wwPDB EM Validation Summary Report

Sep 15, 2026 – 03:22 PM JST

PDB ID	:	9UAS / pdb_00009uas
EMDB ID	:	EMD-63994
Title	:	PSI-LHCE-LHCII from Euglena gracilis
Authors	:	Feng, Y.
Deposited on	:	2025-04-01
Resolution	:	2.35 Å(reported)

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

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

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

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

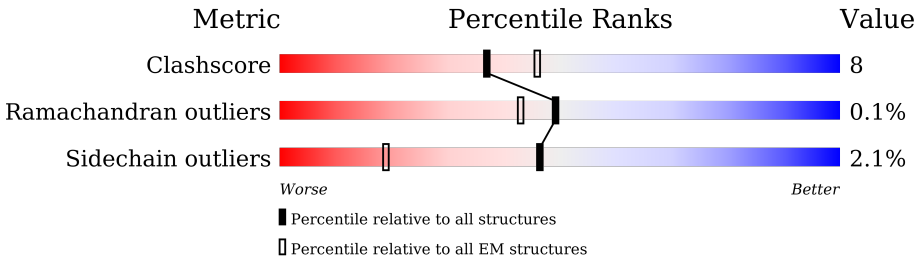
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using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

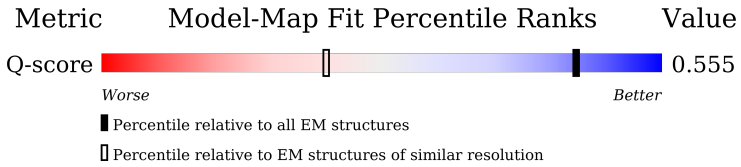
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.35 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.





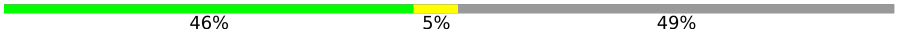
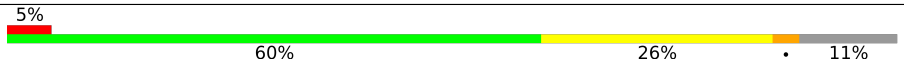
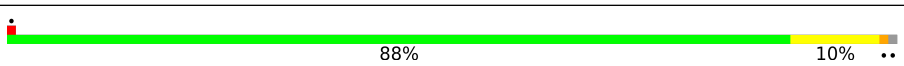
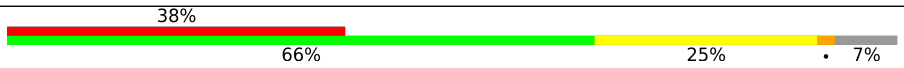
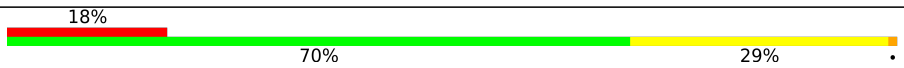
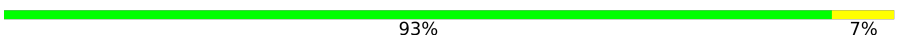
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4607 (1.85 - 2.85)

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	B	734	86% 13%
2	C	81	89% 10%
3	D	193	90% 9%
4	E	158	33% 7% 60%

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Mol	Chain	Length	Quality of chain
5	F	325	
6	G	184	
6	P	184	
7	H	185	
8	I	184	
8	N	184	
9	J	39	
10	K	184	
10	Q	184	
11	L	187	
11	R	187	
12	M	31	
13	O	177	
14	S	180	
15	T	173	
16	U	209	
17	V	196	
18	W	228	
19	X	223	
20	A	756	

2 Entry composition (i)

There are 33 unique types of molecules in this entry. The entry contains 60137 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 A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	732	5868	3859	985	1009	15	0	0

- Molecule 2 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	80	596	363	104	118	11	0	0

- Molecule 3 is a protein called PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	190	1489	948	254	285	2	0	0

- Molecule 4 is a protein called PsaE.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	E	63	509	324	86	99	0	0

- Molecule 5 is a protein called PsaF.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	166	1262	811	210	239	2	0	0

- Molecule 6 is a protein called Lhce5.7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	G	175	1323	853	224	242	4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	P	164	Total	C	N	O	S	0	0
			1243	803	209	227	4		

- Molecule 7 is a protein called Lhce7.3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	173	Total	C	N	O	S	0	0
			1342	862	233	242	5		

- Molecule 8 is a protein called Lhce5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	165	Total	C	N	O	S	0	0
			1242	801	212	225	4		
8	N	170	Total	C	N	O	S	0	0
			1271	819	215	233	4		

- Molecule 9 is a protein called PsaJ.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	37	Total	C	N	O	S	0	0
			305	209	43	52	1		

- Molecule 10 is a protein called LhcE6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	182	Total	C	N	O	S	0	0
			1444	939	246	253	6		
10	Q	182	Total	C	N	O	S	0	0
			1440	938	245	251	6		

- Molecule 11 is a protein called Lhce8.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	178	Total	C	N	O	S	0	0
			1364	876	237	247	4		
11	R	174	Total	C	N	O	S	0	0
			1331	852	232	243	4		

- Molecule 12 is a protein called PsaM.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	31	Total	C	N	O	S	0	0
			242	162	37	42	1		

- Molecule 13 is a protein called LhcE7.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	175	Total	C	N	O	S	0	0
			1359	870	234	250	5		

- Molecule 14 is a protein called Lhce10.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	S	172	Total	C	N	O	S	0	0
			1327	858	219	246	4		

- Molecule 15 is a protein called Lhce11.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	T	167	Total	C	N	O	S	0	0
			1283	824	221	231	7		

- Molecule 16 is a protein called LhcbM4.6.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	U	199	Total	C	N	O	S	0	0
			1517	981	256	275	5		

- Molecule 17 is a protein called LhcbM4.10.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	V	196	Total	C	N	O	S	0	0
			1513	990	253	265	5		

- Molecule 18 is a protein called LhcbM2.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	W	220	Total	C	N	O	S	0	0
			1669	1088	275	302	4		

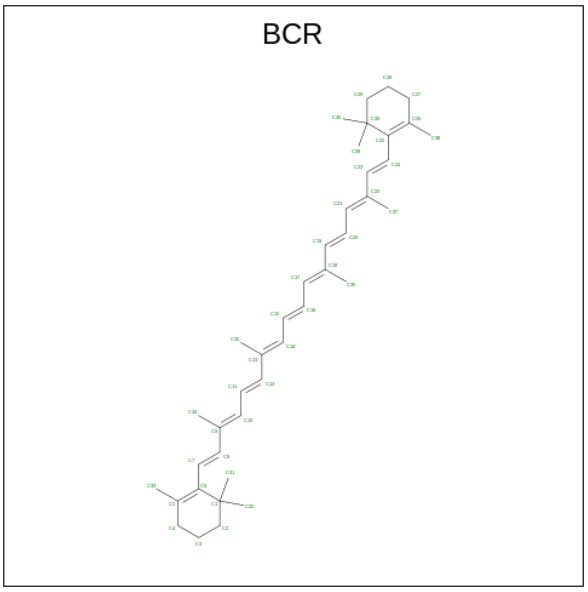
- Molecule 19 is a protein called LhcbM8.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	X	223	Total	C	N	O	S	0	0
			1688	1093	284	306	5		

- Molecule 20 is a protein called PsaA.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	A	740	Total	C	N	O	S	0	0
			5872	3855	992	1004	21		

- Molecule 21 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



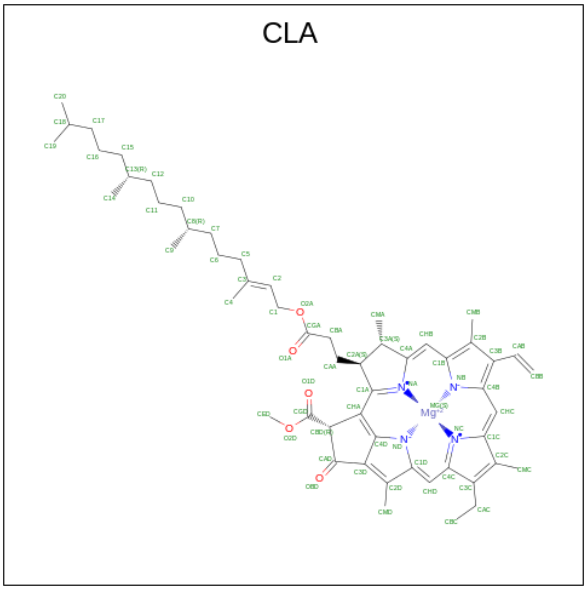
Mol	Chain	Residues	Atoms		AltConf
21	B	1	Total	C	0
			40	40	
21	B	1	Total	C	0
			40	40	
21	B	1	Total	C	0
			40	40	
21	B	1	Total	C	0
			40	40	
21	B	1	Total	C	0
			40	40	
21	B	1	Total	C	0
			40	40	
21	J	1	Total	C	0
			40	40	

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Mol	Chain	Residues	Atoms	AltConf
21	M	1	Total C 40 40	0
21	A	1	Total C 40 40	0
21	A	1	Total C 40 40	0
21	A	1	Total C 40 40	0
21	A	1	Total C 40 40	0

- Molecule 22 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
22	B	1	Total C Mg N O 65 55 1 4 5	0
22	B	1	Total C Mg N O 56 46 1 4 5	0
22	B	1	Total C Mg N O 65 55 1 4 5	0
22	B	1	Total C Mg N O 65 55 1 4 5	0
22	B	1	Total C Mg N O 65 55 1 4 5	0
22	B	1	Total C Mg N O 65 55 1 4 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	F	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	F	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	G	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	G	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
22	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	G	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	G	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	H	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	H	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	H	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	H	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	H	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	H	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	H	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
22	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	I	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	I	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	I	1	Total	C	Mg	N	O	0
			56	46	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	I	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	I	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	I	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
22	I	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	I	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	I	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	I	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	I	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	J	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	K	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	K	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	K	1	Total	C	Mg	N	O	0
			64	55	1	4	4	
22	K	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	K	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	K	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
22	K	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	K	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	K	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
22	K	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	K	1	Total	C	Mg	N	O	0
			53	43	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	K	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	L	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	L	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
22	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	L	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
22	L	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	L	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	L	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	N	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	N	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	N	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	N	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
22	O	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	O	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	O	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	O	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
22	O	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	O	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	O	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	O	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	O	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	O	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	O	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	O	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	P	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
22	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	Q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	Q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	Q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	Q	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
22	Q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	Q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	Q	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	Q	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	Q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	Q	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	Q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	Q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	Q	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	Q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	R	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	R	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	R	1	Total	C	Mg	N	O	0
			56	46	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	R	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	R	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
22	R	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	R	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
22	R	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
22	R	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	R	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	S	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	S	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	S	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	S	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	S	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	S	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	S	1	Total	C	Mg	N	O	0
			51	41	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	T	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	T	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	T	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	T	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	T	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	T	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	T	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	T	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	T	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	T	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	T	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	U	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	U	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	U	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	U	1	Total 57	C 47	Mg 1	N 4	O 5	0
22	U	1	Total 56	C 46	Mg 1	N 4	O 5	0
22	U	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	U	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	U	1	Total 57	C 47	Mg 1	N 4	O 5	0
22	U	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	U	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	U	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
22	U	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	U	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	V	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	V	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	V	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
22	V	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
22	V	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	V	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	V	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
22	V	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	V	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	V	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	V	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	V	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	W	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	W	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	W	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	W	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	W	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
22	W	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	W	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	W	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	W	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	W	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	W	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	W	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	W	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	X	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	X	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	X	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	X	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
22	X	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	X	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	X	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	X	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	X	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	X	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	X	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	X	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	X	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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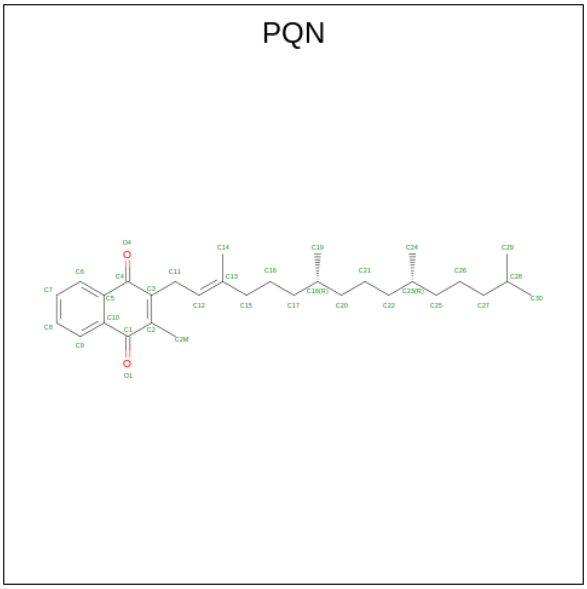
Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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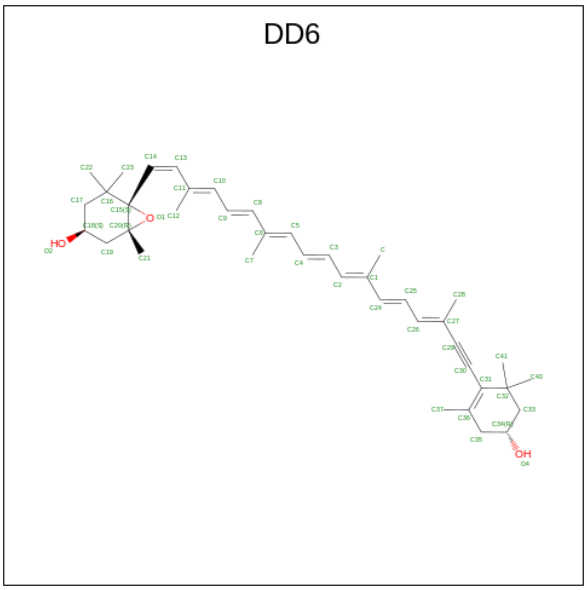
Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 23 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 24 is (3S,3'R,5R,6S,7cis)-7',8'-didehydro-5,6-dihydro-5,6-epoxy-beta,beta-carotene-3,3'-diol (CCD ID: DD6) (formula: $C_{40}H_{54}O_3$) (labeled as "Ligand of Interest" by depositor).



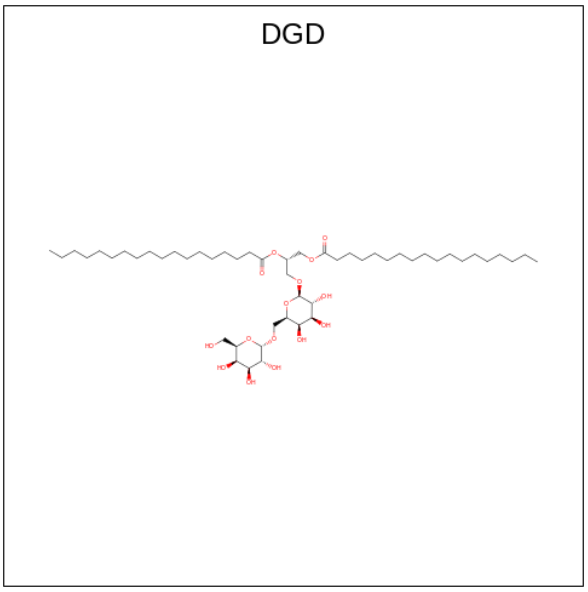
Mol	Chain	Residues	Atoms			AltConf
24	B	1	Total	C	O	0
			43	40	3	
24	F	1	Total	C	O	0
			43	40	3	
24	G	1	Total	C	O	0
			43	40	3	
24	G	1	Total	C	O	0
			43	40	3	
24	H	1	Total	C	O	0
			43	40	3	
24	H	1	Total	C	O	0
			43	40	3	
24	I	1	Total	C	O	0
			43	40	3	
24	I	1	Total	C	O	0
			43	40	3	
24	J	1	Total	C	O	0
			43	40	3	
24	K	1	Total	C	O	0
			43	40	3	
24	K	1	Total	C	O	0
			43	40	3	
24	L	1	Total	C	O	0
			43	40	3	
24	L	1	Total	C	O	0
			43	40	3	
24	L	1	Total	C	O	0
			43	40	3	
24	N	1	Total	C	O	0
			43	40	3	
24	N	1	Total	C	O	0
			43	40	3	
24	O	1	Total	C	O	0
			43	40	3	
24	O	1	Total	C	O	0
			43	40	3	
24	P	1	Total	C	O	0
			43	40	3	
24	P	1	Total	C	O	0
			43	40	3	
24	Q	1	Total	C	O	0
			43	40	3	
24	Q	1	Total	C	O	0
			43	40	3	

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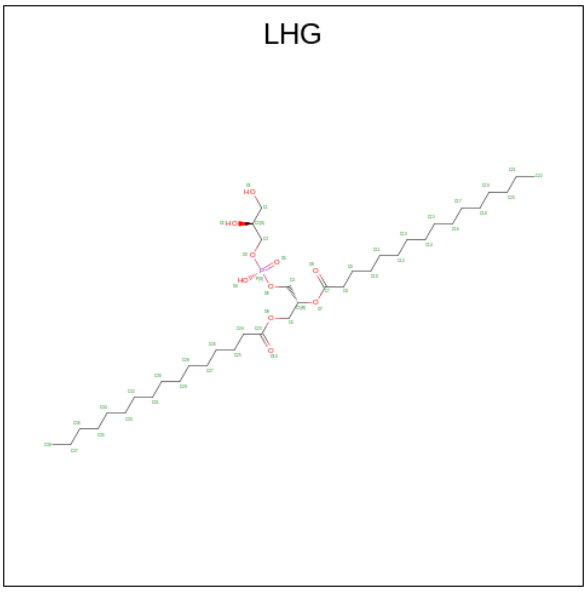
Mol	Chain	Residues	Atoms			AltConf
24	R	1	Total	C	O	0
			43	40	3	
24	R	1	Total	C	O	0
			43	40	3	
24	S	1	Total	C	O	0
			43	40	3	
24	S	1	Total	C	O	0
			43	40	3	
24	T	1	Total	C	O	0
			43	40	3	
24	T	1	Total	C	O	0
			43	40	3	
24	U	1	Total	C	O	0
			43	40	3	
24	U	1	Total	C	O	0
			43	40	3	
24	V	1	Total	C	O	0
			43	40	3	
24	V	1	Total	C	O	0
			43	40	3	
24	W	1	Total	C	O	0
			43	40	3	
24	W	1	Total	C	O	0
			43	40	3	
24	W	1	Total	C	O	0
			43	40	3	
24	X	1	Total	C	O	0
			43	40	3	
24	X	1	Total	C	O	0
			43	40	3	
24	X	1	Total	C	O	0
			43	40	3	
24	X	1	Total	C	O	0
			43	40	3	
24	A	1	Total	C	O	0
			43	40	3	
24	A	1	Total	C	O	0
			43	40	3	
24	A	1	Total	C	O	0
			43	40	3	

- Molecule 25 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
25	B	1	Total 66	C 51	O 15	0
25	F	1	Total 34	C 29	O 5	0
25	O	1	Total 60	C 45	O 15	0

- Molecule 26 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



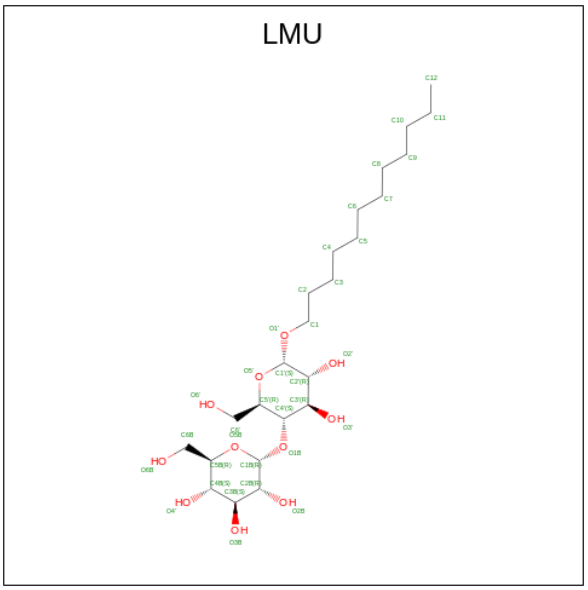
Mol	Chain	Residues	Atoms				AltConf
26	B	1	Total	C	O	P	0
			27	16	10	1	
26	B	1	Total	C	O	P	0
			42	31	10	1	
26	G	1	Total	C	O	P	0
			32	21	10	1	
26	H	1	Total	C	O	P	0
			27	16	10	1	
26	K	1	Total	C	O	P	0
			39	28	10	1	
26	K	1	Total	C	O	P	0
			33	22	10	1	
26	L	1	Total	C	O	P	0
			42	31	10	1	
26	N	1	Total	C	O	P	0
			28	17	10	1	
26	N	1	Total	C	O	P	0
			43	32	10	1	
26	O	1	Total	C	O	P	0
			34	23	10	1	
26	O	1	Total	C	O	P	0
			49	38	10	1	
26	O	1	Total	C	O	P	0
			43	32	10	1	
26	O	1	Total	C	O	P	0
			42	31	10	1	
26	P	1	Total	C	O	P	0
			40	29	10	1	
26	Q	1	Total	C	O	P	0
			44	33	10	1	
26	R	1	Total	C	O	P	0
			42	31	10	1	
26	S	1	Total	C	O	P	0
			32	21	10	1	
26	T	1	Total	C	O	P	0
			42	31	10	1	
26	U	1	Total	C	O	P	0
			25	16	8	1	
26	W	1	Total	C	O	P	0
			42	31	10	1	
26	X	1	Total	C	O	P	0
			42	31	10	1	
26	A	1	Total	C	O	P	0
			49	38	10	1	

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Mol	Chain	Residues	Atoms				AltConf
26	A	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 27 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
27	B	1	Total	C	O	0
			24	18	6	
27	B	1	Total	C	O	0
			24	18	6	
27	B	1	Total	C	O	0
			19	14	5	
27	B	1	Total	C	O	0
			24	18	6	
27	B	1	Total	C	O	0
			24	18	6	
27	B	1	Total	C	O	0
			35	24	11	
27	B	1	Total	C	O	0
			15	14	1	
27	F	1	Total	C	O	0
			21	15	6	
27	F	1	Total	C	O	0
			21	15	6	
27	G	1	Total	C	O	0
			21	15	6	

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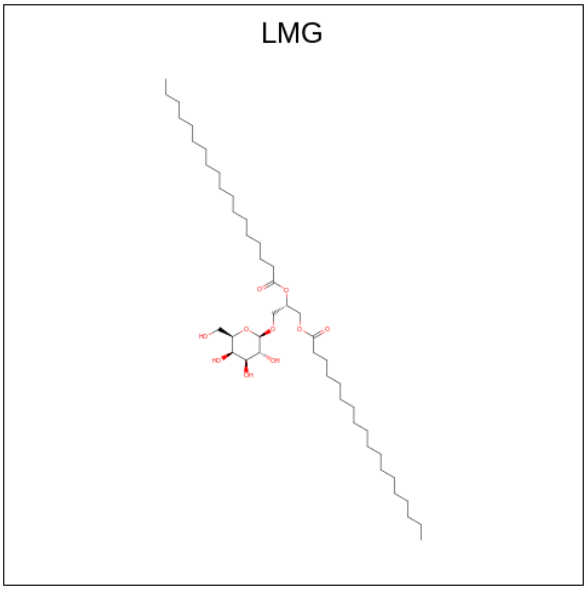
Mol	Chain	Residues	Atoms	AltConf
27	H	1	Total C O 21 15 6	0
27	H	1	Total C O 24 18 6	0
27	H	1	Total C O 33 23 10	0
27	J	1	Total C O 34 24 10	0
27	K	1	Total C O 33 23 10	0
27	L	1	Total C O 24 18 6	0
27	L	1	Total C O 27 21 6	0
27	L	1	Total C O 34 24 10	0
27	M	1	Total C O 24 18 6	0
27	O	1	Total C O 24 18 6	0
27	O	1	Total C O 35 24 11	0
27	O	1	Total C O 26 22 4	0
27	O	1	Total C O 35 24 11	0
27	T	1	Total C O 21 15 6	0
27	T	1	Total C O 24 18 6	0
27	T	1	Total C O 24 18 6	0
27	U	1	Total C O 35 24 11	0
27	U	1	Total C O 35 24 11	0
27	U	1	Total C O 24 18 6	0
27	W	1	Total C O 24 18 6	0
27	X	1	Total C O 24 18 6	0

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Mol	Chain	Residues	Atoms	AltConf
27	X	1	Total C O 35 24 11	0
27	A	1	Total C O 24 18 6	0
27	A	1	Total C O 35 24 11	0
27	A	1	Total C O 21 15 6	0
27	A	1	Total C O 24 18 6	0

- Molecule 28 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



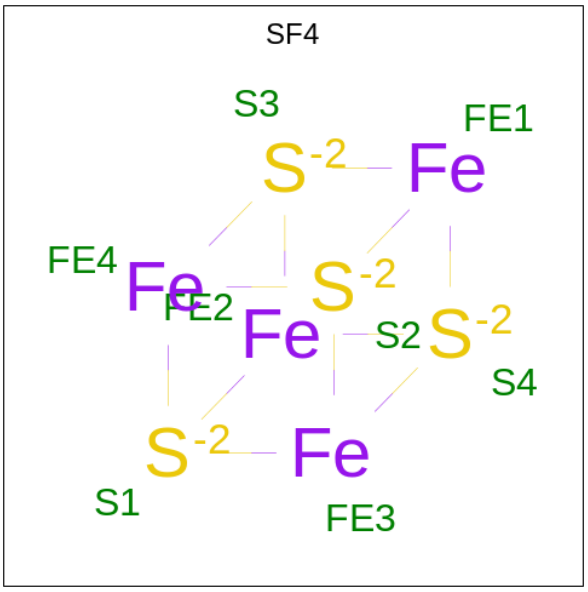
Mol	Chain	Residues	Atoms	AltConf
28	B	1	Total C O 43 33 10	0
28	B	1	Total C O 53 43 10	0
28	F	1	Total C O 42 32 10	0
28	G	1	Total C O 46 36 10	0
28	H	1	Total C O 43 33 10	0
28	H	1	Total C O 40 30 10	0

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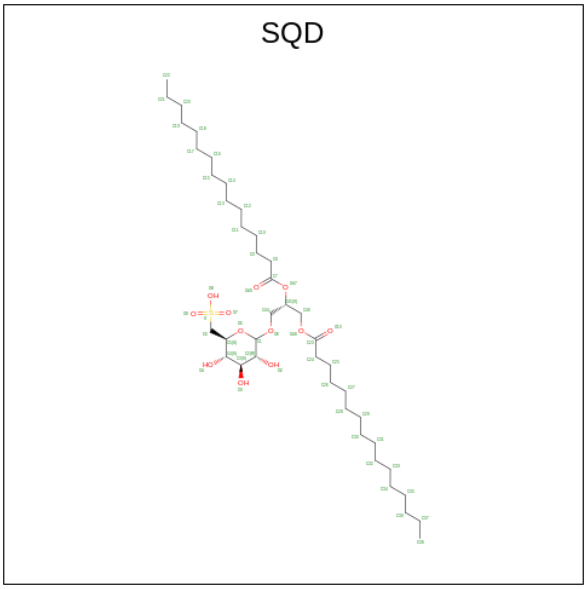
Mol	Chain	Residues	Atoms	AltConf
28	H	1	Total C O 37 27 10	0
28	I	1	Total C O 37 27 10	0
28	I	1	Total C O 50 41 9	0
28	J	1	Total C O 55 45 10	0
28	K	1	Total C O 43 33 10	0
28	K	1	Total C O 49 39 10	0
28	K	1	Total C O 43 33 10	0
28	L	1	Total C O 51 41 10	0
28	N	1	Total C O 44 34 10	0
28	Q	1	Total C O 37 27 10	0
28	T	1	Total C O 41 31 10	0
28	U	1	Total C O 53 43 10	0
28	U	1	Total C O 49 39 10	0
28	W	1	Total C O 48 38 10	0
28	A	1	Total C O 41 31 10	0

- Molecule 29 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



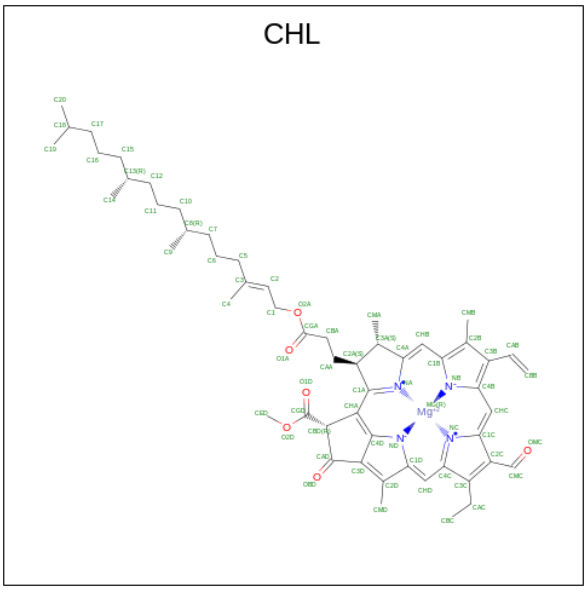
Mol	Chain	Residues	Atoms			AltConf
29	B	1	Total	Fe	S	0
			8	4	4	
29	C	1	Total	Fe	S	0
			8	4	4	
29	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 30 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
30	F	1	Total	C	O	S	0
			42	29	12	1	
30	K	1	Total	C	O	S	0
			43	30	12	1	
30	O	1	Total	C	O	S	0
			42	29	12	1	
30	V	1	Total	C	O	S	0
			27	16	10	1	

- Molecule 31 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



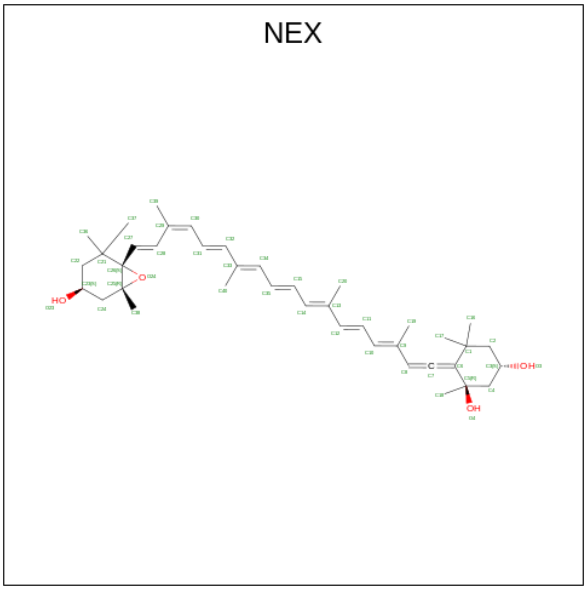
Mol	Chain	Residues	Atoms					AltConf
31	U	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
31	U	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
31	V	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
31	V	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
31	W	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
31	W	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
31	W	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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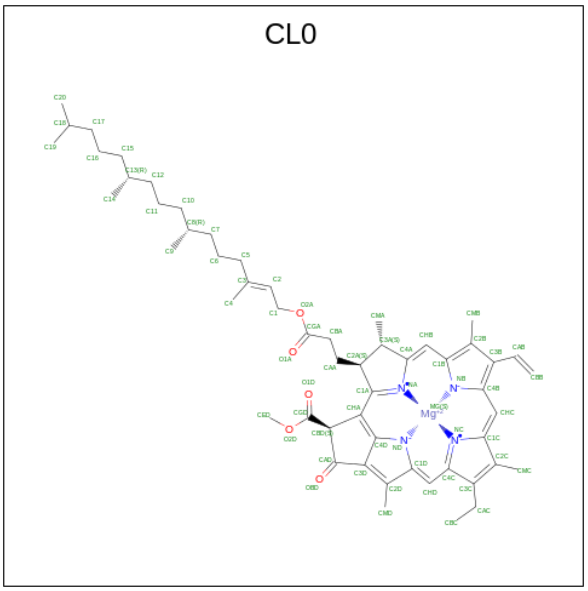
Mol	Chain	Residues	Atoms					AltConf
31	X	1	Total	C	Mg	N	O	0
			46	35	1	4	6	

- Molecule 32 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: $C_{40}H_{56}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
32	U	1	Total	C	O	0
			44	40	4	
32	V	1	Total	C	O	0
			44	40	4	

- Molecule 33 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



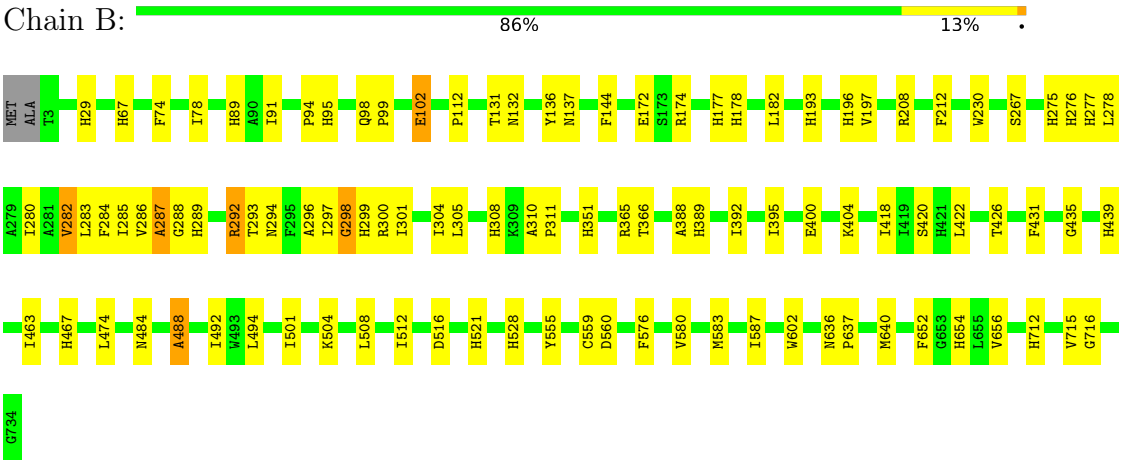
Mol	Chain	Residues	Atoms					AltConf
33	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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.

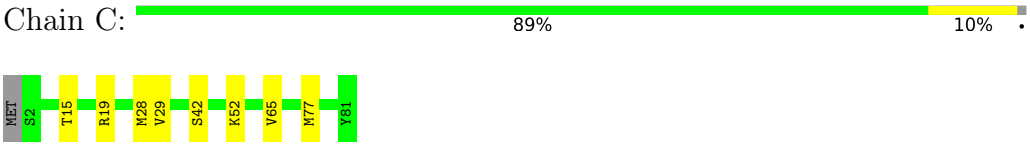
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A2

Chain B:



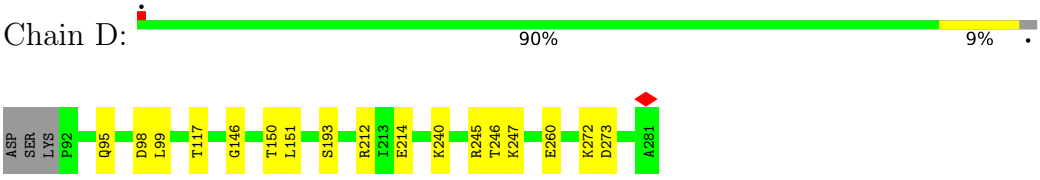
• Molecule 2: Photosystem I iron-sulfur center

Chain C:



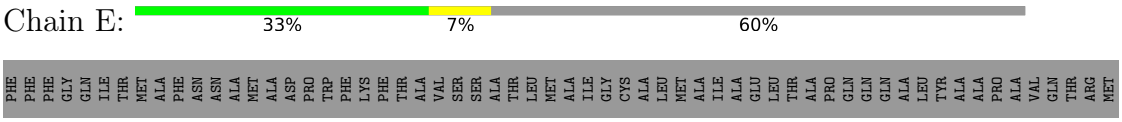
• Molecule 3: PsaD

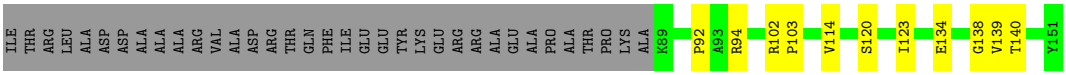
Chain D:



• Molecule 4: PsaE

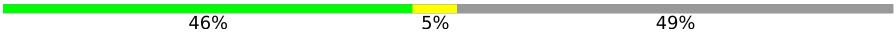
Chain E:

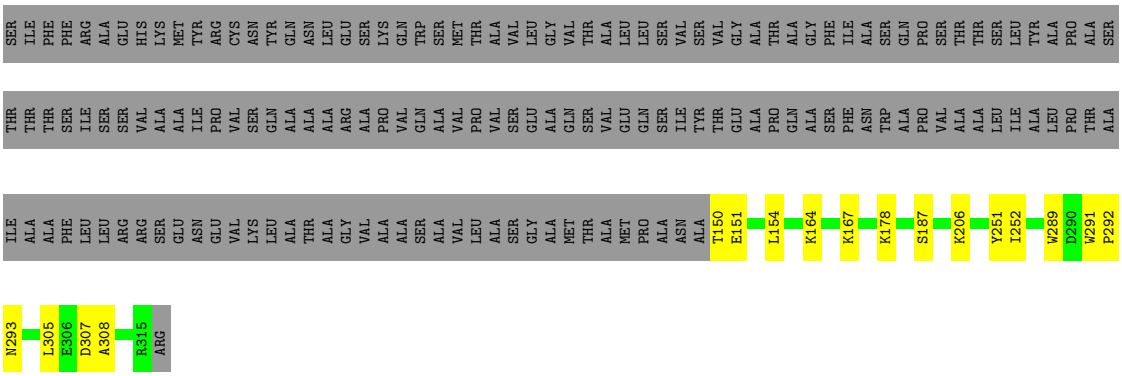




• Molecule 5: PsaF

Chain F:





• Molecule 6: Lhce5.7

Chain G:

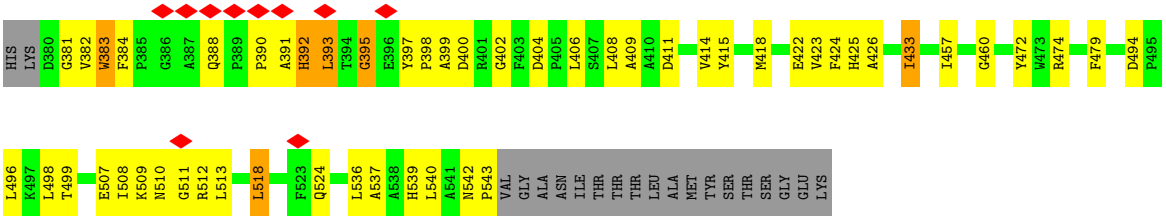




• Molecule 6: Lhce5.7

Chain P:

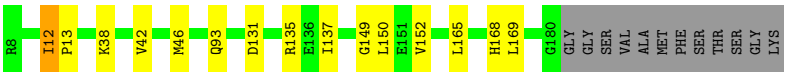




• Molecule 7: Lhce7.3

Chain H:





• Molecule 8: Lhce5

Chain I:



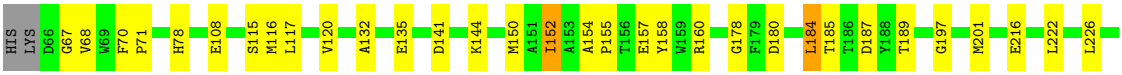


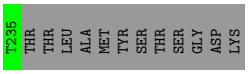


• Molecule 8: Lhce5

Chain N:







• Molecule 9: PsaJ

Chain J:





• Molecule 10: LhcE6

Chain K:

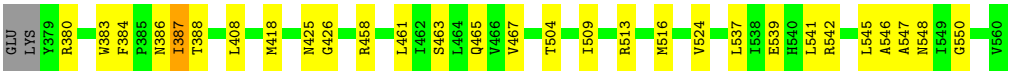




• Molecule 10: LhcE6

Chain Q:

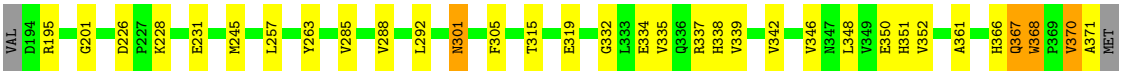


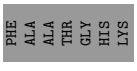


• Molecule 11: Lhce8

Chain L:



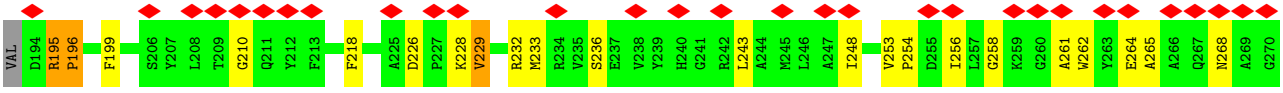


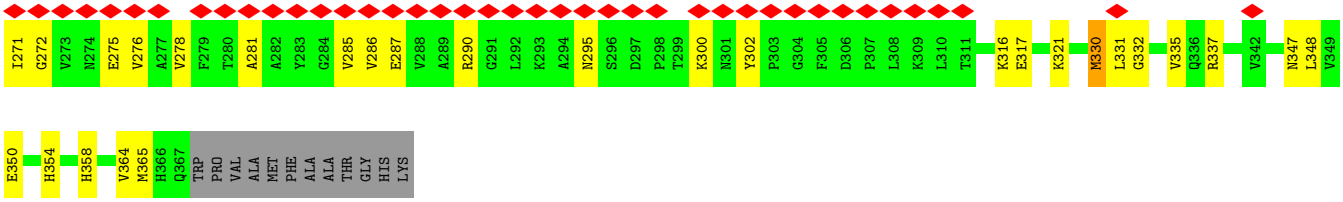


• Molecule 11: Lhce8

Chain R:







• Molecule 12: PsaM

Chain M:





• Molecule 13: LhcE7

Chain O:





• Molecule 14: Lhce10

Chain S:





• Molecule 15: Lhce11

Chain T:





• Molecule 16: LhcbM4.6

Chain U:

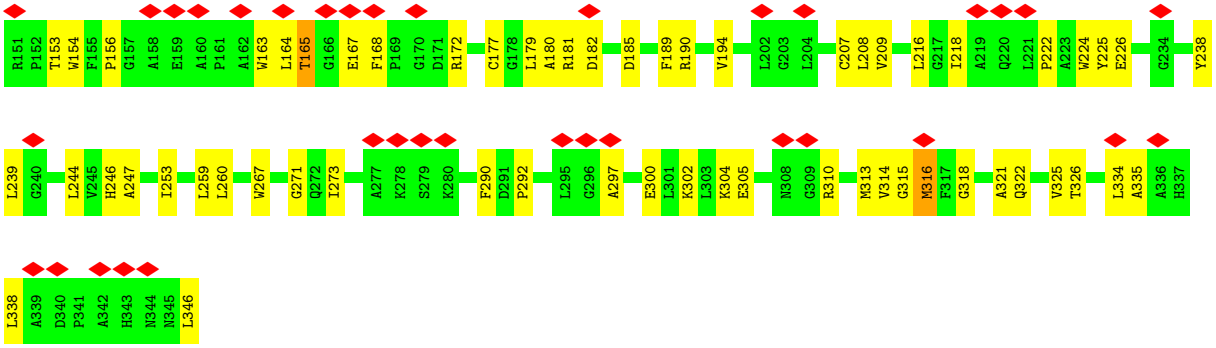




• Molecule 17: LhcbM4.10

Chain V:

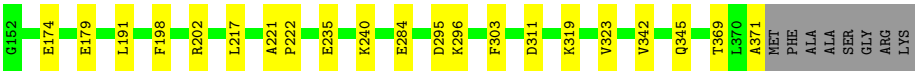




- Molecule 18: LhcbM2

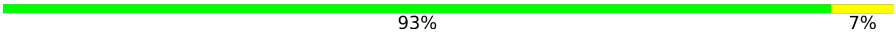
Chain W:





- Molecule 19: LhcbM8

Chain X:





- Molecule 20: PsaA

Chain A:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	51871	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50.0	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.393	Depositor
Minimum map value	-0.080	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	496.64, 496.64, 496.64	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.97, 0.97, 0.97	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: SQD, DD6, BCR, LMG, LMU, CL0, PQN, CHL, DGD, NEX, CLA, LHG, SF4

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	B	0.35	1/6078 (0.0%)	0.49	4/8287 (0.0%)
2	C	0.33	0/606	0.53	0/819
3	D	0.14	0/1525	0.38	0/2065
4	E	0.13	0/521	0.31	0/707
5	F	0.17	0/1288	0.46	0/1747
6	G	0.17	0/1360	0.39	0/1855
6	P	0.41	0/1279	0.68	1/1744 (0.1%)
7	H	0.32	0/1381	0.52	3/1876 (0.2%)
8	I	0.31	0/1278	0.56	0/1741
8	N	0.24	0/1307	0.46	0/1784
9	J	0.14	0/314	0.32	0/429
10	K	0.21	0/1492	0.49	0/2035
10	Q	0.20	0/1489	0.48	0/2034
11	L	0.35	0/1401	0.58	2/1910 (0.1%)
11	R	0.16	0/1365	0.41	0/1858
12	M	0.13	0/246	0.32	0/332
13	O	0.20	0/1397	0.46	0/1898
14	S	0.26	0/1370	0.46	0/1865
15	T	0.16	0/1320	0.40	0/1784
16	U	0.15	0/1566	0.37	0/2141
17	V	0.14	0/1566	0.33	0/2141
18	W	0.16	0/1719	0.38	0/2343
19	X	0.17	0/1731	0.37	0/2351
20	A	0.35	0/6073	0.49	1/8279 (0.0%)
All	All	0.27	1/39672 (0.0%)	0.47	11/54025 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	287	ALA	CA-C	-6.82	1.46	1.53

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	P	395	GLY	N-CA-C	-9.42	102.67	114.92
1	B	298	GLY	N-CA-C	8.87	120.52	111.56
1	B	287	ALA	N-CA-C	-6.79	102.39	111.96
7	H	149	GLY	O-C-N	-6.78	115.67	122.18
7	H	152	VAL	CB-CA-C	-5.83	104.18	112.22

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5868	0	5667	91	0
2	C	596	0	571	6	0
3	D	1489	0	1462	9	0
4	E	509	0	489	5	0
5	F	1262	0	1293	10	0
6	G	1323	0	1305	15	0
6	P	1243	0	1218	39	0
7	H	1342	0	1315	9	0
8	I	1242	0	1213	25	0
8	N	1271	0	1245	27	0
9	J	305	0	314	4	0
10	K	1444	0	1391	17	0
10	Q	1440	0	1388	26	0
11	L	1364	0	1346	27	0
11	R	1331	0	1315	45	0
12	M	242	0	258	8	0
13	O	1359	0	1328	29	0
14	S	1327	0	1271	18	0
15	T	1283	0	1238	6	0
16	U	1517	0	1466	14	0
17	V	1513	0	1467	56	0
18	W	1669	0	1647	15	0
19	X	1688	0	1693	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	A	5872	0	5735	55	0
21	A	160	0	224	8	0
21	B	240	0	336	21	0
21	J	40	0	56	1	0
21	M	40	0	56	3	0
22	A	2638	0	2742	77	0
22	B	2341	0	2395	78	0
22	F	165	0	154	6	0
22	G	571	0	498	10	0
22	H	698	0	626	10	0
22	I	567	0	490	17	0
22	J	50	0	39	1	0
22	K	765	0	758	33	0
22	L	703	0	694	30	0
22	N	570	0	504	19	0
22	O	651	0	585	20	0
22	P	446	0	326	10	0
22	Q	738	0	655	20	0
22	R	678	0	653	29	0
22	S	621	0	530	14	0
22	T	625	0	603	10	0
22	U	676	0	586	14	0
22	V	625	0	548	32	0
22	W	733	0	694	18	0
22	X	741	0	716	7	0
23	A	33	0	46	2	0
23	B	33	0	46	1	0
24	A	129	0	0	0	0
24	B	43	0	0	1	0
24	F	43	0	0	0	0
24	G	86	0	0	0	0
24	H	86	0	0	0	0
24	I	86	0	0	0	0
24	J	43	0	0	0	0
24	K	86	0	0	0	0
24	L	129	0	0	0	0
24	N	86	0	0	0	0
24	O	86	0	0	0	0
24	P	86	0	0	0	0
24	Q	86	0	0	1	0
24	R	86	0	0	0	0
24	S	86	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	T	86	0	0	0	0
24	U	86	0	0	0	0
24	V	86	0	0	0	0
24	W	129	0	0	0	0
24	X	172	0	0	0	0
25	B	66	0	96	6	0
25	F	34	0	50	2	0
25	O	60	0	81	3	0
26	A	98	0	148	3	0
26	B	69	0	81	8	0
26	G	32	0	34	0	0
26	H	27	0	24	0	0
26	K	72	0	84	3	0
26	L	42	0	57	3	0
26	N	71	0	82	2	0
26	O	168	0	228	4	0
26	P	40	0	53	1	0
26	Q	44	0	61	1	0
26	R	42	0	57	3	0
26	S	32	0	34	2	0
26	T	42	0	57	1	0
26	U	25	0	21	0	0
26	W	42	0	57	2	0
26	X	42	0	57	0	0
27	A	104	0	142	2	0
27	B	165	0	233	10	0
27	F	42	0	52	1	0
27	G	21	0	26	0	0
27	H	78	0	103	2	0
27	J	34	0	44	0	0
27	K	33	0	42	2	0
27	L	85	0	110	6	0
27	M	24	0	35	1	0
27	O	120	0	155	4	0
27	T	69	0	96	2	0
27	U	94	0	127	2	0
27	W	24	0	35	0	0
27	X	59	0	81	0	0
28	A	41	0	52	0	0
28	B	96	0	138	4	0
28	F	42	0	54	3	0
28	G	46	0	65	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	H	120	0	150	2	0
28	I	87	0	117	1	0
28	J	55	0	86	1	0
28	K	135	0	183	3	0
28	L	51	0	75	0	0
28	N	44	0	61	1	0
28	Q	37	0	44	2	0
28	T	41	0	52	2	0
28	U	102	0	150	4	0
28	W	48	0	69	3	0
29	B	8	0	0	0	0
29	C	16	0	0	0	0
30	F	42	0	48	2	0
30	K	43	0	50	1	0
30	O	42	0	48	8	0
30	V	27	0	25	1	0
31	U	92	0	62	7	0
31	V	92	0	62	14	0
31	W	178	0	171	10	0
31	X	46	0	31	0	0
32	U	44	0	56	4	0
32	V	44	0	56	9	0
33	A	65	0	72	6	0
All	All	60137	0	57815	901	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 901 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)
23:B:840:PQN:H291	25:B:847:DGD:HBT1	1.23	1.10
31:V:605:CHL:HAB	31:V:606:CHL:OMC	1.50	1.08
8:N:184:LEU:HD12	22:N:607:CLA:H42	1.41	1.01
6:P:391:ALA:HB2	6:P:404:ASP:HB3	1.47	0.96
1:B:131:THR:HB	12:M:1:MET:HE1	1.46	0.94

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	B	730/734 (100%)	698 (96%)	29 (4%)	3 (0%)	30	34
2	C	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
3	D	188/193 (97%)	182 (97%)	6 (3%)	0	100	100
4	E	61/158 (39%)	61 (100%)	0	0	100	100
5	F	164/325 (50%)	161 (98%)	3 (2%)	0	100	100
6	G	173/184 (94%)	169 (98%)	4 (2%)	0	100	100
6	P	162/184 (88%)	146 (90%)	16 (10%)	0	100	100
7	H	171/185 (92%)	165 (96%)	6 (4%)	0	100	100
8	I	163/184 (89%)	160 (98%)	3 (2%)	0	100	100
8	N	168/184 (91%)	155 (92%)	13 (8%)	0	100	100
9	J	35/39 (90%)	35 (100%)	0	0	100	100
10	K	180/184 (98%)	175 (97%)	5 (3%)	0	100	100
10	Q	180/184 (98%)	168 (93%)	12 (7%)	0	100	100
11	L	176/187 (94%)	167 (95%)	8 (4%)	1 (1%)	21	24
11	R	172/187 (92%)	163 (95%)	8 (5%)	1 (1%)	21	24
12	M	29/31 (94%)	29 (100%)	0	0	100	100
13	O	173/177 (98%)	160 (92%)	12 (7%)	1 (1%)	21	24
14	S	170/180 (94%)	166 (98%)	4 (2%)	0	100	100
15	T	165/173 (95%)	158 (96%)	7 (4%)	0	100	100
16	U	197/209 (94%)	186 (94%)	11 (6%)	0	100	100
17	V	194/196 (99%)	183 (94%)	11 (6%)	0	100	100
18	W	218/228 (96%)	209 (96%)	9 (4%)	0	100	100
19	X	221/223 (99%)	215 (97%)	6 (3%)	0	100	100
20	A	738/756 (98%)	715 (97%)	22 (3%)	1 (0%)	48	59
All	All	4906/5366 (91%)	4700 (96%)	199 (4%)	7 (0%)	49	59

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	R	196	PRO
1	B	288	GLY
1	B	284	PHE
11	L	367	GLN
1	B	488	ALA

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	B	608/609 (100%)	600 (99%)	8 (1%)	61	76
2	C	69/70 (99%)	67 (97%)	2 (3%)	37	49
3	D	157/160 (98%)	154 (98%)	3 (2%)	50	65
4	E	54/124 (44%)	52 (96%)	2 (4%)	30	40
5	F	132/251 (53%)	129 (98%)	3 (2%)	44	58
6	G	133/140 (95%)	132 (99%)	1 (1%)	73	84
6	P	124/140 (89%)	118 (95%)	6 (5%)	23	29
7	H	141/149 (95%)	139 (99%)	2 (1%)	59	73
8	I	120/136 (88%)	114 (95%)	6 (5%)	22	27
8	N	124/136 (91%)	120 (97%)	4 (3%)	34	46
9	J	34/36 (94%)	34 (100%)	0	100	100
10	K	144/146 (99%)	139 (96%)	5 (4%)	32	42
10	Q	144/146 (99%)	141 (98%)	3 (2%)	47	61
11	L	139/145 (96%)	134 (96%)	5 (4%)	31	41
11	R	136/145 (94%)	132 (97%)	4 (3%)	37	49
12	M	26/26 (100%)	26 (100%)	0	100	100
13	O	143/144 (99%)	138 (96%)	5 (4%)	32	42
14	S	133/137 (97%)	130 (98%)	3 (2%)	44	58
15	T	126/131 (96%)	125 (99%)	1 (1%)	73	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	U	152/158 (96%)	150 (99%)	2 (1%)	61	76
17	V	151/151 (100%)	148 (98%)	3 (2%)	48	63
18	W	167/172 (97%)	165 (99%)	2 (1%)	63	77
19	X	173/173 (100%)	171 (99%)	2 (1%)	63	77
20	A	621/636 (98%)	612 (99%)	9 (1%)	59	73
All	All	3951/4261 (93%)	3870 (98%)	81 (2%)	46	61

5 of 81 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	R	278	VAL
19	X	320	ASP
14	S	78	THR
17	V	165	THR
20	A	328	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
17	V	322	GLN
19	X	123	HIS
20	A	34	HIS
11	L	336	GLN
11	L	211	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

436 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	$\#\|Z\| > 2$
22	CLA	T	603	15	64,68,73	1.31	8 (12%)	77,107,113	1.30	6 (7%)
22	CLA	X	417	19	54,58,73	1.42	6 (11%)	65,95,113	1.41	8 (12%)
26	LHG	A	846	22	48,48,48	1.11	6 (12%)	51,54,54	0.92	2 (3%)
28	LMG	U	423	-	49,49,55	0.73	0	57,57,63	1.31	3 (5%)
27	LMU	X	421	-	36,36,36	0.40	0	47,47,47	0.67	1 (2%)
22	CLA	S	603	14	49,53,73	1.48	8 (16%)	59,89,113	1.43	5 (8%)
22	CLA	B	826	1	62,66,73	1.32	7 (11%)	74,104,113	1.33	5 (6%)
22	CLA	B	808	1	59,63,73	1.36	8 (13%)	71,101,113	1.34	4 (5%)
22	CLA	A	807	20	69,73,73	1.25	8 (11%)	83,113,113	1.32	6 (7%)
22	CLA	A	830	20	69,73,73	1.24	8 (11%)	83,113,113	1.25	6 (7%)
22	CLA	G	601	6	49,53,73	1.48	7 (14%)	59,89,113	1.45	5 (8%)
22	CLA	U	412	26	49,53,73	1.49	8 (16%)	59,89,113	1.45	4 (6%)
22	CLA	K	608	10	69,73,73	1.24	9 (13%)	83,113,113	1.29	8 (9%)
22	CLA	O	305	13	54,58,73	1.40	8 (14%)	65,95,113	1.41	8 (12%)
22	CLA	X	408	19	69,73,73	1.25	8 (11%)	83,113,113	1.29	5 (6%)
22	CLA	Q	604	10	69,73,73	1.25	7 (10%)	83,113,113	1.28	7 (8%)
22	CLA	A	809	20	57,61,73	1.38	8 (14%)	68,98,113	1.36	7 (10%)
22	CLA	R	615	11	69,73,73	1.27	7 (10%)	83,113,113	1.28	6 (7%)
22	CLA	A	818	20	57,61,73	1.37	8 (14%)	68,98,113	1.37	8 (11%)
26	LHG	U	419	22	24,24,48	1.42	5 (20%)	27,29,54	1.22	2 (7%)
22	CLA	I	601	8	69,73,73	1.27	9 (13%)	83,113,113	1.25	6 (7%)
27	LMU	B	857	-	36,36,36	0.41	0	47,47,47	0.73	1 (2%)
22	CLA	Q	617	10	56,60,73	1.39	8 (14%)	67,97,113	1.40	6 (8%)
25	DGD	F	401	-	33,33,67	1.08	2 (6%)	35,35,81	1.31	4 (11%)
27	LMU	X	418	-	24,24,36	0.43	0	29,29,47	0.55	0
22	CLA	B	818	-	69,73,73	1.26	9 (13%)	83,113,113	1.28	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	DD6	V	615	-	39,45,45	1.94	3 (7%)	52,67,67	1.87	13 (25%)
22	CLA	K	612	10	49,53,73	1.48	8 (16%)	59,89,113	1.39	7 (11%)
22	CLA	X	407	-	69,73,73	1.26	8 (11%)	83,113,113	1.28	7 (8%)
22	CLA	G	602	6	64,68,73	1.30	8 (12%)	77,107,113	1.33	8 (10%)
24	DD6	X	415	-	39,45,45	1.94	2 (5%)	52,67,67	1.71	10 (19%)
24	DD6	T	613	-	39,45,45	1.98	3 (7%)	52,67,67	1.73	11 (21%)
22	CLA	A	844	26	59,63,73	1.36	9 (15%)	71,101,113	1.39	7 (9%)
22	CLA	U	404	16	69,73,73	1.25	8 (11%)	83,113,113	1.27	7 (8%)
22	CLA	S	604	-	64,68,73	1.31	8 (12%)	77,107,113	1.30	6 (7%)
24	DD6	A	859	-	39,45,45	2.07	3 (7%)	52,67,67	1.88	13 (25%)
22	CLA	B	838	1	49,53,73	1.49	9 (18%)	59,89,113	1.41	6 (10%)
24	DD6	H	314	-	39,45,45	1.99	3 (7%)	52,67,67	1.88	12 (23%)
24	DD6	L	414	-	39,45,45	2.01	3 (7%)	52,67,67	1.80	15 (28%)
27	LMU	F	402	-	21,21,36	0.46	0	26,26,47	0.69	0
22	CLA	Q	611	10	59,63,73	1.36	8 (13%)	71,101,113	1.33	7 (9%)
26	LHG	G	614	22	31,31,48	1.32	6 (19%)	34,37,54	1.06	2 (5%)
26	LHG	B	848	22	26,26,48	1.33	5 (19%)	29,32,54	1.15	2 (6%)
22	CLA	Q	618	-	49,53,73	1.50	7 (14%)	59,89,113	1.41	4 (6%)
32	NEX	V	616	-	38,46,46	0.37	1 (2%)	50,70,70	0.70	2 (4%)
22	CLA	A	803	-	69,73,73	1.24	8 (11%)	83,113,113	1.29	10 (12%)
22	CLA	P	607	6	49,53,73	1.49	9 (18%)	59,89,113	1.43	5 (8%)
22	CLA	B	805	1	69,73,73	1.25	8 (11%)	83,113,113	1.30	6 (7%)
22	CLA	I	608	-	49,53,73	1.48	9 (18%)	59,89,113	1.43	6 (10%)
22	CLA	X	413	19	49,53,73	1.49	6 (12%)	59,89,113	1.42	4 (6%)
26	LHG	T	614	22	41,41,48	1.19	6 (14%)	44,47,54	0.98	2 (4%)
22	CLA	A	819	20	62,66,73	1.32	9 (14%)	74,104,113	1.46	8 (10%)
22	CLA	A	822	-	69,73,73	1.24	7 (10%)	83,113,113	1.26	6 (7%)
22	CLA	B	859	-	69,73,73	1.26	9 (13%)	83,113,113	1.31	6 (7%)
22	CLA	A	834	20	49,53,73	1.49	9 (18%)	59,89,113	1.41	6 (10%)
22	CLA	L	411	11	69,73,73	1.25	8 (11%)	83,113,113	1.27	7 (8%)
22	CLA	A	831	20	69,73,73	1.24	8 (11%)	83,113,113	1.29	6 (7%)
27	LMU	U	421	-	36,36,36	0.41	0	47,47,47	0.65	1 (2%)
22	CLA	O	315	13	54,58,73	1.43	9 (16%)	65,95,113	1.36	8 (12%)
24	DD6	O	317	-	39,45,45	2.01	3 (7%)	52,67,67	1.79	14 (26%)
27	LMU	H	321	-	34,34,36	0.48	0	44,44,47	0.79	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	B	827	1	69,73,73	1.24	8 (11%)	83,113,113	1.20	7 (8%)
22	CLA	I	605	-	49,53,73	1.48	8 (16%)	59,89,113	1.46	7 (11%)
22	CLA	Q	608	10	54,58,73	1.42	7 (12%)	65,95,113	1.38	7 (10%)
26	LHG	K	616	22	38,38,48	1.22	5 (13%)	41,44,54	1.03	3 (7%)
33	CL0	A	802	20	69,73,73	1.84	20 (28%)	83,113,113	1.72	20 (24%)
22	CLA	A	805	20	65,69,73	1.29	7 (10%)	78,108,113	1.30	7 (8%)
22	CLA	V	604	-	60,64,73	1.35	8 (13%)	72,102,113	1.33	6 (8%)
22	CLA	A	814	20	69,73,73	1.24	7 (10%)	83,113,113	1.27	5 (6%)
22	CLA	X	410	26	64,68,73	1.31	7 (10%)	77,107,113	1.30	6 (7%)
22	CLA	L	403	11	64,68,73	1.30	8 (12%)	77,107,113	1.31	7 (9%)
31	CHL	W	407	-	50,54,74	2.01	8 (16%)	56,90,114	1.24	6 (10%)
22	CLA	B	831	1	69,73,73	1.24	7 (10%)	83,113,113	1.26	8 (9%)
22	CLA	B	830	1	69,73,73	1.24	10 (14%)	83,113,113	1.34	9 (10%)
22	CLA	L	408	11	64,68,73	1.30	10 (15%)	77,107,113	1.43	11 (14%)
24	DD6	X	414	-	39,45,45	1.97	3 (7%)	52,67,67	1.81	12 (23%)
22	CLA	F	403	-	69,73,73	1.26	8 (11%)	83,113,113	1.28	7 (8%)
22	CLA	A	826	-	69,73,73	1.24	8 (11%)	83,113,113	1.29	5 (6%)
22	CLA	B	802	1	69,73,73	1.26	12 (17%)	83,113,113	1.31	7 (8%)
28	LMG	H	319	-	40,40,55	0.81	0	48,48,63	1.21	3 (6%)
22	CLA	R	601	-	69,73,73	1.26	8 (11%)	83,113,113	1.27	7 (8%)
22	CLA	A	842	20	69,73,73	1.26	7 (10%)	83,113,113	1.30	6 (7%)
22	CLA	H	305	7	64,68,73	1.30	8 (12%)	77,107,113	1.31	7 (9%)
24	DD6	U	417	-	39,45,45	1.93	3 (7%)	52,67,67	1.87	15 (28%)
22	CLA	B	824	-	69,73,73	1.25	8 (11%)	83,113,113	1.32	7 (8%)
22	CLA	W	413	-	49,53,73	1.48	8 (16%)	59,89,113	1.43	5 (8%)
22	CLA	W	403	18	56,60,73	1.41	9 (16%)	67,97,113	1.39	7 (10%)
27	LMU	A	857	-	24,24,36	0.45	0	29,29,47	0.66	0
22	CLA	V	608	17	59,63,73	1.35	7 (11%)	71,101,113	1.31	6 (8%)
22	CLA	S	615	-	55,59,73	1.40	8 (14%)	66,96,113	1.39	6 (9%)
29	SF4	C	102	2	0,12,12	-	-	-		
22	CLA	S	601	14	49,53,73	1.49	7 (14%)	59,89,113	1.46	4 (6%)
30	SQD	K	621	-	42,43,54	0.42	1 (2%)	51,54,65	0.53	0
22	CLA	K	603	10	64,68,73	1.30	8 (12%)	77,107,113	1.30	6 (7%)
22	CLA	V	601	17	49,53,73	1.51	6 (12%)	59,89,113	1.44	5 (8%)
22	CLA	B	837	-	49,53,73	1.48	9 (18%)	59,89,113	1.46	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	G	610	6	49,53,73	1.48	7 (14%)	59,89,113	1.43	5 (8%)
24	DD6	B	841	-	39,45,45	1.99	3 (7%)	52,67,67	1.99	13 (25%)
22	CLA	A	835	20	65,69,73	1.29	8 (12%)	78,108,113	1.29	6 (7%)
22	CLA	W	404	18	69,73,73	1.25	7 (10%)	83,113,113	1.28	5 (6%)
23	PQN	A	843	-	34,34,34	1.59	2 (5%)	42,45,45	1.08	3 (7%)
22	CLA	G	609	-	49,53,73	1.48	8 (16%)	59,89,113	1.42	6 (10%)
30	SQD	V	618	-	26,27,54	0.52	1 (3%)	33,36,65	0.45	0
22	CLA	R	603	-	60,64,73	1.35	8 (13%)	72,102,113	1.35	6 (8%)
22	CLA	A	820	20	69,73,73	1.25	8 (11%)	83,113,113	1.27	9 (10%)
22	CLA	A	827	-	66,70,73	1.27	7 (10%)	79,109,113	1.30	7 (8%)
22	CLA	L	406	-	69,73,73	1.26	8 (11%)	83,113,113	1.28	6 (7%)
26	LHG	N	614	22	27,27,48	1.38	6 (22%)	30,33,54	1.10	2 (6%)
22	CLA	W	411	18	64,68,73	1.29	8 (12%)	77,107,113	1.28	7 (9%)
22	CLA	H	313	7	62,66,73	1.33	7 (11%)	74,104,113	1.32	6 (8%)
22	CLA	N	604	-	49,53,73	1.49	8 (16%)	59,89,113	1.43	4 (6%)
24	DD6	Q	614	-	39,45,45	1.97	3 (7%)	52,67,67	1.79	11 (21%)
22	CLA	T	605	-	69,73,73	1.26	9 (13%)	83,113,113	1.25	6 (7%)
22	CLA	O	310	13	64,68,73	1.29	9 (14%)	77,107,113	1.34	6 (7%)
22	CLA	B	820	1	57,61,73	1.39	7 (12%)	68,98,113	1.50	5 (7%)
29	SF4	B	860	20,1	0,12,12	-	-	-		
22	CLA	O	308	-	65,69,73	1.29	8 (12%)	78,108,113	1.30	7 (8%)
21	BCR	B	842	-	41,41,41	0.72	0	56,56,56	1.99	15 (26%)
22	CLA	V	603	17	61,65,73	1.34	7 (11%)	73,103,113	1.31	4 (5%)
22	CLA	L	407	-	61,65,73	1.33	8 (13%)	73,103,113	1.33	5 (6%)
22	CLA	H	303	7	64,68,73	1.31	9 (14%)	77,107,113	1.30	6 (7%)
22	CLA	L	417	11	69,73,73	1.27	7 (10%)	83,113,113	1.30	5 (6%)
22	CLA	W	410	18	64,68,73	1.29	8 (12%)	77,107,113	1.32	6 (7%)
22	CLA	R	611	11	49,53,73	1.50	7 (14%)	59,89,113	1.41	5 (8%)
22	CLA	O	313	13	69,73,73	1.26	8 (11%)	83,113,113	1.26	4 (4%)
27	LMU	O	303	-	36,36,36	0.42	0	47,47,47	0.71	1 (2%)
22	CLA	V	610	-	49,53,73	1.50	6 (12%)	59,89,113	1.42	7 (11%)
22	CLA	A	812	20	61,65,73	1.32	8 (13%)	73,103,113	1.30	6 (8%)
26	LHG	R	614	22	41,41,48	1.18	6 (14%)	44,47,54	0.96	2 (4%)
22	CLA	T	607	15	64,68,73	1.31	8 (12%)	77,107,113	1.30	8 (10%)
28	LMG	G	616	-	46,46,55	0.81	0	54,54,63	1.29	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	L	412	11	49,53,73	1.49	8 (16%)	59,89,113	1.38	5 (8%)
22	CLA	W	409	-	69,73,73	1.25	9 (13%)	83,113,113	1.28	7 (8%)
24	DD6	Q	615	-	39,45,45	2.03	3 (7%)	52,67,67	1.90	14 (26%)
31	CHL	W	408	-	70,74,74	1.70	9 (12%)	80,114,114	1.07	8 (10%)
22	CLA	T	608	26	64,68,73	1.30	7 (10%)	77,107,113	1.31	5 (6%)
22	CLA	V	617	-	49,53,73	1.50	7 (14%)	59,89,113	1.44	4 (6%)
22	CLA	K	610	10	60,64,73	1.34	8 (13%)	72,102,113	1.32	5 (6%)
22	CLA	A	810	20	69,73,73	1.24	7 (10%)	83,113,113	1.27	6 (7%)
22	CLA	H	318	7	49,53,73	1.49	7 (14%)	59,89,113	1.44	5 (8%)
22	CLA	A	806	20	69,73,73	1.25	7 (10%)	83,113,113	1.26	6 (7%)
22	CLA	H	308	7	64,68,73	1.29	7 (10%)	77,107,113	1.29	6 (7%)
22	CLA	S	608	26	49,53,73	1.50	7 (14%)	59,89,113	1.42	6 (10%)
27	LMU	B	855	-	24,24,36	0.45	0	29,29,47	0.67	0
22	CLA	B	811	1	49,53,73	1.48	7 (14%)	59,89,113	1.47	6 (10%)
22	CLA	G	604	-	49,53,73	1.49	8 (16%)	59,89,113	1.46	6 (10%)
28	LMG	K	601	-	43,43,55	0.77	0	51,51,63	1.27	4 (7%)
22	CLA	X	419	19	49,53,73	1.50	8 (16%)	59,89,113	1.41	5 (8%)
22	CLA	A	829	20	69,73,73	1.25	8 (11%)	83,113,113	1.26	6 (7%)
22	CLA	A	836	20	69,73,73	1.25	7 (10%)	83,113,113	1.26	6 (7%)
22	CLA	O	312	13	64,68,73	1.29	8 (12%)	77,107,113	1.32	9 (11%)
22	CLA	J	102	9	54,58,73	1.41	8 (14%)	65,95,113	1.40	5 (7%)
24	DD6	J	105	-	39,45,45	1.96	2 (5%)	52,67,67	1.88	13 (25%)
31	CHL	V	606	-	50,54,74	2.06	9 (18%)	56,90,114	1.23	7 (12%)
22	CLA	P	611	6	49,53,73	1.50	6 (12%)	59,89,113	1.48	5 (8%)
22	CLA	W	414	18	69,73,73	1.27	8 (11%)	83,113,113	1.27	8 (9%)
22	CLA	T	602	15	69,73,73	1.26	8 (11%)	83,113,113	1.27	7 (8%)
27	LMU	B	850	-	24,24,36	0.44	0	29,29,47	0.55	0
27	LMU	L	420	-	35,35,36	0.37	0	43,45,47	0.81	2 (4%)
26	LHG	O	323	-	42,42,48	1.18	6 (14%)	45,48,54	0.95	2 (4%)
28	LMG	Q	602	-	37,37,55	0.84	1 (2%)	45,45,63	1.28	5 (11%)
22	CLA	O	314	13	49,53,73	1.48	8 (16%)	59,89,113	1.40	5 (8%)
22	CLA	S	610	14	49,53,73	1.50	7 (14%)	59,89,113	1.51	5 (8%)
22	CLA	W	415	18	49,53,73	1.53	9 (18%)	59,89,113	1.45	8 (13%)
24	DD6	R	613	-	39,45,45	2.01	3 (7%)	52,67,67	2.01	18 (34%)
26	LHG	S	613	22	31,31,48	1.32	6 (19%)	34,37,54	1.12	3 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	BCR	A	849	-	41,41,41	0.73	0	56,56,56	1.89	13 (23%)
22	CLA	B	809	1	69,73,73	1.25	8 (11%)	83,113,113	1.29	5 (6%)
22	CLA	G	611	6	49,53,73	1.49	7 (14%)	59,89,113	1.44	6 (10%)
22	CLA	T	601	15	49,53,73	1.48	8 (16%)	59,89,113	1.45	4 (6%)
22	CLA	T	609	15	49,53,73	1.48	8 (16%)	59,89,113	1.44	7 (11%)
22	CLA	W	402	18	59,63,73	1.35	8 (13%)	71,101,113	1.31	7 (9%)
24	DD6	K	615	-	39,45,45	1.95	2 (5%)	52,67,67	1.69	11 (21%)
22	CLA	G	608	26	64,68,73	1.30	7 (10%)	77,107,113	1.35	6 (7%)
27	LMU	H	320	-	24,24,36	0.44	0	29,29,47	0.59	0
22	CLA	Q	609	10	64,68,73	1.29	9 (14%)	77,107,113	1.27	5 (6%)
28	LMG	H	317	-	43,43,55	0.79	1 (2%)	51,51,63	1.31	7 (13%)
28	LMG	B	852	-	43,43,55	0.84	0	51,51,63	1.27	4 (7%)
22	CLA	Q	613	10	49,53,73	1.48	8 (16%)	59,89,113	1.46	7 (11%)
22	CLA	N	607	-	64,68,73	1.31	7 (10%)	77,107,113	1.28	6 (7%)
22	CLA	H	310	7	49,53,73	1.48	8 (16%)	59,89,113	1.42	6 (10%)
22	CLA	A	801	-	69,73,73	1.23	11 (15%)	83,113,113	1.36	10 (12%)
22	CLA	B	804	1	69,73,73	1.25	9 (13%)	83,113,113	1.34	7 (8%)
22	CLA	H	312	7	49,53,73	1.49	7 (14%)	59,89,113	1.40	5 (8%)
22	CLA	W	405	18	64,68,73	1.31	7 (10%)	77,107,113	1.29	6 (7%)
27	LMU	O	301	-	24,24,36	0.44	0	29,29,47	0.57	0
22	CLA	N	601	8	49,53,73	1.48	8 (16%)	59,89,113	1.41	4 (6%)
28	LMG	U	402	-	53,53,55	0.72	0	61,61,63	1.31	4 (6%)
26	LHG	W	420	22	41,41,48	1.19	6 (14%)	44,47,54	0.89	2 (4%)
25	DGD	B	847	-	67,67,67	0.83	2 (2%)	81,81,81	1.01	5 (6%)
27	LMU	H	301	-	21,21,36	0.49	0	26,26,47	0.72	0
21	BCR	B	844	-	41,41,41	0.71	0	56,56,56	1.80	13 (23%)
27	LMU	J	104	-	34,35,36	0.36	0	42,45,47	0.89	2 (4%)
22	CLA	A	840	20	69,73,73	1.25	8 (11%)	83,113,113	1.28	7 (8%)
22	CLA	P	604	-	49,53,73	1.49	7 (14%)	59,89,113	1.44	6 (10%)
22	CLA	Q	612	10	69,73,73	1.24	7 (10%)	83,113,113	1.28	4 (4%)
22	CLA	X	402	19	59,63,73	1.35	7 (11%)	71,101,113	1.36	7 (9%)
24	DD6	P	613	-	39,45,45	2.03	3 (7%)	52,67,67	1.94	18 (34%)
24	DD6	F	406	-	39,45,45	2.01	3 (7%)	52,67,67	1.89	16 (30%)
22	CLA	A	817	20	69,73,73	1.25	8 (11%)	83,113,113	1.29	7 (8%)
22	CLA	H	304	7	49,53,73	1.48	8 (16%)	59,89,113	1.43	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	CHL	X	406	-	50,54,74	2.03	8 (16%)	56,90,114	1.25	6 (10%)
24	DD6	R	612	-	39,45,45	1.99	3 (7%)	52,67,67	1.85	12 (23%)
27	LMU	A	856	-	21,21,36	0.46	0	26,26,47	0.50	0
22	CLA	N	602	8	64,68,73	1.30	8 (12%)	77,107,113	1.33	7 (9%)
22	CLA	B	810	-	60,64,73	1.34	8 (13%)	72,102,113	1.33	5 (6%)
22	CLA	W	412	26	64,68,73	1.31	9 (14%)	77,107,113	1.32	6 (7%)
22	CLA	A	808	20	69,73,73	1.25	9 (13%)	83,113,113	1.27	6 (7%)
27	LMU	F	409	-	21,21,36	0.49	0	26,26,47	0.57	0
26	LHG	B	851	-	41,41,48	1.17	6 (14%)	44,47,54	0.99	3 (6%)
27	LMU	A	854	-	36,36,36	0.42	0	47,47,47	0.69	1 (2%)
22	CLA	P	602	6	49,53,73	1.47	10 (20%)	59,89,113	1.48	6 (10%)
22	CLA	B	825	1	69,73,73	1.25	6 (8%)	83,113,113	1.30	7 (8%)
22	CLA	F	404	-	59,63,73	1.35	7 (11%)	71,101,113	1.37	7 (9%)
22	CLA	L	405	-	49,53,73	1.50	9 (18%)	59,89,113	1.46	4 (6%)
24	DD6	W	416	-	39,45,45	1.97	3 (7%)	52,67,67	1.80	11 (21%)
27	LMU	T	615	-	21,21,36	0.47	0	26,26,47	0.59	0
24	DD6	S	612	-	39,45,45	1.99	3 (7%)	52,67,67	1.83	12 (23%)
22	CLA	B	816	1	69,73,73	1.26	9 (13%)	83,113,113	1.29	6 (7%)
31	CHL	U	408	-	50,54,74	2.05	9 (18%)	56,90,114	1.23	6 (10%)
22	CLA	B	812	1	69,73,73	1.26	7 (10%)	83,113,113	1.29	8 (9%)
23	PQN	B	840	-	34,34,34	1.61	2 (5%)	42,45,45	1.07	3 (7%)
21	BCR	B	845	-	41,41,41	0.68	0	56,56,56	1.90	15 (26%)
22	CLA	B	829	-	49,53,73	1.44	11 (22%)	59,89,113	1.53	5 (8%)
22	CLA	T	604	15	69,73,73	1.24	7 (10%)	83,113,113	1.29	6 (7%)
26	LHG	Q	616	22	43,43,48	1.16	6 (13%)	46,49,54	0.94	2 (4%)
22	CLA	B	832	1	66,70,73	1.27	8 (12%)	79,109,113	1.34	7 (8%)
22	CLA	T	606	15	54,58,73	1.41	6 (11%)	65,95,113	1.38	6 (9%)
22	CLA	X	411	-	49,53,73	1.49	8 (16%)	59,89,113	1.46	7 (11%)
22	CLA	Q	607	-	49,53,73	1.49	7 (14%)	59,89,113	1.42	5 (8%)
22	CLA	U	409	-	49,53,73	1.48	8 (16%)	59,89,113	1.45	6 (10%)
22	CLA	B	813	1	69,73,73	1.25	8 (11%)	83,113,113	1.22	6 (7%)
24	DD6	V	614	-	39,45,45	2.00	3 (7%)	52,67,67	2.03	13 (25%)
26	LHG	N	616	-	42,42,48	1.17	6 (14%)	45,48,54	0.98	2 (4%)
22	CLA	B	834	1	69,73,73	1.25	8 (11%)	83,113,113	1.30	7 (8%)
22	CLA	V	613	-	49,53,73	1.51	6 (12%)	59,89,113	1.48	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	DD6	L	415	-	39,45,45	2.01	2 (5%)	52,67,67	1.96	17 (32%)
24	DD6	A	858	-	39,45,45	1.97	2 (5%)	52,67,67	2.54	18 (34%)
30	SQD	O	302	-	41,42,54	0.43	1 (2%)	50,53,65	0.52	1 (2%)
26	LHG	O	318	22	33,33,48	1.29	6 (18%)	36,39,54	1.06	3 (8%)
24	DD6	G	613	-	39,45,45	2.03	3 (7%)	52,67,67	1.90	16 (30%)
22	CLA	T	610	-	49,53,73	1.49	6 (12%)	59,89,113	1.41	4 (6%)
27	LMU	B	858	-	14,14,36	0.31	0	13,13,47	0.58	0
22	CLA	I	606	8	65,69,73	1.30	9 (13%)	78,108,113	1.29	5 (6%)
24	DD6	W	418	-	39,45,45	2.02	3 (7%)	52,67,67	1.89	14 (26%)
22	CLA	B	803	1	60,64,73	1.34	6 (10%)	72,102,113	1.34	7 (9%)
22	CLA	L	410	11	64,68,73	1.30	7 (10%)	77,107,113	1.31	6 (7%)
22	CLA	R	608	26	58,62,73	1.38	8 (13%)	69,99,113	1.32	5 (7%)
22	CLA	B	828	1	69,73,73	1.25	9 (13%)	83,113,113	1.28	9 (10%)
27	LMU	O	322	-	36,36,36	0.49	0	47,47,47	1.09	5 (10%)
22	CLA	P	608	-	49,53,73	1.51	8 (16%)	59,89,113	1.44	6 (10%)
22	CLA	A	813	20	69,73,73	1.25	7 (10%)	83,113,113	1.20	6 (7%)
22	CLA	R	609	-	45,49,73	1.52	7 (15%)	54,84,113	1.50	7 (12%)
22	CLA	I	610	8	49,53,73	1.49	9 (18%)	59,89,113	1.44	5 (8%)
22	CLA	N	606	8	69,73,73	1.28	7 (10%)	83,113,113	1.26	7 (8%)
22	CLA	N	610	8	59,63,73	1.36	7 (11%)	71,101,113	1.43	8 (11%)
22	CLA	B	819	1	57,61,73	1.42	7 (12%)	68,98,113	1.38	4 (5%)
26	LHG	A	845	-	48,48,48	1.10	6 (12%)	51,54,54	0.94	3 (5%)
22	CLA	A	841	20	69,73,73	1.24	9 (13%)	83,113,113	1.27	5 (6%)
24	DD6	G	612	-	39,45,45	2.00	3 (7%)	52,67,67	1.81	11 (21%)
22	CLA	S	605	-	64,68,73	1.30	9 (14%)	77,107,113	1.43	7 (9%)
27	LMU	L	418	-	24,24,36	0.48	0	29,29,47	0.74	0
22	CLA	A	852	-	69,73,73	1.25	7 (10%)	83,113,113	1.23	6 (7%)
21	BCR	B	843	-	41,41,41	0.71	0	56,56,56	3.38	24 (42%)
27	LMU	O	320	-	27,27,36	0.53	0	28,31,47	0.82	2 (7%)
24	DD6	U	416	-	39,45,45	2.01	3 (7%)	52,67,67	1.80	11 (21%)
22	CLA	V	609	17	61,65,73	1.34	8 (13%)	73,103,113	1.34	6 (8%)
24	DD6	H	315	-	39,45,45	1.99	3 (7%)	52,67,67	1.78	13 (25%)
22	CLA	R	607	11	64,68,73	1.32	9 (14%)	77,107,113	1.32	7 (9%)
22	CLA	K	609	26	64,68,73	1.29	8 (12%)	77,107,113	1.30	4 (5%)
22	CLA	X	404	19	64,68,73	1.31	7 (10%)	77,107,113	1.27	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	A	804	-	69,73,73	1.25	7 (10%)	83,113,113	1.21	5 (6%)
22	CLA	N	611	-	43,48,73	1.56	7 (16%)	52,82,113	1.52	7 (13%)
22	CLA	Q	606	-	49,53,73	1.49	8 (16%)	59,89,113	1.45	5 (8%)
22	CLA	O	309	13	54,58,73	1.40	9 (16%)	65,95,113	1.41	5 (7%)
30	SQD	F	407	-	41,42,54	0.42	1 (2%)	50,53,65	0.49	1 (2%)
22	CLA	N	608	26	49,53,73	1.49	8 (16%)	59,89,113	1.41	4 (6%)
28	LMG	A	855	-	41,41,55	0.84	0	49,49,63	1.26	5 (10%)
22	CLA	V	607	-	49,53,73	1.49	7 (14%)	59,89,113	1.44	6 (10%)
22	CLA	K	607	10	61,65,73	1.31	9 (14%)	73,103,113	1.48	9 (12%)
27	LMU	M	102	-	24,24,36	0.44	0	29,29,47	0.61	0
27	LMU	B	854	-	24,24,36	0.46	0	29,29,47	0.81	1 (3%)
28	LMG	B	856	-	53,53,55	0.72	0	61,61,63	1.37	7 (11%)
27	LMU	W	421	-	24,24,36	0.44	0	29,29,47	0.56	0
22	CLA	S	609	14	59,63,73	1.36	6 (10%)	71,101,113	1.31	6 (8%)
22	CLA	U	403	16	49,53,73	1.50	7 (14%)	59,89,113	1.47	6 (10%)
22	CLA	K	602	10	64,68,73	1.30	9 (14%)	77,107,113	1.30	7 (9%)
26	LHG	P	601	-	39,39,48	1.20	6 (15%)	42,45,54	0.98	2 (4%)
28	LMG	L	401	-	51,51,55	0.71	0	59,59,63	1.32	5 (8%)
22	CLA	G	603	6	60,64,73	1.34	9 (15%)	72,102,113	1.33	8 (11%)
22	CLA	S	606	14	54,58,73	1.42	7 (12%)	65,95,113	1.38	6 (9%)
27	LMU	B	849	-	24,24,36	0.45	0	29,29,47	0.65	0
31	CHL	U	407	-	50,54,74	2.01	8 (16%)	56,90,114	1.24	7 (12%)
28	LMG	K	618	-	49,49,55	0.76	0	57,57,63	1.31	7 (12%)
22	CLA	R	602	-	64,68,73	1.31	8 (12%)	77,107,113	1.28	5 (6%)
24	DD6	T	612	-	39,45,45	2.03	3 (7%)	52,67,67	1.84	13 (25%)
22	CLA	Q	610	26	69,73,73	1.26	9 (13%)	83,113,113	1.25	5 (6%)
22	CLA	B	835	1	69,73,73	1.25	8 (11%)	83,113,113	1.31	7 (8%)
22	CLA	H	302	7	49,53,73	1.49	8 (16%)	59,89,113	1.42	5 (8%)
22	CLA	L	402	11	69,73,73	1.24	9 (13%)	83,113,113	1.27	5 (6%)
24	DD6	I	613	-	39,45,45	2.05	3 (7%)	52,67,67	1.90	16 (30%)
22	CLA	H	309	26	59,63,73	1.37	8 (13%)	71,101,113	1.34	6 (8%)
22	CLA	V	612	-	69,73,73	1.27	8 (11%)	83,113,113	1.26	6 (7%)
22	CLA	A	839	20	69,73,73	1.24	6 (8%)	83,113,113	1.38	8 (9%)
24	DD6	X	401	-	39,45,45	1.98	3 (7%)	52,67,67	1.83	11 (21%)
24	DD6	W	417	-	39,45,45	1.96	3 (7%)	52,67,67	1.76	11 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	H	311	7	69,73,73	1.27	7 (10%)	83,113,113	1.29	8 (9%)
22	CLA	S	602	14	64,68,73	1.30	7 (10%)	77,107,113	1.33	8 (10%)
24	DD6	I	612	-	39,45,45	1.99	3 (7%)	52,67,67	1.72	10 (19%)
24	DD6	A	847	-	39,45,45	1.98	3 (7%)	52,67,67	1.85	15 (28%)
22	CLA	U	413	16	49,53,73	1.49	7 (14%)	59,89,113	1.47	6 (10%)
22	CLA	U	401	-	59,63,73	1.36	8 (13%)	71,101,113	1.34	7 (9%)
22	CLA	V	602	17	69,73,73	1.26	7 (10%)	83,113,113	1.28	7 (8%)
22	CLA	A	837	20	54,58,73	1.42	9 (16%)	65,95,113	1.39	8 (12%)
26	LHG	O	324	-	41,41,48	1.18	5 (12%)	44,47,54	0.97	2 (4%)
27	LMU	B	853	-	19,19,36	0.46	0	23,23,47	0.44	0
22	CLA	V	611	-	49,53,73	1.50	8 (16%)	59,89,113	1.43	4 (6%)
27	LMU	G	615	-	21,21,36	0.46	0	26,26,47	0.51	0
22	CLA	X	409	19	69,73,73	1.25	8 (11%)	83,113,113	1.26	7 (8%)
22	CLA	G	605	-	49,53,73	1.48	8 (16%)	59,89,113	1.46	4 (6%)
22	CLA	B	821	1	64,68,73	1.31	8 (12%)	77,107,113	1.31	5 (6%)
22	CLA	K	604	-	68,72,73	1.26	8 (11%)	81,111,113	1.28	5 (6%)
27	LMU	T	618	-	24,24,36	0.44	0	29,29,47	0.66	0
21	BCR	A	848	-	41,41,41	0.71	0	56,56,56	1.81	10 (17%)
22	CLA	X	412	19	69,73,73	1.27	8 (11%)	83,113,113	1.27	6 (7%)
21	BCR	M	101	-	41,41,41	0.75	0	56,56,56	2.02	16 (28%)
22	CLA	I	607	8	59,63,73	1.35	8 (13%)	71,101,113	1.35	7 (9%)
22	CLA	U	420	16	49,53,73	1.49	8 (16%)	59,89,113	1.43	5 (8%)
28	LMG	J	101	-	55,55,55	0.70	0	63,63,63	1.35	7 (11%)
22	CLA	R	606	11	61,65,73	1.34	6 (9%)	73,103,113	1.29	6 (8%)
24	DD6	N	612	-	39,45,45	1.99	3 (7%)	52,67,67	1.87	13 (25%)
22	CLA	R	604	-	49,53,73	1.49	7 (14%)	59,89,113	1.40	7 (11%)
22	CLA	B	836	1	55,59,73	1.40	8 (14%)	66,96,113	1.37	5 (7%)
22	CLA	O	311	26	64,68,73	1.29	7 (10%)	77,107,113	1.29	6 (7%)
22	CLA	K	617	10	69,73,73	1.25	9 (13%)	83,113,113	1.27	7 (8%)
22	CLA	U	410	16	59,63,73	1.35	8 (13%)	71,101,113	1.33	5 (7%)
22	CLA	N	603	8	69,73,73	1.26	8 (11%)	83,113,113	1.26	7 (8%)
22	CLA	A	821	20	69,73,73	1.24	9 (13%)	83,113,113	1.32	6 (7%)
27	LMU	T	617	-	24,24,36	0.42	0	29,29,47	0.66	0
22	CLA	S	614	-	49,53,73	1.48	8 (16%)	59,89,113	1.45	5 (8%)
27	LMU	A	853	-	24,24,36	0.43	0	29,29,47	0.57	0
29	SF4	C	101	2	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	P	603	6	49,53,73	1.49	6 (12%)	59,89,113	1.30	4 (6%)
22	CLA	A	824	20	69,73,73	1.25	8 (11%)	83,113,113	1.28	7 (8%)
22	CLA	Q	603	10	49,53,73	1.48	8 (16%)	59,89,113	1.47	6 (10%)
28	LMG	W	401	-	48,48,55	0.73	0	56,56,63	1.33	8 (14%)
32	NEX	U	418	-	38,46,46	0.35	1 (2%)	50,70,70	0.67	2 (4%)
22	CLA	W	406	-	60,64,73	1.34	8 (13%)	72,102,113	1.32	5 (6%)
22	CLA	U	411	16	61,65,73	1.32	7 (11%)	73,103,113	1.31	6 (8%)
24	DD6	N	613	-	39,45,45	2.00	3 (7%)	52,67,67	1.86	15 (28%)
22	CLA	A	823	20	49,53,73	1.48	8 (16%)	59,89,113	1.47	6 (10%)
24	DD6	L	413	-	39,45,45	2.00	3 (7%)	52,67,67	1.78	12 (23%)
22	CLA	B	833	1	69,73,73	1.25	8 (11%)	83,113,113	1.26	5 (6%)
22	CLA	B	822	1	69,73,73	1.26	8 (11%)	83,113,113	1.28	6 (7%)
28	LMG	T	616	-	41,41,55	0.84	0	49,49,63	1.24	3 (6%)
26	LHG	O	321	-	48,48,48	1.11	6 (12%)	51,54,54	0.92	2 (3%)
22	CLA	B	815	1	56,60,73	1.39	9 (16%)	67,97,113	1.32	6 (8%)
31	CHL	W	422	-	70,74,74	1.70	8 (11%)	80,114,114	1.07	7 (8%)
22	CLA	K	606	-	54,58,73	1.42	8 (14%)	65,95,113	1.42	6 (9%)
25	DGD	O	304	-	61,61,67	0.87	3 (4%)	75,75,81	1.14	8 (10%)
22	CLA	B	814	1	49,53,73	1.47	8 (16%)	59,89,113	1.42	7 (11%)
22	CLA	R	605	-	69,73,73	1.27	8 (11%)	83,113,113	1.29	6 (7%)
22	CLA	B	817	1	69,73,73	1.25	8 (11%)	83,113,113	1.27	5 (6%)
21	BCR	A	851	-	41,41,41	0.70	0	56,56,56	2.11	16 (28%)
27	LMU	U	422	-	36,36,36	0.44	0	47,47,47	0.79	2 (4%)
22	CLA	I	604	-	49,53,73	1.49	8 (16%)	59,89,113	1.44	5 (8%)
22	CLA	X	405	-	60,64,73	1.34	8 (13%)	72,102,113	1.34	6 (8%)
22	CLA	P	605	-	49,53,73	1.48	8 (16%)	59,89,113	1.44	6 (10%)
22	CLA	U	414	16	65,69,73	1.30	8 (12%)	78,108,113	1.31	5 (6%)
21	BCR	B	846	-	41,41,41	0.71	0	56,56,56	1.82	17 (30%)
22	CLA	B	806	1	69,73,73	1.26	8 (11%)	83,113,113	1.28	6 (7%)
22	CLA	A	811	20	61,65,73	1.33	8 (13%)	73,103,113	1.40	10 (13%)
24	DD6	S	611	-	39,45,45	1.99	3 (7%)	52,67,67	1.78	13 (25%)
26	LHG	X	420	22	41,41,48	1.19	6 (14%)	44,47,54	0.99	2 (4%)
22	CLA	O	306	13	64,68,73	1.30	8 (12%)	77,107,113	1.29	7 (9%)
28	LMG	I	614	-	37,37,55	0.85	0	45,45,63	1.27	5 (11%)
22	CLA	U	415	16	49,53,73	1.49	8 (16%)	59,89,113	1.40	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	K	611	10	69,73,73	1.26	7 (10%)	83,113,113	1.30	5 (6%)
22	CLA	I	602	8	64,68,73	1.31	8 (12%)	77,107,113	1.32	8 (10%)
22	CLA	S	607	14	64,68,73	1.31	7 (10%)	77,107,113	1.29	5 (6%)
22	CLA	B	807	1	69,73,73	1.24	9 (13%)	83,113,113	1.24	5 (6%)
22	CLA	O	307	13	49,53,73	1.48	8 (16%)	59,89,113	1.42	5 (8%)
22	CLA	G	606	6	69,73,73	1.26	8 (11%)	83,113,113	1.23	5 (6%)
22	CLA	K	605	-	69,73,73	1.25	7 (10%)	83,113,113	1.27	4 (4%)
21	BCR	A	850	-	41,41,41	0.71	0	56,56,56	1.97	12 (21%)
22	CLA	I	603	8	60,64,73	1.36	8 (13%)	72,102,113	1.31	7 (9%)
24	DD6	P	612	-	39,45,45	2.04	2 (5%)	52,67,67	2.96	18 (34%)
22	CLA	A	825	20	65,69,73	1.27	6 (9%)	78,108,113	1.29	6 (7%)
28	LMG	F	408	-	42,42,55	0.85	1 (2%)	50,50,63	1.32	4 (8%)
22	CLA	G	607	-	64,68,73	1.29	8 (12%)	77,107,113	1.27	5 (6%)
26	LHG	L	416	22	41,41,48	1.17	6 (14%)	44,47,54	0.99	2 (4%)
22	CLA	Q	601	-	49,53,73	1.51	9 (18%)	59,89,113	1.43	5 (8%)
22	CLA	I	609	8	49,53,73	1.49	8 (16%)	59,89,113	1.47	5 (8%)
28	LMG	I	615	-	49,50,55	0.75	0	54,57,63	1.38	4 (7%)
22	CLA	H	307	7	64,68,73	1.31	7 (10%)	77,107,113	1.29	4 (5%)
26	LHG	K	619	-	32,32,48	1.31	6 (18%)	35,38,54	1.10	2 (5%)
22	CLA	K	613	-	57,61,73	1.38	8 (14%)	68,98,113	1.35	6 (8%)
22	CLA	A	832	20	56,60,73	1.39	8 (14%)	67,97,113	1.36	6 (8%)
22	CLA	A	828	20	69,73,73	1.25	7 (10%)	83,113,113	1.29	7 (8%)
22	CLA	B	823	-	69,73,73	1.25	7 (10%)	83,113,113	1.28	4 (4%)
21	BCR	B	801	-	41,41,41	0.69	0	56,56,56	1.96	16 (28%)
22	CLA	A	816	20	65,69,73	1.29	11 (16%)	78,108,113	1.42	10 (12%)
22	CLA	L	404	-	60,64,73	1.35	8 (13%)	72,102,113	1.36	6 (8%)
24	DD6	X	416	-	39,45,45	2.01	2 (5%)	52,67,67	2.23	15 (28%)
31	CHL	V	605	-	50,54,74	2.03	8 (16%)	56,90,114	1.23	6 (10%)
22	CLA	B	839	26	69,73,73	1.25	8 (11%)	83,113,113	1.29	7 (8%)
22	CLA	T	611	15	69,73,73	1.26	7 (10%)	83,113,113	1.28	5 (6%)
22	CLA	A	815	20	69,73,73	1.25	7 (10%)	83,113,113	1.29	8 (9%)
22	CLA	F	405	5	49,53,73	1.49	8 (16%)	59,89,113	1.38	4 (6%)
22	CLA	P	606	6	49,53,73	1.47	8 (16%)	59,89,113	1.43	5 (8%)
22	CLA	N	609	8	49,53,73	1.49	8 (16%)	59,89,113	1.40	5 (8%)
22	CLA	Q	605	-	60,64,73	1.34	7 (11%)	72,102,113	1.34	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	A	838	20	56,60,73	1.39	9 (16%)	67,97,113	1.43	9 (13%)
27	LMU	K	620	-	34,34,36	0.50	0	44,44,47	1.04	5 (11%)
22	CLA	H	306	-	59,63,73	1.36	9 (15%)	71,101,113	1.34	5 (7%)
22	CLA	R	610	11	69,73,73	1.27	7 (10%)	83,113,113	1.24	7 (8%)
28	LMG	H	322	-	37,37,55	0.85	0	45,45,63	1.23	4 (8%)
26	LHG	H	316	22	26,26,48	1.40	6 (23%)	29,32,54	1.16	2 (6%)
22	CLA	P	610	6	45,49,73	1.54	7 (15%)	54,84,113	1.54	7 (12%)
22	CLA	L	409	26	64,68,73	1.30	9 (14%)	77,107,113	1.30	5 (6%)
22	CLA	X	403	19	69,73,73	1.25	8 (11%)	83,113,113	1.27	6 (7%)
24	DD6	O	316	-	39,45,45	1.96	3 (7%)	52,67,67	1.72	12 (23%)
22	CLA	I	611	8	49,53,73	1.53	8 (16%)	59,89,113	1.45	9 (15%)
22	CLA	N	605	-	49,53,73	1.48	8 (16%)	59,89,113	1.47	6 (10%)
22	CLA	W	419	18	49,53,73	1.49	7 (14%)	59,89,113	1.44	4 (6%)
28	LMG	K	622	-	43,43,55	0.80	0	51,51,63	1.27	5 (9%)
22	CLA	U	406	-	60,64,73	1.35	7 (11%)	72,102,113	1.33	6 (8%)
28	LMG	N	615	-	44,44,55	0.78	0	52,52,63	1.26	4 (7%)
27	LMU	L	419	-	27,27,36	0.41	0	30,30,47	0.75	0
22	CLA	O	319	13	49,53,73	1.48	7 (14%)	59,89,113	1.45	6 (10%)
27	LMU	U	424	-	24,24,36	0.42	0	29,29,47	0.58	0
22	CLA	A	833	20	69,73,73	1.25	8 (11%)	83,113,113	1.28	8 (9%)
24	DD6	K	614	-	39,45,45	1.98	3 (7%)	52,67,67	1.86	15 (28%)
22	CLA	U	405	16	61,65,73	1.34	8 (13%)	73,103,113	1.33	4 (5%)
22	CLA	P	609	-	49,53,73	1.49	9 (18%)	59,89,113	1.41	4 (6%)
21	BCR	J	103	-	41,41,41	0.68	0	56,56,56	1.78	12 (21%)

