3	1	Total C 40 40	0
30	4	1	Total C 40 40	0
30	5	1	Total C 40 40	0

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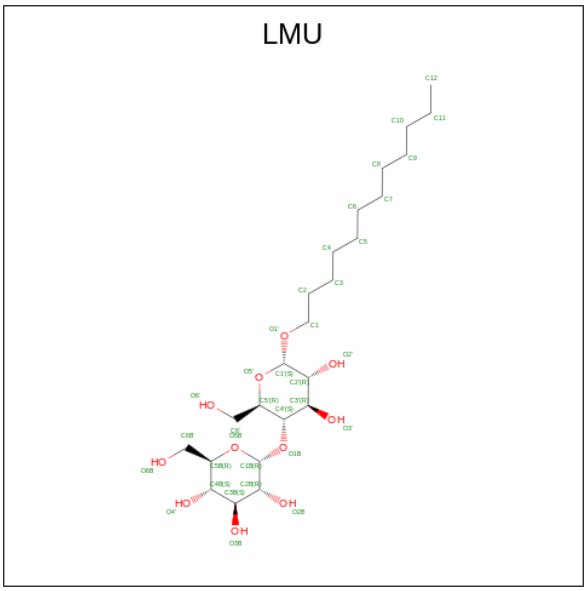
Mol	Chain	Residues	Atoms	AltConf
30	6	1	Total C 40 40	0
30	7	1	Total C 40 40	0
30	7	1	Total C 40 40	0
30	8	1	Total C 40 40	0
30	9	1	Total C 40 40	0

- Molecule 31 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



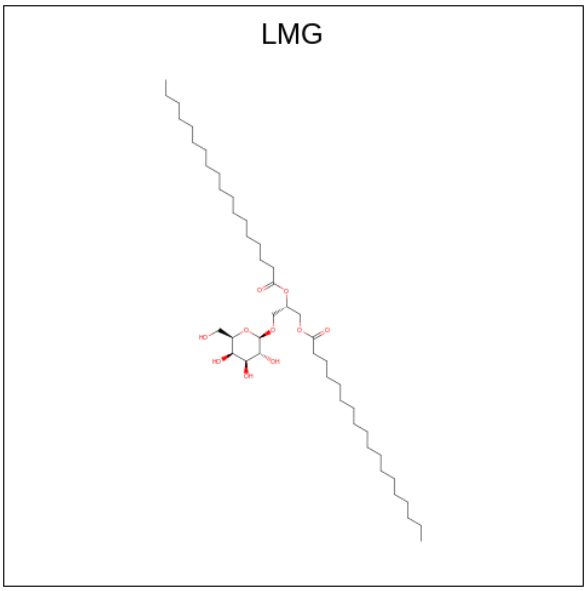
Mol	Chain	Residues	Atoms	AltConf
31	A	1	Total Fe S 8 4 4	0
31	C	1	Total Fe S 8 4 4	0
31	C	1	Total Fe S 8 4 4	0

- Molecule 32 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$).



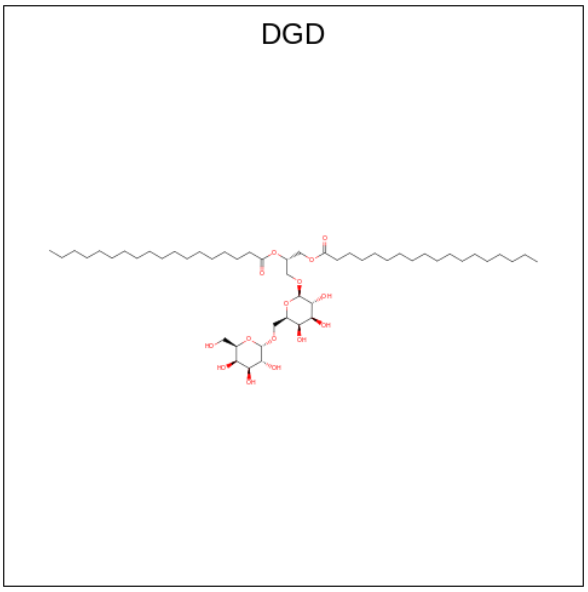
Mol	Chain	Residues	Atoms			AltConf
32	A	1	Total	C	O	0
			35	24	11	
32	A	1	Total	C	O	0
			34	24	10	
32	K	1	Total	C	O	0
			35	24	11	
32	1	1	Total	C	O	0
			35	24	11	
32	5	1	Total	C	O	0
			33	22	11	
32	5	1	Total	C	O	0
			32	21	11	
32	8	1	Total	C	O	0
			35	24	11	

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



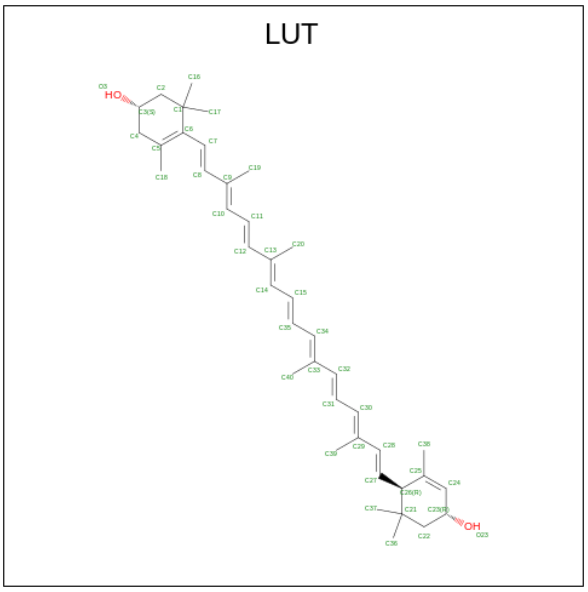
Mol	Chain	Residues	Atoms	AltConf
33	A	1	Total C O 40 30 10	0
33	H	1	Total C O 55 45 10	0
33	J	1	Total C O 42 32 10	0
33	J	1	Total C O 40 30 10	0
33	L	1	Total C O 37 27 10	0
33	4	1	Total C O 40 30 10	0
33	4	1	Total C O 40 30 10	0
33	5	1	Total C O 40 30 10	0
33	8	1	Total C O 46 36 10	0
33	9	1	Total C O 55 45 10	0
33	V	1	Total C O 41 31 10	0

- Molecule 34 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			AltConf
34	B	1	Total	C	O	0
			62	47	15	

- Molecule 35 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3 ,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$).



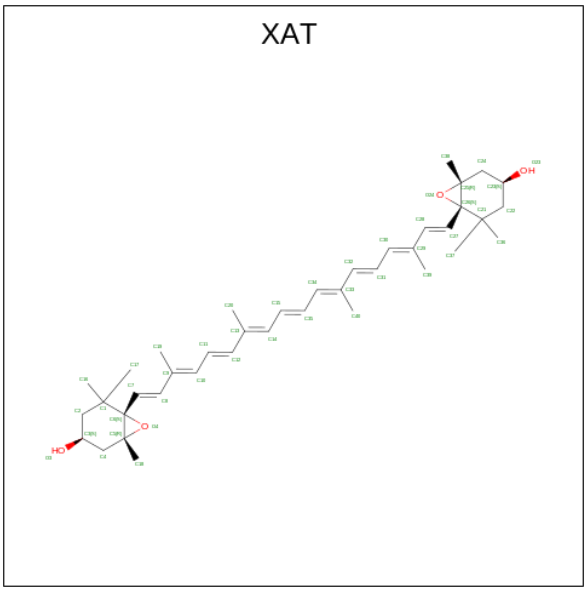
Mol	Chain	Residues	Atoms			AltConf
35	a	1	Total	C	O	0
			42	40	2	
35	1	1	Total	C	O	0
			42	40	2	

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Mol	Chain	Residues	Atoms			AltConf
35	2	1	Total	C	O	0
			42	40	2	
35	3	1	Total	C	O	0
			42	40	2	
35	4	1	Total	C	O	0
			42	40	2	
35	5	1	Total	C	O	0
			42	40	2	
35	6	1	Total	C	O	0
			42	40	2	
35	7	1	Total	C	O	0
			42	40	2	
35	8	1	Total	C	O	0
			42	40	2	
35	9	1	Total	C	O	0
			42	40	2	
35	X	1	Total	C	O	0
			42	40	2	
35	X	1	Total	C	O	0
			42	40	2	
35	Y	1	Total	C	O	0
			42	40	2	
35	Y	1	Total	C	O	0
			42	40	2	
35	Z	1	Total	C	O	0
			42	40	2	
35	Z	1	Total	C	O	0
			42	40	2	
35	U	1	Total	C	O	0
			42	40	2	
35	U	1	Total	C	O	0
			42	40	2	
35	V	1	Total	C	O	0
			42	40	2	
35	V	1	Total	C	O	0
			42	40	2	
35	W	1	Total	C	O	0
			42	40	2	
35	W	1	Total	C	O	0
			42	40	2	

- Molecule 36 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: $C_{40}H_{56}O_4$).



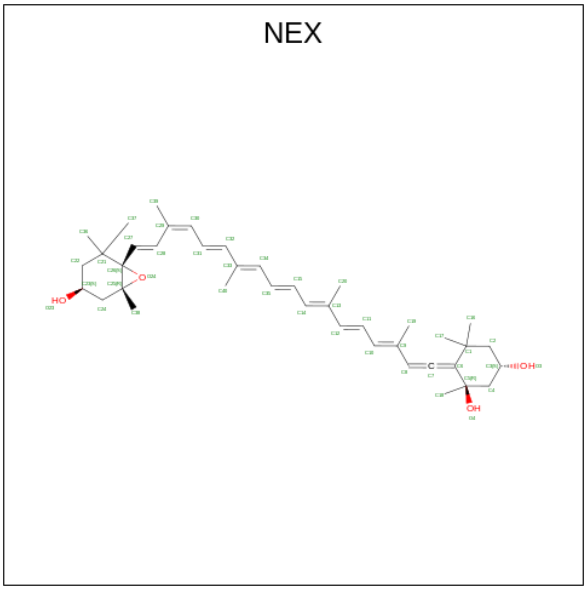
Mol	Chain	Residues	Atoms	AltConf
36	a	1	Total C O 44 40 4	0
36	1	1	Total C O 44 40 4	0
36	2	1	Total C O 44 40 4	0
36	3	1	Total C O 44 40 4	0
36	4	1	Total C O 44 40 4	0
36	5	1	Total C O 44 40 4	0
36	6	1	Total C O 44 40 4	0
36	7	1	Total C O 44 40 4	0
36	8	1	Total C O 44 40 4	0
36	9	1	Total C O 44 40 4	0
36	X	1	Total C O 44 40 4	0
36	Y	1	Total C O 44 40 4	0
36	Z	1	Total C O 44 40 4	0
36	U	1	Total C O 44 40 4	0

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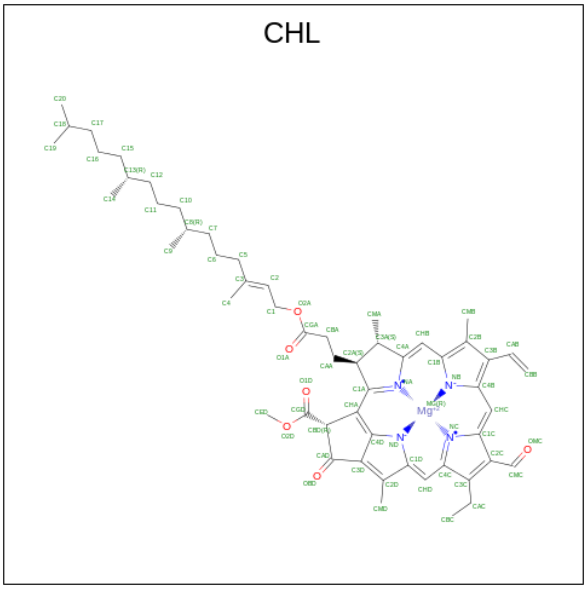
Mol	Chain	Residues	Atoms	AltConf
36	V	1	Total C O 44 40 4	0
36	W	1	Total C O 44 40 4	0

- Molecule 37 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
37	5	1	Total C O 44 40 4	0
37	6	1	Total C O 44 40 4	0
37	X	1	Total C O 44 40 4	0
37	Y	1	Total C O 43 40 3	0
37	Z	1	Total C O 44 40 4	0
37	U	1	Total C O 44 40 4	0
37	V	1	Total C O 44 40 4	0
37	W	1	Total C O 44 40 4	0

- Molecule 38 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
38	X	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	X	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
38	X	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
38	X	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	X	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	X	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	Y	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
38	Y	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
38	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	Y	1	Total	C	Mg	N	O	0
			49	38	1	4	6	
38	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
38	Z	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	Z	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
38	Z	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
38	Z	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	Z	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
38	Z	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	U	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	U	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
38	U	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
38	U	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
38	U	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
38	U	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
38	V	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	V	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
38	V	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
38	V	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
38	V	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
38	V	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
38	W	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	W	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
38	W	1	Total	C	Mg	N	O	0
			46	35	1	4	6	

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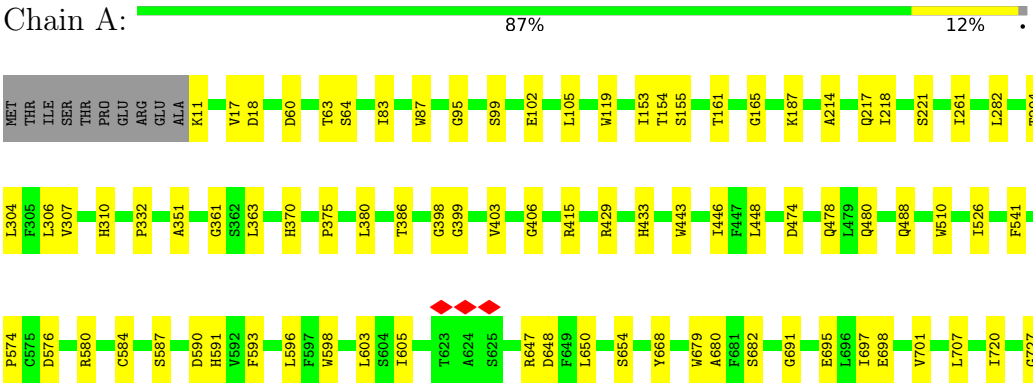
Mol	Chain	Residues	Atoms					AltConf
38	W	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
38	W	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
38	W	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

3 Residue-property plots (i)

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

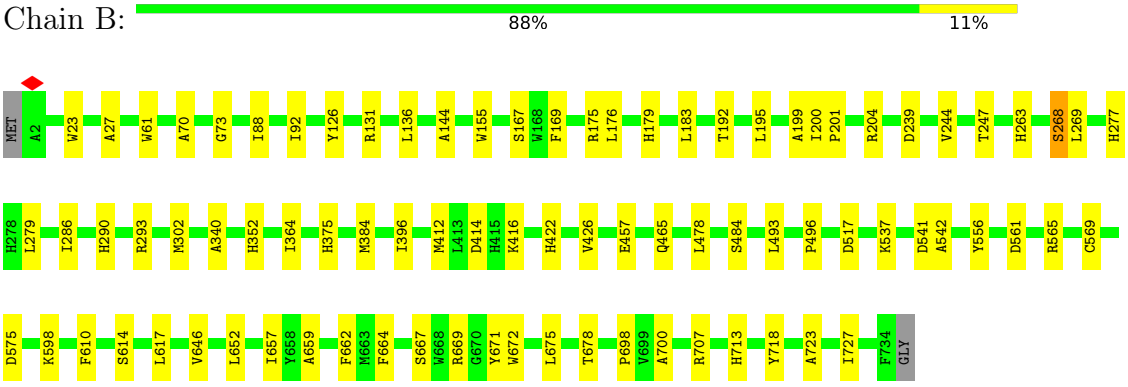
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain A:



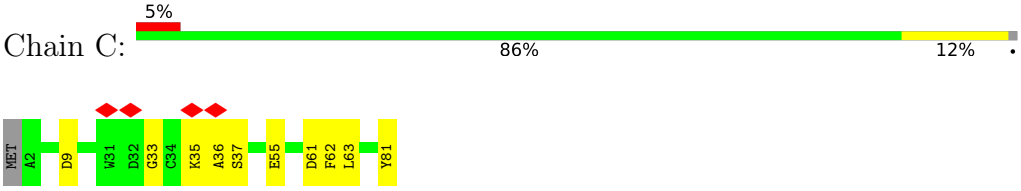
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain B:



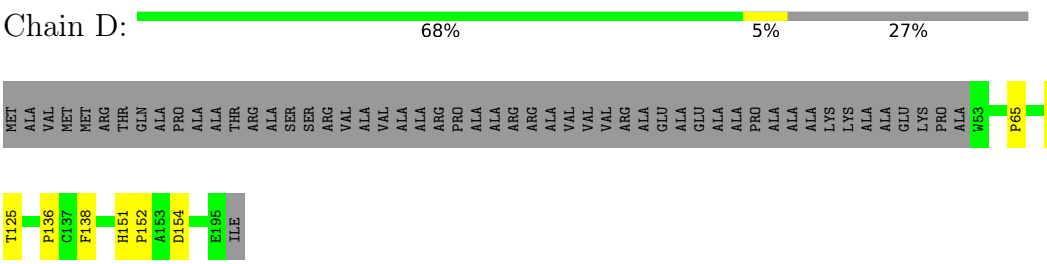
• Molecule 3: Photosystem I iron-sulfur center

Chain C:



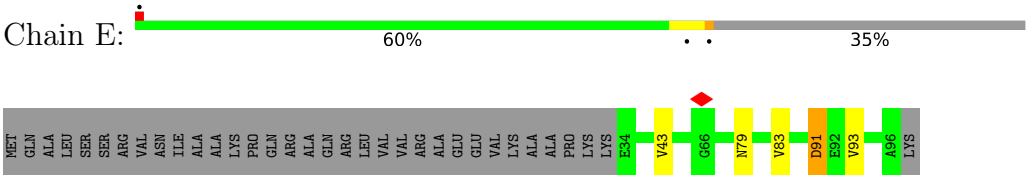
• Molecule 4: Photosystem I reaction center subunit II, chloroplastic

Chain D:



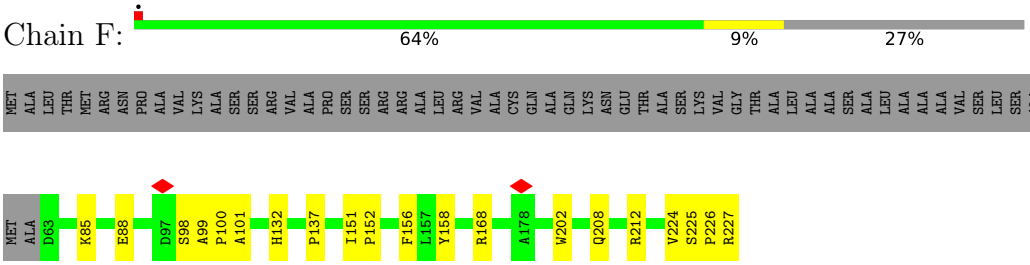
• Molecule 5: Photosystem I reaction center subunit IV, chloroplastic

Chain E:



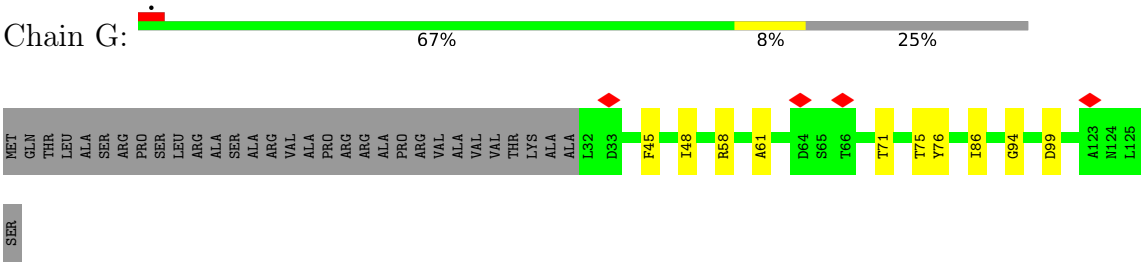
• Molecule 6: Photosystem I reaction center subunit III, chloroplastic

Chain F:



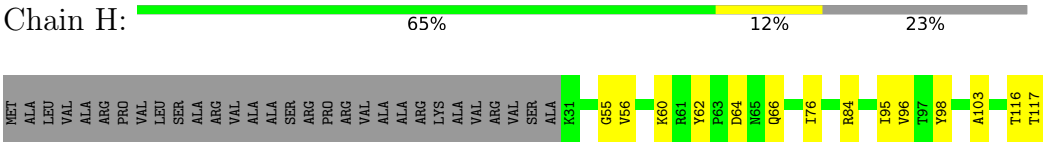
• Molecule 7: Photosystem I reaction center subunit V, chloroplastic

Chain G:



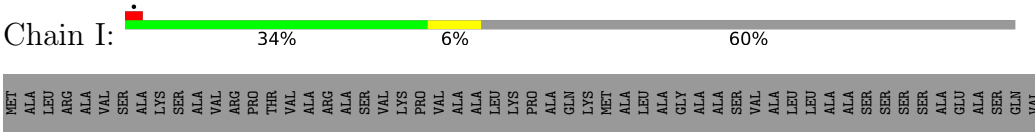
• Molecule 8: Photosystem I reaction center subunit VI, chloroplastic

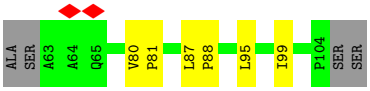
Chain H:



• Molecule 9: Photosystem I reaction center subunit VIII

Chain I:

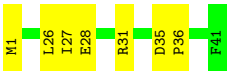




• Molecule 10: Photosystem I reaction center subunit IX

Chain J:

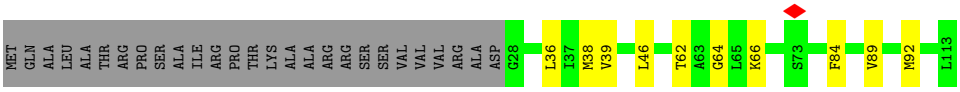




• Molecule 11: Photosystem I reaction center subunit psaK, chloroplastic

Chain K:

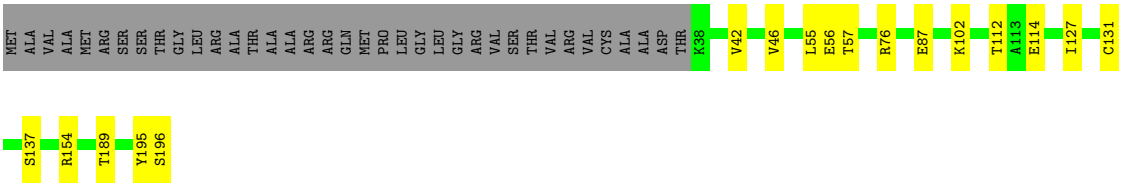




• Molecule 12: PSI subunit V

Chain L:

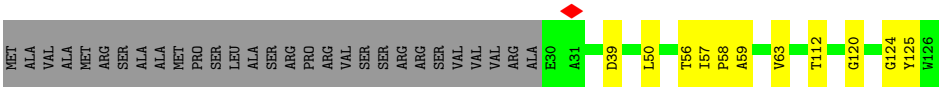




• Molecule 13: Photosystem I subunit O

Chain O:

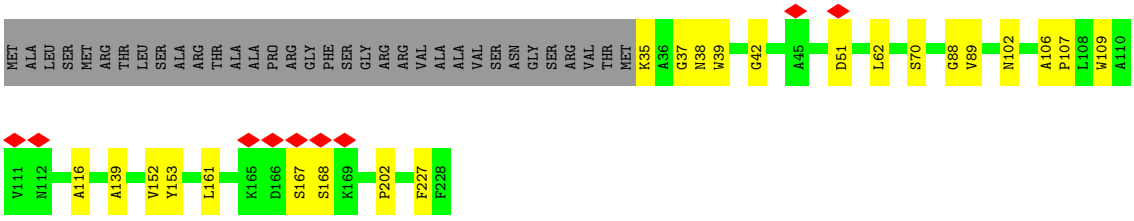




• Molecule 14: Chlorophyll a-b binding protein, chloroplastic

Chain a:

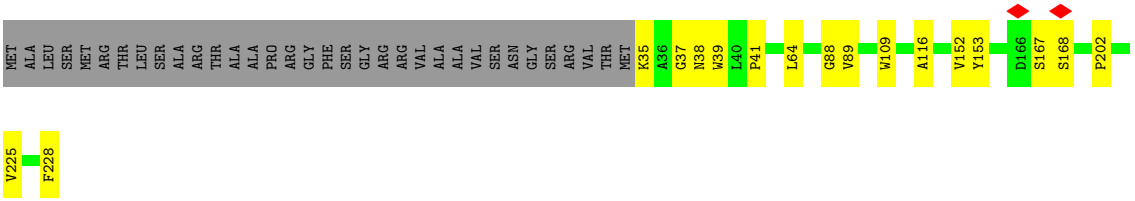




• Molecule 14: Chlorophyll a-b binding protein, chloroplastic

Chain 1:

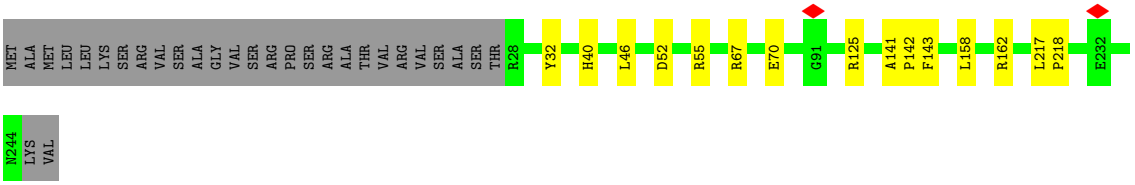




• Molecule 15: Chlorophyll a-b binding protein, chloroplastic

Chain 2:

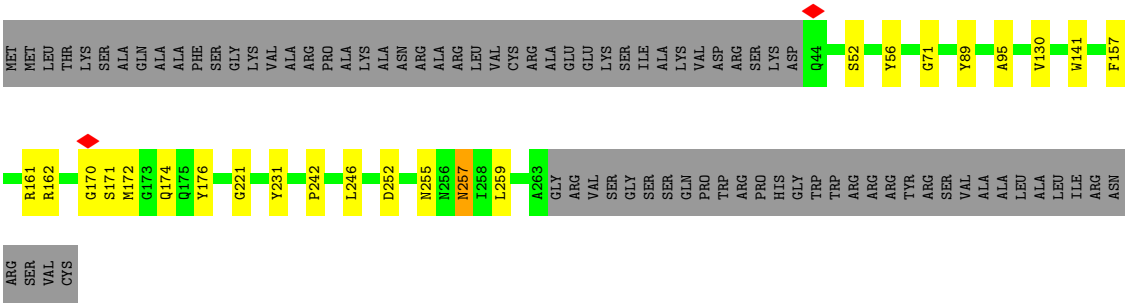




• Molecule 16: Chlorophyll a-b binding protein, chloroplastic

Chain 3:

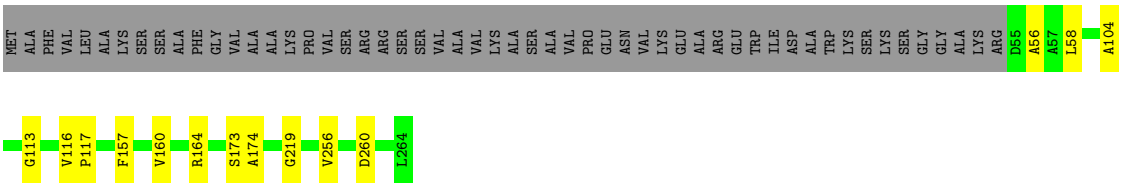




• Molecule 17: Chlorophyll a-b binding protein, chloroplastic

Chain 4:

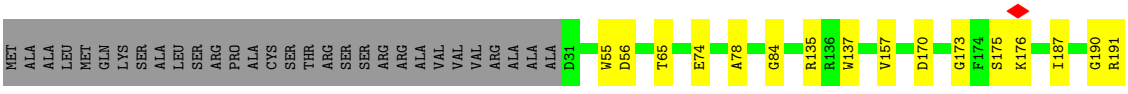


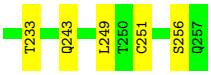


• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain 5:



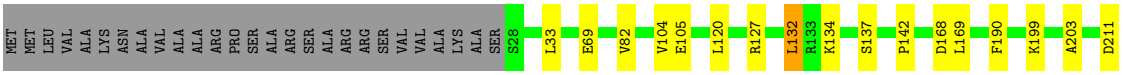




• Molecule 19: Chlorophyll a-b binding protein, chloroplastic

Chain 6:



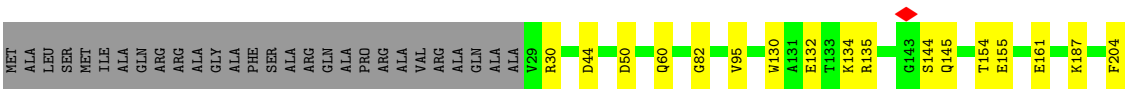


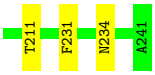


• Molecule 20: Chlorophyll a-b binding protein, chloroplastic

Chain 7:







• Molecule 21: Chlorophyll a-b binding protein, chloroplastic

Chain 8:



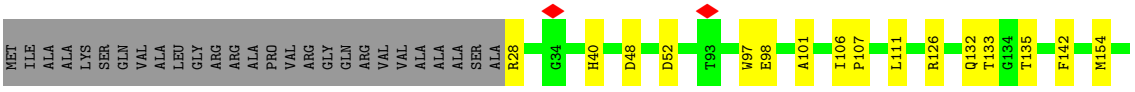


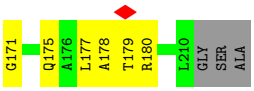


• Molecule 22: Chlorophyll a-b binding protein, chloroplastic

Chain 9:



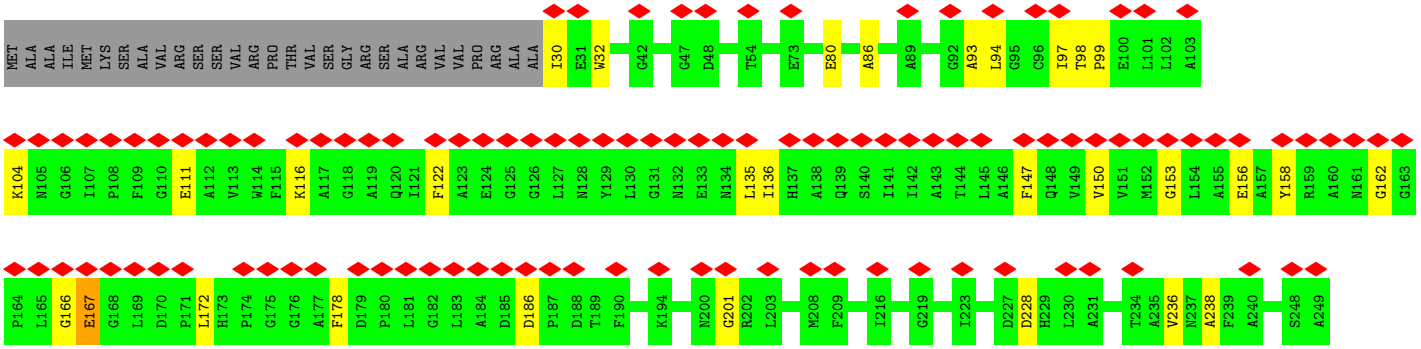




• Molecule 23: Chlorophyll a-b binding protein, chloroplastic

Chain X:

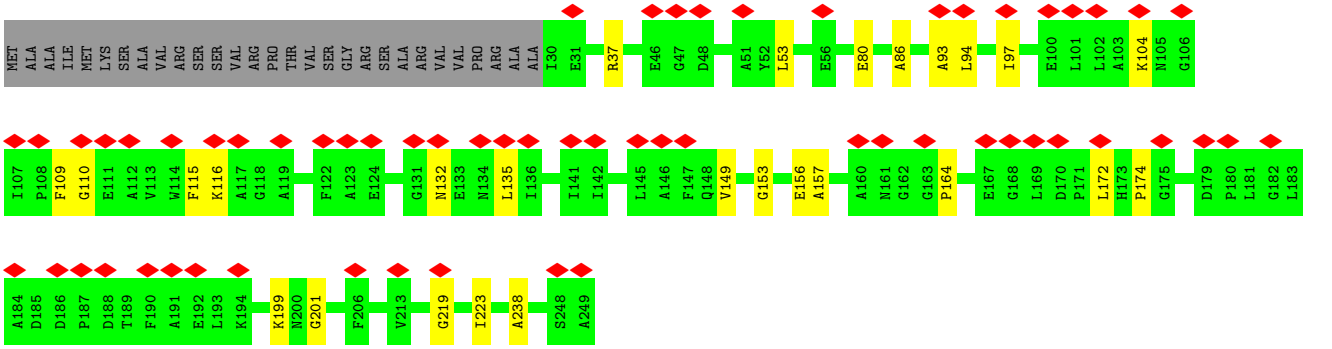




• Molecule 23: Chlorophyll a-b binding protein, chloroplastic

Chain W:

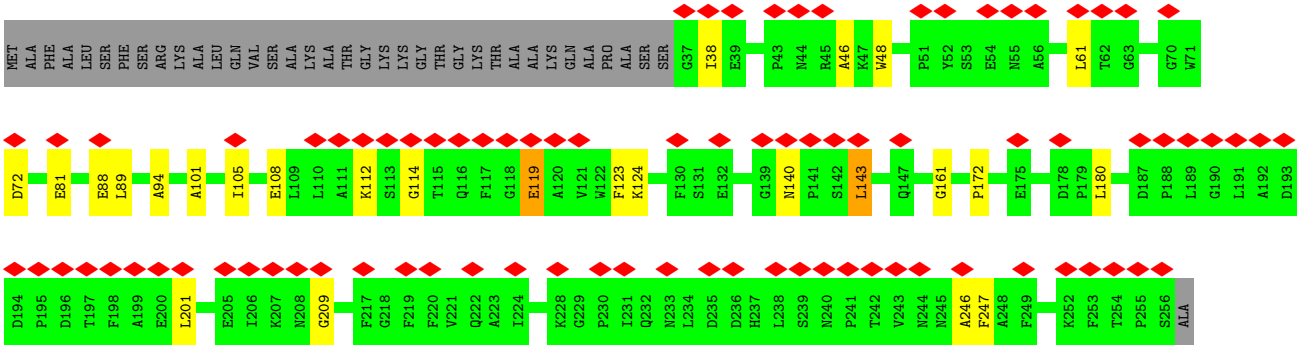




• Molecule 24: Chlorophyll a-b binding protein, chloroplastic

Chain Y:

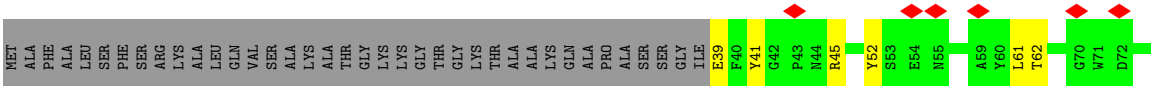


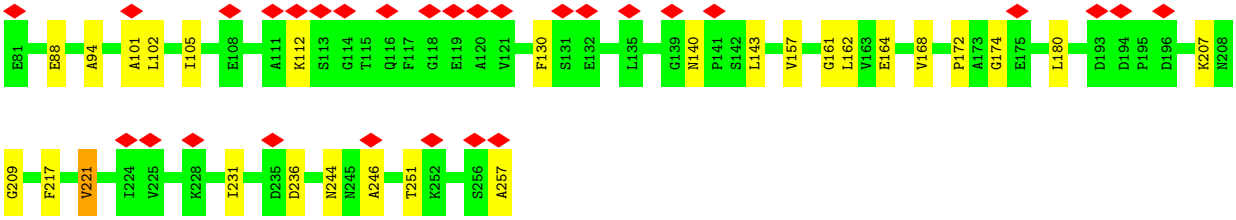


• Molecule 24: Chlorophyll a-b binding protein, chloroplastic

Chain U:



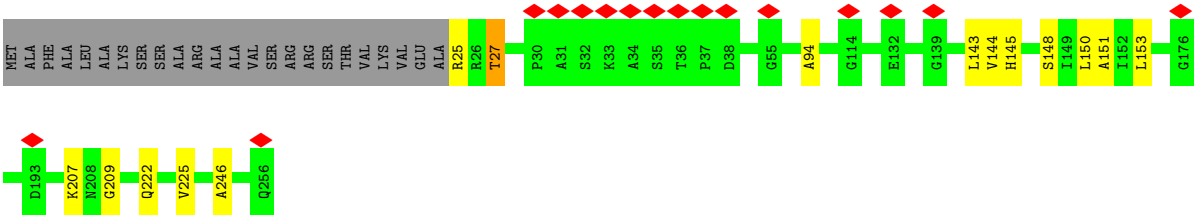




• Molecule 25: Chlorophyll a-b binding protein, chloroplastic

Chain Z:

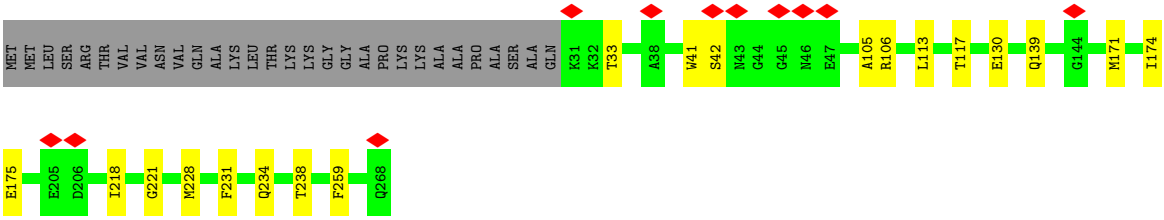




• Molecule 26: Chlorophyll a-b binding protein, chloroplastic

Chain V:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	56601	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	1.5625	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	0.216	Depositor
Minimum map value	-0.116	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	480.0, 480.0, 480.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	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: DGD, XAT, LHG, LMG, LMU, LUT, CLA, TPO, SF4, PQN, CHL, BCR, NEX

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.31	0/6015	0.32	0/8201
2	B	0.29	0/6036	0.34	0/8242
3	C	0.24	0/610	0.37	0/826
4	D	0.24	0/1152	0.36	0/1556
5	E	0.21	0/506	0.30	0/689
6	F	0.23	0/1291	0.33	0/1747
7	G	0.20	0/714	0.33	0/972
8	H	0.23	0/788	0.32	0/1059
9	I	0.28	0/329	0.35	0/456
10	J	0.27	0/349	0.30	0/478
11	K	0.24	0/587	0.38	0/795
12	L	0.27	0/1190	0.36	0/1628
13	O	0.25	0/784	0.35	0/1069
14	1	0.29	0/1490	0.41	0/2028
14	a	0.32	0/1490	0.44	0/2028
15	2	0.22	0/1730	0.35	0/2353
16	3	0.26	0/1726	0.34	0/2342
17	4	0.22	0/1686	0.33	0/2300
18	5	0.24	0/1829	0.36	0/2492
19	6	0.29	0/1833	0.42	0/2505
20	7	0.27	0/1701	0.34	0/2310
21	8	0.27	0/1700	0.35	0/2315
22	9	0.23	0/1444	0.39	0/1964
23	W	0.39	0/1721	0.43	0/2341
23	X	0.24	0/1725	0.47	1/2348 (0.0%)
24	U	0.42	0/1718	0.48	0/2338
24	Y	0.25	0/1727	0.46	0/2350
25	Z	0.13	0/1822	0.30	0/2474
26	V	0.40	0/1856	0.40	0/2518
All	All	0.28	0/47549	0.37	1/64724 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	X	166	GLY	CA-C-O	-6.01	118.31	122.22

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	A	5819	0	5670	68	0
2	B	5824	0	5579	72	0
3	C	600	0	581	6	0
4	D	1124	0	1139	6	0
5	E	496	0	491	4	0
6	F	1265	0	1301	16	0
7	G	699	0	681	9	0
8	H	776	0	765	17	0
9	I	316	0	321	3	0
10	J	337	0	336	5	0
11	K	582	0	620	13	0
12	L	1161	0	1184	16	0
13	O	758	0	740	10	0
14	1	1444	0	1396	12	0
14	a	1444	0	1396	20	0
15	2	1682	0	1665	15	0
16	3	1678	0	1637	19	0
17	4	1631	0	1587	11	0
18	5	1774	0	1746	18	0
19	6	1771	0	1770	19	0
20	7	1649	0	1589	15	0
21	8	1649	0	1629	32	0
22	9	1403	0	1381	21	0
23	W	1671	0	1604	28	0
23	X	1675	0	1617	27	0
24	U	1670	0	1604	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	Y	1679	0	1620	26	0
25	Z	1780	0	1723	14	0
26	V	1815	0	1765	32	0
27	1	666	0	522	1	0
27	2	641	0	533	9	0
27	3	724	0	628	9	0
27	4	778	0	678	8	0
27	5	878	0	758	9	0
27	6	903	0	831	6	0
27	7	756	0	635	5	0
27	8	724	0	629	4	0
27	9	595	0	491	5	0
27	A	2669	0	2693	40	0
27	B	2282	0	2232	40	0
27	F	140	0	113	1	0
27	G	87	0	64	0	0
27	H	104	0	93	1	0
27	J	42	0	31	0	0
27	K	191	0	150	7	0
27	L	235	0	184	4	0
27	O	116	0	61	0	0
27	U	401	0	344	4	0
27	V	415	0	365	4	0
27	W	426	0	377	5	0
27	X	436	0	415	5	0
27	Y	429	0	389	6	0
27	Z	496	0	520	2	0
27	a	710	0	591	2	0
28	A	33	0	46	0	0
28	B	33	0	46	2	0
29	1	49	0	74	0	0
29	2	36	0	42	0	0
29	3	94	0	137	1	0
29	4	49	0	74	0	0
29	5	98	0	148	1	0
29	6	48	0	69	0	0
29	7	37	0	44	1	0
29	8	89	0	124	0	0
29	9	128	0	178	2	0
29	A	79	0	104	0	0
29	B	87	0	120	1	0
29	H	49	0	74	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	O	36	0	42	0	0
29	U	49	0	74	0	0
29	V	48	0	69	2	0
29	W	44	0	61	0	0
29	X	49	0	74	0	0
29	Y	49	0	74	0	0
29	Z	49	0	74	2	0
29	a	43	0	59	0	0
30	1	40	0	56	2	0
30	2	40	0	56	9	0
30	3	120	0	168	15	0
30	4	40	0	56	3	0
30	5	40	0	56	3	0
30	6	40	0	56	3	0
30	7	80	0	112	10	0
30	8	40	0	56	3	0
30	9	40	0	56	5	0
30	A	240	0	336	38	0
30	B	400	0	560	50	0
30	F	40	0	56	8	0
30	G	40	0	56	2	0
30	J	40	0	56	10	0
30	K	80	0	112	17	0
30	L	160	0	224	20	0
30	O	80	0	112	11	0
30	a	40	0	56	2	0
31	A	8	0	0	0	0
31	C	16	0	0	0	0
32	1	35	0	46	0	0
32	5	65	0	76	0	0
32	8	35	0	46	0	0
32	A	69	0	90	1	0
32	K	35	0	46	1	0
33	4	80	0	100	0	0
33	5	40	0	50	1	0
33	8	46	0	65	0	0
33	9	55	0	86	0	0
33	A	40	0	50	1	0
33	H	55	0	86	0	0
33	J	82	0	107	0	0
33	L	37	0	44	1	0
33	V	41	0	52	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	B	62	0	85	3	0
35	1	42	0	56	3	0
35	2	42	0	56	2	0
35	3	42	0	56	3	0
35	4	42	0	56	4	0
35	5	42	0	56	0	0
35	6	42	0	56	3	0
35	7	42	0	56	2	0
35	8	42	0	56	3	0
35	9	42	0	56	2	0
35	U	84	0	112	2	0
35	V	84	0	112	2	0
35	W	84	0	112	2	0
35	X	84	0	112	5	0
35	Y	84	0	112	3	0
35	Z	84	0	112	4	0
35	a	42	0	56	4	0
36	1	44	0	56	1	0
36	2	44	0	56	0	0
36	3	44	0	56	1	0
36	4	44	0	56	0	0
36	5	44	0	56	3	0
36	6	44	0	56	1	0
36	7	44	0	56	2	0
36	8	44	0	56	0	0
36	9	44	0	56	0	0
36	U	44	0	56	3	0
36	V	44	0	56	0	0
36	W	44	0	56	1	0
36	X	44	0	56	0	0
36	Y	44	0	56	1	0
36	Z	44	0	56	1	0
36	a	44	0	56	1	0
37	5	44	0	56	2	0
37	6	44	0	56	1	0
37	U	44	0	56	0	0
37	V	44	0	56	1	0
37	W	44	0	56	2	0
37	X	44	0	56	2	0
37	Y	43	0	55	2	0
37	Z	44	0	56	4	0
38	U	303	0	248	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	V	309	0	253	28	0
38	W	336	0	298	19	0
38	X	354	0	342	16	0
38	Y	335	0	302	19	0
38	Z	338	0	309	17	0
All	All	69647	0	68867	860	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 860 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:U:140:ASN:CB	24:U:143:LEU:HD13	1.49	1.42
12:L:114:GLU:HG2	12:L:189:THR:CG2	1.67	1.24
22:9:133:THR:HG22	22:9:135:THR:CG2	1.71	1.20
22:9:133:THR:CG2	22:9:135:THR:HG22	1.74	1.18
12:L:114:GLU:CG	12:L:189:THR:HG21	1.75	1.16

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	739/751 (98%)	720 (97%)	19 (3%)	0	100	100
2	B	731/735 (100%)	714 (98%)	17 (2%)	0	100	100
3	C	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
4	D	141/196 (72%)	135 (96%)	6 (4%)	0	100	100
5	E	61/97 (63%)	59 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	163/227 (72%)	155 (95%)	8 (5%)	0	100	100
7	G	92/126 (73%)	86 (94%)	6 (6%)	0	100	100
8	H	98/130 (75%)	92 (94%)	6 (6%)	0	100	100
9	I	40/106 (38%)	35 (88%)	5 (12%)	0	100	100
10	J	39/41 (95%)	38 (97%)	1 (3%)	0	100	100
11	K	84/113 (74%)	79 (94%)	5 (6%)	0	100	100
12	L	157/196 (80%)	150 (96%)	7 (4%)	0	100	100
13	O	95/126 (75%)	87 (92%)	8 (8%)	0	100	100
14	1	192/228 (84%)	185 (96%)	7 (4%)	0	100	100
14	a	192/228 (84%)	185 (96%)	7 (4%)	0	100	100
15	2	215/246 (87%)	202 (94%)	13 (6%)	0	100	100
16	3	218/298 (73%)	213 (98%)	5 (2%)	0	100	100
17	4	208/264 (79%)	201 (97%)	7 (3%)	0	100	100
18	5	225/257 (88%)	212 (94%)	13 (6%)	0	100	100
19	6	228/257 (89%)	206 (90%)	22 (10%)	0	100	100
20	7	211/241 (88%)	201 (95%)	10 (5%)	0	100	100
21	8	215/243 (88%)	209 (97%)	6 (3%)	0	100	100
22	9	181/213 (85%)	167 (92%)	14 (8%)	0	100	100
23	W	218/249 (88%)	204 (94%)	14 (6%)	0	100	100
23	X	218/249 (88%)	204 (94%)	13 (6%)	1 (0%)	24	43
24	U	217/257 (84%)	197 (91%)	19 (9%)	1 (0%)	24	43
24	Y	218/257 (85%)	202 (93%)	15 (7%)	1 (0%)	24	43
25	Z	229/256 (90%)	223 (97%)	6 (3%)	0	100	100
26	V	235/268 (88%)	220 (94%)	15 (6%)	0	100	100
All	All	5938/6936 (86%)	5655 (95%)	280 (5%)	3 (0%)	49	69

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
23	X	167	GLU
24	Y	114	GLY
24	U	174	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	601/610 (98%)	601 (100%)	0	100 100
2	B	596/597 (100%)	594 (100%)	2 (0%)	86 94
3	C	69/70 (99%)	69 (100%)	0	100 100
4	D	120/152 (79%)	119 (99%)	1 (1%)	73 86
5	E	54/81 (67%)	53 (98%)	1 (2%)	50 73
6	F	127/169 (75%)	127 (100%)	0	100 100
7	G	70/94 (74%)	70 (100%)	0	100 100
8	H	81/102 (79%)	80 (99%)	1 (1%)	63 80
9	I	33/76 (43%)	33 (100%)	0	100 100
10	J	37/37 (100%)	37 (100%)	0	100 100
11	K	59/80 (74%)	59 (100%)	0	100 100
12	L	121/148 (82%)	120 (99%)	1 (1%)	73 86
13	O	78/101 (77%)	78 (100%)	0	100 100
14	1	137/162 (85%)	136 (99%)	1 (1%)	76 88
14	a	137/162 (85%)	137 (100%)	0	100 100
15	2	173/198 (87%)	173 (100%)	0	100 100
16	3	167/230 (73%)	166 (99%)	1 (1%)	78 89
17	4	165/205 (80%)	165 (100%)	0	100 100
18	5	184/206 (89%)	181 (98%)	3 (2%)	55 76
19	6	184/203 (91%)	182 (99%)	2 (1%)	65 81
20	7	164/181 (91%)	163 (99%)	1 (1%)	78 89
21	8	163/183 (89%)	162 (99%)	1 (1%)	78 89
22	9	140/159 (88%)	140 (100%)	0	100 100
23	W	163/187 (87%)	163 (100%)	0	100 100
23	X	165/187 (88%)	163 (99%)	2 (1%)	63 80
24	U	168/194 (87%)	166 (99%)	2 (1%)	63 80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
24	Y	170/194 (88%)	167 (98%)	3 (2%)	51 74
25	Z	178/195 (91%)	178 (100%)	0	100 100
26	V	178/201 (89%)	178 (100%)	0	100 100
All	All	4682/5364 (87%)	4660 (100%)	22 (0%)	78 90

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
21	8	154	PHE
24	Y	81	GLU
23	X	186	ASP
24	Y	119	GLU
14	1	225	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
15	2	240	ASN
20	7	113	ASN
26	V	158	GLN
16	3	256	ASN
18	5	138	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	TPO	V	33	26	8,10,11	1.54	1 (12%)	10,14,16	1.77	2 (20%)
25	TPO	Z	27	25	8,10,11	1.09	0	10,14,16	1.63	1 (10%)

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	TPO	V	33	26	-	5/9/11/13	-
25	TPO	Z	27	25	-	0/9/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	V	33	TPO	P-O1P	3.17	1.60	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	V	33	TPO	P-OG1-CB	-4.60	109.31	123.21
25	Z	27	TPO	P-OG1-CB	-4.57	109.42	123.21
26	V	33	TPO	CG2-CB-CA	-2.26	108.70	113.16

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	V	33	TPO	N-CA-CB-CG2
26	V	33	TPO	CB-OG1-P-O1P
26	V	33	TPO	CB-OG1-P-O2P
26	V	33	TPO	CB-OG1-P-O3P
26	V	33	TPO	O-C-CA-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	Z	27	TPO	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

471 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
27	CLA	A	845	29	54,58,73	1.40	8 (14%)	65,95,113	1.21	4 (6%)
33	LMG	4	624	-	40,40,55	1.05	2 (5%)	48,48,63	1.20	7 (14%)
27	CLA	Y	613	24	69,73,73	1.27	8 (11%)	83,113,113	1.16	8 (9%)
27	CLA	L	304	-	49,53,73	1.46	8 (16%)	59,89,113	1.23	5 (8%)
32	LMU	K	208	-	36,36,36	1.15	2 (5%)	47,47,47	0.97	2 (4%)
27	CLA	L	302	12	49,53,73	1.47	8 (16%)	59,89,113	1.29	5 (8%)
27	CLA	6	607	-	45,49,73	1.55	10 (22%)	57,84,113	1.37	7 (12%)
27	CLA	a	613	-	58,62,73	1.35	8 (13%)	69,99,113	1.18	6 (8%)
27	CLA	7	606	-	45,49,73	1.52	9 (20%)	54,84,113	1.31	6 (11%)
29	LHG	6	623	27	47,47,48	0.93	2 (4%)	50,53,54	0.90	3 (6%)
38	CHL	Z	601	25	70,74,74	1.91	18 (25%)	80,114,114	2.83	24 (30%)
27	CLA	A	808	1	54,58,73	1.40	8 (14%)	65,95,113	1.28	6 (9%)
27	CLA	A	854	-	69,73,73	1.25	8 (11%)	83,113,113	1.28	8 (9%)
32	LMU	5	629	-	33,33,36	1.18	2 (6%)	44,44,47	1.09	3 (6%)
36	XAT	Y	1622	-	39,47,47	0.89	1 (2%)	54,74,74	3.87	25 (46%)
27	CLA	V	610	26	66,70,73	1.29	8 (12%)	79,109,113	1.17	7 (8%)
27	CLA	A	842	1	69,73,73	1.26	9 (13%)	83,113,113	1.28	8 (9%)
30	BCR	B	849	-	41,41,41	0.72	0	56,56,56	2.49	24 (42%)
27	CLA	9	607	-	49,53,73	1.48	9 (18%)	59,89,113	1.32	7 (11%)
27	CLA	5	606	-	43,48,73	1.56	9 (20%)	51,83,113	1.25	5 (9%)
27	CLA	1	611	29	61,65,73	1.34	8 (13%)	73,103,113	1.20	6 (8%)
27	CLA	6	616	19	69,73,73	1.24	8 (11%)	83,113,113	1.28	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
35	LUT	V	1620	-	42,43,43	0.91	1 (2%)	51,60,60	1.65	11 (21%)
27	CLA	a	604	-	53,57,73	1.41	8 (15%)	62,93,113	1.21	4 (6%)
27	CLA	J	101	10	46,50,73	1.52	9 (19%)	55,85,113	1.30	7 (12%)
29	LHG	H	204	-	48,48,48	0.90	2 (4%)	51,54,54	0.90	1 (1%)
30	BCR	F	305	-	41,41,41	0.81	0	56,56,56	2.29	26 (46%)
27	CLA	W	614	23	49,53,73	1.48	9 (18%)	59,89,113	1.34	6 (10%)
27	CLA	1	607	-	43,48,73	1.52	7 (16%)	51,83,113	1.30	6 (11%)
27	CLA	F	303	-	46,50,73	1.52	10 (21%)	55,85,113	1.36	6 (10%)
27	CLA	A	843	-	68,72,73	1.27	9 (13%)	81,111,113	1.16	7 (8%)
27	CLA	3	610	16	69,73,73	1.24	9 (13%)	83,113,113	1.15	8 (9%)
27	CLA	H	202	8	42,47,73	1.57	8 (19%)	50,82,113	1.27	4 (8%)
38	CHL	Z	606	-	50,54,74	2.33	19 (38%)	56,90,114	2.82	26 (46%)
27	CLA	B	802	2	69,73,73	1.24	9 (13%)	83,113,113	1.10	5 (6%)
27	CLA	U	612	24	47,51,73	1.49	9 (19%)	56,86,113	1.31	4 (7%)
30	BCR	L	301	-	41,41,41	0.72	0	56,56,56	2.26	27 (48%)
27	CLA	1	614	14	40,45,73	1.69	10 (25%)	50,79,113	1.51	10 (20%)
30	BCR	3	620	-	41,41,41	0.85	0	56,56,56	4.30	30 (53%)
27	CLA	A	801	1	69,73,73	1.25	8 (11%)	83,113,113	1.20	8 (9%)
38	CHL	V	609	26	65,69,74	2.05	18 (27%)	74,108,114	2.81	23 (31%)
27	CLA	5	609	18	69,73,73	1.25	8 (11%)	83,113,113	1.17	5 (6%)
27	CLA	A	824	1	69,73,73	1.23	8 (11%)	83,113,113	1.22	6 (7%)
27	CLA	6	612	19	44,49,73	1.51	7 (15%)	52,84,113	1.33	6 (11%)
30	BCR	K	202	-	41,41,41	0.83	0	56,56,56	2.16	18 (32%)
30	BCR	A	851	-	41,41,41	0.88	1 (2%)	56,56,56	2.08	21 (37%)
27	CLA	a	616	14	49,53,73	1.48	7 (14%)	59,89,113	1.30	7 (11%)
27	CLA	B	816	2	58,62,73	1.34	8 (13%)	69,99,113	1.24	6 (8%)
27	CLA	A	804	1	69,73,73	1.23	9 (13%)	83,113,113	1.28	5 (6%)
27	CLA	B	827	2	66,70,73	1.26	9 (13%)	79,109,113	1.22	6 (7%)
27	CLA	1	606	-	41,47,73	1.54	9 (21%)	48,80,113	1.40	6 (12%)
27	CLA	9	604	-	54,58,73	1.47	10 (18%)	68,95,113	1.28	8 (11%)
36	XAT	U	1622	-	39,47,47	1.02	3 (7%)	54,74,74	3.93	24 (44%)
27	CLA	B	810	2	68,72,73	1.27	10 (14%)	81,111,113	1.16	5 (6%)
29	LHG	4	622	27	48,48,48	0.92	2 (4%)	51,54,54	0.89	2 (3%)
33	LMG	A	860	-	40,40,55	1.04	2 (5%)	48,48,63	1.10	4 (8%)
27	CLA	B	836	2	54,58,73	1.42	10 (18%)	65,95,113	1.33	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	CLA	A	812	1	69,73,73	1.23	8 (11%)	83,113,113	1.15	5 (6%)
27	CLA	B	830	2	47,51,73	1.48	8 (17%)	56,86,113	1.26	4 (7%)
29	LHG	Z	2630	27	48,48,48	0.94	2 (4%)	51,54,54	0.85	2 (3%)
27	CLA	a	611	29	41,46,73	1.65	10 (24%)	52,81,113	1.39	8 (15%)
27	CLA	4	602	17	64,68,73	1.30	8 (12%)	77,107,113	1.25	9 (11%)
38	CHL	X	609	23	70,74,74	1.95	18 (25%)	80,114,114	2.79	25 (31%)
30	BCR	B	845	-	41,41,41	0.81	0	56,56,56	2.13	22 (39%)
27	CLA	V	612	26	49,53,73	1.48	9 (18%)	59,89,113	1.36	8 (13%)
27	CLA	6	603	19	55,59,73	1.45	8 (14%)	69,96,113	1.33	9 (13%)
27	CLA	3	603	16	59,63,73	1.36	9 (15%)	71,101,113	1.40	8 (11%)
27	CLA	9	602	22	64,68,73	1.29	9 (14%)	77,107,113	1.25	9 (11%)
35	LUT	Z	1621	-	42,43,43	0.76	0	51,60,60	1.77	13 (25%)
27	CLA	B	814	2	66,70,73	1.25	8 (12%)	79,109,113	1.13	7 (8%)
38	CHL	Y	605	24	46,50,74	2.39	18 (39%)	51,85,114	2.96	26 (50%)
27	CLA	A	805	1	56,60,73	1.37	8 (14%)	67,97,113	1.39	6 (8%)
27	CLA	4	607	-	49,53,73	1.46	8 (16%)	59,89,113	1.33	6 (10%)
27	CLA	9	603	22	48,52,73	1.56	10 (20%)	61,88,113	1.35	8 (13%)
27	CLA	1	616	14	47,51,73	1.57	8 (17%)	60,87,113	1.41	9 (15%)
29	LHG	V	2630	27	47,47,48	0.89	2 (4%)	50,53,54	1.12	3 (6%)
27	CLA	V	614	26	49,53,73	1.50	9 (18%)	59,89,113	1.30	6 (10%)
38	CHL	X	606	-	48,52,74	2.26	17 (35%)	53,87,114	2.89	25 (47%)
35	LUT	X	1620	-	42,43,43	0.80	0	51,60,60	1.93	10 (19%)
33	LMG	J	104	-	40,40,55	1.06	2 (5%)	48,48,63	1.17	4 (8%)
27	CLA	Y	614	24	52,56,73	1.46	7 (13%)	62,92,113	1.24	6 (9%)
35	LUT	4	619	-	42,43,43	0.78	0	51,60,60	1.76	16 (31%)
27	CLA	B	808	2	69,73,73	1.22	8 (11%)	83,113,113	1.15	8 (9%)
27	CLA	Z	614	25	58,62,73	1.38	7 (12%)	69,99,113	1.18	6 (8%)
29	LHG	O	2631	-	35,35,48	1.08	2 (5%)	38,41,54	1.07	3 (7%)
27	CLA	4	604	-	58,62,73	1.41	9 (15%)	73,100,113	1.25	8 (10%)
27	CLA	A	821	1	57,61,73	1.38	8 (14%)	68,98,113	1.29	6 (8%)
27	CLA	Z	613	25	69,73,73	1.26	6 (8%)	83,113,113	1.14	6 (7%)
27	CLA	2	610	15	59,63,73	1.34	9 (15%)	71,101,113	1.30	9 (12%)
33	LMG	8	626	-	46,46,55	0.97	2 (4%)	54,54,63	1.10	4 (7%)
30	BCR	J	102	-	41,41,41	0.76	0	56,56,56	2.18	23 (41%)
27	CLA	A	834	1	69,73,73	1.24	9 (13%)	83,113,113	1.24	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	CLA	A	836	1	69,73,73	1.24	9 (13%)	83,113,113	1.18	6 (7%)
27	CLA	5	602	18	69,73,73	1.24	9 (13%)	83,113,113	1.17	6 (7%)
27	CLA	a	610	14	63,67,73	1.30	8 (12%)	76,106,113	1.21	7 (9%)
27	CLA	3	613	16	56,61,73	1.38	8 (14%)	66,98,113	1.20	7 (10%)
32	LMU	A	857	-	36,36,36	1.14	2 (5%)	47,47,47	0.98	1 (2%)
27	CLA	A	831	1	69,73,73	1.25	8 (11%)	83,113,113	1.10	5 (6%)
27	CLA	a	607	-	49,53,73	1.47	8 (16%)	59,89,113	1.26	6 (10%)
27	CLA	6	602	19	69,73,73	1.26	9 (13%)	83,113,113	1.17	7 (8%)
37	NEX	W	1623	-	38,46,46	0.91	1 (2%)	50,70,70	2.48	16 (32%)
27	CLA	A	806	1	69,73,73	1.24	9 (13%)	83,113,113	1.29	6 (7%)
27	CLA	8	608	-	55,59,73	1.40	9 (16%)	66,96,113	1.31	6 (9%)
27	CLA	B	823	2	49,53,73	1.49	9 (18%)	59,89,113	1.22	7 (11%)
27	CLA	2	613	15	69,73,73	1.23	8 (11%)	83,113,113	1.11	6 (7%)
31	SF4	A	853	1,2	0,12,12	-	-	-		
35	LUT	8	619	-	42,43,43	0.81	1 (2%)	51,60,60	1.66	13 (25%)
27	CLA	W	611	29	61,65,73	1.31	9 (14%)	73,103,113	1.25	7 (9%)
38	CHL	V	607	-	50,54,74	2.23	19 (38%)	56,90,114	2.78	26 (46%)
35	LUT	1	617	-	42,43,43	0.83	1 (2%)	51,60,60	1.77	14 (27%)
27	CLA	B	835	-	49,53,73	1.47	7 (14%)	59,89,113	1.24	5 (8%)
27	CLA	a	601	14	57,62,73	1.36	8 (14%)	68,100,113	1.21	8 (11%)
27	CLA	1	603	14	56,61,73	1.37	9 (16%)	66,98,113	1.33	7 (10%)
36	XAT	1	618	-	39,47,47	0.90	0	54,74,74	2.51	22 (40%)
38	CHL	Y	608	-	53,57,74	2.26	19 (35%)	59,93,114	2.72	27 (45%)
27	CLA	8	604	-	54,58,73	1.38	8 (14%)	65,95,113	1.29	6 (9%)
27	CLA	B	804	2	45,49,73	1.49	8 (17%)	54,84,113	1.28	5 (9%)
27	CLA	3	608	-	59,63,73	1.40	9 (15%)	71,101,113	1.21	6 (8%)
27	CLA	3	604	-	69,73,73	1.24	8 (11%)	83,113,113	1.19	5 (6%)
30	BCR	6	622	-	41,41,41	0.72	1 (2%)	56,56,56	3.46	27 (48%)
38	CHL	U	606	-	48,52,74	2.19	17 (35%)	53,87,114	2.87	25 (47%)
27	CLA	O	2002	-	41,46,73	1.66	9 (21%)	52,81,113	1.31	5 (9%)
30	BCR	3	622	-	41,41,41	0.73	0	56,56,56	2.30	19 (33%)
30	BCR	4	621	-	41,41,41	0.78	1 (2%)	56,56,56	2.47	24 (42%)
27	CLA	U	603	24	56,60,73	1.38	10 (17%)	67,97,113	1.36	6 (8%)
27	CLA	W	613	23	69,73,73	1.25	8 (11%)	83,113,113	1.19	6 (7%)
38	CHL	Z	609	25	70,74,74	2.01	18 (25%)	80,114,114	2.71	25 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	LMU	A	858	-	34,35,36	1.23	3 (8%)	42,45,47	0.92	1 (2%)
27	CLA	B	825	-	53,57,73	1.39	8 (15%)	62,93,113	1.25	6 (9%)
37	NEX	Y	1623	-	40,45,46	1.03	2 (5%)	50,67,70	2.47	16 (32%)
38	CHL	V	601	26	70,74,74	1.91	18 (25%)	80,114,114	2.84	24 (30%)
27	CLA	2	604	-	46,50,73	1.51	9 (19%)	55,85,113	1.25	6 (10%)
38	CHL	X	605	23	50,54,74	2.30	19 (38%)	56,90,114	2.84	27 (48%)
27	CLA	3	602	16	64,68,73	1.29	9 (14%)	77,107,113	1.14	7 (9%)
27	CLA	B	812	2	47,51,73	1.49	8 (17%)	56,86,113	1.32	7 (12%)
27	CLA	Y	611	29	47,51,73	1.50	7 (14%)	56,86,113	1.30	5 (8%)
27	CLA	X	614	23	46,50,73	1.51	7 (15%)	55,85,113	1.27	5 (9%)
35	LUT	Z	1620	-	42,43,43	0.75	1 (2%)	51,60,60	1.78	12 (23%)
27	CLA	2	609	15	49,53,73	1.48	8 (16%)	59,89,113	1.28	6 (10%)
38	CHL	W	609	23	70,74,74	1.94	18 (25%)	80,114,114	2.79	25 (31%)
30	BCR	a	619	-	41,41,41	0.73	0	56,56,56	2.41	22 (39%)
27	CLA	K	201	11	49,53,73	1.47	7 (14%)	59,89,113	1.19	4 (6%)
27	CLA	A	823	1	46,50,73	1.50	8 (17%)	55,85,113	1.27	5 (9%)
27	CLA	W	604	-	51,55,73	1.44	8 (15%)	61,91,113	1.26	6 (9%)
37	NEX	5	624	-	38,46,46	1.04	1 (2%)	50,70,70	2.16	13 (26%)
27	CLA	A	837	1	49,53,73	1.46	9 (18%)	59,89,113	1.37	7 (11%)
30	BCR	B	843	-	41,41,41	0.78	0	56,56,56	1.80	16 (28%)
27	CLA	5	608	-	54,58,73	1.41	9 (16%)	65,95,113	1.24	7 (10%)
27	CLA	A	841	1	69,73,73	1.23	9 (13%)	83,113,113	1.19	6 (7%)
27	CLA	7	615	-	45,50,73	1.59	8 (17%)	56,85,113	1.28	5 (8%)
27	CLA	a	606	-	47,52,73	1.49	9 (19%)	55,87,113	1.28	5 (9%)
32	LMU	1	621	-	36,36,36	1.17	2 (5%)	47,47,47	0.95	1 (2%)
27	CLA	7	613	20	69,73,73	1.24	8 (11%)	83,113,113	1.12	6 (7%)
27	CLA	5	618	18	43,48,73	1.62	9 (20%)	54,83,113	1.40	7 (12%)
27	CLA	V	611	29	47,51,73	1.47	8 (17%)	56,86,113	1.35	4 (7%)
27	CLA	A	807	1	69,73,73	1.25	10 (14%)	83,113,113	1.27	7 (8%)
27	CLA	6	606	-	43,48,73	1.56	8 (18%)	51,83,113	1.24	5 (9%)
35	LUT	a	617	-	42,43,43	0.82	1 (2%)	51,60,60	1.77	14 (27%)
27	CLA	Y	604	-	54,58,73	1.42	8 (14%)	65,95,113	1.20	7 (10%)
35	LUT	Y	1621	-	42,43,43	0.78	0	51,60,60	1.75	13 (25%)
30	BCR	A	850	-	41,41,41	0.78	1 (2%)	56,56,56	2.16	22 (39%)
27	CLA	O	2003	-	43,48,73	1.57	8 (18%)	51,83,113	1.25	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
36	XAT	5	621	-	39,47,47	0.89	1 (2%)	54,74,74	2.52	22 (40%)
27	CLA	5	616	18	45,50,73	1.58	9 (20%)	56,85,113	1.25	6 (10%)
27	CLA	A	840	1	56,60,73	1.39	9 (16%)	67,97,113	1.34	8 (11%)
27	CLA	7	610	20	69,73,73	1.23	8 (11%)	83,113,113	1.18	9 (10%)
33	LMG	J	103	-	42,42,55	1.01	2 (4%)	50,50,63	1.09	2 (4%)
27	CLA	4	610	17	65,69,73	1.27	8 (12%)	78,108,113	1.19	7 (8%)
27	CLA	U	611	29	46,50,73	1.47	9 (19%)	55,85,113	1.33	5 (9%)
27	CLA	a	609	14	67,72,73	1.27	8 (11%)	80,112,113	1.15	6 (7%)
33	LMG	9	625	-	55,55,55	0.89	2 (3%)	63,63,63	0.95	2 (3%)
33	LMG	V	2631	-	41,41,55	1.01	2 (4%)	49,49,63	1.16	4 (8%)
27	CLA	G	204	7	49,53,73	1.48	9 (18%)	59,89,113	1.36	8 (13%)
27	CLA	B	815	2	47,51,73	1.48	8 (17%)	56,86,113	1.27	4 (7%)
27	CLA	B	831	2	69,73,73	1.23	8 (11%)	83,113,113	1.27	8 (9%)
31	SF4	C	102	3	0,12,12	-	-	-		
27	CLA	B	817	2	63,67,73	1.30	9 (14%)	75,105,113	1.33	9 (12%)
27	CLA	6	610	19	69,73,73	1.26	9 (13%)	83,113,113	1.11	7 (8%)
27	CLA	7	616	20	47,51,73	1.58	9 (19%)	60,87,113	1.32	7 (11%)
27	CLA	K	204	11	49,53,73	1.47	9 (18%)	59,89,113	1.39	6 (10%)
30	BCR	A	856	-	41,41,41	0.77	0	56,56,56	2.14	19 (33%)
38	CHL	W	601	23	70,74,74	1.91	18 (25%)	80,114,114	2.90	26 (32%)
30	BCR	A	848	-	41,41,41	0.82	0	56,56,56	1.97	14 (25%)
27	CLA	Z	610	25	69,73,73	1.26	7 (10%)	83,113,113	1.17	8 (9%)
27	CLA	A	838	1	54,58,73	1.38	8 (14%)	65,95,113	1.37	8 (12%)
27	CLA	F	304	6	45,49,73	1.50	8 (17%)	54,84,113	1.34	6 (11%)
38	CHL	Z	605	25	48,52,74	2.27	18 (37%)	53,87,114	2.81	27 (50%)
27	CLA	9	613	22	69,73,73	1.26	8 (11%)	83,113,113	1.16	6 (7%)
27	CLA	V	604	-	54,58,73	1.42	8 (14%)	65,95,113	1.29	4 (6%)
27	CLA	a	614	14	58,62,73	1.36	9 (15%)	67,99,113	1.30	9 (13%)
27	CLA	3	617	16	43,48,73	1.52	8 (18%)	51,83,113	1.39	6 (11%)
27	CLA	Y	612	24	49,53,73	1.50	7 (14%)	59,89,113	1.31	6 (10%)
30	BCR	A	852	-	41,41,41	0.85	1 (2%)	56,56,56	2.47	25 (44%)
27	CLA	X	602	23	69,73,73	1.27	8 (11%)	83,113,113	1.12	5 (6%)
36	XAT	7	620	-	39,47,47	0.91	1 (2%)	54,74,74	2.48	22 (40%)
27	CLA	3	615	-	43,48,73	1.57	8 (18%)	51,83,113	1.42	7 (13%)
27	CLA	7	608	-	54,58,73	1.40	8 (14%)	65,95,113	1.25	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	CLA	B	837	2	69,73,73	1.26	9 (13%)	83,113,113	1.23	9 (10%)
30	BCR	9	621	-	41,41,41	0.76	0	56,56,56	2.08	18 (32%)
37	NEX	X	1623	-	38,46,46	0.93	1 (2%)	50,70,70	2.44	16 (32%)
27	CLA	7	607	-	46,50,73	1.48	8 (17%)	55,85,113	1.27	4 (7%)
27	CLA	2	601	15	69,73,73	1.24	6 (8%)	83,113,113	1.37	8 (9%)
27	CLA	L	303	12	69,73,73	1.24	7 (10%)	83,113,113	1.23	7 (8%)
27	CLA	X	612	23	47,51,73	1.50	8 (17%)	56,86,113	1.31	6 (10%)
30	BCR	A	849	-	41,41,41	0.82	0	56,56,56	2.24	19 (33%)
27	CLA	8	611	29	46,50,73	1.48	8 (17%)	55,85,113	1.25	5 (9%)
27	CLA	B	838	2	50,54,73	1.43	9 (18%)	60,90,113	1.36	7 (11%)
35	LUT	V	1621	-	42,43,43	0.97	2 (4%)	51,60,60	1.74	12 (23%)
27	CLA	5	607	-	69,73,73	1.25	10 (14%)	83,113,113	1.30	6 (7%)
27	CLA	8	612	21	44,49,73	1.53	8 (18%)	52,84,113	1.35	4 (7%)
38	CHL	W	607	-	69,73,74	1.98	20 (28%)	80,113,114	2.78	25 (31%)
29	LHG	8	623	-	39,39,48	1.02	2 (5%)	42,45,54	1.09	3 (7%)
27	CLA	4	613	17	69,73,73	1.25	8 (11%)	83,113,113	1.15	7 (8%)
29	LHG	B	854	-	48,48,48	0.94	2 (4%)	51,54,54	1.03	3 (5%)
27	CLA	B	822	2	46,50,73	1.48	8 (17%)	55,85,113	1.27	7 (12%)
38	CHL	U	601	24	70,74,74	1.92	18 (25%)	80,114,114	2.89	26 (32%)
30	BCR	1	619	-	41,41,41	0.72	0	56,56,56	2.42	22 (39%)
38	CHL	Y	601	24	70,74,74	1.91	18 (25%)	80,114,114	2.87	25 (31%)
27	CLA	B	840	2	69,73,73	1.25	8 (11%)	83,113,113	1.20	5 (6%)
27	CLA	H	203	-	69,73,73	1.24	8 (11%)	83,113,113	1.25	6 (7%)
38	CHL	X	607	-	70,74,74	1.92	19 (27%)	80,114,114	2.95	26 (32%)
27	CLA	8	614	21	57,61,73	1.37	9 (15%)	68,98,113	1.28	8 (11%)
30	BCR	K	207	-	41,41,41	0.75	0	56,56,56	2.93	23 (41%)
38	CHL	W	606	-	50,54,74	2.26	18 (36%)	56,90,114	4.50	28 (50%)
27	CLA	8	607	-	45,49,73	1.58	9 (20%)	57,84,113	1.37	7 (12%)
38	CHL	Z	607	-	70,74,74	1.90	18 (25%)	80,114,114	2.94	23 (28%)
27	CLA	B	839	-	69,73,73	1.25	8 (11%)	83,113,113	1.11	4 (4%)
27	CLA	8	601	21	69,73,73	1.24	8 (11%)	83,113,113	1.19	6 (7%)
27	CLA	A	835	1	65,69,73	1.29	9 (13%)	78,108,113	1.22	7 (8%)
27	CLA	2	606	-	49,53,73	1.48	9 (18%)	59,89,113	1.36	5 (8%)
30	BCR	B	801	-	41,41,41	0.84	0	56,56,56	2.10	20 (35%)
38	CHL	Y	607	-	70,74,74	1.97	20 (28%)	80,114,114	2.88	28 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	CLA	W	603	23	56,60,73	1.38	11 (19%)	67,97,113	1.37	6 (8%)
27	CLA	A	819	1	63,67,73	1.29	10 (15%)	75,105,113	1.29	7 (9%)
27	CLA	8	602	21	64,68,73	1.29	9 (14%)	77,107,113	1.20	6 (7%)
35	LUT	2	619	-	42,43,43	0.82	1 (2%)	51,60,60	1.84	11 (21%)
30	BCR	B	848	-	41,41,41	0.78	0	56,56,56	2.20	20 (35%)
34	DGD	B	850	-	63,63,67	0.84	2 (3%)	77,77,81	1.03	4 (5%)
27	CLA	8	613	21	69,73,73	1.26	9 (13%)	83,113,113	1.16	7 (8%)
29	LHG	2	622	27	35,35,48	1.08	2 (5%)	38,41,54	0.98	1 (2%)
27	CLA	K	206	11	49,53,73	1.49	7 (14%)	59,89,113	1.33	4 (6%)
27	CLA	U	602	24	63,67,73	1.30	9 (14%)	75,105,113	1.25	4 (5%)
30	BCR	8	621	-	41,41,41	0.83	0	56,56,56	2.52	17 (30%)
27	CLA	A	813	1	58,62,73	1.35	8 (13%)	69,99,113	1.29	8 (11%)
36	XAT	3	619	-	39,47,47	0.89	1 (2%)	54,74,74	2.56	22 (40%)
27	CLA	2	611	29	46,50,73	1.50	8 (17%)	55,85,113	1.30	5 (9%)
29	LHG	3	624	27	48,48,48	0.92	2 (4%)	51,54,54	0.97	3 (5%)
29	LHG	1	620	27	48,48,48	0.91	2 (4%)	51,54,54	0.97	3 (5%)
30	BCR	7	621	-	41,41,41	0.75	0	56,56,56	2.34	23 (41%)
27	CLA	L	306	-	43,48,73	1.53	8 (18%)	51,83,113	1.34	4 (7%)
27	CLA	A	825	1	69,73,73	1.24	8 (11%)	83,113,113	1.17	6 (7%)
27	CLA	Y	603	24	59,63,73	1.37	7 (11%)	71,101,113	1.26	6 (8%)
27	CLA	3	611	29	41,46,73	1.65	9 (21%)	52,81,113	1.34	6 (11%)
37	NEX	Z	1623	-	38,46,46	1.14	2 (5%)	50,70,70	2.34	15 (30%)
29	LHG	B	851	27	37,37,48	1.08	2 (5%)	40,43,54	1.13	3 (7%)
27	CLA	2	607	-	49,53,73	1.47	10 (20%)	59,89,113	1.36	5 (8%)
27	CLA	1	612	14	49,53,73	1.47	8 (16%)	59,89,113	1.28	4 (6%)
27	CLA	5	610	18	58,62,73	1.34	8 (13%)	69,99,113	1.24	8 (11%)
35	LUT	3	618	-	42,43,43	0.82	1 (2%)	51,60,60	1.67	12 (23%)
27	CLA	A	815	1	54,58,73	1.41	9 (16%)	65,95,113	1.31	4 (6%)
36	XAT	X	1622	-	39,47,47	0.91	1 (2%)	54,74,74	3.87	25 (46%)
29	LHG	W	2630	27	43,43,48	0.96	2 (4%)	46,49,54	0.96	2 (4%)
27	CLA	6	618	19	43,48,73	1.60	11 (25%)	54,83,113	1.42	7 (12%)
38	CHL	V	605	26	48,52,74	2.23	16 (33%)	53,87,114	2.79	25 (47%)
27	CLA	a	612	14	49,53,73	1.47	8 (16%)	59,89,113	1.29	4 (6%)
27	CLA	A	833	1	49,53,73	1.47	9 (18%)	59,89,113	1.35	6 (10%)
27	CLA	9	610	22	61,65,73	1.33	9 (14%)	73,103,113	1.20	9 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	LHG	Y	2630	27	48,48,48	0.95	2 (4%)	51,54,54	0.97	2 (3%)
27	CLA	5	603	18	58,62,73	1.43	10 (17%)	73,100,113	1.30	8 (10%)
29	LHG	9	622	27	29,29,48	1.19	2 (6%)	32,35,54	1.03	1 (3%)
27	CLA	B	826	2	66,70,73	1.27	9 (13%)	79,109,113	1.29	8 (10%)
27	CLA	A	829	1	69,73,73	1.24	10 (14%)	83,113,113	1.16	7 (8%)
38	CHL	Y	606	-	50,54,74	2.30	19 (38%)	56,90,114	2.82	25 (44%)
35	LUT	U	1621	-	42,43,43	0.96	2 (4%)	51,60,60	1.70	11 (21%)
27	CLA	B	811	2	57,60,73	1.48	11 (19%)	68,97,113	1.26	7 (10%)
28	PQN	A	844	-	34,34,34	3.46	11 (32%)	42,45,45	1.59	4 (9%)
27	CLA	B	828	2	69,73,73	1.25	9 (13%)	83,113,113	1.15	10 (12%)
36	XAT	Z	1622	-	39,47,47	0.90	1 (2%)	54,74,74	3.78	25 (46%)
27	CLA	7	603	20	47,52,73	1.50	9 (19%)	56,88,113	1.44	7 (12%)
27	CLA	A	817	-	49,53,73	1.46	8 (16%)	59,89,113	1.43	7 (11%)
35	LUT	6	619	-	42,43,43	0.82	1 (2%)	51,60,60	1.83	13 (25%)
27	CLA	B	834	2	64,68,73	1.29	8 (12%)	77,107,113	1.23	6 (7%)
29	LHG	7	622	27	36,36,48	1.05	2 (5%)	39,42,54	0.85	2 (5%)
27	CLA	2	612	15	48,52,73	1.50	8 (16%)	58,88,113	1.30	6 (10%)
37	NEX	6	624	-	38,46,46	1.09	1 (2%)	50,70,70	2.10	15 (30%)
27	CLA	1	613	-	69,73,73	1.24	8 (11%)	83,113,113	1.13	7 (8%)
38	CHL	U	607	-	50,54,74	2.21	16 (32%)	56,90,114	2.80	29 (51%)
35	LUT	W	1621	-	42,43,43	0.96	2 (4%)	51,60,60	1.70	12 (23%)
30	BCR	O	2005	-	41,41,41	0.80	1 (2%)	56,56,56	3.00	25 (44%)
35	LUT	W	1620	-	42,43,43	0.90	1 (2%)	51,60,60	1.83	9 (17%)
27	CLA	A	802	2	69,73,73	1.23	9 (13%)	83,113,113	1.24	6 (7%)
27	CLA	4	606	-	43,48,73	1.55	8 (18%)	51,83,113	1.31	7 (13%)
27	CLA	V	602	26	64,68,73	1.30	11 (17%)	77,107,113	1.24	8 (10%)
27	CLA	5	604	-	67,71,73	1.32	9 (13%)	84,111,113	1.20	9 (10%)
27	CLA	B	833	2	69,73,73	1.24	8 (11%)	83,113,113	1.17	9 (10%)
27	CLA	3	606	-	57,62,73	1.36	9 (15%)	68,100,113	1.22	6 (8%)
36	XAT	V	1622	-	39,47,47	0.97	2 (5%)	54,74,74	2.58	19 (35%)
27	CLA	5	613	18	68,72,73	1.26	8 (11%)	81,111,113	1.15	5 (6%)
27	CLA	W	610	23	59,63,73	1.35	9 (15%)	71,101,113	1.17	7 (9%)
29	LHG	U	2630	27	48,48,48	0.92	2 (4%)	51,54,54	0.92	2 (3%)
27	CLA	W	612	23	49,53,73	1.48	9 (18%)	59,89,113	1.32	4 (6%)
27	CLA	A	826	-	68,72,73	1.27	10 (14%)	81,111,113	1.24	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	CLA	X	603	23	66,70,73	1.30	8 (12%)	79,109,113	1.21	6 (7%)
27	CLA	3	614	16	43,48,73	1.55	10 (23%)	51,83,113	1.31	5 (9%)
27	CLA	B	819	-	59,63,73	1.36	8 (13%)	71,101,113	1.24	8 (11%)
27	CLA	1	604	-	53,57,73	1.41	8 (15%)	62,93,113	1.22	4 (6%)
27	CLA	2	603	15	47,52,73	1.54	9 (19%)	56,88,113	1.33	5 (8%)
30	BCR	O	2004	-	41,41,41	0.77	0	56,56,56	2.38	19 (33%)
35	LUT	Y	1620	-	42,43,43	0.80	1 (2%)	51,60,60	1.94	11 (21%)
31	SF4	C	101	3	0,12,12	-	-	-		
37	NEX	V	1623	-	38,46,46	0.90	2 (5%)	50,70,70	2.25	12 (24%)
27	CLA	Y	610	24	69,73,73	1.28	8 (11%)	83,113,113	1.13	8 (9%)
27	CLA	4	609	17	61,65,73	1.32	8 (13%)	73,103,113	1.23	7 (9%)
27	CLA	3	609	16	64,68,73	1.28	8 (12%)	77,107,113	1.34	8 (10%)
36	XAT	a	618	-	39,47,47	0.89	1 (2%)	54,74,74	2.51	22 (40%)
27	CLA	B	841	29	69,73,73	1.25	10 (14%)	83,113,113	1.20	6 (7%)
27	CLA	8	616	-	47,51,73	1.58	9 (19%)	60,87,113	1.33	7 (11%)
27	CLA	4	612	17	44,49,73	1.53	8 (18%)	52,84,113	1.33	4 (7%)
27	CLA	9	609	22	65,69,73	1.29	8 (12%)	78,108,113	1.17	5 (6%)
32	LMU	5	628	-	34,34,36	1.16	2 (5%)	45,45,47	1.16	6 (13%)
27	CLA	6	620	-	68,72,73	1.24	9 (13%)	81,111,113	1.12	5 (6%)
27	CLA	a	608	-	47,52,73	1.49	8 (17%)	56,88,113	1.26	6 (10%)
27	CLA	U	614	24	46,50,73	1.50	9 (19%)	55,85,113	1.31	5 (9%)
36	XAT	9	620	-	39,47,47	0.92	1 (2%)	54,74,74	2.41	20 (37%)
27	CLA	K	203	-	60,64,73	1.35	9 (15%)	72,102,113	1.32	10 (13%)
35	LUT	5	620	-	42,43,43	0.84	1 (2%)	51,60,60	1.97	11 (21%)
27	CLA	B	824	-	69,73,73	1.25	9 (13%)	83,113,113	1.16	4 (4%)
38	CHL	Y	609	24	70,74,74	1.96	18 (25%)	80,114,114	2.74	24 (30%)
30	BCR	L	308	-	41,41,41	0.82	2 (4%)	56,56,56	2.31	27 (48%)
27	CLA	U	613	24	63,67,73	1.30	8 (12%)	75,105,113	1.22	6 (8%)
27	CLA	2	614	15	45,50,73	1.51	8 (17%)	53,85,113	1.24	6 (11%)
27	CLA	4	603	17	48,52,73	1.56	9 (18%)	61,88,113	1.42	8 (13%)
27	CLA	4	601	17	69,73,73	1.24	8 (11%)	83,113,113	1.22	6 (7%)
27	CLA	F	301	-	61,65,73	1.35	9 (14%)	73,103,113	1.17	6 (8%)
30	BCR	L	305	-	41,41,41	0.75	0	56,56,56	2.07	23 (41%)
27	CLA	6	613	-	67,72,73	1.27	9 (13%)	80,112,113	1.11	6 (7%)
29	LHG	a	620	27	42,42,48	0.98	2 (4%)	45,48,54	1.01	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	CLA	6	608	-	49,53,73	1.48	8 (16%)	59,89,113	1.31	6 (10%)
27	CLA	4	611	29	46,50,73	1.49	8 (17%)	55,85,113	1.28	6 (10%)
27	CLA	X	611	29	49,53,73	1.50	7 (14%)	59,89,113	1.33	7 (11%)
27	CLA	B	829	2	69,73,73	1.24	8 (11%)	83,113,113	1.16	6 (7%)
35	LUT	7	619	-	42,43,43	0.85	2 (4%)	51,60,60	1.82	11 (21%)
27	CLA	A	818	1	64,68,73	1.27	8 (12%)	77,107,113	1.23	7 (9%)
27	CLA	A	839	1	59,63,73	1.35	9 (15%)	71,101,113	1.24	7 (9%)
27	CLA	U	604	-	53,56,73	1.49	9 (16%)	57,91,113	1.30	5 (8%)
29	LHG	X	2630	27	48,48,48	0.96	2 (4%)	51,54,54	0.97	2 (3%)
27	CLA	A	832	1	54,58,73	1.43	8 (14%)	65,95,113	1.26	9 (13%)
27	CLA	7	604	-	54,58,73	1.42	8 (14%)	65,95,113	1.22	7 (10%)
27	CLA	Z	602	25	64,68,73	1.32	7 (10%)	77,107,113	1.15	6 (7%)
27	CLA	5	617	18	54,58,73	1.40	8 (14%)	65,95,113	1.24	7 (10%)
27	CLA	A	803	-	69,73,73	1.25	8 (11%)	83,113,113	1.17	4 (4%)
27	CLA	B	805	2	69,73,73	1.25	9 (13%)	83,113,113	1.24	6 (7%)
27	CLA	6	604	-	69,73,73	1.24	8 (11%)	83,113,113	1.13	8 (9%)
33	LMG	5	627	-	40,40,55	1.05	2 (5%)	48,48,63	1.01	2 (4%)
29	LHG	3	623	-	44,44,48	0.96	2 (4%)	47,50,54	1.05	3 (6%)
30	BCR	B	844	-	41,41,41	0.87	1 (2%)	56,56,56	2.11	20 (35%)
38	CHL	X	608	-	70,74,74	1.95	19 (27%)	80,114,114	2.83	22 (27%)
27	CLA	V	613	26	69,73,73	1.27	8 (11%)	83,113,113	1.19	5 (6%)
27	CLA	6	609	19	49,53,73	1.47	9 (18%)	59,89,113	1.30	5 (8%)
27	CLA	A	809	1	69,73,73	1.21	8 (11%)	83,113,113	1.23	6 (7%)
27	CLA	8	603	21	48,52,73	1.56	10 (20%)	61,88,113	1.47	8 (13%)
36	XAT	4	620	-	39,47,47	0.88	0	54,74,74	2.49	23 (42%)
27	CLA	7	614	20	46,50,73	1.49	10 (21%)	55,85,113	1.28	7 (12%)
27	CLA	X	604	-	53,57,73	1.43	8 (15%)	62,93,113	1.20	6 (9%)
27	CLA	X	610	23	69,73,73	1.28	7 (10%)	83,113,113	1.13	8 (9%)
38	CHL	U	609	24	64,68,74	2.03	18 (28%)	72,106,114	2.90	25 (34%)
35	LUT	U	1620	-	42,43,43	0.90	1 (2%)	51,60,60	1.83	10 (19%)
27	CLA	5	601	18	60,64,73	1.33	8 (13%)	72,102,113	1.34	7 (9%)
36	XAT	2	620	-	39,47,47	0.93	0	54,74,74	2.50	21 (38%)
27	CLA	5	614	18	48,52,73	1.49	8 (16%)	55,87,113	1.32	8 (14%)
27	CLA	Z	612	25	69,73,73	1.27	5 (7%)	83,113,113	1.13	4 (4%)
27	CLA	X	613	23	69,73,73	1.27	8 (11%)	83,113,113	1.16	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	CLA	B	818	2	64,68,73	1.28	8 (12%)	77,107,113	1.36	8 (10%)
38	CHL	Z	608	-	54,58,74	2.22	17 (31%)	59,94,114	2.70	26 (44%)
27	CLA	A	822	-	69,73,73	1.26	9 (13%)	83,113,113	1.30	11 (13%)
38	CHL	W	605	23	50,54,74	2.26	17 (34%)	56,90,114	2.86	26 (46%)
27	CLA	1	610	14	42,47,73	1.53	8 (19%)	51,81,113	1.47	8 (15%)
27	CLA	4	608	-	69,73,73	1.26	8 (11%)	83,113,113	1.18	8 (9%)
27	CLA	7	609	20	47,52,73	1.48	8 (17%)	55,87,113	1.24	5 (9%)
27	CLA	Z	603	25	69,73,73	1.24	7 (10%)	83,113,113	1.24	4 (4%)
27	CLA	A	816	1	69,73,73	1.26	8 (11%)	83,113,113	1.24	5 (6%)
27	CLA	3	612	16	47,51,73	1.51	8 (17%)	56,86,113	1.31	7 (12%)
27	CLA	4	616	17	47,51,73	1.59	8 (17%)	60,87,113	1.31	5 (8%)
27	CLA	O	2001	13	40,46,73	1.59	8 (20%)	48,80,113	1.31	6 (12%)
29	LHG	9	624	-	48,48,48	0.95	2 (4%)	51,54,54	1.00	2 (3%)
27	CLA	1	608	-	47,52,73	1.50	8 (17%)	56,88,113	1.26	6 (10%)
38	CHL	U	605	24	47,51,74	2.24	16 (34%)	52,86,114	2.95	26 (50%)
38	CHL	W	608	-	51,55,74	2.22	16 (31%)	57,91,114	2.70	25 (43%)
27	CLA	6	617	19	49,53,73	1.46	8 (16%)	59,89,113	1.26	5 (8%)
29	LHG	A	847	27	29,29,48	1.17	2 (6%)	32,35,54	1.04	2 (6%)
27	CLA	4	614	17	60,64,73	1.34	8 (13%)	72,102,113	1.25	9 (12%)
27	CLA	Z	611	29	69,73,73	1.24	5 (7%)	83,113,113	1.14	5 (6%)
32	LMU	8	625	-	36,36,36	1.15	2 (5%)	47,47,47	1.02	3 (6%)
35	LUT	X	1621	-	42,43,43	0.79	1 (2%)	51,60,60	1.75	13 (25%)
27	CLA	5	619	-	47,51,73	1.58	8 (17%)	60,87,113	1.38	9 (15%)
38	CHL	V	606	-	48,52,74	2.17	17 (35%)	53,87,114	2.91	23 (43%)
27	CLA	1	602	14	65,69,73	1.29	9 (13%)	78,108,113	1.20	6 (7%)
27	CLA	9	611	29	46,50,73	1.50	8 (17%)	55,85,113	1.26	4 (7%)
27	CLA	6	611	29	46,50,73	1.49	9 (19%)	55,85,113	1.29	6 (10%)
27	CLA	B	821	2	47,51,73	1.60	10 (21%)	55,86,113	1.32	7 (12%)
27	CLA	8	610	21	64,68,73	1.27	8 (12%)	77,107,113	1.32	9 (11%)
27	CLA	a	602	14	65,69,73	1.28	9 (13%)	78,108,113	1.19	6 (7%)
27	CLA	9	612	22	44,49,73	1.53	7 (15%)	52,84,113	1.35	5 (9%)
30	BCR	B	847	-	41,41,41	0.82	0	56,56,56	2.08	15 (26%)
29	LHG	8	622	27	48,48,48	0.92	2 (4%)	51,54,54	0.85	2 (3%)
38	CHL	X	601	23	70,74,74	1.91	18 (25%)	80,114,114	2.88	24 (30%)
29	LHG	9	623	-	48,48,48	0.92	2 (4%)	51,54,54	1.06	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	CLA	a	603	14	58,62,73	1.36	9 (15%)	69,99,113	1.35	7 (10%)
27	CLA	A	811	1	69,73,73	1.23	8 (11%)	83,113,113	1.13	7 (8%)
30	BCR	L	309	-	41,41,41	0.68	0	56,56,56	1.97	18 (32%)
27	CLA	W	602	23	64,68,73	1.29	9 (14%)	77,107,113	1.24	4 (5%)
27	CLA	Z	604	-	61,65,73	1.35	6 (9%)	73,103,113	1.20	7 (9%)
27	CLA	9	601	22	49,53,73	1.48	8 (16%)	59,89,113	1.31	8 (13%)
36	XAT	W	1622	-	39,47,47	1.01	3 (7%)	54,74,74	3.94	24 (44%)
27	CLA	U	610	24	60,64,73	1.35	9 (15%)	72,102,113	1.18	7 (9%)
27	CLA	B	803	-	69,73,73	1.23	9 (13%)	83,113,113	1.14	4 (4%)
29	LHG	A	846	-	48,48,48	0.91	2 (4%)	51,54,54	0.90	2 (3%)
27	CLA	2	616	-	47,51,73	1.57	9 (19%)	60,87,113	1.31	7 (11%)
27	CLA	B	820	2	54,58,73	1.39	9 (16%)	65,95,113	1.32	8 (12%)
29	LHG	5	623	27	48,48,48	0.92	2 (4%)	51,54,54	0.83	2 (3%)
27	CLA	3	607	16	60,64,73	1.38	9 (15%)	75,102,113	1.32	9 (12%)
27	CLA	5	611	29	46,50,73	1.48	8 (17%)	55,85,113	1.26	6 (10%)
30	BCR	2	623	-	41,41,41	0.78	0	56,56,56	2.33	21 (37%)
27	CLA	B	809	2	69,73,73	1.26	9 (13%)	83,113,113	1.24	7 (8%)
27	CLA	2	602	15	67,72,73	1.25	10 (14%)	80,112,113	1.17	4 (5%)
36	XAT	6	621	-	39,47,47	0.87	0	54,74,74	2.39	20 (37%)
27	CLA	Y	602	24	62,66,73	1.34	7 (11%)	74,104,113	1.16	5 (6%)
33	LMG	L	2631	-	37,37,55	1.10	2 (5%)	45,45,63	1.11	3 (6%)
30	BCR	G	205	-	41,41,41	0.79	0	56,56,56	1.96	15 (26%)
38	CHL	U	608	-	48,52,74	2.21	16 (33%)	53,87,114	2.76	23 (43%)
27	CLA	6	614	19	64,68,73	1.30	8 (12%)	77,107,113	1.18	9 (11%)
33	LMG	4	623	-	40,40,55	1.05	2 (5%)	48,48,63	1.14	4 (8%)
27	CLA	1	601	14	57,62,73	1.37	9 (15%)	68,100,113	1.20	8 (11%)
27	CLA	B	813	2	69,73,73	1.27	10 (14%)	83,113,113	1.22	8 (9%)
27	CLA	1	609	14	44,48,73	1.60	9 (20%)	56,83,113	1.41	8 (14%)
27	CLA	8	606	-	68,72,73	1.26	9 (13%)	82,112,113	1.15	6 (7%)
27	CLA	7	611	29	63,67,73	1.29	8 (12%)	75,105,113	1.16	8 (10%)
27	CLA	V	603	26	49,53,73	1.48	10 (20%)	59,89,113	1.40	3 (5%)
29	LHG	5	625	-	48,48,48	0.93	2 (4%)	51,54,54	1.06	3 (5%)
30	BCR	3	621	-	41,41,41	0.81	0	56,56,56	1.79	14 (25%)
35	LUT	9	619	-	42,43,43	0.79	0	51,60,60	1.73	14 (27%)
27	CLA	L	307	-	43,48,73	1.55	8 (18%)	51,83,113	1.36	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	CLA	G	203	7	46,50,73	1.50	8 (17%)	55,85,113	1.34	5 (9%)
27	CLA	B	806	2	69,73,73	1.26	9 (13%)	83,113,113	1.23	5 (6%)
27	CLA	6	601	19	69,73,73	1.25	8 (11%)	83,113,113	1.21	8 (9%)
27	CLA	5	612	18	44,49,73	1.52	8 (18%)	52,84,113	1.29	3 (5%)
27	CLA	A	827	-	62,66,73	1.32	9 (14%)	74,104,113	1.22	7 (9%)
28	PQN	B	842	-	34,34,34	3.39	10 (29%)	42,45,45	1.59	6 (14%)
27	CLA	A	810	1	54,58,73	1.43	10 (18%)	65,95,113	1.35	8 (12%)
30	BCR	7	623	-	41,41,41	0.68	0	56,56,56	2.22	26 (46%)
30	BCR	B	853	-	41,41,41	0.75	0	56,56,56	1.70	13 (23%)
37	NEX	U	1623	-	38,46,46	0.93	2 (5%)	50,70,70	2.48	15 (30%)
27	CLA	8	609	21	49,53,73	1.46	8 (16%)	59,89,113	1.28	7 (11%)
27	CLA	A	820	1	69,73,73	1.25	8 (11%)	83,113,113	1.23	6 (7%)
27	CLA	7	601	20	64,68,73	1.27	9 (14%)	77,107,113	1.31	9 (11%)
27	CLA	B	807	2	56,60,73	1.38	9 (16%)	67,97,113	1.33	10 (14%)
36	XAT	8	620	-	39,47,47	0.95	1 (2%)	54,74,74	2.56	26 (48%)
38	CHL	V	608	-	52,56,74	2.19	18 (34%)	58,92,114	2.67	25 (43%)
27	CLA	A	830	1	69,73,73	1.25	9 (13%)	83,113,113	1.25	6 (7%)
30	BCR	5	622	-	41,41,41	0.73	0	56,56,56	2.34	21 (37%)
27	CLA	9	606	-	43,48,73	1.57	8 (18%)	51,83,113	1.34	6 (11%)
30	BCR	B	846	-	41,41,41	0.76	1 (2%)	56,56,56	2.23	21 (37%)
27	CLA	A	828	1	69,73,73	1.24	10 (14%)	83,113,113	1.18	7 (8%)
27	CLA	B	832	2	64,68,73	1.30	8 (12%)	77,107,113	1.23	9 (11%)
27	CLA	7	612	20	48,52,73	1.50	8 (16%)	58,88,113	1.33	3 (5%)
27	CLA	9	614	22	49,53,73	1.48	8 (16%)	59,89,113	1.33	9 (15%)
33	LMG	H	205	-	55,55,55	0.89	2 (3%)	63,63,63	1.12	6 (9%)
27	CLA	7	602	20	69,73,73	1.24	10 (14%)	83,113,113	1.15	4 (4%)
27	CLA	4	618	17	43,48,73	1.60	8 (18%)	54,83,113	1.44	7 (12%)
30	BCR	B	852	-	41,41,41	0.80	0	56,56,56	3.56	24 (42%)
27	CLA	A	814	1	69,73,73	1.26	9 (13%)	83,113,113	1.29	8 (9%)

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
27	CLA	A	845	29	-	4/21/97/115	-
33	LMG	4	624	-	-	8/35/55/70	0/1/1/1
27	CLA	Y	613	24	-	18/39/115/115	-
27	CLA	L	304	-	-	1/15/91/115	-
32	LMU	K	208	-	-	14/21/61/61	0/2/2/2
27	CLA	L	302	12	-	4/15/91/115	-
27	CLA	6	607	-	-	5/10/86/115	-
27	CLA	a	613	-	-	10/26/102/115	-
27	CLA	7	606	-	-	2/10/86/115	-
29	LHG	6	623	27	-	25/52/52/53	-
38	CHL	Z	601	25	-	22/41/117/117	-
27	CLA	A	808	1	-	3/21/97/115	-
27	CLA	A	854	-	-	13/39/115/115	-
32	LMU	5	629	-	-	11/18/58/61	0/2/2/2
36	XAT	Y	1622	-	-	0/31/93/93	0/4/4/4
27	CLA	V	610	26	-	7/36/112/115	-
27	CLA	A	842	1	-	18/39/115/115	-
30	BCR	B	849	-	-	3/29/63/63	0/2/2/2
27	CLA	9	607	-	-	8/15/91/115	-
27	CLA	5	606	-	-	3/8/84/115	-
27	CLA	1	611	29	-	7/30/106/115	-
27	CLA	6	616	19	-	22/39/115/115	-
35	LUT	V	1620	-	-	0/29/67/67	0/2/2/2
27	CLA	a	604	-	-	11/20/96/115	-
27	CLA	J	101	10	-	6/12/88/115	-
29	LHG	H	204	-	-	17/53/53/53	-
30	BCR	F	305	-	-	6/29/63/63	0/2/2/2
27	CLA	W	614	23	-	5/15/91/115	-
27	CLA	1	607	-	-	1/8/84/115	-
27	CLA	F	303	-	-	6/12/88/115	-
27	CLA	A	843	-	-	13/37/113/115	-
27	CLA	3	610	16	-	12/39/115/115	-
27	CLA	H	202	8	-	3/6/82/115	-
38	CHL	Z	606	-	-	4/17/93/117	-
27	CLA	B	802	2	-	22/39/115/115	-
27	CLA	U	612	24	-	4/13/89/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	BCR	L	301	-	-	4/29/63/63	0/2/2/2
27	CLA	1	614	14	-	2/4/76/115	-
30	BCR	3	620	-	-	4/29/63/63	0/2/2/2
27	CLA	A	801	1	-	10/39/115/115	-
38	CHL	V	609	26	-	18/35/111/117	-
27	CLA	5	609	18	-	13/39/115/115	-
27	CLA	A	824	1	-	10/39/115/115	-
27	CLA	6	612	19	-	2/10/86/115	-
30	BCR	K	202	-	-	4/29/63/63	0/2/2/2
30	BCR	A	851	-	-	2/29/63/63	0/2/2/2
27	CLA	a	616	14	-	5/15/91/115	-
27	CLA	B	816	2	-	12/25/101/115	-
27	CLA	A	804	1	-	16/39/115/115	-
27	CLA	B	827	2	-	17/36/112/115	-
27	CLA	1	606	-	-	3/7/79/115	-
27	CLA	9	604	-	-	3/20/96/115	-
36	XAT	U	1622	-	-	1/31/93/93	0/4/4/4
27	CLA	B	810	2	-	15/37/113/115	-
29	LHG	4	622	27	-	10/53/53/53	-
33	LMG	A	860	-	-	9/35/55/70	0/1/1/1
27	CLA	B	836	2	-	4/21/97/115	-
27	CLA	A	812	1	-	6/39/115/115	-
27	CLA	B	830	2	-	4/13/89/115	-
29	LHG	Z	2630	27	-	17/53/53/53	-
27	CLA	a	611	29	-	3/4/80/115	-
27	CLA	4	602	17	-	5/33/109/115	-
38	CHL	X	609	23	-	19/41/117/117	-
30	BCR	B	845	-	-	9/29/63/63	0/2/2/2
27	CLA	V	612	26	-	4/15/91/115	-
27	CLA	6	603	19	-	4/22/98/115	-
27	CLA	3	603	16	-	6/27/103/115	-
27	CLA	9	602	22	-	7/33/109/115	-
35	LUT	Z	1621	-	-	2/29/67/67	0/2/2/2
27	CLA	B	814	2	-	10/36/112/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	CHL	Y	605	24	-	2/12/88/117	-
27	CLA	A	805	1	-	5/24/100/115	-
27	CLA	4	607	-	-	6/15/91/115	-
27	CLA	9	603	22	-	2/13/89/115	-
27	CLA	1	616	14	-	5/11/87/115	-
29	LHG	V	2630	27	-	9/52/52/53	-
27	CLA	V	614	26	-	5/15/91/115	-
38	CHL	X	606	-	-	0/15/91/117	-
35	LUT	X	1620	-	-	2/29/67/67	0/2/2/2
33	LMG	J	104	-	-	15/35/55/70	0/1/1/1
27	CLA	Y	614	24	-	9/19/95/115	-
35	LUT	4	619	-	-	4/29/67/67	0/2/2/2
27	CLA	B	808	2	-	14/39/115/115	-
27	CLA	Z	614	25	-	9/26/102/115	-
29	LHG	O	2631	-	-	17/40/40/53	-
27	CLA	4	604	-	-	8/25/101/115	-
27	CLA	A	821	1	-	14/25/101/115	-
27	CLA	Z	613	25	-	16/39/115/115	-
27	CLA	2	610	15	-	9/27/103/115	-
33	LMG	8	626	-	-	15/41/61/70	0/1/1/1
30	BCR	J	102	-	-	3/29/63/63	0/2/2/2
27	CLA	A	834	1	-	15/39/115/115	-
27	CLA	A	836	1	-	5/39/115/115	-
27	CLA	5	602	18	-	14/39/115/115	-
27	CLA	a	610	14	-	2/31/107/115	-
27	CLA	3	613	16	-	8/23/99/115	-
32	LMU	A	857	-	-	3/21/61/61	0/2/2/2
27	CLA	A	831	1	-	12/39/115/115	-
27	CLA	a	607	-	-	3/15/91/115	-
27	CLA	6	602	19	-	10/39/115/115	-
37	NEX	W	1623	-	-	4/27/83/83	0/3/3/3
27	CLA	A	806	1	-	16/39/115/115	-
27	CLA	8	608	-	-	9/23/99/115	-
27	CLA	B	823	2	-	8/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	2	613	15	-	7/39/115/115	-
31	SF4	A	853	1,2	-	-	0/6/5/5
35	LUT	8	619	-	-	1/29/67/67	0/2/2/2
27	CLA	W	611	29	-	14/30/106/115	-
38	CHL	V	607	-	-	2/17/93/117	-
35	LUT	1	617	-	-	0/29/67/67	0/2/2/2
27	CLA	B	835	-	-	5/15/91/115	-
27	CLA	a	601	14	-	4/25/101/115	-
27	CLA	1	603	14	-	4/23/99/115	-
36	XAT	1	618	-	-	0/31/93/93	0/4/4/4
38	CHL	Y	608	-	-	6/21/97/117	-
27	CLA	8	604	-	-	4/21/97/115	-
27	CLA	B	804	2	-	0/10/86/115	-
27	CLA	3	608	-	-	4/27/103/115	-
27	CLA	3	604	-	-	9/39/115/115	-
30	BCR	6	622	-	-	5/29/63/63	0/2/2/2
38	CHL	U	606	-	-	0/15/91/117	-
27	CLA	O	2002	-	-	0/4/80/115	-
30	BCR	3	622	-	-	2/29/63/63	0/2/2/2
30	BCR	4	621	-	-	4/29/63/63	0/2/2/2
27	CLA	U	603	24	-	10/24/100/115	-
27	CLA	W	613	23	-	14/39/115/115	-
38	CHL	Z	609	25	-	20/41/117/117	-
32	LMU	A	858	-	-	12/21/57/61	0/2/2/2
27	CLA	B	825	-	-	4/20/96/115	-
37	NEX	Y	1623	-	-	3/27/80/83	0/3/3/3
38	CHL	V	601	26	-	16/41/117/117	-
27	CLA	2	604	-	-	7/11/87/115	-
38	CHL	X	605	23	-	3/17/93/117	-
27	CLA	3	602	16	-	4/33/109/115	-
27	CLA	B	812	2	-	3/13/89/115	-
27	CLA	Y	611	29	-	8/13/89/115	-
27	CLA	X	614	23	-	6/12/88/115	-
35	LUT	Z	1620	-	-	0/29/67/67	0/2/2/2
27	CLA	2	609	15	-	2/15/91/115	-
38	CHL	W	609	23	-	18/41/117/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	BCR	a	619	-	-	4/29/63/63	0/2/2/2
27	CLA	K	201	11	-	6/15/91/115	-
27	CLA	A	823	1	-	4/12/88/115	-
27	CLA	W	604	-	-	4/18/94/115	-
37	NEX	5	624	-	-	2/27/83/83	0/3/3/3
27	CLA	A	837	1	-	11/15/91/115	-
30	BCR	B	843	-	-	4/29/63/63	0/2/2/2
27	CLA	5	608	-	-	6/21/97/115	-
27	CLA	A	841	1	-	18/39/115/115	-
27	CLA	7	615	-	-	6/8/84/115	-
27	CLA	a	606	-	-	4/12/88/115	-
32	LMU	1	621	-	-	7/21/61/61	0/2/2/2
27	CLA	7	613	20	-	13/39/115/115	-
27	CLA	5	618	18	-	0/8/84/115	-
27	CLA	V	611	29	-	5/13/89/115	-
27	CLA	A	807	1	-	20/39/115/115	-
27	CLA	6	606	-	-	0/8/84/115	-
35	LUT	a	617	-	-	0/29/67/67	0/2/2/2
27	CLA	Y	604	-	-	5/21/97/115	-
35	LUT	Y	1621	-	-	1/29/67/67	0/2/2/2
30	BCR	A	850	-	-	2/29/63/63	0/2/2/2
27	CLA	O	2003	-	-	4/8/84/115	-
36	XAT	5	621	-	-	0/31/93/93	0/4/4/4
27	CLA	5	616	18	-	3/8/84/115	-
27	CLA	A	840	1	-	5/24/100/115	-
27	CLA	7	610	20	-	2/39/115/115	-
33	LMG	J	103	-	-	5/37/57/70	0/1/1/1
27	CLA	4	610	17	-	8/35/111/115	-
27	CLA	U	611	29	-	8/12/88/115	-
27	CLA	a	609	14	-	14/37/113/115	-
33	LMG	9	625	-	-	16/50/70/70	0/1/1/1
33	LMG	V	2631	-	-	9/36/56/70	0/1/1/1
27	CLA	G	204	7	-	5/15/91/115	-
27	CLA	B	815	2	-	0/13/89/115	-
27	CLA	B	831	2	-	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	SF4	C	102	3	-	-	0/6/5/5
27	CLA	B	817	2	-	9/32/108/115	-
27	CLA	6	610	19	-	9/39/115/115	-
27	CLA	7	616	20	-	2/11/87/115	-
27	CLA	K	204	11	-	5/15/91/115	-
30	BCR	A	856	-	-	2/29/63/63	0/2/2/2
38	CHL	W	601	23	-	20/41/117/117	-
30	BCR	A	848	-	-	1/29/63/63	0/2/2/2
27	CLA	Z	610	25	-	11/39/115/115	-
27	CLA	A	838	1	-	7/21/97/115	-
27	CLA	F	304	6	-	6/10/86/115	-
38	CHL	Z	605	25	-	1/15/91/117	-
27	CLA	9	613	22	-	8/39/115/115	-
27	CLA	V	604	-	-	4/21/97/115	-
27	CLA	a	614	14	-	9/27/99/115	-
27	CLA	3	617	16	-	2/8/84/115	-
27	CLA	Y	612	24	-	6/15/91/115	-
30	BCR	A	852	-	-	8/29/63/63	0/2/2/2
27	CLA	X	602	23	-	10/39/115/115	-
36	XAT	7	620	-	-	0/31/93/93	0/4/4/4
27	CLA	3	615	-	-	2/8/84/115	-
27	CLA	7	608	-	-	3/21/97/115	-
27	CLA	B	837	2	-	12/39/115/115	-
30	BCR	9	621	-	-	4/29/63/63	0/2/2/2
37	NEX	X	1623	-	-	3/27/83/83	0/3/3/3
27	CLA	7	607	-	-	4/12/88/115	-
27	CLA	2	601	15	-	14/39/115/115	-
27	CLA	L	303	12	-	15/39/115/115	-
27	CLA	X	612	23	-	4/13/89/115	-
30	BCR	A	849	-	-	5/29/63/63	0/2/2/2
27	CLA	8	611	29	-	4/12/88/115	-
27	CLA	B	838	2	-	3/17/93/115	-
35	LUT	V	1621	-	-	2/29/67/67	0/2/2/2
27	CLA	5	607	-	-	14/39/115/115	-
27	CLA	8	612	21	-	2/10/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	CHL	W	607	-	-	27/39/115/117	-
29	LHG	8	623	-	-	10/44/44/53	-
27	CLA	4	613	17	-	14/39/115/115	-
29	LHG	B	854	-	-	17/53/53/53	-
27	CLA	B	822	2	-	4/12/88/115	-
38	CHL	U	601	24	-	23/41/117/117	-
30	BCR	1	619	-	-	4/29/63/63	0/2/2/2
38	CHL	Y	601	24	-	24/41/117/117	-
27	CLA	B	840	2	-	5/39/115/115	-
27	CLA	H	203	-	-	14/39/115/115	-
38	CHL	X	607	-	-	19/41/117/117	-
27	CLA	8	614	21	-	11/25/101/115	-
30	BCR	K	207	-	-	1/29/63/63	0/2/2/2
38	CHL	W	606	-	-	2/17/93/117	-
27	CLA	8	607	-	-	5/10/86/115	-
38	CHL	Z	607	-	-	21/41/117/117	-
27	CLA	B	839	-	-	16/39/115/115	-
27	CLA	8	601	21	-	16/39/115/115	-
27	CLA	A	835	1	-	13/35/111/115	-
27	CLA	2	606	-	-	5/15/91/115	-
30	BCR	B	801	-	-	4/29/63/63	0/2/2/2
38	CHL	Y	607	-	-	23/41/117/117	-
27	CLA	W	603	23	-	10/24/100/115	-
27	CLA	A	819	1	-	6/32/108/115	-
27	CLA	8	602	21	-	8/33/109/115	-
35	LUT	2	619	-	-	1/29/67/67	0/2/2/2
30	BCR	B	848	-	-	3/29/63/63	0/2/2/2
34	DGD	B	850	-	-	16/51/91/95	0/2/2/2
27	CLA	8	613	21	-	15/39/115/115	-
29	LHG	2	622	27	-	13/40/40/53	-
27	CLA	K	206	11	-	7/15/91/115	-
27	CLA	U	602	24	-	7/32/108/115	-
30	BCR	8	621	-	-	4/29/63/63	0/2/2/2
27	CLA	A	813	1	-	6/26/102/115	-
36	XAT	3	619	-	-	0/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	2	611	29	-	5/12/88/115	-
29	LHG	3	624	27	-	23/53/53/53	-
29	LHG	1	620	27	-	11/53/53/53	-
30	BCR	7	621	-	-	5/29/63/63	0/2/2/2
27	CLA	L	306	-	-	0/8/84/115	-
27	CLA	A	825	1	-	21/39/115/115	-
27	CLA	Y	603	24	-	9/27/103/115	-
27	CLA	3	611	29	-	2/4/80/115	-
37	NEX	Z	1623	-	-	3/27/83/83	0/3/3/3
29	LHG	B	851	27	-	11/42/42/53	-
27	CLA	2	607	-	-	5/15/91/115	-
27	CLA	1	612	14	-	5/15/91/115	-
27	CLA	5	610	18	-	4/26/102/115	-
35	LUT	3	618	-	-	0/29/67/67	0/2/2/2
27	CLA	A	815	1	-	10/21/97/115	-
36	XAT	X	1622	-	-	0/31/93/93	0/4/4/4
29	LHG	W	2630	27	-	10/48/48/53	-
27	CLA	6	618	19	-	0/8/84/115	-
38	CHL	V	605	26	-	0/15/91/117	-
27	CLA	a	612	14	-	5/15/91/115	-
27	CLA	A	833	1	-	5/15/91/115	-
27	CLA	9	610	22	-	5/30/106/115	-
29	LHG	Y	2630	27	-	11/53/53/53	-
27	CLA	5	603	18	-	6/25/101/115	-
29	LHG	9	622	27	-	12/34/34/53	-
27	CLA	B	826	2	-	6/36/112/115	-
27	CLA	A	829	1	-	15/39/115/115	-
38	CHL	Y	606	-	-	2/17/93/117	-
35	LUT	U	1621	-	-	1/29/67/67	0/2/2/2
27	CLA	B	811	2	-	8/23/95/115	-
28	PQN	A	844	-	-	11/23/43/43	0/2/2/2
27	CLA	B	828	2	-	15/39/115/115	-
36	XAT	Z	1622	-	-	0/31/93/93	0/4/4/4
27	CLA	7	603	20	-	3/13/89/115	-
27	CLA	A	817	-	-	4/15/91/115	-
35	LUT	6	619	-	-	0/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	B	834	2	-	7/33/109/115	-
29	LHG	7	622	27	-	21/41/41/53	-
27	CLA	2	612	15	-	7/13/89/115	-
37	NEX	6	624	-	-	2/27/83/83	0/3/3/3
27	CLA	1	613	-	-	15/39/115/115	-
38	CHL	U	607	-	-	5/17/93/117	-
35	LUT	W	1621	-	-	1/29/67/67	0/2/2/2
30	BCR	O	2005	-	-	5/29/63/63	0/2/2/2
35	LUT	W	1620	-	-	2/29/67/67	0/2/2/2
27	CLA	A	802	2	-	9/39/115/115	-
27	CLA	4	606	-	-	4/8/84/115	-
27	CLA	V	602	26	-	4/33/109/115	-
27	CLA	5	604	-	-	18/35/111/115	-
27	CLA	B	833	2	-	10/39/115/115	-
27	CLA	3	606	-	-	7/25/101/115	-
36	XAT	V	1622	-	-	0/31/93/93	0/4/4/4
27	CLA	5	613	18	-	18/37/113/115	-
27	CLA	W	610	23	-	7/27/103/115	-
29	LHG	U	2630	27	-	12/53/53/53	-
27	CLA	W	612	23	-	6/15/91/115	-
27	CLA	A	826	-	-	10/37/113/115	-
27	CLA	X	603	23	-	9/36/112/115	-
27	CLA	3	614	16	-	3/8/84/115	-
27	CLA	B	819	-	-	9/27/103/115	-
27	CLA	1	604	-	-	11/20/96/115	-
27	CLA	2	603	15	-	4/13/89/115	-
30	BCR	O	2004	-	-	3/29/63/63	0/2/2/2
35	LUT	Y	1620	-	-	2/29/67/67	0/2/2/2
31	SF4	C	101	3	-	-	0/6/5/5
37	NEX	V	1623	-	-	4/27/83/83	0/3/3/3
27	CLA	Y	610	24	-	9/39/115/115	-
27	CLA	4	609	17	-	4/30/106/115	-
27	CLA	3	609	16	-	15/33/109/115	-
36	XAT	a	618	-	-	0/31/93/93	0/4/4/4
27	CLA	B	841	29	-	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	8	616	-	-	4/11/87/115	-
27	CLA	4	612	17	-	2/10/86/115	-
27	CLA	9	609	22	-	8/35/111/115	-
32	LMU	5	628	-	-	9/19/59/61	0/2/2/2
27	CLA	6	620	-	-	11/37/113/115	-
27	CLA	a	608	-	-	5/13/89/115	-
27	CLA	U	614	24	-	6/12/88/115	-
36	XAT	9	620	-	-	0/31/93/93	0/4/4/4
27	CLA	K	203	-	-	8/29/105/115	-
35	LUT	5	620	-	-	1/29/67/67	0/2/2/2
27	CLA	B	824	-	-	13/39/115/115	-
38	CHL	Y	609	24	-	16/41/117/117	-
30	BCR	L	308	-	-	2/29/63/63	0/2/2/2
27	CLA	U	613	24	-	12/32/108/115	-
27	CLA	2	614	15	-	0/11/87/115	-
27	CLA	4	603	17	-	2/13/89/115	-
27	CLA	4	601	17	-	15/39/115/115	-
27	CLA	F	301	-	-	10/30/106/115	-
30	BCR	L	305	-	-	2/29/63/63	0/2/2/2
27	CLA	6	613	-	-	16/37/113/115	-
29	LHG	a	620	27	-	10/47/47/53	-
27	CLA	6	608	-	-	6/15/91/115	-
27	CLA	4	611	29	-	4/12/88/115	-
27	CLA	X	611	29	-	10/15/91/115	-
27	CLA	B	829	2	-	11/39/115/115	-
35	LUT	7	619	-	-	1/29/67/67	0/2/2/2
27	CLA	A	818	1	-	14/33/109/115	-
27	CLA	A	839	1	-	6/27/103/115	-
27	CLA	U	604	-	-	6/20/92/115	-
29	LHG	X	2630	27	-	11/53/53/53	-
27	CLA	A	832	1	-	8/21/97/115	-
27	CLA	7	604	-	-	9/21/97/115	-
27	CLA	Z	602	25	-	4/33/109/115	-
27	CLA	5	617	18	-	9/21/97/115	-
27	CLA	A	803	-	-	3/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	B	805	2	-	15/39/115/115	-
27	CLA	6	604	-	-	15/39/115/115	-
33	LMG	5	627	-	-	11/35/55/70	0/1/1/1
29	LHG	3	623	-	-	20/49/49/53	-
30	BCR	B	844	-	-	2/29/63/63	0/2/2/2
38	CHL	X	608	-	-	23/41/117/117	-
27	CLA	V	613	26	-	18/39/115/115	-
27	CLA	6	609	19	-	2/15/91/115	-
27	CLA	A	809	1	-	11/39/115/115	-
27	CLA	8	603	21	-	4/13/89/115	-
36	XAT	4	620	-	-	0/31/93/93	0/4/4/4
27	CLA	7	614	20	-	5/12/88/115	-
27	CLA	X	604	-	-	7/20/96/115	-
27	CLA	X	610	23	-	9/39/115/115	-
38	CHL	U	609	24	-	11/34/110/117	-
35	LUT	U	1620	-	-	2/29/67/67	0/2/2/2
27	CLA	5	601	18	-	4/29/105/115	-
36	XAT	2	620	-	-	0/31/93/93	0/4/4/4
27	CLA	5	614	18	-	10/15/87/115	-
27	CLA	Z	612	25	-	6/39/115/115	-
27	CLA	X	613	23	-	18/39/115/115	-
27	CLA	B	818	2	-	15/33/109/115	-
38	CHL	Z	608	-	-	6/22/98/117	-
27	CLA	A	822	-	-	7/39/115/115	-
38	CHL	W	605	23	-	5/17/93/117	-
27	CLA	1	610	14	-	1/8/80/115	-
27	CLA	4	608	-	-	14/39/115/115	-
27	CLA	7	609	20	-	4/12/88/115	-
27	CLA	Z	603	25	-	21/39/115/115	-
27	CLA	A	816	1	-	10/39/115/115	-
27	CLA	3	612	16	-	1/13/89/115	-
27	CLA	4	616	17	-	9/11/87/115	-
27	CLA	O	2001	13	-	3/6/78/115	-
29	LHG	9	624	-	-	20/53/53/53	-
27	CLA	1	608	-	-	5/13/89/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	CHL	U	605	24	-	3/14/90/117	-
38	CHL	W	608	-	-	5/19/95/117	-
27	CLA	6	617	19	-	9/15/91/115	-
29	LHG	A	847	27	-	7/34/34/53	-
27	CLA	4	614	17	-	11/29/105/115	-
27	CLA	Z	611	29	-	6/39/115/115	-
32	LMU	8	625	-	-	9/21/61/61	0/2/2/2
35	LUT	X	1621	-	-	1/29/67/67	0/2/2/2
27	CLA	5	619	-	-	6/11/87/115	-
38	CHL	V	606	-	-	3/15/91/117	-
27	CLA	1	602	14	-	3/35/111/115	-
27	CLA	9	611	29	-	5/12/88/115	-
27	CLA	6	611	29	-	4/12/88/115	-
27	CLA	B	821	2	-	4/13/89/115	-
27	CLA	8	610	21	-	8/33/109/115	-
27	CLA	a	602	14	-	3/35/111/115	-
27	CLA	9	612	22	-	2/10/86/115	-
30	BCR	B	847	-	-	2/29/63/63	0/2/2/2
29	LHG	8	622	27	-	9/53/53/53	-
38	CHL	X	601	23	-	24/41/117/117	-
29	LHG	9	623	-	-	16/53/53/53	-
27	CLA	a	603	14	-	3/25/101/115	-
27	CLA	A	811	1	-	11/39/115/115	-
30	BCR	L	309	-	-	1/29/63/63	0/2/2/2
27	CLA	W	602	23	-	7/33/109/115	-
27	CLA	Z	604	-	-	6/30/106/115	-
27	CLA	9	601	22	-	4/15/91/115	-
36	XAT	W	1622	-	-	1/31/93/93	0/4/4/4
27	CLA	U	610	24	-	7/29/105/115	-
27	CLA	B	803	-	-	11/39/115/115	-
29	LHG	A	846	-	-	14/53/53/53	-
27	CLA	2	616	-	-	4/11/87/115	-
27	CLA	B	820	2	-	3/21/97/115	-
29	LHG	5	623	27	-	14/53/53/53	-
27	CLA	3	607	16	-	10/28/104/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	5	611	29	-	7/12/88/115	-
30	BCR	2	623	-	-	4/29/63/63	0/2/2/2
27	CLA	B	809	2	-	15/39/115/115	-
27	CLA	2	602	15	-	9/37/113/115	-
36	XAT	6	621	-	-	0/31/93/93	0/4/4/4
27	CLA	Y	602	24	-	7/31/107/115	-
33	LMG	L	2631	-	-	8/32/52/70	0/1/1/1
30	BCR	G	205	-	-	1/29/63/63	0/2/2/2
38	CHL	U	608	-	-	3/15/91/117	-
27	CLA	6	614	19	-	11/33/109/115	-
33	LMG	4	623	-	-	5/35/55/70	0/1/1/1
27	CLA	1	601	14	-	4/25/101/115	-
27	CLA	B	813	2	-	19/39/115/115	-
27	CLA	1	609	14	-	3/8/84/115	-
27	CLA	8	606	-	-	7/37/113/115	-
27	CLA	7	611	29	-	6/31/107/115	-
27	CLA	V	603	26	-	5/15/91/115	-
29	LHG	5	625	-	-	16/53/53/53	-
30	BCR	3	621	-	-	0/29/63/63	0/2/2/2
35	LUT	9	619	-	-	1/29/67/67	0/2/2/2
27	CLA	L	307	-	-	2/8/84/115	-
27	CLA	G	203	7	-	4/12/88/115	-
27	CLA	B	806	2	-	16/39/115/115	-
27	CLA	6	601	19	-	14/39/115/115	-
27	CLA	5	612	18	-	3/10/86/115	-
27	CLA	A	827	-	-	7/31/107/115	-
28	PQN	B	842	-	-	5/23/43/43	0/2/2/2
27	CLA	A	810	1	-	10/21/97/115	-
30	BCR	7	623	-	-	4/29/63/63	0/2/2/2
30	BCR	B	853	-	-	4/29/63/63	0/2/2/2
37	NEX	U	1623	-	-	4/27/83/83	0/3/3/3
27	CLA	8	609	21	-	6/15/91/115	-
27	CLA	A	820	1	-	13/39/115/115	-
27	CLA	7	601	20	-	10/33/109/115	-
27	CLA	B	807	2	-	3/24/100/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	XAT	8	620	-	-	0/31/93/93	0/4/4/4
38	CHL	V	608	-	-	5/20/96/117	-
27	CLA	A	830	1	-	11/39/115/115	-
30	BCR	5	622	-	-	3/29/63/63	0/2/2/2
27	CLA	9	606	-	-	4/8/84/115	-
30	BCR	B	846	-	-	2/29/63/63	0/2/2/2
27	CLA	A	828	1	-	9/39/115/115	-
27	CLA	B	832	2	-	9/33/109/115	-
27	CLA	7	612	20	-	5/13/89/115	-
27	CLA	9	614	22	-	6/15/91/115	-
33	LMG	H	205	-	-	8/50/70/70	0/1/1/1
27	CLA	7	602	20	-	13/39/115/115	-
27	CLA	4	618	17	-	2/8/84/115	-
30	BCR	B	852	-	-	7/29/63/63	0/2/2/2
27	CLA	A	814	1	-	16/39/115/115	-

The worst 5 of 3337 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	A	844	PQN	C12-C13	9.80	1.56	1.33
28	B	842	PQN	C12-C13	9.64	1.56	1.33
28	B	842	PQN	O4-C4	7.84	1.39	1.23
28	A	844	PQN	O4-C4	7.82	1.39	1.23
28	A	844	PQN	O1-C1	7.65	1.39	1.23

The worst 5 of 4544 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	W	606	CHL	O2A-CGA-O1A	-17.62	79.39	123.30
30	B	852	BCR	C32-C1-C6	-14.75	86.38	110.30
38	W	606	CHL	O2A-CGA-CBA	14.42	160.37	114.03
30	6	622	BCR	C40-C30-C25	-14.02	87.56	110.30
36	U	1622	XAT	C37-C21-C36	-14.00	86.72	107.37

There are no chirality outliers.

5 of 3485 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	A	801	CLA	CBD-CGD-O2D-CED
27	A	801	CLA	O1D-CGD-O2D-CED
27	A	804	CLA	C1A-C2A-CAA-CBA
27	A	804	CLA	C3A-C2A-CAA-CBA
27	A	805	CLA	C3A-C2A-CAA-CBA

There are no ring outliers.

232 monomers are involved in 515 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	Y	613	CLA	2	0
32	K	208	LMU	1	0
38	Z	601	CHL	7	0
27	A	808	CLA	2	0
27	A	854	CLA	7	0
36	Y	1622	XAT	1	0
27	V	610	CLA	1	0
30	B	849	BCR	4	0
27	1	611	CLA	1	0
27	6	616	CLA	1	0
35	V	1620	LUT	2	0
30	F	305	BCR	8	0
27	F	303	CLA	1	0
27	A	843	CLA	1	0
38	Z	606	CHL	3	0
27	B	802	CLA	2	0
30	L	301	BCR	7	0
30	3	620	BCR	2	0
27	A	801	CLA	2	0
38	V	609	CHL	4	0
30	K	202	BCR	8	0
30	A	851	BCR	4	0
27	B	827	CLA	1	0
36	U	1622	XAT	3	0
33	A	860	LMG	1	0
27	B	836	CLA	1	0
27	A	812	CLA	1	0
27	B	830	CLA	1	0
29	Z	2630	LHG	2	0
27	a	611	CLA	1	0
38	X	609	CHL	2	0
30	B	845	BCR	3	0
27	3	603	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	Z	1621	LUT	1	0
38	Y	605	CHL	1	0
29	V	2630	LHG	2	0
38	X	606	CHL	1	0
35	X	1620	LUT	3	0
35	4	619	LUT	4	0
27	B	808	CLA	6	0
27	Z	613	CLA	2	0
27	2	610	CLA	1	0
30	J	102	BCR	10	0
27	A	834	CLA	3	0
27	5	602	CLA	1	0
32	A	857	LMU	1	0
37	W	1623	NEX	2	0
27	2	613	CLA	1	0
35	8	619	LUT	3	0
27	W	611	CLA	1	0
38	V	607	CHL	5	0
35	1	617	LUT	3	0
27	B	835	CLA	1	0
36	1	618	XAT	1	0
38	Y	608	CHL	2	0
27	8	604	CLA	1	0
27	B	804	CLA	1	0
27	3	608	CLA	1	0
30	6	622	BCR	3	0
38	U	606	CHL	2	0
30	3	622	BCR	4	0
30	4	621	BCR	3	0
27	W	613	CLA	2	0
38	Z	609	CHL	5	0
27	B	825	CLA	1	0
37	Y	1623	NEX	2	0
38	V	601	CHL	5	0
38	X	605	CHL	1	0
27	3	602	CLA	1	0
27	Y	611	CLA	3	0
35	Z	1620	LUT	3	0
38	W	609	CHL	4	0
30	a	619	BCR	2	0
27	K	201	CLA	6	0
27	W	604	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	5	624	NEX	2	0
30	B	843	BCR	7	0
27	A	841	CLA	1	0
27	7	613	CLA	3	0
27	V	611	CLA	1	0
27	6	606	CLA	1	0
35	a	617	LUT	4	0
30	A	850	BCR	5	0
36	5	621	XAT	3	0
27	4	610	CLA	2	0
27	U	611	CLA	1	0
33	V	2631	LMG	3	0
27	B	817	CLA	1	0
27	K	204	CLA	1	0
30	A	856	BCR	10	0
38	W	601	CHL	3	0
30	A	848	BCR	4	0
38	Z	605	CHL	1	0
27	9	613	CLA	1	0
27	3	617	CLA	3	0
30	A	852	BCR	11	0
36	7	620	XAT	2	0
27	7	608	CLA	1	0
27	B	837	CLA	1	0
30	9	621	BCR	5	0
37	X	1623	NEX	2	0
27	2	601	CLA	5	0
27	L	303	CLA	2	0
30	A	849	BCR	4	0
27	8	611	CLA	1	0
27	5	607	CLA	1	0
38	W	607	CHL	7	0
27	4	613	CLA	1	0
38	U	601	CHL	3	0
30	1	619	BCR	2	0
38	Y	601	CHL	3	0
27	B	840	CLA	3	0
27	H	203	CLA	1	0
38	X	607	CHL	4	0
30	K	207	BCR	9	0
38	W	606	CHL	3	0
38	Z	607	CHL	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	B	839	CLA	1	0
30	B	801	BCR	9	0
38	Y	607	CHL	6	0
27	A	819	CLA	1	0
35	2	619	LUT	2	0
30	B	848	BCR	8	0
34	B	850	DGD	3	0
27	8	613	CLA	2	0
30	8	621	BCR	3	0
36	3	619	XAT	1	0
30	7	621	BCR	3	0
27	A	825	CLA	1	0
37	Z	1623	NEX	4	0
29	B	851	LHG	1	0
35	3	618	LUT	3	0
27	6	618	CLA	1	0
38	V	605	CHL	4	0
27	9	610	CLA	3	0
27	5	603	CLA	1	0
27	B	826	CLA	2	0
27	A	829	CLA	4	0
38	Y	606	CHL	3	0
27	B	828	CLA	1	0
36	Z	1622	XAT	1	0
27	A	817	CLA	1	0
35	6	619	LUT	3	0
27	B	834	CLA	1	0
29	7	622	LHG	1	0
37	6	624	NEX	1	0
38	U	607	CHL	2	0
30	O	2005	BCR	8	0
35	W	1620	LUT	2	0
27	A	802	CLA	2	0
27	V	602	CLA	1	0
27	B	833	CLA	2	0
27	3	606	CLA	2	0
27	W	610	CLA	1	0
27	B	819	CLA	2	0
27	2	603	CLA	2	0
30	O	2004	BCR	3	0
35	Y	1620	LUT	3	0
37	V	1623	NEX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	Y	610	CLA	1	0
27	4	609	CLA	1	0
27	3	609	CLA	1	0
36	a	618	XAT	1	0
27	9	609	CLA	1	0
38	Y	609	CHL	6	0
27	U	613	CLA	2	0
27	4	601	CLA	1	0
30	L	305	BCR	6	0
27	6	613	CLA	1	0
27	X	611	CLA	3	0
35	7	619	LUT	2	0
27	A	818	CLA	1	0
27	U	604	CLA	1	0
27	5	617	CLA	1	0
27	A	803	CLA	5	0
33	5	627	LMG	1	0
29	3	623	LHG	1	0
30	B	844	BCR	4	0
38	X	608	CHL	5	0
27	V	613	CLA	1	0
27	A	809	CLA	2	0
38	U	609	CHL	7	0
35	U	1620	LUT	2	0
27	X	613	CLA	2	0
27	B	818	CLA	3	0
38	Z	608	CHL	1	0
38	W	605	CHL	3	0
27	4	608	CLA	1	0
27	A	816	CLA	4	0
27	3	612	CLA	1	0
27	4	616	CLA	1	0
29	9	624	LHG	1	0
38	U	605	CHL	3	0
38	W	608	CHL	1	0
27	4	614	CLA	1	0
35	X	1621	LUT	2	0
27	5	619	CLA	5	0
38	V	606	CHL	3	0
27	6	611	CLA	1	0
27	B	821	CLA	2	0
30	B	847	BCR	5	0

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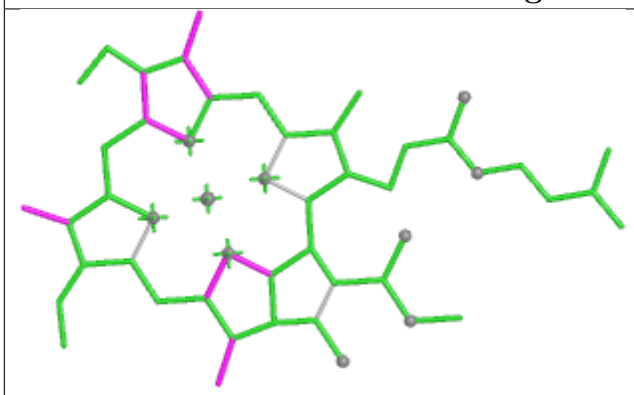
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	X	601	CHL	3	0
29	9	623	LHG	2	0
27	a	603	CLA	1	0
27	A	811	CLA	1	0
30	L	309	BCR	7	0
36	W	1622	XAT	1	0
27	B	803	CLA	4	0
30	2	623	BCR	9	0
27	B	809	CLA	1	0
36	6	621	XAT	1	0
33	L	2631	LMG	1	0
30	G	205	BCR	2	0
38	U	608	CHL	1	0
27	B	813	CLA	1	0
27	8	606	CLA	1	0
29	5	625	LHG	1	0
30	3	621	BCR	9	0
35	9	619	LUT	2	0
27	L	307	CLA	2	0
27	6	601	CLA	1	0
28	B	842	PQN	2	0
30	7	623	BCR	7	0
30	B	853	BCR	2	0
27	A	820	CLA	3	0
27	7	601	CLA	1	0
38	V	608	CHL	12	0
30	5	622	BCR	3	0
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27	B	832	CLA	2	0
27	9	614	CLA	1	0
30	B	852	BCR	5	0

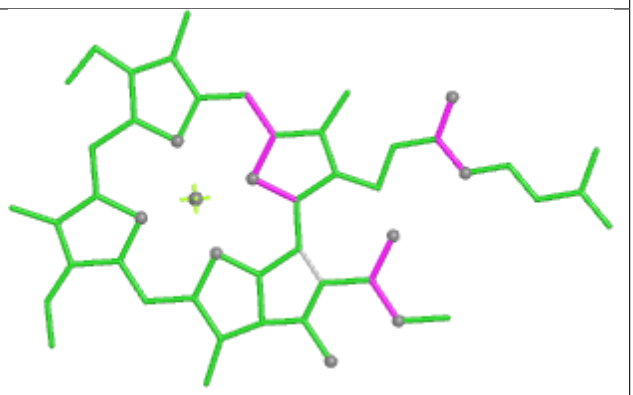
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

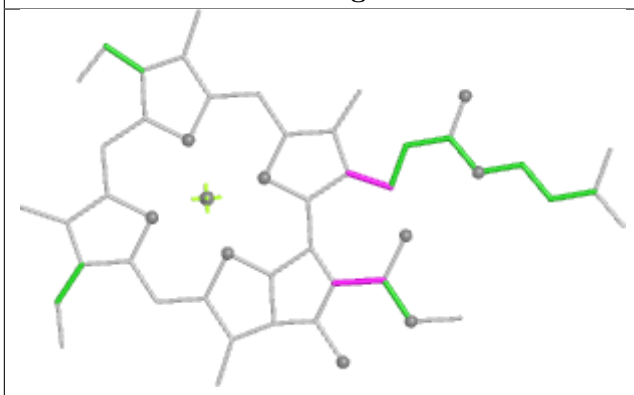
Ligand CLA A 845



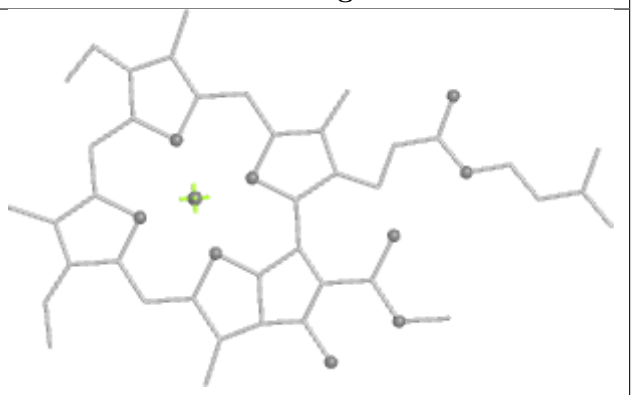
Bond lengths



Bond angles

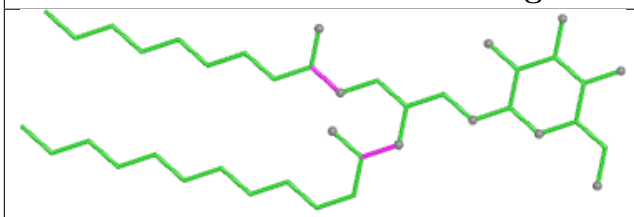


Torsions

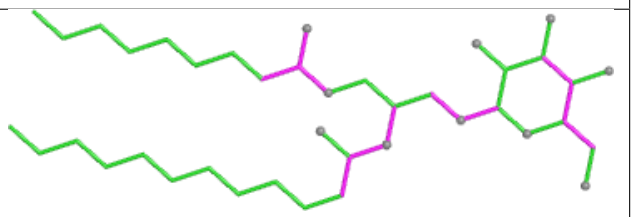


Rings

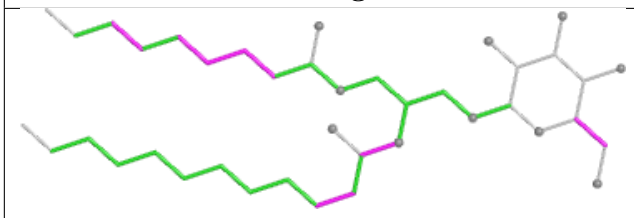
Ligand LMG 4 624



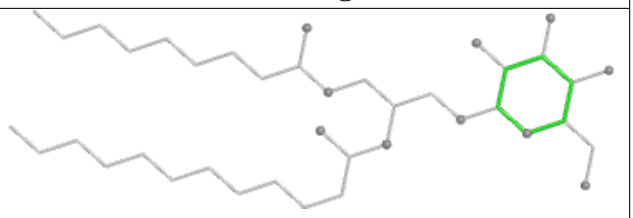
Bond lengths



Bond angles

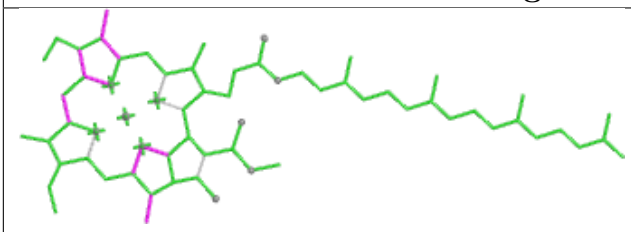


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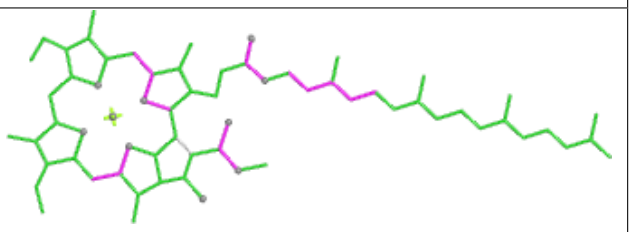


Rings

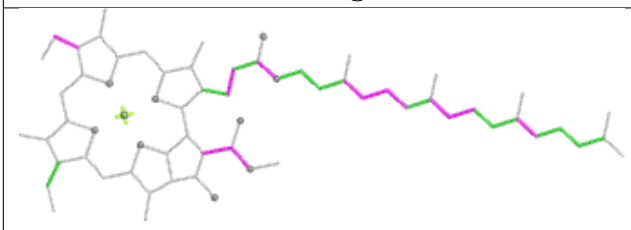
Ligand CLA Y 613



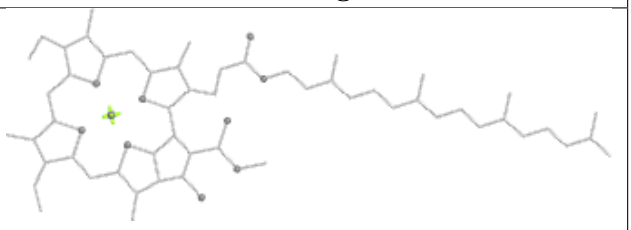
Bond lengths



Bond angles

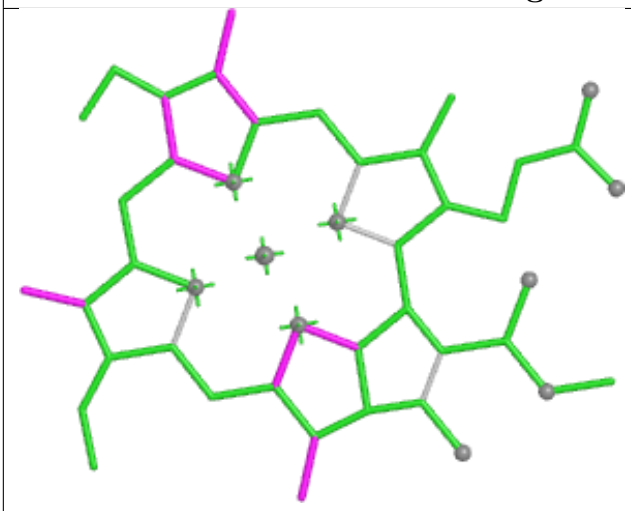


Torsions

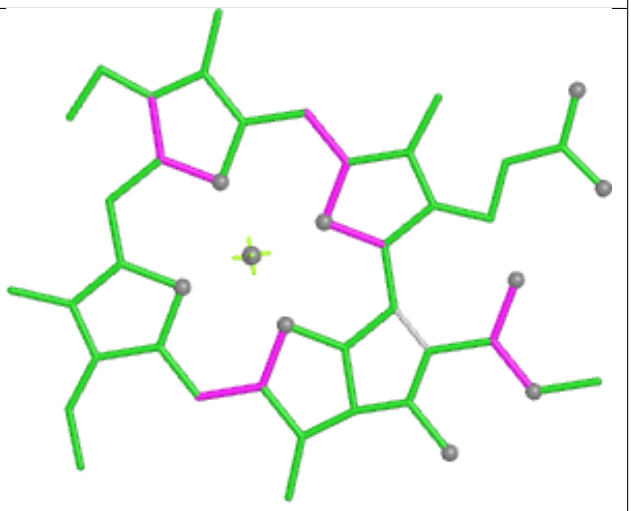


Rings

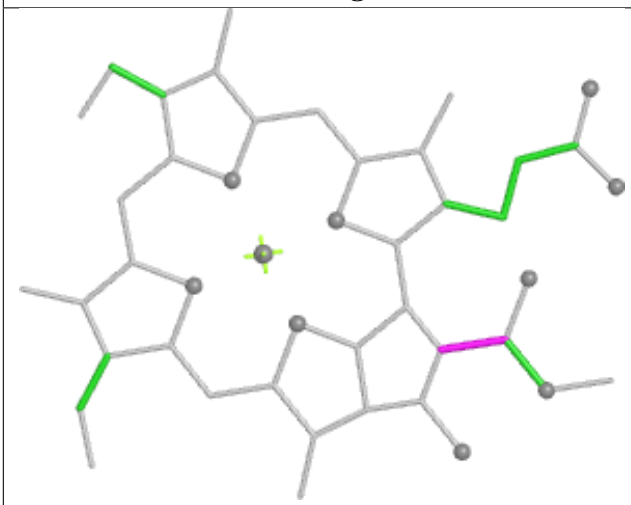
Ligand CLA L 304



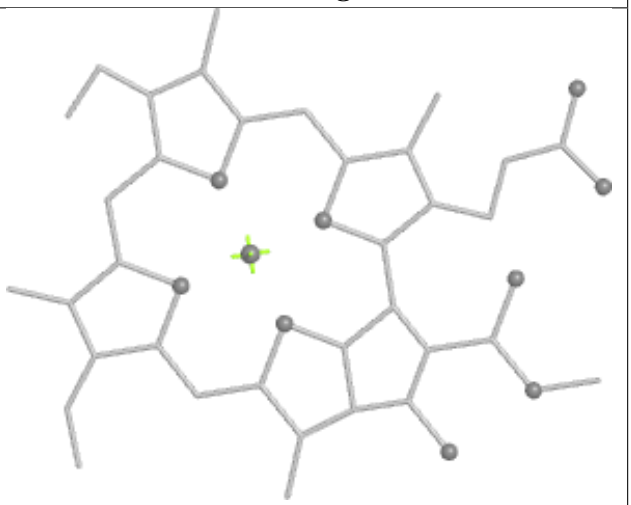
Bond lengths



Bond angles

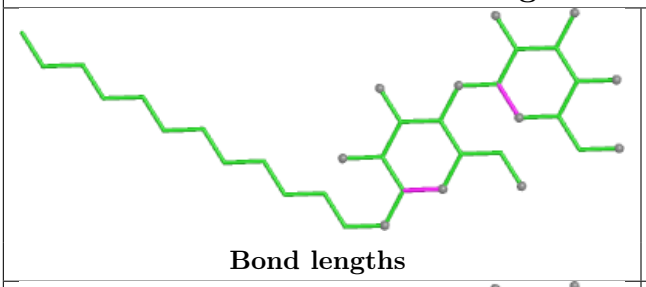


Torsions

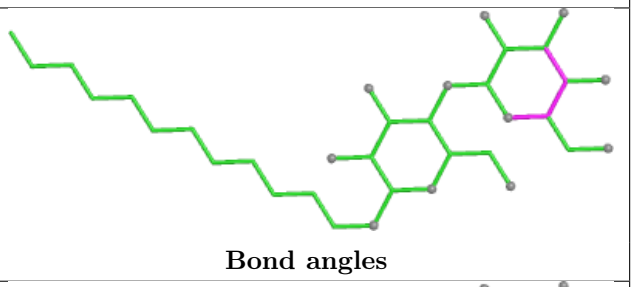


Rings

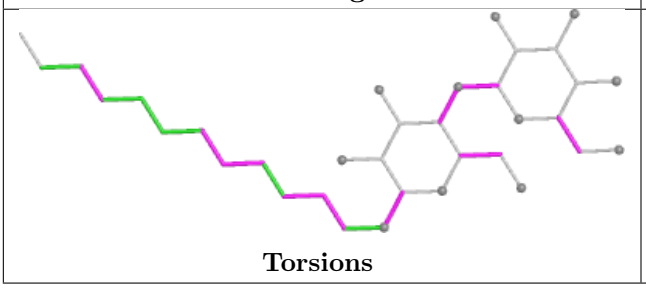
Ligand LMU K 208



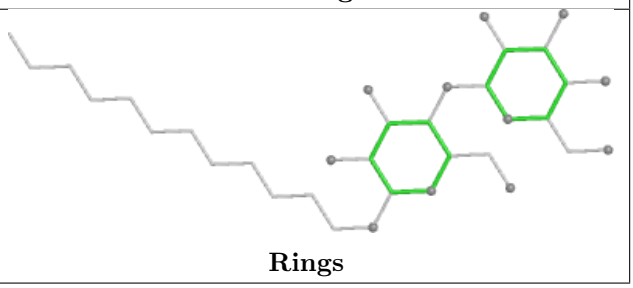
Bond lengths



Bond angles

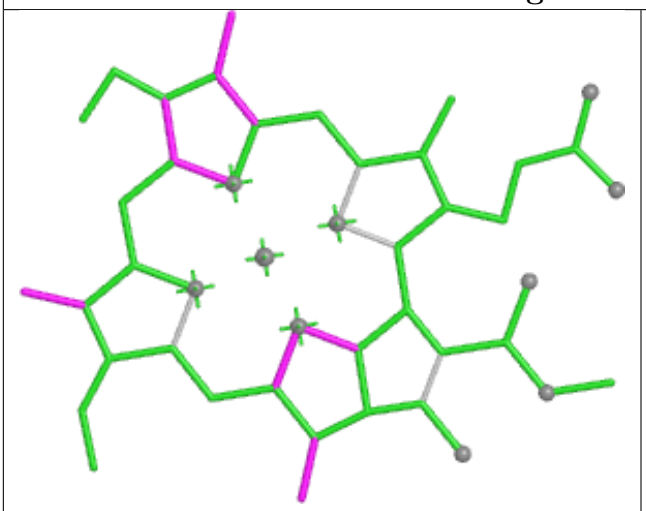


Torsions

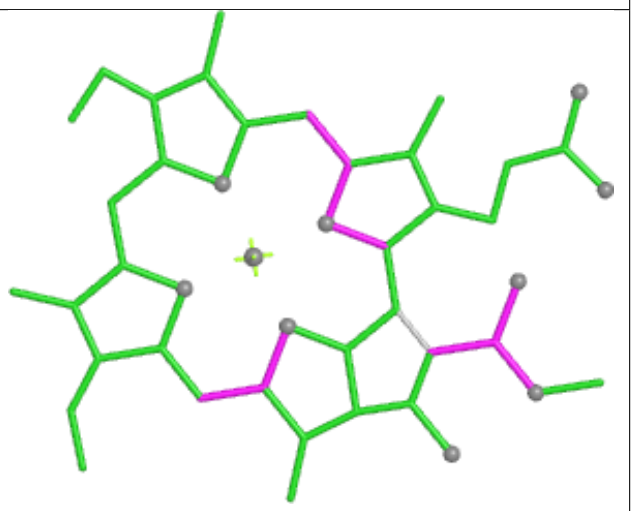


Rings

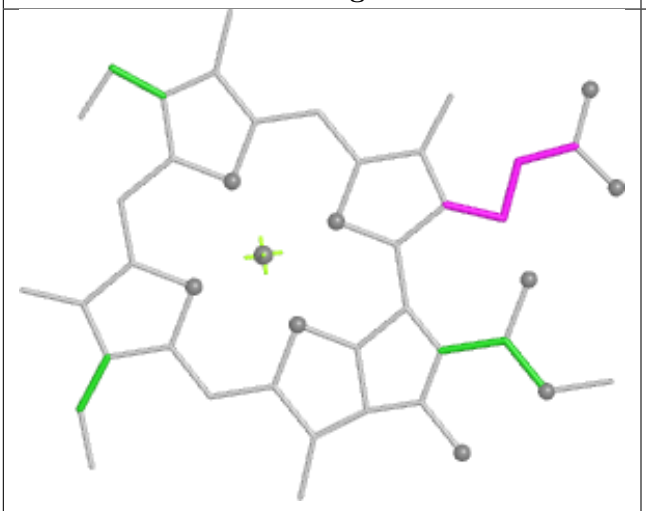
Ligand CLA L 302



Bond lengths



Bond angles

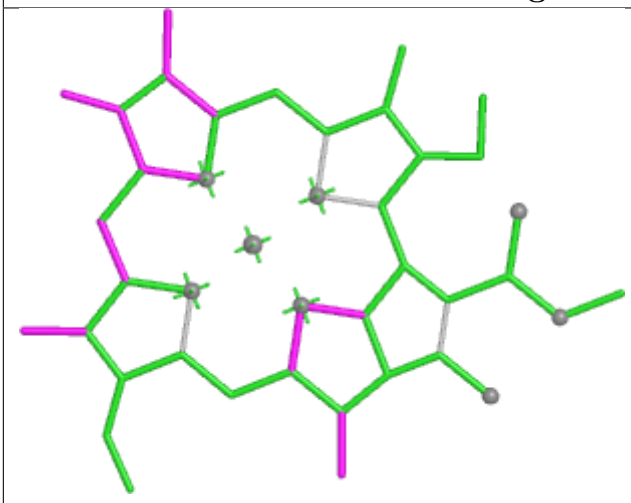


Torsions

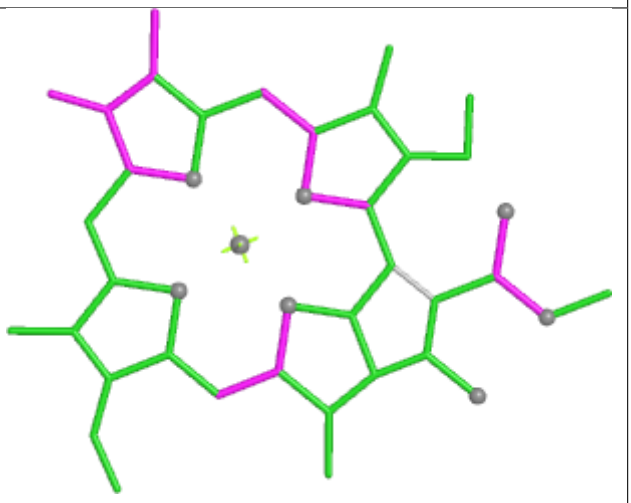


Rings

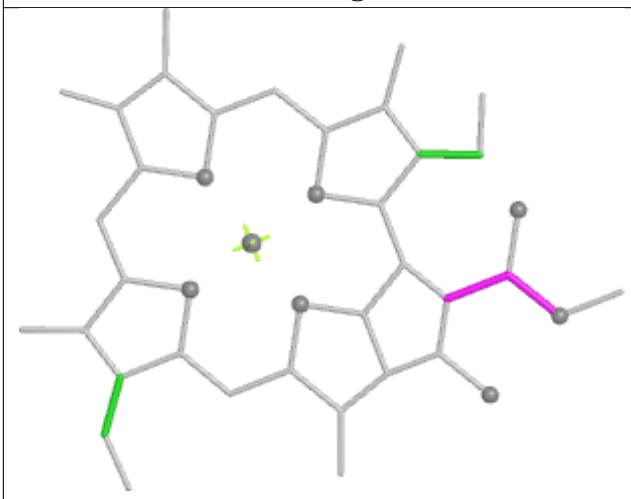
Ligand CLA 6 607



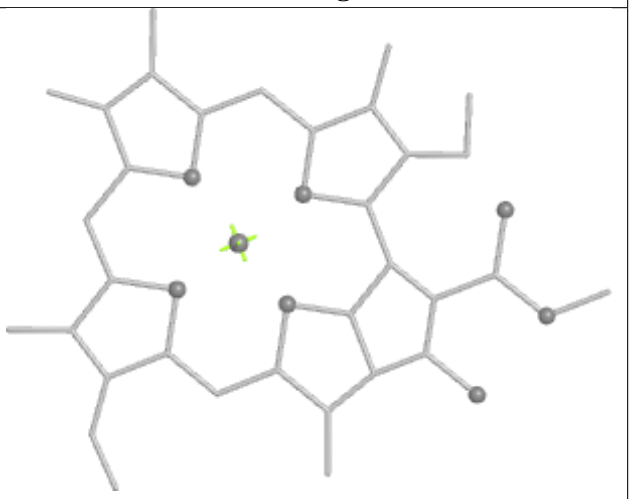
Bond lengths



Bond angles

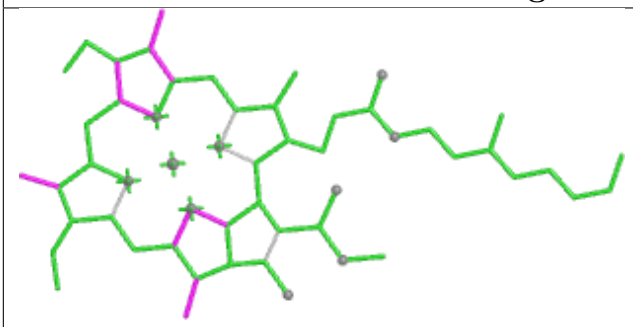


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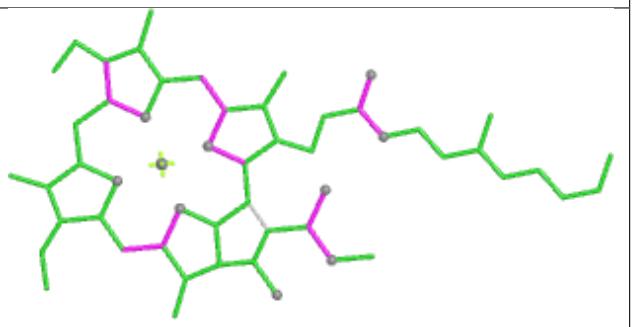


Rings

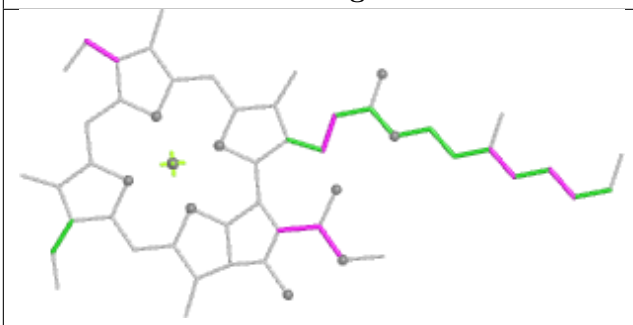
Ligand CLA a 613



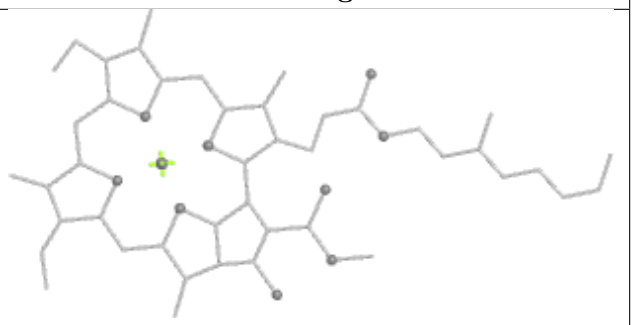
Bond lengths



Bond angles

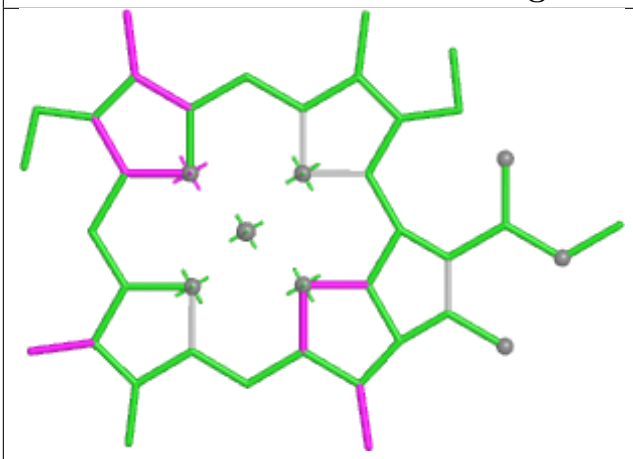


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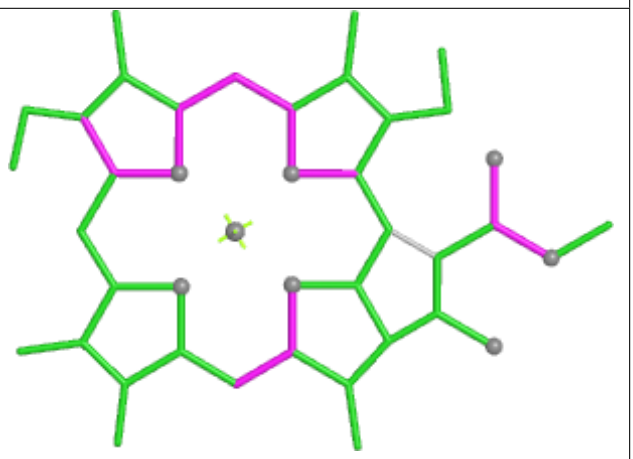


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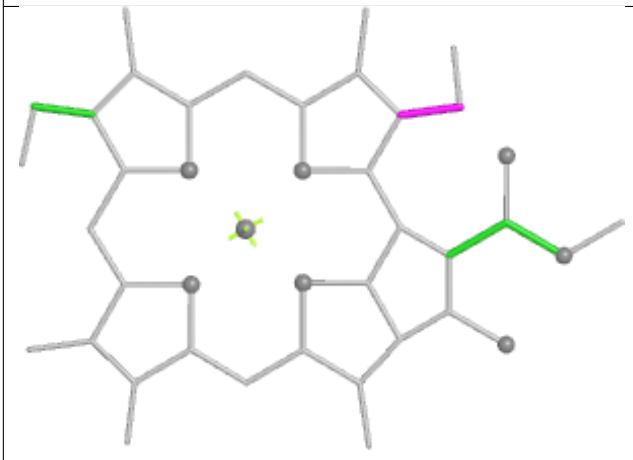
Ligand CLA 7 606



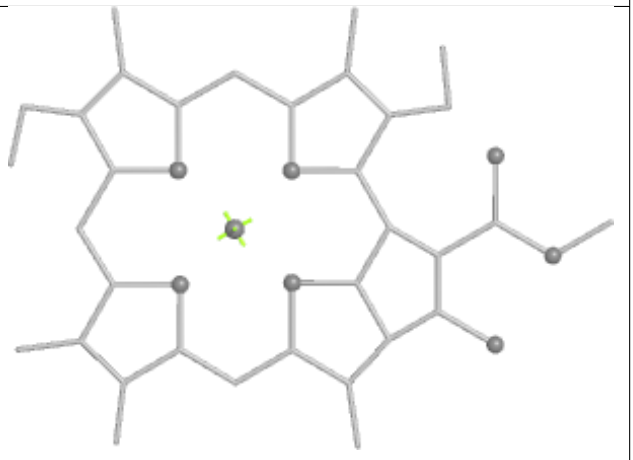
Bond lengths



Bond angles

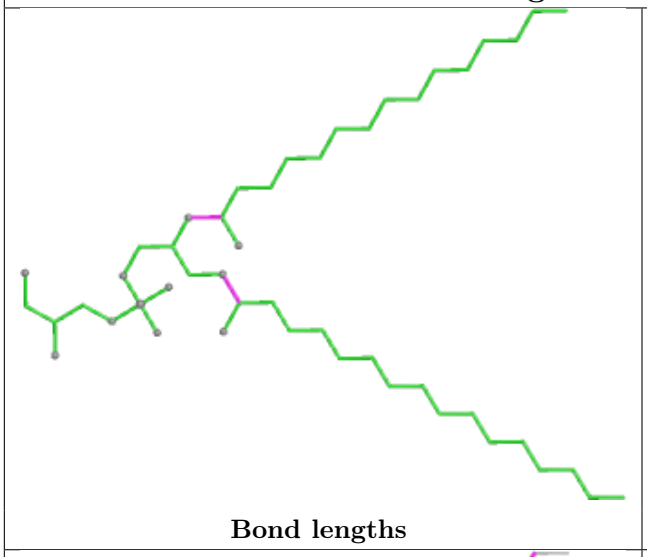


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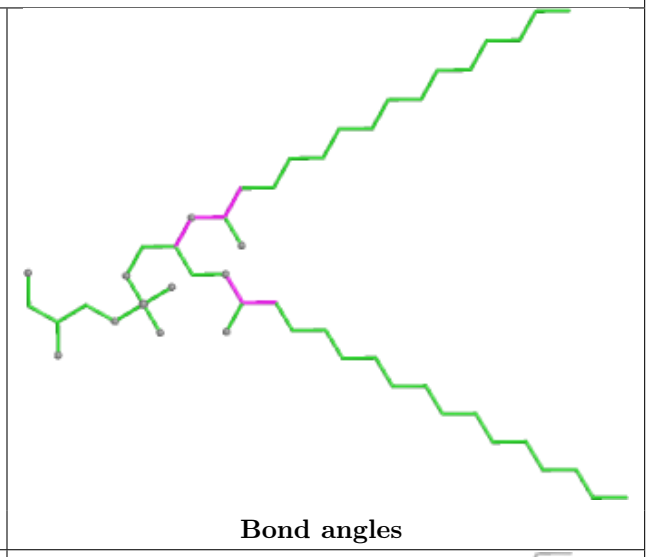


Rings

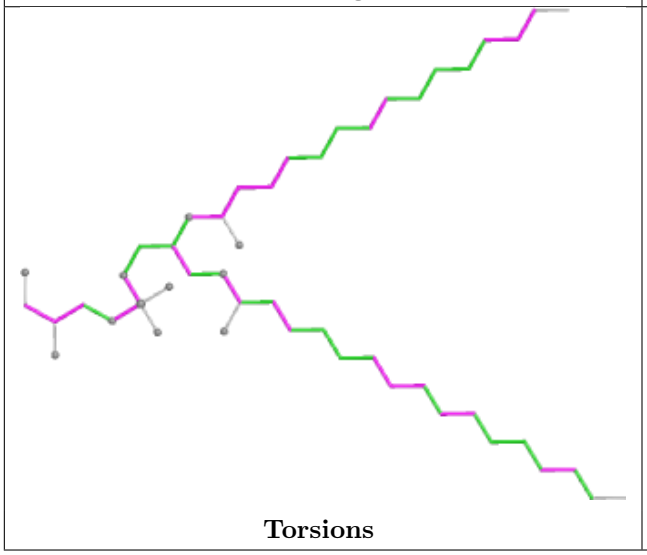
Ligand LHG 6 623



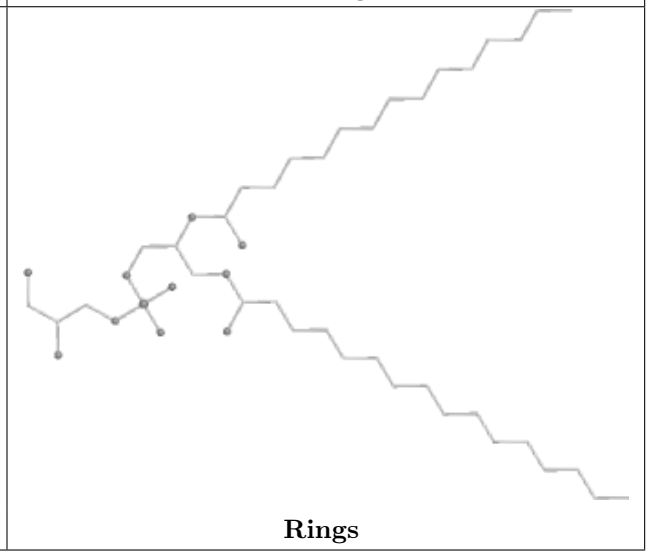
Bond lengths



Bond angles

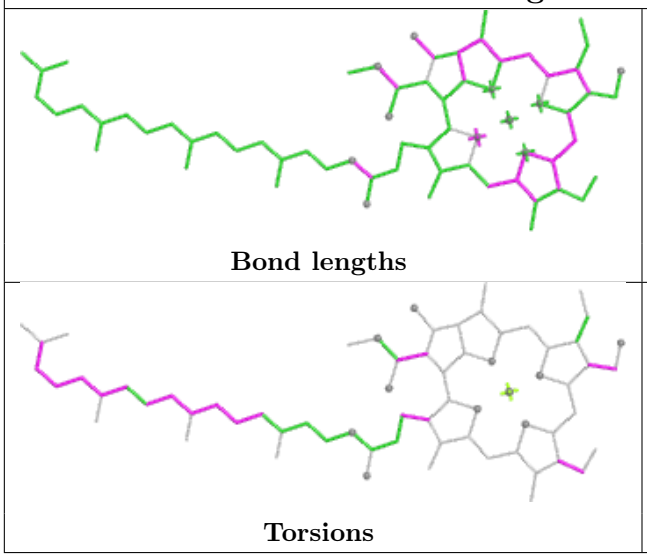


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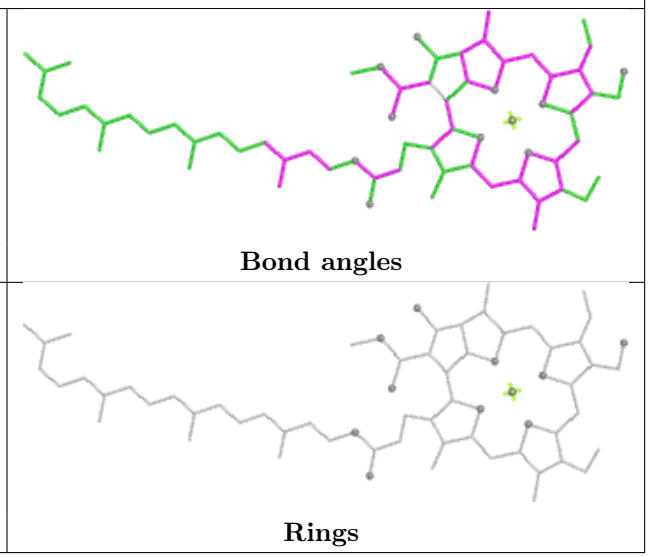


