wwPDB EM Validation Summary Report

Aug 6, 2026 – 04:55 AM JST

PDB ID	:	7DZ8 / pdb_00007dz8
EMDB ID	:	EMD-30926
Title	:	State transition supercomplex PSI-LHCI-LHCII from the LhcbM1 lacking mutant of Chlamydomonas reinhardtii
Authors	:	Pan, X.W.; Li, A.J.; Liu, Z.F.; Li, M.
Deposited on	:	2021-01-23
Resolution	:	3.16 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:

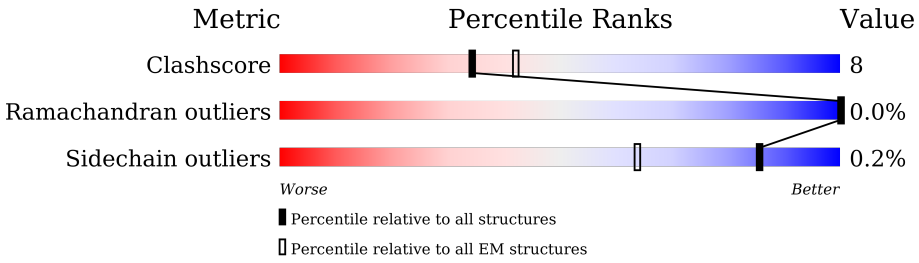
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using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

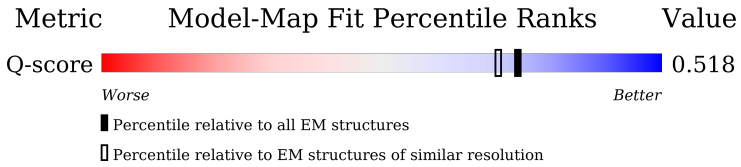
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.16 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	14474 (2.66 - 3.66)

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	84% 15% •
2	B	735	82% 18%
3	C	81	78% 19% •••
4	D	196	62% 10% • 27%

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Mol	Chain	Length	Quality of chain
5	E	97	60% 5% 35%
6	F	227	65% 7% 27%
7	G	126	65% 10% 25%
8	H	130	67% 10% 23%
9	I	106	29% 10% 60%
10	J	41	93% 7%
11	K	113	65% 11% 24%
12	L	196	72% 9% 19%
13	O	126	64% 13% 23%
14	1	228	65% 19% 15%
14	a	228	68% 16% 15%
15	2	246	77% 11% 12%
16	3	298	63% 11% 26%
17	4	264	70% 9% 20%
18	5	257	74% 14% 12%
19	6	257	81% 9% 11%
20	7	241	80% 8% 12%
21	8	243	80% 9% 11%
22	9	213	71% 15% 14%
23	W	249	71% 17% 12%
23	X	249	70% 18% 11%
24	U	257	66% 19% 15%
24	Y	257	73% 12% 15%
24	Z	257	70% 16% 14%
25	V	268	73% 16% 11%

2 Entry composition (i)

There are 37 unique types of molecules in this entry. The entry contains 69460 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	1	194	Total	C	N	O	S	0	0
			1444	941	240	260	3		
14	a	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	216	Total	C	N	O	S	0	0
			1641	1067	279	291	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	221	Total	C	N	O	S	0	0
			1680	1091	274	310	5		
23	W	220	Total	C	N	O	S	0	0
			1671	1085	273	308	5		

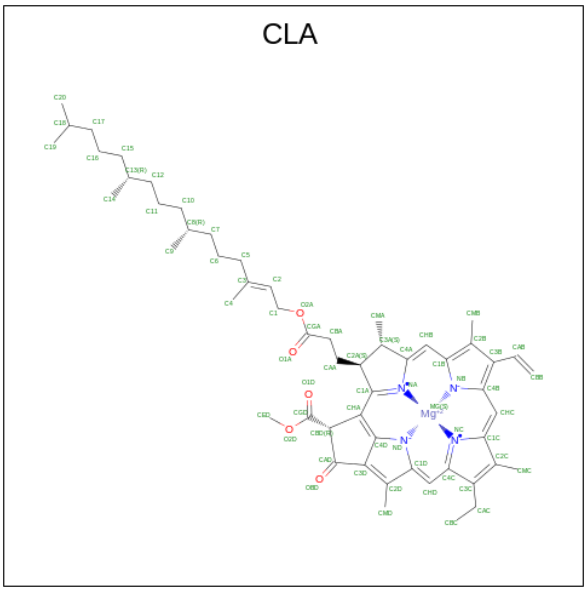
- Molecule 24 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	219	Total	C	N	O	S	0	0
			1675	1084	272	314	5		
24	Z	221	Total	C	N	O	S	0	0
			1684	1089	274	316	5		
24	U	219	Total	C	N	O	S	0	0
			1669	1080	272	312	5		

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

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

- Molecule 26 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
26	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	A	1	Total 52	C 42	Mg 1	N 4	O 5	0
26	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
26	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
26	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	A	1	Total 54	C 44	Mg 1	N 4	O 5	0
26	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

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

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

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Mol	Chain	Residues	Atoms					AltConf
26	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
26	B	1	Total	C	Mg	N	O	0
			54	45	1	4	4	
26	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			43	33	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
26	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
26	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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

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Mol	Chain	Residues	Atoms					AltConf
26	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	L	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
26	L	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
26	O	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
26	O	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
26	O	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
26	1	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
26	1	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
26	1	1	Total	C	Mg	N	O	0
			53	44	1	4	4	
26	1	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	1	1	Total	C	Mg	N	O	0
			39	32	1	4	2	
26	1	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
26	1	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
26	1	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
26	1	1	Total	C	Mg	N	O	0
			39	31	1	4	3	
26	1	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
26	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	1	1	Total	C	Mg	N	O	0
			37	29	1	4	3	
26	1	1	Total	C	Mg	N	O	0
			43	33	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
26	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
26	a	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
26	a	1	Total	C	Mg	N	O	0
			54	45	1	4	4	
26	a	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	a	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
26	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	a	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
26	a	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
26	a	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
26	a	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
26	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
26	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
26	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	2	1	Total	C	Mg	N	O	0
			63	54	1	3	5	
26	2	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
26	2	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
26	2	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
26	2	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
26	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
26	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
26	2	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
26	2	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
26	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	2	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
26	2	1	Total	C	Mg	N	O	0
			43	33	1	4	5	
26	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
26	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	3	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
26	3	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
26	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
26	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	3	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
26	3	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
26	3	1	Total	C	Mg	N	O	0
			53	44	1	4	4	
26	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
26	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
26	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
26	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
26	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	4	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
26	4	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
26	4	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
26	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	4	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
26	4	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
26	4	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
26	4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
26	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	4	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
26	4	1	Total	C	Mg	N	O	0
			43	33	1	4	5	
26	4	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
26	5	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
26	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	5	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
26	5	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
26	5	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
26	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
26	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	5	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
26	5	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
26	5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
26	5	1	Total	C	Mg	N	O	0
			64	55	1	4	4	
26	5	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
26	5	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
26	5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
26	5	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
26	5	1	Total	C	Mg	N	O	0
			43	33	1	4	5	
26	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	6	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
26	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	6	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
26	6	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
26	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	6	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
26	6	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
26	6	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
26	6	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	6	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
26	6	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
26	7	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	7	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
26	7	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
26	7	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
26	7	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
26	7	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
26	7	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
26	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	7	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
26	7	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
26	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	7	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
26	7	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
26	7	1	Total	C	Mg	N	O	0
			43	33	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
26	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	8	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	8	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
26	8	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
26	8	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
26	8	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
26	8	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
26	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	8	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	8	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
26	8	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
26	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	8	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
26	8	1	Total	C	Mg	N	O	0
			43	33	1	4	5	
26	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	9	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	9	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
26	9	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
26	9	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
26	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	9	1	Total	C	Mg	N	O	0
			61	51	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
26	9	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
26	9	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
26	9	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
26	9	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	X	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	X	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
26	X	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	X	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	X	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	X	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
26	X	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	X	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
26	Y	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
26	Y	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
26	Y	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
26	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	Y	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
26	Y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	Y	1	Total	C	Mg	N	O	0
			48	38	1	4	5	

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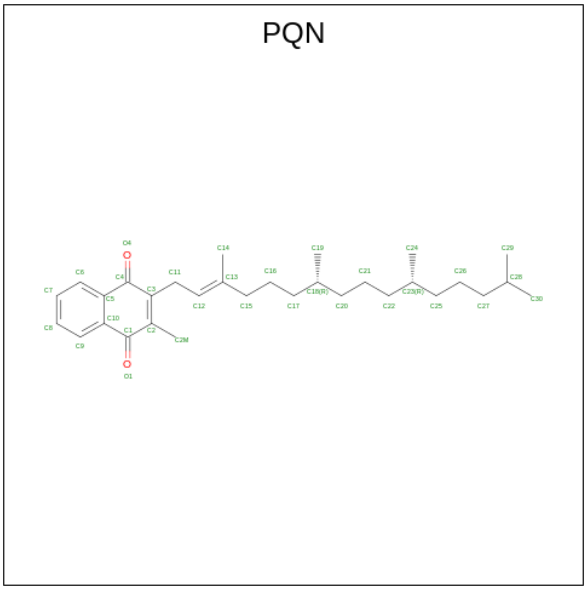
Mol	Chain	Residues	Atoms					AltConf
26	Z	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
26	Z	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
26	Z	1	Total	C	Mg	N	O	0
			49	40	1	4	4	
26	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	Z	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
26	Z	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	Z	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
26	U	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
26	U	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
26	U	1	Total	C	Mg	N	O	0
			48	39	1	4	4	
26	U	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
26	U	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
26	U	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
26	U	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
26	U	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
26	V	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	V	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	V	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
26	V	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
26	V	1	Total	C	Mg	N	O	0
			43	35	1	4	3	

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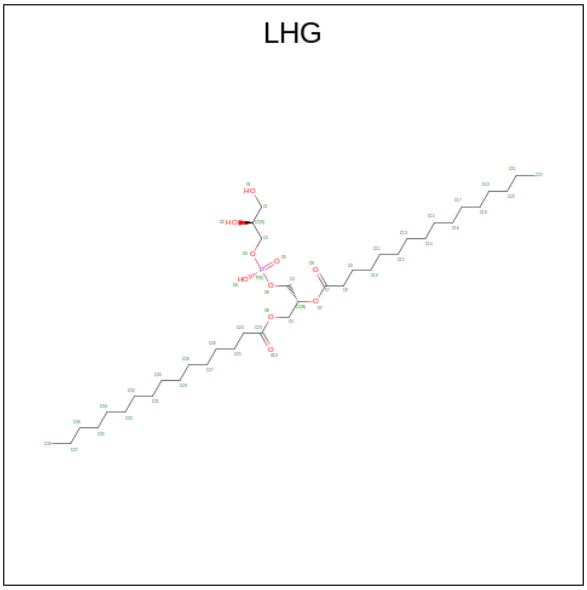
Mol	Chain	Residues	Atoms					AltConf
26	V	1	Total 45	C 35	Mg 1	N 4	O 5	0
26	V	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	V	1	Total 45	C 35	Mg 1	N 4	O 5	0
26	W	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	W	1	Total 52	C 42	Mg 1	N 4	O 5	0
26	W	1	Total 47	C 37	Mg 1	N 4	O 5	0
26	W	1	Total 55	C 45	Mg 1	N 4	O 5	0
26	W	1	Total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

- Molecule 27 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



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

- Molecule 28 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



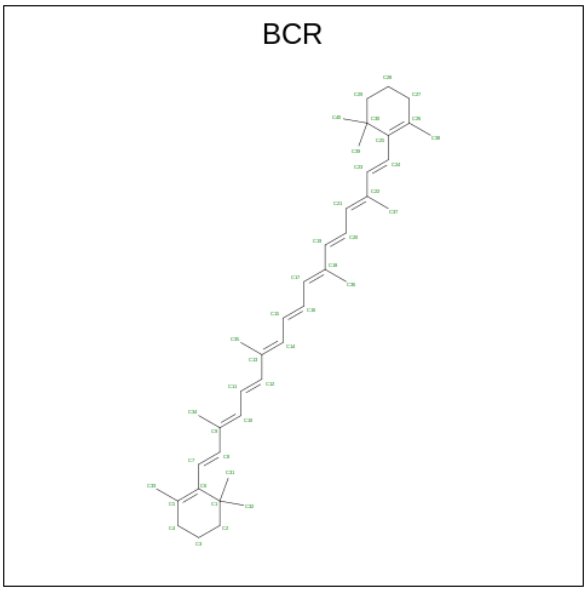
Mol	Chain	Residues	Atoms				AltConf
28	A	1	Total 49	C 38	O 10	P 1	0
28	A	1	Total 30	C 19	O 10	P 1	0
28	A	1	Total 49	C 38	O 10	P 1	0
28	B	1	Total 38	C 27	O 10	P 1	0
28	H	1	Total 49	C 38	O 10	P 1	0
28	O	1	Total 36	C 25	O 10	P 1	0
28	1	1	Total 49	C 38	O 10	P 1	0
28	a	1	Total 43	C 32	O 10	P 1	0
28	2	1	Total 36	C 25	O 10	P 1	0

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Mol	Chain	Residues	Atoms				AltConf
28	3	1	Total	C	O	P	0
			45	34	10	1	
28	3	1	Total	C	O	P	0
			49	38	10	1	
28	4	1	Total	C	O	P	0
			49	38	10	1	
28	5	1	Total	C	O	P	0
			49	38	10	1	
28	5	1	Total	C	O	P	0
			49	38	10	1	
28	6	1	Total	C	O	P	0
			48	37	10	1	
28	7	1	Total	C	O	P	0
			37	26	10	1	
28	8	1	Total	C	O	P	0
			49	38	10	1	
28	8	1	Total	C	O	P	0
			40	29	10	1	
28	9	1	Total	C	O	P	0
			30	19	10	1	
28	9	1	Total	C	O	P	0
			49	38	10	1	
28	9	1	Total	C	O	P	0
			49	38	10	1	
28	X	1	Total	C	O	P	0
			49	38	10	1	
28	Y	1	Total	C	O	P	0
			49	38	10	1	
28	Z	1	Total	C	O	P	0
			49	38	10	1	
28	U	1	Total	C	O	P	0
			49	38	10	1	
28	V	1	Total	C	O	P	0
			36	25	10	1	
28	W	1	Total	C	O	P	0
			34	23	10	1	

- Molecule 29 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



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

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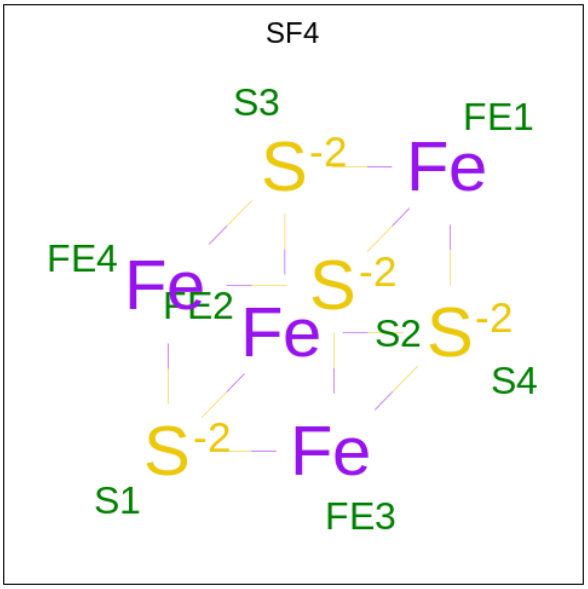
Mol	Chain	Residues	Atoms	AltConf
29	B	1	Total C 40 40	0
29	B	1	Total C 40 40	0
29	F	1	Total C 40 40	0
29	G	1	Total C 40 40	0
29	J	1	Total C 40 40	0
29	K	1	Total C 40 40	0
29	K	1	Total C 40 40	0
29	L	1	Total C 40 40	0
29	L	1	Total C 40 40	0
29	L	1	Total C 40 40	0
29	L	1	Total C 40 40	0
29	O	1	Total C 40 40	0
29	O	1	Total C 40 40	0
29	1	1	Total C 40 40	0
29	a	1	Total C 40 40	0
29	2	1	Total C 40 40	0
29	3	1	Total C 40 40	0
29	3	1	Total C 40 40	0
29	3	1	Total C 40 40	0
29	4	1	Total C 40 40	0
29	5	1	Total C 40 40	0

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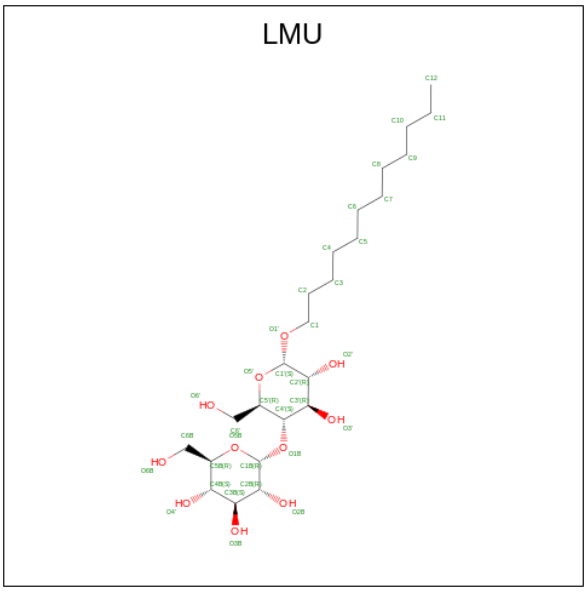
Mol	Chain	Residues	Atoms	AltConf
29	6	1	Total C 40 40	0
29	7	1	Total C 40 40	0
29	7	1	Total C 40 40	0
29	8	1	Total C 40 40	0
29	9	1	Total C 40 40	0

- Molecule 30 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



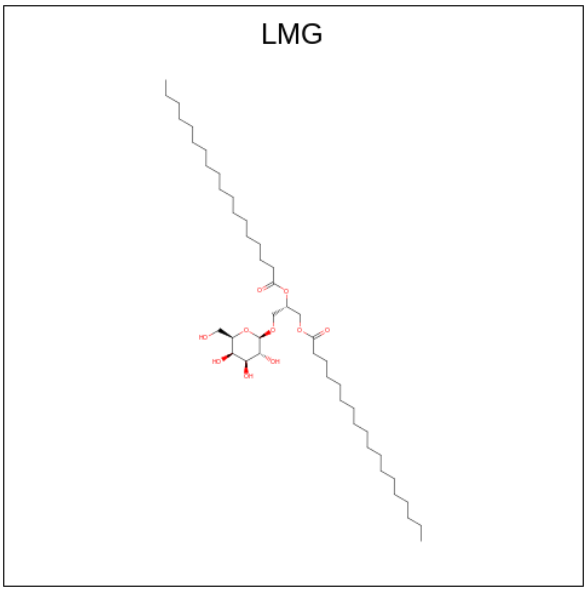
Mol	Chain	Residues	Atoms	AltConf
30	A	1	Total Fe S 8 4 4	0
30	C	1	Total Fe S 8 4 4	0
30	C	1	Total Fe S 8 4 4	0

- Molecule 31 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$).



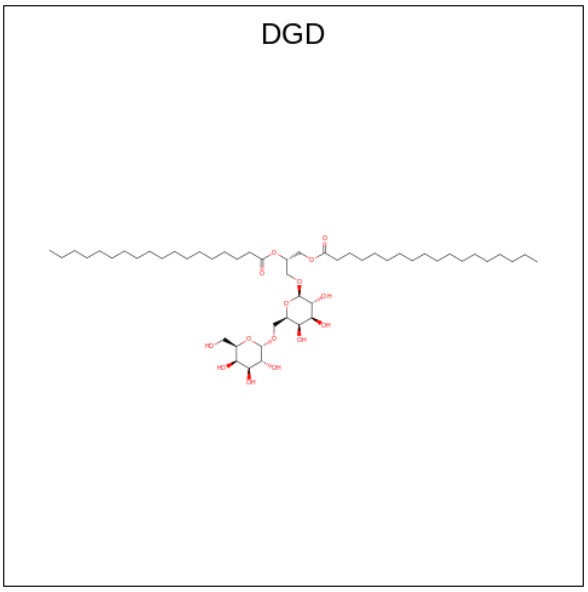
Mol	Chain	Residues	Atoms	AltConf
31	A	1	Total C O 35 24 11	0
31	A	1	Total C O 34 24 10	0
31	K	1	Total C O 35 24 11	0
31	1	1	Total C O 35 24 11	0
31	5	1	Total C O 33 22 11	0
31	5	1	Total C O 32 21 11	0
31	8	1	Total C O 35 24 11	0

- Molecule 32 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



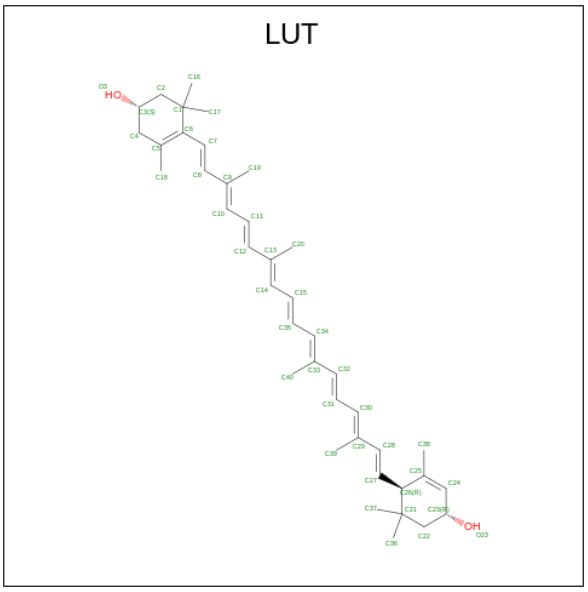
Mol	Chain	Residues	Atoms	AltConf
32	A	1	Total C O 40 30 10	0
32	H	1	Total C O 55 45 10	0
32	J	1	Total C O 42 32 10	0
32	J	1	Total C O 40 30 10	0
32	L	1	Total C O 37 27 10	0
32	4	1	Total C O 40 30 10	0
32	4	1	Total C O 40 30 10	0
32	5	1	Total C O 40 30 10	0
32	8	1	Total C O 46 36 10	0
32	9	1	Total C O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

- Molecule 33 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



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

- Molecule 34 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3 ,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$).



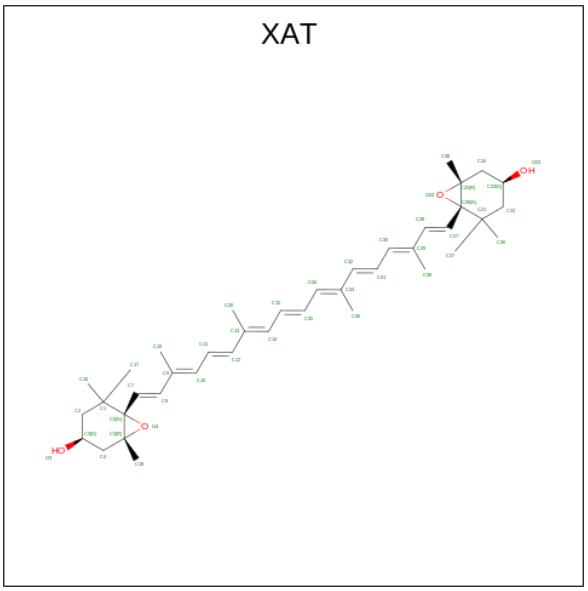
Mol	Chain	Residues	Atoms			AltConf
34	1	1	Total	C	O	0
			42	40	2	
34	a	1	Total	C	O	0
			42	40	2	

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Mol	Chain	Residues	Atoms	AltConf
34	2	1	Total C O 42 40 2	0
34	3	1	Total C O 42 40 2	0
34	4	1	Total C O 42 40 2	0
34	5	1	Total C O 42 40 2	0
34	6	1	Total C O 42 40 2	0
34	7	1	Total C O 42 40 2	0
34	8	1	Total C O 42 40 2	0
34	9	1	Total C O 42 40 2	0
34	X	1	Total C O 42 40 2	0
34	X	1	Total C O 42 40 2	0
34	Y	1	Total C O 42 40 2	0
34	Y	1	Total C O 42 40 2	0
34	Z	1	Total C O 42 40 2	0
34	Z	1	Total C O 42 40 2	0
34	U	1	Total C O 42 40 2	0
34	U	1	Total C O 42 40 2	0
34	V	1	Total C O 42 40 2	0
34	V	1	Total C O 42 40 2	0
34	W	1	Total C O 42 40 2	0
34	W	1	Total C O 42 40 2	0

- Molecule 35 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: $C_{40}H_{56}O_4$).



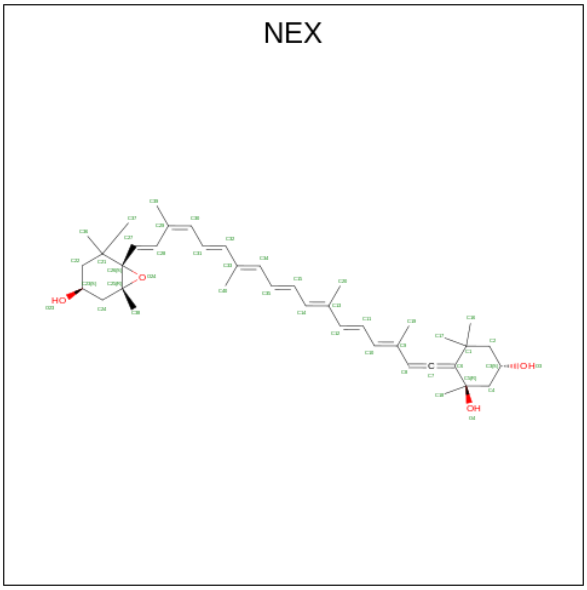
Mol	Chain	Residues	Atoms	AltConf
35	1	1	Total C O 44 40 4	0
35	a	1	Total C O 44 40 4	0
35	2	1	Total C O 44 40 4	0
35	3	1	Total C O 44 40 4	0
35	4	1	Total C O 44 40 4	0
35	5	1	Total C O 44 40 4	0
35	6	1	Total C O 44 40 4	0
35	7	1	Total C O 44 40 4	0
35	8	1	Total C O 44 40 4	0
35	9	1	Total C O 44 40 4	0
35	X	1	Total C O 44 40 4	0
35	Y	1	Total C O 44 40 4	0
35	Z	1	Total C O 44 40 4	0
35	U	1	Total C O 44 40 4	0

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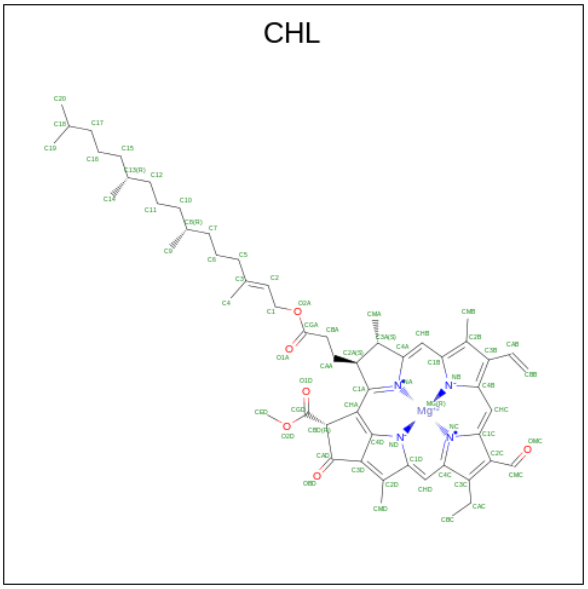
Mol	Chain	Residues	Atoms	AltConf
35	V	1	Total C O 44 40 4	0
35	W	1	Total C O 44 40 4	0

- Molecule 36 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
36	5	1	Total C O 44 40 4	0
36	6	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
36	V	1	Total C O 44 40 4	0
36	W	1	Total C O 44 40 4	0

- Molecule 37 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
37	X	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
37	X	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
37	X	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
37	X	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
37	X	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	X	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
37	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
37	Y	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
37	Y	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
37	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
37	Y	1	Total	C	Mg	N	O	0
			49	38	1	4	6	
37	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
37	Z	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
37	Z	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
37	Z	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
37	Z	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
37	Z	1	Total	C	Mg	N	O	0
			49	38	1	4	6	
37	Z	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
37	U	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
37	U	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
37	U	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
37	U	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
37	U	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
37	U	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
37	V	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
37	V	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
37	V	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
37	V	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
37	V	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
37	V	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
37	W	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
37	W	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
37	W	1	Total	C	Mg	N	O	0
			46	35	1	4	6	

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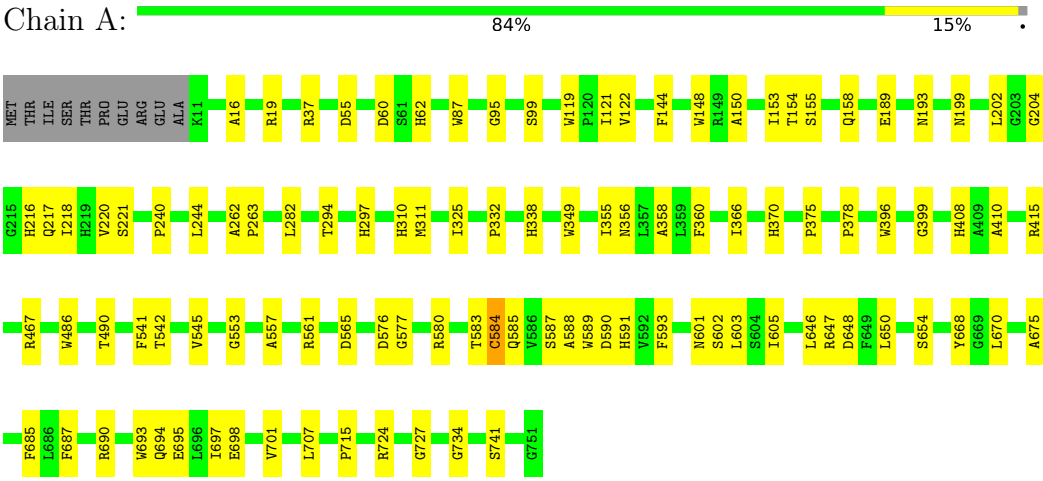
Mol	Chain	Residues	Atoms					AltConf
37	W	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
37	W	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
37	W	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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.

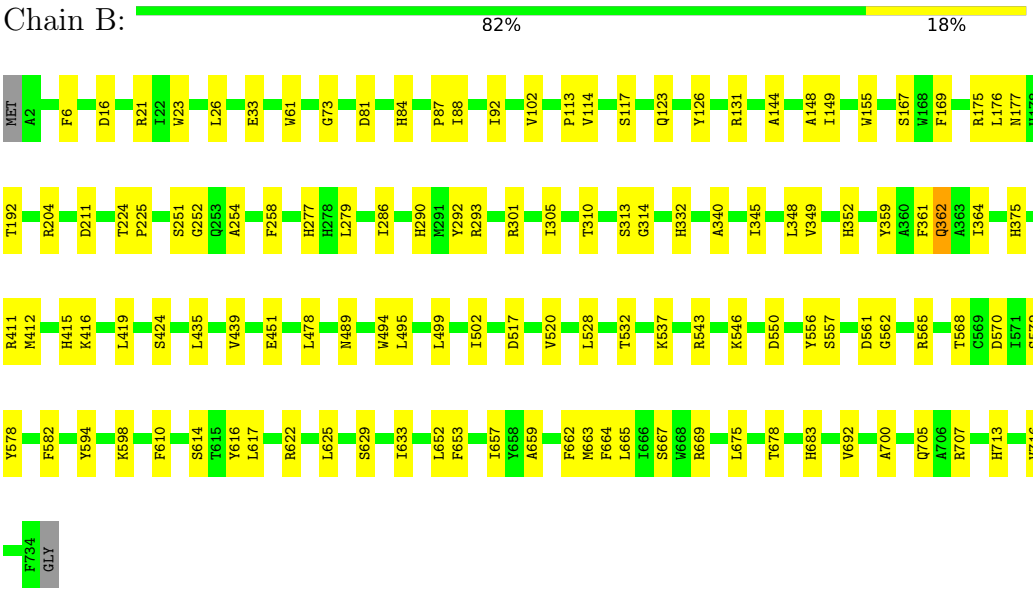
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain A:



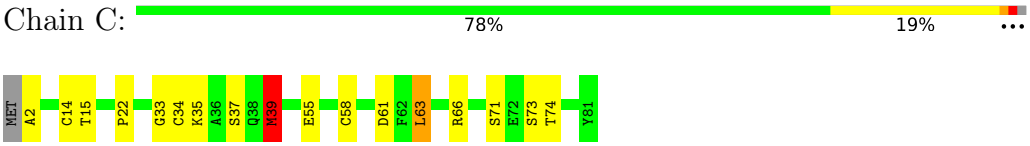
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain B:



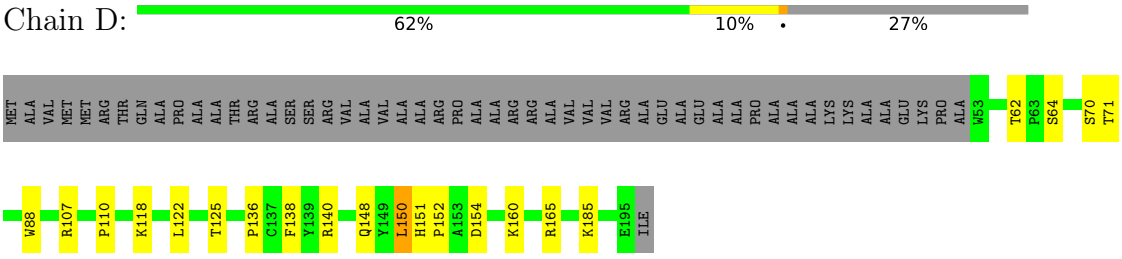
• Molecule 3: Photosystem I iron-sulfur center

Chain C:



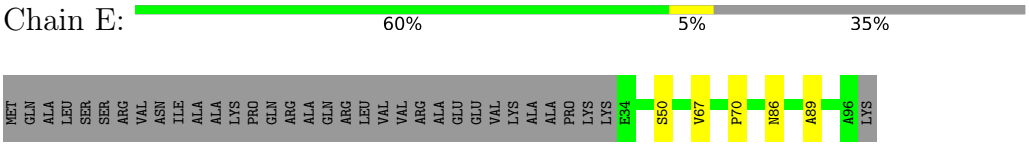
• Molecule 4: Photosystem I reaction center subunit II, chloroplastic

Chain D:



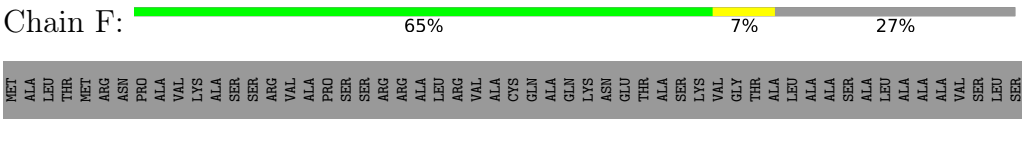
• Molecule 5: Photosystem I reaction center subunit IV, chloroplastic

Chain E:



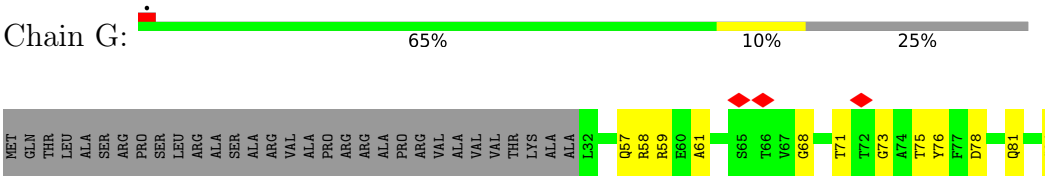
• Molecule 6: Photosystem I reaction center subunit III, chloroplastic

Chain F:



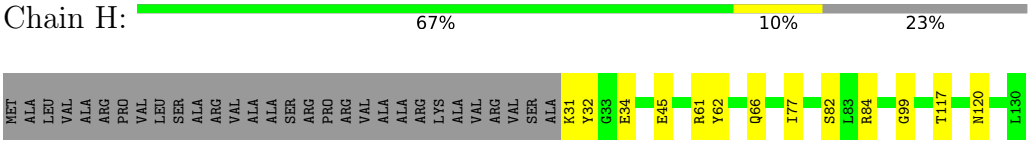
• Molecule 7: Photosystem I reaction center subunit V, chloroplastic

Chain G:



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

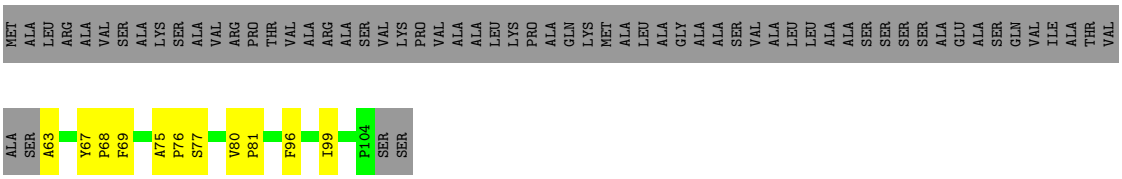
Chain H:



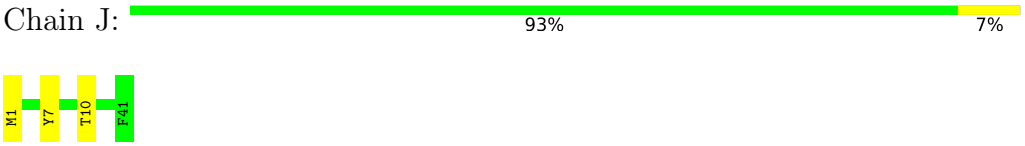
• Molecule 9: Photosystem I reaction center subunit VIII

Chain I:

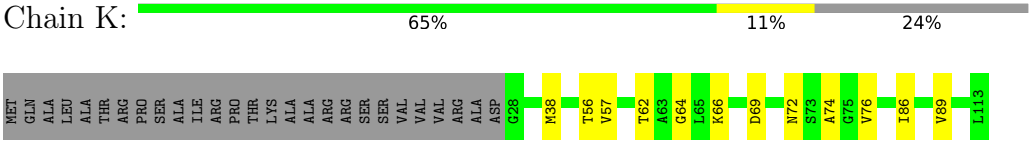




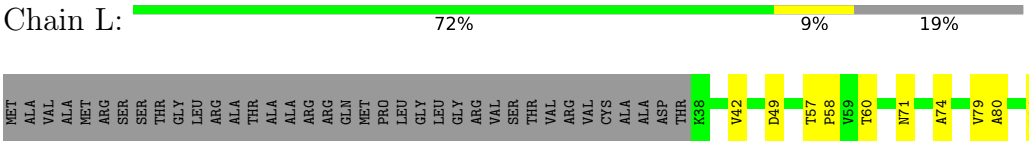
• Molecule 10: Photosystem I reaction center subunit IX



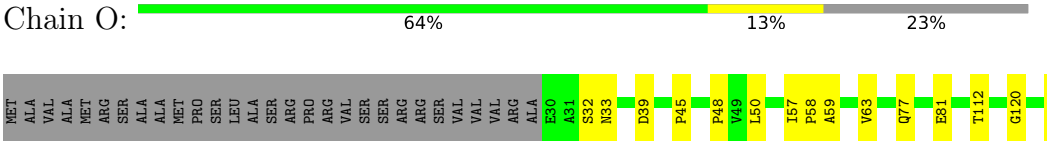
• Molecule 11: Photosystem I reaction center subunit psaK, chloroplastic



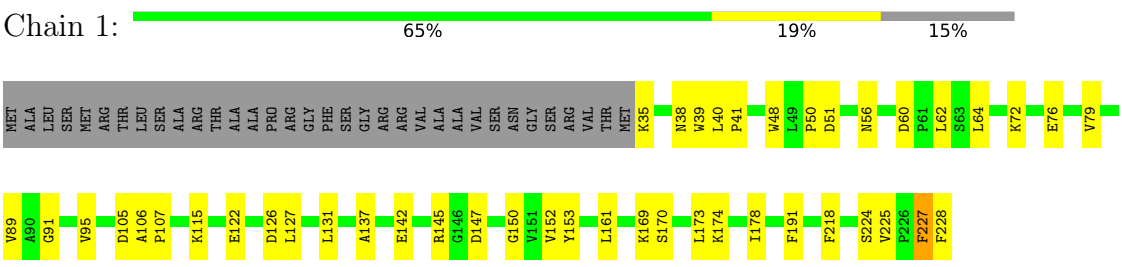
• Molecule 12: PSI subunit V



• Molecule 13: Photosystem I subunit O

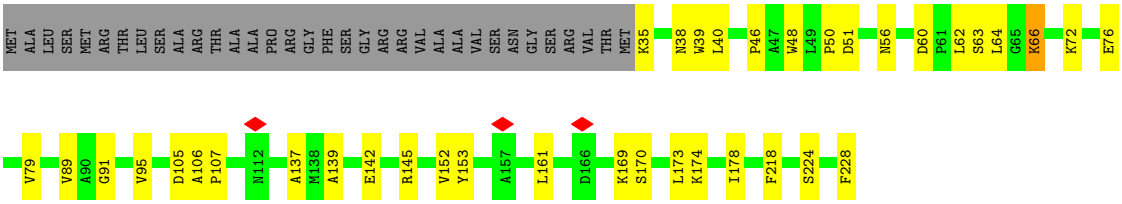


• Molecule 14: Chlorophyll a-b binding protein, chloroplastic

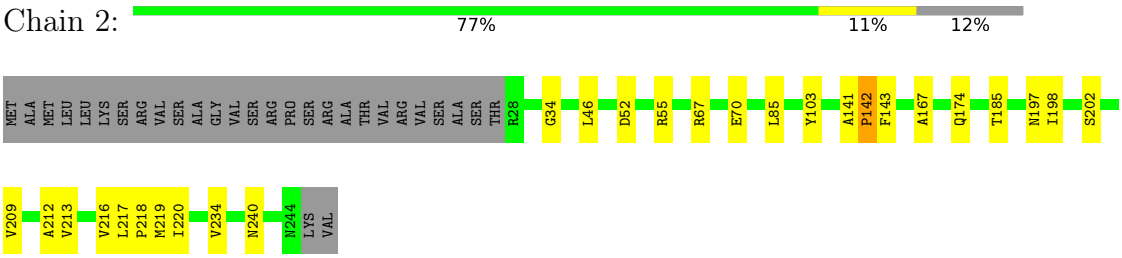


• Molecule 14: Chlorophyll a-b binding protein, chloroplastic

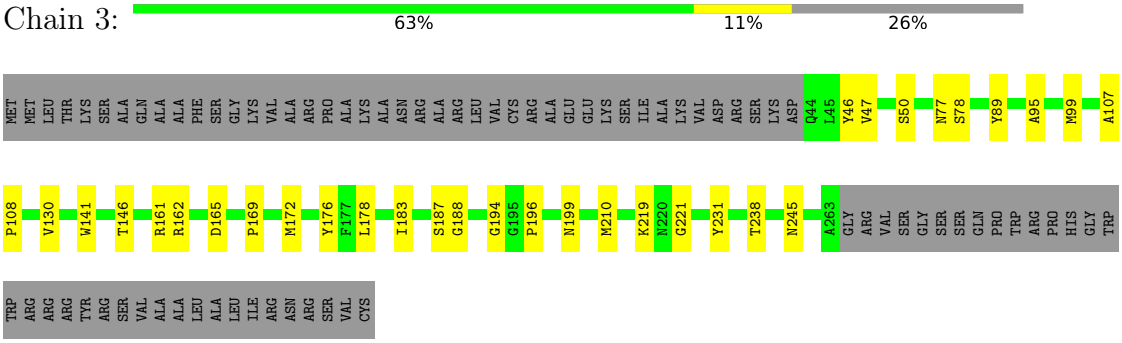




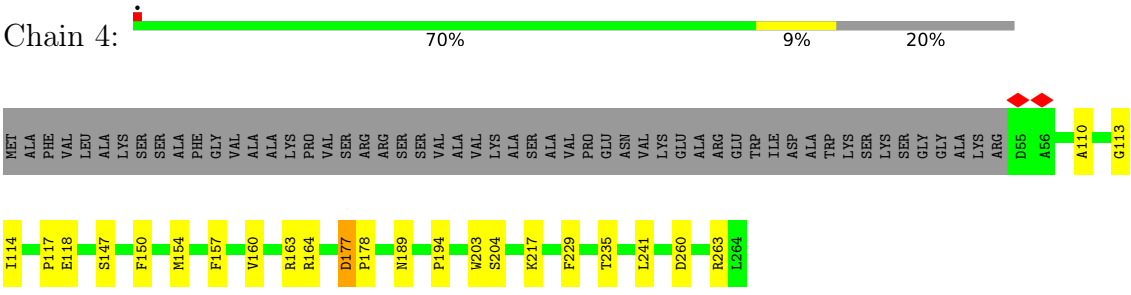
• Molecule 15: Chlorophyll a-b binding protein, chloroplastic



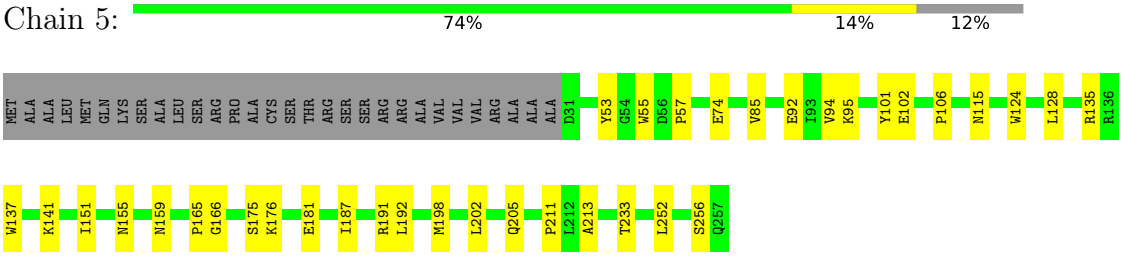
• Molecule 16: Chlorophyll a-b binding protein, chloroplastic



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

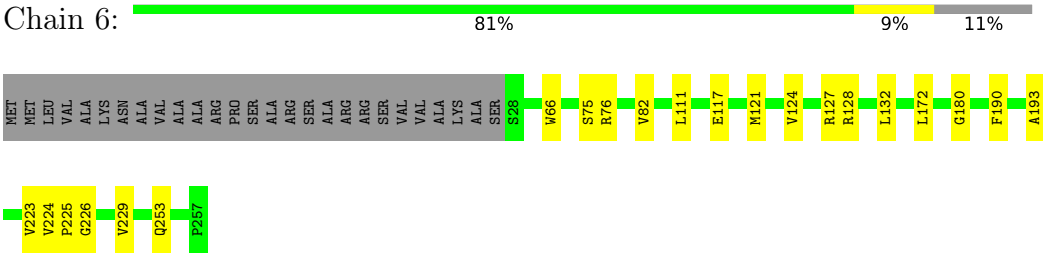


• Molecule 18: Chlorophyll a-b binding protein, chloroplastic



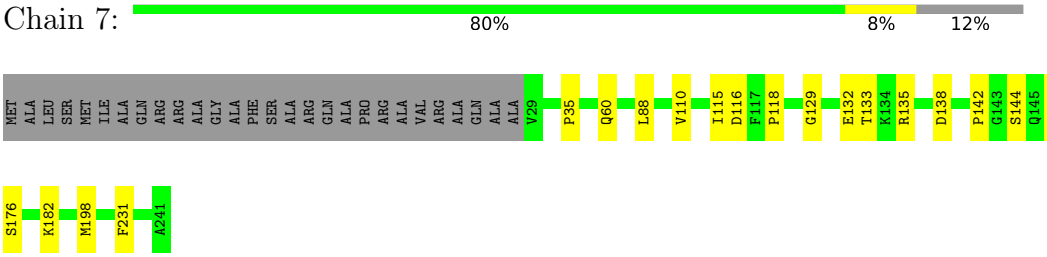
• Molecule 19: Chlorophyll a-b binding protein, chloroplastic

Chain 6:



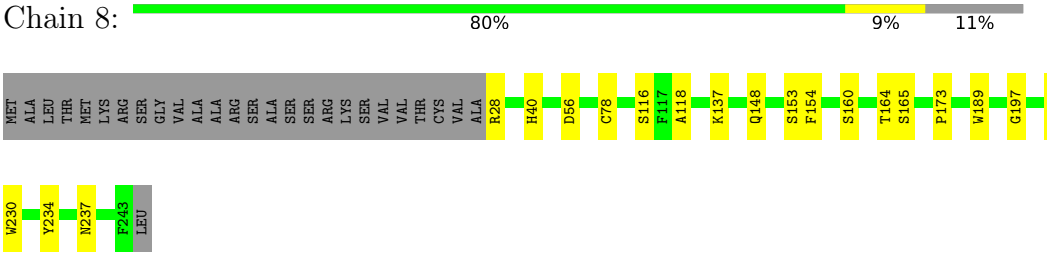
• Molecule 20: Chlorophyll a-b binding protein, chloroplastic

Chain 7:



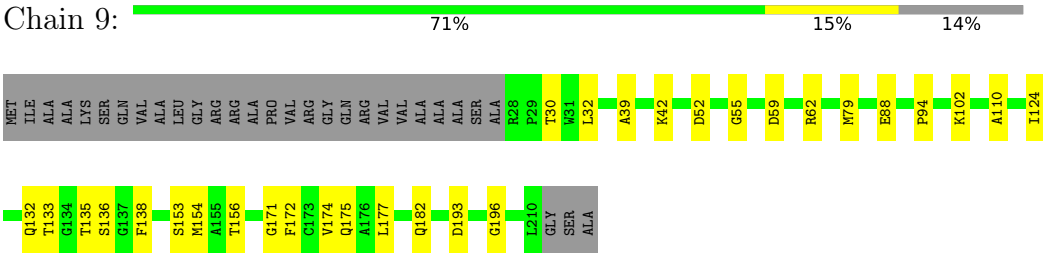
• Molecule 21: Chlorophyll a-b binding protein, chloroplastic

Chain 8:



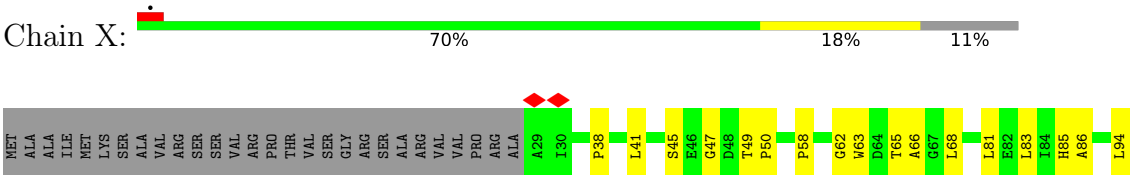
• Molecule 22: Chlorophyll a-b binding protein, chloroplastic

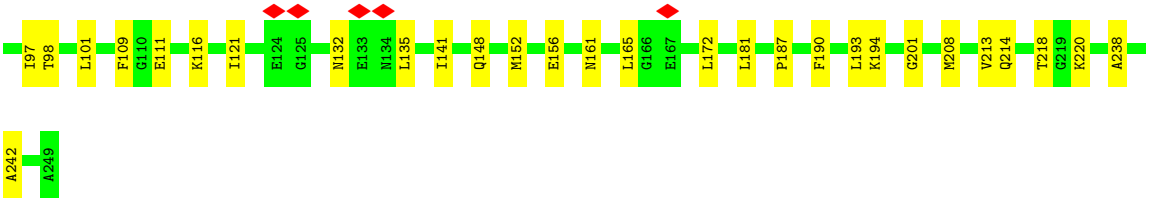
Chain 9:



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

Chain X:

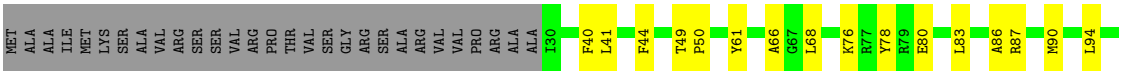


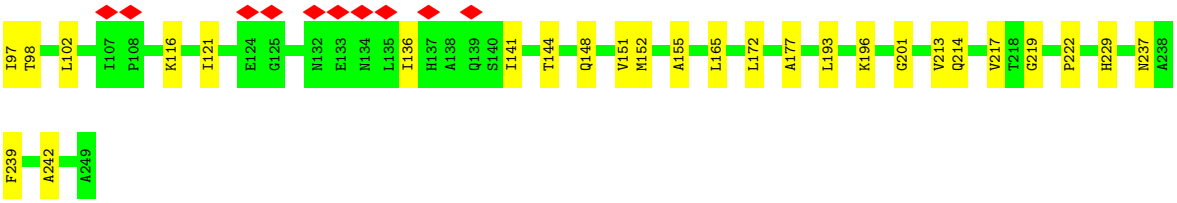


• Molecule 23: Chlorophyll a-b binding protein, chloroplastic

Chain W:





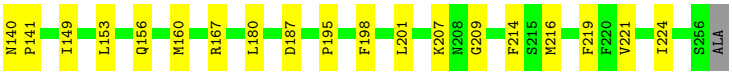


• Molecule 24: Chlorophyll a-b binding protein, chloroplastic

Chain Y:







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

Chain Z:







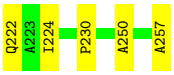
• Molecule 24: Chlorophyll a-b binding protein, chloroplastic

Chain U:





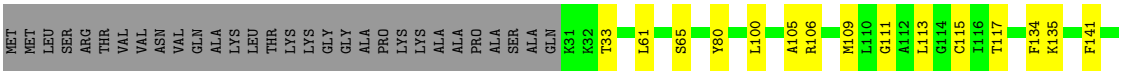


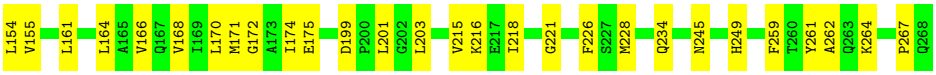


• Molecule 25: Chlorophyll a-b binding protein, chloroplastic

Chain V:







4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	123997	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	0.116	Depositor
Minimum map value	-0.049	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	360.0, 360.0, 360.0	wwPDB
Map dimensions	360, 360, 360	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: SF4, LHG, LMG, NEX, LMU, CLA, DGD, BCR, LUT, XAT, TPO, CHL, PQN

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	0.53	0/6015	0.39	0/8201
2	B	0.52	0/6036	0.45	5/8242 (0.1%)
3	C	0.51	0/610	0.62	1/826 (0.1%)
4	D	0.44	0/1152	0.46	1/1556 (0.1%)
5	E	0.41	0/506	0.34	0/689
6	F	0.39	0/1291	0.37	0/1747
7	G	0.27	0/714	0.34	0/972
8	H	0.39	0/788	0.37	0/1059
9	I	0.52	0/329	0.46	0/456
10	J	0.45	0/349	0.33	0/478
11	K	0.38	0/587	0.42	0/795
12	L	0.47	0/1190	0.41	0/1628
13	O	0.40	0/784	0.39	0/1069
14	1	0.37	0/1490	0.46	0/2028
14	a	0.37	0/1490	0.46	0/2028
15	2	0.38	0/1730	0.43	0/2353
16	3	0.43	0/1726	0.38	0/2342
17	4	0.29	0/1686	0.34	0/2300
18	5	0.37	0/1829	0.40	0/2492
19	6	0.34	0/1833	0.38	0/2505
20	7	0.44	0/1701	0.38	0/2310
21	8	0.40	0/1692	0.37	0/2304
22	9	0.36	0/1444	0.43	0/1964
23	W	0.22	0/1721	0.54	0/2341
23	X	0.24	0/1730	0.54	0/2355
24	U	0.23	0/1717	0.55	1/2336 (0.0%)
24	Y	0.25	0/1723	0.53	0/2345
24	Z	0.23	0/1732	0.53	0/2357
25	V	0.22	0/1856	0.46	0/2518
All	All	0.41	0/47451	0.44	8/64596 (0.0%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	150	LEU	N-CA-C	7.75	122.50	112.12
24	U	116	GLN	N-CA-C	6.74	118.62	111.28
2	B	495	LEU	N-CA-C	5.71	121.31	113.77
2	B	362	GLN	N-CA-C	-5.51	101.81	110.36
2	B	310	THR	CA-C-N	-5.44	114.78	120.38

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	87	0
2	B	5824	0	5579	104	0
3	C	600	0	581	15	0
4	D	1124	0	1139	16	0
5	E	496	0	491	5	0
6	F	1265	0	1301	19	0
7	G	699	0	681	11	0
8	H	776	0	765	10	0
9	I	316	0	321	9	0
10	J	337	0	336	2	0
11	K	582	0	620	10	0
12	L	1161	0	1184	15	0
13	O	758	0	740	13	0
14	1	1444	0	1396	34	0
14	a	1444	0	1396	27	0
15	2	1682	0	1665	22	0
16	3	1678	0	1637	25	0
17	4	1631	0	1587	18	0
18	5	1774	0	1746	42	0
19	6	1771	0	1770	21	0
20	7	1649	0	1589	15	0
21	8	1641	0	1618	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	9	1403	0	1381	21	0
23	W	1671	0	1604	30	0
23	X	1680	0	1622	32	0
24	U	1669	0	1603	40	0
24	Y	1675	0	1617	26	0
24	Z	1684	0	1625	29	0
25	V	1815	0	1766	50	0
26	1	666	0	522	6	0
26	2	637	0	530	4	0
26	3	724	0	628	5	0
26	4	778	0	678	7	0
26	5	878	0	758	17	0
26	6	903	0	831	11	0
26	7	756	0	635	13	0
26	8	724	0	629	8	0
26	9	595	0	491	4	0
26	A	2669	0	2693	56	0
26	B	2284	0	2237	33	0
26	F	140	0	113	6	0
26	G	87	0	64	0	0
26	H	104	0	93	0	0
26	J	42	0	31	0	0
26	K	191	0	150	3	0
26	L	235	0	184	7	0
26	O	116	0	61	0	0
26	U	400	0	342	11	0
26	V	415	0	365	11	0
26	W	426	0	377	12	0
26	X	436	0	415	16	0
26	Y	429	0	389	10	0
26	Z	427	0	386	17	0
26	a	710	0	591	8	0
27	A	33	0	46	2	0
27	B	33	0	46	3	0
28	1	49	0	74	0	0
28	2	36	0	42	0	0
28	3	94	0	137	3	0
28	4	49	0	74	0	0
28	5	98	0	148	6	0
28	6	48	0	69	0	0
28	7	37	0	44	0	0
28	8	89	0	124	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	9	128	0	178	1	0
28	A	128	0	178	0	0
28	B	38	0	46	0	0
28	H	49	0	74	0	0
28	O	36	0	42	1	0
28	U	49	0	74	1	0
28	V	36	0	42	3	0
28	W	34	0	38	1	0
28	X	49	0	74	6	0
28	Y	49	0	74	6	0
28	Z	49	0	74	9	0
28	a	43	0	59	1	0
29	1	40	0	56	2	0
29	2	40	0	56	5	0
29	3	120	0	168	19	0
29	4	40	0	56	5	0
29	5	40	0	56	2	0
29	6	40	0	56	1	0
29	7	80	0	112	8	0
29	8	40	0	56	3	0
29	9	40	0	56	7	0
29	A	240	0	336	42	0
29	B	400	0	560	44	0
29	F	40	0	56	7	0
29	G	40	0	56	4	0
29	J	40	0	56	8	0
29	K	80	0	112	8	0
29	L	160	0	224	29	0
29	O	80	0	112	9	0
29	a	40	0	56	3	0
30	A	8	0	0	0	0
30	C	16	0	0	1	0
31	1	35	0	46	0	0
31	5	65	0	76	0	0
31	8	35	0	46	0	0
31	A	69	0	90	1	0
31	K	35	0	46	0	0
32	4	80	0	100	0	0
32	5	40	0	50	1	0
32	8	46	0	65	3	0
32	9	55	0	86	2	0
32	A	40	0	50	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	H	55	0	86	0	0
32	J	82	0	107	0	0
32	L	37	0	44	0	0
32	V	55	0	86	2	0
33	B	62	0	85	1	0
34	1	42	0	56	6	0
34	2	42	0	56	7	0
34	3	42	0	56	7	0
34	4	42	0	56	3	0
34	5	42	0	56	4	0
34	6	42	0	56	5	0
34	7	42	0	56	3	0
34	8	42	0	56	6	0
34	9	42	0	56	5	0
34	U	84	0	112	8	0
34	V	84	0	112	10	0
34	W	84	0	112	8	0
34	X	84	0	112	12	0
34	Y	84	0	112	9	0
34	Z	84	0	112	10	0
34	a	42	0	56	5	0
35	1	44	0	56	3	0
35	2	44	0	56	1	0
35	3	44	0	56	2	0
35	4	44	0	56	3	0
35	5	44	0	56	2	0
35	6	44	0	56	1	0
35	7	44	0	56	1	0
35	8	44	0	56	1	0
35	9	44	0	56	0	0
35	U	44	0	56	5	0
35	V	44	0	56	6	0
35	W	44	0	56	3	0
35	X	44	0	56	3	0
35	Y	44	0	56	3	0
35	Z	44	0	56	5	0
35	a	44	0	56	3	0
36	5	44	0	56	1	0
36	6	44	0	56	6	0
36	U	44	0	56	0	0
36	V	44	0	56	11	0
36	W	44	0	56	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	X	44	0	56	2	0
36	Y	44	0	56	2	0
36	Z	44	0	56	3	0
37	U	303	0	248	14	0
37	V	309	0	253	15	0
37	W	336	0	298	9	0
37	X	353	0	342	15	0
37	Y	335	0	302	16	0
37	Z	335	0	302	14	0
All	All	69460	0	68604	1115	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 8.

The worst 5 of 1115 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)
21:8:78:CYS:SG	21:8:201:MET:HE2	1.64	1.34
25:V:174:ILE:CG2	36:V:1623:NEX:H15	1.78	1.14
21:8:78:CYS:SG	21:8:201:MET:CE	2.44	1.06
18:5:192:LEU:CD1	26:5:611:CLA:HMD1	1.87	1.04
25:V:174:ILE:HG22	36:V:1623:NEX:H201	1.42	1.00

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%)	713 (96%)	26 (4%)	0	100	100
2	B	731/735 (100%)	701 (96%)	30 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	78/81 (96%)	67 (86%)	11 (14%)	0	100	100
4	D	141/196 (72%)	135 (96%)	6 (4%)	0	100	100
5	E	61/97 (63%)	57 (93%)	4 (7%)	0	100	100
6	F	163/227 (72%)	156 (96%)	7 (4%)	0	100	100
7	G	92/126 (73%)	86 (94%)	6 (6%)	0	100	100
8	H	98/130 (75%)	94 (96%)	4 (4%)	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%)	78 (93%)	6 (7%)	0	100	100
12	L	157/196 (80%)	146 (93%)	11 (7%)	0	100	100
13	O	95/126 (75%)	87 (92%)	8 (8%)	0	100	100
14	1	192/228 (84%)	186 (97%)	6 (3%)	0	100	100
14	a	192/228 (84%)	186 (97%)	6 (3%)	0	100	100
15	2	215/246 (87%)	203 (94%)	10 (5%)	2 (1%)	14	43
16	3	218/298 (73%)	211 (97%)	7 (3%)	0	100	100
17	4	208/264 (79%)	202 (97%)	6 (3%)	0	100	100
18	5	225/257 (88%)	211 (94%)	14 (6%)	0	100	100
19	6	228/257 (89%)	210 (92%)	18 (8%)	0	100	100
20	7	211/241 (88%)	197 (93%)	14 (7%)	0	100	100
21	8	214/243 (88%)	210 (98%)	4 (2%)	0	100	100
22	9	181/213 (85%)	165 (91%)	16 (9%)	0	100	100
23	W	218/249 (88%)	202 (93%)	16 (7%)	0	100	100
23	X	219/249 (88%)	194 (89%)	25 (11%)	0	100	100
24	U	217/257 (84%)	196 (90%)	21 (10%)	0	100	100
24	Y	217/257 (84%)	198 (91%)	19 (9%)	0	100	100
24	Z	219/257 (85%)	204 (93%)	15 (7%)	0	100	100
25	V	235/268 (88%)	222 (94%)	13 (6%)	0	100	100
All	All	5927/6937 (85%)	5590 (94%)	335 (6%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	2	142	PRO

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Mol	Chain	Res	Type
15	2	143	PHE

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%)	600 (100%)	1 (0%)	87 87
2	B	596/597 (100%)	596 (100%)	0	100 100
3	C	69/70 (99%)	67 (97%)	2 (3%)	37 63
4	D	120/152 (79%)	120 (100%)	0	100 100
5	E	54/81 (67%)	54 (100%)	0	100 100
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%)	81 (100%)	0	100 100
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%)	121 (100%)	0	100 100
13	O	78/101 (77%)	78 (100%)	0	100 100
14	1	137/162 (85%)	135 (98%)	2 (2%)	57 72
14	a	137/162 (85%)	135 (98%)	2 (2%)	57 72
15	2	173/198 (87%)	173 (100%)	0	100 100
16	3	167/230 (73%)	167 (100%)	0	100 100
17	4	165/205 (80%)	164 (99%)	1 (1%)	78 81
18	5	184/206 (89%)	184 (100%)	0	100 100
19	6	184/203 (91%)	184 (100%)	0	100 100
20	7	164/181 (91%)	164 (100%)	0	100 100
21	8	162/183 (88%)	162 (100%)	0	100 100
22	9	140/159 (88%)	140 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
23	W	164/187 (88%)	164 (100%)	0	100 100
23	X	165/187 (88%)	164 (99%)	1 (1%)	78 81
24	U	168/194 (87%)	168 (100%)	0	100 100
24	Y	170/194 (88%)	170 (100%)	0	100 100
24	Z	170/194 (88%)	170 (100%)	0	100 100
25	V	178/201 (89%)	178 (100%)	0	100 100
All	All	4674/5363 (87%)	4665 (100%)	9 (0%)	85 87

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	4	177	ASP
23	X	165	LEU
14	1	72	LYS
14	1	227	PHE
14	a	66	LYS

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

Mol	Chain	Res	Type
13	O	82	ASN
24	U	147	GLN
15	2	196	ASN
23	W	161	ASN
23	X	161	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\| > 2$
25	TPO	V	33	25	8,10,11	1.56	1 (12%)	10,14,16	1.95	2 (20%)

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
25	TPO	V	33	25	-	3/9/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	V	33	TPO	P-O1P	3.28	1.61	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	V	33	TPO	P-OG1-CB	-5.21	107.48	123.21
25	V	33	TPO	CG2-CB-CA	-2.55	108.14	113.16

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	V	33	TPO	N-CA-CB-CG2
25	V	33	TPO	N-CA-CB-OG1
25	V	33	TPO	C-CA-CB-CG2

There are no ring outliers.

No monomer is involved in short contacts.

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	$\#\|Z\| > 2$
26	CLA	A	832	1	54,58,73	1.45	10 (18%)	65,95,113	1.46	11 (16%)
26	CLA	4	607	-	49,53,73	1.49	8 (16%)	59,89,113	1.27	6 (10%)
35	XAT	6	621	-	39,47,47	0.98	3 (7%)	54,74,74	2.42	23 (42%)
37	CHL	W	601	23	70,74,74	1.98	19 (27%)	80,114,114	2.76	24 (30%)
26	CLA	A	835	1	65,69,73	1.30	10 (15%)	78,108,113	1.28	8 (10%)
26	CLA	J	101	10	46,50,73	1.50	8 (17%)	55,85,113	1.29	6 (10%)
28	LHG	7	622	26	36,36,48	1.05	2 (5%)	39,42,54	1.02	3 (7%)
26	CLA	W	614	23	49,53,73	1.46	6 (12%)	59,89,113	1.38	3 (5%)
26	CLA	B	810	2	68,72,73	1.26	11 (16%)	81,111,113	1.38	9 (11%)
28	LHG	A	846	-	48,48,48	0.91	2 (4%)	51,54,54	0.87	2 (3%)
28	LHG	8	622	26	48,48,48	0.91	2 (4%)	51,54,54	0.86	2 (3%)
26	CLA	F	304	6	45,49,73	1.52	8 (17%)	54,84,113	1.37	6 (11%)
32	LMG	H	205	-	55,55,55	0.86	2 (3%)	63,63,63	1.11	6 (9%)
26	CLA	8	612	21	44,49,73	1.51	8 (18%)	52,84,113	1.37	4 (7%)
26	CLA	9	611	28	46,50,73	1.50	7 (15%)	55,85,113	1.23	2 (3%)
26	CLA	B	812	2	47,51,73	1.48	8 (17%)	56,86,113	1.27	5 (8%)
26	CLA	O	2001	13	40,46,73	1.60	9 (22%)	48,80,113	1.35	5 (10%)
26	CLA	2	607	-	47,52,73	1.48	9 (19%)	56,88,113	1.38	7 (12%)
26	CLA	V	612	25	49,53,73	1.47	8 (16%)	59,89,113	1.35	5 (8%)
26	CLA	B	827	2	66,70,73	1.27	10 (15%)	79,109,113	1.34	9 (11%)
26	CLA	5	607	-	69,73,73	1.26	10 (14%)	83,113,113	1.23	8 (9%)
26	CLA	3	617	16	43,48,73	1.52	9 (20%)	51,83,113	1.40	6 (11%)
32	LMG	L	2631	-	37,37,55	1.08	2 (5%)	45,45,63	1.18	4 (8%)
26	CLA	U	613	24	63,67,73	1.33	8 (12%)	75,105,113	1.20	7 (9%)
37	CHL	Y	601	24	70,74,74	1.95	19 (27%)	80,114,114	2.86	24 (30%)
26	CLA	3	611	28	41,46,73	1.62	7 (17%)	52,81,113	1.31	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
35	XAT	1	618	-	39,47,47	0.91	0	54,74,74	2.46	21 (38%)
26	CLA	4	608	-	69,73,73	1.25	8 (11%)	83,113,113	1.19	8 (9%)
37	CHL	X	608	-	70,73,74	1.99	16 (22%)	75,112,114	2.82	21 (28%)
28	LHG	A	847	26	29,29,48	1.16	2 (6%)	32,35,54	1.04	3 (9%)
26	CLA	Y	614	24	52,56,73	1.42	6 (11%)	62,92,113	1.29	8 (12%)
29	BCR	G	205	-	41,41,41	0.80	1 (2%)	56,56,56	1.97	15 (26%)
32	LMG	4	623	-	40,40,55	1.07	2 (5%)	48,48,63	1.15	5 (10%)
26	CLA	1	606	-	41,47,73	1.59	9 (21%)	48,80,113	1.38	6 (12%)
36	NEX	6	624	-	38,46,46	1.13	3 (7%)	50,70,70	2.40	18 (36%)
26	CLA	Z	613	24	69,73,73	1.26	9 (13%)	83,113,113	1.22	5 (6%)
26	CLA	B	817	2	63,67,73	1.32	9 (14%)	75,105,113	1.31	6 (8%)
26	CLA	8	606	-	68,72,73	1.29	9 (13%)	82,112,113	1.13	7 (8%)
34	LUT	5	620	-	42,43,43	0.84	1 (2%)	51,60,60	1.91	15 (29%)
26	CLA	2	604	-	46,50,73	1.50	8 (17%)	55,85,113	1.33	8 (14%)
26	CLA	A	837	1	49,53,73	1.51	11 (22%)	59,89,113	1.50	8 (13%)
32	LMG	V	2631	-	55,55,55	0.87	2 (3%)	63,63,63	1.11	5 (7%)
26	CLA	Z	604	-	54,57,73	1.50	9 (16%)	60,93,113	1.33	8 (13%)
36	NEX	5	624	-	38,46,46	1.08	1 (2%)	50,70,70	2.27	18 (36%)
26	CLA	A	829	1	69,73,73	1.27	8 (11%)	83,113,113	1.35	9 (10%)
26	CLA	6	613	-	67,72,73	1.30	9 (13%)	80,112,113	1.22	8 (10%)
29	BCR	3	622	-	41,41,41	0.89	1 (2%)	56,56,56	2.23	18 (32%)
26	CLA	G	204	7	49,53,73	1.50	9 (18%)	59,89,113	1.33	7 (11%)
26	CLA	B	828	2	69,73,73	1.28	9 (13%)	83,113,113	1.18	7 (8%)
35	XAT	4	620	-	39,47,47	0.94	2 (5%)	54,74,74	2.49	24 (44%)
26	CLA	A	838	1	54,58,73	1.42	12 (22%)	65,95,113	1.36	6 (9%)
26	CLA	7	611	28	63,67,73	1.31	9 (14%)	75,105,113	1.21	7 (9%)
37	CHL	V	608	-	52,56,74	2.17	17 (32%)	58,92,114	3.35	23 (39%)
26	CLA	4	616	17	47,51,73	1.58	9 (19%)	60,87,113	1.30	5 (8%)
26	CLA	B	839	-	69,73,73	1.28	12 (17%)	83,113,113	1.17	6 (7%)
29	BCR	4	621	-	41,41,41	0.83	1 (2%)	56,56,56	2.03	18 (32%)
37	CHL	V	609	25	65,69,74	2.00	18 (27%)	74,108,114	3.01	25 (33%)
26	CLA	8	608	-	55,59,73	1.41	10 (18%)	66,96,113	1.40	9 (13%)
28	LHG	Y	2630	26	48,48,48	0.92	2 (4%)	51,54,54	1.01	2 (3%)
28	LHG	Z	2630	26	48,48,48	0.92	2 (4%)	51,54,54	0.97	2 (3%)
26	CLA	6	611	28	46,50,73	1.49	8 (17%)	55,85,113	1.30	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	CLA	K	206	11	49,53,73	1.50	8 (16%)	59,89,113	1.26	4 (6%)
26	CLA	U	612	24	46,50,73	1.50	5 (10%)	55,85,113	1.45	6 (10%)
28	LHG	2	622	26	35,35,48	1.05	2 (5%)	38,41,54	1.16	3 (7%)
26	CLA	1	601	14	57,62,73	1.36	9 (15%)	68,100,113	1.23	8 (11%)
29	BCR	6	622	-	41,41,41	0.75	0	56,56,56	2.46	25 (44%)
26	CLA	3	607	16	60,64,73	1.38	8 (13%)	75,102,113	1.23	7 (9%)
37	CHL	U	605	24	47,51,74	2.39	18 (38%)	52,86,114	3.23	21 (40%)
26	CLA	B	811	2	57,60,73	1.50	11 (19%)	68,97,113	1.35	8 (11%)
26	CLA	8	607	-	45,49,73	1.60	11 (24%)	57,84,113	1.33	6 (10%)
32	LMG	5	627	-	40,40,55	1.03	2 (5%)	48,48,63	1.02	3 (6%)
37	CHL	Z	605	24	46,50,74	2.34	18 (39%)	51,85,114	3.55	24 (47%)
29	BCR	A	848	-	41,41,41	1.01	3 (7%)	56,56,56	2.24	14 (25%)
26	CLA	A	810	1	54,58,73	1.45	8 (14%)	65,95,113	1.38	8 (12%)
26	CLA	a	614	14	58,62,73	1.37	8 (13%)	67,99,113	1.34	6 (8%)
34	LUT	a	617	-	42,43,43	0.80	1 (2%)	51,60,60	1.90	16 (31%)
26	CLA	A	825	1	69,73,73	1.27	9 (13%)	83,113,113	1.20	6 (7%)
27	PQN	A	844	-	34,34,34	3.31	9 (26%)	42,45,45	2.07	4 (9%)
26	CLA	Z	612	24	49,53,73	1.48	7 (14%)	59,89,113	1.32	7 (11%)
26	CLA	2	616	-	47,51,73	1.57	9 (19%)	60,87,113	1.33	6 (10%)
26	CLA	B	809	2	69,73,73	1.29	10 (14%)	83,113,113	1.29	8 (9%)
26	CLA	1	608	-	47,52,73	1.50	9 (19%)	56,88,113	1.30	7 (12%)
26	CLA	A	801	1	69,73,73	1.27	11 (15%)	83,113,113	1.28	7 (8%)
26	CLA	X	614	23	46,50,73	1.52	8 (17%)	55,85,113	1.30	5 (9%)
30	SF4	C	101	3	0,12,12	-	-	-		
26	CLA	Y	611	28	47,51,73	1.48	7 (14%)	56,86,113	1.27	4 (7%)
26	CLA	5	614	18	48,52,73	1.49	9 (18%)	55,87,113	1.32	5 (9%)
26	CLA	7	614	20	46,50,73	1.50	9 (19%)	55,85,113	1.31	6 (10%)
26	CLA	A	826	-	68,72,73	1.28	11 (16%)	81,111,113	1.25	7 (8%)
26	CLA	W	611	28	61,65,73	1.33	6 (9%)	73,103,113	1.15	7 (9%)
26	CLA	V	602	25	64,68,73	1.29	8 (12%)	77,107,113	1.23	8 (10%)
29	BCR	A	850	-	41,41,41	0.93	1 (2%)	56,56,56	2.02	14 (25%)
26	CLA	7	603	20	47,52,73	1.52	10 (21%)	56,88,113	1.50	7 (12%)
26	CLA	a	602	14	65,69,73	1.34	11 (16%)	78,108,113	1.24	8 (10%)
26	CLA	a	611	28	41,46,73	1.64	10 (24%)	52,81,113	1.40	10 (19%)
26	CLA	7	606	-	45,49,73	1.54	11 (24%)	54,84,113	1.28	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	CLA	3	602	16	64,68,73	1.31	8 (12%)	77,107,113	1.20	8 (10%)
26	CLA	W	602	23	64,68,73	1.31	9 (14%)	77,107,113	1.17	8 (10%)
26	CLA	O	2003	-	43,48,73	1.54	9 (20%)	51,83,113	1.28	3 (5%)
31	LMU	5	628	-	34,34,36	1.19	2 (5%)	45,45,47	1.14	5 (11%)
29	BCR	a	619	-	41,41,41	0.84	0	56,56,56	2.38	22 (39%)
26	CLA	A	802	2	69,73,73	1.28	10 (14%)	83,113,113	1.39	10 (12%)
26	CLA	A	841	1	69,73,73	1.26	9 (13%)	83,113,113	1.20	6 (7%)
26	CLA	8	613	21	69,73,73	1.27	9 (13%)	83,113,113	1.16	6 (7%)
26	CLA	U	611	28	46,50,73	1.51	6 (13%)	55,85,113	1.33	4 (7%)
26	CLA	6	609	19	49,53,73	1.50	9 (18%)	59,89,113	1.31	6 (10%)
26	CLA	U	604	-	53,56,73	1.52	10 (18%)	57,91,113	1.38	8 (14%)
26	CLA	A	818	1	64,68,73	1.30	10 (15%)	77,107,113	1.28	8 (10%)
29	BCR	L	301	-	41,41,41	0.80	0	56,56,56	2.26	24 (42%)
26	CLA	A	812	1	69,73,73	1.26	9 (13%)	83,113,113	1.19	5 (6%)
26	CLA	6	602	19	69,73,73	1.28	9 (13%)	83,113,113	1.18	8 (9%)
26	CLA	a	607	-	49,53,73	1.52	10 (20%)	59,89,113	1.21	5 (8%)
26	CLA	B	840	2	69,73,73	1.33	10 (14%)	83,113,113	1.26	5 (6%)
34	LUT	X	1621	-	42,43,43	0.81	0	51,60,60	1.74	15 (29%)
26	CLA	B	803	-	69,73,73	1.25	11 (15%)	83,113,113	1.26	6 (7%)
26	CLA	3	604	-	69,73,73	1.27	9 (13%)	83,113,113	1.19	8 (9%)
35	XAT	a	618	-	39,47,47	0.90	0	54,74,74	2.47	21 (38%)
28	LHG	9	622	26	29,29,48	1.18	2 (6%)	32,35,54	1.02	1 (3%)
26	CLA	A	843	-	68,72,73	1.29	10 (14%)	81,111,113	1.25	9 (11%)
36	NEX	V	1623	-	38,46,46	0.94	2 (5%)	50,70,70	2.30	18 (36%)
26	CLA	A	828	1	69,73,73	1.27	11 (15%)	83,113,113	1.31	10 (12%)
29	BCR	K	202	-	41,41,41	0.94	2 (4%)	56,56,56	2.28	21 (37%)
26	CLA	9	614	22	49,53,73	1.48	9 (18%)	59,89,113	1.24	7 (11%)
26	CLA	X	602	23	69,73,73	1.25	9 (13%)	83,113,113	1.20	6 (7%)
32	LMG	J	104	-	40,40,55	1.02	2 (5%)	48,48,63	1.30	6 (12%)
26	CLA	7	607	-	46,50,73	1.49	8 (17%)	55,85,113	1.20	4 (7%)
26	CLA	U	614	24	46,50,73	1.49	7 (15%)	55,85,113	1.36	5 (9%)
31	LMU	1	621	-	36,36,36	1.15	2 (5%)	47,47,47	1.00	1 (2%)
29	BCR	7	623	-	41,41,41	0.87	0	56,56,56	2.01	17 (30%)
29	BCR	3	620	-	41,41,41	0.80	0	56,56,56	2.38	23 (41%)
26	CLA	B	836	2	54,58,73	1.43	11 (20%)	65,95,113	1.46	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
37	CHL	X	609	23	70,74,74	1.94	19 (27%)	80,114,114	2.83	25 (31%)
29	BCR	L	308	-	41,41,41	0.81	0	56,56,56	2.33	23 (41%)
29	BCR	B	844	-	41,41,41	1.08	4 (9%)	56,56,56	2.60	26 (46%)
26	CLA	Y	602	24	62,66,73	1.32	8 (12%)	74,104,113	1.23	8 (10%)
26	CLA	A	817	-	49,53,73	1.50	9 (18%)	59,89,113	1.41	6 (10%)
26	CLA	4	611	28	46,50,73	1.46	7 (15%)	55,85,113	1.35	8 (14%)
26	CLA	H	203	-	69,73,73	1.25	8 (11%)	83,113,113	1.23	5 (6%)
31	LMU	8	625	-	36,36,36	1.10	2 (5%)	47,47,47	1.24	3 (6%)
28	LHG	U	2630	26	48,48,48	0.94	2 (4%)	51,54,54	1.08	4 (7%)
30	SF4	A	853	1,2	0,12,12	-	-	-		
26	CLA	1	611	28	61,65,73	1.33	8 (13%)	73,103,113	1.20	8 (10%)
26	CLA	6	616	19	69,73,73	1.26	10 (14%)	83,113,113	1.29	10 (12%)
26	CLA	a	613	-	58,62,73	1.40	10 (17%)	69,99,113	1.23	6 (8%)
28	LHG	3	623	-	44,44,48	0.93	2 (4%)	47,50,54	1.00	3 (6%)
31	LMU	A	857	-	36,36,36	1.09	2 (5%)	47,47,47	1.37	8 (17%)
26	CLA	B	825	-	53,57,73	1.42	8 (15%)	62,93,113	1.35	8 (12%)
26	CLA	1	610	14	42,47,73	1.56	8 (19%)	51,81,113	1.39	7 (13%)
36	NEX	Y	1623	-	38,46,46	0.98	1 (2%)	50,70,70	2.52	16 (32%)
26	CLA	V	604	-	54,58,73	1.40	8 (14%)	65,95,113	1.31	7 (10%)
26	CLA	5	619	-	47,51,73	1.60	9 (19%)	60,87,113	1.42	8 (13%)
26	CLA	F	301	-	61,65,73	1.35	9 (14%)	73,103,113	1.18	6 (8%)
26	CLA	9	610	22	61,65,73	1.36	9 (14%)	73,103,113	1.27	8 (10%)
26	CLA	9	603	22	48,52,73	1.60	13 (27%)	61,88,113	1.40	6 (9%)
28	LHG	B	851	26	37,37,48	1.04	2 (5%)	40,43,54	1.14	4 (10%)
26	CLA	B	814	2	68,72,73	1.25	9 (13%)	81,111,113	1.29	6 (7%)
26	CLA	9	607	-	49,53,73	1.45	9 (18%)	59,89,113	1.28	6 (10%)
26	CLA	1	604	-	53,57,73	1.42	8 (15%)	62,93,113	1.28	5 (8%)
28	LHG	4	622	26	48,48,48	0.91	2 (4%)	51,54,54	0.82	2 (3%)
26	CLA	V	611	28	47,51,73	1.50	7 (14%)	56,86,113	1.25	3 (5%)
37	CHL	U	608	-	48,52,74	2.21	16 (33%)	53,87,114	3.48	22 (41%)
26	CLA	Z	614	24	52,56,73	1.45	7 (13%)	62,92,113	1.28	6 (9%)
32	LMG	4	624	-	40,40,55	1.03	2 (5%)	48,48,63	1.15	5 (10%)
37	CHL	U	607	-	50,54,74	2.27	19 (38%)	56,90,114	3.35	22 (39%)
26	CLA	2	606	-	47,51,73	1.49	10 (21%)	56,86,113	1.32	5 (8%)
26	CLA	6	608	-	49,53,73	1.48	8 (16%)	59,89,113	1.35	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	CLA	8	601	21	69,73,73	1.30	8 (11%)	83,113,113	1.18	6 (7%)
26	CLA	5	603	18	58,62,73	1.43	11 (18%)	73,100,113	1.35	6 (8%)
26	CLA	A	824	1	69,73,73	1.26	10 (14%)	83,113,113	1.30	6 (7%)
26	CLA	3	615	-	43,48,73	1.53	8 (18%)	51,83,113	1.31	6 (11%)
37	CHL	Z	608	-	53,57,74	2.22	19 (35%)	59,93,114	3.23	22 (37%)
37	CHL	Z	607	-	70,74,74	1.92	18 (25%)	80,114,114	2.90	21 (26%)
37	CHL	W	605	23	50,54,74	2.28	20 (40%)	56,90,114	3.38	22 (39%)
29	BCR	B	801	-	41,41,41	0.94	1 (2%)	56,56,56	2.10	18 (32%)
26	CLA	B	806	2	69,73,73	1.30	13 (18%)	83,113,113	1.38	8 (9%)
26	CLA	B	816	2	58,62,73	1.35	9 (15%)	69,99,113	1.30	8 (11%)
26	CLA	4	606	-	43,48,73	1.55	9 (20%)	51,83,113	1.28	6 (11%)
37	CHL	V	607	-	50,54,74	2.27	19 (38%)	56,90,114	3.25	23 (41%)
37	CHL	X	606	-	48,52,74	2.28	16 (33%)	53,87,114	3.31	21 (39%)
26	CLA	U	603	24	56,60,73	1.38	7 (12%)	67,97,113	1.36	7 (10%)
26	CLA	K	201	11	49,53,73	1.46	7 (14%)	59,89,113	1.24	4 (6%)
26	CLA	Z	603	24	59,63,73	1.35	7 (11%)	71,101,113	1.41	8 (11%)
26	CLA	5	618	18	43,48,73	1.61	10 (23%)	54,83,113	1.36	7 (12%)
26	CLA	A	808	1	54,58,73	1.41	8 (14%)	65,95,113	1.35	7 (10%)
31	LMU	K	208	-	36,36,36	1.14	2 (5%)	47,47,47	1.00	3 (6%)
26	CLA	3	614	16	43,48,73	1.55	9 (20%)	51,83,113	1.36	6 (11%)
26	CLA	A	807	1	69,73,73	1.29	11 (15%)	83,113,113	1.27	6 (7%)
26	CLA	a	610	14	63,67,73	1.31	8 (12%)	76,106,113	1.15	6 (7%)
26	CLA	A	840	1	56,60,73	1.39	11 (19%)	67,97,113	1.41	9 (13%)
26	CLA	L	306	-	43,48,73	1.53	8 (18%)	51,83,113	1.35	3 (5%)
28	LHG	1	620	26	48,48,48	0.92	2 (4%)	51,54,54	0.79	2 (3%)
26	CLA	7	615	-	45,50,73	1.60	10 (22%)	56,85,113	1.33	5 (8%)
34	LUT	X	1620	-	42,43,43	0.73	0	51,60,60	1.54	9 (17%)
26	CLA	A	809	1	69,73,73	1.27	11 (15%)	83,113,113	1.31	7 (8%)
26	CLA	1	616	14	47,51,73	1.56	8 (17%)	60,87,113	1.46	9 (15%)
28	LHG	H	204	-	48,48,48	0.92	2 (4%)	51,54,54	0.94	2 (3%)
26	CLA	2	611	28	46,50,73	1.48	8 (17%)	55,85,113	1.35	6 (10%)
26	CLA	B	834	2	64,68,73	1.30	10 (15%)	77,107,113	1.24	7 (9%)
29	BCR	F	305	-	41,41,41	0.89	1 (2%)	56,56,56	2.34	20 (35%)
26	CLA	2	610	15	59,63,73	1.37	9 (15%)	71,101,113	1.23	7 (9%)
26	CLA	8	609	21	49,53,73	1.48	8 (16%)	59,89,113	1.33	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	CLA	B	818	2	64,68,73	1.32	11 (17%)	77,107,113	1.36	8 (10%)
26	CLA	5	610	18	58,62,73	1.36	9 (15%)	69,99,113	1.22	6 (8%)
26	CLA	A	816	1	69,73,73	1.26	11 (15%)	83,113,113	1.29	7 (8%)
26	CLA	3	612	16	47,51,73	1.51	9 (19%)	56,86,113	1.24	6 (10%)
26	CLA	9	613	22	69,73,73	1.27	9 (13%)	83,113,113	1.24	6 (7%)
26	CLA	9	602	22	64,68,73	1.31	9 (14%)	77,107,113	1.27	8 (10%)
35	XAT	9	620	-	39,47,47	0.99	2 (5%)	54,74,74	2.51	19 (35%)
37	CHL	X	601	23	70,74,74	1.91	19 (27%)	80,114,114	2.85	28 (35%)
26	CLA	5	613	18	68,72,73	1.23	9 (13%)	81,111,113	1.28	8 (9%)
26	CLA	Y	610	24	69,73,73	1.26	9 (13%)	83,113,113	1.14	7 (8%)
26	CLA	3	603	16	59,63,73	1.36	11 (18%)	71,101,113	1.39	6 (8%)
35	XAT	V	1622	-	39,47,47	0.87	0	54,74,74	2.68	20 (37%)
35	XAT	3	619	-	39,47,47	0.98	2 (5%)	54,74,74	2.60	19 (35%)
28	LHG	9	624	-	48,48,48	0.93	2 (4%)	51,54,54	0.87	2 (3%)
26	CLA	5	604	-	67,71,73	1.36	9 (13%)	84,111,113	1.20	9 (10%)
26	CLA	2	601	15	69,73,73	1.23	10 (14%)	83,113,113	1.34	8 (9%)
36	NEX	X	1623	-	38,46,46	0.90	1 (2%)	50,70,70	4.33	20 (40%)
34	LUT	V	1621	-	42,43,43	0.79	0	51,60,60	1.99	16 (31%)
35	XAT	W	1622	-	39,47,47	0.92	1 (2%)	54,74,74	4.26	25 (46%)
26	CLA	W	610	23	59,63,73	1.34	6 (10%)	71,101,113	1.26	9 (12%)
26	CLA	W	603	23	56,60,73	1.37	6 (10%)	67,97,113	1.40	8 (11%)
37	CHL	V	606	-	48,52,74	2.16	18 (37%)	53,87,114	3.32	23 (43%)
26	CLA	4	613	17	69,73,73	1.29	10 (14%)	83,113,113	1.27	9 (10%)
26	CLA	4	602	17	64,68,73	1.34	9 (14%)	77,107,113	1.22	7 (9%)
26	CLA	7	601	20	64,68,73	1.33	11 (17%)	77,107,113	1.31	9 (11%)
36	NEX	U	1623	-	38,46,46	0.93	1 (2%)	50,70,70	2.60	20 (40%)
26	CLA	6	610	19	69,73,73	1.28	8 (11%)	83,113,113	1.18	7 (8%)
26	CLA	5	617	18	54,58,73	1.41	11 (20%)	65,95,113	1.26	6 (9%)
26	CLA	B	819	-	59,63,73	1.37	8 (13%)	71,101,113	1.22	9 (12%)
26	CLA	A	831	1	69,73,73	1.29	11 (15%)	83,113,113	1.22	7 (8%)
37	CHL	W	608	-	51,55,74	2.25	18 (35%)	57,91,114	3.26	21 (36%)
26	CLA	7	612	20	48,52,73	1.50	8 (16%)	58,88,113	1.29	4 (6%)
35	XAT	X	1622	-	39,47,47	0.87	0	54,74,74	2.63	20 (37%)
26	CLA	X	610	23	69,73,73	1.26	8 (11%)	83,113,113	1.17	7 (8%)
29	BCR	1	619	-	41,41,41	0.83	0	56,56,56	2.38	22 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	CLA	a	609	14	67,72,73	1.26	8 (11%)	80,112,113	1.19	6 (7%)
29	BCR	8	621	-	41,41,41	0.75	0	56,56,56	2.77	21 (37%)
26	CLA	1	603	14	56,61,73	1.36	8 (14%)	66,98,113	1.34	4 (6%)
26	CLA	W	612	23	49,53,73	1.48	8 (16%)	59,89,113	1.40	6 (10%)
28	LHG	5	623	26	48,48,48	0.93	2 (4%)	51,54,54	0.87	2 (3%)
35	XAT	7	620	-	39,47,47	0.99	2 (5%)	54,74,74	2.50	18 (33%)
26	CLA	A	845	28	54,58,73	1.44	10 (18%)	65,95,113	1.36	7 (10%)
35	XAT	2	620	-	39,47,47	1.05	2 (5%)	54,74,74	2.48	26 (48%)
29	BCR	5	622	-	41,41,41	0.87	2 (4%)	56,56,56	2.31	19 (33%)
37	CHL	V	601	25	70,74,74	1.95	19 (27%)	80,114,114	2.80	24 (30%)
26	CLA	X	604	-	53,57,73	1.44	6 (11%)	62,93,113	1.24	5 (8%)
37	CHL	X	605	-	50,54,74	2.42	19 (38%)	56,90,114	3.08	21 (37%)
26	CLA	5	601	18	60,64,73	1.33	7 (11%)	72,102,113	1.30	5 (6%)
26	CLA	5	612	18	44,49,73	1.52	7 (15%)	52,84,113	1.28	4 (7%)
26	CLA	9	609	22	65,69,73	1.30	9 (13%)	78,108,113	1.23	5 (6%)
26	CLA	2	609	15	49,53,73	1.52	9 (18%)	59,89,113	1.27	7 (11%)
35	XAT	8	620	-	39,47,47	1.02	2 (5%)	54,74,74	2.45	24 (44%)
26	CLA	6	617	19	49,53,73	1.46	8 (16%)	59,89,113	1.30	7 (11%)
34	LUT	U	1621	-	42,43,43	0.75	0	51,60,60	1.55	9 (17%)
26	CLA	4	610	17	65,69,73	1.27	7 (10%)	78,108,113	1.21	6 (7%)
26	CLA	8	616	21	47,51,73	1.58	7 (14%)	60,87,113	1.38	9 (15%)
26	CLA	B	807	2	56,60,73	1.44	12 (21%)	67,97,113	1.39	9 (13%)
26	CLA	L	302	12	49,53,73	1.53	8 (16%)	59,89,113	1.33	6 (10%)
32	LMG	A	860	-	40,40,55	1.00	2 (5%)	48,48,63	1.09	4 (8%)
37	CHL	U	609	24	64,68,74	2.01	17 (26%)	72,106,114	2.95	25 (34%)
29	BCR	B	847	-	41,41,41	0.92	2 (4%)	56,56,56	2.20	16 (28%)
26	CLA	3	610	16	69,73,73	1.28	8 (11%)	83,113,113	1.16	6 (7%)
34	LUT	Y	1621	-	42,43,43	0.87	1 (2%)	51,60,60	1.87	14 (27%)
26	CLA	a	608	-	47,52,73	1.50	8 (17%)	56,88,113	1.31	7 (12%)
26	CLA	9	601	22	49,53,73	1.48	8 (16%)	59,89,113	1.31	5 (8%)
26	CLA	B	808	2	69,73,73	1.27	9 (13%)	83,113,113	1.23	9 (10%)
26	CLA	V	610	25	66,70,73	1.26	7 (10%)	79,109,113	1.20	8 (10%)
26	CLA	A	834	1	69,73,73	1.30	11 (15%)	83,113,113	1.34	9 (10%)
26	CLA	3	613	16	56,61,73	1.39	9 (16%)	66,98,113	1.17	5 (7%)
26	CLA	Y	613	24	69,73,73	1.25	8 (11%)	83,113,113	1.20	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	LHG	A	861	-	48,48,48	0.94	2 (4%)	51,54,54	1.00	2 (3%)
26	CLA	B	815	2	47,51,73	1.48	9 (19%)	56,86,113	1.26	4 (7%)
26	CLA	4	614	17	60,64,73	1.34	8 (13%)	72,102,113	1.25	7 (9%)
35	XAT	5	621	-	39,47,47	0.95	2 (5%)	54,74,74	2.52	18 (33%)
26	CLA	9	612	22	44,49,73	1.53	6 (13%)	52,84,113	1.21	3 (5%)
26	CLA	A	820	1	69,73,73	1.26	11 (15%)	83,113,113	1.28	9 (10%)
28	LHG	8	623	-	39,39,48	1.03	2 (5%)	42,45,54	1.07	2 (4%)
37	CHL	Y	609	24	70,74,74	1.93	20 (28%)	80,114,114	2.85	25 (31%)
26	CLA	a	606	-	47,52,73	1.52	9 (19%)	55,87,113	1.26	4 (7%)
26	CLA	B	822	2	46,50,73	1.48	9 (19%)	55,85,113	1.29	6 (10%)
26	CLA	A	811	1	69,73,73	1.28	9 (13%)	83,113,113	1.24	5 (6%)
26	CLA	6	607	-	45,49,73	1.58	9 (20%)	57,84,113	1.35	6 (10%)
26	CLA	6	620	-	68,72,73	1.25	8 (11%)	81,111,113	1.20	5 (6%)
34	LUT	6	619	-	42,43,43	0.77	1 (2%)	51,60,60	2.07	18 (35%)
26	CLA	A	814	1	69,73,73	1.26	11 (15%)	83,113,113	1.40	10 (12%)
35	XAT	Y	1622	-	39,47,47	0.92	0	54,74,74	2.75	22 (40%)
26	CLA	1	614	14	40,45,73	1.67	9 (22%)	50,79,113	1.53	9 (18%)
26	CLA	W	604	-	51,55,73	1.47	8 (15%)	61,91,113	1.28	7 (11%)
26	CLA	K	203	-	60,64,73	1.35	10 (16%)	72,102,113	1.38	10 (13%)
31	LMU	A	858	-	34,35,36	1.26	4 (11%)	42,45,47	0.99	2 (4%)
34	LUT	Z	1621	-	42,43,43	0.79	0	51,60,60	1.41	8 (15%)
26	CLA	2	614	15	45,50,73	1.53	9 (20%)	53,85,113	1.36	8 (15%)
26	CLA	X	603	23	66,70,73	1.29	6 (9%)	79,109,113	1.29	5 (6%)
34	LUT	V	1620	-	42,43,43	0.75	0	51,60,60	1.65	10 (19%)
26	CLA	9	604	-	54,58,73	1.48	9 (16%)	68,95,113	1.30	8 (11%)
37	CHL	U	606	-	48,52,74	2.18	18 (37%)	53,87,114	3.36	21 (39%)
26	CLA	2	613	15	69,73,73	1.24	7 (10%)	83,113,113	1.12	5 (6%)
26	CLA	B	823	2	49,53,73	1.49	10 (20%)	59,89,113	1.36	7 (11%)
26	CLA	B	830	2	47,51,73	1.50	8 (17%)	56,86,113	1.37	8 (14%)
26	CLA	Z	602	24	62,66,73	1.32	8 (12%)	74,104,113	1.22	6 (8%)
26	CLA	A	804	1	69,73,73	1.25	10 (14%)	83,113,113	1.29	7 (8%)
37	CHL	W	609	23	70,74,74	1.98	18 (25%)	80,114,114	2.78	22 (27%)
26	CLA	5	609	18	69,73,73	1.29	9 (13%)	83,113,113	1.22	8 (9%)
29	BCR	A	856	-	41,41,41	0.91	2 (4%)	56,56,56	1.97	17 (30%)
34	LUT	7	619	-	42,43,43	0.91	2 (4%)	51,60,60	1.99	14 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	CLA	6	606	-	43,48,73	1.55	8 (18%)	51,83,113	1.25	5 (9%)
26	CLA	A	833	1	49,53,73	1.49	10 (20%)	59,89,113	1.50	11 (18%)
26	CLA	G	203	7	46,50,73	1.49	8 (17%)	55,85,113	1.38	6 (10%)
37	CHL	Z	609	24	70,74,74	1.95	19 (27%)	80,114,114	2.84	25 (31%)
26	CLA	B	835	-	49,53,73	1.49	10 (20%)	59,89,113	1.33	7 (11%)
26	CLA	7	604	-	54,58,73	1.40	9 (16%)	65,95,113	1.23	6 (9%)
37	CHL	Z	606	-	50,54,74	2.29	19 (38%)	56,90,114	3.30	25 (44%)
26	CLA	7	616	20	47,51,73	1.59	10 (21%)	60,87,113	1.37	7 (11%)
26	CLA	B	804	2	45,49,73	1.48	9 (20%)	54,84,113	1.36	4 (7%)
26	CLA	U	602	24	63,67,73	1.31	8 (12%)	75,105,113	1.20	6 (8%)
34	LUT	U	1620	-	42,43,43	0.74	0	51,60,60	1.60	10 (19%)
29	BCR	A	851	-	41,41,41	0.91	1 (2%)	56,56,56	2.29	24 (42%)
37	CHL	X	607	-	70,74,74	1.86	18 (25%)	80,114,114	2.97	24 (30%)
26	CLA	B	833	2	69,73,73	1.26	9 (13%)	83,113,113	1.15	5 (6%)
26	CLA	V	614	25	49,53,73	1.46	8 (16%)	59,89,113	1.33	6 (10%)
26	CLA	a	601	14	57,62,73	1.36	9 (15%)	68,100,113	1.24	8 (11%)
30	SF4	C	102	3	0,12,12	-	-	-		
26	CLA	2	603	15	47,52,73	1.51	9 (19%)	56,88,113	1.31	7 (12%)
31	LMU	5	629	-	33,33,36	1.21	2 (6%)	44,44,47	1.27	6 (13%)
29	BCR	B	846	-	41,41,41	0.81	1 (2%)	56,56,56	2.34	21 (37%)
26	CLA	1	602	14	65,69,73	1.33	10 (15%)	78,108,113	1.25	8 (10%)
28	LHG	V	2630	26	35,35,48	1.07	2 (5%)	38,41,54	1.08	2 (5%)
29	BCR	B	843	-	41,41,41	1.04	4 (9%)	56,56,56	1.94	18 (32%)
26	CLA	a	604	-	53,57,73	1.42	8 (15%)	62,93,113	1.27	4 (6%)
34	LUT	Z	1620	-	42,43,43	0.78	0	51,60,60	1.80	12 (23%)
26	CLA	A	854	-	69,73,73	1.30	10 (14%)	83,113,113	1.31	8 (9%)
26	CLA	a	612	14	49,53,73	1.48	9 (18%)	59,89,113	1.38	5 (8%)
36	NEX	Z	1623	-	38,46,46	1.02	1 (2%)	50,70,70	2.64	19 (38%)
26	CLA	7	610	20	69,73,73	1.29	9 (13%)	83,113,113	1.11	6 (7%)
26	CLA	A	836	1	69,73,73	1.25	10 (14%)	83,113,113	1.26	7 (8%)
26	CLA	4	609	17	61,65,73	1.33	7 (11%)	73,103,113	1.18	5 (6%)
34	LUT	2	619	-	42,43,43	0.91	2 (4%)	51,60,60	1.95	14 (27%)
26	CLA	4	603	17	48,52,73	1.56	10 (20%)	61,88,113	1.40	9 (14%)
26	CLA	6	601	19	69,73,73	1.24	8 (11%)	83,113,113	1.13	6 (7%)
28	LHG	a	620	26	42,42,48	0.98	2 (4%)	45,48,54	0.82	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	CLA	K	204	11	49,53,73	1.49	9 (18%)	59,89,113	1.45	5 (8%)
34	LUT	3	618	-	42,43,43	0.83	1 (2%)	51,60,60	2.01	12 (23%)
26	CLA	B	832	2	64,68,73	1.34	9 (14%)	77,107,113	1.32	8 (10%)
26	CLA	5	616	18	45,50,73	1.60	11 (24%)	56,85,113	1.30	4 (7%)
26	CLA	A	822	-	69,73,73	1.31	9 (13%)	83,113,113	1.28	11 (13%)
29	BCR	B	845	-	41,41,41	0.93	1 (2%)	56,56,56	2.50	23 (41%)
37	CHL	V	605	25	48,52,74	2.30	18 (37%)	53,87,114	3.30	20 (37%)
26	CLA	B	824	-	69,73,73	1.27	10 (14%)	83,113,113	1.16	5 (6%)
36	NEX	W	1623	-	38,46,46	0.90	2 (5%)	50,70,70	2.54	12 (24%)
26	CLA	L	303	12	69,73,73	1.26	9 (13%)	83,113,113	1.27	8 (9%)
28	LHG	X	2630	26	48,48,48	0.92	2 (4%)	51,54,54	1.02	3 (5%)
37	CHL	U	601	24	70,74,74	1.97	20 (28%)	80,114,114	2.75	23 (28%)
29	BCR	9	621	-	41,41,41	0.76	1 (2%)	56,56,56	2.90	18 (32%)
26	CLA	3	608	-	59,63,73	1.38	11 (18%)	71,101,113	1.18	4 (5%)
26	CLA	B	838	2	50,54,73	1.47	10 (20%)	60,90,113	1.38	7 (11%)
26	CLA	A	803	-	69,73,73	1.32	12 (17%)	83,113,113	1.21	4 (4%)
26	CLA	6	612	19	44,49,73	1.52	8 (18%)	52,84,113	1.26	5 (9%)
26	CLA	X	613	23	69,73,73	1.25	8 (11%)	83,113,113	1.14	6 (7%)
26	CLA	Y	612	24	49,53,73	1.48	7 (14%)	59,89,113	1.32	4 (6%)
29	BCR	2	623	-	41,41,41	0.86	1 (2%)	56,56,56	2.36	20 (35%)
26	CLA	1	607	-	43,48,73	1.59	10 (23%)	51,83,113	1.24	5 (9%)
34	LUT	9	619	-	42,43,43	0.87	1 (2%)	51,60,60	1.90	14 (27%)
34	LUT	W	1621	-	42,43,43	0.69	0	51,60,60	1.78	13 (25%)
26	CLA	8	610	21	64,68,73	1.28	8 (12%)	77,107,113	1.31	8 (10%)
37	CHL	W	606	-	50,54,74	2.20	19 (38%)	56,90,114	3.24	24 (42%)
26	CLA	8	603	21	48,52,73	1.58	9 (18%)	61,88,113	1.51	8 (13%)
26	CLA	A	823	1	46,50,73	1.49	9 (19%)	55,85,113	1.36	4 (7%)
26	CLA	X	612	23	47,51,73	1.49	7 (14%)	56,86,113	1.38	7 (12%)
26	CLA	W	613	23	69,73,73	1.25	8 (11%)	83,113,113	1.14	3 (3%)
29	BCR	L	309	-	41,41,41	0.78	0	56,56,56	2.40	25 (44%)
26	CLA	5	611	28	46,50,73	1.48	7 (15%)	55,85,113	1.27	7 (12%)
26	CLA	7	609	20	47,52,73	1.50	9 (19%)	55,87,113	1.24	5 (9%)
26	CLA	A	819	1	63,67,73	1.34	12 (19%)	75,105,113	1.36	7 (9%)
26	CLA	B	813	2	69,73,73	1.30	11 (15%)	83,113,113	1.21	7 (8%)
29	BCR	B	852	-	41,41,41	0.82	0	56,56,56	4.21	30 (53%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	CLA	6	603	19	55,59,73	1.46	10 (18%)	69,96,113	1.40	7 (10%)
26	CLA	U	610	24	60,64,73	1.32	7 (11%)	72,102,113	1.27	5 (6%)
26	CLA	Y	604	-	54,58,73	1.43	8 (14%)	65,95,113	1.23	4 (6%)
33	DGD	B	850	-	63,63,67	0.83	2 (3%)	77,77,81	1.24	7 (9%)
34	LUT	4	619	-	42,43,43	0.80	1 (2%)	51,60,60	2.02	18 (35%)
26	CLA	8	604	-	54,58,73	1.41	8 (14%)	65,95,113	1.39	9 (13%)
37	CHL	Y	605	24	46,50,74	2.47	20 (43%)	51,85,114	3.36	23 (45%)
28	LHG	3	624	26	48,48,48	0.91	2 (4%)	51,54,54	0.97	3 (5%)
26	CLA	3	609	16	64,68,73	1.33	9 (14%)	77,107,113	1.26	7 (9%)
26	CLA	3	606	-	57,62,73	1.35	9 (15%)	68,100,113	1.36	8 (11%)
26	CLA	O	2002	-	41,46,73	1.64	9 (21%)	52,81,113	1.36	7 (13%)
26	CLA	2	612	15	48,52,73	1.49	8 (16%)	58,88,113	1.29	3 (5%)
34	LUT	1	617	-	42,43,43	0.80	1 (2%)	51,60,60	1.89	16 (31%)
28	LHG	5	625	-	48,48,48	0.91	2 (4%)	51,54,54	1.02	3 (5%)
32	LMG	J	103	-	42,42,55	0.98	2 (4%)	50,50,63	1.22	6 (12%)
26	CLA	A	821	1	57,61,73	1.37	8 (14%)	68,98,113	1.30	7 (10%)
26	CLA	A	830	1	69,73,73	1.27	10 (14%)	83,113,113	1.24	7 (8%)
26	CLA	8	611	28	46,50,73	1.50	8 (17%)	55,85,113	1.29	5 (9%)
26	CLA	Z	611	28	46,50,73	1.55	9 (19%)	58,85,113	1.38	7 (12%)
26	CLA	B	826	2	66,70,73	1.29	9 (13%)	79,109,113	1.45	6 (7%)
29	BCR	J	102	-	41,41,41	0.93	2 (4%)	56,56,56	2.40	22 (39%)
26	CLA	4	618	17	43,48,73	1.60	8 (18%)	54,83,113	1.33	5 (9%)
29	BCR	B	849	-	41,41,41	0.93	2 (4%)	56,56,56	2.53	19 (33%)
37	CHL	W	607	-	69,73,74	2.00	19 (27%)	80,113,114	2.71	24 (30%)
26	CLA	1	613	-	69,73,73	1.28	10 (14%)	83,113,113	1.15	6 (7%)
26	CLA	6	604	-	69,73,73	1.25	8 (11%)	83,113,113	1.11	7 (8%)
28	LHG	W	2630	26	33,33,48	1.13	2 (6%)	36,39,54	1.17	3 (8%)
26	CLA	8	602	21	64,68,73	1.34	9 (14%)	77,107,113	1.31	10 (12%)
26	CLA	X	611	28	49,53,73	1.48	7 (14%)	59,89,113	1.29	5 (8%)
26	CLA	F	303	-	46,50,73	1.53	10 (21%)	55,85,113	1.38	7 (12%)
26	CLA	Y	603	24	59,63,73	1.35	7 (11%)	71,101,113	1.39	7 (9%)
37	CHL	Z	601	24	70,74,74	1.91	18 (25%)	80,114,114	2.87	23 (28%)
26	CLA	4	612	17	44,49,73	1.53	7 (15%)	52,84,113	1.26	3 (5%)
28	LHG	9	623	-	48,48,48	0.91	2 (4%)	51,54,54	0.96	2 (3%)
26	CLA	B	805	2	69,73,73	1.27	10 (14%)	83,113,113	1.25	10 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	CLA	V	613	25	69,73,73	1.25	8 (11%)	83,113,113	1.17	5 (6%)
26	CLA	5	606	-	43,48,73	1.55	8 (18%)	51,83,113	1.31	6 (11%)
26	CLA	B	802	2	69,73,73	1.25	10 (14%)	83,113,113	1.24	7 (8%)
26	CLA	B	841	28	69,73,73	1.25	9 (13%)	83,113,113	1.23	7 (8%)
26	CLA	1	612	14	49,53,73	1.46	9 (18%)	59,89,113	1.37	5 (8%)
26	CLA	A	827	-	62,66,73	1.34	9 (14%)	74,104,113	1.20	6 (8%)
37	CHL	Y	608	-	53,57,74	2.18	18 (33%)	59,93,114	3.31	24 (40%)
26	CLA	B	831	2	69,73,73	1.25	9 (13%)	83,113,113	1.19	6 (7%)
28	LHG	O	2631	-	35,35,48	1.07	2 (5%)	38,41,54	1.12	3 (7%)
26	CLA	6	614	19	64,68,73	1.31	8 (12%)	77,107,113	1.21	8 (10%)
37	CHL	Y	607	-	70,74,74	1.87	17 (24%)	80,114,114	2.89	23 (28%)
26	CLA	5	608	-	54,58,73	1.43	9 (16%)	65,95,113	1.22	6 (9%)
26	CLA	a	616	14	49,53,73	1.47	6 (12%)	59,89,113	1.39	8 (13%)
26	CLA	7	608	-	54,58,73	1.42	11 (20%)	65,95,113	1.34	8 (12%)
26	CLA	4	604	-	58,62,73	1.42	9 (15%)	73,100,113	1.31	8 (10%)
26	CLA	B	820	2	54,58,73	1.40	10 (18%)	65,95,113	1.37	6 (9%)
27	PQN	B	842	-	34,34,34	3.33	8 (23%)	42,45,45	2.02	7 (16%)
26	CLA	B	837	2	69,73,73	1.29	11 (15%)	83,113,113	1.32	10 (12%)
26	CLA	7	613	20	69,73,73	1.27	9 (13%)	83,113,113	1.24	6 (7%)
26	CLA	4	601	17	69,73,73	1.24	9 (13%)	83,113,113	1.23	5 (6%)
26	CLA	7	602	20	69,73,73	1.30	10 (14%)	83,113,113	1.22	7 (8%)
26	CLA	A	806	1	69,73,73	1.31	11 (15%)	83,113,113	1.40	12 (14%)
29	BCR	3	621	-	41,41,41	0.83	1 (2%)	56,56,56	1.84	15 (26%)
35	XAT	Z	1622	-	39,47,47	0.93	0	54,74,74	2.87	21 (38%)
26	CLA	Z	610	24	69,73,73	1.23	9 (13%)	83,113,113	1.19	8 (9%)
26	CLA	B	829	2	69,73,73	1.31	11 (15%)	83,113,113	1.31	10 (12%)
26	CLA	L	304	-	49,53,73	1.46	8 (16%)	59,89,113	1.30	6 (10%)
29	BCR	O	2004	-	41,41,41	0.82	0	56,56,56	1.96	14 (25%)
26	CLA	V	603	25	49,53,73	1.47	7 (14%)	59,89,113	1.46	4 (6%)
26	CLA	A	813	1	58,62,73	1.39	9 (15%)	69,99,113	1.32	8 (11%)
26	CLA	6	618	19	43,48,73	1.60	9 (20%)	54,83,113	1.43	7 (12%)
32	LMG	9	625	-	55,55,55	0.88	2 (3%)	63,63,63	1.03	6 (9%)
32	LMG	8	626	-	46,46,55	0.97	2 (4%)	54,54,63	1.10	4 (7%)
26	CLA	A	815	1	54,58,73	1.43	9 (16%)	65,95,113	1.34	5 (7%)
26	CLA	L	307	8	43,48,73	1.52	9 (20%)	51,83,113	1.42	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	CLA	9	606	-	43,48,73	1.56	10 (23%)	51,83,113	1.32	4 (7%)
26	CLA	A	842	1	69,73,73	1.31	10 (14%)	83,113,113	1.35	11 (13%)
29	BCR	A	852	-	41,41,41	0.97	1 (2%)	56,56,56	2.56	26 (46%)
26	CLA	a	603	14	58,62,73	1.34	8 (13%)	69,99,113	1.33	4 (5%)
29	BCR	A	849	-	41,41,41	0.85	0	56,56,56	2.22	21 (37%)
26	CLA	1	609	14	44,48,73	1.57	9 (20%)	56,83,113	1.48	9 (16%)
35	XAT	U	1622	-	39,47,47	0.92	1 (2%)	54,74,74	4.40	22 (40%)
26	CLA	A	839	1	59,63,73	1.40	10 (16%)	71,101,113	1.34	9 (12%)
34	LUT	8	619	-	42,43,43	0.86	1 (2%)	51,60,60	1.87	11 (21%)
29	BCR	O	2005	-	41,41,41	0.88	1 (2%)	56,56,56	3.05	23 (41%)
28	LHG	6	623	26	47,47,48	0.91	2 (4%)	50,53,54	0.96	3 (6%)
29	BCR	B	848	-	41,41,41	0.84	1 (2%)	56,56,56	2.53	14 (25%)
29	BCR	7	621	-	41,41,41	0.80	1 (2%)	56,56,56	2.28	22 (39%)
26	CLA	H	202	-	42,47,73	1.57	7 (16%)	50,82,113	1.25	3 (6%)
26	CLA	2	602	15	61,69,73	1.33	8 (13%)	70,102,113	0.96	3 (4%)
26	CLA	5	602	18	69,73,73	1.27	9 (13%)	83,113,113	1.19	7 (8%)
29	BCR	L	305	-	41,41,41	0.89	0	56,56,56	2.52	25 (44%)
26	CLA	A	805	1	56,60,73	1.41	10 (17%)	67,97,113	1.49	11 (16%)
26	CLA	B	821	2	47,51,73	1.61	9 (19%)	55,86,113	1.34	6 (10%)
34	LUT	W	1620	-	42,43,43	0.72	0	51,60,60	1.59	11 (21%)
29	BCR	K	207	-	41,41,41	0.85	1 (2%)	56,56,56	2.72	21 (37%)
34	LUT	Y	1620	-	42,43,43	0.80	0	51,60,60	3.18	18 (35%)
29	BCR	B	853	-	41,41,41	0.87	3 (7%)	56,56,56	1.81	14 (25%)
26	CLA	8	614	21	57,61,73	1.39	10 (17%)	68,98,113	1.31	7 (10%)
37	CHL	Y	606	-	50,54,74	2.24	17 (34%)	56,90,114	3.23	22 (39%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	A	832	1	-	11/21/97/115	-
26	CLA	4	607	-	-	5/15/91/115	-
35	XAT	6	621	-	-	0/31/93/93	0/4/4/4
37	CHL	W	601	23	-	19/41/117/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	A	835	1	-	14/35/111/115	-
26	CLA	J	101	10	-	7/12/88/115	-
28	LHG	7	622	26	-	19/41/41/53	-
26	CLA	W	614	23	-	8/15/91/115	-
26	CLA	B	810	2	-	20/37/113/115	-
28	LHG	A	846	-	-	15/53/53/53	-
28	LHG	8	622	26	-	13/53/53/53	-
26	CLA	F	304	6	-	5/10/86/115	-
32	LMG	H	205	-	-	14/50/70/70	0/1/1/1
26	CLA	8	612	21	-	2/10/86/115	-
26	CLA	9	611	28	-	5/12/88/115	-
26	CLA	B	812	2	-	5/13/89/115	-
26	CLA	O	2001	13	-	2/6/78/115	-
26	CLA	2	607	-	-	2/13/89/115	-
26	CLA	V	612	25	-	7/15/91/115	-
26	CLA	B	827	2	-	12/36/112/115	-
26	CLA	5	607	-	-	15/39/115/115	-
26	CLA	3	617	16	-	1/8/84/115	-
32	LMG	L	2631	-	-	4/32/52/70	0/1/1/1
26	CLA	U	613	24	-	13/32/108/115	-
37	CHL	Y	601	24	-	21/41/117/117	-
26	CLA	3	611	28	-	3/4/80/115	-
35	XAT	1	618	-	-	0/31/93/93	0/4/4/4
26	CLA	4	608	-	-	11/39/115/115	-
37	CHL	X	608	-	-	21/41/113/117	-
28	LHG	A	847	26	-	6/34/34/53	-
26	CLA	Y	614	24	-	10/19/95/115	-
29	BCR	G	205	-	-	2/29/63/63	0/2/2/2
32	LMG	4	623	-	-	6/35/55/70	0/1/1/1
26	CLA	1	606	-	-	3/7/79/115	-
36	NEX	6	624	-	-	3/27/83/83	0/3/3/3
26	CLA	Z	613	24	-	8/39/115/115	-
26	CLA	B	817	2	-	10/32/108/115	-
26	CLA	8	606	-	-	8/37/113/115	-
34	LUT	5	620	-	-	0/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	2	604	-	-	3/11/87/115	-
26	CLA	A	837	1	-	9/15/91/115	-
32	LMG	V	2631	-	-	12/50/70/70	0/1/1/1
26	CLA	Z	604	-	-	5/21/93/115	-
36	NEX	5	624	-	-	2/27/83/83	0/3/3/3
26	CLA	A	829	1	-	10/39/115/115	-
26	CLA	6	613	-	-	15/37/113/115	-
29	BCR	3	622	-	-	3/29/63/63	0/2/2/2
26	CLA	G	204	7	-	7/15/91/115	-
26	CLA	B	828	2	-	17/39/115/115	-
35	XAT	4	620	-	-	2/31/93/93	0/4/4/4
26	CLA	A	838	1	-	8/21/97/115	-
26	CLA	7	611	28	-	6/31/107/115	-
37	CHL	V	608	-	-	7/20/96/117	-
26	CLA	4	616	17	-	7/11/87/115	-
26	CLA	B	839	-	-	14/39/115/115	-
29	BCR	4	621	-	-	2/29/63/63	0/2/2/2
37	CHL	V	609	25	-	13/35/111/117	-
26	CLA	8	608	-	-	7/23/99/115	-
28	LHG	Y	2630	26	-	13/53/53/53	-
28	LHG	Z	2630	26	-	19/53/53/53	-
26	CLA	6	611	28	-	5/12/88/115	-
26	CLA	K	206	11	-	6/15/91/115	-
26	CLA	U	612	24	-	5/12/88/115	-
28	LHG	2	622	26	-	9/40/40/53	-
26	CLA	1	601	14	-	4/25/101/115	-
29	BCR	6	622	-	-	2/29/63/63	0/2/2/2
26	CLA	3	607	16	-	6/28/104/115	-
37	CHL	U	605	24	-	6/14/90/117	-
26	CLA	B	811	2	-	11/23/95/115	-
26	CLA	8	607	-	-	2/10/86/115	-
32	LMG	5	627	-	-	7/35/55/70	0/1/1/1
37	CHL	Z	605	24	-	6/12/88/117	-
29	BCR	A	848	-	-	3/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	A	810	1	-	7/21/97/115	-
26	CLA	a	614	14	-	9/27/99/115	-
34	LUT	a	617	-	-	4/29/67/67	0/2/2/2
26	CLA	A	825	1	-	17/39/115/115	-
27	PQN	A	844	-	-	6/23/43/43	0/2/2/2
26	CLA	Z	612	24	-	8/15/91/115	-
26	CLA	2	616	-	-	3/11/87/115	-
26	CLA	B	809	2	-	11/39/115/115	-
26	CLA	1	608	-	-	4/13/89/115	-
26	CLA	A	801	1	-	10/39/115/115	-
26	CLA	X	614	23	-	3/12/88/115	-
30	SF4	C	101	3	-	-	0/6/5/5
26	CLA	Y	611	28	-	9/13/89/115	-
26	CLA	5	614	18	-	9/15/87/115	-
26	CLA	7	614	20	-	3/12/88/115	-
26	CLA	A	826	-	-	8/37/113/115	-
26	CLA	W	611	28	-	9/30/106/115	-
26	CLA	V	602	25	-	8/33/109/115	-
29	BCR	A	850	-	-	2/29/63/63	0/2/2/2
26	CLA	7	603	20	-	7/13/89/115	-
26	CLA	a	602	14	-	5/35/111/115	-
26	CLA	a	611	28	-	0/4/80/115	-
26	CLA	7	606	-	-	2/10/86/115	-
26	CLA	3	602	16	-	3/33/109/115	-
26	CLA	W	602	23	-	12/33/109/115	-
26	CLA	O	2003	-	-	6/8/84/115	-
31	LMU	5	628	-	-	10/19/59/61	0/2/2/2
29	BCR	a	619	-	-	3/29/63/63	0/2/2/2
26	CLA	A	802	2	-	12/39/115/115	-
26	CLA	A	841	1	-	18/39/115/115	-
26	CLA	8	613	21	-	18/39/115/115	-
26	CLA	U	611	28	-	4/12/88/115	-
26	CLA	6	609	19	-	7/15/91/115	-
26	CLA	U	604	-	-	7/20/92/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	A	818	1	-	15/33/109/115	-
29	BCR	L	301	-	-	4/29/63/63	0/2/2/2
26	CLA	A	812	1	-	9/39/115/115	-
26	CLA	6	602	19	-	9/39/115/115	-
26	CLA	a	607	-	-	6/15/91/115	-
26	CLA	B	840	2	-	9/39/115/115	-
34	LUT	X	1621	-	-	3/29/67/67	0/2/2/2
26	CLA	B	803	-	-	12/39/115/115	-
26	CLA	3	604	-	-	7/39/115/115	-
35	XAT	a	618	-	-	0/31/93/93	0/4/4/4
28	LHG	9	622	26	-	10/34/34/53	-
26	CLA	A	843	-	-	14/37/113/115	-
36	NEX	V	1623	-	-	7/27/83/83	0/3/3/3
26	CLA	A	828	1	-	16/39/115/115	-
29	BCR	K	202	-	-	4/29/63/63	0/2/2/2
26	CLA	9	614	22	-	5/15/91/115	-
26	CLA	X	602	23	-	13/39/115/115	-
32	LMG	J	104	-	-	12/35/55/70	0/1/1/1
26	CLA	7	607	-	-	1/12/88/115	-
26	CLA	U	614	24	-	5/12/88/115	-
31	LMU	1	621	-	-	7/21/61/61	0/2/2/2
29	BCR	7	623	-	-	3/29/63/63	0/2/2/2
29	BCR	3	620	-	-	4/29/63/63	0/2/2/2
26	CLA	B	836	2	-	5/21/97/115	-
37	CHL	X	609	23	-	26/41/117/117	-
29	BCR	L	308	-	-	6/29/63/63	0/2/2/2
29	BCR	B	844	-	-	2/29/63/63	0/2/2/2
26	CLA	Y	602	24	-	14/31/107/115	-
26	CLA	A	817	-	-	2/15/91/115	-
26	CLA	4	611	28	-	9/12/88/115	-
26	CLA	H	203	-	-	17/39/115/115	-
31	LMU	8	625	-	-	12/21/61/61	0/2/2/2
28	LHG	U	2630	26	-	21/53/53/53	-
30	SF4	A	853	1,2	-	-	0/6/5/5
26	CLA	1	611	28	-	7/30/106/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	6	616	19	-	18/39/115/115	-
26	CLA	a	613	-	-	9/26/102/115	-
28	LHG	3	623	-	-	15/49/49/53	-
31	LMU	A	857	-	-	9/21/61/61	0/2/2/2
26	CLA	B	825	-	-	4/20/96/115	-
26	CLA	1	610	14	-	2/8/80/115	-
36	NEX	Y	1623	-	-	6/27/83/83	0/3/3/3
26	CLA	V	604	-	-	8/21/97/115	-
26	CLA	5	619	-	-	10/11/87/115	-
26	CLA	F	301	-	-	14/30/106/115	-
26	CLA	9	610	22	-	5/30/106/115	-
26	CLA	9	603	22	-	5/13/89/115	-
28	LHG	B	851	26	-	14/42/42/53	-
26	CLA	B	814	2	-	15/38/114/115	-
26	CLA	9	607	-	-	11/15/91/115	-
26	CLA	1	604	-	-	8/20/96/115	-
28	LHG	4	622	26	-	8/53/53/53	-
26	CLA	V	611	28	-	7/13/89/115	-
37	CHL	U	608	-	-	7/15/91/117	-
26	CLA	Z	614	24	-	9/19/95/115	-
32	LMG	4	624	-	-	5/35/55/70	0/1/1/1
37	CHL	U	607	-	-	11/17/93/117	-
26	CLA	2	606	-	-	3/13/89/115	-
26	CLA	6	608	-	-	8/15/91/115	-
26	CLA	8	601	21	-	16/39/115/115	-
26	CLA	5	603	18	-	5/25/101/115	-
26	CLA	A	824	1	-	11/39/115/115	-
26	CLA	3	615	-	-	3/8/84/115	-
37	CHL	Z	608	-	-	8/21/97/117	-
37	CHL	Z	607	-	-	22/41/117/117	-
37	CHL	W	605	23	-	12/17/93/117	-
29	BCR	B	801	-	-	4/29/63/63	0/2/2/2
26	CLA	B	806	2	-	19/39/115/115	-
26	CLA	B	816	2	-	10/25/101/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	4	606	-	-	4/8/84/115	-
37	CHL	V	607	-	-	12/17/93/117	-
37	CHL	X	606	-	-	6/15/91/117	-
26	CLA	U	603	24	-	10/24/100/115	-
26	CLA	K	201	11	-	7/15/91/115	-
26	CLA	Z	603	24	-	11/27/103/115	-
26	CLA	5	618	18	-	3/8/84/115	-
26	CLA	A	808	1	-	3/21/97/115	-
31	LMU	K	208	-	-	10/21/61/61	0/2/2/2
26	CLA	3	614	16	-	2/8/84/115	-
26	CLA	A	807	1	-	20/39/115/115	-
26	CLA	a	610	14	-	7/31/107/115	-
26	CLA	A	840	1	-	5/24/100/115	-
26	CLA	L	306	-	-	1/8/84/115	-
28	LHG	1	620	26	-	9/53/53/53	-
26	CLA	7	615	-	-	6/8/84/115	-
34	LUT	X	1620	-	-	4/29/67/67	0/2/2/2
26	CLA	A	809	1	-	11/39/115/115	-
26	CLA	1	616	14	-	7/11/87/115	-
28	LHG	H	204	-	-	15/53/53/53	-
26	CLA	2	611	28	-	4/12/88/115	-
26	CLA	B	834	2	-	5/33/109/115	-
29	BCR	F	305	-	-	6/29/63/63	0/2/2/2
26	CLA	2	610	15	-	5/27/103/115	-
26	CLA	8	609	21	-	2/15/91/115	-
26	CLA	B	818	2	-	11/33/109/115	-
26	CLA	5	610	18	-	6/26/102/115	-
26	CLA	A	816	1	-	15/39/115/115	-
26	CLA	3	612	16	-	5/13/89/115	-
26	CLA	9	613	22	-	14/39/115/115	-
26	CLA	9	602	22	-	7/33/109/115	-
35	XAT	9	620	-	-	0/31/93/93	0/4/4/4
37	CHL	X	601	23	-	21/41/117/117	-
26	CLA	5	613	18	-	16/37/113/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	Y	610	24	-	10/39/115/115	-
26	CLA	3	603	16	-	10/27/103/115	-
35	XAT	V	1622	-	-	2/31/93/93	0/4/4/4
35	XAT	3	619	-	-	0/31/93/93	0/4/4/4
28	LHG	9	624	-	-	17/53/53/53	-
26	CLA	5	604	-	-	12/35/111/115	-
26	CLA	2	601	15	-	8/39/115/115	-
36	NEX	X	1623	-	-	5/27/83/83	0/3/3/3
34	LUT	V	1621	-	-	3/29/67/67	0/2/2/2
35	XAT	W	1622	-	-	2/31/93/93	0/4/4/4
26	CLA	W	610	23	-	7/27/103/115	-
26	CLA	W	603	23	-	9/24/100/115	-
37	CHL	V	606	-	-	6/15/91/117	-
26	CLA	4	613	17	-	13/39/115/115	-
26	CLA	4	602	17	-	8/33/109/115	-
26	CLA	7	601	20	-	8/33/109/115	-
36	NEX	U	1623	-	-	6/27/83/83	0/3/3/3
26	CLA	6	610	19	-	12/39/115/115	-
26	CLA	5	617	18	-	12/21/97/115	-
26	CLA	B	819	-	-	8/27/103/115	-
26	CLA	A	831	1	-	16/39/115/115	-
37	CHL	W	608	-	-	11/19/95/117	-
26	CLA	7	612	20	-	4/13/89/115	-
35	XAT	X	1622	-	-	3/31/93/93	0/4/4/4
26	CLA	X	610	23	-	13/39/115/115	-
29	BCR	1	619	-	-	3/29/63/63	0/2/2/2
26	CLA	a	609	14	-	15/37/113/115	-
29	BCR	8	621	-	-	2/29/63/63	0/2/2/2
26	CLA	1	603	14	-	7/23/99/115	-
26	CLA	W	612	23	-	7/15/91/115	-
28	LHG	5	623	26	-	15/53/53/53	-
35	XAT	7	620	-	-	0/31/93/93	0/4/4/4
26	CLA	A	845	28	-	7/21/97/115	-
35	XAT	2	620	-	-	0/31/93/93	0/4/4/4
29	BCR	5	622	-	-	1/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	CHL	V	601	25	-	13/41/117/117	-
26	CLA	X	604	-	-	11/20/96/115	-
37	CHL	X	605	-	-	9/17/93/117	-
26	CLA	5	601	18	-	3/29/105/115	-
26	CLA	5	612	18	-	2/10/86/115	-
26	CLA	9	609	22	-	4/35/111/115	-
26	CLA	2	609	15	-	5/15/91/115	-
35	XAT	8	620	-	-	0/31/93/93	0/4/4/4
26	CLA	6	617	19	-	9/15/91/115	-
34	LUT	U	1621	-	-	5/29/67/67	0/2/2/2
26	CLA	4	610	17	-	8/35/111/115	-
26	CLA	8	616	21	-	5/11/87/115	-
26	CLA	B	807	2	-	4/24/100/115	-
26	CLA	L	302	12	-	8/15/91/115	-
32	LMG	A	860	-	-	9/35/55/70	0/1/1/1
37	CHL	U	609	24	-	14/34/110/117	-
29	BCR	B	847	-	-	2/29/63/63	0/2/2/2
26	CLA	3	610	16	-	14/39/115/115	-
34	LUT	Y	1621	-	-	3/29/67/67	0/2/2/2
26	CLA	a	608	-	-	4/13/89/115	-
26	CLA	9	601	22	-	8/15/91/115	-
26	CLA	B	808	2	-	13/39/115/115	-
26	CLA	V	610	25	-	9/36/112/115	-
26	CLA	A	834	1	-	12/39/115/115	-
26	CLA	3	613	16	-	7/23/99/115	-
26	CLA	Y	613	24	-	16/39/115/115	-
28	LHG	A	861	-	-	18/53/53/53	-
26	CLA	B	815	2	-	2/13/89/115	-
26	CLA	4	614	17	-	9/29/105/115	-
35	XAT	5	621	-	-	0/31/93/93	0/4/4/4
26	CLA	9	612	22	-	2/10/86/115	-
26	CLA	A	820	1	-	8/39/115/115	-
28	LHG	8	623	-	-	12/44/44/53	-
37	CHL	Y	609	24	-	17/41/117/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	a	606	-	-	8/12/88/115	-
26	CLA	B	822	2	-	7/12/88/115	-
26	CLA	A	811	1	-	15/39/115/115	-
26	CLA	6	607	-	-	2/10/86/115	-
26	CLA	6	620	-	-	12/37/113/115	-
34	LUT	6	619	-	-	4/29/67/67	0/2/2/2
26	CLA	A	814	1	-	18/39/115/115	-
35	XAT	Y	1622	-	-	3/31/93/93	0/4/4/4
26	CLA	1	614	14	-	0/4/76/115	-
26	CLA	W	604	-	-	6/18/94/115	-
26	CLA	K	203	-	-	10/29/105/115	-
31	LMU	A	858	-	-	10/21/57/61	0/2/2/2
34	LUT	Z	1621	-	-	3/29/67/67	0/2/2/2
26	CLA	2	614	15	-	0/11/87/115	-
26	CLA	X	603	23	-	15/36/112/115	-
34	LUT	V	1620	-	-	4/29/67/67	0/2/2/2
26	CLA	9	604	-	-	8/20/96/115	-
37	CHL	U	606	-	-	8/15/91/117	-
26	CLA	2	613	15	-	10/39/115/115	-
26	CLA	B	823	2	-	7/15/91/115	-
26	CLA	B	830	2	-	4/13/89/115	-
26	CLA	Z	602	24	-	7/31/107/115	-
26	CLA	A	804	1	-	16/39/115/115	-
37	CHL	W	609	23	-	13/41/117/117	-
26	CLA	5	609	18	-	12/39/115/115	-
29	BCR	A	856	-	-	2/29/63/63	0/2/2/2
34	LUT	7	619	-	-	2/29/67/67	0/2/2/2
26	CLA	6	606	-	-	2/8/84/115	-
26	CLA	A	833	1	-	5/15/91/115	-
26	CLA	G	203	7	-	5/12/88/115	-
37	CHL	Z	609	24	-	18/41/117/117	-
26	CLA	B	835	-	-	2/15/91/115	-
26	CLA	7	604	-	-	8/21/97/115	-
37	CHL	Z	606	-	-	8/17/93/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	7	616	20	-	8/11/87/115	-
26	CLA	B	804	2	-	3/10/86/115	-
26	CLA	U	602	24	-	18/32/108/115	-
34	LUT	U	1620	-	-	7/29/67/67	0/2/2/2
29	BCR	A	851	-	-	2/29/63/63	0/2/2/2
37	CHL	X	607	-	-	27/41/117/117	-
26	CLA	B	833	2	-	13/39/115/115	-
26	CLA	V	614	25	-	6/15/91/115	-
26	CLA	a	601	14	-	4/25/101/115	-
30	SF4	C	102	3	-	-	0/6/5/5
26	CLA	2	603	15	-	7/13/89/115	-
31	LMU	5	629	-	-	11/18/58/61	0/2/2/2
29	BCR	B	846	-	-	0/29/63/63	0/2/2/2
26	CLA	1	602	14	-	5/35/111/115	-
28	LHG	V	2630	26	-	6/40/40/53	-
29	BCR	B	843	-	-	4/29/63/63	0/2/2/2
26	CLA	a	604	-	-	8/20/96/115	-
34	LUT	Z	1620	-	-	5/29/67/67	0/2/2/2
26	CLA	A	854	-	-	9/39/115/115	-
26	CLA	a	612	14	-	6/15/91/115	-
36	NEX	Z	1623	-	-	6/27/83/83	0/3/3/3
26	CLA	7	610	20	-	7/39/115/115	-
26	CLA	A	836	1	-	9/39/115/115	-
26	CLA	4	609	17	-	5/30/106/115	-
34	LUT	2	619	-	-	2/29/67/67	0/2/2/2
26	CLA	4	603	17	-	5/13/89/115	-
26	CLA	6	601	19	-	17/39/115/115	-
28	LHG	a	620	26	-	7/47/47/53	-
26	CLA	K	204	11	-	5/15/91/115	-
34	LUT	3	618	-	-	4/29/67/67	0/2/2/2
26	CLA	B	832	2	-	12/33/109/115	-
26	CLA	5	616	18	-	4/8/84/115	-
26	CLA	A	822	-	-	6/39/115/115	-
29	BCR	B	845	-	-	9/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	CHL	V	605	25	-	7/15/91/117	-
26	CLA	B	824	-	-	10/39/115/115	-
36	NEX	W	1623	-	-	6/27/83/83	0/3/3/3
26	CLA	L	303	12	-	14/39/115/115	-
28	LHG	X	2630	26	-	13/53/53/53	-
37	CHL	U	601	24	-	19/41/117/117	-
29	BCR	9	621	-	-	4/29/63/63	0/2/2/2
26	CLA	3	608	-	-	10/27/103/115	-
26	CLA	B	838	2	-	3/17/93/115	-
26	CLA	A	803	-	-	9/39/115/115	-
26	CLA	6	612	19	-	3/10/86/115	-
26	CLA	X	613	23	-	14/39/115/115	-
26	CLA	Y	612	24	-	7/15/91/115	-
29	BCR	2	623	-	-	4/29/63/63	0/2/2/2
26	CLA	1	607	-	-	2/8/84/115	-
34	LUT	9	619	-	-	4/29/67/67	0/2/2/2
34	LUT	W	1621	-	-	5/29/67/67	0/2/2/2
26	CLA	8	610	21	-	9/33/109/115	-
37	CHL	W	606	-	-	4/17/93/117	-
26	CLA	8	603	21	-	4/13/89/115	-
26	CLA	A	823	1	-	1/12/88/115	-
26	CLA	X	612	23	-	8/13/89/115	-
26	CLA	W	613	23	-	22/39/115/115	-
29	BCR	L	309	-	-	3/29/63/63	0/2/2/2
26	CLA	5	611	28	-	2/12/88/115	-
26	CLA	7	609	20	-	6/12/88/115	-
26	CLA	A	819	1	-	5/32/108/115	-
26	CLA	B	813	2	-	20/39/115/115	-
29	BCR	B	852	-	-	6/29/63/63	0/2/2/2
26	CLA	6	603	19	-	5/22/98/115	-
26	CLA	U	610	24	-	4/29/105/115	-
26	CLA	Y	604	-	-	8/21/97/115	-
33	DGD	B	850	-	-	15/51/91/95	0/2/2/2
34	LUT	4	619	-	-	4/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	8	604	-	-	6/21/97/115	-
37	CHL	Y	605	24	-	6/12/88/117	-
28	LHG	3	624	26	-	14/53/53/53	-
26	CLA	3	609	16	-	14/33/109/115	-
26	CLA	3	606	-	-	4/25/101/115	-
26	CLA	O	2002	-	-	0/4/80/115	-
26	CLA	2	612	15	-	7/13/89/115	-
34	LUT	1	617	-	-	4/29/67/67	0/2/2/2
28	LHG	5	625	-	-	14/53/53/53	-
32	LMG	J	103	-	-	10/37/57/70	0/1/1/1
26	CLA	A	821	1	-	14/25/101/115	-
26	CLA	A	830	1	-	13/39/115/115	-
26	CLA	8	611	28	-	6/12/88/115	-
26	CLA	Z	611	28	-	5/11/87/115	-
26	CLA	B	826	2	-	14/36/112/115	-
29	BCR	J	102	-	-	2/29/63/63	0/2/2/2
26	CLA	4	618	17	-	2/8/84/115	-
29	BCR	B	849	-	-	5/29/63/63	0/2/2/2
37	CHL	W	607	-	-	21/39/115/117	-
26	CLA	1	613	-	-	17/39/115/115	-
26	CLA	6	604	-	-	18/39/115/115	-
28	LHG	W	2630	26	-	13/38/38/53	-
26	CLA	8	602	21	-	14/33/109/115	-
26	CLA	X	611	28	-	6/15/91/115	-
26	CLA	F	303	-	-	7/12/88/115	-
26	CLA	Y	603	24	-	12/27/103/115	-
37	CHL	Z	601	24	-	16/41/117/117	-
26	CLA	4	612	17	-	4/10/86/115	-
28	LHG	9	623	-	-	20/53/53/53	-
26	CLA	B	805	2	-	11/39/115/115	-
26	CLA	V	613	25	-	20/39/115/115	-
26	CLA	5	606	-	-	3/8/84/115	-
26	CLA	B	802	2	-	18/39/115/115	-
26	CLA	B	841	28	-	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	1	612	14	-	6/15/91/115	-
26	CLA	A	827	-	-	7/31/107/115	-
37	CHL	Y	608	-	-	8/21/97/117	-
26	CLA	B	831	2	-	12/39/115/115	-
28	LHG	O	2631	-	-	13/40/40/53	-
26	CLA	6	614	19	-	9/33/109/115	-
37	CHL	Y	607	-	-	21/41/117/117	-
26	CLA	5	608	-	-	6/21/97/115	-
26	CLA	a	616	14	-	7/15/91/115	-
26	CLA	7	608	-	-	4/21/97/115	-
26	CLA	4	604	-	-	9/25/101/115	-
26	CLA	B	820	2	-	3/21/97/115	-
27	PQN	B	842	-	-	7/23/43/43	0/2/2/2
26	CLA	B	837	2	-	10/39/115/115	-
26	CLA	7	613	20	-	18/39/115/115	-
26	CLA	4	601	17	-	16/39/115/115	-
26	CLA	7	602	20	-	11/39/115/115	-
26	CLA	A	806	1	-	13/39/115/115	-
29	BCR	3	621	-	-	0/29/63/63	0/2/2/2
35	XAT	Z	1622	-	-	4/31/93/93	0/4/4/4
26	CLA	Z	610	24	-	9/39/115/115	-
26	CLA	B	829	2	-	8/39/115/115	-
26	CLA	L	304	-	-	3/15/91/115	-
29	BCR	O	2004	-	-	2/29/63/63	0/2/2/2
26	CLA	V	603	25	-	6/15/91/115	-
26	CLA	A	813	1	-	7/26/102/115	-
26	CLA	6	618	19	-	1/8/84/115	-
32	LMG	9	625	-	-	11/50/70/70	0/1/1/1
32	LMG	8	626	-	-	16/41/61/70	0/1/1/1
26	CLA	A	815	1	-	12/21/97/115	-
26	CLA	L	307	8	-	2/8/84/115	-
26	CLA	9	606	-	-	2/8/84/115	-
26	CLA	A	842	1	-	18/39/115/115	-
29	BCR	A	852	-	-	8/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	a	603	14	-	10/25/101/115	-
29	BCR	A	849	-	-	5/29/63/63	0/2/2/2
26	CLA	1	609	14	-	3/8/84/115	-
35	XAT	U	1622	-	-	4/31/93/93	0/4/4/4
26	CLA	A	839	1	-	10/27/103/115	-
34	LUT	8	619	-	-	4/29/67/67	0/2/2/2
29	BCR	O	2005	-	-	2/29/63/63	0/2/2/2
28	LHG	6	623	26	-	19/52/52/53	-
29	BCR	B	848	-	-	4/29/63/63	0/2/2/2
29	BCR	7	621	-	-	2/29/63/63	0/2/2/2
26	CLA	H	202	-	-	4/6/82/115	-
26	CLA	2	602	15	-	18/49/99/115	-
26	CLA	5	602	18	-	10/39/115/115	-
29	BCR	L	305	-	-	2/29/63/63	0/2/2/2
26	CLA	A	805	1	-	7/24/100/115	-
26	CLA	B	821	2	-	5/13/89/115	-
34	LUT	W	1620	-	-	6/29/67/67	0/2/2/2
29	BCR	K	207	-	-	2/29/63/63	0/2/2/2
34	LUT	Y	1620	-	-	5/29/67/67	0/2/2/2
29	BCR	B	853	-	-	4/29/63/63	0/2/2/2
26	CLA	8	614	21	-	8/25/101/115	-
37	CHL	Y	606	-	-	8/17/93/117	-

The worst 5 of 3510 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	842	PQN	C12-C13	9.58	1.56	1.33
27	A	844	PQN	C12-C13	9.30	1.55	1.33
27	B	842	PQN	O4-C4	7.74	1.39	1.23
27	A	844	PQN	O4-C4	7.72	1.39	1.23
27	A	844	PQN	O1-C1	7.56	1.39	1.23

The worst 5 of 4551 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	X	1623	NEX	C17-C1-C6	-20.23	92.37	110.47
35	U	1622	XAT	C37-C21-C36	-17.41	81.69	107.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	W	1622	XAT	C37-C21-C36	-17.39	81.72	107.37
29	B	852	BCR	C32-C1-C6	-16.31	83.85	110.30
35	U	1622	XAT	C37-C21-C22	-15.46	82.13	108.98

There are no chirality outliers.

5 of 3788 torsion outliers are listed below:

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

There are no ring outliers.

290 monomers are involved in 664 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	4	607	CLA	1	0
35	6	621	XAT	1	0
37	W	601	CHL	3	0
26	A	835	CLA	2	0
26	W	614	CLA	4	0
26	F	304	CLA	1	0
26	8	612	CLA	2	0
26	V	612	CLA	2	0
26	B	827	CLA	1	0
26	5	607	CLA	2	0
26	U	613	CLA	3	0
37	Y	601	CHL	6	0
35	1	618	XAT	3	0
37	X	608	CHL	3	0
29	G	205	BCR	4	0
26	1	606	CLA	1	0
36	6	624	NEX	6	0
26	Z	613	CLA	4	0
26	B	817	CLA	1	0
26	8	606	CLA	1	0
34	5	620	LUT	4	0
26	A	837	CLA	1	0
32	V	2631	LMG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	5	624	NEX	1	0
26	A	829	CLA	5	0
29	3	622	BCR	7	0
26	B	828	CLA	2	0
35	4	620	XAT	3	0
26	7	611	CLA	4	0
37	V	608	CHL	2	0
26	4	616	CLA	1	0
26	B	839	CLA	1	0
29	4	621	BCR	5	0
37	V	609	CHL	3	0
28	Y	2630	LHG	6	0
28	Z	2630	LHG	9	0
26	1	601	CLA	2	0
29	6	622	BCR	1	0
37	U	605	CHL	1	0
32	5	627	LMG	1	0
29	A	848	BCR	3	0
34	a	617	LUT	5	0
26	A	825	CLA	3	0
27	A	844	PQN	2	0
26	Z	612	CLA	1	0
26	X	614	CLA	1	0
26	7	614	CLA	2	0
26	V	602	CLA	3	0
29	A	850	BCR	8	0
26	a	611	CLA	1	0
26	W	602	CLA	2	0
29	a	619	BCR	3	0
26	A	802	CLA	3	0
26	A	841	CLA	4	0
26	8	613	CLA	2	0
26	6	609	CLA	1	0
26	U	604	CLA	3	0
26	A	818	CLA	1	0
29	L	301	BCR	10	0
26	A	812	CLA	1	0
26	6	602	CLA	1	0
26	a	607	CLA	1	0
26	B	840	CLA	1	0
34	X	1621	LUT	6	0
26	B	803	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	a	618	XAT	3	0
28	9	622	LHG	1	0
26	A	843	CLA	2	0
36	V	1623	NEX	11	0
29	K	202	BCR	5	0
26	X	602	CLA	4	0
29	7	623	BCR	5	0
29	3	620	BCR	8	0
37	X	609	CHL	4	0
29	L	308	BCR	7	0
29	B	844	BCR	6	0
26	Y	602	CLA	2	0
26	4	611	CLA	1	0
28	U	2630	LHG	1	0
26	1	611	CLA	1	0
26	6	616	CLA	1	0
26	a	613	CLA	1	0
28	3	623	LHG	1	0
31	A	857	LMU	1	0
26	B	825	CLA	2	0
36	Y	1623	NEX	2	0
26	5	619	CLA	3	0
26	F	301	CLA	1	0
26	9	610	CLA	1	0
26	1	604	CLA	1	0
37	U	608	CHL	3	0
26	Z	614	CLA	1	0
37	U	607	CHL	2	0
26	2	606	CLA	1	0
26	6	608	CLA	1	0
26	5	603	CLA	1	0
26	A	824	CLA	2	0
37	Z	608	CHL	2	0
37	Z	607	CHL	3	0
37	W	605	CHL	2	0
29	B	801	BCR	7	0
26	B	816	CLA	1	0
26	4	606	CLA	1	0
37	V	607	CHL	4	0
26	Z	603	CLA	1	0
26	A	808	CLA	2	0
26	A	807	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	A	840	CLA	1	0
26	7	615	CLA	1	0
34	X	1620	LUT	6	0
26	A	809	CLA	1	0
26	B	834	CLA	3	0
29	F	305	BCR	7	0
26	B	818	CLA	1	0
26	5	610	CLA	1	0
26	A	816	CLA	1	0
26	3	612	CLA	1	0
26	9	613	CLA	2	0
37	X	601	CHL	7	0
26	5	613	CLA	1	0
26	Y	610	CLA	2	0
35	V	1622	XAT	6	0
35	3	619	XAT	2	0
36	X	1623	NEX	2	0
34	V	1621	LUT	5	0
35	W	1622	XAT	3	0
26	W	610	CLA	1	0
26	W	603	CLA	2	0
37	V	606	CHL	2	0
26	7	601	CLA	1	0
26	6	610	CLA	3	0
26	B	819	CLA	1	0
26	A	831	CLA	1	0
35	X	1622	XAT	3	0
26	X	610	CLA	3	0
29	1	619	BCR	2	0
29	8	621	BCR	3	0
26	W	612	CLA	1	0
28	5	623	LHG	6	0
35	7	620	XAT	1	0
35	2	620	XAT	1	0
29	5	622	BCR	2	0
37	V	601	CHL	4	0
26	X	604	CLA	1	0
26	9	609	CLA	1	0
35	8	620	XAT	1	0
34	U	1621	LUT	2	0
26	L	302	CLA	3	0
32	A	860	LMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	U	609	CHL	3	0
29	B	847	BCR	4	0
26	3	610	CLA	1	0
34	Y	1621	LUT	4	0
26	B	808	CLA	3	0
26	V	610	CLA	3	0
26	A	834	CLA	2	0
26	3	613	CLA	1	0
26	Y	613	CLA	4	0
35	5	621	XAT	2	0
26	A	820	CLA	2	0
37	Y	609	CHL	3	0
26	a	606	CLA	1	0
26	B	822	CLA	1	0
26	6	607	CLA	1	0
34	6	619	LUT	5	0
35	Y	1622	XAT	3	0
26	K	203	CLA	1	0
34	Z	1621	LUT	4	0
26	X	603	CLA	1	0
34	V	1620	LUT	5	0
37	U	606	CHL	2	0
26	2	613	CLA	3	0
26	B	830	CLA	1	0
26	Z	602	CLA	4	0
37	W	609	CHL	1	0
29	A	856	BCR	10	0
34	7	619	LUT	3	0
26	6	606	CLA	1	0
37	Z	609	CHL	3	0
26	B	835	CLA	1	0
26	7	604	CLA	1	0
37	Z	606	CHL	3	0
26	7	616	CLA	1	0
26	U	602	CLA	1	0
34	U	1620	LUT	6	0
29	A	851	BCR	6	0
37	X	607	CHL	2	0
26	B	833	CLA	2	0
26	V	614	CLA	1	0
26	a	601	CLA	3	0
30	C	102	SF4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	B	846	BCR	3	0
28	V	2630	LHG	3	0
29	B	843	BCR	9	0
26	a	604	CLA	1	0
34	Z	1620	LUT	6	0
26	A	854	CLA	5	0
36	Z	1623	NEX	3	0
26	4	609	CLA	1	0
34	2	619	LUT	7	0
26	6	601	CLA	1	0
28	a	620	LHG	1	0
26	K	204	CLA	2	0
34	3	618	LUT	7	0
26	A	822	CLA	4	0
29	B	845	BCR	3	0
37	V	605	CHL	1	0
26	B	824	CLA	1	0
36	W	1623	NEX	2	0
26	L	303	CLA	2	0
28	X	2630	LHG	6	0
37	U	601	CHL	4	0
29	9	621	BCR	7	0
26	3	608	CLA	1	0
26	A	803	CLA	3	0
26	X	613	CLA	4	0
29	2	623	BCR	5	0
26	1	607	CLA	1	0
34	9	619	LUT	5	0
34	W	1621	LUT	4	0
26	8	610	CLA	1	0
37	W	606	CHL	1	0
26	X	612	CLA	1	0
26	W	613	CLA	4	0
29	L	309	BCR	4	0
26	5	611	CLA	7	0
26	7	609	CLA	1	0
26	A	819	CLA	2	0
26	B	813	CLA	2	0
29	B	852	BCR	6	0
26	U	610	CLA	4	0
33	B	850	DGD	1	0
34	4	619	LUT	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	8	604	CLA	1	0
37	Y	605	CHL	1	0
28	3	624	LHG	2	0
26	3	606	CLA	1	0
34	1	617	LUT	6	0
26	A	821	CLA	1	0
26	A	830	CLA	1	0
26	8	611	CLA	2	0
26	Z	611	CLA	3	0
29	J	102	BCR	8	0
26	4	618	CLA	1	0
29	B	849	BCR	2	0
37	W	607	CHL	3	0
26	1	613	CLA	1	0
28	W	2630	LHG	1	0
26	X	611	CLA	2	0
26	F	303	CLA	4	0
26	Y	603	CLA	3	0
37	Z	601	CHL	4	0
26	V	613	CLA	4	0
26	B	802	CLA	1	0
26	A	827	CLA	1	0
37	Y	608	CHL	2	0
28	O	2631	LHG	1	0
26	6	614	CLA	2	0
37	Y	607	CHL	3	0
27	B	842	PQN	3	0
26	B	837	CLA	2	0
26	7	613	CLA	2	0
26	4	601	CLA	1	0
26	7	602	CLA	1	0
26	A	806	CLA	2	0
29	3	621	BCR	4	0
35	Z	1622	XAT	5	0
26	Z	610	CLA	5	0
29	O	2004	BCR	3	0
32	9	625	LMG	2	0
32	8	626	LMG	3	0
26	A	815	CLA	2	0
26	L	307	CLA	2	0
29	A	852	BCR	10	0
26	a	603	CLA	1	0

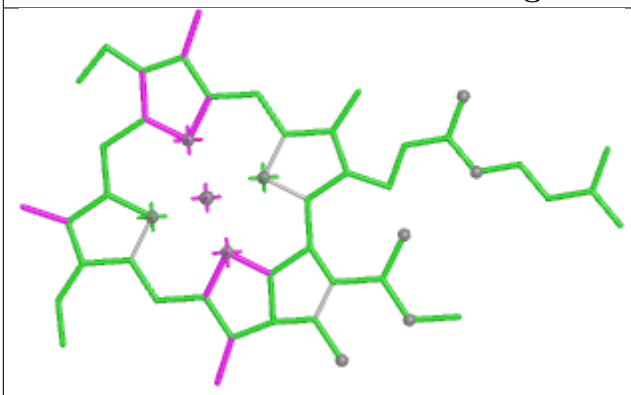
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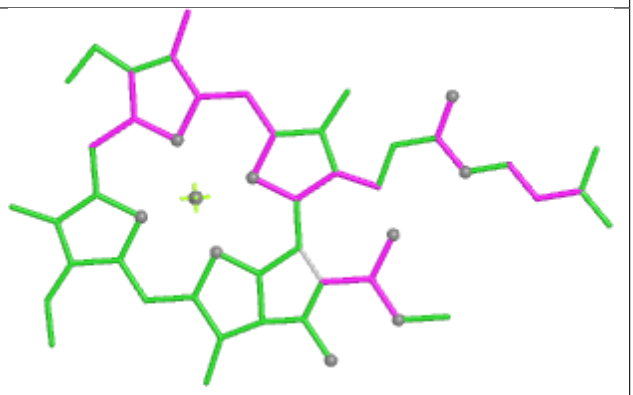
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35	U	1622	XAT	5	0
34	8	619	LUT	6	0
29	O	2005	BCR	6	0
29	B	848	BCR	2	0
29	7	621	BCR	3	0
26	5	602	CLA	2	0
29	L	305	BCR	8	0
26	A	805	CLA	1	0
26	B	821	CLA	3	0
34	W	1620	LUT	4	0
29	K	207	BCR	3	0
34	Y	1620	LUT	5	0
29	B	853	BCR	3	0
37	Y	606	CHL	2	0

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

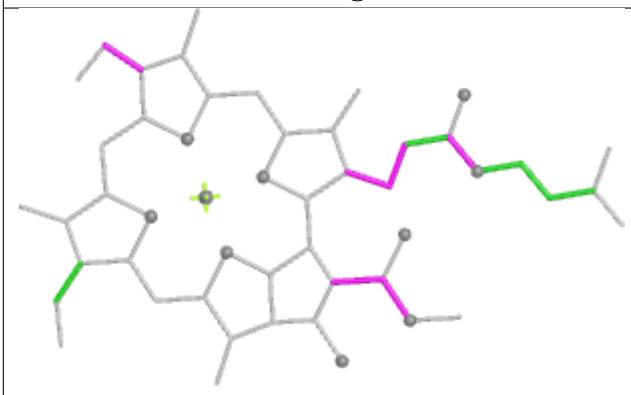
Ligand CLA A 832



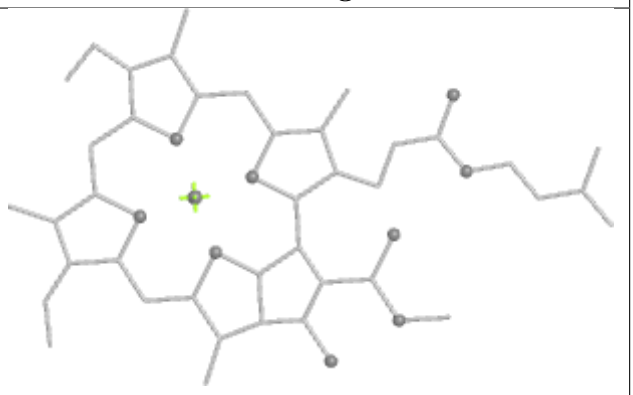
Bond lengths



Bond angles

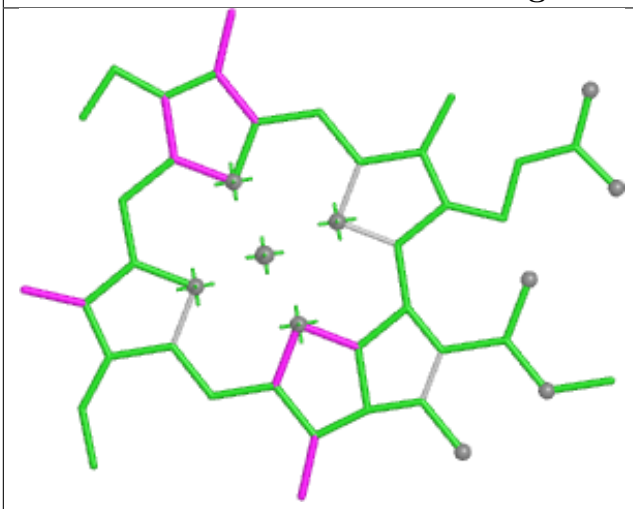


Torsions

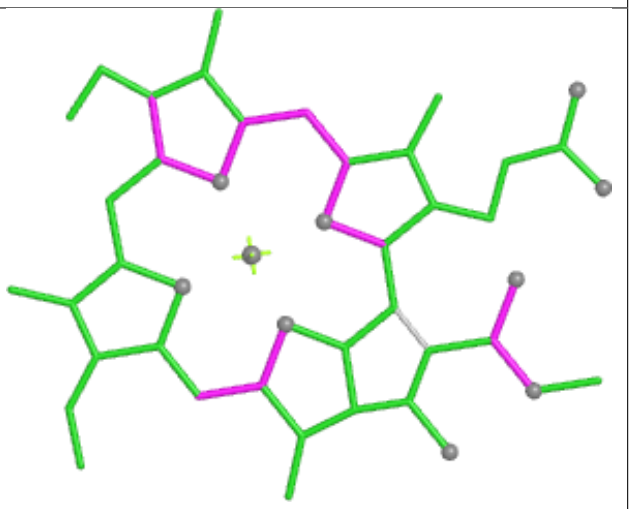


Rings

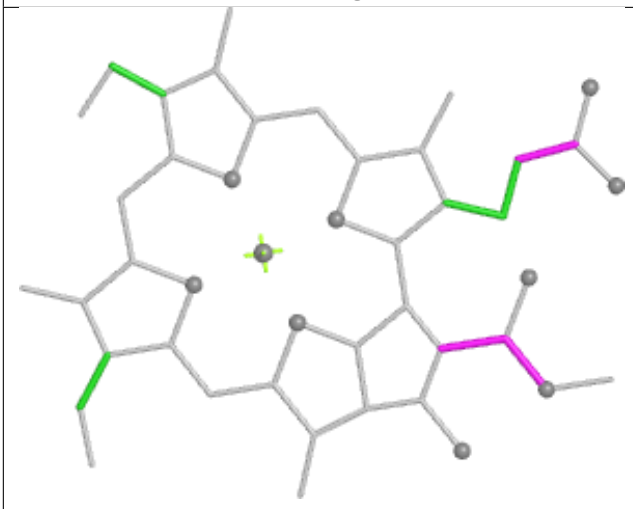
Ligand CLA 4 607



Bond lengths



Bond angles

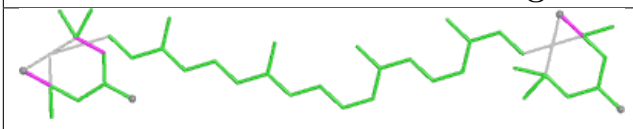


Torsions

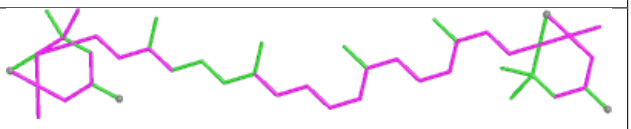


Rings

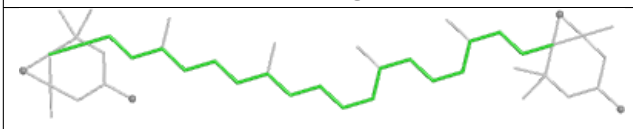
Ligand XAT 6 621



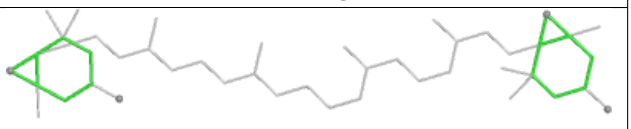
Bond lengths



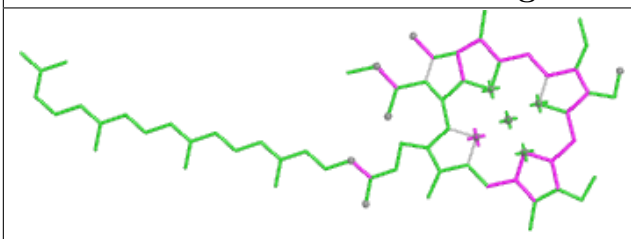
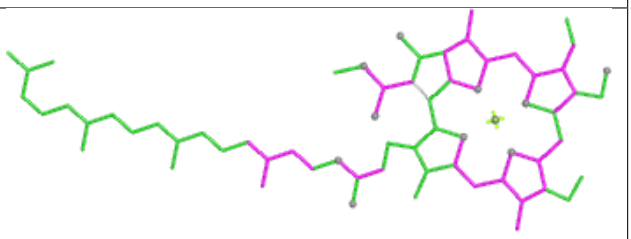
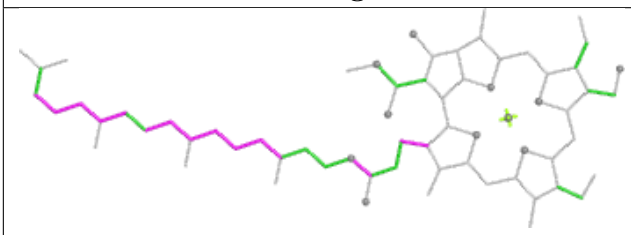
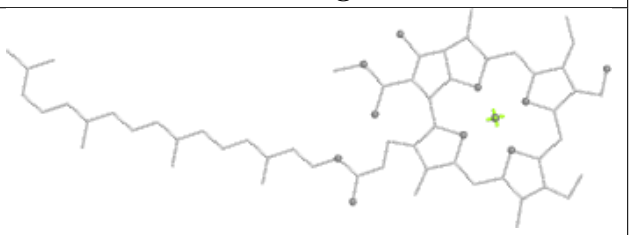
Bond angles

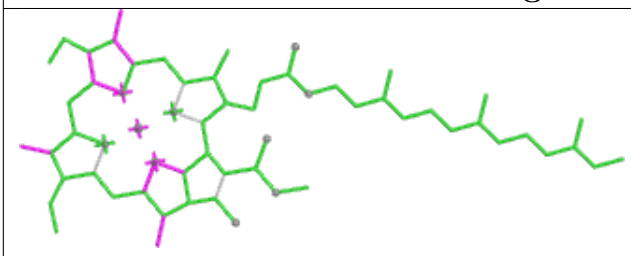
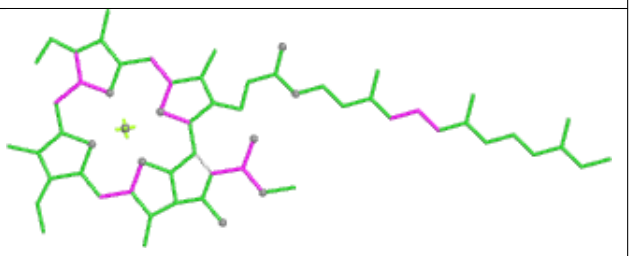
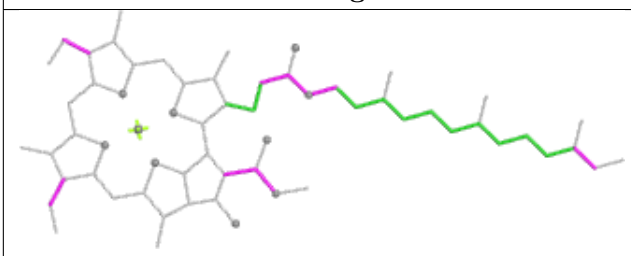
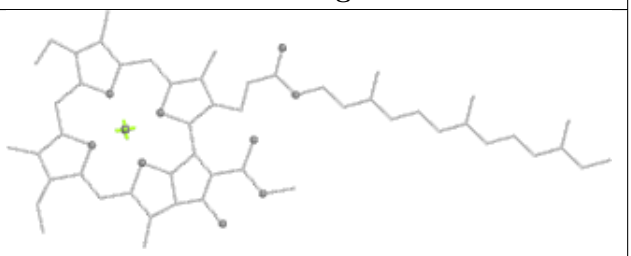


Torsions

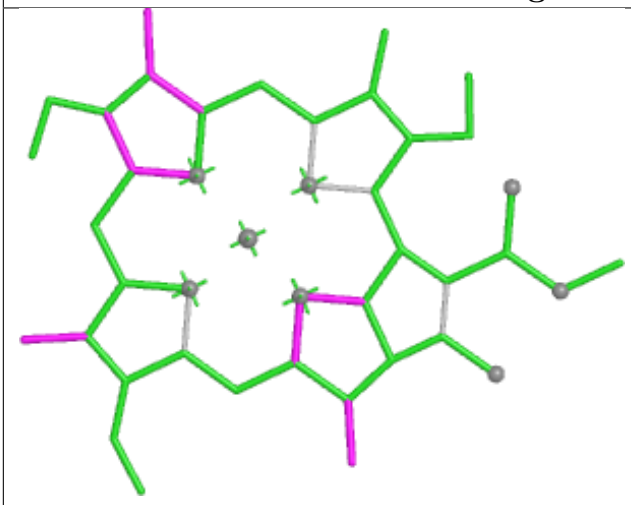


Rings

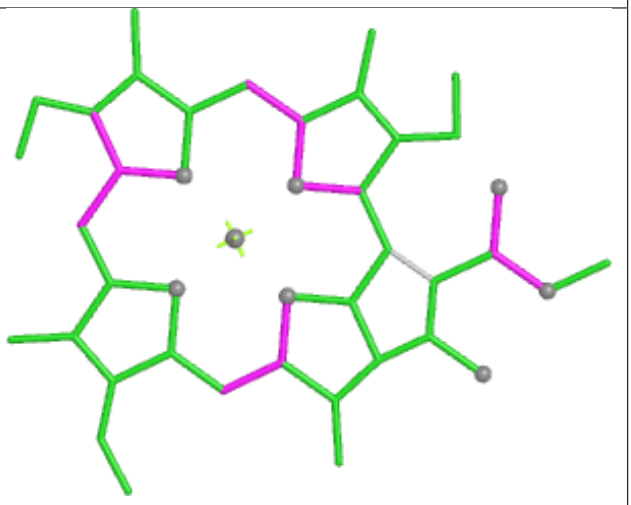
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 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 835	
 Bond lengths	 Bond angles
 Torsions	 Rings

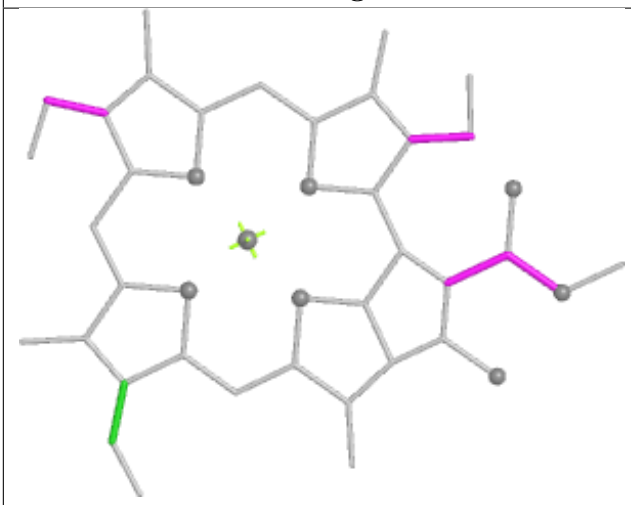
Ligand CLA J 101



Bond lengths



Bond angles

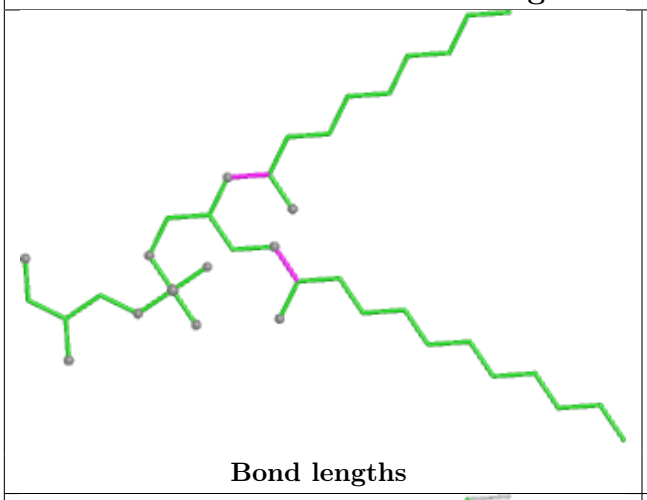


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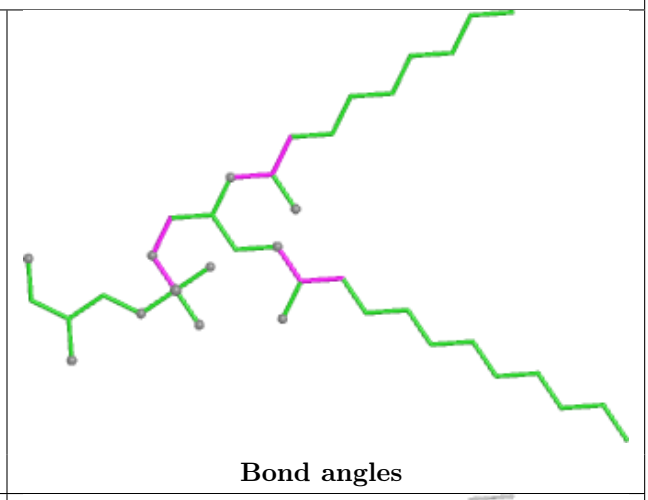


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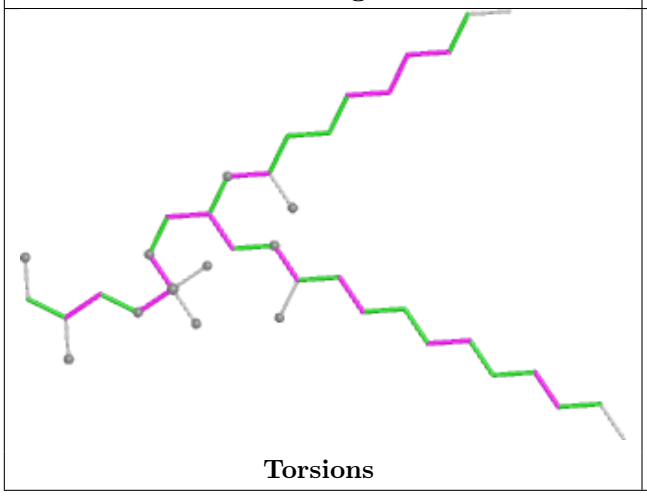
Ligand LHG 7 622



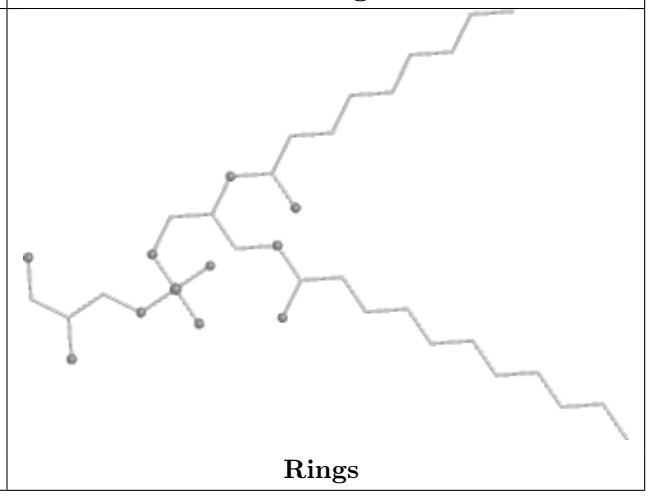
Bond lengths



Bond angles

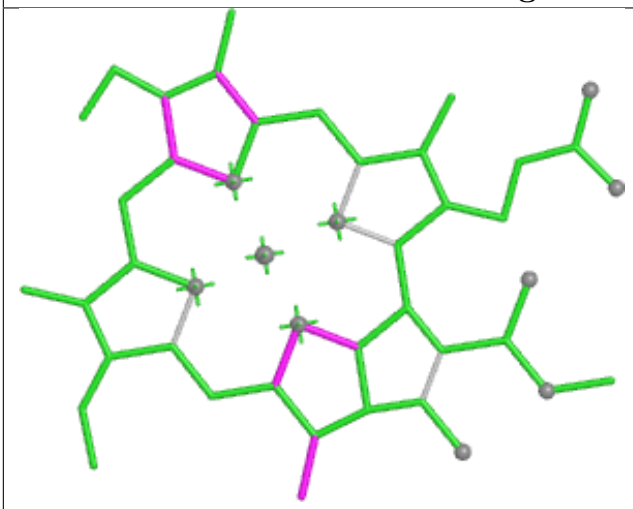


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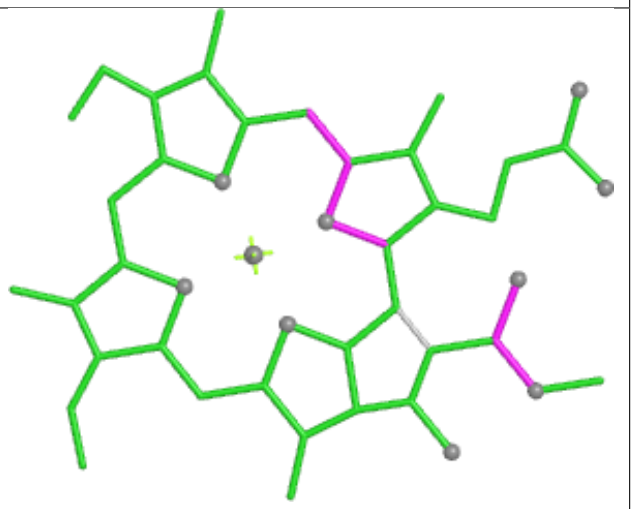