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
22	CLA	T	603	15	-	8/33/109/115	-
22	CLA	X	417	19	-	5/21/97/115	-
26	LHG	A	846	22	-	27/53/53/53	-
28	LMG	U	423	-	-	20/44/64/70	0/1/1/1
27	LMU	X	421	-	-	3/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	S	603	14	-	3/15/91/115	-
22	CLA	B	826	1	-	10/31/107/115	-
22	CLA	B	808	1	-	7/27/103/115	-
22	CLA	A	807	20	-	13/39/115/115	-
22	CLA	A	830	20	-	13/39/115/115	-
22	CLA	G	601	6	-	6/15/91/115	-
22	CLA	U	412	26	-	3/15/91/115	-
22	CLA	K	608	10	-	11/39/115/115	-
22	CLA	O	305	13	-	4/21/97/115	-
22	CLA	X	408	19	-	12/39/115/115	-
22	CLA	Q	604	10	-	16/39/115/115	-
22	CLA	A	809	20	-	1/25/101/115	-
22	CLA	R	615	11	-	13/39/115/115	-
22	CLA	A	818	20	-	4/25/101/115	-
26	LHG	U	419	22	-	15/28/28/53	-
22	CLA	I	601	8	-	15/39/115/115	-
27	LMU	B	857	-	-	4/21/61/61	0/2/2/2
22	CLA	Q	617	10	-	5/24/100/115	-
25	DGD	F	401	-	-	19/35/35/95	-
27	LMU	X	418	-	-	1/15/35/61	0/1/1/2
22	CLA	B	818	-	-	12/39/115/115	-
24	DD6	V	615	-	-	3/26/80/80	0/3/3/3
22	CLA	K	612	10	-	2/15/91/115	-
22	CLA	X	407	-	-	4/39/115/115	-
22	CLA	G	602	6	-	4/33/109/115	-
24	DD6	X	415	-	-	1/26/80/80	0/3/3/3
24	DD6	T	613	-	-	1/26/80/80	0/3/3/3
22	CLA	A	844	26	-	12/27/103/115	-
22	CLA	U	404	16	-	14/39/115/115	-
22	CLA	S	604	-	-	9/33/109/115	-
24	DD6	A	859	-	-	1/26/80/80	0/3/3/3
22	CLA	B	838	1	-	7/15/91/115	-
24	DD6	H	314	-	-	1/26/80/80	0/3/3/3
24	DD6	L	414	-	-	2/26/80/80	0/3/3/3
27	LMU	F	402	-	-	1/12/32/61	0/1/1/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	Q	611	10	-	9/27/103/115	-
26	LHG	G	614	22	-	13/36/36/53	-
26	LHG	B	848	22	-	10/31/31/53	-
22	CLA	Q	618	-	-	9/15/91/115	-
32	NEX	V	616	-	-	4/27/83/83	0/3/3/3
22	CLA	A	803	-	-	12/39/115/115	-
22	CLA	P	607	6	-	4/15/91/115	-
22	CLA	B	805	1	-	7/39/115/115	-
22	CLA	I	608	-	-	5/15/91/115	-
22	CLA	X	413	19	-	3/15/91/115	-
26	LHG	T	614	22	-	27/46/46/53	-
22	CLA	A	819	20	-	11/31/107/115	-
22	CLA	A	822	-	-	8/39/115/115	-
22	CLA	B	859	-	-	12/39/115/115	-
22	CLA	A	834	20	-	5/15/91/115	-
22	CLA	L	411	11	-	14/39/115/115	-
22	CLA	A	831	20	-	6/39/115/115	-
27	LMU	U	421	-	-	7/21/61/61	0/2/2/2
22	CLA	O	315	13	-	4/21/97/115	-
24	DD6	O	317	-	-	0/26/80/80	0/3/3/3
27	LMU	H	321	-	-	1/19/56/61	0/2/2/2
22	CLA	B	827	1	-	9/39/115/115	-
22	CLA	I	605	-	-	2/15/91/115	-
22	CLA	Q	608	10	-	3/21/97/115	-
26	LHG	K	616	22	-	18/43/43/53	-
33	CL0	A	802	20	-	6/39/115/115	-
22	CLA	A	805	20	-	9/35/111/115	-
22	CLA	V	604	-	-	9/29/105/115	-
22	CLA	A	814	20	-	9/39/115/115	-
22	CLA	X	410	26	-	12/33/109/115	-
22	CLA	L	403	11	-	5/33/109/115	-
31	CHL	W	407	-	-	2/17/93/117	-
22	CLA	B	831	1	-	7/39/115/115	-
22	CLA	B	830	1	-	9/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	L	408	11	-	6/33/109/115	-
24	DD6	X	414	-	-	1/26/80/80	0/3/3/3
22	CLA	F	403	-	-	11/39/115/115	-
22	CLA	A	826	-	-	8/39/115/115	-
22	CLA	B	802	1	-	6/39/115/115	-
28	LMG	H	319	-	-	19/35/55/70	0/1/1/1
22	CLA	R	601	-	-	19/39/115/115	-
22	CLA	A	842	20	-	12/39/115/115	-
22	CLA	H	305	7	-	11/33/109/115	-
24	DD6	U	417	-	-	1/26/80/80	0/3/3/3
22	CLA	B	824	-	-	11/39/115/115	-
22	CLA	W	413	-	-	6/15/91/115	-
22	CLA	W	403	18	-	7/24/100/115	-
27	LMU	A	857	-	-	3/15/35/61	0/1/1/2
22	CLA	V	608	17	-	8/27/103/115	-
22	CLA	S	615	-	-	4/23/99/115	-
29	SF4	C	102	2	-	-	0/6/5/5
22	CLA	S	601	14	-	6/15/91/115	-
30	SQD	K	621	-	-	5/38/58/69	0/1/1/1
22	CLA	K	603	10	-	7/33/109/115	-
22	CLA	V	601	17	-	6/15/91/115	-
22	CLA	B	837	-	-	3/15/91/115	-
22	CLA	G	610	6	-	5/15/91/115	-
24	DD6	B	841	-	-	1/26/80/80	0/3/3/3
22	CLA	A	835	20	-	9/35/111/115	-
22	CLA	W	404	18	-	10/39/115/115	-
23	PQN	A	843	-	-	4/23/43/43	0/2/2/2
22	CLA	G	609	-	-	4/15/91/115	-
30	SQD	V	618	-	-	4/19/39/69	0/1/1/1
22	CLA	R	603	-	-	10/29/105/115	-
22	CLA	A	820	20	-	12/39/115/115	-
22	CLA	A	827	-	-	5/36/112/115	-
22	CLA	L	406	-	-	10/39/115/115	-
26	LHG	N	614	22	-	9/32/32/53	-
22	CLA	W	411	18	-	10/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	H	313	7	-	10/31/107/115	-
22	CLA	N	604	-	-	6/15/91/115	-
24	DD6	Q	614	-	-	1/26/80/80	0/3/3/3
22	CLA	T	605	-	-	15/39/115/115	-
22	CLA	O	310	13	-	9/33/109/115	-
22	CLA	B	820	1	-	8/25/101/115	-
29	SF4	B	860	20,1	-	-	0/6/5/5
22	CLA	O	308	-	-	14/35/111/115	-
21	BCR	B	842	-	-	2/29/63/63	0/2/2/2
22	CLA	V	603	17	-	11/30/106/115	-
22	CLA	L	407	-	-	11/30/106/115	-
22	CLA	H	303	7	-	11/33/109/115	-
22	CLA	L	417	11	-	8/39/115/115	-
22	CLA	W	410	18	-	10/33/109/115	-
22	CLA	R	611	11	-	6/15/91/115	-
22	CLA	O	313	13	-	14/39/115/115	-
27	LMU	O	303	-	-	2/21/61/61	0/2/2/2
22	CLA	V	610	-	-	4/15/91/115	-
22	CLA	A	812	20	-	10/30/106/115	-
26	LHG	R	614	22	-	20/46/46/53	-
22	CLA	T	607	15	-	9/33/109/115	-
28	LMG	G	616	-	-	21/41/61/70	0/1/1/1
22	CLA	L	412	11	-	5/15/91/115	-
22	CLA	W	409	-	-	10/39/115/115	-
24	DD6	Q	615	-	-	0/26/80/80	0/3/3/3
31	CHL	W	408	-	-	5/41/117/117	-
22	CLA	T	608	26	-	4/33/109/115	-
22	CLA	V	617	-	-	10/15/91/115	-
22	CLA	K	610	10	-	8/29/105/115	-
22	CLA	A	810	20	-	10/39/115/115	-
22	CLA	H	318	7	-	6/15/91/115	-
22	CLA	A	806	20	-	10/39/115/115	-
22	CLA	H	308	7	-	6/33/109/115	-
22	CLA	S	608	26	-	9/15/91/115	-
27	LMU	B	855	-	-	2/15/35/61	0/1/1/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	811	1	-	2/15/91/115	-
22	CLA	G	604	-	-	0/15/91/115	-
28	LMG	K	601	-	-	24/38/58/70	0/1/1/1
22	CLA	X	419	19	-	9/15/91/115	-
22	CLA	A	829	20	-	15/39/115/115	-
22	CLA	A	836	20	-	12/39/115/115	-
22	CLA	O	312	13	-	8/33/109/115	-
22	CLA	J	102	9	-	7/21/97/115	-
24	DD6	J	105	-	-	3/26/80/80	0/3/3/3
31	CHL	V	606	-	-	1/17/93/117	-
22	CLA	P	611	6	-	6/15/91/115	-
22	CLA	W	414	18	-	10/39/115/115	-
22	CLA	T	602	15	-	9/39/115/115	-
27	LMU	B	850	-	-	3/15/35/61	0/1/1/2
27	LMU	L	420	-	-	4/21/57/61	1/2/2/2
26	LHG	O	323	-	-	19/47/47/53	-
28	LMG	Q	602	-	-	11/32/52/70	0/1/1/1
22	CLA	O	314	13	-	1/15/91/115	-
22	CLA	S	610	14	-	4/15/91/115	-
22	CLA	W	415	18	-	6/15/91/115	-
24	DD6	R	613	-	-	1/26/80/80	0/3/3/3
26	LHG	S	613	22	-	13/36/36/53	-
21	BCR	A	849	-	-	0/29/63/63	0/2/2/2
22	CLA	B	809	1	-	3/39/115/115	-
22	CLA	G	611	6	-	5/15/91/115	-
22	CLA	T	601	15	-	5/15/91/115	-
22	CLA	T	609	15	-	5/15/91/115	-
22	CLA	W	402	18	-	2/27/103/115	-
24	DD6	K	615	-	-	0/26/80/80	0/3/3/3
22	CLA	G	608	26	-	16/33/109/115	-
27	LMU	H	320	-	-	2/15/35/61	0/1/1/2
22	CLA	Q	609	10	-	9/33/109/115	-
28	LMG	H	317	-	-	13/38/58/70	0/1/1/1
28	LMG	B	852	-	-	15/38/58/70	0/1/1/1
22	CLA	Q	613	10	-	6/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	N	607	-	-	14/33/109/115	-
22	CLA	H	310	7	-	3/15/91/115	-
22	CLA	A	801	-	-	15/39/115/115	-
22	CLA	B	804	1	-	15/39/115/115	-
22	CLA	H	312	7	-	3/15/91/115	-
22	CLA	W	405	18	-	3/33/109/115	-
27	LMU	O	301	-	-	1/15/35/61	0/1/1/2
22	CLA	N	601	8	-	6/15/91/115	-
28	LMG	U	402	-	-	25/48/68/70	0/1/1/1
26	LHG	W	420	22	-	22/46/46/53	-
25	DGD	B	847	-	-	33/55/95/95	0/2/2/2
27	LMU	H	301	-	-	2/12/32/61	0/1/1/2
21	BCR	B	844	-	-	1/29/63/63	0/2/2/2
27	LMU	J	104	-	-	9/21/57/61	0/2/2/2
22	CLA	A	840	20	-	16/39/115/115	-
22	CLA	P	604	-	-	6/15/91/115	-
22	CLA	Q	612	10	-	15/39/115/115	-
22	CLA	X	402	19	-	11/27/103/115	-
24	DD6	P	613	-	-	4/26/80/80	0/3/3/3
24	DD6	F	406	-	-	7/26/80/80	0/3/3/3
22	CLA	A	817	20	-	16/39/115/115	-
22	CLA	H	304	7	-	6/15/91/115	-
31	CHL	X	406	-	-	0/17/93/117	-
24	DD6	R	612	-	-	1/26/80/80	0/3/3/3
27	LMU	A	856	-	-	0/12/32/61	0/1/1/2
22	CLA	N	602	8	-	5/33/109/115	-
22	CLA	B	810	-	-	4/29/105/115	-
22	CLA	W	412	26	-	5/33/109/115	-
22	CLA	A	808	20	-	12/39/115/115	-
27	LMU	F	409	-	-	4/12/32/61	0/1/1/2
26	LHG	B	851	-	-	22/46/46/53	-
27	LMU	A	854	-	-	3/21/61/61	0/2/2/2
22	CLA	P	602	6	-	10/15/91/115	-
22	CLA	B	825	1	-	10/39/115/115	-
22	CLA	F	404	-	-	10/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	L	405	-	-	3/15/91/115	-
24	DD6	W	416	-	-	1/26/80/80	0/3/3/3
27	LMU	T	615	-	-	0/12/32/61	0/1/1/2
24	DD6	S	612	-	-	1/26/80/80	0/3/3/3
22	CLA	B	816	1	-	13/39/115/115	-
31	CHL	U	408	-	-	1/17/93/117	-
22	CLA	B	812	1	-	18/39/115/115	-
23	PQN	B	840	-	-	0/23/43/43	0/2/2/2
21	BCR	B	845	-	-	2/29/63/63	0/2/2/2
22	CLA	B	829	-	-	7/15/91/115	-
22	CLA	T	604	15	-	18/39/115/115	-
26	LHG	Q	616	22	-	15/48/48/53	-
22	CLA	B	832	1	-	12/36/112/115	-
22	CLA	T	606	15	-	5/21/97/115	-
22	CLA	X	411	-	-	3/15/91/115	-
22	CLA	Q	607	-	-	5/15/91/115	-
22	CLA	U	409	-	-	6/15/91/115	-
22	CLA	B	813	1	-	10/39/115/115	-
24	DD6	V	614	-	-	1/26/80/80	0/3/3/3
26	LHG	N	616	-	-	23/47/47/53	-
22	CLA	B	834	1	-	7/39/115/115	-
22	CLA	V	613	-	-	11/15/91/115	-
24	DD6	L	415	-	-	3/26/80/80	0/3/3/3
24	DD6	A	858	-	-	5/26/80/80	0/3/3/3
30	SQD	O	302	-	-	5/37/57/69	0/1/1/1
26	LHG	O	318	22	-	16/38/38/53	-
24	DD6	G	613	-	-	1/26/80/80	0/3/3/3
22	CLA	T	610	-	-	7/15/91/115	-
27	LMU	B	858	-	-	2/12/12/61	-
22	CLA	I	606	8	-	12/35/111/115	-
24	DD6	W	418	-	-	1/26/80/80	0/3/3/3
22	CLA	B	803	1	-	7/29/105/115	-
22	CLA	L	410	11	-	8/33/109/115	-
22	CLA	R	608	26	-	10/26/102/115	-
22	CLA	B	828	1	-	15/39/115/115	-
27	LMU	O	322	-	-	5/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	P	608	-	-	9/15/91/115	-
22	CLA	A	813	20	-	10/39/115/115	-
22	CLA	R	609	-	-	3/10/86/115	-
22	CLA	I	610	8	-	8/15/91/115	-
22	CLA	N	606	8	-	13/39/115/115	-
22	CLA	N	610	8	-	18/27/103/115	-
22	CLA	B	819	1	-	9/25/101/115	-
26	LHG	A	845	-	-	25/53/53/53	-
22	CLA	A	841	20	-	12/39/115/115	-
24	DD6	G	612	-	-	0/26/80/80	0/3/3/3
22	CLA	S	605	-	-	14/33/109/115	-
27	LMU	L	418	-	-	0/15/35/61	0/1/1/2
22	CLA	A	852	-	-	14/39/115/115	-
21	BCR	B	843	-	-	4/29/63/63	0/2/2/2
27	LMU	O	320	-	-	1/17/35/61	0/2/2/2
24	DD6	U	416	-	-	1/26/80/80	0/3/3/3
22	CLA	V	609	17	-	8/30/106/115	-
24	DD6	H	315	-	-	1/26/80/80	0/3/3/3
22	CLA	R	607	11	-	17/33/109/115	-
22	CLA	K	609	26	-	13/33/109/115	-
22	CLA	X	404	19	-	8/33/109/115	-
22	CLA	A	804	-	-	6/39/115/115	-
22	CLA	N	611	-	-	4/10/82/115	-
22	CLA	Q	606	-	-	7/15/91/115	-
22	CLA	O	309	13	-	4/21/97/115	-
30	SQD	F	407	-	-	2/37/57/69	0/1/1/1
22	CLA	N	608	26	-	7/15/91/115	-
28	LMG	A	855	-	-	12/36/56/70	0/1/1/1
22	CLA	V	607	-	-	3/15/91/115	-
22	CLA	K	607	10	-	9/30/106/115	-
27	LMU	M	102	-	-	4/15/35/61	0/1/1/2
27	LMU	B	854	-	-	3/15/35/61	0/1/1/2
28	LMG	B	856	-	-	26/48/68/70	0/1/1/1
27	LMU	W	421	-	-	4/15/35/61	0/1/1/2
22	CLA	S	609	14	-	9/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	U	403	16	-	8/15/91/115	-
22	CLA	K	602	10	-	11/33/109/115	-
26	LHG	P	601	-	-	23/44/44/53	-
28	LMG	L	401	-	-	20/46/66/70	0/1/1/1
22	CLA	G	603	6	-	10/29/105/115	-
22	CLA	S	606	14	-	4/21/97/115	-
27	LMU	B	849	-	-	2/15/35/61	0/1/1/2
31	CHL	U	407	-	-	0/17/93/117	-
28	LMG	K	618	-	-	24/44/64/70	0/1/1/1
22	CLA	R	602	-	-	12/33/109/115	-
24	DD6	T	612	-	-	1/26/80/80	0/3/3/3
22	CLA	Q	610	26	-	16/39/115/115	-
22	CLA	B	835	1	-	11/39/115/115	-
22	CLA	H	302	7	-	4/15/91/115	-
22	CLA	L	402	11	-	17/39/115/115	-
24	DD6	I	613	-	-	0/26/80/80	0/3/3/3
22	CLA	H	309	26	-	10/27/103/115	-
22	CLA	V	612	-	-	15/39/115/115	-
22	CLA	A	839	20	-	6/39/115/115	-
24	DD6	X	401	-	-	0/26/80/80	0/3/3/3
24	DD6	W	417	-	-	1/26/80/80	0/3/3/3
22	CLA	H	311	7	-	16/39/115/115	-
22	CLA	S	602	14	-	9/33/109/115	-
24	DD6	I	612	-	-	0/26/80/80	0/3/3/3
24	DD6	A	847	-	-	1/26/80/80	0/3/3/3
22	CLA	U	413	16	-	5/15/91/115	-
22	CLA	U	401	-	-	9/27/103/115	-
22	CLA	V	602	17	-	8/39/115/115	-
22	CLA	A	837	20	-	6/21/97/115	-
26	LHG	O	324	-	-	25/46/46/53	-
27	LMU	B	853	-	-	0/10/27/61	0/1/1/2
22	CLA	V	611	-	-	5/15/91/115	-
27	LMU	G	615	-	-	0/12/32/61	0/1/1/2
22	CLA	X	409	19	-	10/39/115/115	-
22	CLA	G	605	-	-	3/15/91/115	-
22	CLA	B	821	1	-	11/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	K	604	-	-	19/37/113/115	-
27	LMU	T	618	-	-	1/15/35/61	0/1/1/2
21	BCR	A	848	-	-	0/29/63/63	0/2/2/2
22	CLA	X	412	19	-	12/39/115/115	-
21	BCR	M	101	-	-	2/29/63/63	0/2/2/2
22	CLA	I	607	8	-	4/27/103/115	-
22	CLA	U	420	16	-	9/15/91/115	-
28	LMG	J	101	-	-	23/50/70/70	0/1/1/1
22	CLA	R	606	11	-	12/30/106/115	-
24	DD6	N	612	-	-	0/26/80/80	0/3/3/3
22	CLA	R	604	-	-	5/15/91/115	-
22	CLA	B	836	1	-	2/23/99/115	-
22	CLA	O	311	26	-	9/33/109/115	-
22	CLA	K	617	10	-	12/39/115/115	-
22	CLA	U	410	16	-	7/27/103/115	-
22	CLA	N	603	8	-	10/39/115/115	-
22	CLA	A	821	20	-	15/39/115/115	-
27	LMU	T	617	-	-	3/15/35/61	0/1/1/2
22	CLA	S	614	-	-	0/15/91/115	-
27	LMU	A	853	-	-	0/15/35/61	0/1/1/2
29	SF4	C	101	2	-	-	0/6/5/5
22	CLA	P	603	6	-	5/15/91/115	-
22	CLA	A	824	20	-	25/39/115/115	-
22	CLA	Q	603	10	-	4/15/91/115	-
28	LMG	W	401	-	-	19/43/63/70	0/1/1/1
32	NEX	U	418	-	-	4/27/83/83	0/3/3/3
22	CLA	W	406	-	-	2/29/105/115	-
22	CLA	U	411	16	-	7/30/106/115	-
24	DD6	N	613	-	-	4/26/80/80	0/3/3/3
22	CLA	A	823	20	-	5/15/91/115	-
24	DD6	L	413	-	-	1/26/80/80	0/3/3/3
22	CLA	B	833	1	-	9/39/115/115	-
22	CLA	B	822	1	-	10/39/115/115	-
28	LMG	T	616	-	-	16/36/56/70	0/1/1/1
26	LHG	O	321	-	-	30/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	815	1	-	3/24/100/115	-
31	CHL	W	422	-	-	11/41/117/117	-
22	CLA	K	606	-	-	1/21/97/115	-
25	DGD	O	304	-	-	31/49/89/95	0/2/2/2
22	CLA	B	814	1	-	6/15/91/115	-
22	CLA	R	605	-	-	15/39/115/115	-
22	CLA	B	817	1	-	15/39/115/115	-
21	BCR	A	851	-	-	4/29/63/63	0/2/2/2
27	LMU	U	422	-	-	5/21/61/61	0/2/2/2
22	CLA	I	604	-	-	1/15/91/115	-
22	CLA	X	405	-	-	8/29/105/115	-
22	CLA	P	605	-	-	8/15/91/115	-
22	CLA	U	414	16	-	14/35/111/115	-
21	BCR	B	846	-	-	6/29/63/63	0/2/2/2
22	CLA	B	806	1	-	13/39/115/115	-
22	CLA	A	811	20	-	10/30/106/115	-
24	DD6	S	611	-	-	1/26/80/80	0/3/3/3
26	LHG	X	420	22	-	28/46/46/53	-
22	CLA	O	306	13	-	7/33/109/115	-
28	LMG	I	614	-	-	10/32/52/70	0/1/1/1
22	CLA	U	415	16	-	7/15/91/115	-
22	CLA	K	611	10	-	11/39/115/115	-
22	CLA	I	602	8	-	3/33/109/115	-
22	CLA	S	607	14	-	9/33/109/115	-
22	CLA	B	807	1	-	15/39/115/115	-
22	CLA	O	307	13	-	3/15/91/115	-
22	CLA	G	606	6	-	12/39/115/115	-
22	CLA	K	605	-	-	19/39/115/115	-
21	BCR	A	850	-	-	4/29/63/63	0/2/2/2
22	CLA	I	603	8	-	9/29/105/115	-
24	DD6	P	612	-	-	6/26/80/80	0/3/3/3
22	CLA	A	825	20	-	17/35/111/115	-
28	LMG	F	408	-	-	18/37/57/70	0/1/1/1
22	CLA	G	607	-	-	3/33/109/115	-
26	LHG	L	416	22	-	20/46/46/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	Q	601	-	-	6/15/91/115	-
22	CLA	I	609	8	-	4/15/91/115	-
28	LMG	I	615	-	-	26/46/62/70	0/1/1/1
22	CLA	H	307	7	-	11/33/109/115	-
26	LHG	K	619	-	-	19/37/37/53	-
22	CLA	K	613	-	-	5/25/101/115	-
22	CLA	A	832	20	-	5/24/100/115	-
22	CLA	A	828	20	-	8/39/115/115	-
22	CLA	B	823	-	-	10/39/115/115	-
21	BCR	B	801	-	-	4/29/63/63	0/2/2/2
22	CLA	A	816	20	-	14/35/111/115	-
22	CLA	L	404	-	-	12/29/105/115	-
24	DD6	X	416	-	-	5/26/80/80	0/3/3/3
31	CHL	V	605	-	-	0/17/93/117	-
22	CLA	B	839	26	-	3/39/115/115	-
22	CLA	T	611	15	-	15/39/115/115	-
22	CLA	A	815	20	-	6/39/115/115	-
22	CLA	F	405	5	-	7/15/91/115	-
22	CLA	P	606	6	-	6/15/91/115	-
22	CLA	N	609	8	-	4/15/91/115	-
22	CLA	Q	605	-	-	3/29/105/115	-
22	CLA	A	838	20	-	7/24/100/115	-
27	LMU	K	620	-	-	6/19/56/61	0/2/2/2
22	CLA	H	306	-	-	10/27/103/115	-
22	CLA	R	610	11	-	12/39/115/115	-
28	LMG	H	322	-	-	15/32/52/70	0/1/1/1
26	LHG	H	316	22	-	5/31/31/53	-
22	CLA	P	610	6	-	5/10/86/115	-
22	CLA	L	409	26	-	6/33/109/115	-
22	CLA	X	403	19	-	9/39/115/115	-
24	DD6	O	316	-	-	1/26/80/80	0/3/3/3
22	CLA	I	611	8	-	6/15/91/115	-
22	CLA	N	605	-	-	1/15/91/115	-
22	CLA	W	419	18	-	6/15/91/115	-
28	LMG	K	622	-	-	15/38/58/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	U	406	-	-	7/29/105/115	-
28	LMG	N	615	-	-	24/39/59/70	0/1/1/1
27	LMU	L	419	-	-	6/21/34/61	1/1/1/2
22	CLA	O	319	13	-	1/15/91/115	-
27	LMU	U	424	-	-	2/15/35/61	0/1/1/2
22	CLA	A	833	20	-	6/39/115/115	-
24	DD6	K	614	-	-	0/26/80/80	0/3/3/3
22	CLA	U	405	16	-	5/30/106/115	-
22	CLA	P	609	-	-	8/15/91/115	-
21	BCR	J	103	-	-	2/29/63/63	0/2/2/2

The worst 5 of 2549 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	859	DD6	C29-C27	-8.82	1.25	1.42
24	I	613	DD6	C29-C27	-8.81	1.25	1.42
24	W	418	DD6	C29-C27	-8.76	1.25	1.42
24	P	612	DD6	C29-C27	-8.75	1.25	1.42
24	Q	615	DD6	C29-C27	-8.72	1.25	1.42

The worst 5 of 2728 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	843	BCR	C40-C30-C25	-13.35	88.64	110.30
24	P	612	DD6	C9-C10-C11	-9.93	113.14	127.31
24	P	612	DD6	C4-C5-C6	-9.08	114.35	127.31
24	X	416	DD6	C4-C5-C6	-8.39	115.34	127.31
21	B	843	BCR	C40-C30-C39	-8.38	82.82	108.53

There are no chirality outliers.

5 of 3518 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	B	801	BCR	C7-C8-C9-C10
21	B	801	BCR	C7-C8-C9-C34
21	B	842	BCR	C21-C22-C23-C24
21	B	842	BCR	C37-C22-C23-C24
21	B	845	BCR	C21-C22-C23-C24

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	L	420	LMU	C1'-C2'-C3'-C4'-C5'-O5'
27	L	419	LMU	C1'-C2'-C3'-C4'-C5'-O5'

291 monomers are involved in 581 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	A	846	LHG	2	0
28	U	423	LMG	2	0
22	A	807	CLA	1	0
22	A	830	CLA	1	0
22	G	601	CLA	1	0
22	U	412	CLA	1	0
22	K	608	CLA	4	0
22	O	305	CLA	1	0
22	X	408	CLA	1	0
22	Q	604	CLA	5	0
22	A	809	CLA	1	0
22	R	615	CLA	2	0
22	I	601	CLA	2	0
25	F	401	DGD	2	0
22	B	818	CLA	1	0
22	G	602	CLA	1	0
22	A	844	CLA	4	0
22	U	404	CLA	2	0
22	S	604	CLA	1	0
22	B	838	CLA	3	0
22	Q	611	CLA	1	0
26	B	848	LHG	1	0
32	V	616	NEX	9	0
22	A	803	CLA	1	0
22	P	607	CLA	1	0
22	B	805	CLA	1	0
22	I	608	CLA	2	0
22	X	413	CLA	1	0
26	T	614	LHG	1	0
22	A	819	CLA	1	0
22	A	822	CLA	3	0
22	B	859	CLA	2	0
22	A	834	CLA	1	0
22	L	411	CLA	1	0
22	A	831	CLA	2	0
27	U	421	LMU	1	0
22	O	315	CLA	2	0
27	H	321	LMU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	827	CLA	1	0
22	Q	608	CLA	3	0
26	K	616	LHG	3	0
33	A	802	CL0	6	0
22	A	805	CLA	2	0
22	V	604	CLA	7	0
22	A	814	CLA	4	0
31	W	407	CHL	6	0
22	B	831	CLA	2	0
22	B	830	CLA	4	0
22	L	408	CLA	12	0
22	F	403	CLA	2	0
22	B	802	CLA	2	0
28	H	319	LMG	1	0
22	R	601	CLA	6	0
22	A	842	CLA	4	0
22	H	305	CLA	1	0
22	B	824	CLA	3	0
22	W	413	CLA	2	0
27	A	857	LMU	1	0
22	V	608	CLA	1	0
22	S	601	CLA	1	0
30	K	621	SQD	1	0
22	K	603	CLA	2	0
22	V	601	CLA	4	0
22	G	610	CLA	1	0
24	B	841	DD6	1	0
22	W	404	CLA	2	0
23	A	843	PQN	2	0
22	G	609	CLA	3	0
30	V	618	SQD	1	0
22	A	820	CLA	1	0
22	A	827	CLA	2	0
22	L	406	CLA	1	0
26	N	614	LHG	1	0
22	W	411	CLA	2	0
22	H	313	CLA	1	0
22	N	604	CLA	1	0
24	Q	614	DD6	1	0
22	T	605	CLA	4	0
22	O	310	CLA	1	0
22	B	820	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	O	308	CLA	4	0
21	B	842	BCR	2	0
22	V	603	CLA	2	0
22	L	417	CLA	7	0
22	W	410	CLA	3	0
22	R	611	CLA	2	0
22	O	313	CLA	3	0
22	A	812	CLA	3	0
26	R	614	LHG	3	0
22	T	607	CLA	1	0
22	L	412	CLA	3	0
22	W	409	CLA	4	0
31	W	408	CHL	8	0
22	T	608	CLA	2	0
22	V	617	CLA	1	0
22	A	806	CLA	4	0
22	H	308	CLA	2	0
22	S	608	CLA	2	0
27	B	855	LMU	1	0
22	B	811	CLA	1	0
28	K	601	LMG	3	0
22	X	419	CLA	2	0
22	A	829	CLA	1	0
22	A	836	CLA	2	0
22	O	312	CLA	1	0
22	J	102	CLA	1	0
31	V	606	CHL	14	0
22	W	414	CLA	1	0
27	L	420	LMU	2	0
28	Q	602	LMG	2	0
22	O	314	CLA	1	0
22	S	610	CLA	2	0
22	W	415	CLA	1	0
26	S	613	LHG	2	0
21	A	849	BCR	3	0
22	B	809	CLA	4	0
22	G	611	CLA	1	0
22	W	402	CLA	2	0
22	G	608	CLA	4	0
22	Q	609	CLA	1	0
22	Q	613	CLA	2	0
22	N	607	CLA	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	H	310	CLA	1	0
22	A	801	CLA	1	0
22	B	804	CLA	2	0
22	H	312	CLA	3	0
27	O	301	LMU	4	0
22	N	601	CLA	1	0
28	U	402	LMG	2	0
26	W	420	LHG	2	0
25	B	847	DGD	6	0
27	H	301	LMU	1	0
21	B	844	BCR	5	0
22	A	840	CLA	3	0
22	Q	612	CLA	1	0
22	A	817	CLA	2	0
22	N	602	CLA	1	0
22	B	810	CLA	1	0
22	W	412	CLA	2	0
22	A	808	CLA	1	0
27	F	409	LMU	1	0
26	B	851	LHG	7	0
27	A	854	LMU	1	0
22	P	602	CLA	2	0
22	B	825	CLA	3	0
22	F	404	CLA	4	0
22	B	816	CLA	2	0
31	U	408	CHL	4	0
22	B	812	CLA	1	0
23	B	840	PQN	1	0
21	B	845	BCR	2	0
22	B	829	CLA	3	0
22	T	604	CLA	1	0
26	Q	616	LHG	1	0
22	B	832	CLA	3	0
22	T	606	CLA	1	0
22	X	411	CLA	1	0
22	Q	607	CLA	2	0
22	U	409	CLA	1	0
22	B	813	CLA	3	0
26	N	616	LHG	1	0
22	B	834	CLA	5	0
22	V	613	CLA	1	0
30	O	302	SQD	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	O	318	LHG	1	0
27	B	858	LMU	1	0
22	I	606	CLA	2	0
22	B	803	CLA	2	0
22	L	410	CLA	3	0
22	B	828	CLA	2	0
22	P	608	CLA	2	0
22	A	813	CLA	2	0
22	N	606	CLA	4	0
22	N	610	CLA	3	0
22	B	819	CLA	1	0
26	A	845	LHG	1	0
22	A	841	CLA	3	0
22	S	605	CLA	4	0
22	A	852	CLA	4	0
21	B	843	BCR	3	0
22	V	609	CLA	2	0
22	R	607	CLA	3	0
22	K	609	CLA	2	0
22	X	404	CLA	1	0
22	A	804	CLA	3	0
22	O	309	CLA	3	0
30	F	407	SQD	2	0
22	V	607	CLA	2	0
22	K	607	CLA	9	0
27	M	102	LMU	1	0
27	B	854	LMU	8	0
28	B	856	LMG	4	0
22	S	609	CLA	1	0
26	P	601	LHG	1	0
22	G	603	CLA	2	0
22	S	606	CLA	1	0
31	U	407	CHL	3	0
22	R	602	CLA	4	0
22	Q	610	CLA	2	0
22	B	835	CLA	2	0
22	L	402	CLA	2	0
22	V	612	CLA	7	0
22	A	839	CLA	1	0
22	H	311	CLA	2	0
22	S	602	CLA	1	0
22	U	401	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	V	602	CLA	5	0
22	X	409	CLA	1	0
22	B	821	CLA	2	0
22	K	604	CLA	6	0
27	T	618	LMU	2	0
21	A	848	BCR	2	0
21	M	101	BCR	3	0
22	I	607	CLA	3	0
22	U	420	CLA	1	0
28	J	101	LMG	1	0
22	R	606	CLA	3	0
22	R	604	CLA	5	0
22	B	836	CLA	2	0
22	O	311	CLA	3	0
22	K	617	CLA	2	0
22	N	603	CLA	2	0
22	A	821	CLA	1	0
22	P	603	CLA	1	0
22	A	824	CLA	4	0
22	Q	603	CLA	1	0
28	W	401	LMG	3	0
32	U	418	NEX	4	0
22	W	406	CLA	3	0
22	U	411	CLA	1	0
22	A	823	CLA	1	0
22	B	833	CLA	4	0
22	B	822	CLA	3	0
28	T	616	LMG	2	0
26	O	321	LHG	3	0
22	B	815	CLA	3	0
31	W	422	CHL	2	0
22	K	606	CLA	2	0
25	O	304	DGD	3	0
22	B	814	CLA	1	0
22	R	605	CLA	5	0
22	B	817	CLA	1	0
21	A	851	BCR	3	0
22	P	605	CLA	1	0
21	B	846	BCR	1	0
22	B	806	CLA	4	0
22	A	811	CLA	1	0
24	S	611	DD6	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	U	415	CLA	2	0
22	K	611	CLA	3	0
22	I	602	CLA	1	0
22	S	607	CLA	1	0
22	B	807	CLA	2	0
22	O	307	CLA	1	0
22	K	605	CLA	3	0
22	I	603	CLA	3	0
22	A	825	CLA	2	0
28	F	408	LMG	3	0
26	L	416	LHG	3	0
22	Q	601	CLA	1	0
28	I	615	LMG	1	0
22	H	307	CLA	1	0
22	K	613	CLA	4	0
22	A	832	CLA	3	0
22	A	828	CLA	4	0
22	B	823	CLA	3	0
21	B	801	BCR	8	0
22	A	816	CLA	2	0
22	L	404	CLA	6	0
31	V	605	CHL	12	0
22	B	839	CLA	2	0
22	T	611	CLA	1	0
22	A	815	CLA	2	0
22	P	606	CLA	3	0
22	Q	605	CLA	1	0
22	A	838	CLA	3	0
27	K	620	LMU	2	0
22	R	610	CLA	3	0
28	H	322	LMG	1	0
22	P	610	CLA	1	0
22	L	409	CLA	2	0
22	X	403	CLA	1	0
22	I	611	CLA	4	0
22	U	406	CLA	1	0
28	N	615	LMG	1	0
27	L	419	LMU	4	0
27	U	424	LMU	1	0
22	A	833	CLA	1	0
22	U	405	CLA	3	0
22	P	609	CLA	1	0

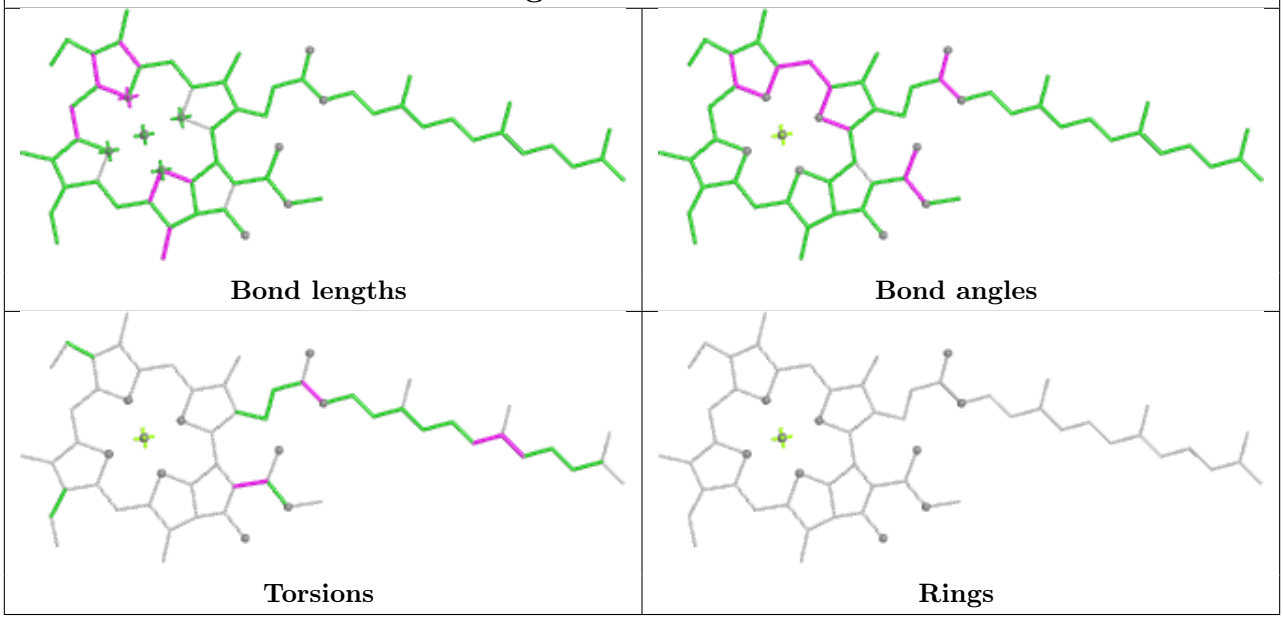
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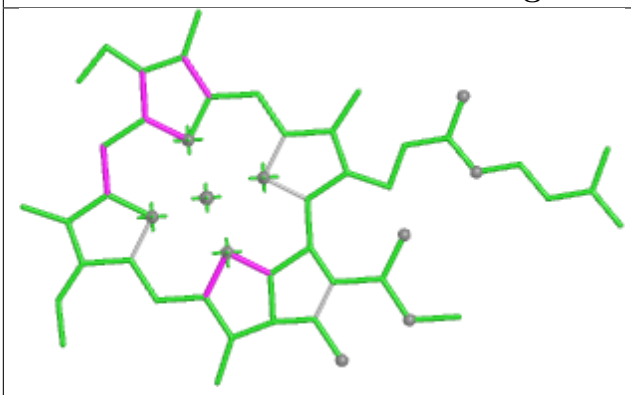
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	J	103	BCR	1	0

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

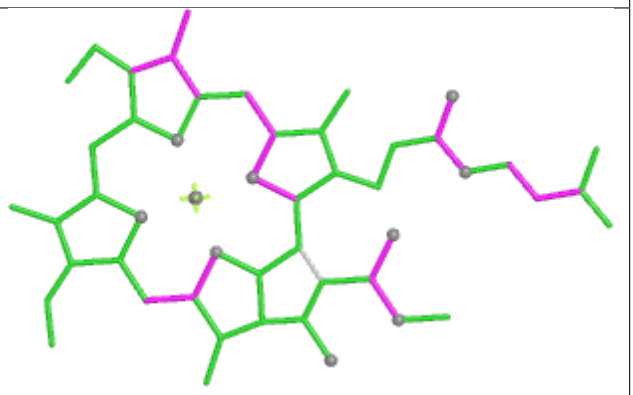
Ligand CLA T 603



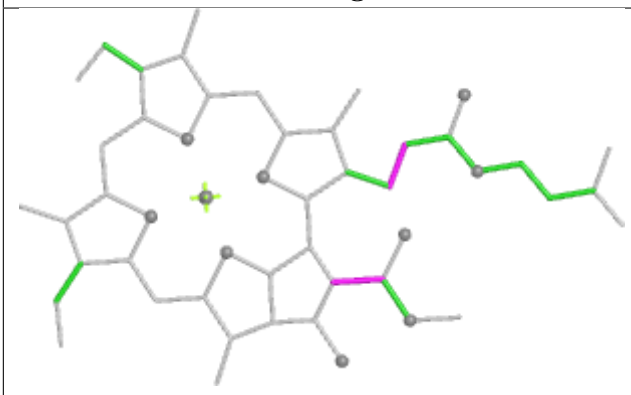
Ligand CLA X 417



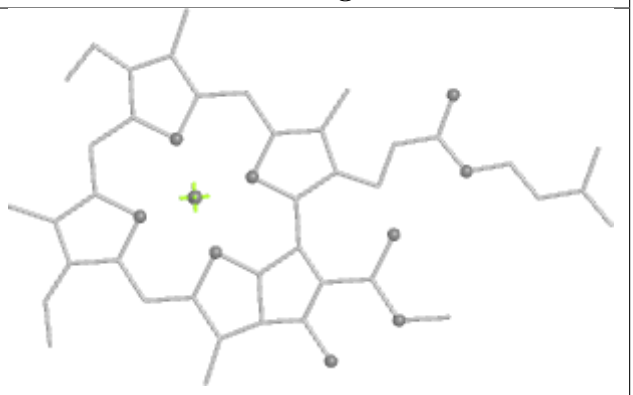
Bond lengths



Bond angles

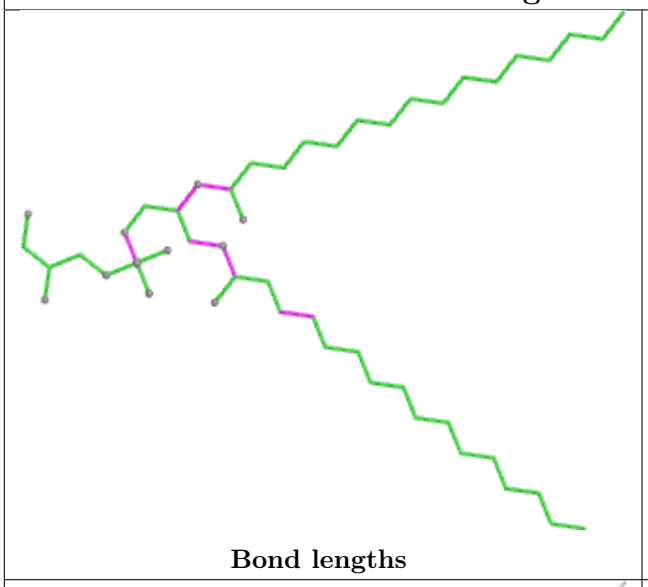


Torsions

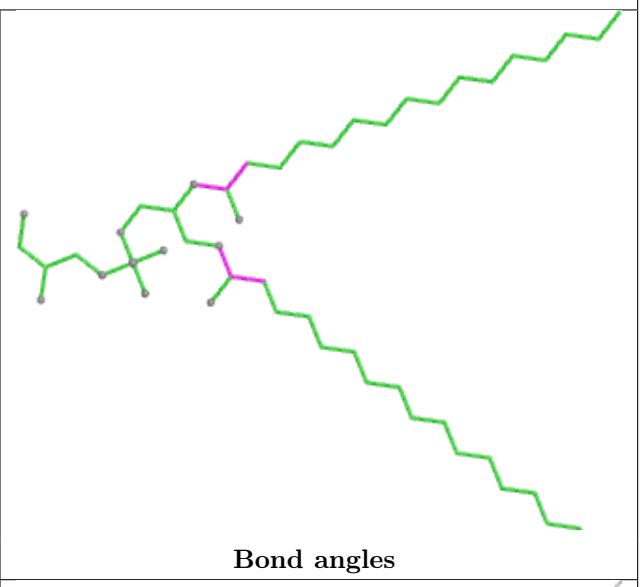


Rings

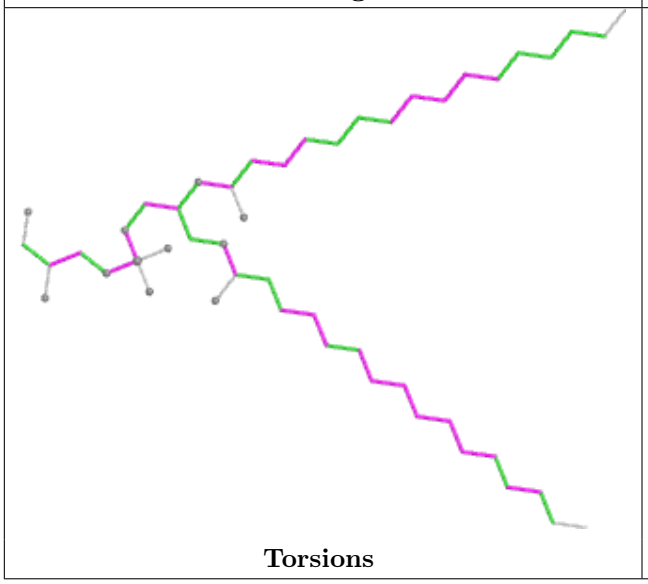
Ligand LHG A 846



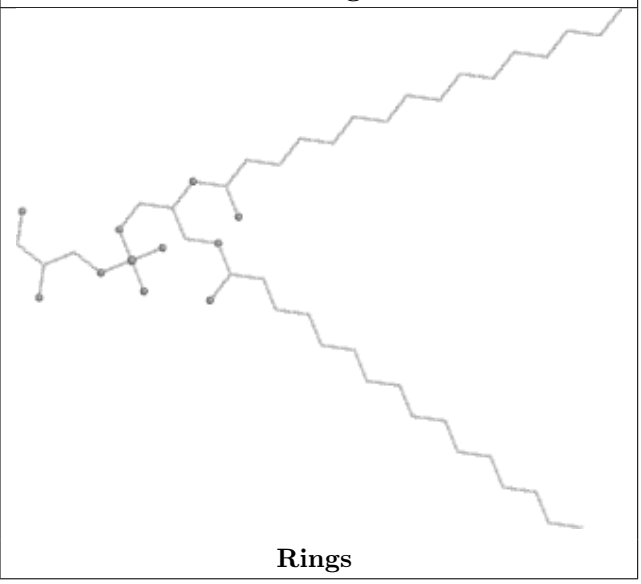
Bond lengths



Bond angles

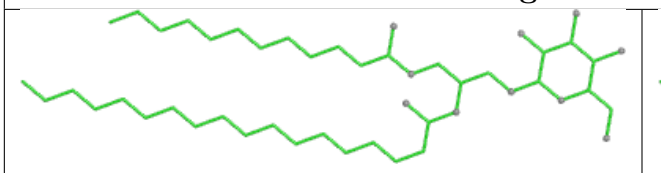


Torsions



Rings

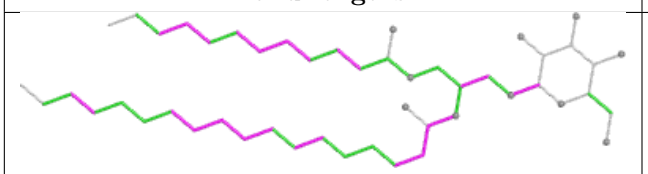
Ligand LMG U 423



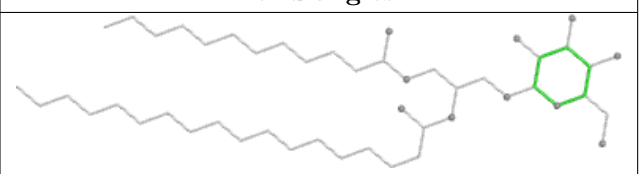
Bond lengths



Bond angles

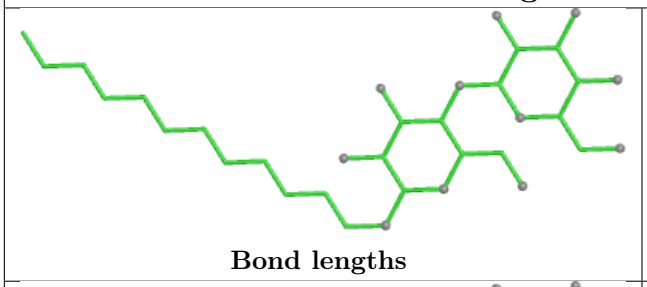


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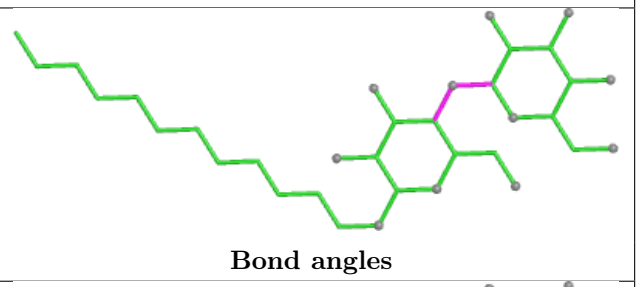


Rings

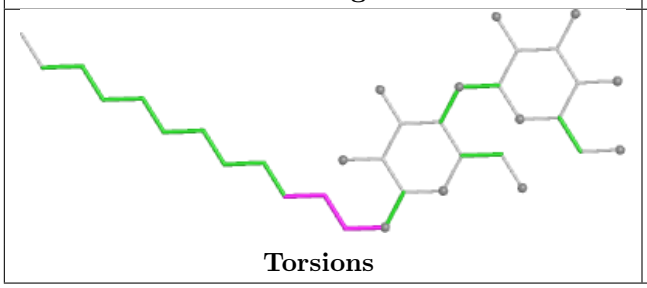
Ligand LMU X 421



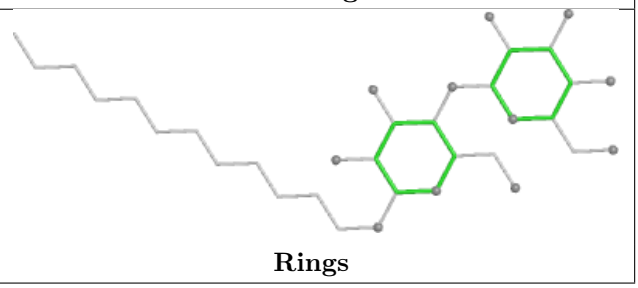
Bond lengths



Bond angles

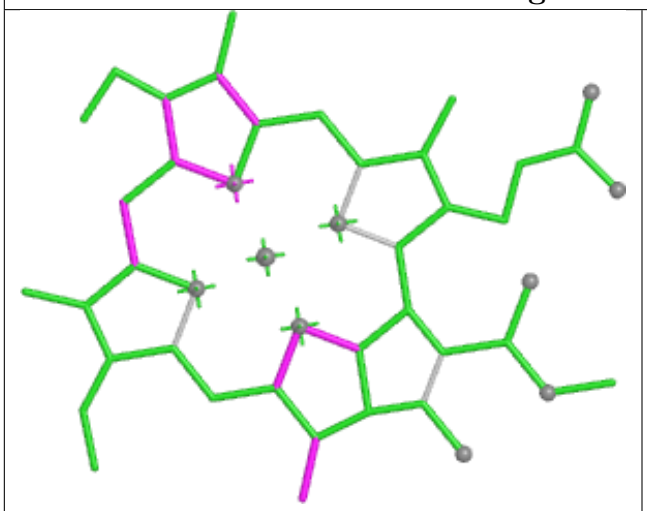


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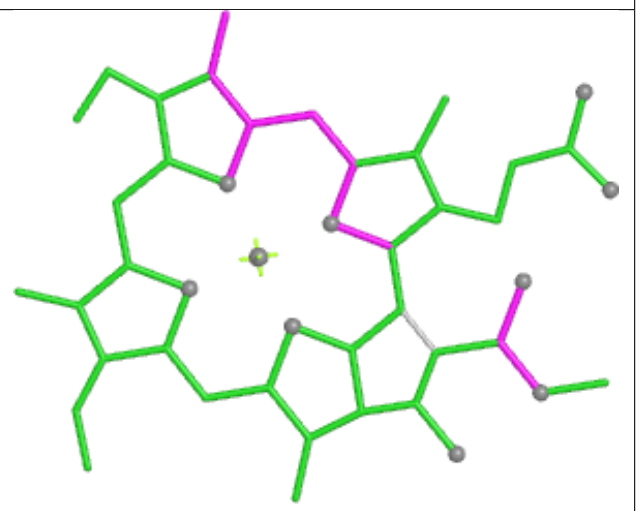


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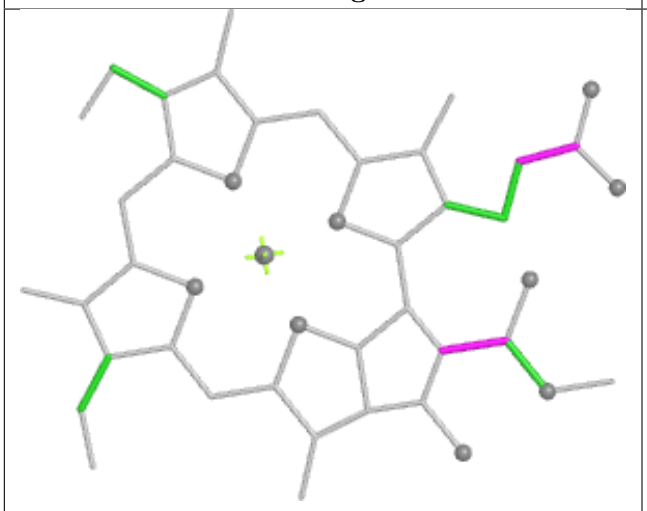
Ligand CLA S 603



Bond lengths



Bond angles

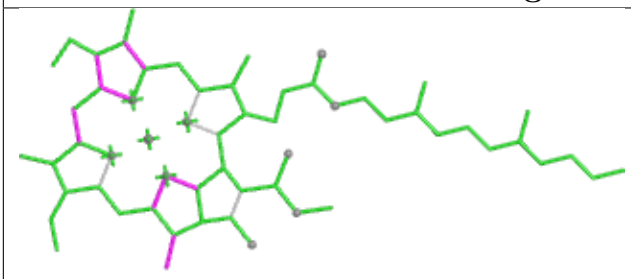


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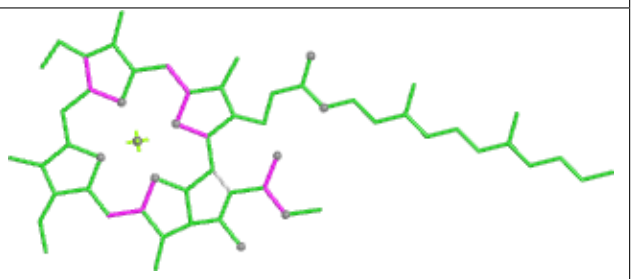


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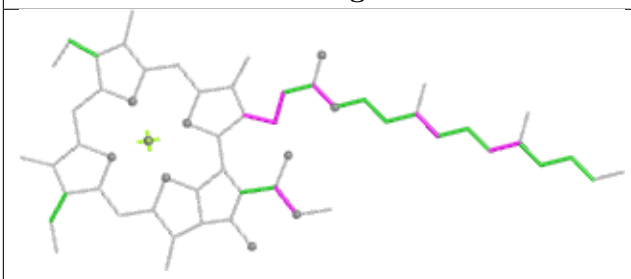
Ligand CLA B 826



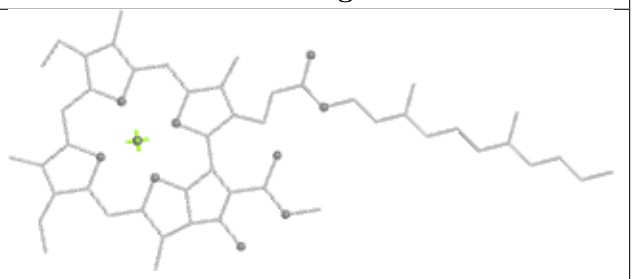
Bond lengths



Bond angles

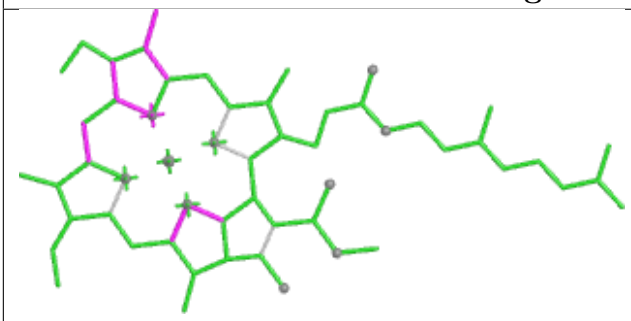


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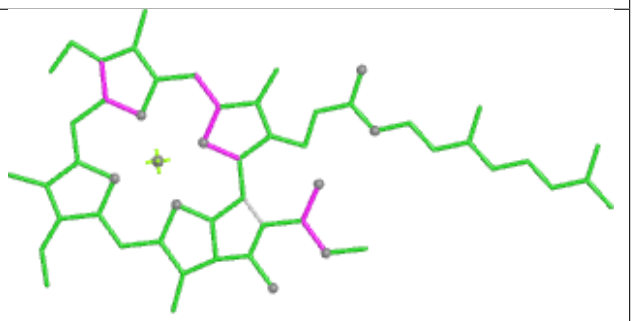