Rings

Ligand CHL Z 601



Bond lengths

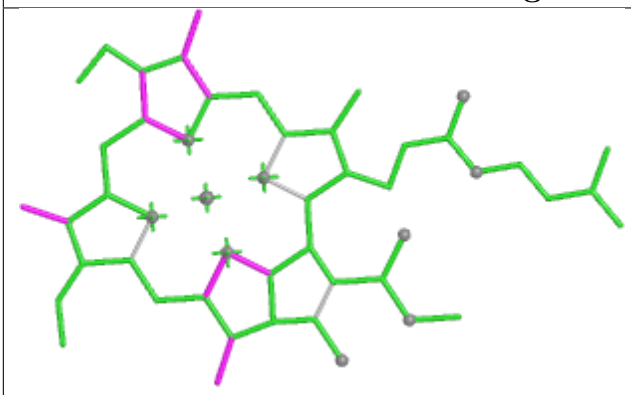


Bond angles

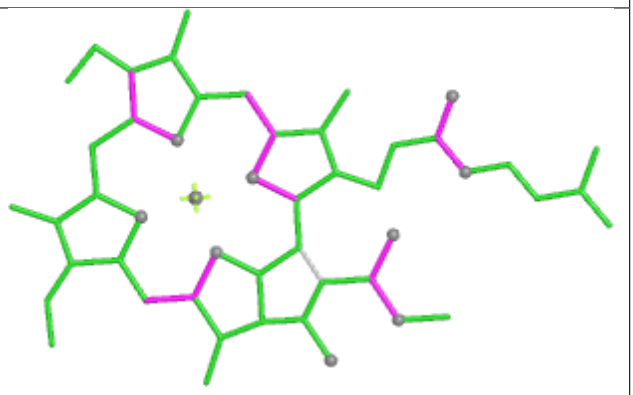
Torsions

Rings

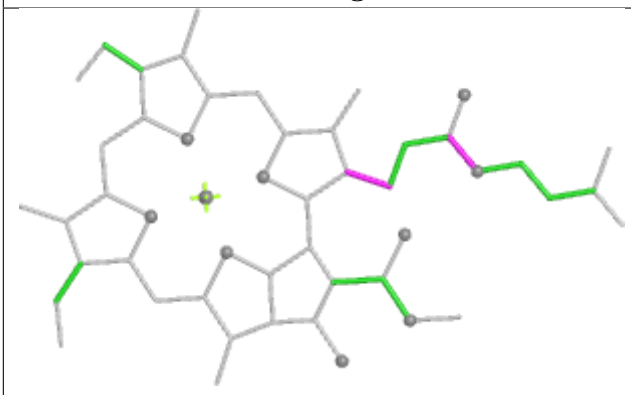
Ligand CLA A 808



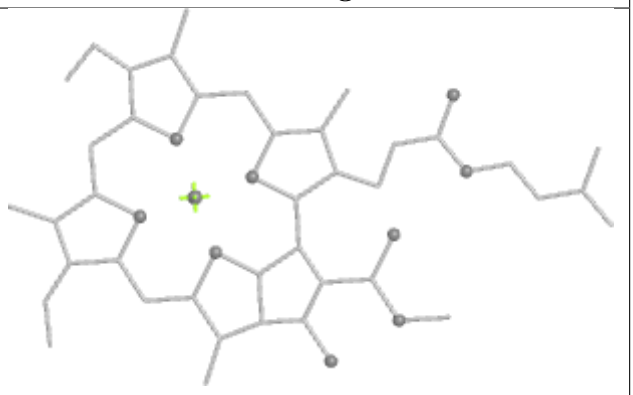
Bond lengths



Bond angles

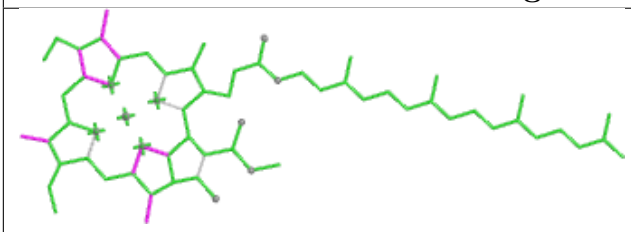


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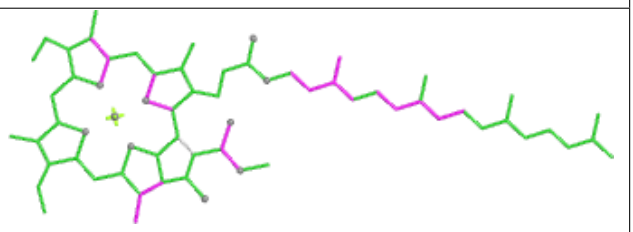


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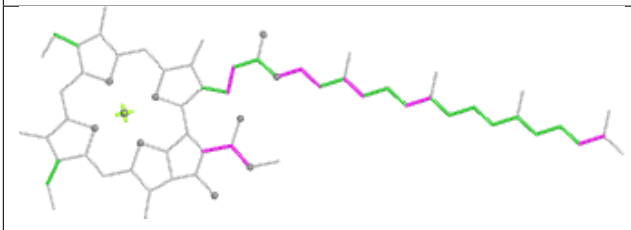
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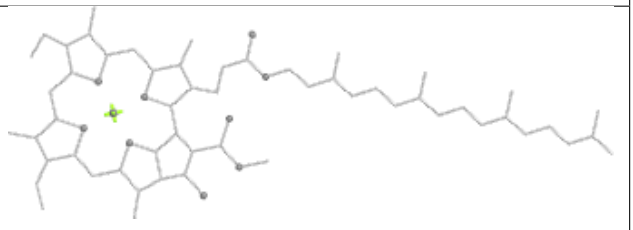
Bond lengths



Bond angles

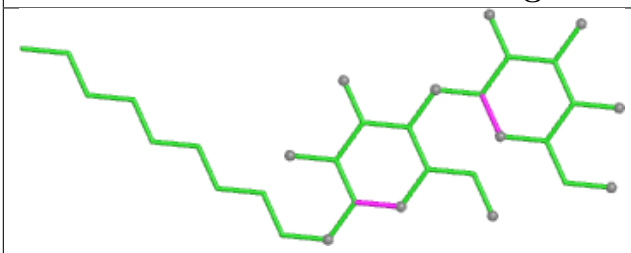


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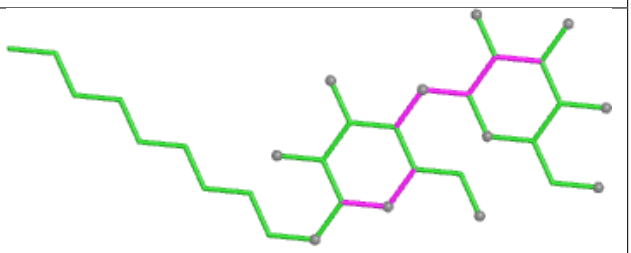


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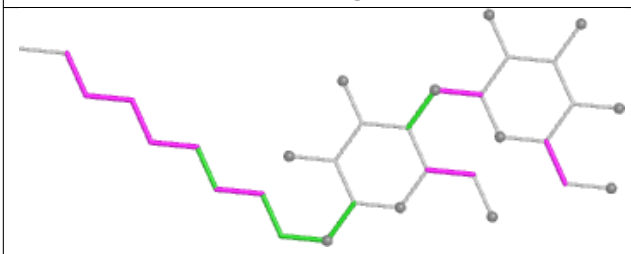
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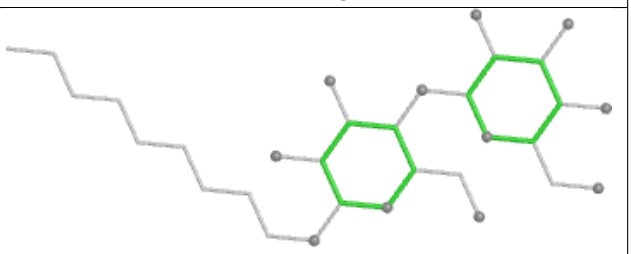
Bond lengths



Bond angles

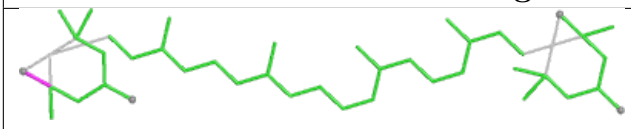


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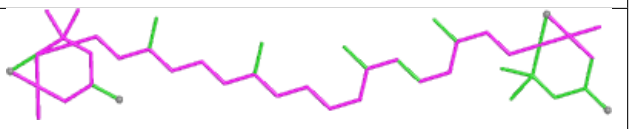


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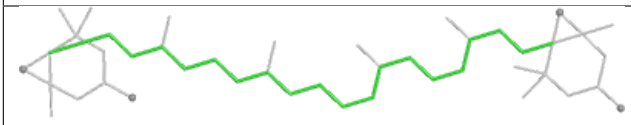
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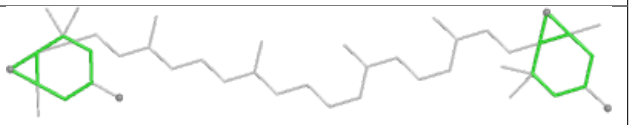
Bond lengths



Bond angles

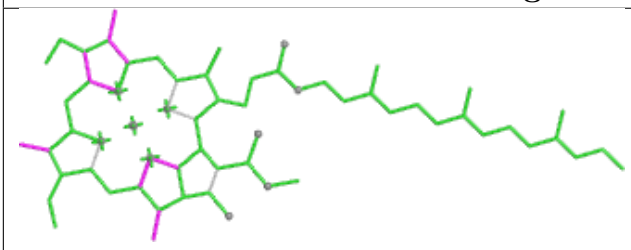


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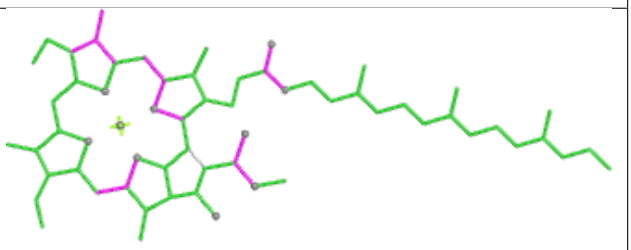


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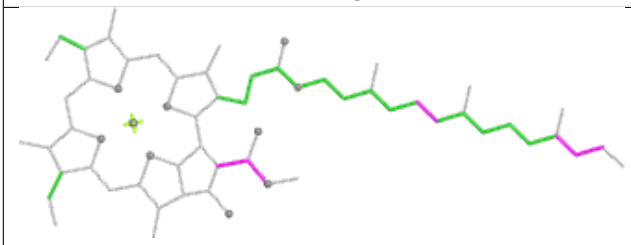
Ligand CLA V 610



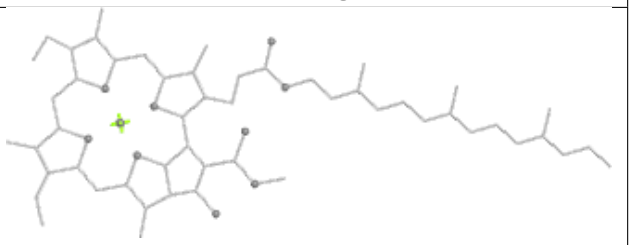
Bond lengths



Bond angles

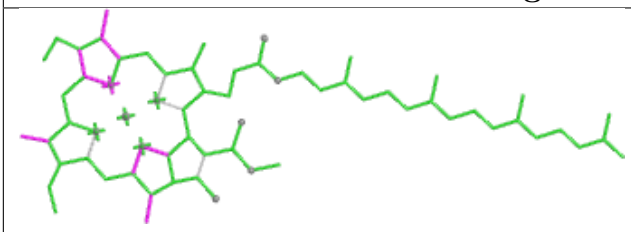


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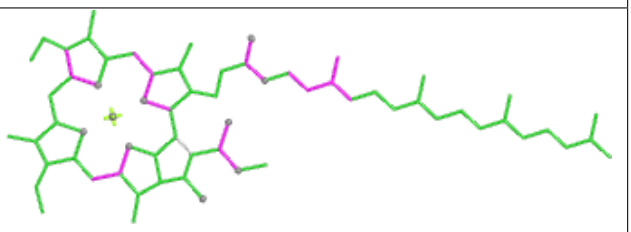


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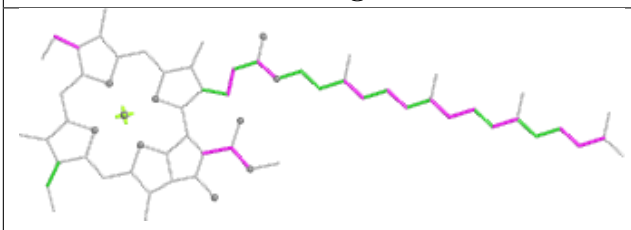
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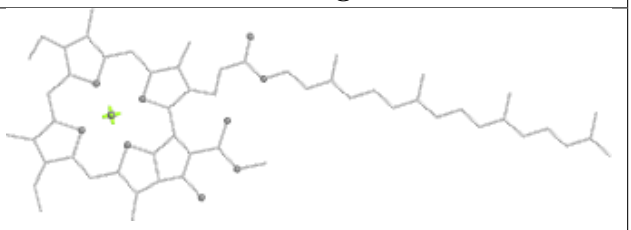
Bond lengths



Bond angles



Torsions



Rings

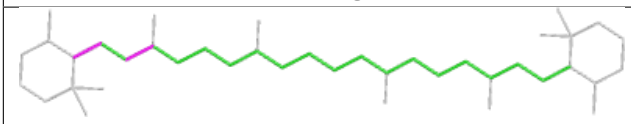
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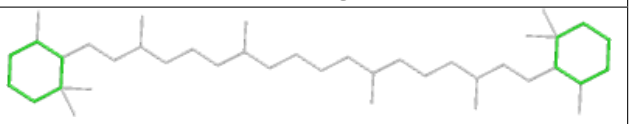
Bond lengths



Bond angles

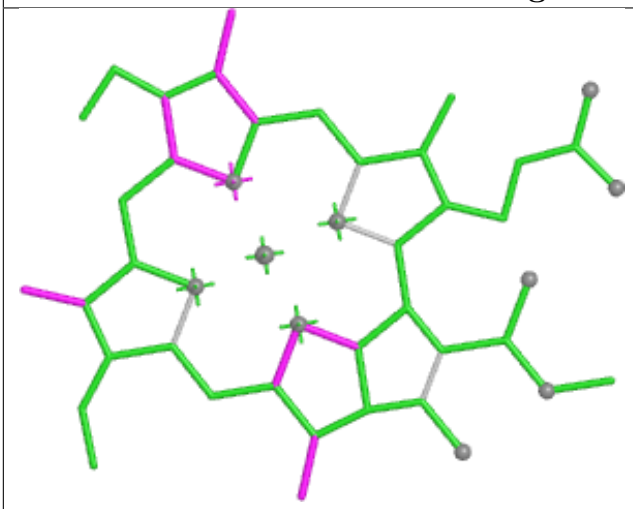


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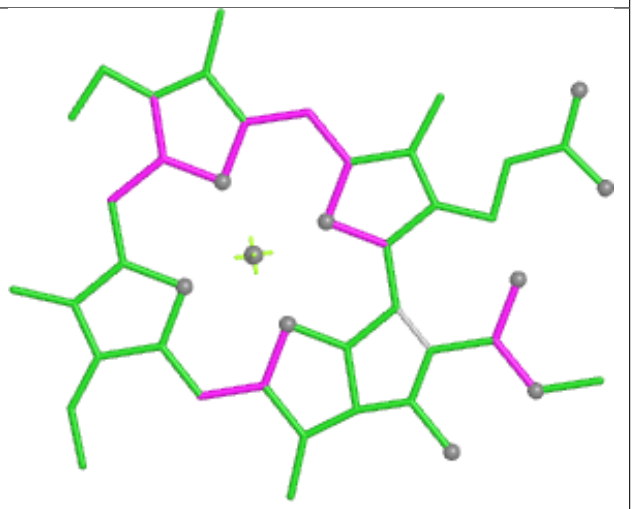


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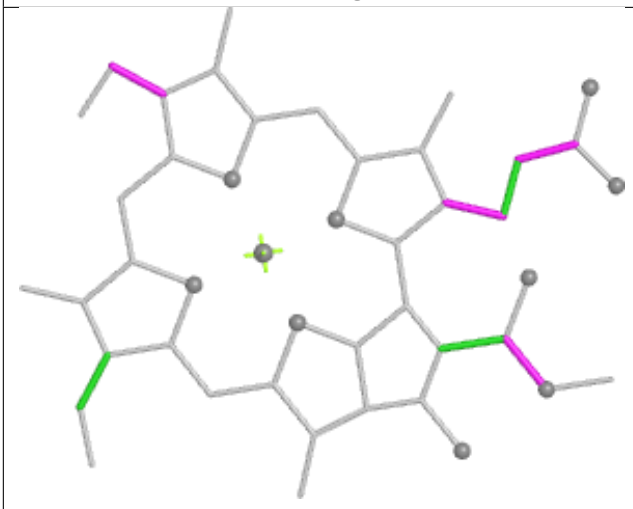
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Bond lengths



Bond angles

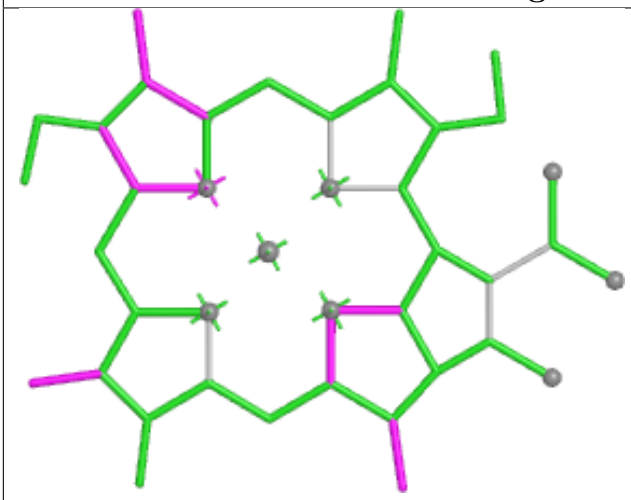


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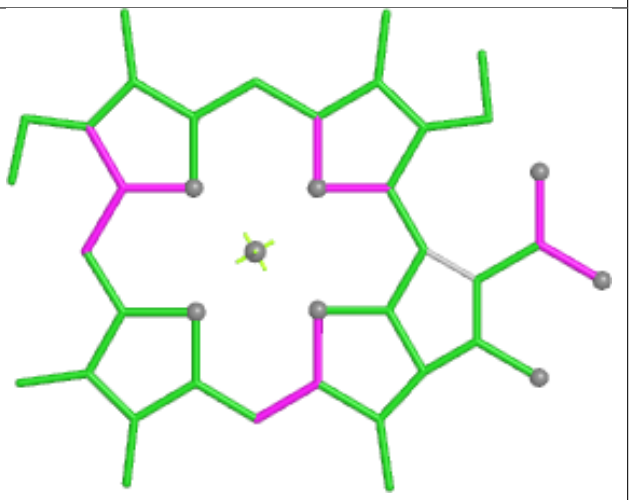


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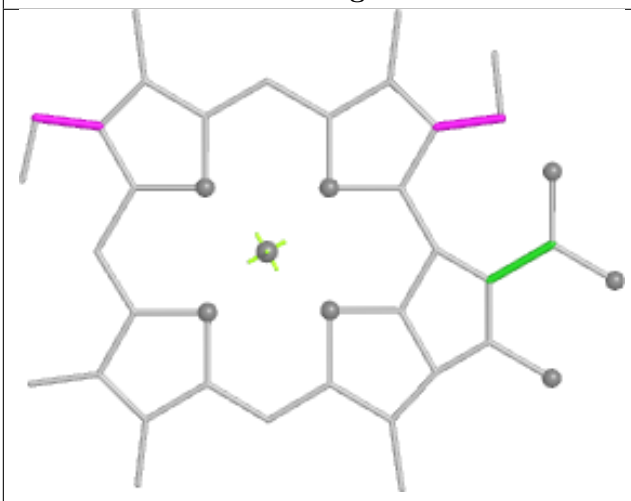
Ligand CLA 5 606



Bond lengths



Bond angles

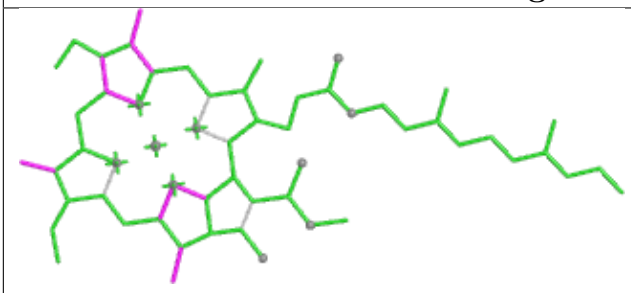


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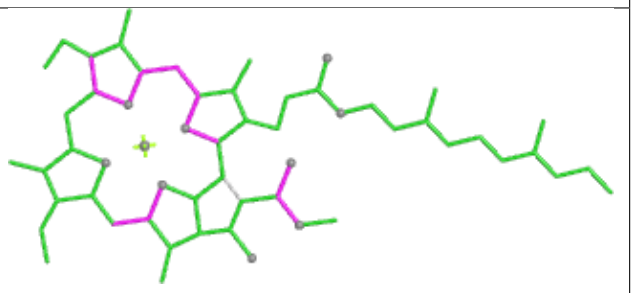


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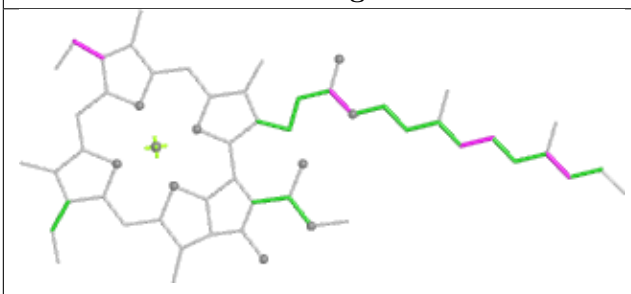
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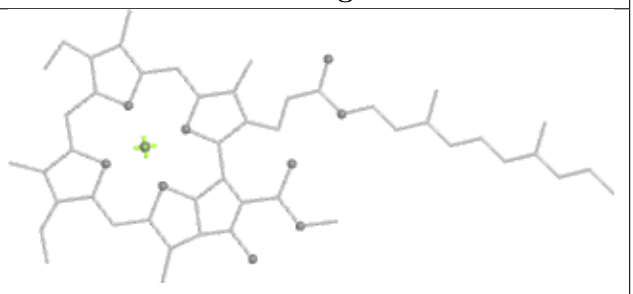
Bond lengths



Bond angles

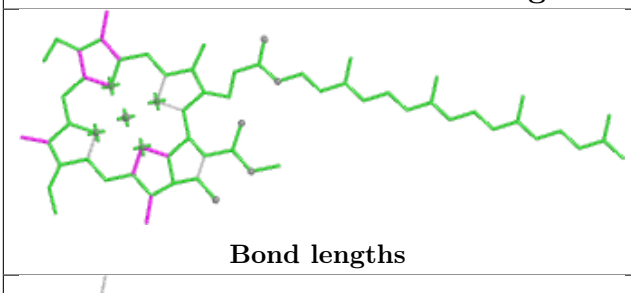


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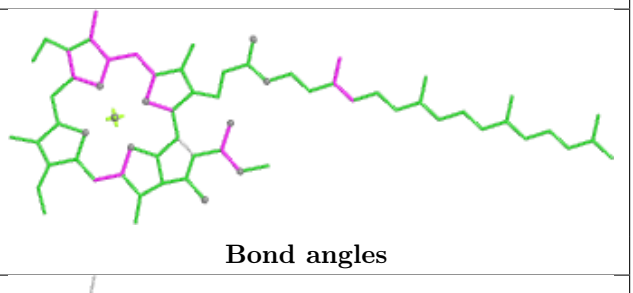


Rings

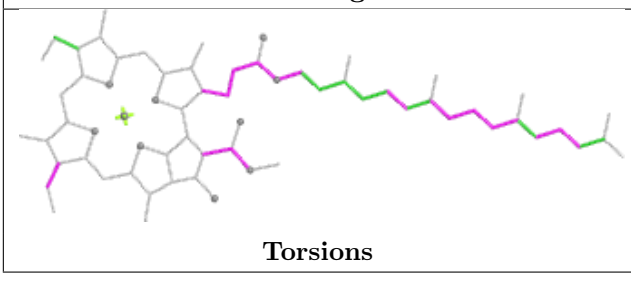
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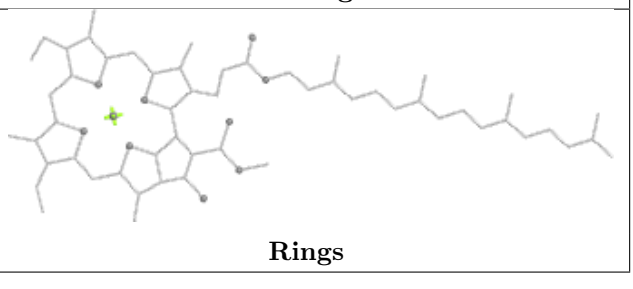
Bond lengths



Bond angles

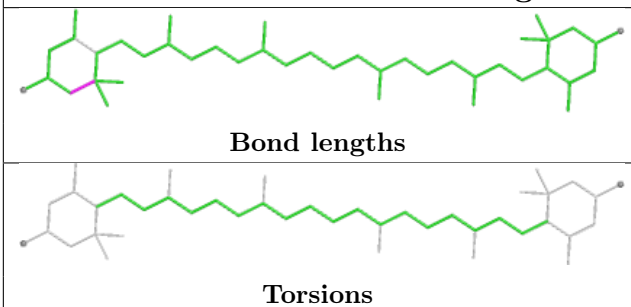


Torsions

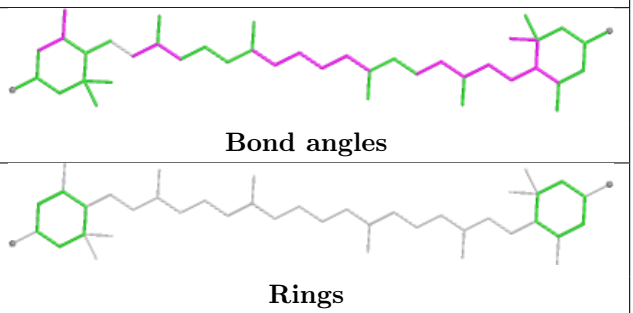


Rings

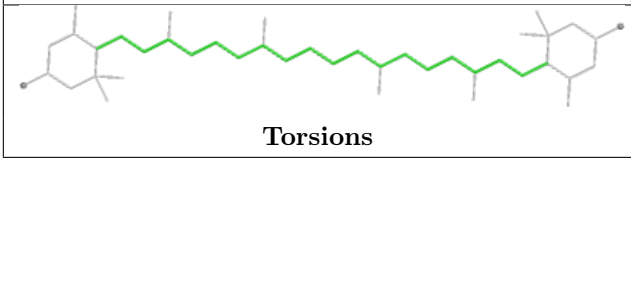
Ligand LUT V 1620



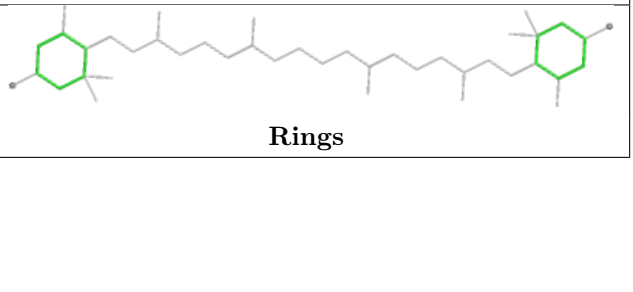
Bond lengths



Bond angles

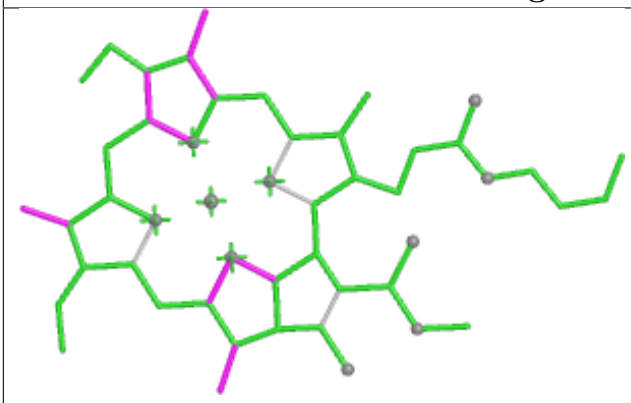


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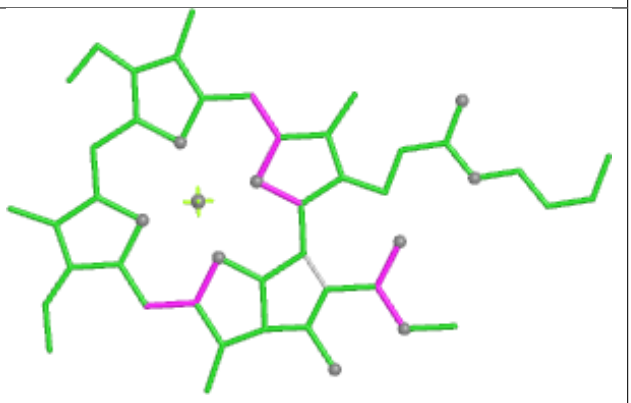


Rings

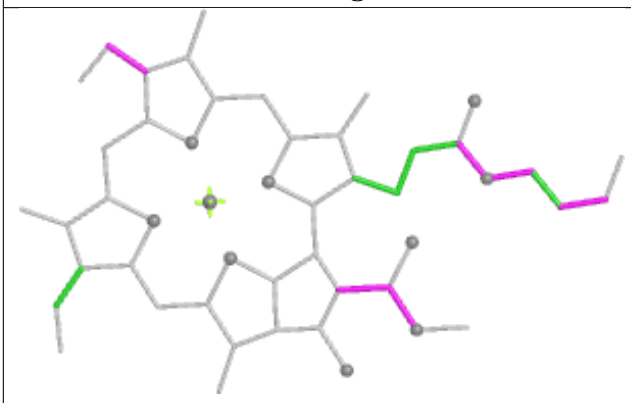
Ligand CLA a 604



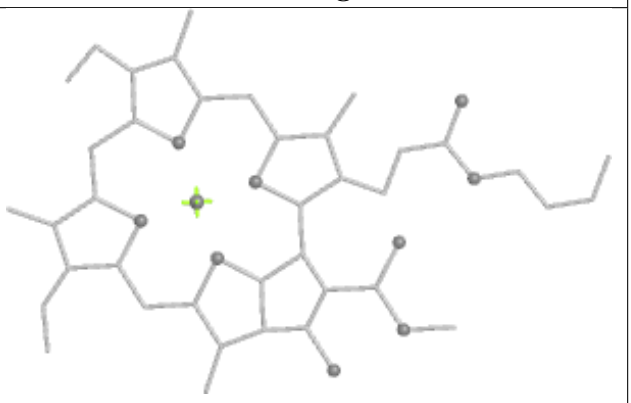
Bond lengths



Bond angles

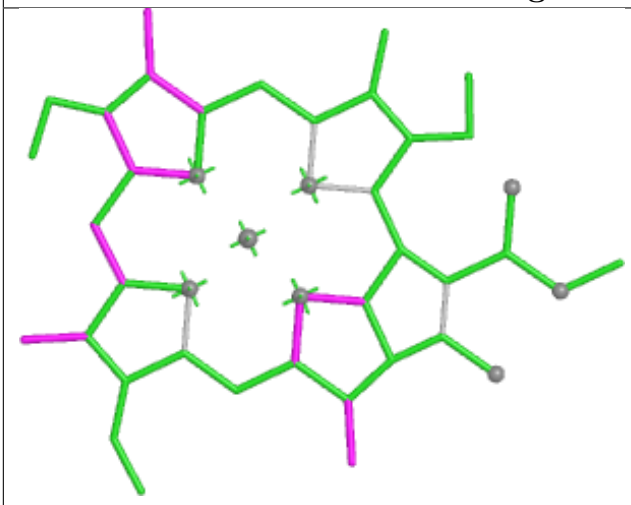


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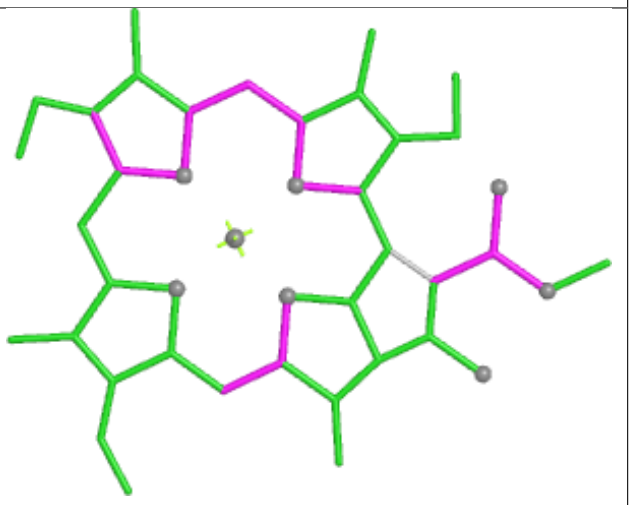


Rings

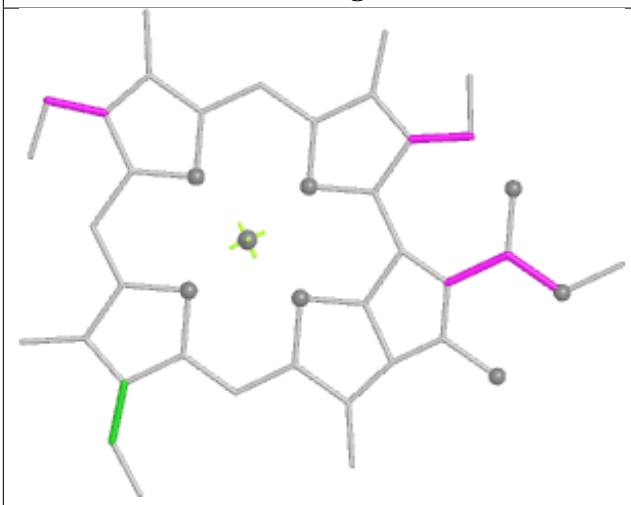
Ligand CLA J 101



Bond lengths



Bond angles

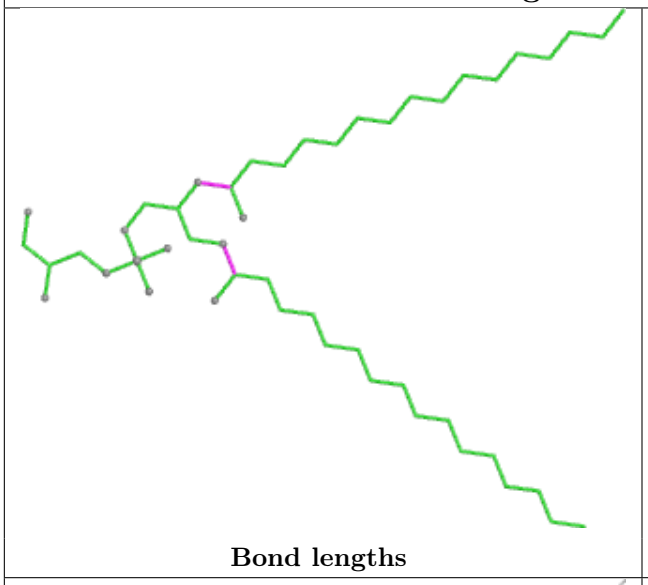


Torsions

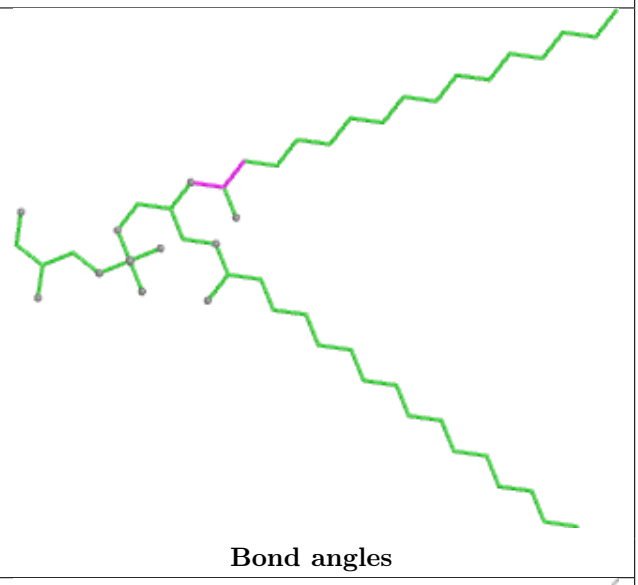


Rings

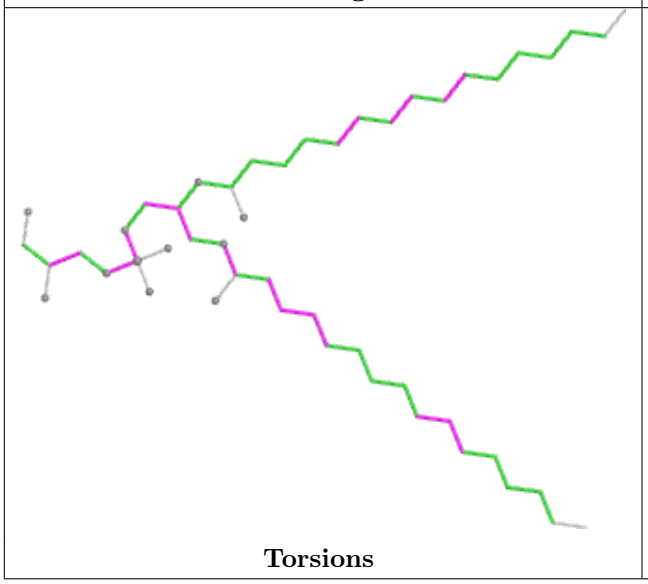
Ligand LHG H 204



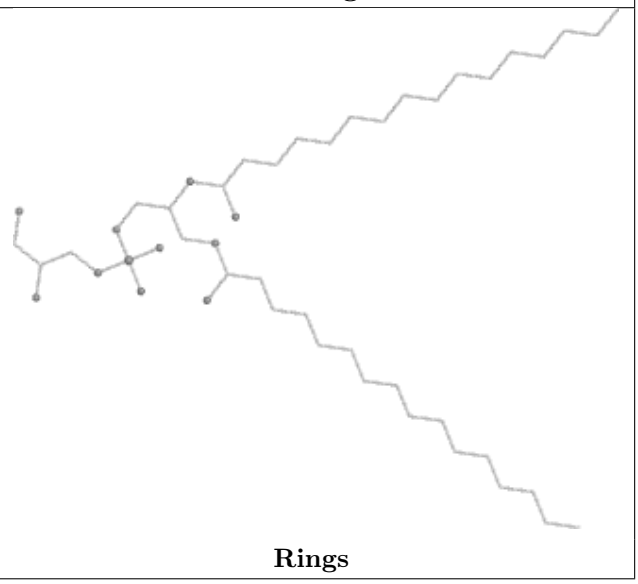
Bond lengths



Bond angles



Torsions



Rings

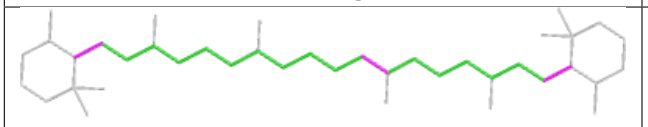
Ligand BCR F 305



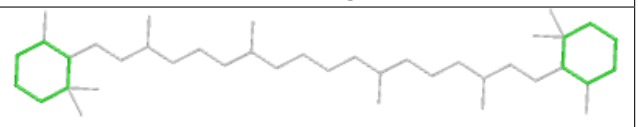
Bond lengths



Bond angles

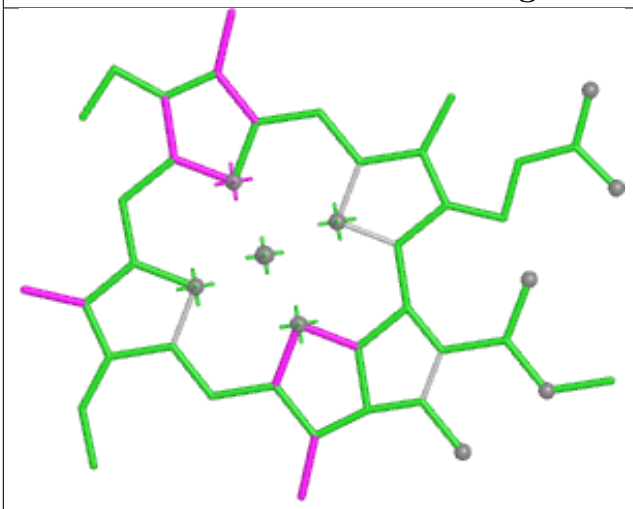


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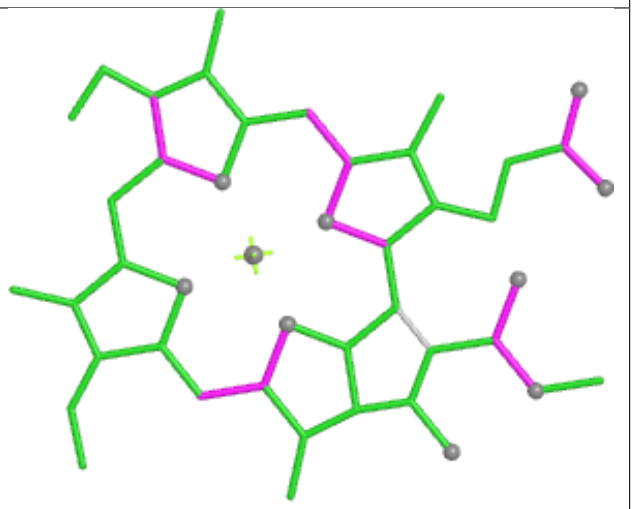


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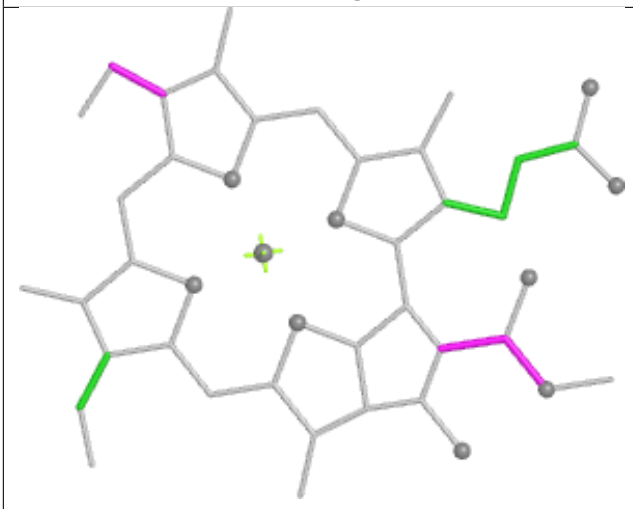
Ligand CLA W 614



Bond lengths



Bond angles

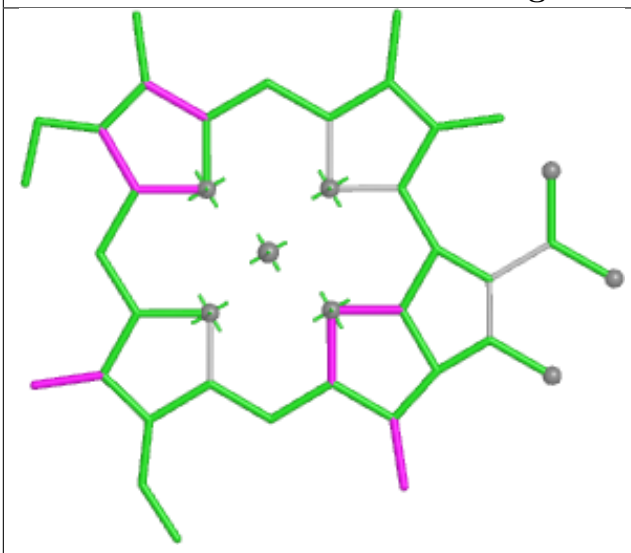


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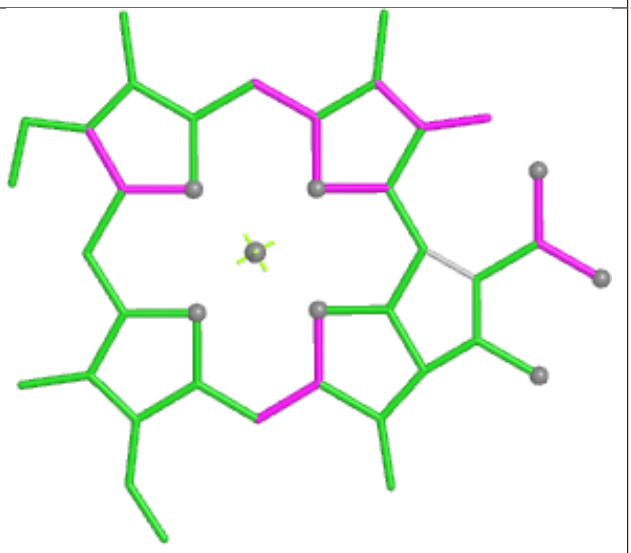


Rings

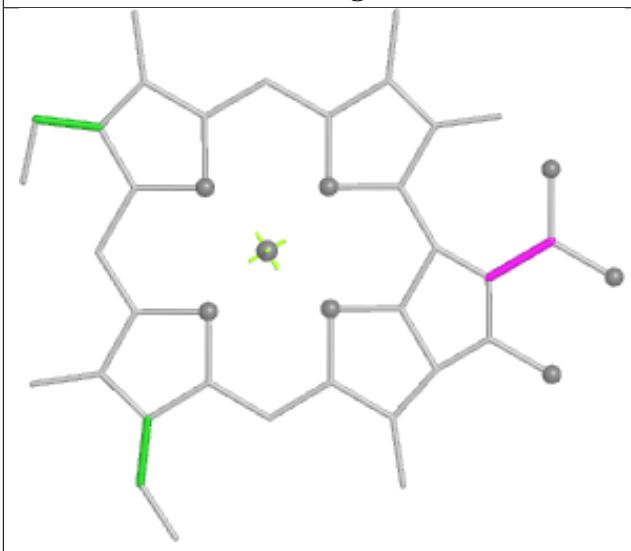
Ligand CLA 1 607



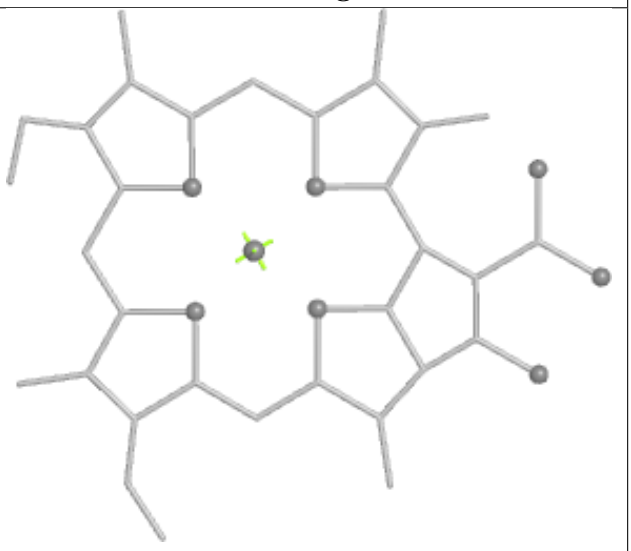
Bond lengths



Bond angles

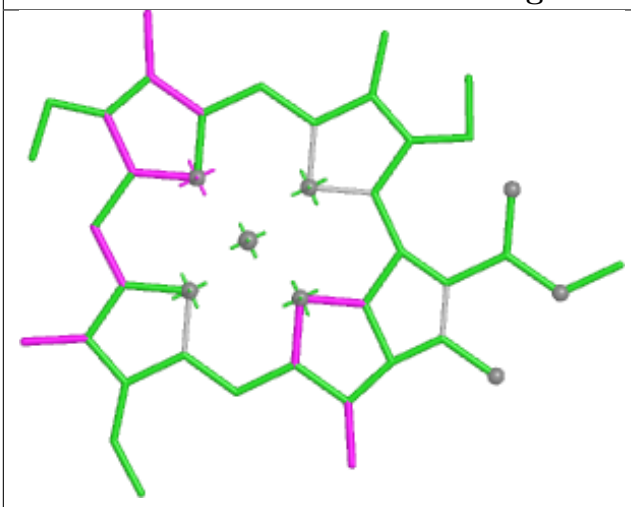


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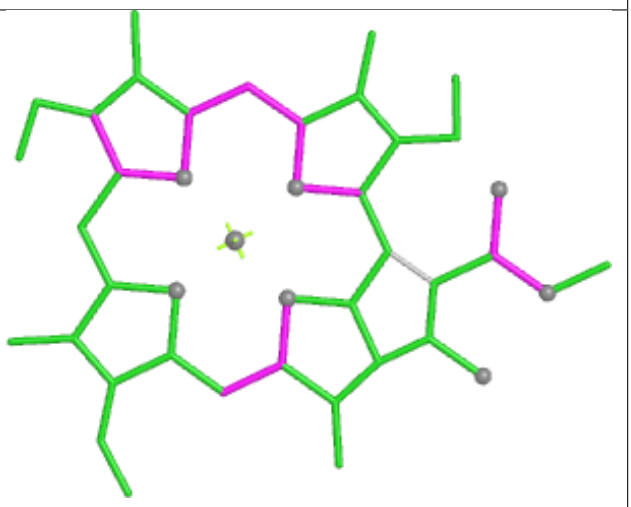


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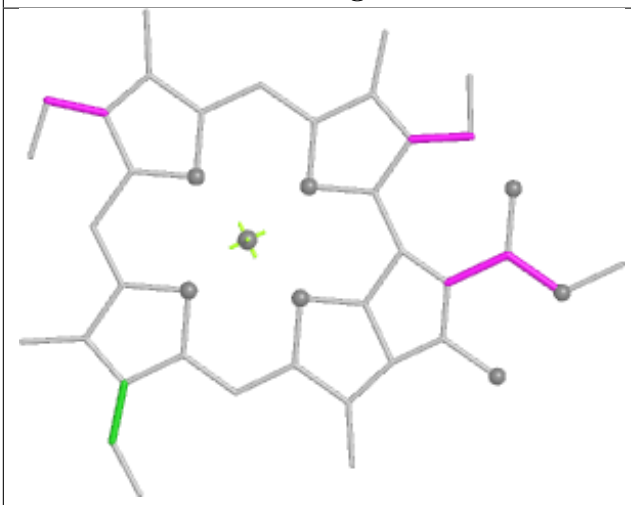
Ligand CLA F 303



Bond lengths



Bond angles

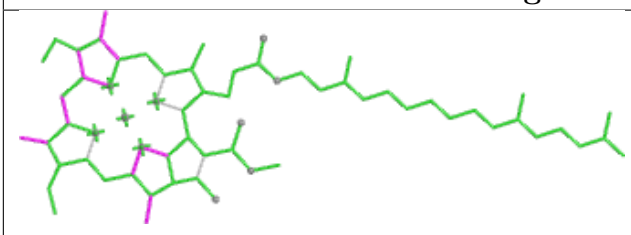


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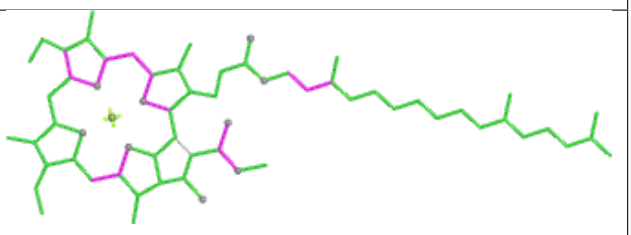


Rings

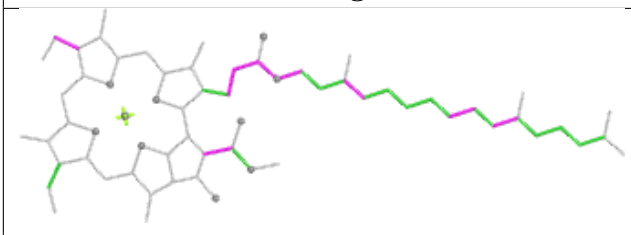
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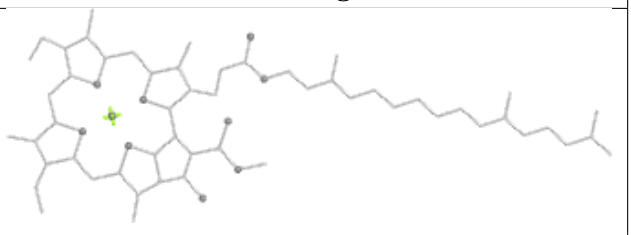
Bond lengths



Bond angles

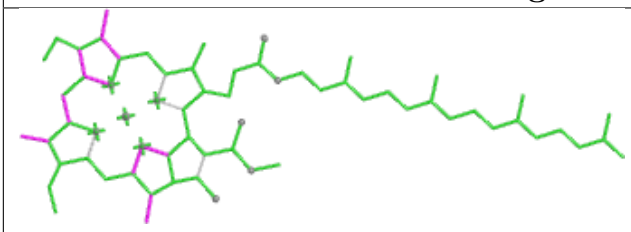


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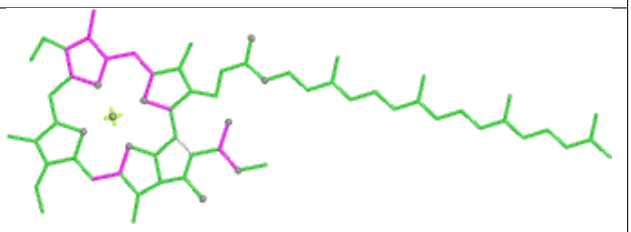


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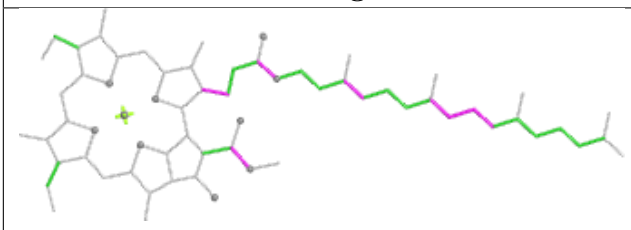
Ligand CLA 3 610



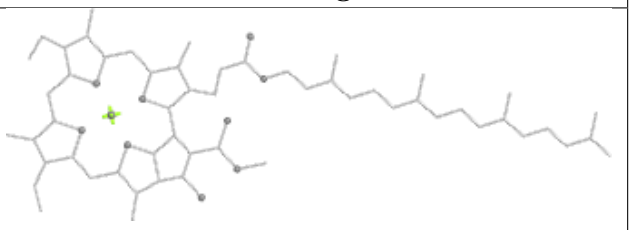
Bond lengths



Bond angles

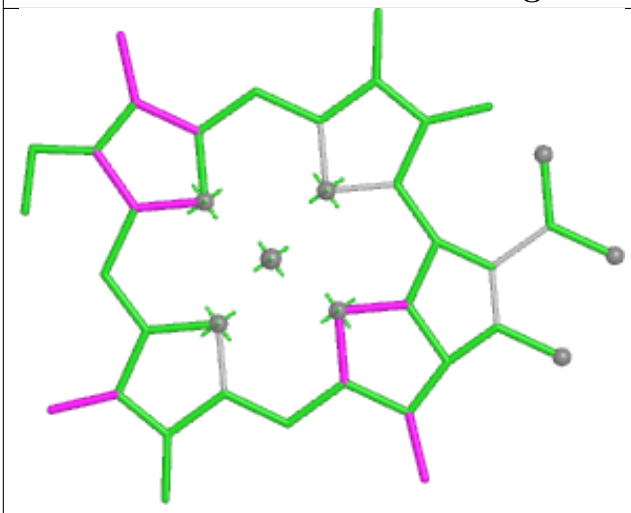


Torsions



Rings

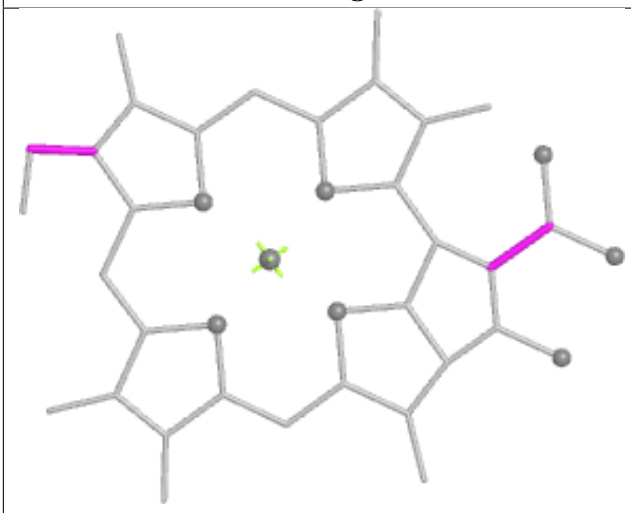
Ligand CLA H 202



Bond lengths



Bond angles

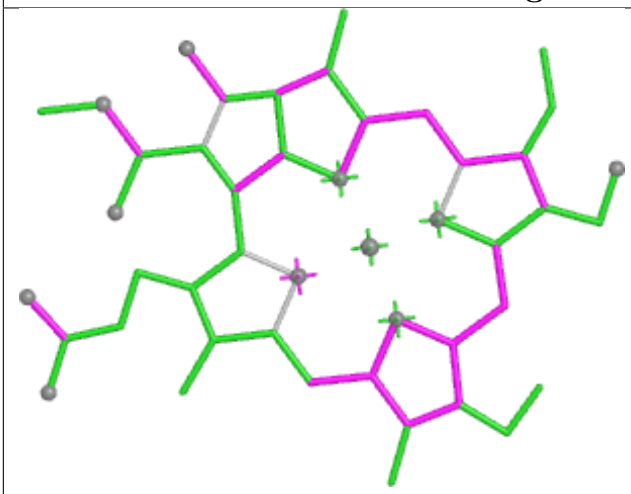


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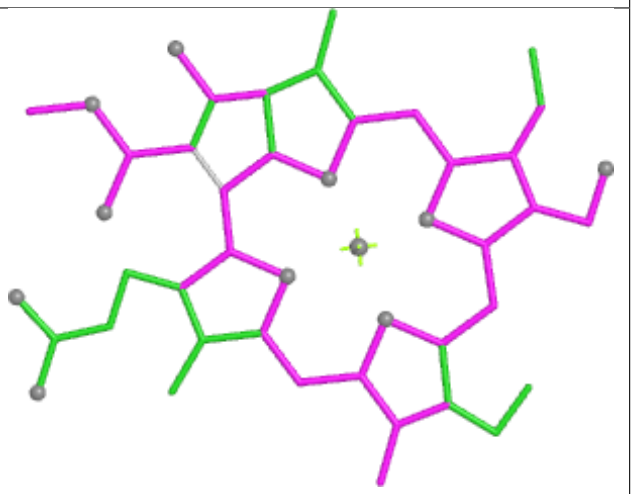


Rings

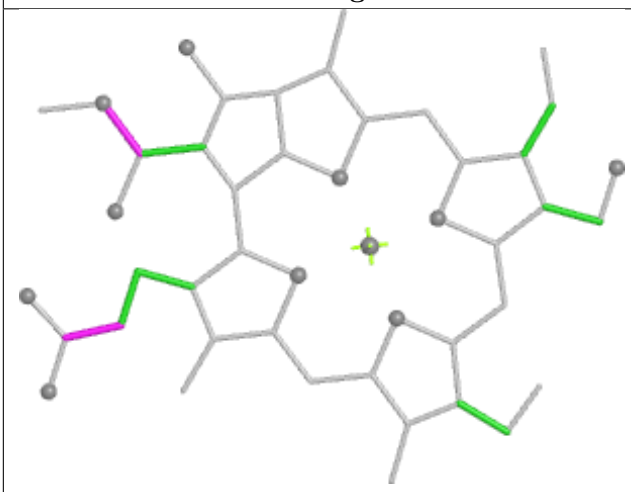
Ligand CHL Z 606



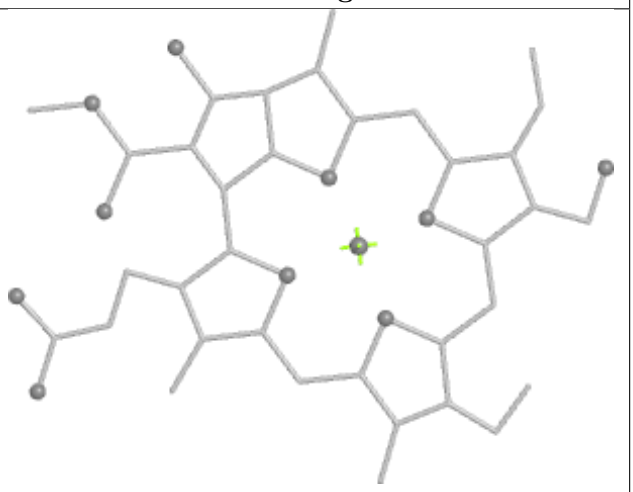
Bond lengths



Bond angles

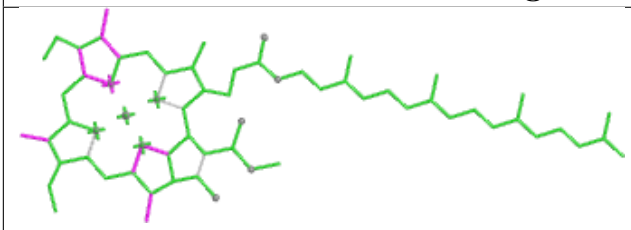


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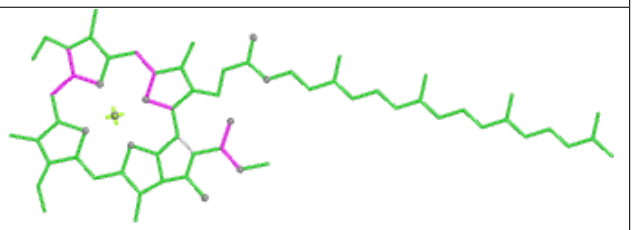


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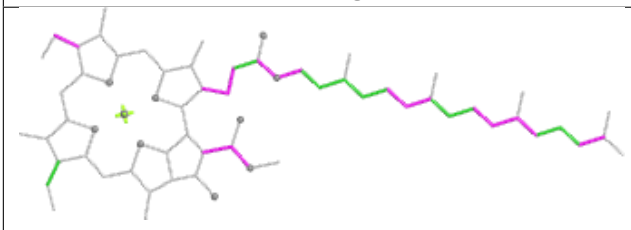
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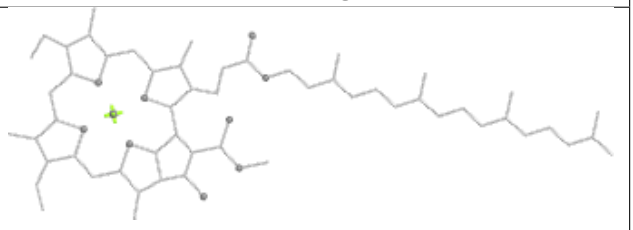
Bond lengths



Bond angles

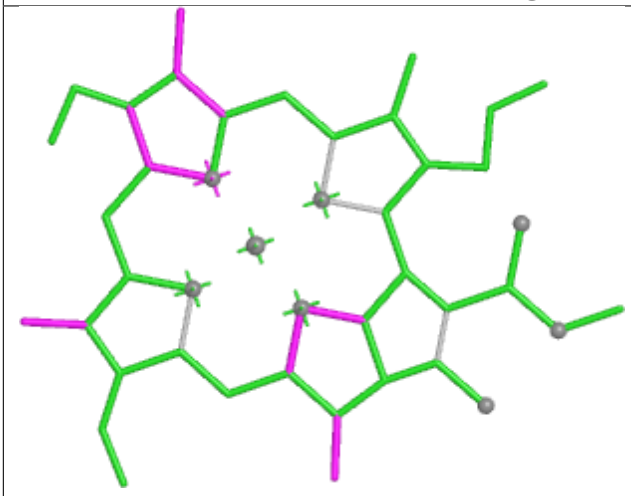


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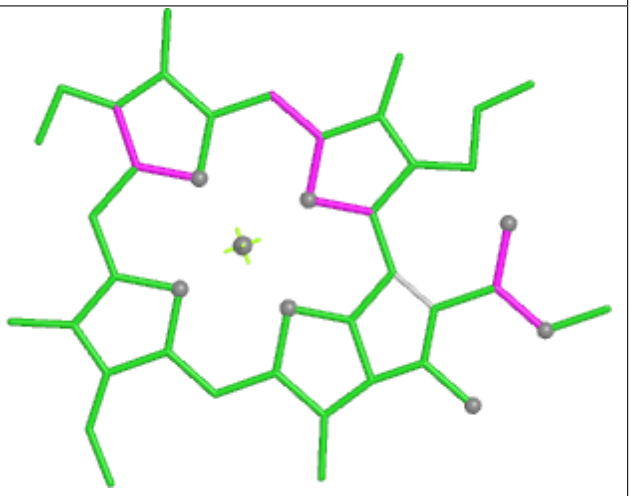


Rings

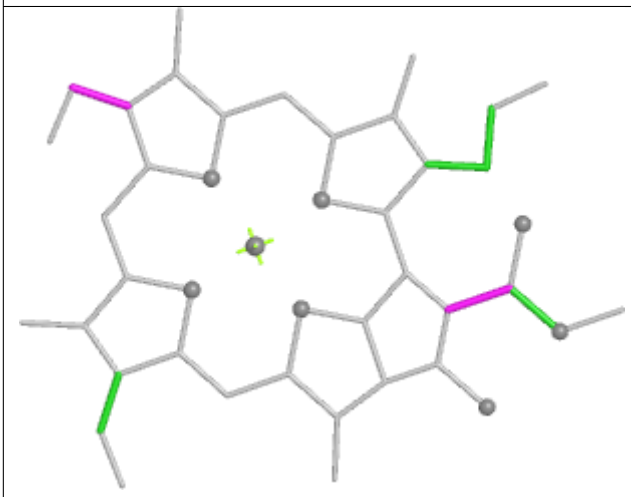
Ligand CLA U 612



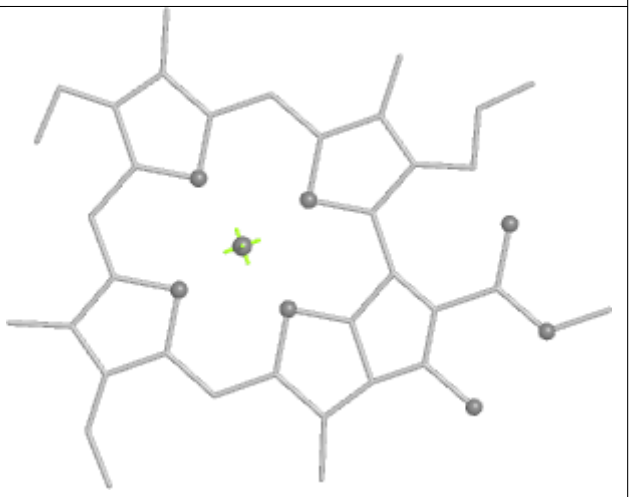
Bond lengths



Bond angles

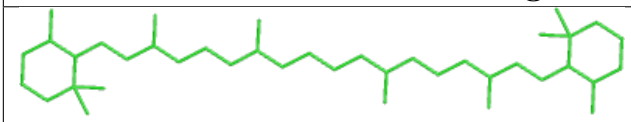


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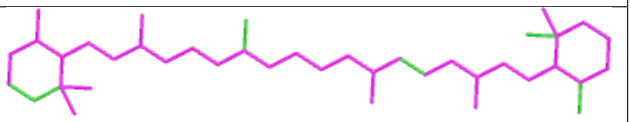


Rings

Ligand BCR L 301



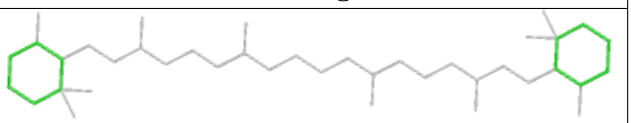
Bond lengths



Bond angles

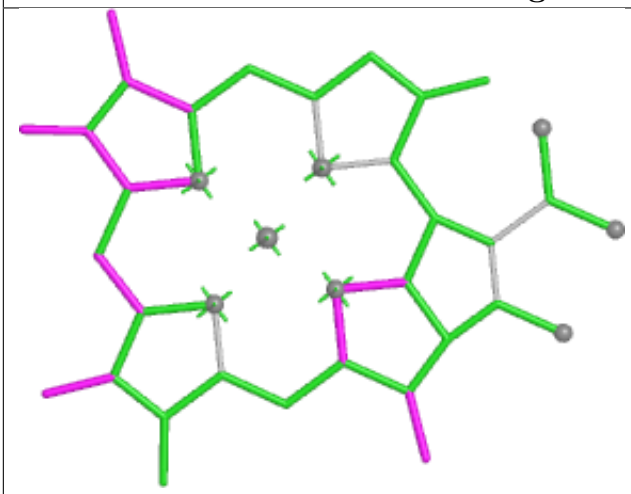


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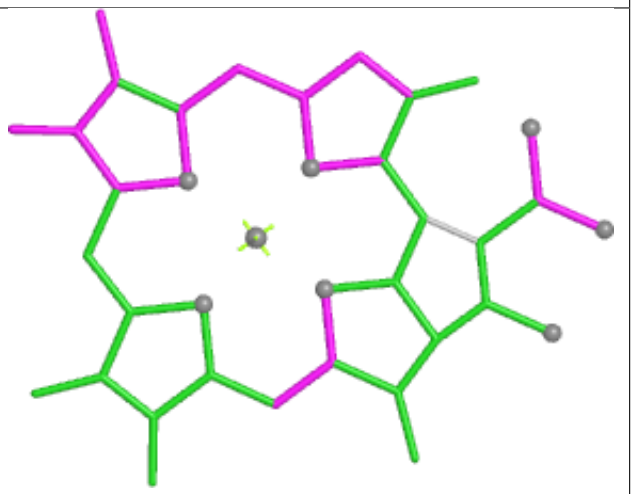


Rings

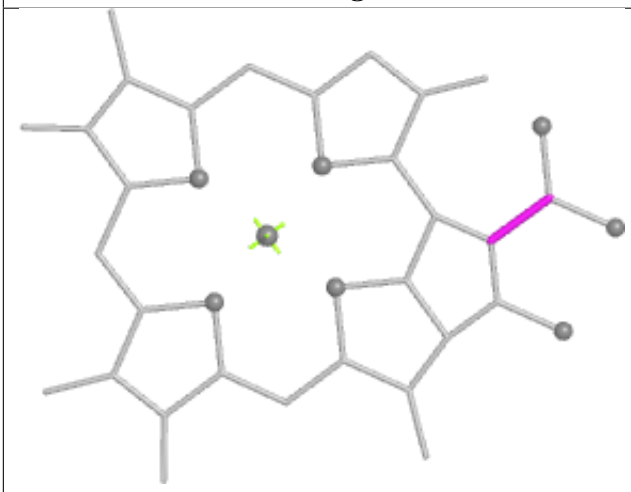
Ligand CLA 1 614



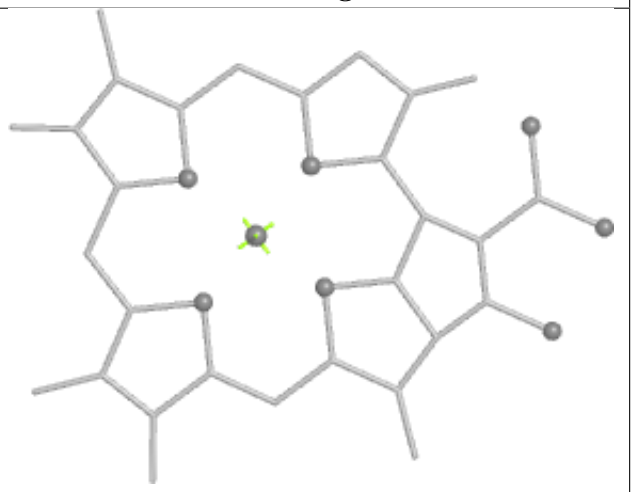
Bond lengths



Bond angles

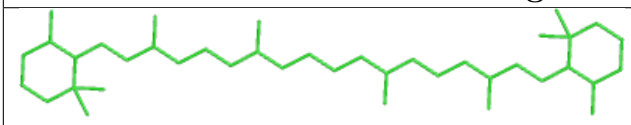


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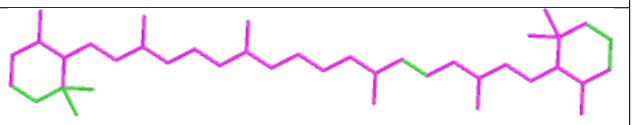


Rings

Ligand BCR 3 620



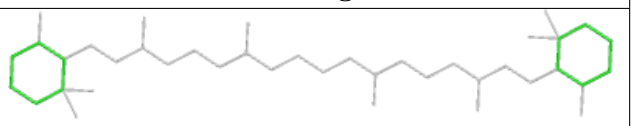
Bond lengths



Bond angles

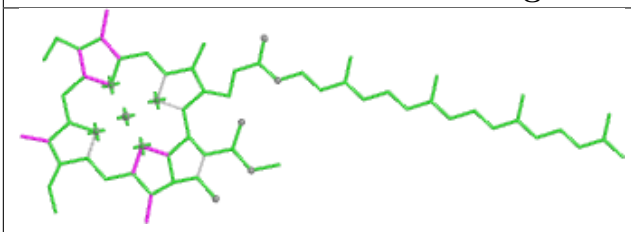


Torsions

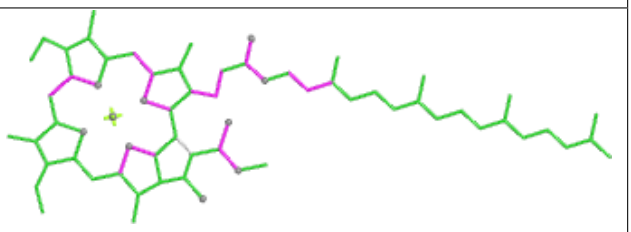


Rings

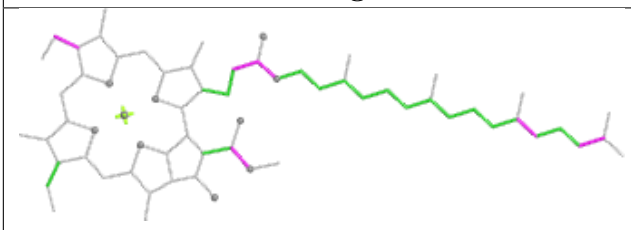
Ligand CLA A 801



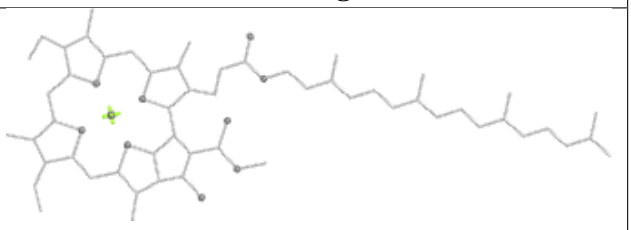
Bond lengths



Bond angles

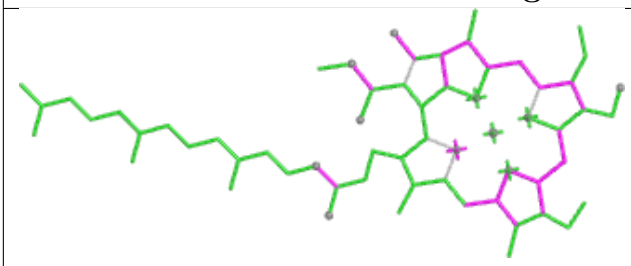


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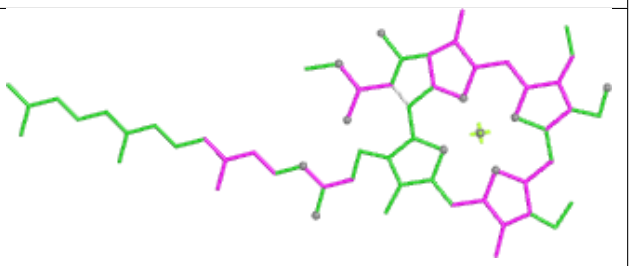


Rings

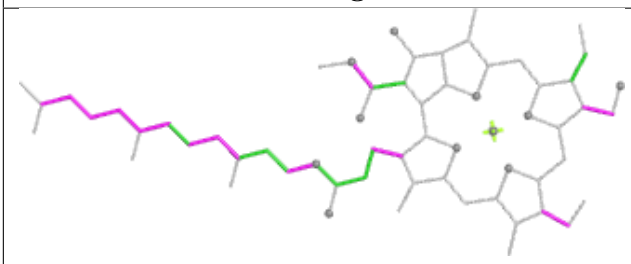
Ligand CHL V 609



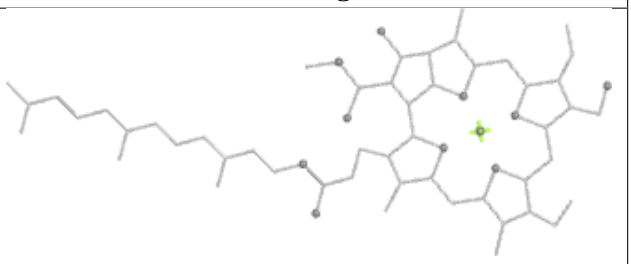
Bond lengths



Bond angles

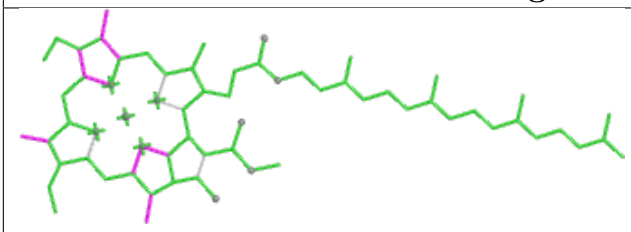


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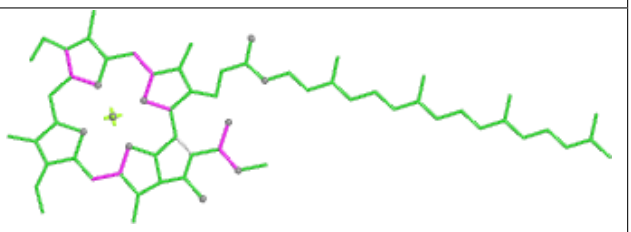


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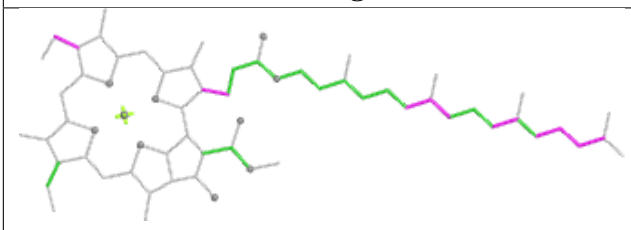
Ligand CLA 5 609



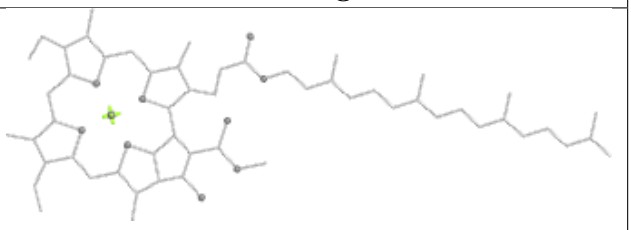
Bond lengths



Bond angles

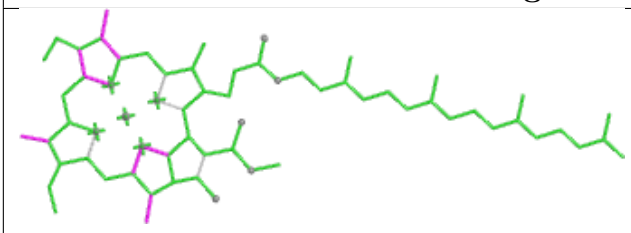


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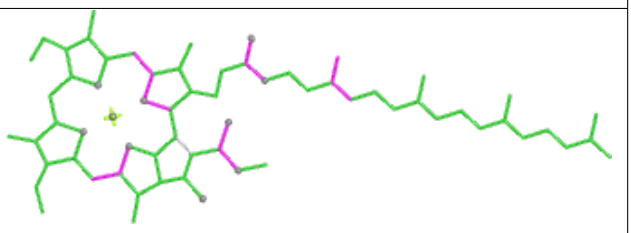


Rings

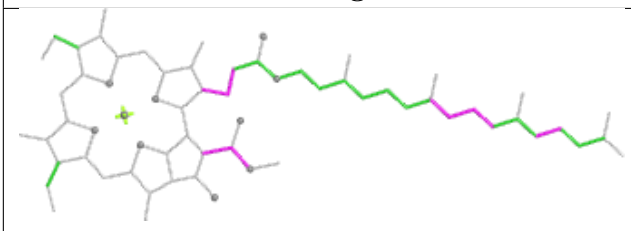
Ligand CLA A 824



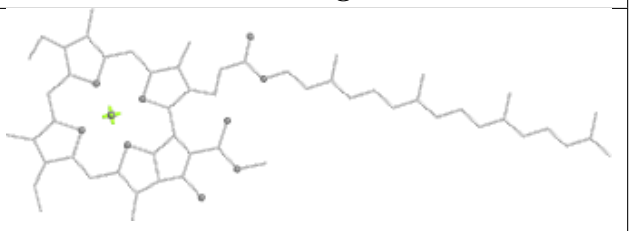
Bond lengths



Bond angles

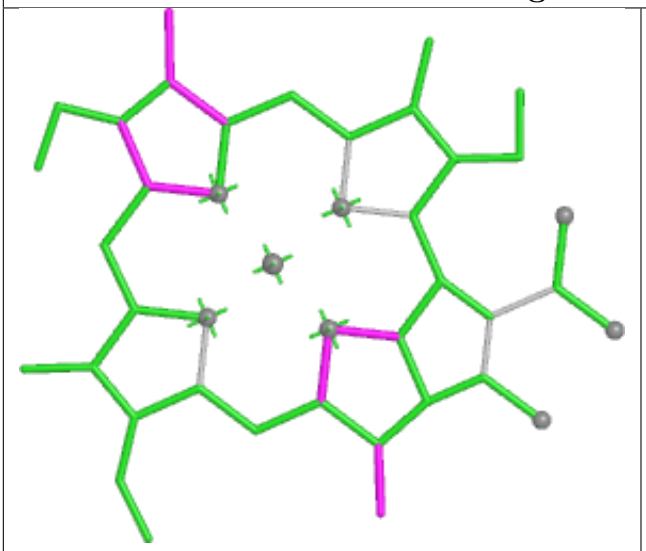


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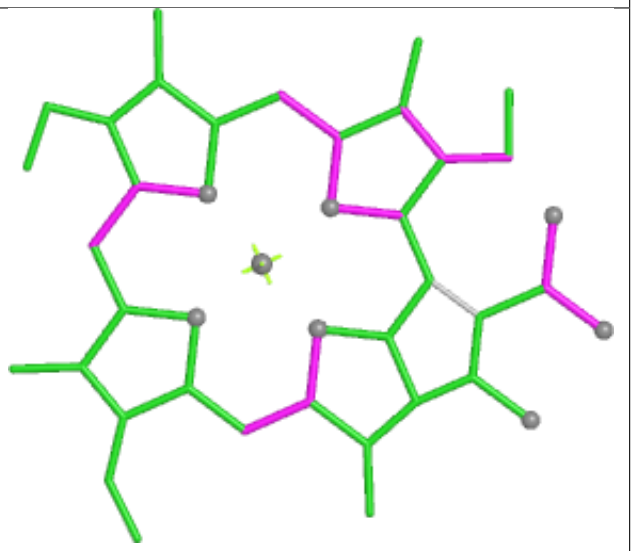


Rings

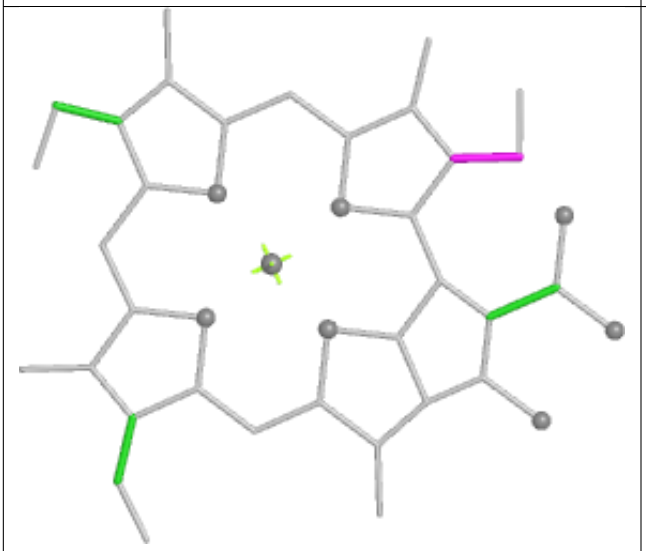
Ligand CLA 6 612



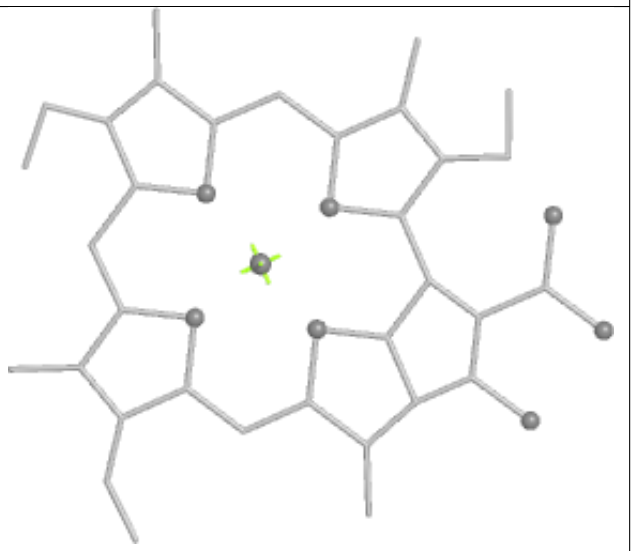
Bond lengths



Bond angles

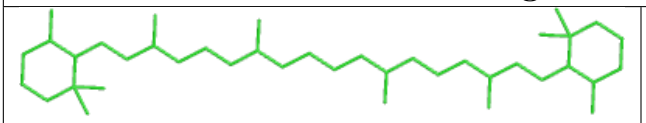


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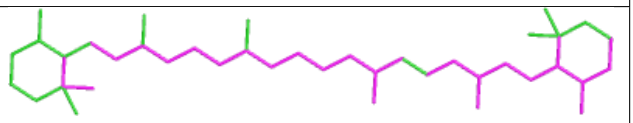


Rings

Ligand BCR K 202



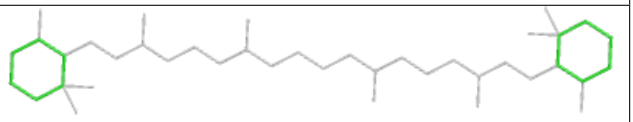
Bond lengths



Bond angles

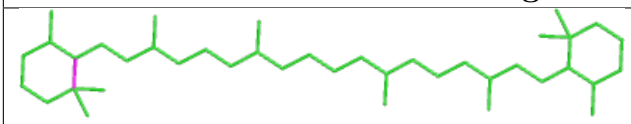


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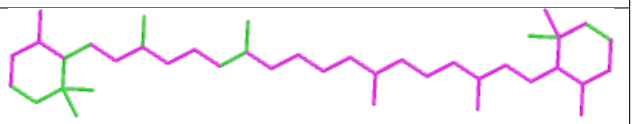


Rings

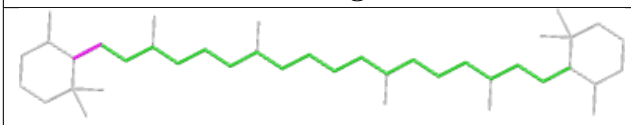
Ligand BCR A 851



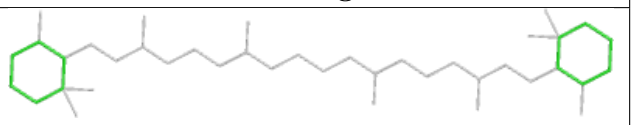
Bond lengths



Bond angles

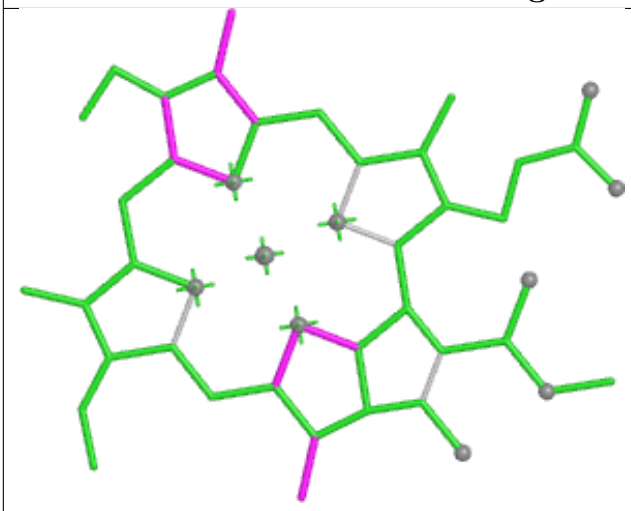


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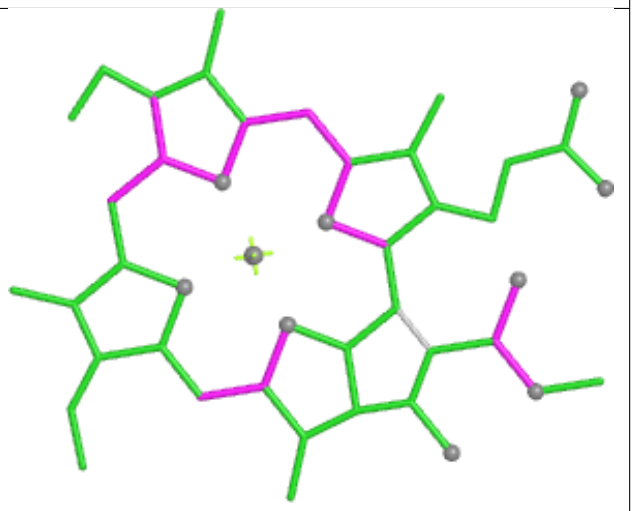


Rings

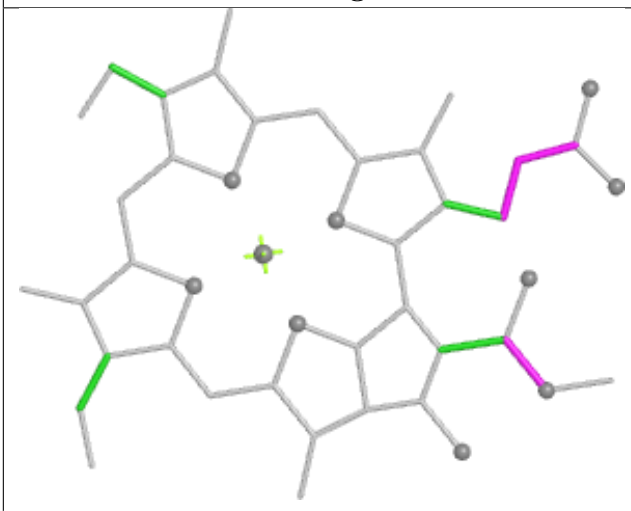
Ligand CLA a 616



Bond lengths



Bond angles

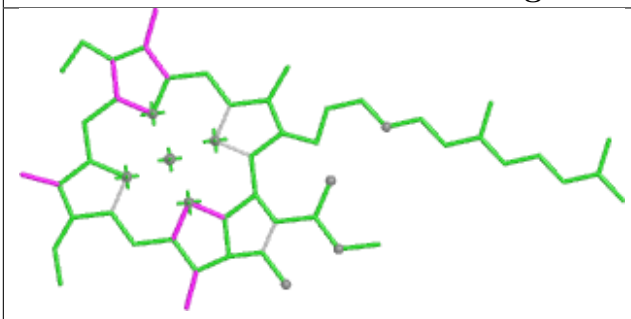


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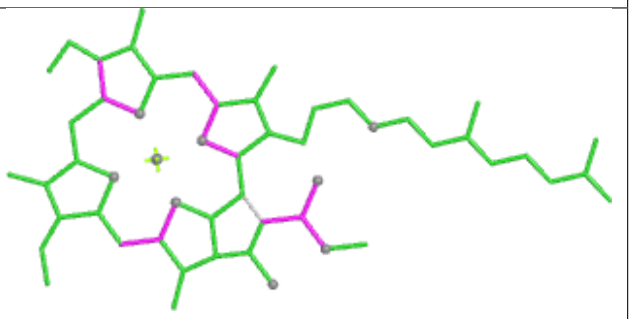


Rings

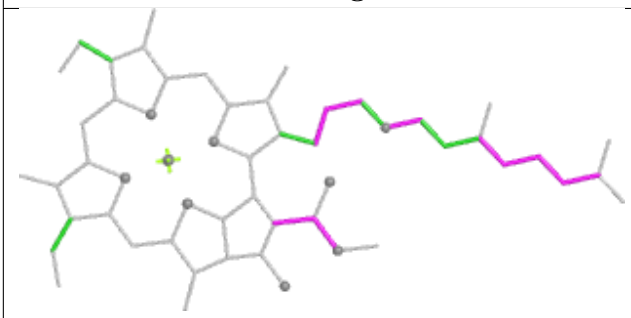
Ligand CLA B 816



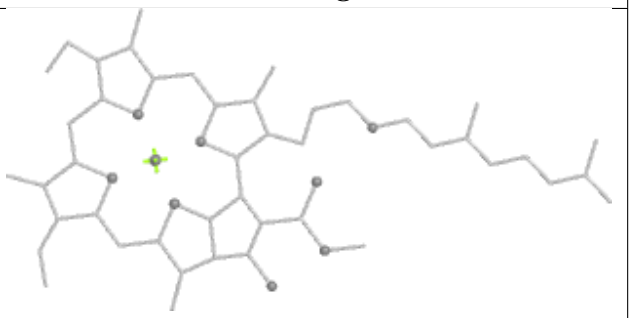
Bond lengths



Bond angles

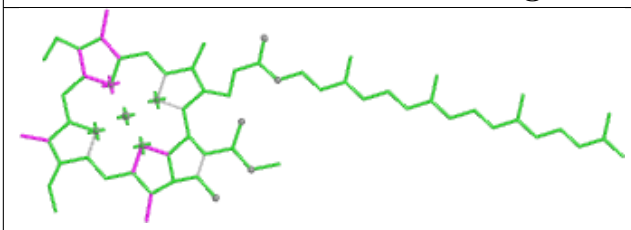


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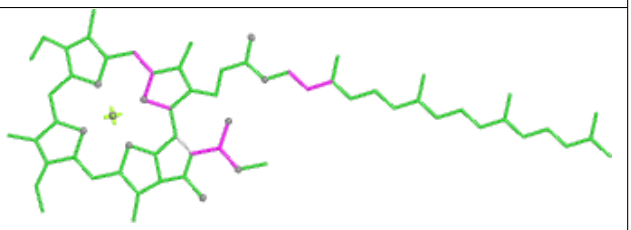


Rings

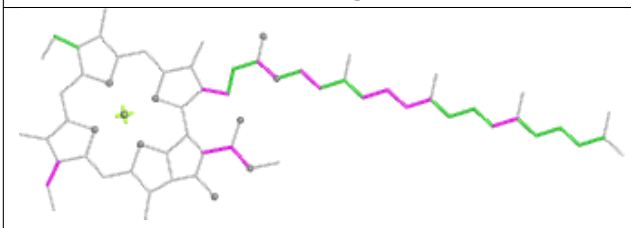
Ligand CLA A 804



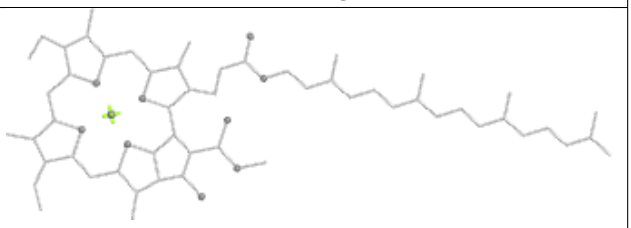
Bond lengths



Bond angles

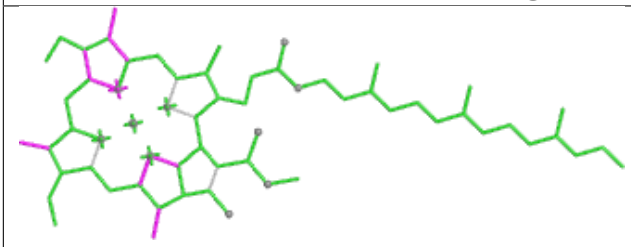


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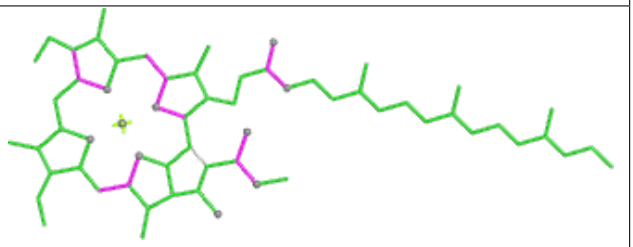


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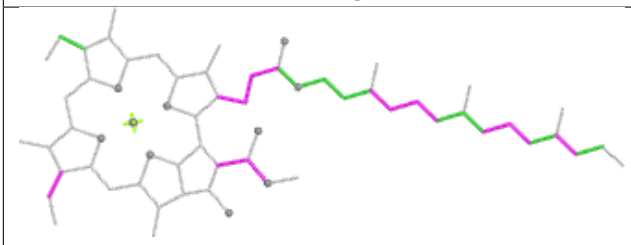
Ligand CLA B 827



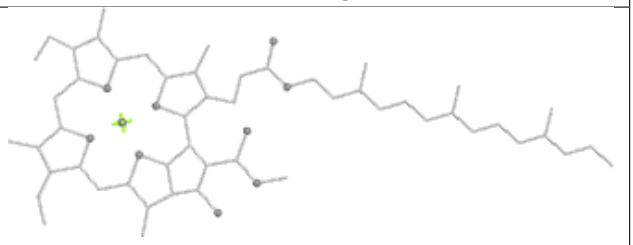
Bond lengths



Bond angles

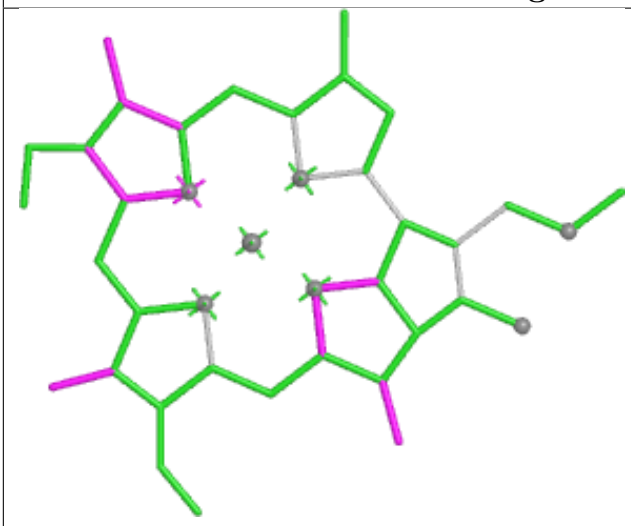


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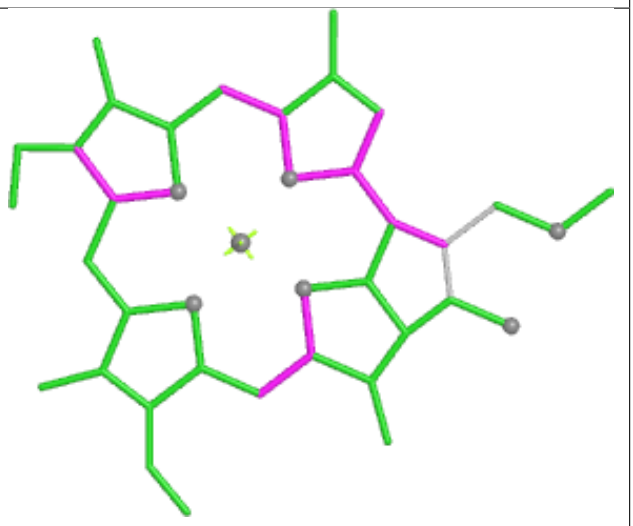


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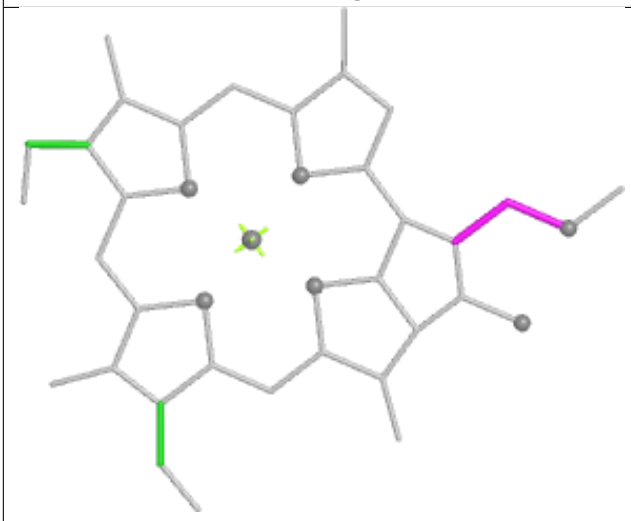
Ligand CLA 1 606



Bond lengths



Bond angles

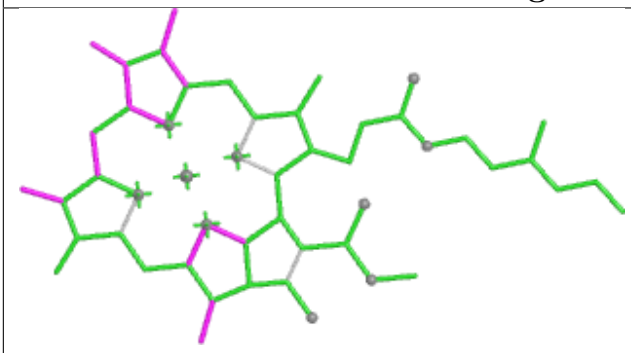


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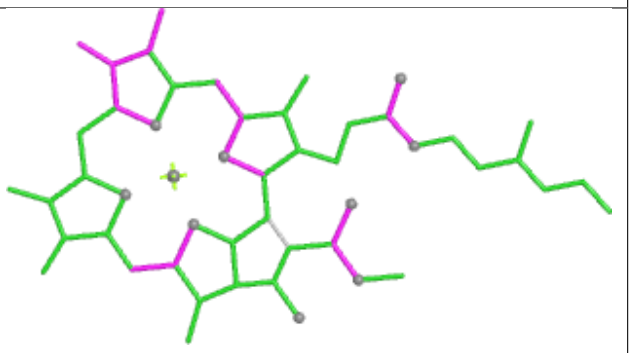


Rings

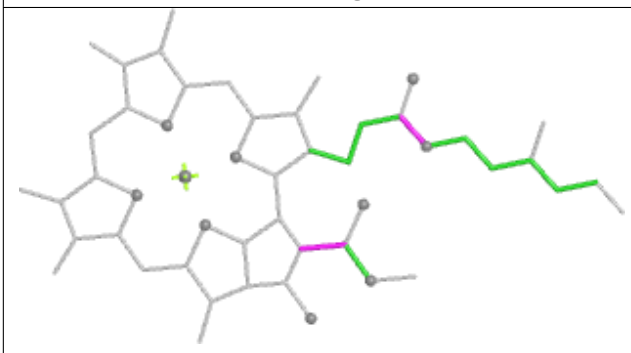
Ligand CLA 9 604



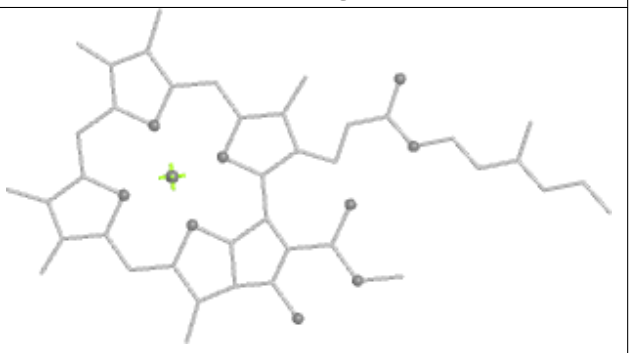
Bond lengths



Bond angles

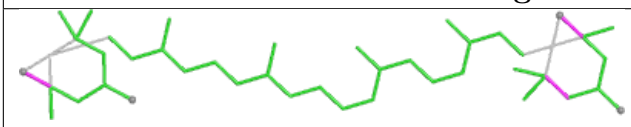


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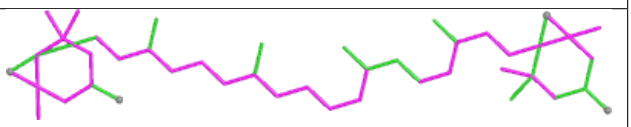


Rings

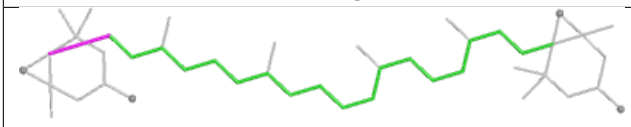
Ligand XAT U 1622



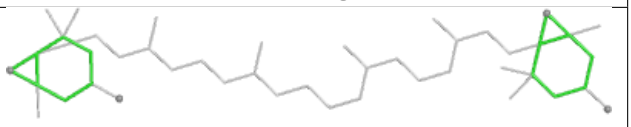
Bond lengths



Bond angles

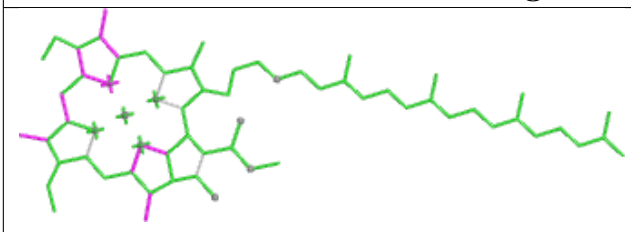


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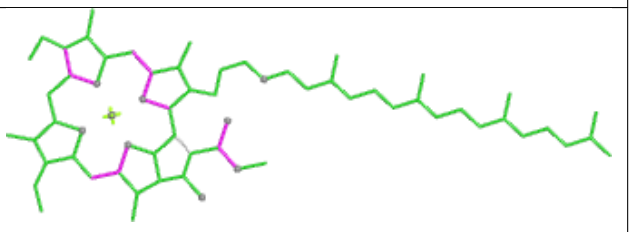


Rings

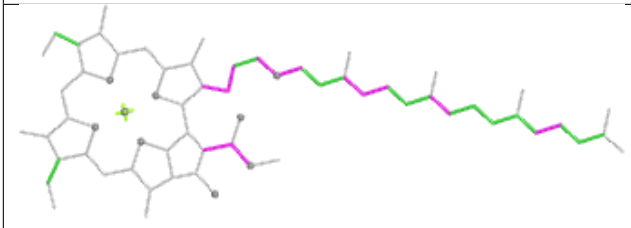
Ligand CLA B 810



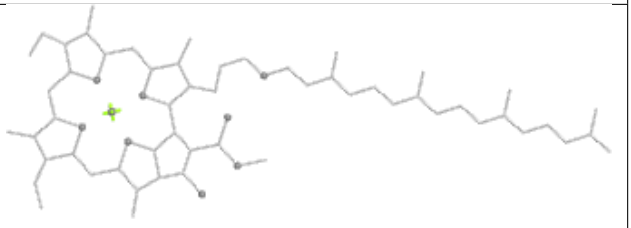
Bond lengths



Bond angles

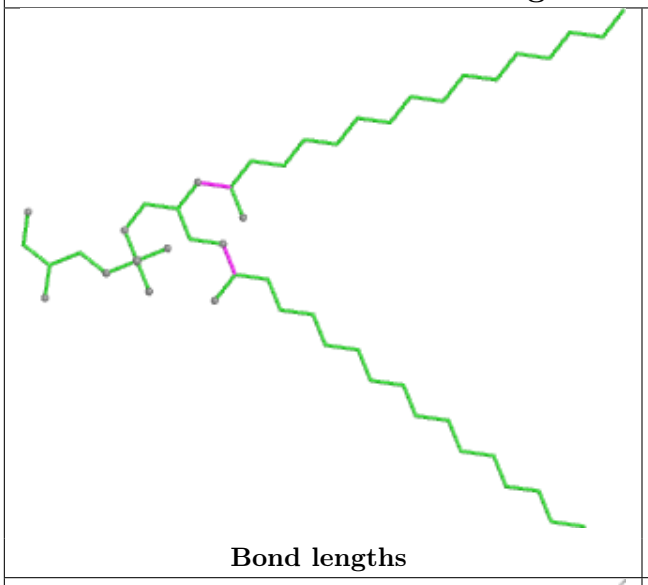


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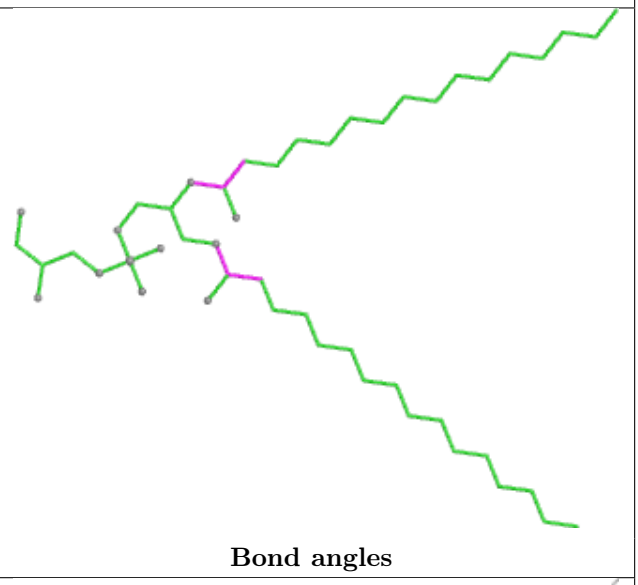


Rings

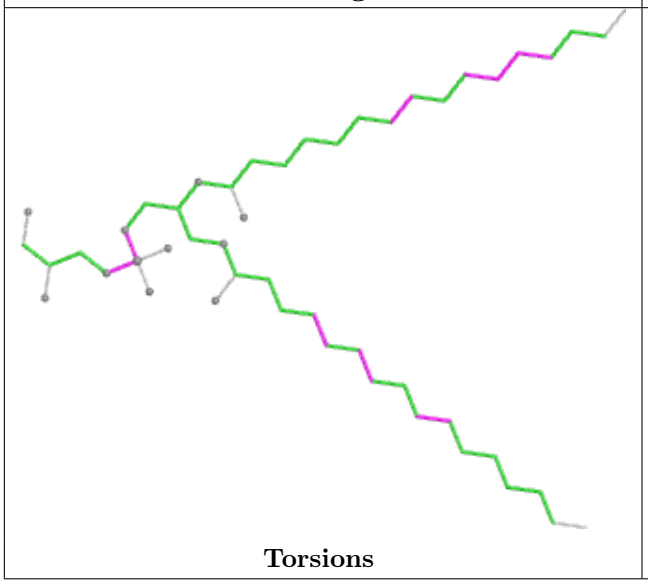
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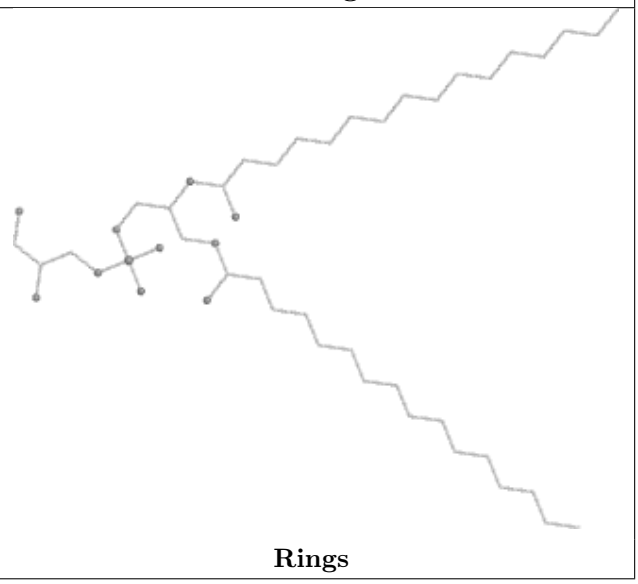
Bond lengths



Bond angles

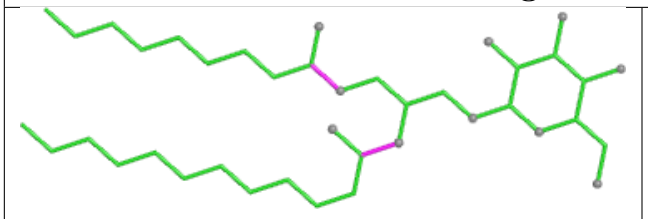


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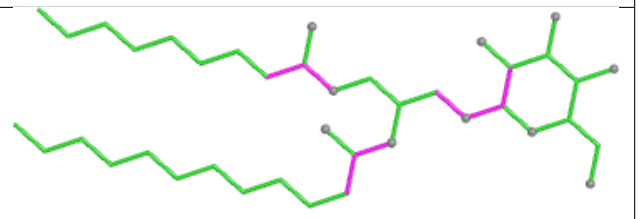


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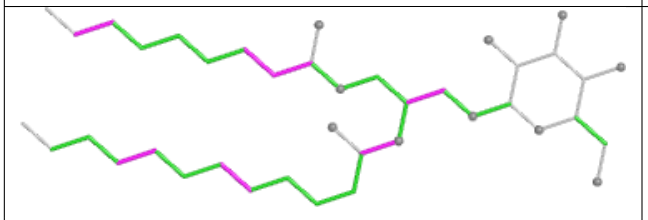
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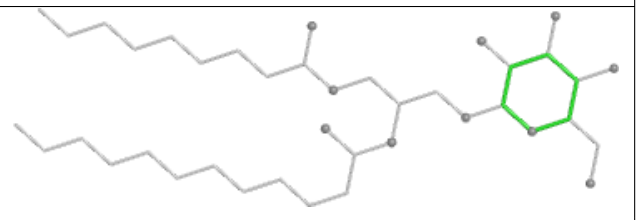
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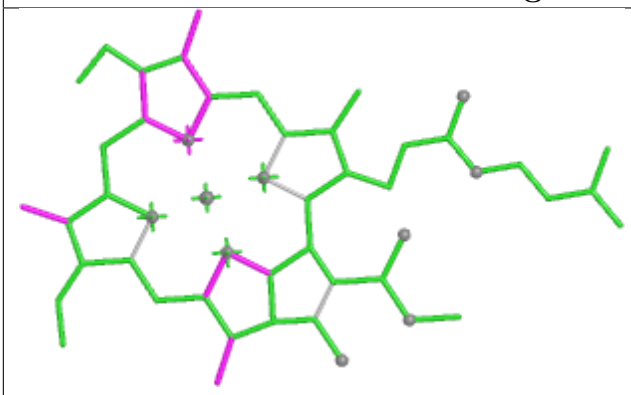


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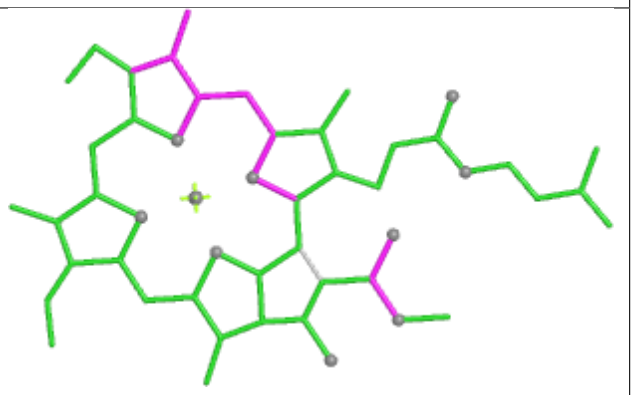


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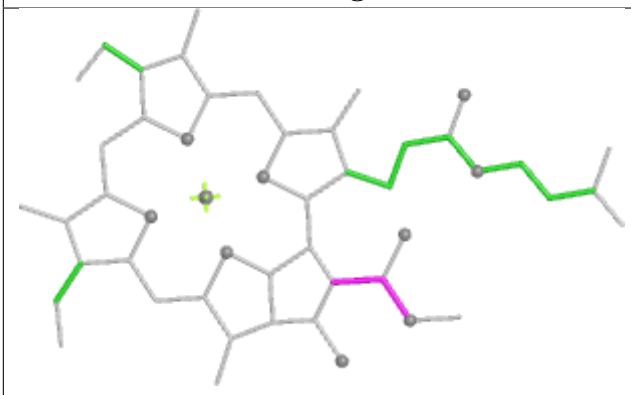
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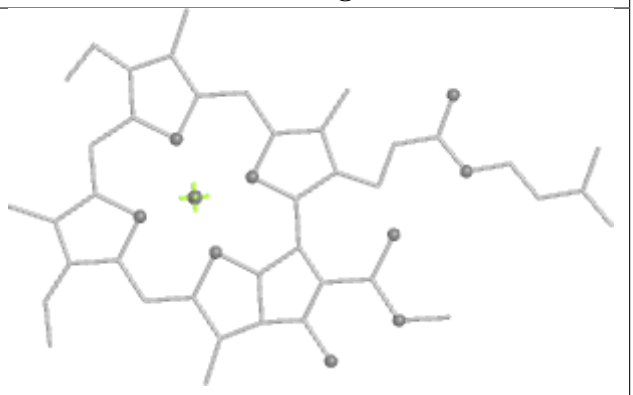
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Bond angles

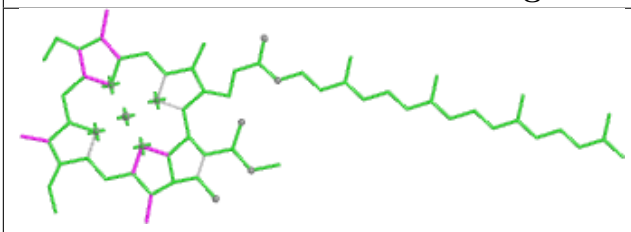


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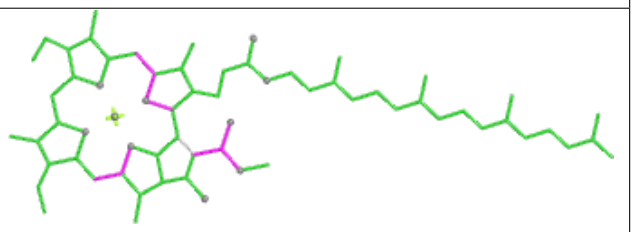


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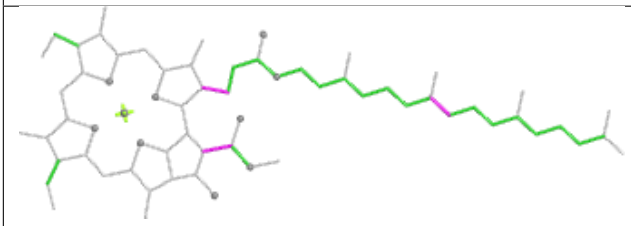
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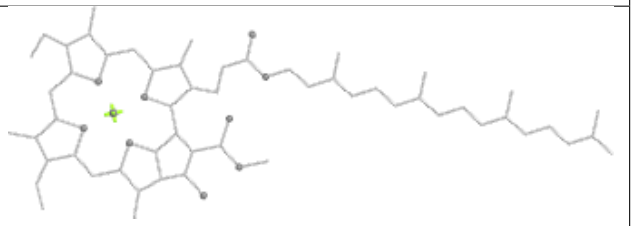
Bond lengths



Bond angles

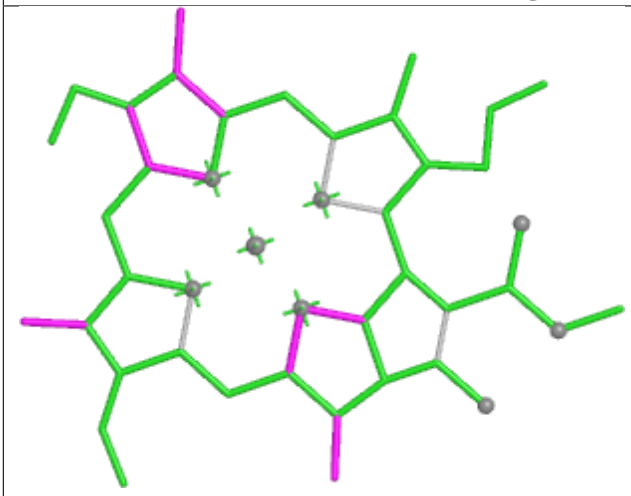


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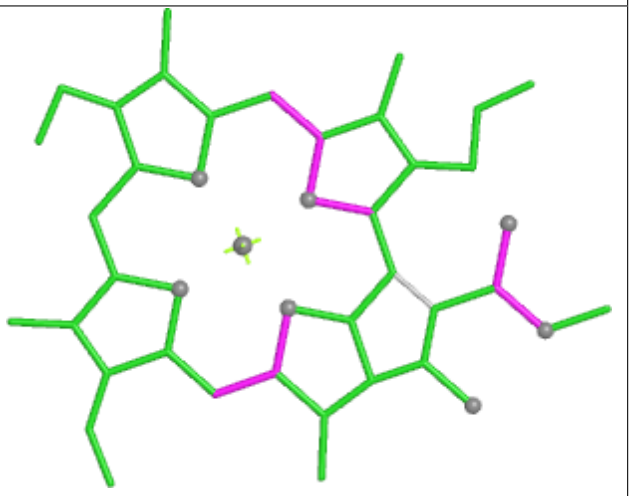


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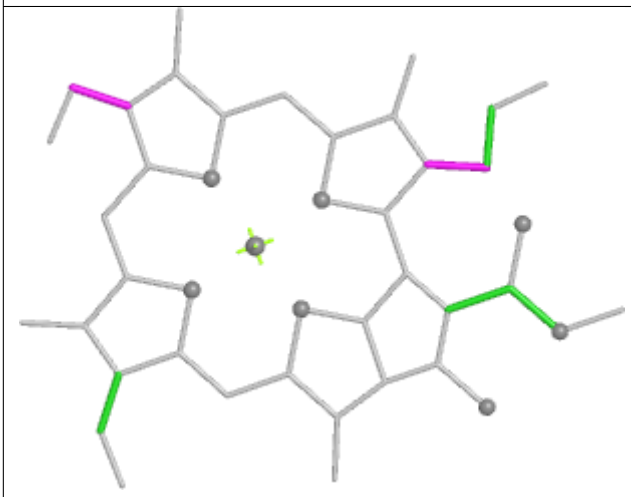
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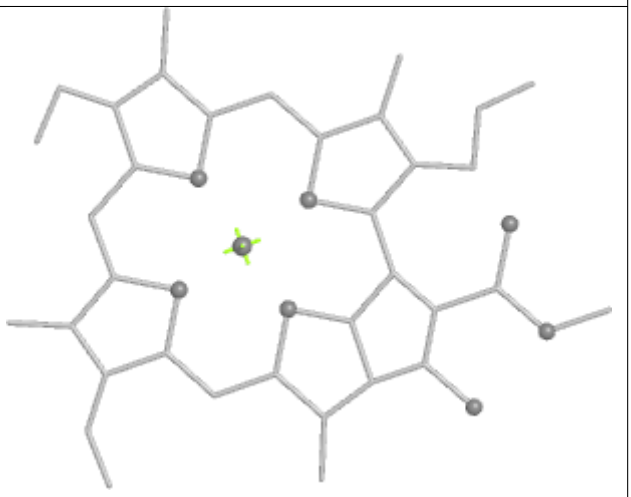
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Bond angles

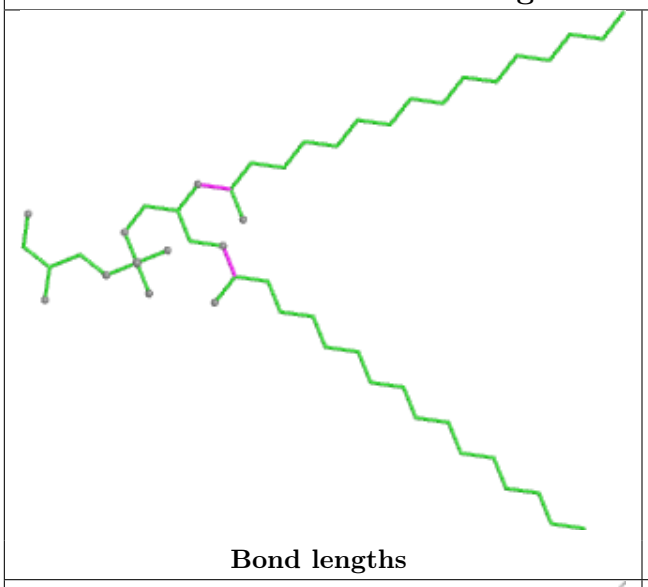


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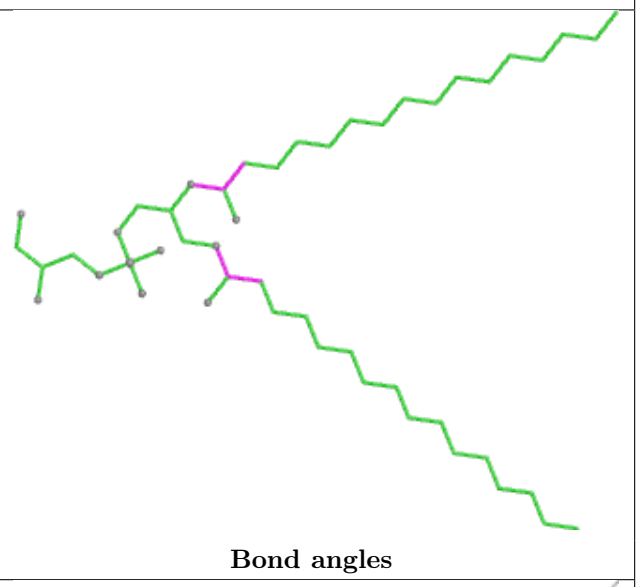


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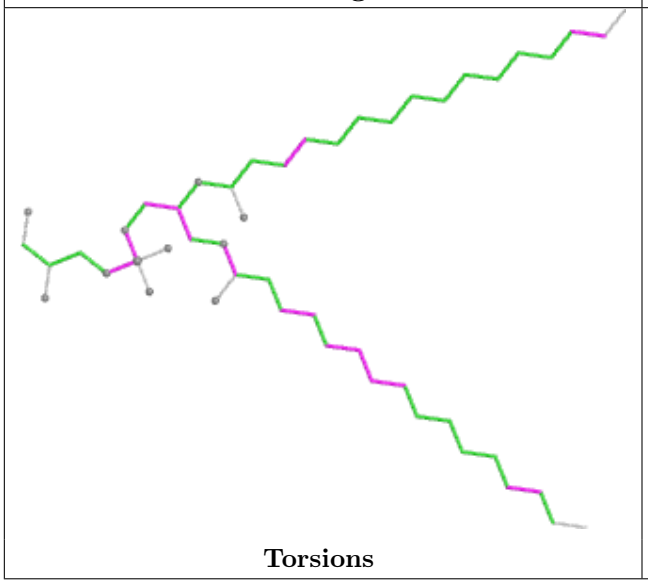
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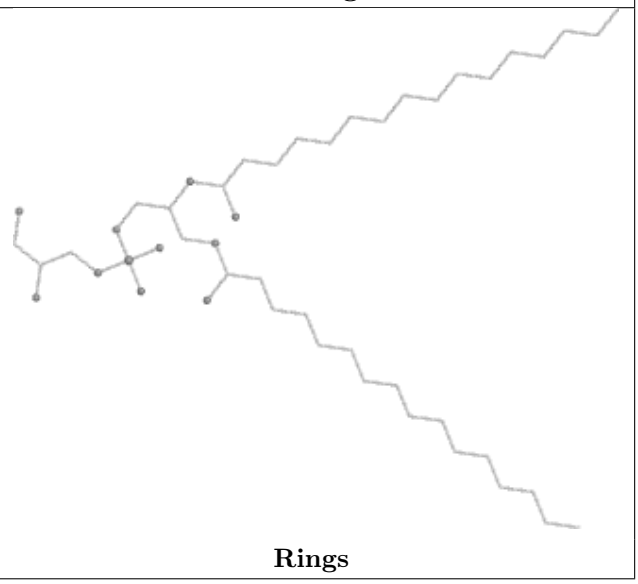
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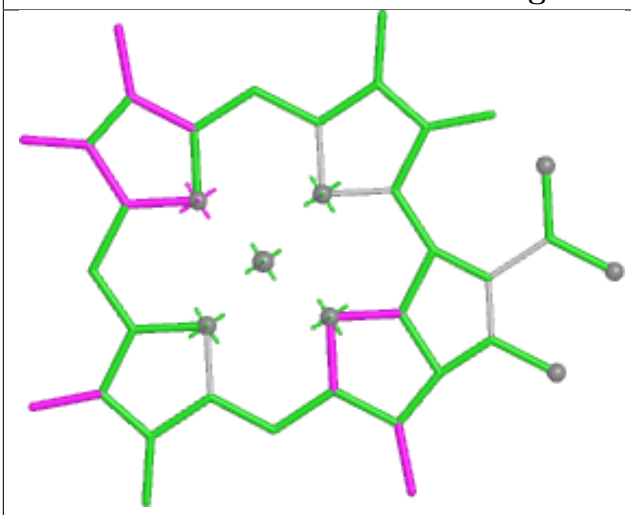


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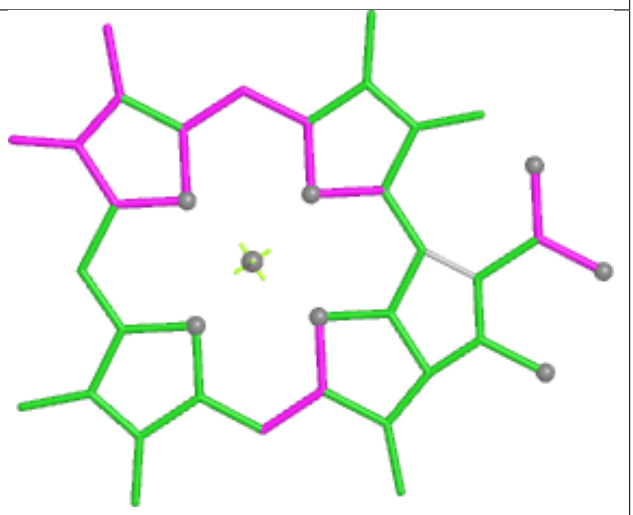


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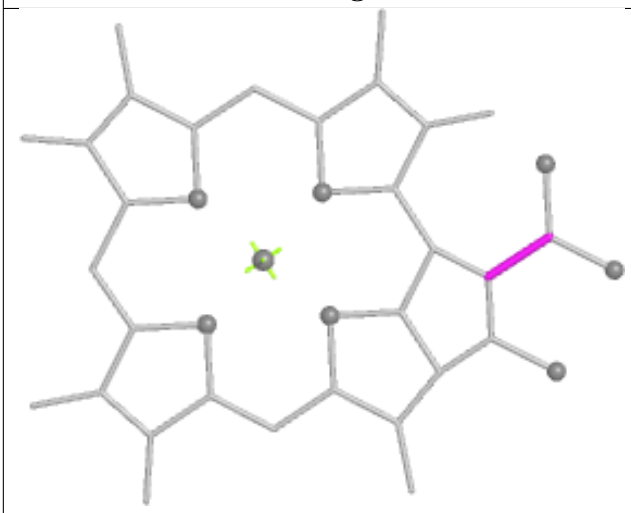
Ligand CLA a 611



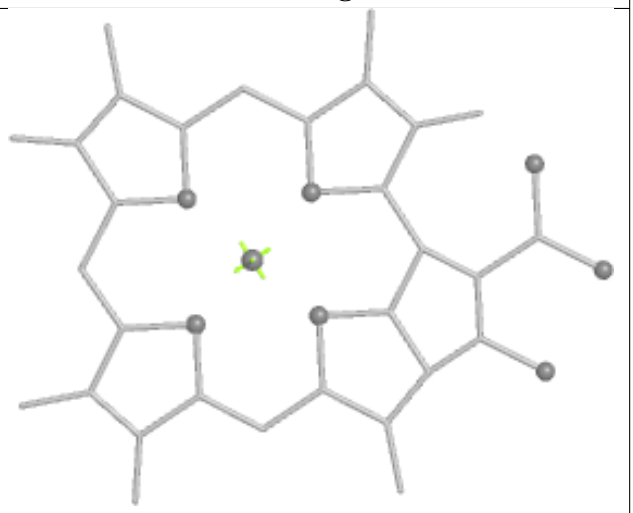
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Bond angles

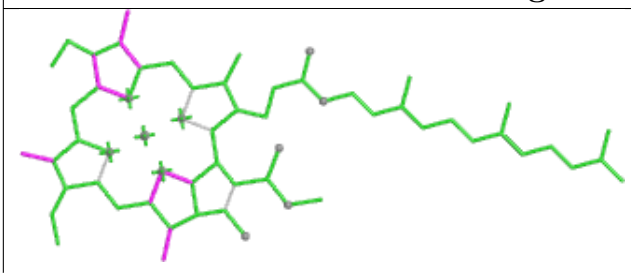


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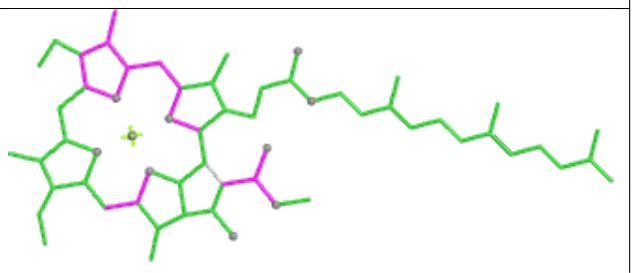


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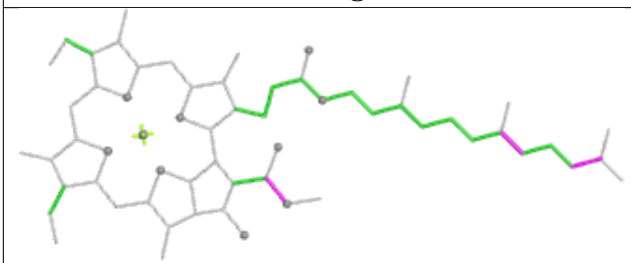
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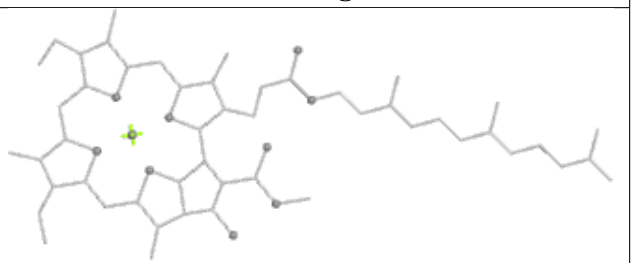
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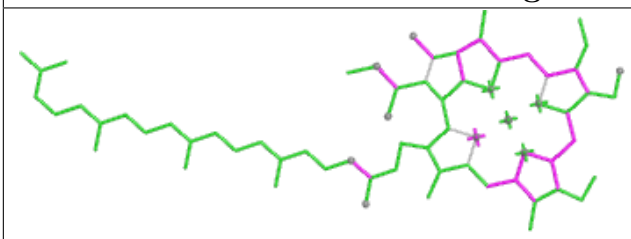


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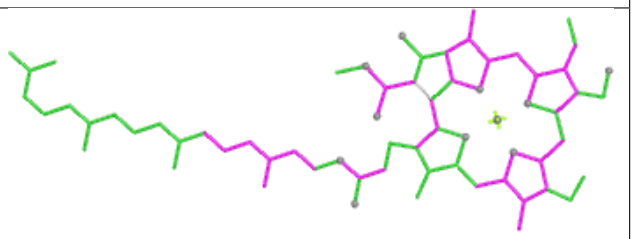


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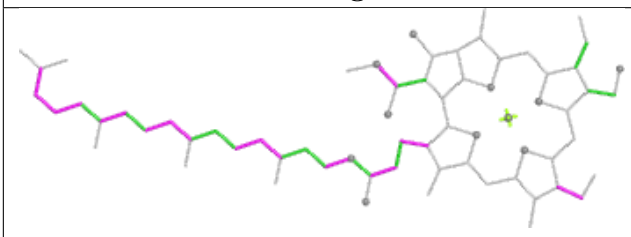
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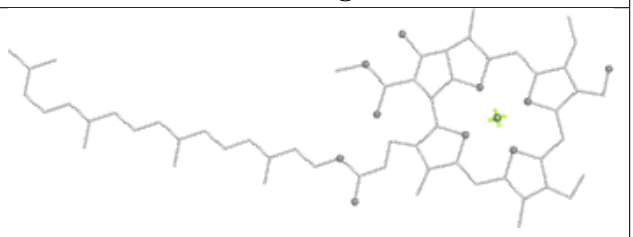
Bond lengths



Bond angles

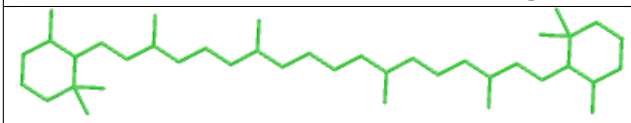


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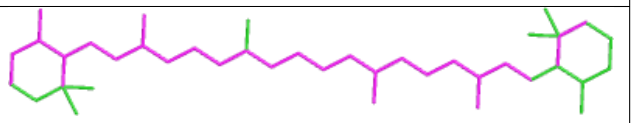


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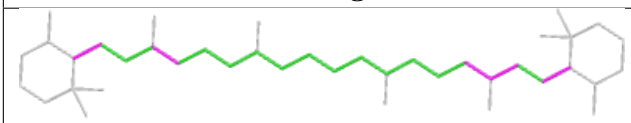
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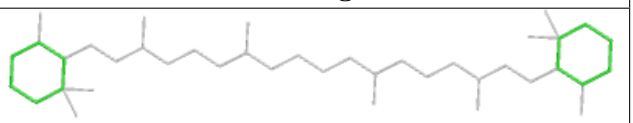
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Bond angles

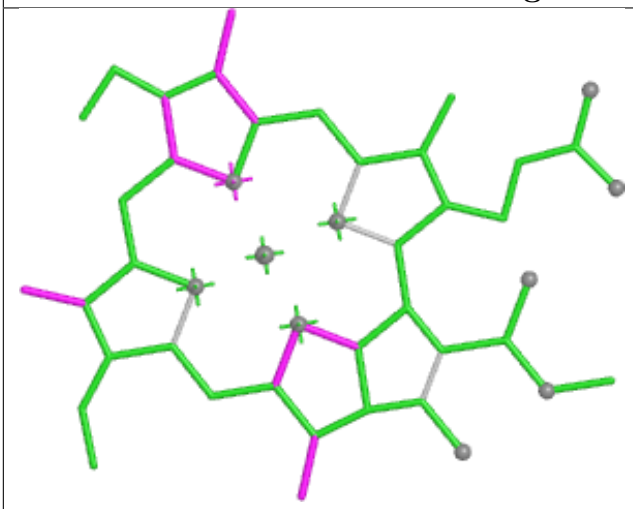


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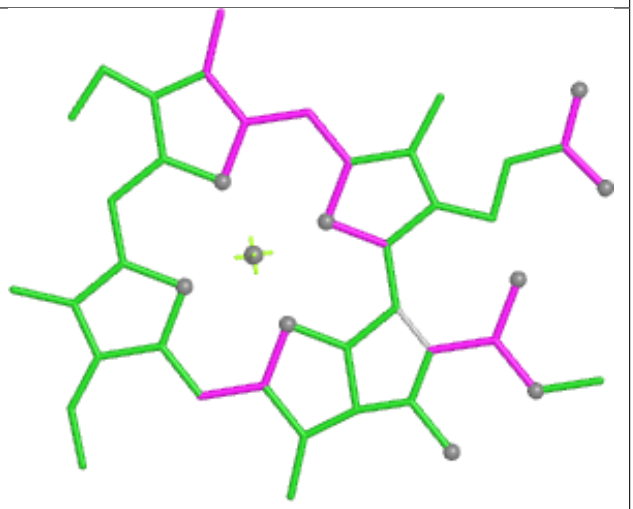


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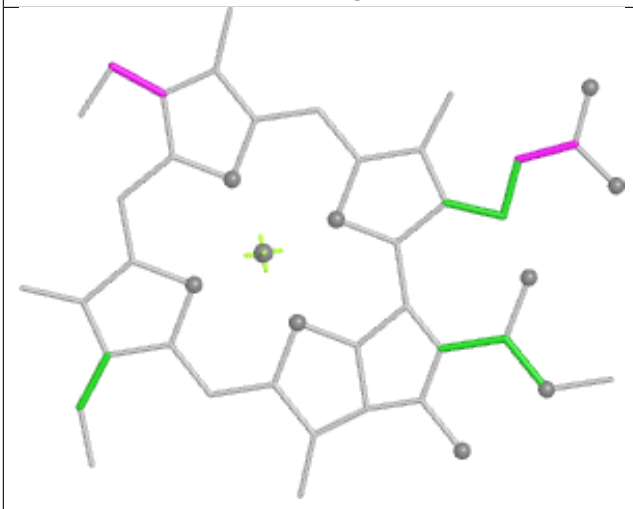
Ligand CLA V 612



Bond lengths



Bond angles

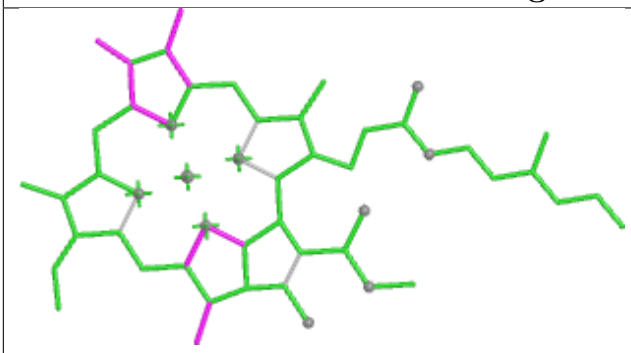


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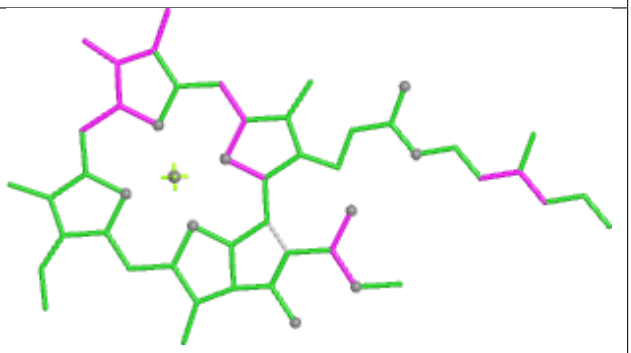


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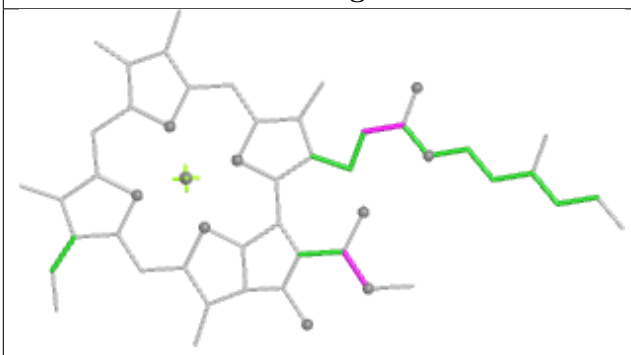
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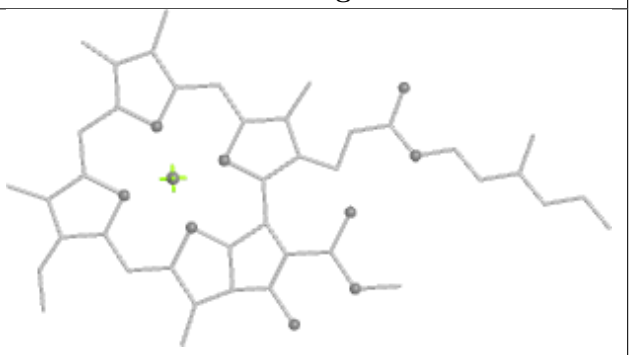
Bond lengths



Bond angles

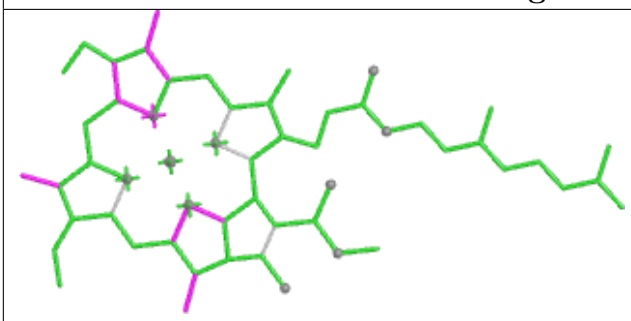


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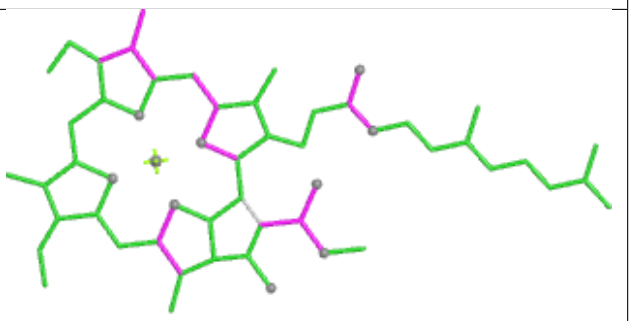


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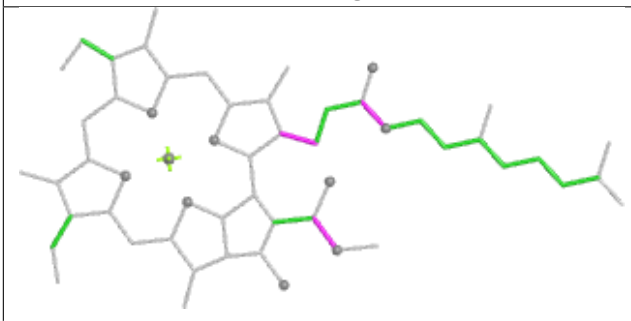
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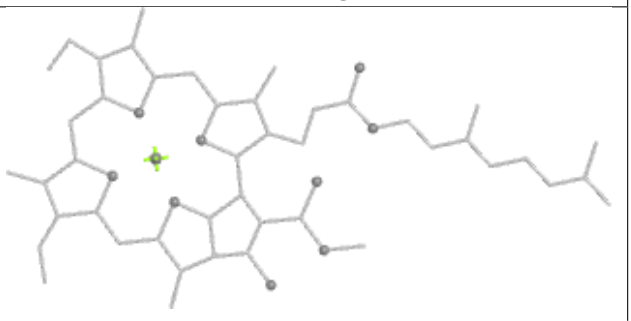
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Bond angles

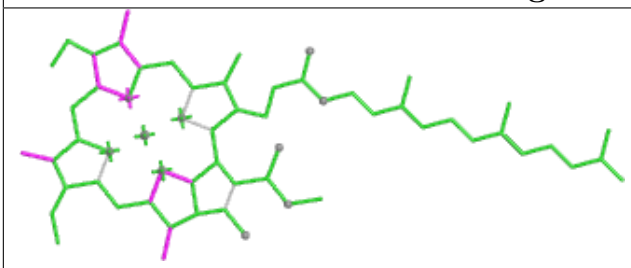


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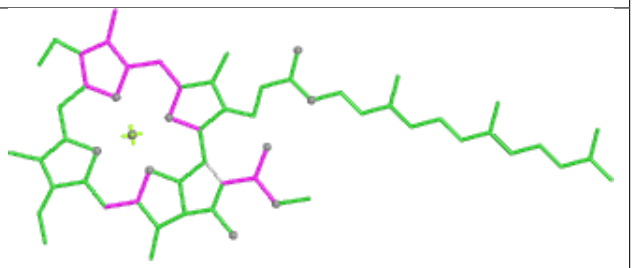


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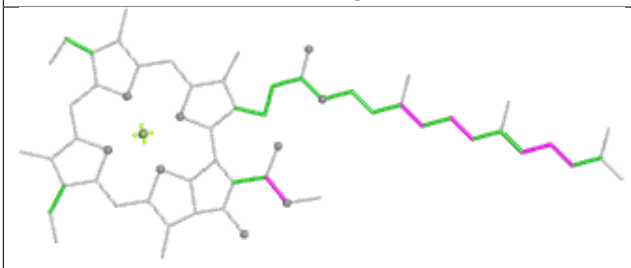
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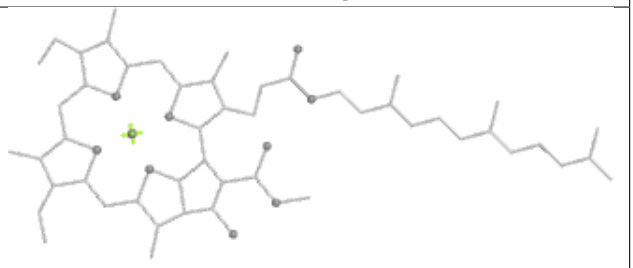
Bond lengths



Bond angles

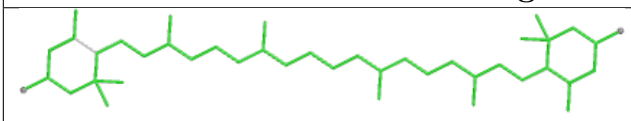


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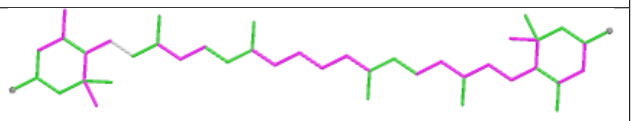


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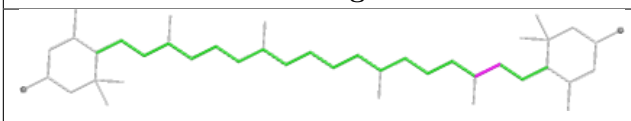
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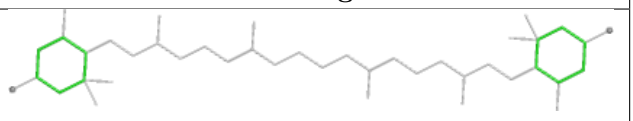
Bond lengths



Bond angles

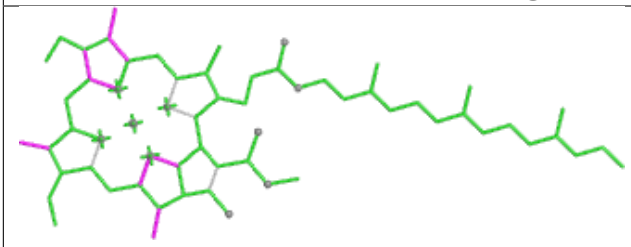


Torsions

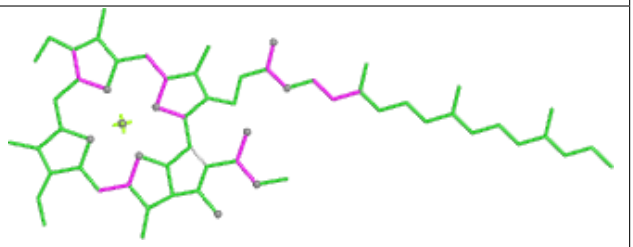


Rings

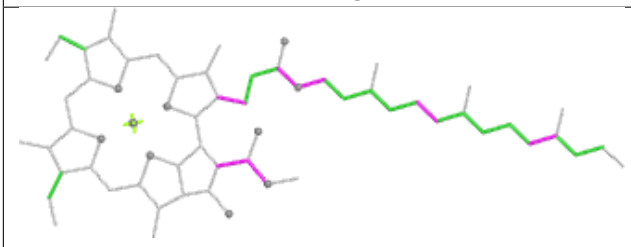
Ligand CLA B 814



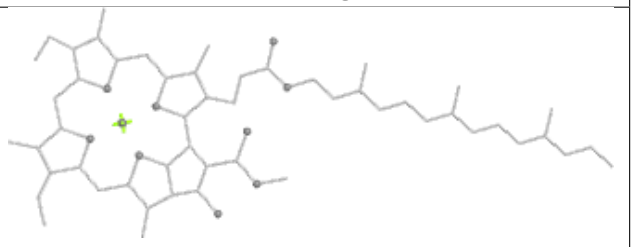
Bond lengths



Bond angles

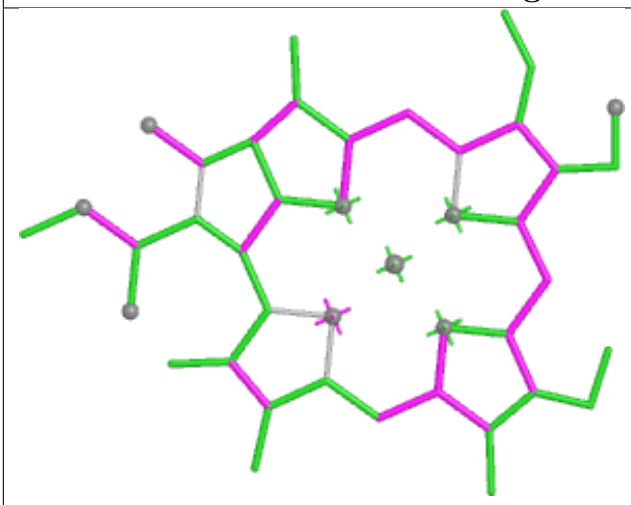


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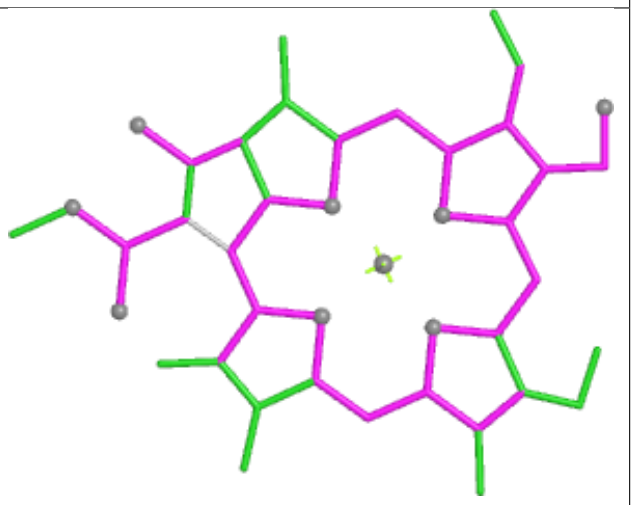


Rings

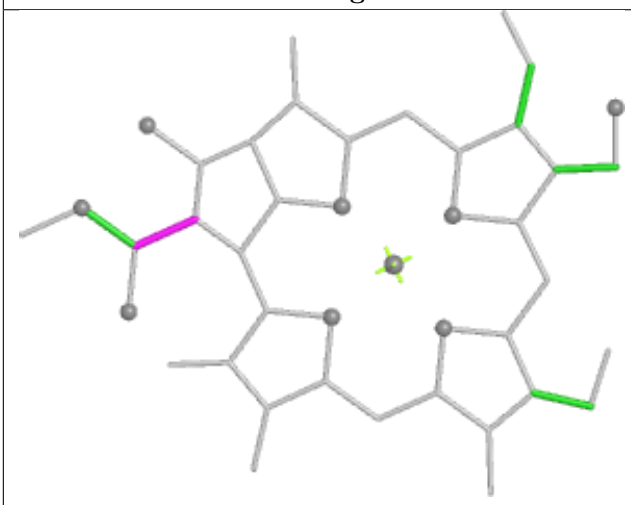
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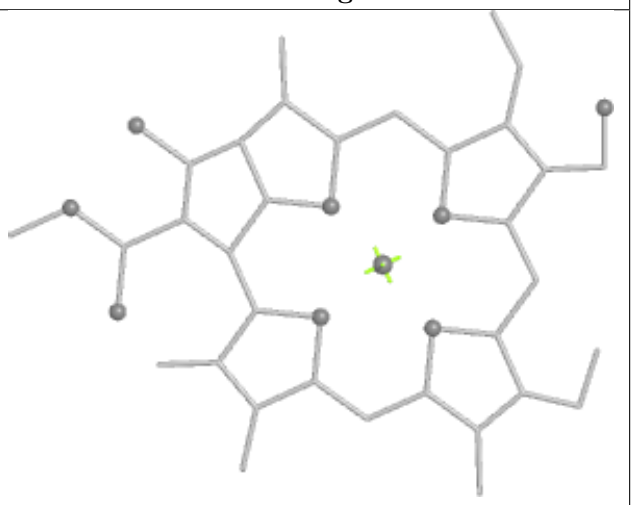
Bond lengths



Bond angles

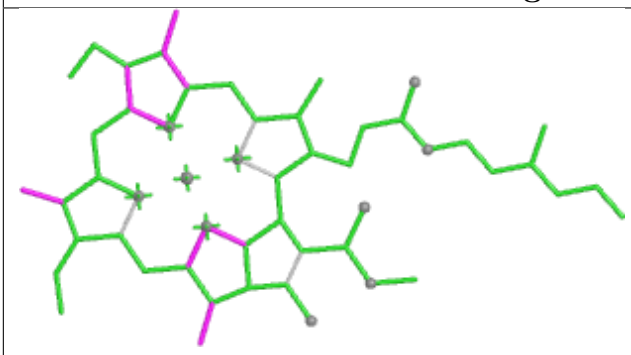


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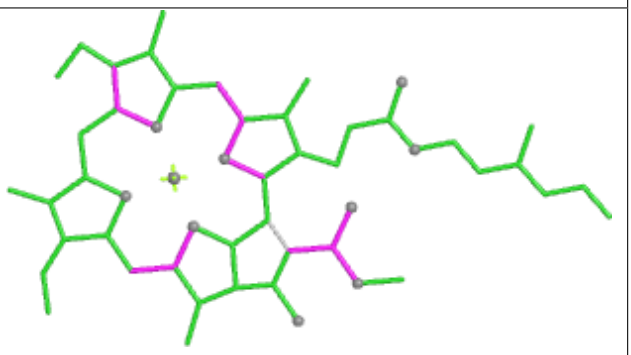


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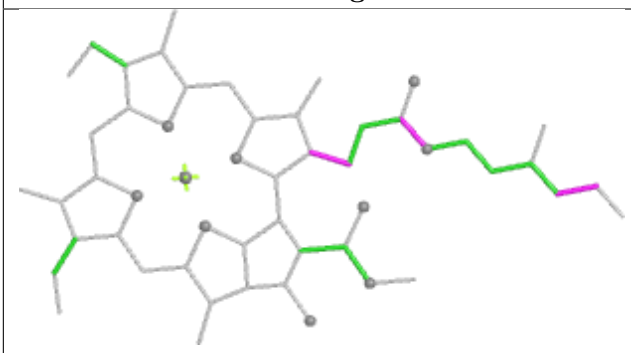
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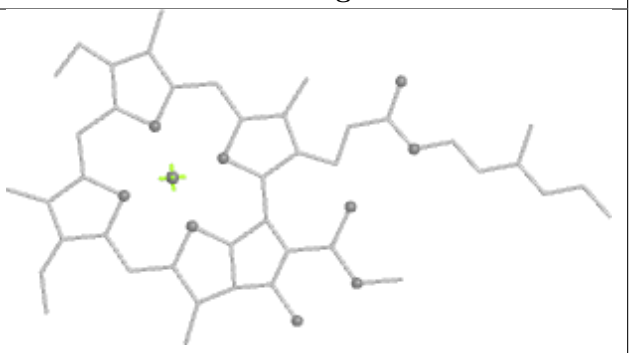
Bond lengths



Bond angles

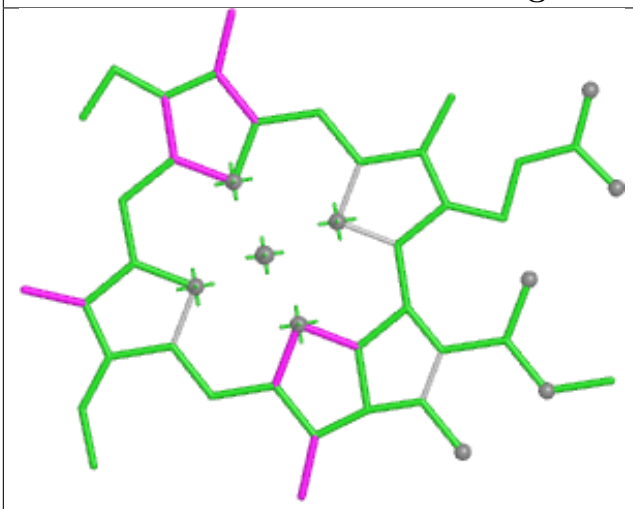


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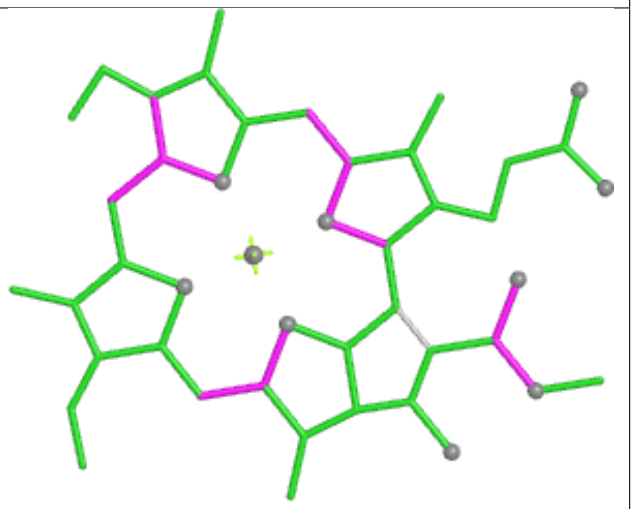


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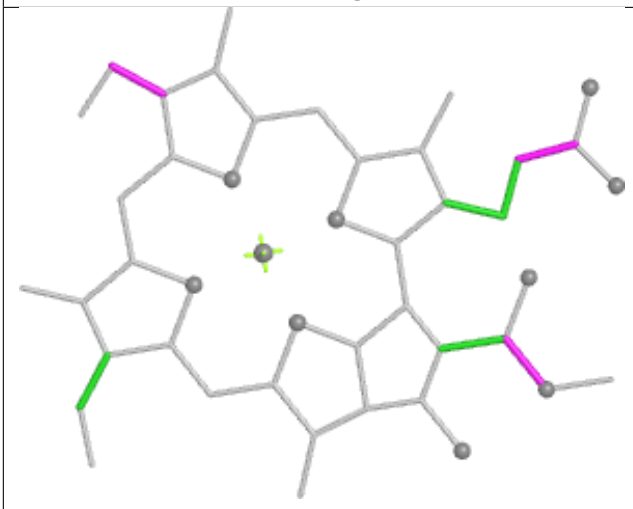
Ligand CLA 4 607



Bond lengths



Bond angles

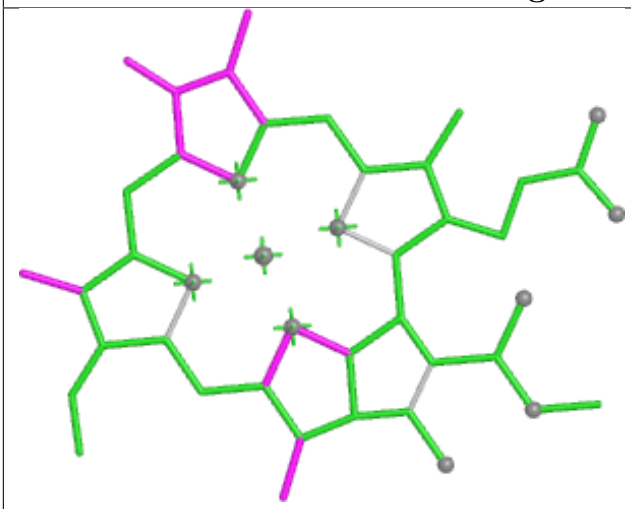


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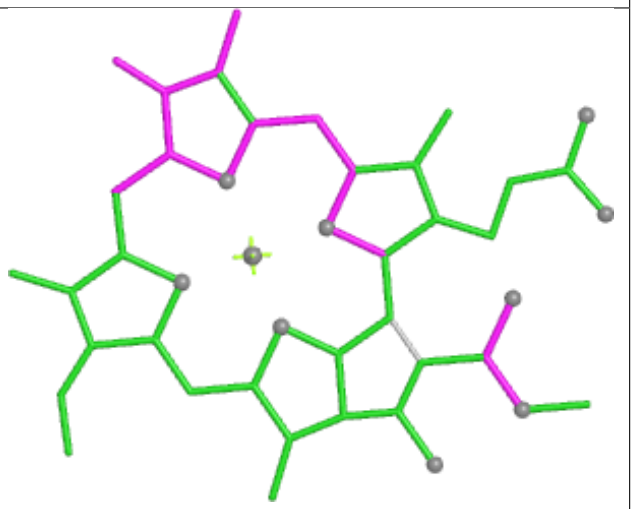


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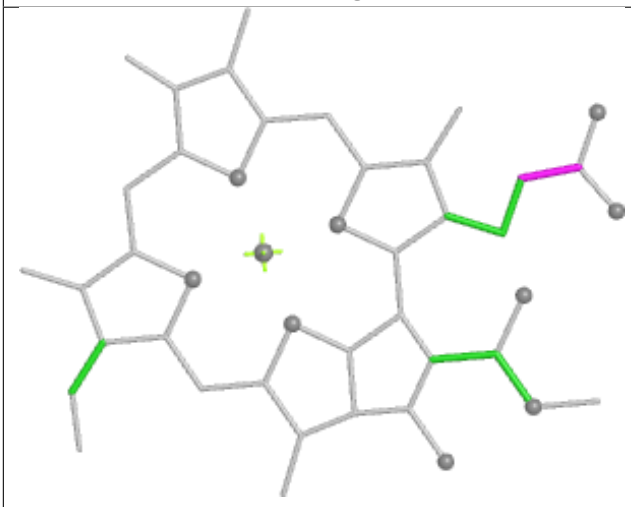
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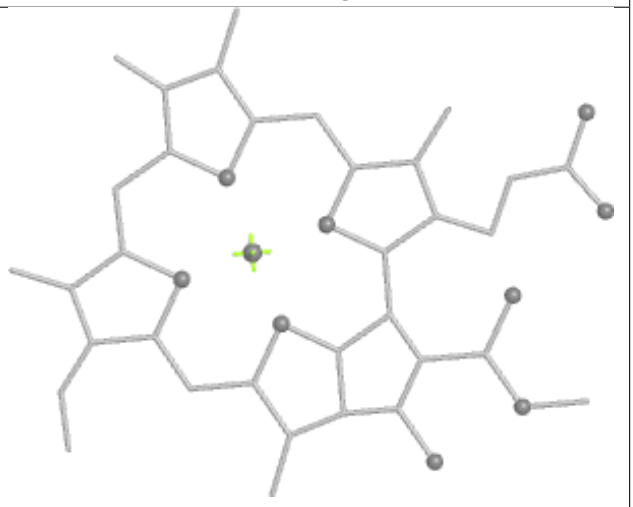
Bond lengths



Bond angles

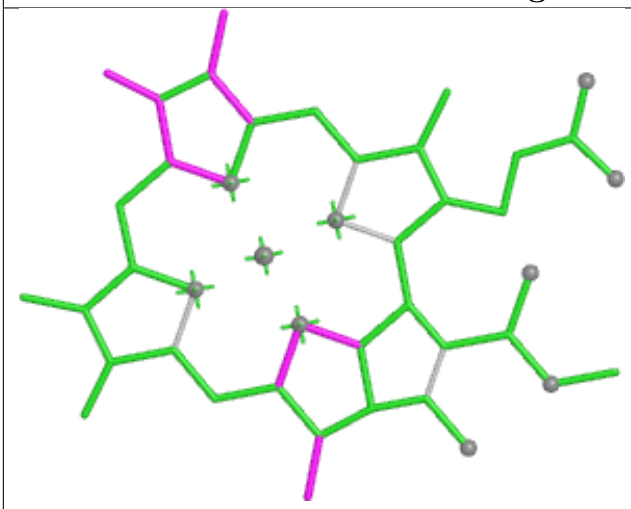


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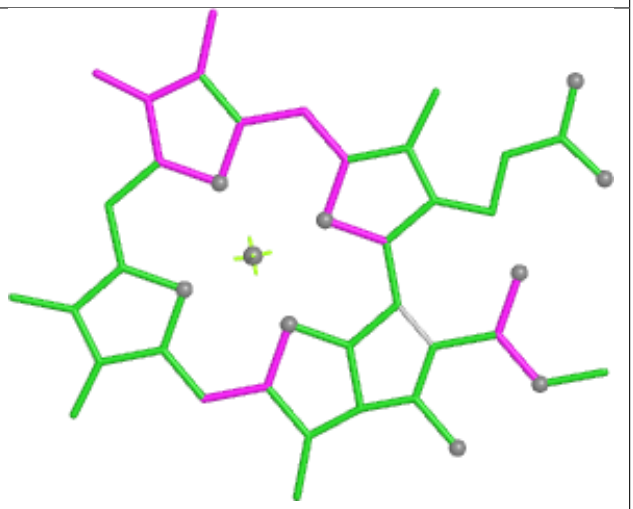


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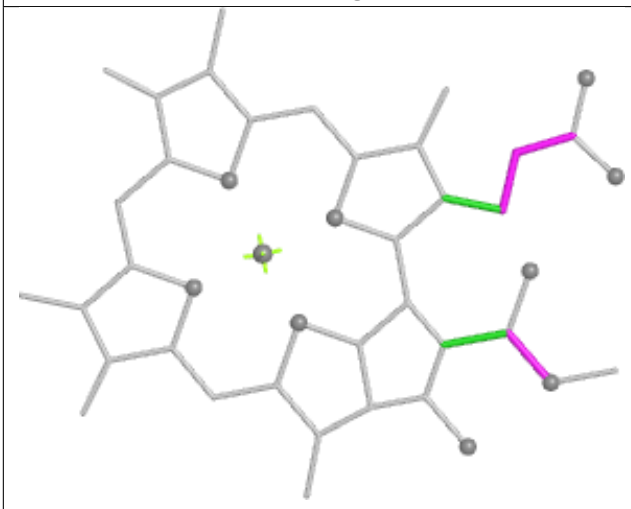
Ligand CLA 1 616



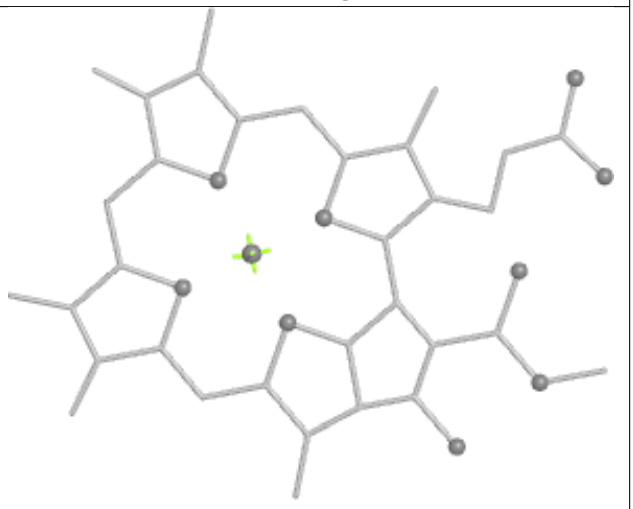
Bond lengths



Bond angles

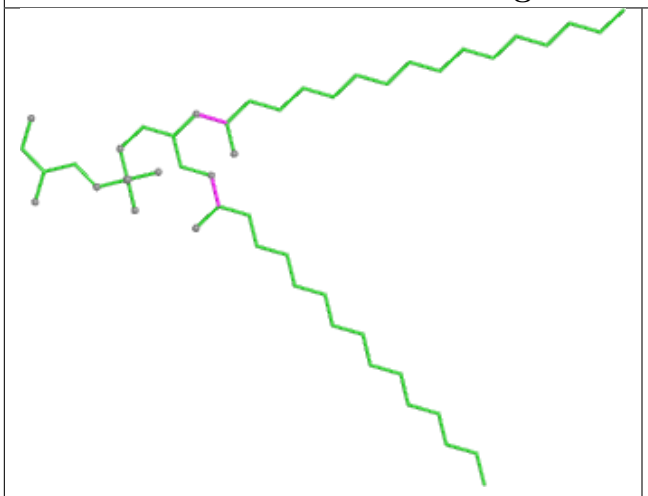


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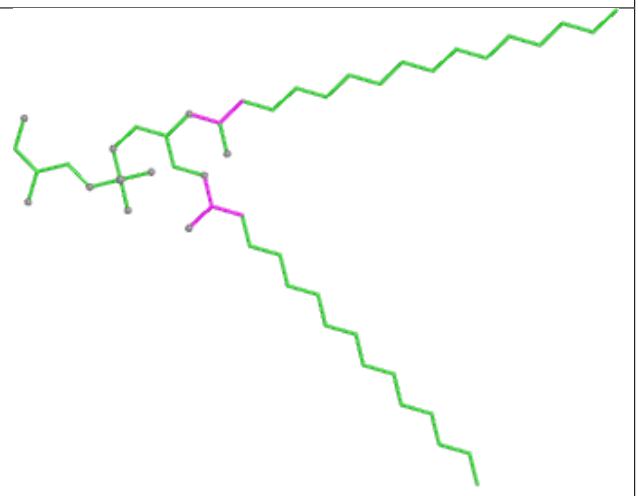