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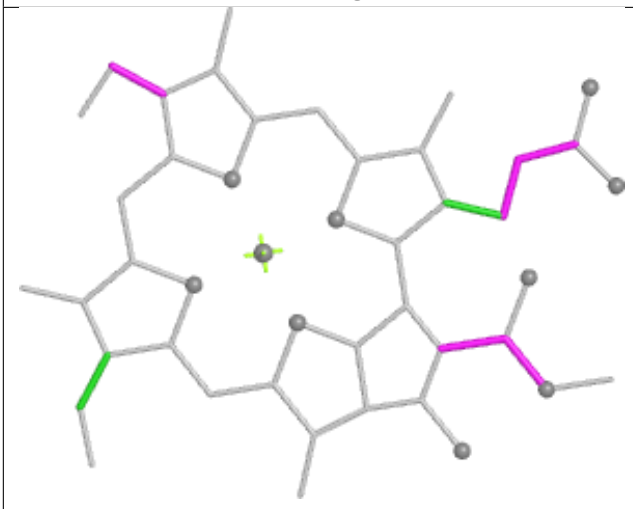
Ligand CLA W 614



Bond lengths



Bond angles

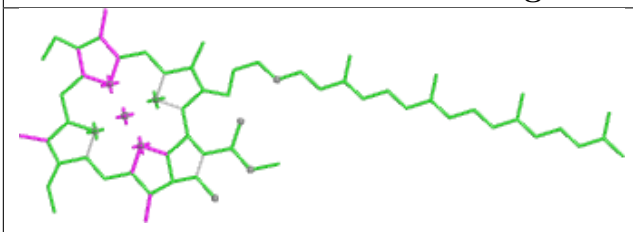


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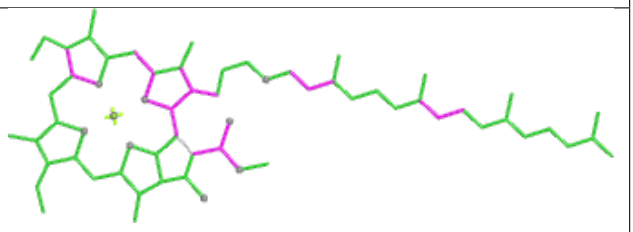


Rings

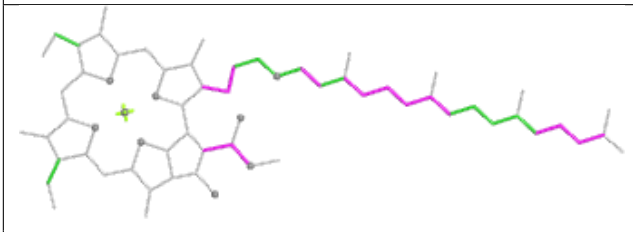
Ligand CLA B 810



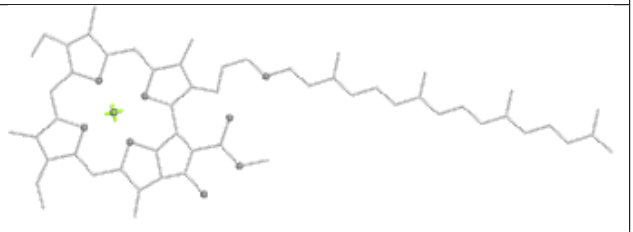
Bond lengths



Bond angles

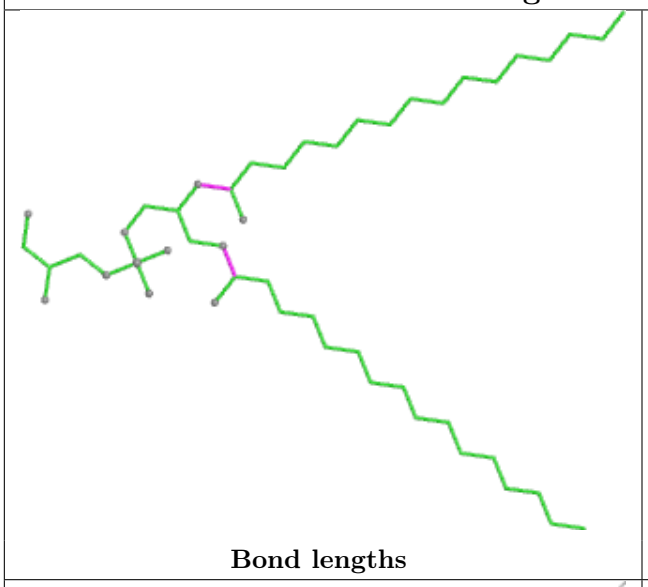


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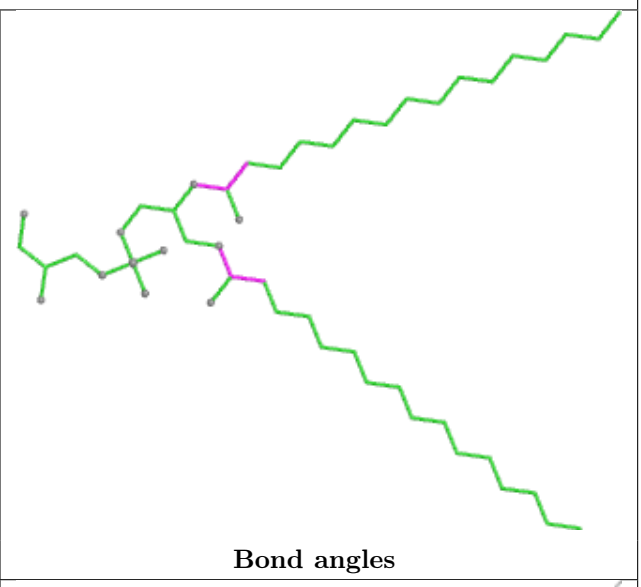


Rings

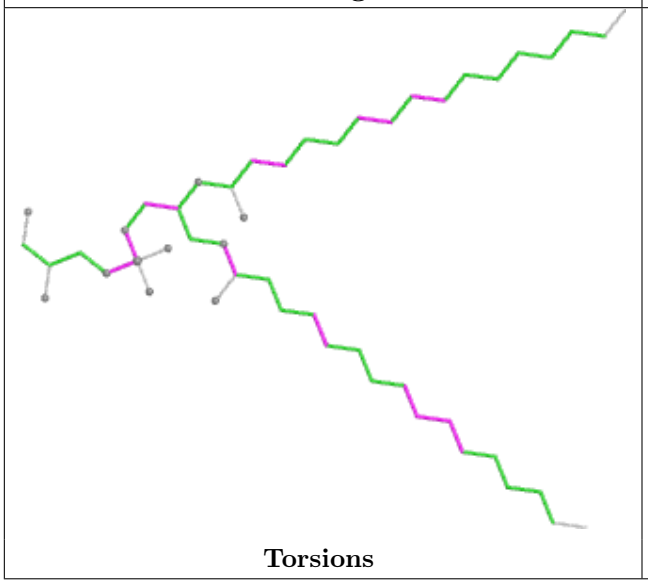
Ligand LHG A 846



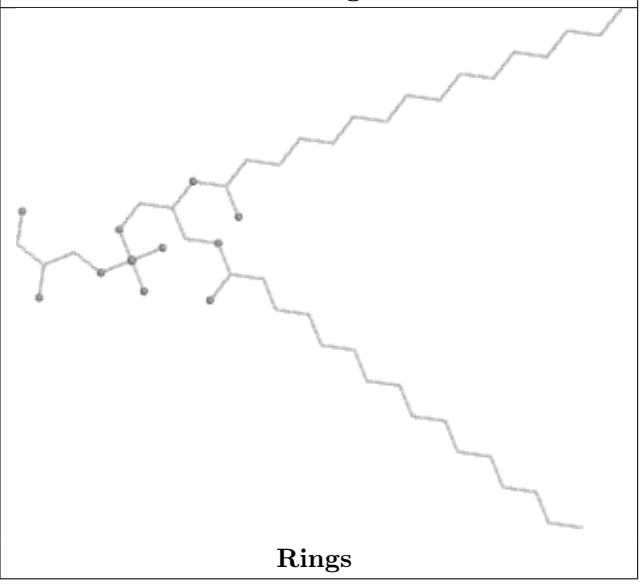
Bond lengths



Bond angles

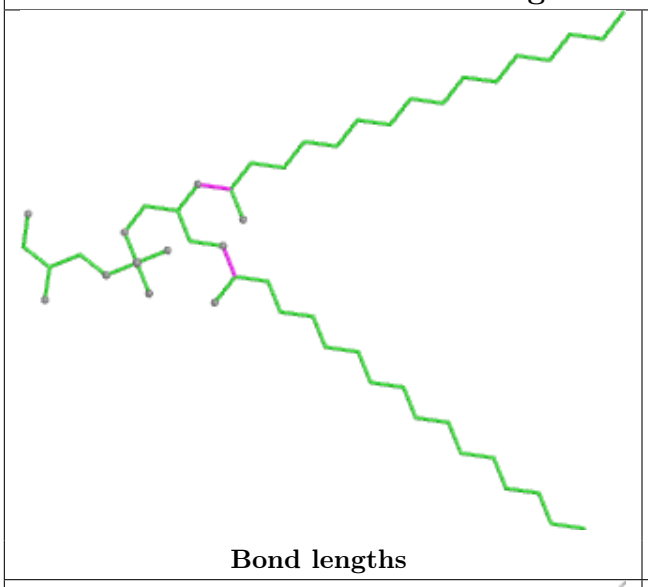


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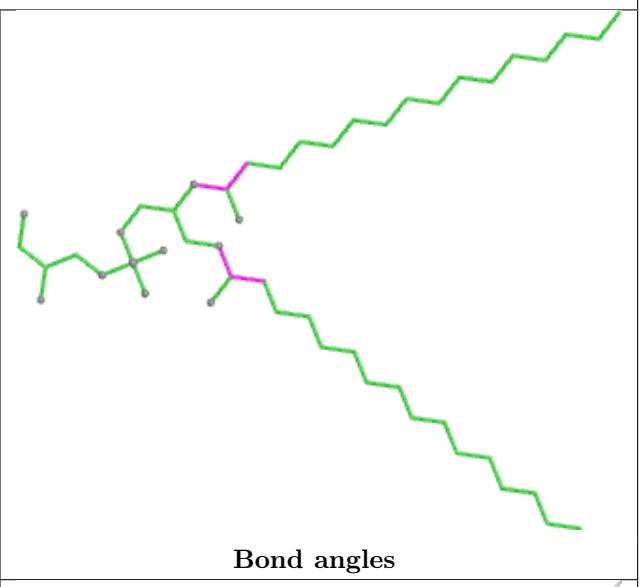


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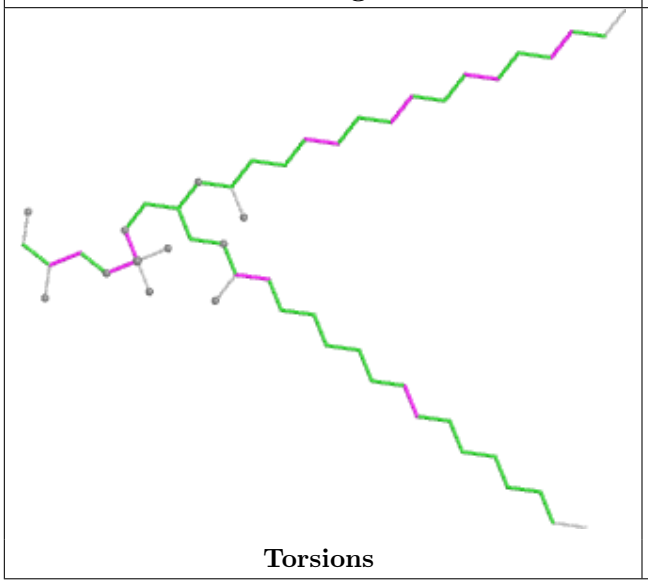
Ligand LHG 8 622



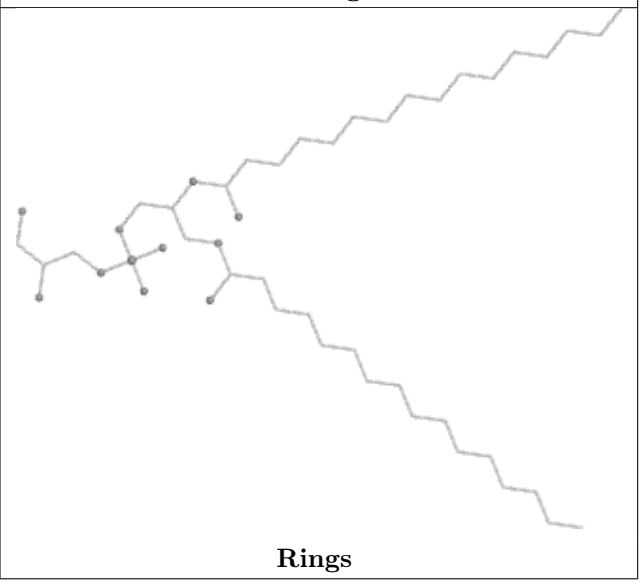
Bond lengths



Bond angles

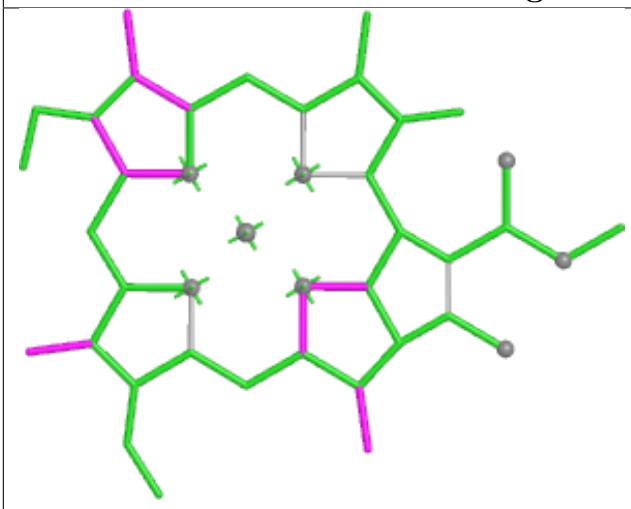


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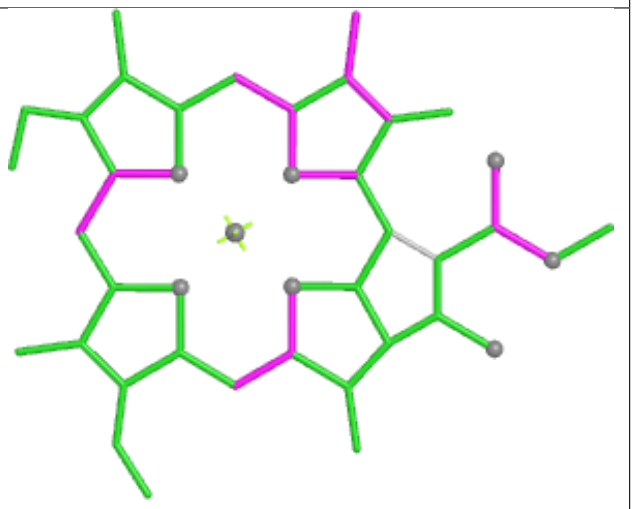


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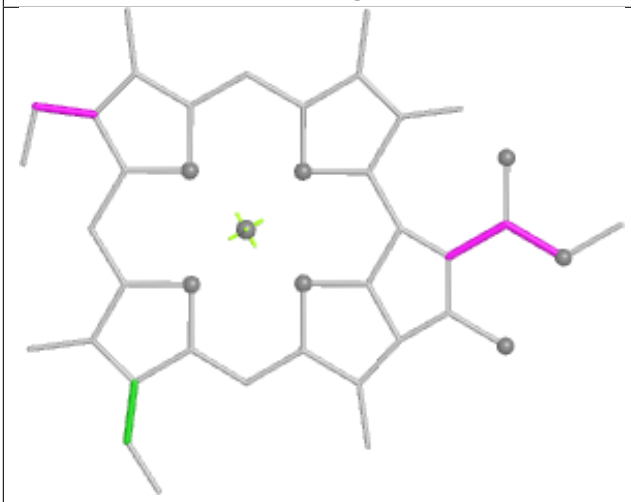
Ligand CLA F 304



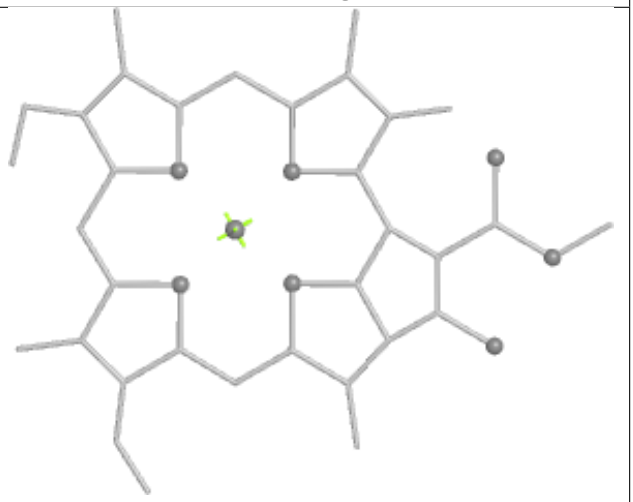
Bond lengths



Bond angles

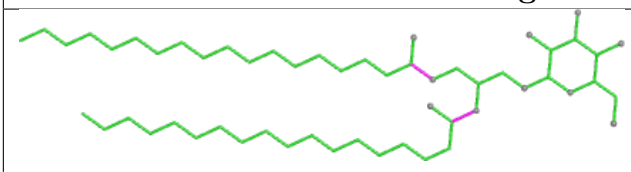


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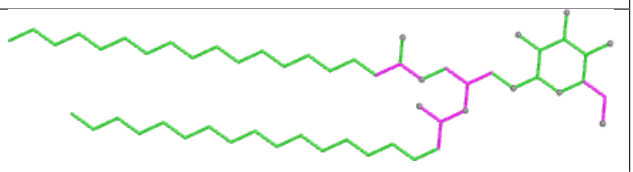


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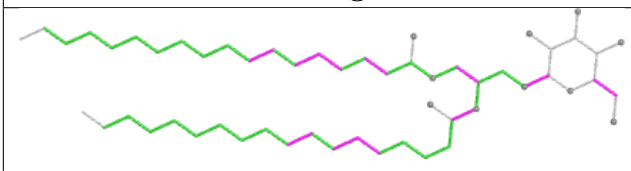
Ligand LMG H 205



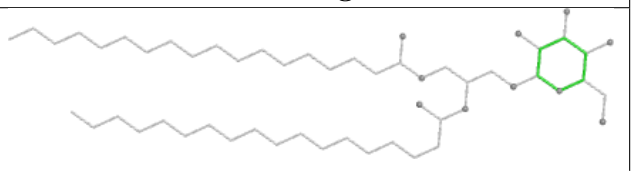
Bond lengths



Bond angles

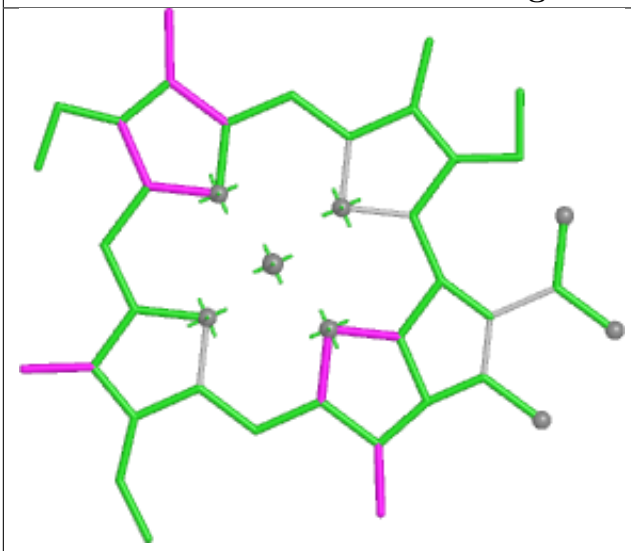


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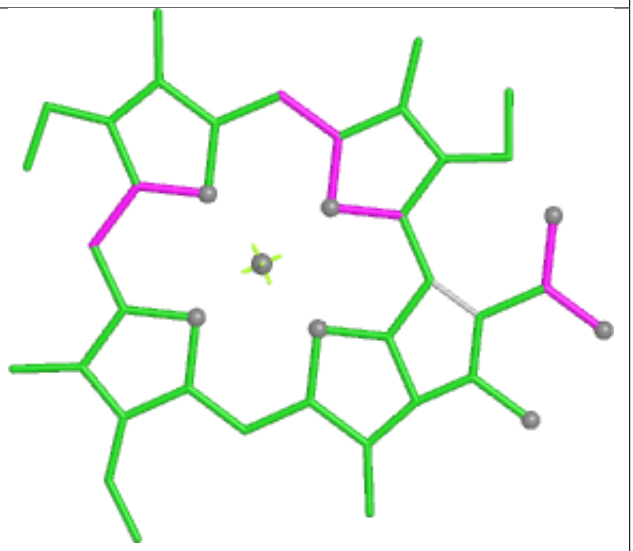


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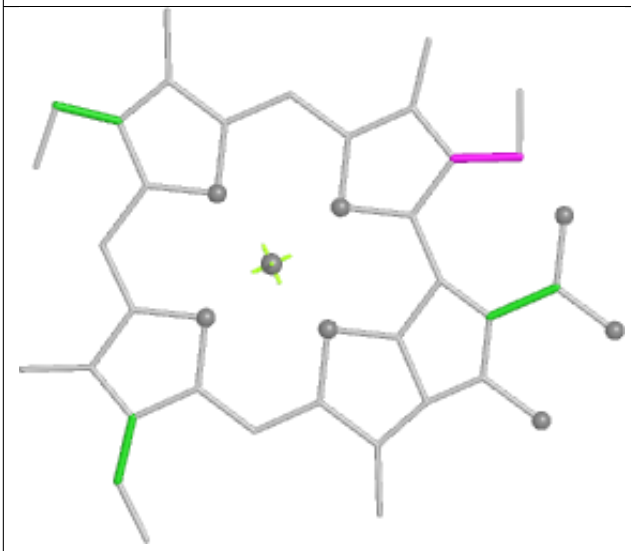
Ligand CLA 8 612



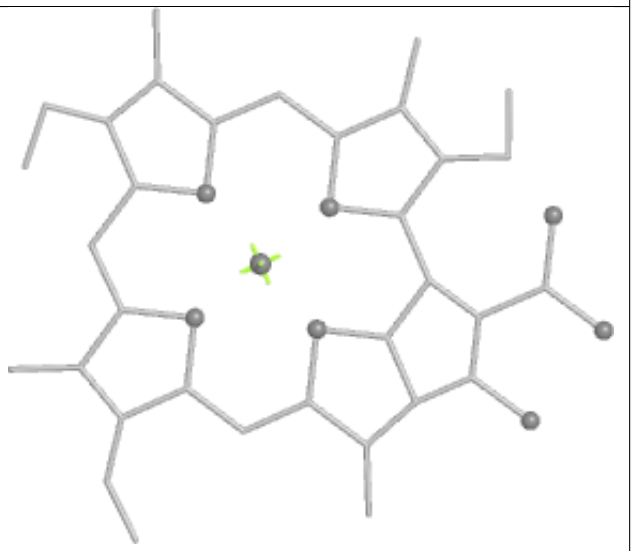
Bond lengths



Bond angles

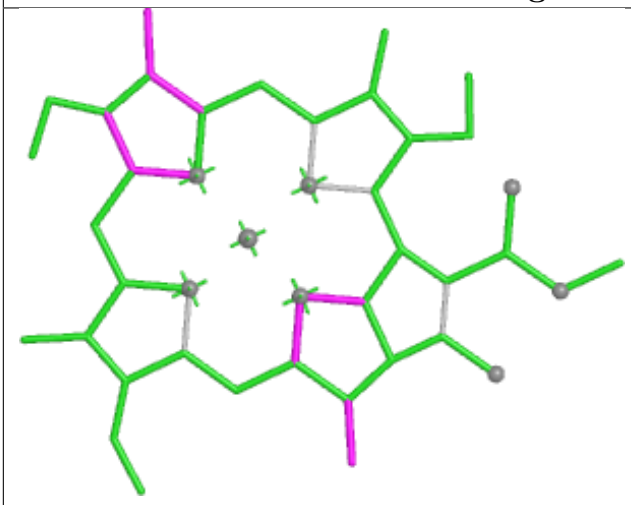


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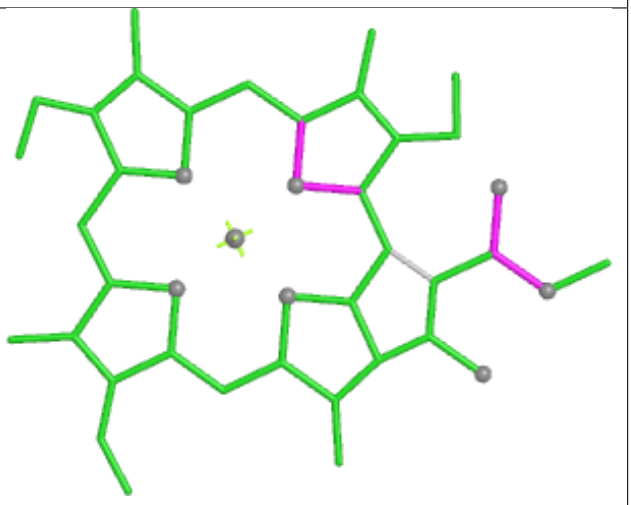


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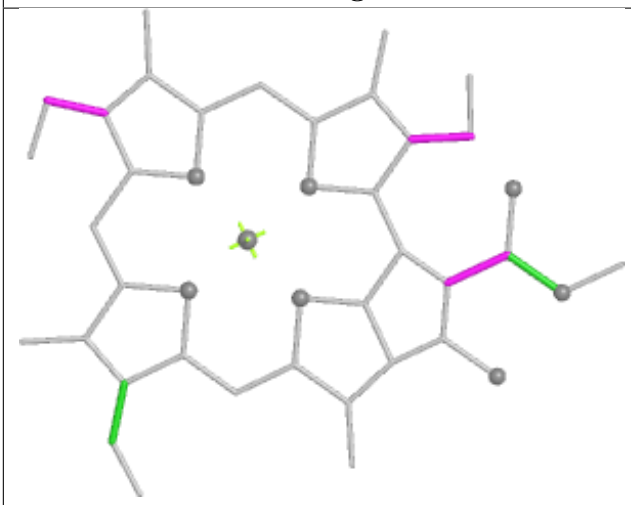
Ligand CLA 9 611



Bond lengths



Bond angles

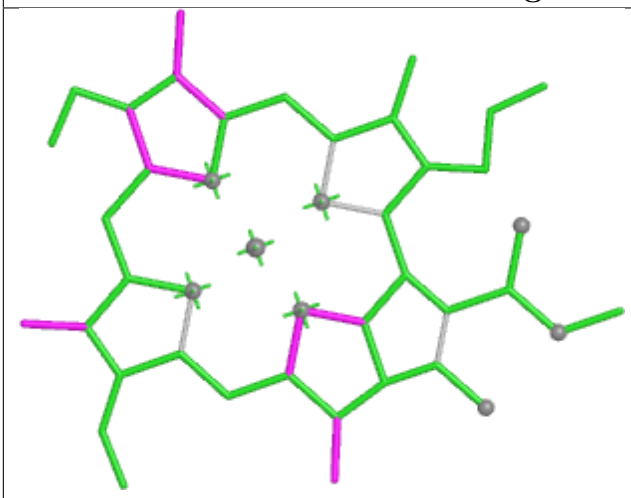


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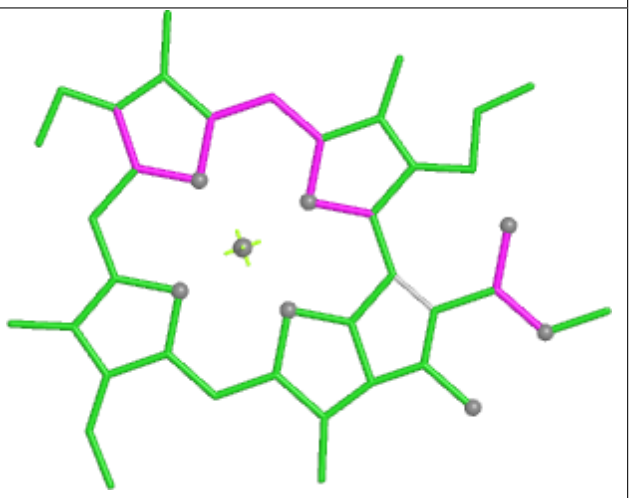


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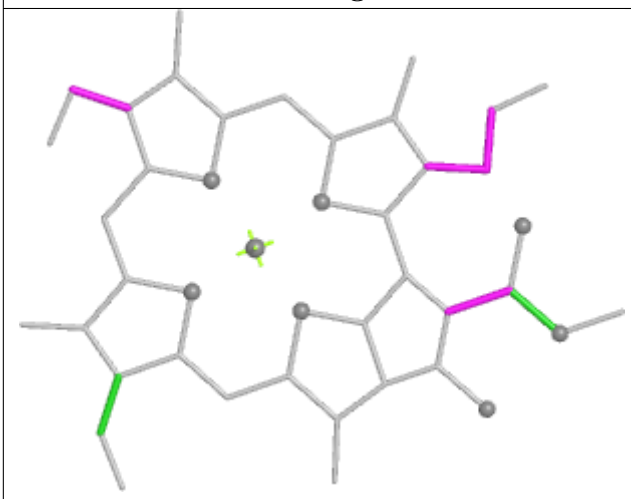
Ligand CLA B 812



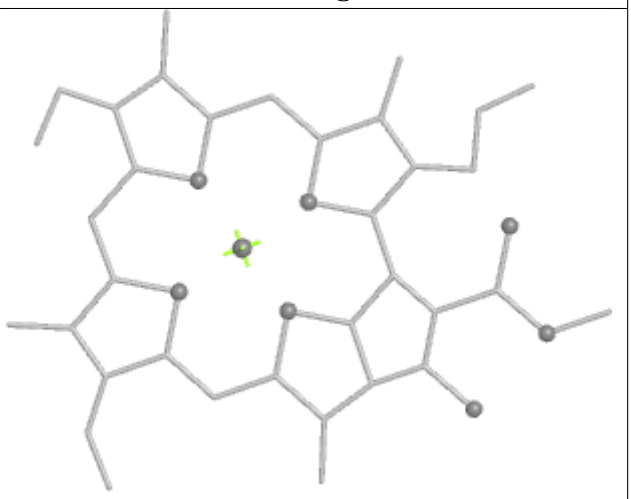
Bond lengths



Bond angles

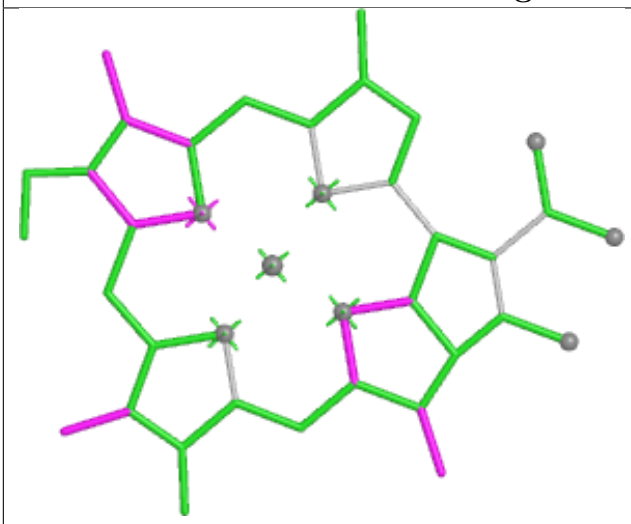


Torsions



Rings

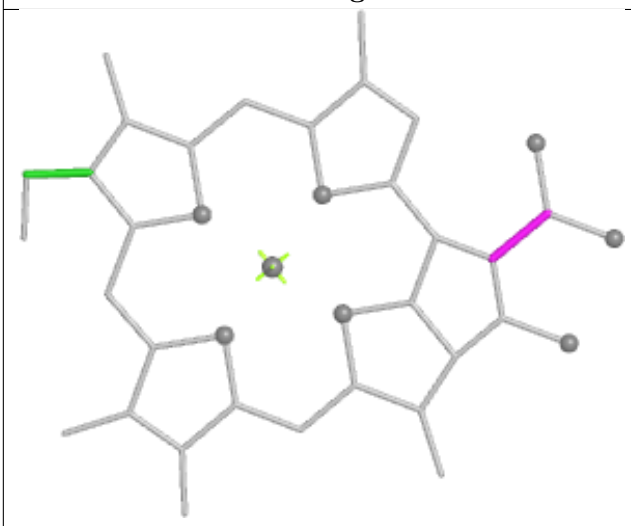
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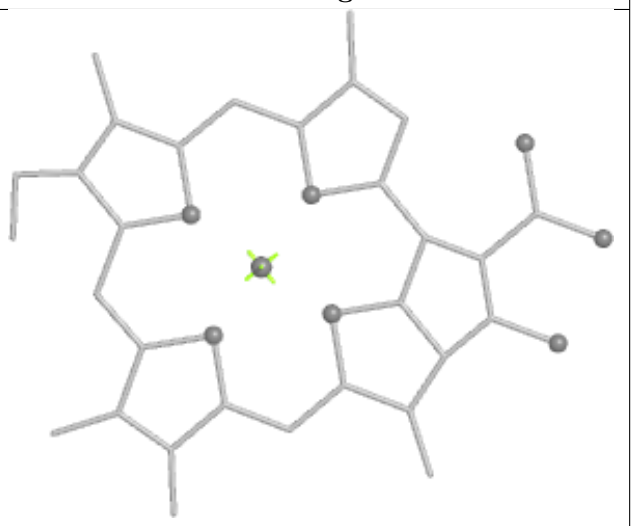
Bond lengths



Bond angles

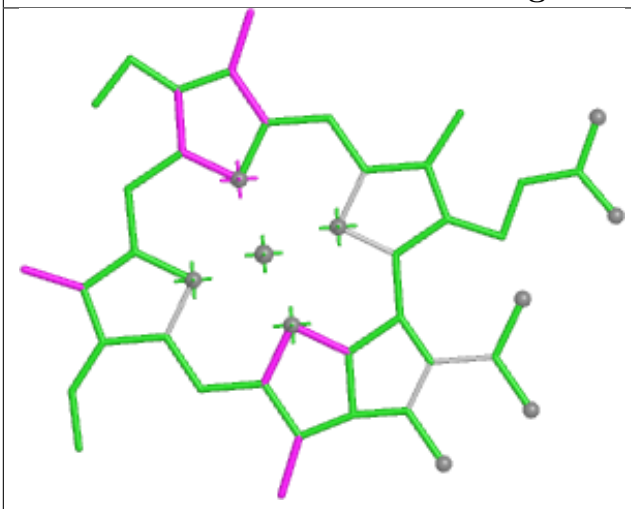


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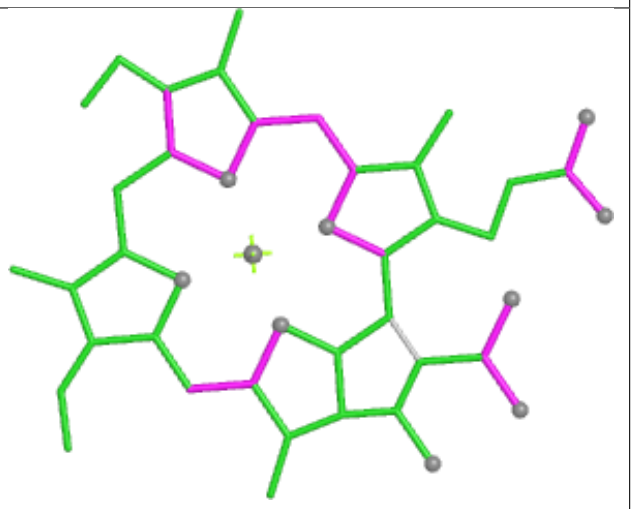


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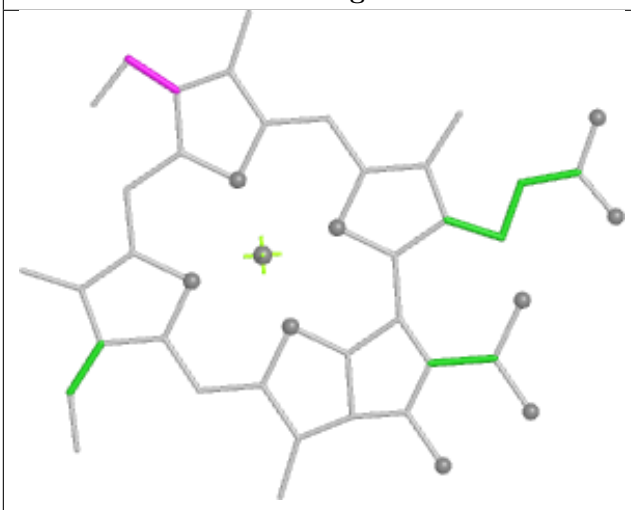
Ligand CLA 2 607



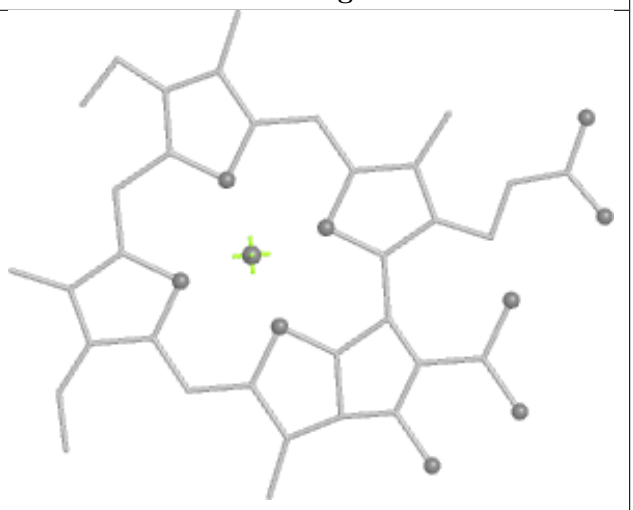
Bond lengths



Bond angles

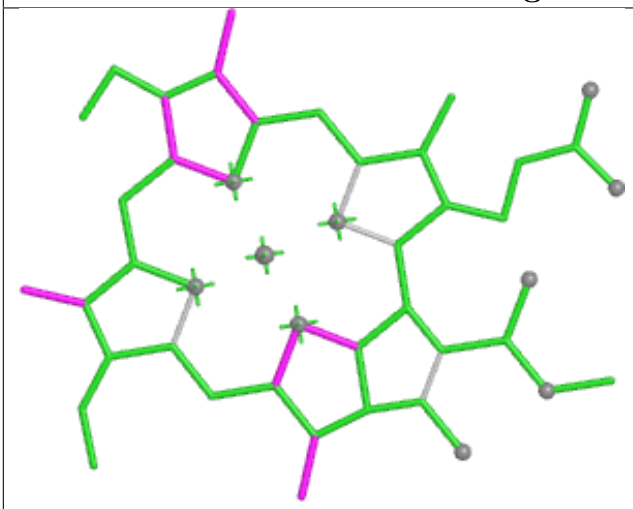


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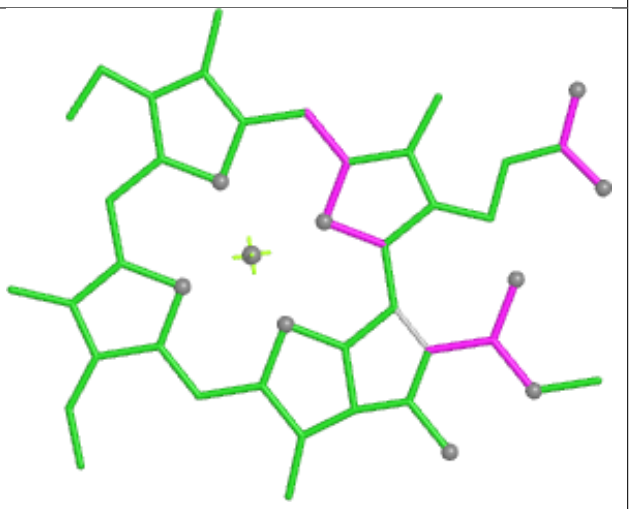


Rings

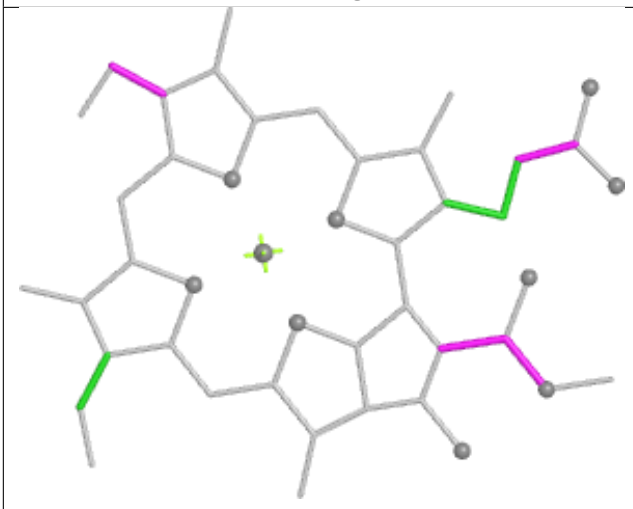
Ligand CLA V 612



Bond lengths



Bond angles

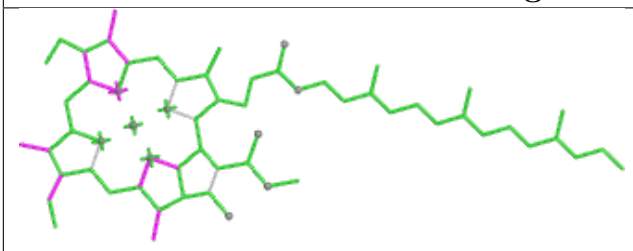


Torsions

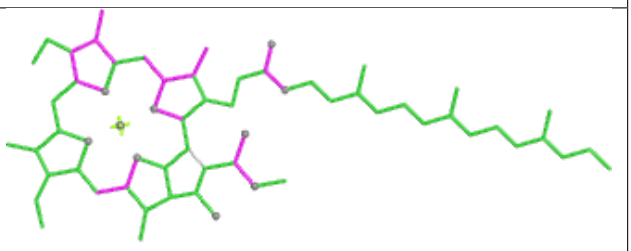


Rings

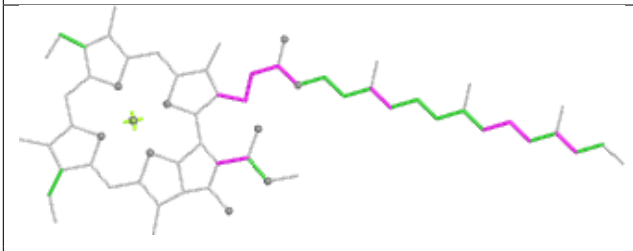
Ligand CLA B 827



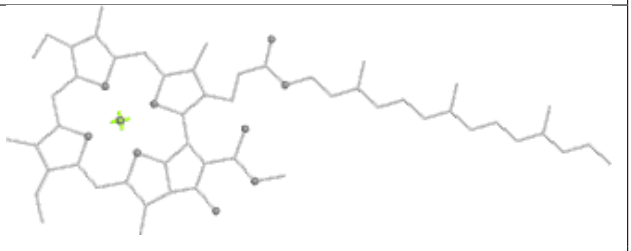
Bond lengths



Bond angles

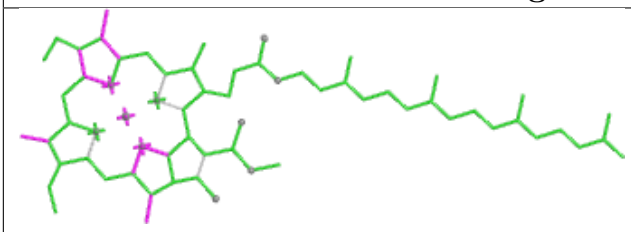


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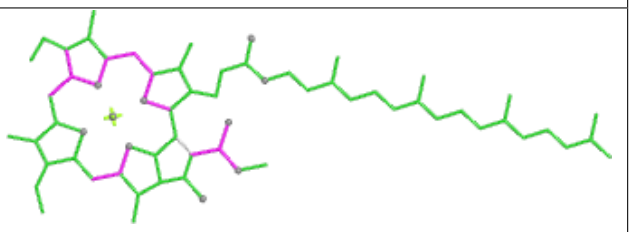


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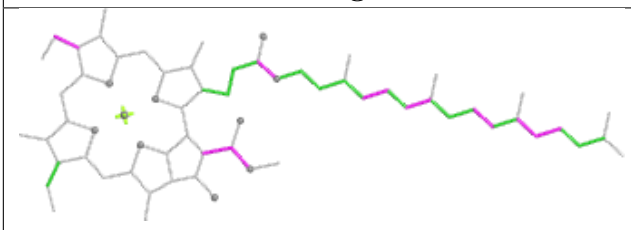
Ligand CLA 5 607



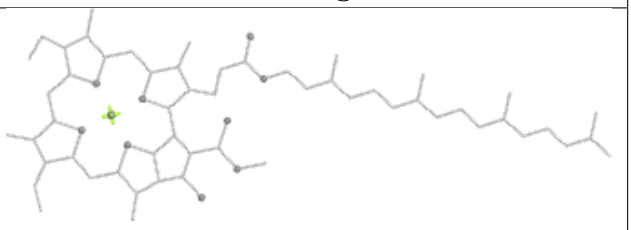
Bond lengths



Bond angles

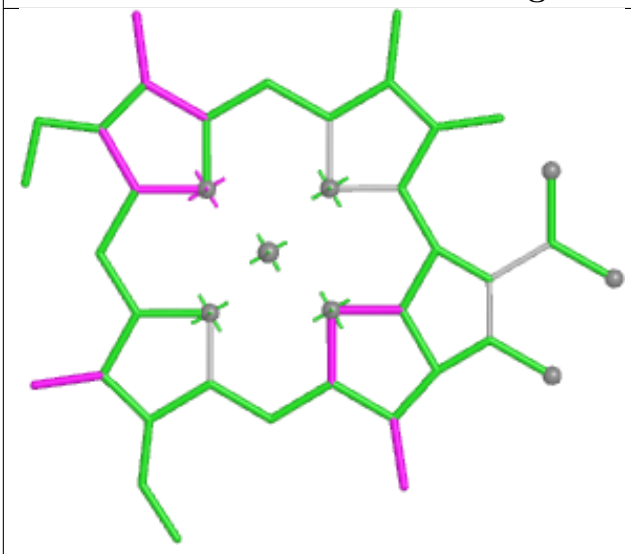


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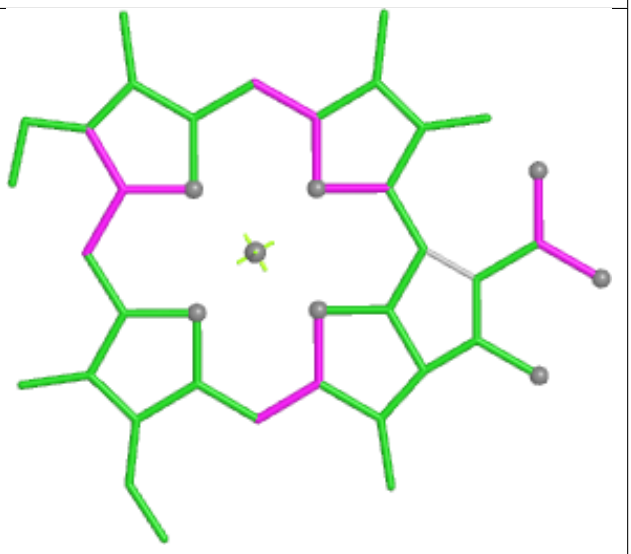


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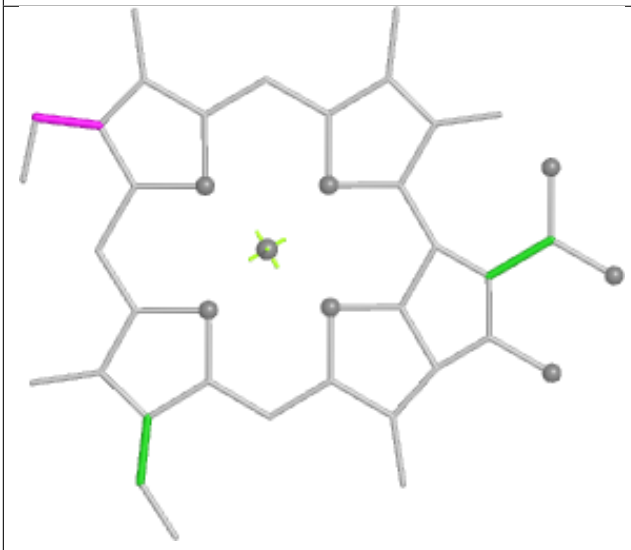
Ligand CLA 3 617



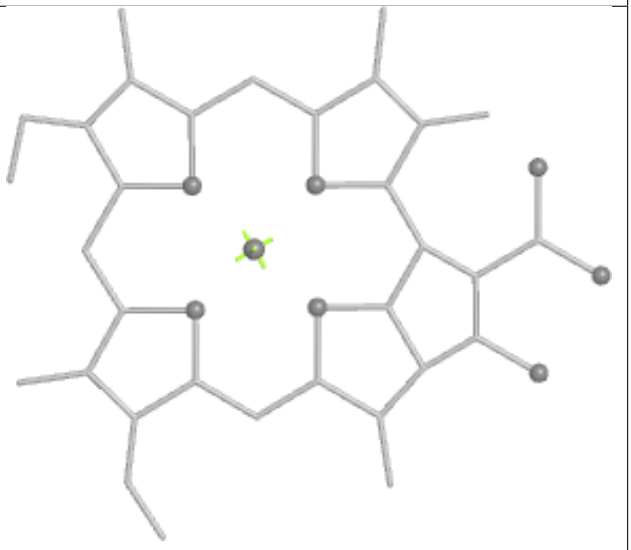
Bond lengths



Bond angles

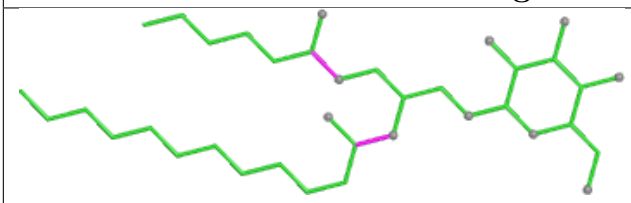


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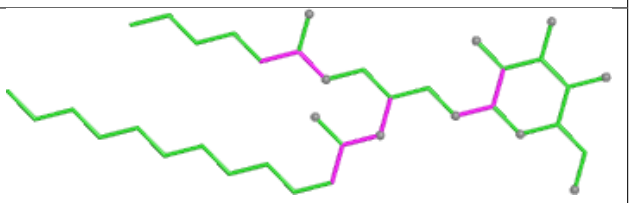


Rings

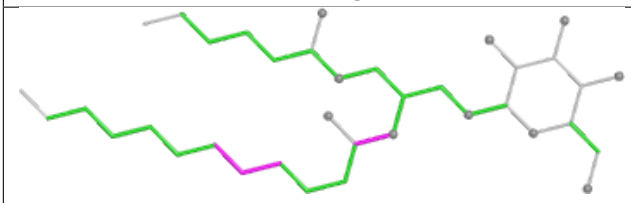
Ligand LMG L 2631



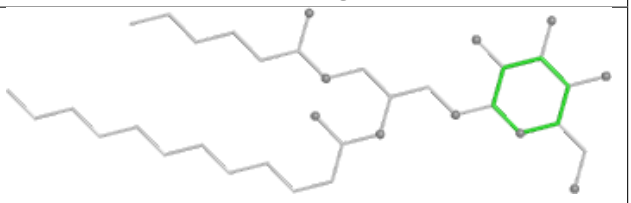
Bond lengths



Bond angles

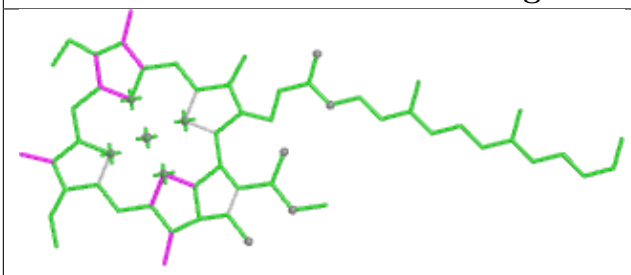


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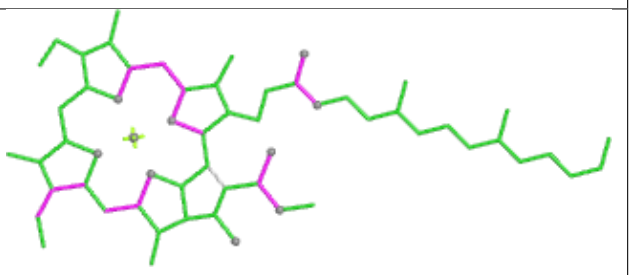


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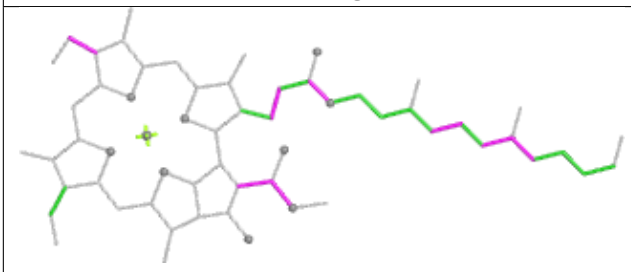
Ligand CLA U 613



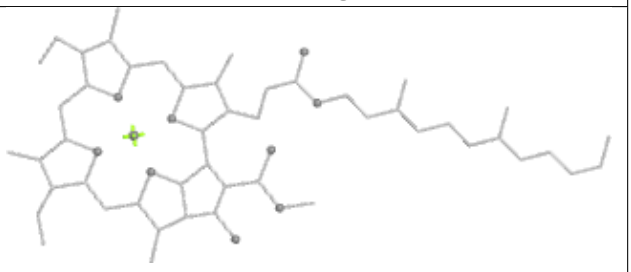
Bond lengths



Bond angles

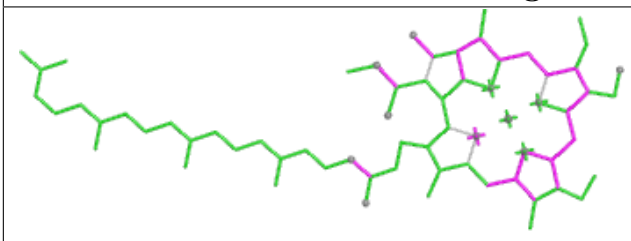


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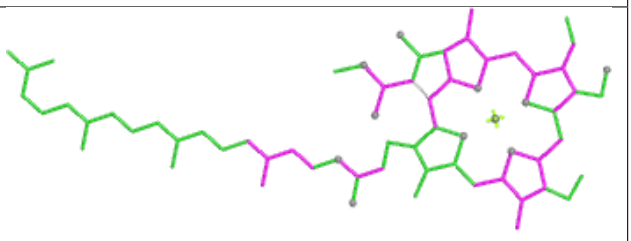


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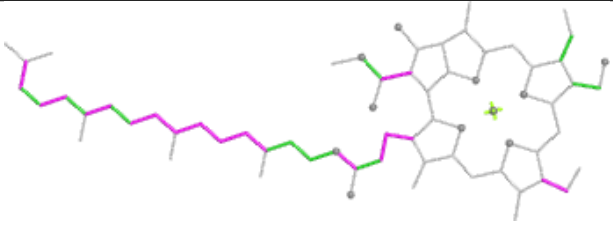
Ligand CHL Y 601



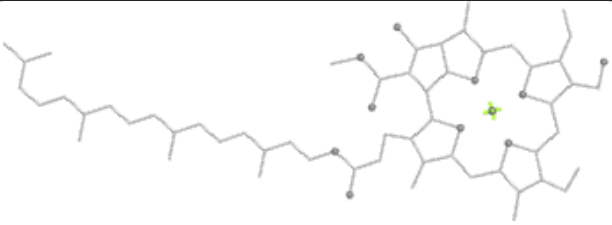
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Bond angles

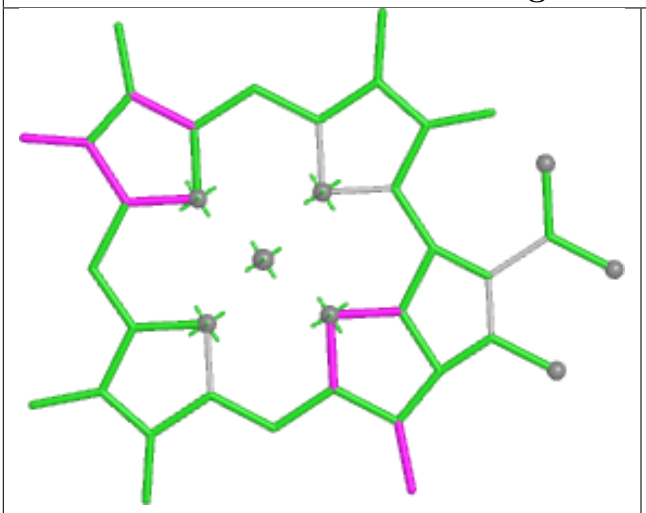


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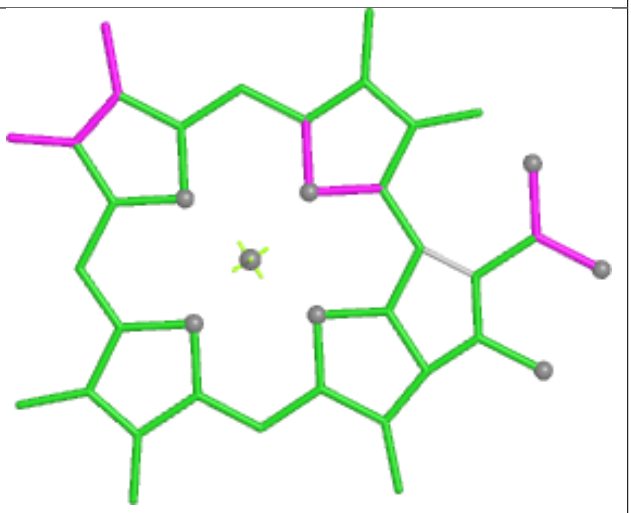


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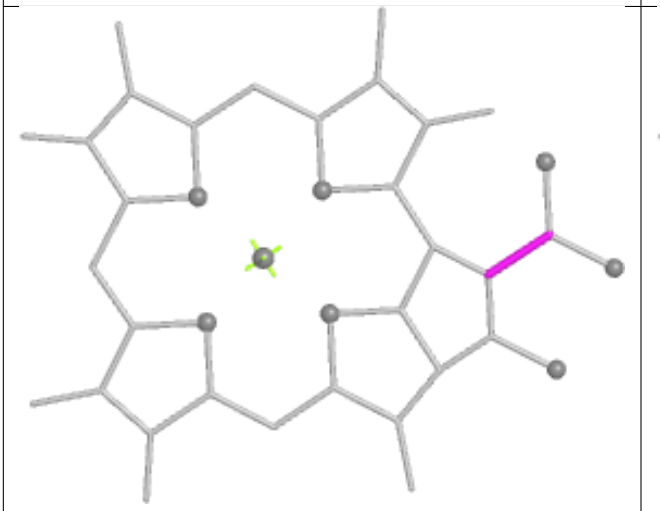
Ligand CLA 3 611



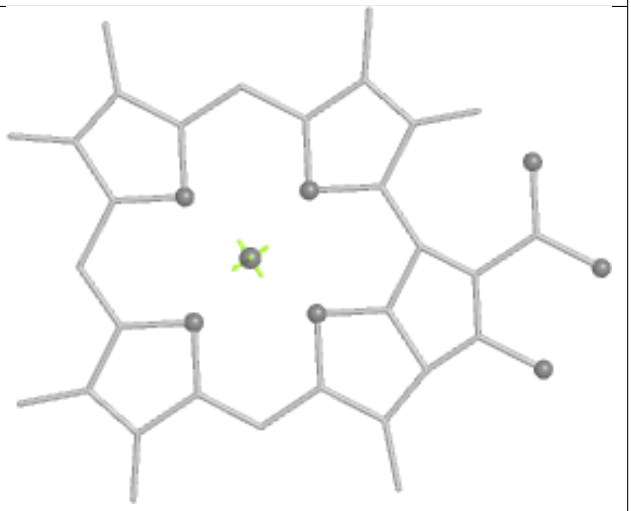
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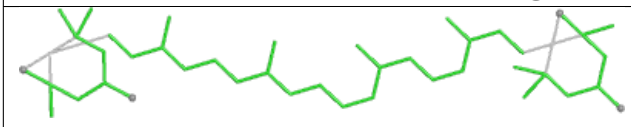


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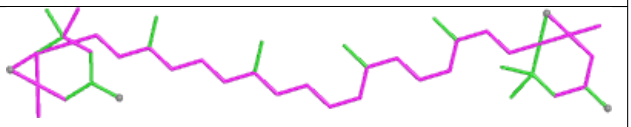


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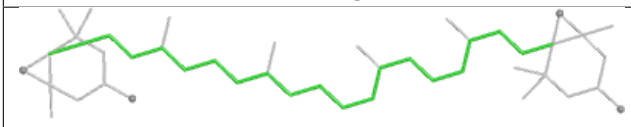
Ligand XAT 1 618



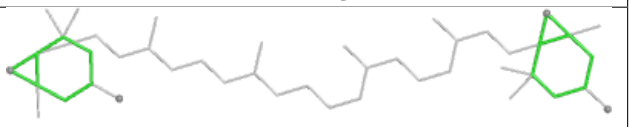
Bond lengths



Bond angles

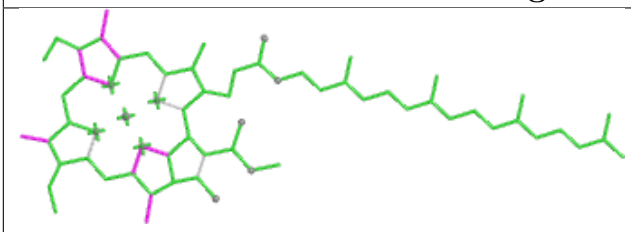


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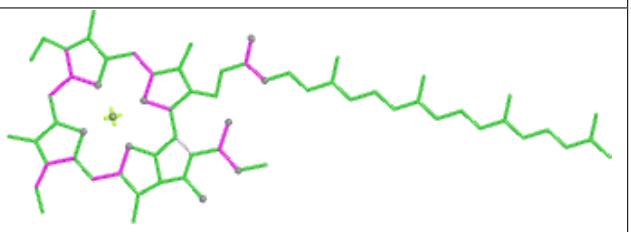


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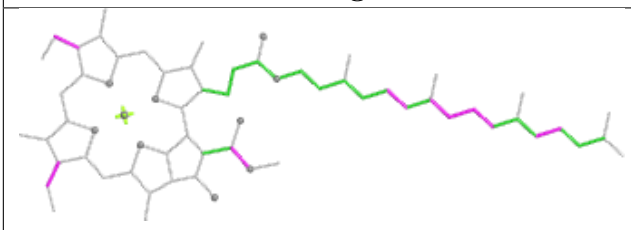
Ligand CLA 4 608



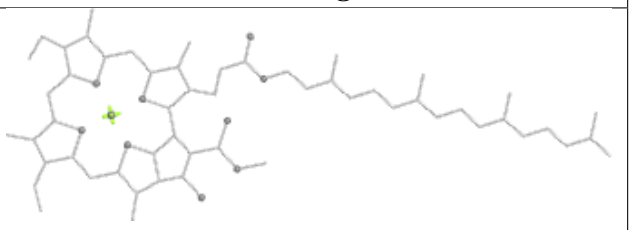
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Bond angles

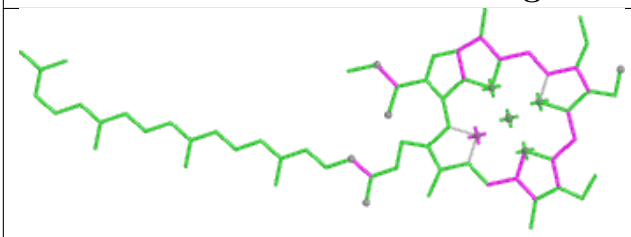


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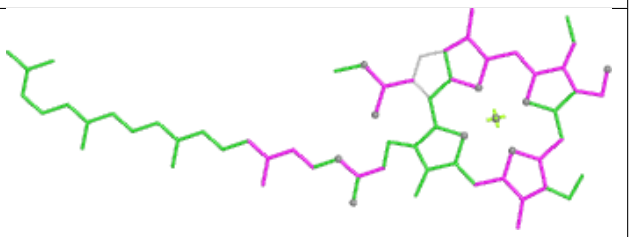


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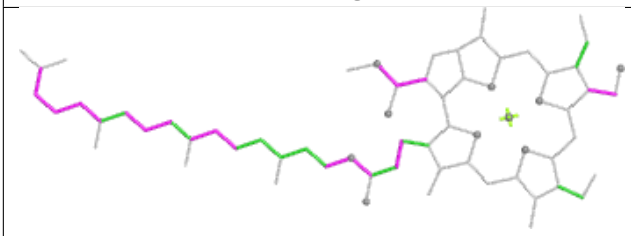
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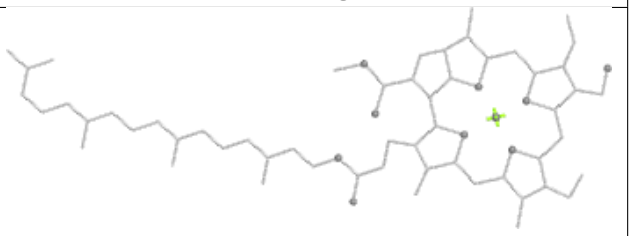
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Bond angles

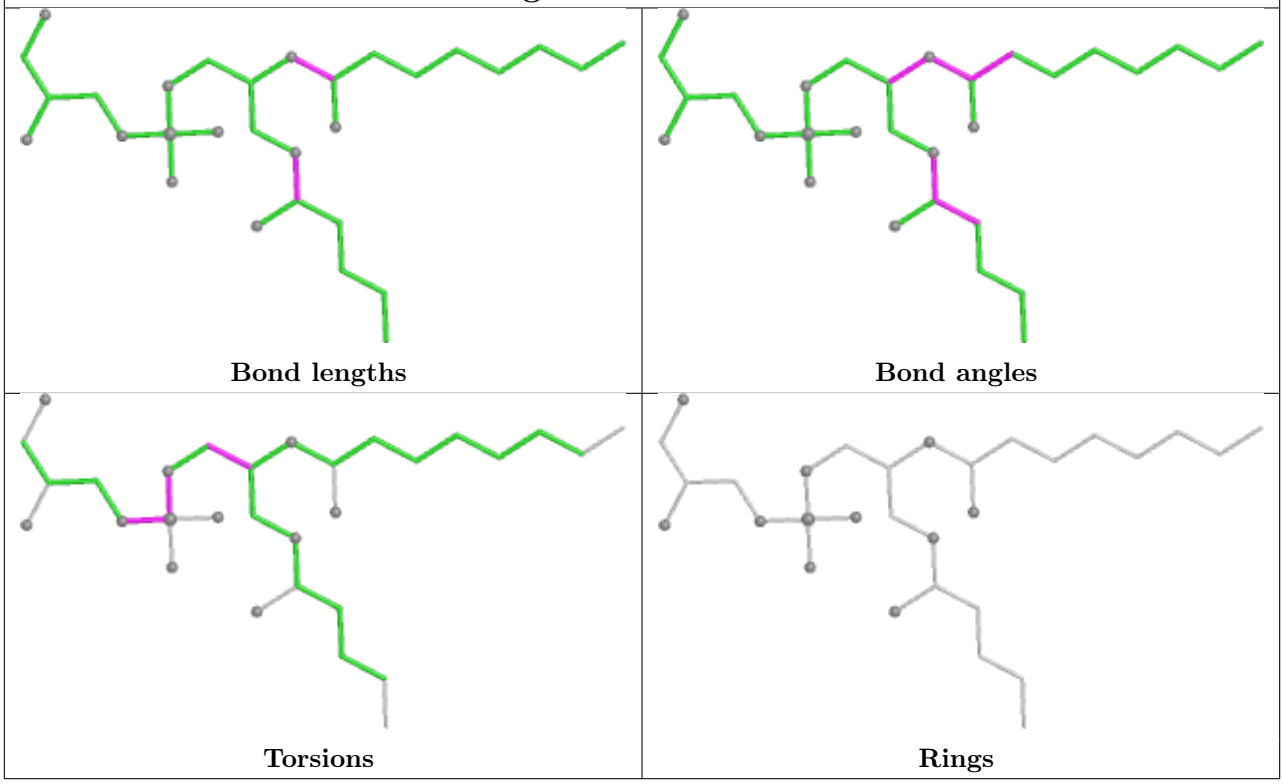


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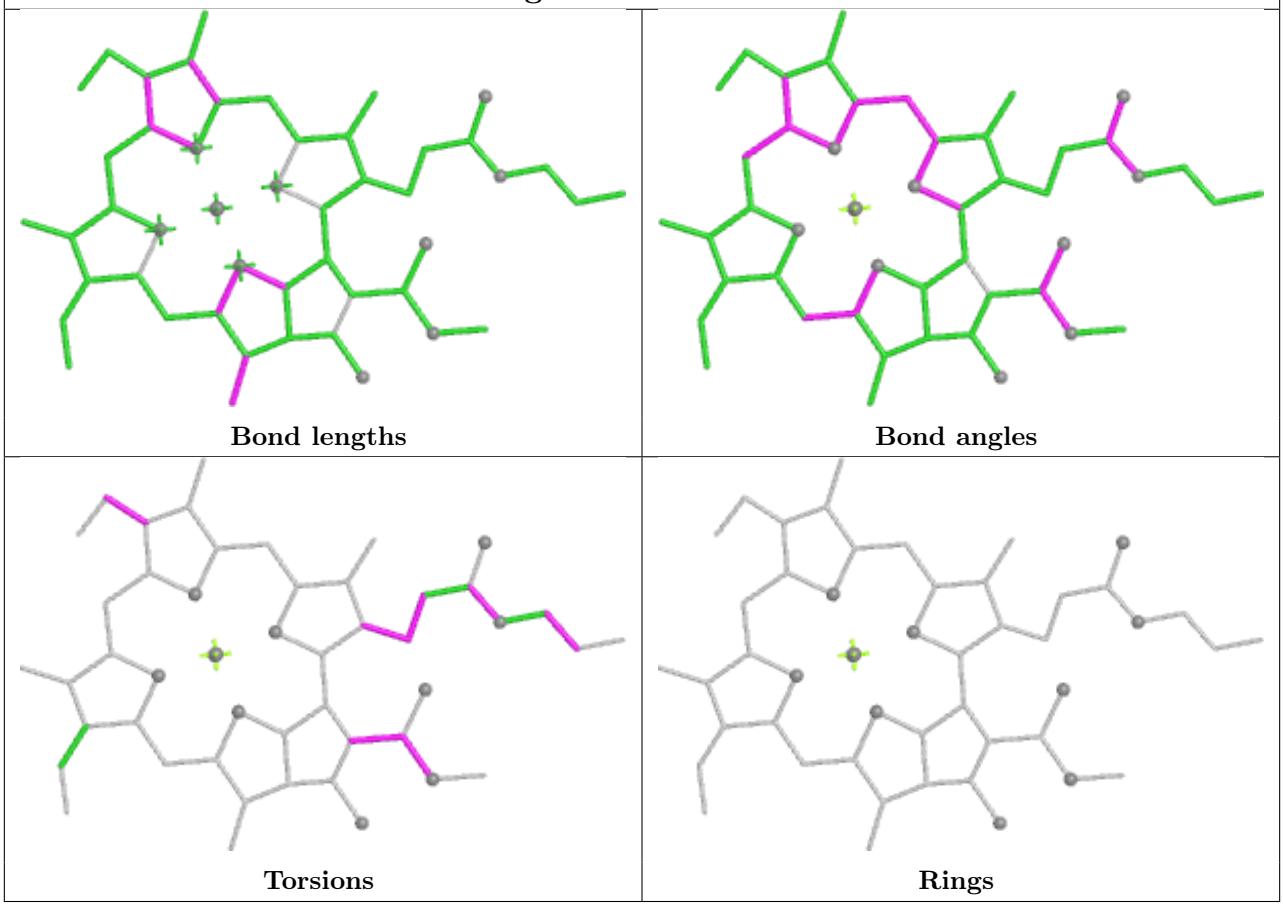


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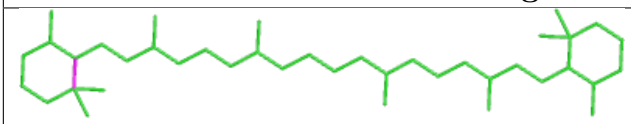
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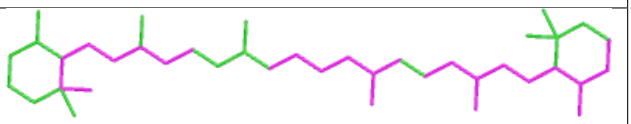
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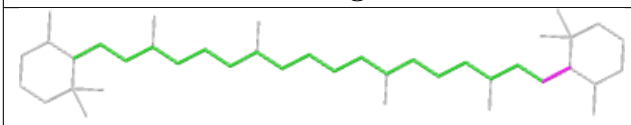
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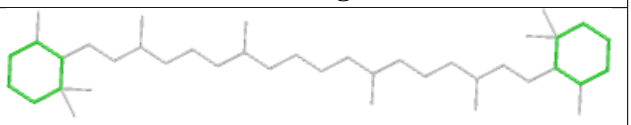
Bond lengths



Bond angles

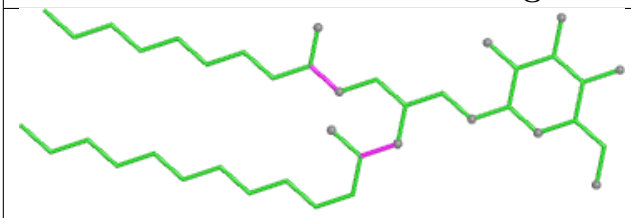


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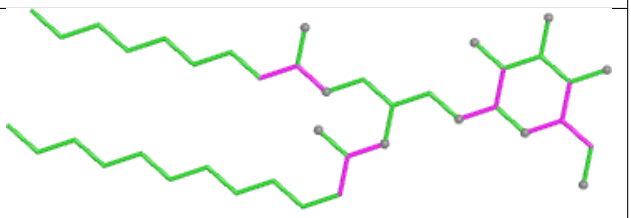


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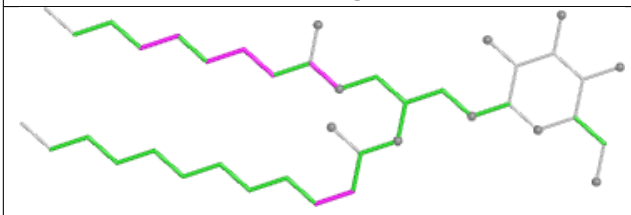
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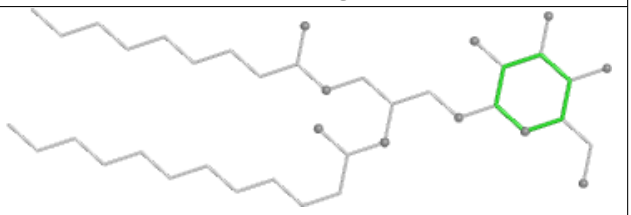
Bond lengths



Bond angles

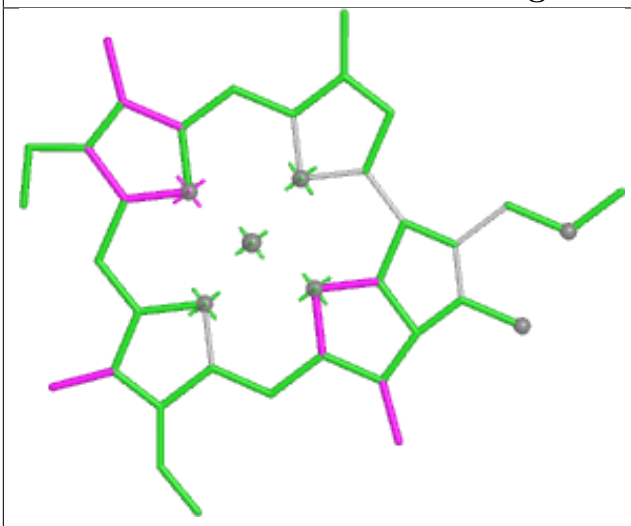


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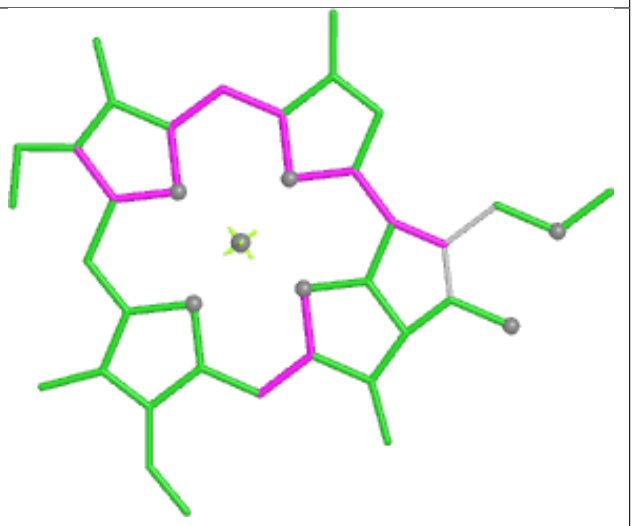


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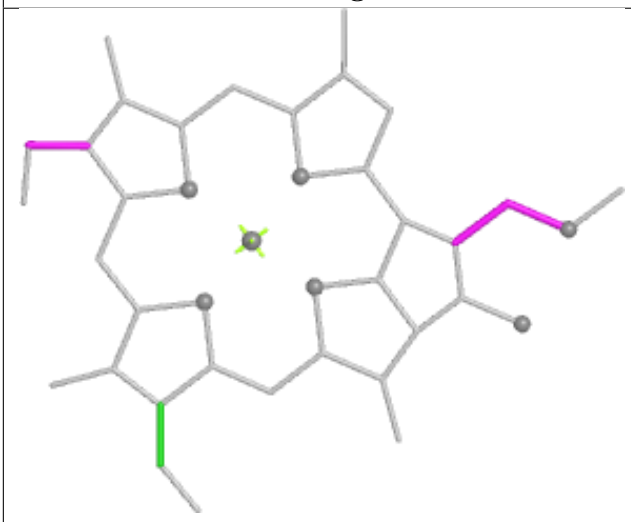
Ligand CLA 1 606



Bond lengths



Bond angles

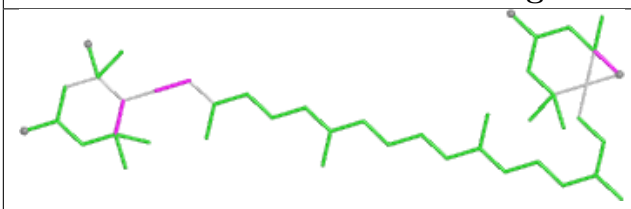


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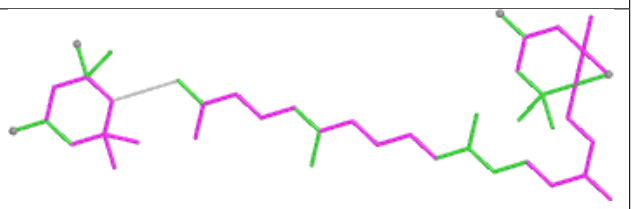


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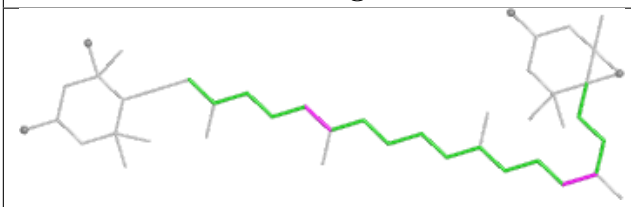
Ligand NEX 6 624



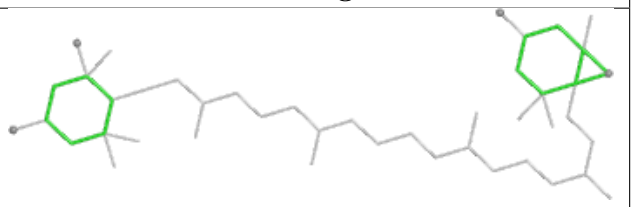
Bond lengths



Bond angles

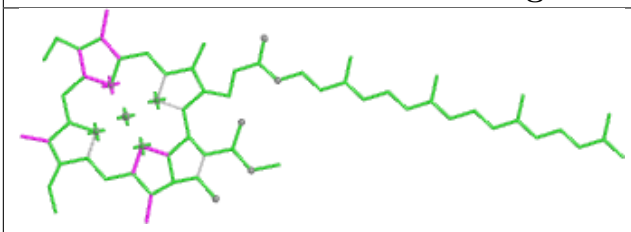


Torsions

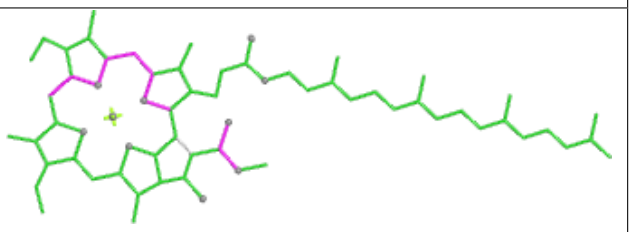


Rings

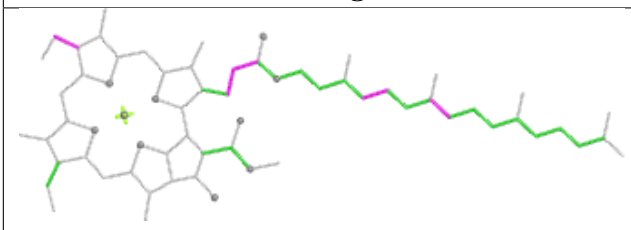
Ligand CLA Z 613



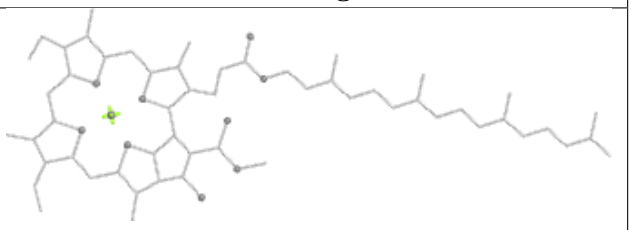
Bond lengths



Bond angles

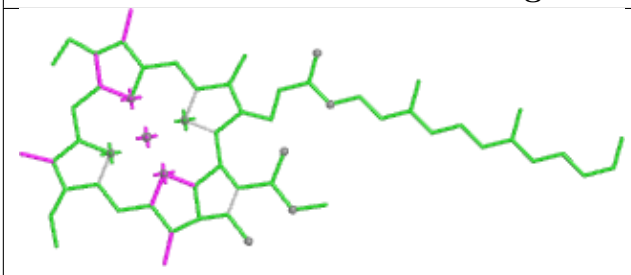


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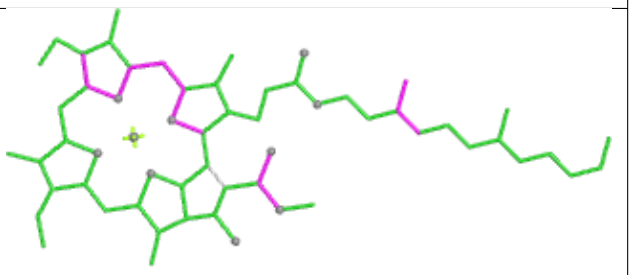


Rings

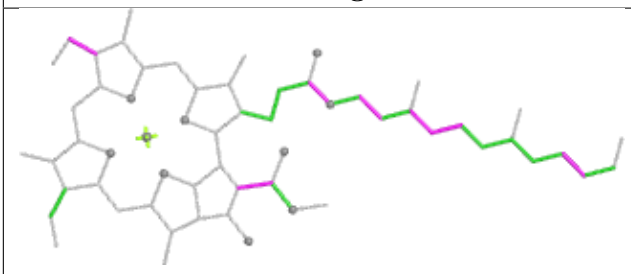
Ligand CLA B 817



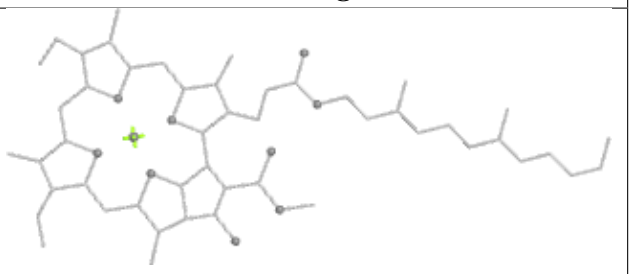
Bond lengths



Bond angles

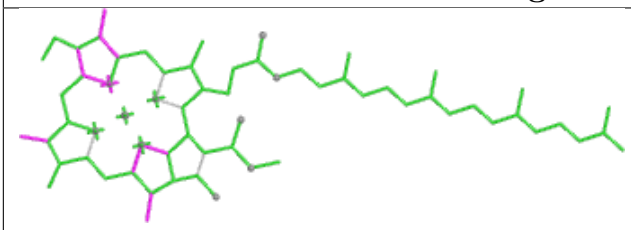


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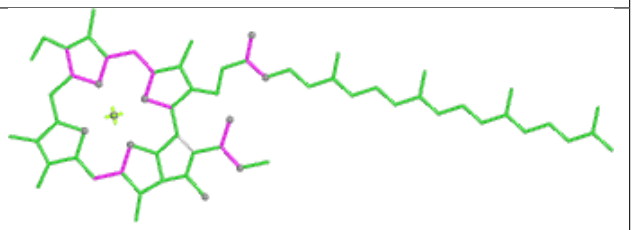


Rings

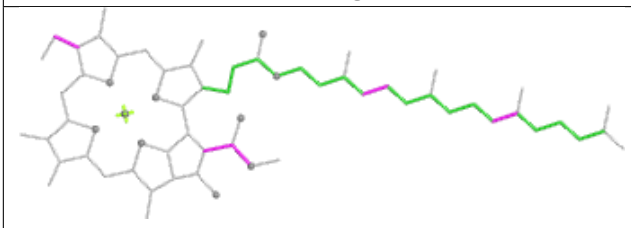
Ligand CLA 8 606



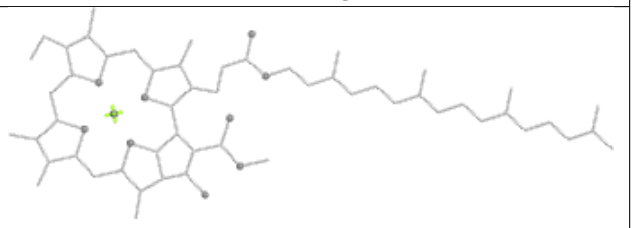
Bond lengths



Bond angles



Torsions

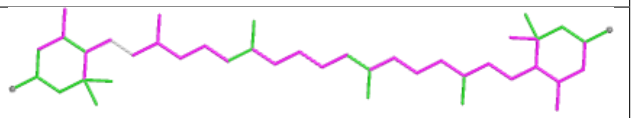


Rings

Ligand LUT 5 620



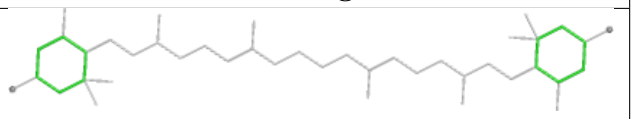
Bond lengths



Bond angles

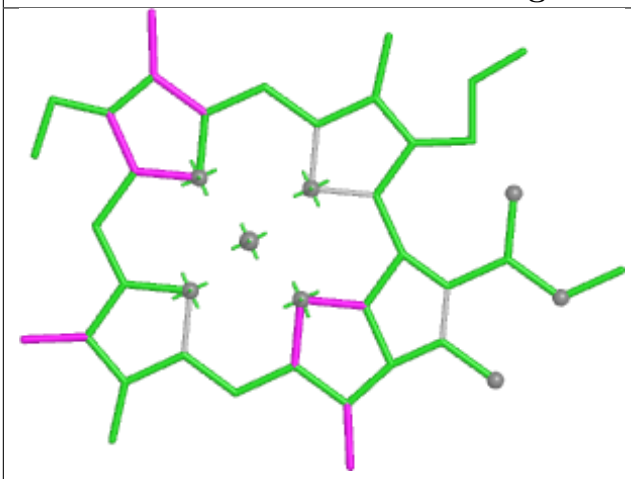


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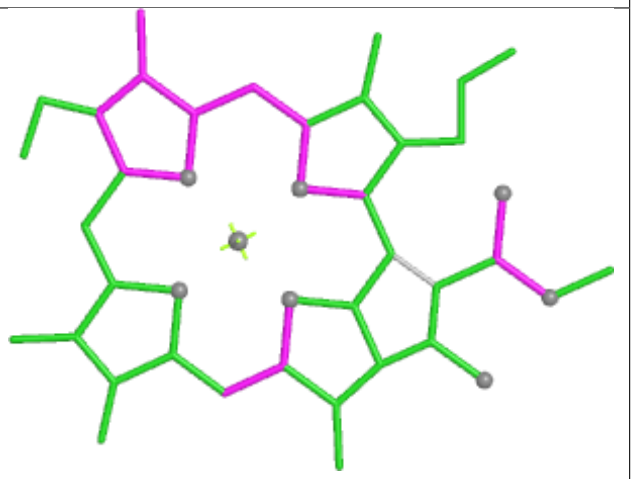


Rings

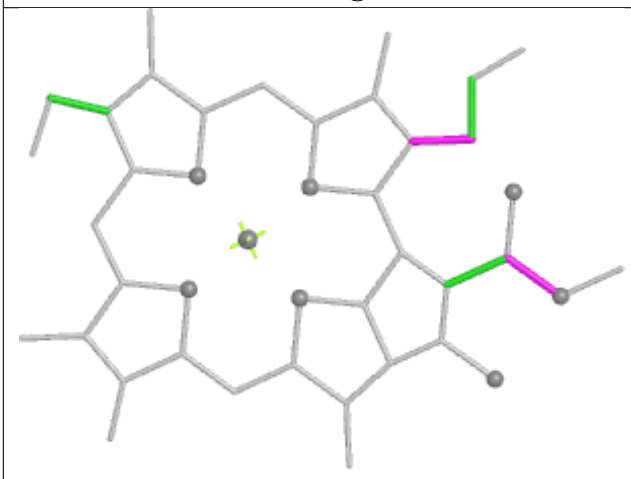
Ligand CLA 2 604



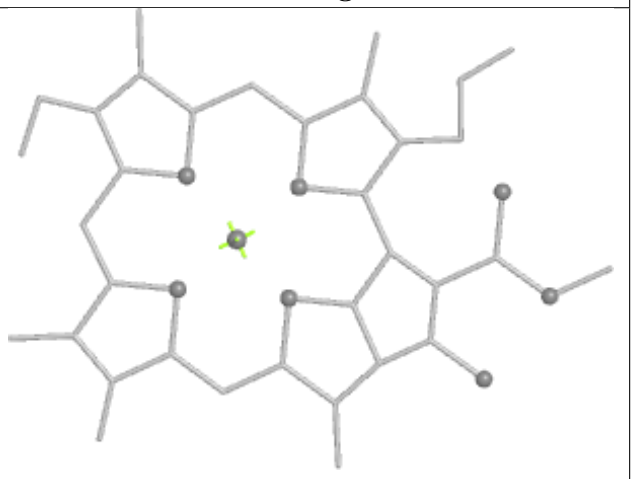
Bond lengths



Bond angles

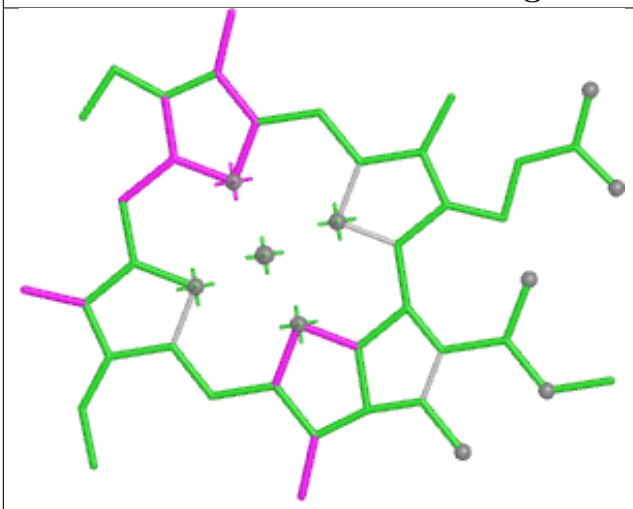


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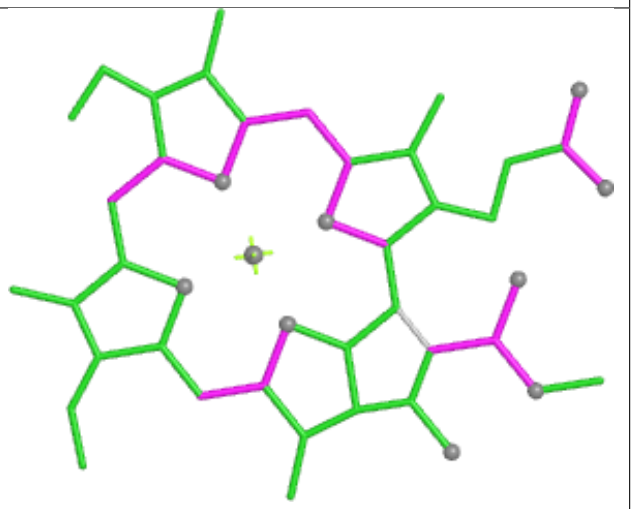


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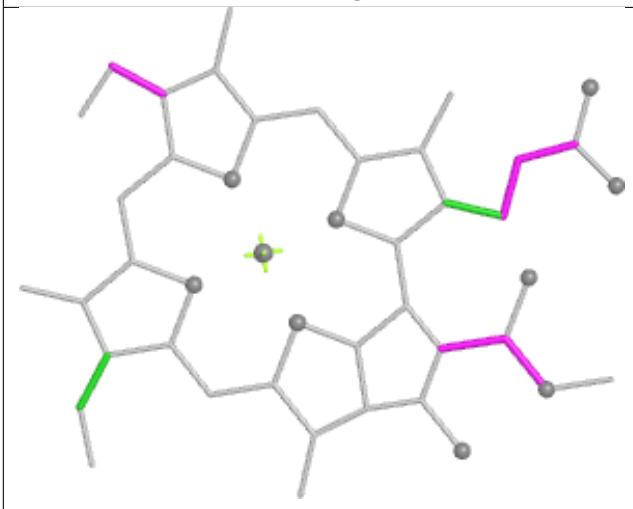
Ligand CLA A 837



Bond lengths



Bond angles

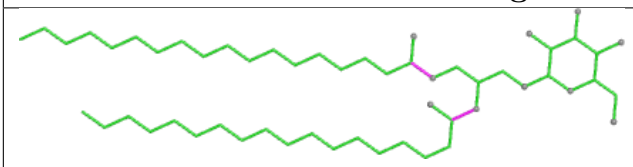


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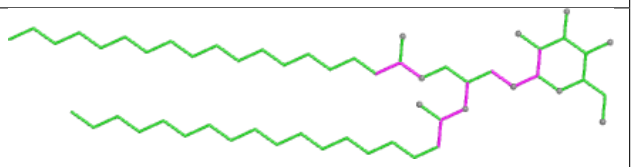


Rings

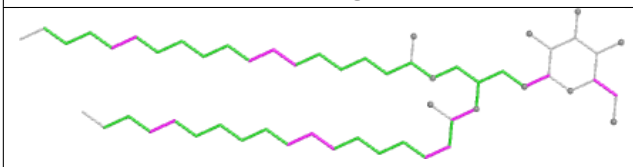
Ligand LMG V 2631



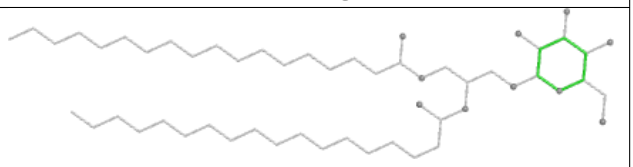
Bond lengths



Bond angles

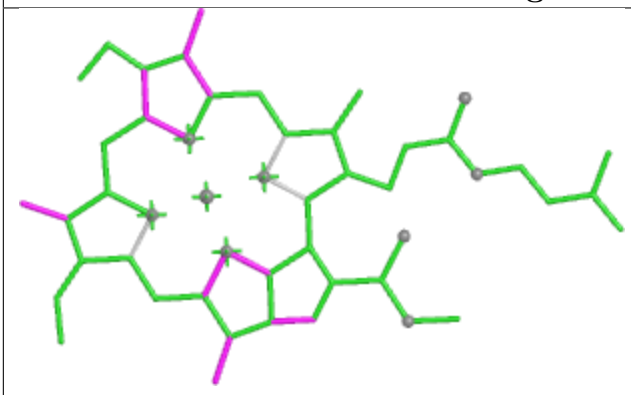


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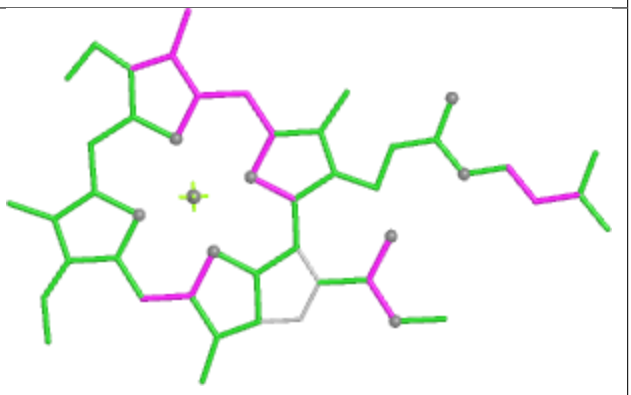


Rings

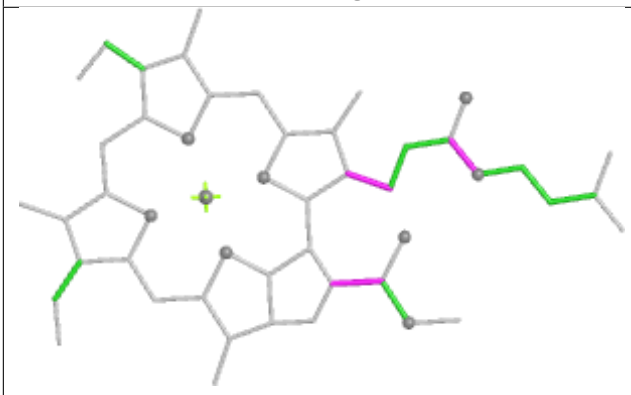
Ligand CLA Z 604



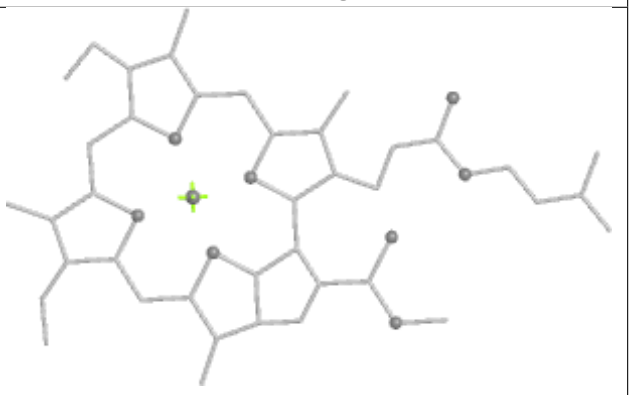
Bond lengths



Bond angles

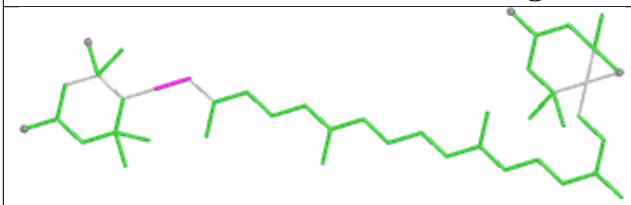


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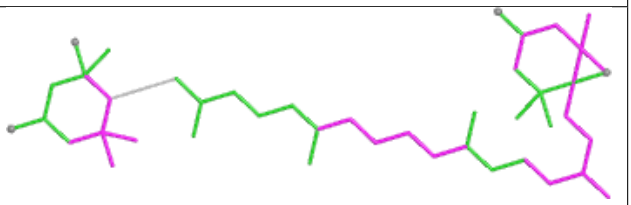


Rings

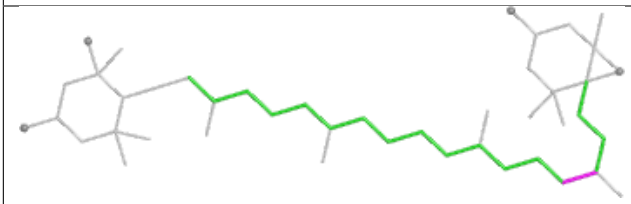
Ligand NEX 5 624



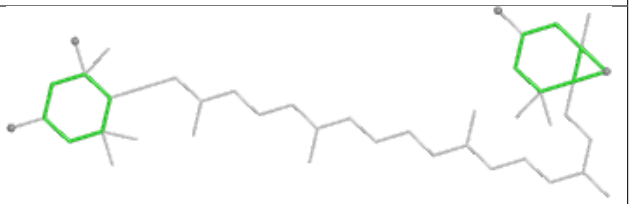
Bond lengths



Bond angles

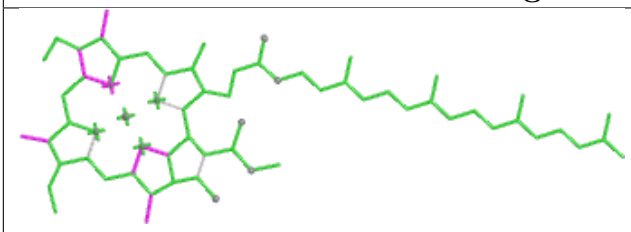


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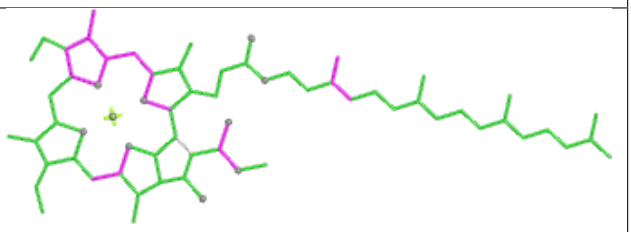


Rings

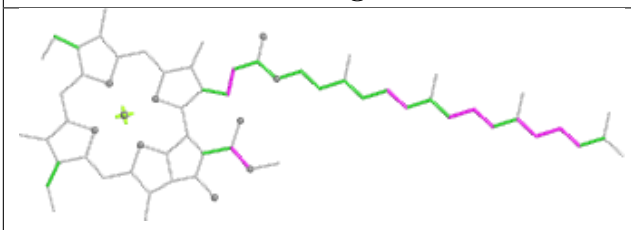
Ligand CLA A 829



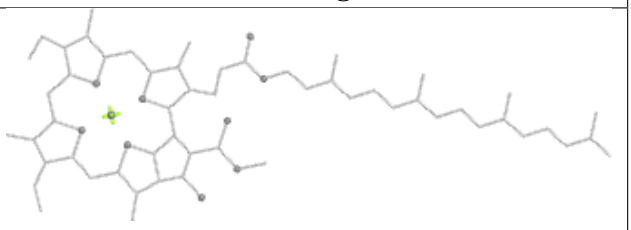
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Bond angles

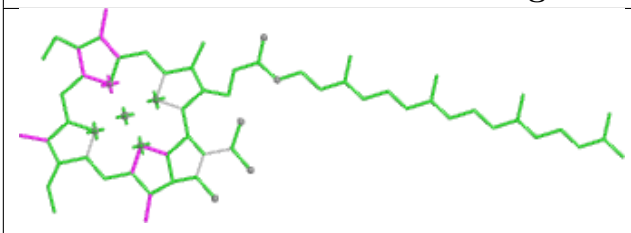


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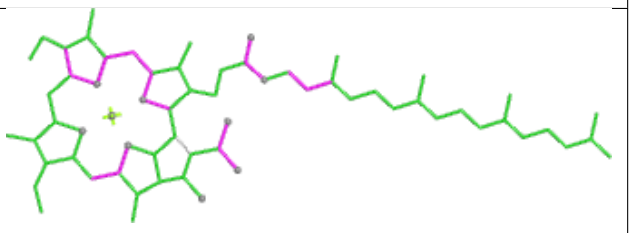


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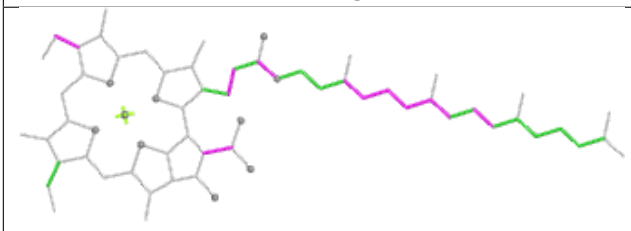
Ligand CLA 6 613



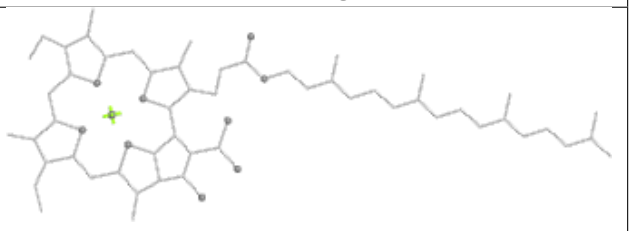
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Bond angles

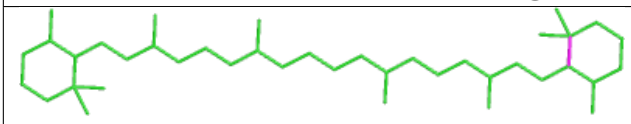


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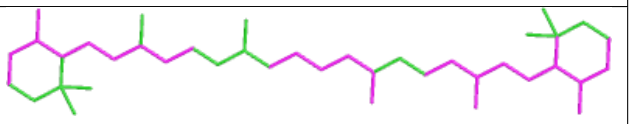


Rings

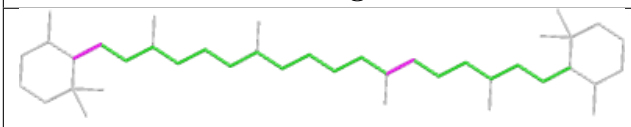
Ligand BCR 3 622



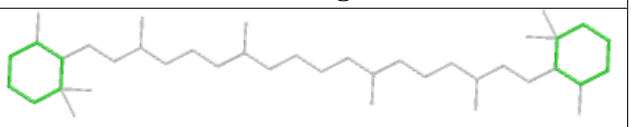
Bond lengths



Bond angles

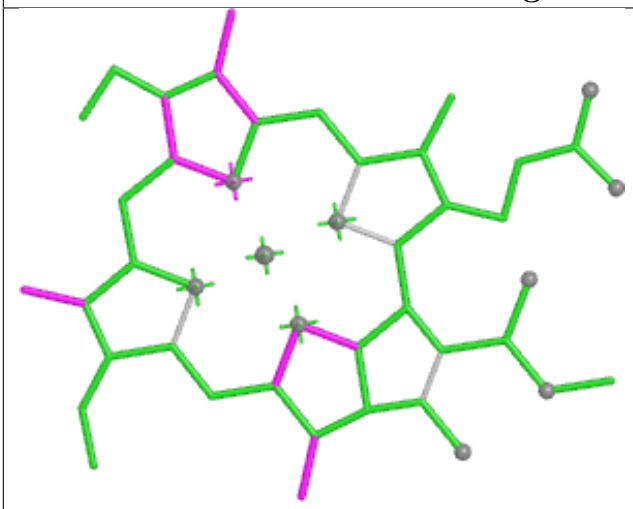


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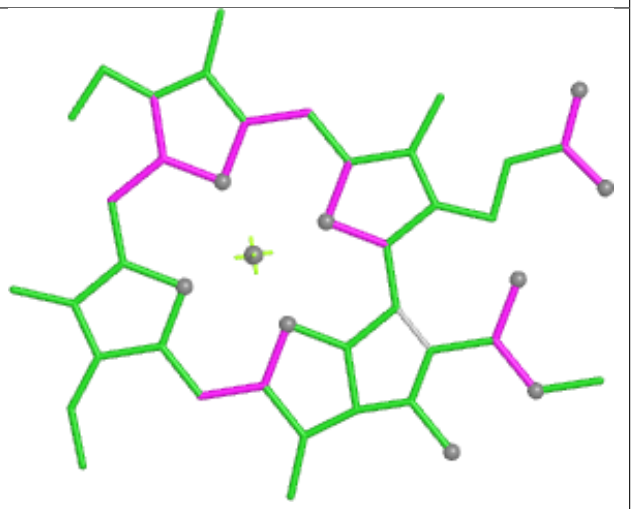


Rings

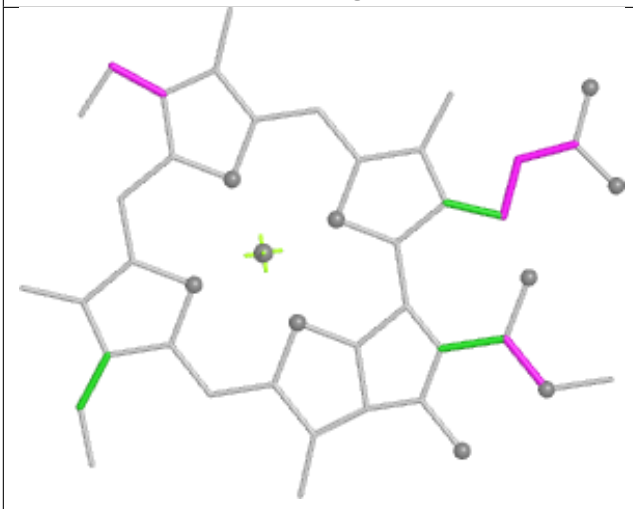
Ligand CLA G 204



Bond lengths



Bond angles

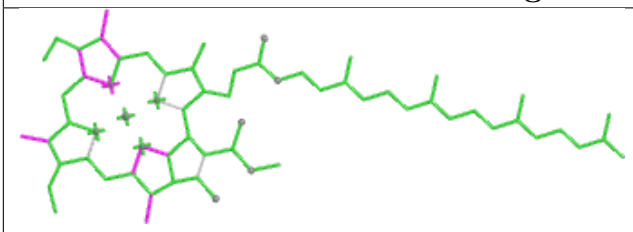


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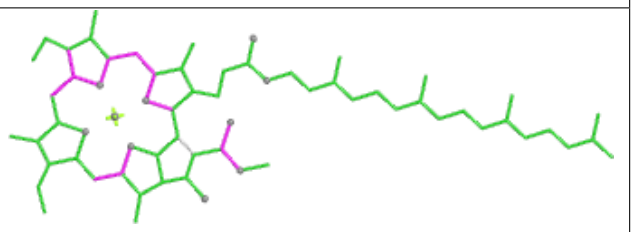


Rings

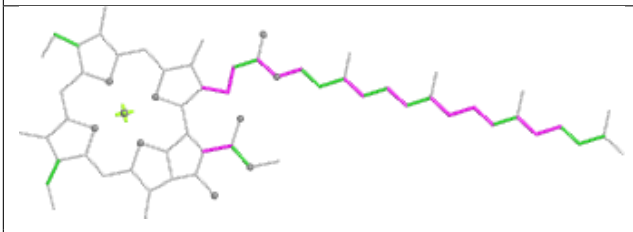
Ligand CLA B 828



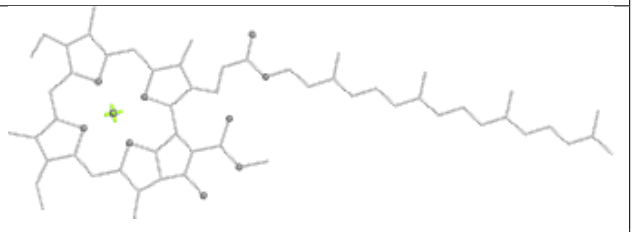
Bond lengths



Bond angles

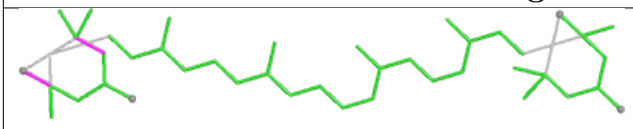


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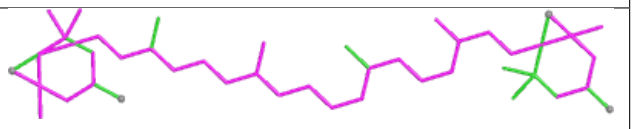


Rings

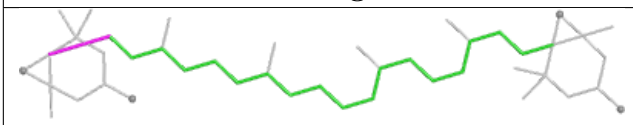
Ligand XAT 4 620



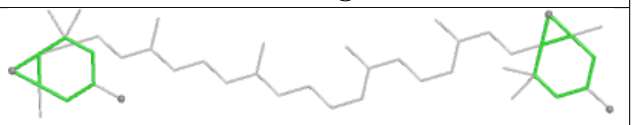
Bond lengths



Bond angles

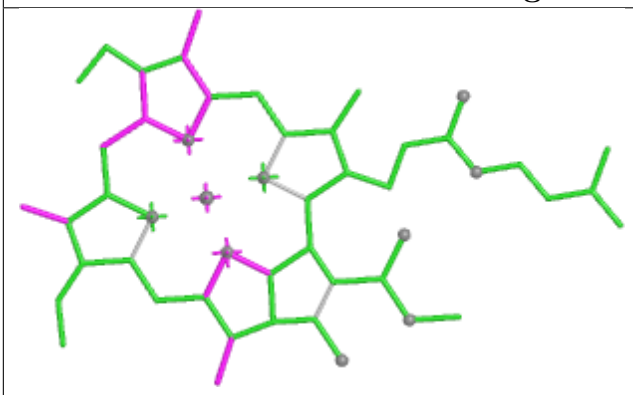


Torsions

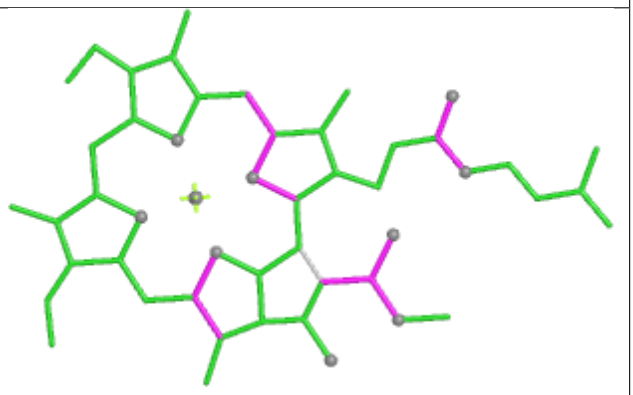


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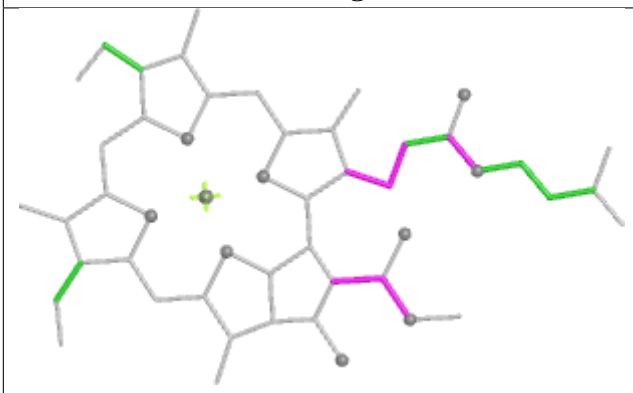
Ligand CLA A 838



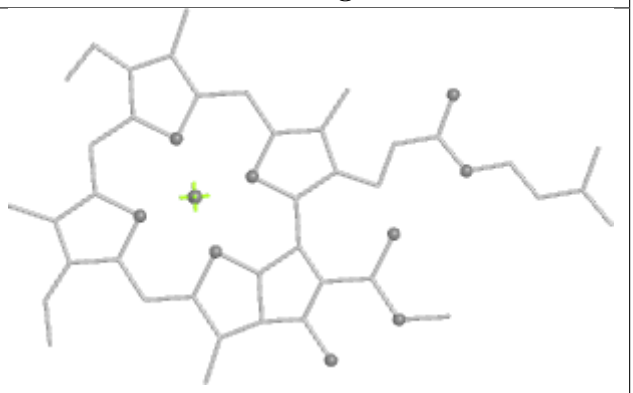
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Bond angles

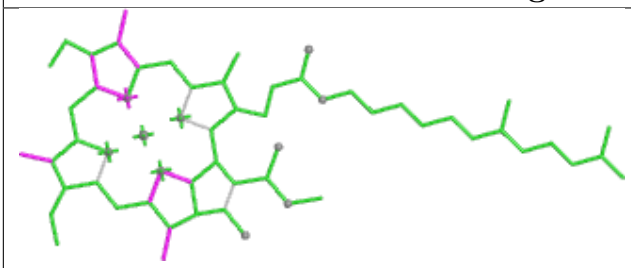


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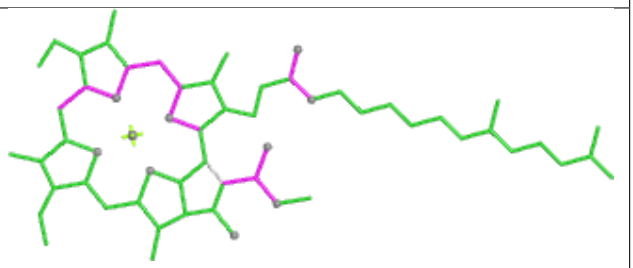


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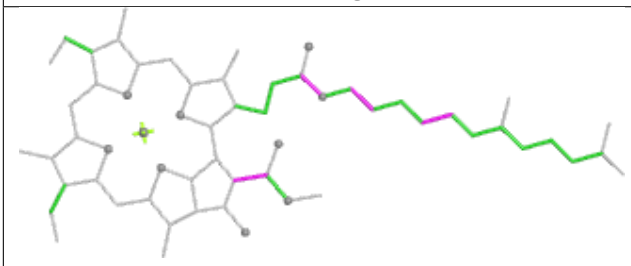
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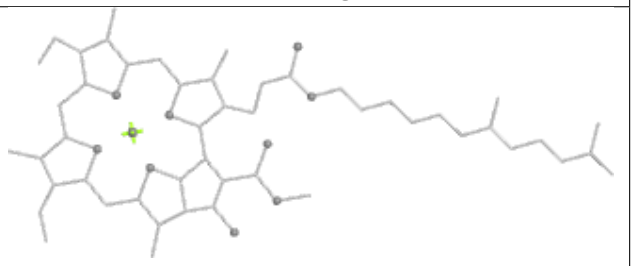
Bond lengths



Bond angles

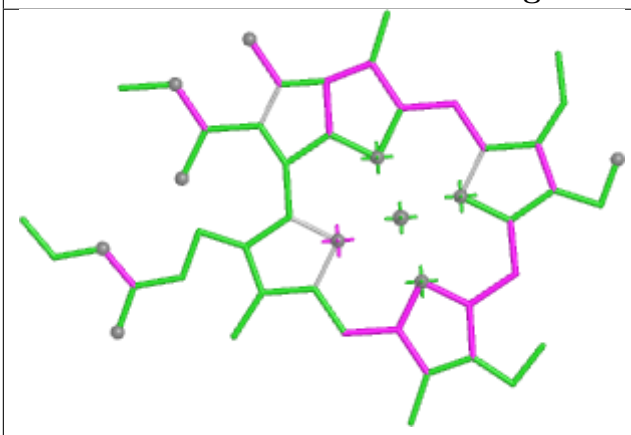


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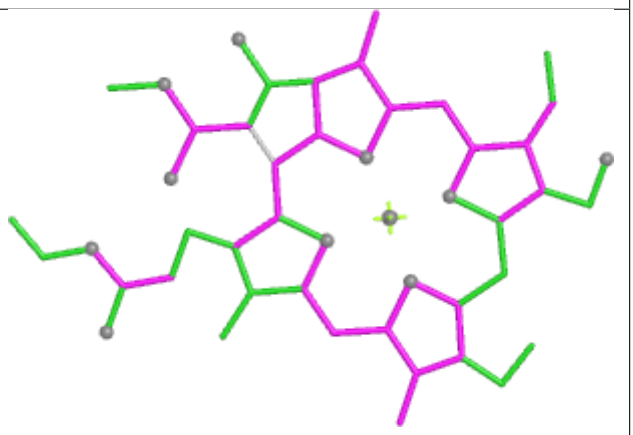


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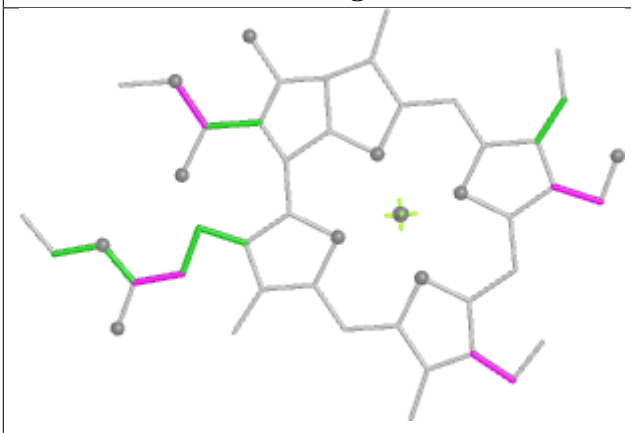
Ligand CHL V 608



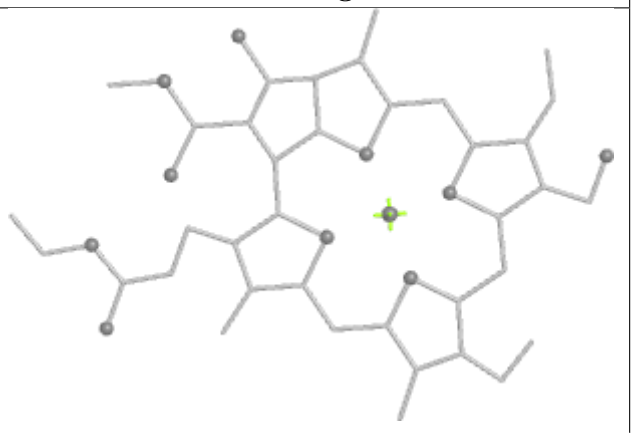
Bond lengths



Bond angles

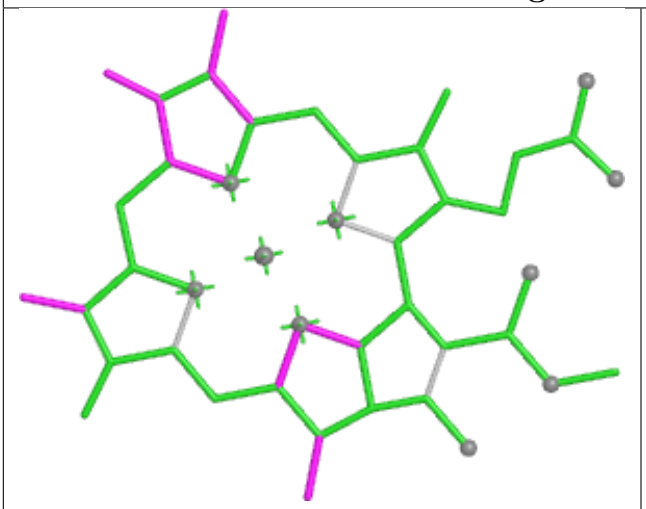


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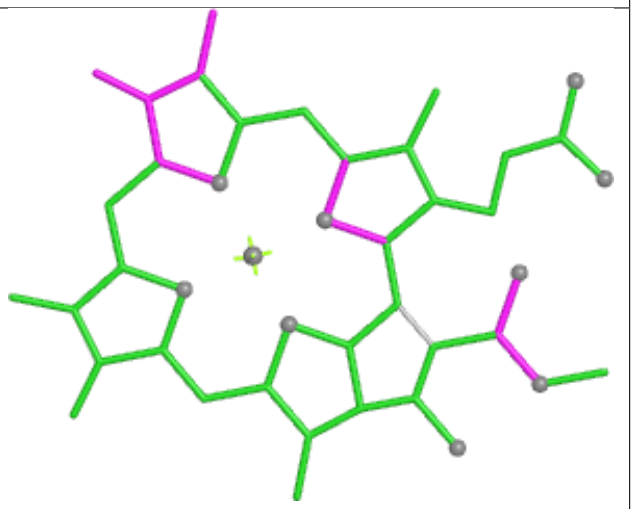


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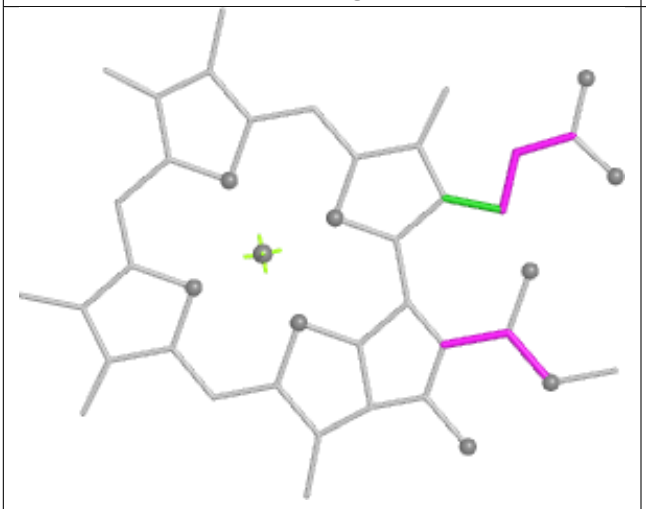
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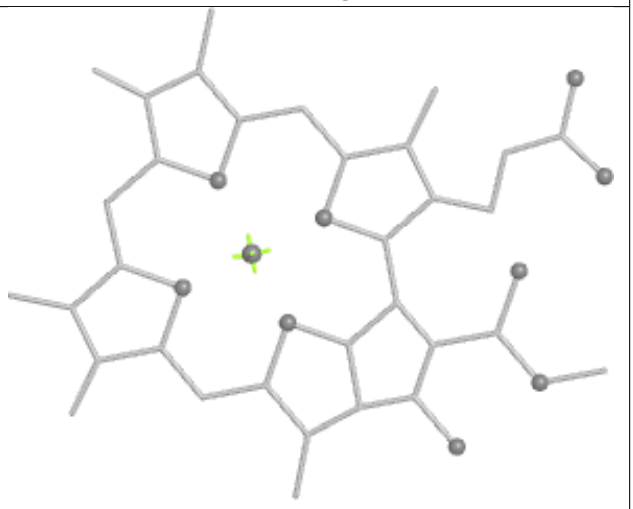
Bond lengths



Bond angles

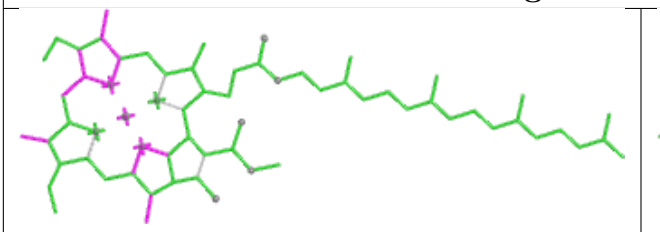


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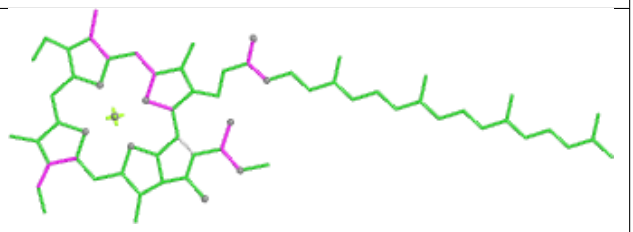


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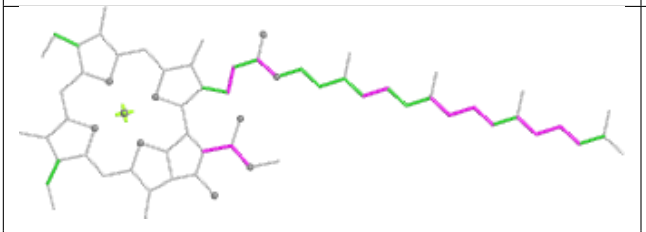
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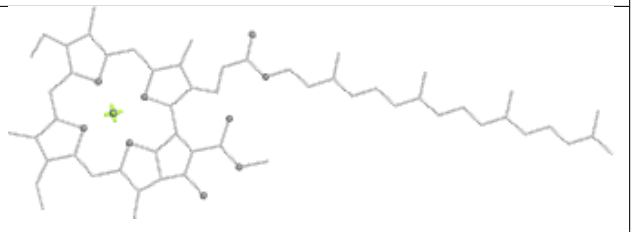
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Bond angles

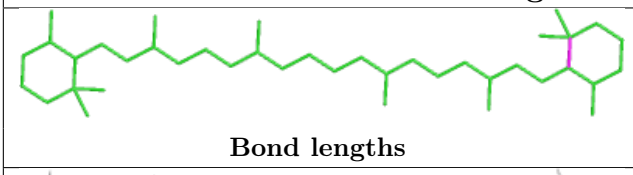


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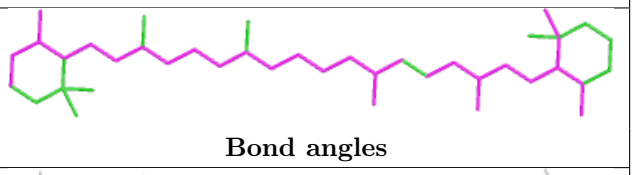


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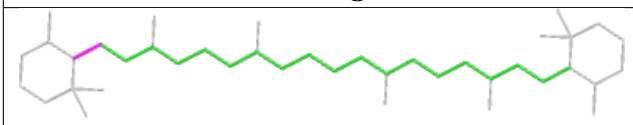
Ligand BCR 4 621



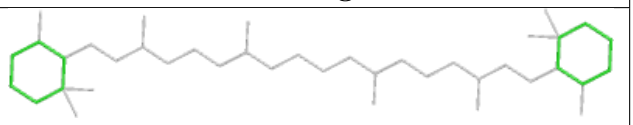
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Bond angles

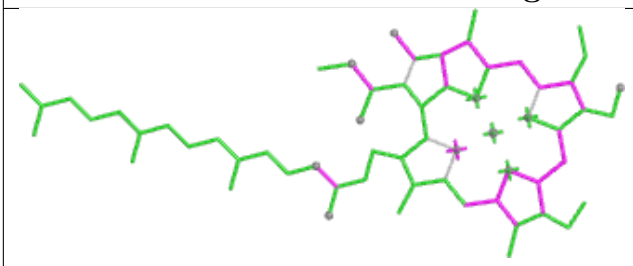


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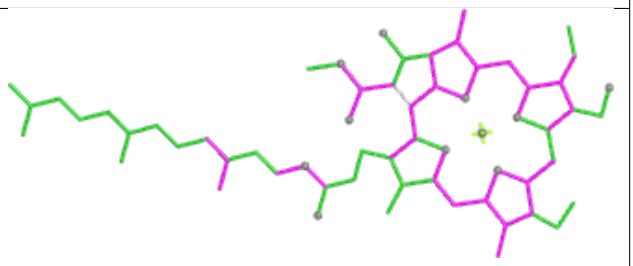


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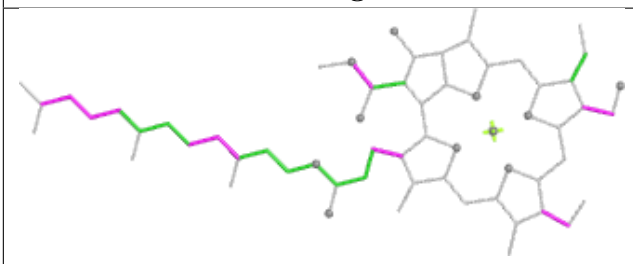
Ligand CHL V 609



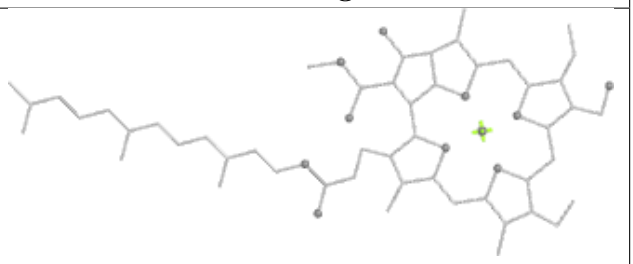
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Bond angles

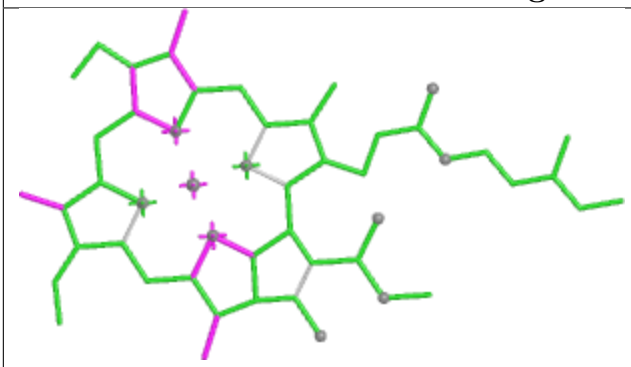


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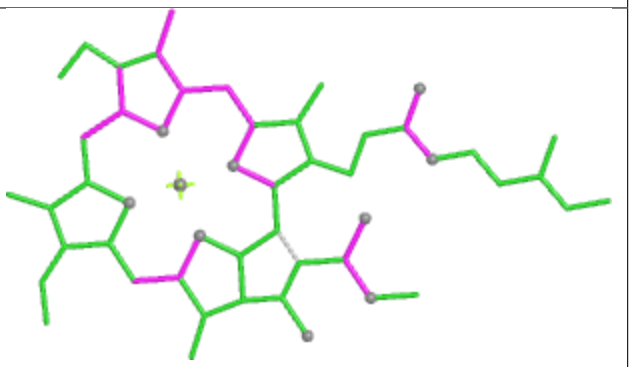


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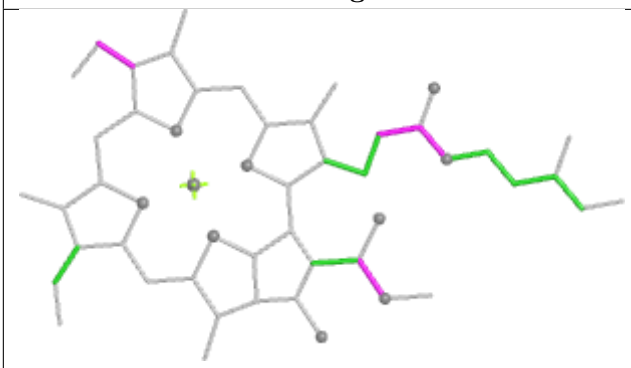
Ligand CLA 8 608



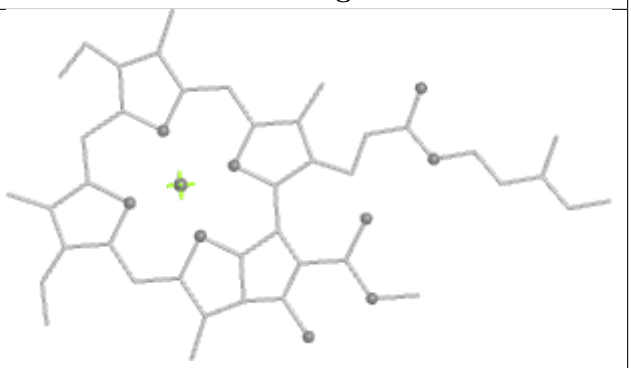
Bond lengths



Bond angles

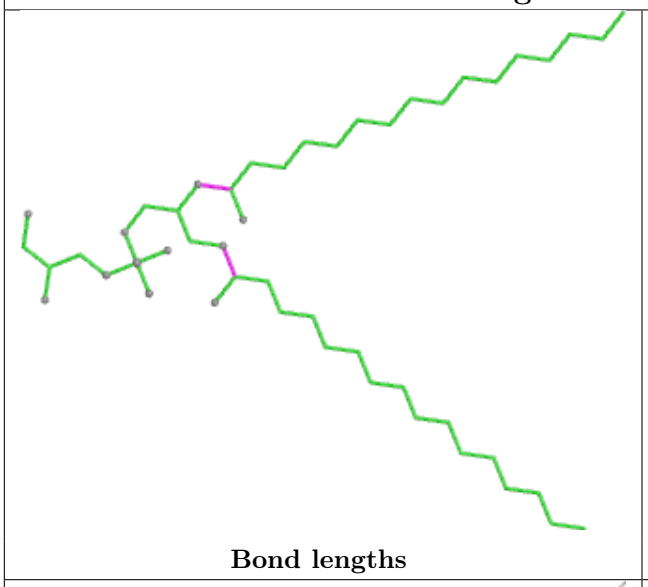


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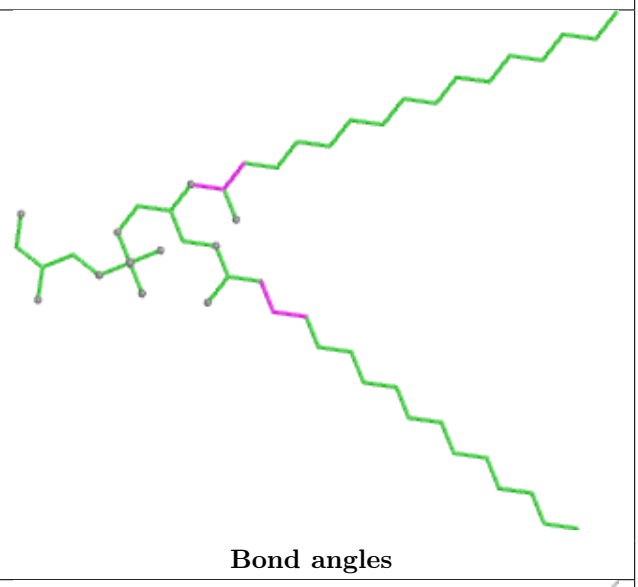


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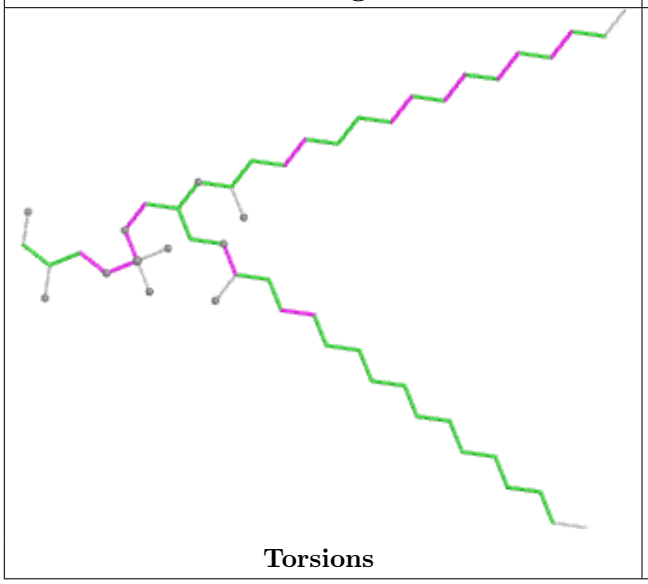
Ligand LHG Y 2630



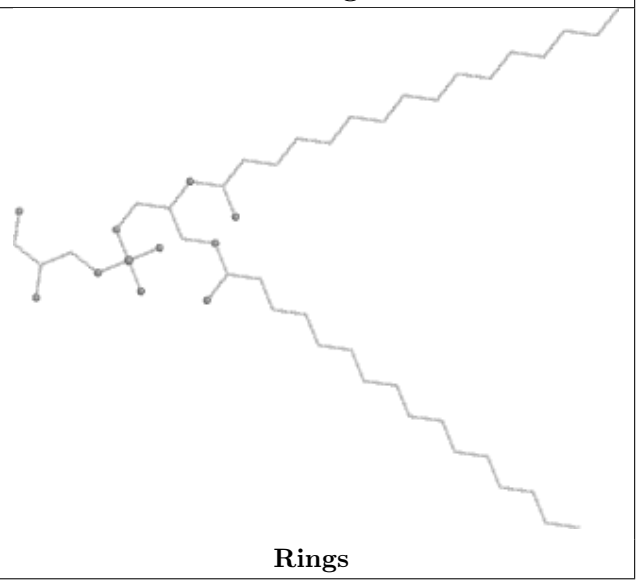
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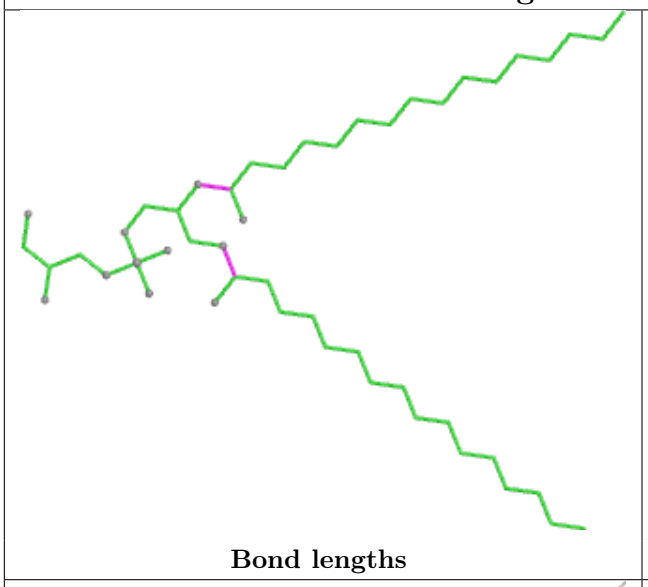


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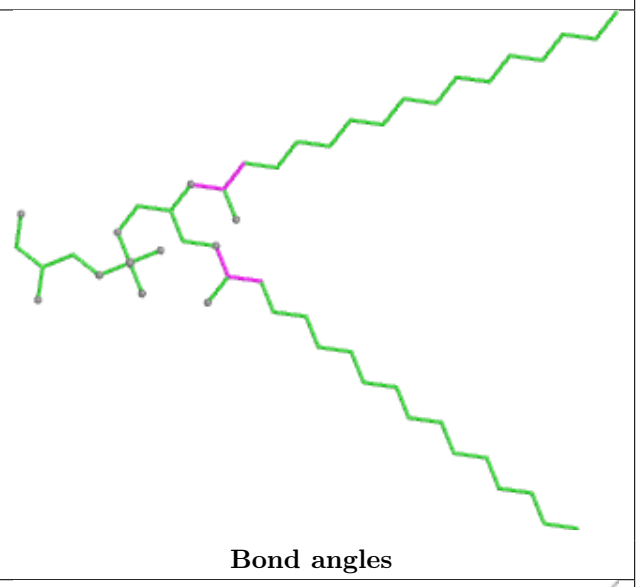


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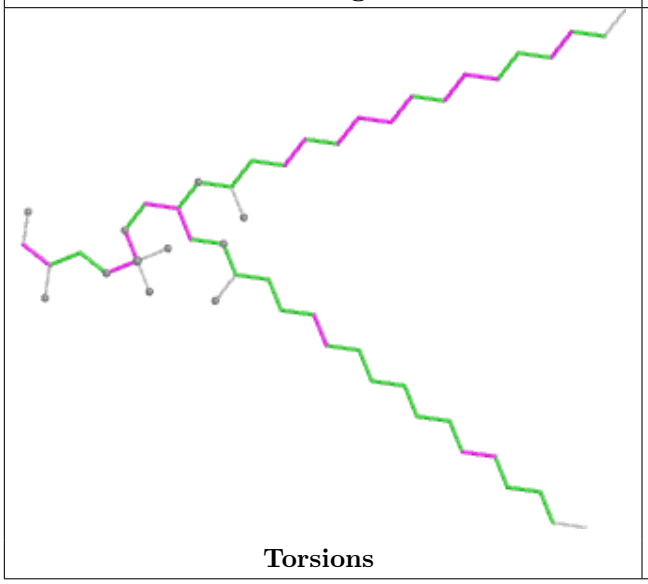
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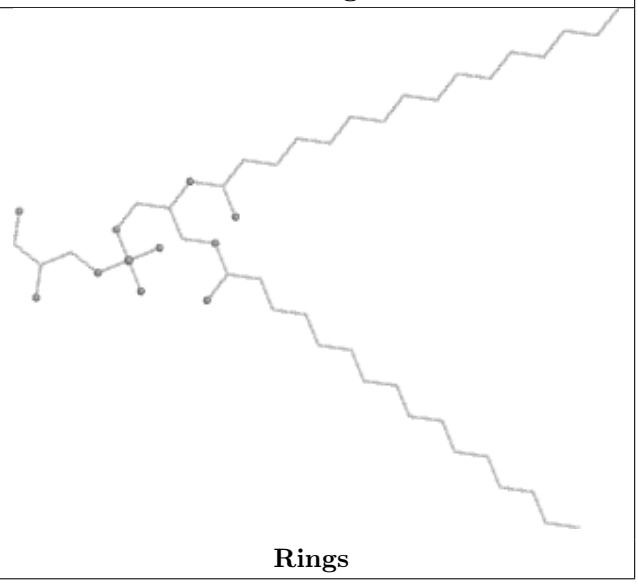
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Bond angles

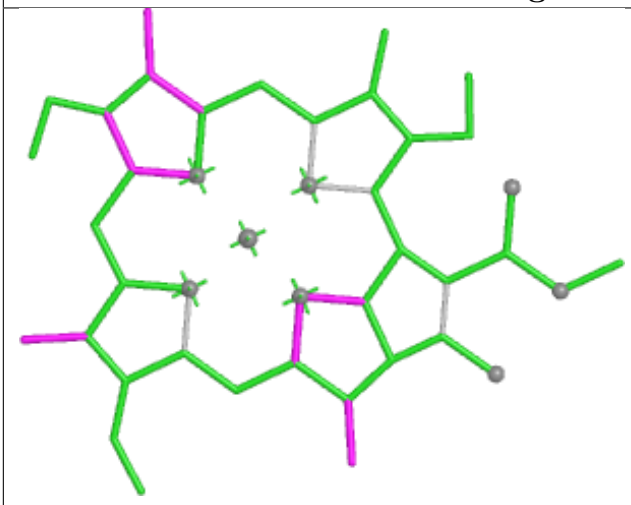


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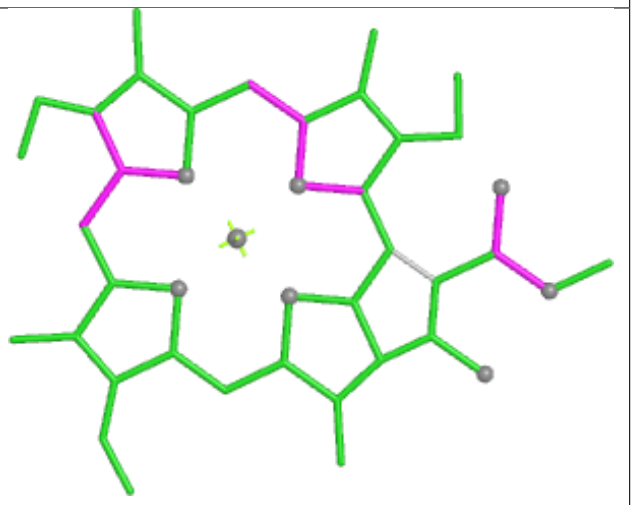


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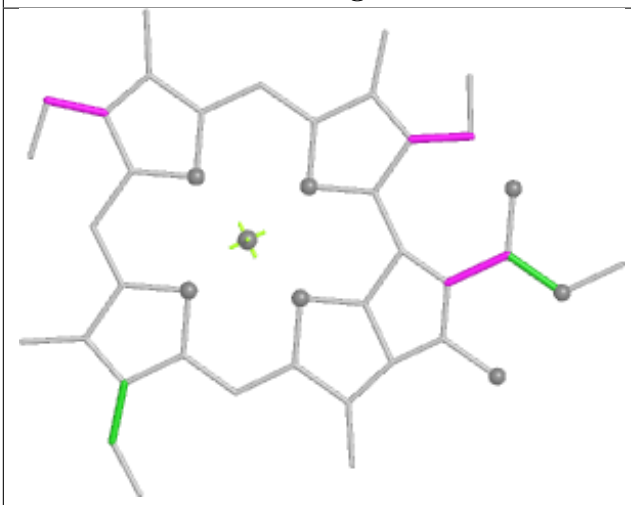
Ligand CLA 6 611



Bond lengths



Bond angles

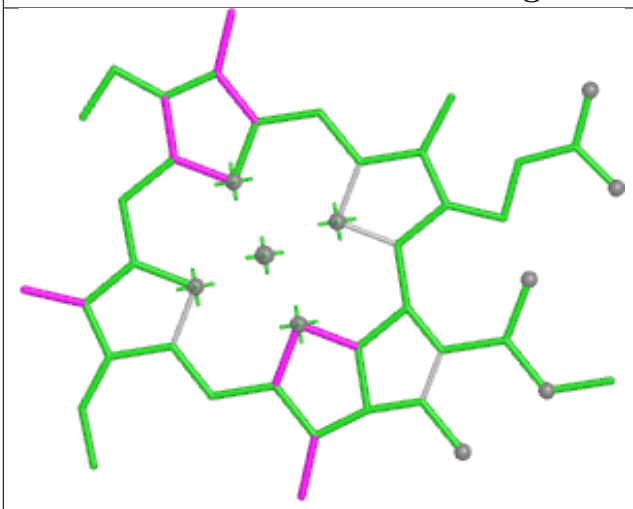


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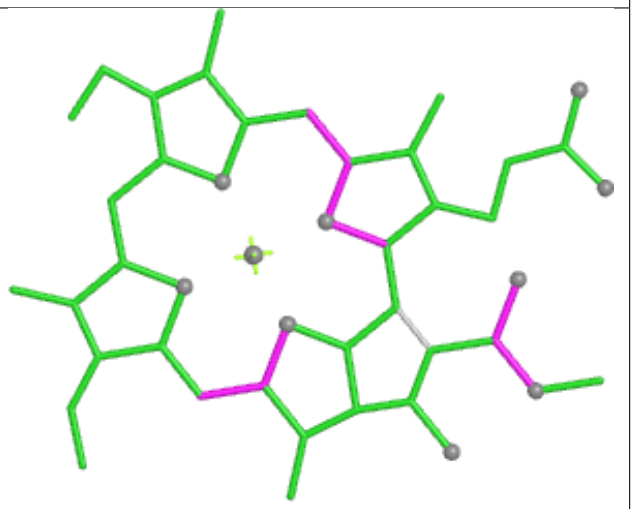


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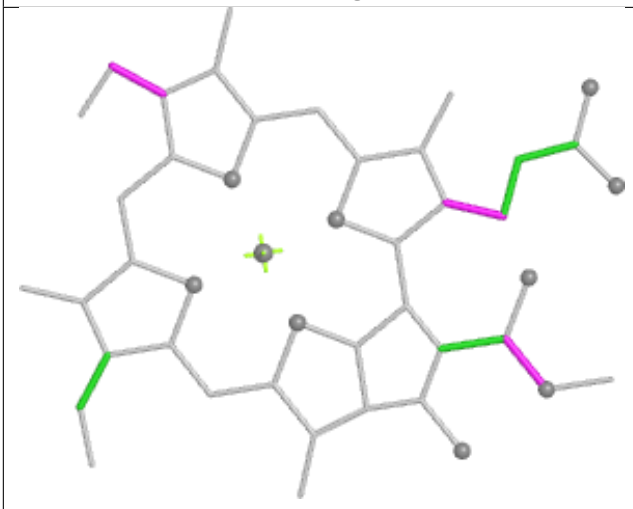
Ligand CLA K 206



Bond lengths



Bond angles

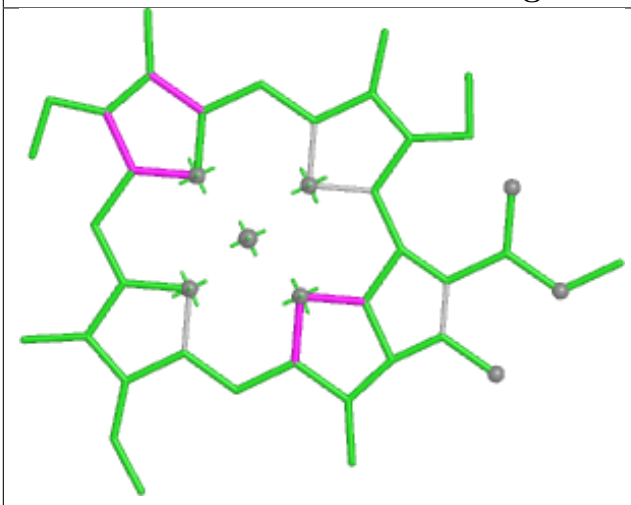


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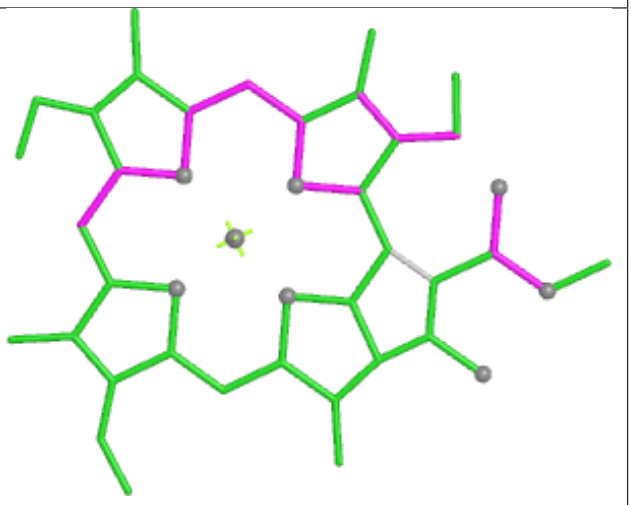


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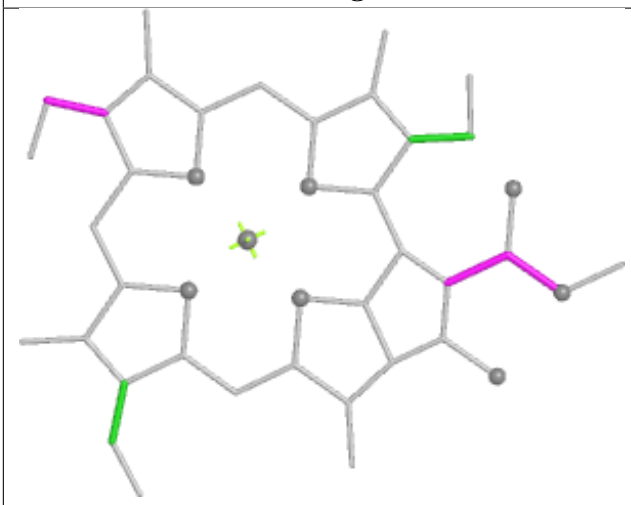
Ligand CLA U 612



Bond lengths



Bond angles

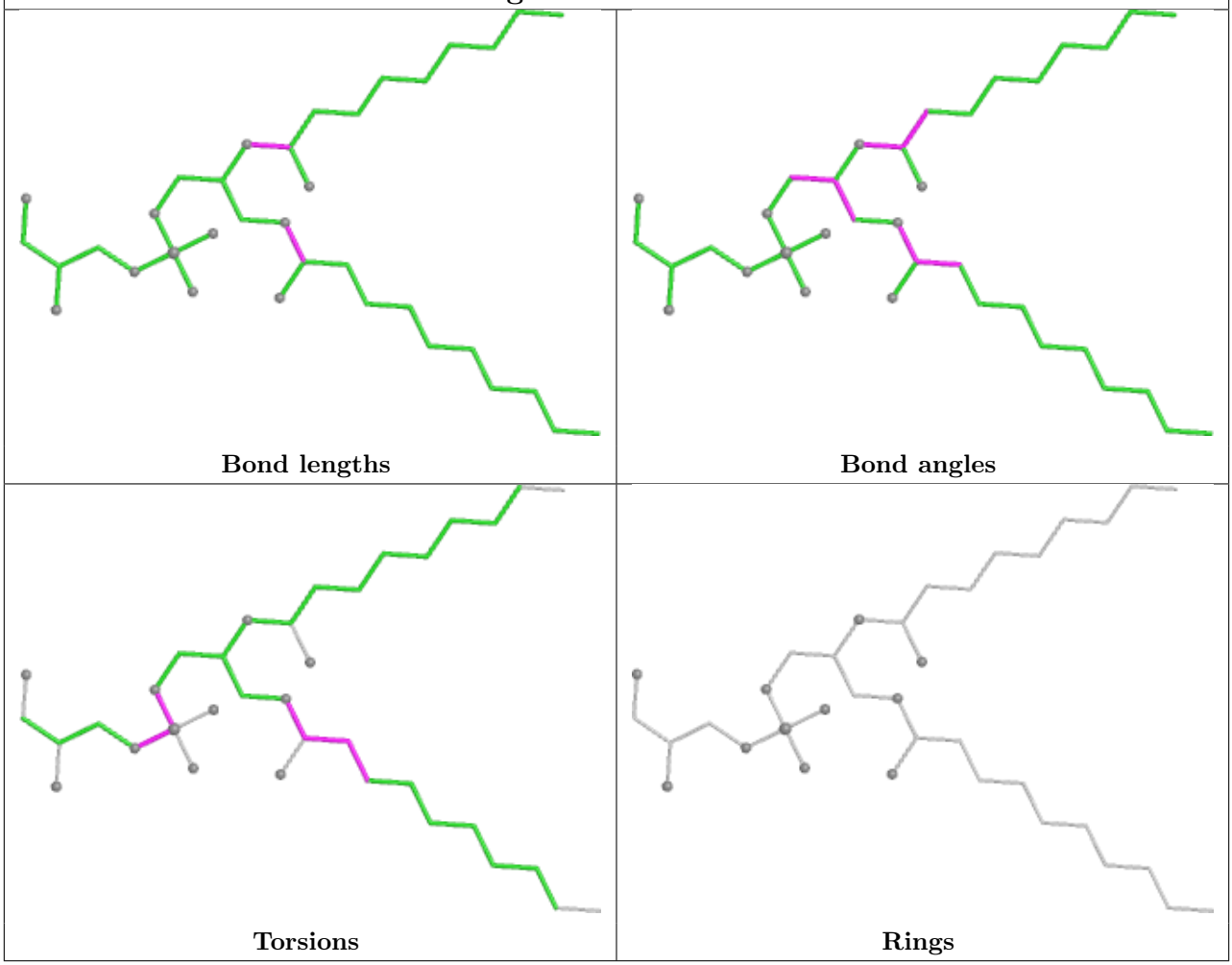


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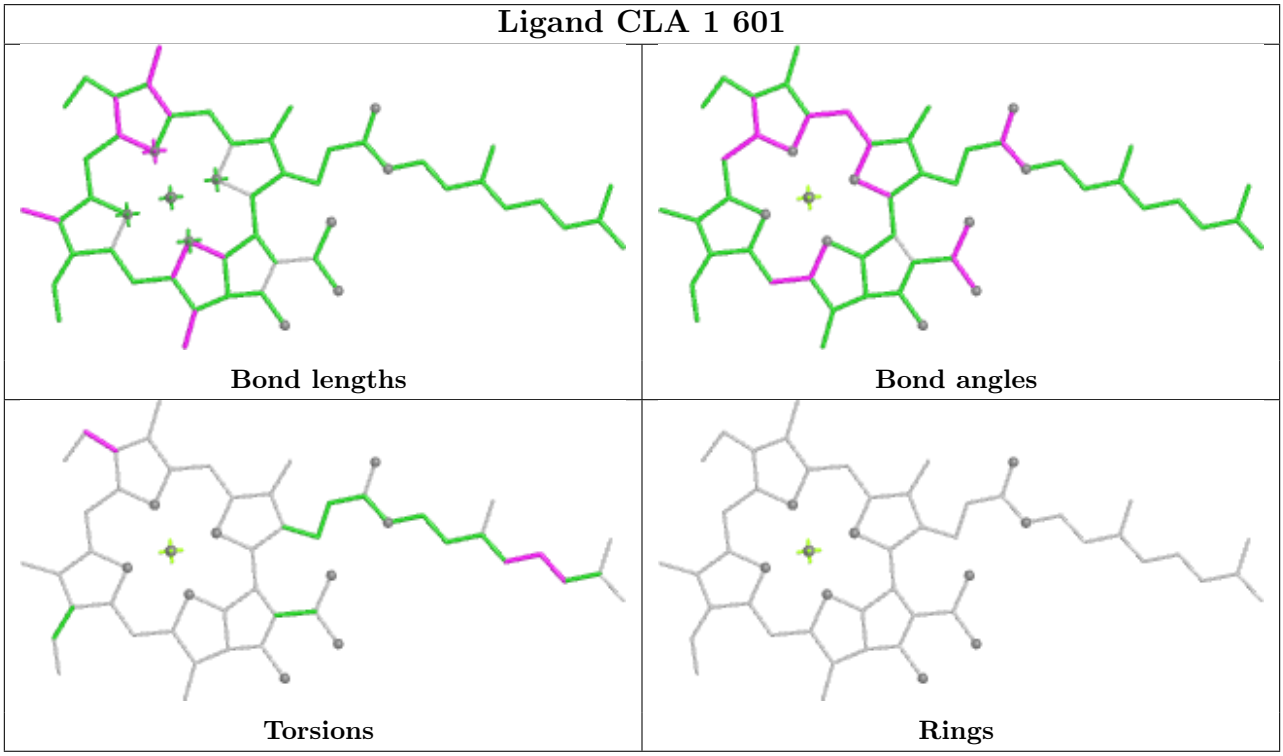


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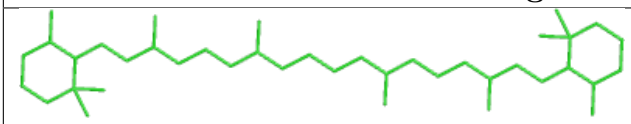
Ligand LHG 2 622



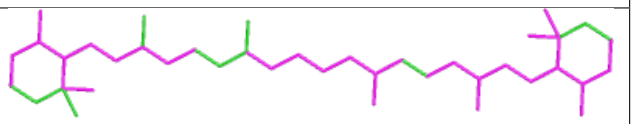
Ligand CLA 1 601



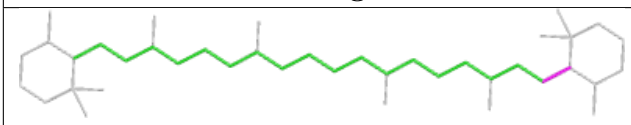
Ligand BCR 6 622



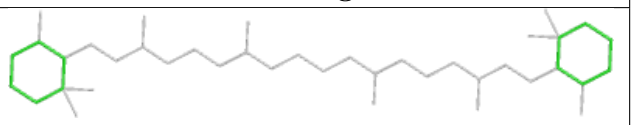
Bond lengths



Bond angles

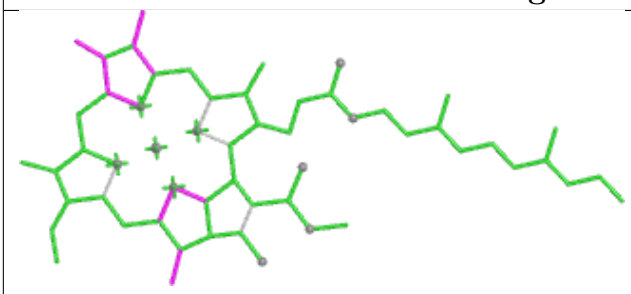


Torsions

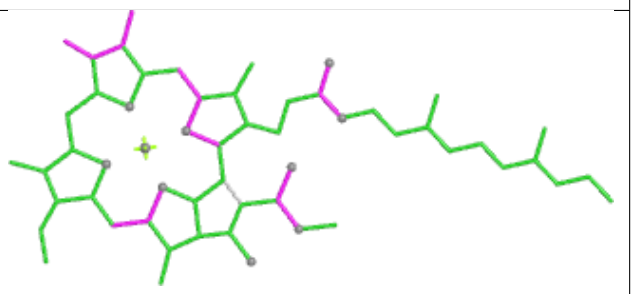


Rings

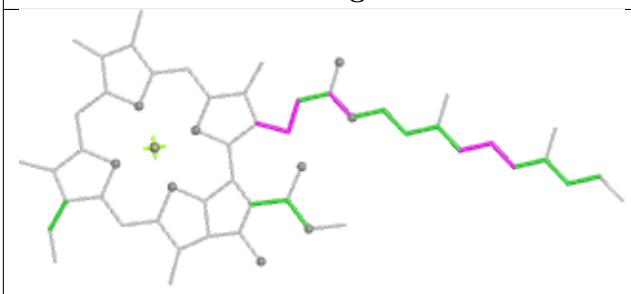
Ligand CLA 3 607



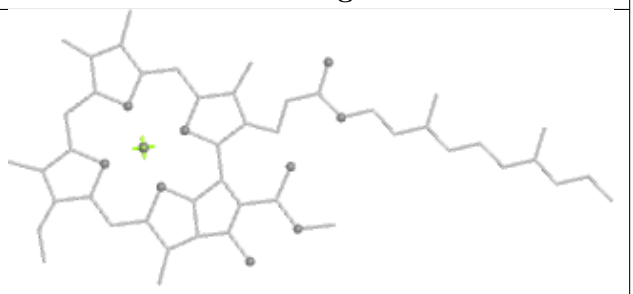
Bond lengths



Bond angles

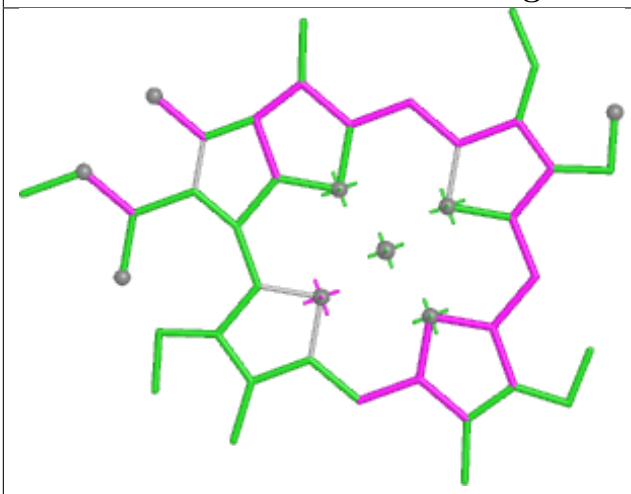


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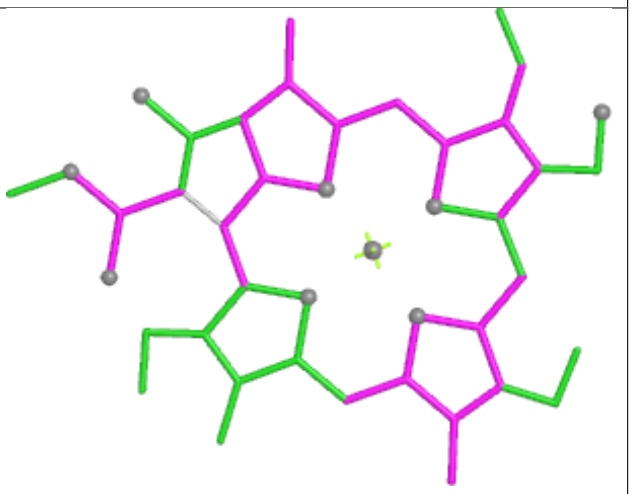


Rings

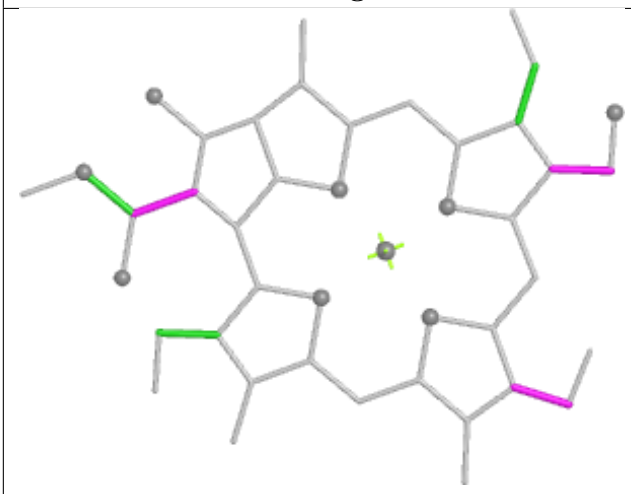
Ligand CHL U 605



Bond lengths



Bond angles

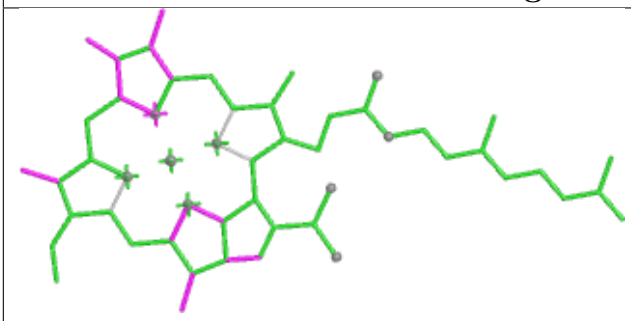


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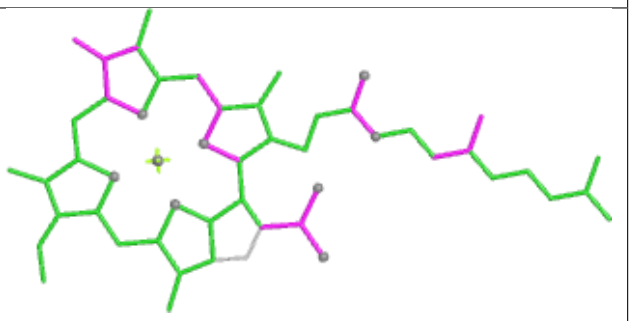


Rings

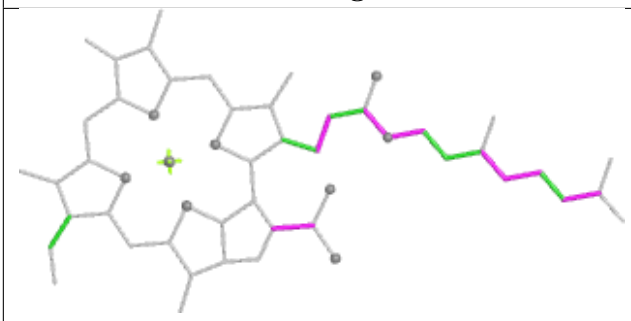
Ligand CLA B 811



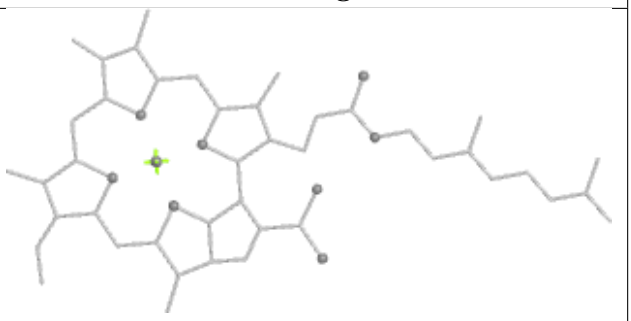
Bond lengths



Bond angles

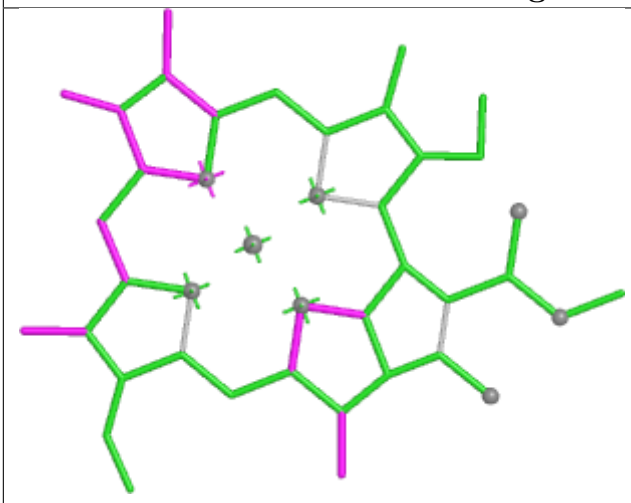


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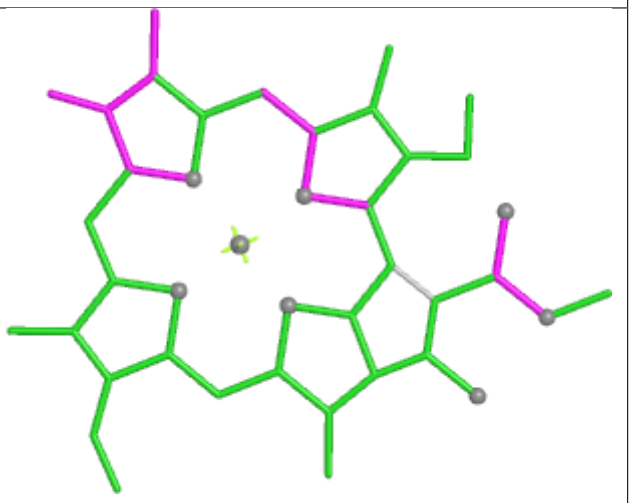


Rings

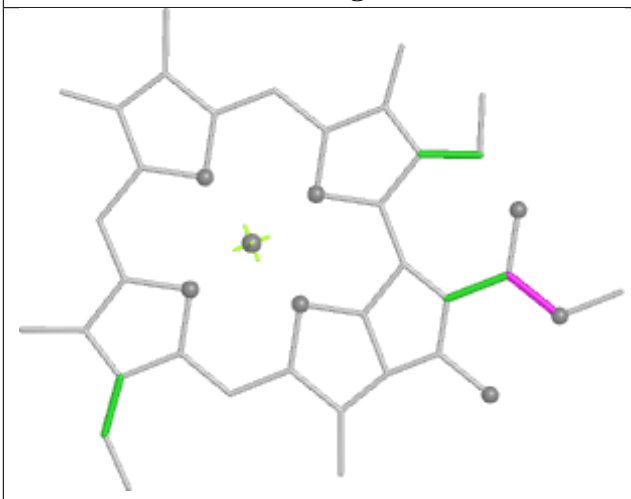
Ligand CLA 8 607



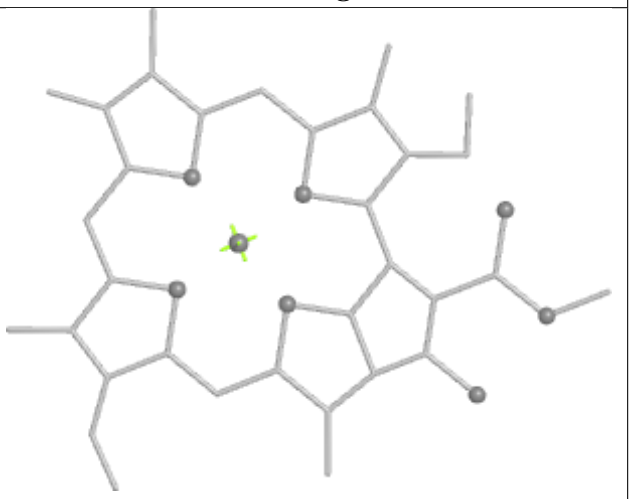
Bond lengths



Bond angles

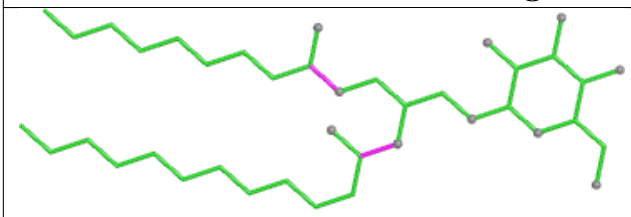


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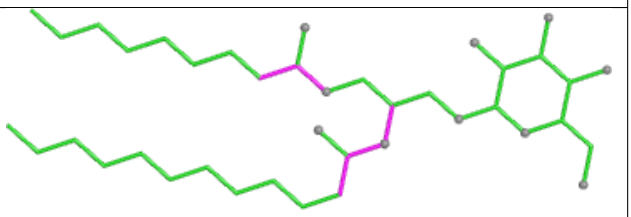


Rings

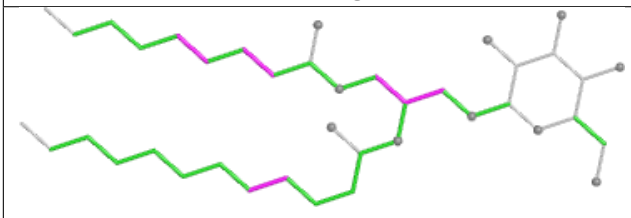
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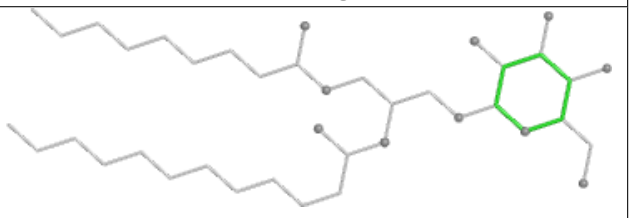
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Bond angles