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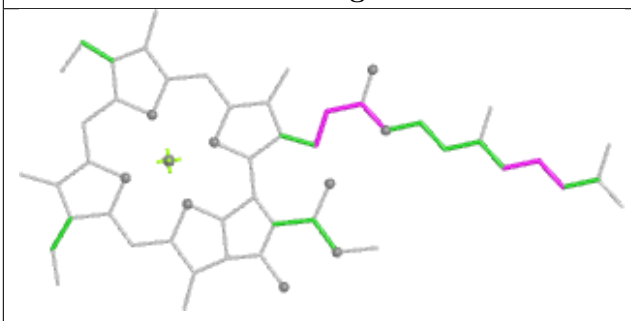
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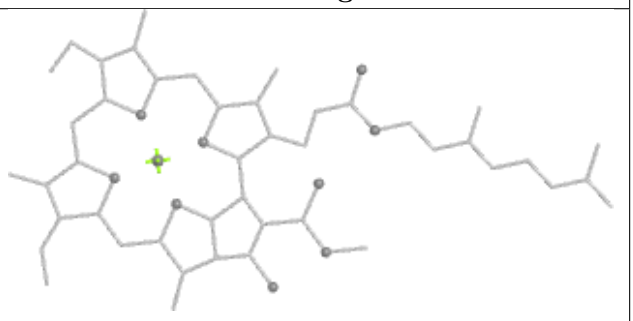
Bond lengths



Bond angles

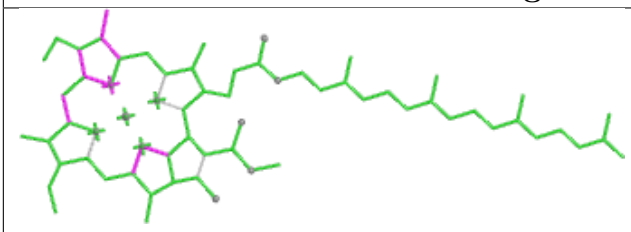


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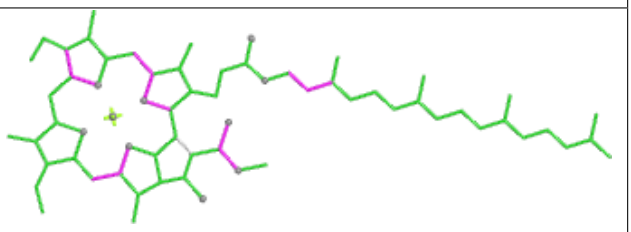


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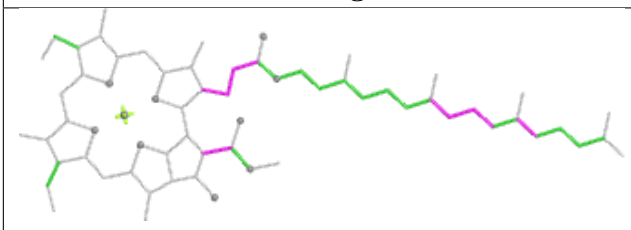
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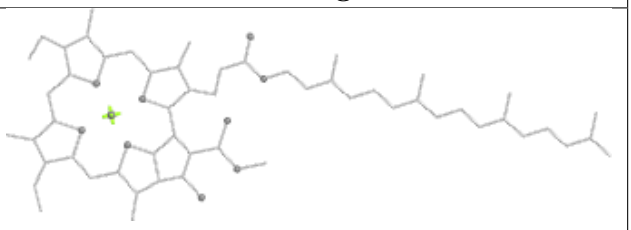
Bond lengths



Bond angles

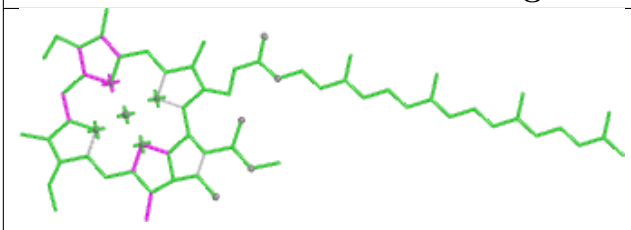


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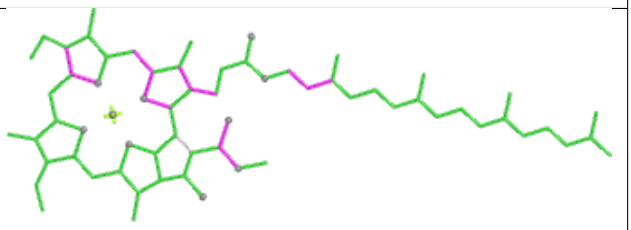


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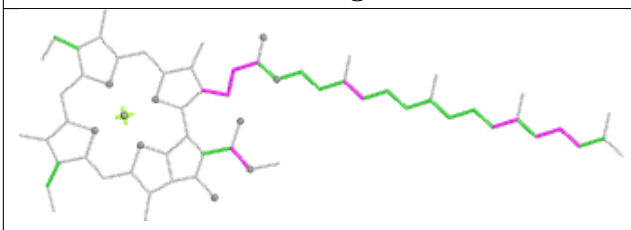
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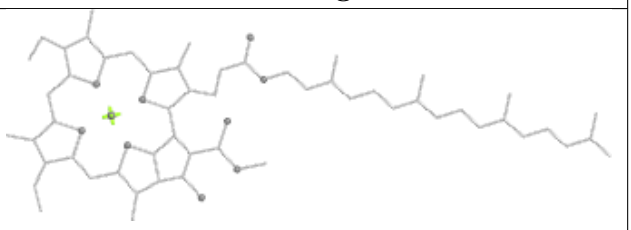
Bond lengths



Bond angles

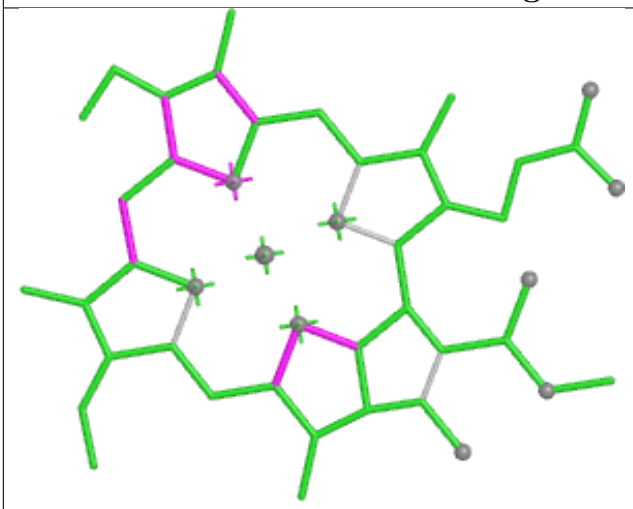


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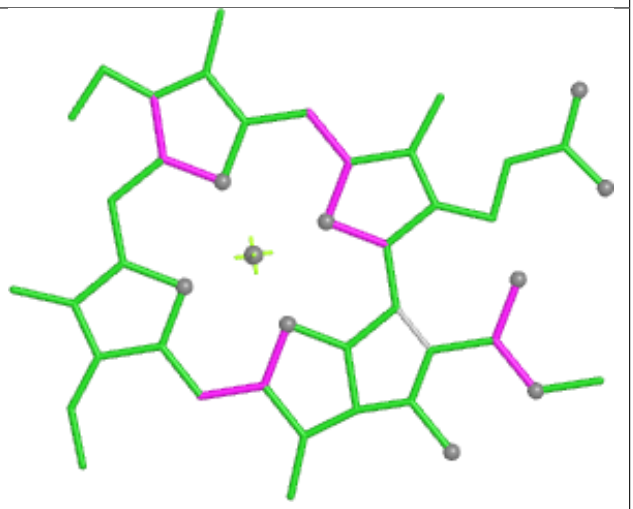


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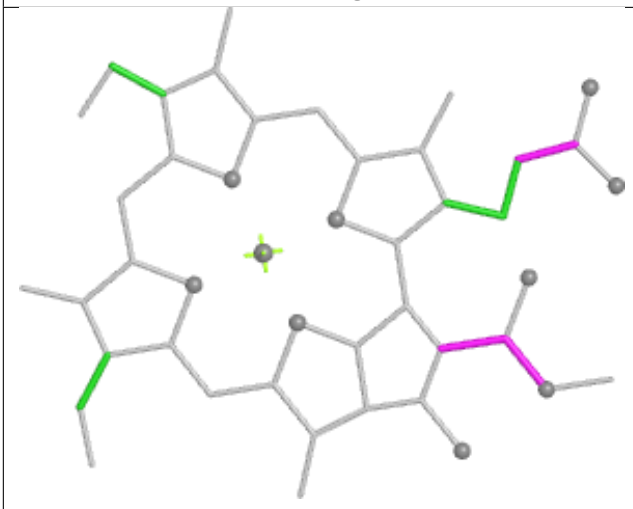
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Bond lengths



Bond angles

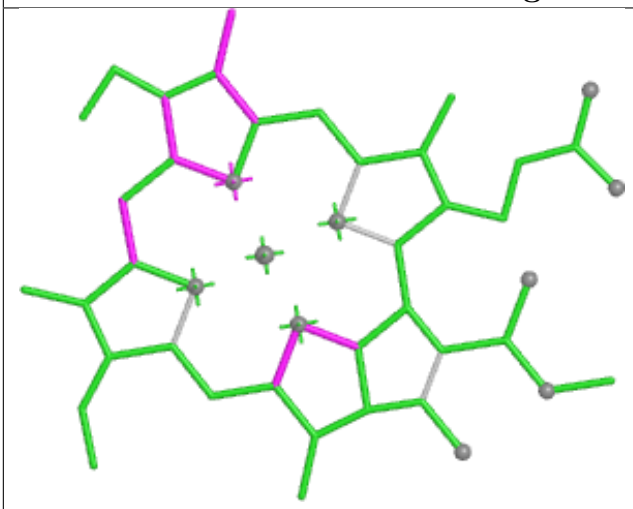


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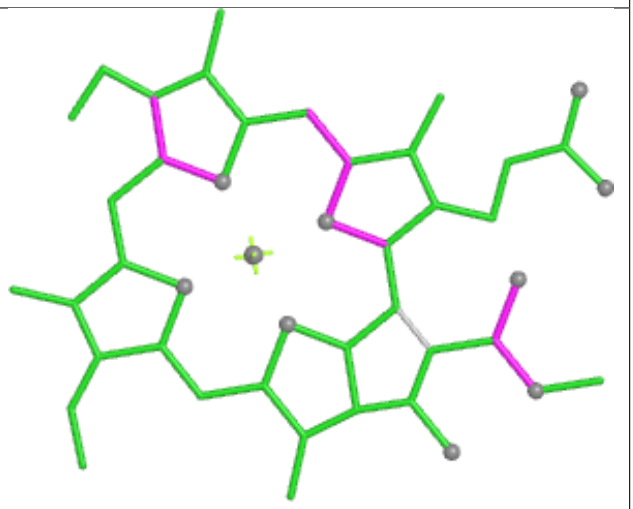


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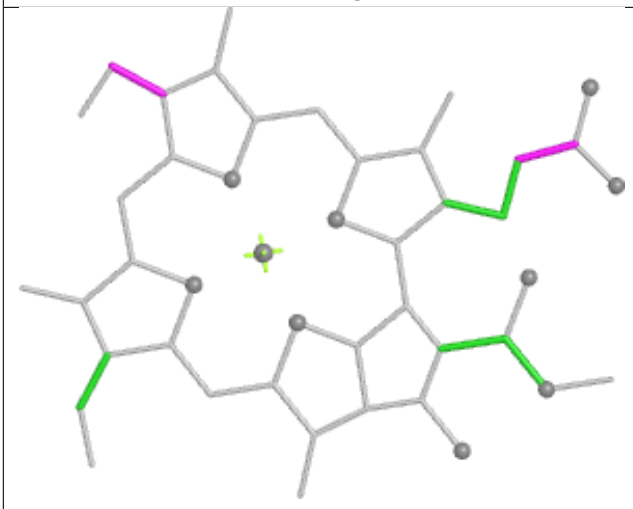
Ligand CLA U 412



Bond lengths



Bond angles

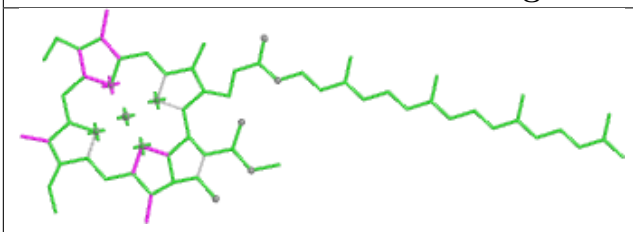


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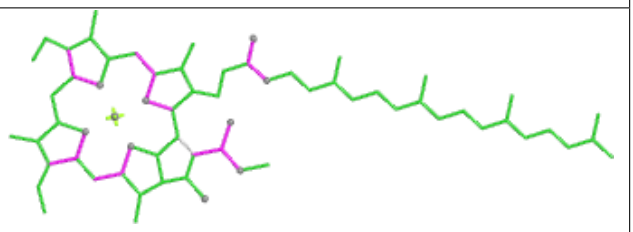


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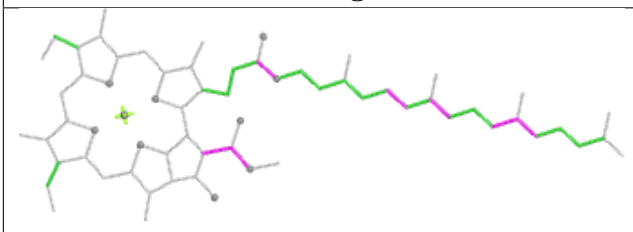
Ligand CLA K 608



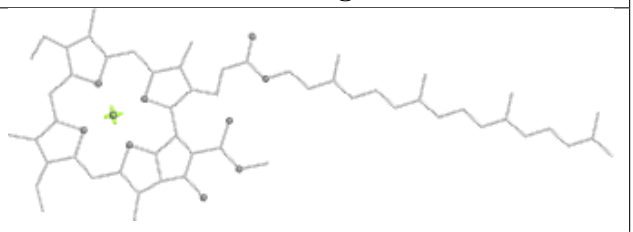
Bond lengths



Bond angles

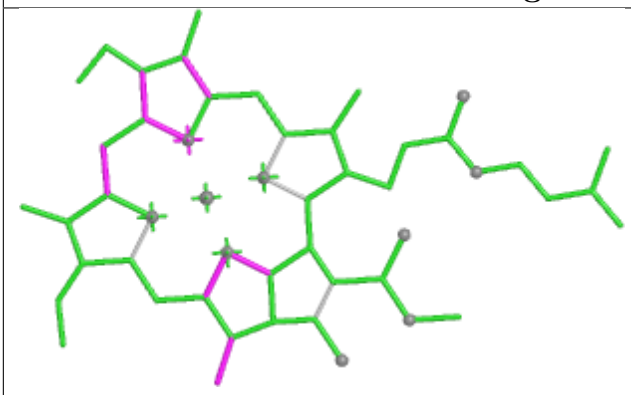


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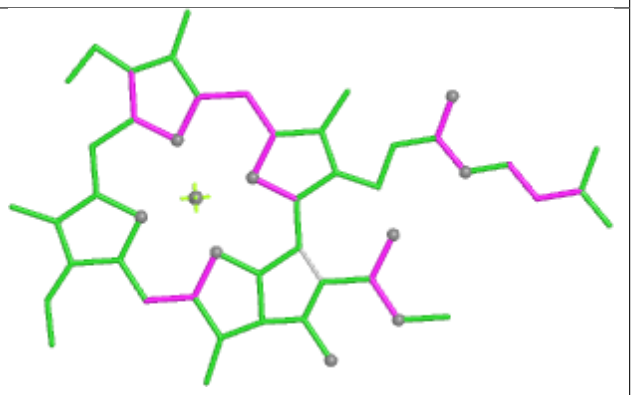


Rings

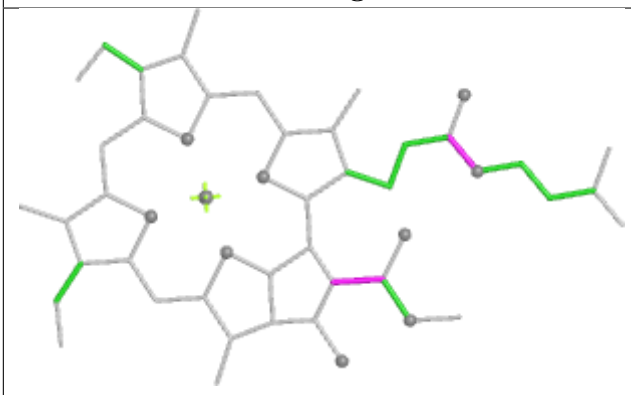
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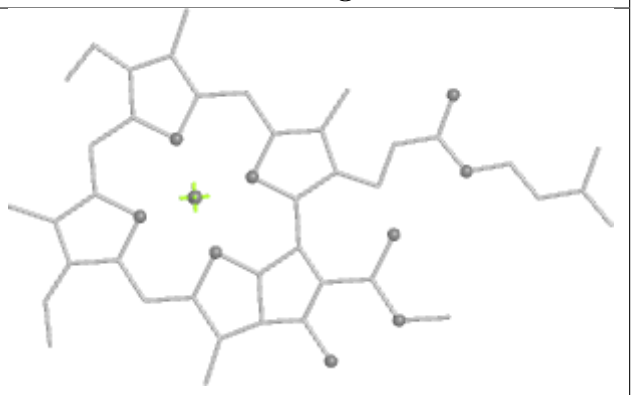
Bond lengths



Bond angles

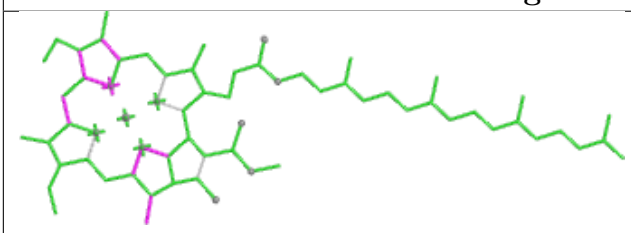


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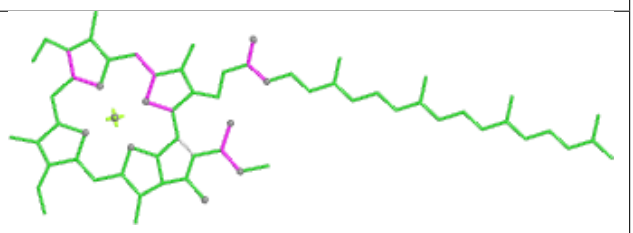


Rings

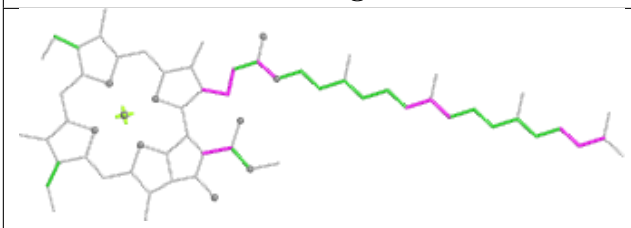
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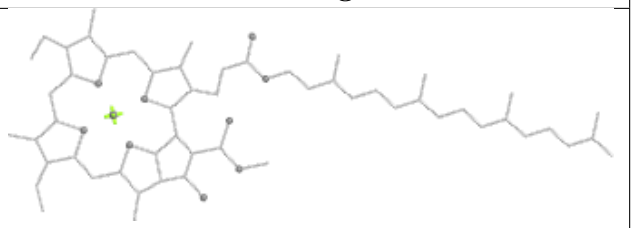
Bond lengths



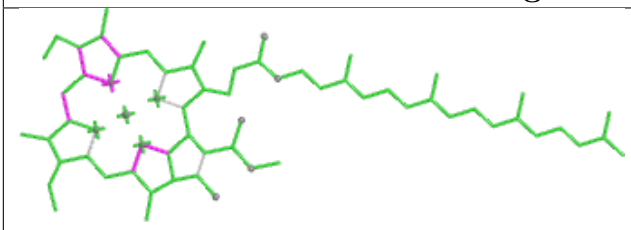
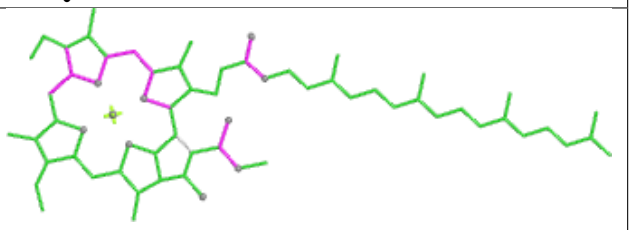
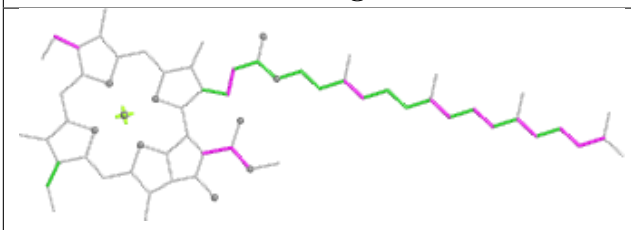
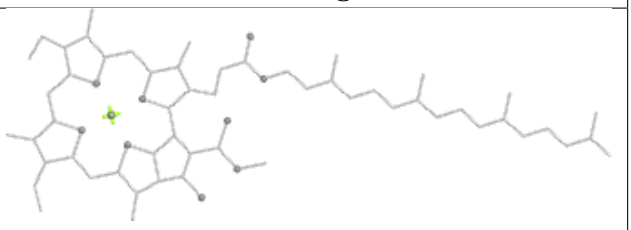
Bond angles

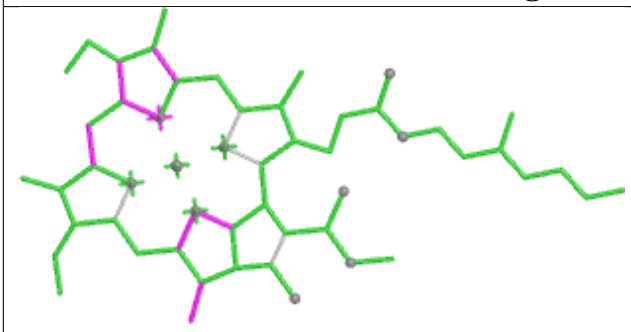
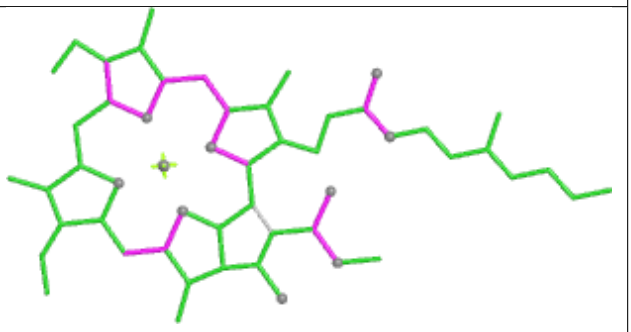
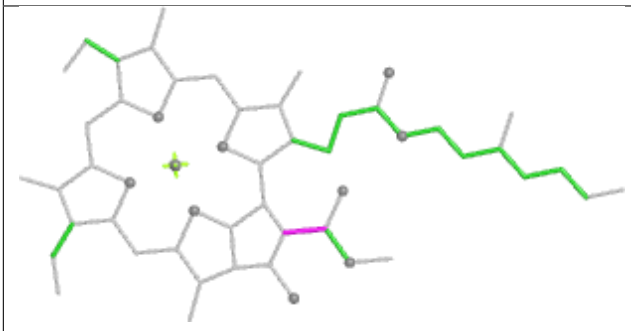
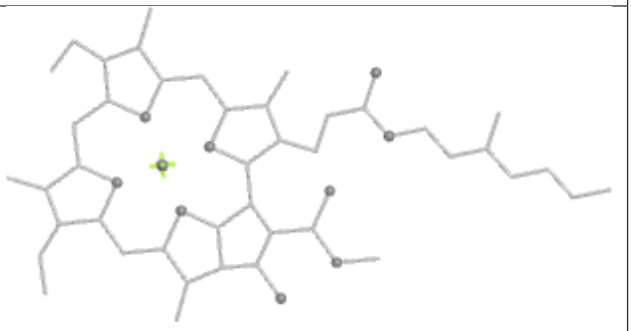


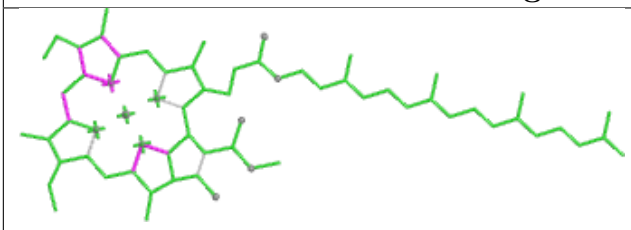
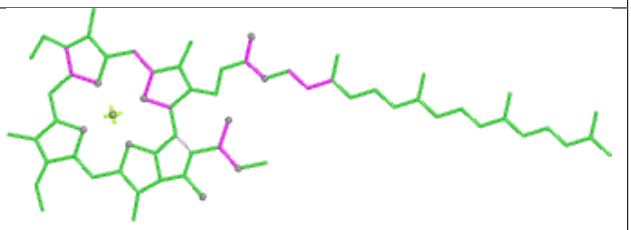
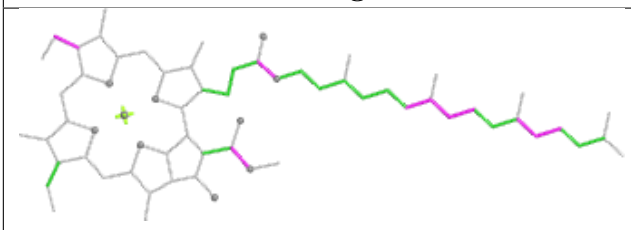
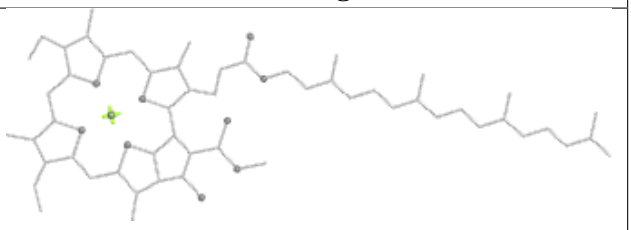
Torsions

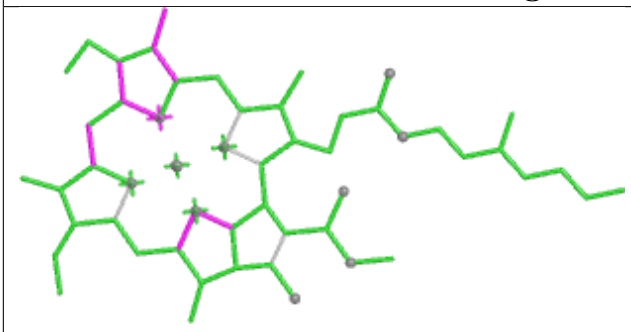
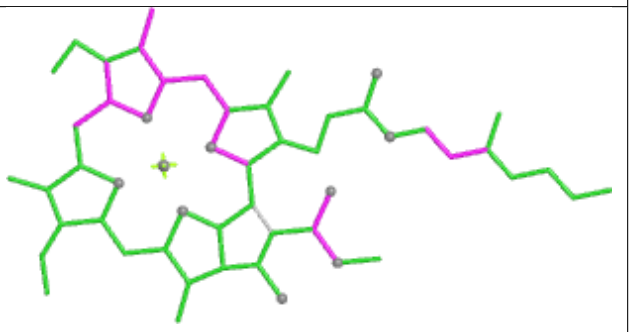
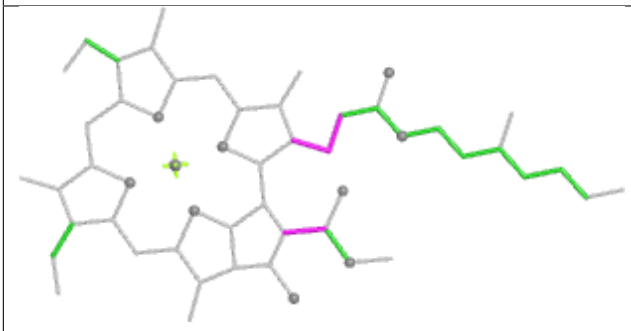
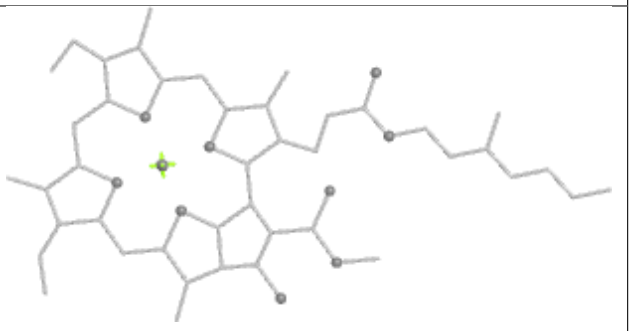


Rings

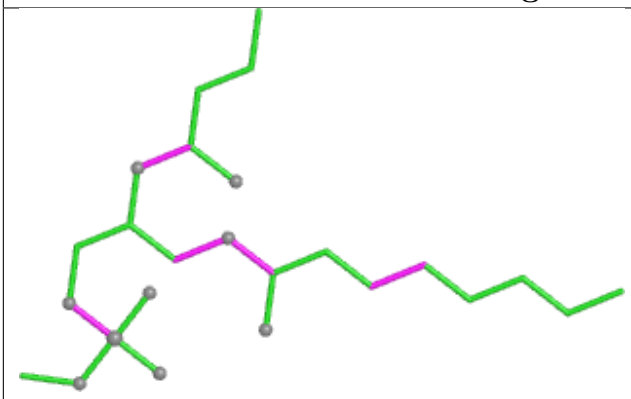
Ligand CLA Q 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 809	
 Bond lengths	 Bond angles
 Torsions	 Rings

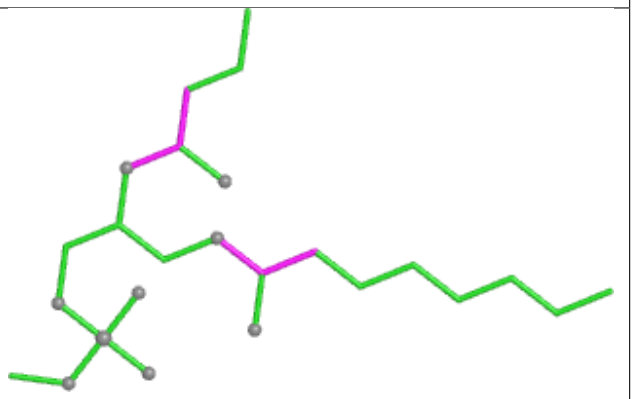
Ligand CLA R 615	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 818	
 Bond lengths	 Bond angles
 Torsions	 Rings

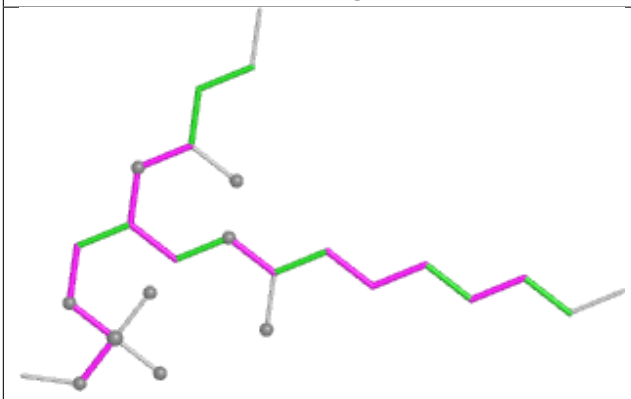
Ligand LHG U 419



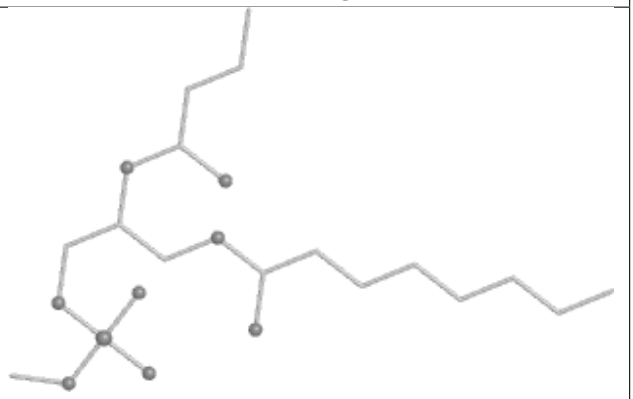
Bond lengths



Bond angles

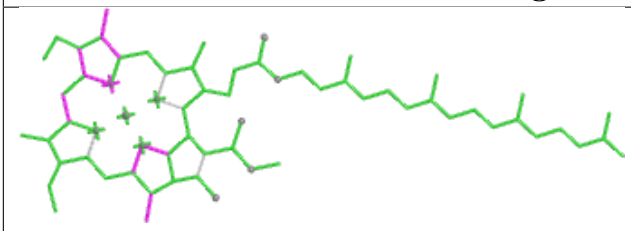


Torsions

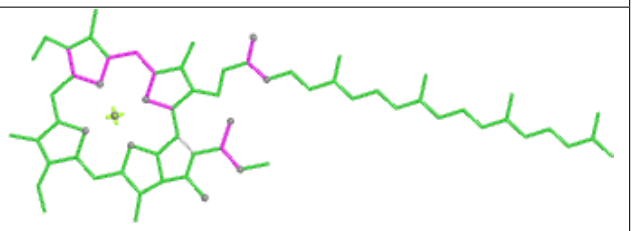


Rings

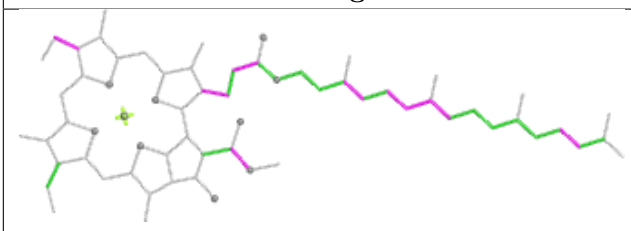
Ligand CLA I 601



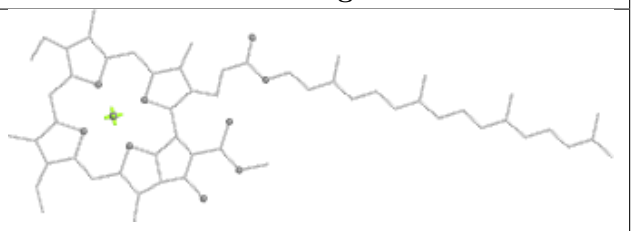
Bond lengths



Bond angles

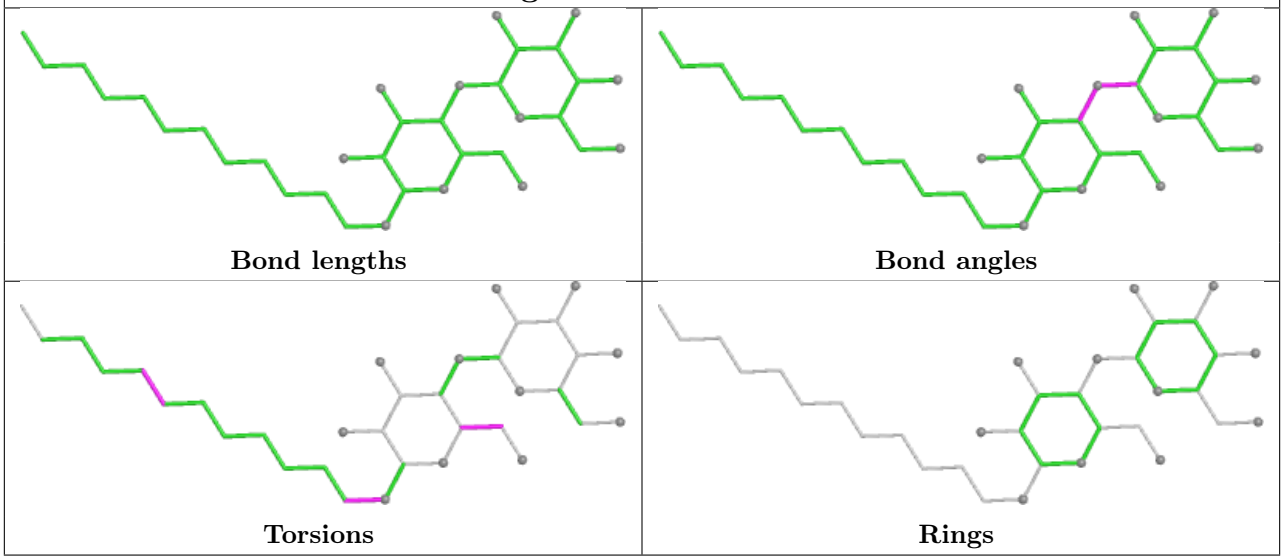


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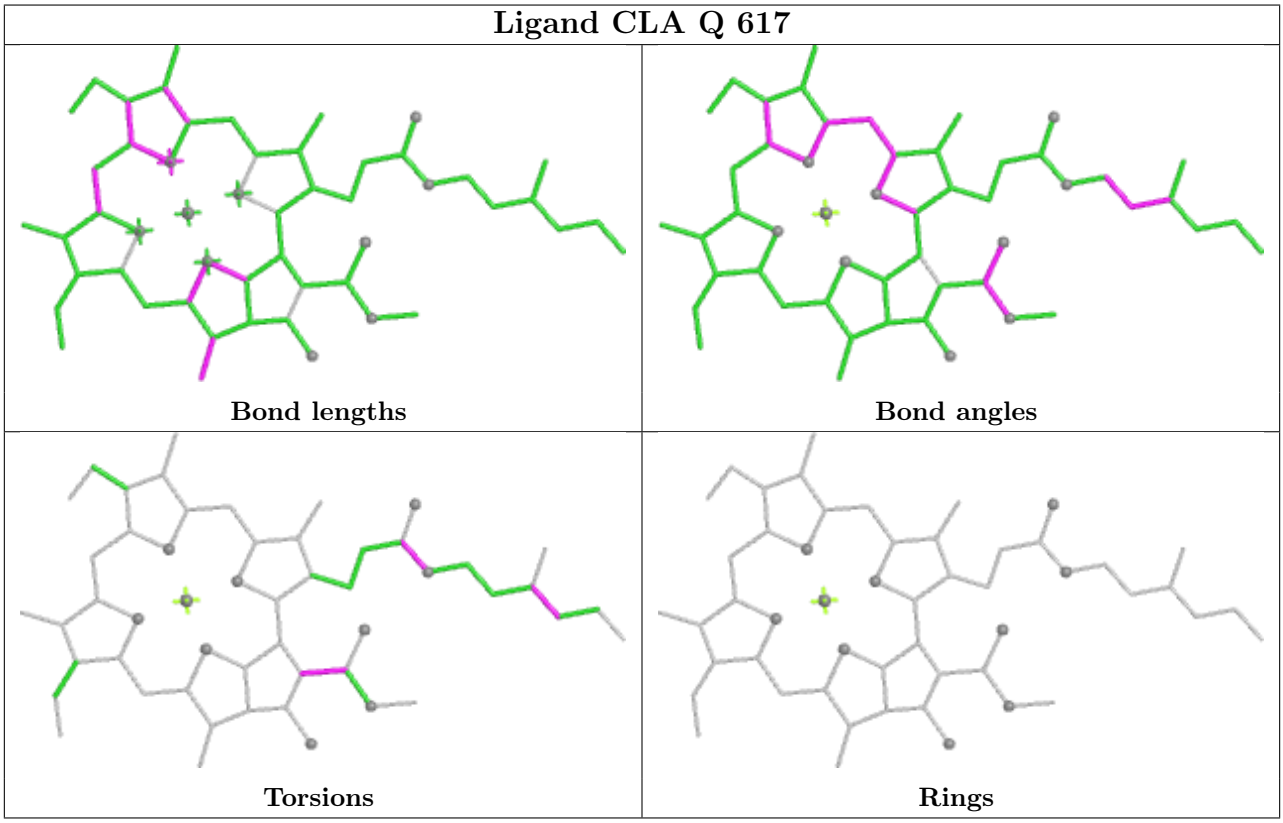


Rings

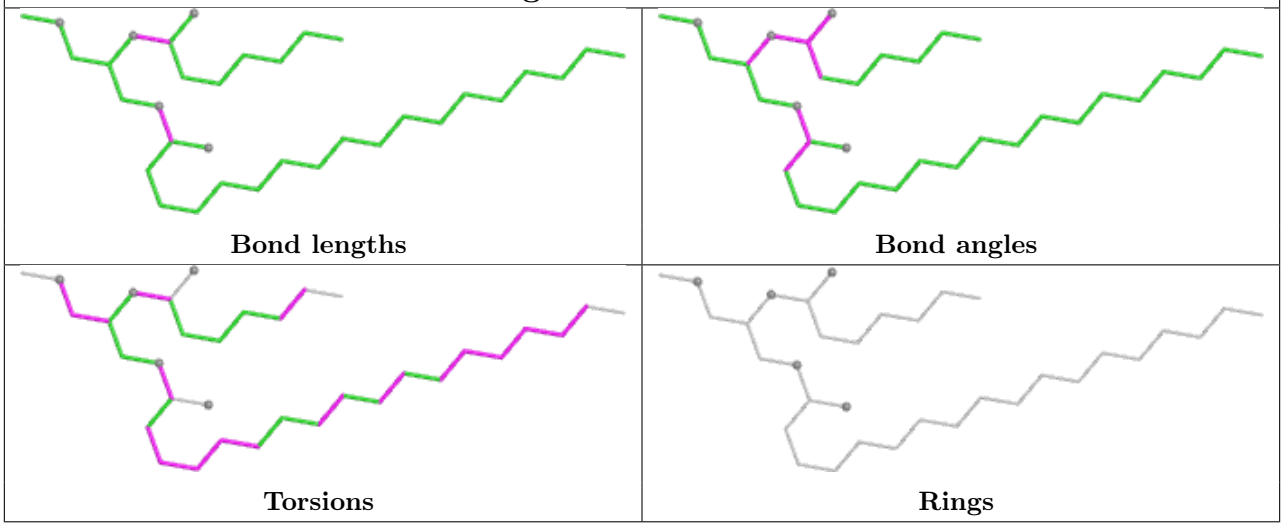
Ligand LMU B 857



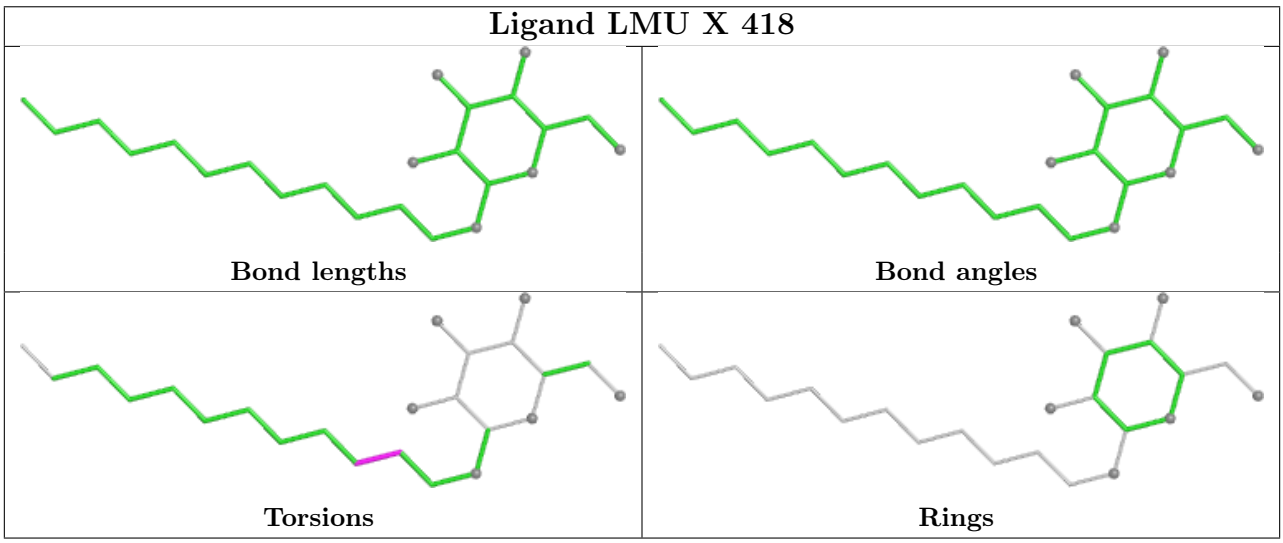
Ligand CLA Q 617



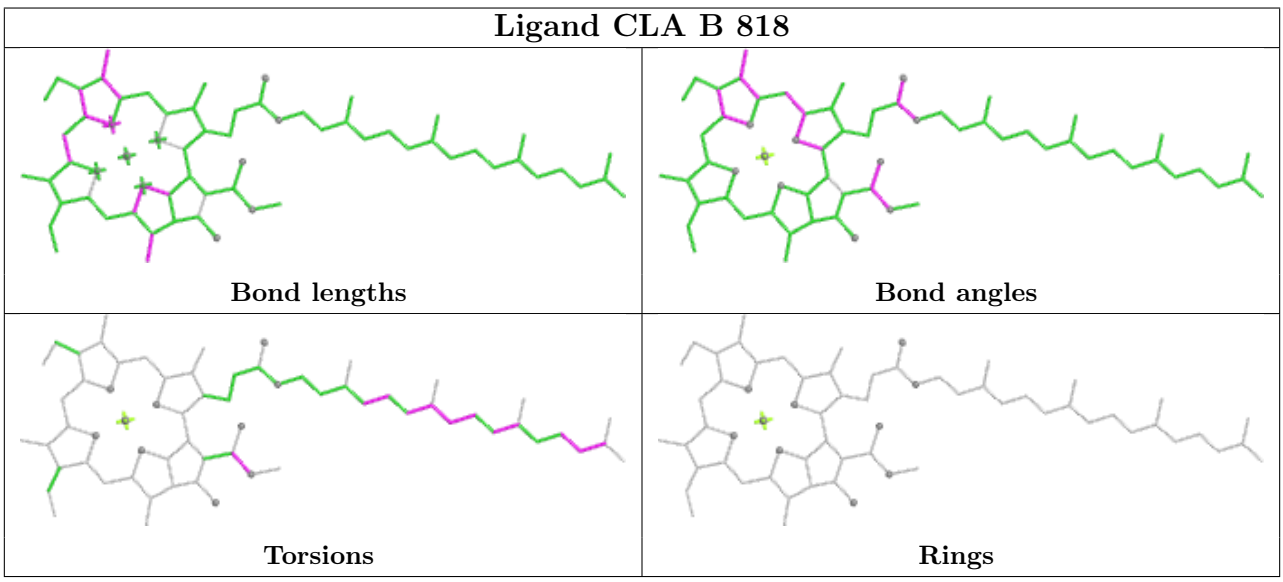
Ligand DGD F 401



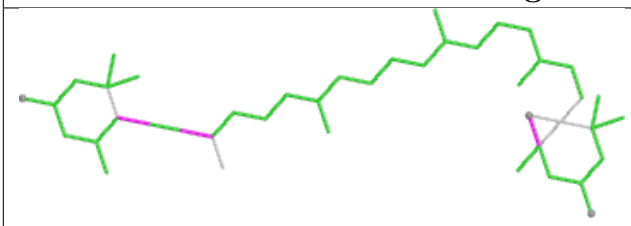
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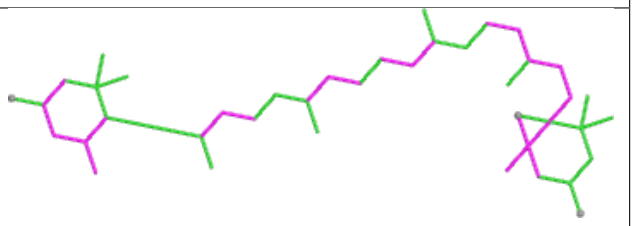
Ligand CLA B 818



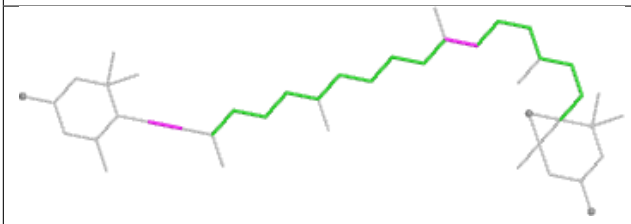
Ligand DD6 V 615



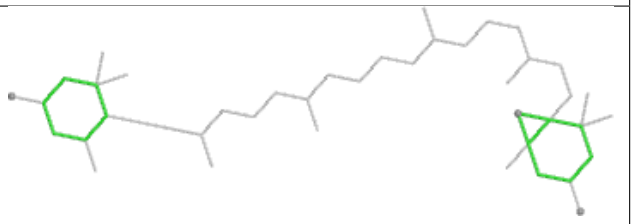
Bond lengths



Bond angles

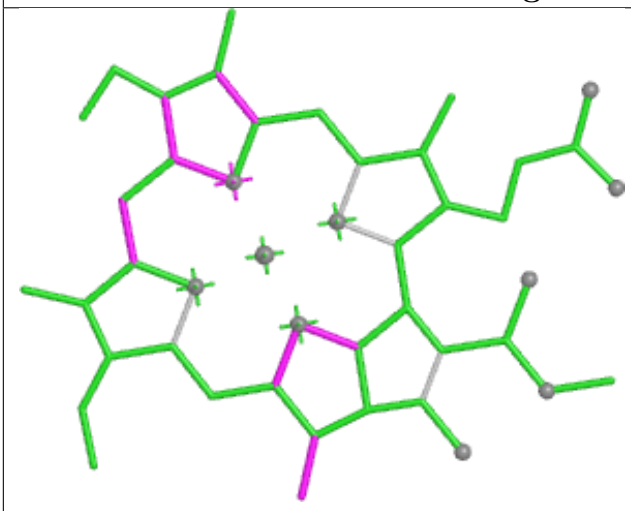


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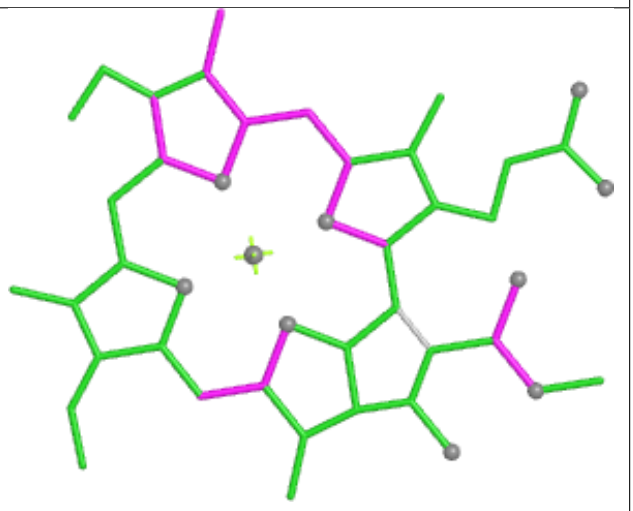


Rings

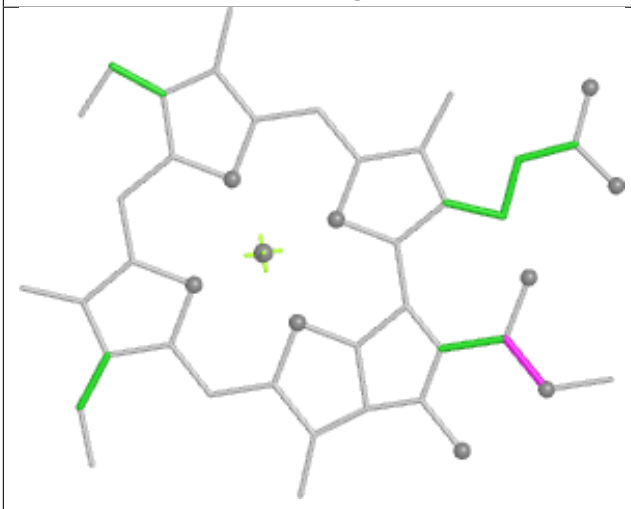
Ligand CLA K 612



Bond lengths



Bond angles

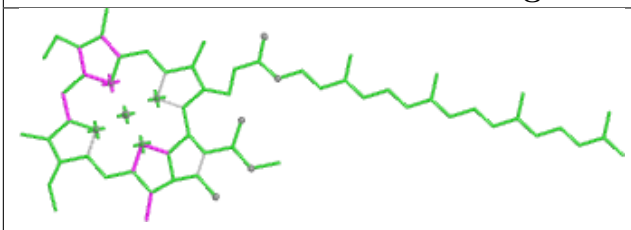


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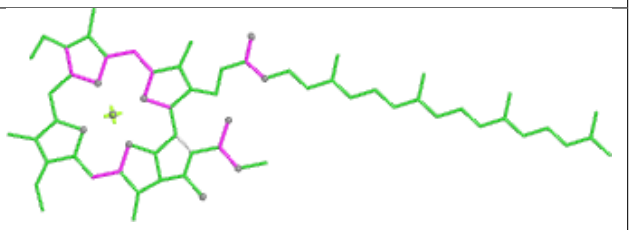


Rings

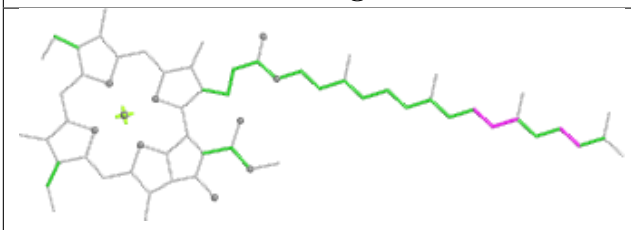
Ligand CLA X 407



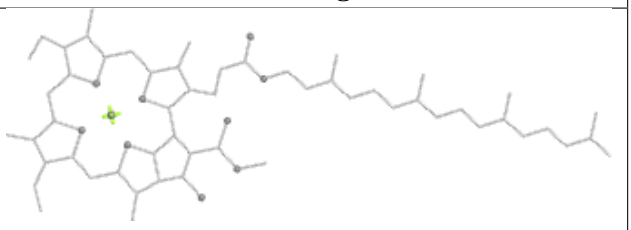
Bond lengths



Bond angles

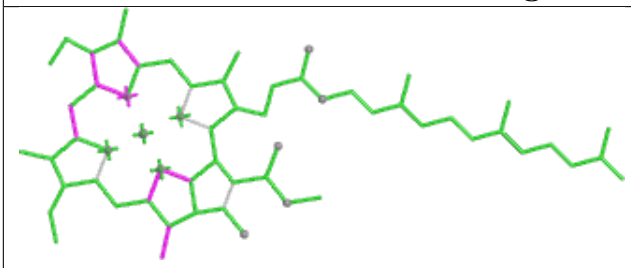


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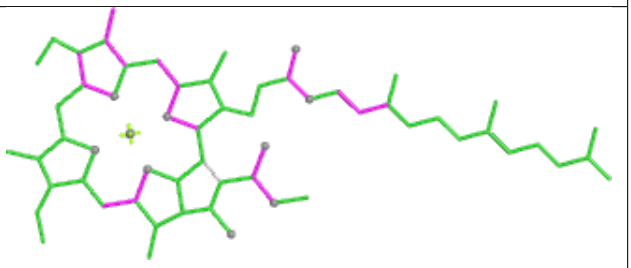


Rings

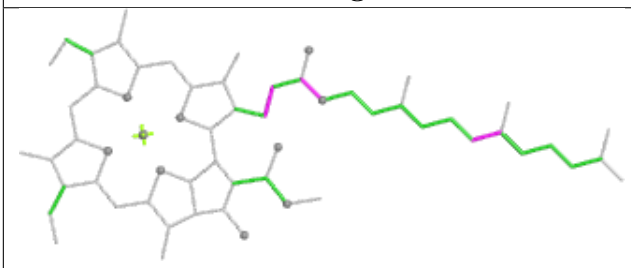
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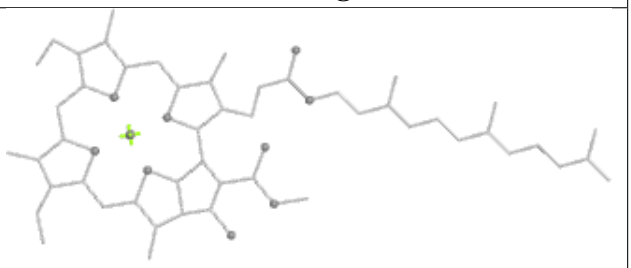
Bond lengths



Bond angles

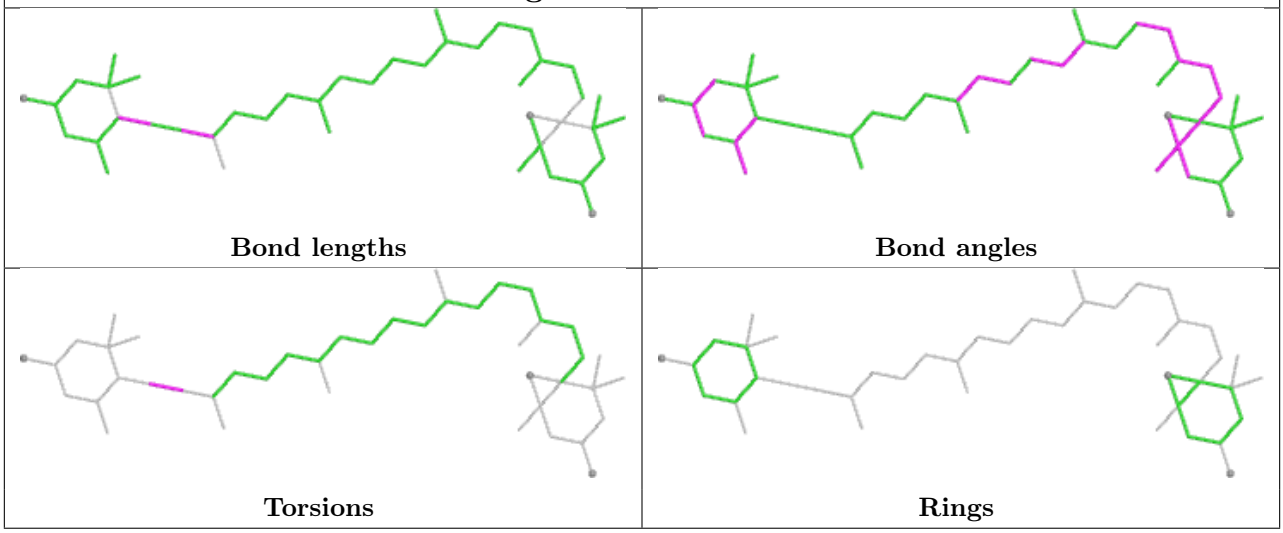


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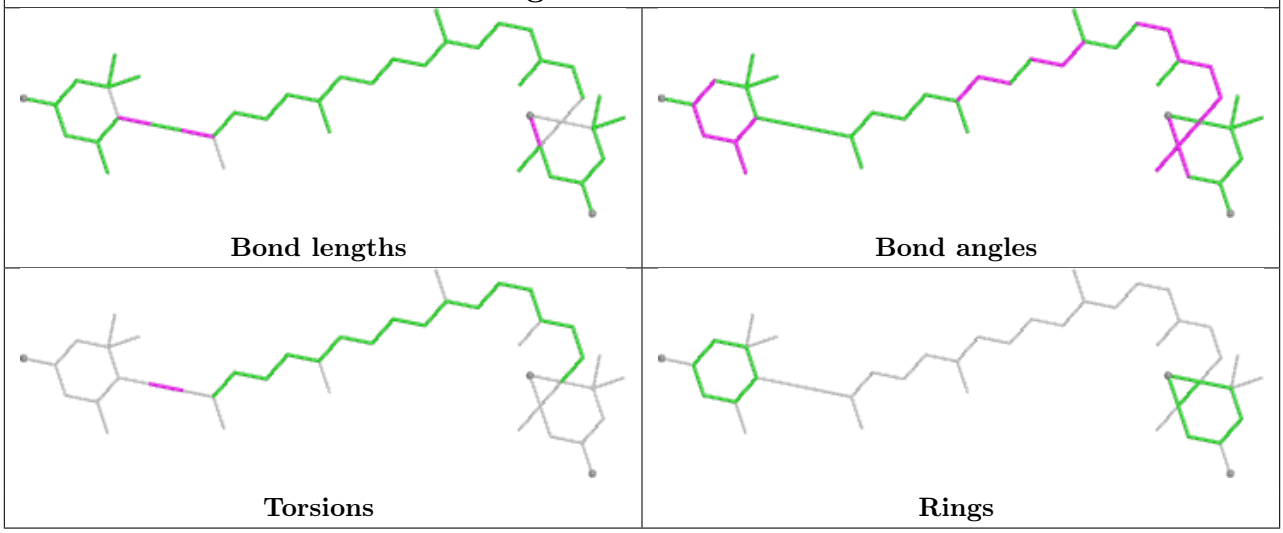


Rings

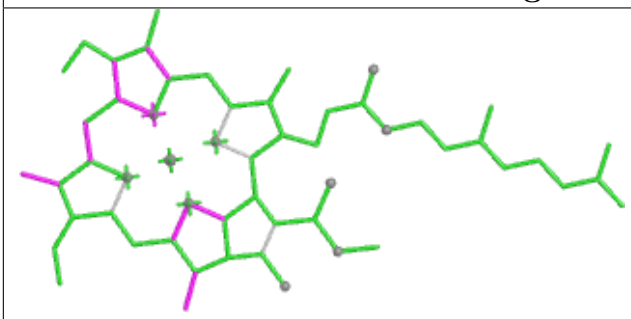
Ligand DD6 X 415



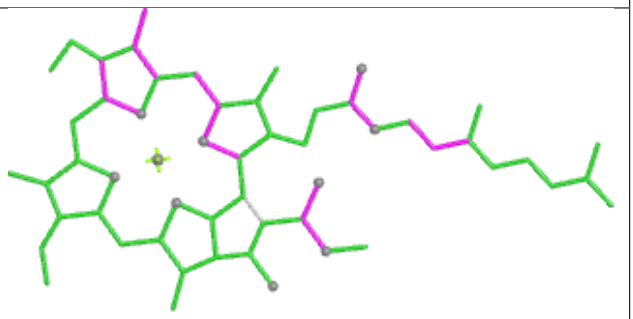
Ligand DD6 T 613



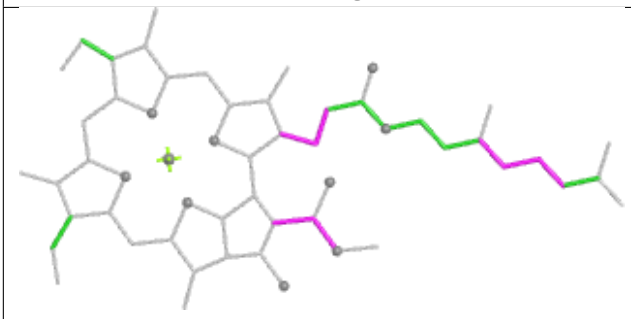
Ligand CLA A 844



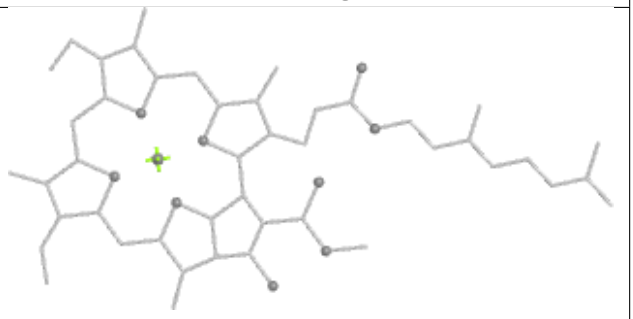
Bond lengths



Bond angles

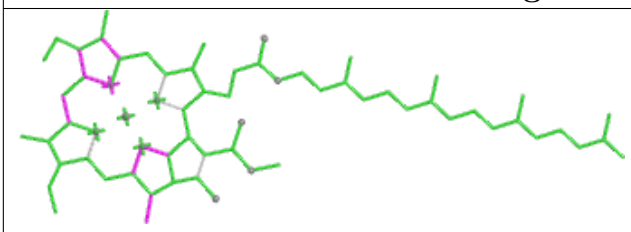


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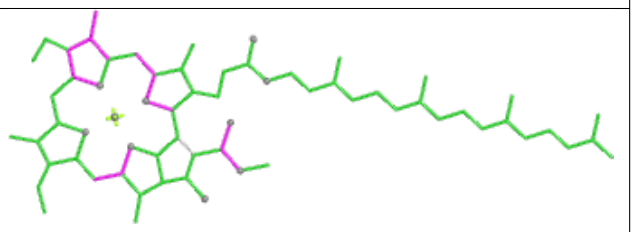


Rings

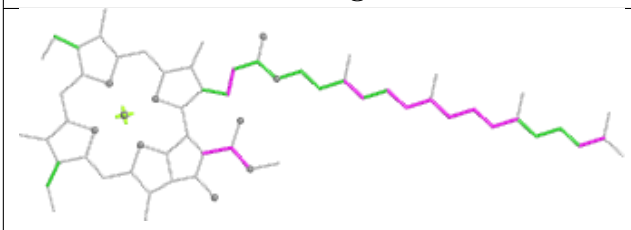
Ligand CLA U 404



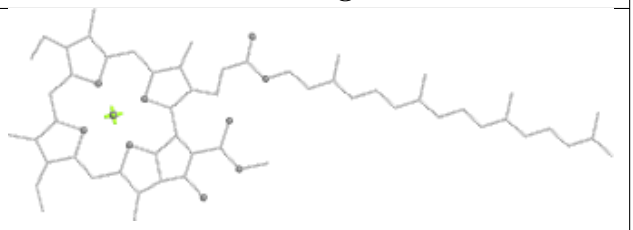
Bond lengths



Bond angles

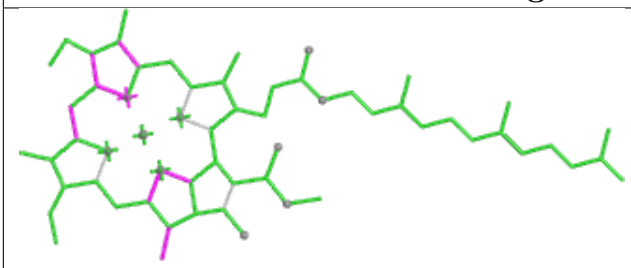


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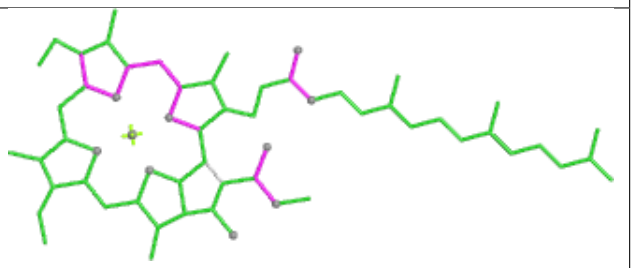


Rings

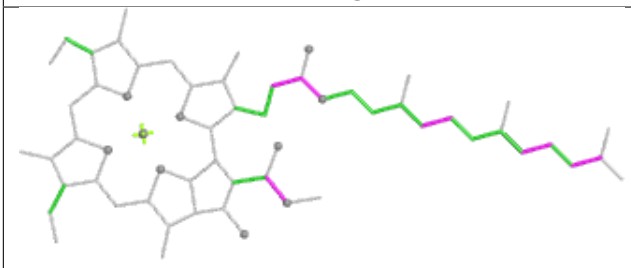
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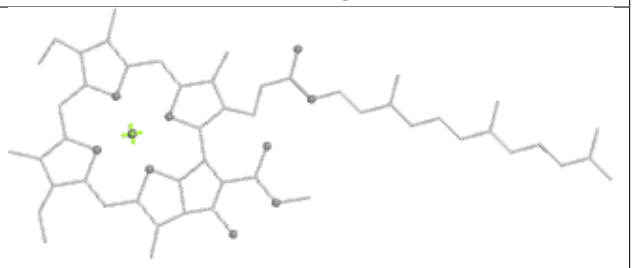
Bond lengths



Bond angles

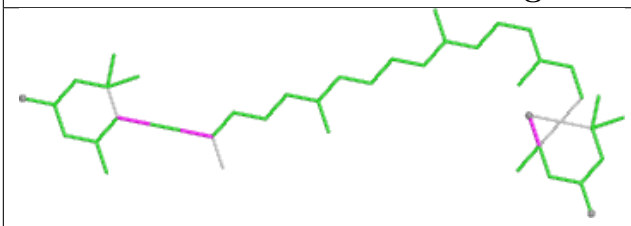


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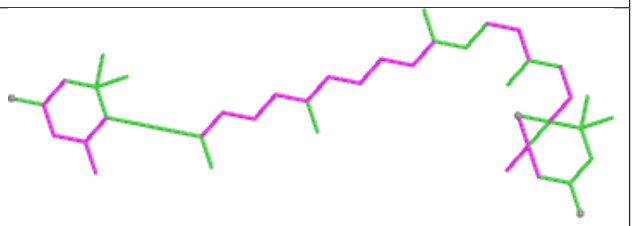


Rings

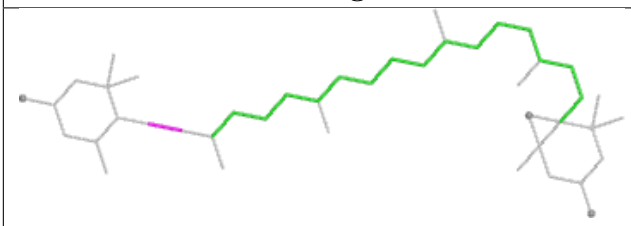
Ligand DD6 A 859



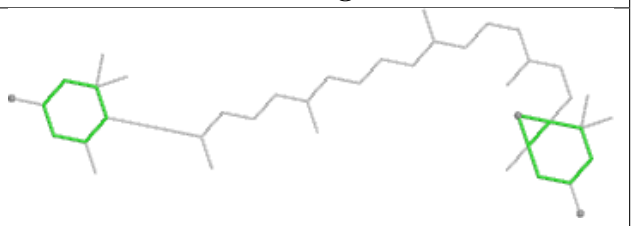
Bond lengths



Bond angles

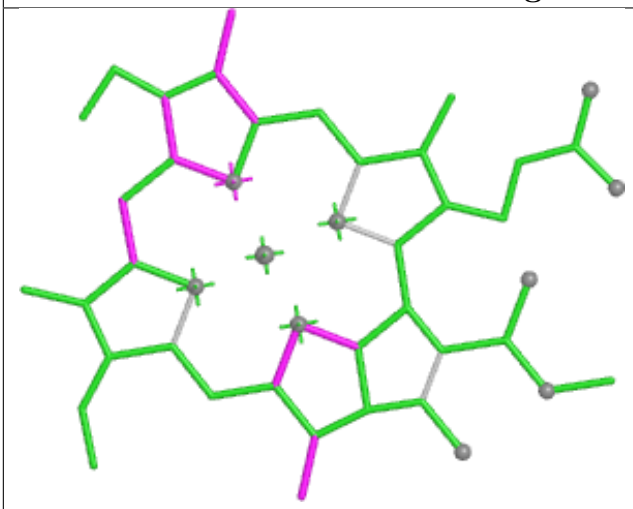


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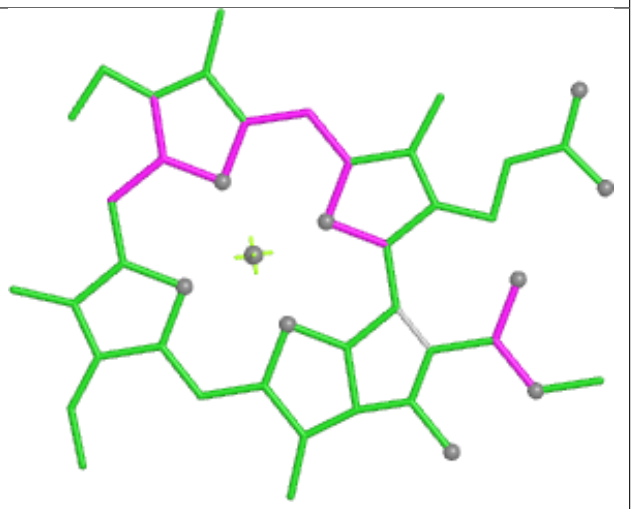


Rings

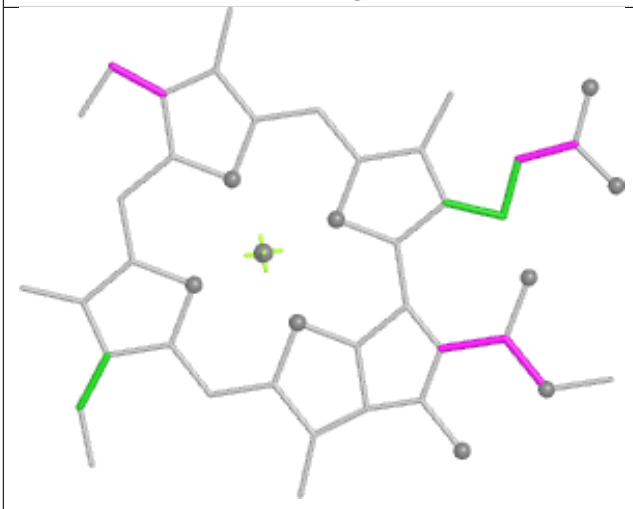
Ligand CLA B 838



Bond lengths



Bond angles

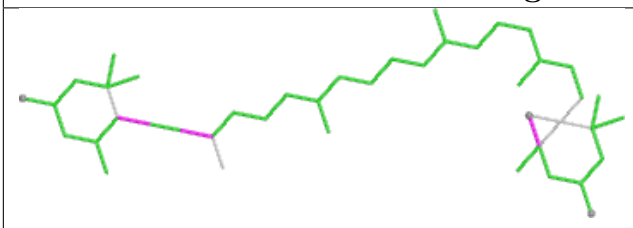


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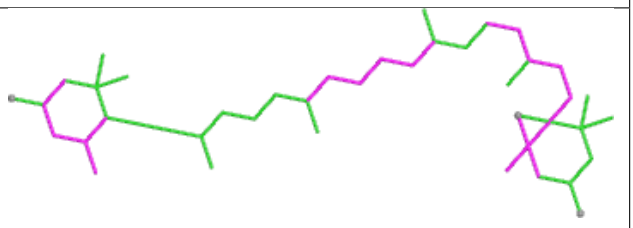


Rings

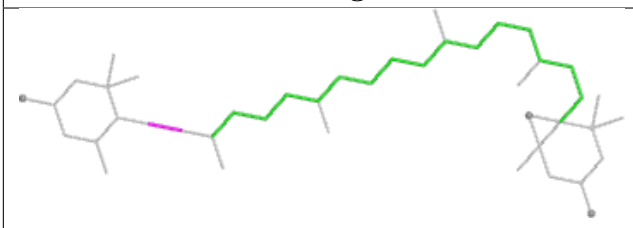
Ligand DD6 H 314



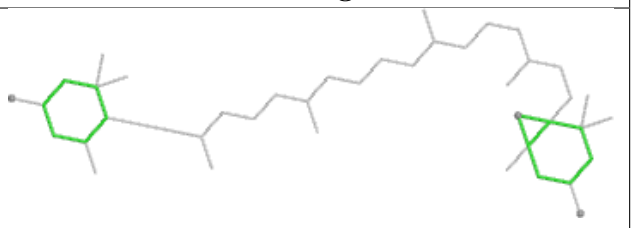
Bond lengths



Bond angles

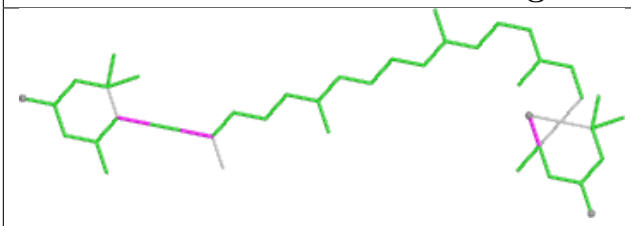


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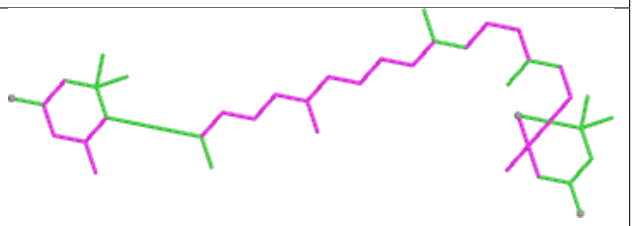


Rings

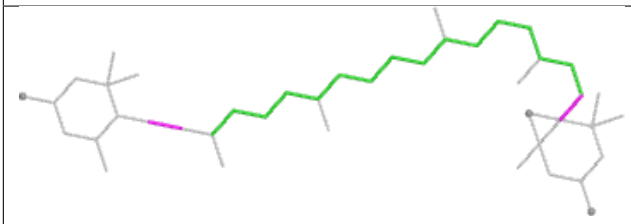
Ligand DD6 L 414



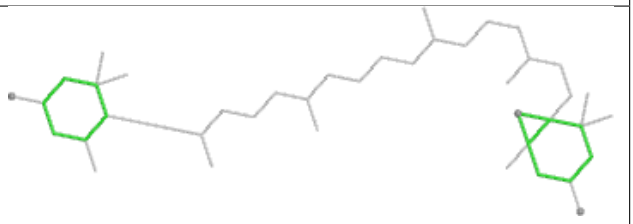
Bond lengths



Bond angles

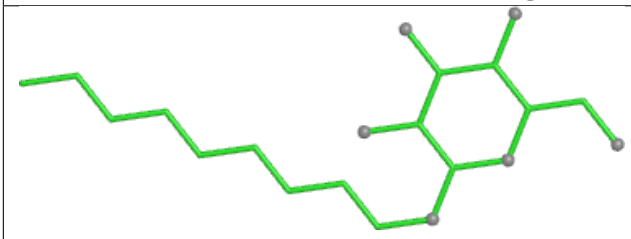


Torsions

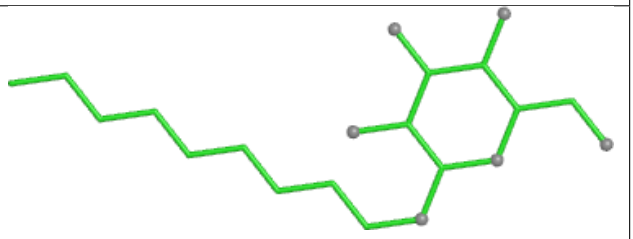


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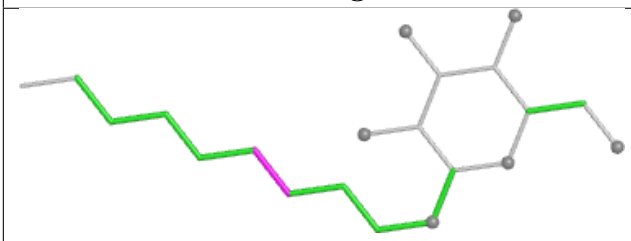
Ligand LMU F 402



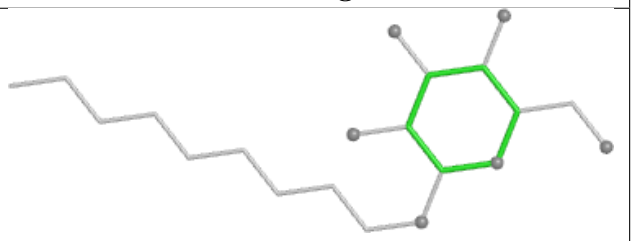
Bond lengths



Bond angles

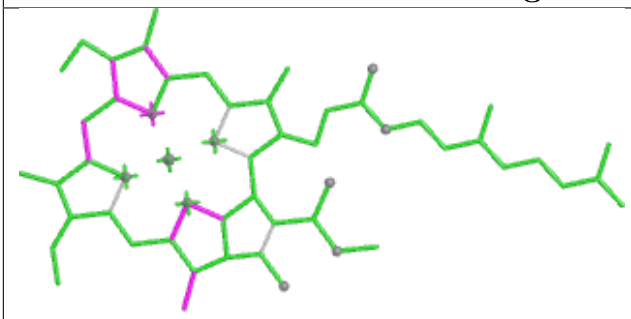


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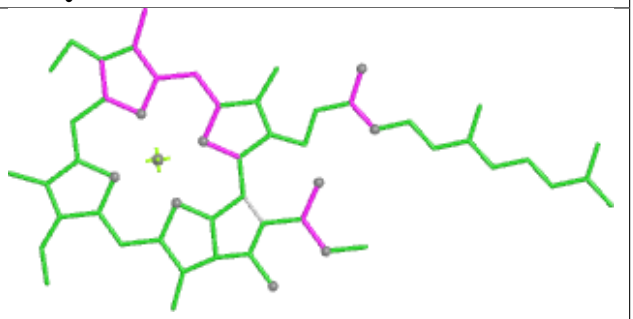