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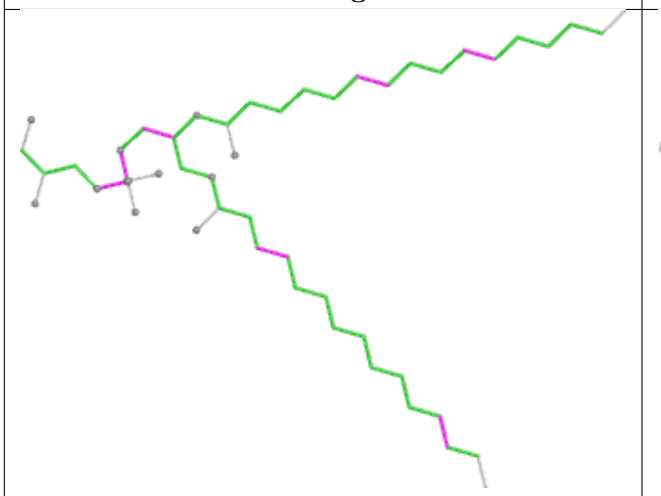
Ligand LHG V 2630



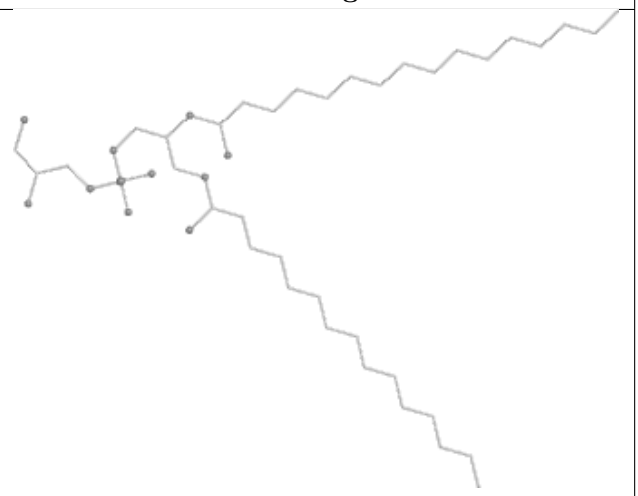
Bond lengths



Bond angles

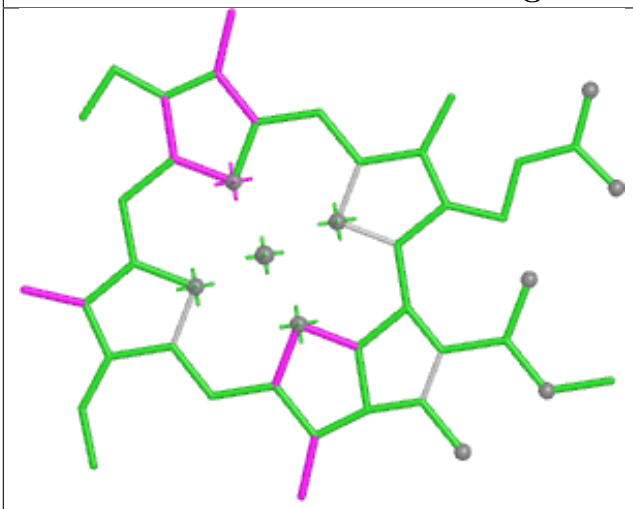


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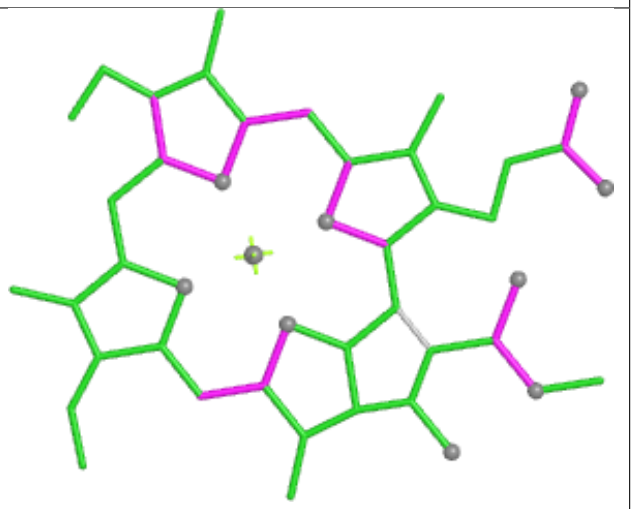


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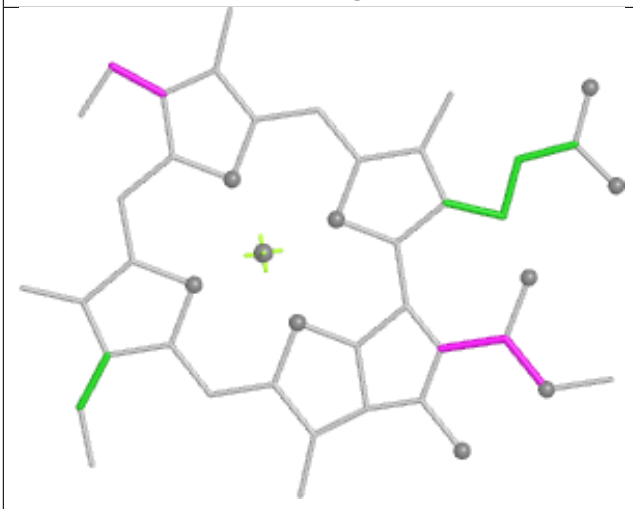
Ligand CLA V 614



Bond lengths



Bond angles

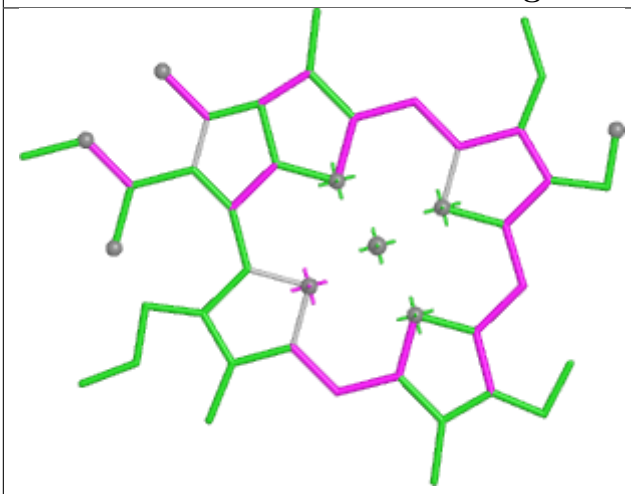


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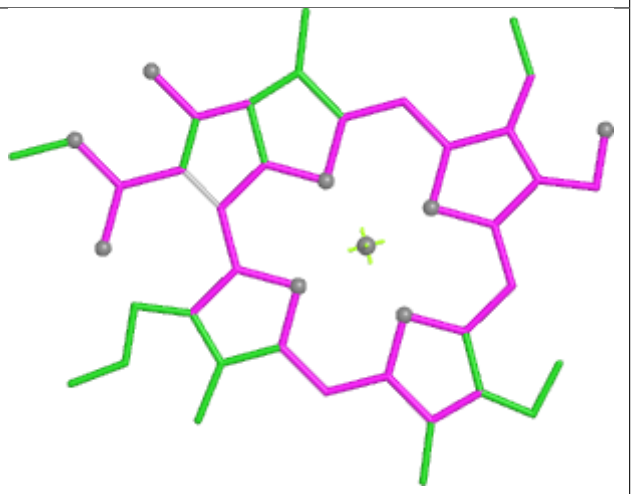


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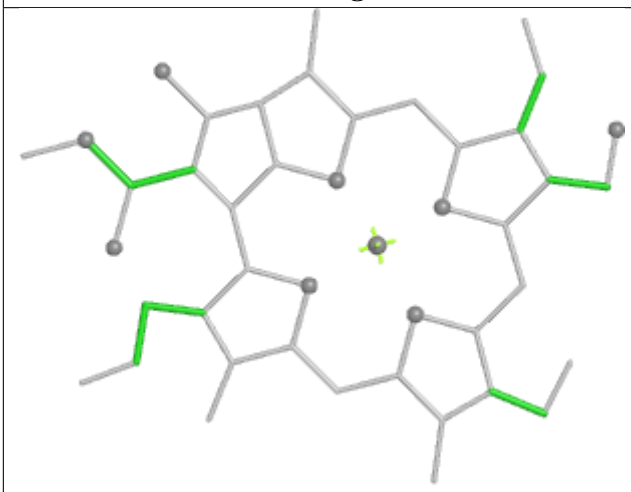
Ligand CHL X 606



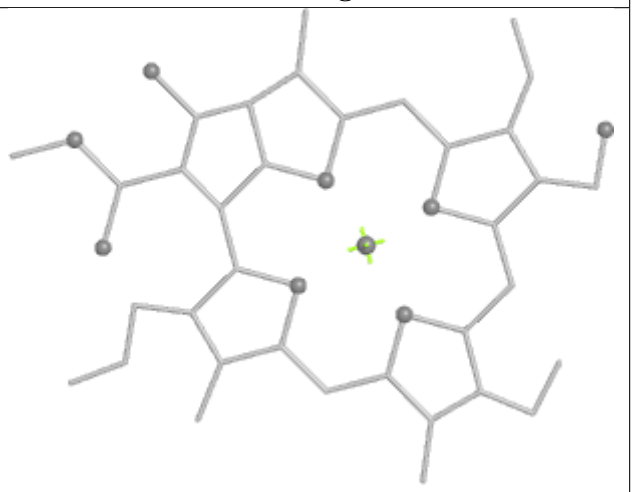
Bond lengths



Bond angles

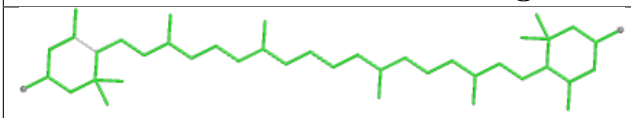


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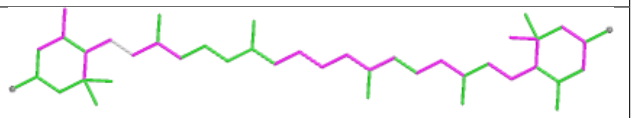


Rings

Ligand LUT X 1620



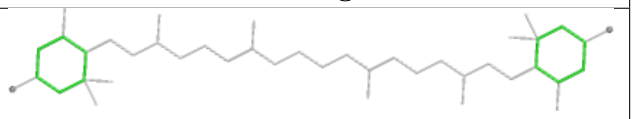
Bond lengths



Bond angles

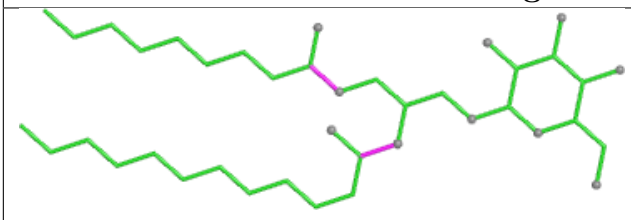


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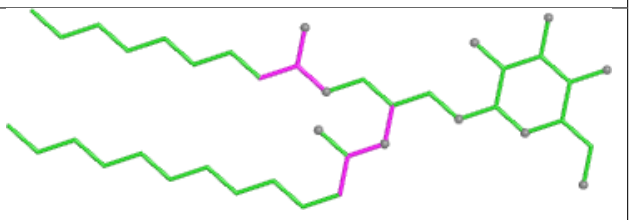


Rings

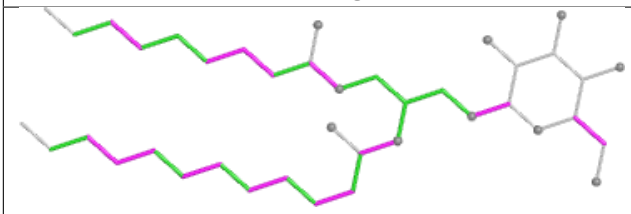
Ligand LMG J 104



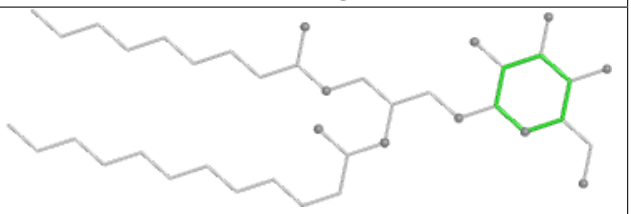
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Bond angles

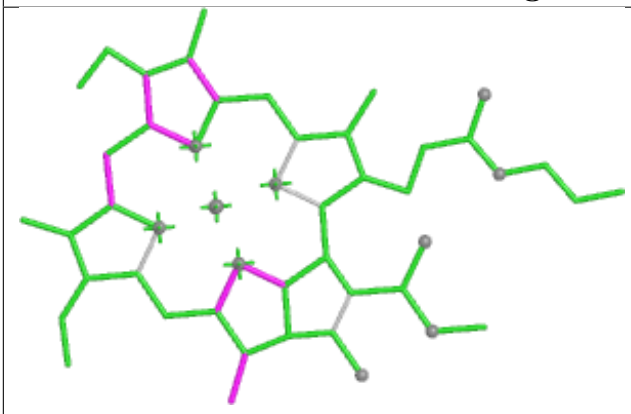


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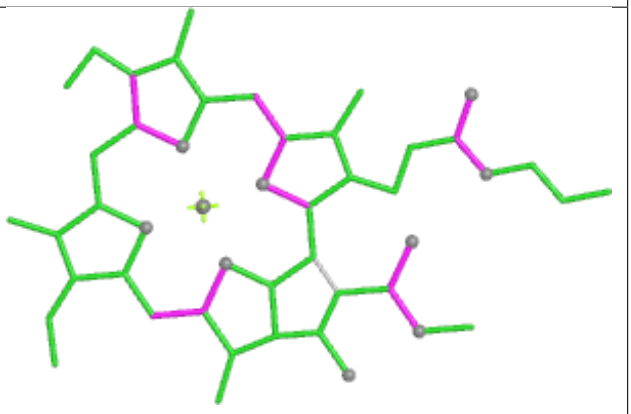


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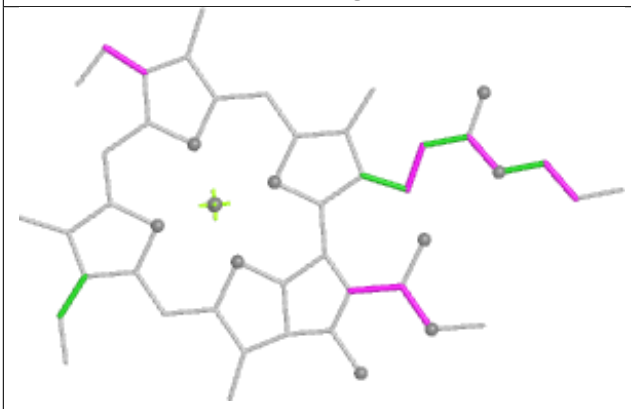
Ligand CLA Y 614



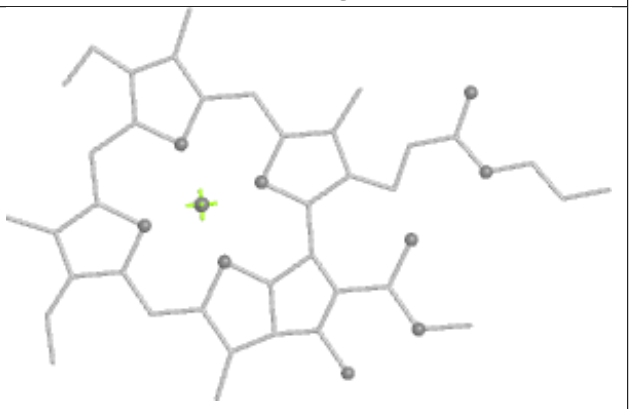
Bond lengths



Bond angles

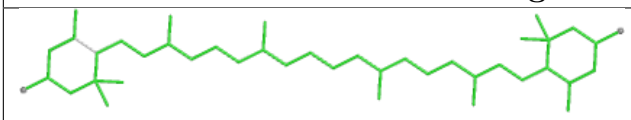


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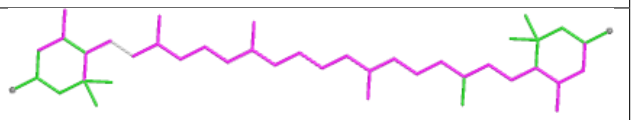


Rings

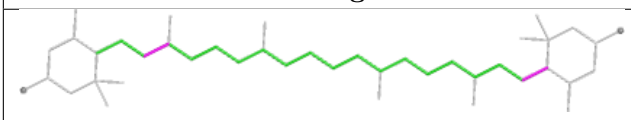
Ligand LUT 4 619



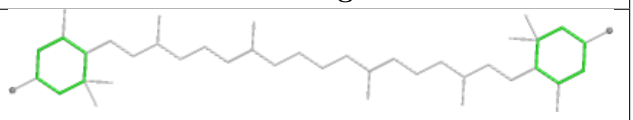
Bond lengths



Bond angles

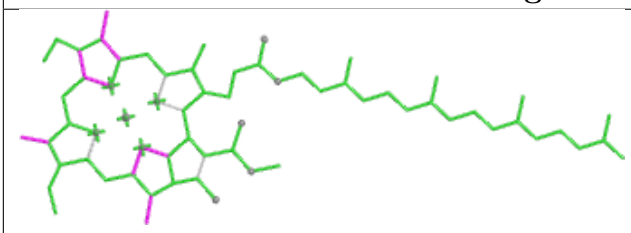


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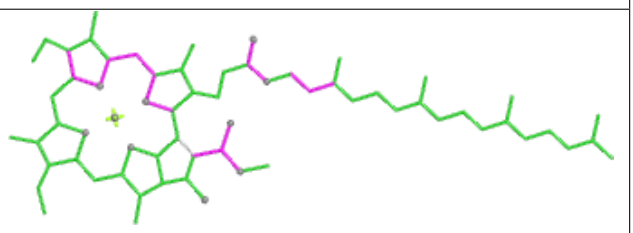


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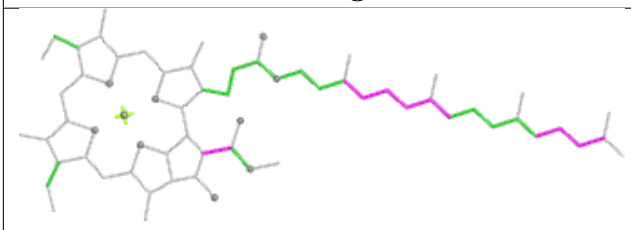
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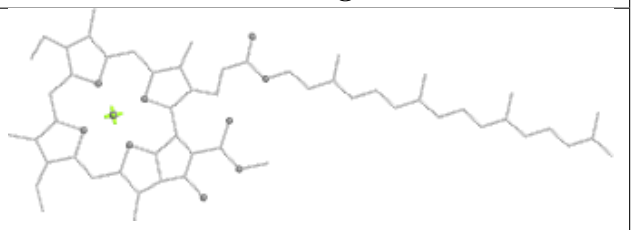
Bond lengths



Bond angles

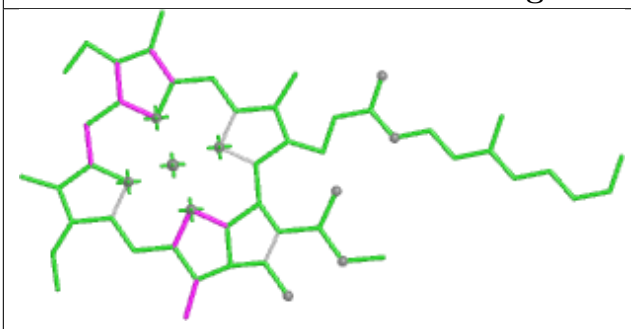


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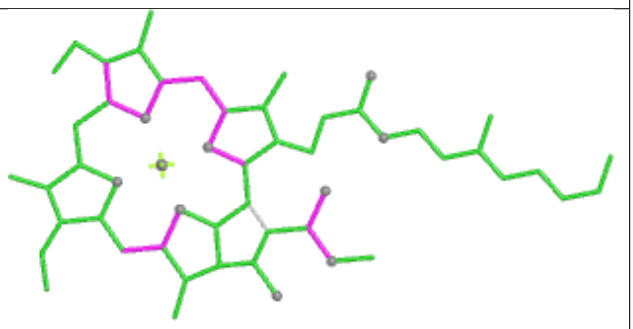


Rings

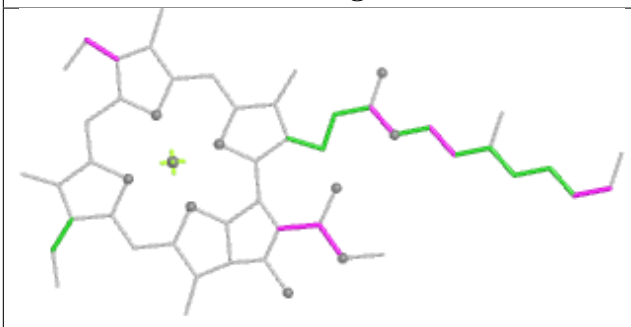
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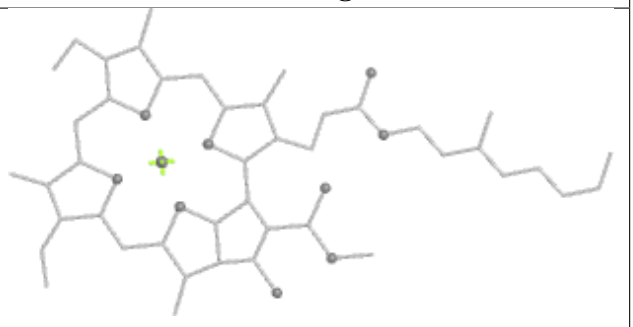
Bond lengths



Bond angles

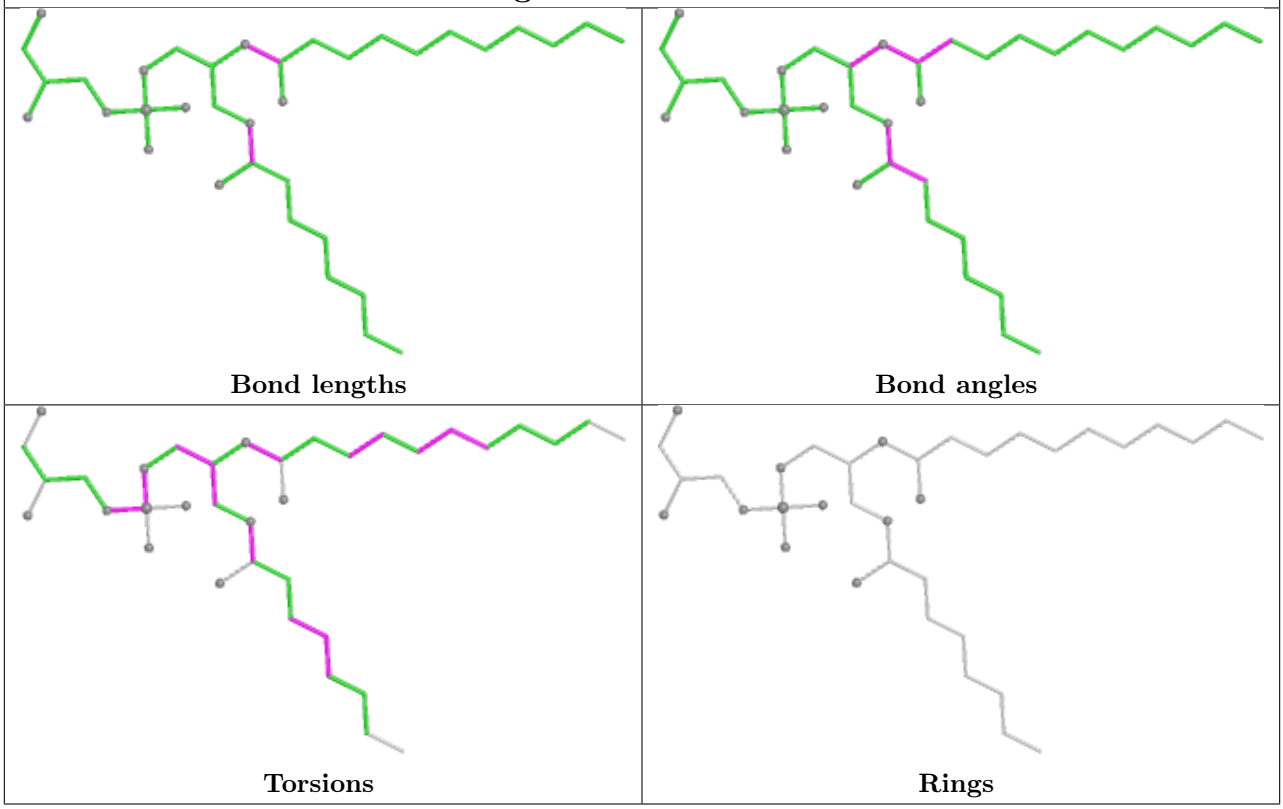


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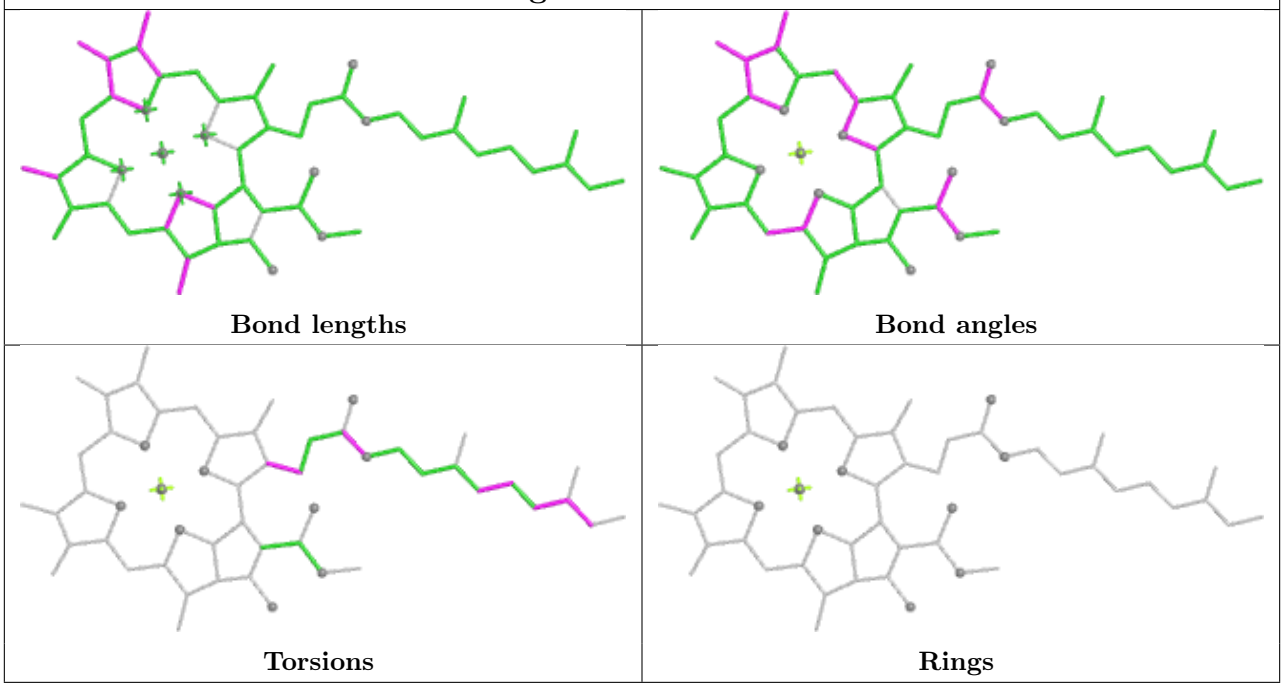


Rings

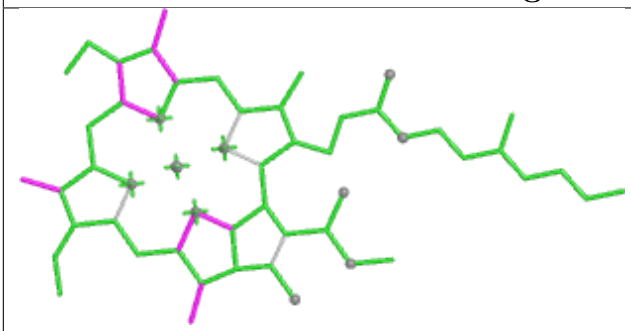
Ligand LHG O 2631



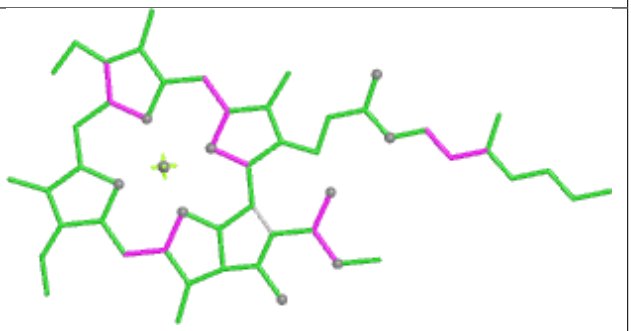
Ligand CLA 4 604



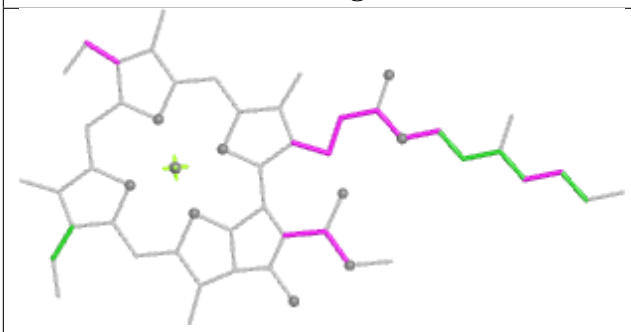
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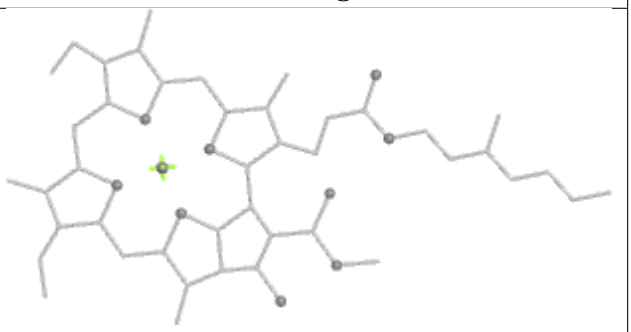
Bond lengths



Bond angles

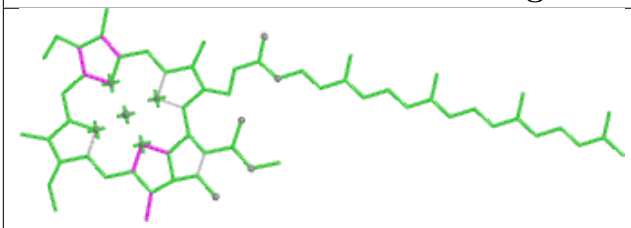


Torsions

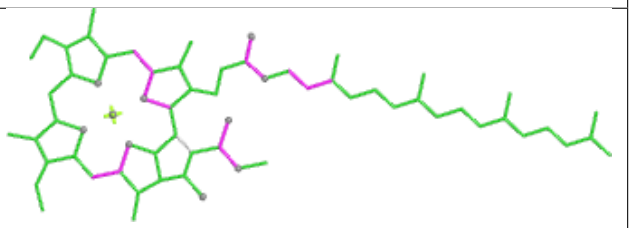


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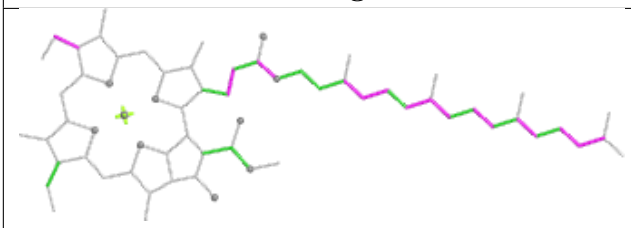
Ligand CLA Z 613



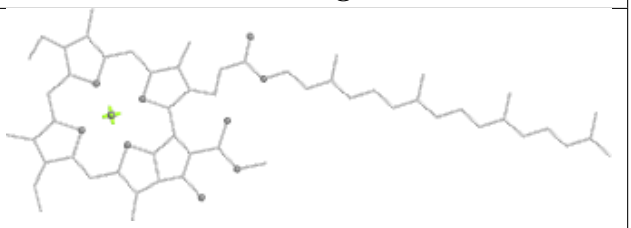
Bond lengths



Bond angles

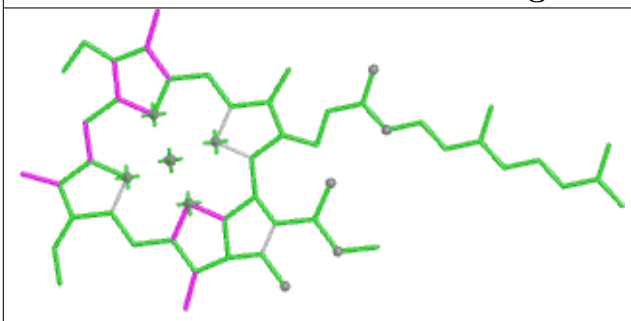


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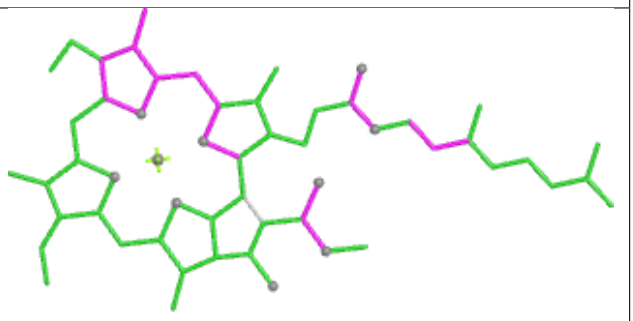


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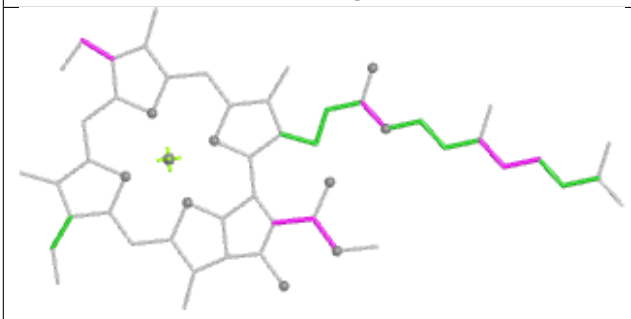
Ligand CLA 2 610



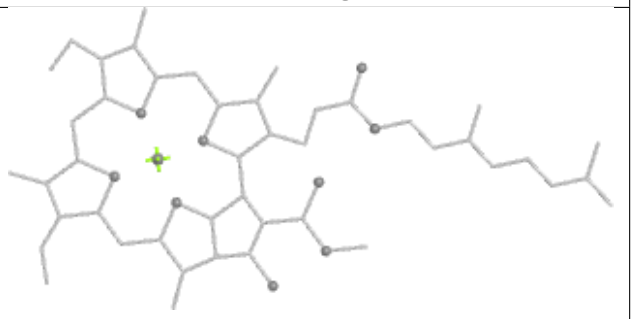
Bond lengths



Bond angles

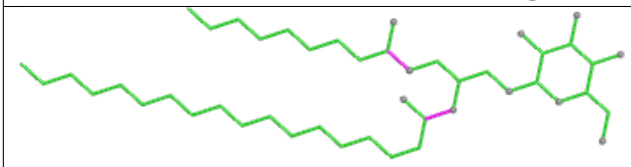


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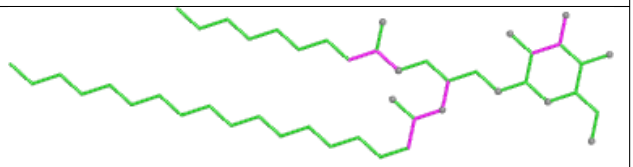


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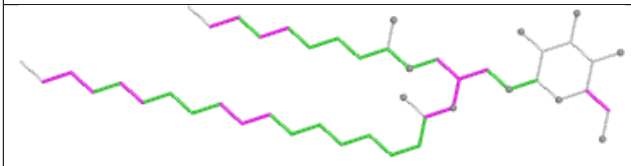
Ligand LMG 8 626



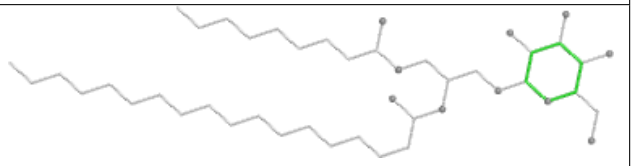
Bond lengths



Bond angles



Torsions



Rings

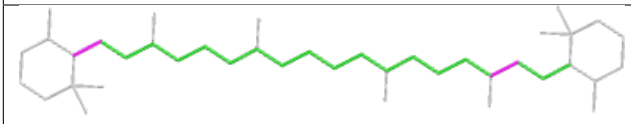
Ligand BCR J 102



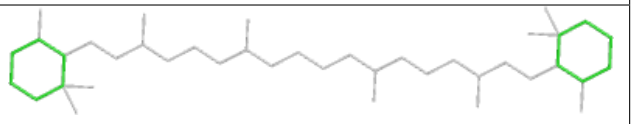
Bond lengths



Bond angles

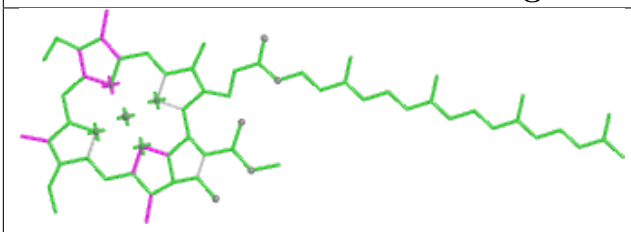


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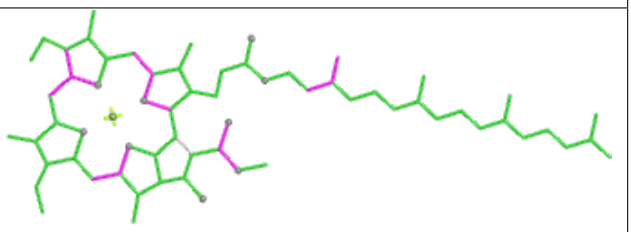


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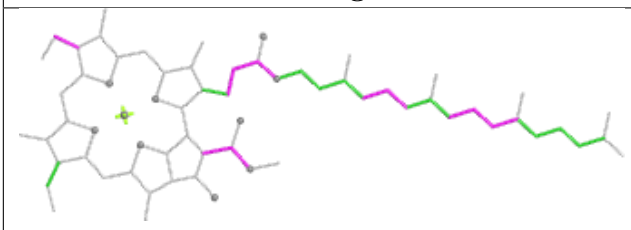
Ligand CLA A 834



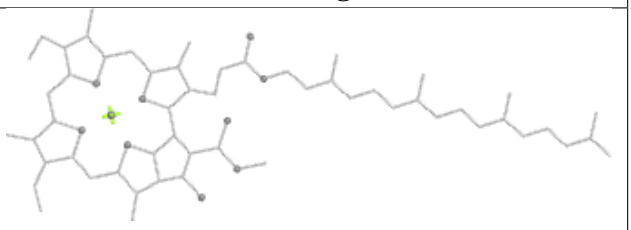
Bond lengths



Bond angles

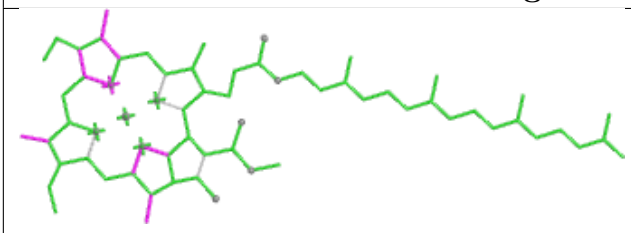


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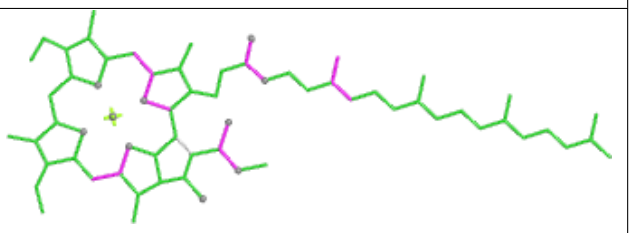


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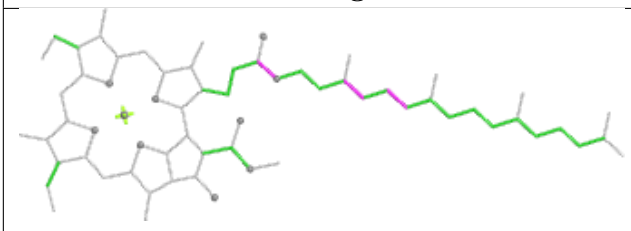
Ligand CLA A 836



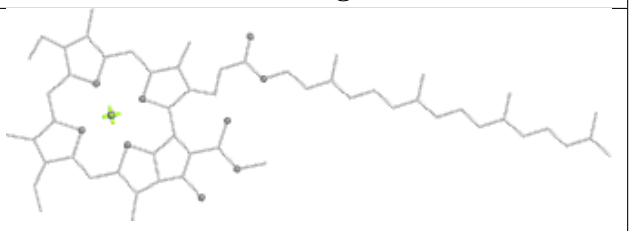
Bond lengths



Bond angles

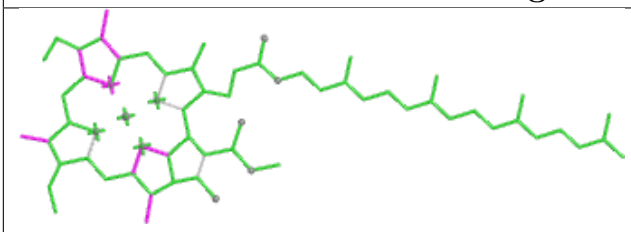


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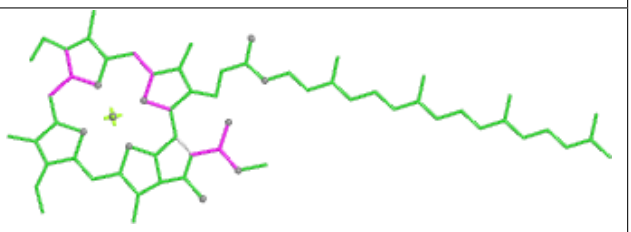


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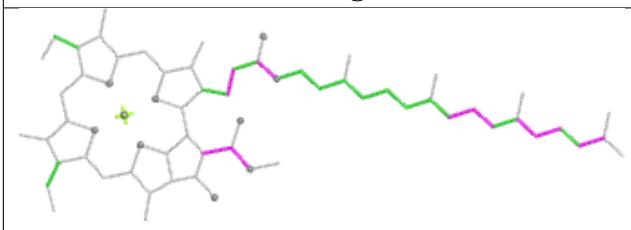
Ligand CLA 5 602



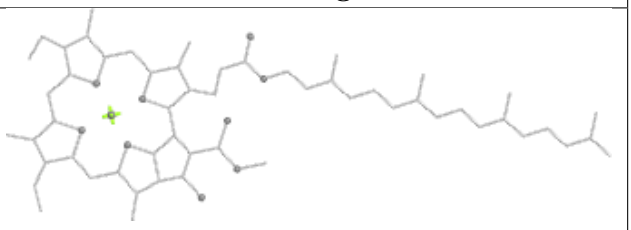
Bond lengths



Bond angles

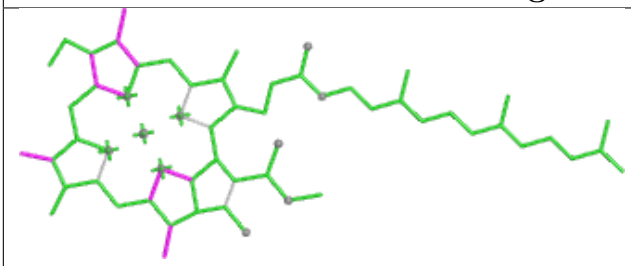


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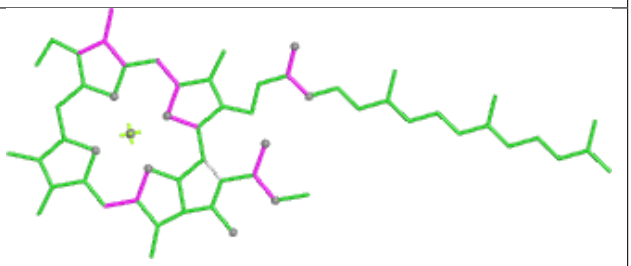


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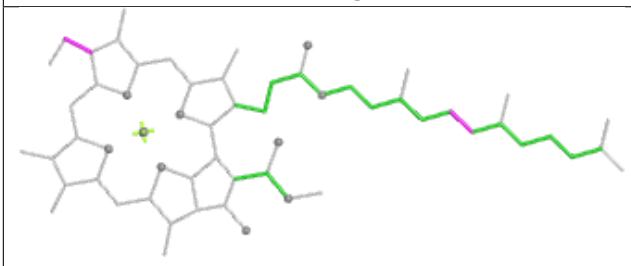
Ligand CLA a 610



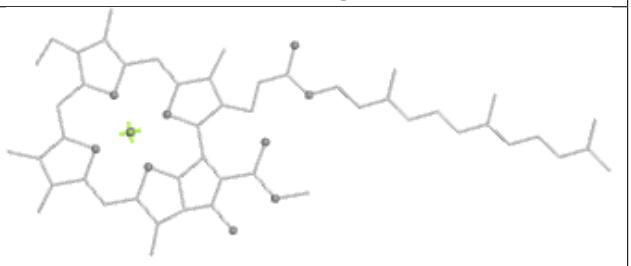
Bond lengths



Bond angles

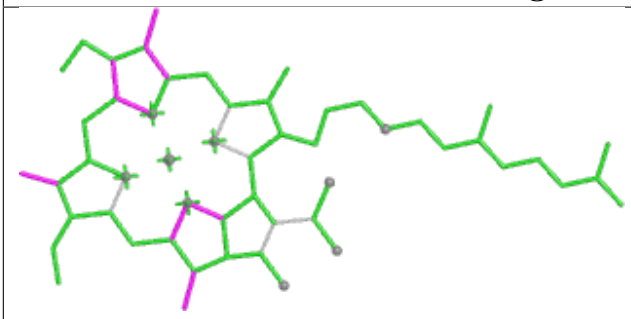


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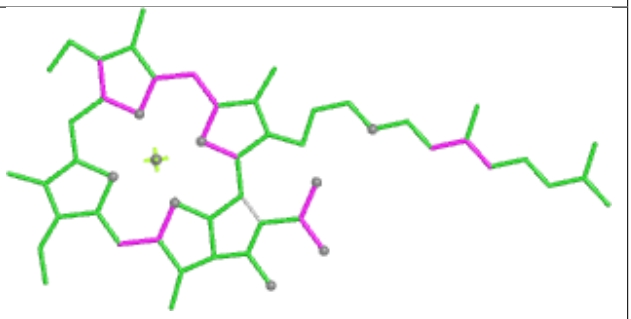


Rings

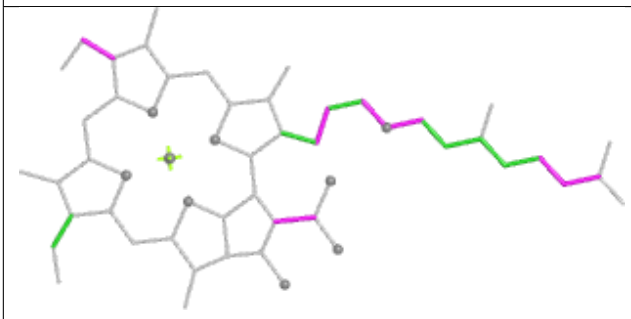
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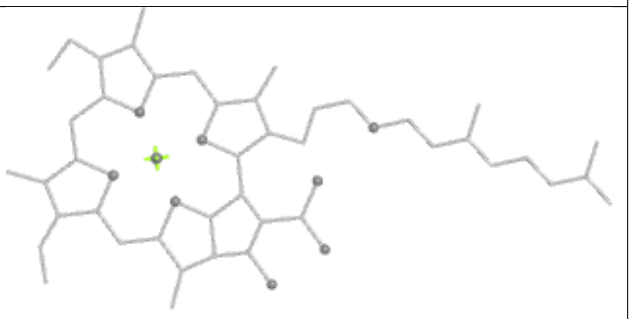
Bond lengths



Bond angles

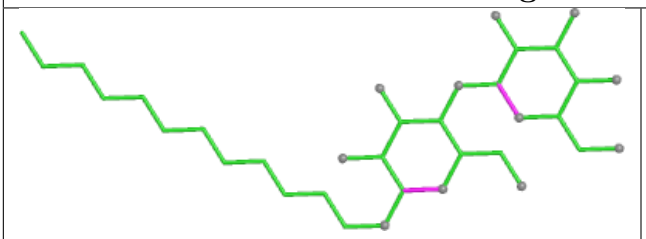


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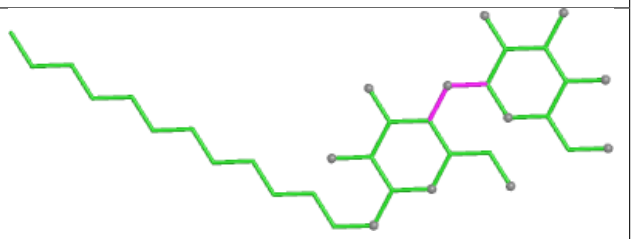


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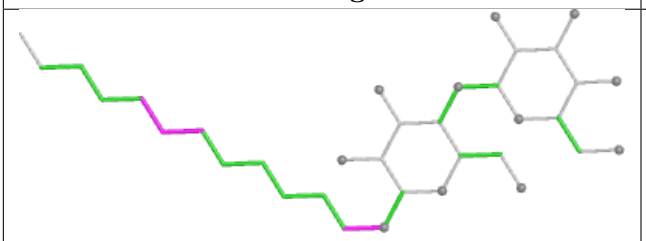
Ligand LMU A 857



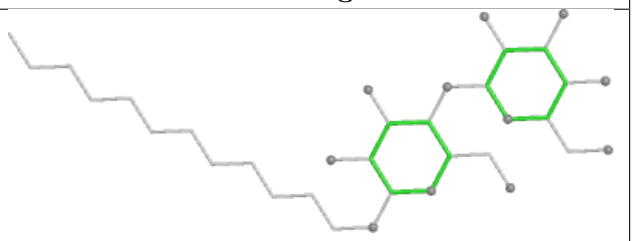
Bond lengths



Bond angles

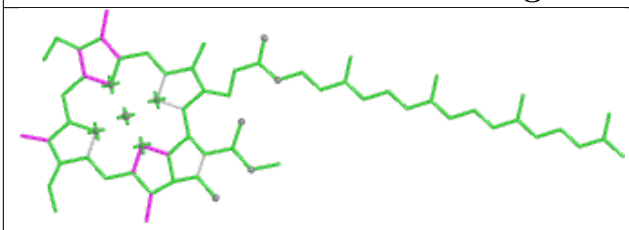


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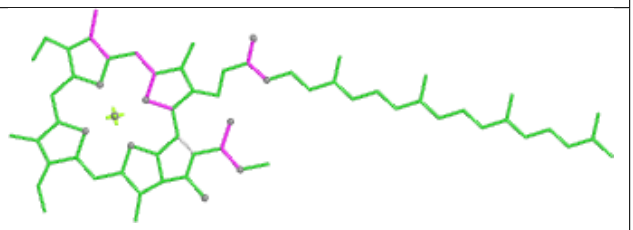


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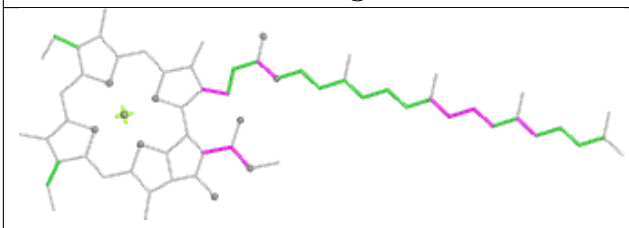
Ligand CLA A 831



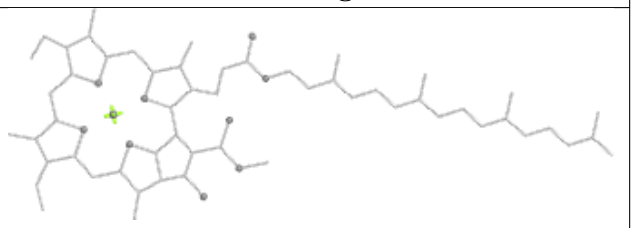
Bond lengths



Bond angles

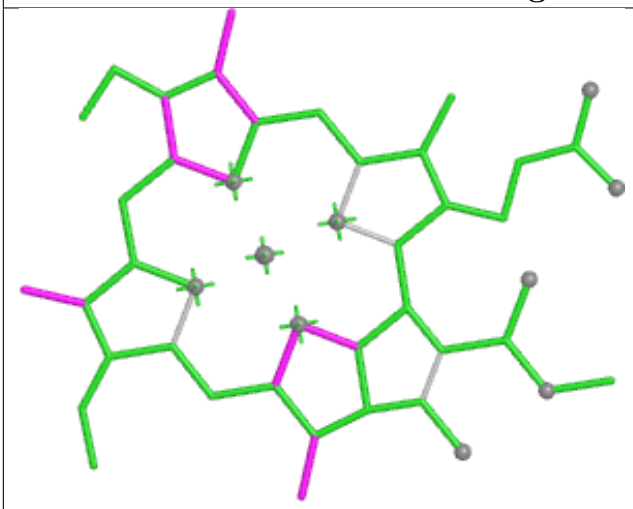


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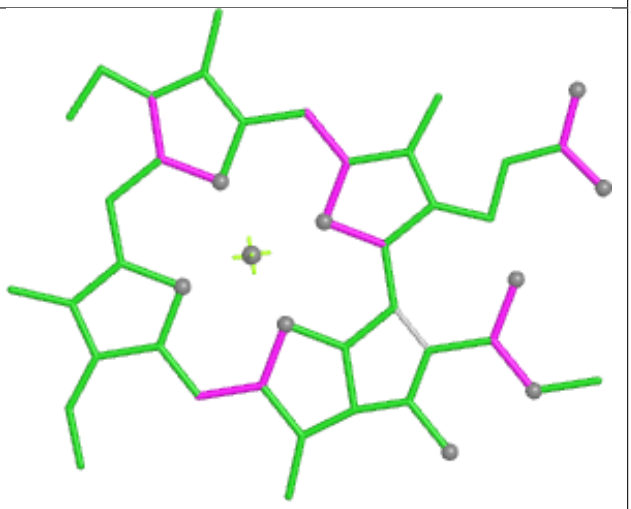


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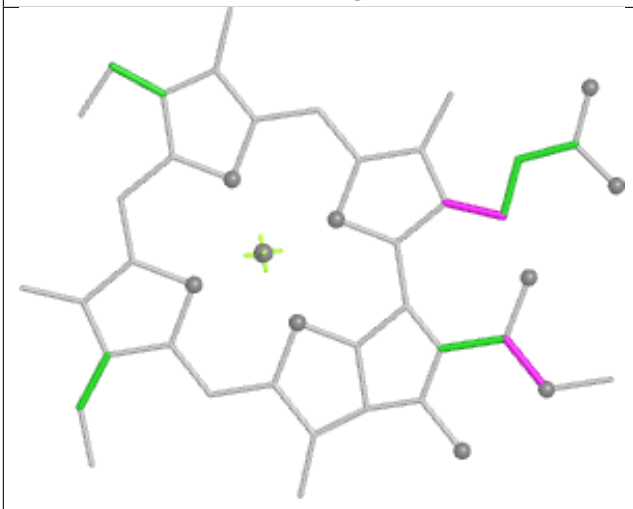
Ligand CLA a 607



Bond lengths



Bond angles

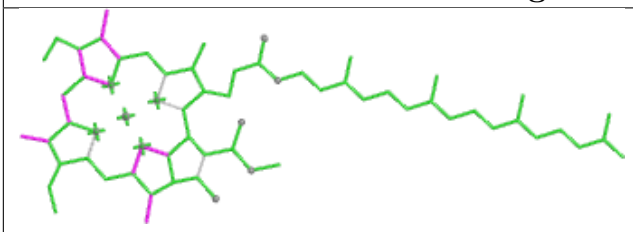


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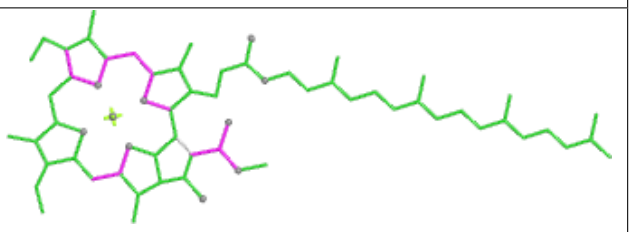


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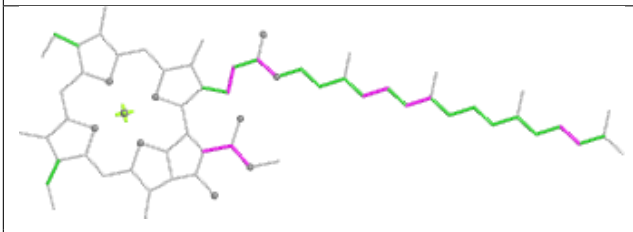
Ligand CLA 6 602



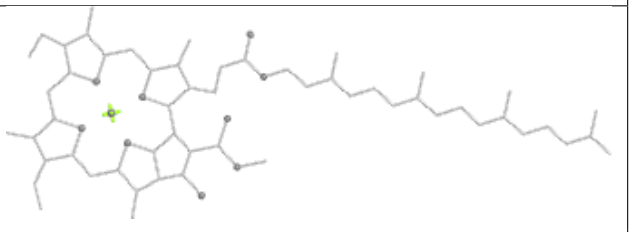
Bond lengths



Bond angles

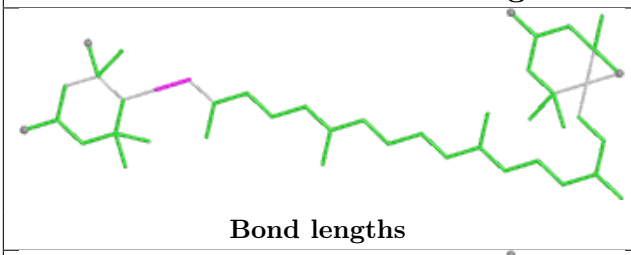


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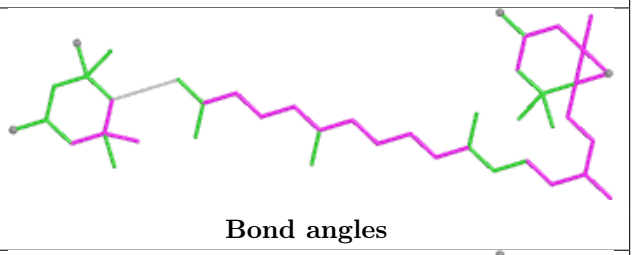


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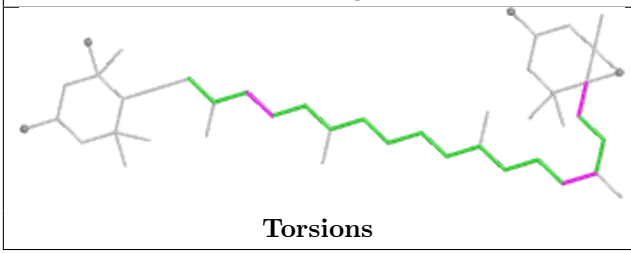
Ligand NEX W 1623



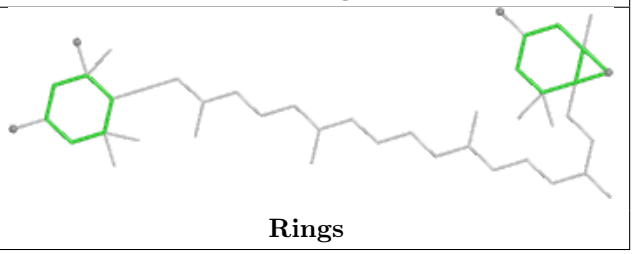
Bond lengths



Bond angles

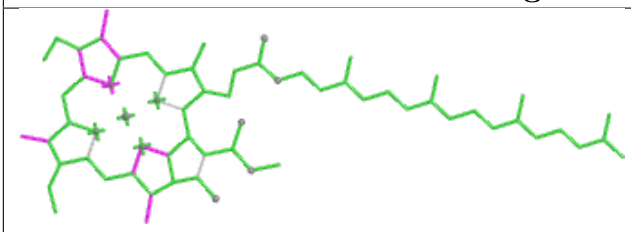


Torsions

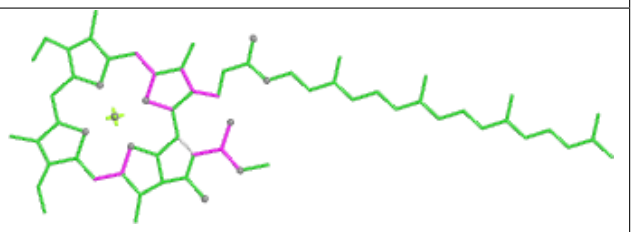


Rings

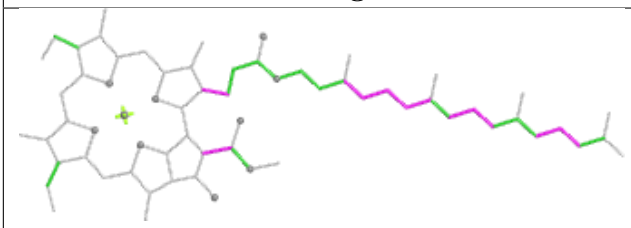
Ligand CLA A 806



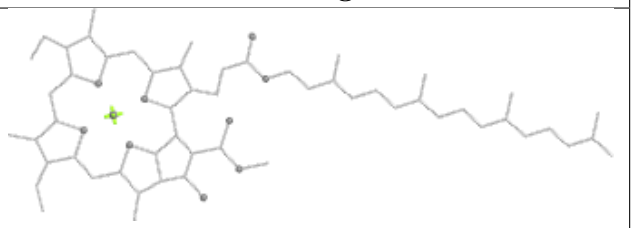
Bond lengths



Bond angles

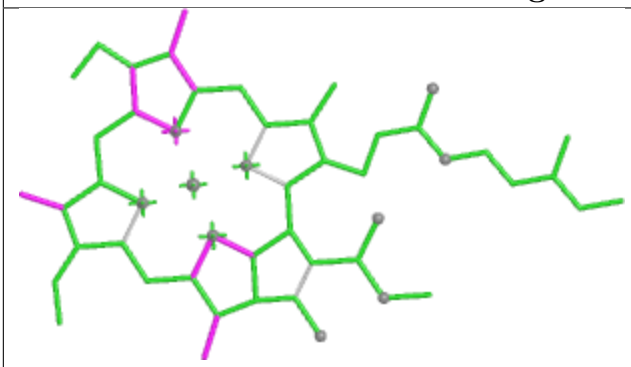


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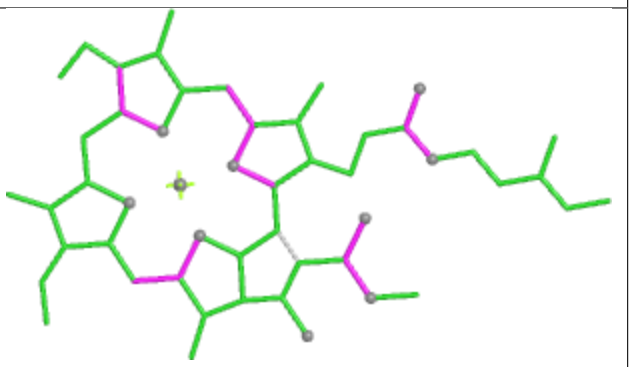


Rings

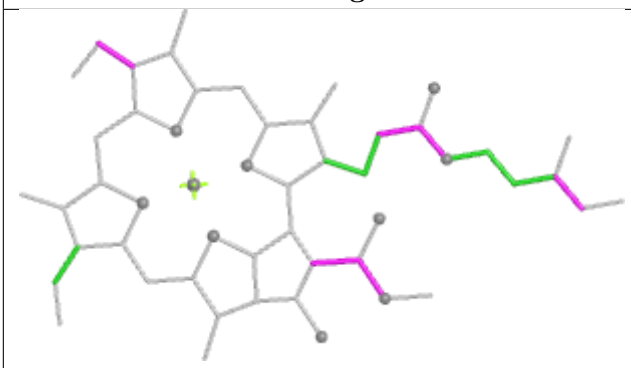
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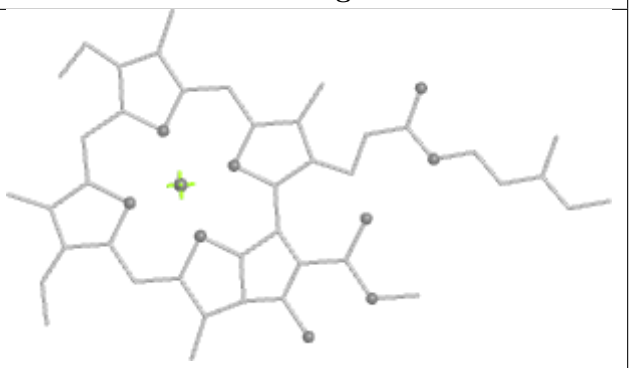
Bond lengths



Bond angles

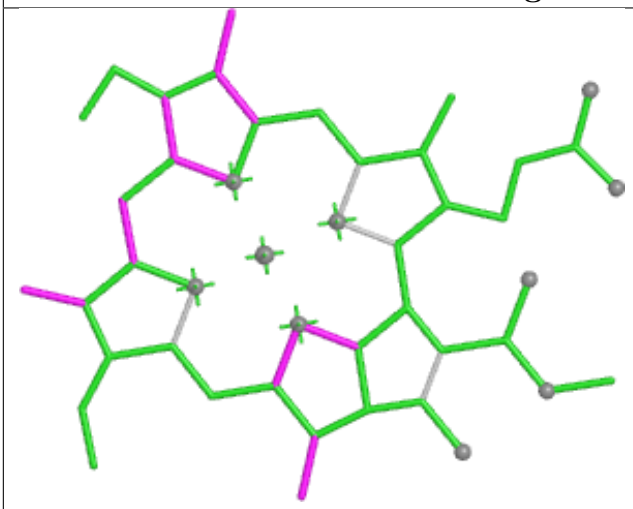


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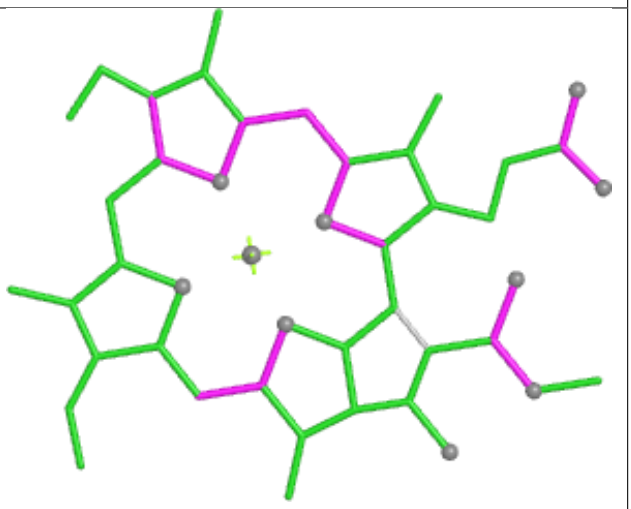


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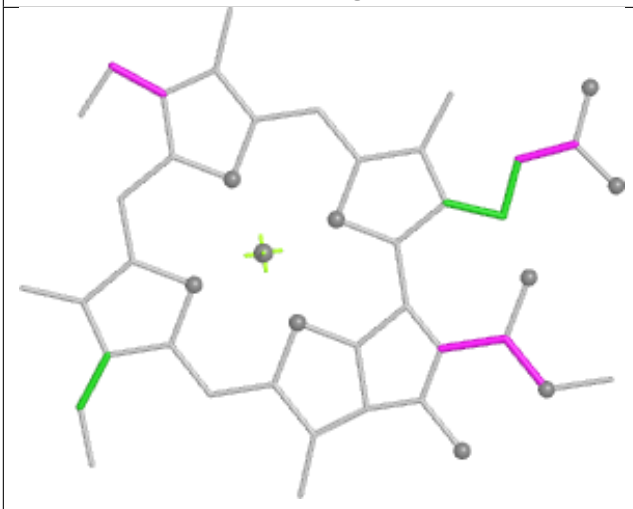
Ligand CLA B 823



Bond lengths



Bond angles

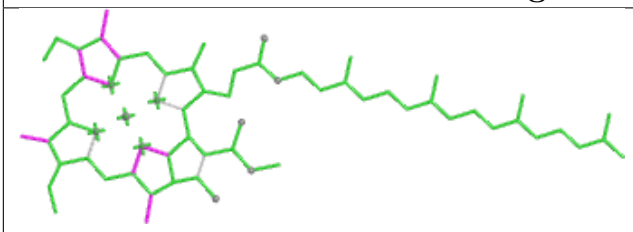


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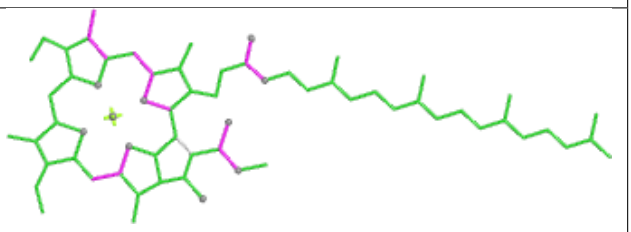


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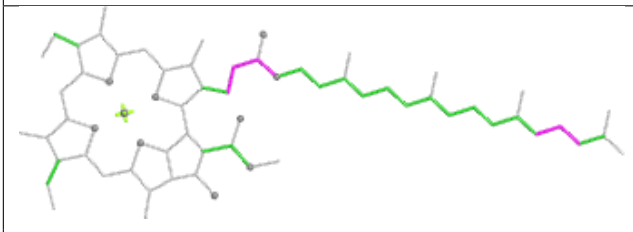
Ligand CLA 2 613



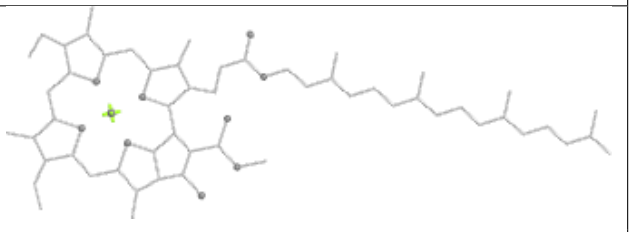
Bond lengths



Bond angles

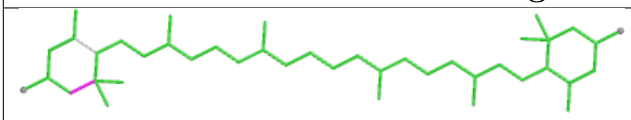


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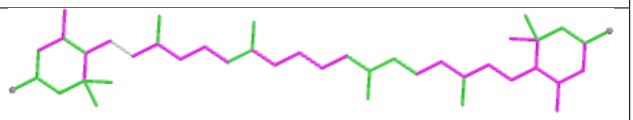


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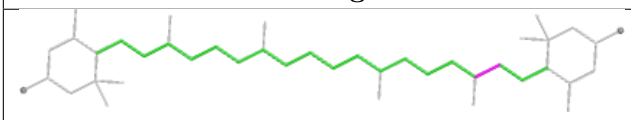
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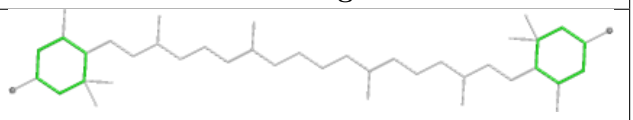
Bond lengths



Bond angles

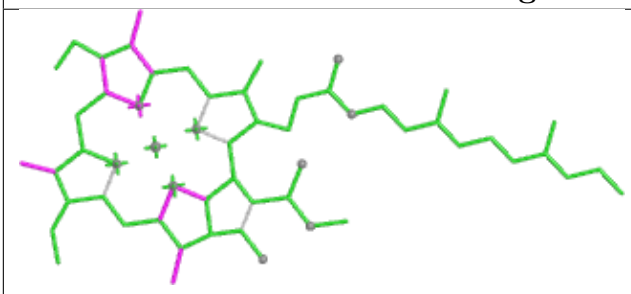


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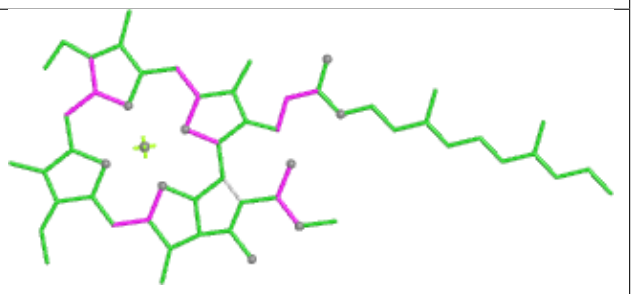


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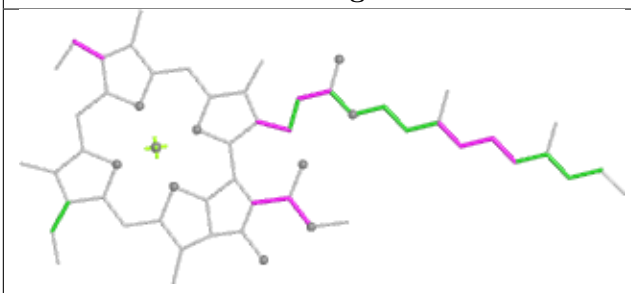
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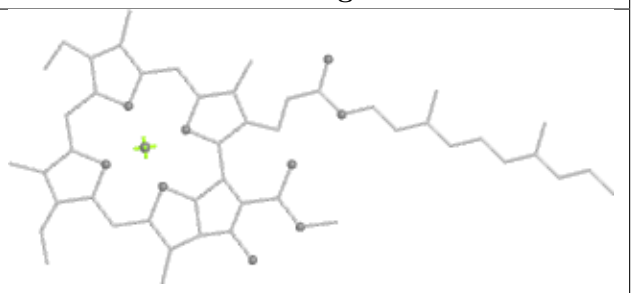
Bond lengths



Bond angles

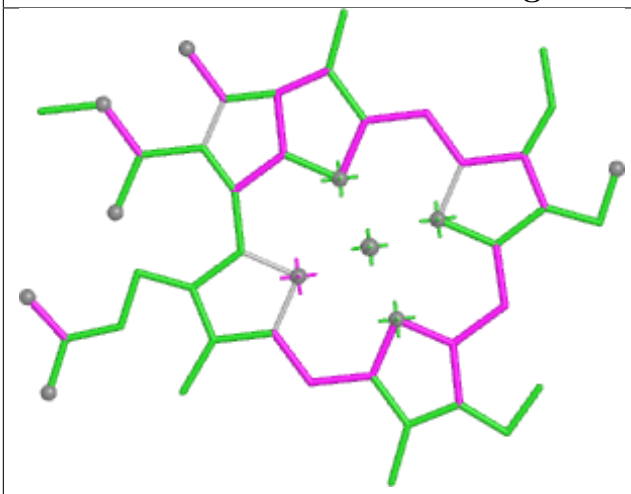


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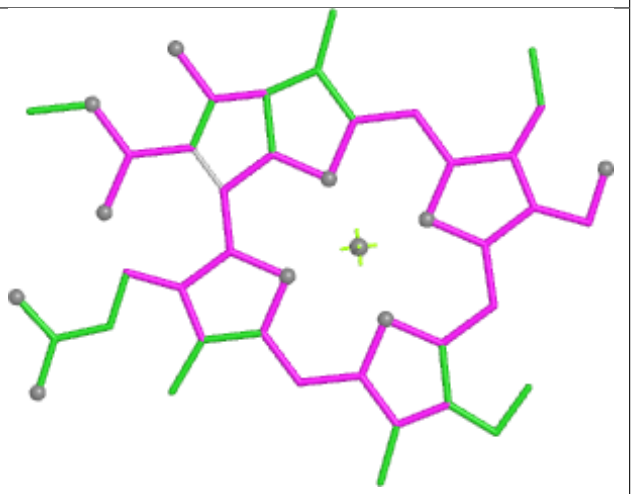


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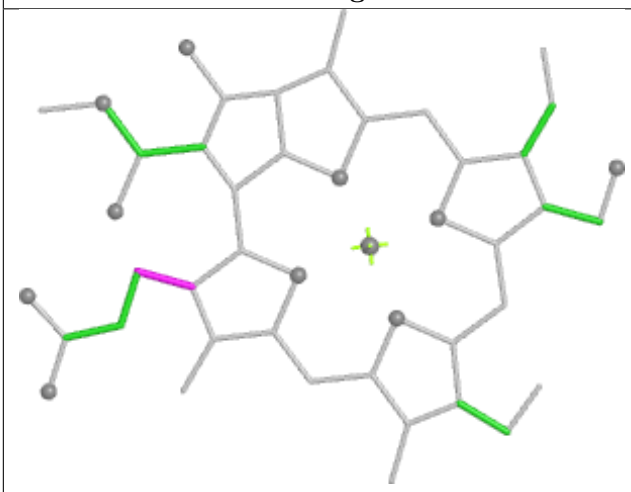
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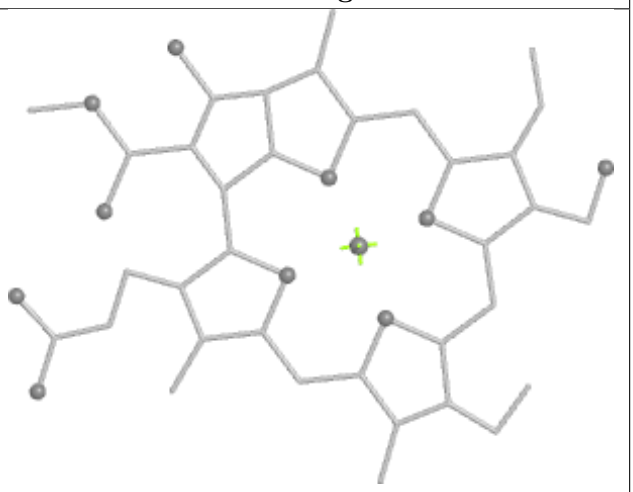
Bond lengths



Bond angles



Torsions

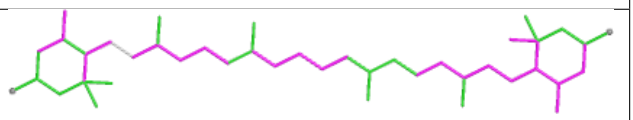


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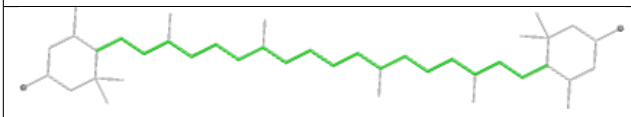
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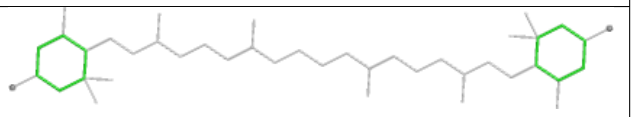
Bond lengths



Bond angles

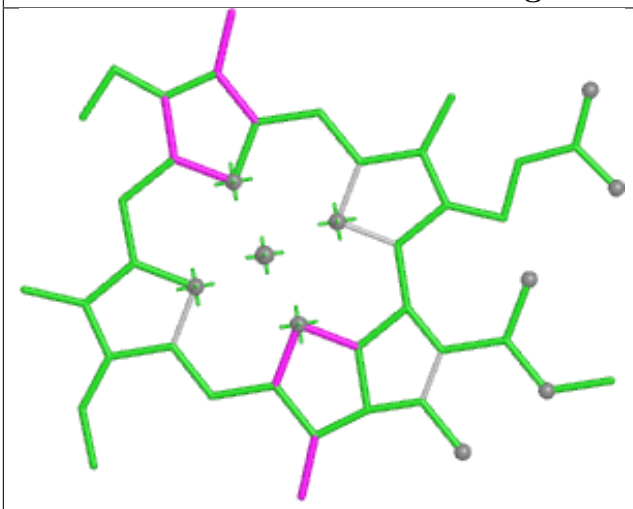


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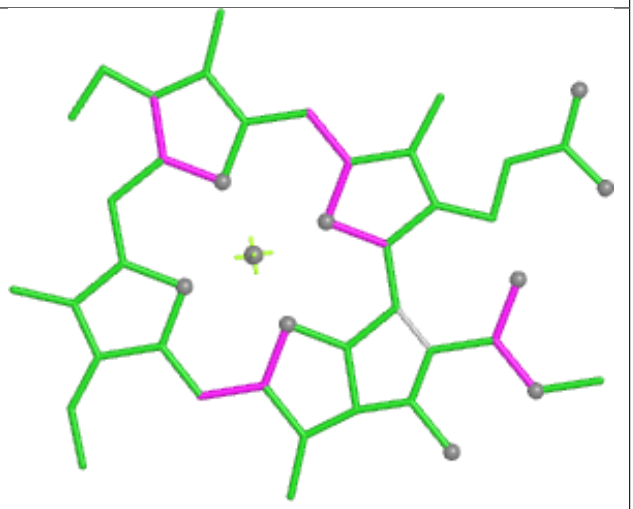


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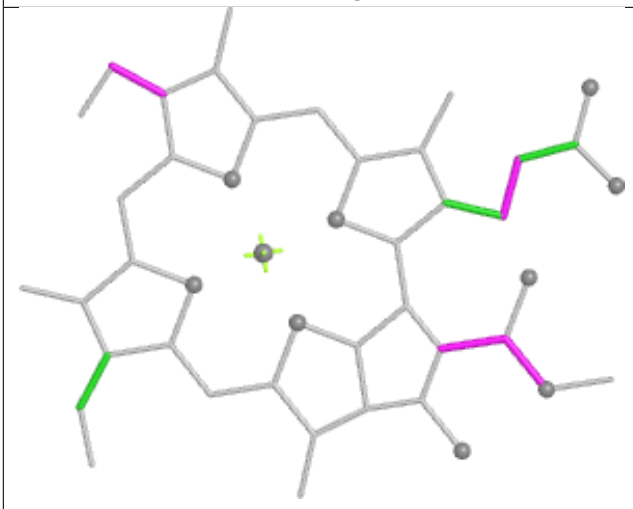
Ligand CLA B 835



Bond lengths



Bond angles

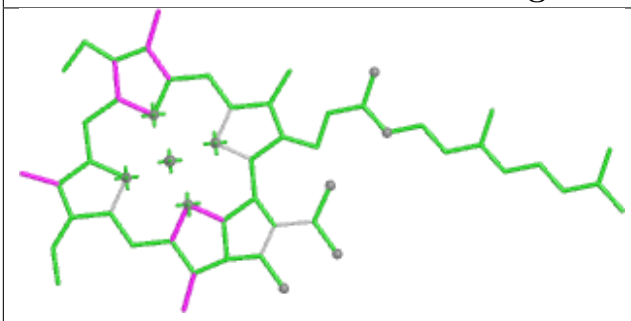


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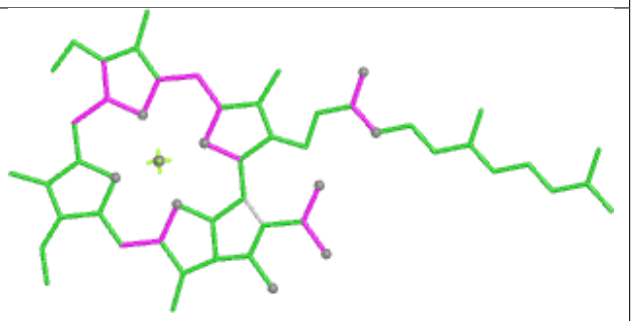


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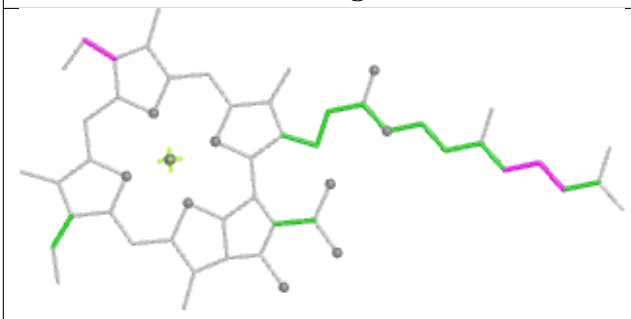
Ligand CLA a 601



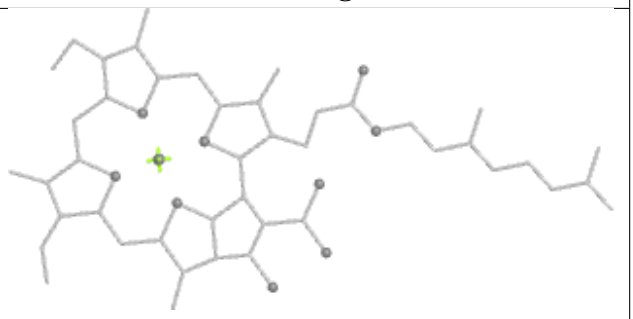
Bond lengths



Bond angles

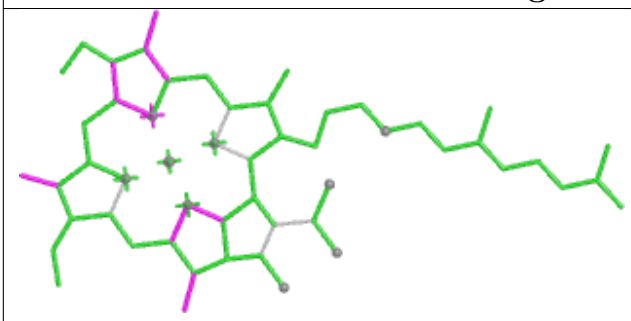


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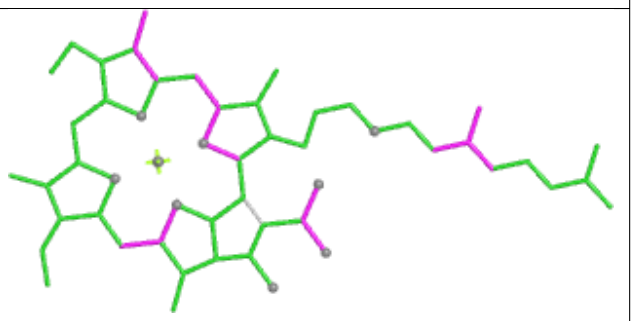


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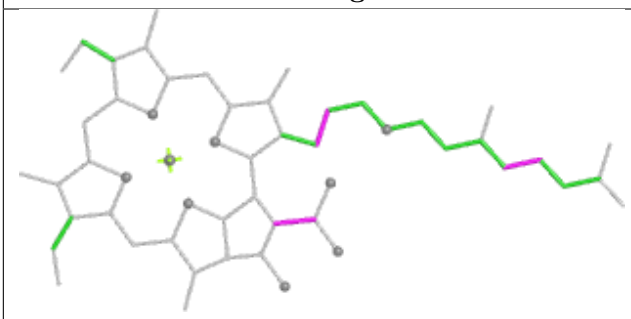
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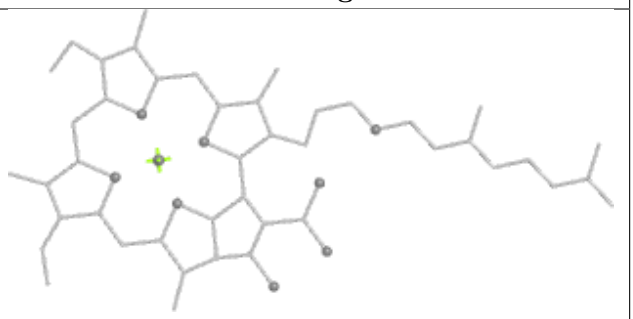
Bond lengths



Bond angles

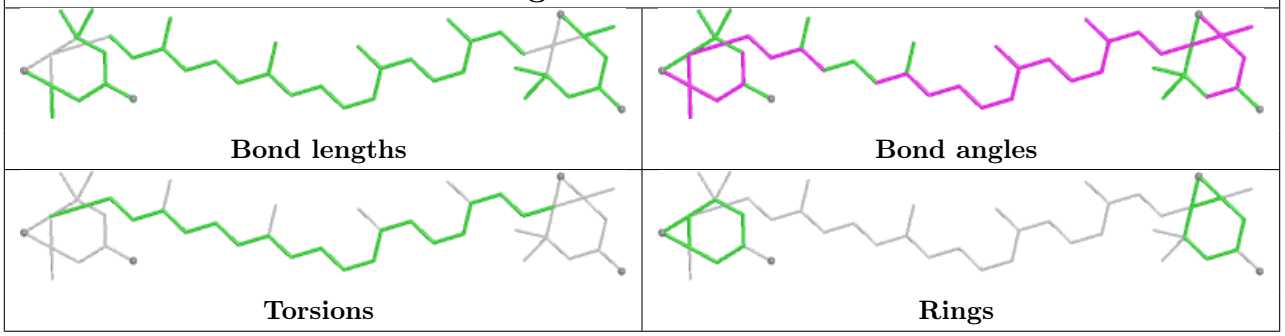


Torsions



Rings

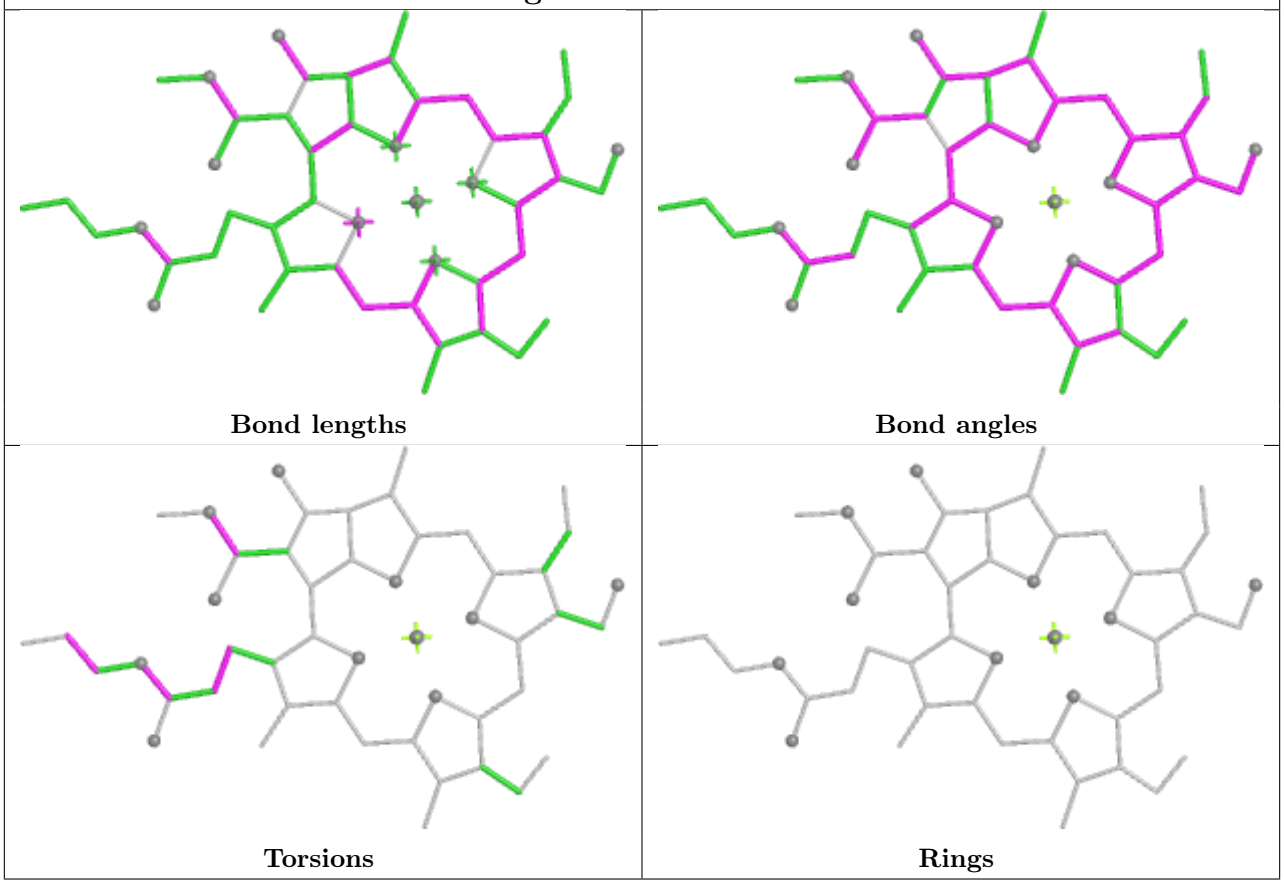
Ligand XAT 1 618



Bond lengths | Bond angles

Torsions | Rings

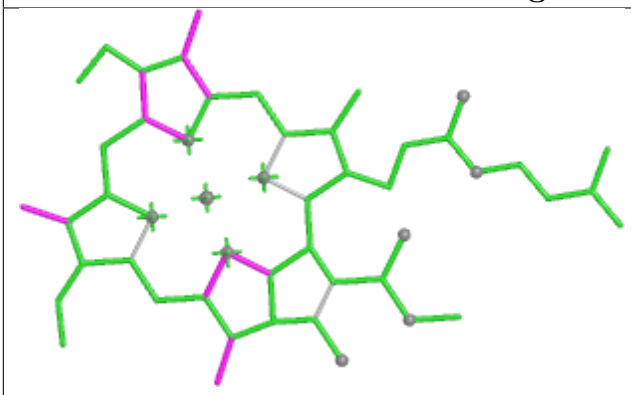
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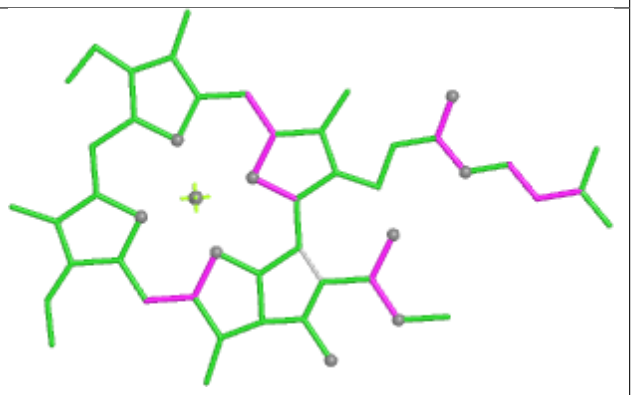
Bond lengths | Bond angles

Torsions | Rings

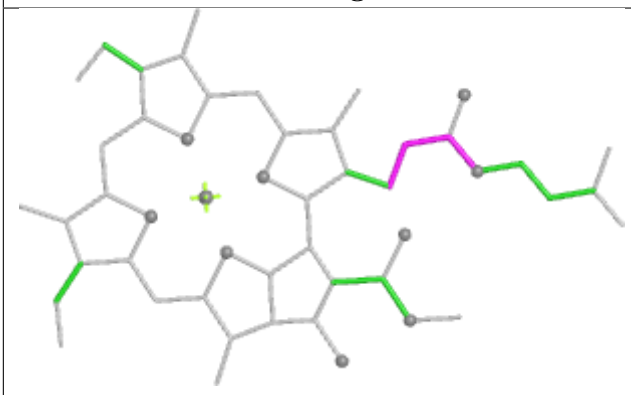
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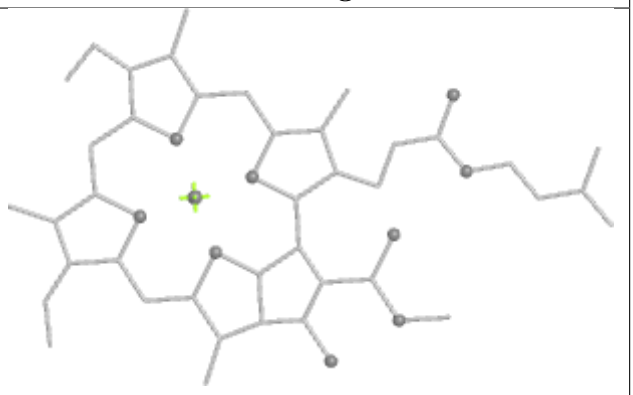
Bond lengths



Bond angles

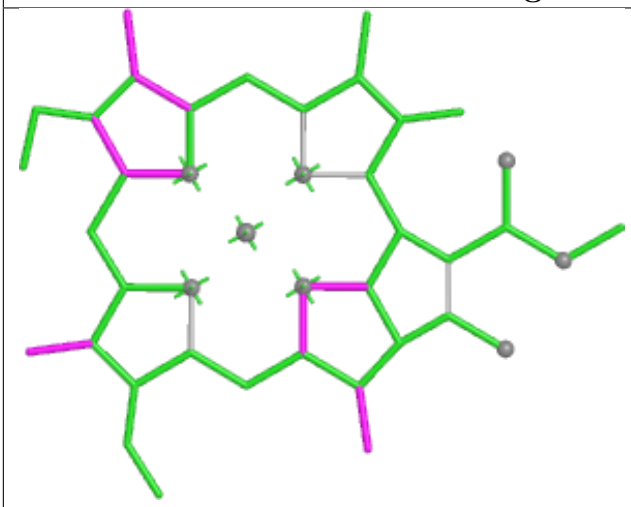


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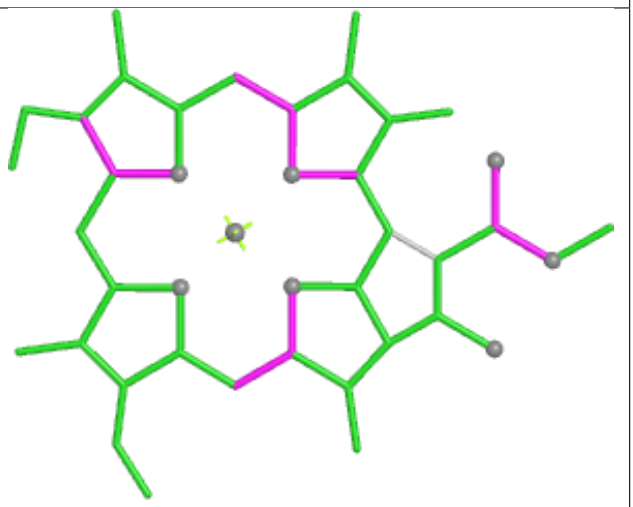


Rings

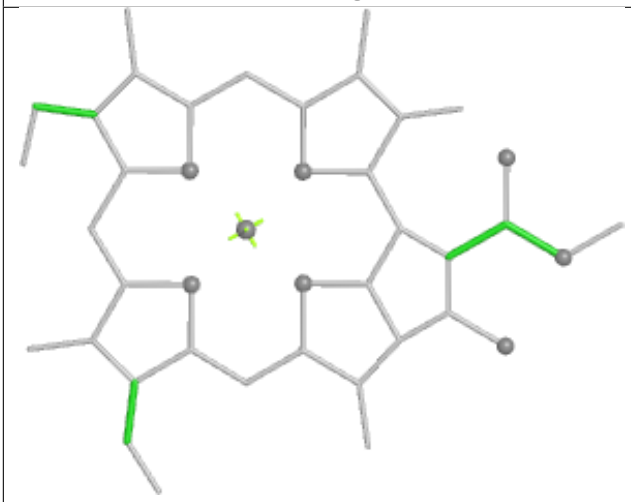
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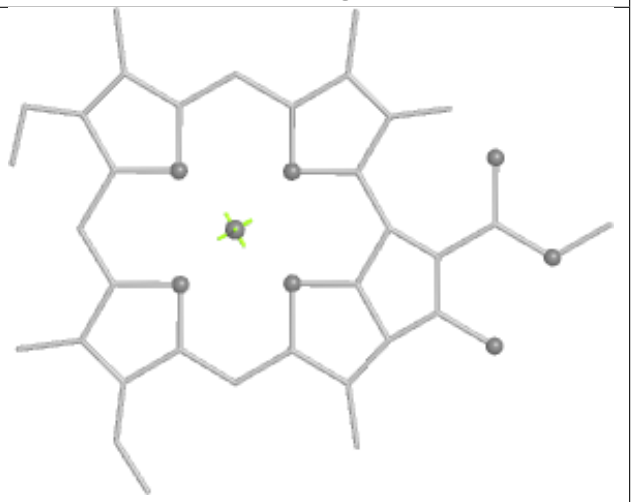
Bond lengths



Bond angles

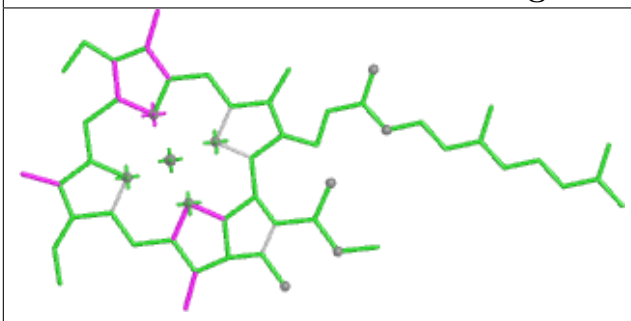


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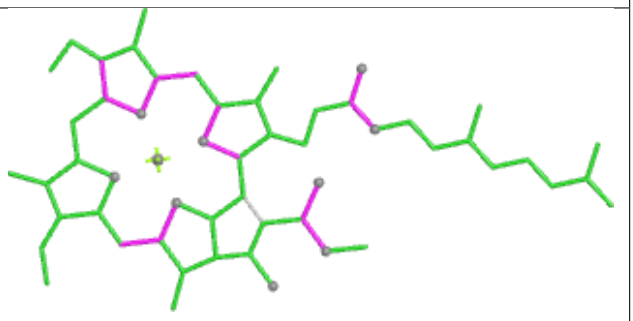


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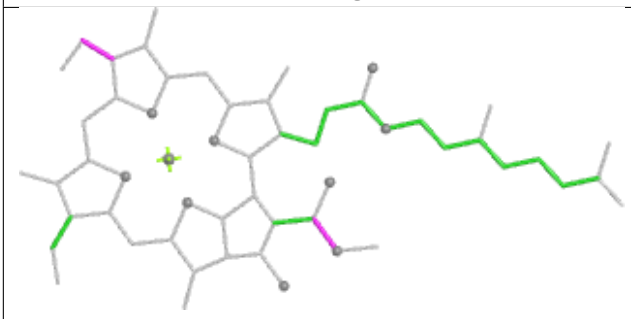
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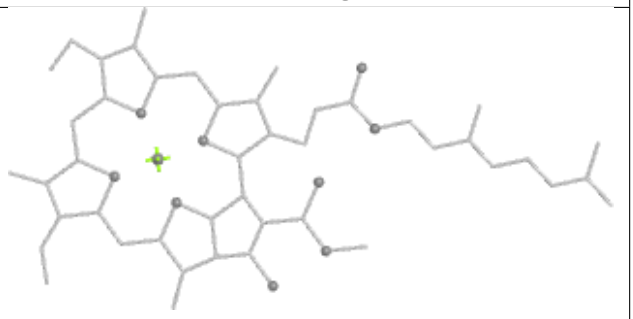
Bond lengths



Bond angles

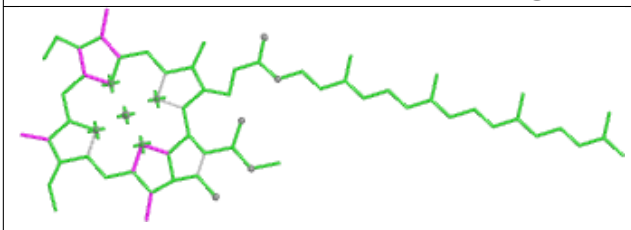


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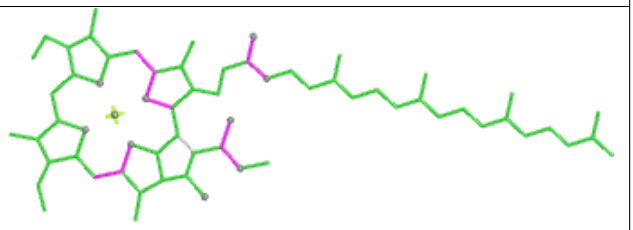


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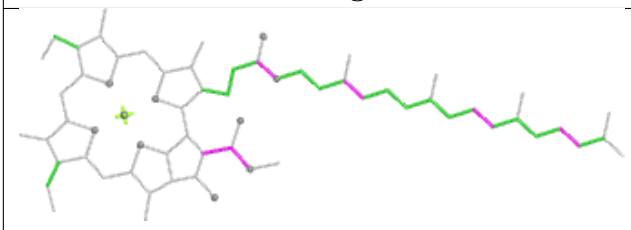
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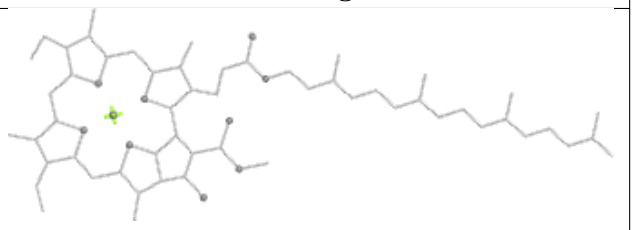
Bond lengths



Bond angles

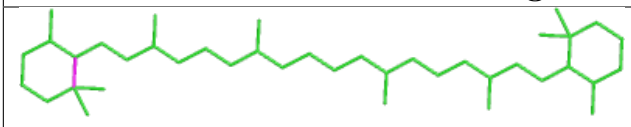


Torsions

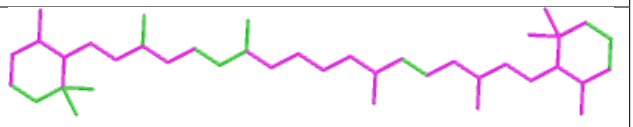


Rings

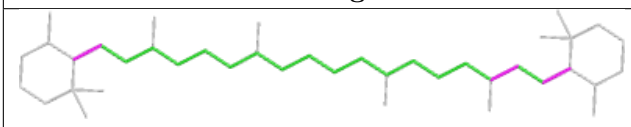
Ligand BCR 6 622



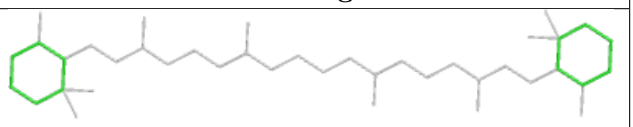
Bond lengths



Bond angles

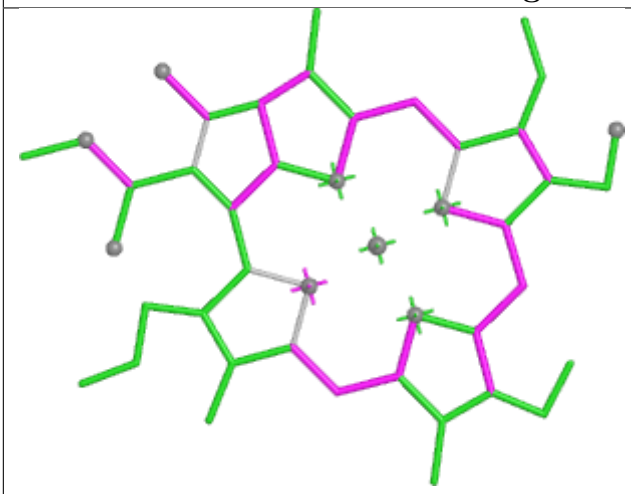


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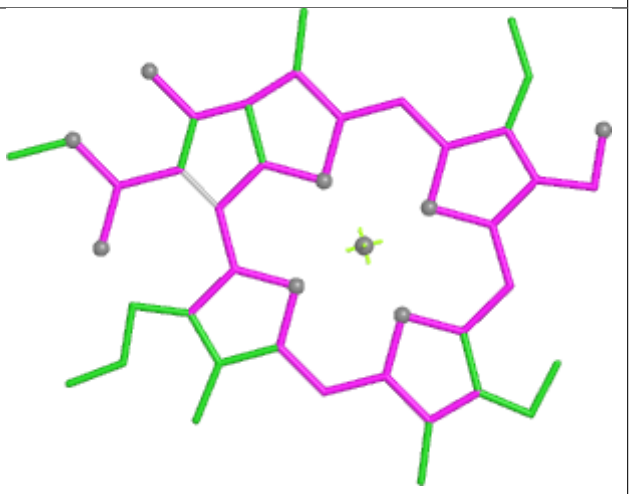


Rings

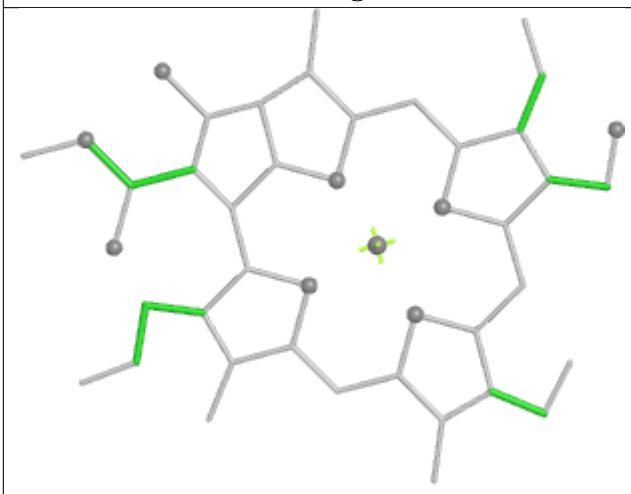
Ligand CHL U 606



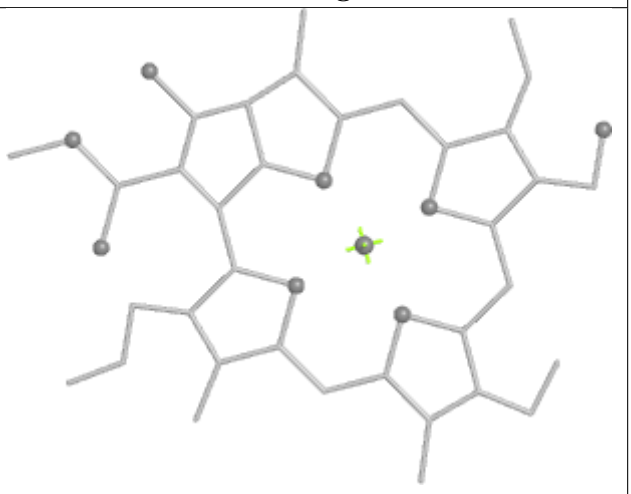
Bond lengths



Bond angles

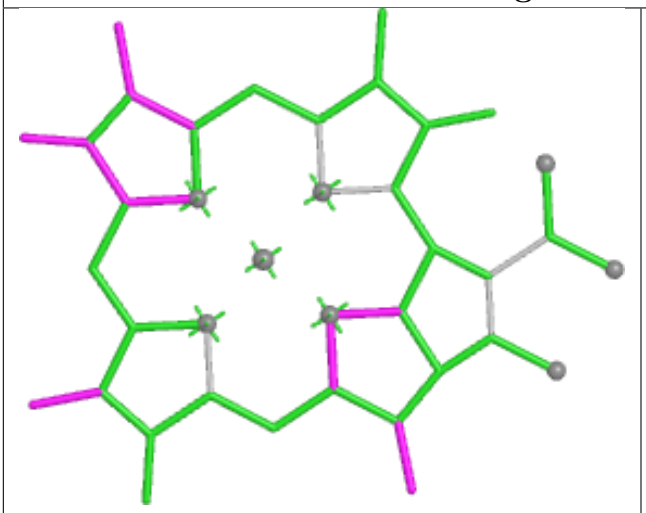


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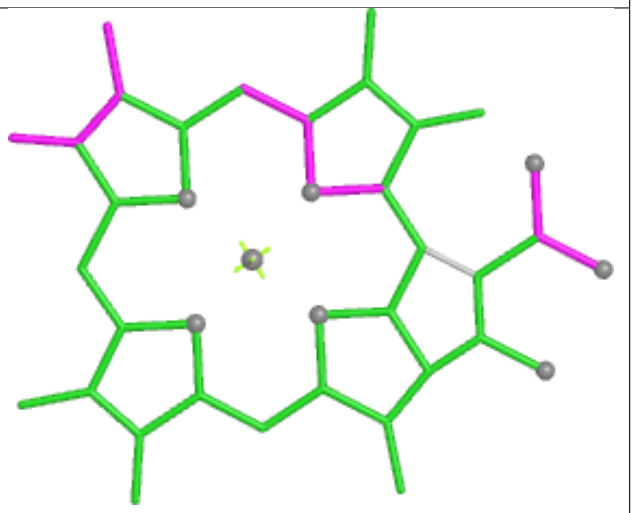


Rings

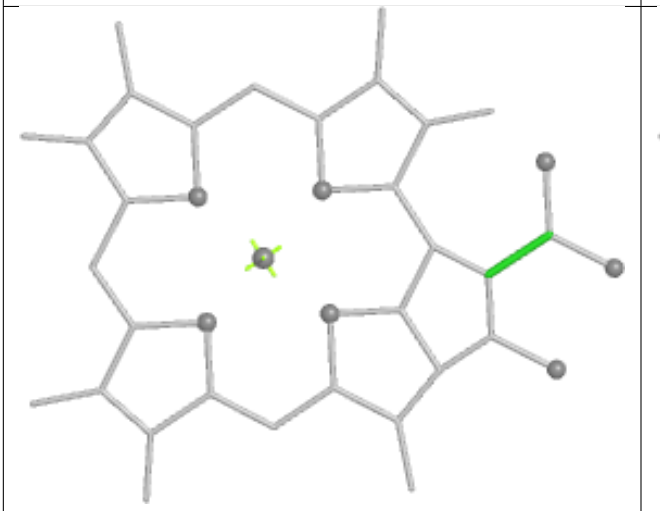
Ligand CLA O 2002



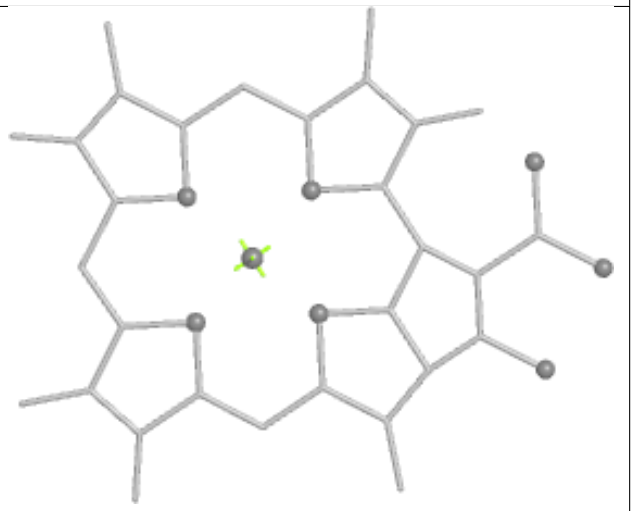
Bond lengths



Bond angles

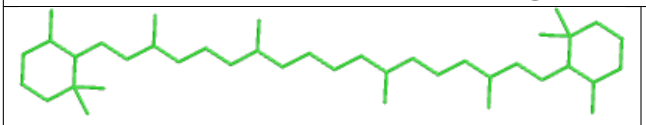


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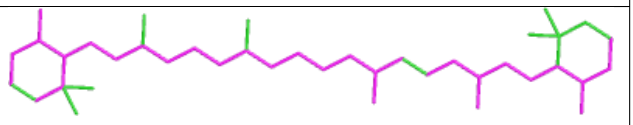


Rings

Ligand BCR 3 622



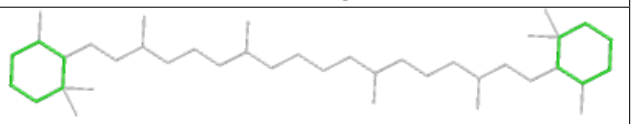
Bond lengths



Bond angles

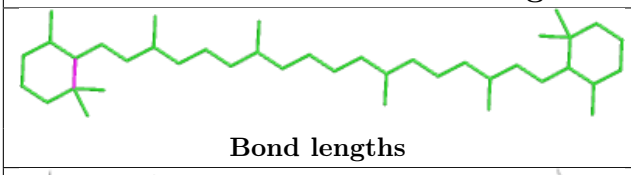


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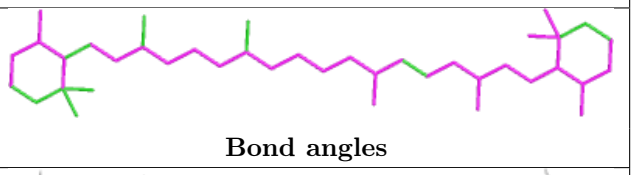


Rings

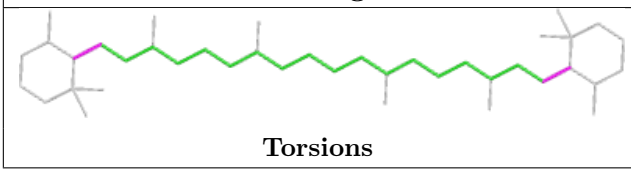
Ligand BCR 4 621



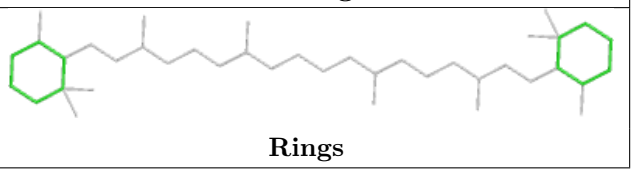
Bond lengths



Bond angles

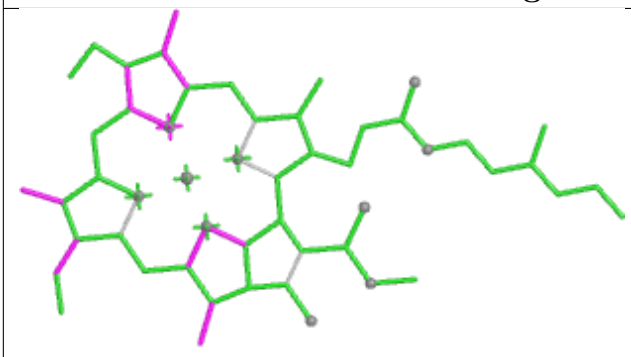


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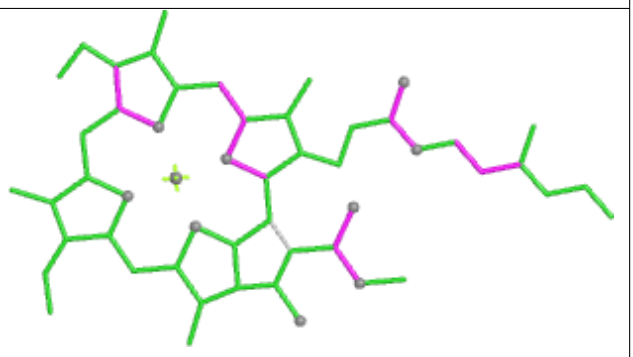


Rings

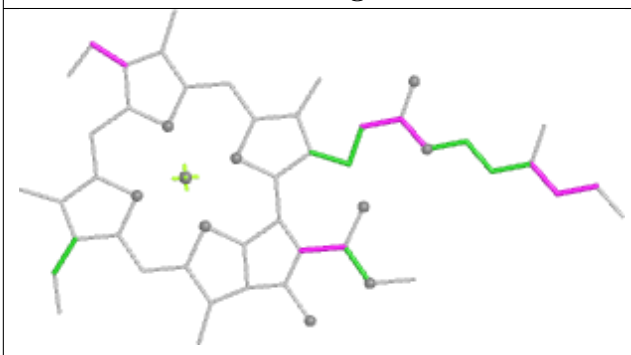
Ligand CLA U 603



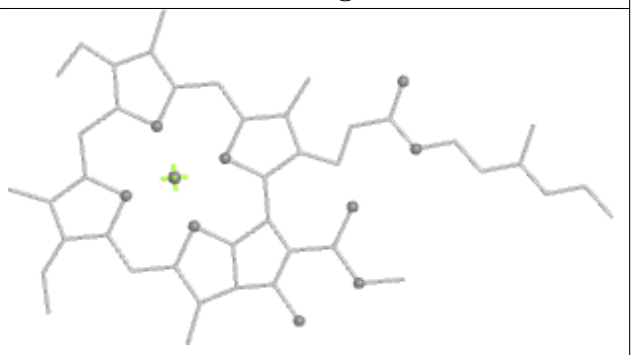
Bond lengths



Bond angles

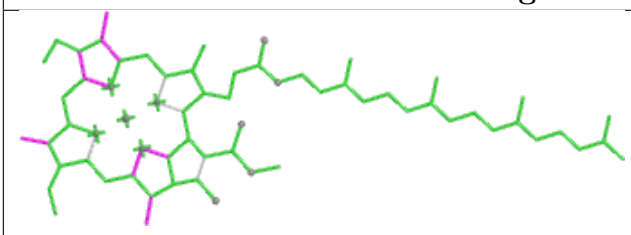


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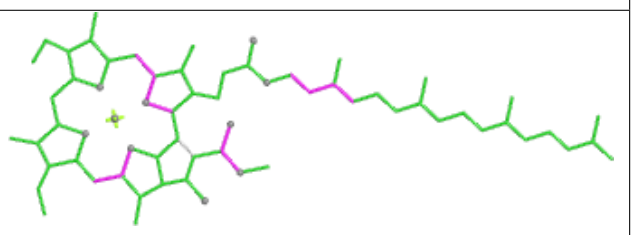


Rings

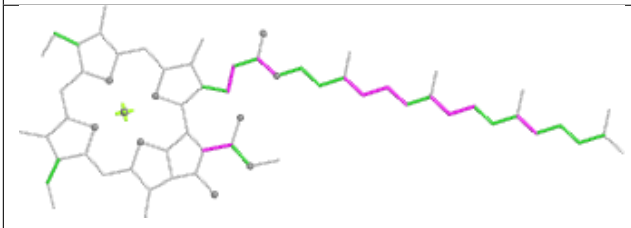
Ligand CLA W 613



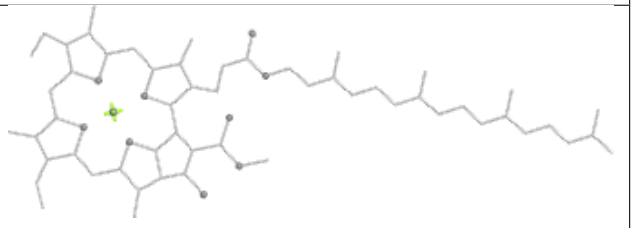
Bond lengths



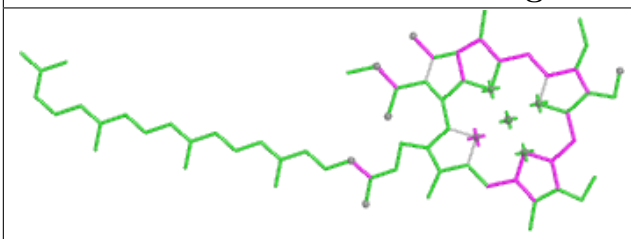
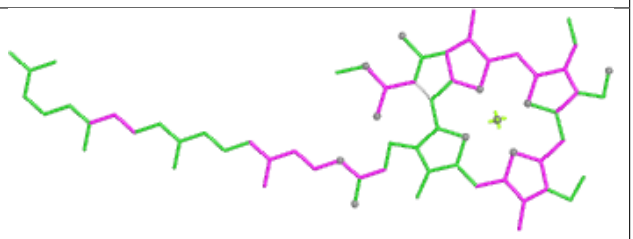
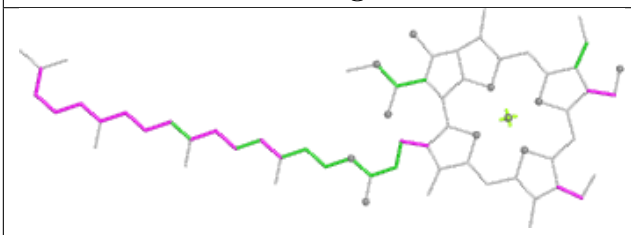
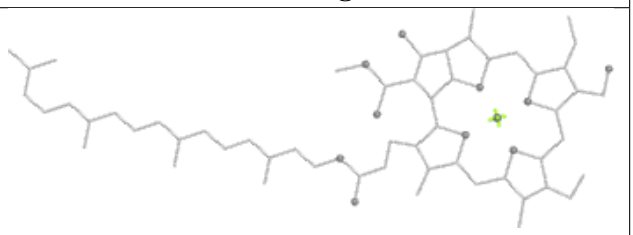
Bond angles

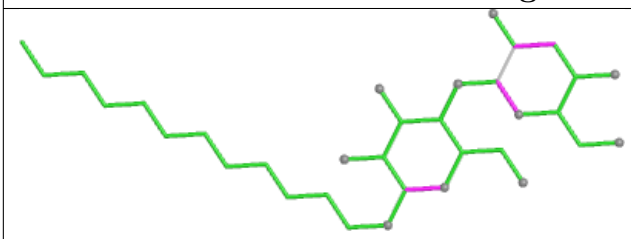
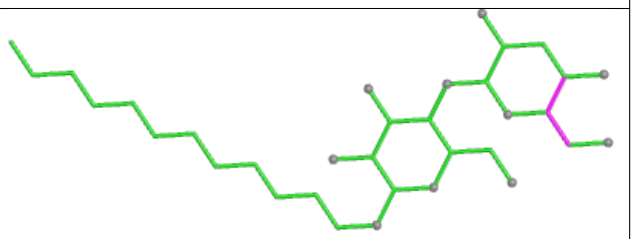
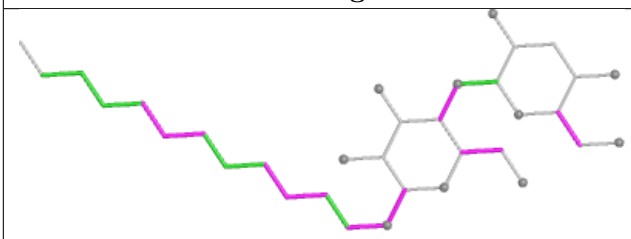
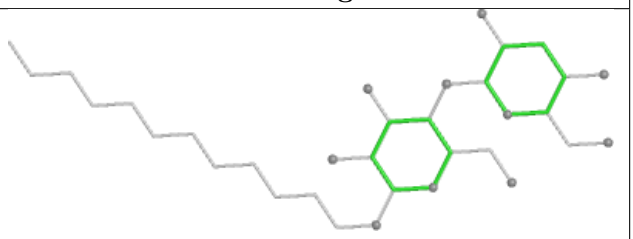


Torsions

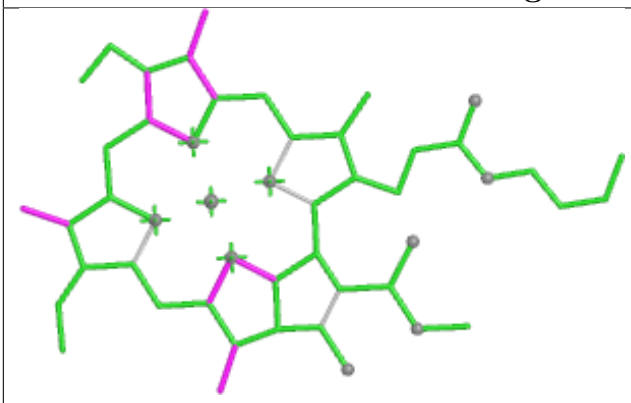


Rings

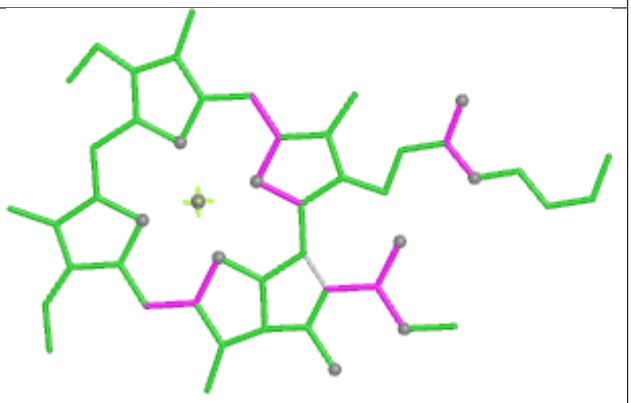
Ligand CHL Z 609	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMU A 858	
 Bond lengths	 Bond angles
 Torsions	 Rings

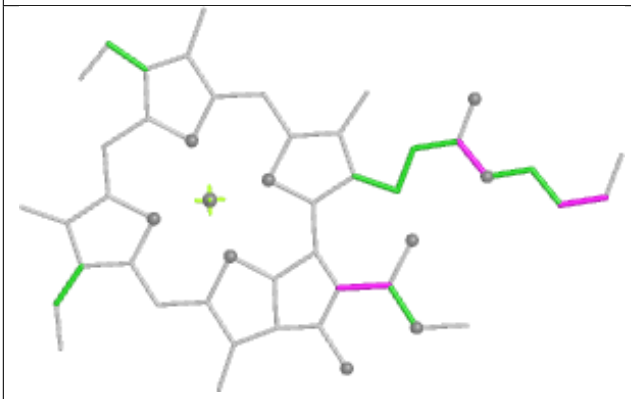
Ligand CLA B 825



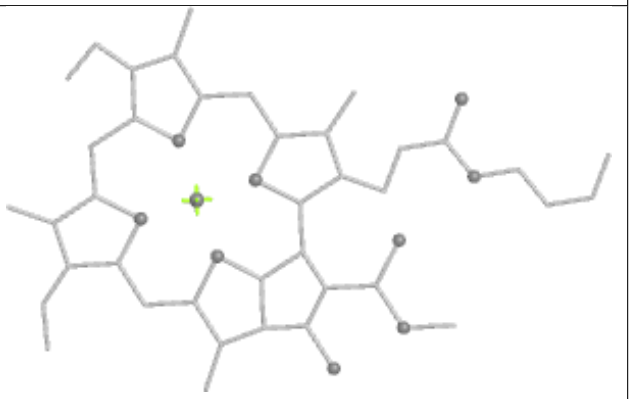
Bond lengths



Bond angles

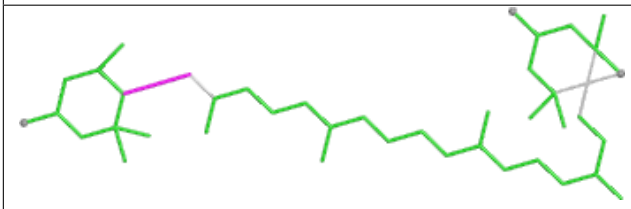


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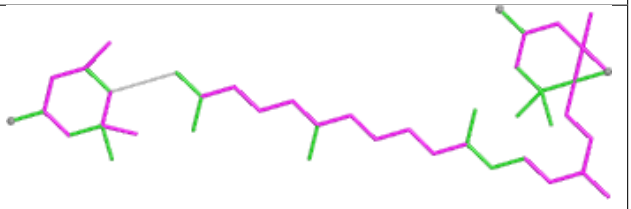


Rings

Ligand NEX Y 1623



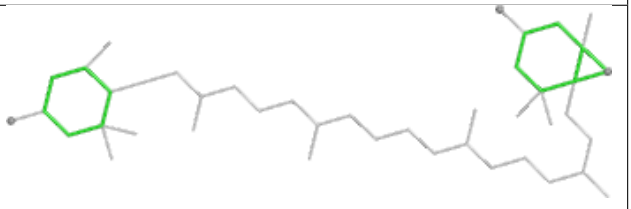
Bond lengths



Bond angles

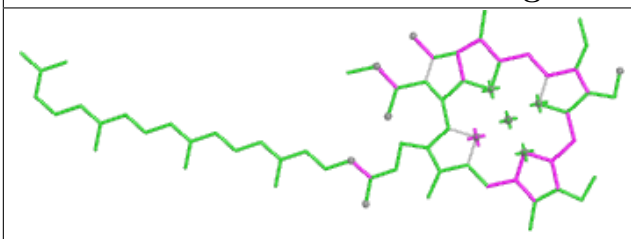


Torsions

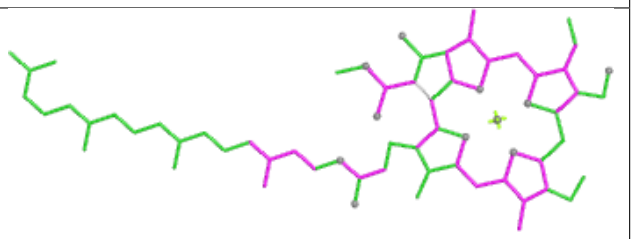


Rings

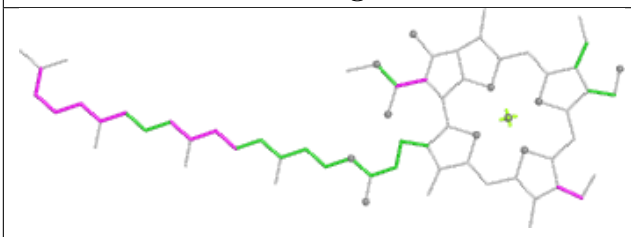
Ligand CHL V 601



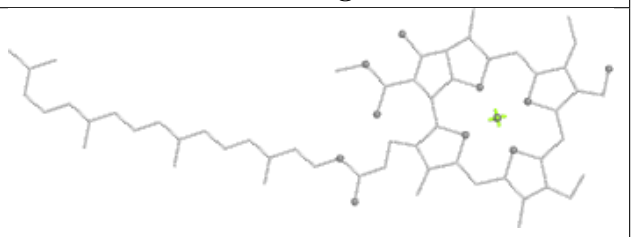
Bond lengths



Bond angles

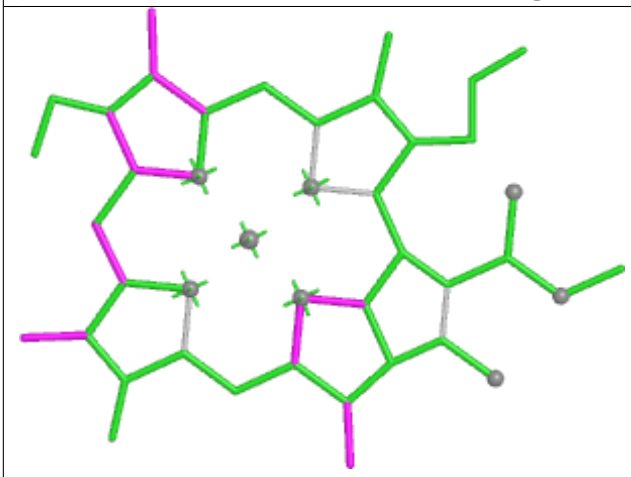


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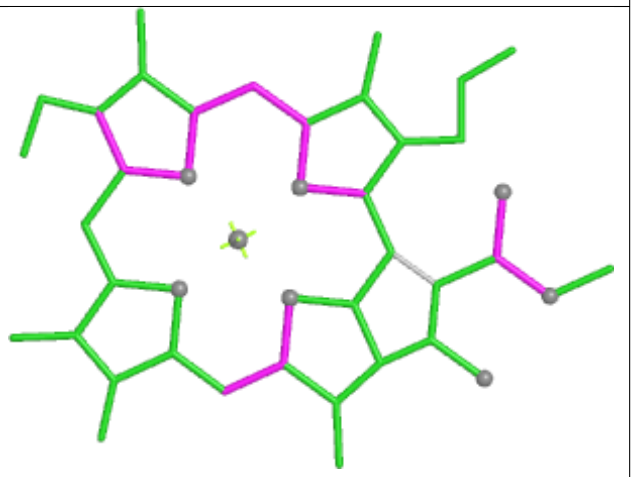


Rings

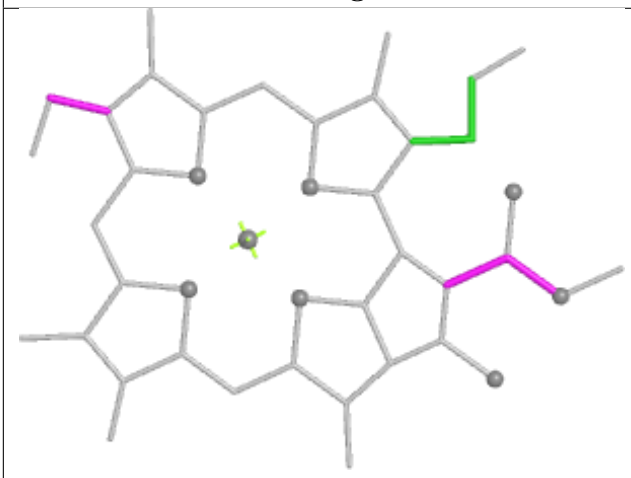
Ligand CLA 2 604



Bond lengths



Bond angles

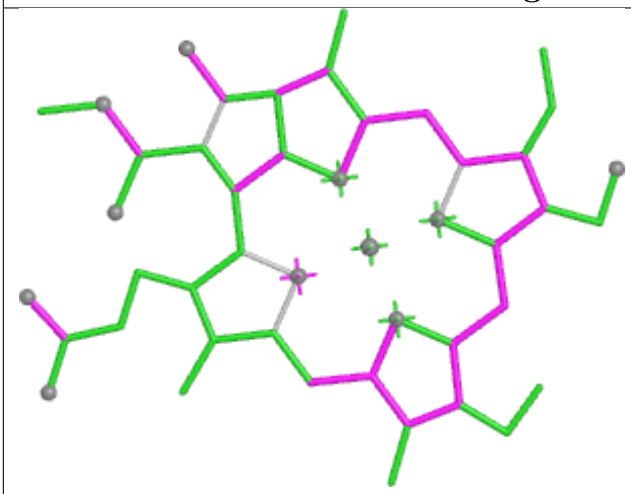


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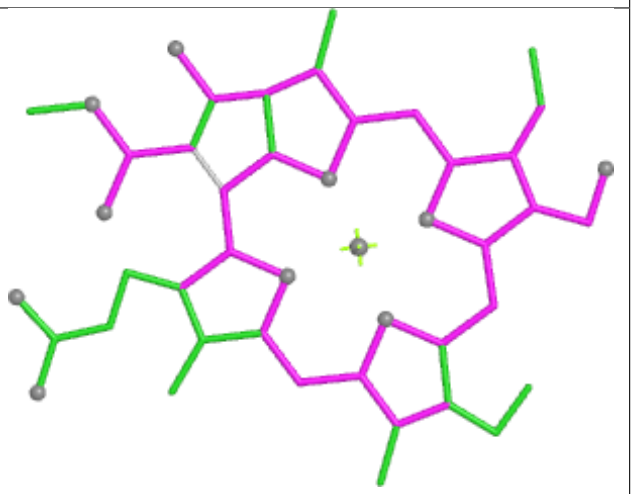


Rings

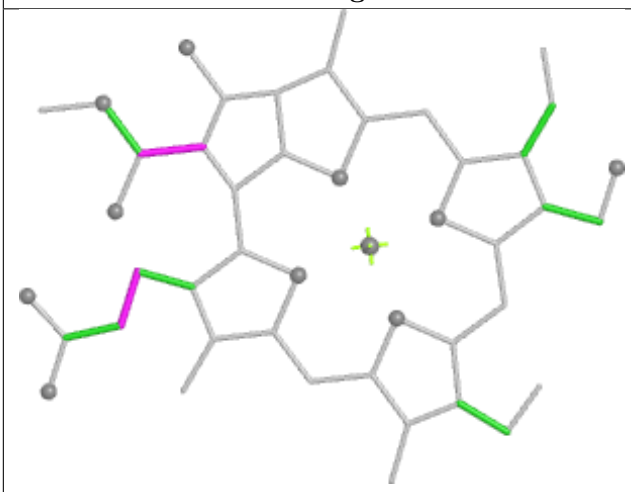
Ligand CHL X 605



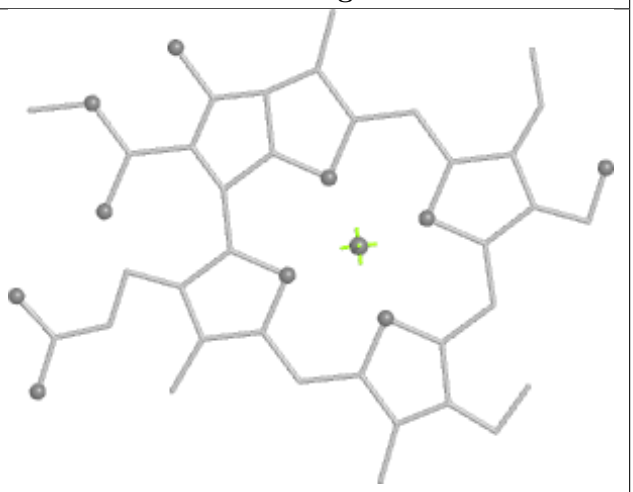
Bond lengths



Bond angles

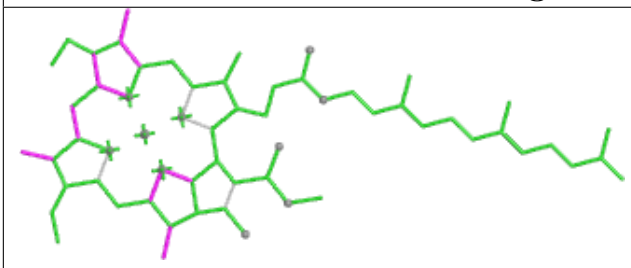


Torsions

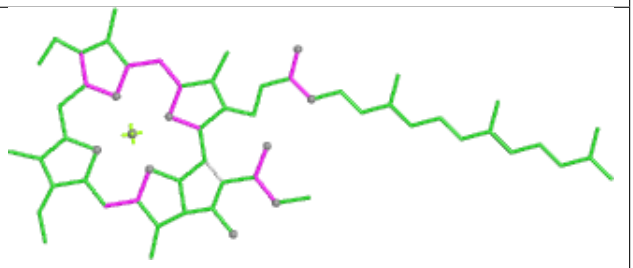


Rings

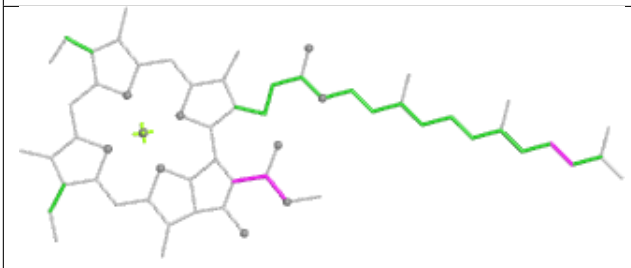
Ligand CLA 3 602



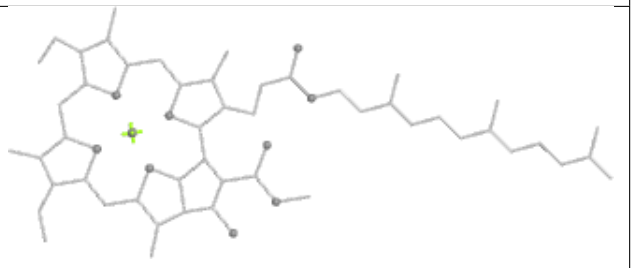
Bond lengths



Bond angles

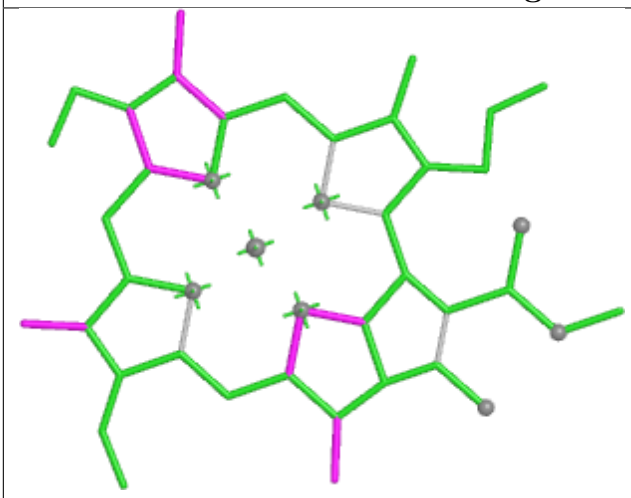


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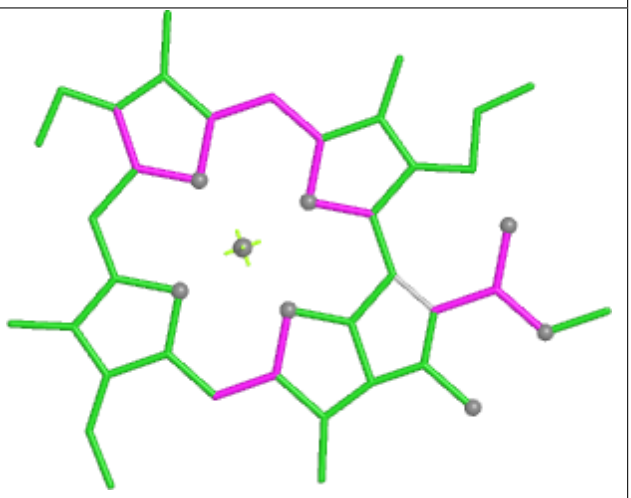


Rings

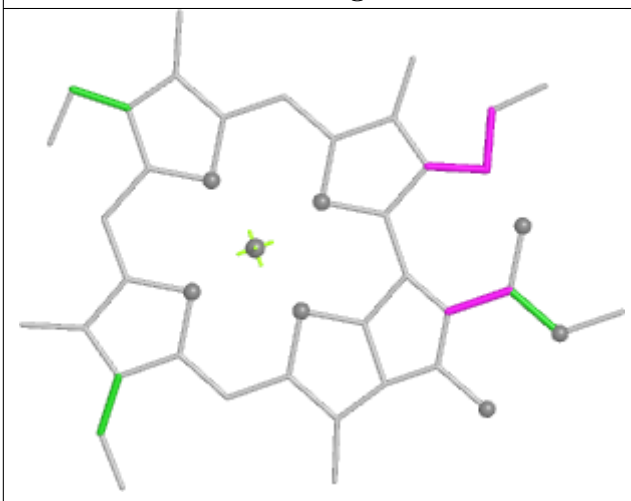
Ligand CLA B 812



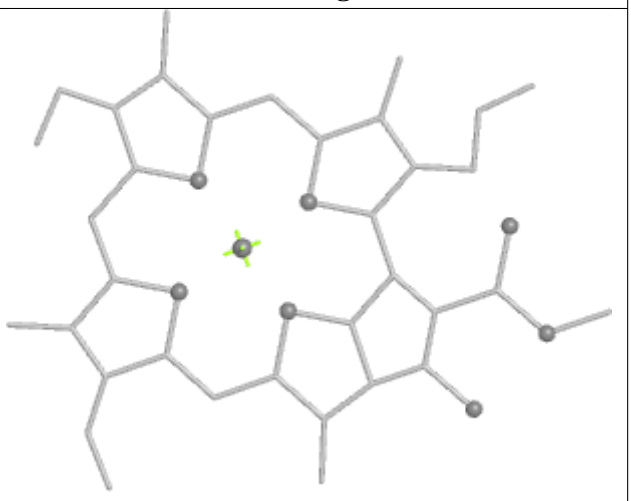
Bond lengths



Bond angles

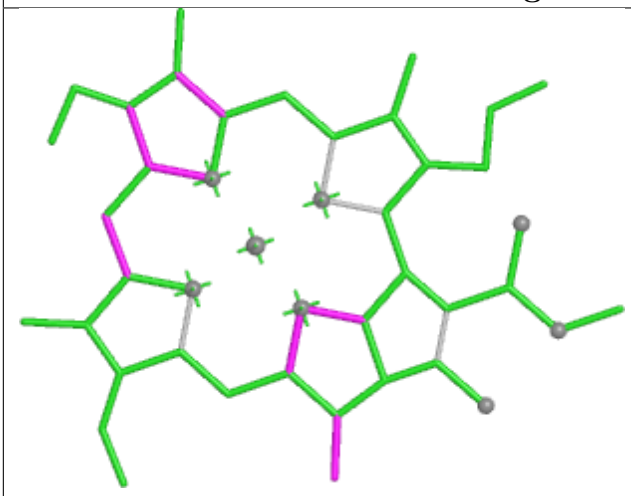


Torsions

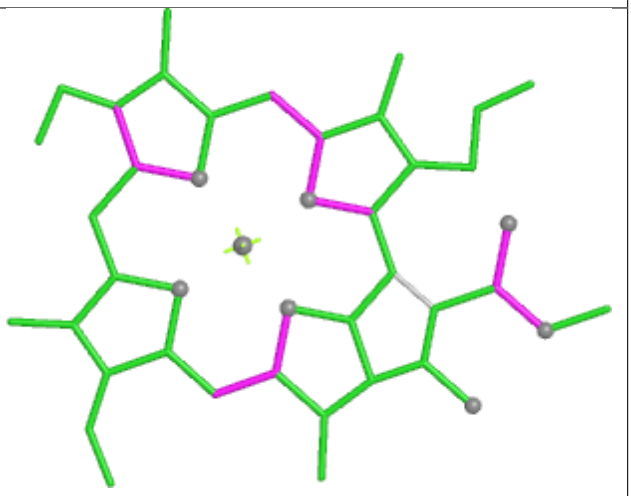


Rings

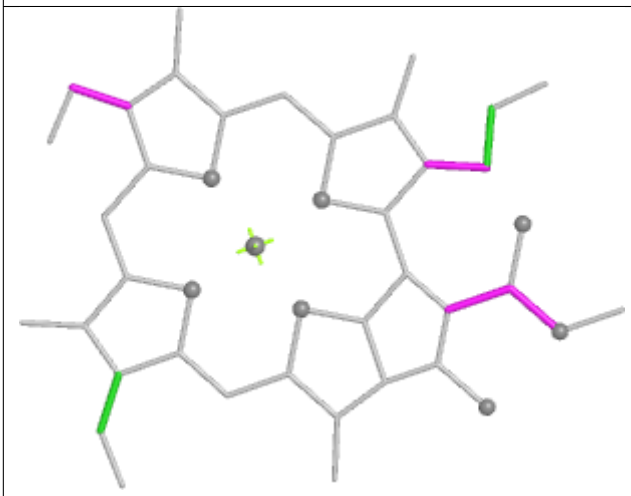
Ligand CLA Y 611



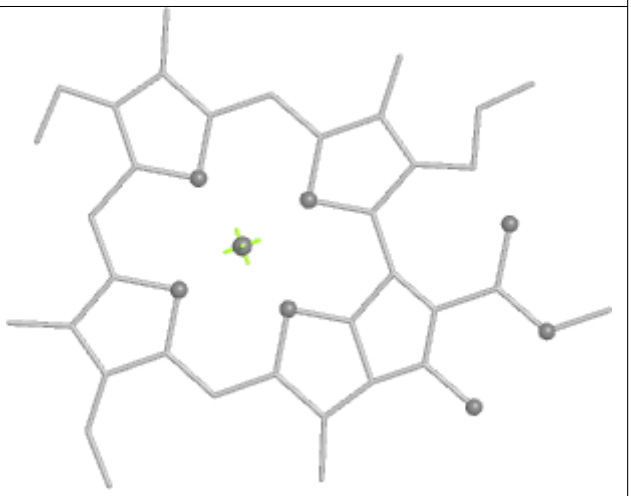
Bond lengths



Bond angles

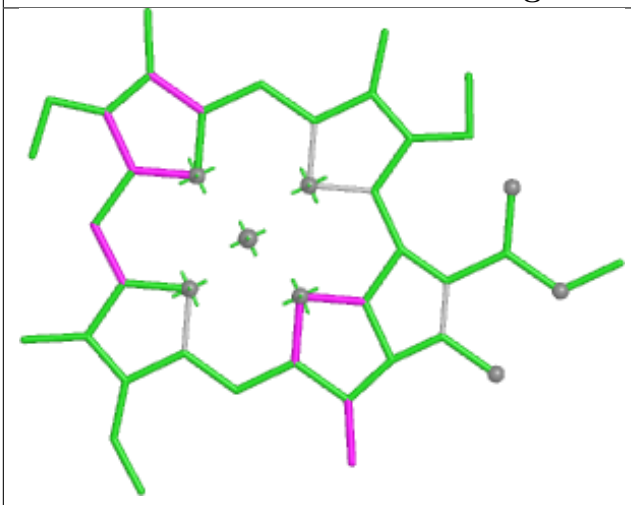


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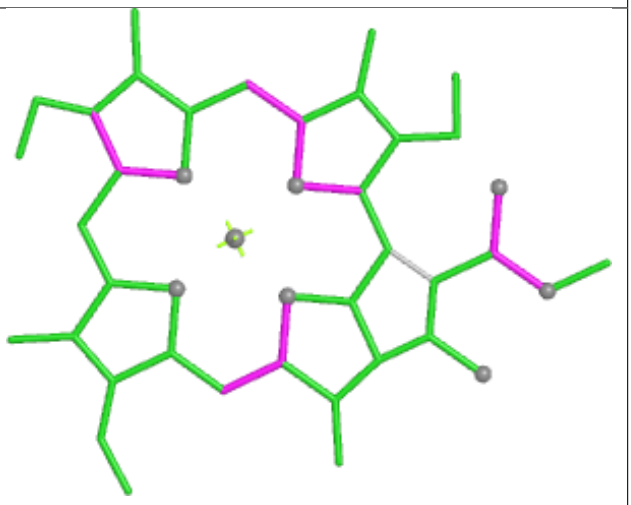


Rings

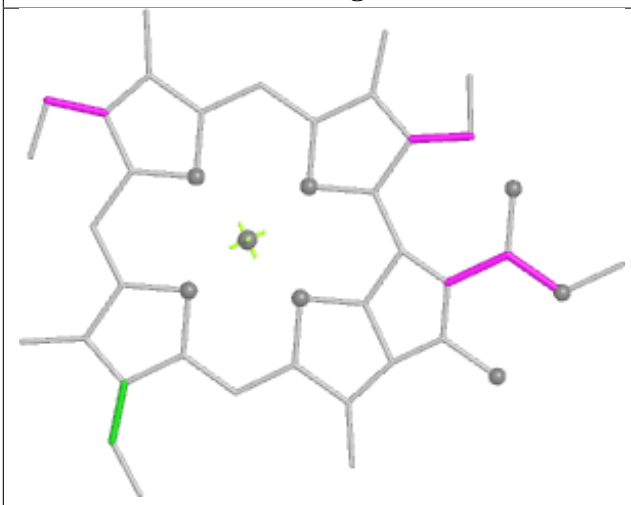
Ligand CLA X 614



Bond lengths



Bond angles



Torsions

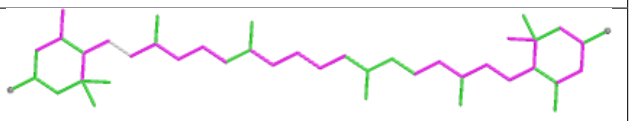


Rings

Ligand LUT Z 1620



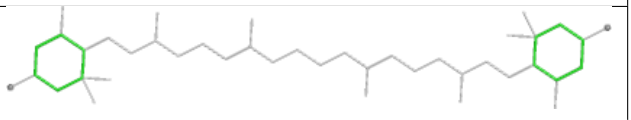
Bond lengths



Bond angles

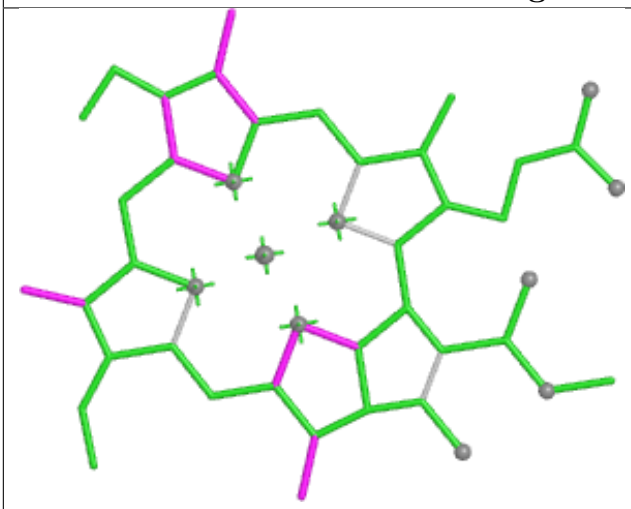


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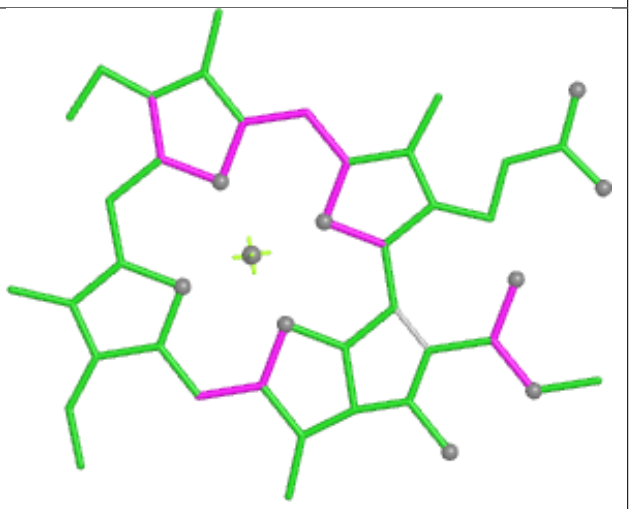


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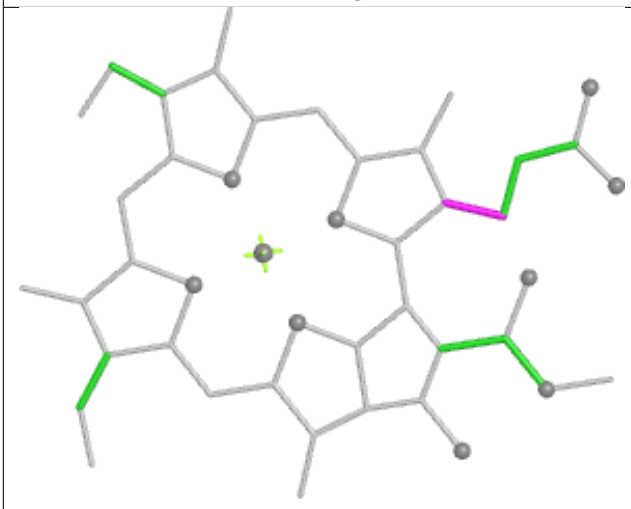
Ligand CLA 2 609



Bond lengths



Bond angles

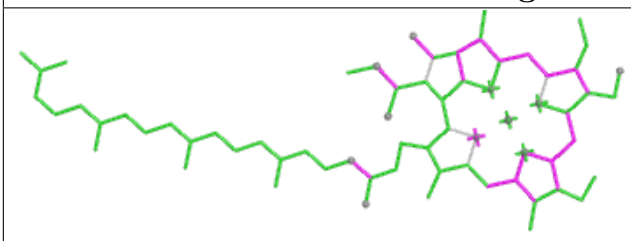


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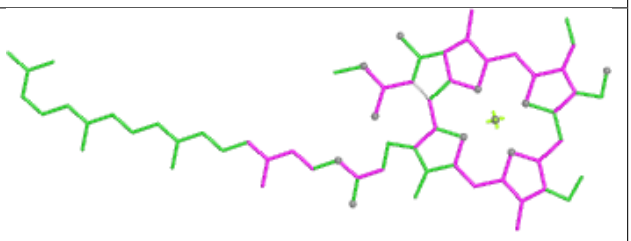


Rings

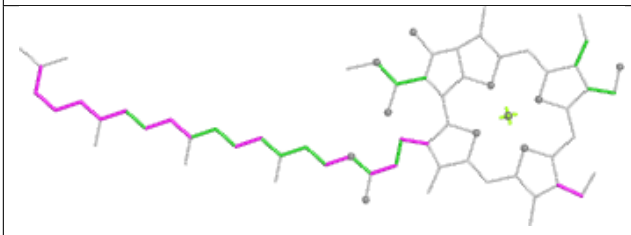
Ligand CHL W 609



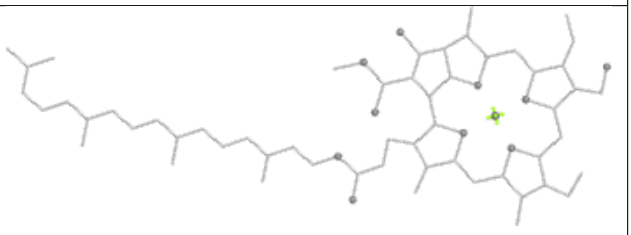
Bond lengths



Bond angles

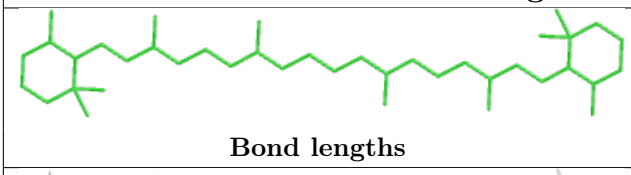


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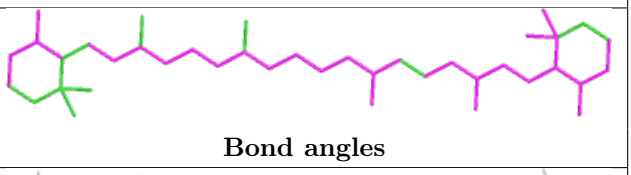


Rings

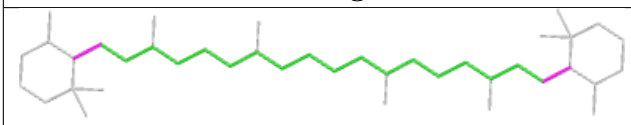
Ligand BCR a 619



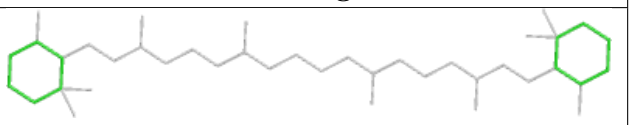
Bond lengths



Bond angles

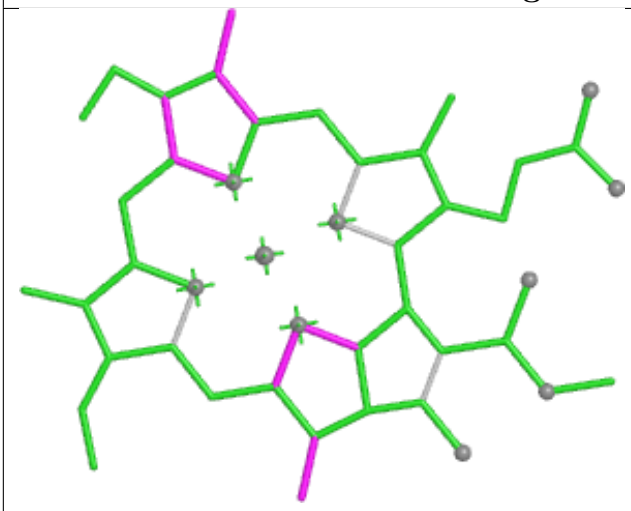


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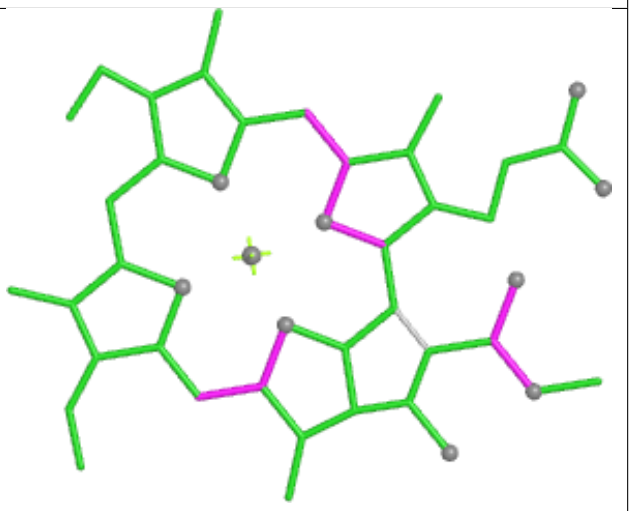


Rings

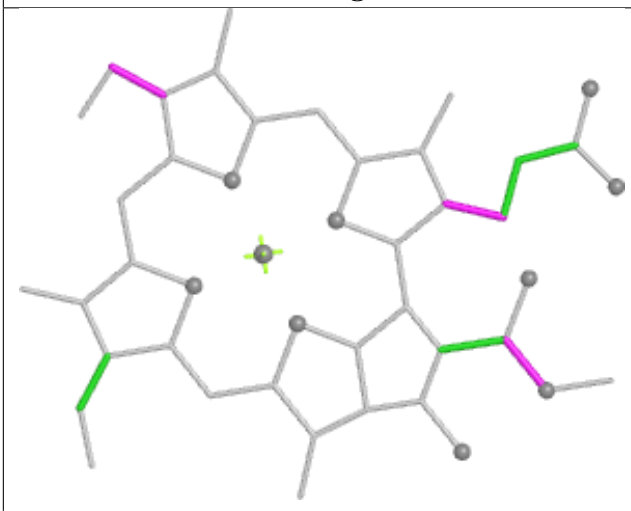
Ligand CLA K 201



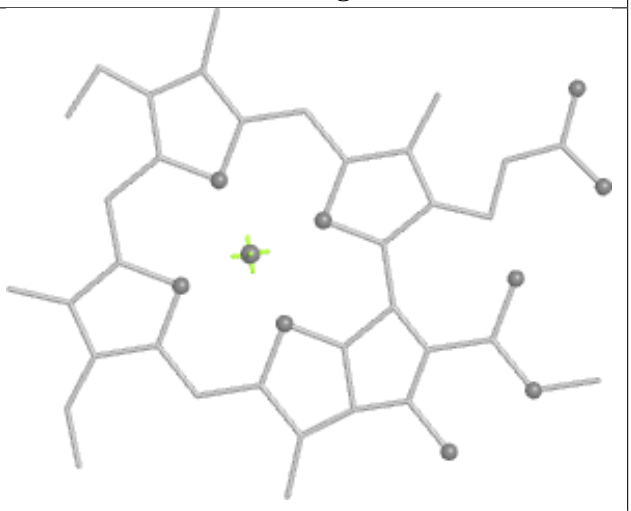
Bond lengths



Bond angles

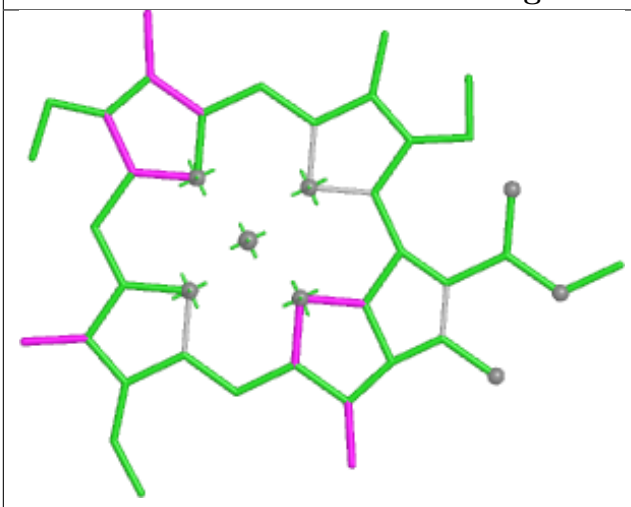


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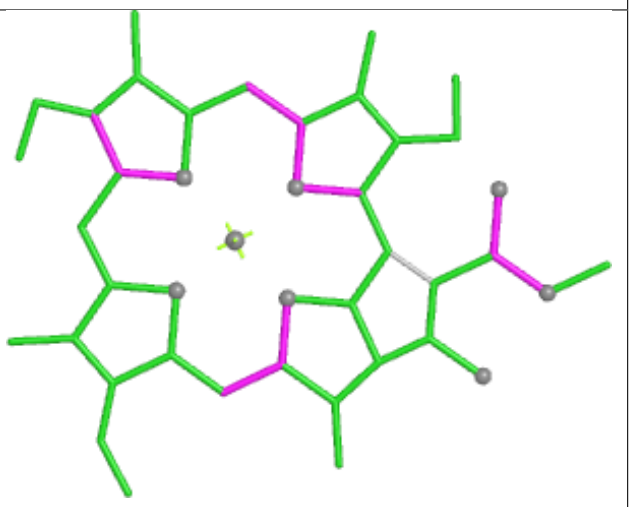


Rings

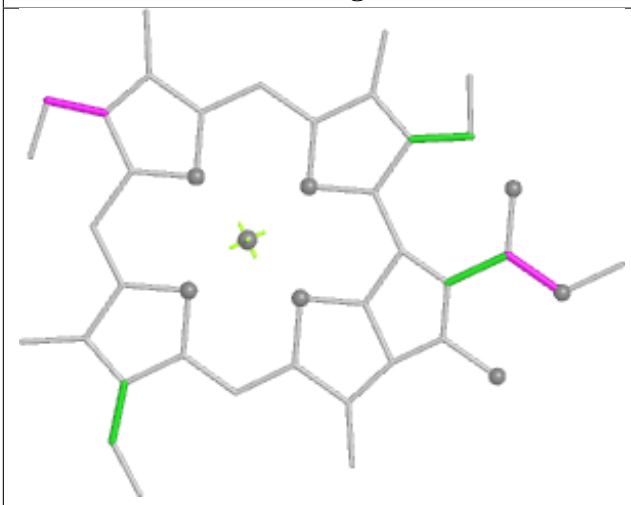
Ligand CLA A 823



Bond lengths



Bond angles

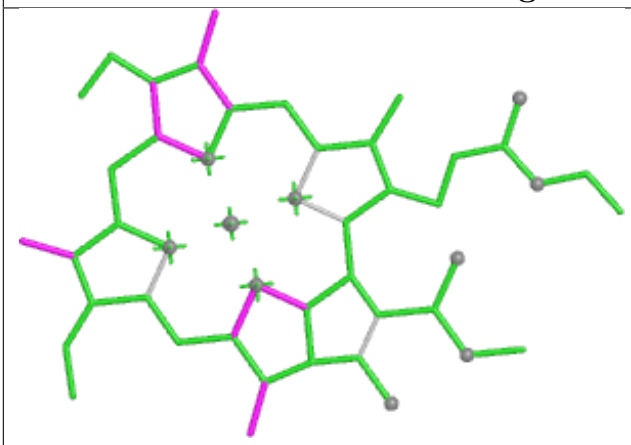


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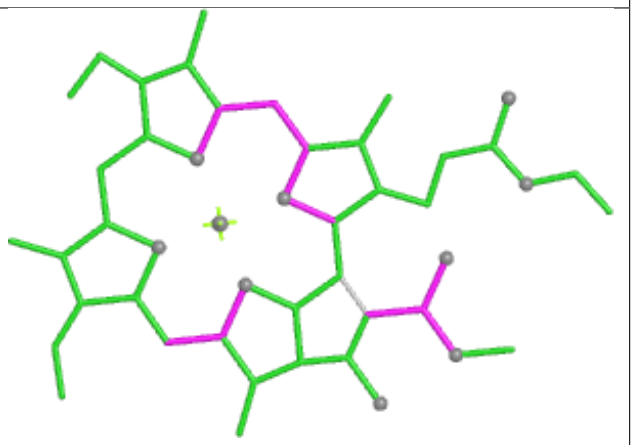


Rings

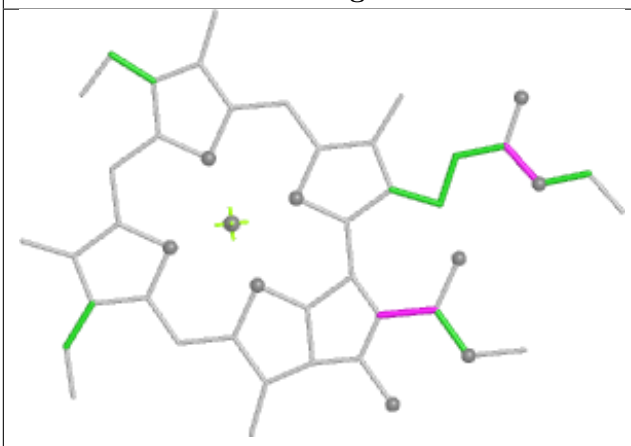
Ligand CLA W 604



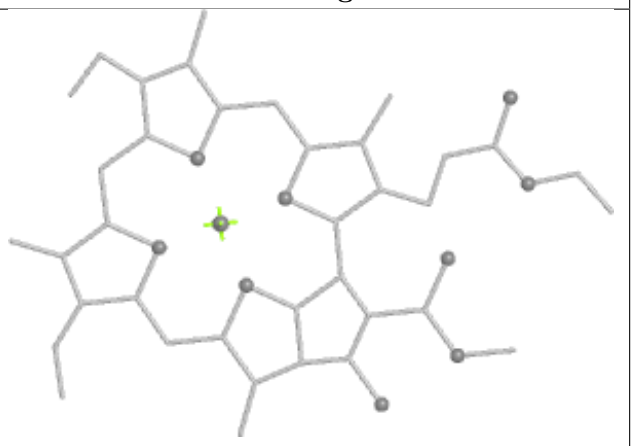
Bond lengths



Bond angles

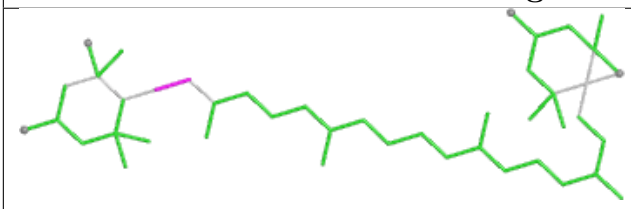


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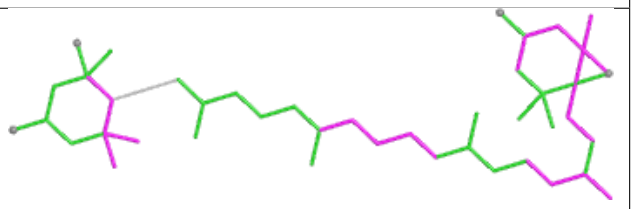