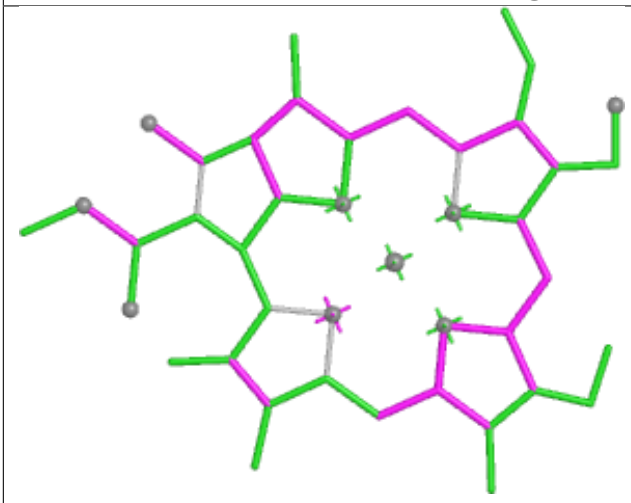


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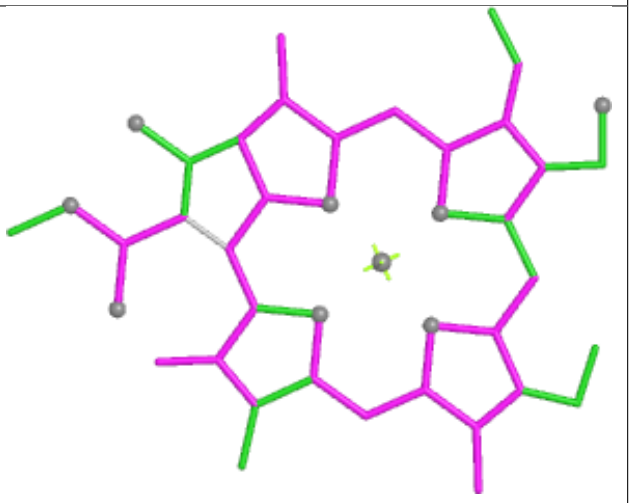


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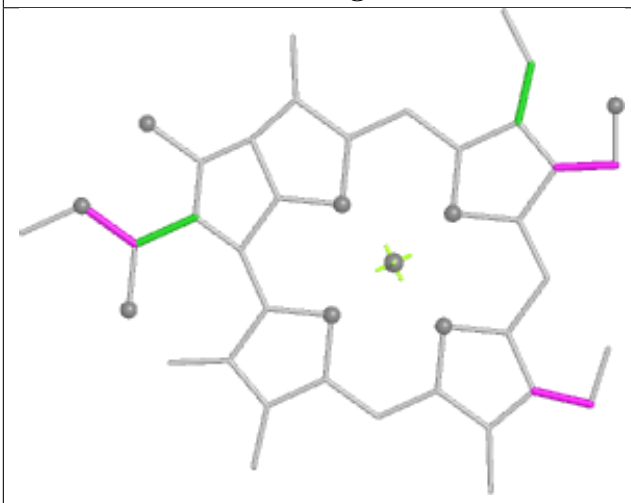
Ligand CHL Z 605



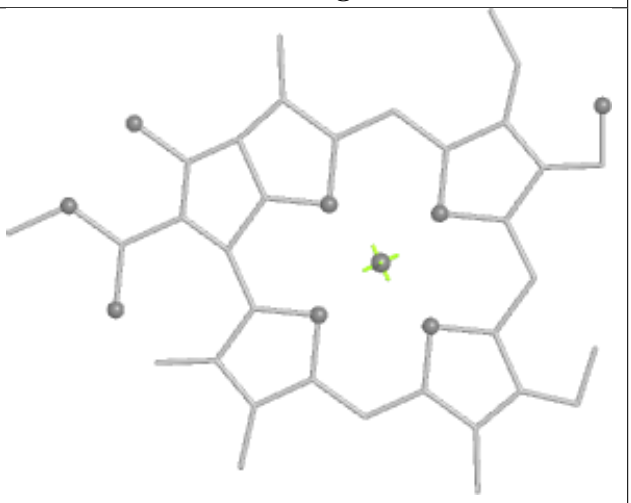
Bond lengths



Bond angles

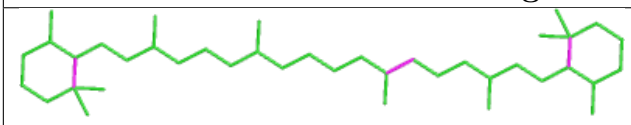


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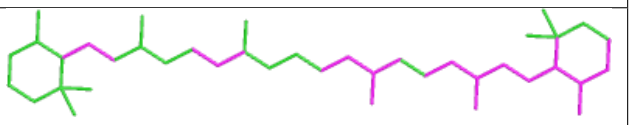


Rings

Ligand BCR A 848



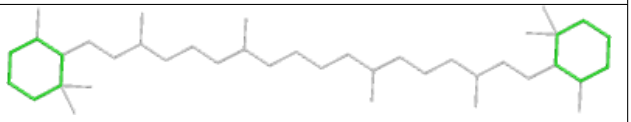
Bond lengths



Bond angles

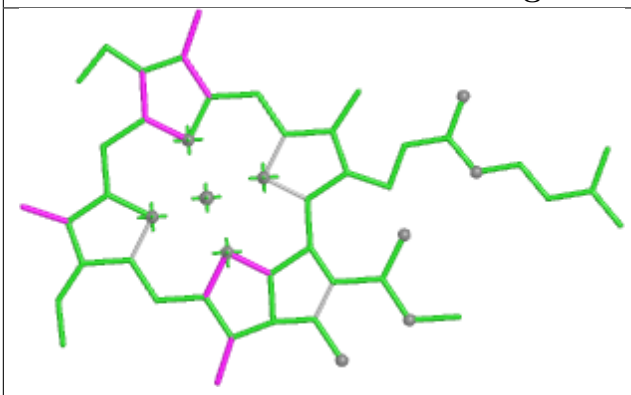


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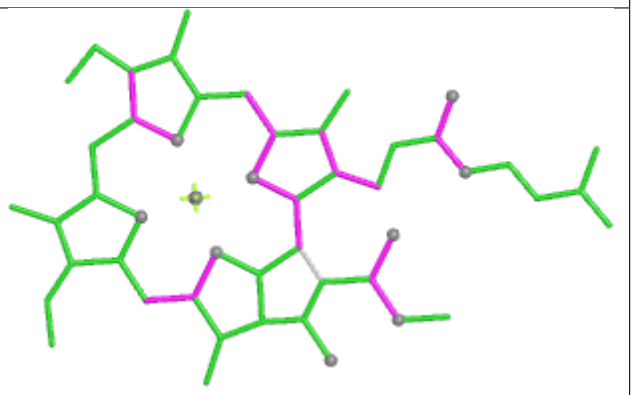


Rings

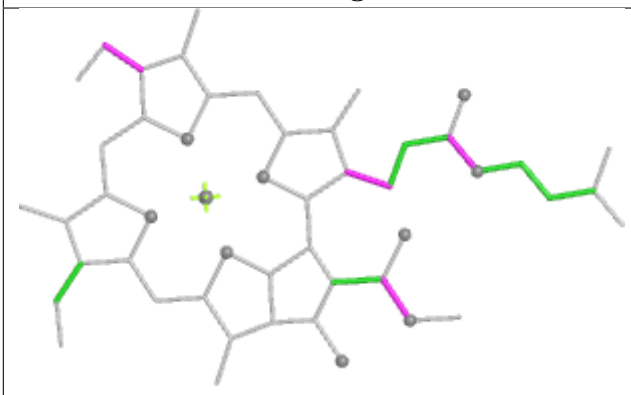
Ligand CLA A 810



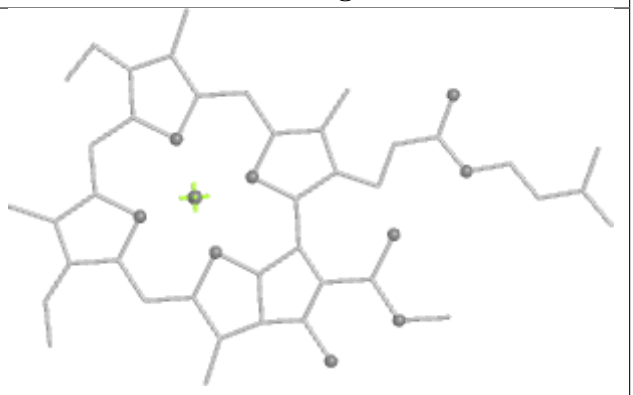
Bond lengths



Bond angles

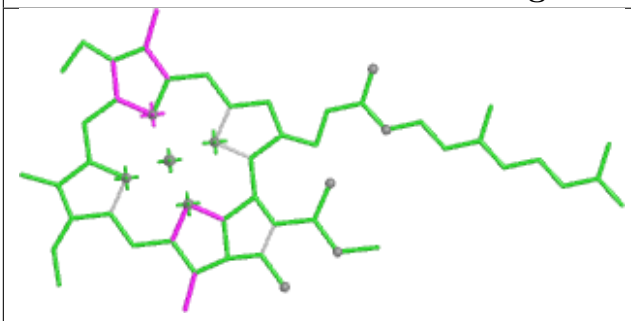


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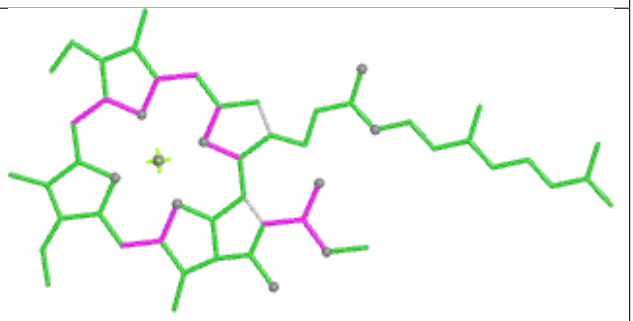


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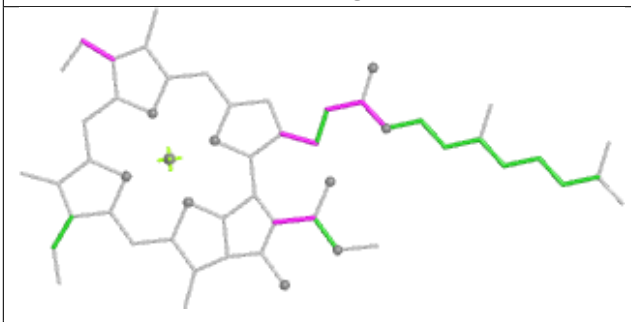
Ligand CLA a 614



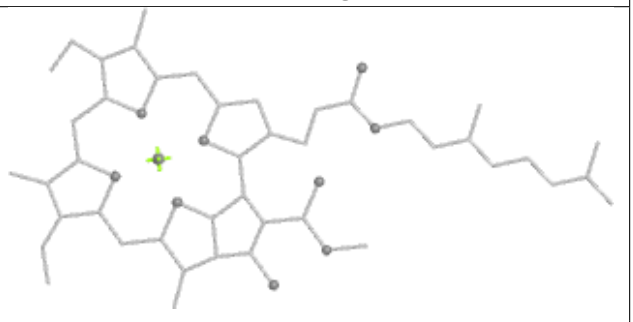
Bond lengths



Bond angles

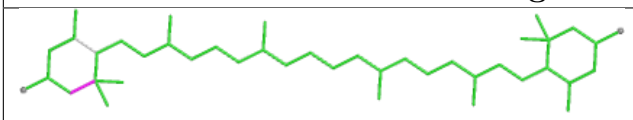


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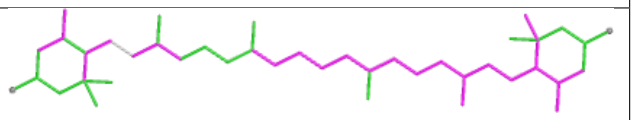


Rings

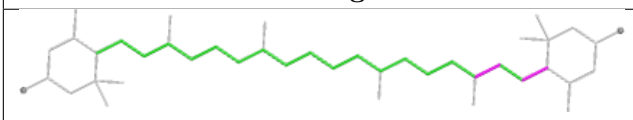
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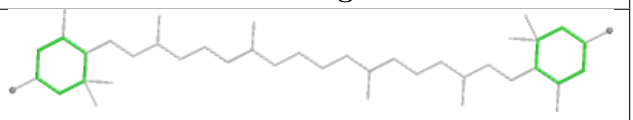
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Bond angles

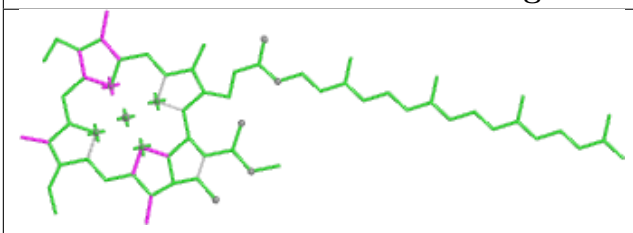


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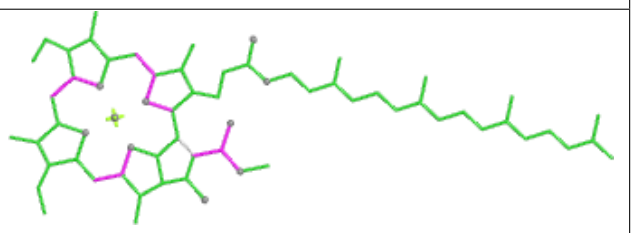


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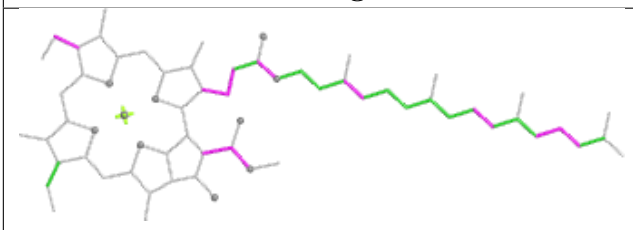
Ligand CLA A 825



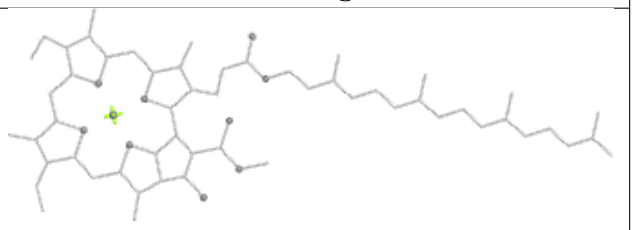
Bond lengths



Bond angles

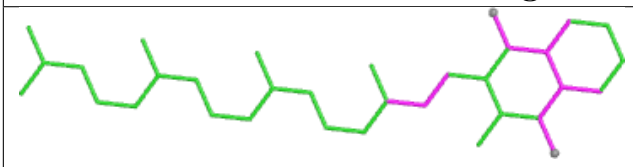


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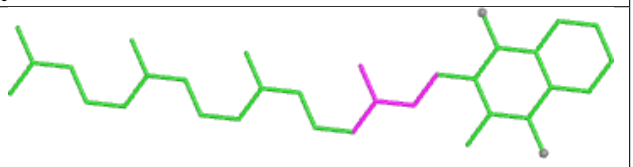


Rings

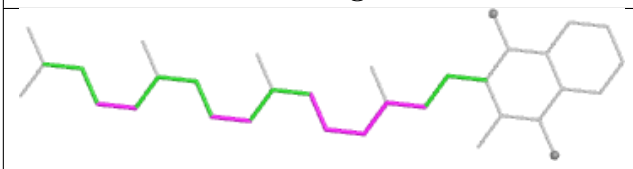
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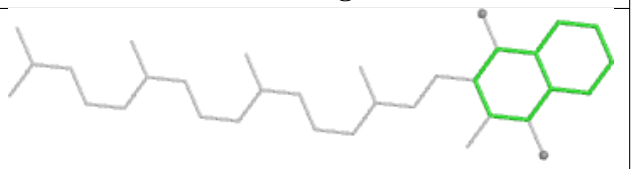
Bond lengths



Bond angles

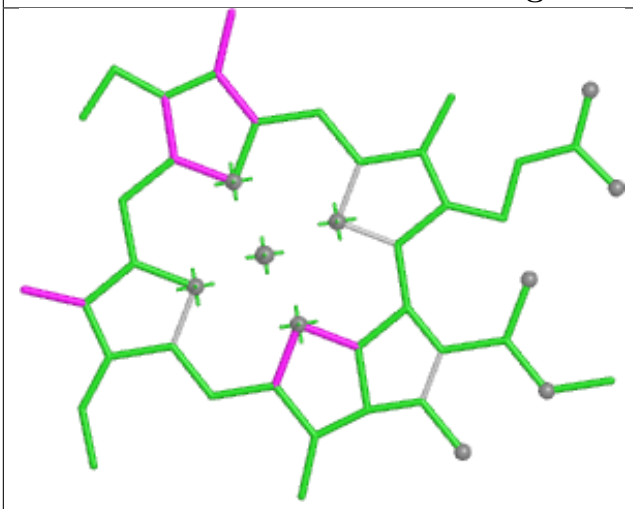


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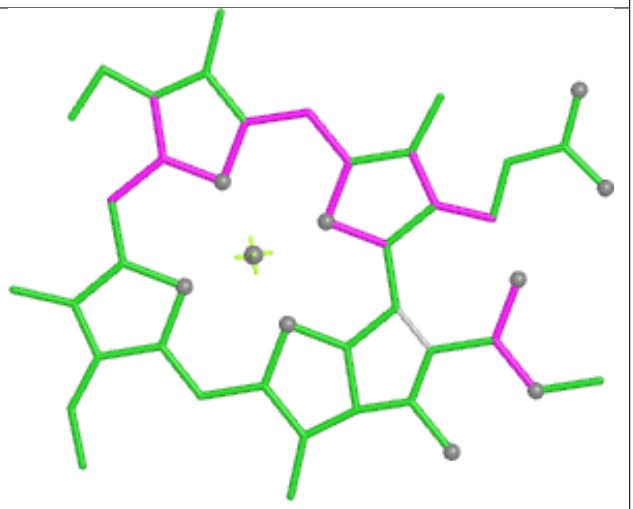


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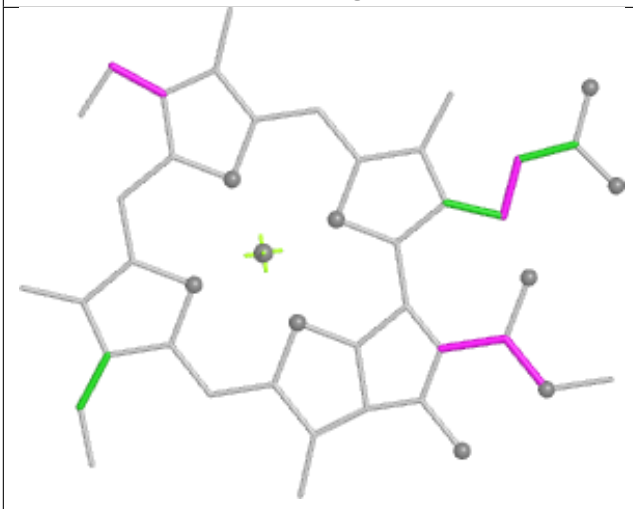
Ligand CLA Z 612



Bond lengths



Bond angles

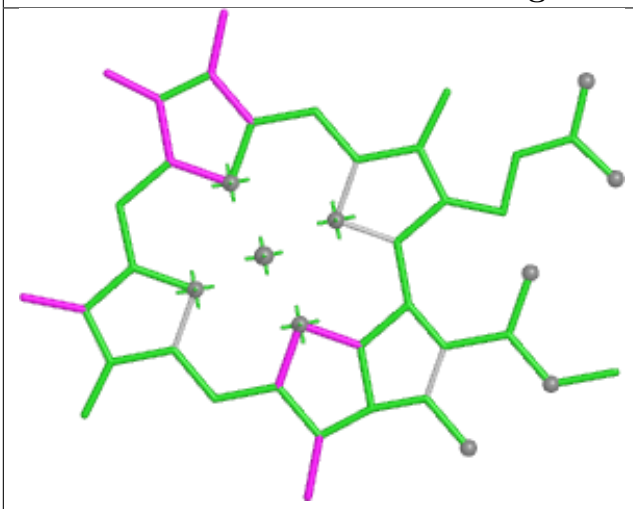


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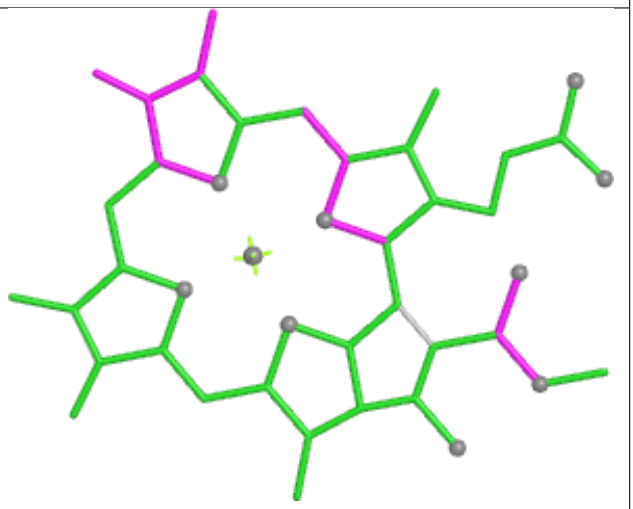


Rings

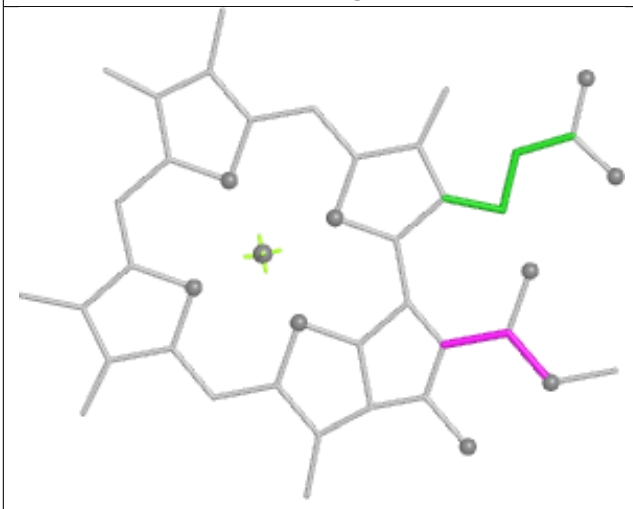
Ligand CLA 2 616



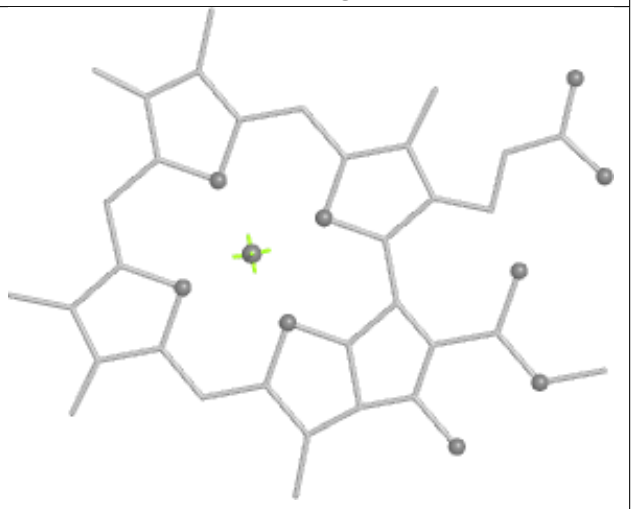
Bond lengths



Bond angles

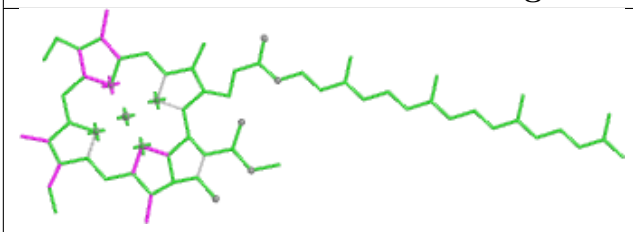


Torsions

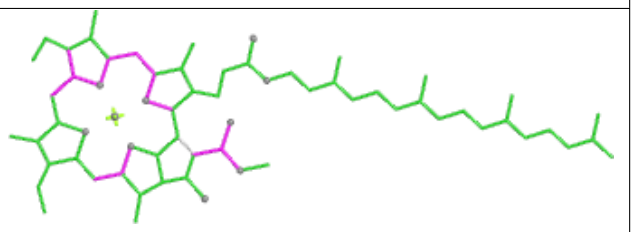


Rings

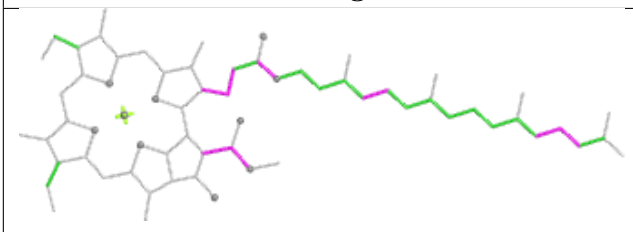
Ligand CLA B 809



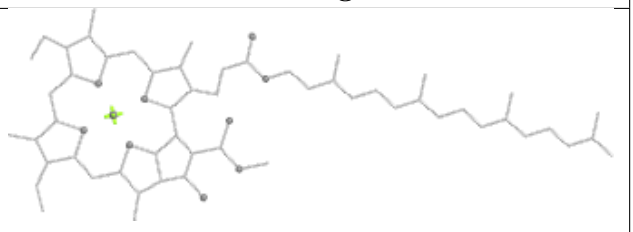
Bond lengths



Bond angles

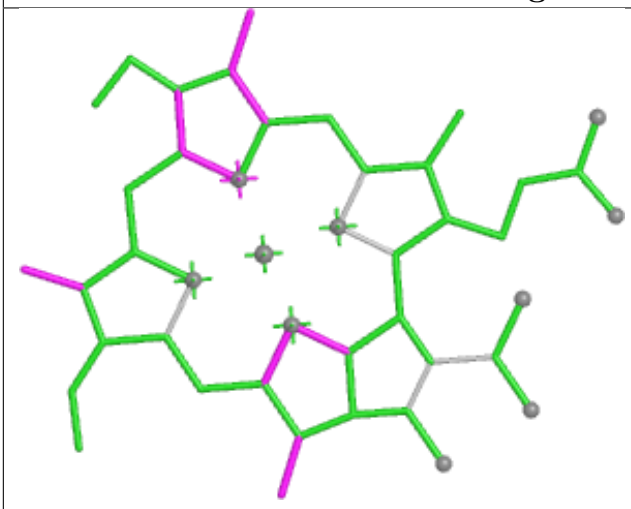


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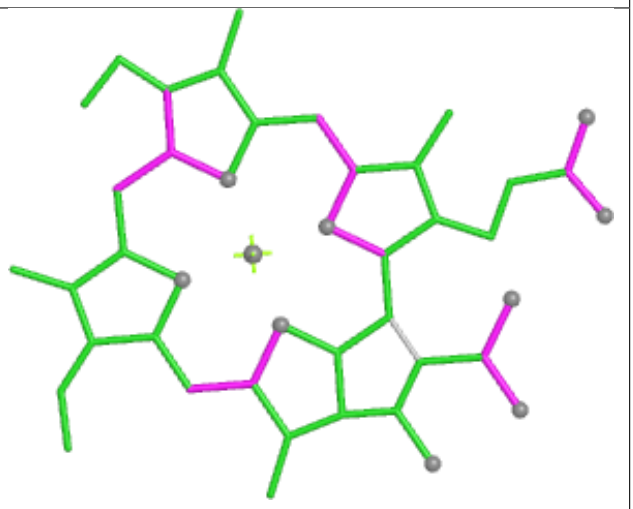


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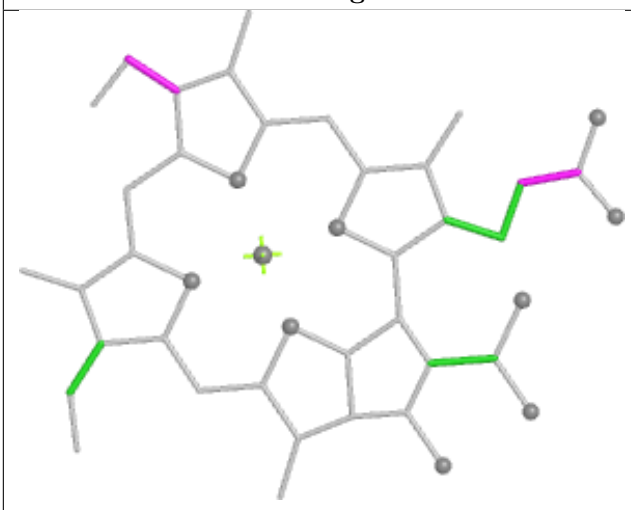
Ligand CLA 1 608



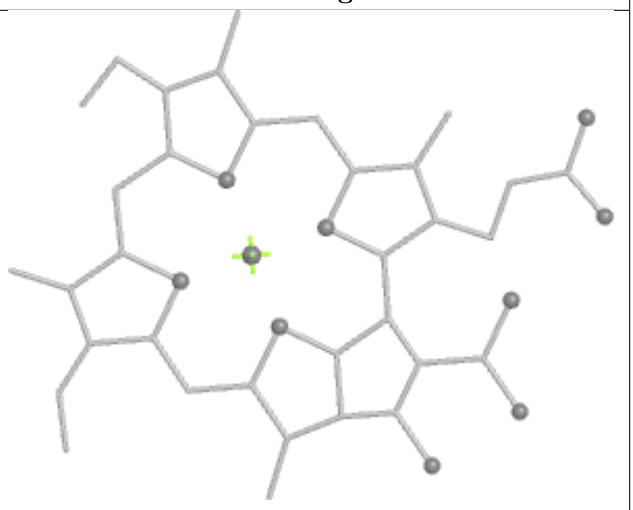
Bond lengths



Bond angles

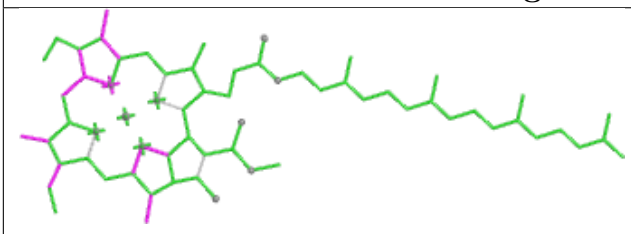


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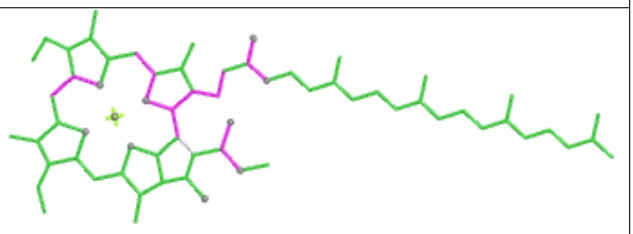


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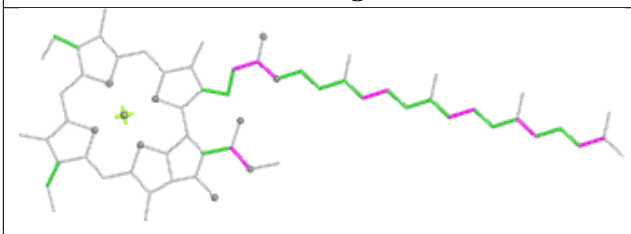
Ligand CLA A 801



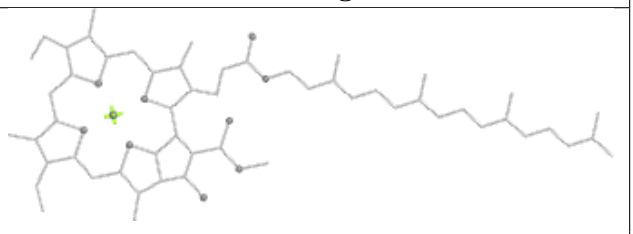
Bond lengths



Bond angles

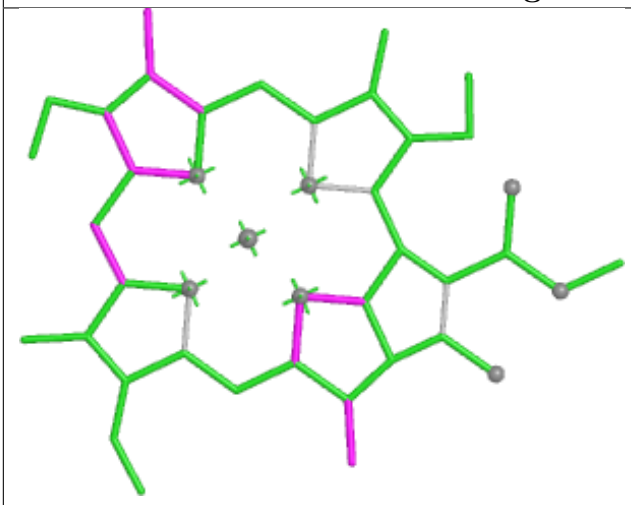


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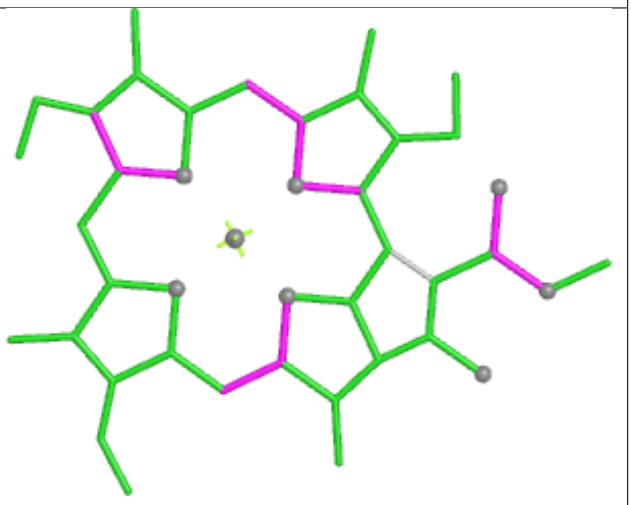


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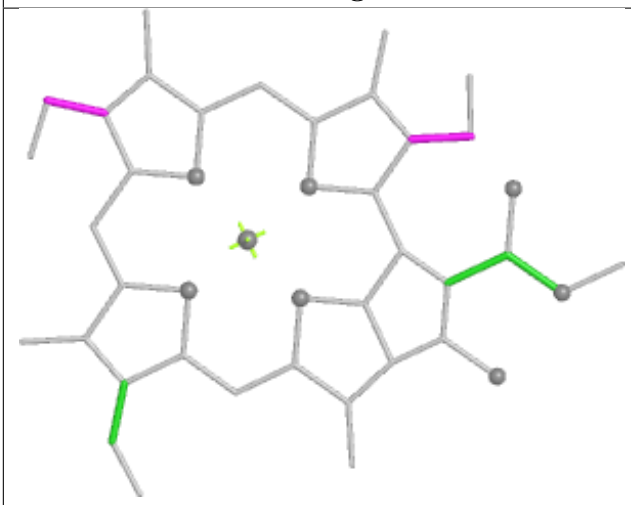
Ligand CLA X 614



Bond lengths



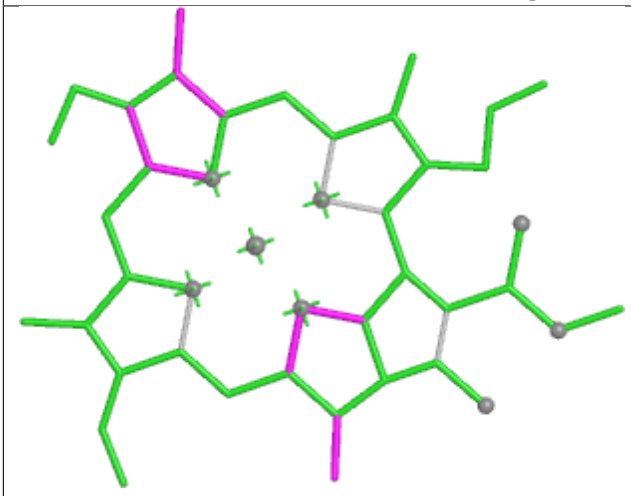
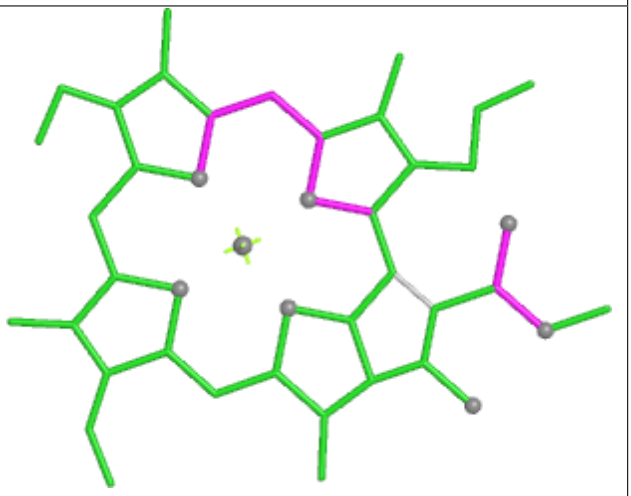
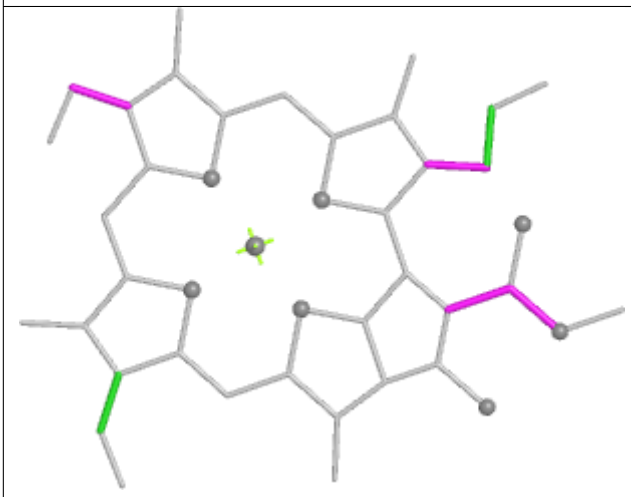
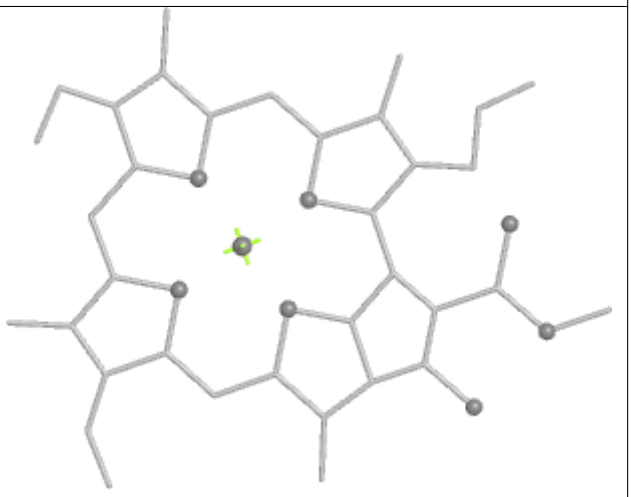
Bond angles



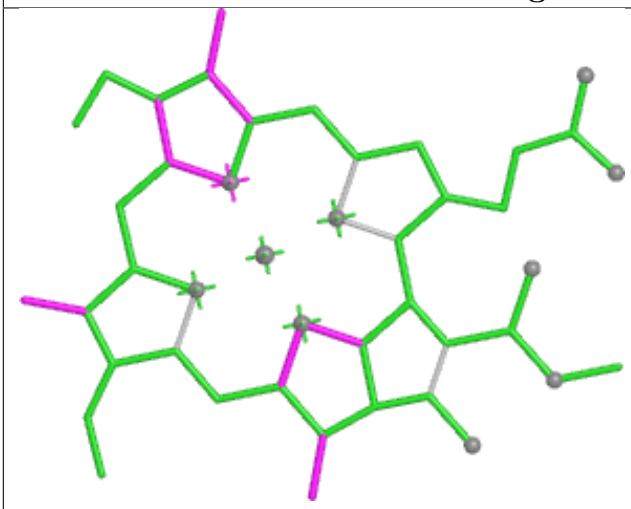
Torsions



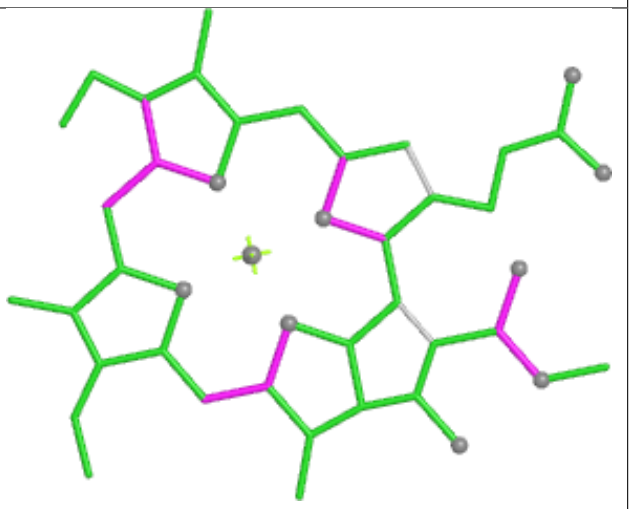
Rings

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

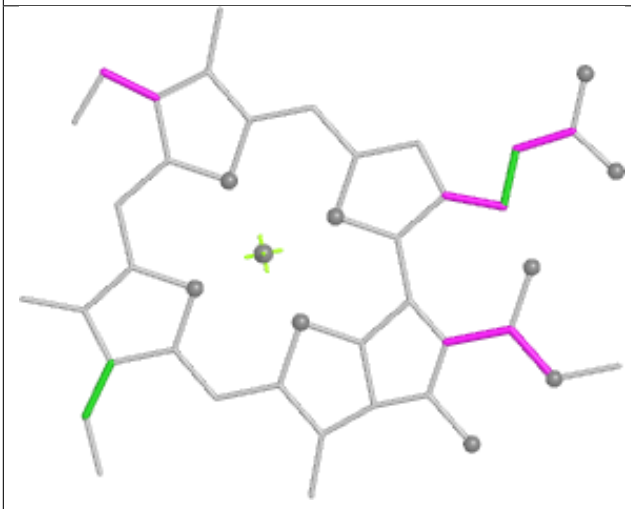
Ligand CLA 5 614



Bond lengths



Bond angles

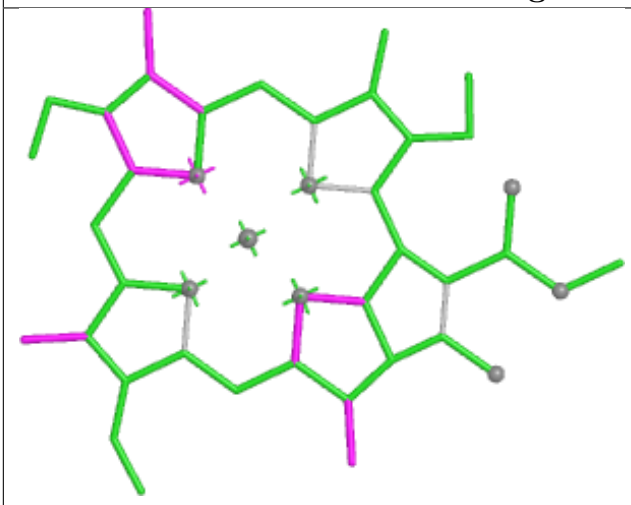


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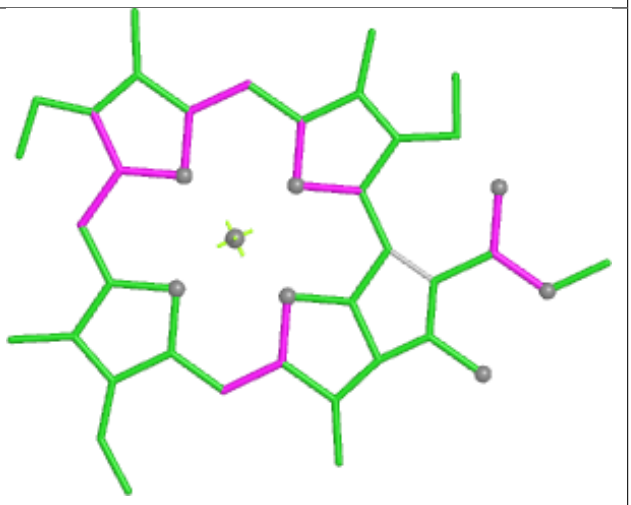


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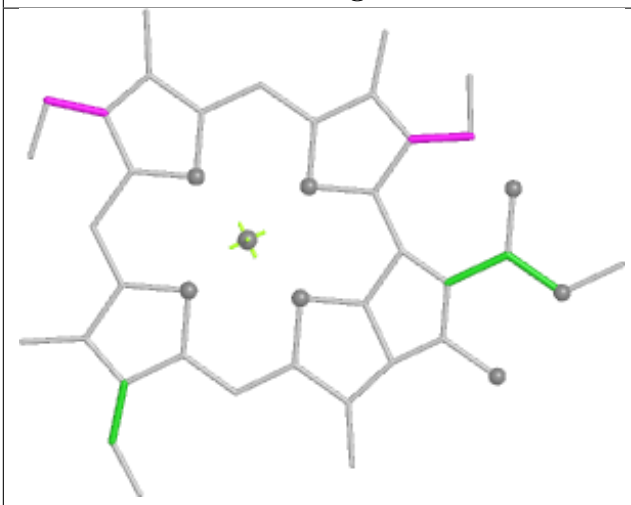
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Bond lengths



Bond angles

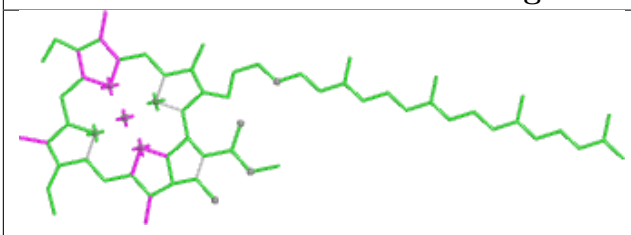


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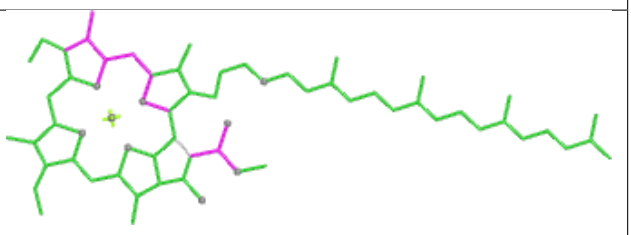


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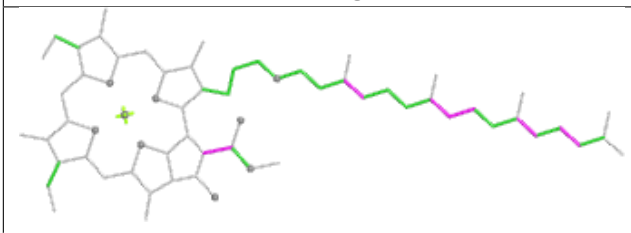
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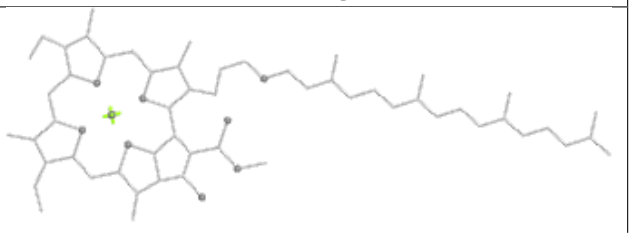
Bond lengths



Bond angles

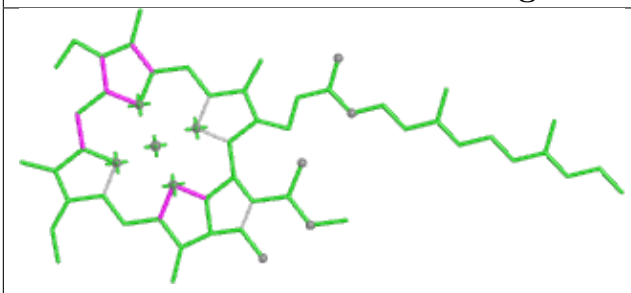


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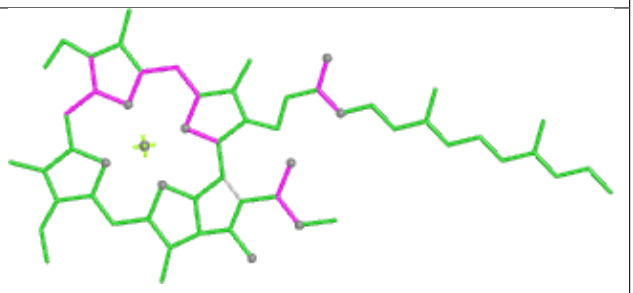


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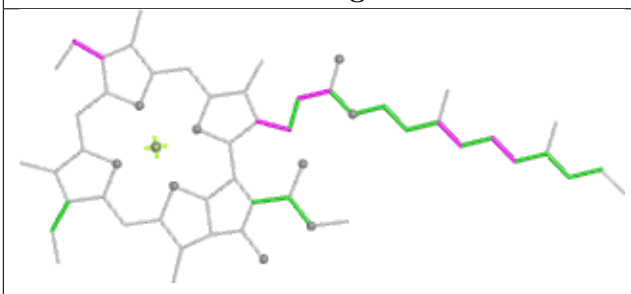
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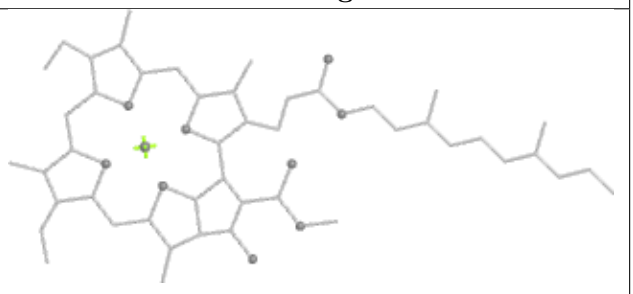
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Bond angles

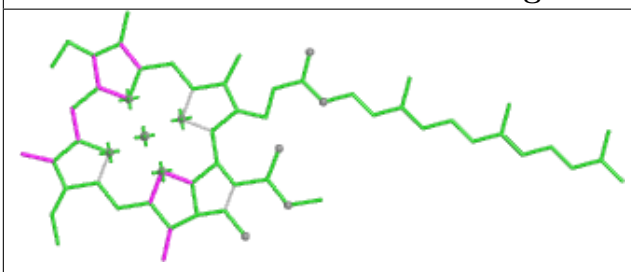


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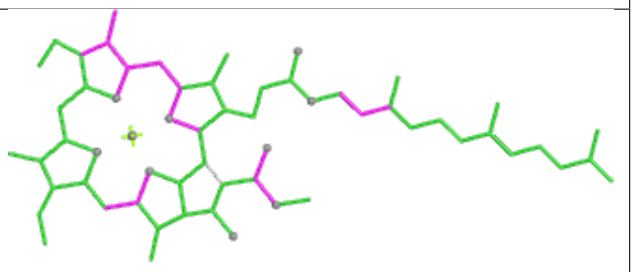


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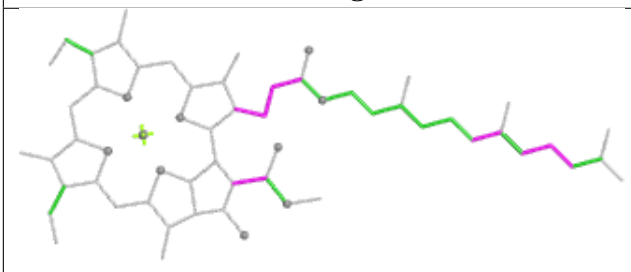
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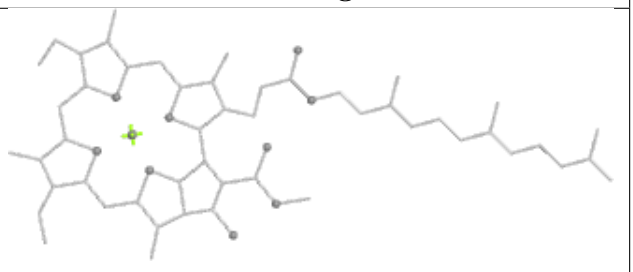
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Bond angles

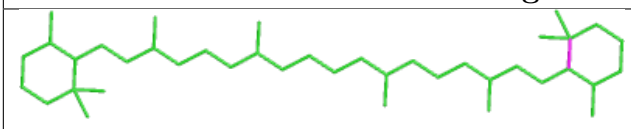


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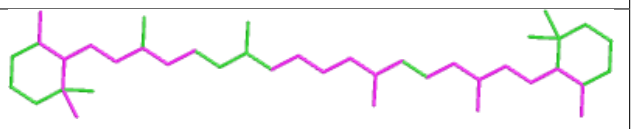


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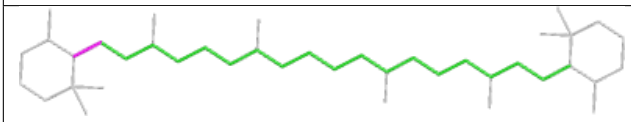
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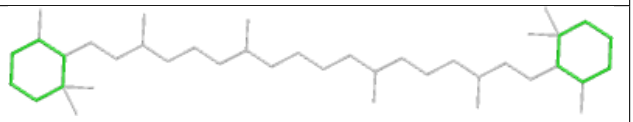
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Bond angles

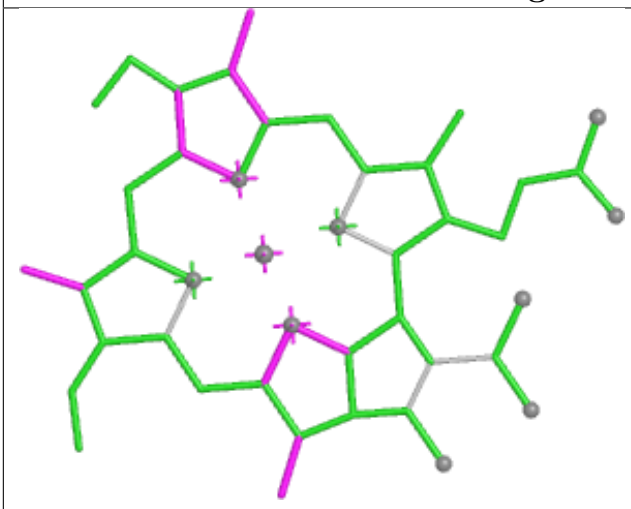


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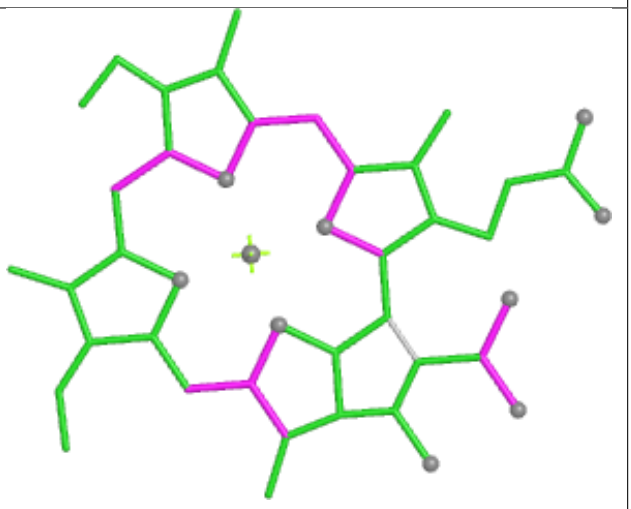


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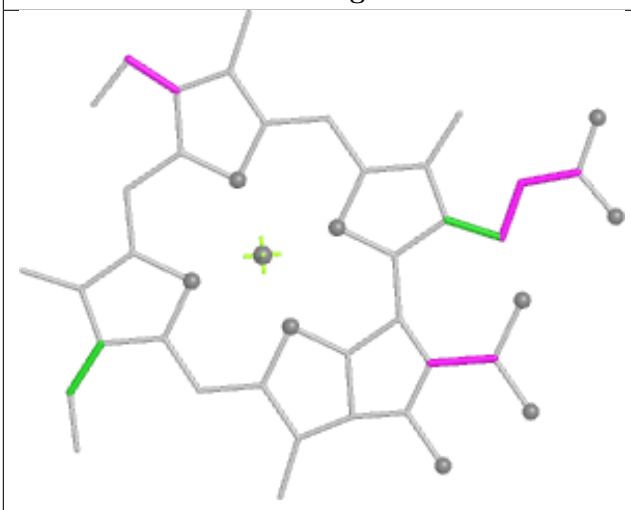
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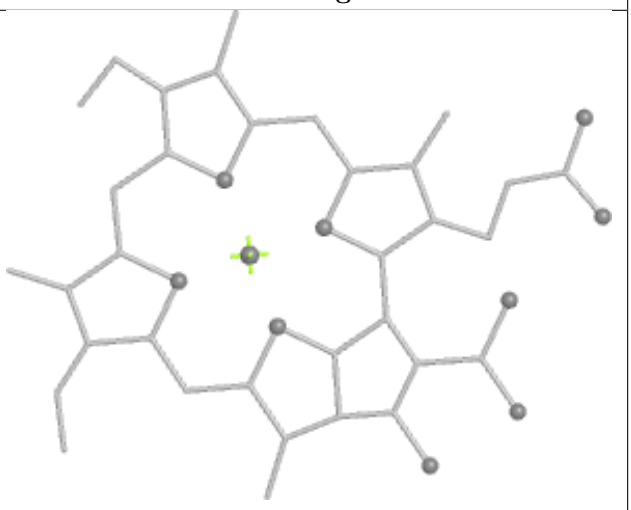
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Bond angles

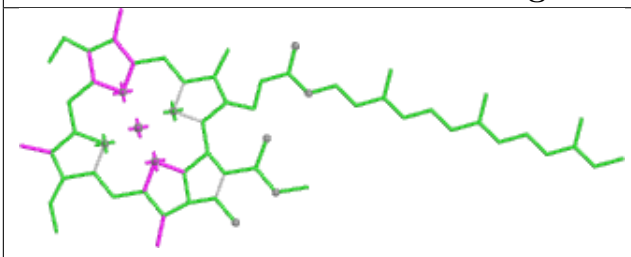


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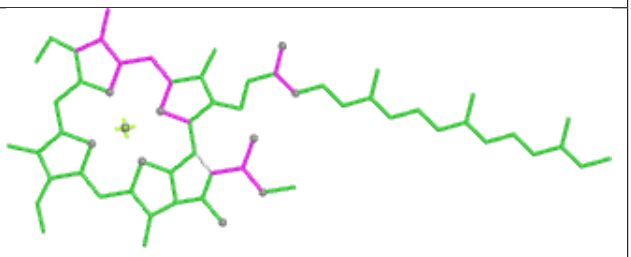


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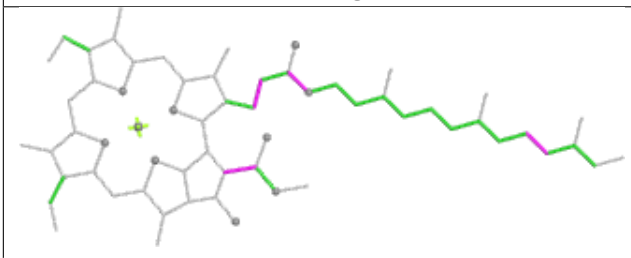
Ligand CLA a 602



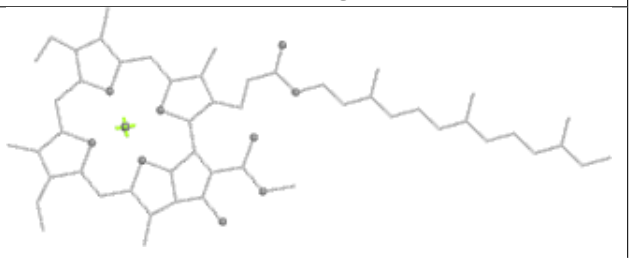
Bond lengths



Bond angles

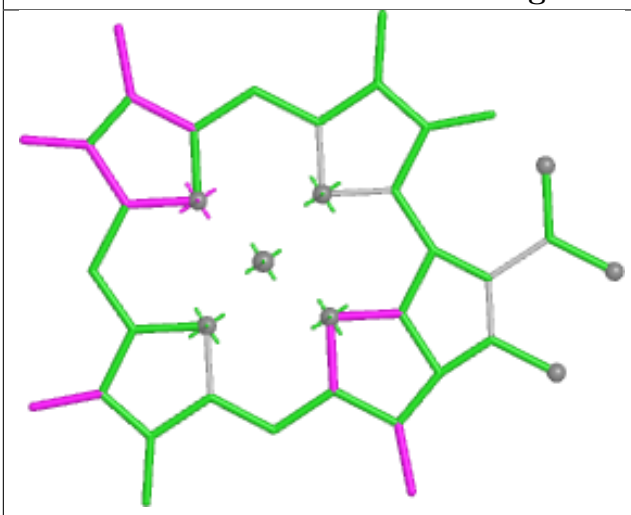


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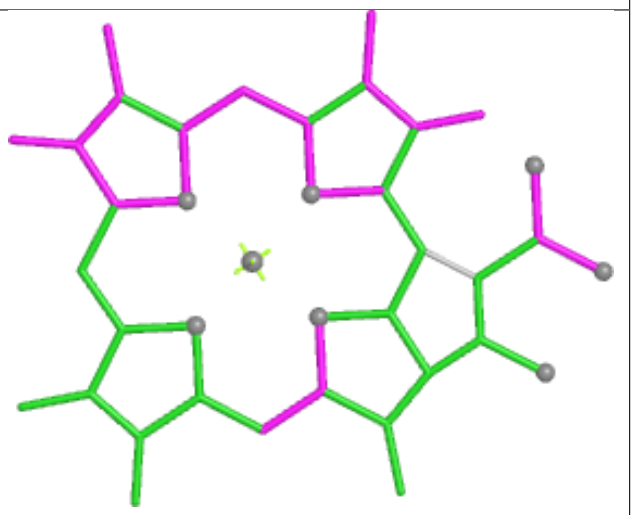


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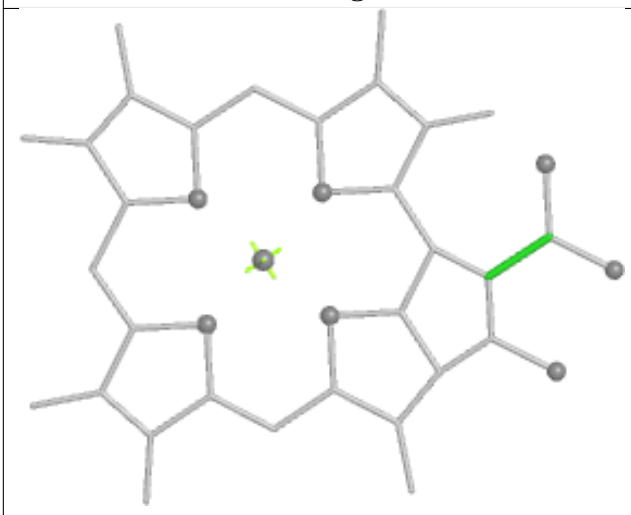
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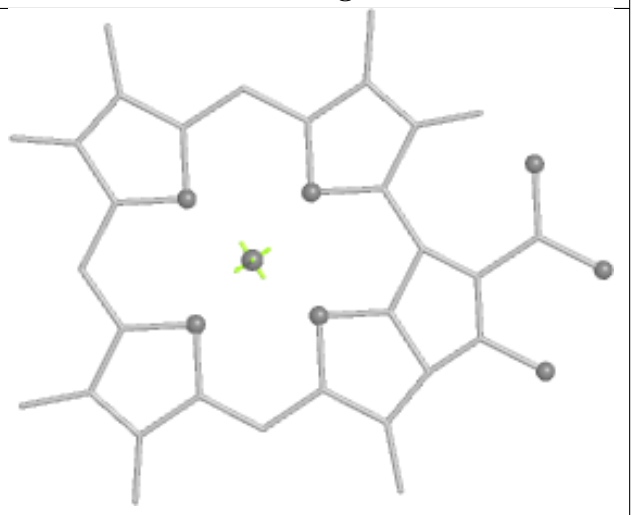
Bond lengths



Bond angles

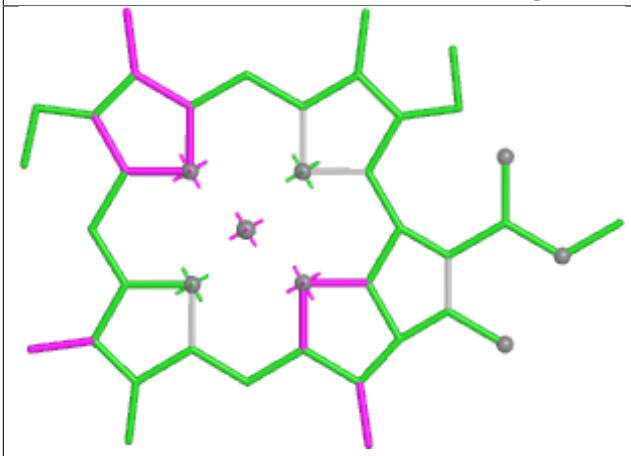


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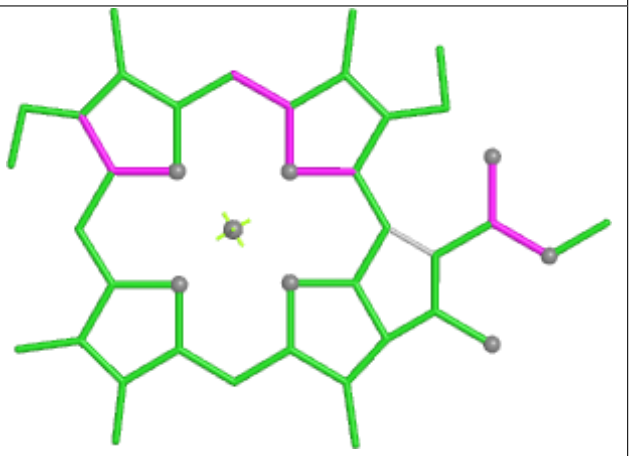


Rings

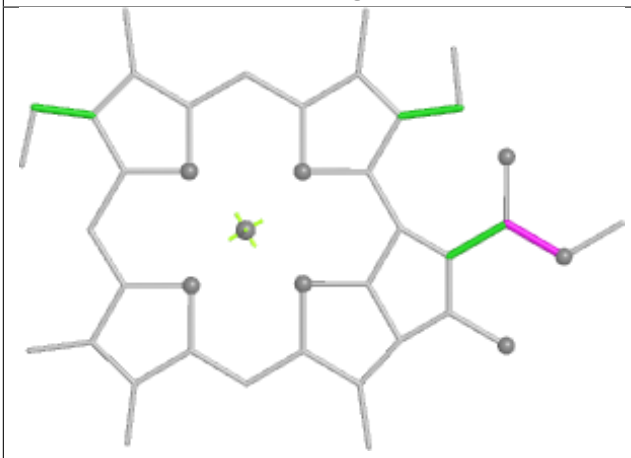
Ligand CLA 7 606



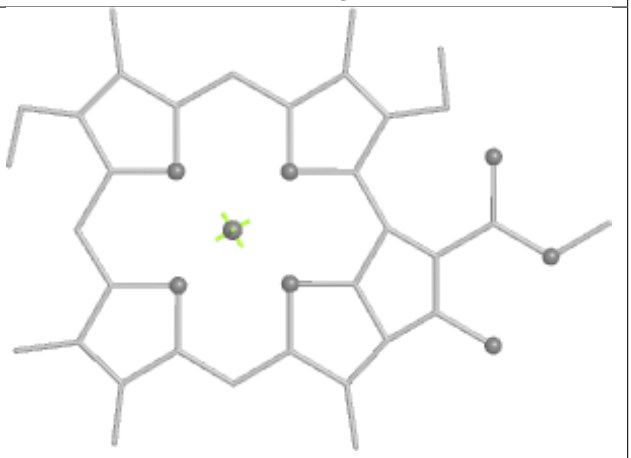
Bond lengths



Bond angles

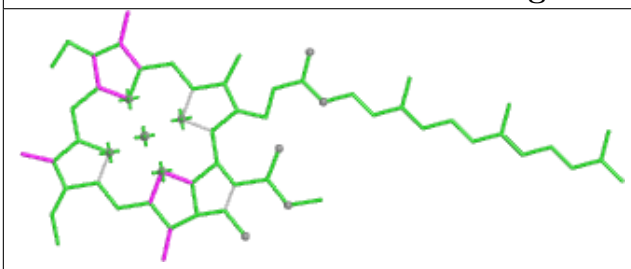


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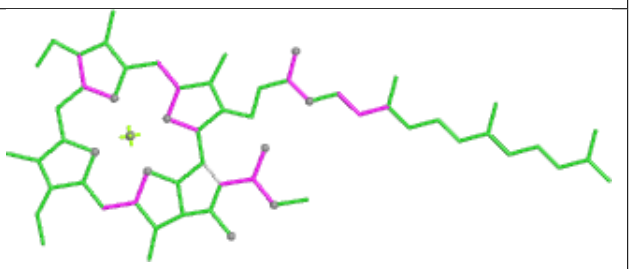


Rings

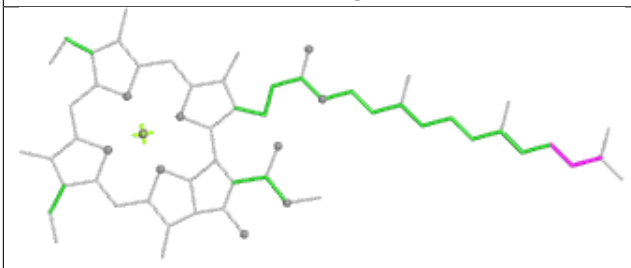
Ligand CLA 3 602



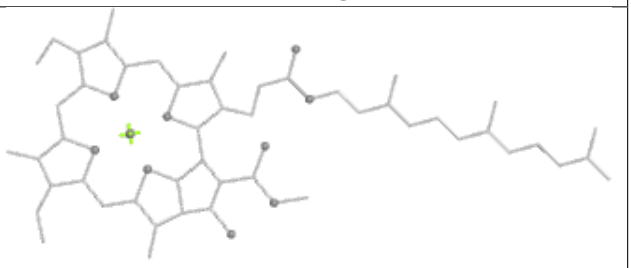
Bond lengths



Bond angles

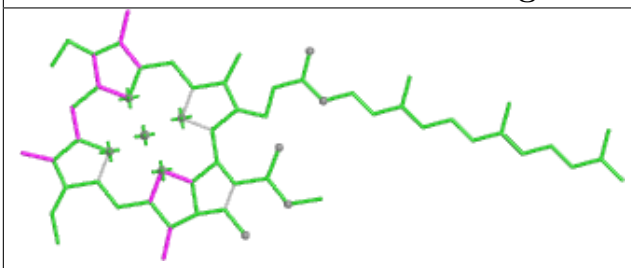


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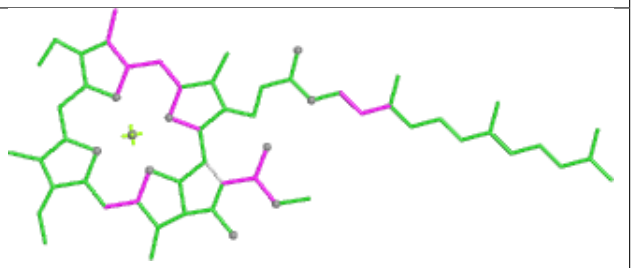


Rings

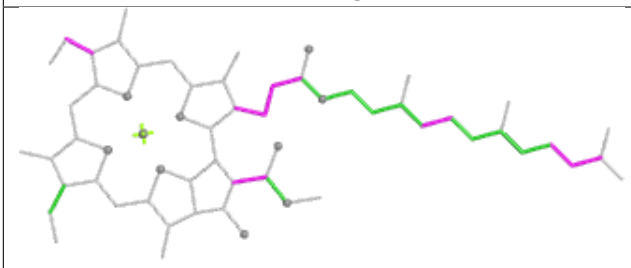
Ligand CLA W 602



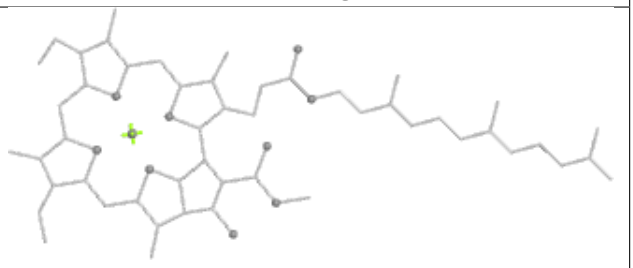
Bond lengths



Bond angles

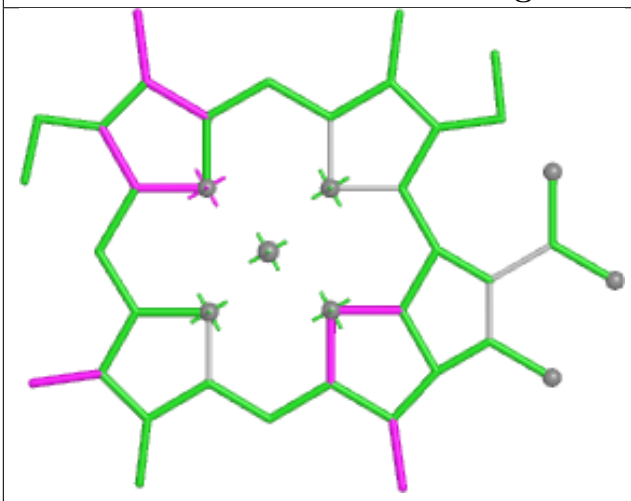


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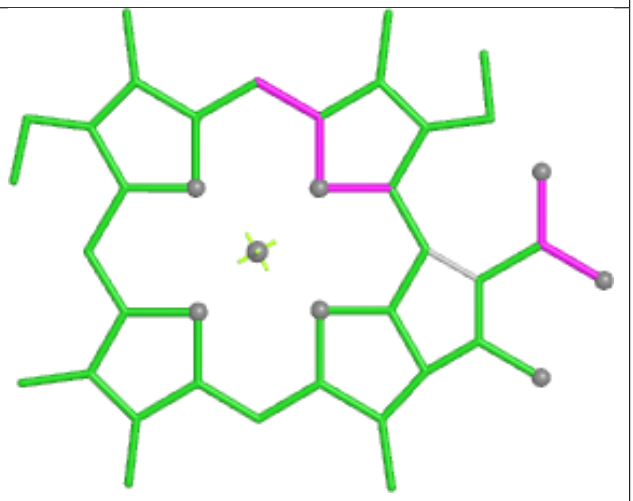


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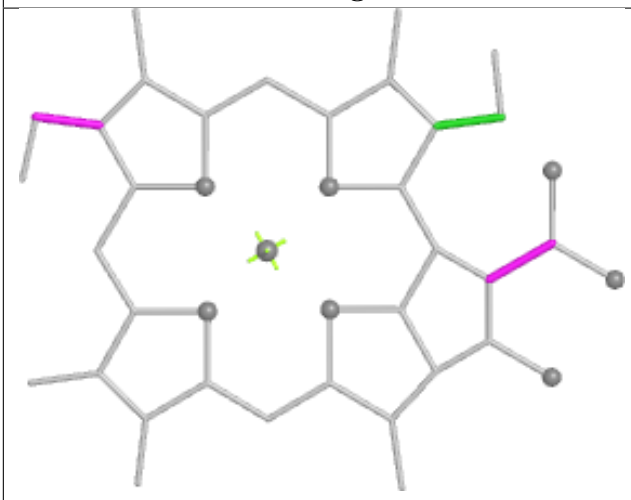
Ligand CLA O 2003



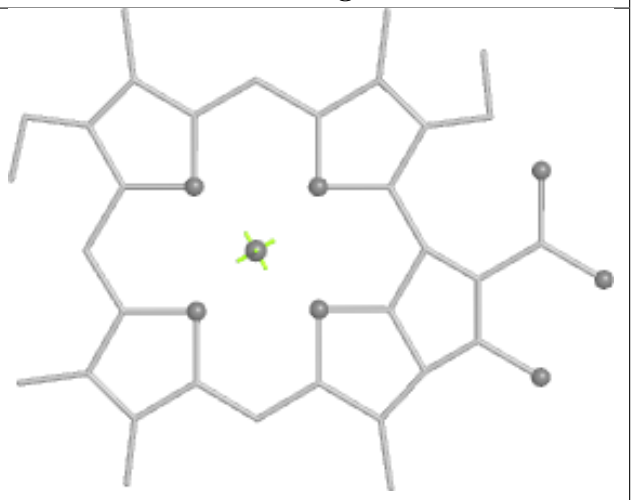
Bond lengths



Bond angles

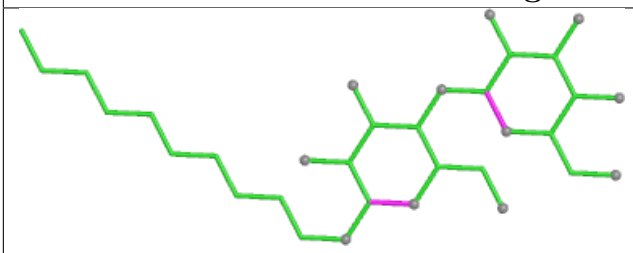


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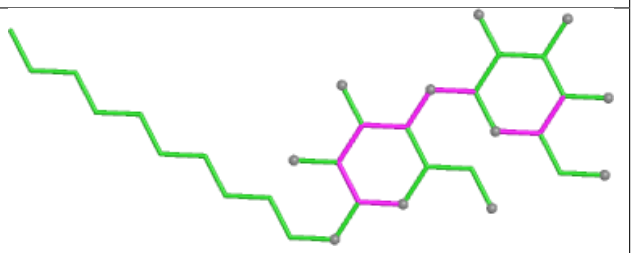


Rings

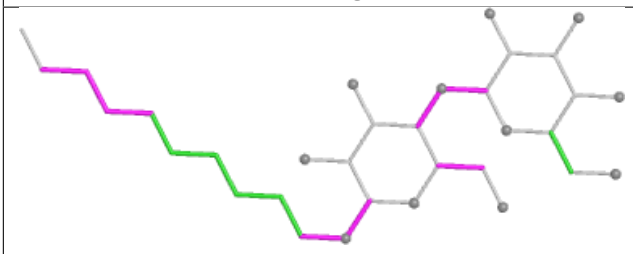
Ligand LMU 5 628



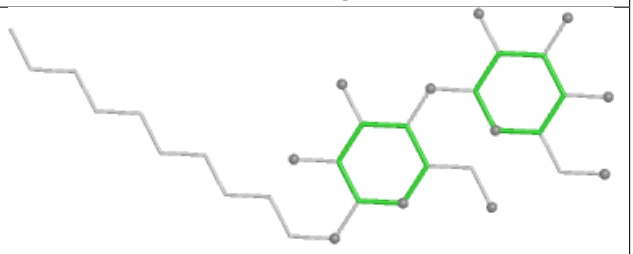
Bond lengths



Bond angles

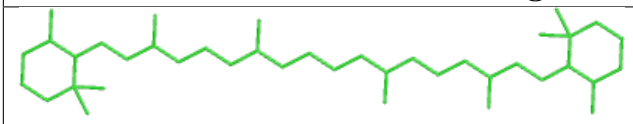


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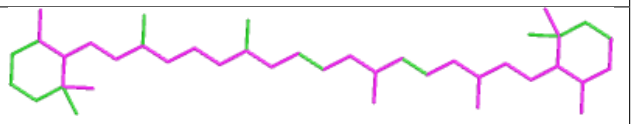


Rings

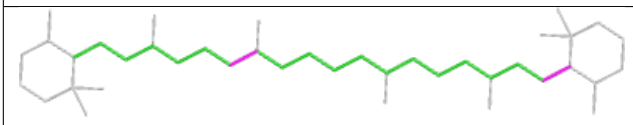
Ligand BCR a 619



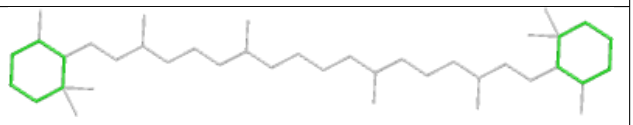
Bond lengths



Bond angles

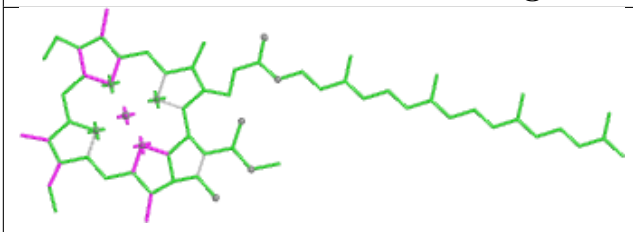


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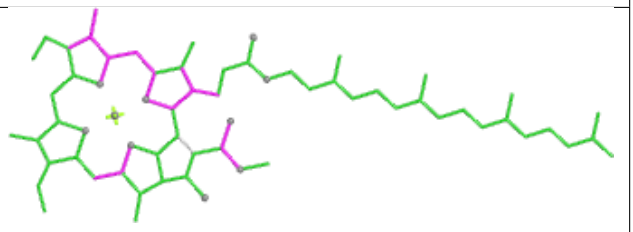


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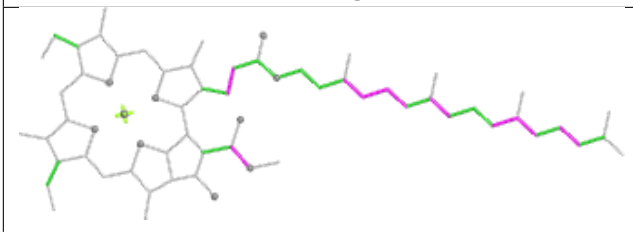
Ligand CLA A 802



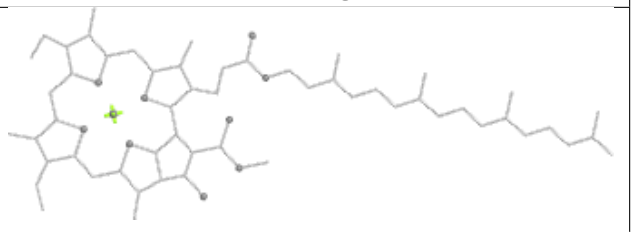
Bond lengths



Bond angles

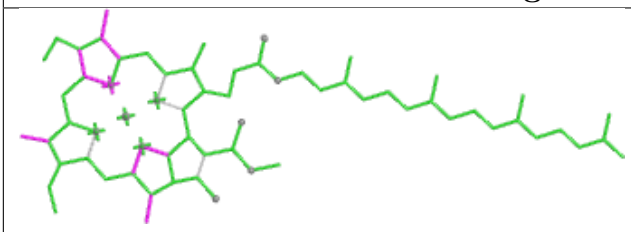


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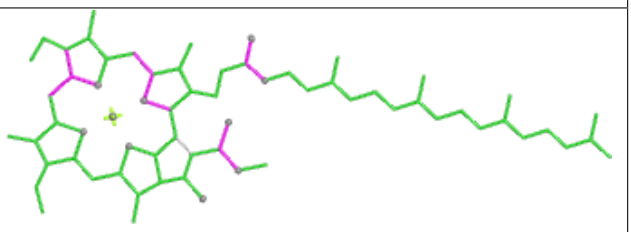


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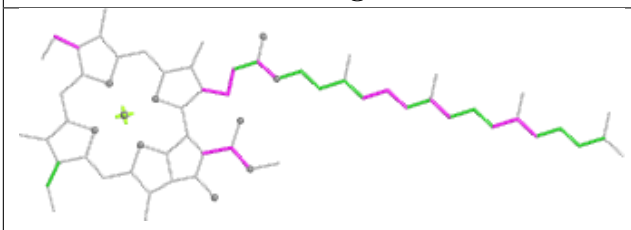
Ligand CLA A 841



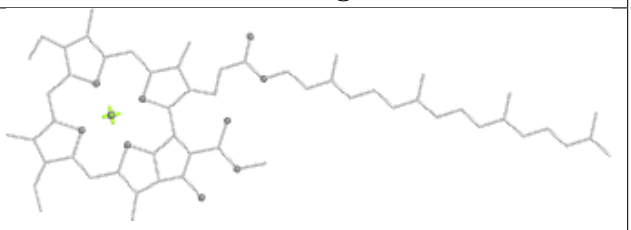
Bond lengths



Bond angles

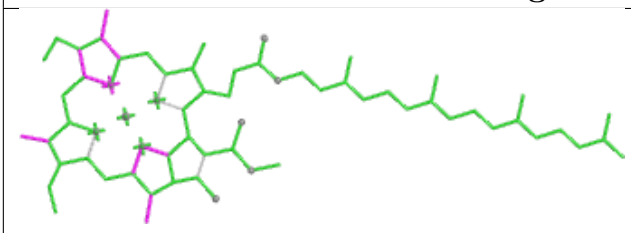


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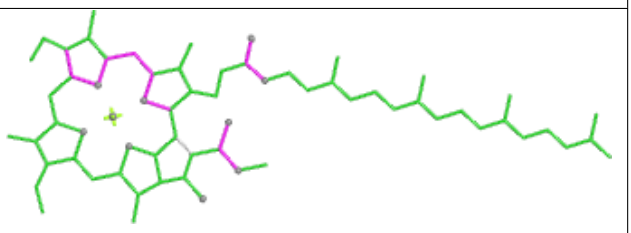


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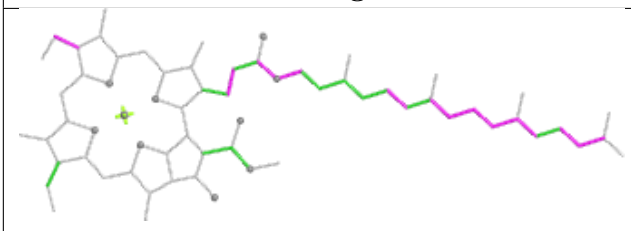
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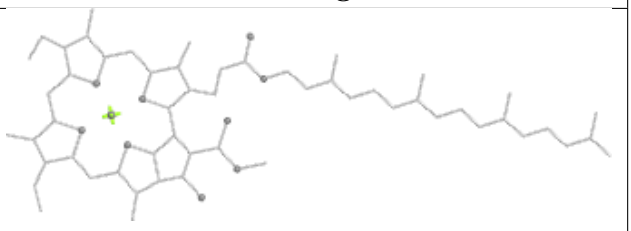
Bond lengths



Bond angles

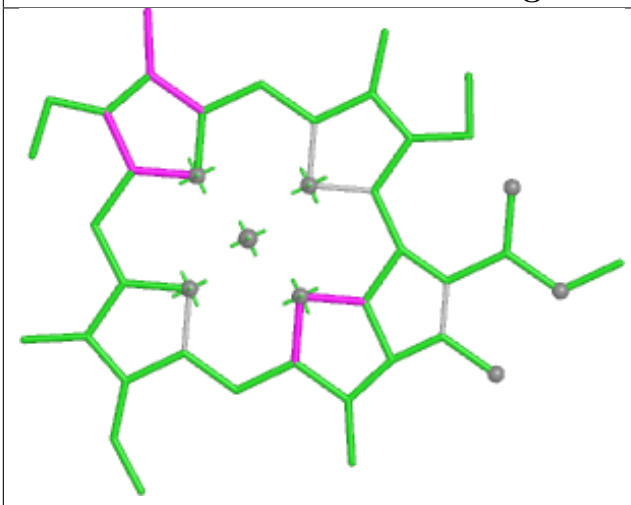


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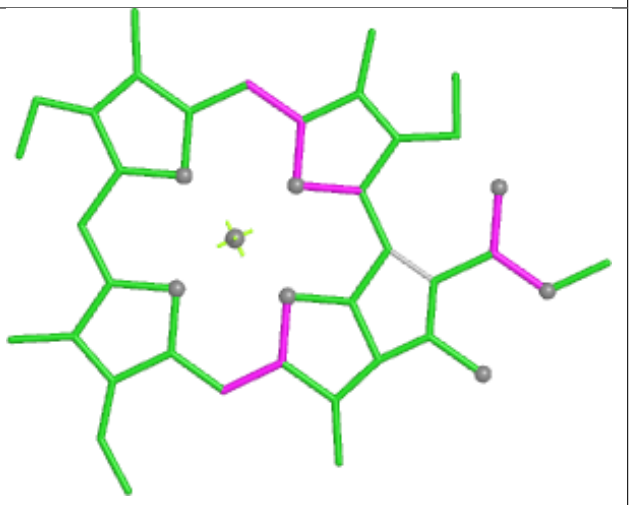


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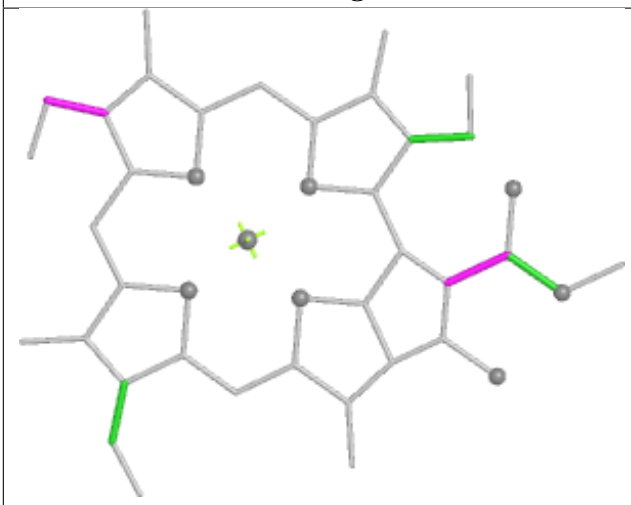
Ligand CLA U 611



Bond lengths



Bond angles

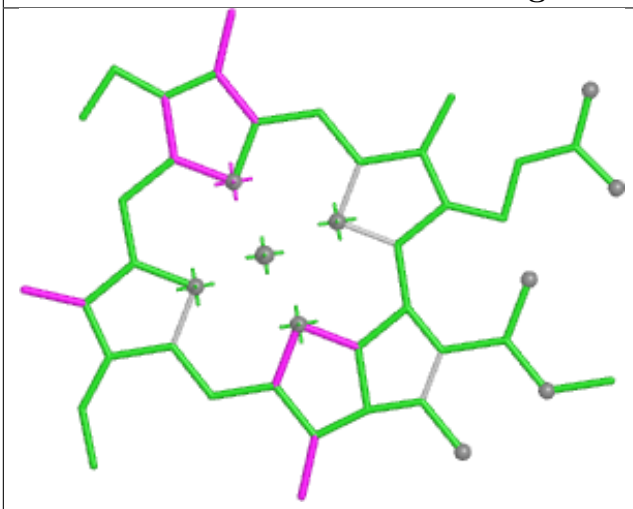


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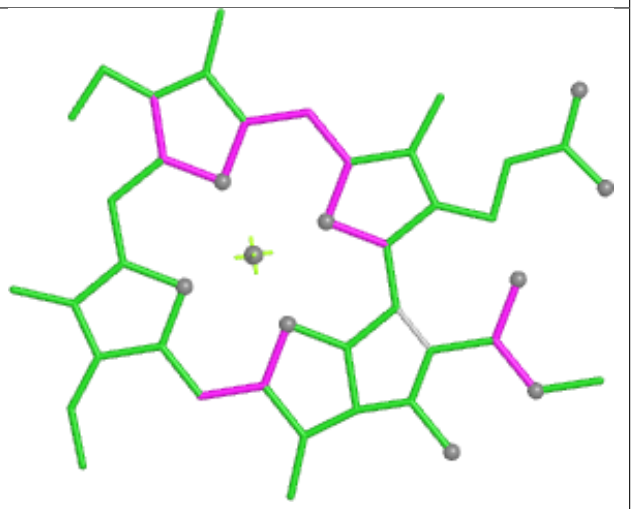


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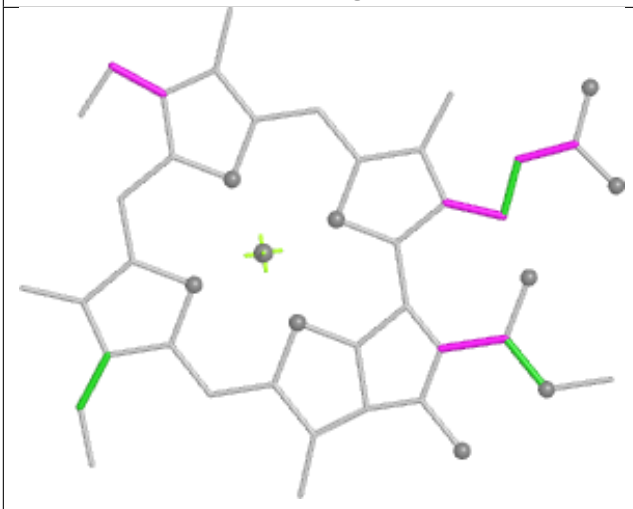
Ligand CLA 6 609



Bond lengths



Bond angles

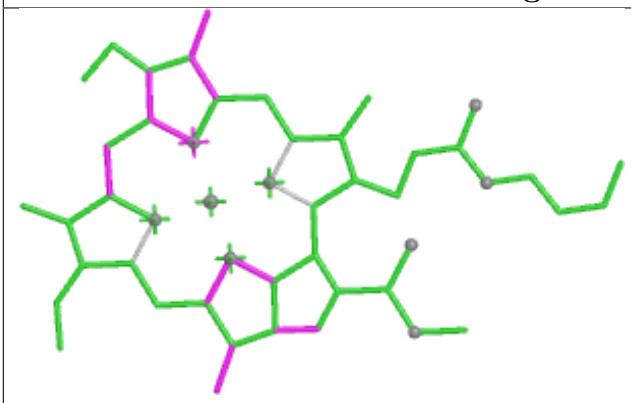


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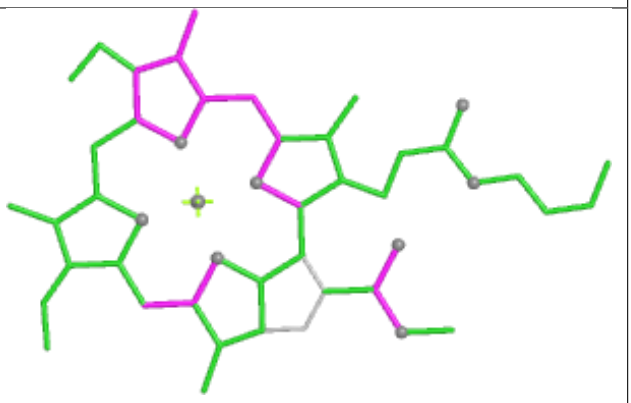


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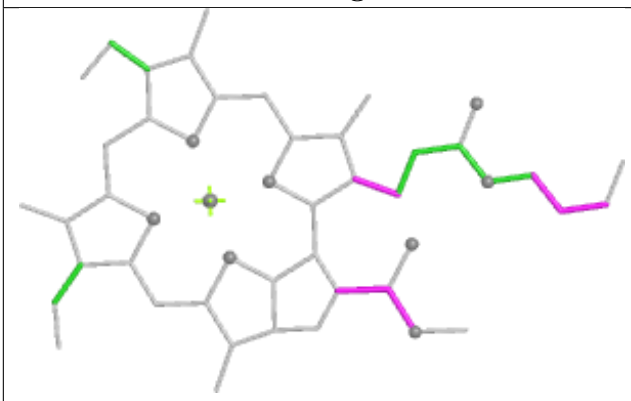
Ligand CLA U 604



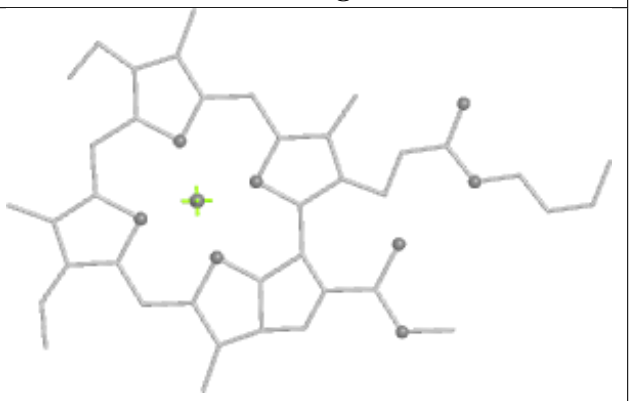
Bond lengths



Bond angles

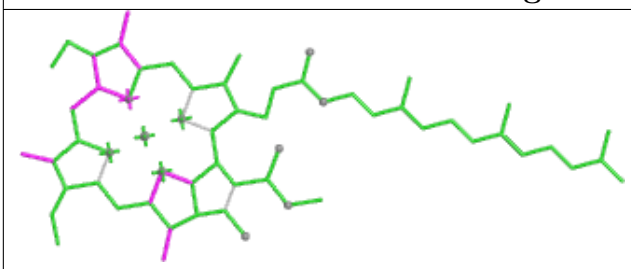


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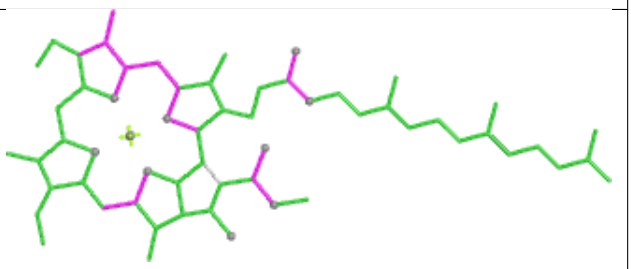


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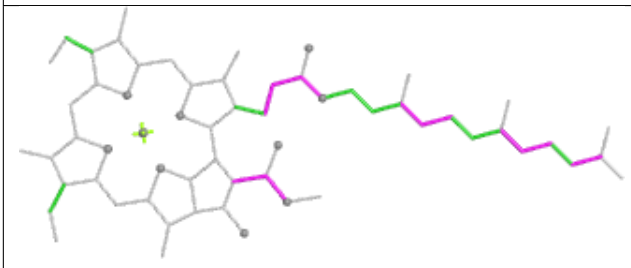
Ligand CLA A 818



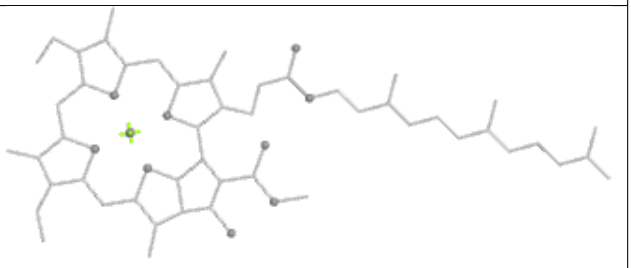
Bond lengths



Bond angles

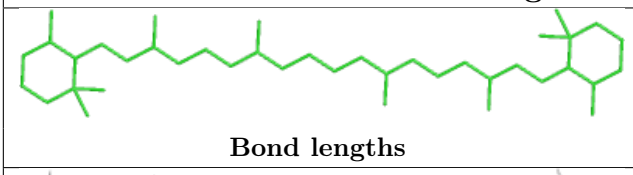


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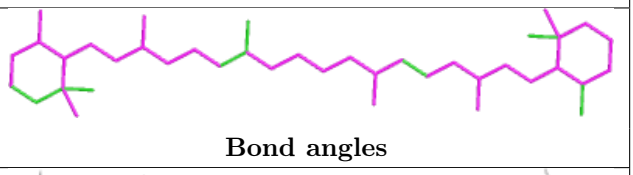


Rings

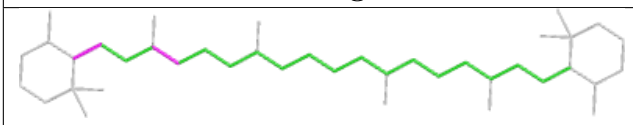
Ligand BCR L 301



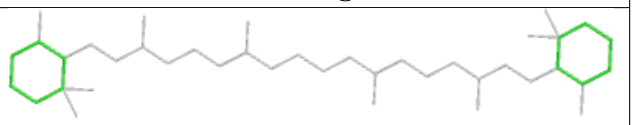
Bond lengths



Bond angles

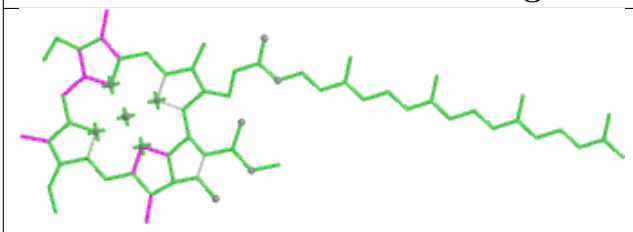


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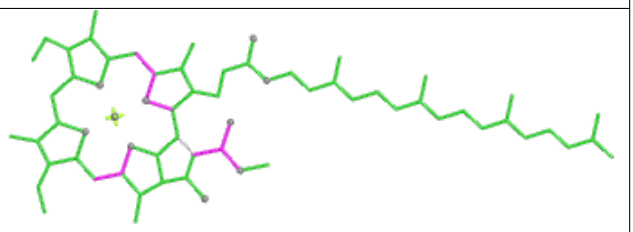


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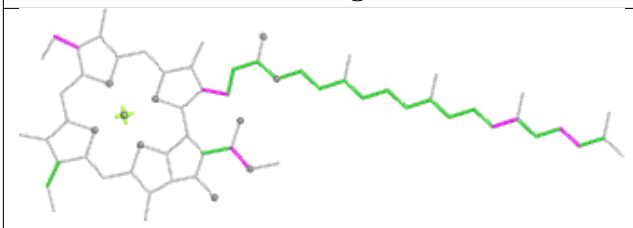
Ligand CLA A 812



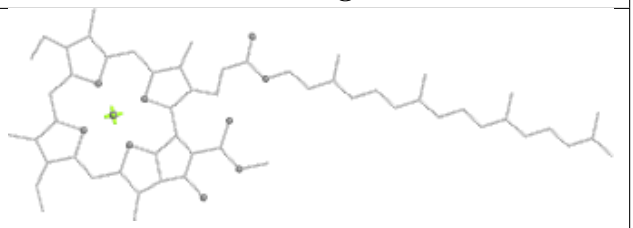
Bond lengths



Bond angles

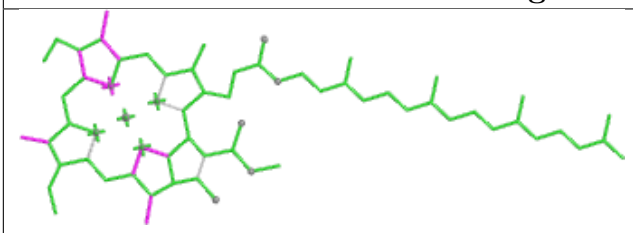


Torsions

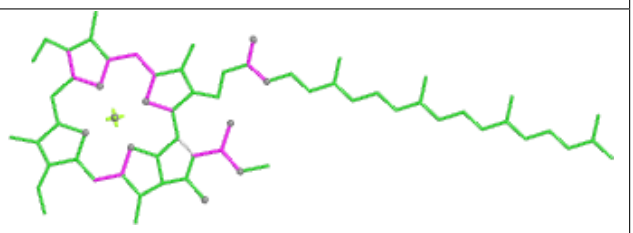


Rings

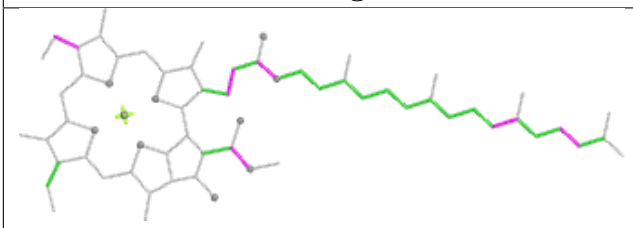
Ligand CLA 6 602



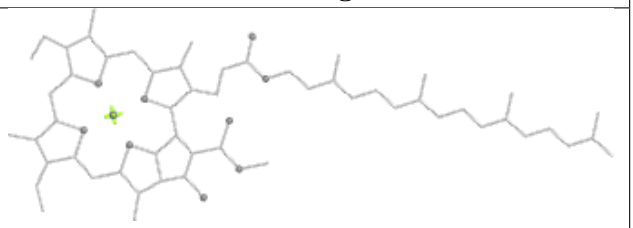
Bond lengths



Bond angles

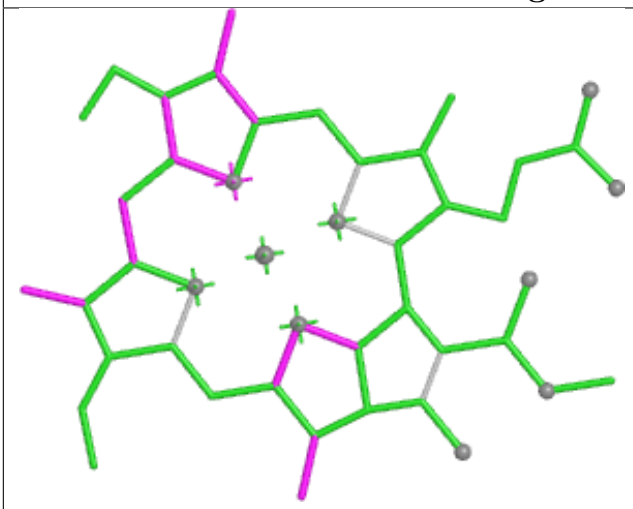


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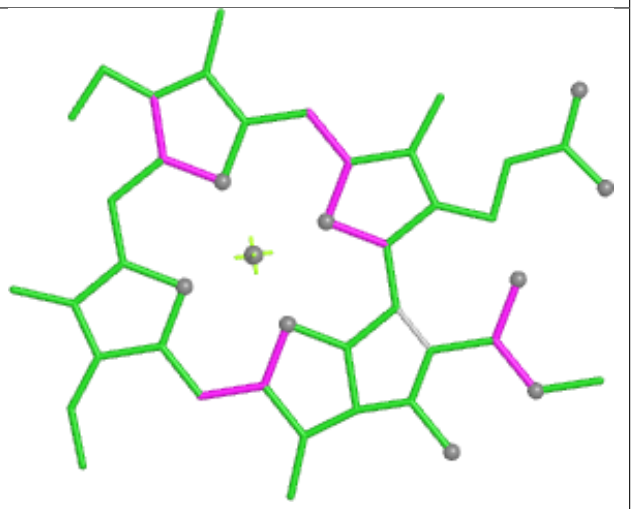


Rings

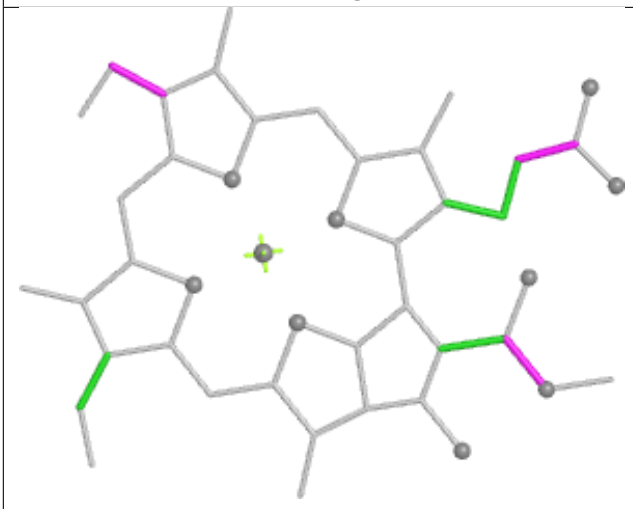
Ligand CLA a 607



Bond lengths



Bond angles

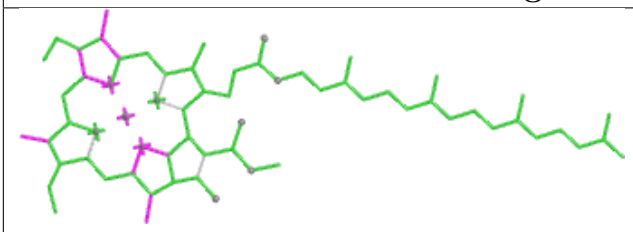


Torsions

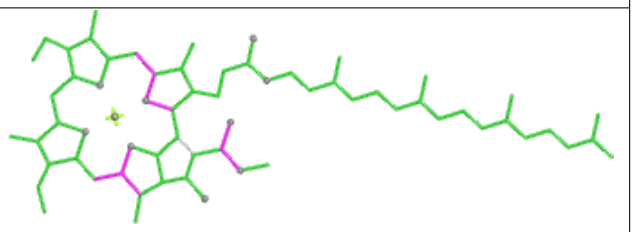


Rings

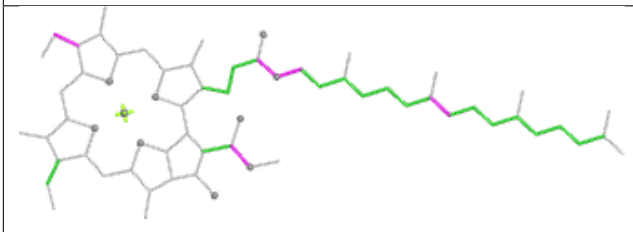
Ligand CLA B 840



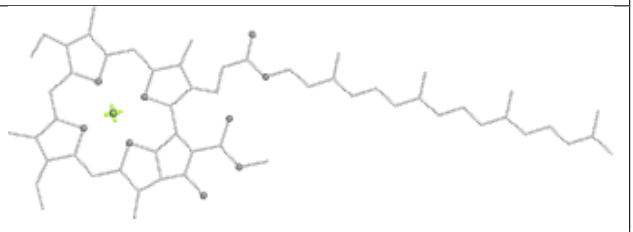
Bond lengths



Bond angles

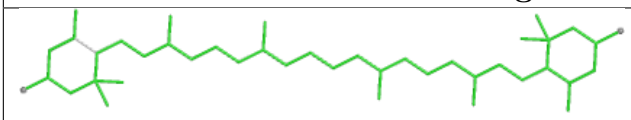


Torsions

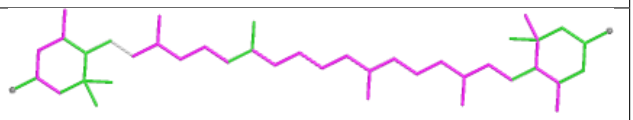


Rings

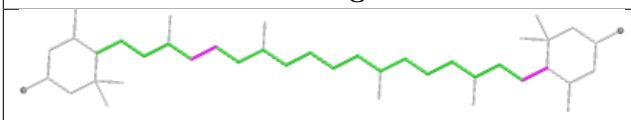
Ligand LUT X 1621



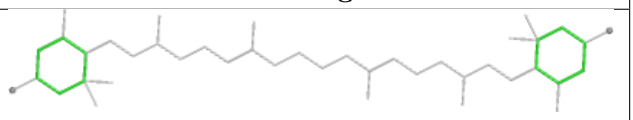
Bond lengths



Bond angles

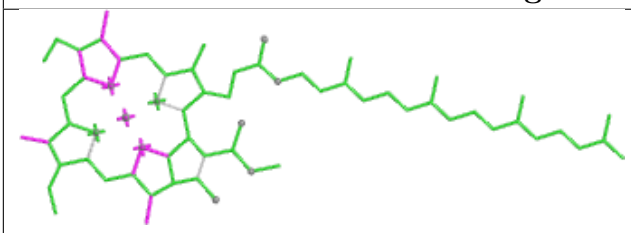


Torsions

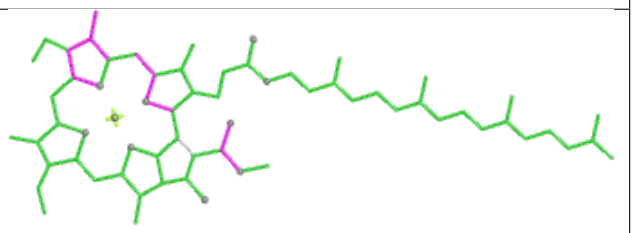


Rings

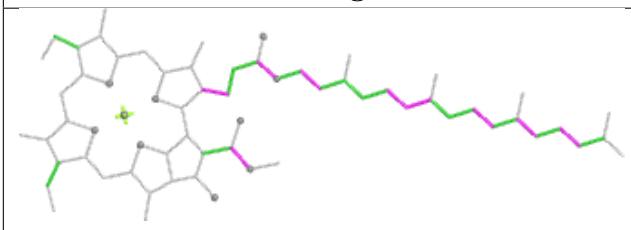
Ligand CLA B 803



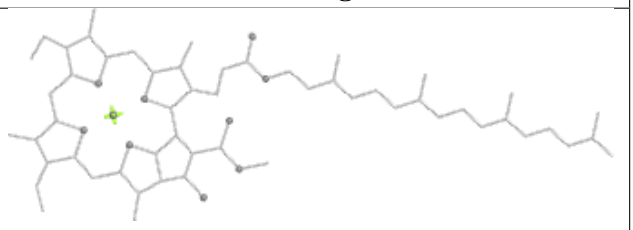
Bond lengths



Bond angles

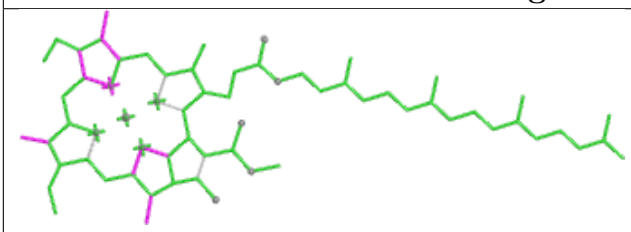


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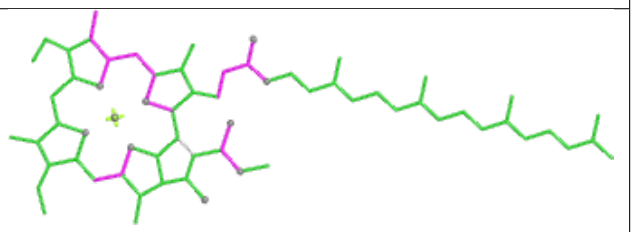


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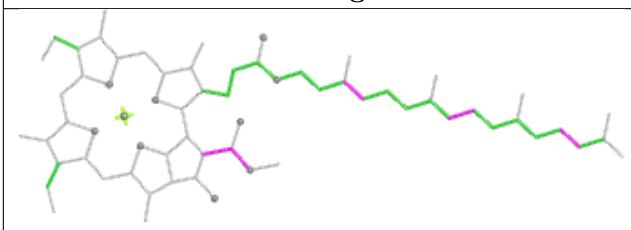
Ligand CLA 3 604



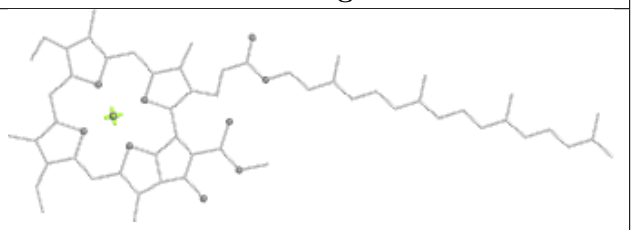
Bond lengths



Bond angles

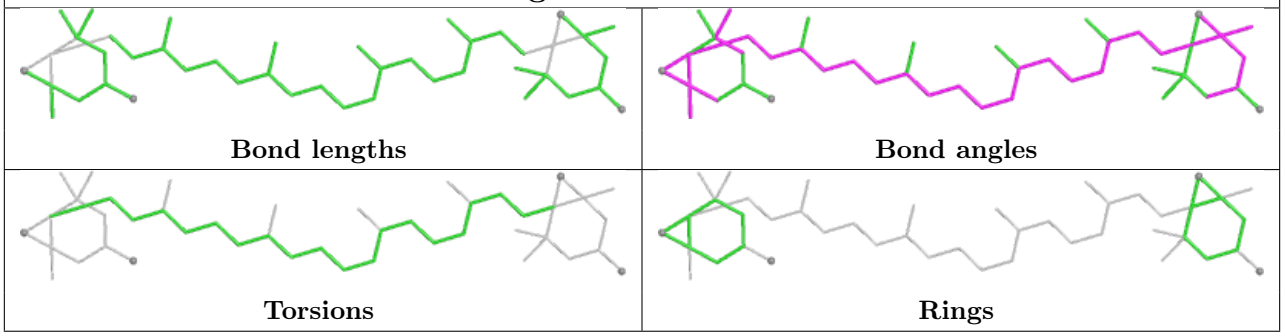


Torsions



Rings

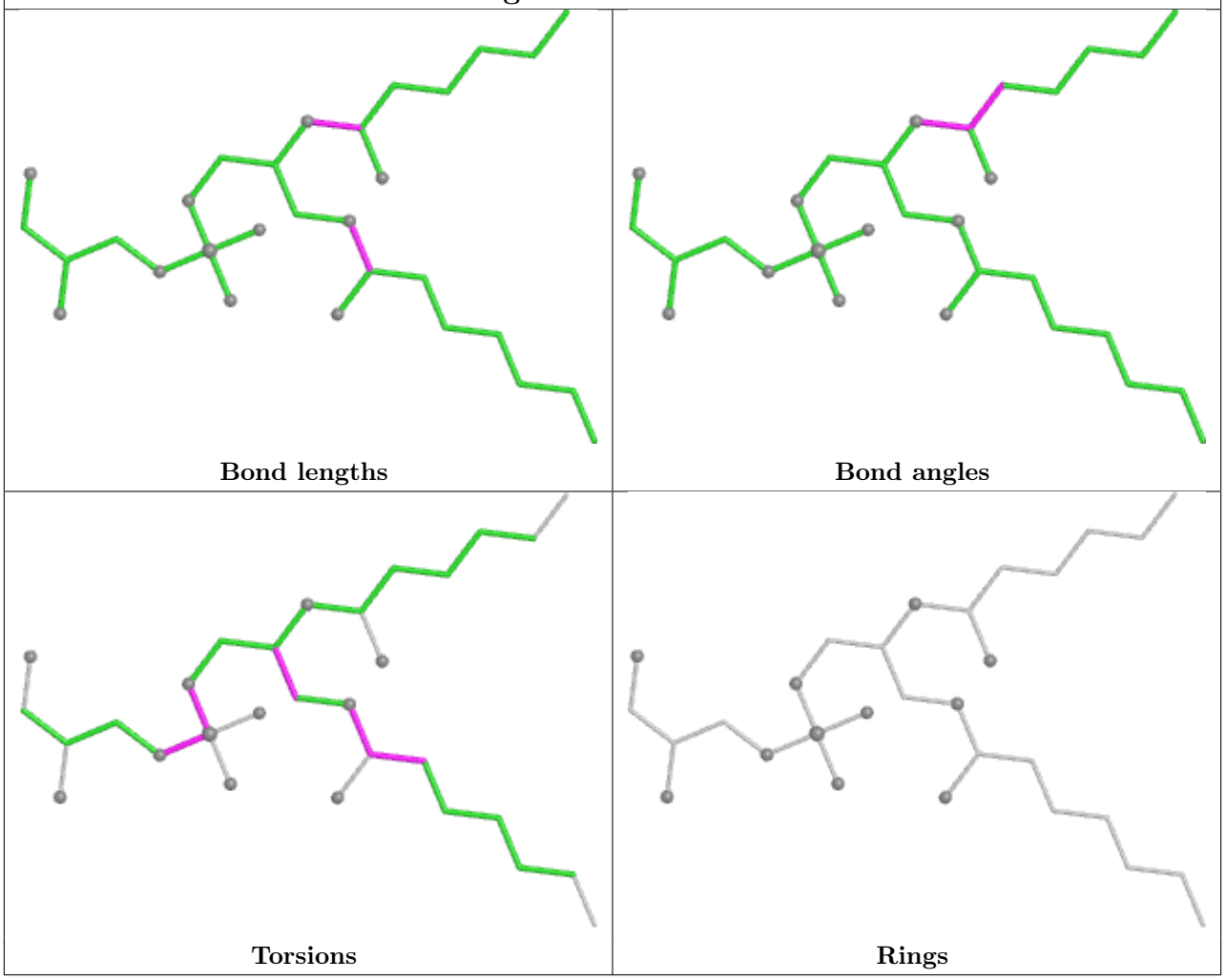
Ligand XAT a 618



Bond lengths | Bond angles

Torsions | Rings

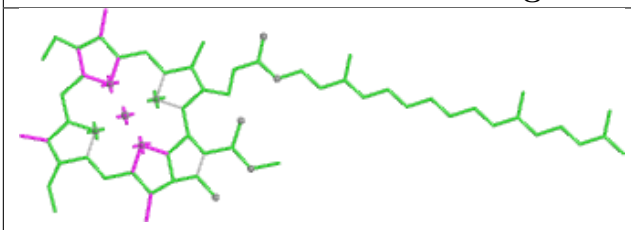
Ligand LHG 9 622



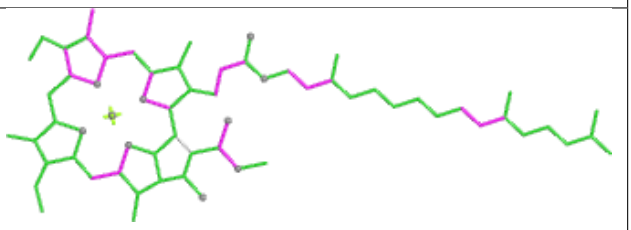
Bond lengths | Bond angles

Torsions | Rings

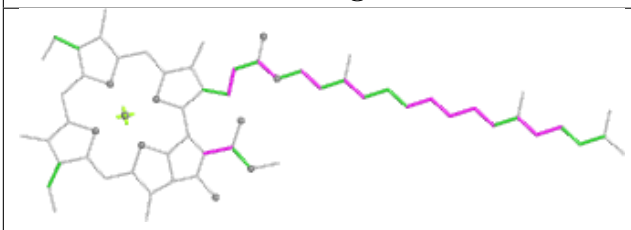
Ligand CLA A 843



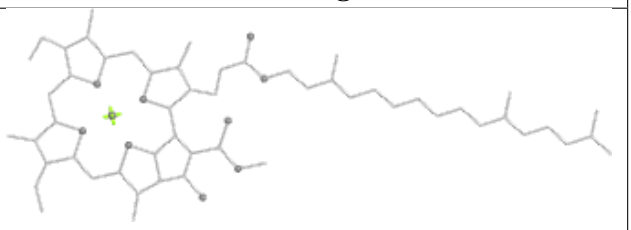
Bond lengths



Bond angles

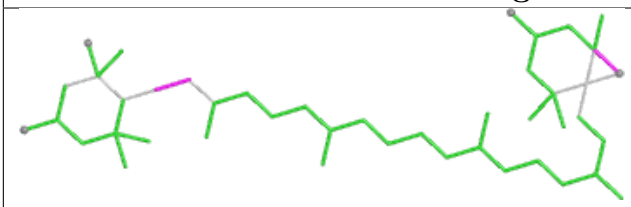


Torsions

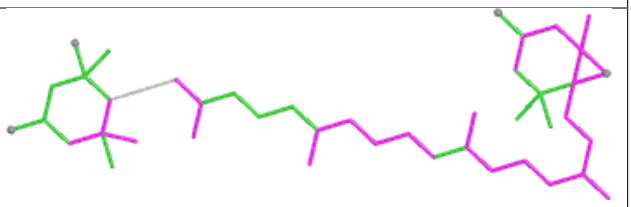


Rings

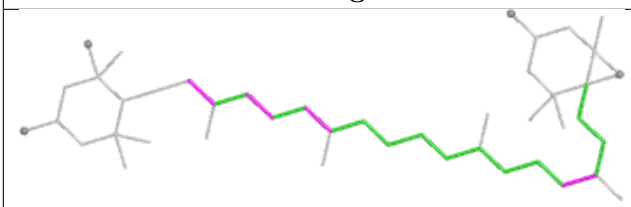
Ligand NEX V 1623



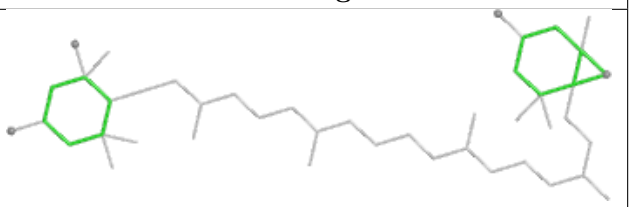
Bond lengths



Bond angles

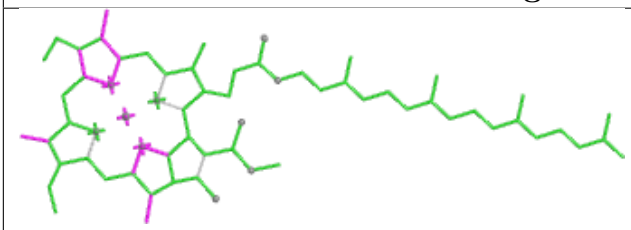


Torsions

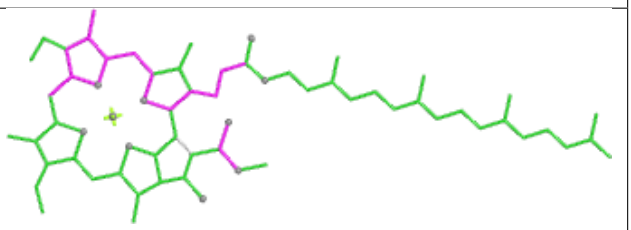


Rings

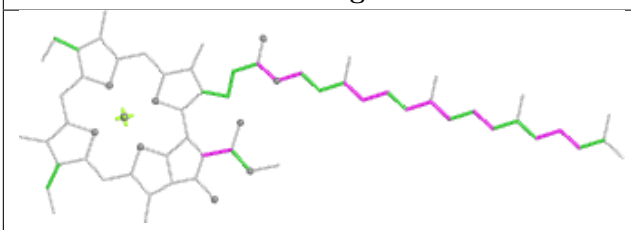
Ligand CLA A 828



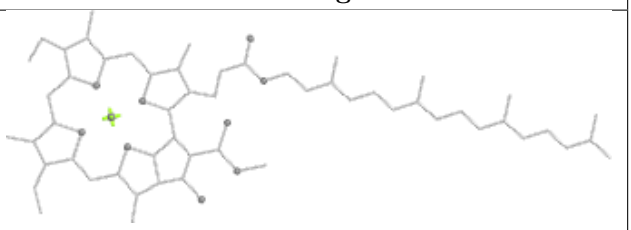
Bond lengths



Bond angles

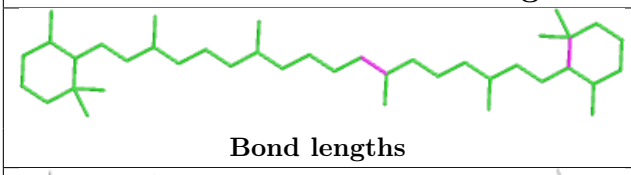


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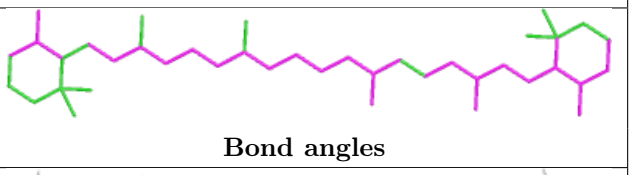


Rings

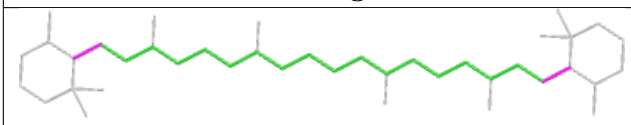
Ligand BCR K 202



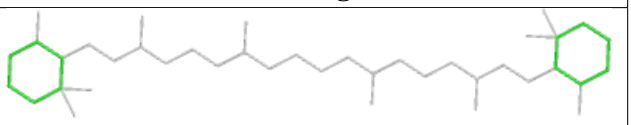
Bond lengths



Bond angles

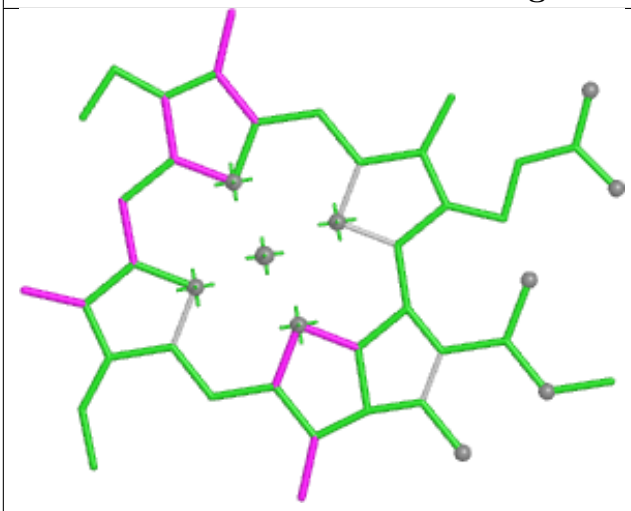


Torsions

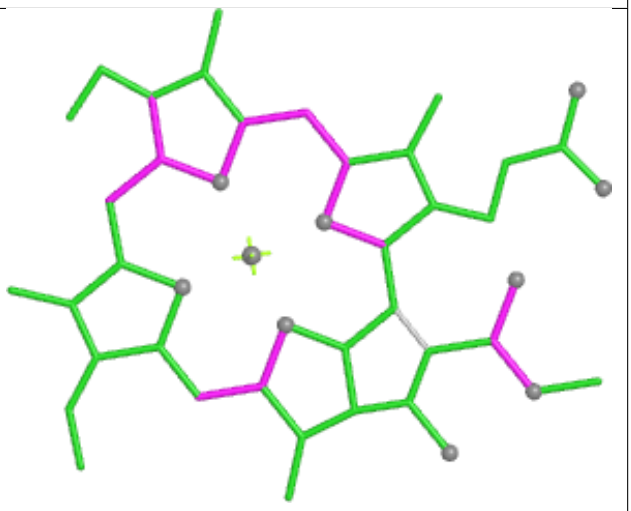


Rings

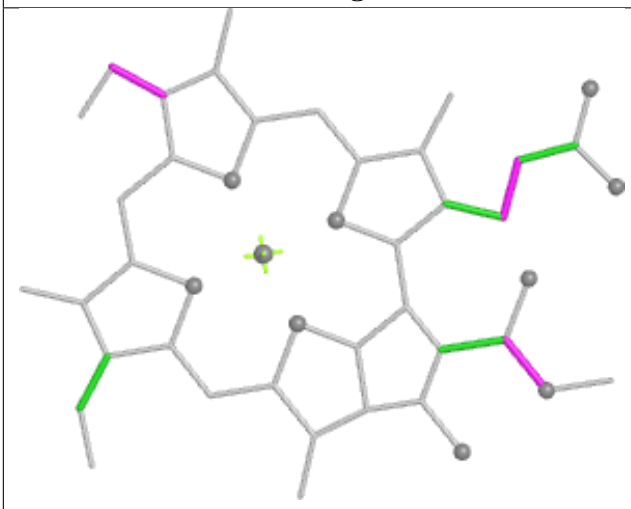
Ligand CLA 9 614



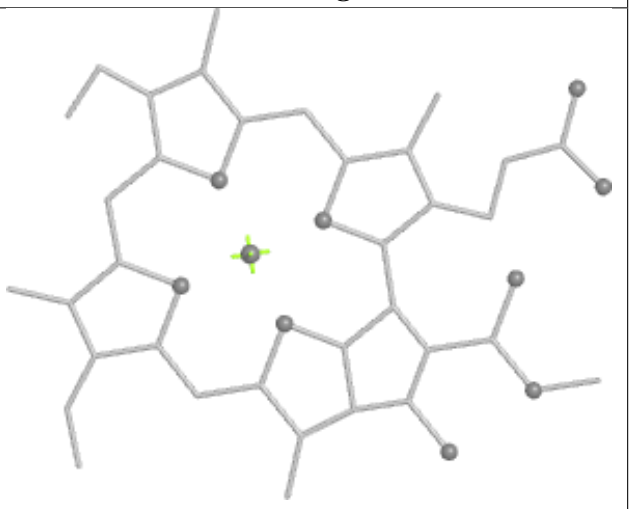
Bond lengths



Bond angles

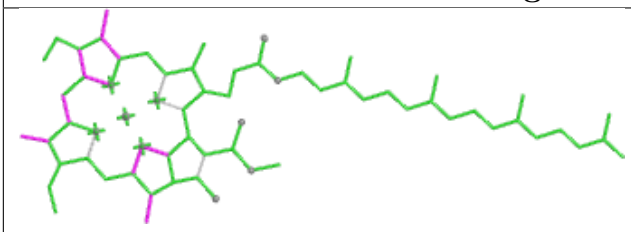


Torsions

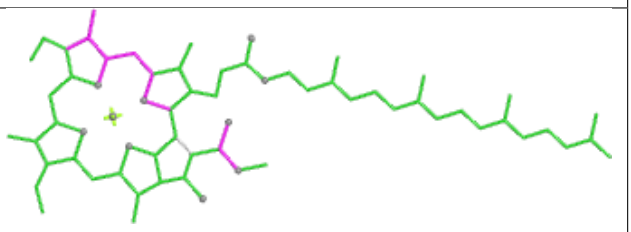


Rings

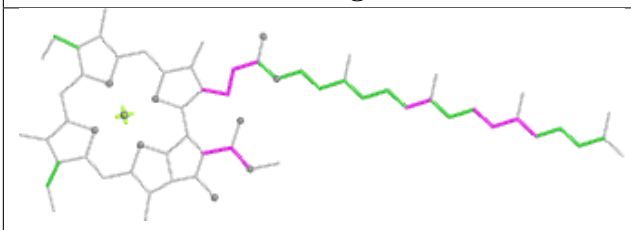
Ligand CLA X 602



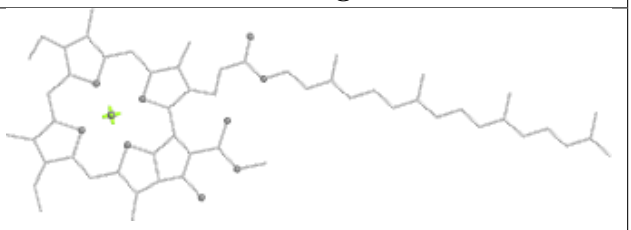
Bond lengths



Bond angles

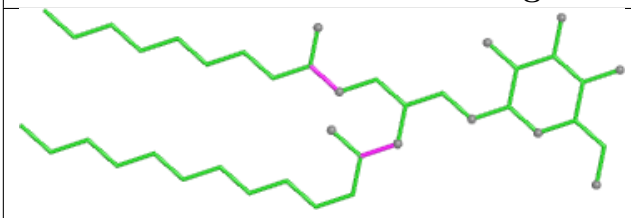


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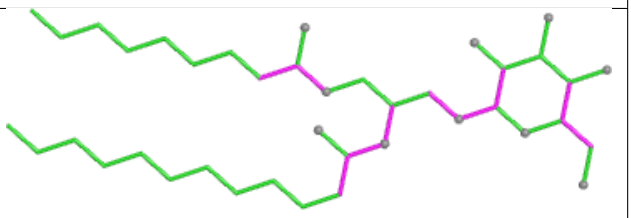


Rings

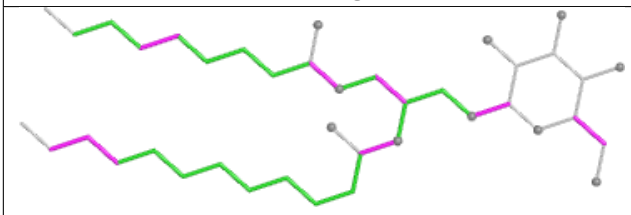
Ligand LMG J 104



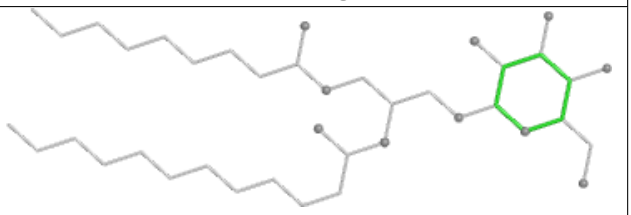
Bond lengths



Bond angles

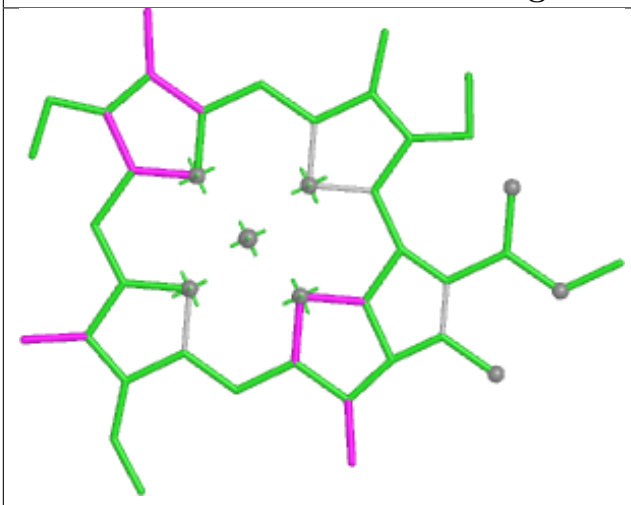


Torsions

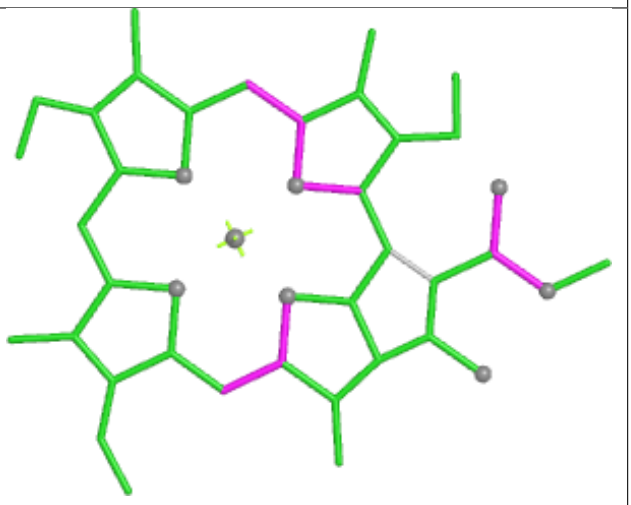


Rings

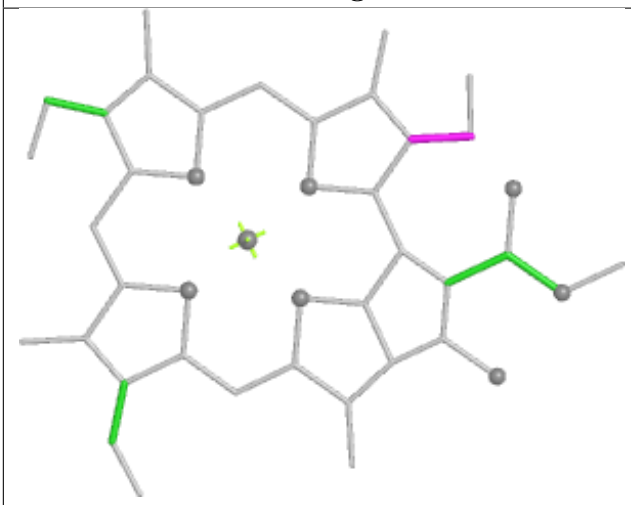
Ligand CLA 7 607



Bond lengths



Bond angles

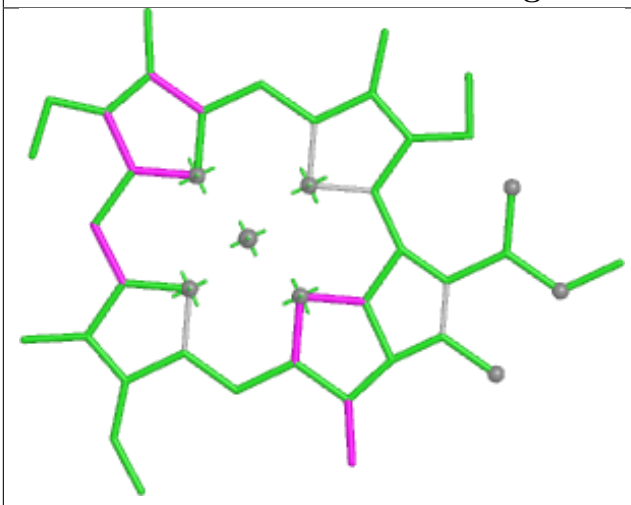


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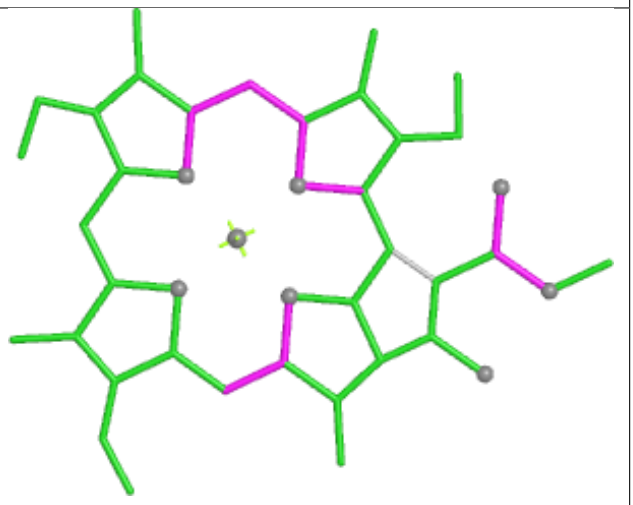


Rings

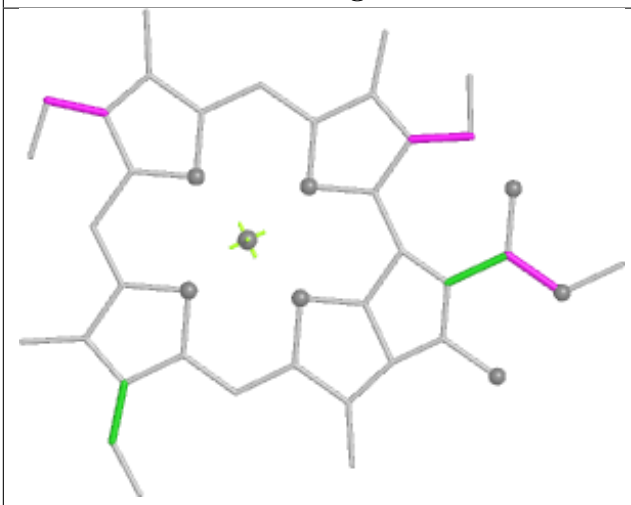
Ligand CLA U 614



Bond lengths



Bond angles

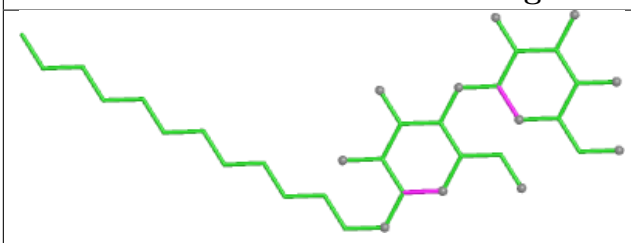


Torsions

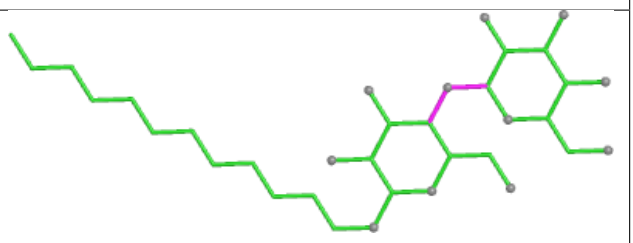


Rings

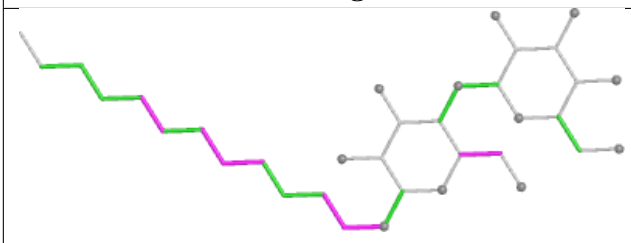
Ligand LMU 1 621



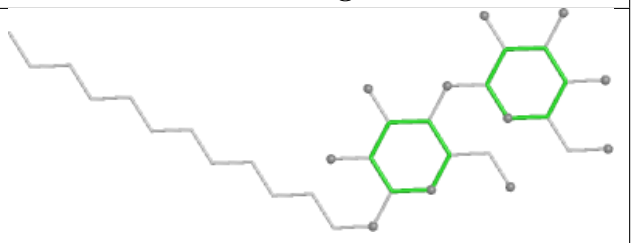
Bond lengths



Bond angles

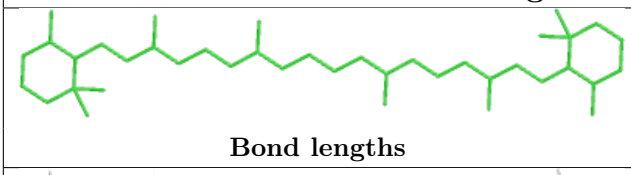


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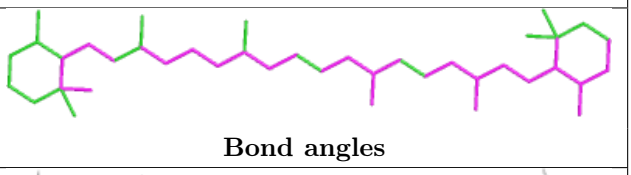


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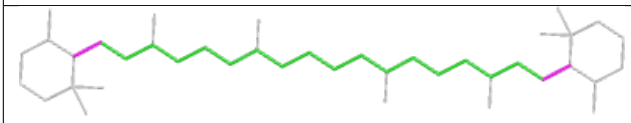
Ligand BCR 7 623



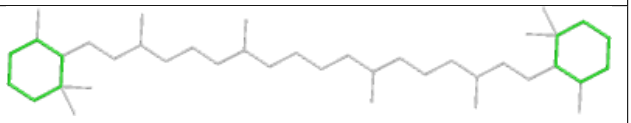
Bond lengths



Bond angles



Torsions



Rings

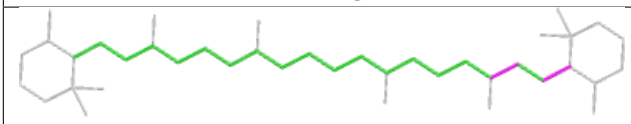
Ligand BCR 3 620



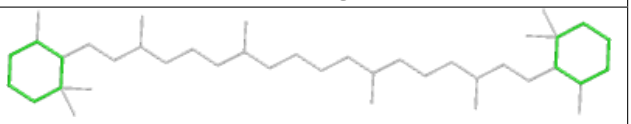
Bond lengths



Bond angles

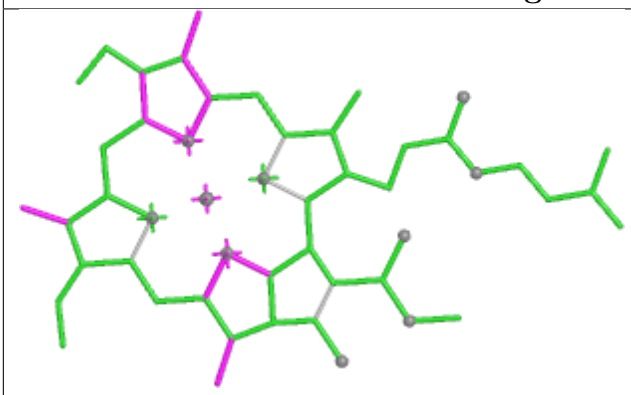


Torsions

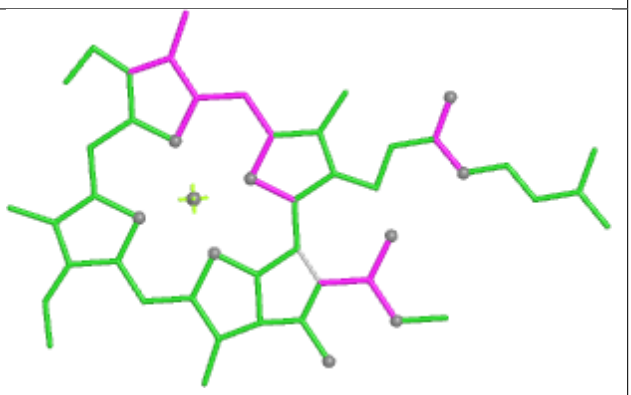


Rings

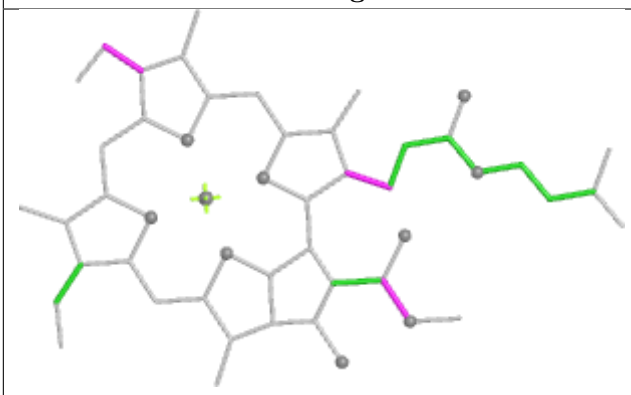
Ligand CLA B 836



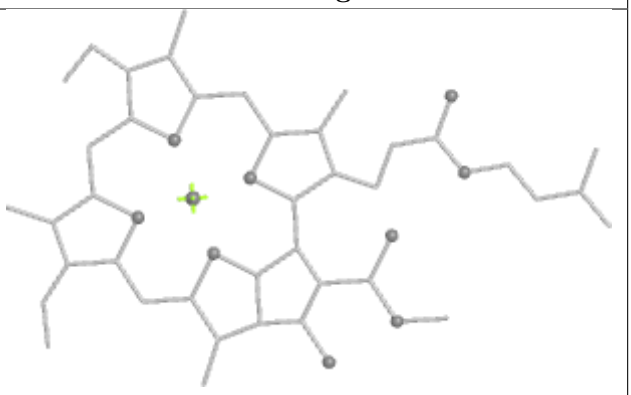
Bond lengths



Bond angles

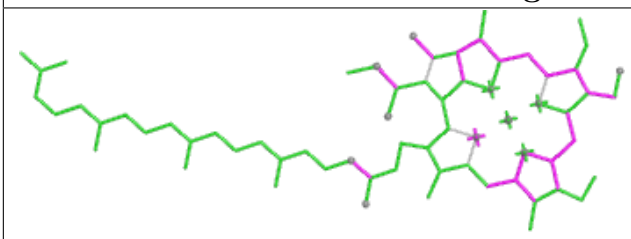


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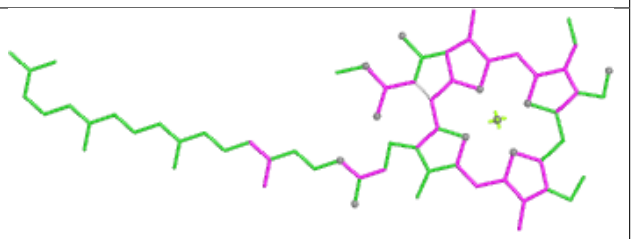


Rings

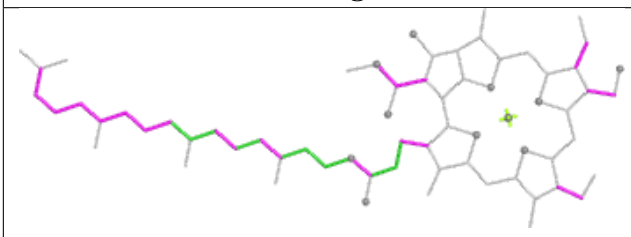
Ligand CHL X 609



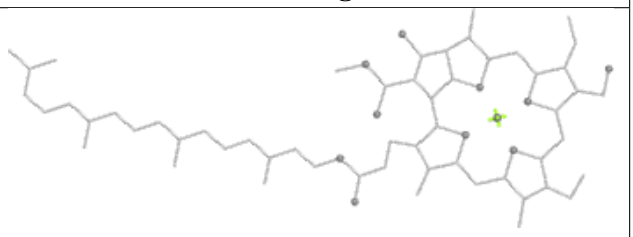
Bond lengths



Bond angles

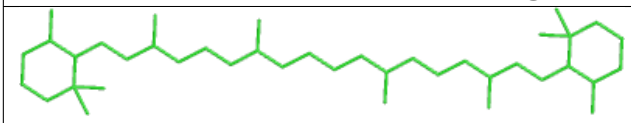


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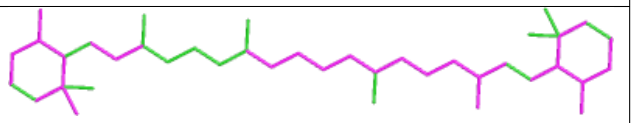


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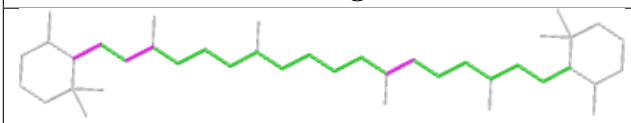
Ligand BCR L 308



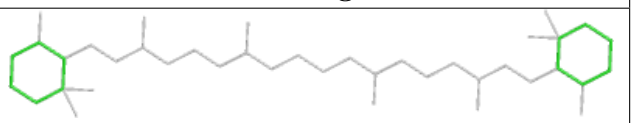
Bond lengths



Bond angles

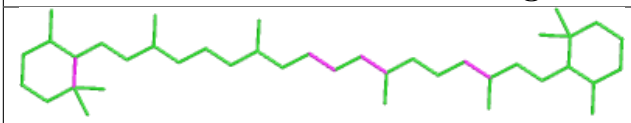


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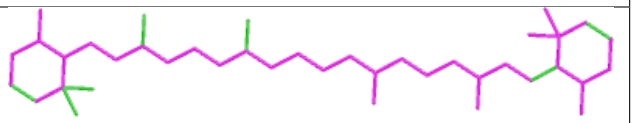


Rings

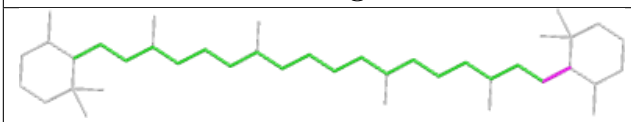
Ligand BCR B 844



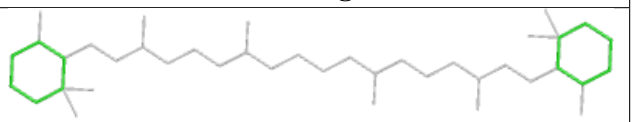
Bond lengths



Bond angles

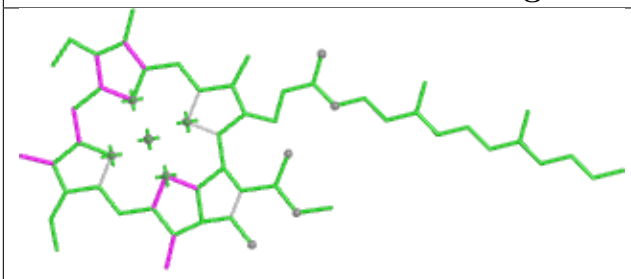


Torsions

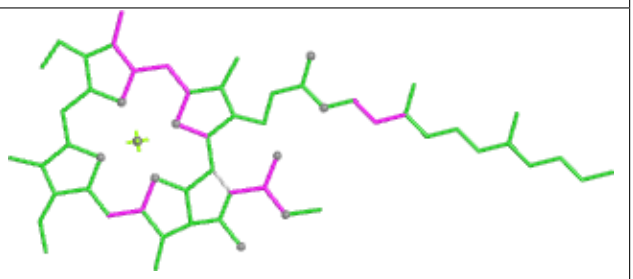


Rings

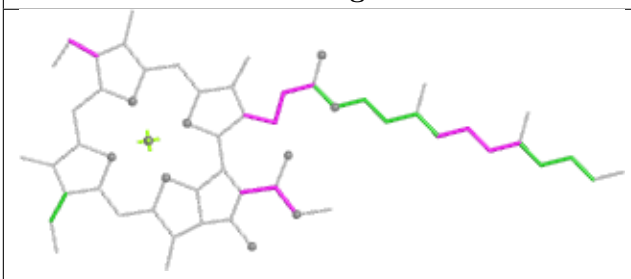
Ligand CLA Y 602



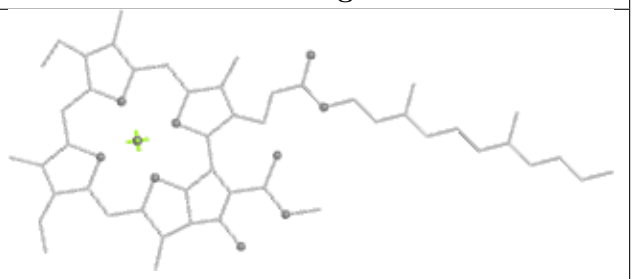
Bond lengths



Bond angles

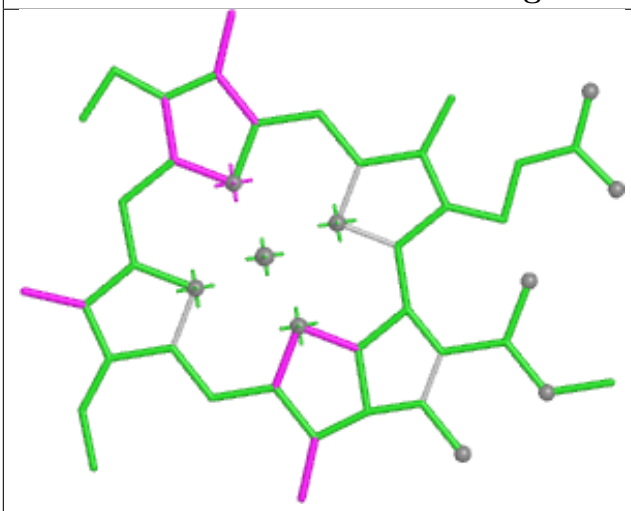


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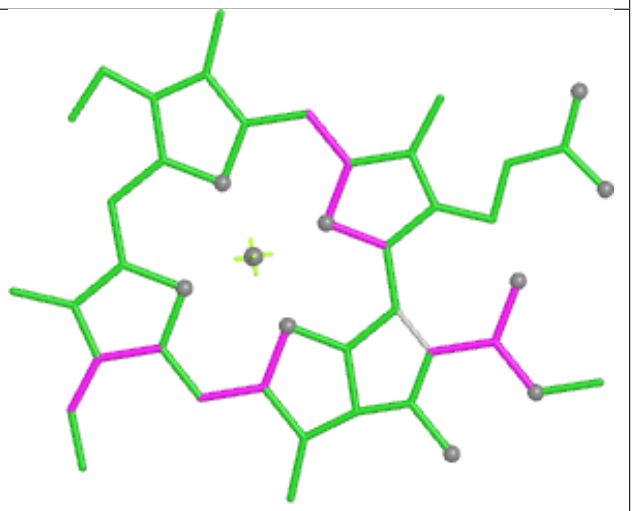


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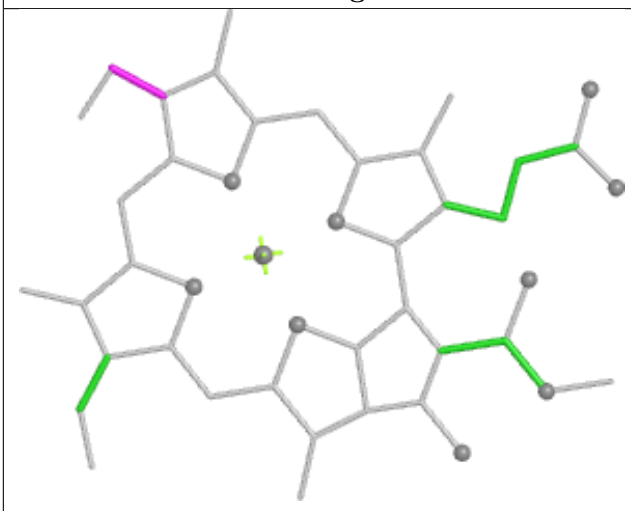
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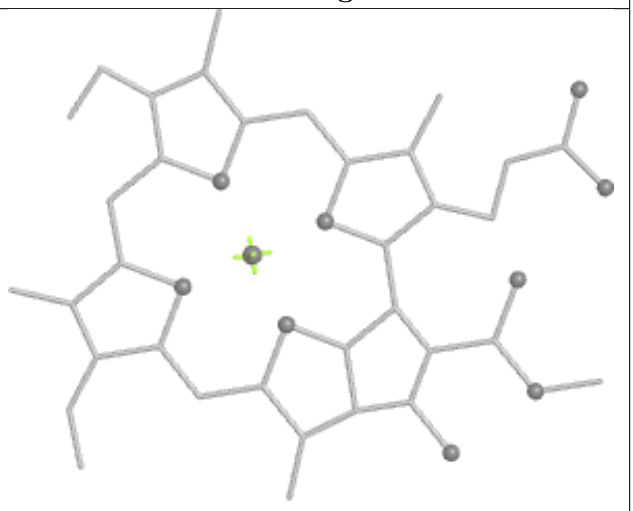
Bond lengths



Bond angles

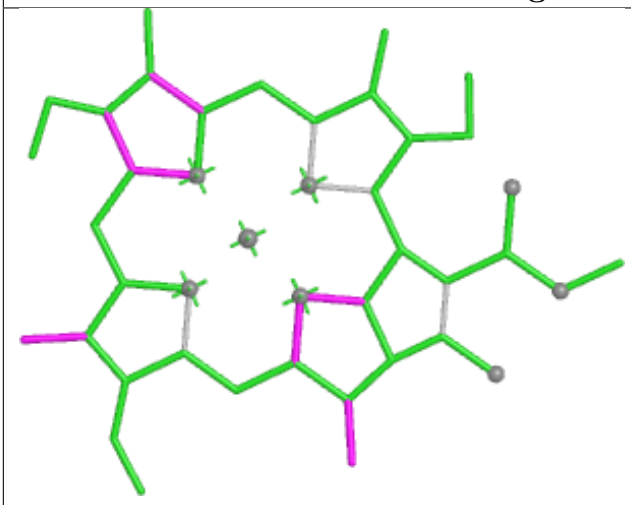


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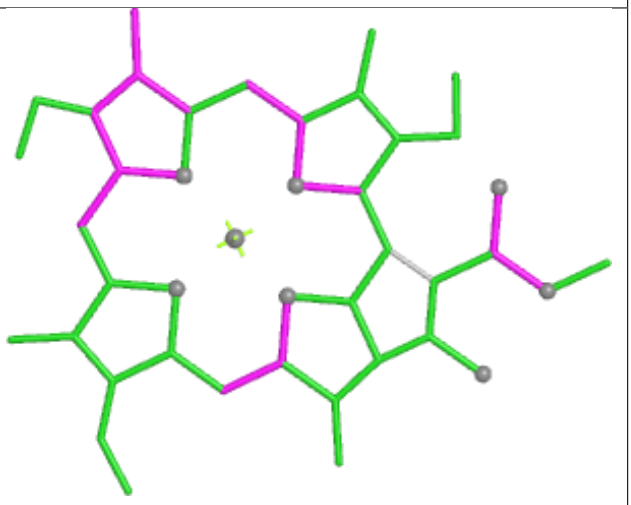


Rings

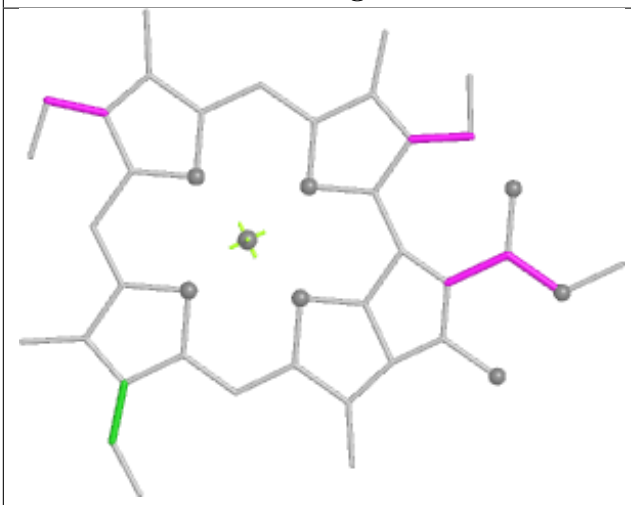
Ligand CLA 4 611



Bond lengths



Bond angles

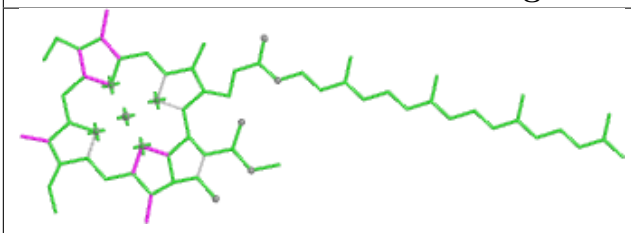


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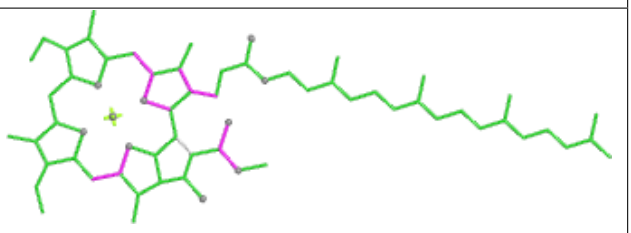


Rings

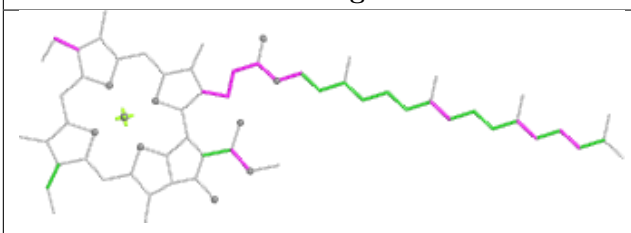
Ligand CLA H 203



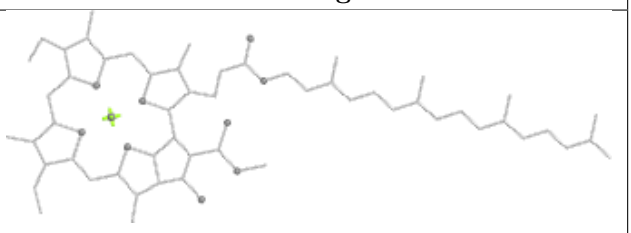
Bond lengths



Bond angles

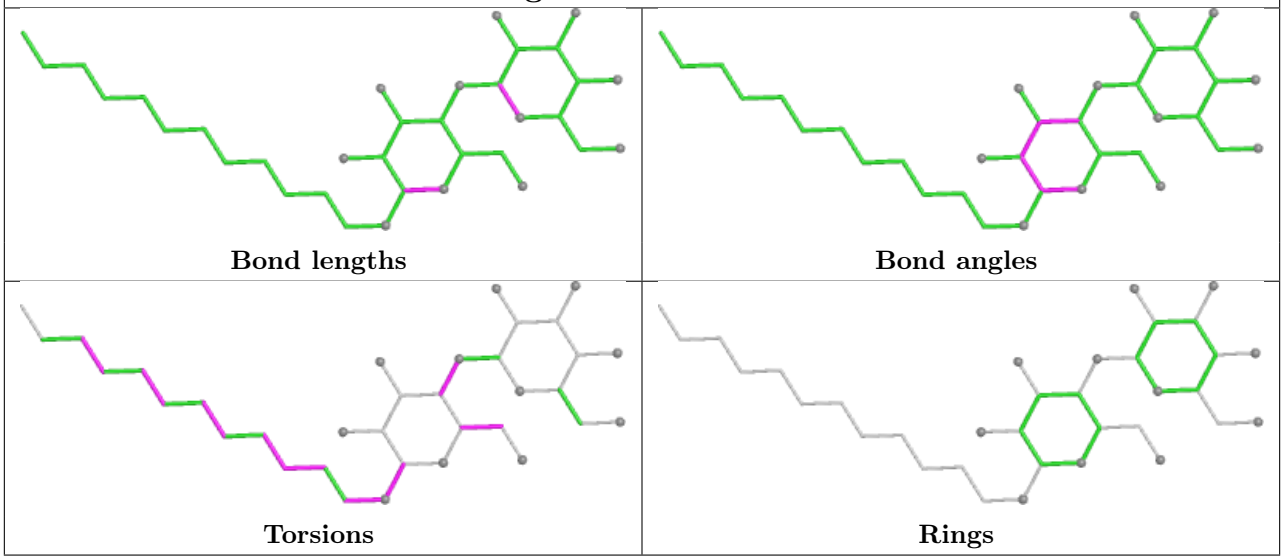


Torsions

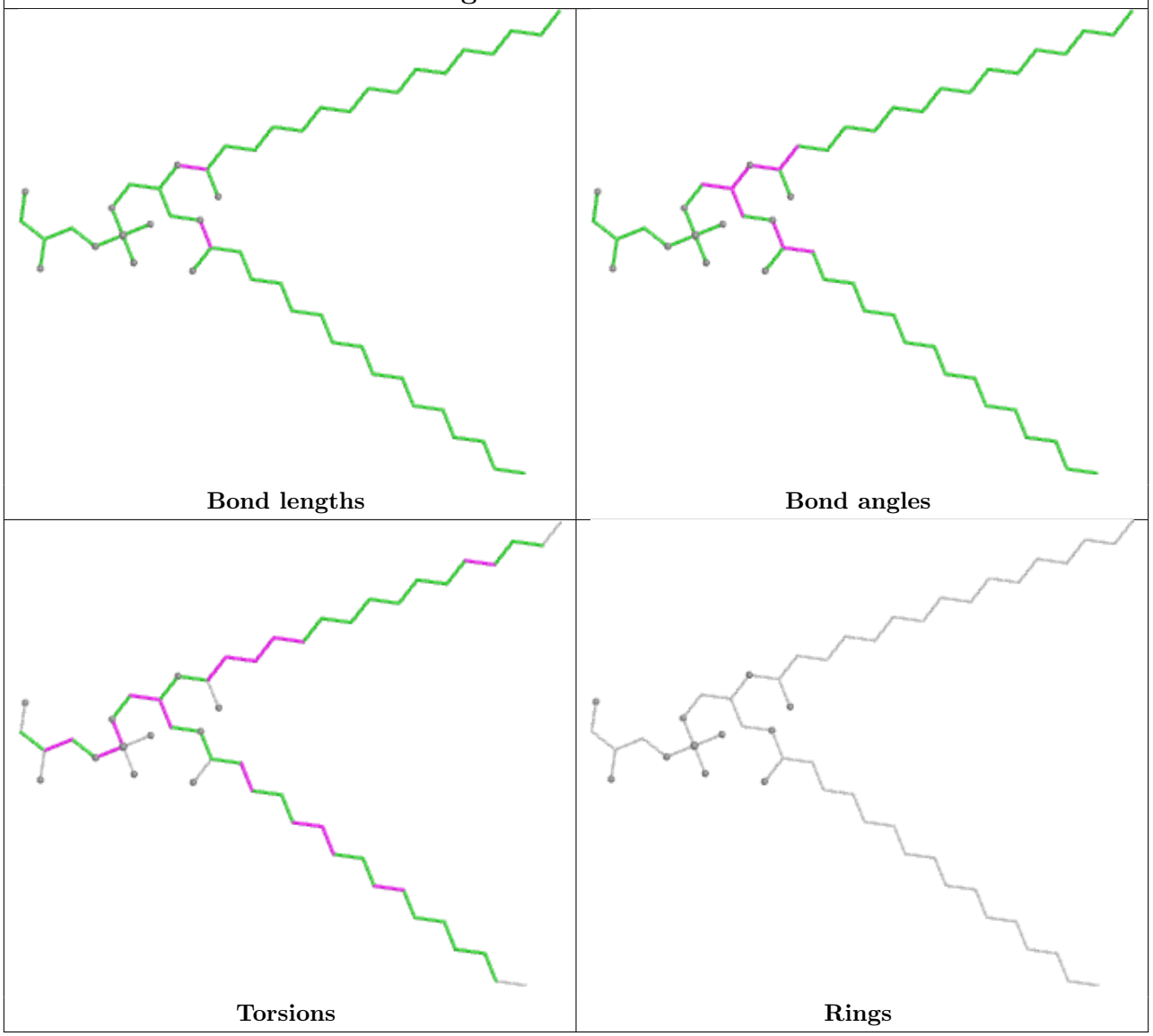


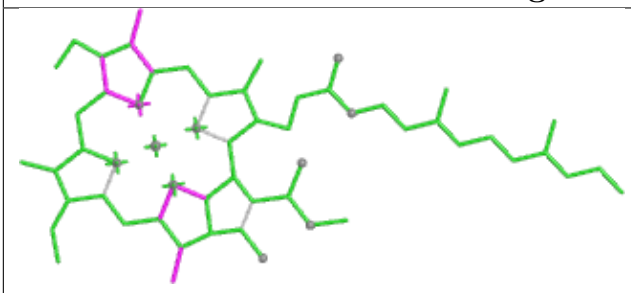
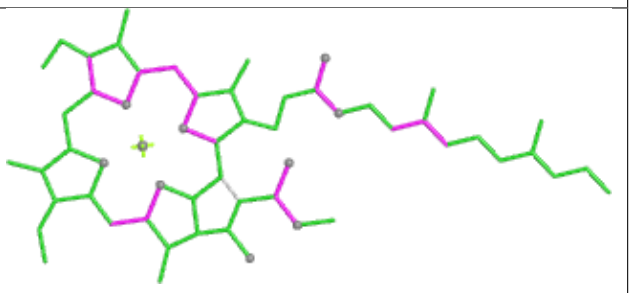
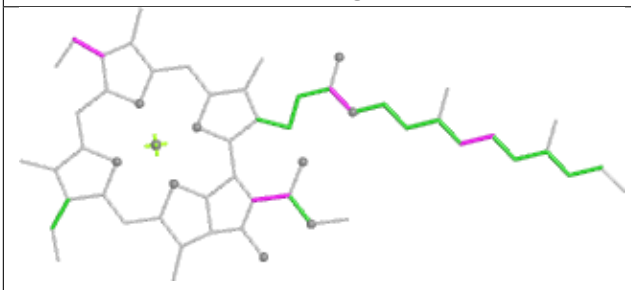
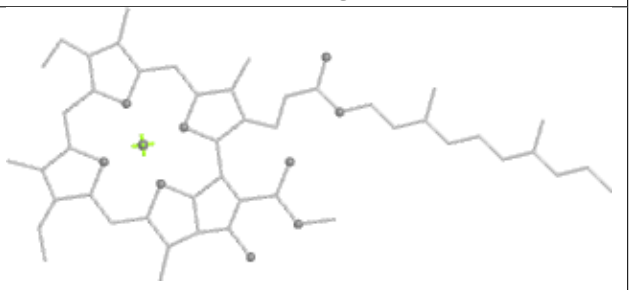
Rings

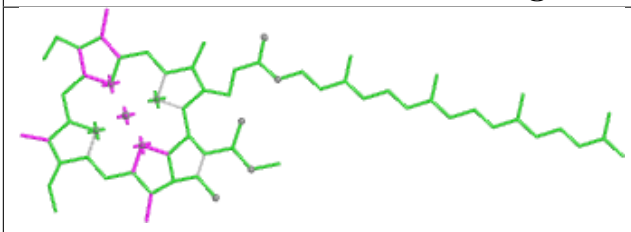
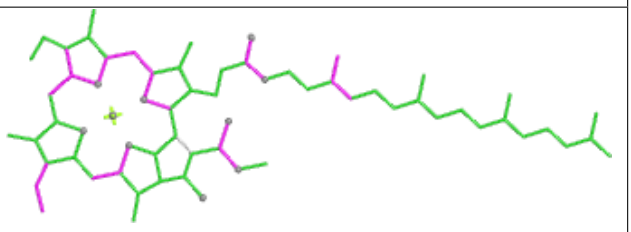
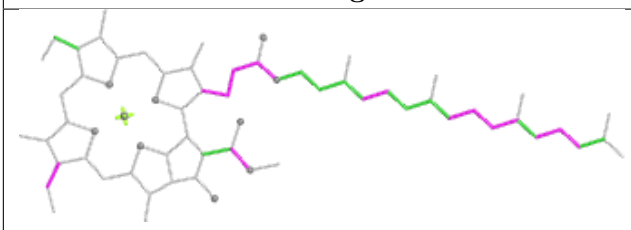
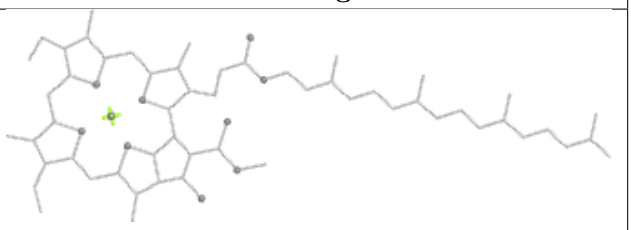
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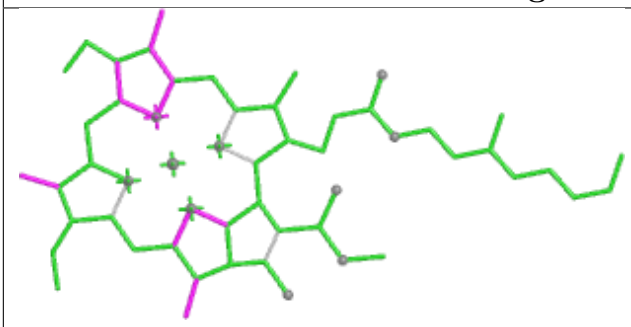
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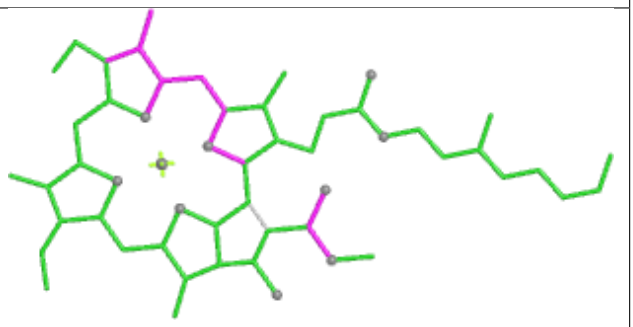
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Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA 6 616	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