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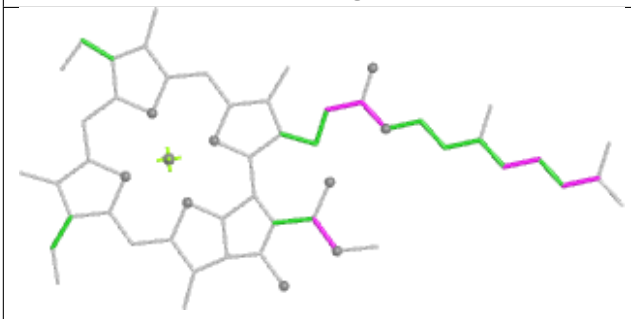
Ligand CLA Q 611



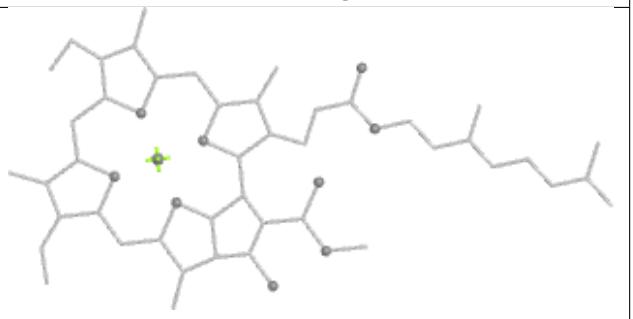
Bond lengths



Bond angles

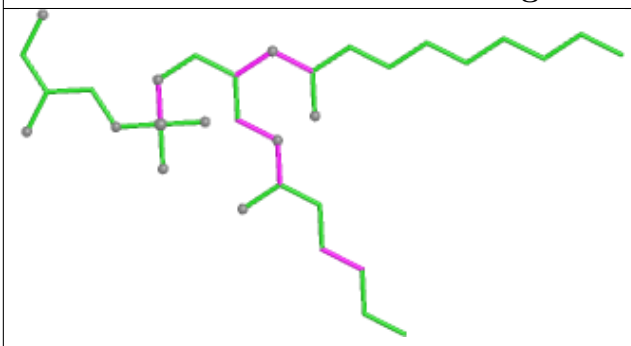


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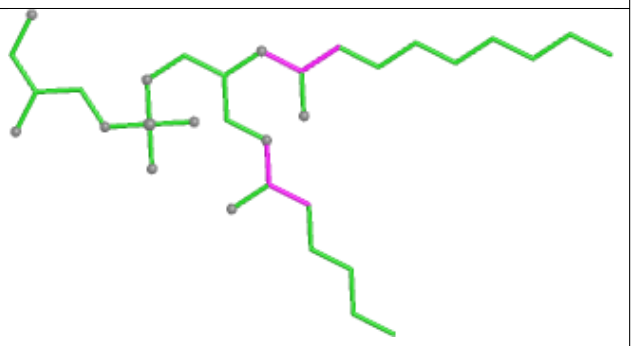


Rings

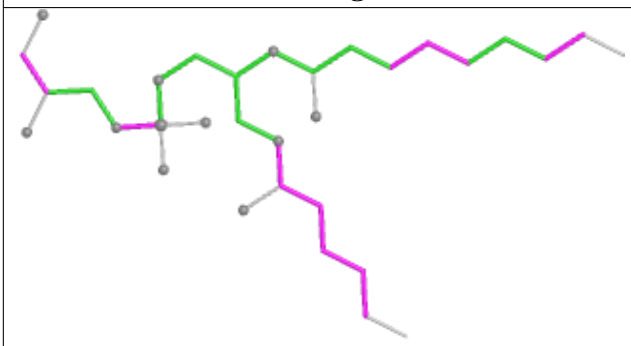
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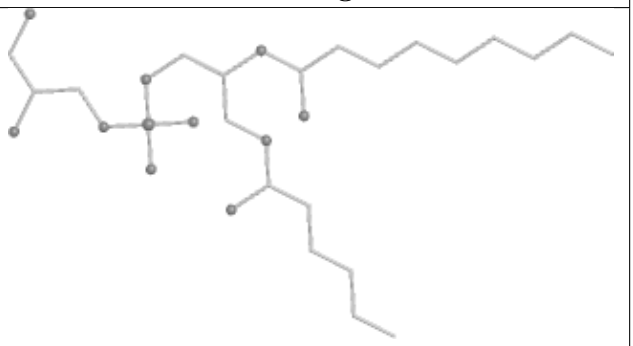
Bond lengths



Bond angles

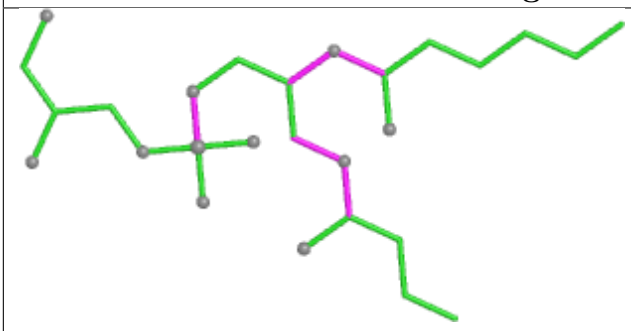


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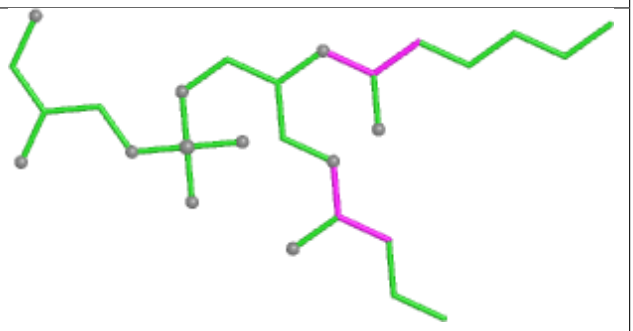


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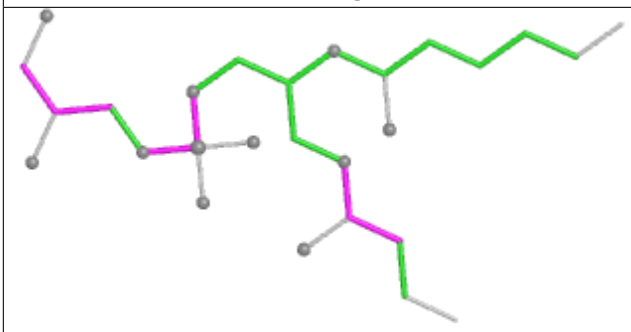
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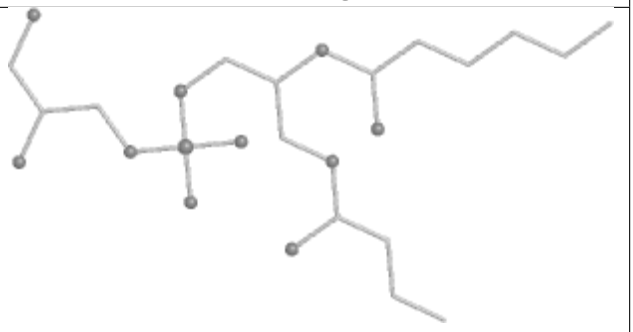
Bond lengths



Bond angles

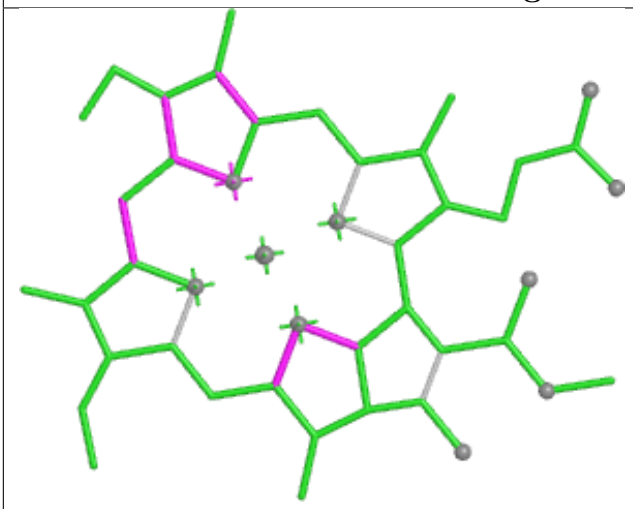


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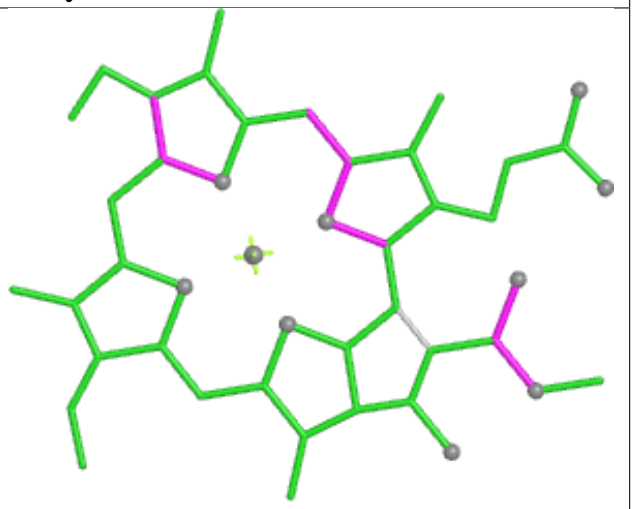


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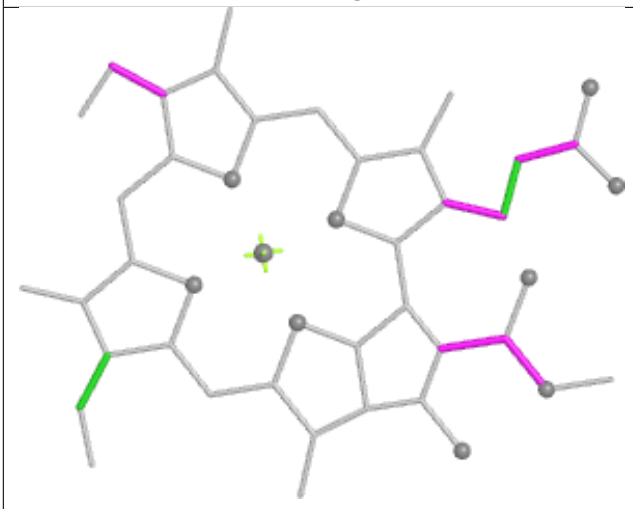
Ligand CLA Q 618



Bond lengths



Bond angles

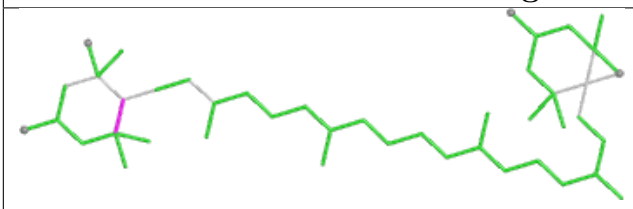


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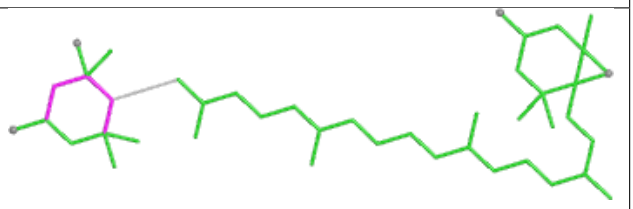


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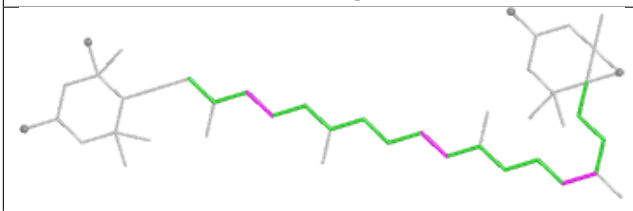
Ligand NEX V 616



Bond lengths



Bond angles

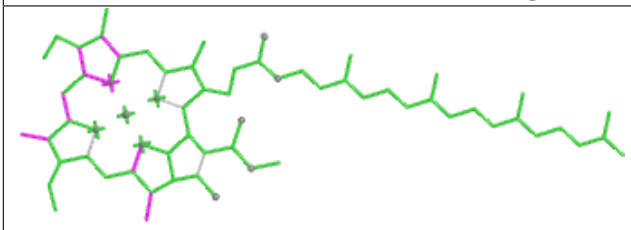


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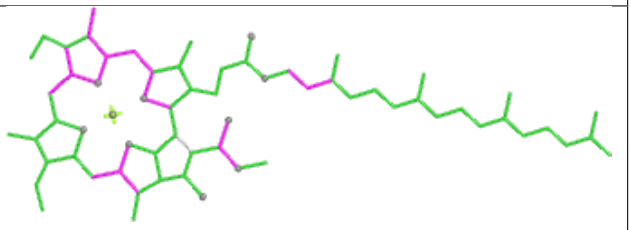


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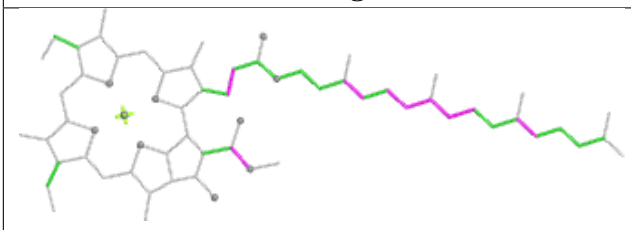
Ligand CLA A 803



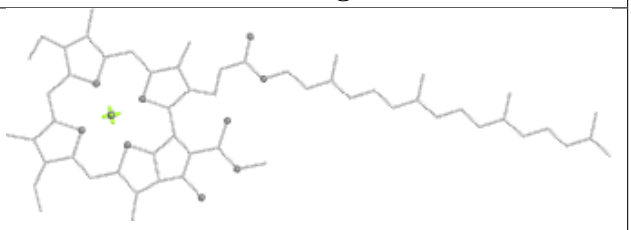
Bond lengths



Bond angles

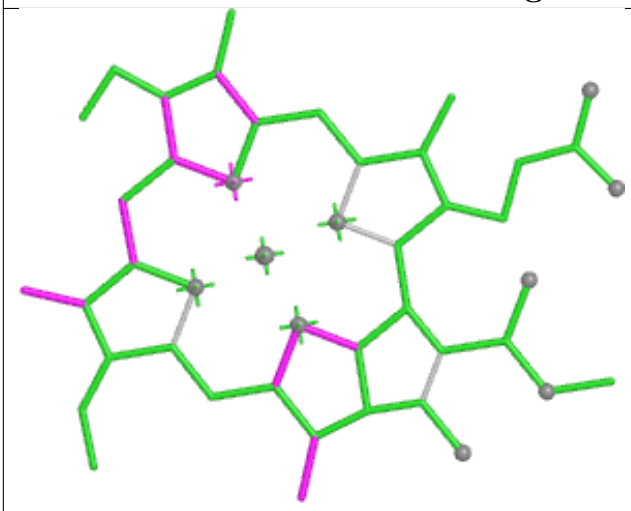


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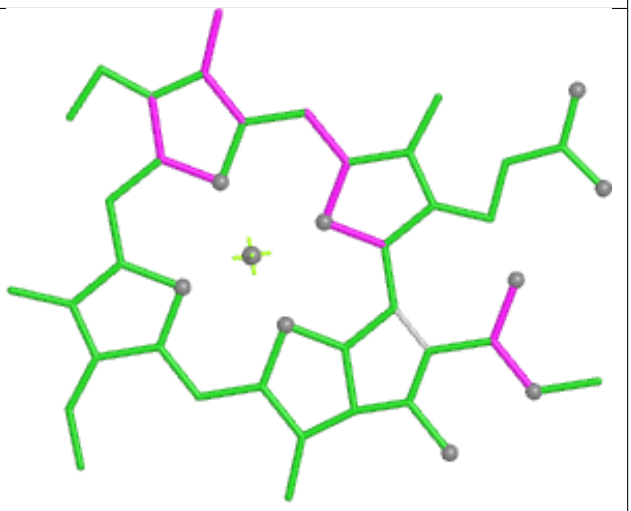


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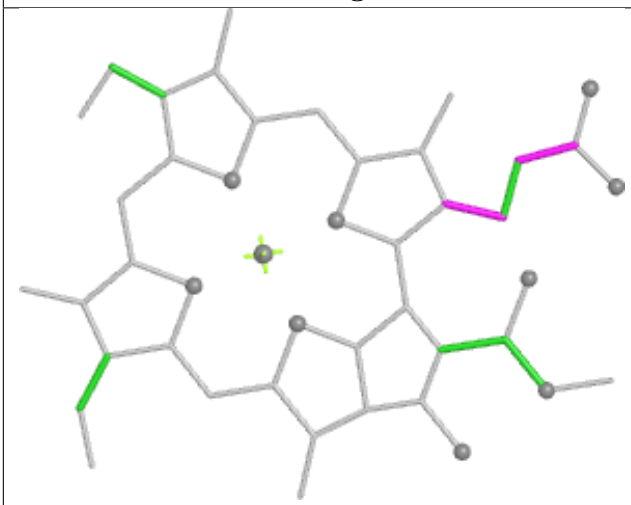
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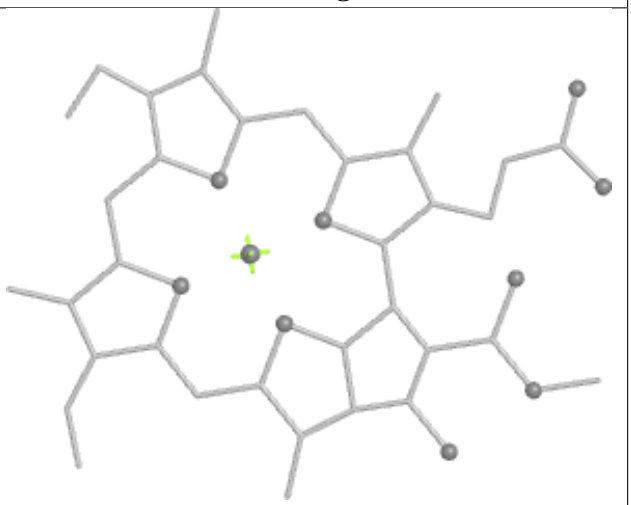
Bond lengths



Bond angles

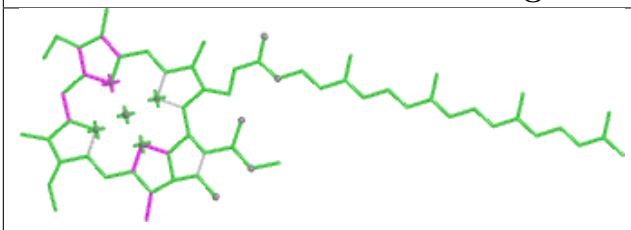


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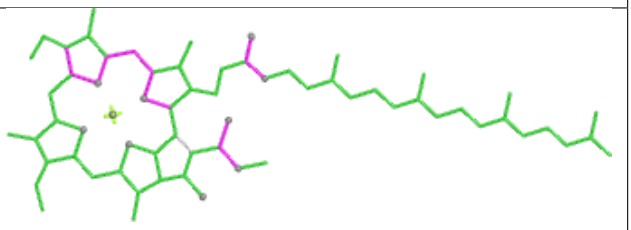


Rings

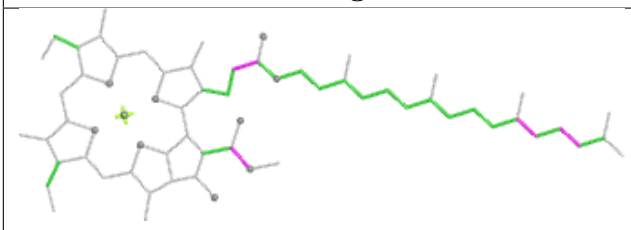
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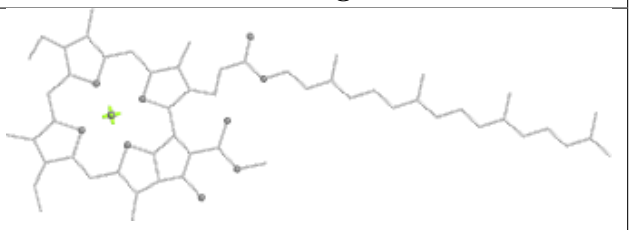
Bond lengths



Bond angles

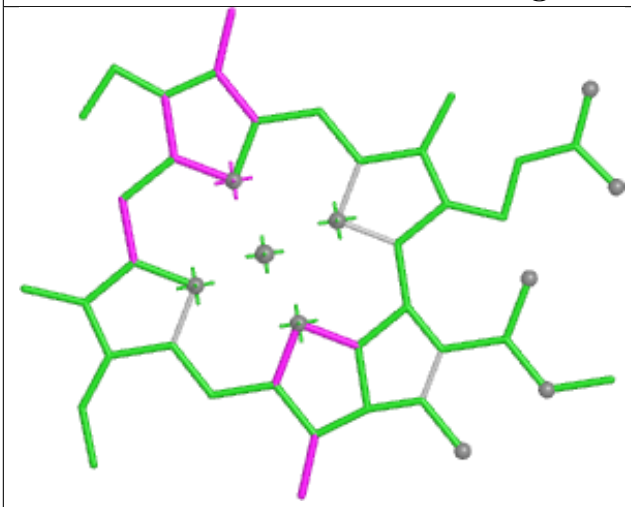


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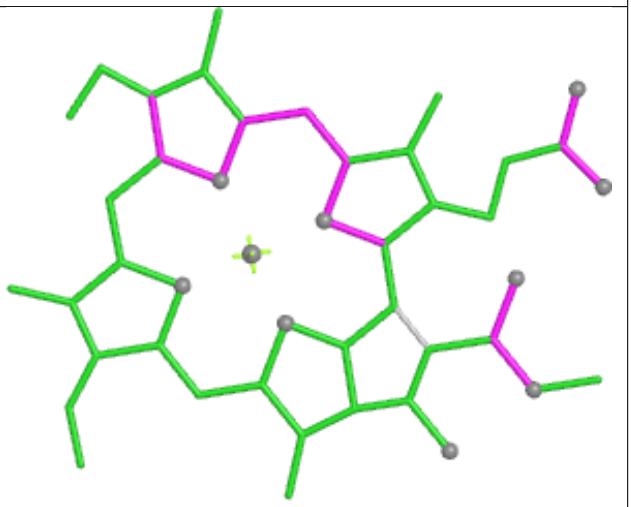


Rings

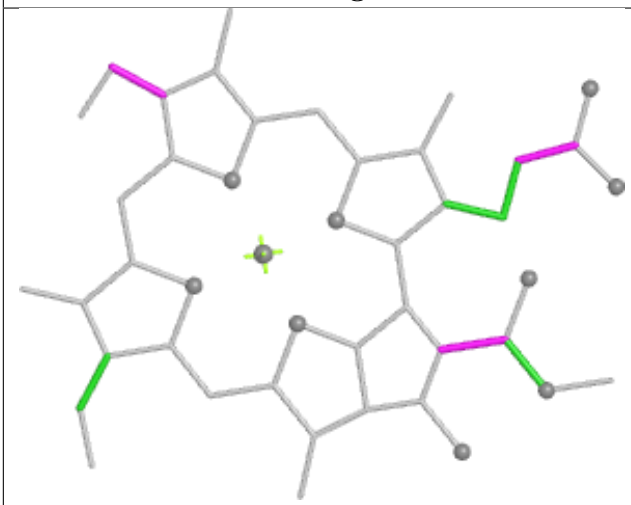
Ligand CLA I 608



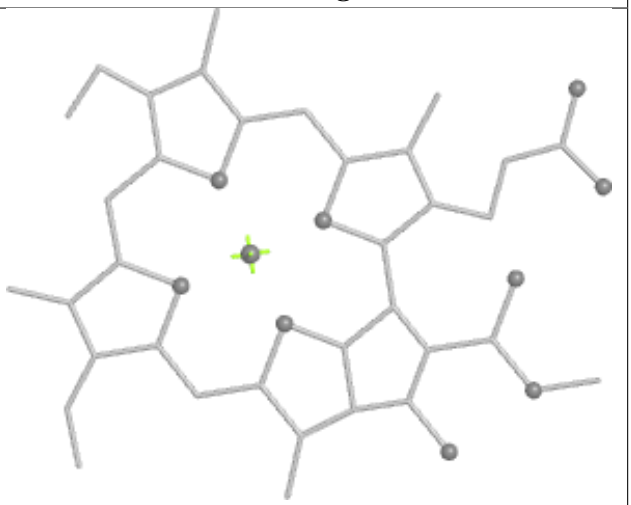
Bond lengths



Bond angles

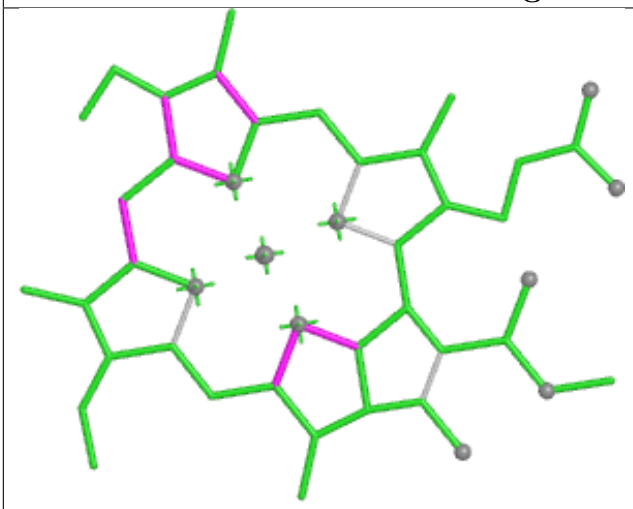


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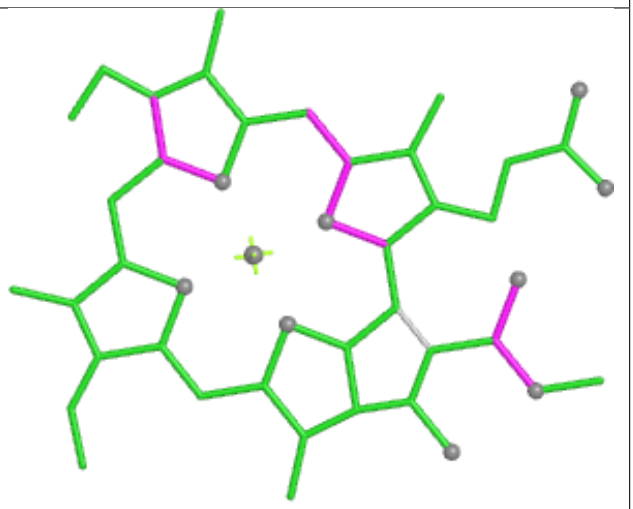


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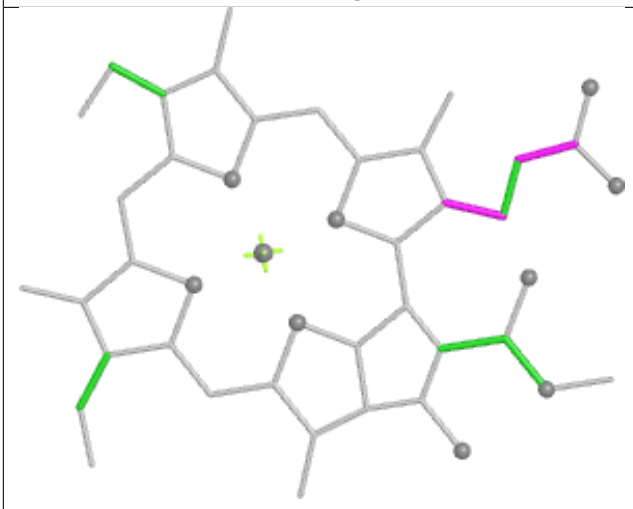
Ligand CLA X 413



Bond lengths



Bond angles

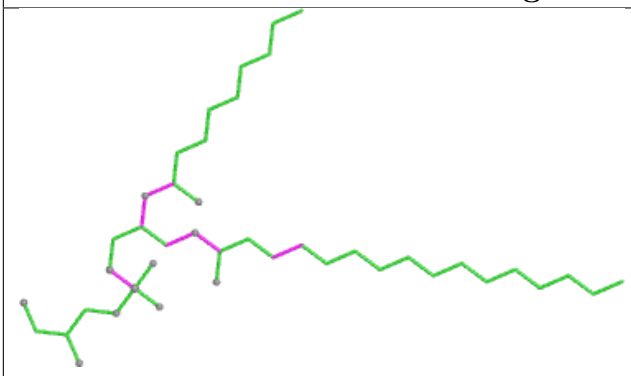


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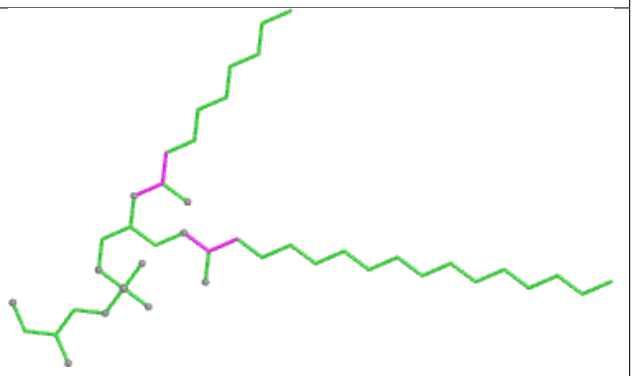


Rings

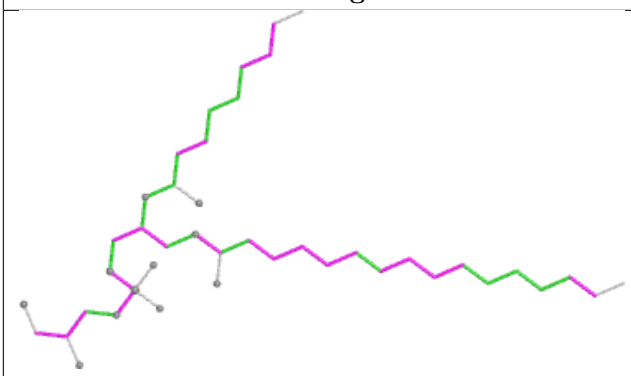
Ligand LHG T 614



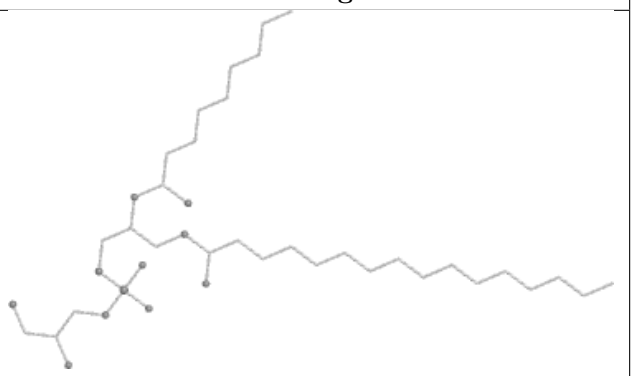
Bond lengths



Bond angles

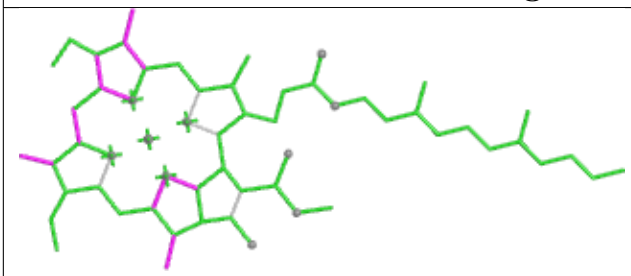


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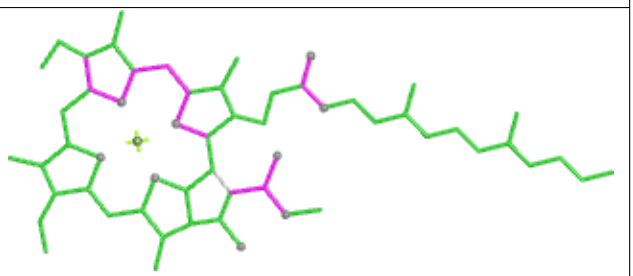


Rings

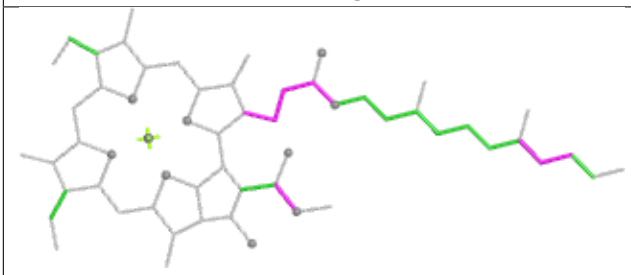
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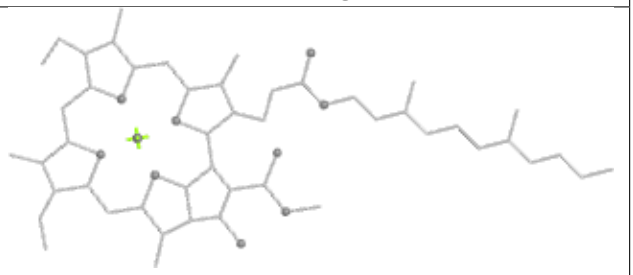
Bond lengths



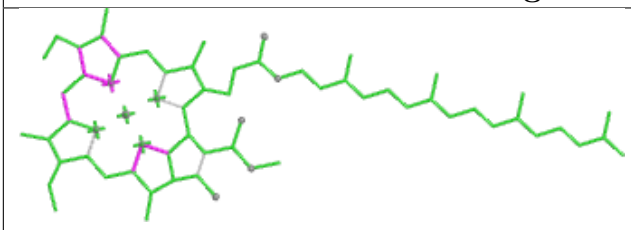
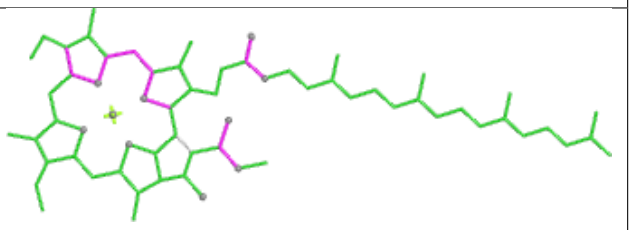
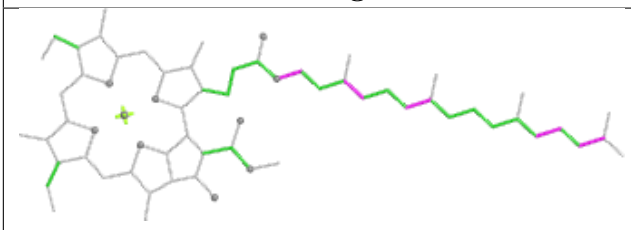
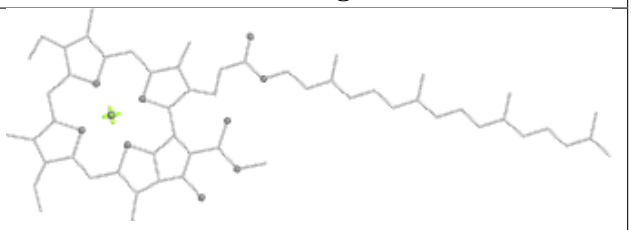
Bond angles

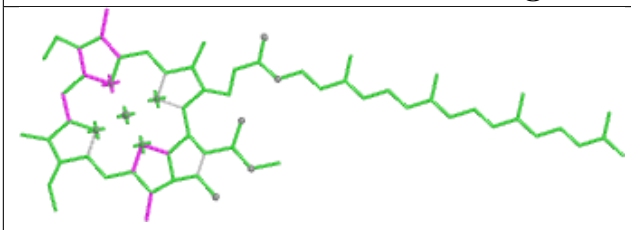
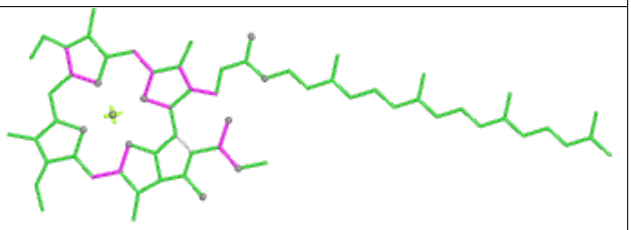
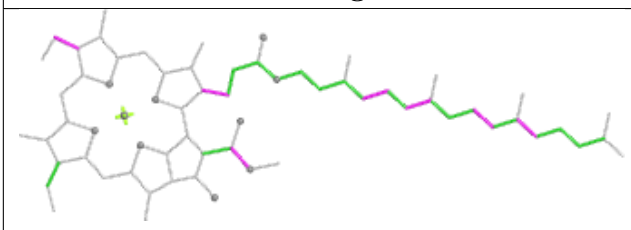
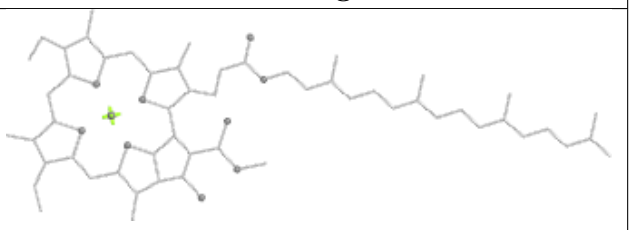


Torsions

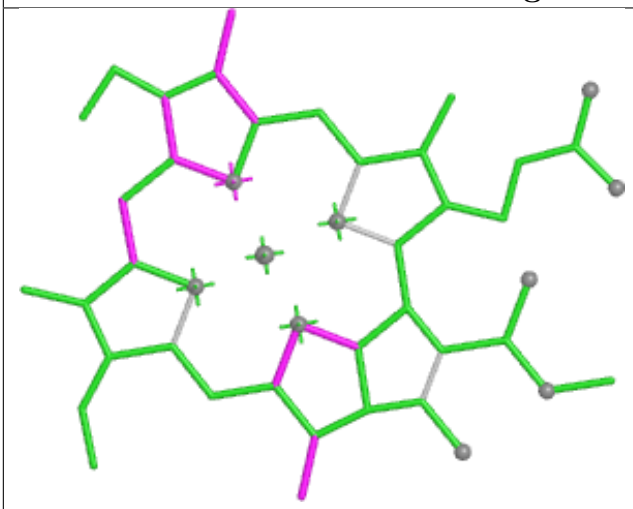


Rings

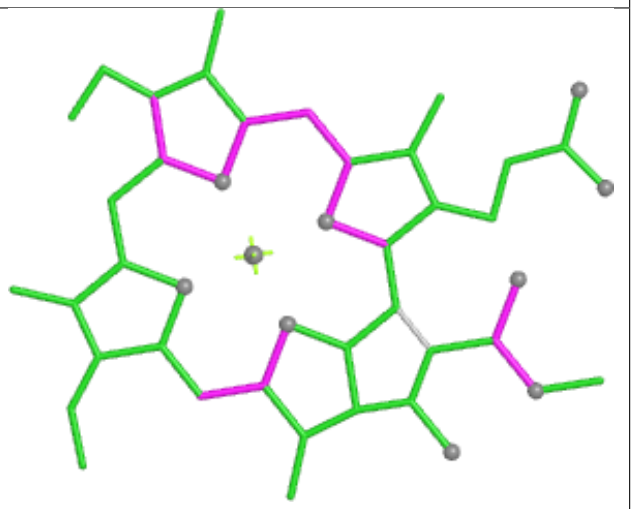
Ligand CLA A 822	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA B 859	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

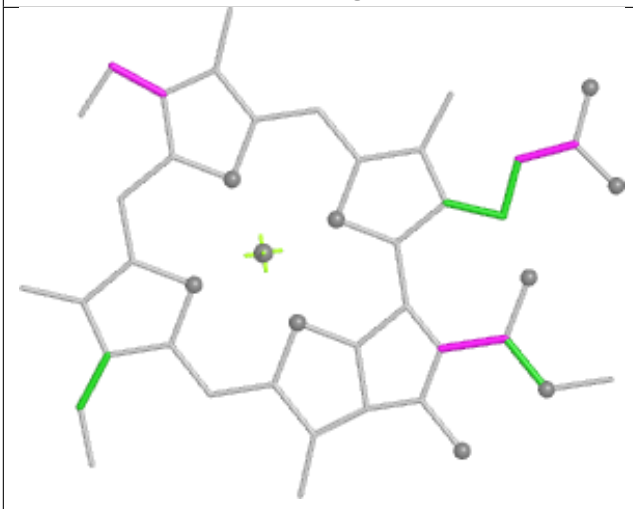
Ligand CLA A 834



Bond lengths



Bond angles

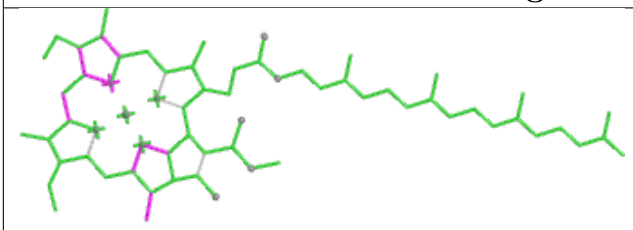


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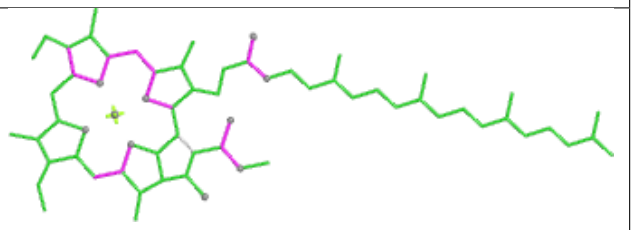


Rings

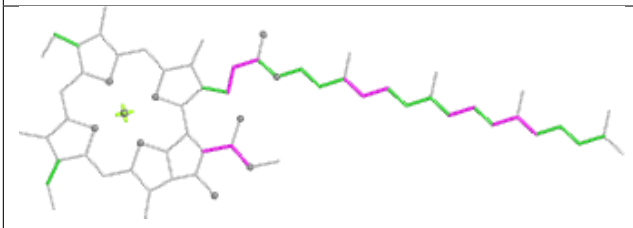
Ligand CLA L 411



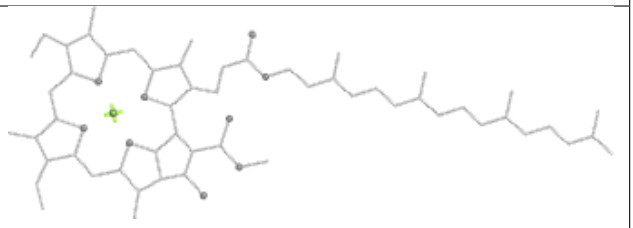
Bond lengths



Bond angles

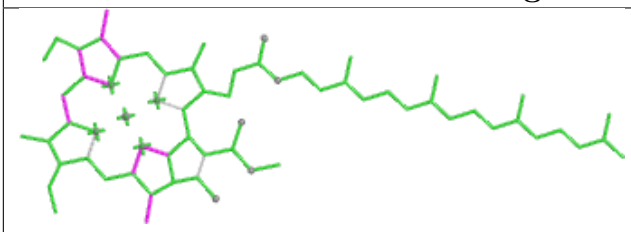


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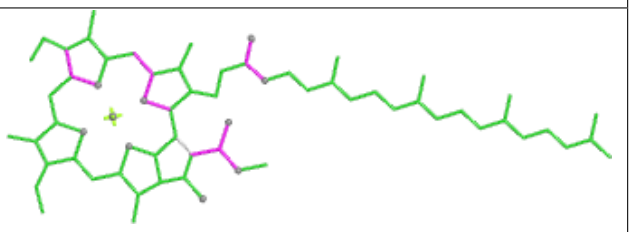


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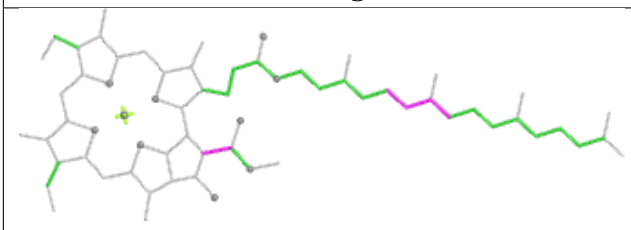
Ligand CLA A 831



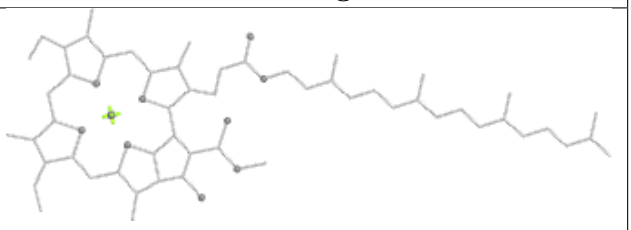
Bond lengths



Bond angles

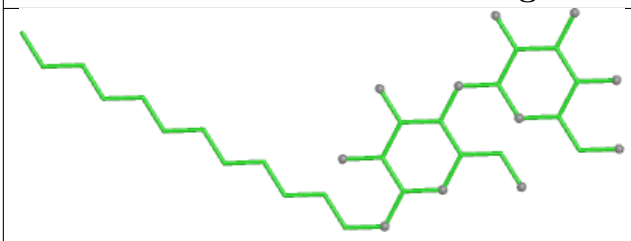


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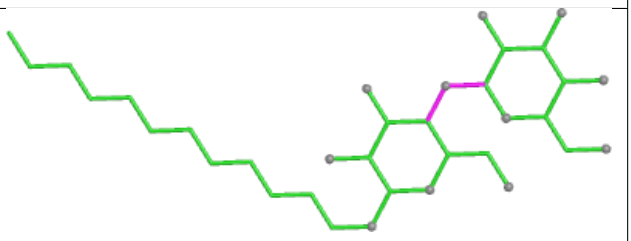


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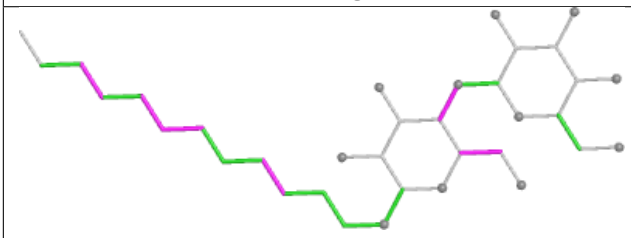
Ligand LMU U 421



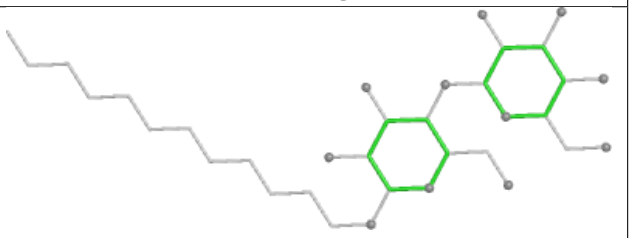
Bond lengths



Bond angles

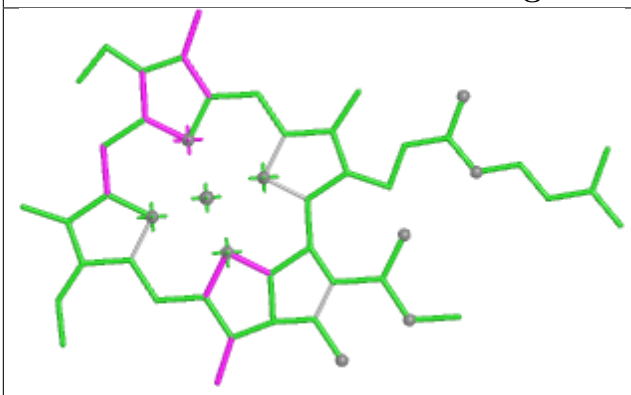


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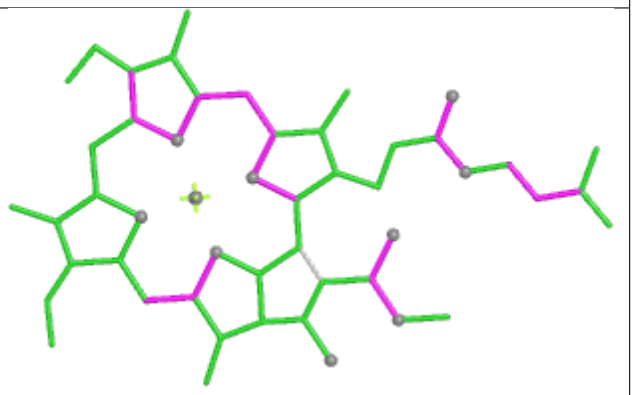


Rings

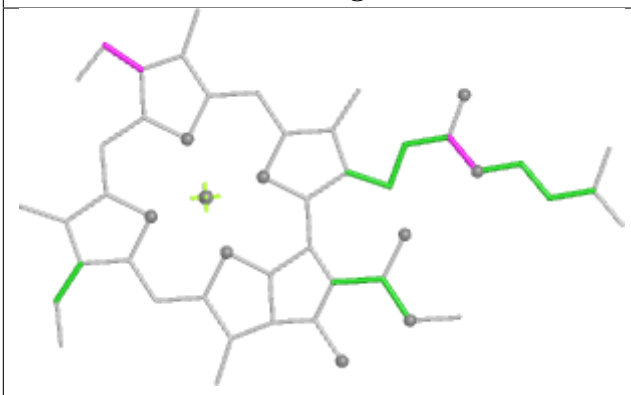
Ligand CLA O 315



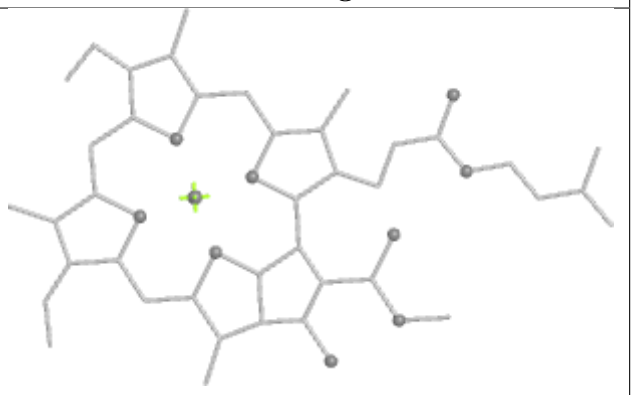
Bond lengths



Bond angles

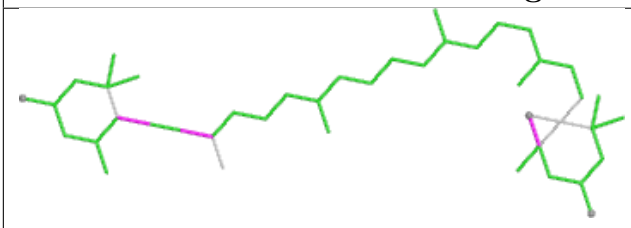


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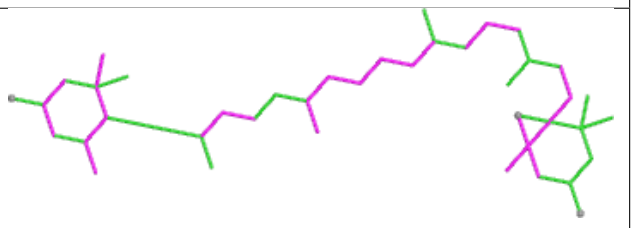


Rings

Ligand DD6 O 317



Bond lengths



Bond angles

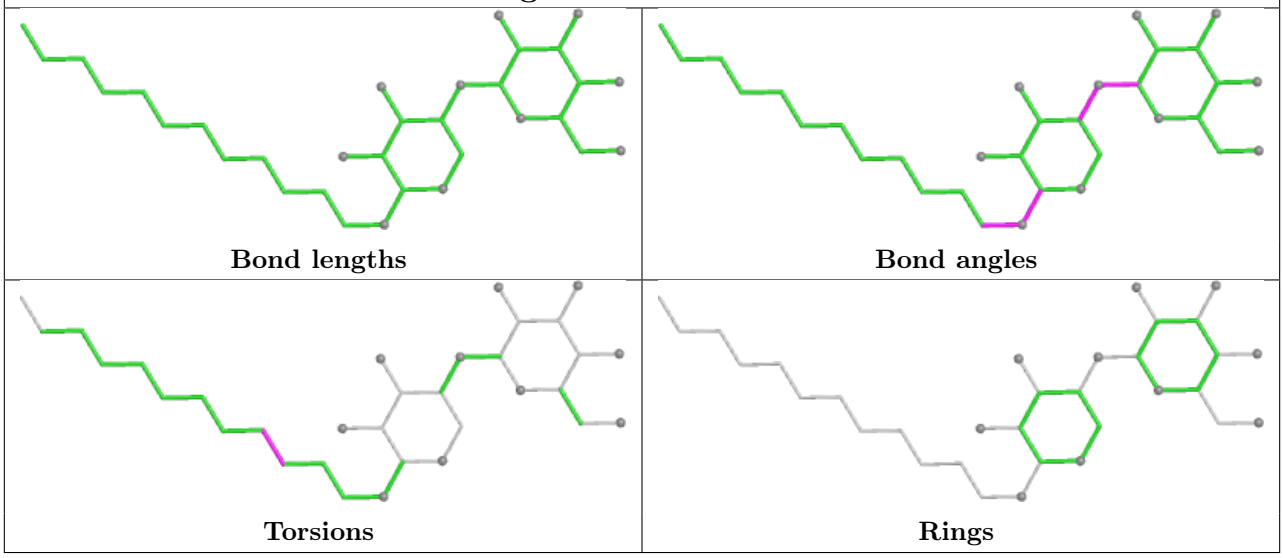


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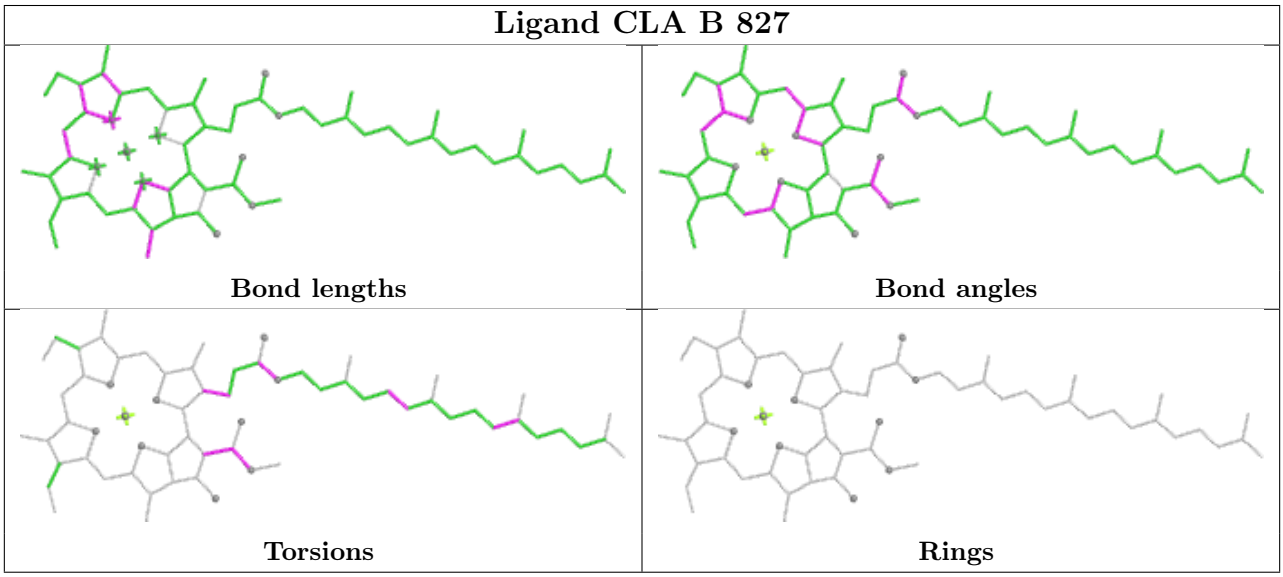


Rings

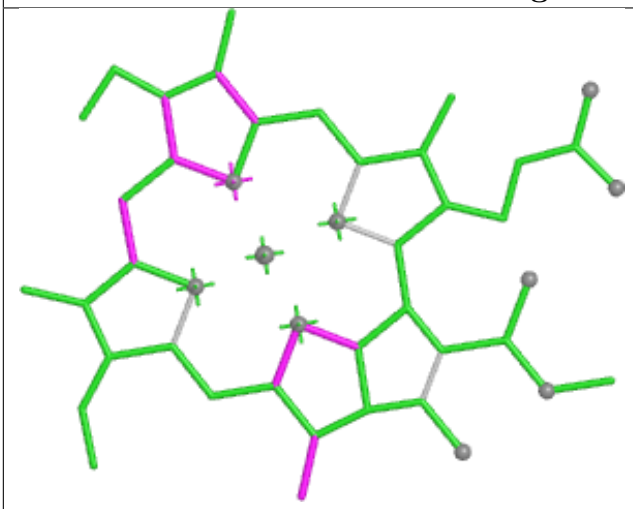
Ligand LMU H 321



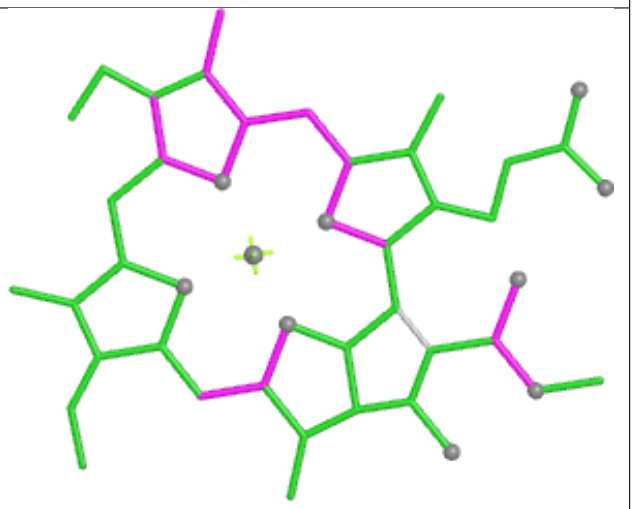
Ligand CLA B 827



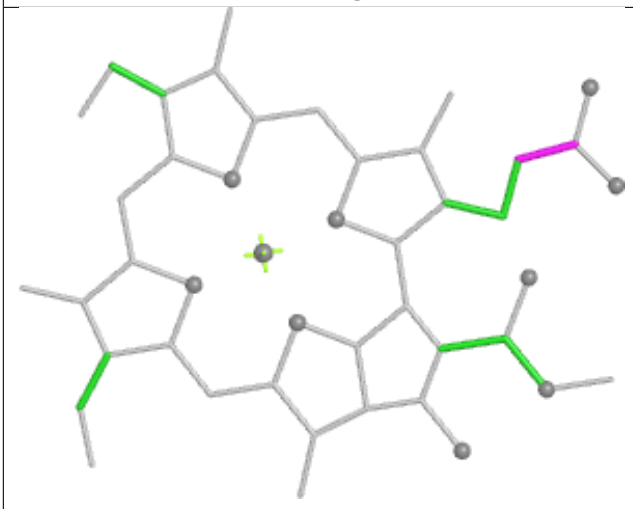
Ligand CLA I 605



Bond lengths



Bond angles

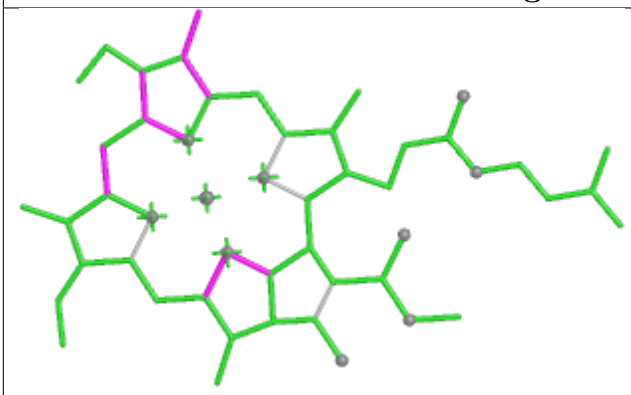


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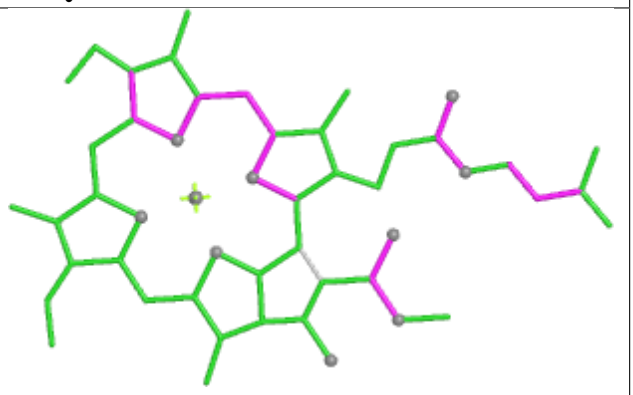


Rings

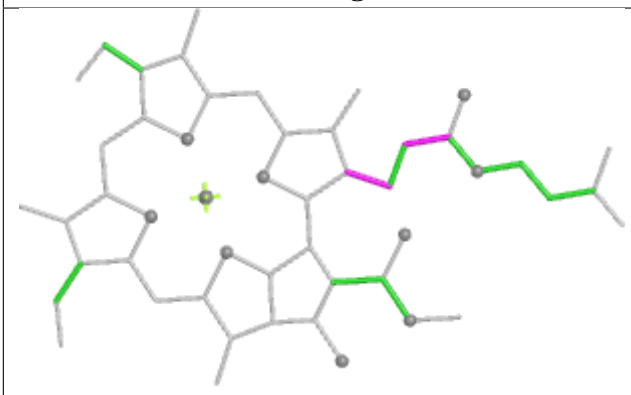
Ligand CLA Q 608



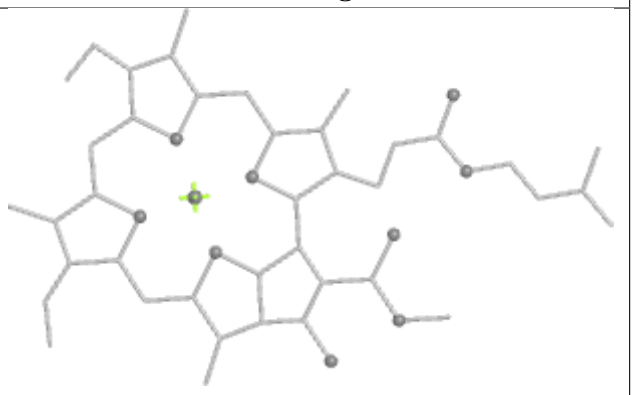
Bond lengths



Bond angles

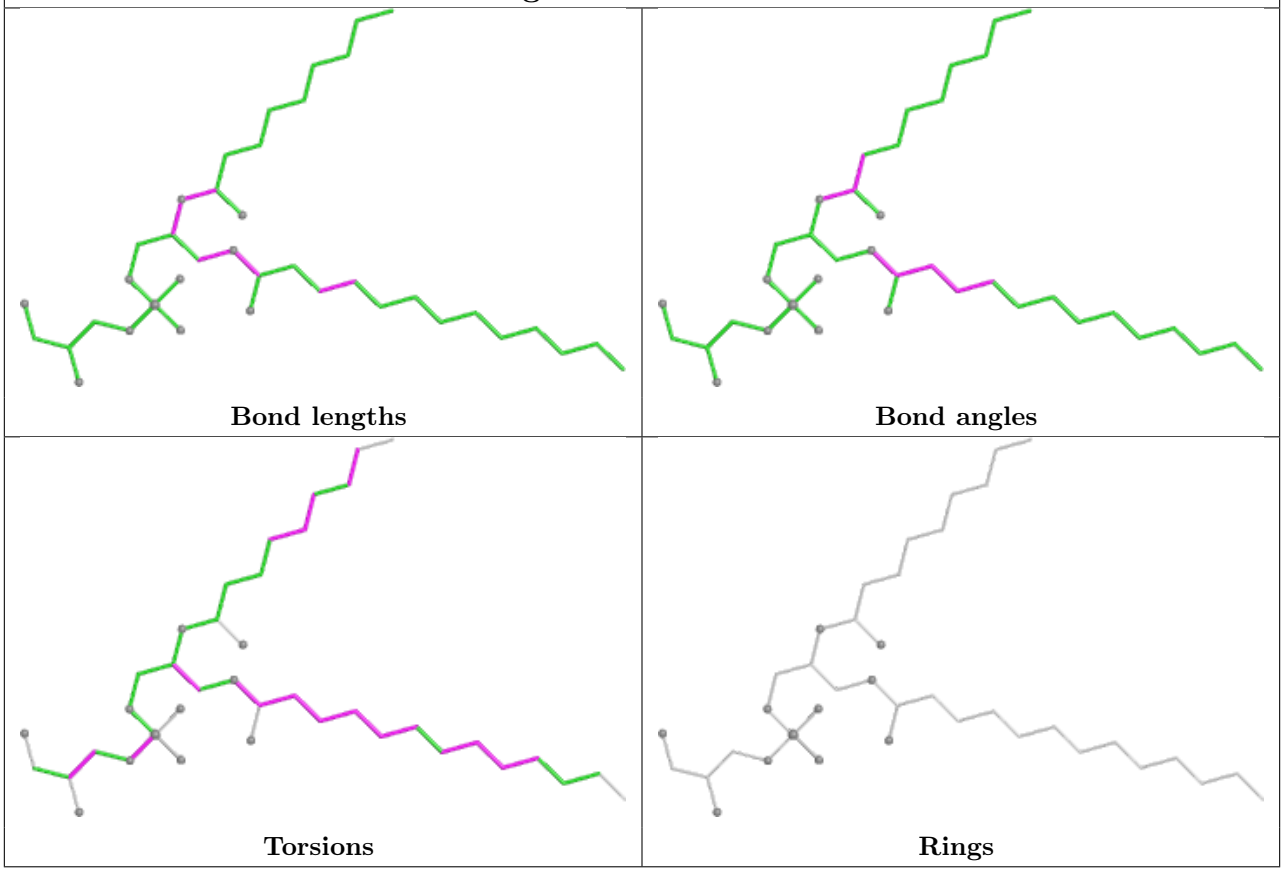


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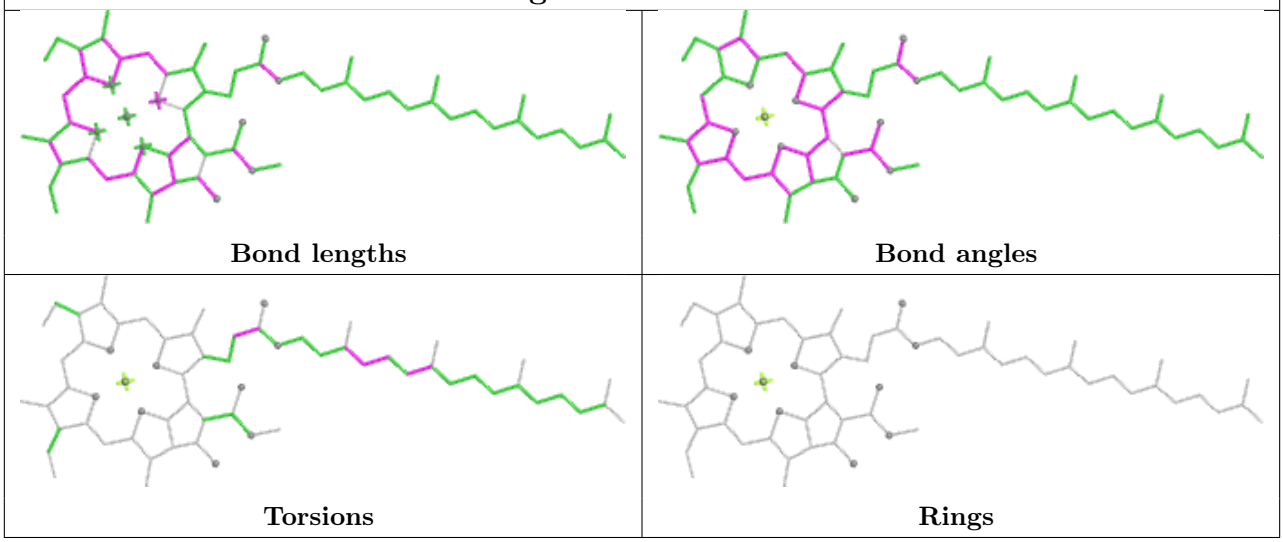


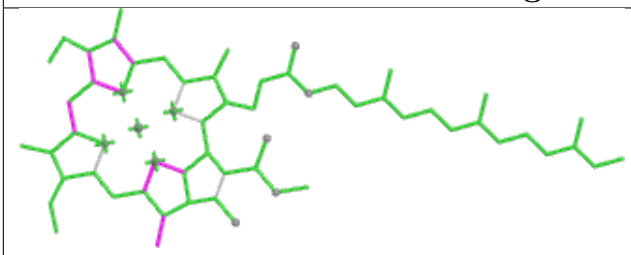
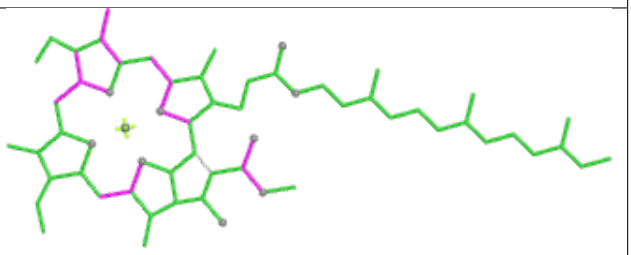
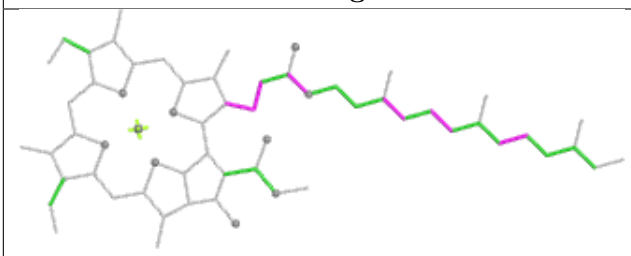
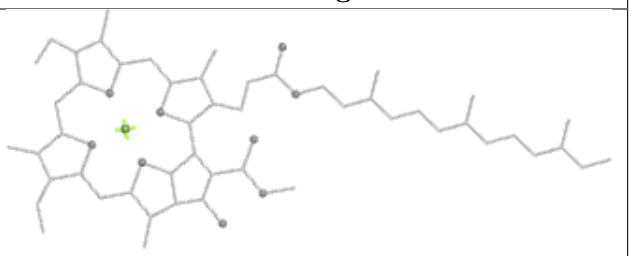
Rings

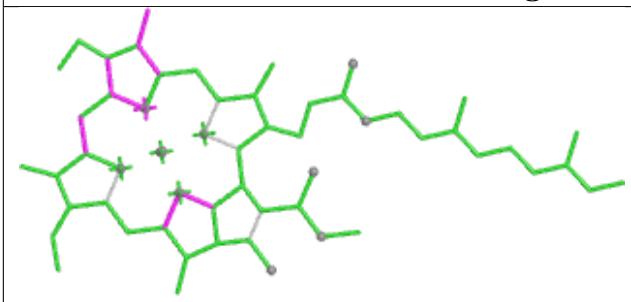
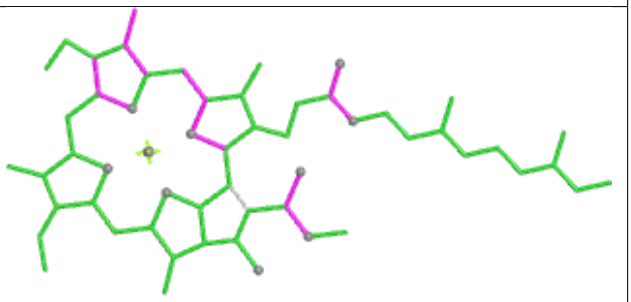
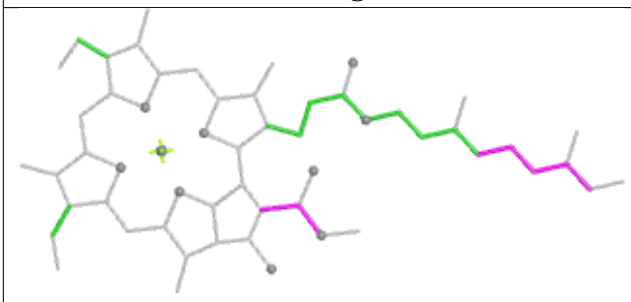
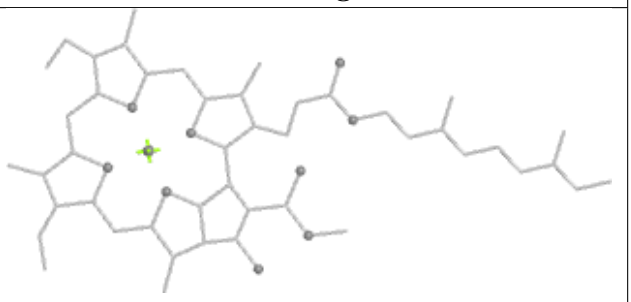
Ligand LHG K 616

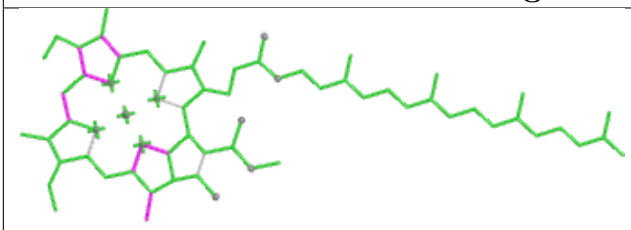
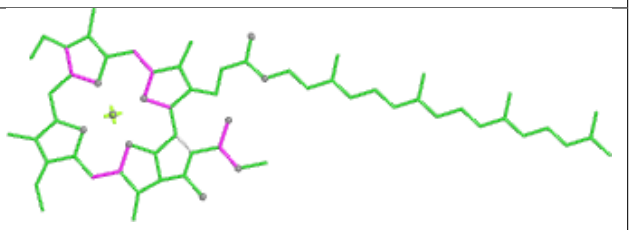
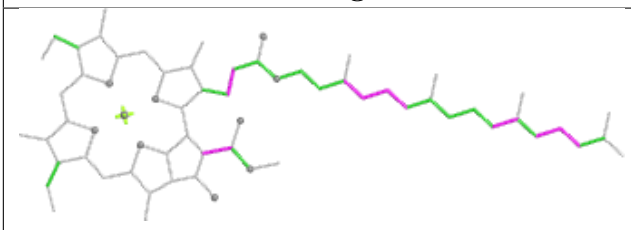
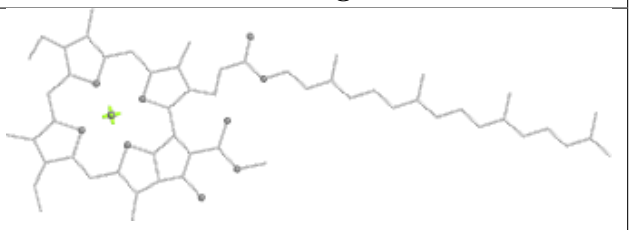


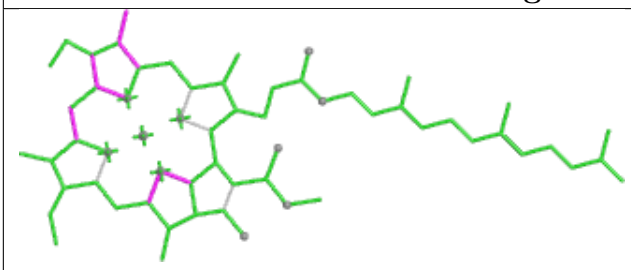
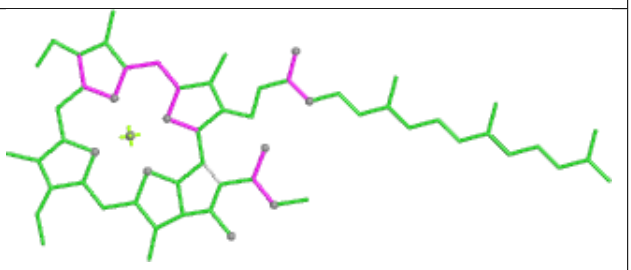
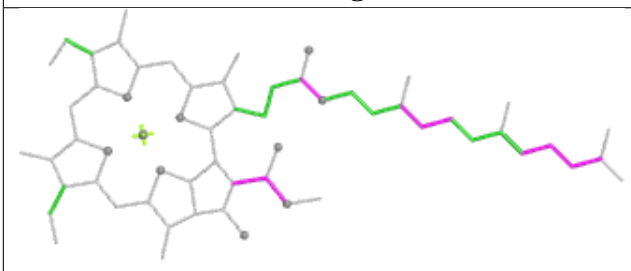
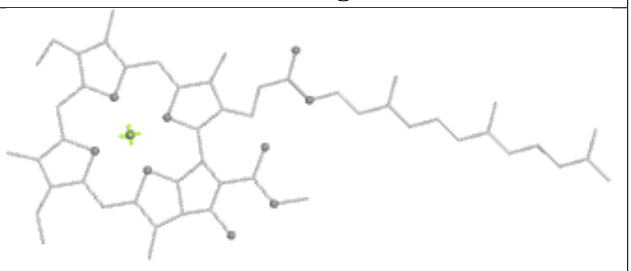
Ligand CL0 A 802



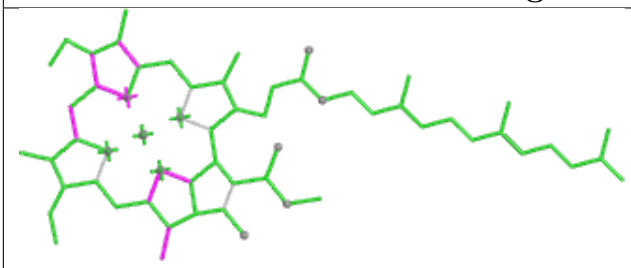
Ligand CLA A 805	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA V 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

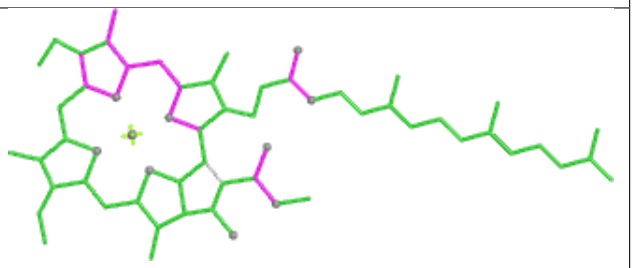
Ligand CLA A 814	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA X 410	
	