Rings

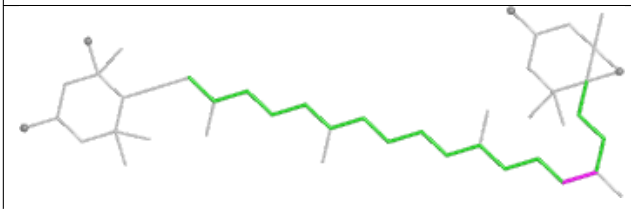
Ligand NEX 5 624



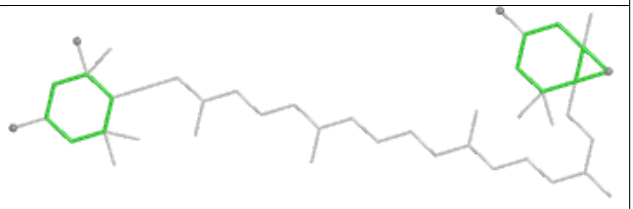
Bond lengths



Bond angles

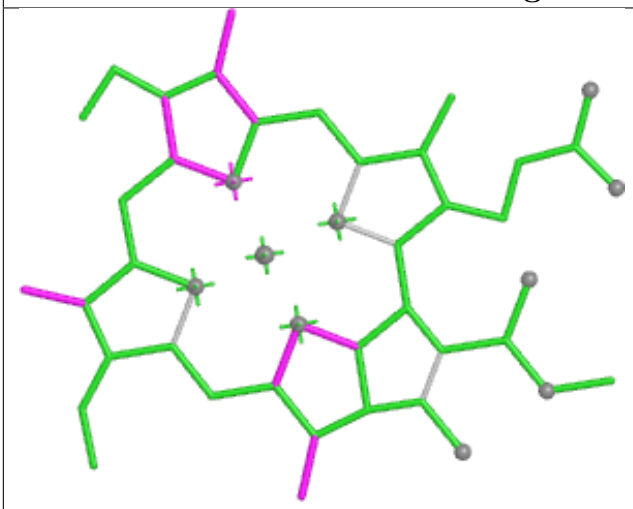


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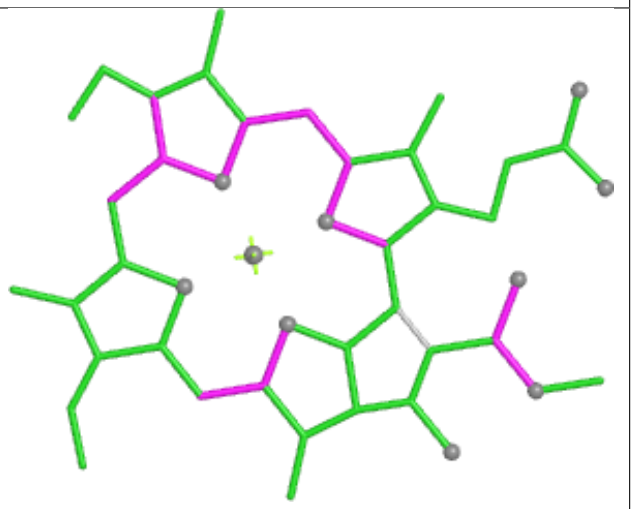


Rings

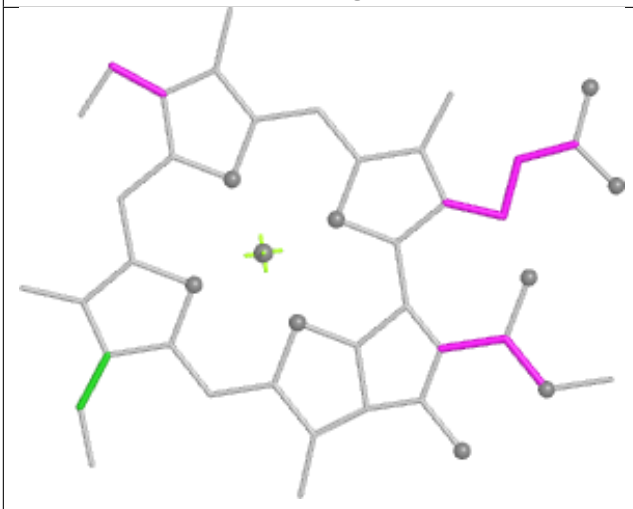
Ligand CLA A 837



Bond lengths



Bond angles

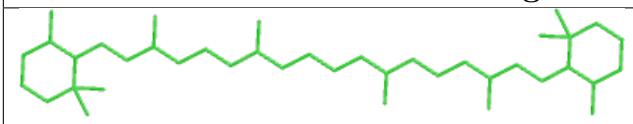


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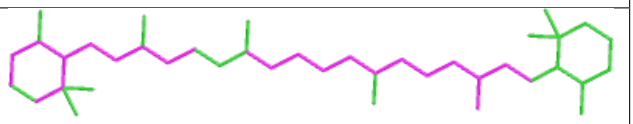


Rings

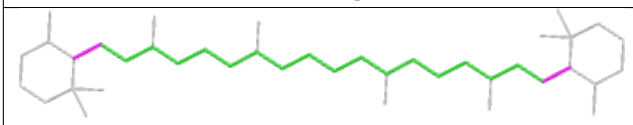
Ligand BCR B 843



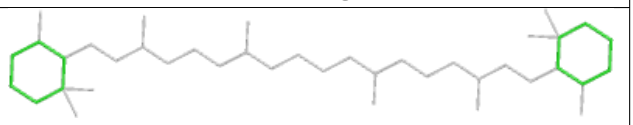
Bond lengths



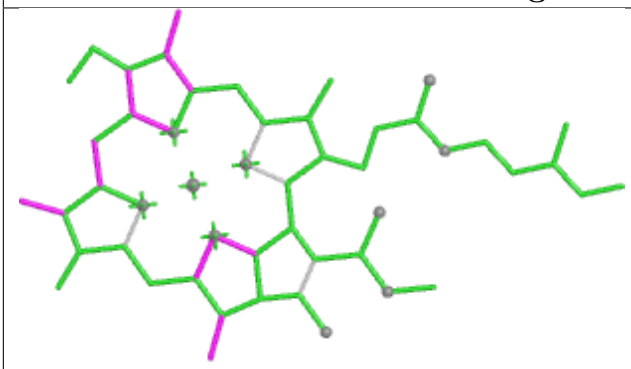
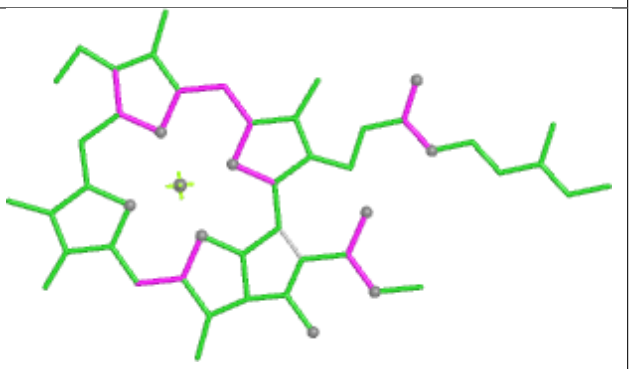
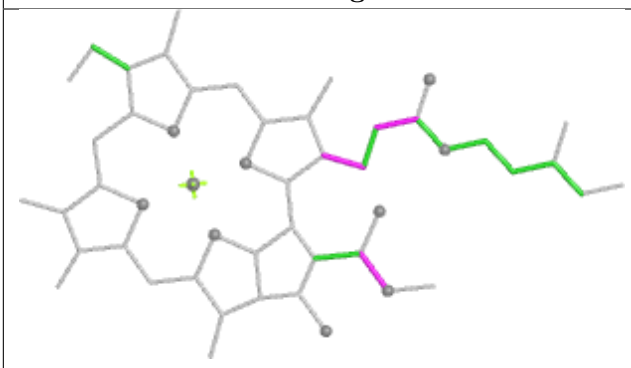
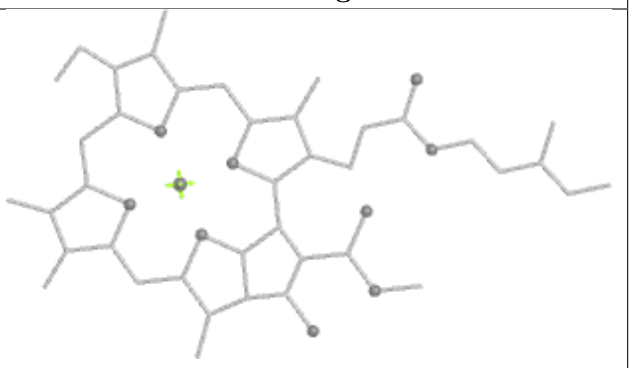
Bond angles

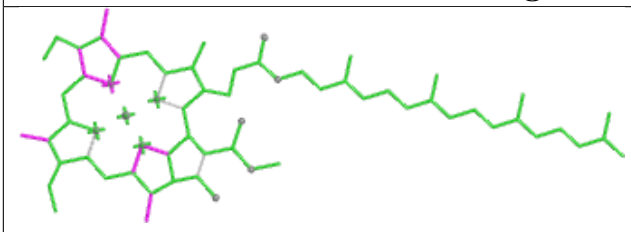
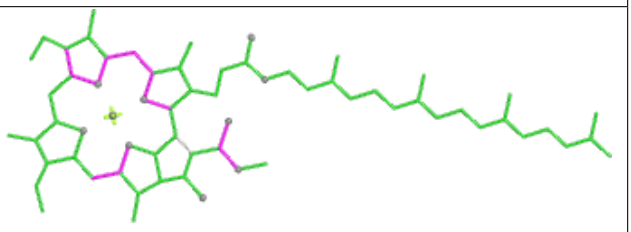
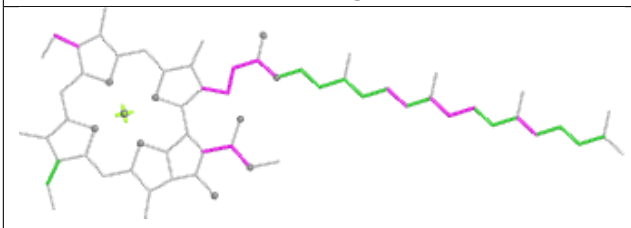
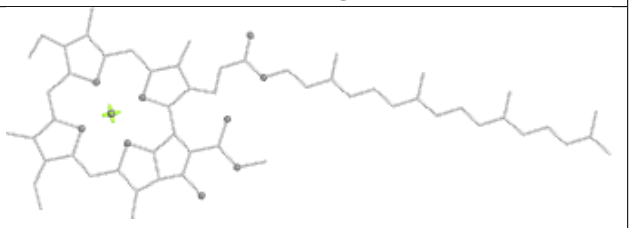


Torsions

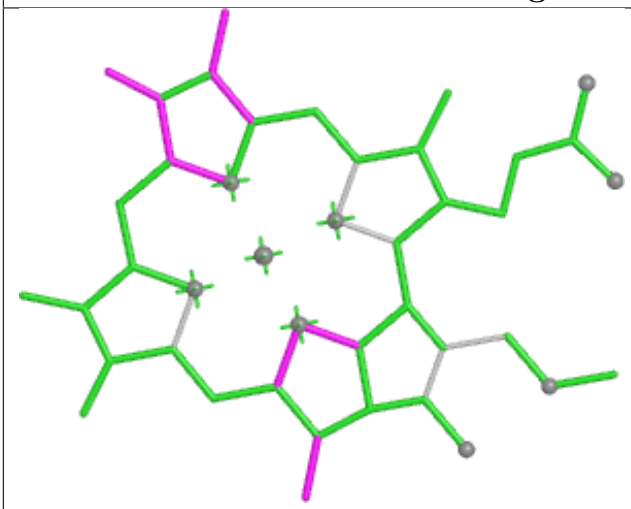


Rings

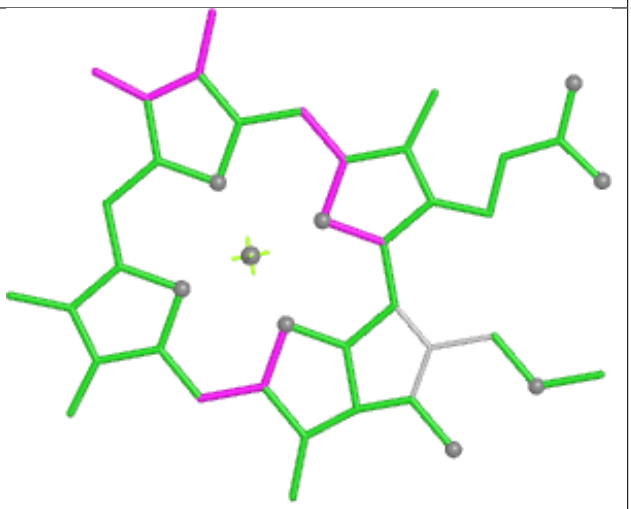
Ligand CLA 5 608	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 841	
	
Bond lengths	Bond angles
	
Torsions	Rings

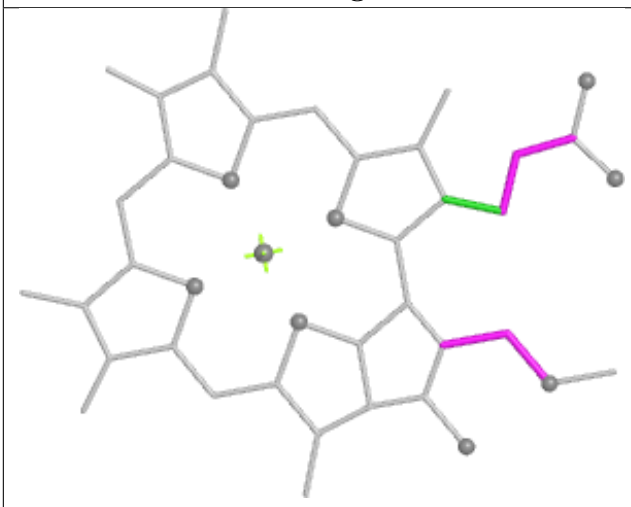
Ligand CLA 7 615



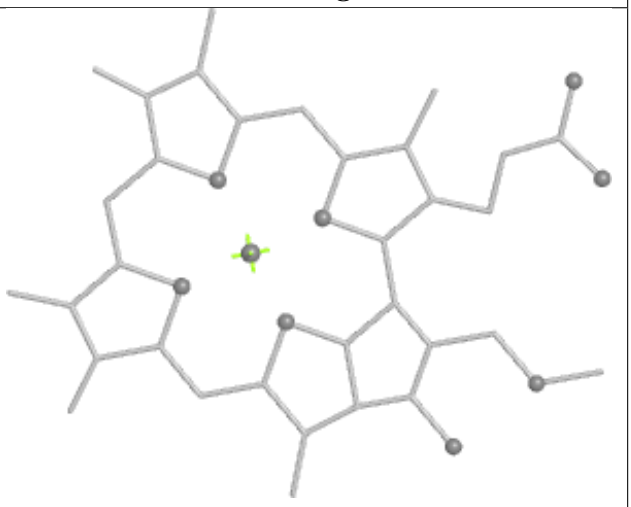
Bond lengths



Bond angles

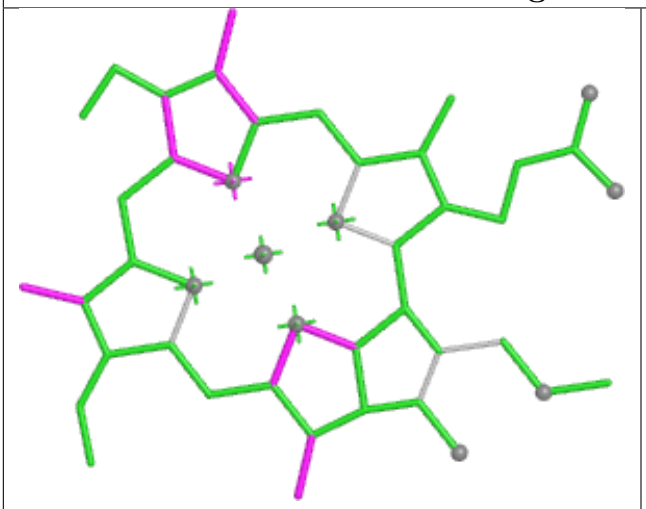


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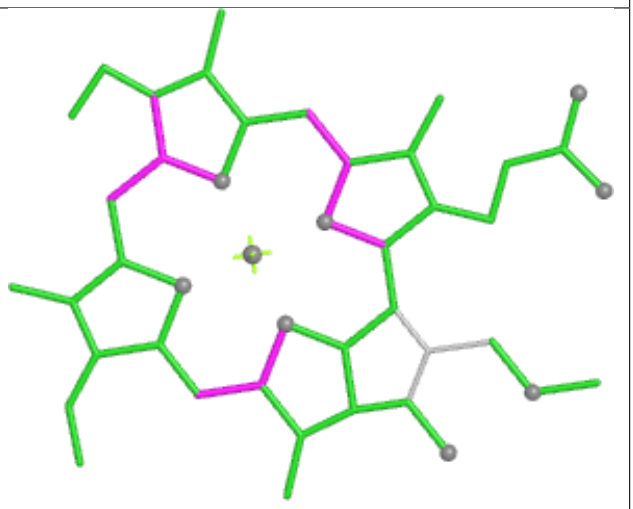


Rings

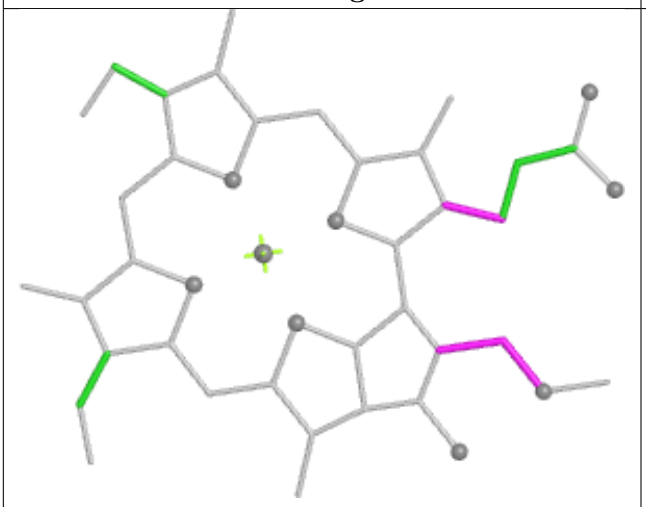
Ligand CLA a 606



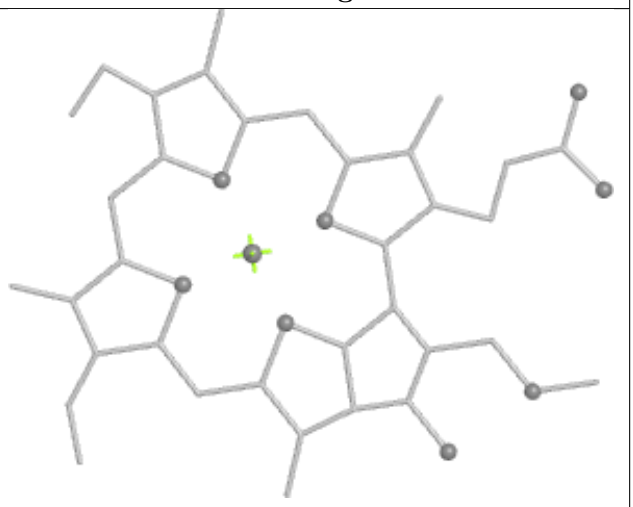
Bond lengths



Bond angles

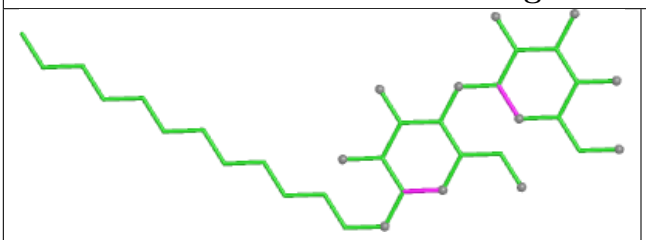


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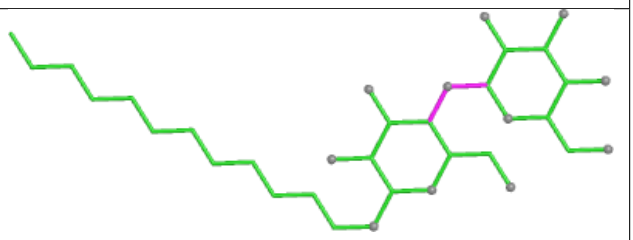


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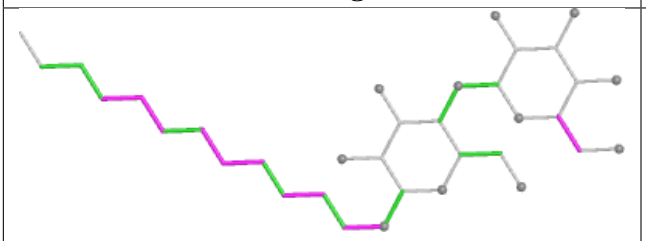
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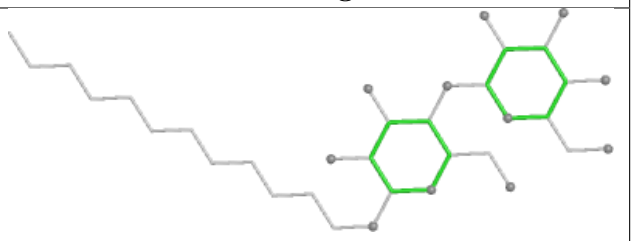
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Bond angles

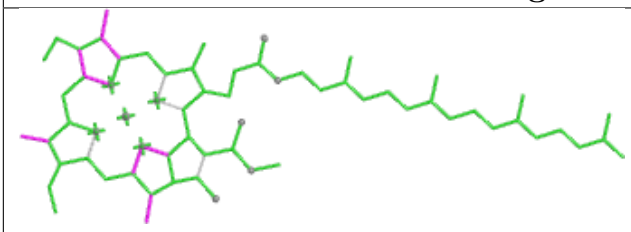


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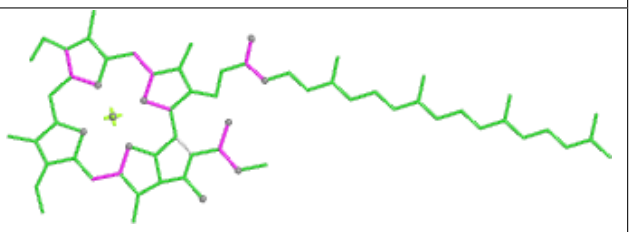


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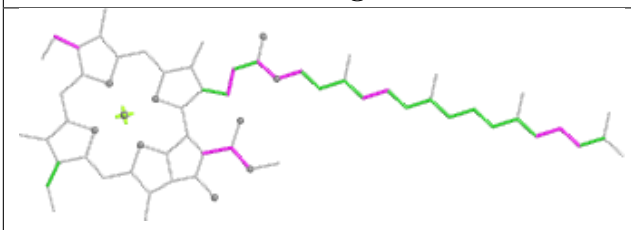
Ligand CLA 7 613



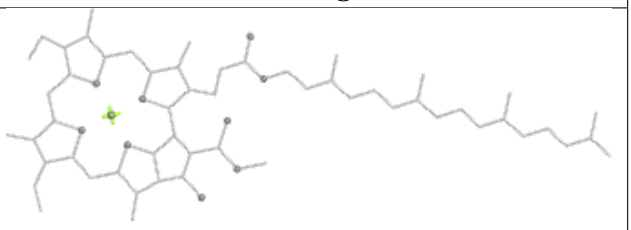
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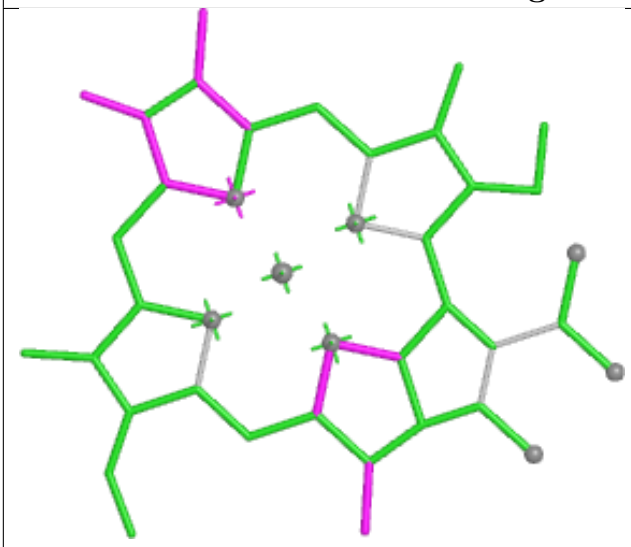


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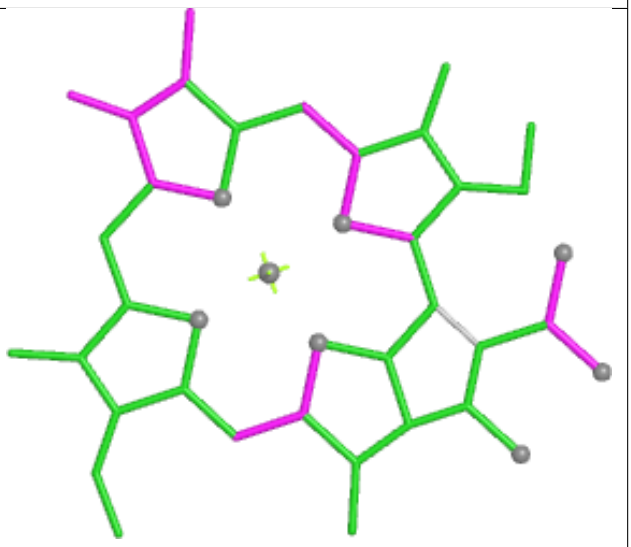


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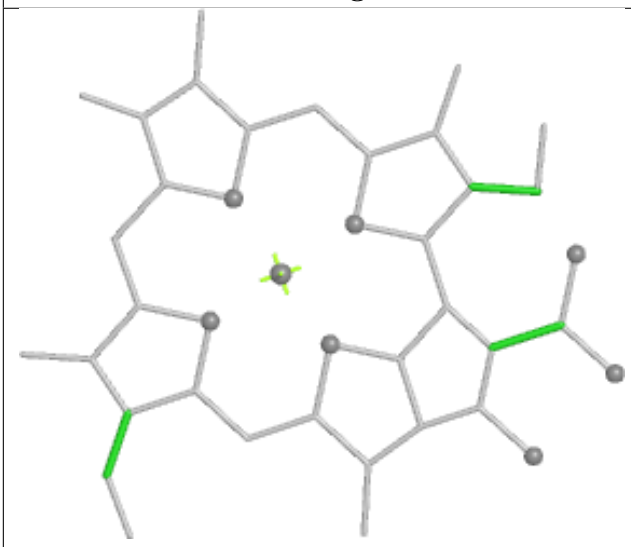
Ligand CLA 5 618



Bond lengths



Bond angles

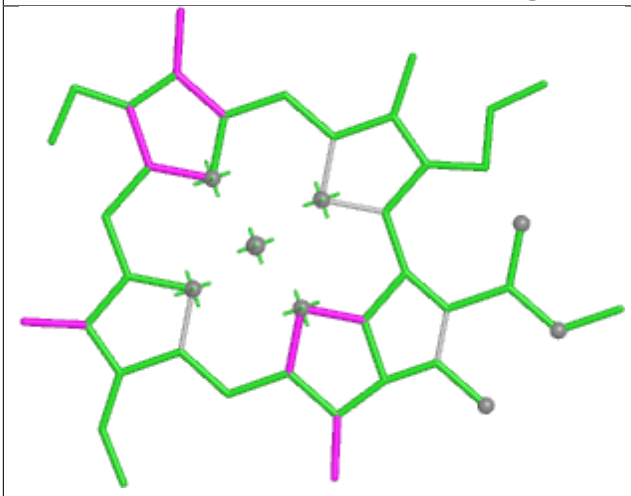


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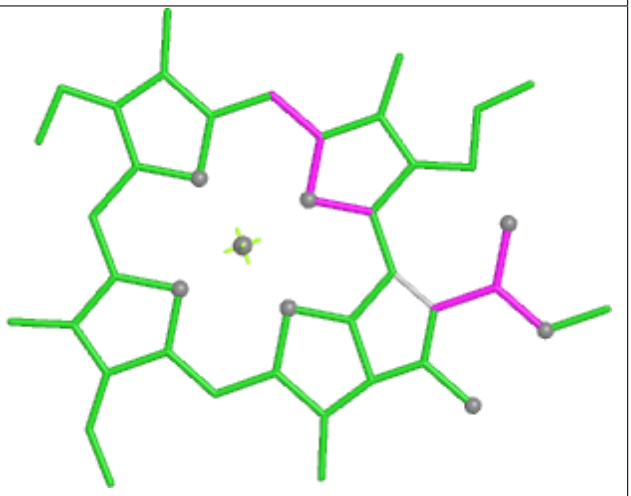


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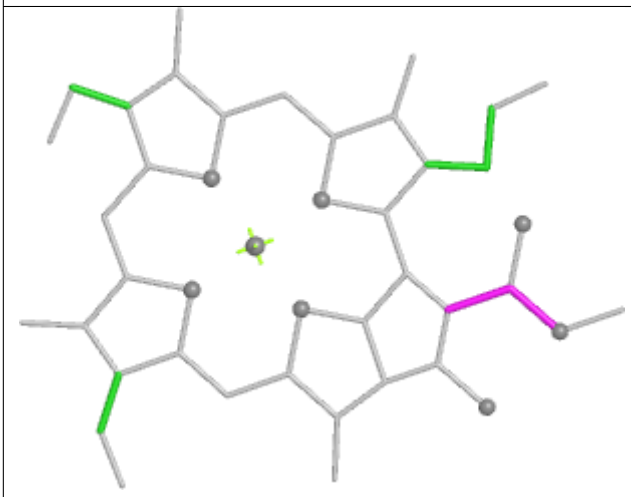
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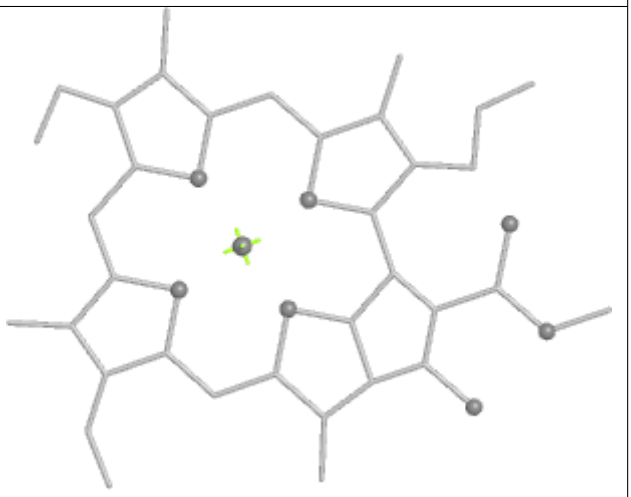
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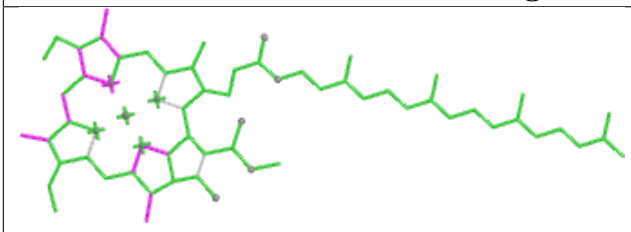


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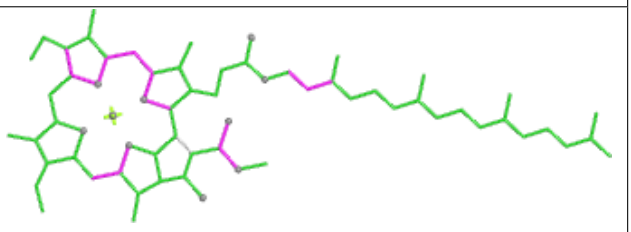


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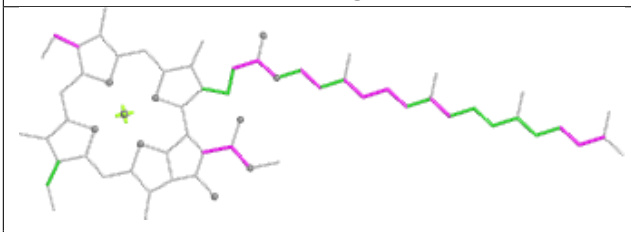
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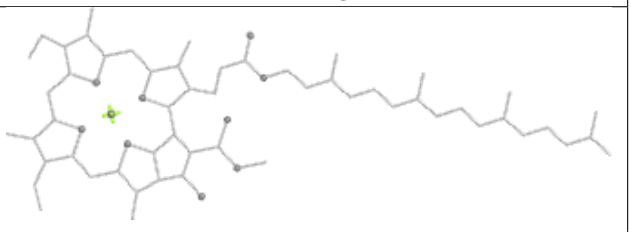
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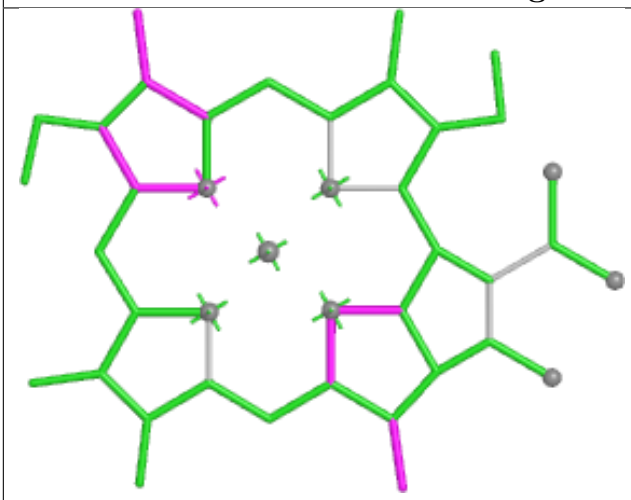


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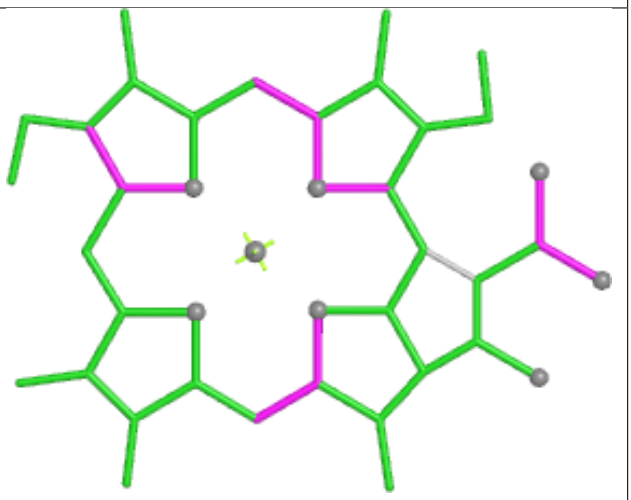


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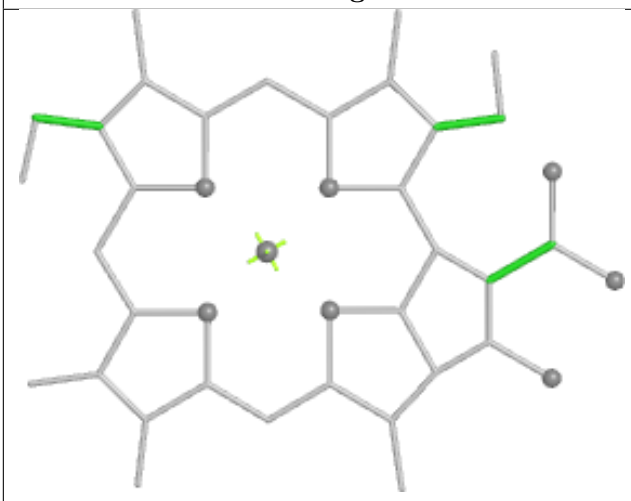
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Bond lengths



Bond angles

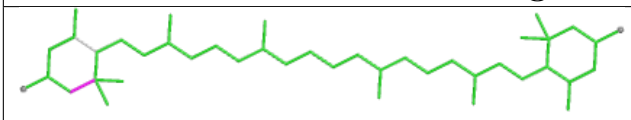


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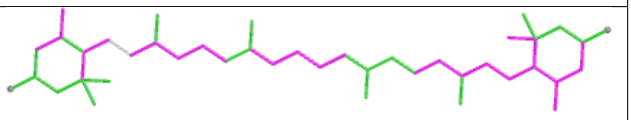


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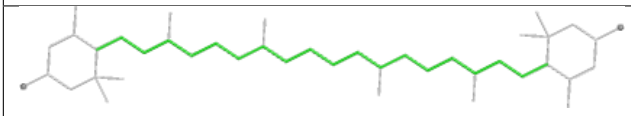
Ligand LUT a 617



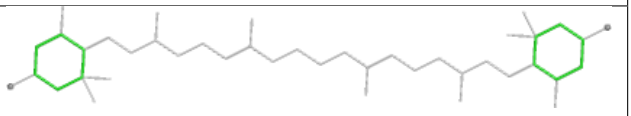
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Bond angles

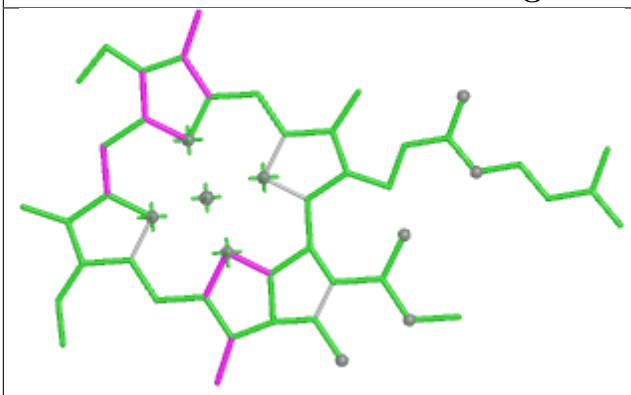


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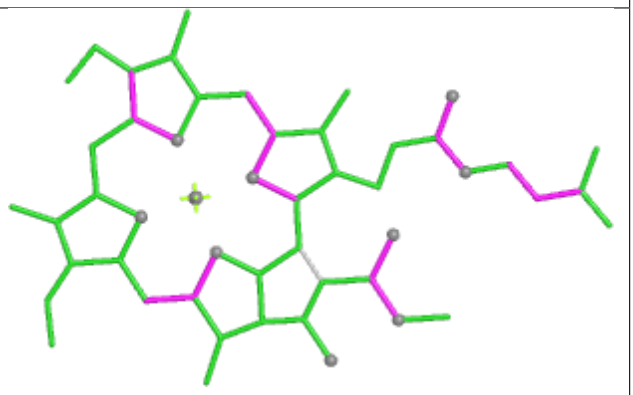


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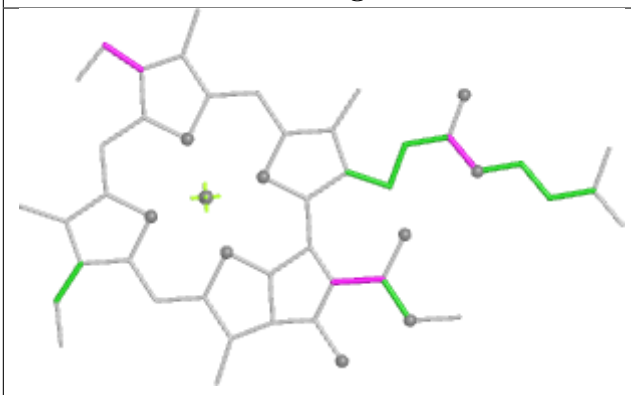
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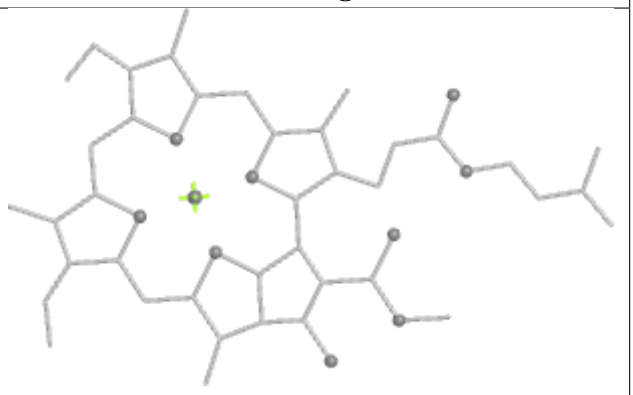
Bond lengths



Bond angles



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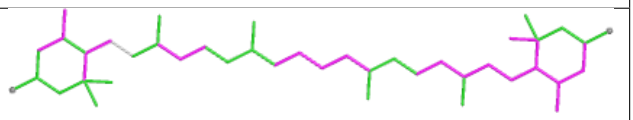


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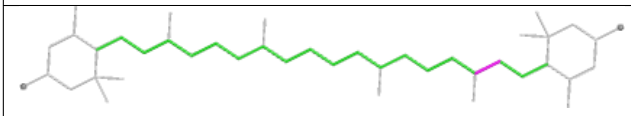
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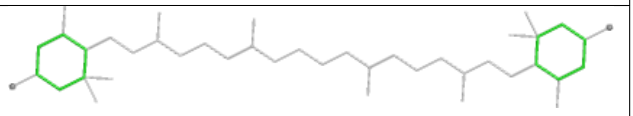
Bond lengths



Bond angles

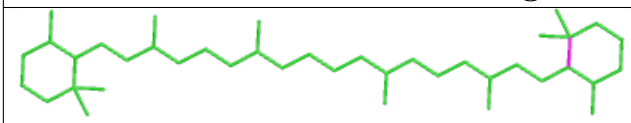


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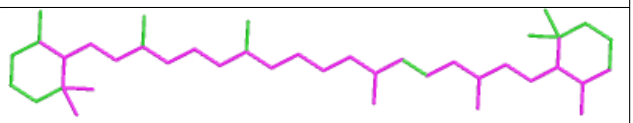


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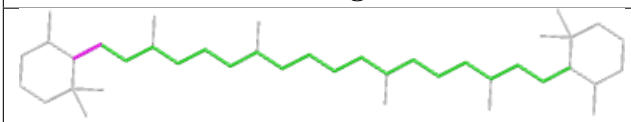
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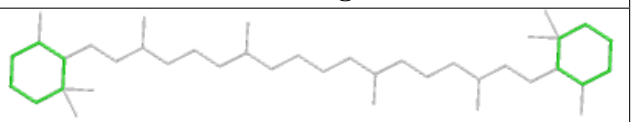
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Bond angles

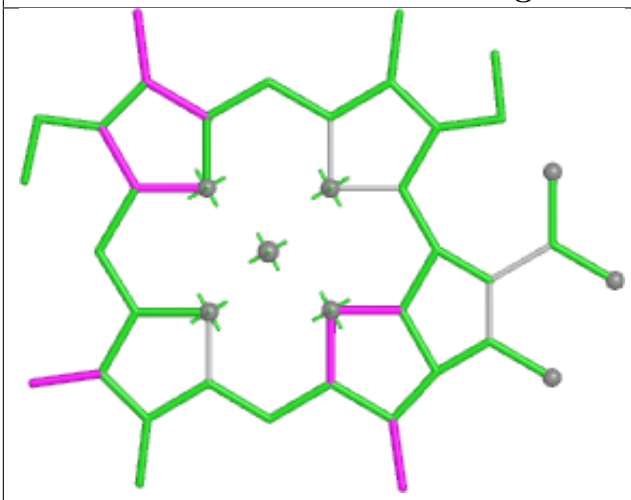


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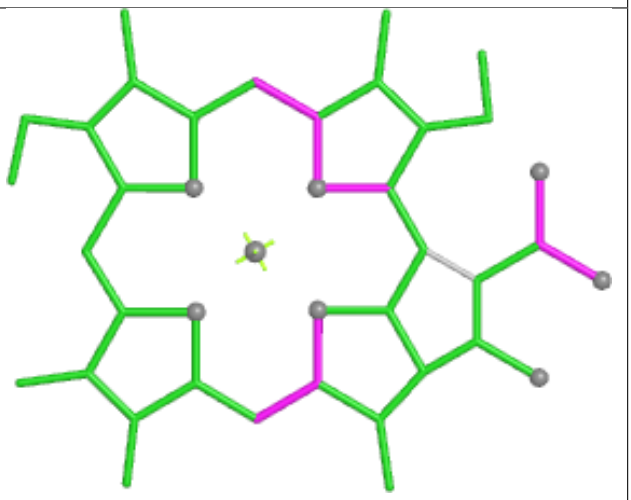


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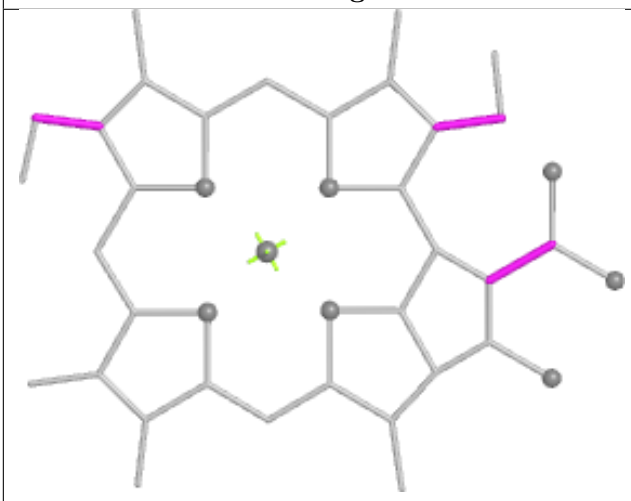
Ligand CLA O 2003



Bond lengths



Bond angles

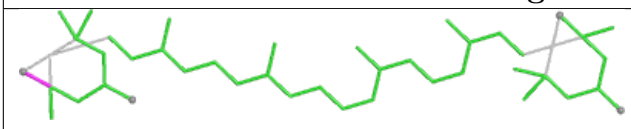


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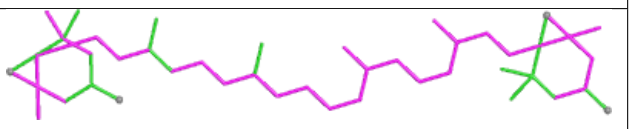


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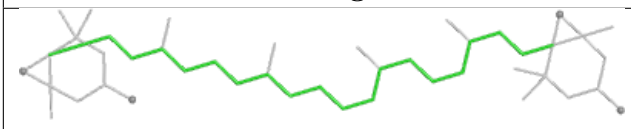
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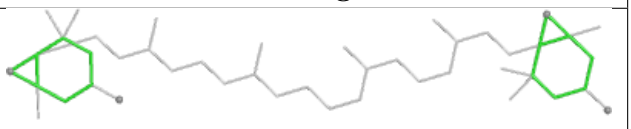
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Bond angles

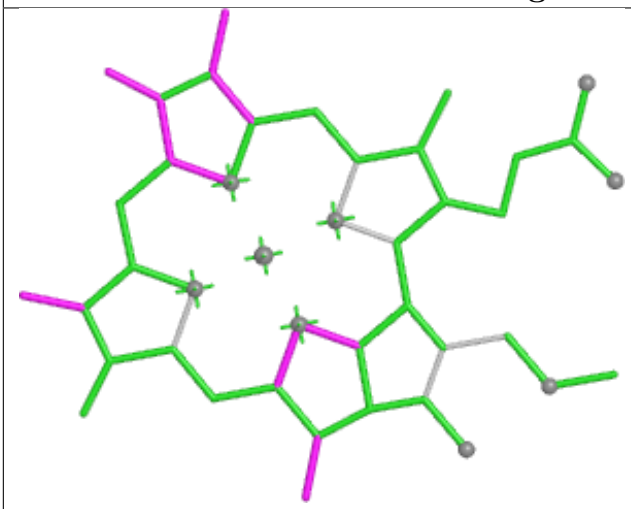


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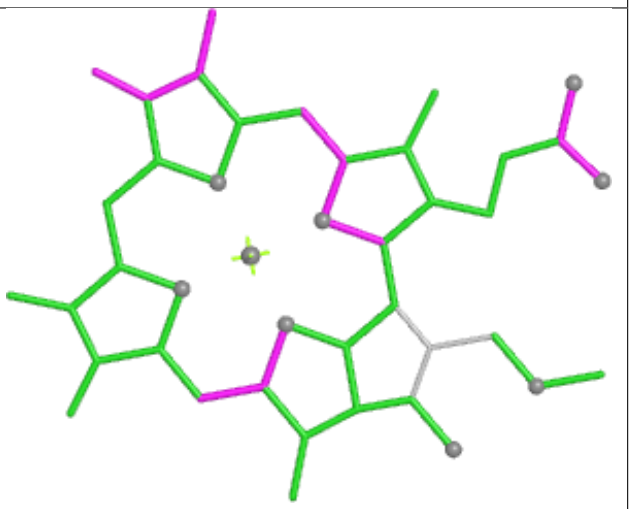


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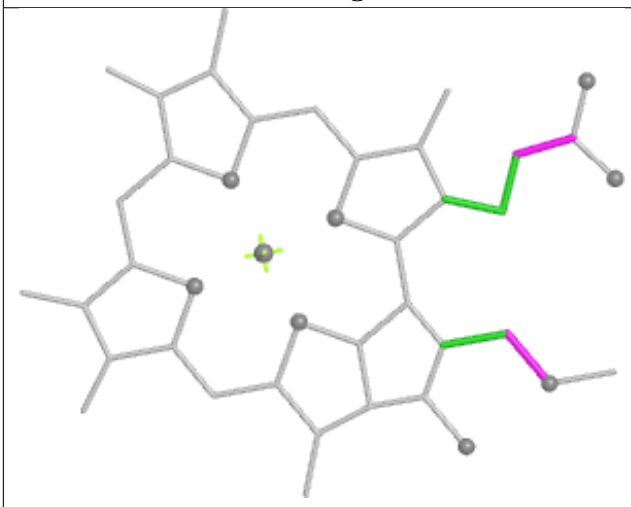
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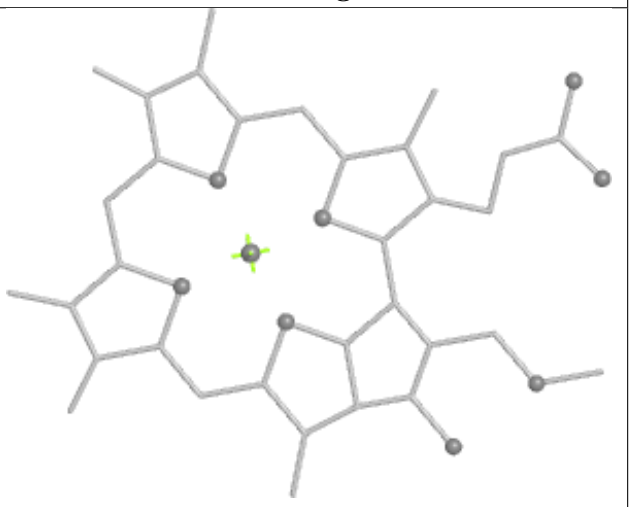
Bond lengths



Bond angles

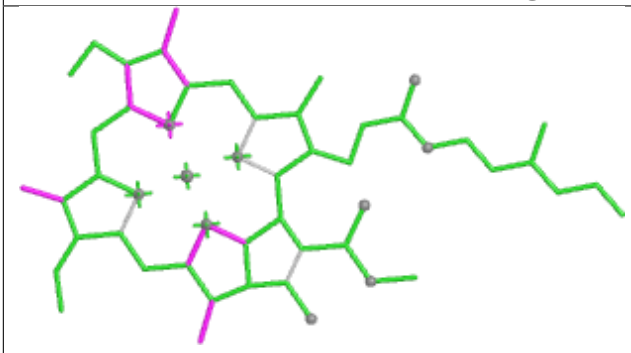


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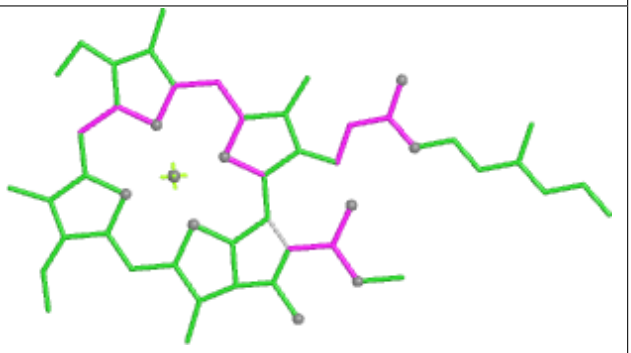


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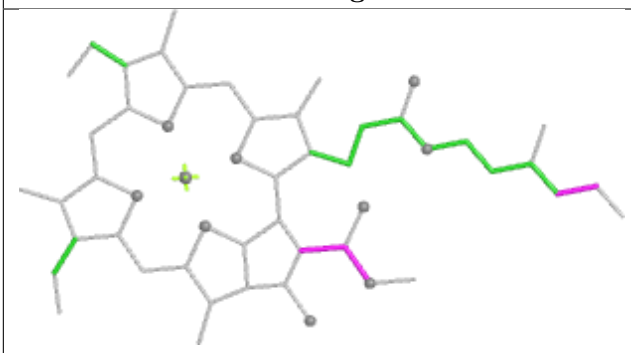
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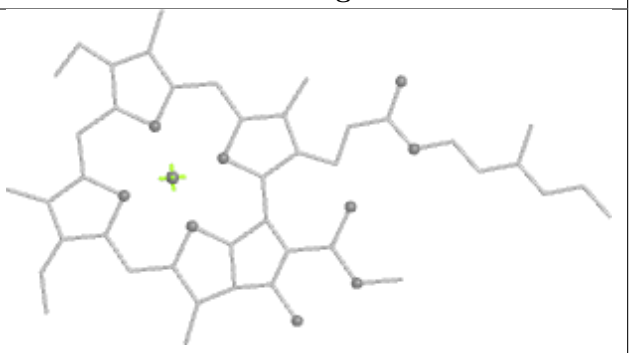
Bond lengths



Bond angles

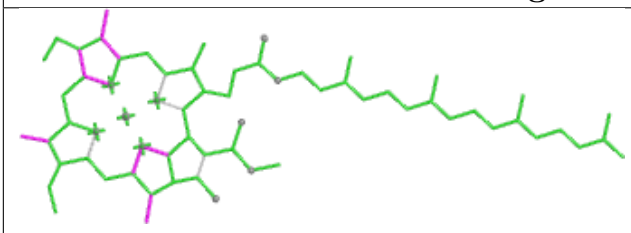


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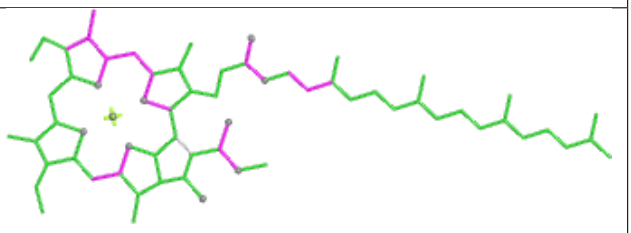


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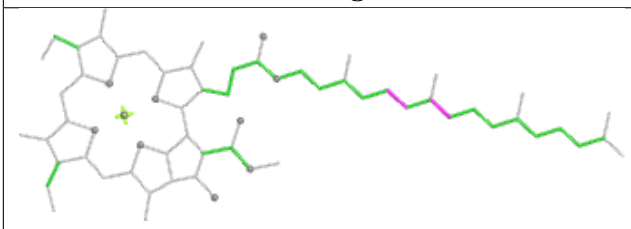
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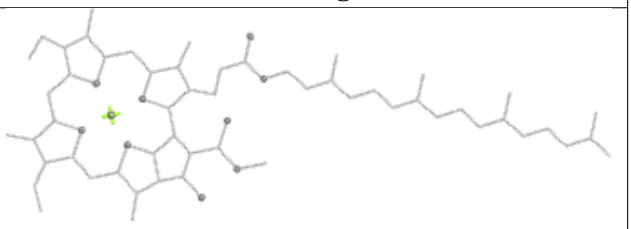
Bond lengths



Bond angles

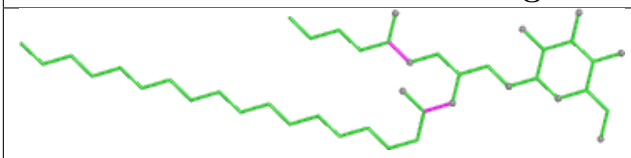


Torsions

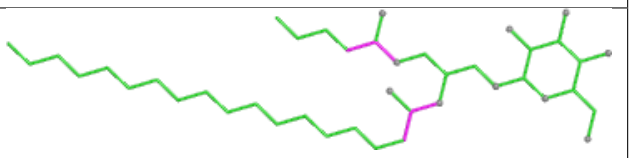


Rings

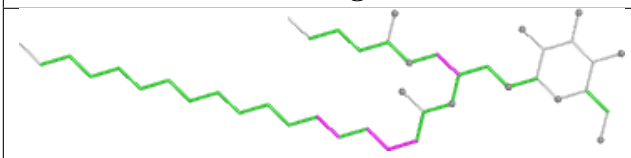
Ligand LMG J 103



Bond lengths



Bond angles

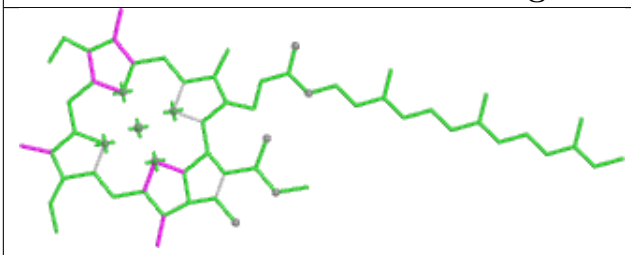


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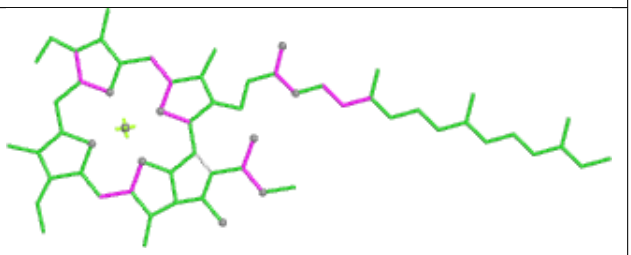


Rings

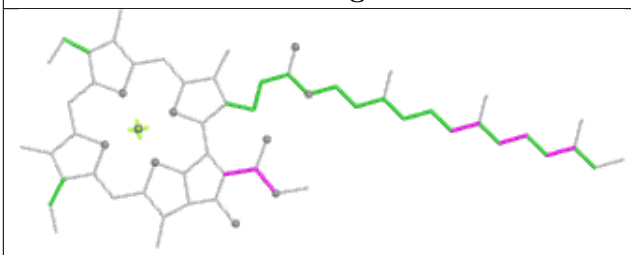
Ligand CLA 4 610



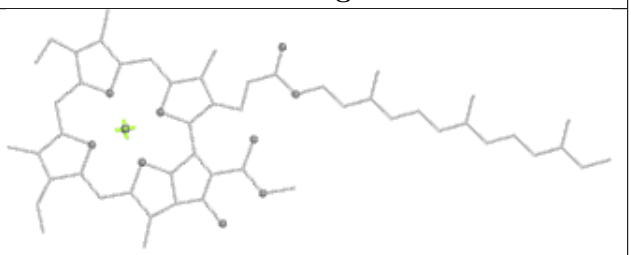
Bond lengths



Bond angles

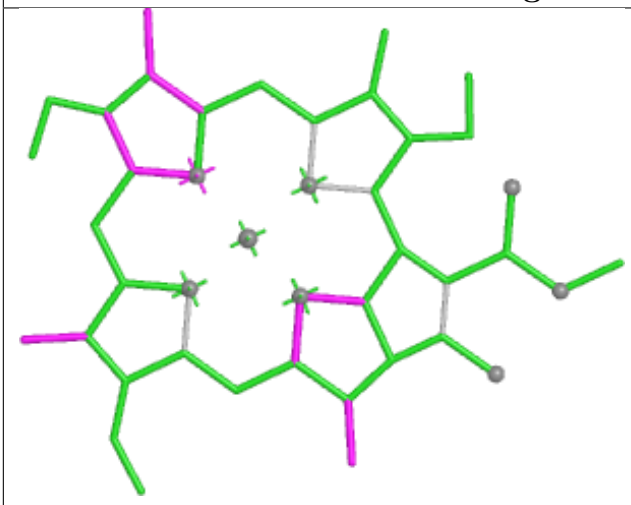


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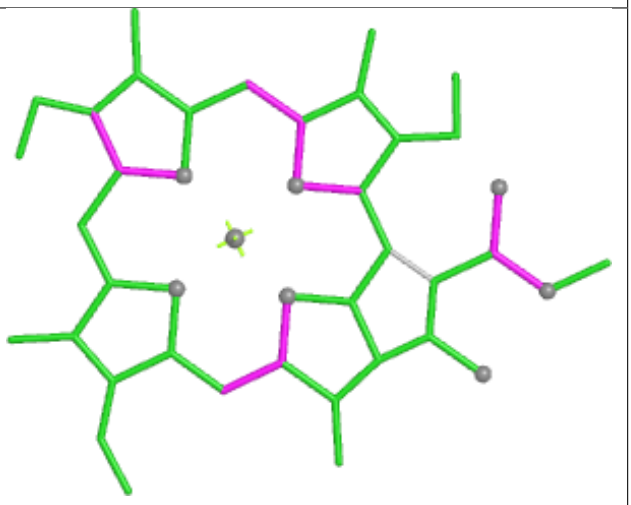


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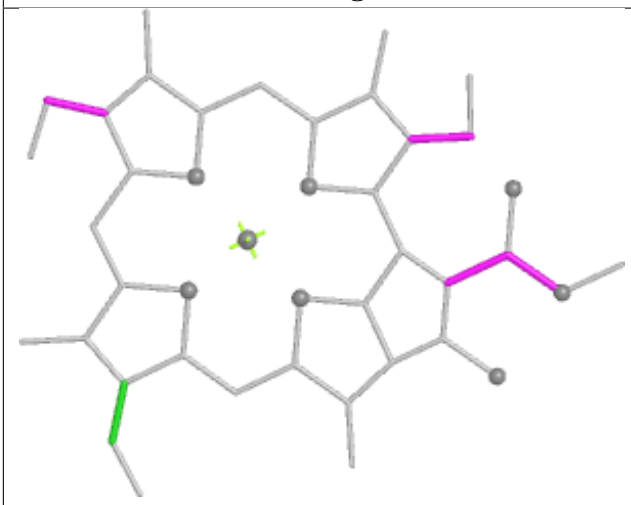
Ligand CLA U 611



Bond lengths



Bond angles

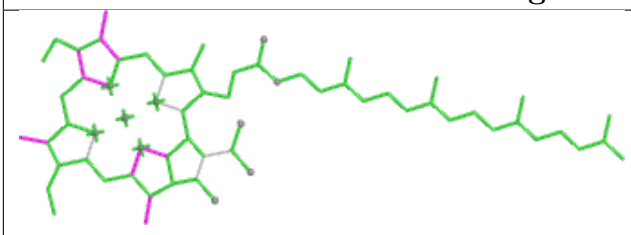


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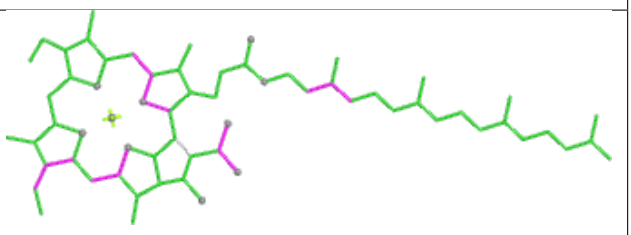


Rings

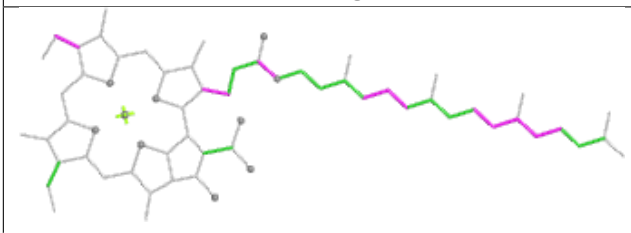
Ligand CLA a 609



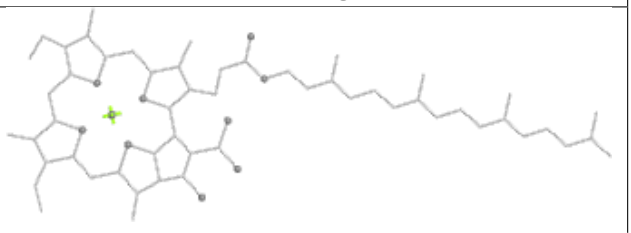
Bond lengths



Bond angles

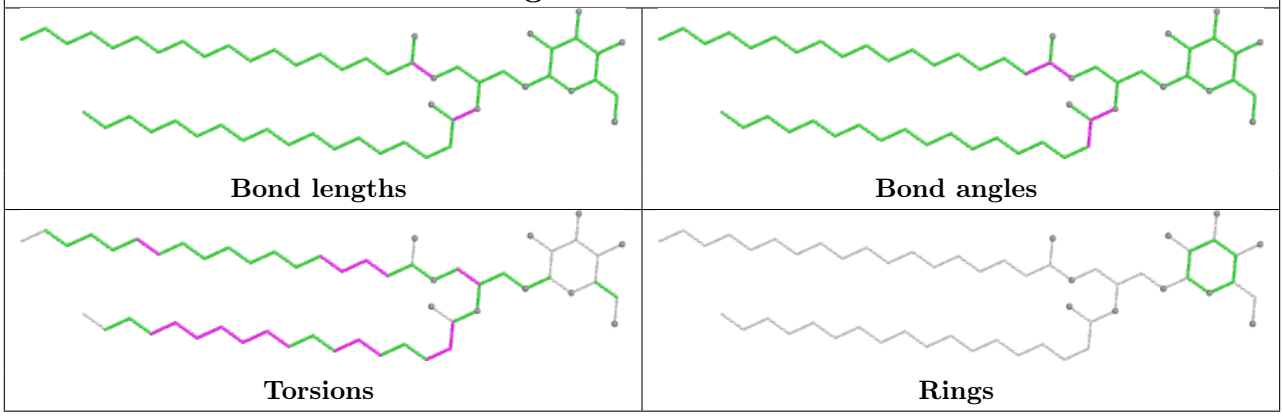


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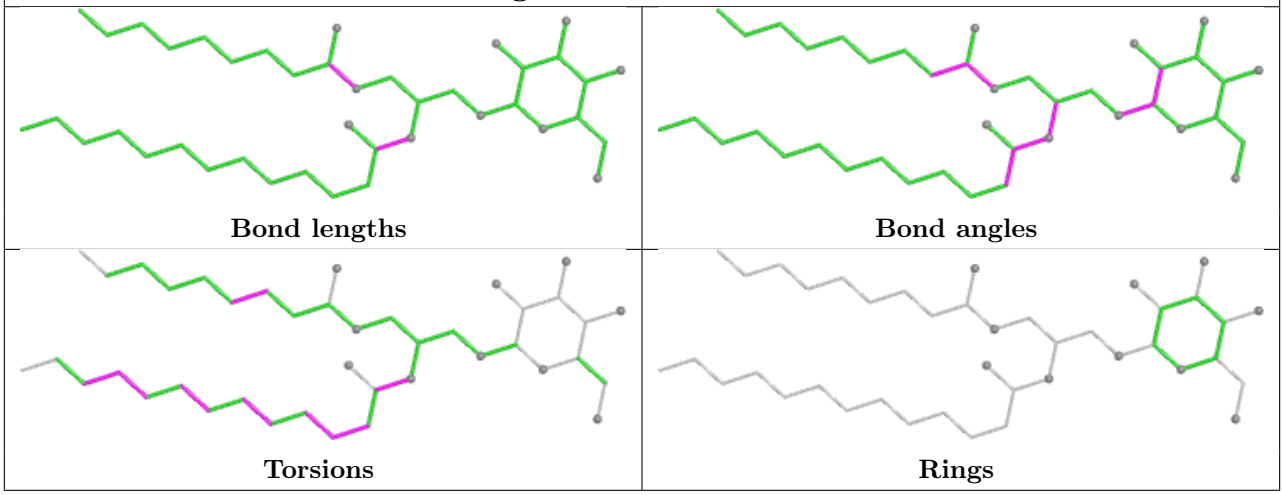


Rings

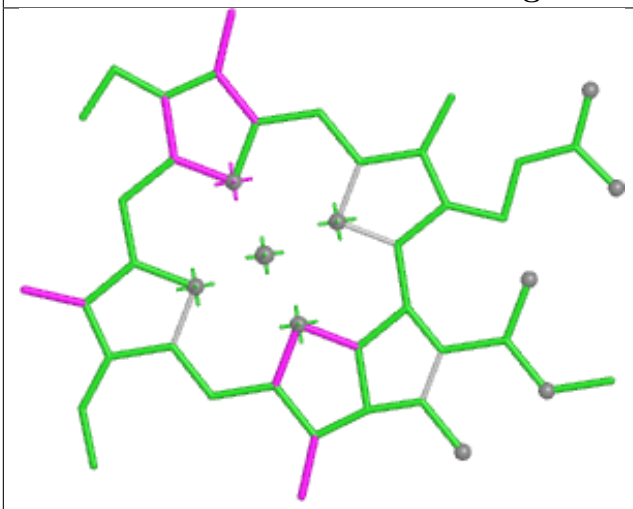
Ligand LMG 9 625



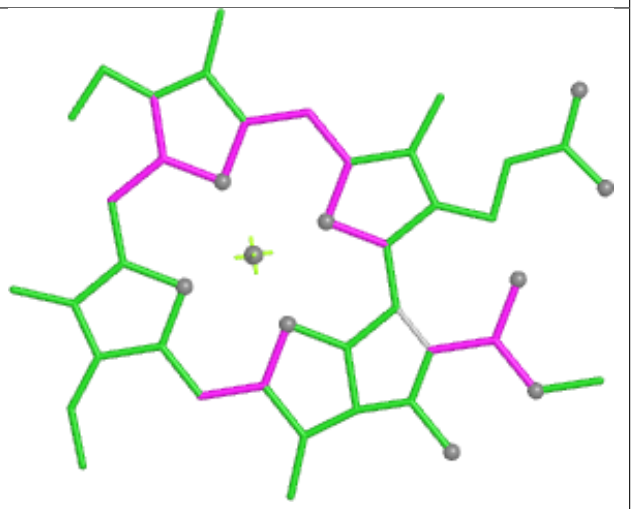
Ligand LMG V 2631



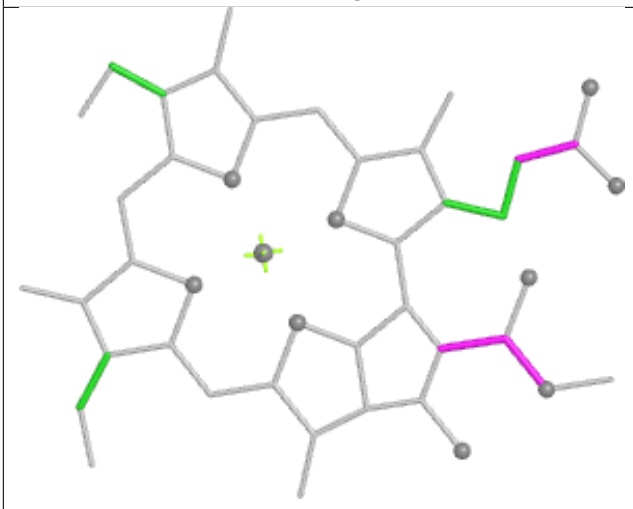
Ligand CLA G 204



Bond lengths



Bond angles

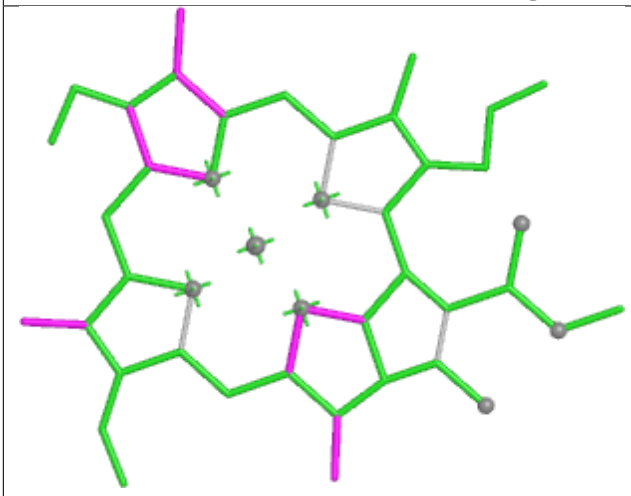


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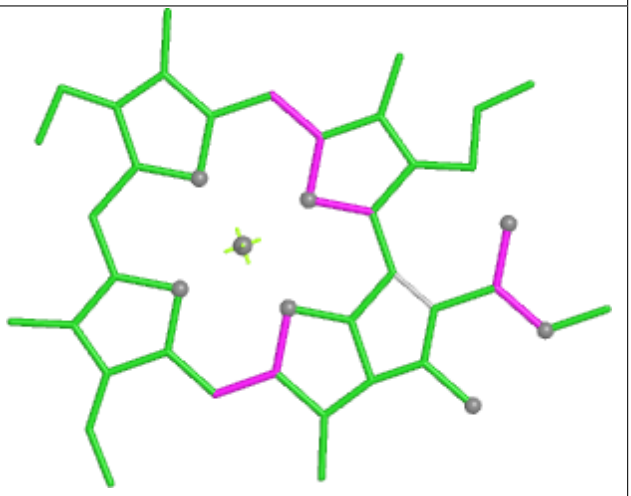


Rings

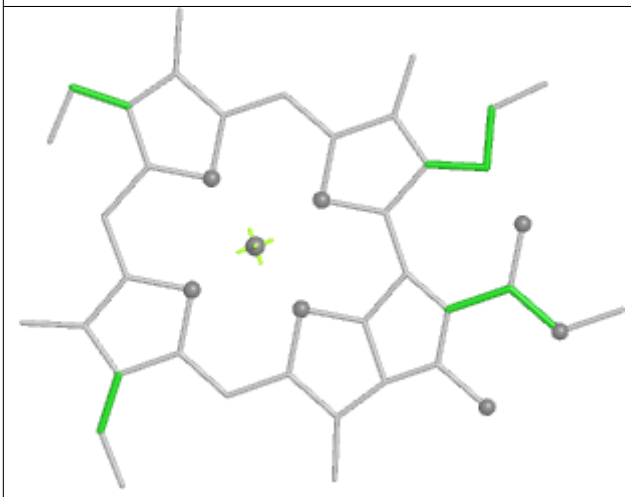
Ligand CLA B 815



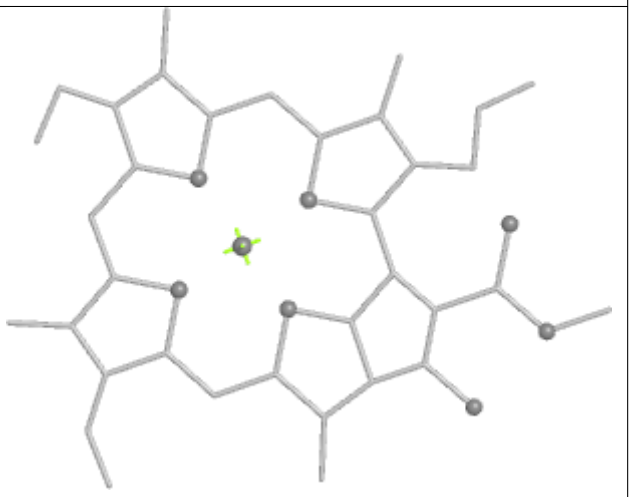
Bond lengths



Bond angles

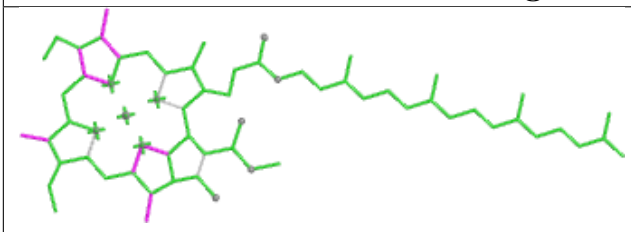


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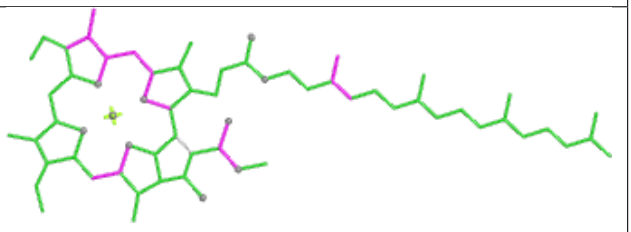


Rings

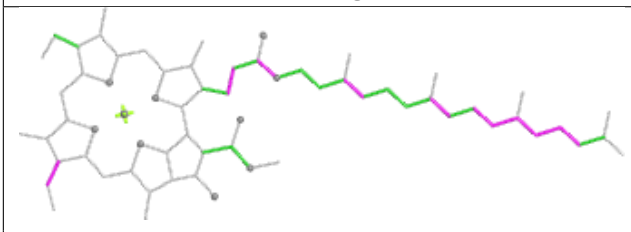
Ligand CLA B 831



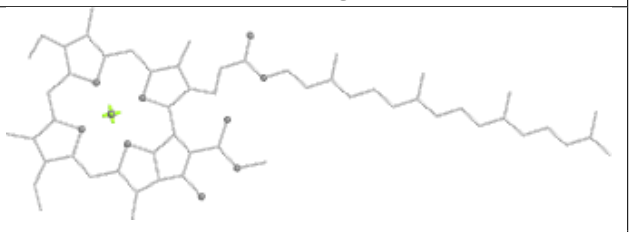
Bond lengths



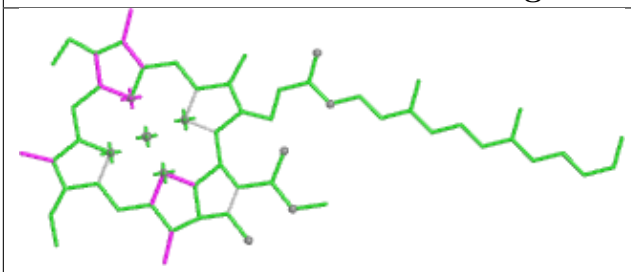
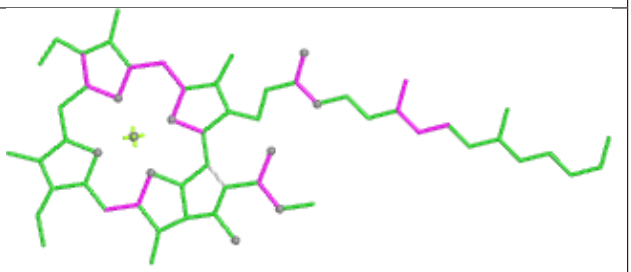
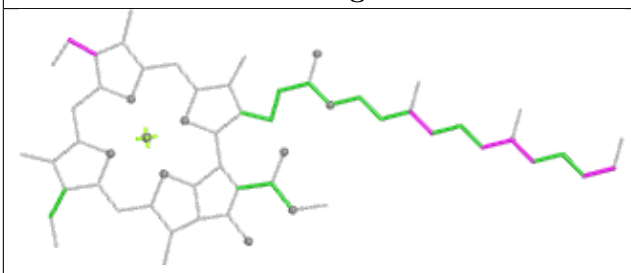
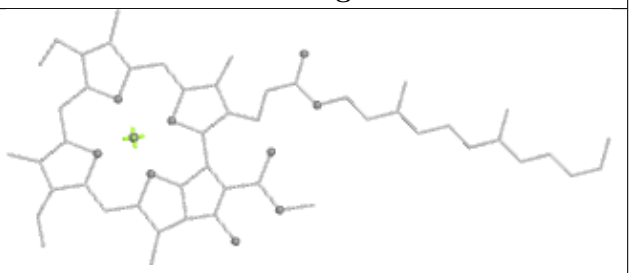
Bond angles

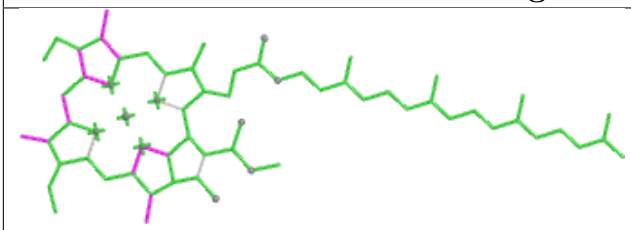
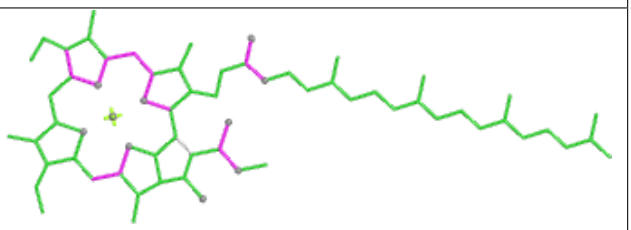
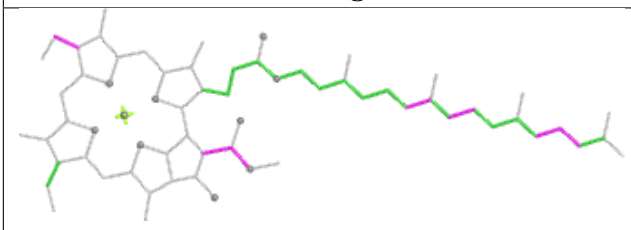
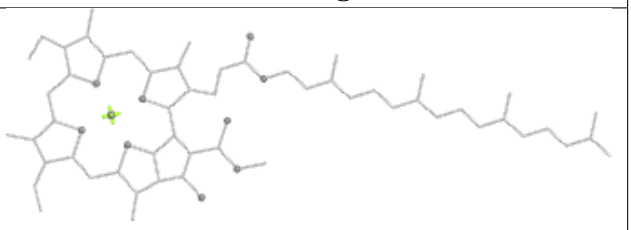


Torsions

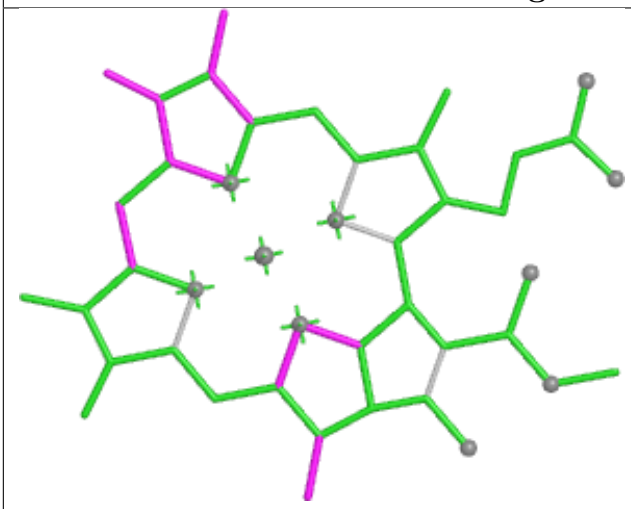


Rings

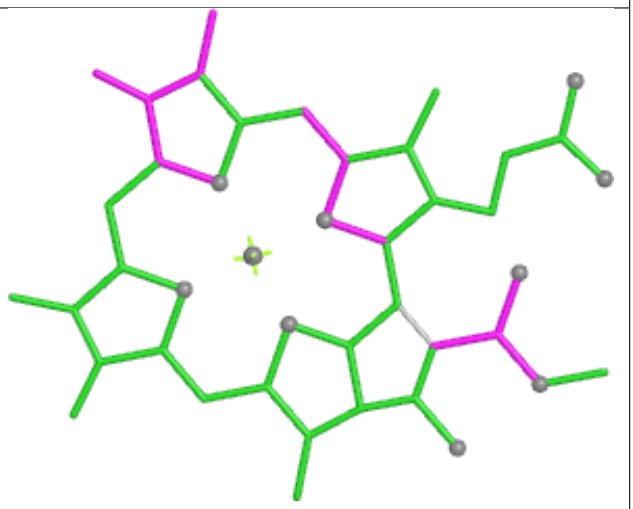
Ligand CLA B 817	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 6 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

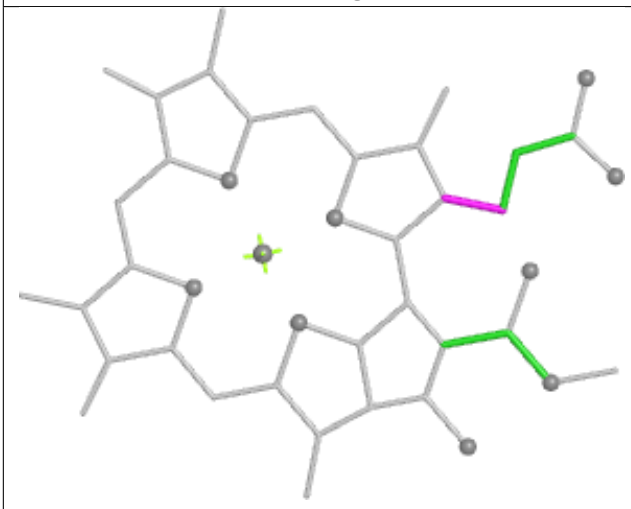
Ligand CLA 7 616



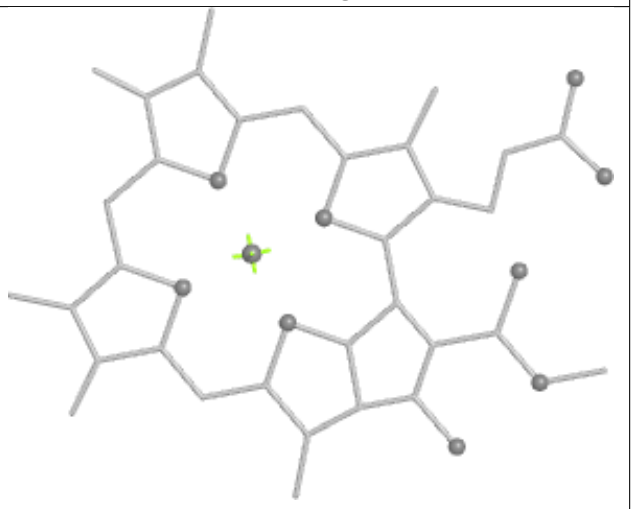
Bond lengths



Bond angles

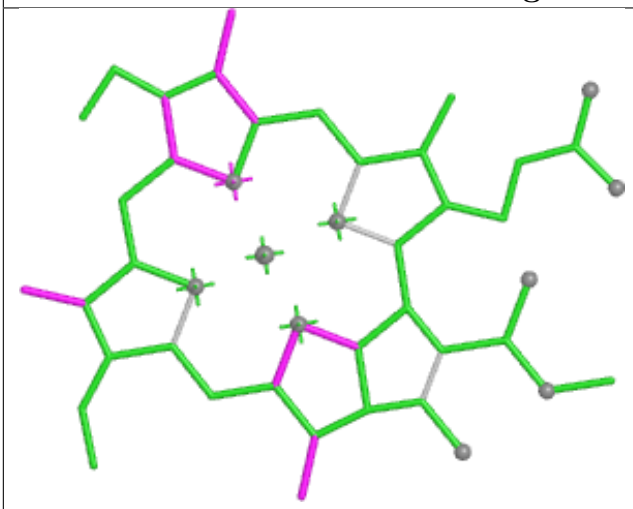


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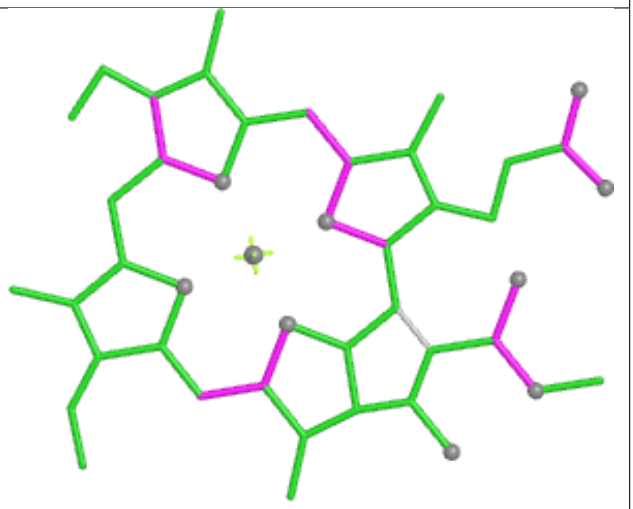


Rings

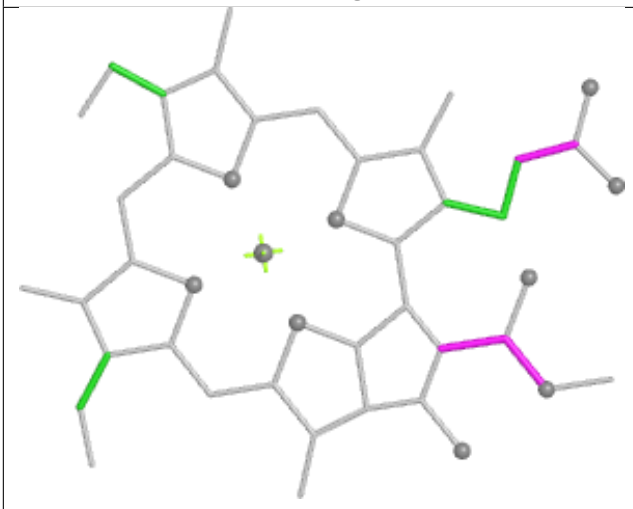
Ligand CLA K 204



Bond lengths



Bond angles

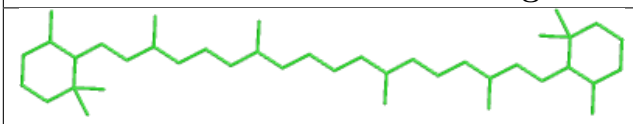


Torsions

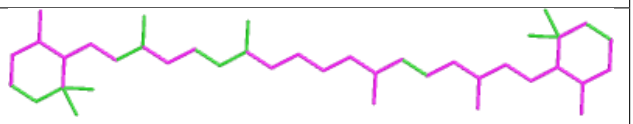


Rings

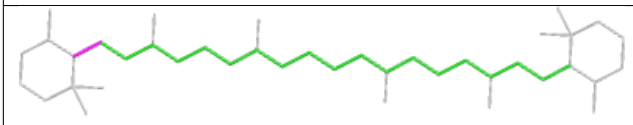
Ligand BCR A 856



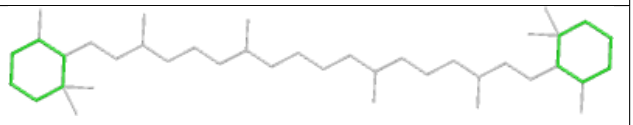
Bond lengths



Bond angles

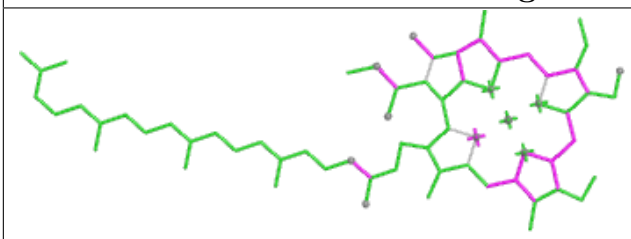


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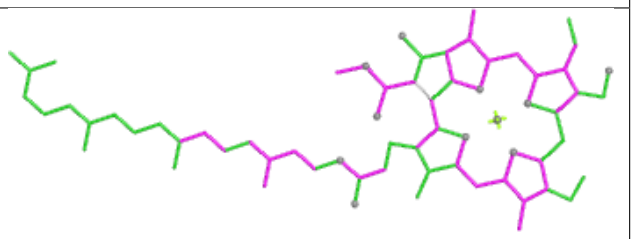


Rings

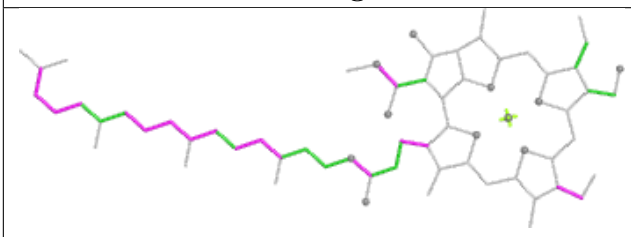
Ligand CHL W 601



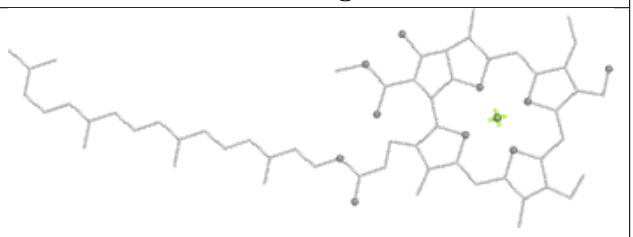
Bond lengths



Bond angles

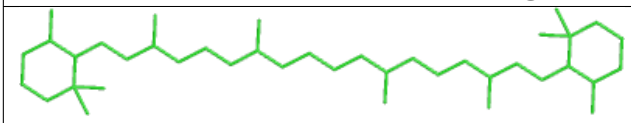


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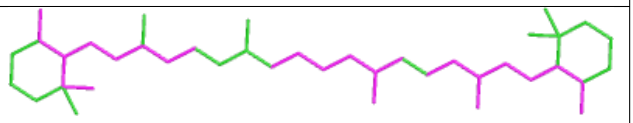


Rings

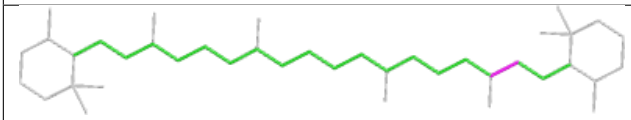
Ligand BCR A 848



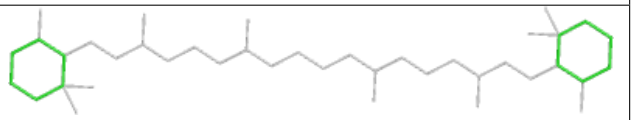
Bond lengths



Bond angles

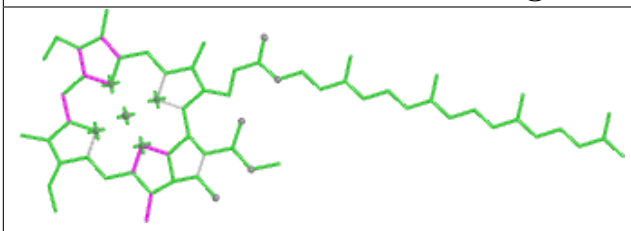


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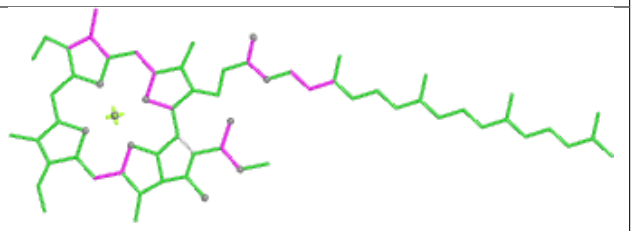


Rings

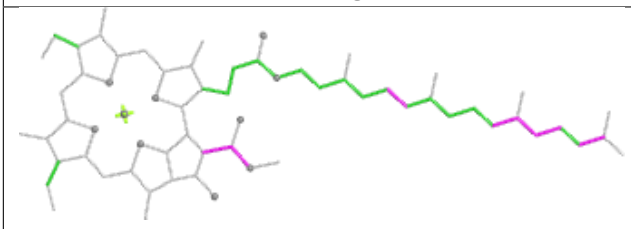
Ligand CLA Z 610



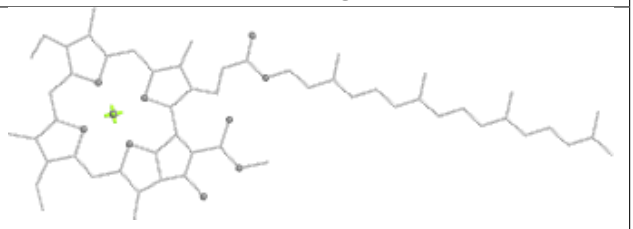
Bond lengths



Bond angles

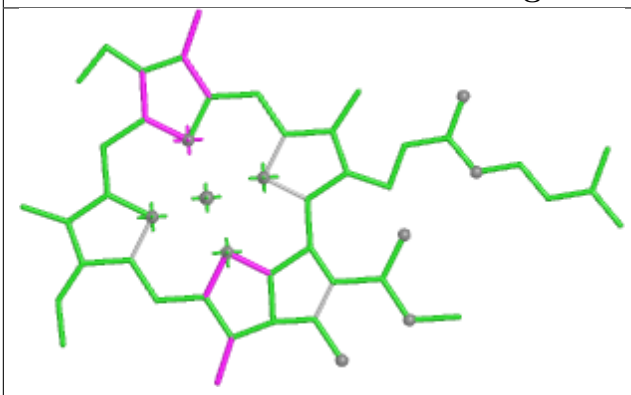


Torsions

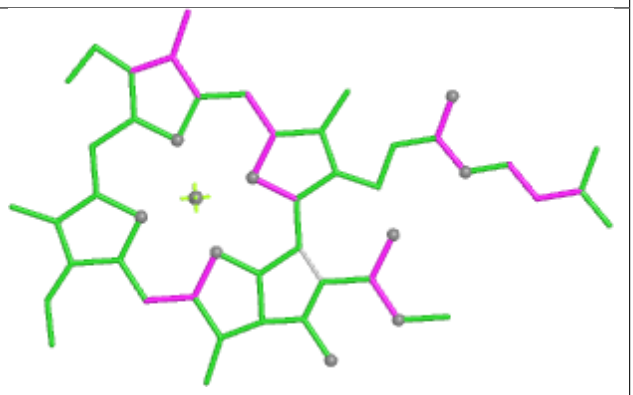


Rings

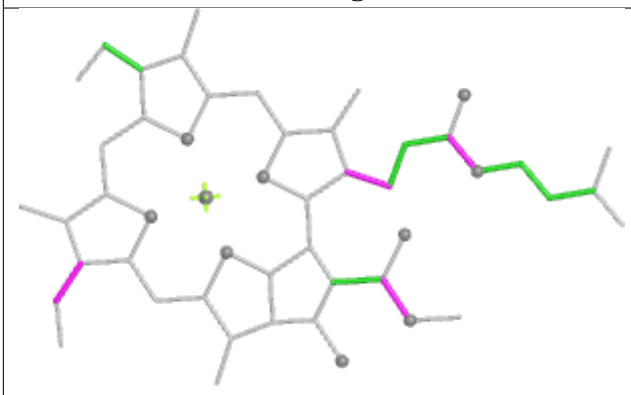
Ligand CLA A 838



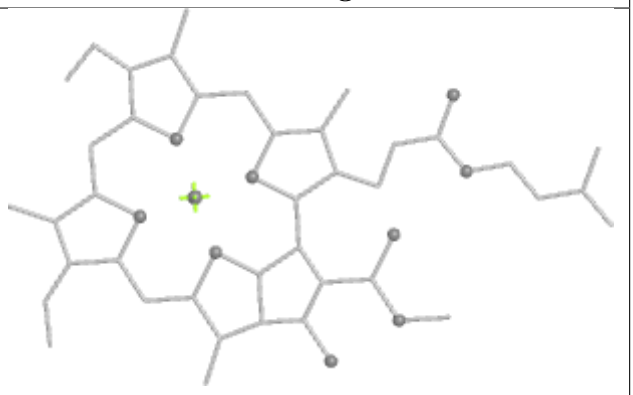
Bond lengths



Bond angles

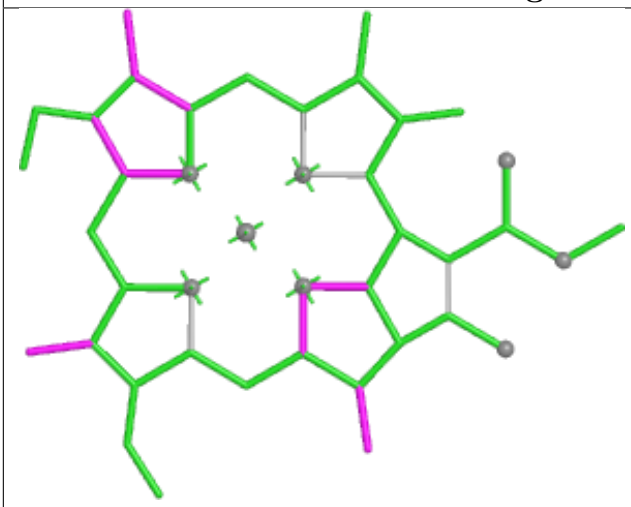


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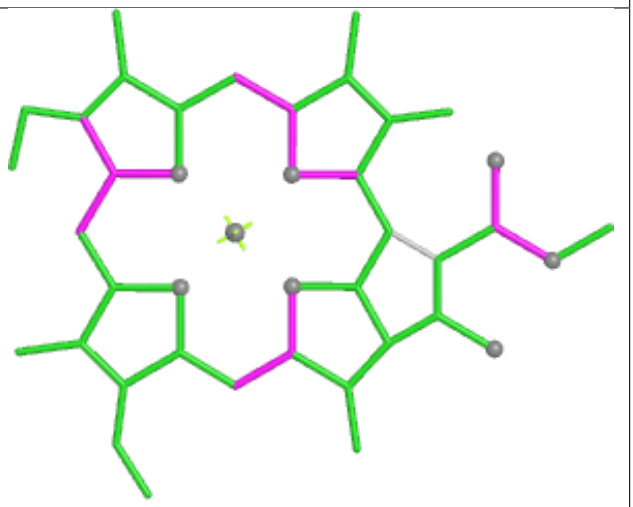


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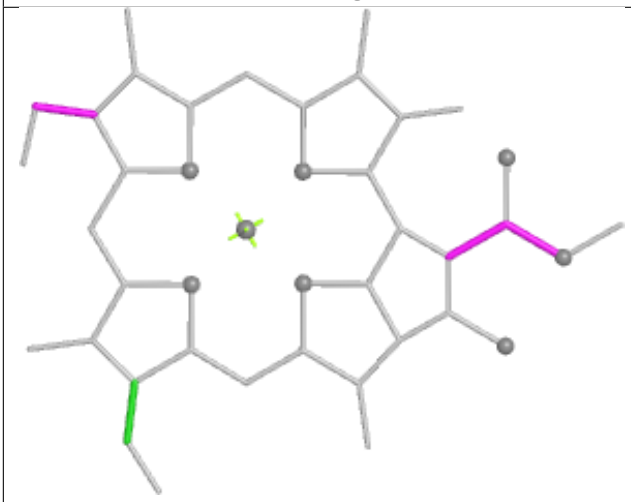
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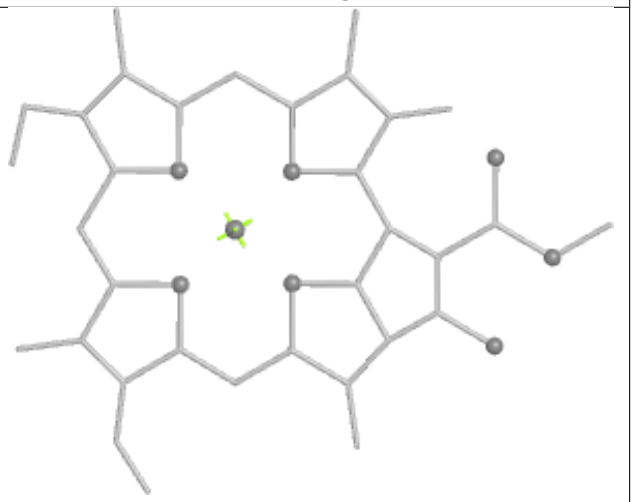
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Bond angles

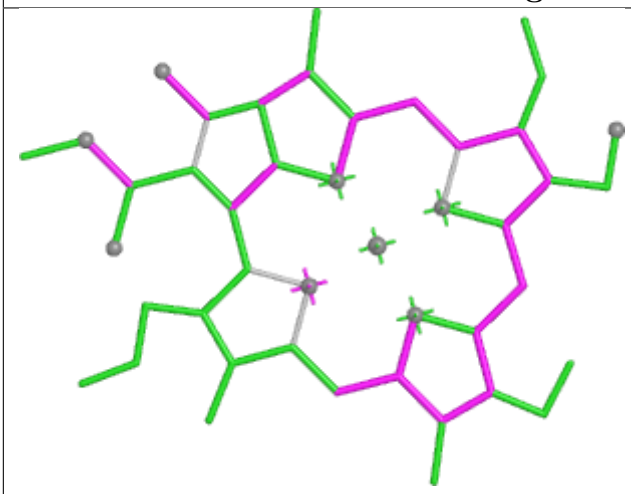


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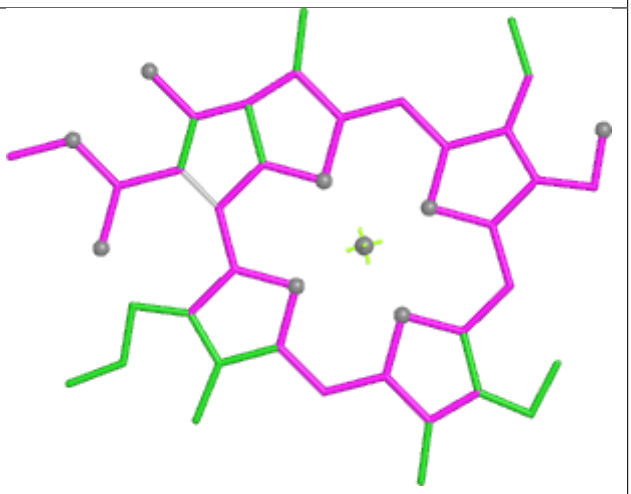


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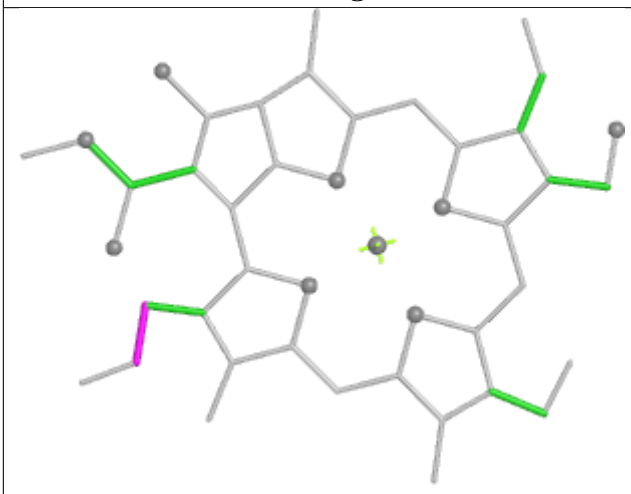
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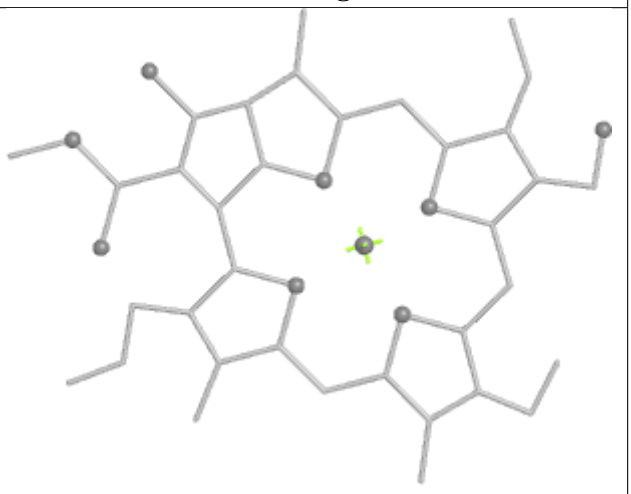
Bond lengths



Bond angles

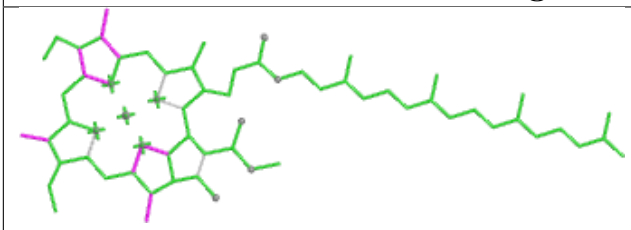


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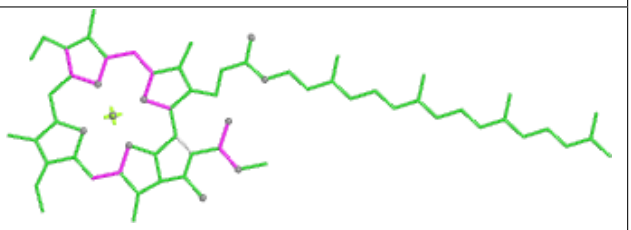


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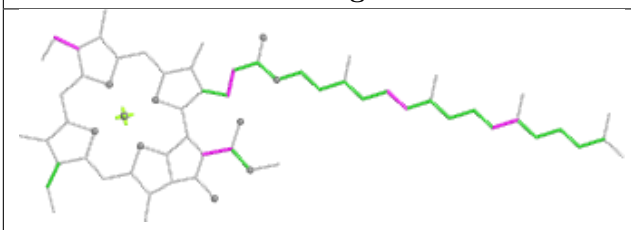
Ligand CLA 9 613



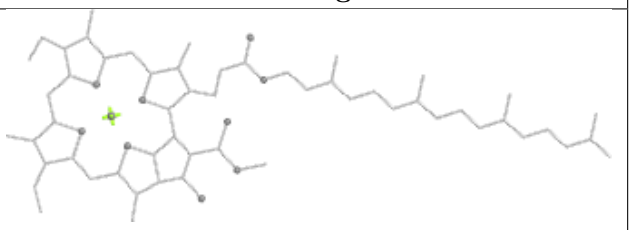
Bond lengths



Bond angles

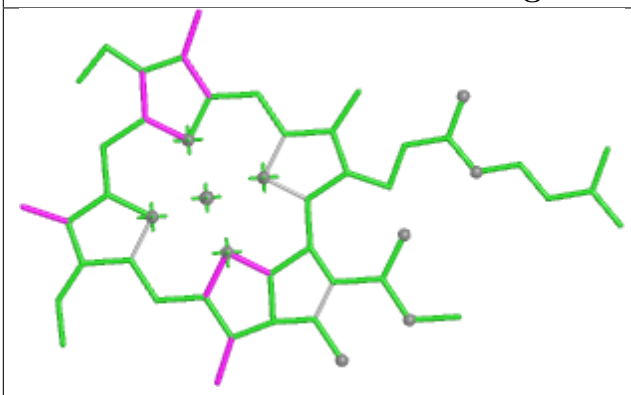


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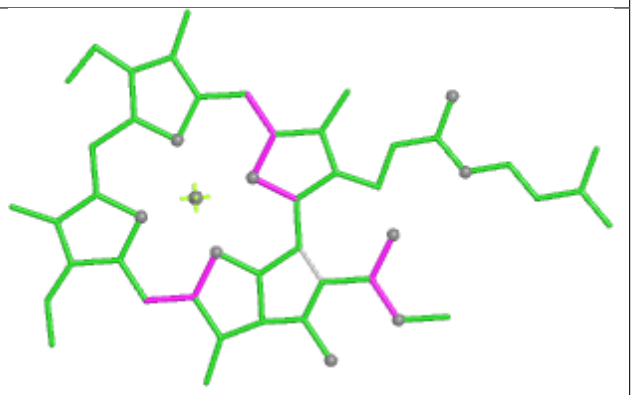


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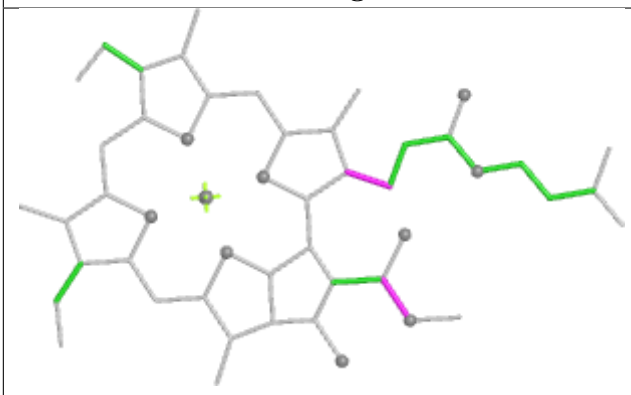
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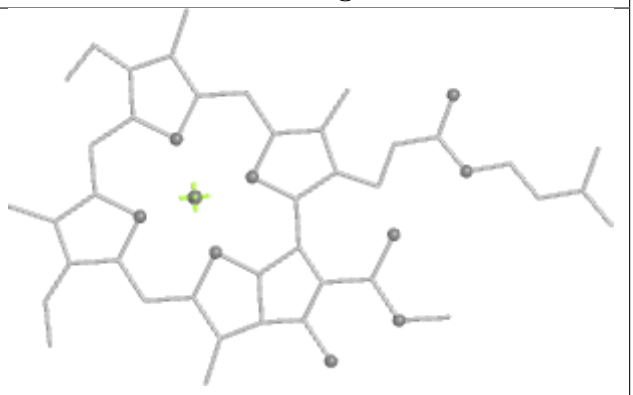
Bond lengths



Bond angles

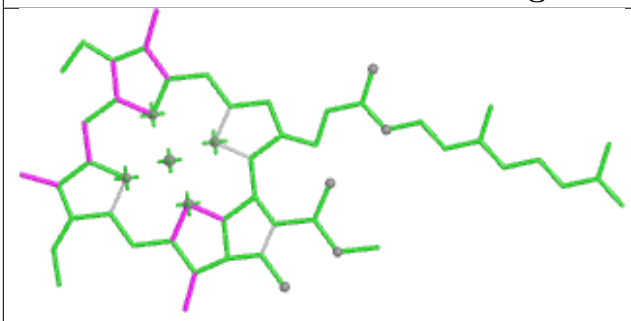


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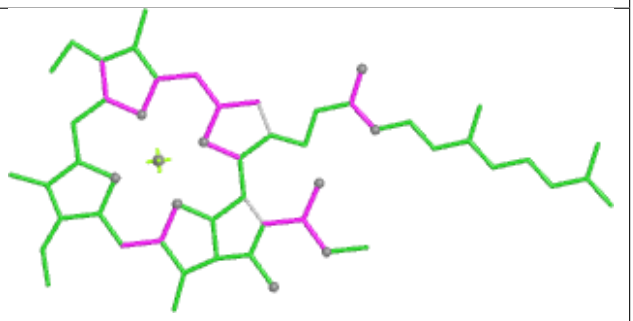


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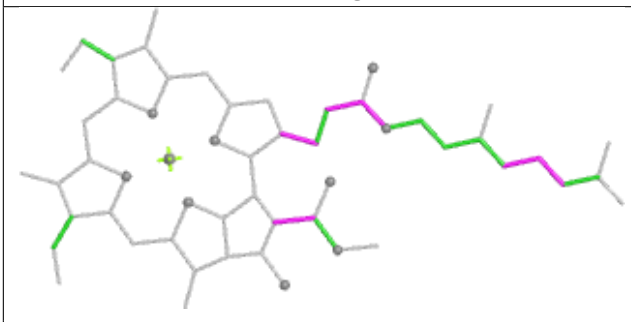
Ligand CLA a 614



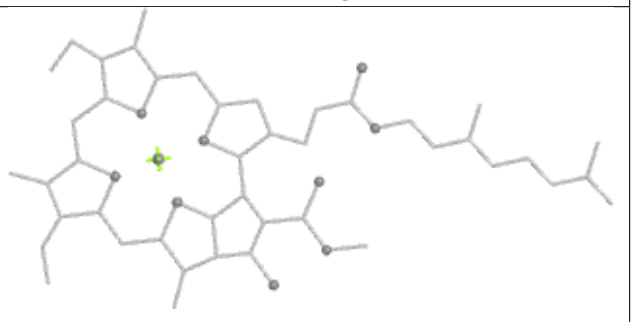
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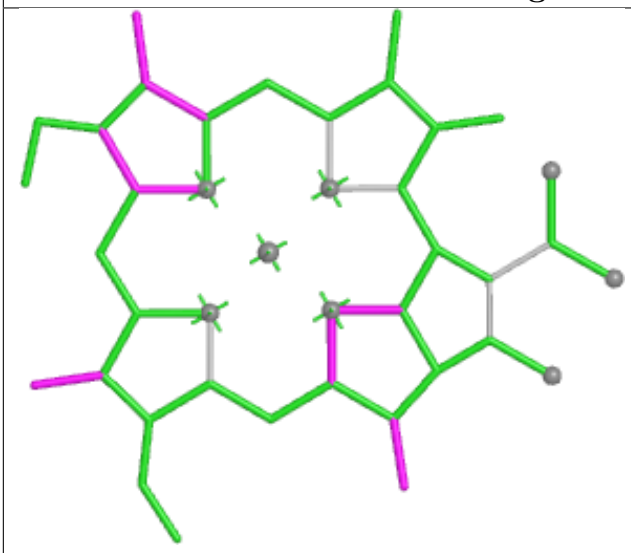


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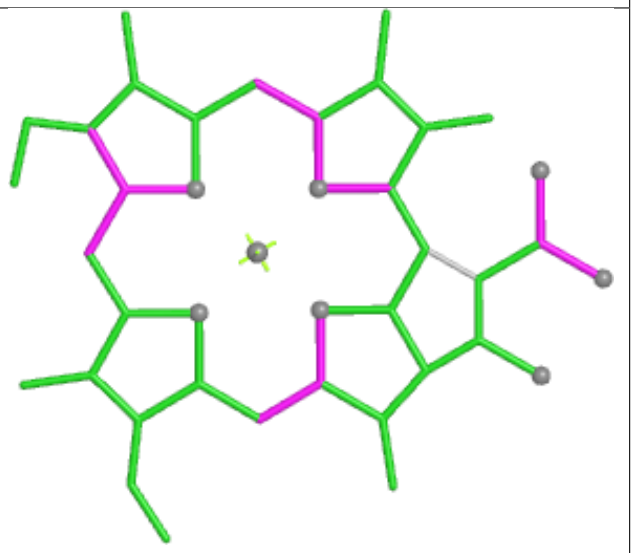


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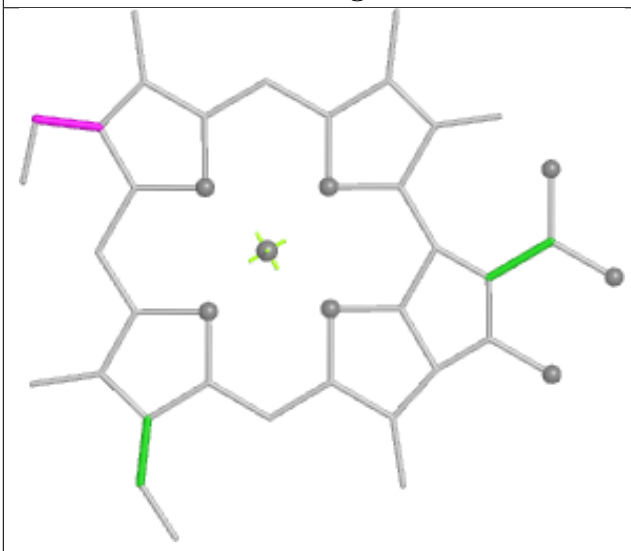
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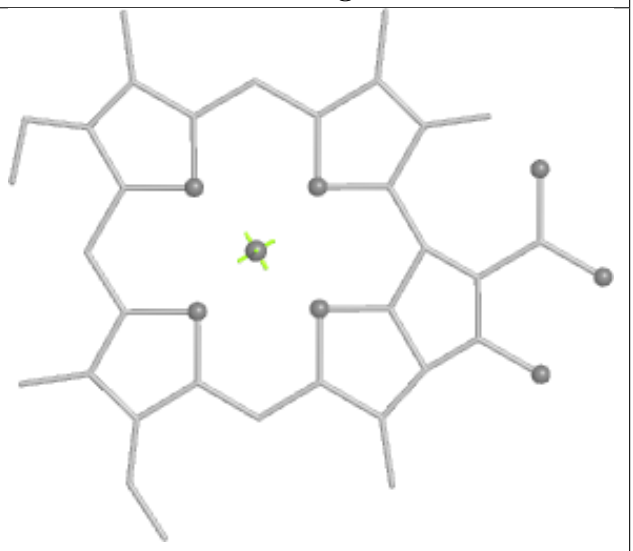
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Bond angles

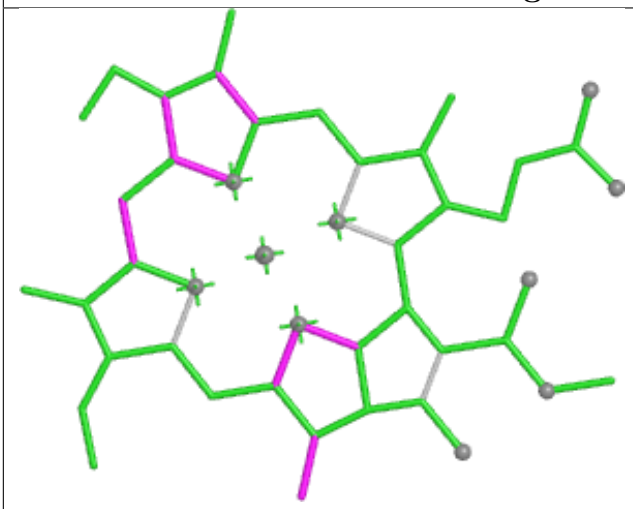


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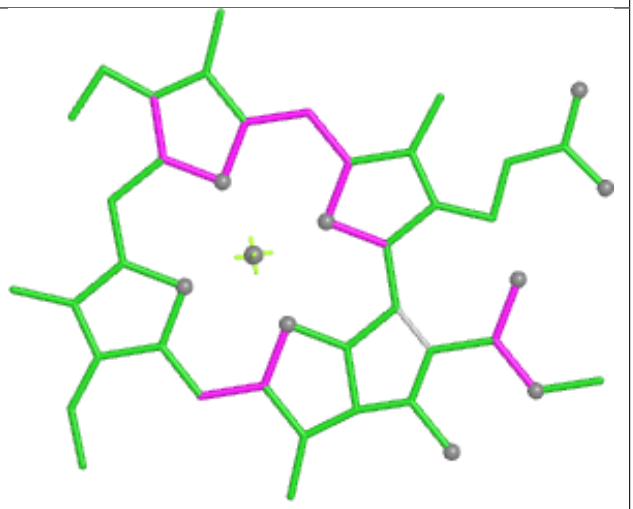


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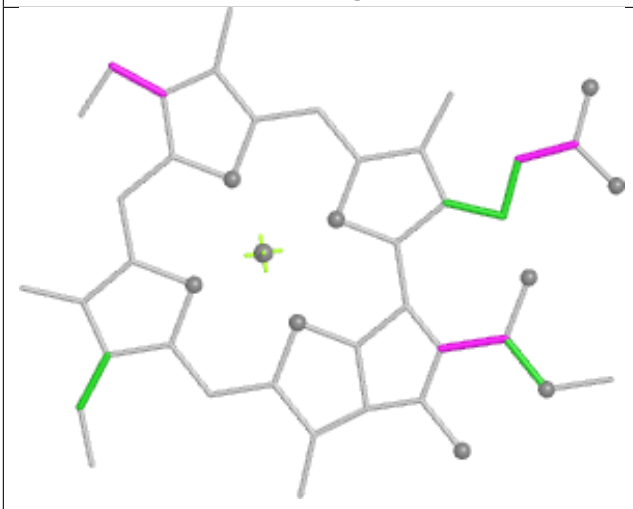
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Bond lengths



Bond angles

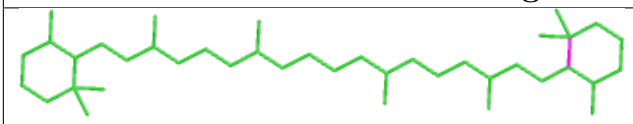


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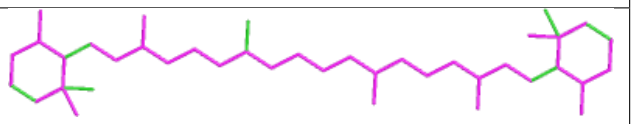


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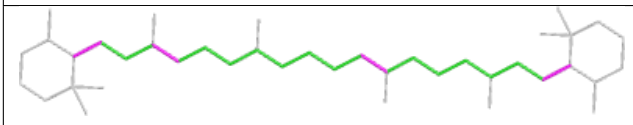
Ligand BCR A 852



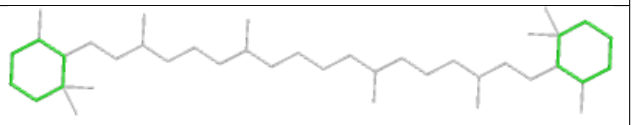
Bond lengths



Bond angles

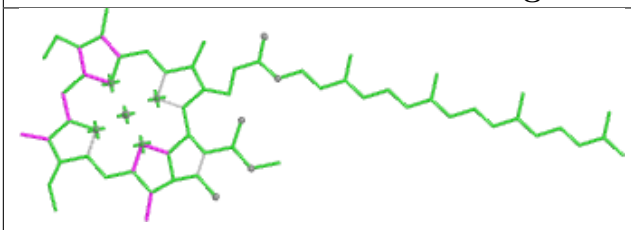


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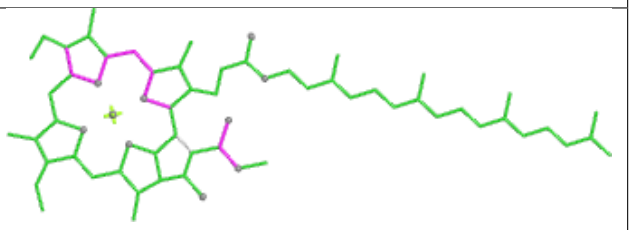


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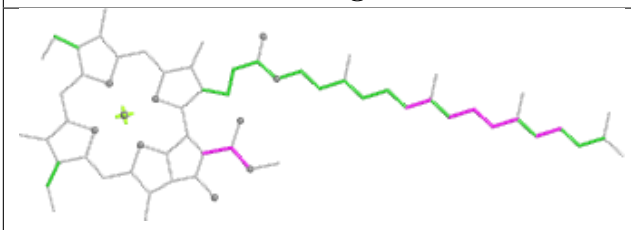
Ligand CLA X 602



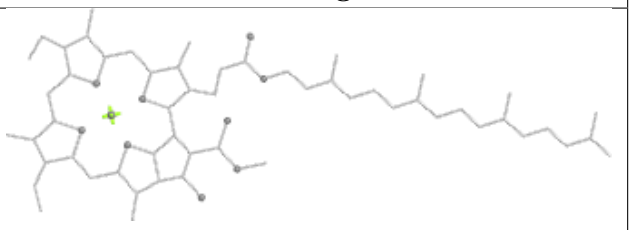
Bond lengths



Bond angles

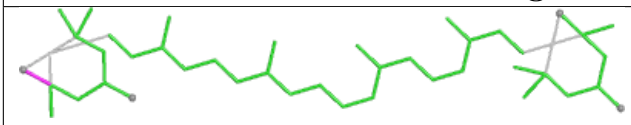


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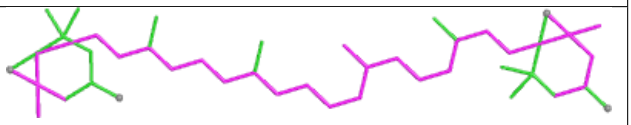


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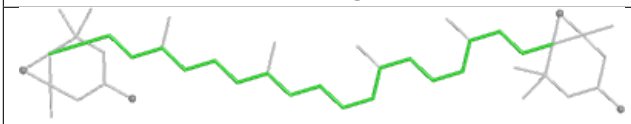
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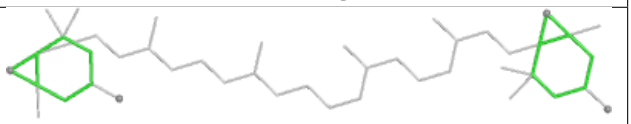
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Bond angles

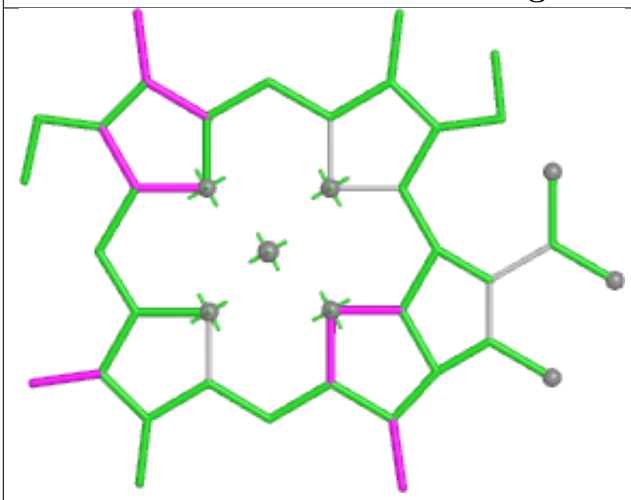


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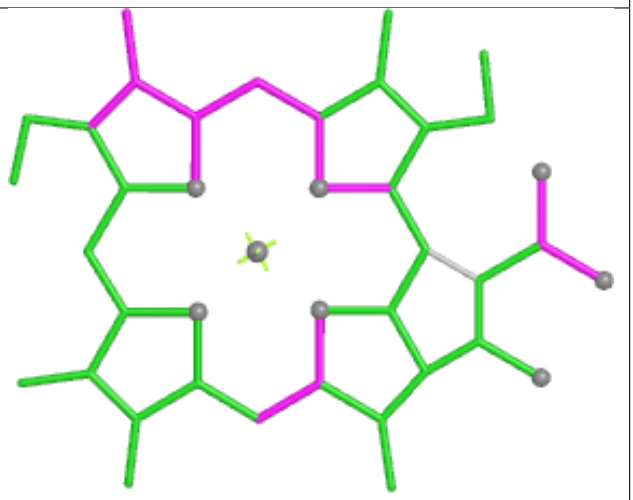


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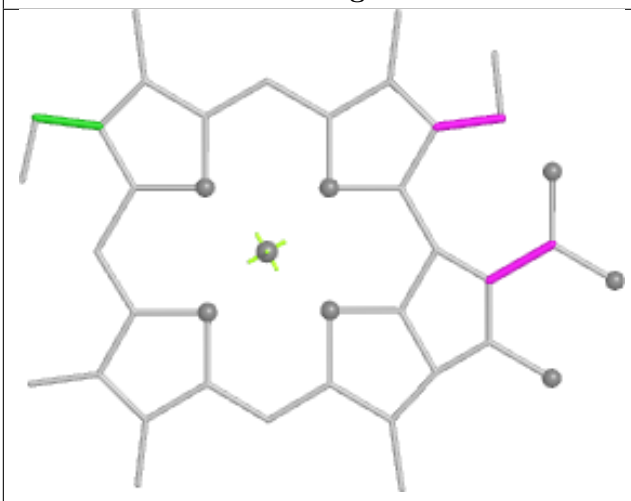
Ligand CLA 3 615



Bond lengths



Bond angles

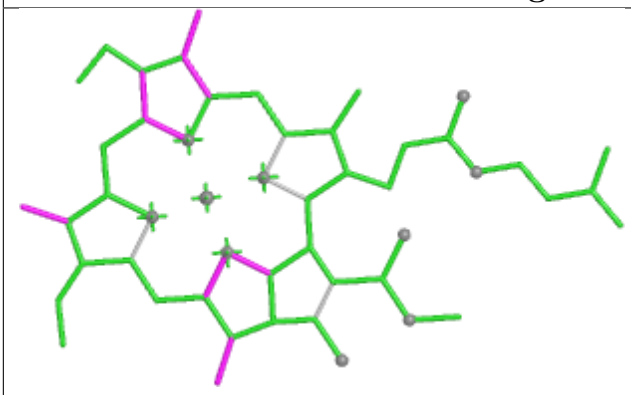


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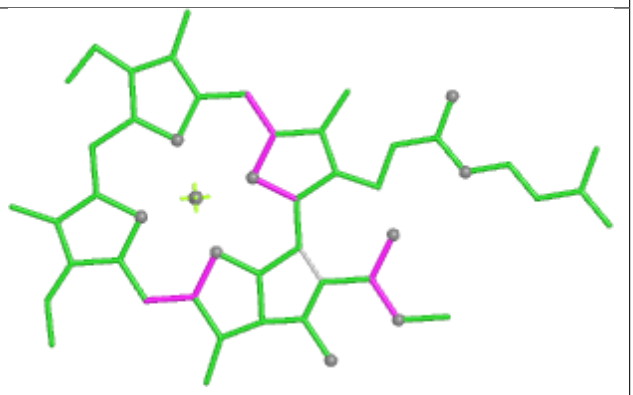


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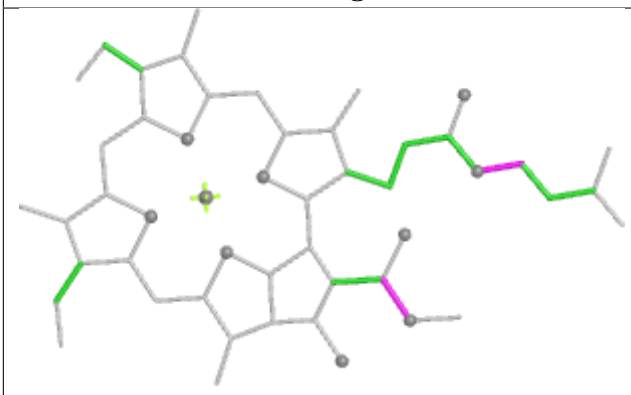
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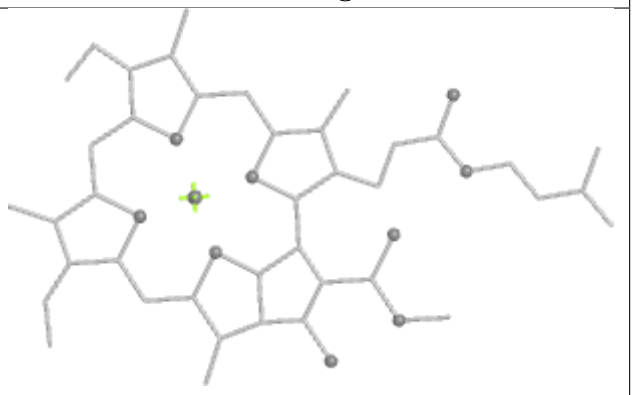
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Bond angles

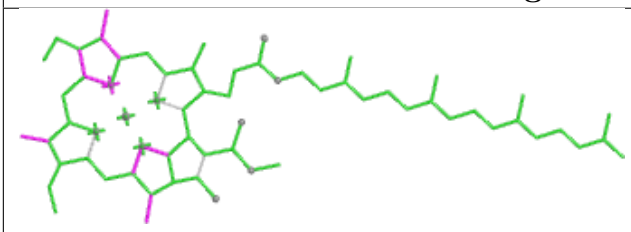


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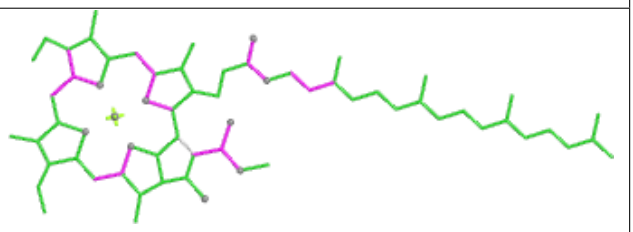


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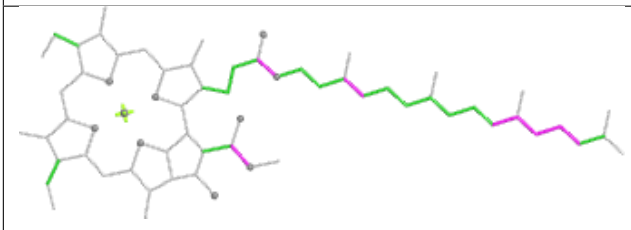
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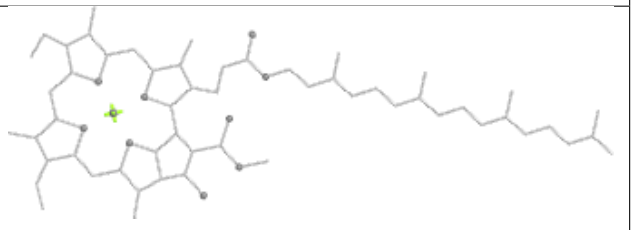
Bond lengths



Bond angles

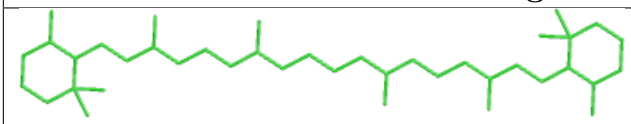


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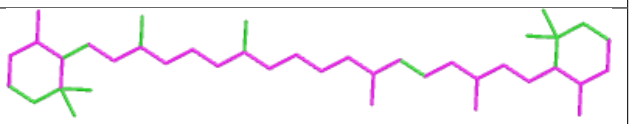


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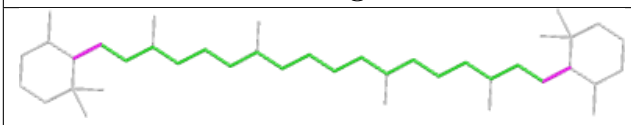
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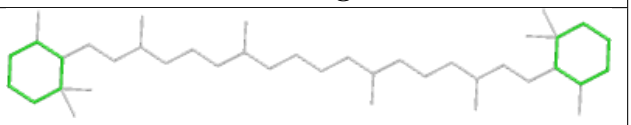
Bond lengths



Bond angles



Torsions

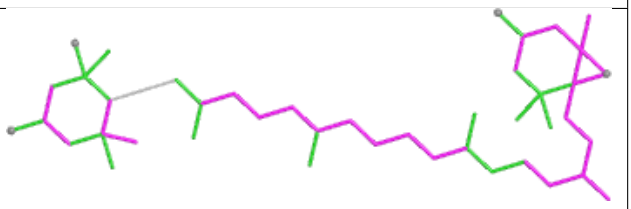


Rings

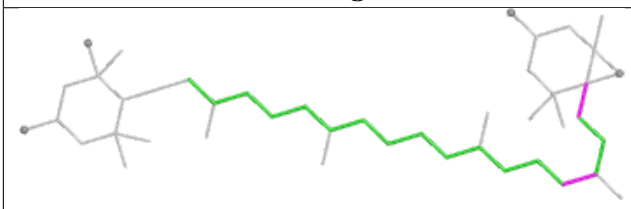
Ligand NEX X 1623



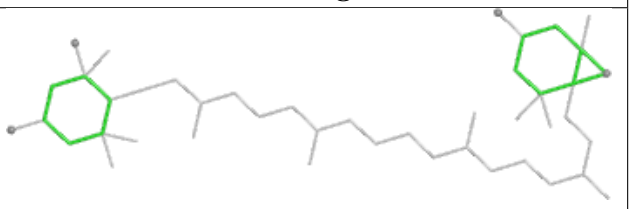
Bond lengths



Bond angles

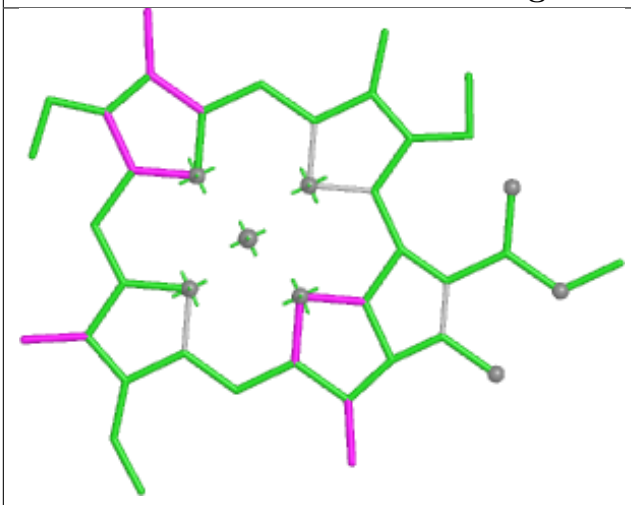


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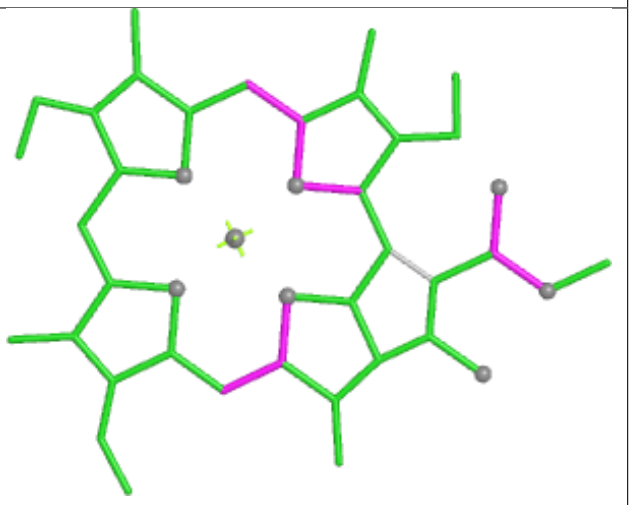


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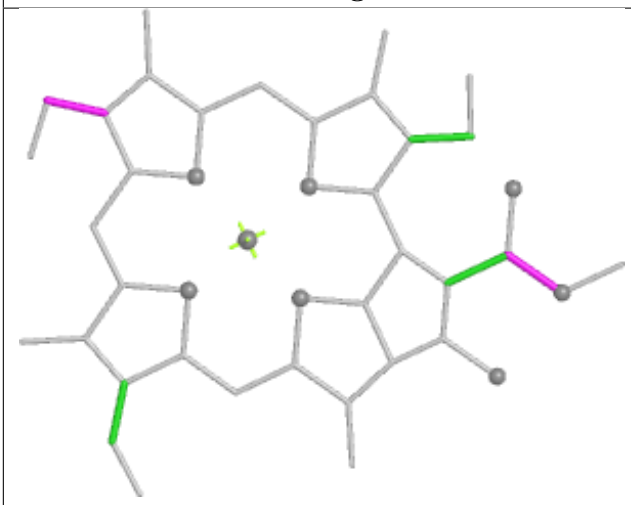
Ligand CLA 7 607



Bond lengths



Bond angles

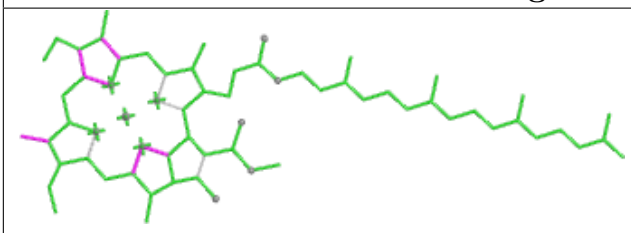


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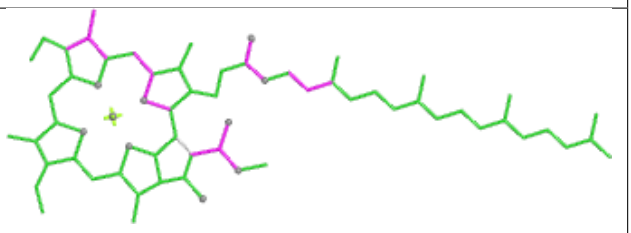


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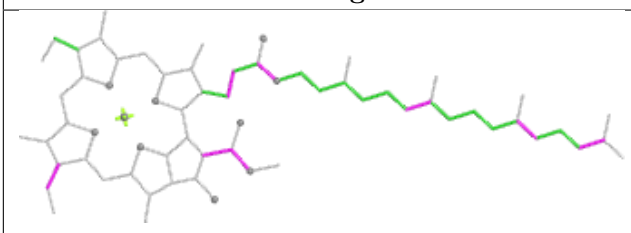
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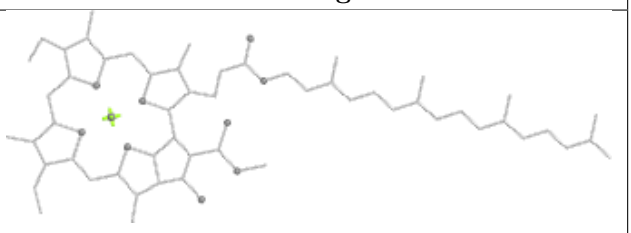
Bond lengths



Bond angles

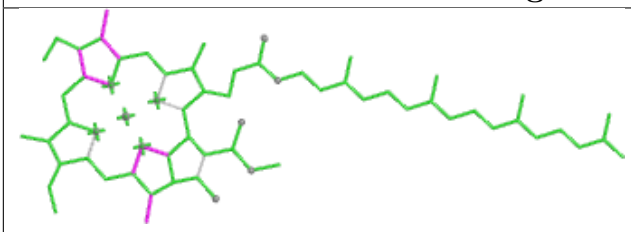


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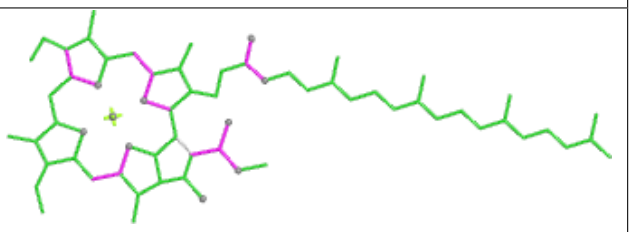


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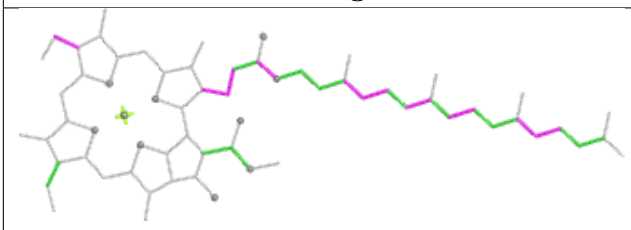
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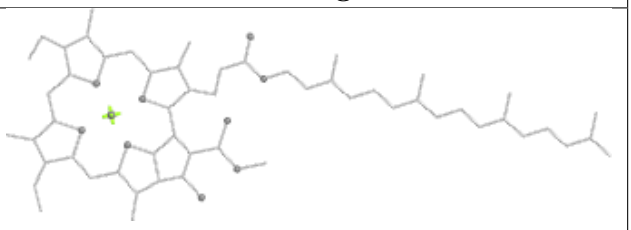
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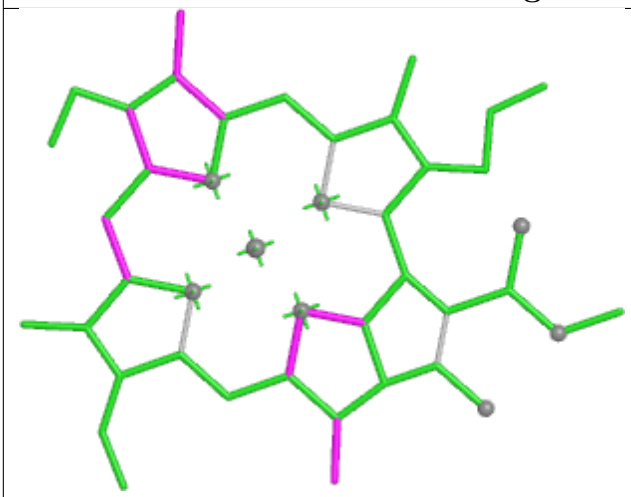


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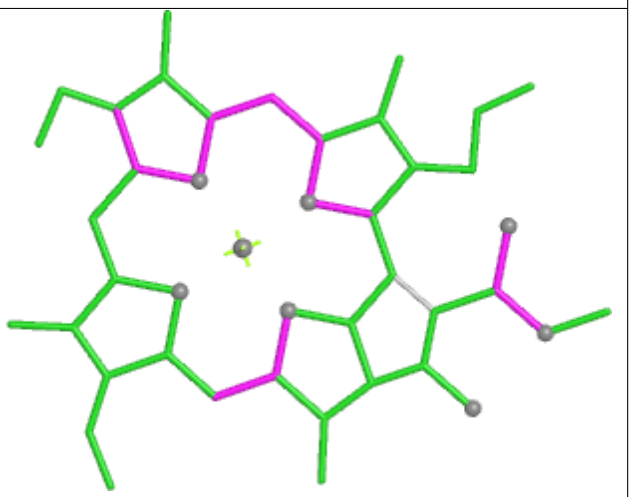


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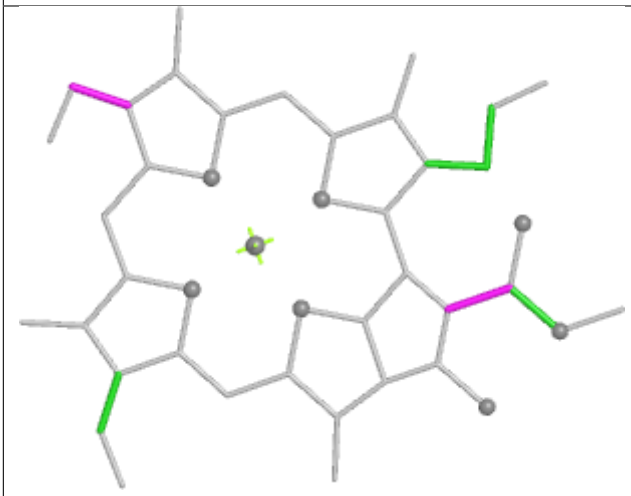
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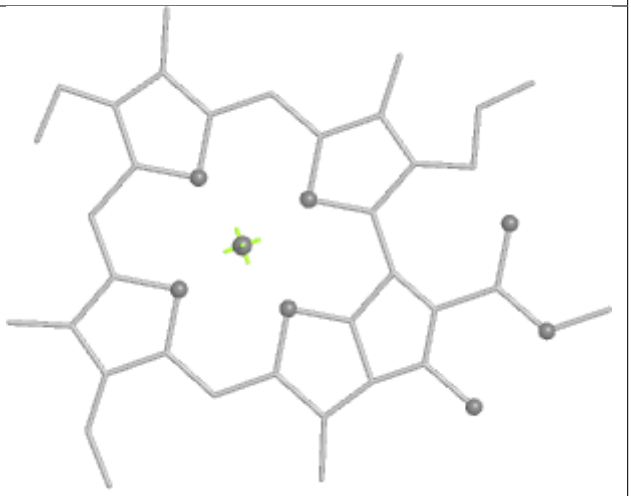
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Bond angles

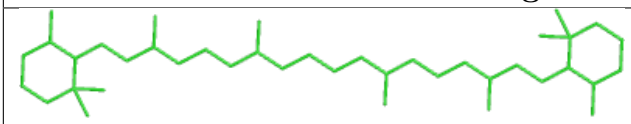


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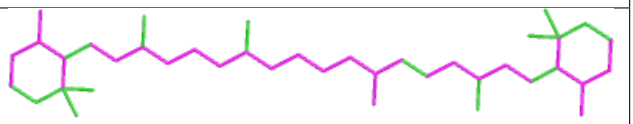


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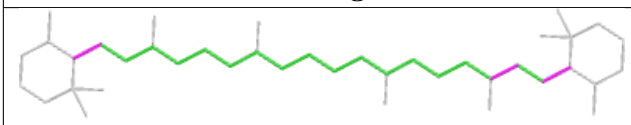
Ligand BCR A 849



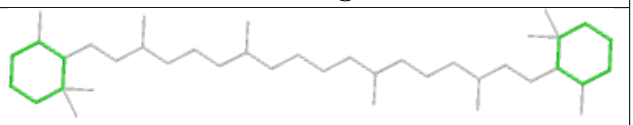
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Bond angles

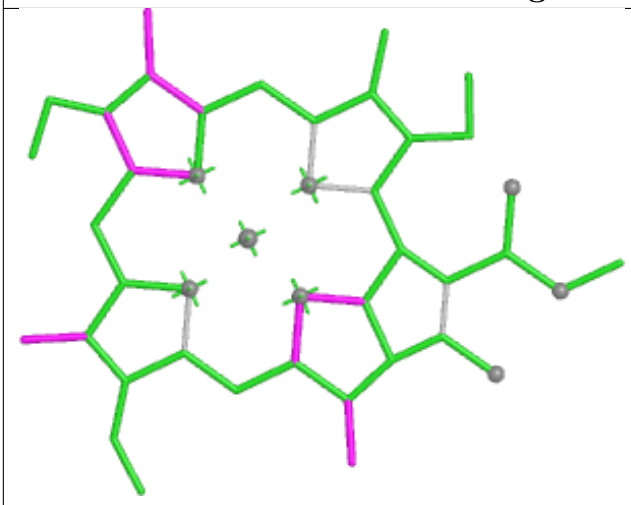


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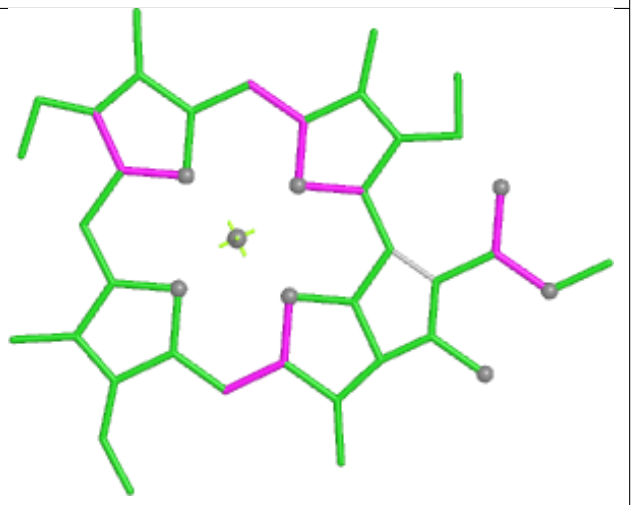


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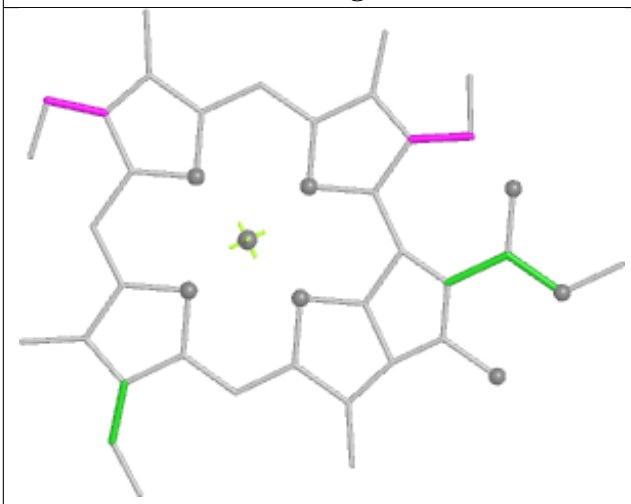
Ligand CLA 8 611



Bond lengths



Bond angles

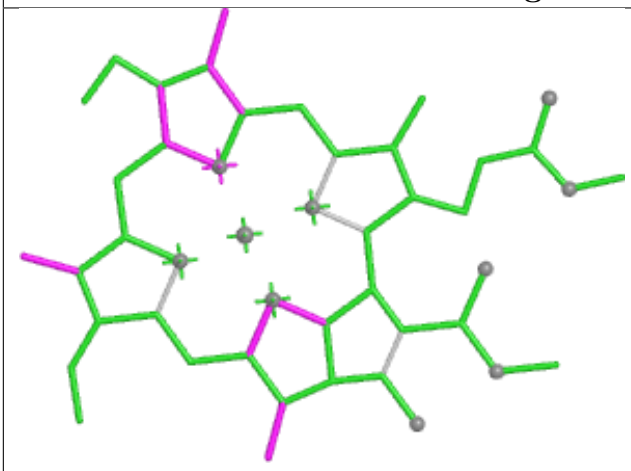


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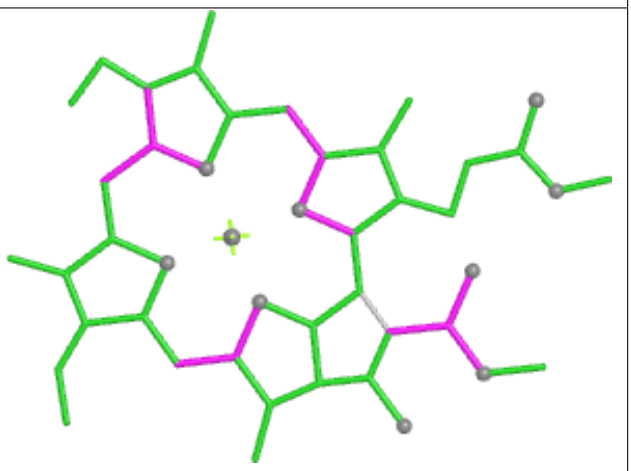


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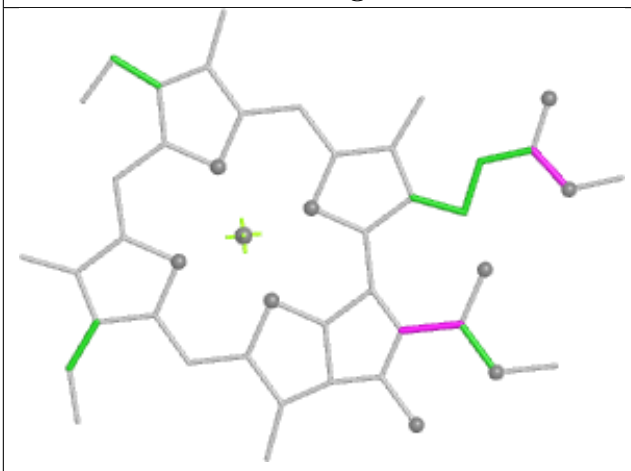
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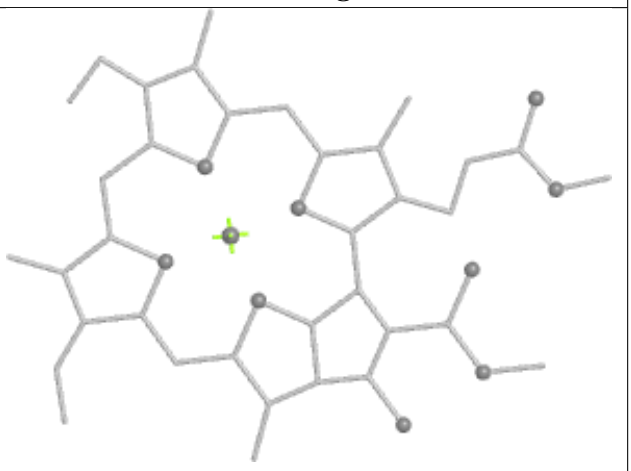
Bond lengths



Bond angles



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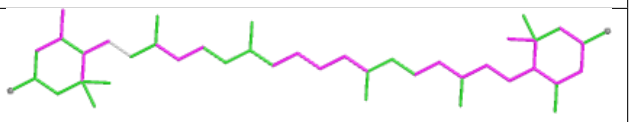


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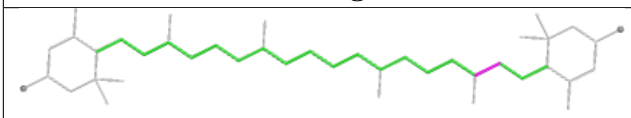
Ligand LUT V 1621



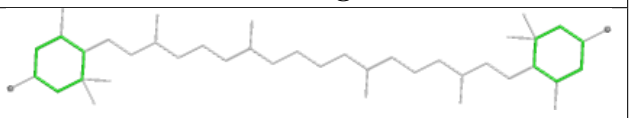
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Bond angles

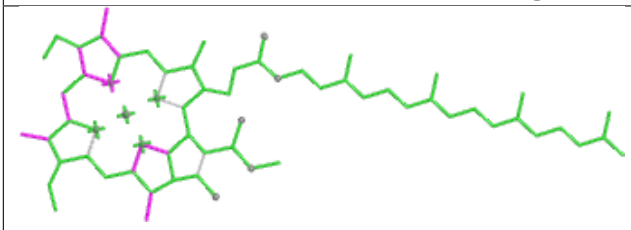


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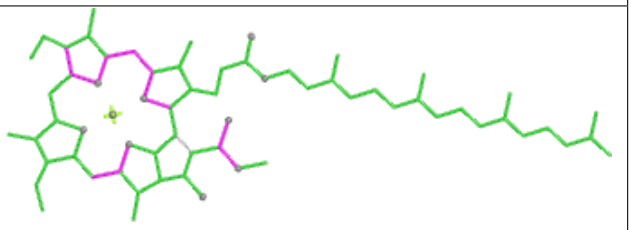


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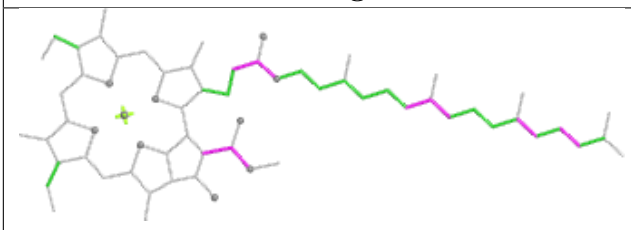
Ligand CLA 5 607



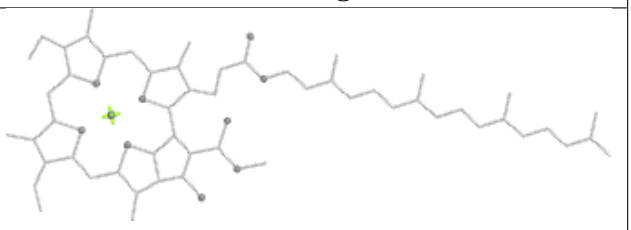
Bond lengths



Bond angles

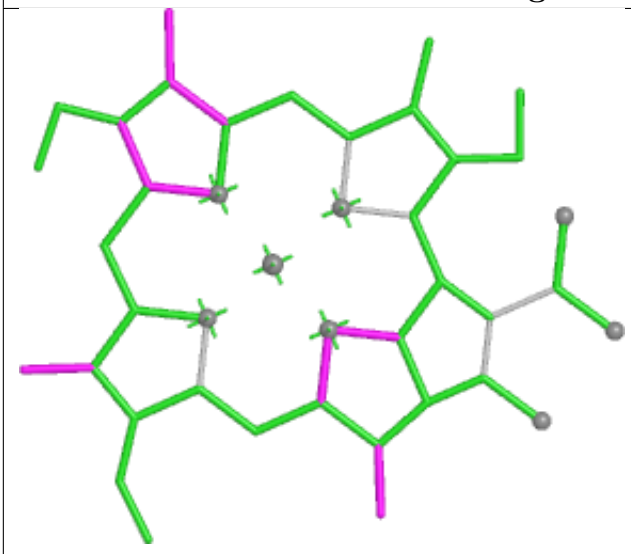


Torsions



Rings

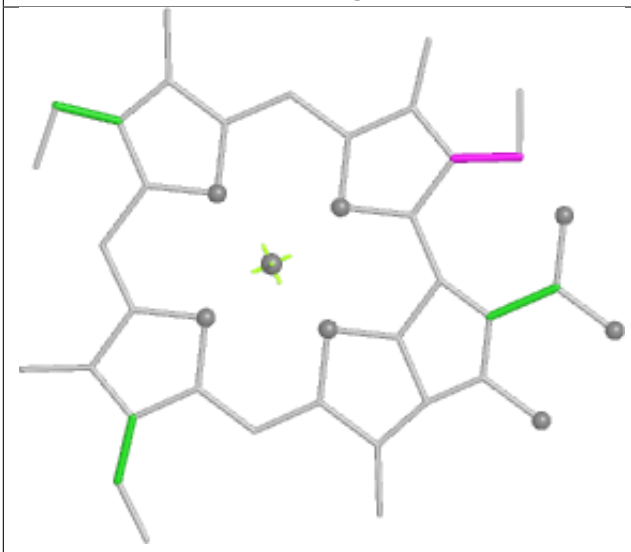
Ligand CLA 8 612



Bond lengths



Bond angles

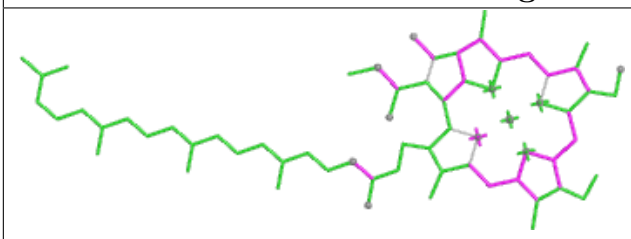


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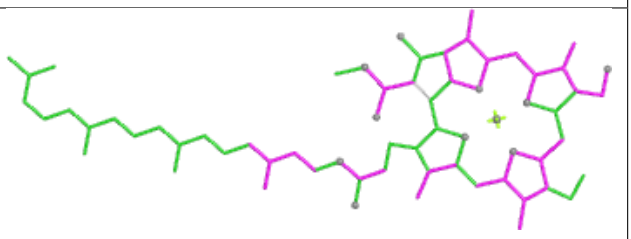


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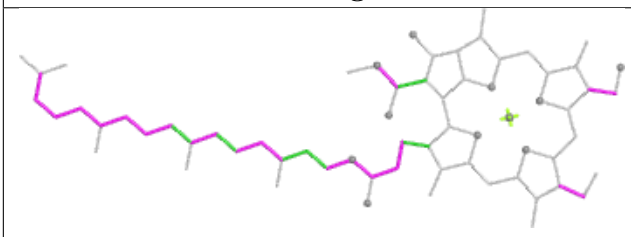
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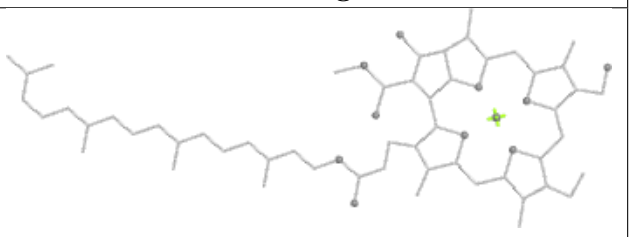
Bond lengths



Bond angles

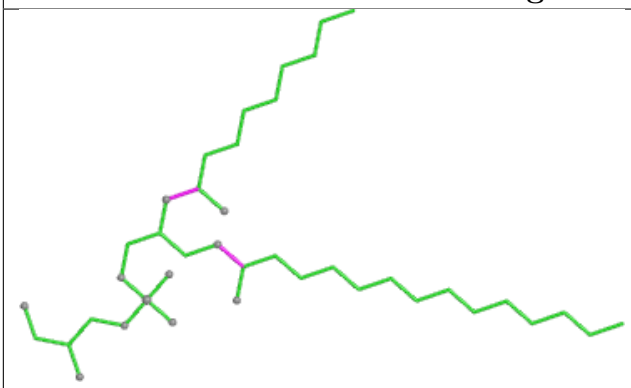


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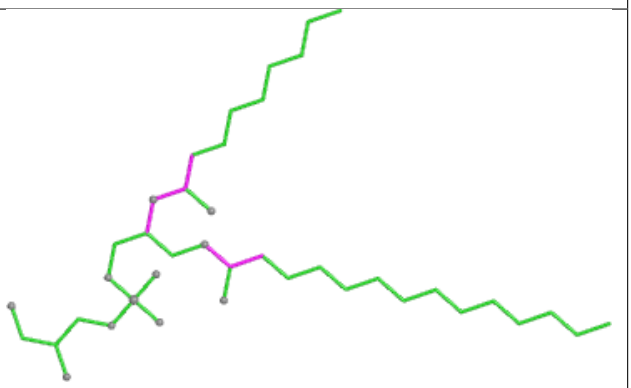


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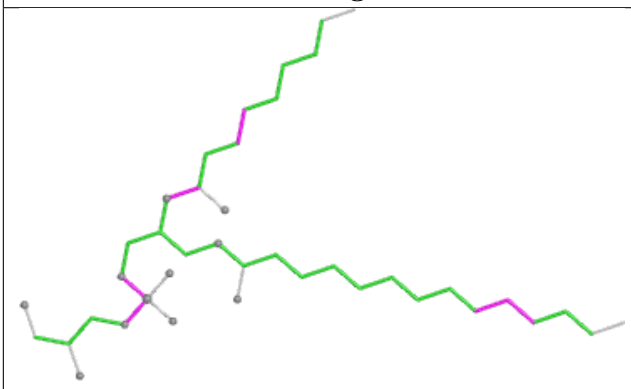
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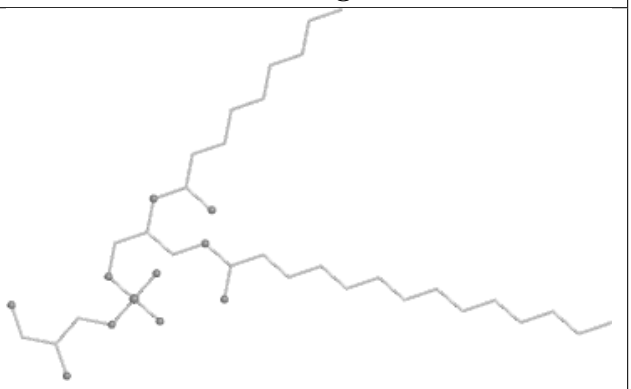
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Bond angles

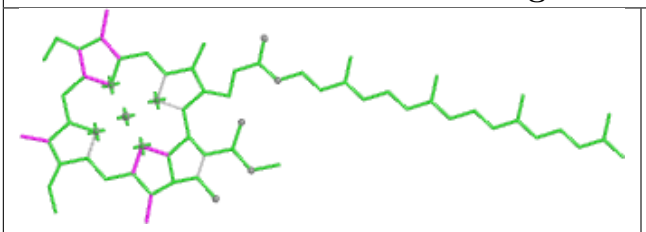


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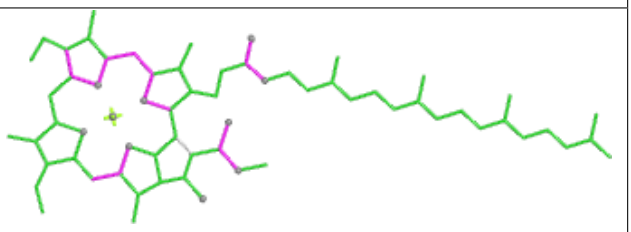


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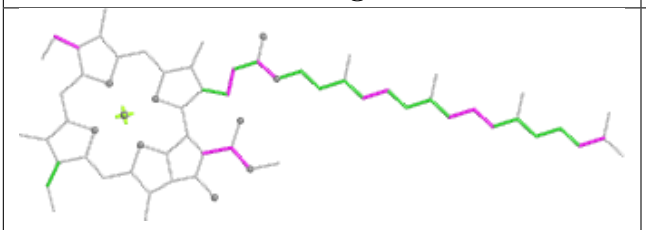
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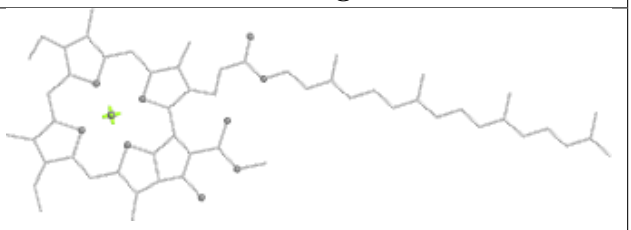
Bond lengths



Bond angles

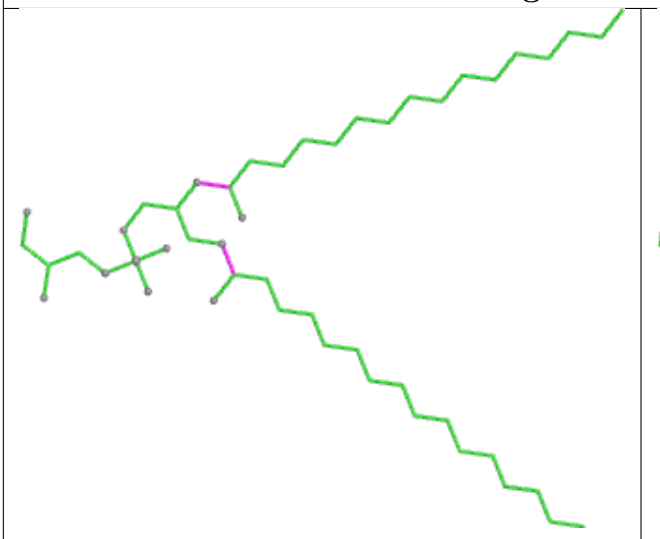


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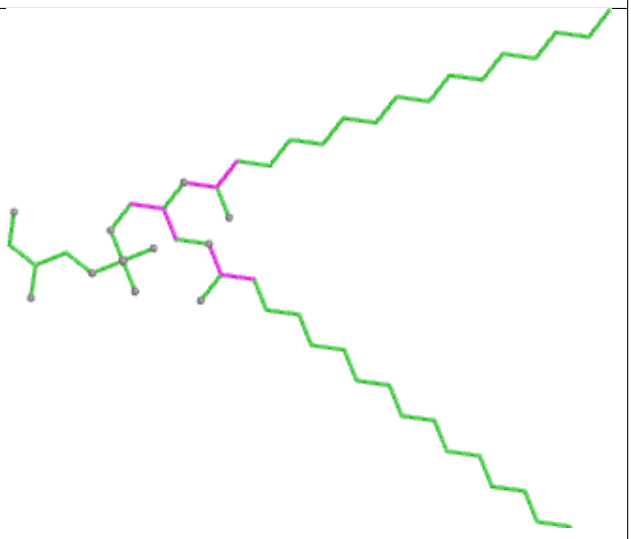