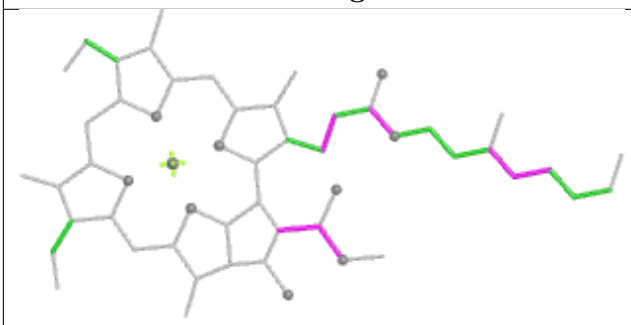
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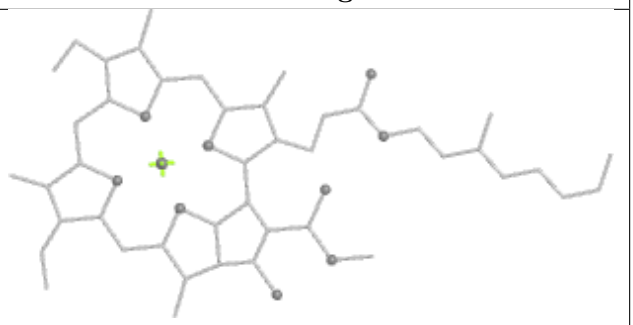
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Bond angles

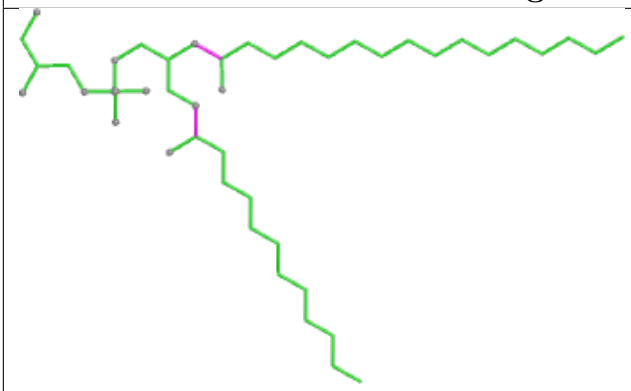


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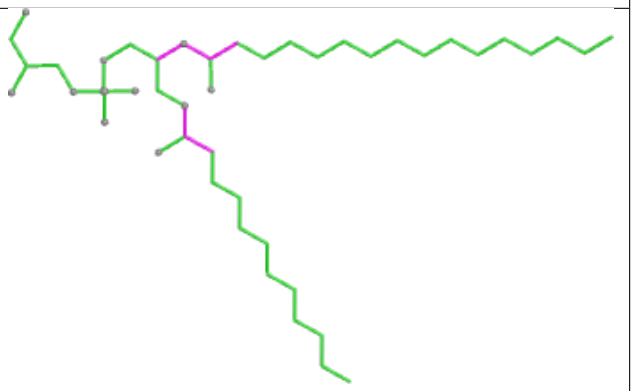


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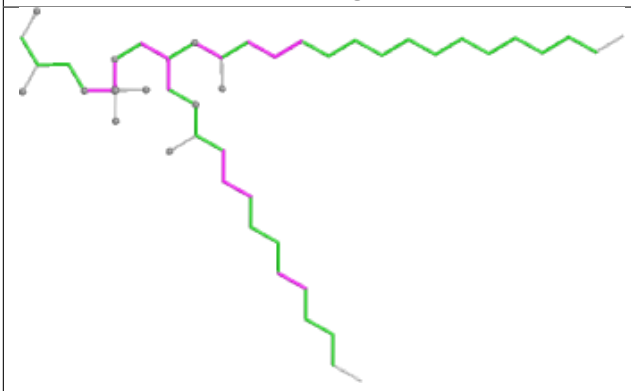
Ligand LHG 3 623



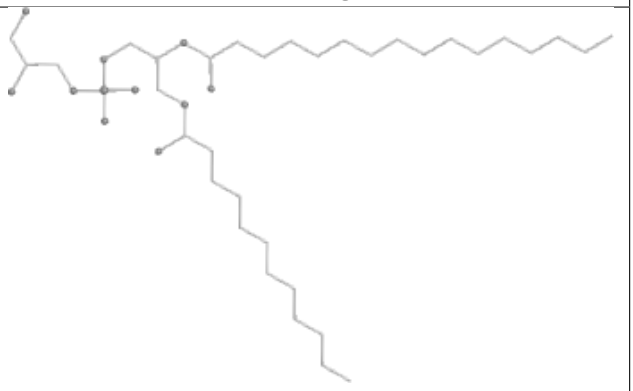
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Bond angles

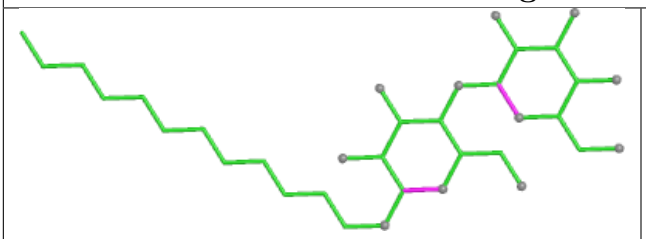


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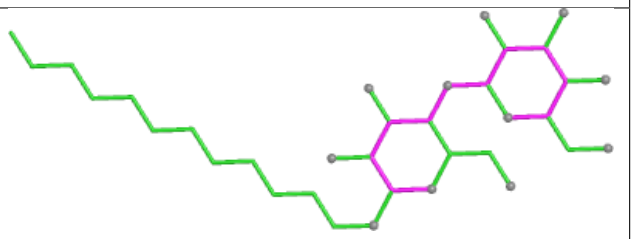


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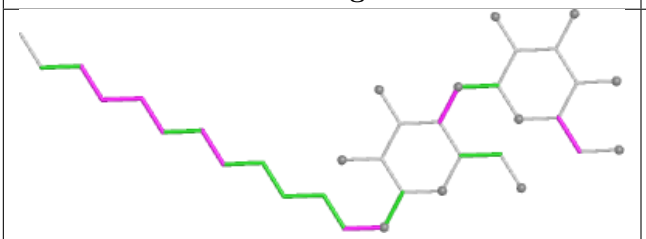
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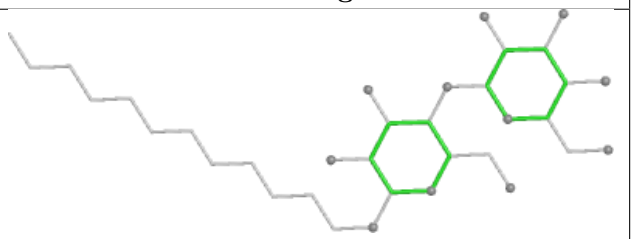
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Bond angles

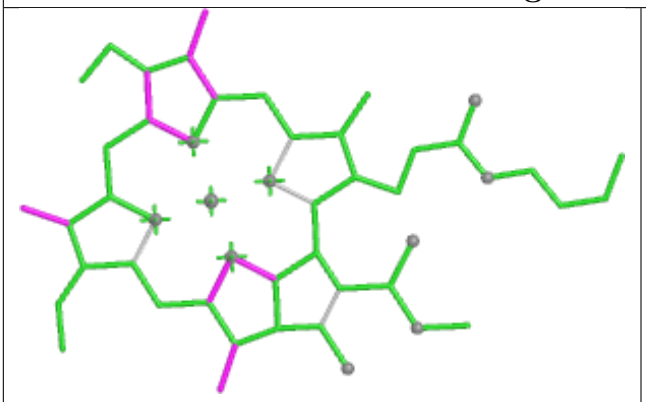


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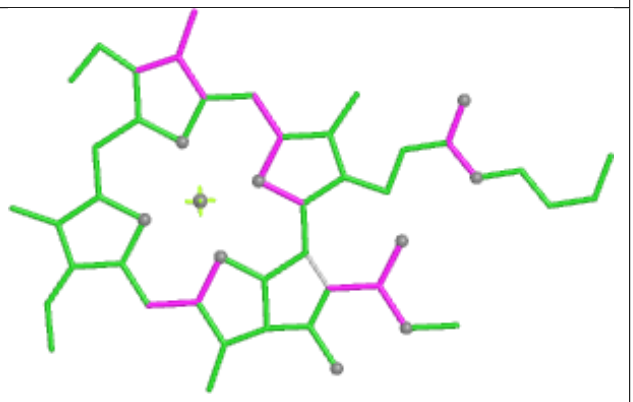


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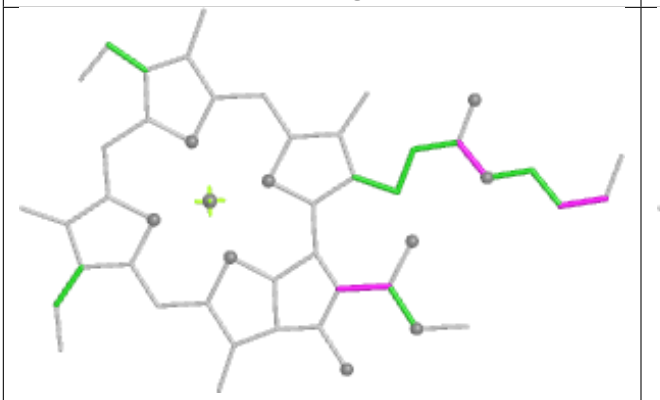
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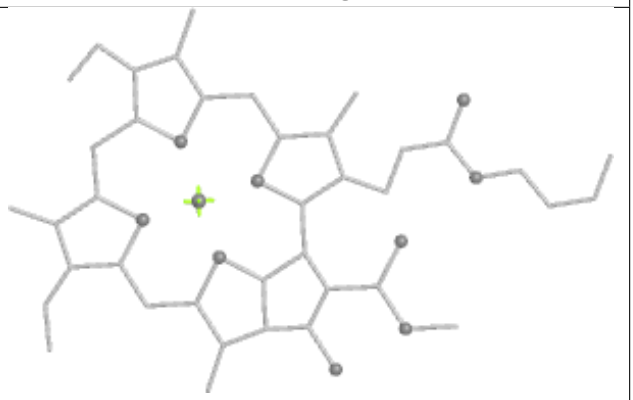
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Bond angles

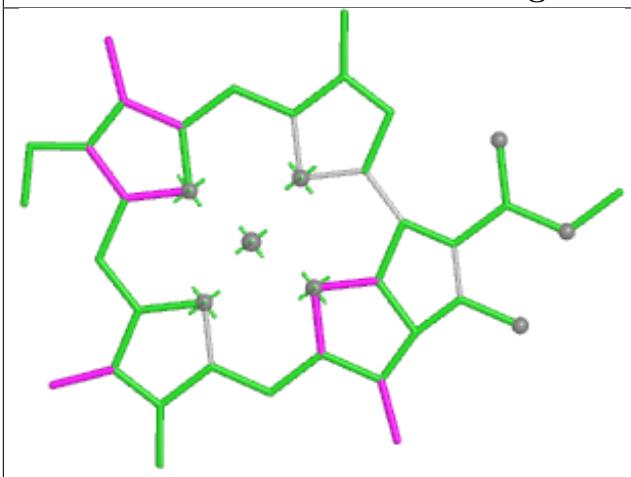


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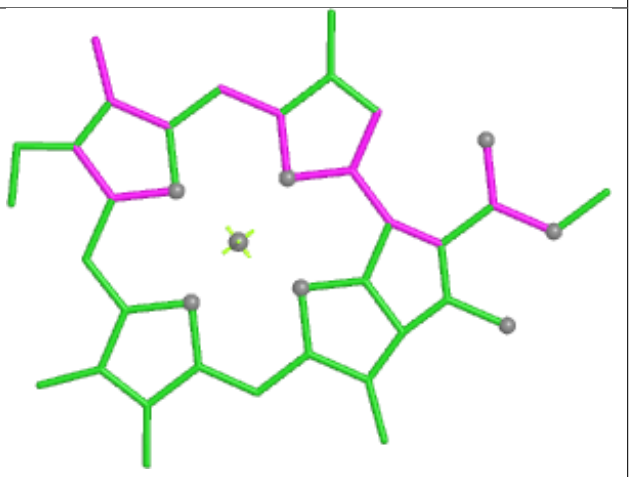


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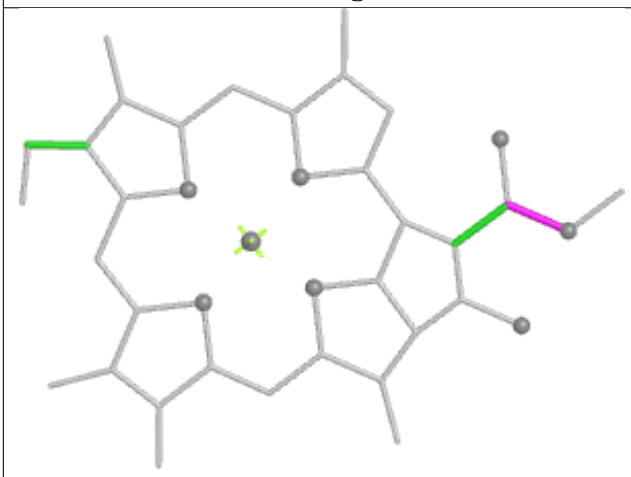
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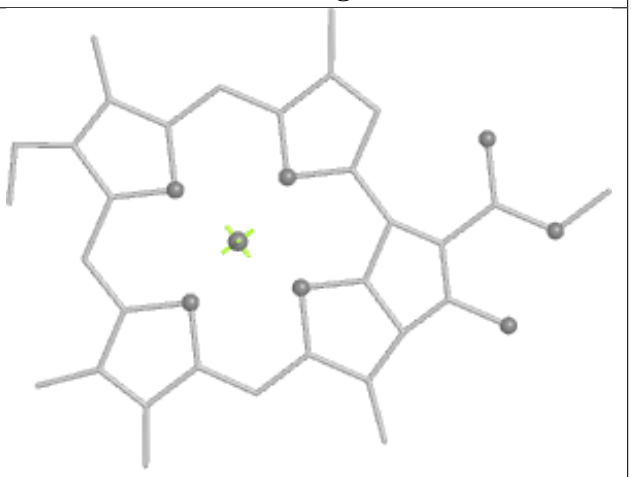
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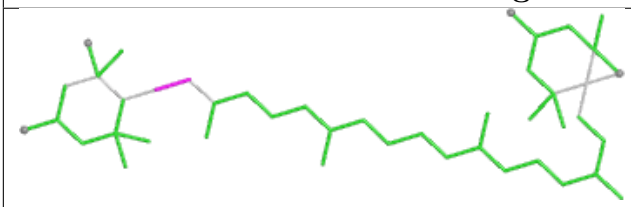


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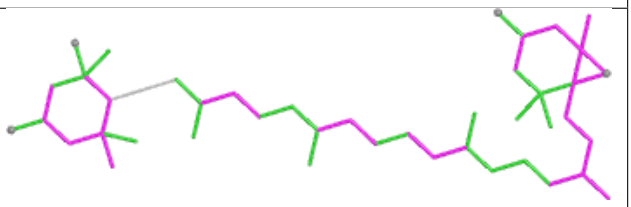


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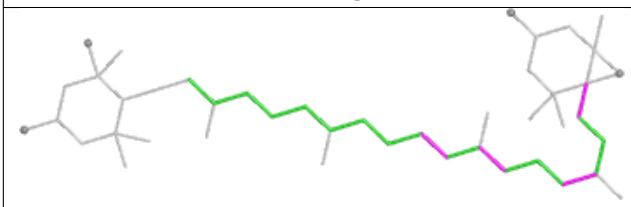
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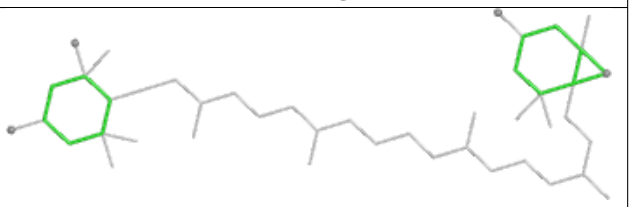
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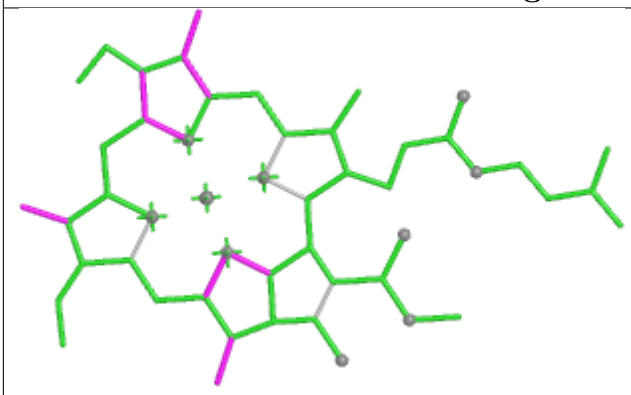


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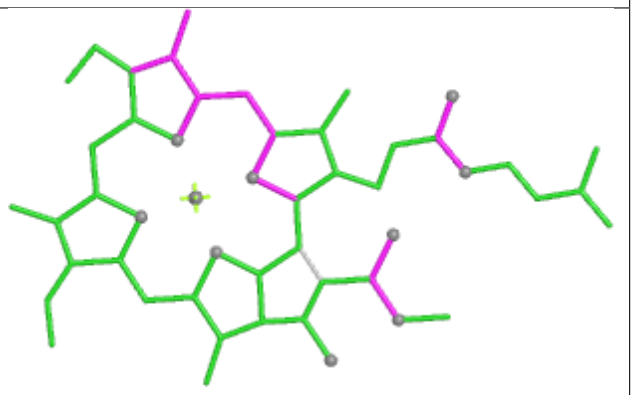


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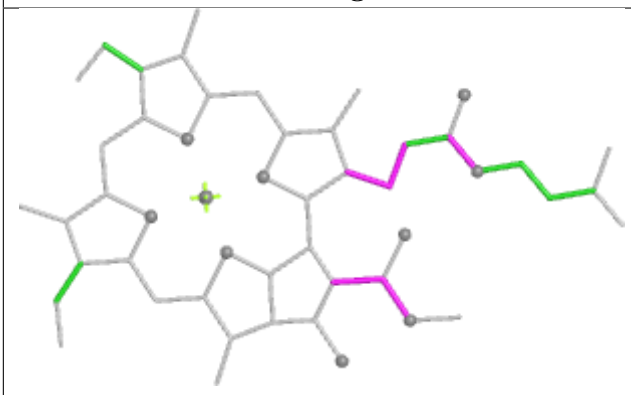
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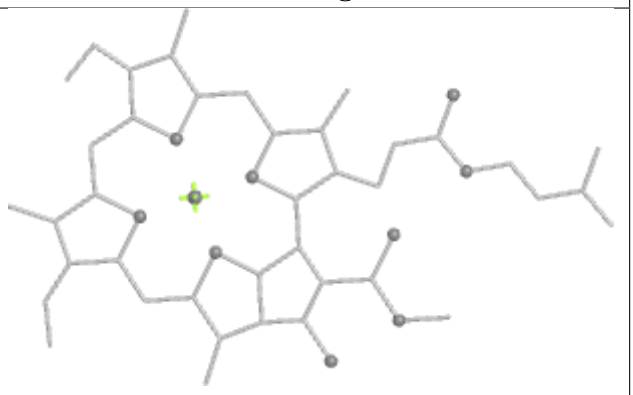
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Bond angles

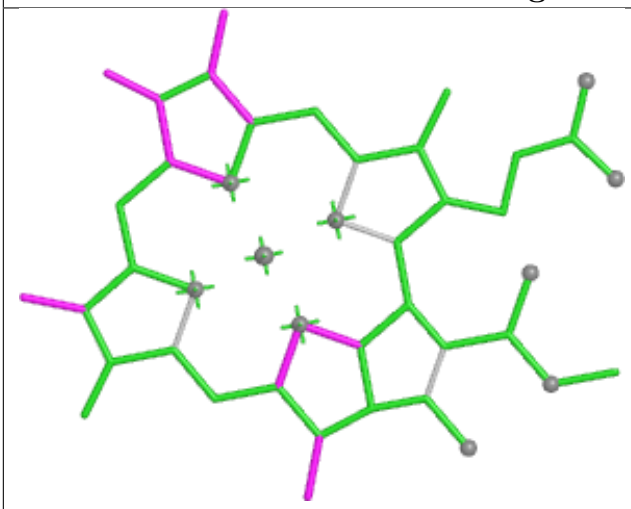


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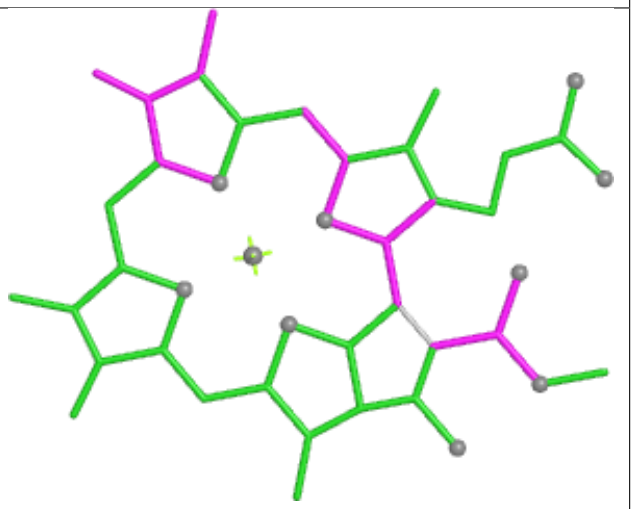


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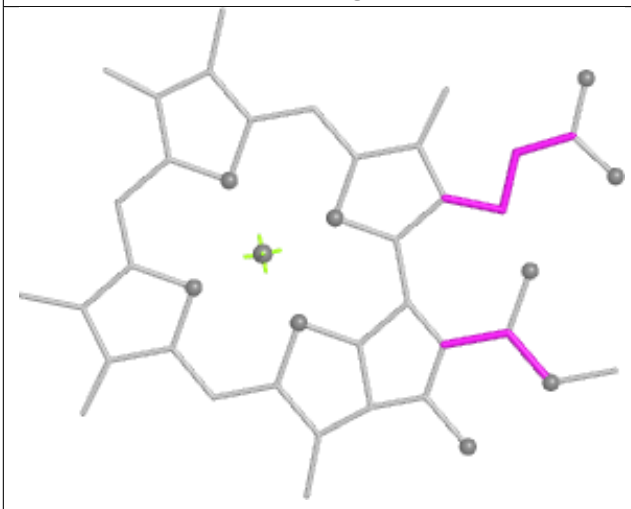
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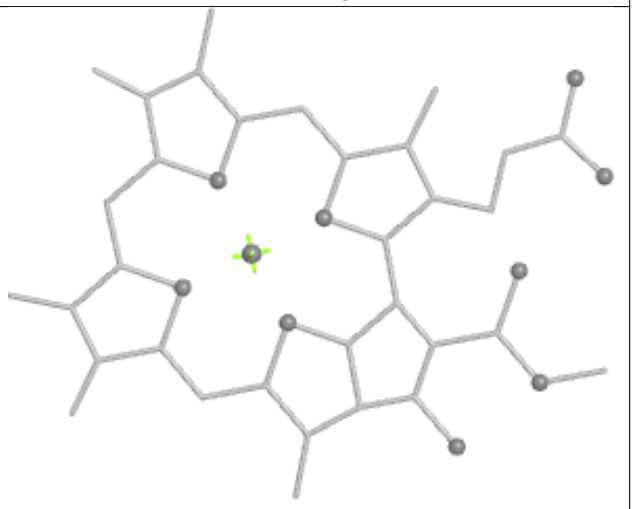
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Bond angles

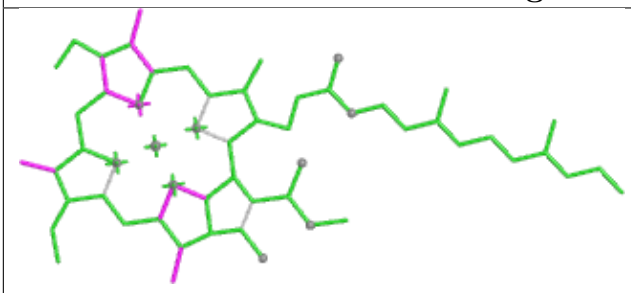


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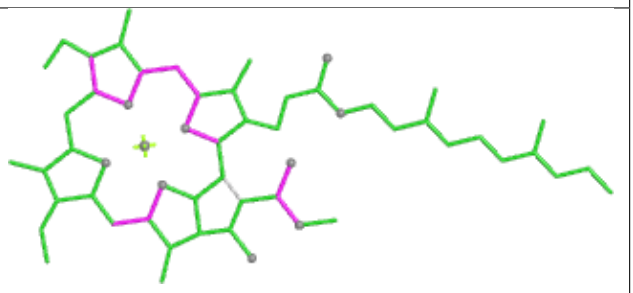


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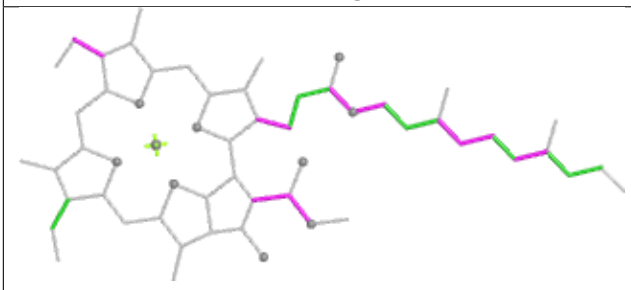
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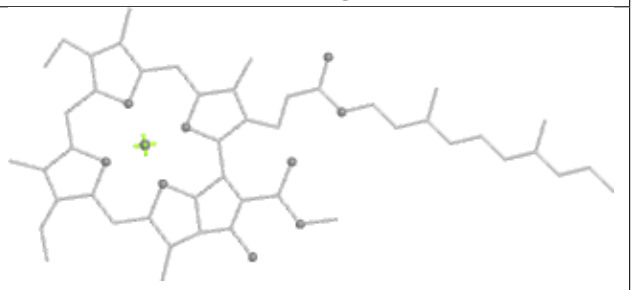
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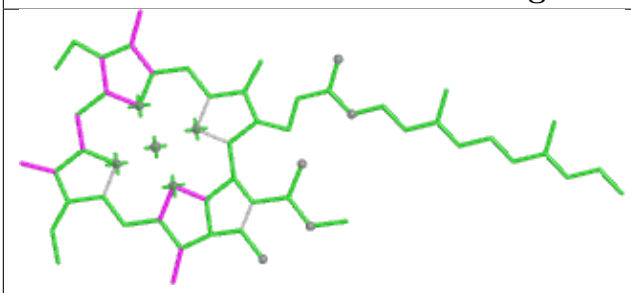


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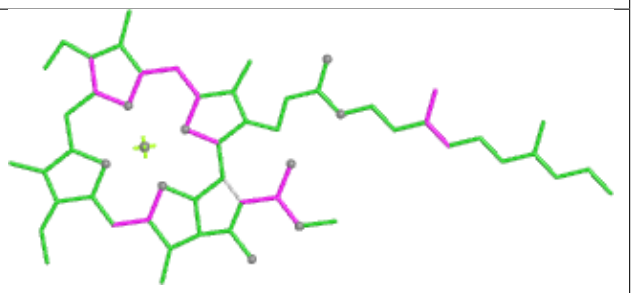


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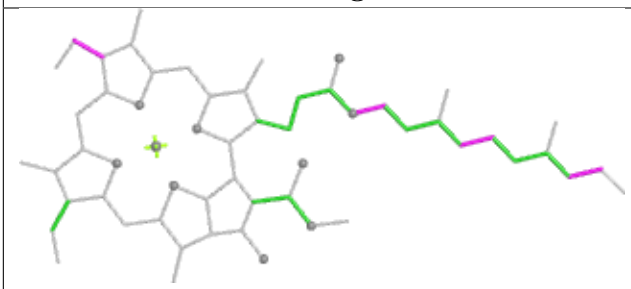
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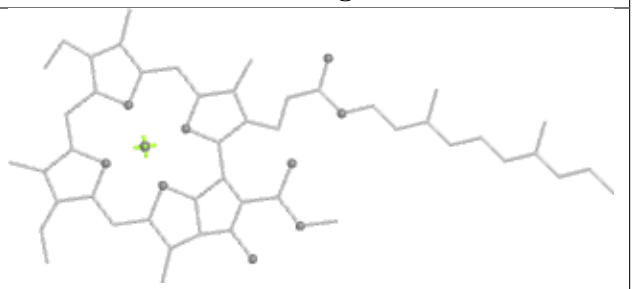
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Bond angles

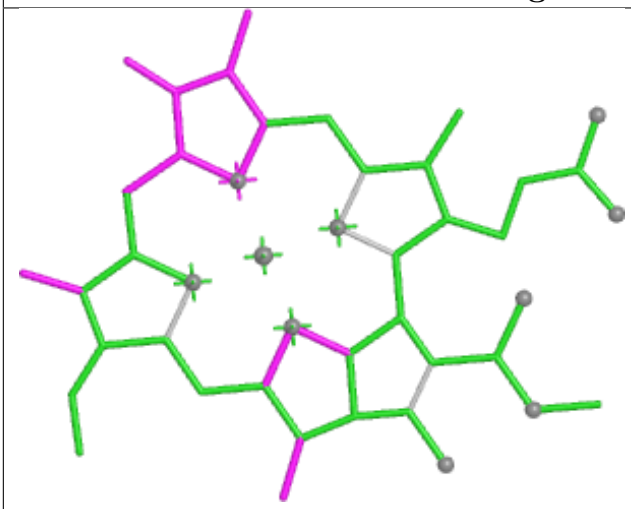


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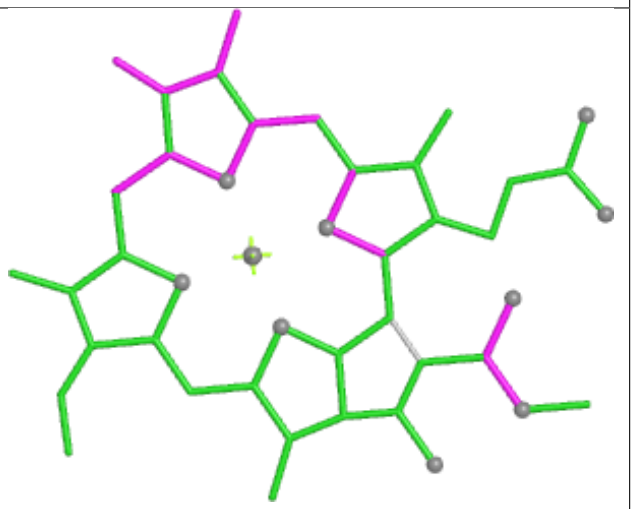


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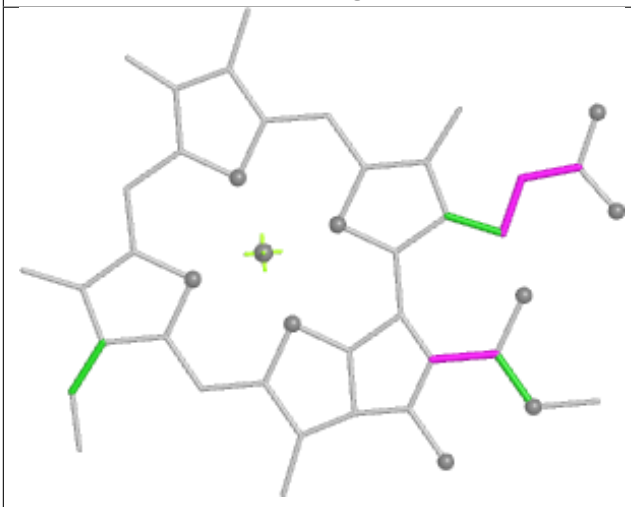
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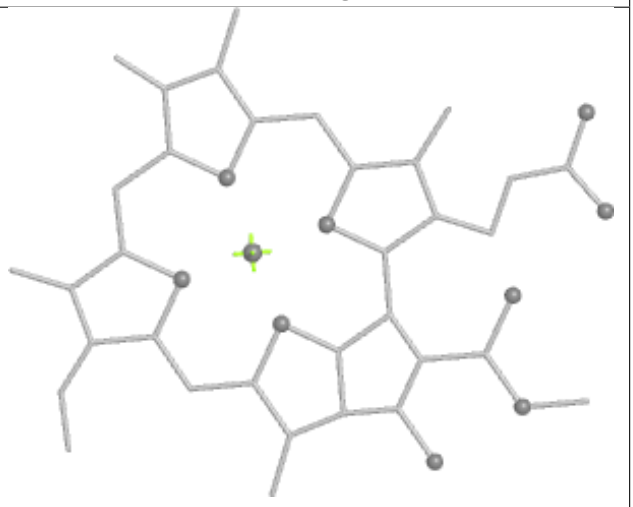
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Bond angles

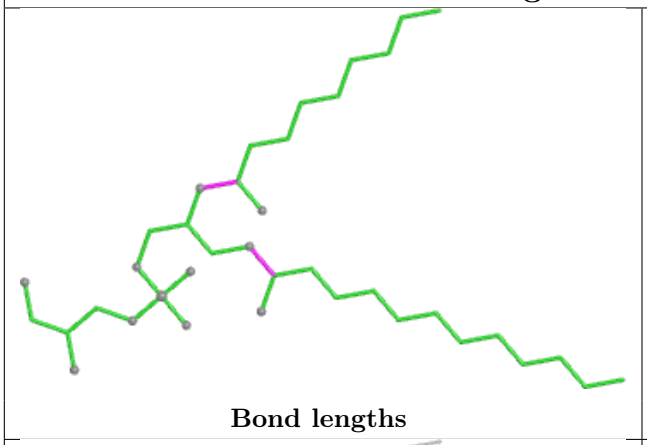


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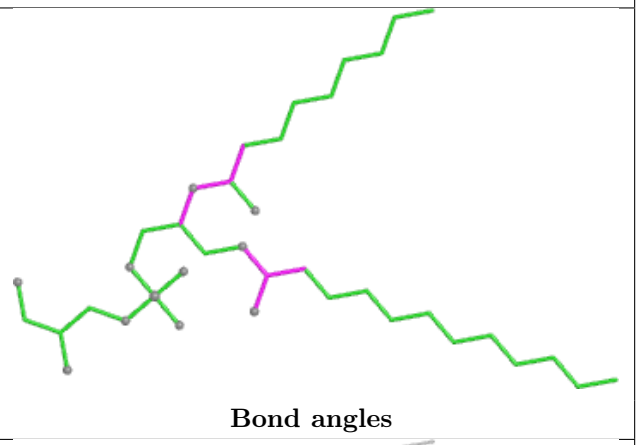


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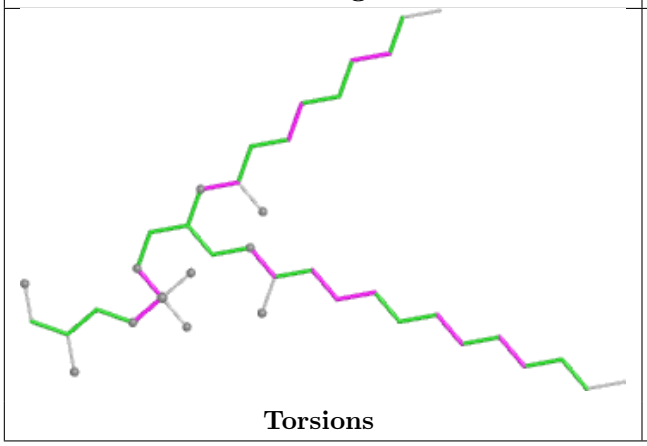
Ligand LHG B 851



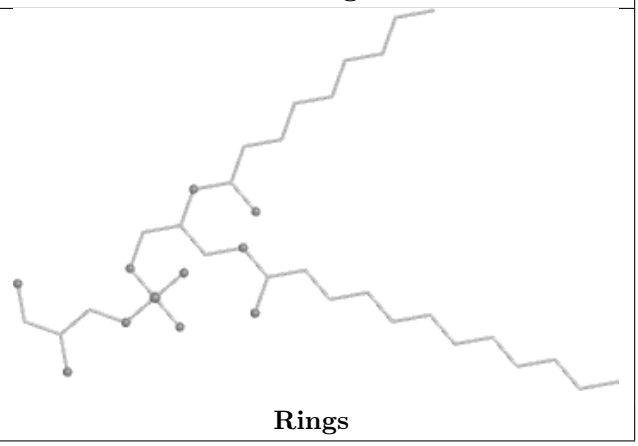
Bond lengths



Bond angles

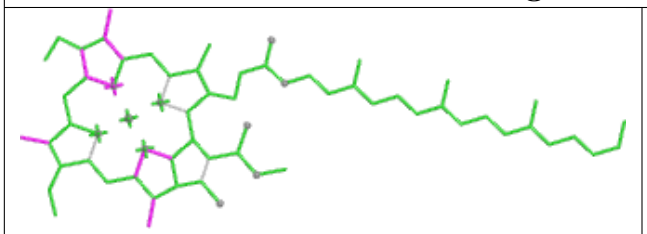


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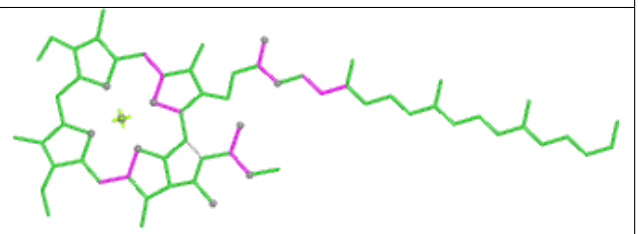


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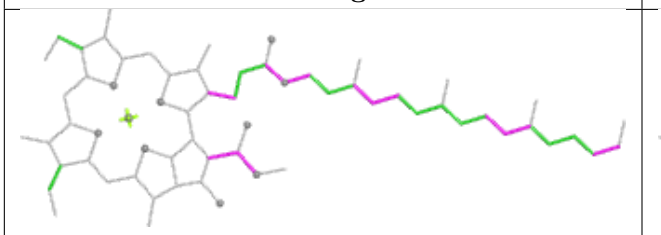
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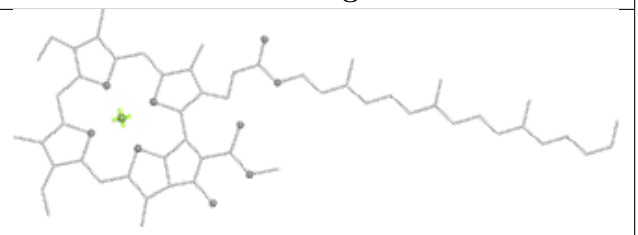
Bond lengths



Bond angles

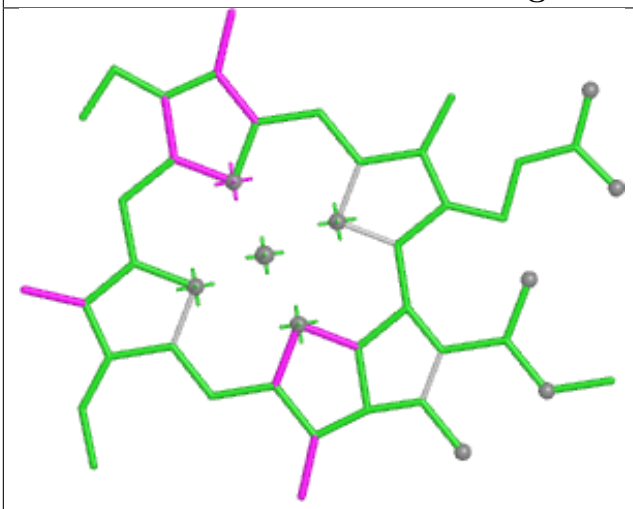


Torsions

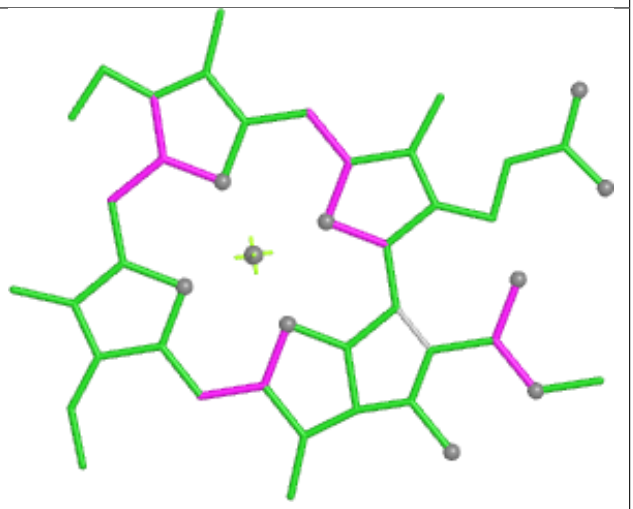


Rings

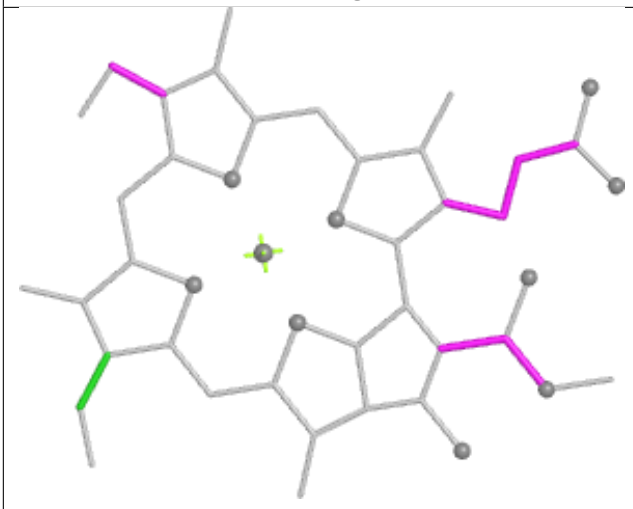
Ligand CLA 9 607



Bond lengths



Bond angles

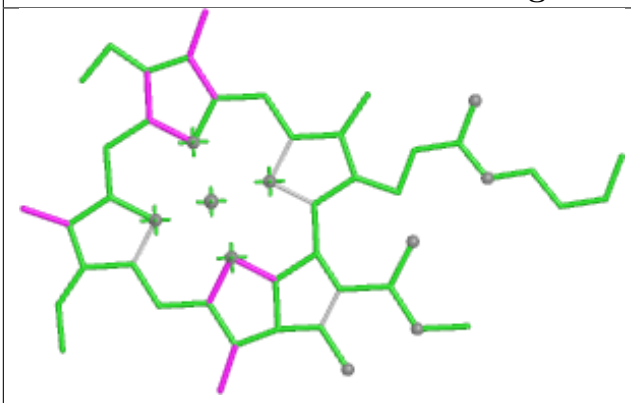


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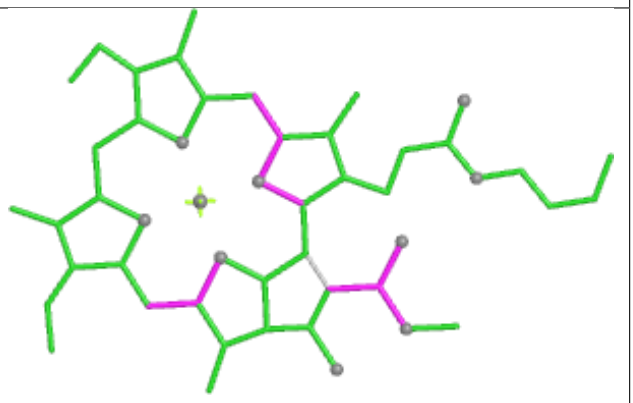


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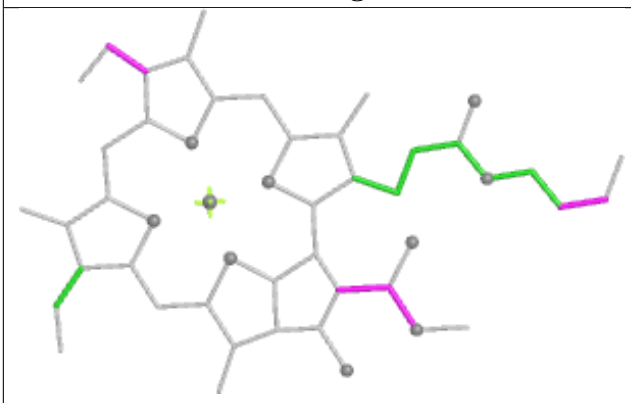
Ligand CLA 1 604



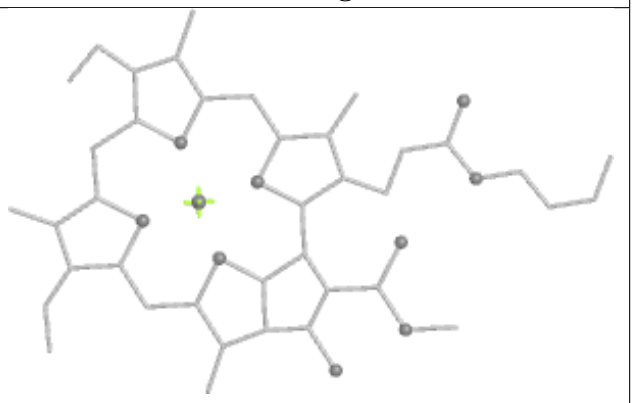
Bond lengths



Bond angles

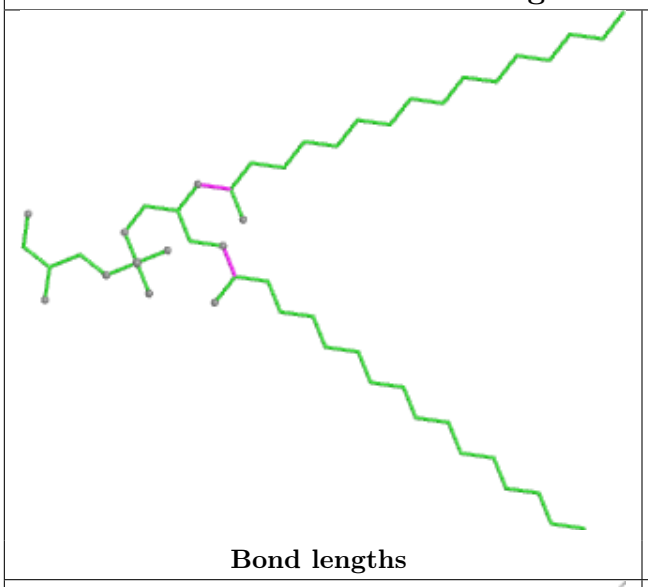


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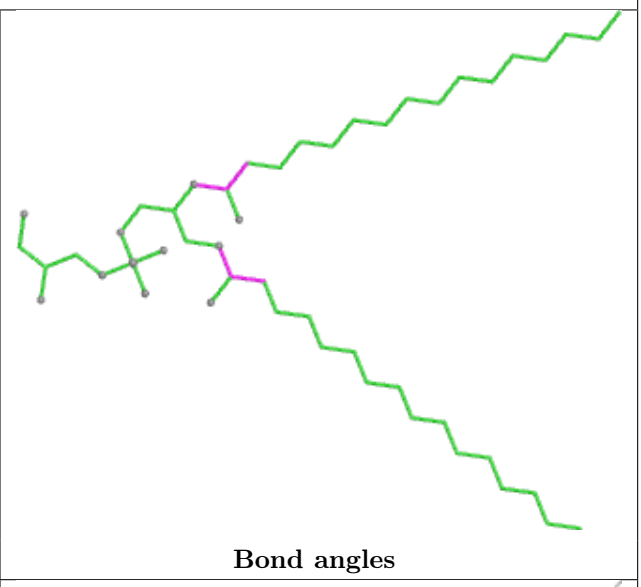


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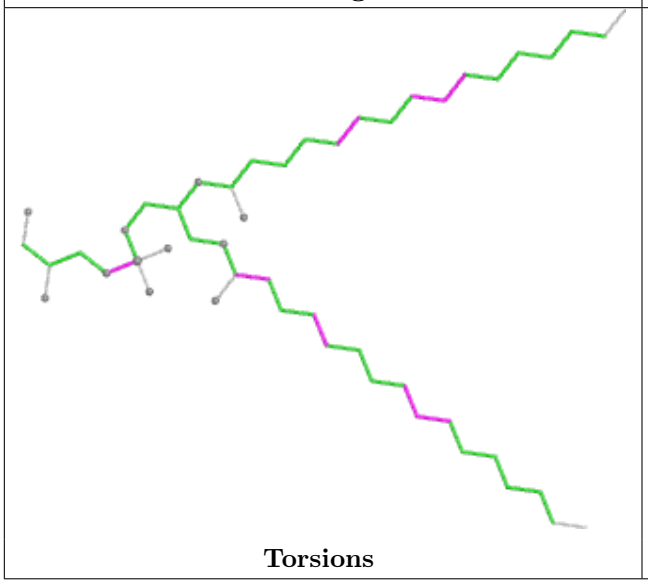
Ligand LHG 4 622



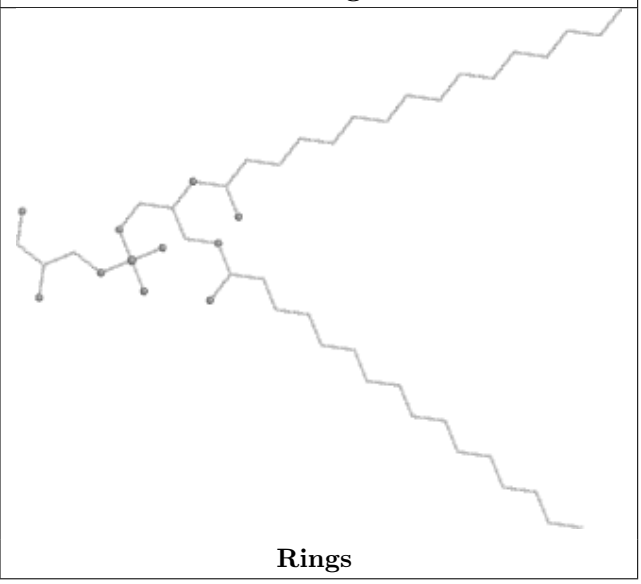
Bond lengths



Bond angles

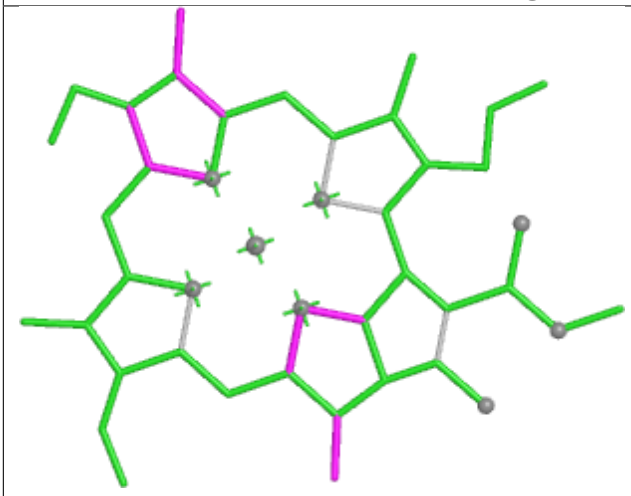


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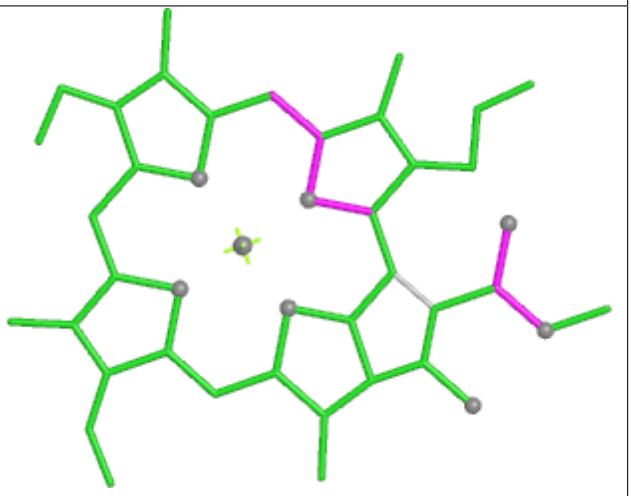


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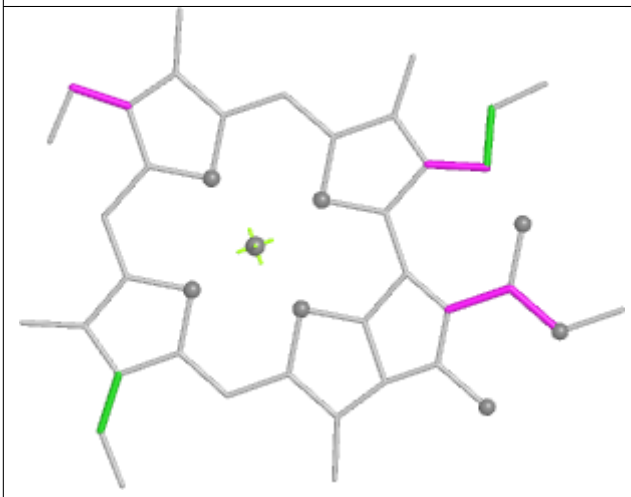
Ligand CLA V 611



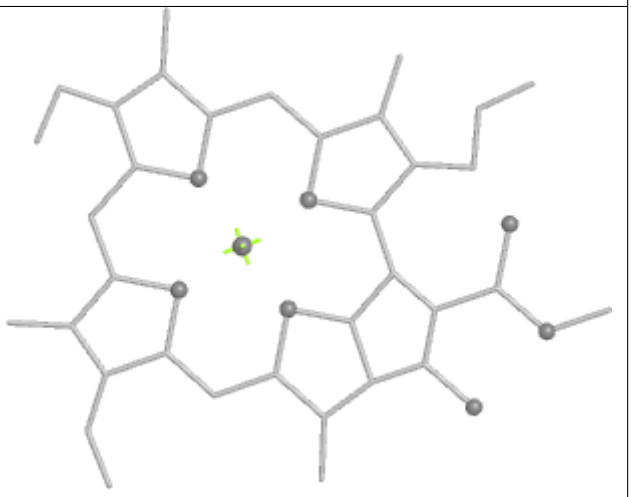
Bond lengths



Bond angles

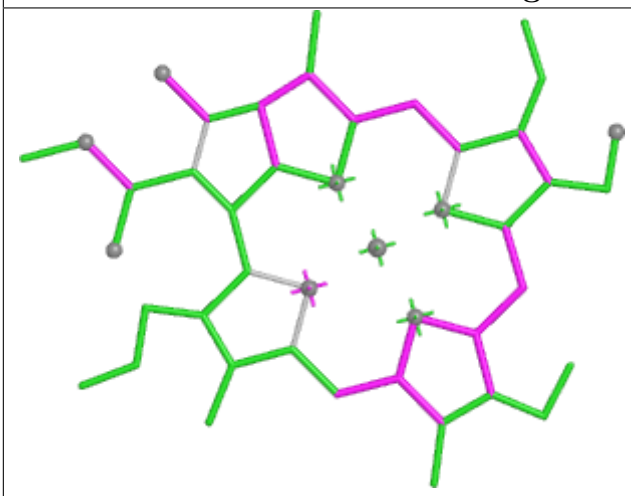


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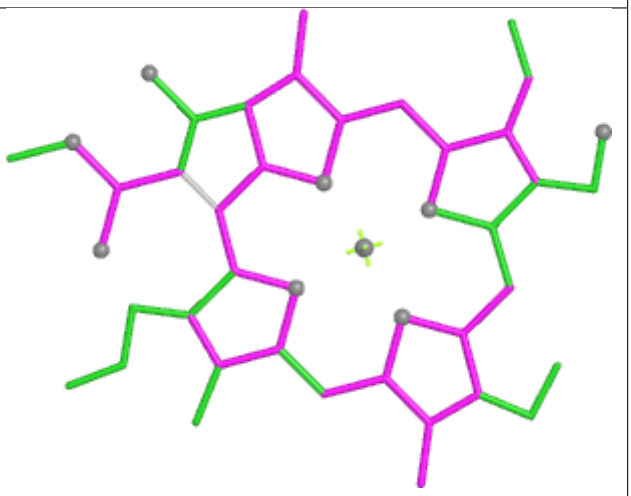


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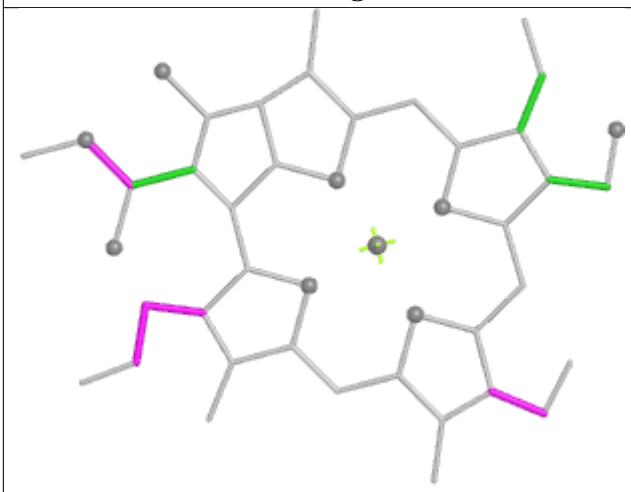
Ligand CHL U 608



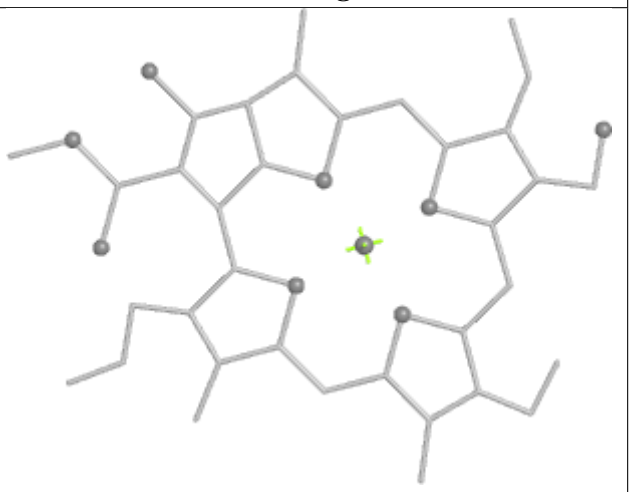
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Bond angles

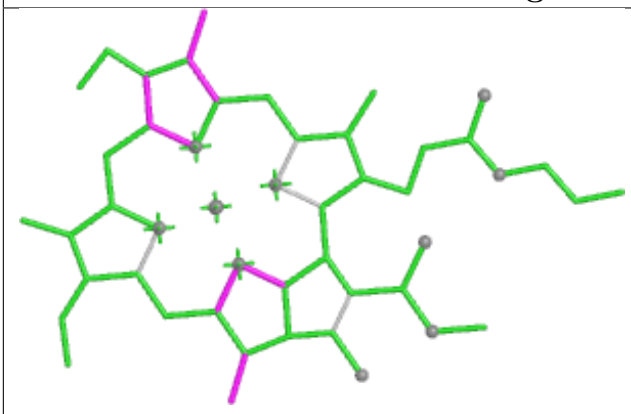


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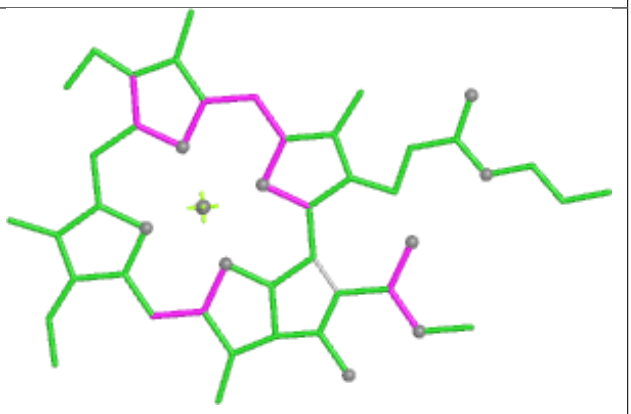


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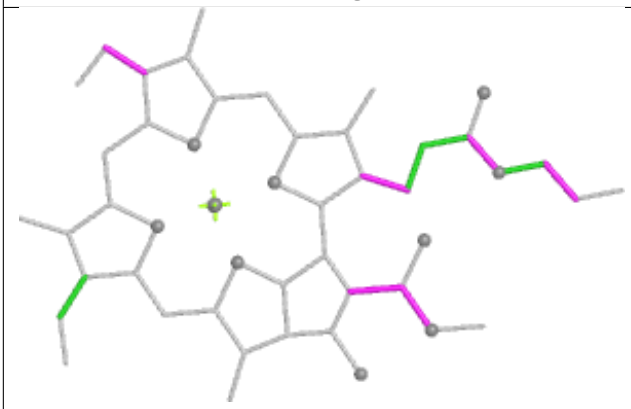
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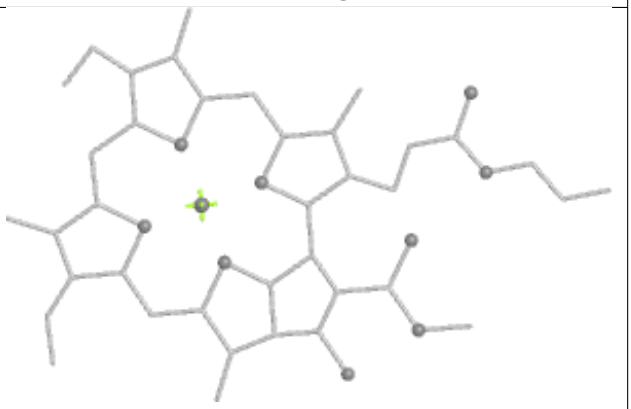
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Bond angles

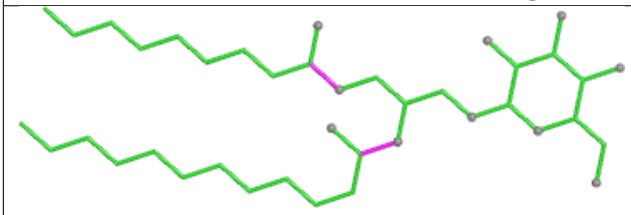


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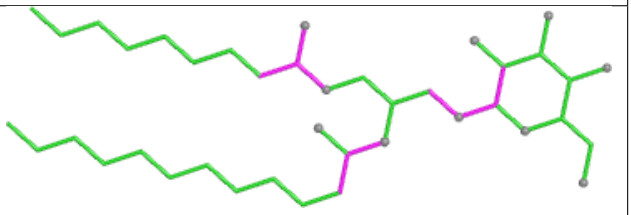


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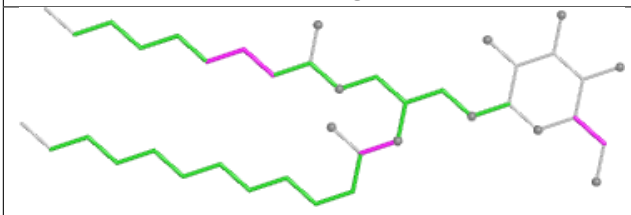
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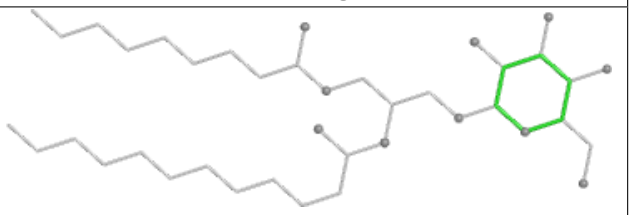
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Bond angles

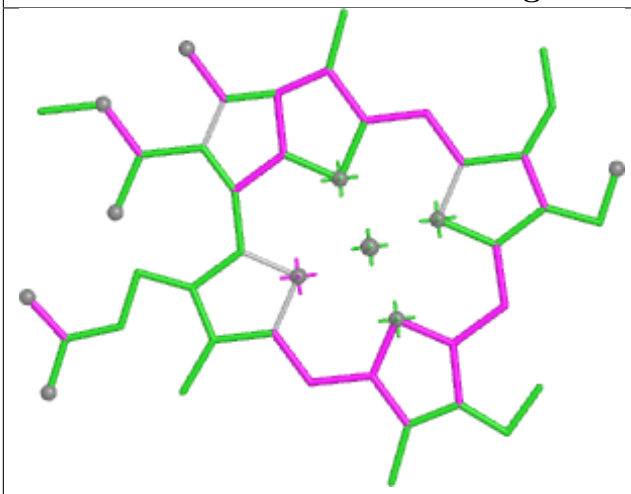


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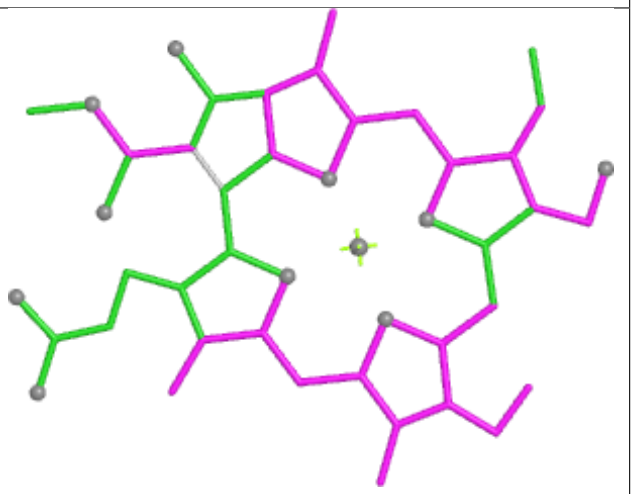


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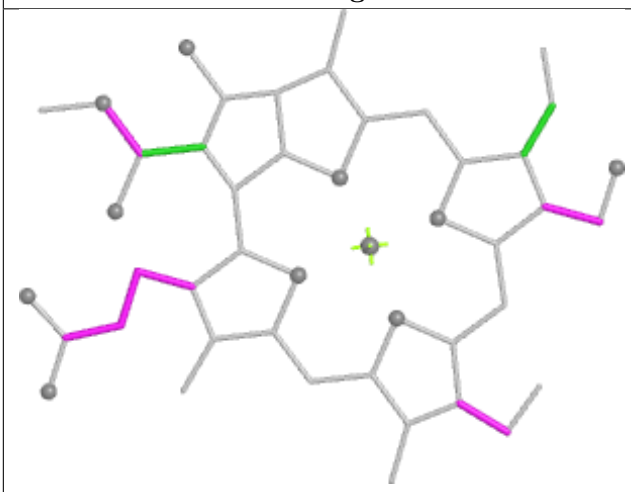
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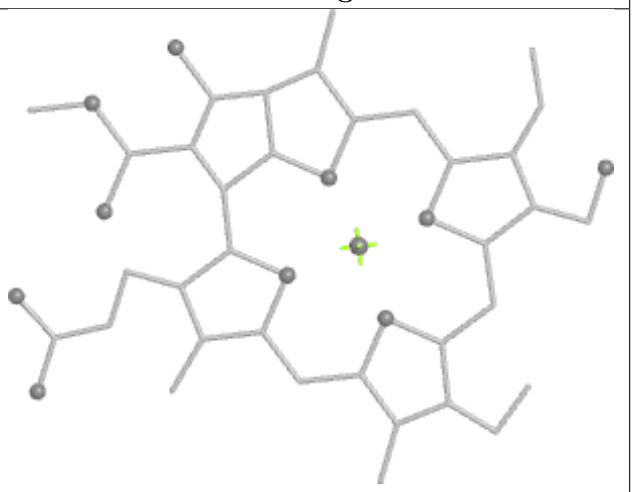
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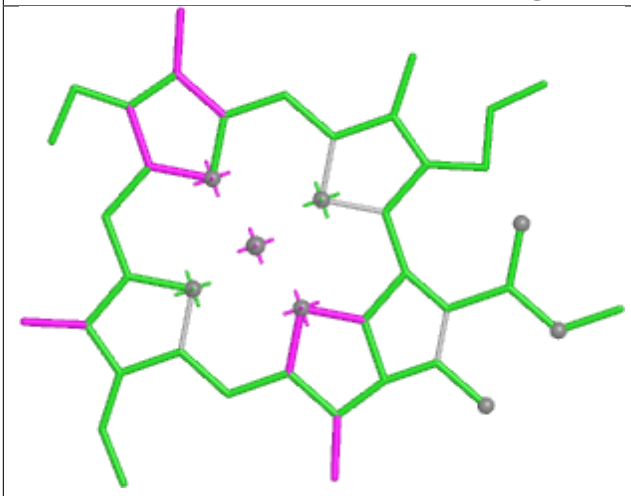


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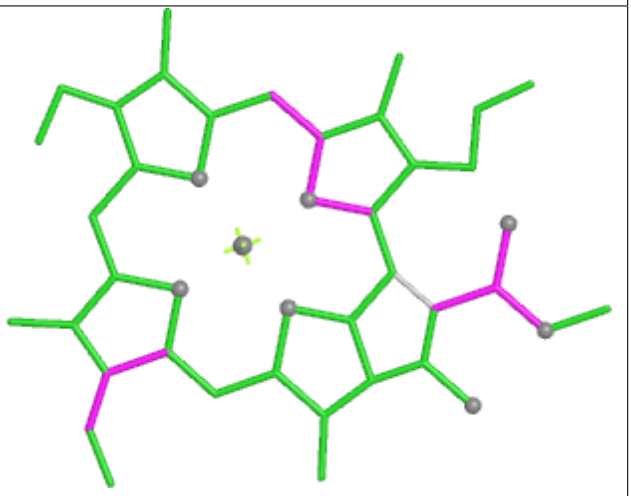


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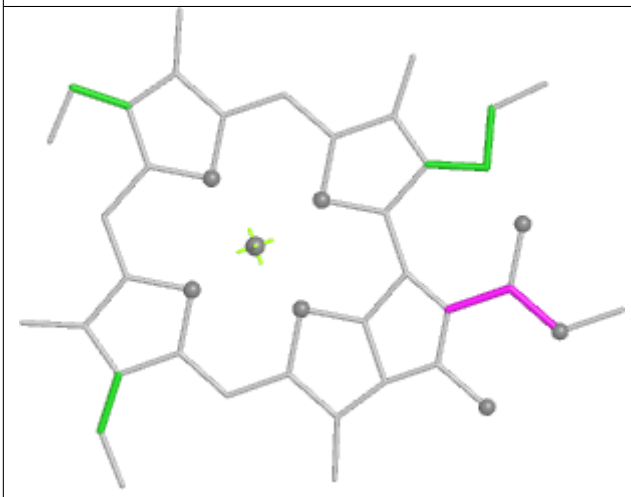
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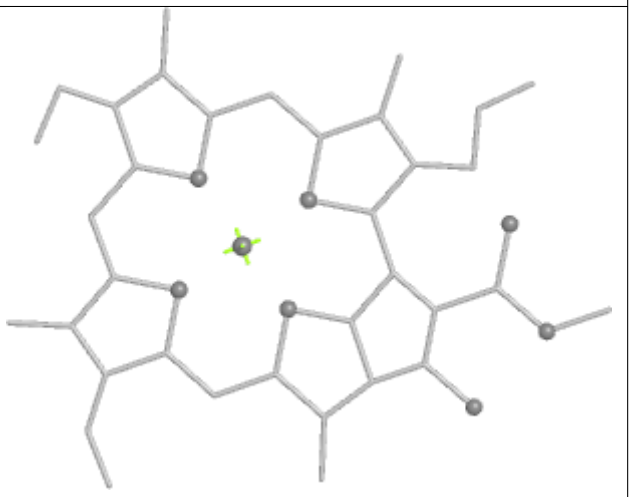
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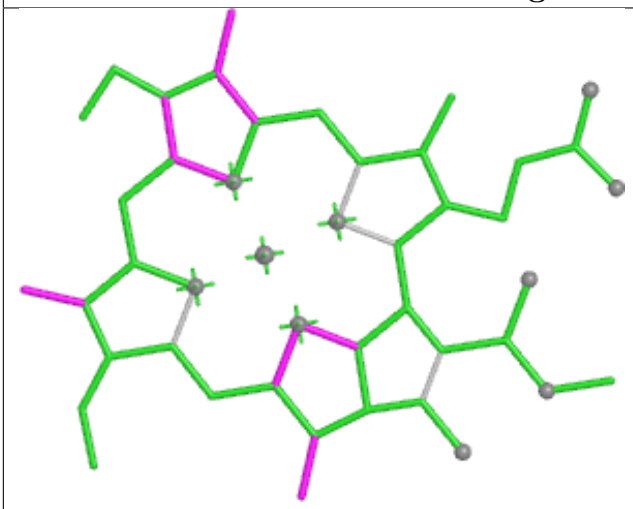


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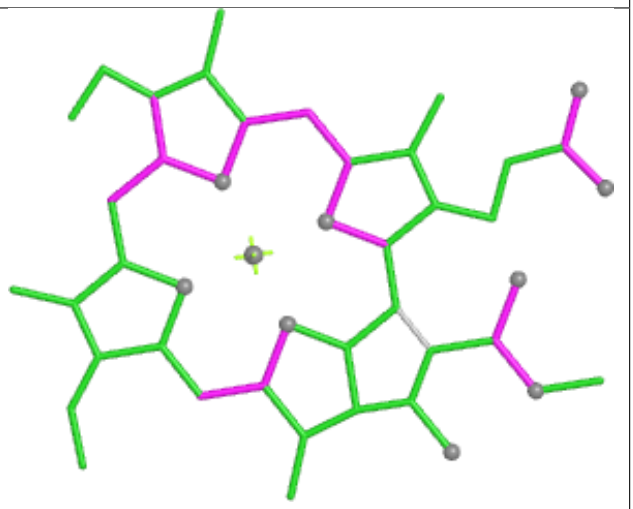


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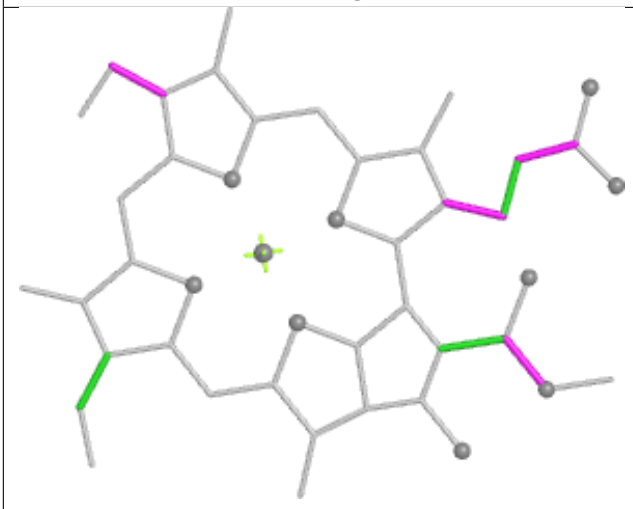
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Bond lengths



Bond angles

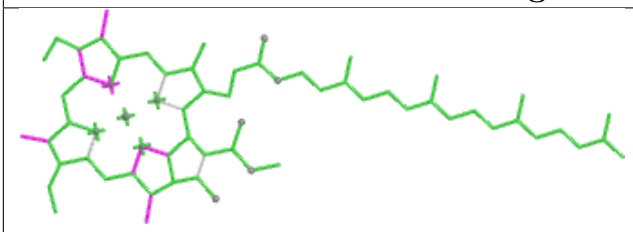


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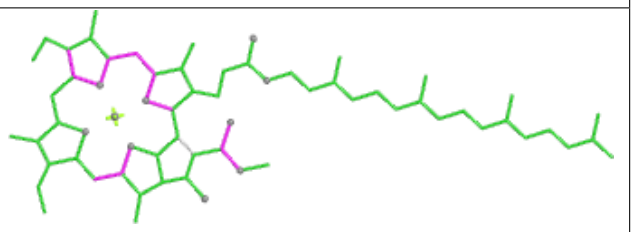


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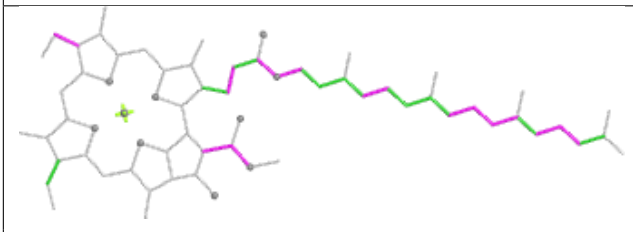
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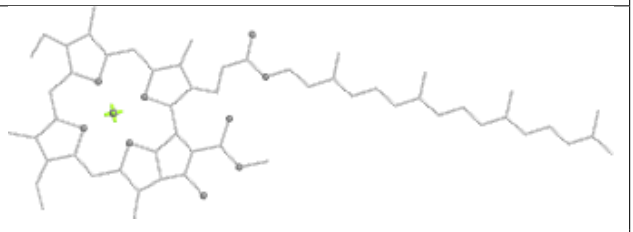
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Bond angles

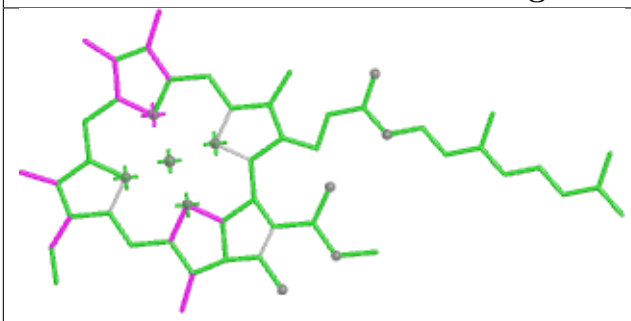


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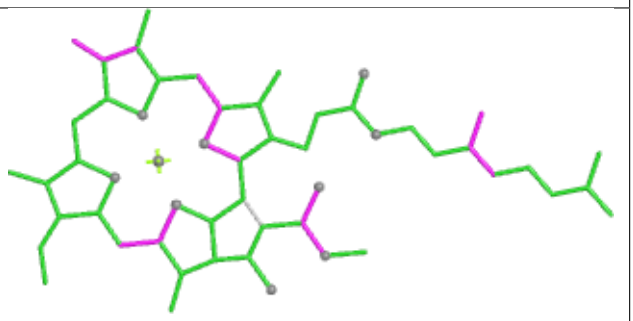


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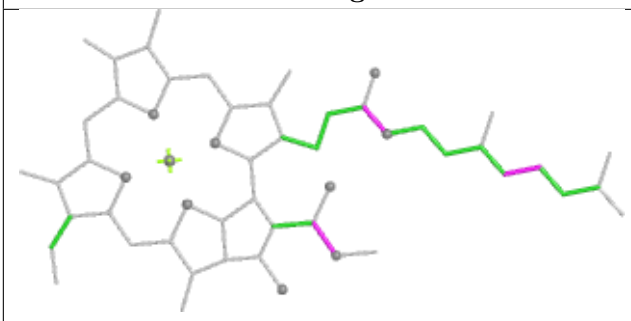
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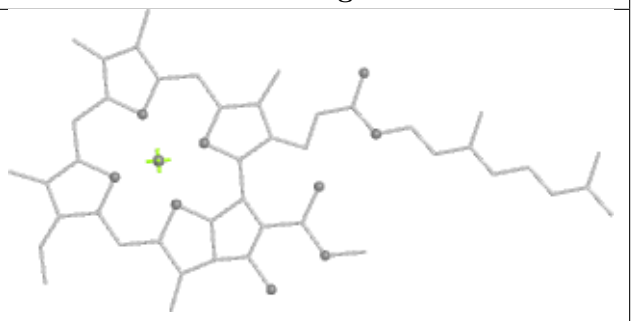
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Bond angles

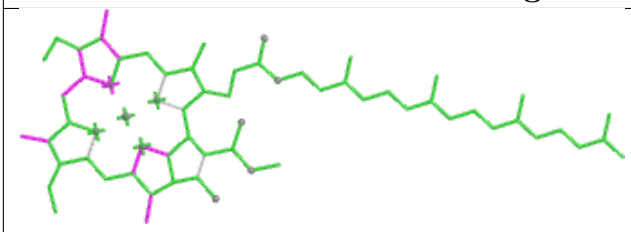


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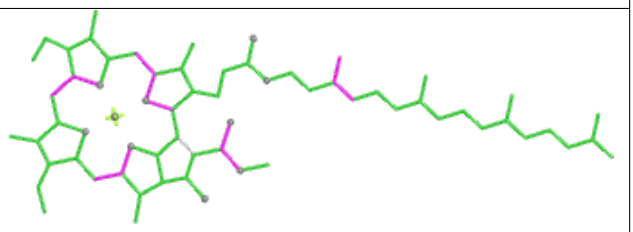


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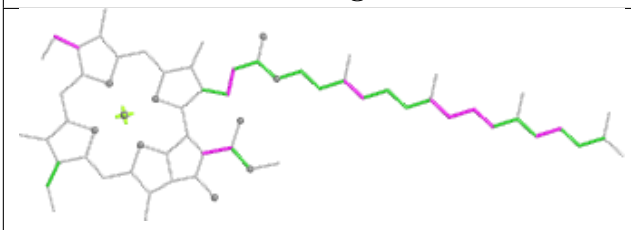
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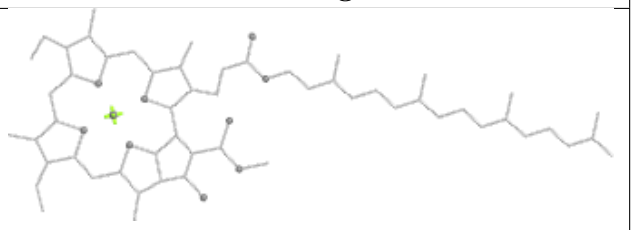
Bond lengths



Bond angles

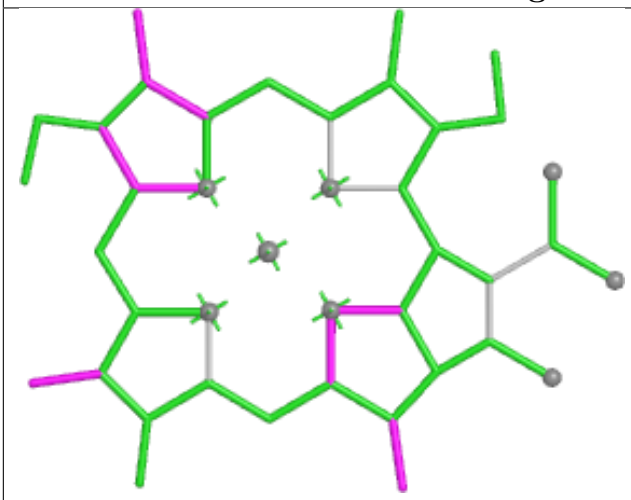


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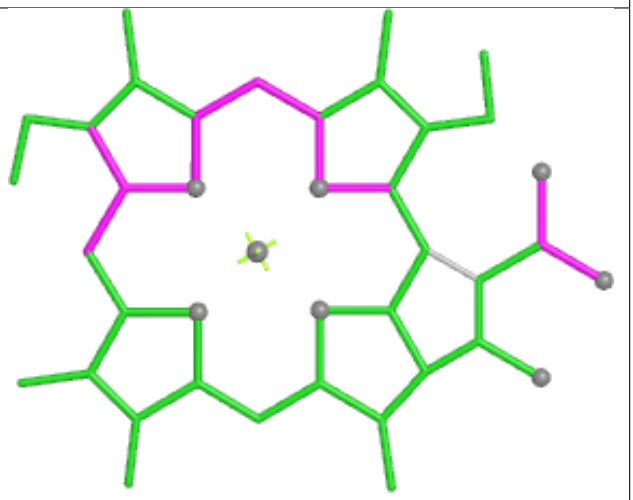


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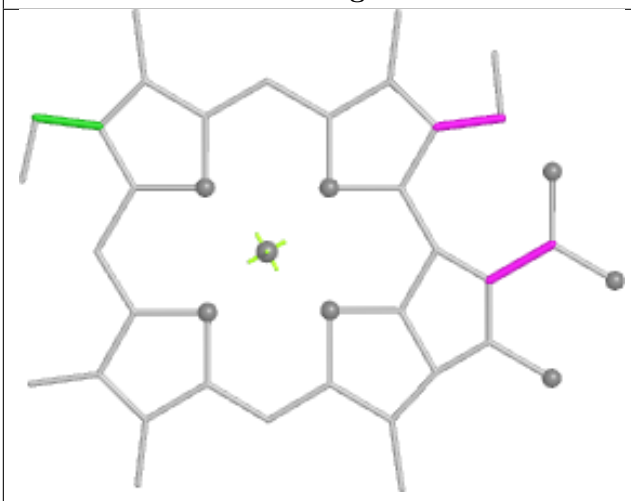
Ligand CLA 3 615



Bond lengths



Bond angles

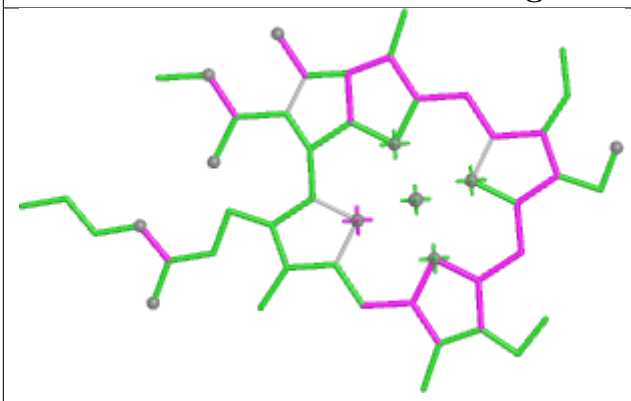


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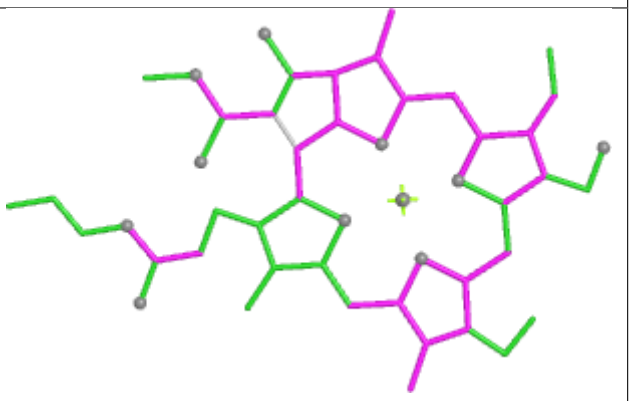


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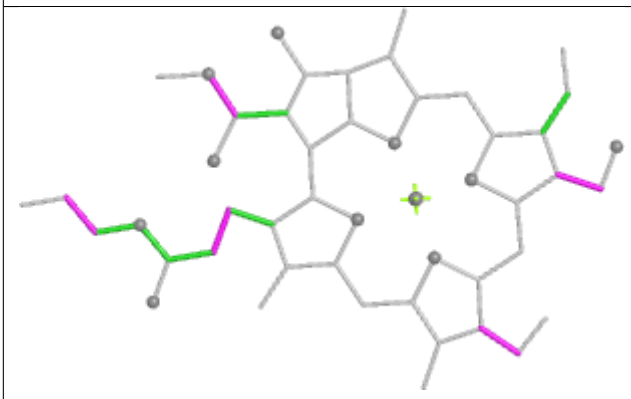
Ligand CHL Z 608



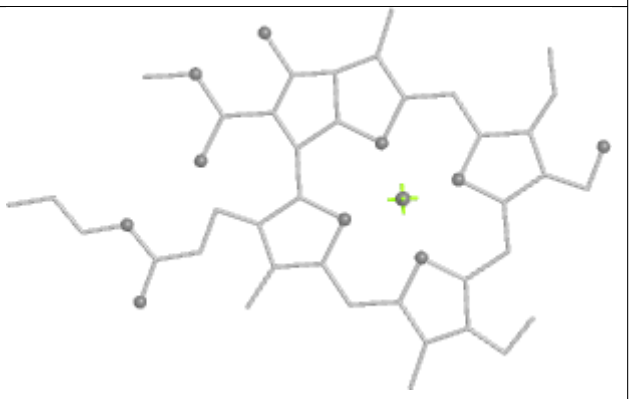
Bond lengths



Bond angles

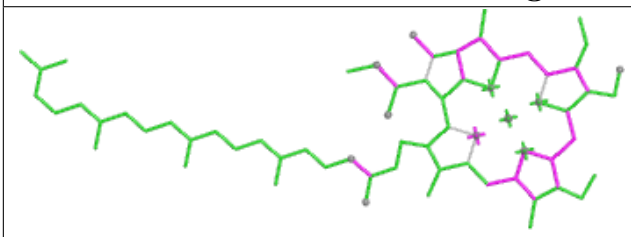


Torsions

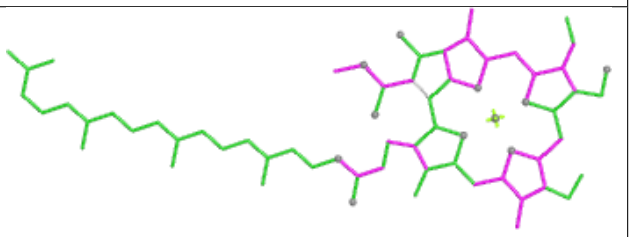


Rings

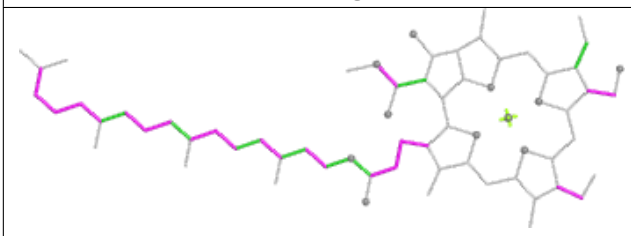
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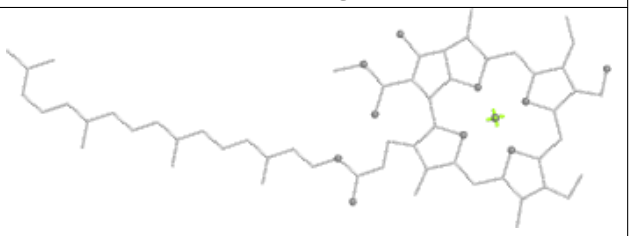
Bond lengths



Bond angles

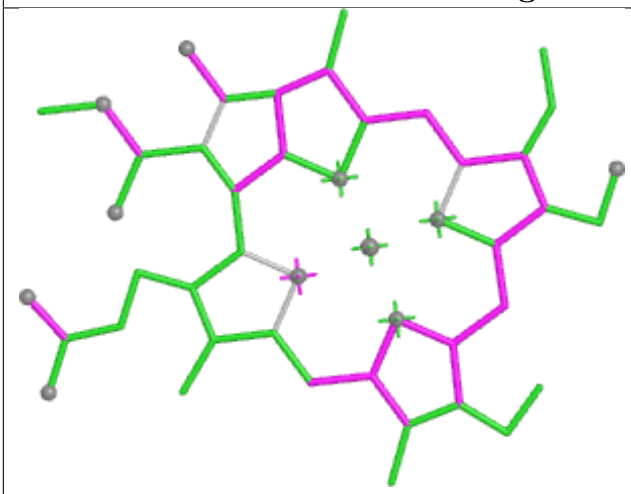


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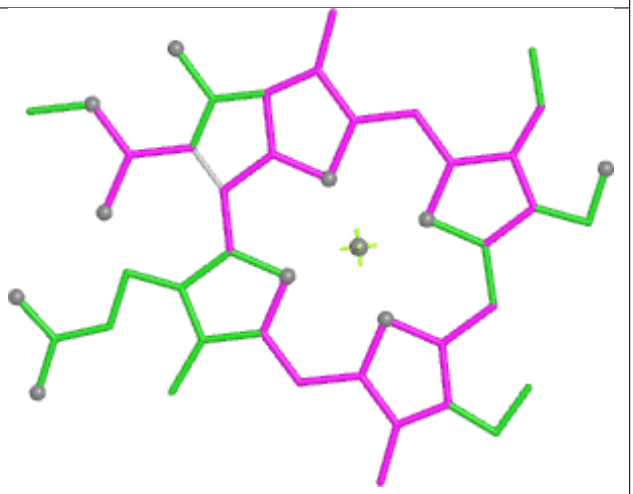


Rings

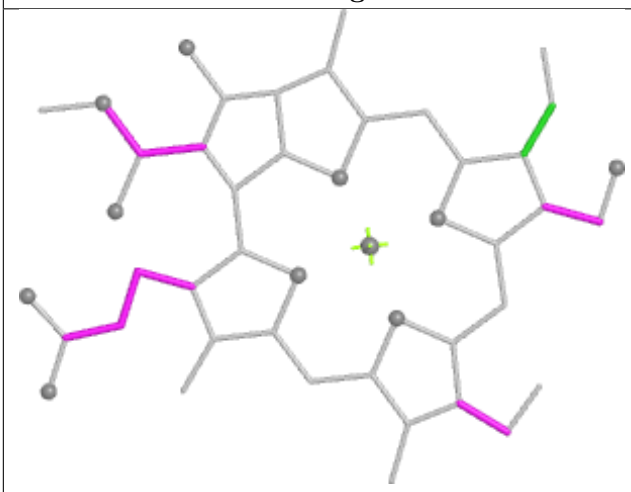
Ligand CHL W 605



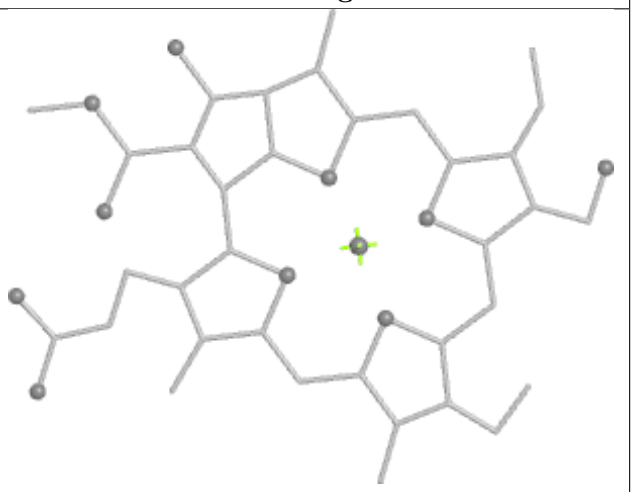
Bond lengths



Bond angles



Torsions

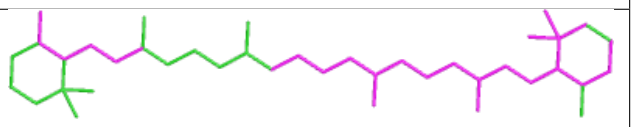


Rings

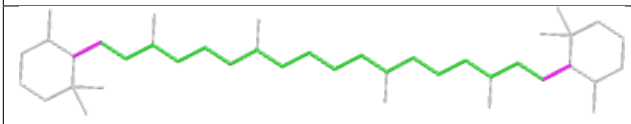
Ligand BCR B 801



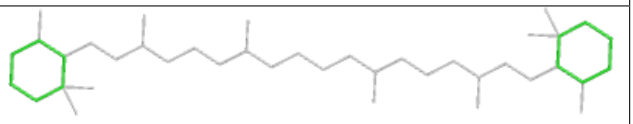
Bond lengths



Bond angles

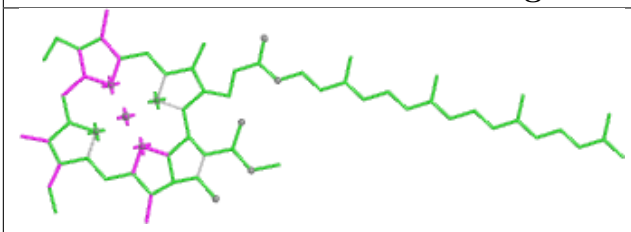


Torsions

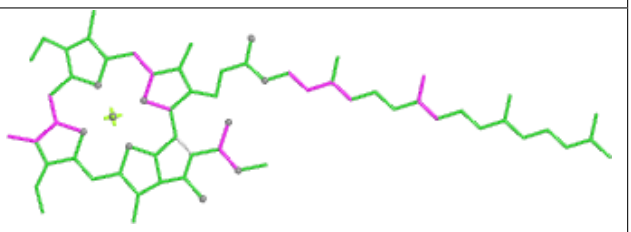


Rings

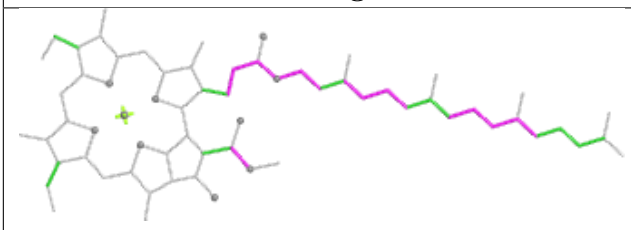
Ligand CLA B 806



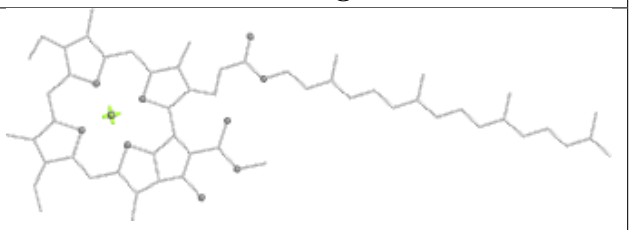
Bond lengths



Bond angles

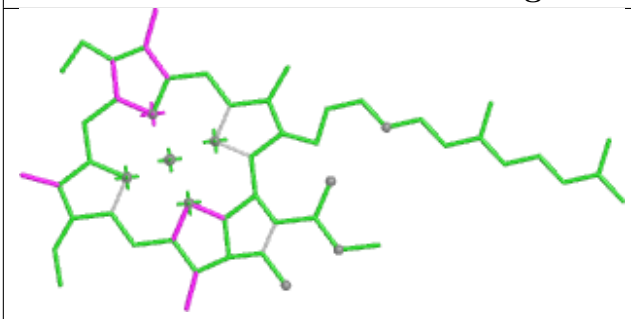


Torsions

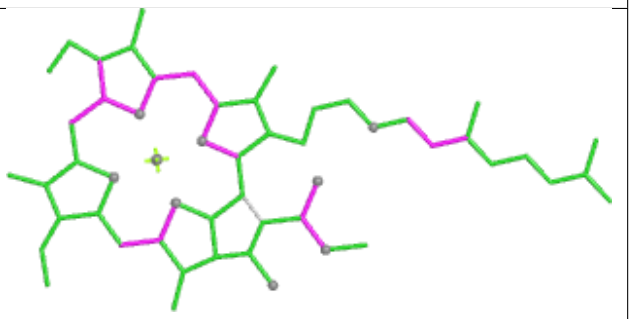


Rings

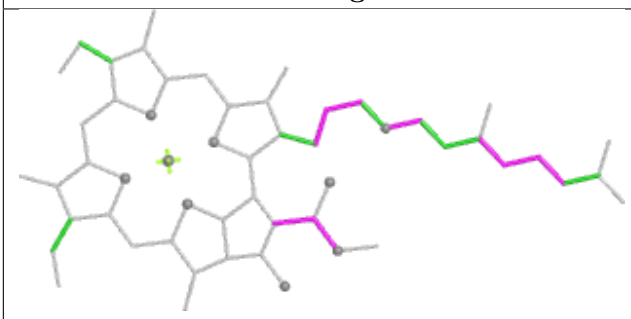
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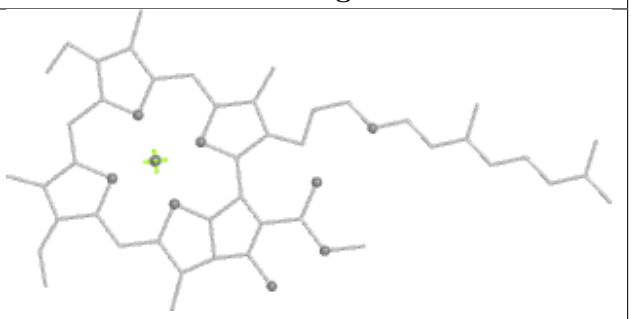
Bond lengths



Bond angles

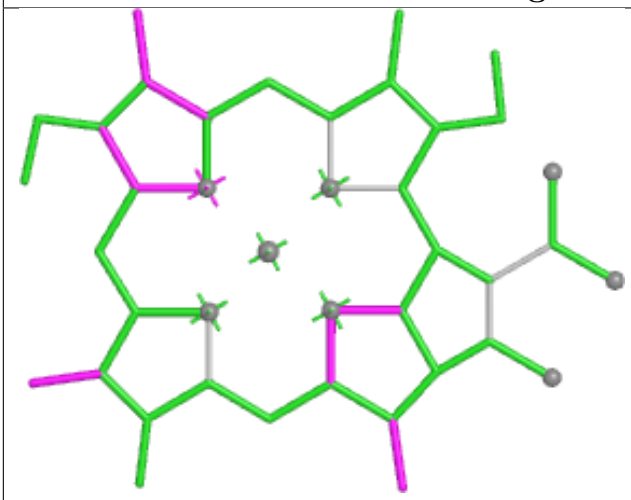


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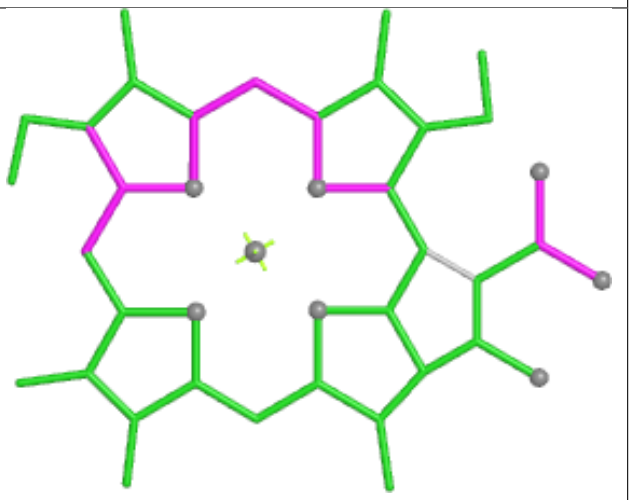


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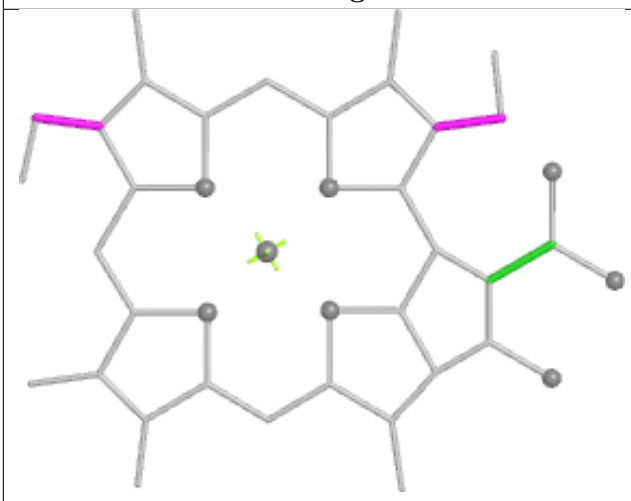
Ligand CLA 4 606



Bond lengths



Bond angles

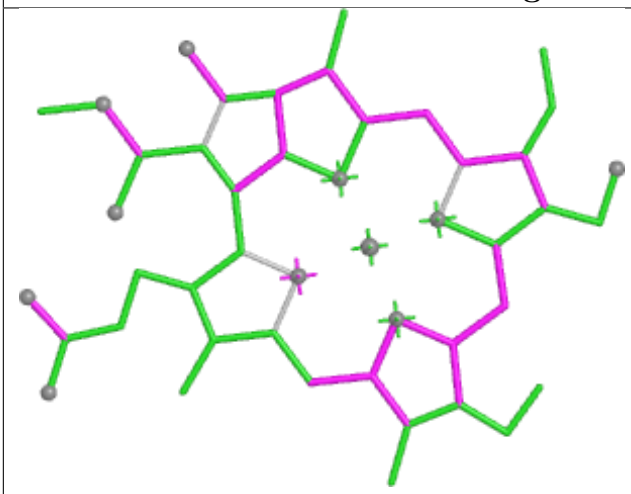


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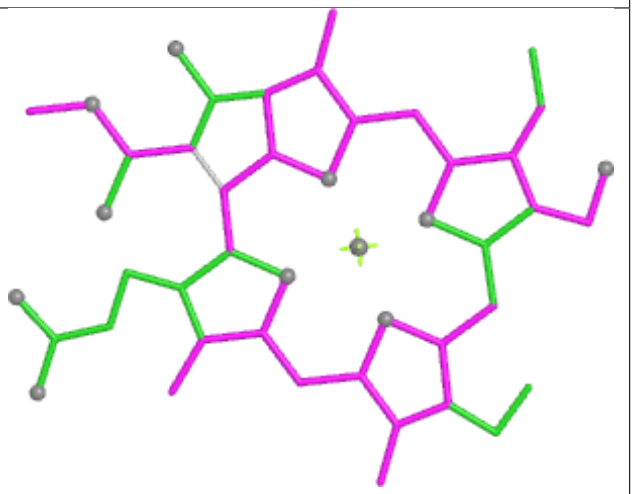


Rings

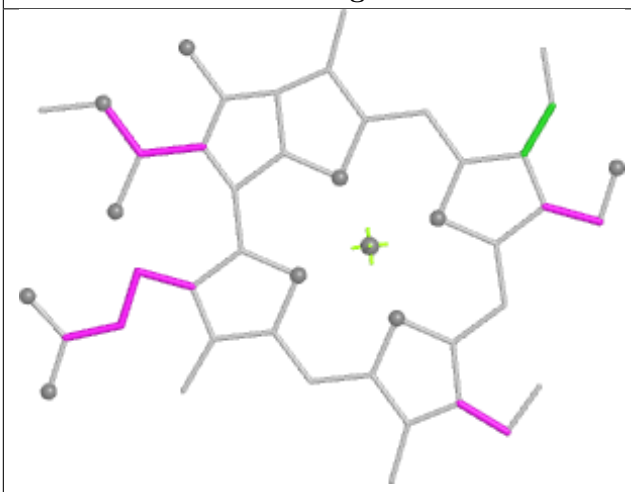
Ligand CHL V 607



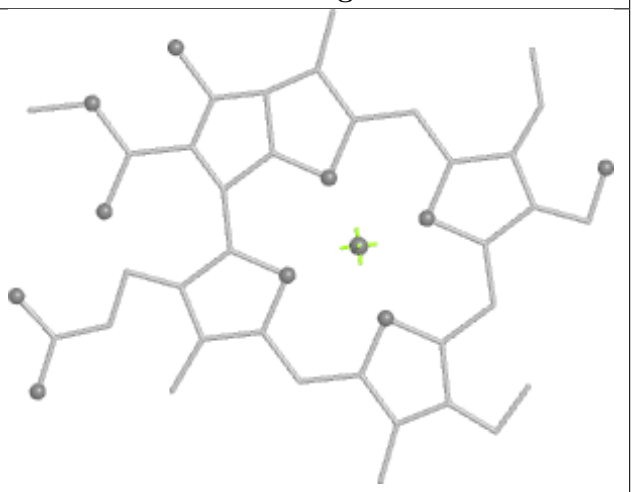
Bond lengths



Bond angles

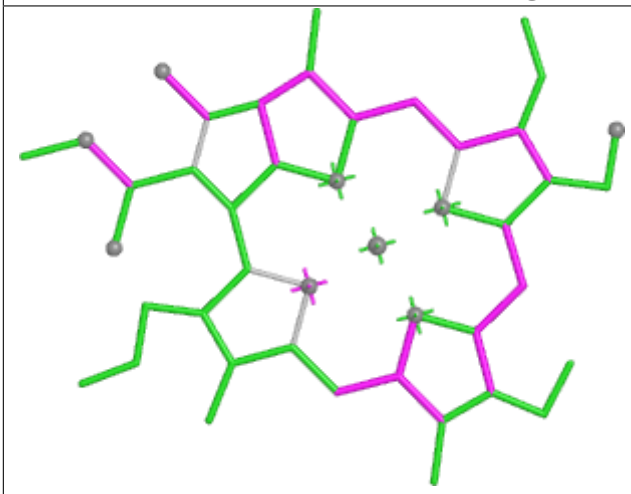


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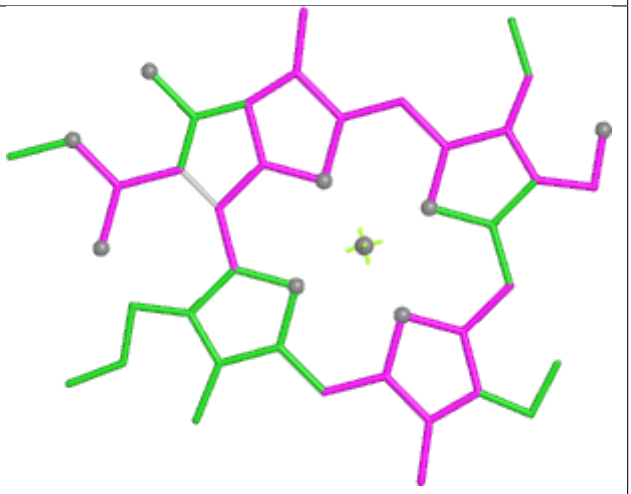


Rings

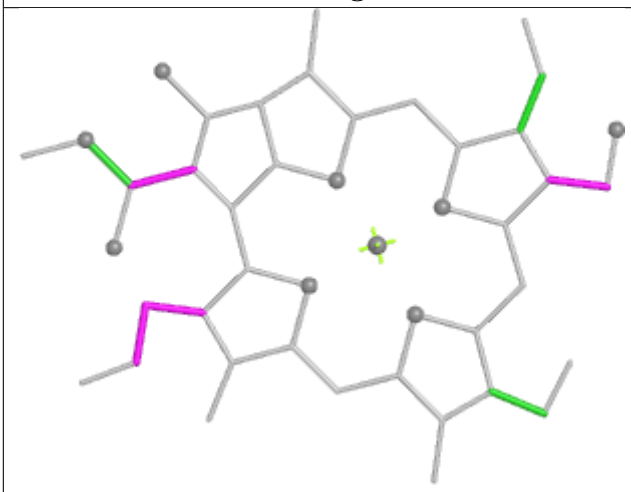
Ligand CHL X 606



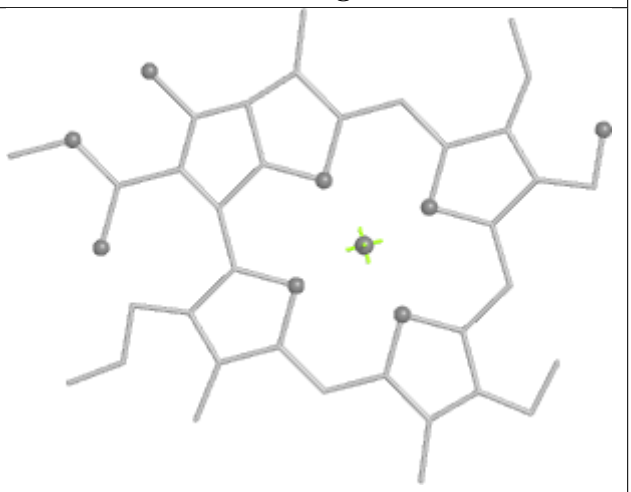
Bond lengths



Bond angles

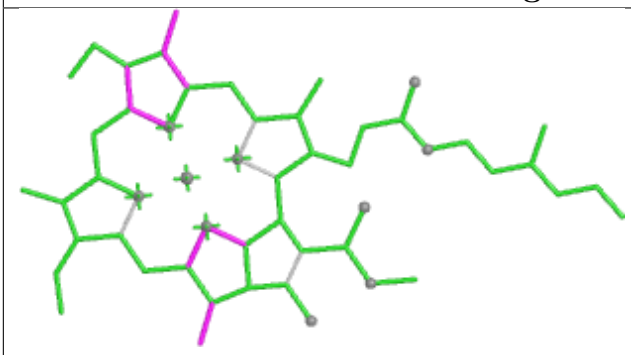


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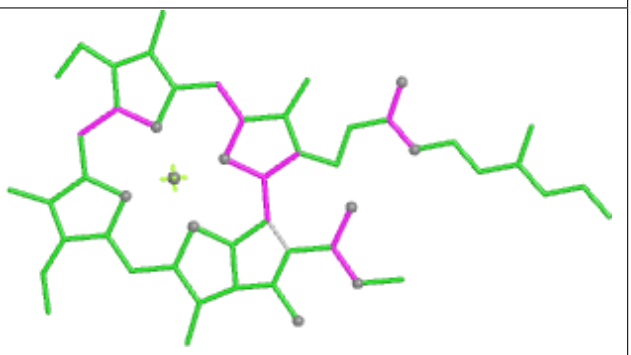


Rings

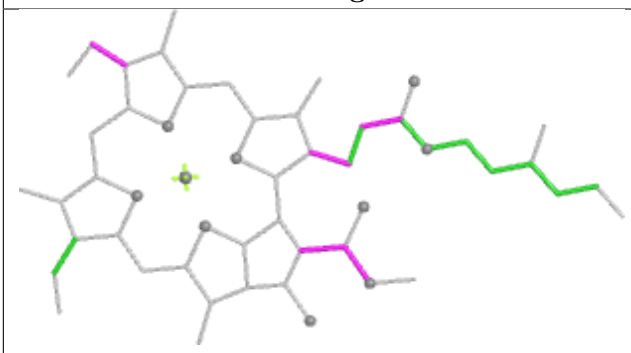
Ligand CLA U 603



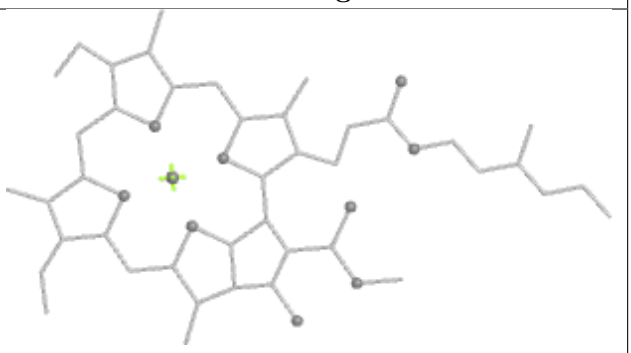
Bond lengths



Bond angles

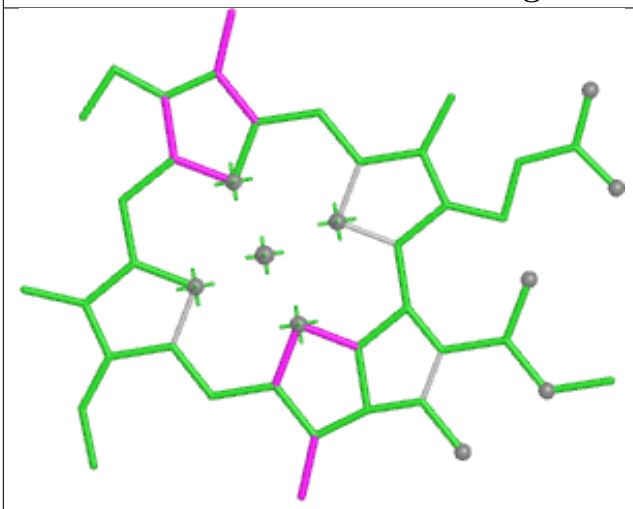


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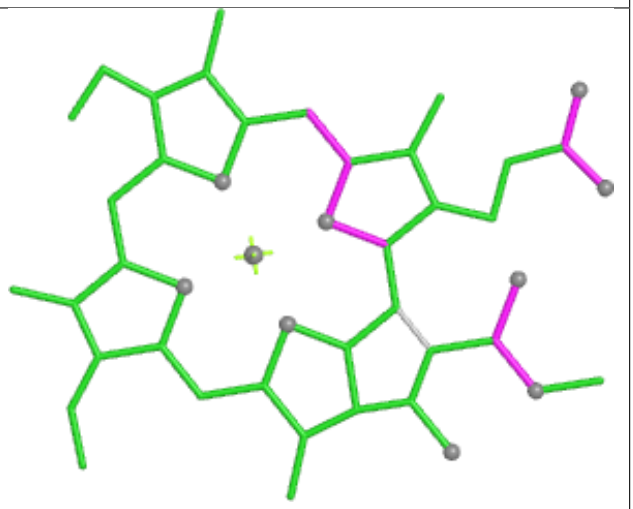


Rings

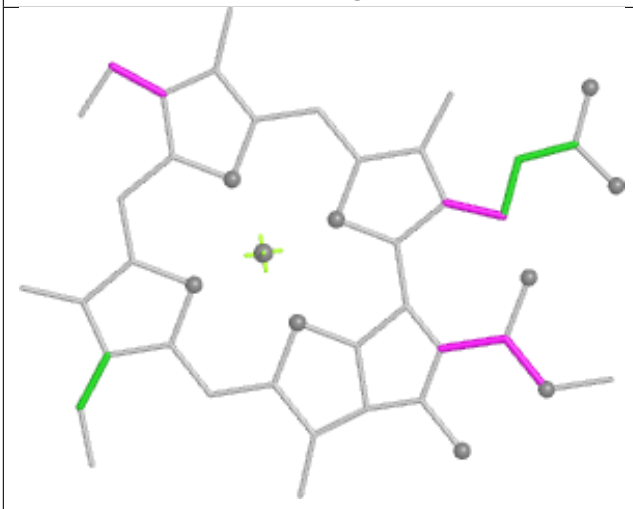
Ligand CLA K 201



Bond lengths



Bond angles

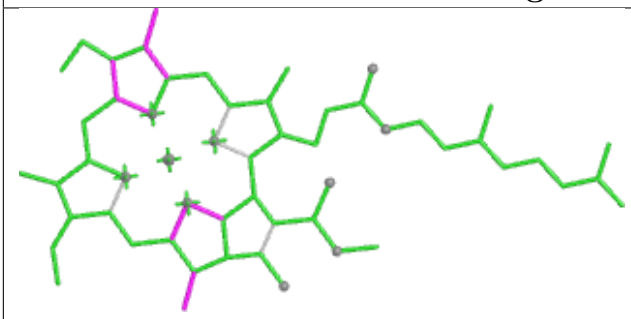


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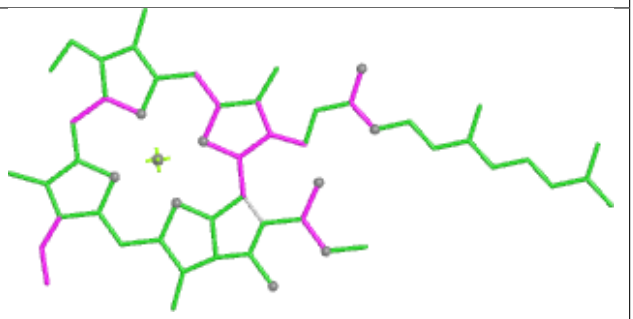


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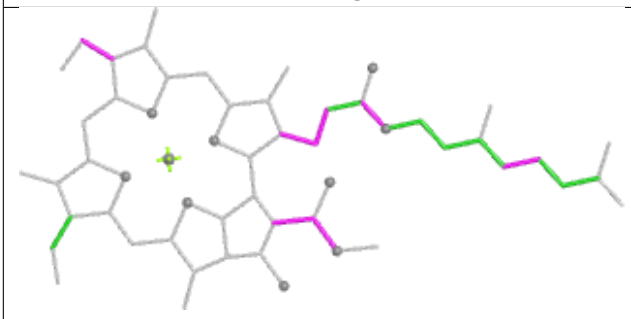
Ligand CLA Z 603



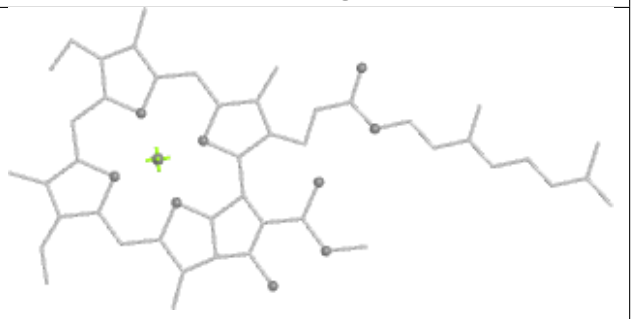
Bond lengths



Bond angles

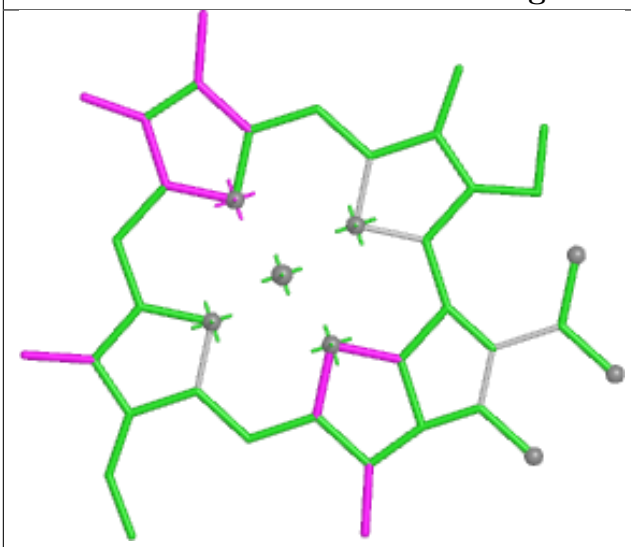


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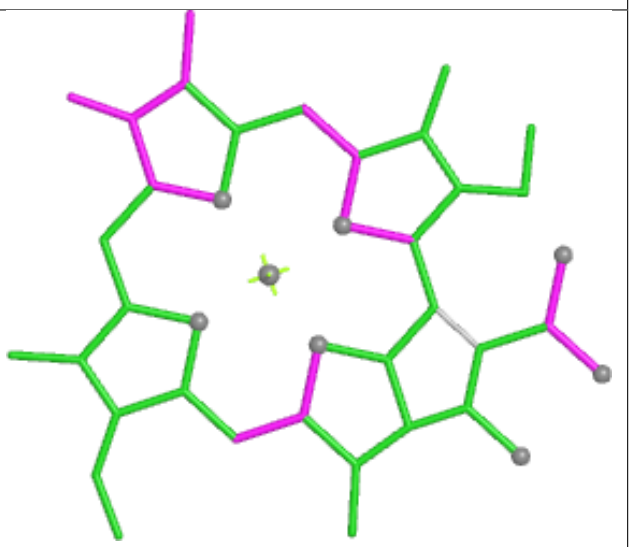


Rings

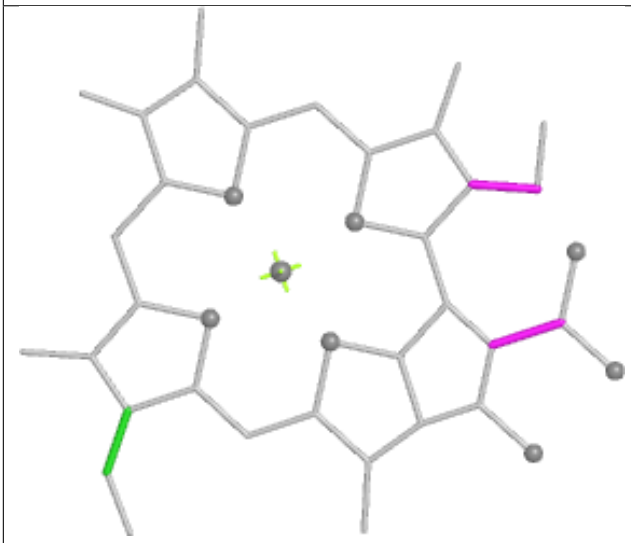
Ligand CLA 5 618



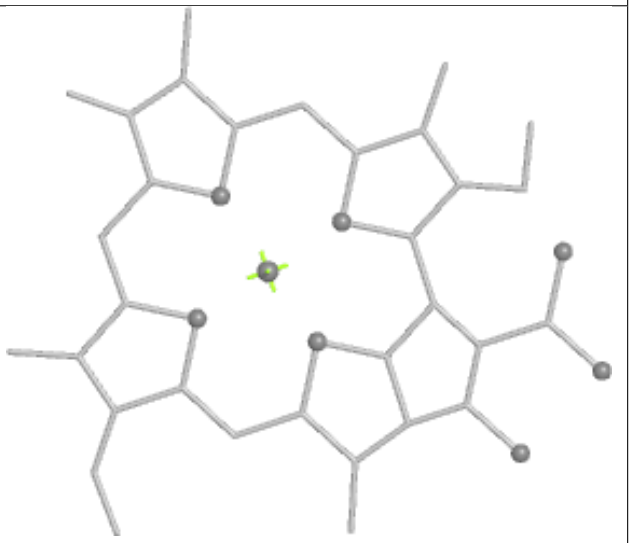
Bond lengths



Bond angles

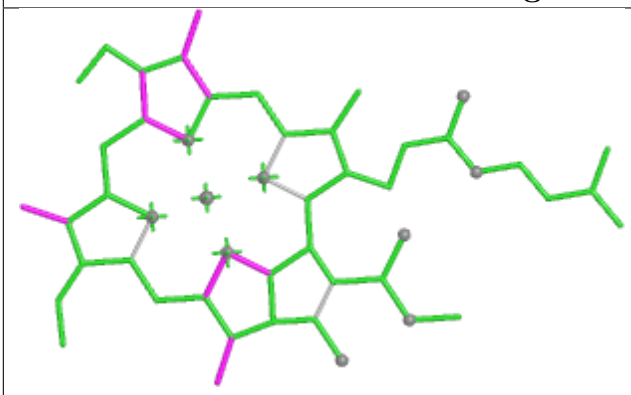


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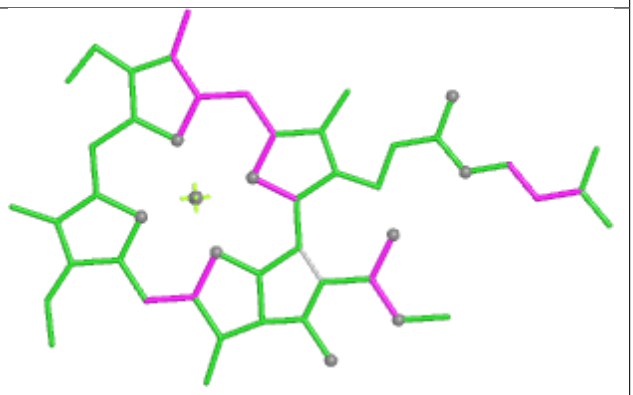


Rings

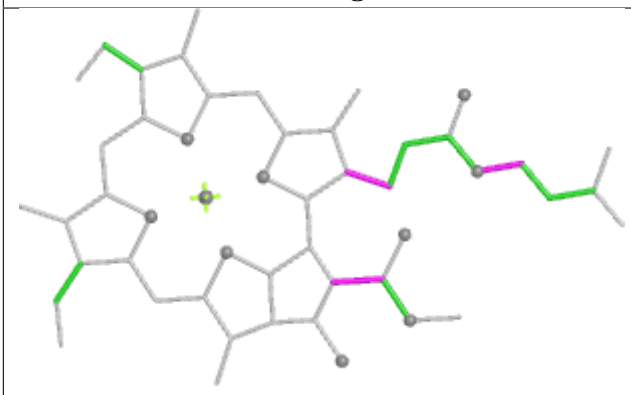
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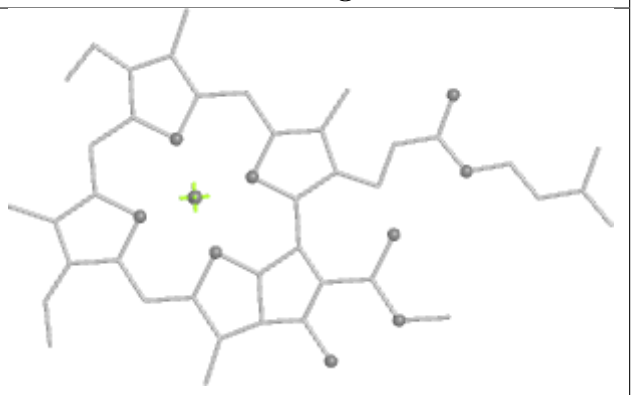
Bond lengths



Bond angles

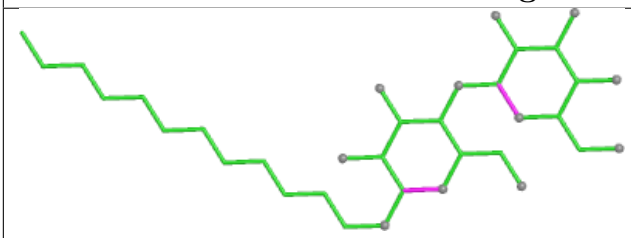


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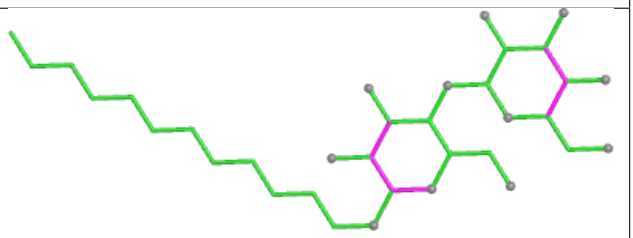


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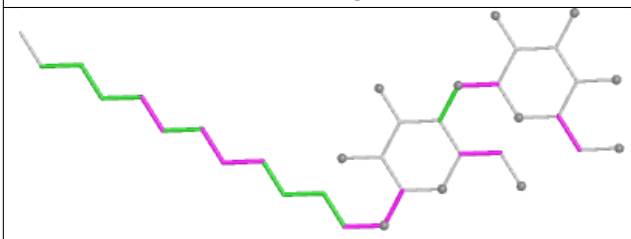
Ligand LMU K 208



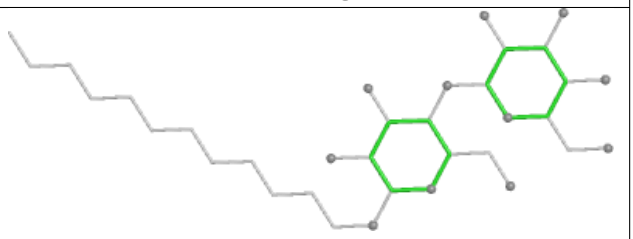
Bond lengths



Bond angles

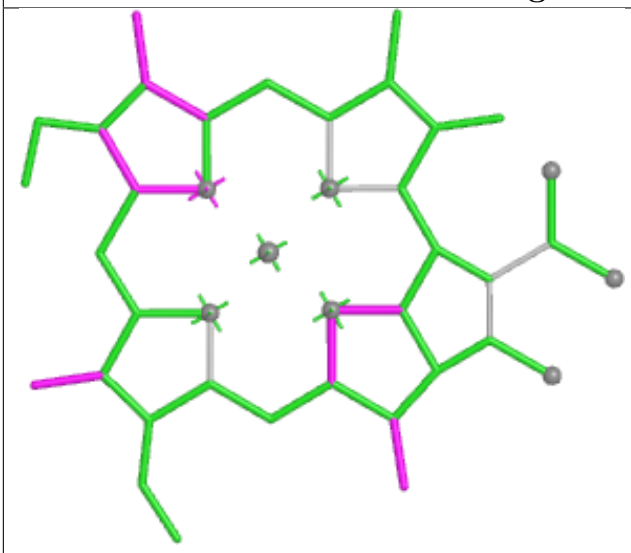


Torsions

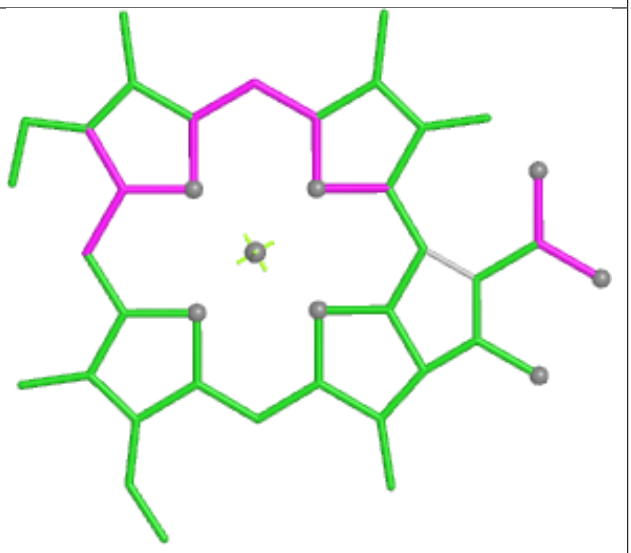


Rings

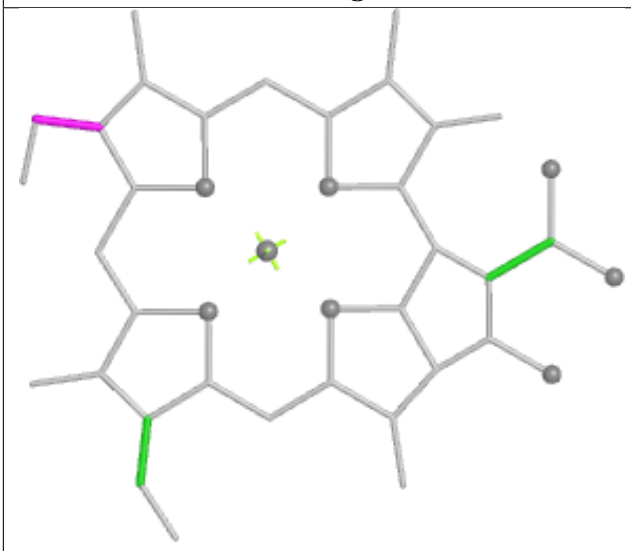
Ligand CLA 3 614



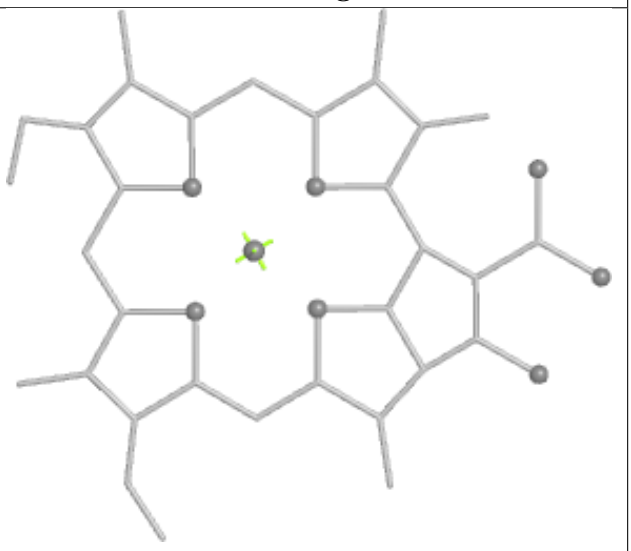
Bond lengths



Bond angles

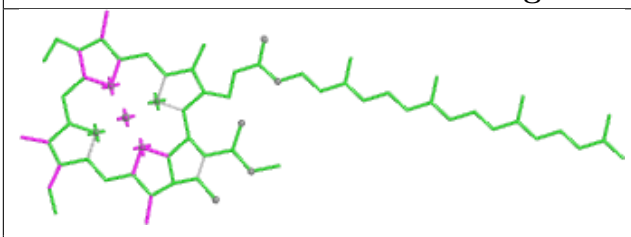


Torsions

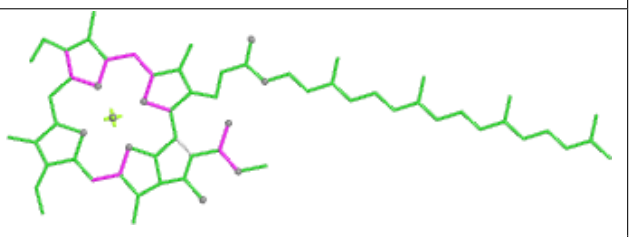


Rings

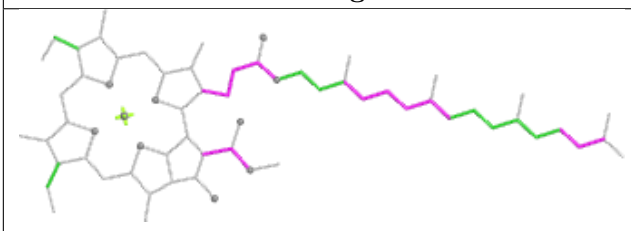
Ligand CLA A 807



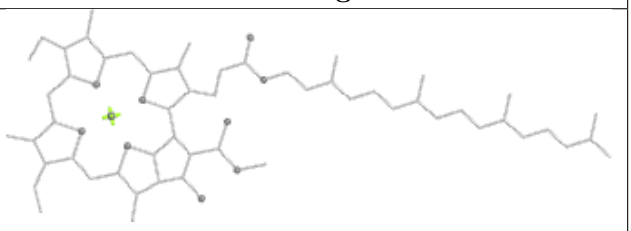
Bond lengths



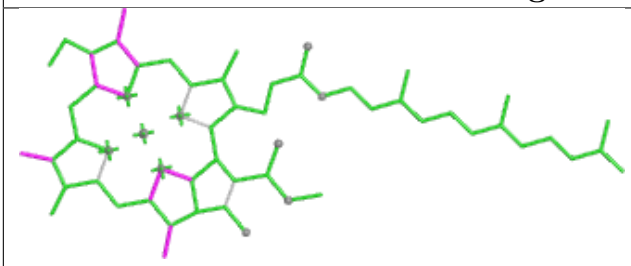
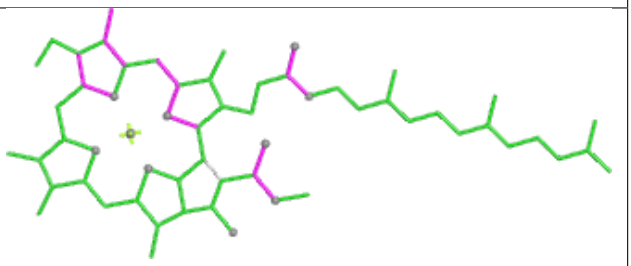
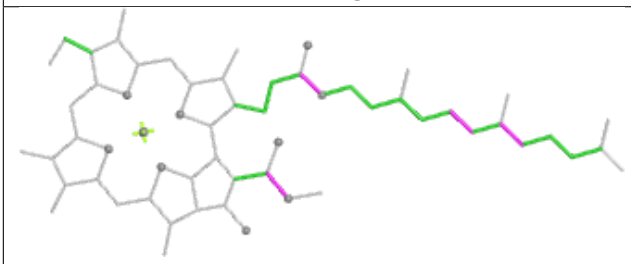
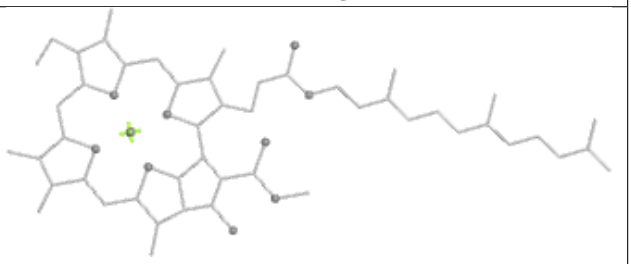
Bond angles

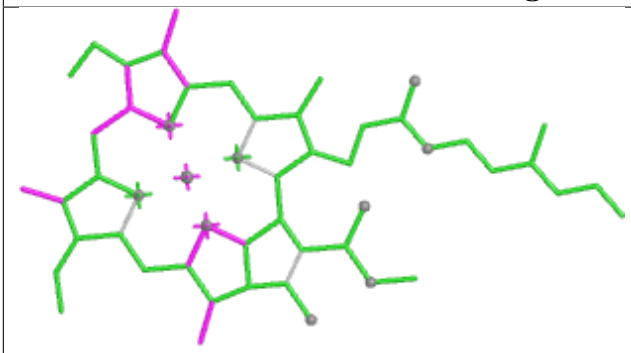
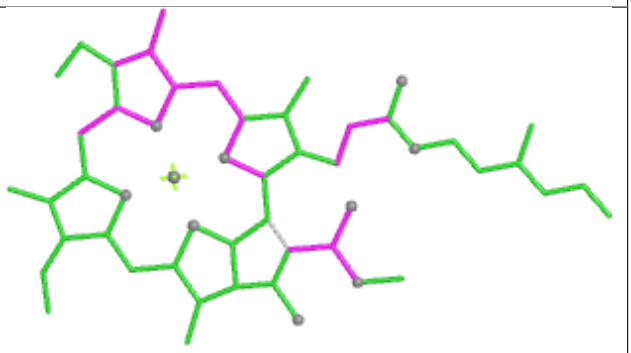
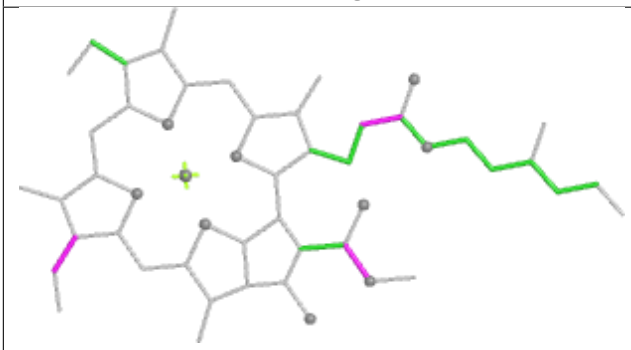
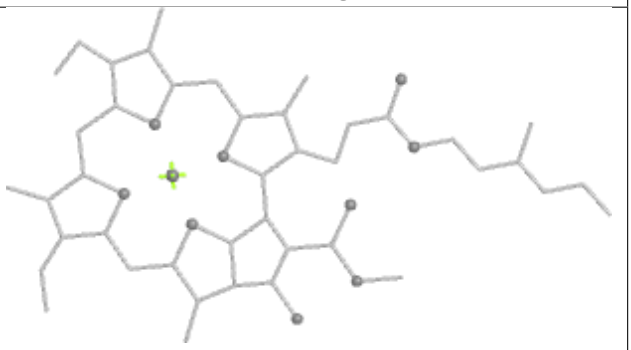


Torsions

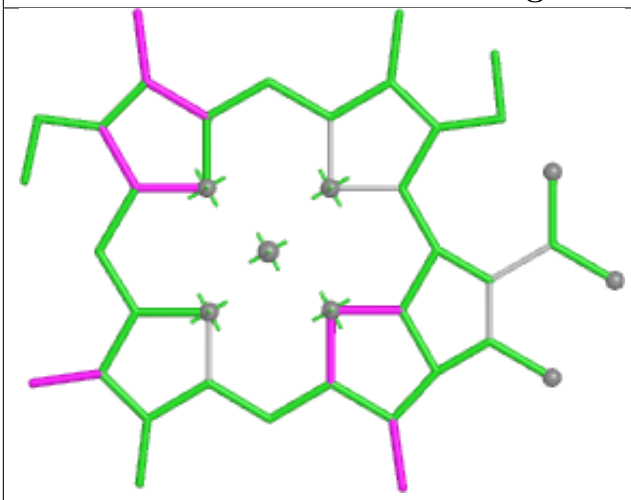


Rings

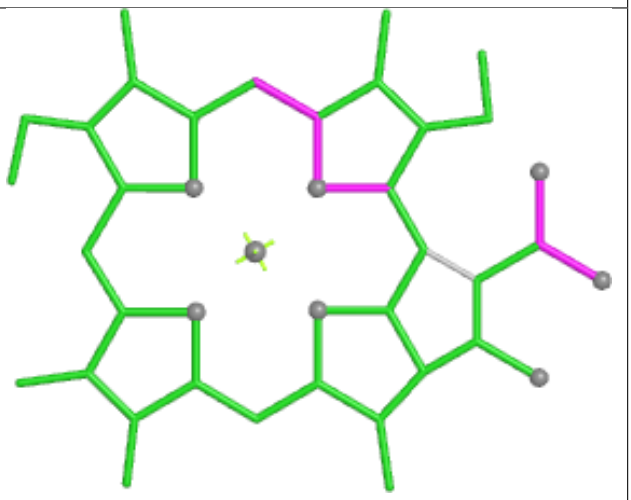
Ligand CLA a 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 840	
 Bond lengths	 Bond angles
 Torsions	 Rings

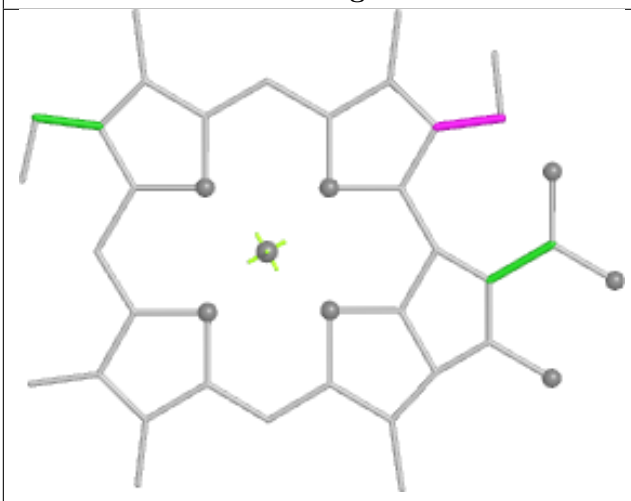
Ligand CLA L 306



Bond lengths



Bond angles

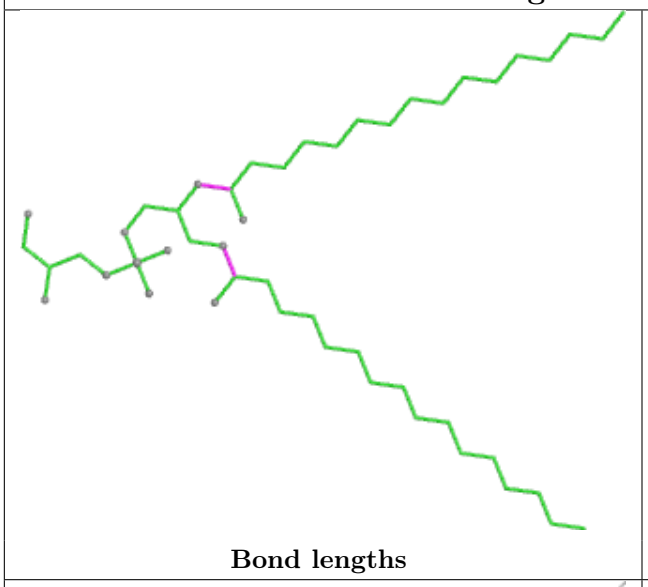


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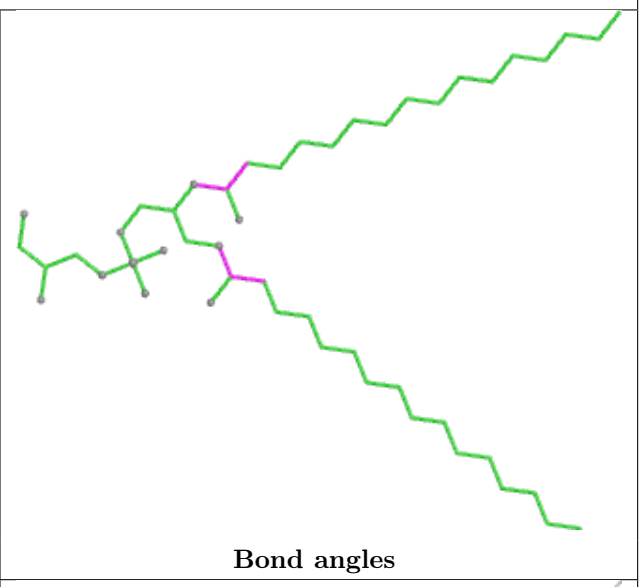


Rings

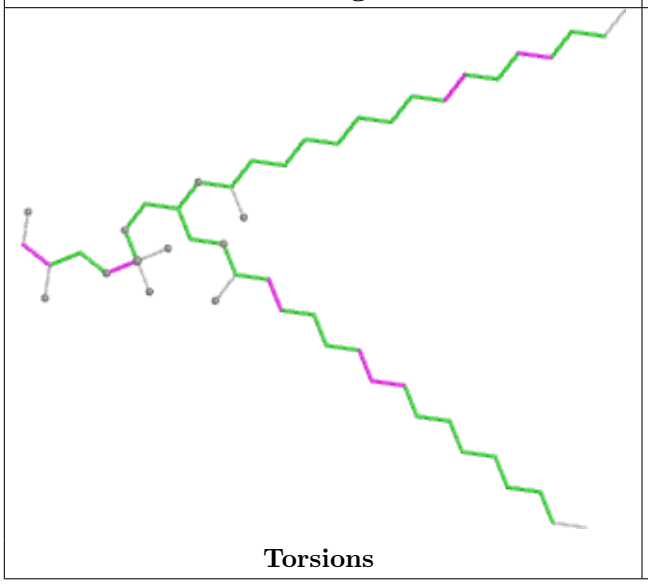
Ligand LHG 1 620



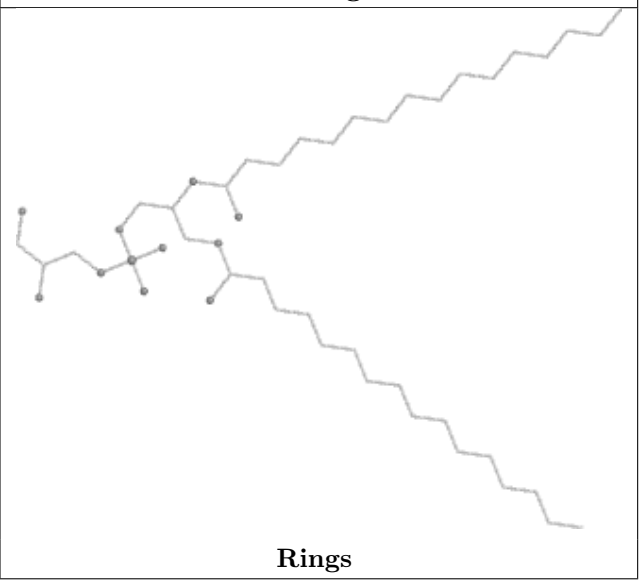
Bond lengths



Bond angles

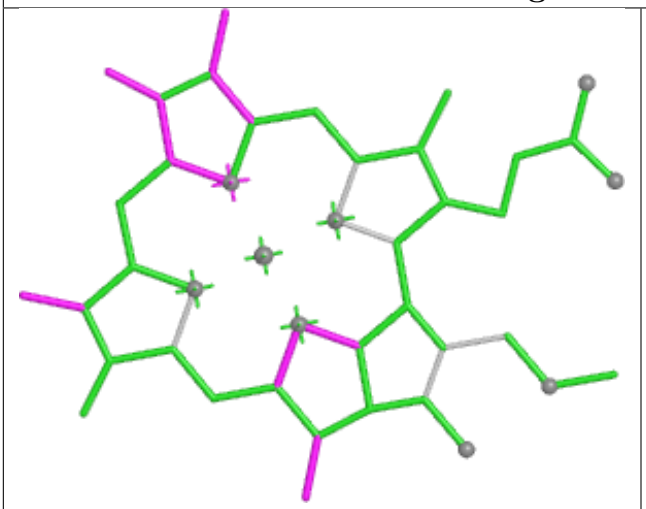


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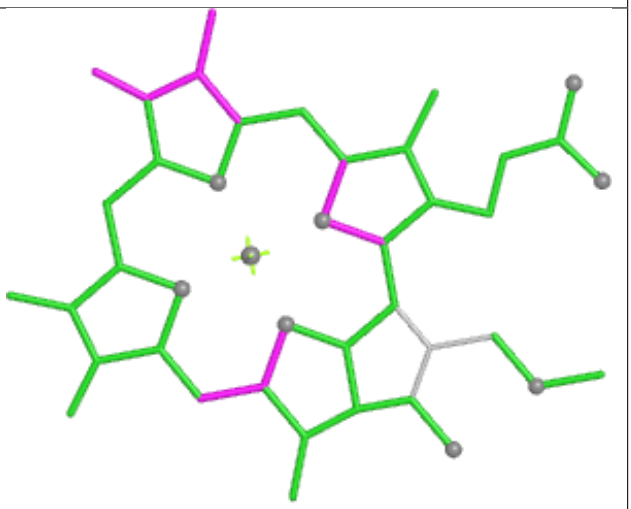


Rings

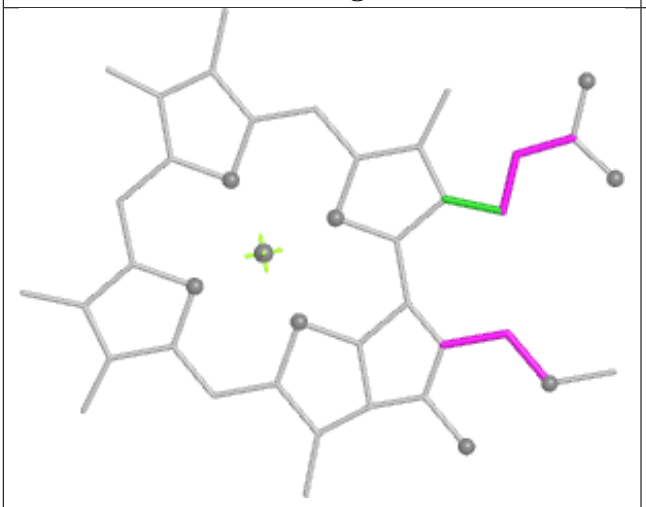
Ligand CLA 7 615



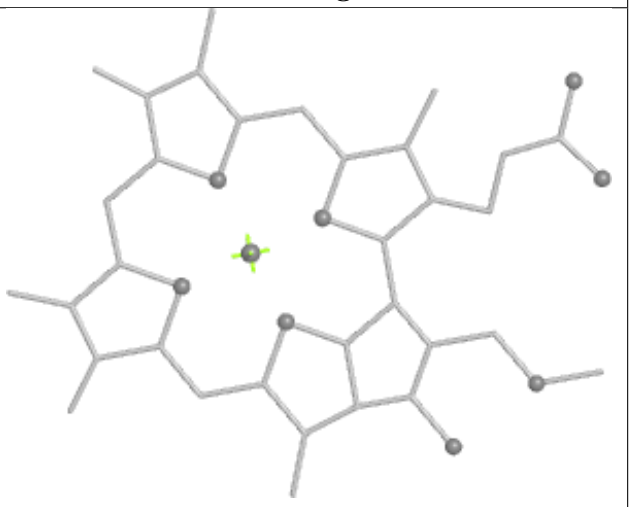
Bond lengths



Bond angles

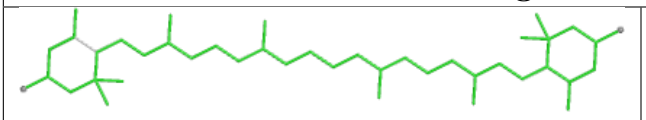


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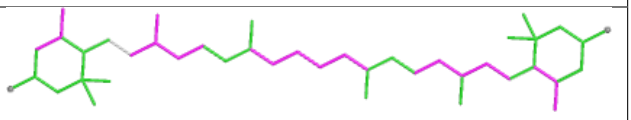


Rings

Ligand LUT X 1620



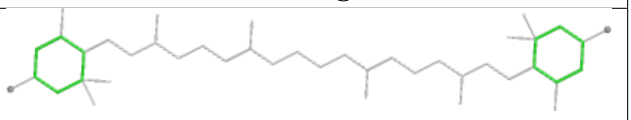
Bond lengths



Bond angles

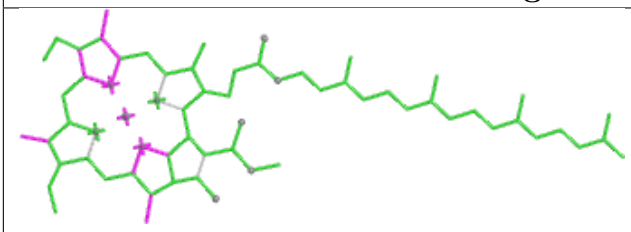


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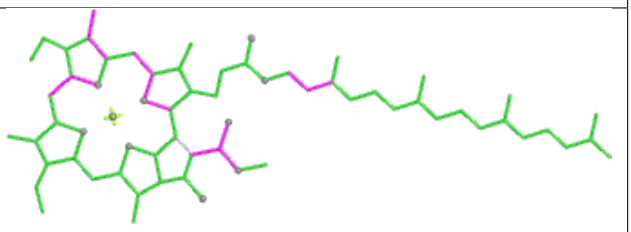


Rings

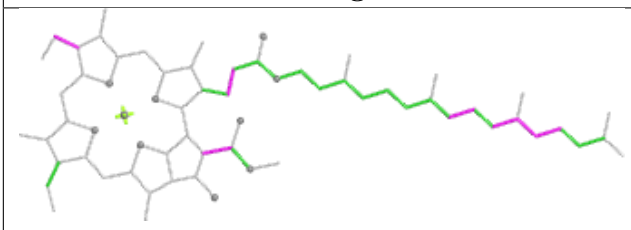
Ligand CLA A 809



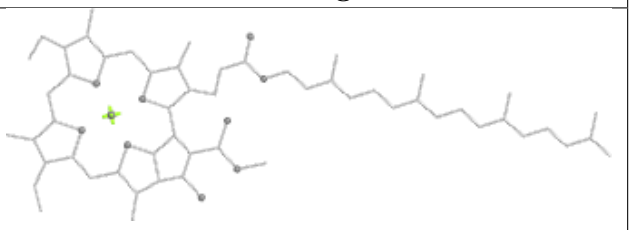
Bond lengths



Bond angles

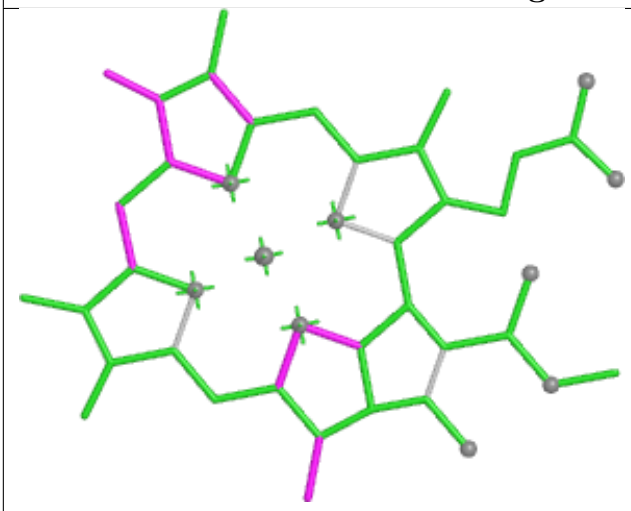


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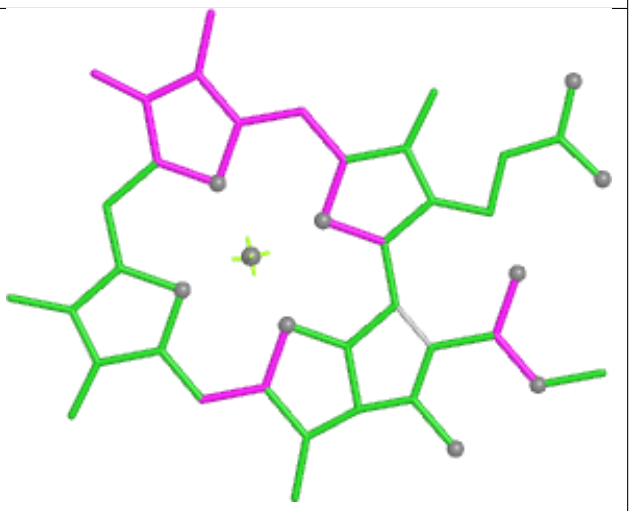


Rings

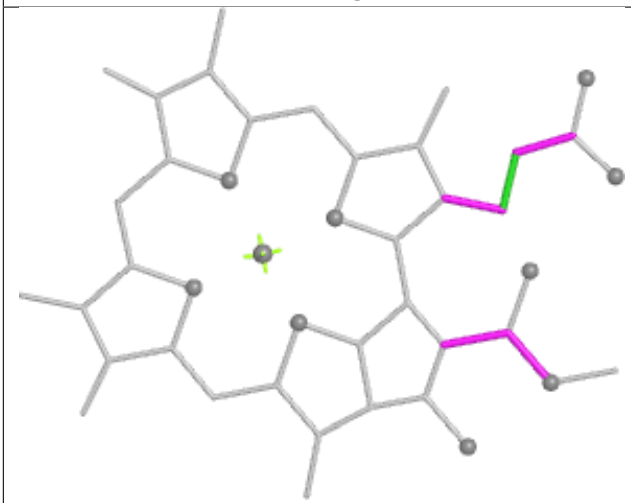
Ligand CLA 1 616



Bond lengths



Bond angles

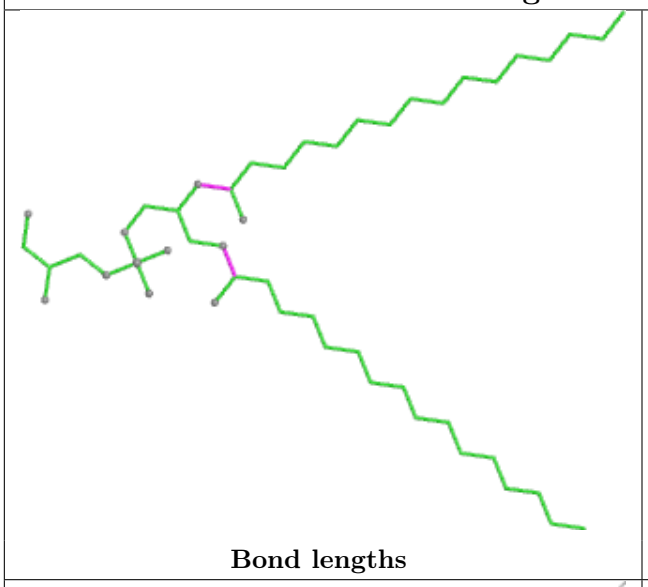


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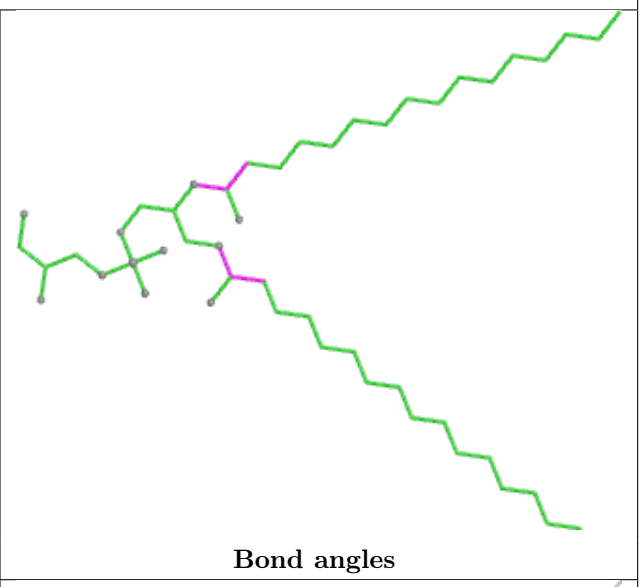


Rings

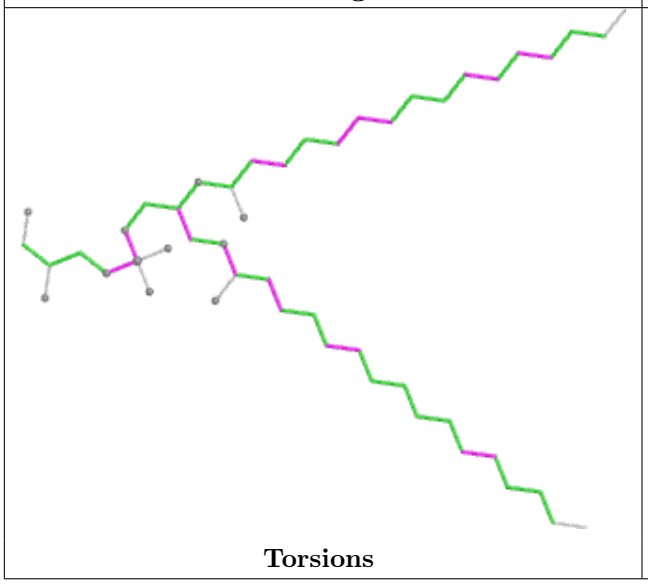
Ligand LHG H 204



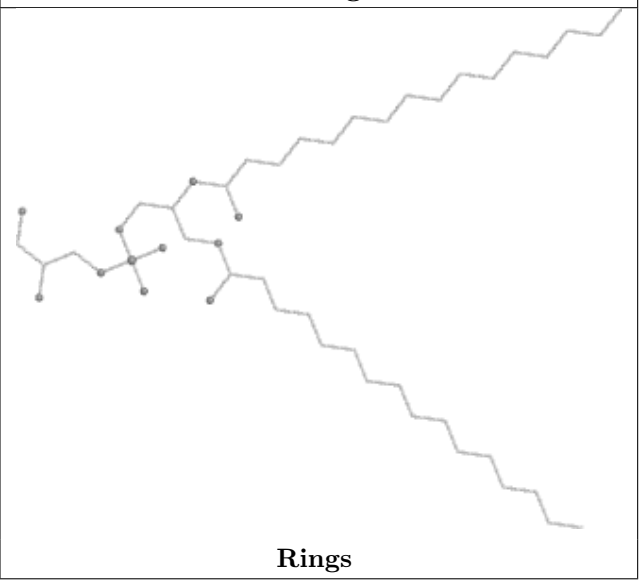
Bond lengths



Bond angles

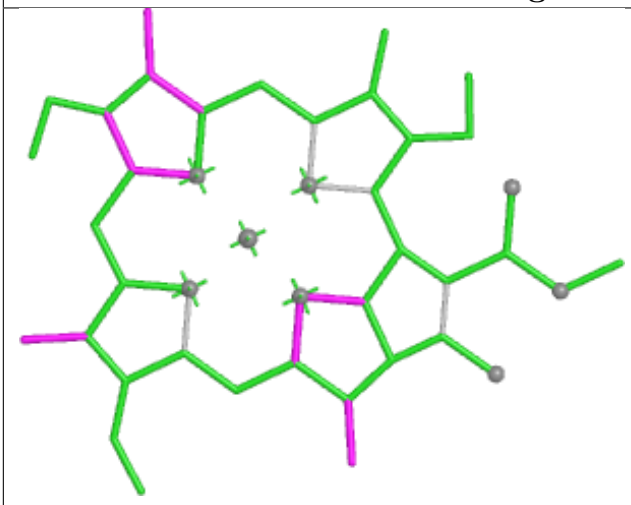


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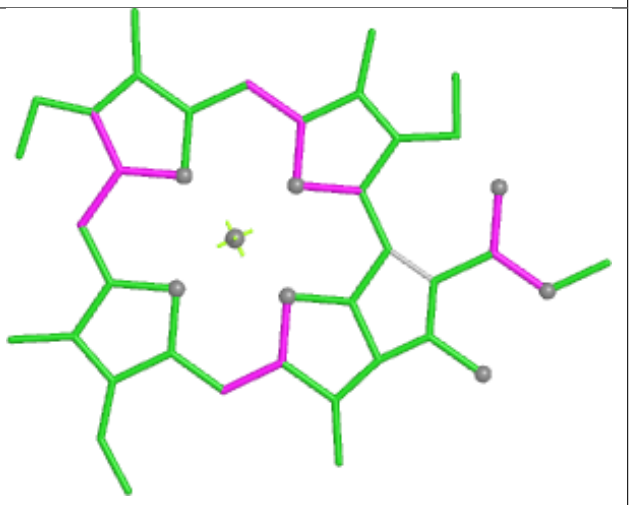


Rings

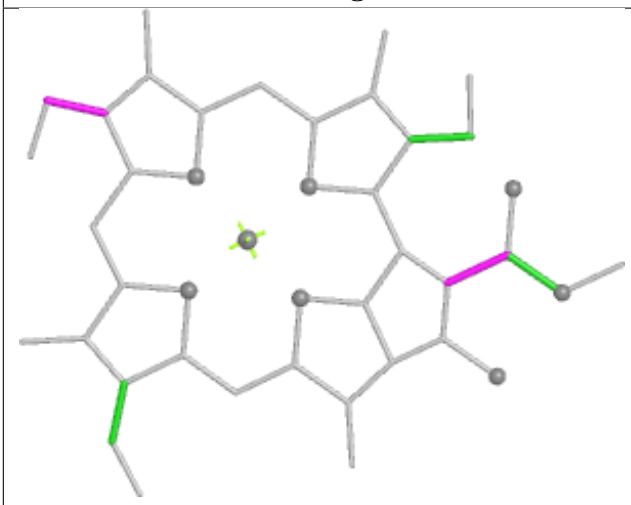
Ligand CLA 2 611



Bond lengths



Bond angles

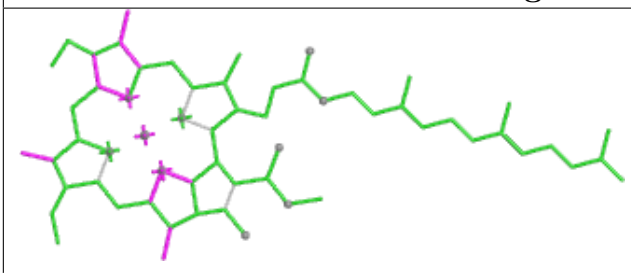


Torsions

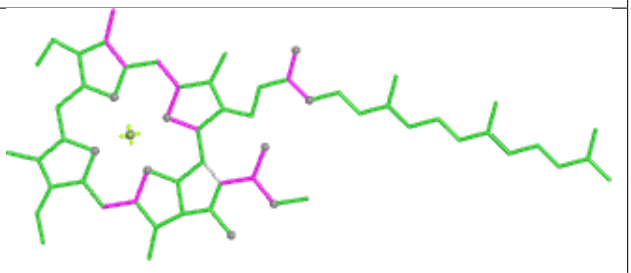


Rings

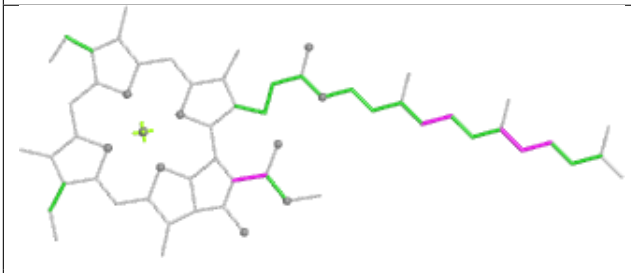
Ligand CLA B 834



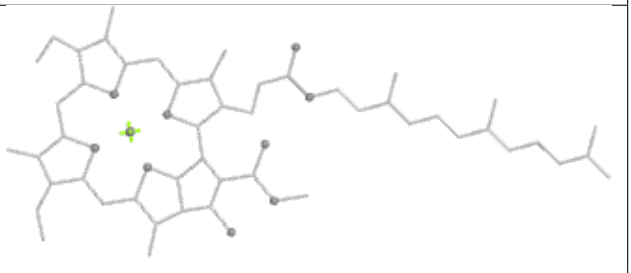
Bond lengths



Bond angles

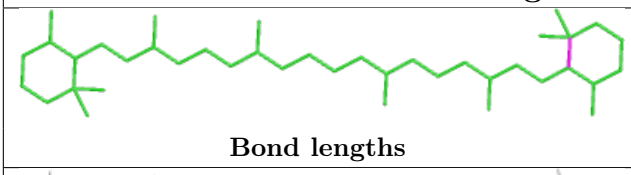


Torsions

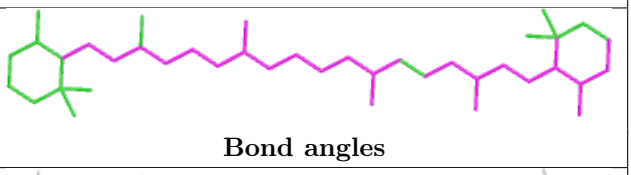


Rings

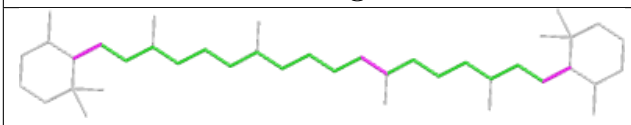
Ligand BCR F 305



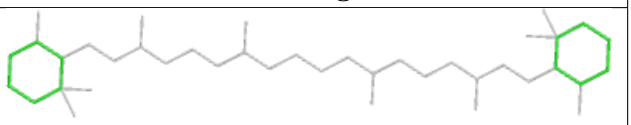
Bond lengths



Bond angles

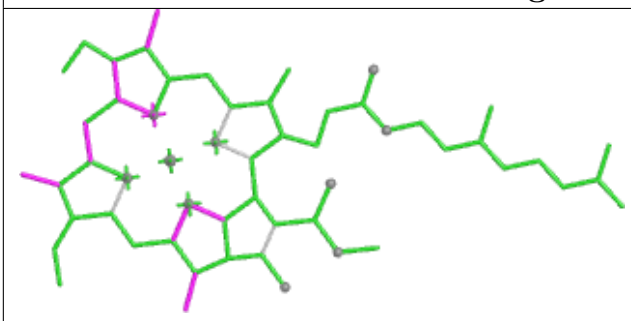


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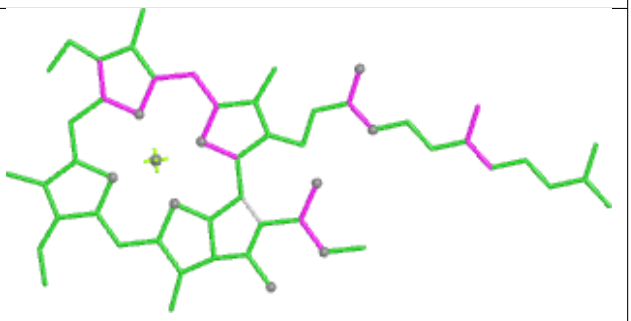


Rings

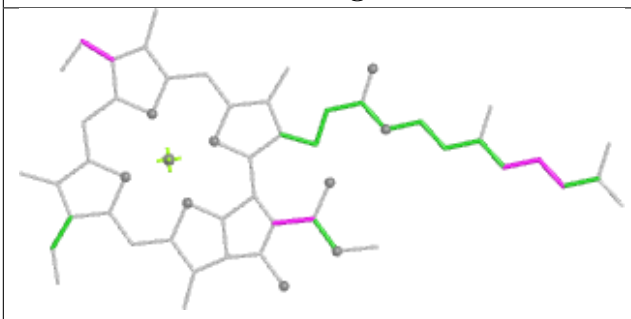
Ligand CLA 2 610



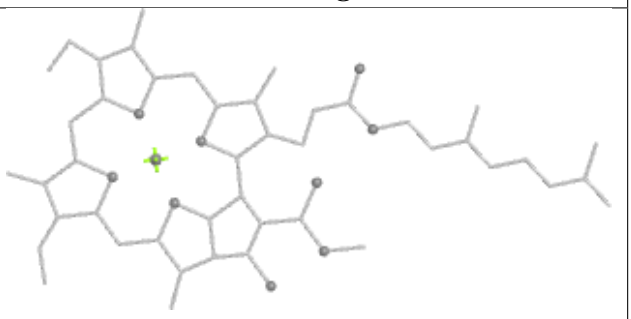
Bond lengths



Bond angles

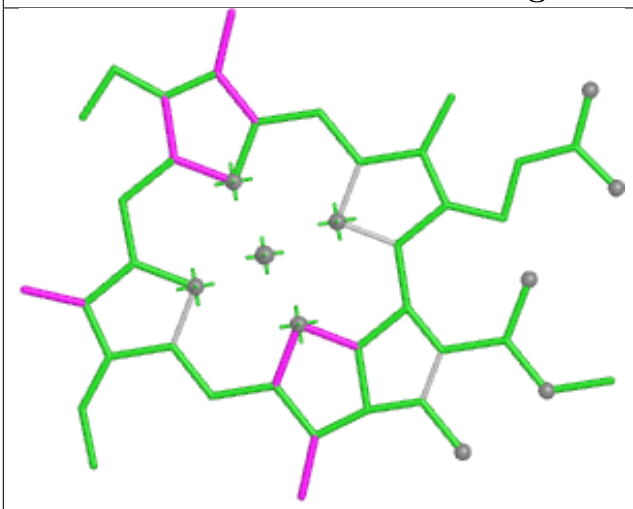


Torsions

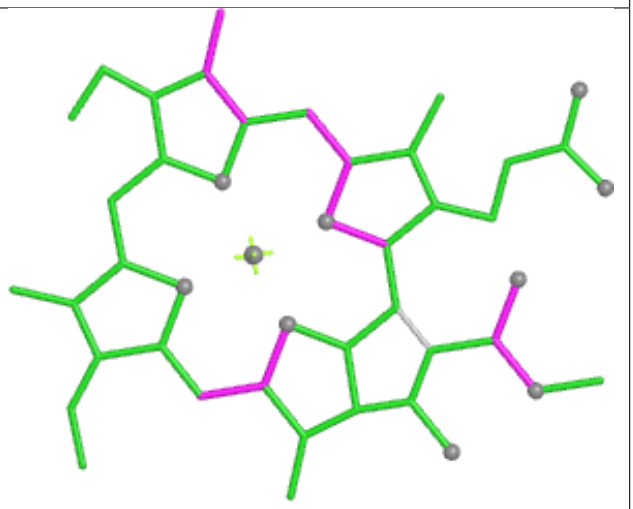


Rings

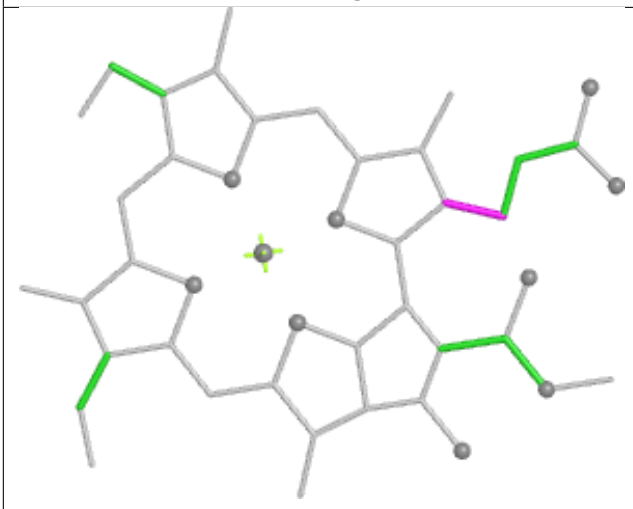
Ligand CLA 8 609



Bond lengths



Bond angles

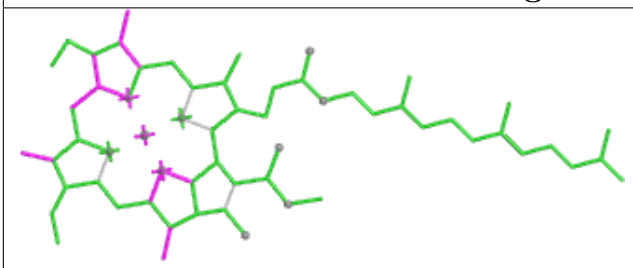


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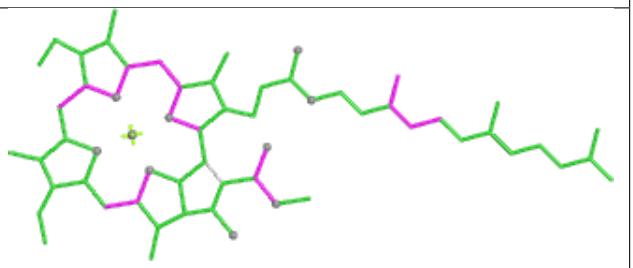