Bond lengths	Bond angles
	
Torsions	Rings

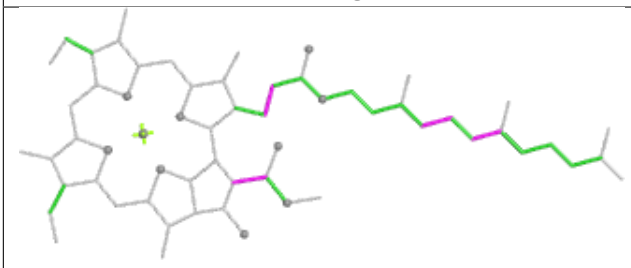
Ligand CLA L 403



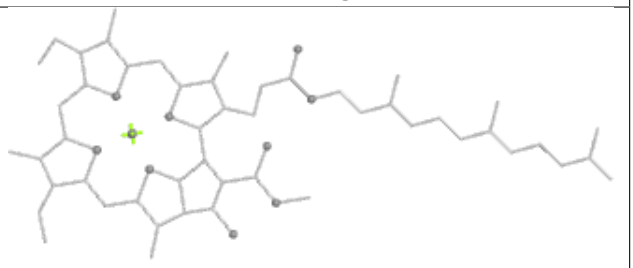
Bond lengths



Bond angles

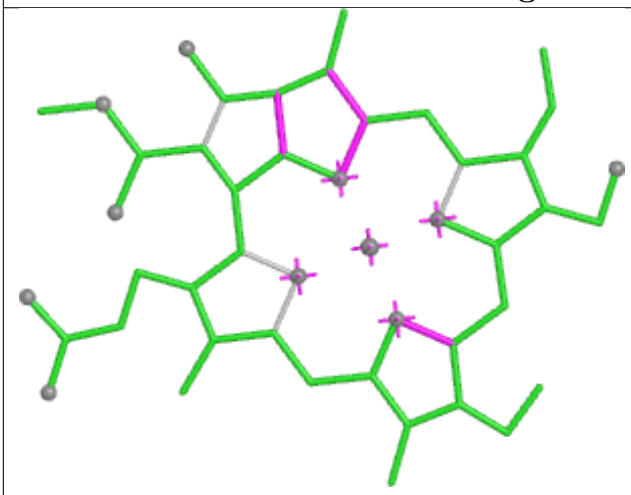


Torsions

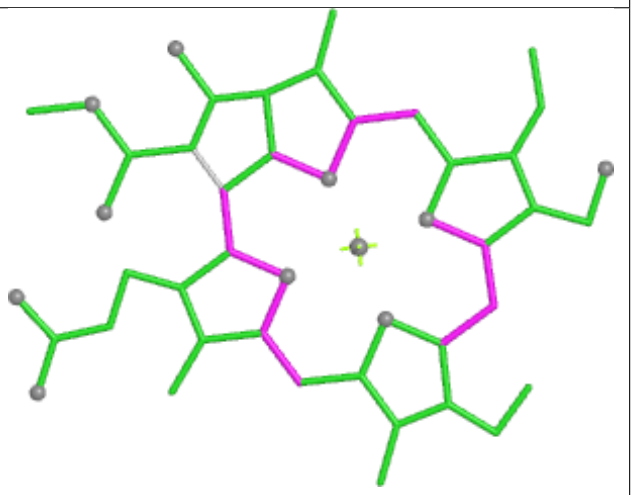


Rings

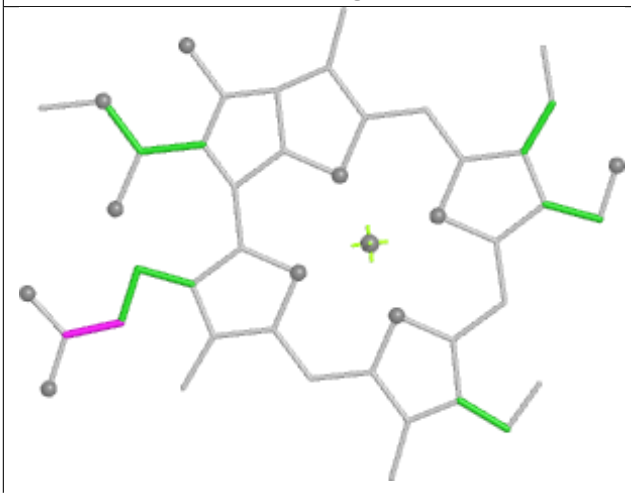
Ligand CHL W 407



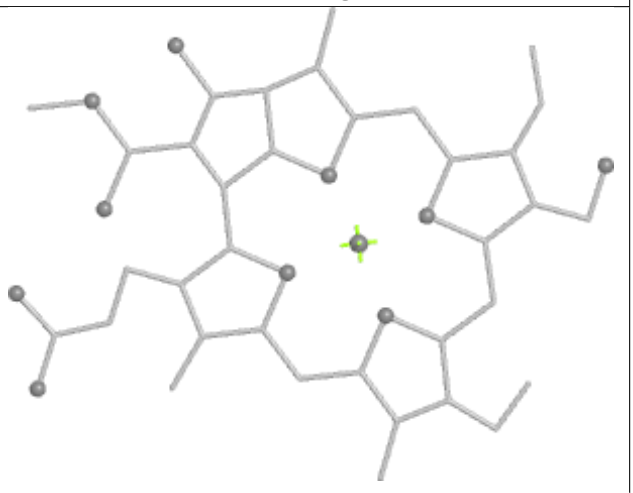
Bond lengths



Bond angles

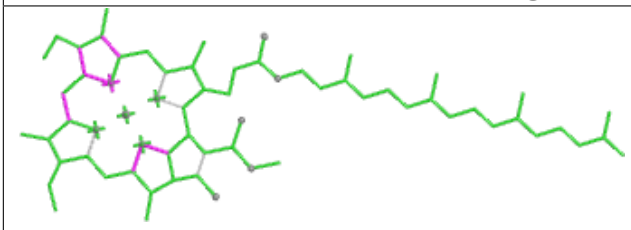


Torsions

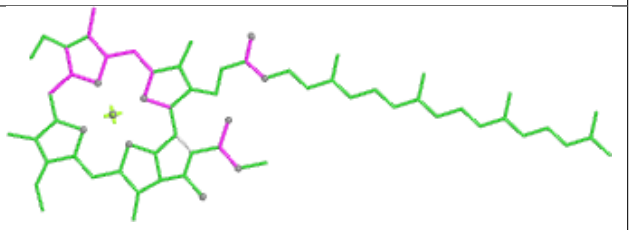


Rings

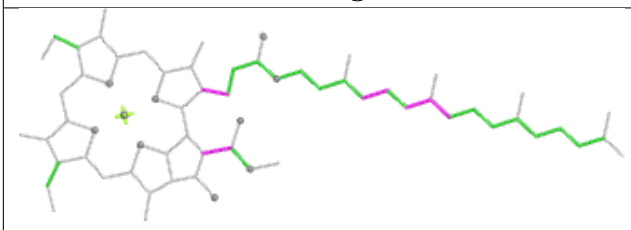
Ligand CLA B 831



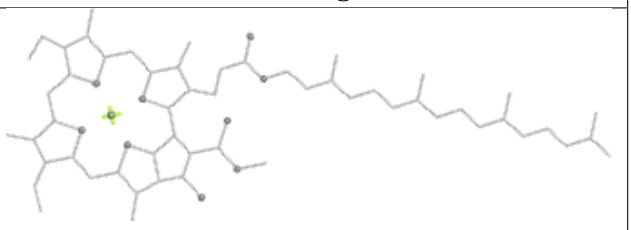
Bond lengths



Bond angles

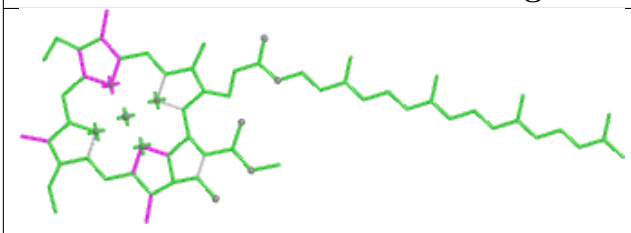


Torsions

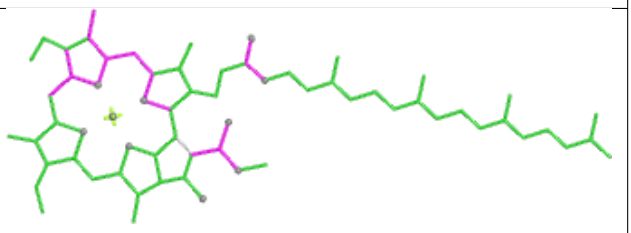


Rings

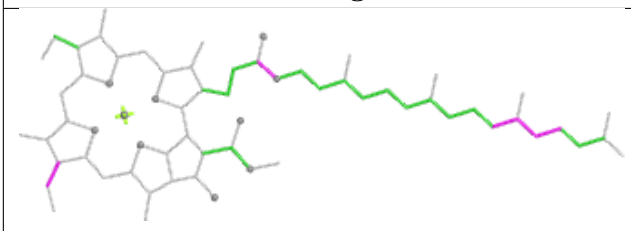
Ligand CLA B 830



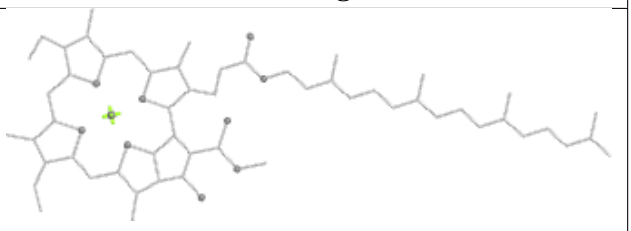
Bond lengths



Bond angles

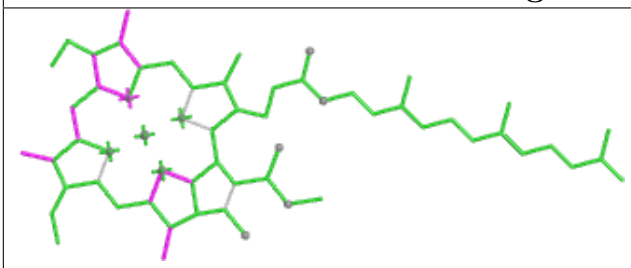


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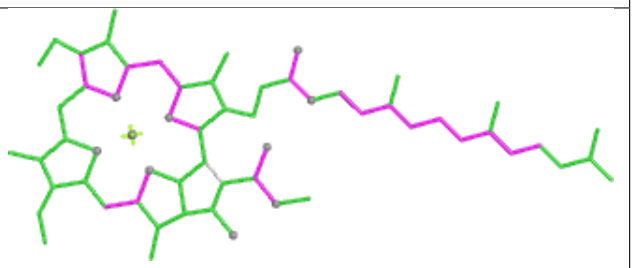


Rings

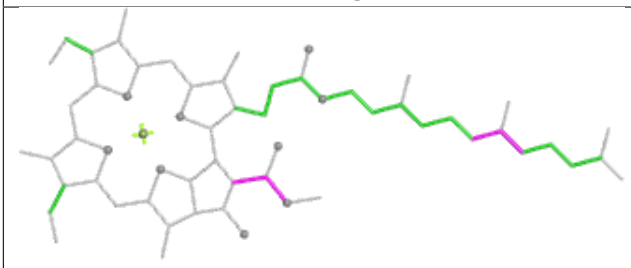
Ligand CLA L 408



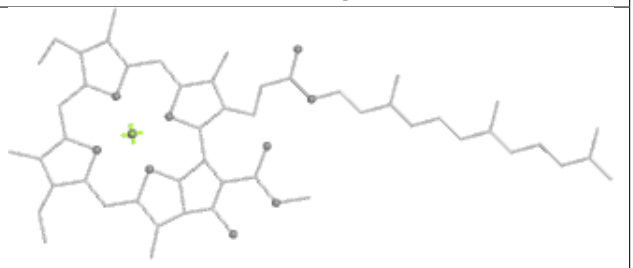
Bond lengths



Bond angles

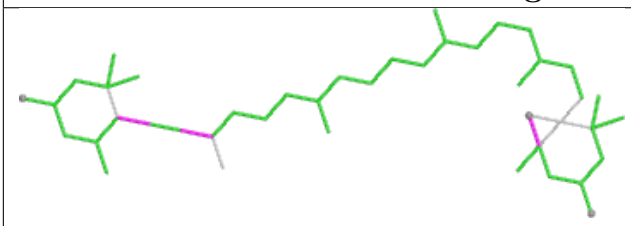


Torsions

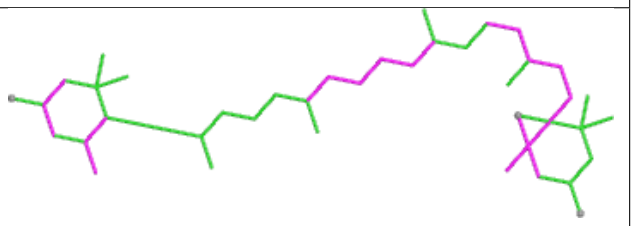


Rings

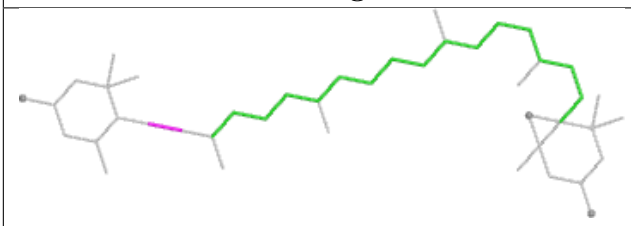
Ligand DD6 X 414



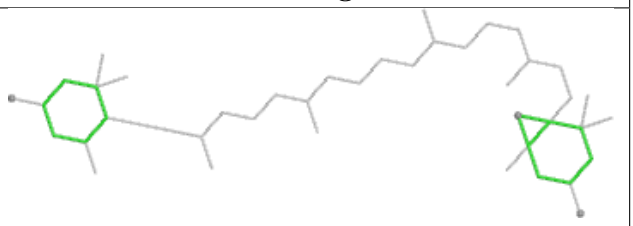
Bond lengths



Bond angles

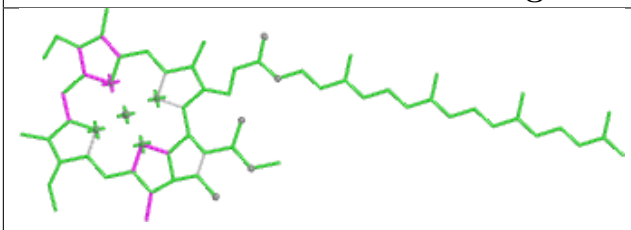


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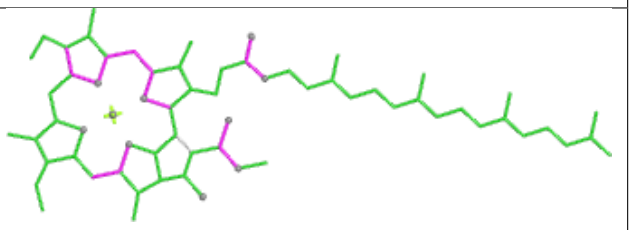


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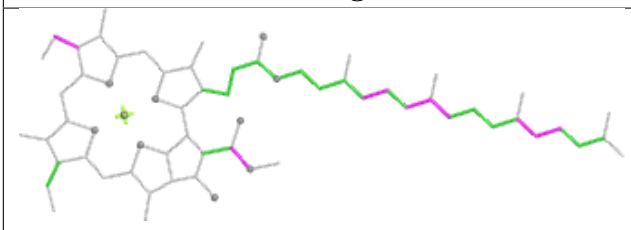
Ligand CLA F 403



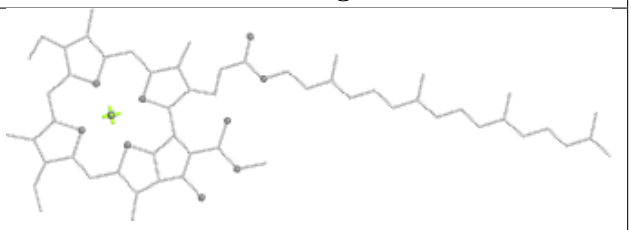
Bond lengths



Bond angles

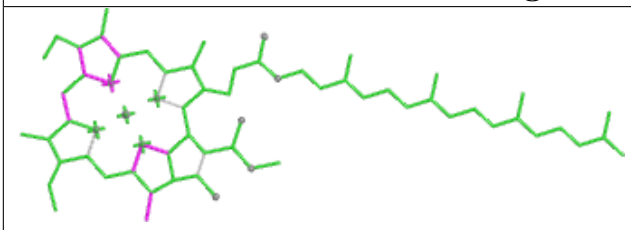


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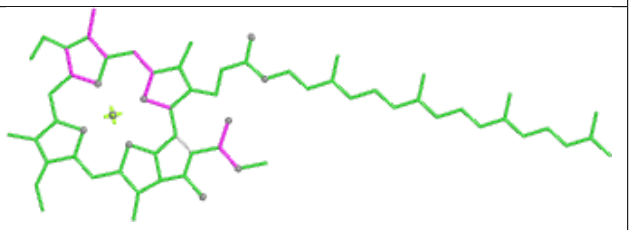


Rings

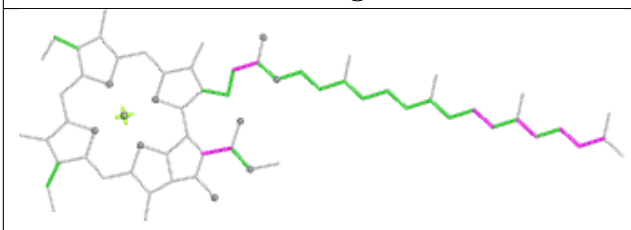
Ligand CLA A 826



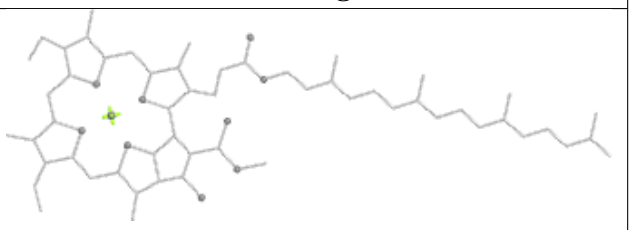
Bond lengths



Bond angles

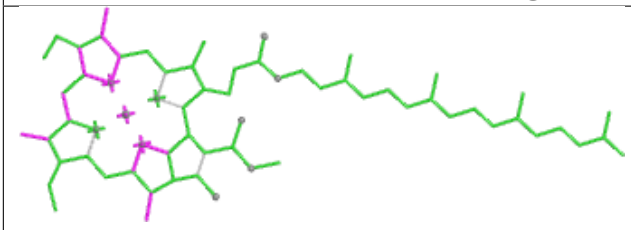


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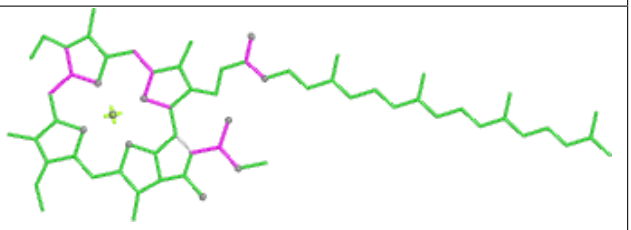


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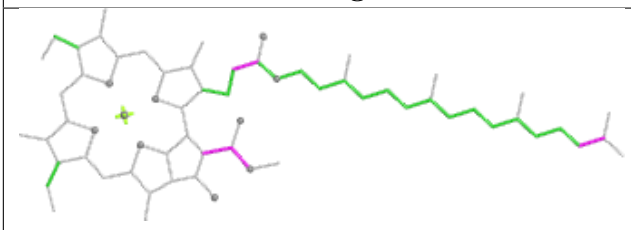
Ligand CLA B 802



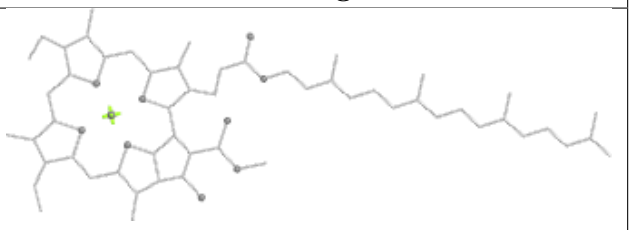
Bond lengths



Bond angles

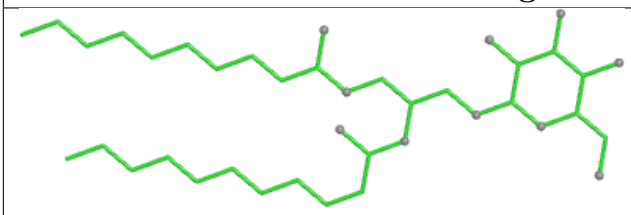


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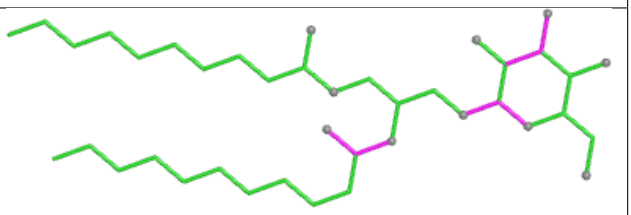


Rings

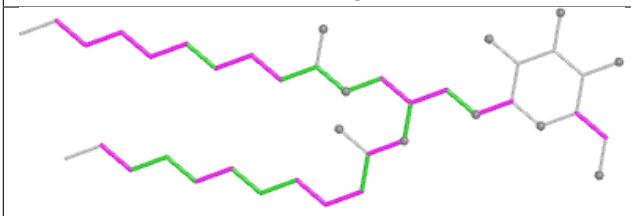
Ligand LMG H 319



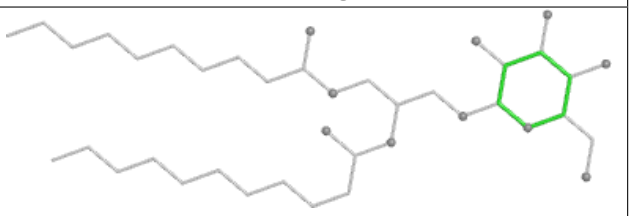
Bond lengths



Bond angles

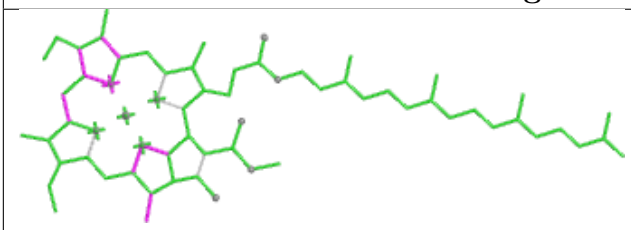


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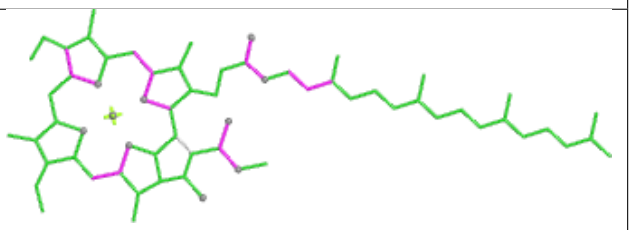


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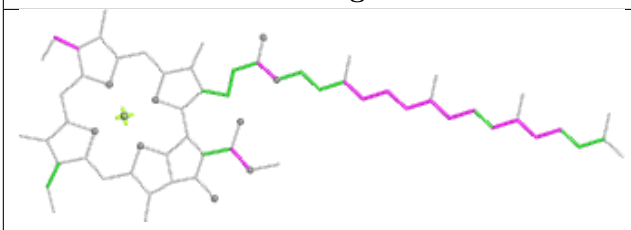
Ligand CLA R 601



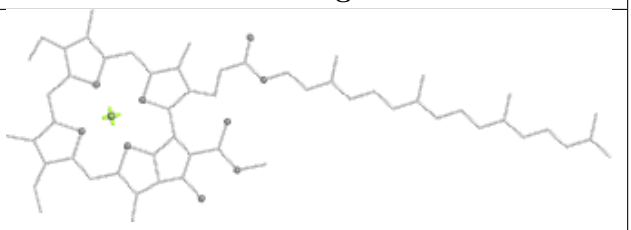
Bond lengths



Bond angles

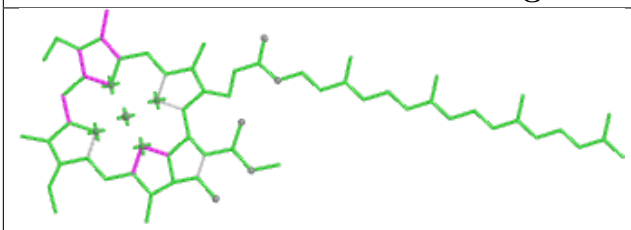


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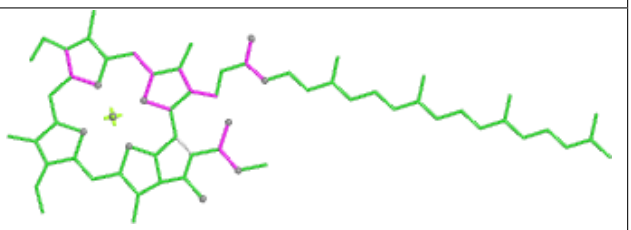


Rings

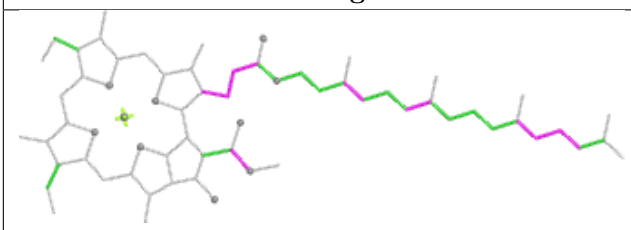
Ligand CLA A 842



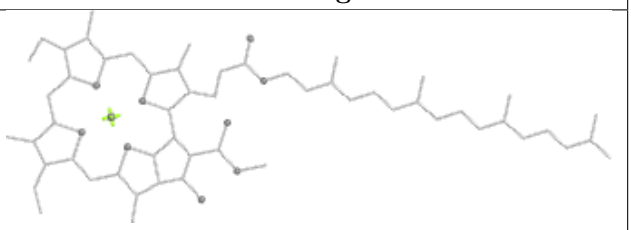
Bond lengths



Bond angles

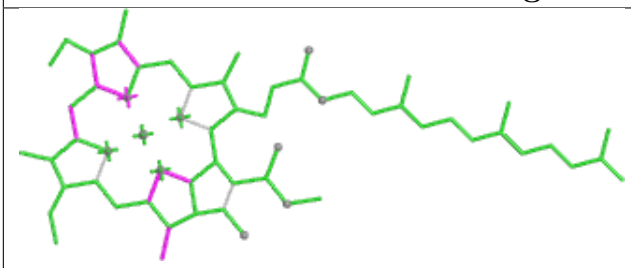


Torsions

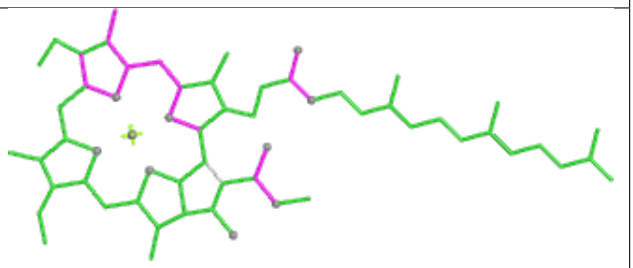


Rings

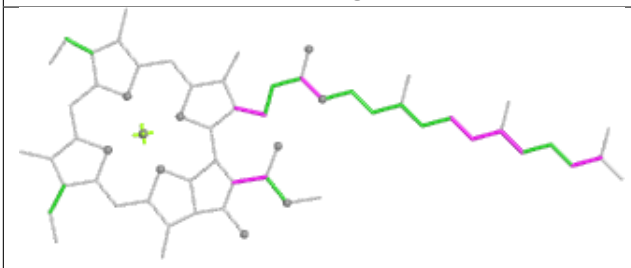
Ligand CLA H 305



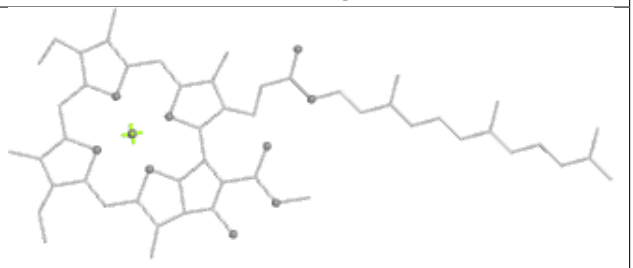
Bond lengths



Bond angles

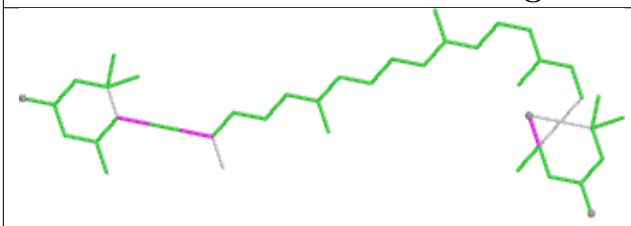


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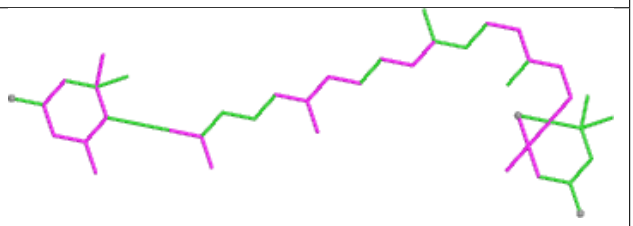


Rings

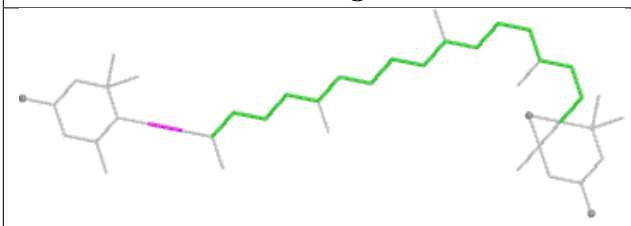
Ligand DD6 U 417



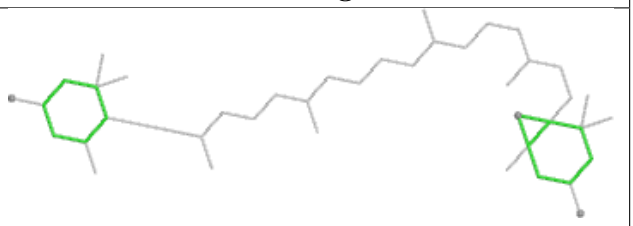
Bond lengths



Bond angles

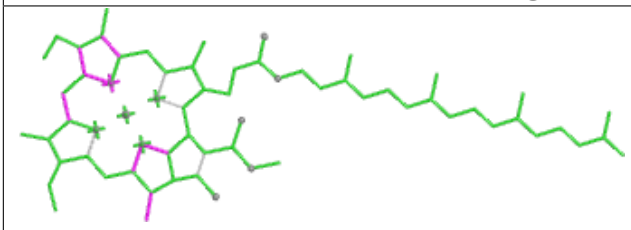


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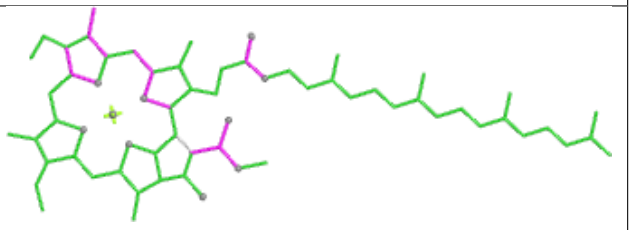


Rings

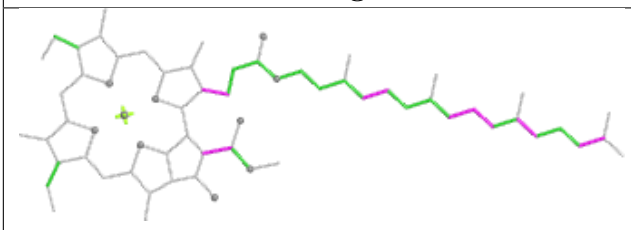
Ligand CLA B 824



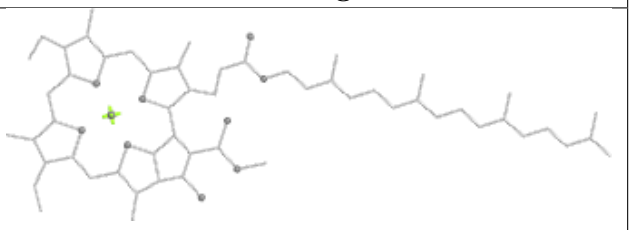
Bond lengths



Bond angles

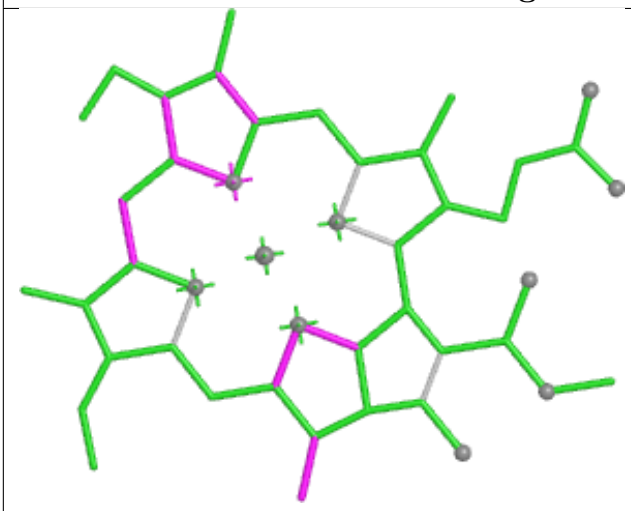


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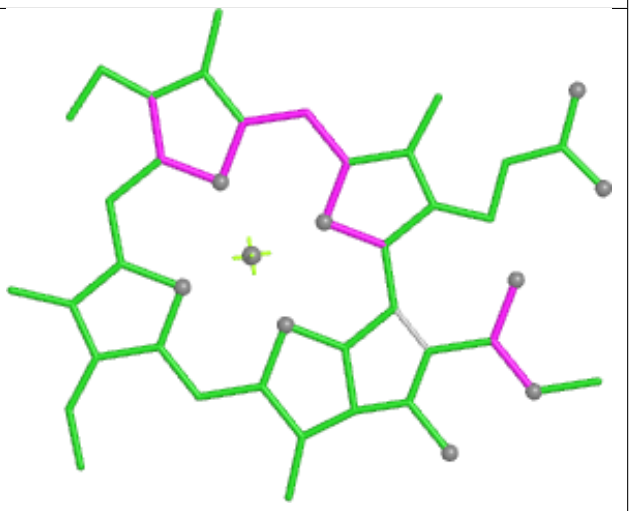


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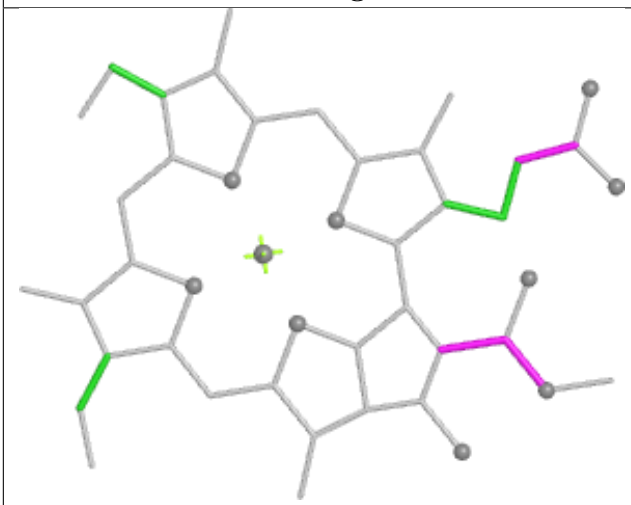
Ligand CLA W 413



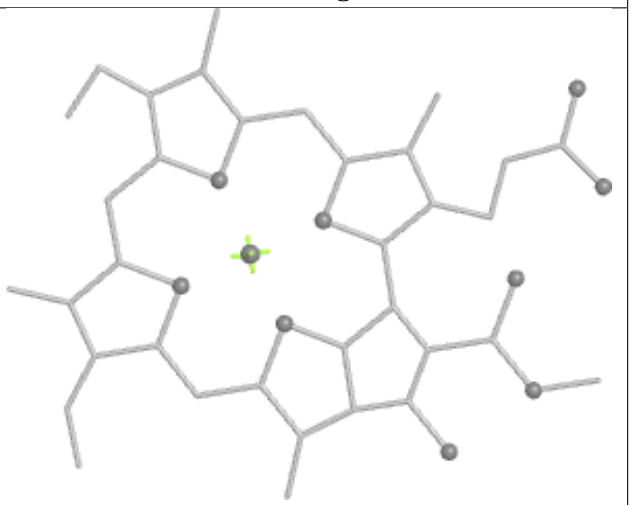
Bond lengths



Bond angles

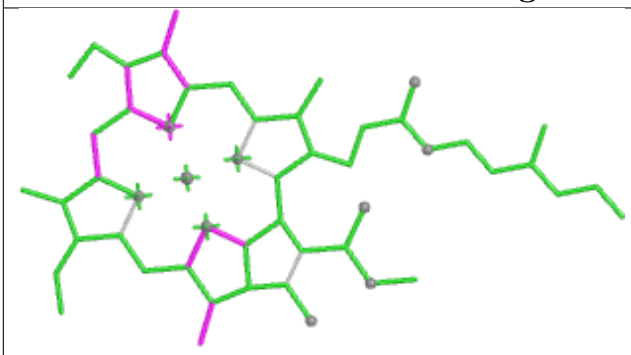


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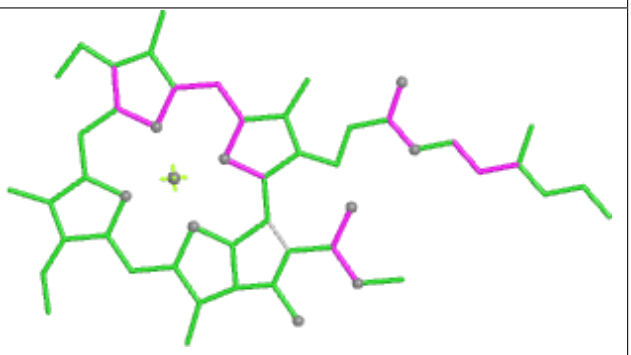


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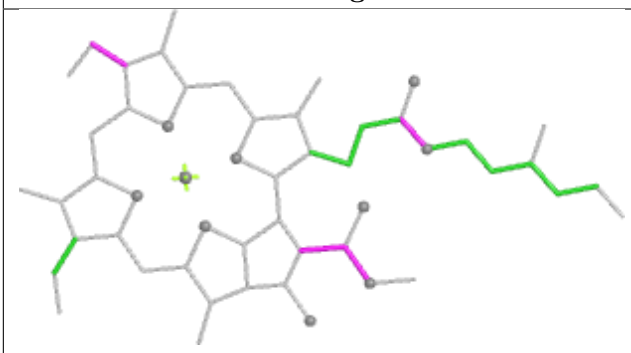
Ligand CLA W 403



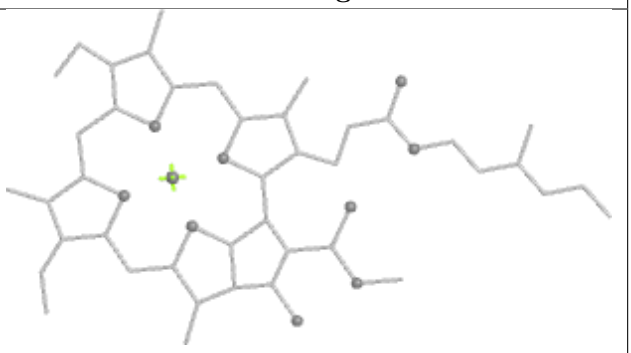
Bond lengths



Bond angles

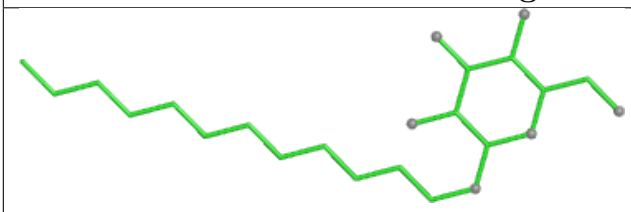


Torsions

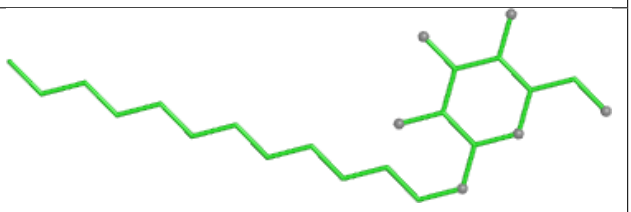


Rings

Ligand LMU A 857



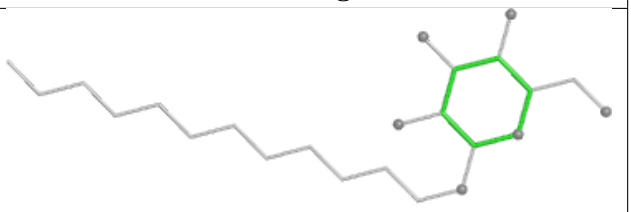
Bond lengths



Bond angles

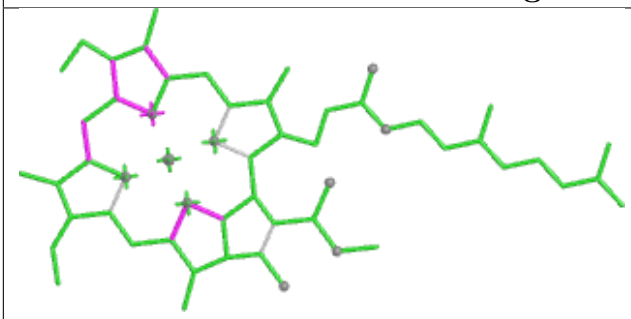


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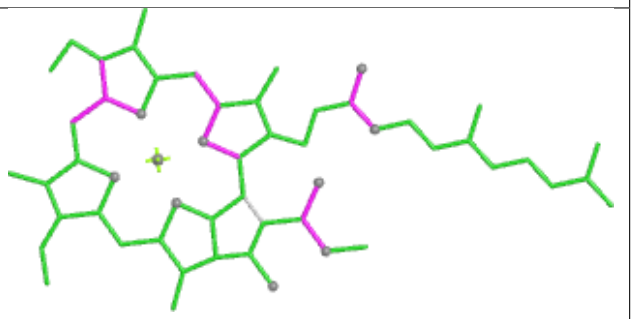


Rings

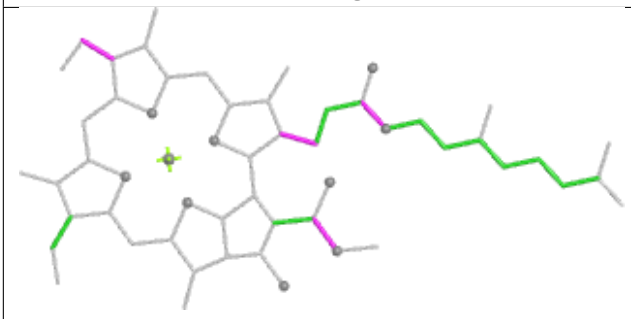
Ligand CLA V 608



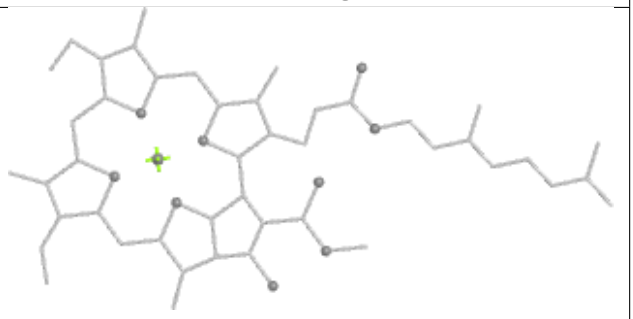
Bond lengths



Bond angles

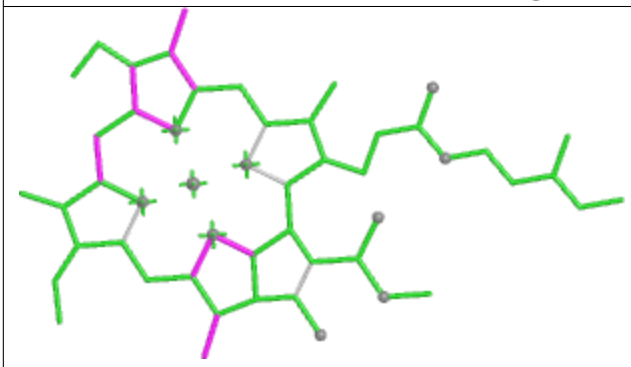


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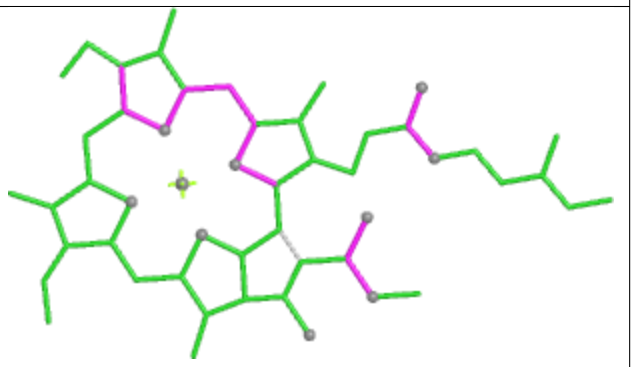


Rings

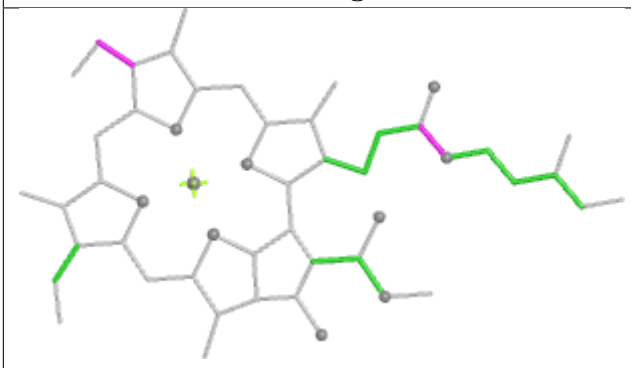
Ligand CLA S 615



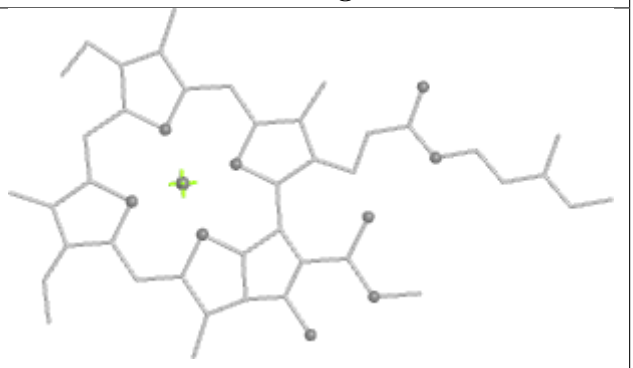
Bond lengths



Bond angles

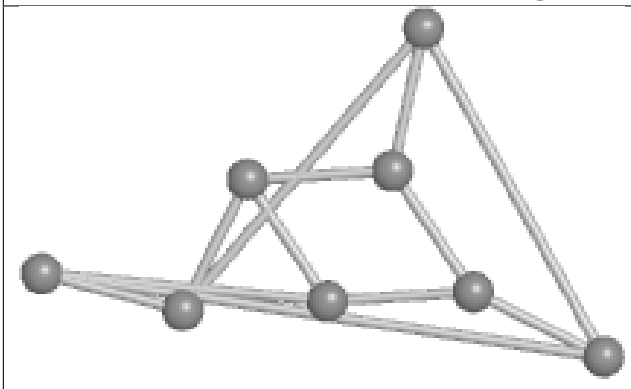


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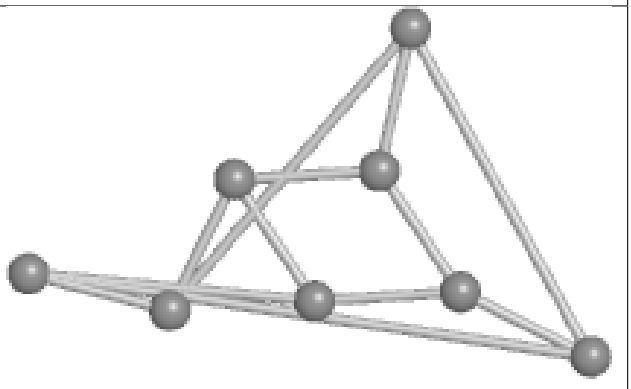


Rings

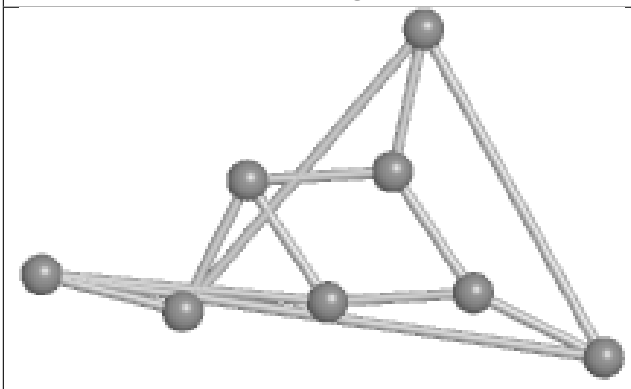
Ligand SF4 C 102



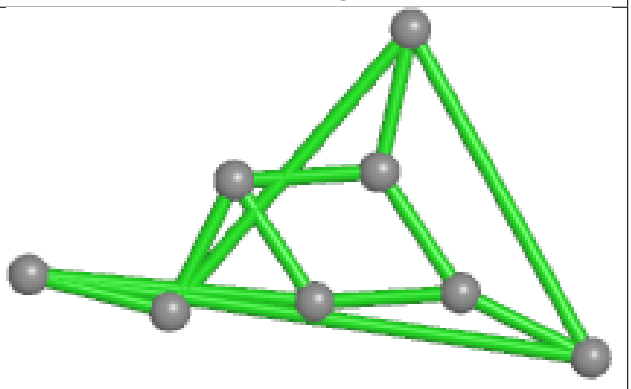
Bond lengths



Bond angles

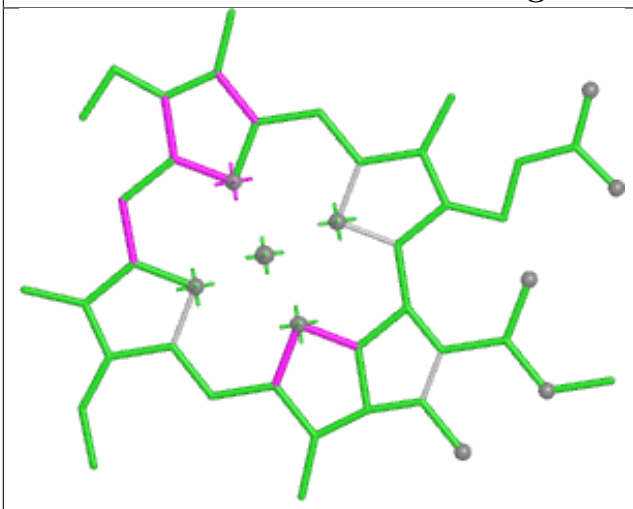


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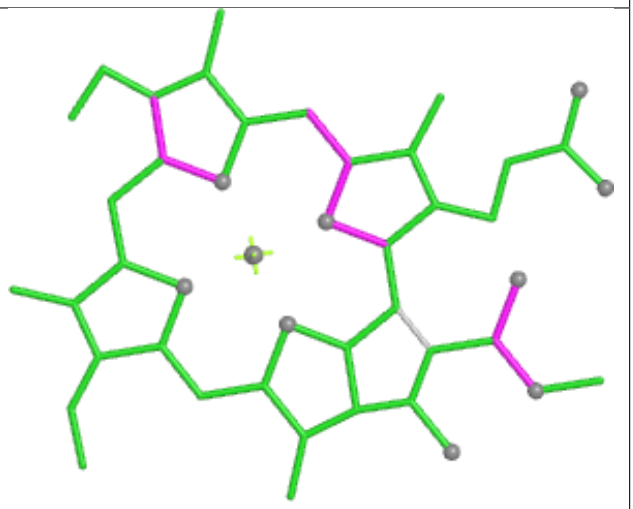


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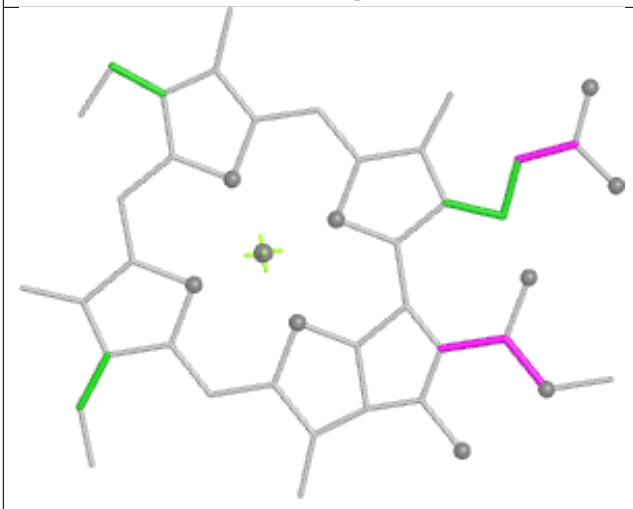
Ligand CLA S 601



Bond lengths



Bond angles

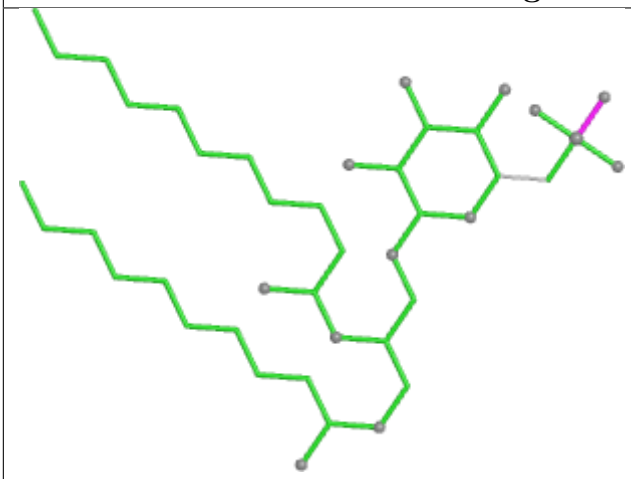


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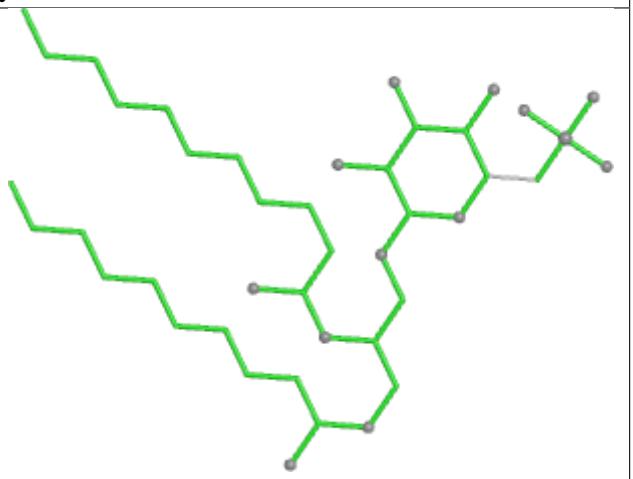


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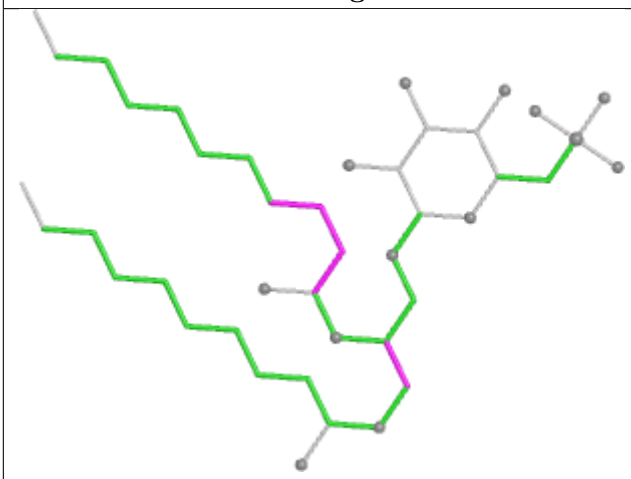
Ligand SQD K 621



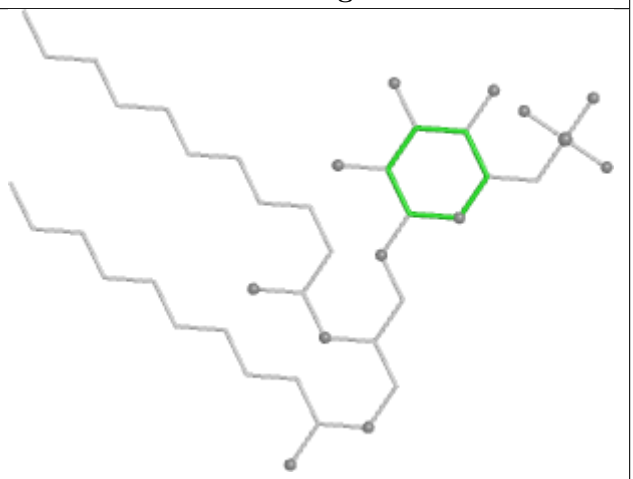
Bond lengths



Bond angles

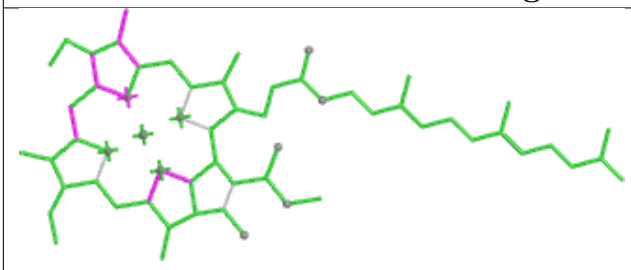


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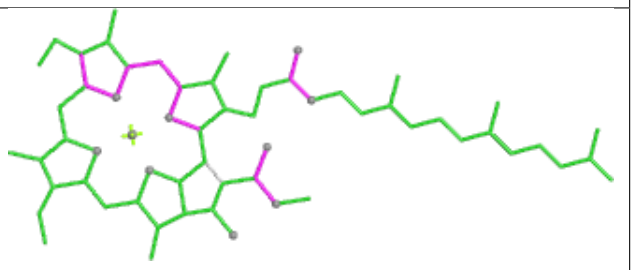


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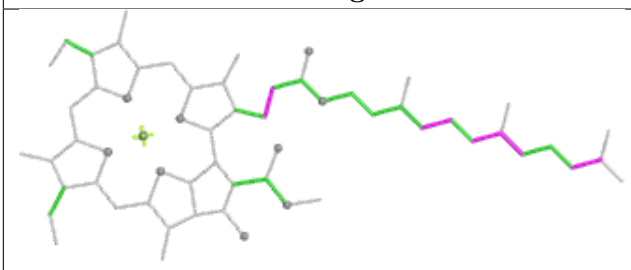
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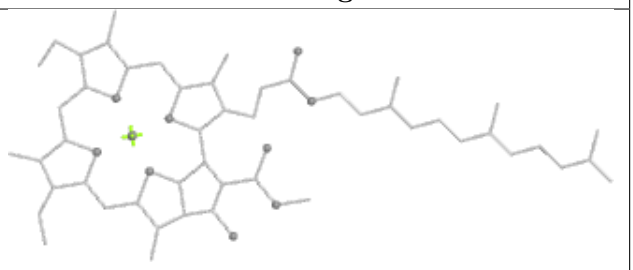
Bond lengths



Bond angles

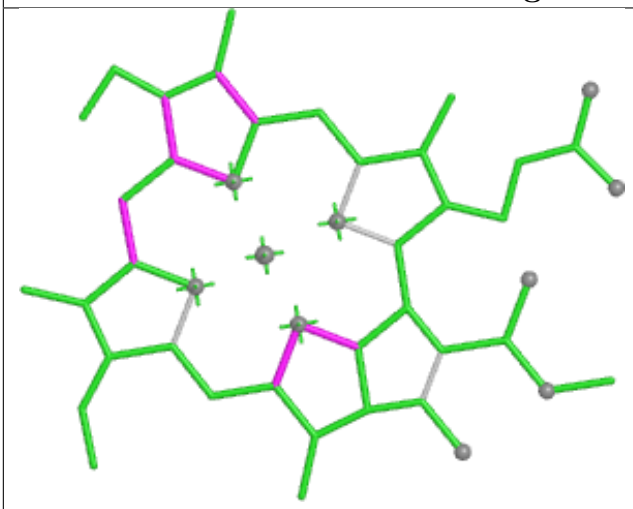


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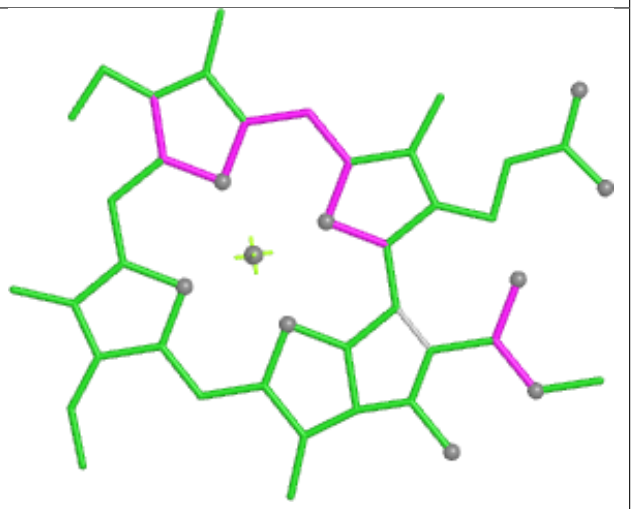


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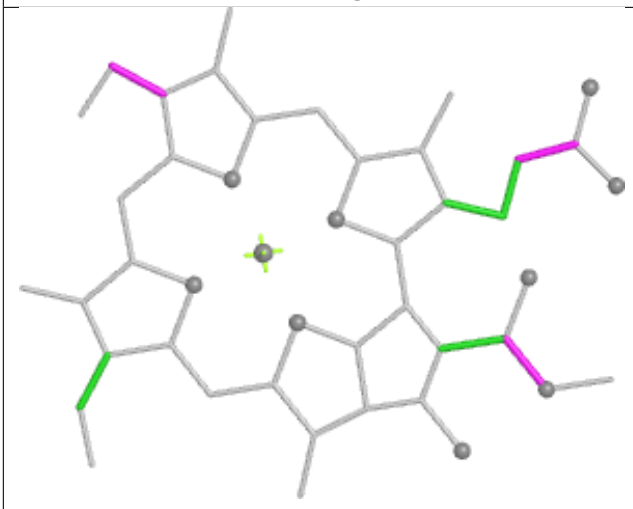
Ligand CLA V 601



Bond lengths



Bond angles

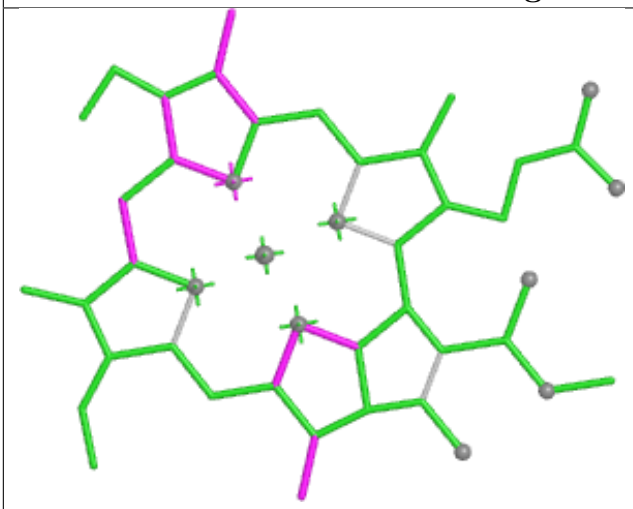


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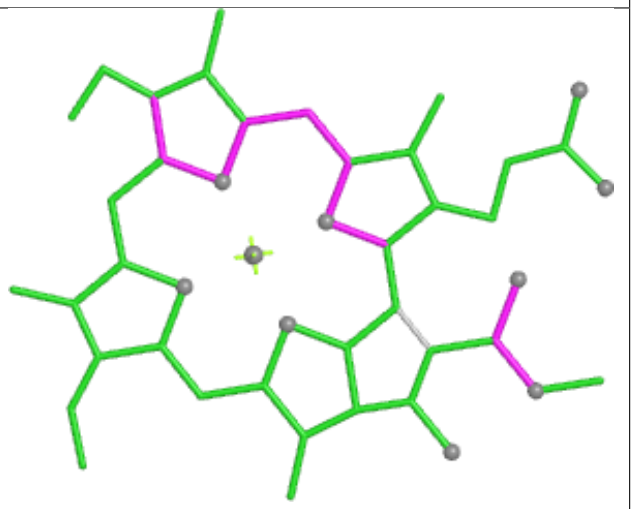


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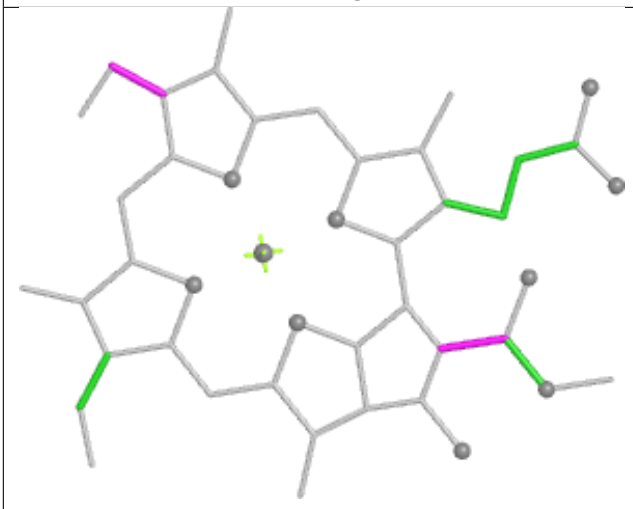
Ligand CLA B 837



Bond lengths



Bond angles

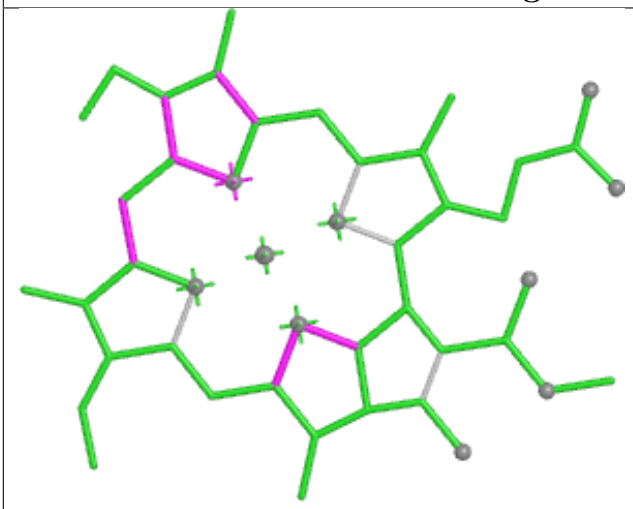


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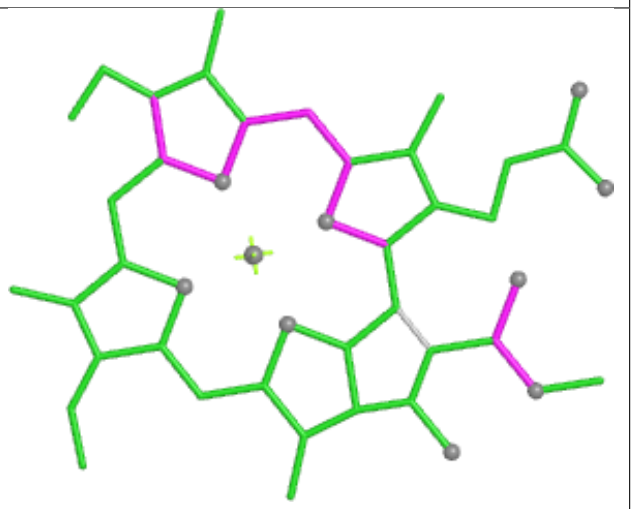


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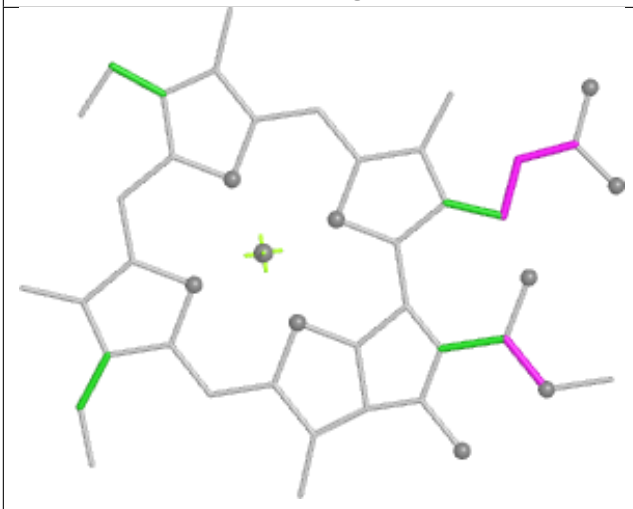
Ligand CLA G 610



Bond lengths



Bond angles

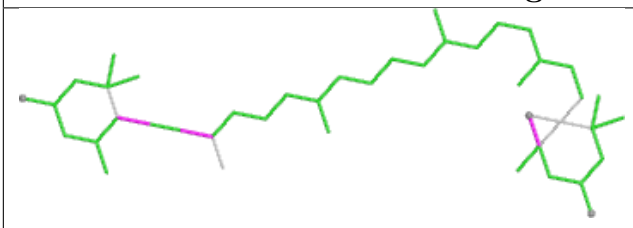


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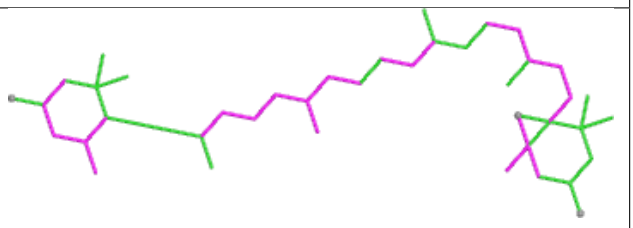


Rings

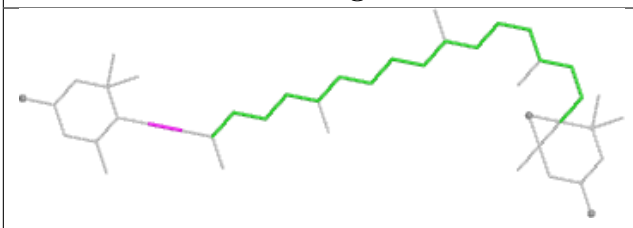
Ligand DD6 B 841



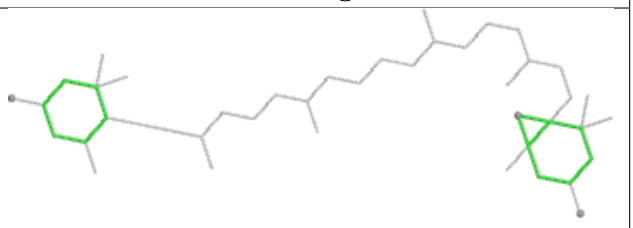
Bond lengths



Bond angles

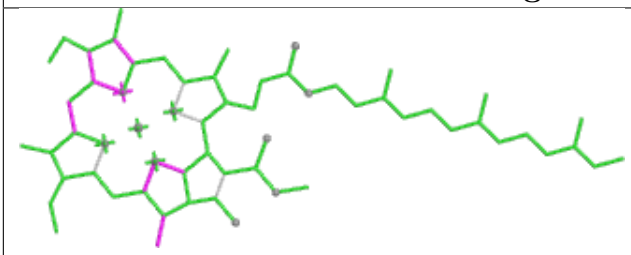


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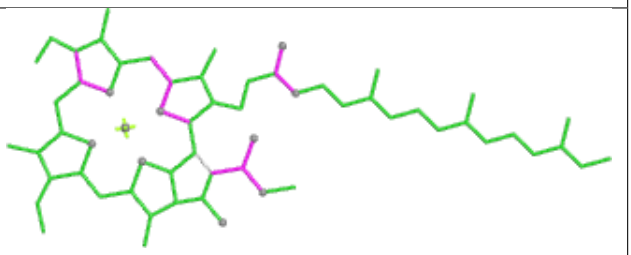


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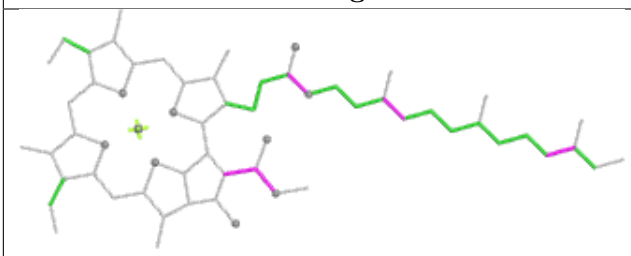
Ligand CLA A 835



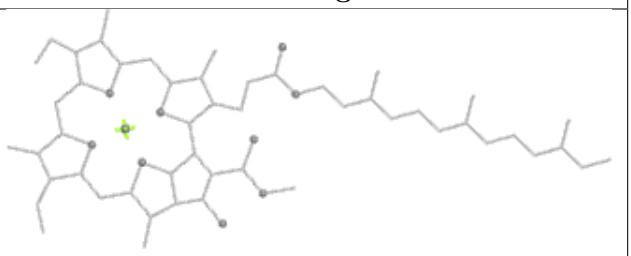
Bond lengths



Bond angles

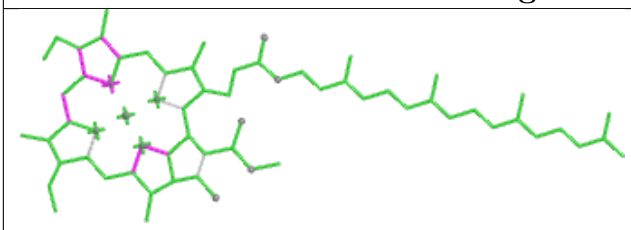


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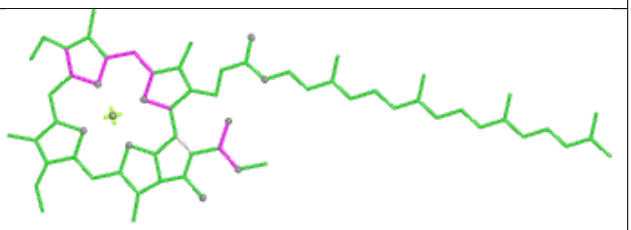


Rings

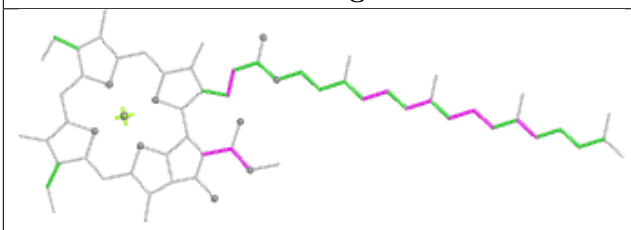
Ligand CLA W 404



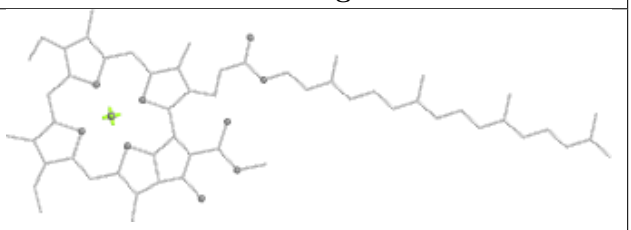
Bond lengths



Bond angles

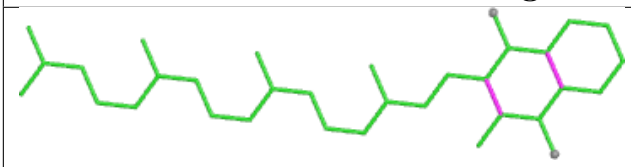


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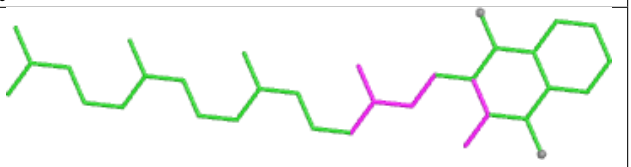


Rings

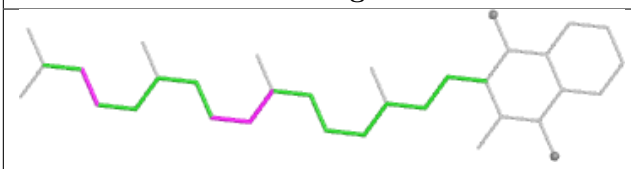
Ligand PQN A 843



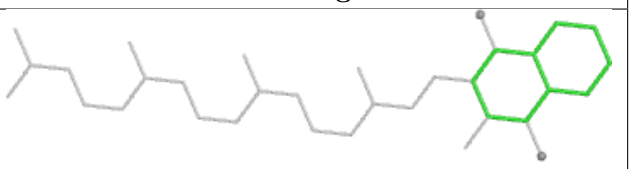
Bond lengths



Bond angles

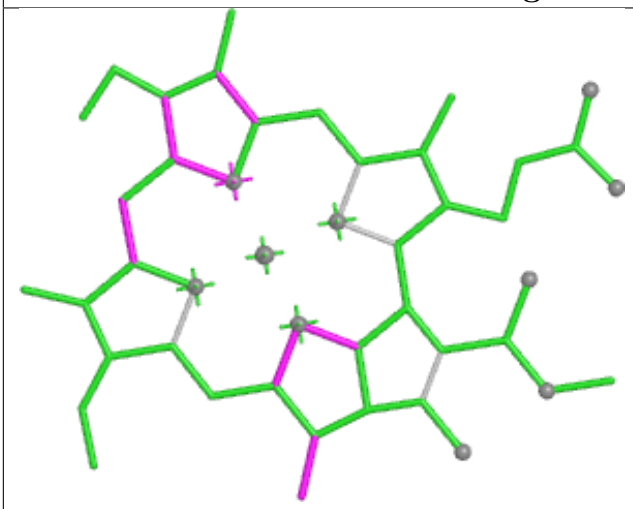


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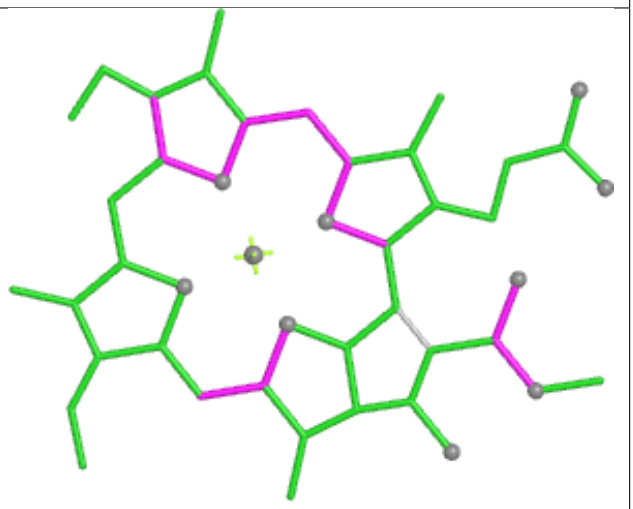


Rings

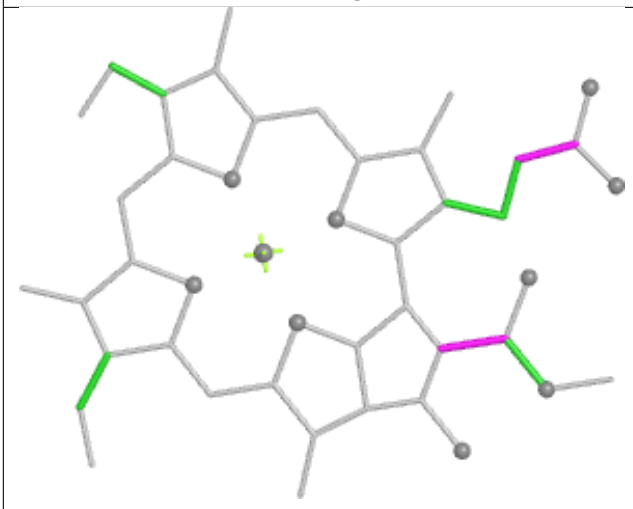
Ligand CLA G 609



Bond lengths



Bond angles

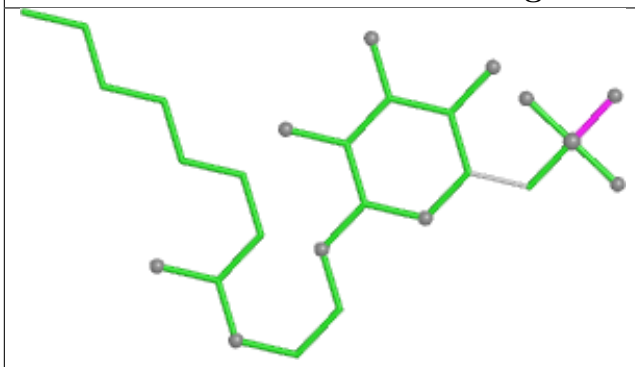


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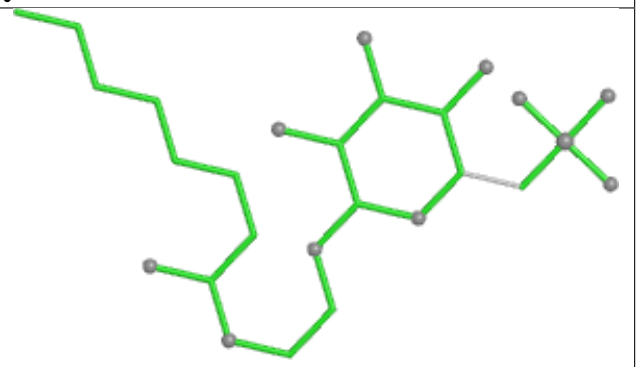