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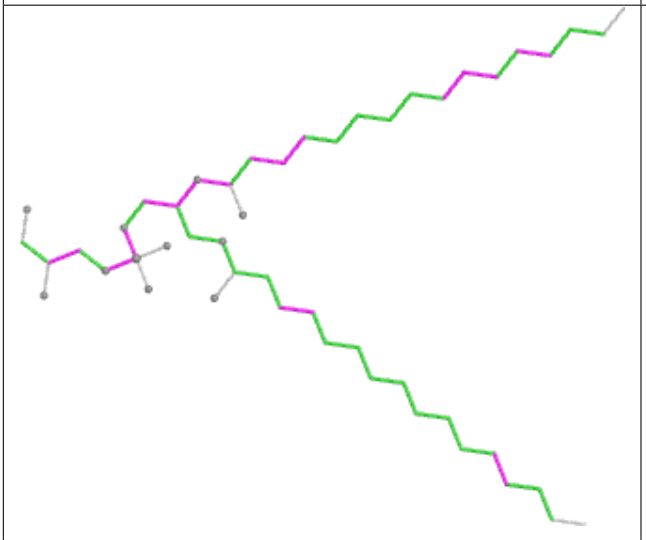
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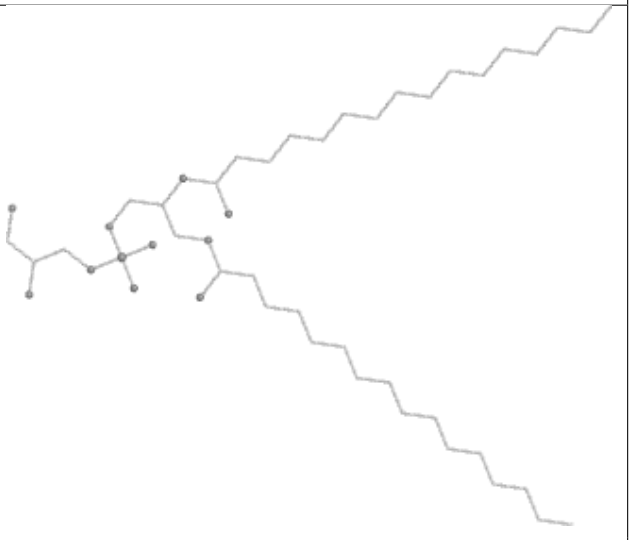
Bond lengths



Bond angles

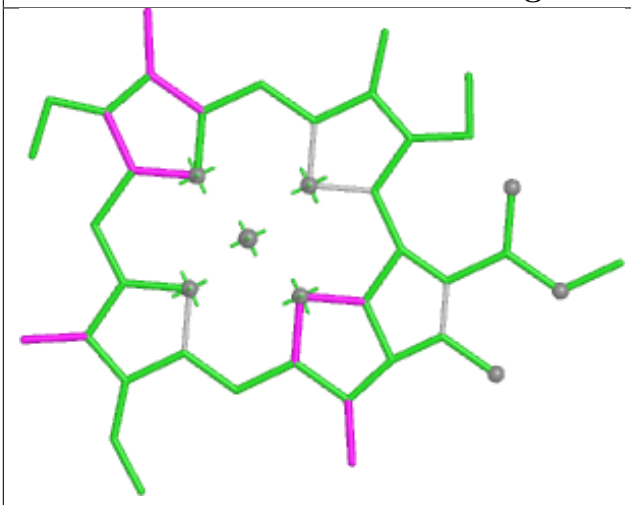


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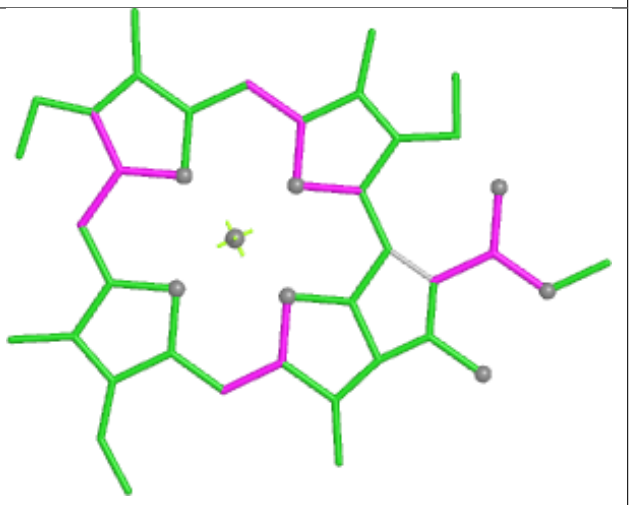


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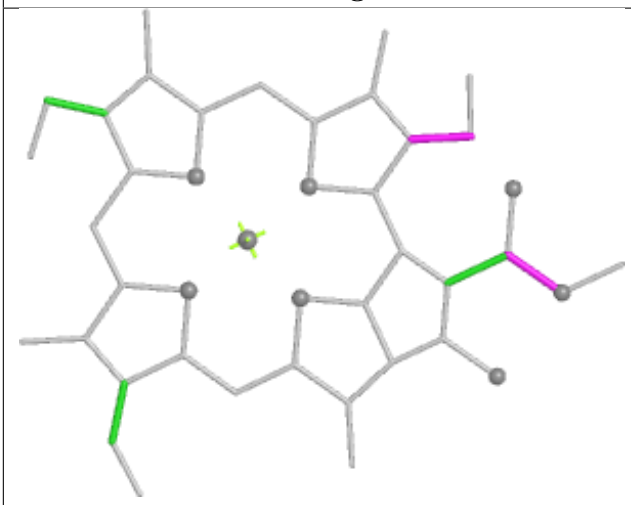
Ligand CLA B 822



Bond lengths



Bond angles

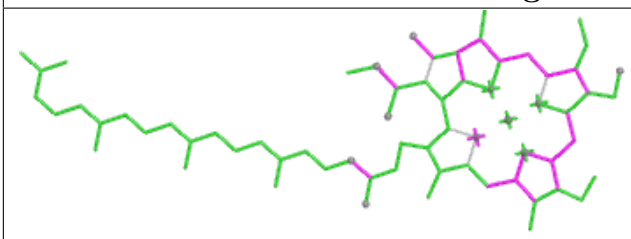


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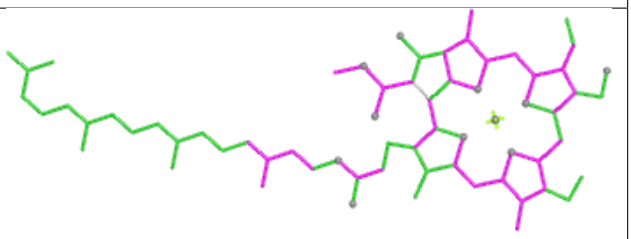


Rings

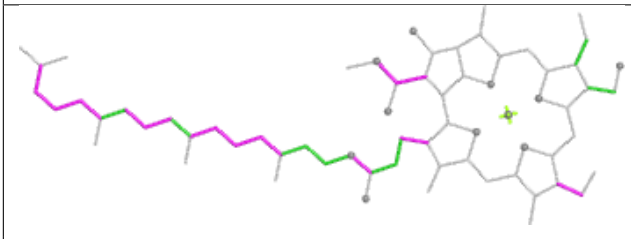
Ligand CHL U 601



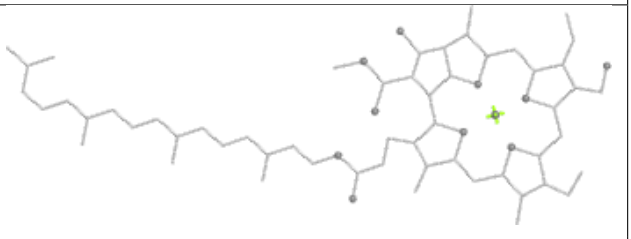
Bond lengths



Bond angles

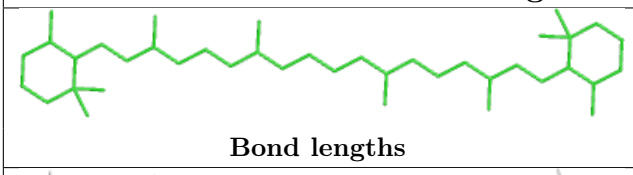


Torsions

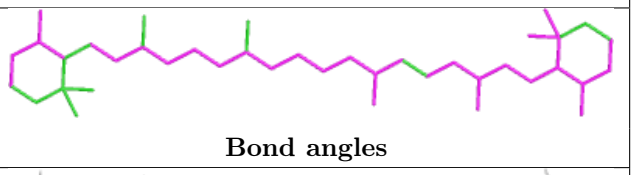


Rings

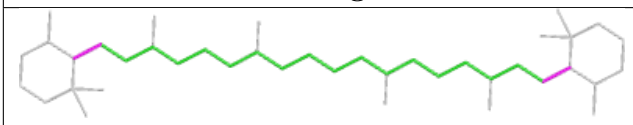
Ligand BCR 1 619



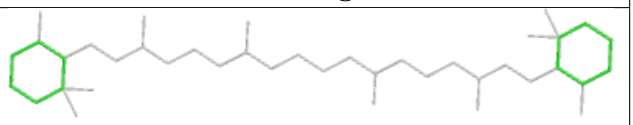
Bond lengths



Bond angles

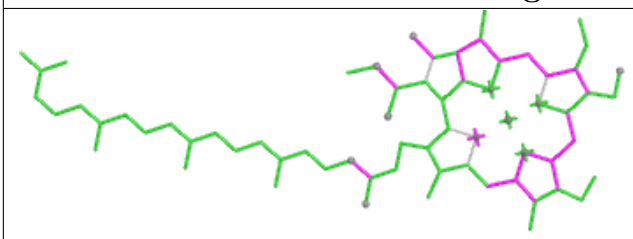


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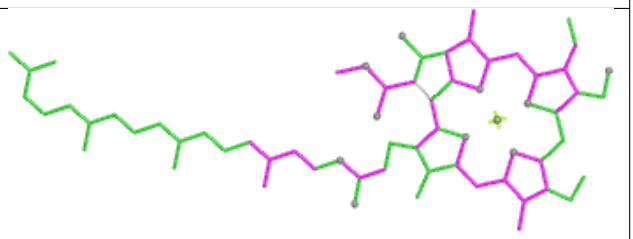


Rings

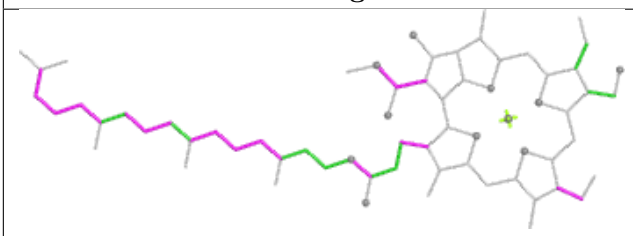
Ligand CHL Y 601



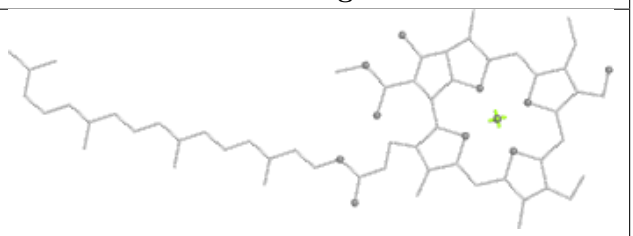
Bond lengths



Bond angles

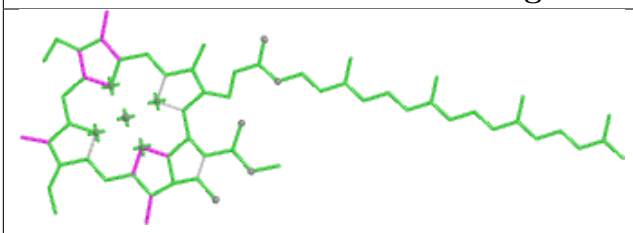


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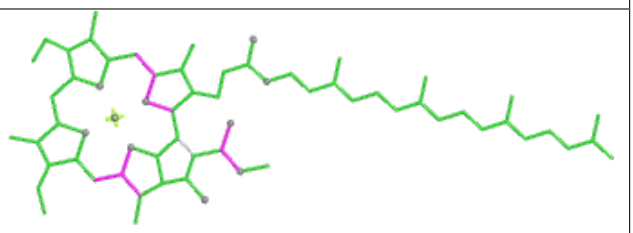


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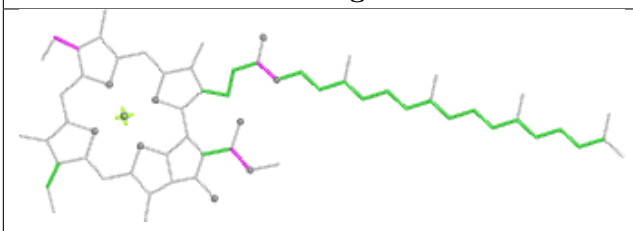
Ligand CLA B 840



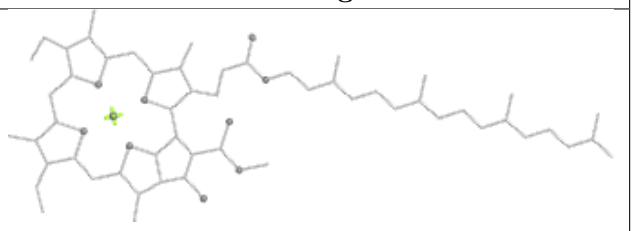
Bond lengths



Bond angles

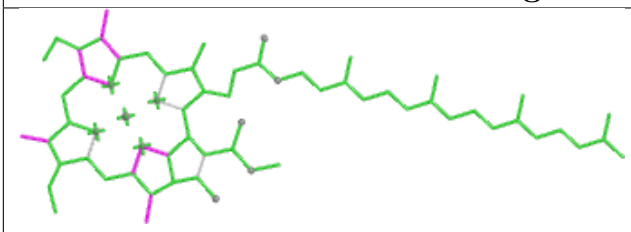


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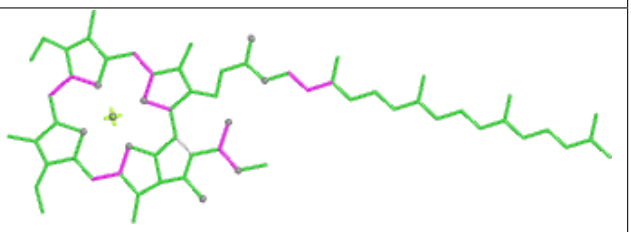


Rings

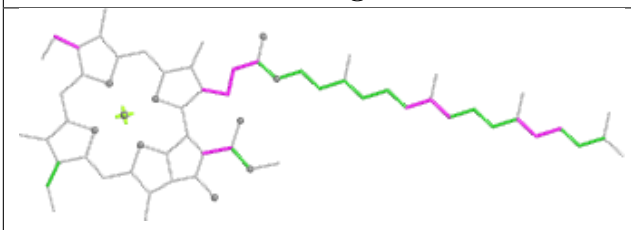
Ligand CLA H 203



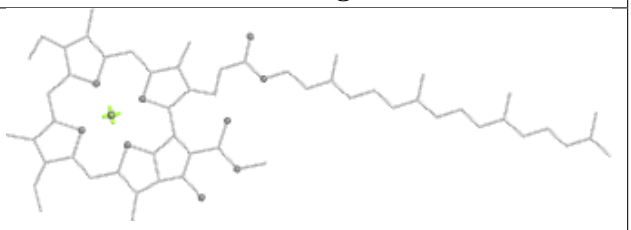
Bond lengths



Bond angles

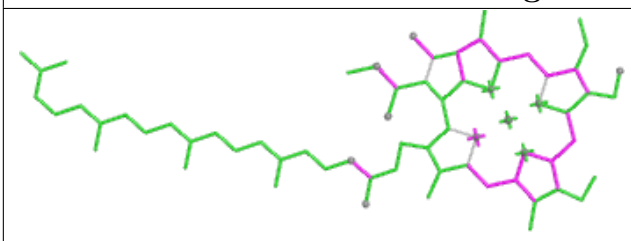


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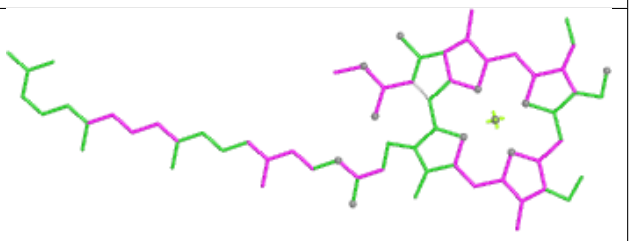


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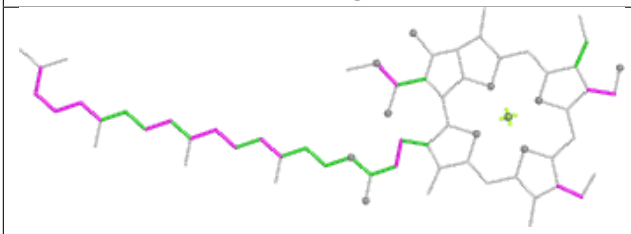
Ligand CHL X 607



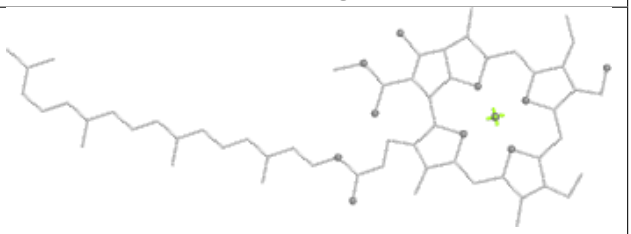
Bond lengths



Bond angles

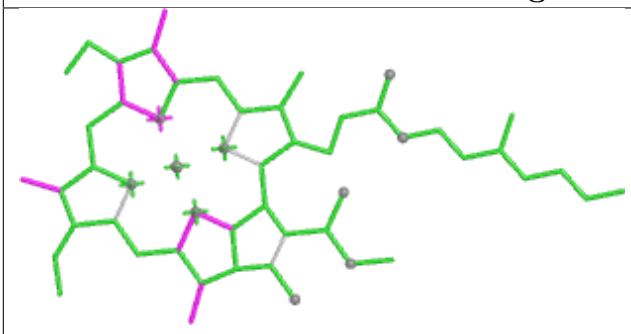


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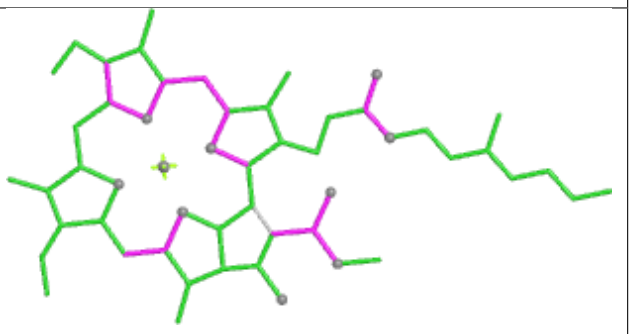


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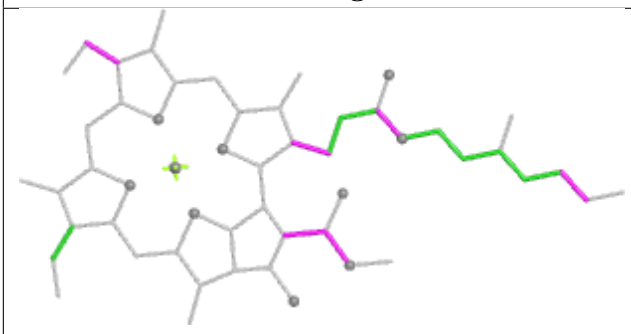
Ligand CLA 8 614



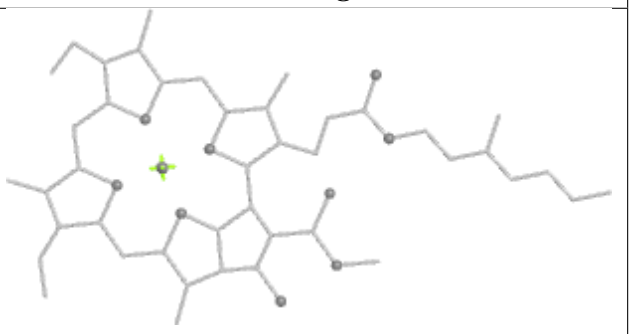
Bond lengths



Bond angles



Torsions

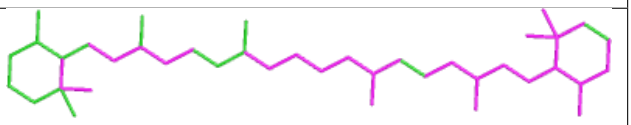


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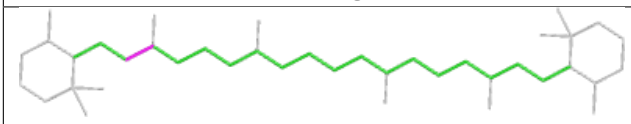
Ligand BCR K 207



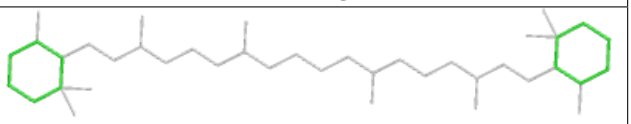
Bond lengths



Bond angles

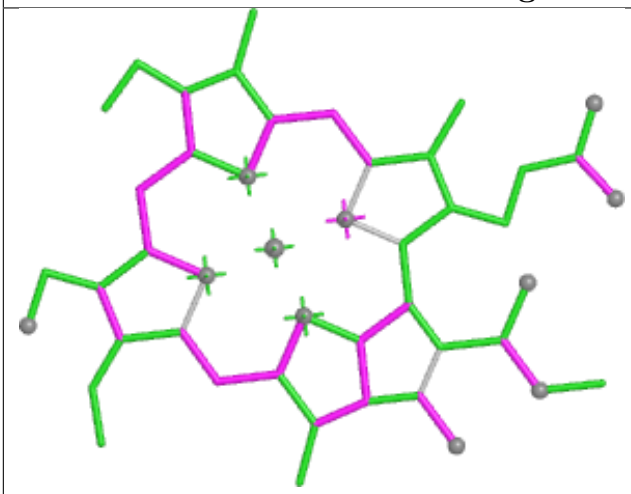


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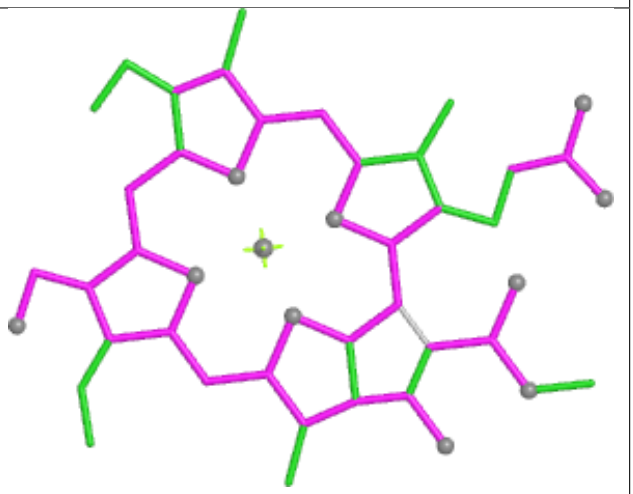


Rings

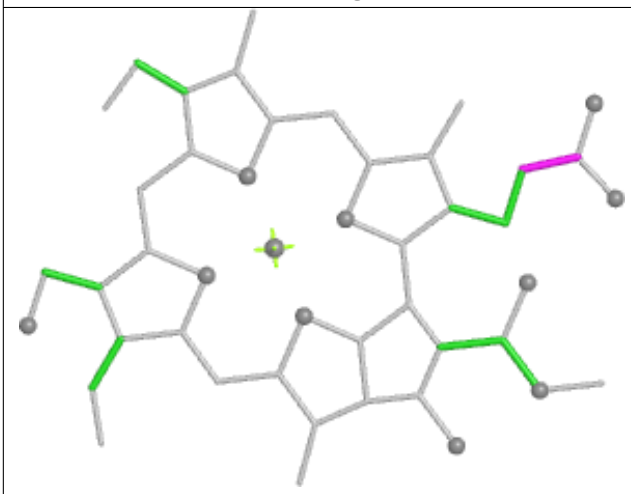
Ligand CHL W 606



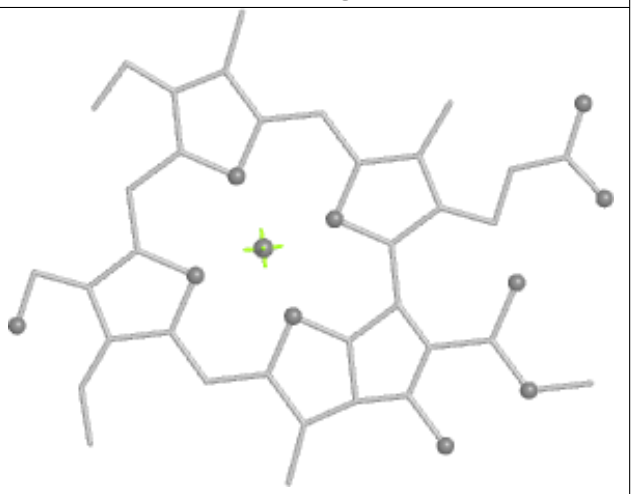
Bond lengths



Bond angles

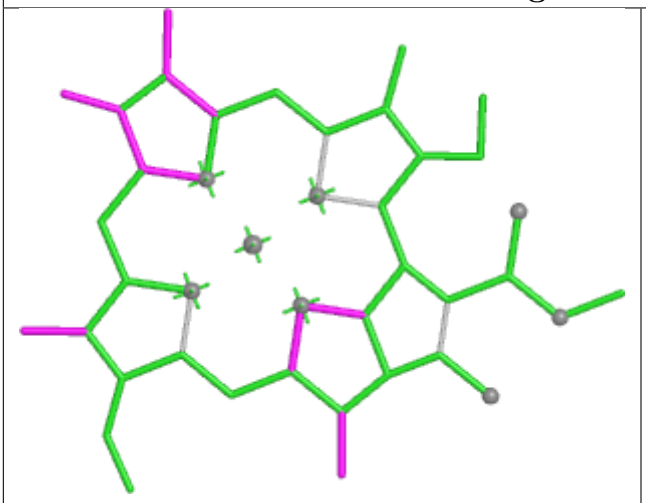


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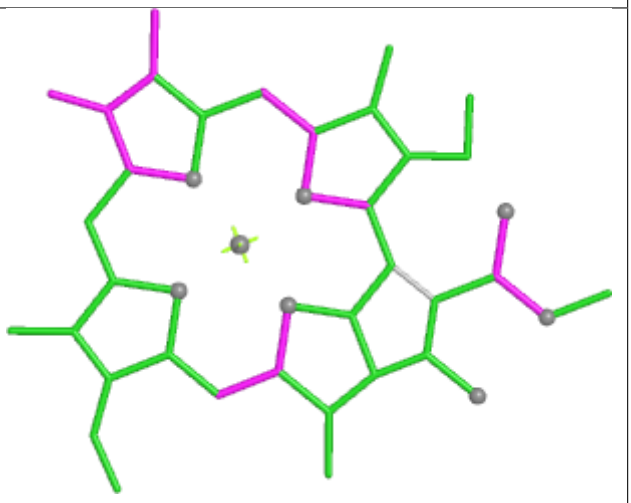


Rings

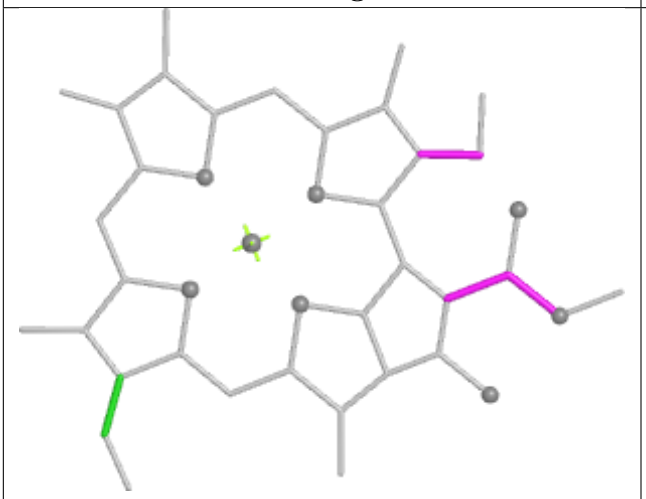
Ligand CLA 8 607



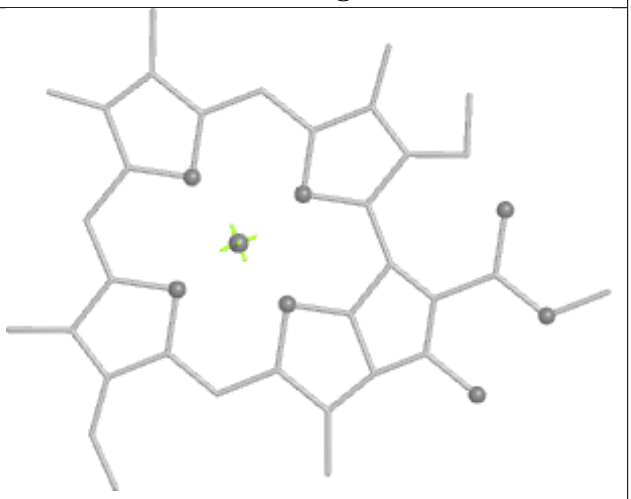
Bond lengths



Bond angles

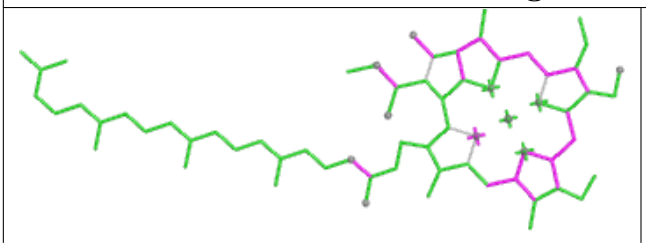


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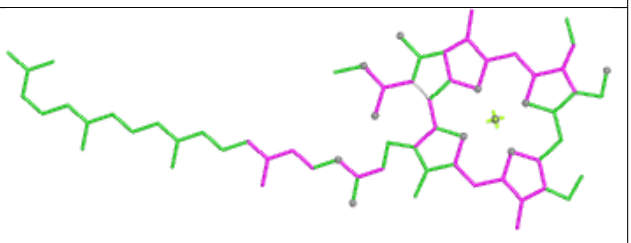


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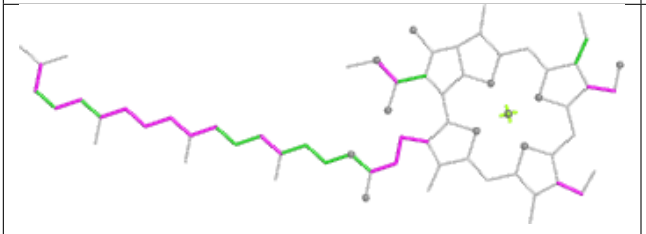
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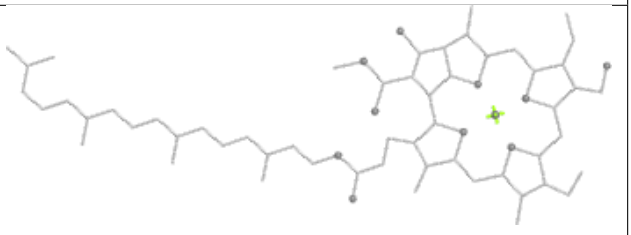
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Bond angles

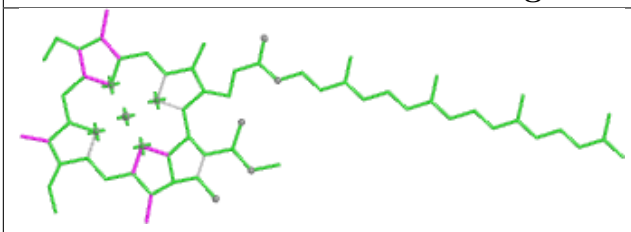


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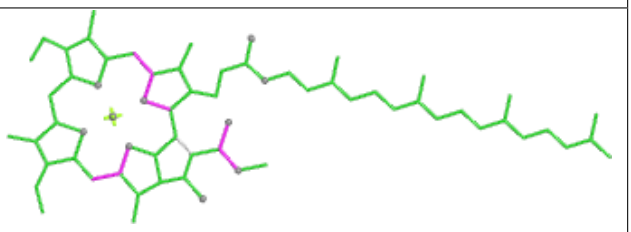


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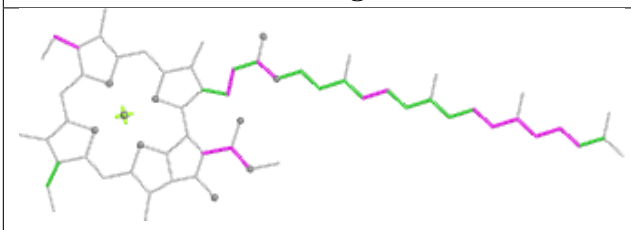
Ligand CLA B 839



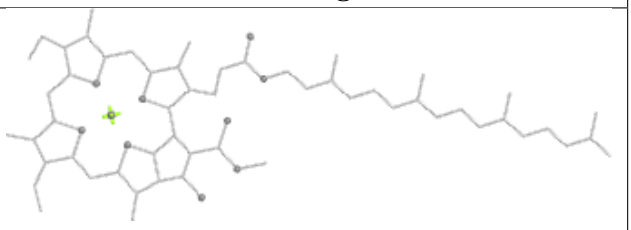
Bond lengths



Bond angles

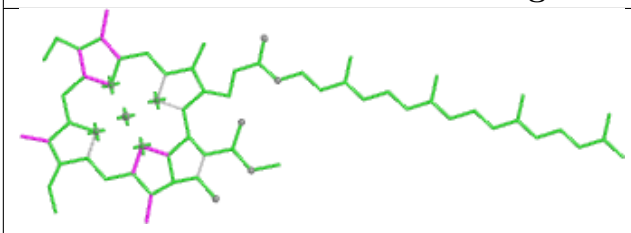


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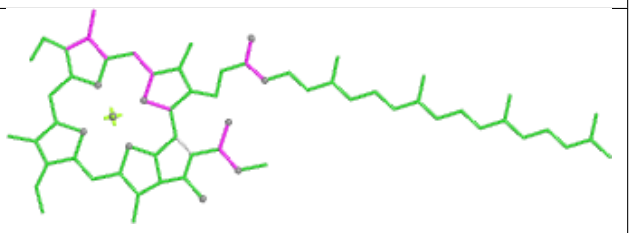


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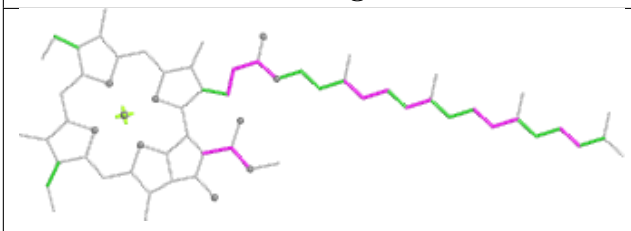
Ligand CLA 8 601



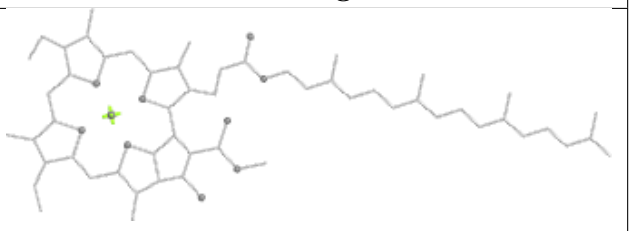
Bond lengths



Bond angles

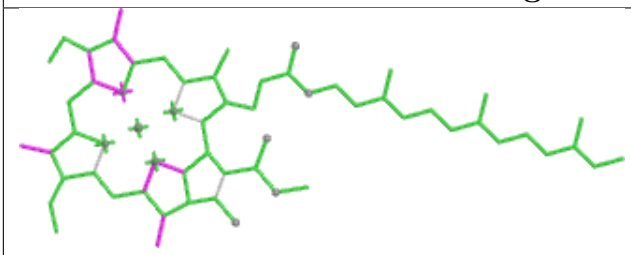


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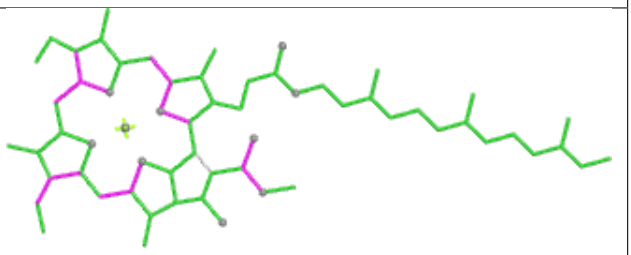


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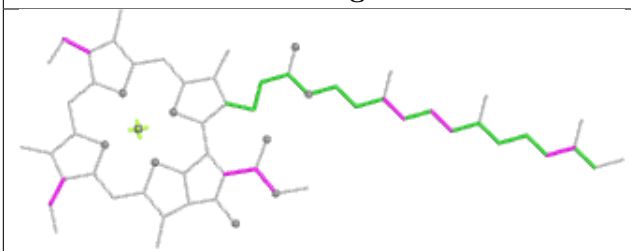
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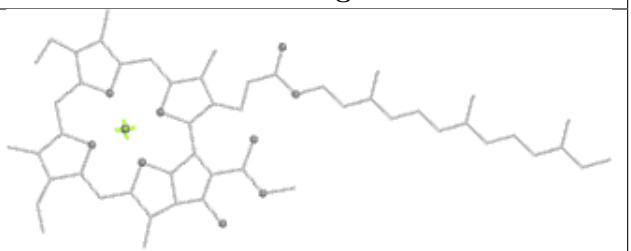
Bond lengths



Bond angles

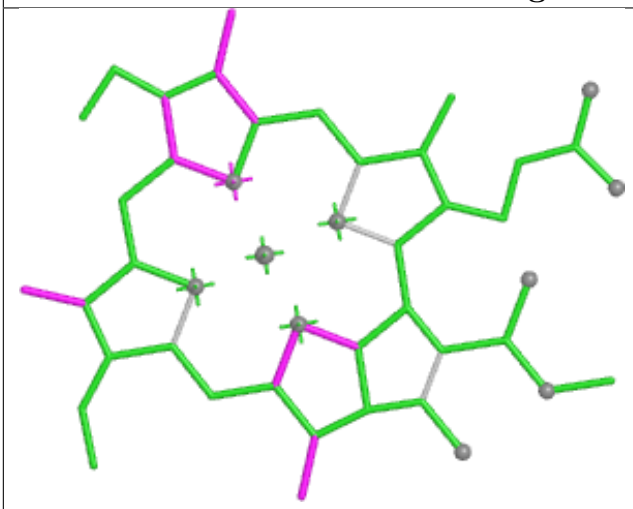


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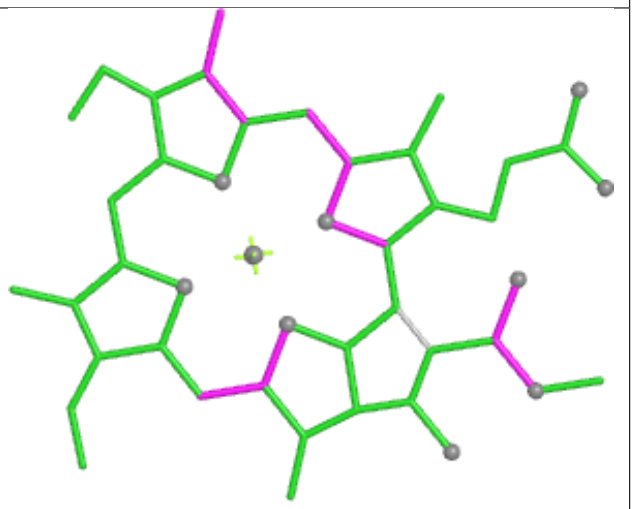


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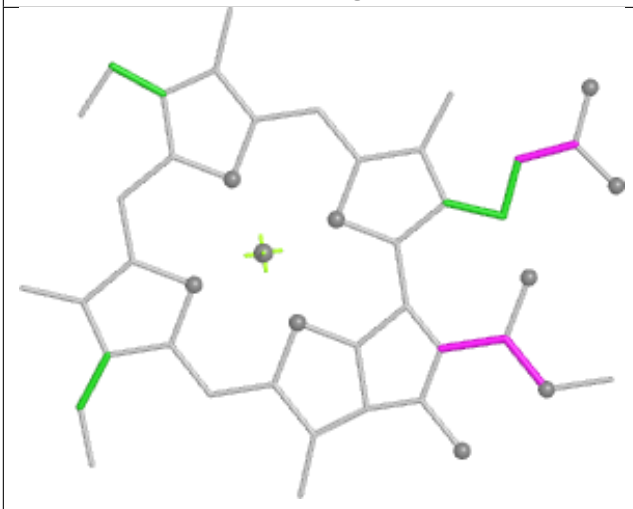
Ligand CLA 2 606



Bond lengths



Bond angles

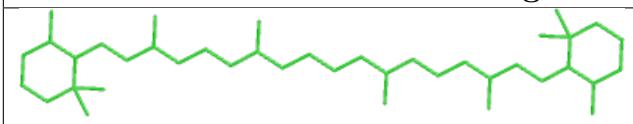


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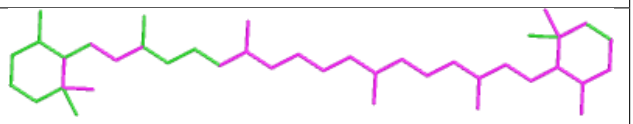


Rings

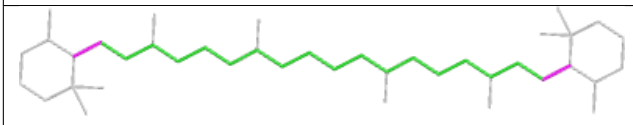
Ligand BCR B 801



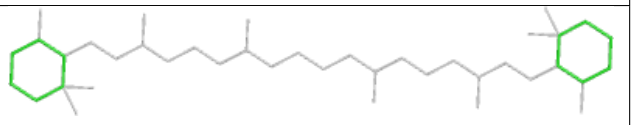
Bond lengths



Bond angles

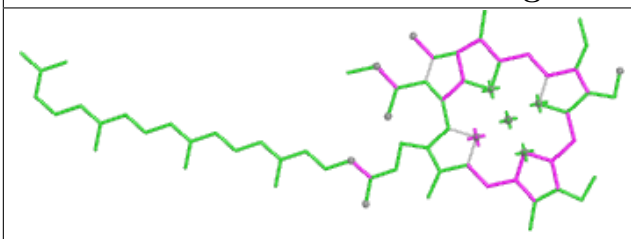


Torsions

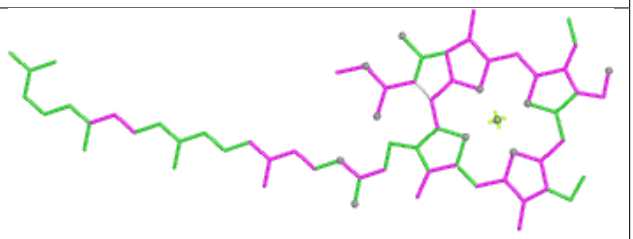


Rings

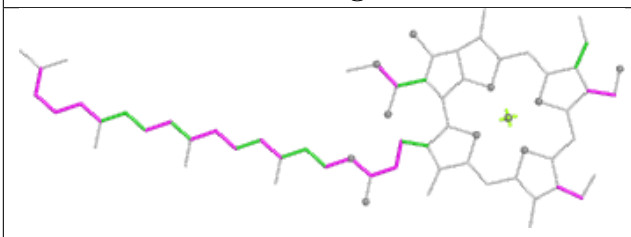
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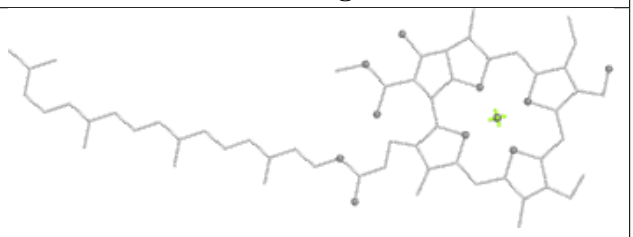
Bond lengths



Bond angles

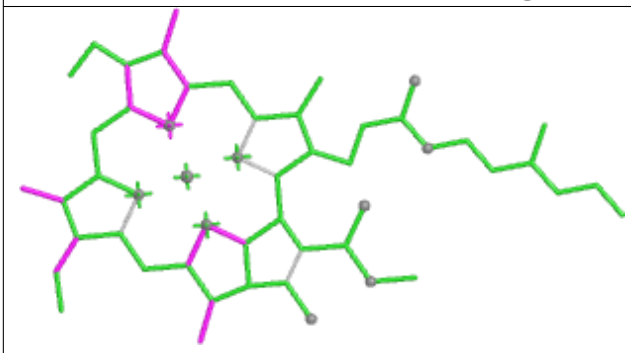


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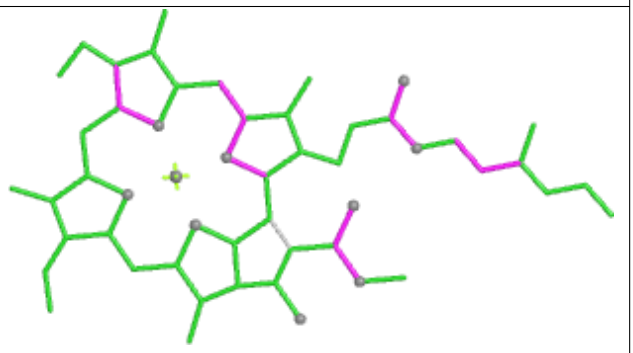


Rings

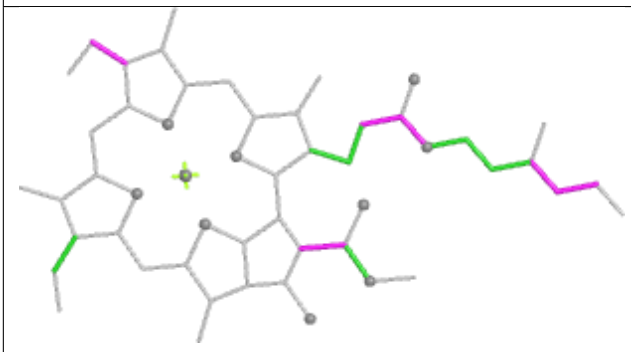
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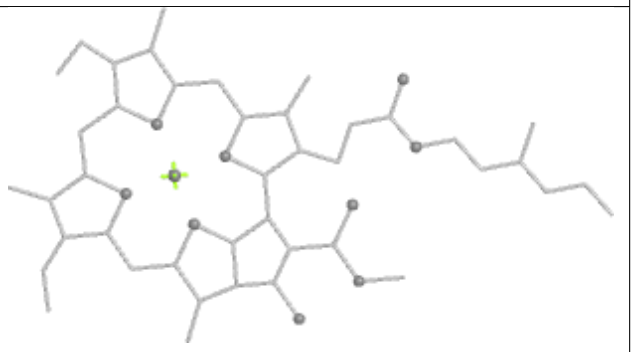
Bond lengths



Bond angles

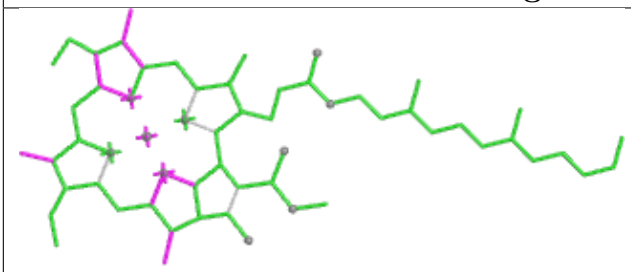


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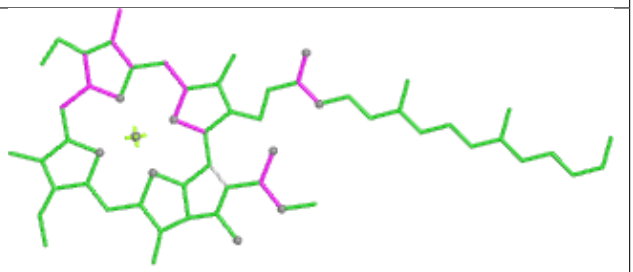


Rings

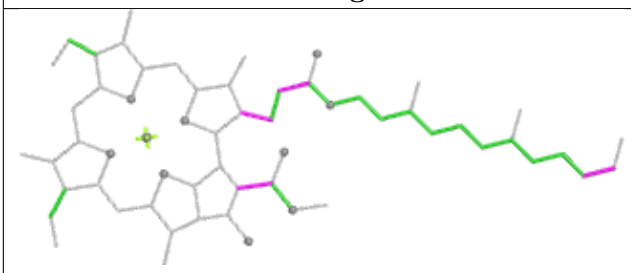
Ligand CLA A 819



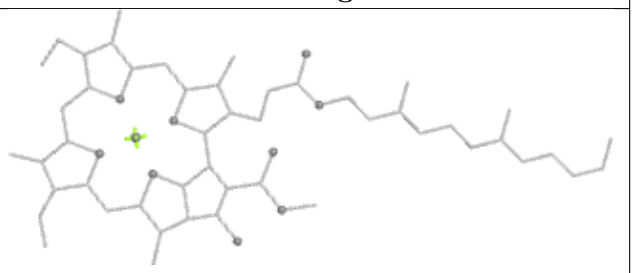
Bond lengths



Bond angles

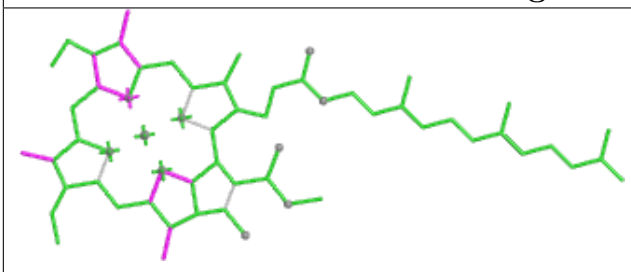


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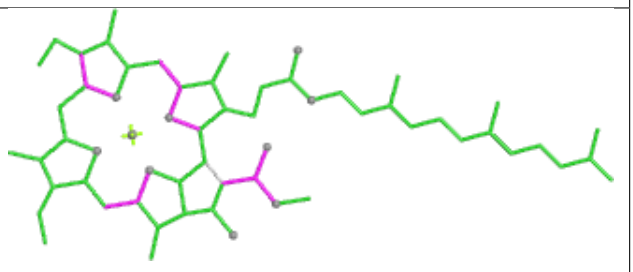


Rings

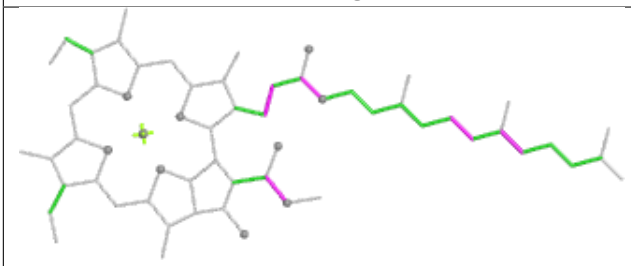
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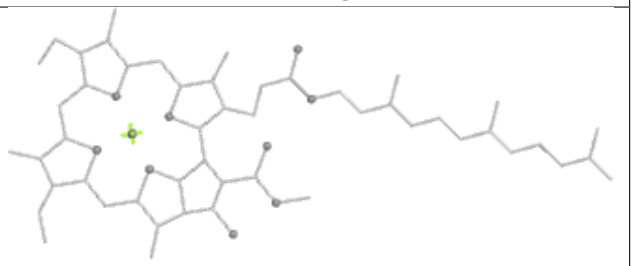
Bond lengths



Bond angles

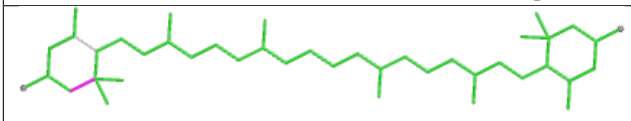


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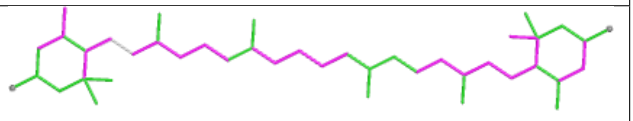


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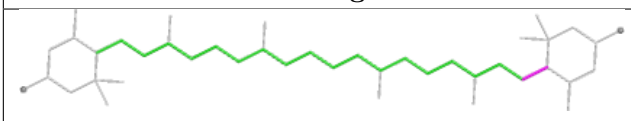
Ligand LUT 2 619



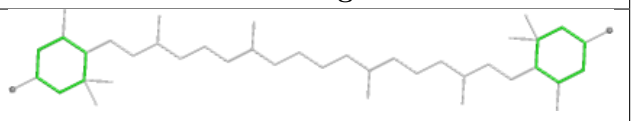
Bond lengths



Bond angles

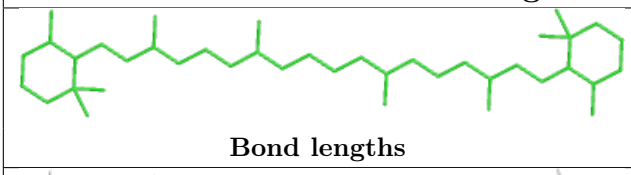


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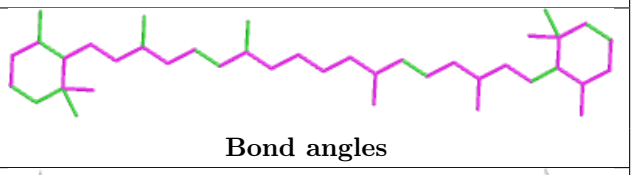


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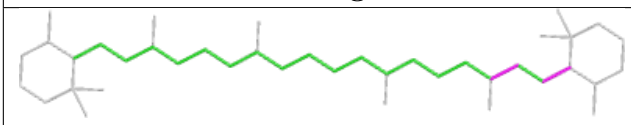
Ligand BCR B 848



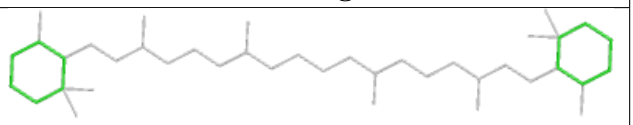
Bond lengths



Bond angles

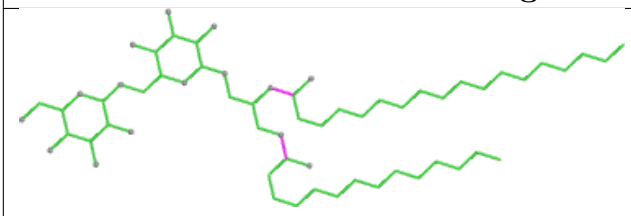


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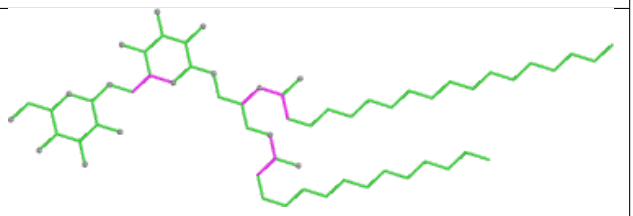


Rings

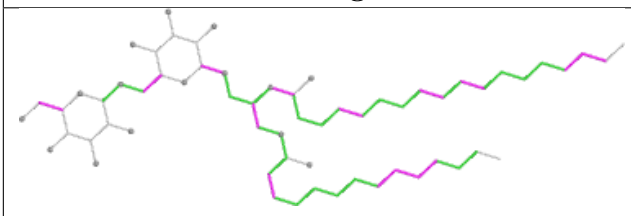
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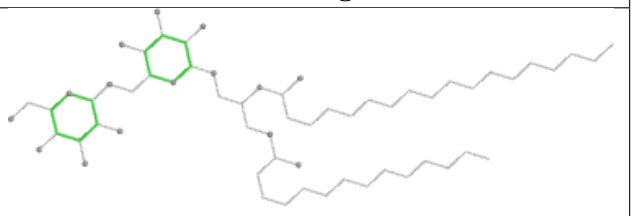
Bond lengths



Bond angles

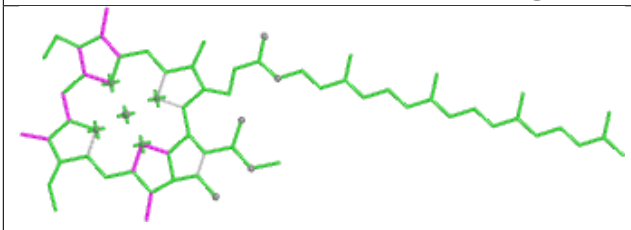


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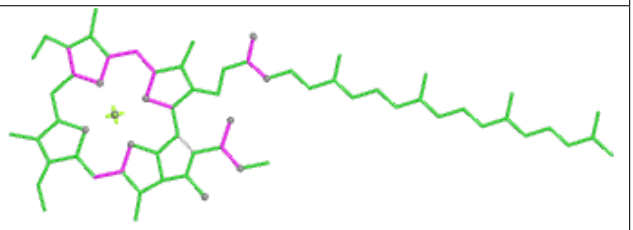


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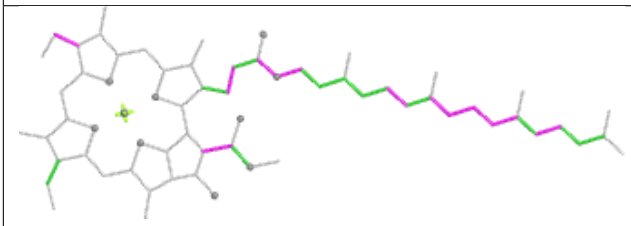
Ligand CLA 8 613



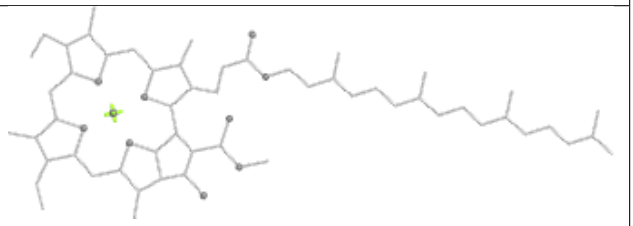
Bond lengths



Bond angles

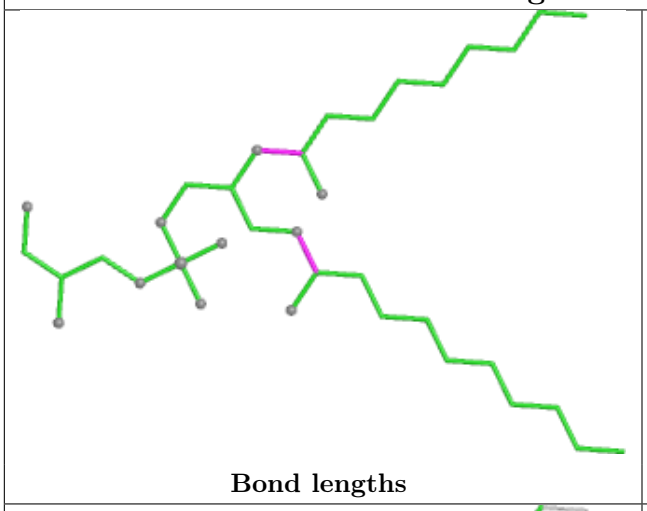


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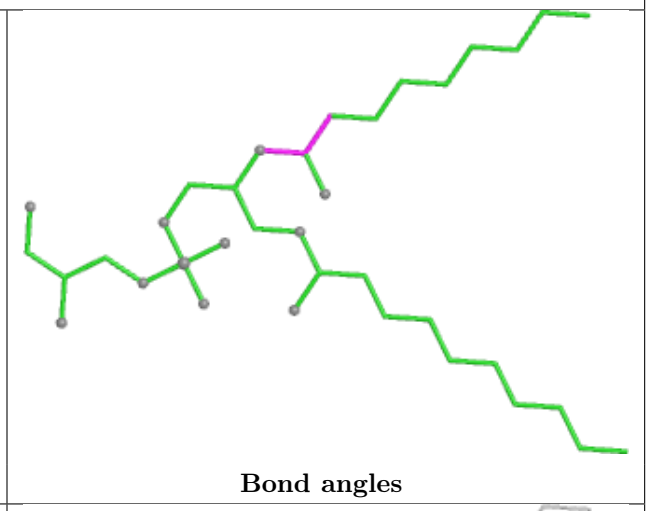


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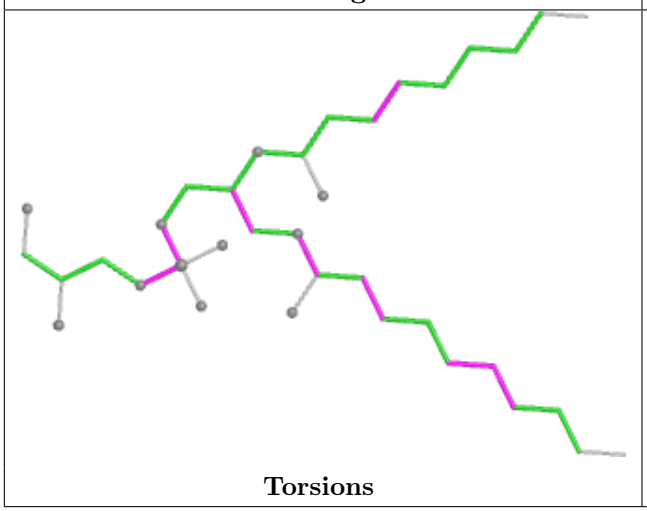
Ligand LHG 2 622



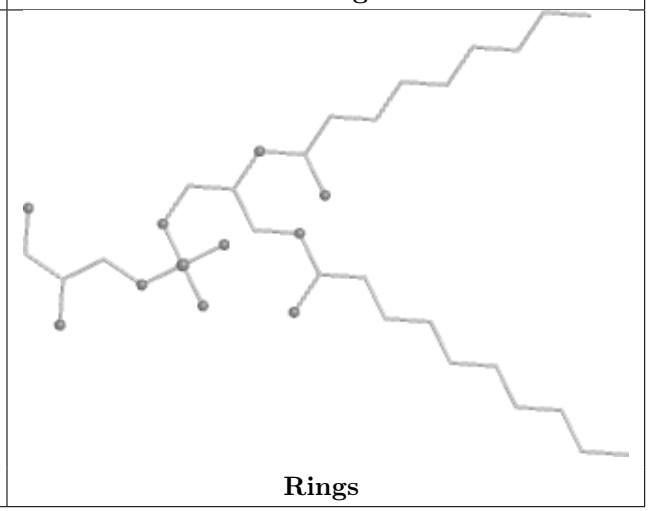
Bond lengths



Bond angles

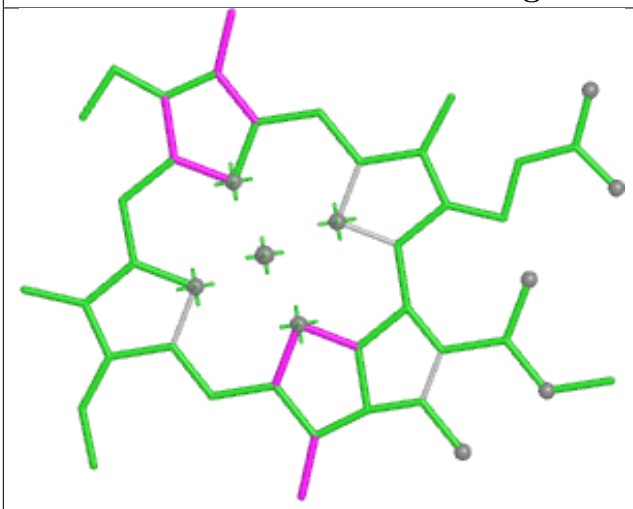


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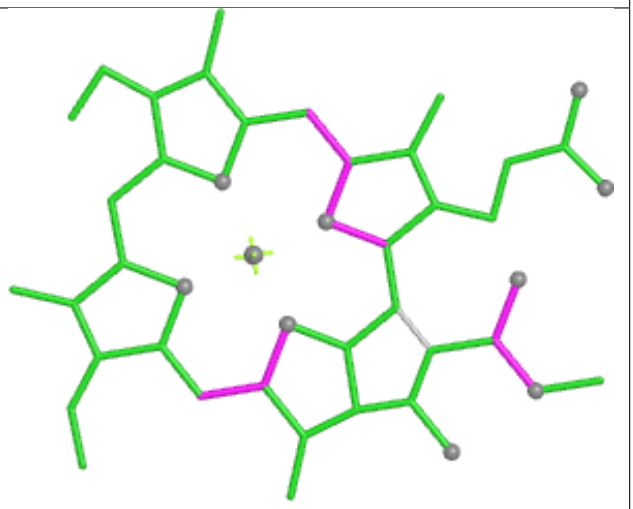


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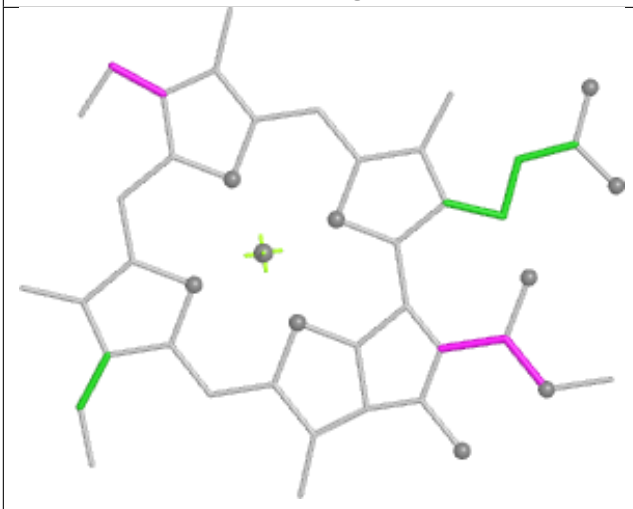
Ligand CLA K 206



Bond lengths



Bond angles

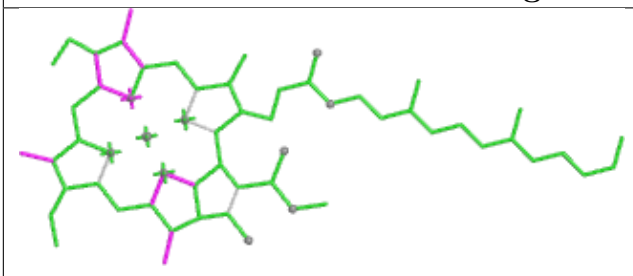


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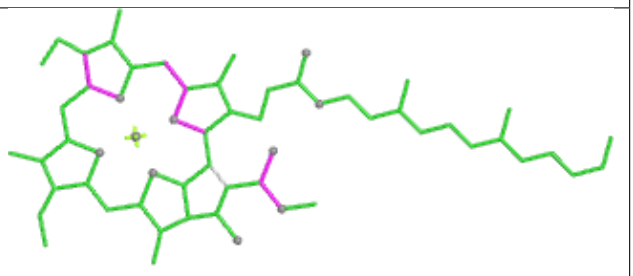


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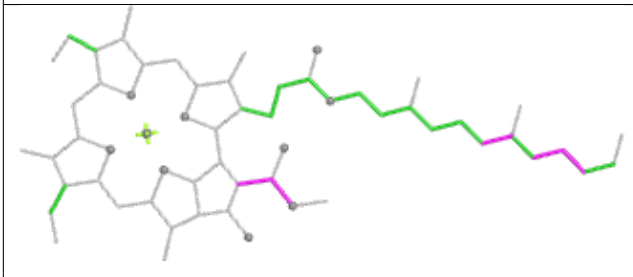
Ligand CLA U 602



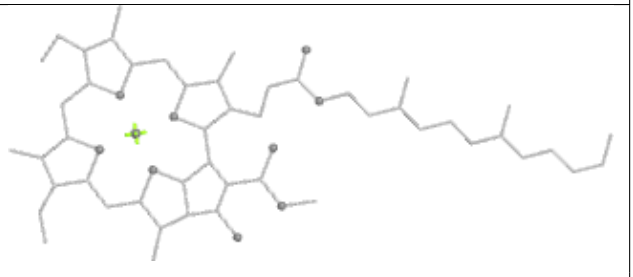
Bond lengths



Bond angles

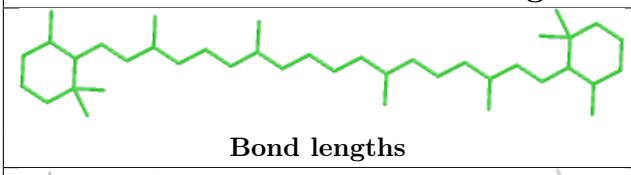


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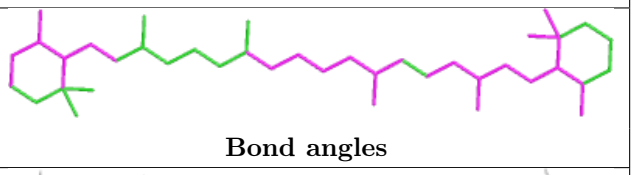


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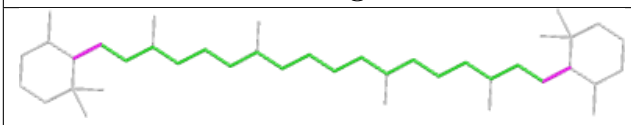
Ligand BCR 8 621



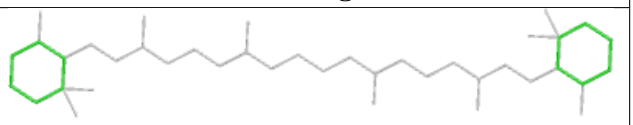
Bond lengths



Bond angles

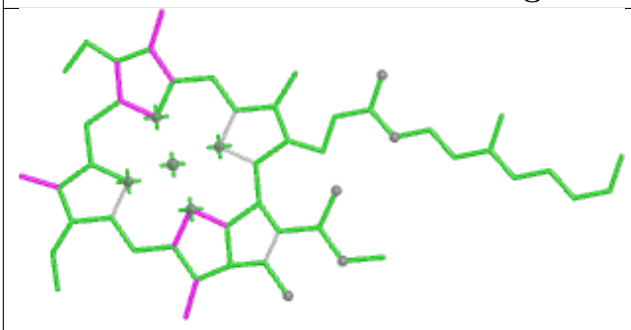


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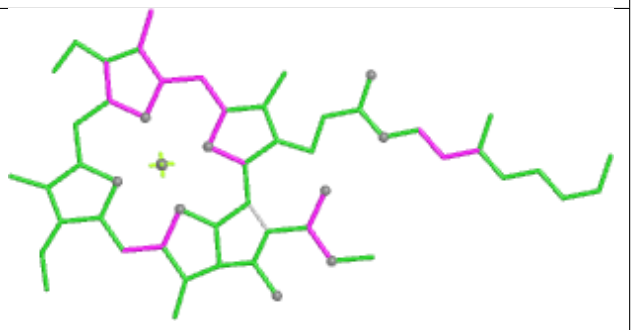


Rings

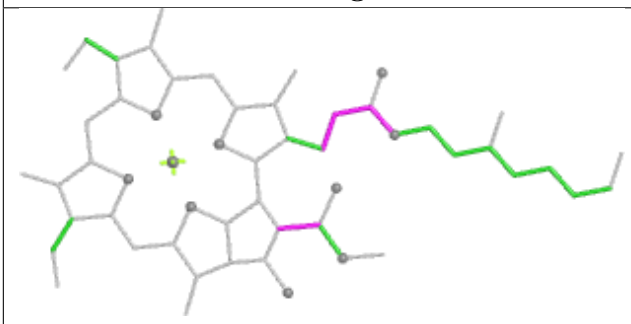
Ligand CLA A 813



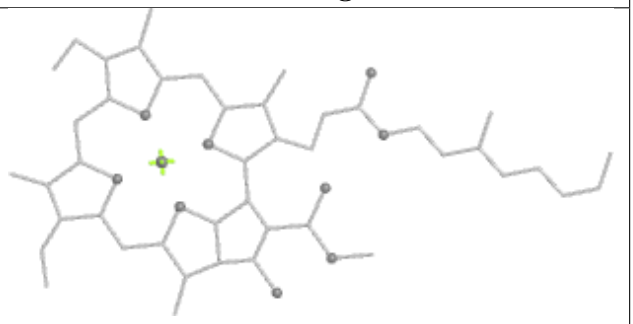
Bond lengths



Bond angles

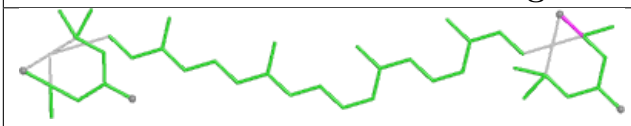


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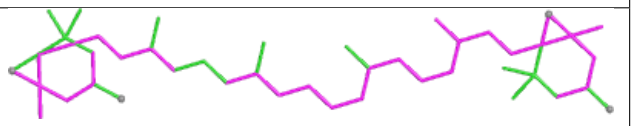


Rings

Ligand XAT 3 619



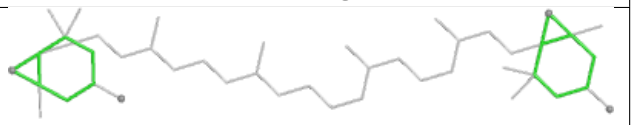
Bond lengths



Bond angles

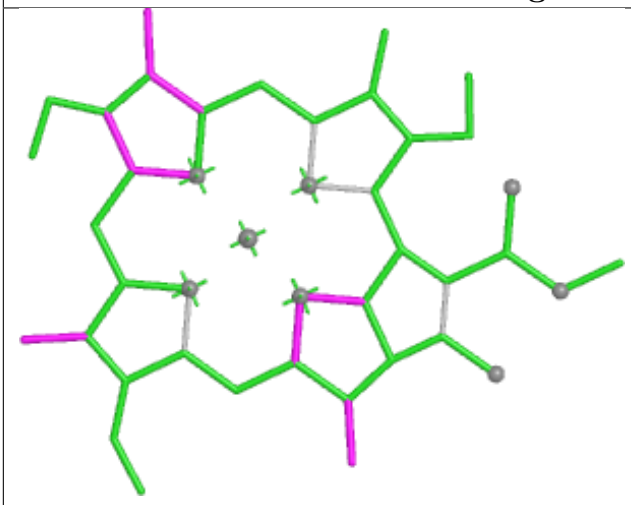


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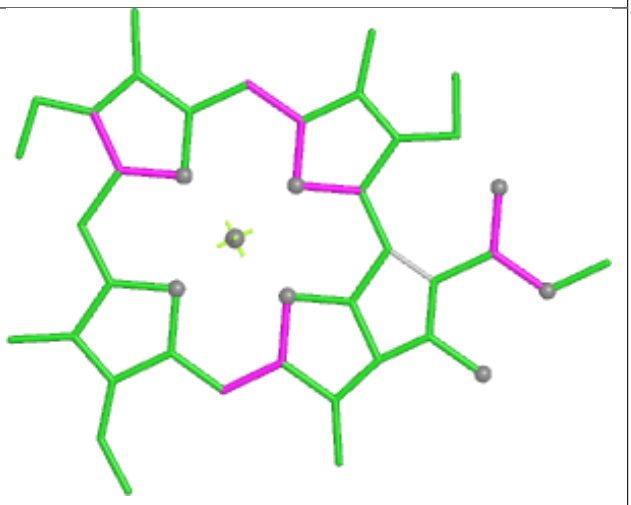


Rings

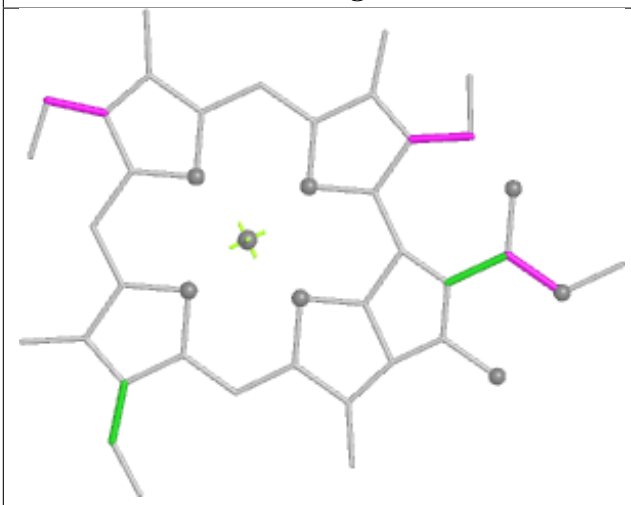
Ligand CLA 2 611



Bond lengths



Bond angles

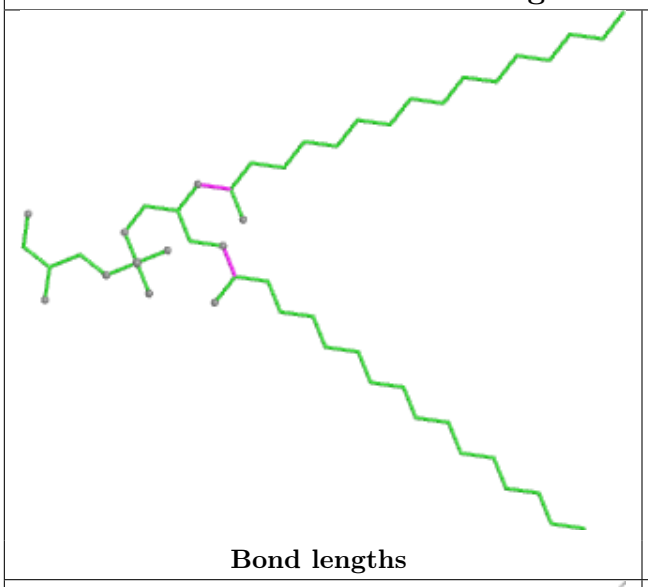


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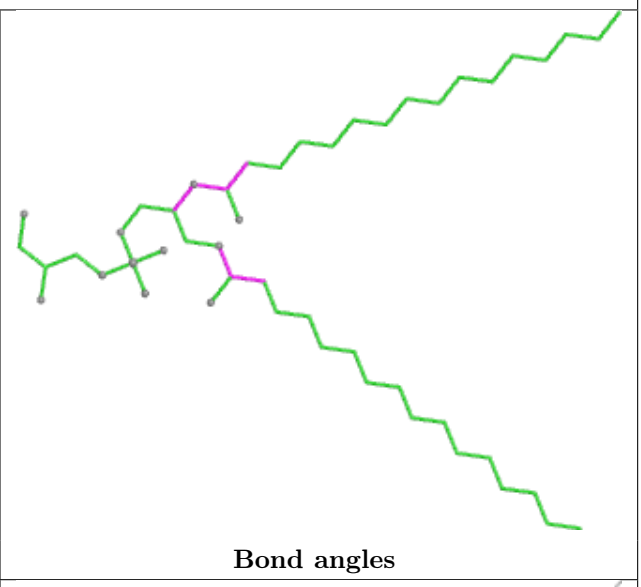


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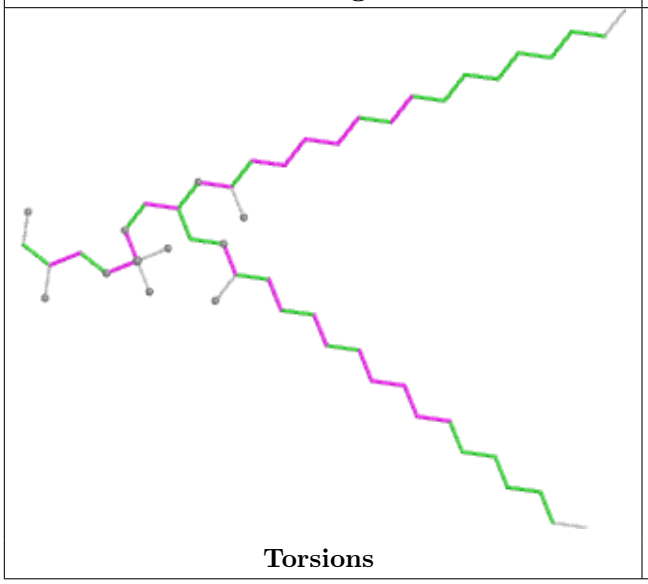
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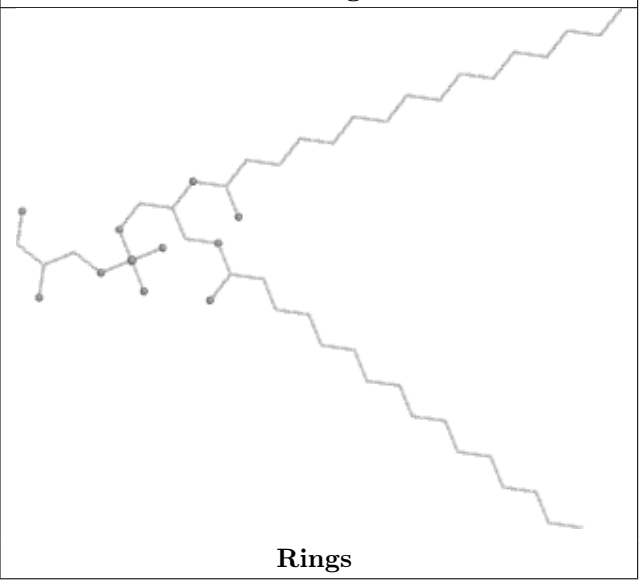
Bond lengths



Bond angles

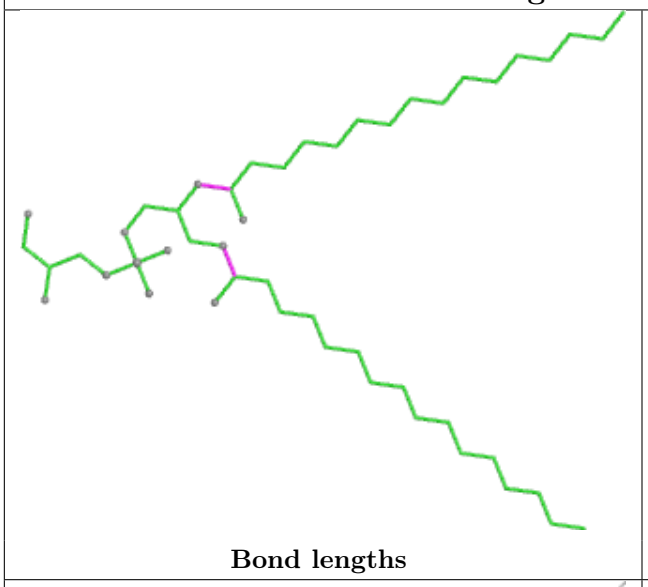


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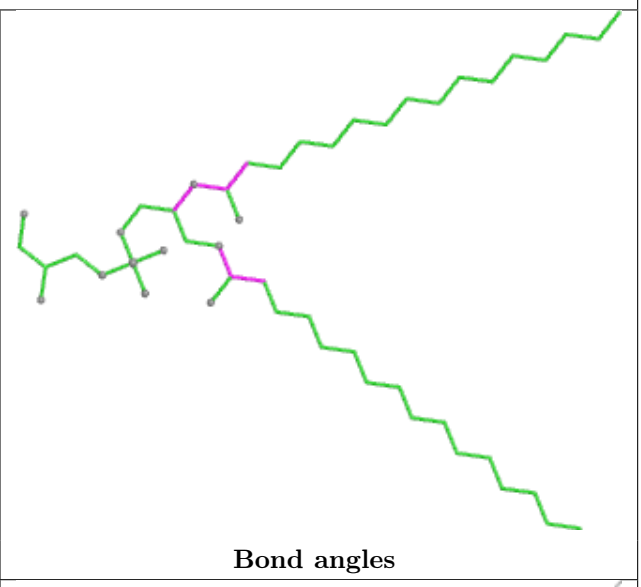


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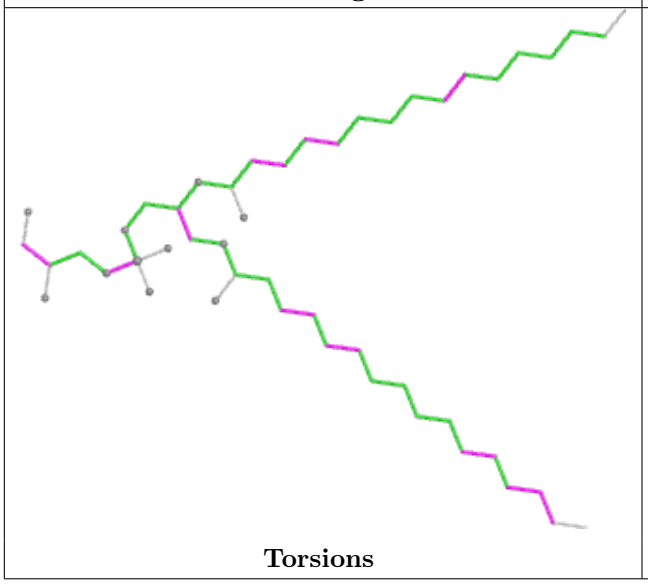
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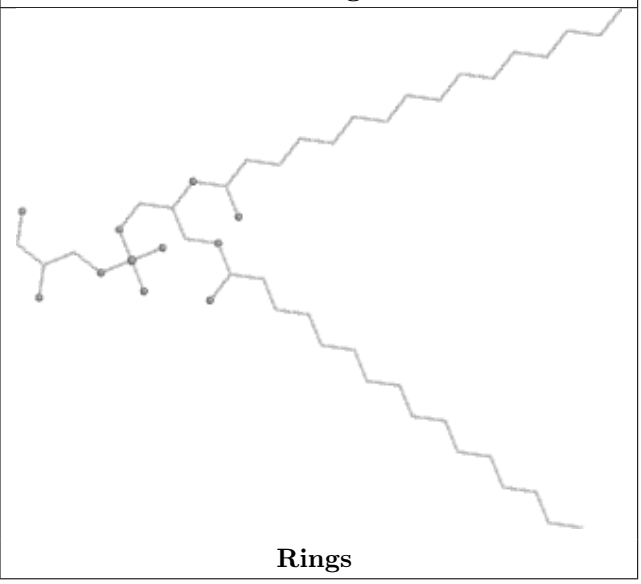
Bond lengths



Bond angles



Torsions

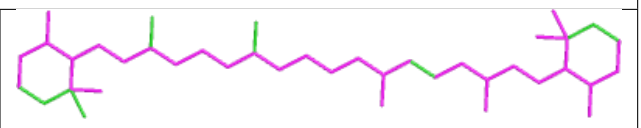


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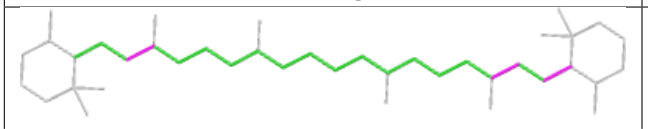
Ligand BCR 7 621



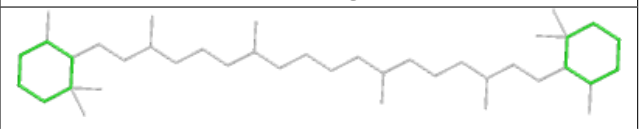
Bond lengths



Bond angles

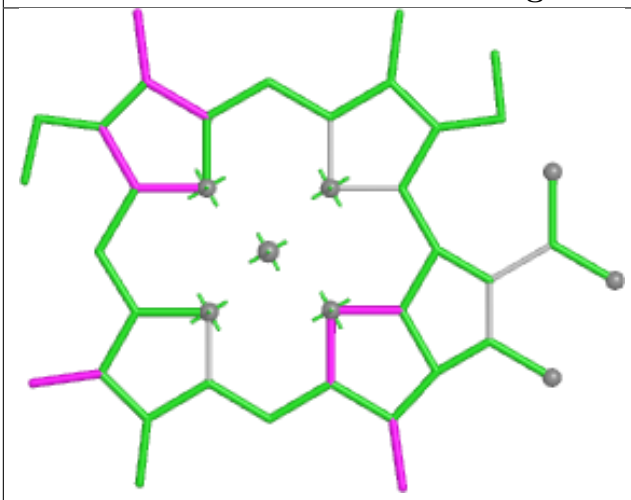


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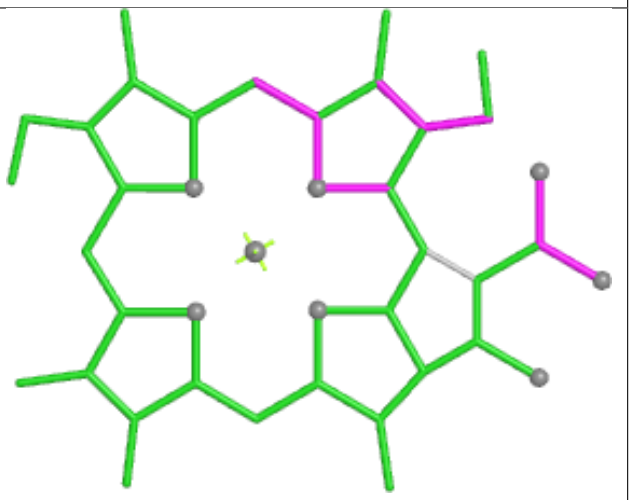


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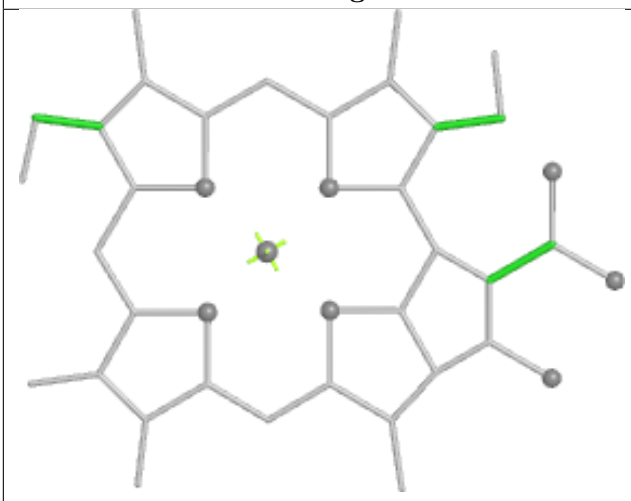
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Bond lengths



Bond angles

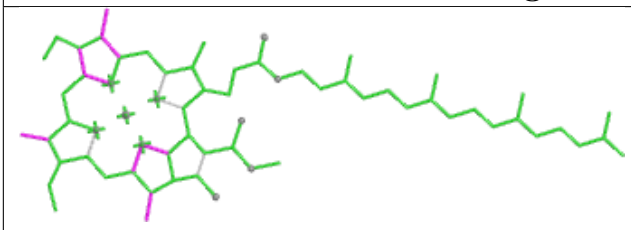


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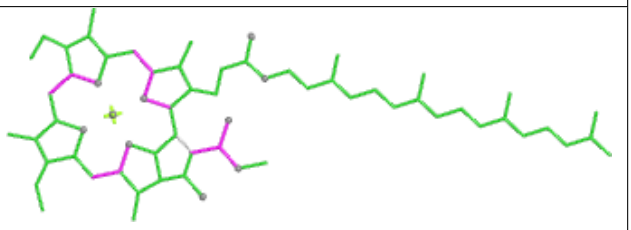


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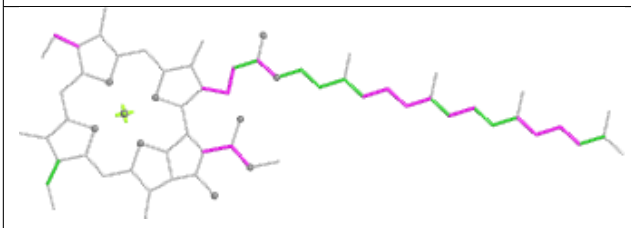
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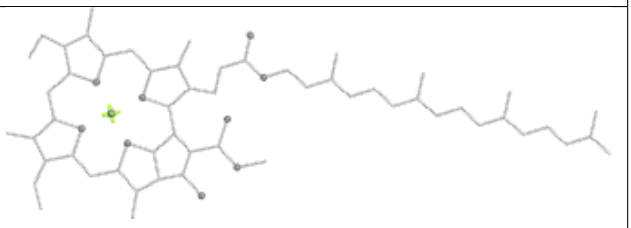
Bond lengths



Bond angles

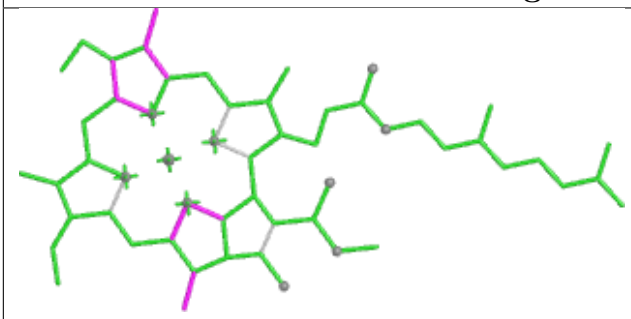


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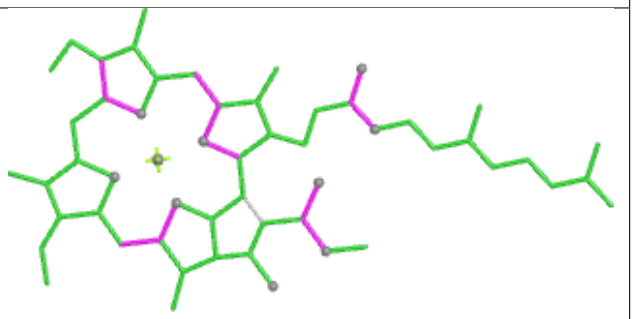


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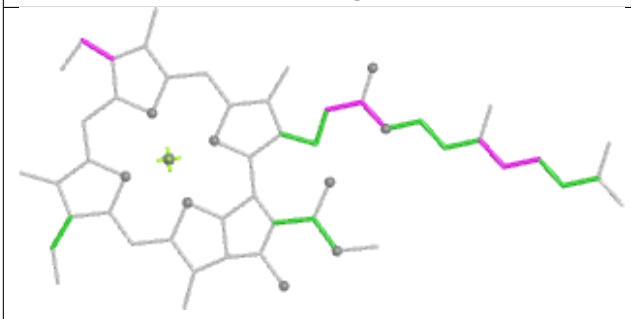
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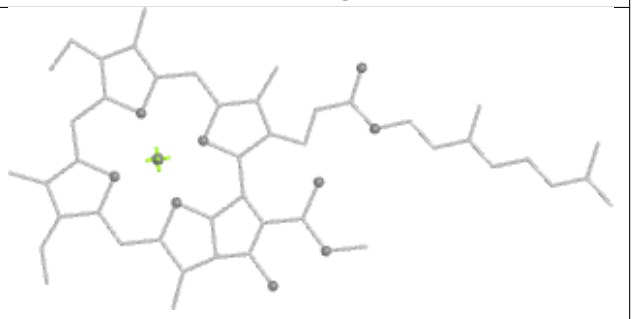
Bond lengths



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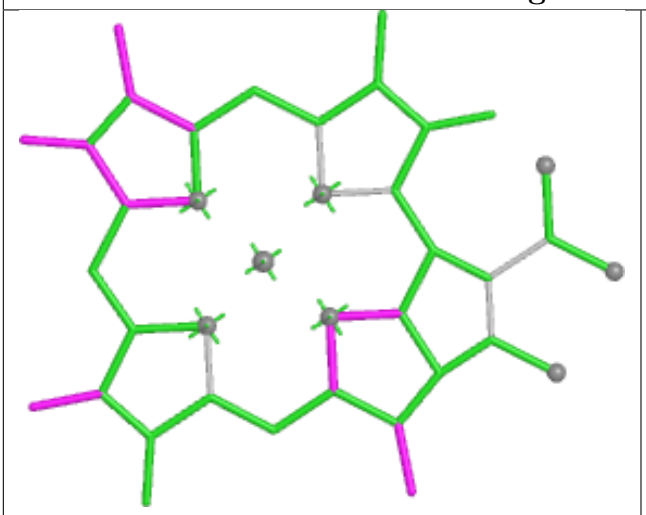


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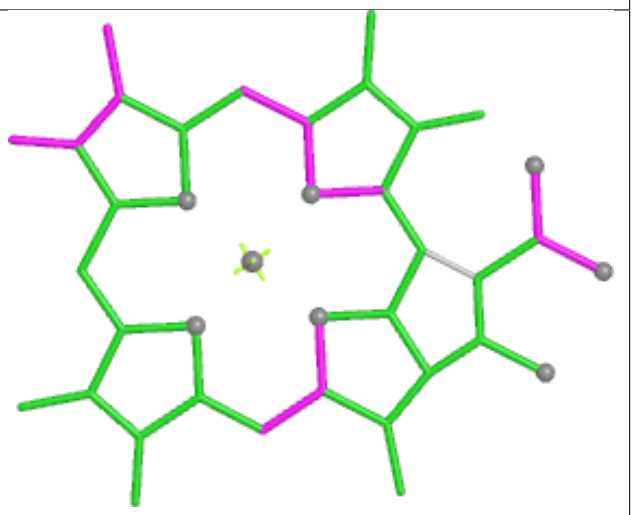


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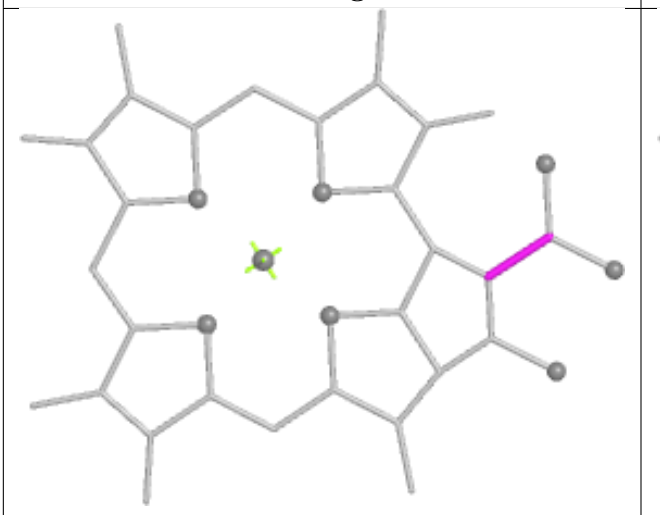
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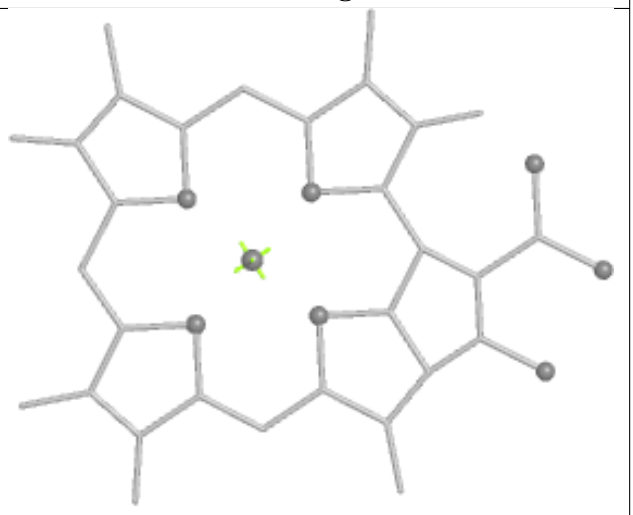
Bond lengths



Bond angles

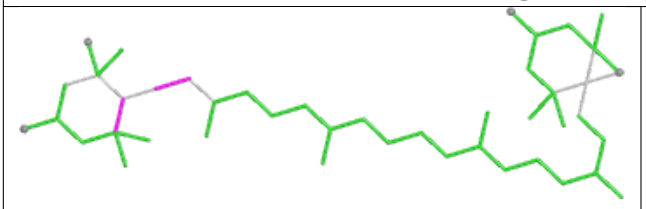


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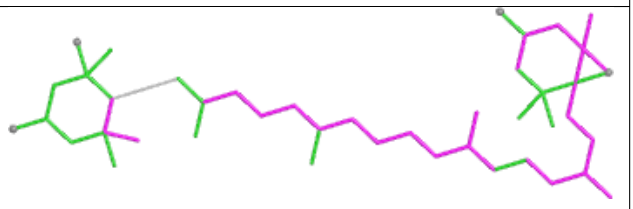


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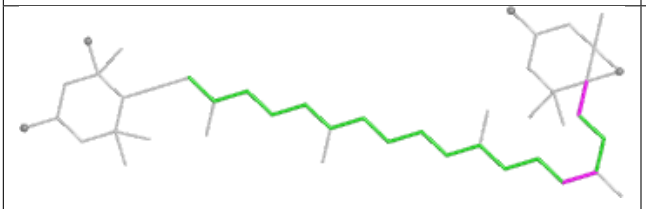
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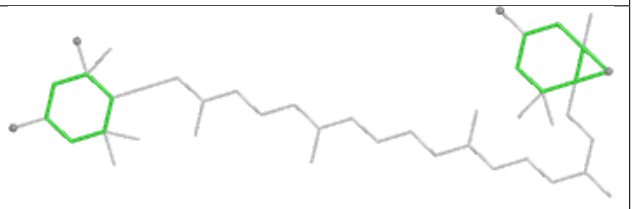
Bond lengths



Bond angles

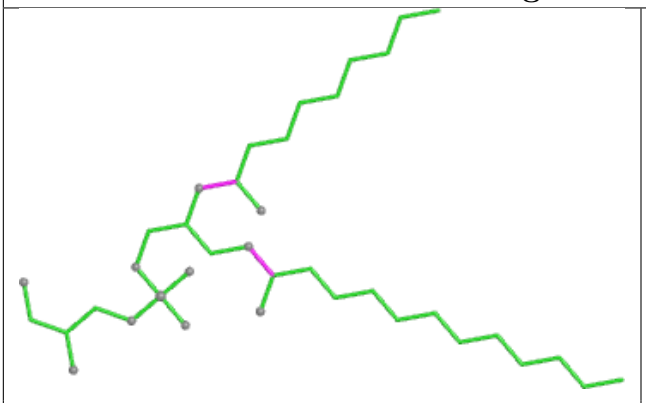


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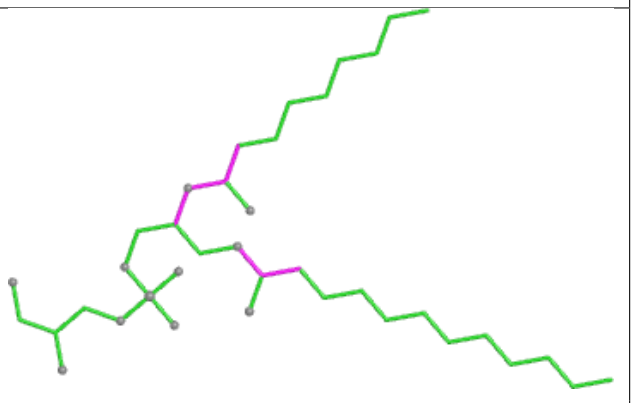


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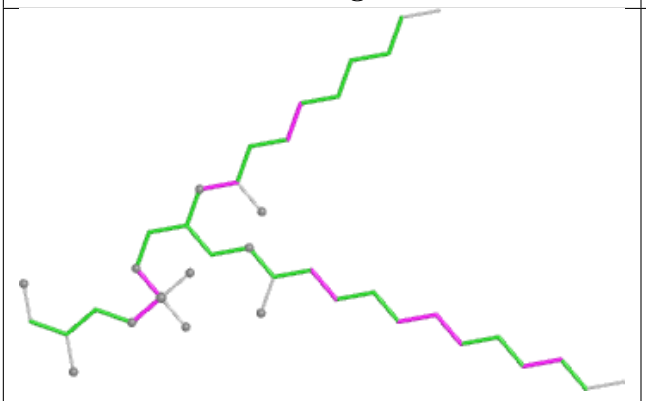
Ligand LHG B 851



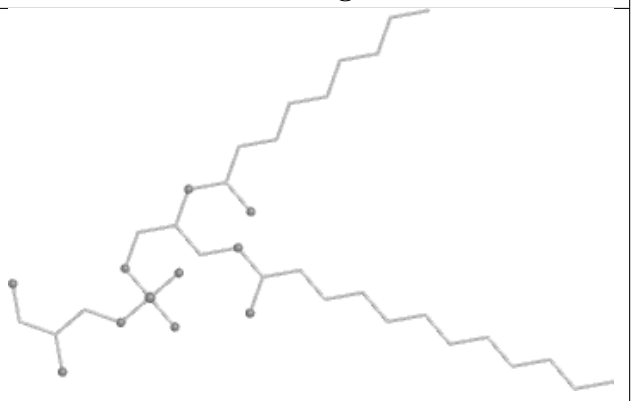
Bond lengths



Bond angles

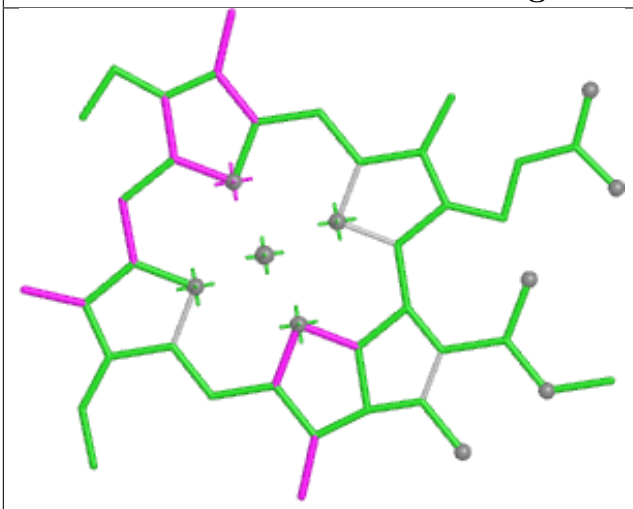


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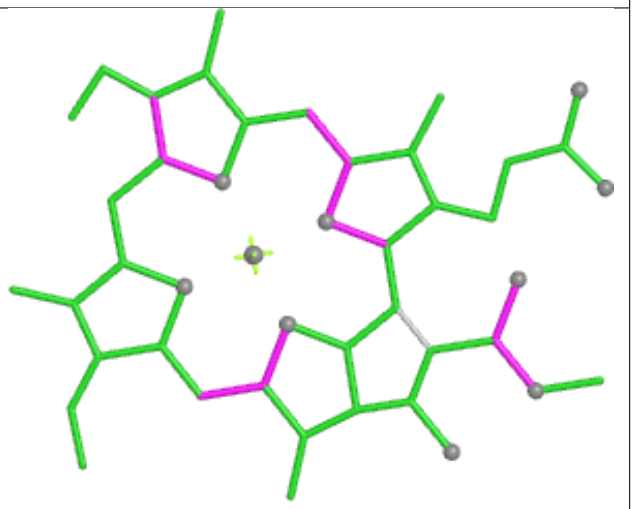


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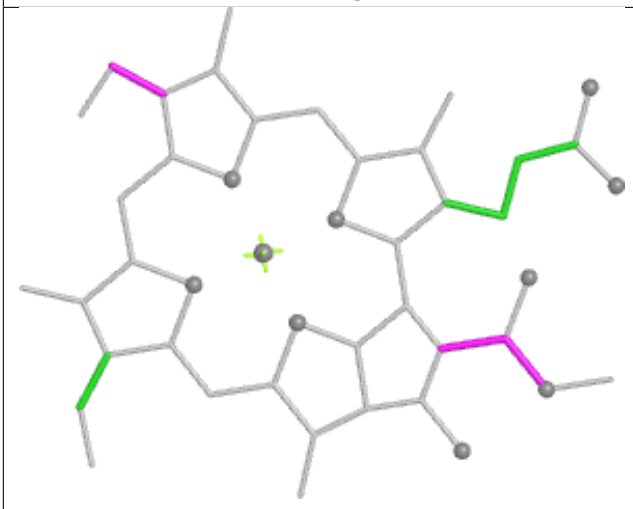
Ligand CLA 2 607



Bond lengths



Bond angles

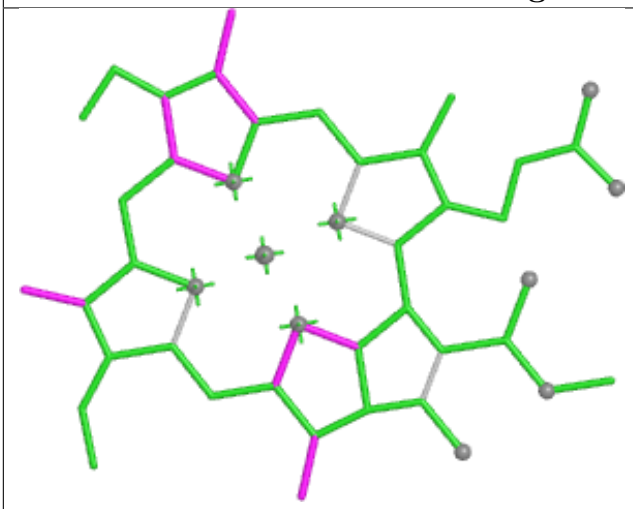


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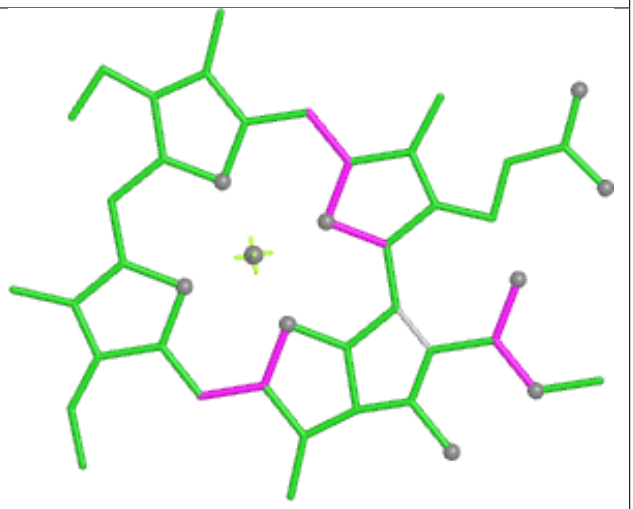


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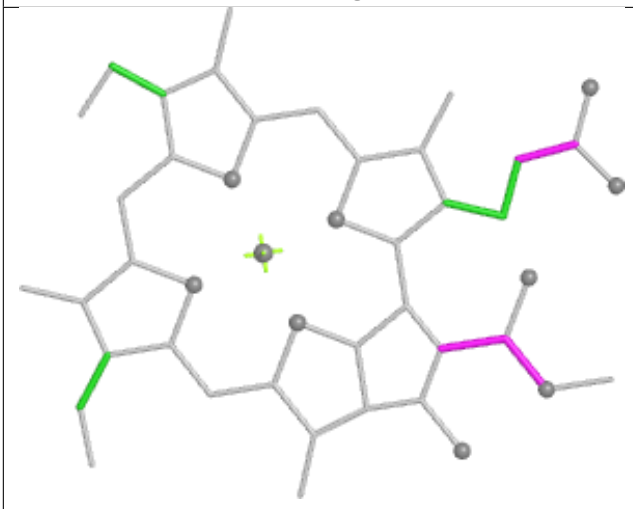
Ligand CLA 1 612



Bond lengths



Bond angles

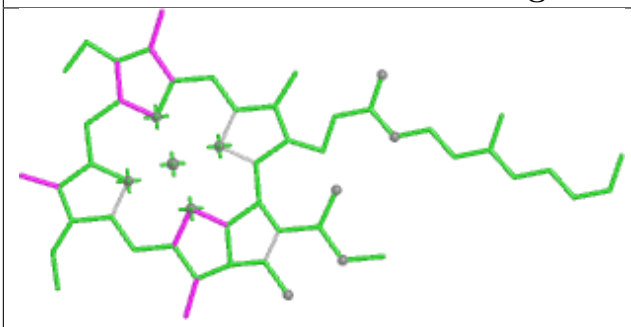


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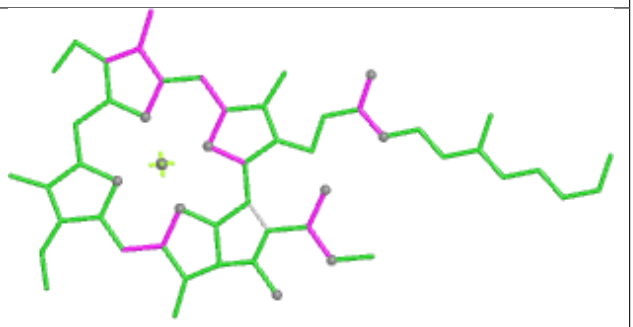


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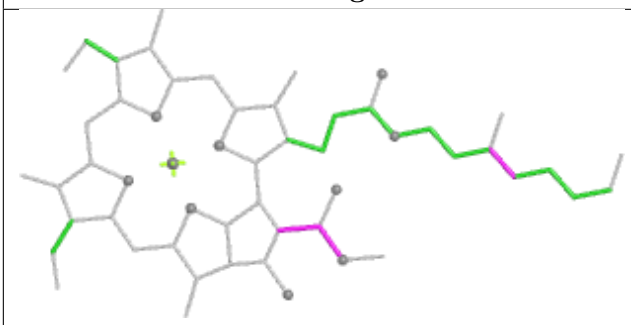
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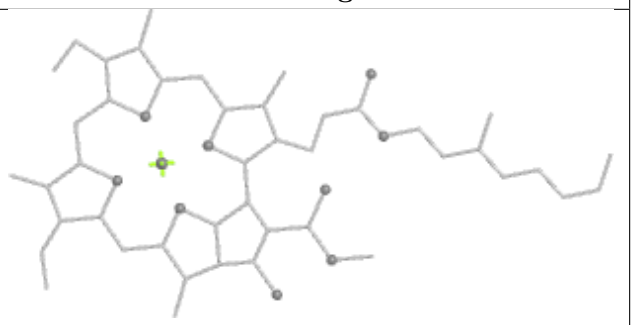
Bond lengths



Bond angles



Torsions

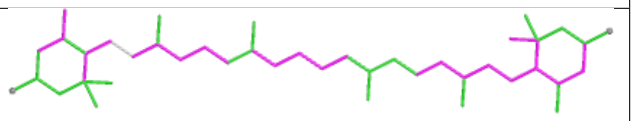


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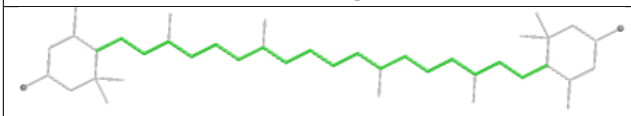
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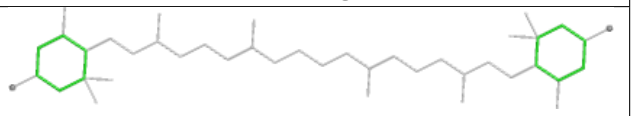
Bond lengths



Bond angles

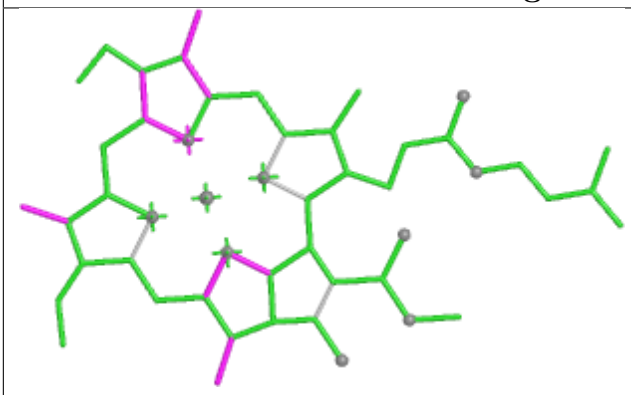


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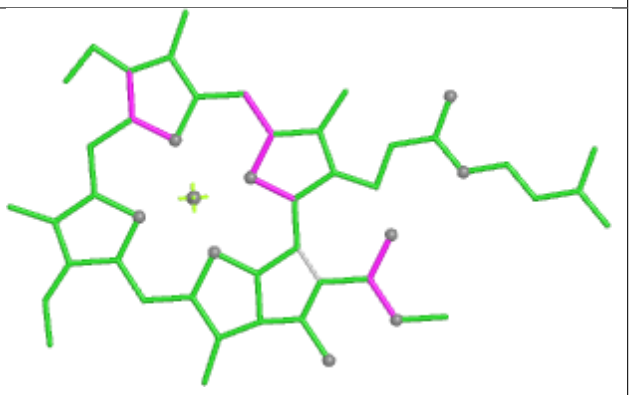


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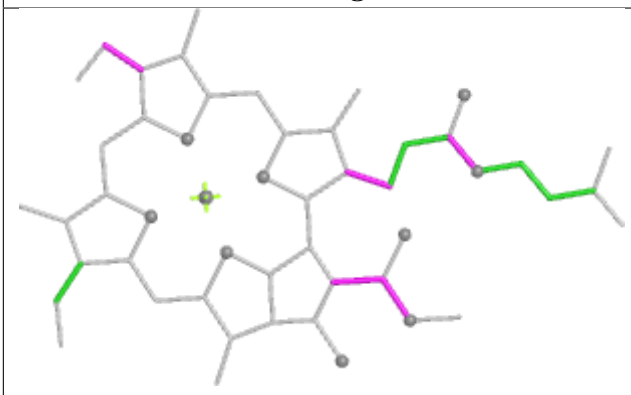
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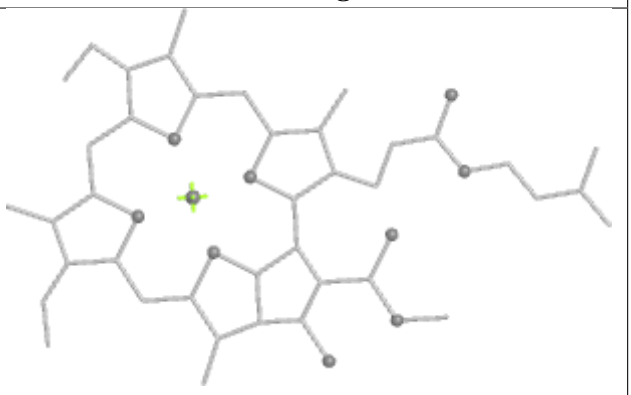
Bond lengths



Bond angles

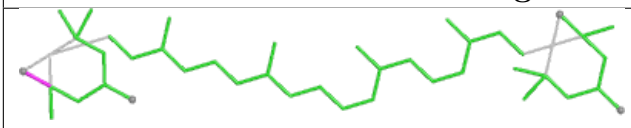


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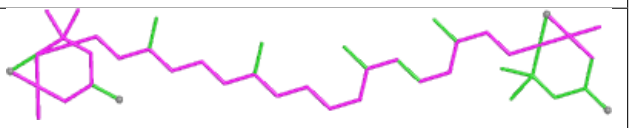


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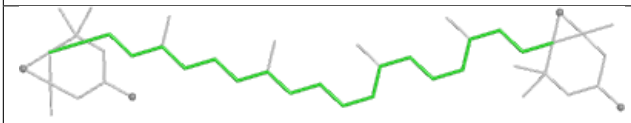
Ligand XAT X 1622



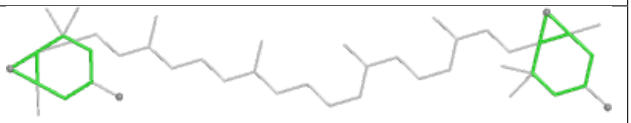
Bond lengths



Bond angles

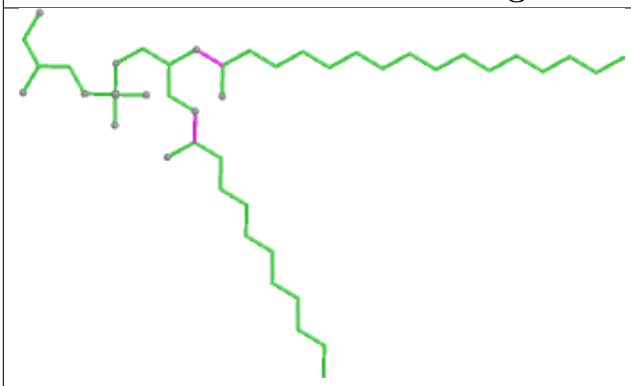


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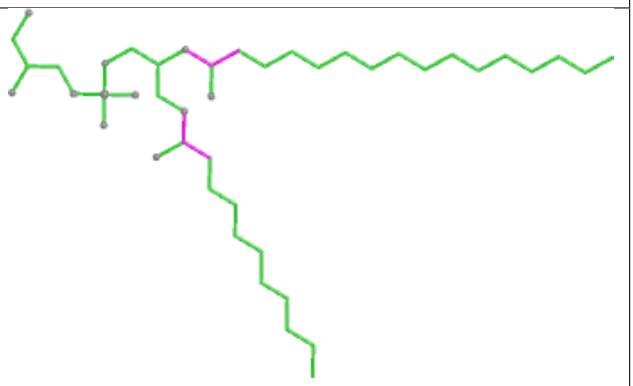


Rings

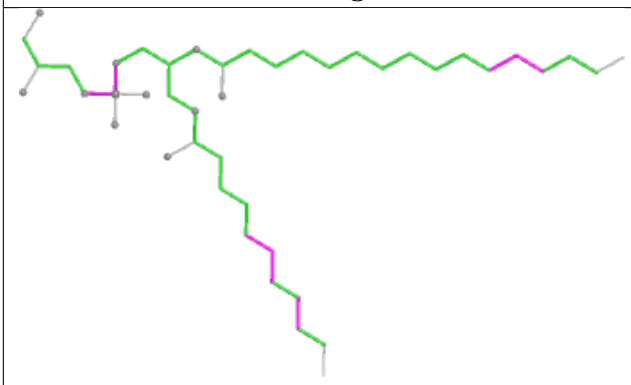
Ligand LHG W 2630



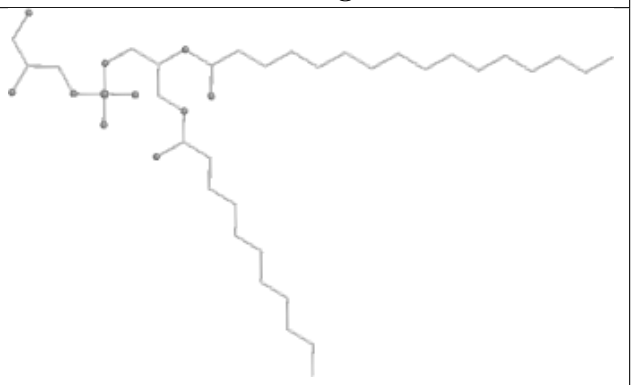
Bond lengths



Bond angles

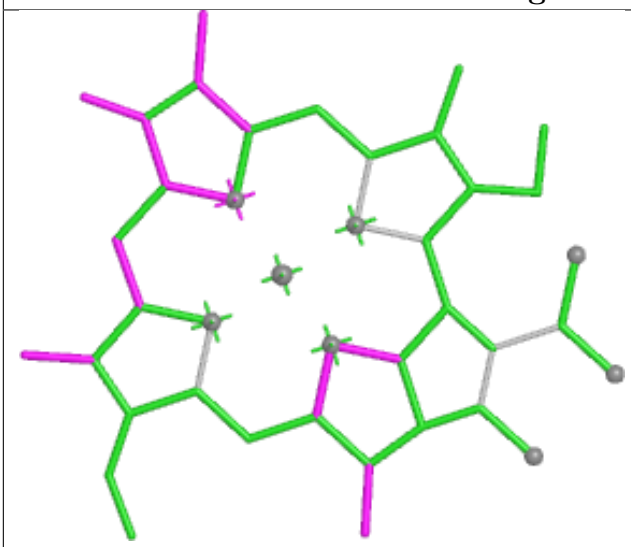


Torsions

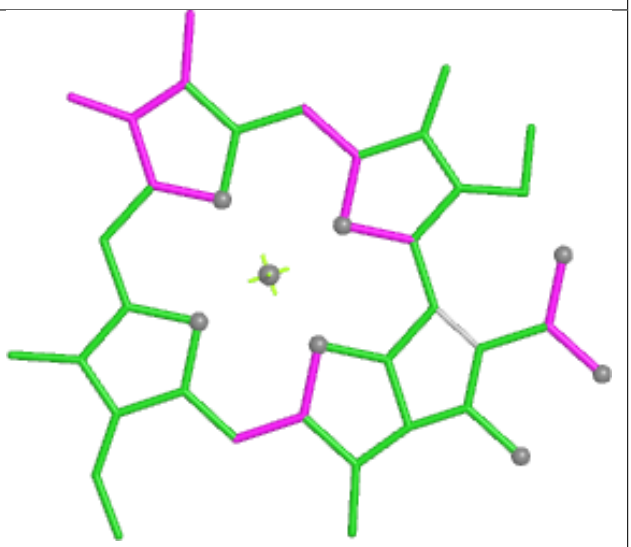


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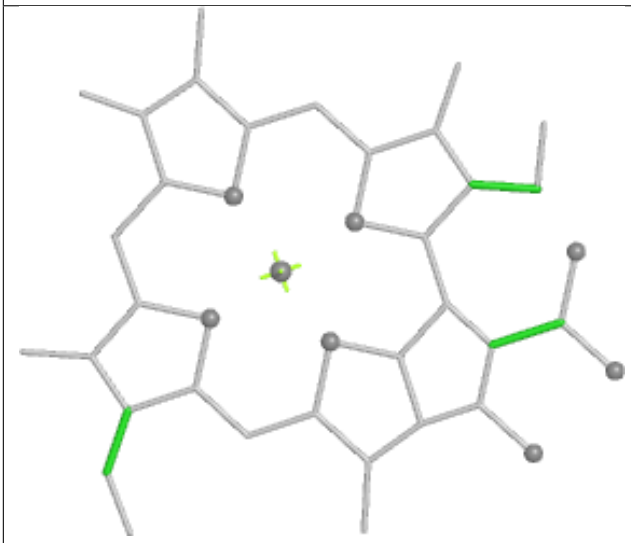
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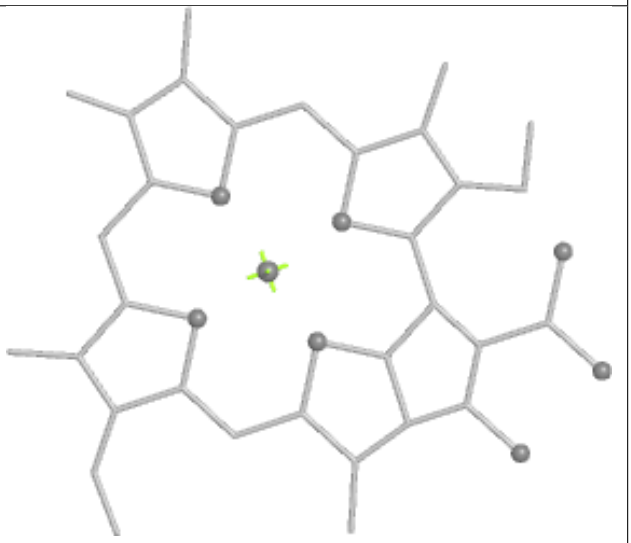
Bond lengths



Bond angles

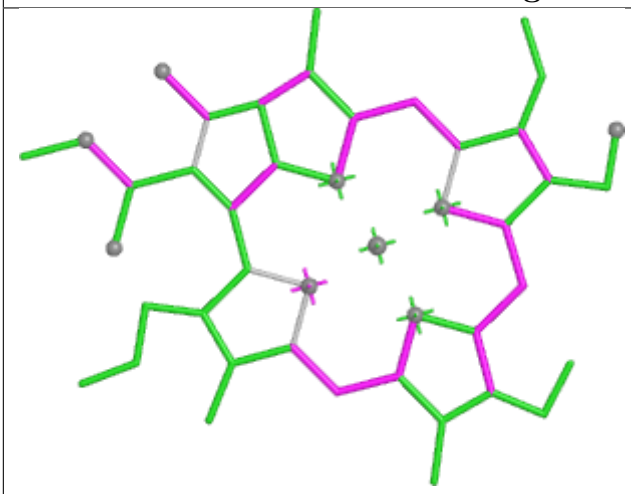


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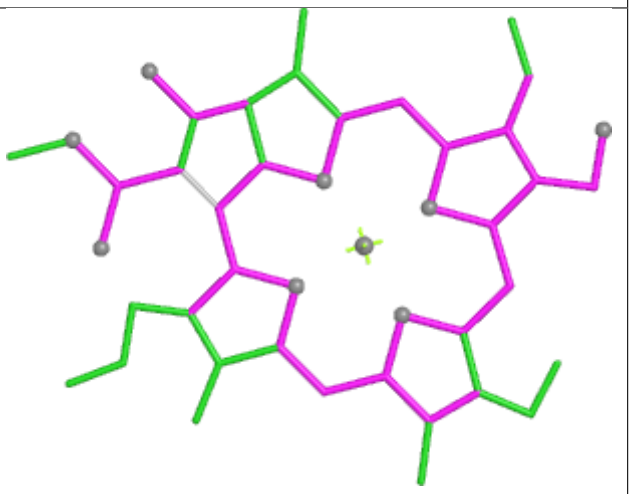


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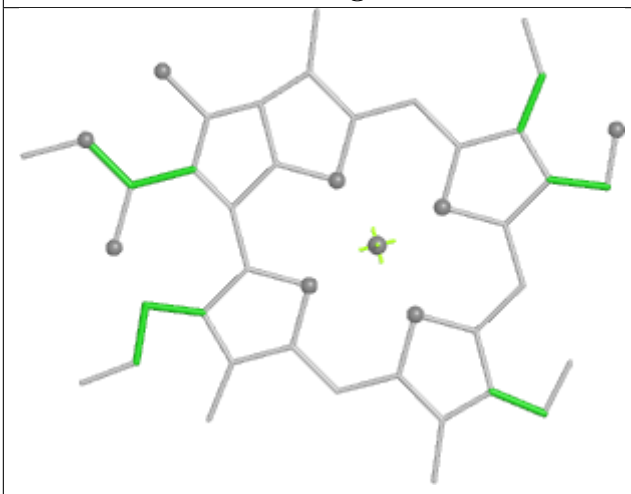
Ligand CHL V 605



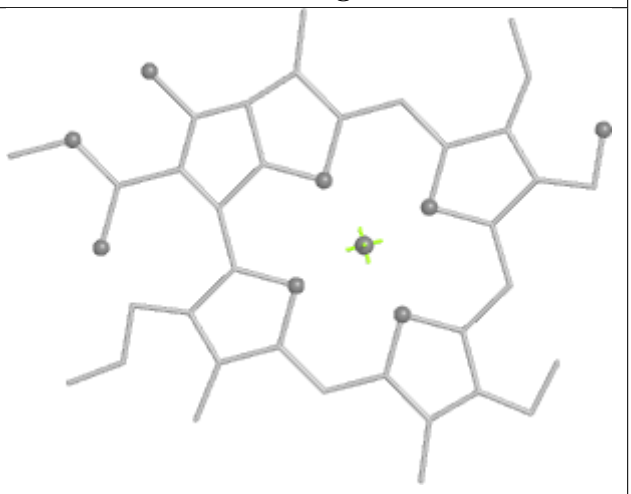
Bond lengths



Bond angles

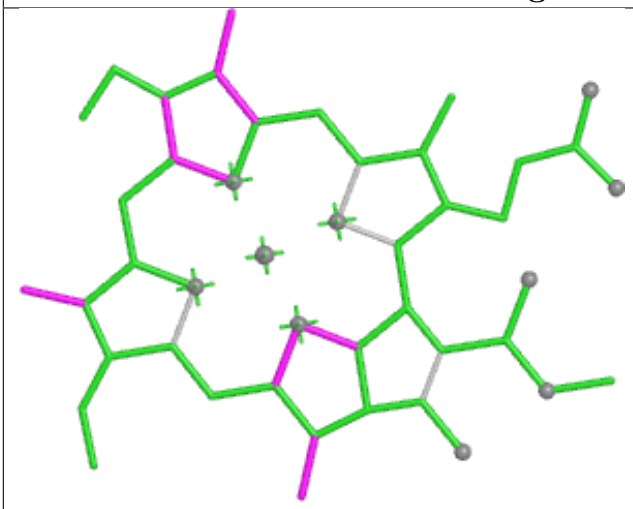


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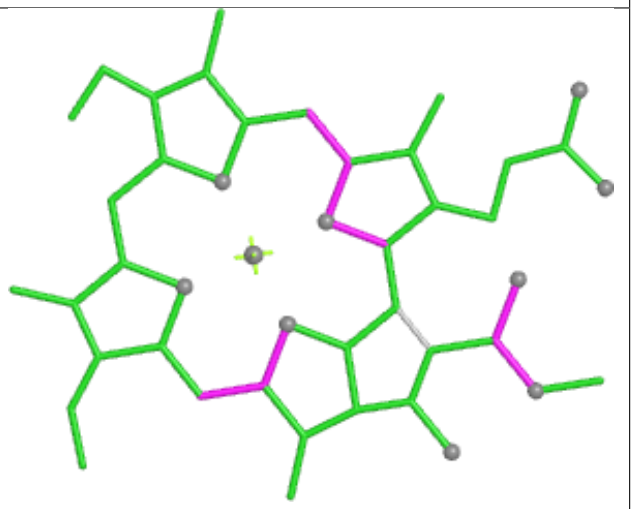


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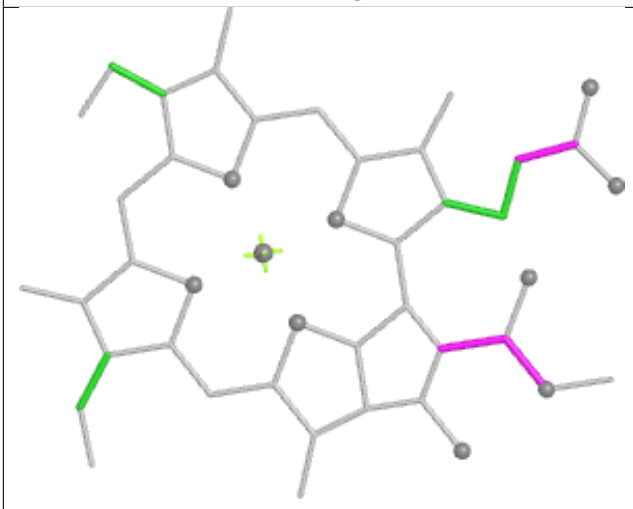
Ligand CLA a 612



Bond lengths



Bond angles

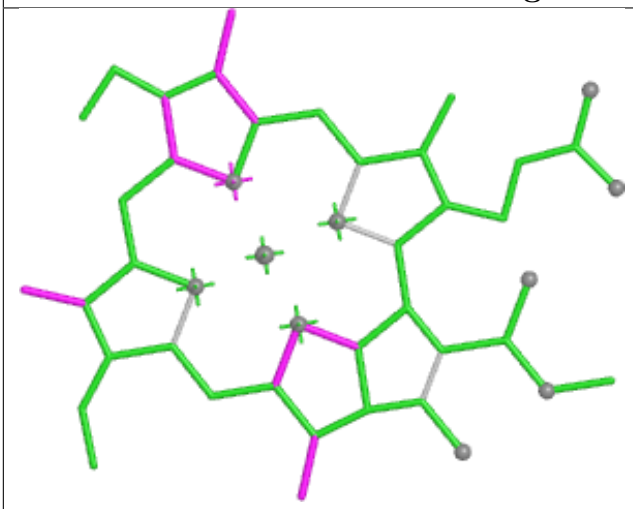


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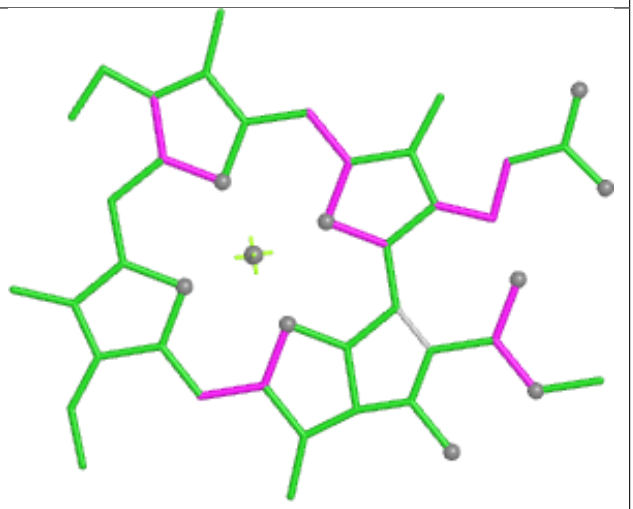


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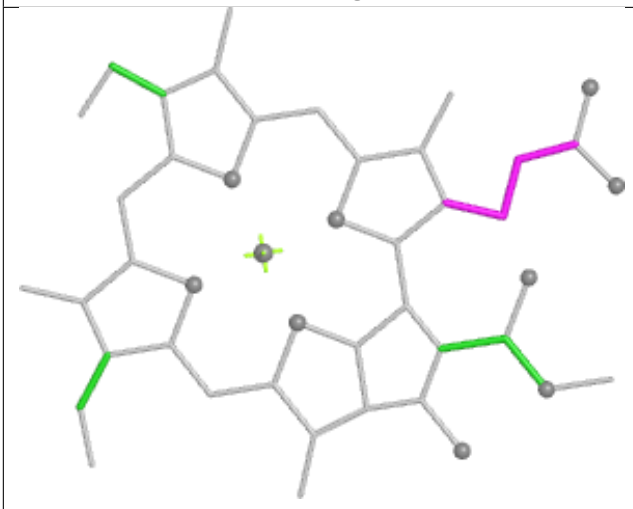
Ligand CLA A 833



Bond lengths



Bond angles

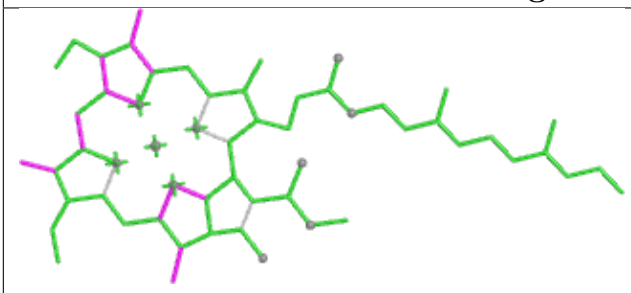


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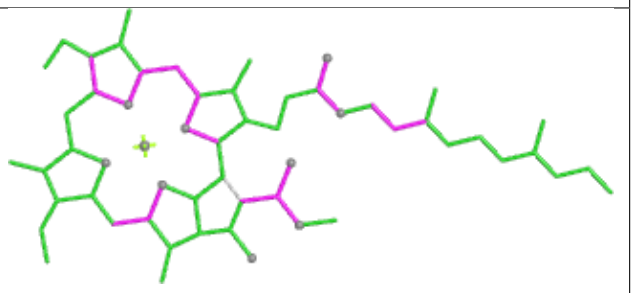


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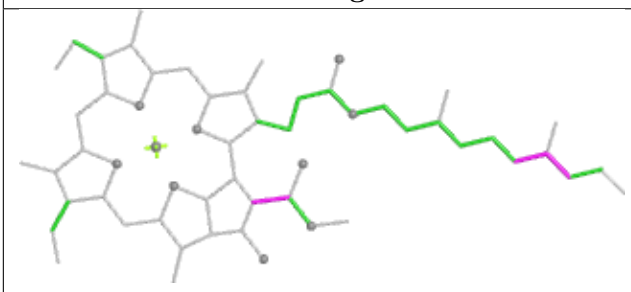
Ligand CLA 9 610



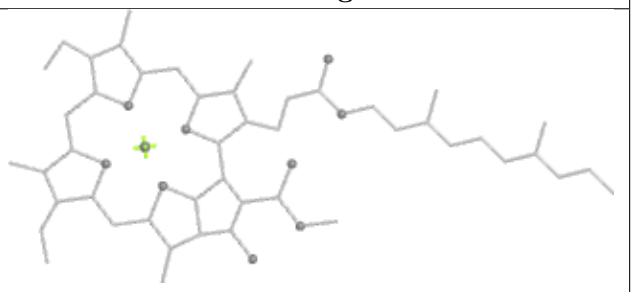
Bond lengths



Bond angles

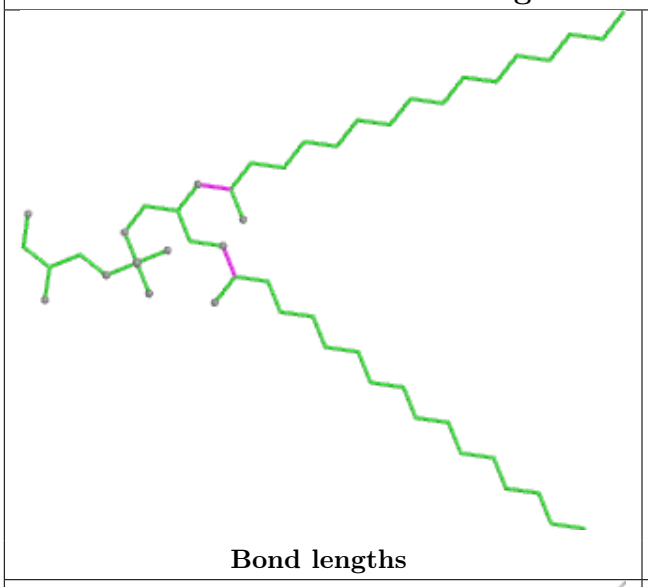


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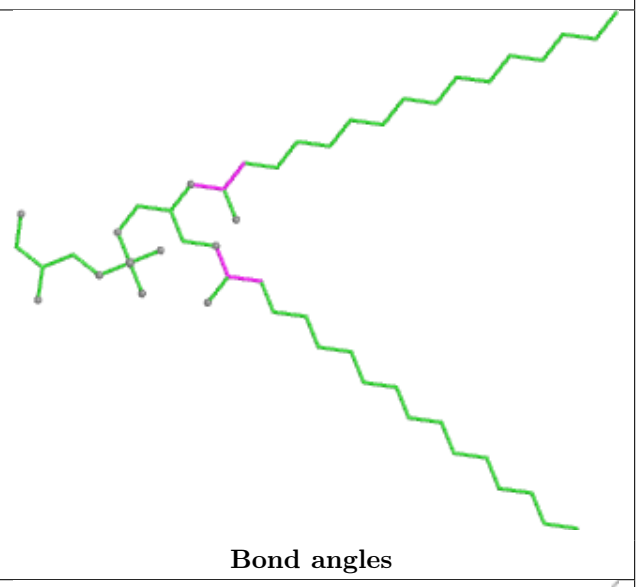


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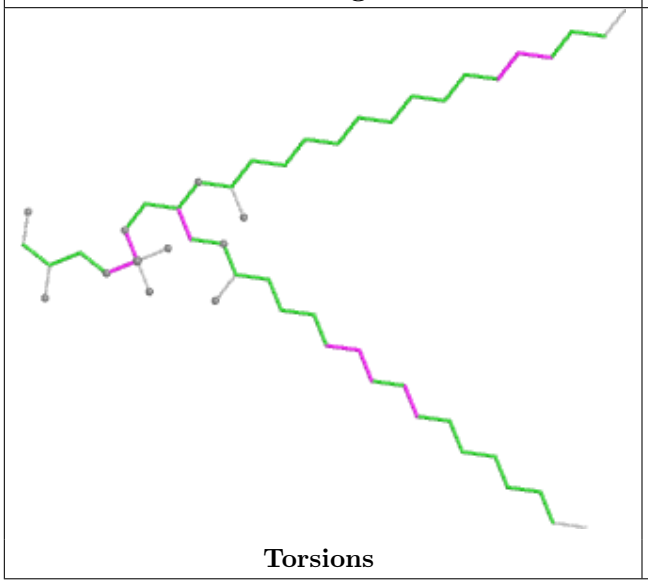
Ligand LHG Y 2630



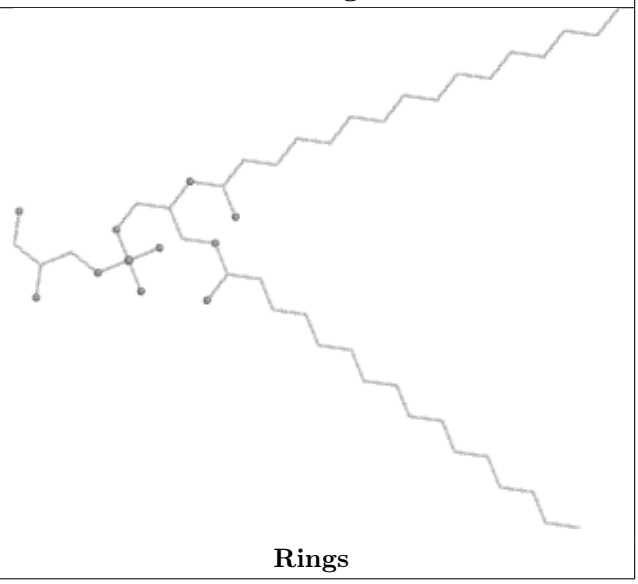
Bond lengths



Bond angles

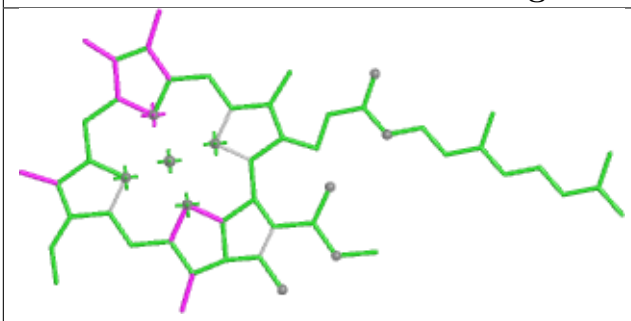


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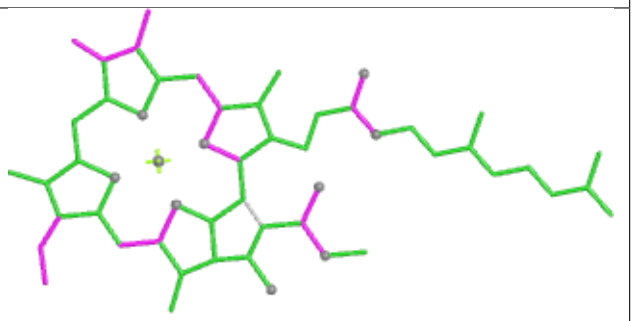


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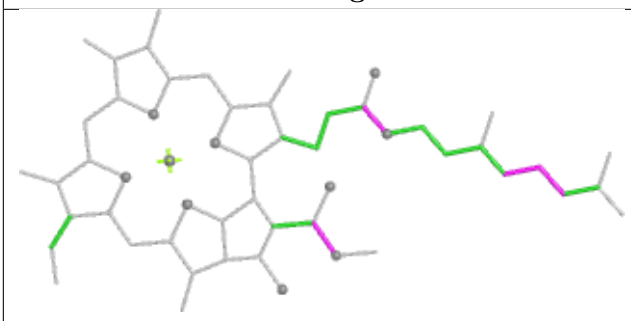
Ligand CLA 5 603



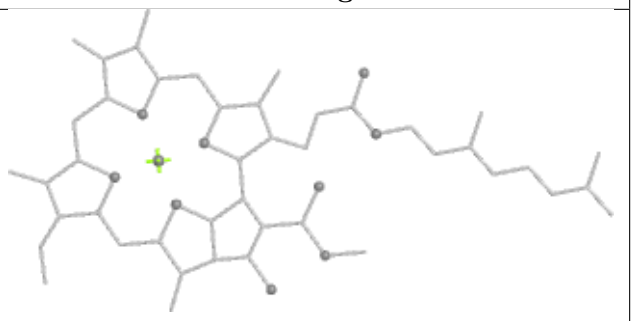
Bond lengths



Bond angles

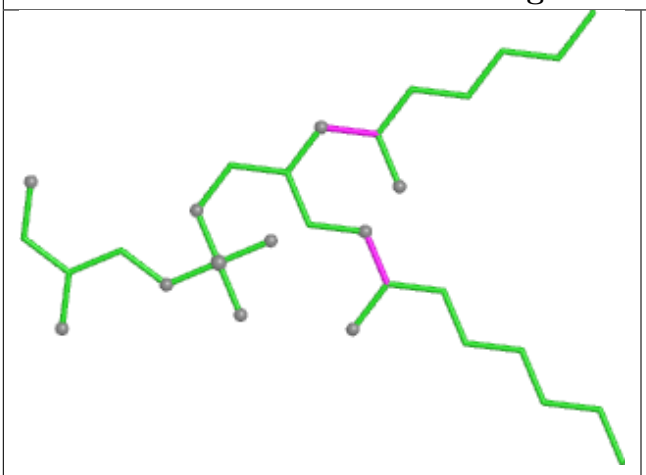


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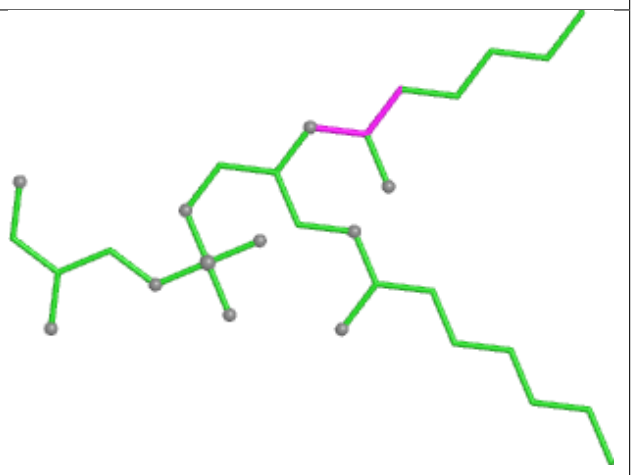


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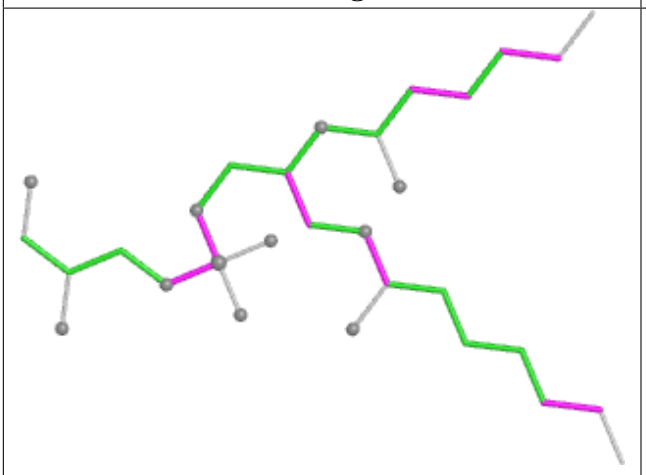
Ligand LHG 9 622



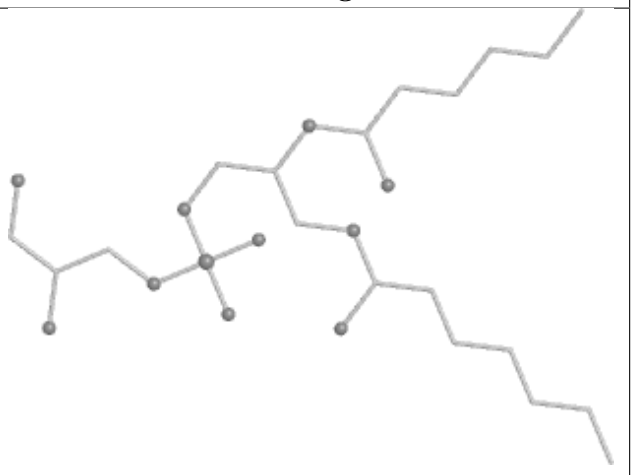
Bond lengths



Bond angles

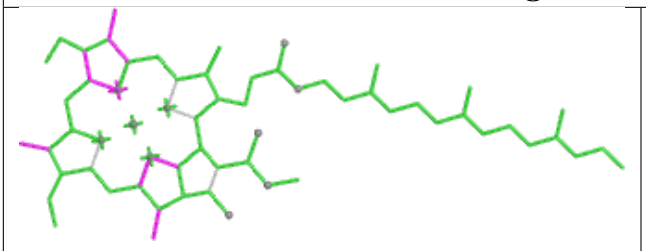


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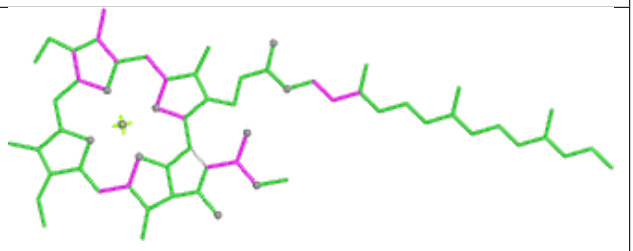


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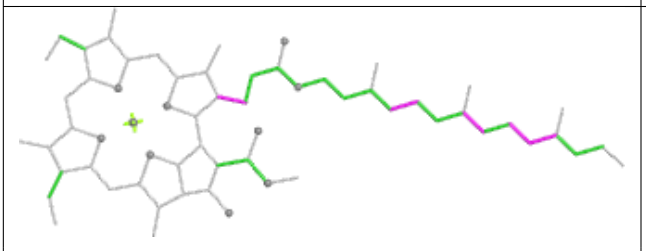
Ligand CLA B 826



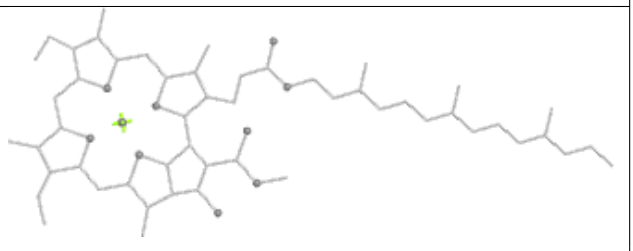
Bond lengths



Bond angles

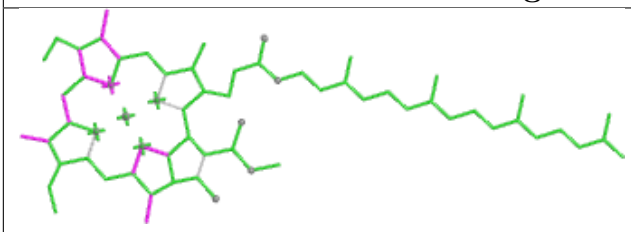


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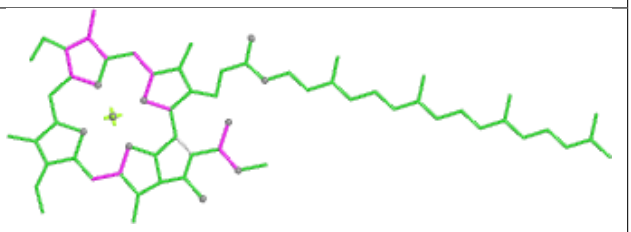


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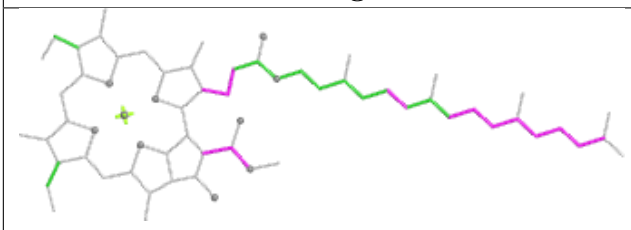
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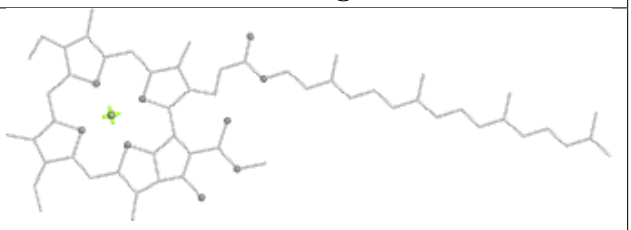
Bond lengths



Bond angles

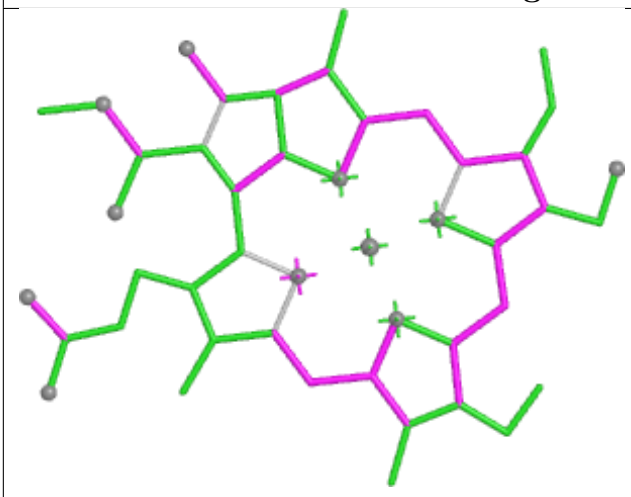


Torsions



Rings

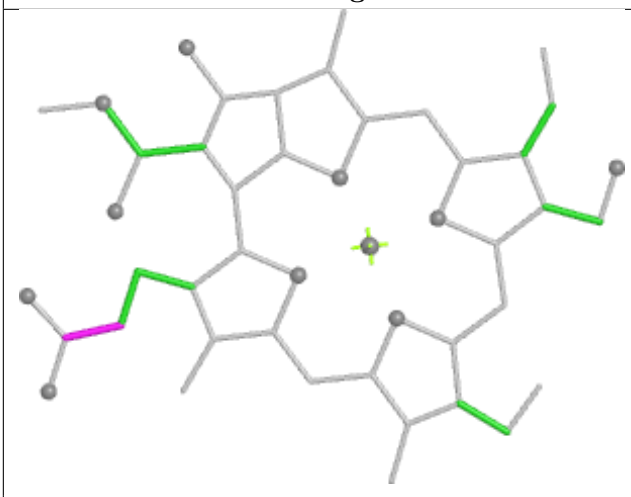
Ligand CHL Y 606



Bond lengths



Bond angles

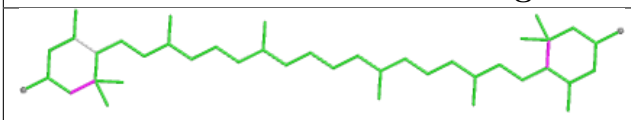


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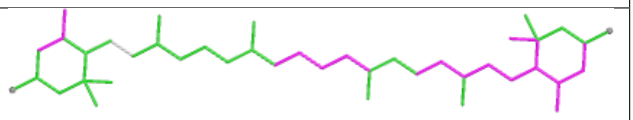


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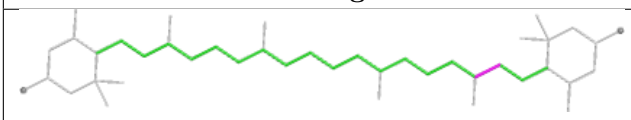
Ligand LUT U 1621



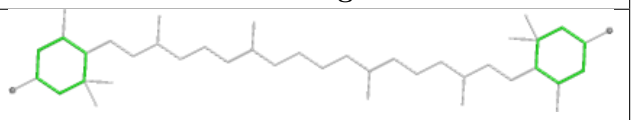
Bond lengths



Bond angles

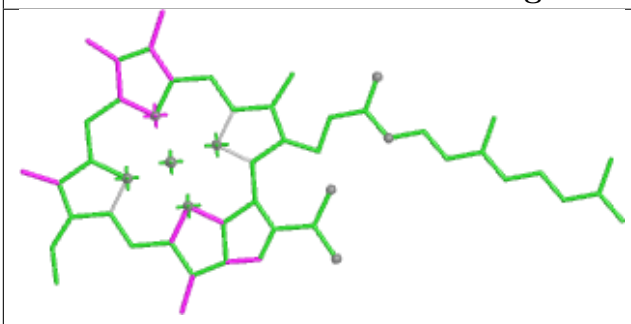


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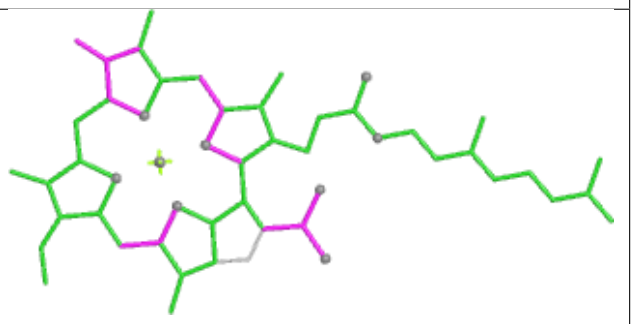


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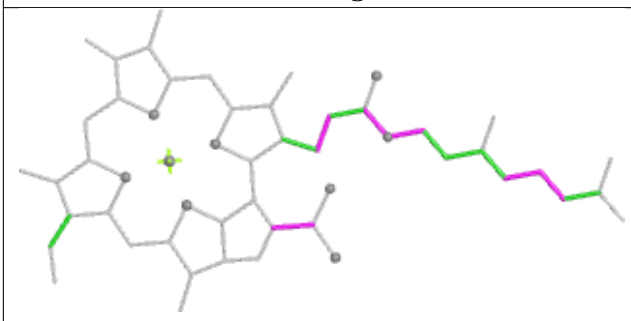
Ligand CLA B 811



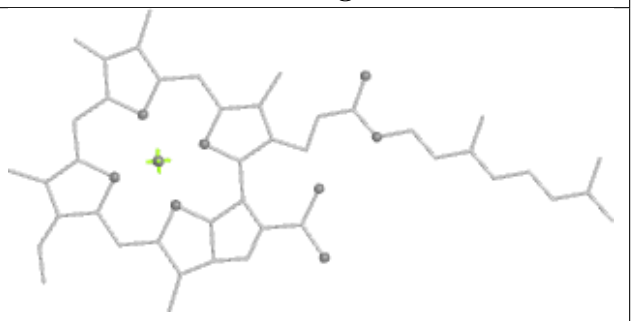
Bond lengths



Bond angles

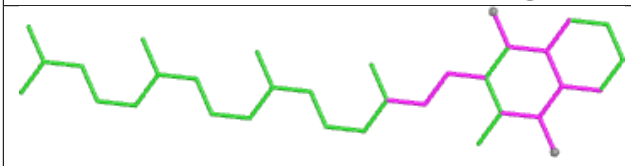


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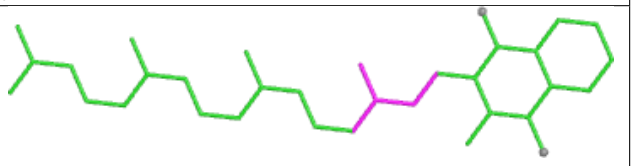


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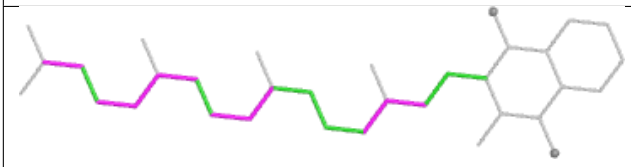
Ligand PQN A 844



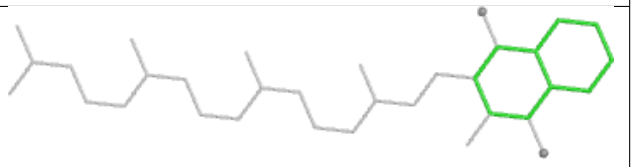
Bond lengths



Bond angles

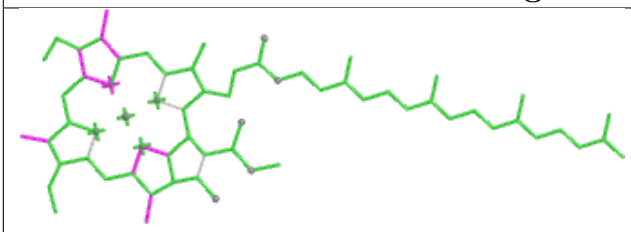


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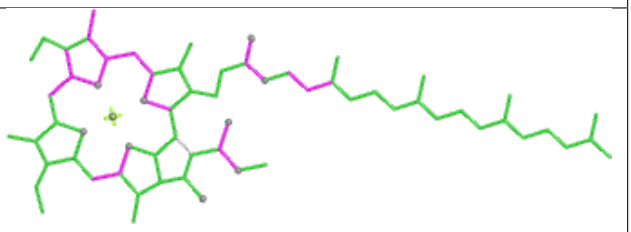


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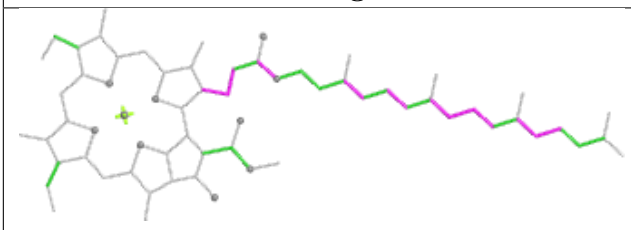
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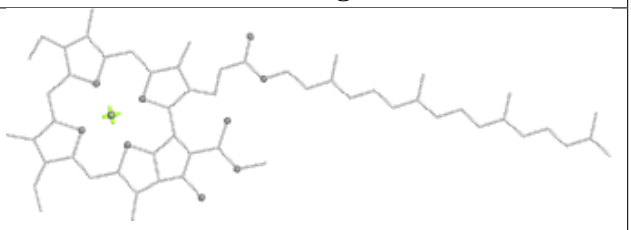
Bond lengths



Bond angles



Torsions

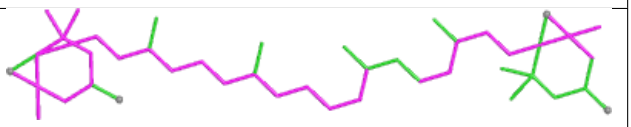


Rings

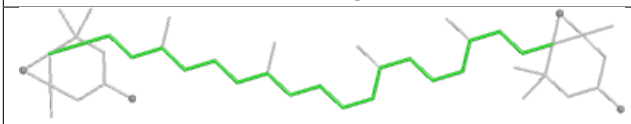
Ligand XAT Z 1622



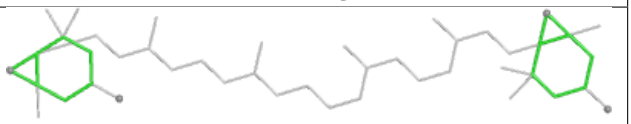
Bond lengths



Bond angles

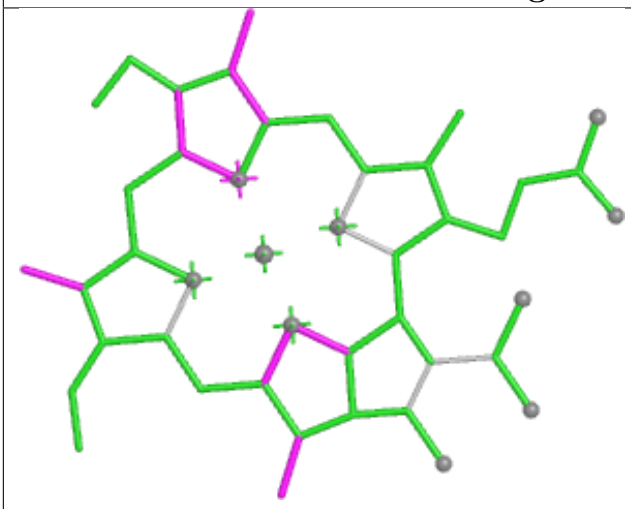


Torsions

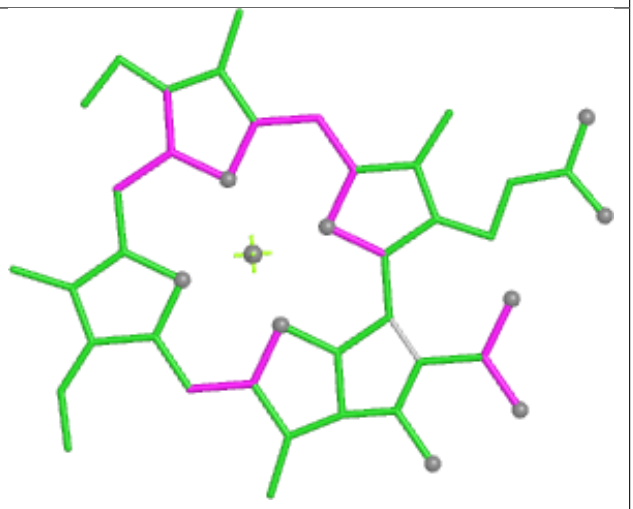


Rings

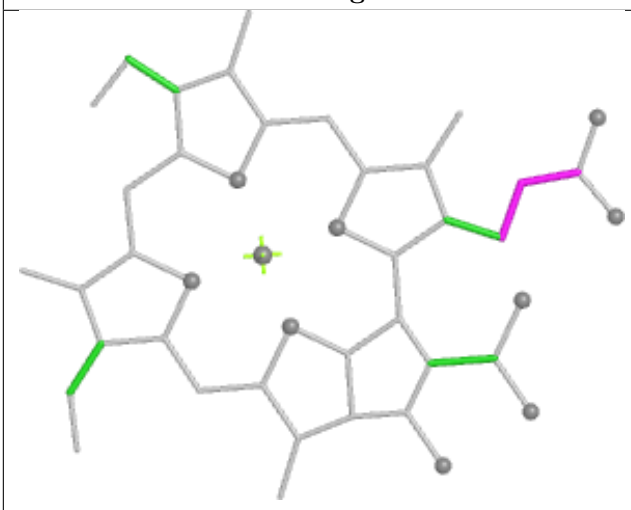
Ligand CLA 7 603



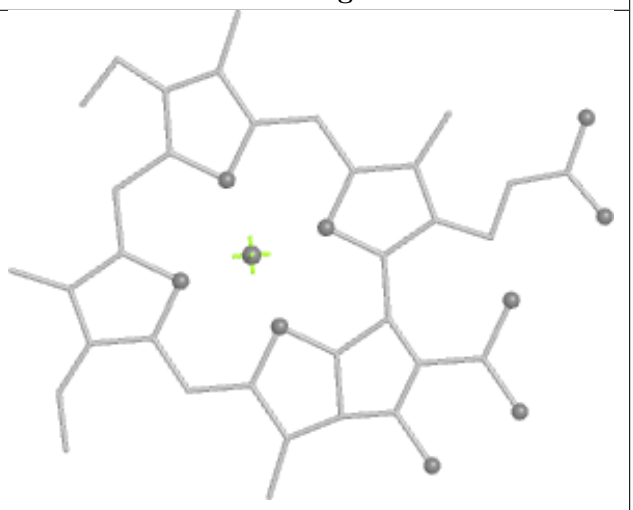
Bond lengths



Bond angles

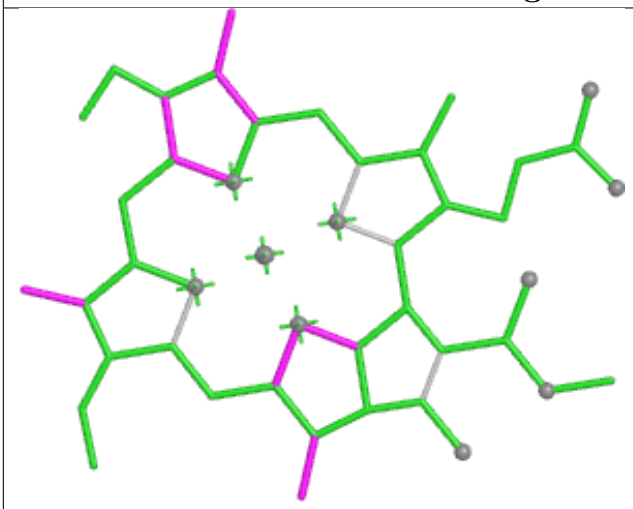


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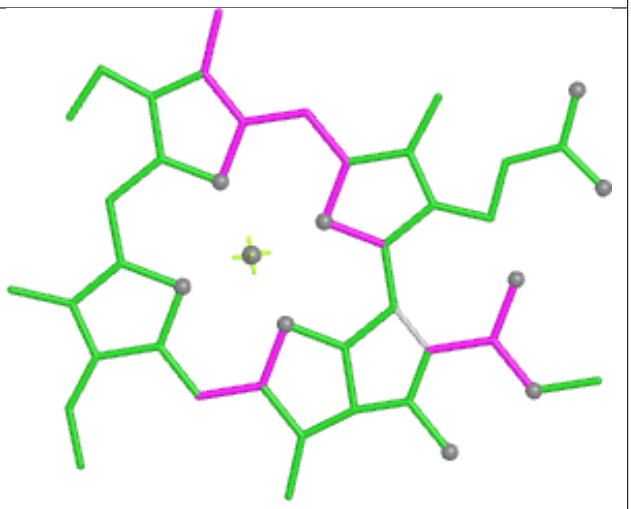


Rings

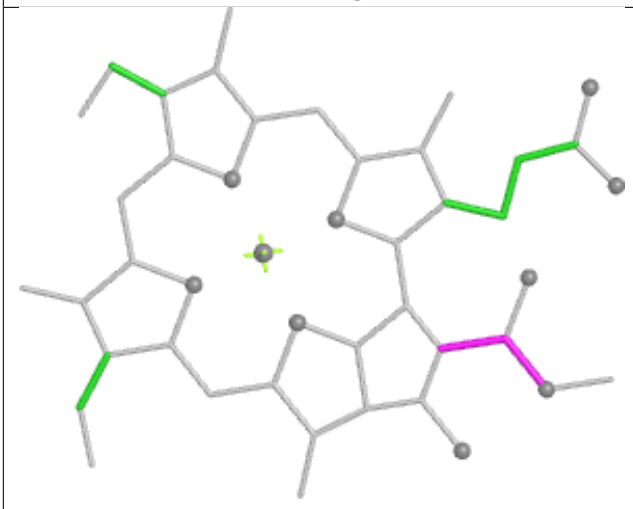
Ligand CLA A 817



Bond lengths



Bond angles

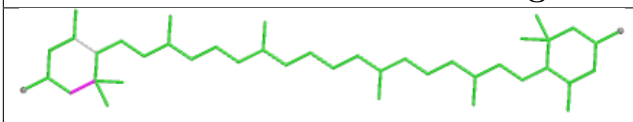


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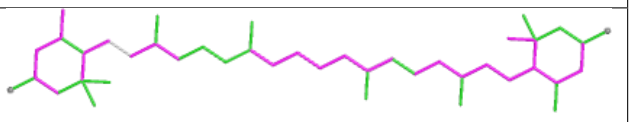