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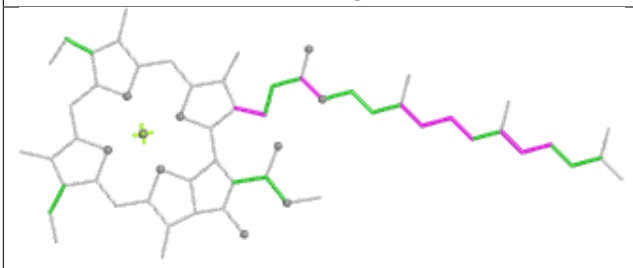
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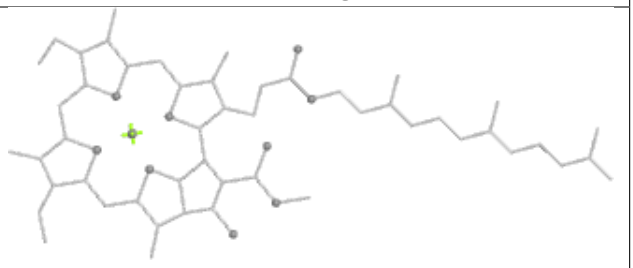
Bond lengths



Bond angles

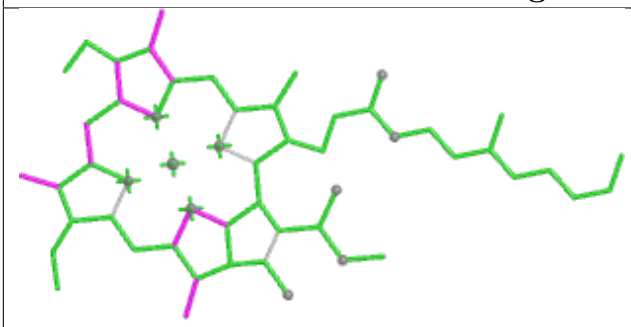


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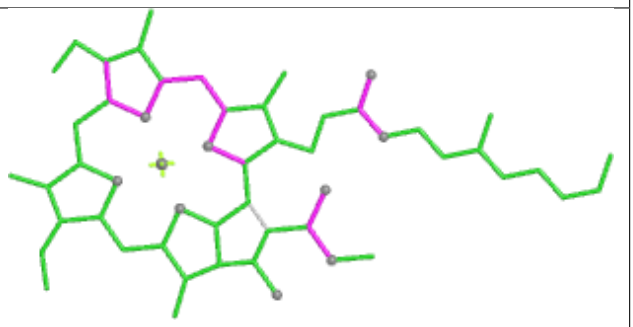


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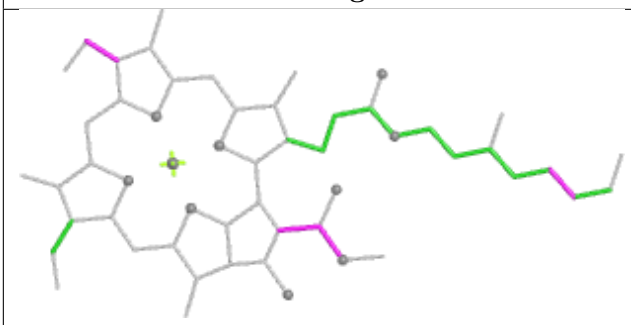
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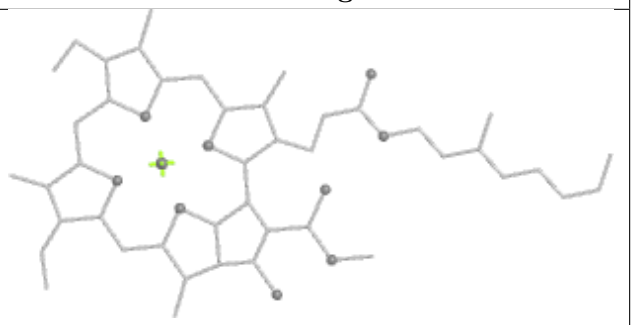
Bond lengths



Bond angles

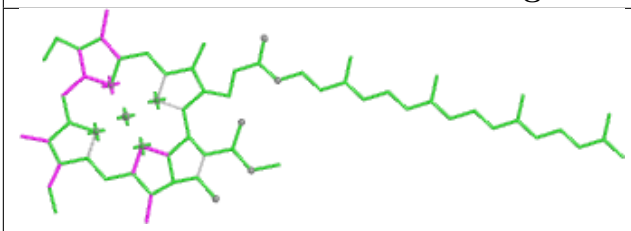


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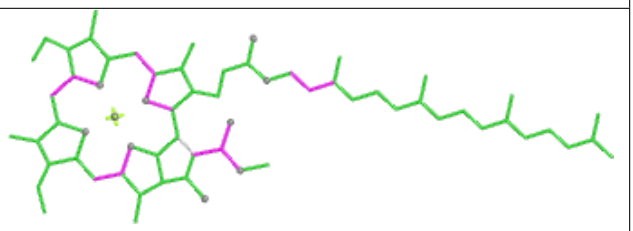


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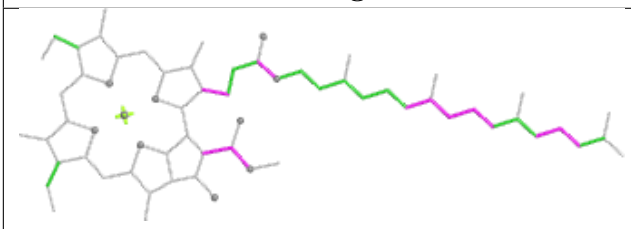
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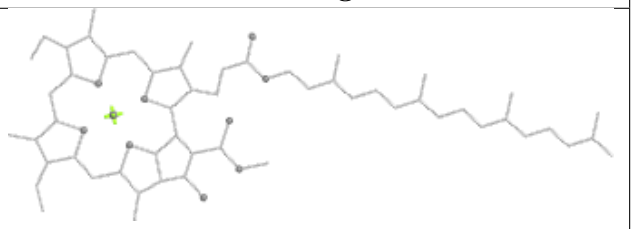
Bond lengths



Bond angles

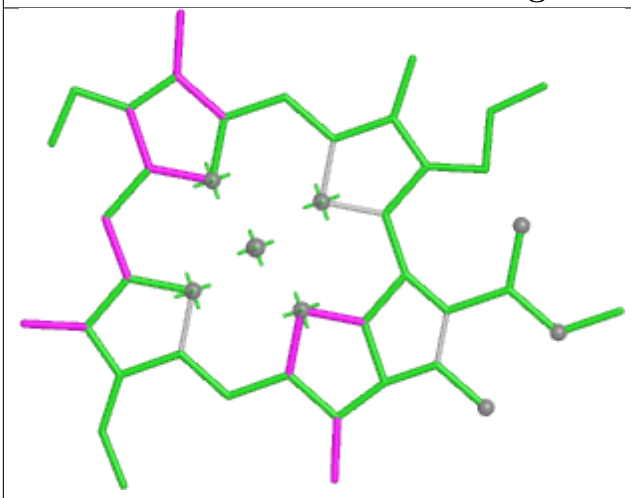


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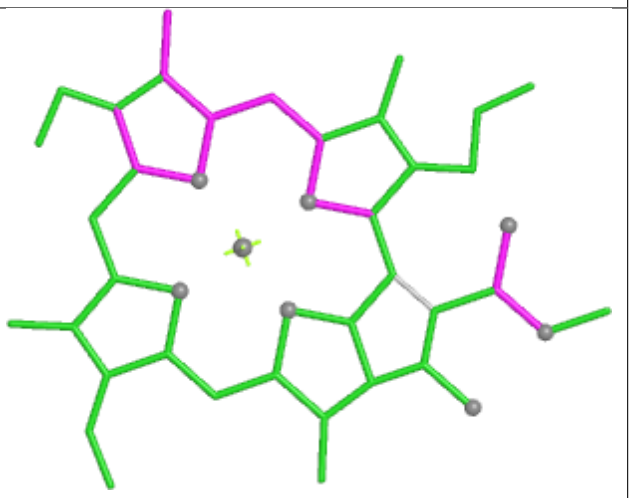


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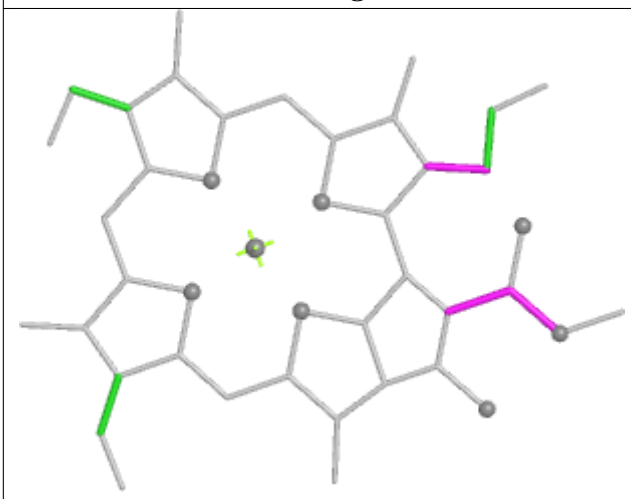
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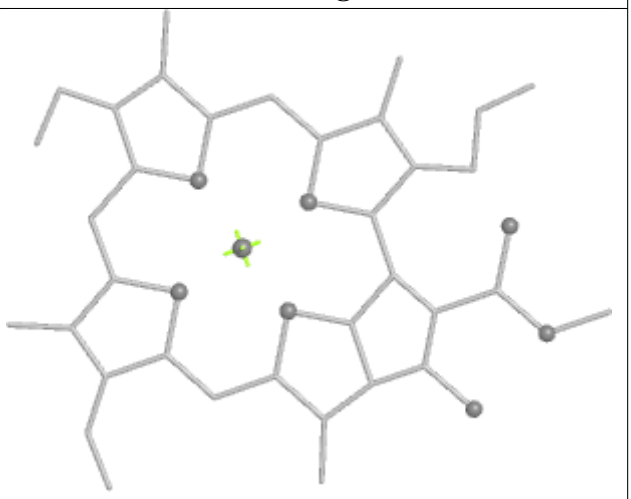
Bond lengths



Bond angles

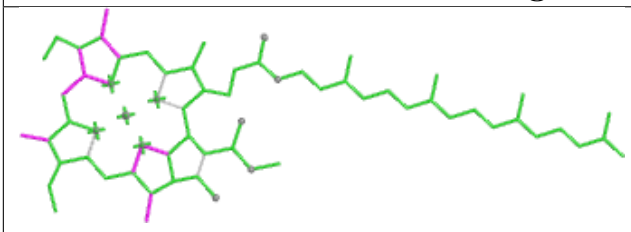


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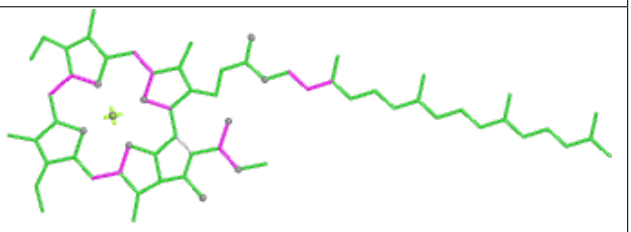


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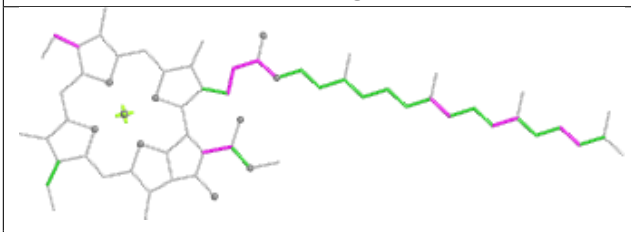
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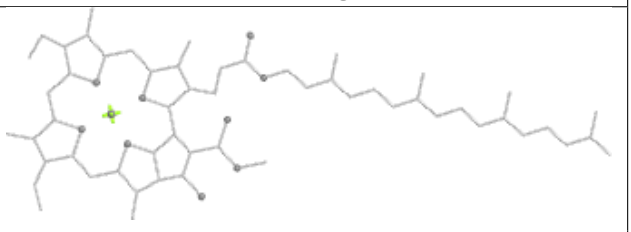
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Bond angles

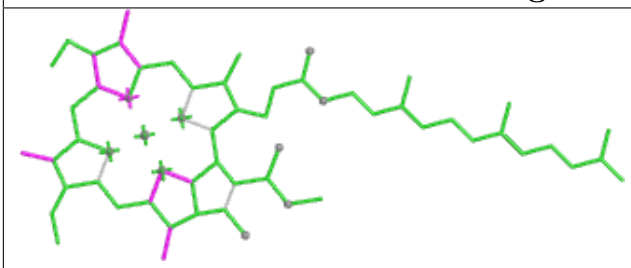


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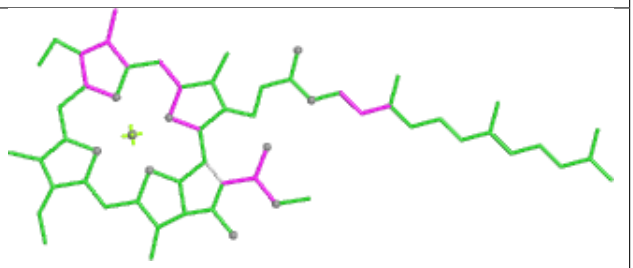


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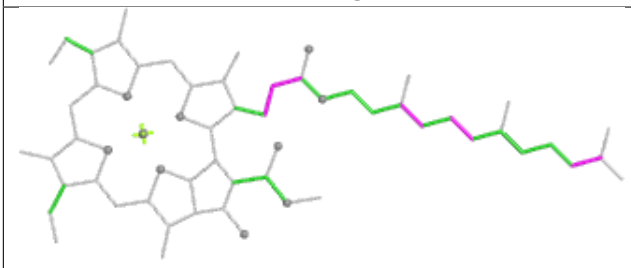
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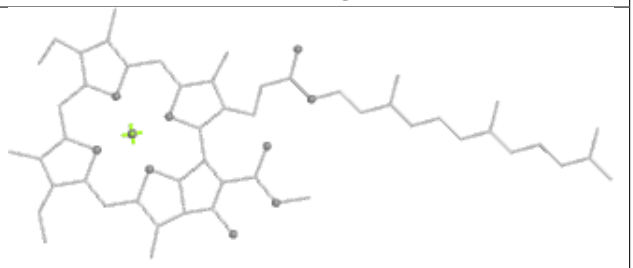
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Bond angles

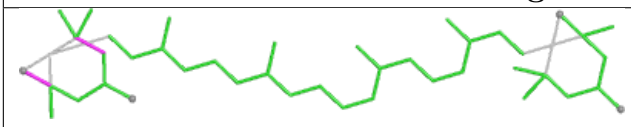


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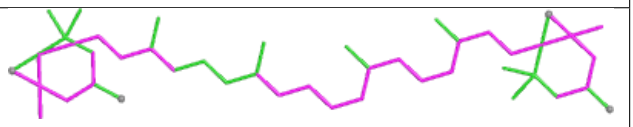


Rings

Ligand XAT 9 620



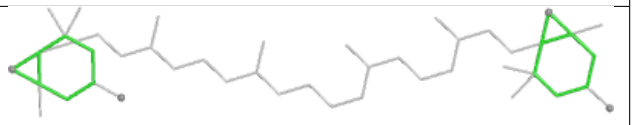
Bond lengths



Bond angles

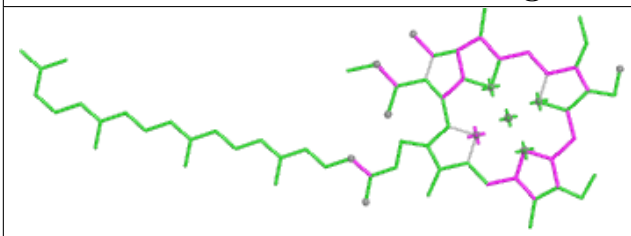


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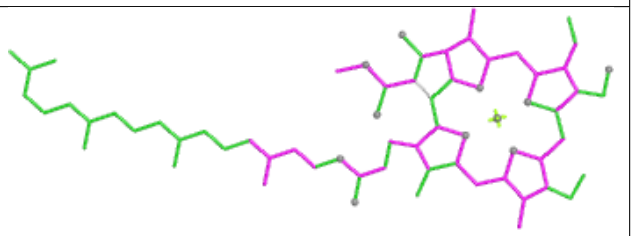


Rings

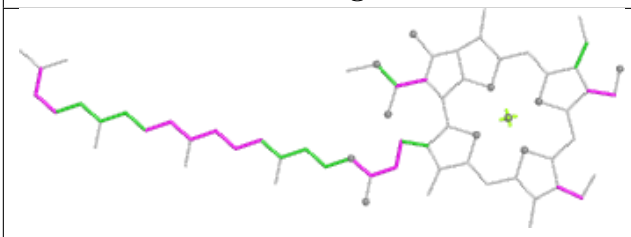
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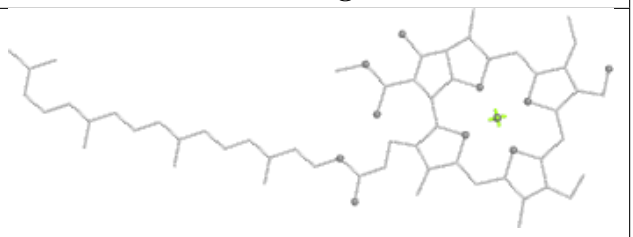
Bond lengths



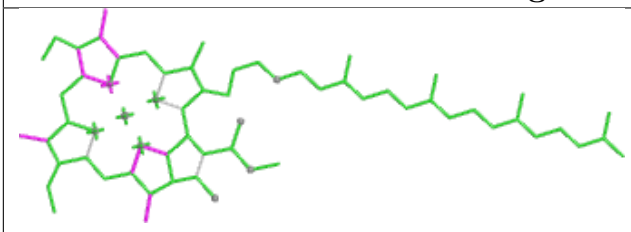
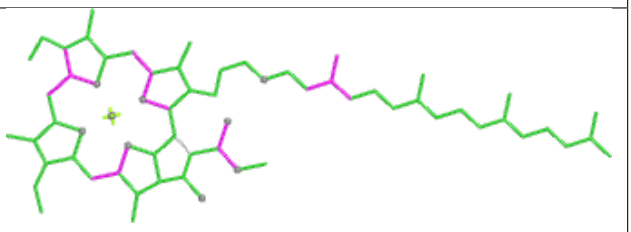
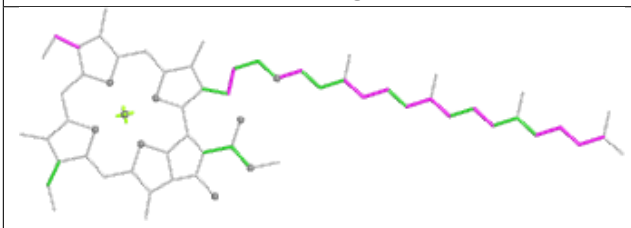
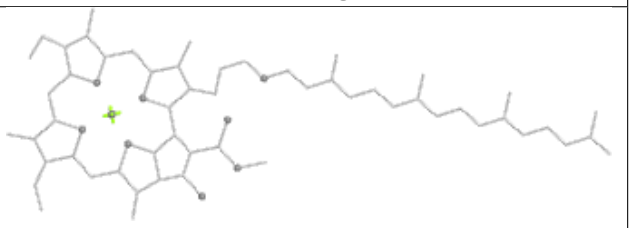
Bond angles

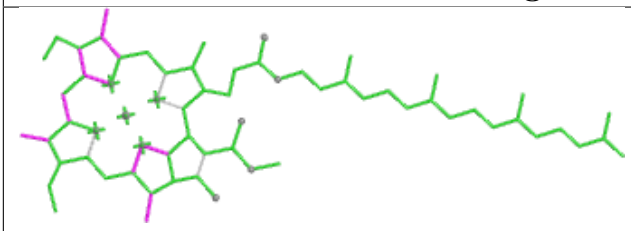
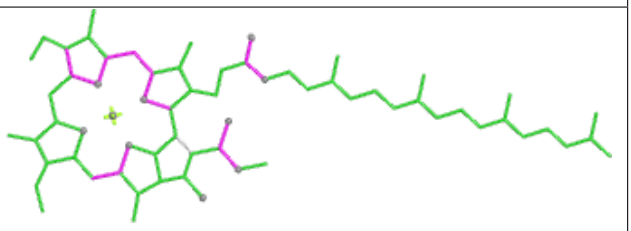
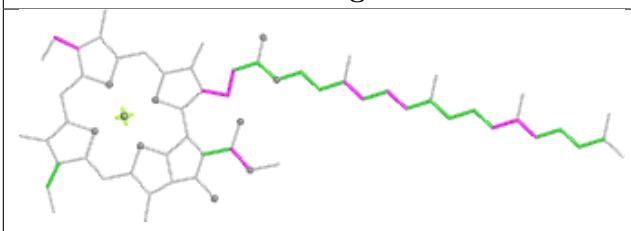
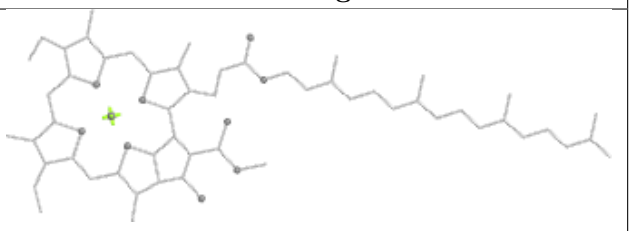


Torsions

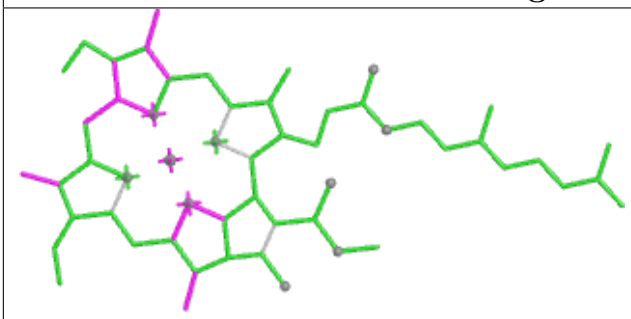


Rings

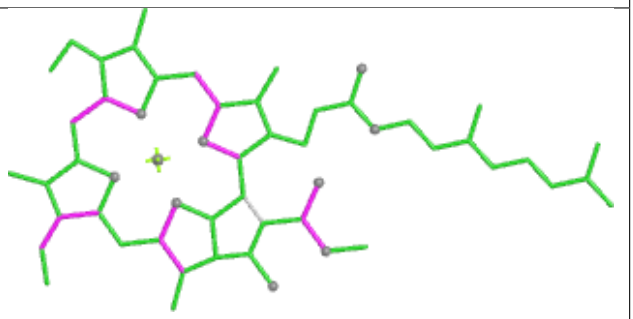
Ligand CLA 5 613	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA Y 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

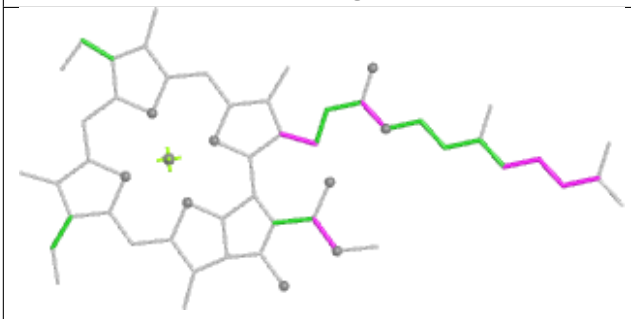
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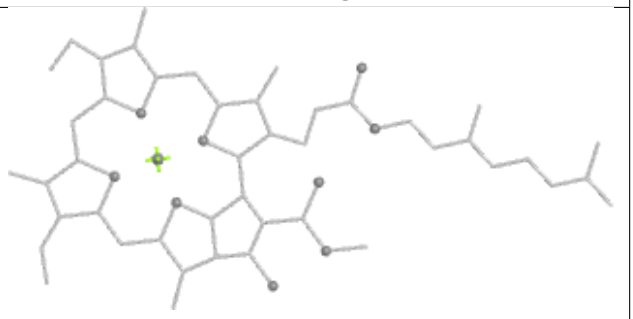
Bond lengths



Bond angles

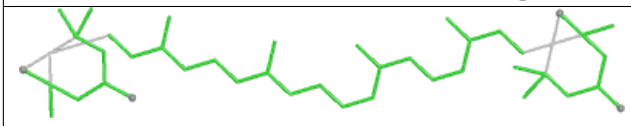


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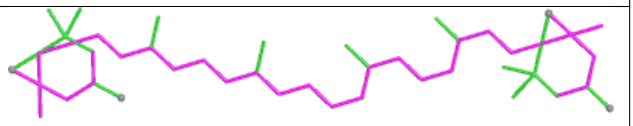


Rings

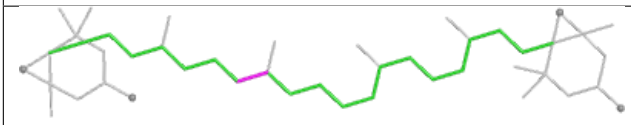
Ligand XAT V 1622



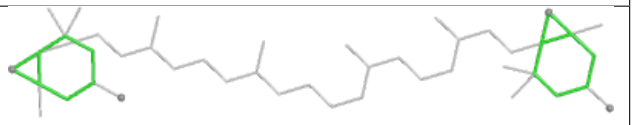
Bond lengths



Bond angles

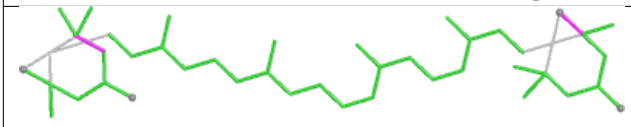


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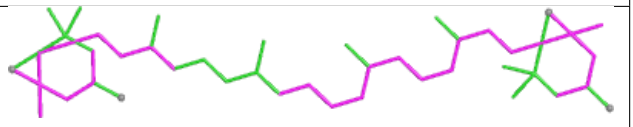


Rings

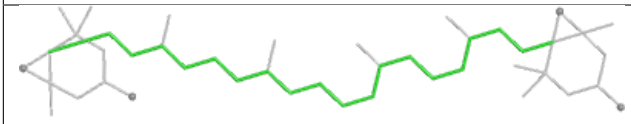
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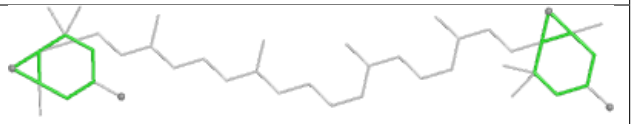
Bond lengths



Bond angles

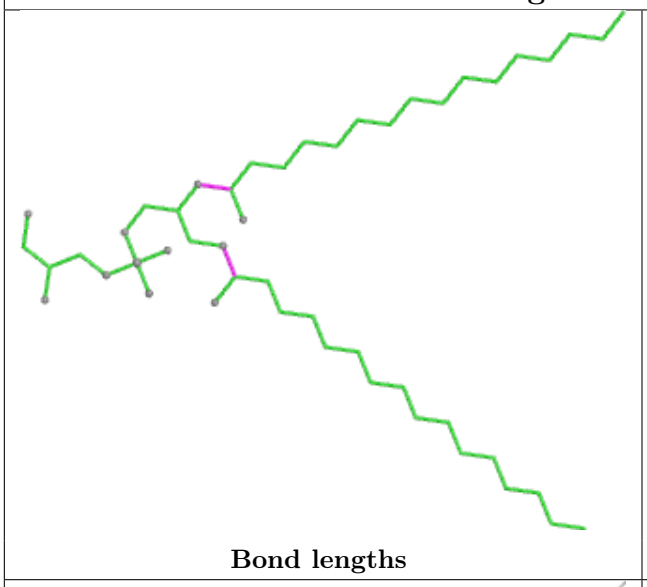


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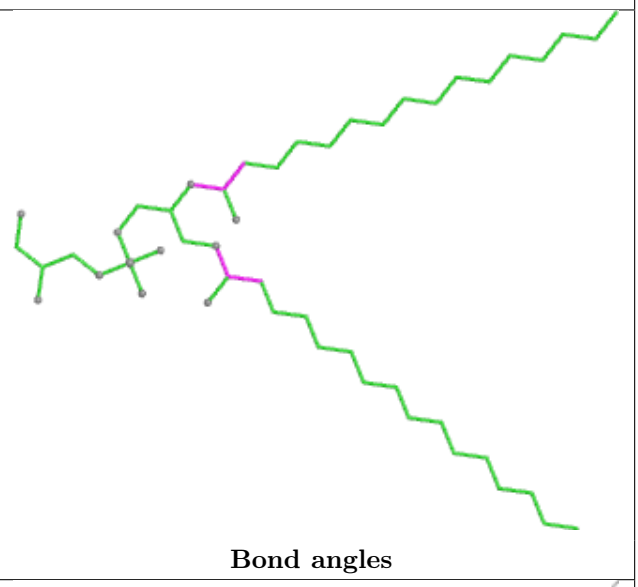


Rings

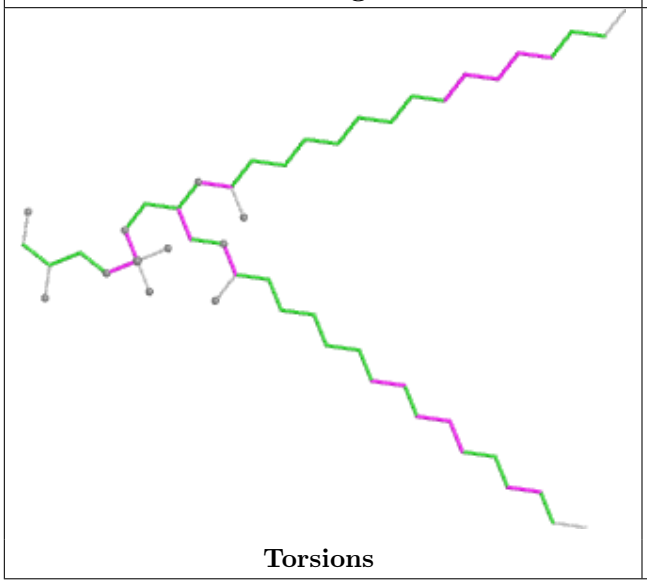
Ligand LHG 9 624



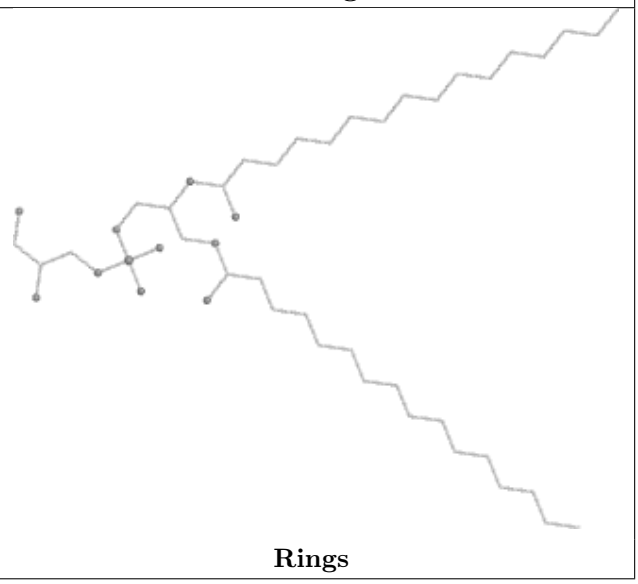
Bond lengths



Bond angles

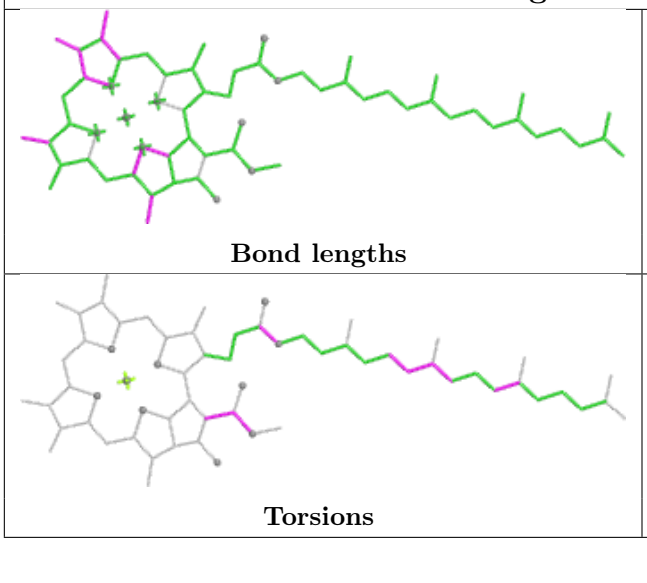


Torsions

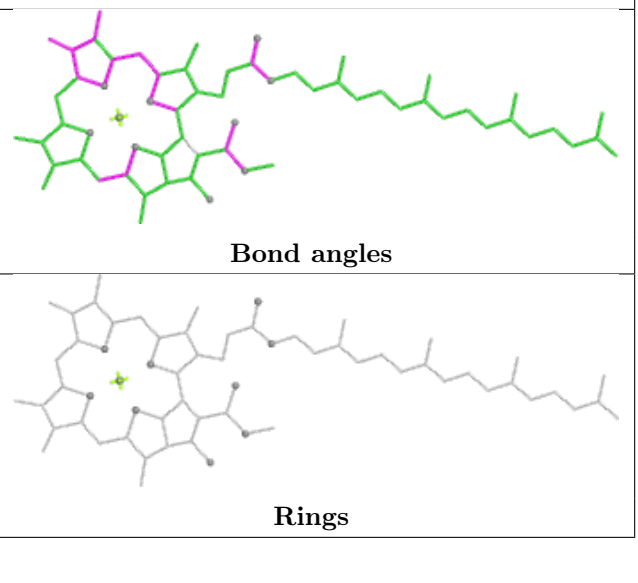


Rings

Ligand CLA 5 604



Bond lengths

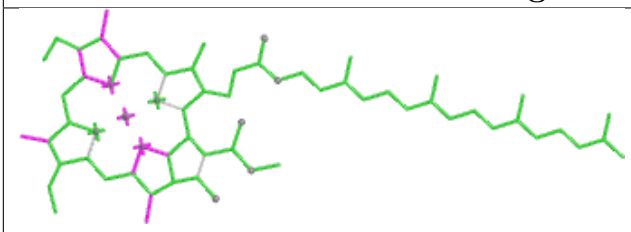


Bond angles

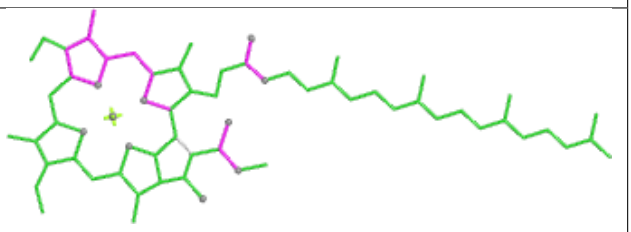
Torsions

Rings

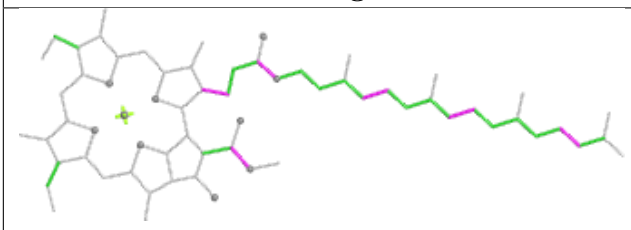
Ligand CLA 2 601



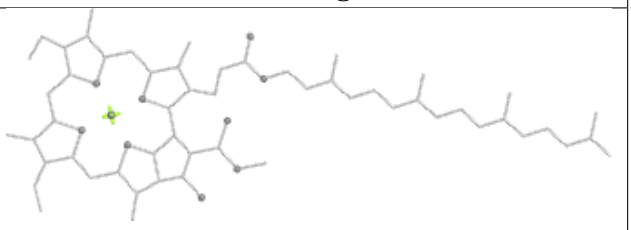
Bond lengths



Bond angles



Torsions



Rings

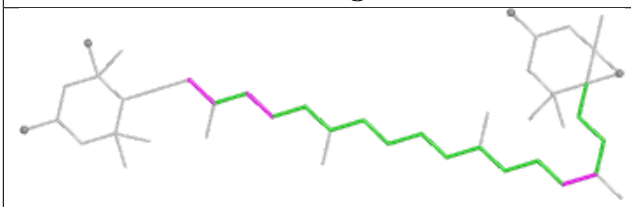
Ligand NEX X 1623



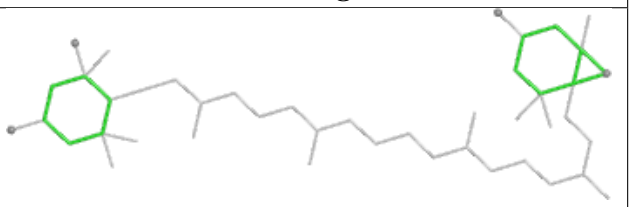
Bond lengths



Bond angles

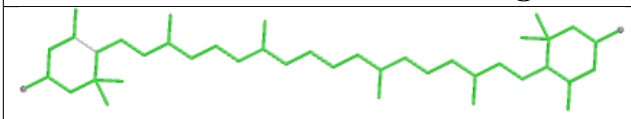


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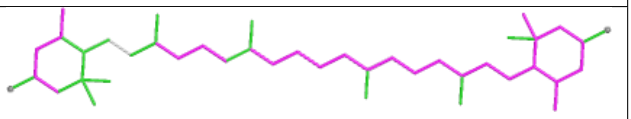


Rings

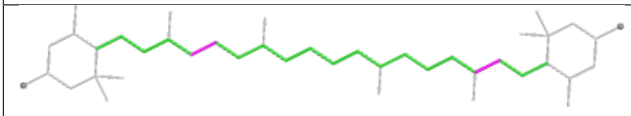
Ligand LUT V 1621



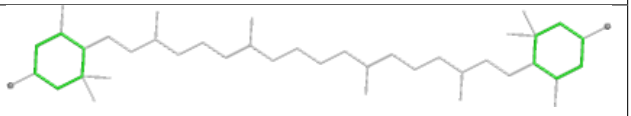
Bond lengths



Bond angles

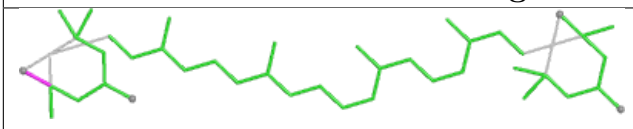


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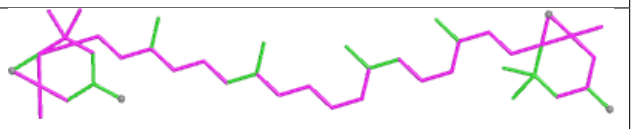


Rings

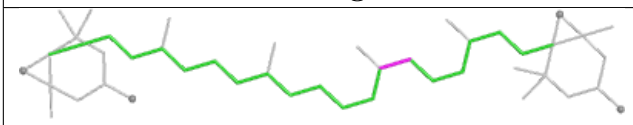
Ligand XAT W 1622



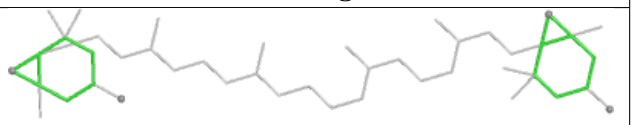
Bond lengths



Bond angles

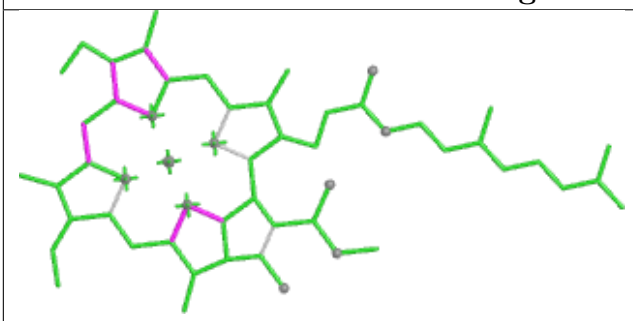


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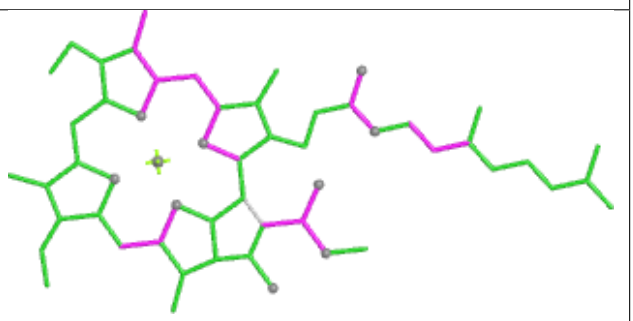


Rings

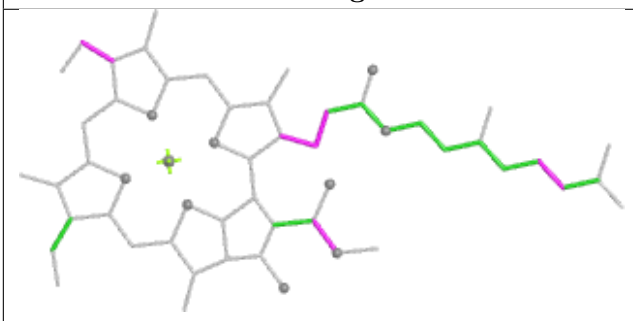
Ligand CLA W 610



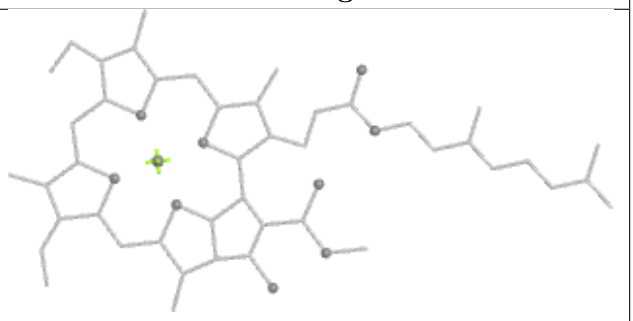
Bond lengths



Bond angles

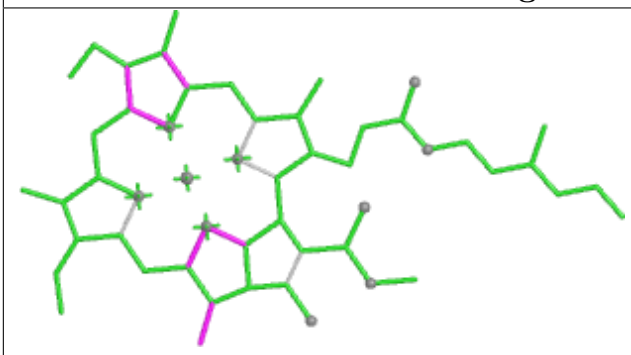


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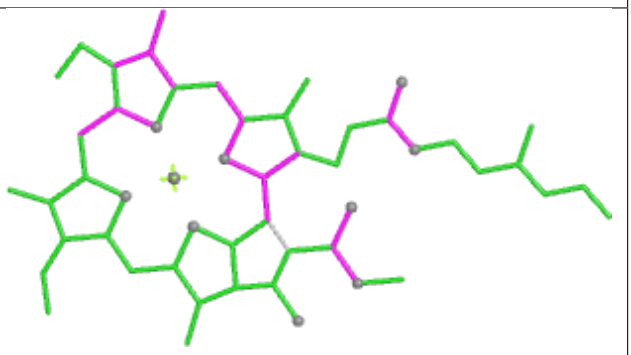


Rings

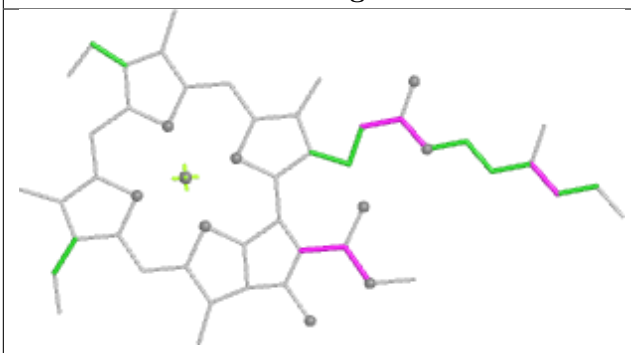
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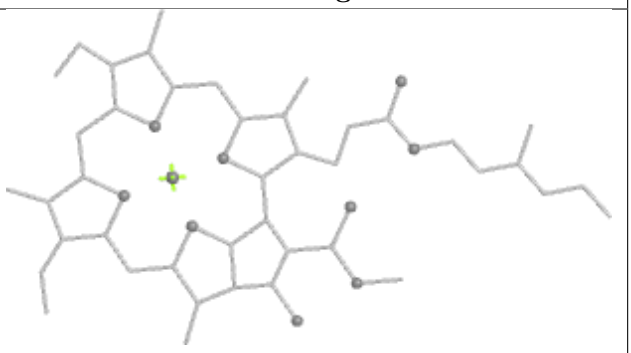
Bond lengths



Bond angles

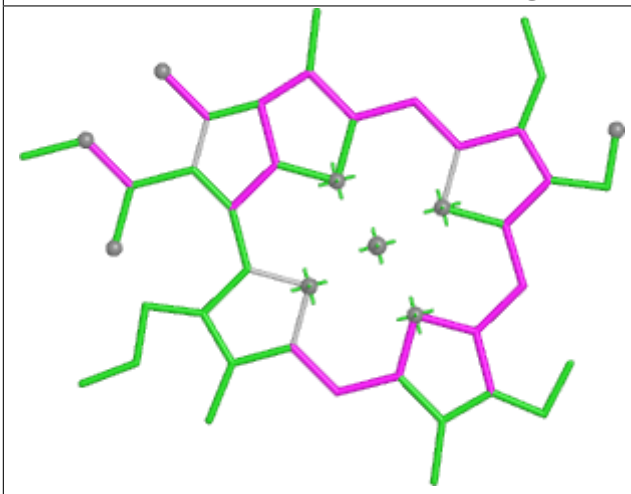


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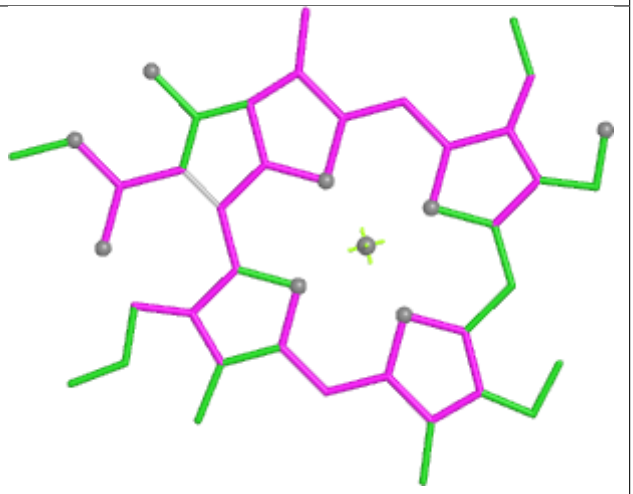


Rings

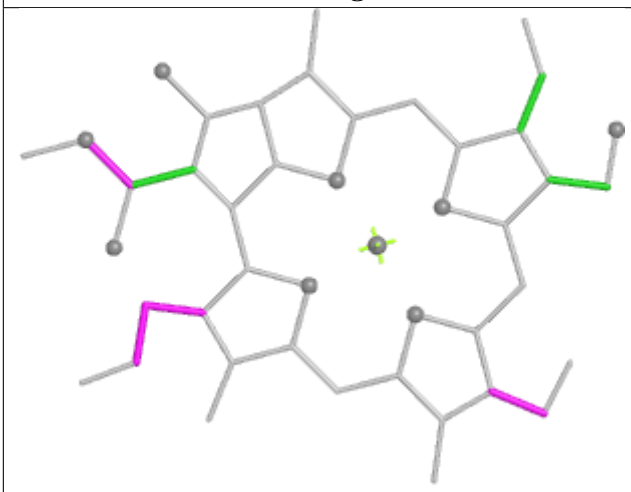
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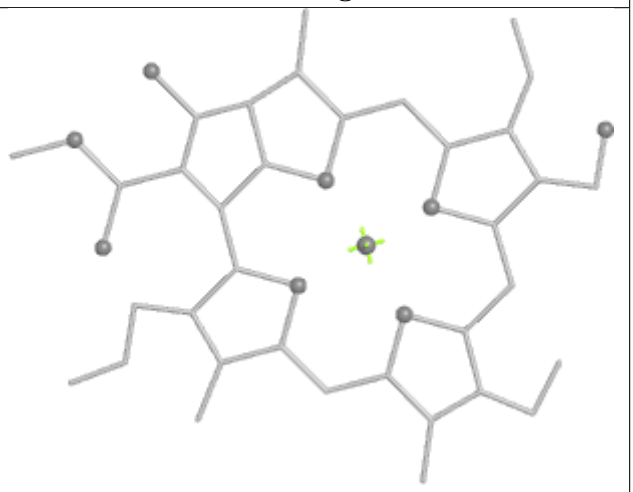
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Bond angles

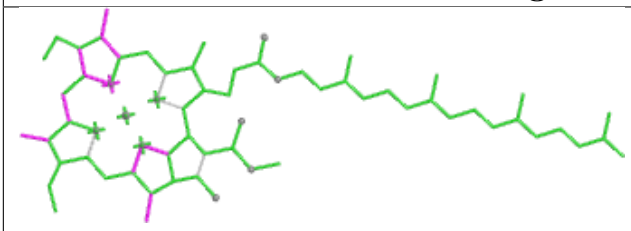


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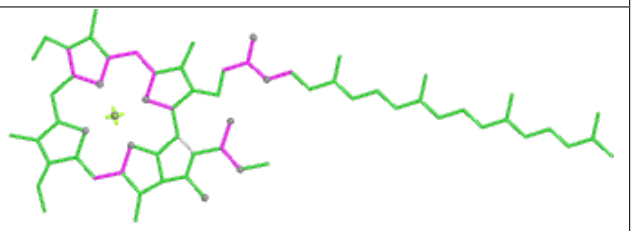


Rings

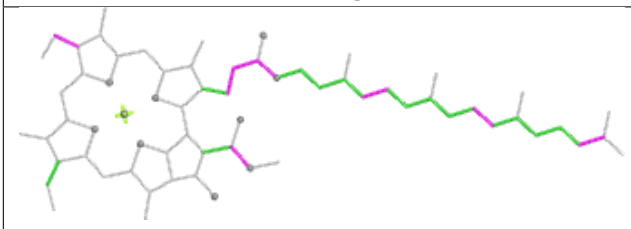
Ligand CLA 4 613



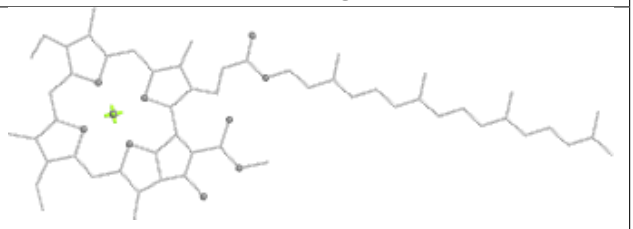
Bond lengths



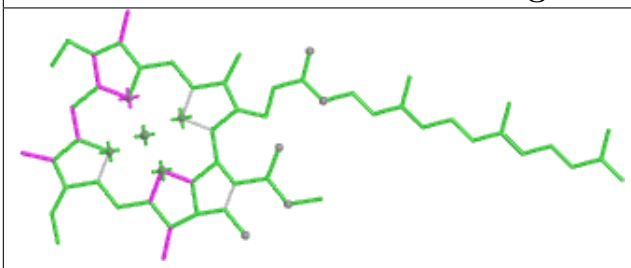
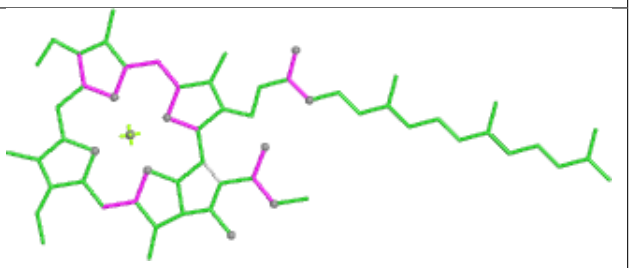
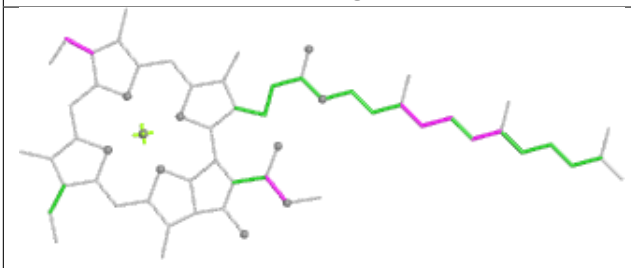
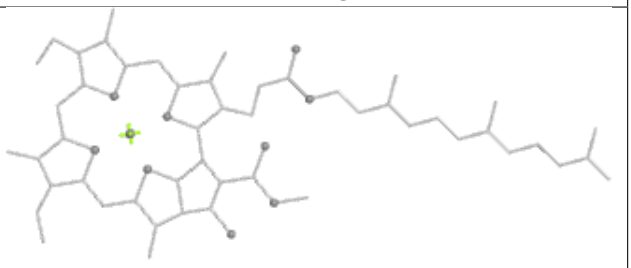
Bond angles

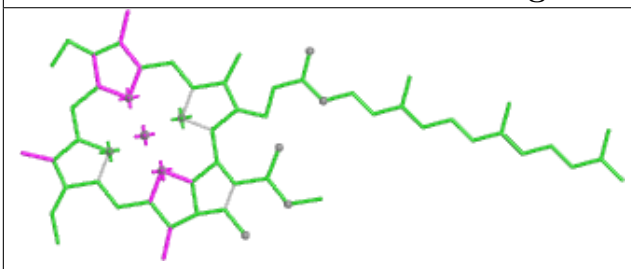
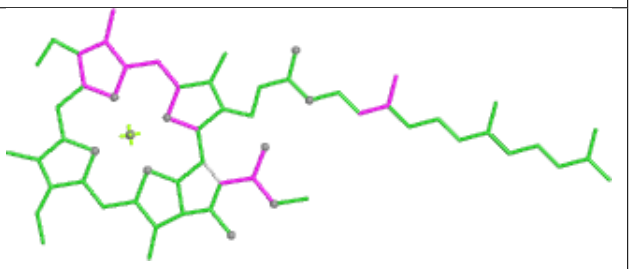
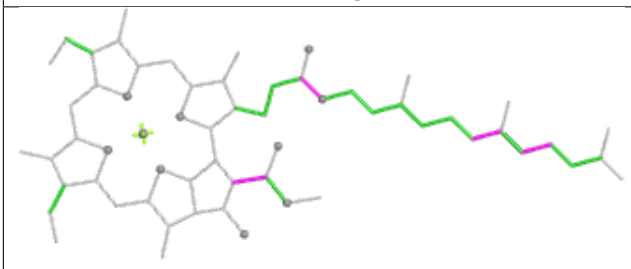
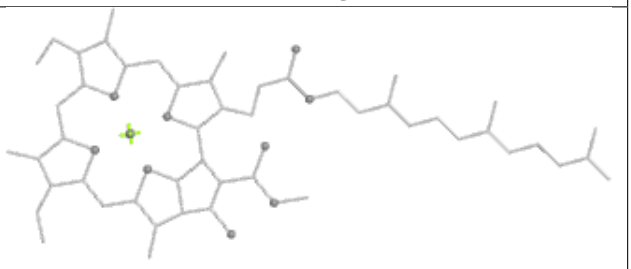


Torsions

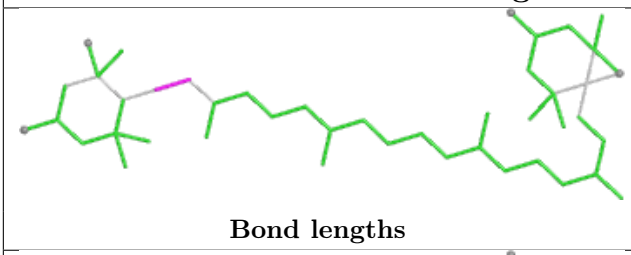


Rings

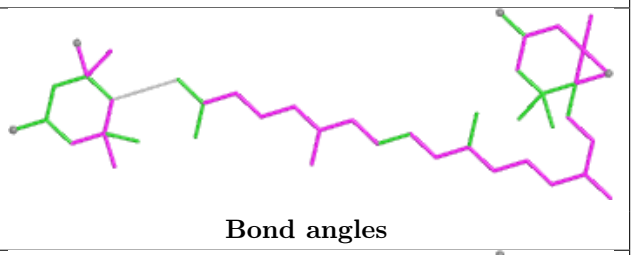
Ligand CLA 4 602	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA 7 601	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

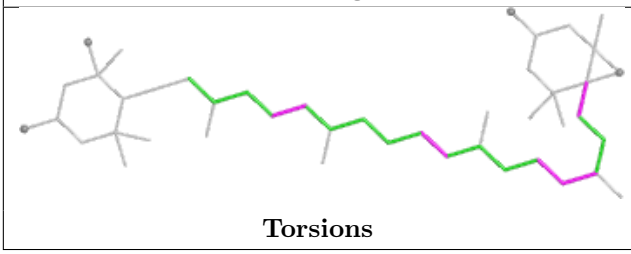
Ligand NEX U 1623



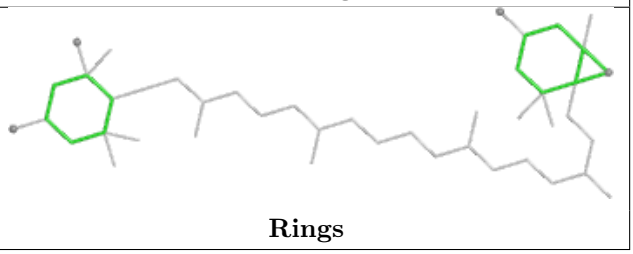
Bond lengths



Bond angles

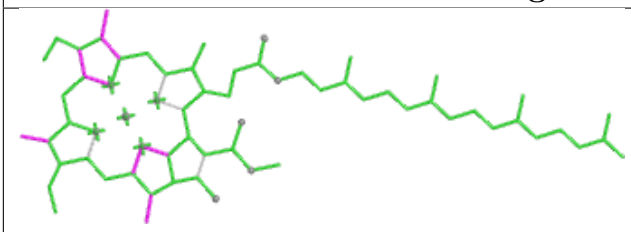


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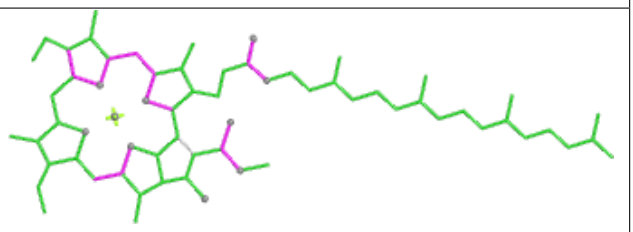


Rings

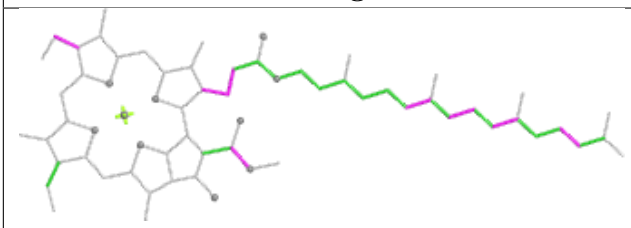
Ligand CLA 6 610



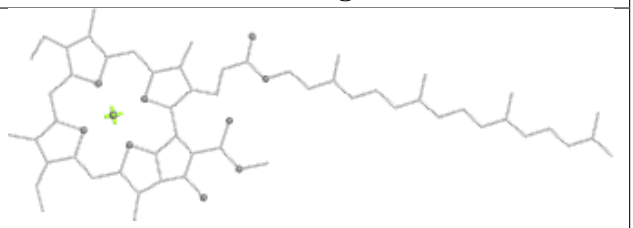
Bond lengths



Bond angles

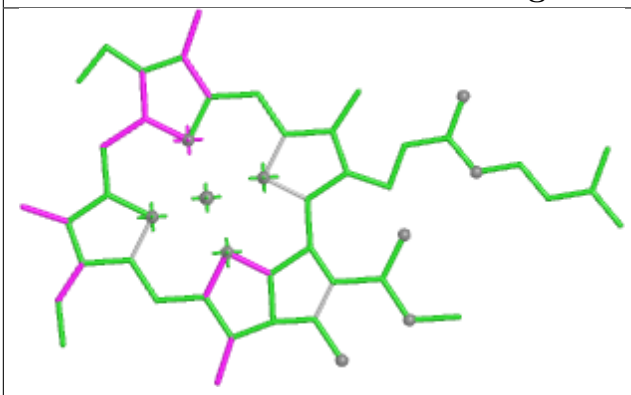


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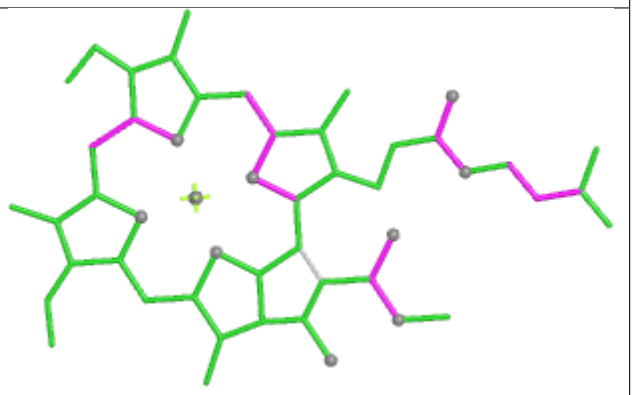


Rings

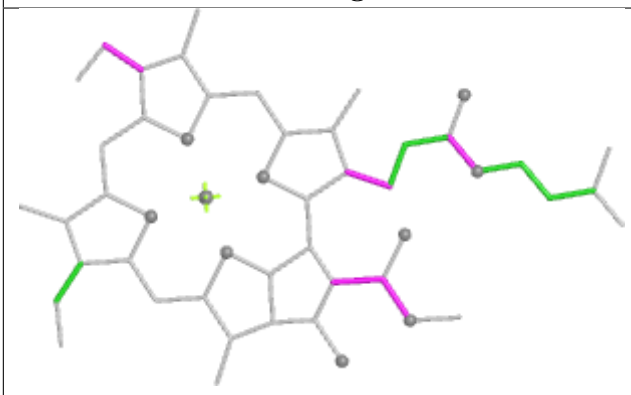
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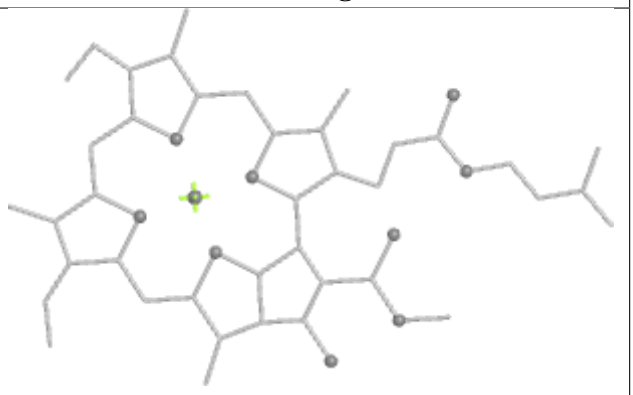
Bond lengths



Bond angles

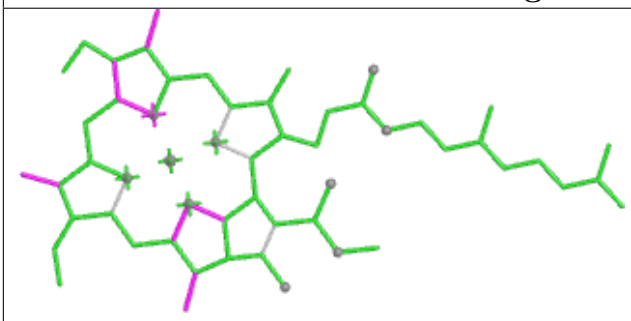


Torsions

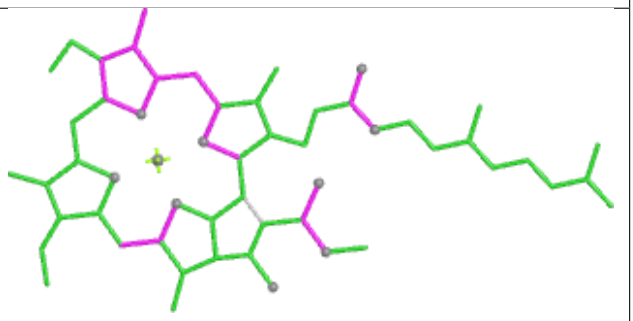


Rings

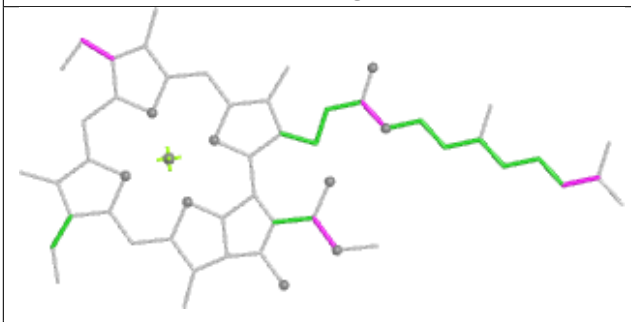
Ligand CLA B 819



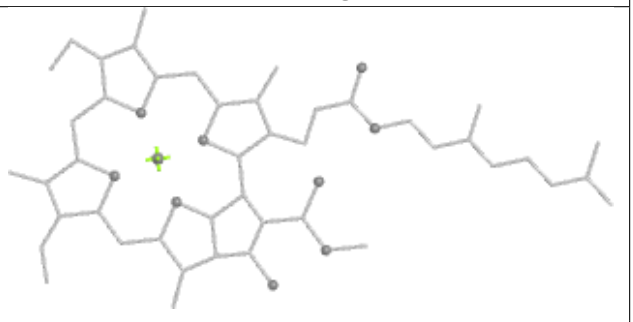
Bond lengths



Bond angles

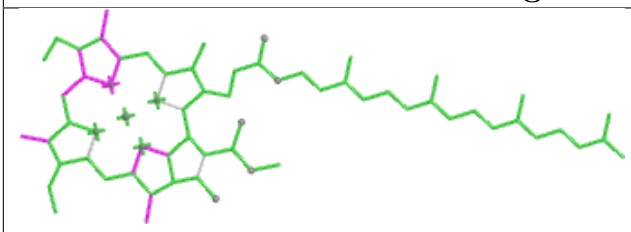


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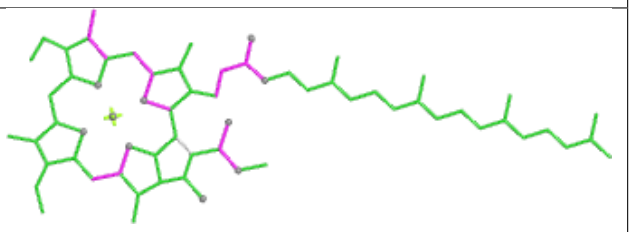


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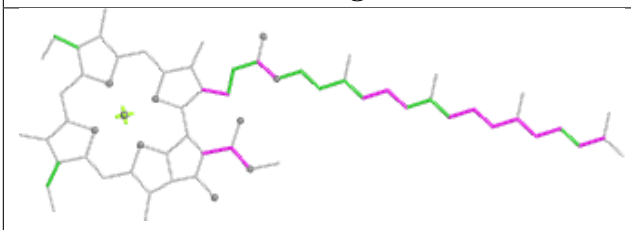
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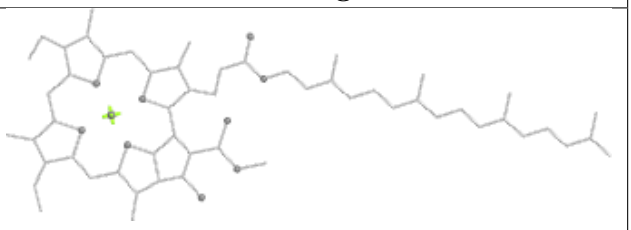
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Bond angles

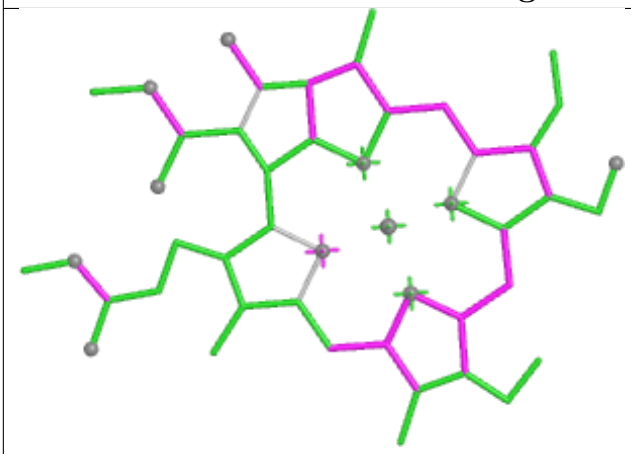


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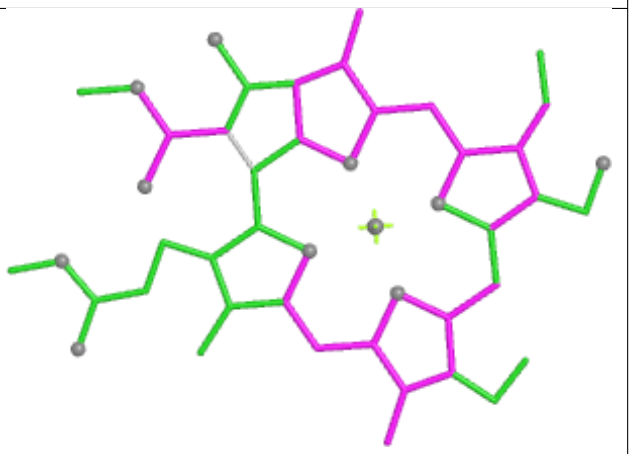


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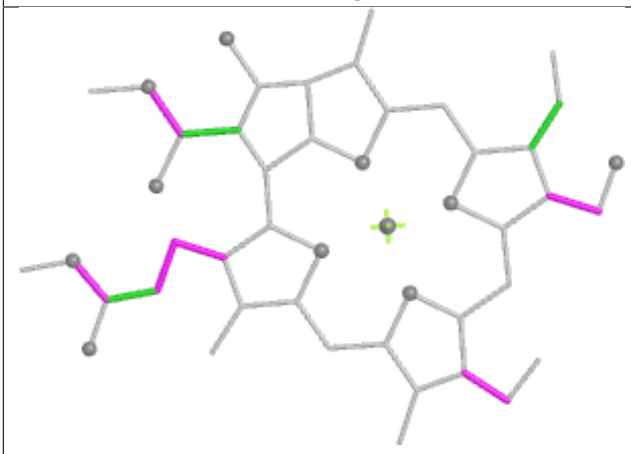
Ligand CHL W 608



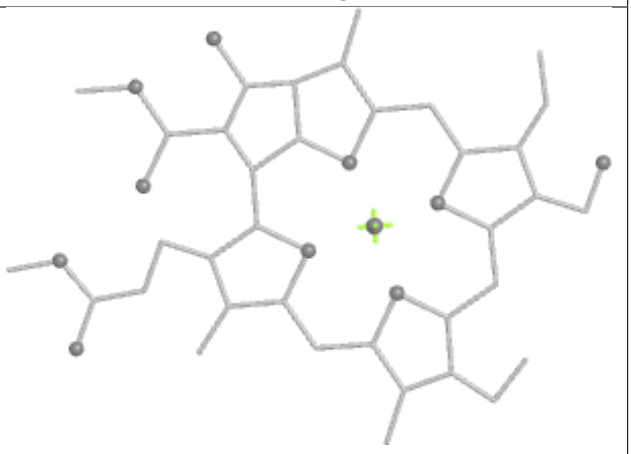
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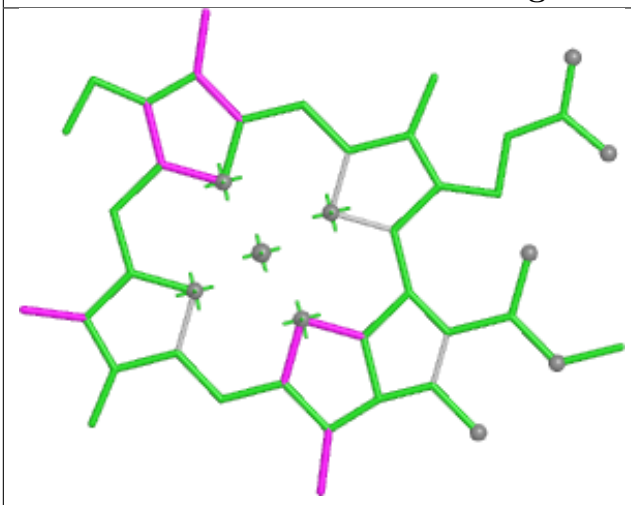


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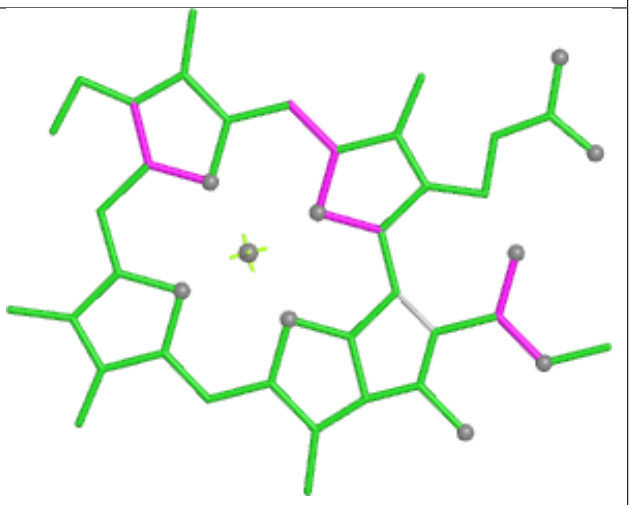


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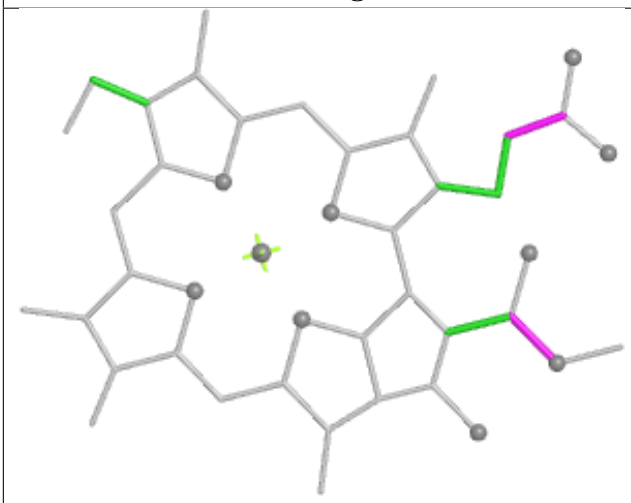
Ligand CLA 7 612



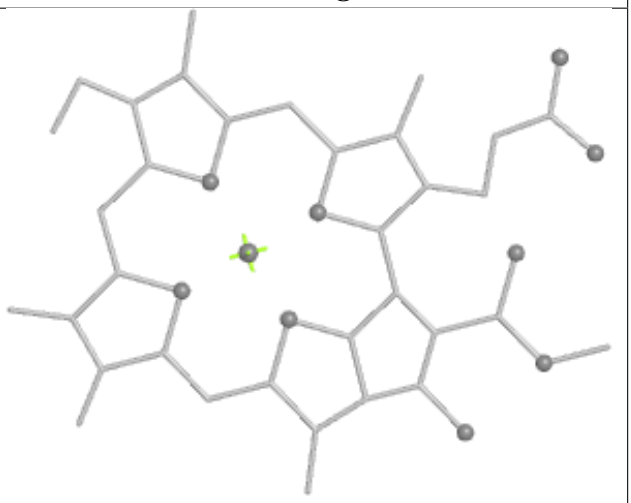
Bond lengths



Bond angles

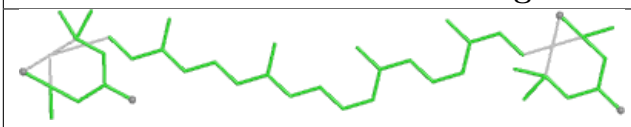


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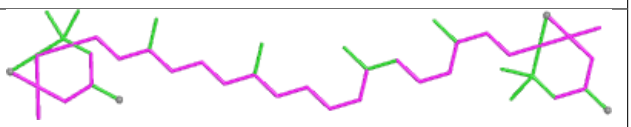


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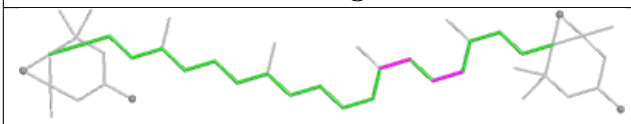
Ligand XAT X 1622



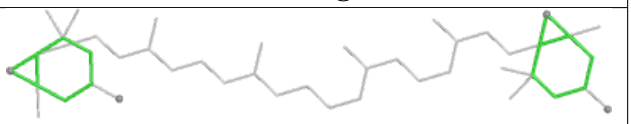
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Bond angles

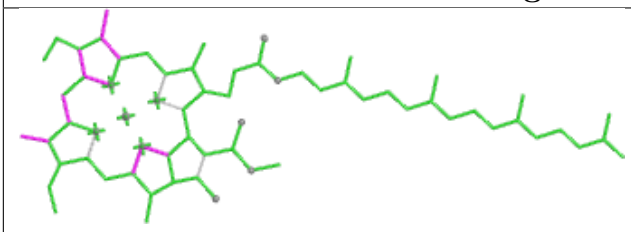


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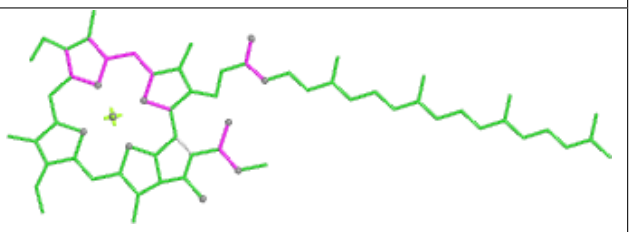


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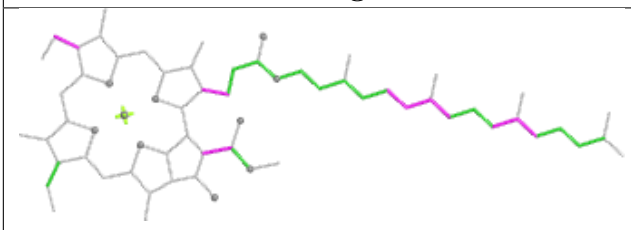
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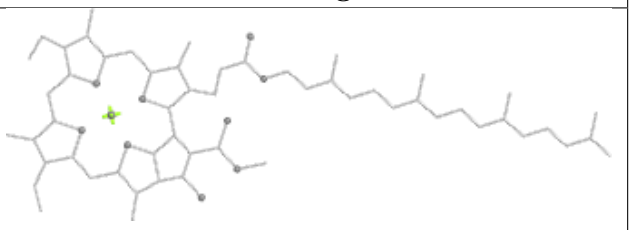
Bond lengths



Bond angles



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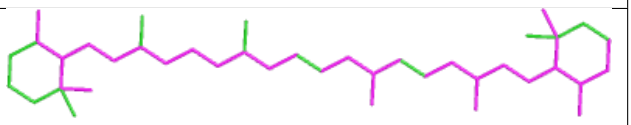


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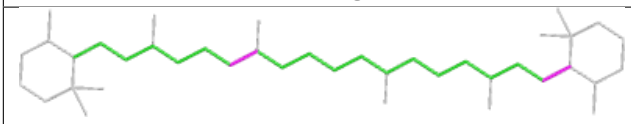
Ligand BCR 1 619



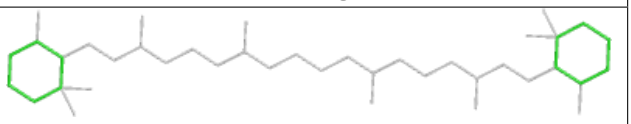
Bond lengths



Bond angles

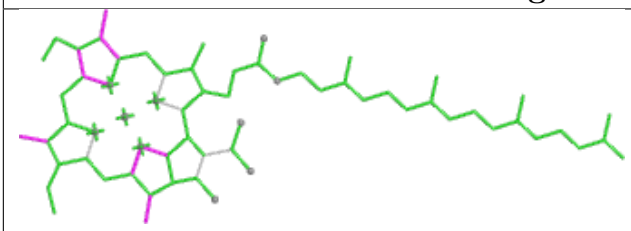


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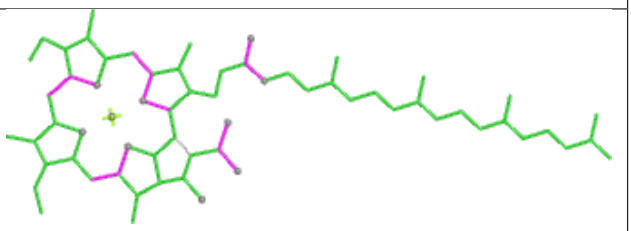


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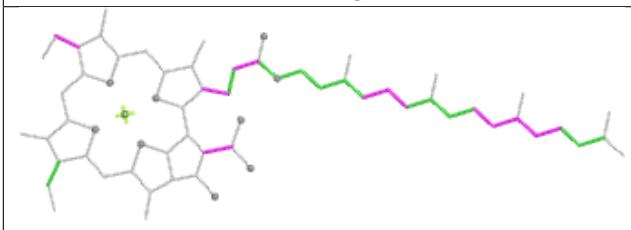
Ligand CLA a 609



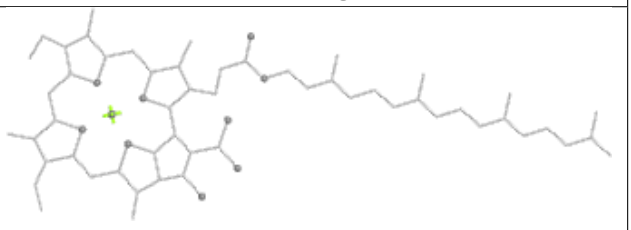
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Bond angles

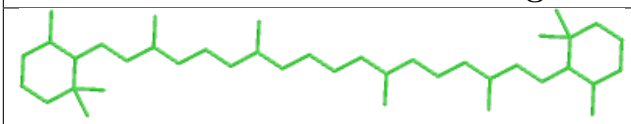


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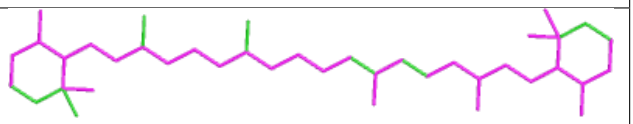


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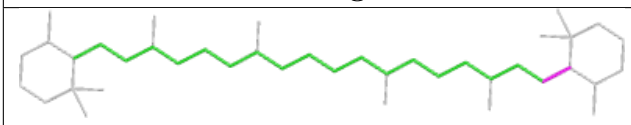
Ligand BCR 8 621



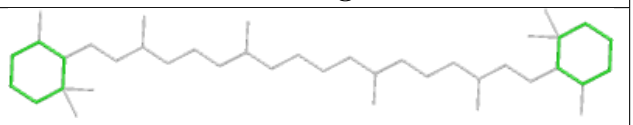
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Bond angles

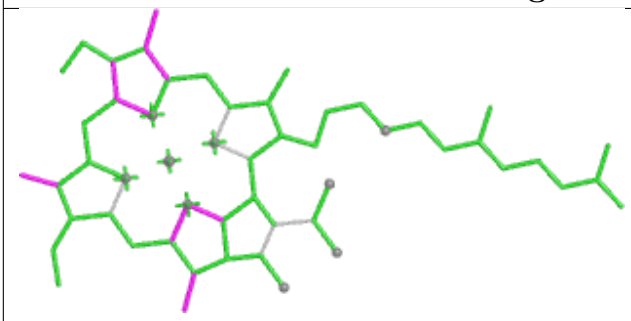


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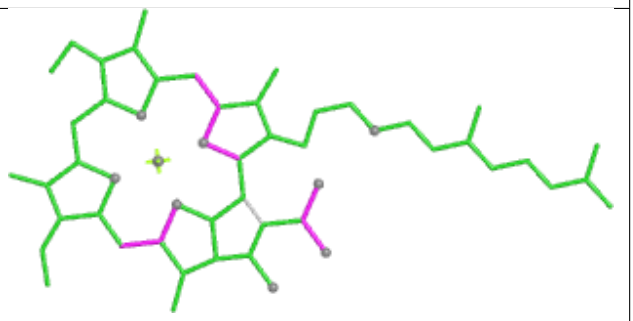


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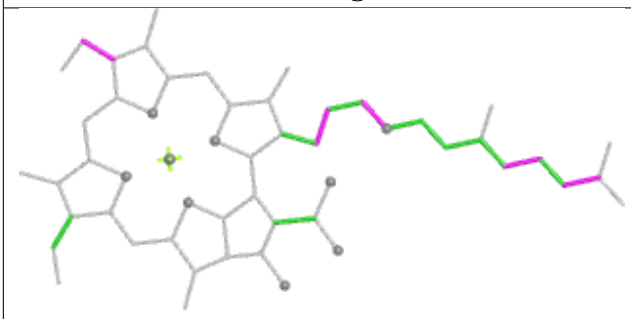
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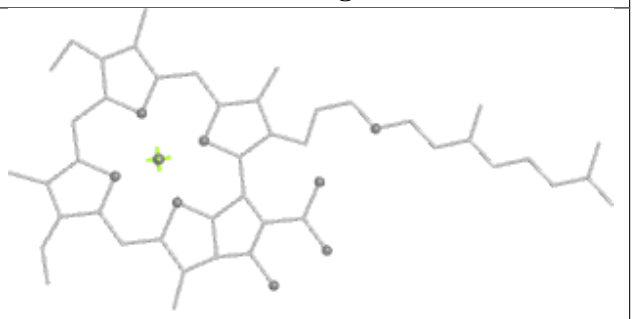
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Bond angles

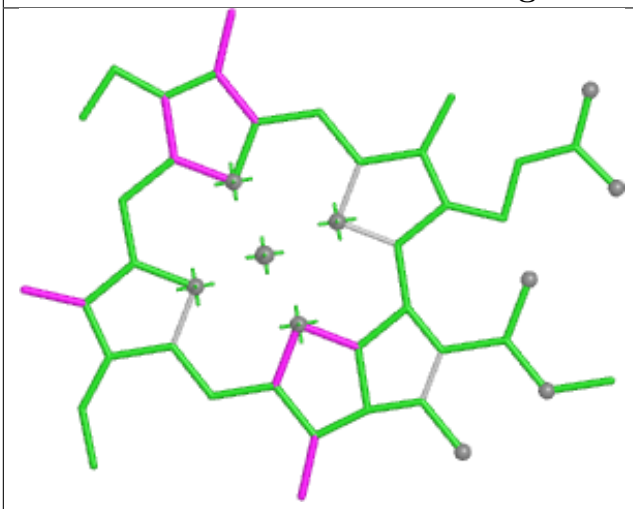


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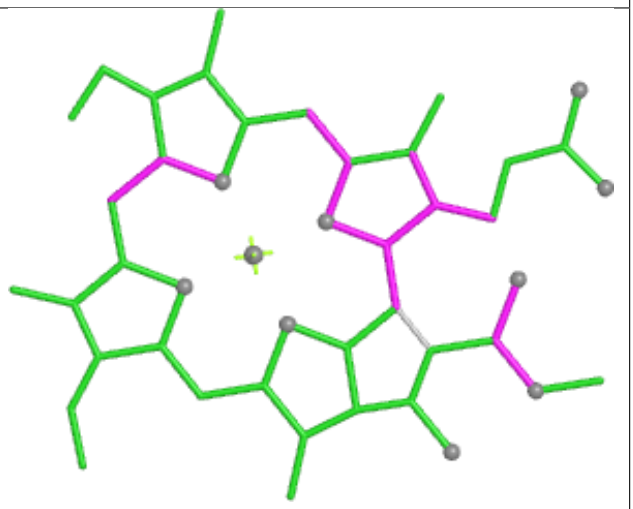


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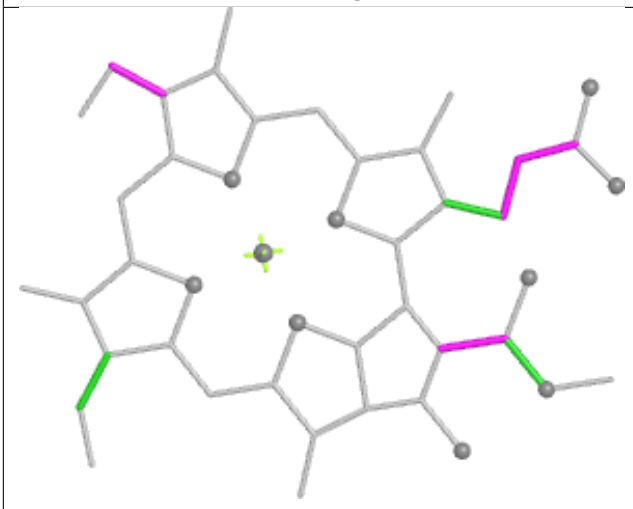
Ligand CLA W 612



Bond lengths



Bond angles

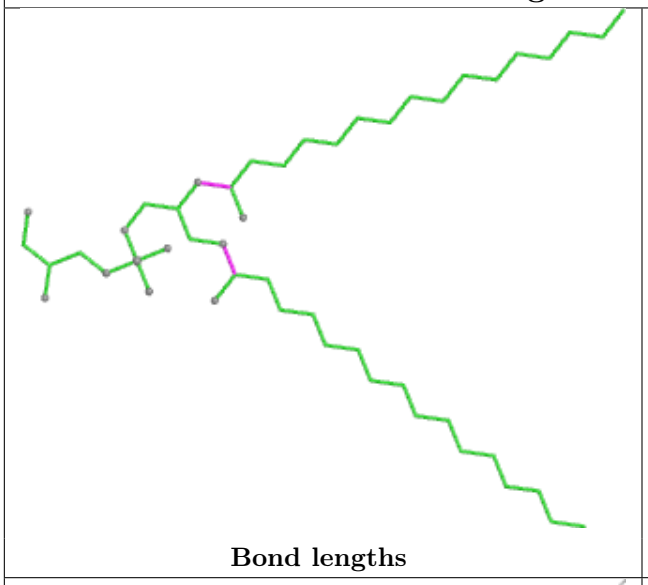


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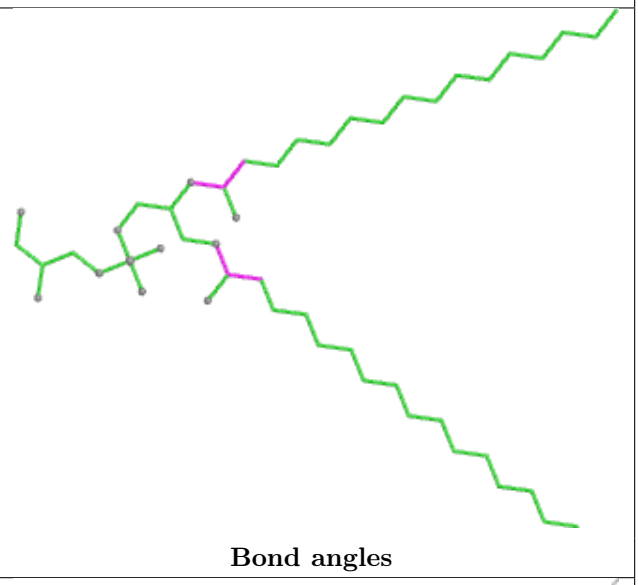


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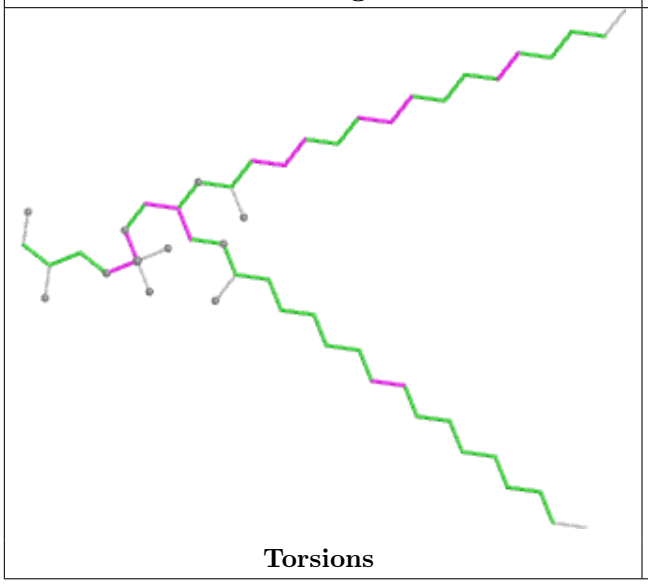
Ligand LHG 5 623



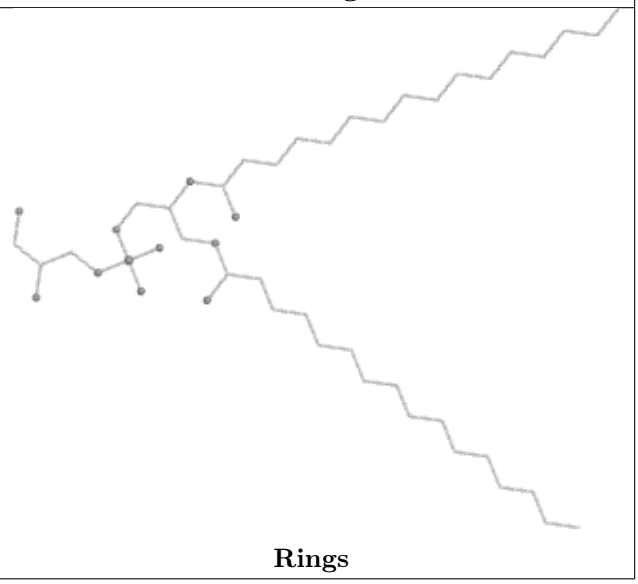
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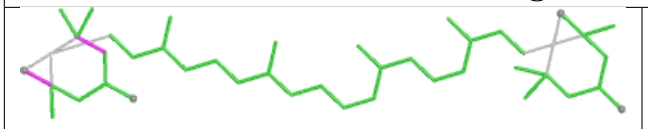


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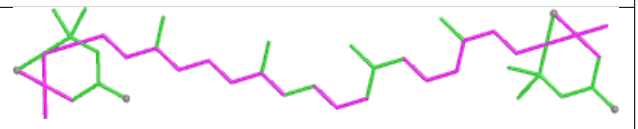


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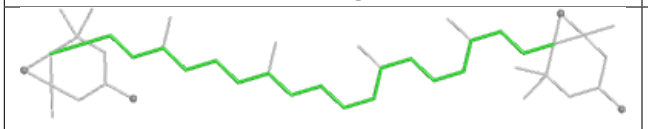
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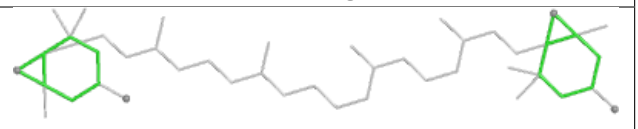
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Bond angles

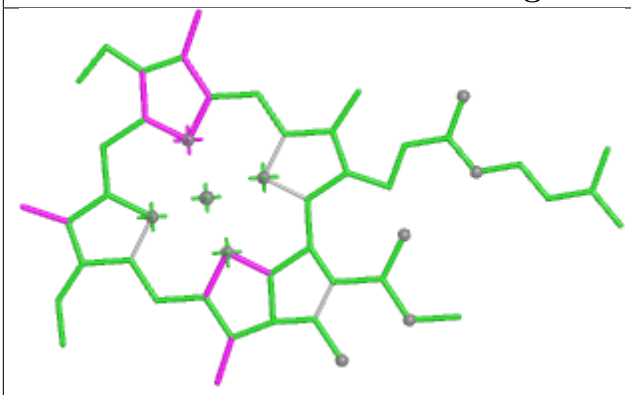


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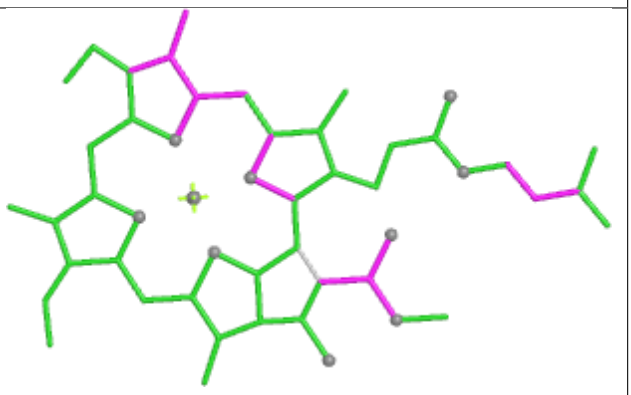


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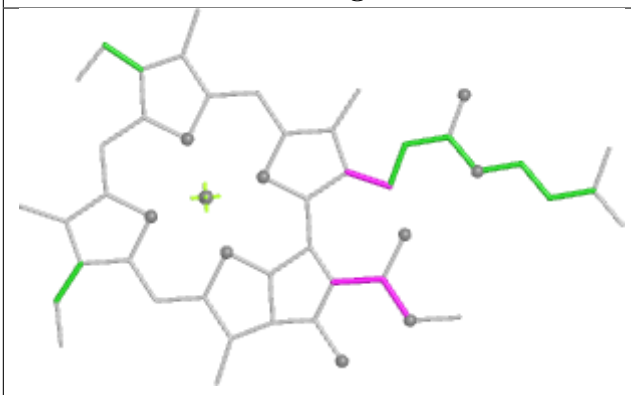
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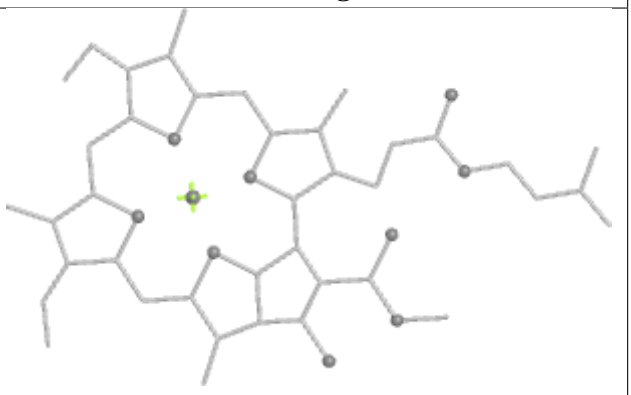
Bond lengths



Bond angles

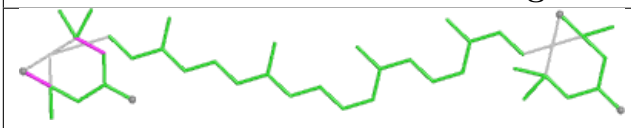


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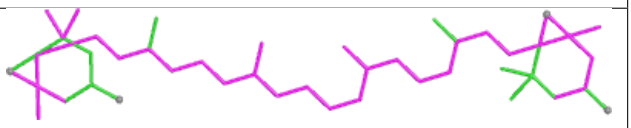


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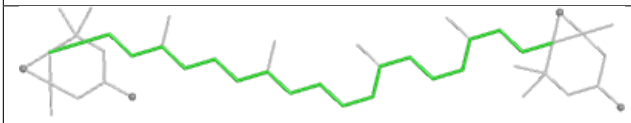
Ligand XAT 2 620



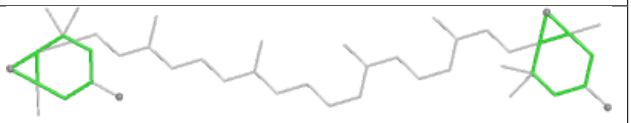
Bond lengths



Bond angles

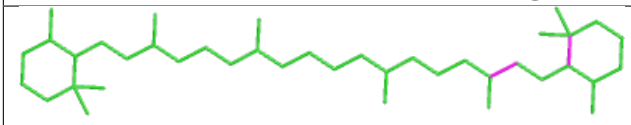


Torsions

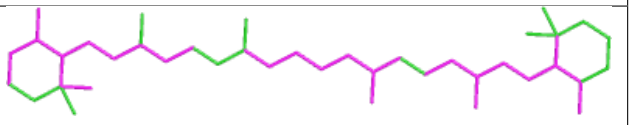


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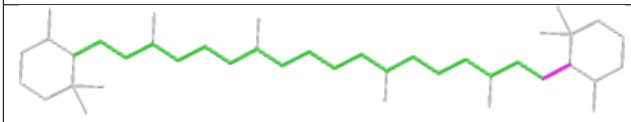
Ligand BCR 5 622



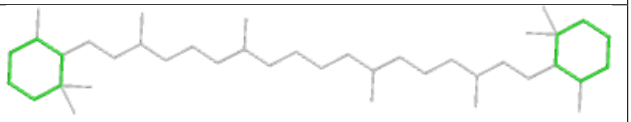
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Bond angles

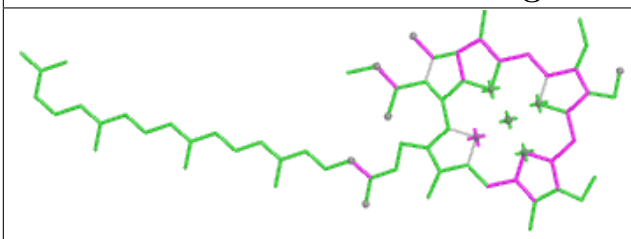


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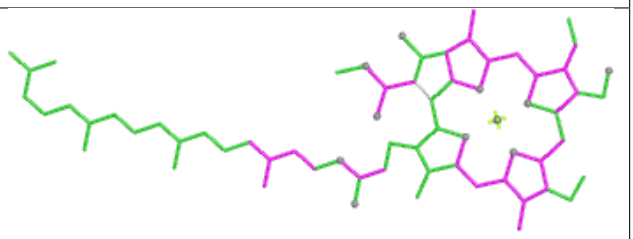


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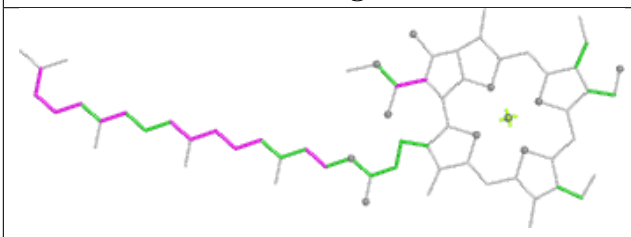
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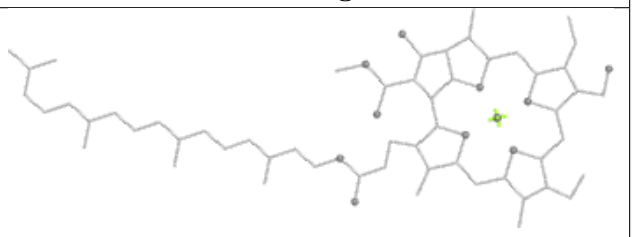
Bond lengths



Bond angles

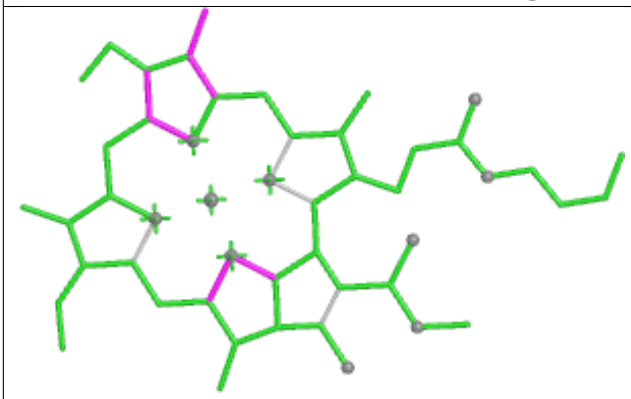


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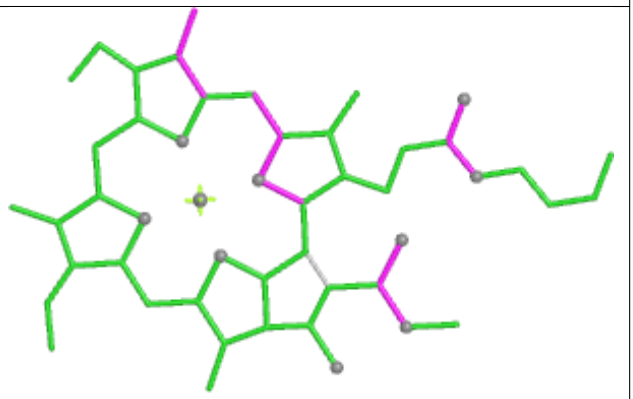


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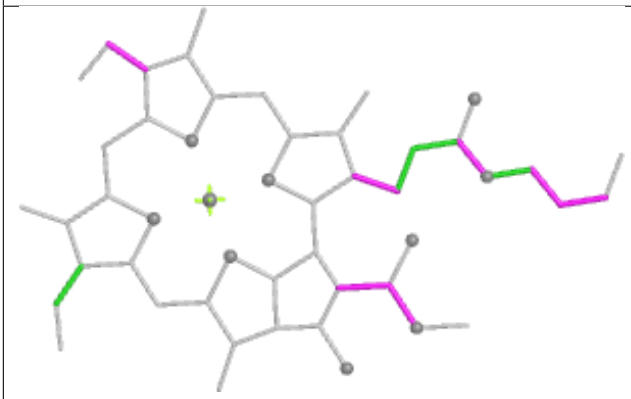
Ligand CLA X 604



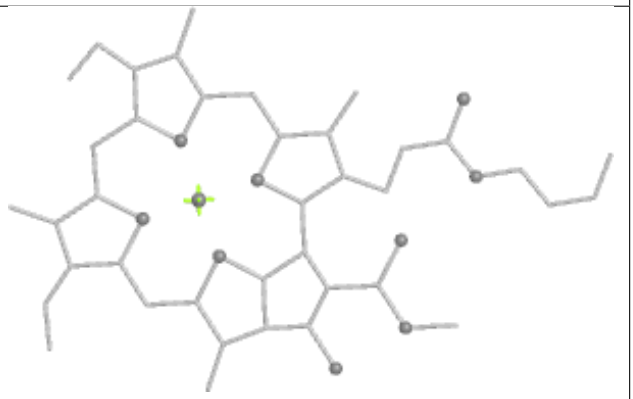
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Bond angles

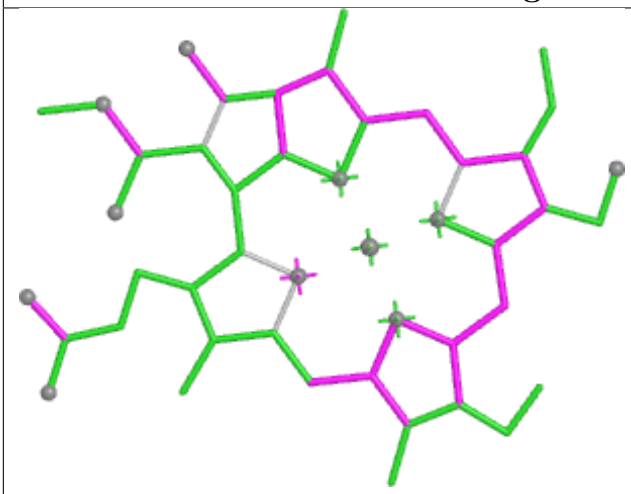


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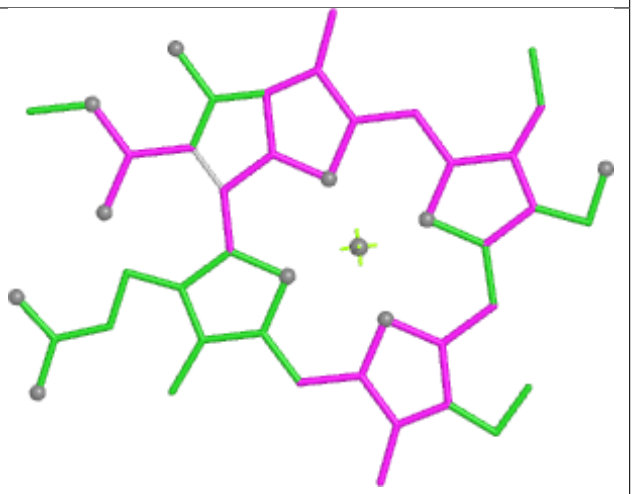


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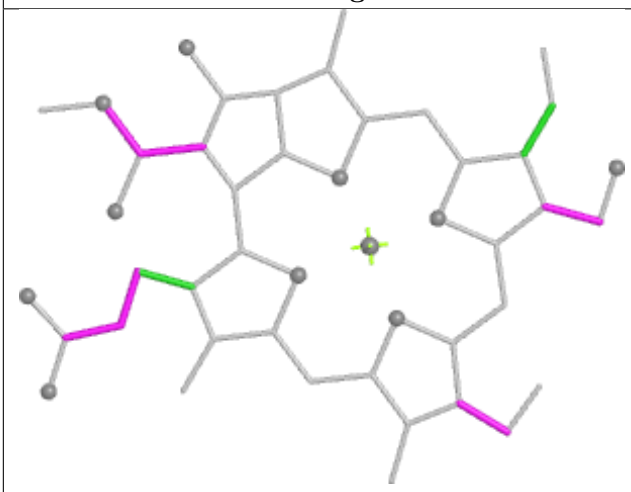
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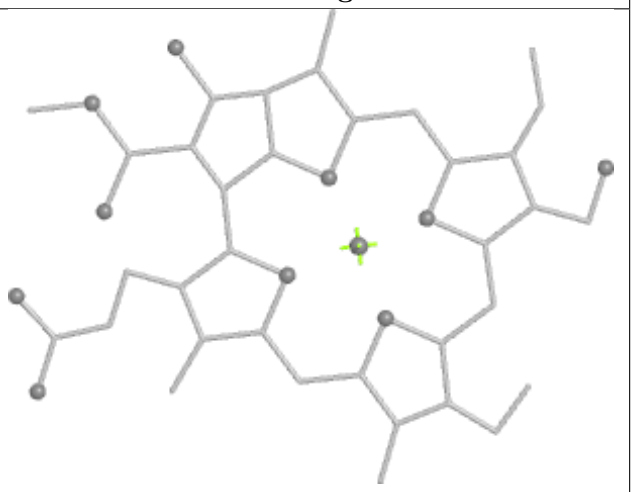
Bond lengths



Bond angles

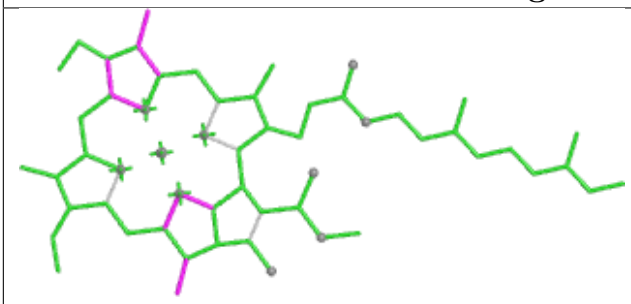


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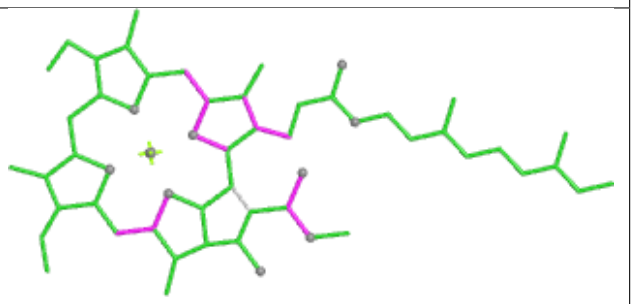


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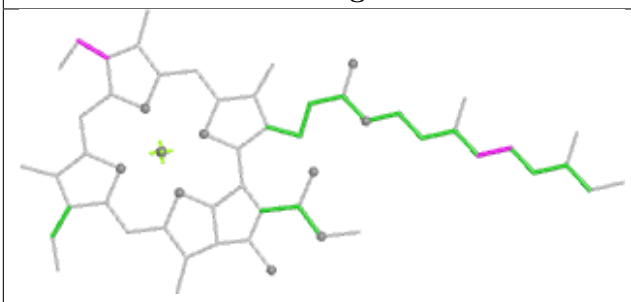
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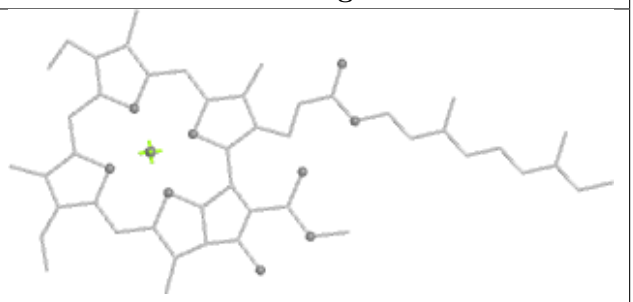
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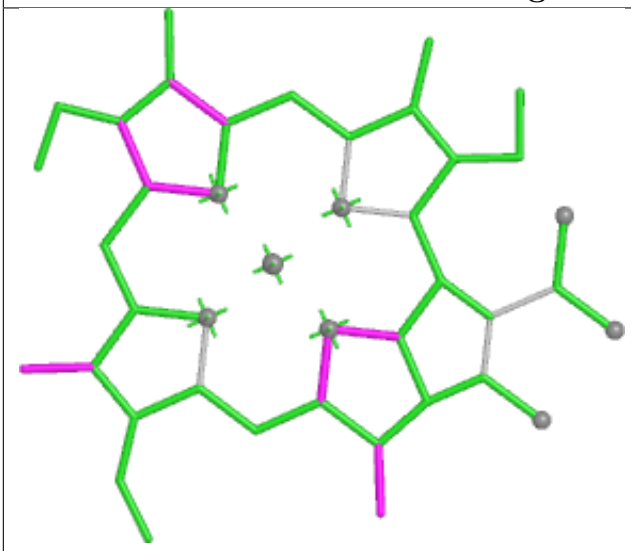


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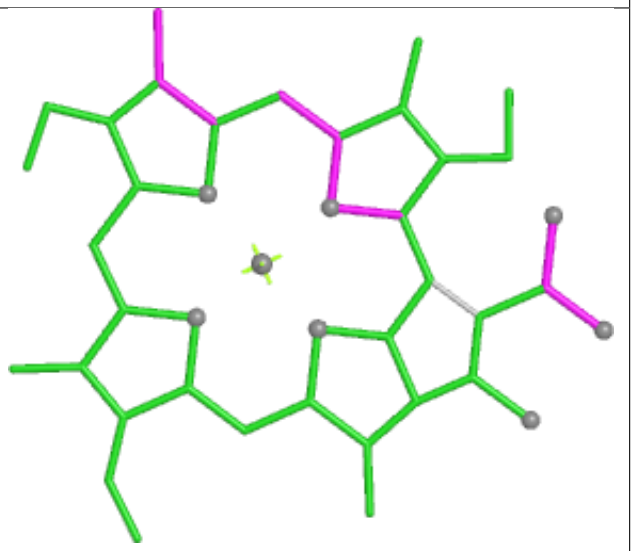


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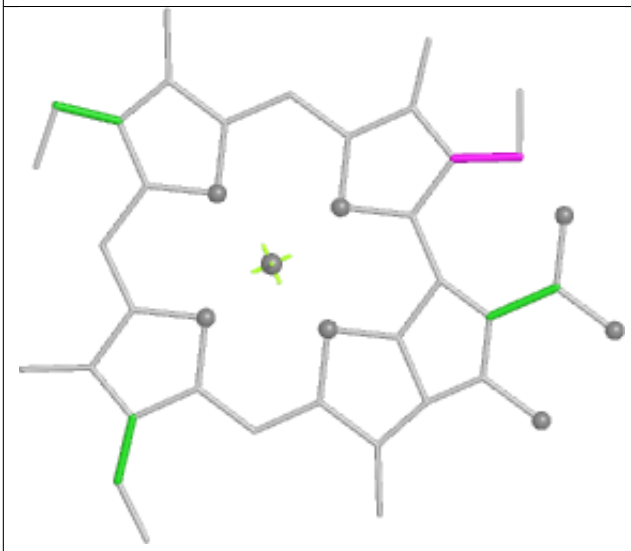
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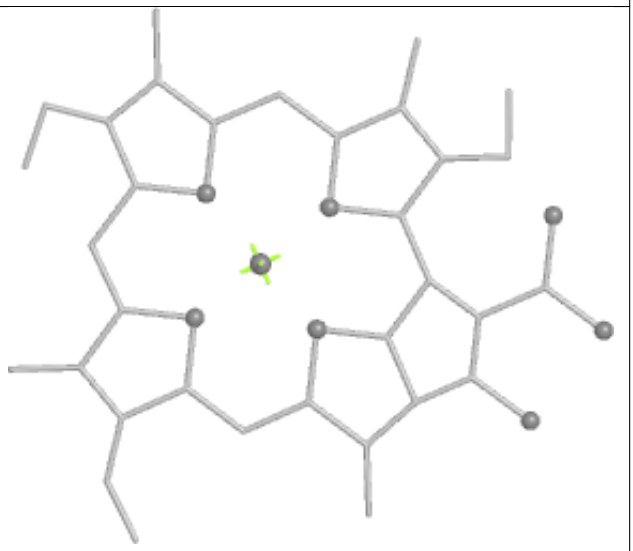
Bond lengths



Bond angles

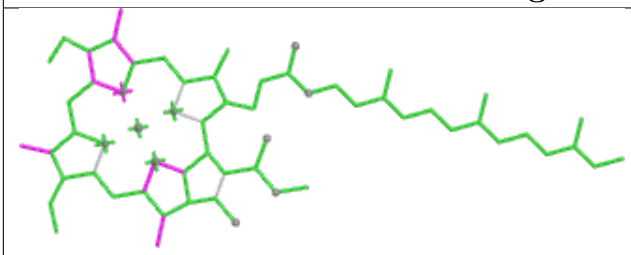


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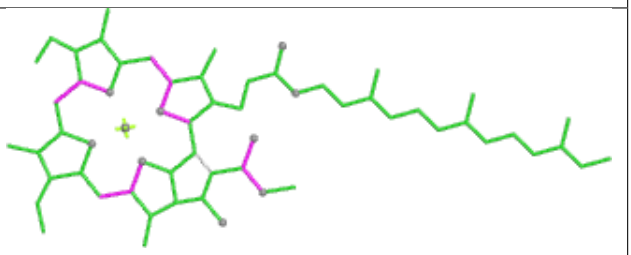


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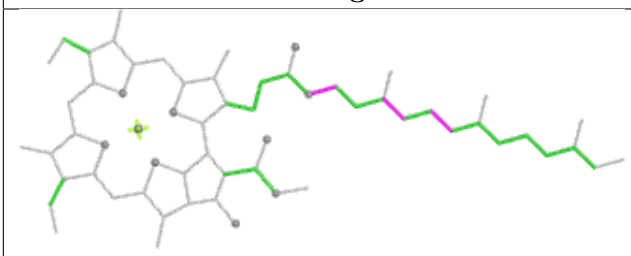
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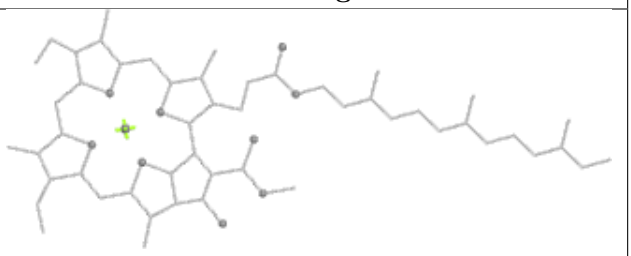
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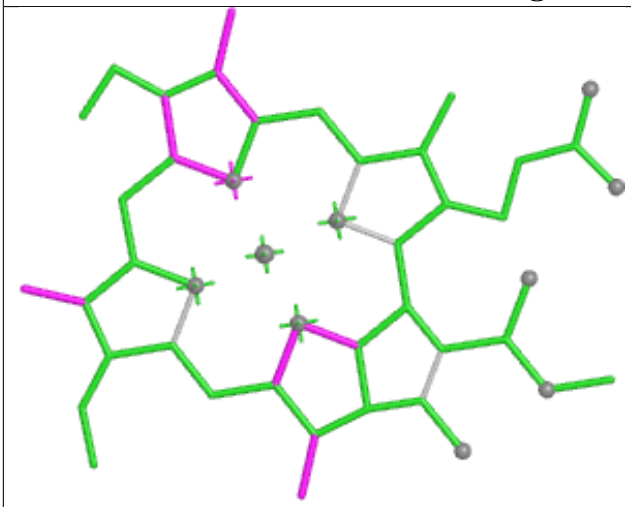


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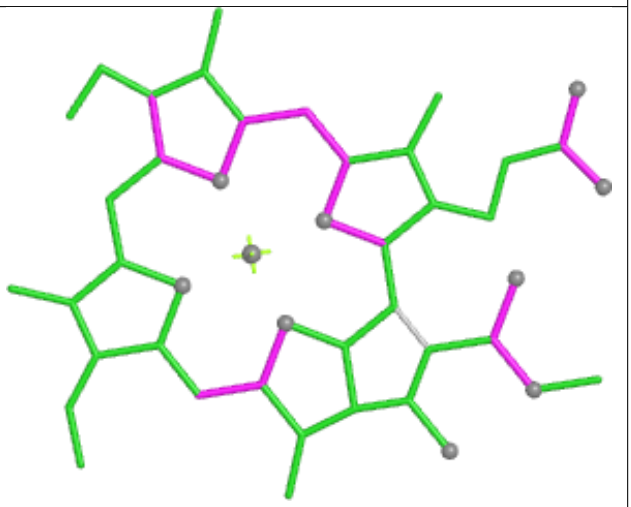


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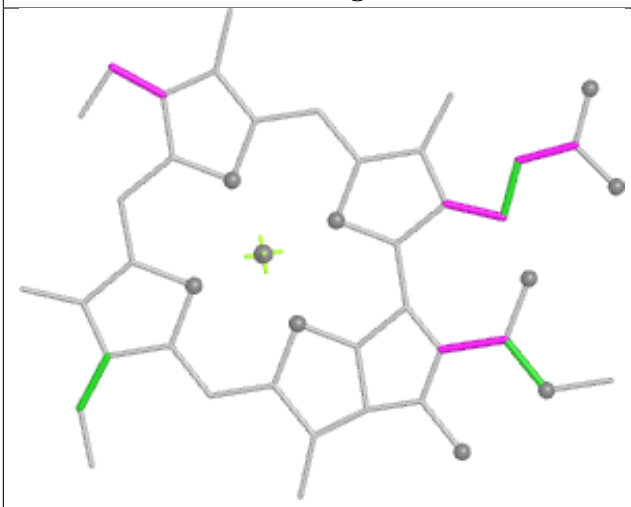
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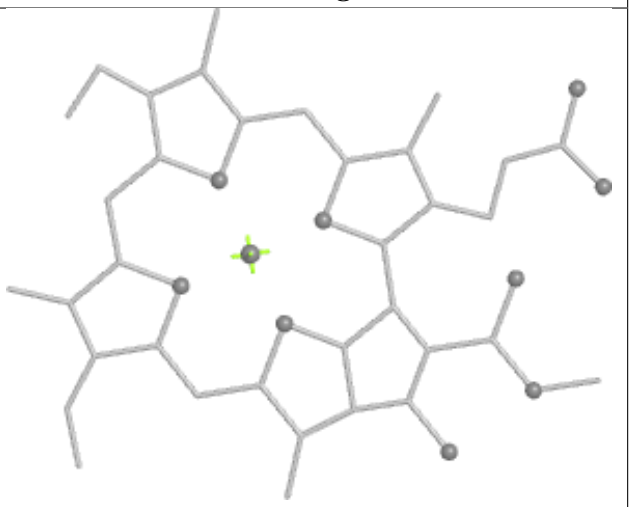
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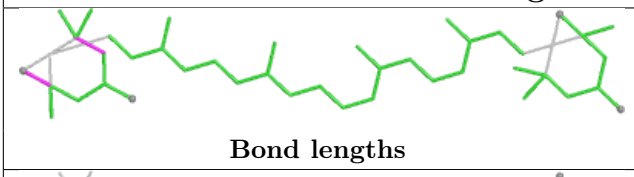


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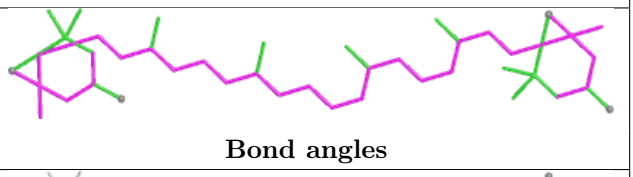


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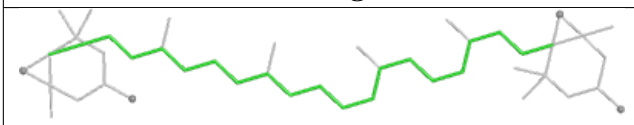
Ligand XAT 8 620



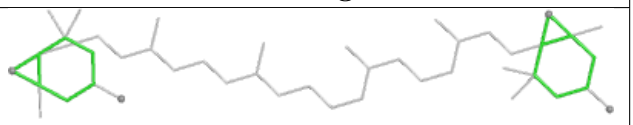
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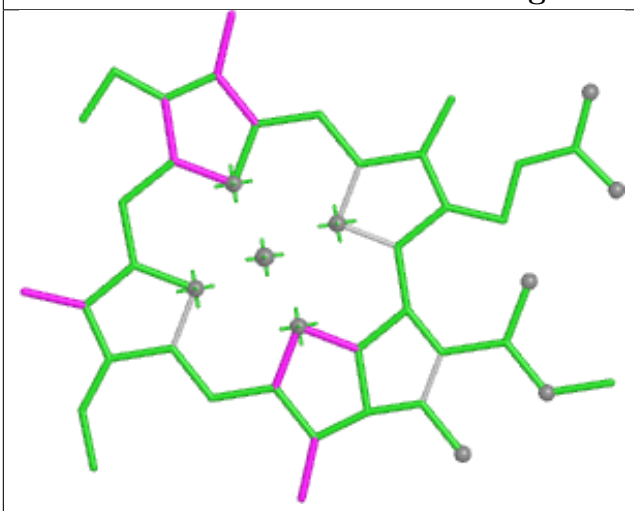


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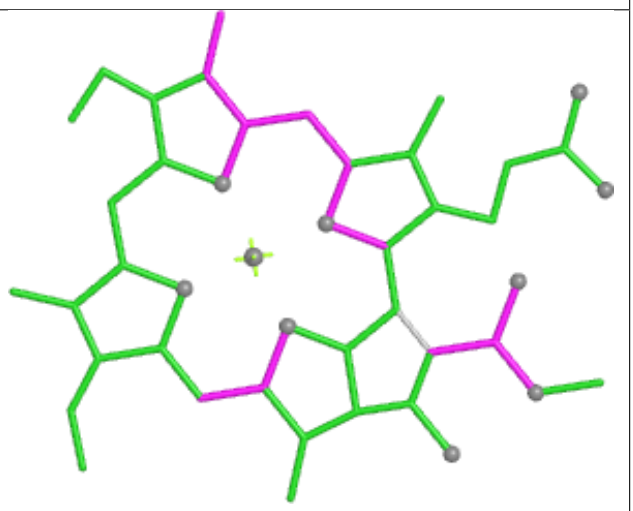


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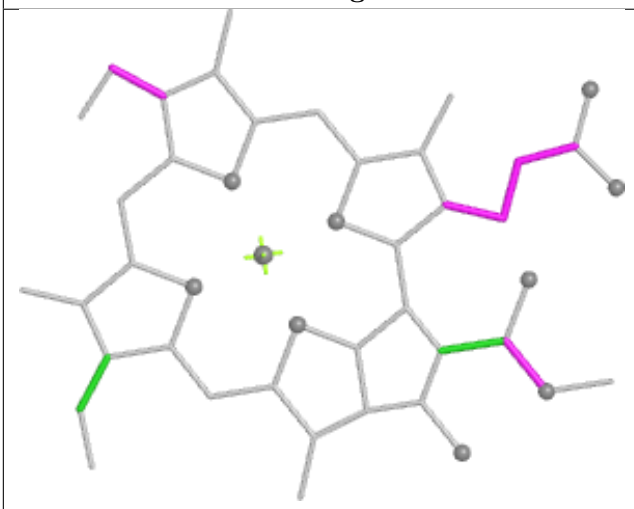
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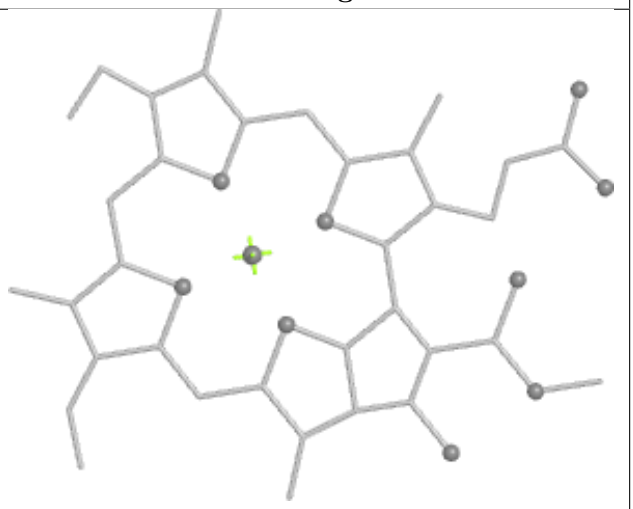
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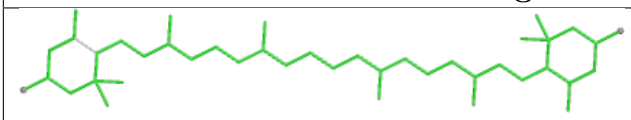


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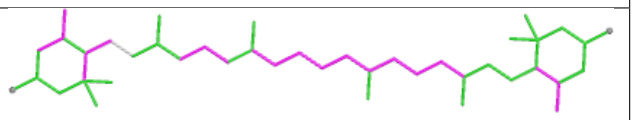


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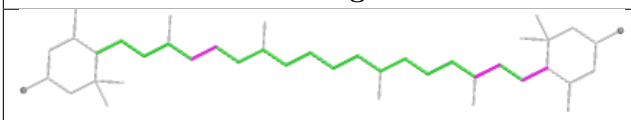
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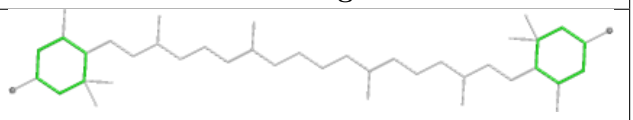
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Bond angles

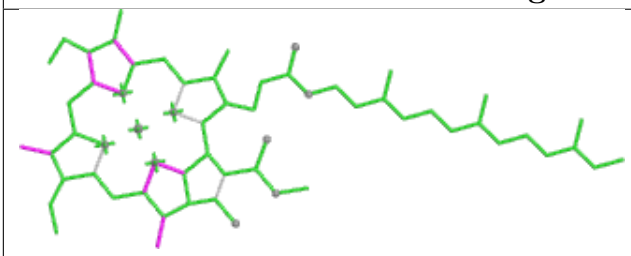


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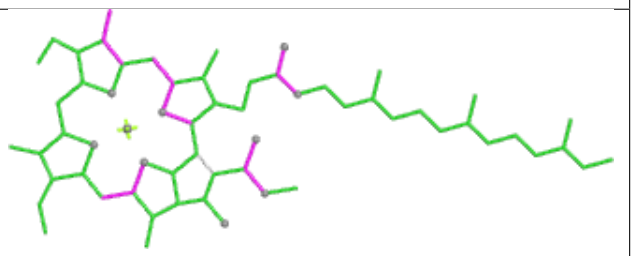


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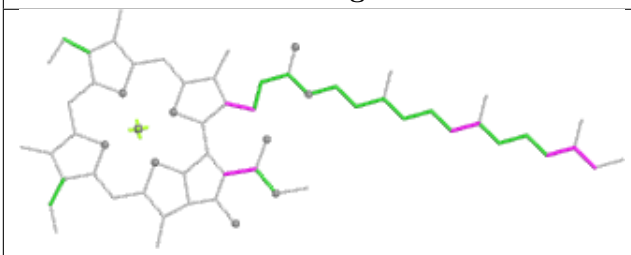
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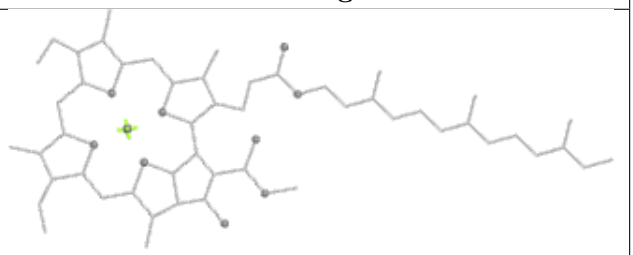
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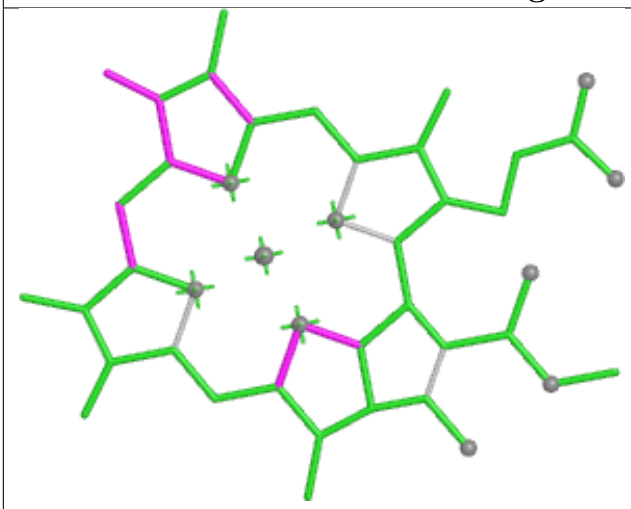


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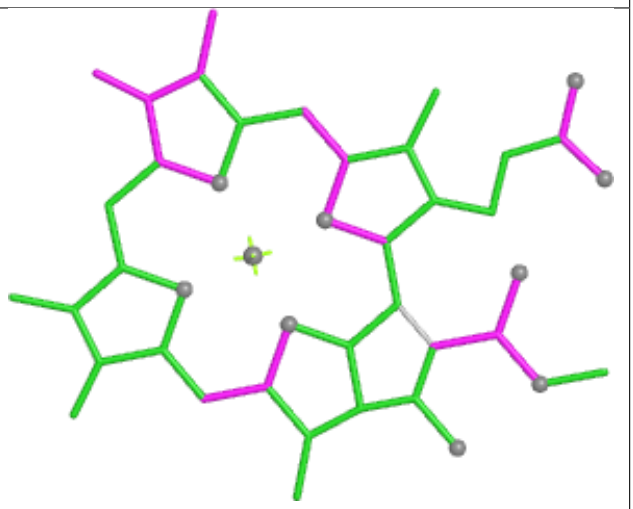


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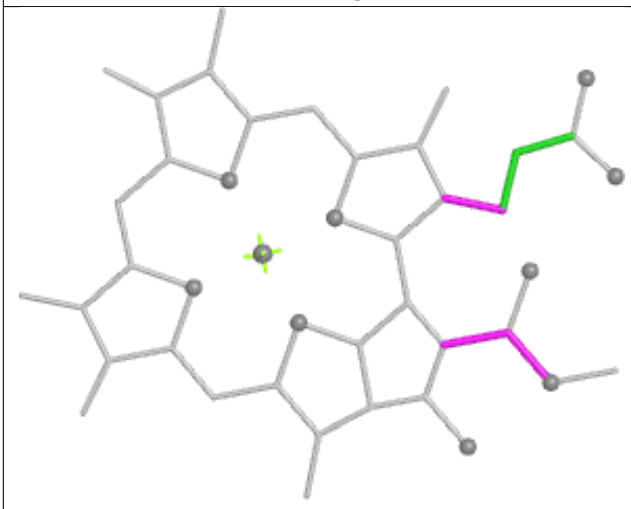
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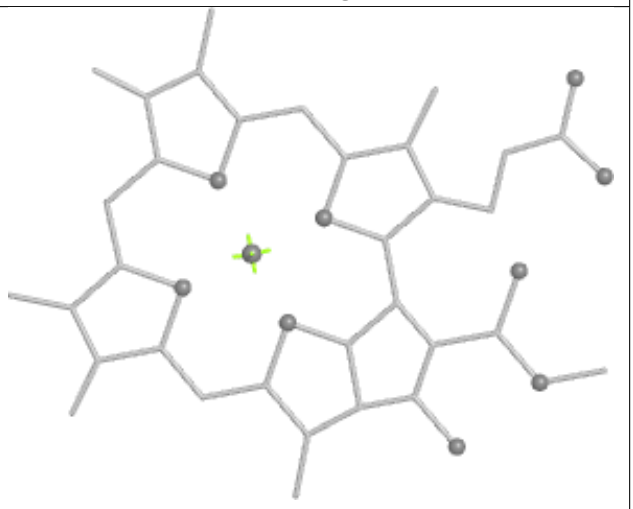
Bond lengths



Bond angles

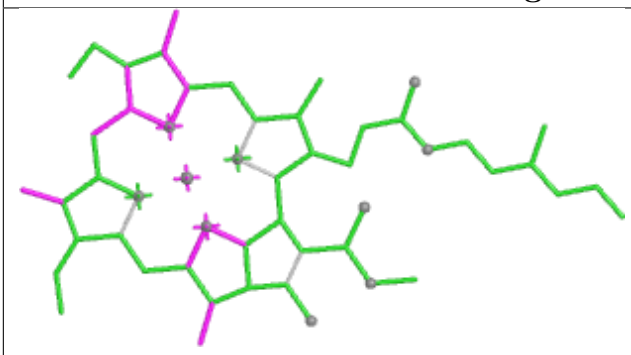


Torsions

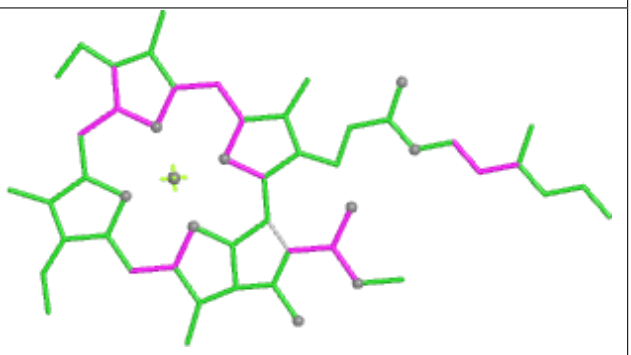


Rings

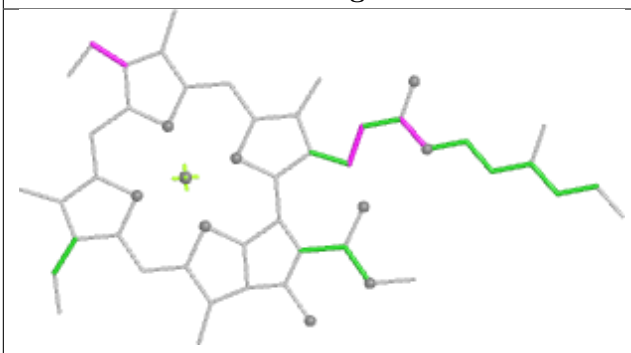
Ligand CLA B 807



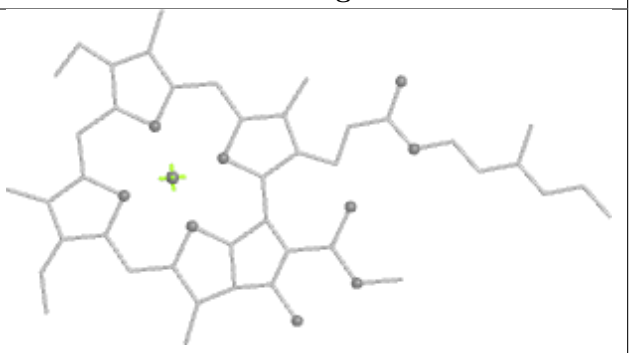
Bond lengths



Bond angles

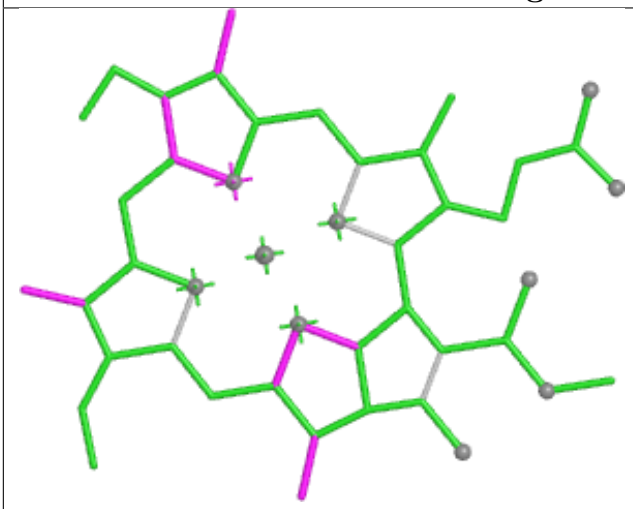


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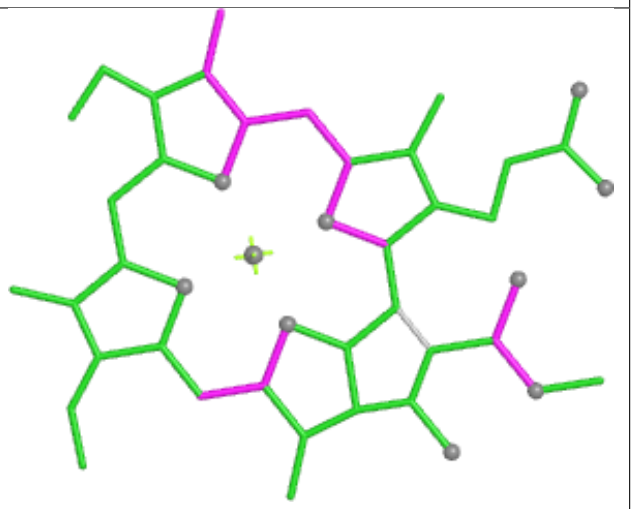


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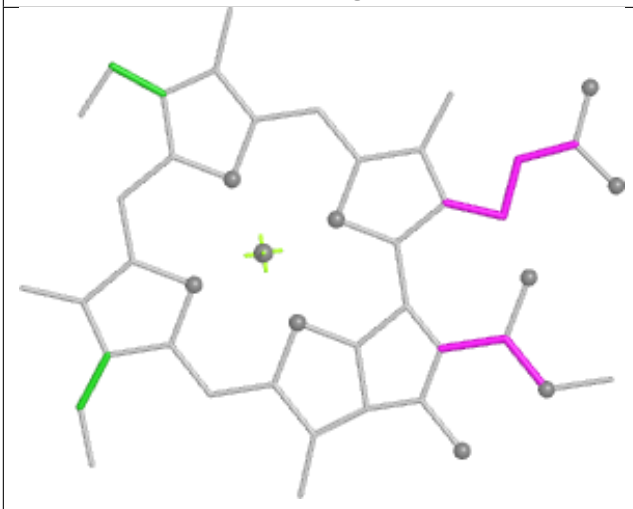
Ligand CLA L 302



Bond lengths



Bond angles

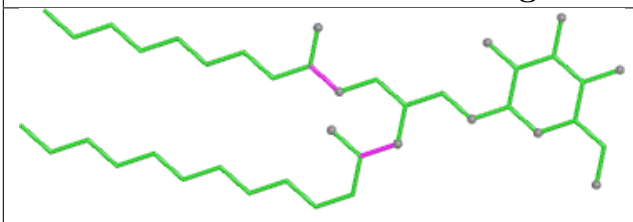


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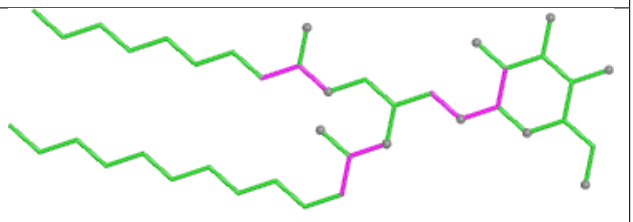


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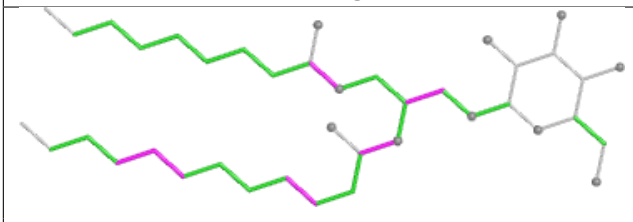
Ligand LMG A 860



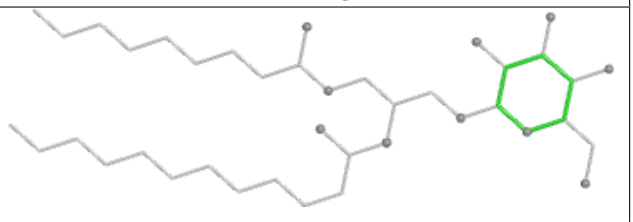
Bond lengths



Bond angles

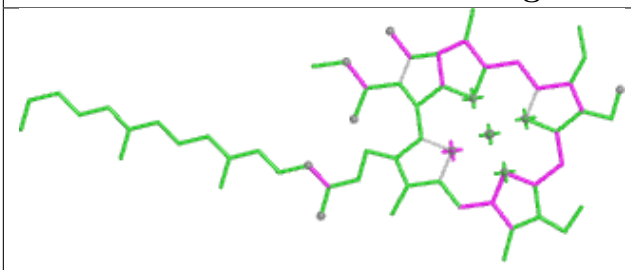


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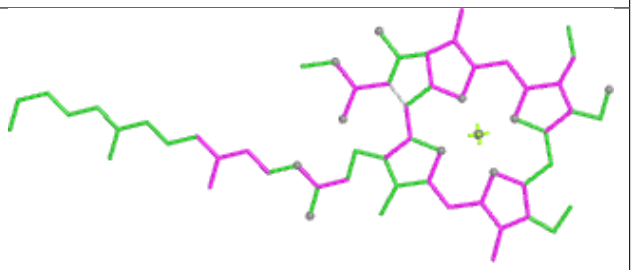


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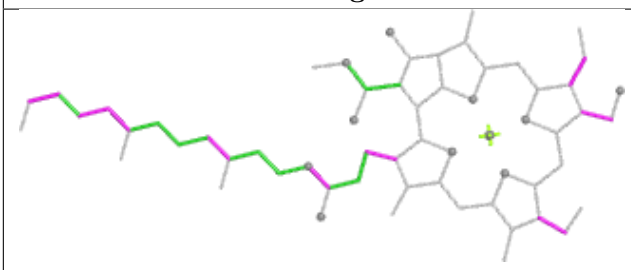
Ligand CHL U 609



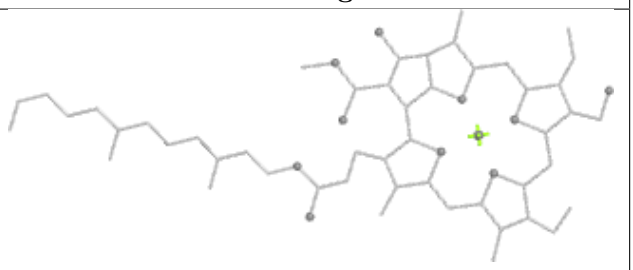
Bond lengths



Bond angles

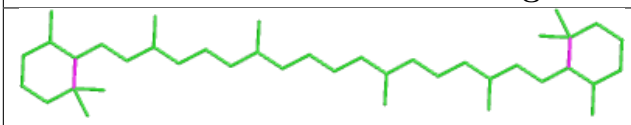


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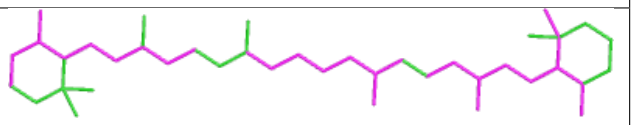


Rings

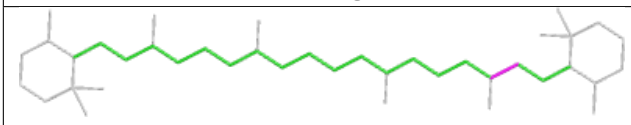
Ligand BCR B 847



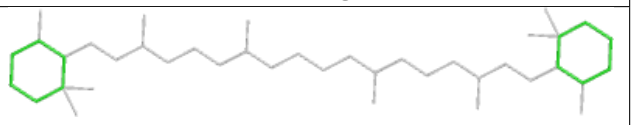
Bond lengths



Bond angles

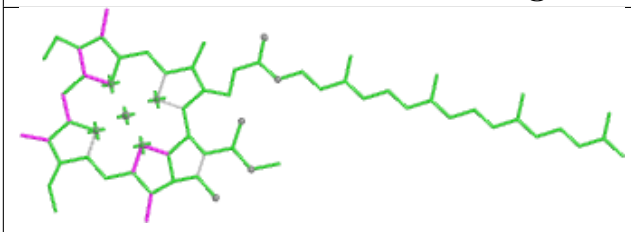


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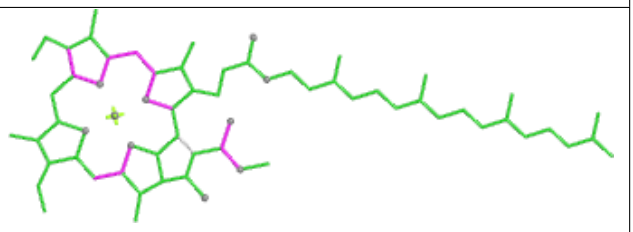


Rings

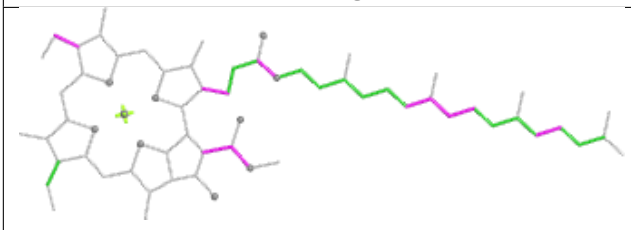
Ligand CLA 3 610



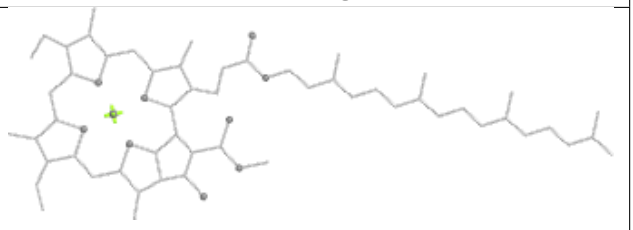
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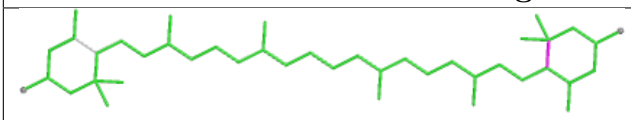


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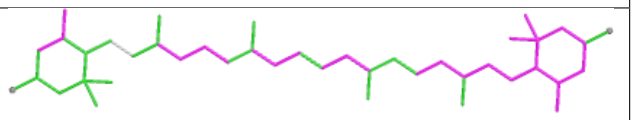


Rings

Ligand LUT Y 1621



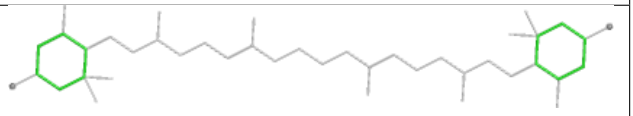
Bond lengths



Bond angles

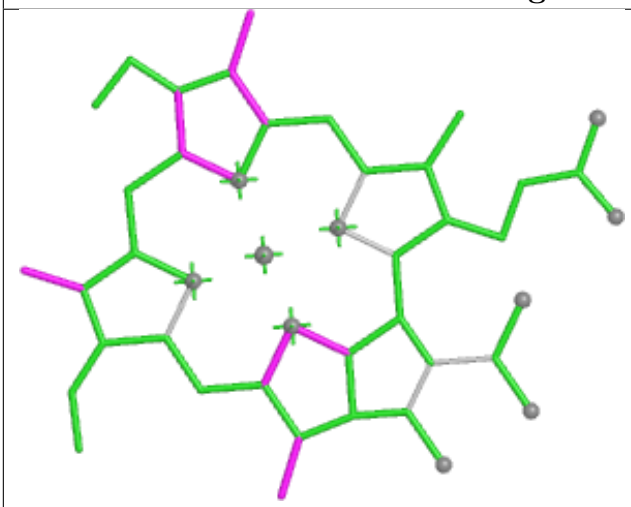


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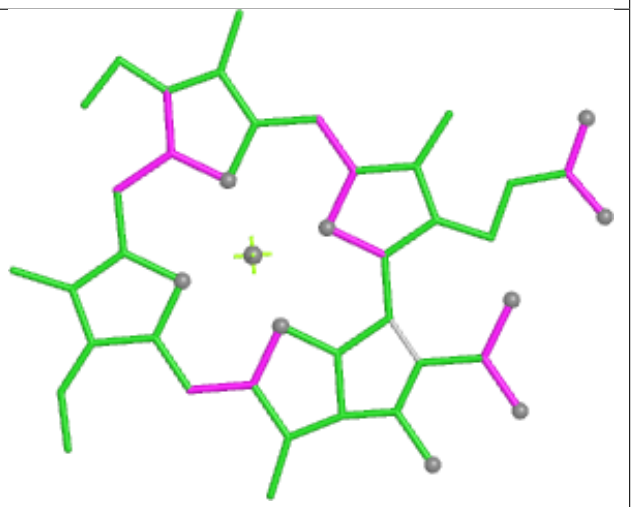


Rings

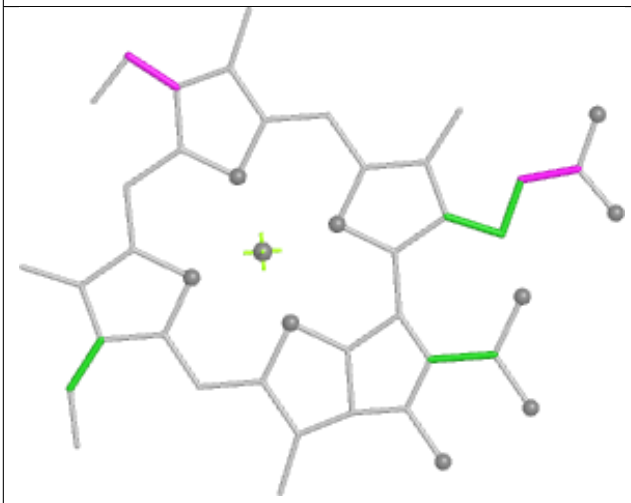
Ligand CLA a 608



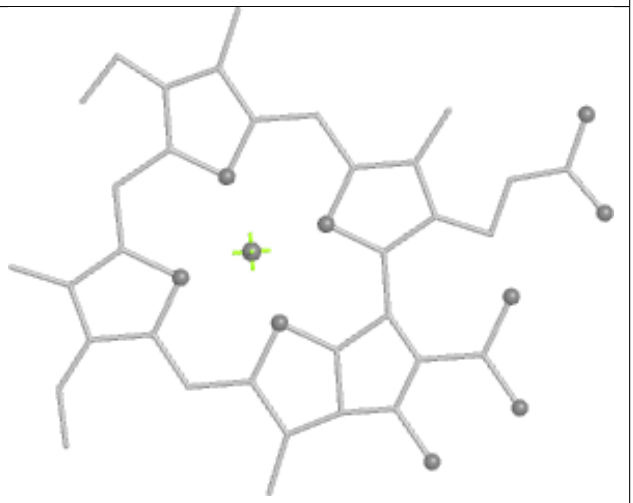
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Bond angles

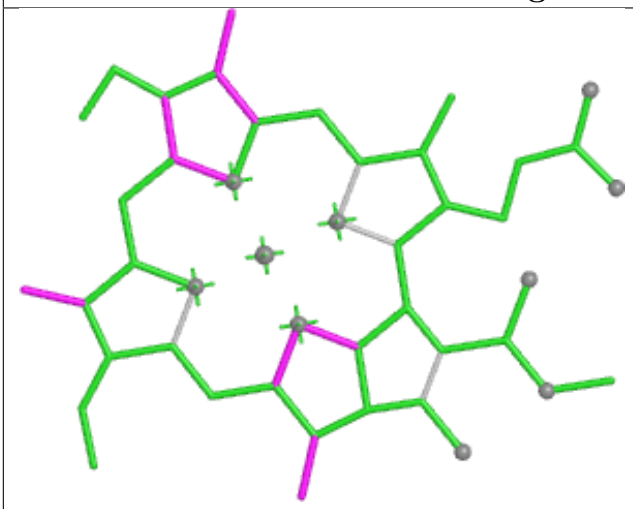


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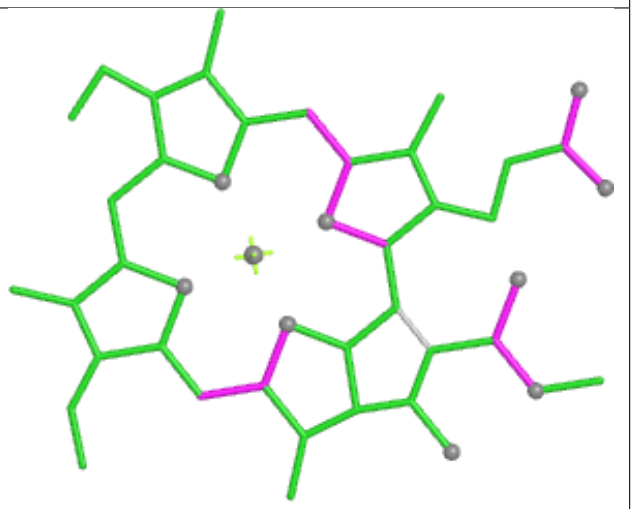


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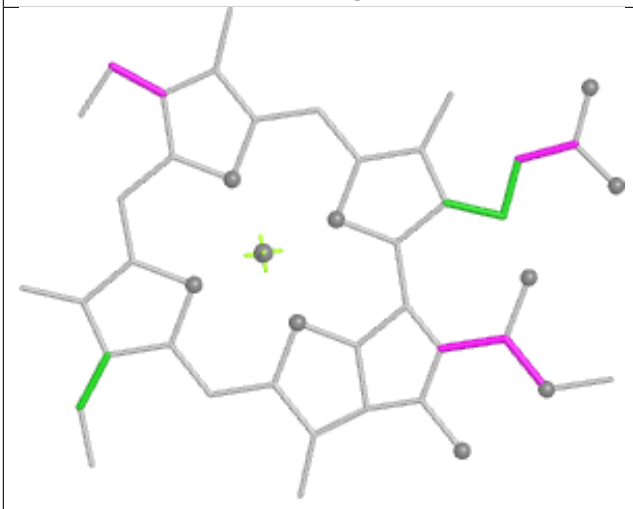
Ligand CLA 9 601



Bond lengths



Bond angles

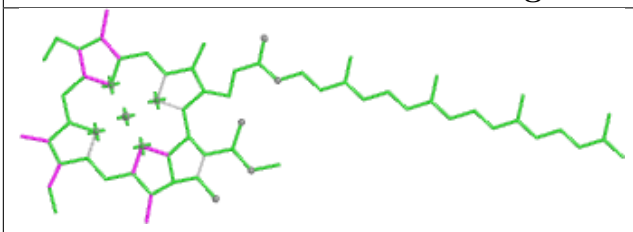


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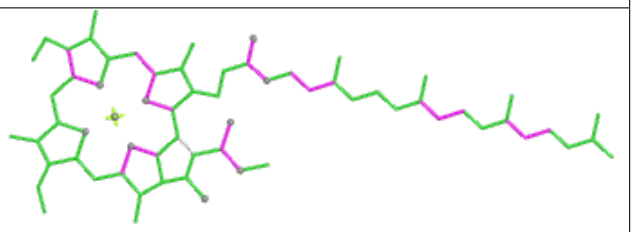


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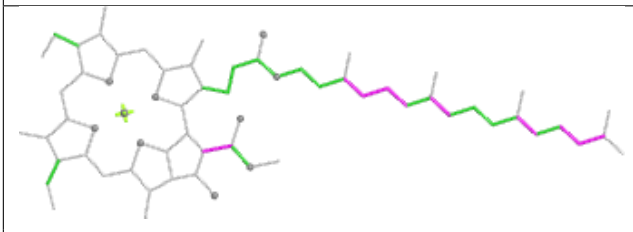
Ligand CLA B 808



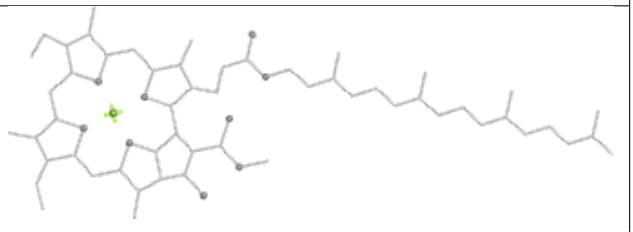
Bond lengths



Bond angles

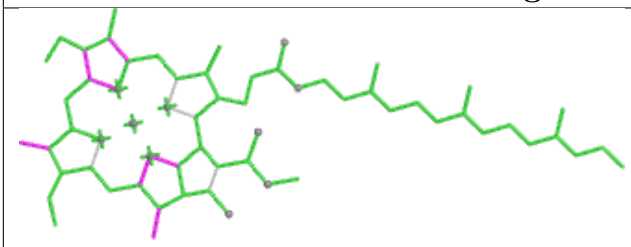


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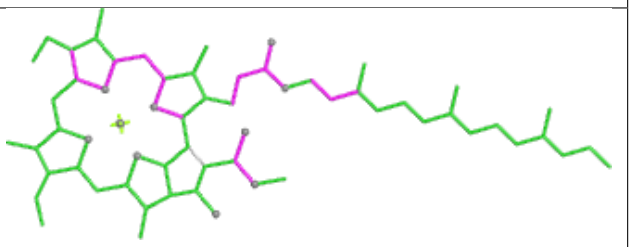


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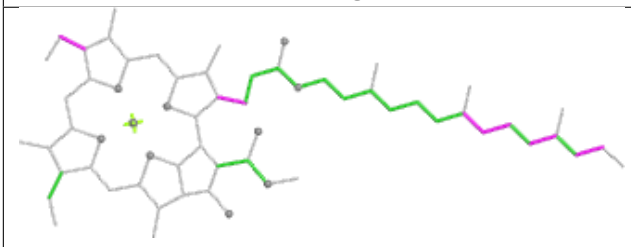
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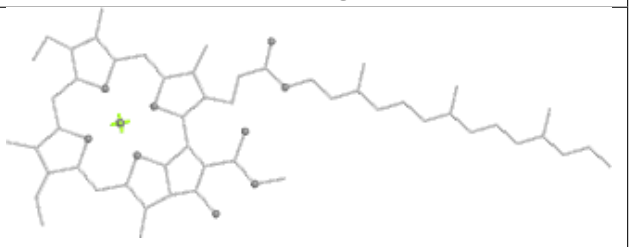
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Bond angles

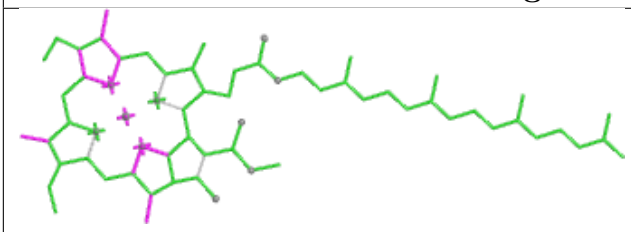


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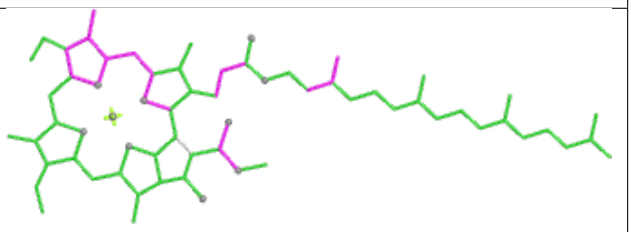


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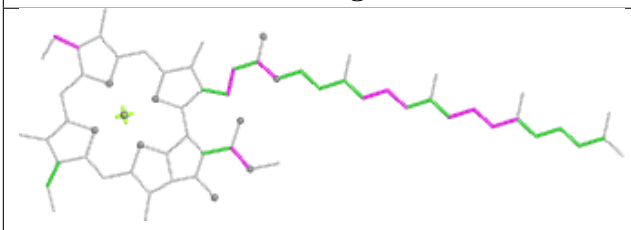
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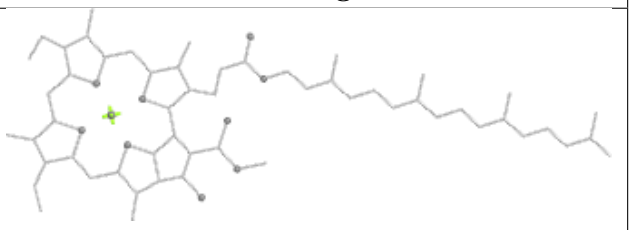
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Bond angles

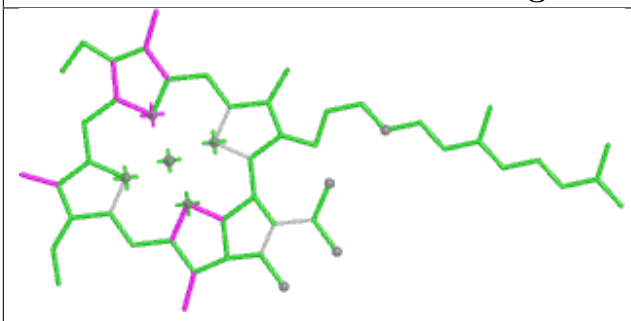


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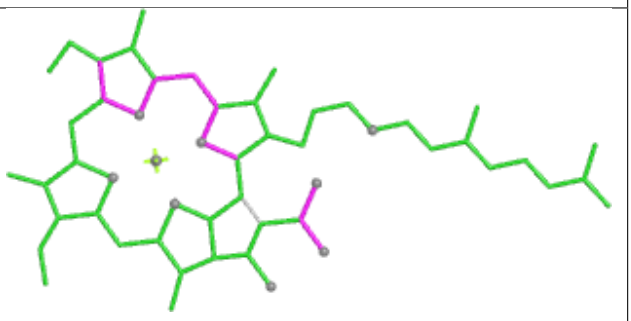


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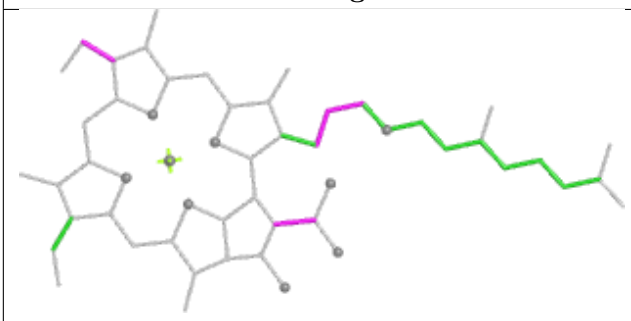
Ligand CLA 3 613



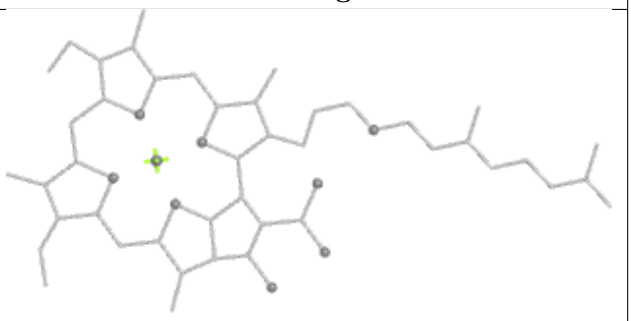
Bond lengths



Bond angles

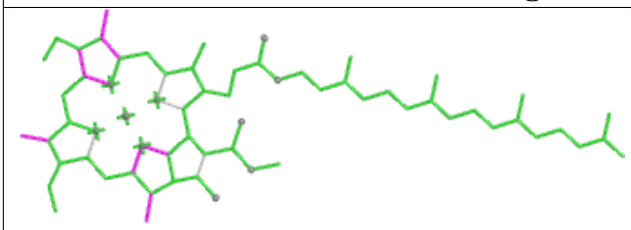


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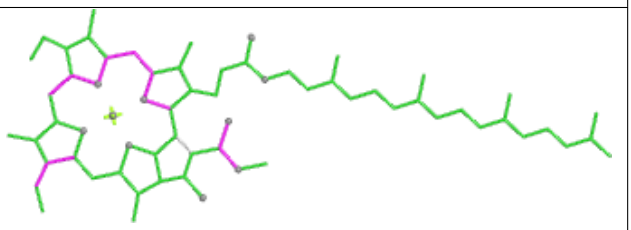


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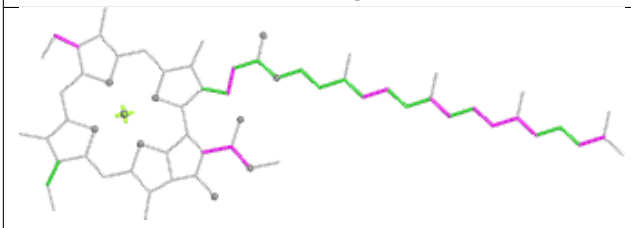
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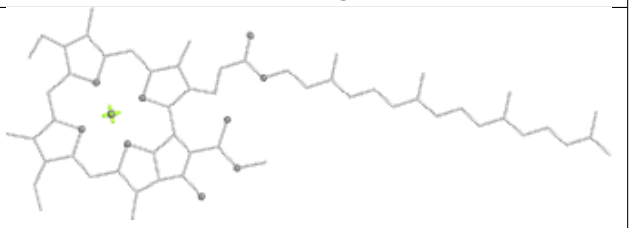
Bond lengths



Bond angles

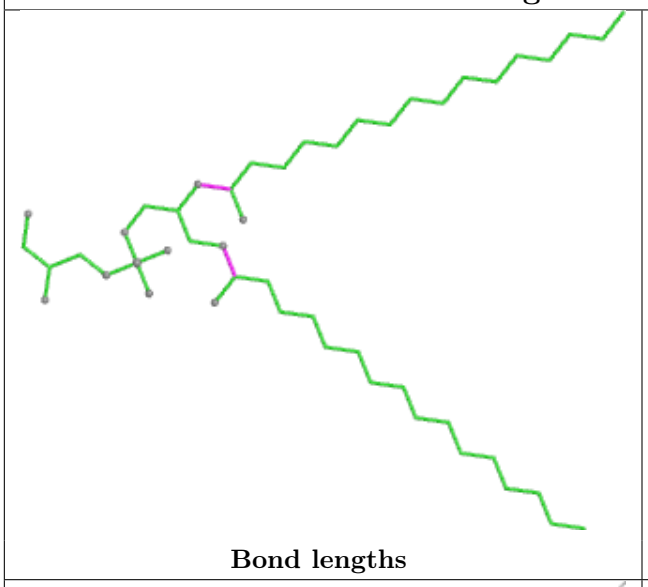


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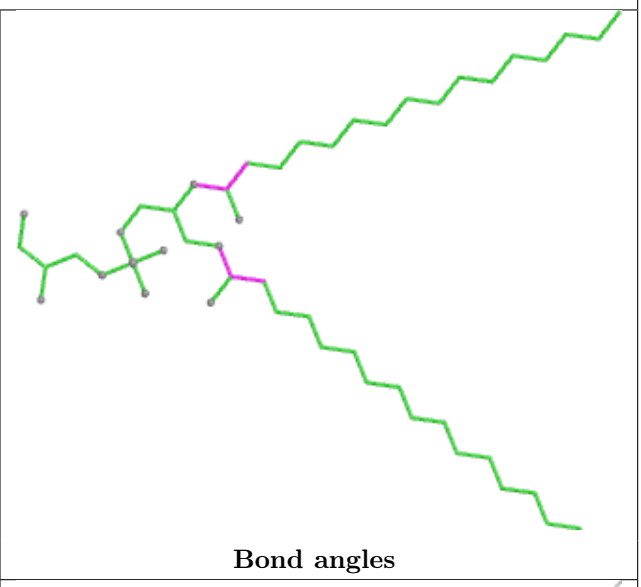


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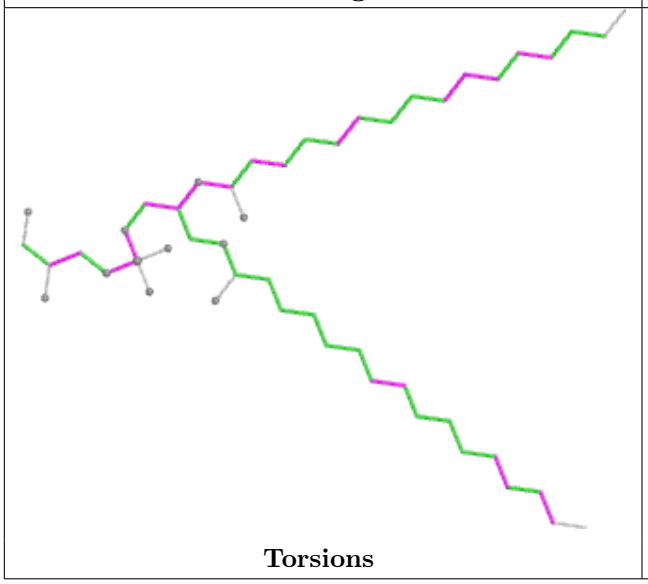
Ligand LHG A 861



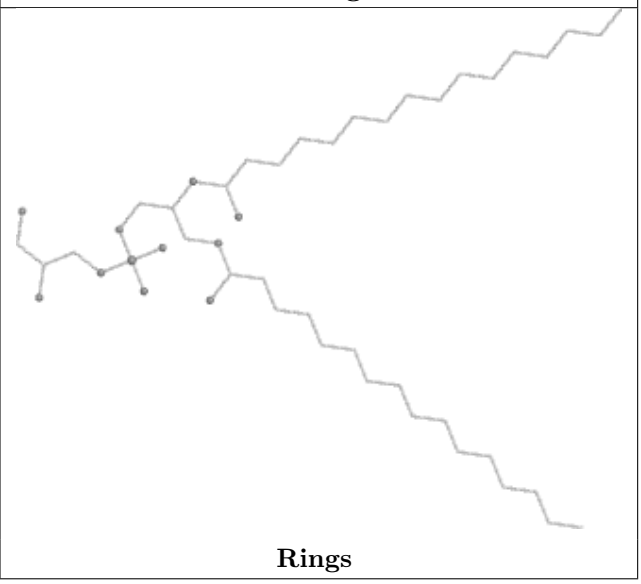
Bond lengths



Bond angles

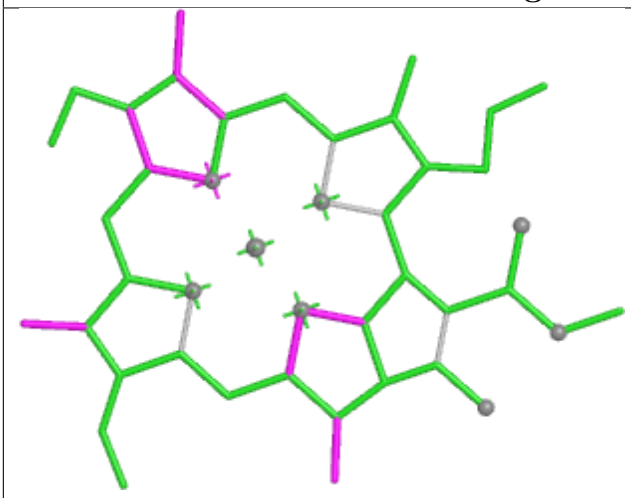


Torsions

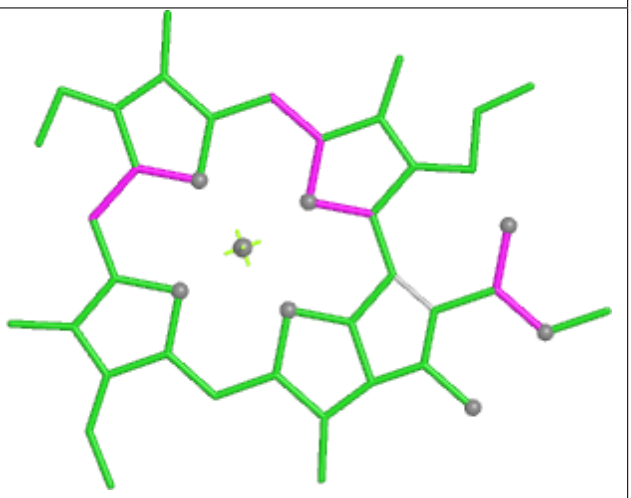


Rings

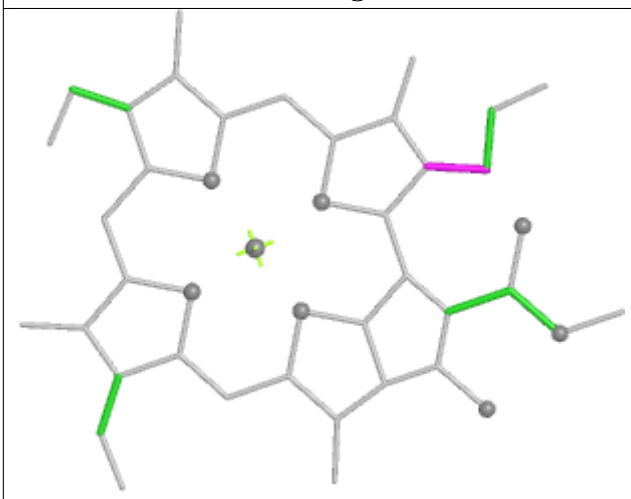
Ligand CLA B 815



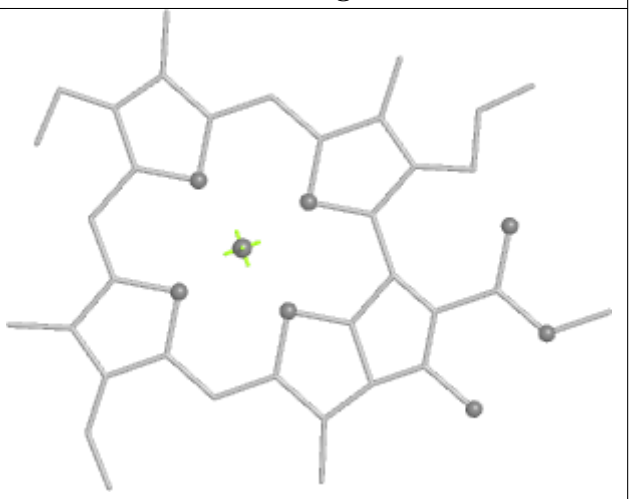
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Bond angles