Rings

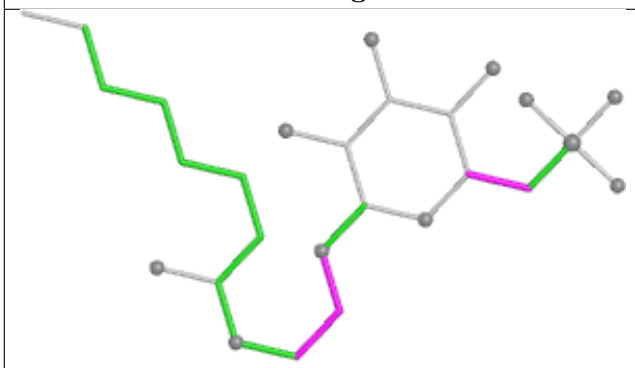
Ligand SQD V 618



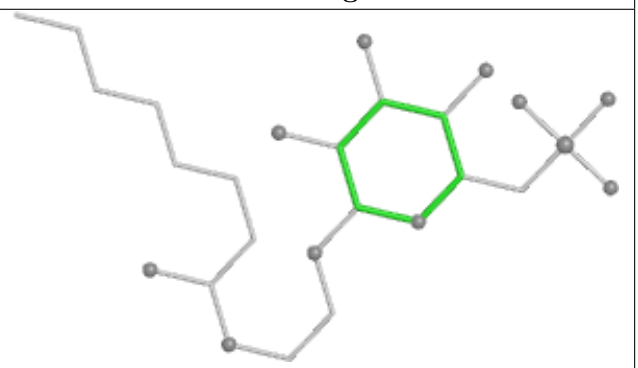
Bond lengths



Bond angles

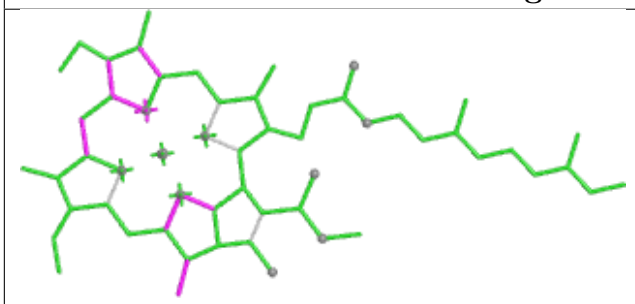


Torsions

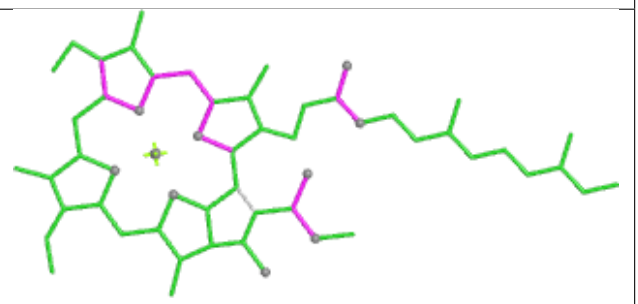


Rings

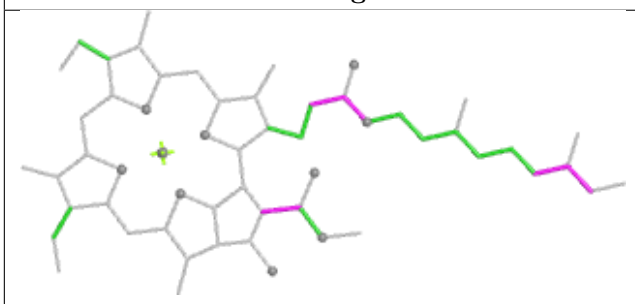
Ligand CLA R 603



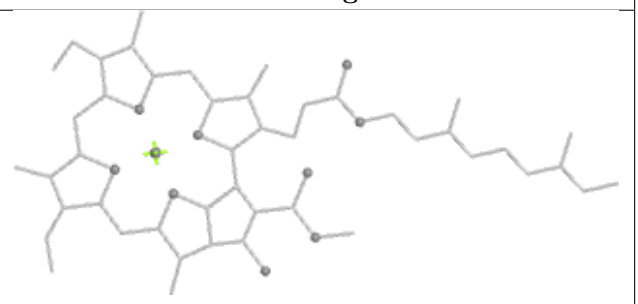
Bond lengths



Bond angles

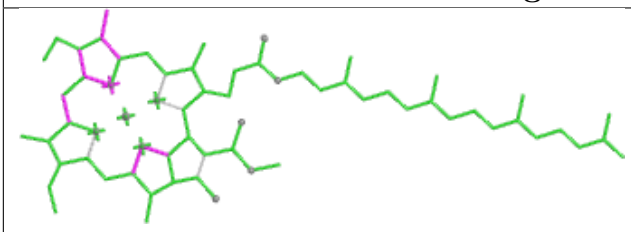


Torsions

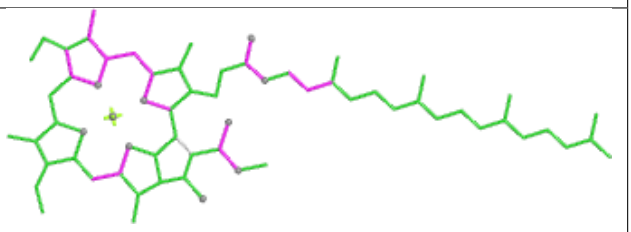


Rings

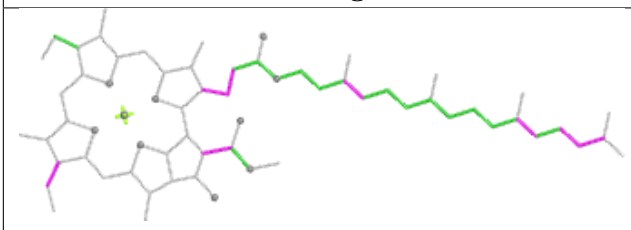
Ligand CLA A 820



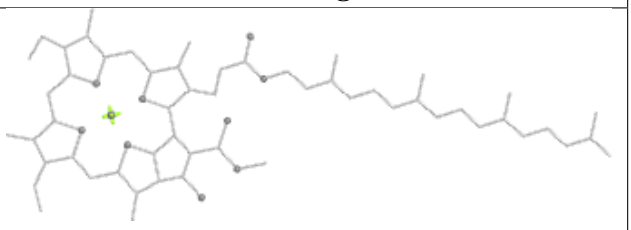
Bond lengths



Bond angles

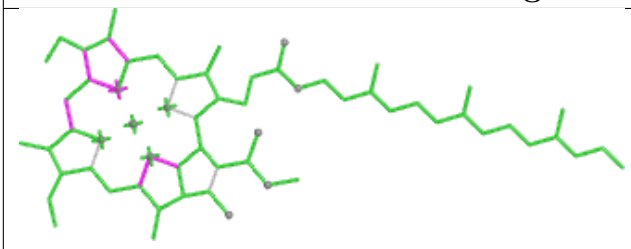


Torsions

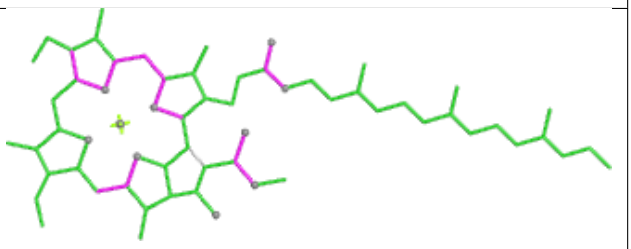


Rings

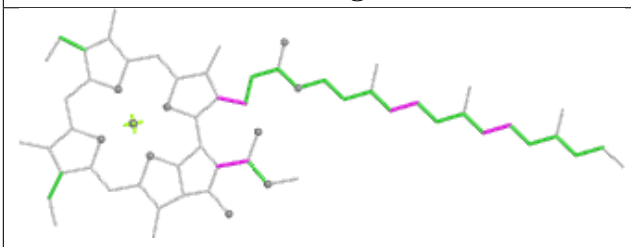
Ligand CLA A 827



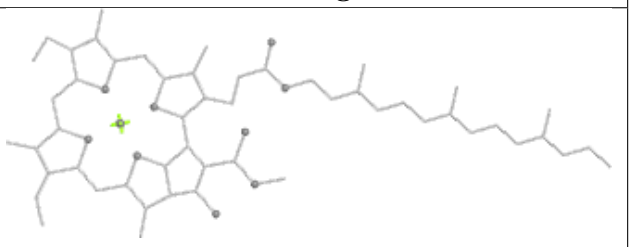
Bond lengths



Bond angles

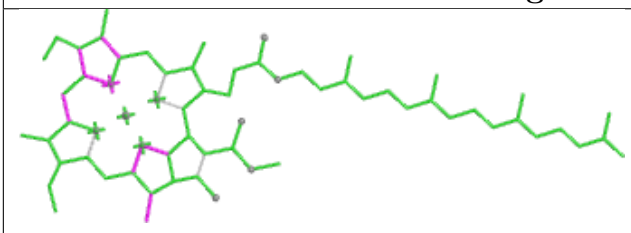


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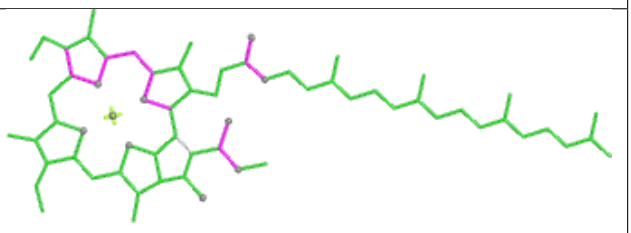


Rings

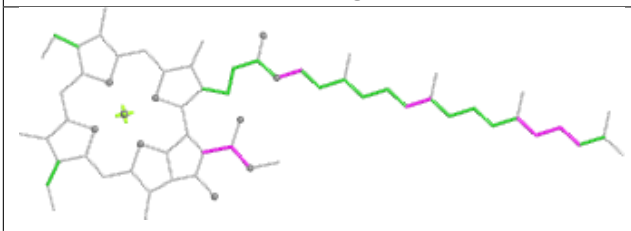
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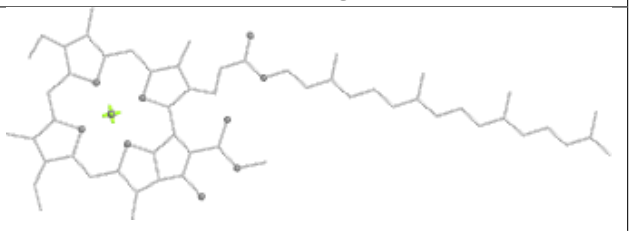
Bond lengths



Bond angles

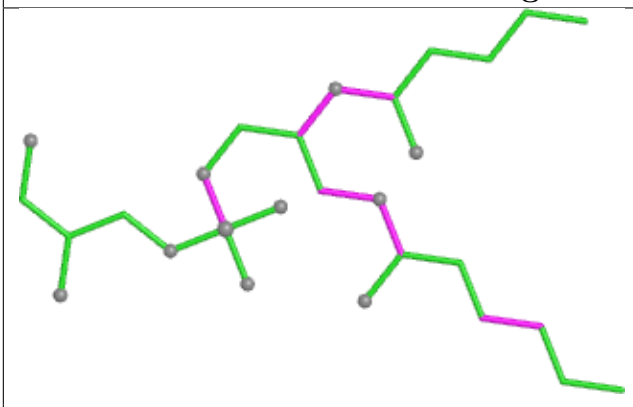


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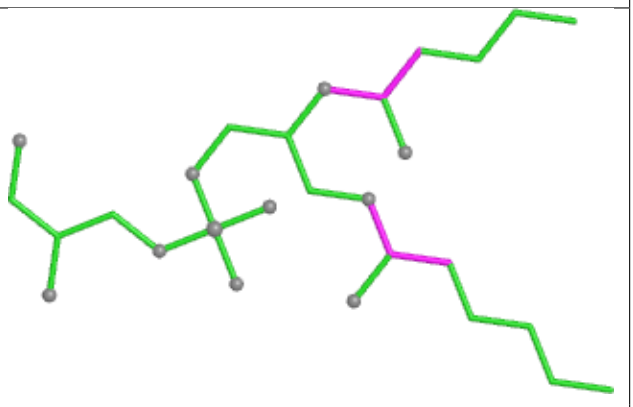


Rings

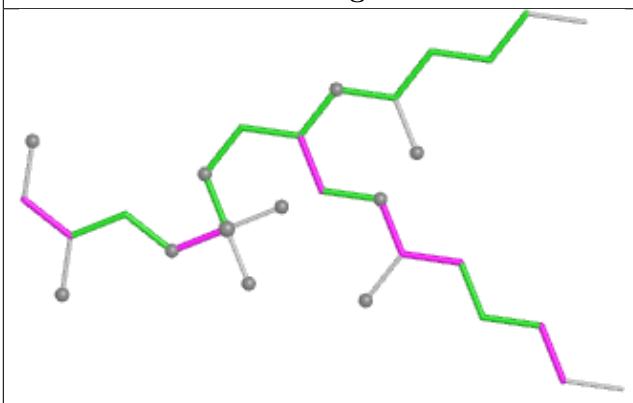
Ligand LHG N 614



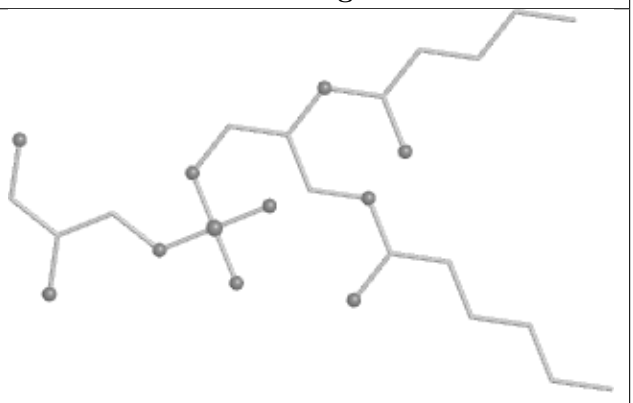
Bond lengths



Bond angles

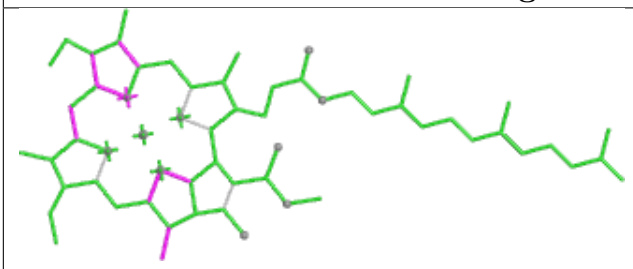


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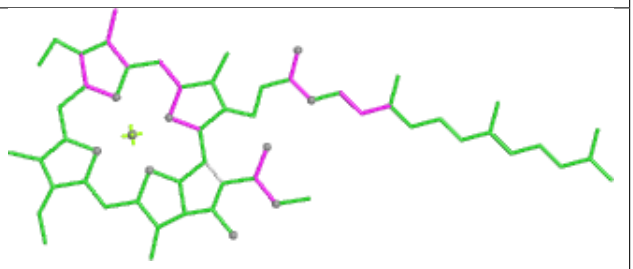


Rings

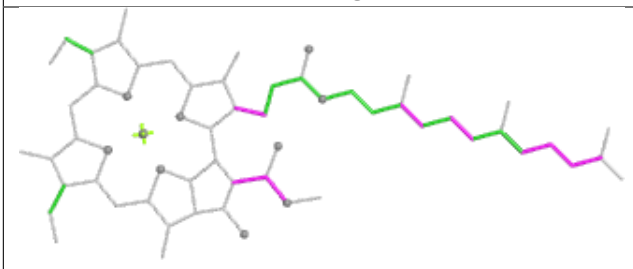
Ligand CLA W 411



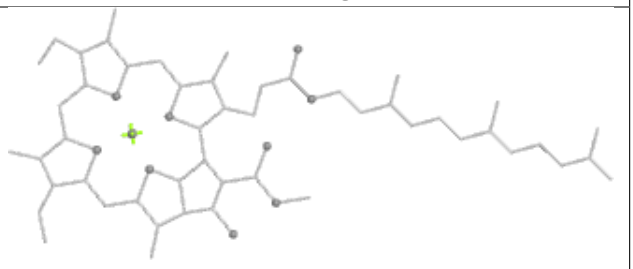
Bond lengths



Bond angles

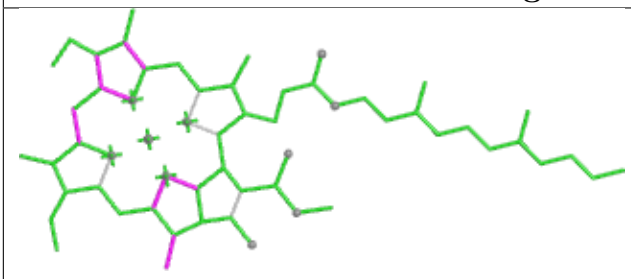


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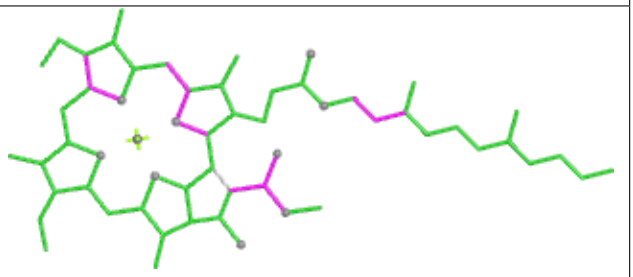


Rings

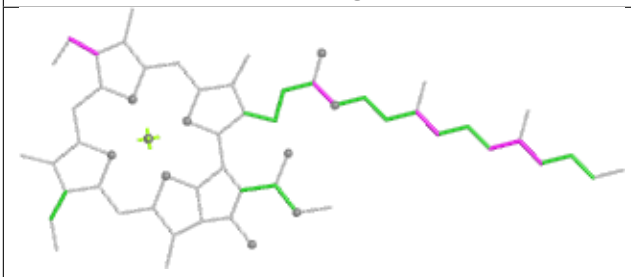
Ligand CLA H 313



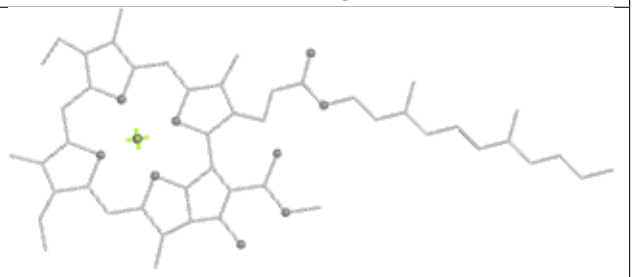
Bond lengths



Bond angles

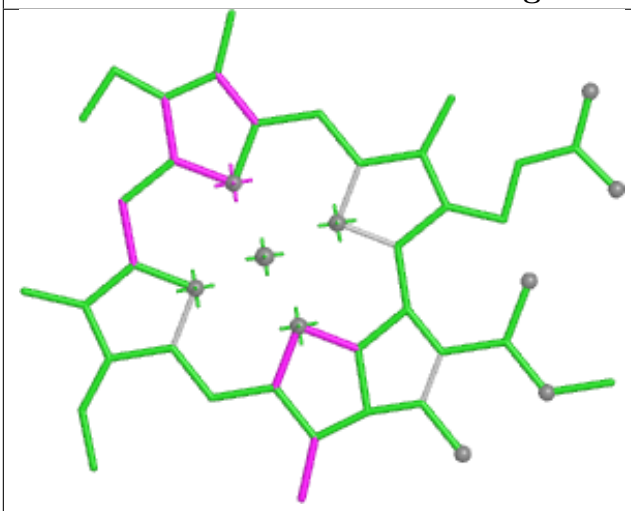


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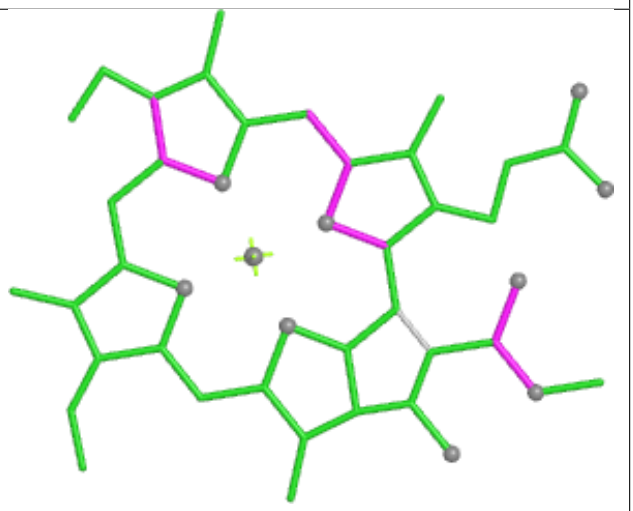


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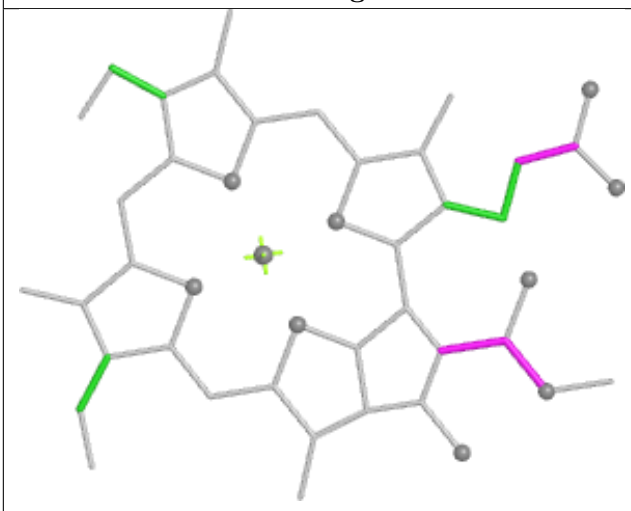
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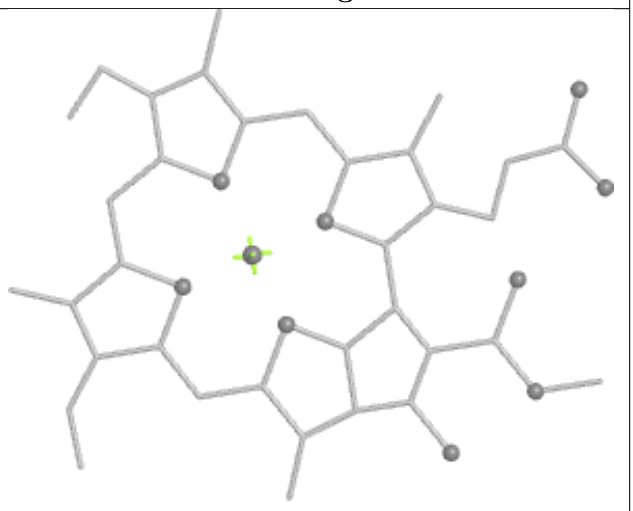
Bond lengths



Bond angles

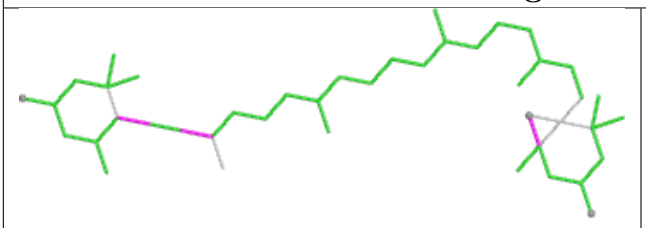


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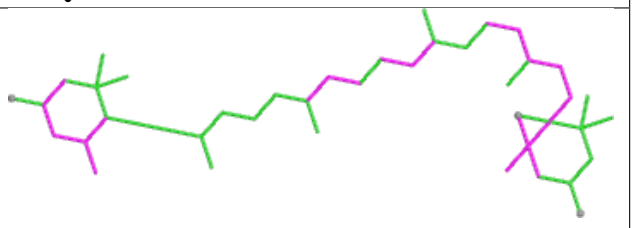


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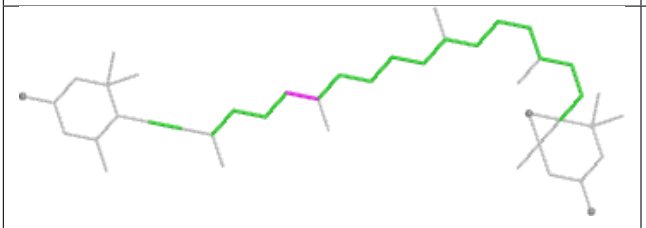
Ligand DD6 Q 614



Bond lengths



Bond angles

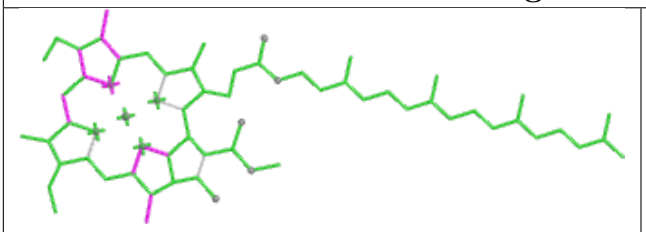


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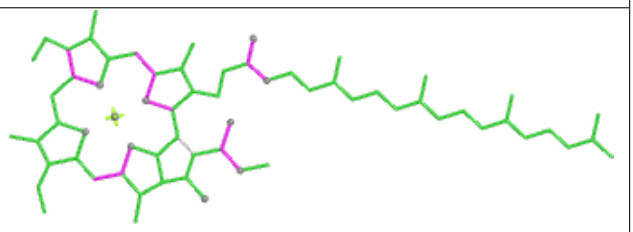


Rings

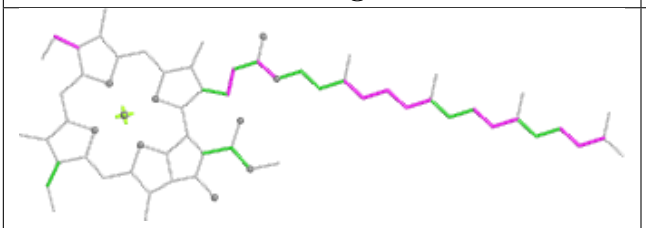
Ligand CLA T 605



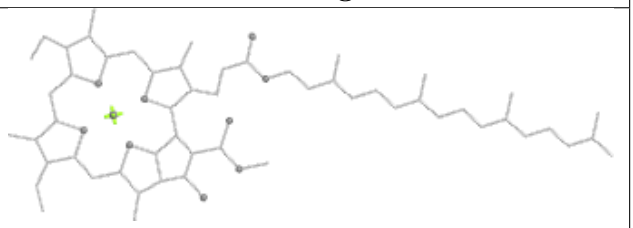
Bond lengths



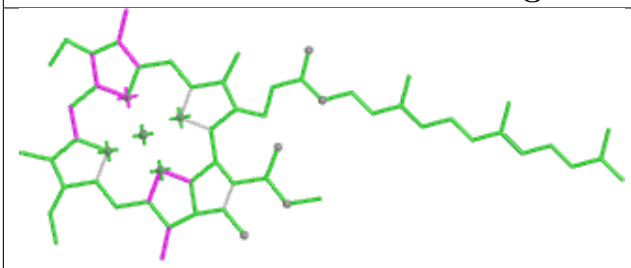
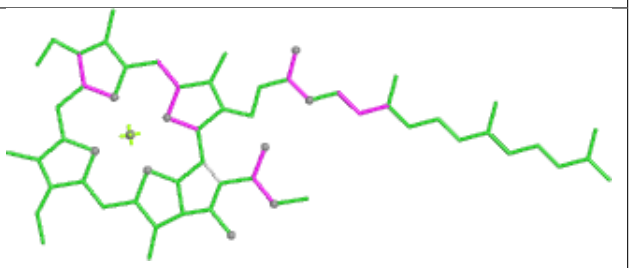
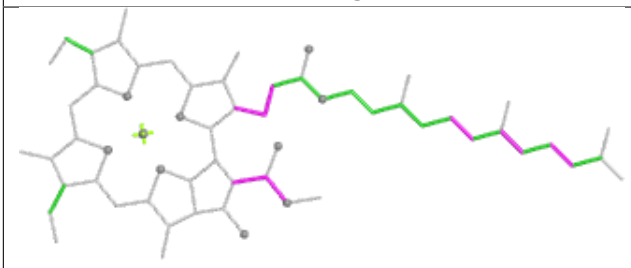
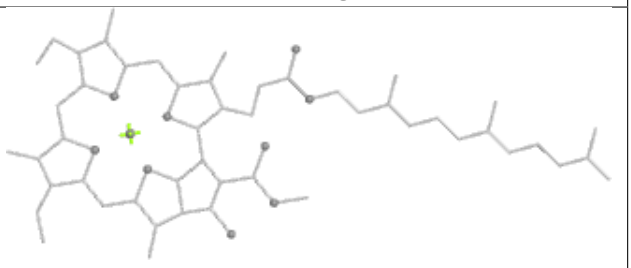
Bond angles

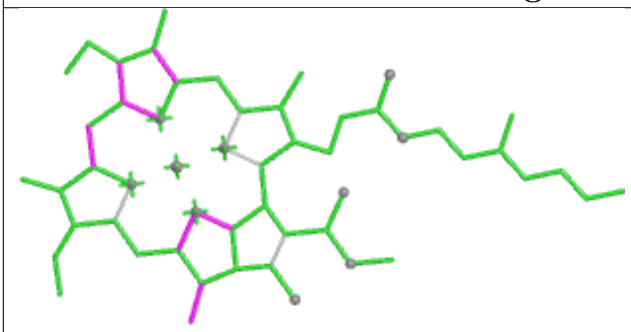
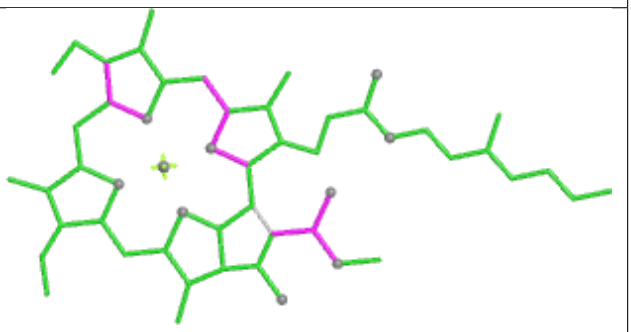
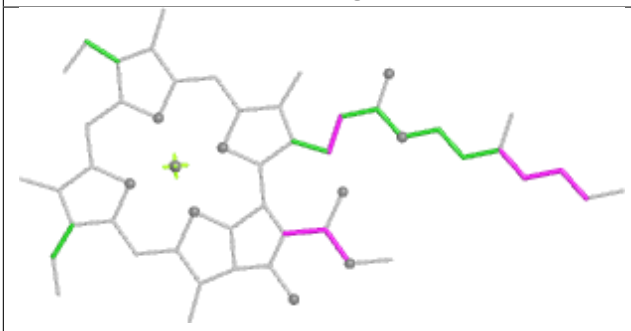
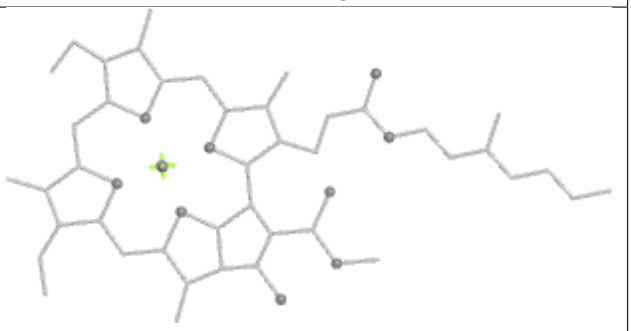


Torsions

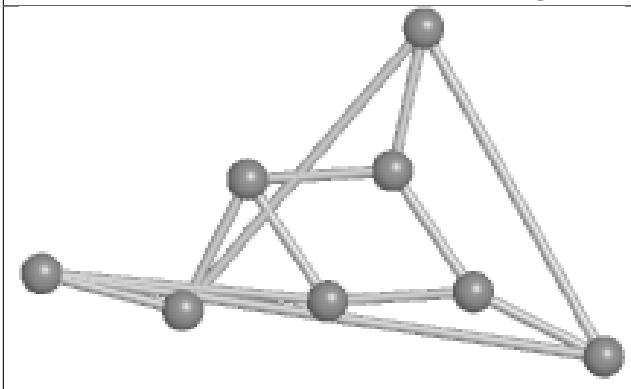


Rings

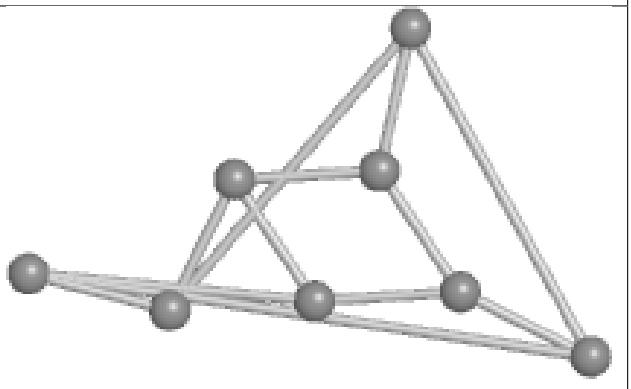
Ligand CLA O 310	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 820	
	
Bond lengths	Bond angles
	
Torsions	Rings

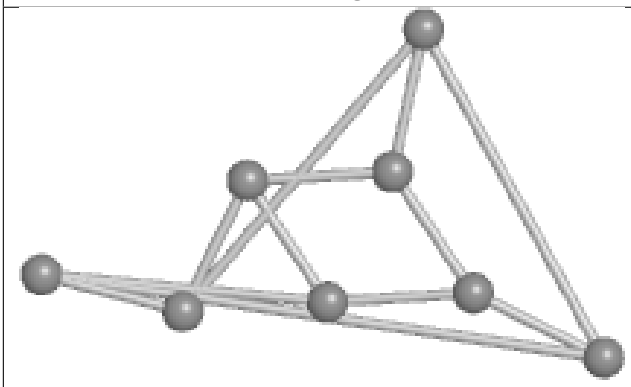
Ligand SF4 B 860



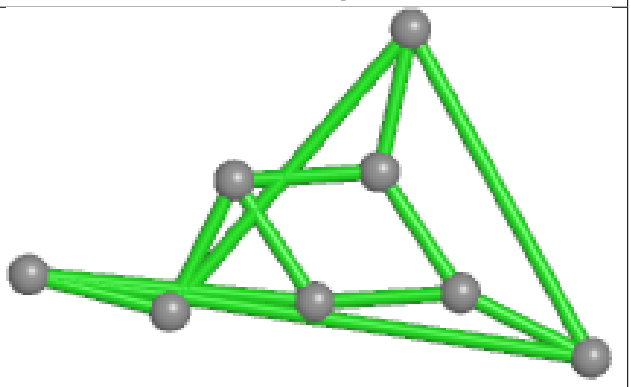
Bond lengths



Bond angles

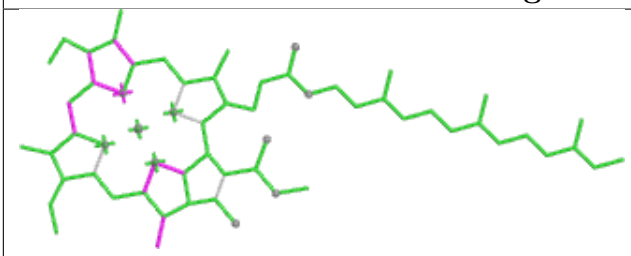


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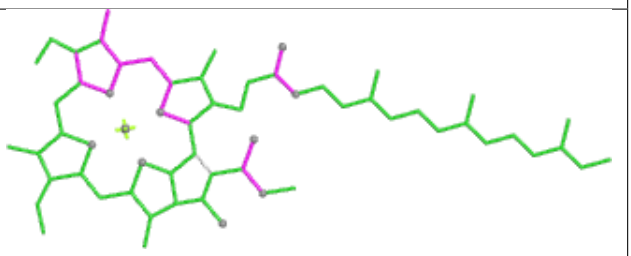


Rings

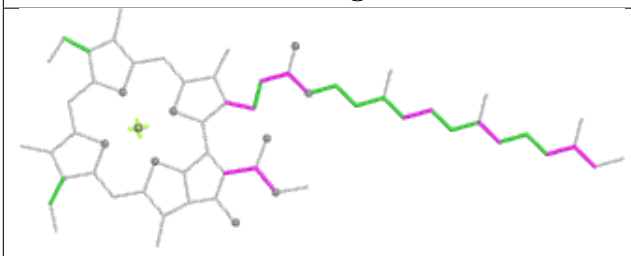
Ligand CLA O 308



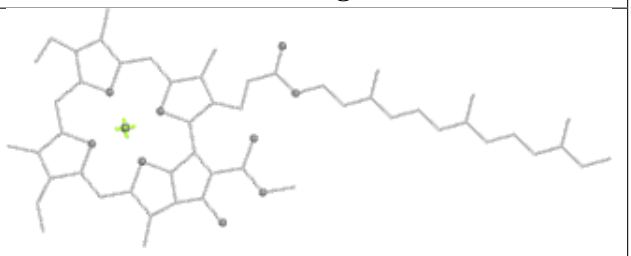
Bond lengths



Bond angles

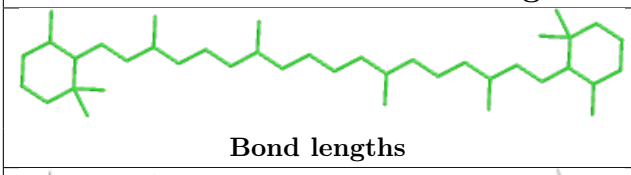


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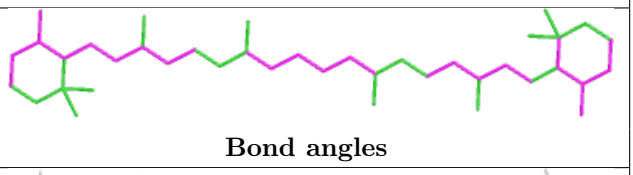


Rings

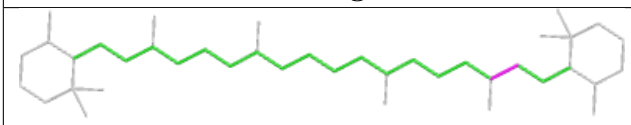
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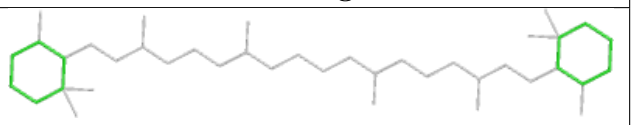
Bond lengths



Bond angles

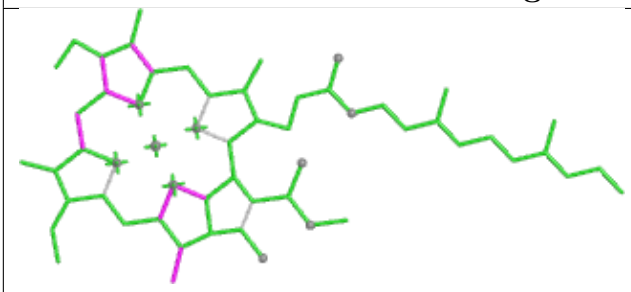


Torsions

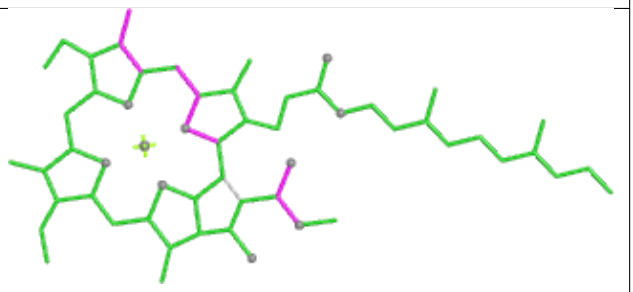


Rings

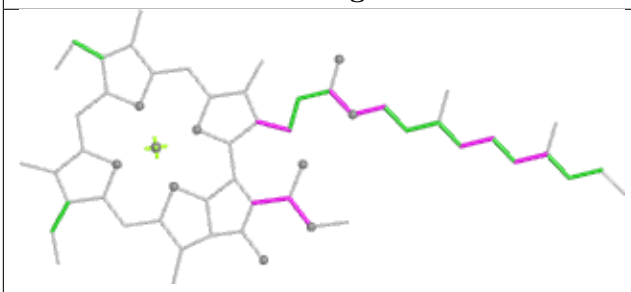
Ligand CLA V 603



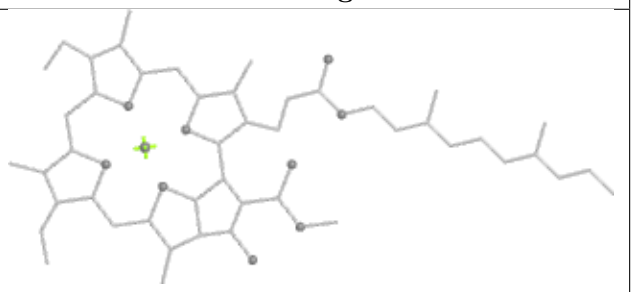
Bond lengths



Bond angles

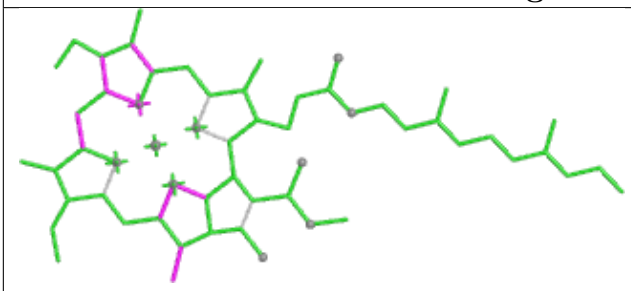


Torsions

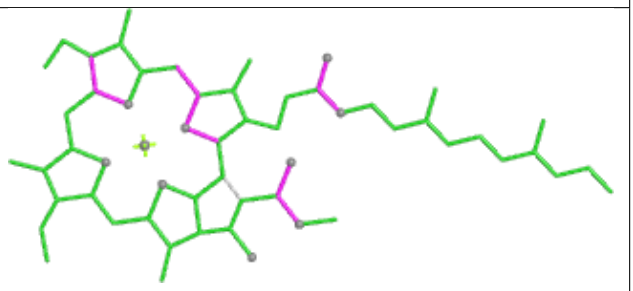


Rings

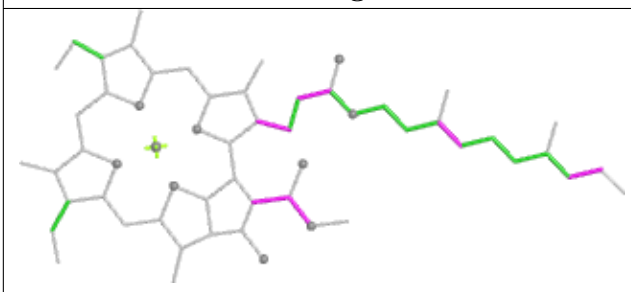
Ligand CLA L 407



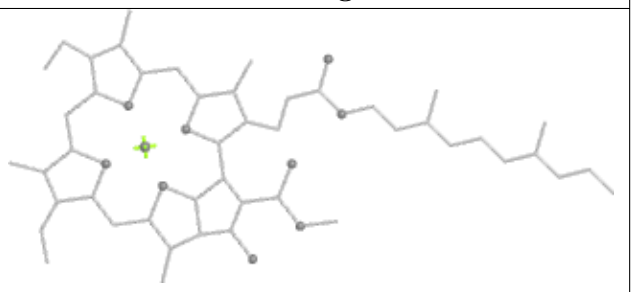
Bond lengths



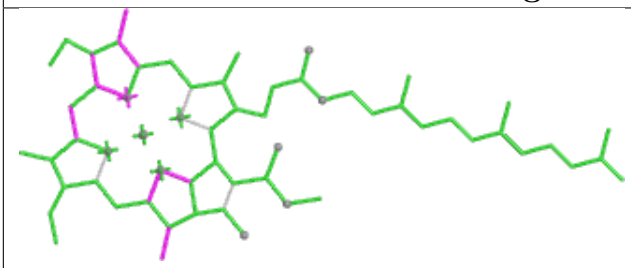
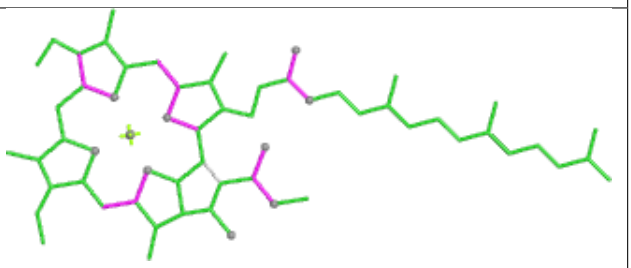
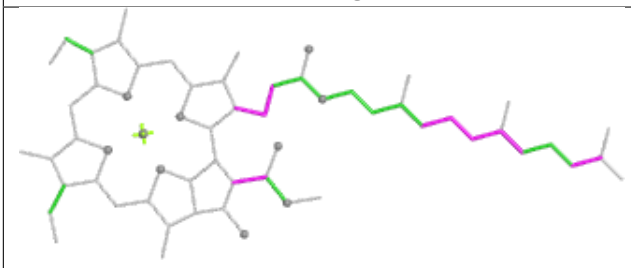
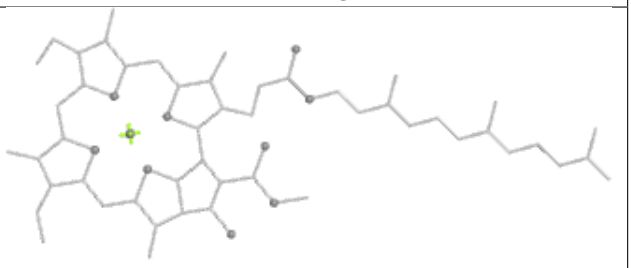
Bond angles

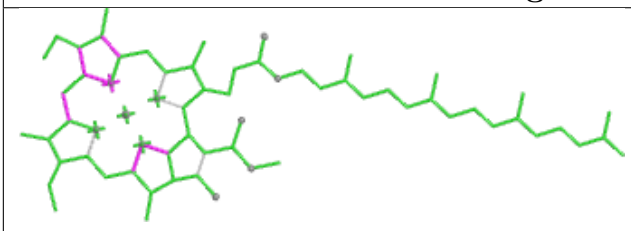
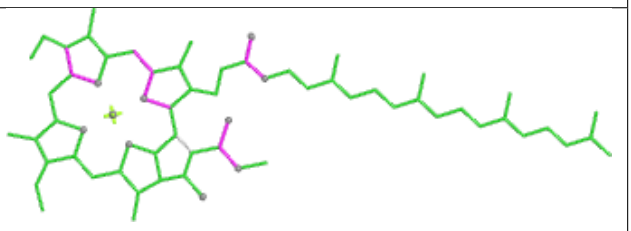
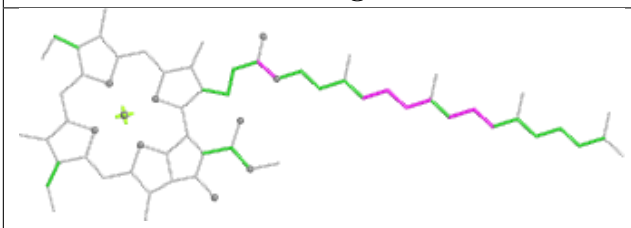
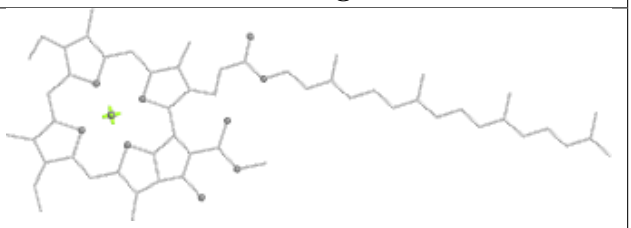


Torsions

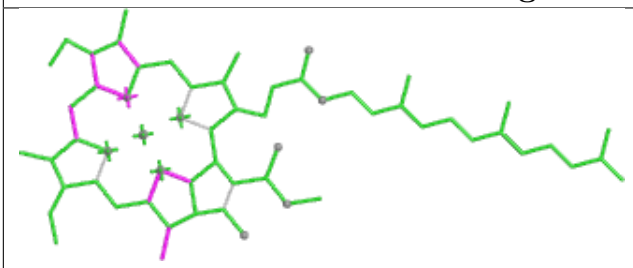


Rings

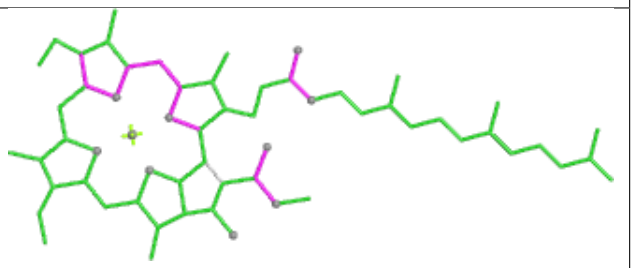
Ligand CLA H 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA L 417	
 Bond lengths	 Bond angles
 Torsions	 Rings

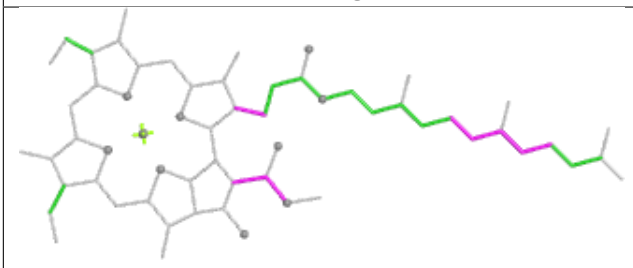
Ligand CLA W 410



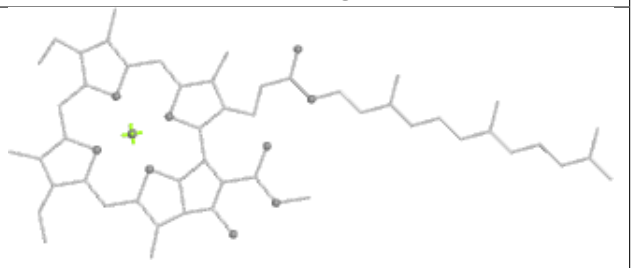
Bond lengths



Bond angles

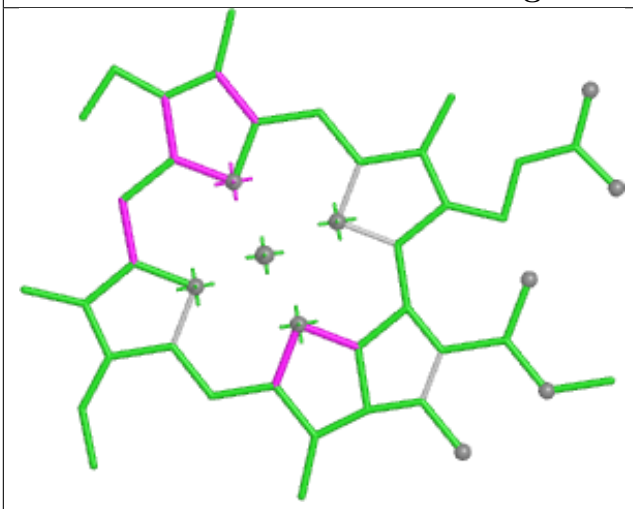


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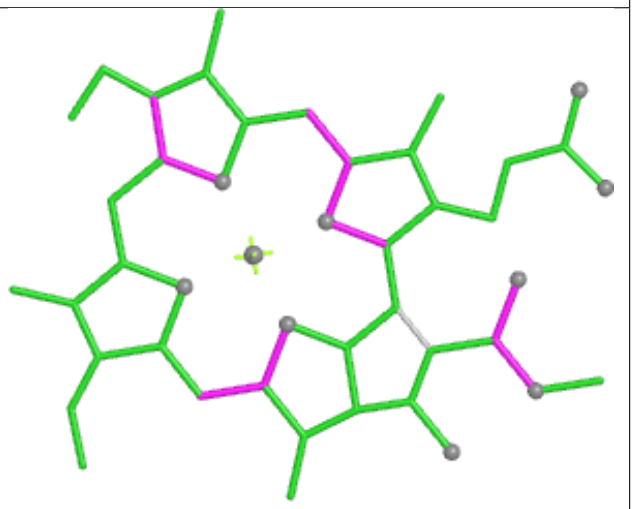


Rings

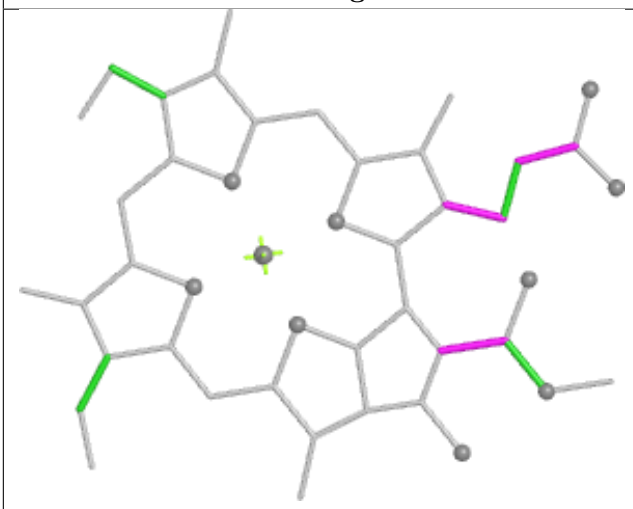
Ligand CLA R 611



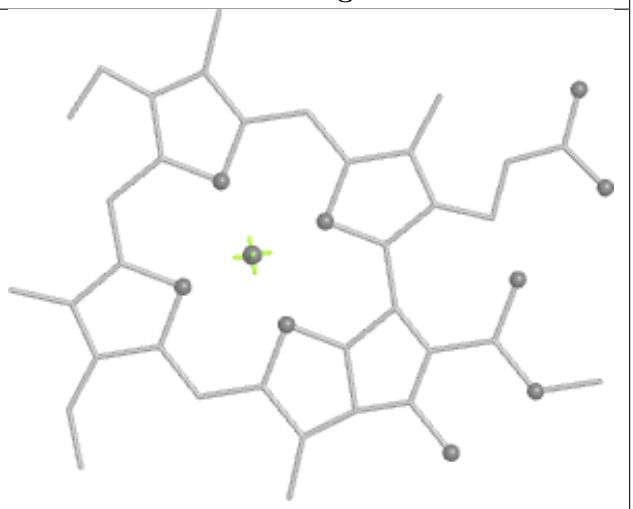
Bond lengths



Bond angles

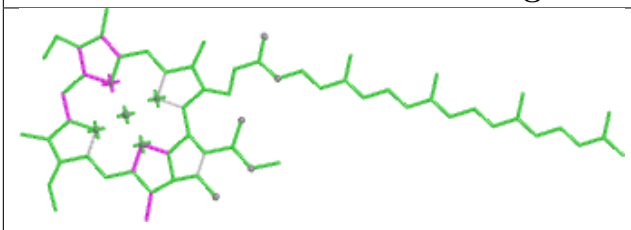


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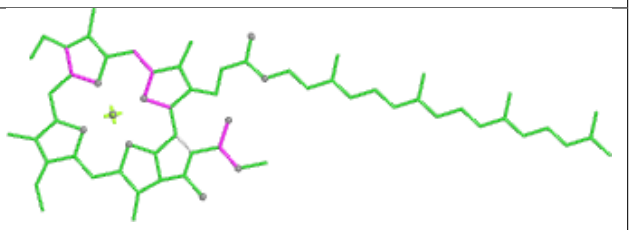


Rings

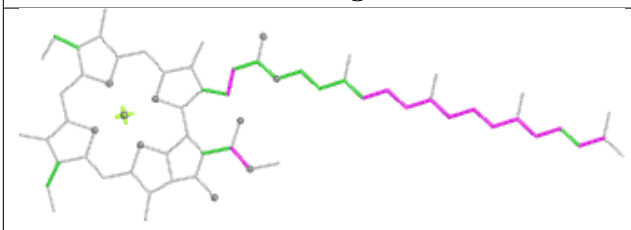
Ligand CLA O 313



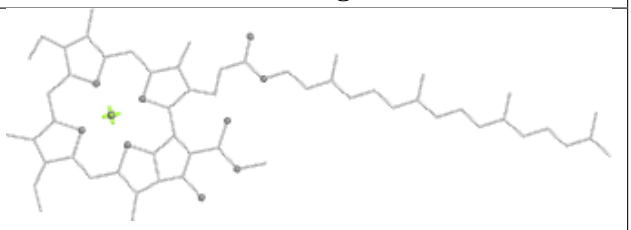
Bond lengths



Bond angles

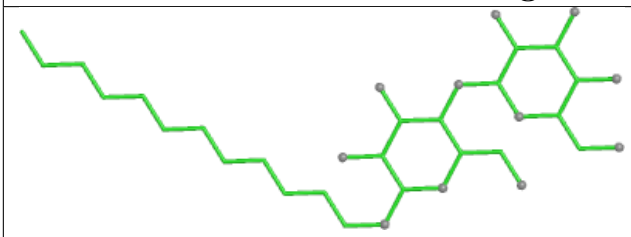


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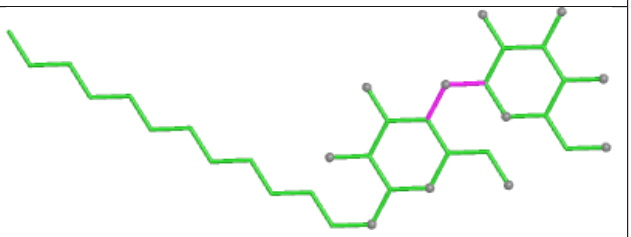


Rings

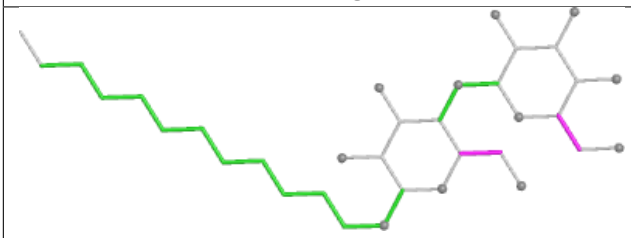
Ligand LMU O 303



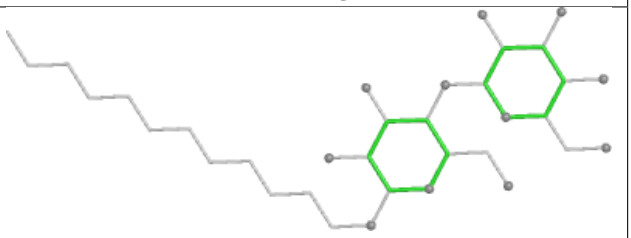
Bond lengths



Bond angles

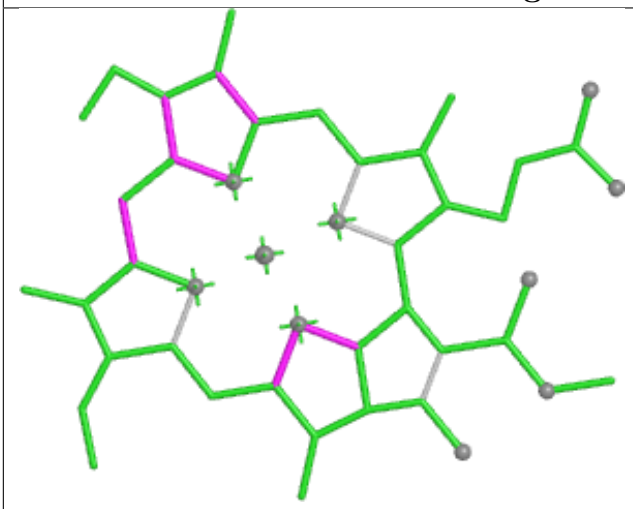


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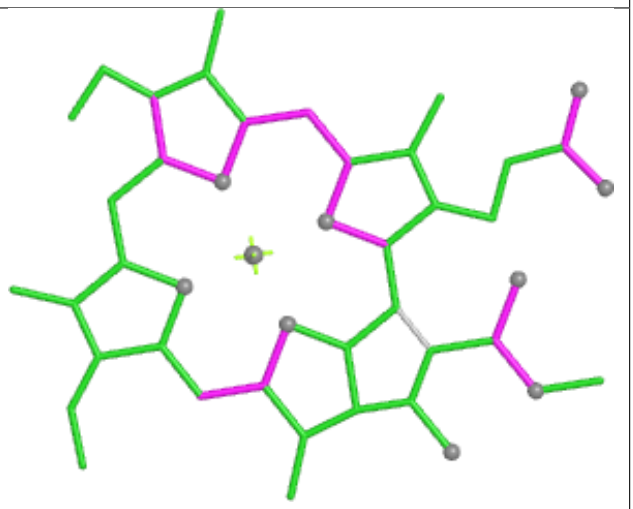


Rings

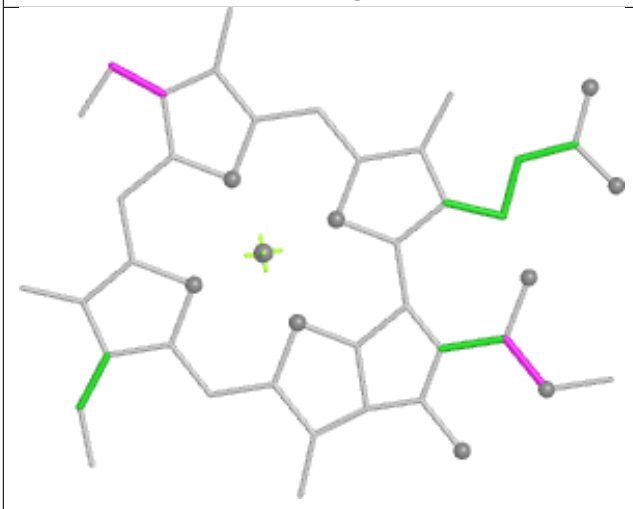
Ligand CLA V 610



Bond lengths



Bond angles

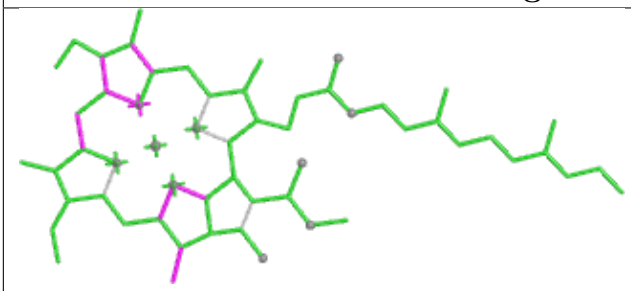


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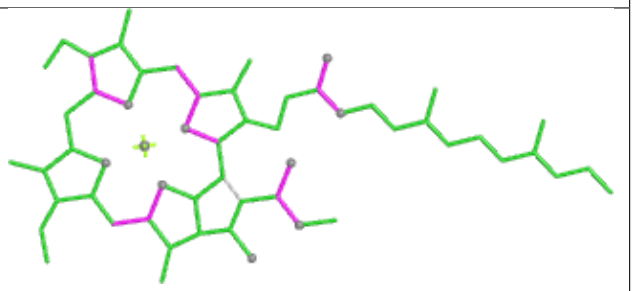


Rings

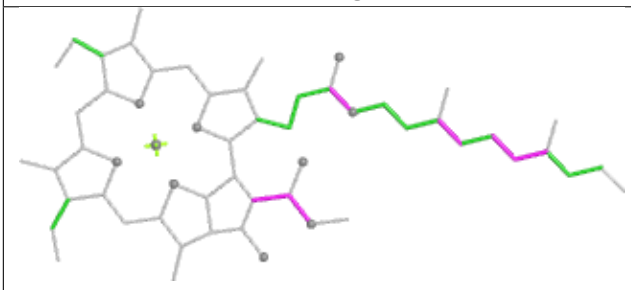
Ligand CLA A 812



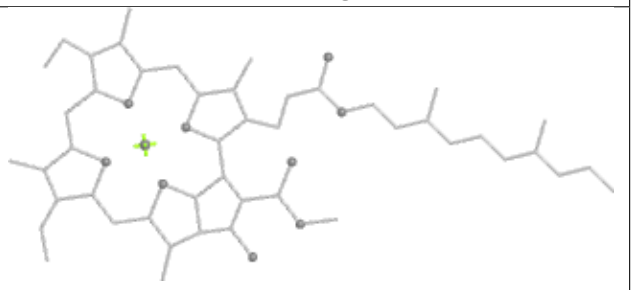
Bond lengths



Bond angles

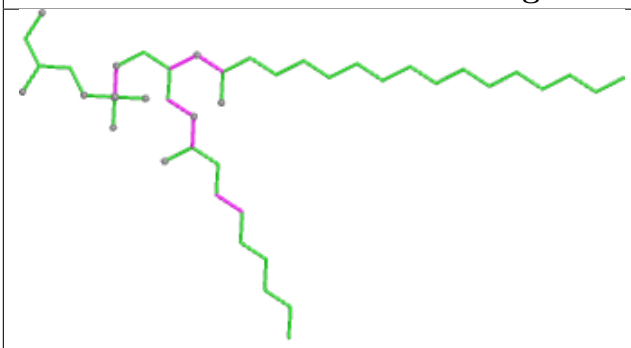


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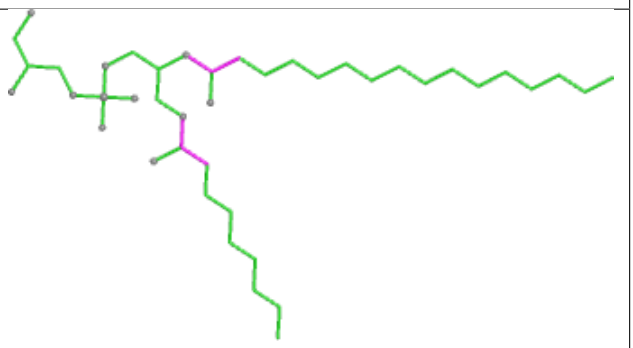


Rings

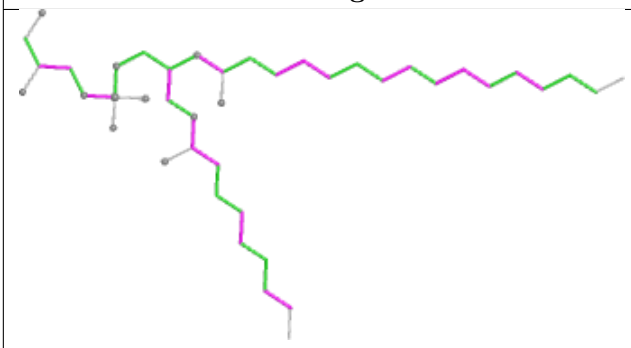
Ligand LHG R 614



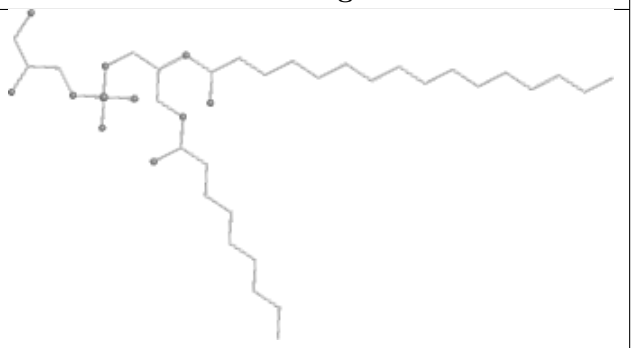
Bond lengths



Bond angles

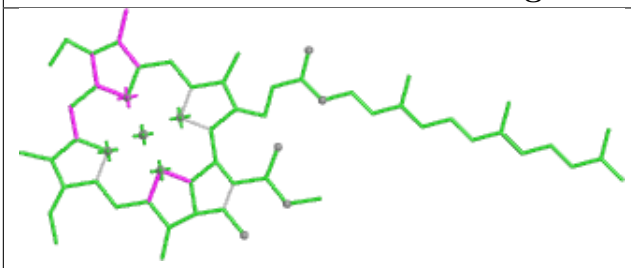


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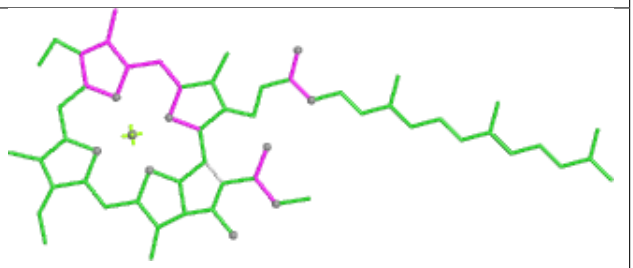


Rings

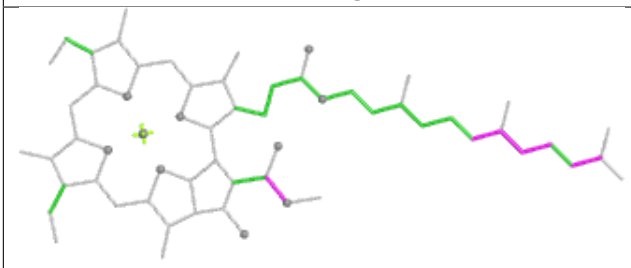
Ligand CLA T 607



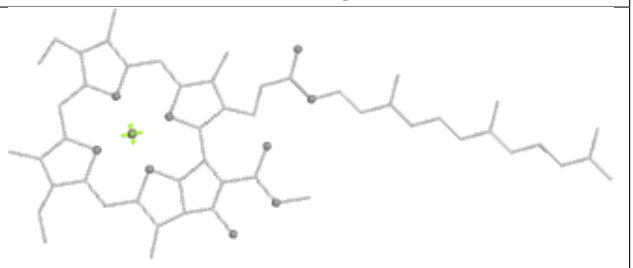
Bond lengths



Bond angles

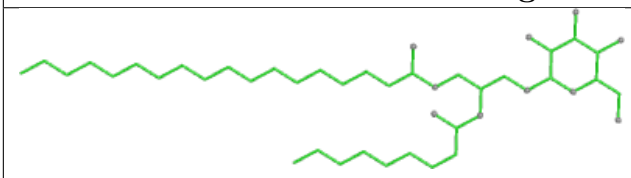


Torsions

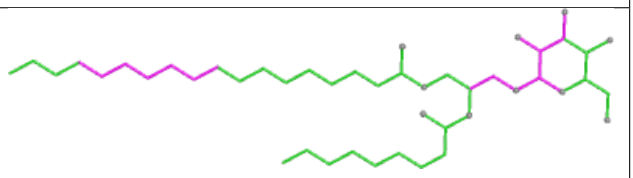


Rings

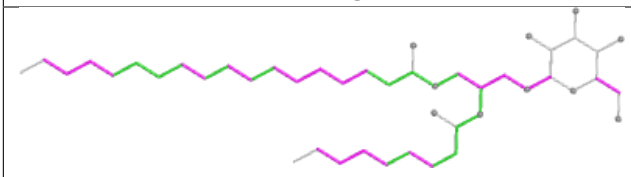
Ligand LMG G 616



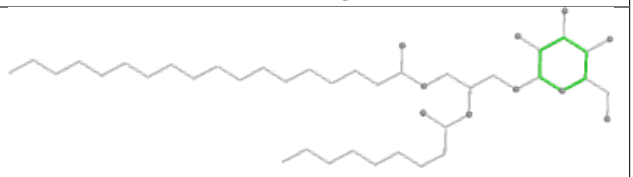
Bond lengths



Bond angles

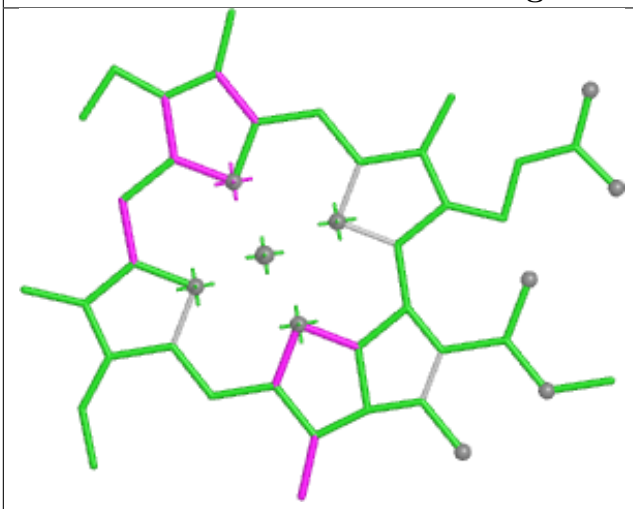


Torsions

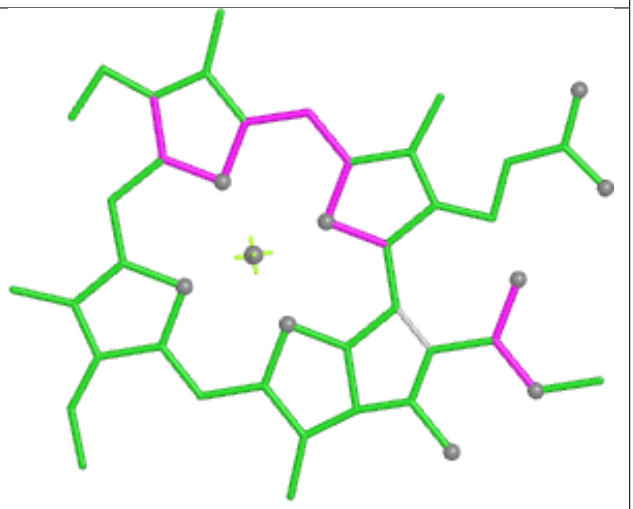


Rings

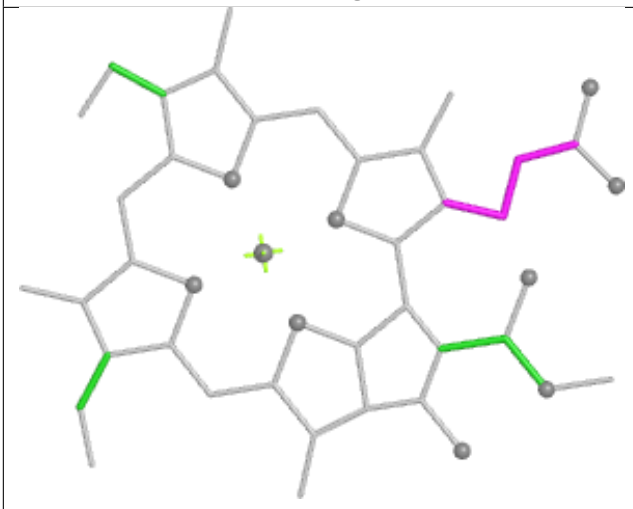
Ligand CLA L 412



Bond lengths



Bond angles

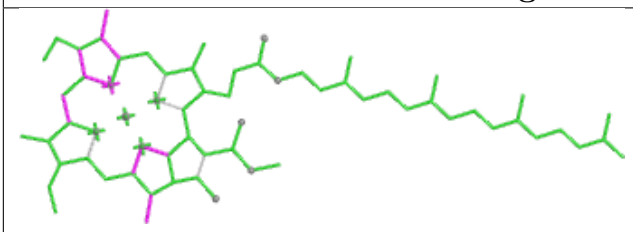


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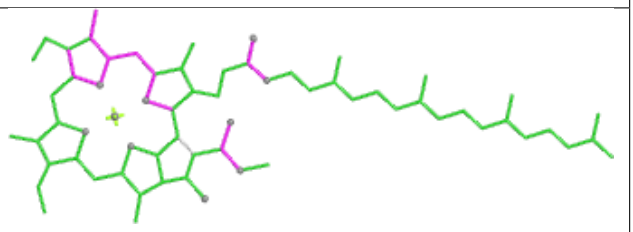


Rings

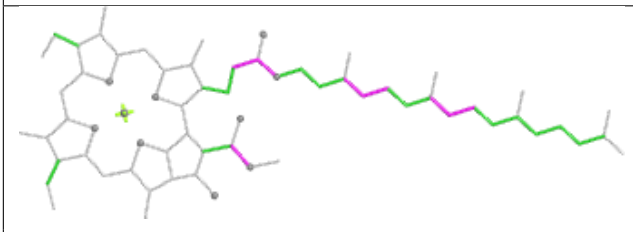
Ligand CLA W 409



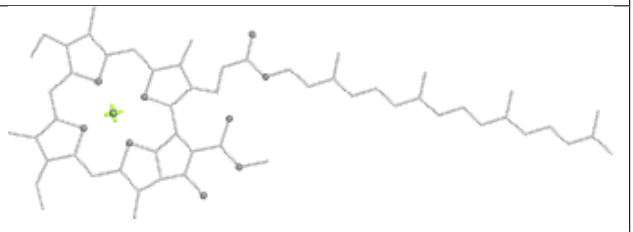
Bond lengths



Bond angles

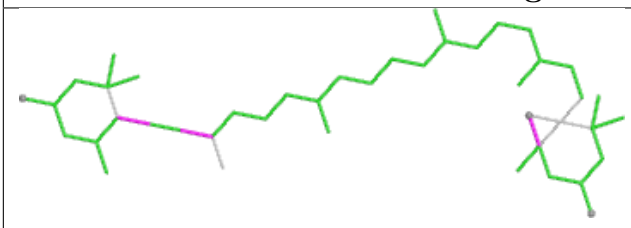


Torsions

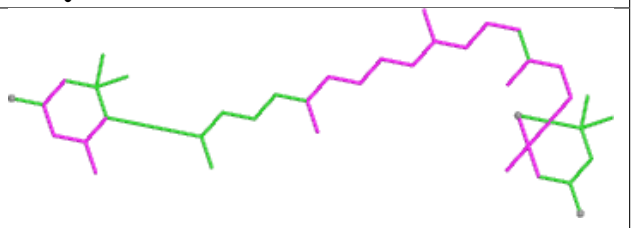


Rings

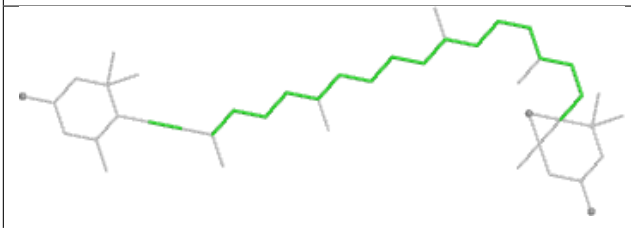
Ligand DD6 Q 615



Bond lengths



Bond angles

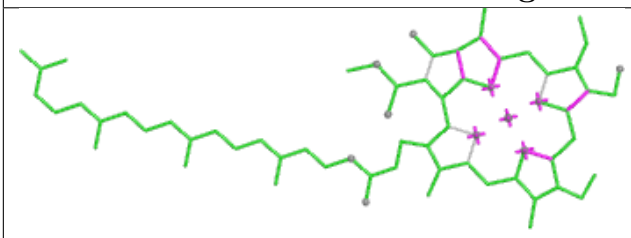


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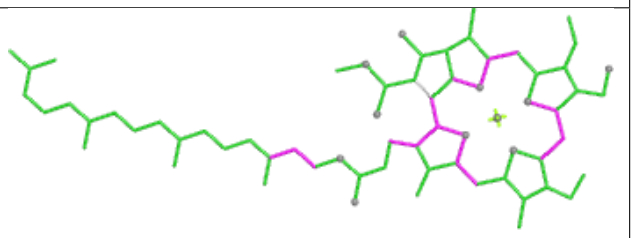