Rings

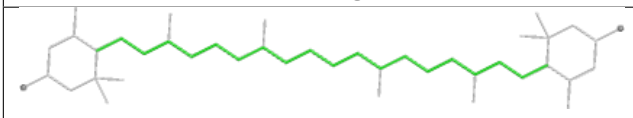
Ligand LUT 6 619



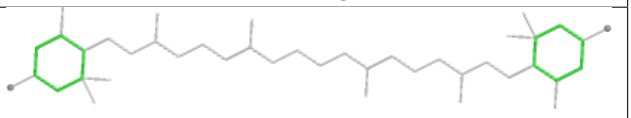
Bond lengths



Bond angles

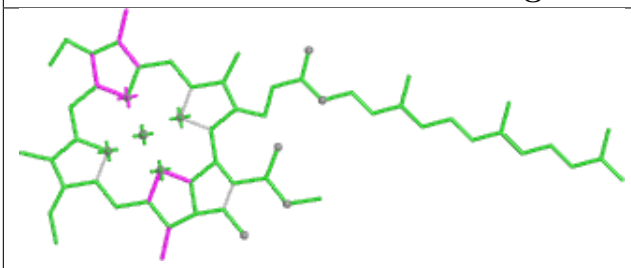


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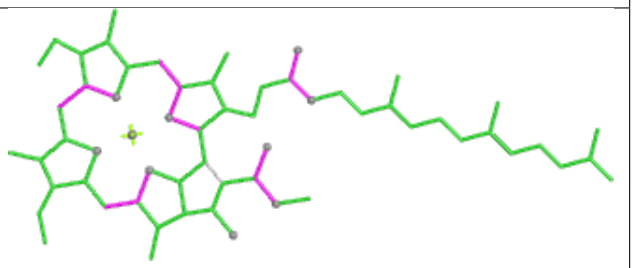


Rings

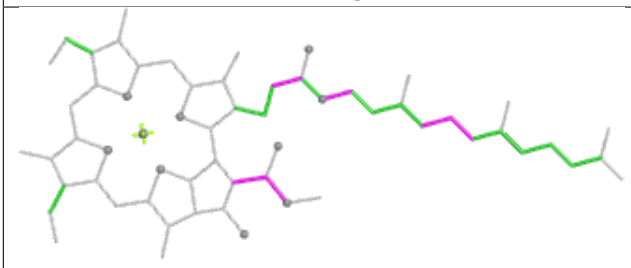
Ligand CLA B 834



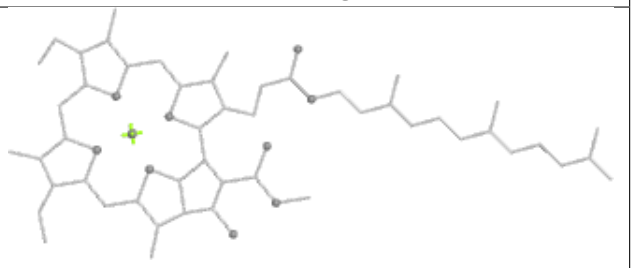
Bond lengths



Bond angles

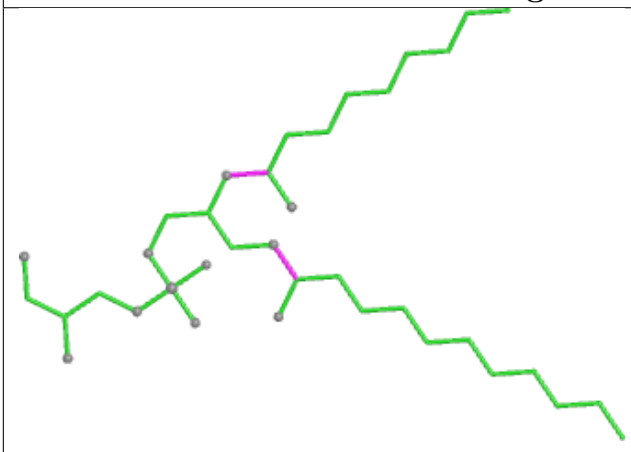


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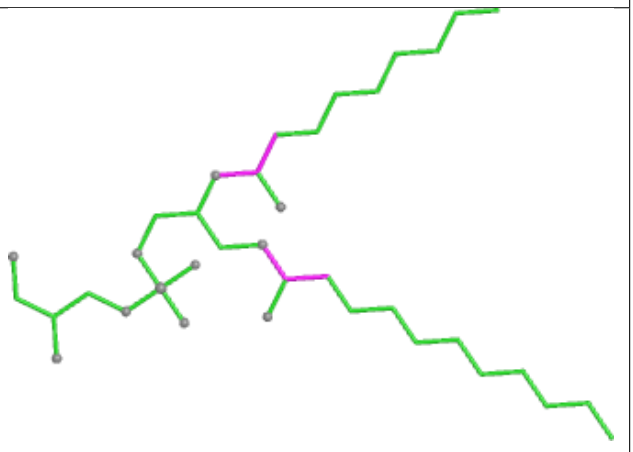


Rings

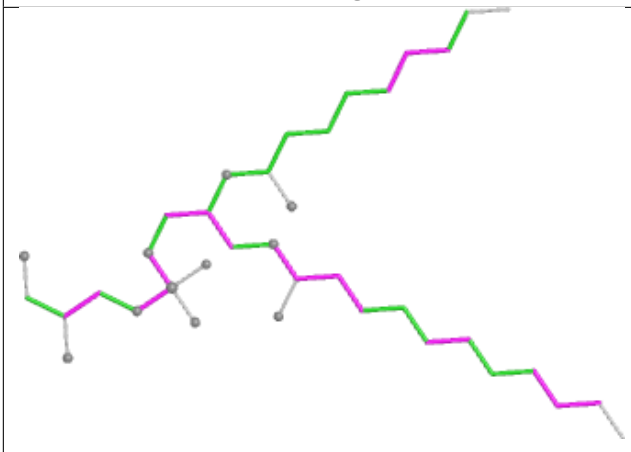
Ligand LHG 7 622



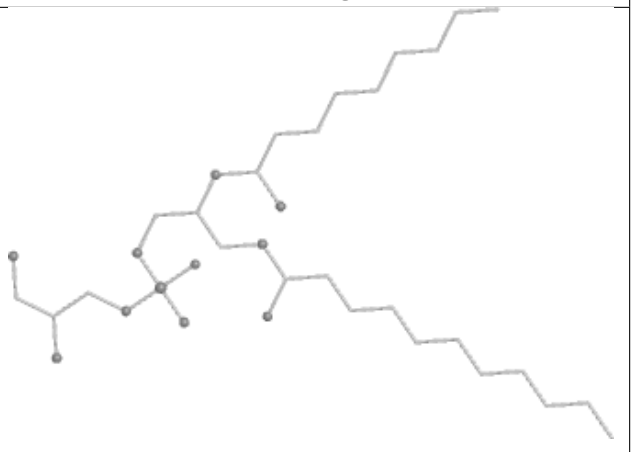
Bond lengths



Bond angles

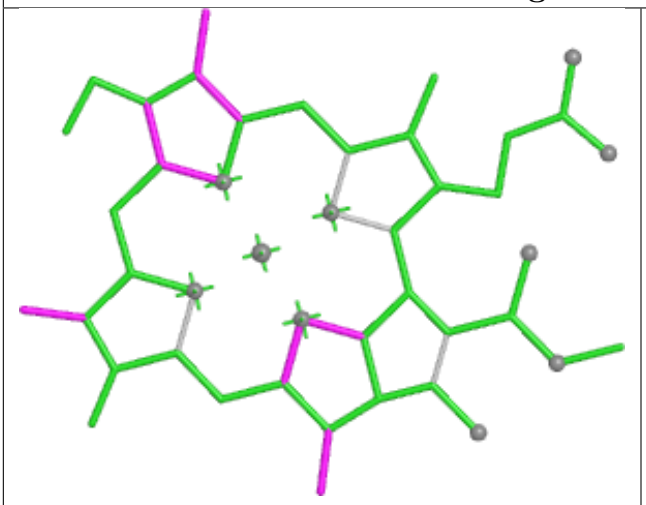


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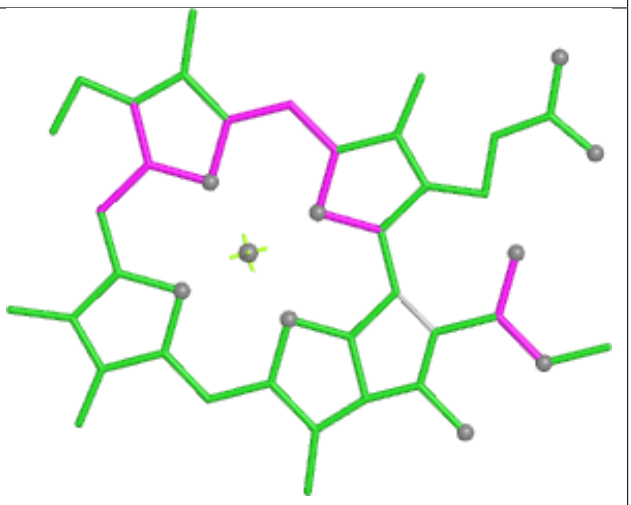


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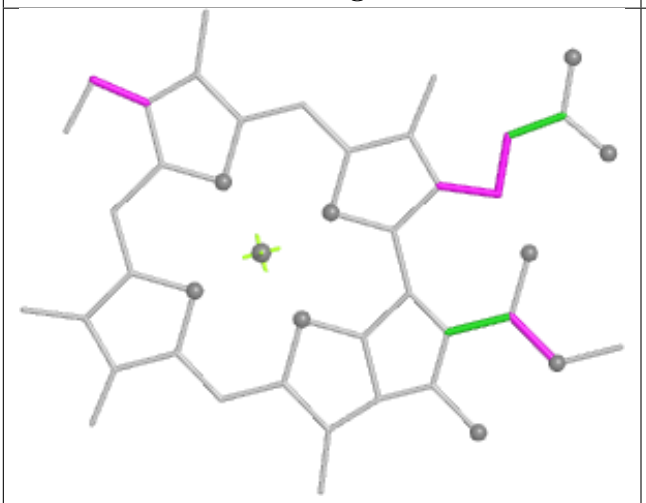
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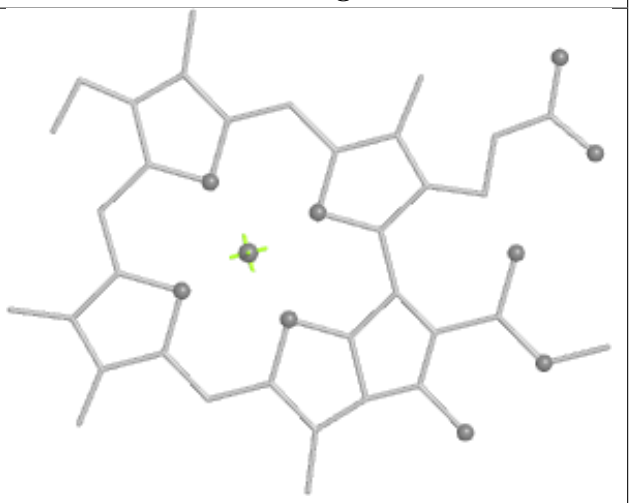
Bond lengths



Bond angles

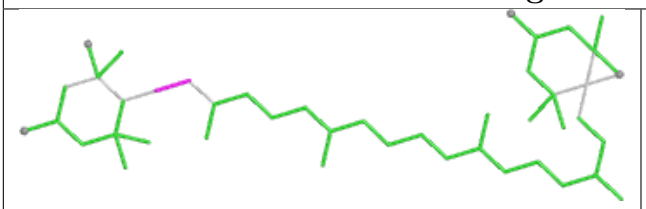


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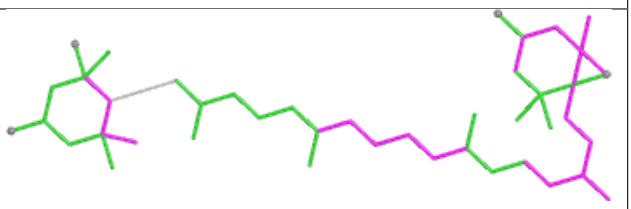


Rings

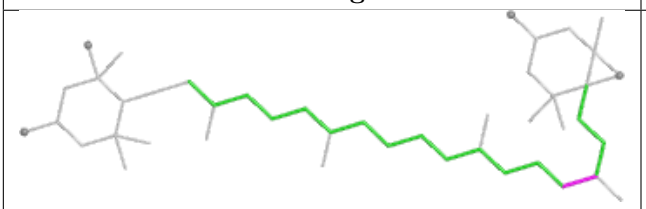
Ligand NEX 6 624



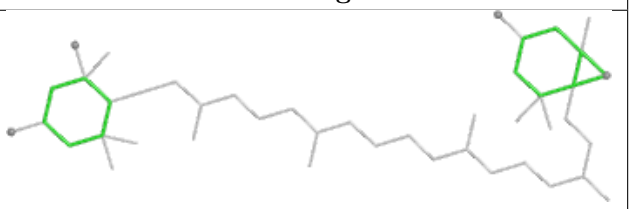
Bond lengths



Bond angles

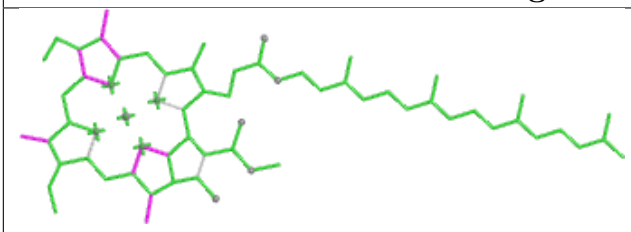


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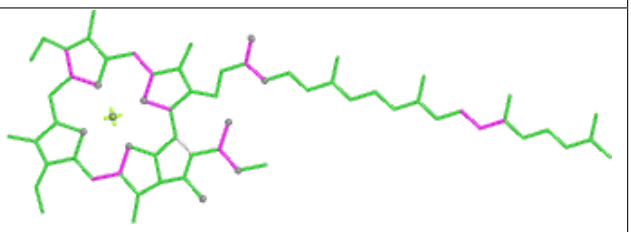


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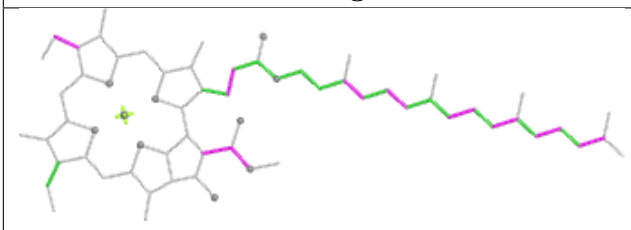
Ligand CLA 1 613



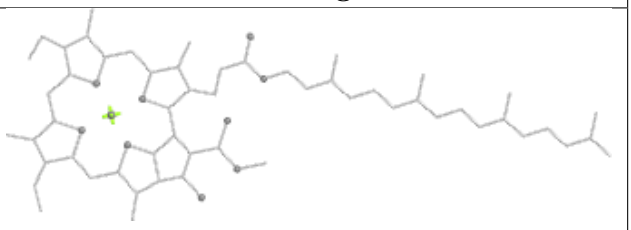
Bond lengths



Bond angles

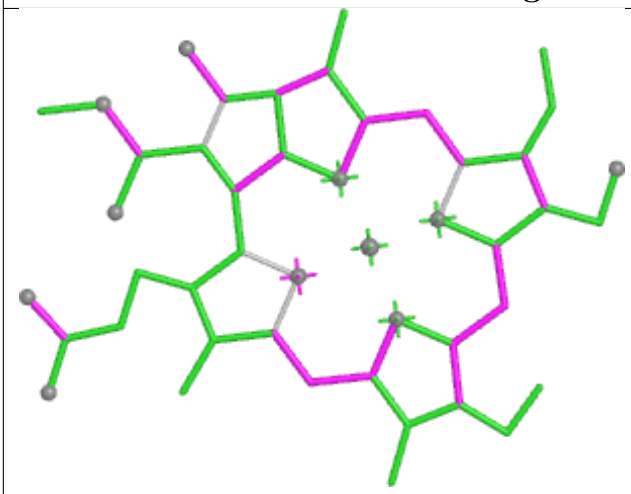


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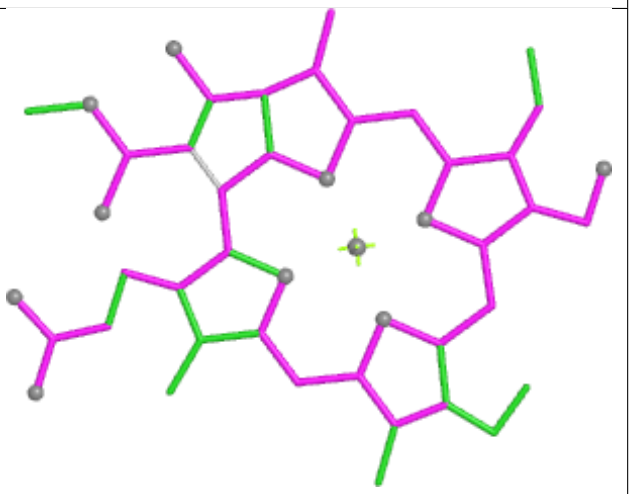


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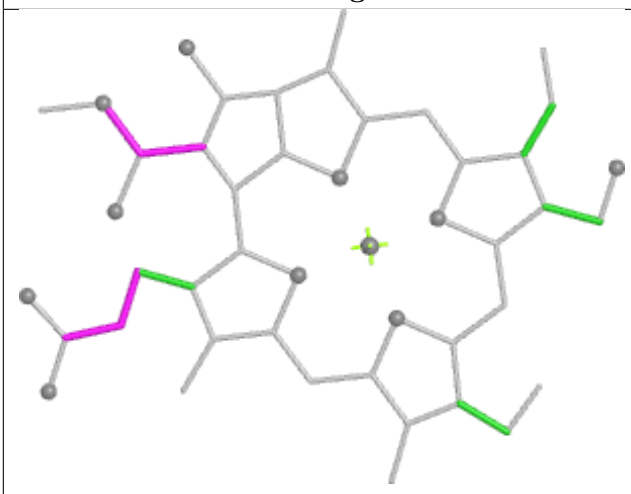
Ligand CHL U 607



Bond lengths



Bond angles

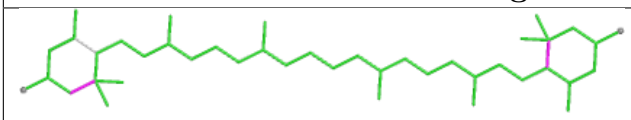


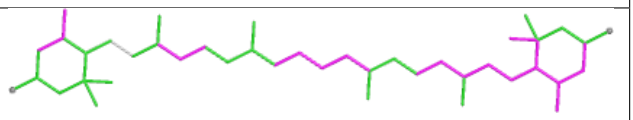
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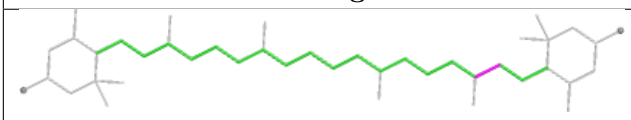


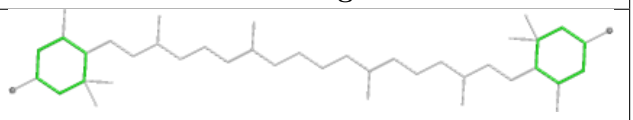
Rings

Ligand LUT W 1621


Bond lengths

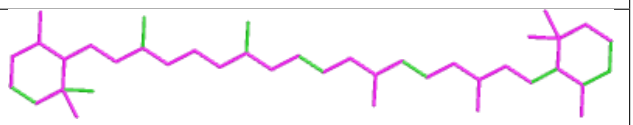

Bond angles

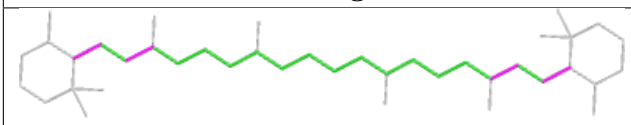

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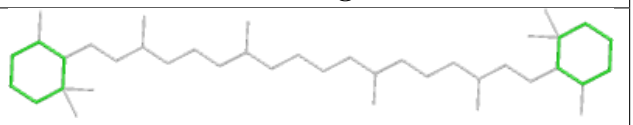

Rings

Ligand BCR O 2005

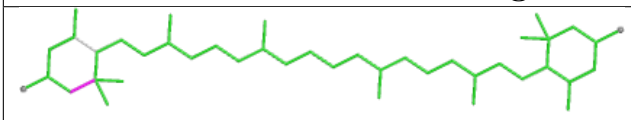

Bond lengths

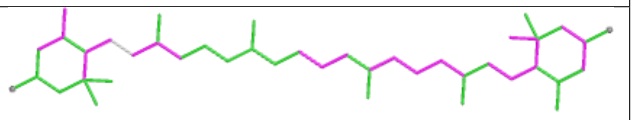

Bond angles

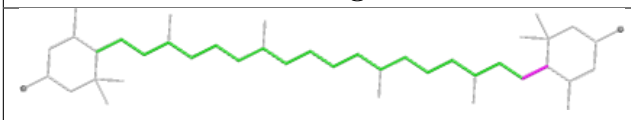

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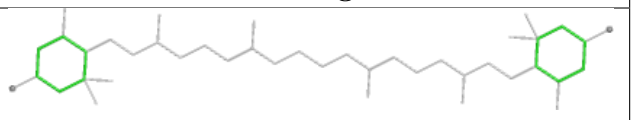

Rings

Ligand LUT W 1620

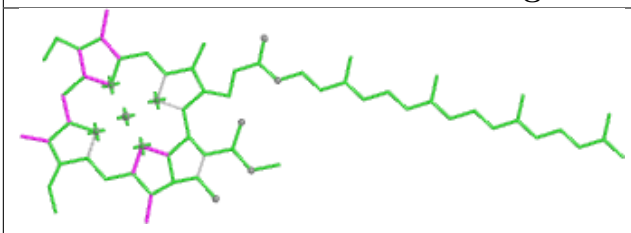

Bond lengths

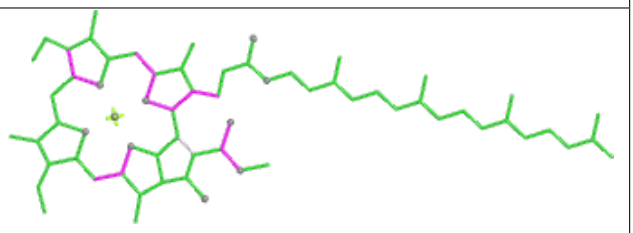

Bond angles

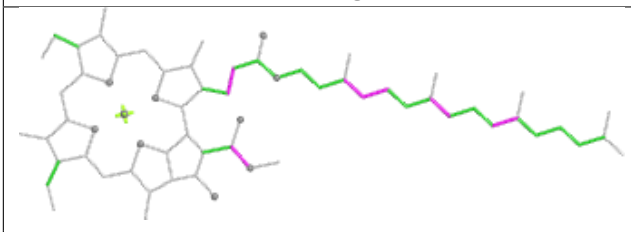

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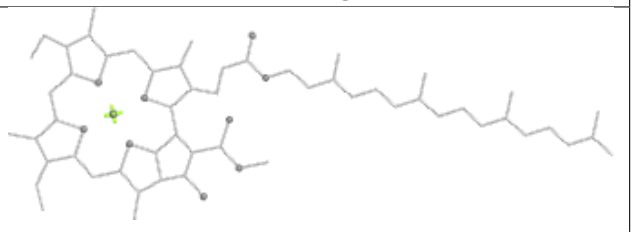

Rings

Ligand CLA A 802

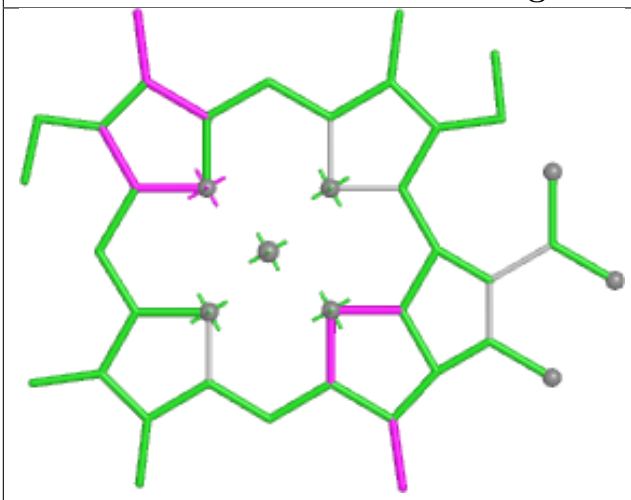

Bond lengths


Bond angles

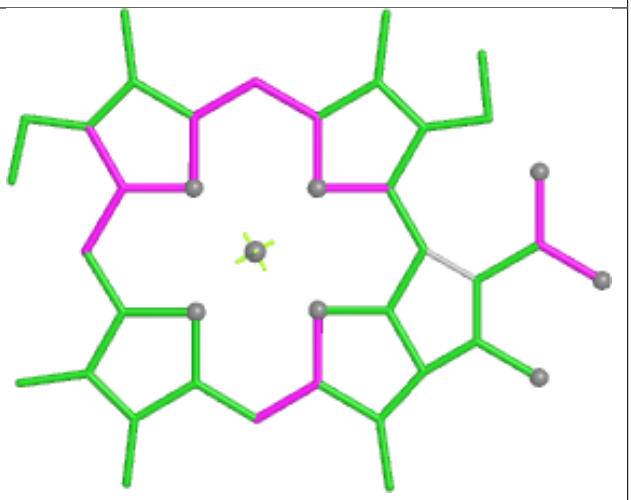

Torsions


Rings

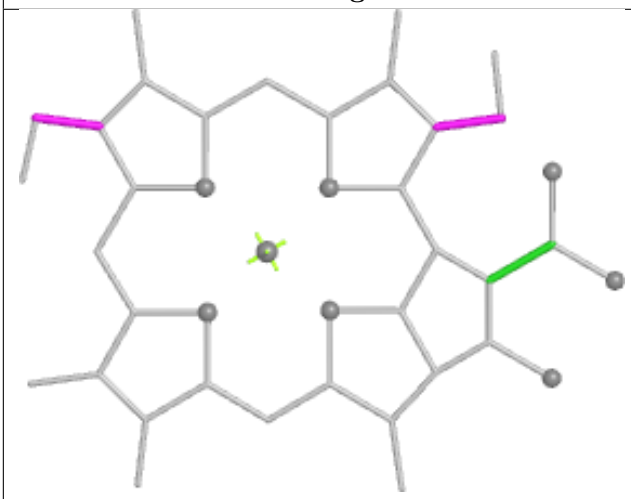
Ligand CLA 4 606



Bond lengths



Bond angles

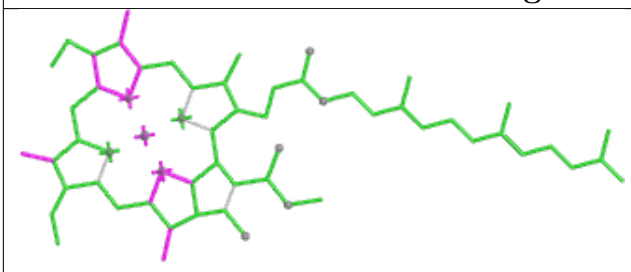


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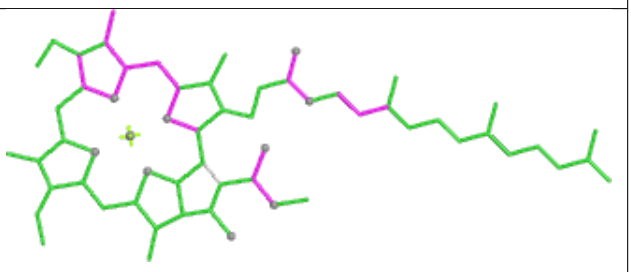


Rings

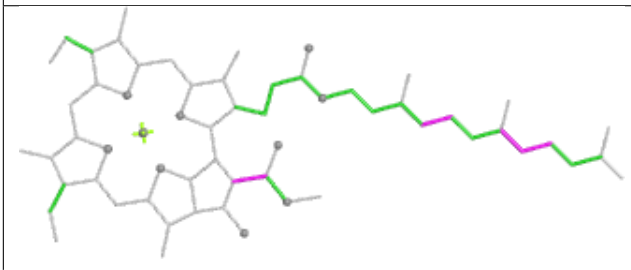
Ligand CLA V 602



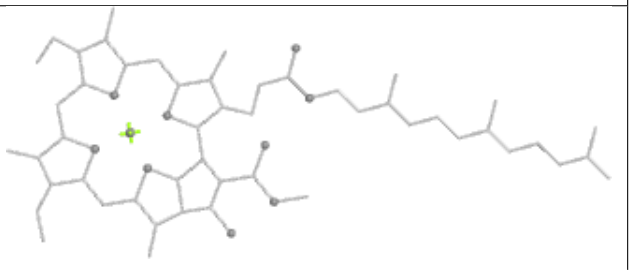
Bond lengths



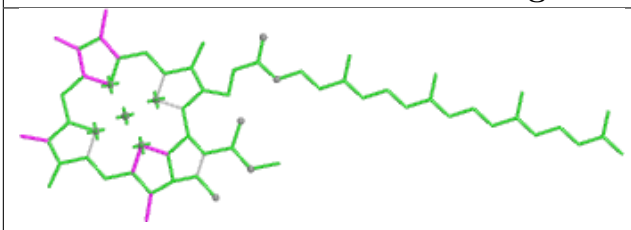
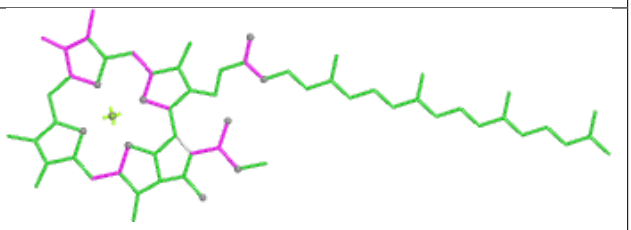
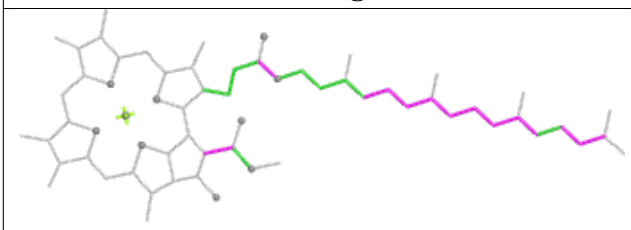
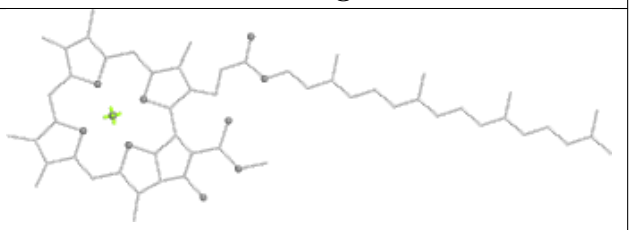
Bond angles

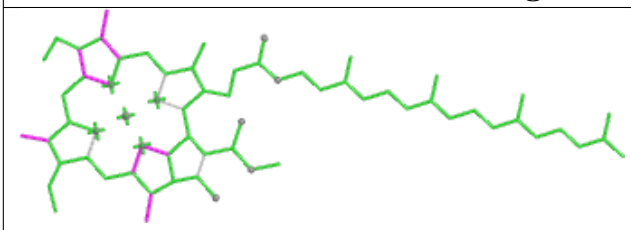
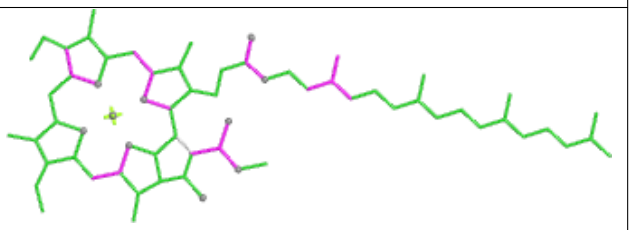
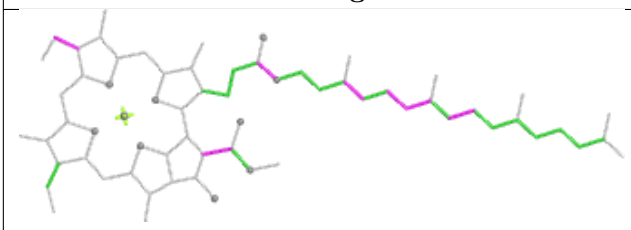
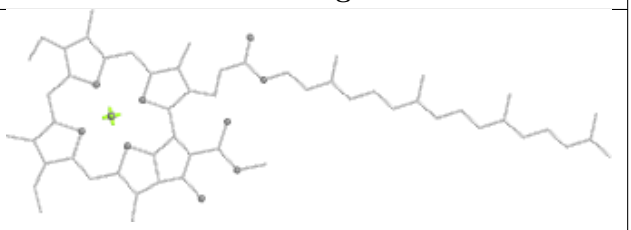


Torsions

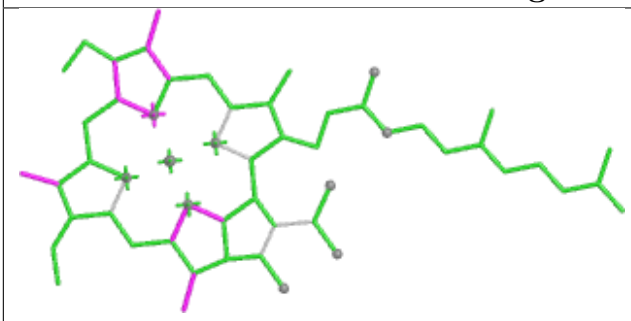


Rings

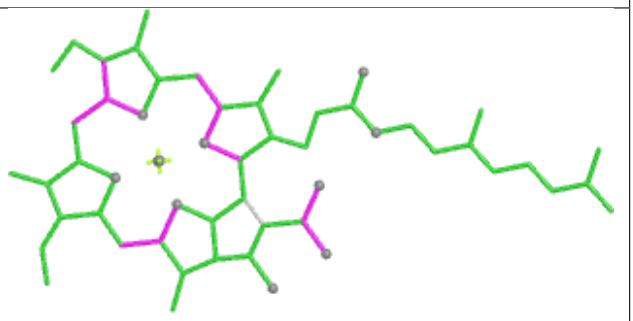
Ligand CLA 5 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 833	
 Bond lengths	 Bond angles
 Torsions	 Rings

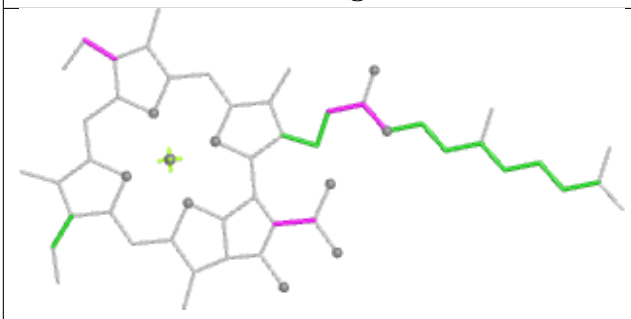
Ligand CLA 3 606



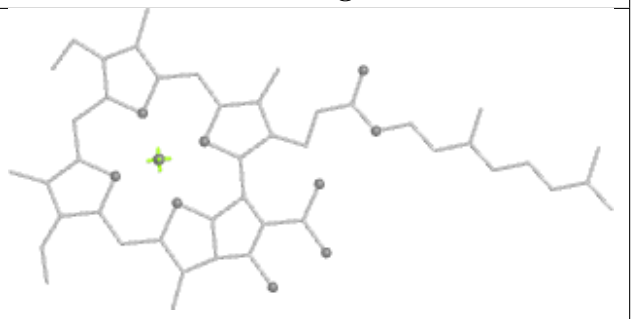
Bond lengths



Bond angles

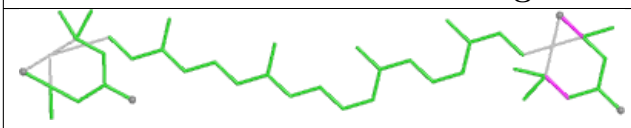


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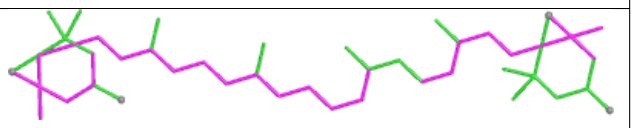


Rings

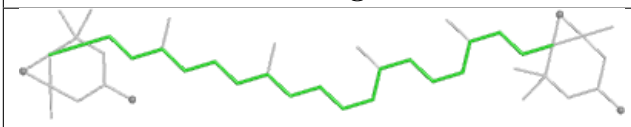
Ligand XAT V 1622



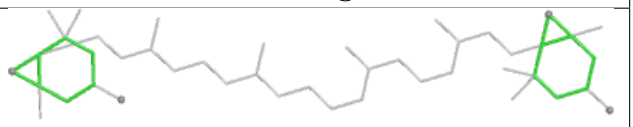
Bond lengths



Bond angles

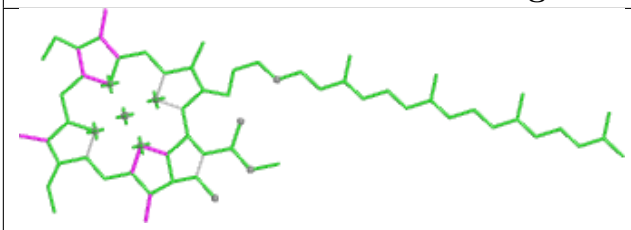


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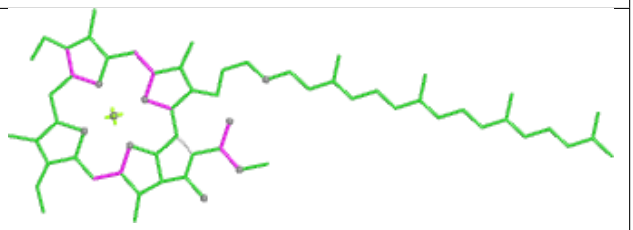


Rings

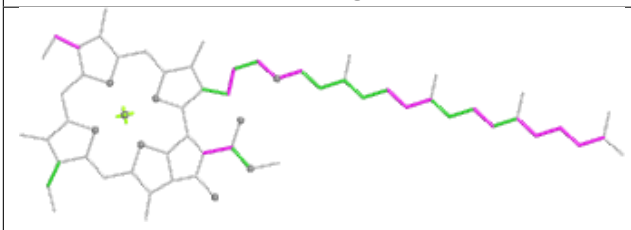
Ligand CLA 5 613



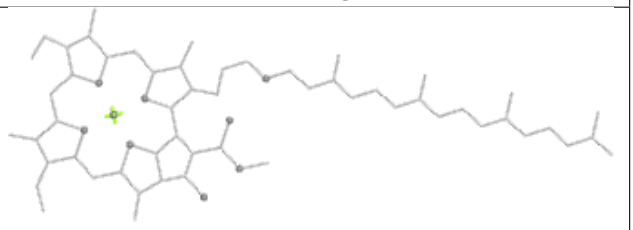
Bond lengths



Bond angles

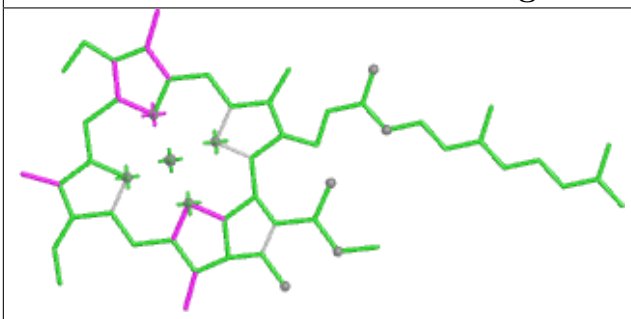


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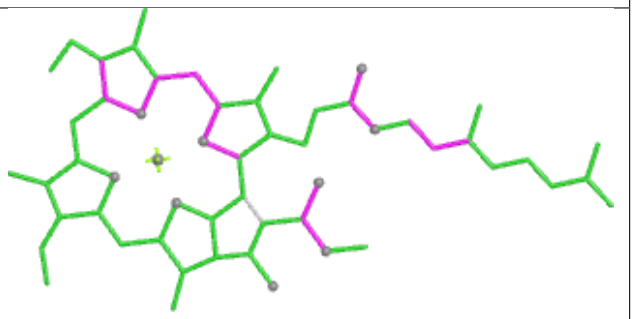


Rings

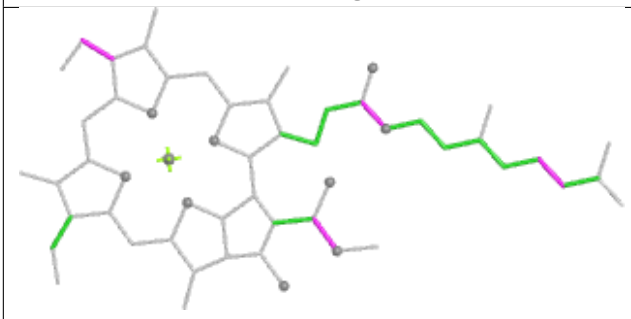
Ligand CLA W 610



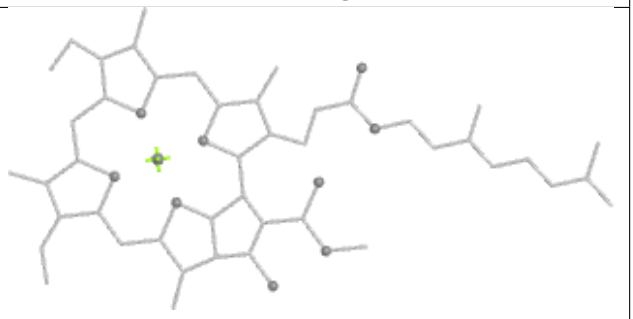
Bond lengths



Bond angles

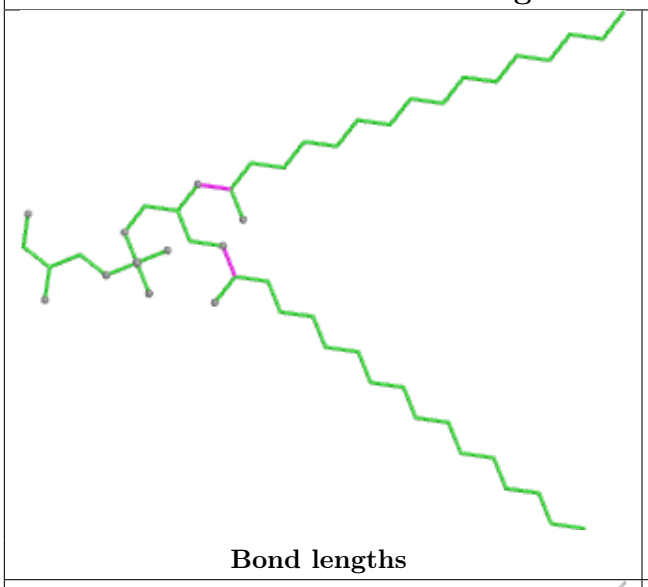


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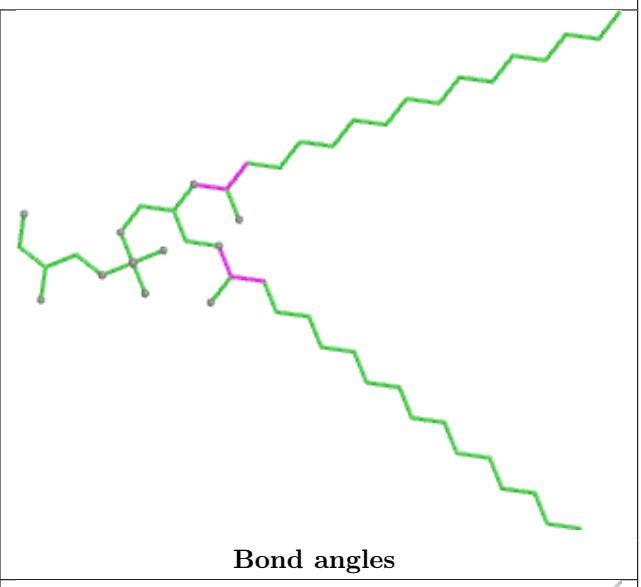


Rings

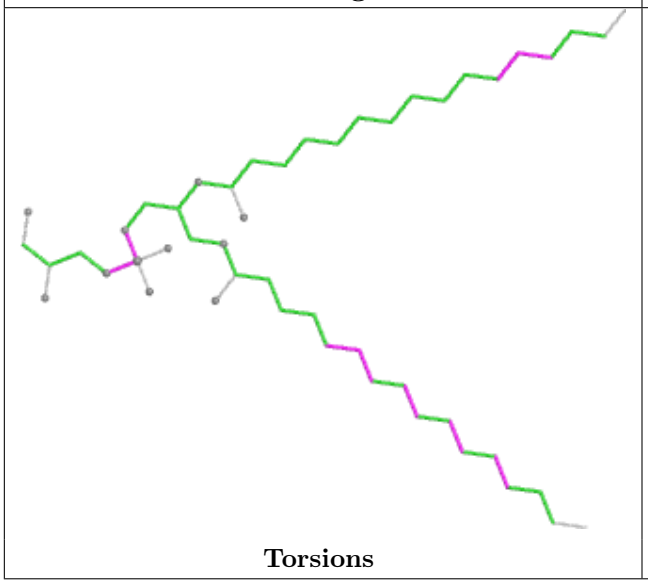
Ligand LHG U 2630



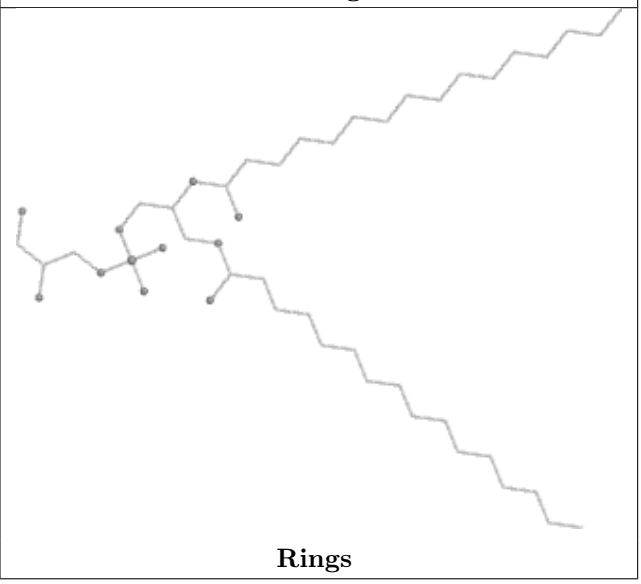
Bond lengths



Bond angles

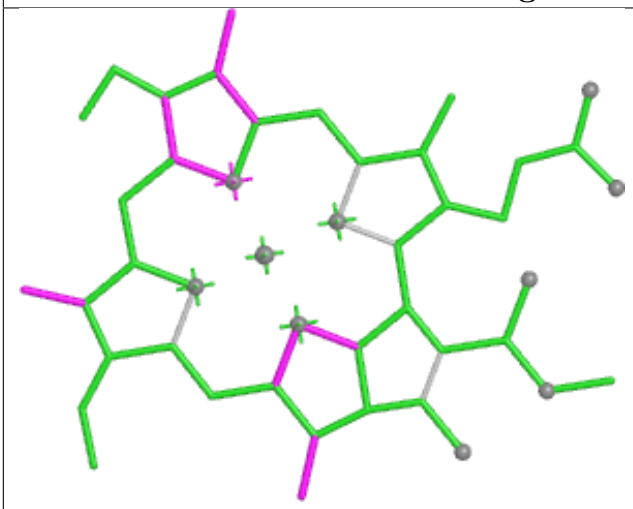


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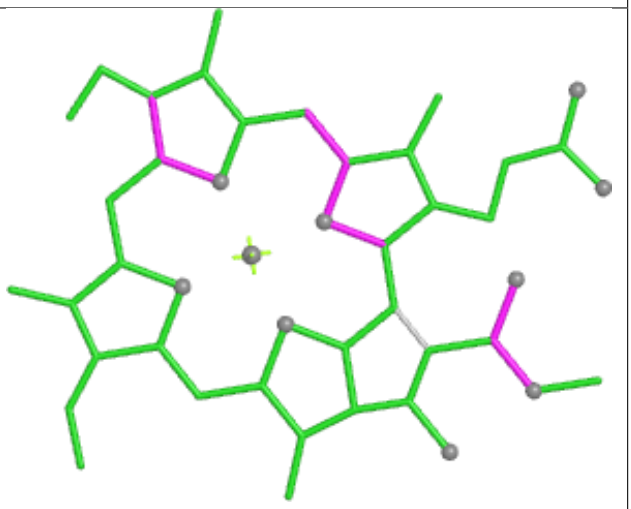


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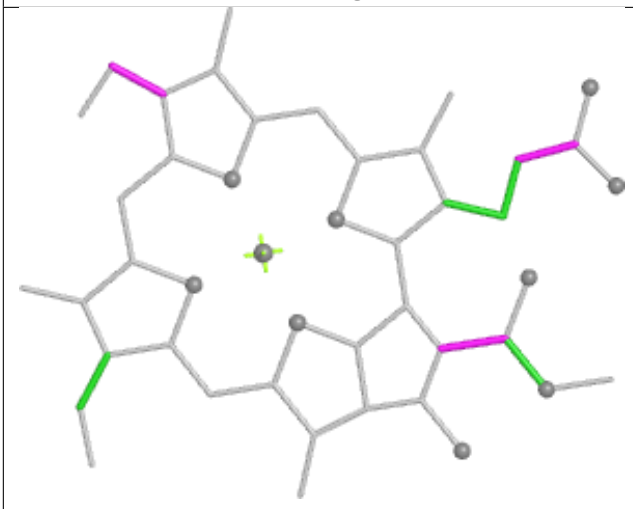
Ligand CLA W 612



Bond lengths



Bond angles

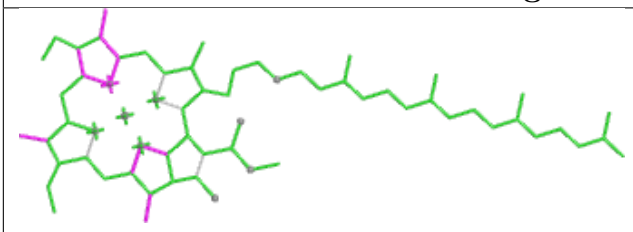


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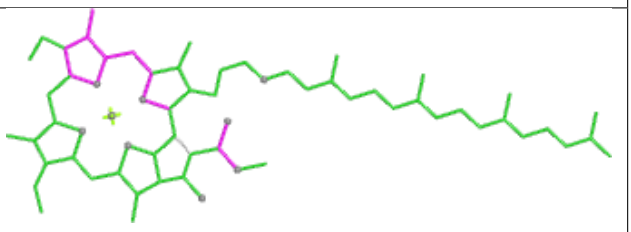


Rings

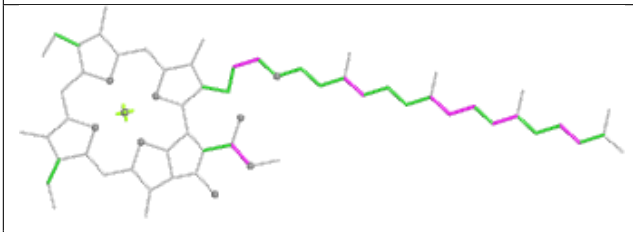
Ligand CLA A 826



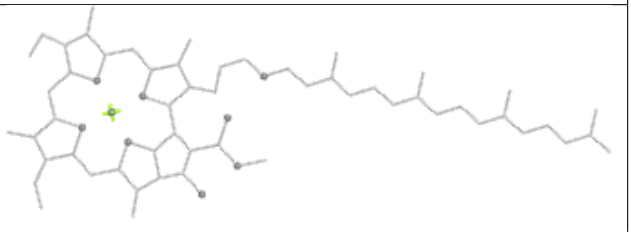
Bond lengths



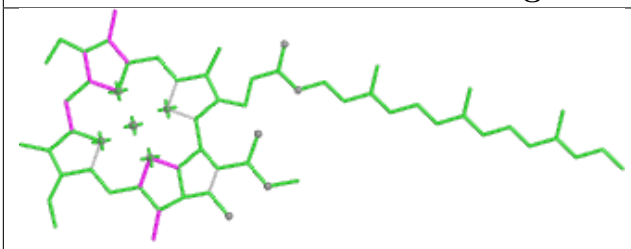
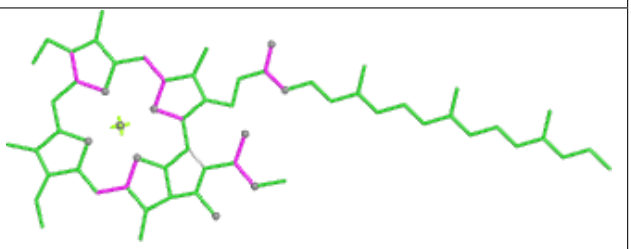
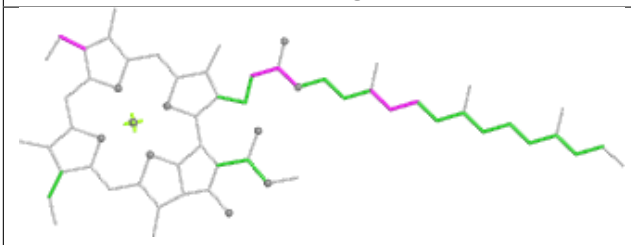
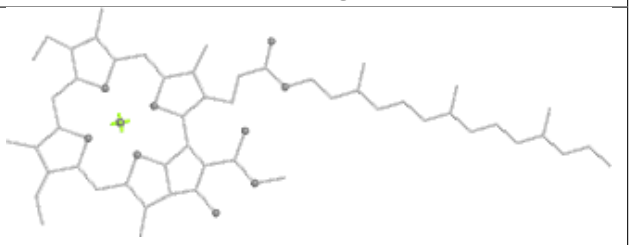
Bond angles



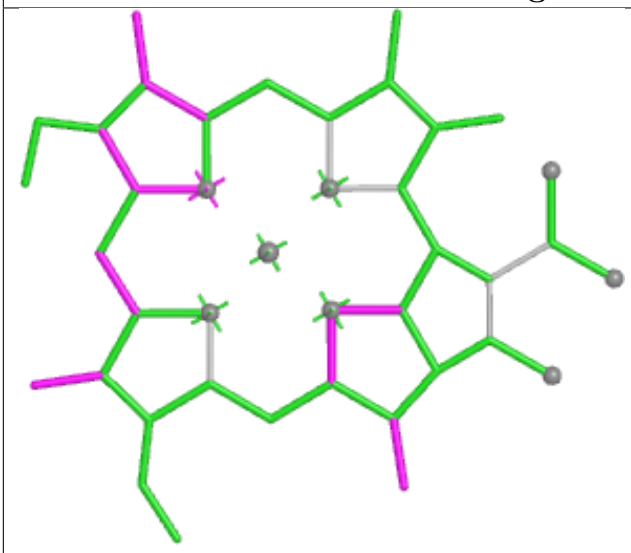
Torsions



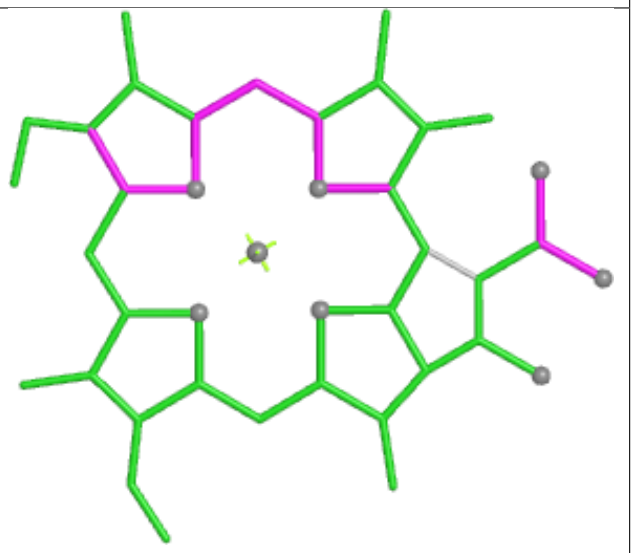
Rings

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

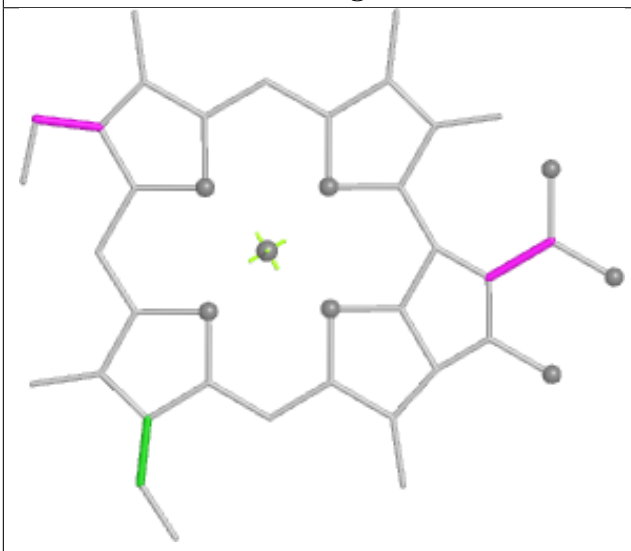
Ligand CLA 3 614



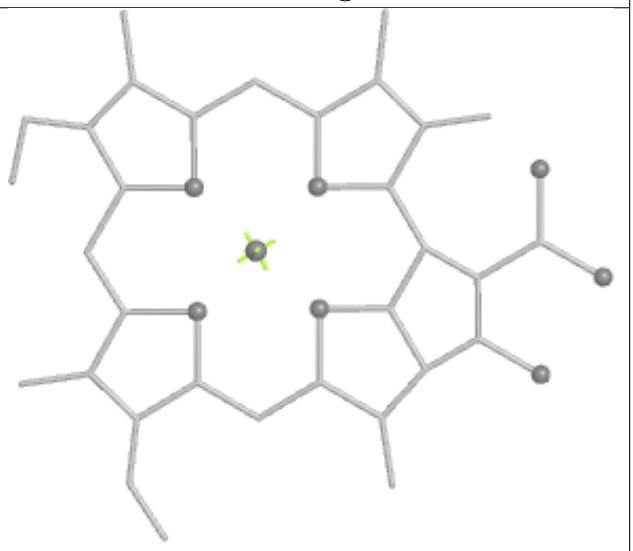
Bond lengths



Bond angles

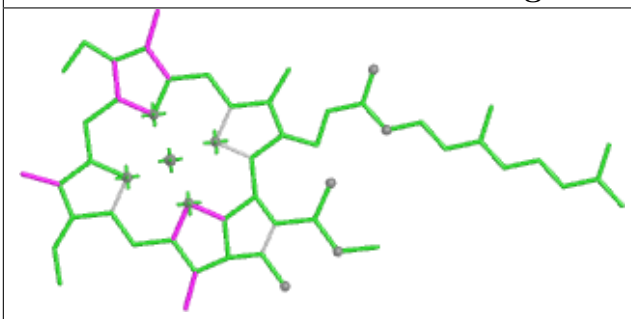


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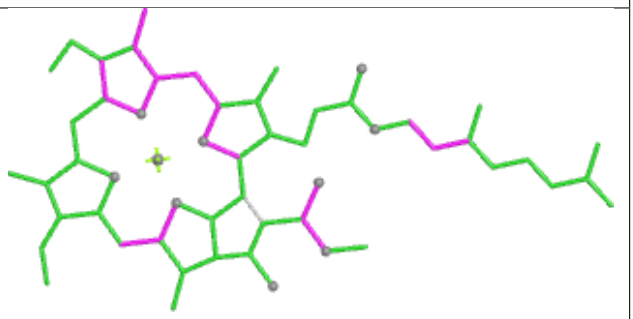


Rings

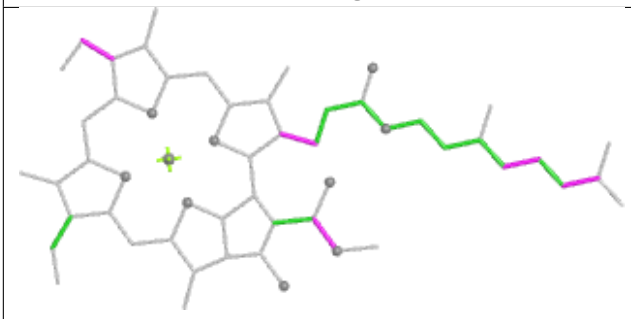
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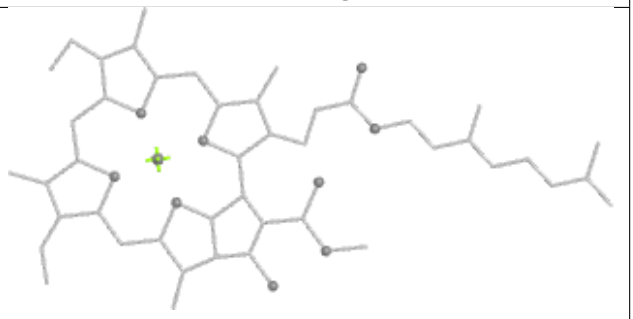
Bond lengths



Bond angles

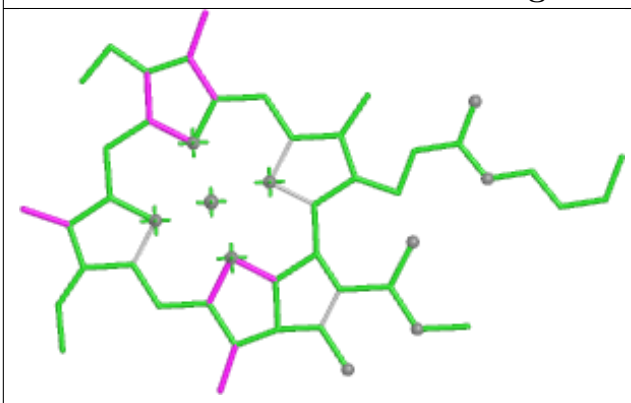


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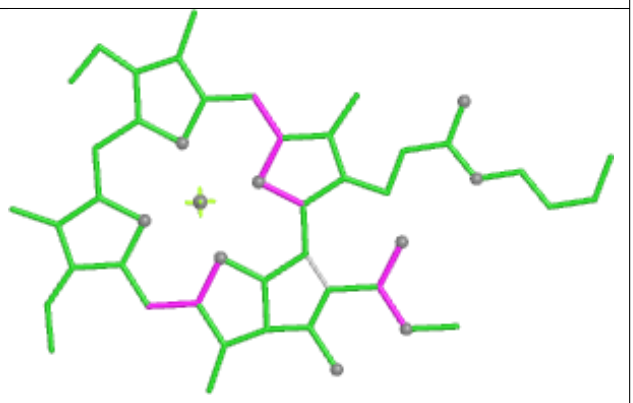


Rings

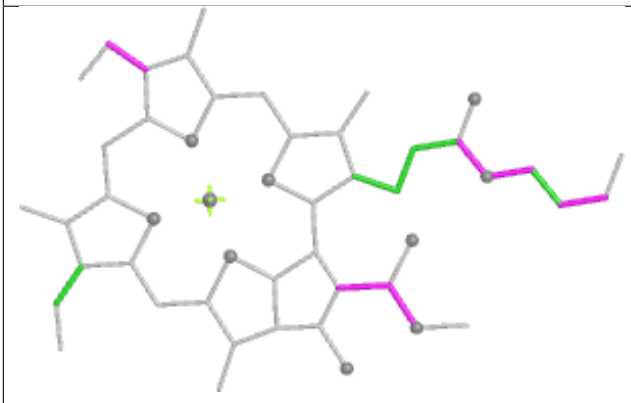
Ligand CLA 1 604



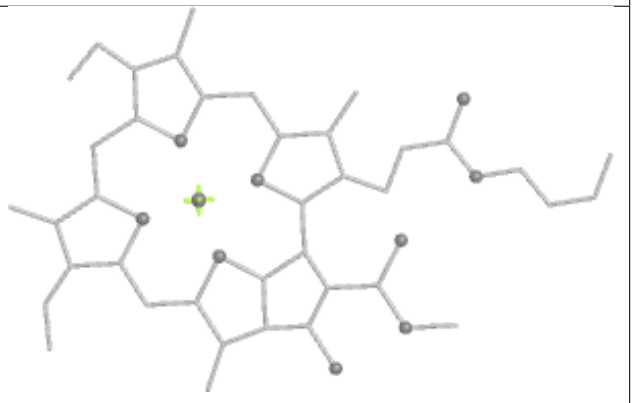
Bond lengths



Bond angles

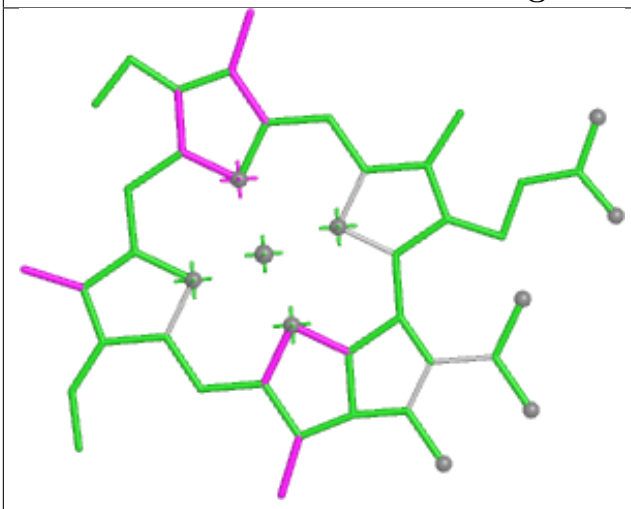


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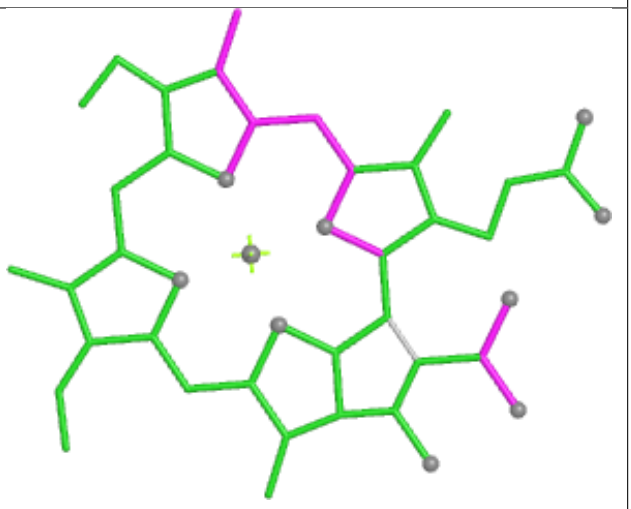


Rings

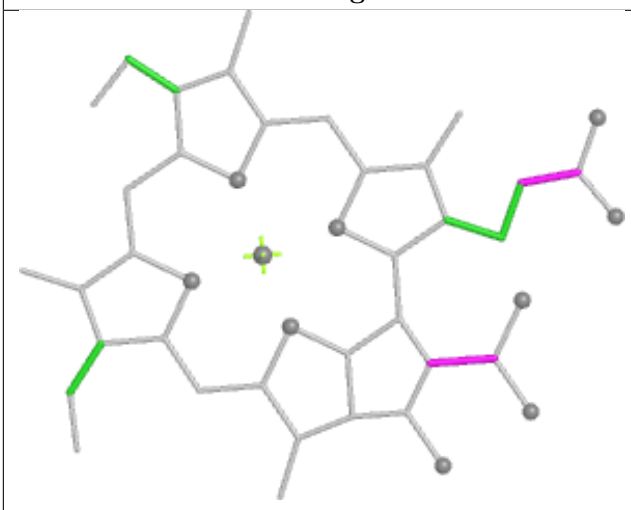
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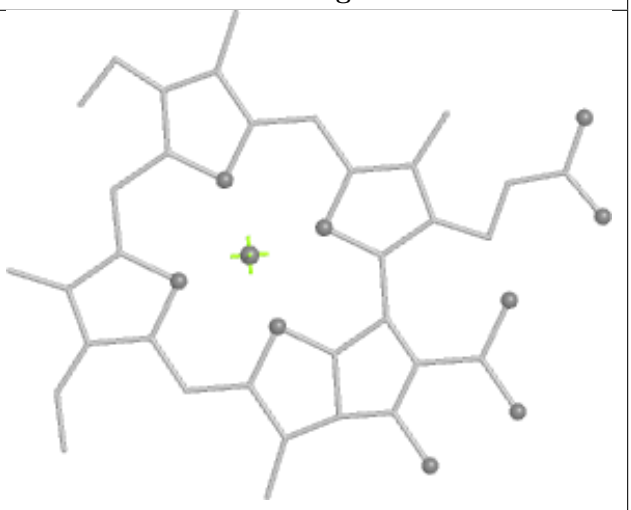
Bond lengths



Bond angles

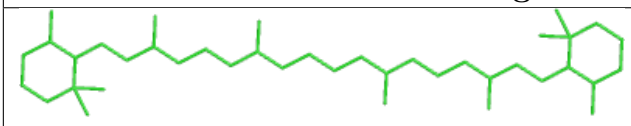


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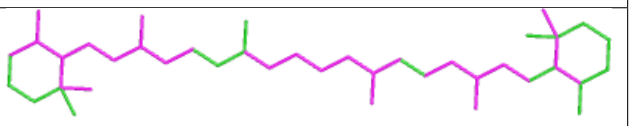


Rings

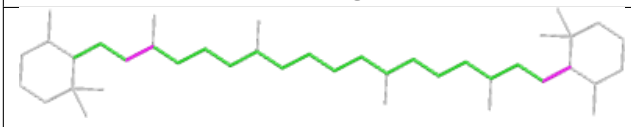
Ligand BCR O 2004



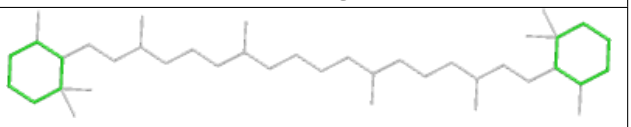
Bond lengths



Bond angles

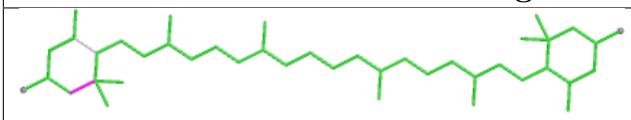


Torsions

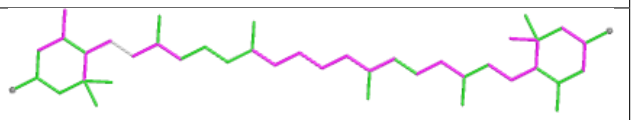


Rings

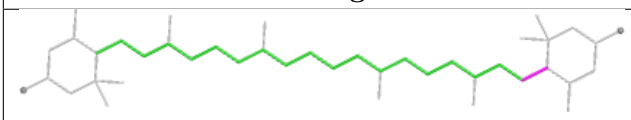
Ligand LUT Y 1620



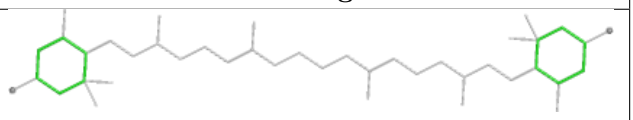
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Bond angles

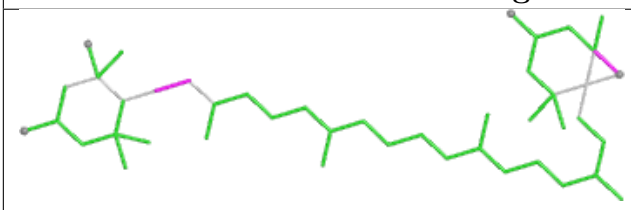


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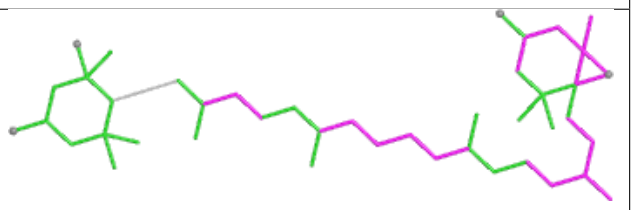


Rings

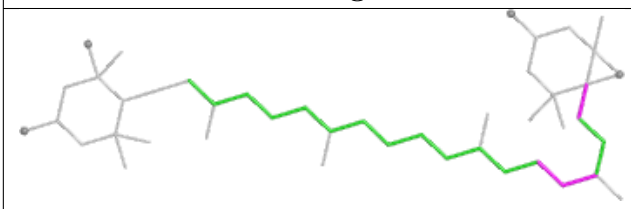
Ligand NEX V 1623



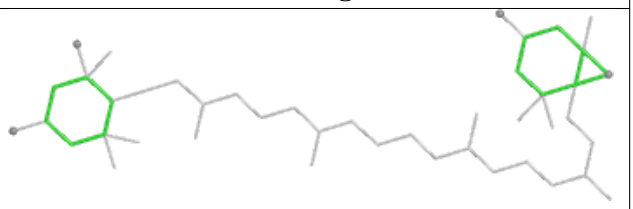
Bond lengths



Bond angles

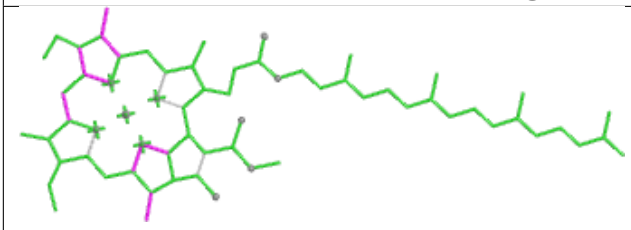


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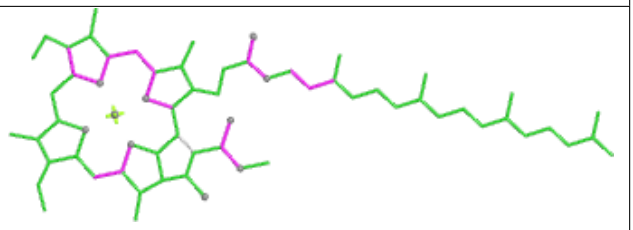


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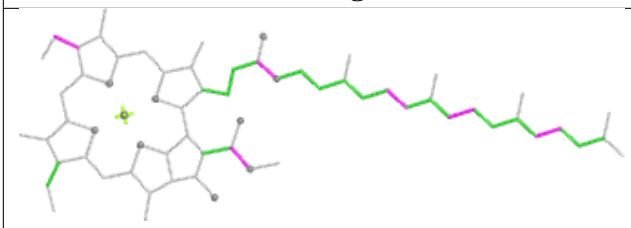
Ligand CLA Y 610



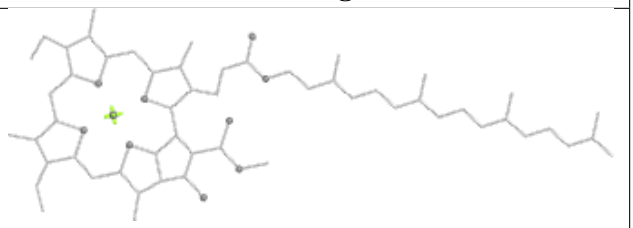
Bond lengths



Bond angles

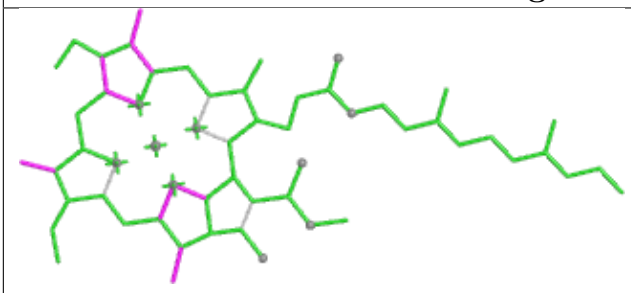


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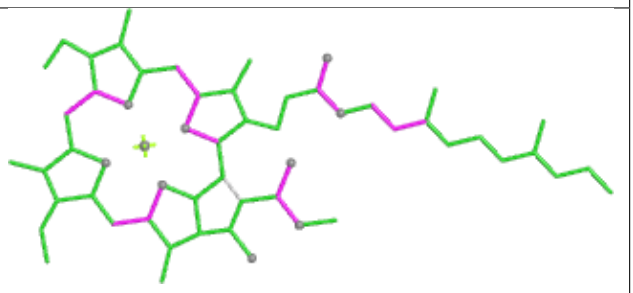


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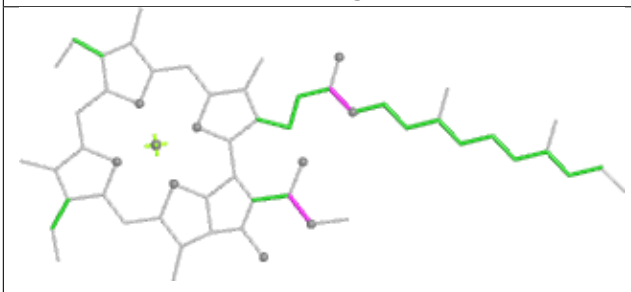
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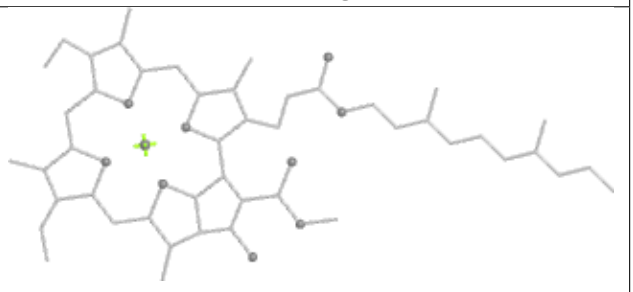
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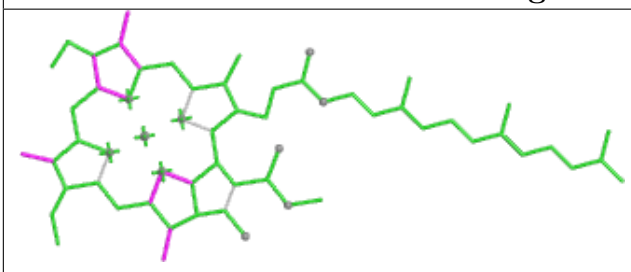


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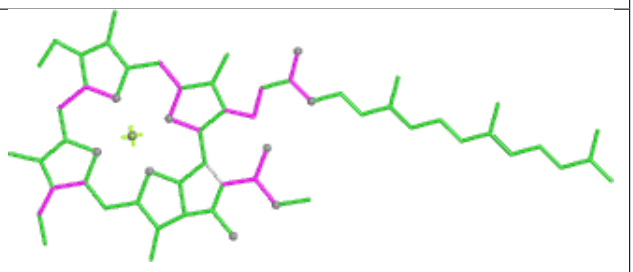


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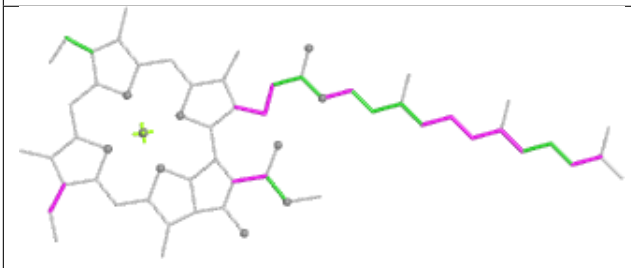
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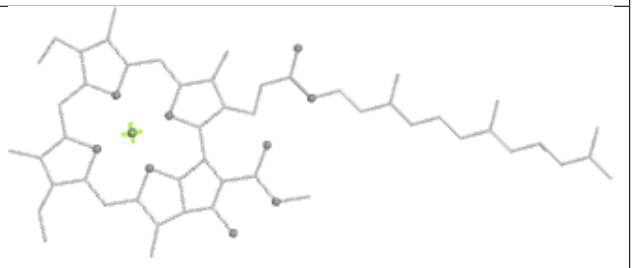
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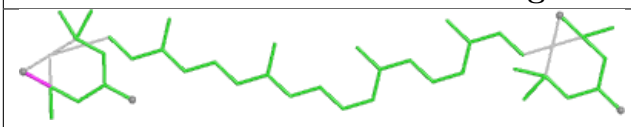


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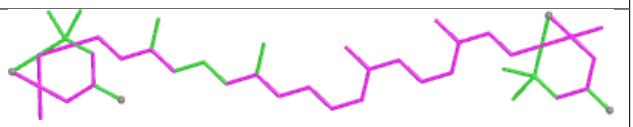


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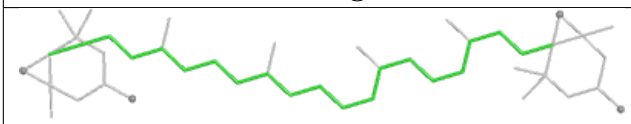
Ligand XAT a 618



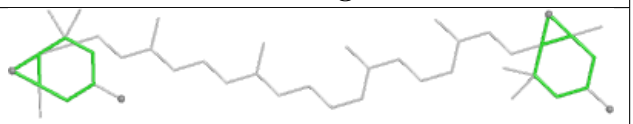
Bond lengths



Bond angles

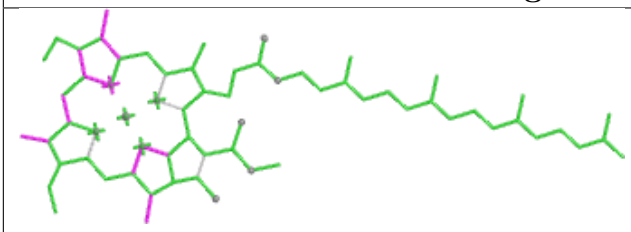


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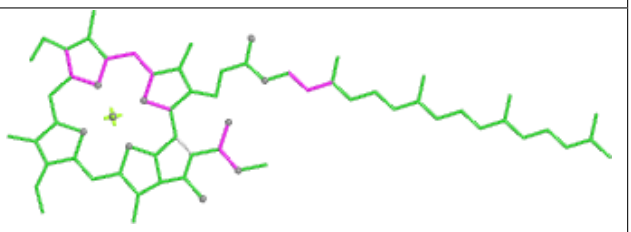


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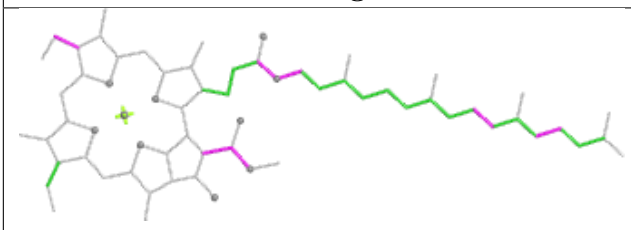
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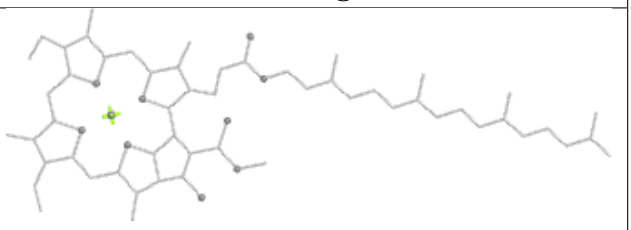
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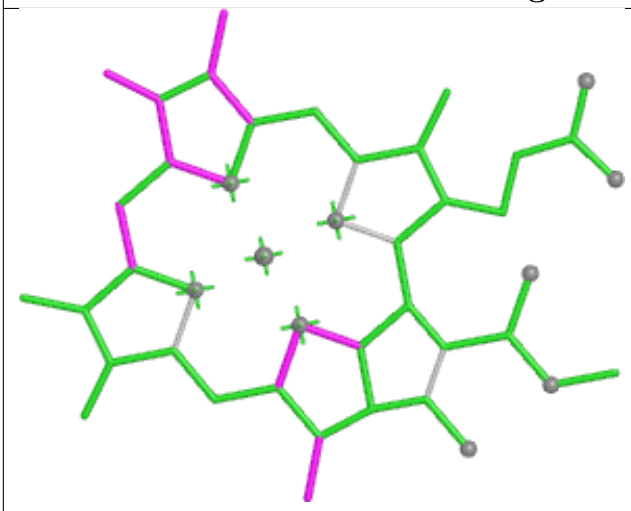


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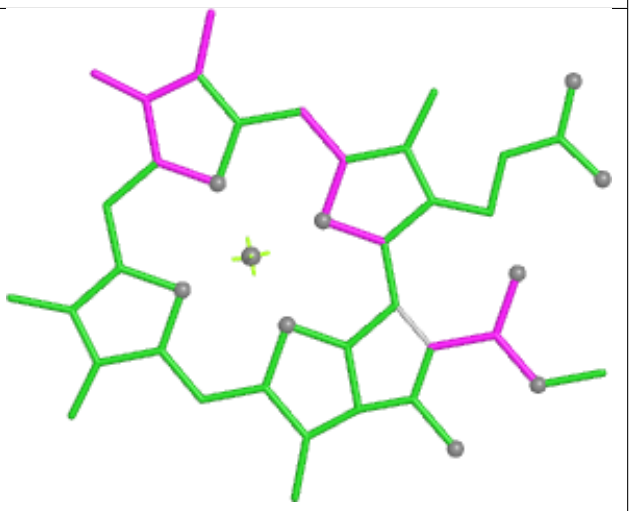


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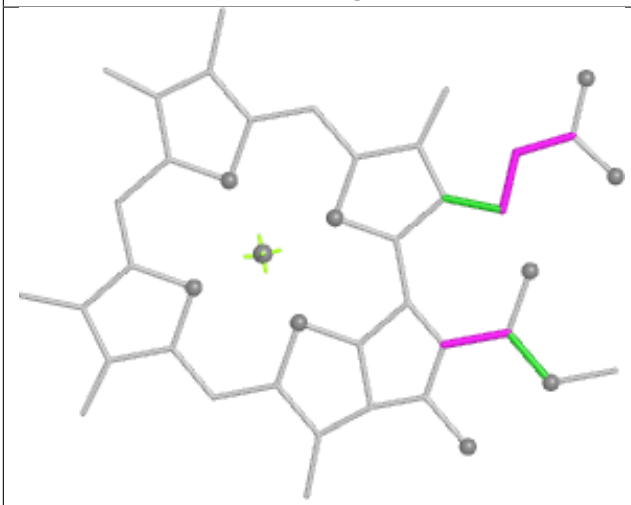
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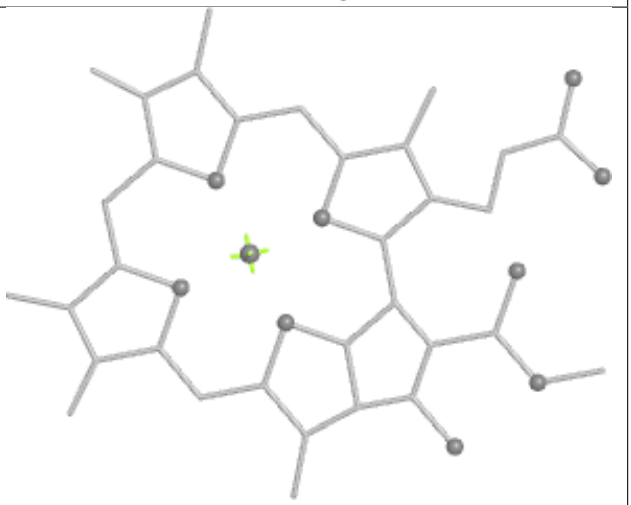
Bond lengths



Bond angles

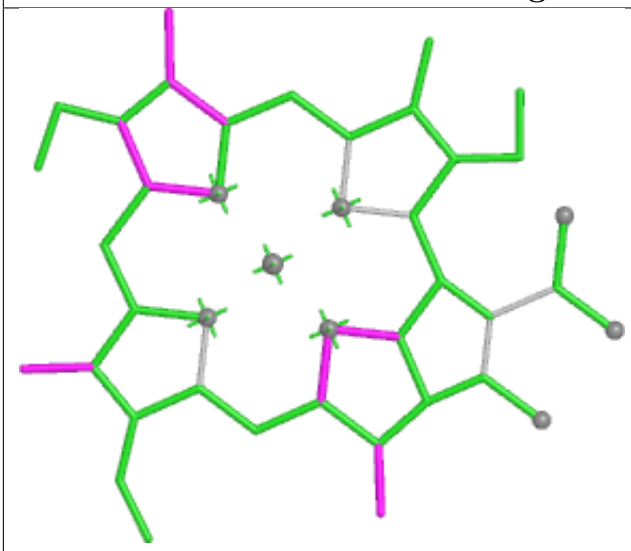


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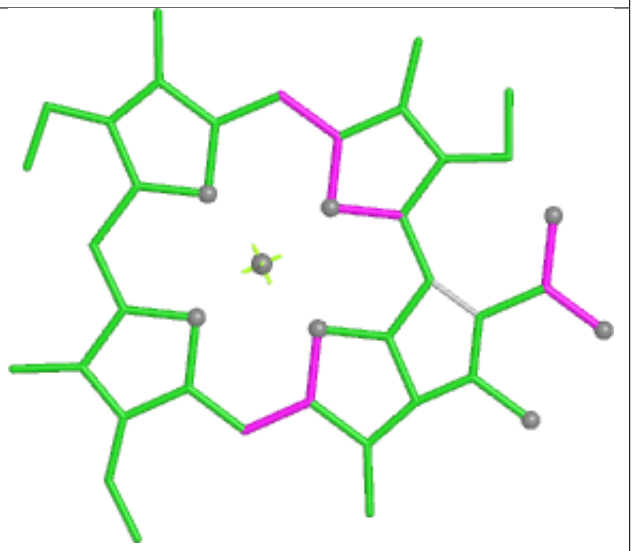


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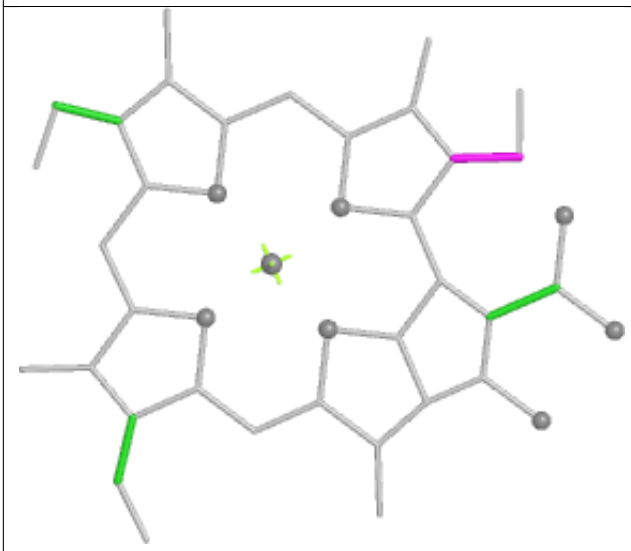
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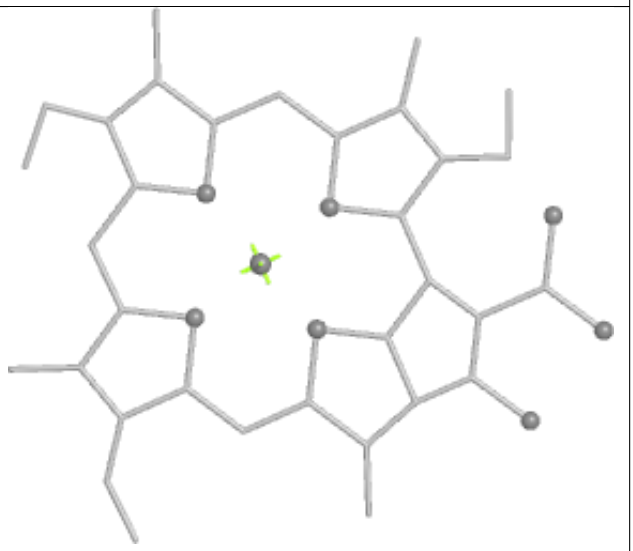
Bond lengths



Bond angles

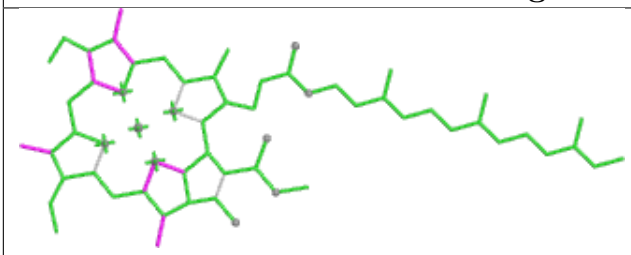


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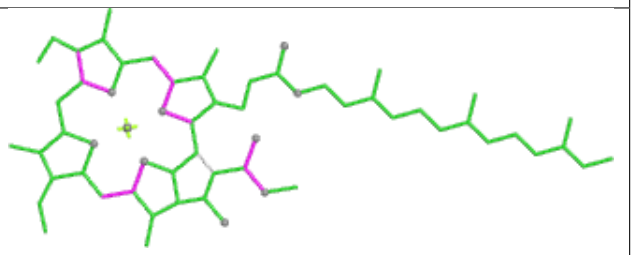


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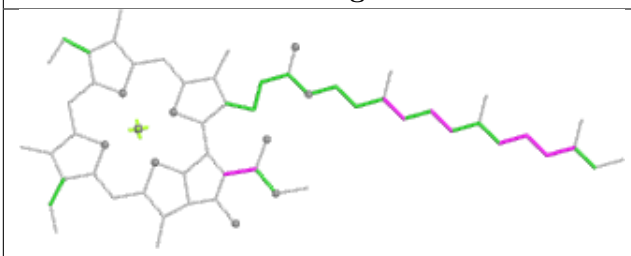
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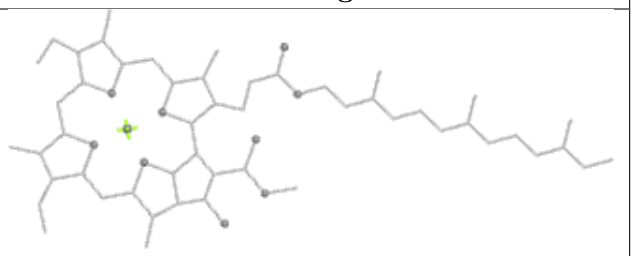
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Bond angles

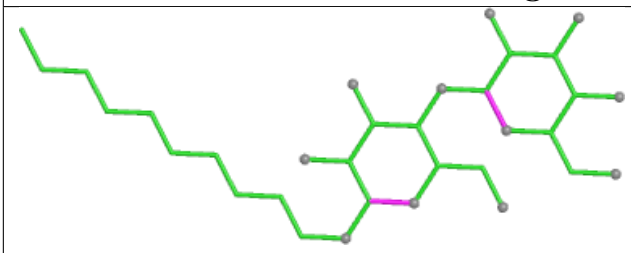


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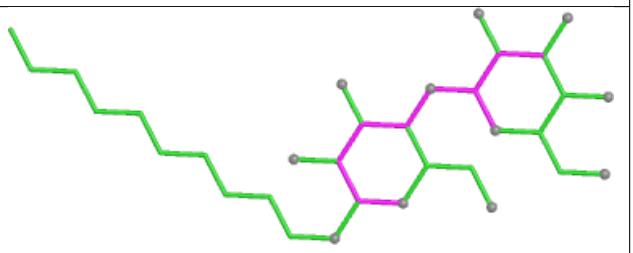


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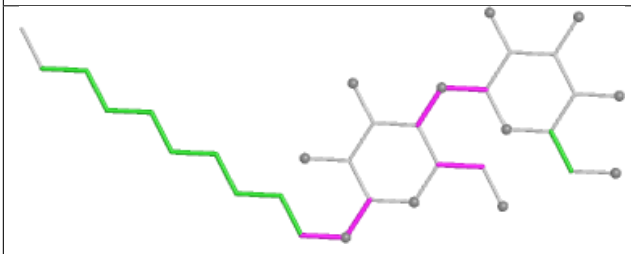
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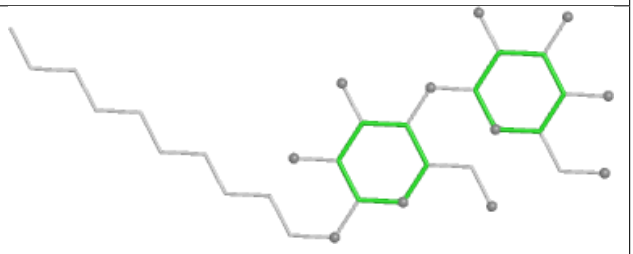
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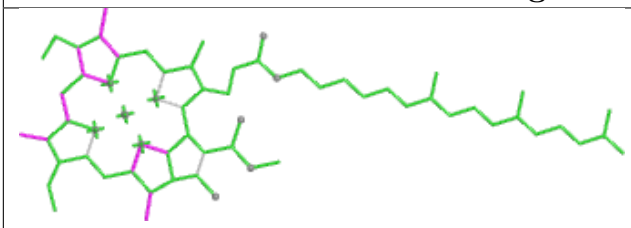


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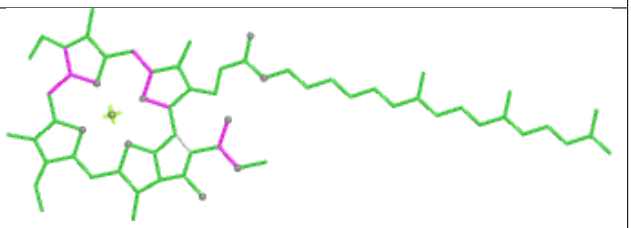


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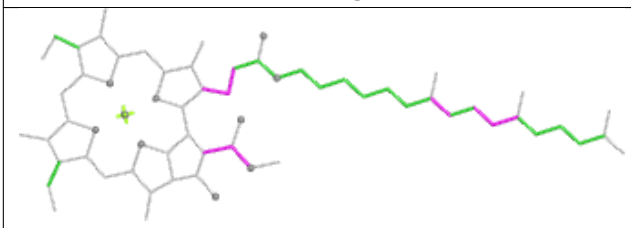
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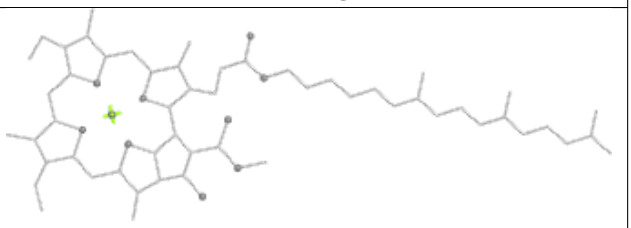
Bond lengths



Bond angles

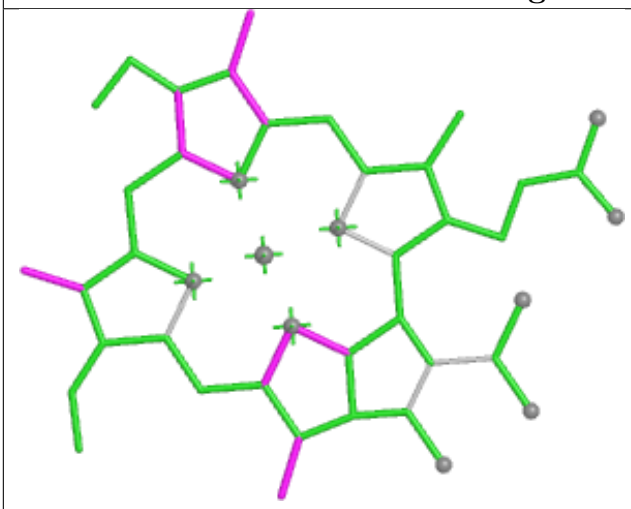


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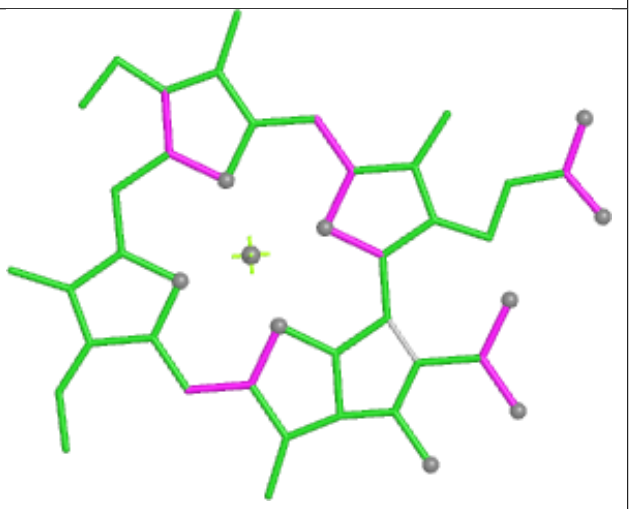


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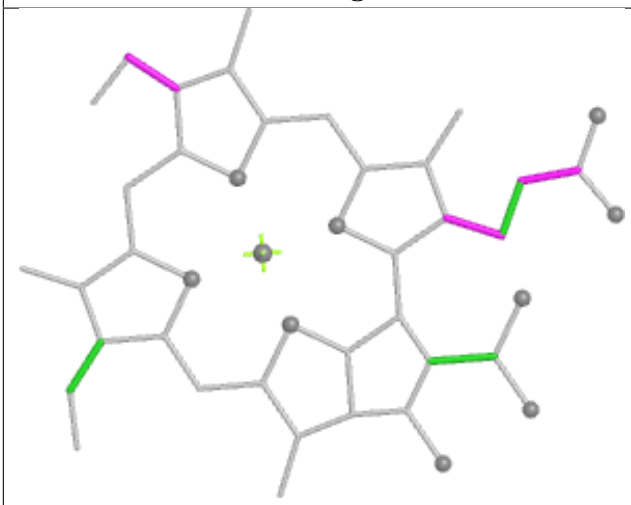
Ligand CLA a 608



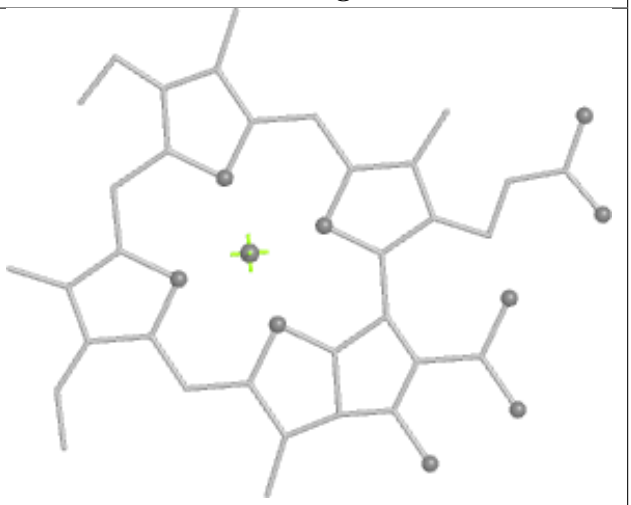
Bond lengths



Bond angles

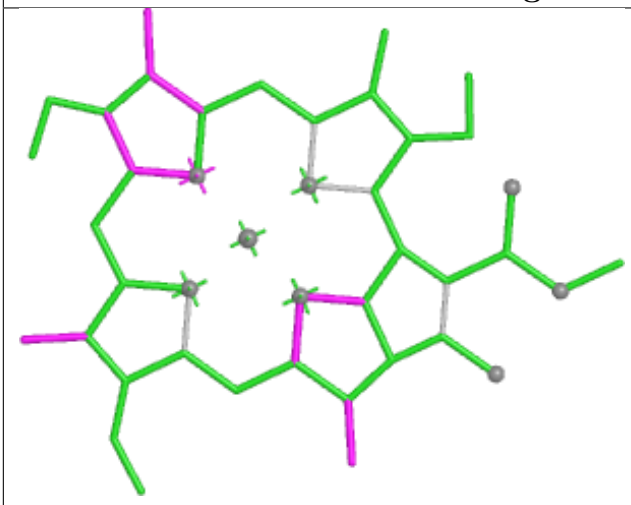


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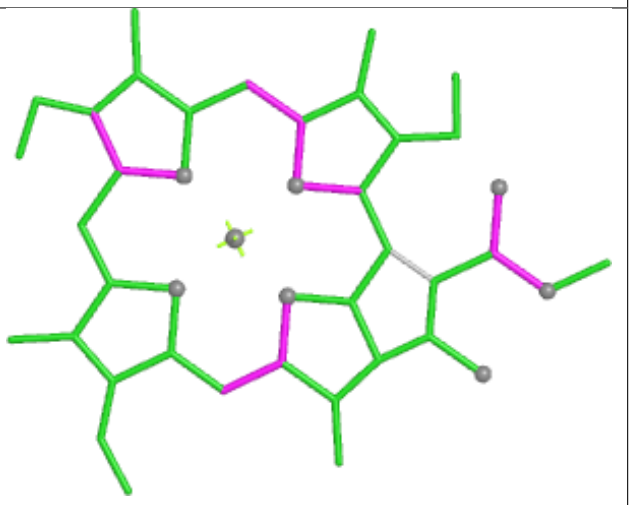


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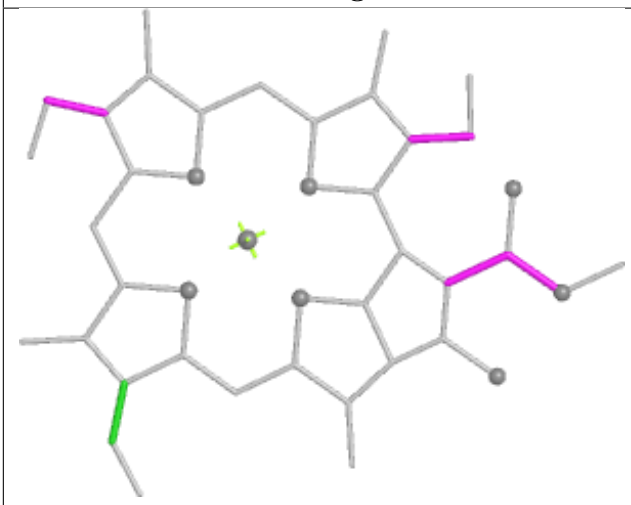
Ligand CLA U 614



Bond lengths



Bond angles

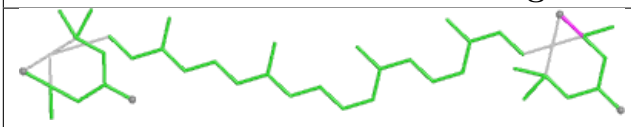


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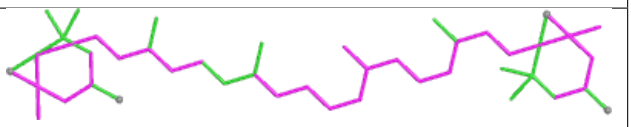


Rings

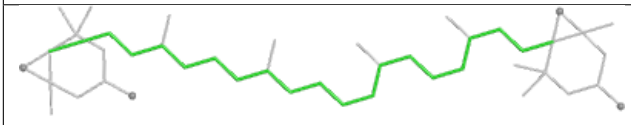
Ligand XAT 9 620



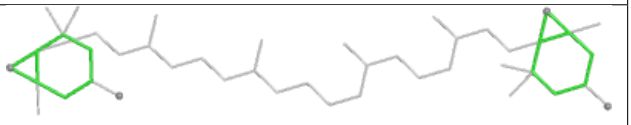
Bond lengths



Bond angles

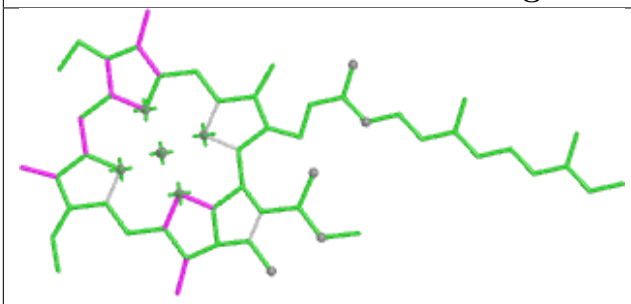


Torsions

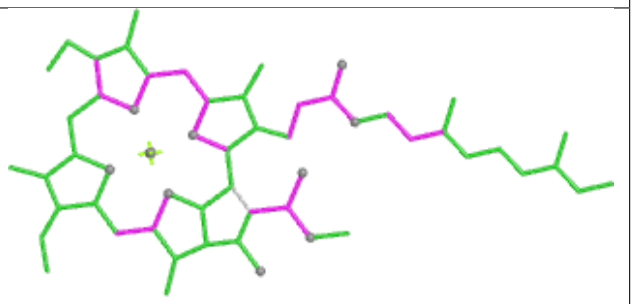


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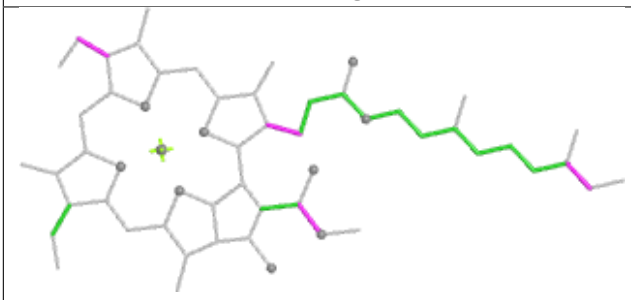
Ligand CLA K 203



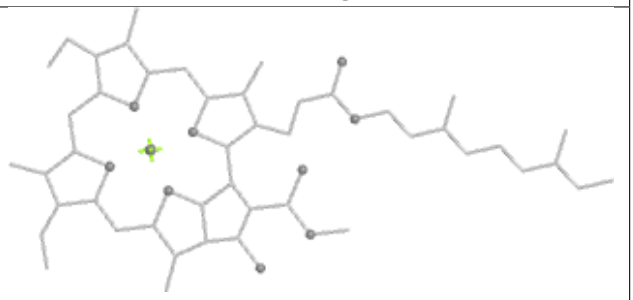
Bond lengths



Bond angles

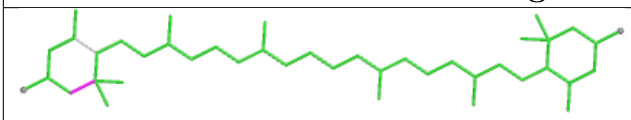


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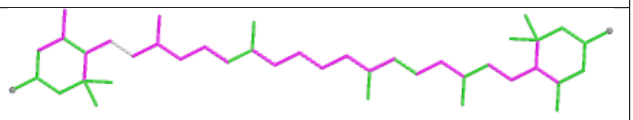


Rings

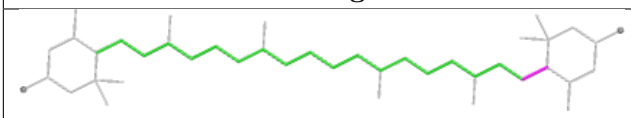
Ligand LUT 5 620



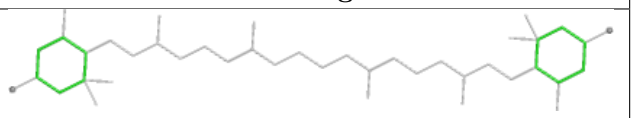
Bond lengths



Bond angles

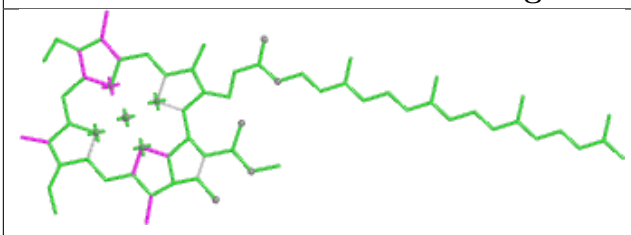


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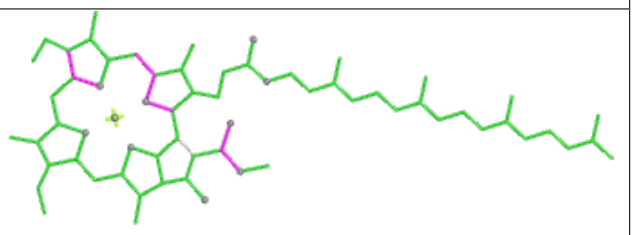


Rings

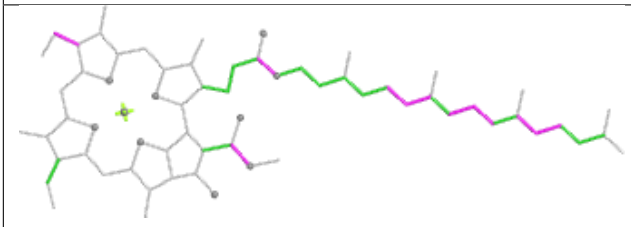
Ligand CLA B 824



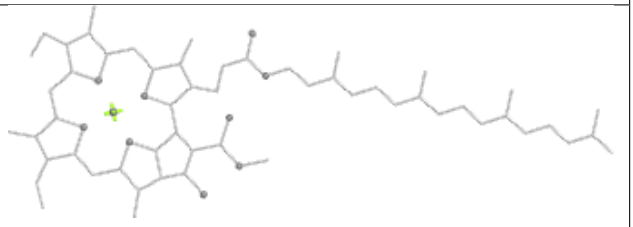
Bond lengths



Bond angles

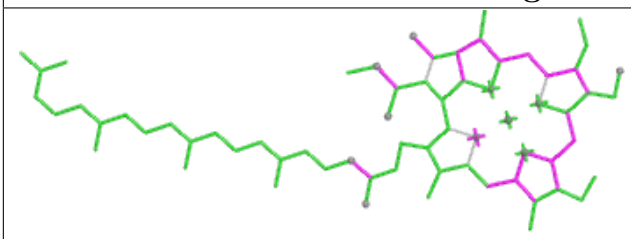


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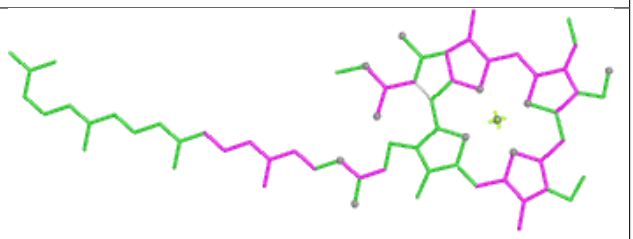


Rings

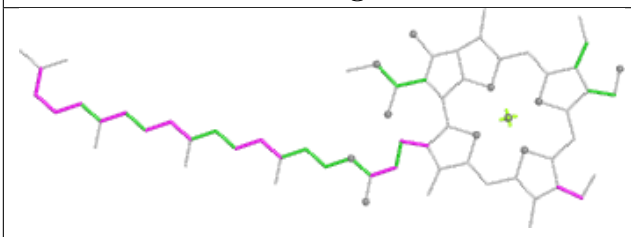
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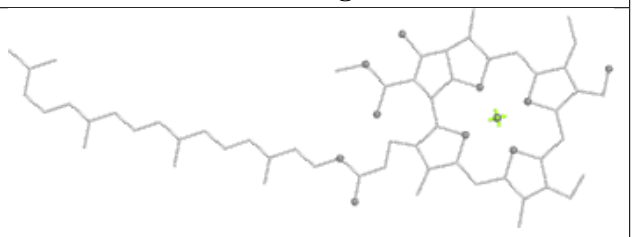
Bond lengths



Bond angles

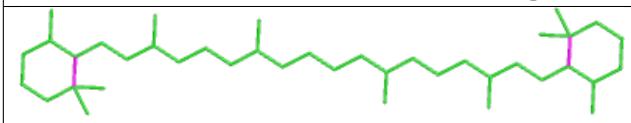


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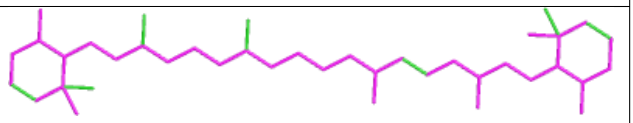


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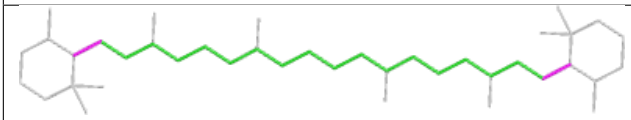
Ligand BCR L 308



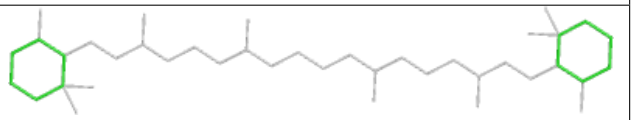
Bond lengths



Bond angles

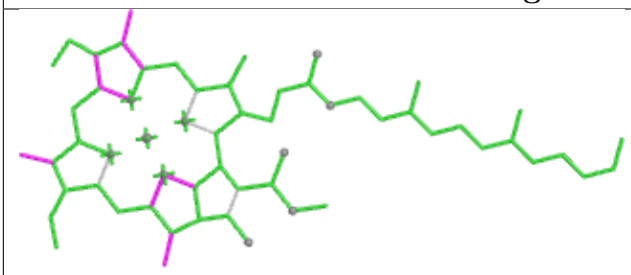


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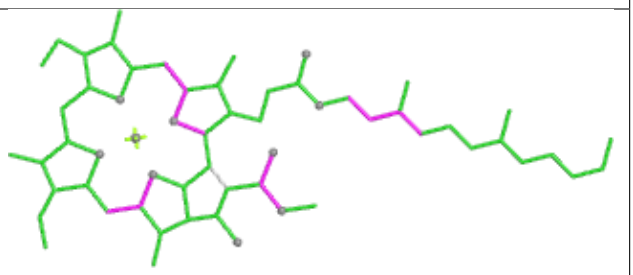


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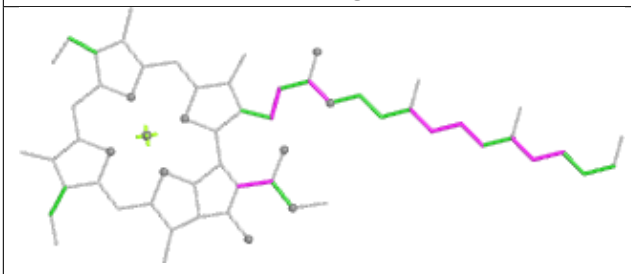
Ligand CLA U 613



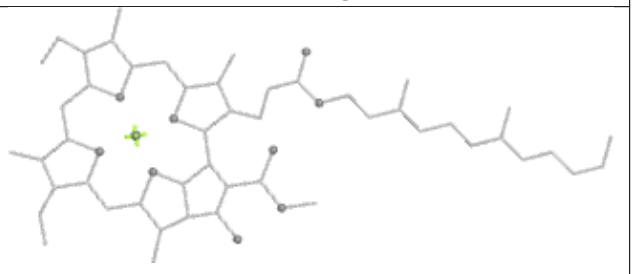
Bond lengths



Bond angles

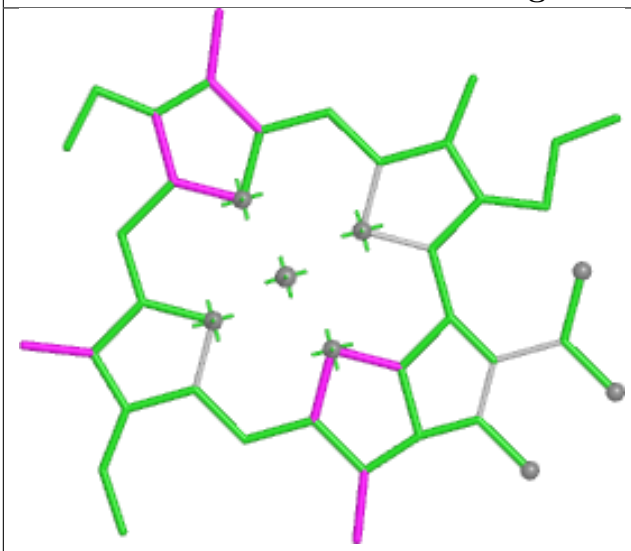


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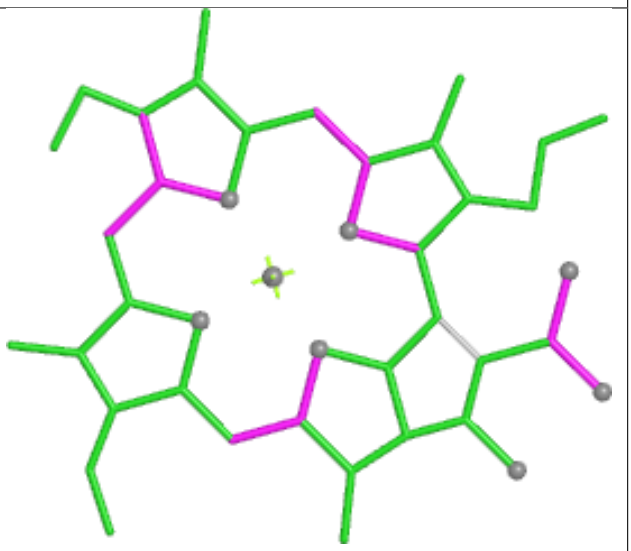


Rings

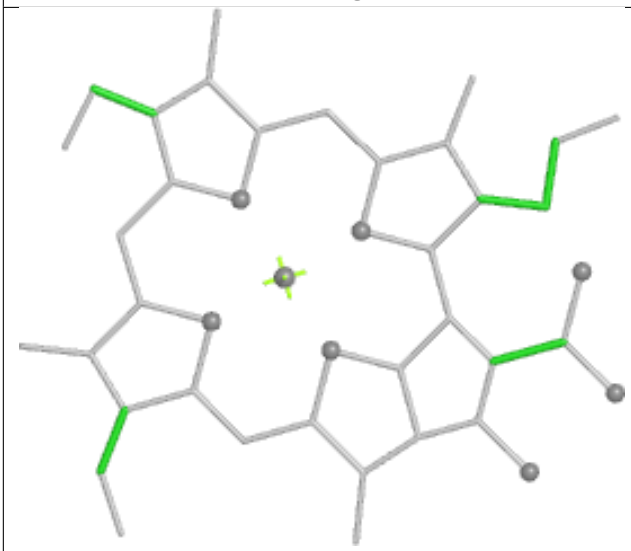
Ligand CLA 2 614



Bond lengths



Bond angles

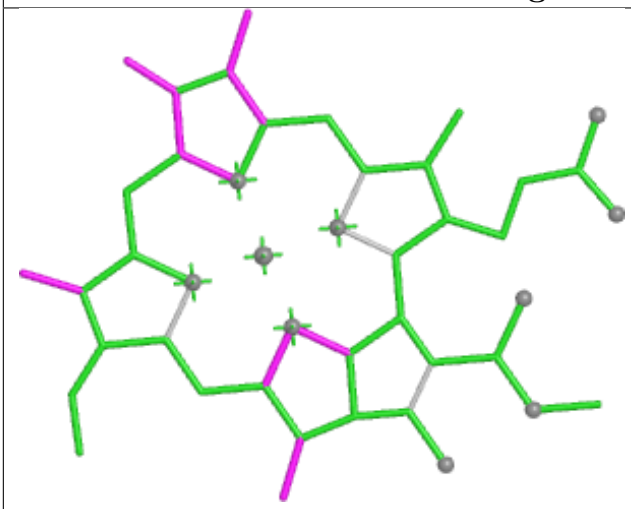


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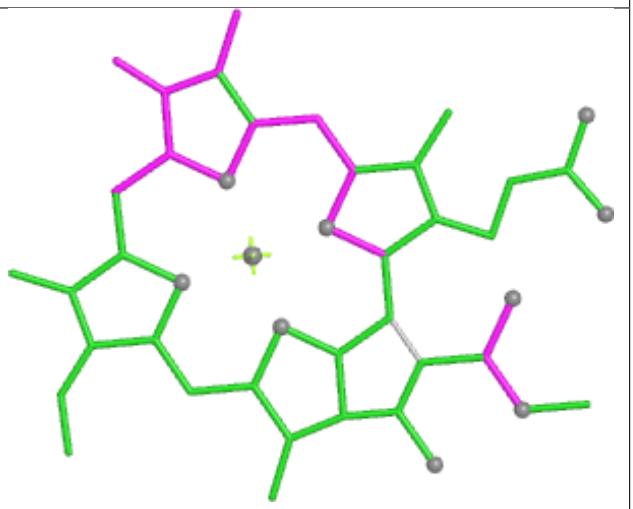


Rings

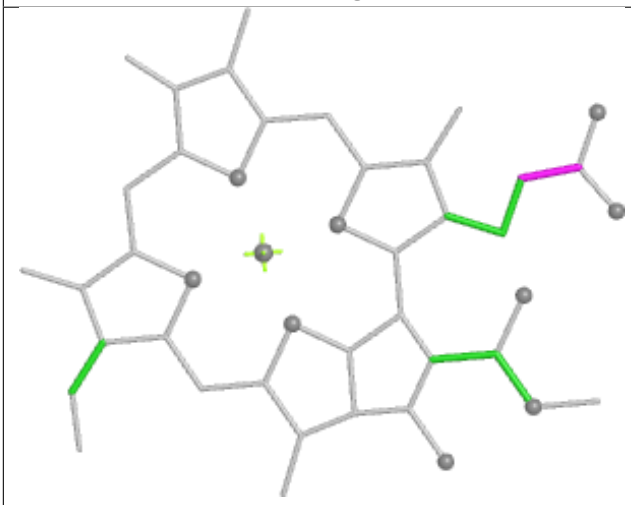
Ligand CLA 4 603



Bond lengths



Bond angles

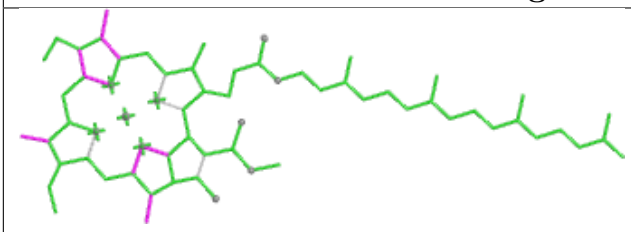


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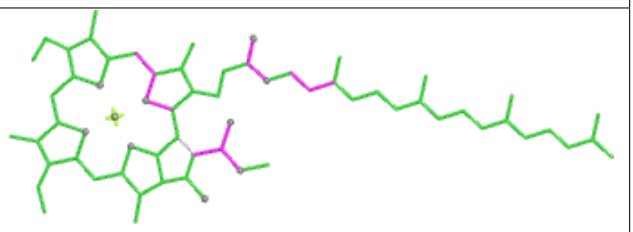


Rings

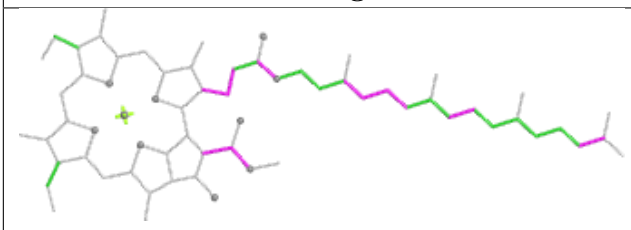
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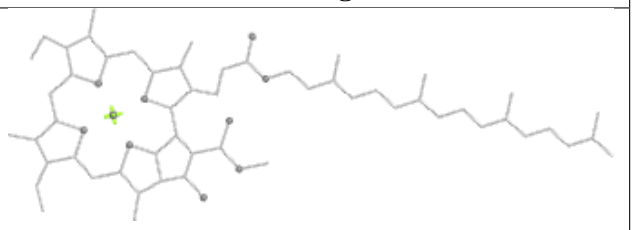
Bond lengths



Bond angles

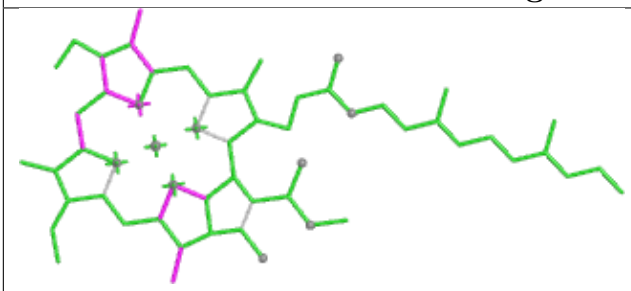


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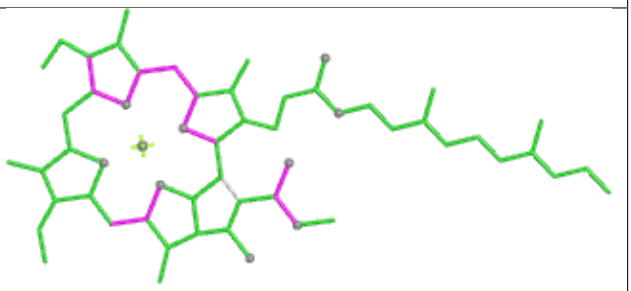


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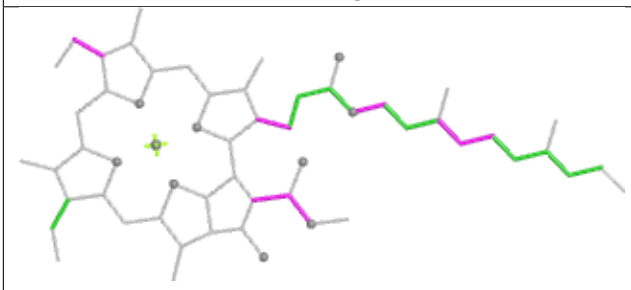
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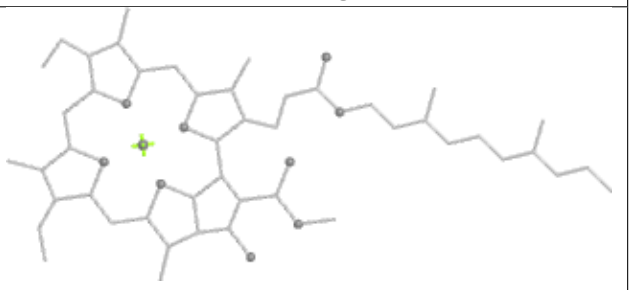
Bond lengths



Bond angles



Torsions

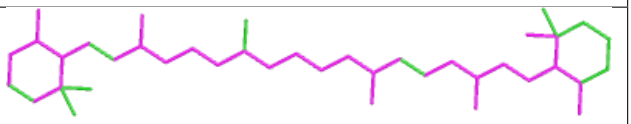


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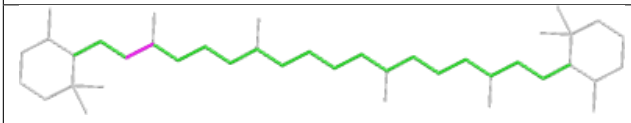
Ligand BCR L 305



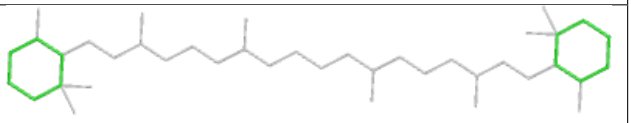
Bond lengths



Bond angles

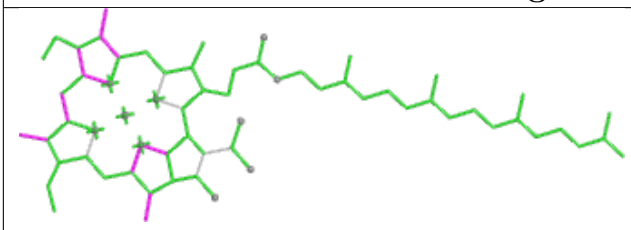


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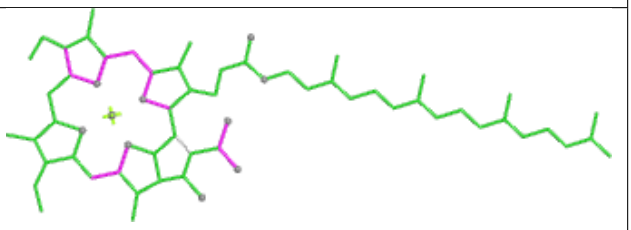


Rings

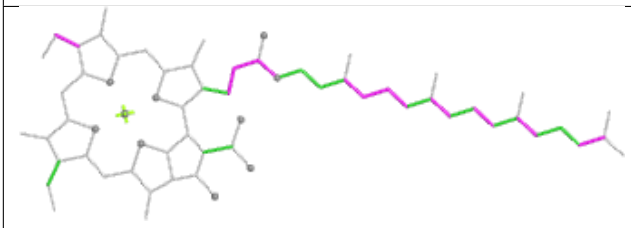
Ligand CLA 6 613



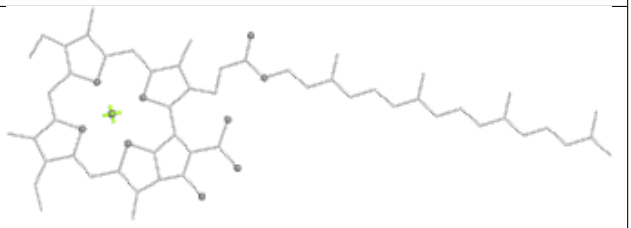
Bond lengths



Bond angles

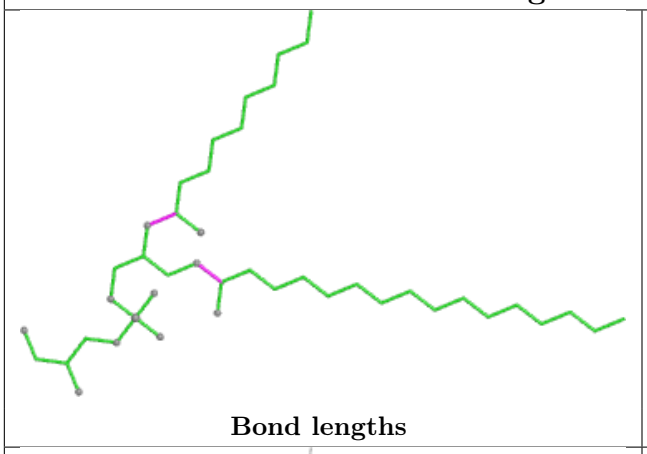


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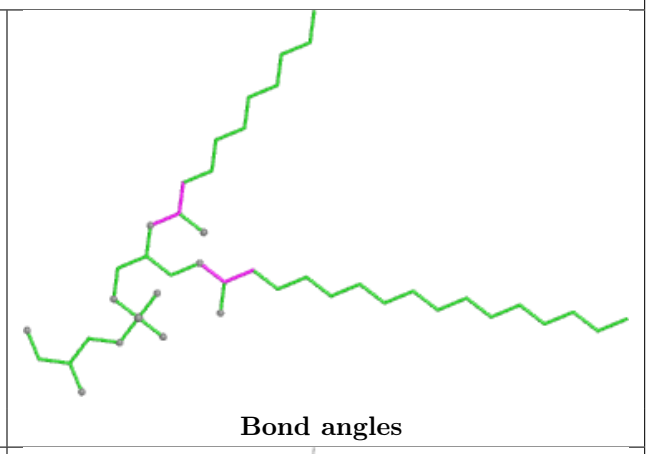


Rings

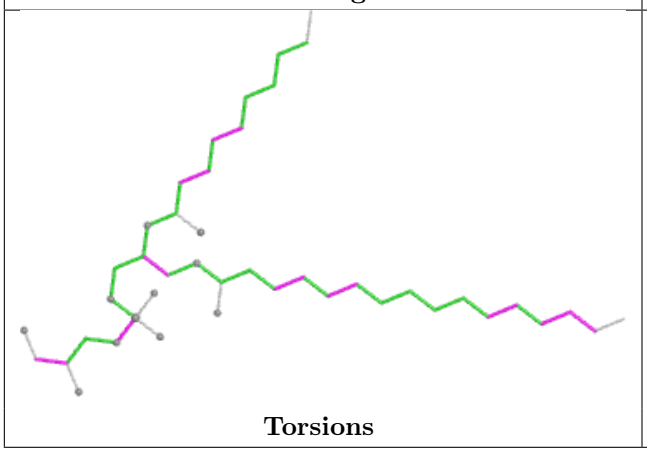
Ligand LHG a 620



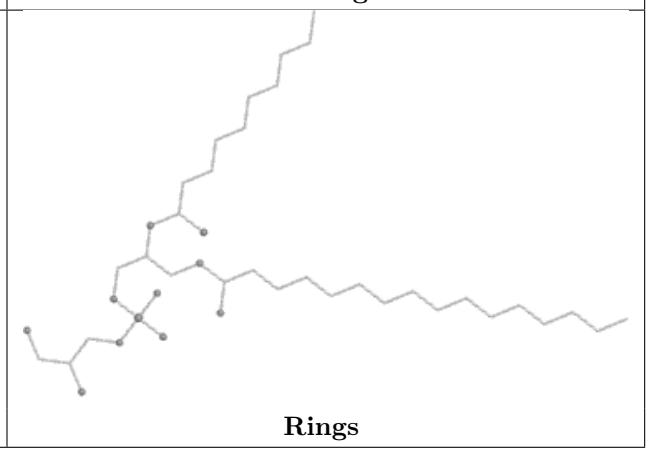
Bond lengths



Bond angles

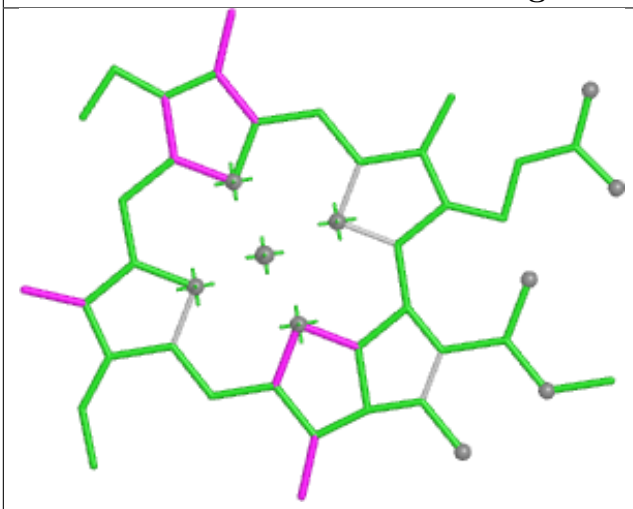


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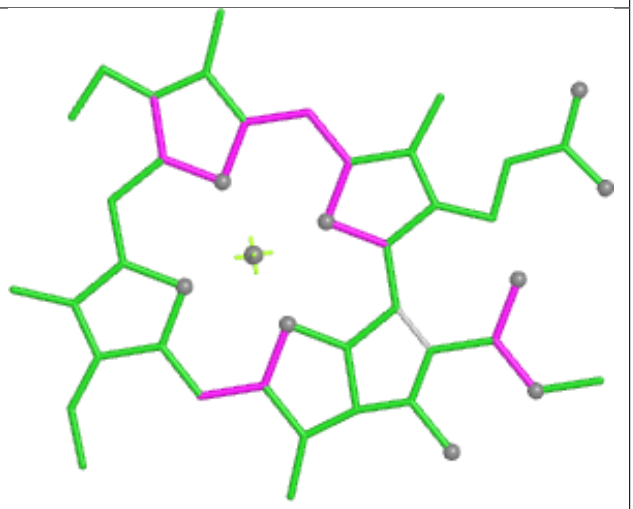


Rings

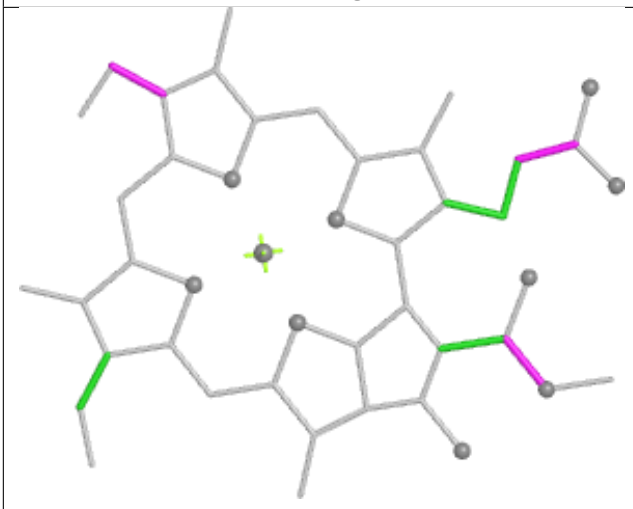
Ligand CLA 6 608



Bond lengths



Bond angles

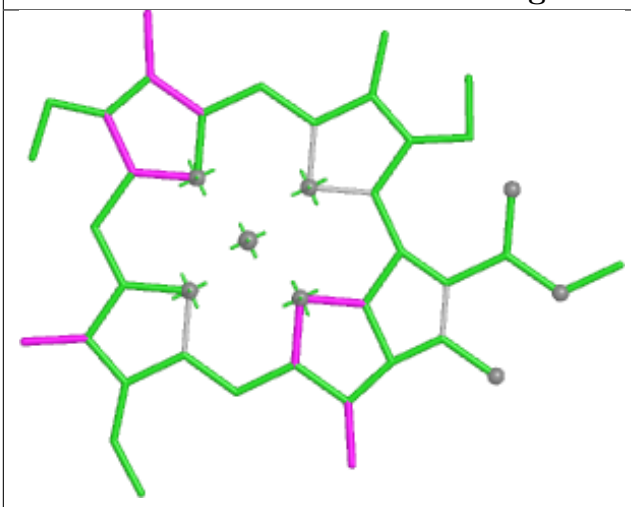


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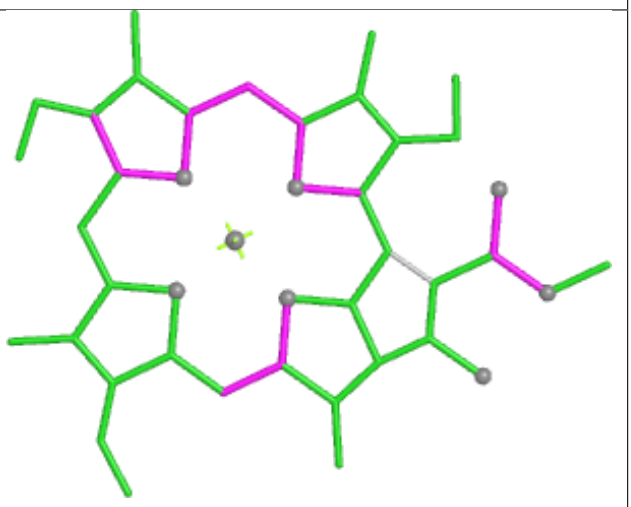


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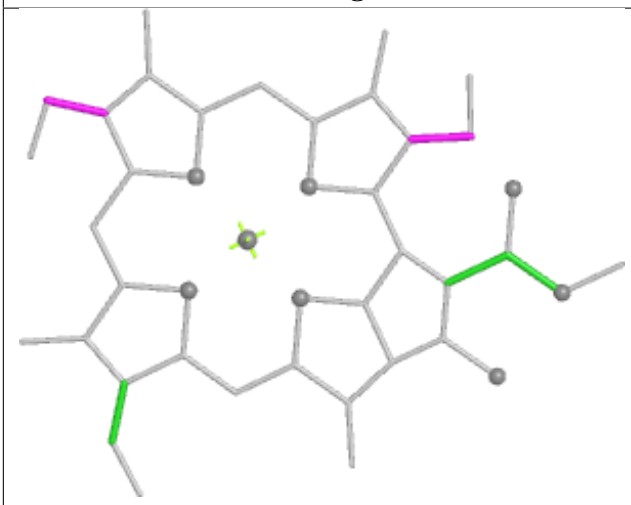
Ligand CLA 4 611



Bond lengths



Bond angles

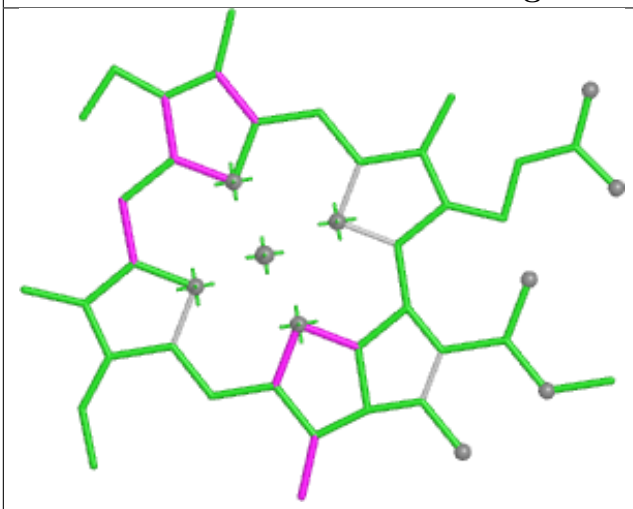


Torsions

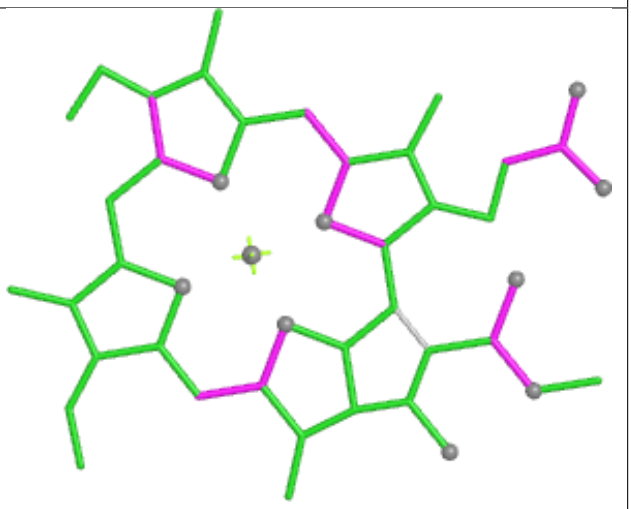


Rings

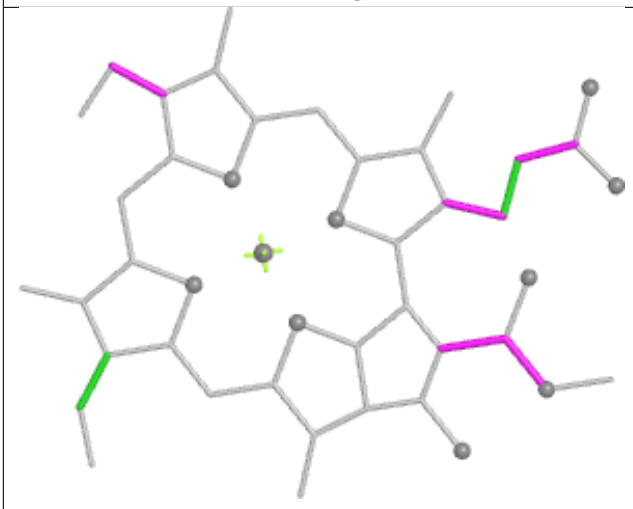
Ligand CLA X 611



Bond lengths



Bond angles

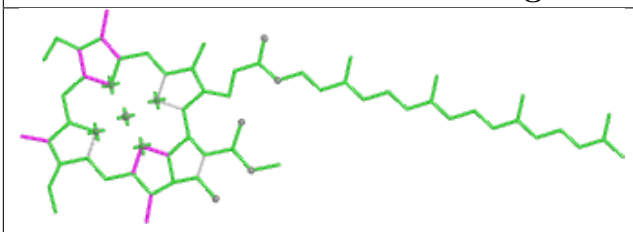


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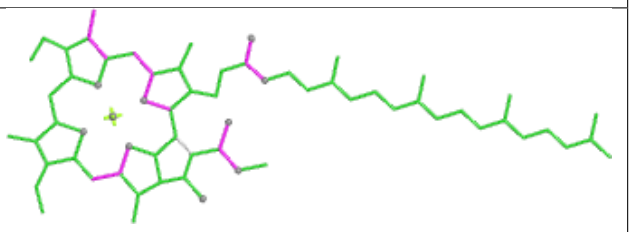


Rings

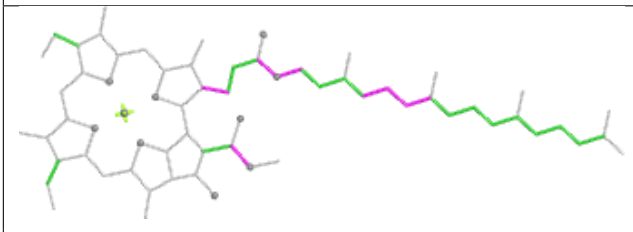
Ligand CLA B 829



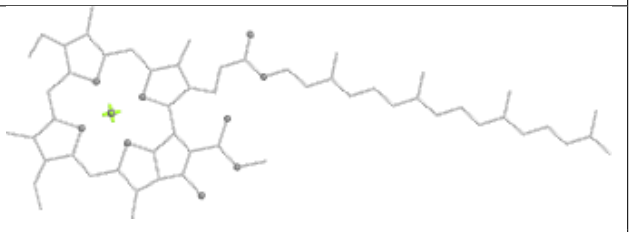
Bond lengths



Bond angles

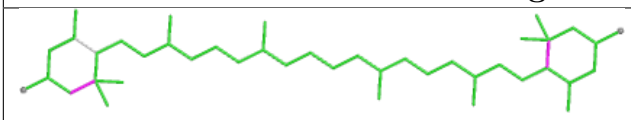


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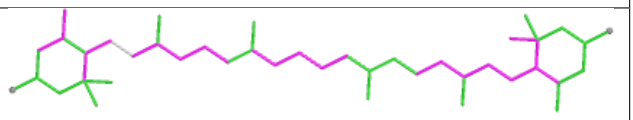


Rings

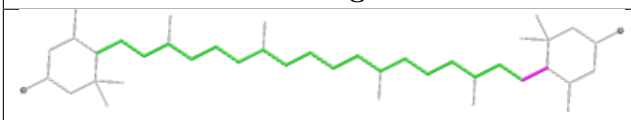
Ligand LUT 7 619



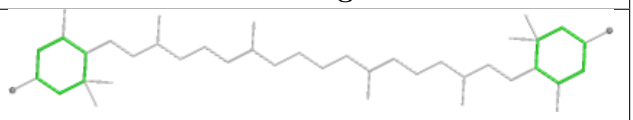
Bond lengths



Bond angles

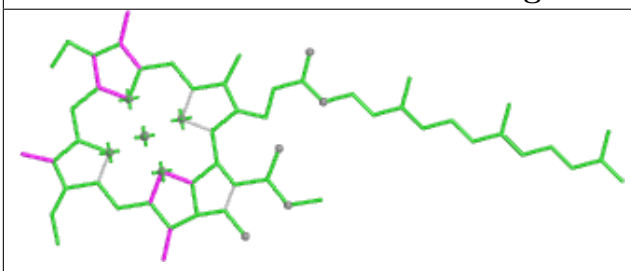


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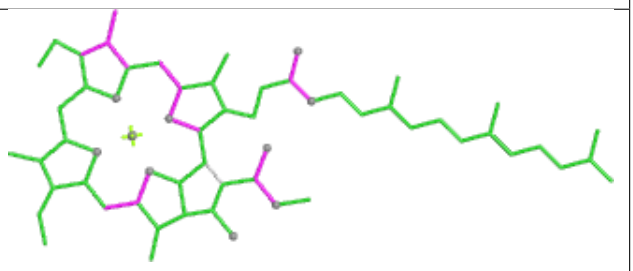


Rings

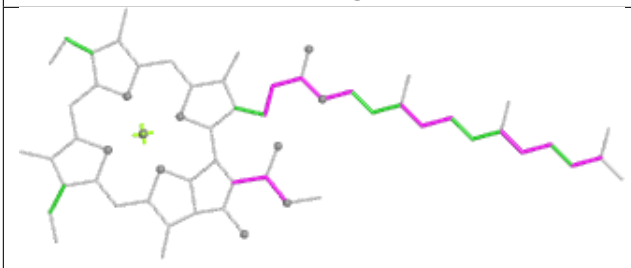
Ligand CLA A 818



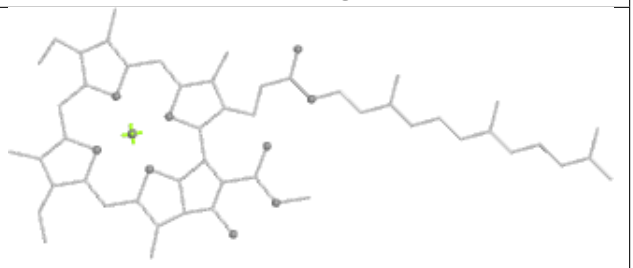
Bond lengths



Bond angles

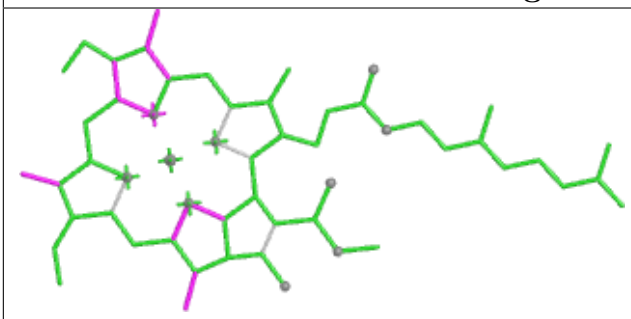


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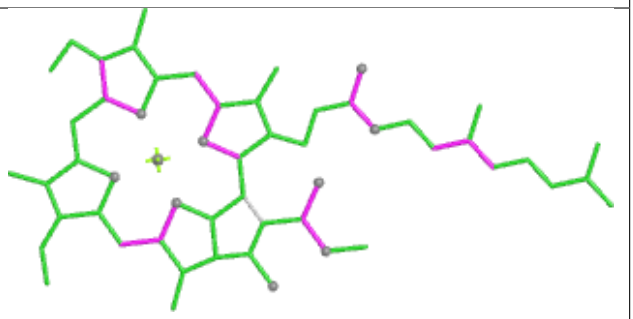


Rings

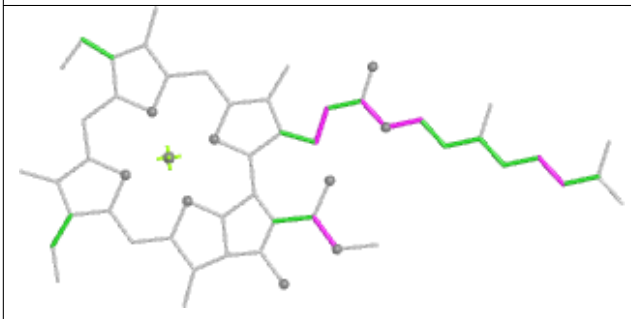
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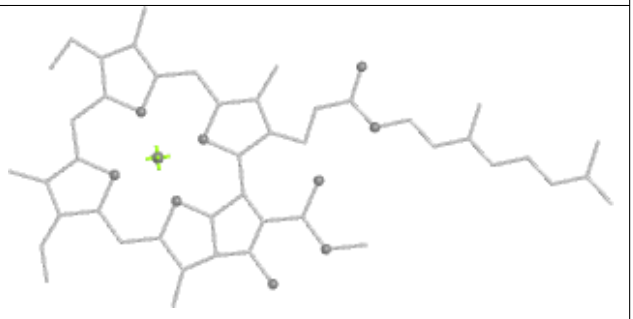
Bond lengths



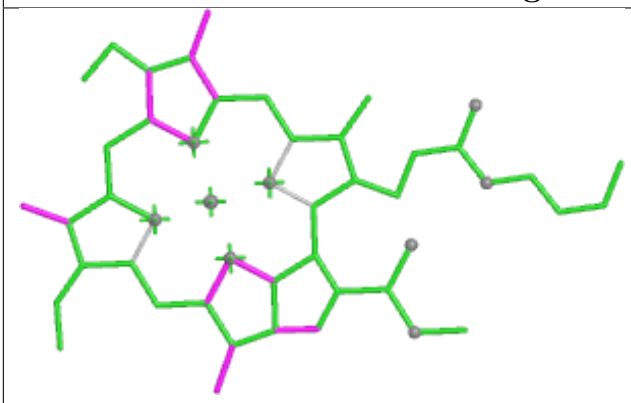
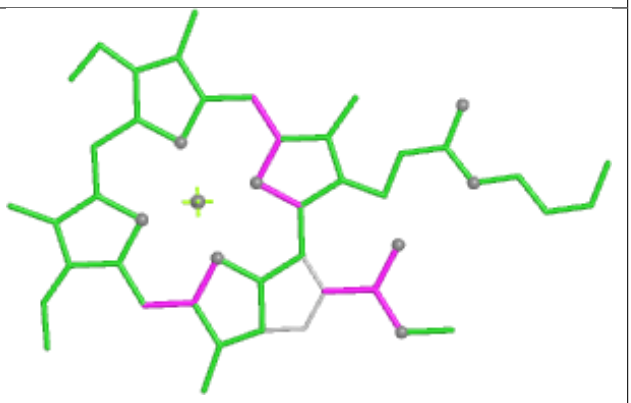
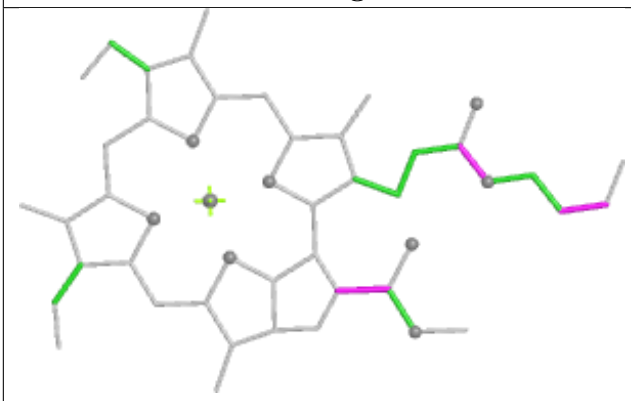
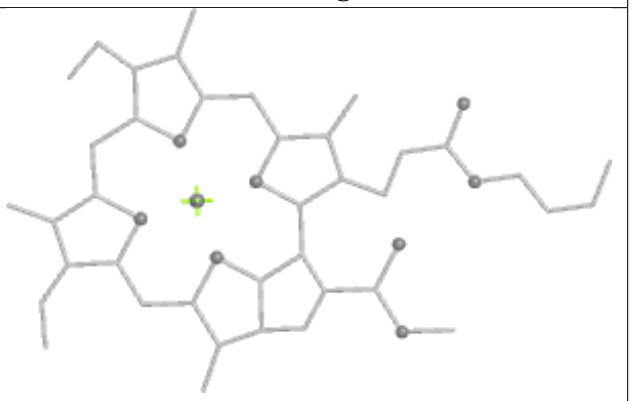
Bond angles



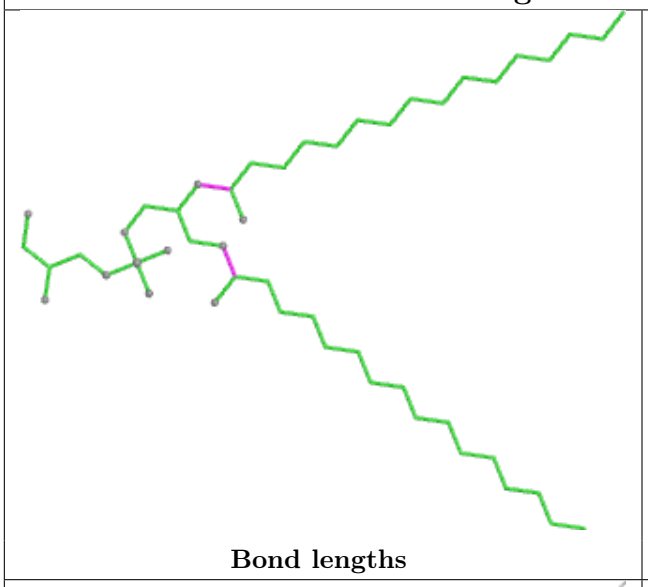
Torsions



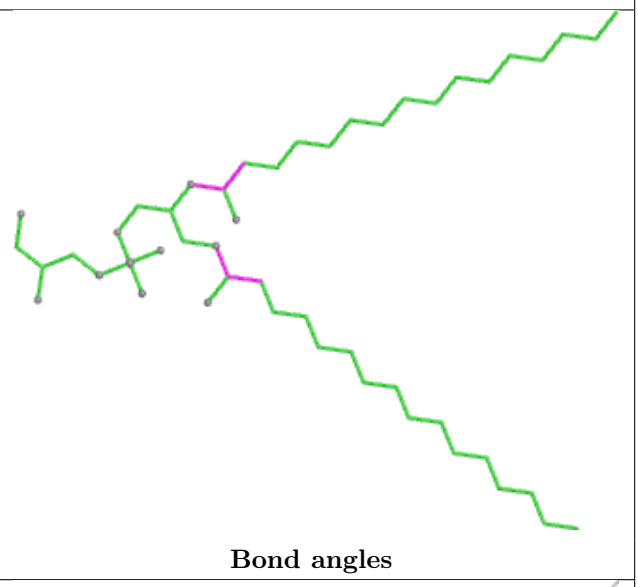
Rings

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

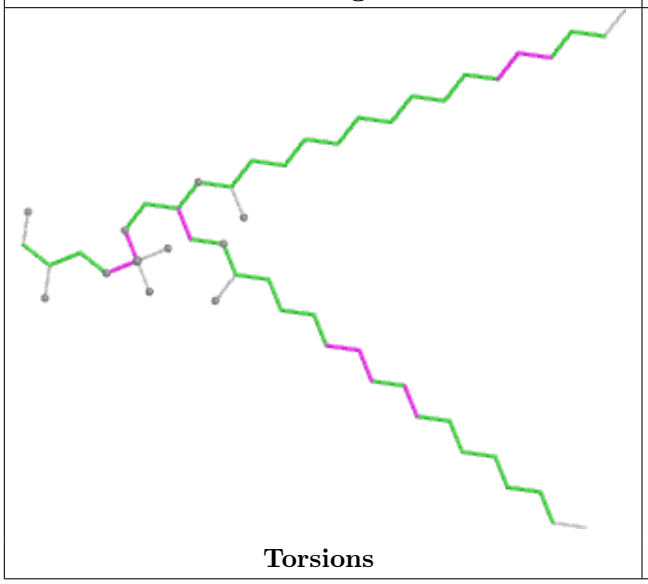
Ligand LHG X 2630



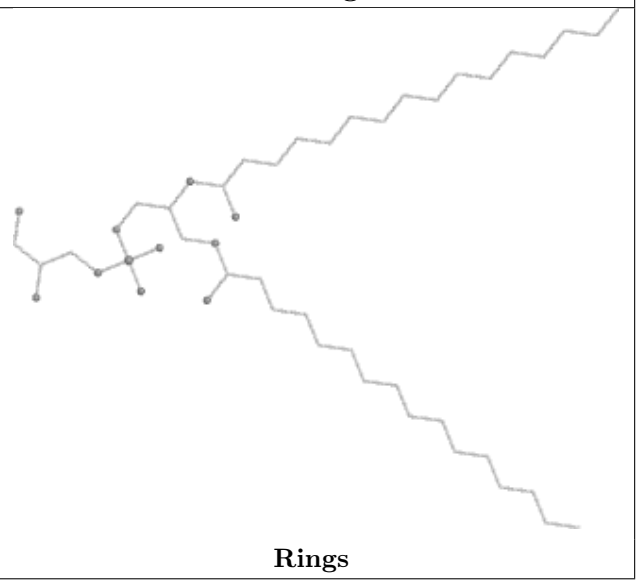
Bond lengths



Bond angles

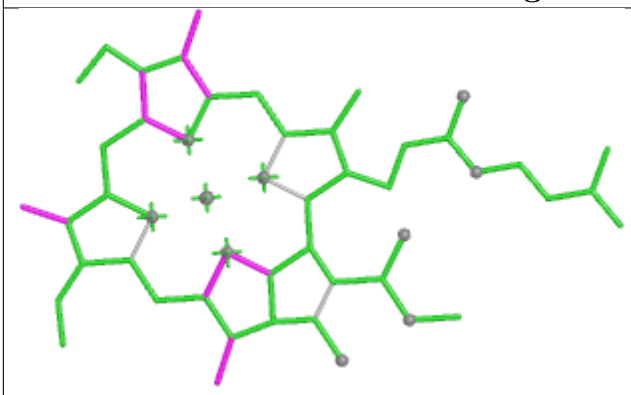


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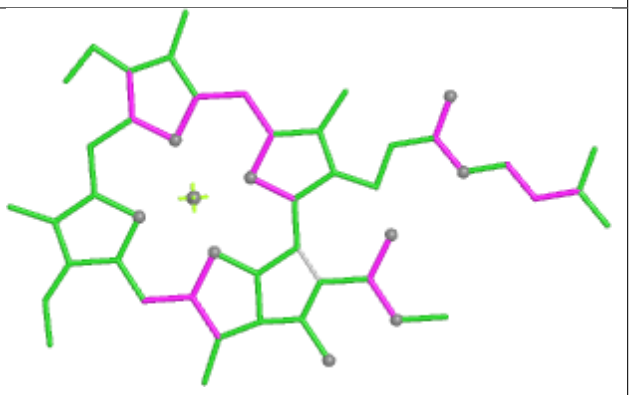


Rings

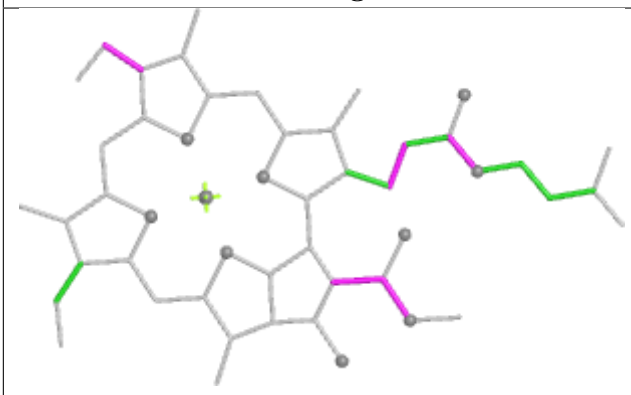
Ligand CLA A 832



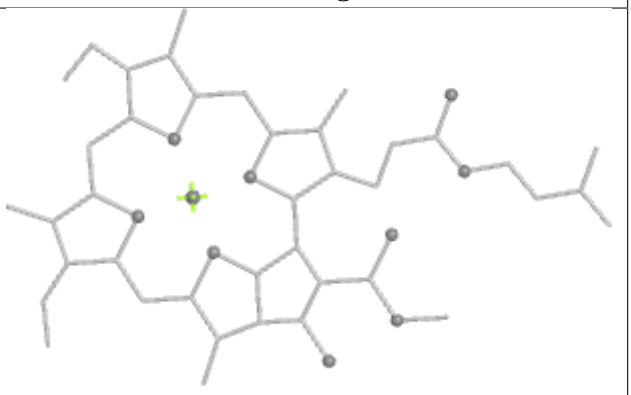
Bond lengths



Bond angles

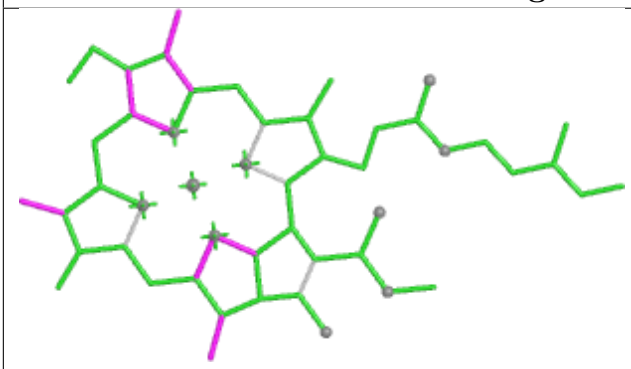


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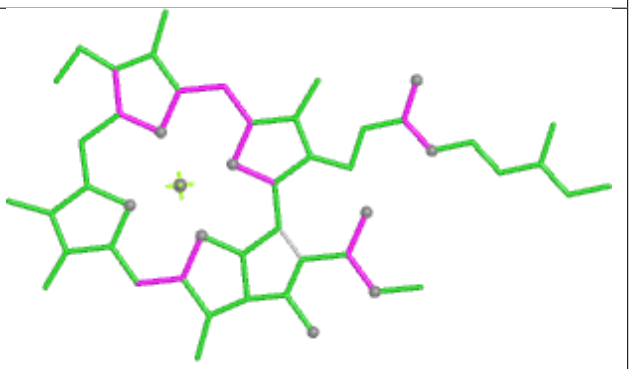


Rings

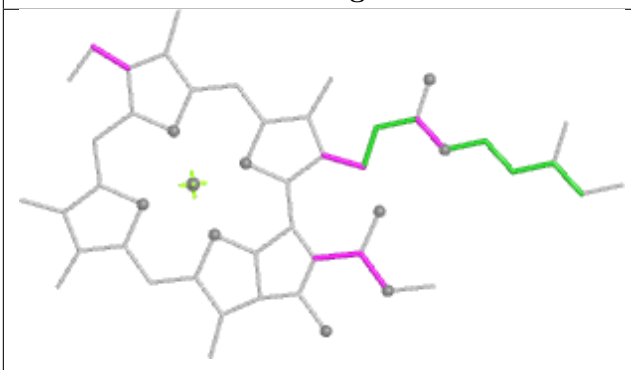
Ligand CLA 7 604



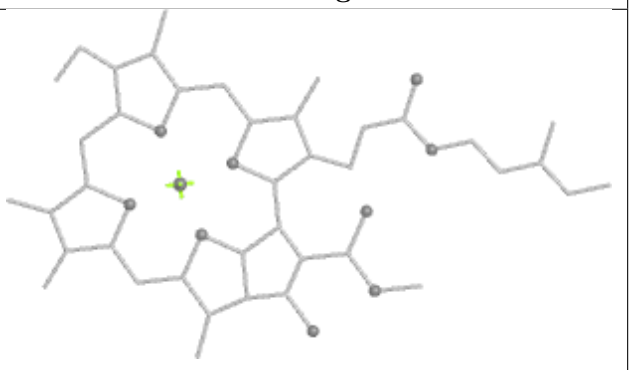
Bond lengths



Bond angles

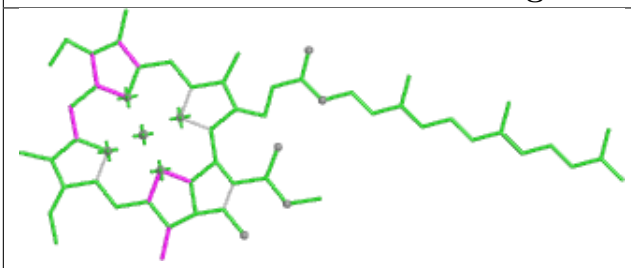


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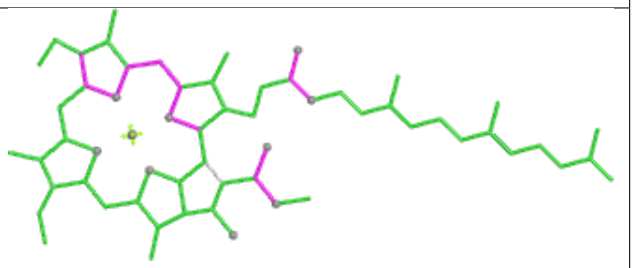


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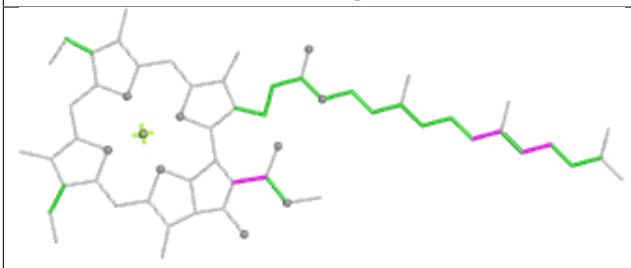
Ligand CLA Z 602



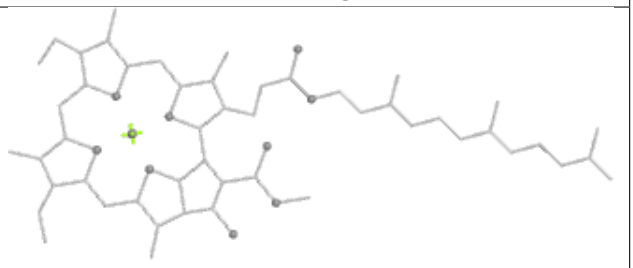
Bond lengths



Bond angles

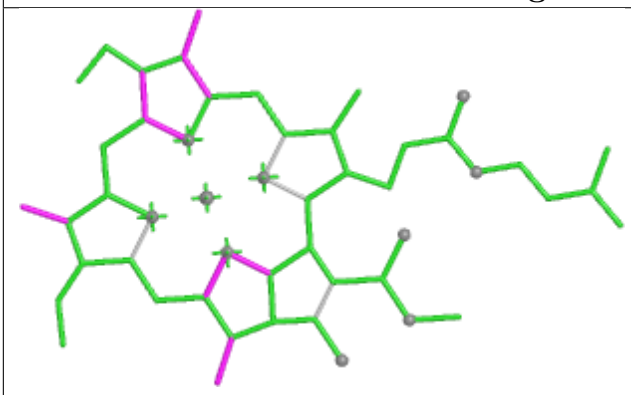


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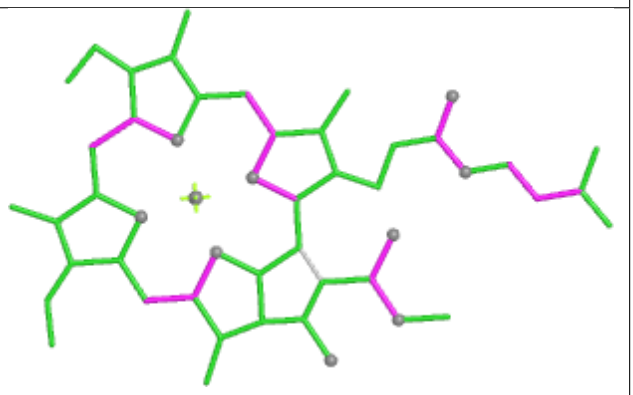