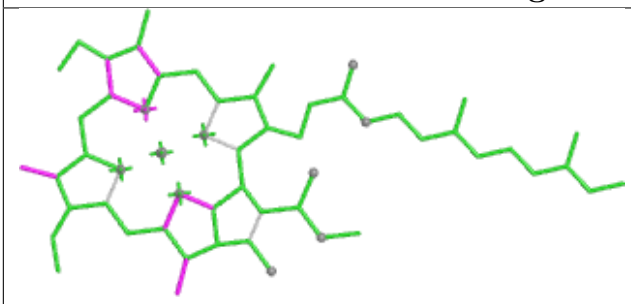


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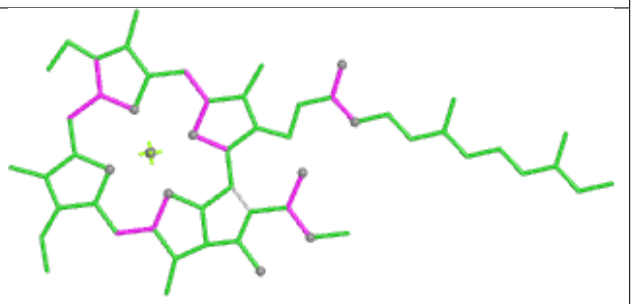


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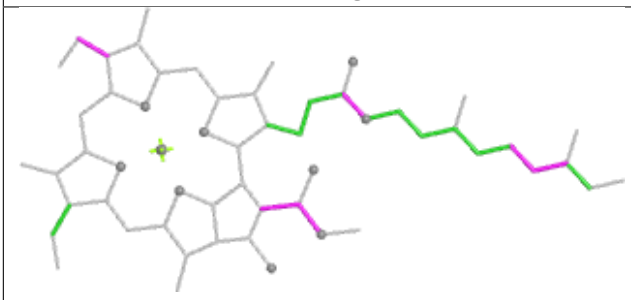
Ligand CLA 4 614



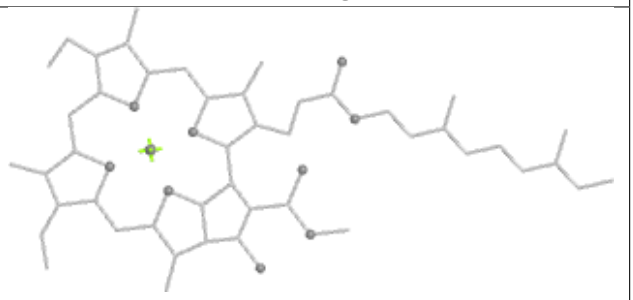
Bond lengths



Bond angles

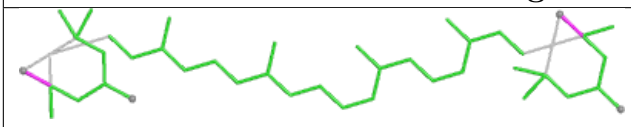


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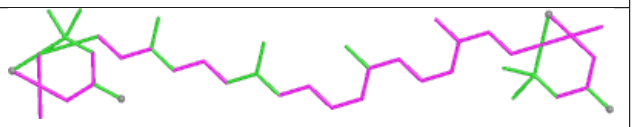


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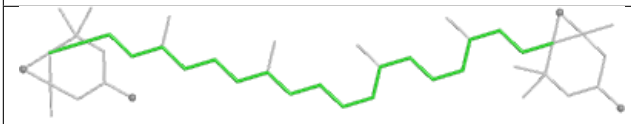
Ligand XAT 5 621



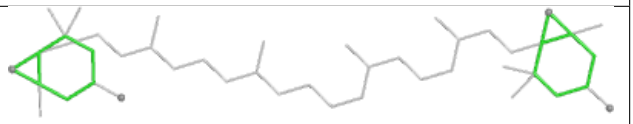
Bond lengths



Bond angles

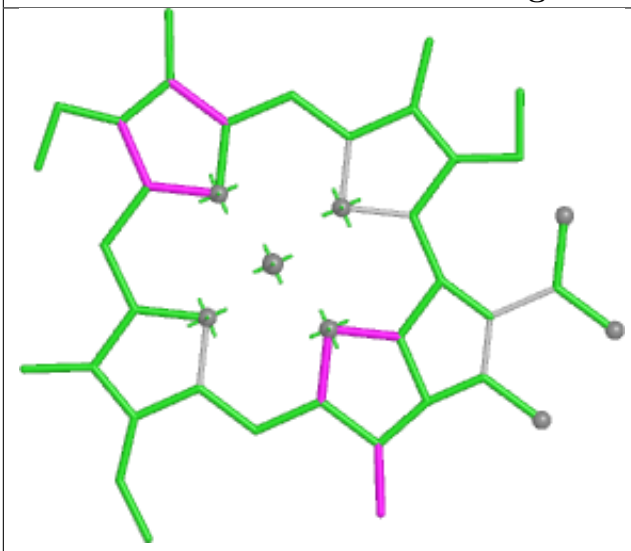


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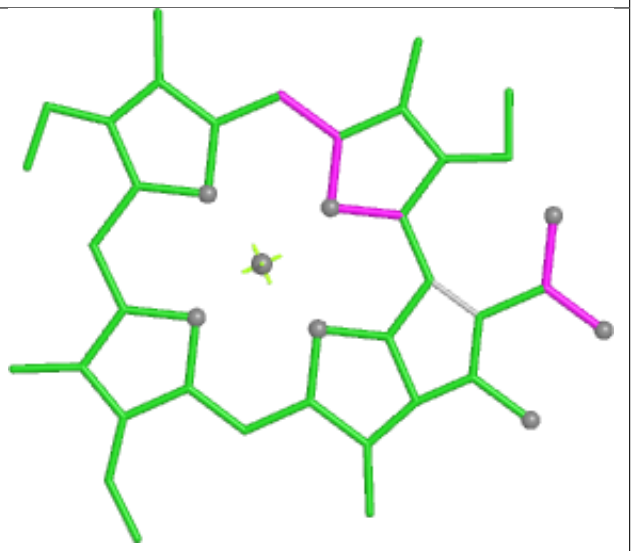


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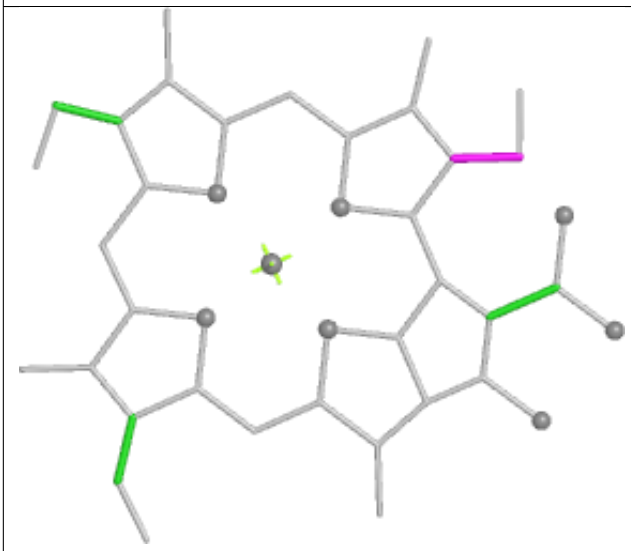
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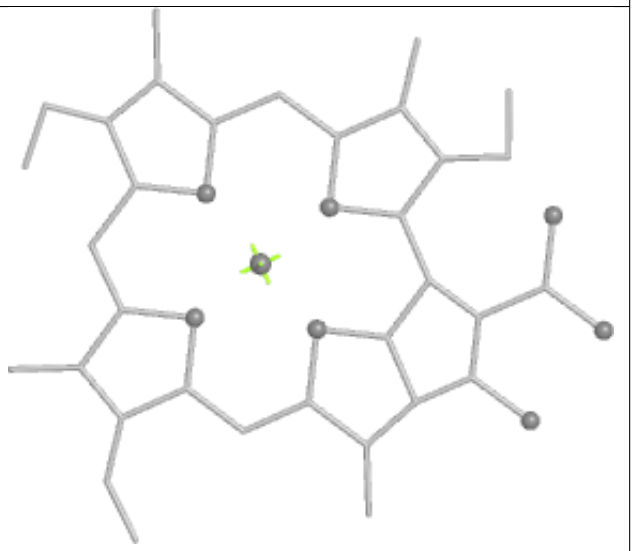
Bond lengths



Bond angles

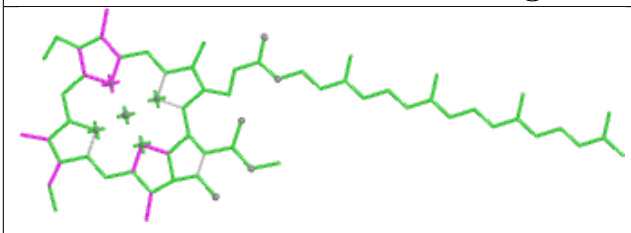


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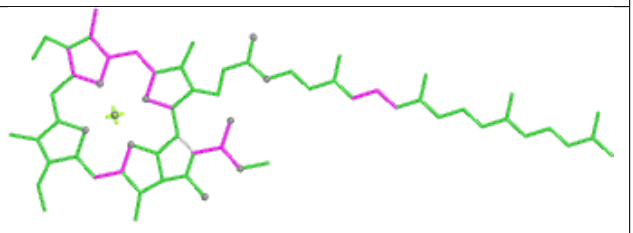


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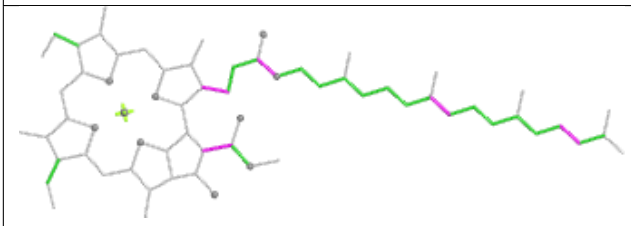
Ligand CLA A 820



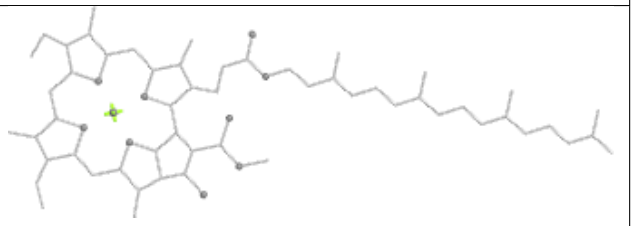
Bond lengths



Bond angles

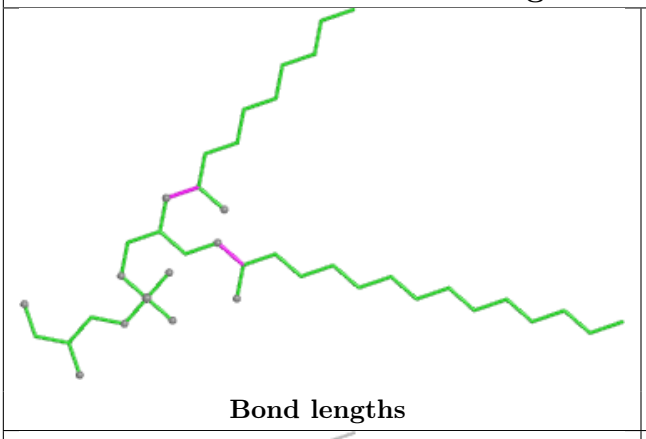


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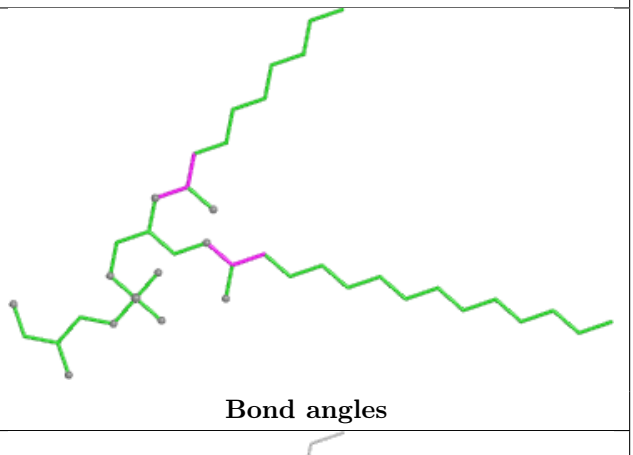


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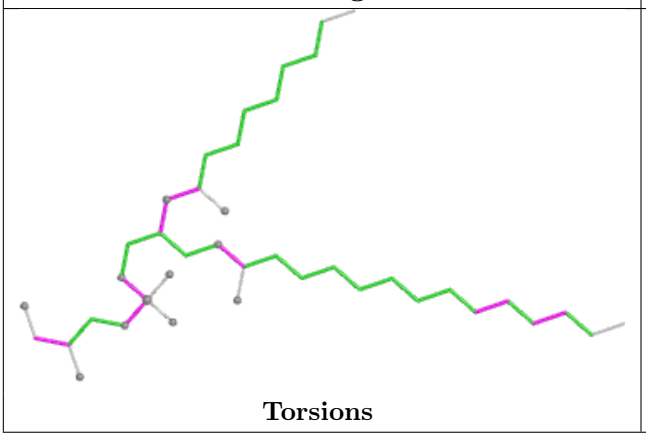
Ligand LHG 8 623



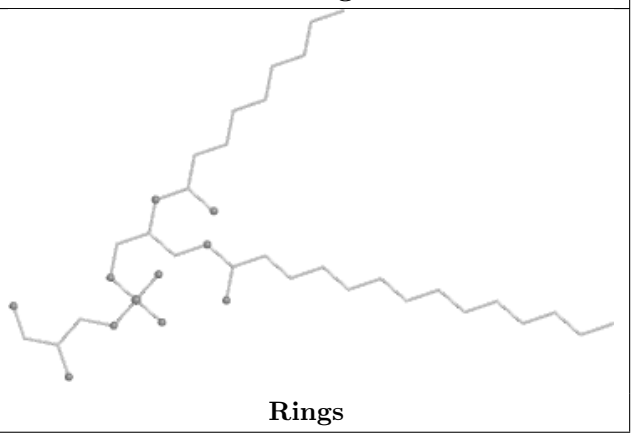
Bond lengths



Bond angles

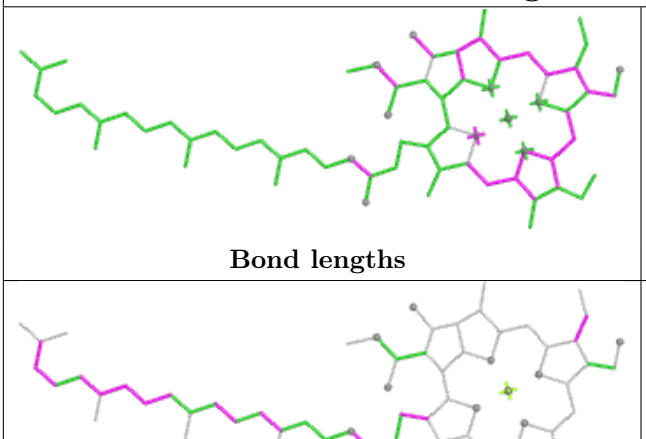


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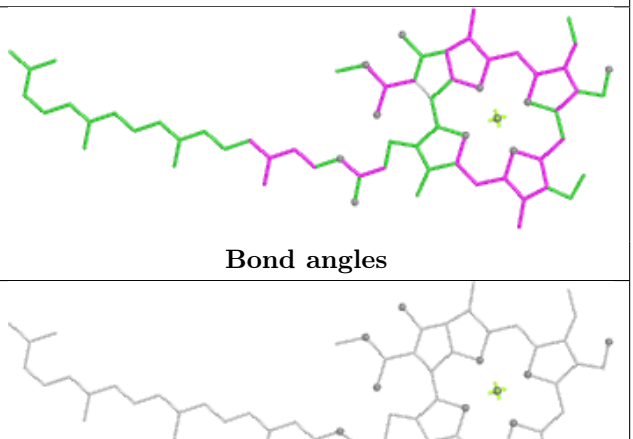


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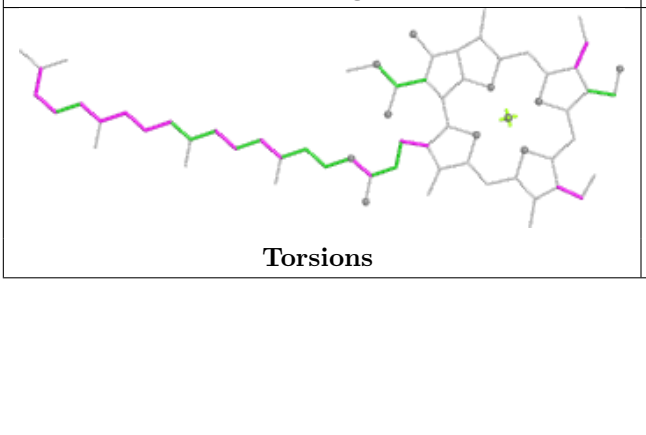
Ligand CHL Y 609



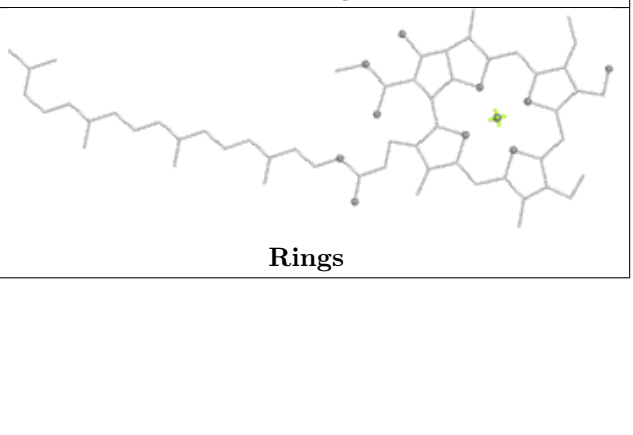
Bond lengths



Bond angles

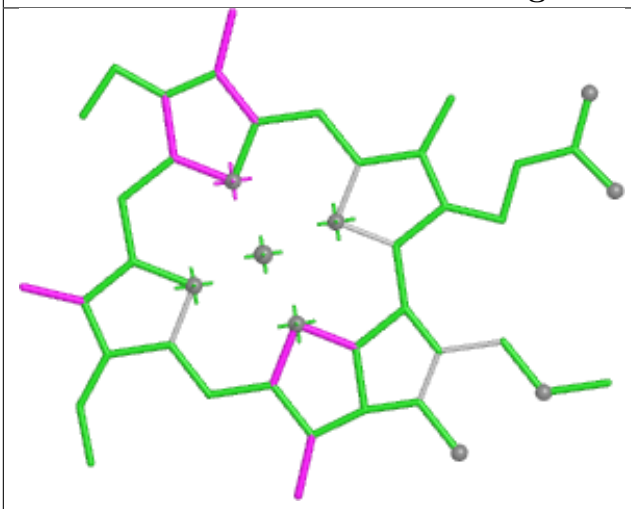


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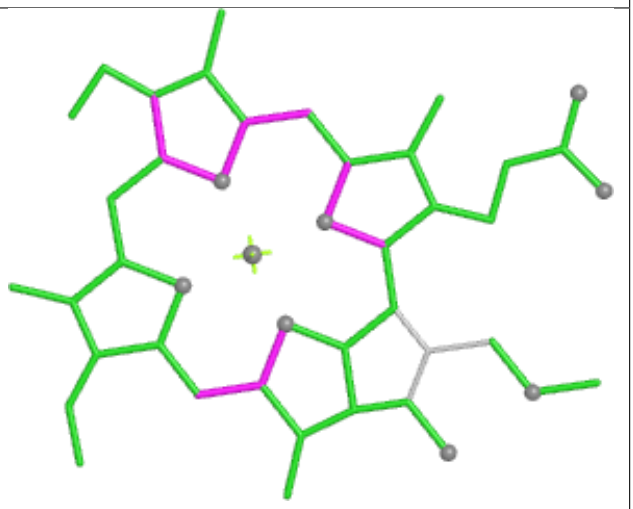


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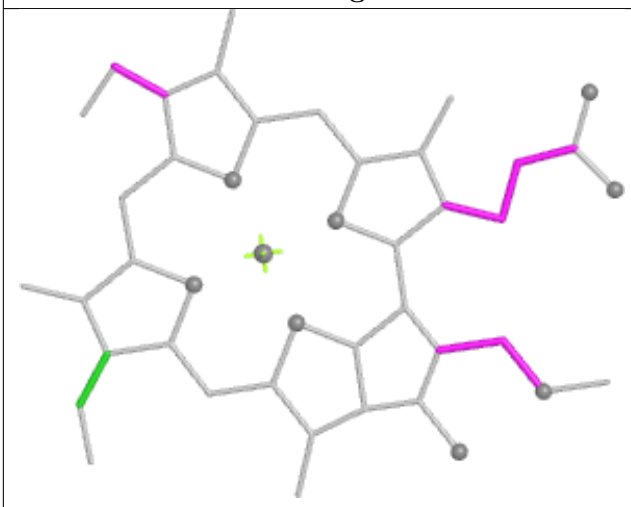
Ligand CLA a 606



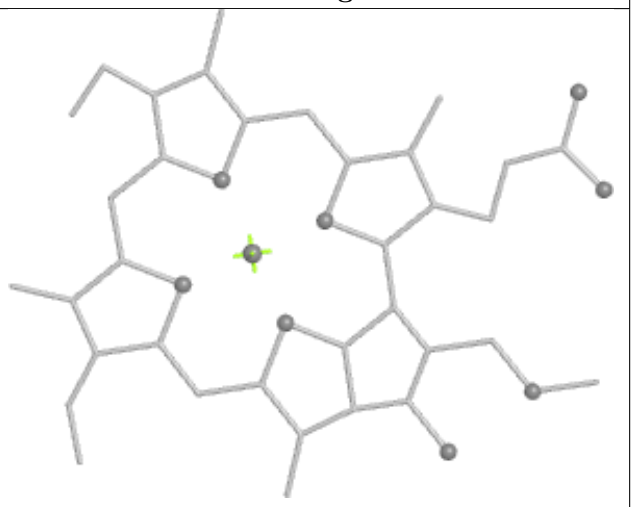
Bond lengths



Bond angles

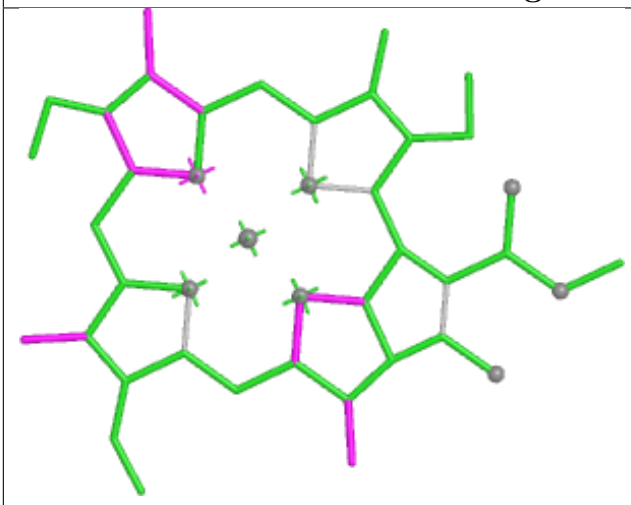


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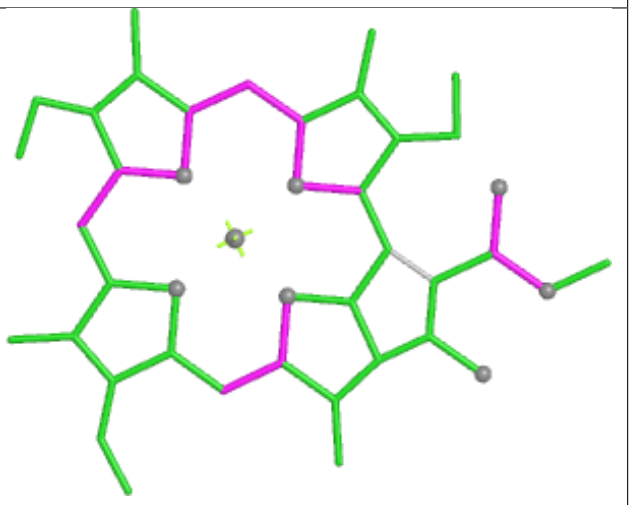


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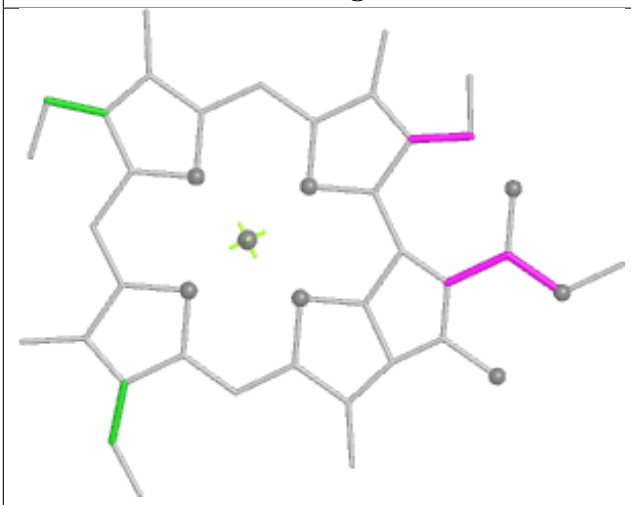
Ligand CLA B 822



Bond lengths



Bond angles

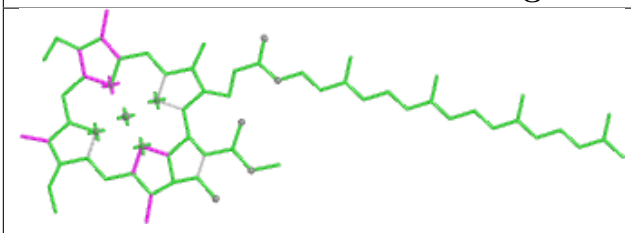


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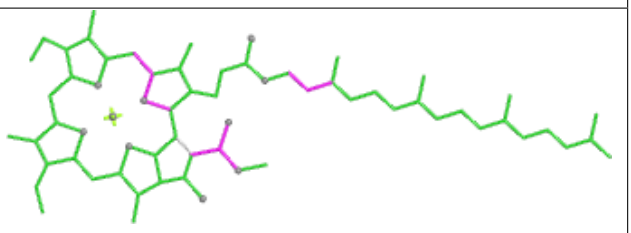


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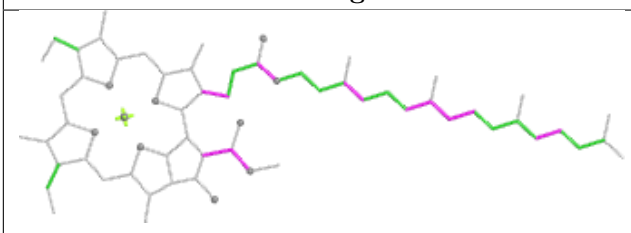
Ligand CLA A 811



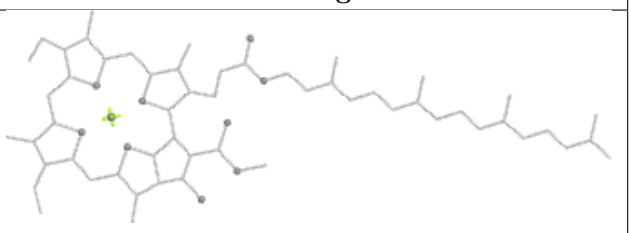
Bond lengths



Bond angles

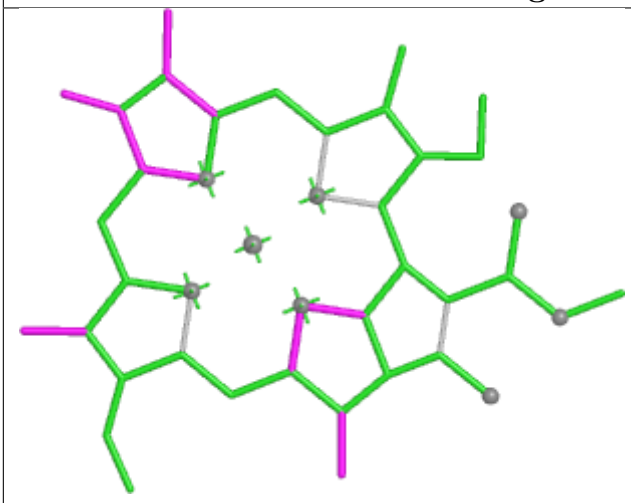


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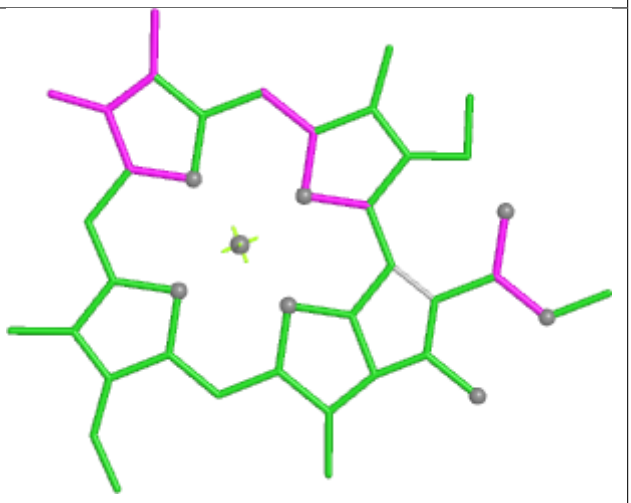


Rings

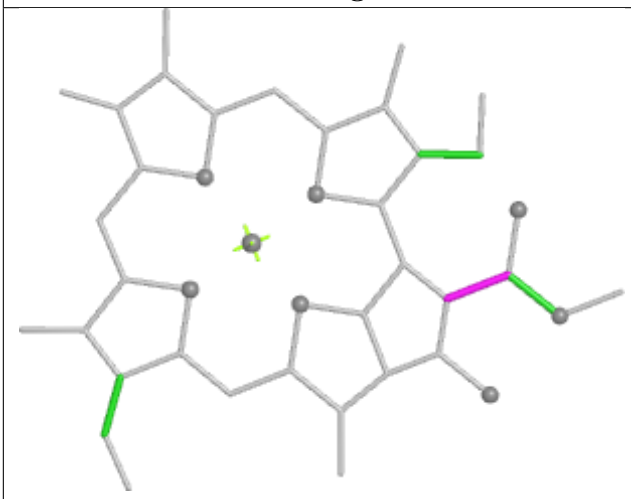
Ligand CLA 6 607



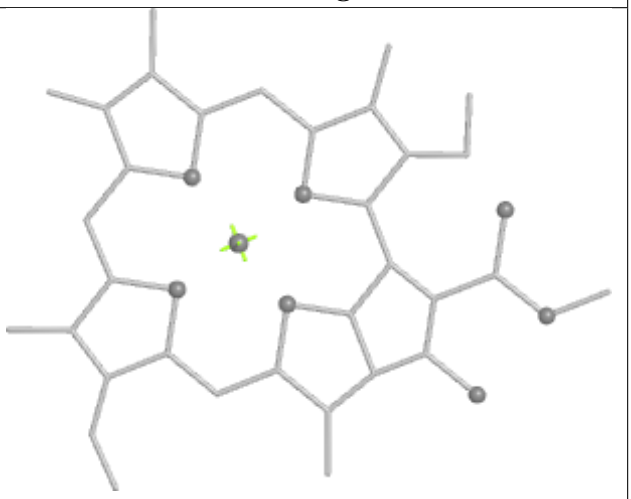
Bond lengths



Bond angles

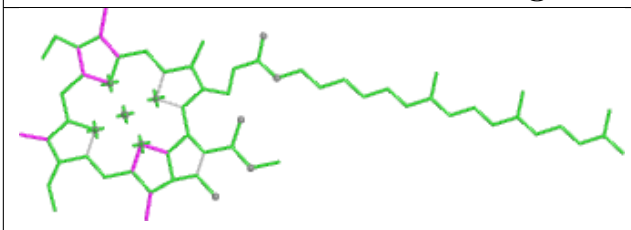


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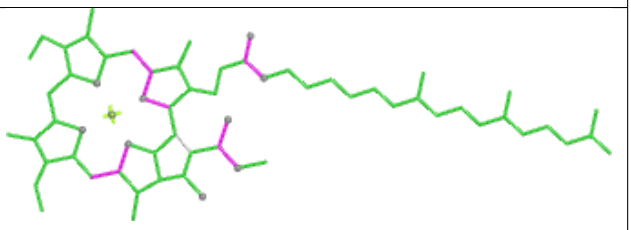


Rings

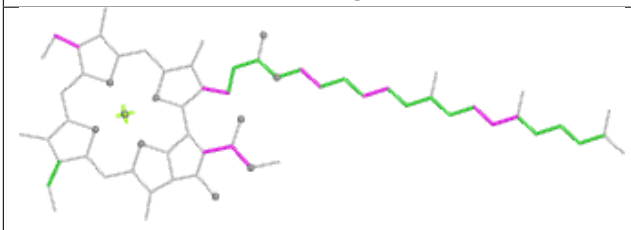
Ligand CLA 6 620



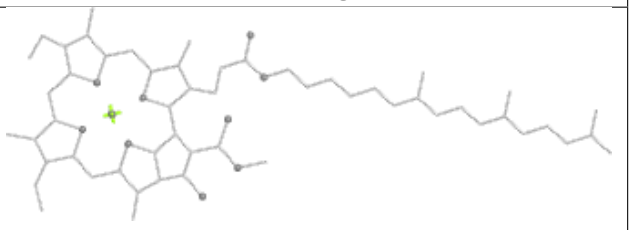
Bond lengths



Bond angles

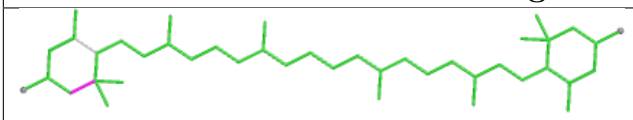


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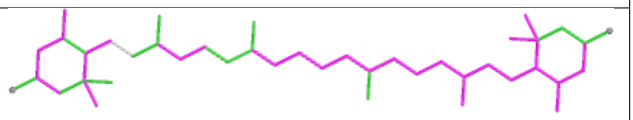


Rings

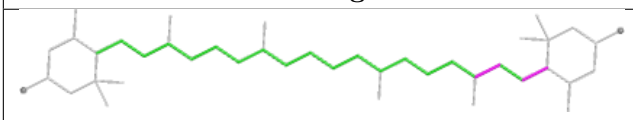
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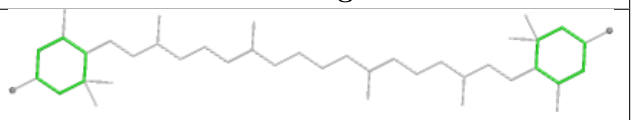
Bond lengths



Bond angles

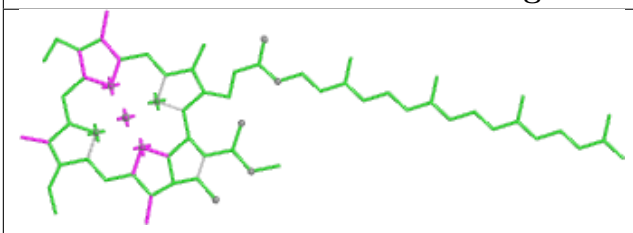


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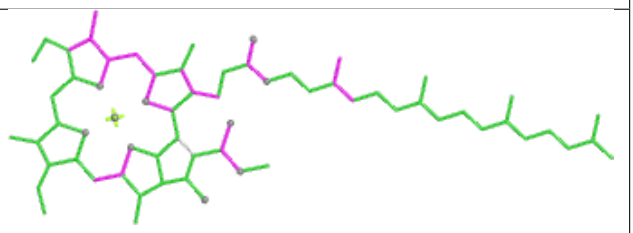


Rings

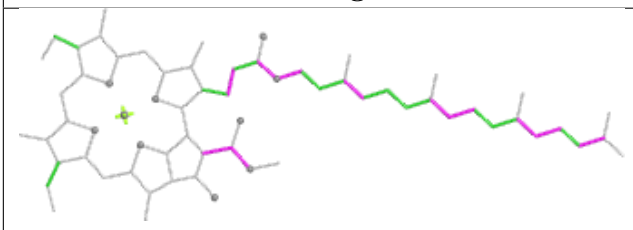
Ligand CLA A 814



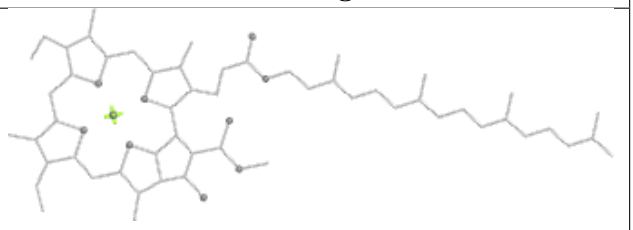
Bond lengths



Bond angles

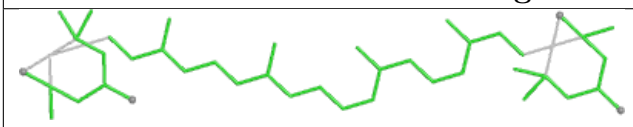


Torsions

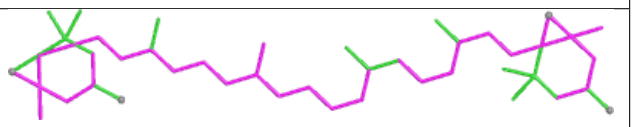


Rings

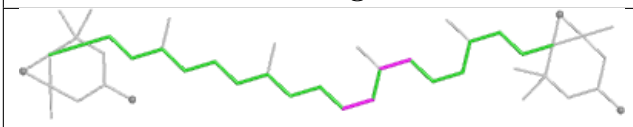
Ligand XAT Y 1622



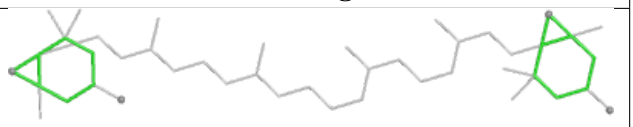
Bond lengths



Bond angles

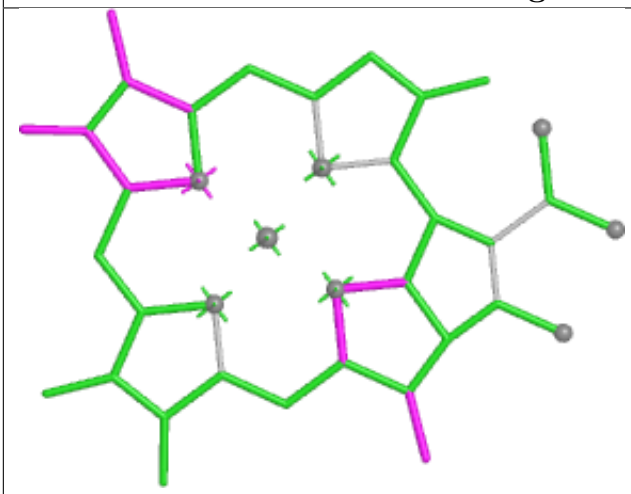


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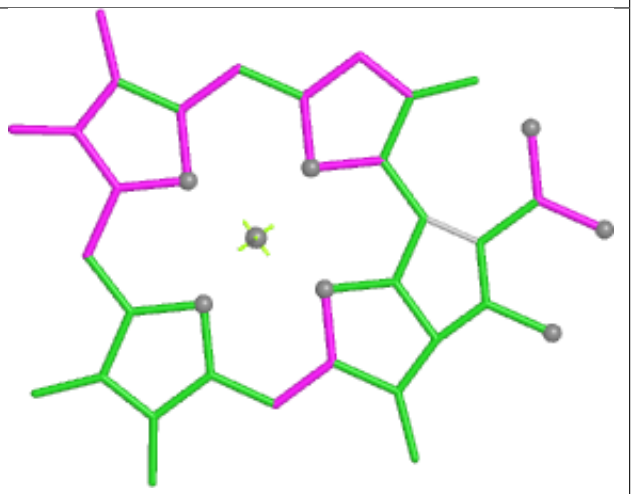


Rings

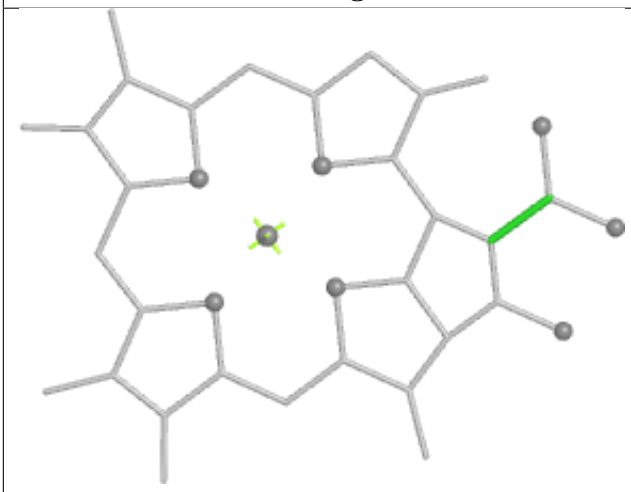
Ligand CLA 1 614



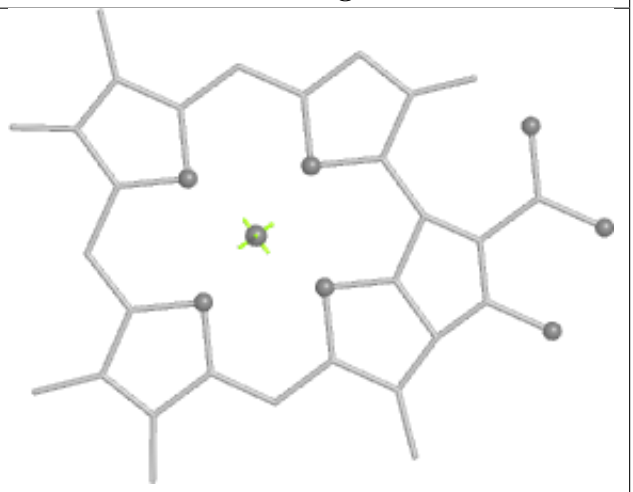
Bond lengths



Bond angles

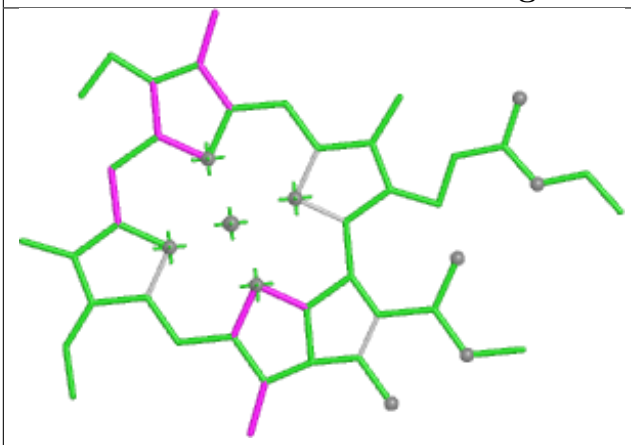


Torsions

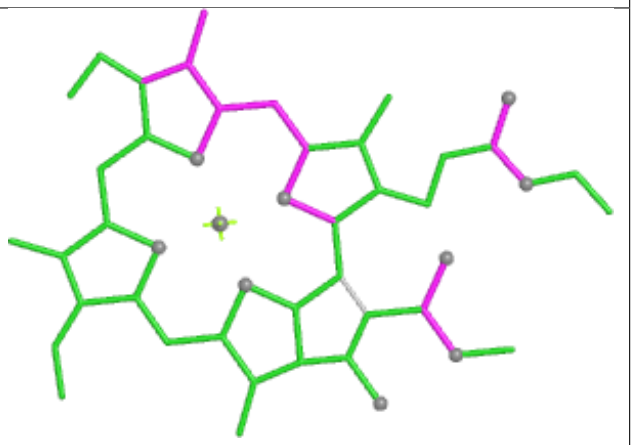


Rings

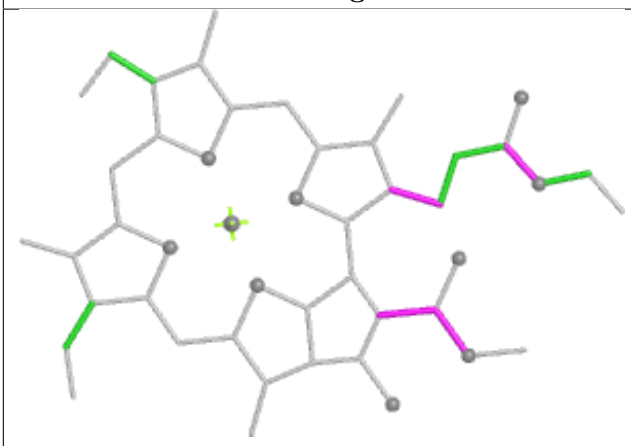
Ligand CLA W 604



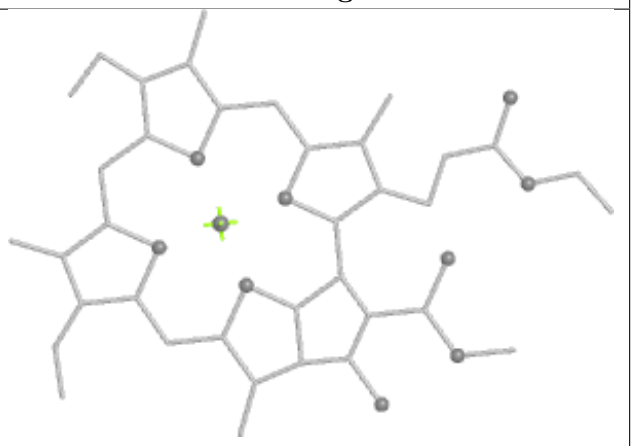
Bond lengths



Bond angles

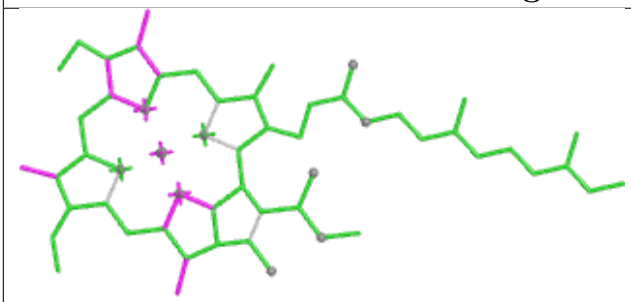


Torsions

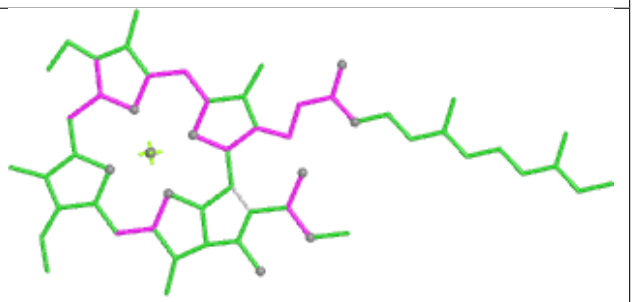


Rings

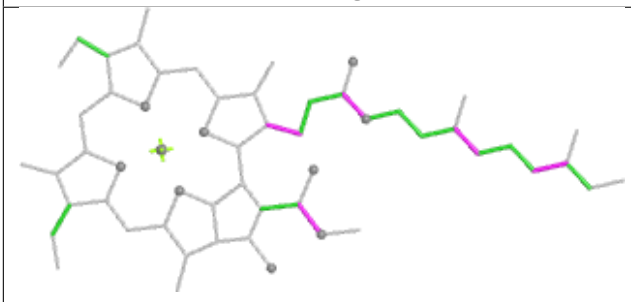
Ligand CLA K 203



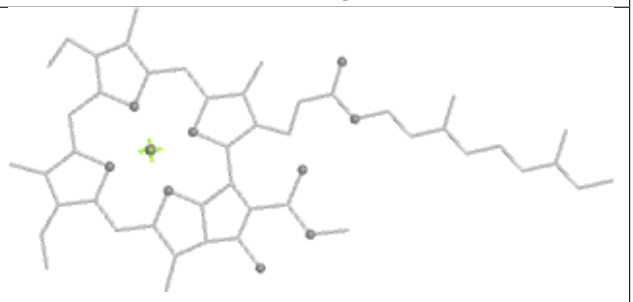
Bond lengths



Bond angles

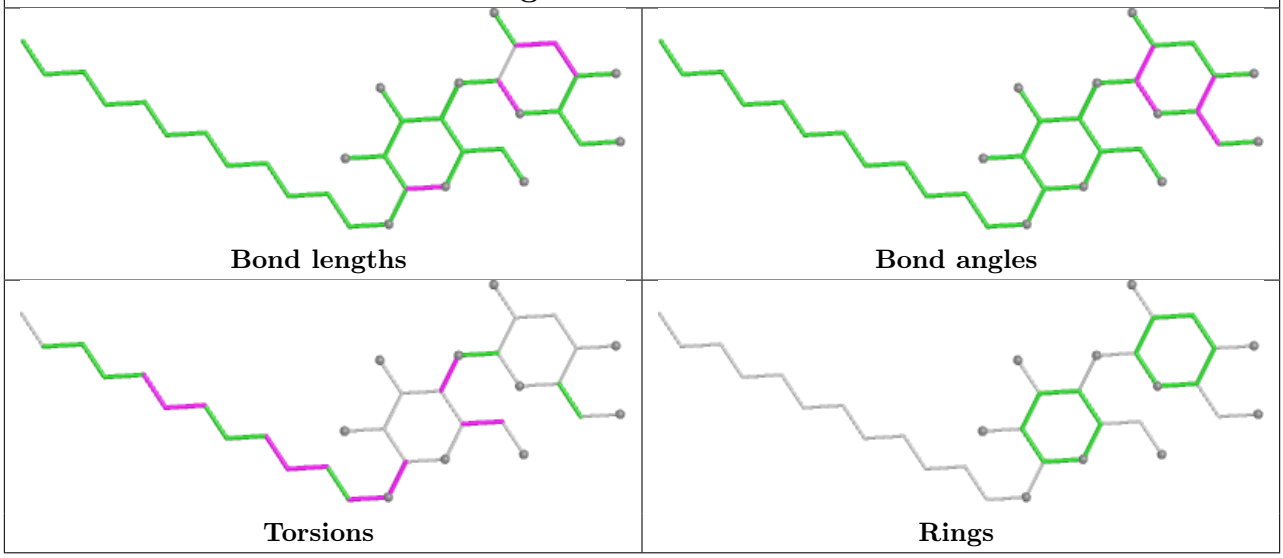


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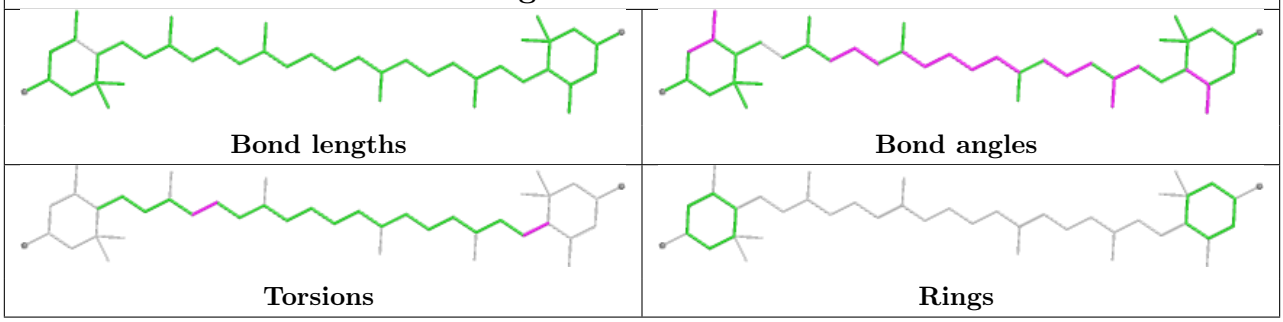


Rings

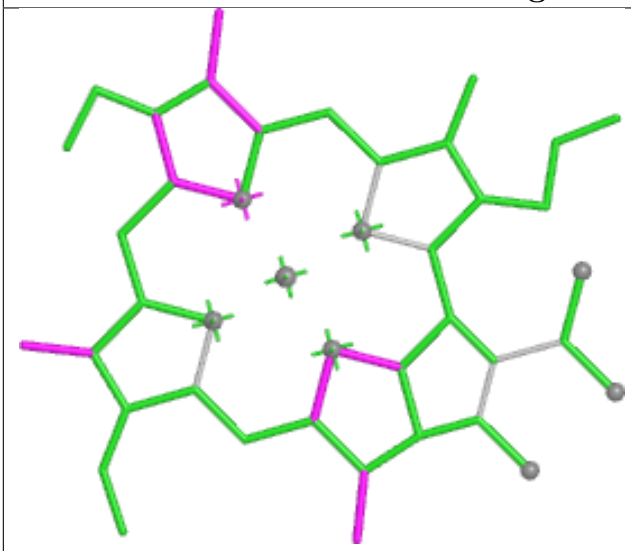
Ligand LMU A 858



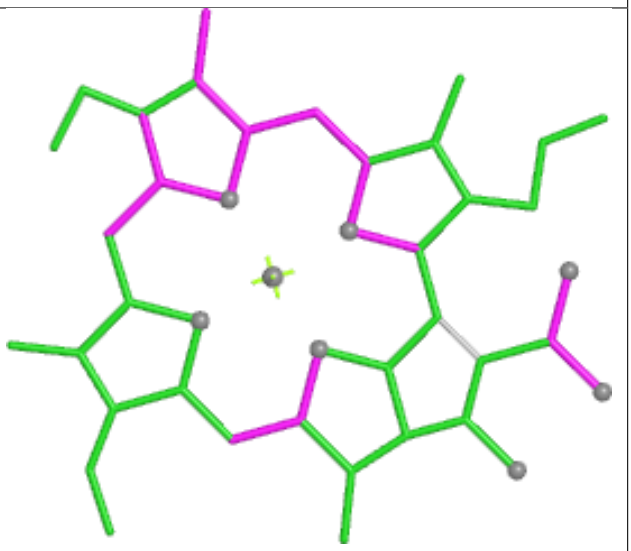
Ligand LUT Z 1621



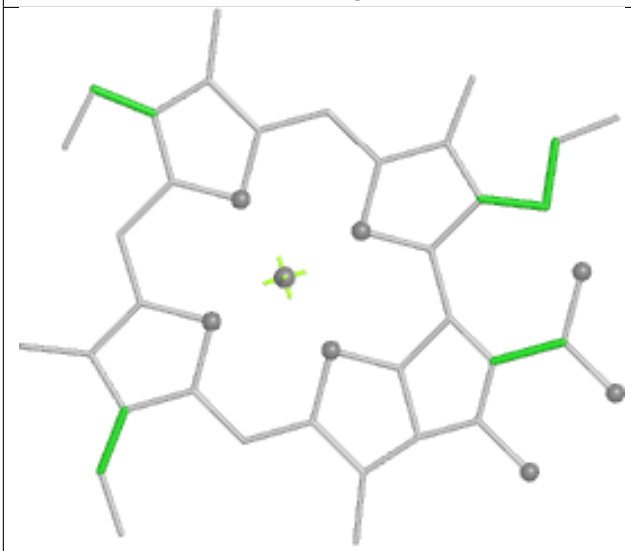
Ligand CLA 2 614



Bond lengths



Bond angles

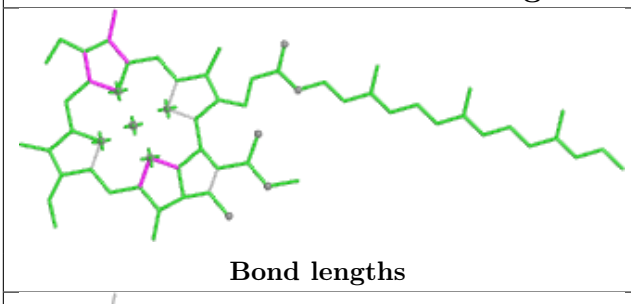


Torsions

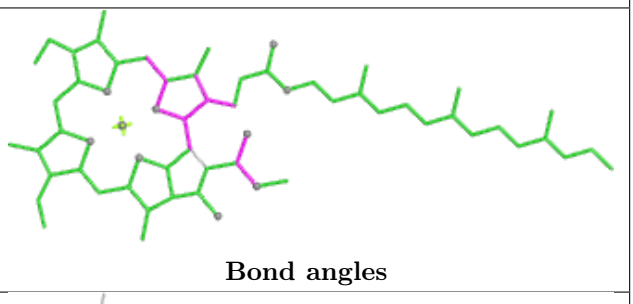


Rings

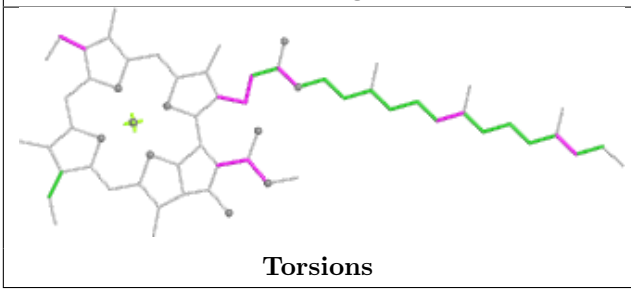
Ligand CLA X 603



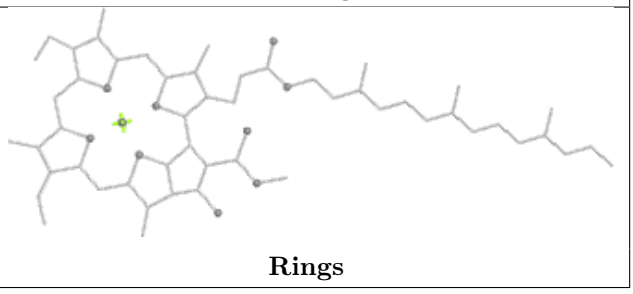
Bond lengths



Bond angles



Torsions

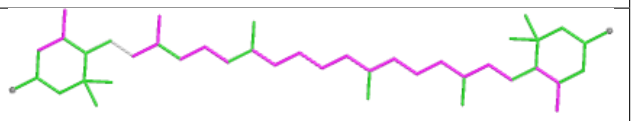


Rings

Ligand LUT V 1620



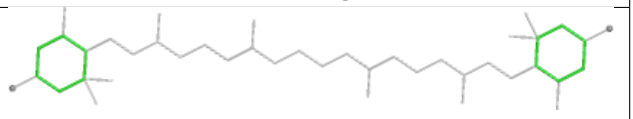
Bond lengths



Bond angles

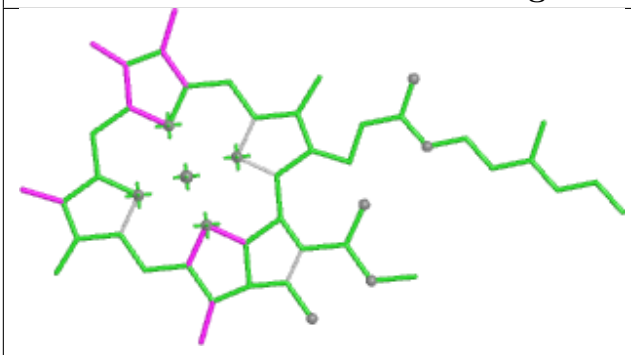


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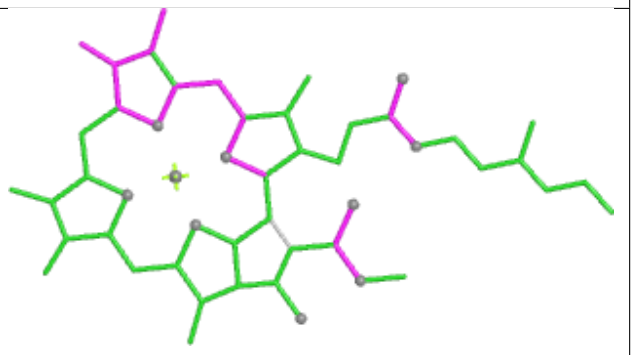


Rings

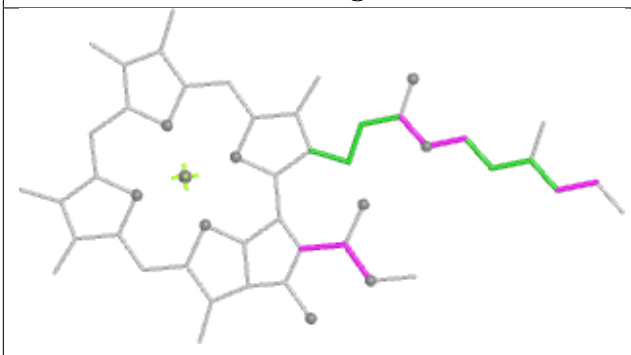
Ligand CLA 9 604



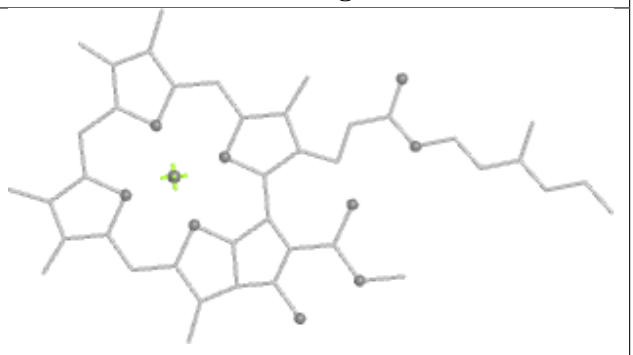
Bond lengths



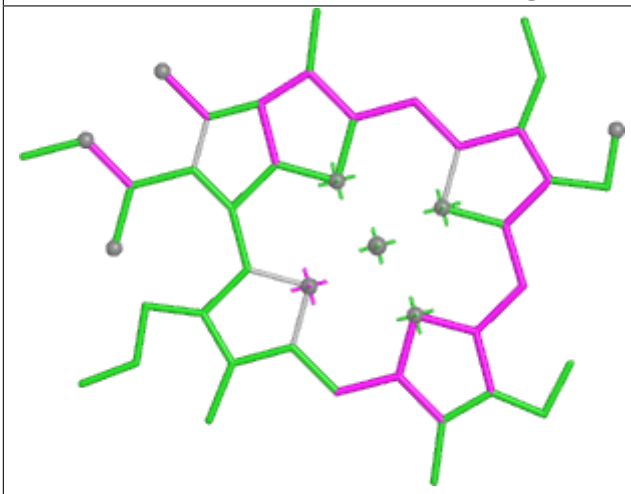
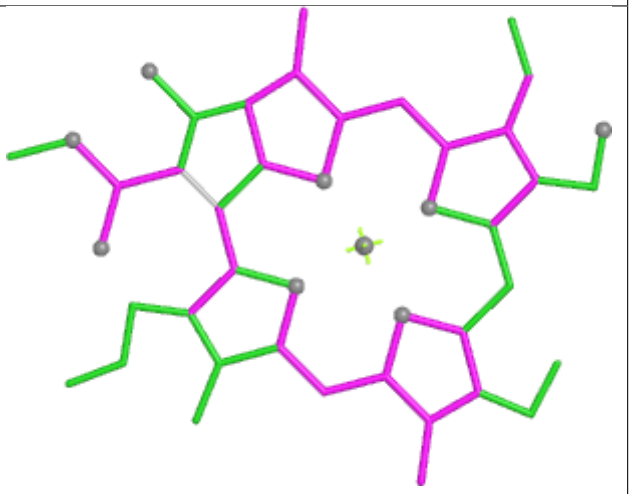
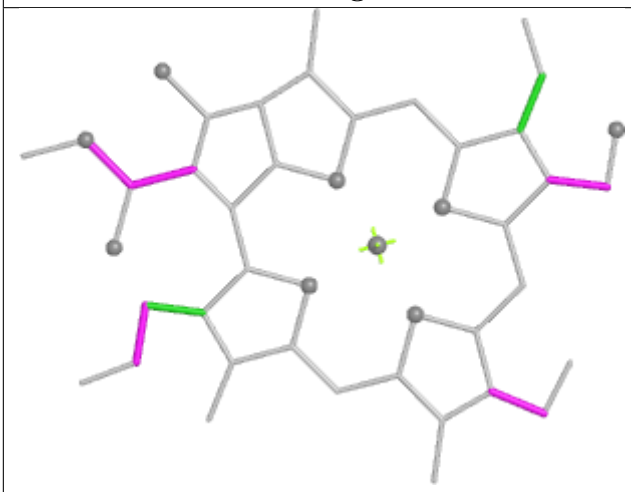
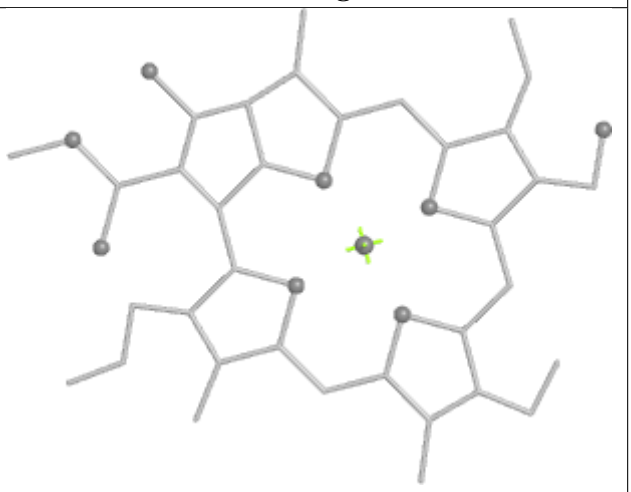
Bond angles

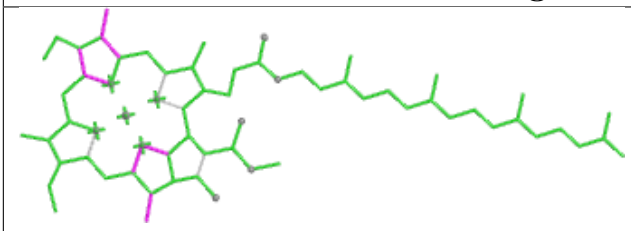
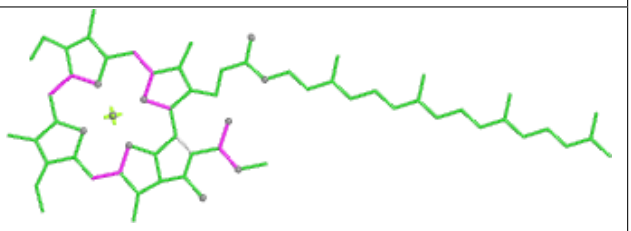
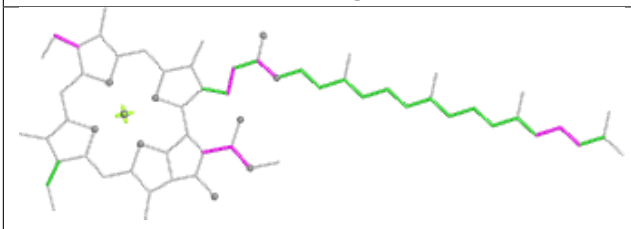
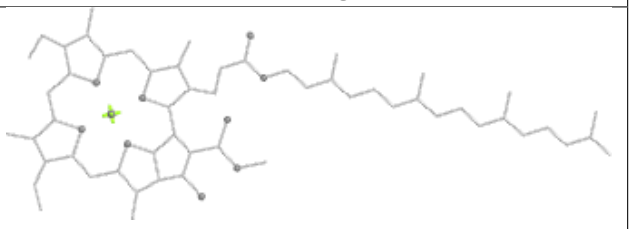


Torsions

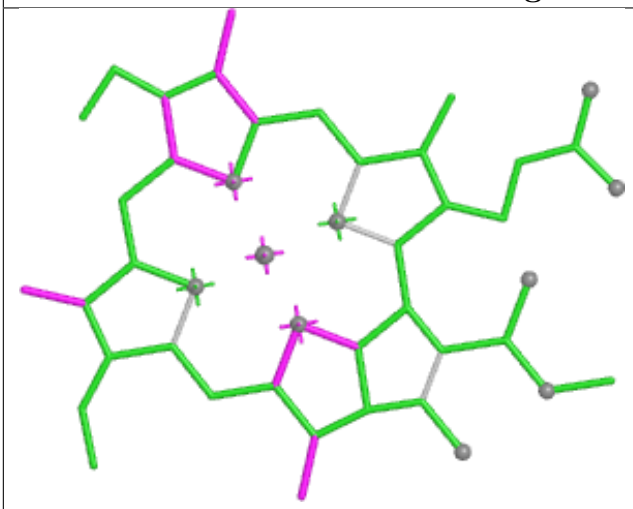


Rings

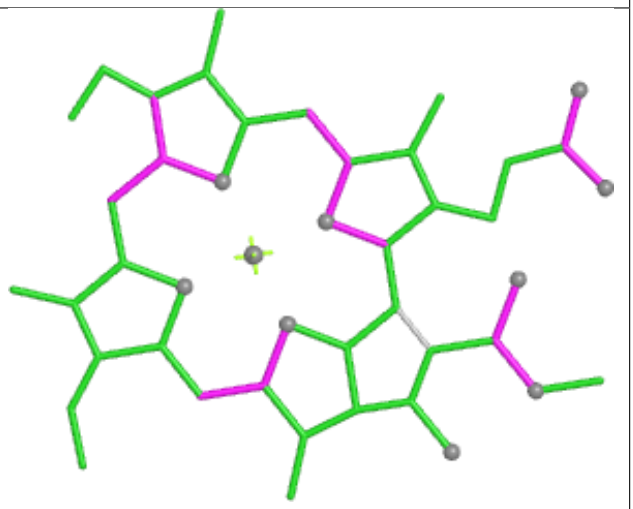
Ligand CHL U 606	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 2 613	
	
Bond lengths	Bond angles
	
Torsions	Rings

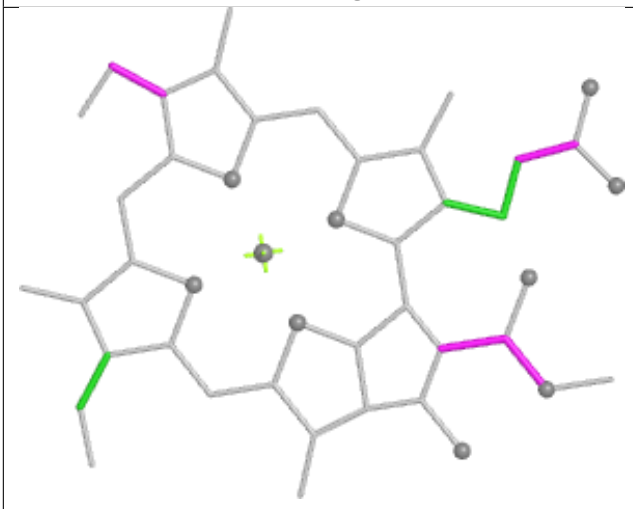
Ligand CLA B 823



Bond lengths



Bond angles

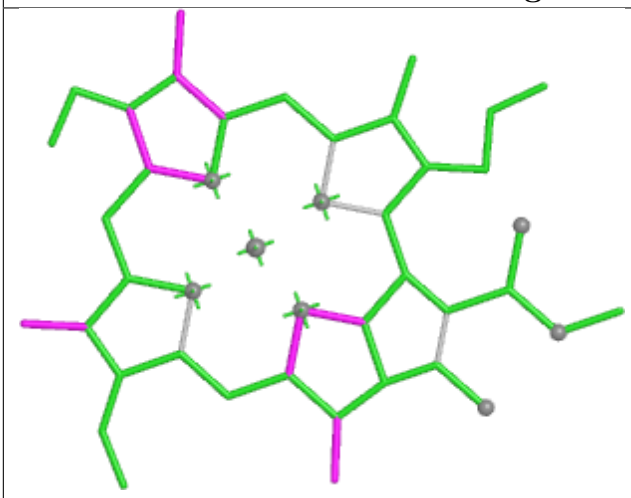


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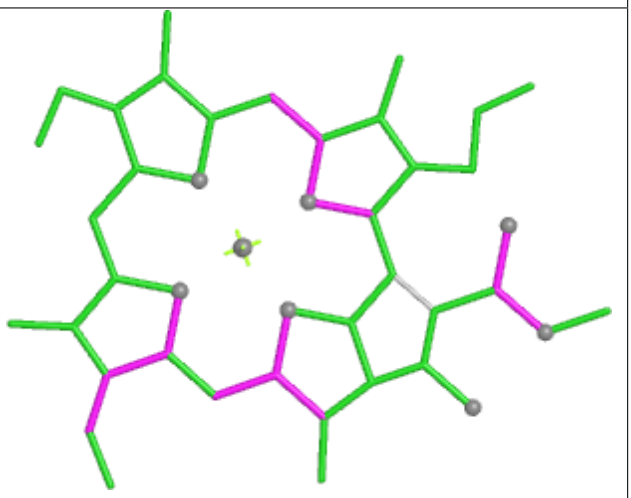


Rings

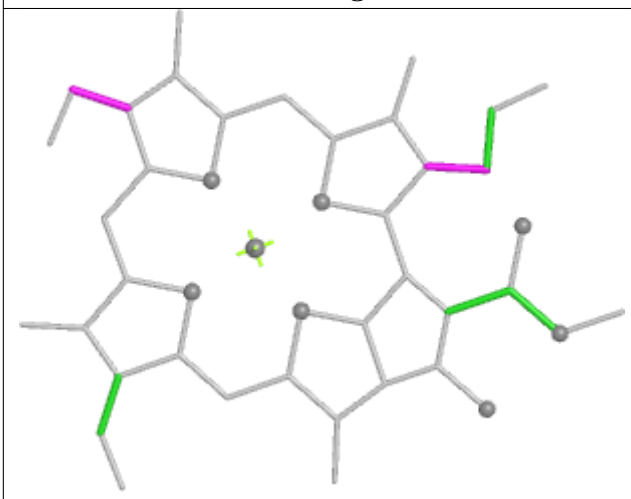
Ligand CLA B 830



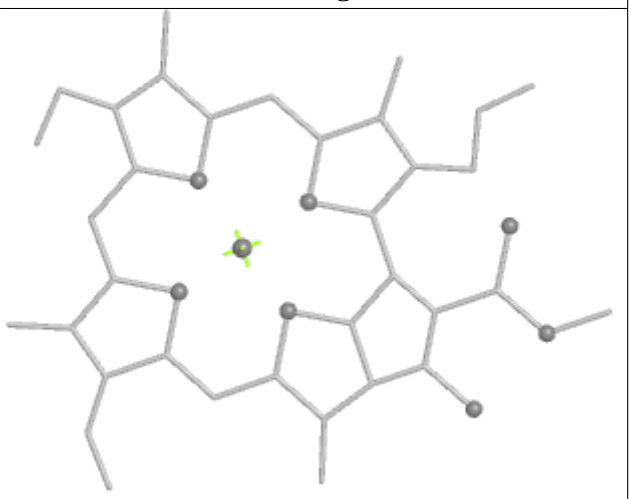
Bond lengths



Bond angles

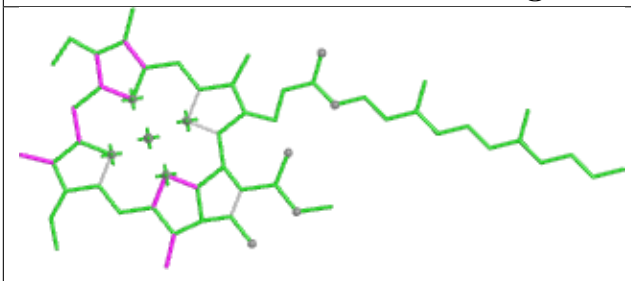


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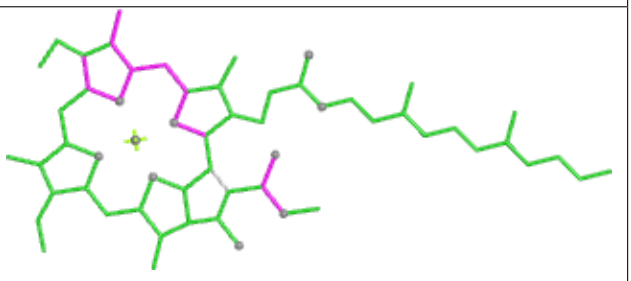


Rings

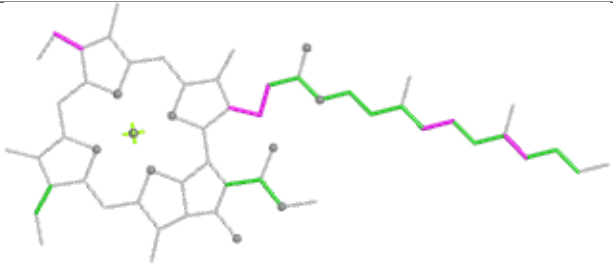
Ligand CLA Z 602



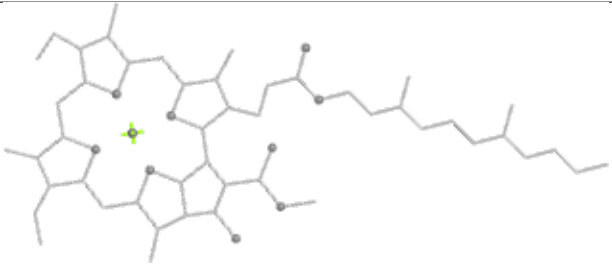
Bond lengths



Bond angles

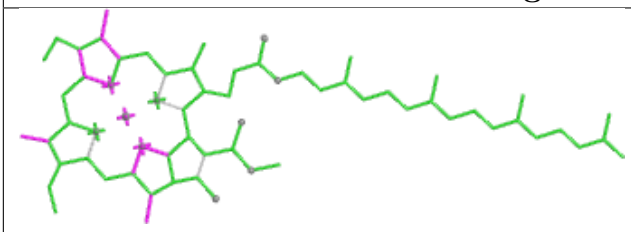


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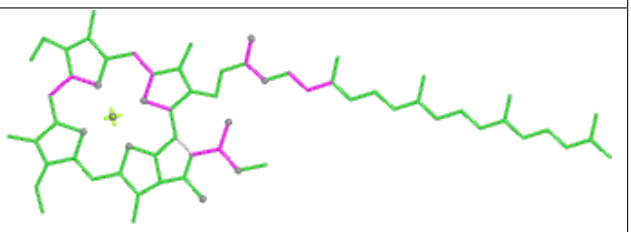


Rings

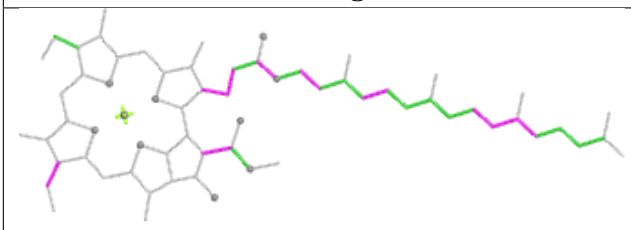
Ligand CLA A 804



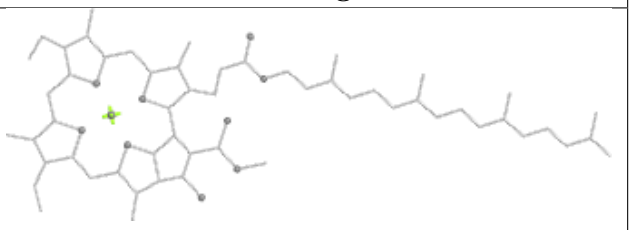
Bond lengths



Bond angles

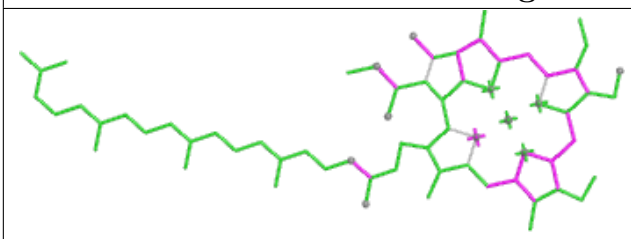


Torsions

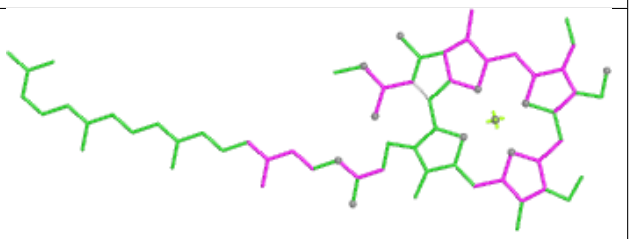


Rings

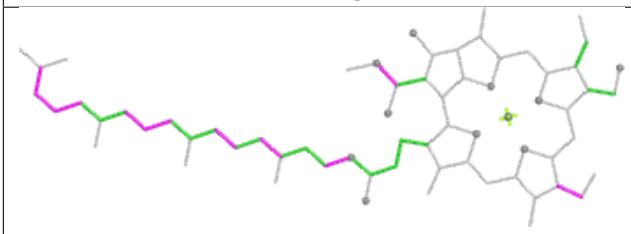
Ligand CHL W 609



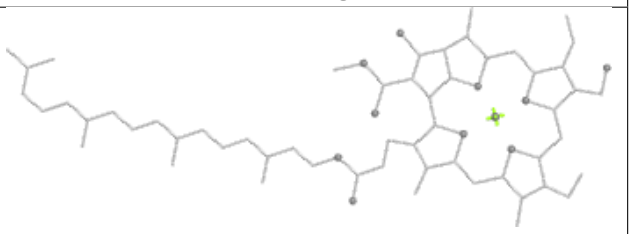
Bond lengths



Bond angles

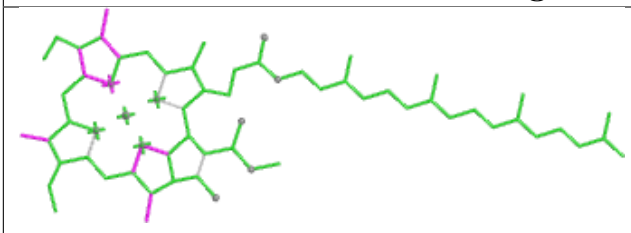


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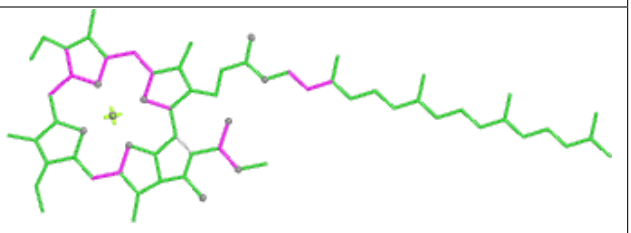


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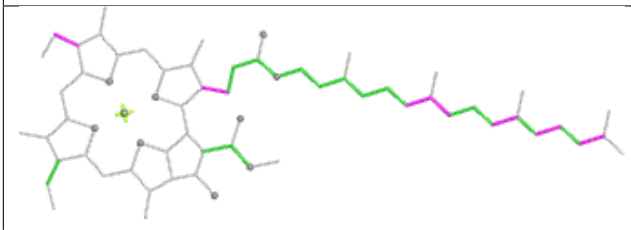
Ligand CLA 5 609



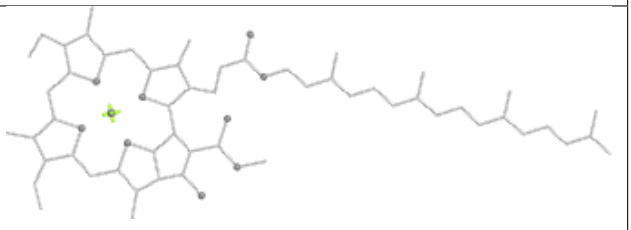
Bond lengths



Bond angles

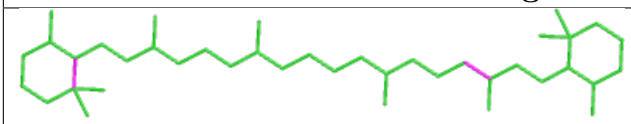


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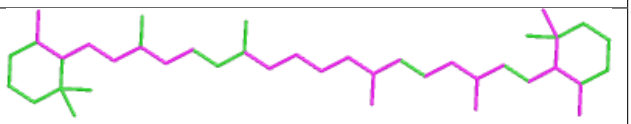


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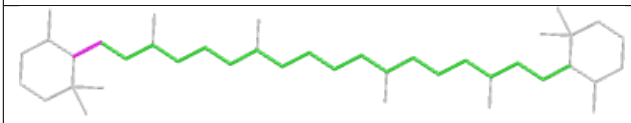
Ligand BCR A 856



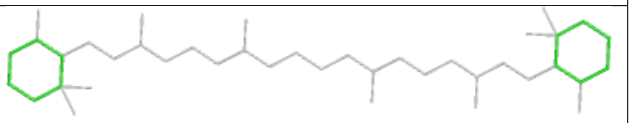
Bond lengths



Bond angles



Torsions



Rings

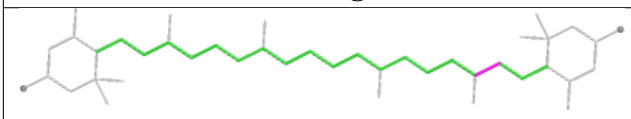
Ligand LUT 7 619



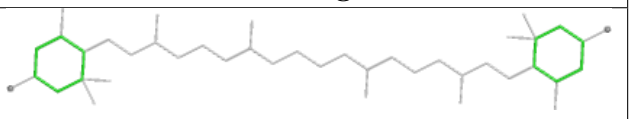
Bond lengths



Bond angles

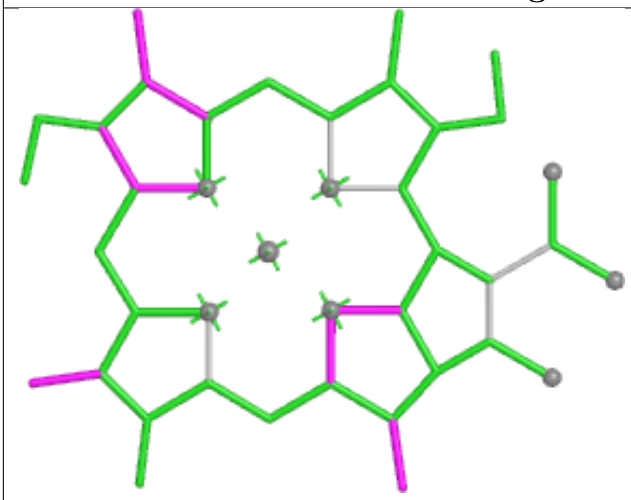


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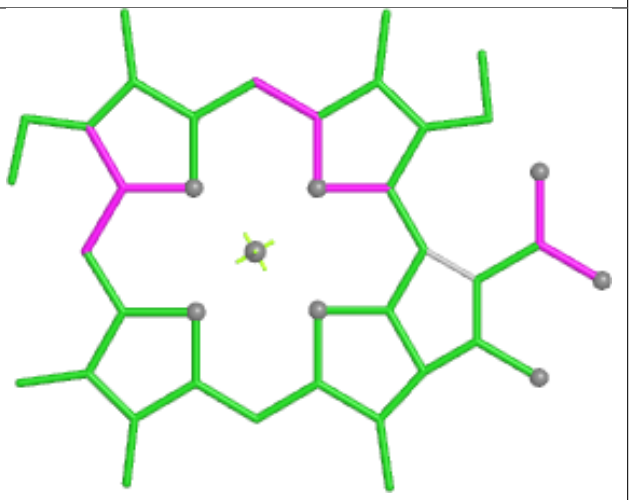


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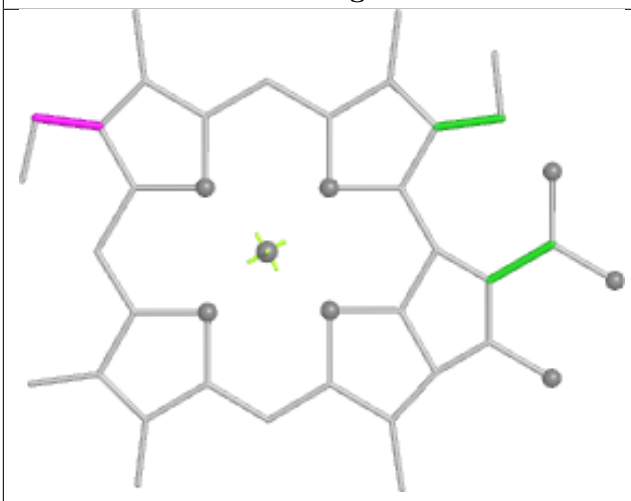
Ligand CLA 6 606



Bond lengths



Bond angles

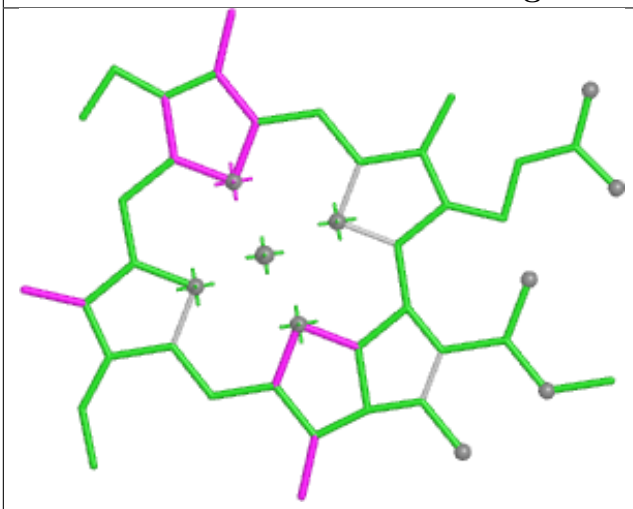


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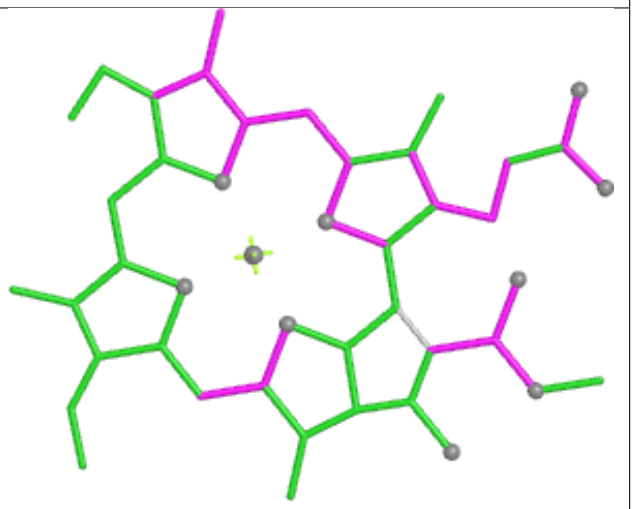


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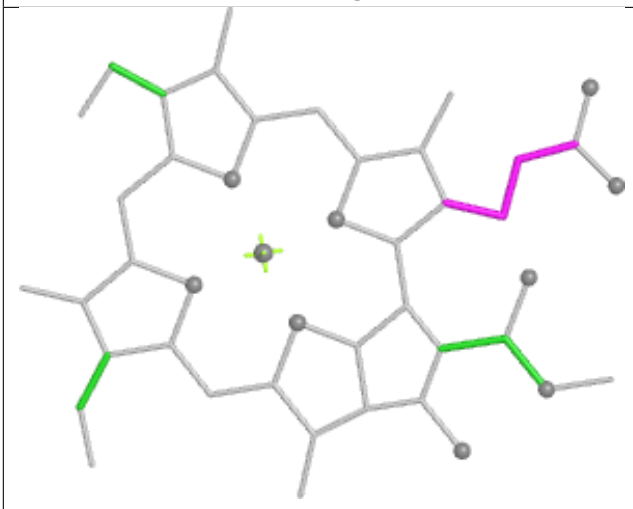
Ligand CLA A 833



Bond lengths



Bond angles

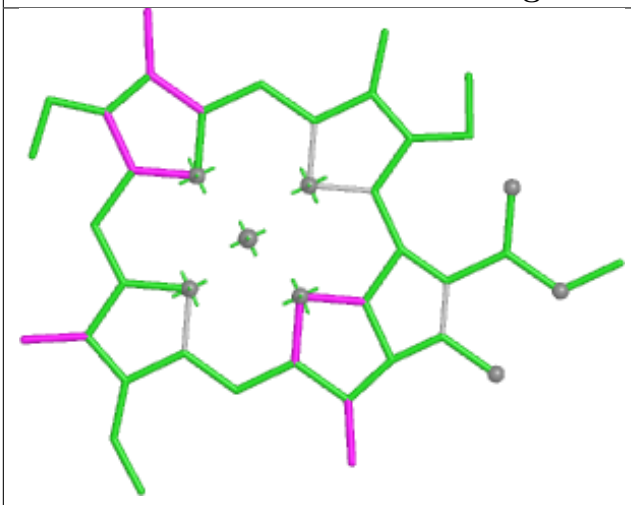


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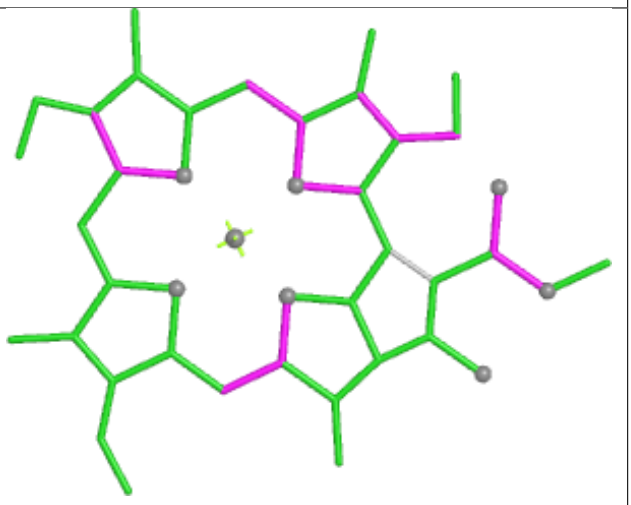


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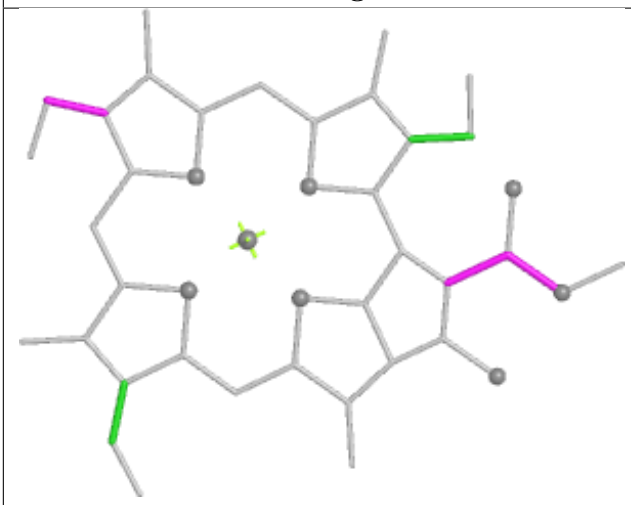
Ligand CLA G 203



Bond lengths



Bond angles

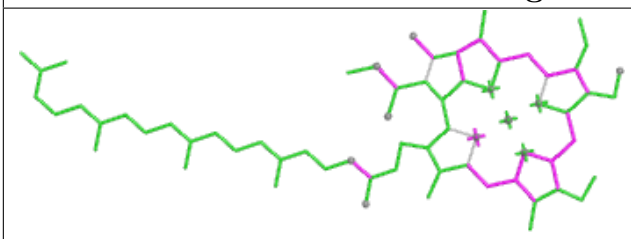


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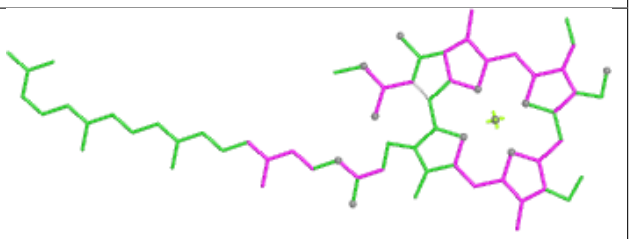


Rings

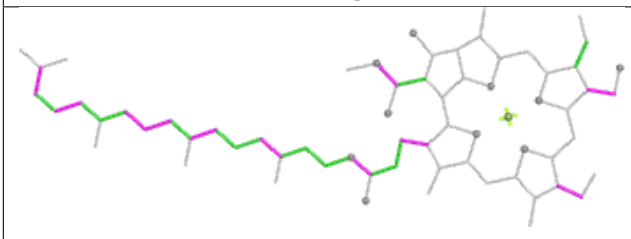
Ligand CHL Z 609



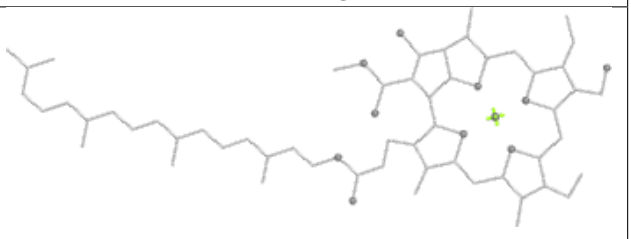
Bond lengths



Bond angles

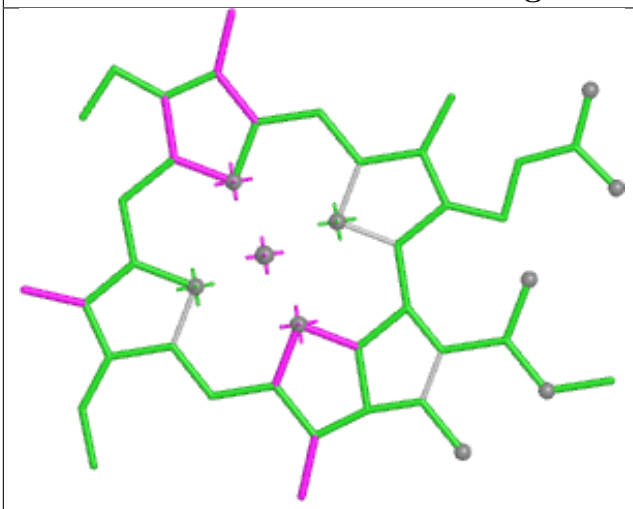


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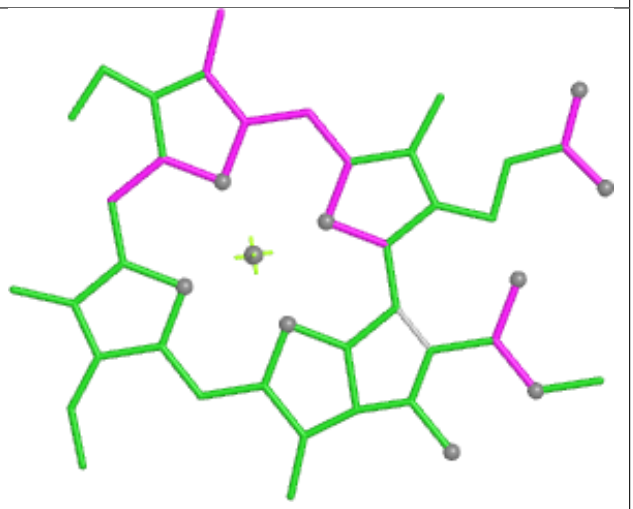


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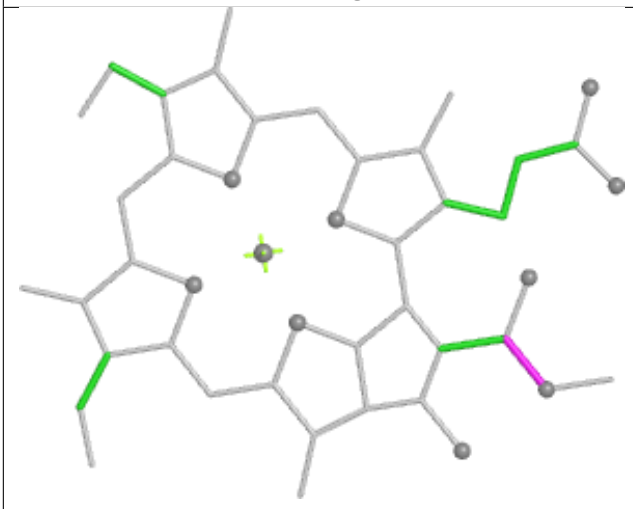
Ligand CLA B 835



Bond lengths



Bond angles

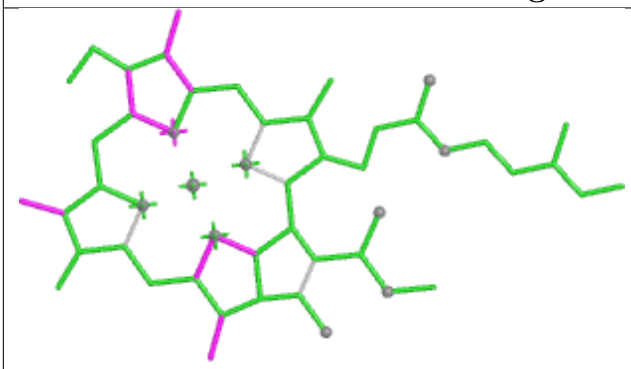


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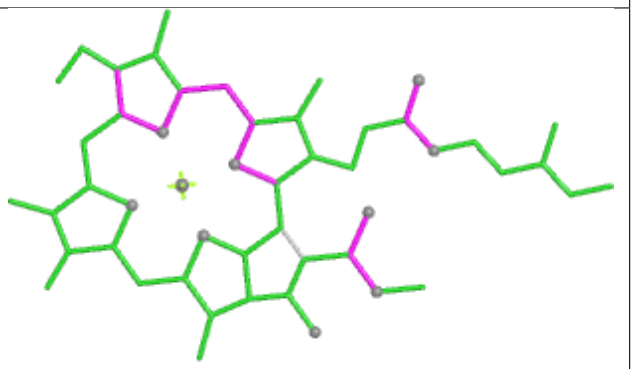


Rings

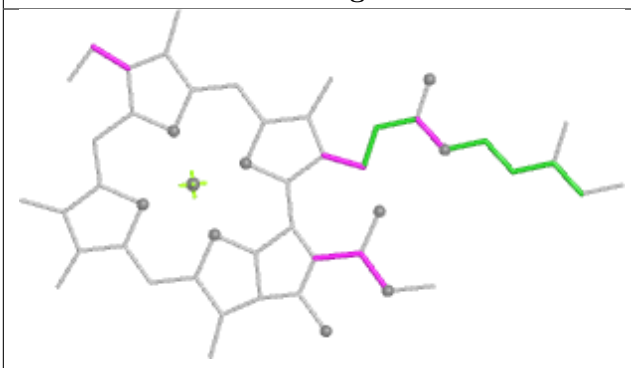
Ligand CLA 7 604



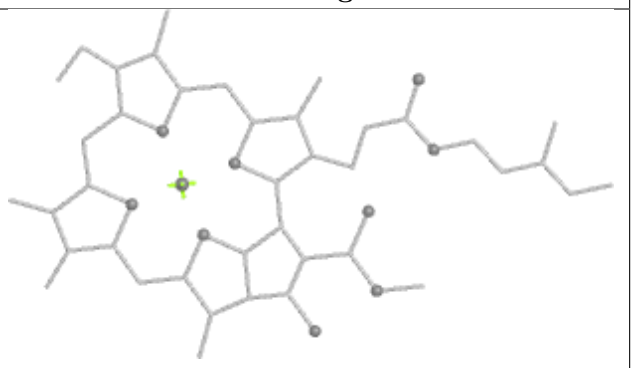
Bond lengths



Bond angles

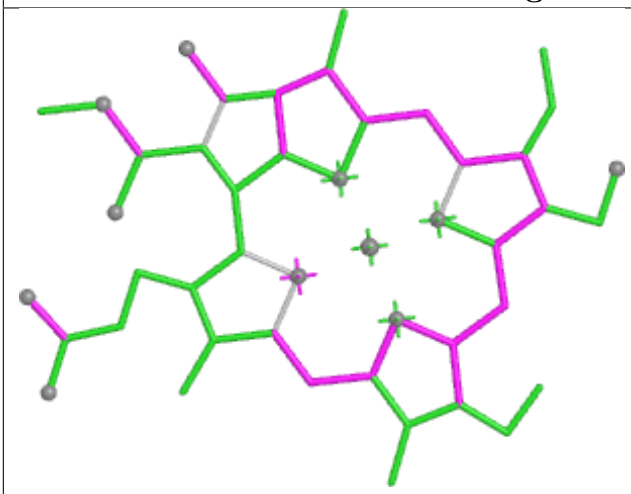


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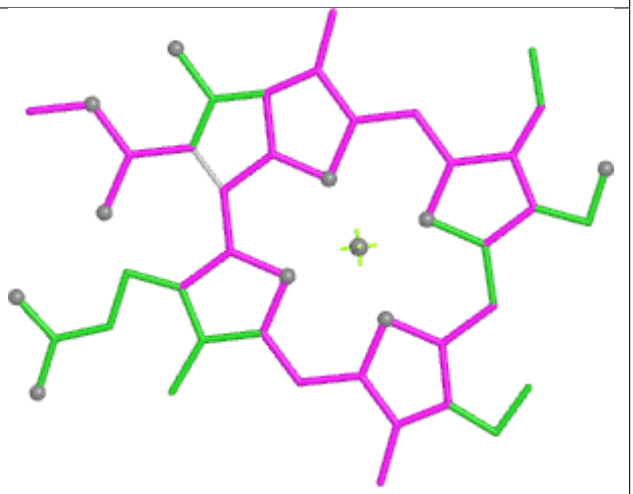


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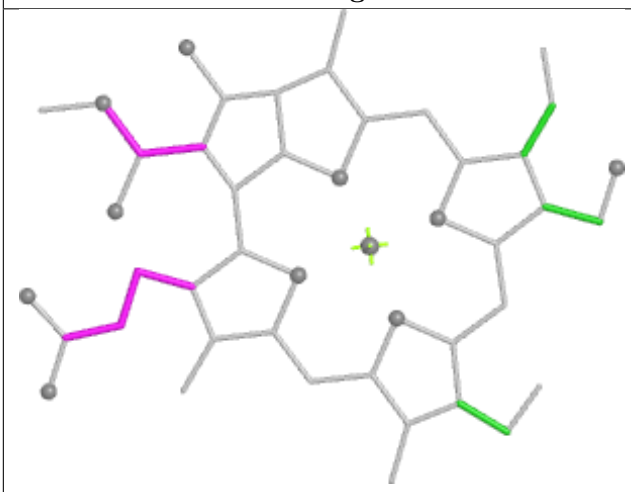
Ligand CHL Z 606



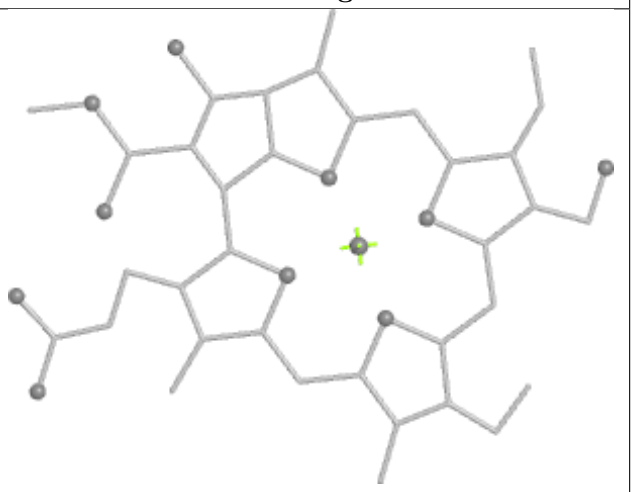
Bond lengths



Bond angles

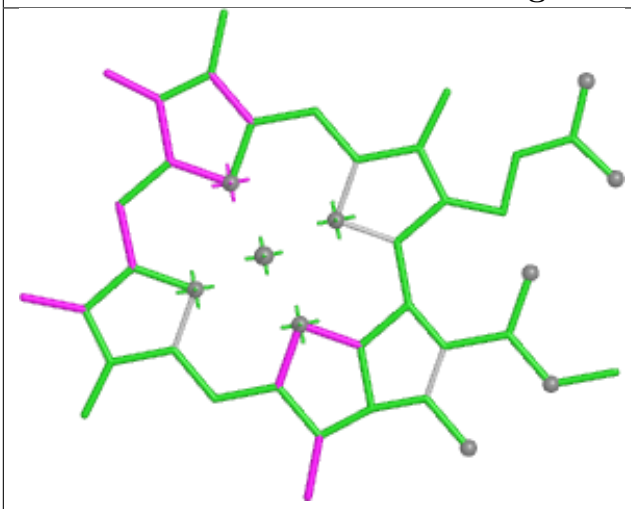


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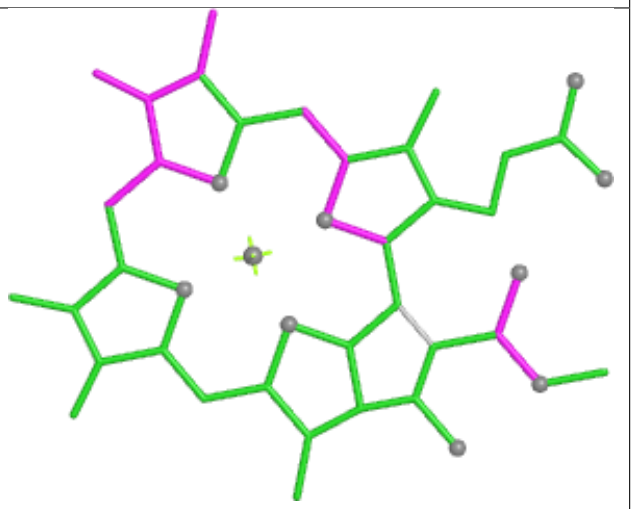


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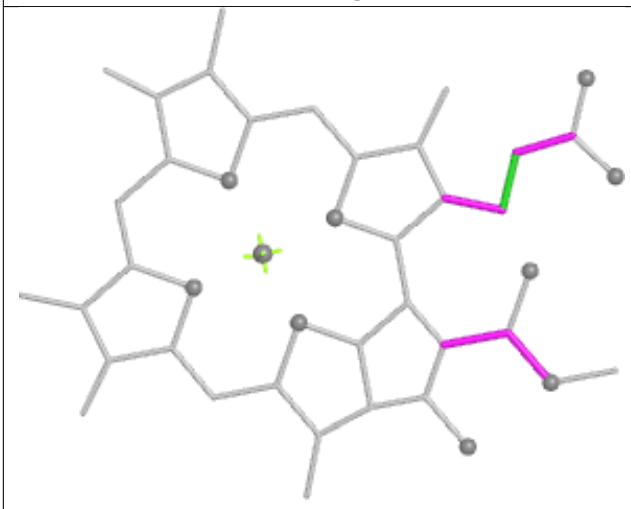
Ligand CLA 7 616



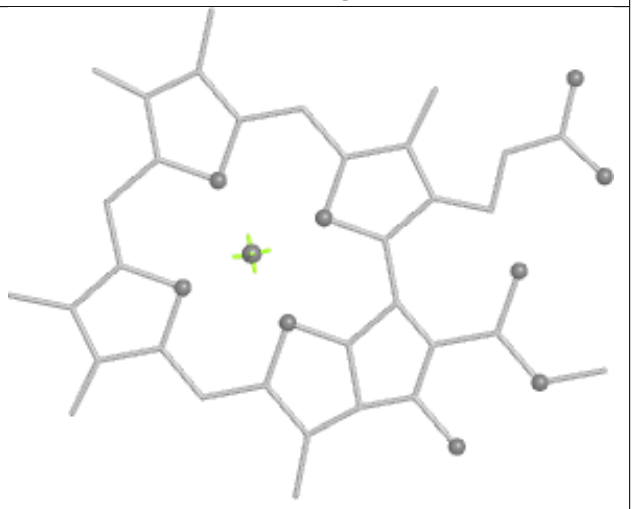
Bond lengths



Bond angles

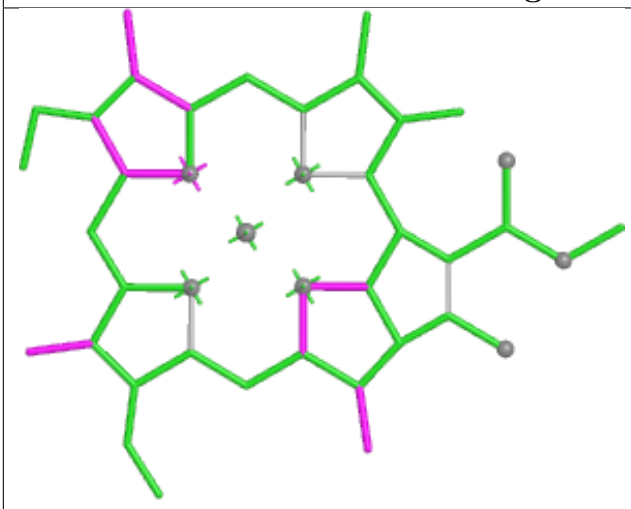


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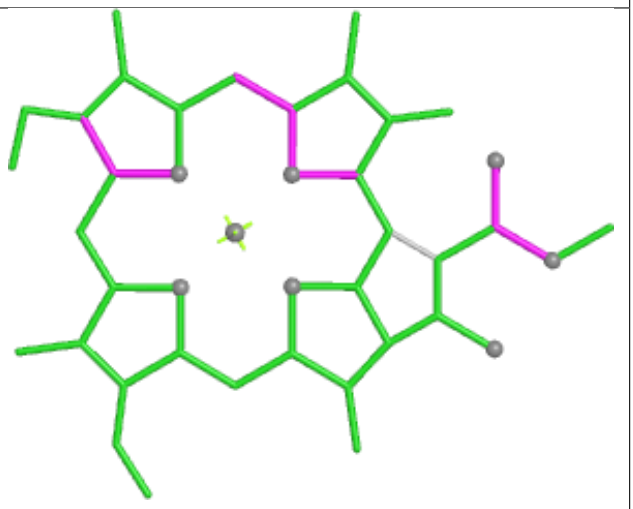


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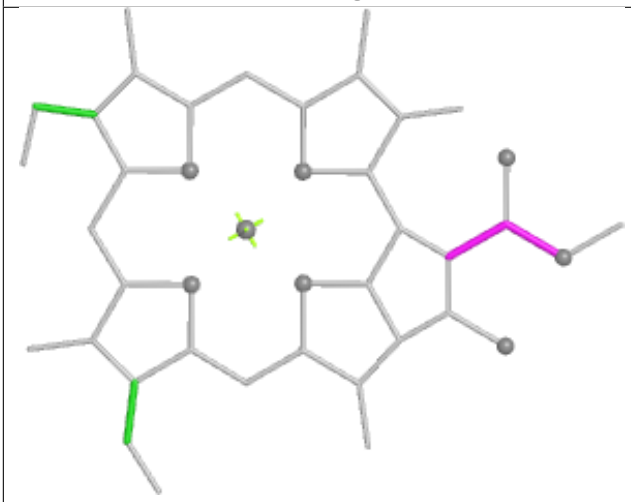
Ligand CLA B 804



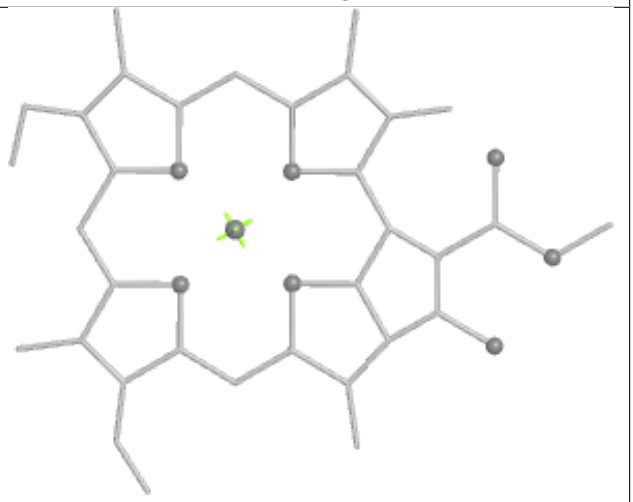
Bond lengths



Bond angles

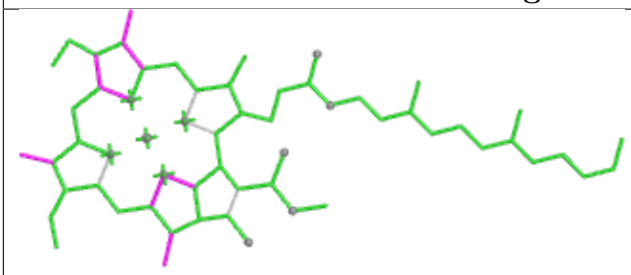


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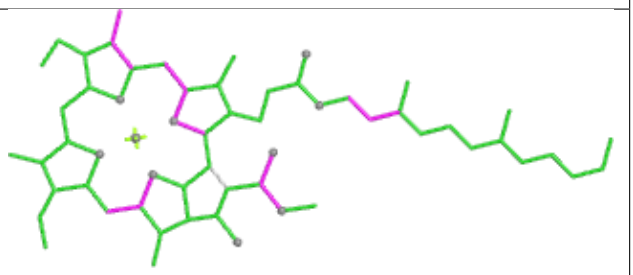


Rings

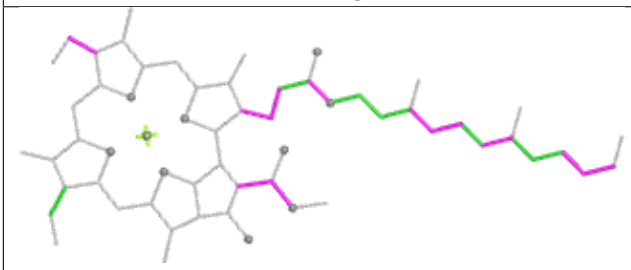
Ligand CLA U 602



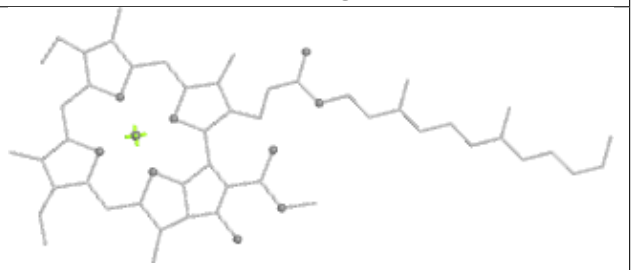
Bond lengths



Bond angles

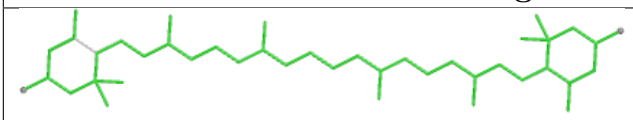


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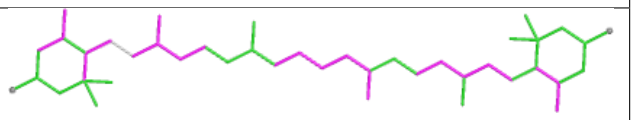


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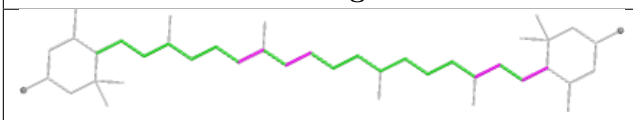
Ligand LUT U 1620



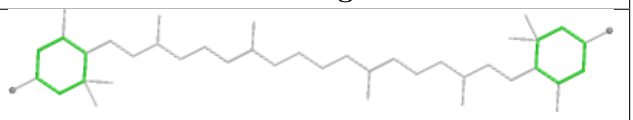
Bond lengths



Bond angles



Torsions

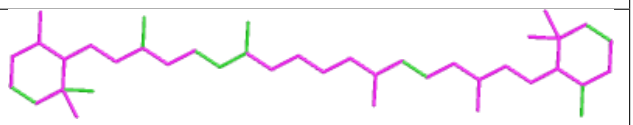


Rings

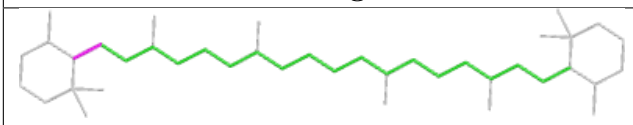
Ligand BCR A 851



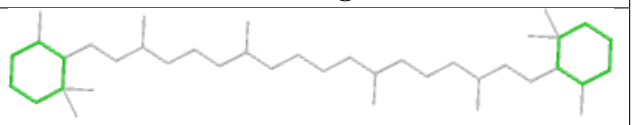
Bond lengths



Bond angles

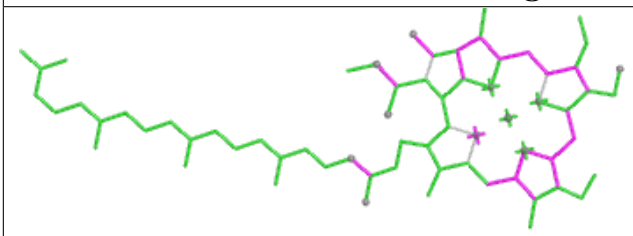


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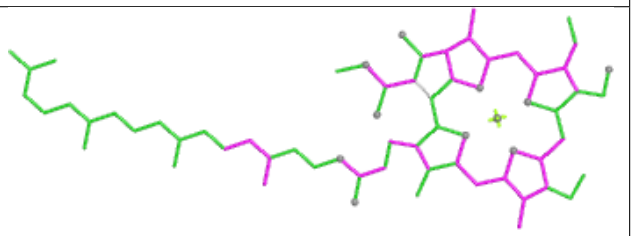


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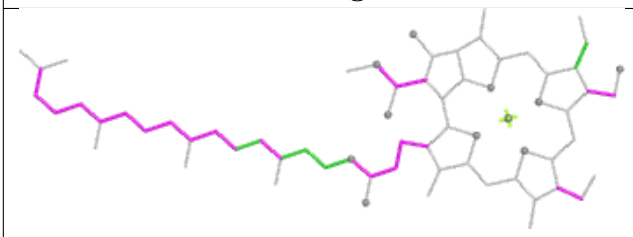
Ligand CHL X 607



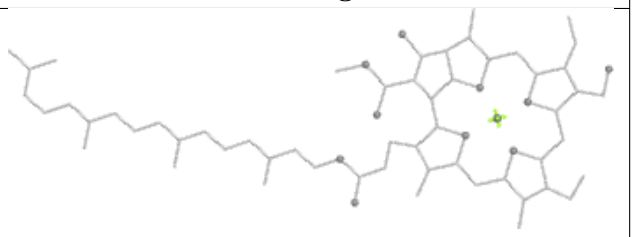
Bond lengths



Bond angles

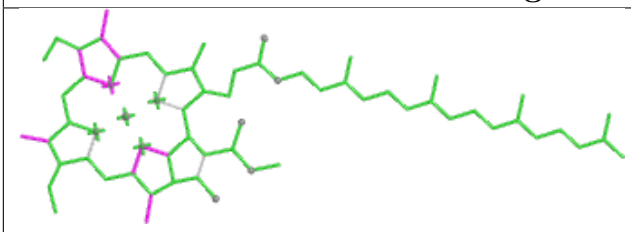


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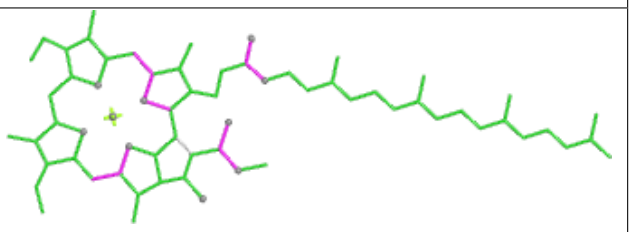


Rings

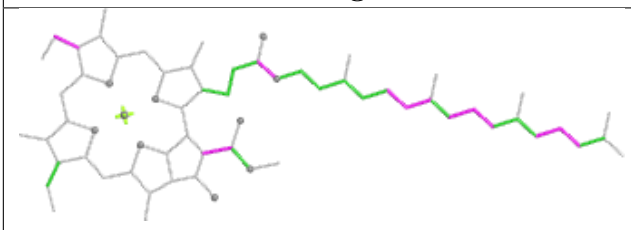
Ligand CLA B 833



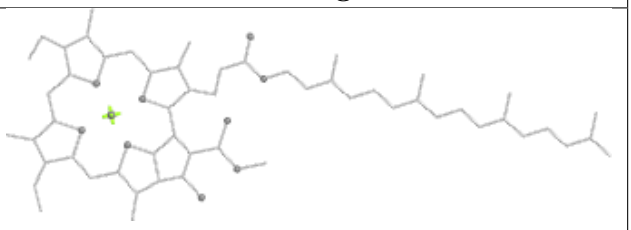
Bond lengths



Bond angles

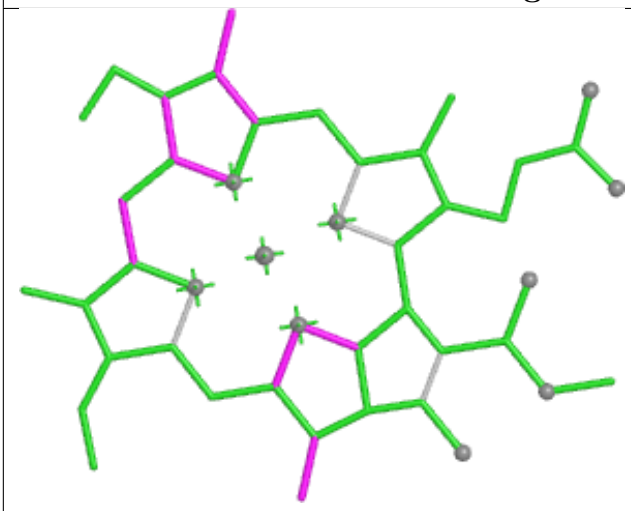


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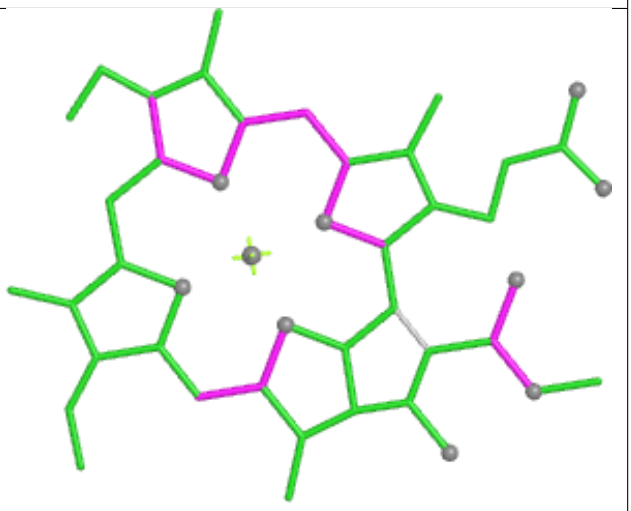


Rings

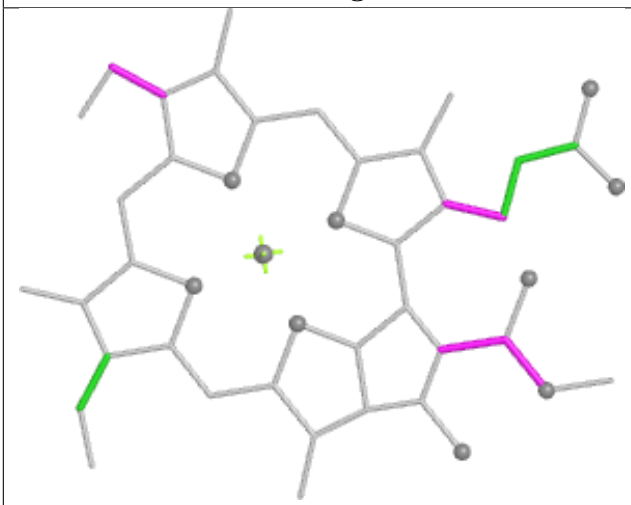
Ligand CLA V 614



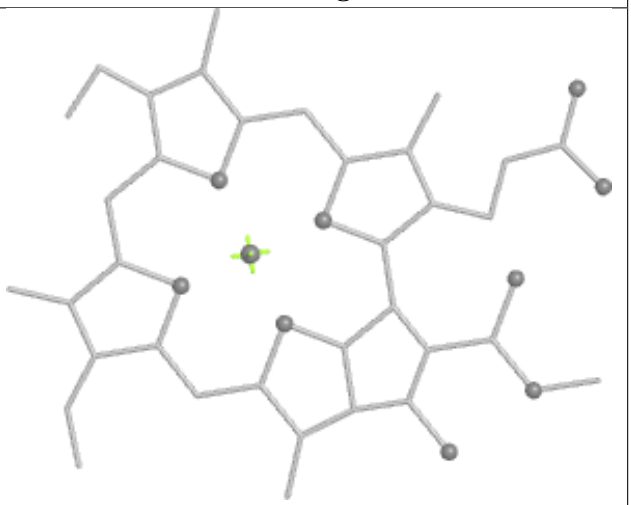
Bond lengths



Bond angles

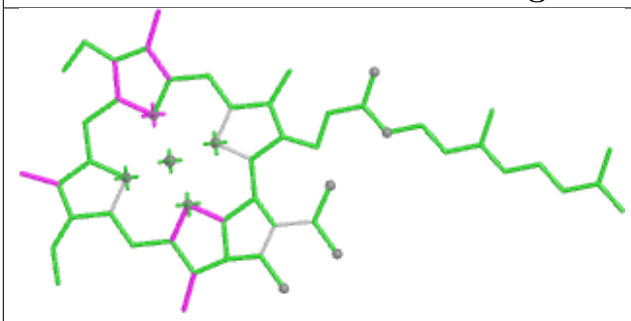


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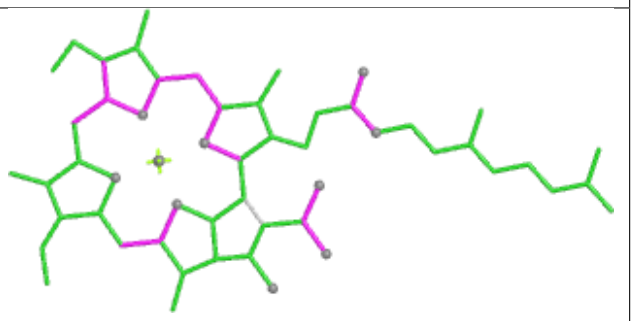


Rings

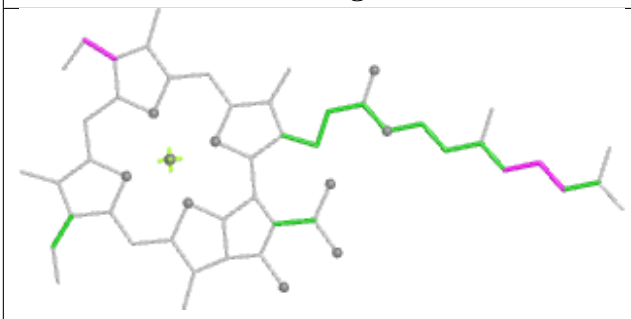
Ligand CLA a 601



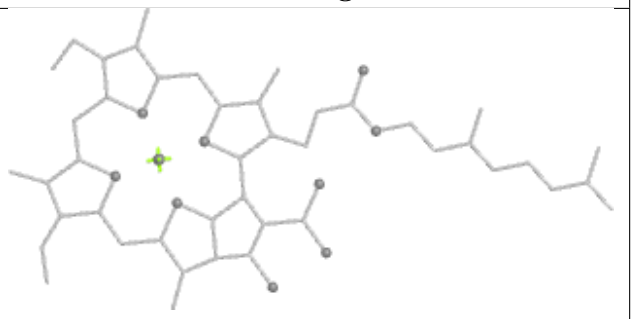
Bond lengths



Bond angles

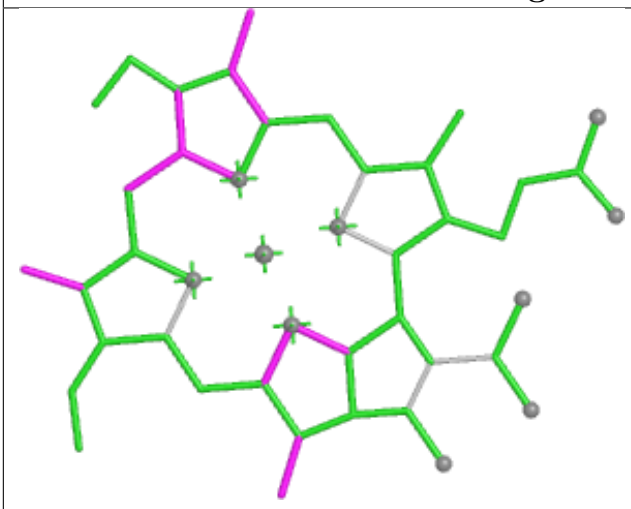


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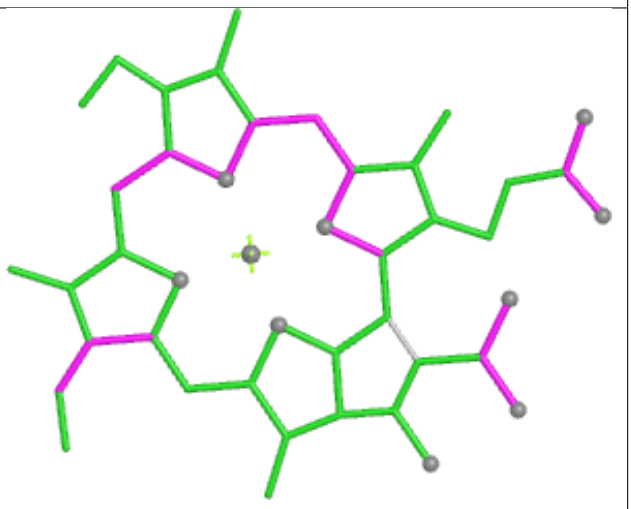


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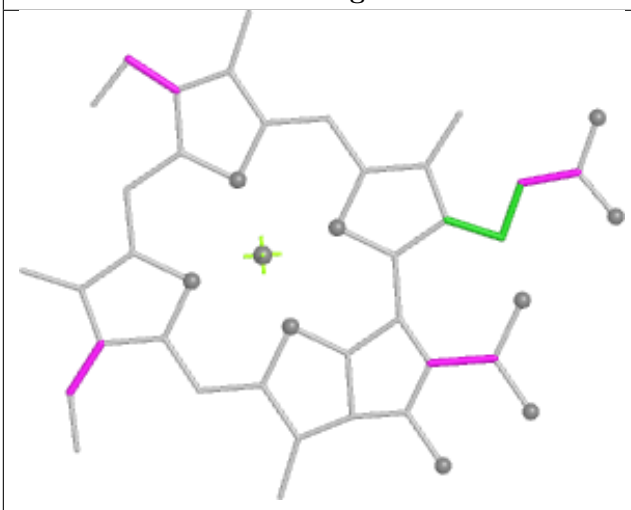
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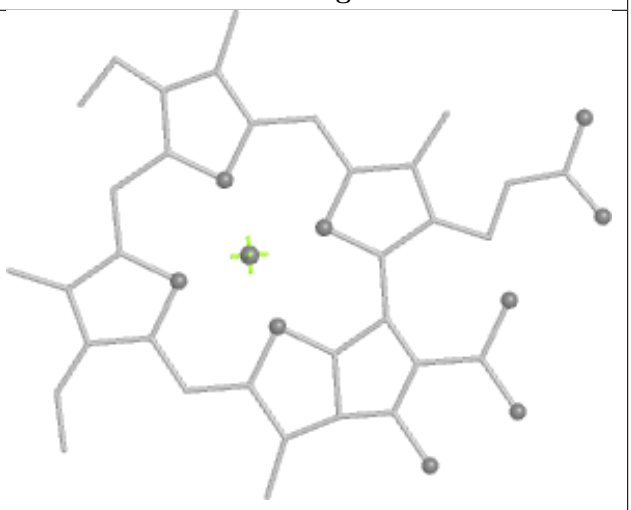
Bond lengths



Bond angles

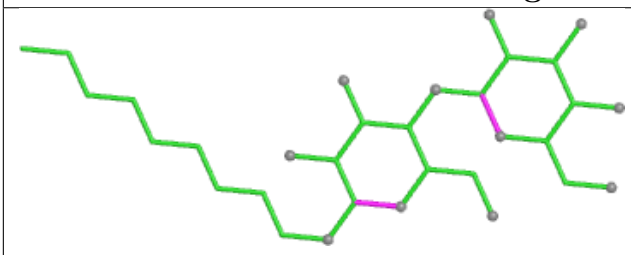


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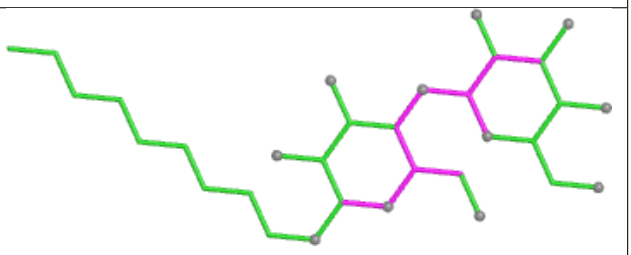


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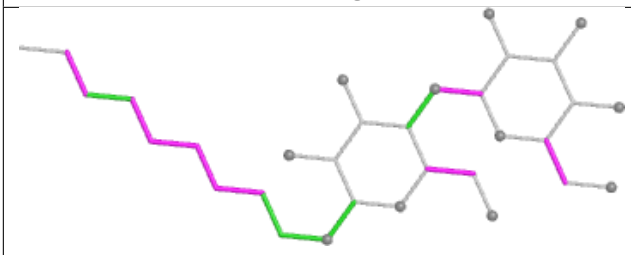
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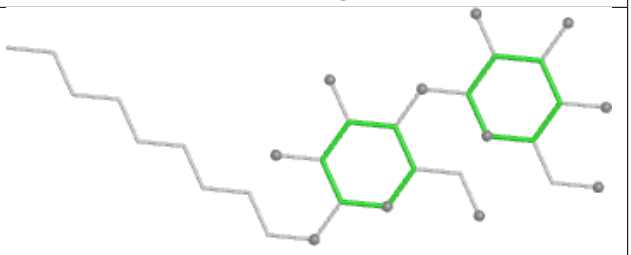
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Bond angles

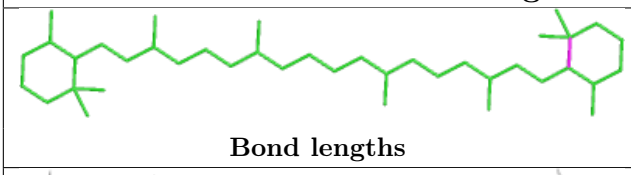


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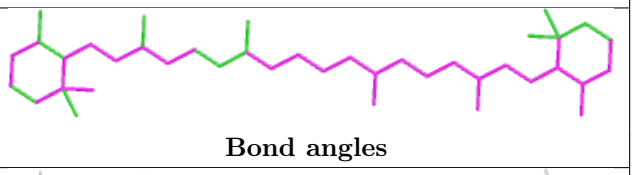


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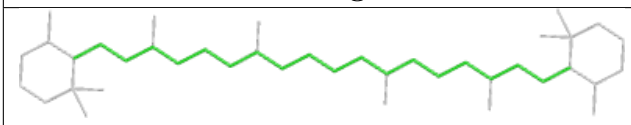
Ligand BCR B 846



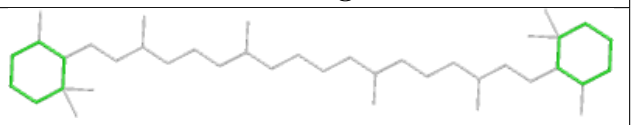
Bond lengths



Bond angles

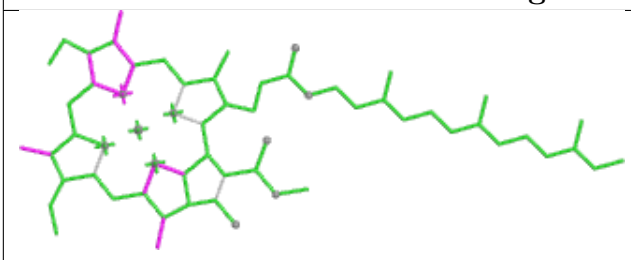


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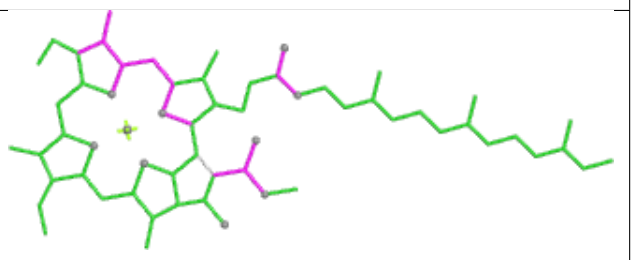


Rings

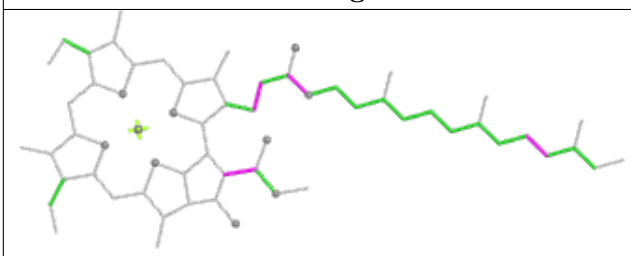
Ligand CLA 1 602



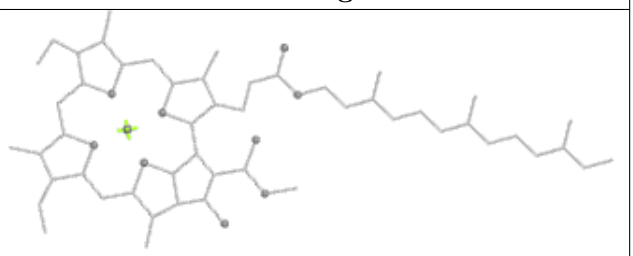
Bond lengths



Bond angles

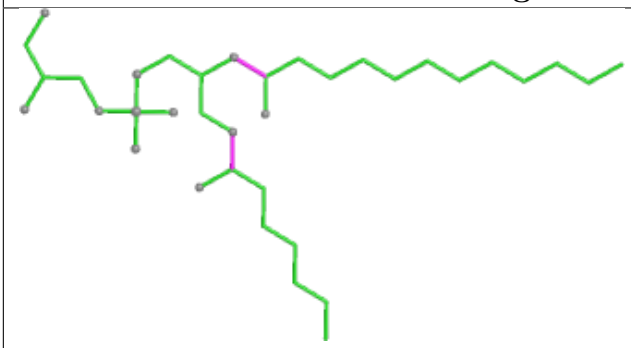


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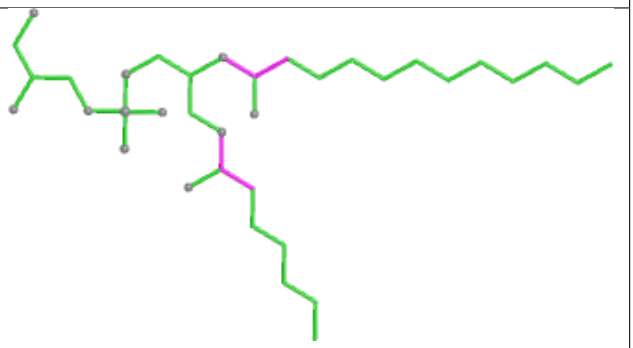


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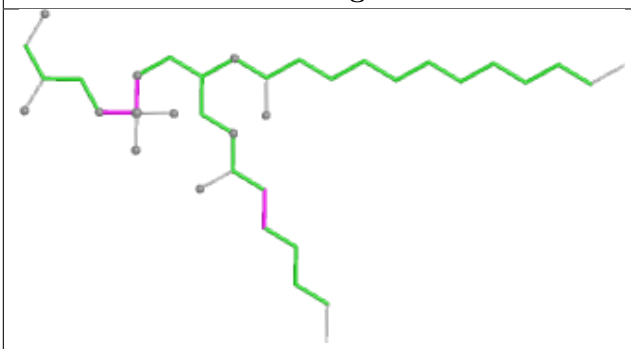
Ligand LHG V 2630



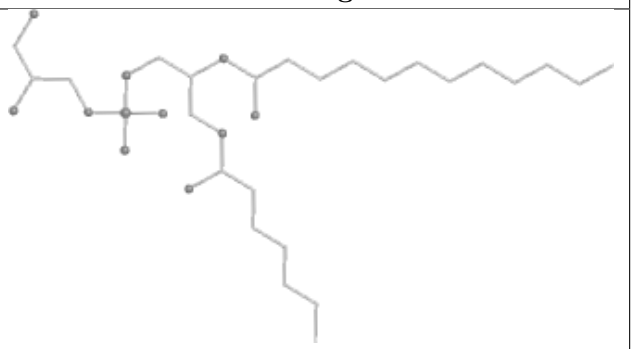
Bond lengths



Bond angles

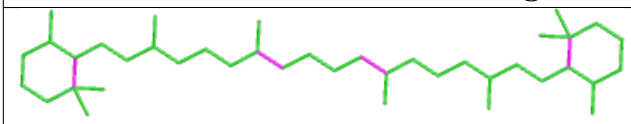


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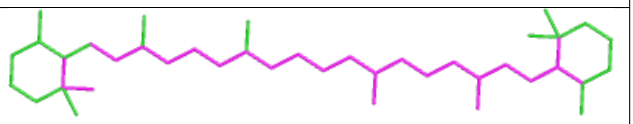


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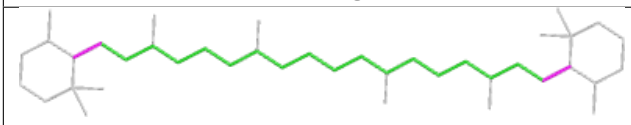
Ligand BCR B 843



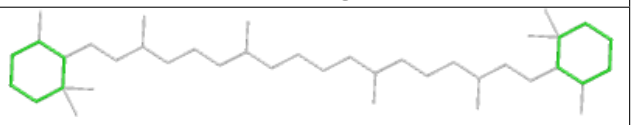
Bond lengths



Bond angles

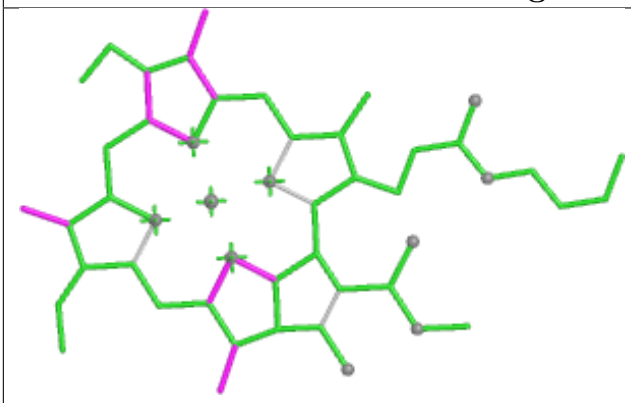


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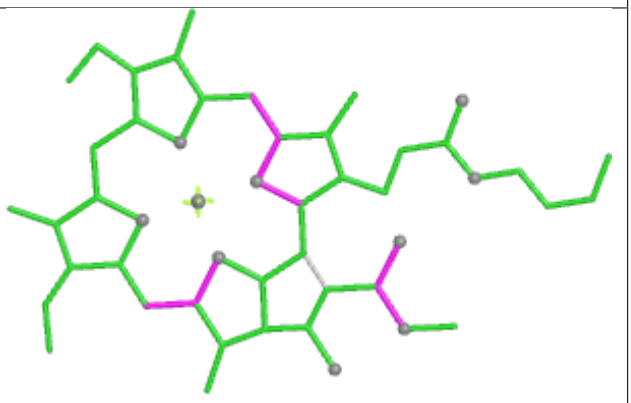


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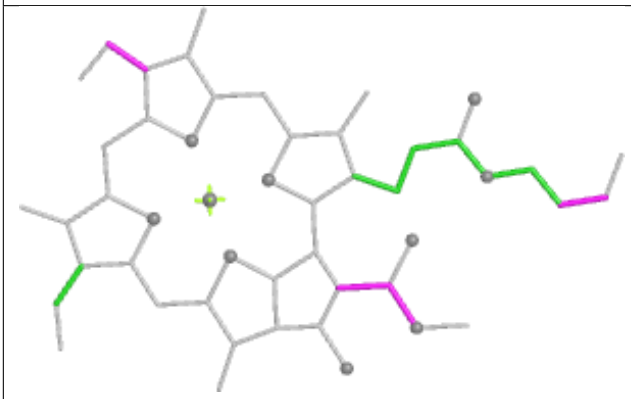
Ligand CLA a 604



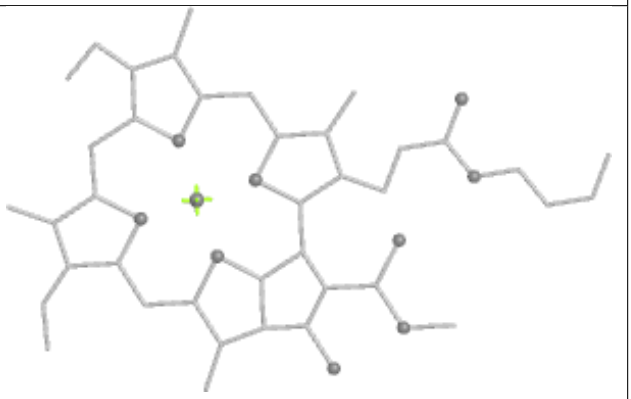
Bond lengths



Bond angles



Torsions

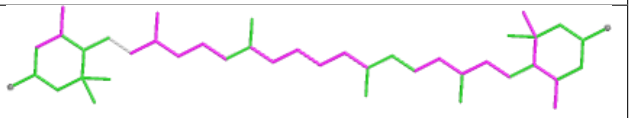


Rings

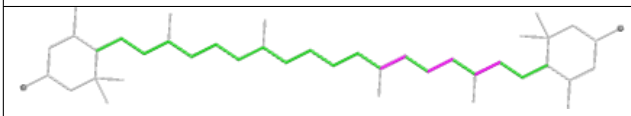
Ligand LUT Z 1620



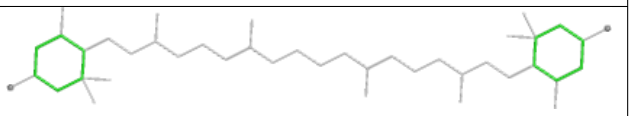
Bond lengths



Bond angles

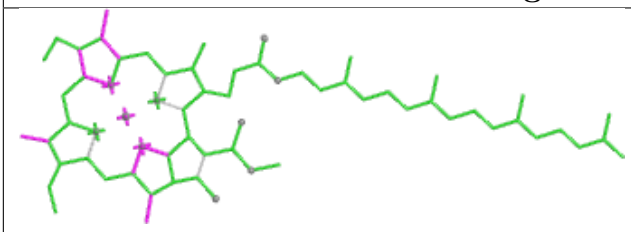


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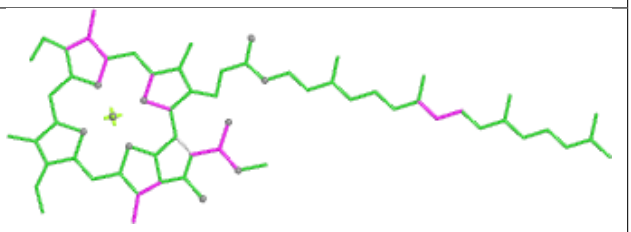


Rings

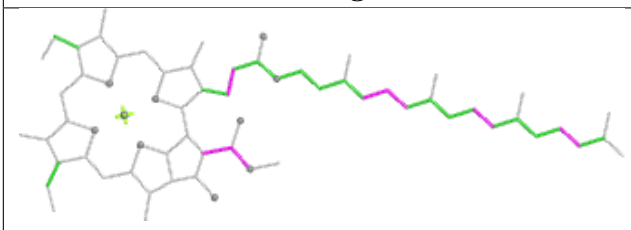
Ligand CLA A 854



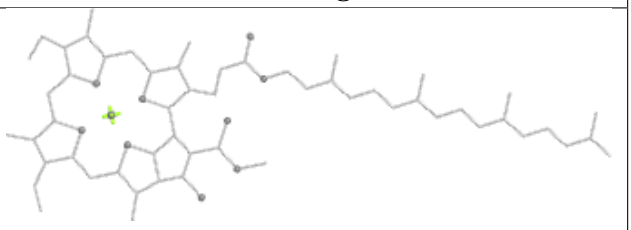
Bond lengths



Bond angles

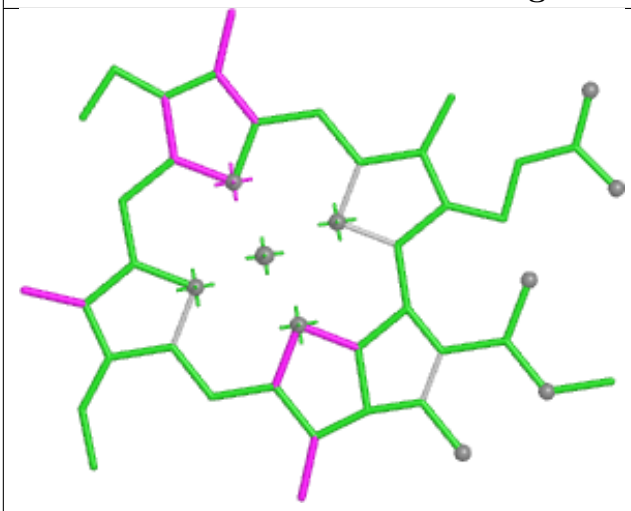


Torsions

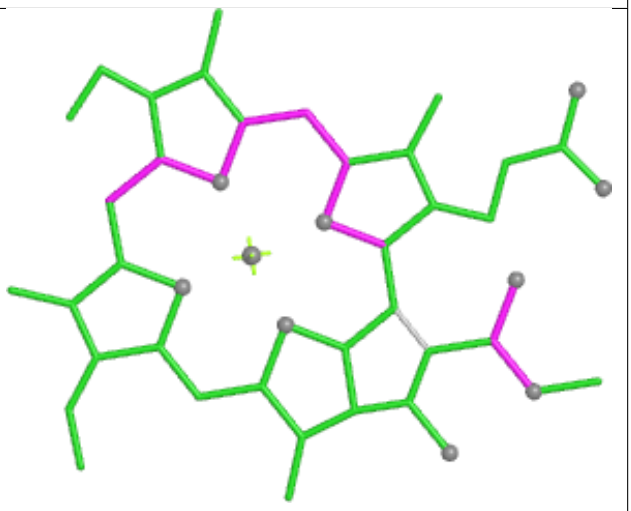


Rings

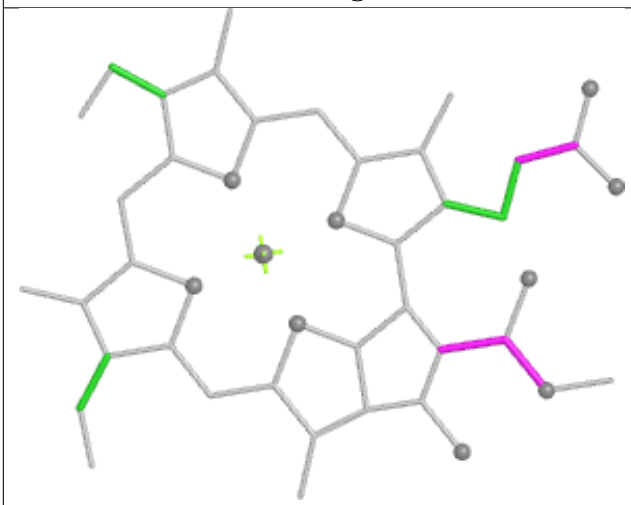
Ligand CLA a 612



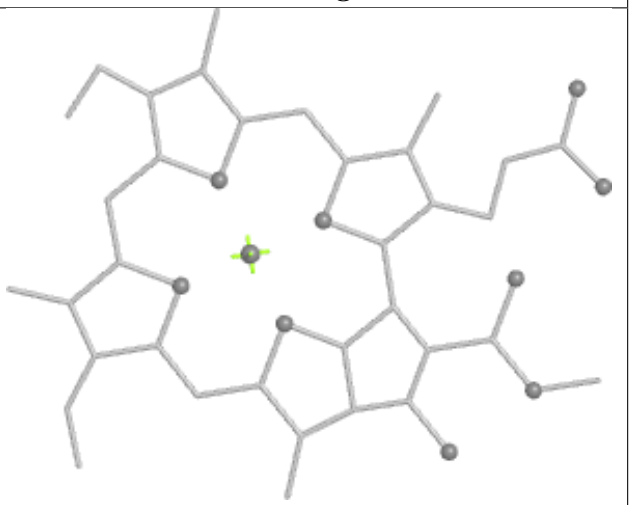
Bond lengths



Bond angles

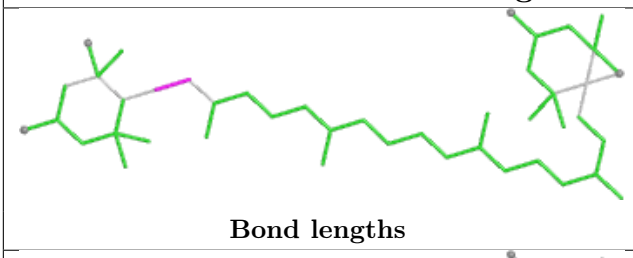


Torsions

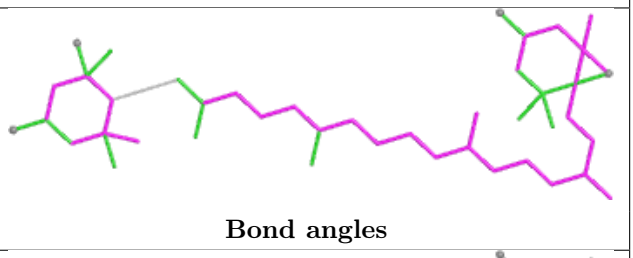


Rings

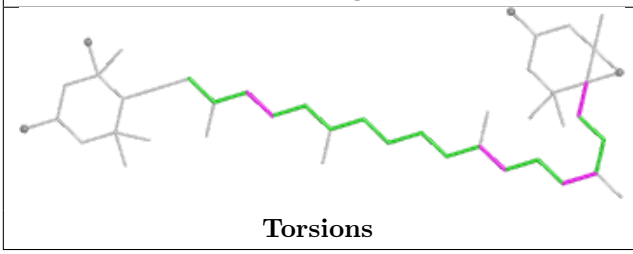
Ligand NEX Z 1623



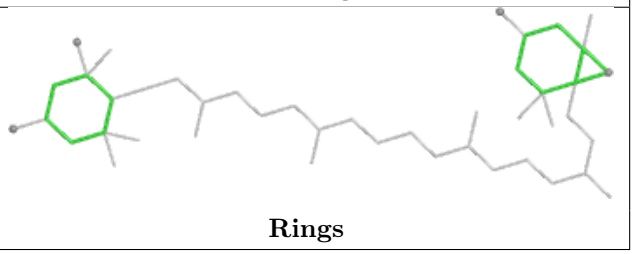
Bond lengths



Bond angles

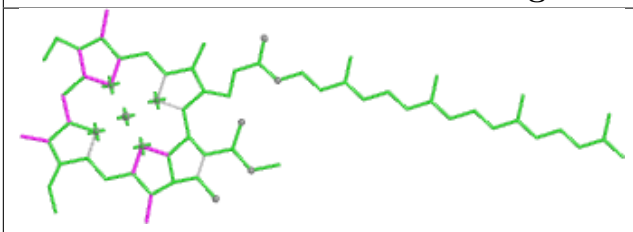


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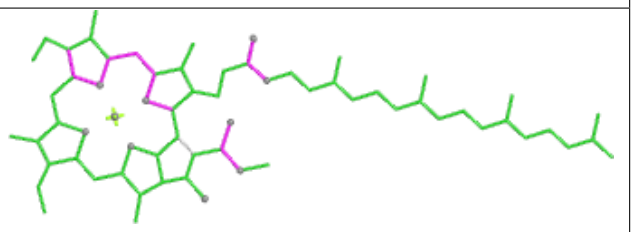


Rings

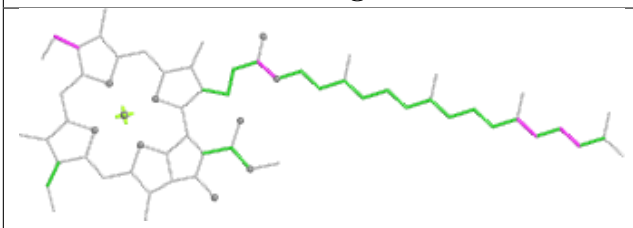
Ligand CLA 7 610



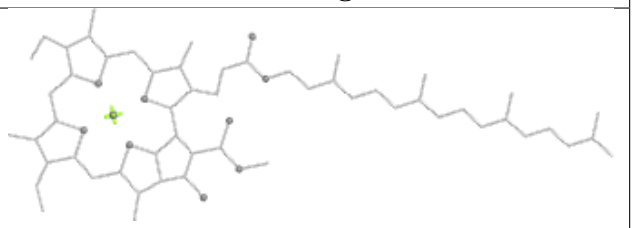
Bond lengths



Bond angles

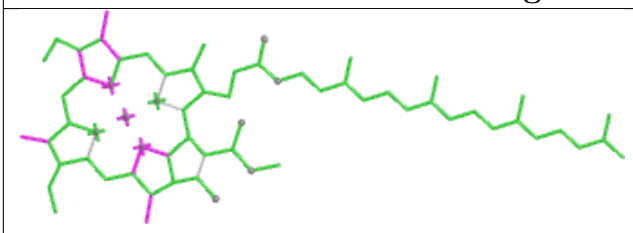


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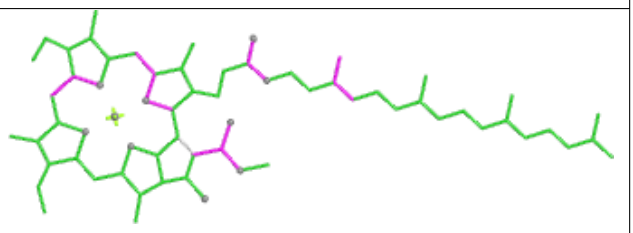


Rings

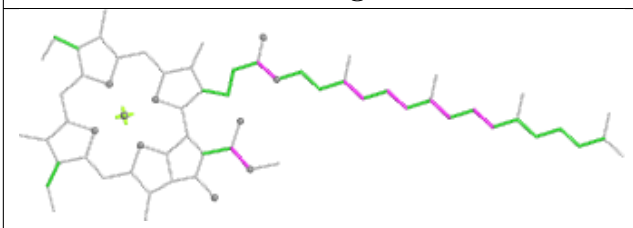
Ligand CLA A 836



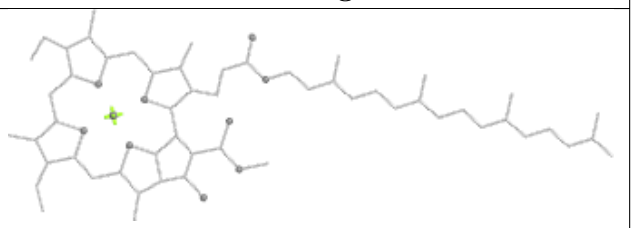
Bond lengths



Bond angles

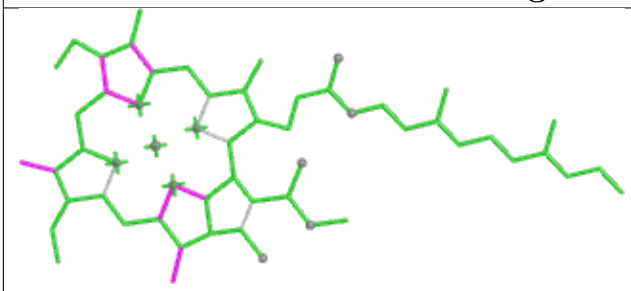


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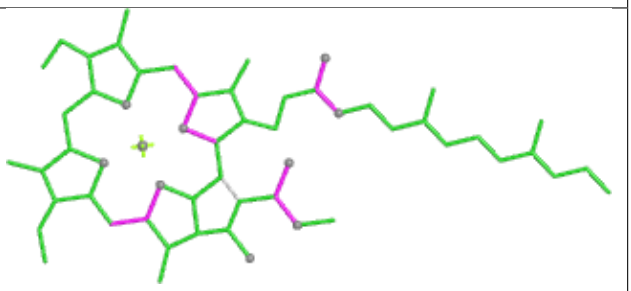


Rings

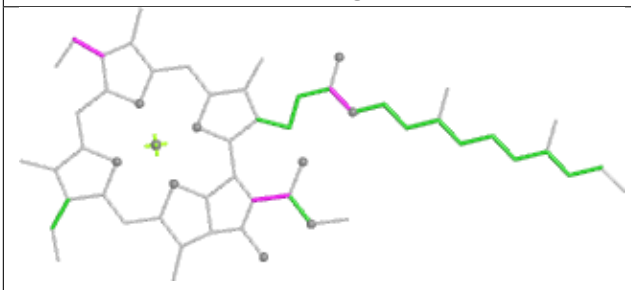
Ligand CLA 4 609



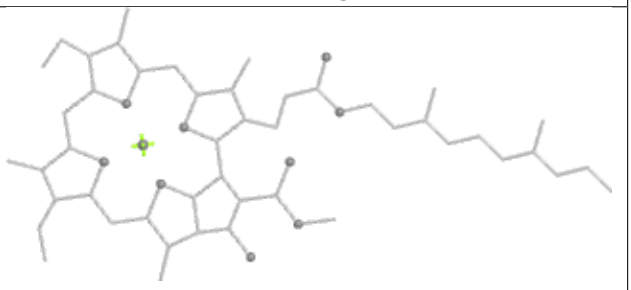
Bond lengths



Bond angles



Torsions

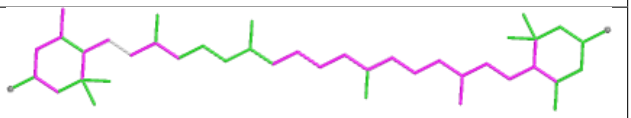


Rings

Ligand LUT 2 619



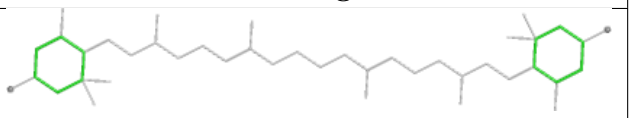
Bond lengths



Bond angles

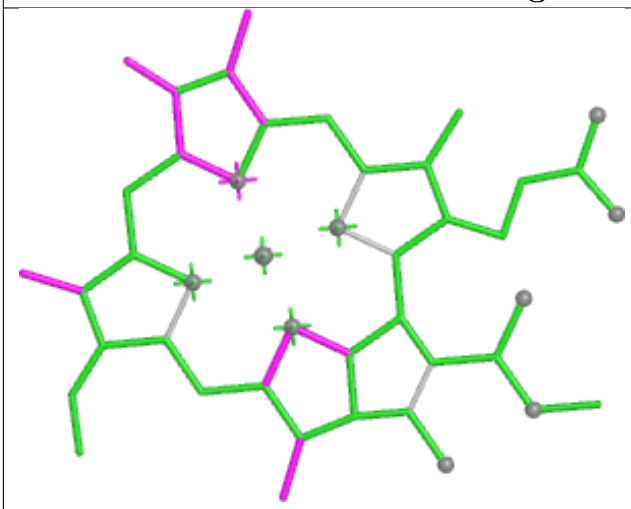


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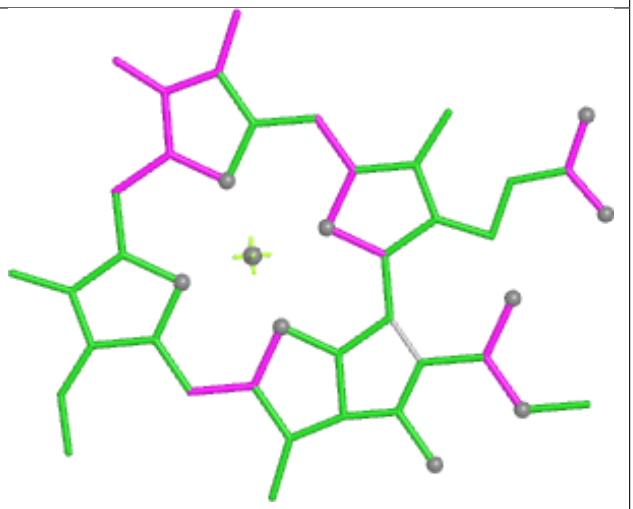


Rings

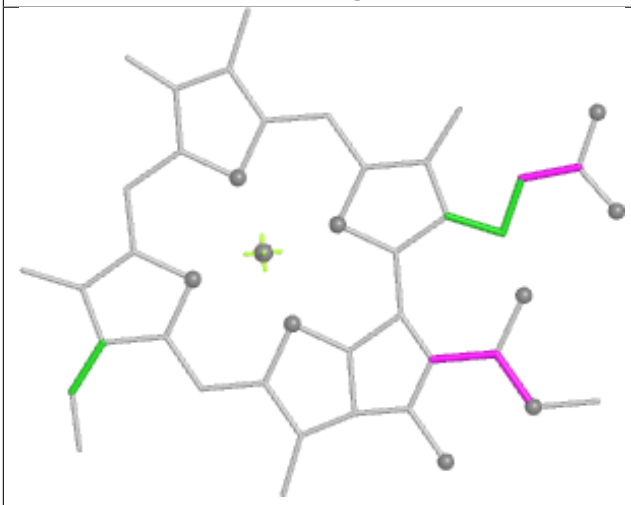
Ligand CLA 4 603



Bond lengths



Bond angles

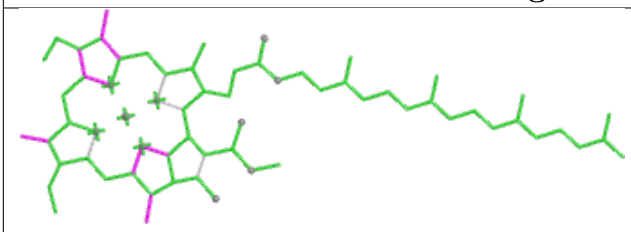


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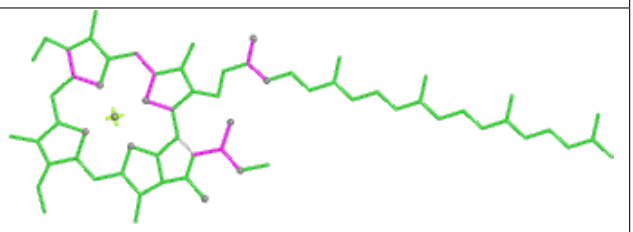


Rings

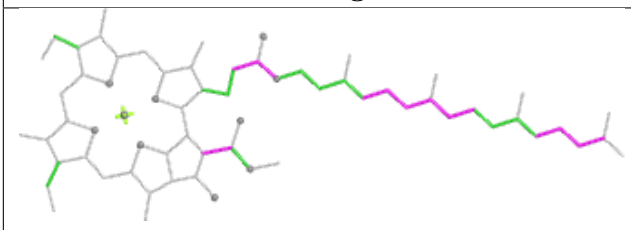
Ligand CLA 6 601



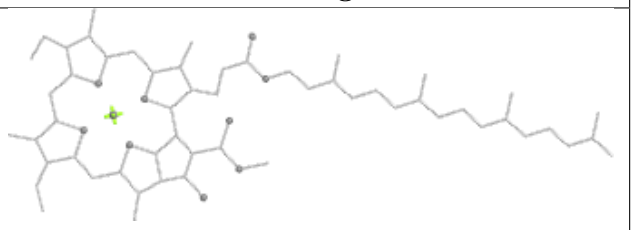
Bond lengths



Bond angles

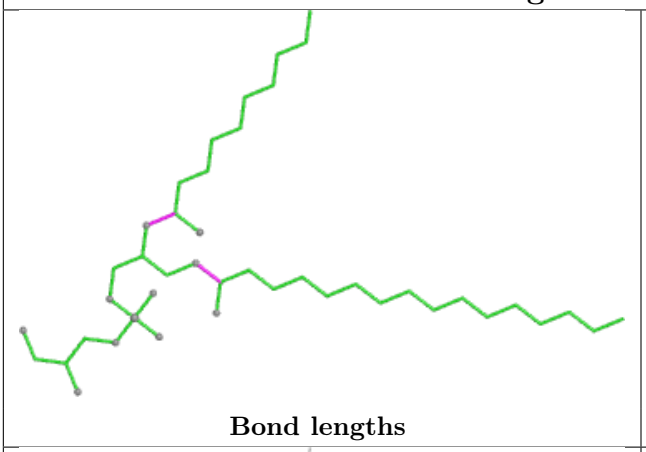


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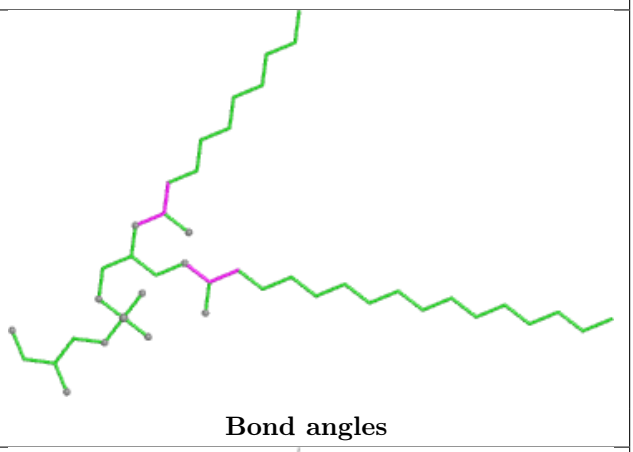


Rings

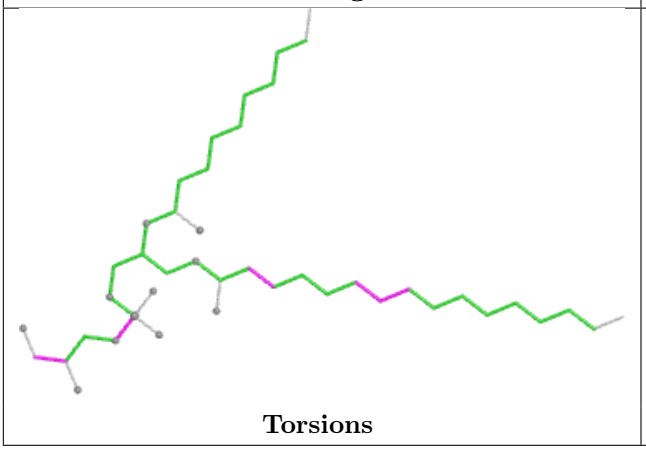
Ligand LHG a 620



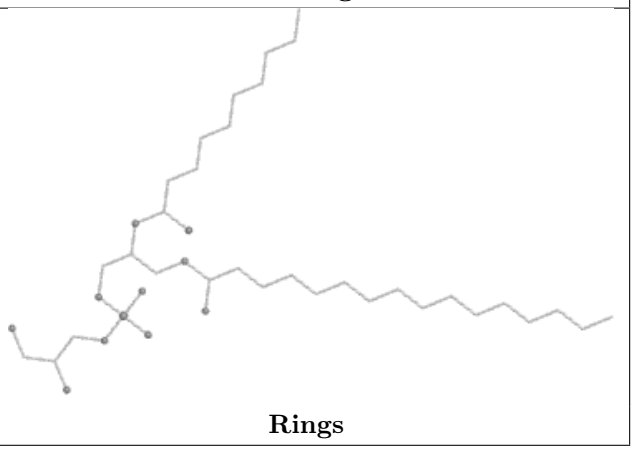
Bond lengths



Bond angles

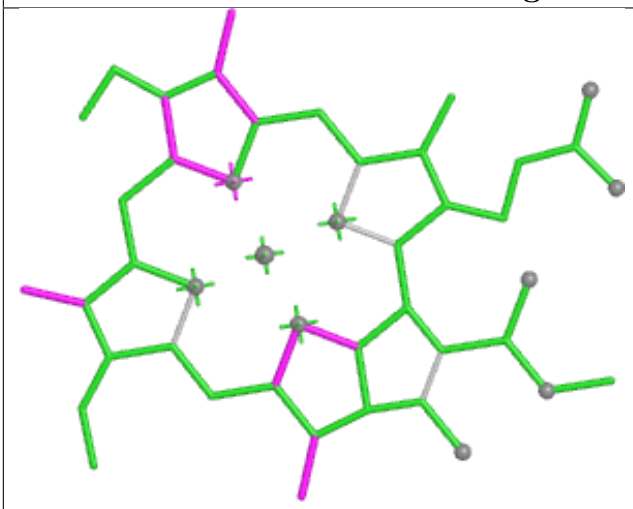


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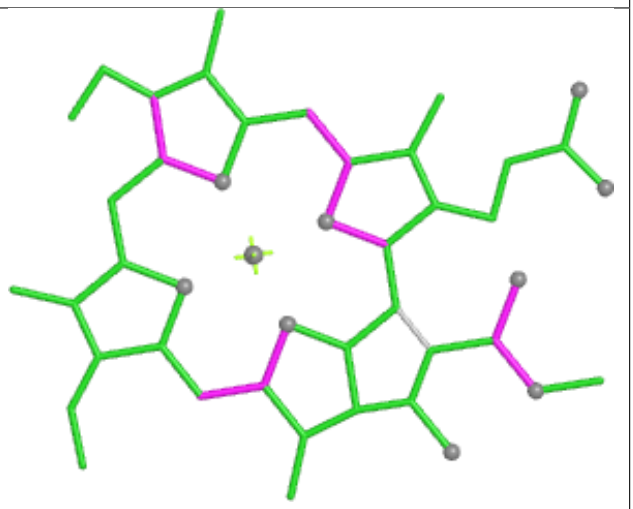