Rings

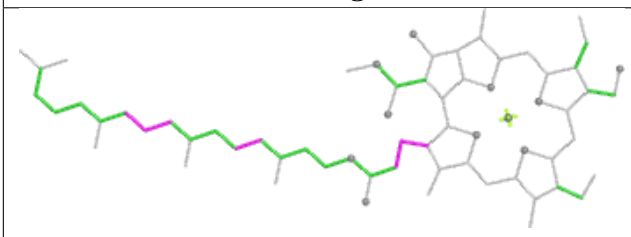
Ligand CHL W 408



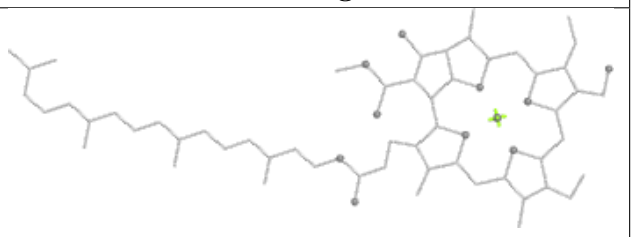
Bond lengths



Bond angles

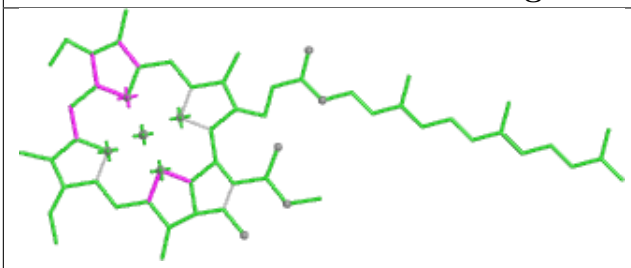


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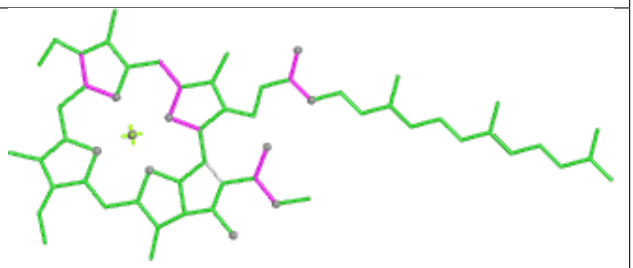


Rings

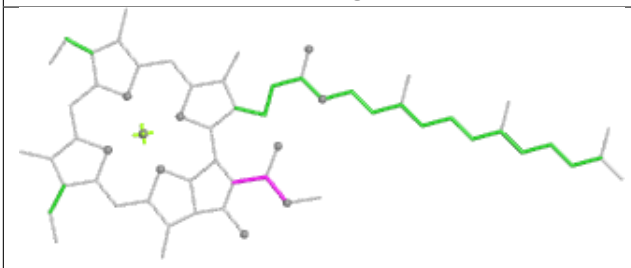
Ligand CLA T 608



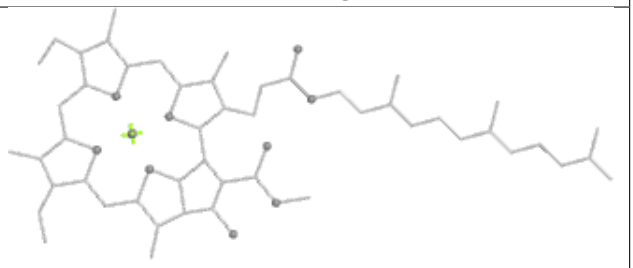
Bond lengths



Bond angles

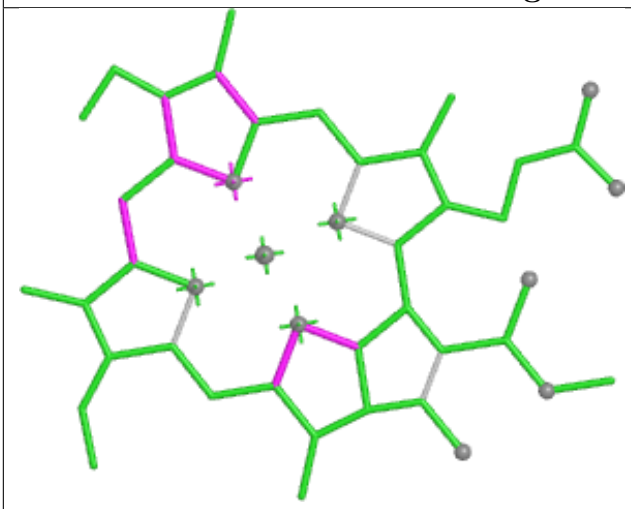


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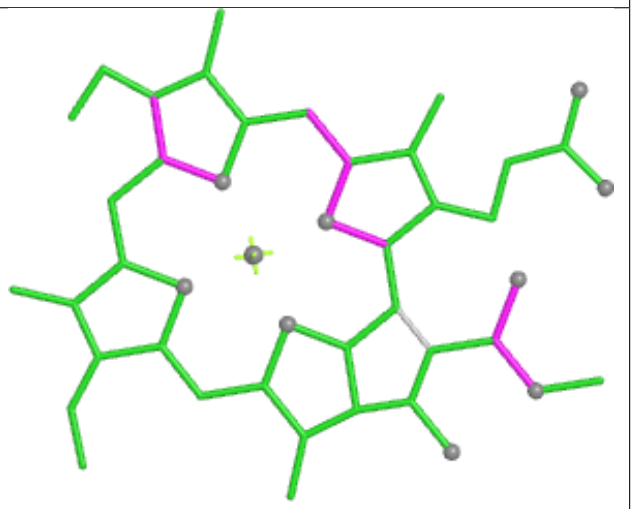


Rings

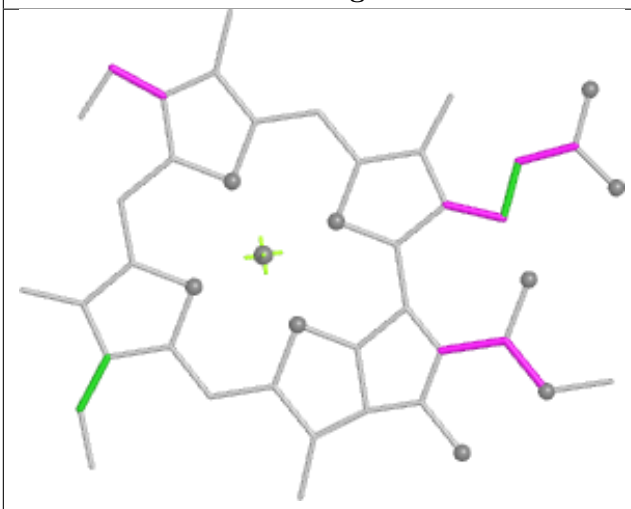
Ligand CLA V 617



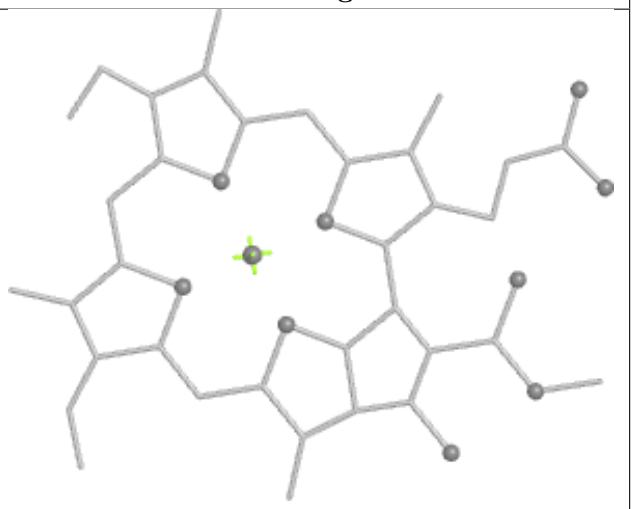
Bond lengths



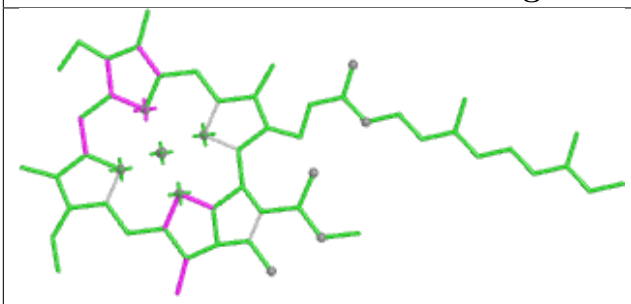
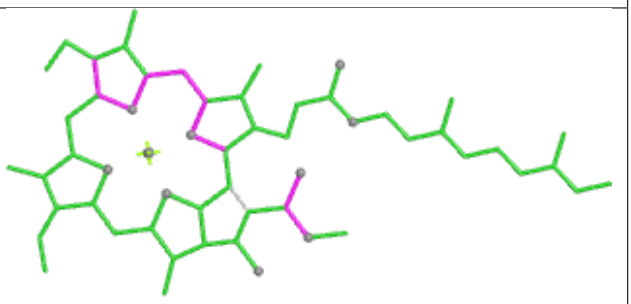
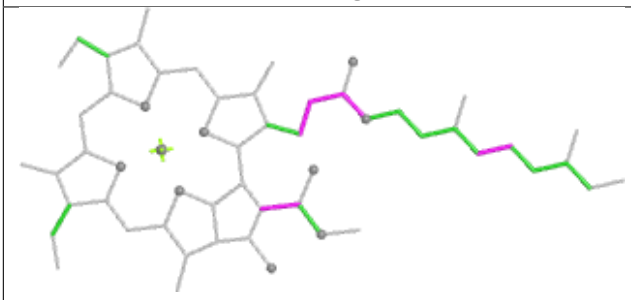
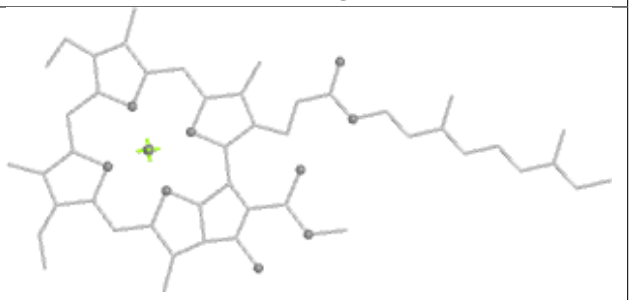
Bond angles

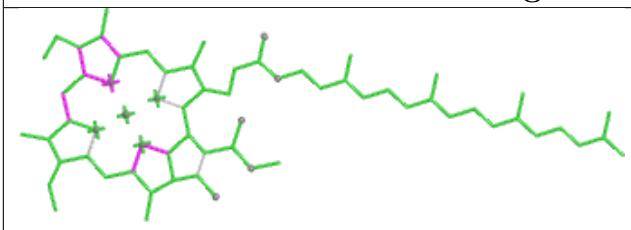
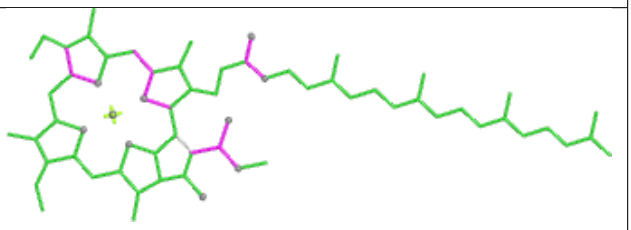
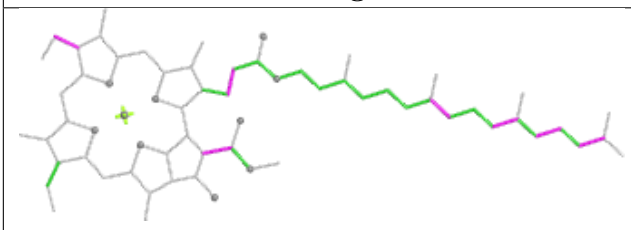
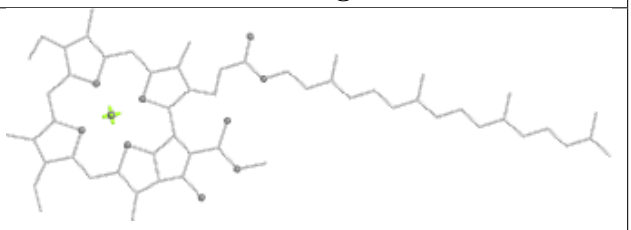


Torsions

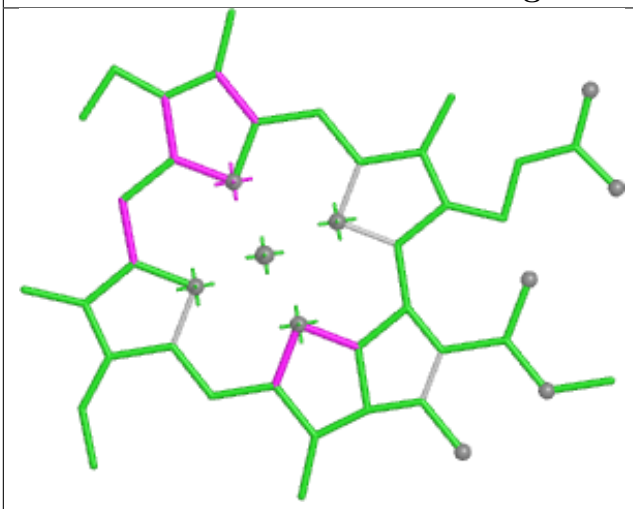


Rings

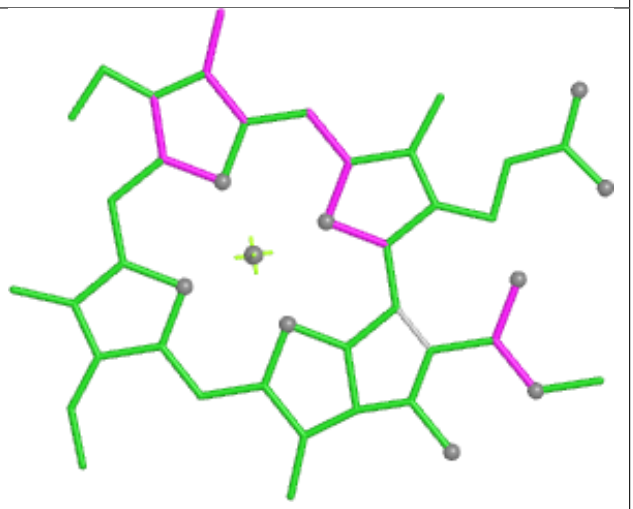
Ligand CLA K 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 810	
	
Bond lengths	Bond angles
	
Torsions	Rings

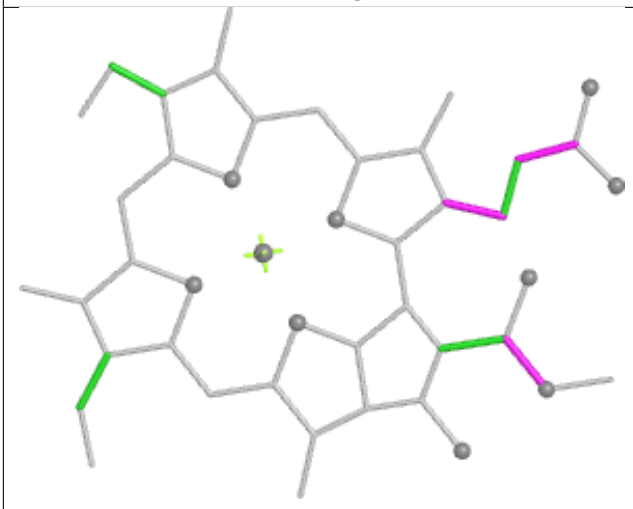
Ligand CLA H 318



Bond lengths



Bond angles

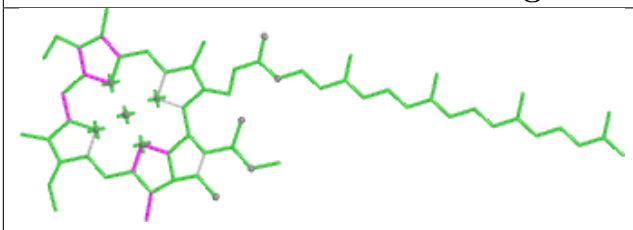


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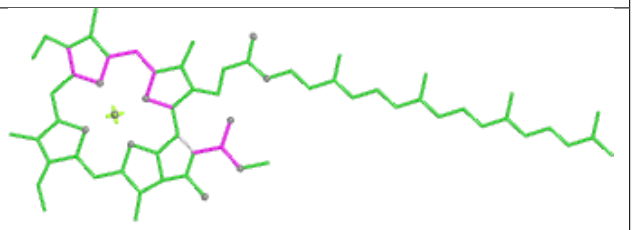


Rings

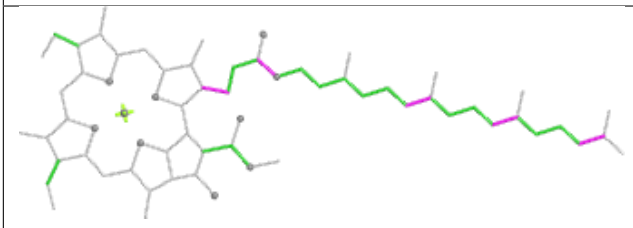
Ligand CLA A 806



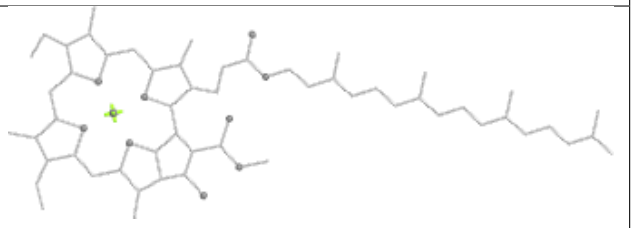
Bond lengths



Bond angles

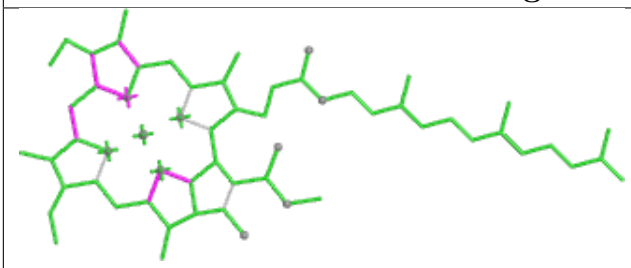


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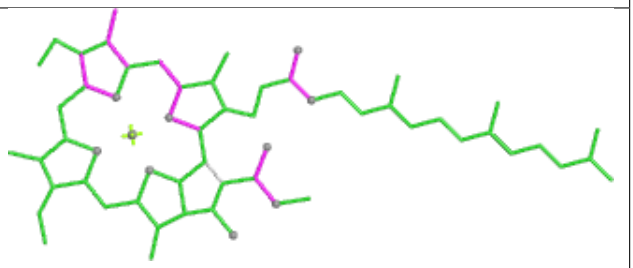


Rings

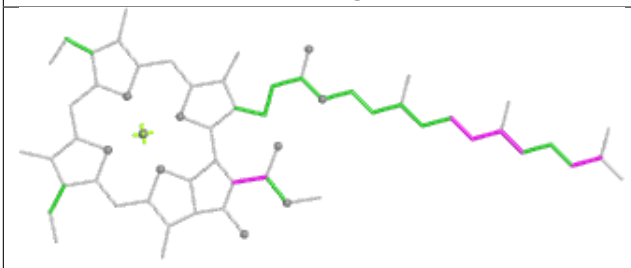
Ligand CLA H 308



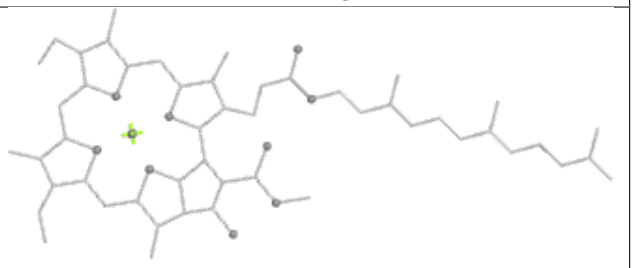
Bond lengths



Bond angles

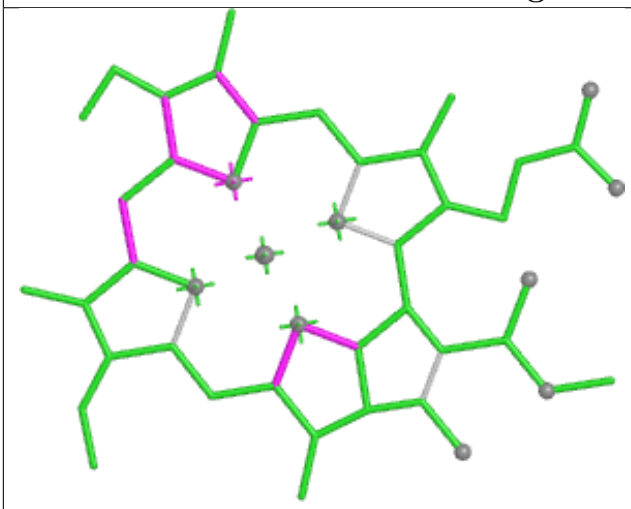


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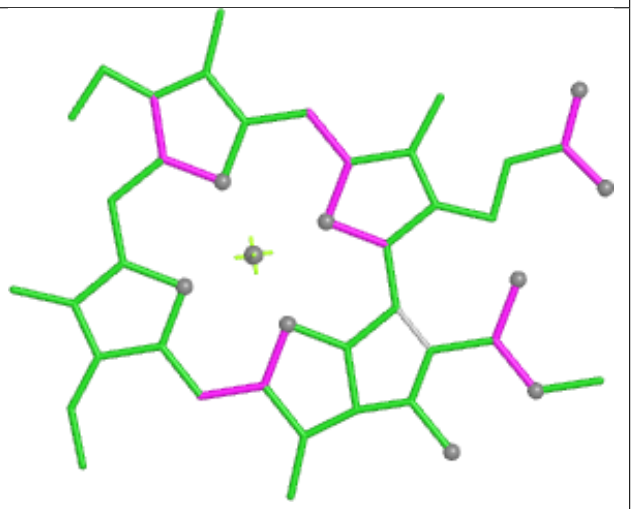


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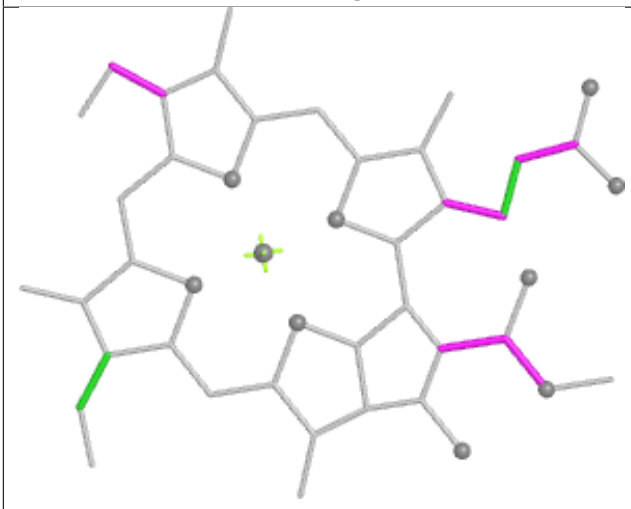
Ligand CLA S 608



Bond lengths



Bond angles

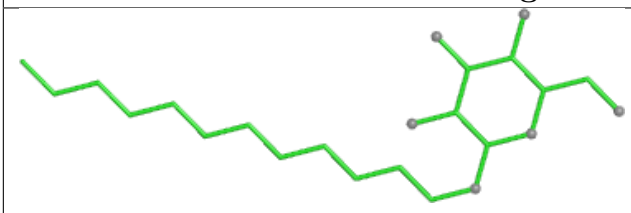


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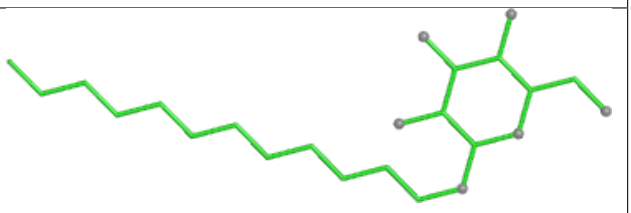


Rings

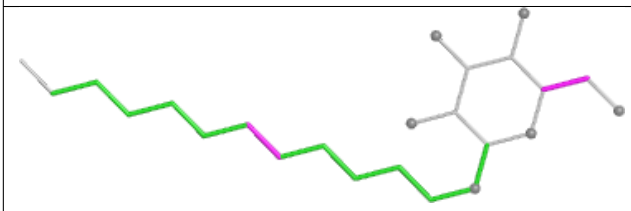
Ligand LMU B 855



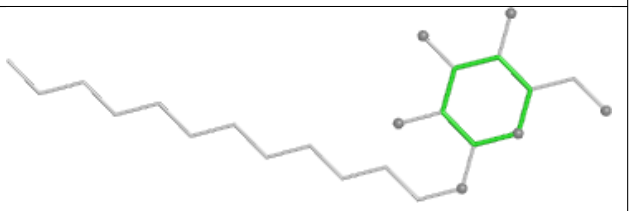
Bond lengths



Bond angles

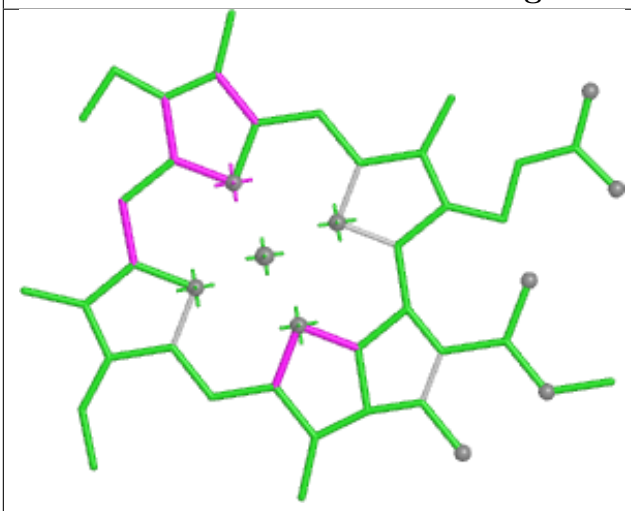


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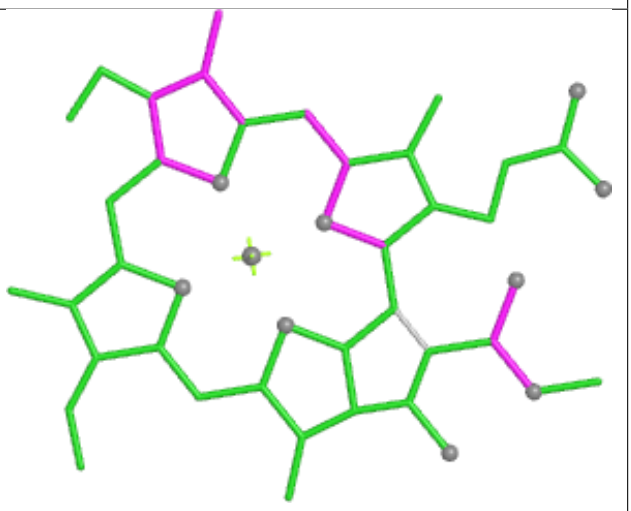


Rings

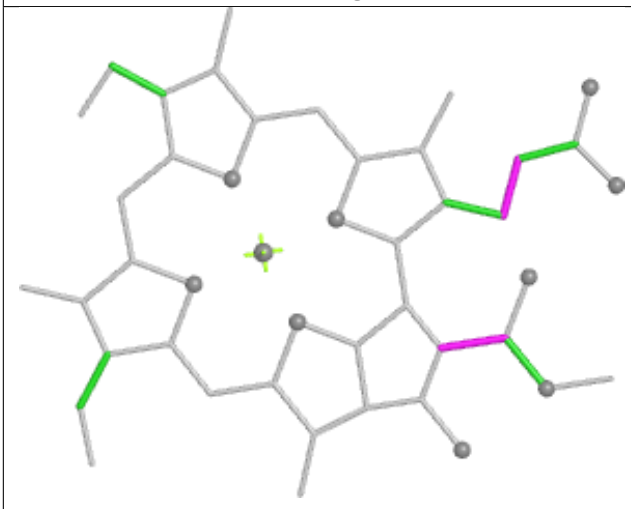
Ligand CLA B 811



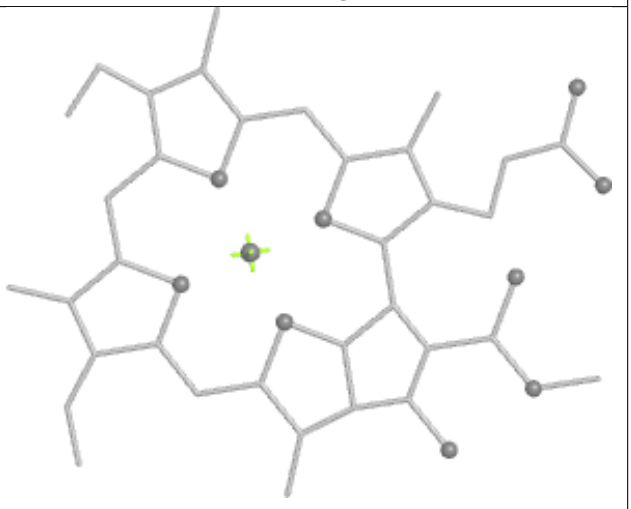
Bond lengths



Bond angles

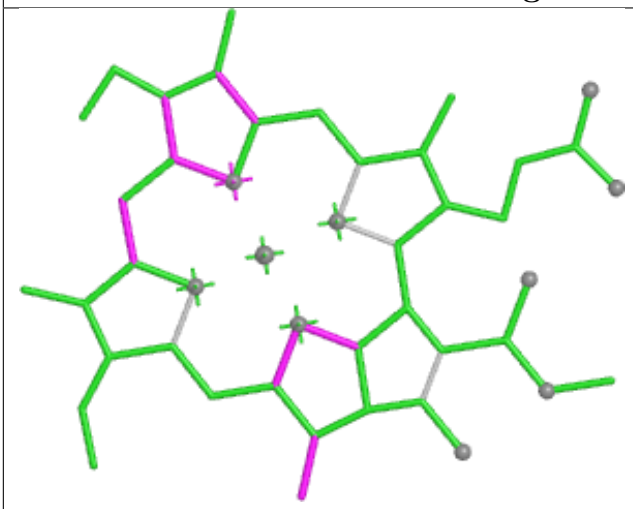


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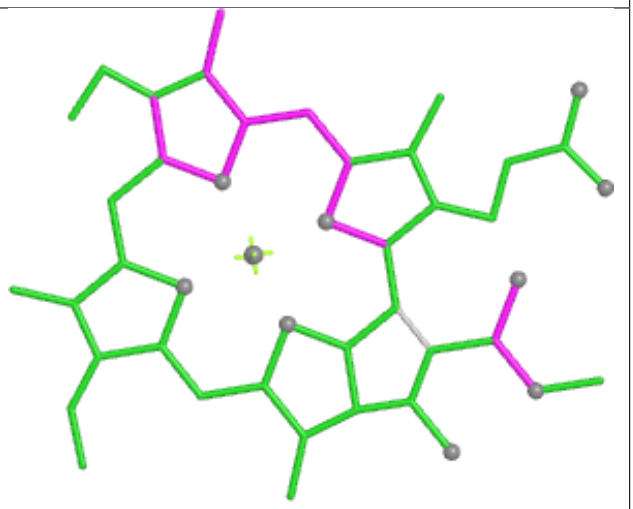


Rings

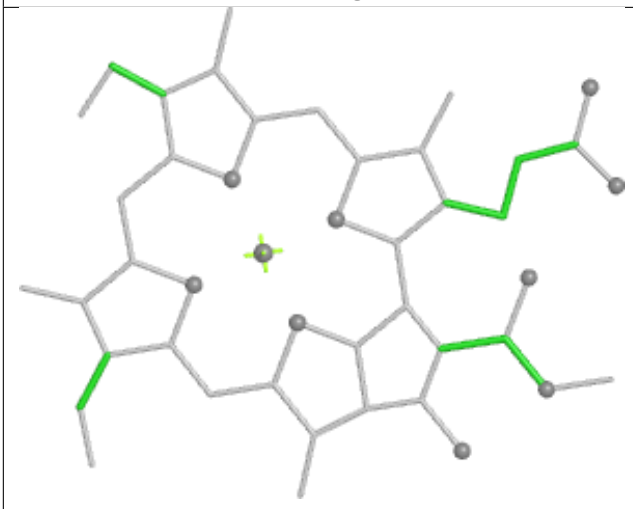
Ligand CLA G 604



Bond lengths



Bond angles

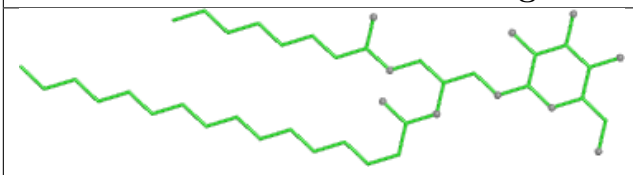


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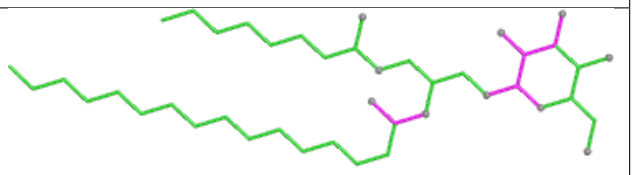


Rings

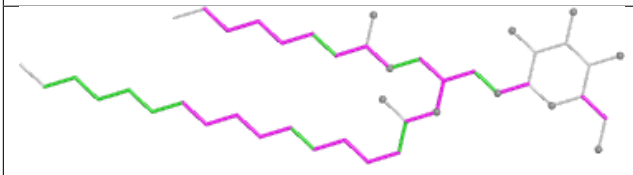
Ligand LMG K 601



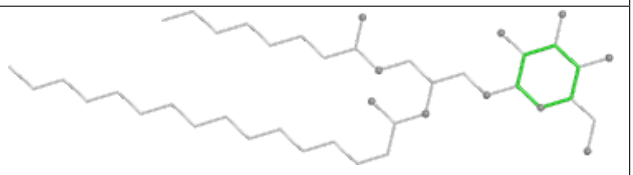
Bond lengths



Bond angles

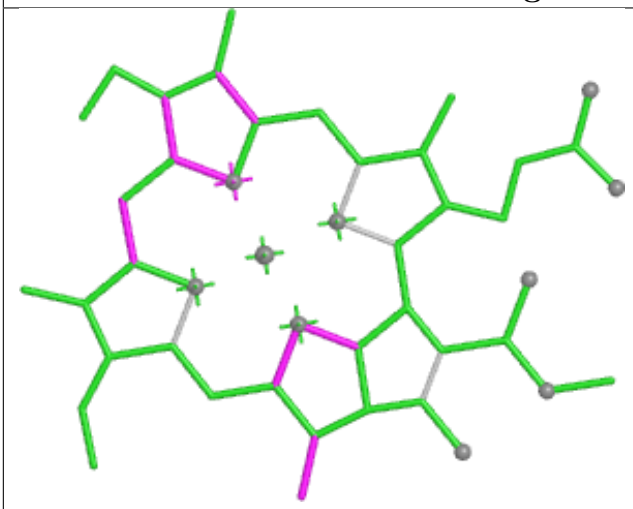


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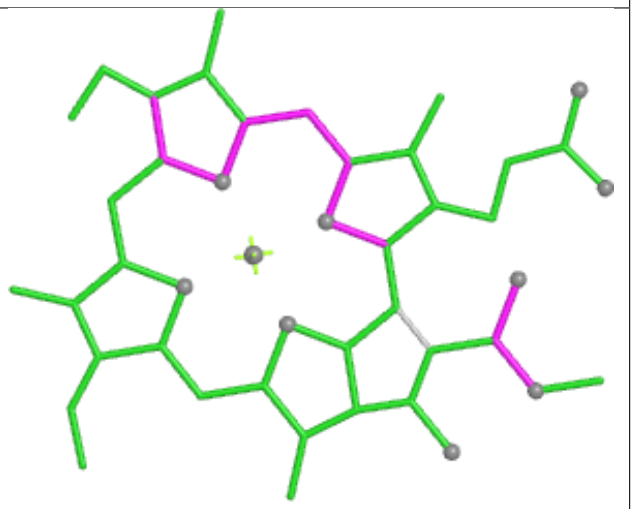


Rings

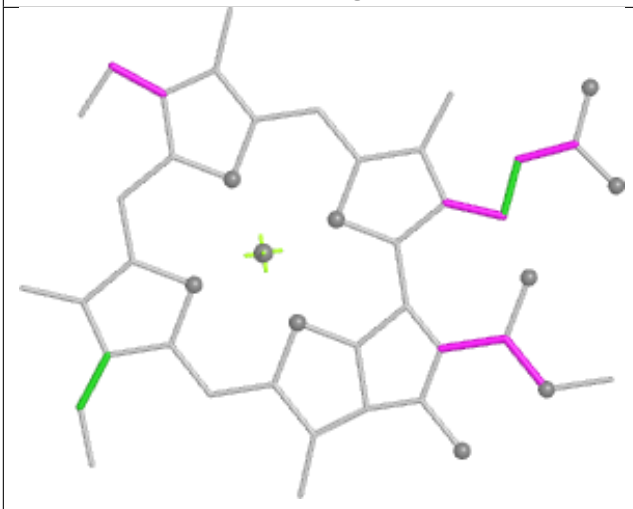
Ligand CLA X 419



Bond lengths



Bond angles

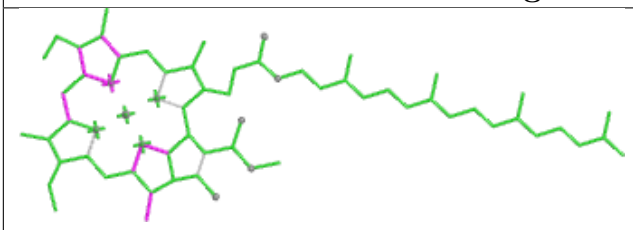


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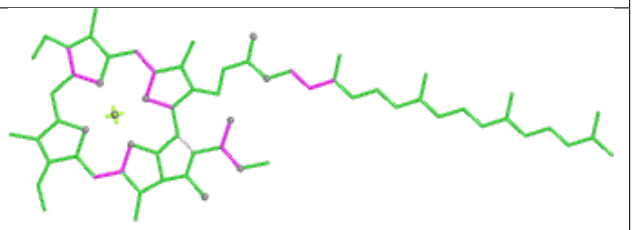


Rings

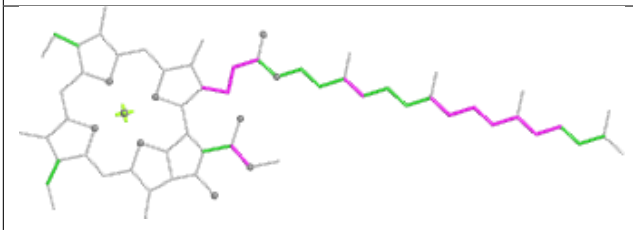
Ligand CLA A 829



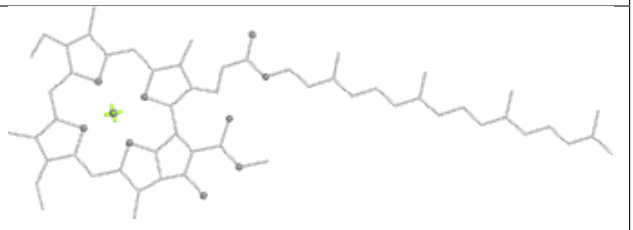
Bond lengths



Bond angles

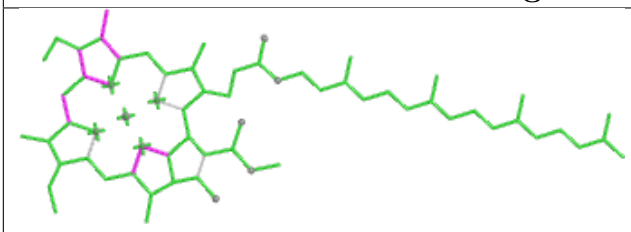


Torsions

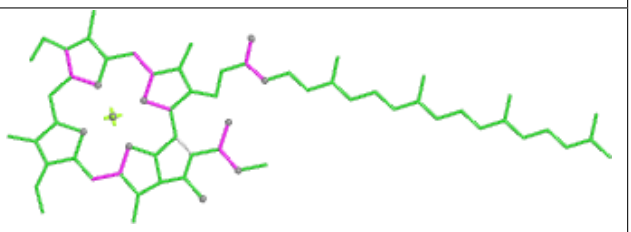


Rings

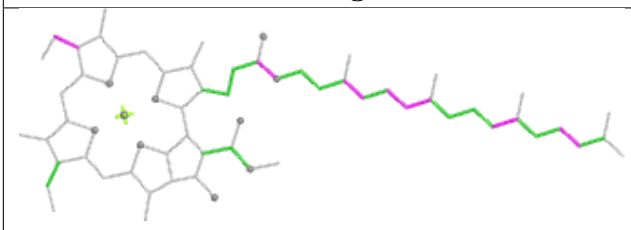
Ligand CLA A 836



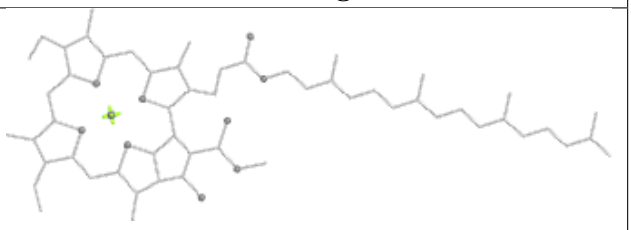
Bond lengths



Bond angles

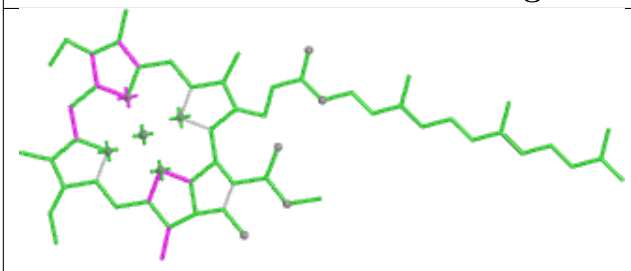


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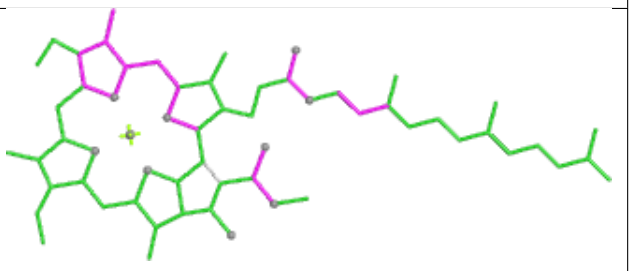


Rings

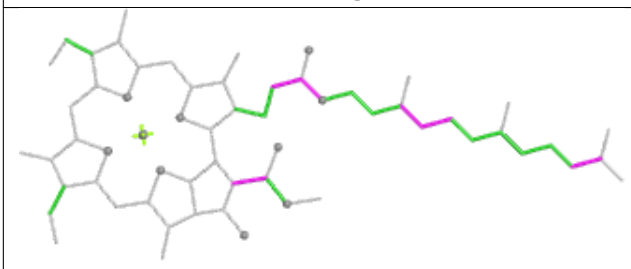
Ligand CLA O 312



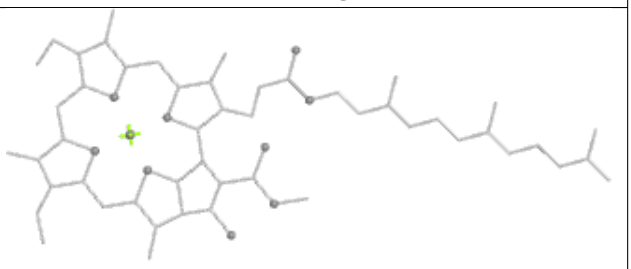
Bond lengths



Bond angles

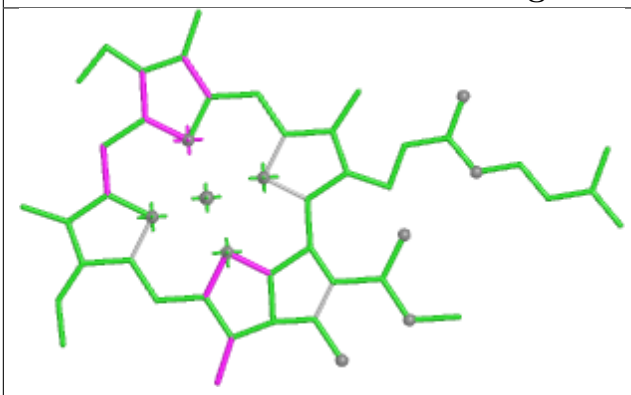


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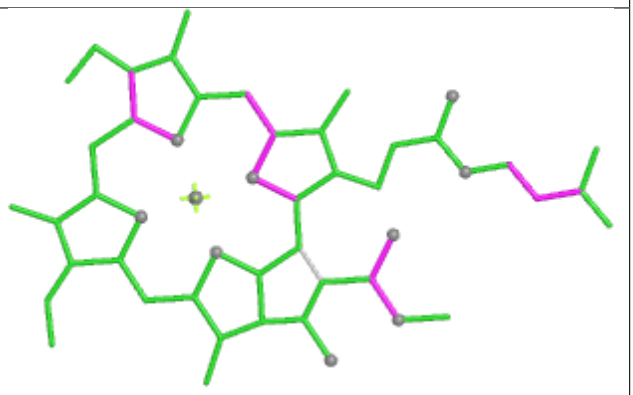


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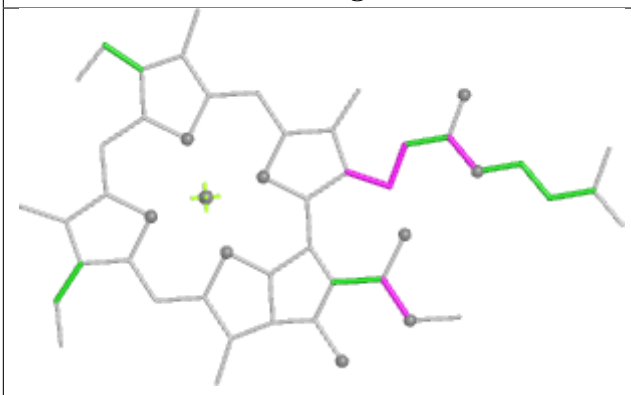
Ligand CLA J 102



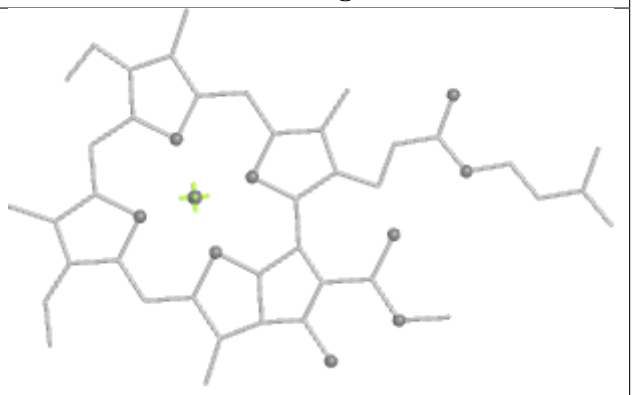
Bond lengths



Bond angles

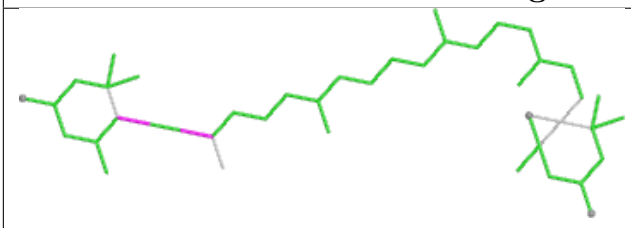


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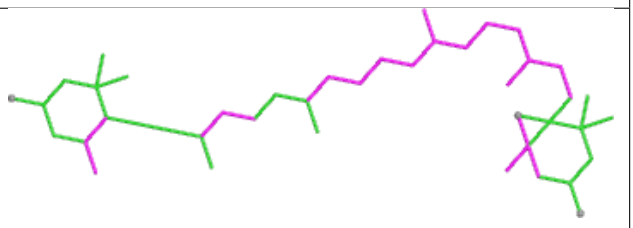


Rings

Ligand DD6 J 105



Bond lengths



Bond angles

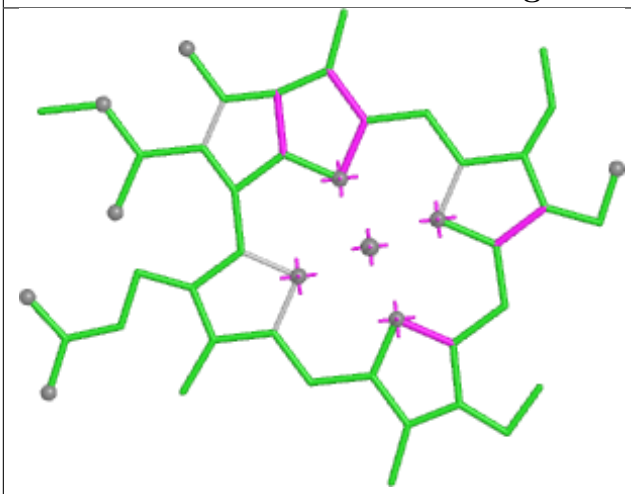


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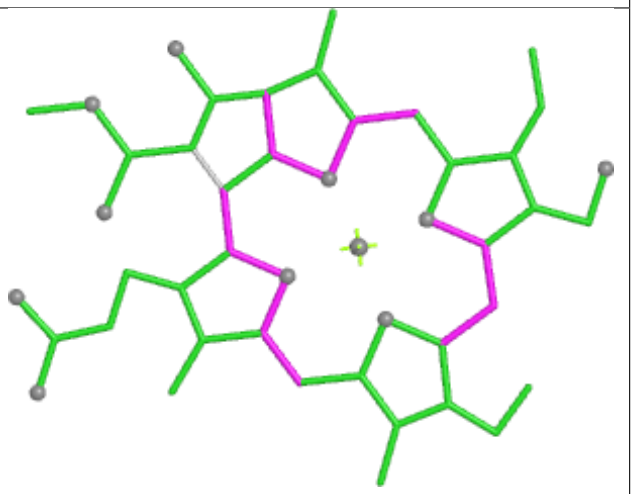


Rings

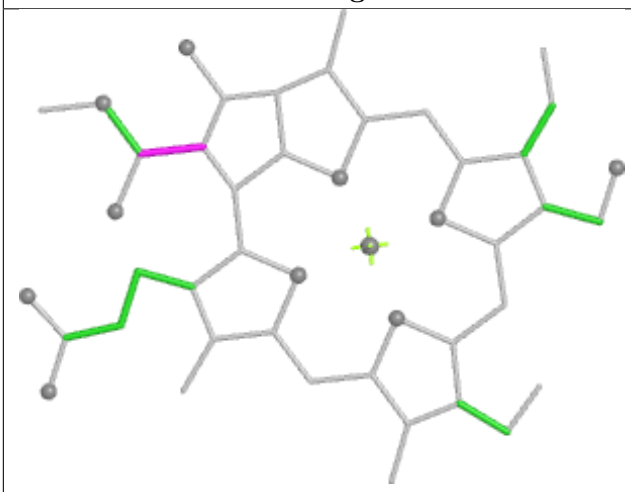
Ligand CHL V 606



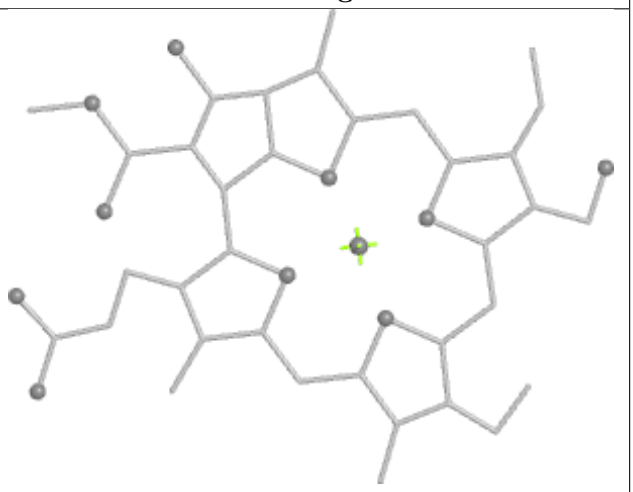
Bond lengths



Bond angles

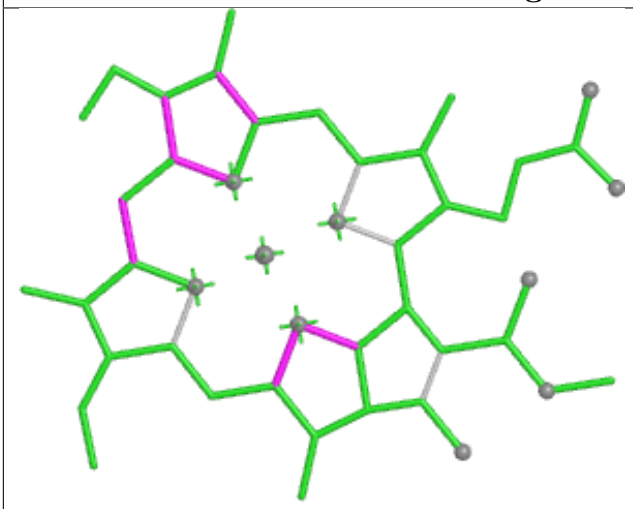


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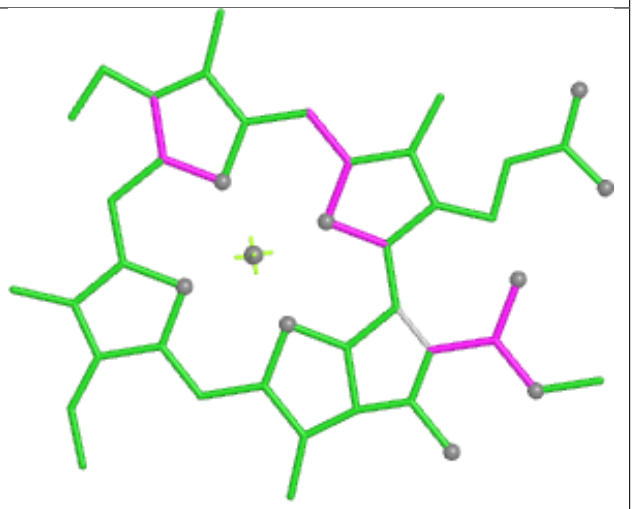


Rings

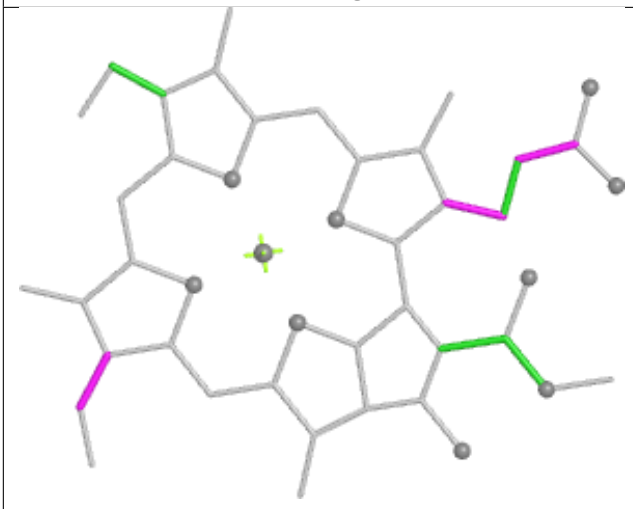
Ligand CLA P 611



Bond lengths



Bond angles

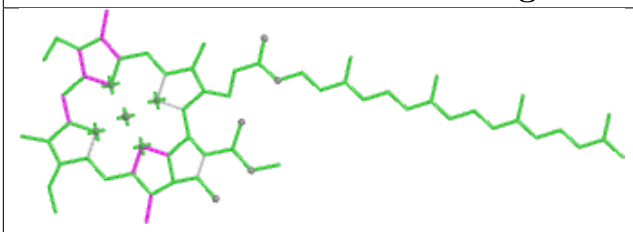


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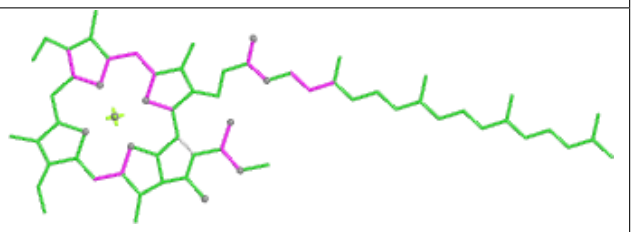


Rings

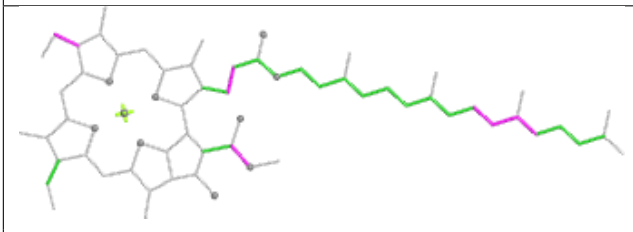
Ligand CLA W 414



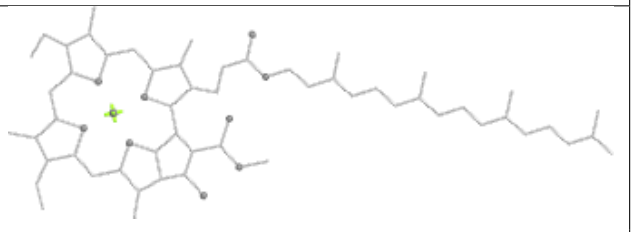
Bond lengths



Bond angles

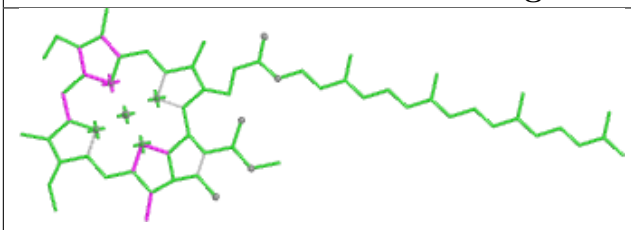


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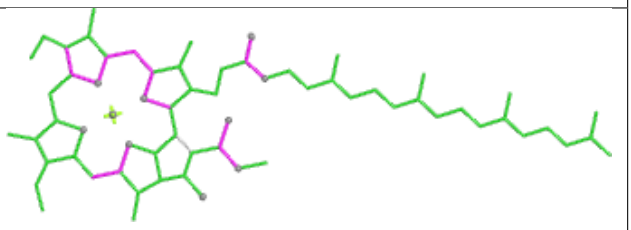


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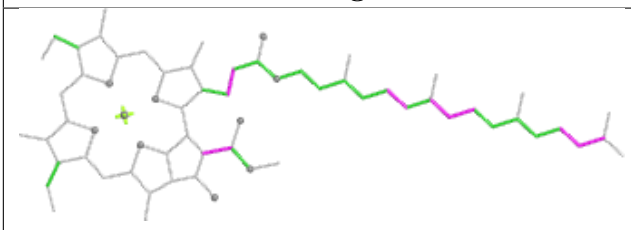
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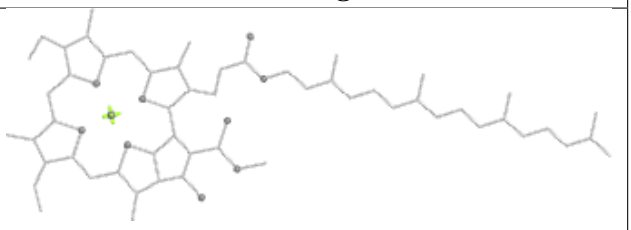
Bond lengths



Bond angles

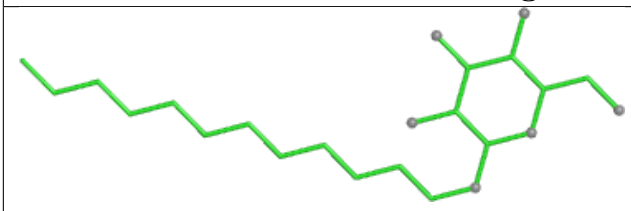


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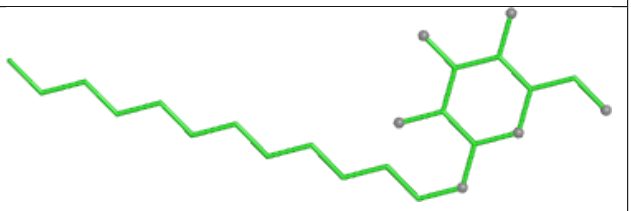


Rings

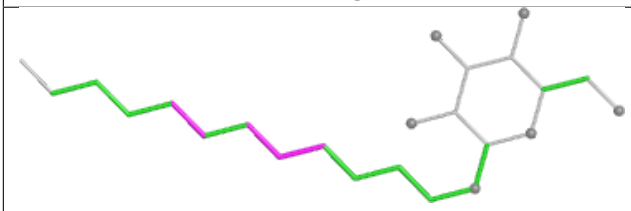
Ligand LMU B 850



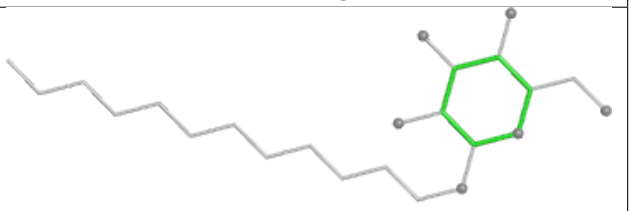
Bond lengths



Bond angles

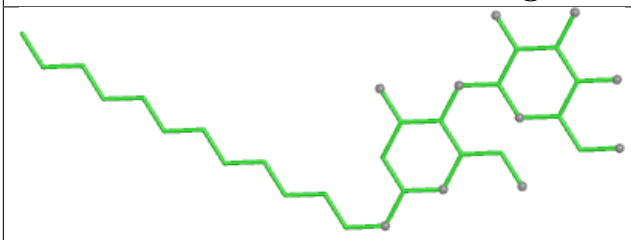


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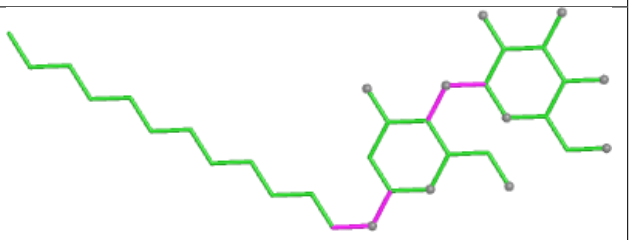


Rings

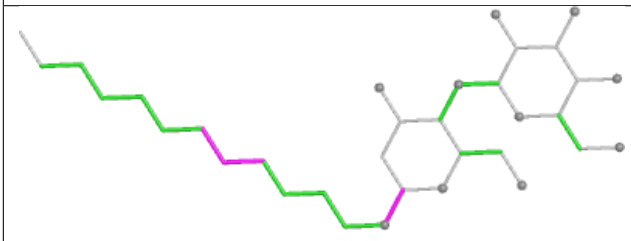
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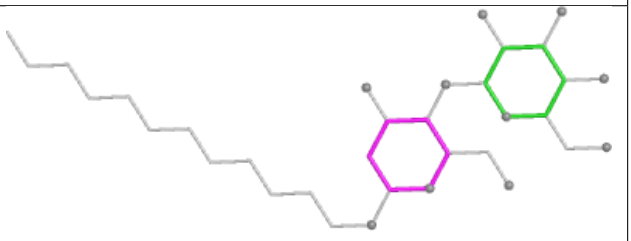
Bond lengths



Bond angles

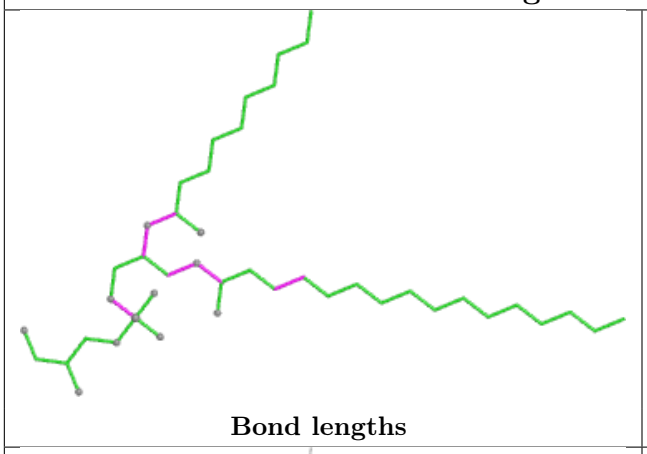


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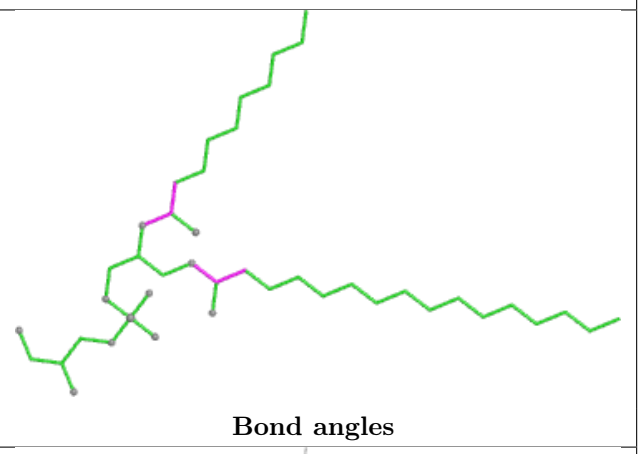


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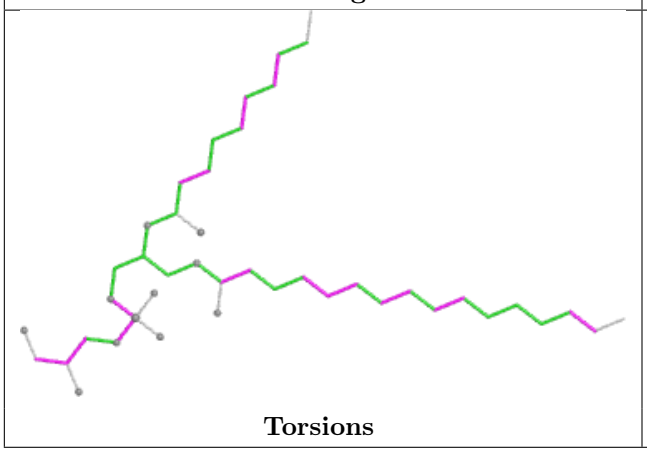
Ligand LHG O 323



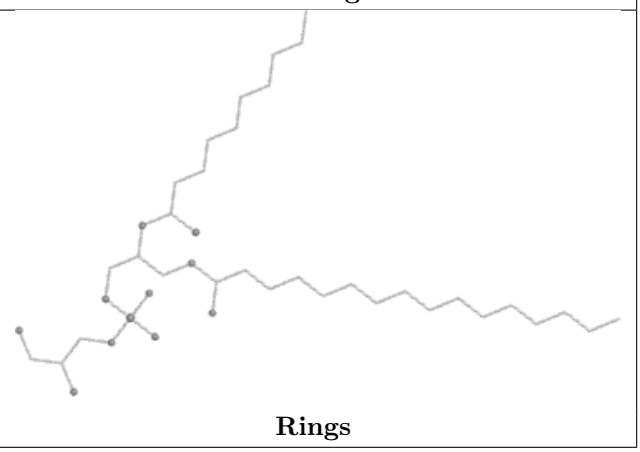
Bond lengths



Bond angles

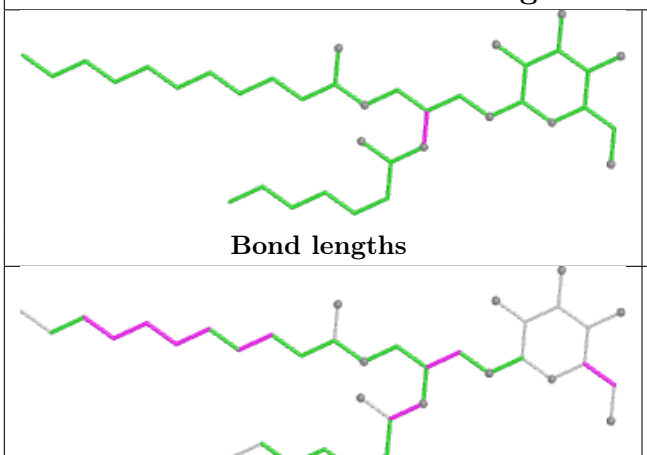


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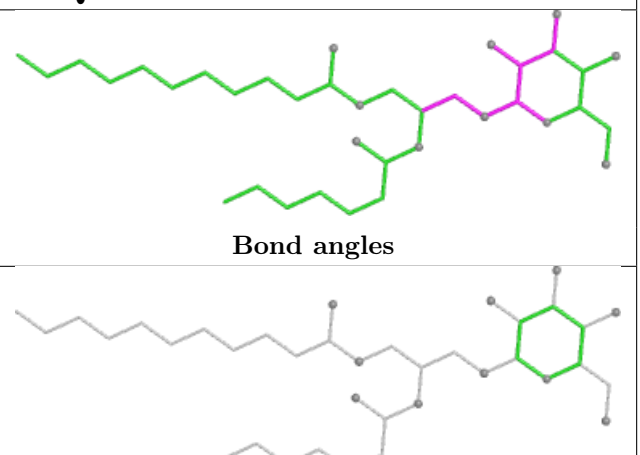


Rings

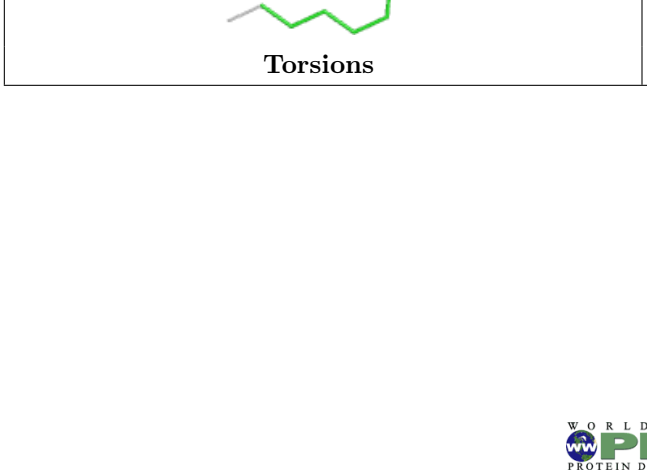
Ligand LMG Q 602



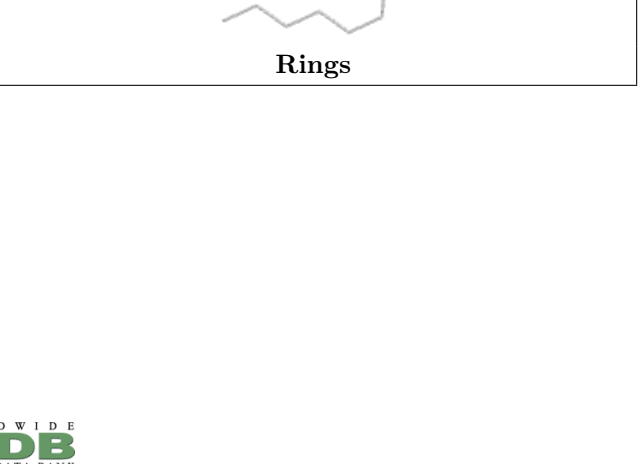
Bond lengths



Bond angles

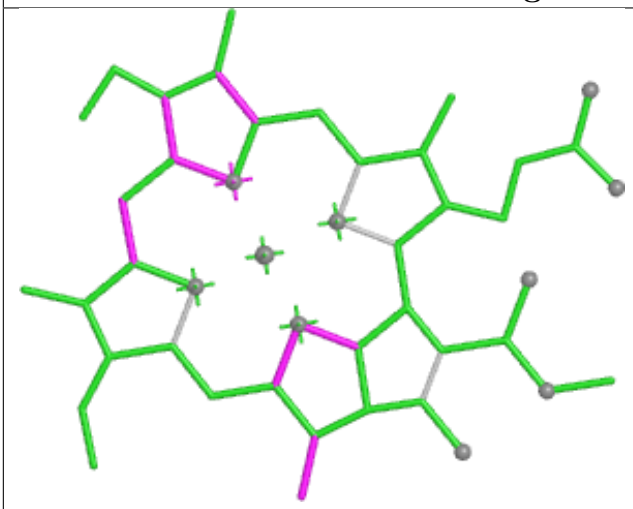


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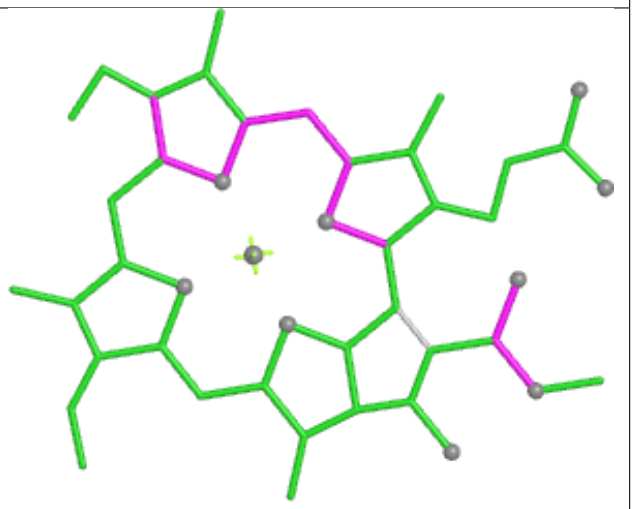


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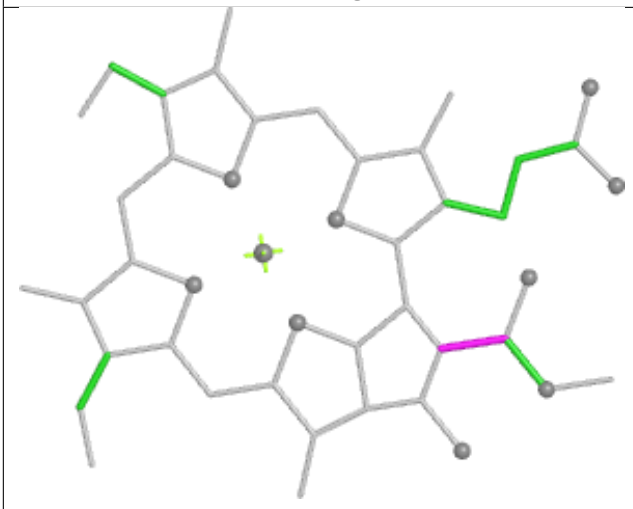
Ligand CLA O 314



Bond lengths



Bond angles

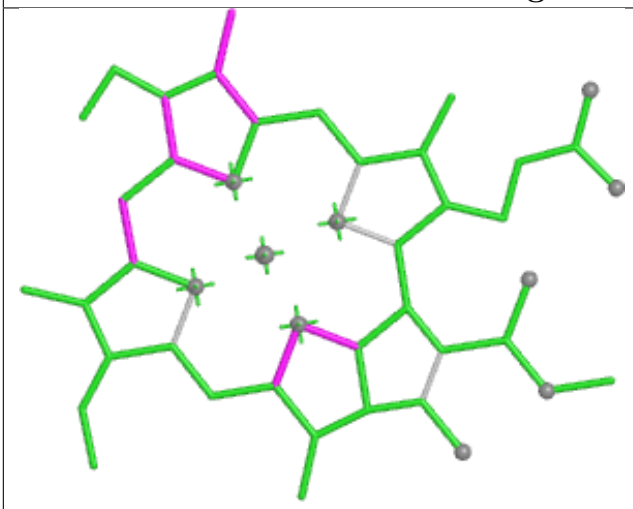


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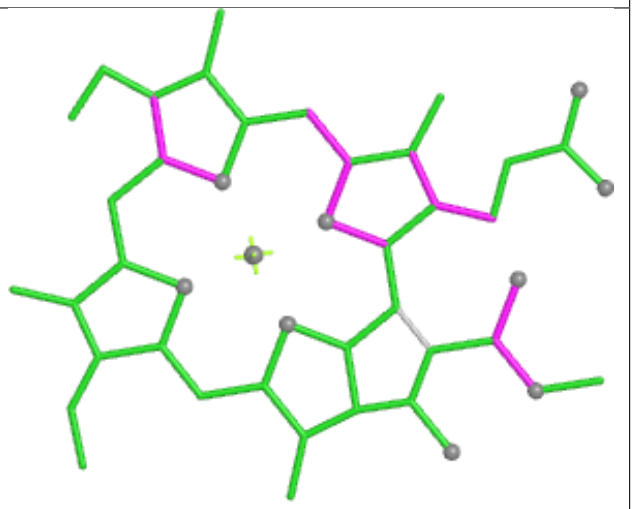


Rings

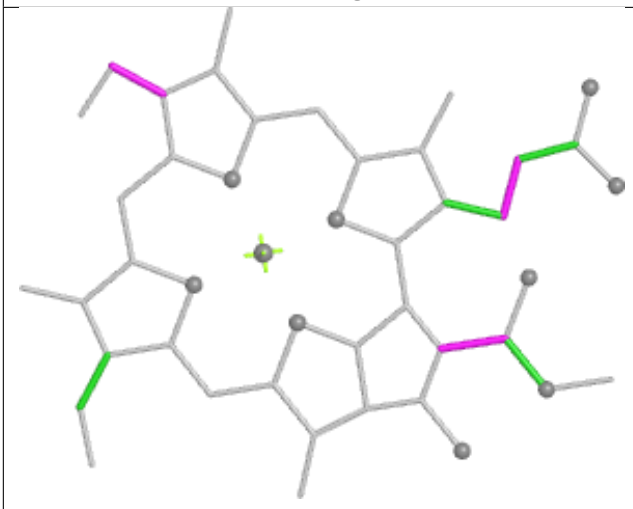
Ligand CLA S 610



Bond lengths



Bond angles

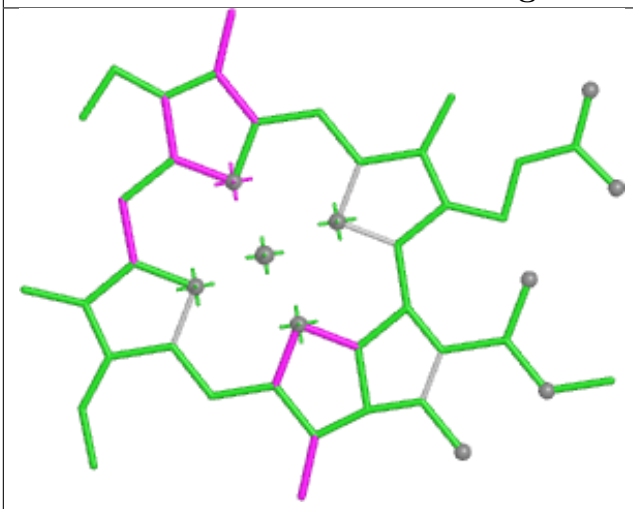


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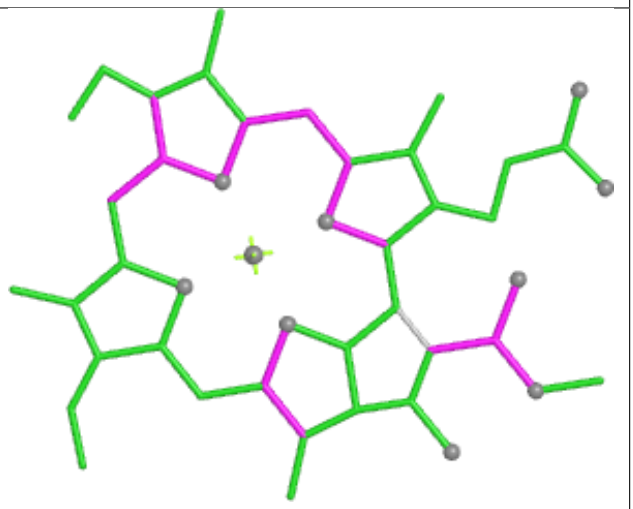


Rings

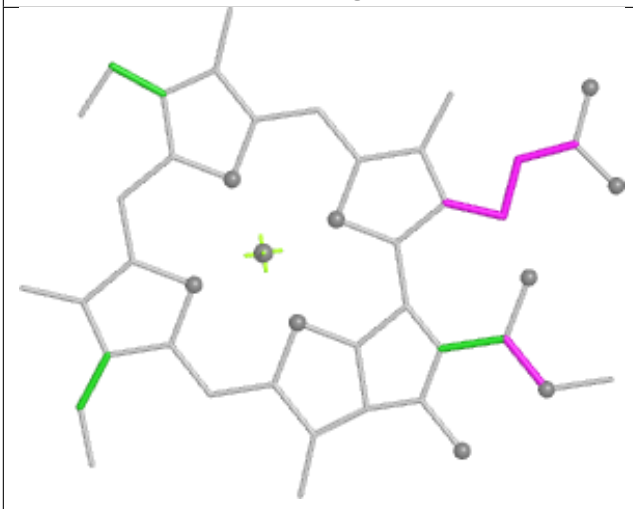
Ligand CLA W 415



Bond lengths



Bond angles

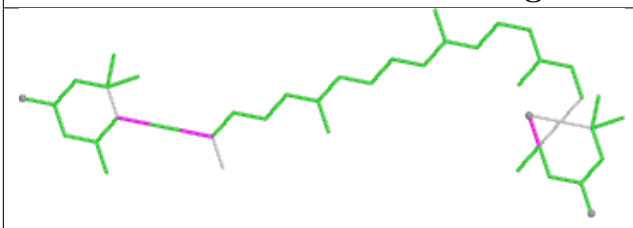


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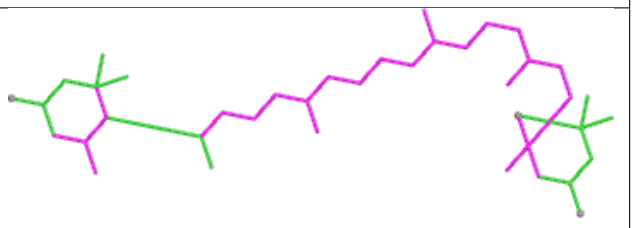