Rings

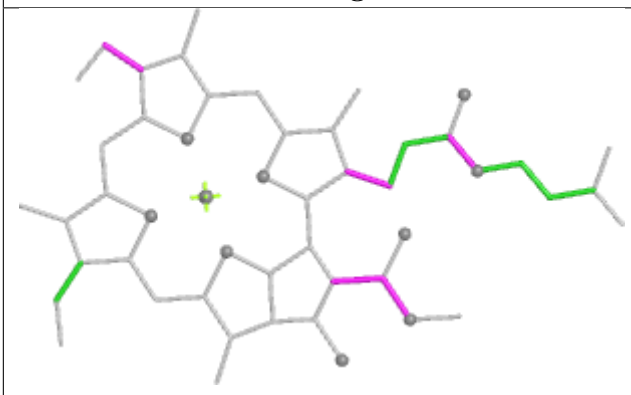
Ligand CLA 5 617



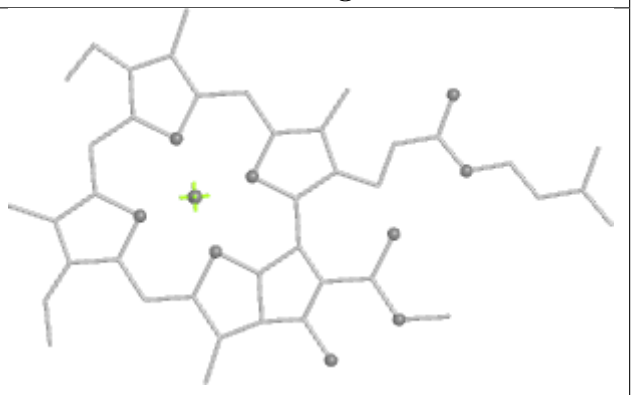
Bond lengths



Bond angles

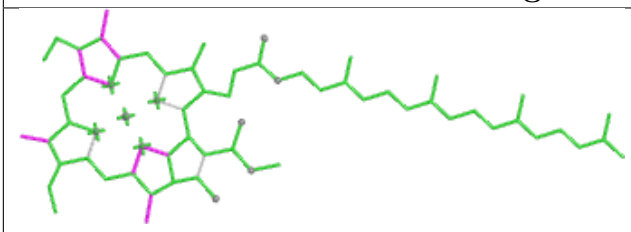


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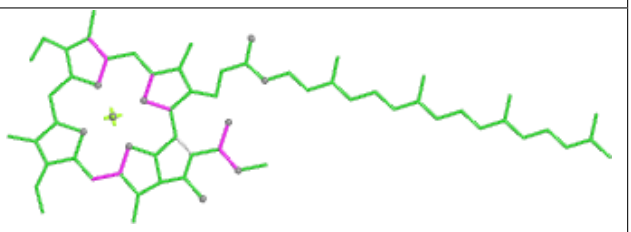


Rings

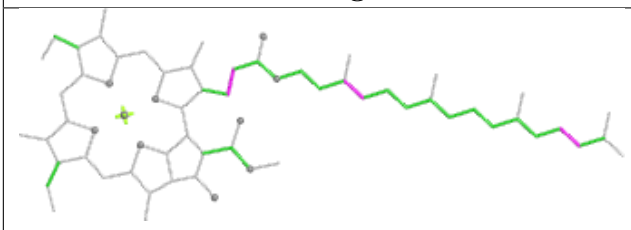
Ligand CLA A 803



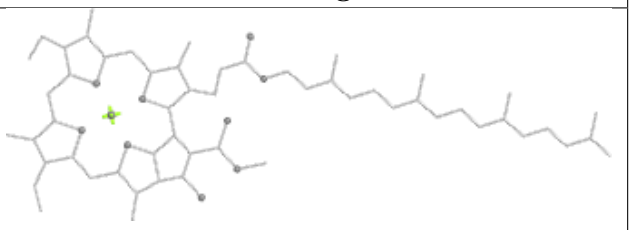
Bond lengths



Bond angles

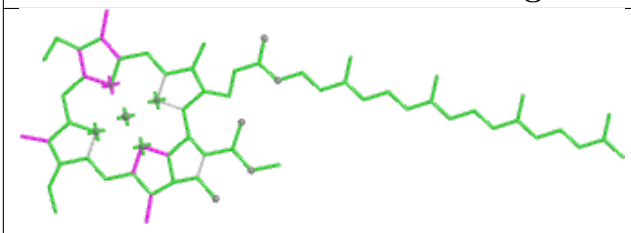


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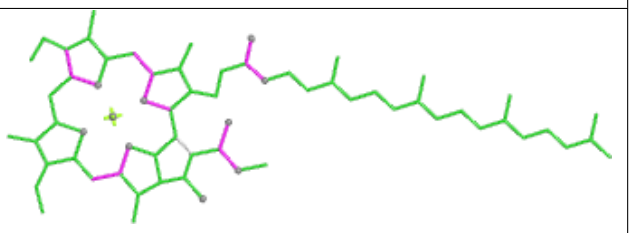


Rings

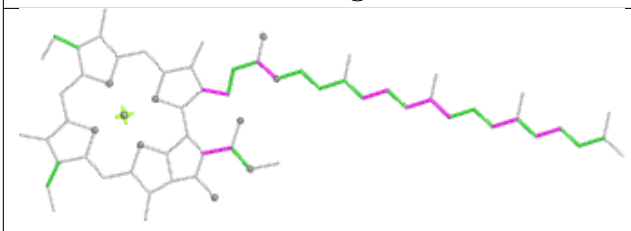
Ligand CLA B 805



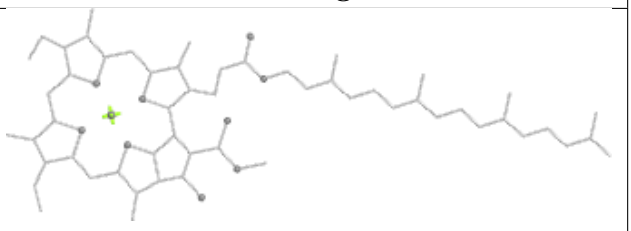
Bond lengths



Bond angles

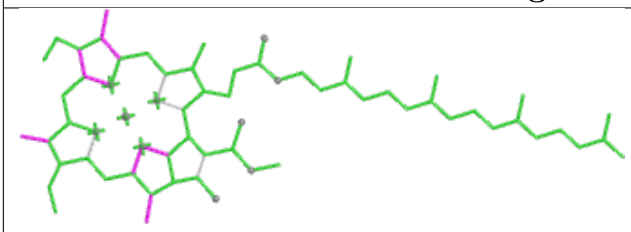


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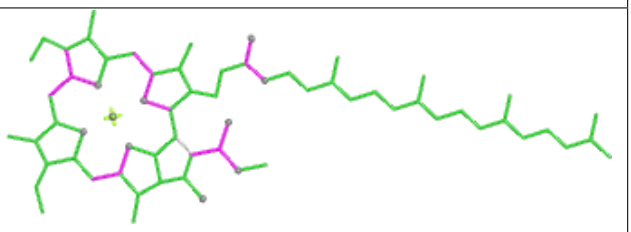


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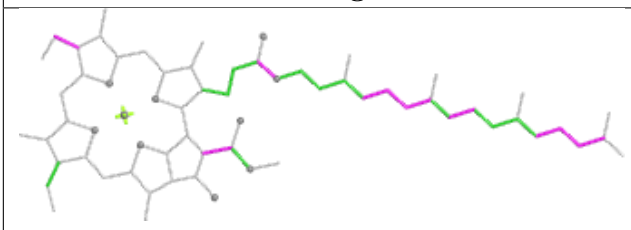
Ligand CLA 6 604



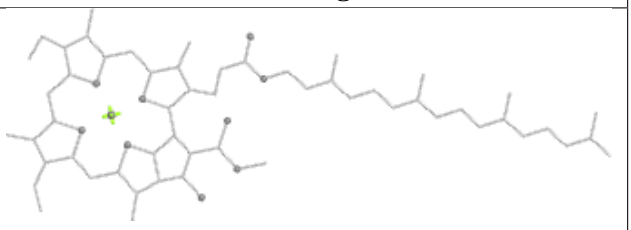
Bond lengths



Bond angles

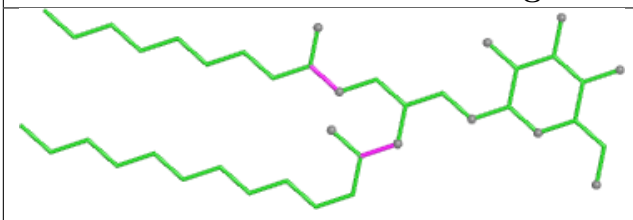


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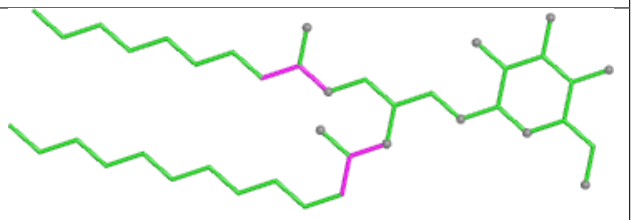


Rings

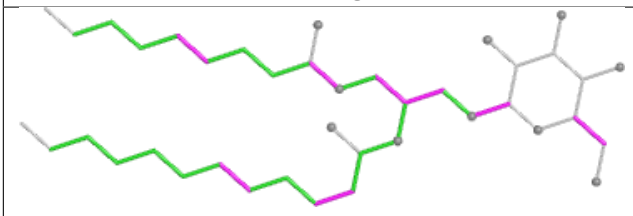
Ligand LMG 5 627



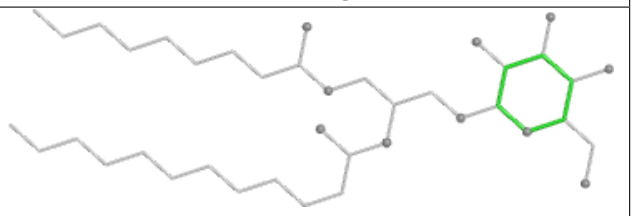
Bond lengths



Bond angles

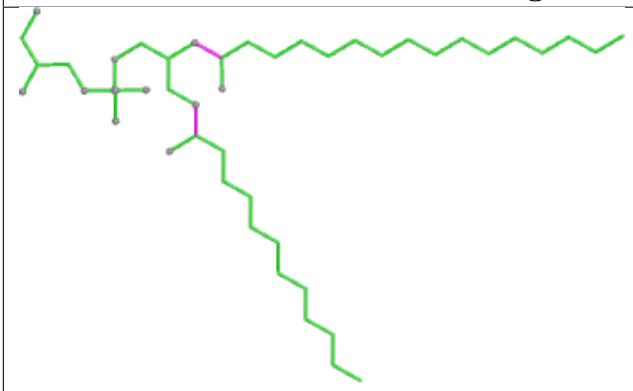


Torsions

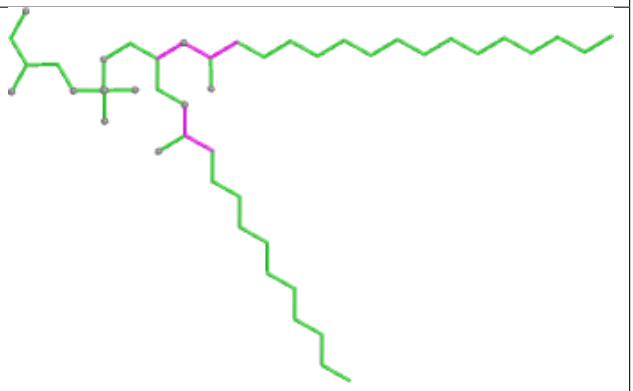


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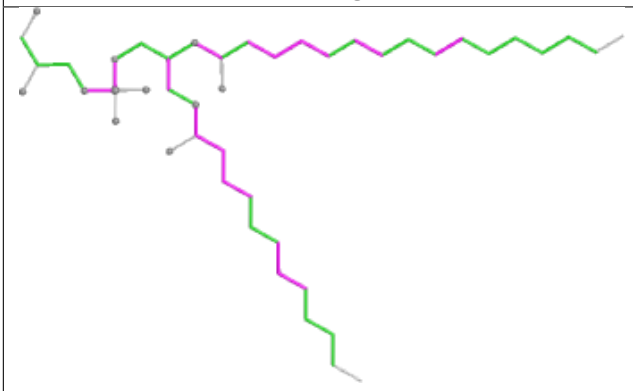
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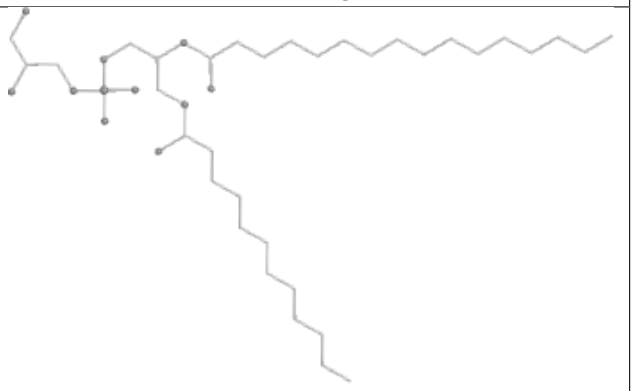
Bond lengths



Bond angles

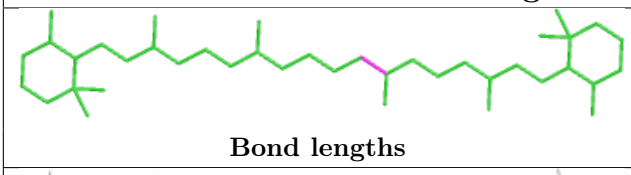


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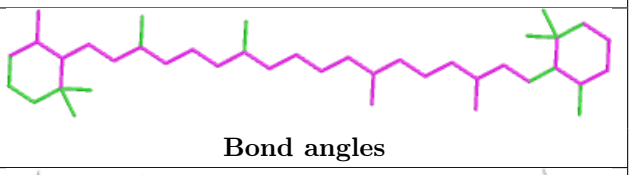


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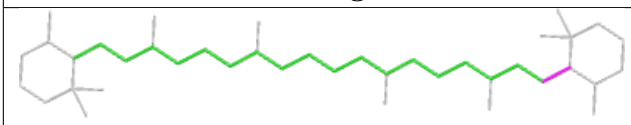
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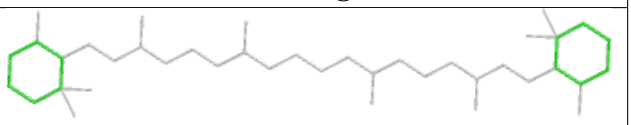
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Bond angles

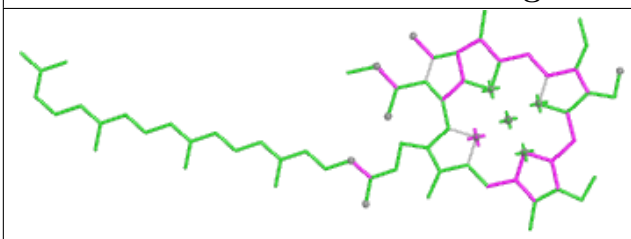


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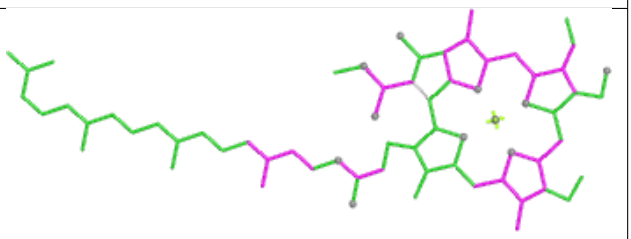


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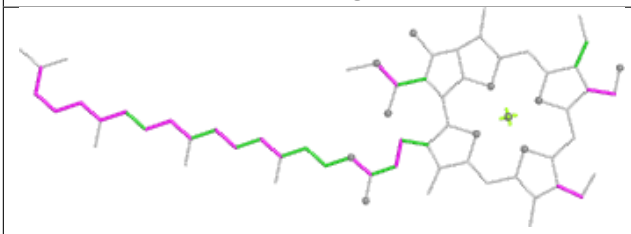
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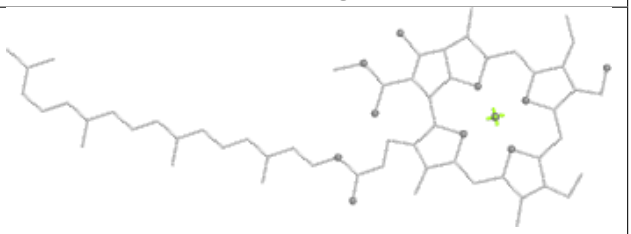
Bond lengths



Bond angles

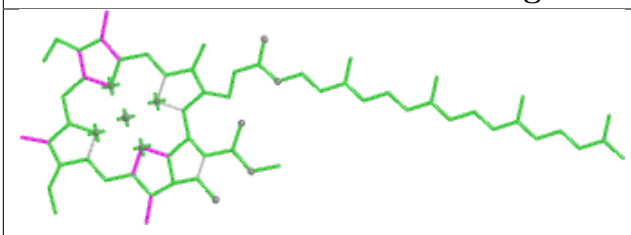


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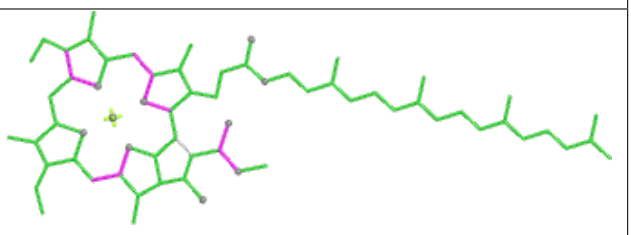


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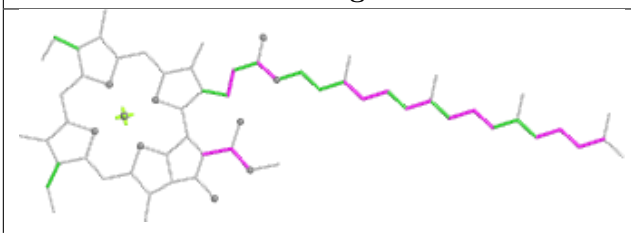
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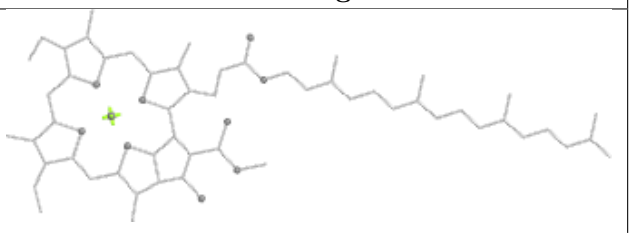
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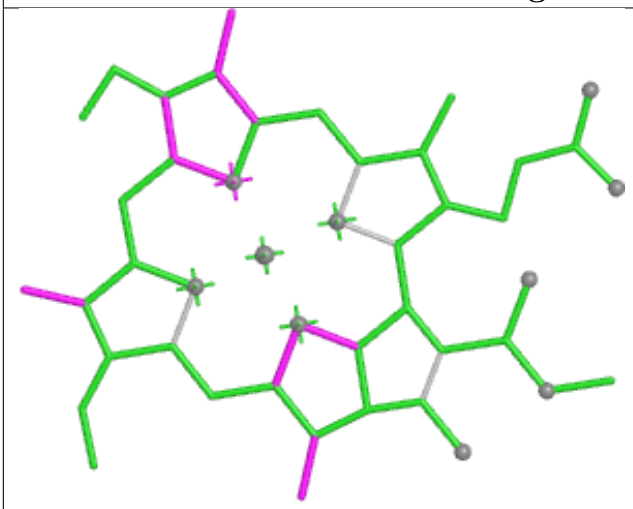


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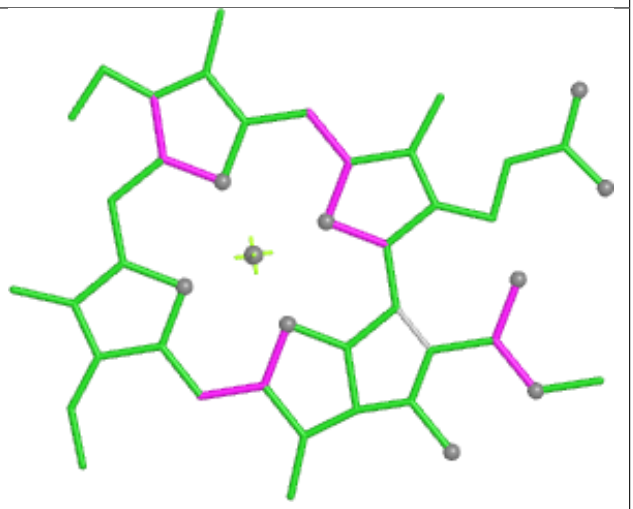


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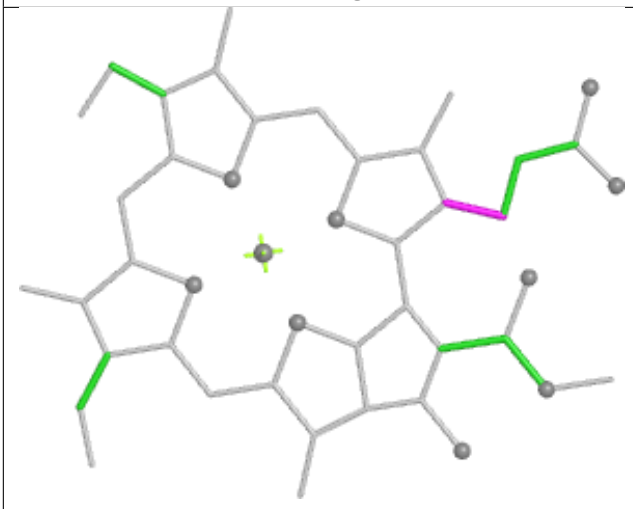
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Bond lengths



Bond angles

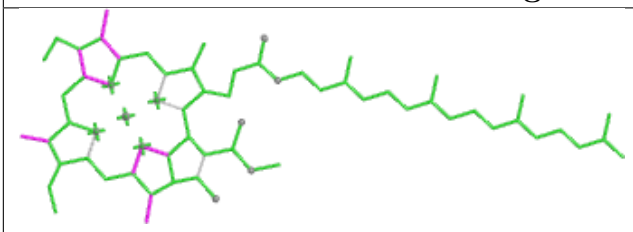


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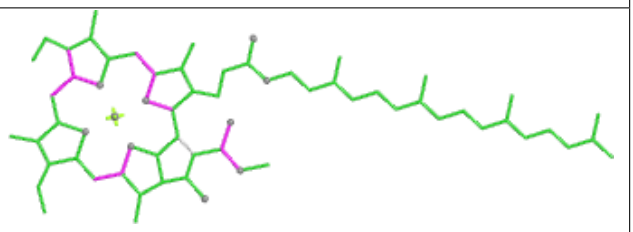


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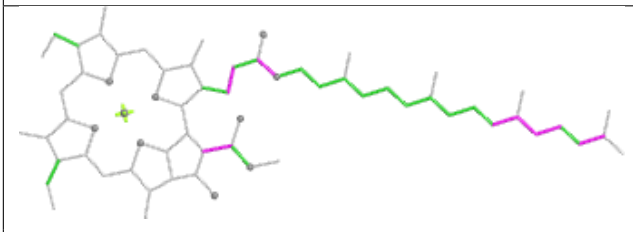
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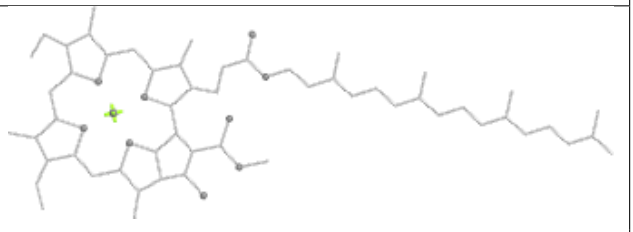
Bond lengths



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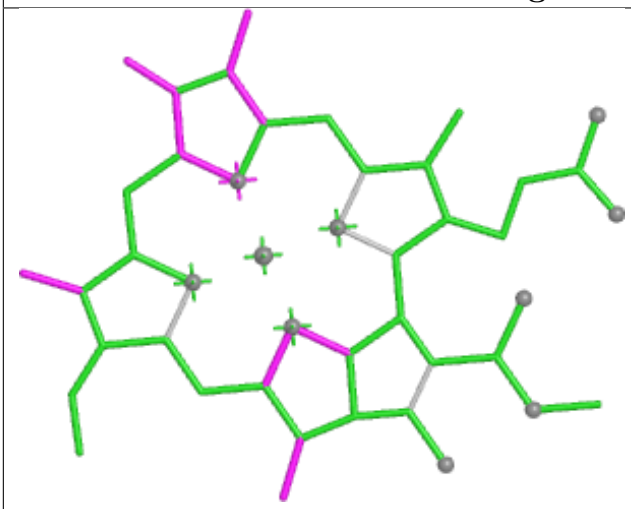


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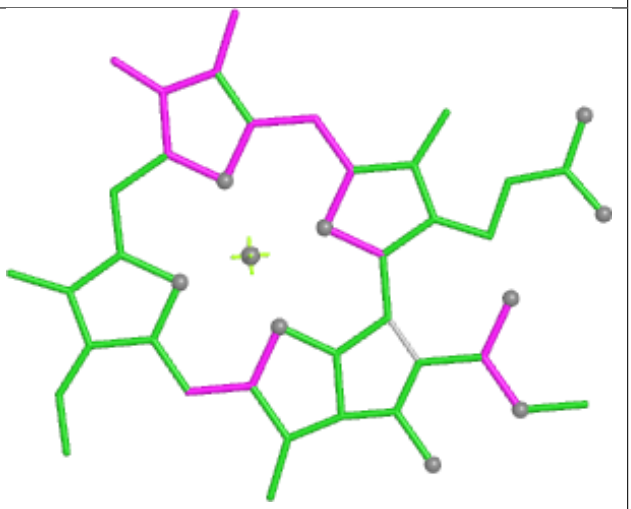


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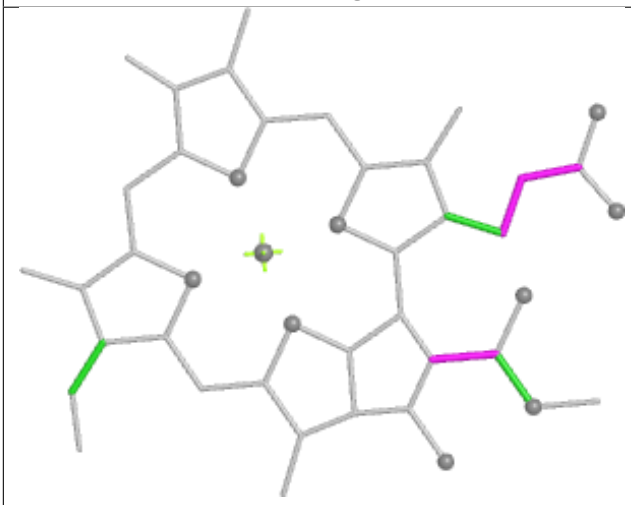
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Bond lengths



Bond angles

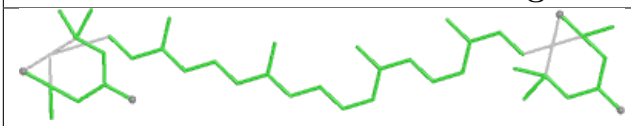


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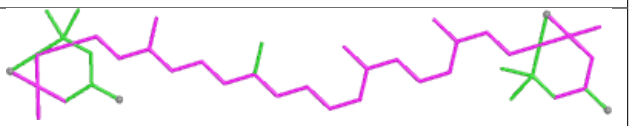


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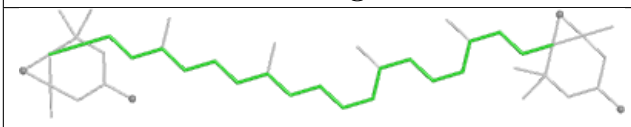
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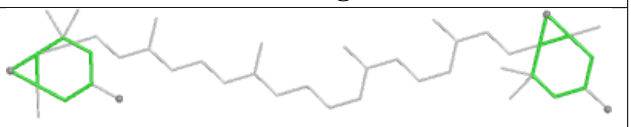
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Bond angles

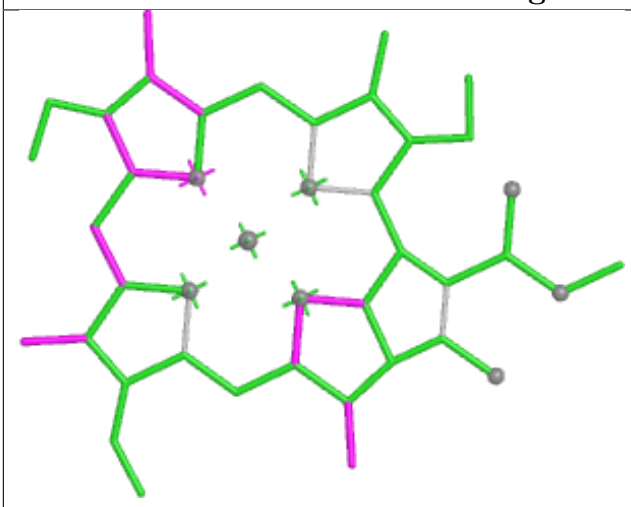


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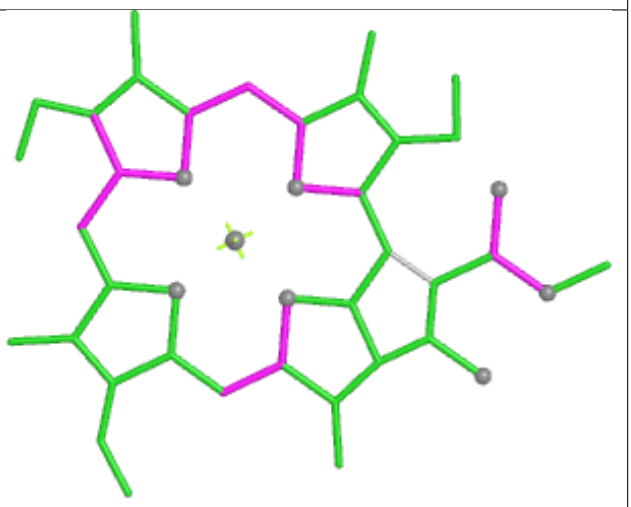


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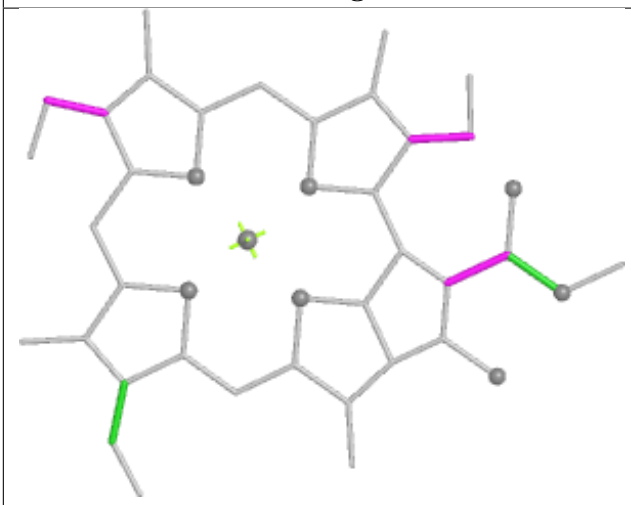
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Bond lengths



Bond angles

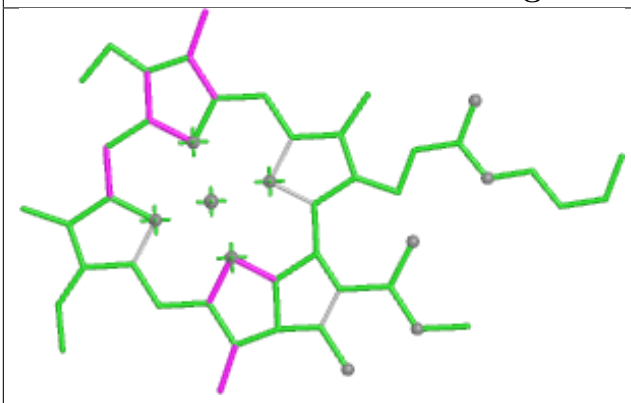


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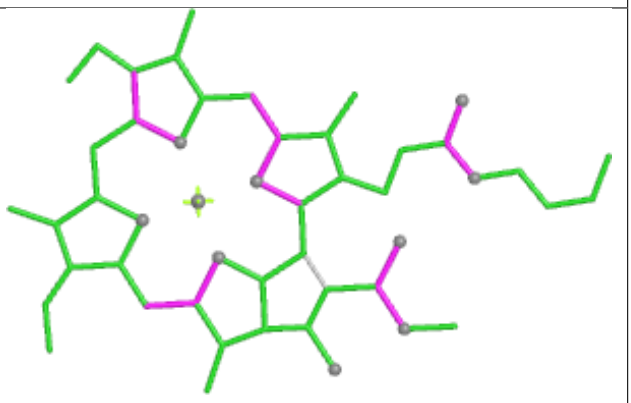


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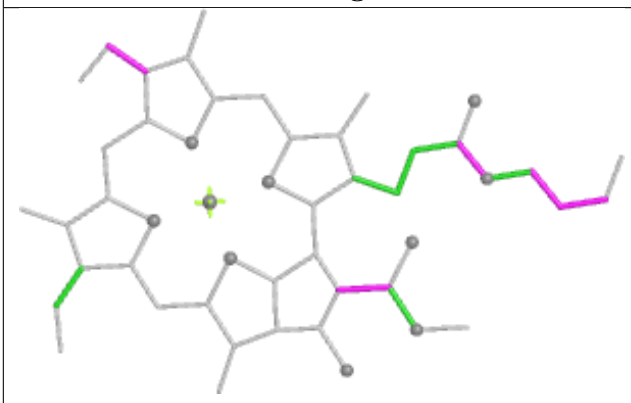
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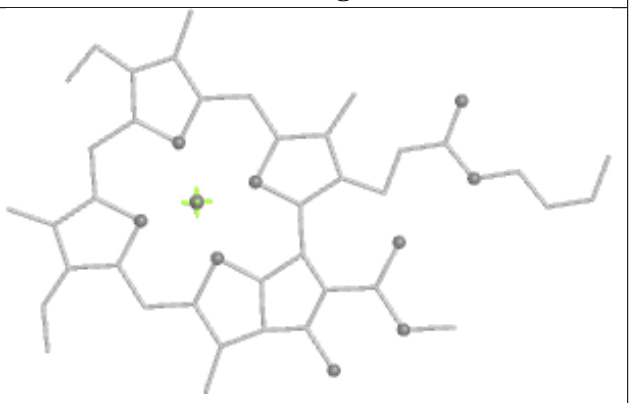
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Bond angles

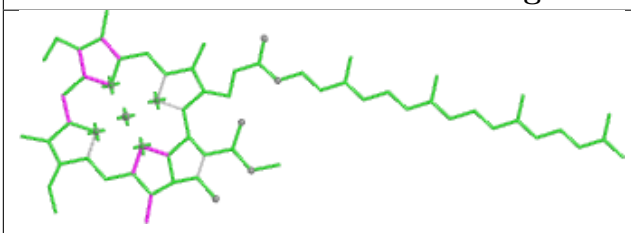


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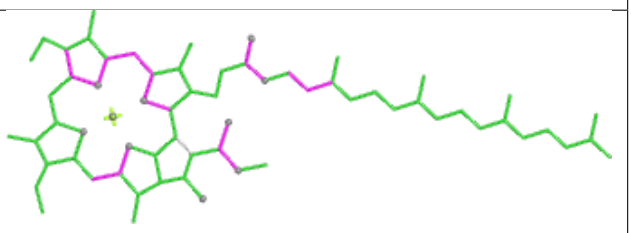


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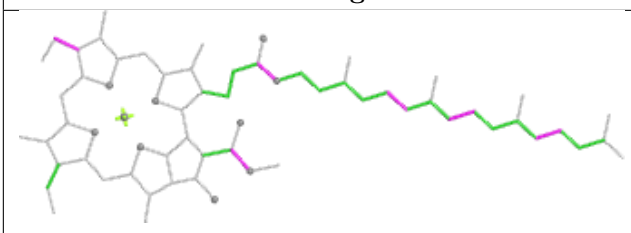
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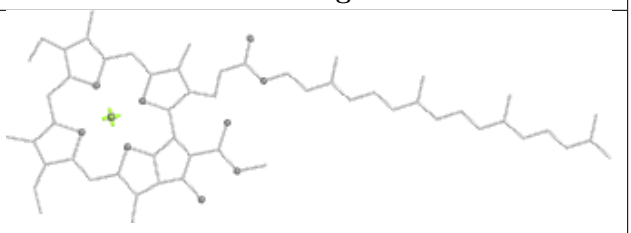
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Bond angles

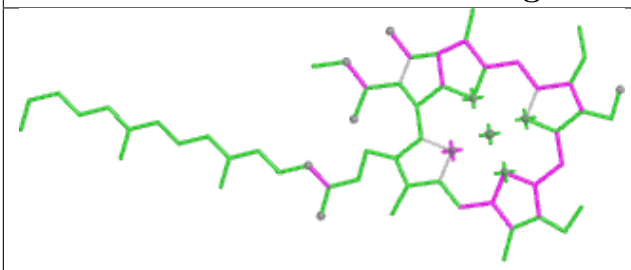


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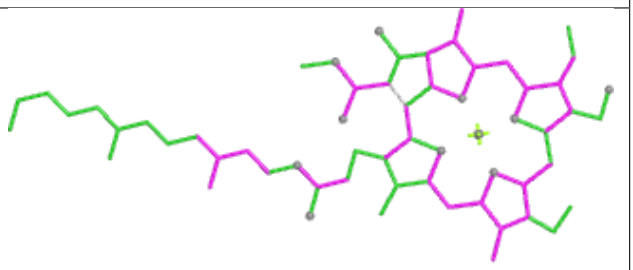


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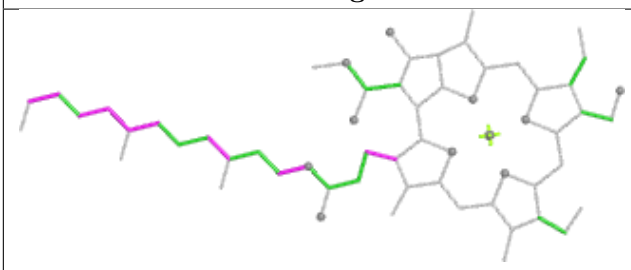
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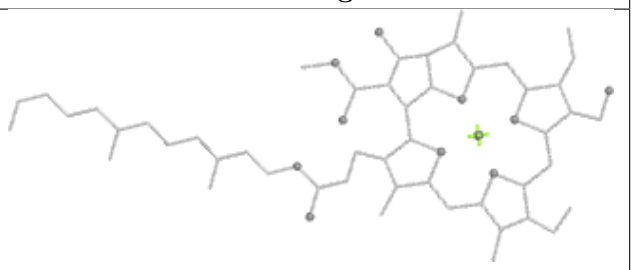
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Bond angles

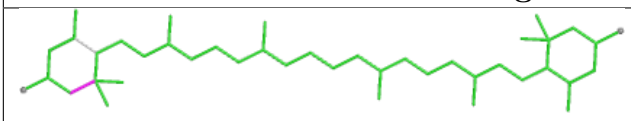


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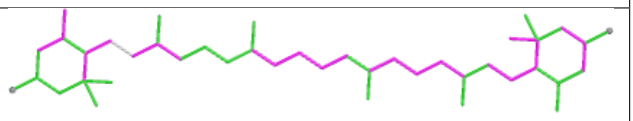


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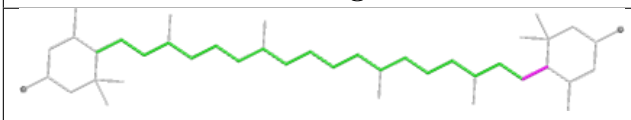
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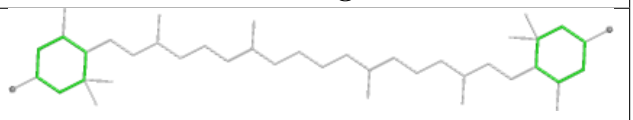
Bond lengths



Bond angles

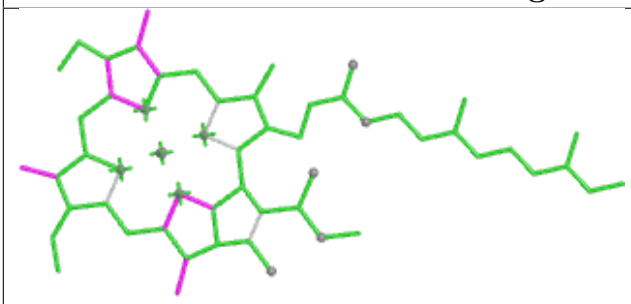


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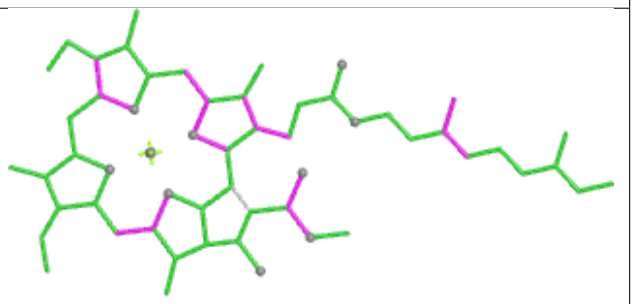


Rings

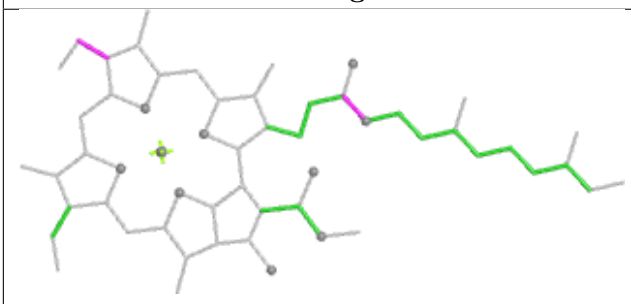
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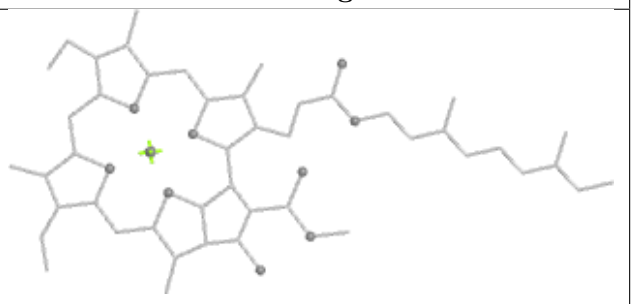
Bond lengths



Bond angles

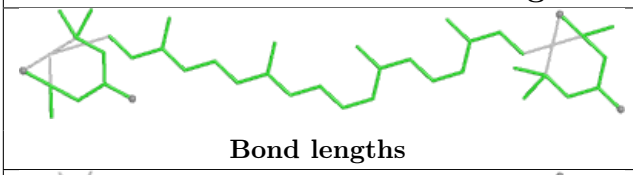


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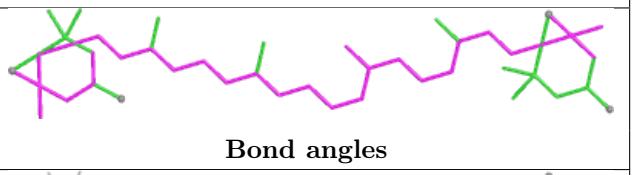


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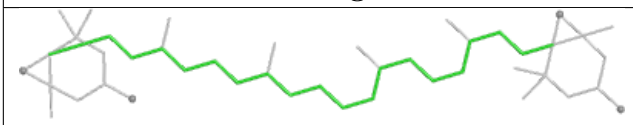
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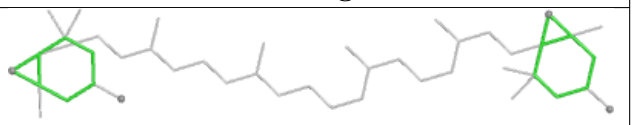
Bond lengths



Bond angles

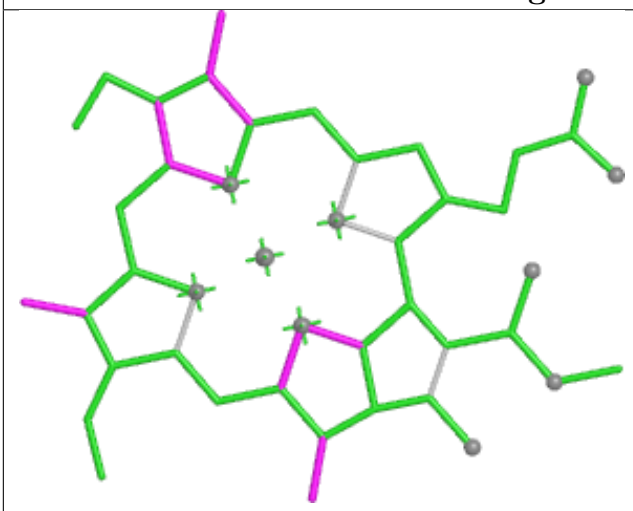


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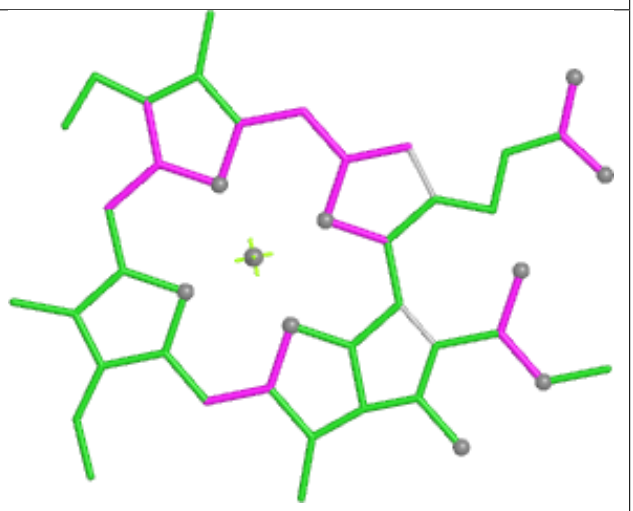


Rings

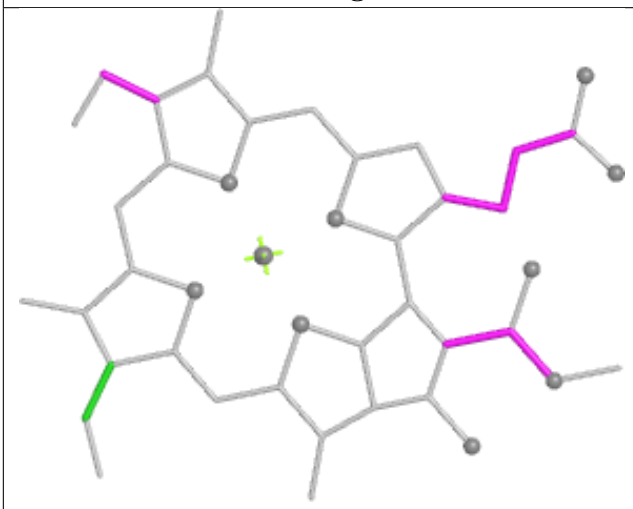
Ligand CLA 5 614



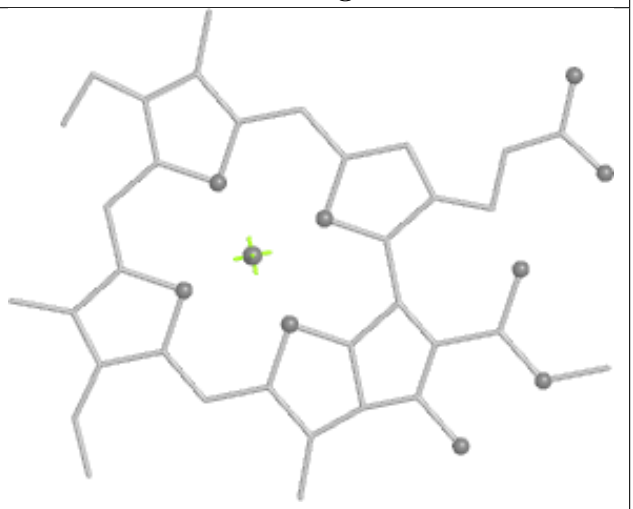
Bond lengths



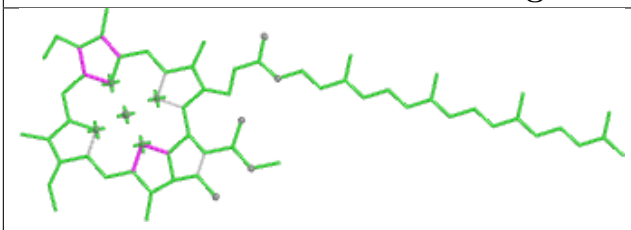
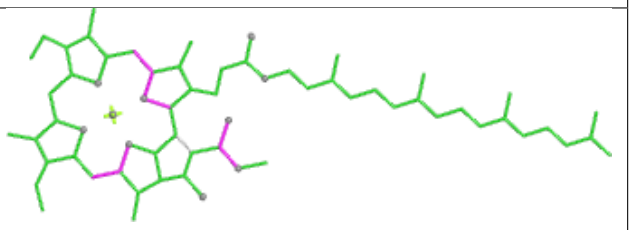
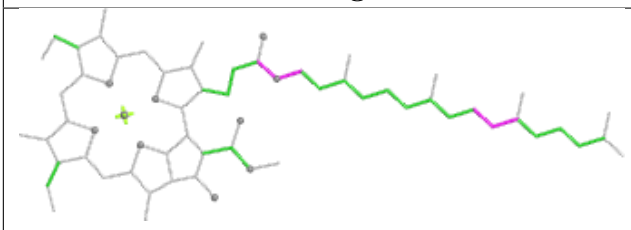
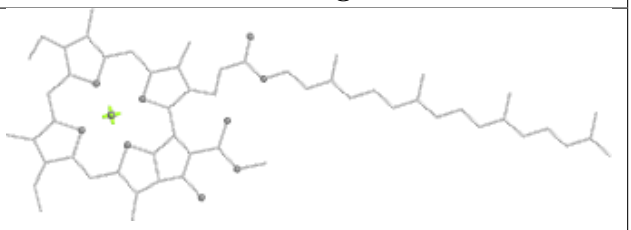
Bond angles

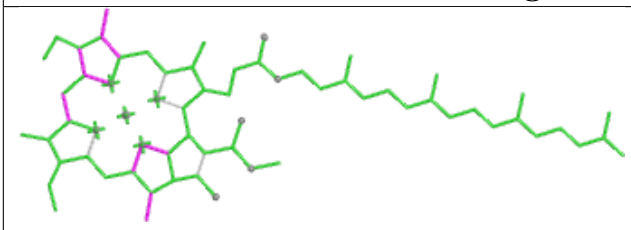
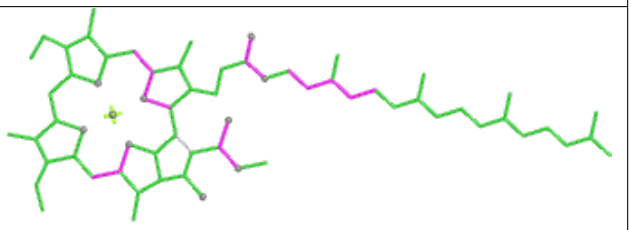
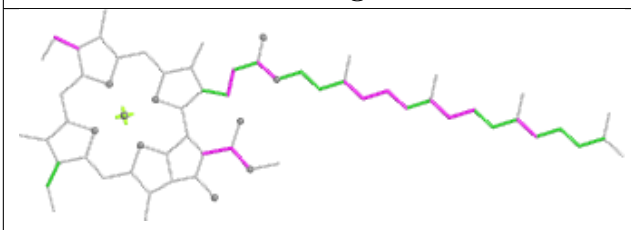
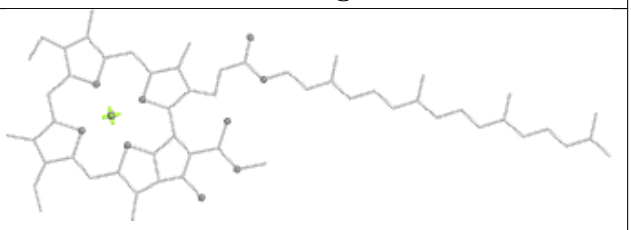


Torsions

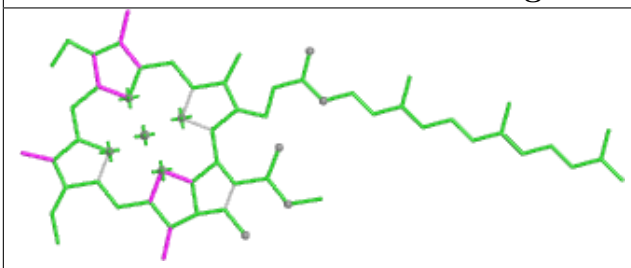


Rings

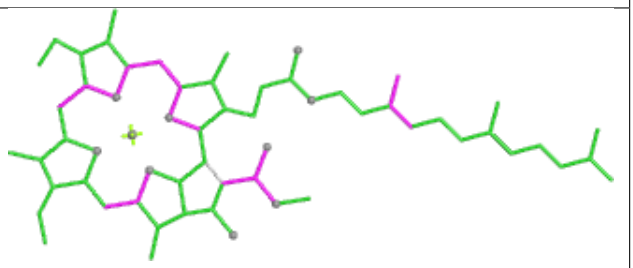
Ligand CLA Z 612	
 Bond lengths	 Bond angles
 Torsions	 Rings

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 Bond lengths	 Bond angles
 Torsions	 Rings

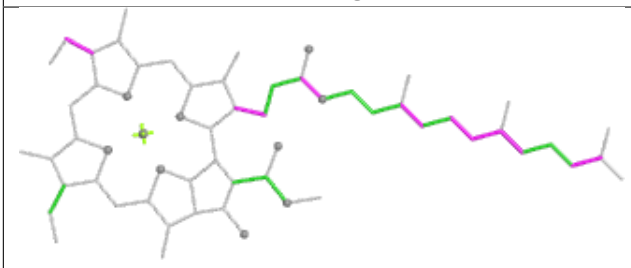
Ligand CLA B 818



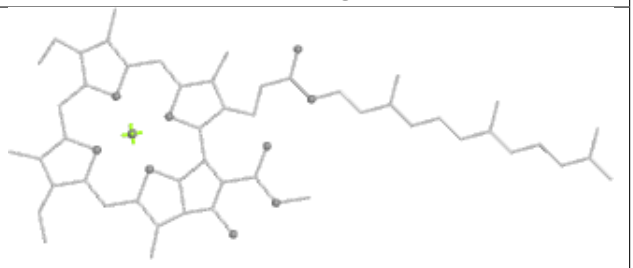
Bond lengths



Bond angles

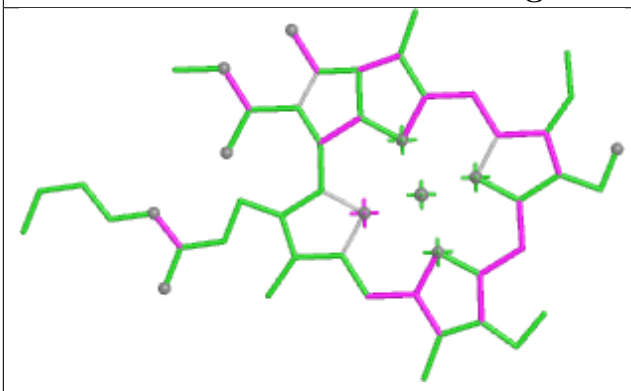


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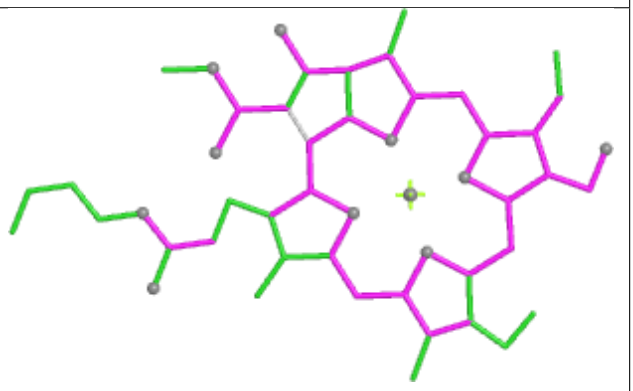


Rings

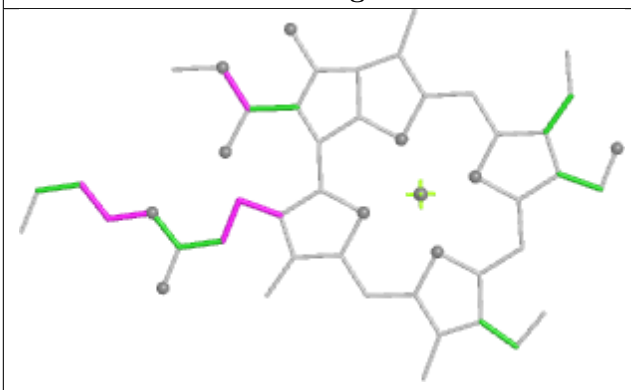
Ligand CHL Z 608



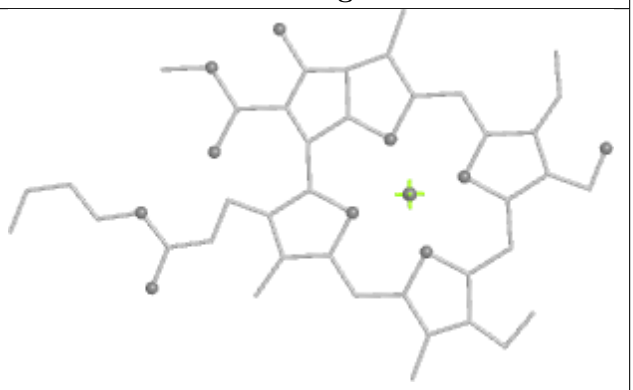
Bond lengths



Bond angles

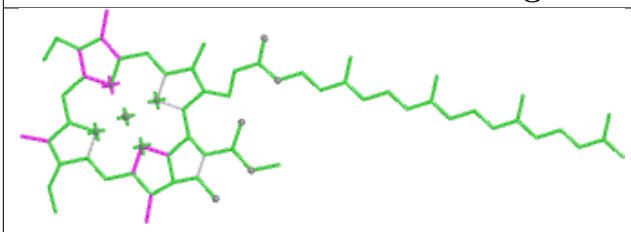


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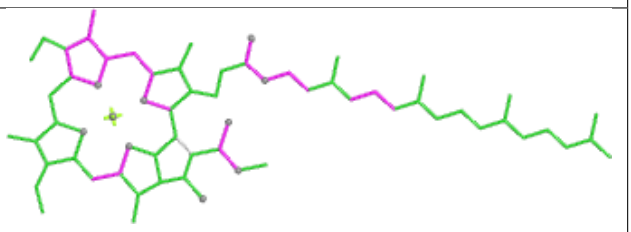


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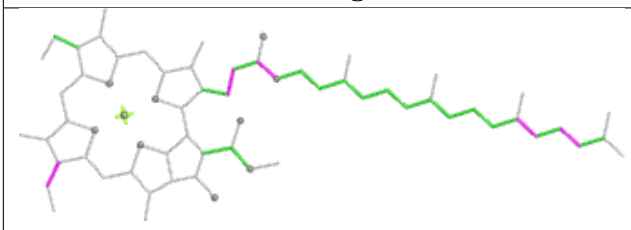
Ligand CLA A 822



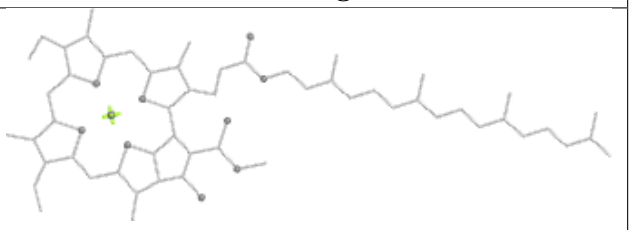
Bond lengths



Bond angles

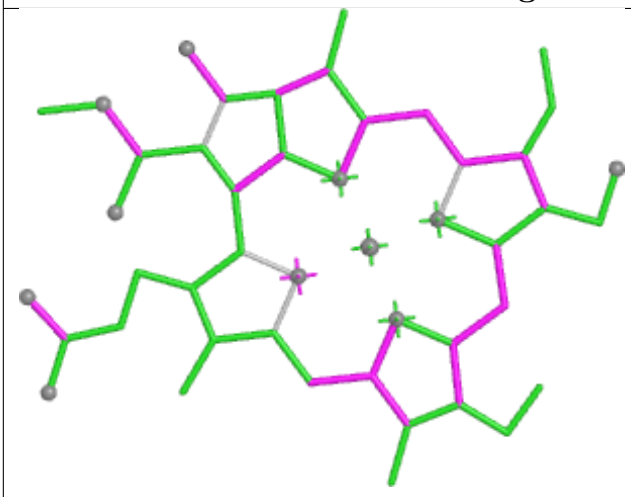


Torsions



Rings

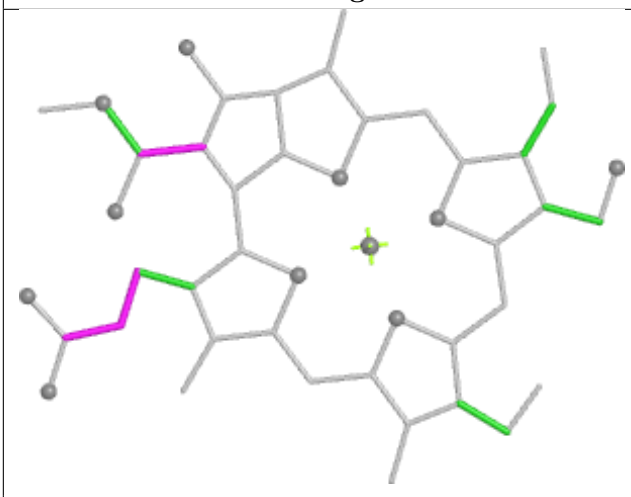
Ligand CHL W 605



Bond lengths



Bond angles

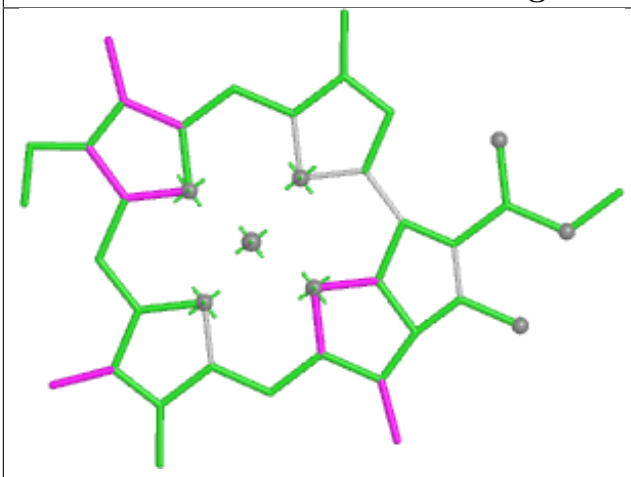


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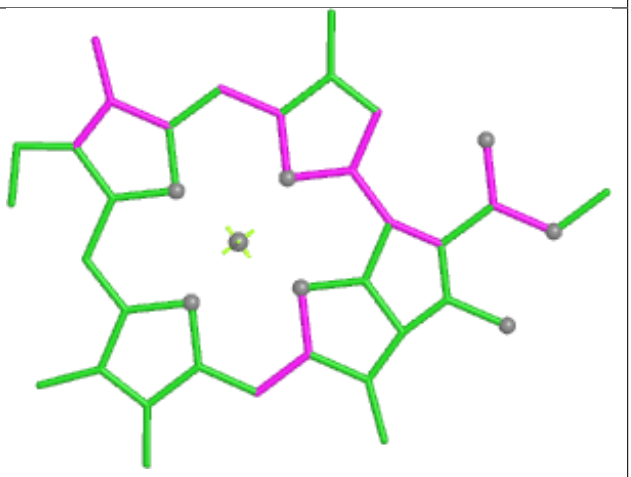


Rings

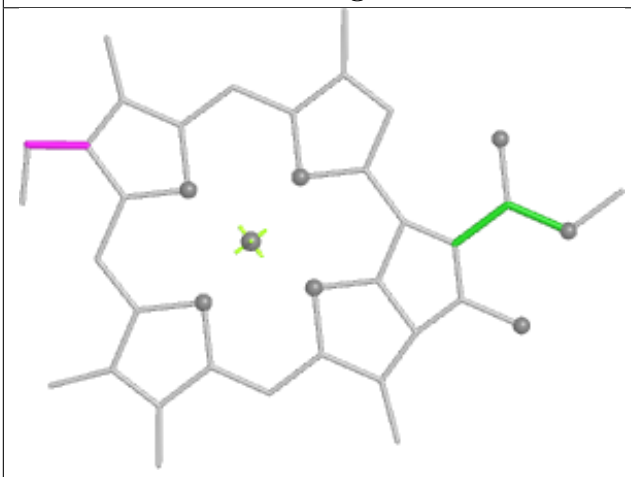
Ligand CLA 1 610



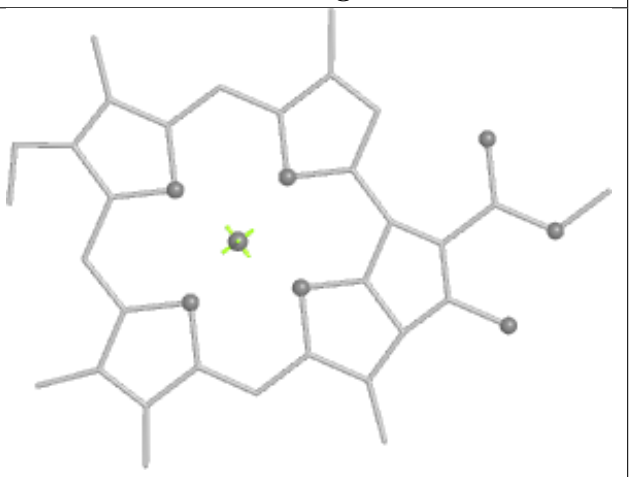
Bond lengths



Bond angles

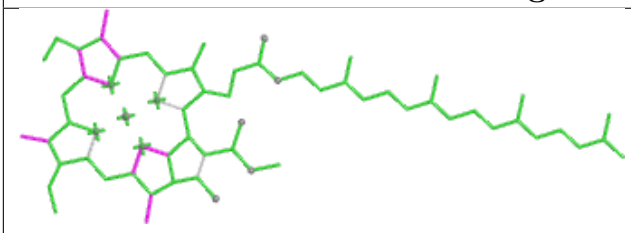


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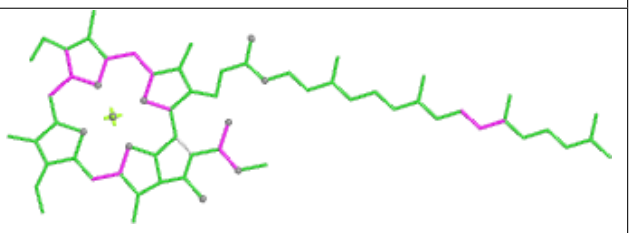


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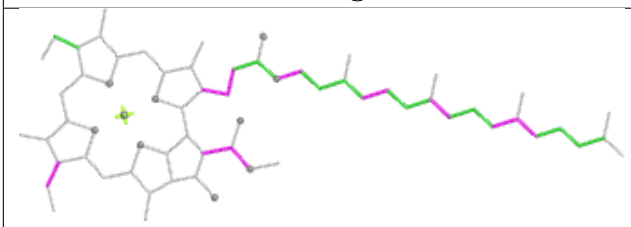
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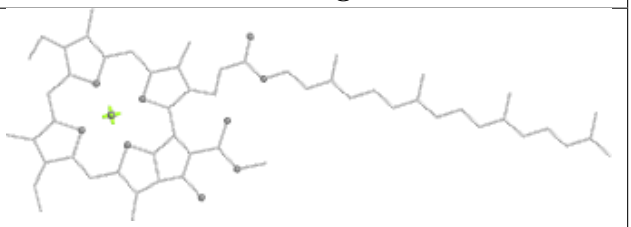
Bond lengths



Bond angles

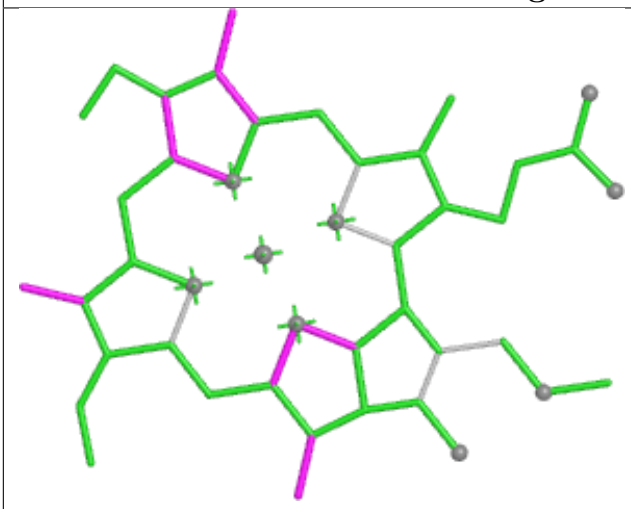


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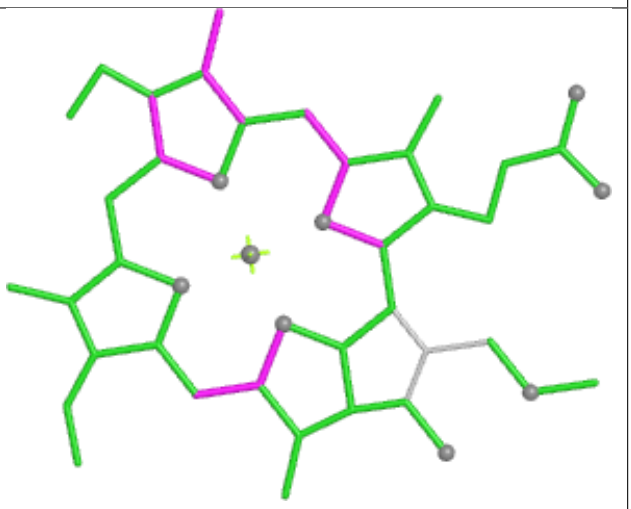


Rings

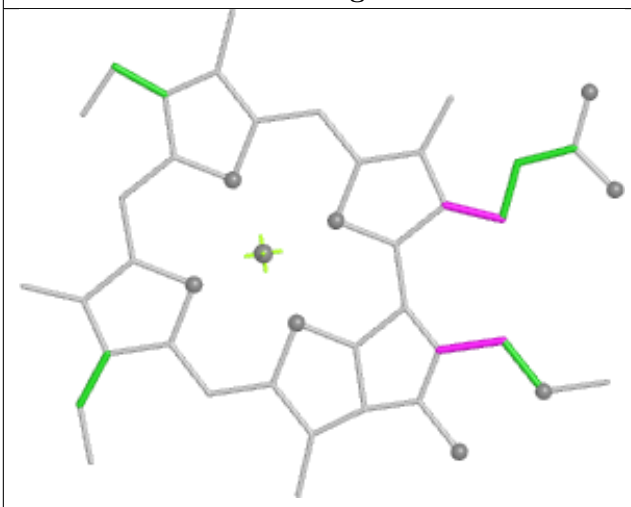
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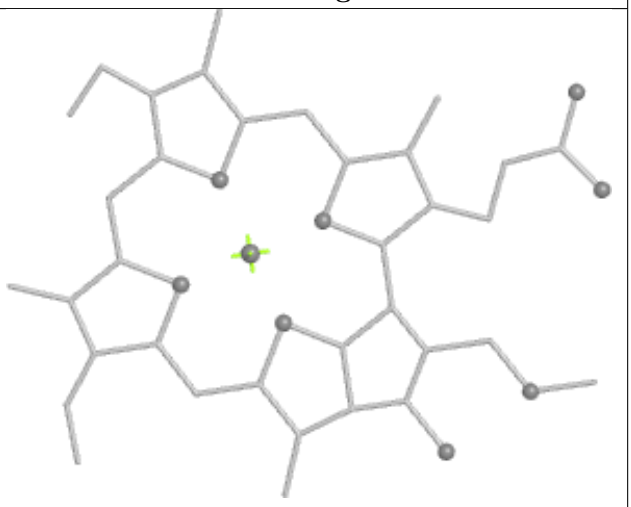
Bond lengths



Bond angles

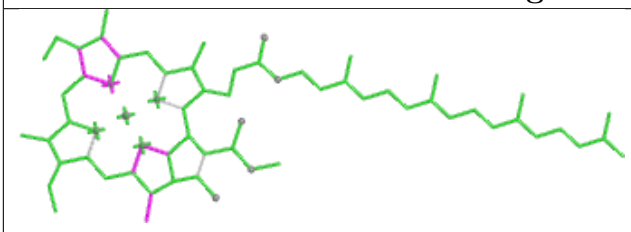


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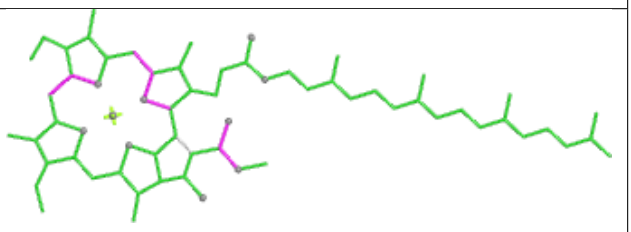


Rings

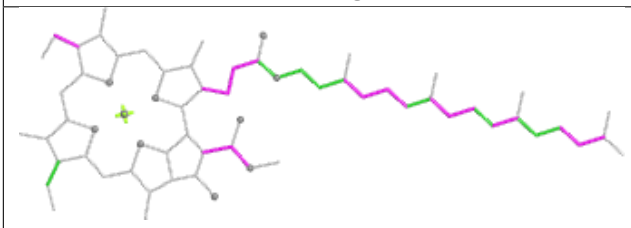
Ligand CLA Z 603



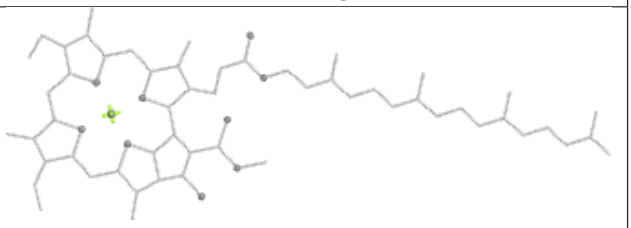
Bond lengths



Bond angles

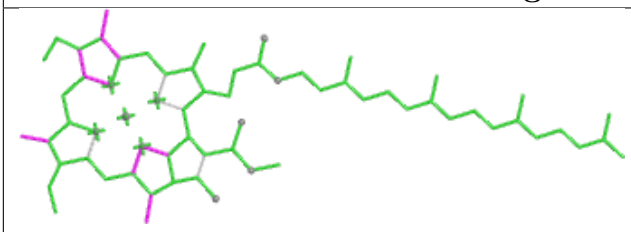


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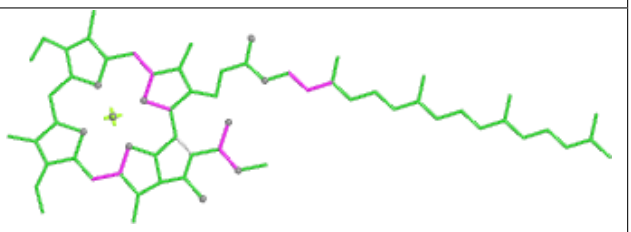


Rings

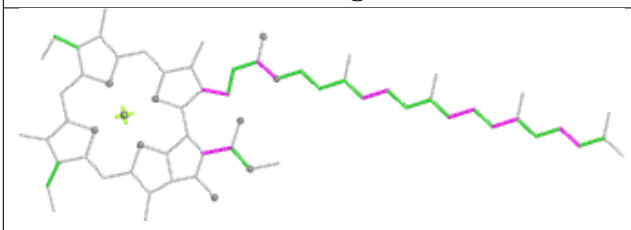
Ligand CLA A 816



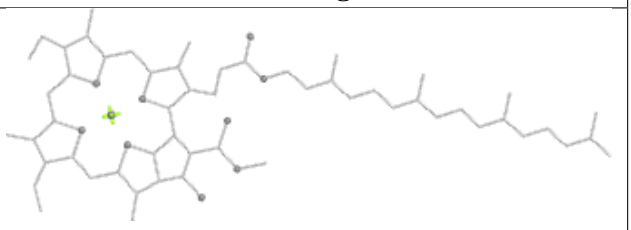
Bond lengths



Bond angles

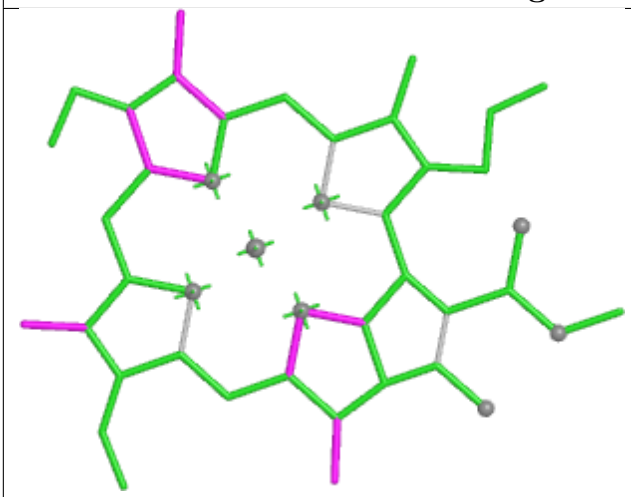


Torsions



Rings

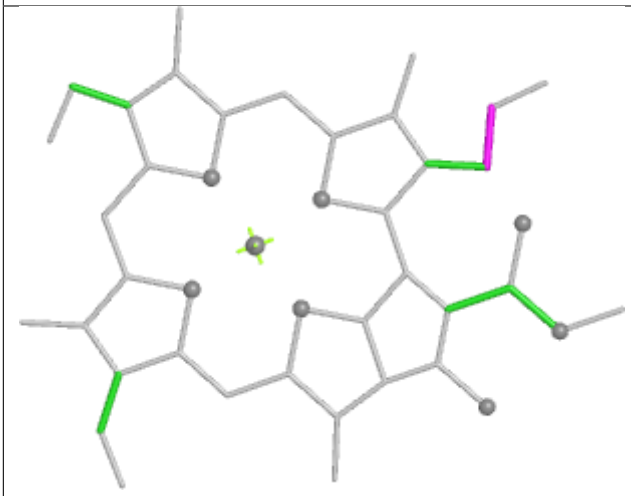
Ligand CLA 3 612



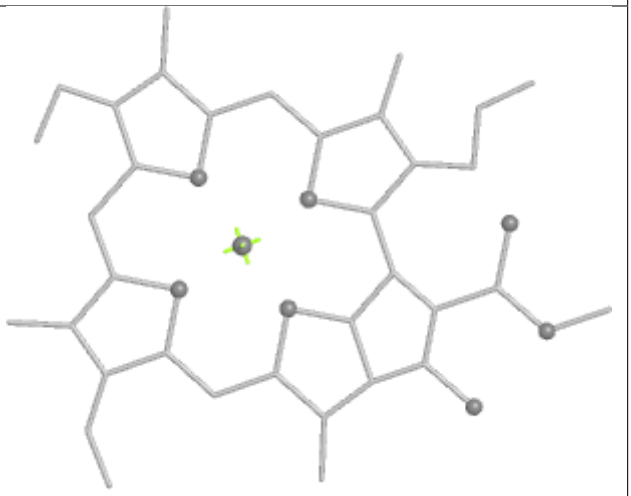
Bond lengths



Bond angles

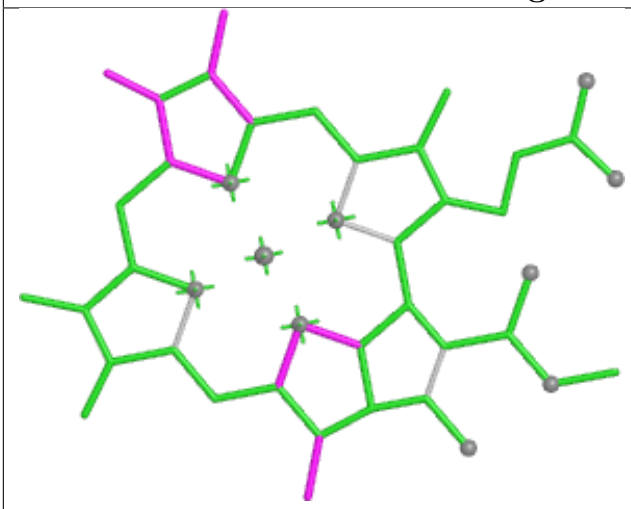


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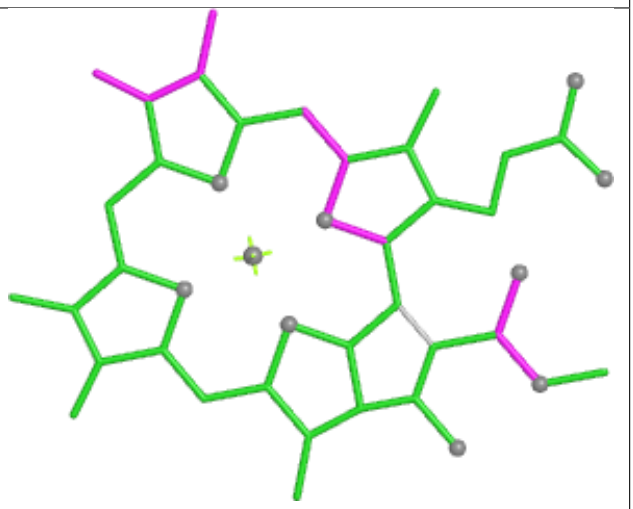


Rings

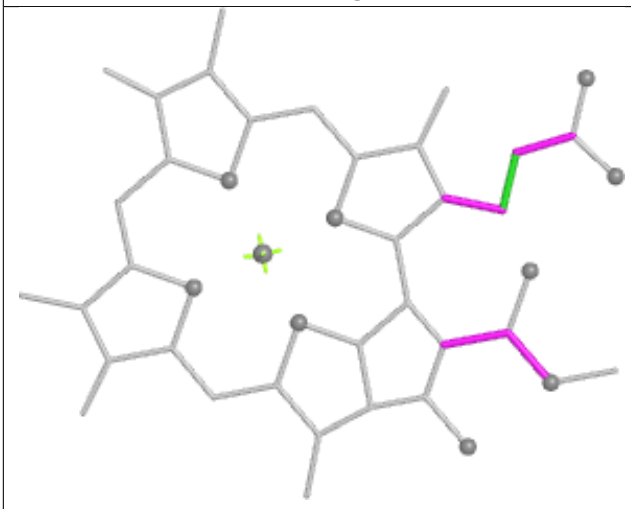
Ligand CLA 4 616



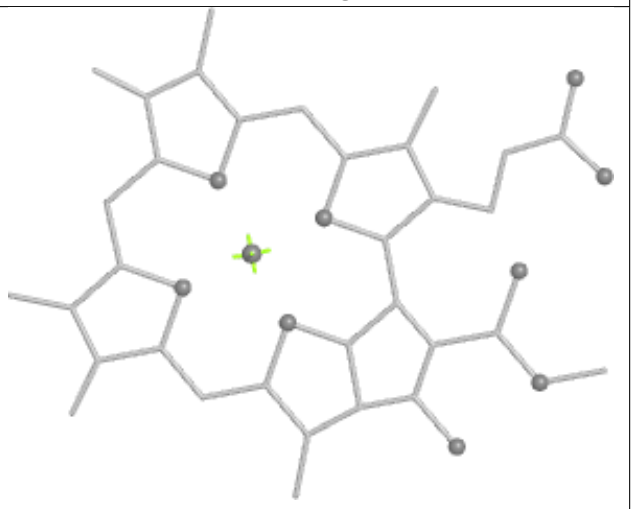
Bond lengths



Bond angles

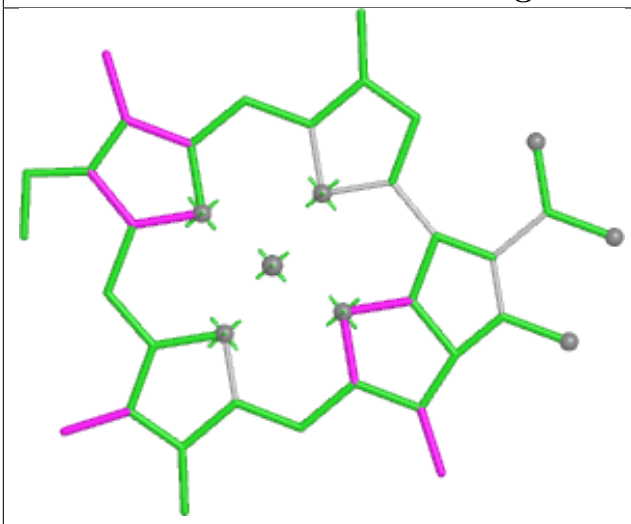


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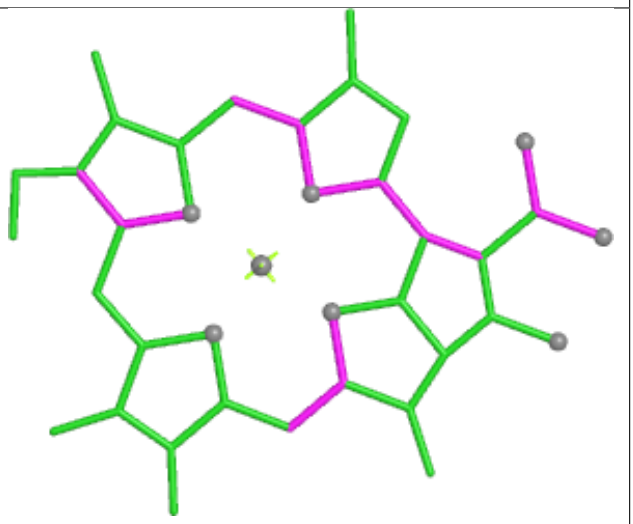


Rings

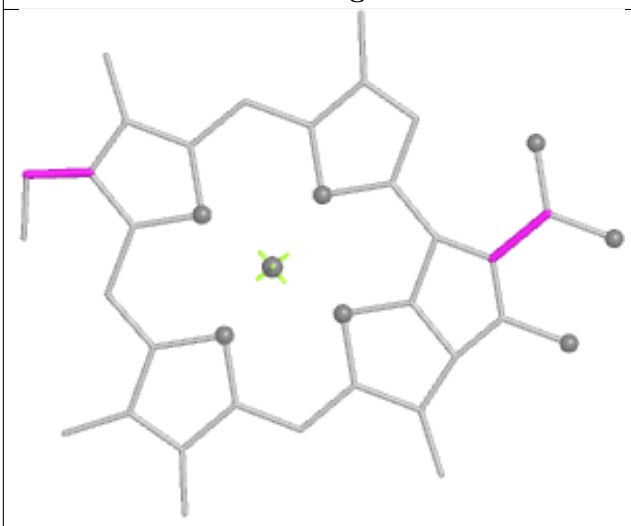
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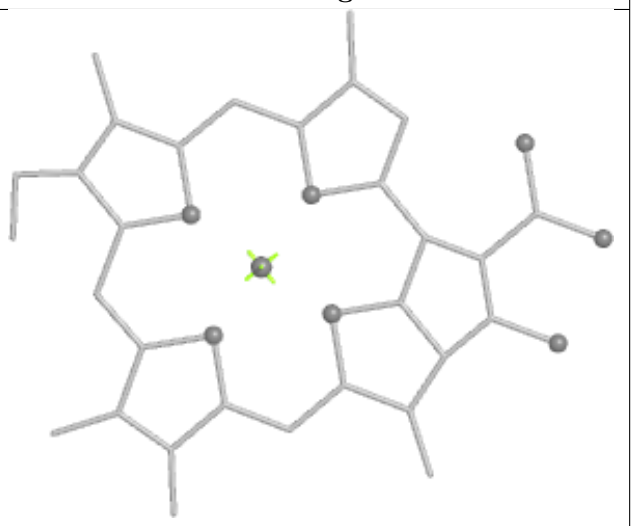
Bond lengths



Bond angles

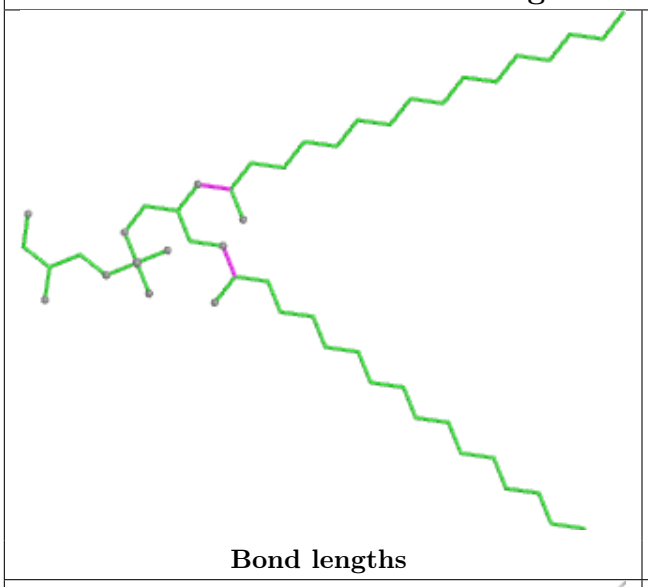


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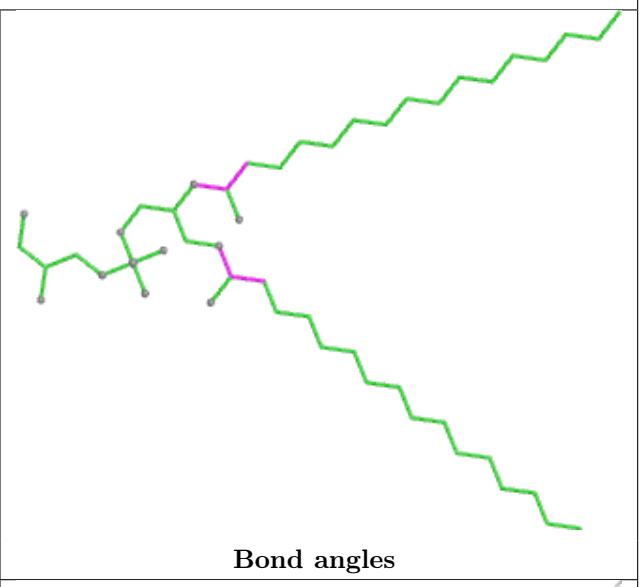


Rings

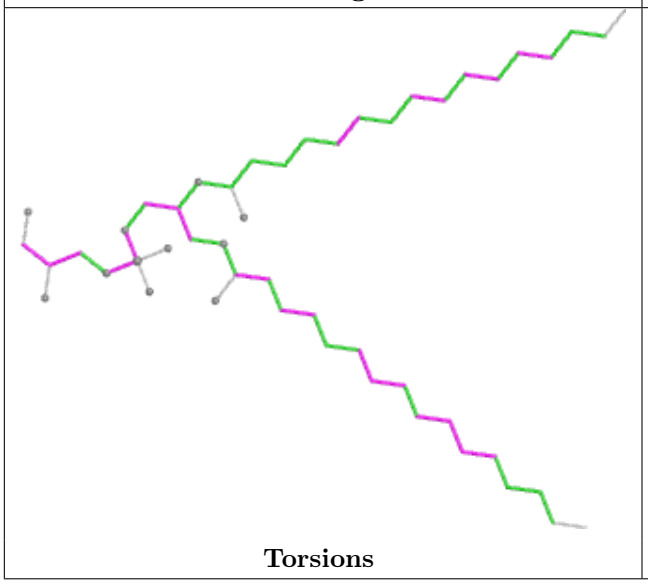
Ligand LHG 9 624



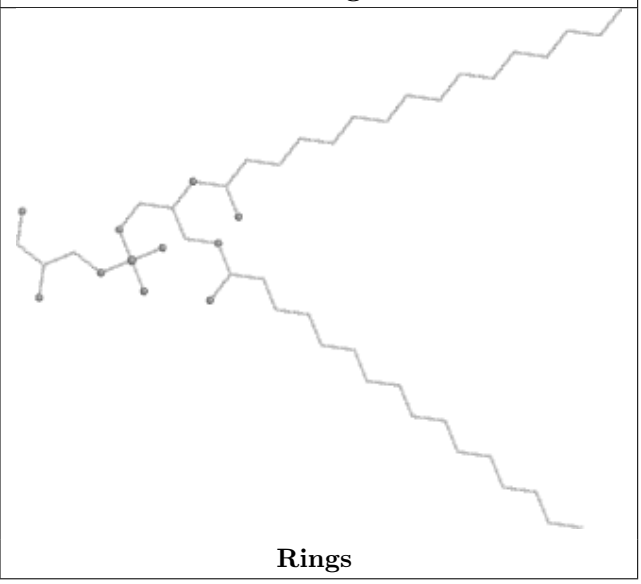
Bond lengths



Bond angles

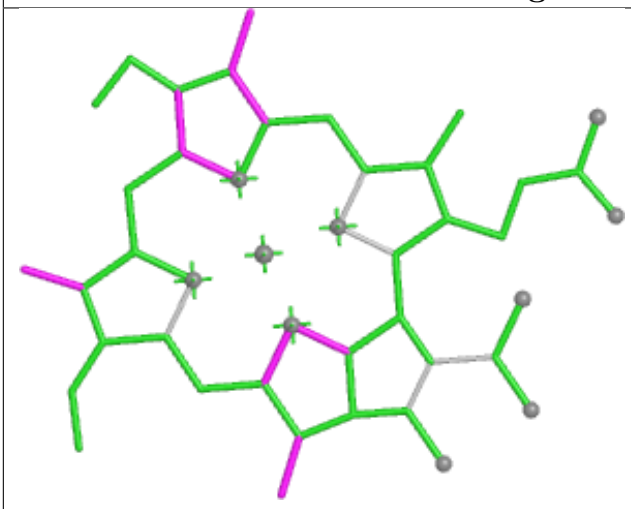


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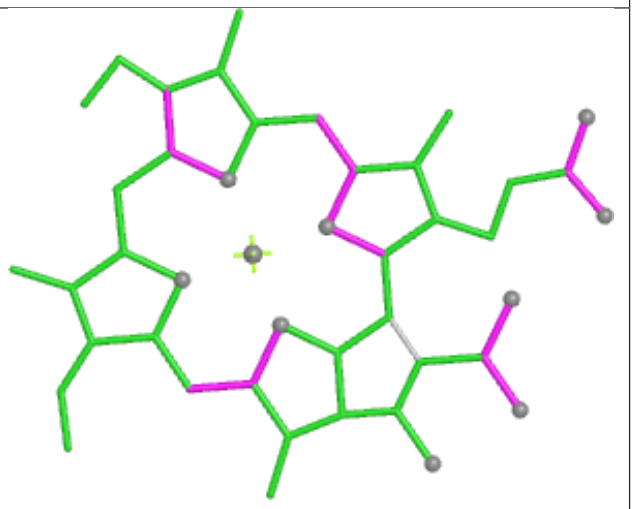


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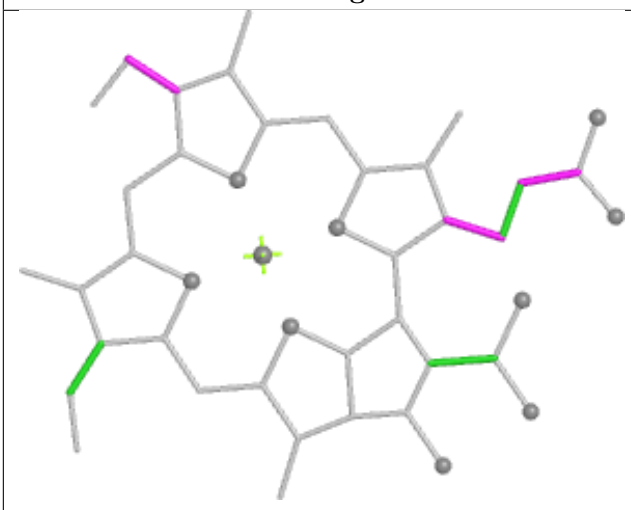
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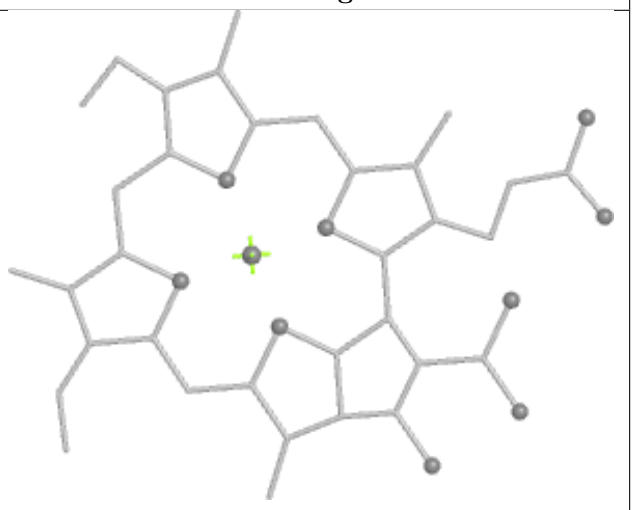
Bond lengths



Bond angles

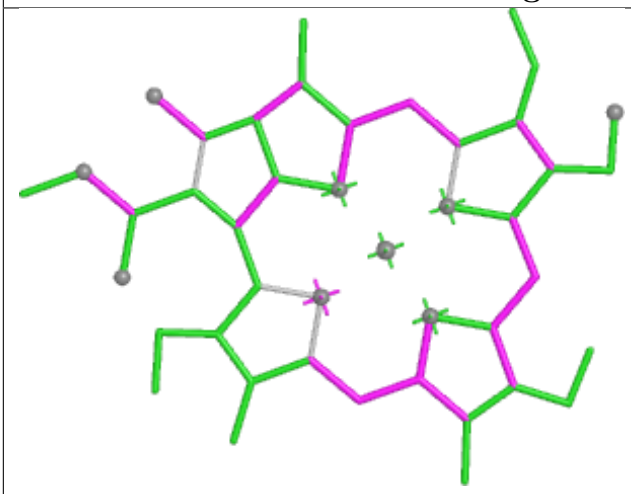


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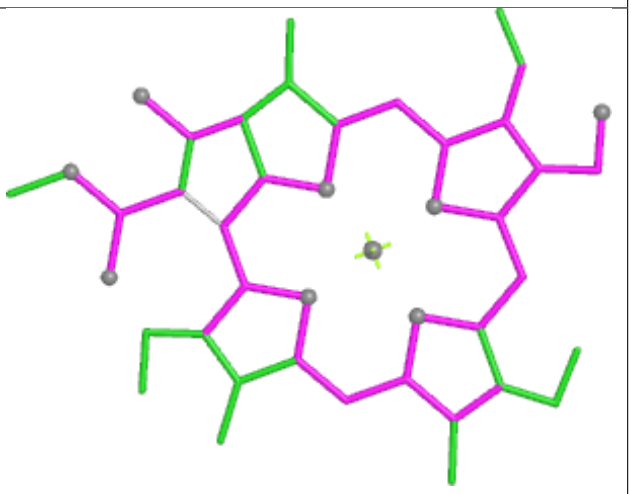


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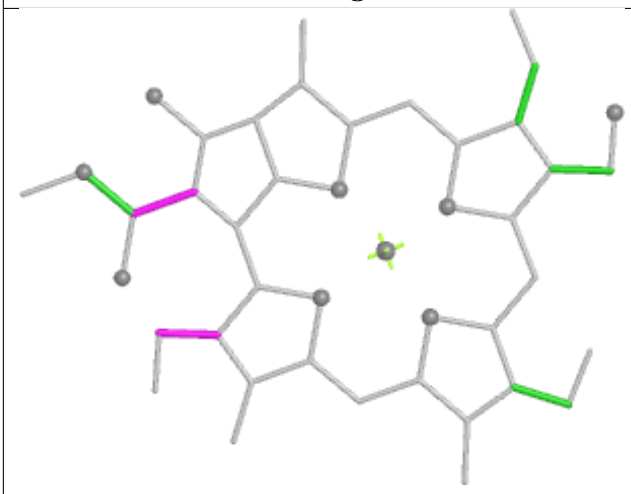
Ligand CHL U 605



Bond lengths



Bond angles

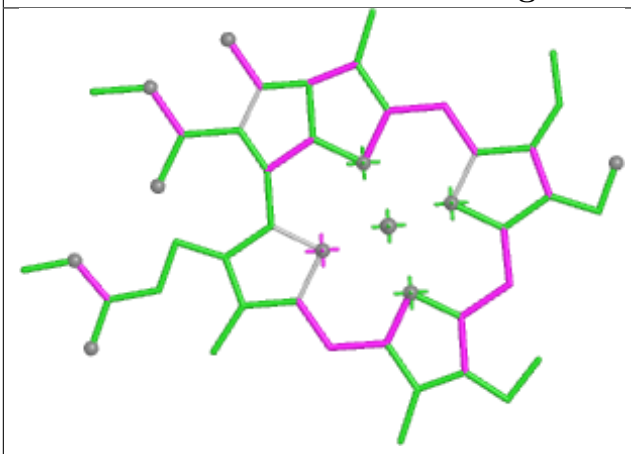


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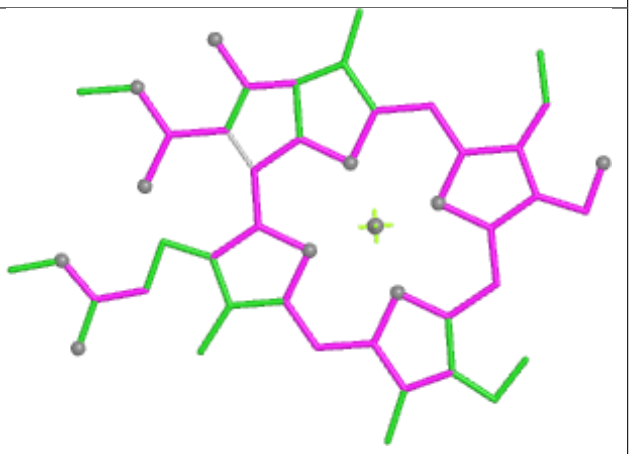


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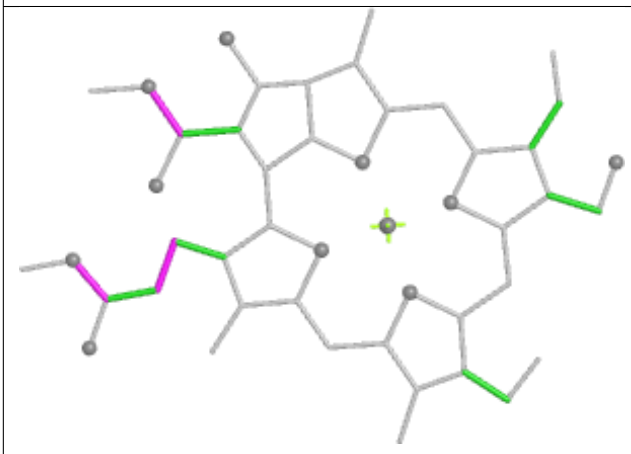
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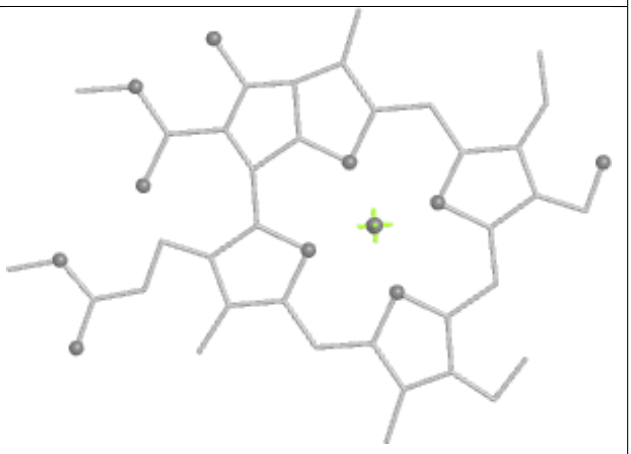
Bond lengths



Bond angles

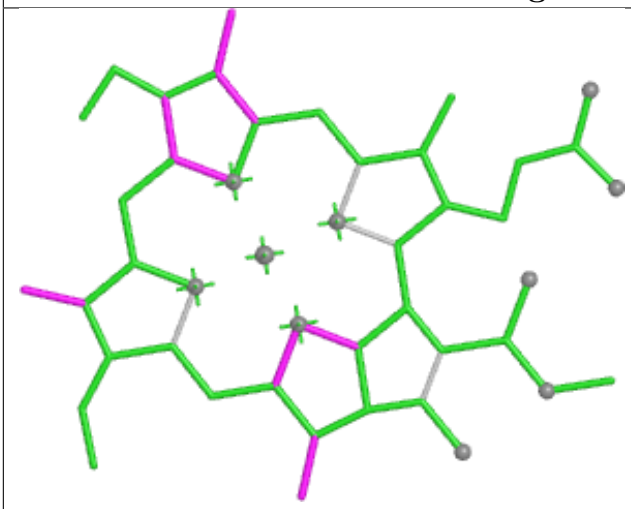


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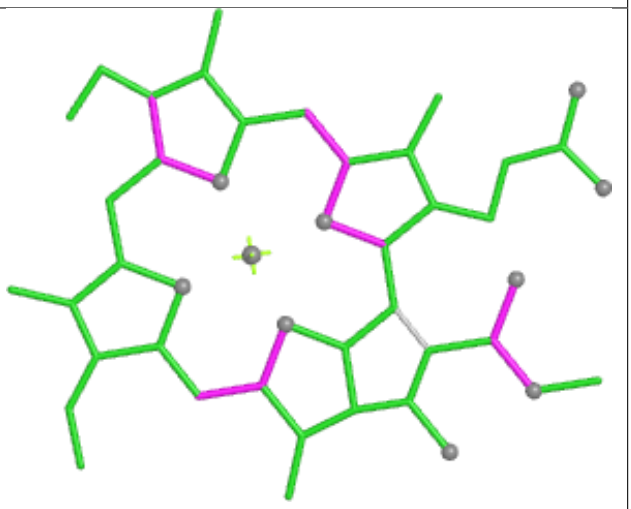


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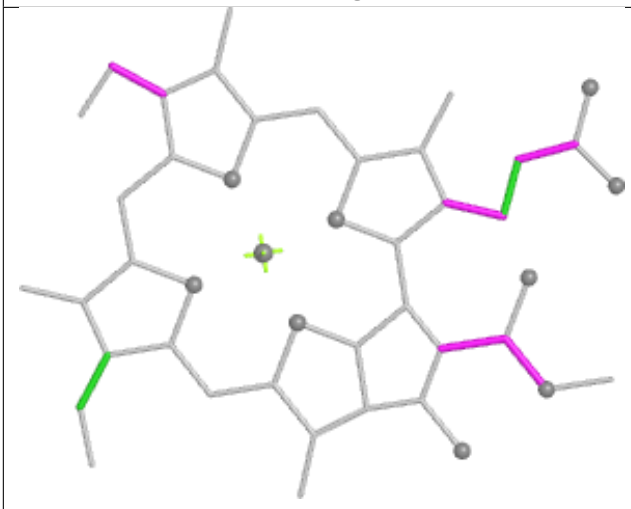
Ligand CLA 6 617



Bond lengths



Bond angles

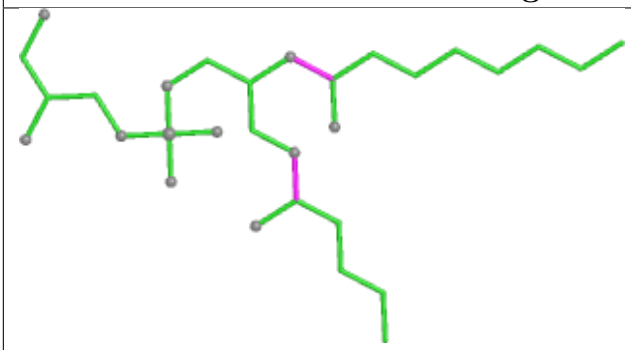


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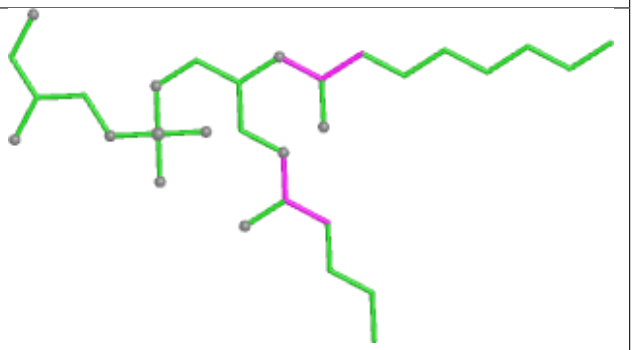


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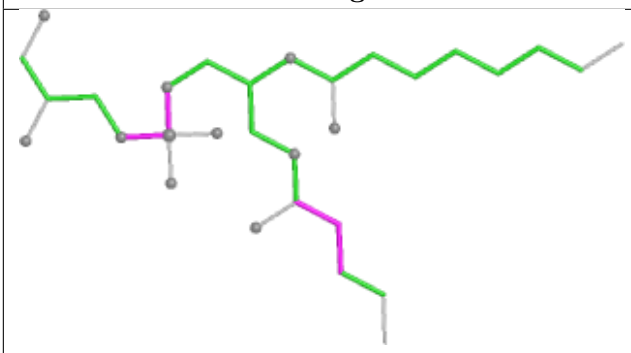
Ligand LHG A 847



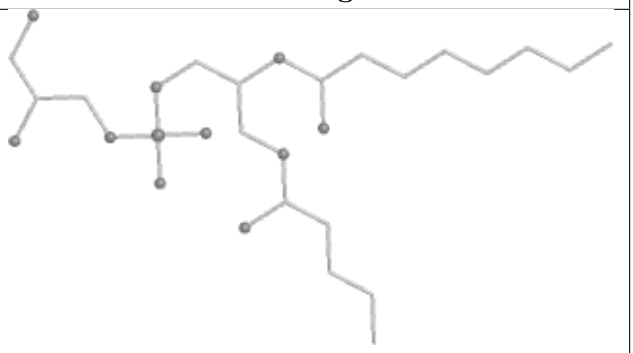
Bond lengths



Bond angles

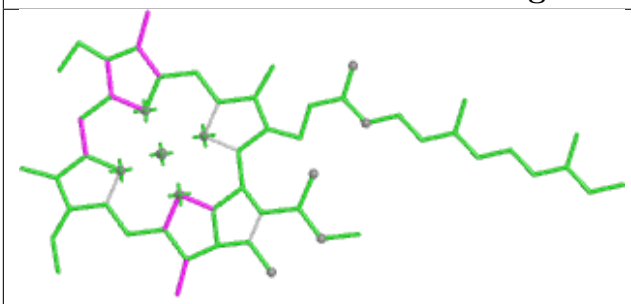


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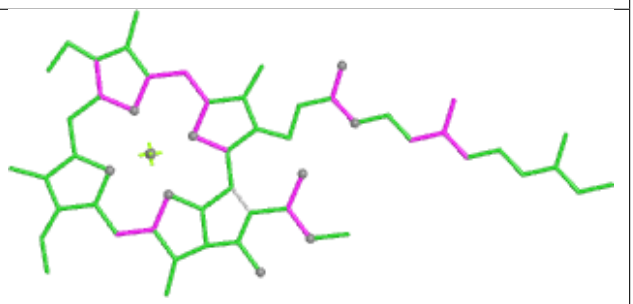


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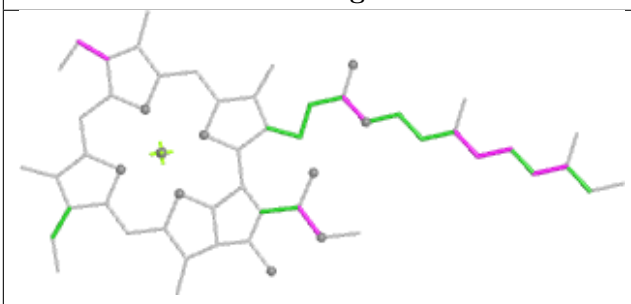
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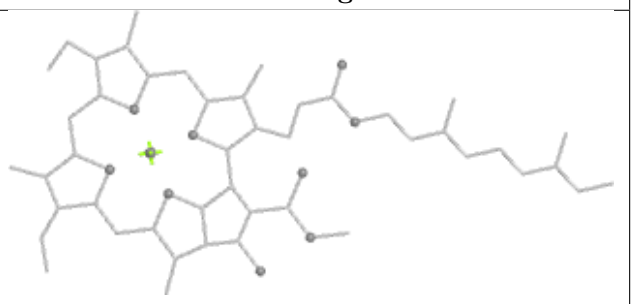
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Bond angles

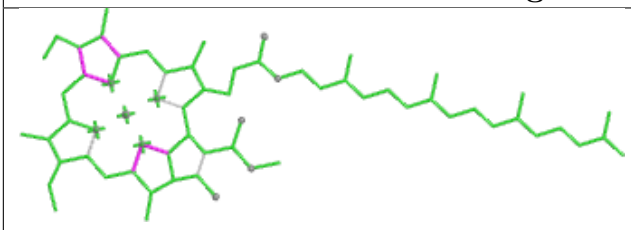


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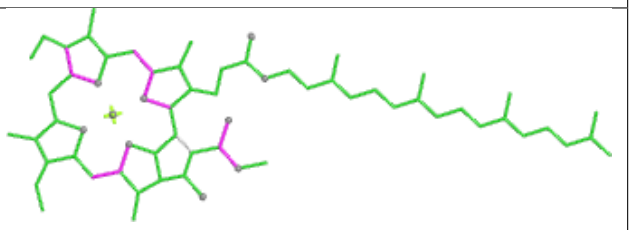


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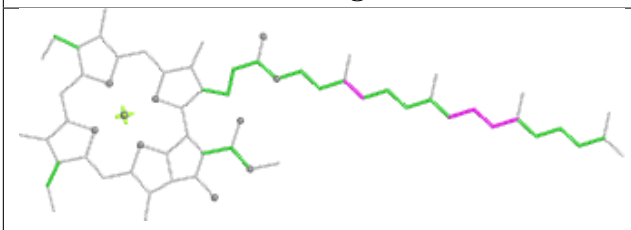
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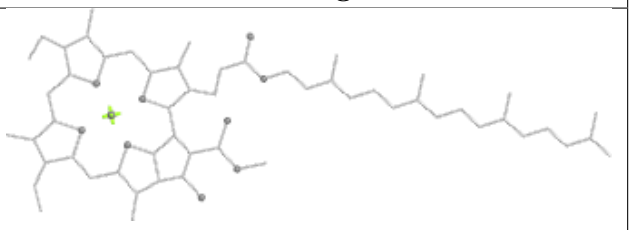
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Bond angles

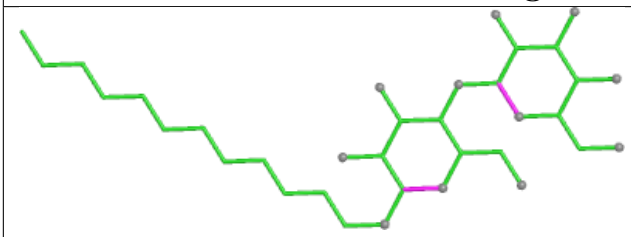


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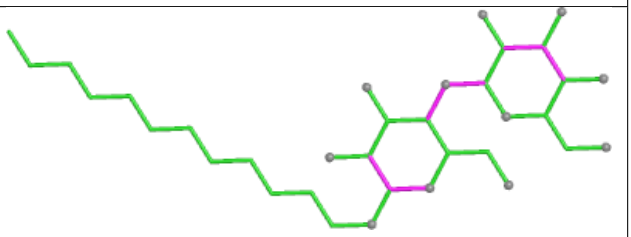


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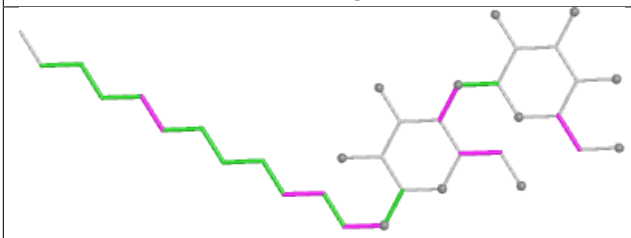
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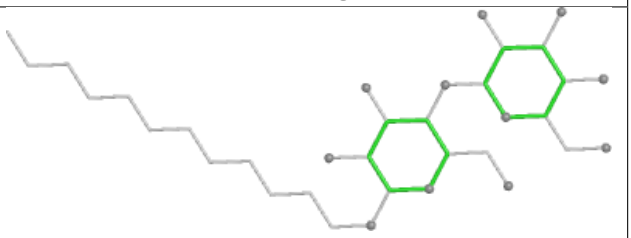
Bond lengths



Bond angles



Torsions

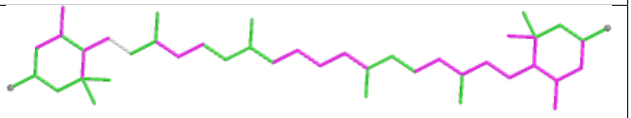


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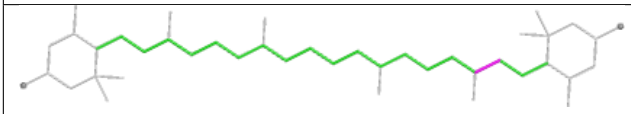
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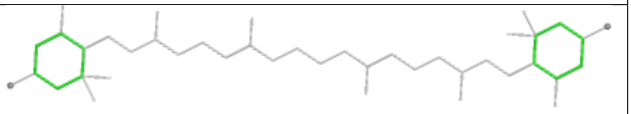
Bond lengths



Bond angles

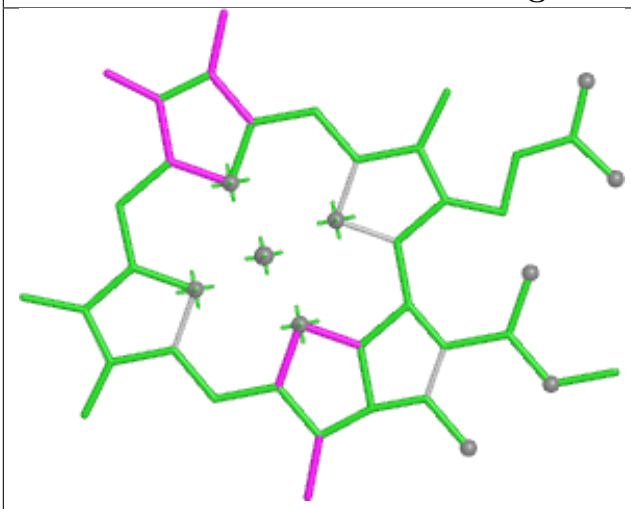


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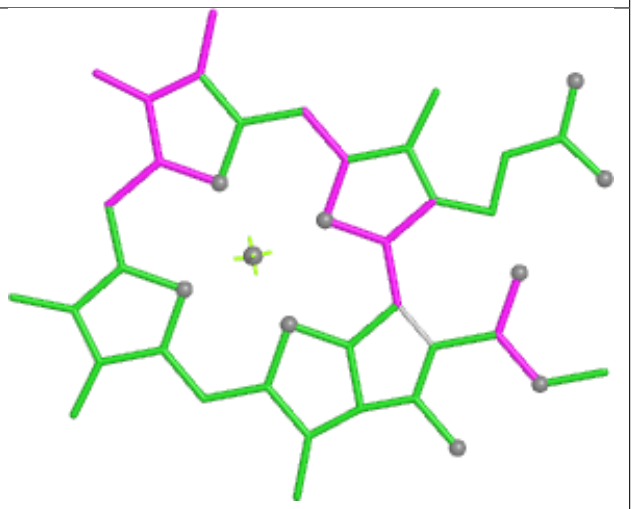


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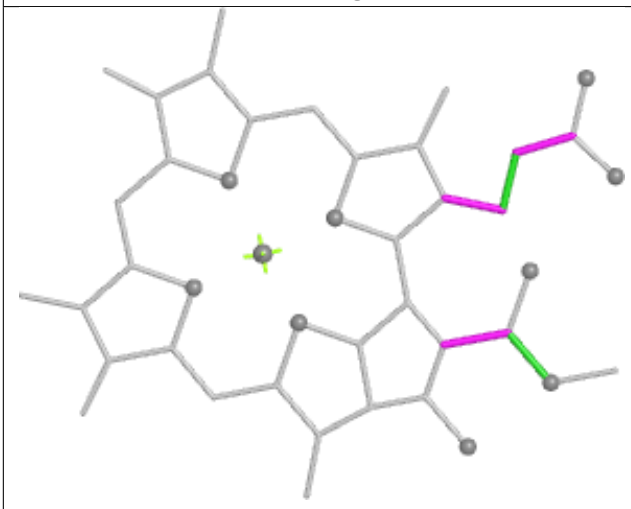
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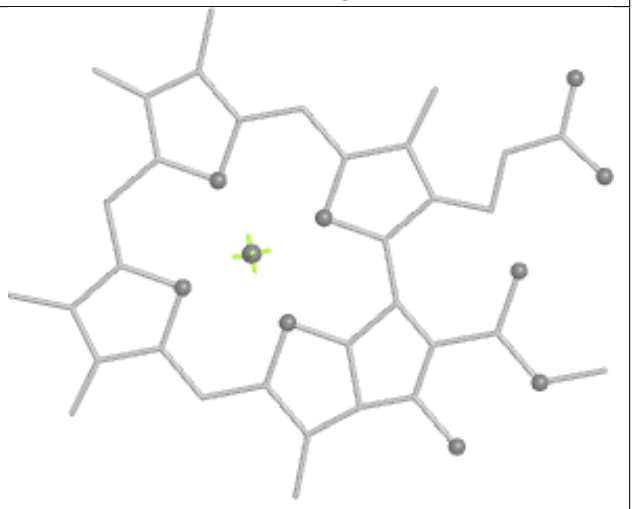
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Bond angles

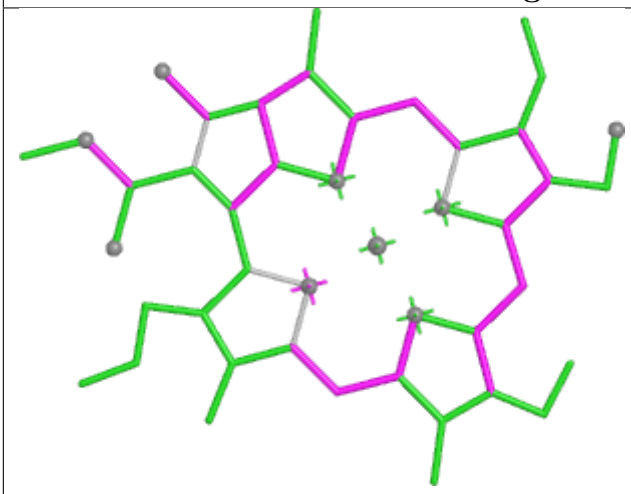


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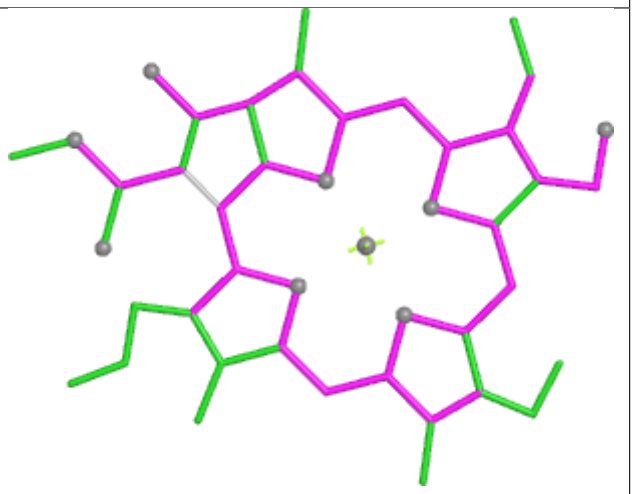


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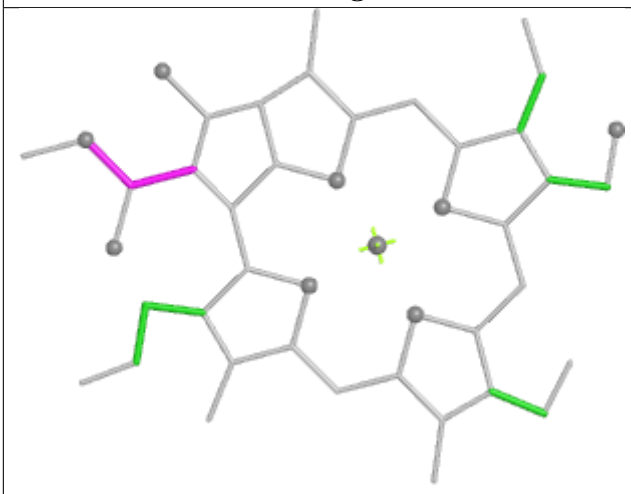
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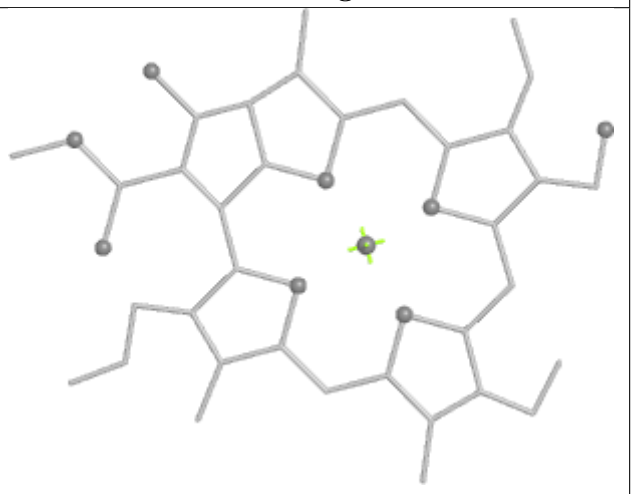
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Bond angles

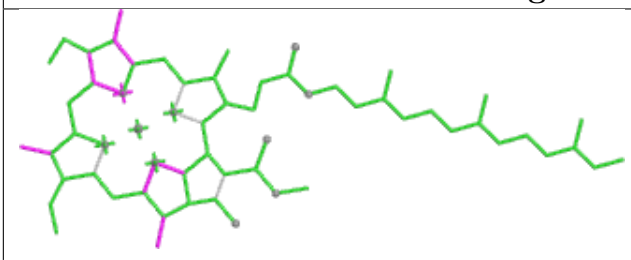


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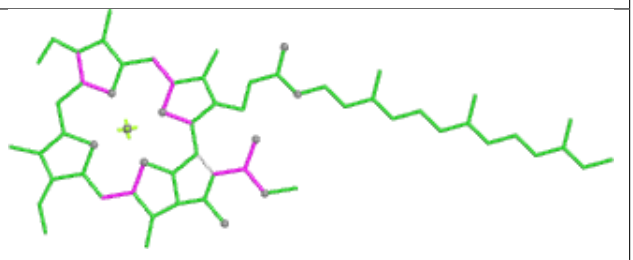


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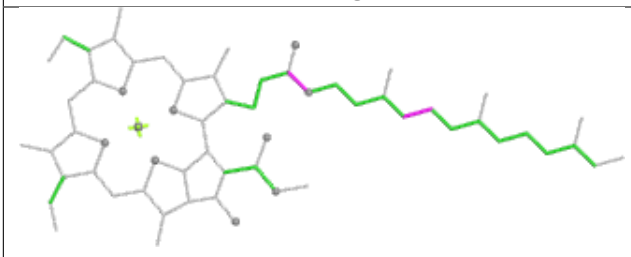
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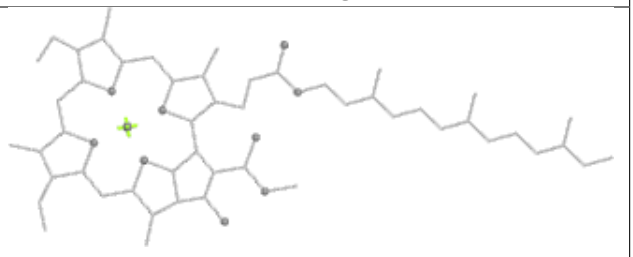
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Bond angles

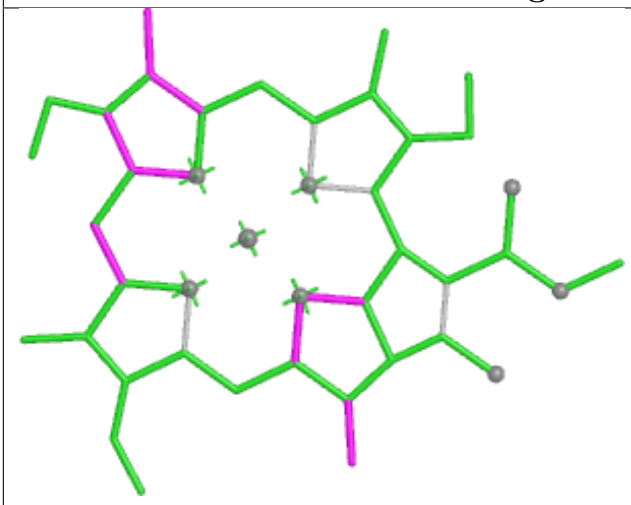


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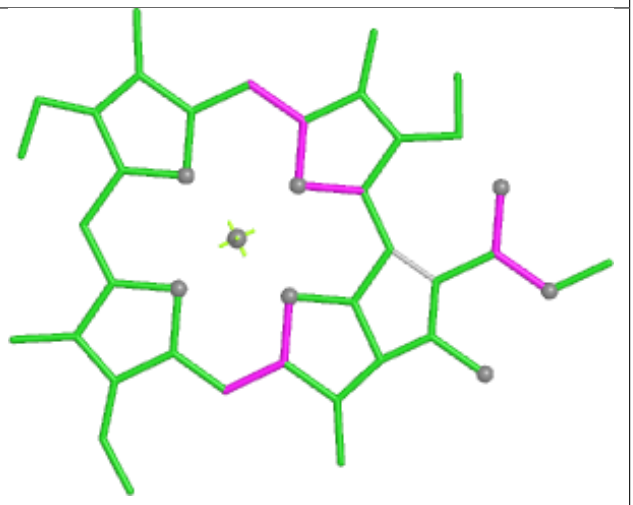


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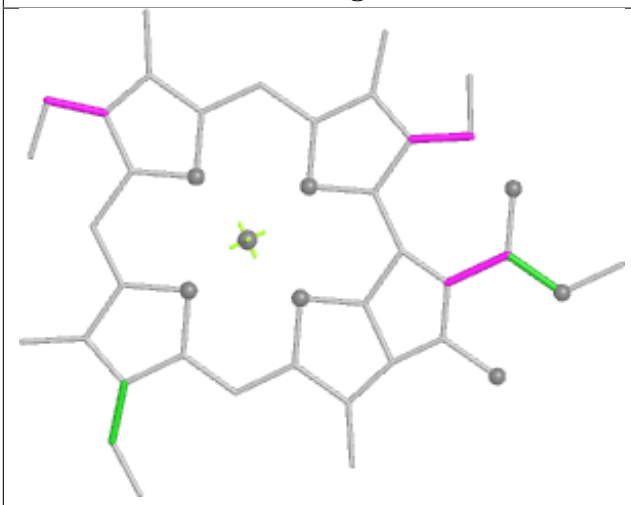
Ligand CLA 9 611



Bond lengths



Bond angles

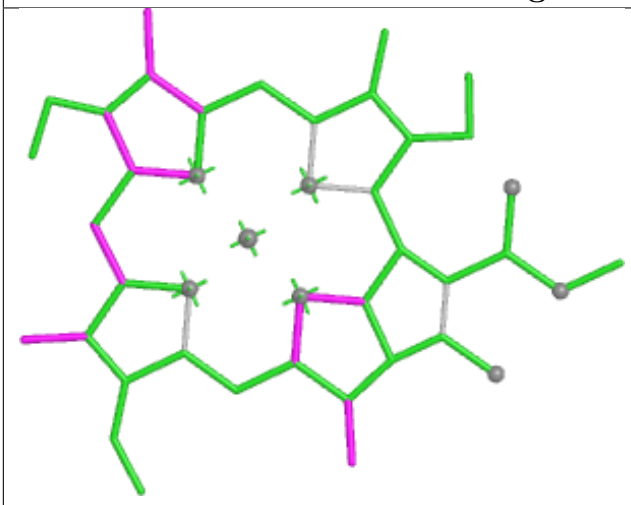


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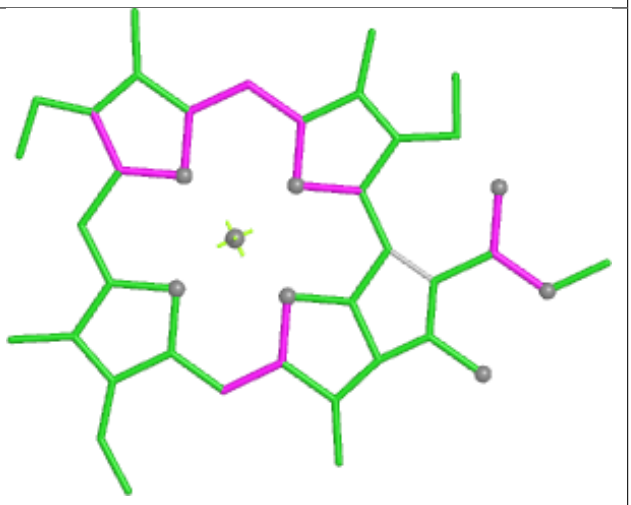


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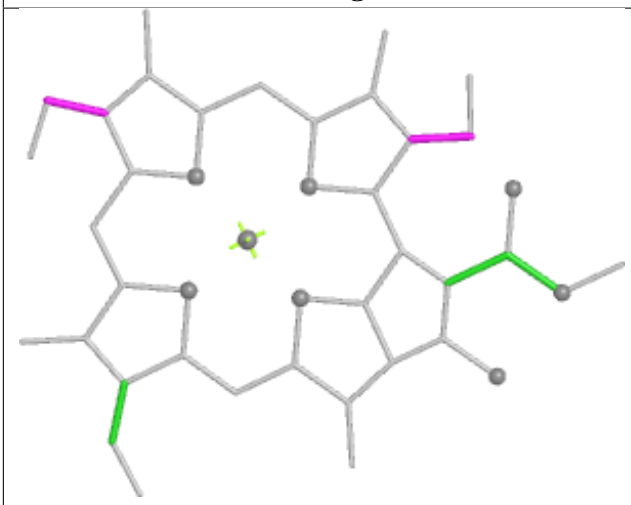
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Bond lengths



Bond angles

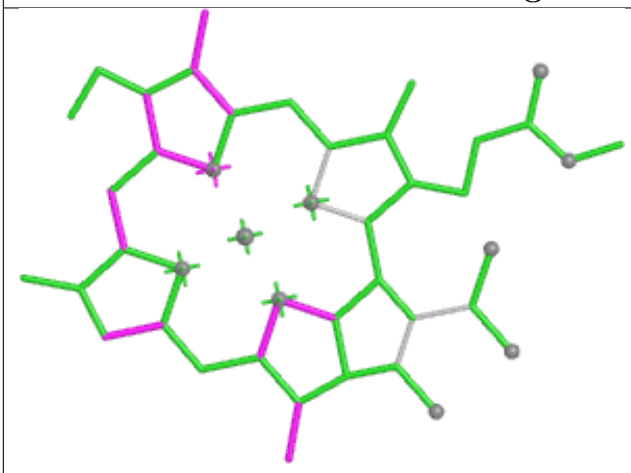


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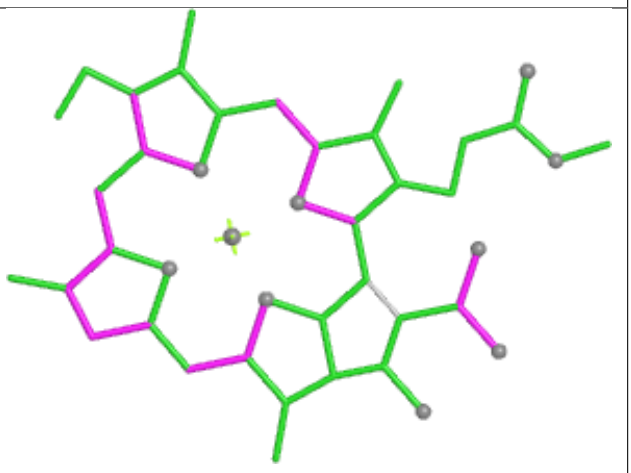


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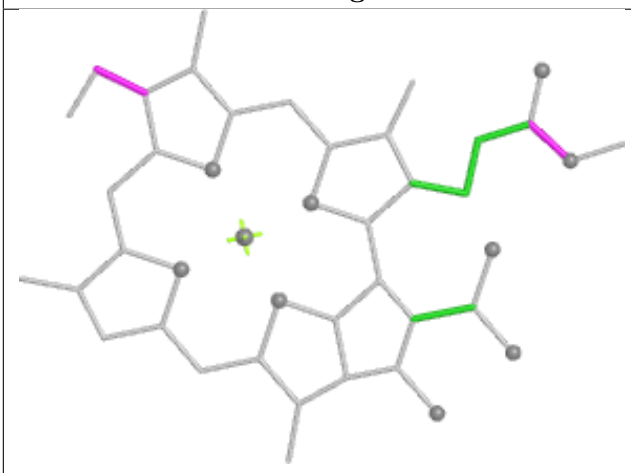
Ligand CLA B 821



Bond lengths



Bond angles

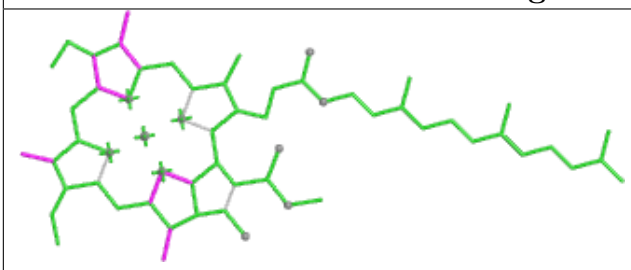


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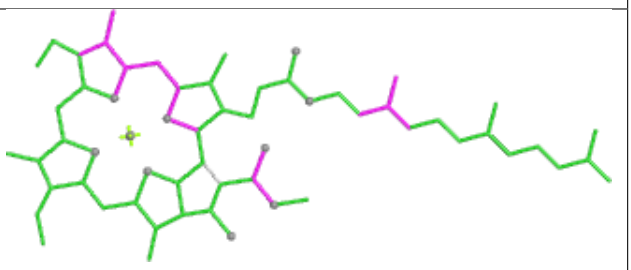


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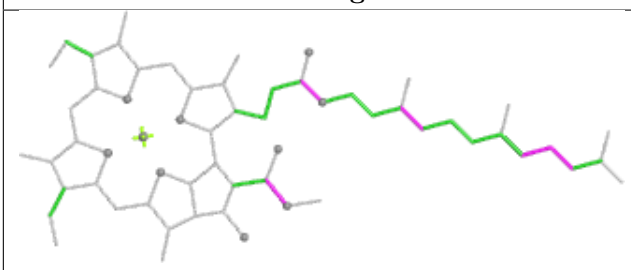
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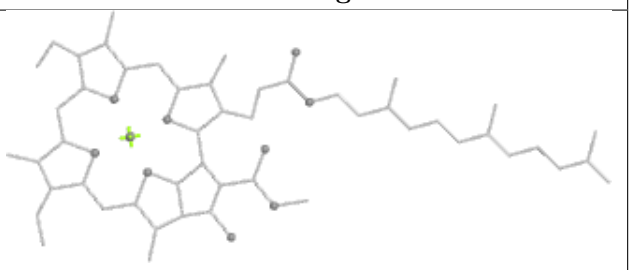
Bond lengths



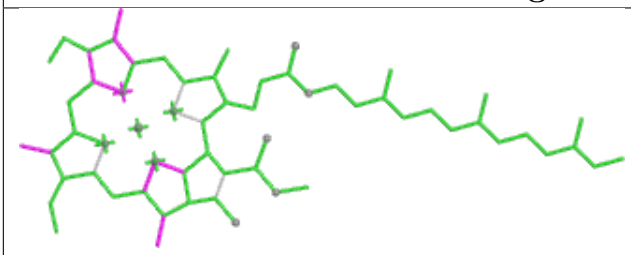
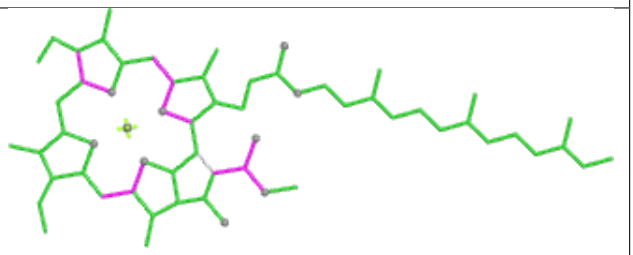
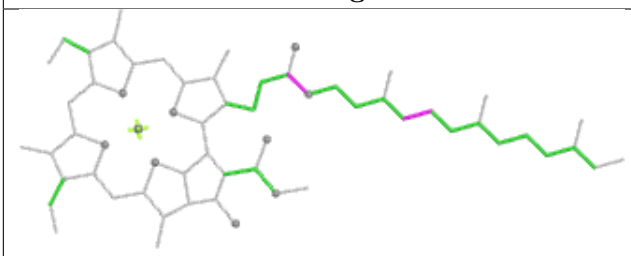
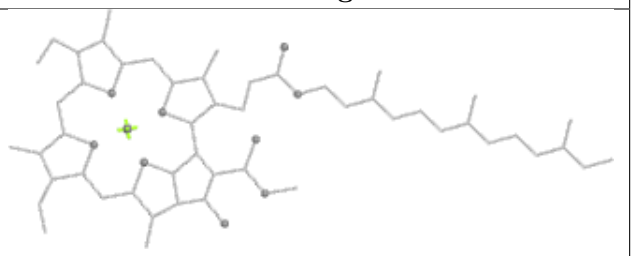
Bond angles



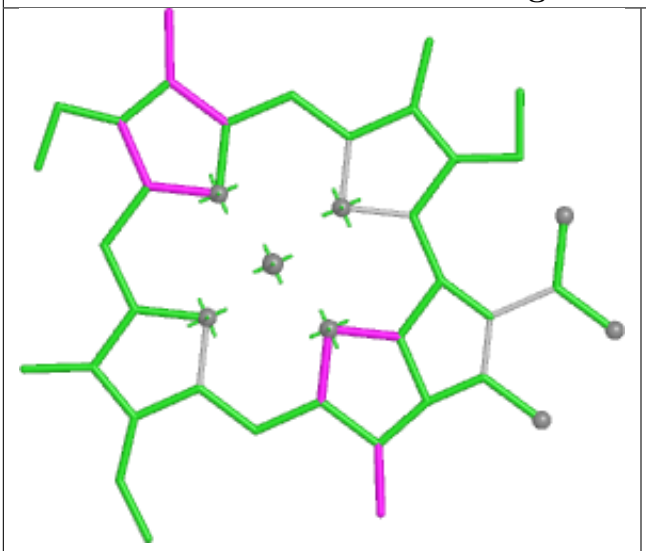
Torsions



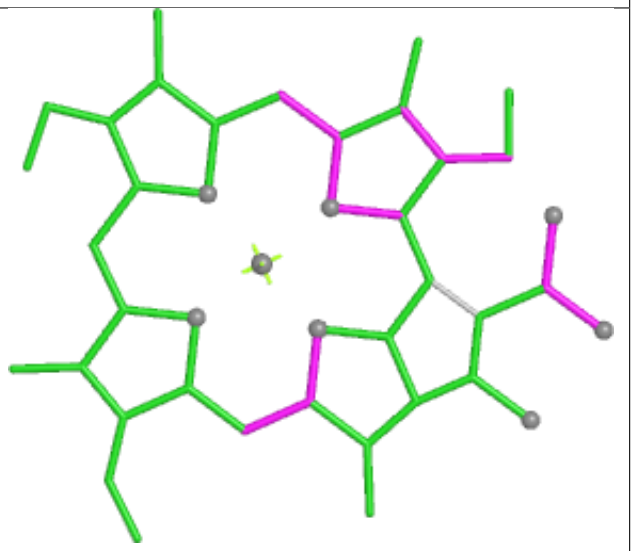
Rings

Ligand CLA a 602	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

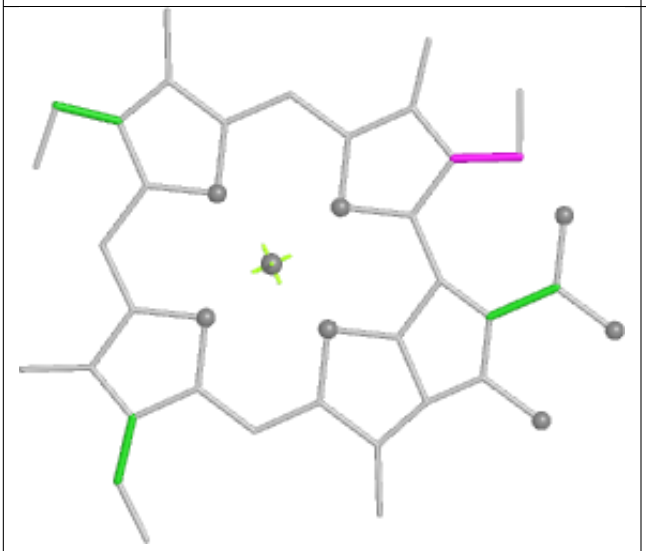
Ligand CLA 9 612



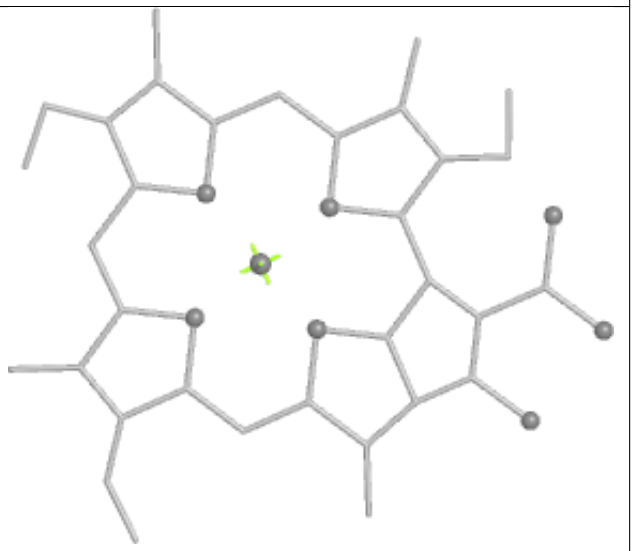
Bond lengths



Bond angles

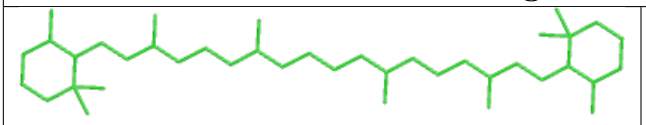


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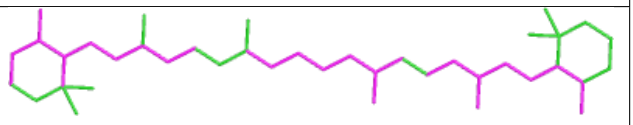


Rings

Ligand BCR B 847



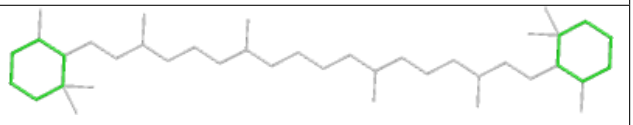
Bond lengths



Bond angles

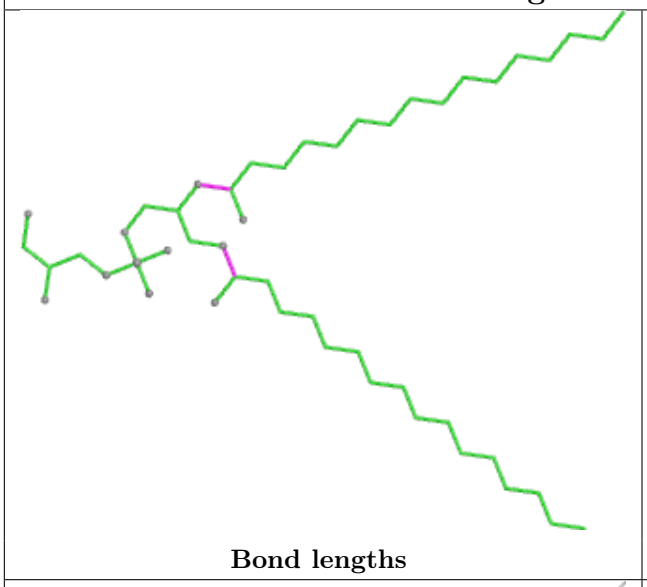


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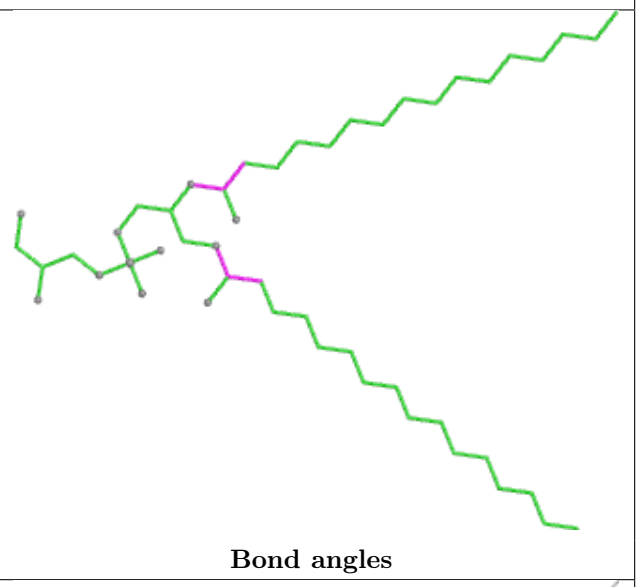


Rings

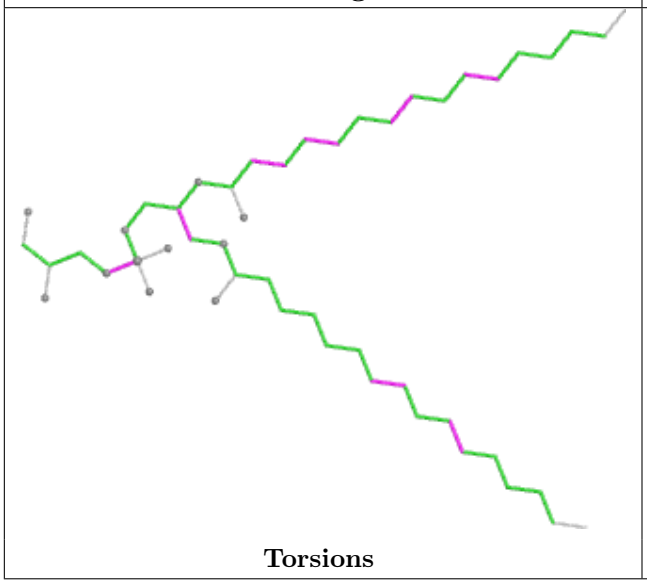
Ligand LHG 8 622



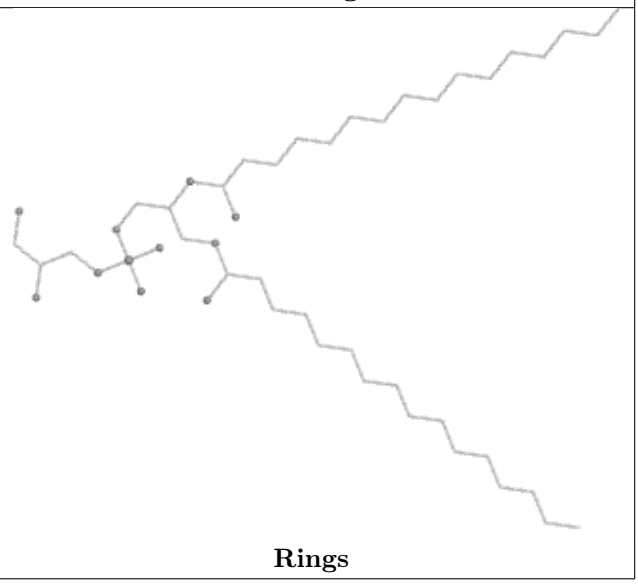
Bond lengths



Bond angles

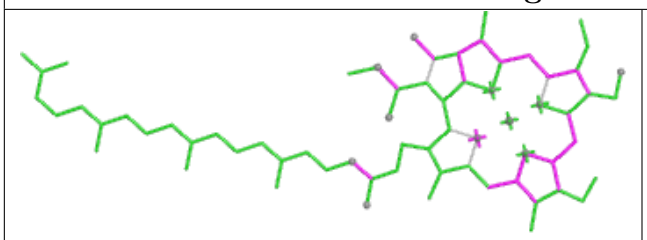


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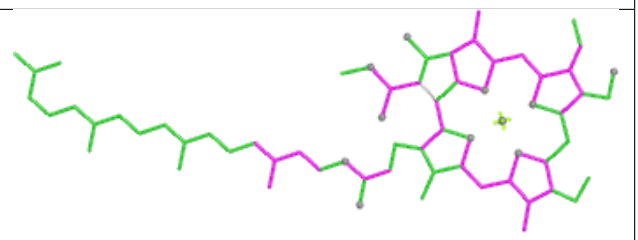


Rings

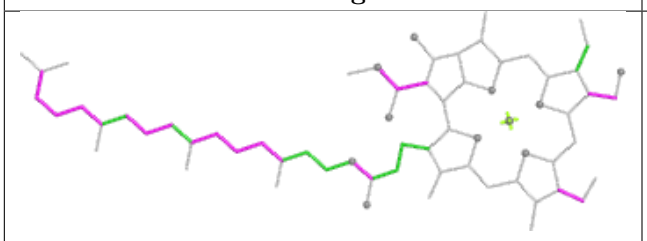
Ligand CHL X 601



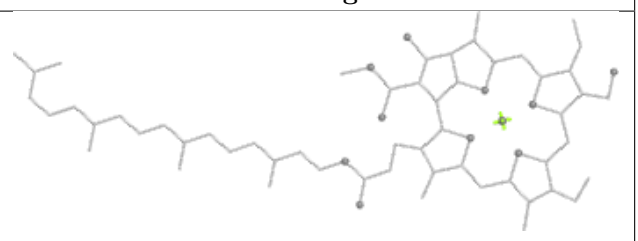
Bond lengths



Bond angles

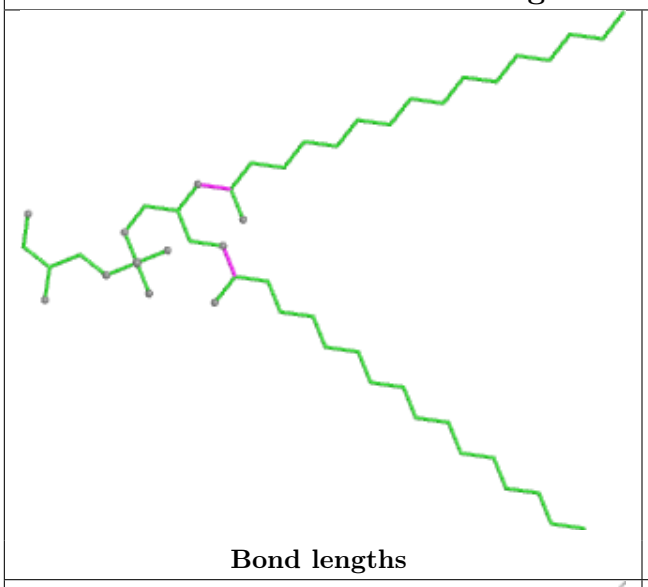


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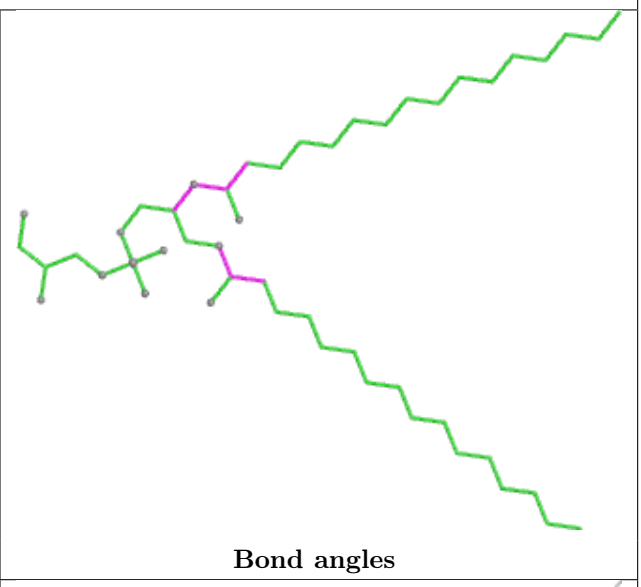


Rings

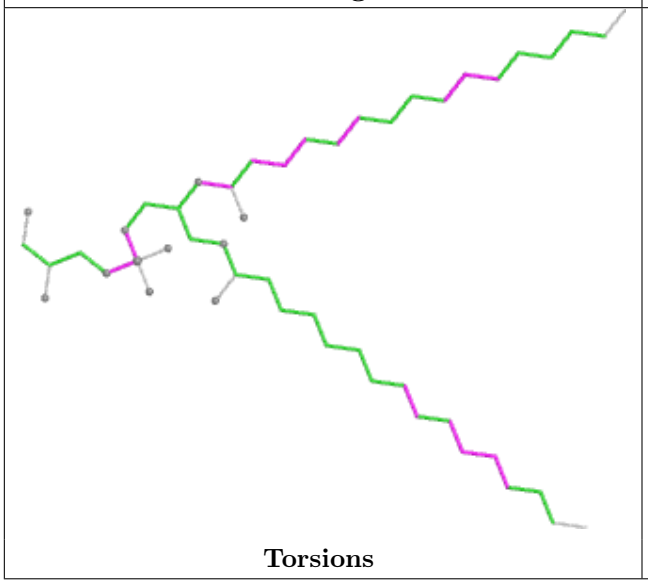
Ligand LHG 9 623



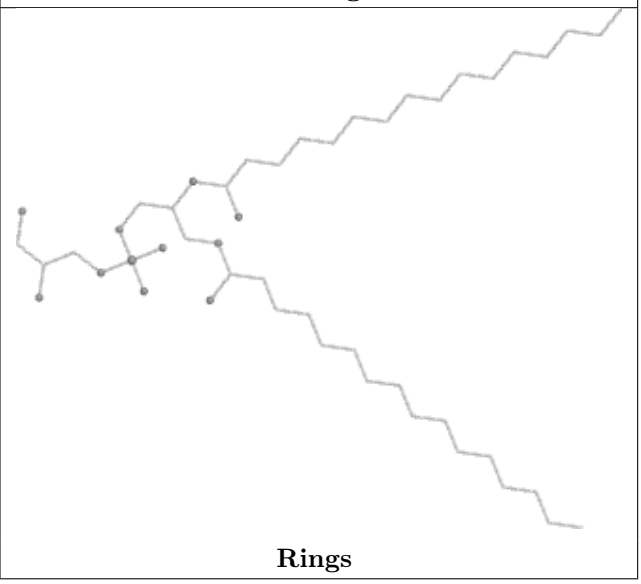
Bond lengths



Bond angles

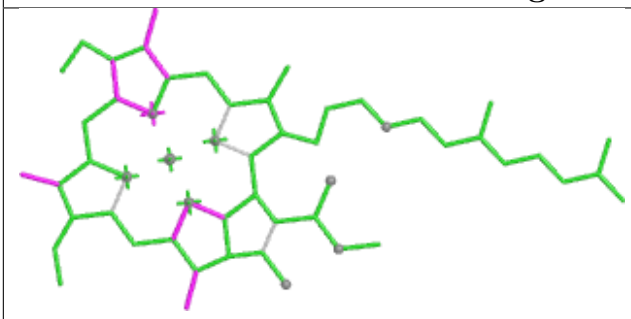


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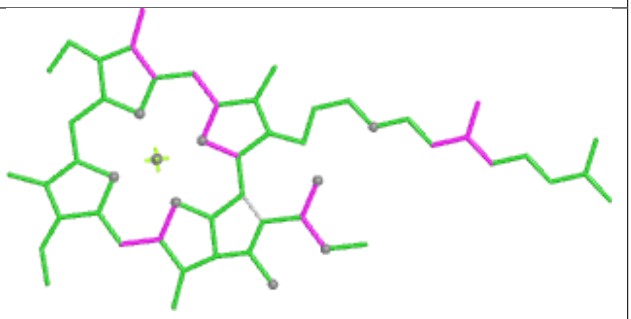


Rings

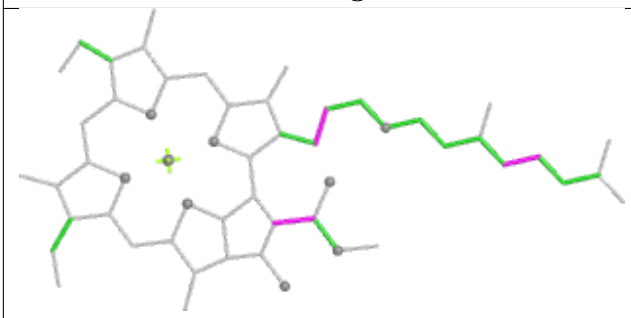
Ligand CLA a 603



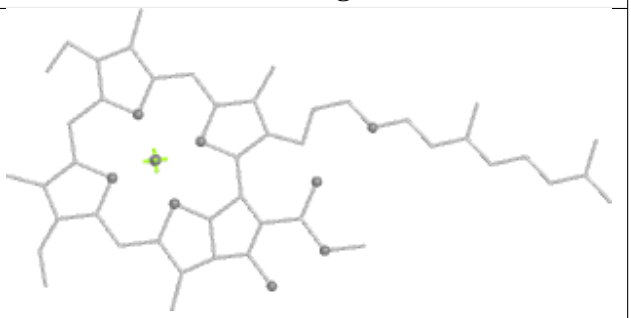
Bond lengths



Bond angles

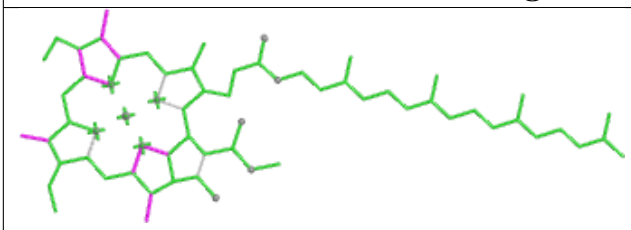


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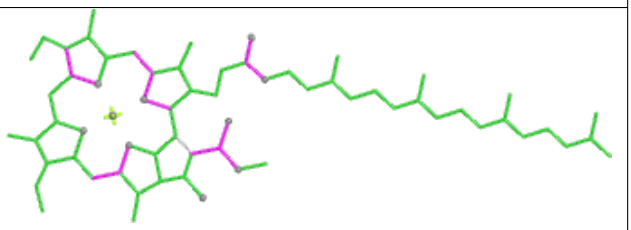


Rings

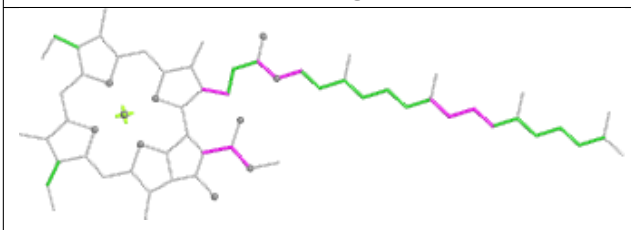
Ligand CLA A 811



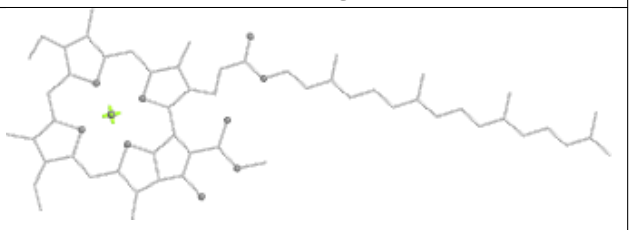
Bond lengths



Bond angles

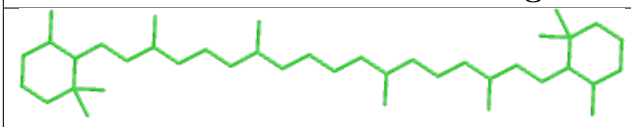


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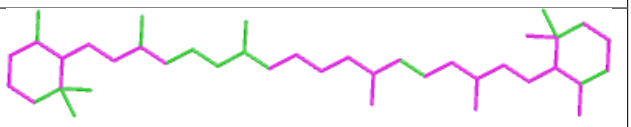


Rings

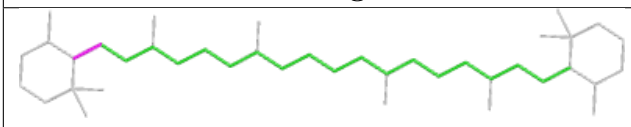
Ligand BCR L 309



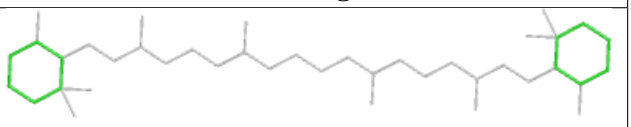
Bond lengths



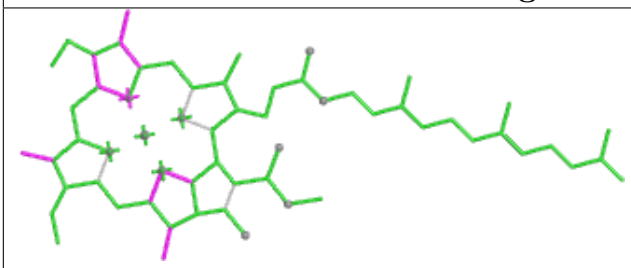
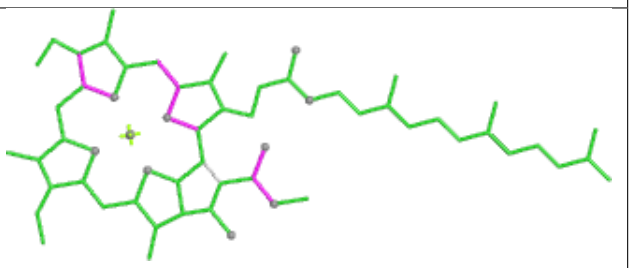
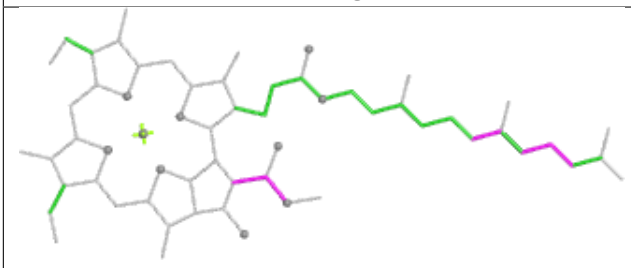
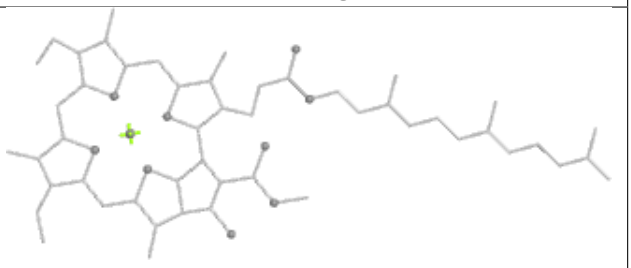
Bond angles

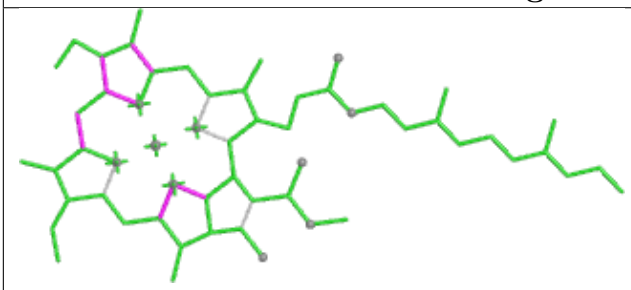
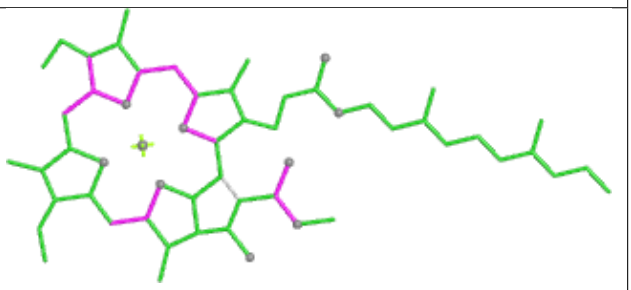
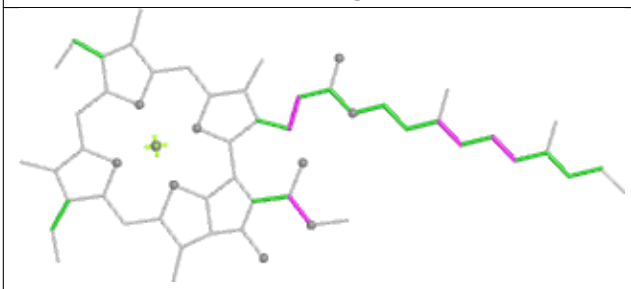
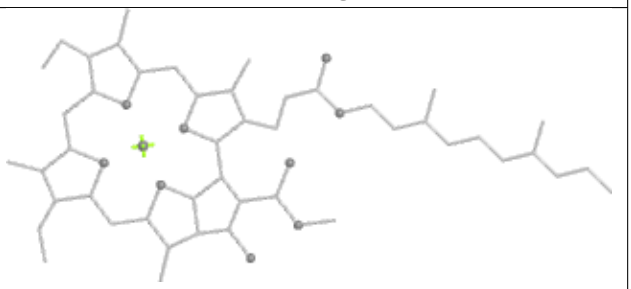


Torsions

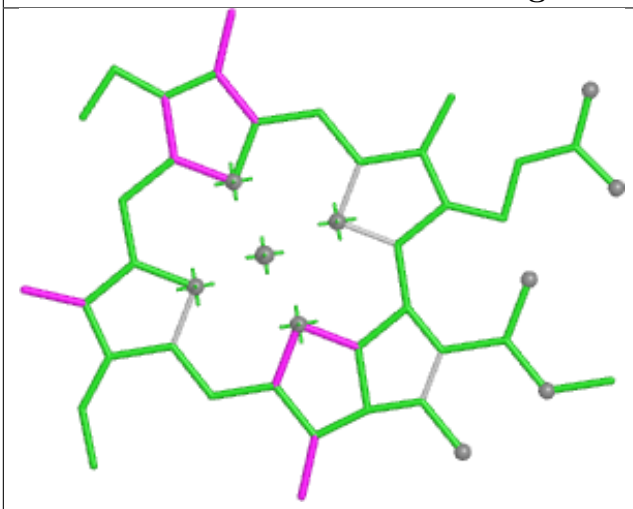


Rings

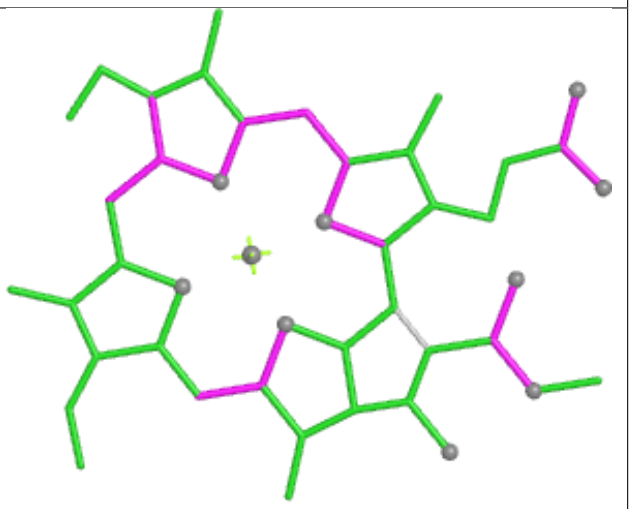
Ligand CLA W 602	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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

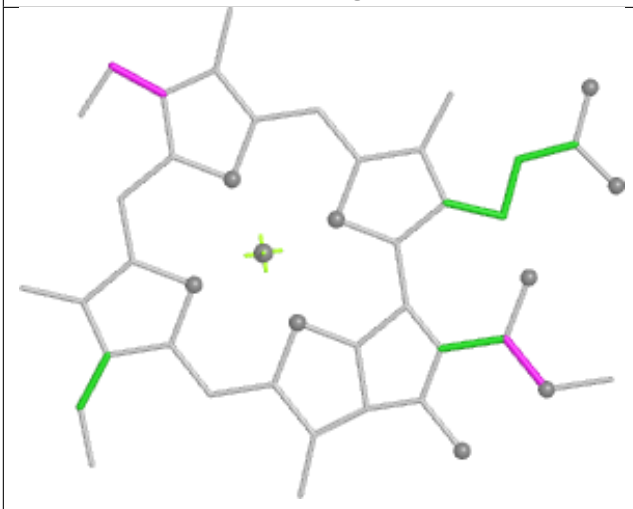
Ligand CLA 9 601



Bond lengths



Bond angles

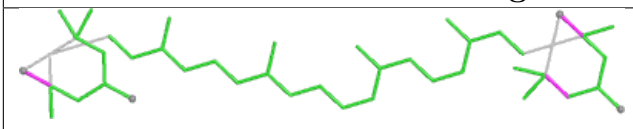


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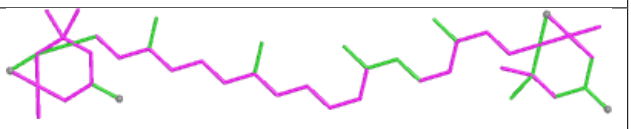