Rings

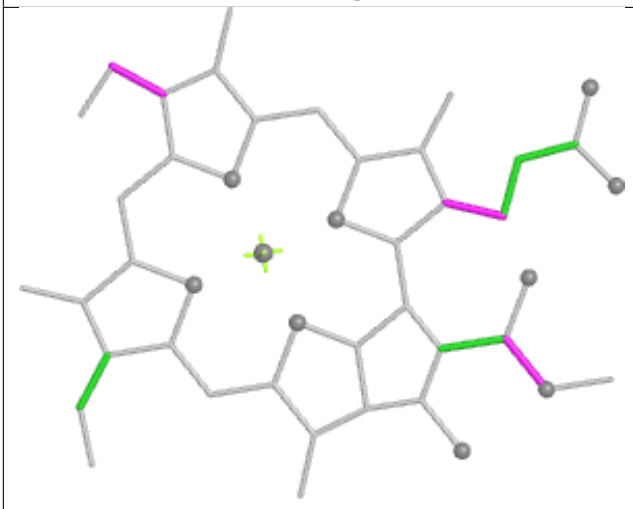
Ligand CLA K 204



Bond lengths



Bond angles

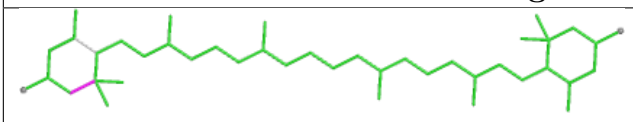


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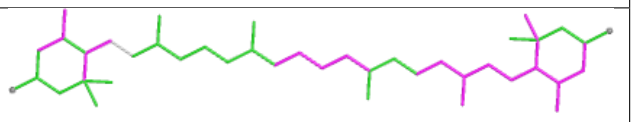


Rings

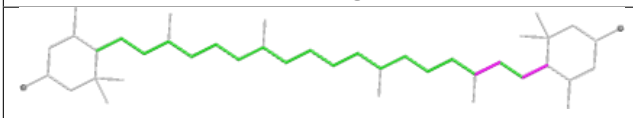
Ligand LUT 3 618



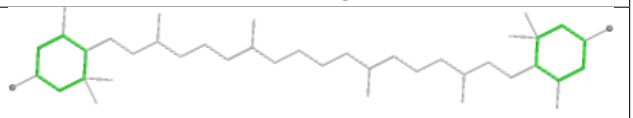
Bond lengths



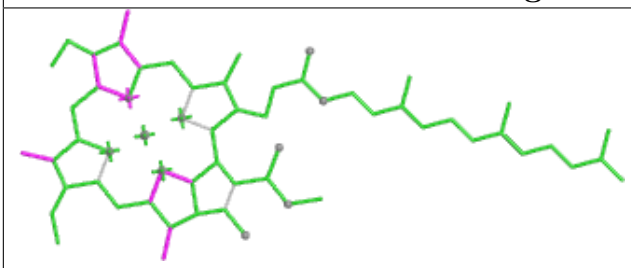
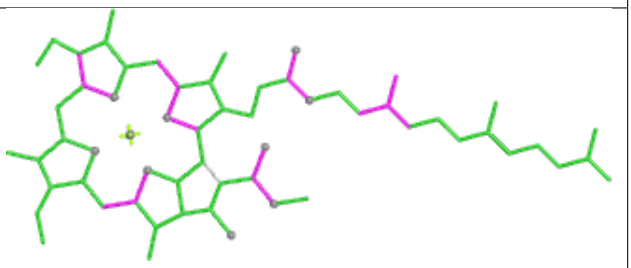
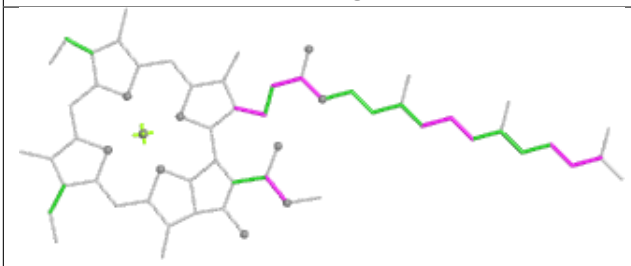
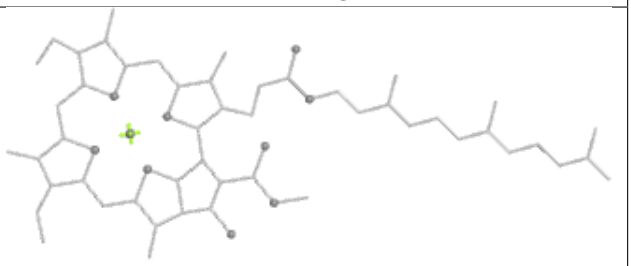
Bond angles

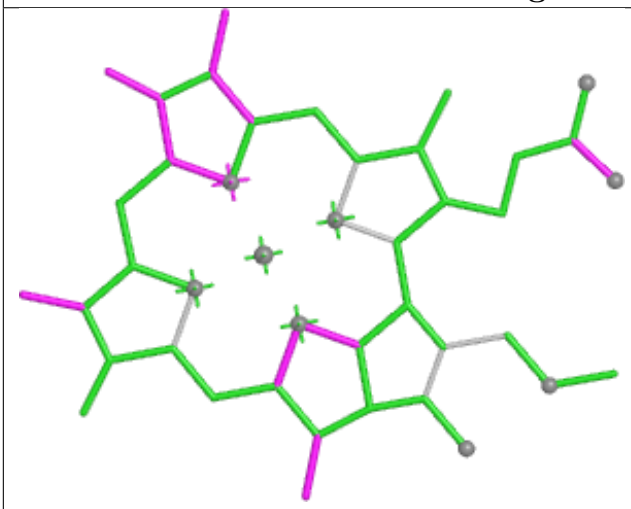
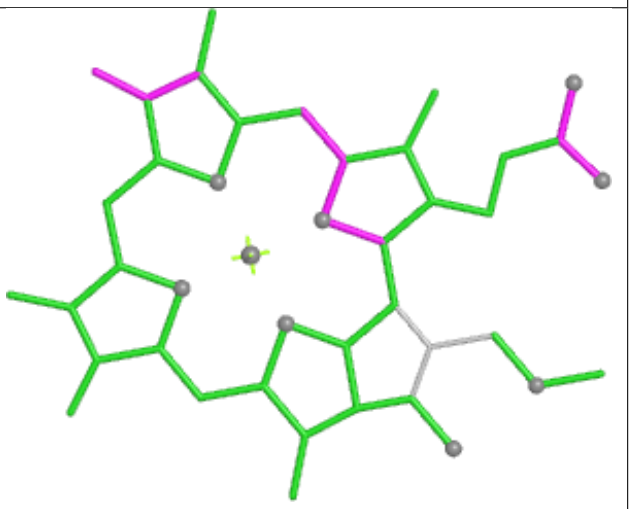
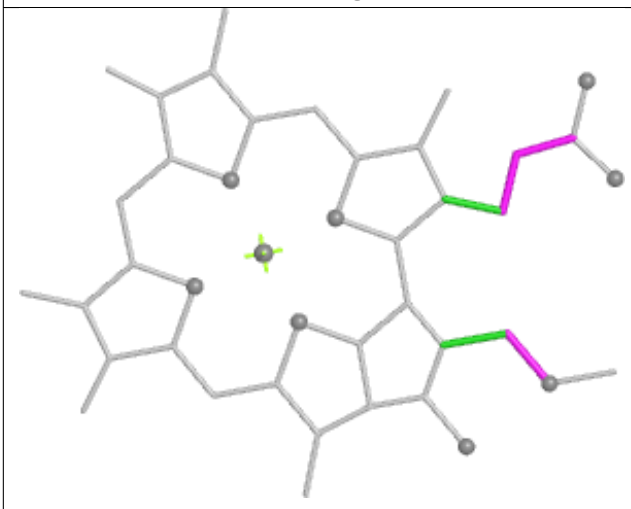


Torsions

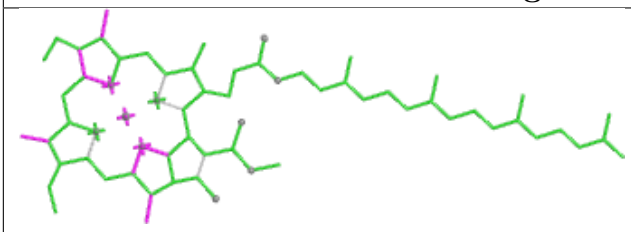


Rings

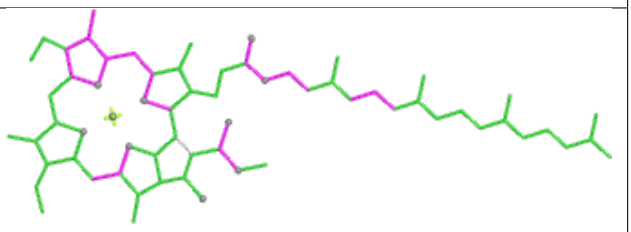
Ligand CLA B 832	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 5 616	
	
Bond lengths	Bond angles
	
Torsions	Rings

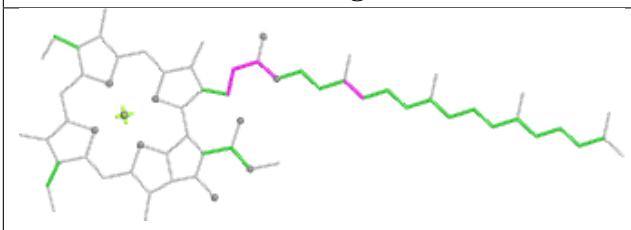
Ligand CLA A 822



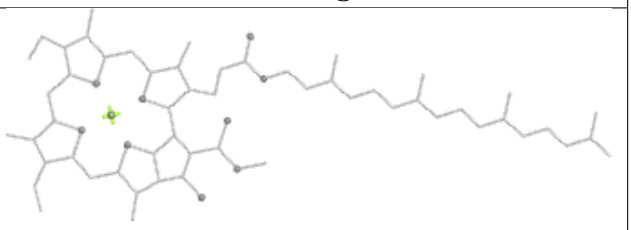
Bond lengths



Bond angles



Torsions



Rings

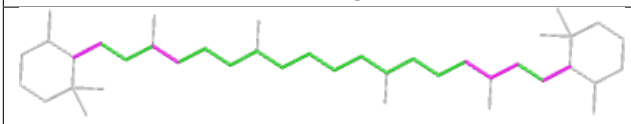
Ligand BCR B 845



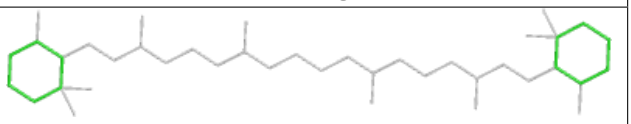
Bond lengths



Bond angles

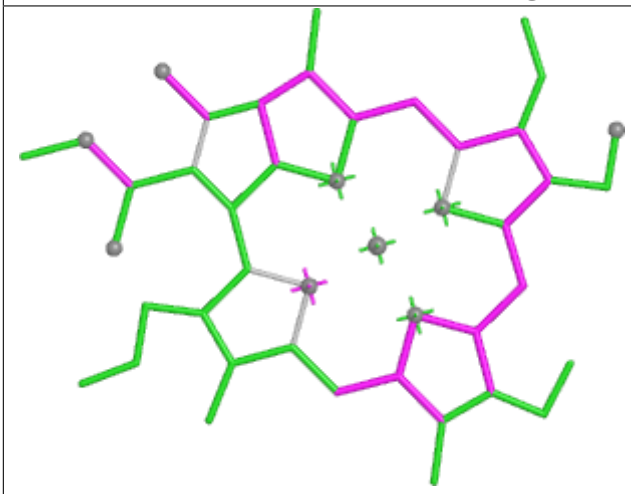


Torsions

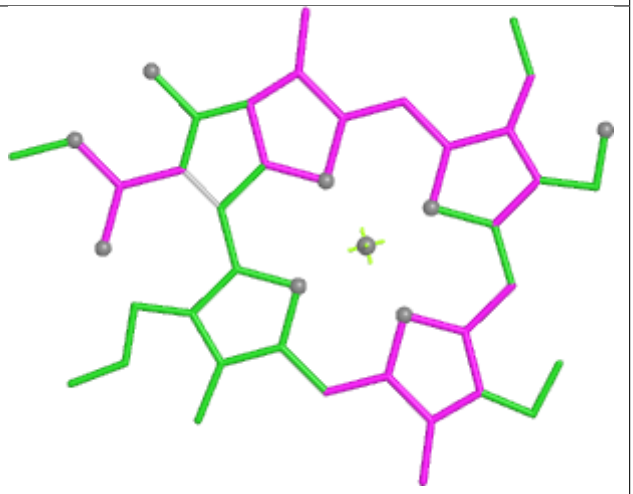


Rings

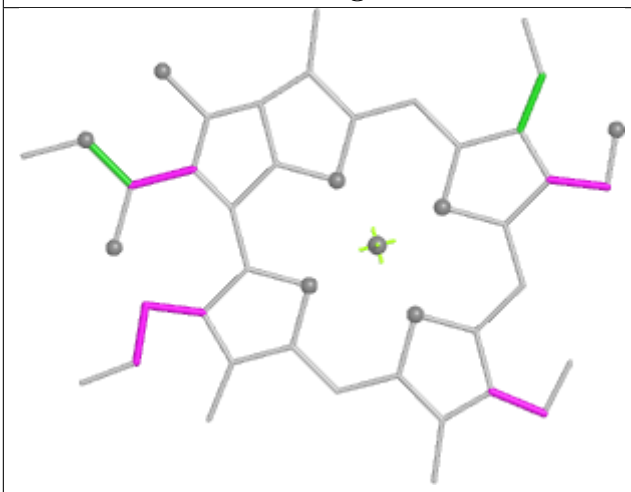
Ligand CHL V 605



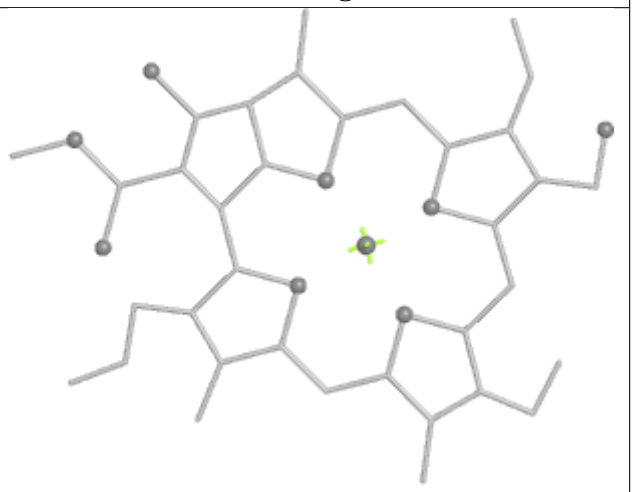
Bond lengths



Bond angles

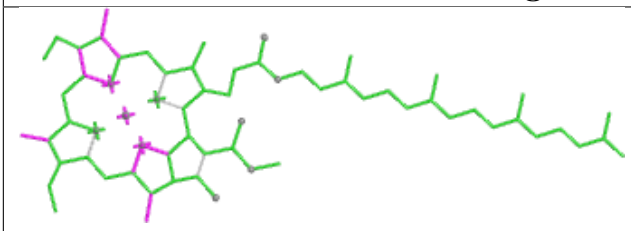


Torsions

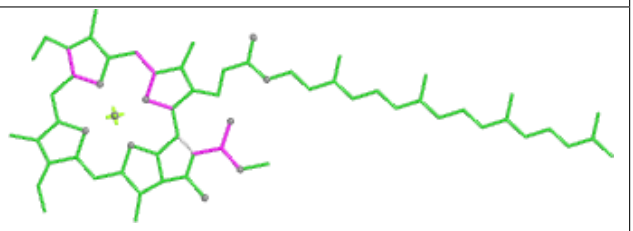


Rings

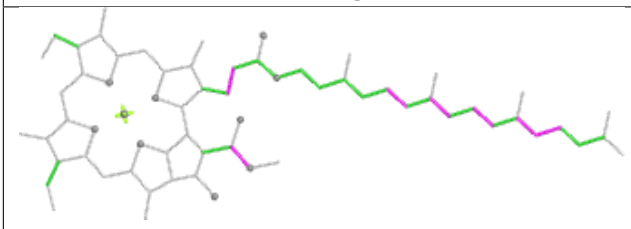
Ligand CLA B 824



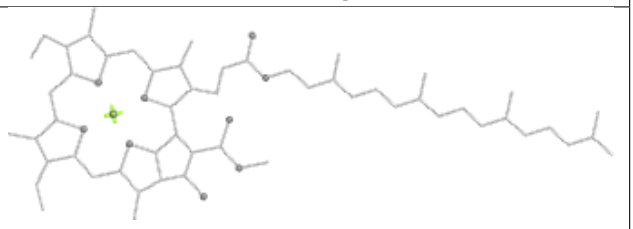
Bond lengths



Bond angles

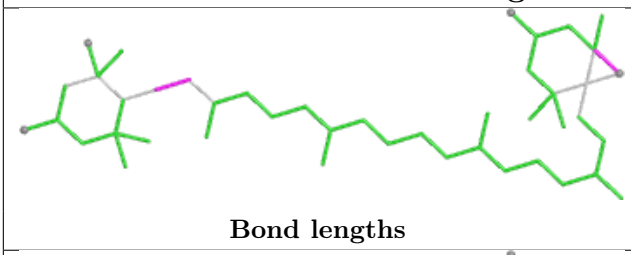


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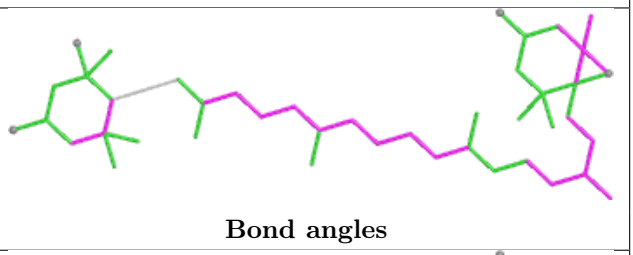


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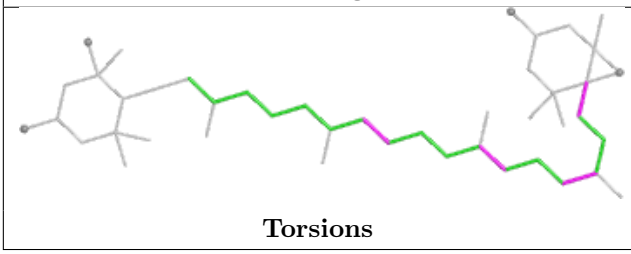
Ligand NEX W 1623



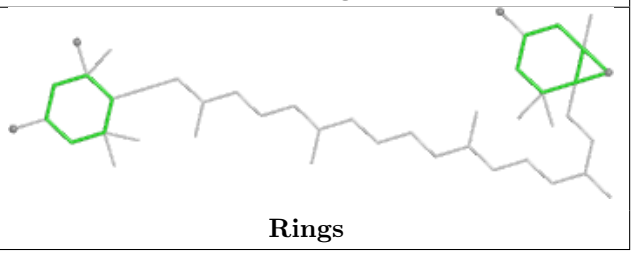
Bond lengths



Bond angles

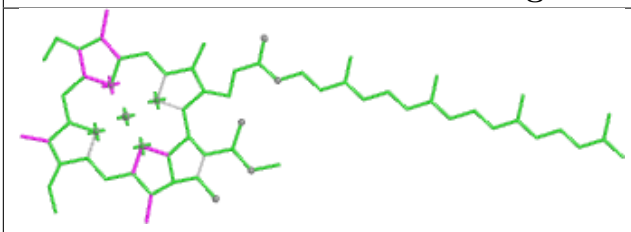


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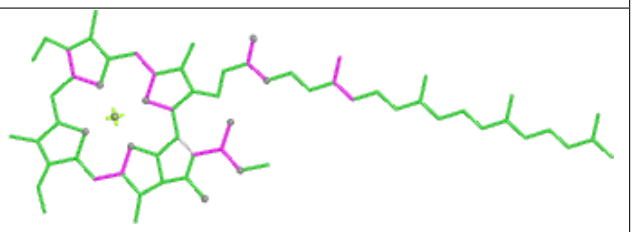


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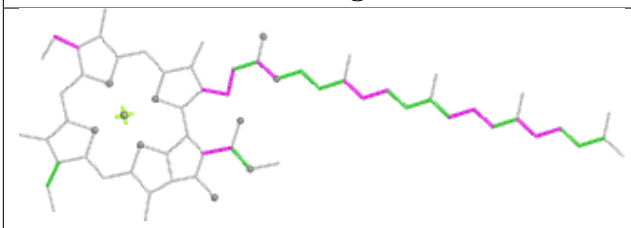
Ligand CLA L 303



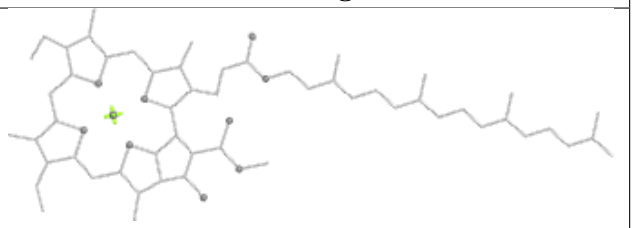
Bond lengths



Bond angles

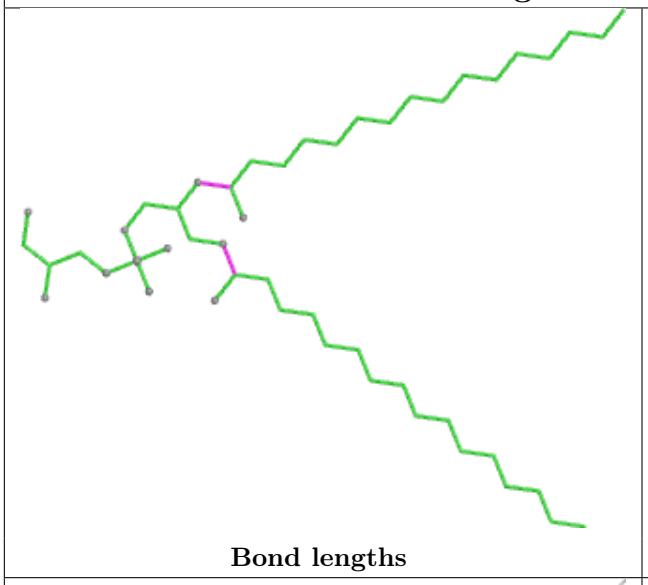


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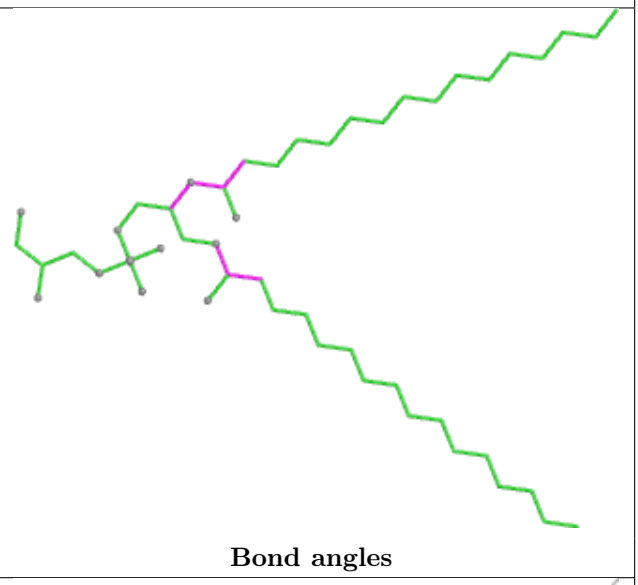


Rings

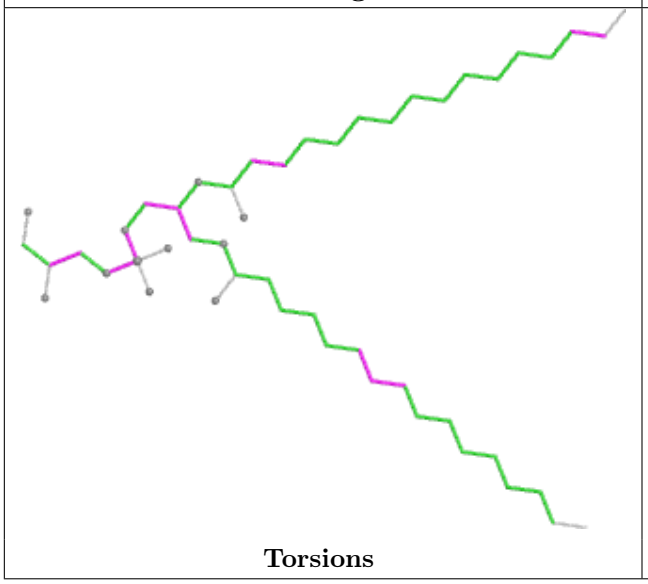
Ligand LHG X 2630



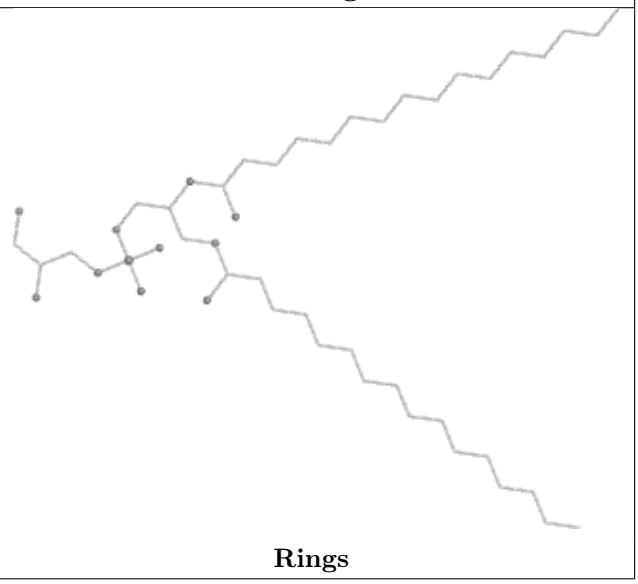
Bond lengths



Bond angles

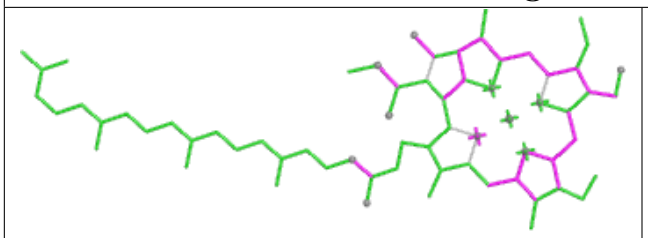


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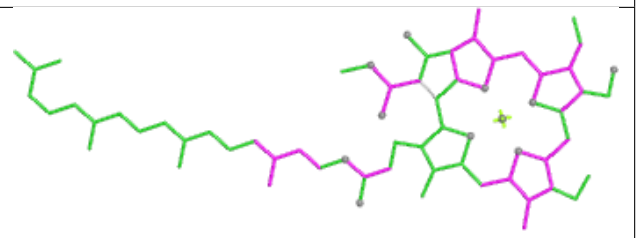


Rings

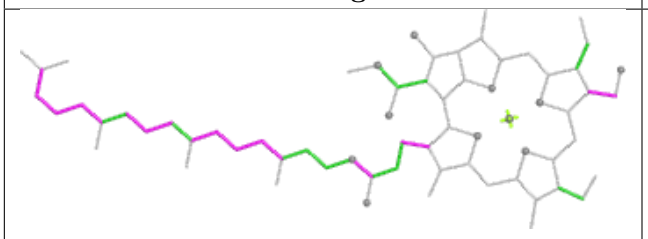
Ligand CHL U 601



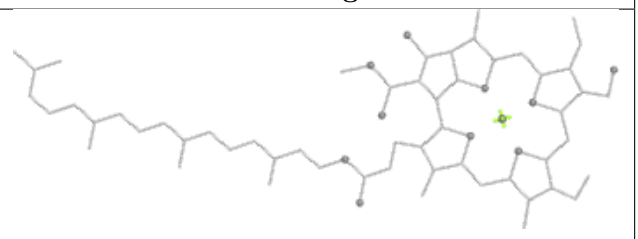
Bond lengths



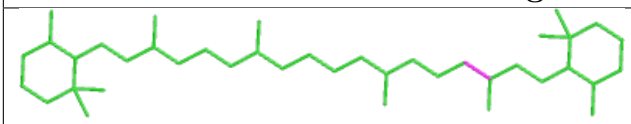
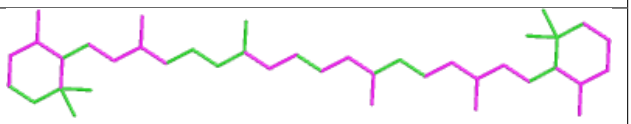
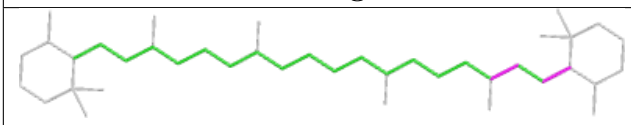
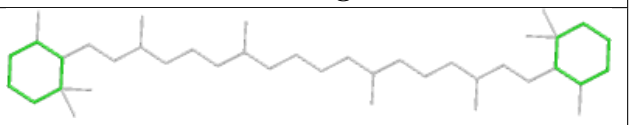
Bond angles

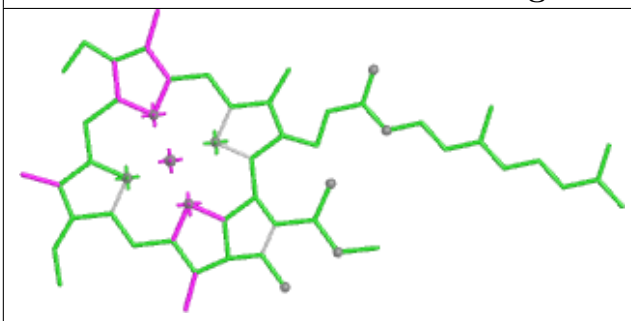
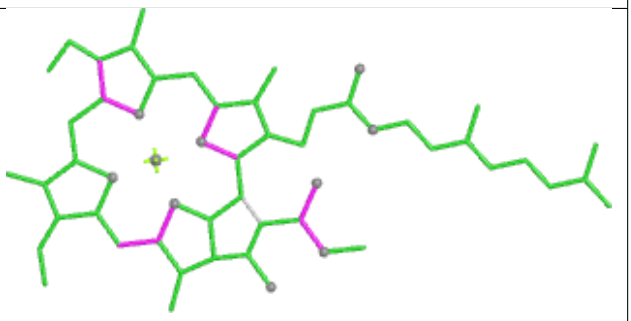
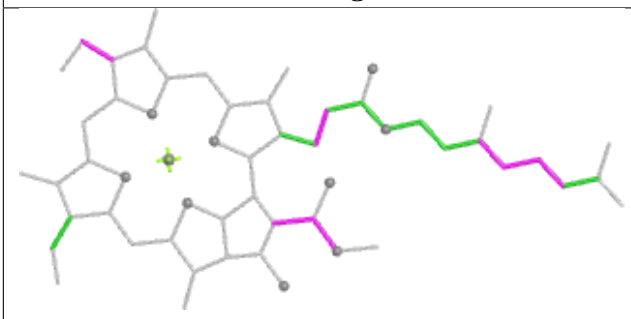
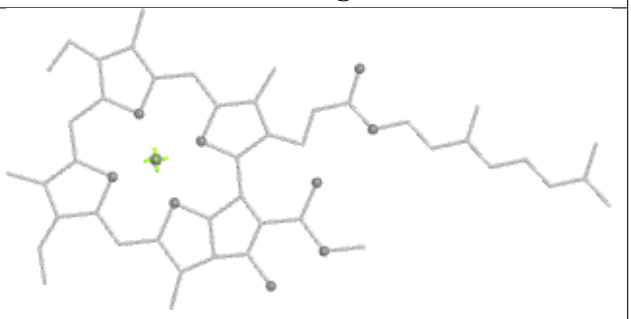


Torsions

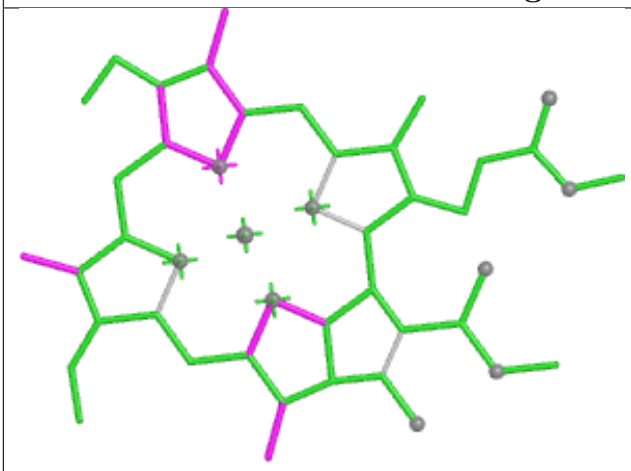


Rings

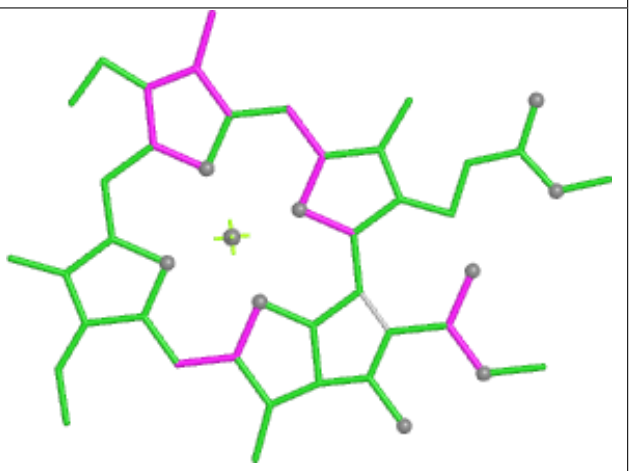
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 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 3 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

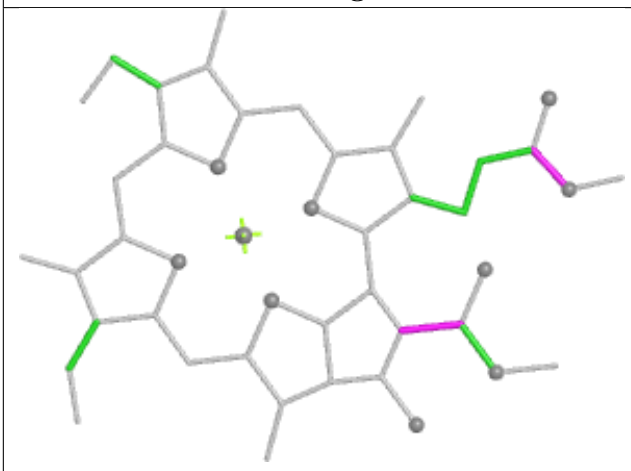
Ligand CLA B 838



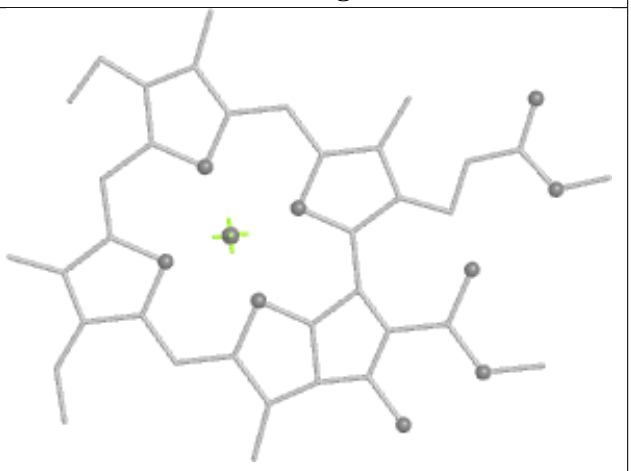
Bond lengths



Bond angles

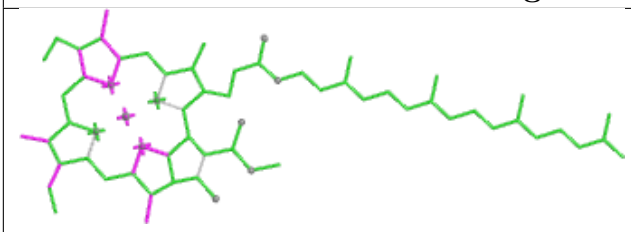


Torsions

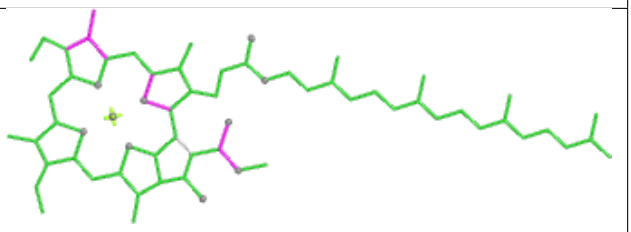


Rings

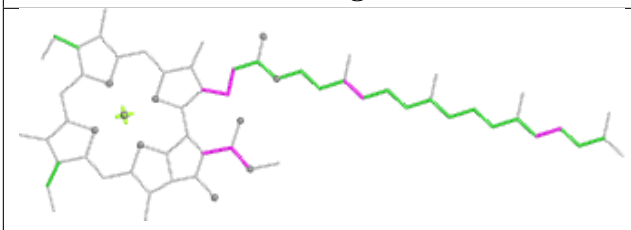
Ligand CLA A 803



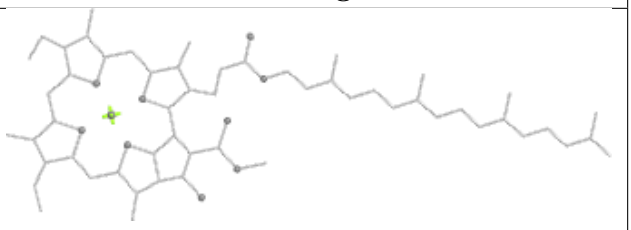
Bond lengths



Bond angles

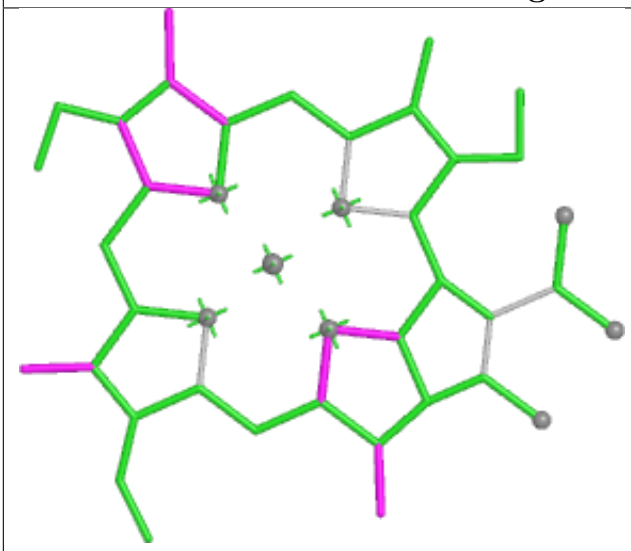


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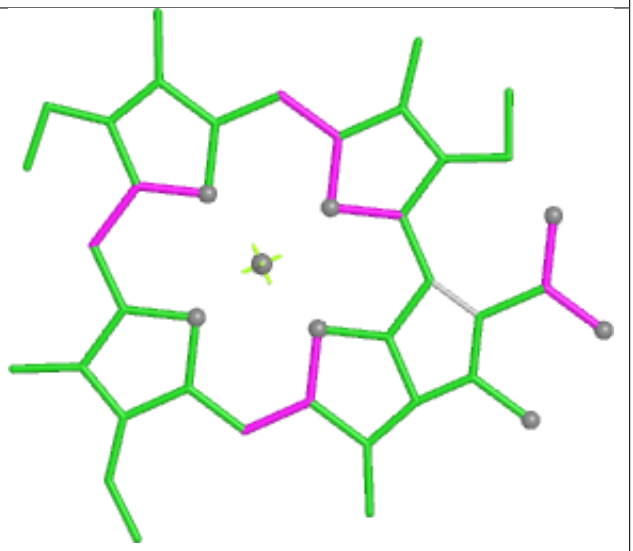


Rings

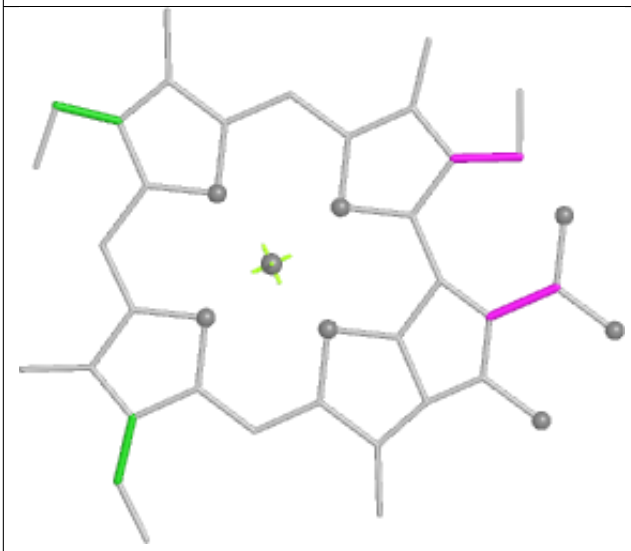
Ligand CLA 6 612



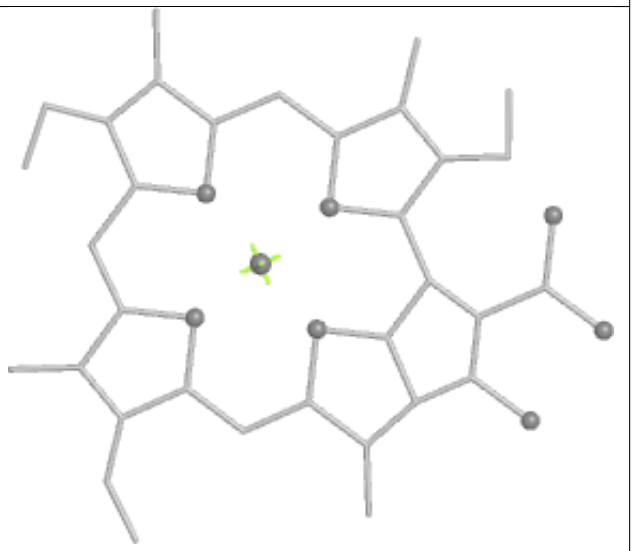
Bond lengths



Bond angles

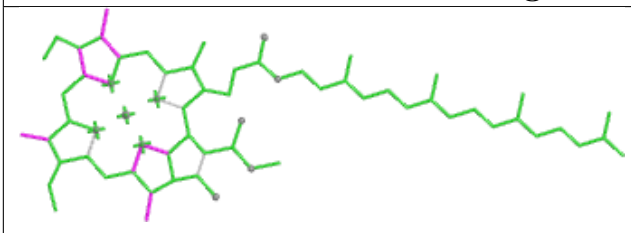


Torsions

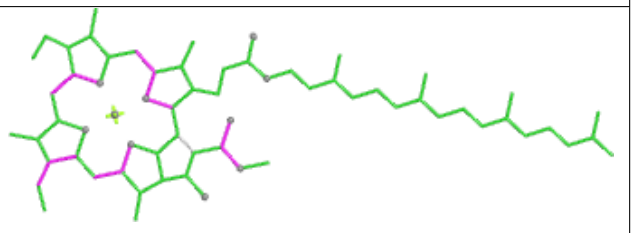


Rings

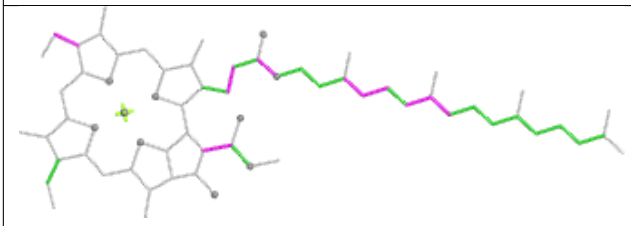
Ligand CLA X 613



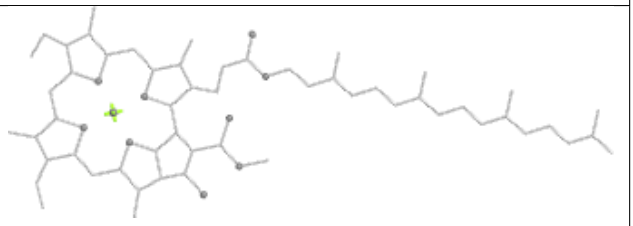
Bond lengths



Bond angles

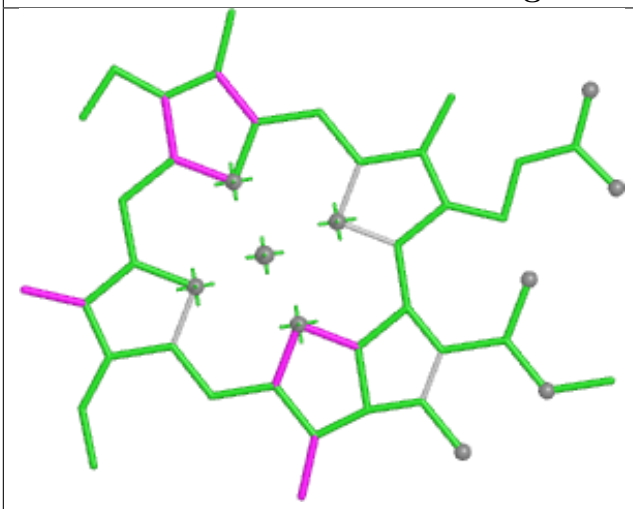


Torsions

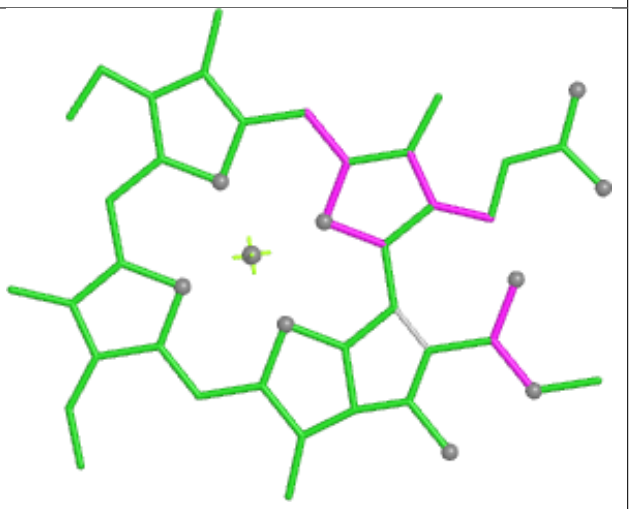


Rings

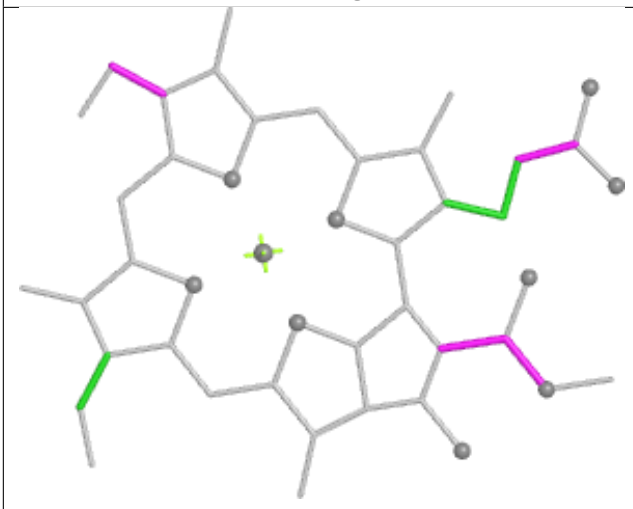
Ligand CLA Y 612



Bond lengths



Bond angles

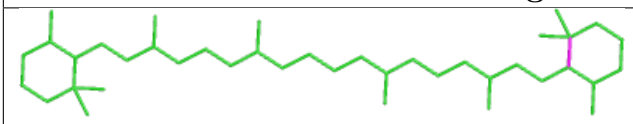


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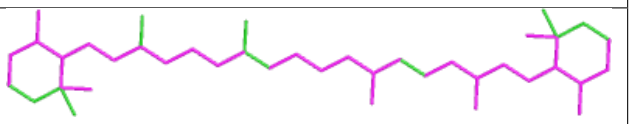


Rings

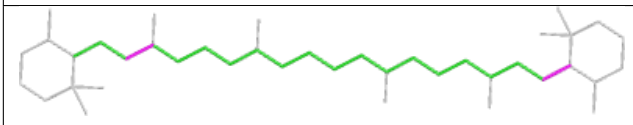
Ligand BCR 2 623



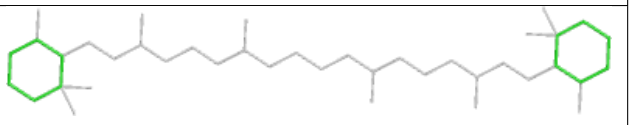
Bond lengths



Bond angles

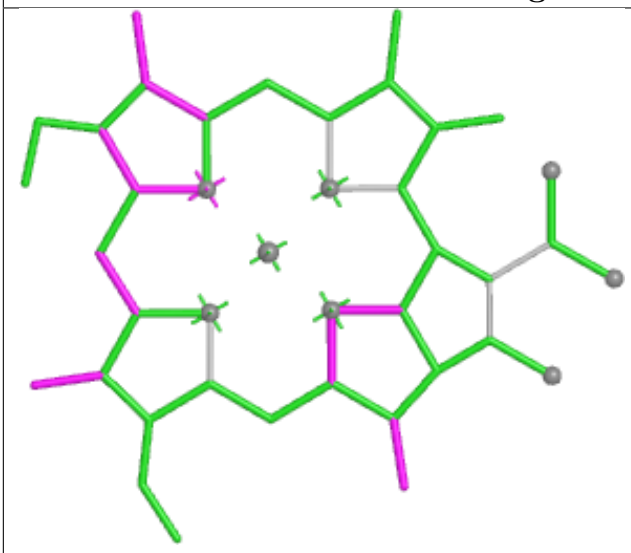


Torsions

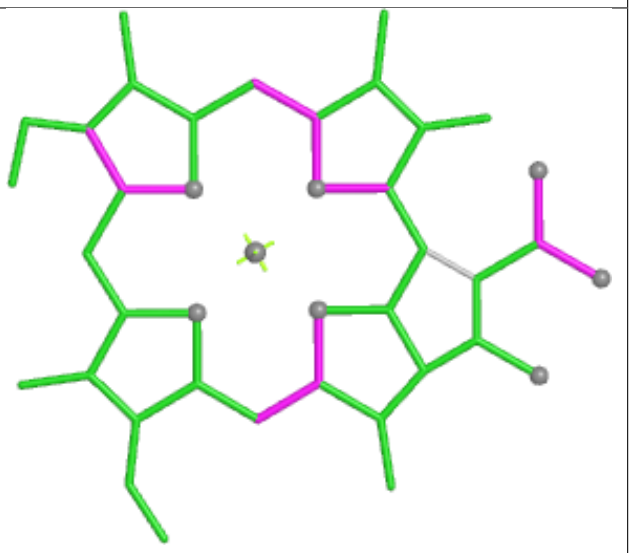


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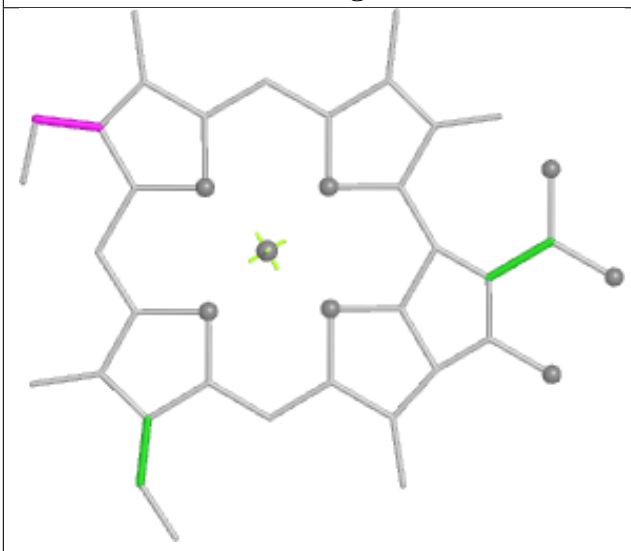
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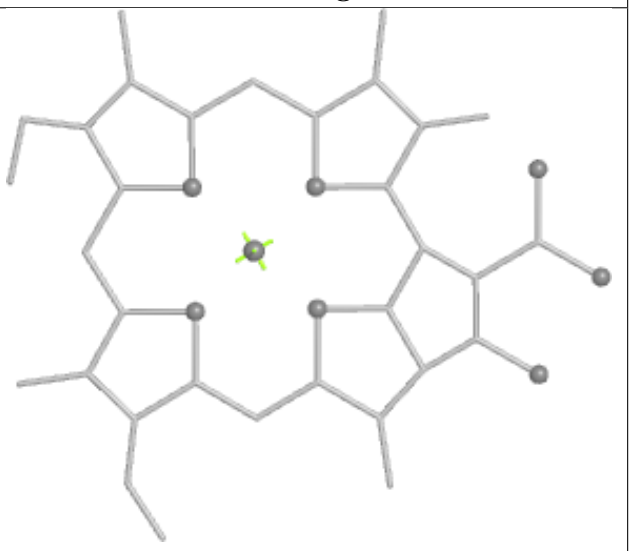
Bond lengths



Bond angles

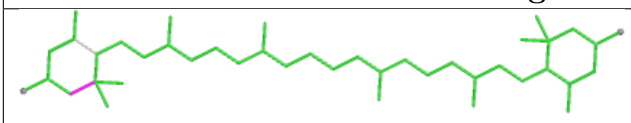


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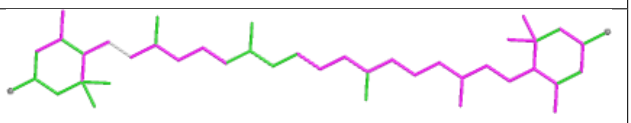


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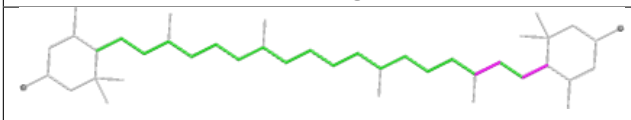
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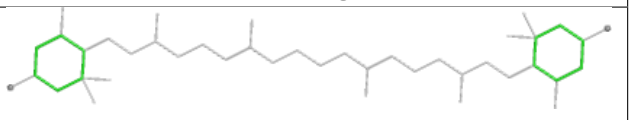
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Bond angles

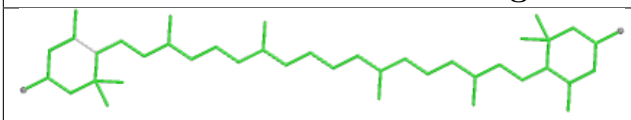


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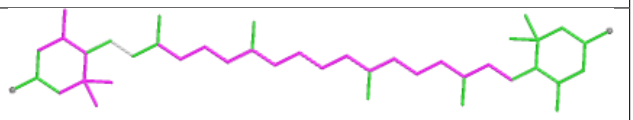


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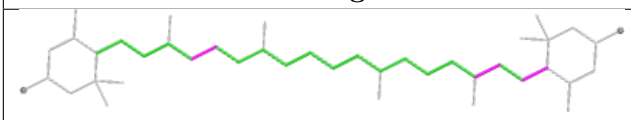
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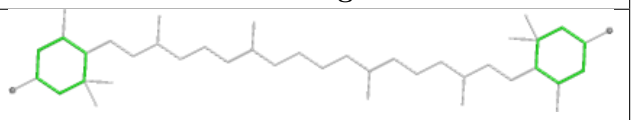
Bond lengths



Bond angles

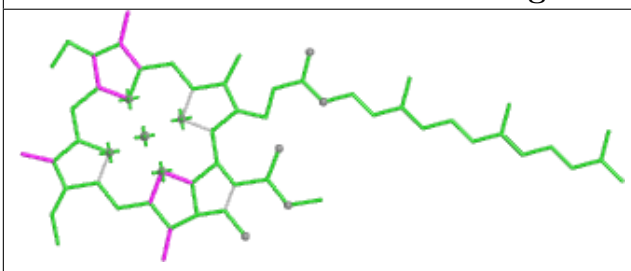


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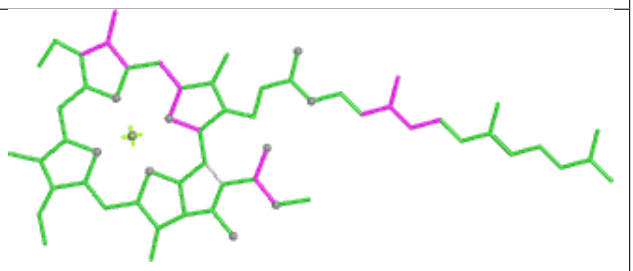


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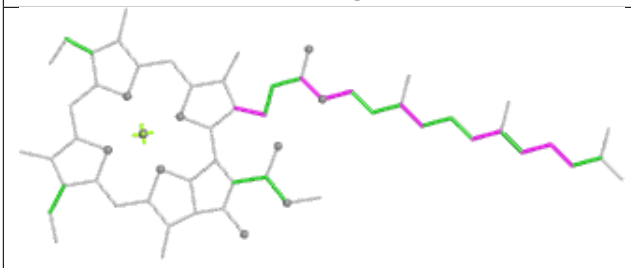
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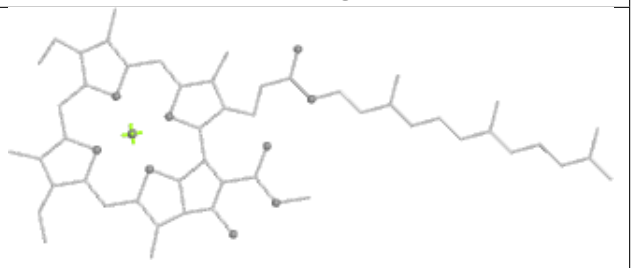
Bond lengths



Bond angles

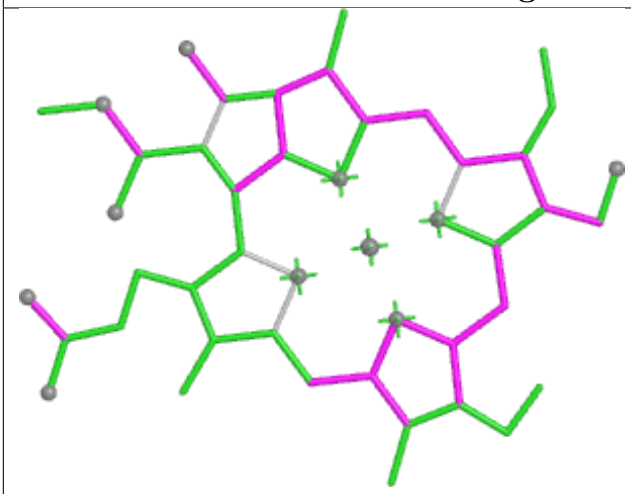


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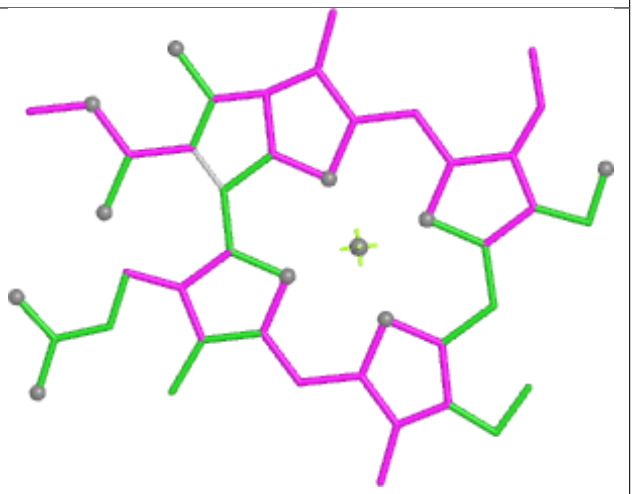


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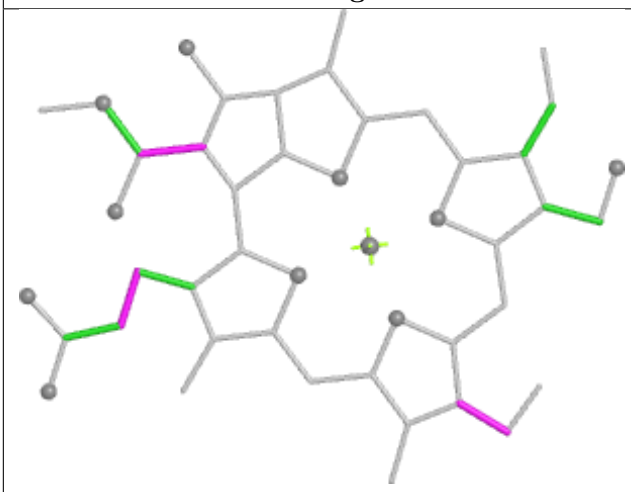
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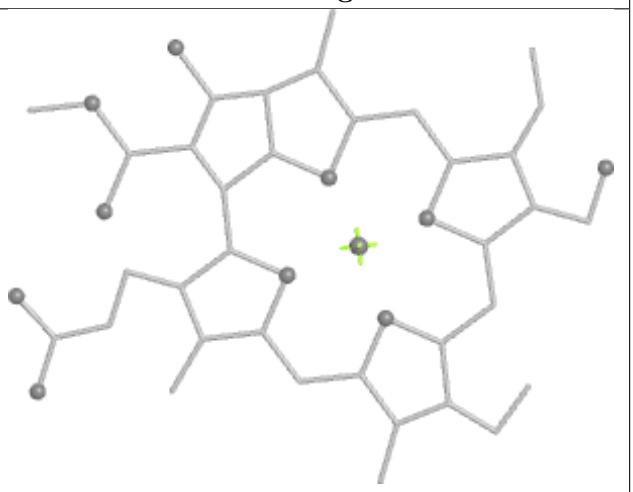
Bond lengths



Bond angles

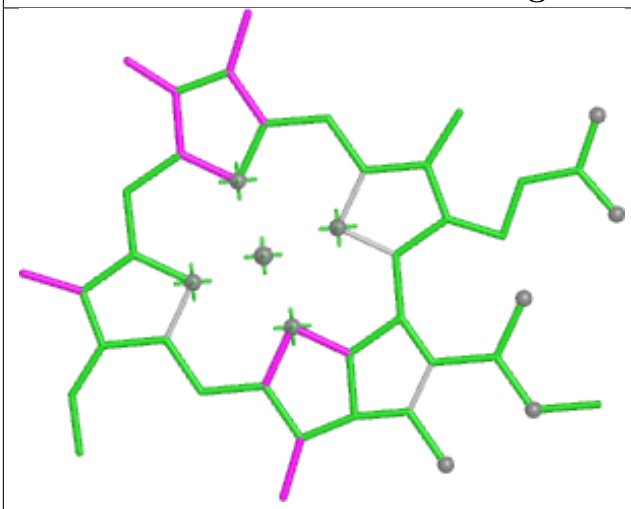


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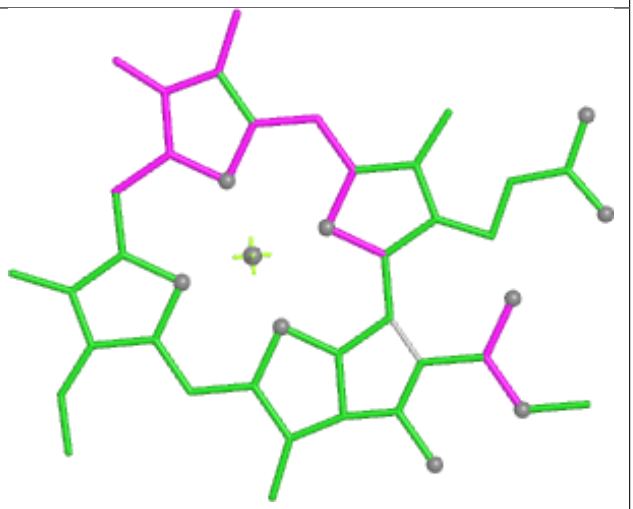


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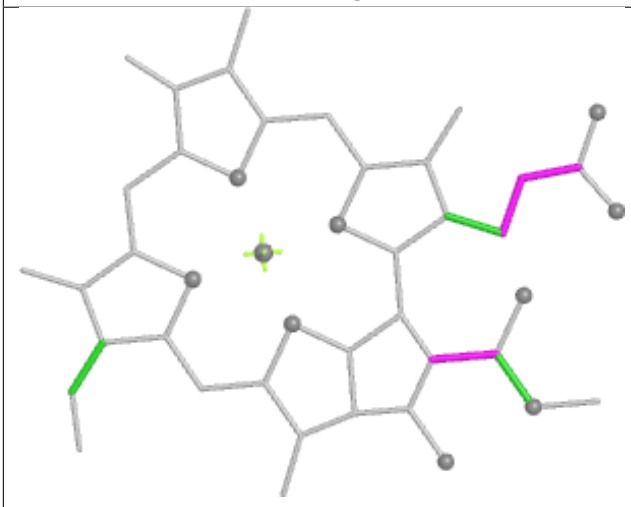
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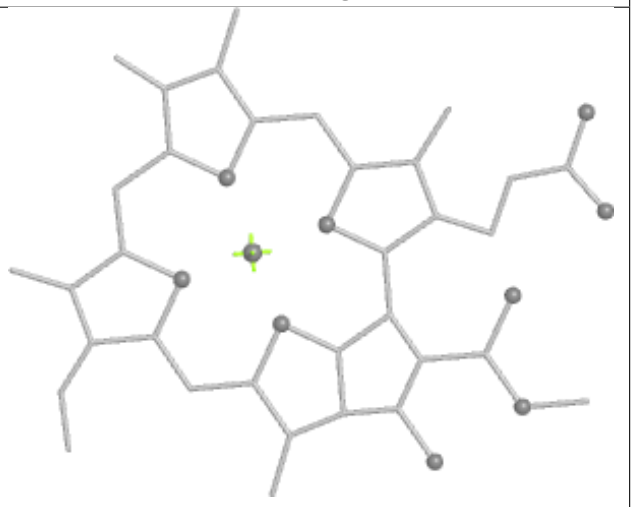
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Bond angles

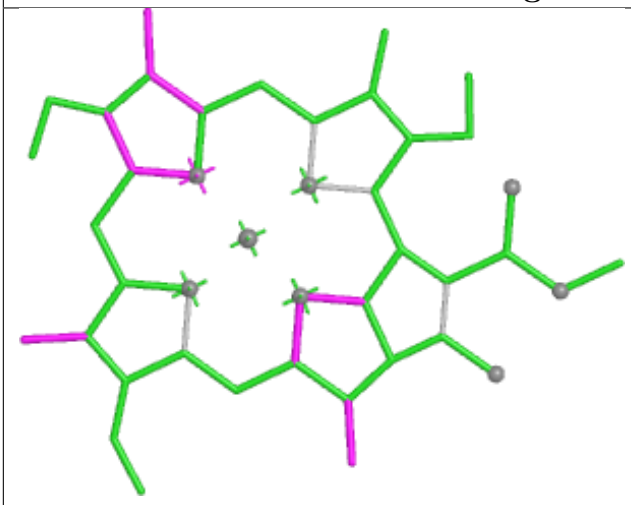


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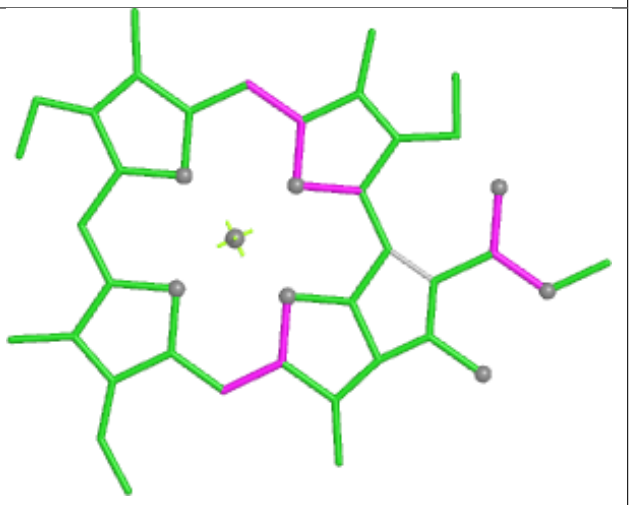


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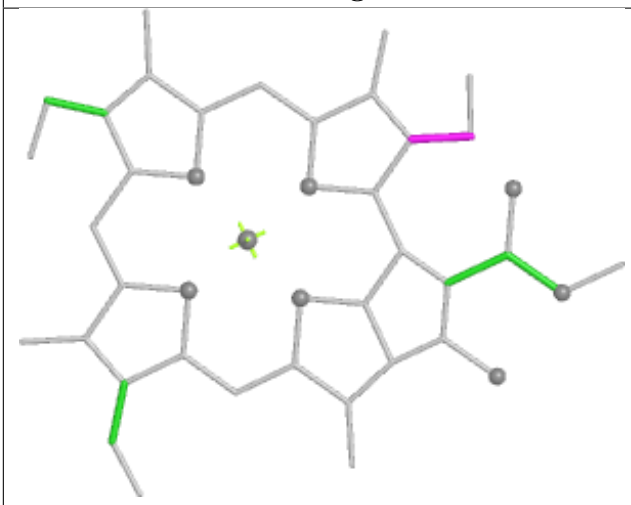
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Bond lengths



Bond angles

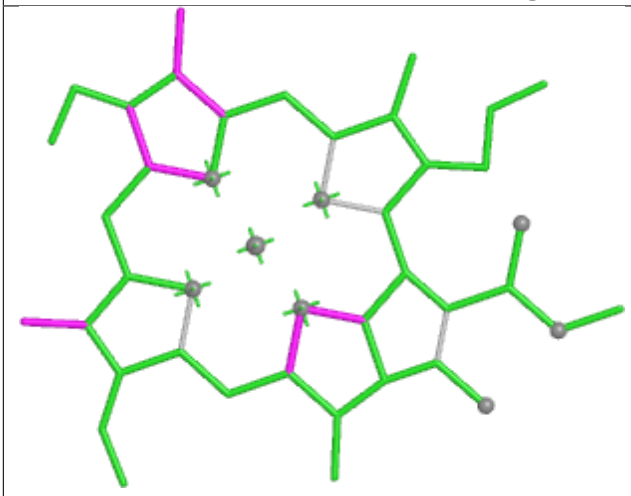


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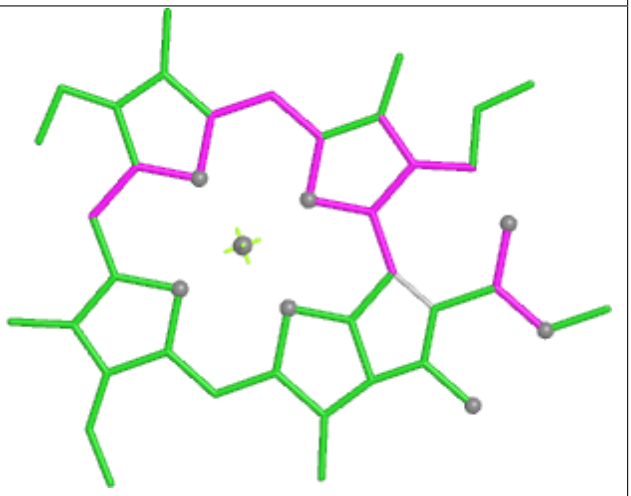


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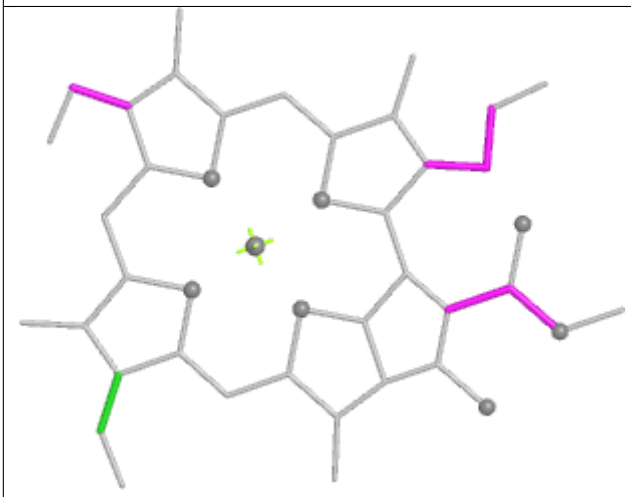
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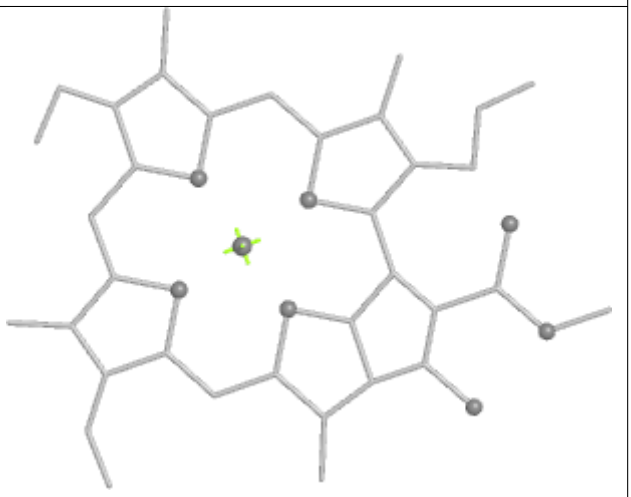
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Bond angles

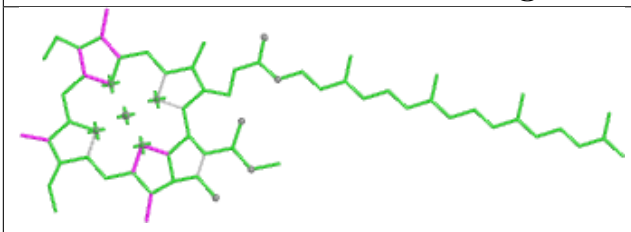


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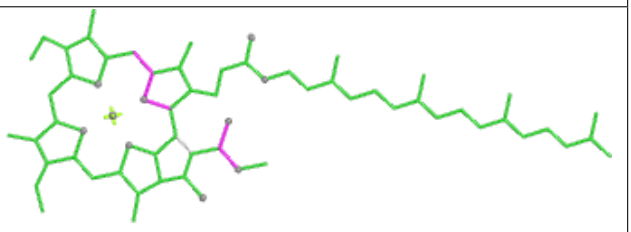


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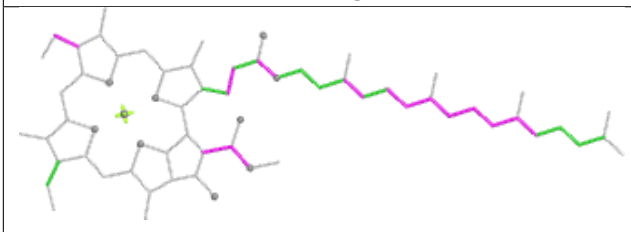
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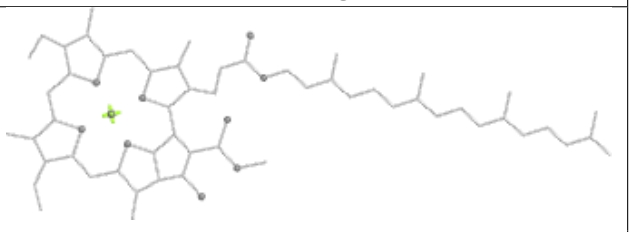
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Bond angles

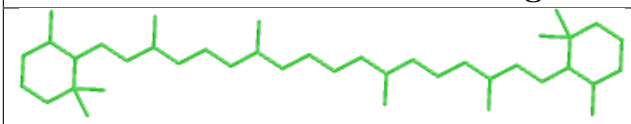


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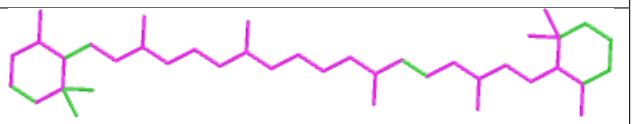


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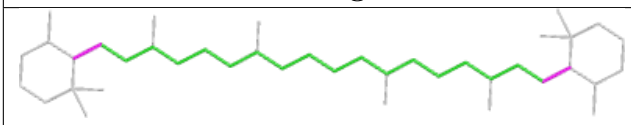
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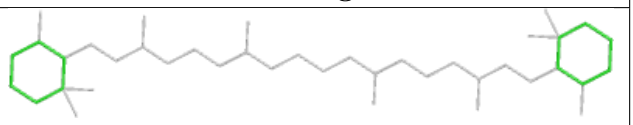
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Bond angles

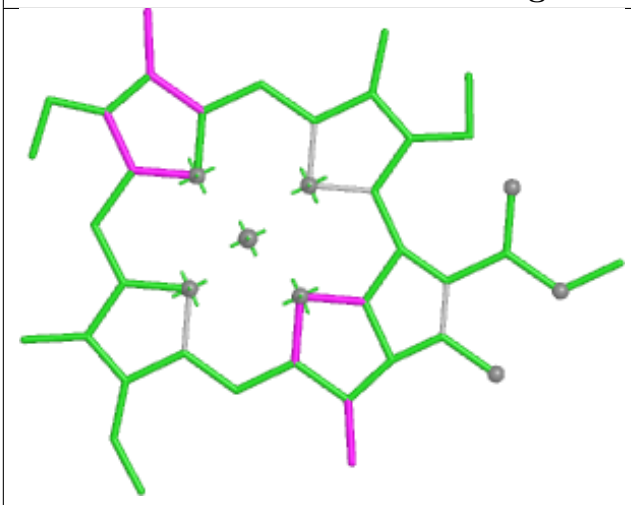


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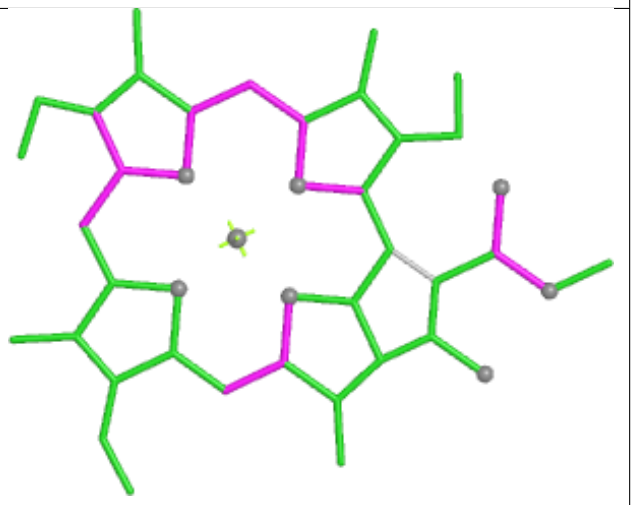


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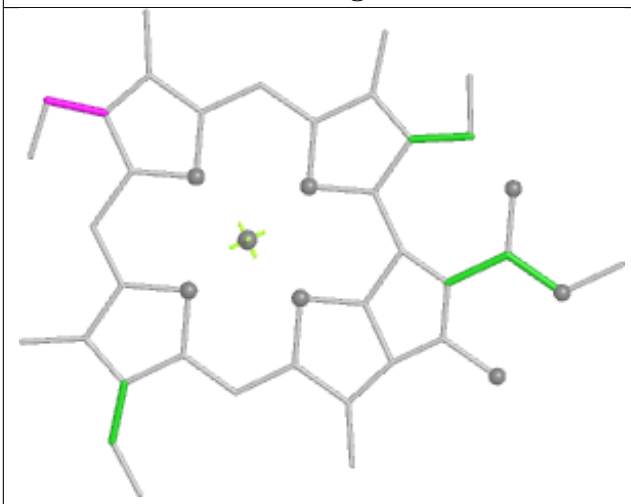
Ligand CLA 5 611



Bond lengths



Bond angles

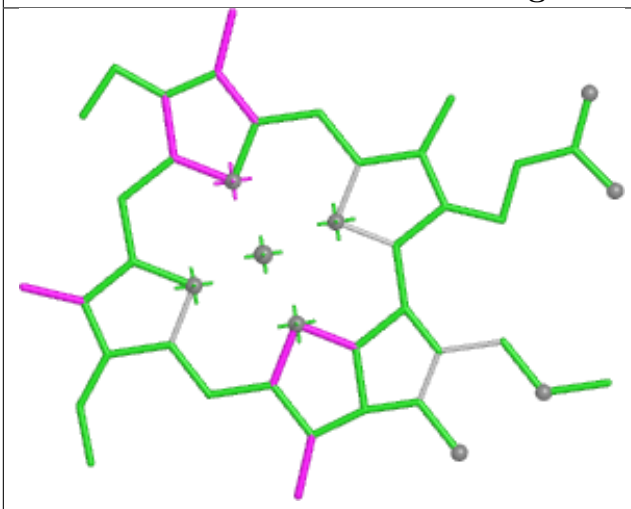


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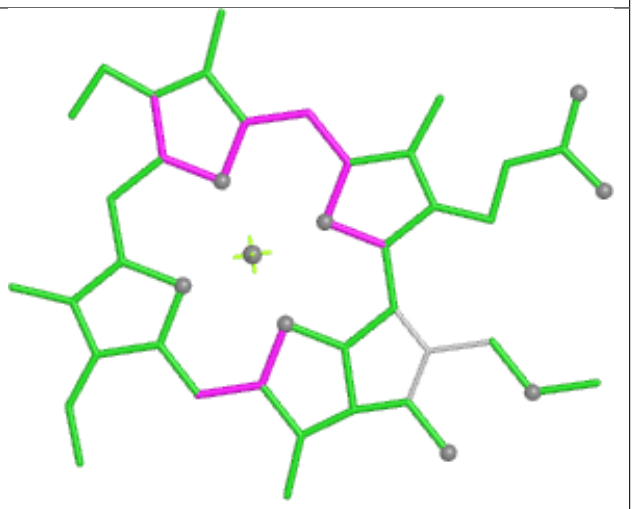


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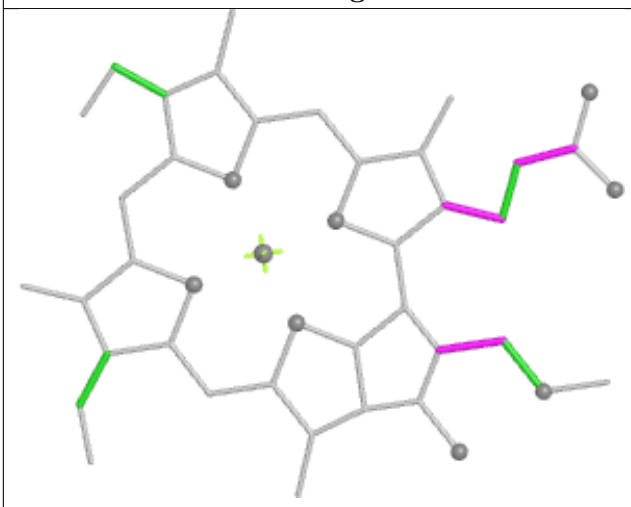
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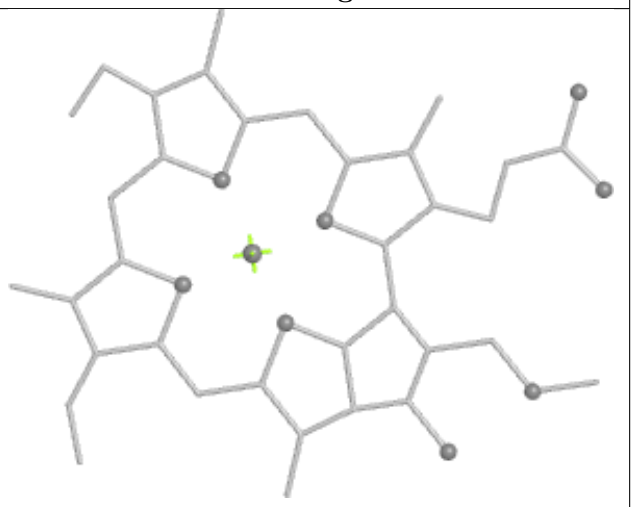
Bond lengths



Bond angles

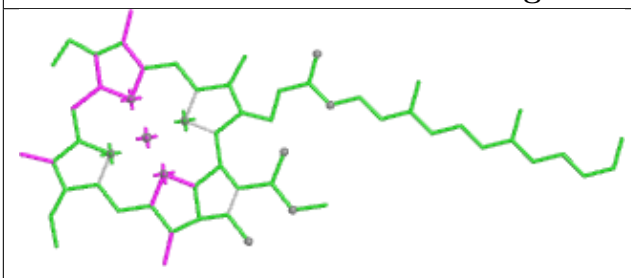


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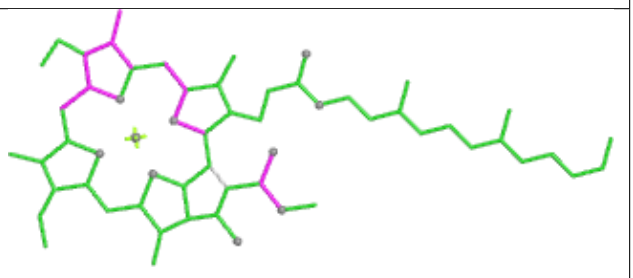


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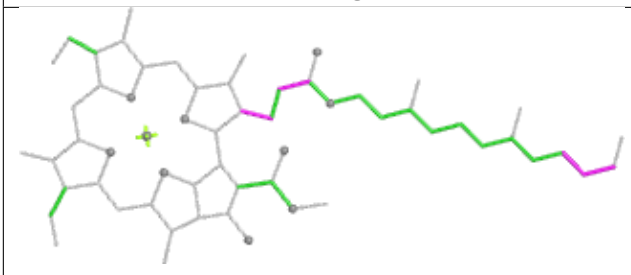
Ligand CLA A 819



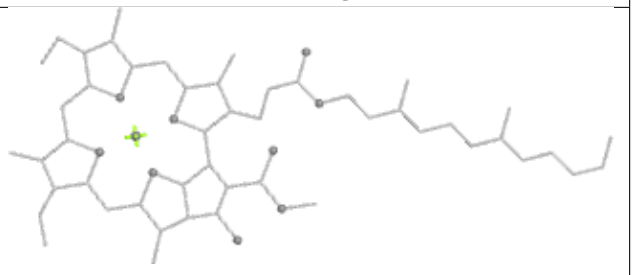
Bond lengths



Bond angles

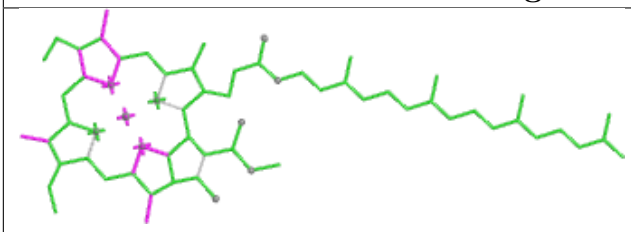


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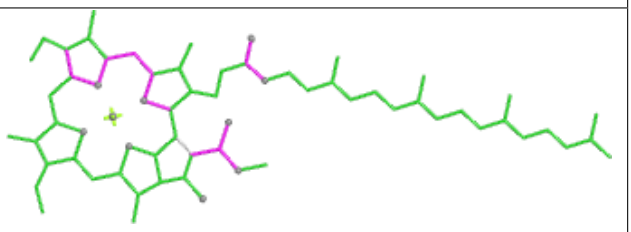


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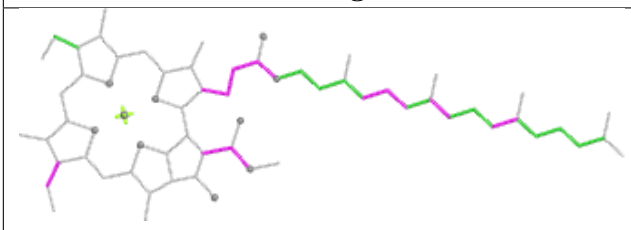
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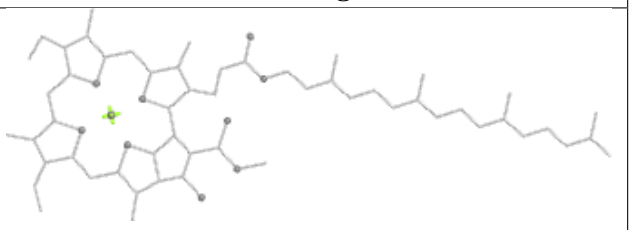
Bond lengths



Bond angles



Torsions



Rings

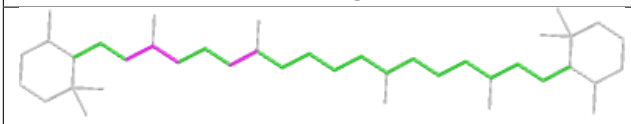
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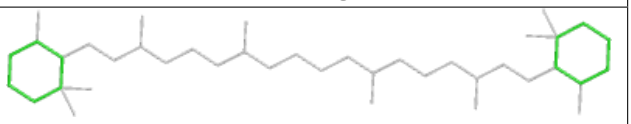
Bond lengths



Bond angles

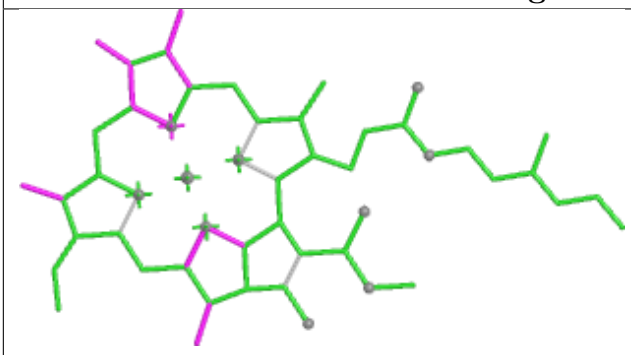


Torsions

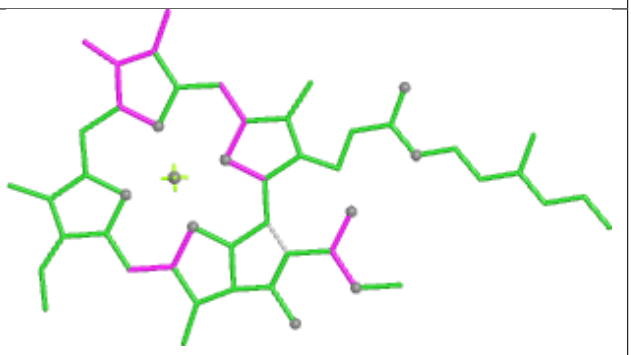


Rings

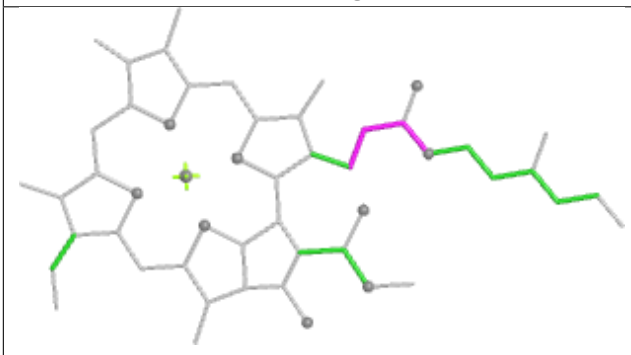
Ligand CLA 6 603



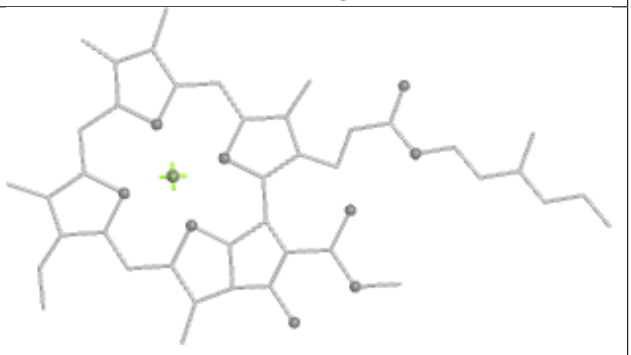
Bond lengths



Bond angles

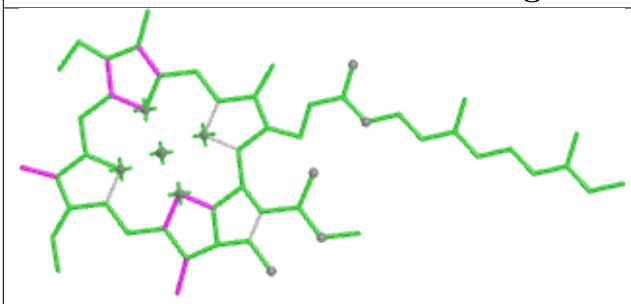


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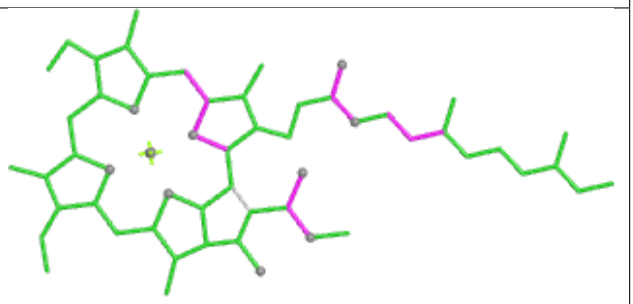


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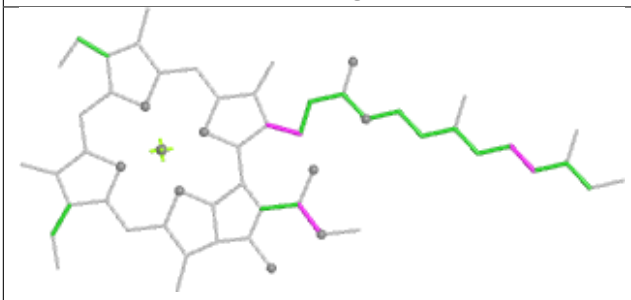
Ligand CLA U 610



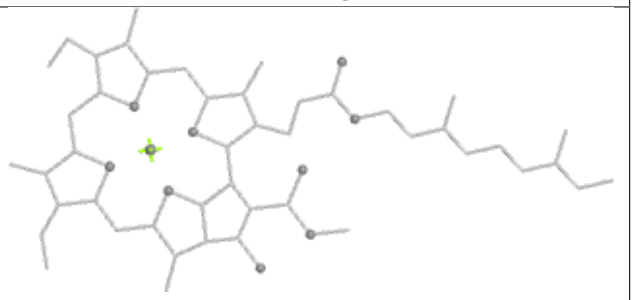
Bond lengths



Bond angles

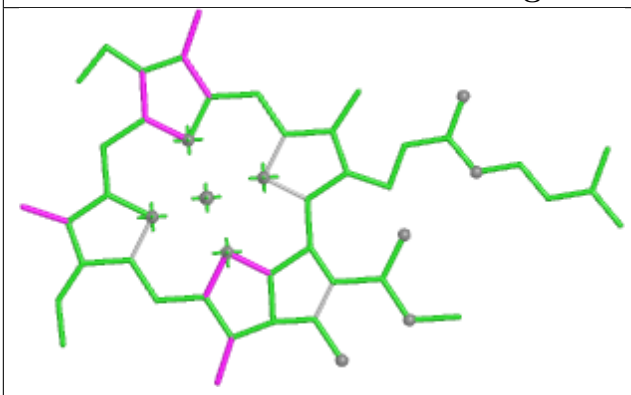


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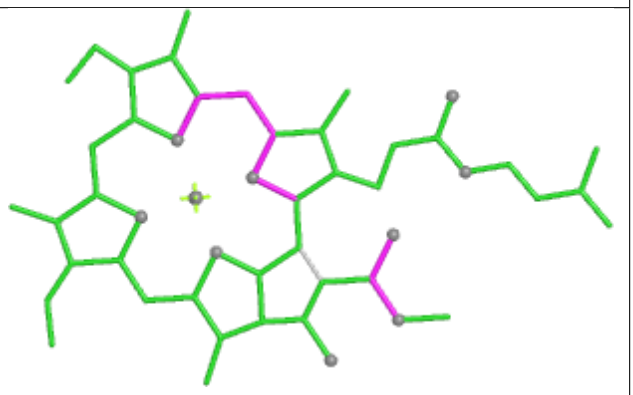


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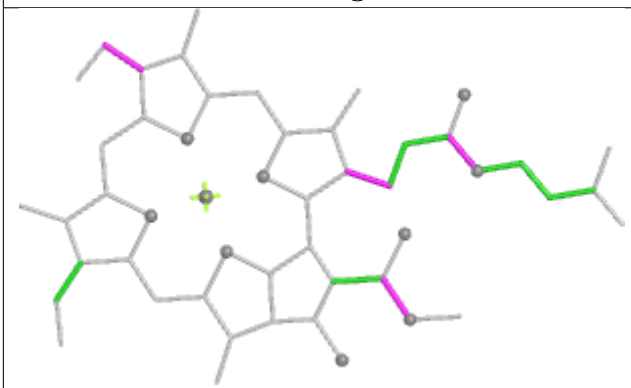
Ligand CLA Y 604



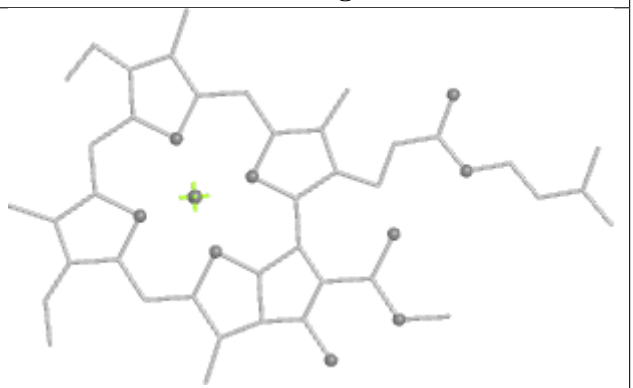
Bond lengths



Bond angles

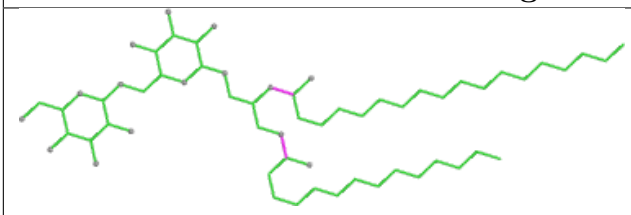


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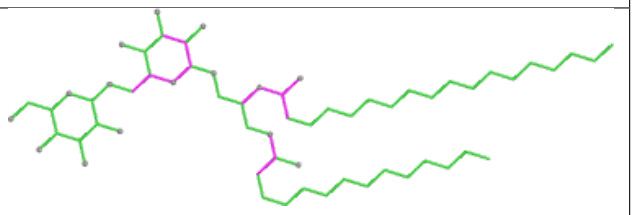


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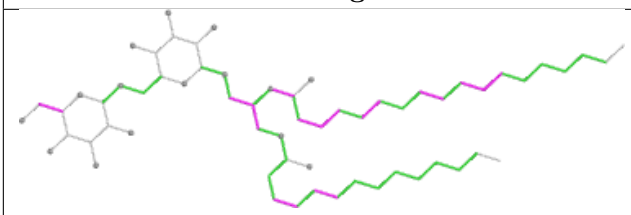
Ligand DGD B 850



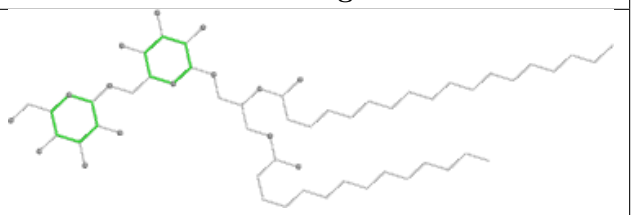
Bond lengths



Bond angles



Torsions

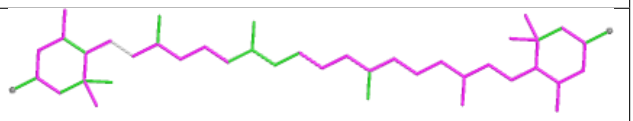


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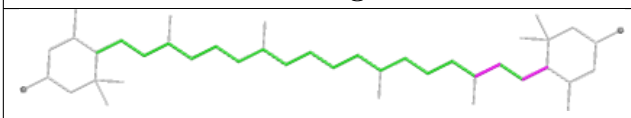
Ligand LUT 4 619



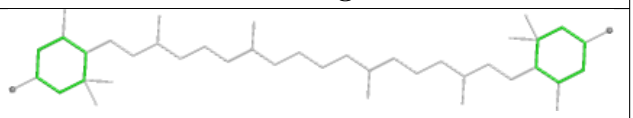
Bond lengths



Bond angles

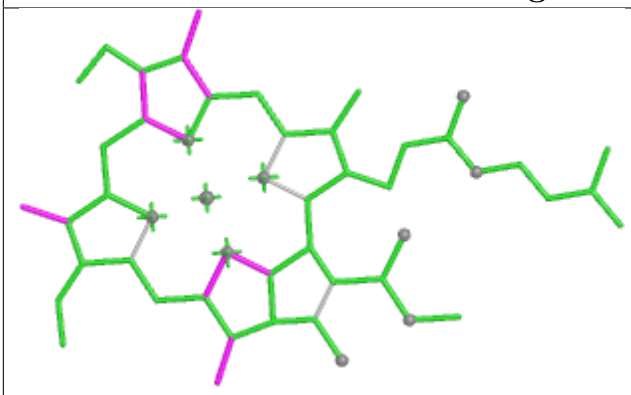


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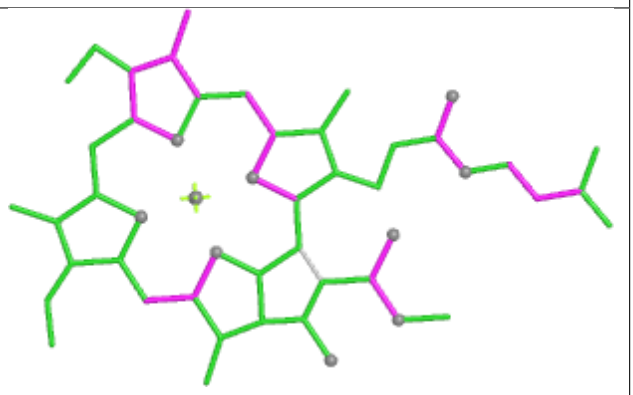


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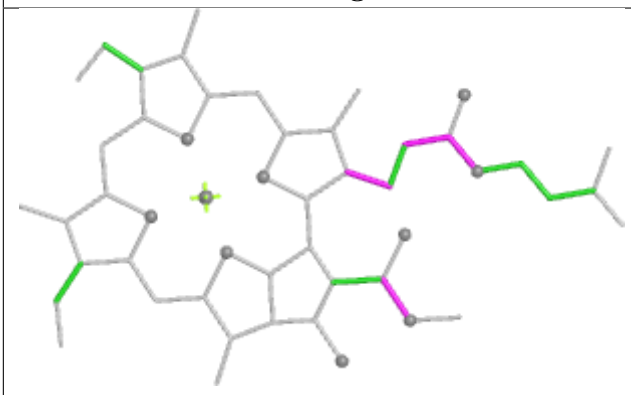
Ligand CLA 8 604



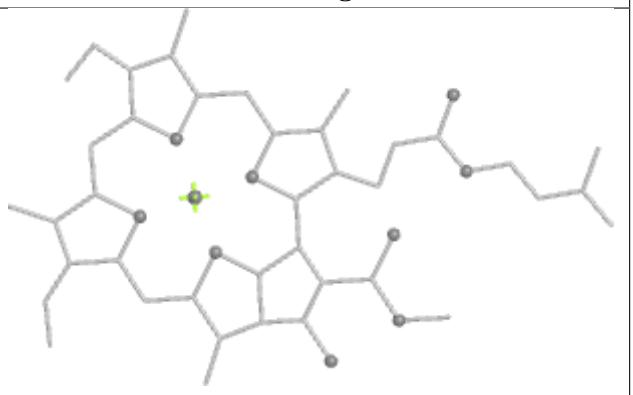
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Bond angles

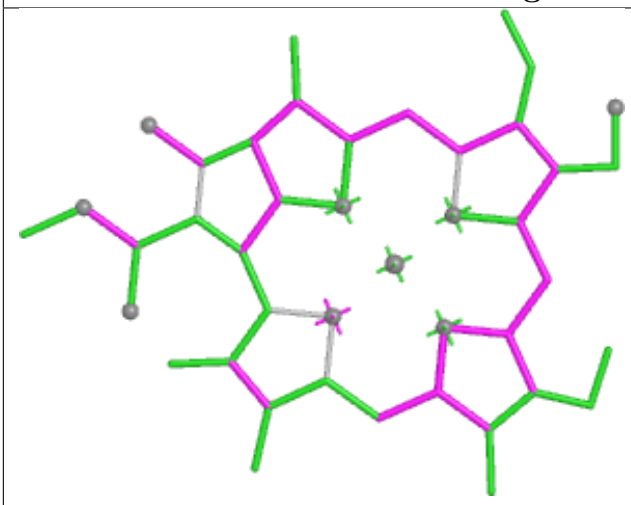


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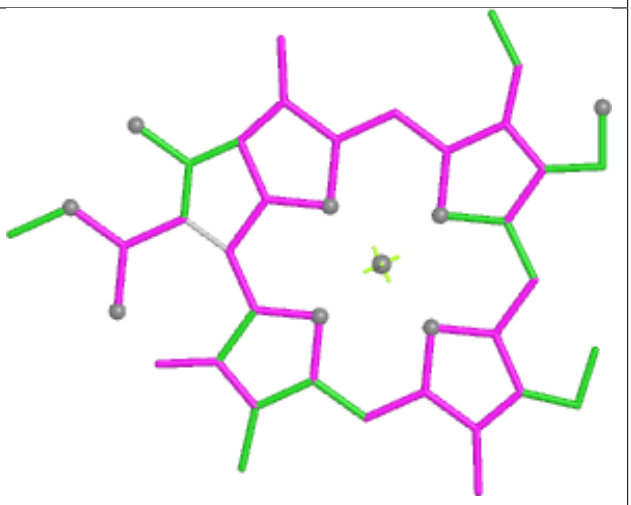


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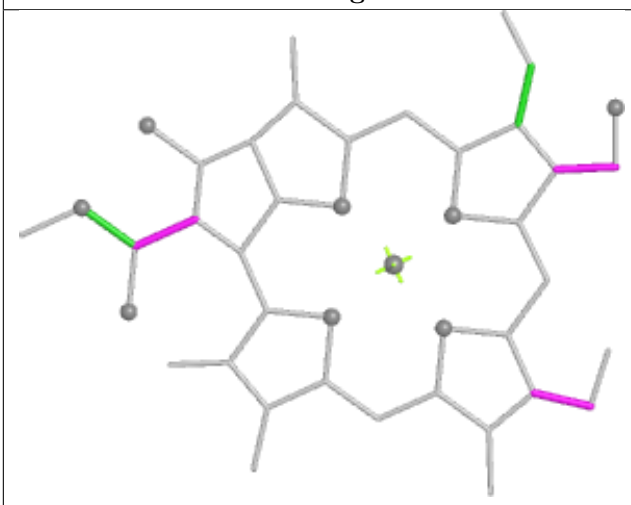
Ligand CHL Y 605



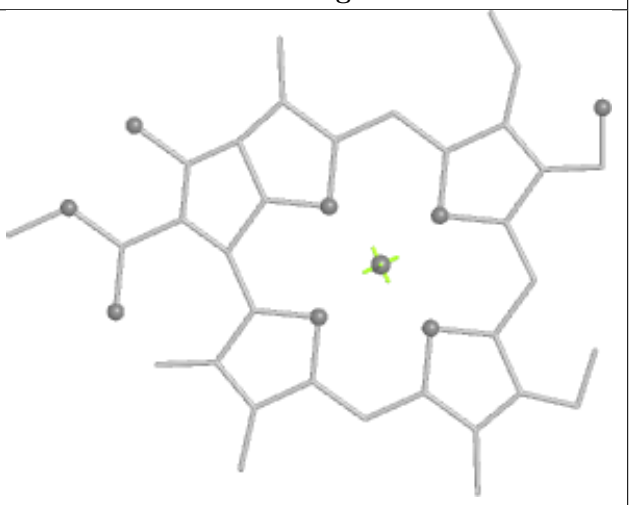
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Bond angles

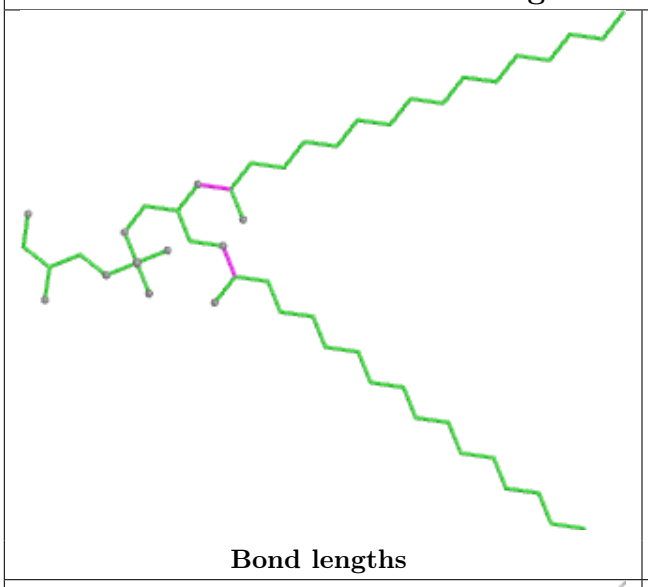


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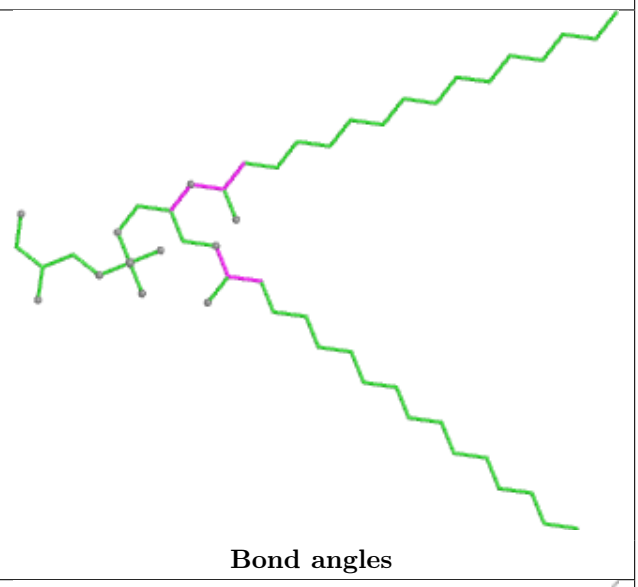


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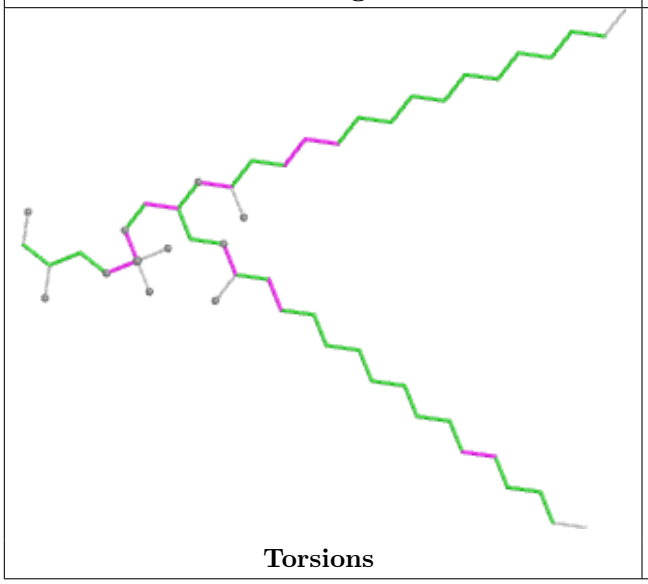
Ligand LHG 3 624



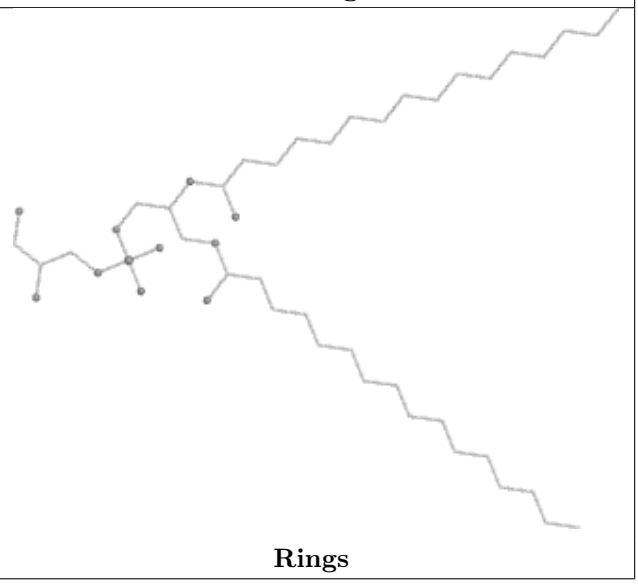
Bond lengths



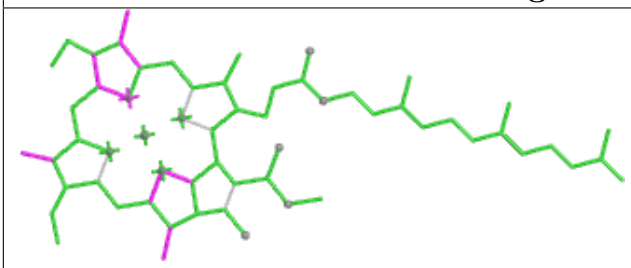
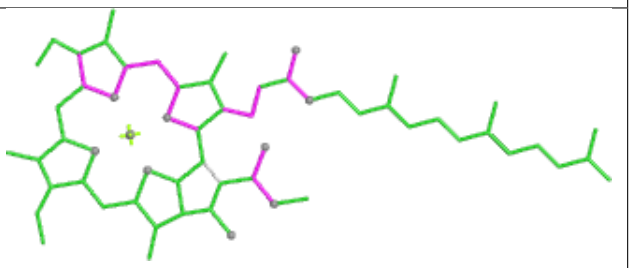
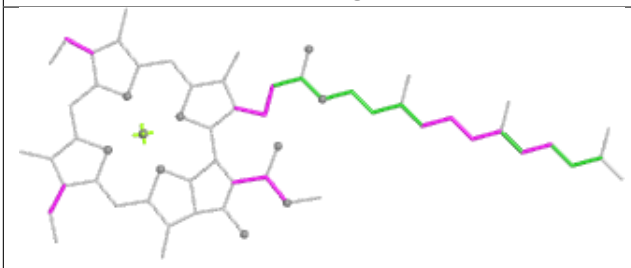
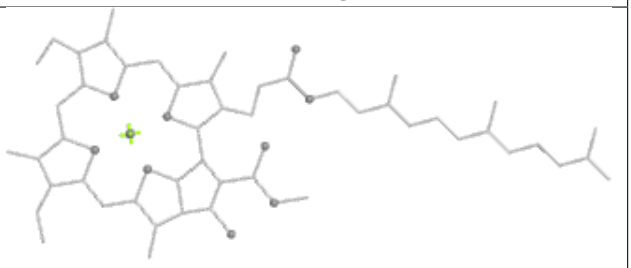
Bond angles

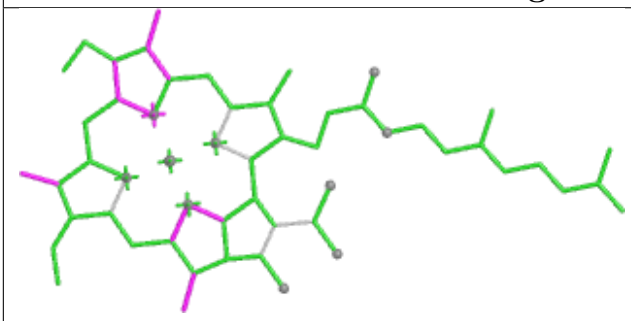
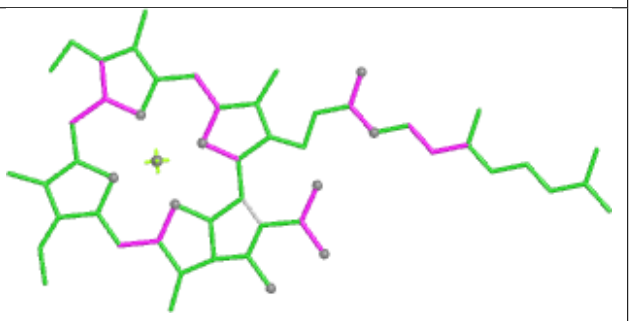
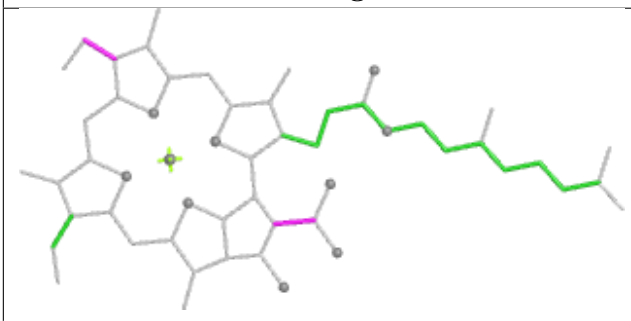
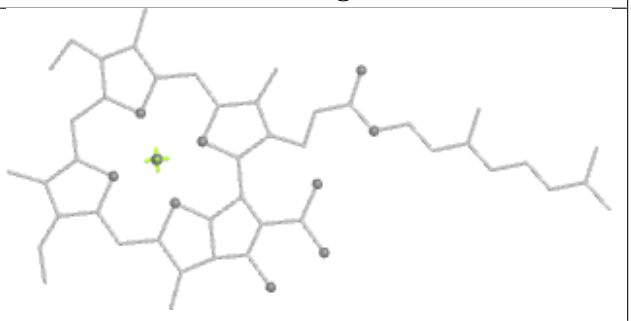


Torsions

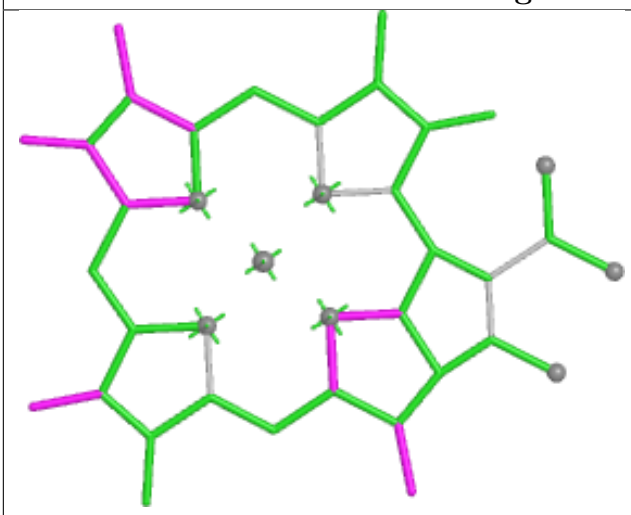


Rings

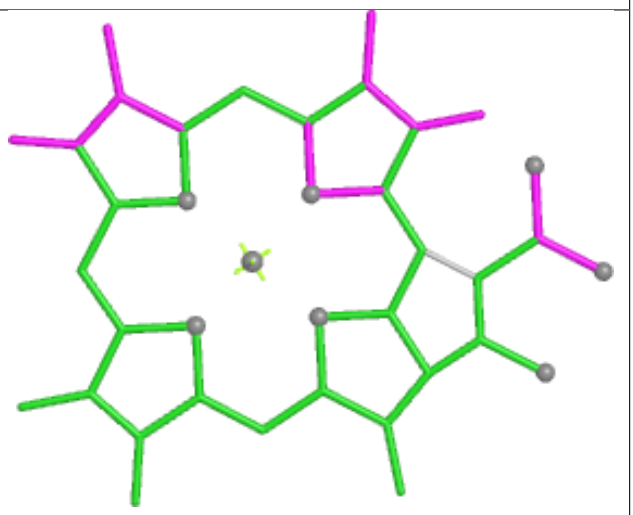
Ligand CLA 3 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 3 606	
	
Bond lengths	Bond angles
	
Torsions	Rings

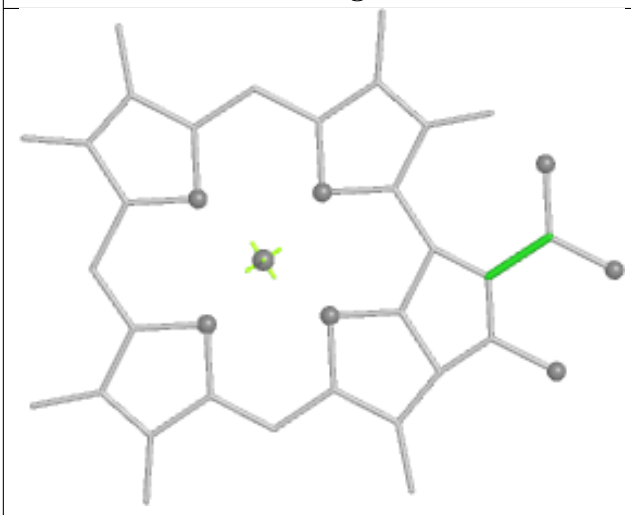
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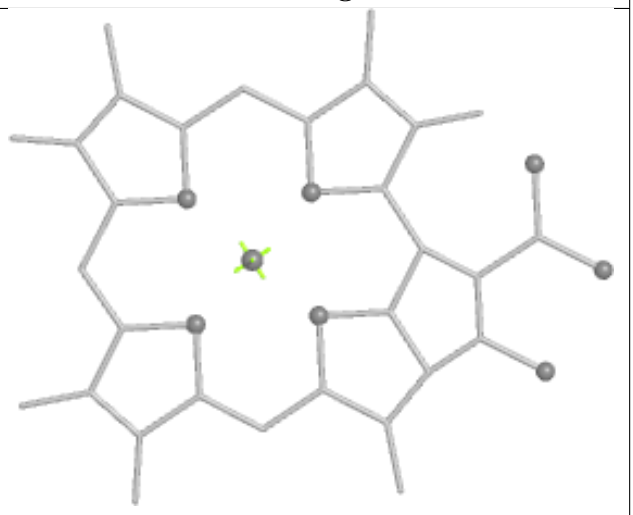
Bond lengths



Bond angles

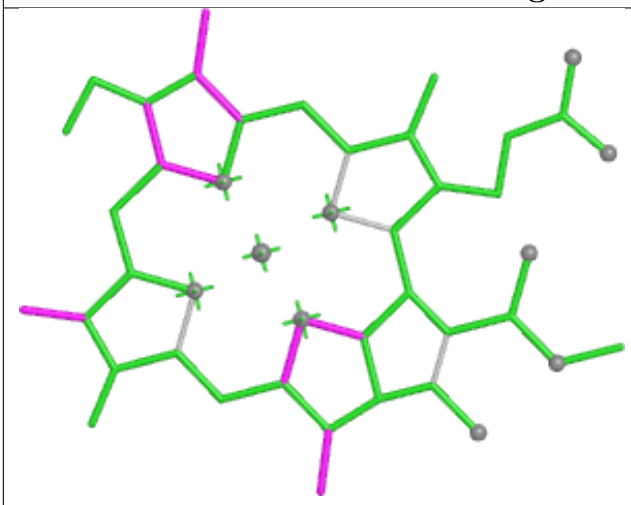


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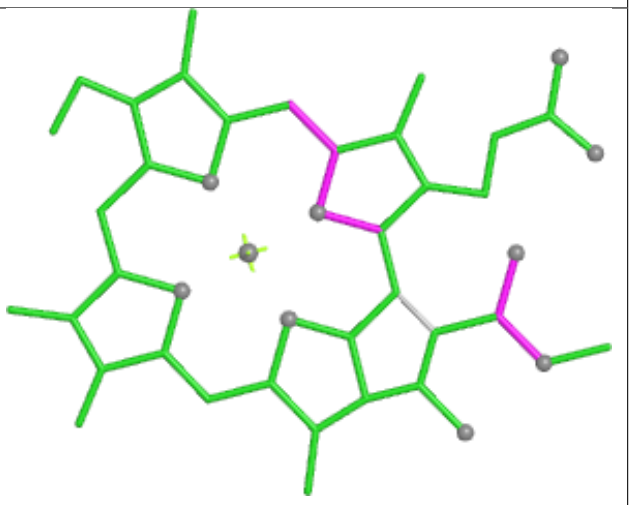


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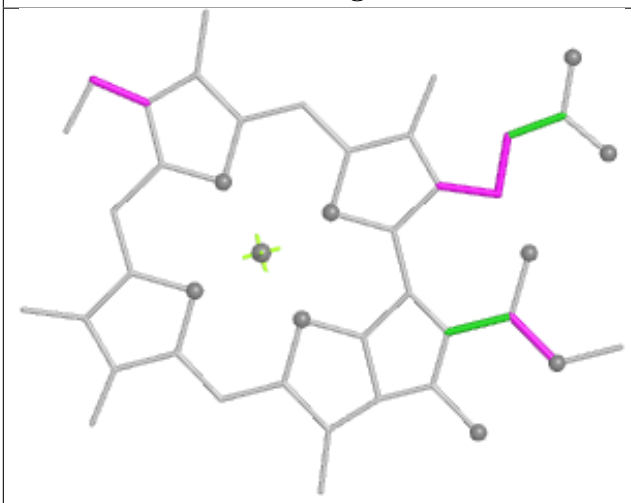
Ligand CLA 2 612



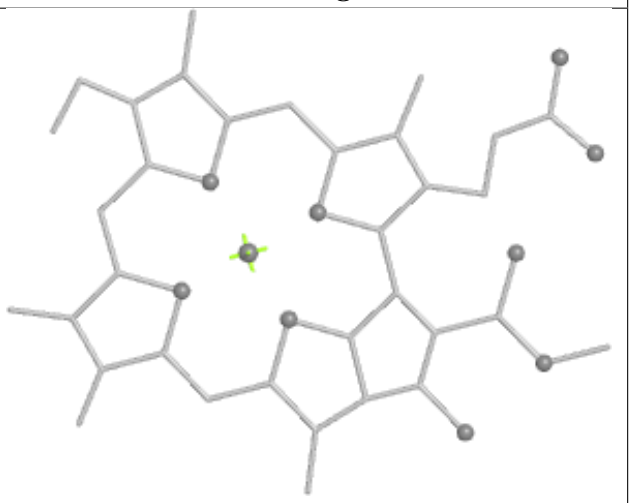
Bond lengths



Bond angles

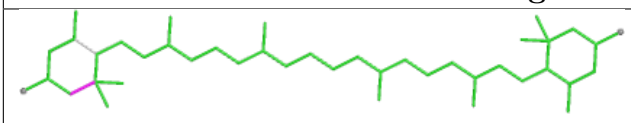


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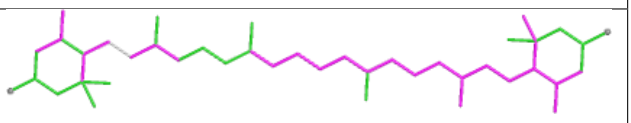


Rings

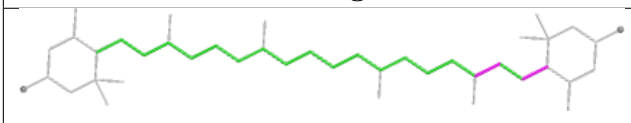
Ligand LUT 1 617



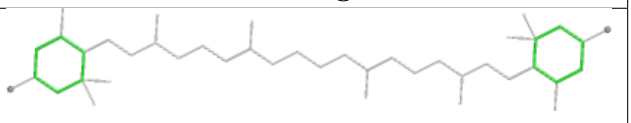
Bond lengths



Bond angles

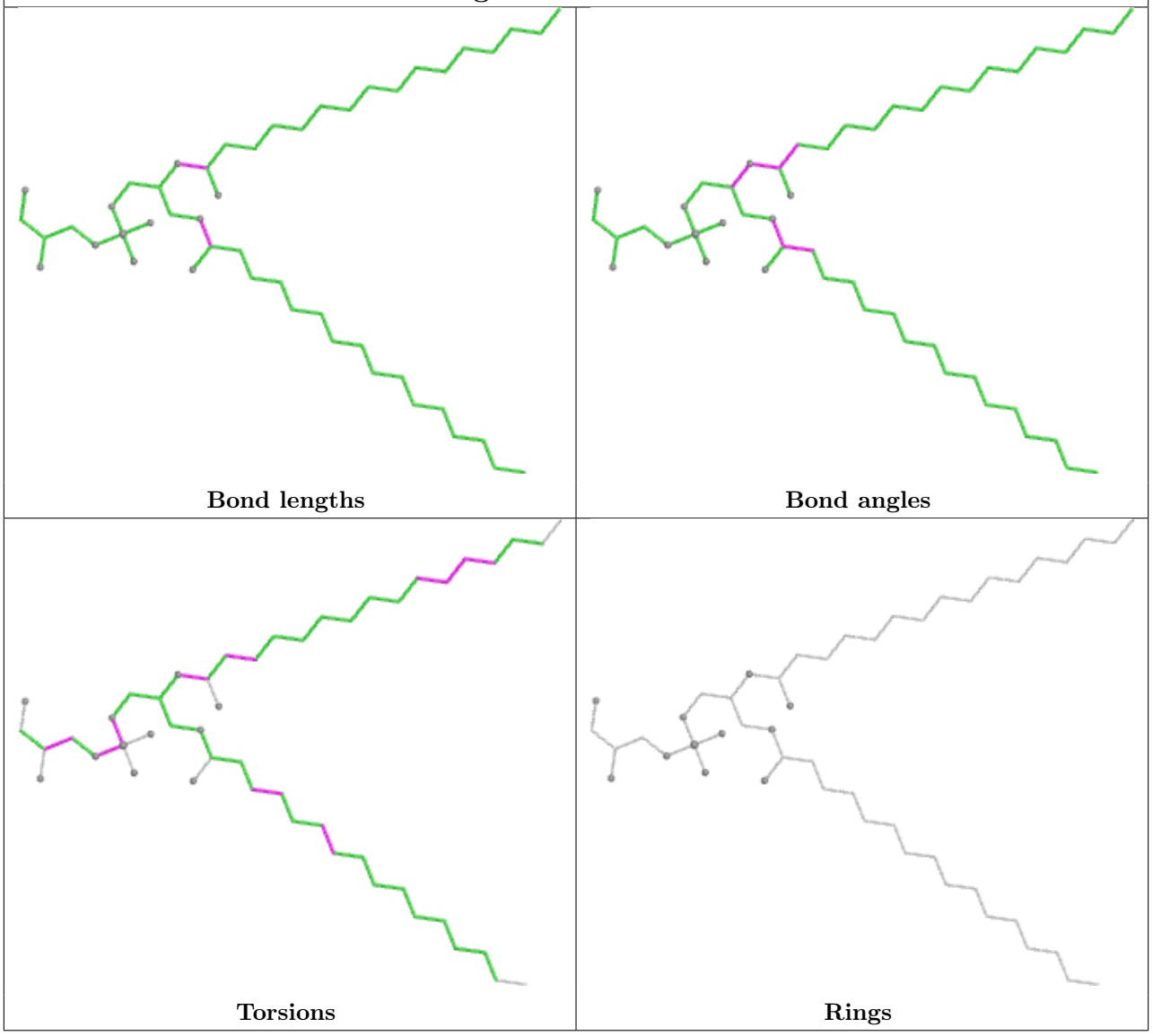


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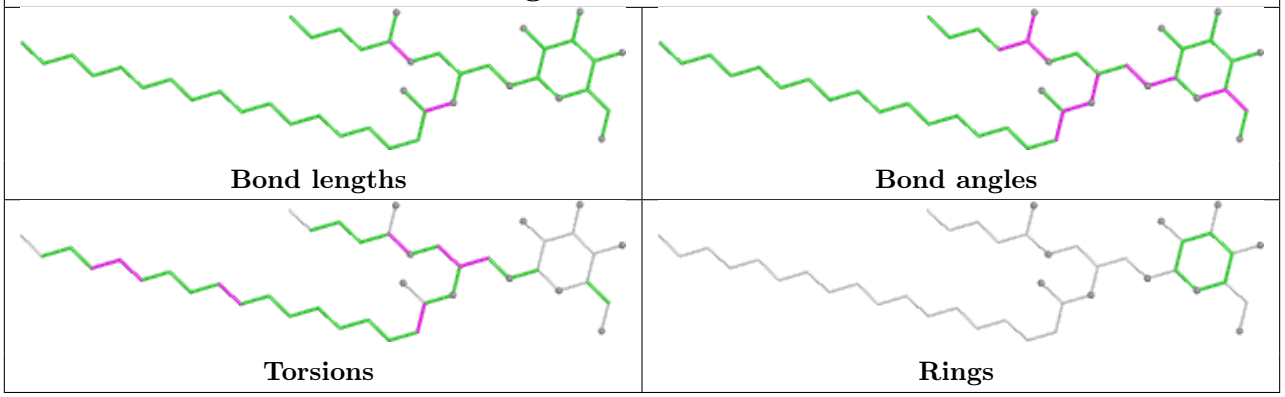


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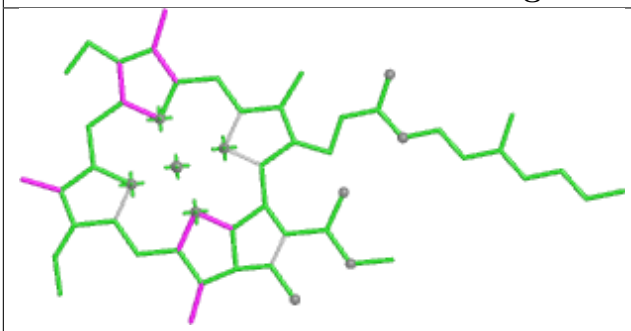
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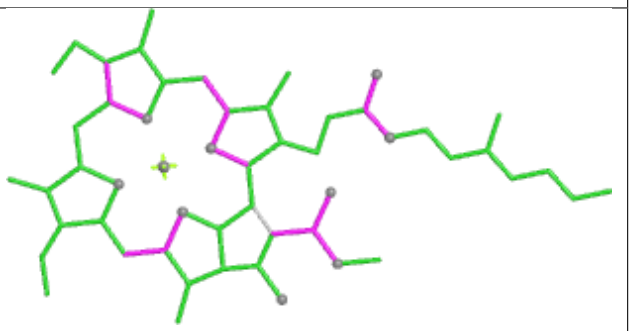
Ligand LMG J 103



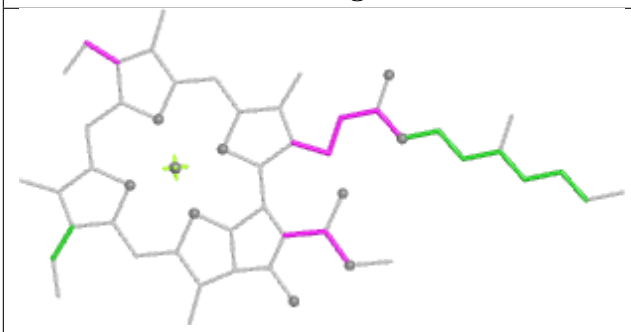
Ligand CLA A 821



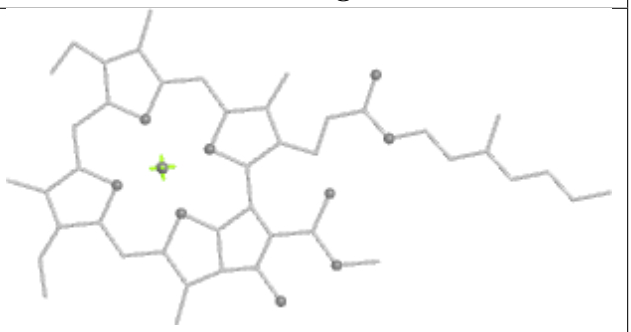
Bond lengths



Bond angles

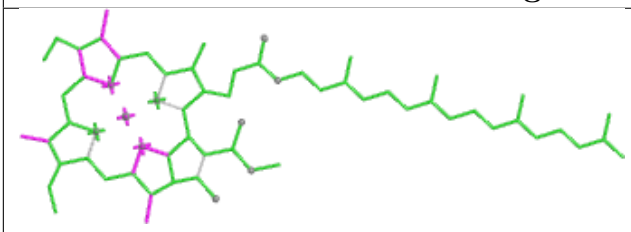


Torsions

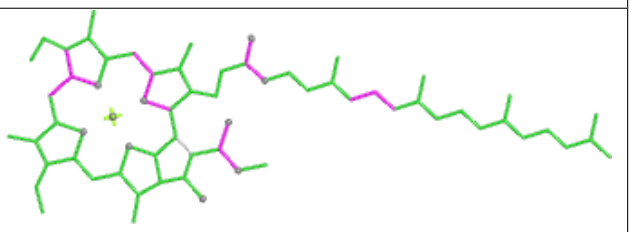


Rings

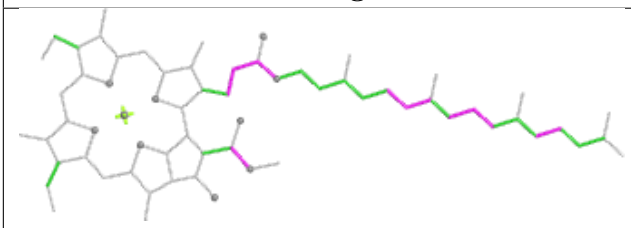
Ligand CLA A 830



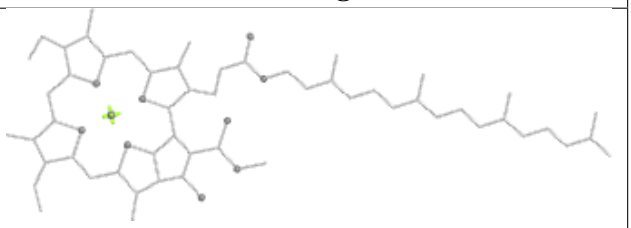
Bond lengths



Bond angles

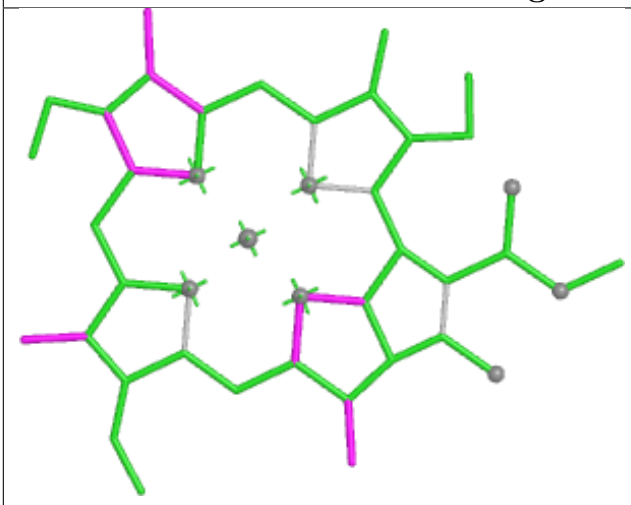


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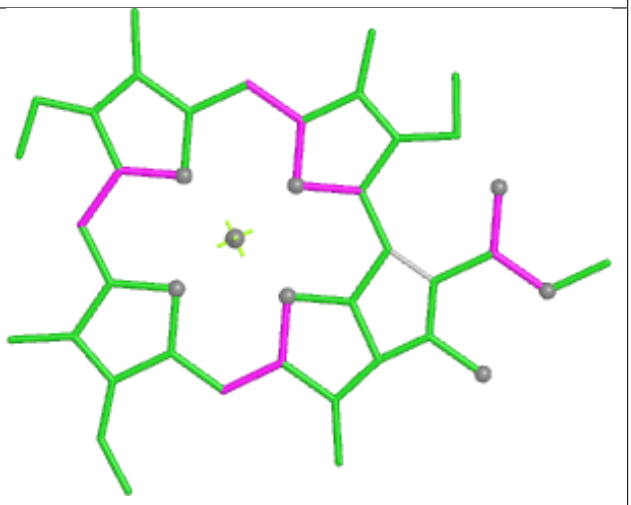


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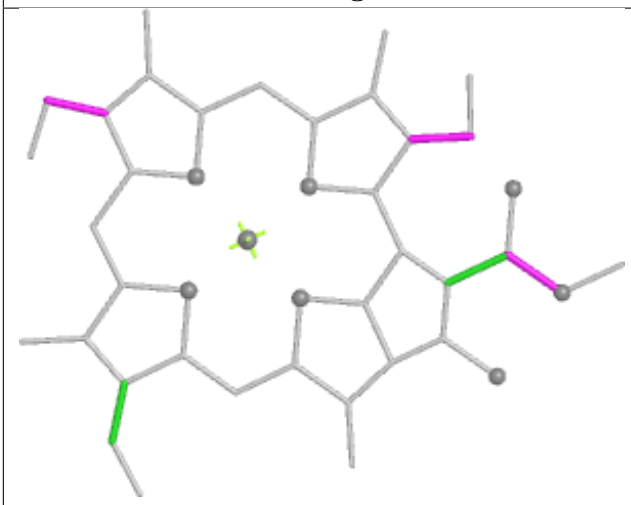
Ligand CLA 8 611



Bond lengths



Bond angles

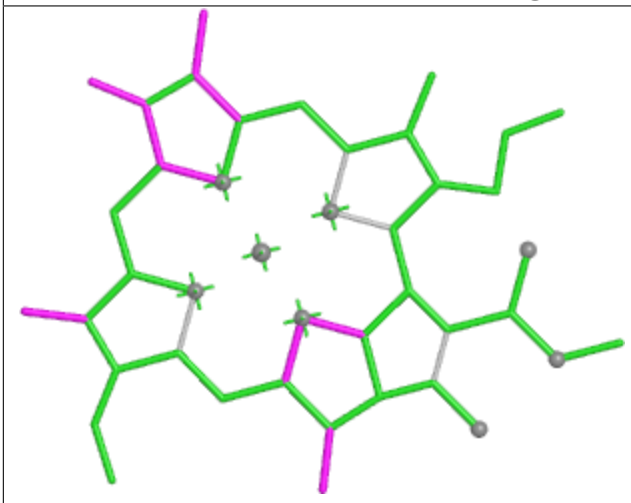


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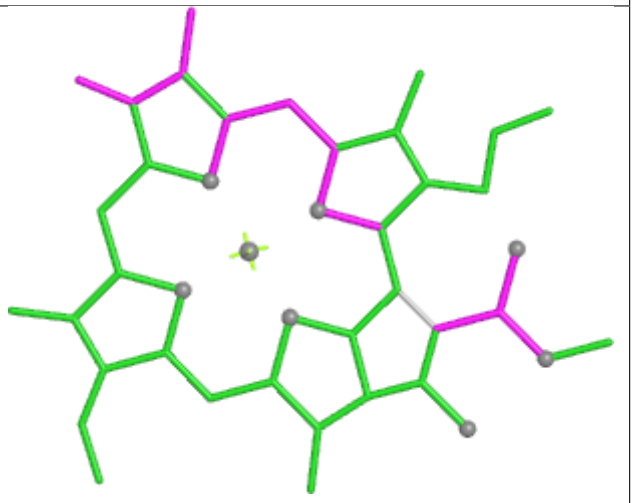


Rings

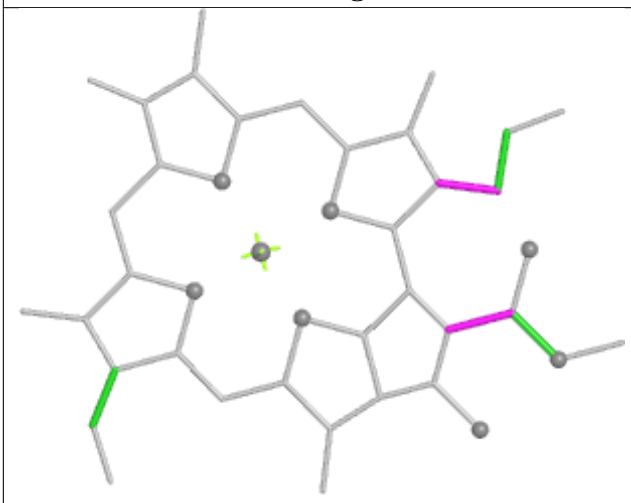
Ligand CLA Z 611



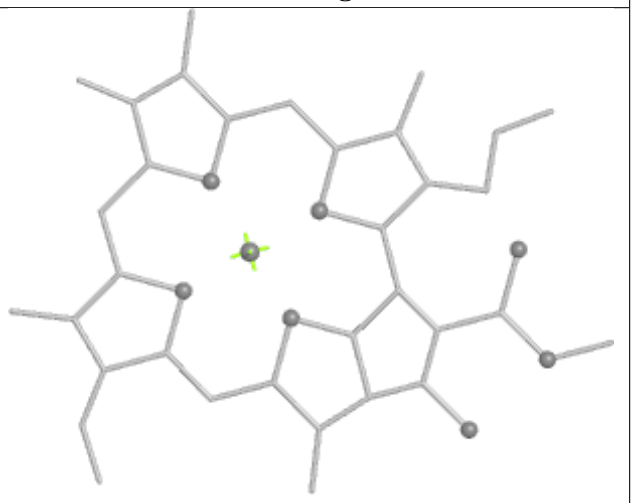
Bond lengths



Bond angles

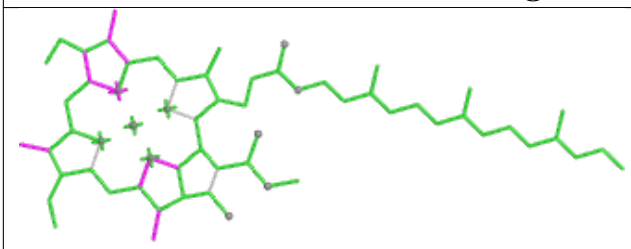


Torsions

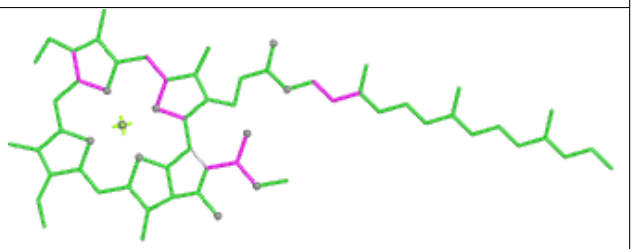


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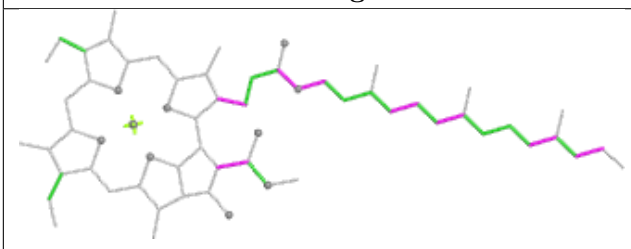
Ligand CLA B 826



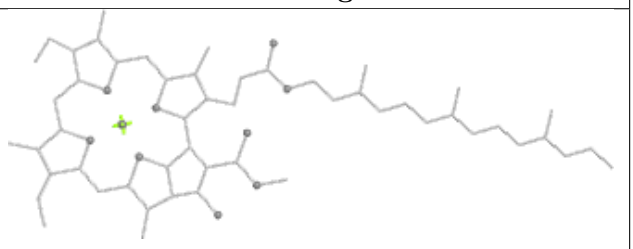
Bond lengths



Bond angles

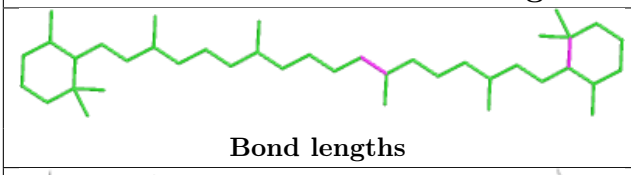


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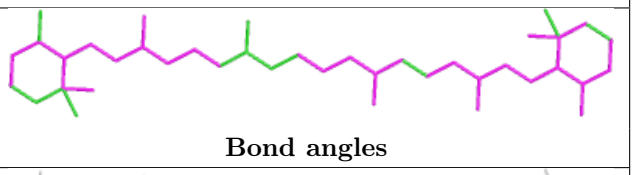


Rings

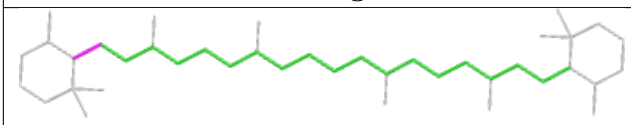
Ligand BCR J 102



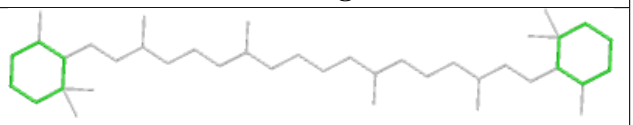
Bond lengths



Bond angles

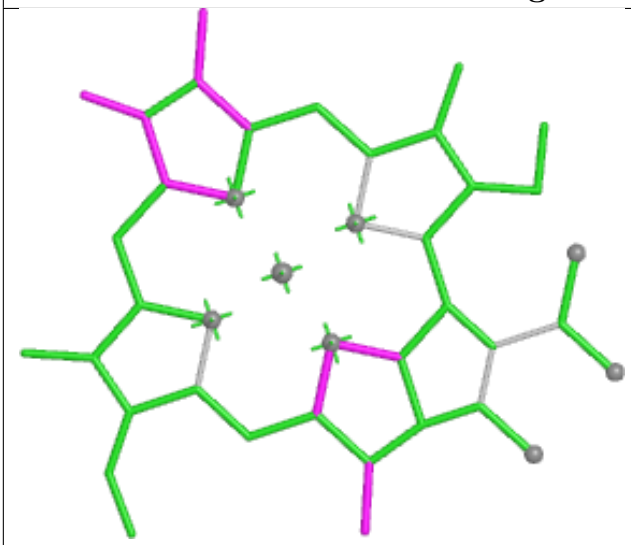


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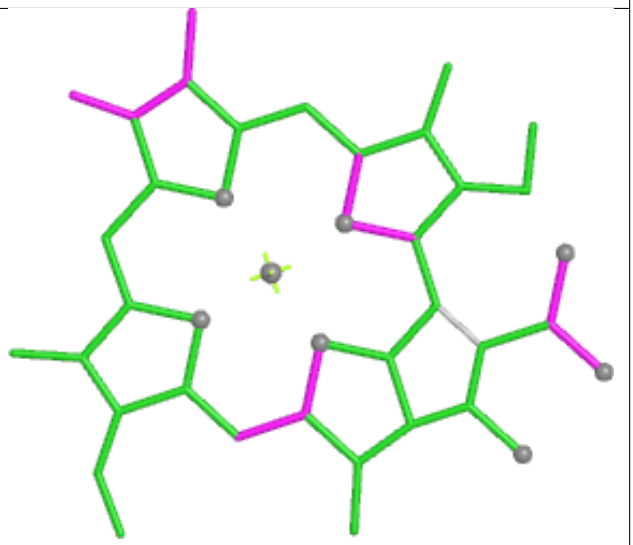


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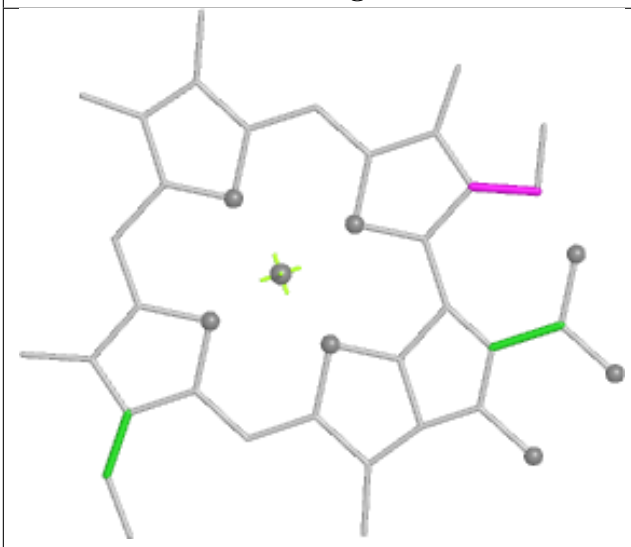
Ligand CLA 4 618



Bond lengths



Bond angles

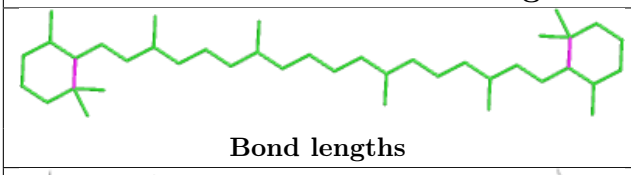


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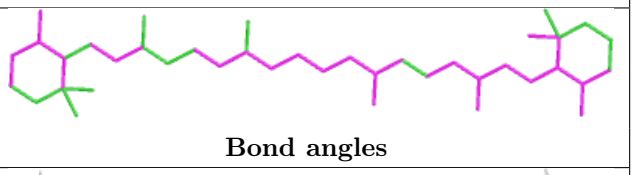


Rings

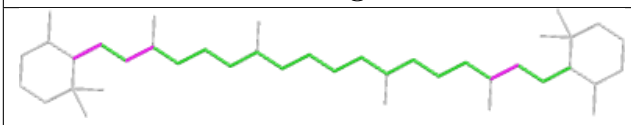
Ligand BCR B 849



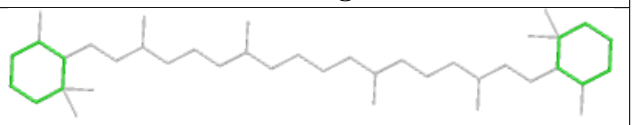
Bond lengths



Bond angles

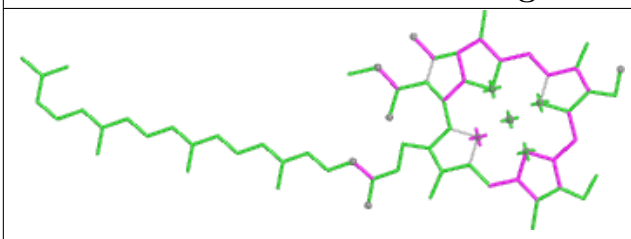


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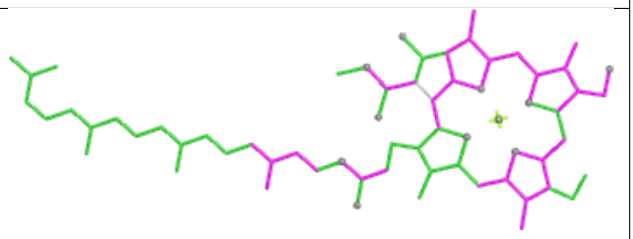


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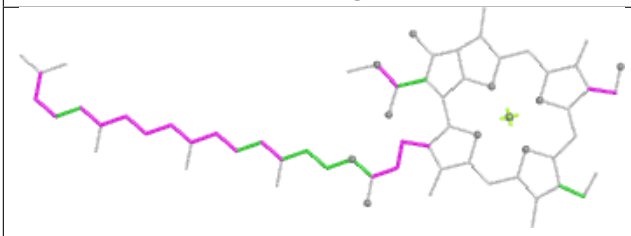
Ligand CHL W 607



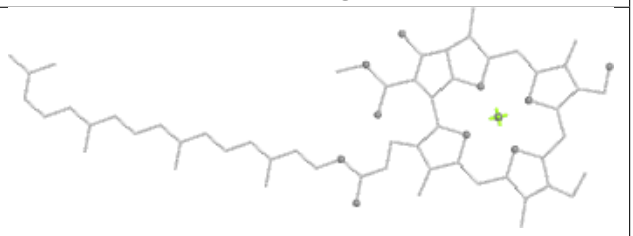
Bond lengths



Bond angles

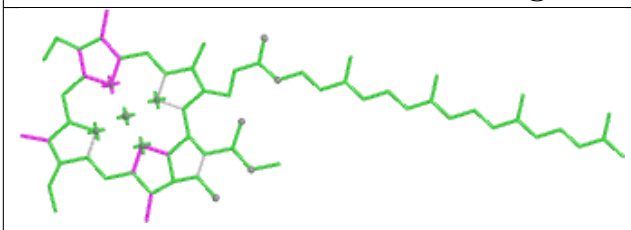


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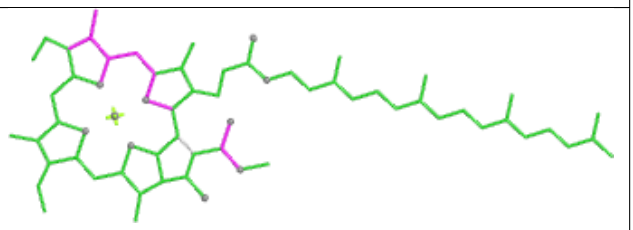


Rings

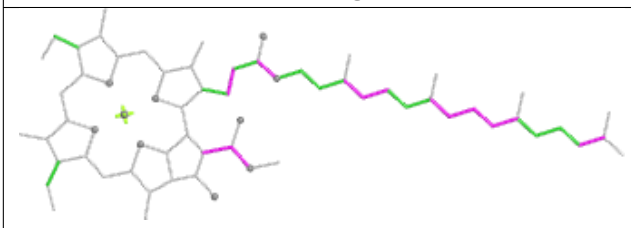
Ligand CLA 1 613



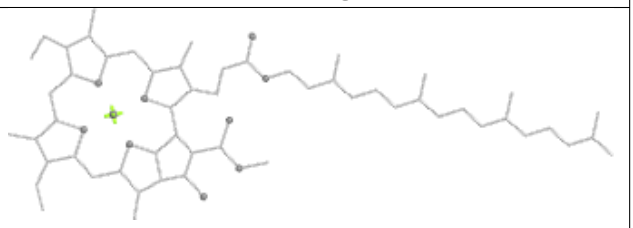
Bond lengths



Bond angles

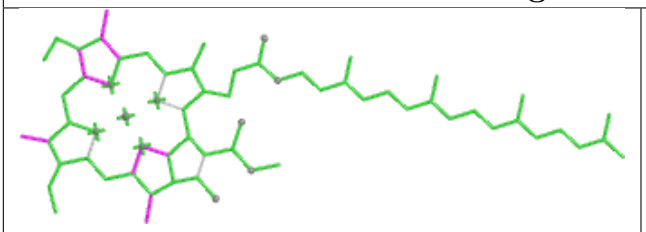


Torsions

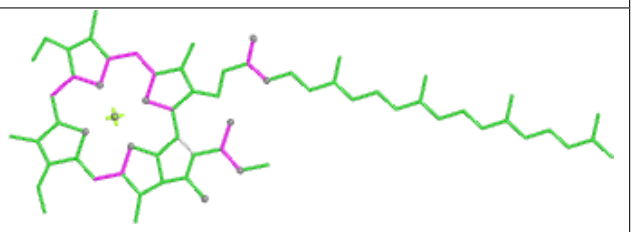


Rings

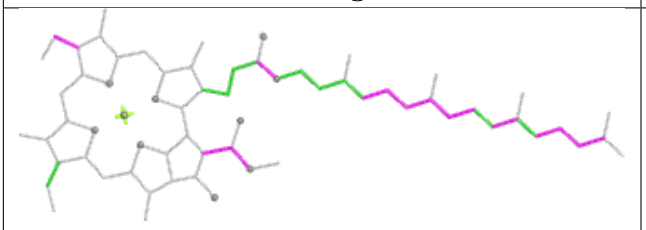
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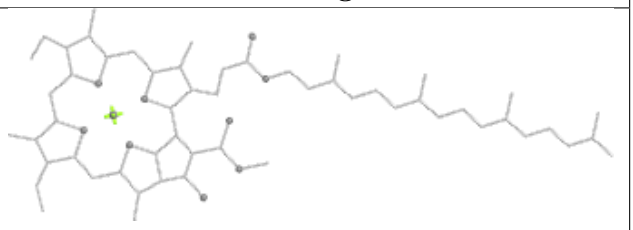
Bond lengths



Bond angles

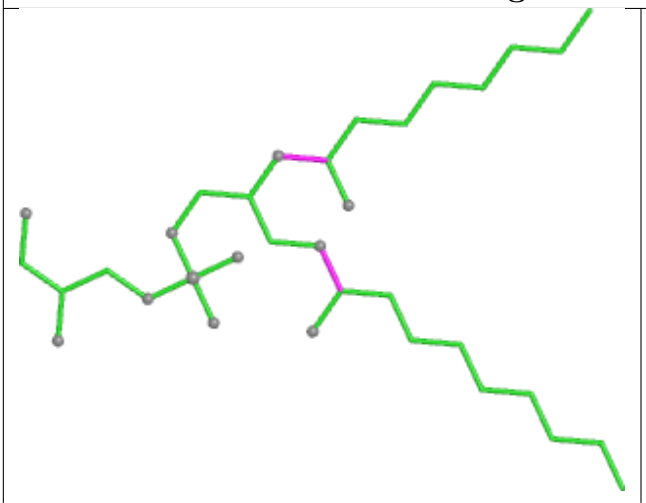


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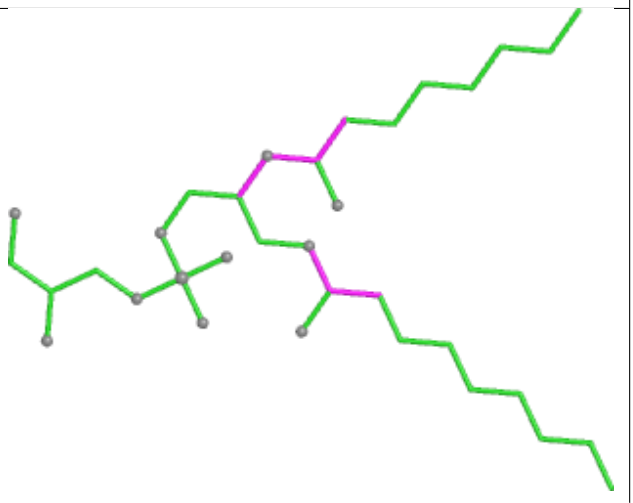


Rings

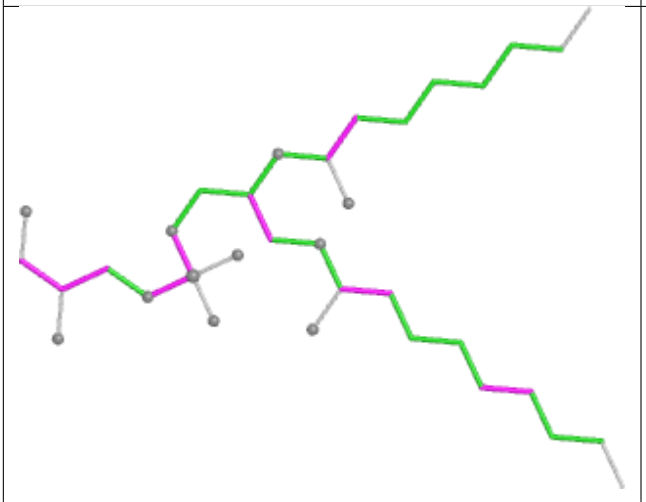
Ligand LHG W 2630



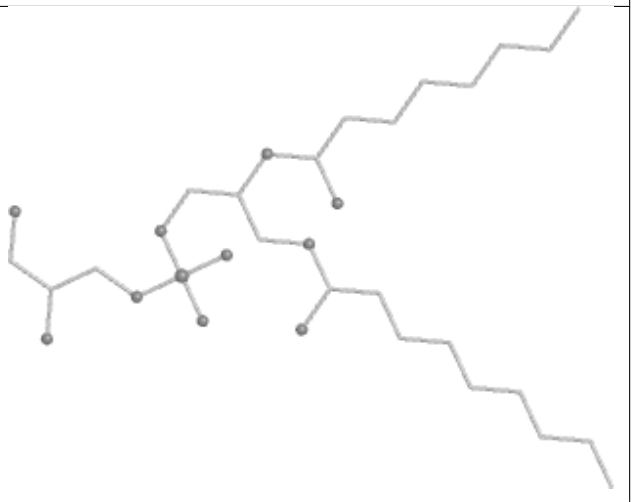
Bond lengths



Bond angles

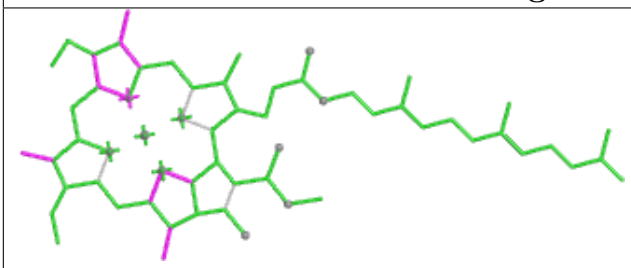


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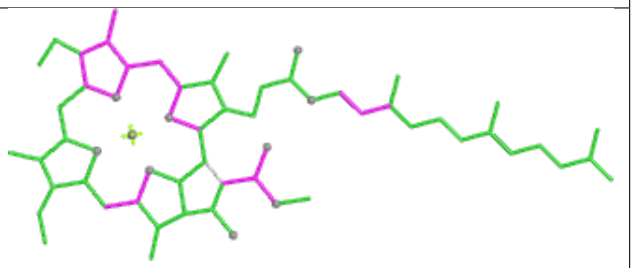


Rings

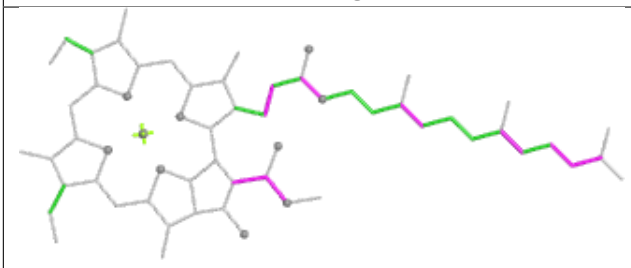
Ligand CLA 8 602



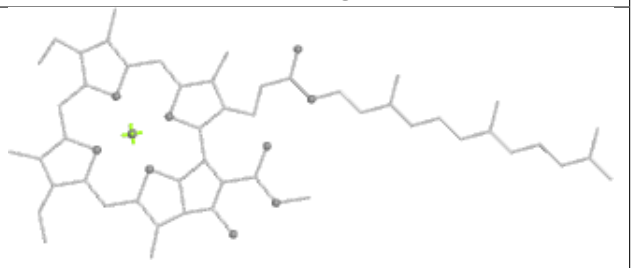
Bond lengths



Bond angles

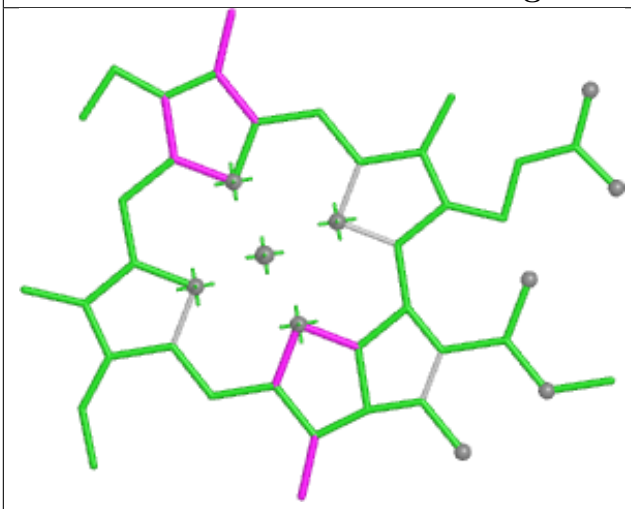


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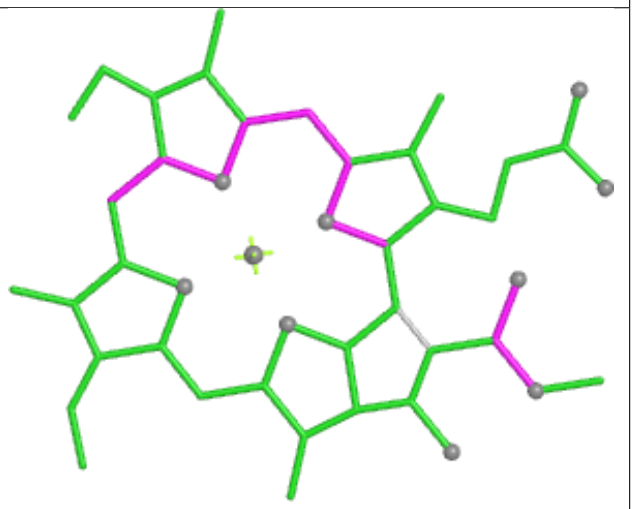


Rings

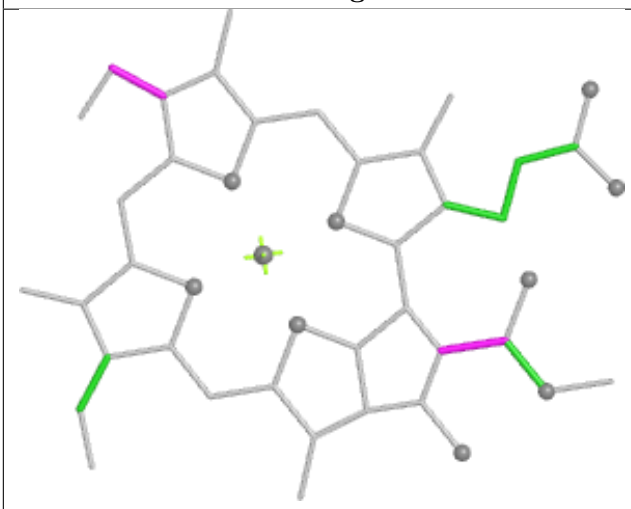
Ligand CLA X 611



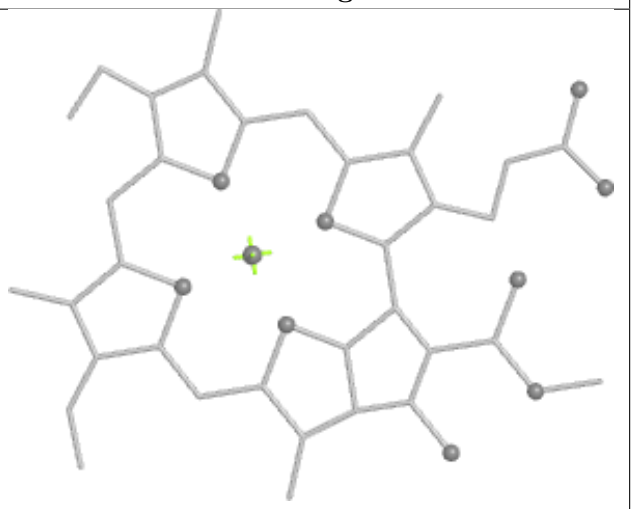
Bond lengths



Bond angles

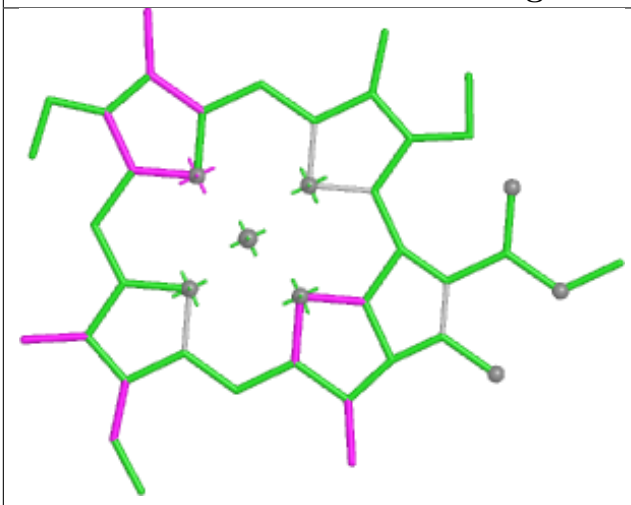


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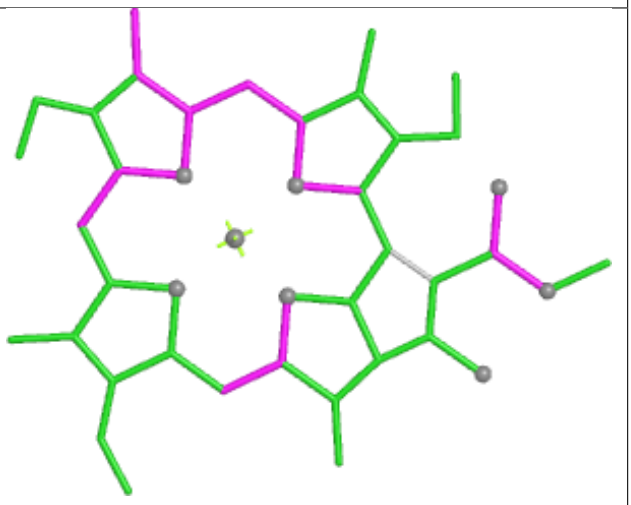


Rings

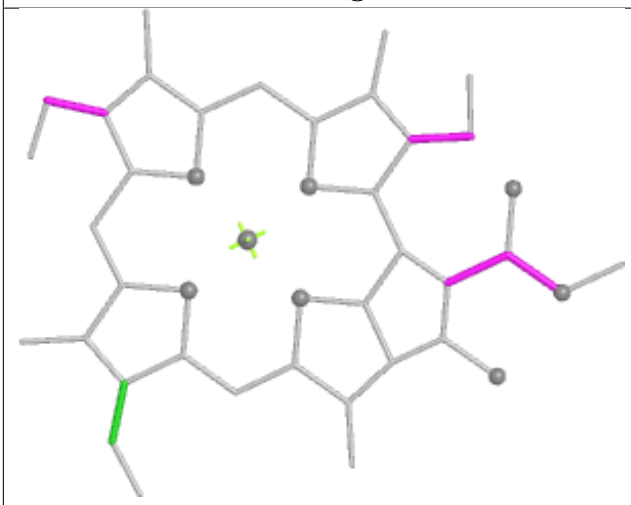
Ligand CLA F 303



Bond lengths



Bond angles

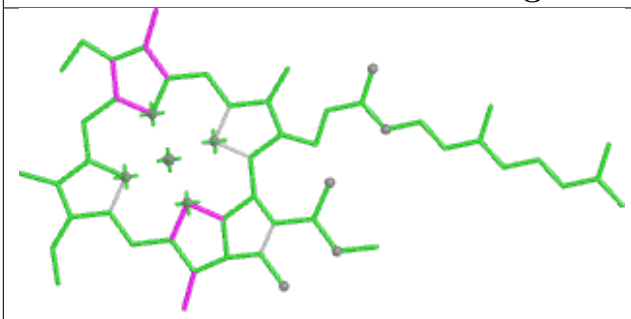


Torsions

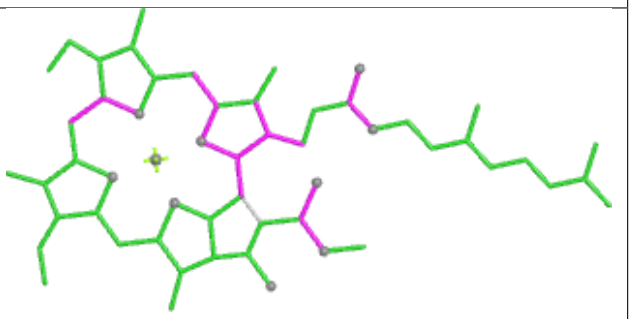


Rings

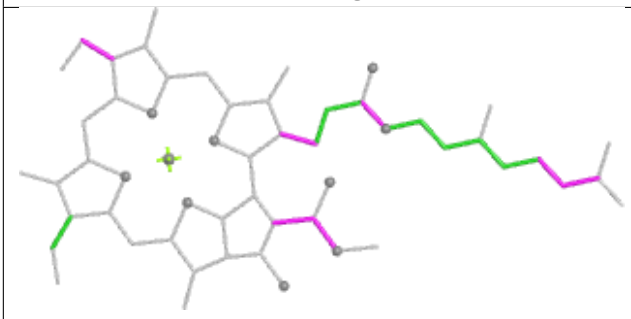
Ligand CLA Y 603



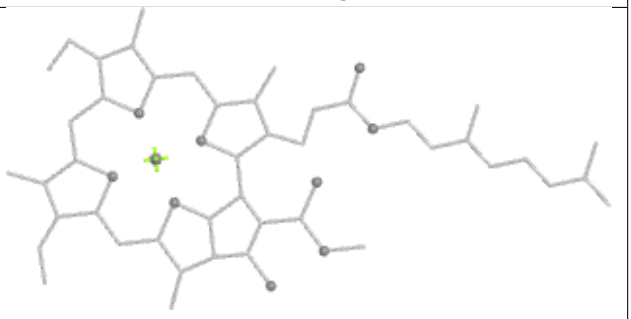
Bond lengths



Bond angles

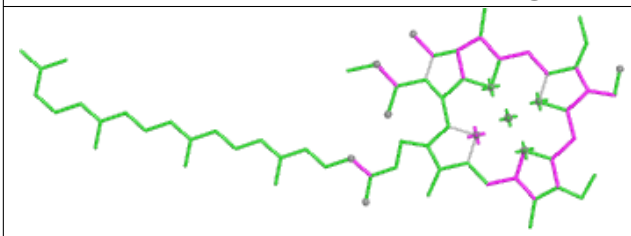


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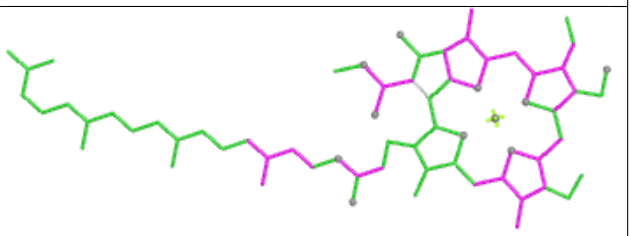


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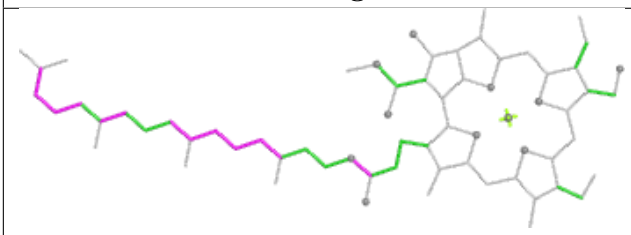
Ligand CHL Z 601



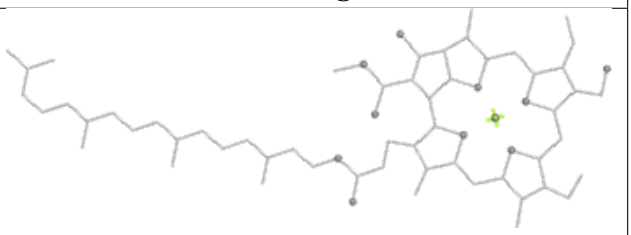
Bond lengths



Bond angles

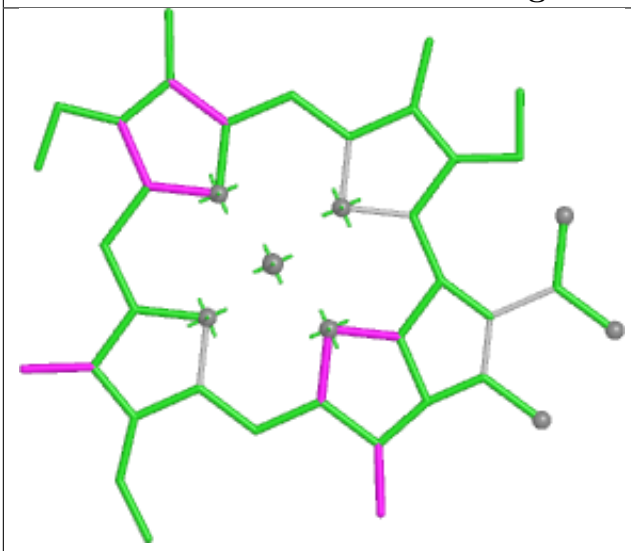


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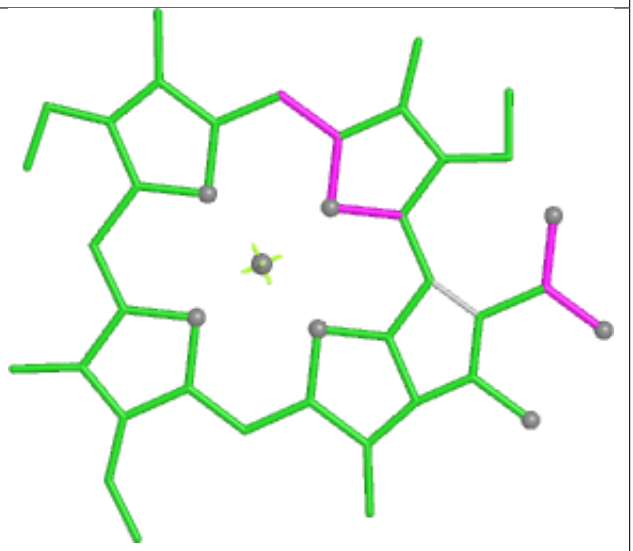


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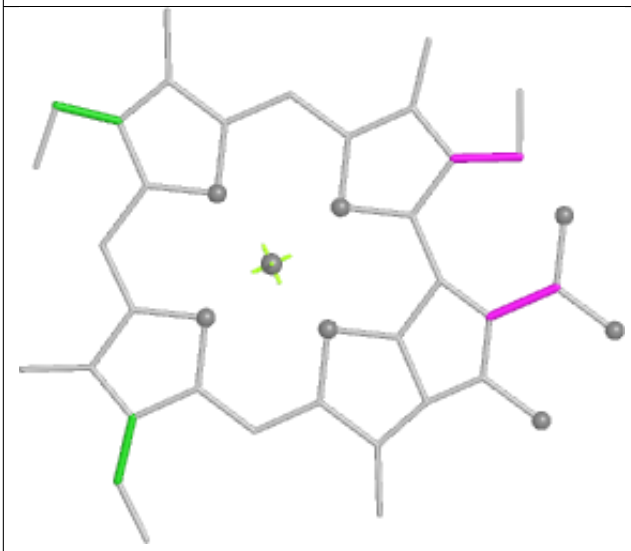
Ligand CLA 4 612



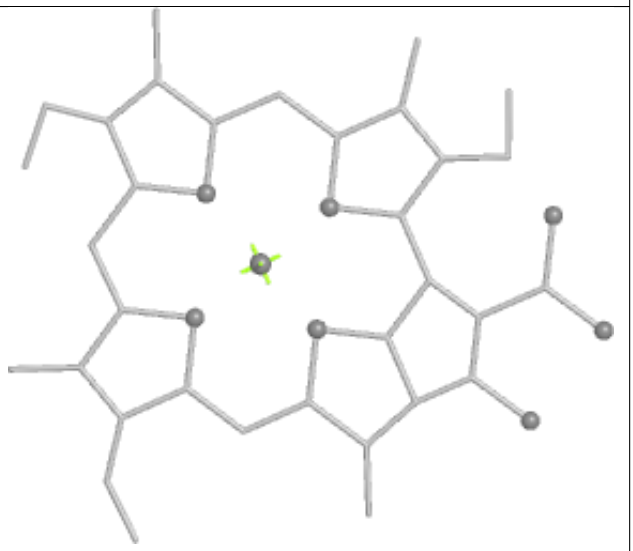
Bond lengths



Bond angles

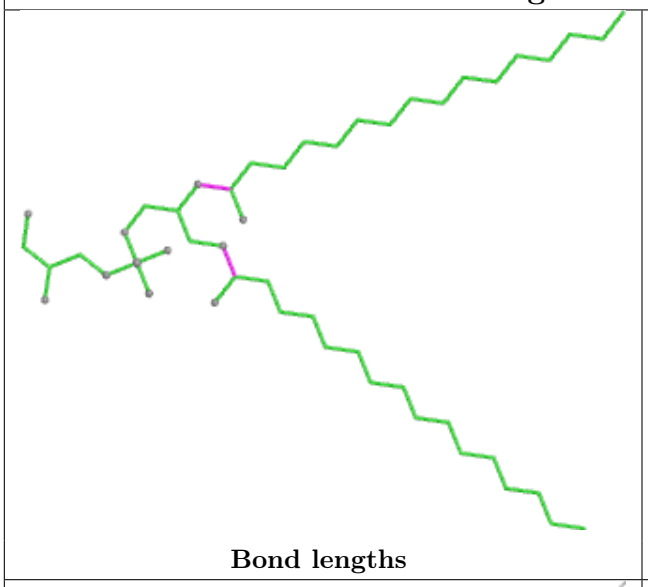


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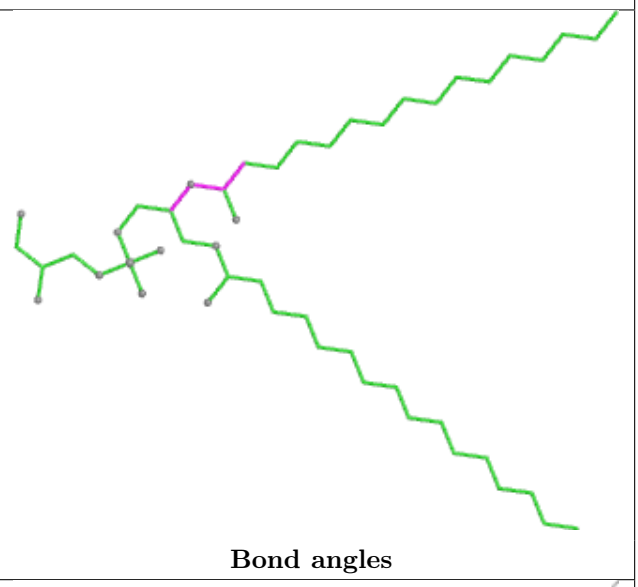


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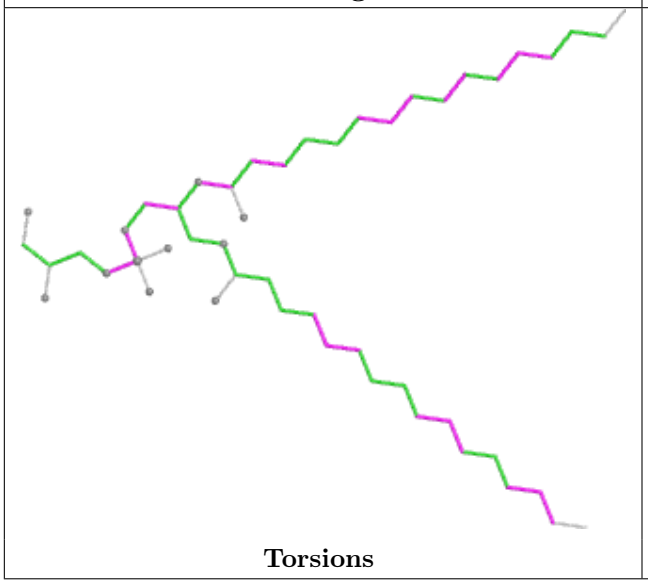
Ligand LHG 9 623



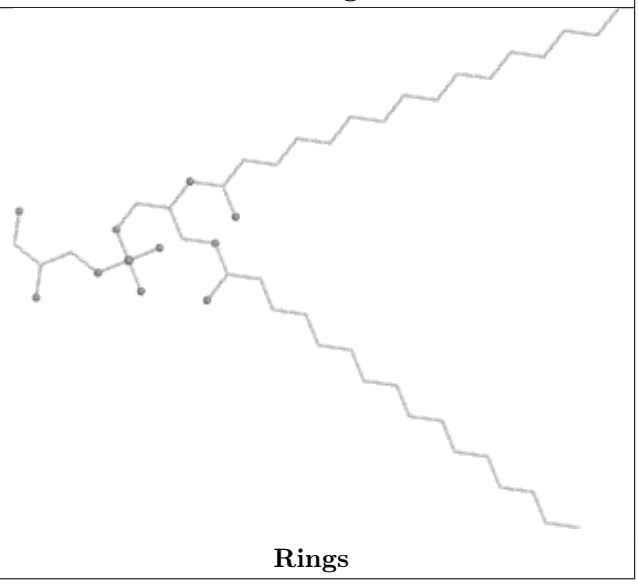
Bond lengths



Bond angles

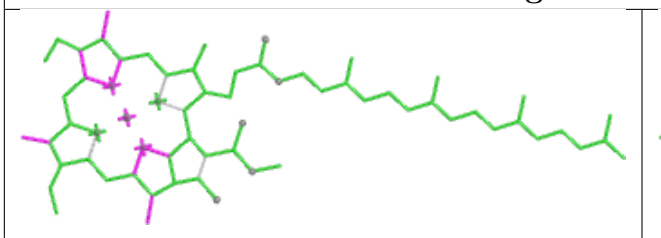


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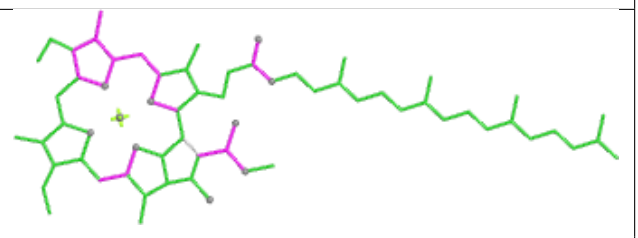


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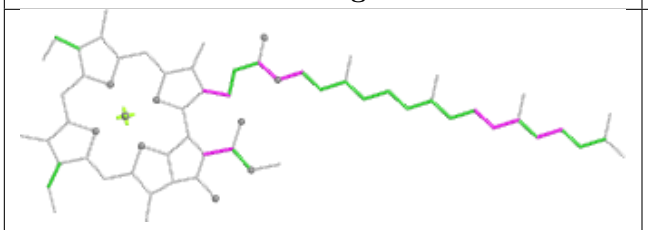
Ligand CLA B 805



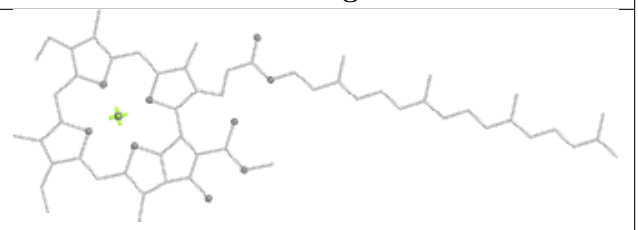
Bond lengths



Bond angles

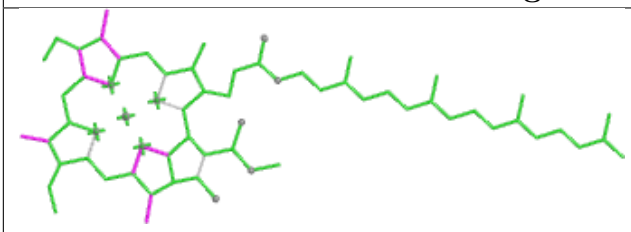


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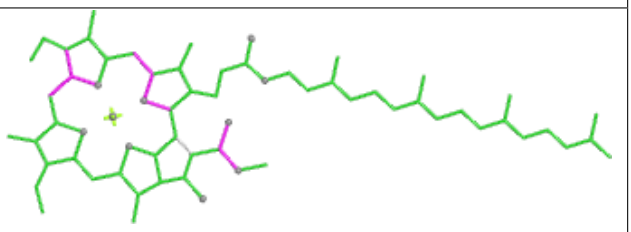


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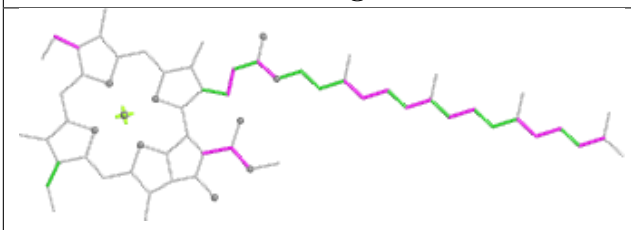
Ligand CLA V 613



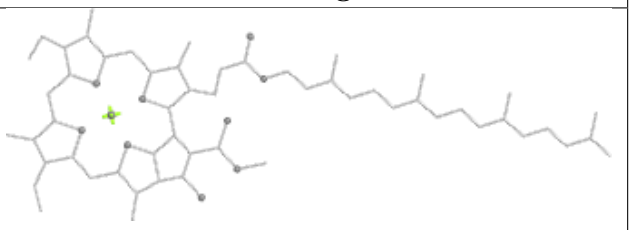
Bond lengths



Bond angles

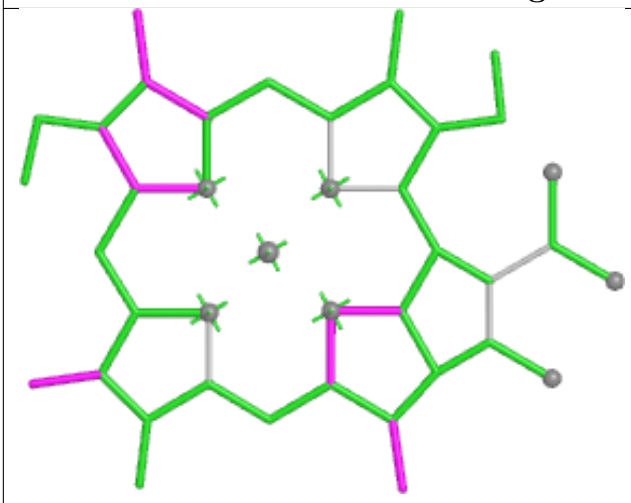


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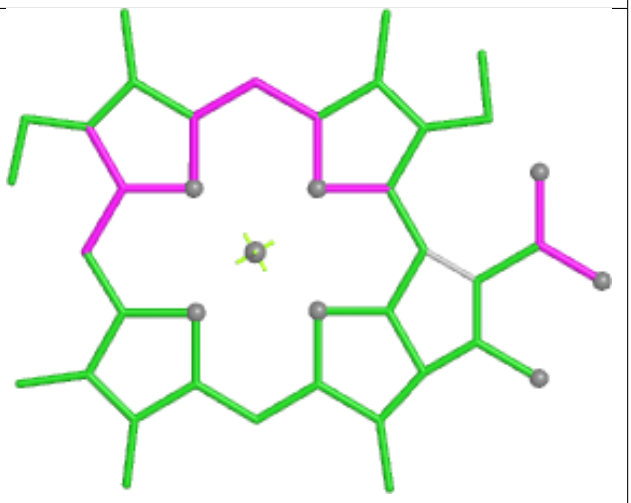


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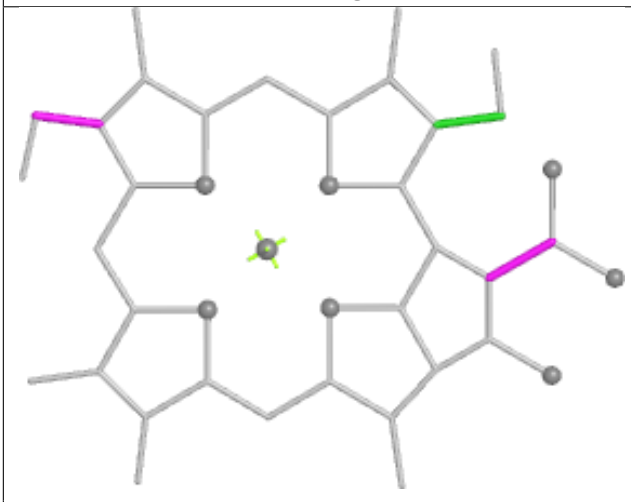
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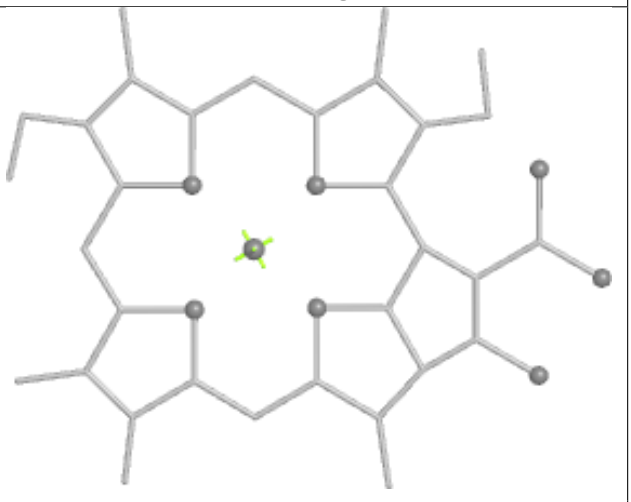
Bond lengths



Bond angles

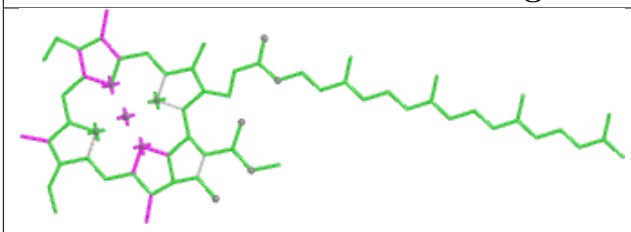


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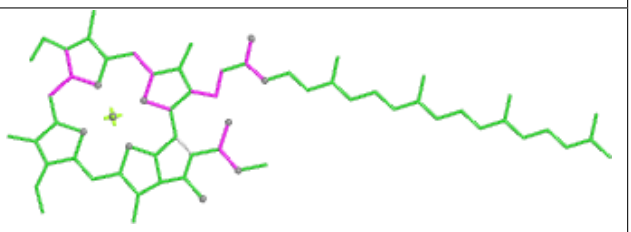


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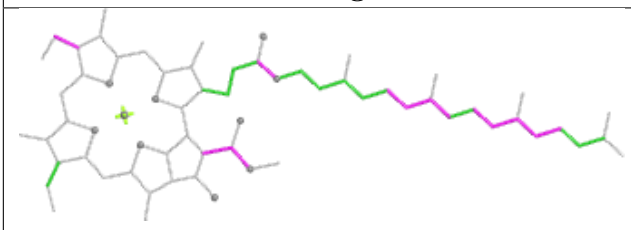
Ligand CLA B 802



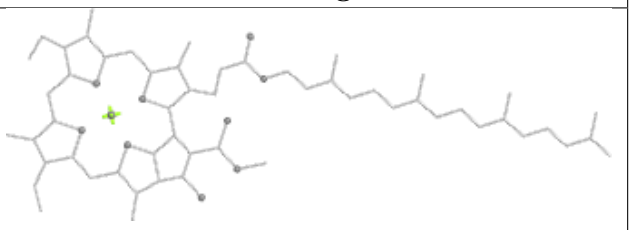
Bond lengths



Bond angles

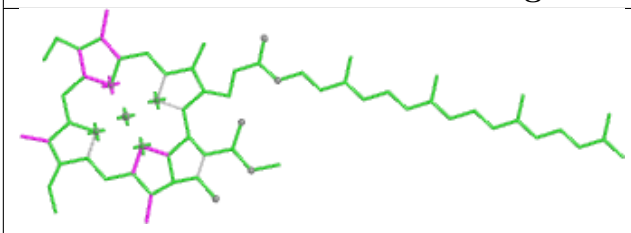


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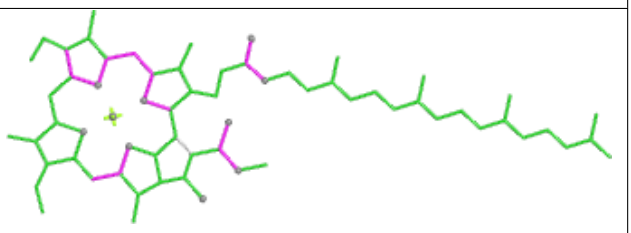


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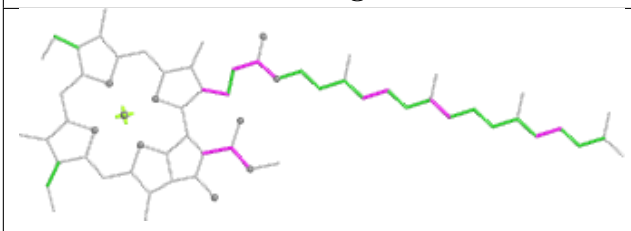
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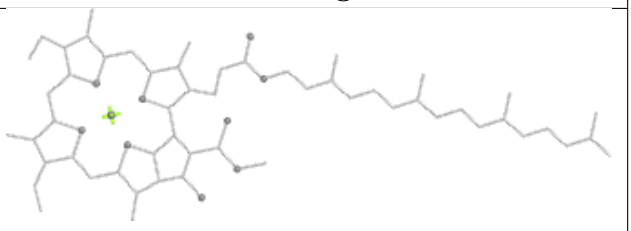
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Bond angles

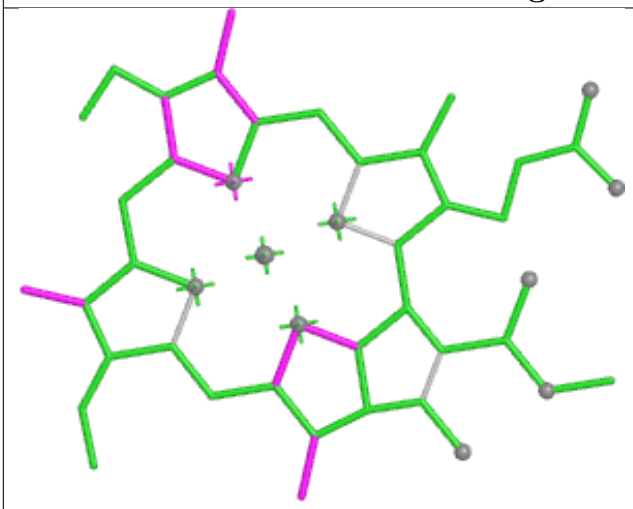


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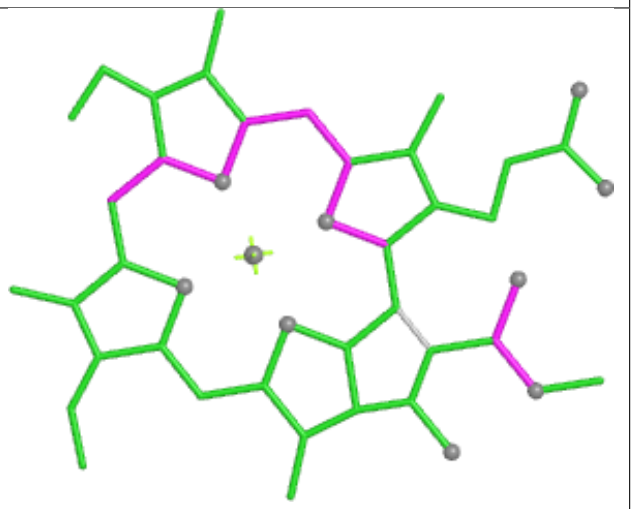


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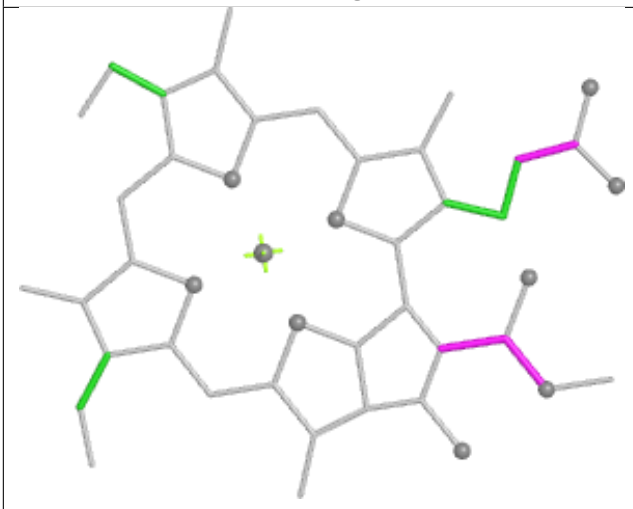
Ligand CLA 1 612



Bond lengths



Bond angles

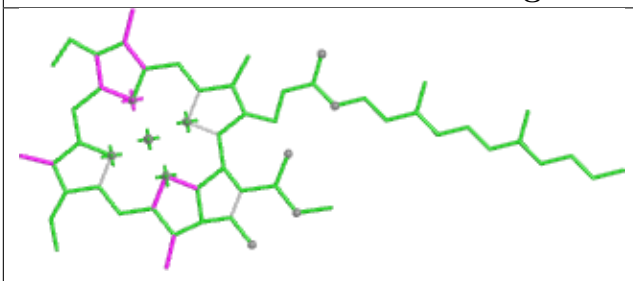


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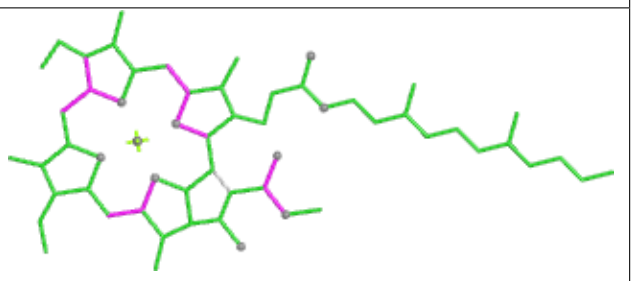


Rings

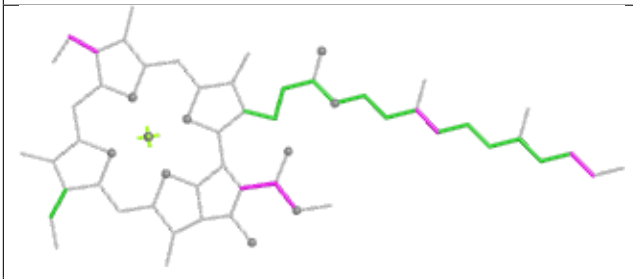
Ligand CLA A 827



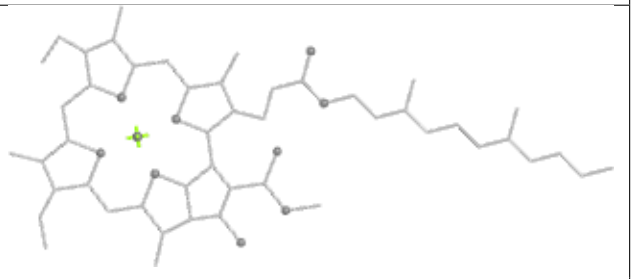
Bond lengths



Bond angles

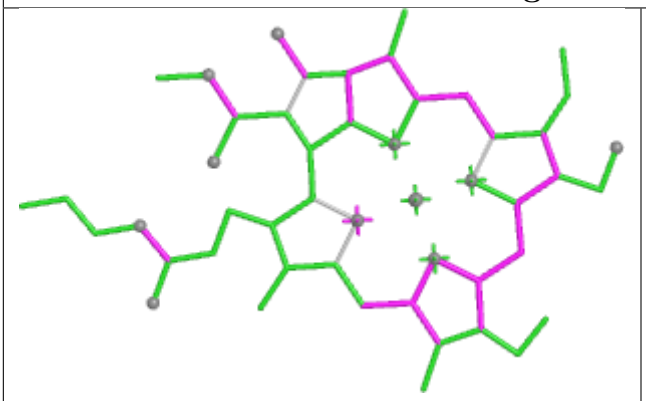


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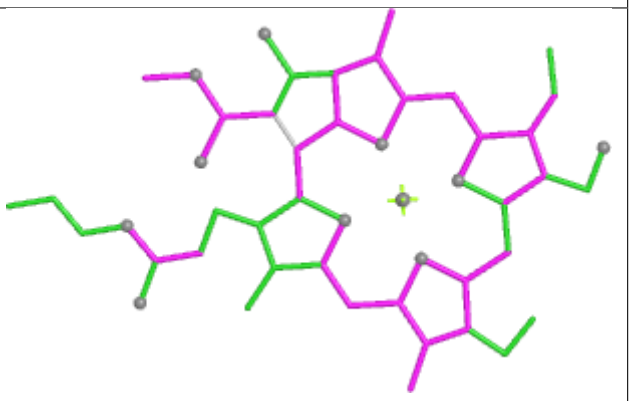


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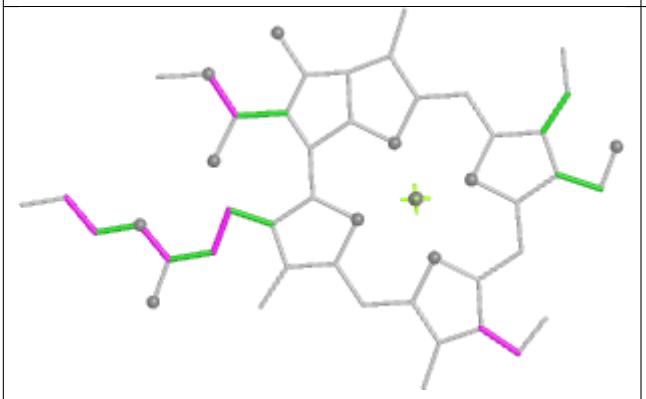
Ligand CHL Y 608



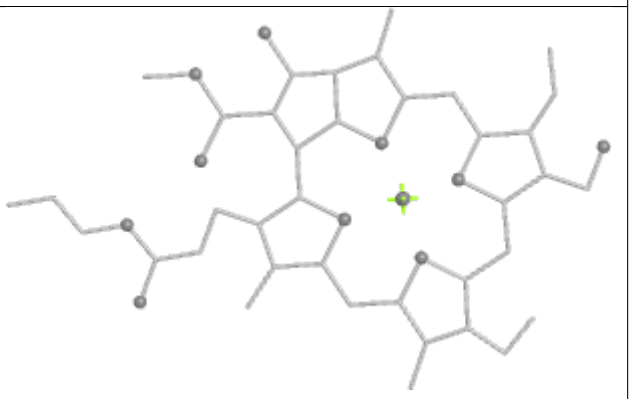
Bond lengths



Bond angles

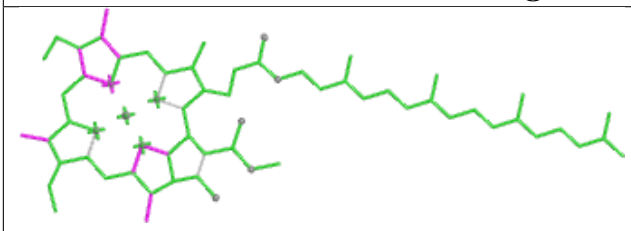


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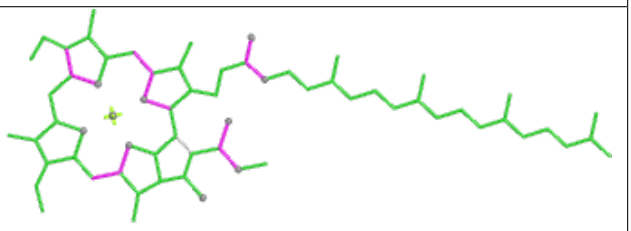


Rings

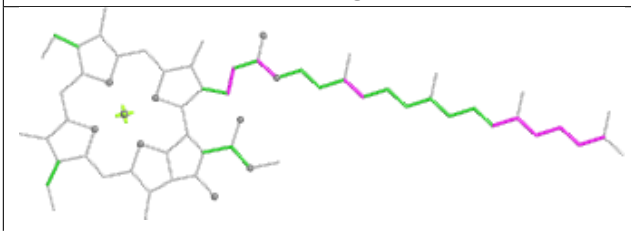
Ligand CLA B 831



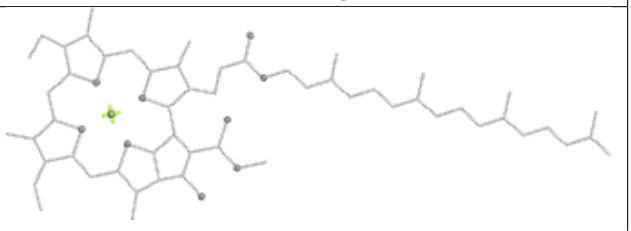
Bond lengths



Bond angles

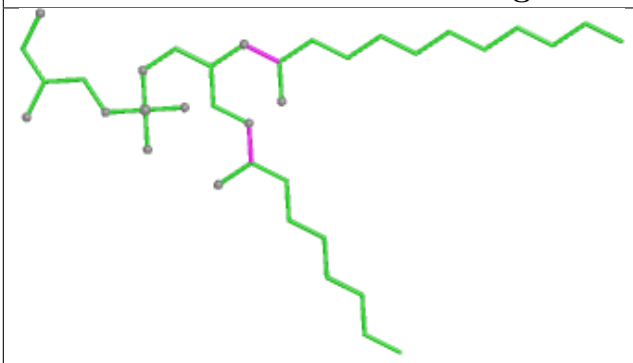


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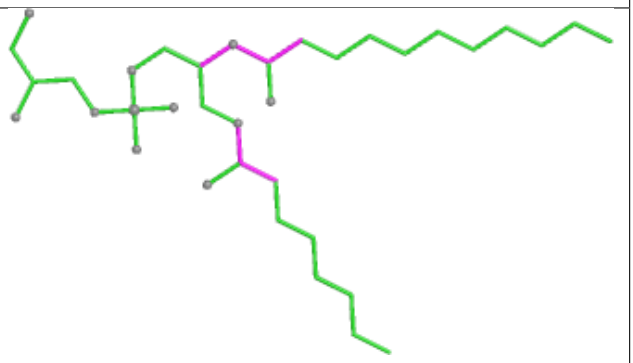


Rings

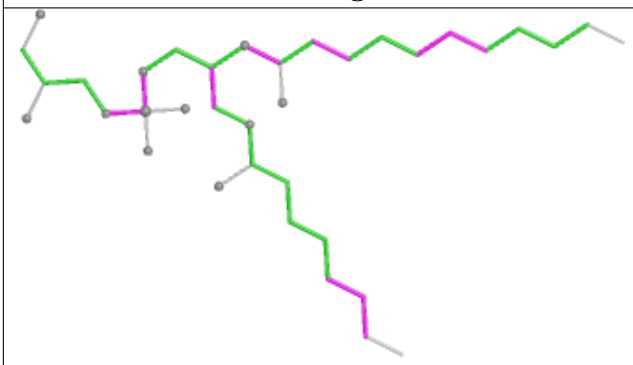
Ligand LHG O 2631



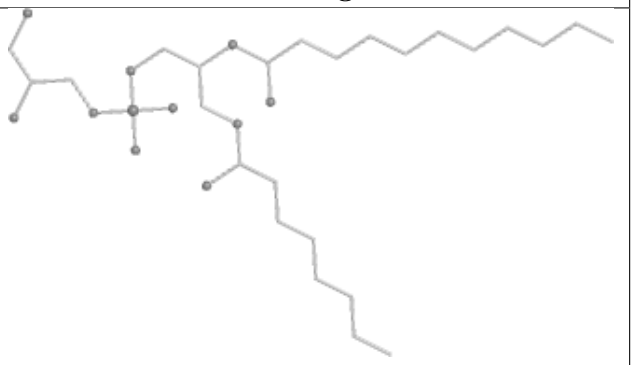
Bond lengths



Bond angles

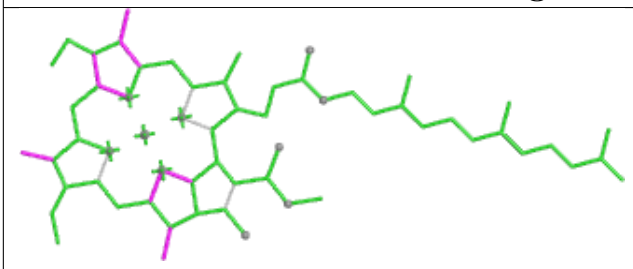


Torsions

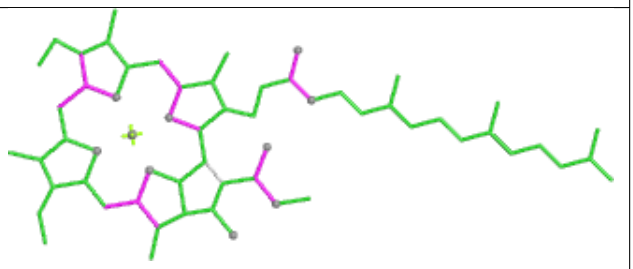


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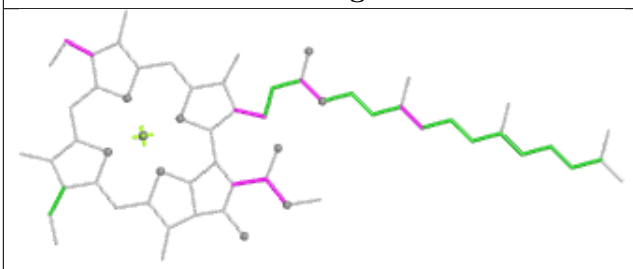
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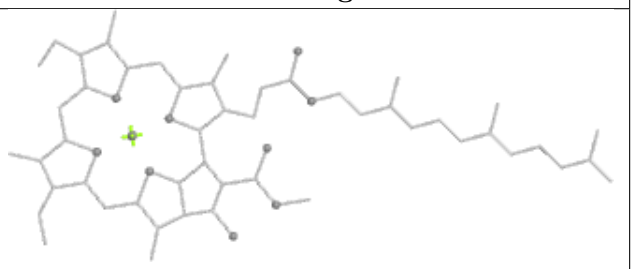
Bond lengths



Bond angles

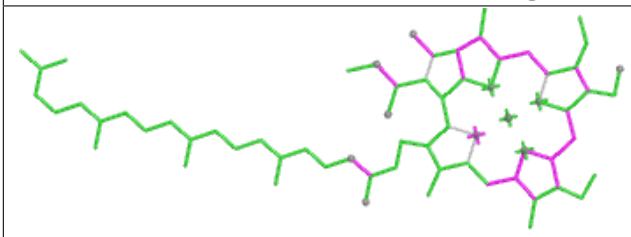


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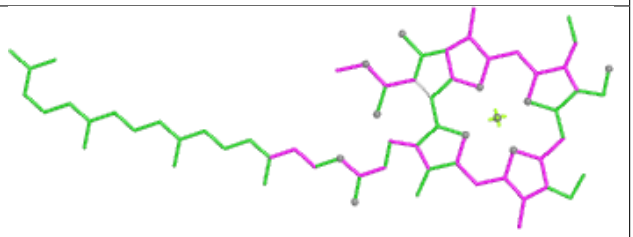


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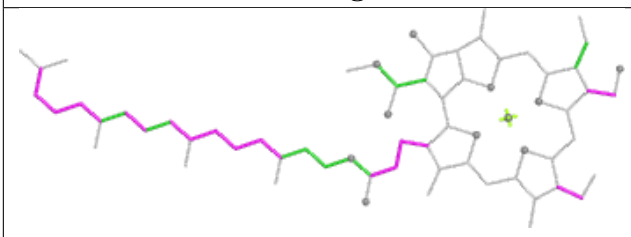
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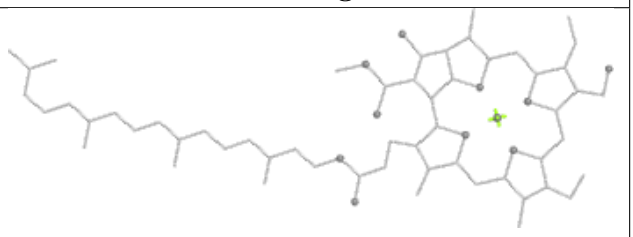
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Bond angles

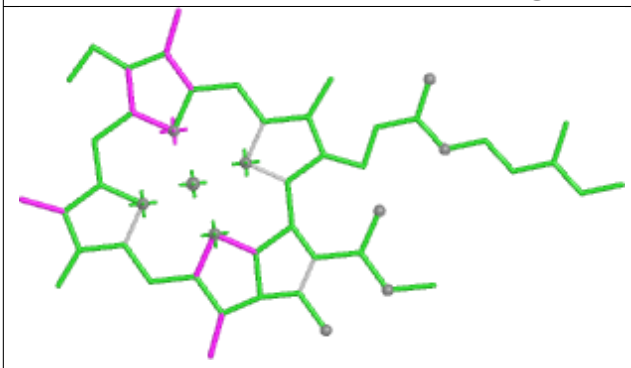


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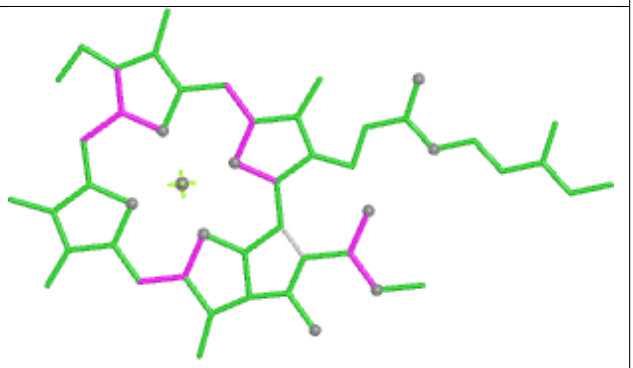


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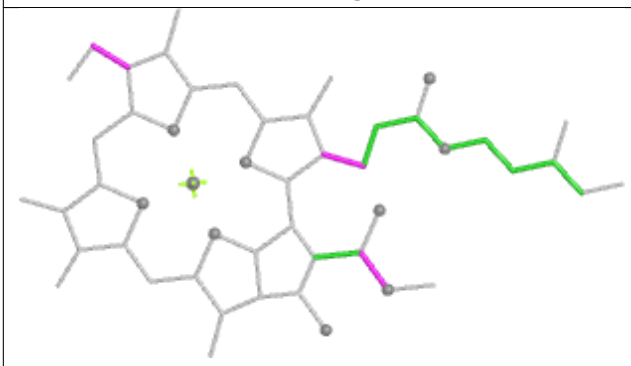
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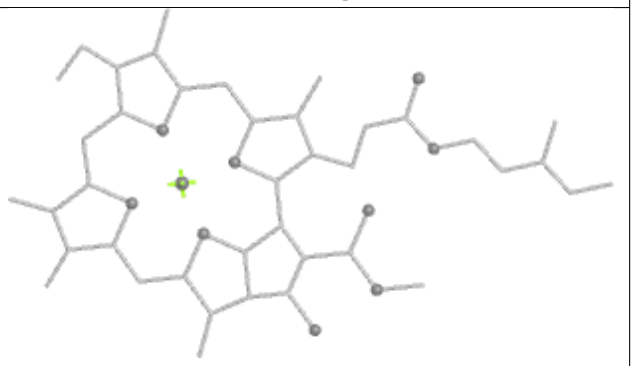
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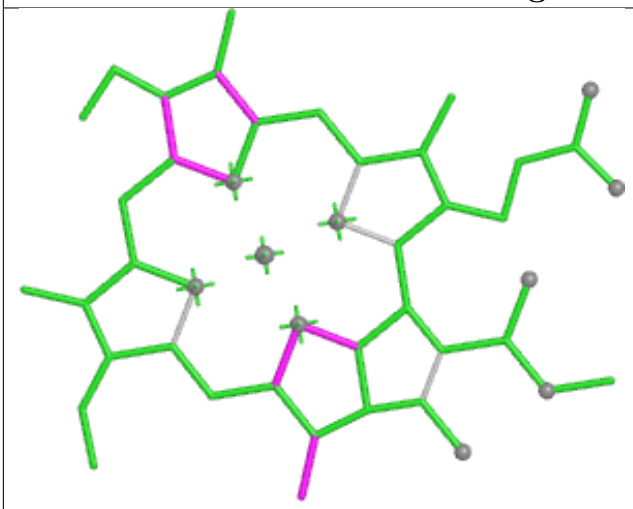


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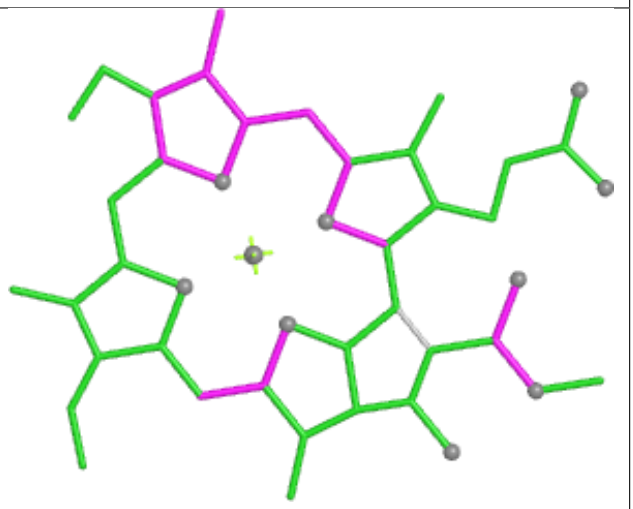


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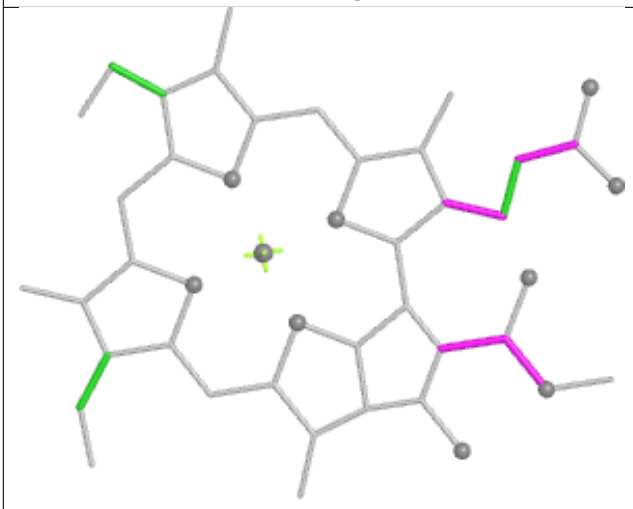
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Bond lengths



Bond angles

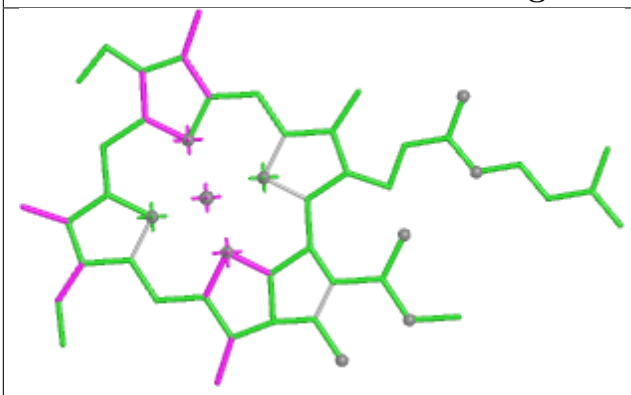


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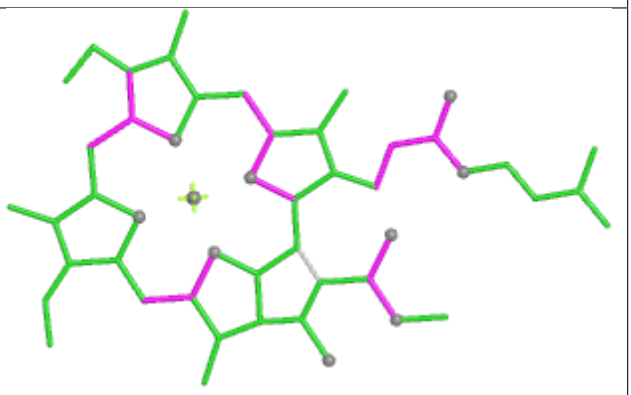


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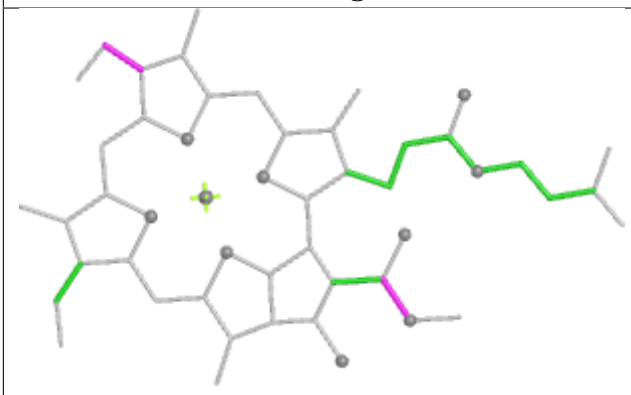
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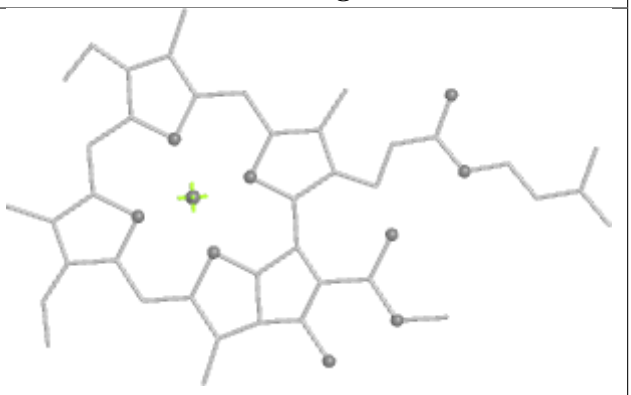
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Bond angles

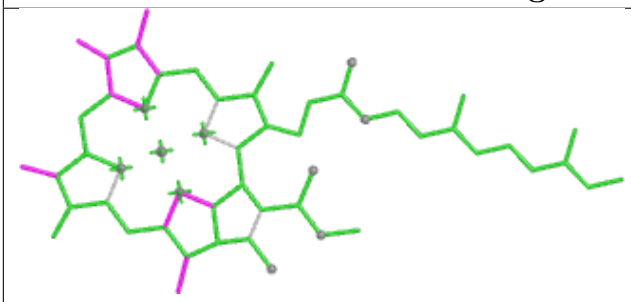


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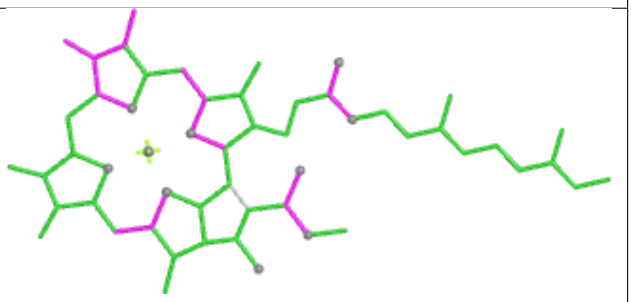


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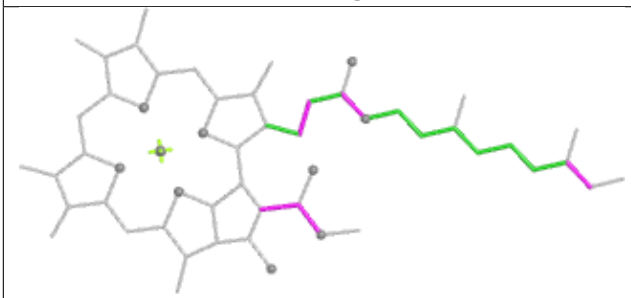
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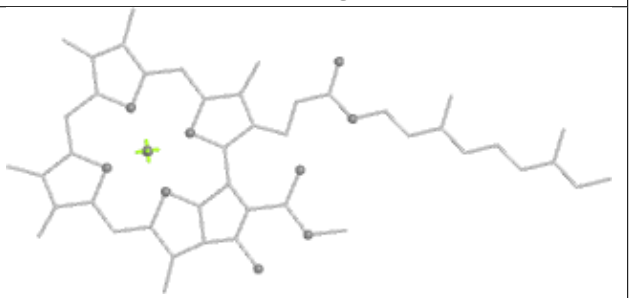
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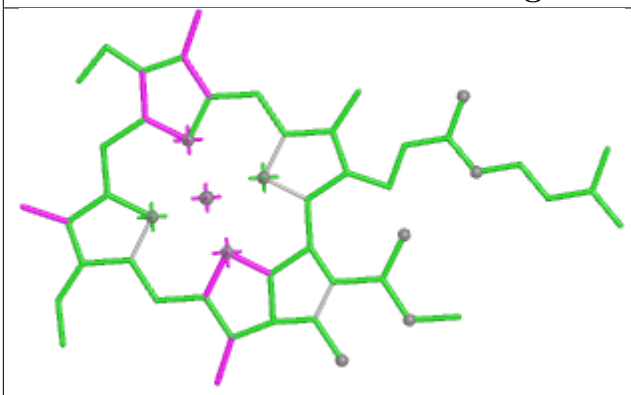


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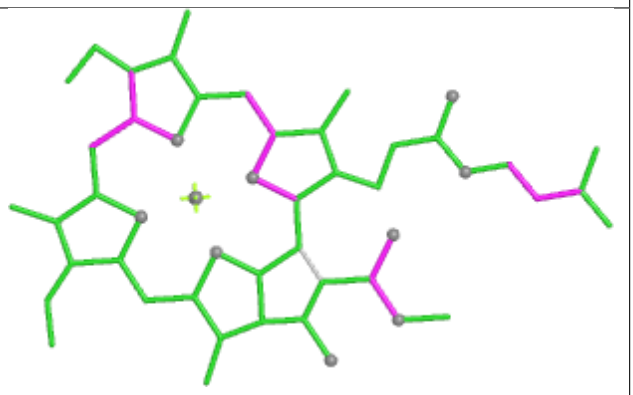


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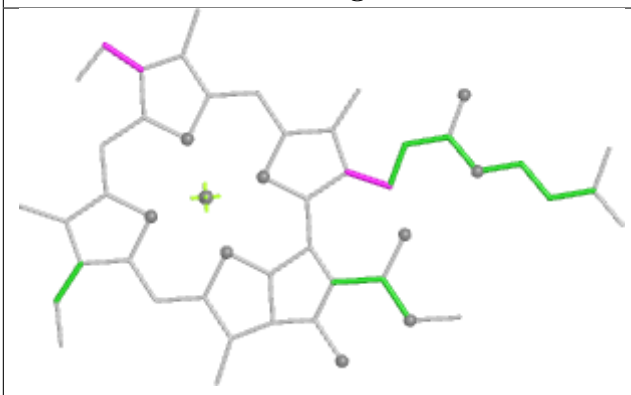
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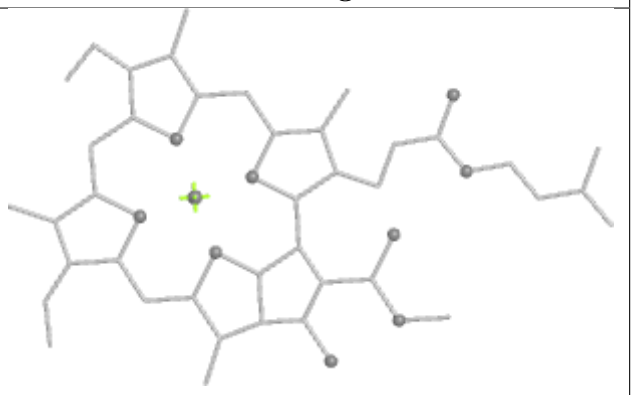
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Bond angles

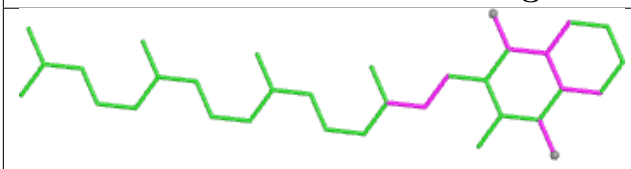


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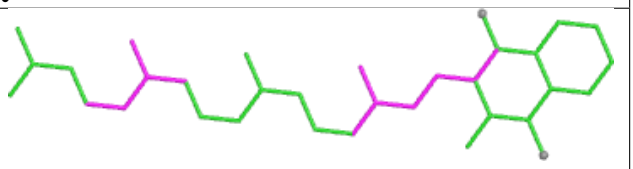


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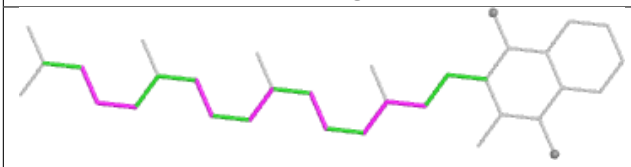
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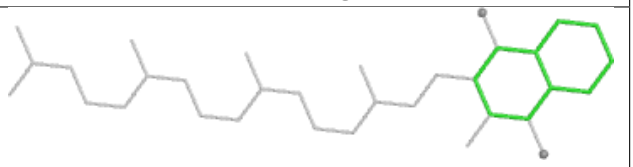
Bond lengths



Bond angles

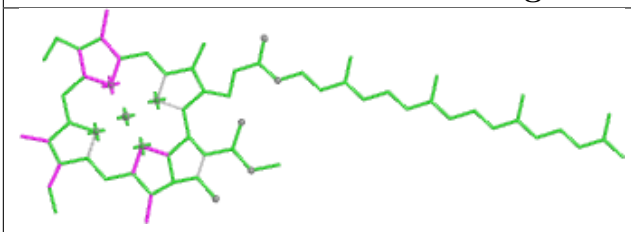


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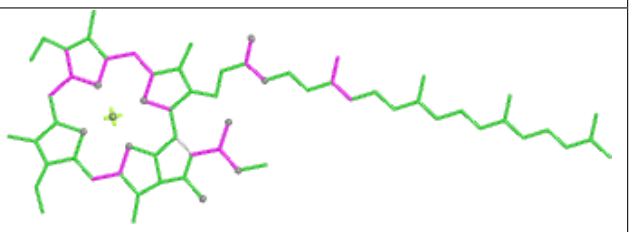


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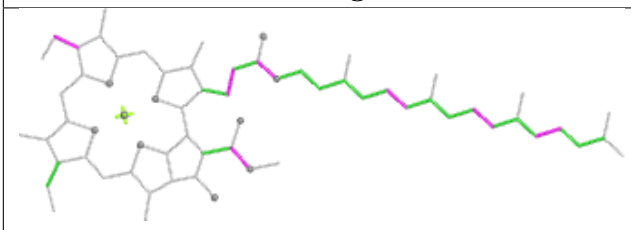
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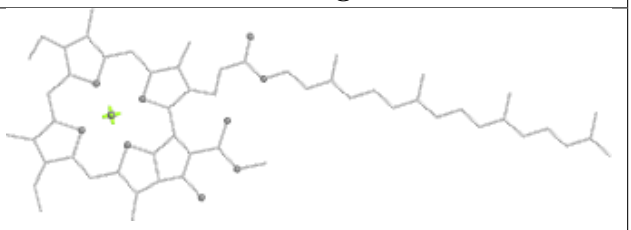
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Bond angles

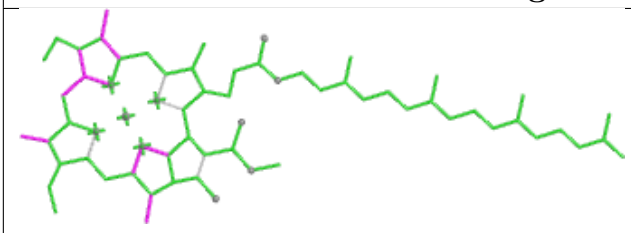


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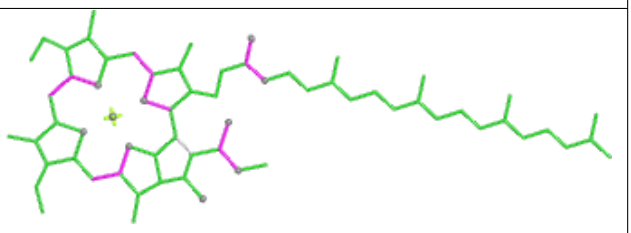


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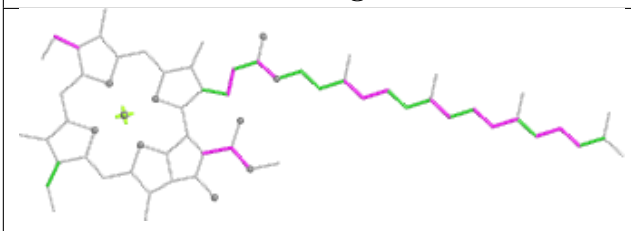
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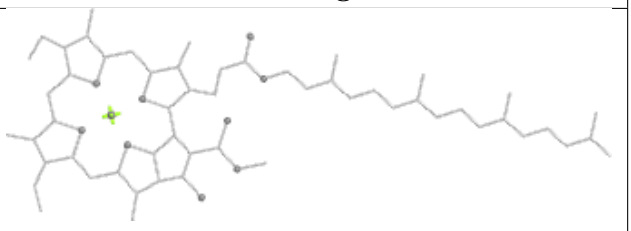
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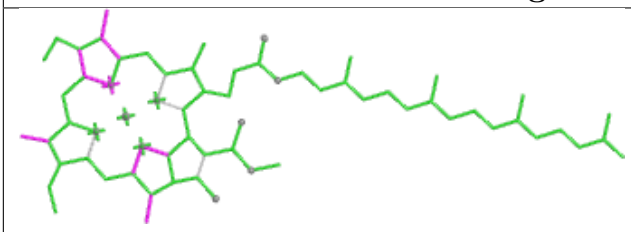


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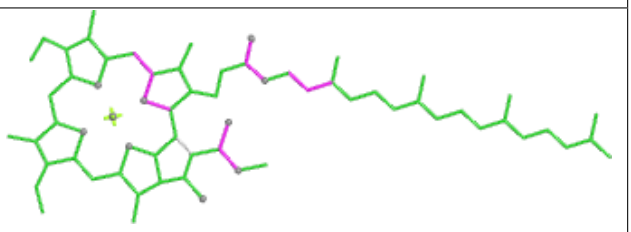


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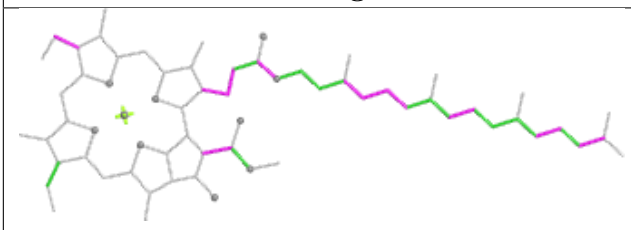
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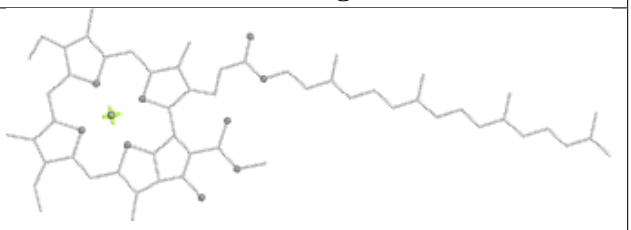
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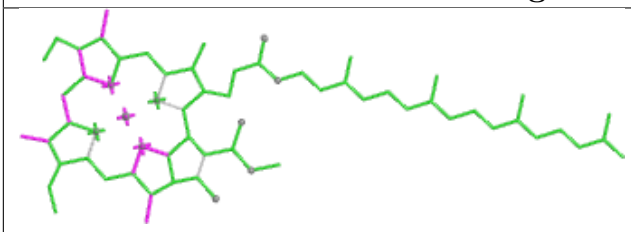


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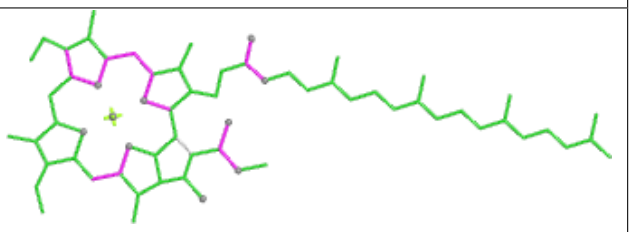


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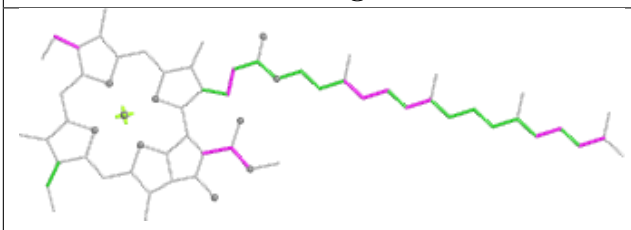
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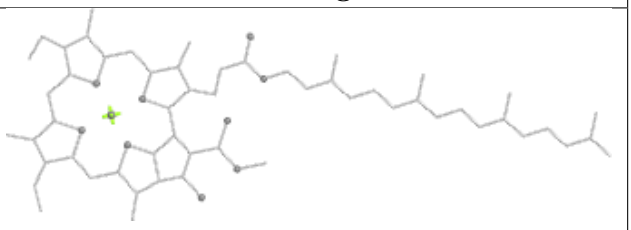
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Bond angles

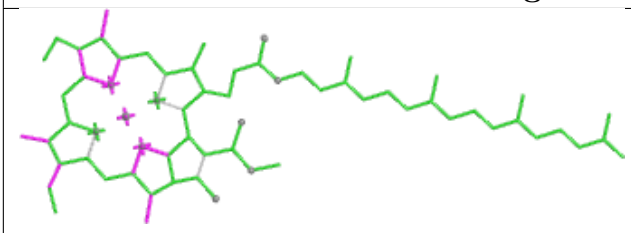


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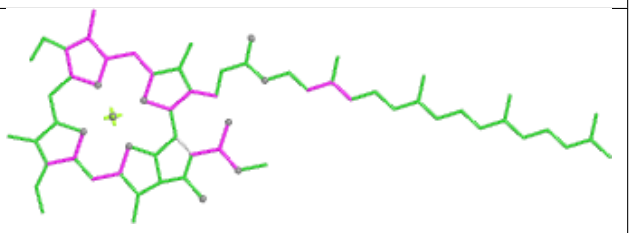


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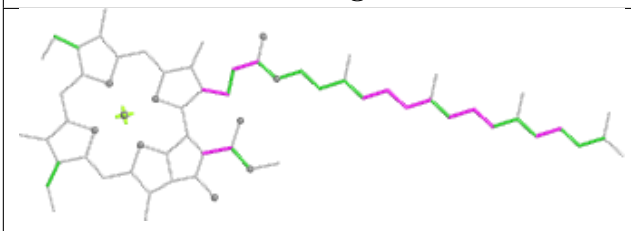
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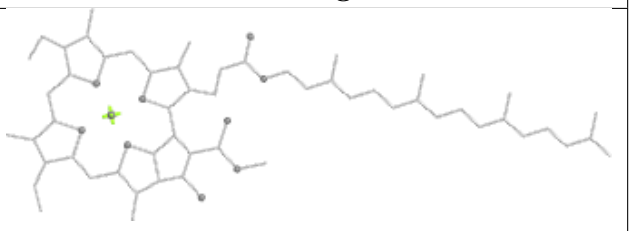
Bond lengths



Bond angles

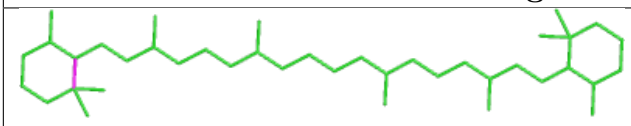


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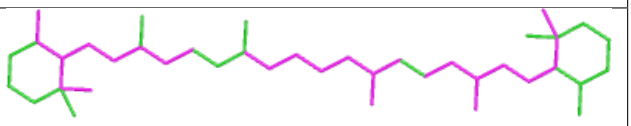


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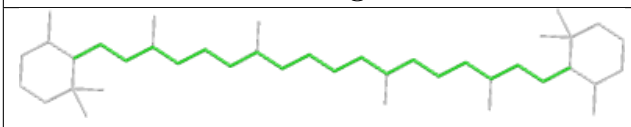
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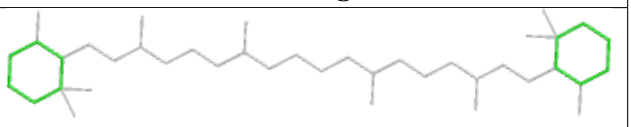
Bond lengths



Bond angles

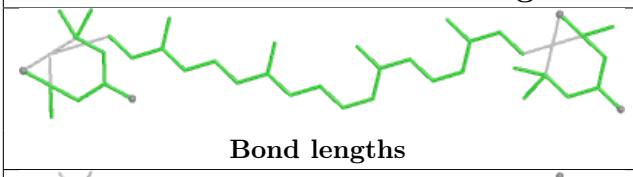


Torsions

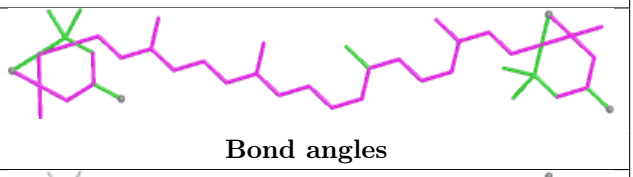


Rings

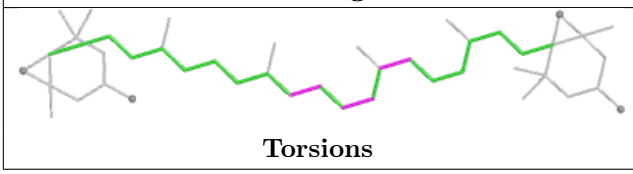
Ligand XAT Z 1622



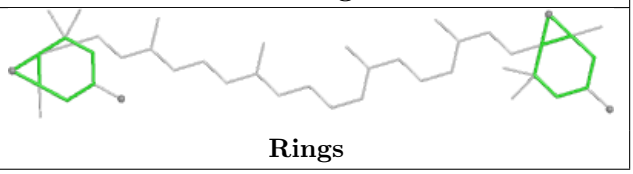
Bond lengths



Bond angles

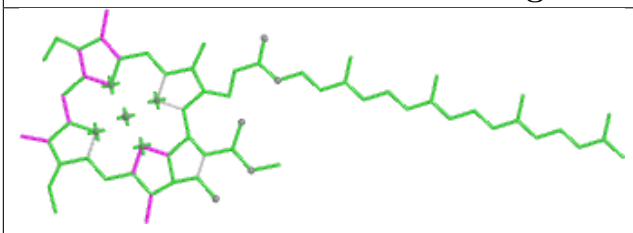


Torsions

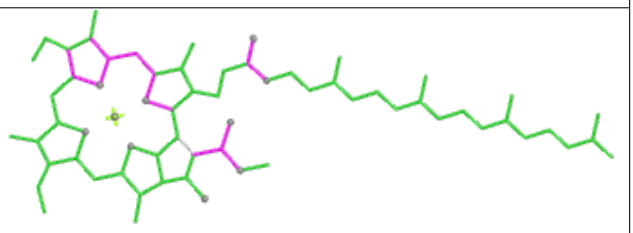


Rings

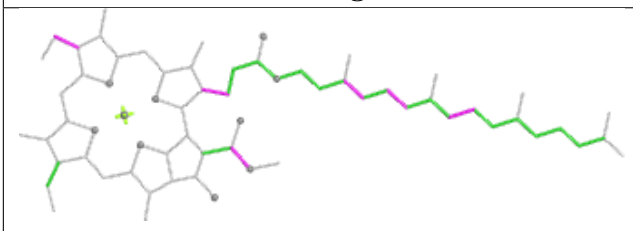
Ligand CLA Z 610



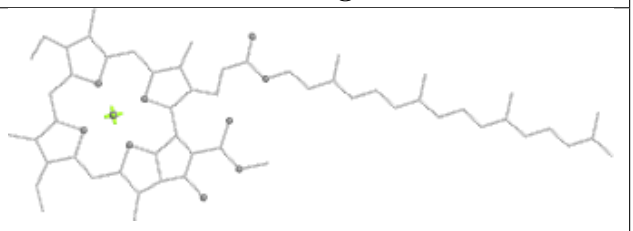
Bond lengths



Bond angles

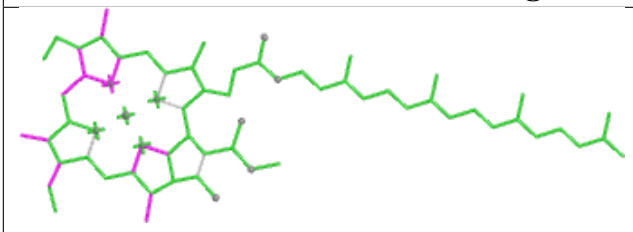


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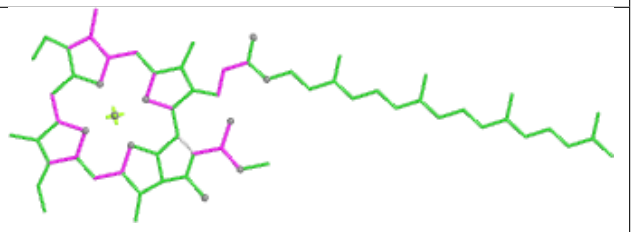


Rings

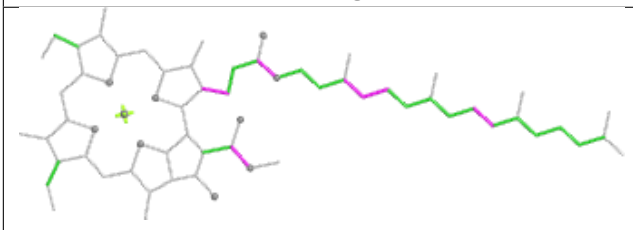
Ligand CLA B 829



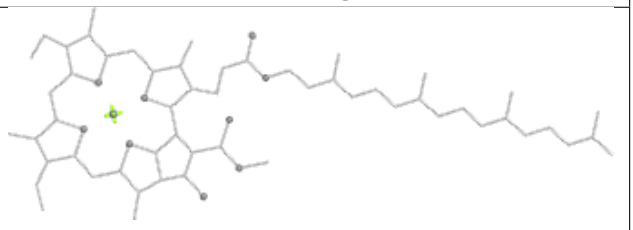
Bond lengths



Bond angles

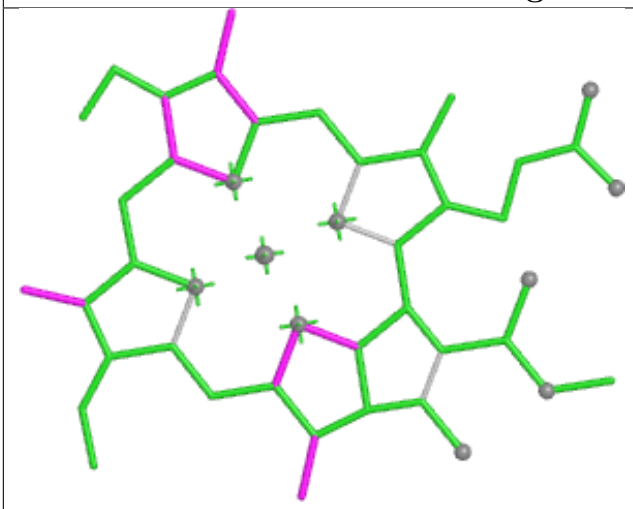


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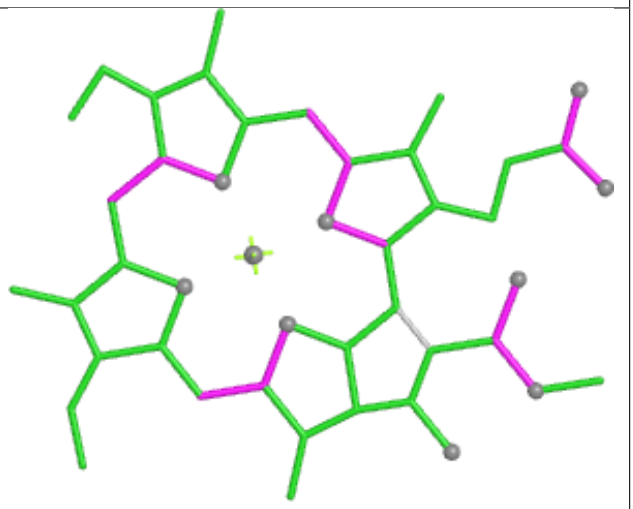


Rings

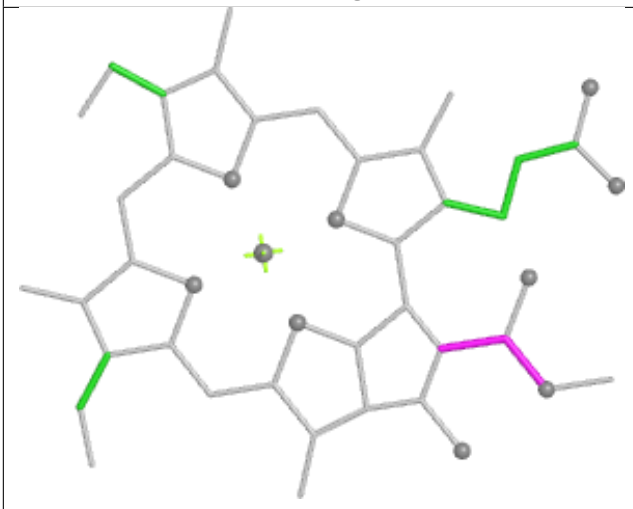
Ligand CLA L 304



Bond lengths



Bond angles

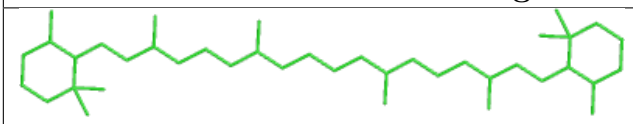


Torsions

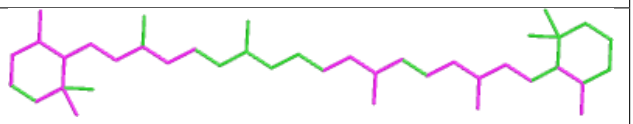


Rings

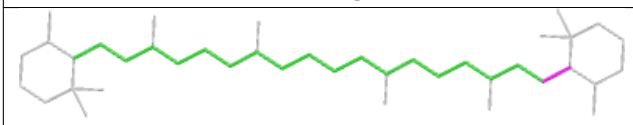
Ligand BCR O 2004



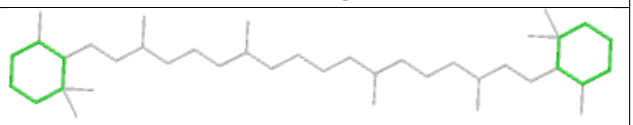
Bond lengths



Bond angles

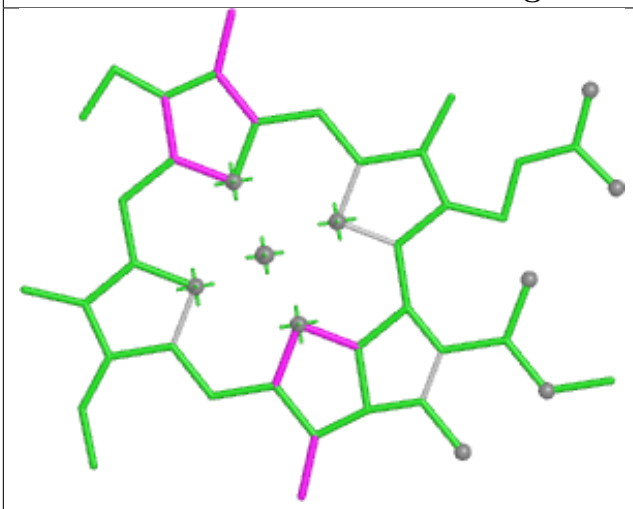


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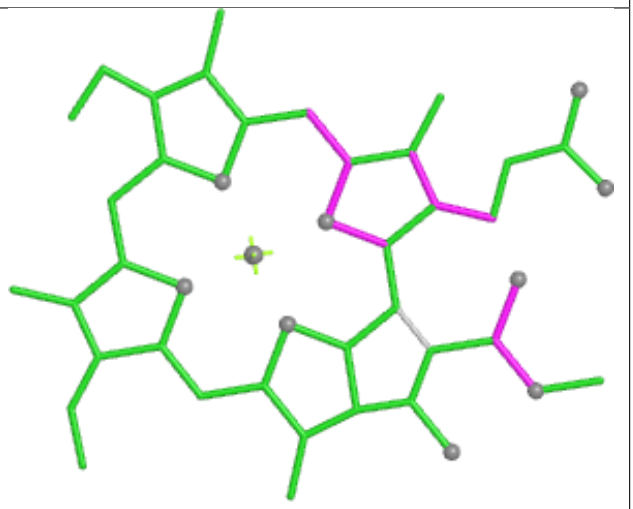


Rings

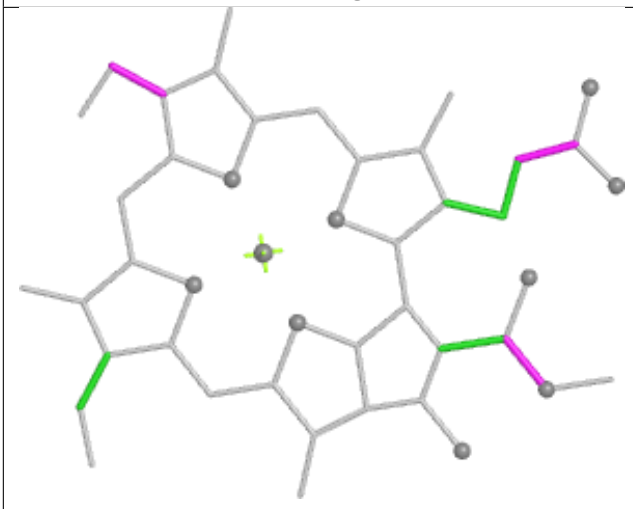
Ligand CLA V 603



Bond lengths



Bond angles

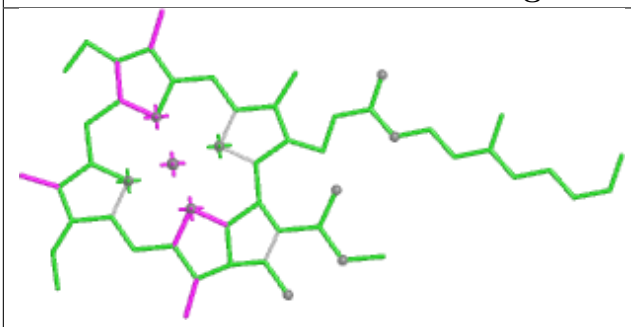


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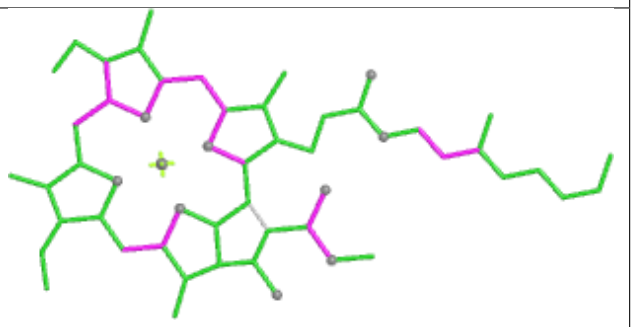


Rings

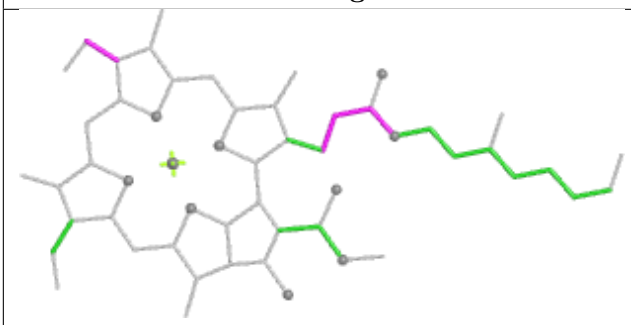
Ligand CLA A 813



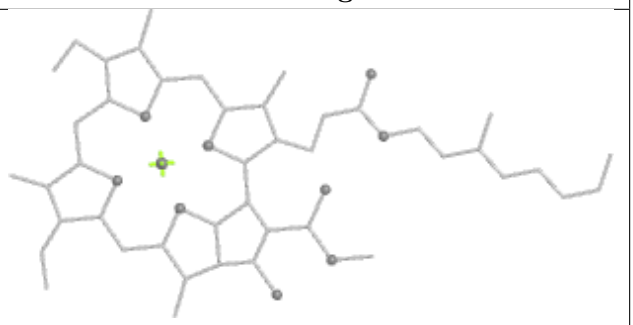
Bond lengths



Bond angles

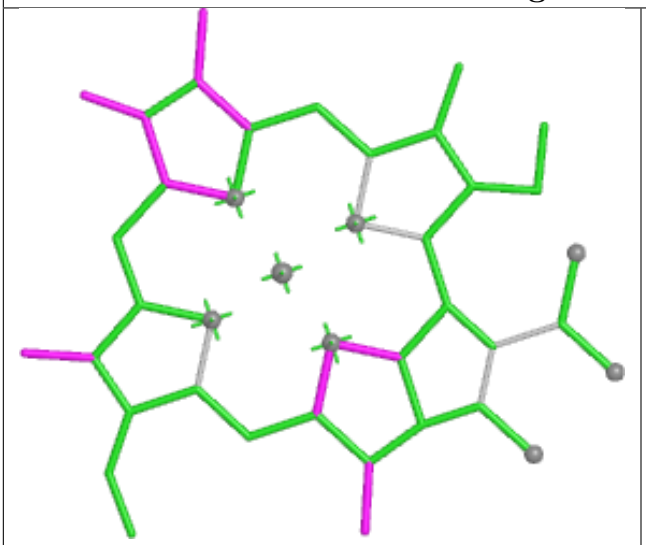


Torsions



Rings

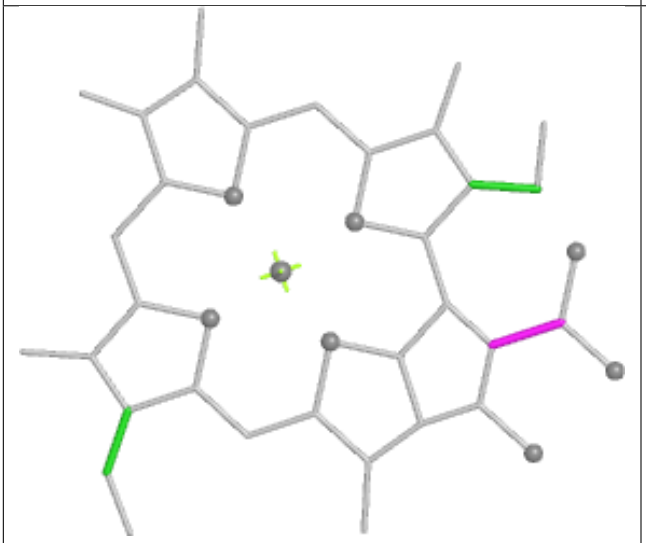
Ligand CLA 6 618



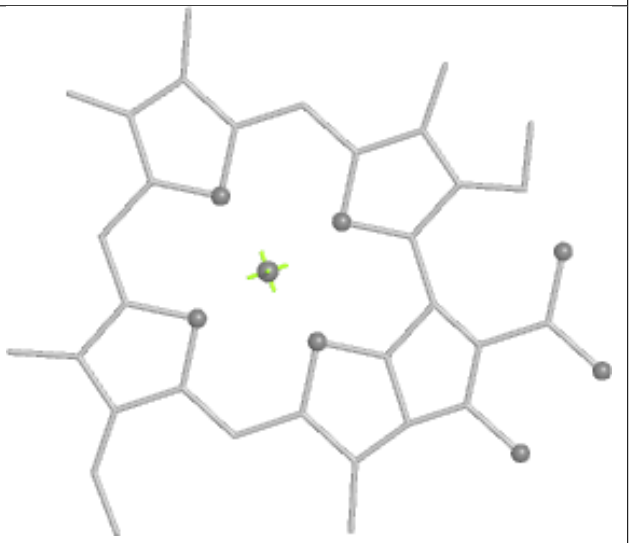
Bond lengths



Bond angles

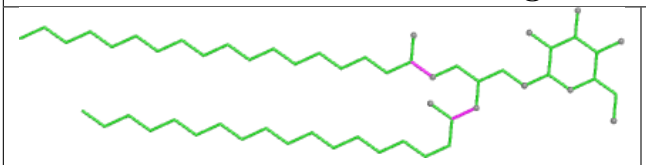


Torsions

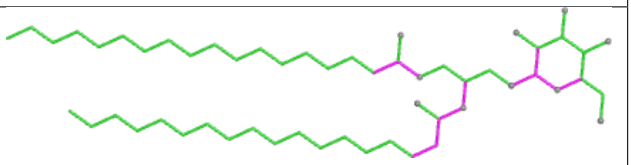


Rings

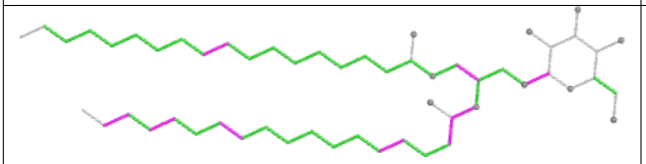
Ligand LMG 9 625



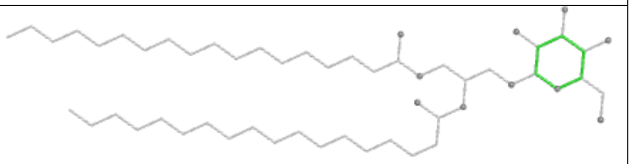
Bond lengths



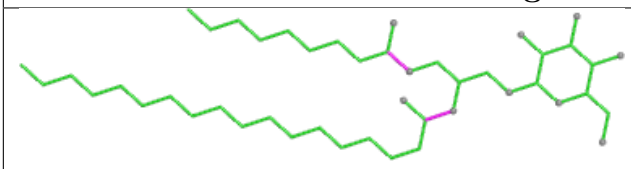
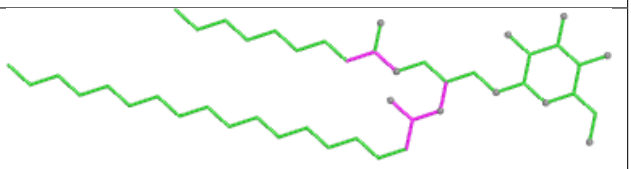
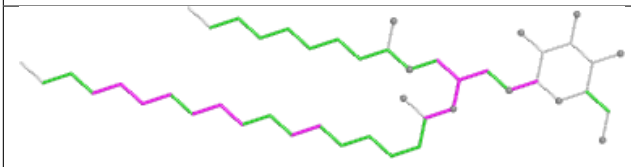
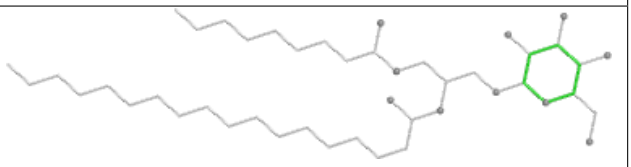
Bond angles

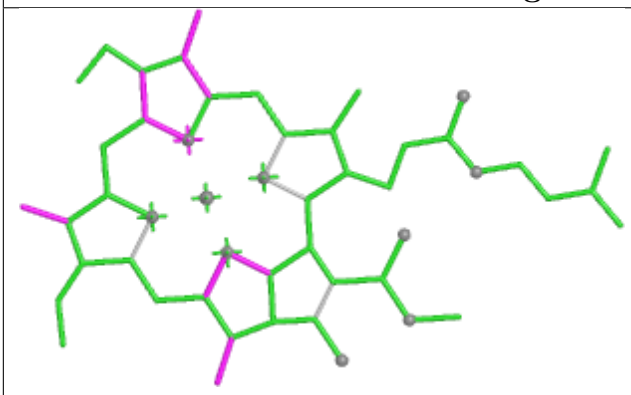
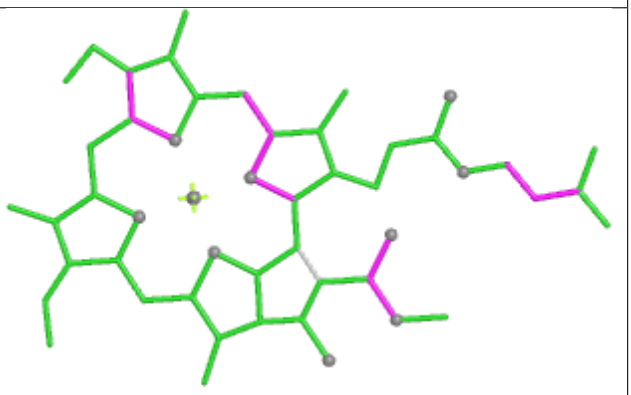
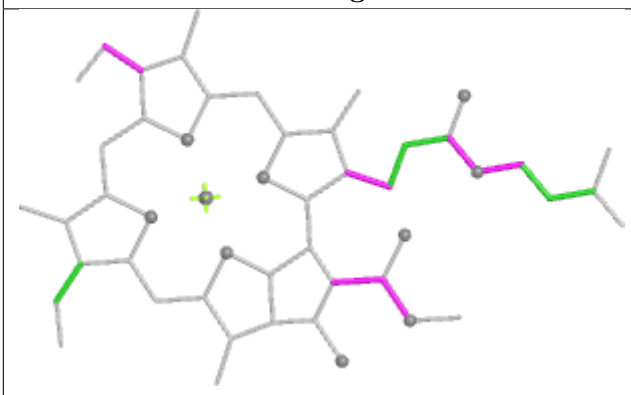
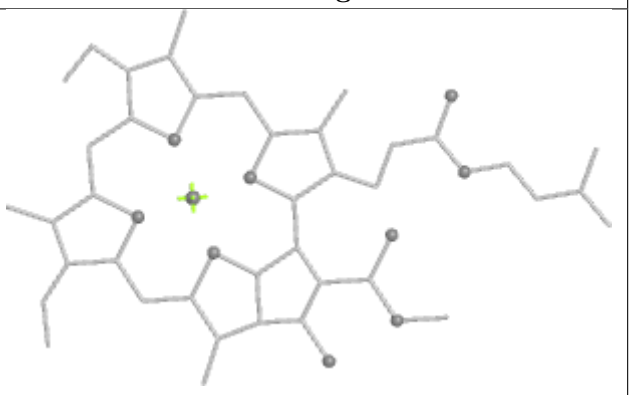


Torsions

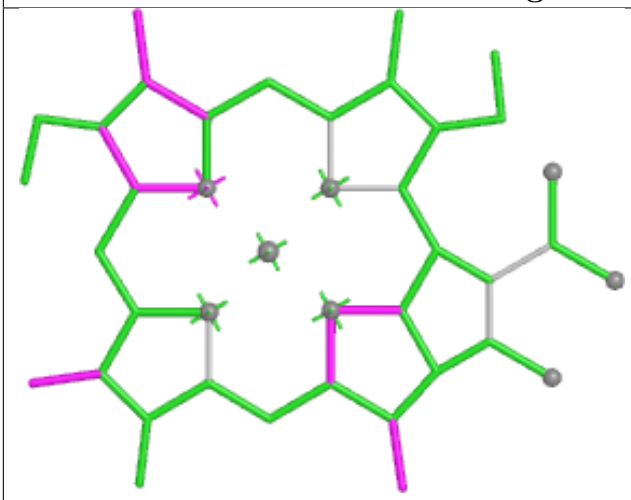


Rings

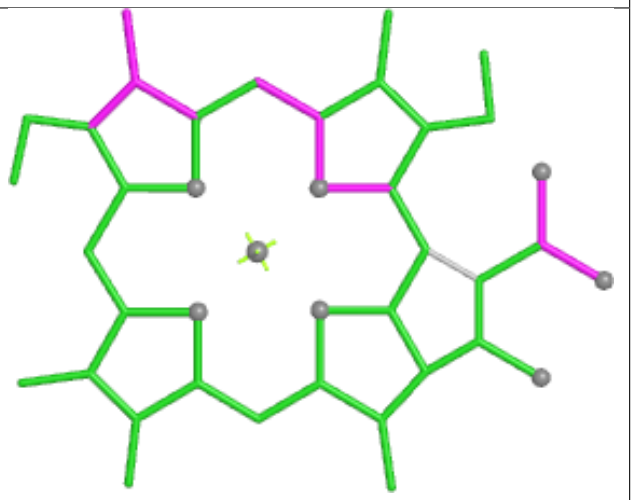
Ligand LMG 8 626	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 815	
 Bond lengths	 Bond angles
 Torsions	 Rings

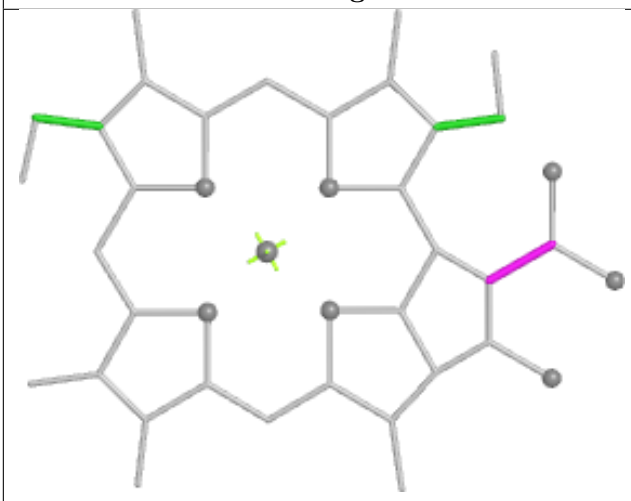
Ligand CLA L 307



Bond lengths



Bond angles

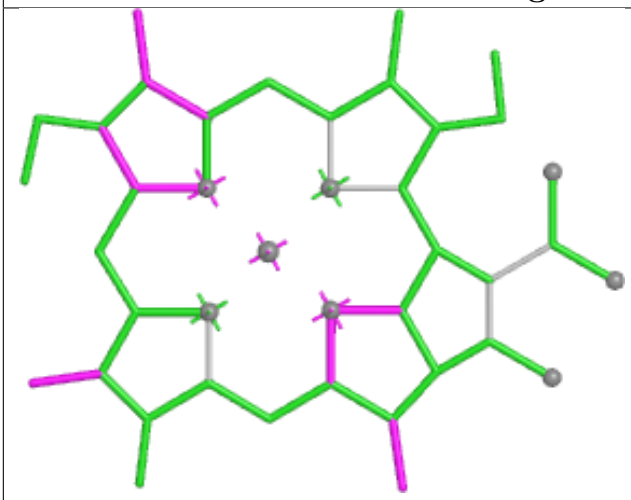


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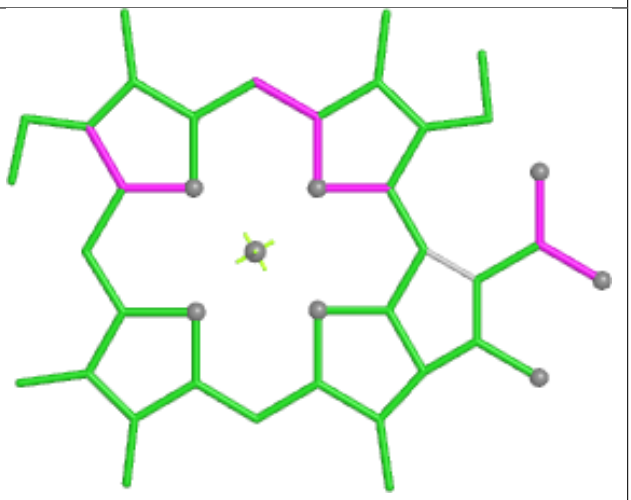


Rings

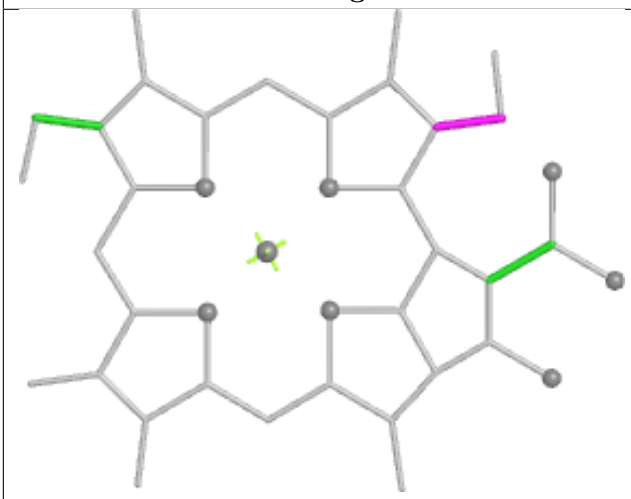
Ligand CLA 9 606



Bond lengths



Bond angles

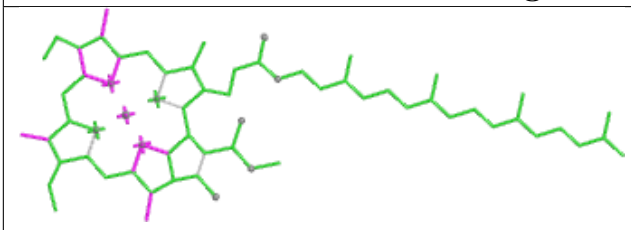


Torsions

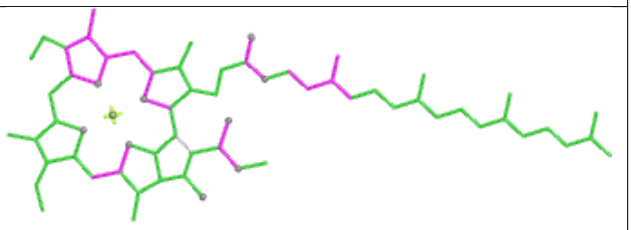


Rings

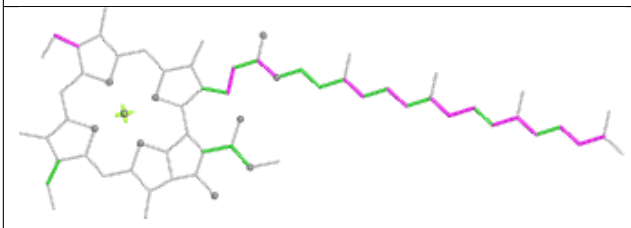
Ligand CLA A 842



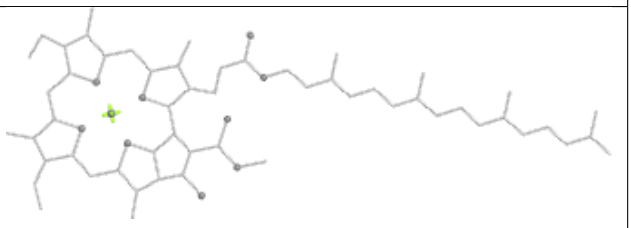
Bond lengths



Bond angles

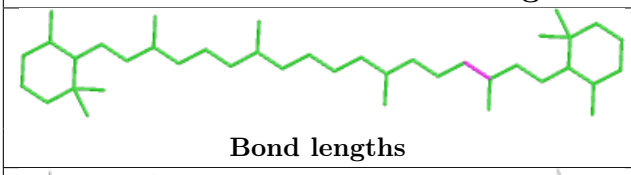


Torsions

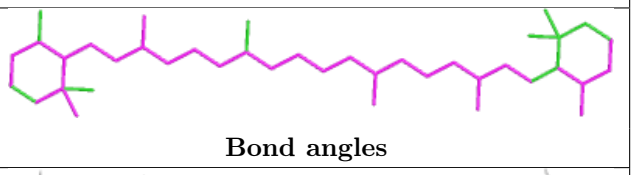


Rings

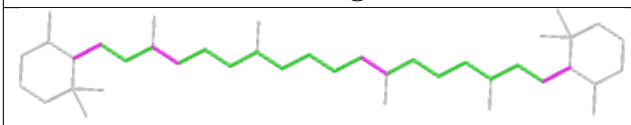
Ligand BCR A 852



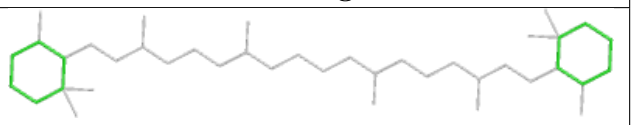
Bond lengths



Bond angles

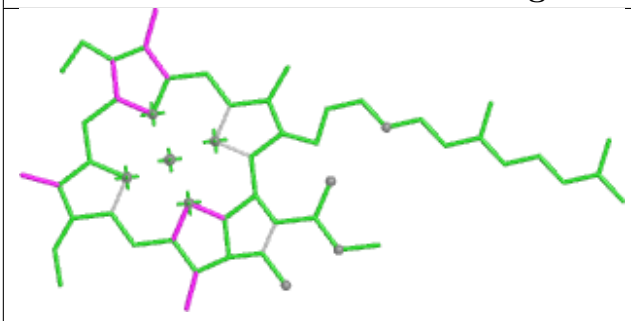


Torsions

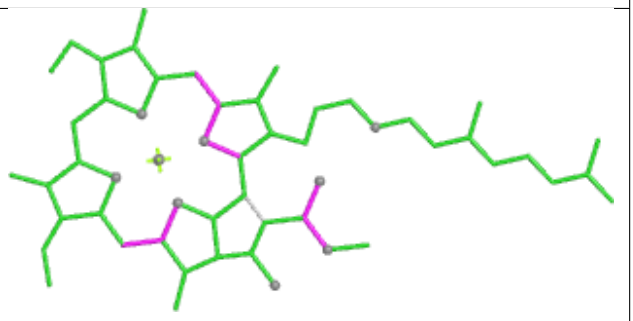


Rings

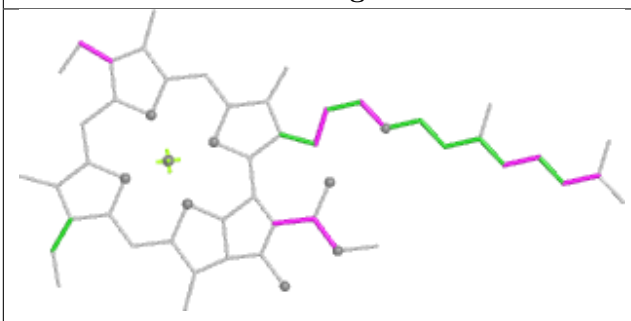
Ligand CLA a 603



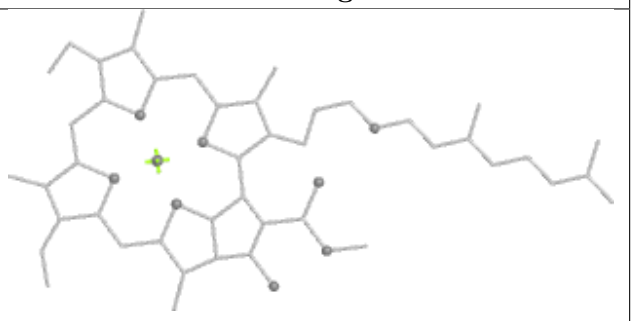
Bond lengths



Bond angles

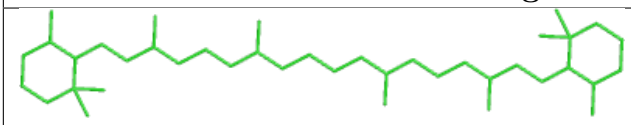


Torsions

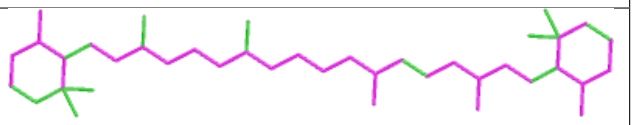


Rings

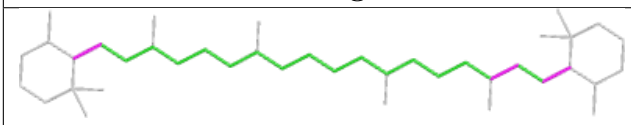
Ligand BCR A 849



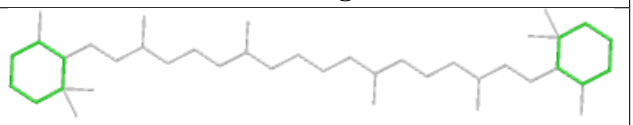
Bond lengths



Bond angles

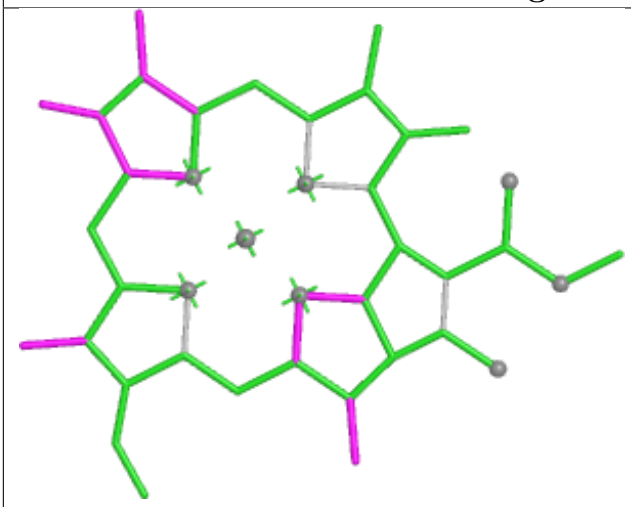


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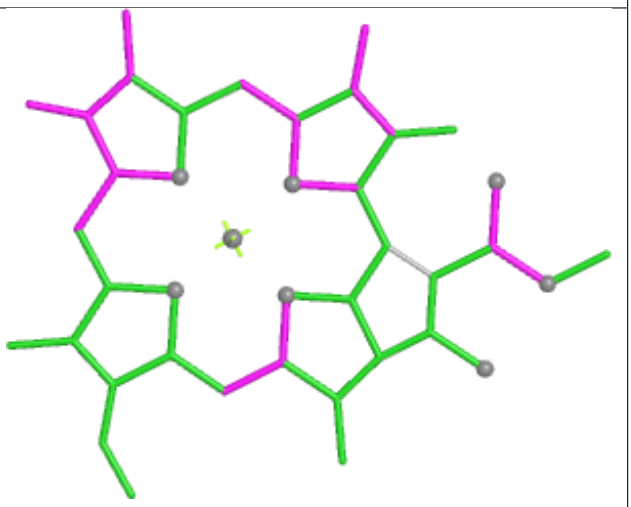


Rings

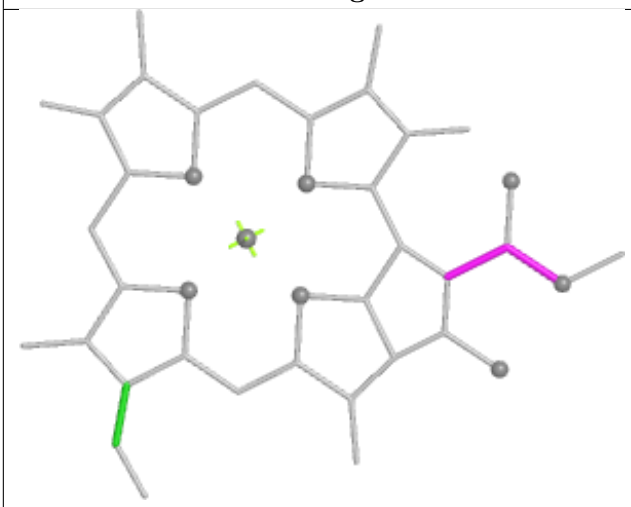
Ligand CLA 1 609



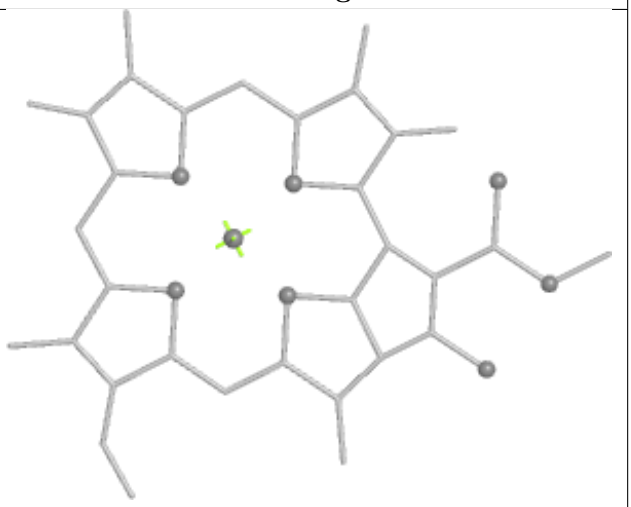
Bond lengths



Bond angles

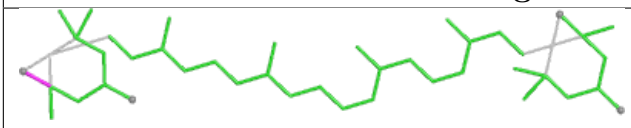


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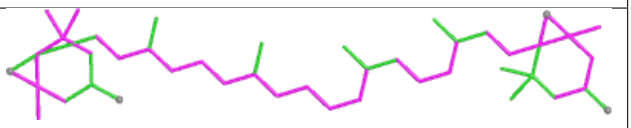


Rings

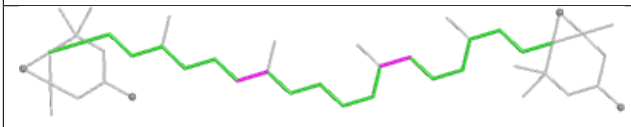
Ligand XAT U 1622



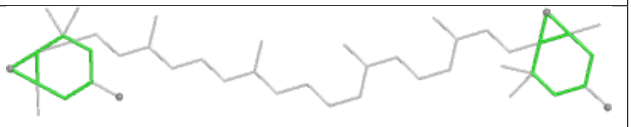
Bond lengths



Bond angles

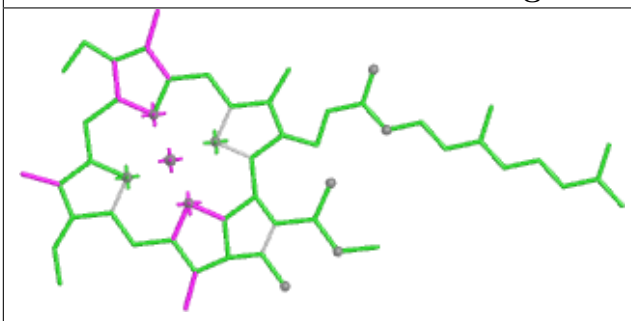


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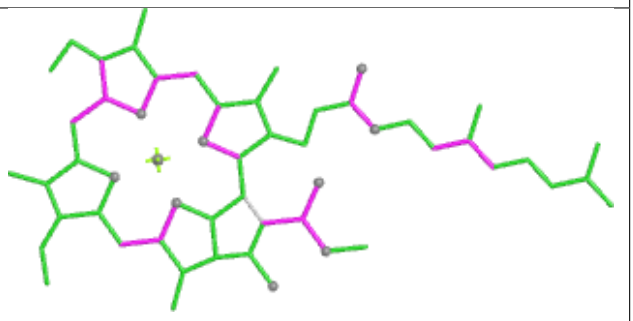


Rings

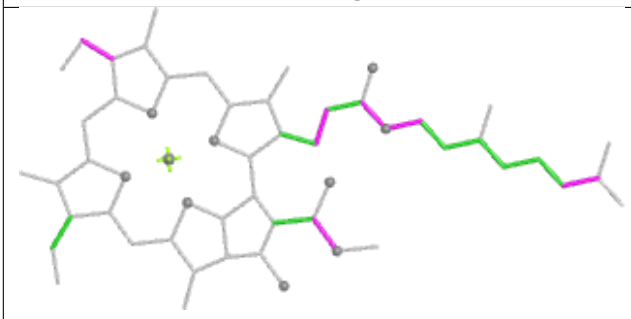
Ligand CLA A 839



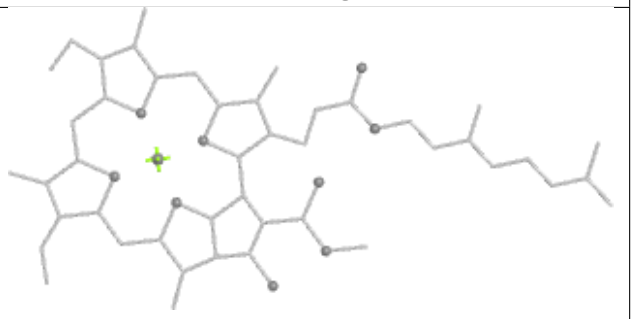
Bond lengths



Bond angles

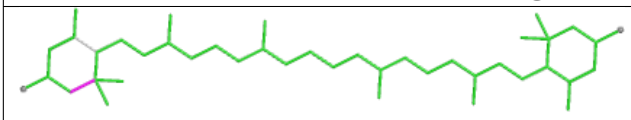


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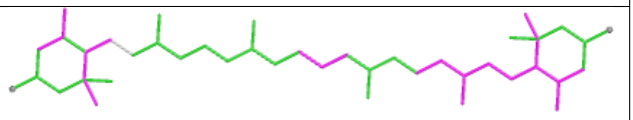


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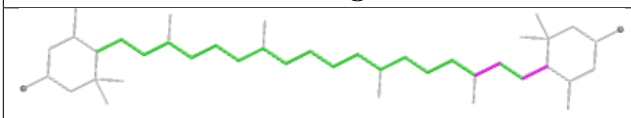
Ligand LUT 8 619



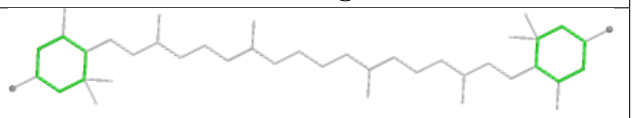
Bond lengths



Bond angles

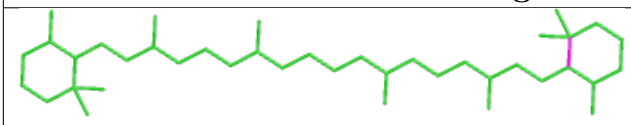


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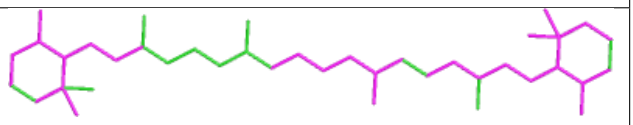


Rings

Ligand BCR O 2005



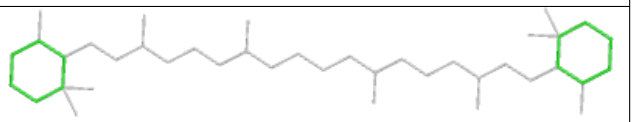
Bond lengths



Bond angles

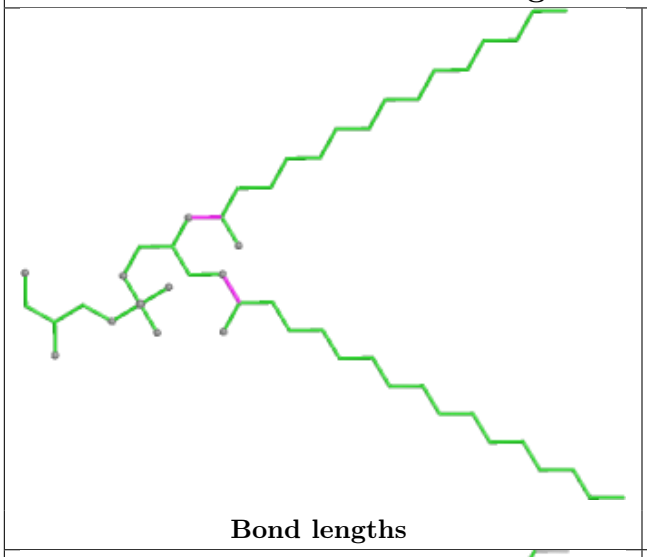


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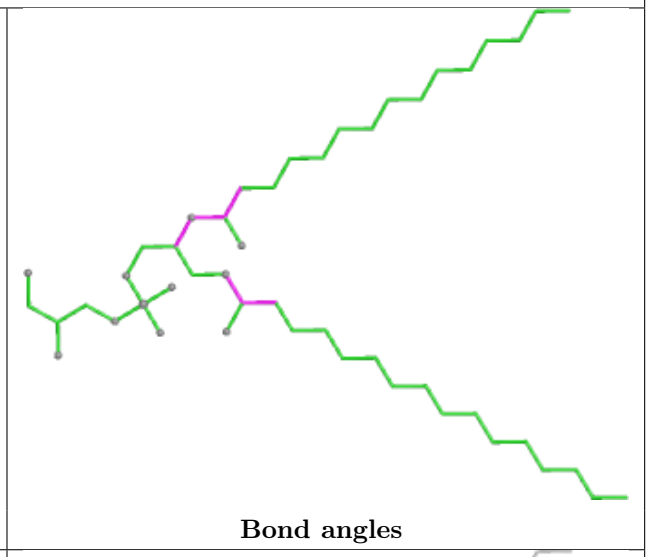


Rings

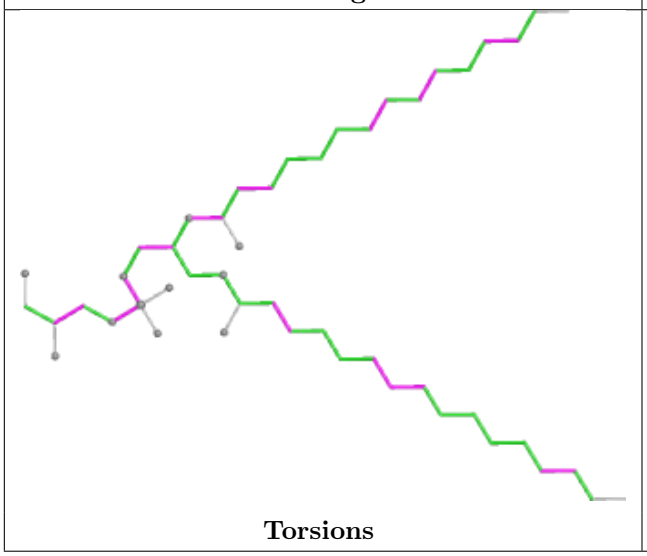
Ligand LHG 6 623



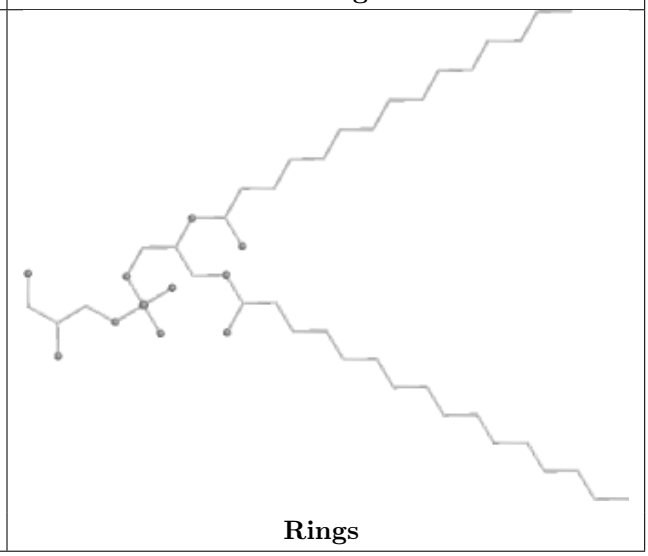
Bond lengths



Bond angles

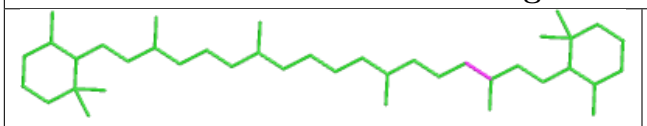


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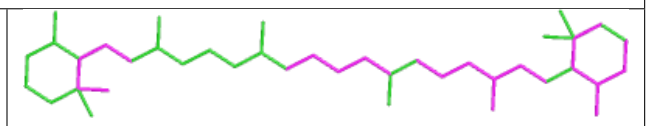


Rings

Ligand BCR B 848



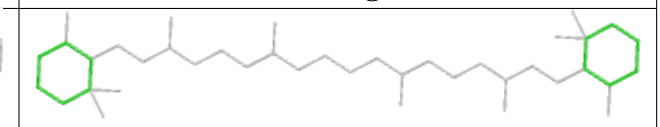
Bond lengths



Bond angles

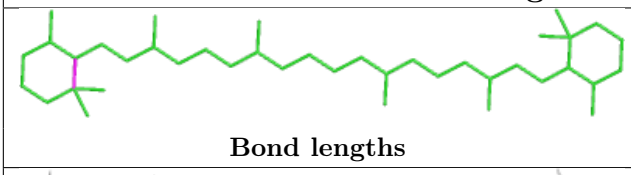


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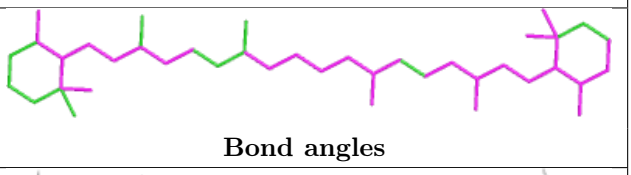


Rings

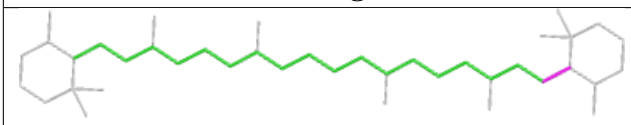
Ligand BCR 7 621



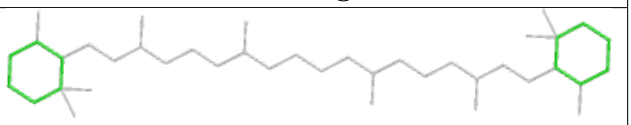
Bond lengths



Bond angles

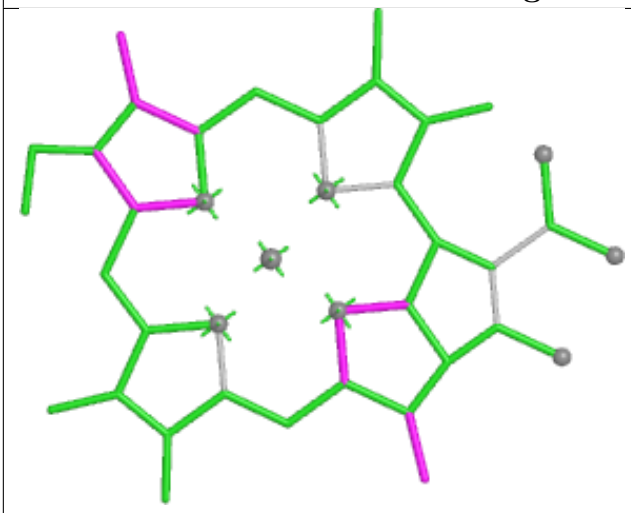


Torsions



Rings

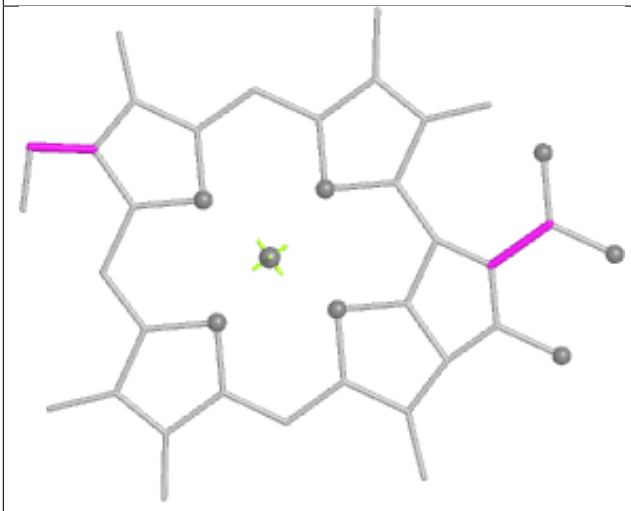
Ligand CLA H 202



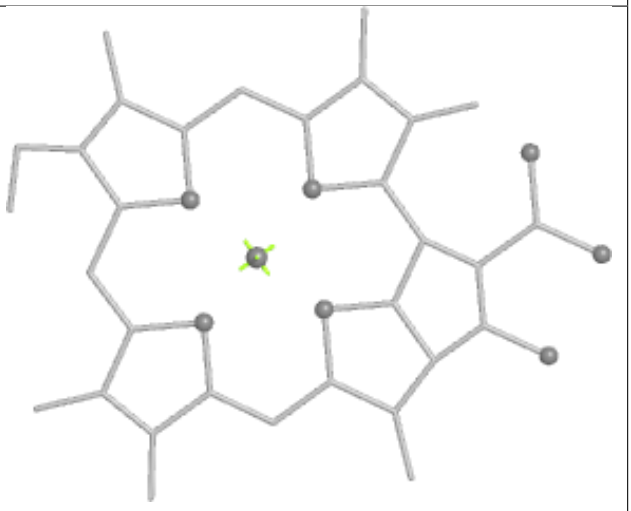
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Bond angles

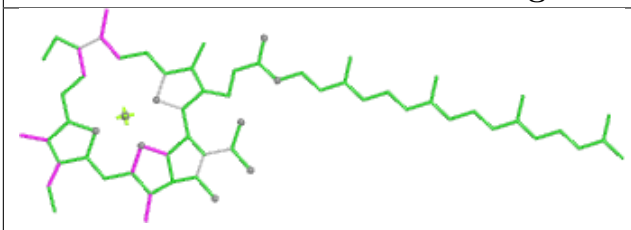


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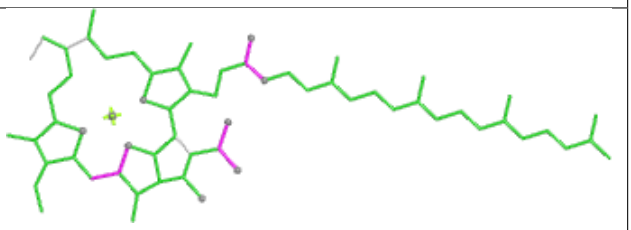


Rings

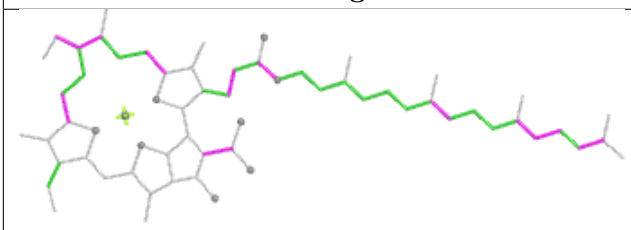
Ligand CLA 2 602



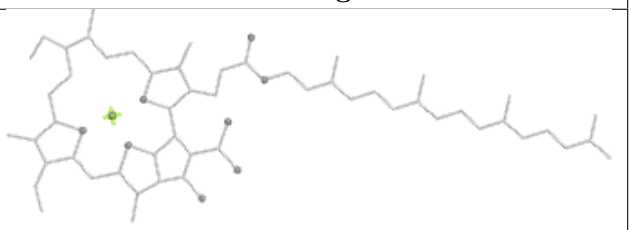
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Bond angles

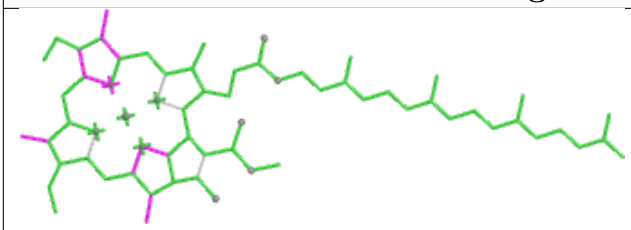


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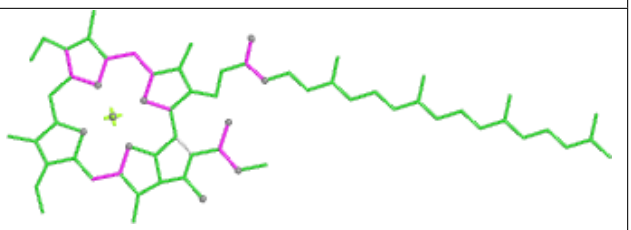


Rings

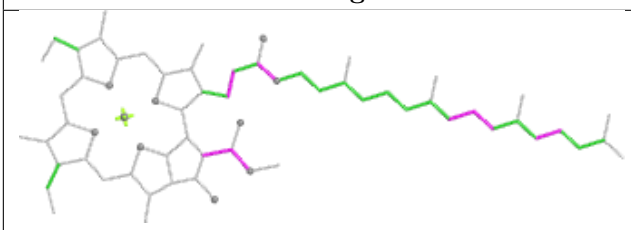
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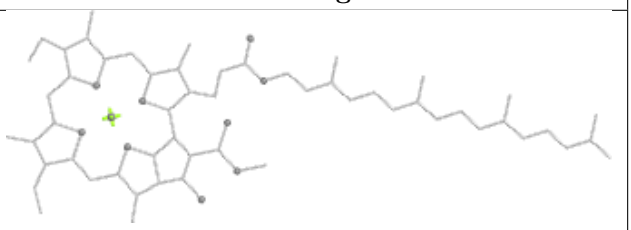
Bond lengths



Bond angles

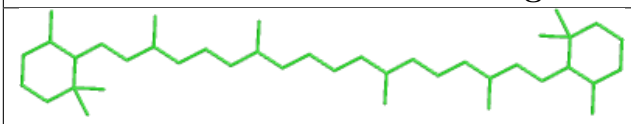


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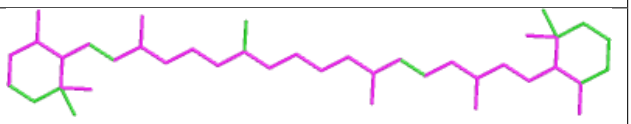


Rings

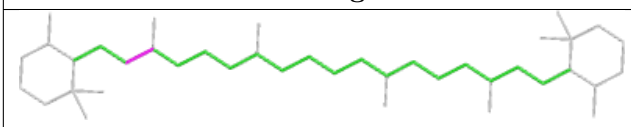
Ligand BCR L 305



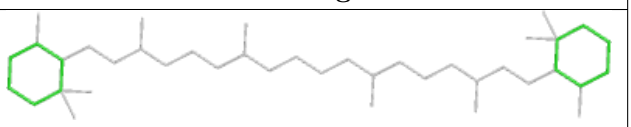
Bond lengths



Bond angles

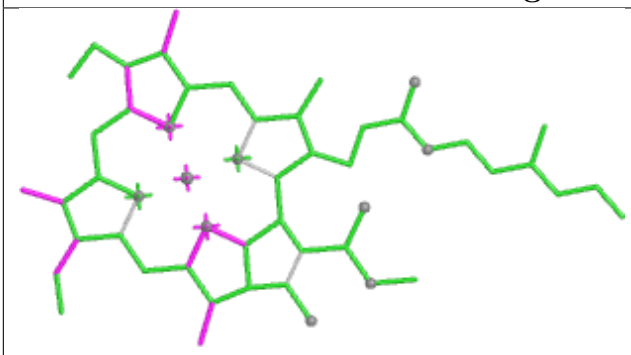


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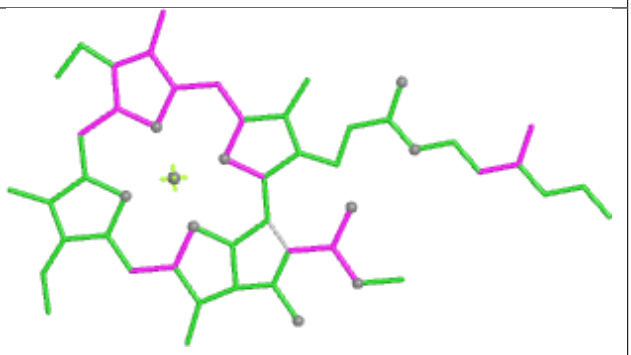


Rings

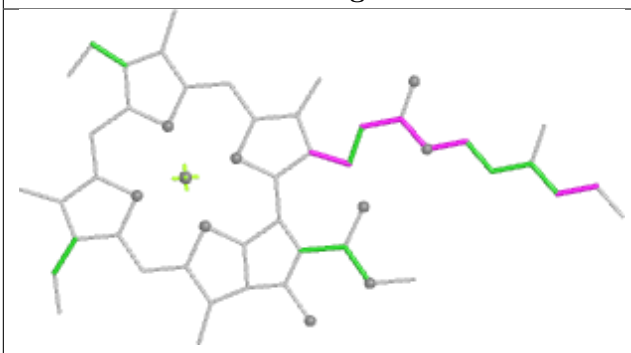
Ligand CLA A 805



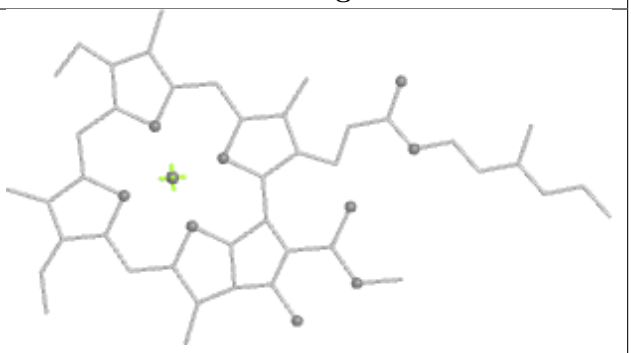
Bond lengths



Bond angles

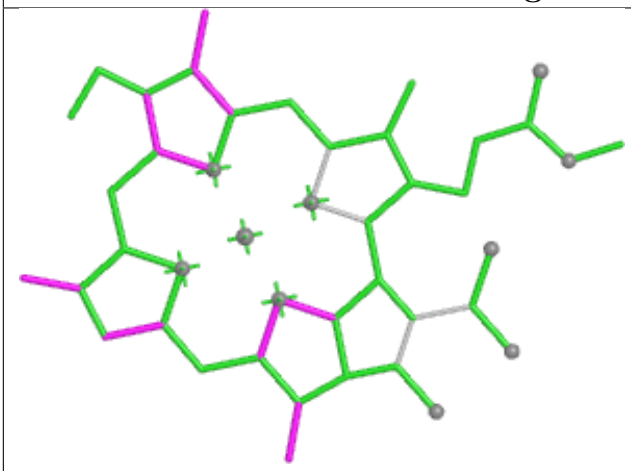


Torsions

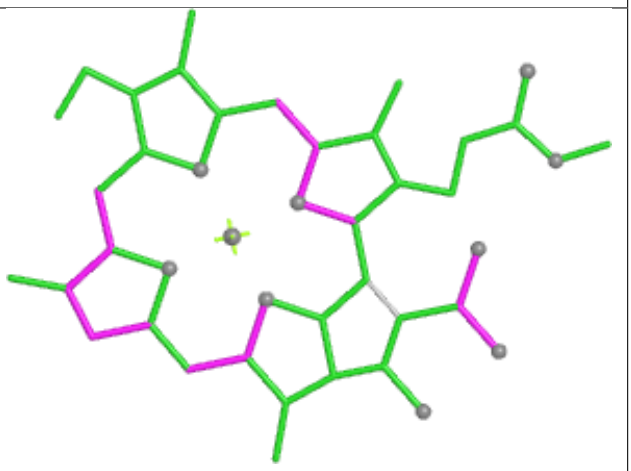


Rings

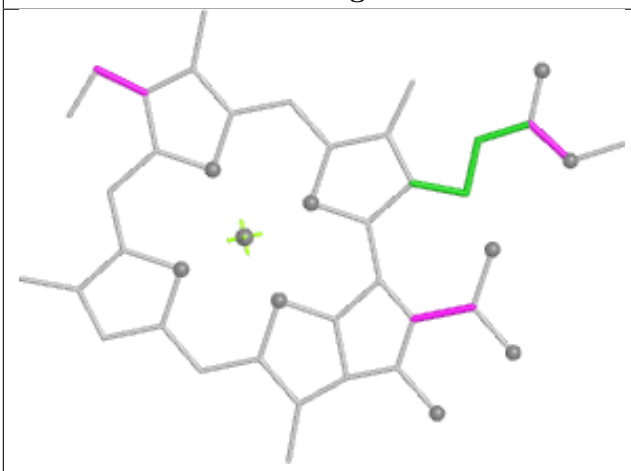
Ligand CLA B 821



Bond lengths



Bond angles

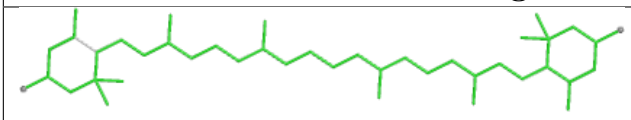


Torsions

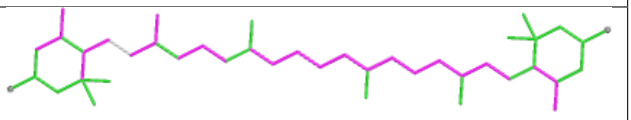


Rings

Ligand LUT W 1620



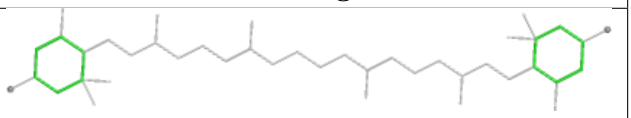
Bond lengths



Bond angles



Torsions

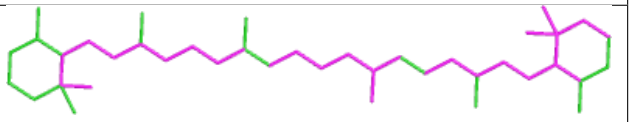


Rings

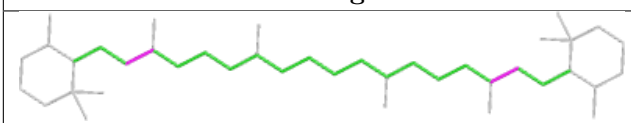
Ligand BCR K 207



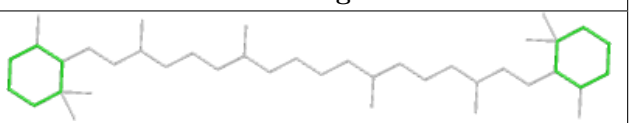
Bond lengths



Bond angles

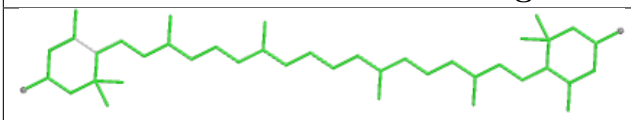


Torsions

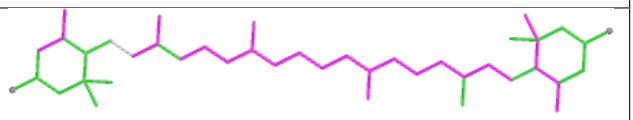


Rings

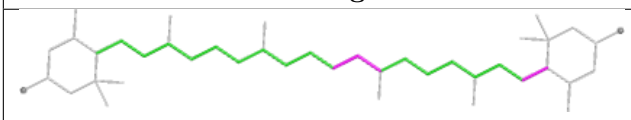
Ligand LUT Y 1620



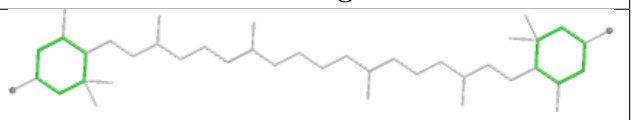
Bond lengths



Bond angles



Torsions

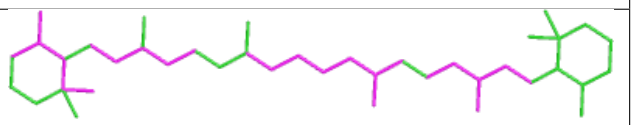


Rings

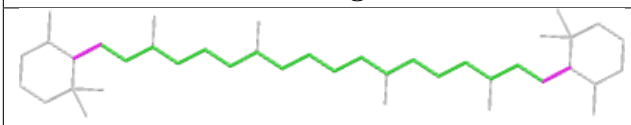
Ligand BCR B 853



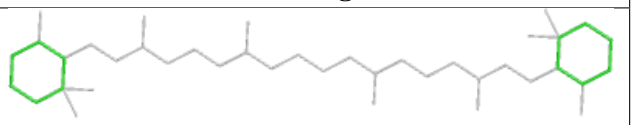
Bond lengths



Bond angles

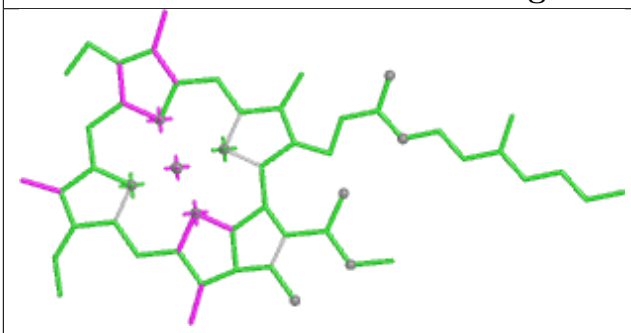


Torsions

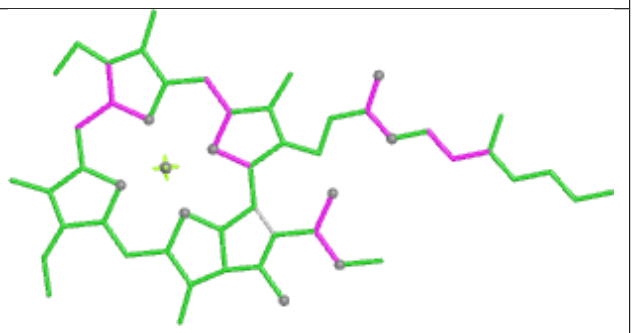


Rings

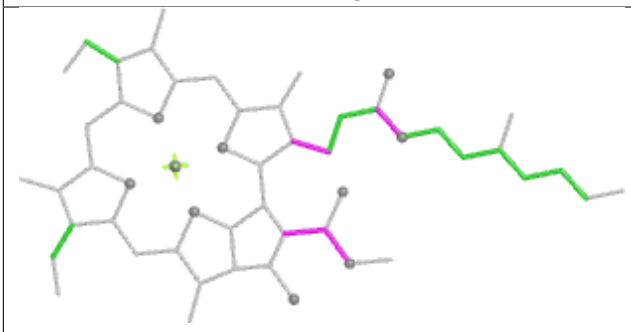
Ligand CLA 8 614



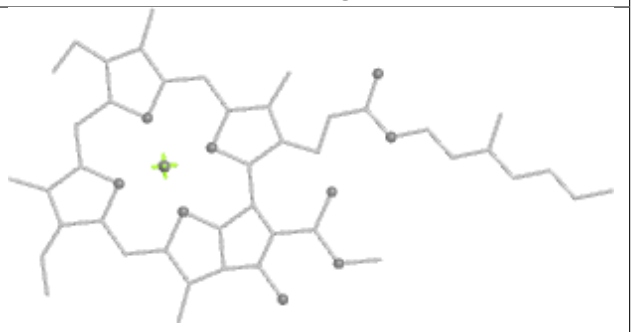
Bond lengths



Bond angles

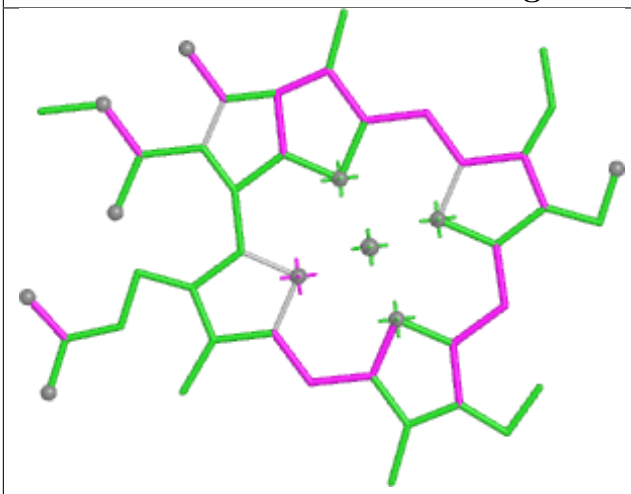


Torsions

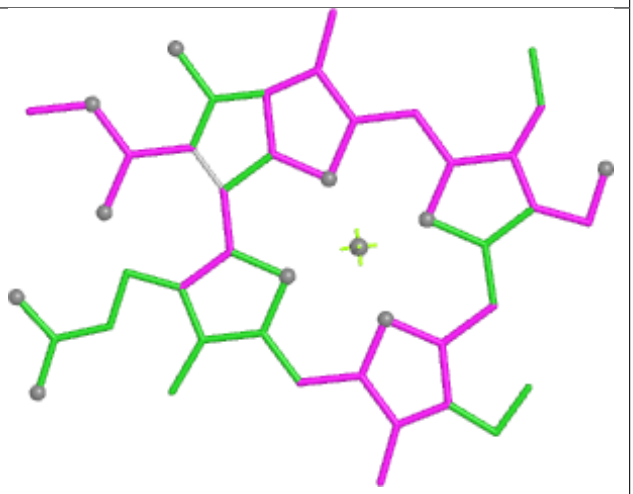


Rings

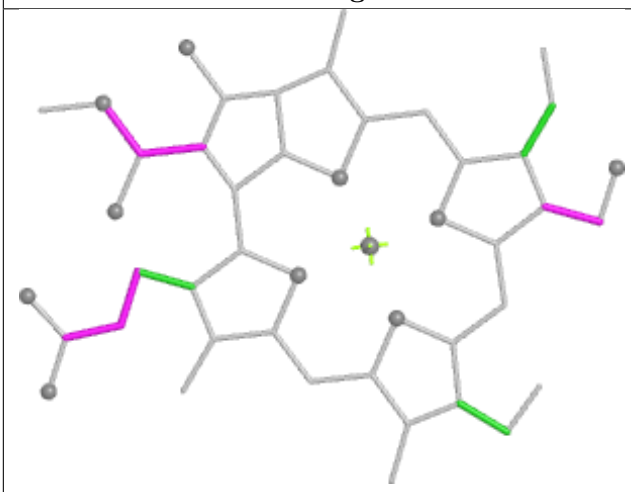
Ligand CHL Y 606



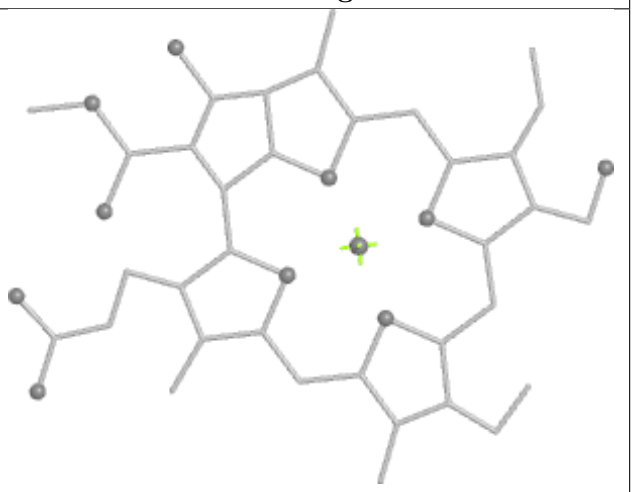
Bond lengths



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.

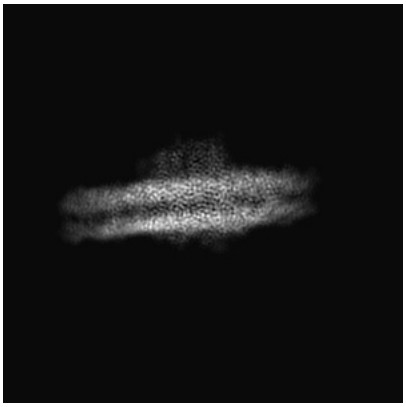
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-30926. 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

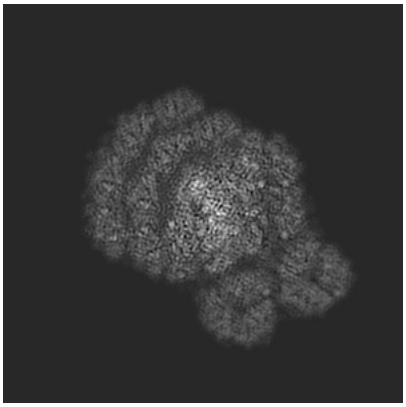
6.1.1 Primary map



X



Y



Z

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

6.2 Central slices

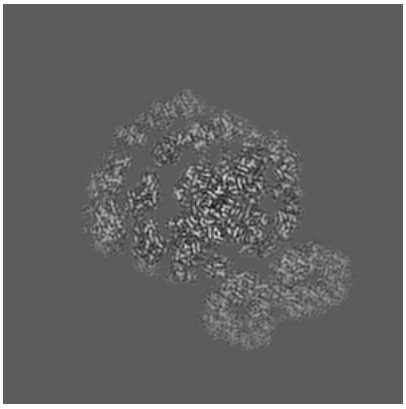
6.2.1 Primary map



X Index: 180



Y Index: 180



Z Index: 180

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

6.3 Largest variance slices (i)

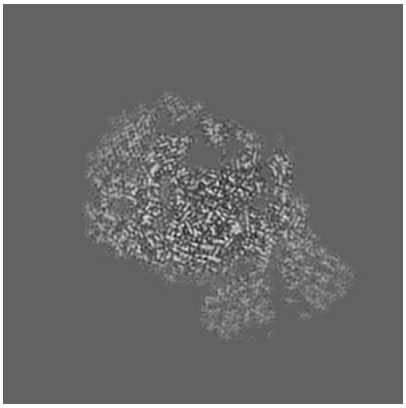
6.3.1 Primary map



X Index: 194



Y Index: 153

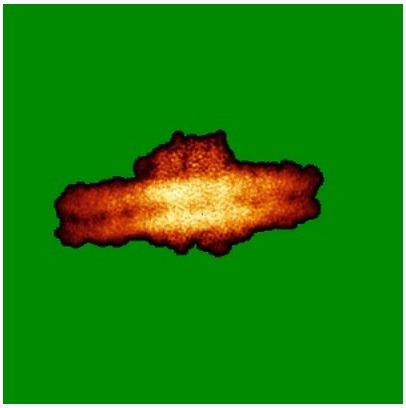


Z Index: 190

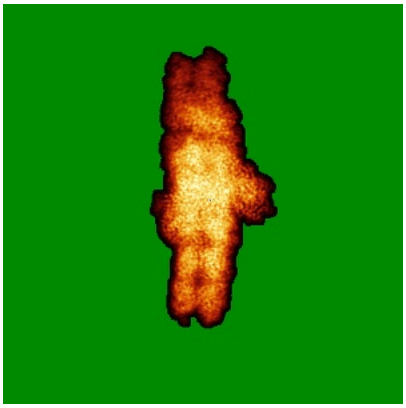
The images above show the largest variance slices of the map in three orthogonal directions.

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

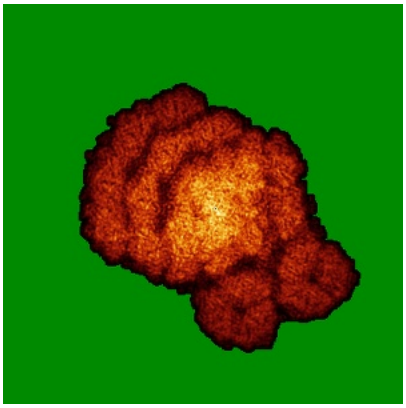
6.4.1 Primary map



X



Y

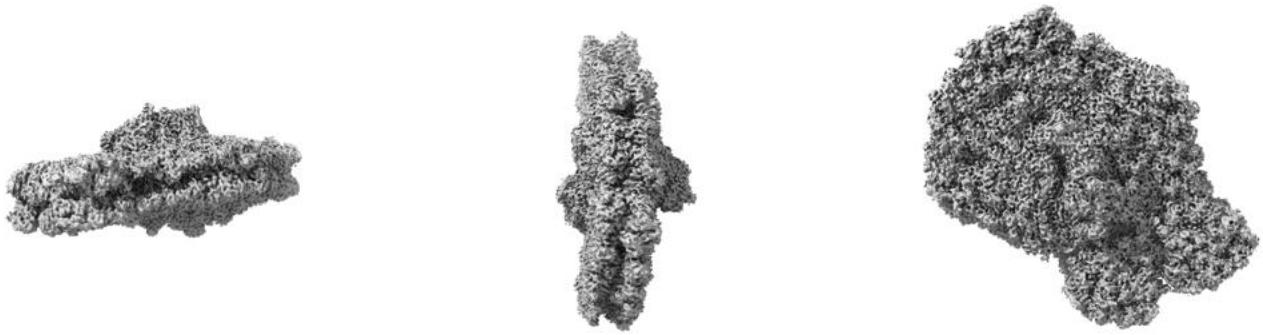


Z

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

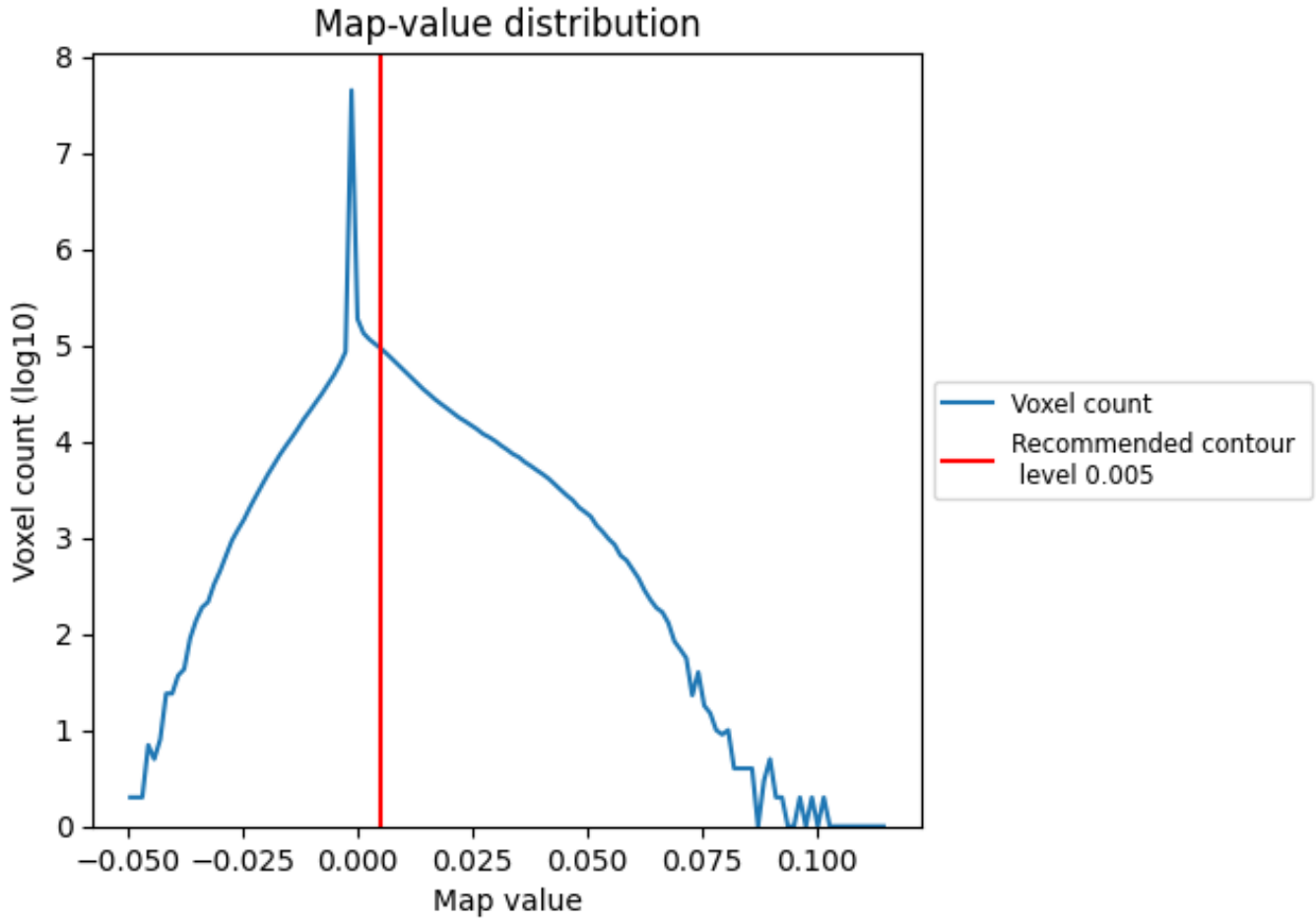
6.6 Mask visualisation (i)

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

7 Map analysis

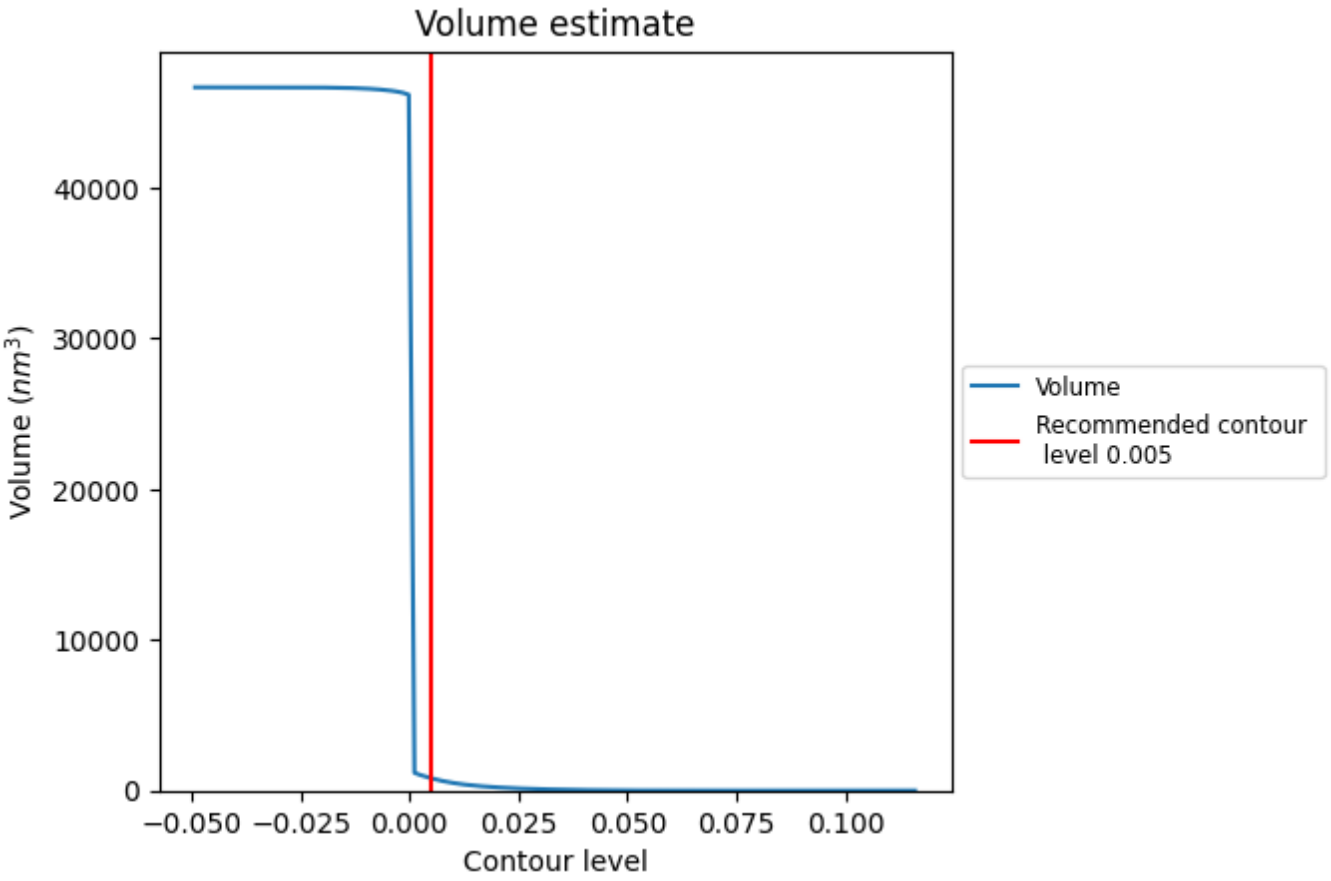
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

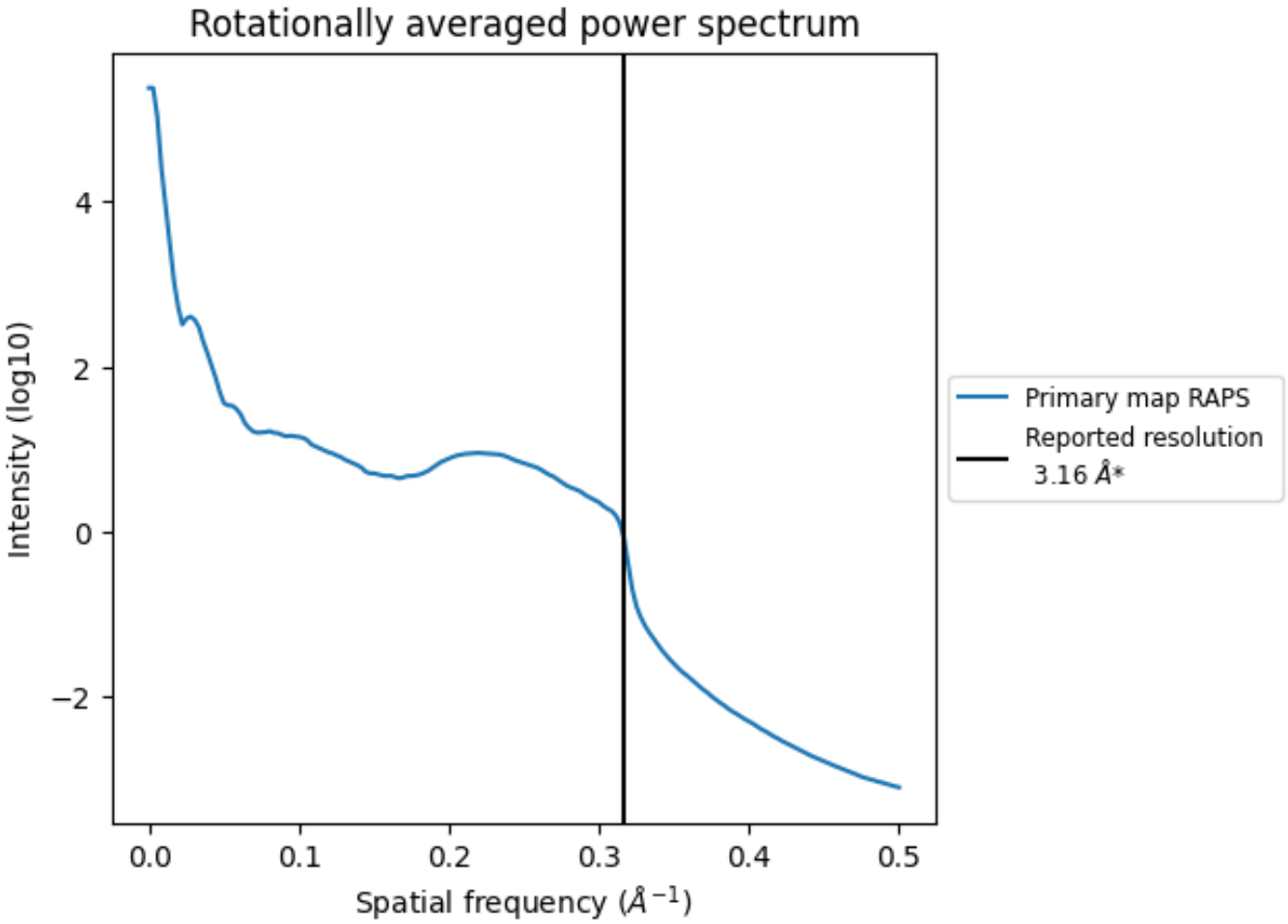
7.2 Volume estimate



The volume at the recommended contour level is 811 nm^3; this corresponds to an approximate mass of 733 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 0.316 $Å^{-1}$

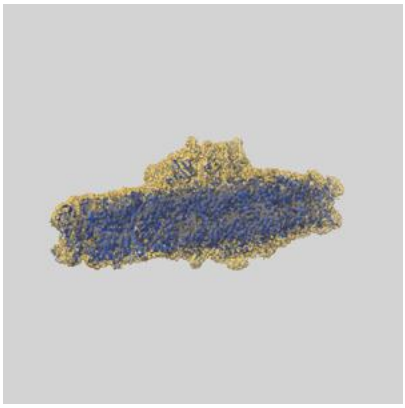
8 Fourier-Shell correlation

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

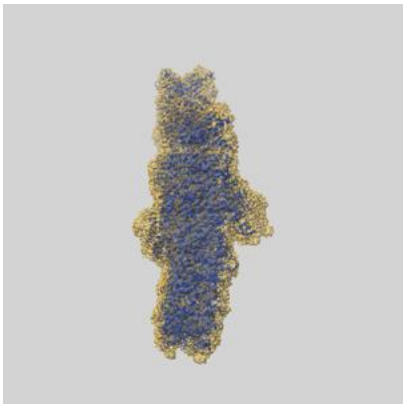
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-30926 and PDB model 7DZ8. Per-residue inclusion information can be found in section 3 on page 37.

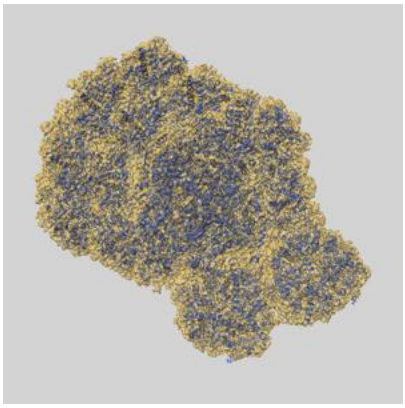
9.1 Map-model overlay



X



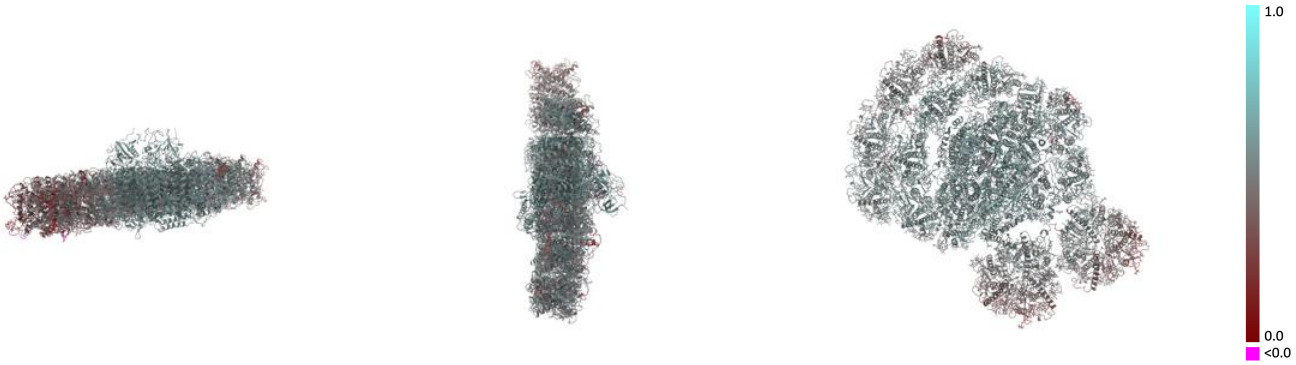
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.005 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.

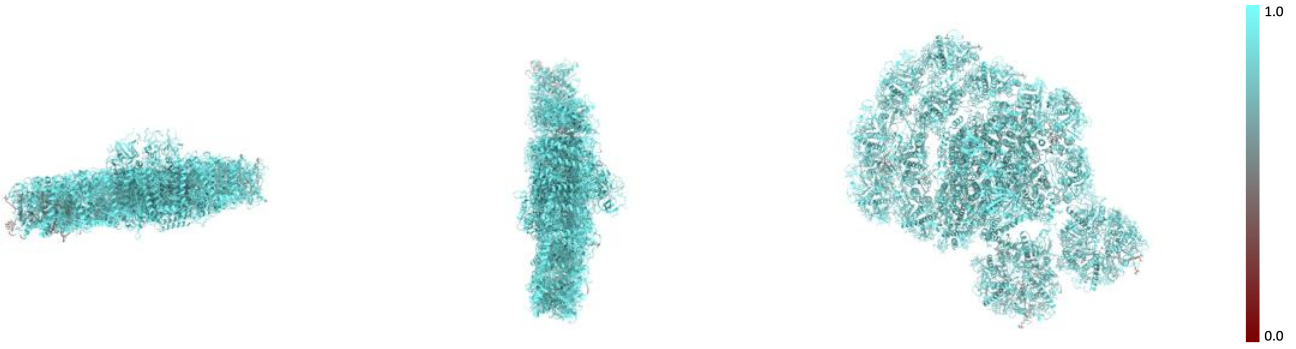
9.2 Q-score mapped to coordinate model



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.

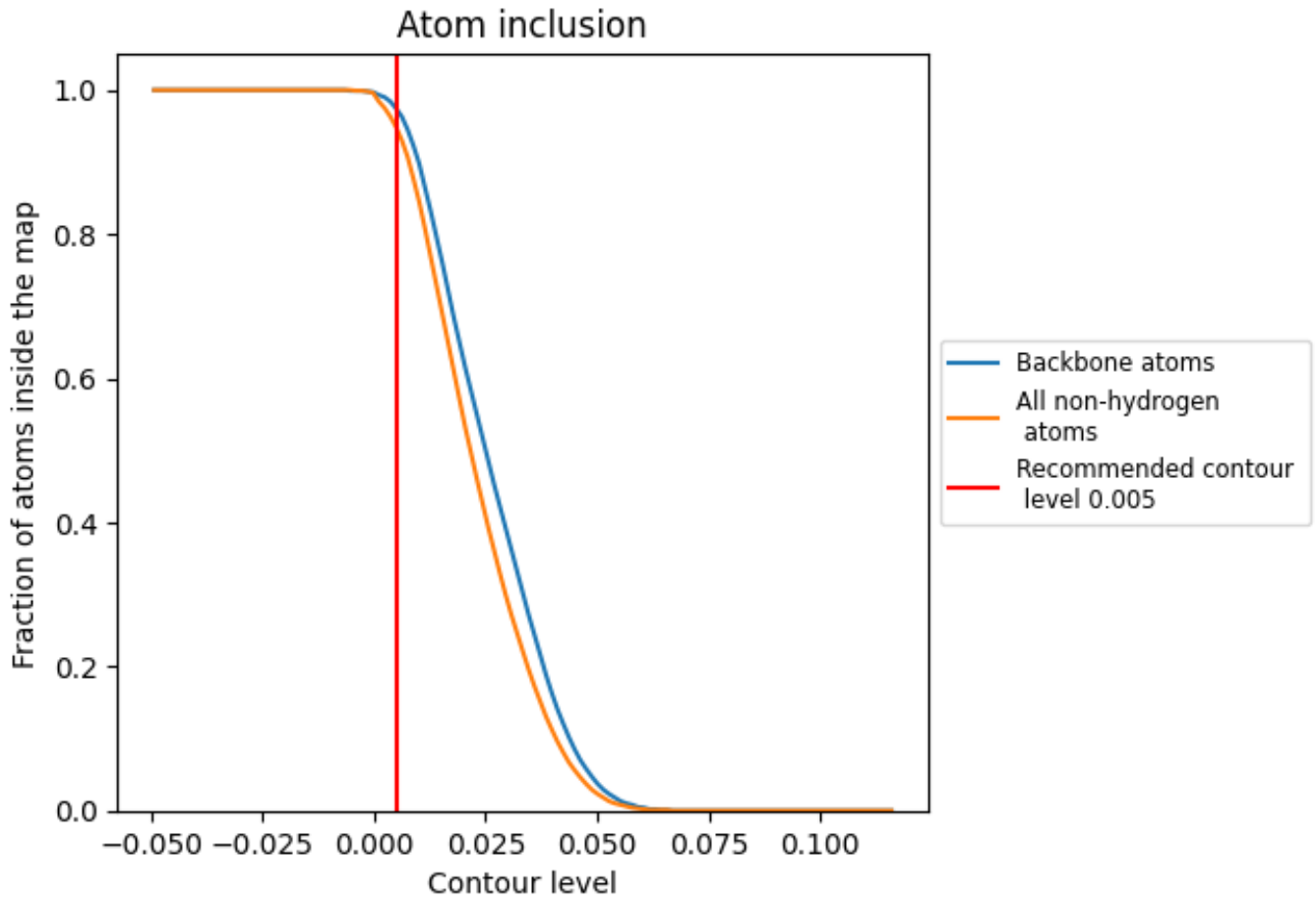
9.3 Atom inclusion mapped to coordinate model



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 (0.005).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 95% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9480	0.5180
1	0.9450	0.5180
2	0.9720	0.5370
3	0.9620	0.5530
4	0.9300	0.4740
5	0.9380	0.5160
6	0.9480	0.5130
7	0.9750	0.5640
8	0.9680	0.5530
9	0.9410	0.5060
A	0.9810	0.5850
B	0.9750	0.5810
C	0.9700	0.5390
D	0.9900	0.5690
E	0.9900	0.5660
F	0.9890	0.5650
G	0.9410	0.5040
H	0.9700	0.5480
I	0.9430	0.5380
J	0.9610	0.5550
K	0.9690	0.5310
L	0.9740	0.5570
O	0.9750	0.5400
U	0.9200	0.4270
V	0.9480	0.4950
W	0.8530	0.3620
X	0.8550	0.3700
Y	0.8830	0.4070
Z	0.9350	0.4990
a	0.8970	0.4270