Rings

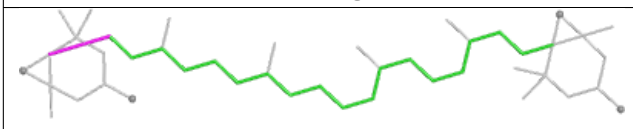
Ligand XAT W 1622



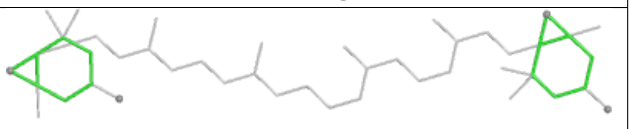
Bond lengths



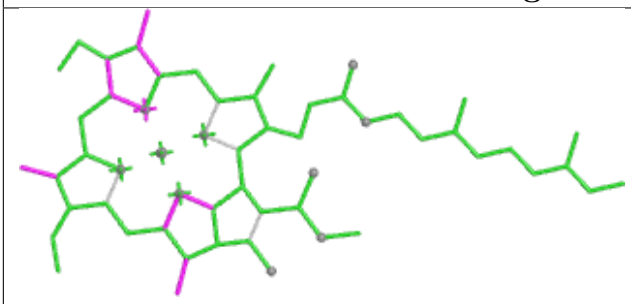
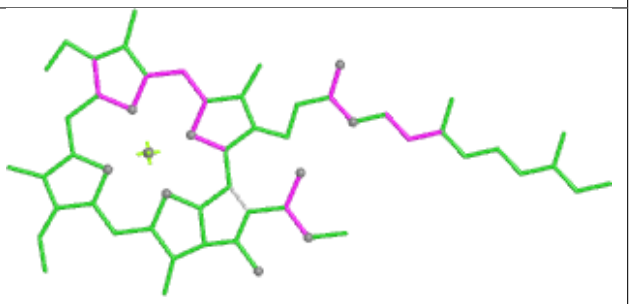
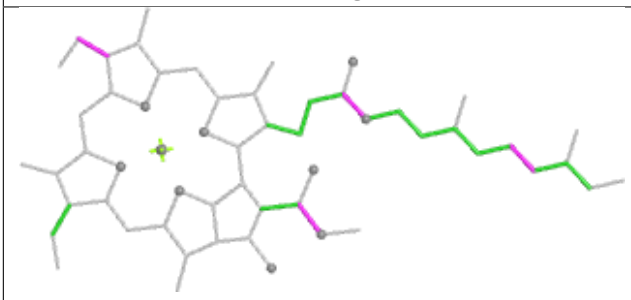
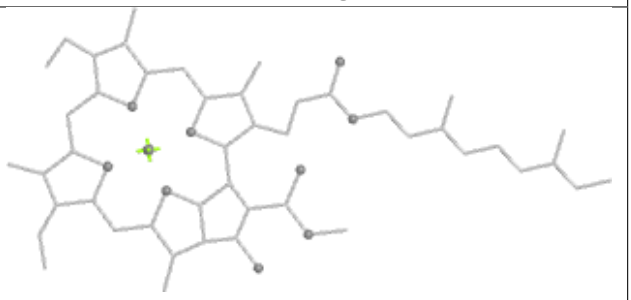
Bond angles

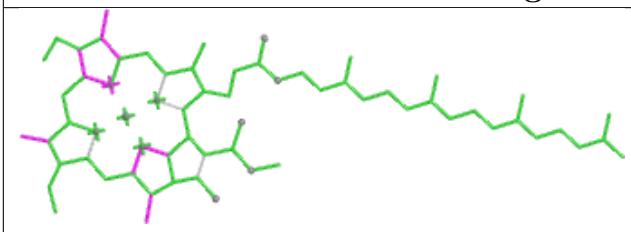
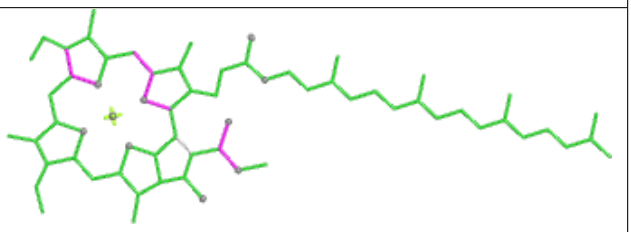
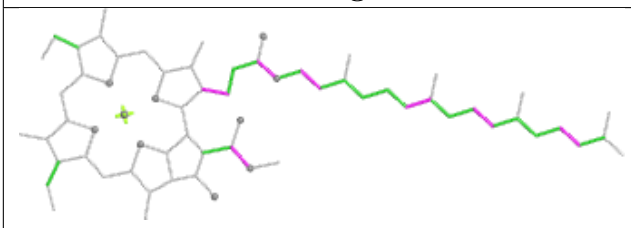
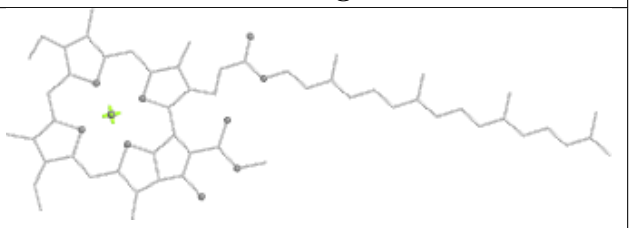


Torsions

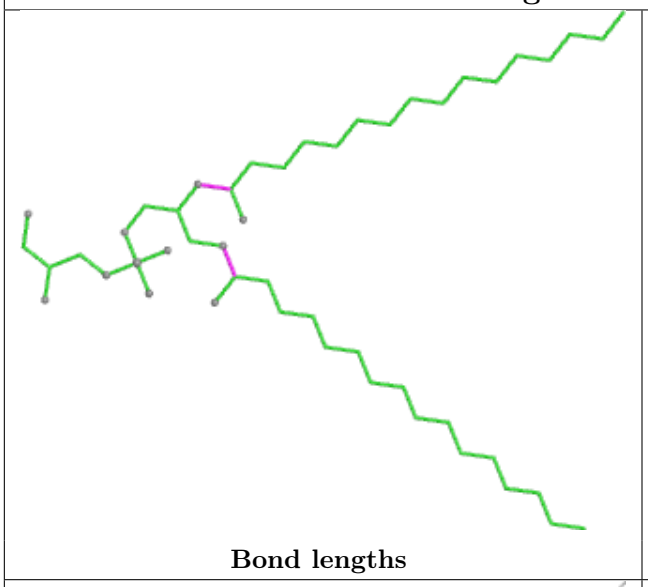


Rings

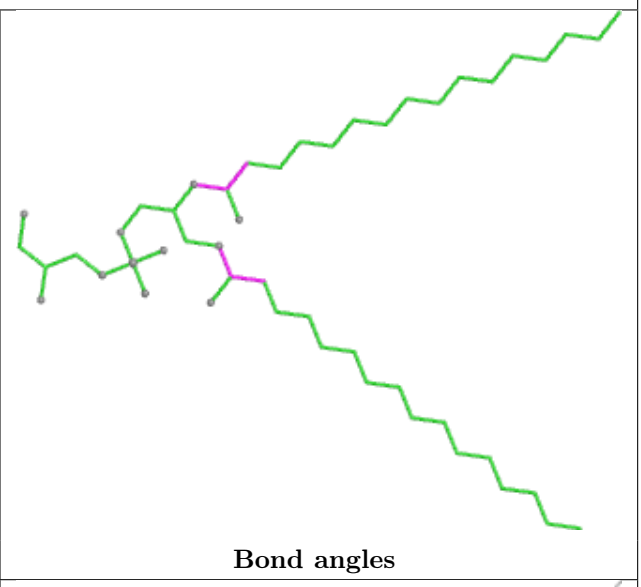
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Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 803	
	
Bond lengths	Bond angles
	
Torsions	Rings

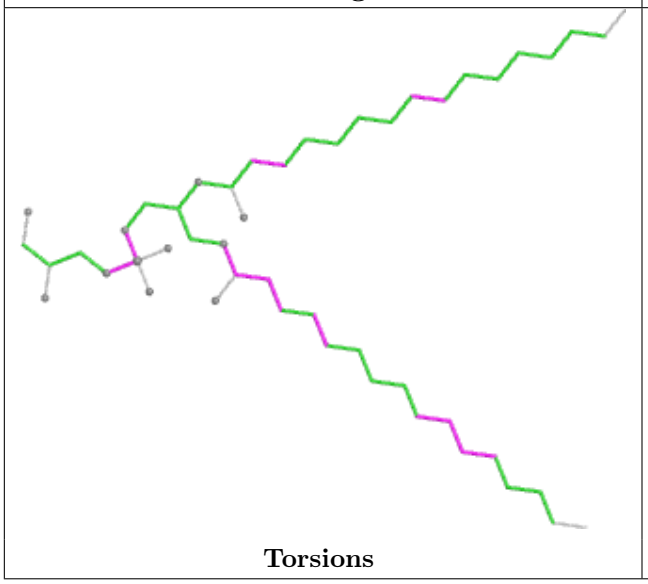
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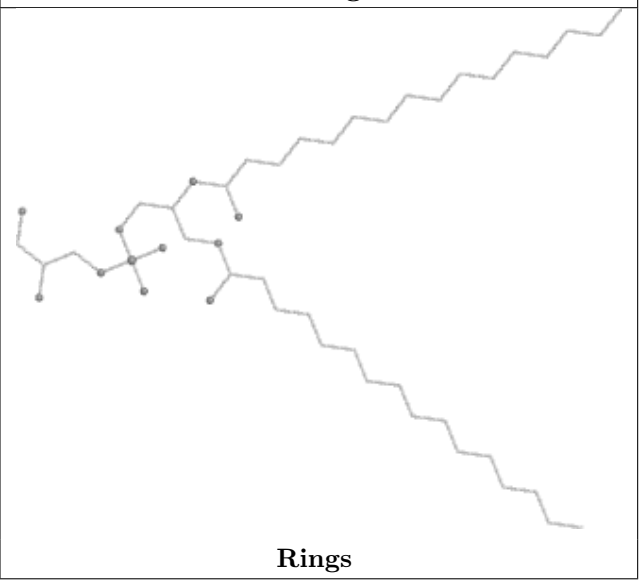
Bond lengths



Bond angles

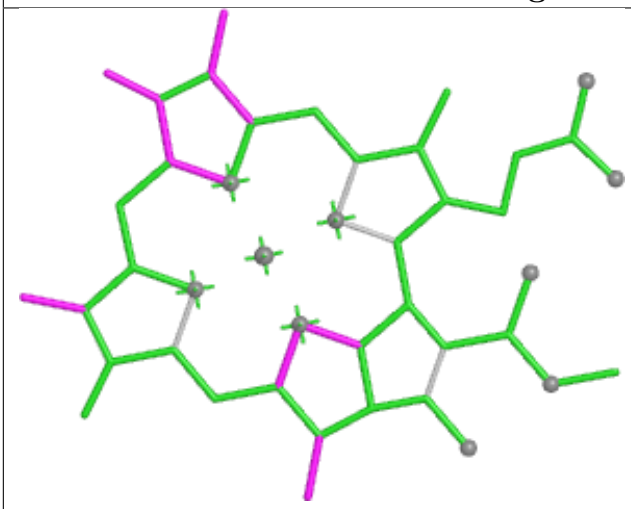


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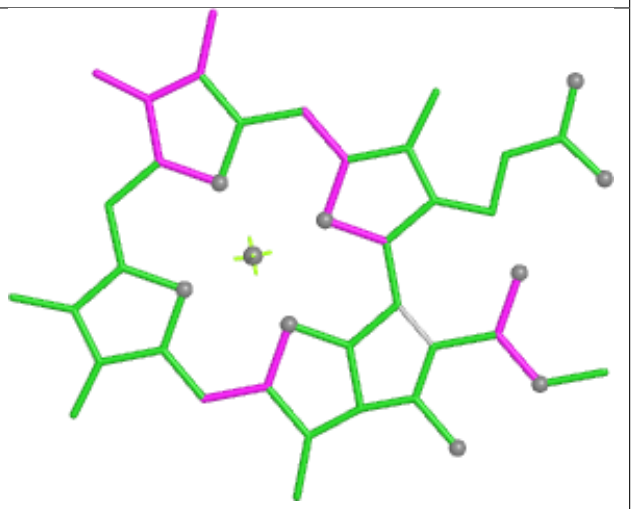


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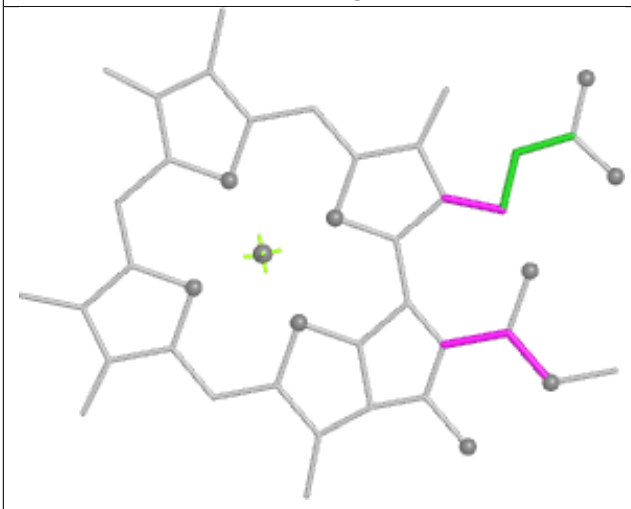
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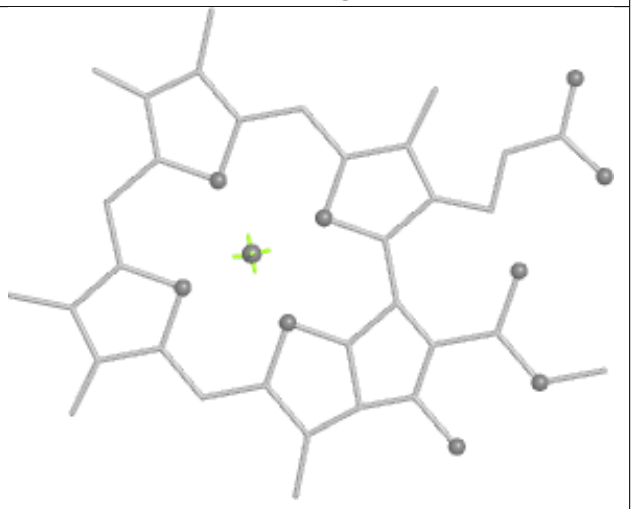
Bond lengths



Bond angles

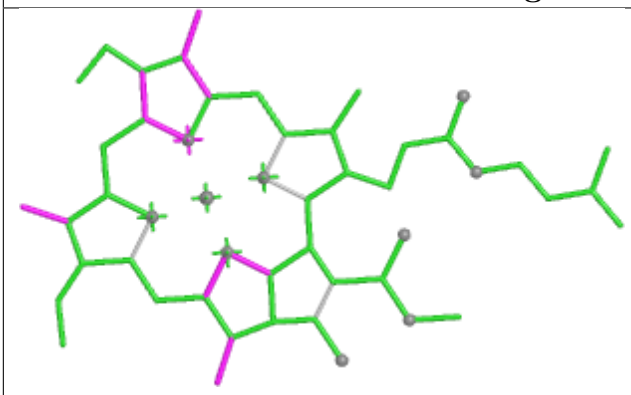


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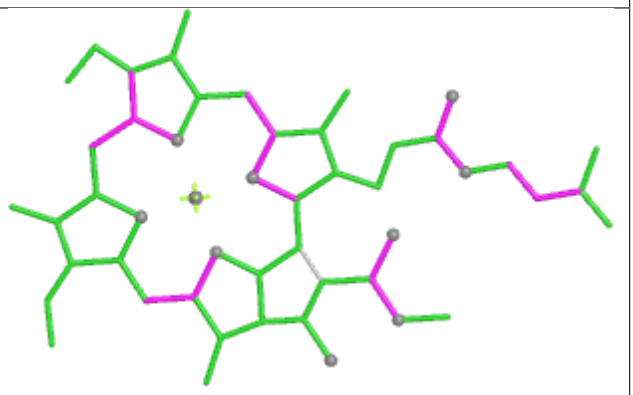


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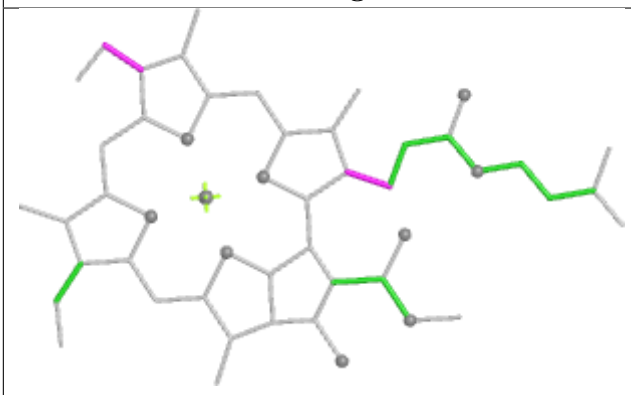
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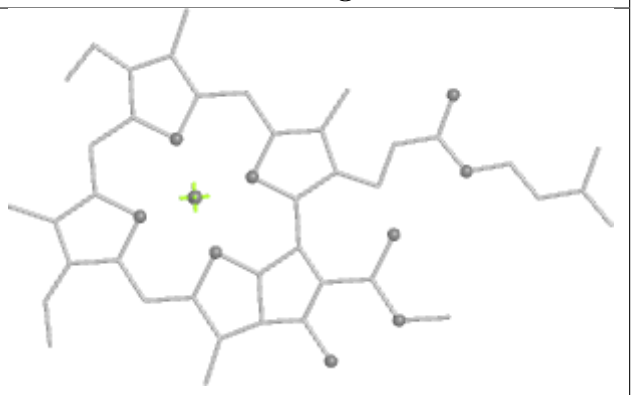
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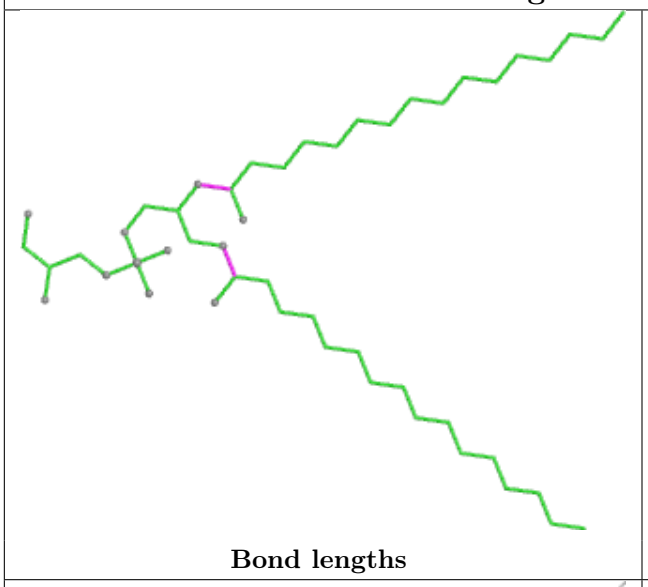


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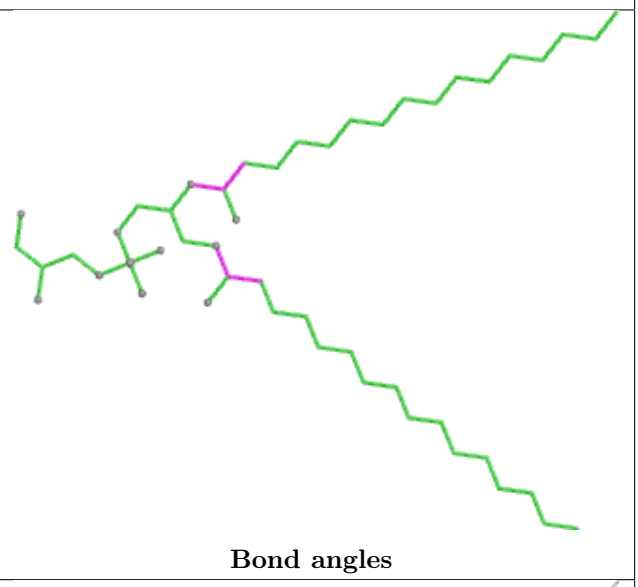


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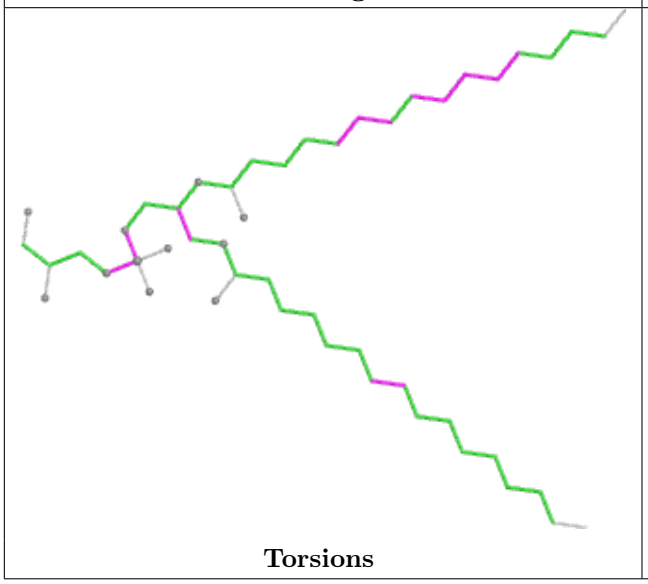
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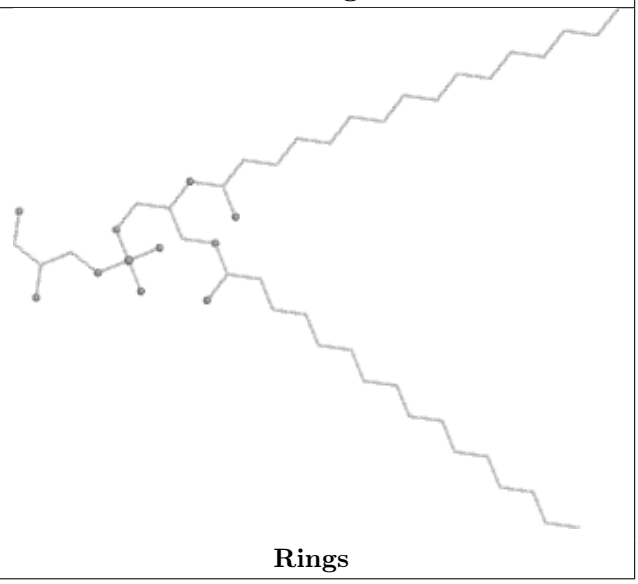
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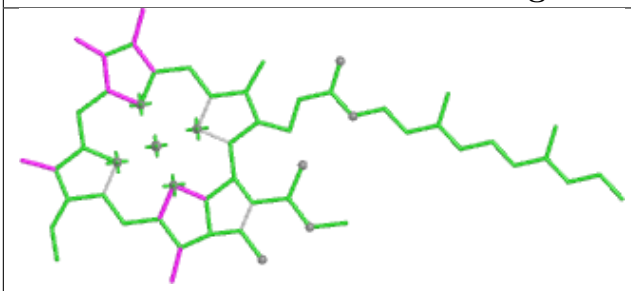


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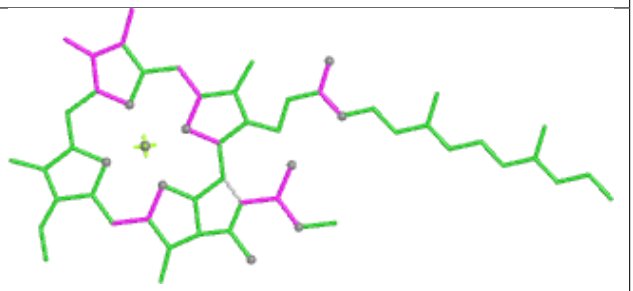


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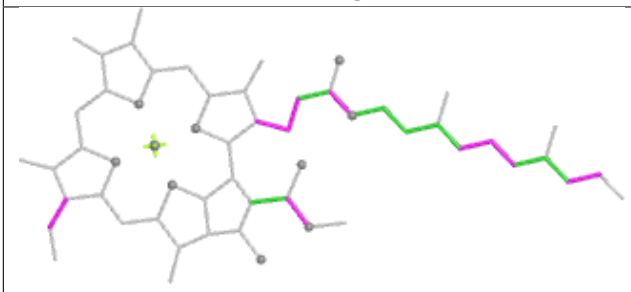
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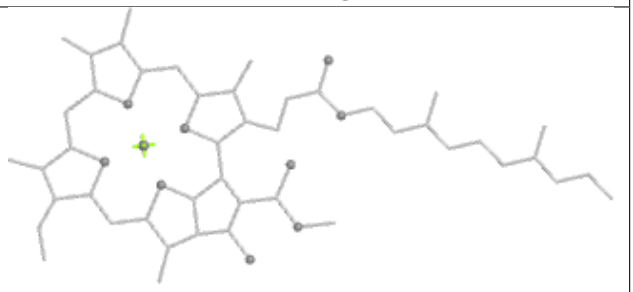
Bond lengths



Bond angles

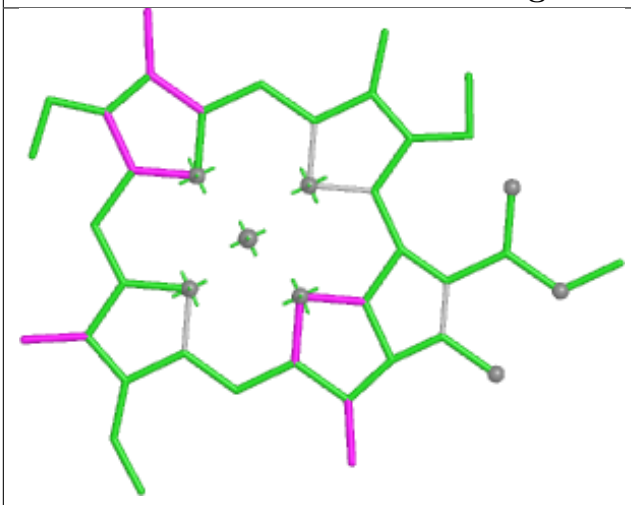


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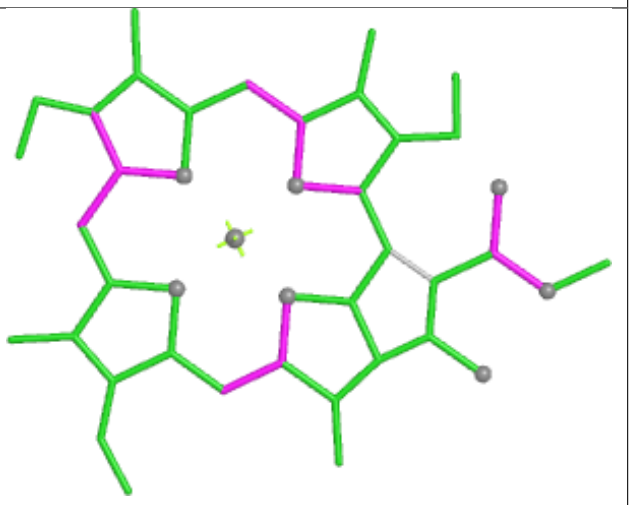


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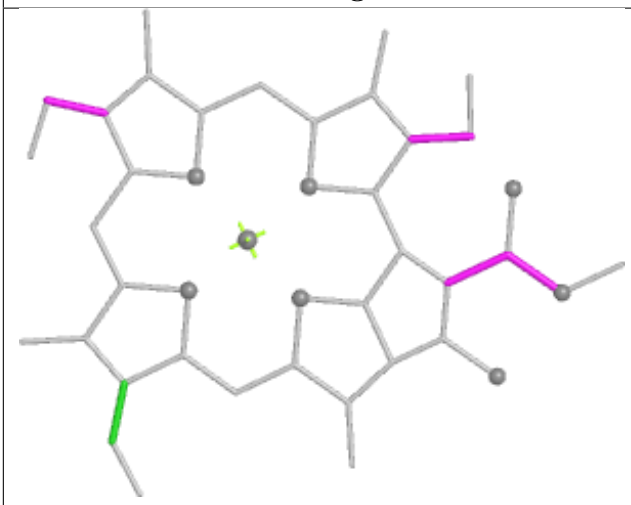
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Bond lengths



Bond angles



Torsions

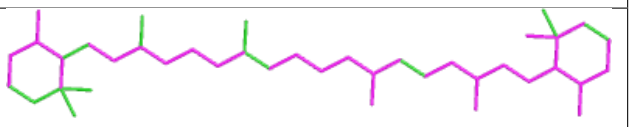


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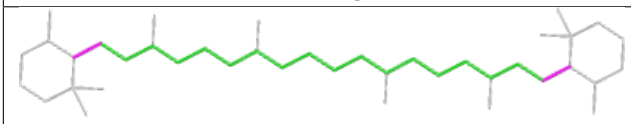
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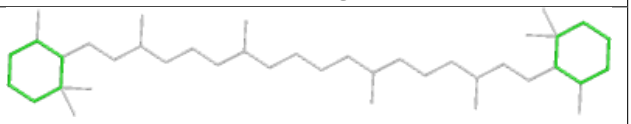
Bond lengths



Bond angles

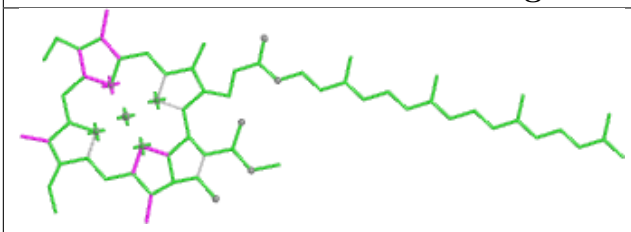


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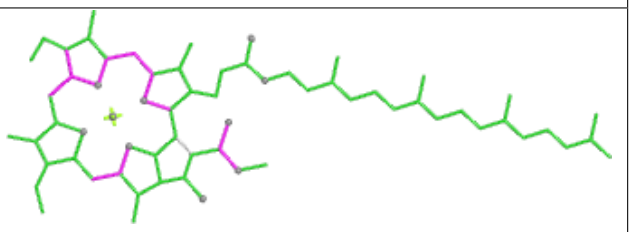


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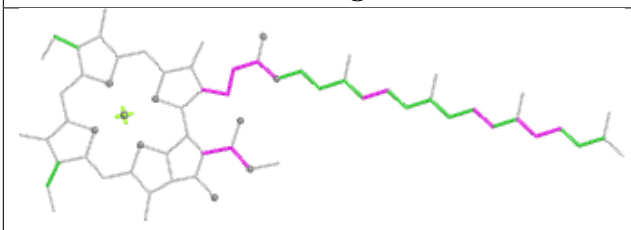
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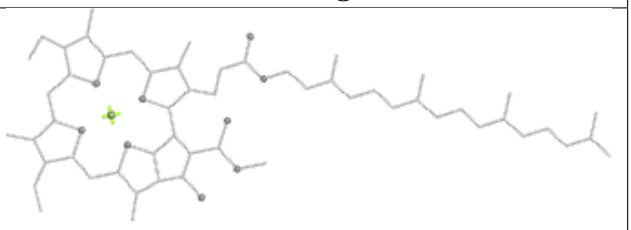
Bond lengths



Bond angles

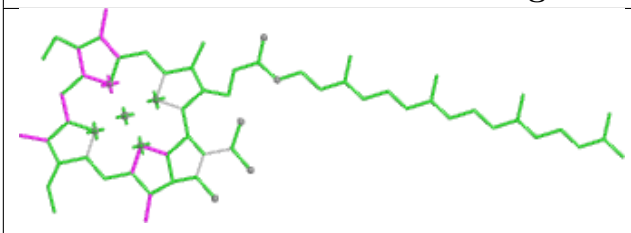


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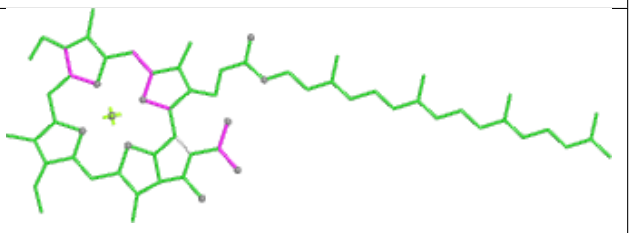


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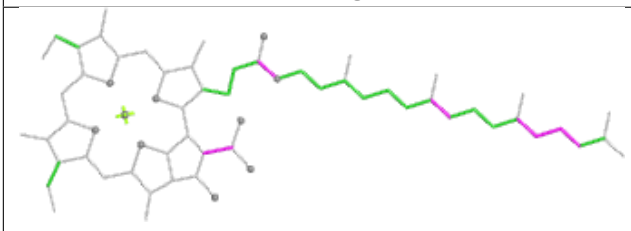
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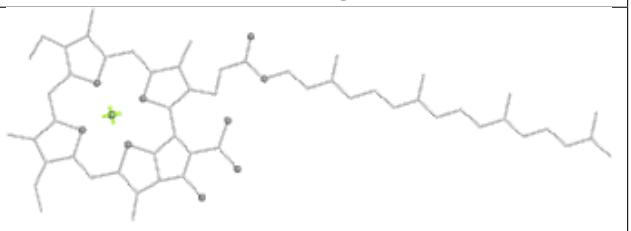
Bond lengths



Bond angles

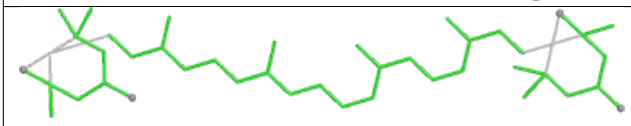


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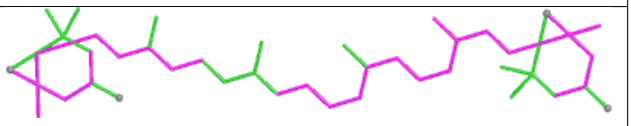


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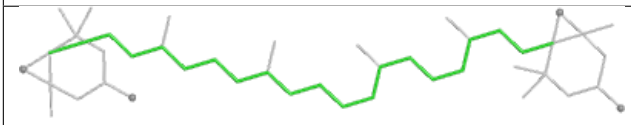
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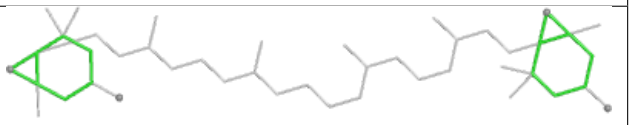
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Bond angles

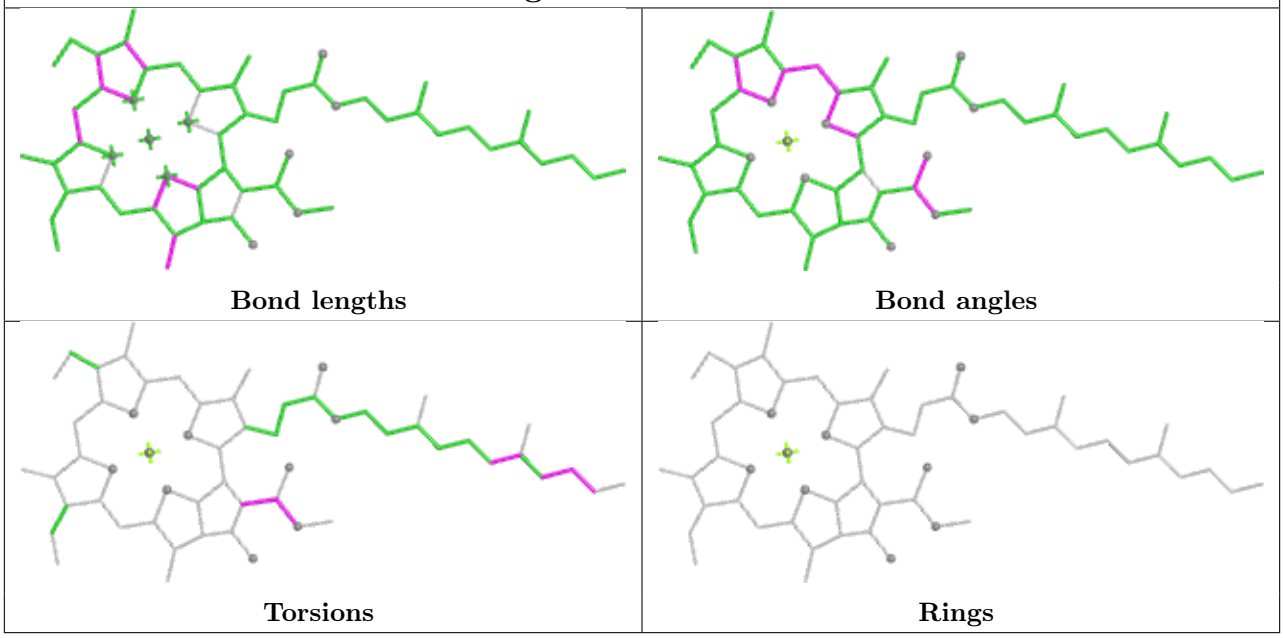


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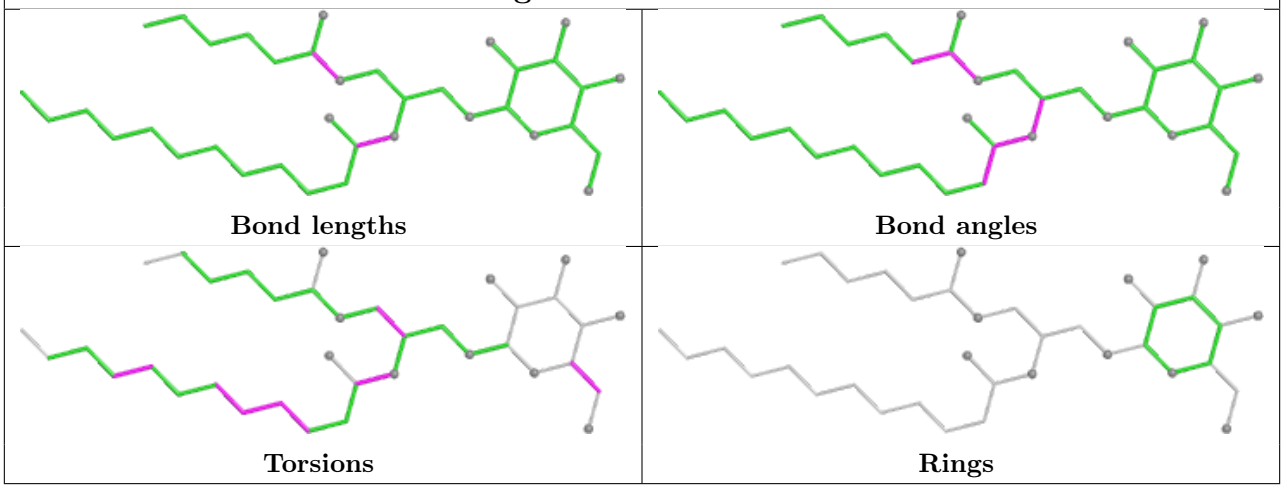


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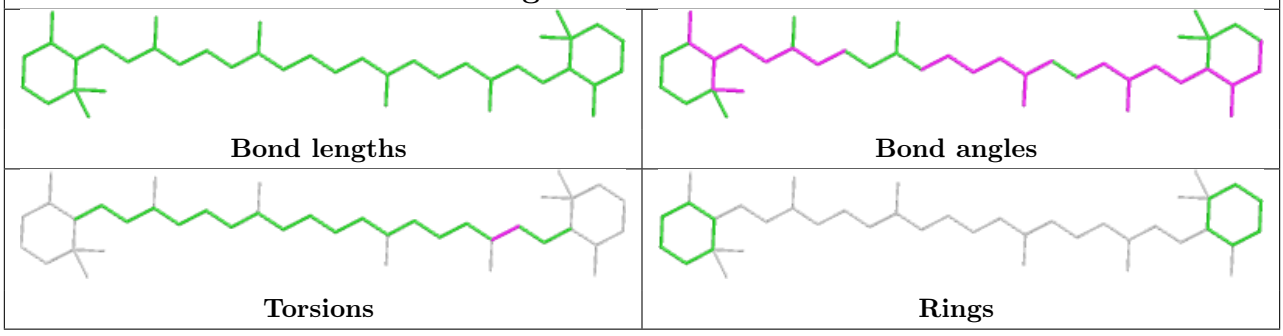
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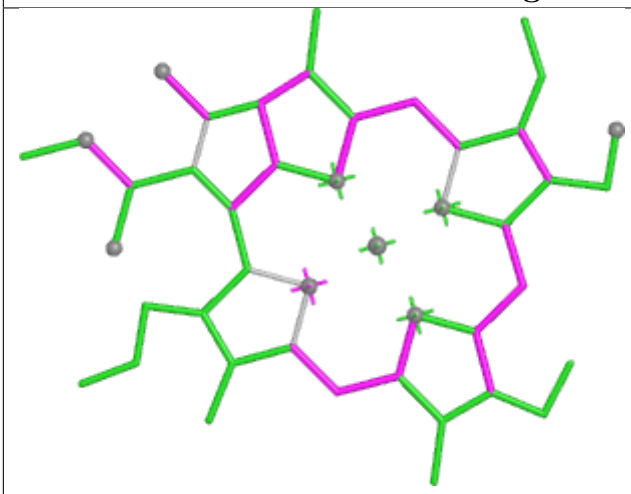
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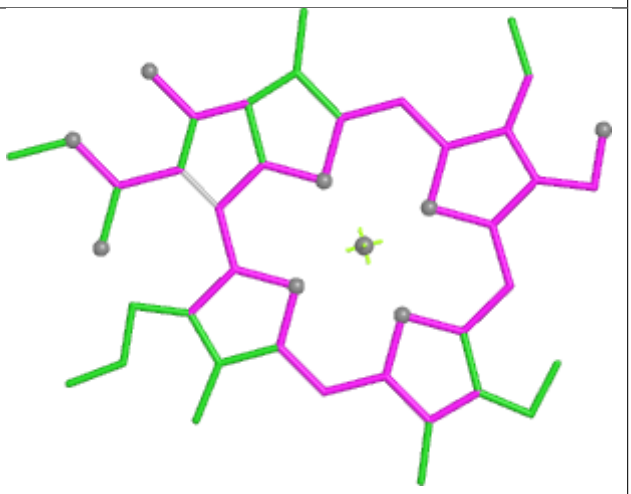
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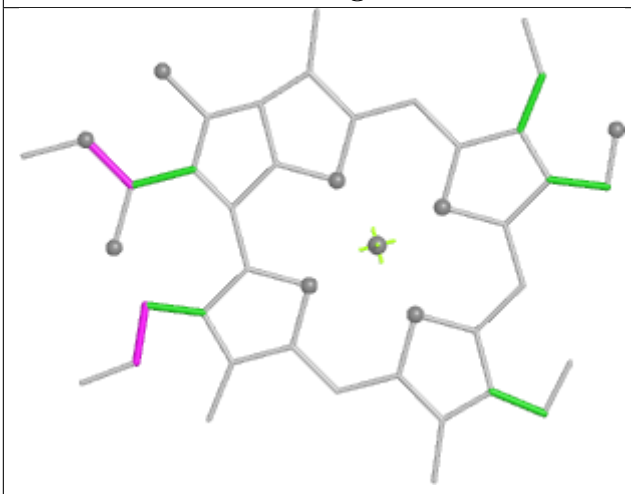
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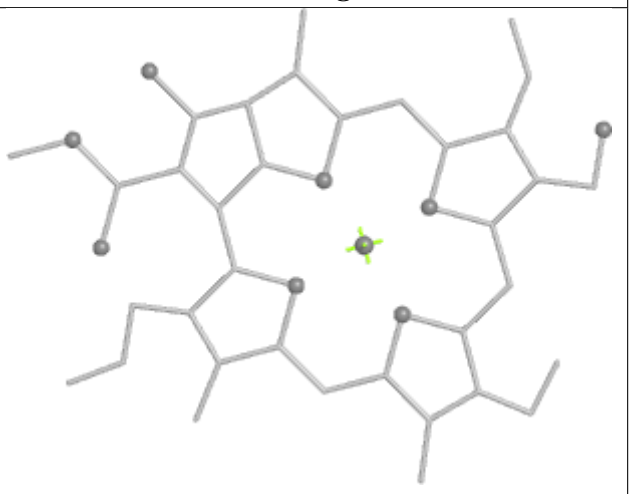
Bond lengths



Bond angles

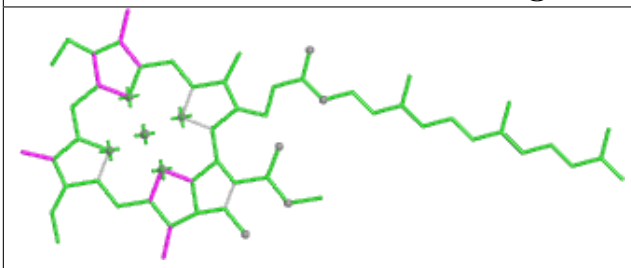


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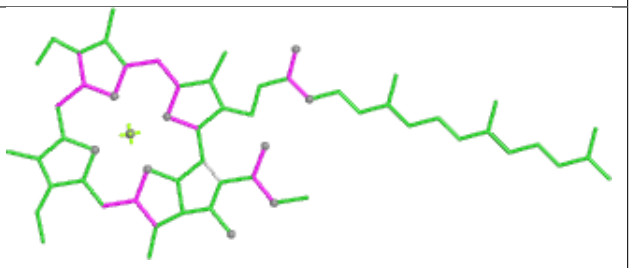


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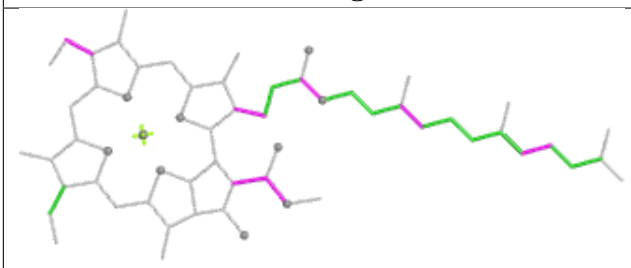
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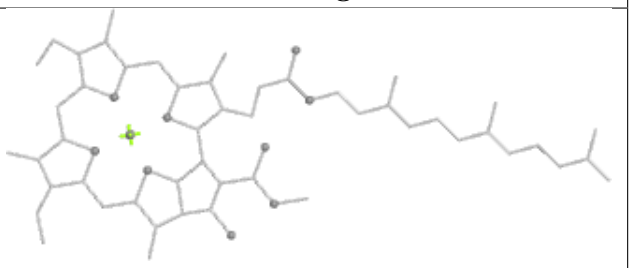
Bond lengths



Bond angles

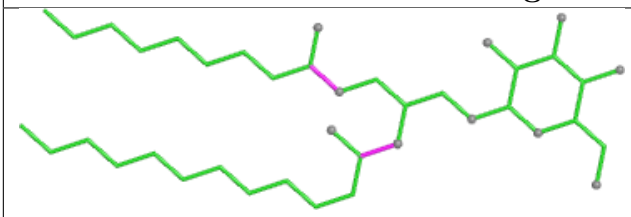


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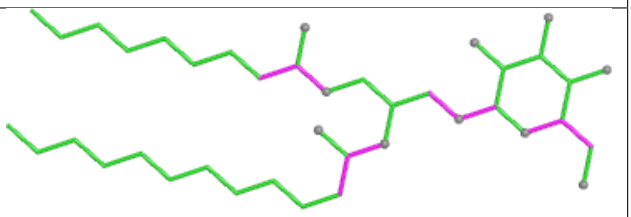


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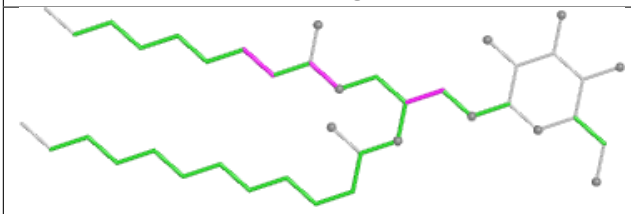
Ligand LMG 4 623



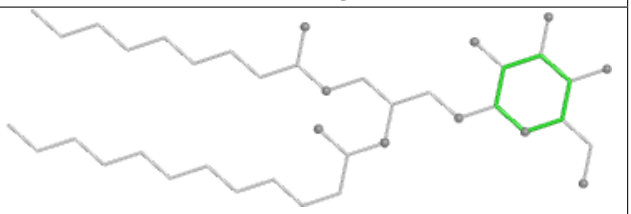
Bond lengths



Bond angles

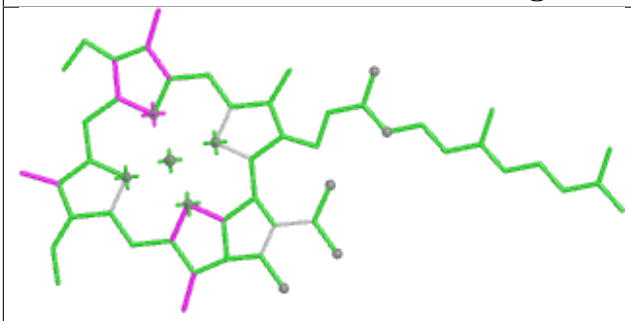


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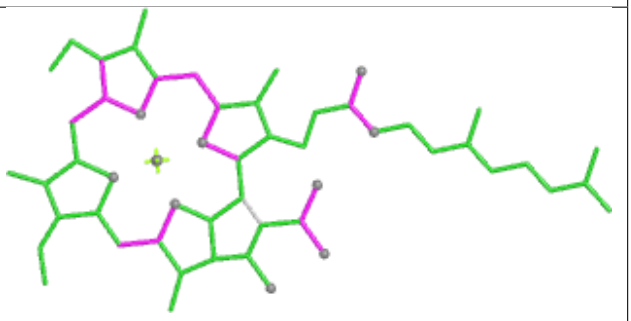


Rings

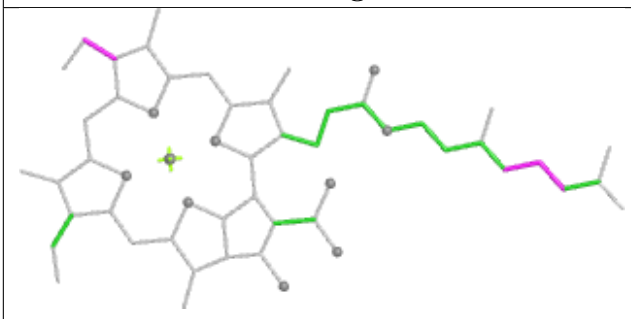
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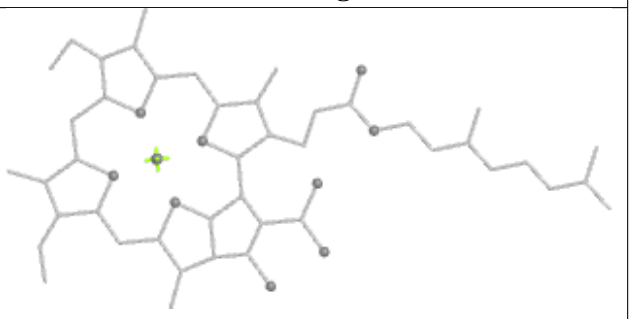
Bond lengths



Bond angles

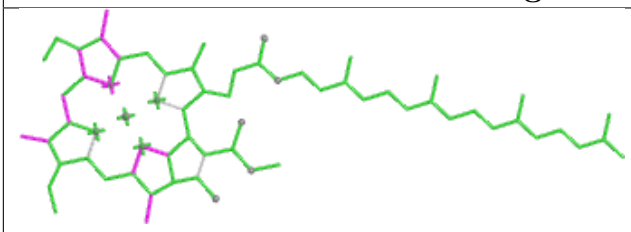


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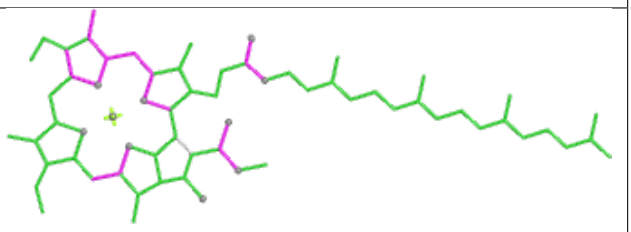


Rings

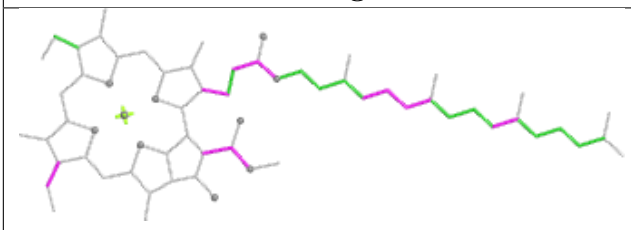
Ligand CLA B 813



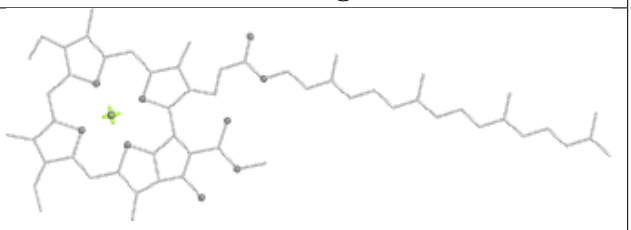
Bond lengths



Bond angles

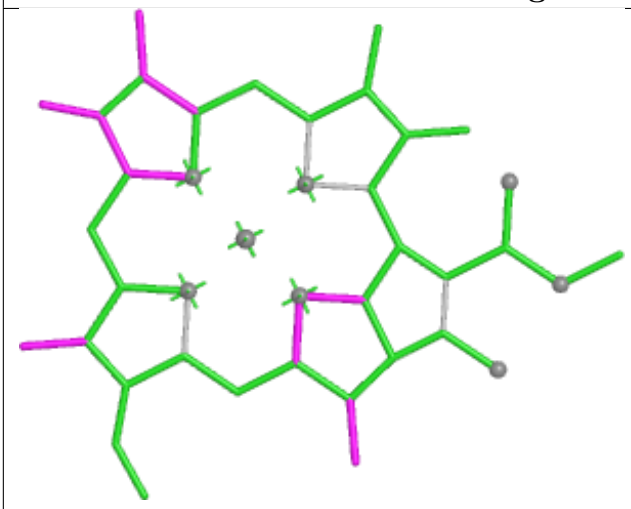


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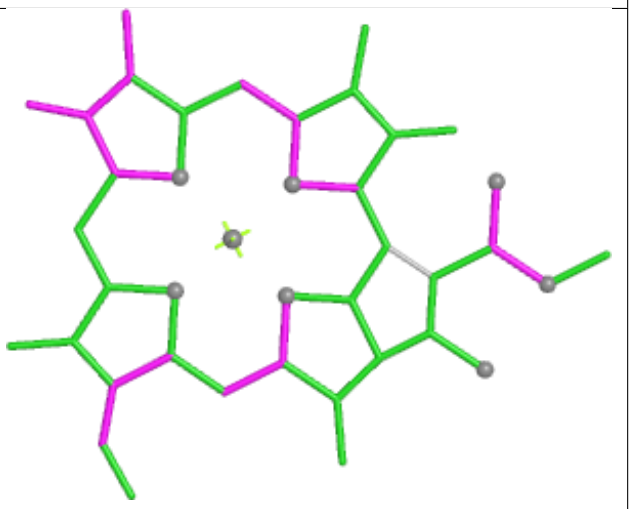


Rings

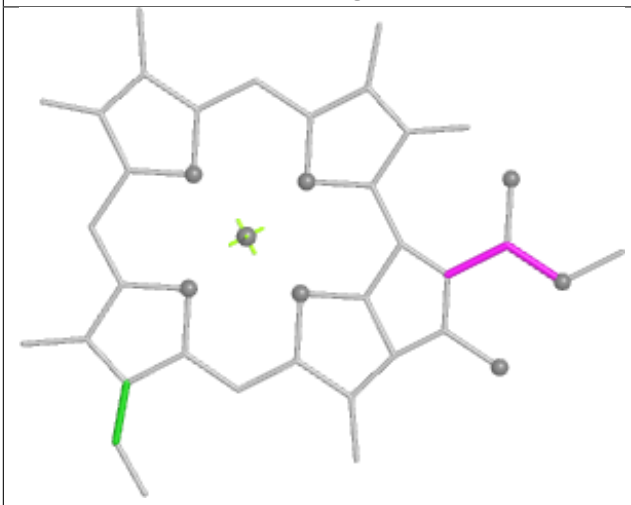
Ligand CLA 1 609



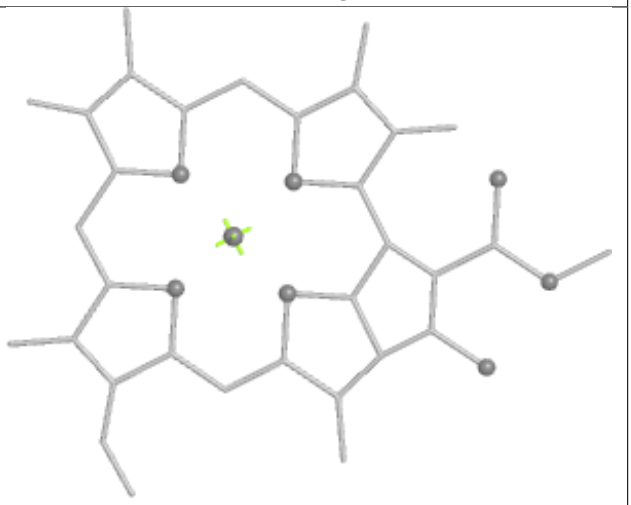
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Bond angles

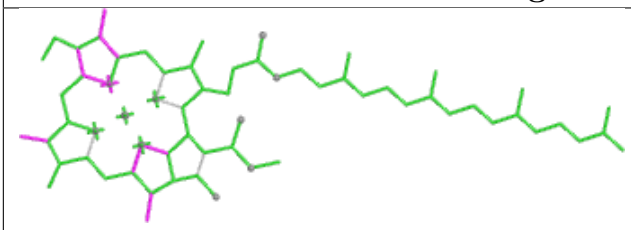


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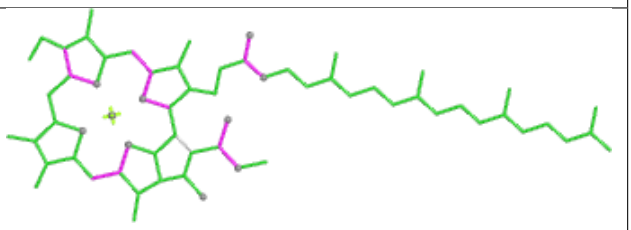


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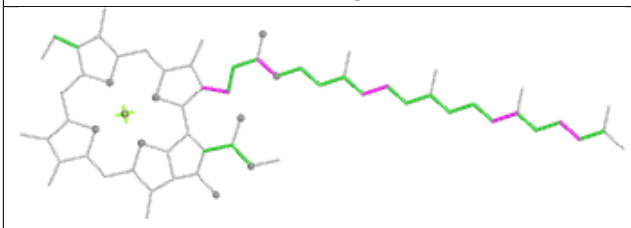
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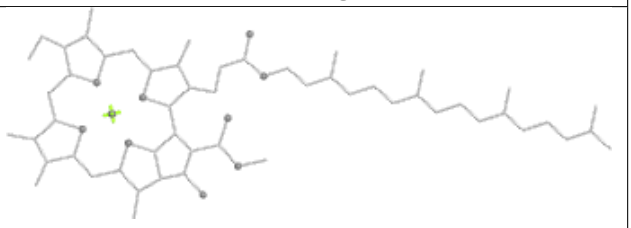
Bond lengths



Bond angles

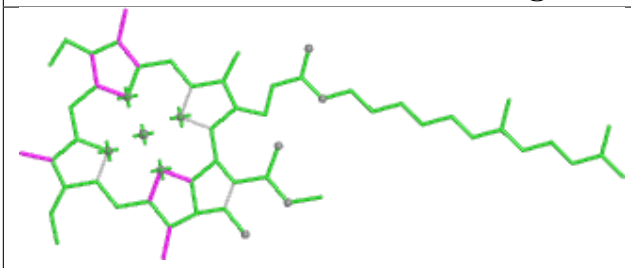


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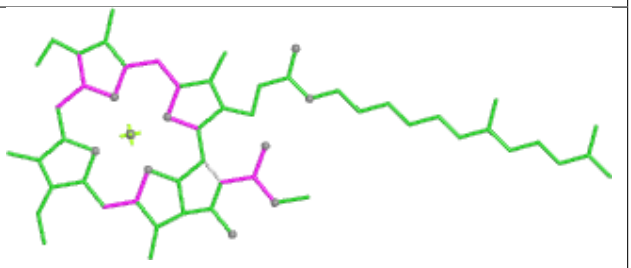


Rings

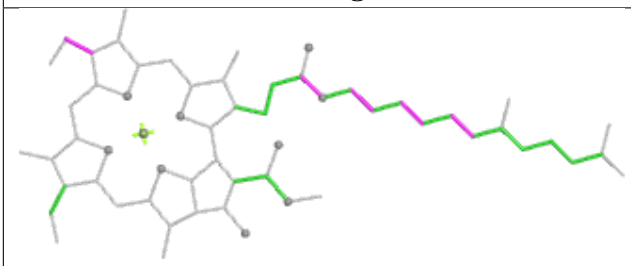
Ligand CLA 7 611



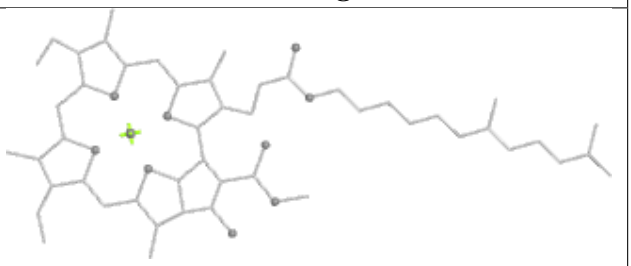
Bond lengths



Bond angles

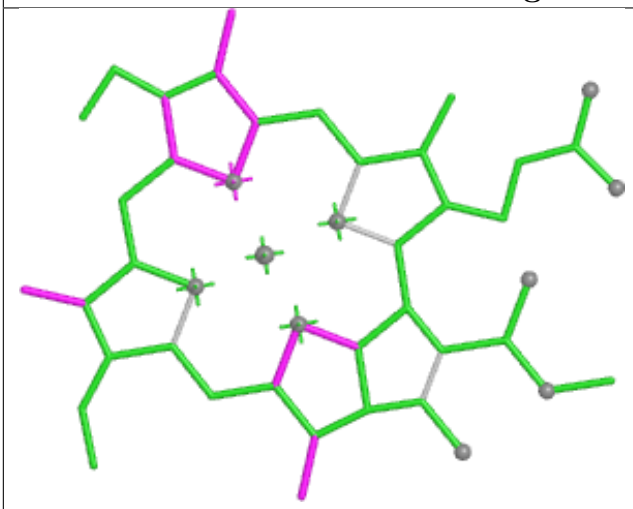


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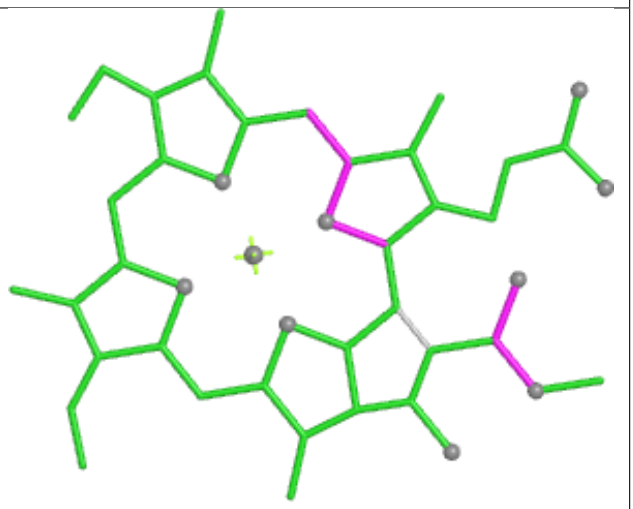


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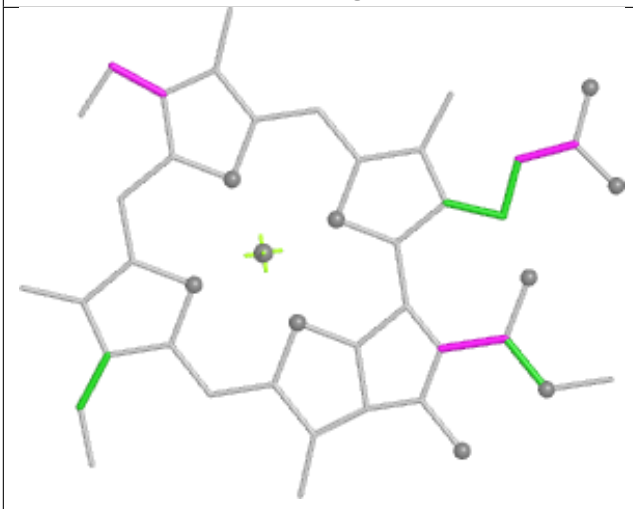
Ligand CLA V 603



Bond lengths



Bond angles

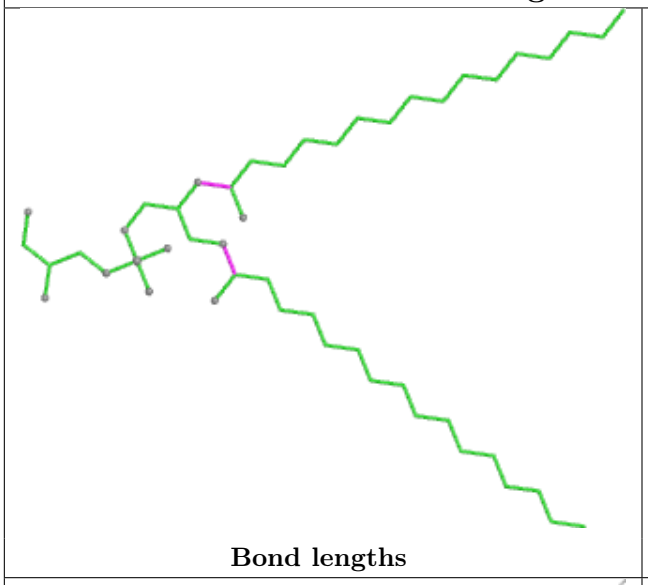


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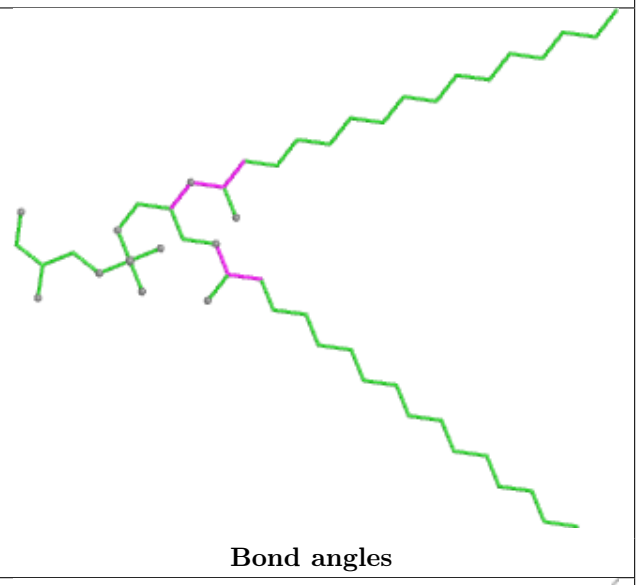


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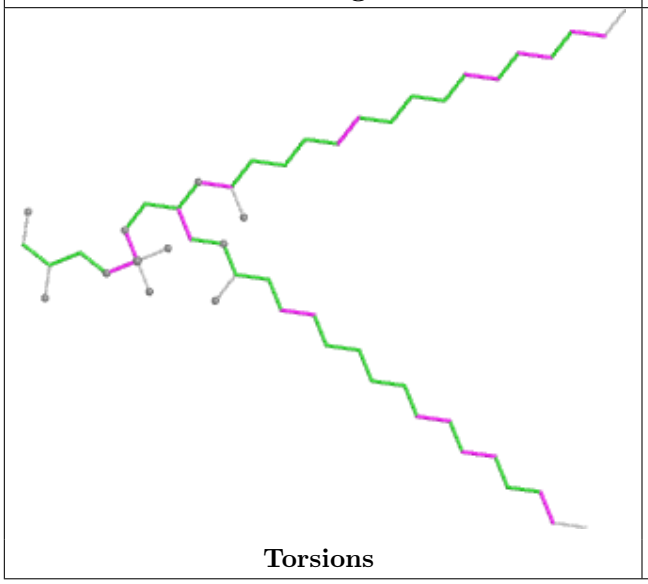
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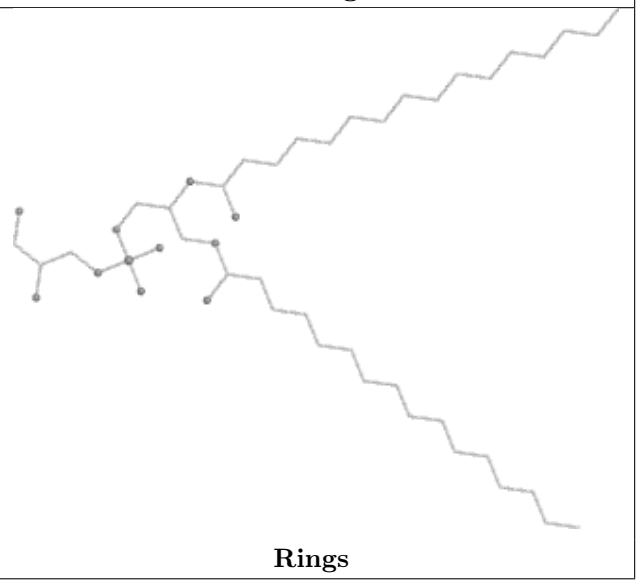
Bond lengths



Bond angles



Torsions

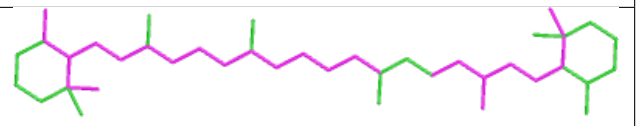


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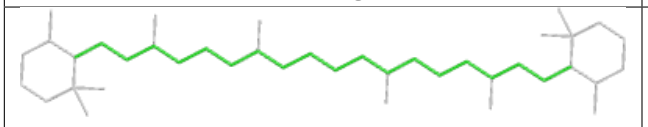
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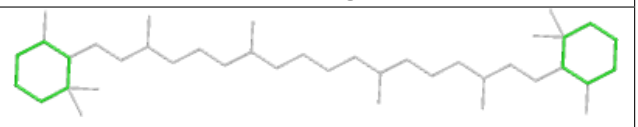
Bond lengths



Bond angles

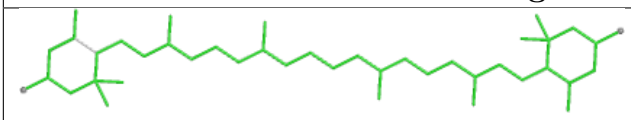


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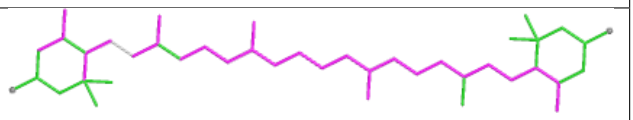


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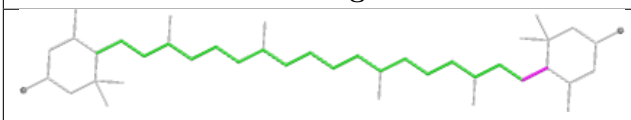
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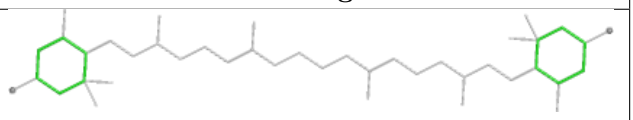
Bond lengths



Bond angles

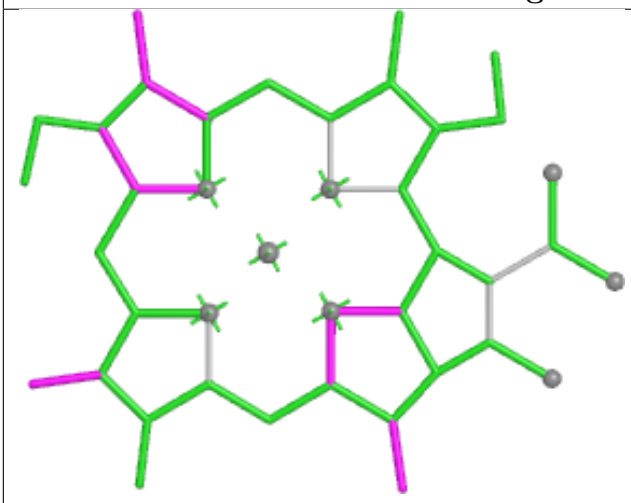


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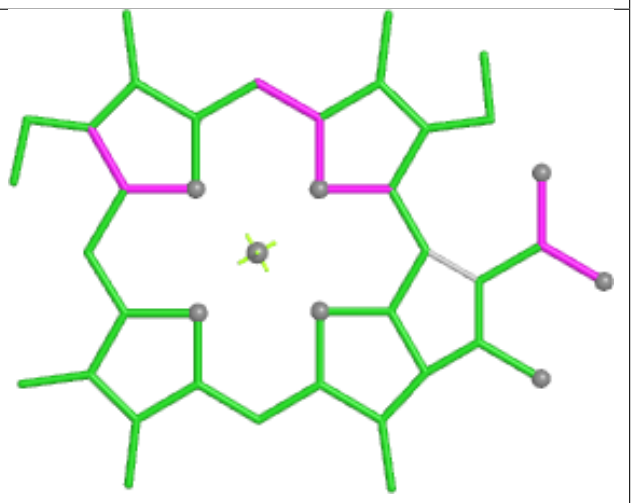


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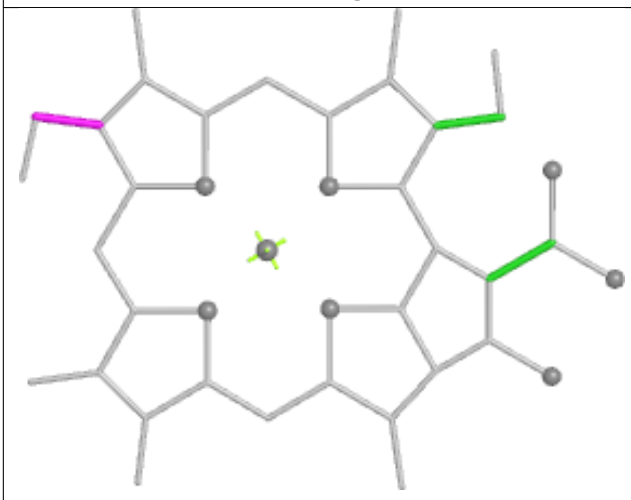
Ligand CLA L 307



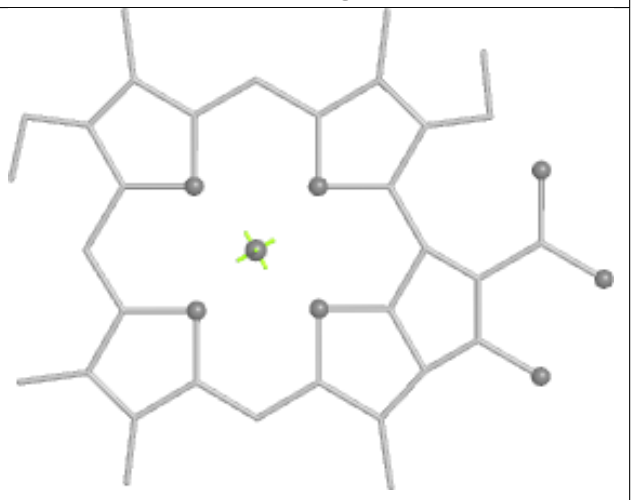
Bond lengths



Bond angles

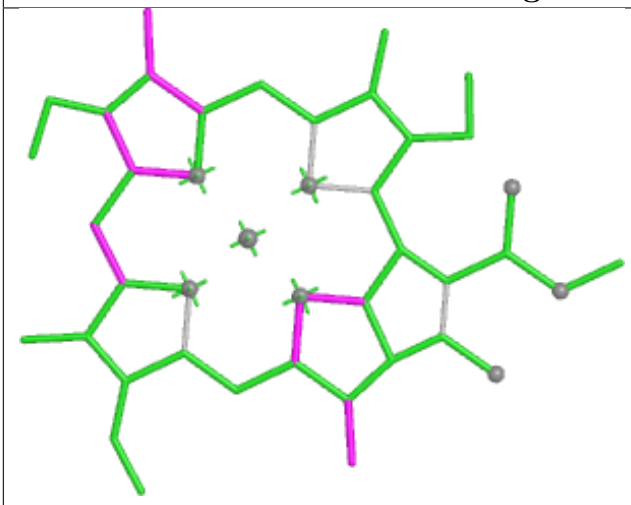


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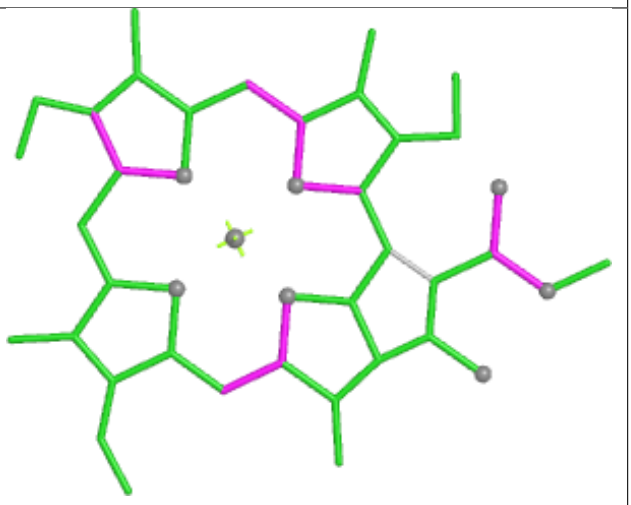


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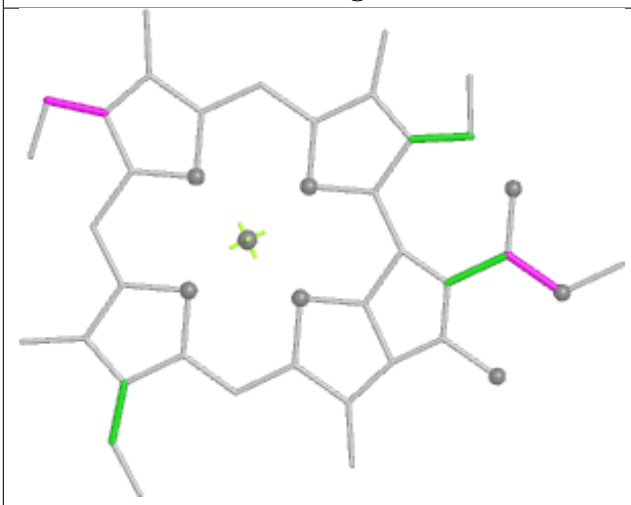
Ligand CLA G 203



Bond lengths



Bond angles

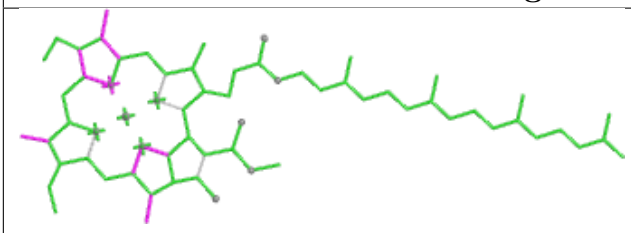


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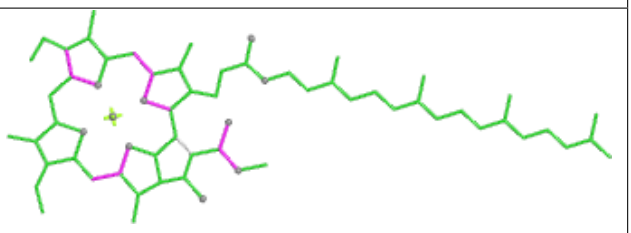


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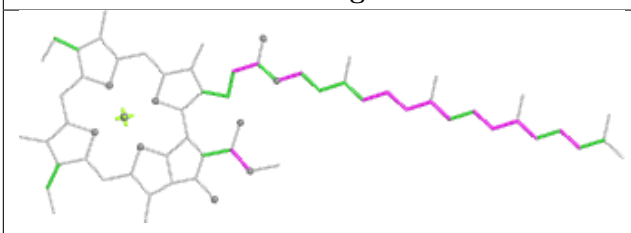
Ligand CLA B 806



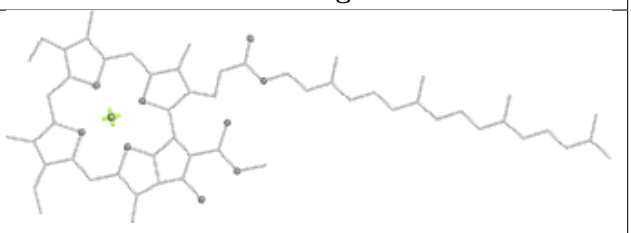
Bond lengths



Bond angles

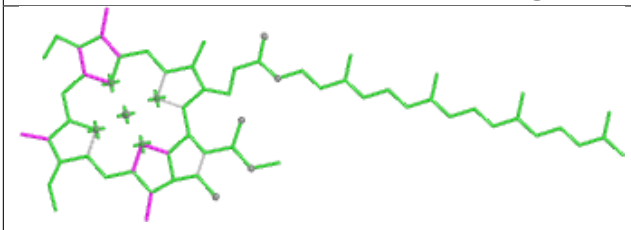


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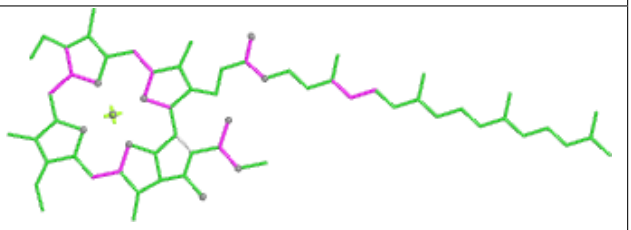


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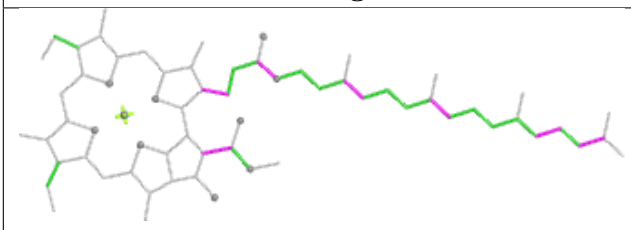
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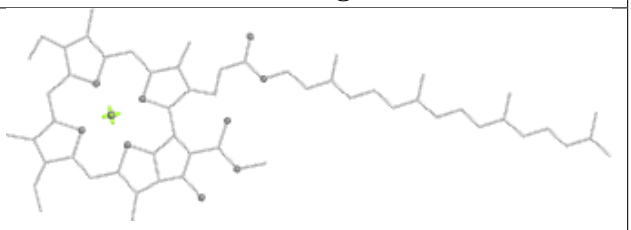
Bond lengths



Bond angles

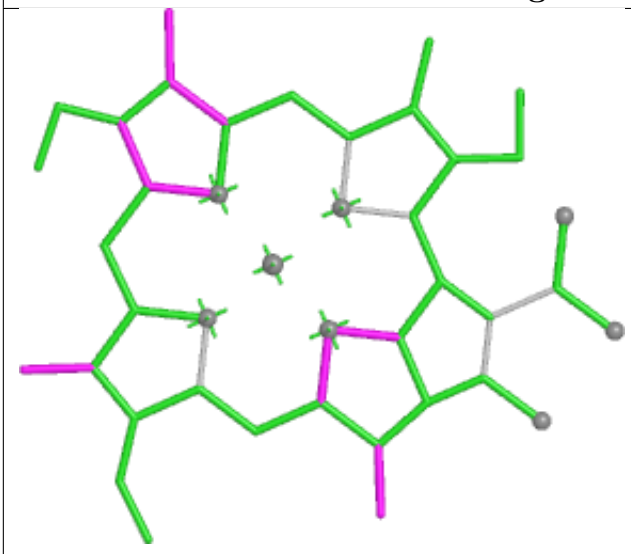


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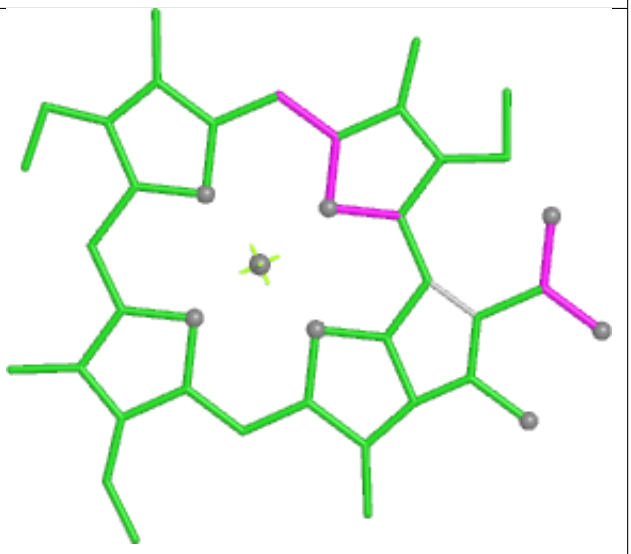


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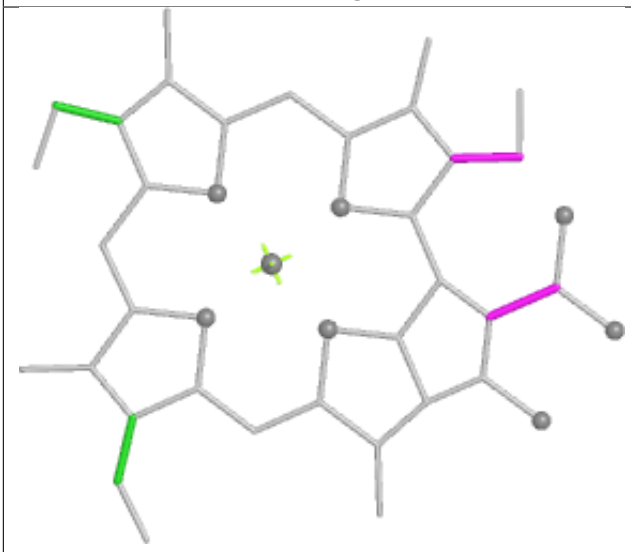
Ligand CLA 5 612



Bond lengths



Bond angles

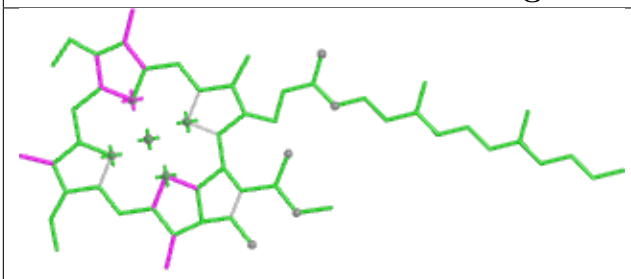


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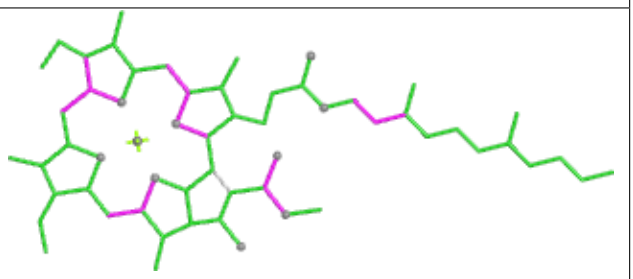


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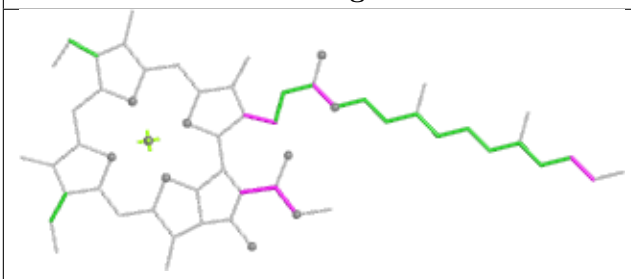
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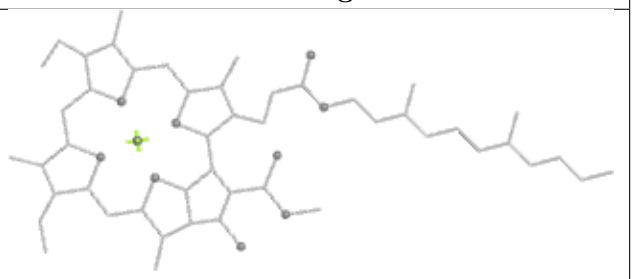
Bond lengths



Bond angles

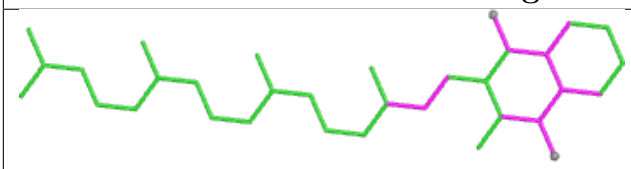


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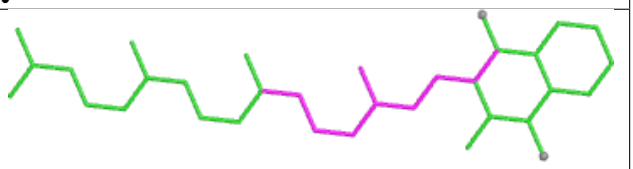


Rings

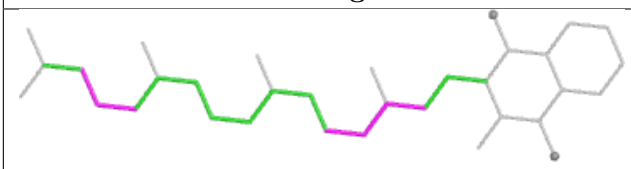
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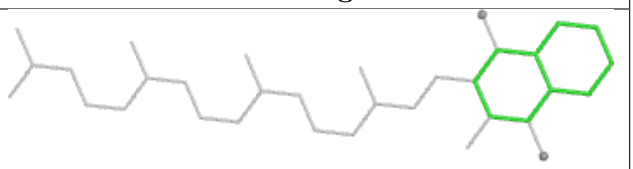
Bond lengths



Bond angles

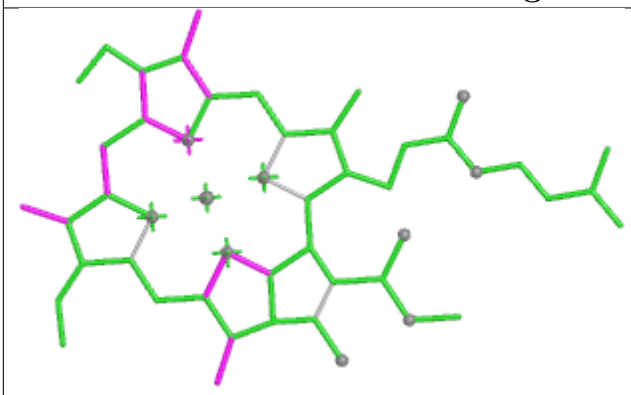


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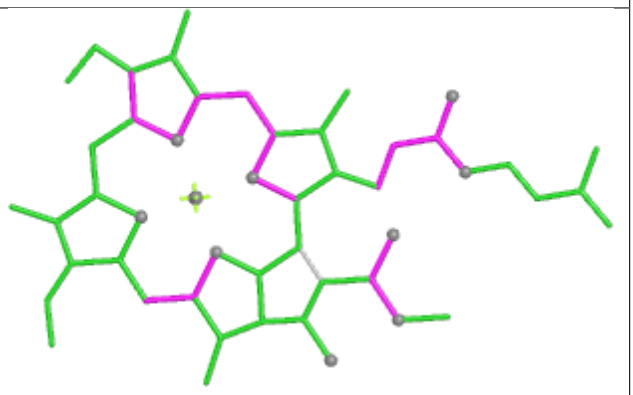


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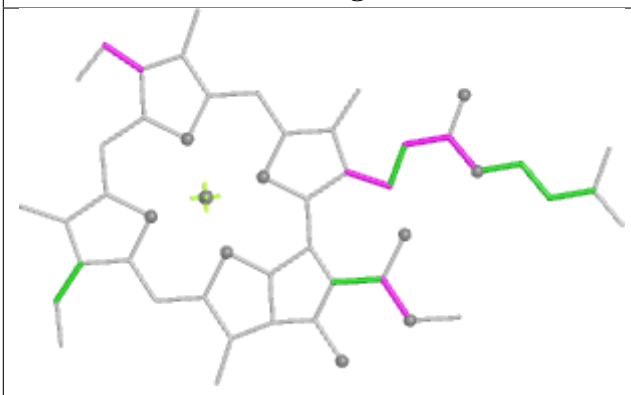
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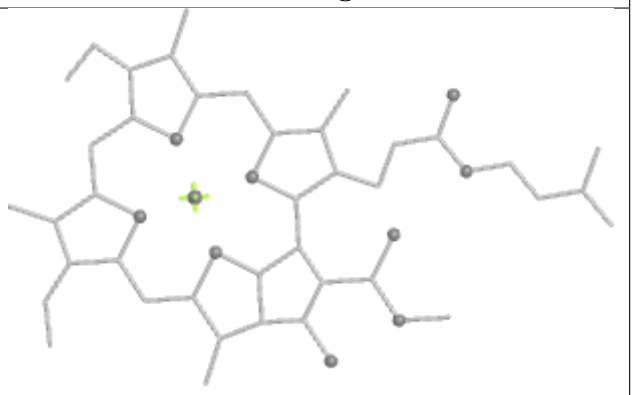
Bond lengths



Bond angles



Torsions

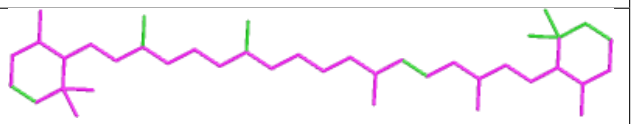


Rings

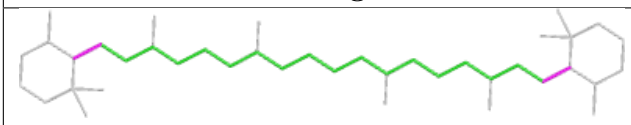
Ligand BCR 7 623



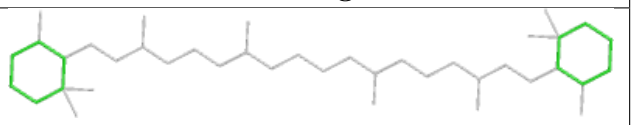
Bond lengths



Bond angles

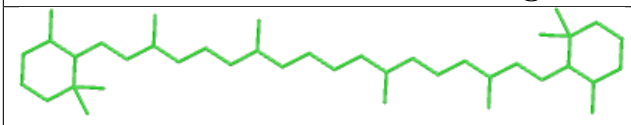


Torsions

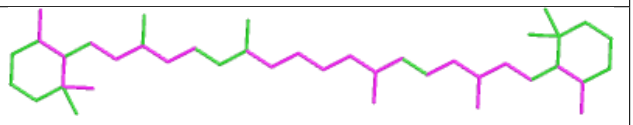


Rings

Ligand BCR B 853



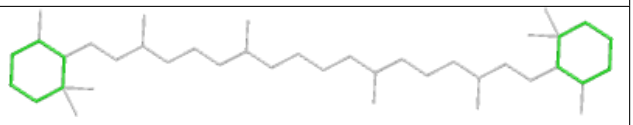
Bond lengths



Bond angles

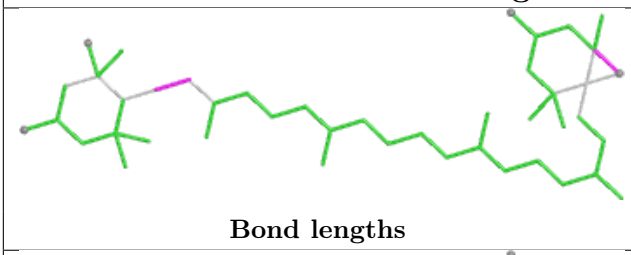


Torsions

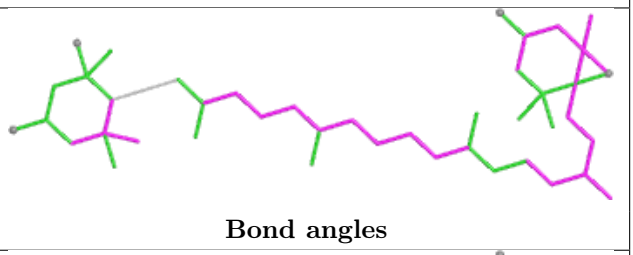


Rings

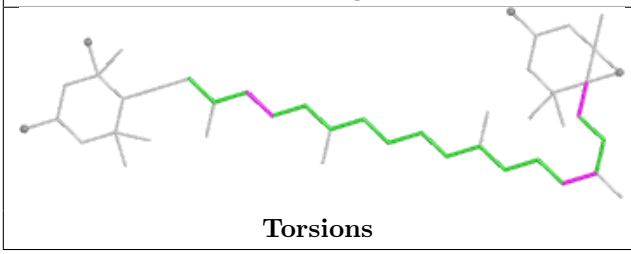
Ligand NEX U 1623



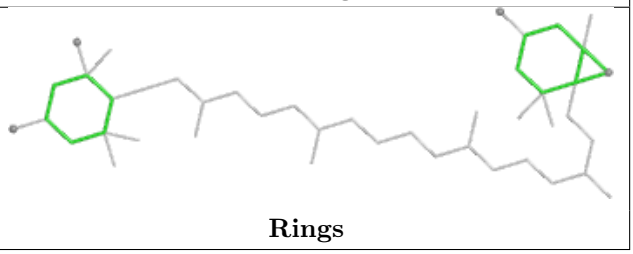
Bond lengths



Bond angles

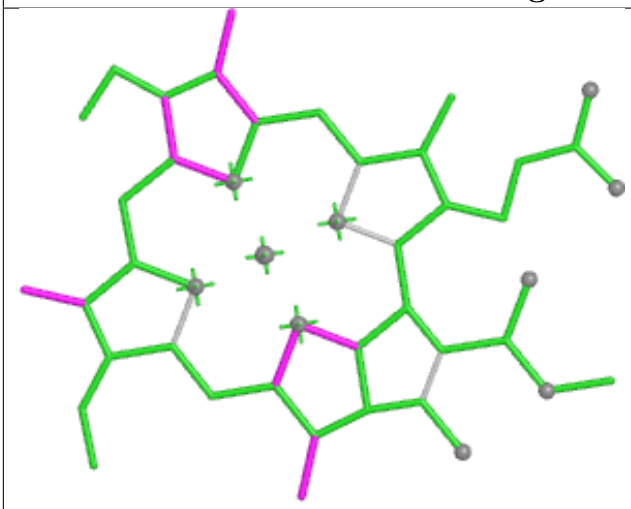


Torsions

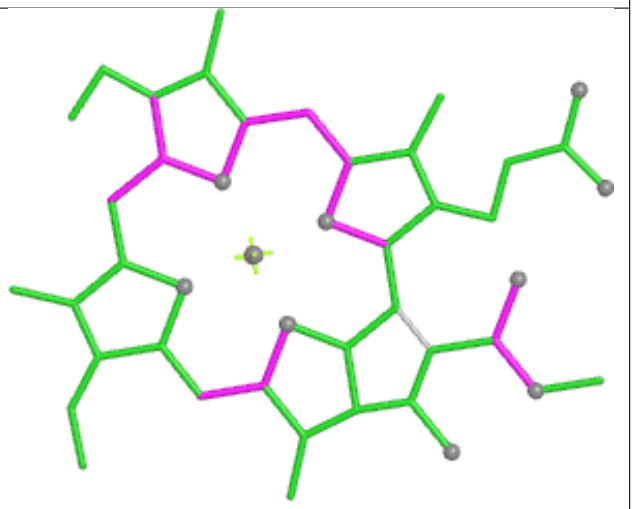


Rings

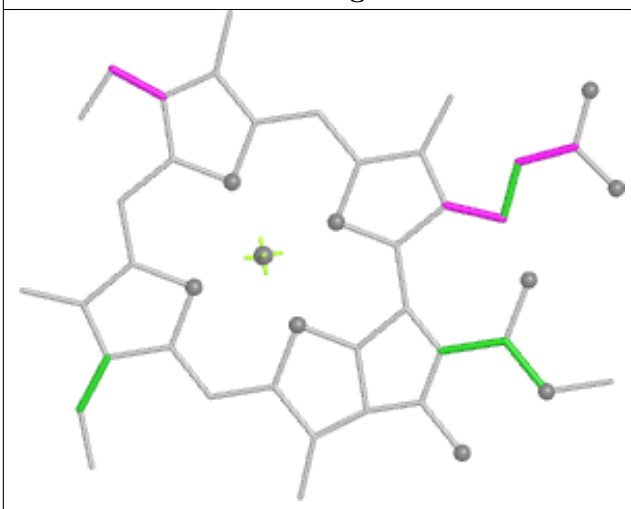
Ligand CLA 8 609



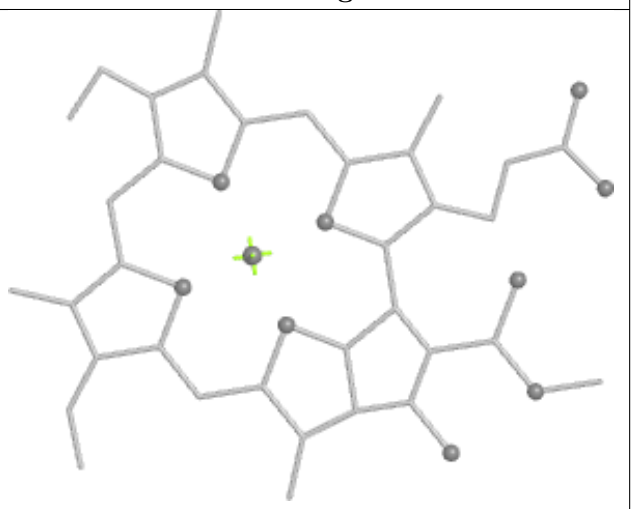
Bond lengths



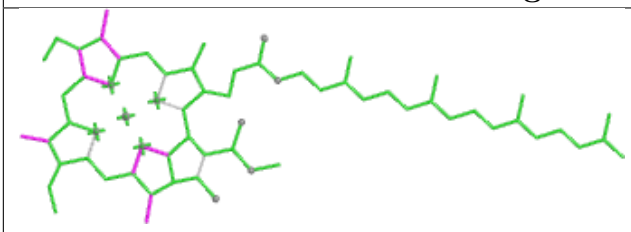
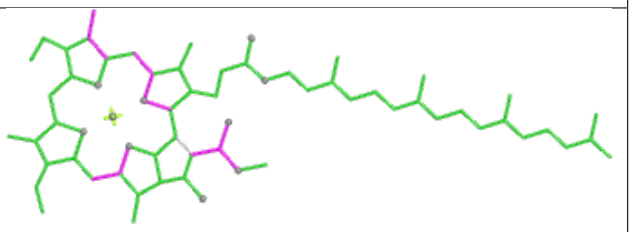
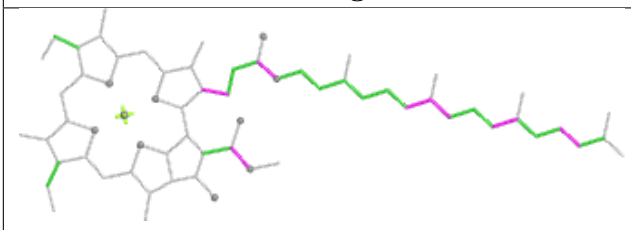
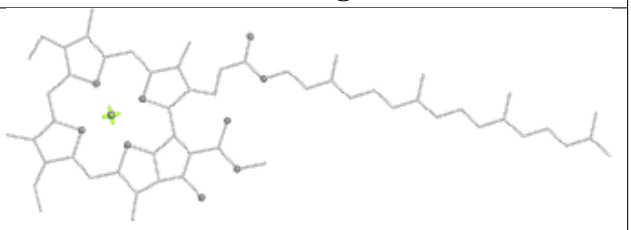
Bond angles

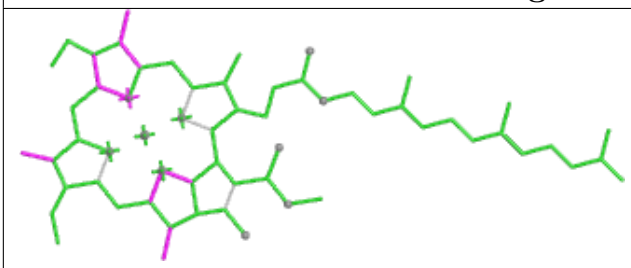
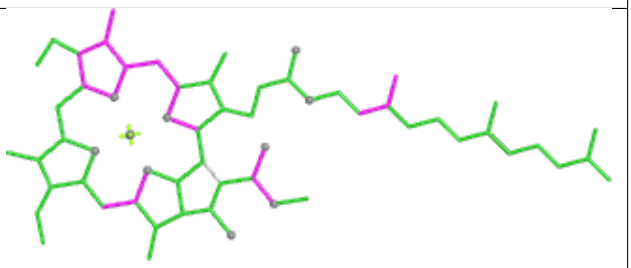
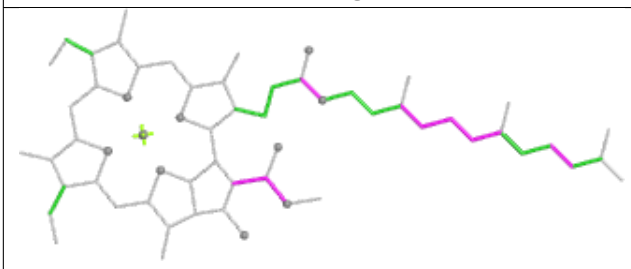
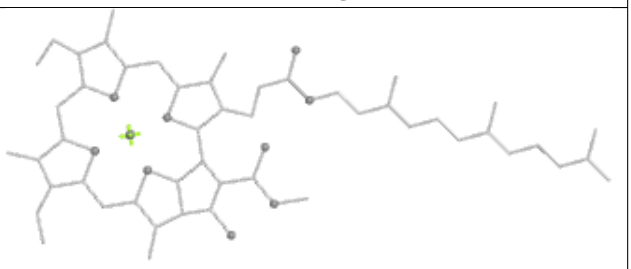


Torsions

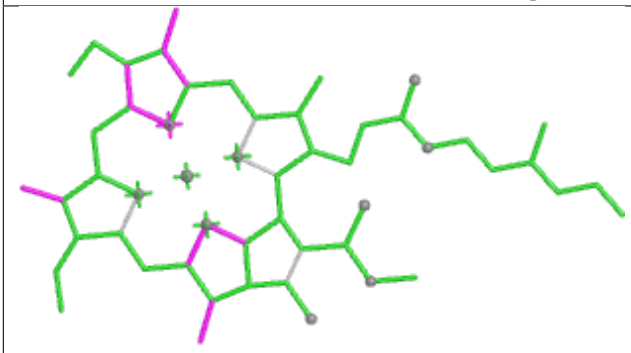


Rings

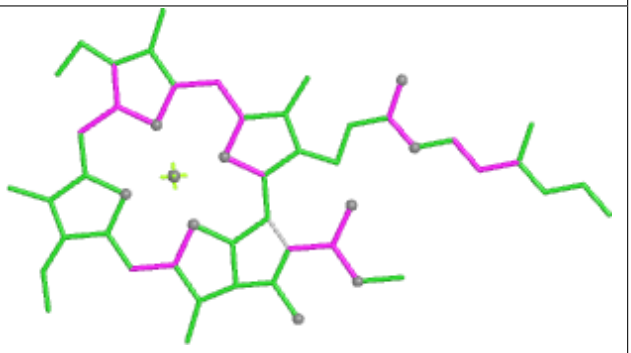
Ligand CLA A 820	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 7 601	
	
Bond lengths	Bond angles
	
Torsions	Rings

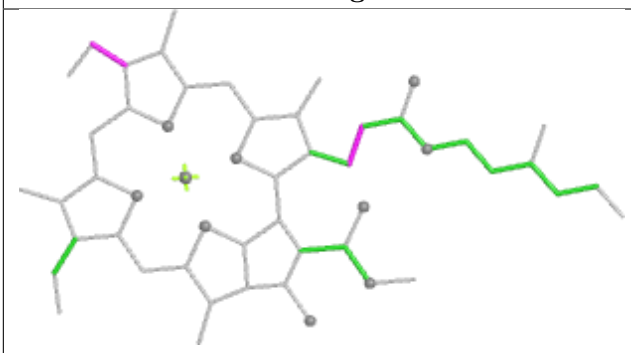
Ligand CLA B 807



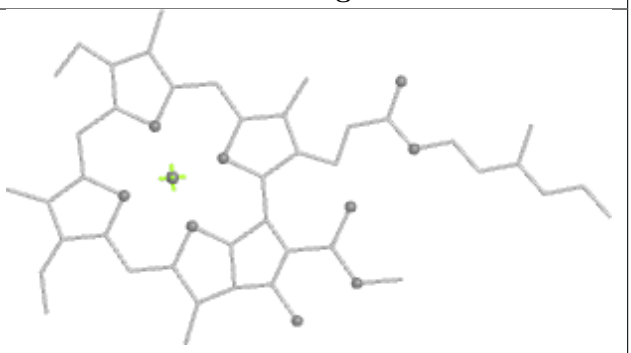
Bond lengths



Bond angles

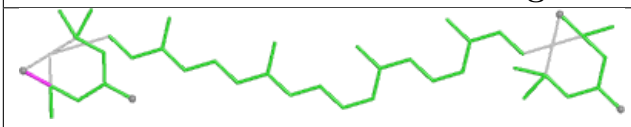


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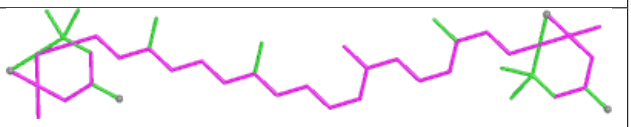


Rings

Ligand XAT 8 620



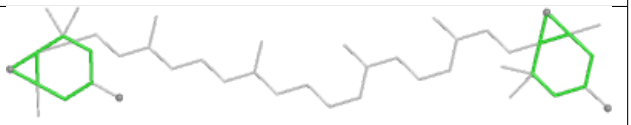
Bond lengths



Bond angles

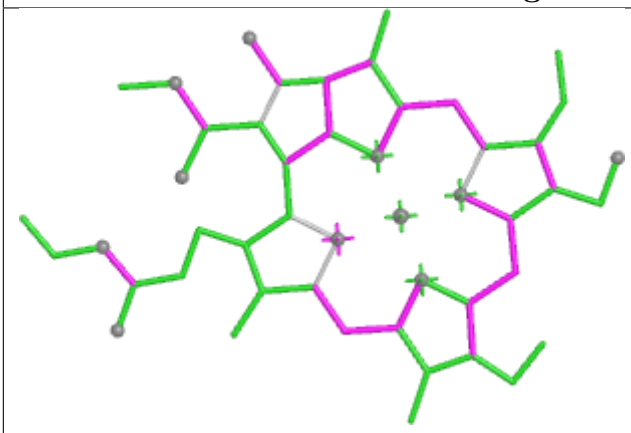


Torsions

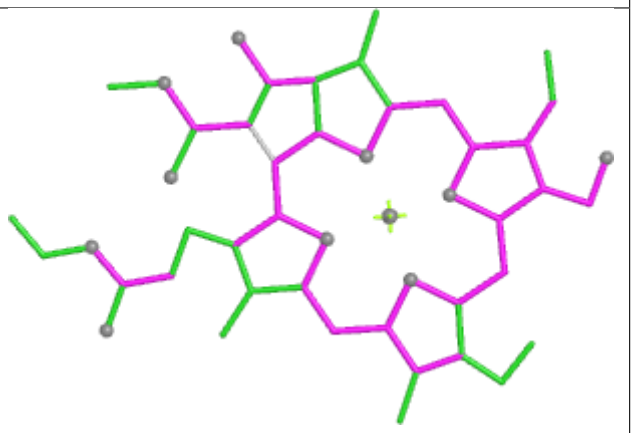


Rings

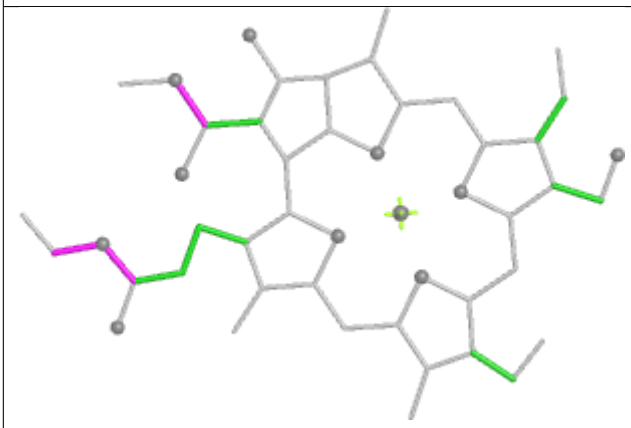
Ligand CHL V 608



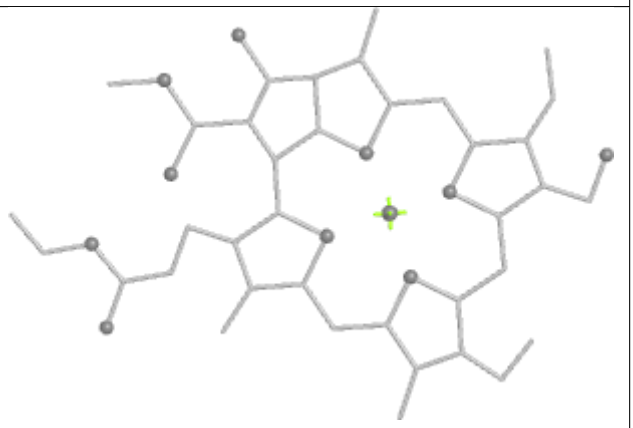
Bond lengths



Bond angles

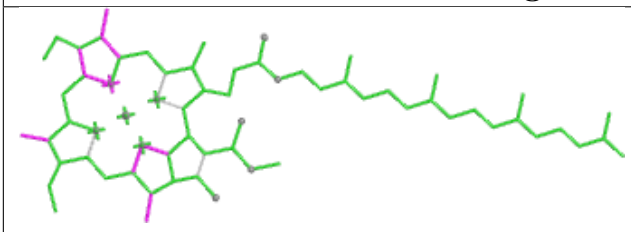


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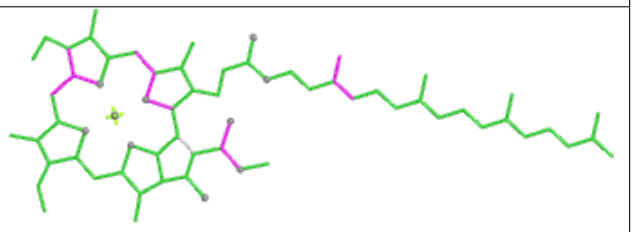


Rings

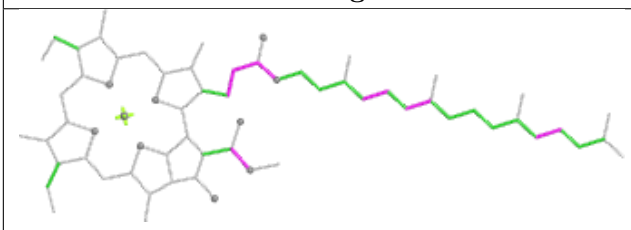
Ligand CLA A 830



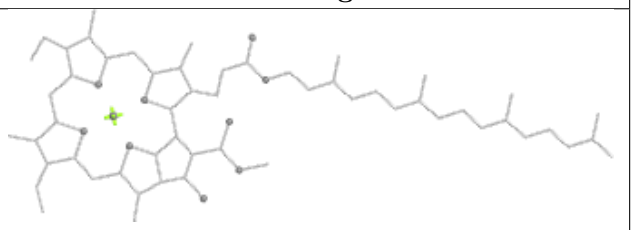
Bond lengths



Bond angles

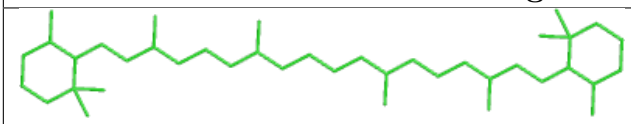


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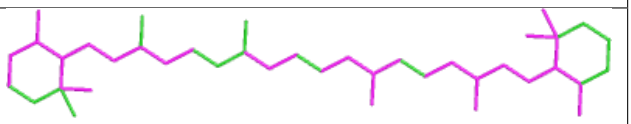


Rings

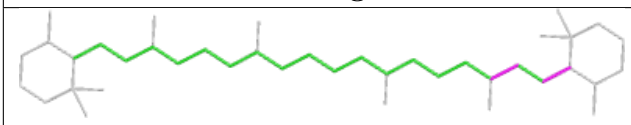
Ligand BCR 5 622



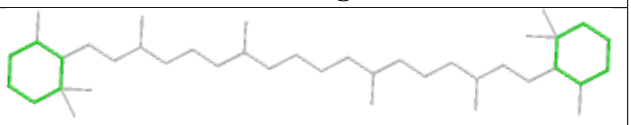
Bond lengths



Bond angles

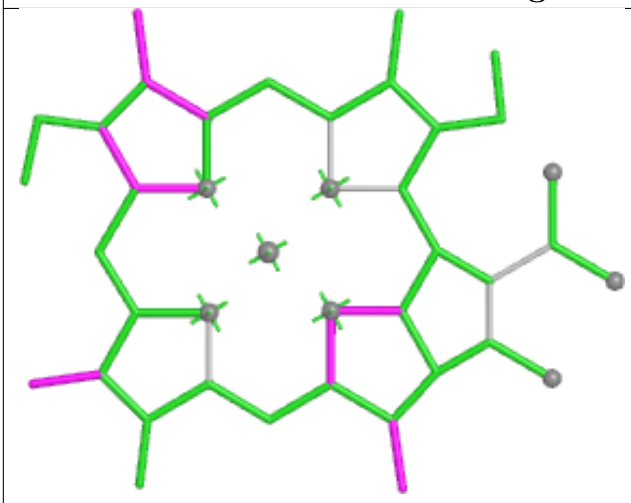


Torsions

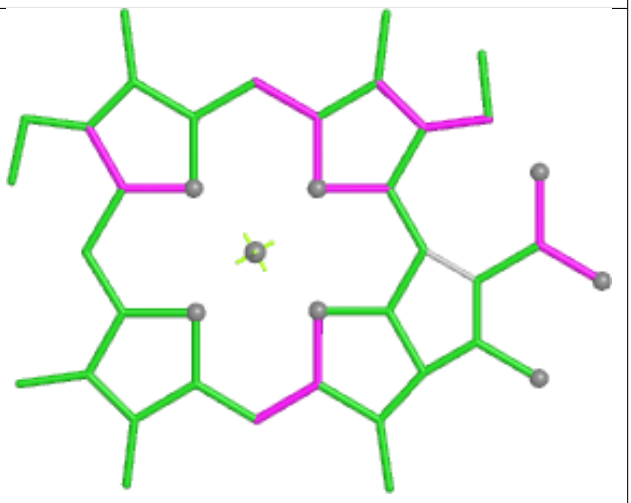


Rings

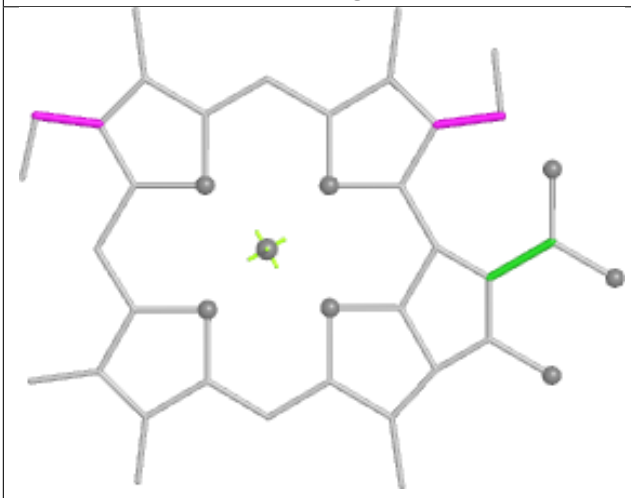
Ligand CLA 9 606



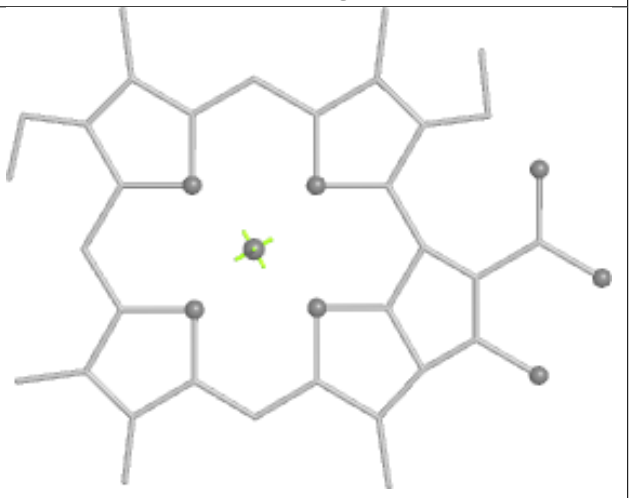
Bond lengths



Bond angles

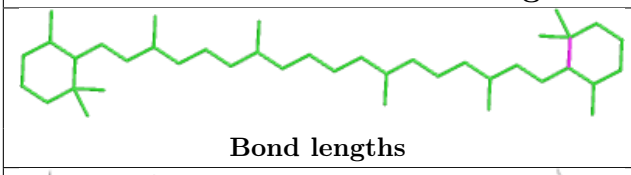


Torsions

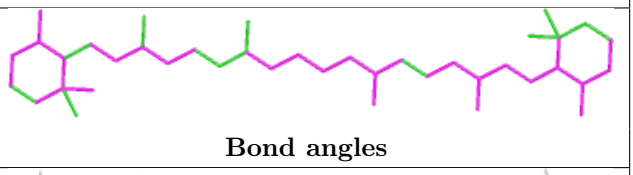


Rings

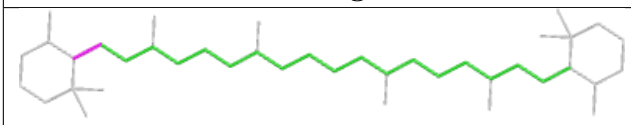
Ligand BCR B 846



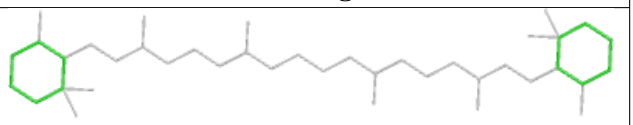
Bond lengths



Bond angles

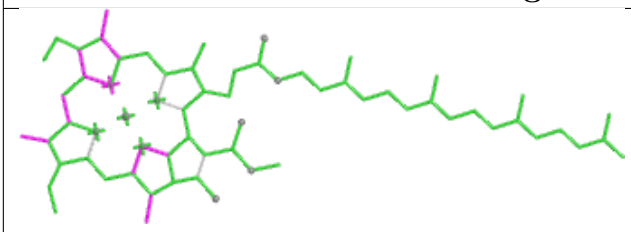


Torsions

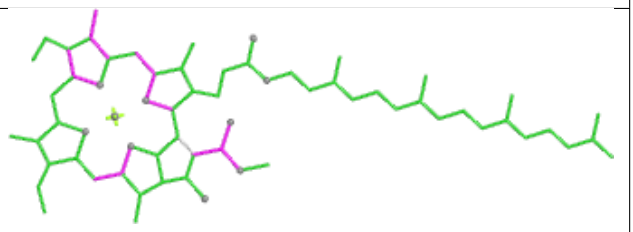


Rings

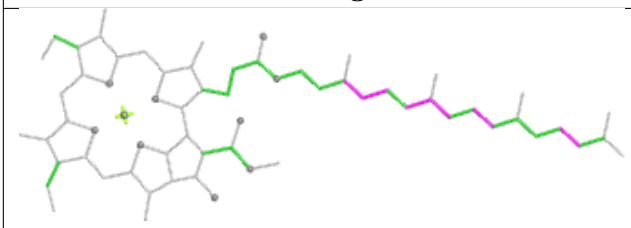
Ligand CLA A 828



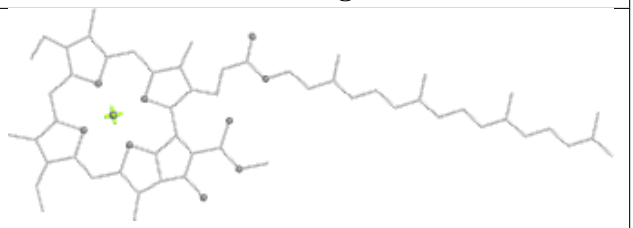
Bond lengths



Bond angles

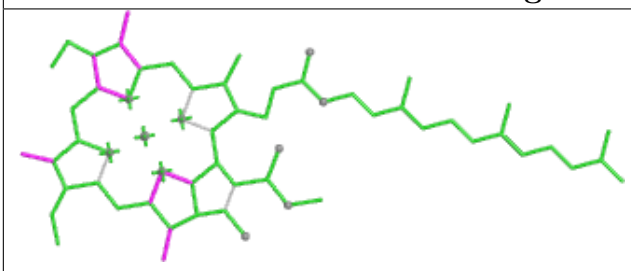


Torsions

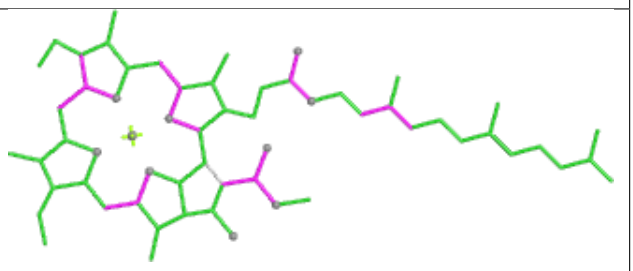


Rings

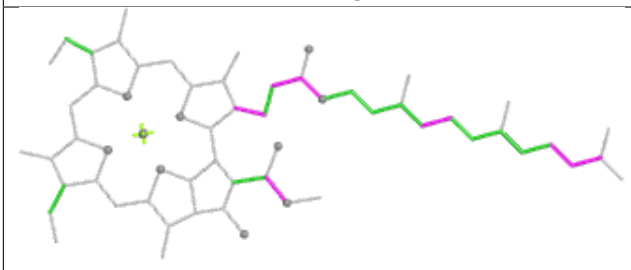
Ligand CLA B 832



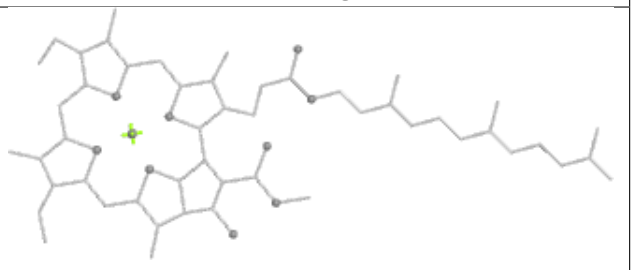
Bond lengths



Bond angles

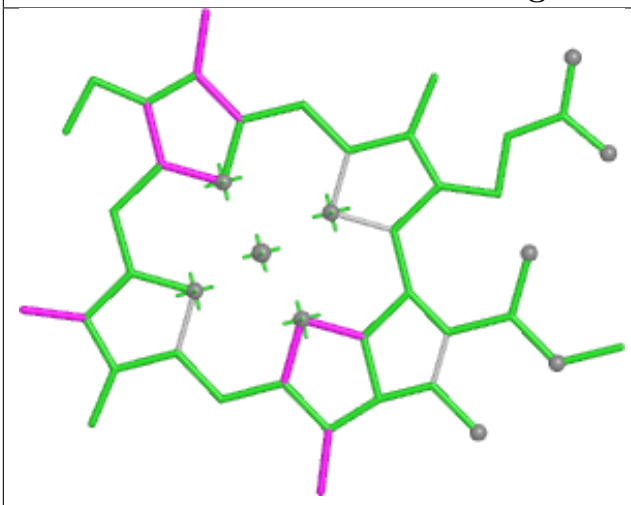


Torsions

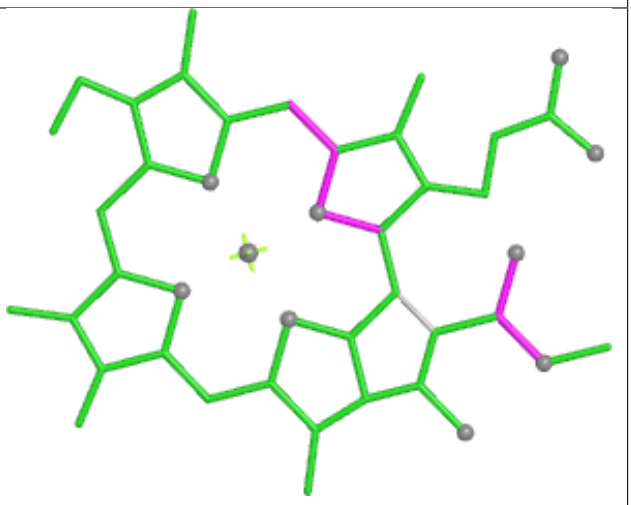


Rings

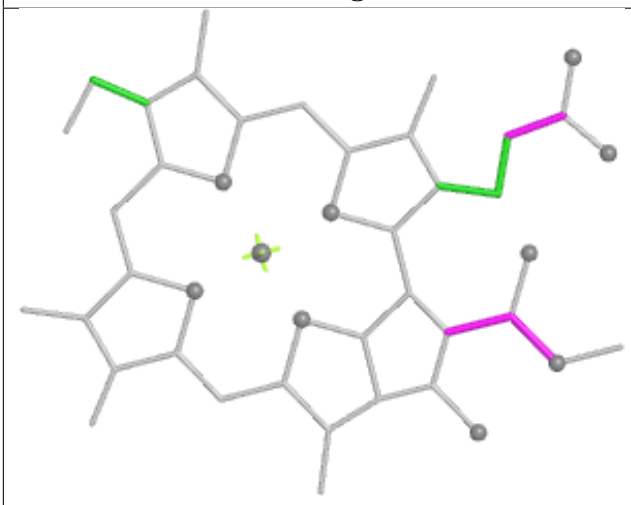
Ligand CLA 7 612



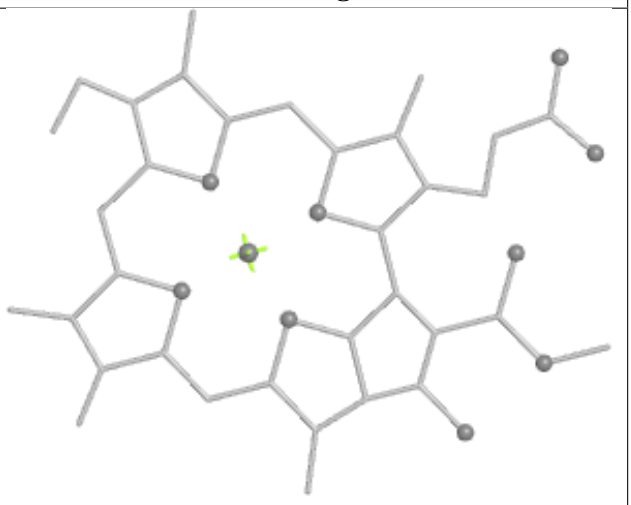
Bond lengths



Bond angles

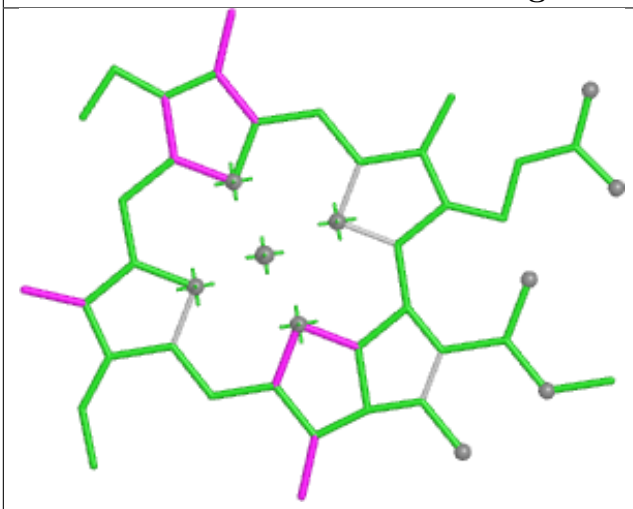


Torsions

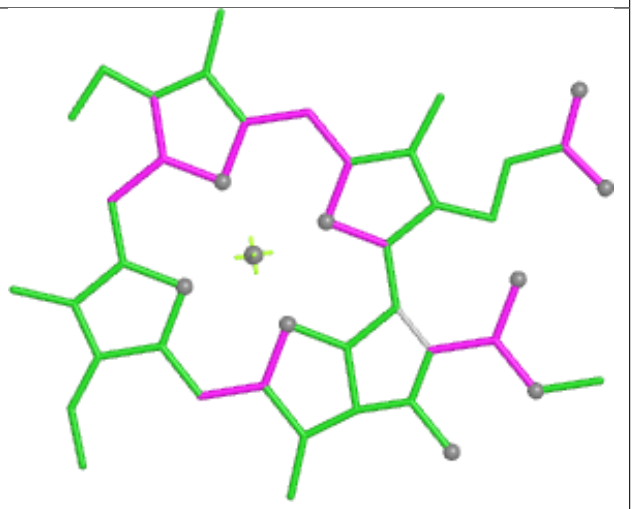


Rings

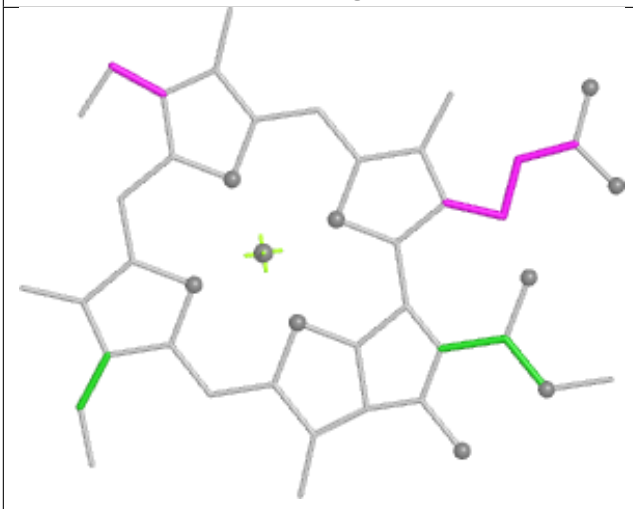
Ligand CLA 9 614



Bond lengths



Bond angles

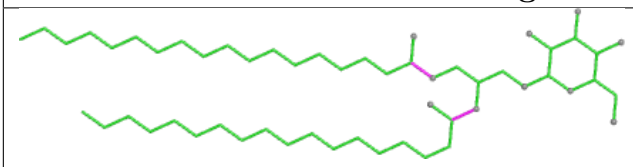


Torsions

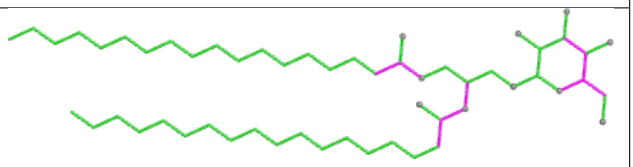


Rings

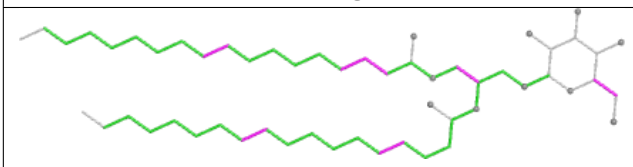
Ligand LMG H 205



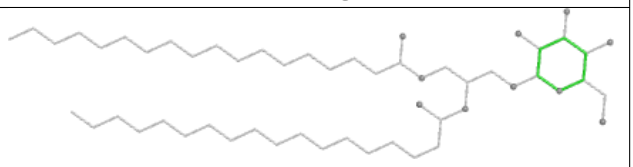
Bond lengths



Bond angles

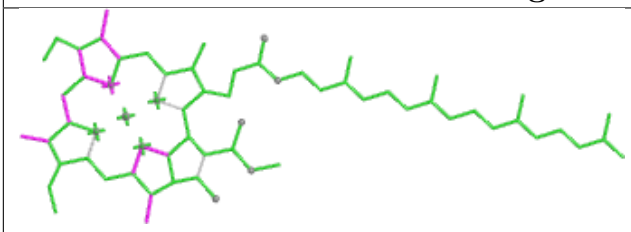


Torsions

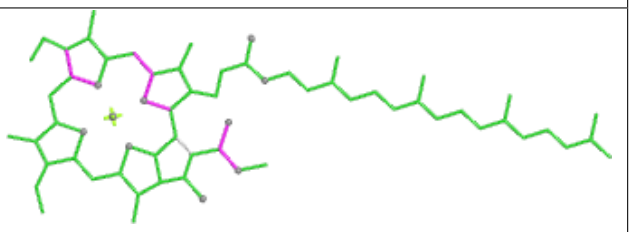


Rings

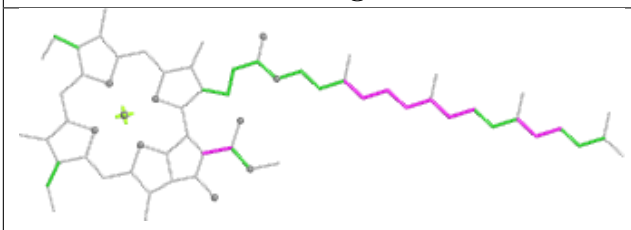
Ligand CLA 7 602



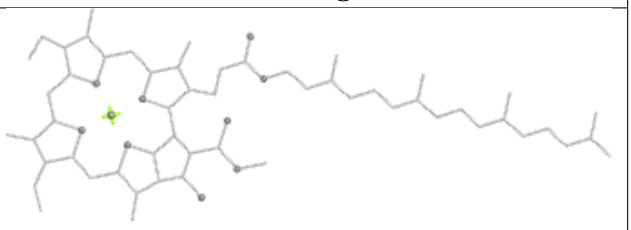
Bond lengths



Bond angles

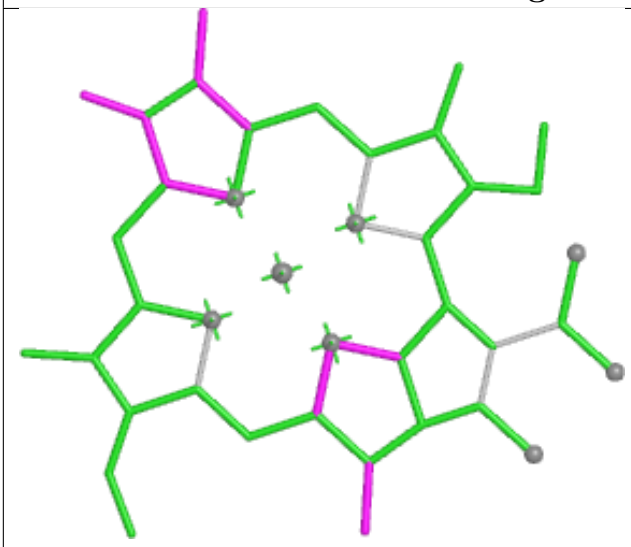


Torsions

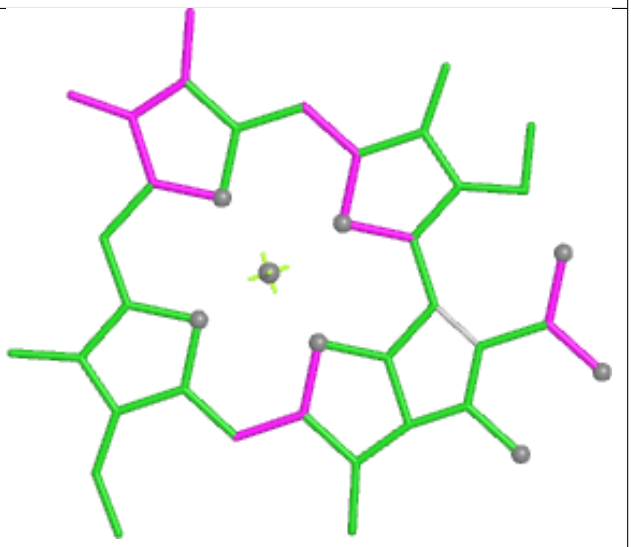


Rings

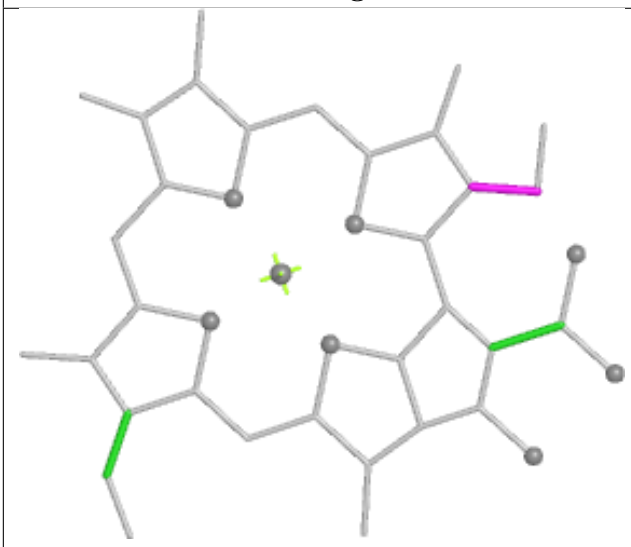
Ligand CLA 4 618



Bond lengths



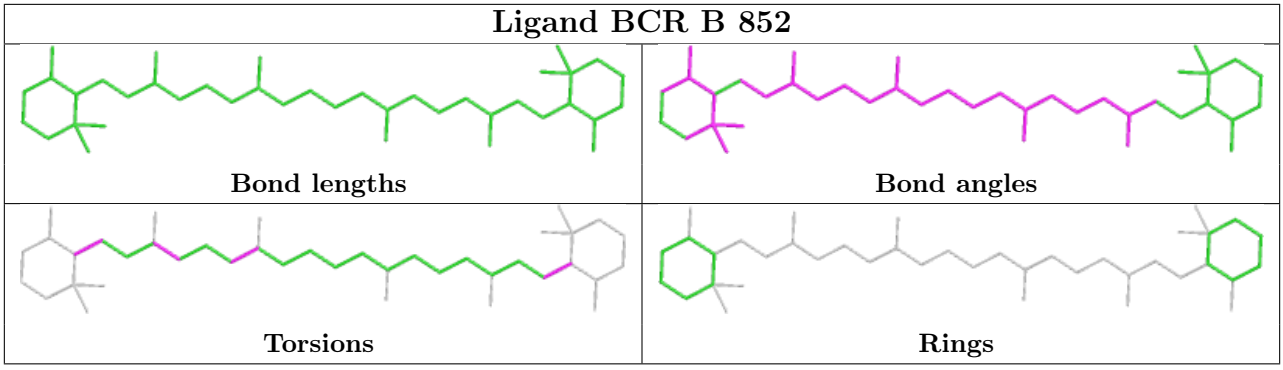
Bond angles

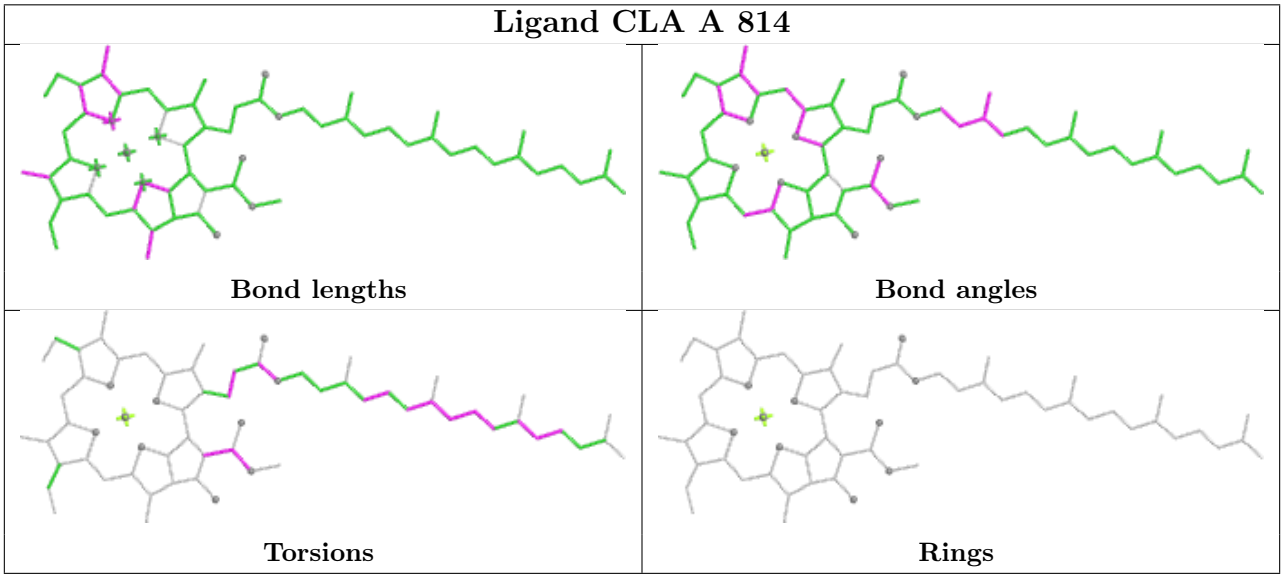


Torsions



Rings





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.

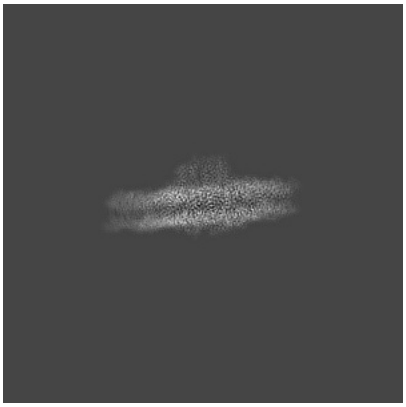
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-30925. These allow visual inspection of the internal detail of the map and identification of artifacts.

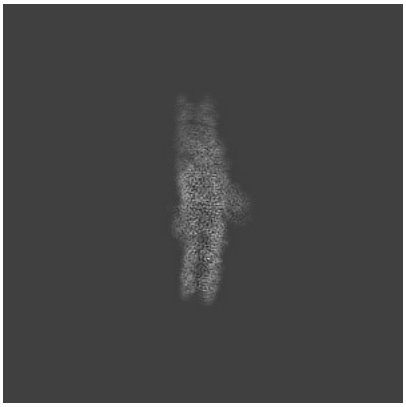
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

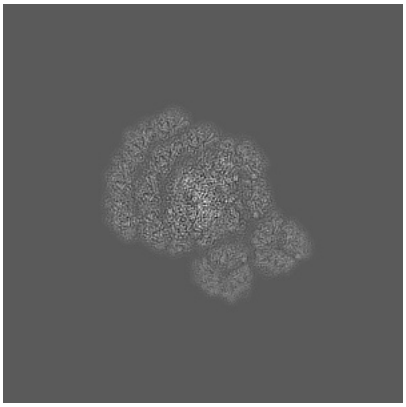
6.1.1 Primary map



X



Y

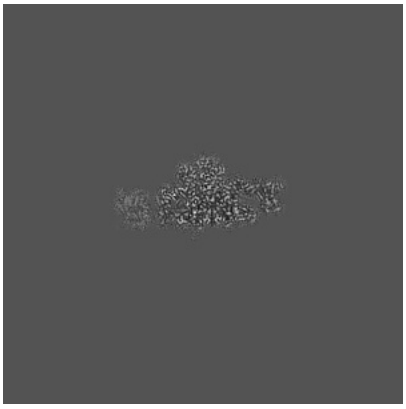


Z

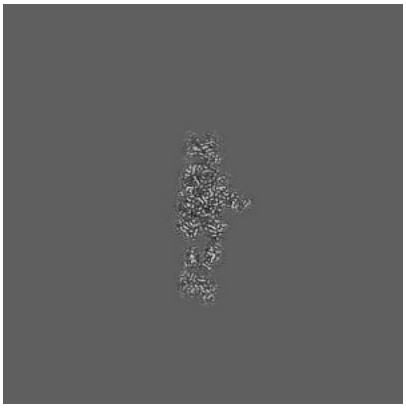
The images above show the map projected in three orthogonal directions.

6.2 Central slices

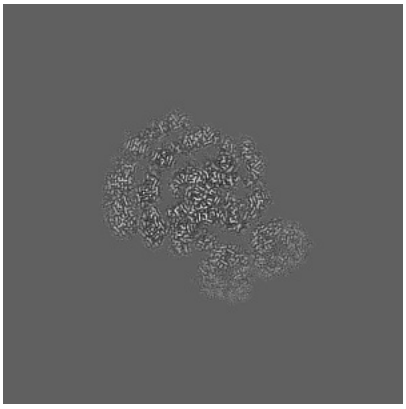
6.2.1 Primary map



X Index: 240



Y Index: 240

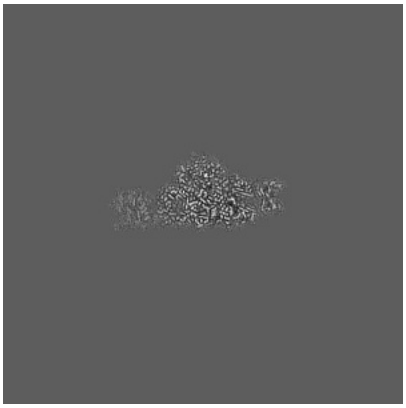


Z Index: 240

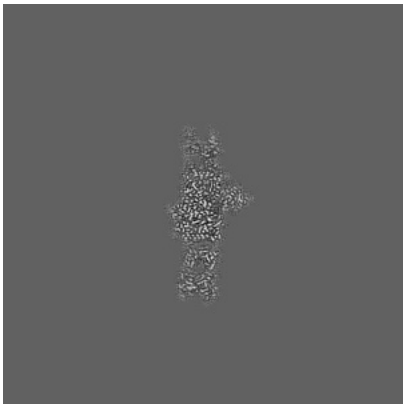
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

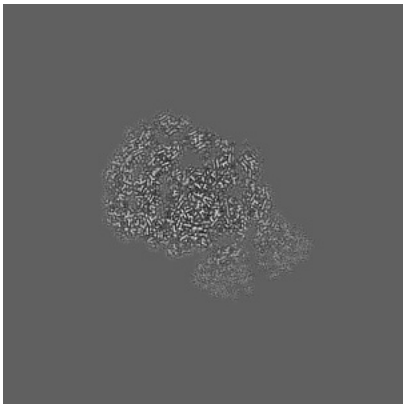
6.3.1 Primary map



X Index: 243



Y Index: 231

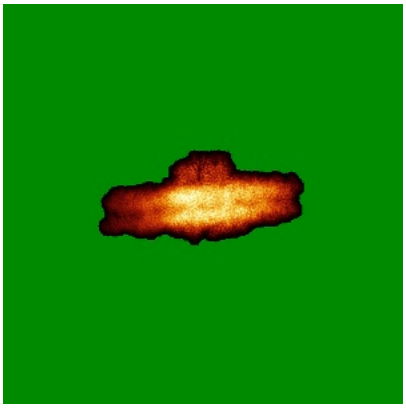


Z Index: 248

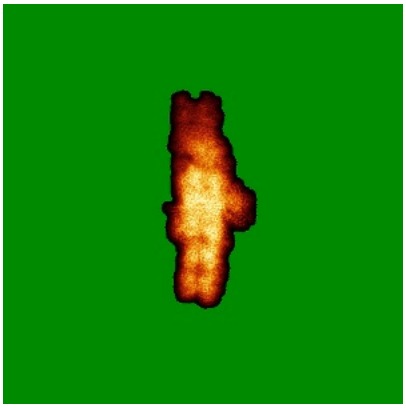
The images above show the largest variance slices of the map in three orthogonal directions.

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

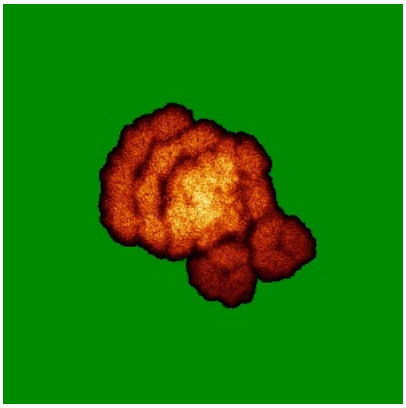
6.4.1 Primary map



X



Y

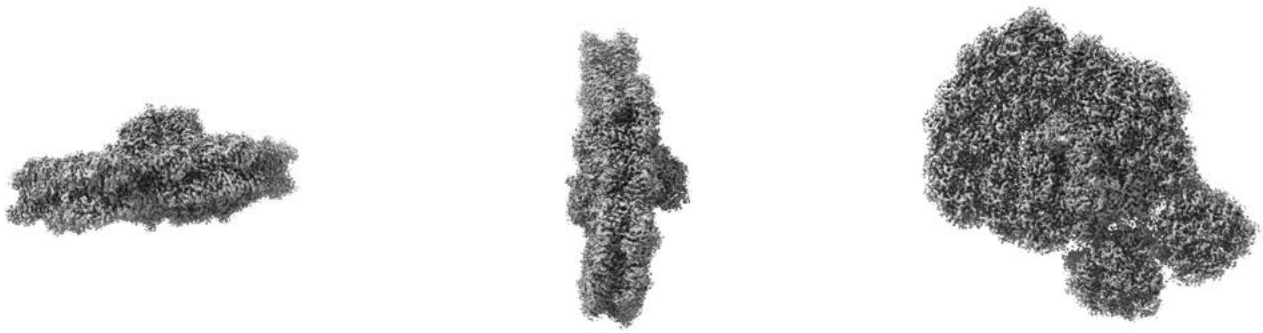


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

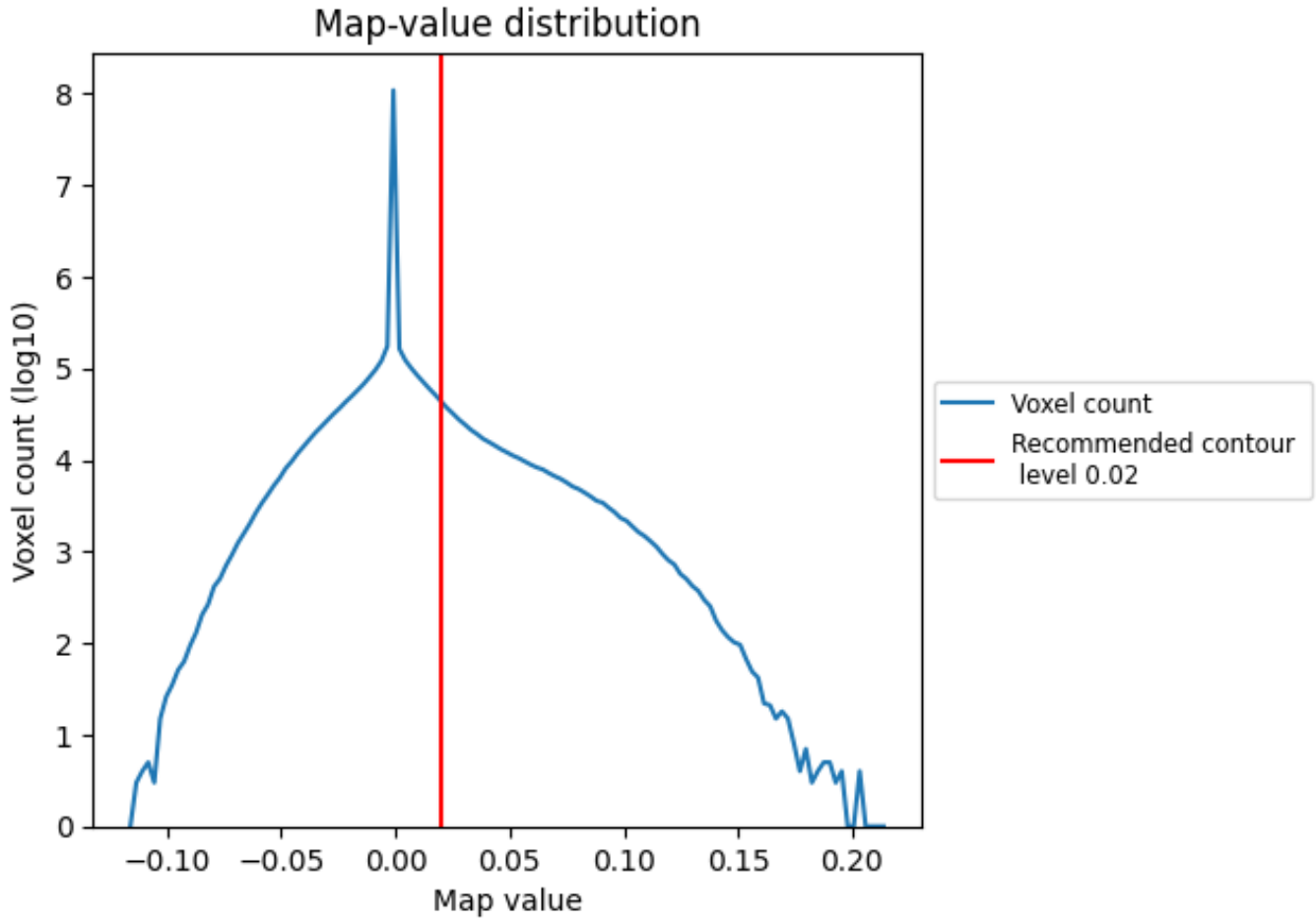
6.6 Mask visualisation (i)

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

7 Map analysis

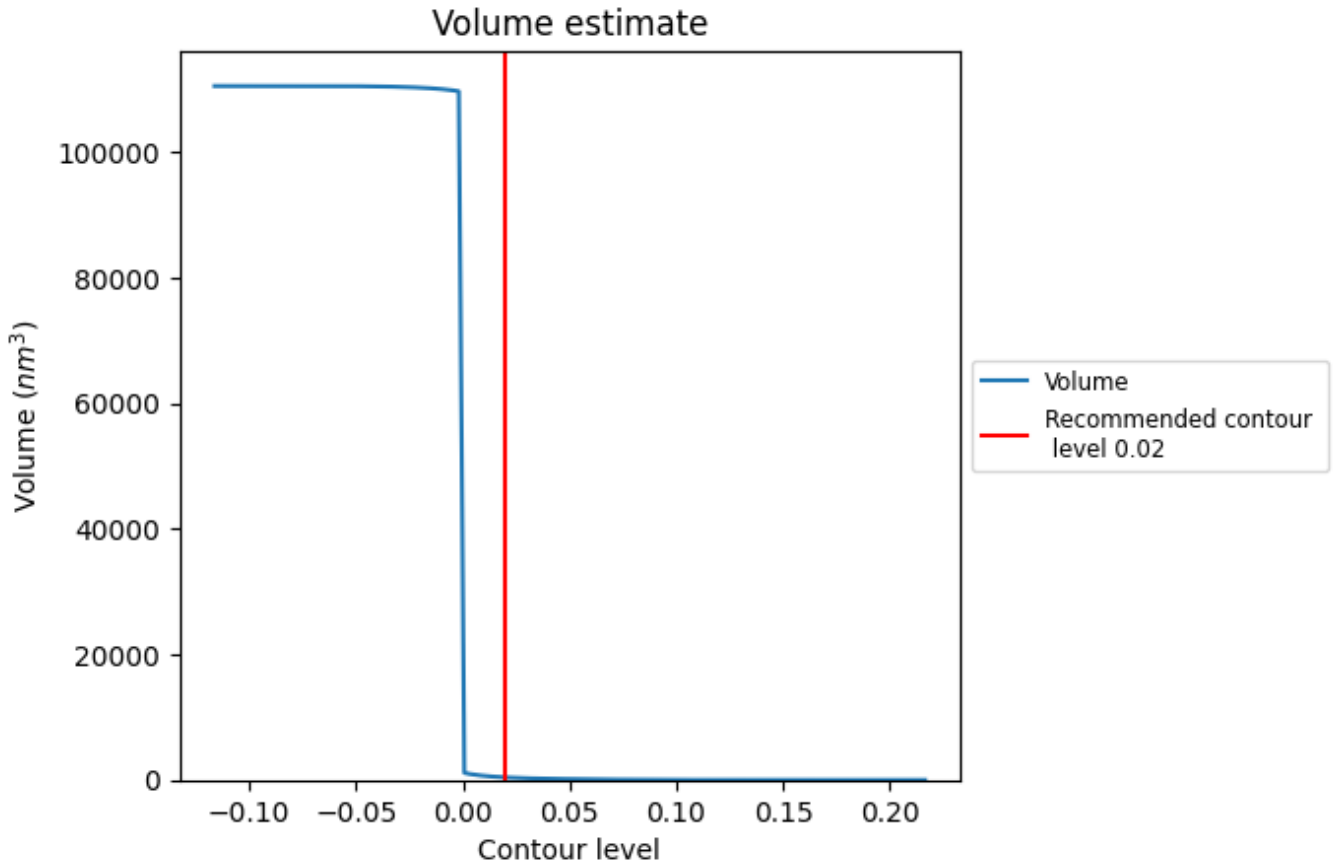
This section contains the results of statistical analysis of the map.

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.

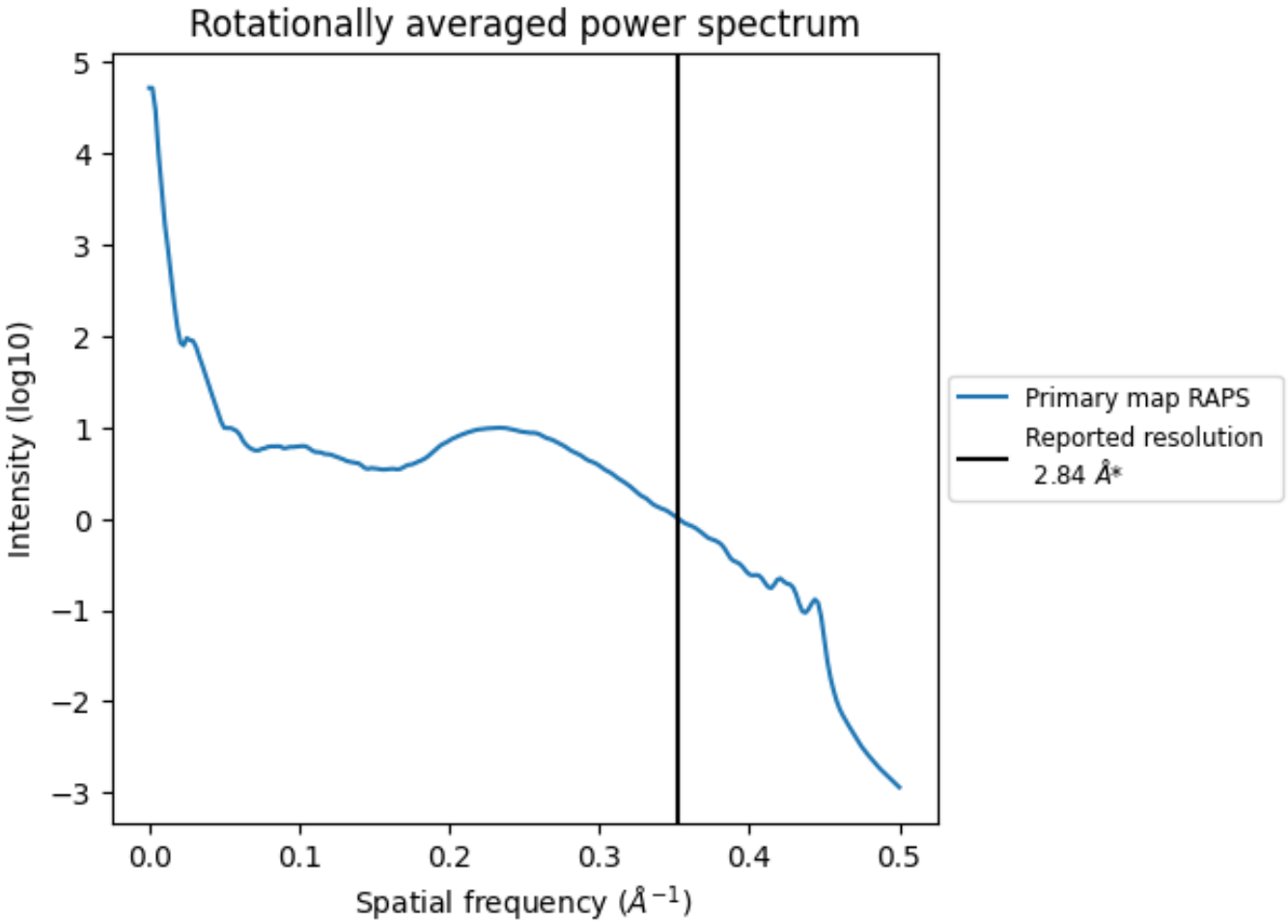
7.2 Volume estimate (i)



The volume at the recommended contour level is 408 nm^3; this corresponds to an approximate mass of 369 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 0.352 Å^{-1}

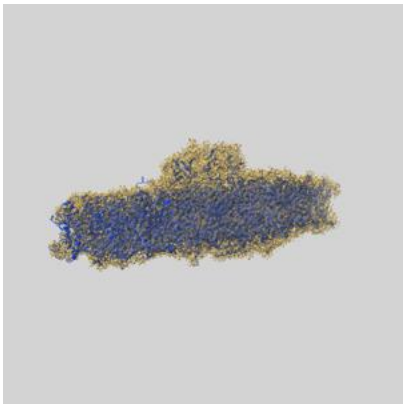
8 Fourier-Shell correlation

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

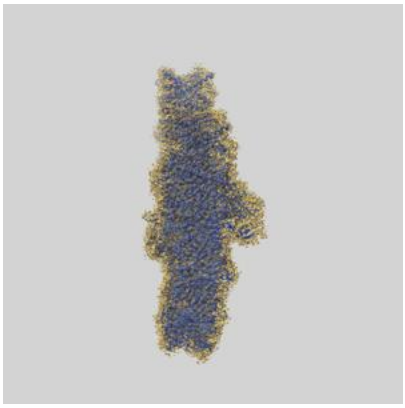
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-30925 and PDB model 7DZ7. Per-residue inclusion information can be found in section 3 on page 37.

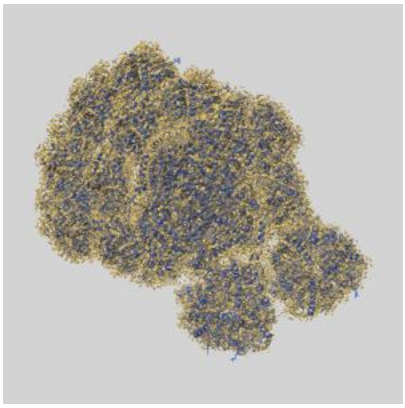
9.1 Map-model overlay



X



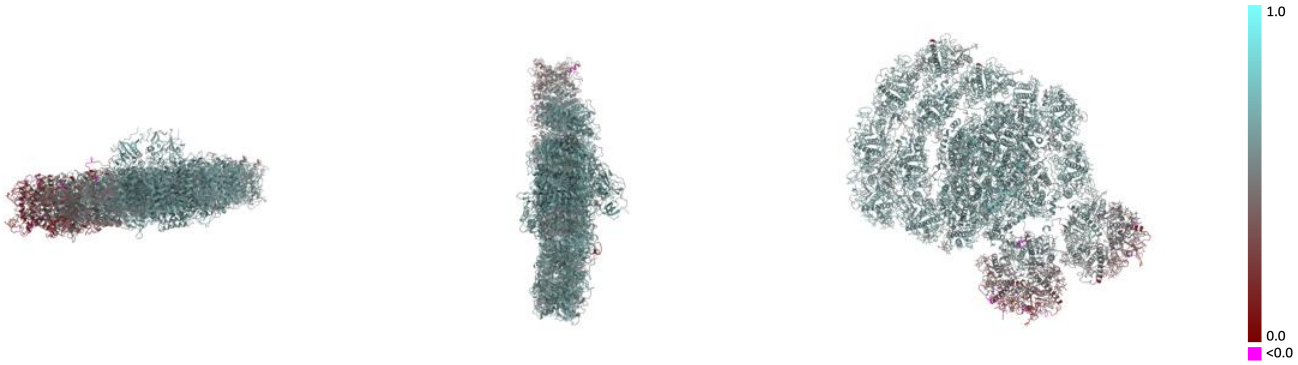
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

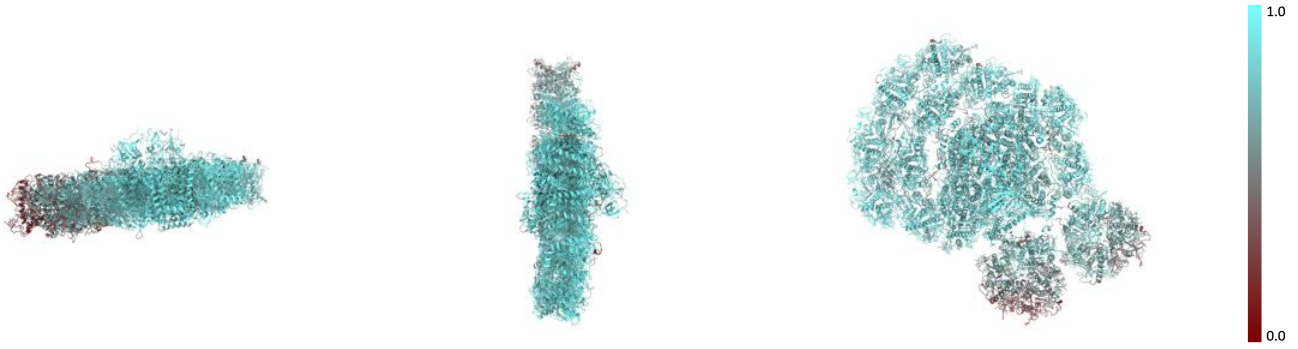
9.2 Q-score mapped to coordinate model



X Y Z

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

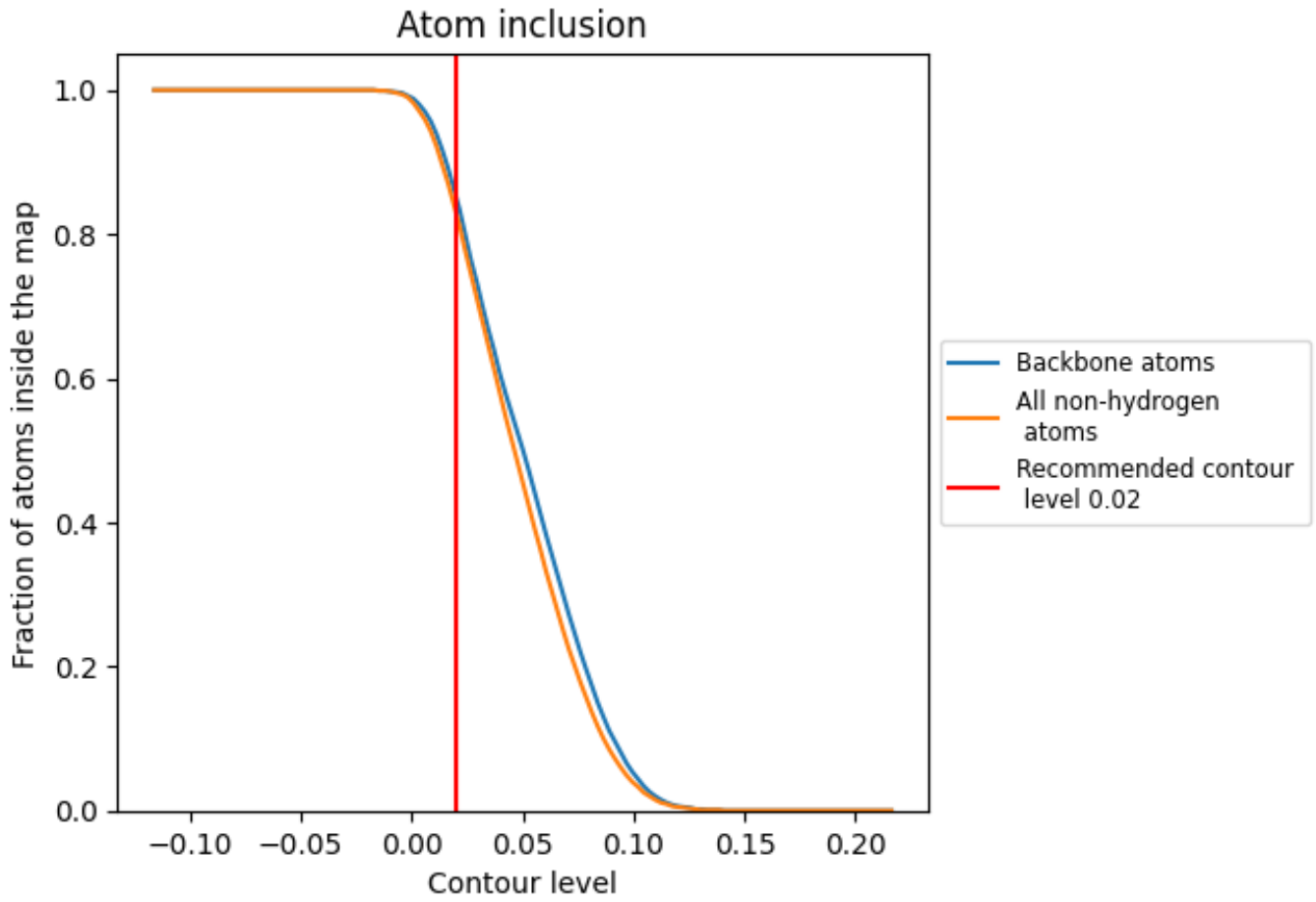
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 83% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8300	0.5670
1	0.8790	0.5940
2	0.8800	0.5990
3	0.9020	0.6140
4	0.8490	0.5800
5	0.8630	0.5940
6	0.8900	0.5990
7	0.9060	0.6200
8	0.8970	0.6110
9	0.8670	0.5870
A	0.9410	0.6400
B	0.9360	0.6400
C	0.9190	0.6060
D	0.9060	0.6130
E	0.9070	0.6130
F	0.8790	0.6120
G	0.8270	0.5770
H	0.8620	0.5940
I	0.8530	0.5910
J	0.8680	0.6090
K	0.8660	0.5900
L	0.9110	0.6180
O	0.8830	0.5910
U	0.6390	0.4250
V	0.7890	0.5490
W	0.5720	0.3910
X	0.4220	0.2990
Y	0.4770	0.3310
Z	0.7410	0.5250
a	0.8060	0.5410