Rings

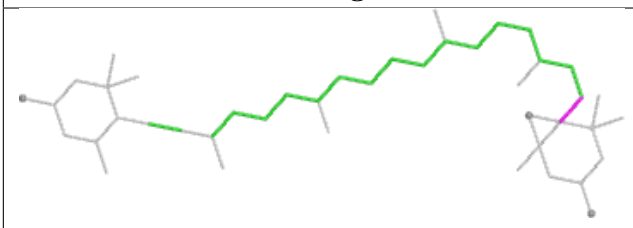
Ligand DD6 R 613



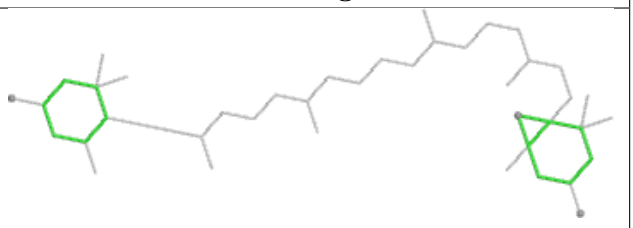
Bond lengths



Bond angles

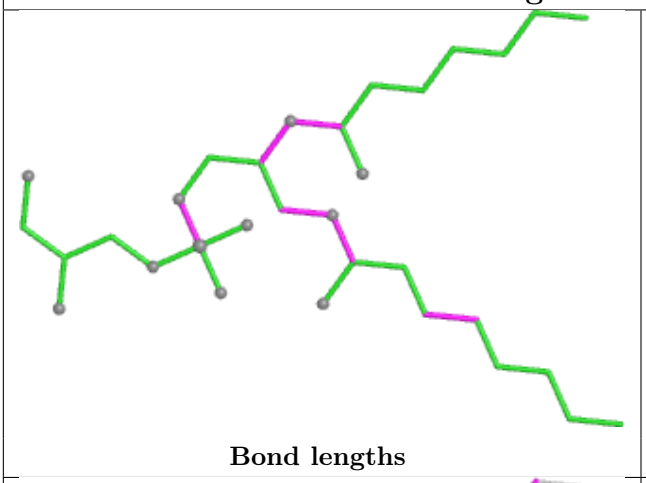


Torsions

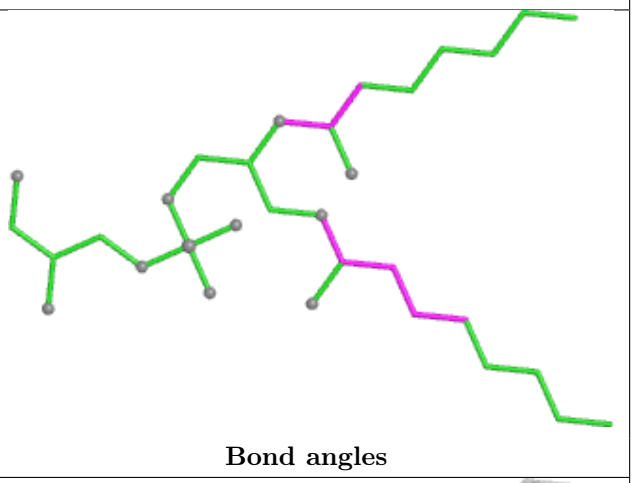


Rings

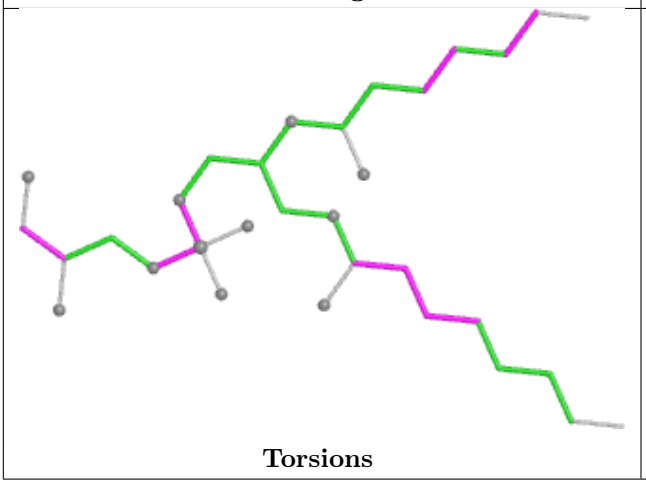
Ligand LHG S 613



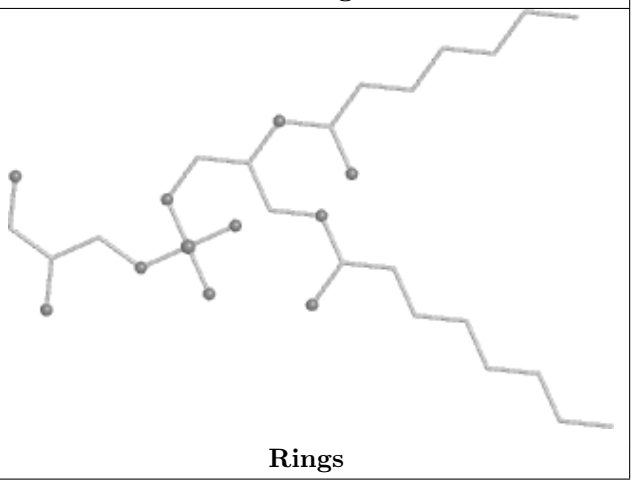
Bond lengths



Bond angles

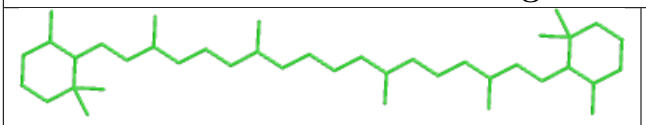


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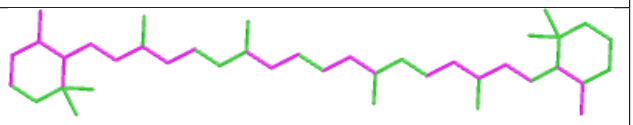


Rings

Ligand BCR A 849



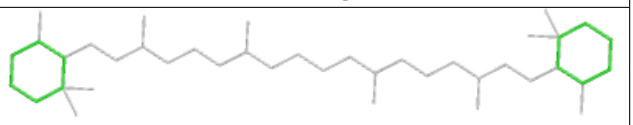
Bond lengths



Bond angles

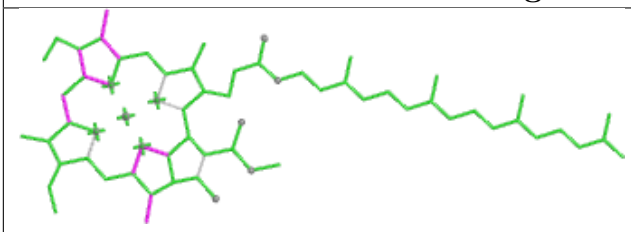


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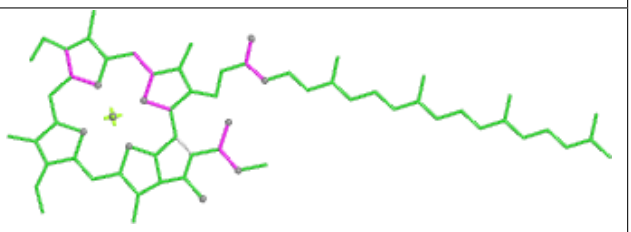


Rings

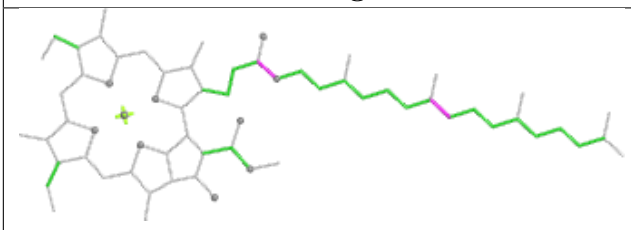
Ligand CLA B 809



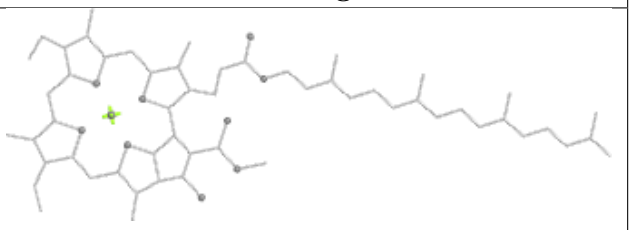
Bond lengths



Bond angles

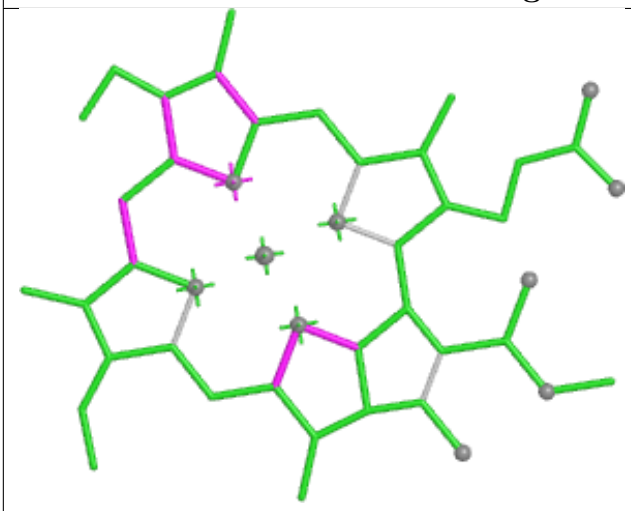


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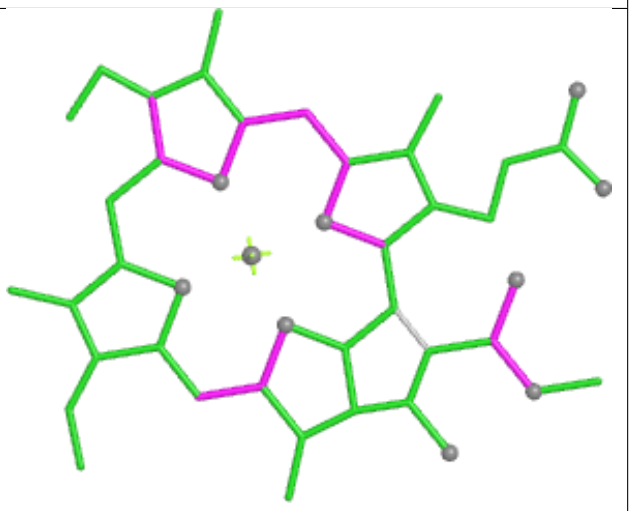


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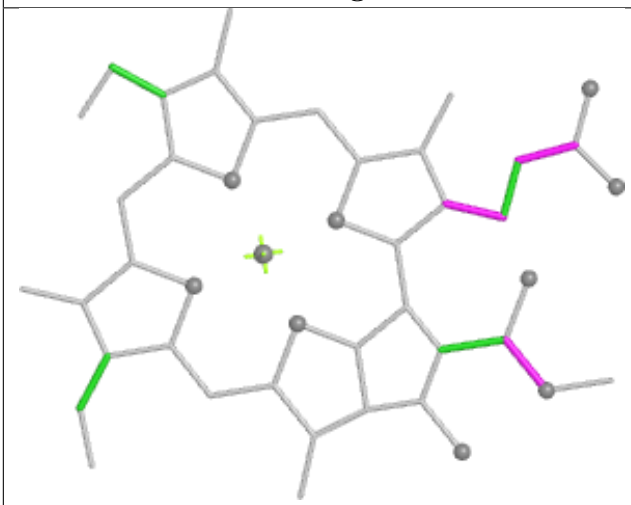
Ligand CLA G 611



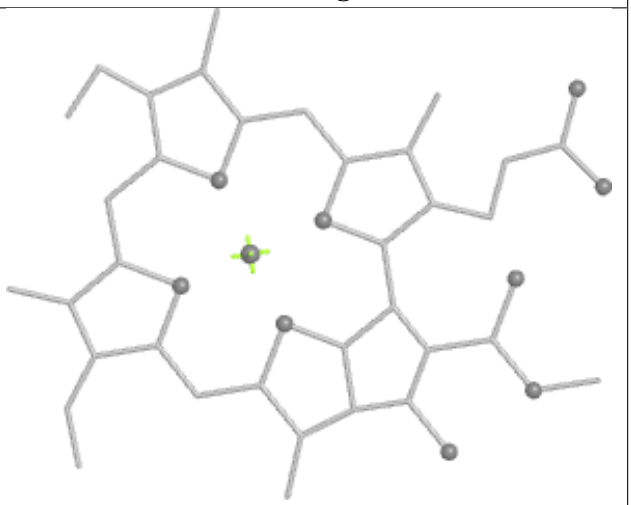
Bond lengths



Bond angles

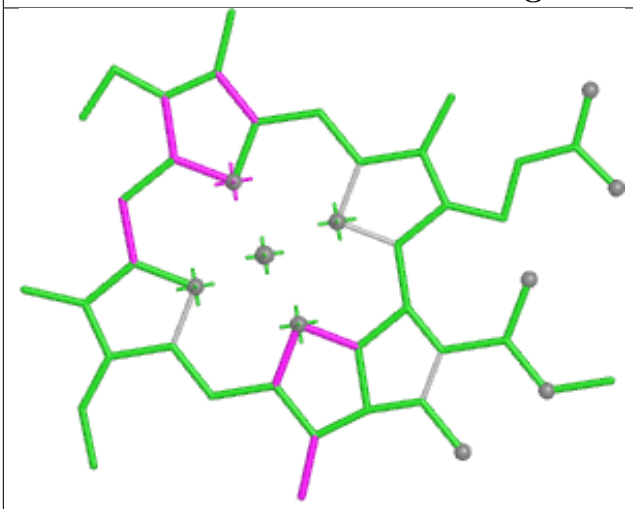


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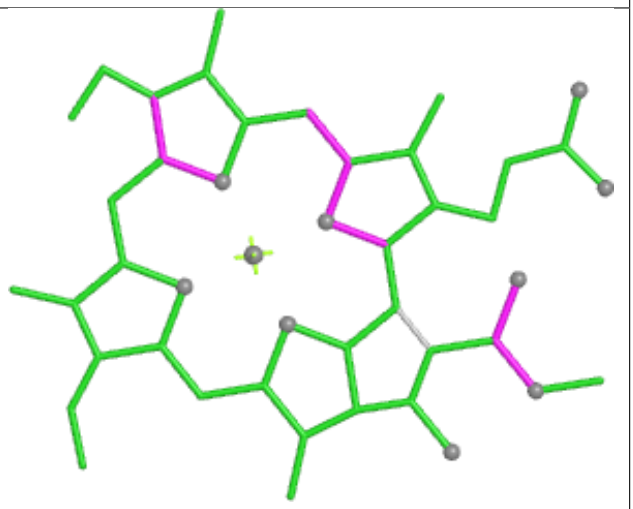


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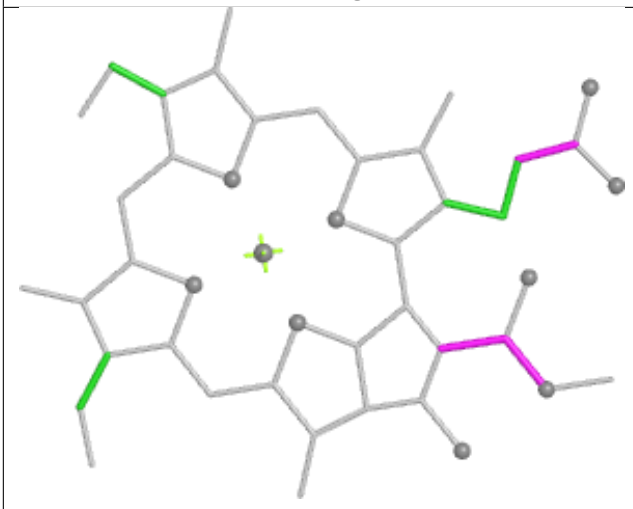
Ligand CLA T 601



Bond lengths



Bond angles

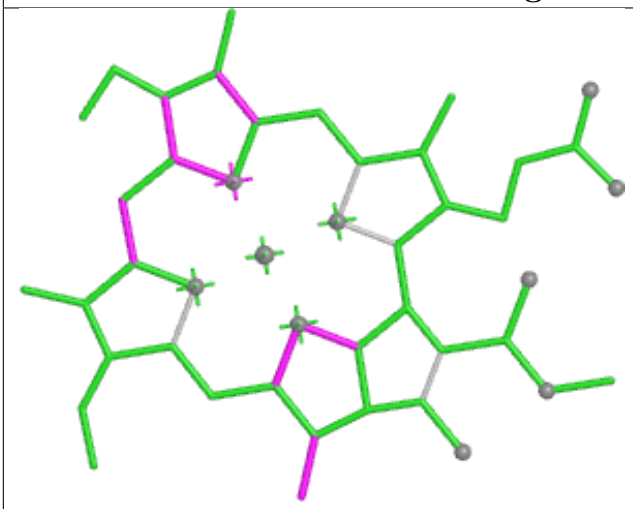


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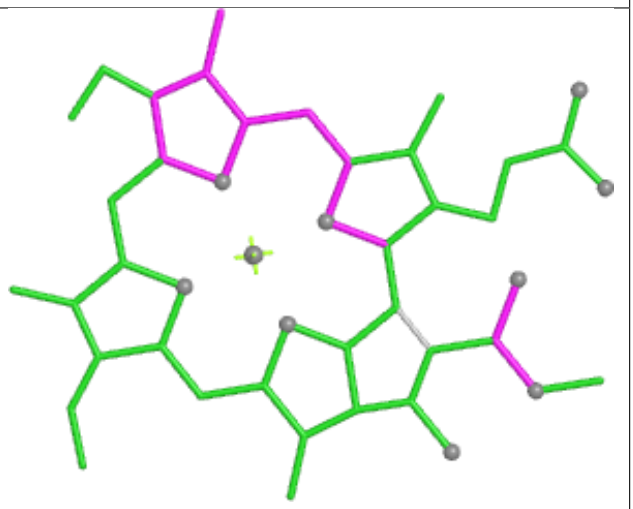


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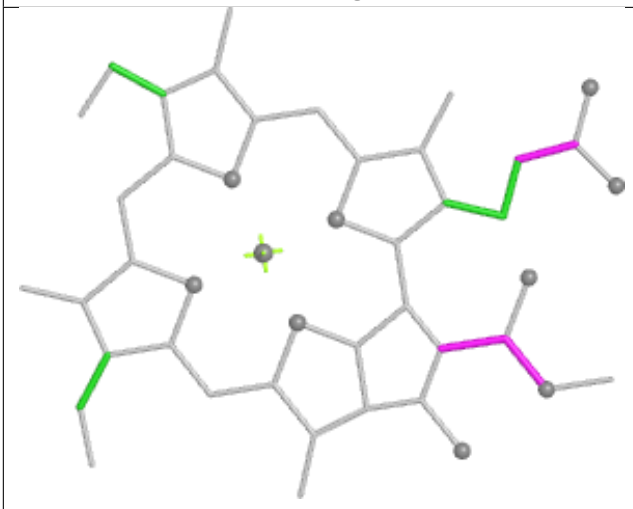
Ligand CLA T 609



Bond lengths



Bond angles

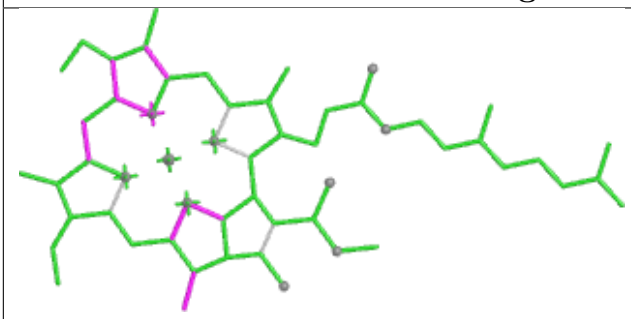


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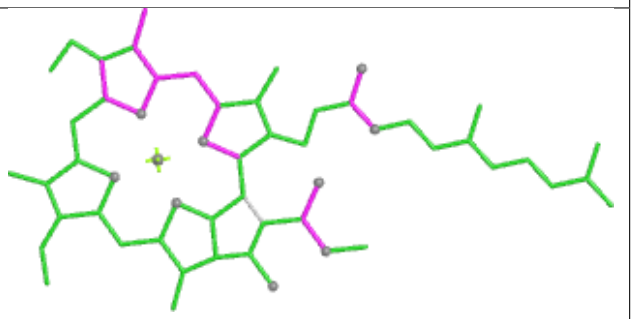


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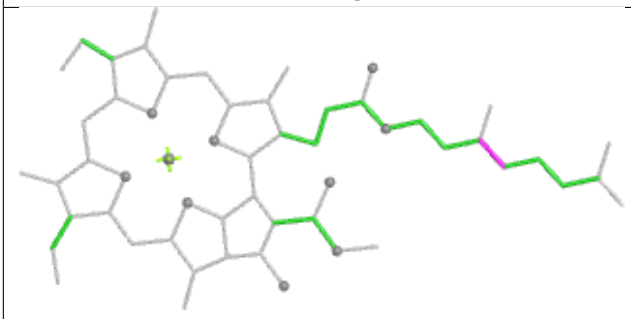
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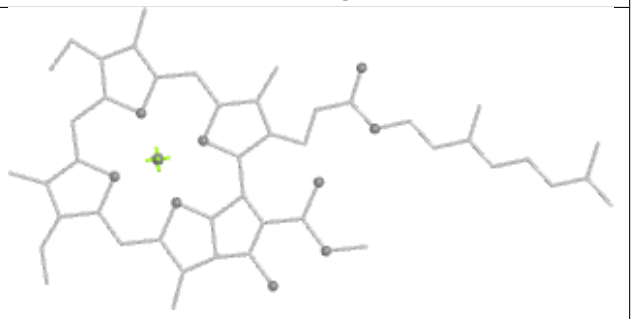
Bond lengths



Bond angles

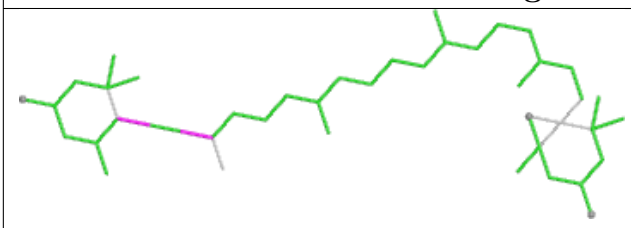


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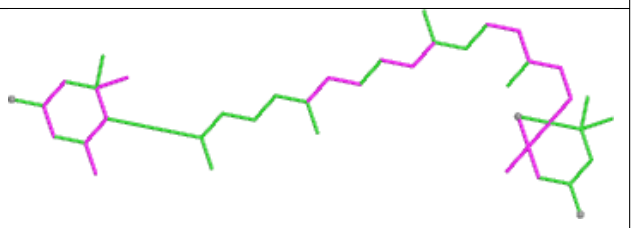


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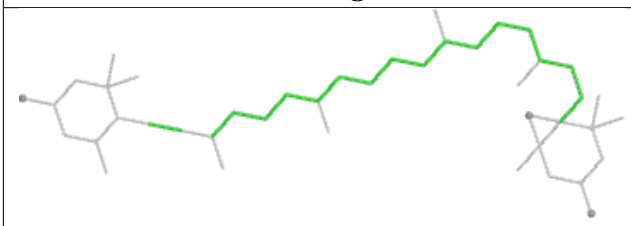
Ligand DD6 K 615



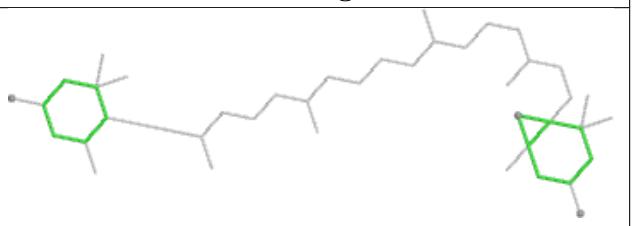
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Bond angles

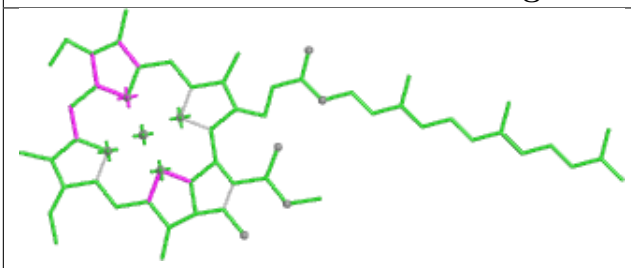


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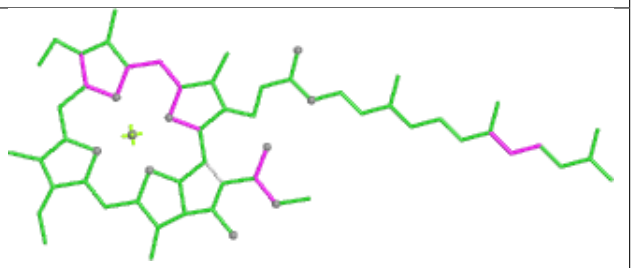


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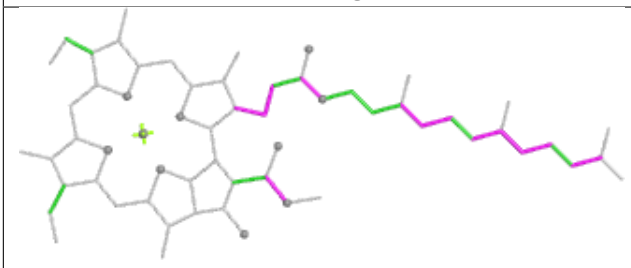
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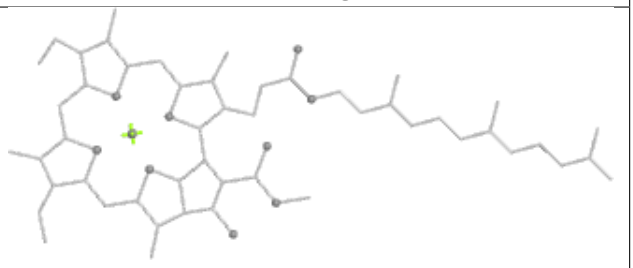
Bond lengths



Bond angles

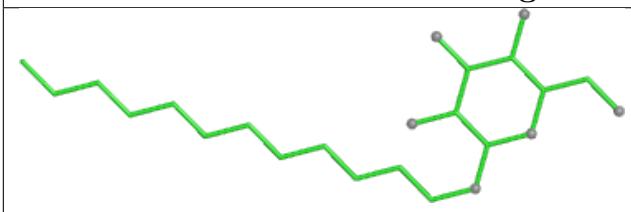


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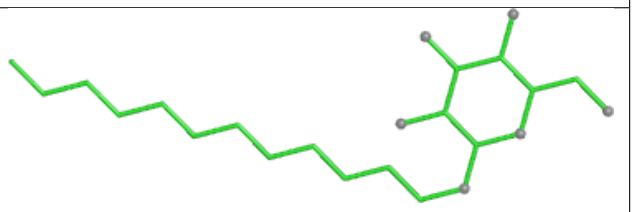


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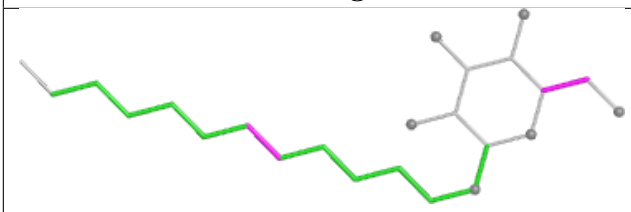
Ligand LMU H 320



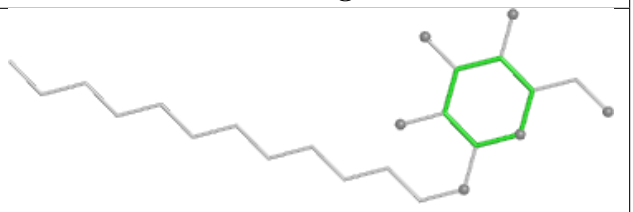
Bond lengths



Bond angles

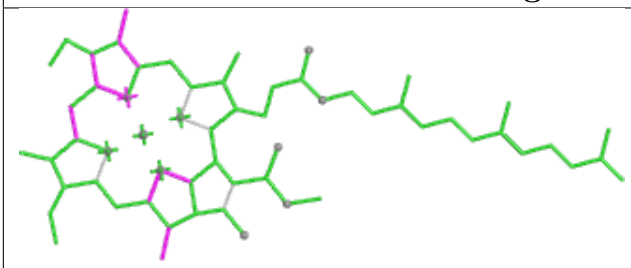


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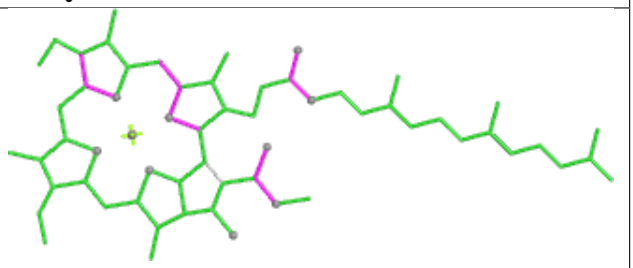


Rings

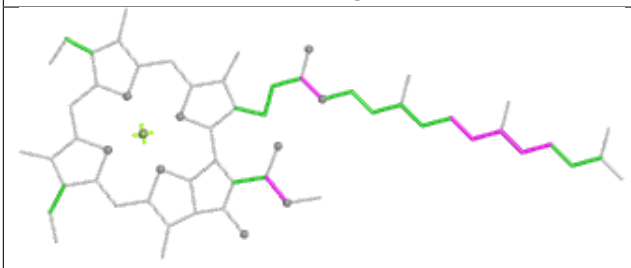
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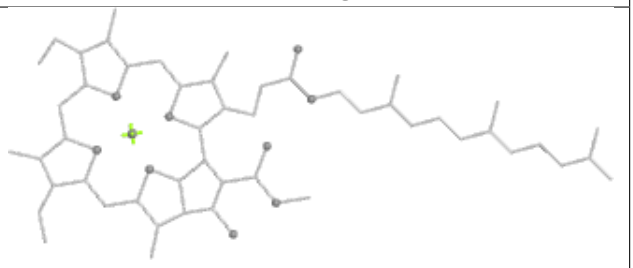
Bond lengths



Bond angles

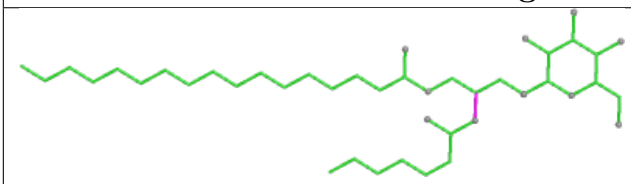


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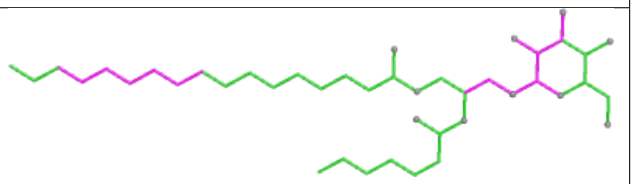


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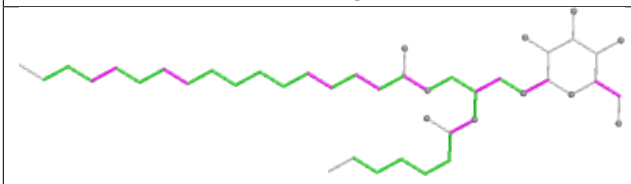
Ligand LMG H 317



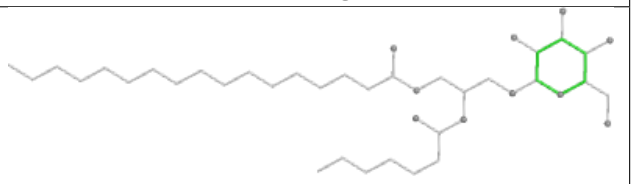
Bond lengths



Bond angles

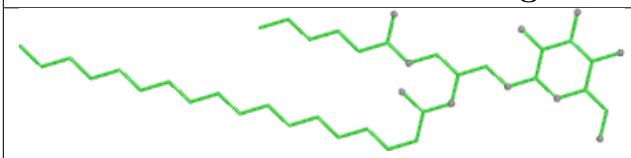


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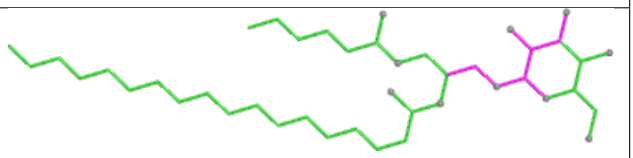


Rings

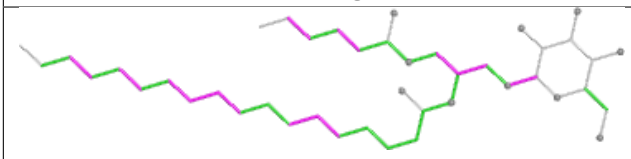
Ligand LMG B 852



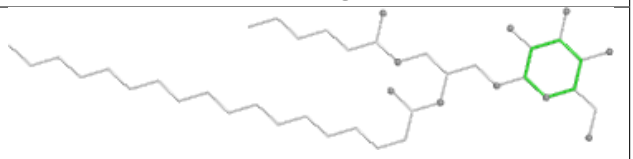
Bond lengths



Bond angles

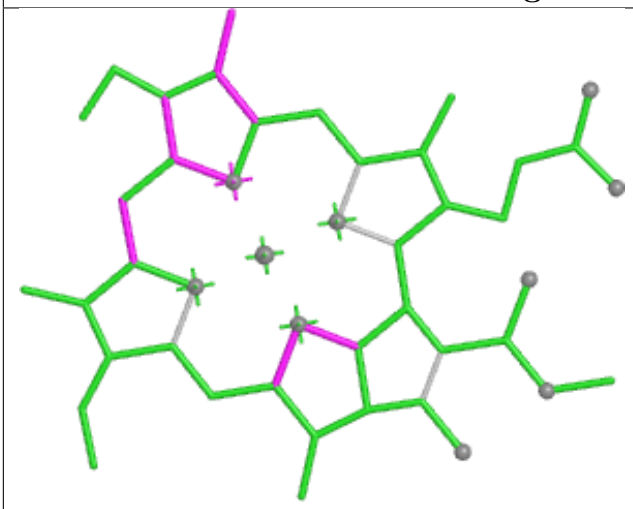


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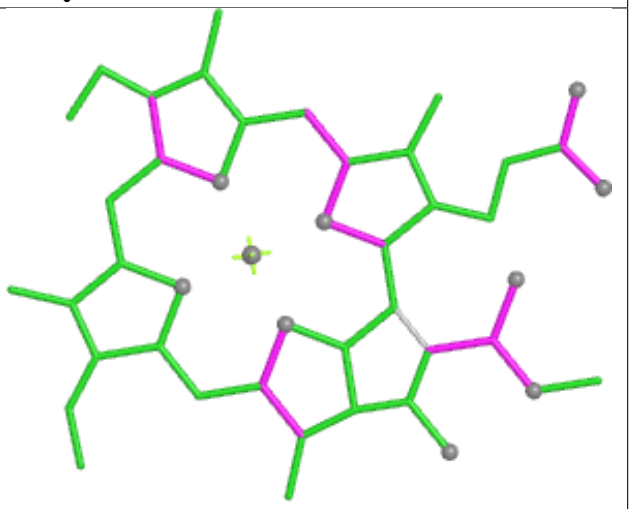


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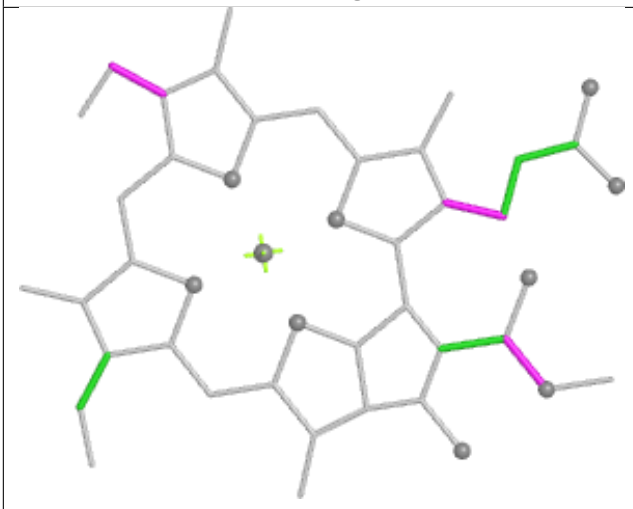
Ligand CLA Q 613



Bond lengths



Bond angles

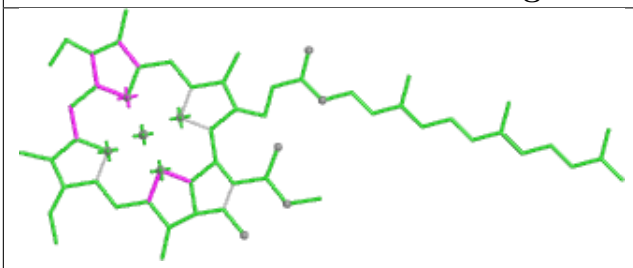


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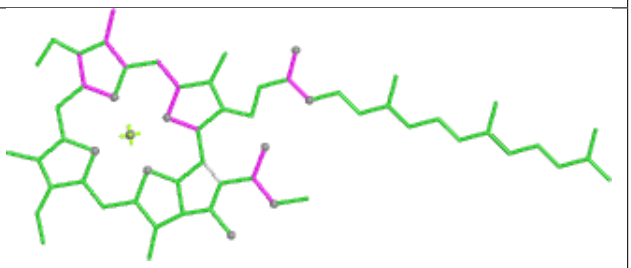


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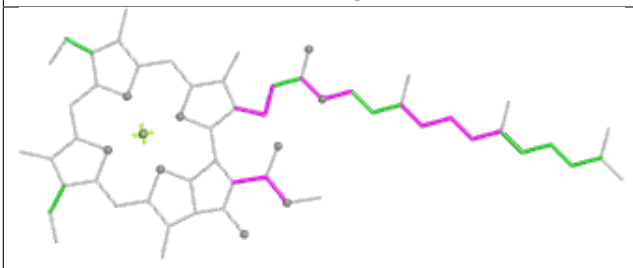
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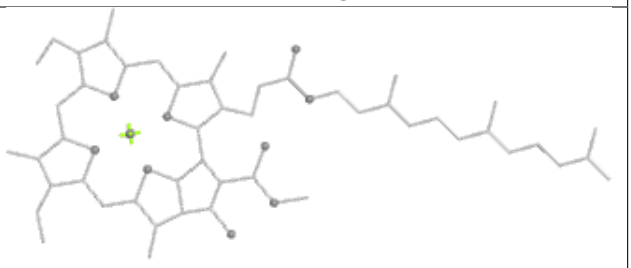
Bond lengths



Bond angles

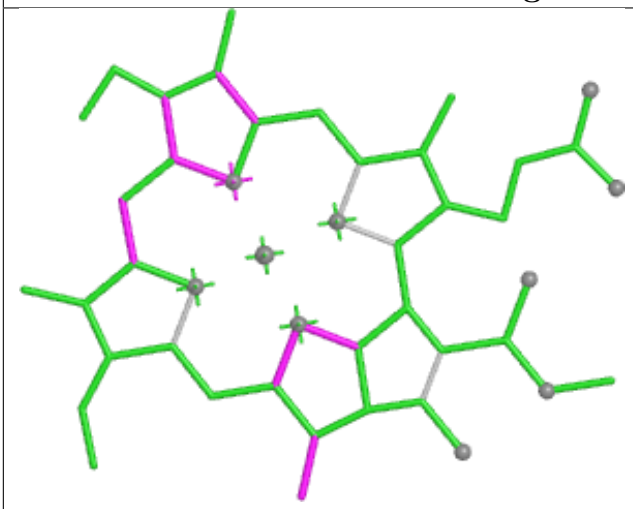


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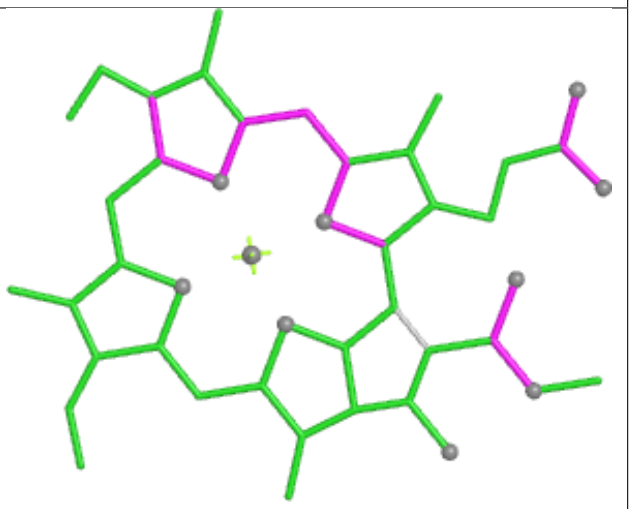


Rings

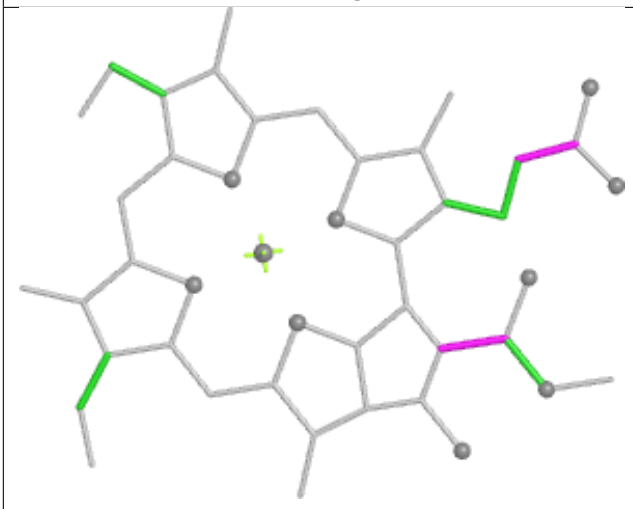
Ligand CLA H 310



Bond lengths



Bond angles

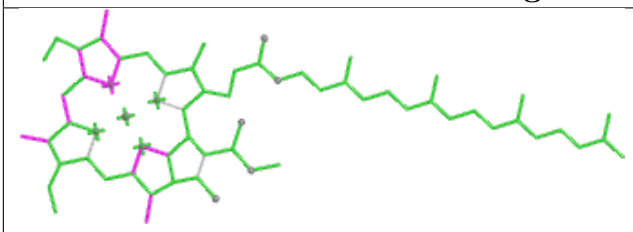


Torsions

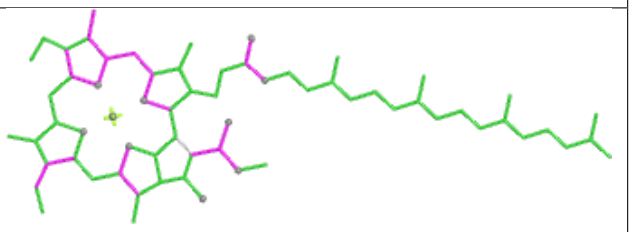


Rings

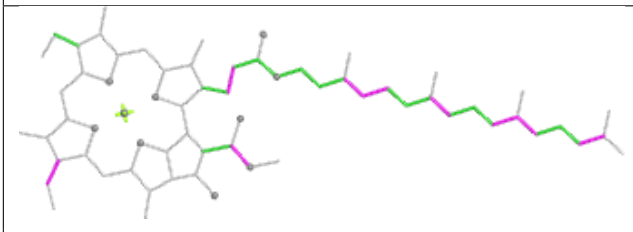
Ligand CLA A 801



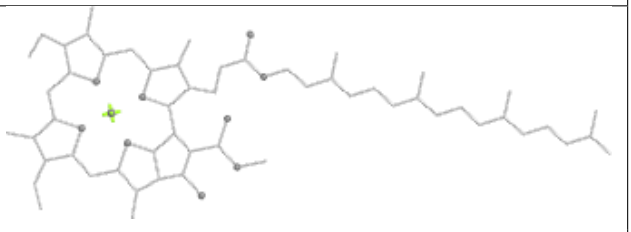
Bond lengths



Bond angles

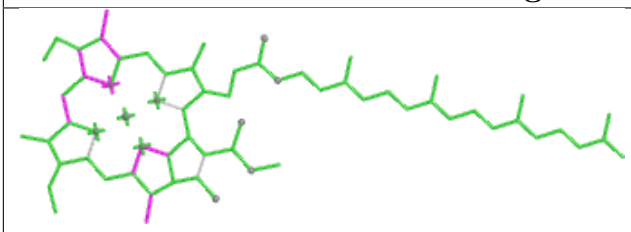


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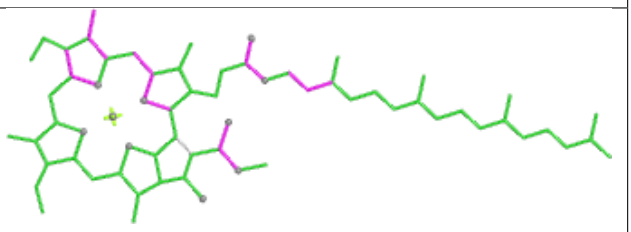


Rings

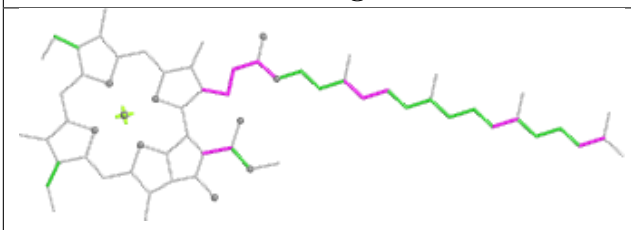
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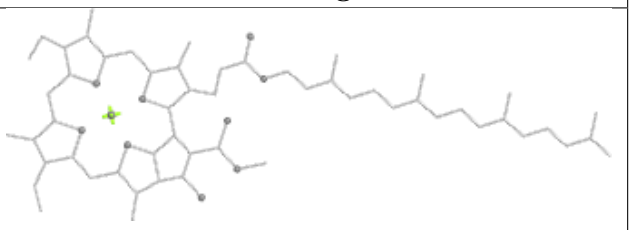
Bond lengths



Bond angles

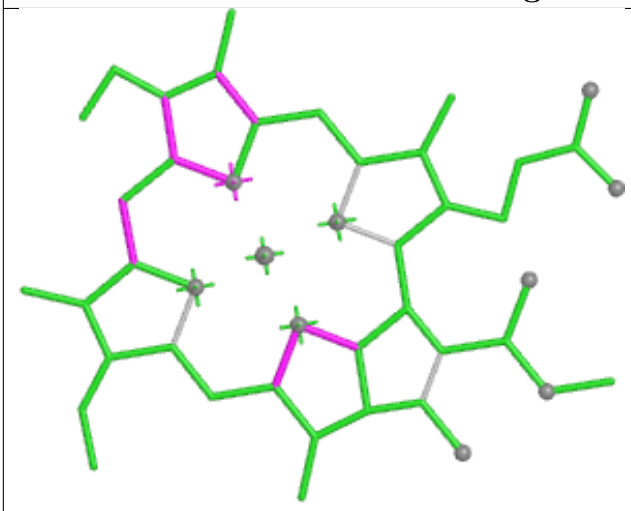


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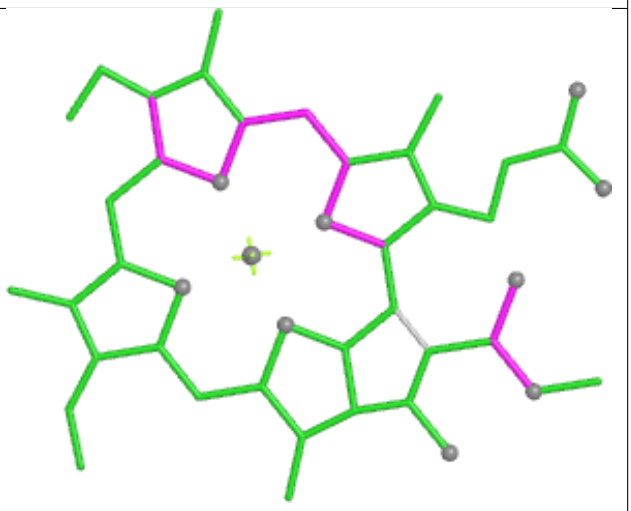


Rings

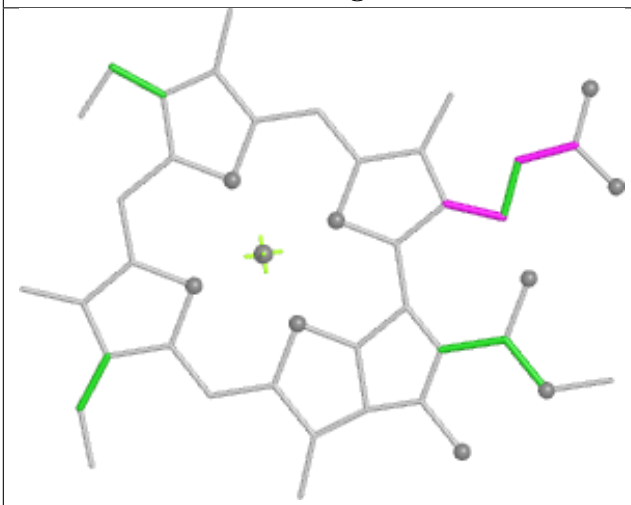
Ligand CLA H 312



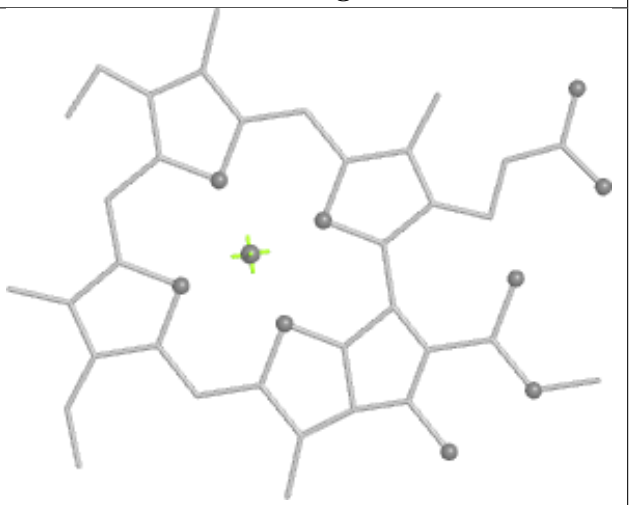
Bond lengths



Bond angles

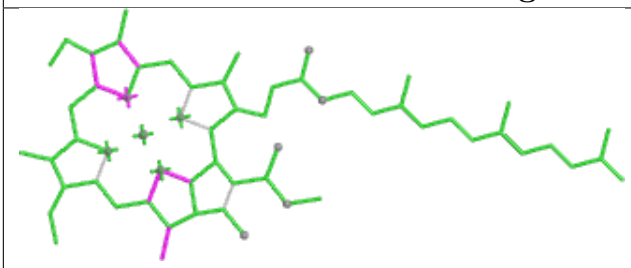


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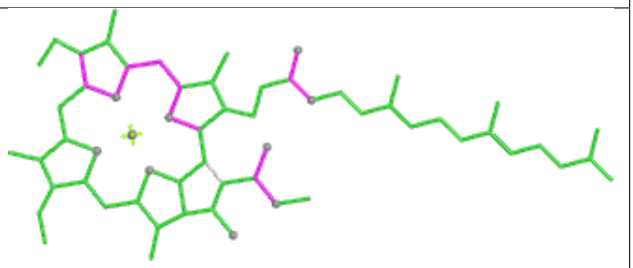


Rings

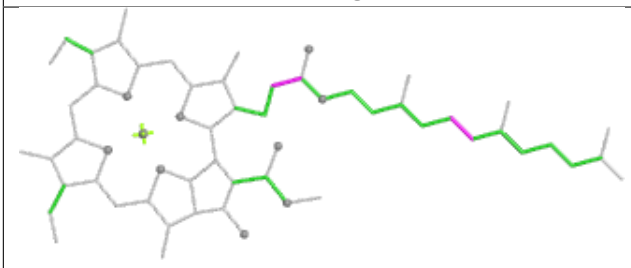
Ligand CLA W 405



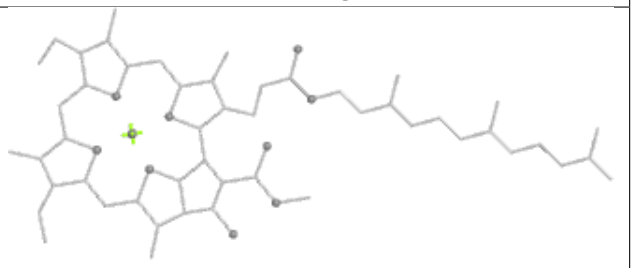
Bond lengths



Bond angles

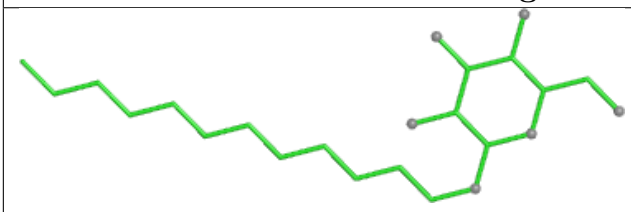


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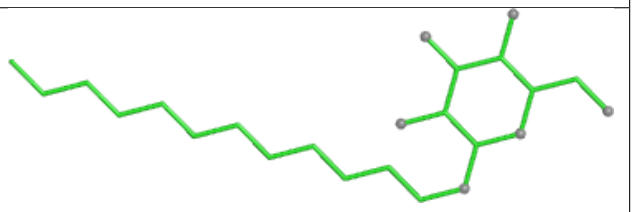


Rings

Ligand LMU O 301



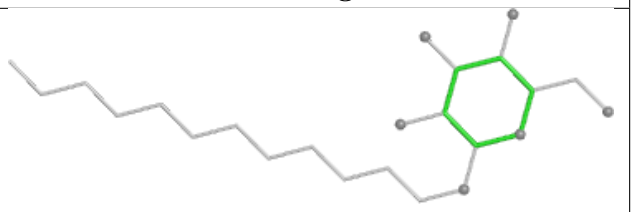
Bond lengths



Bond angles

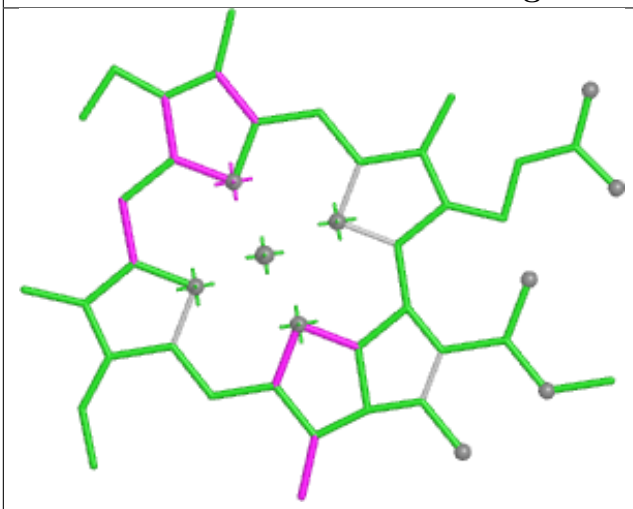


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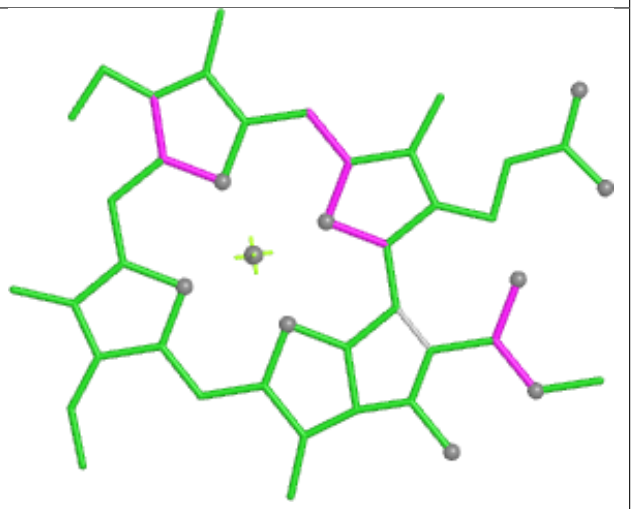


Rings

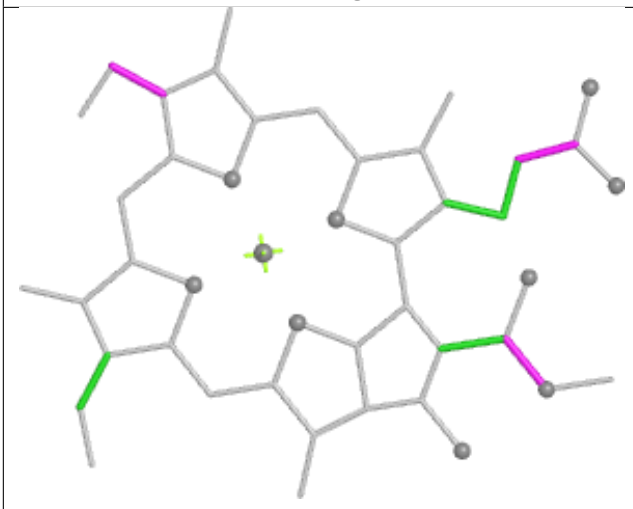
Ligand CLA N 601



Bond lengths



Bond angles

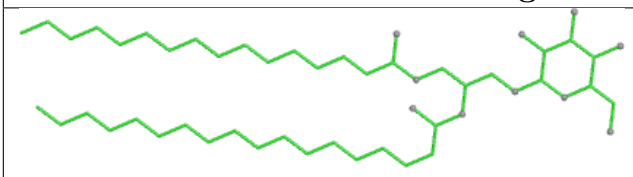


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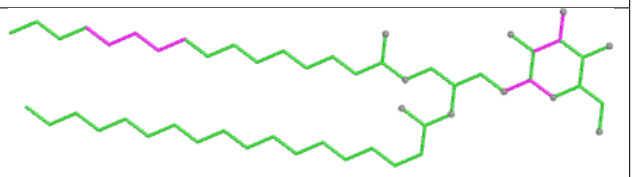


Rings

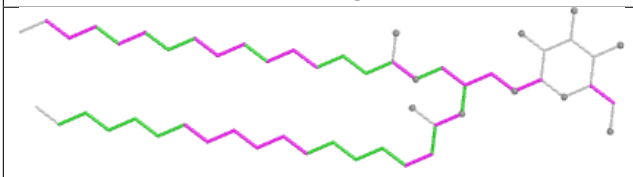
Ligand LMG U 402



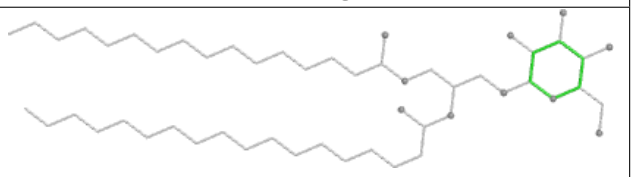
Bond lengths



Bond angles

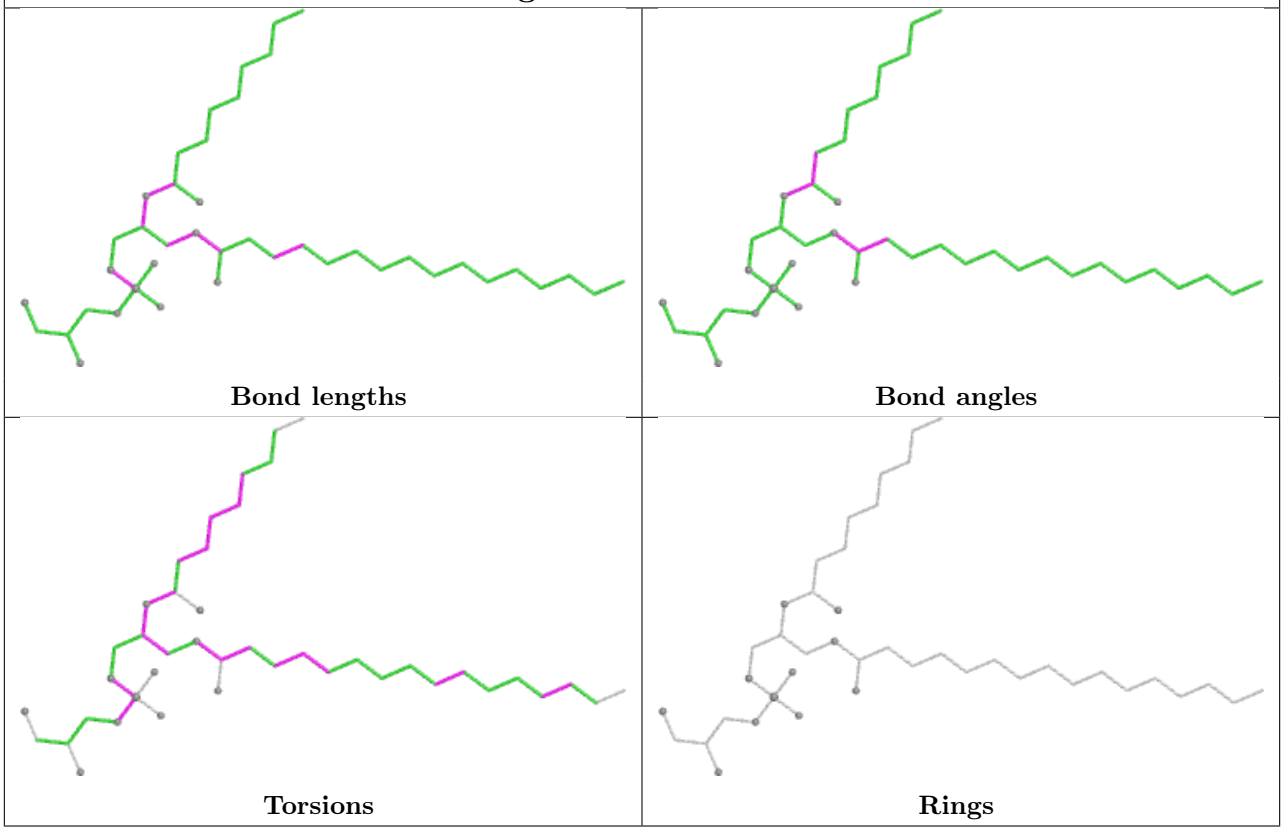


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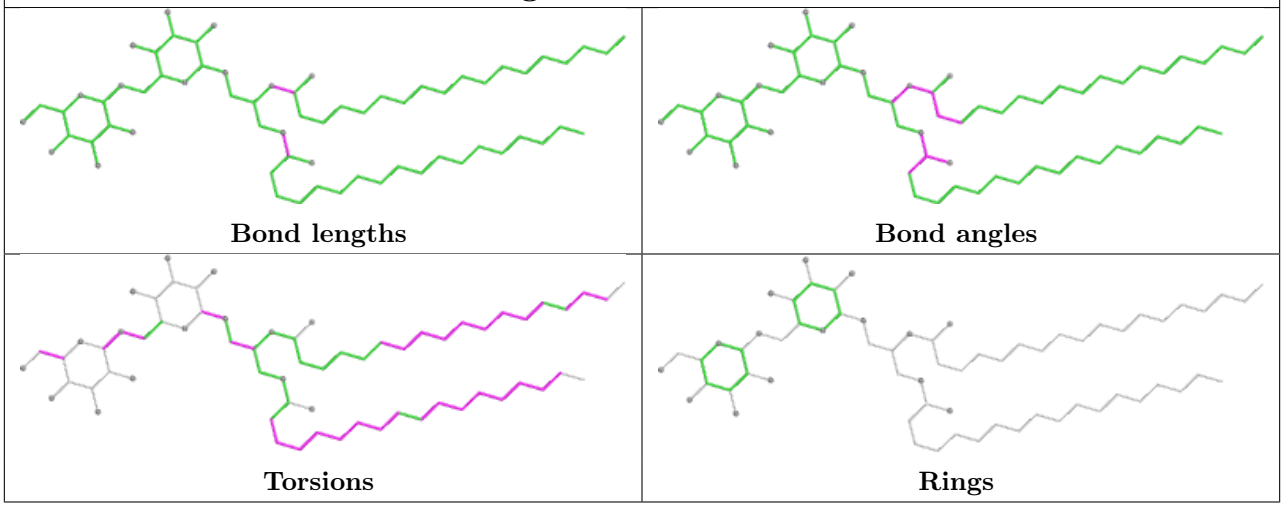


Rings

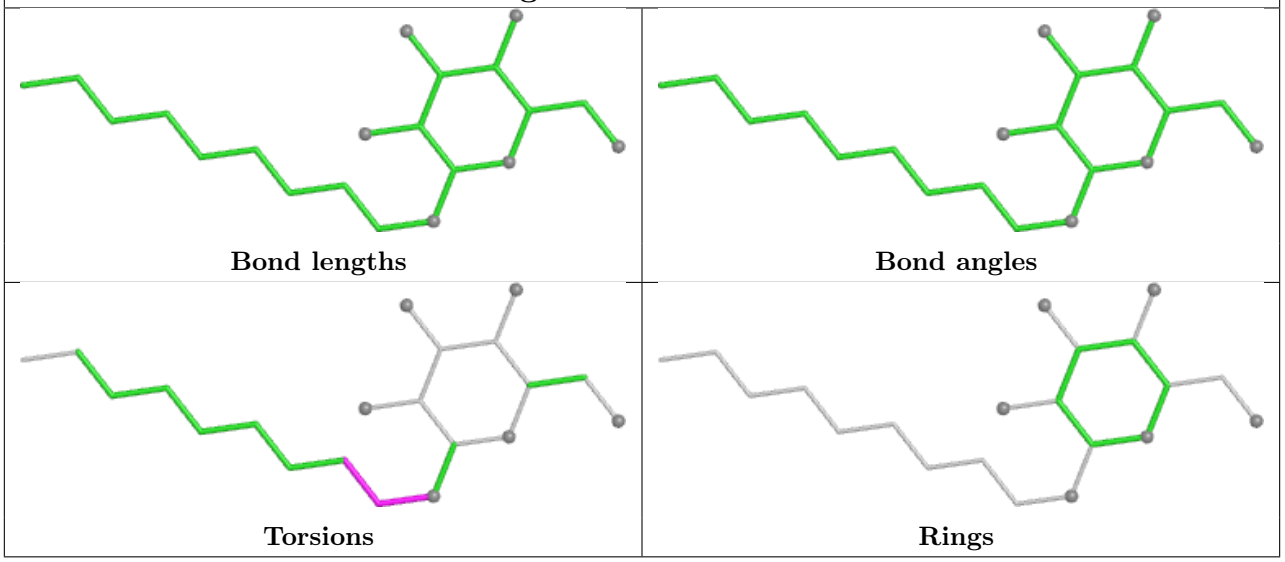
Ligand LHG W 420



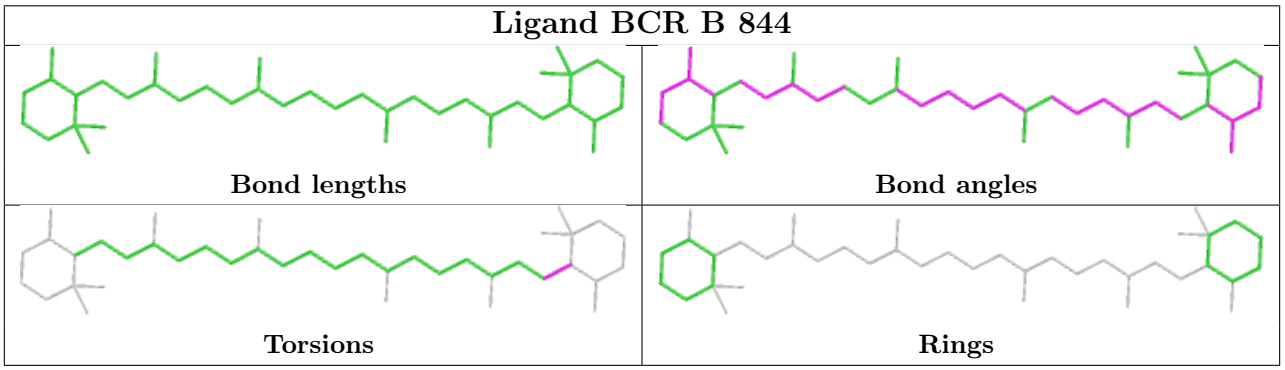
Ligand DGD B 847



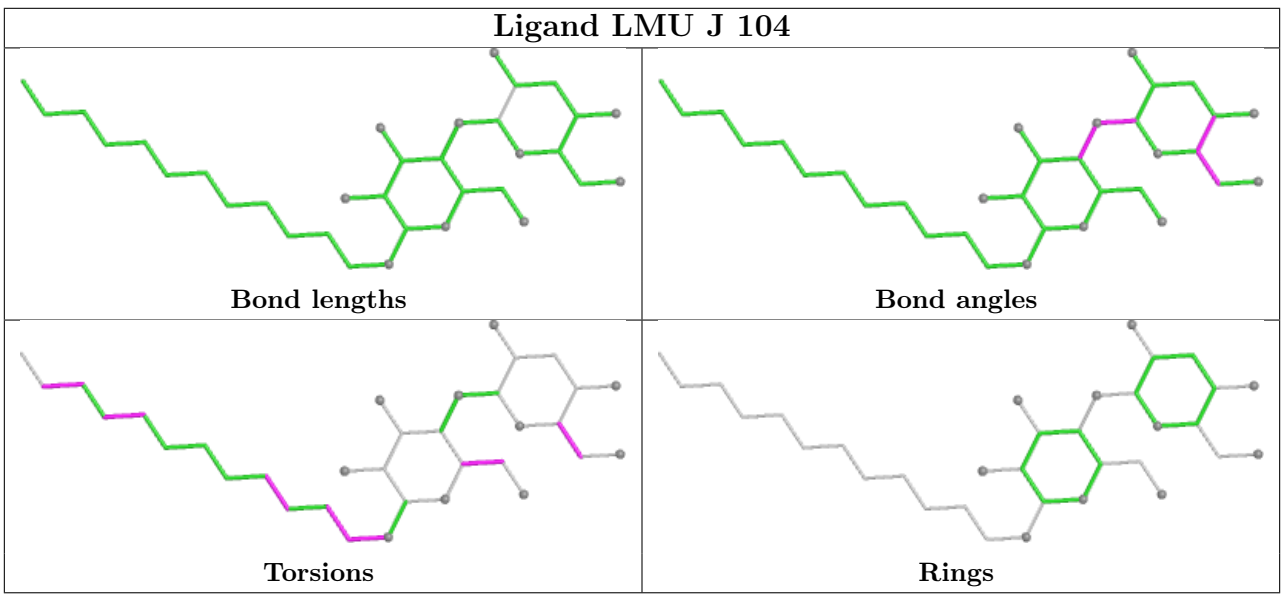
Ligand LMU H 301



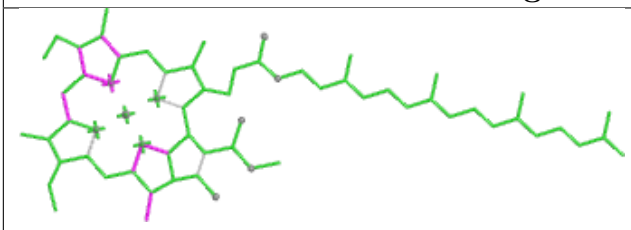
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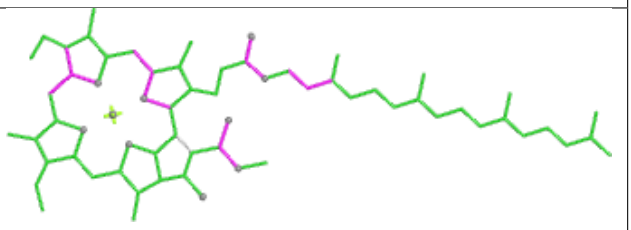
Ligand LMU J 104



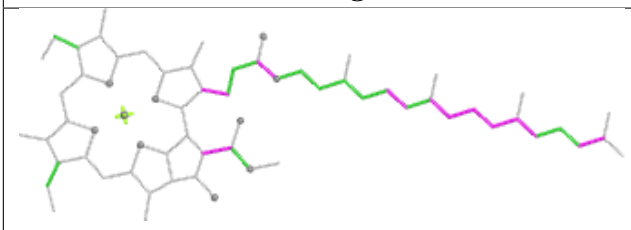
Ligand CLA A 840



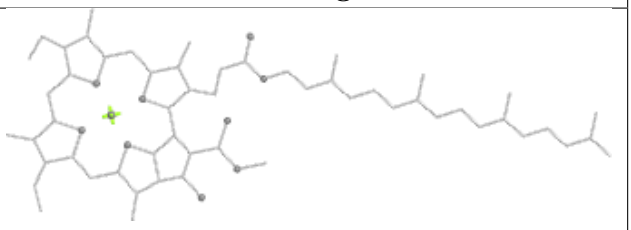
Bond lengths



Bond angles

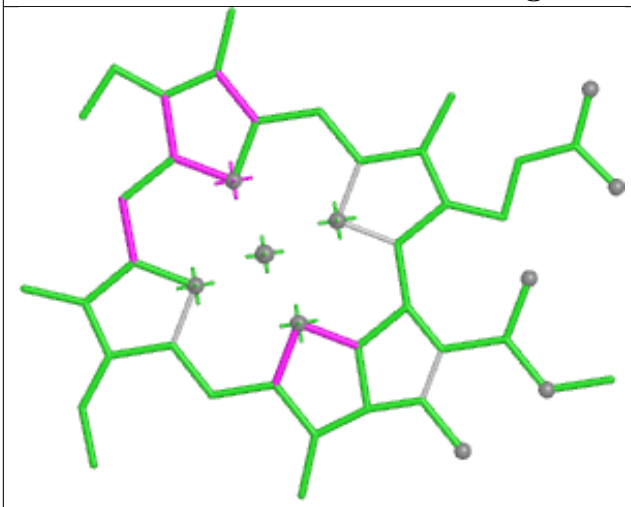


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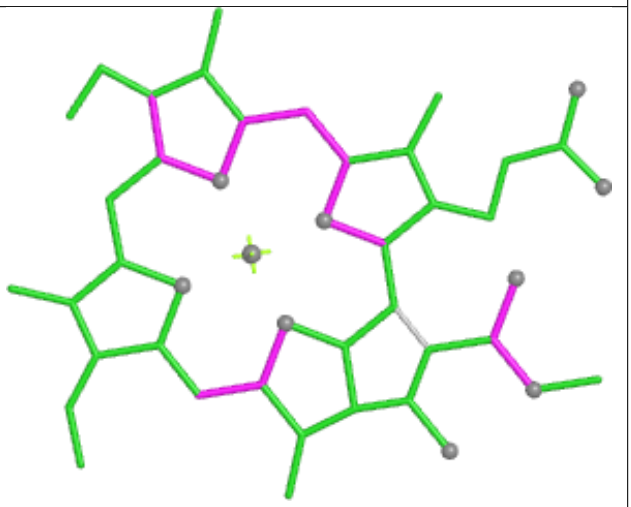


Rings

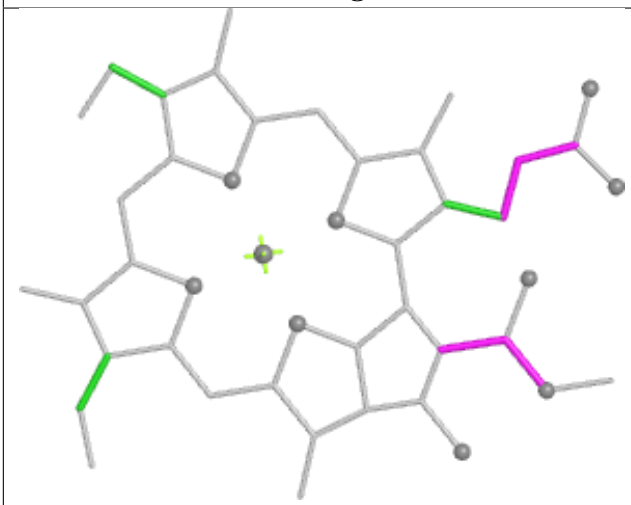
Ligand CLA P 604



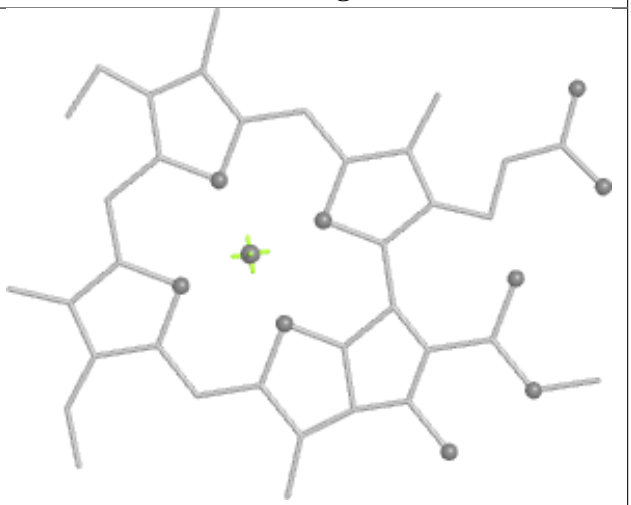
Bond lengths



Bond angles

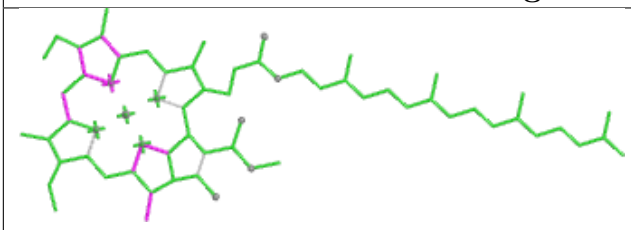


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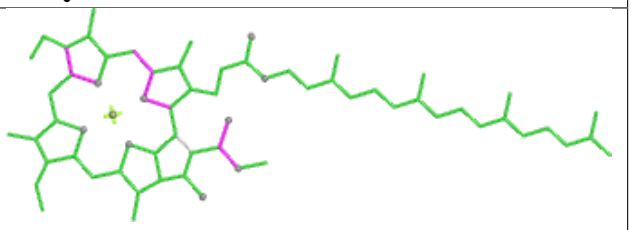


Rings

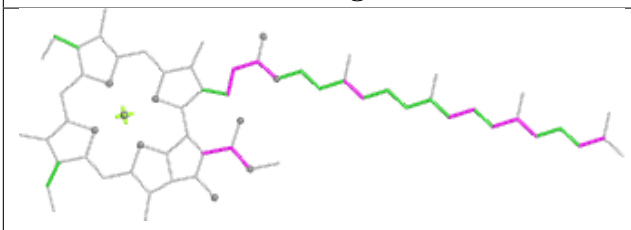
Ligand CLA Q 612



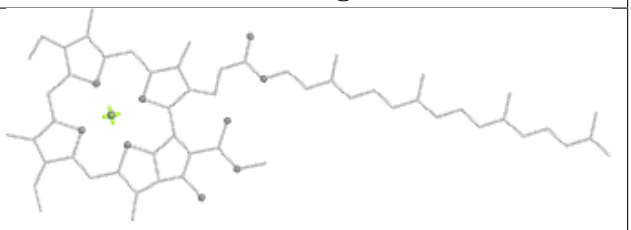
Bond lengths



Bond angles

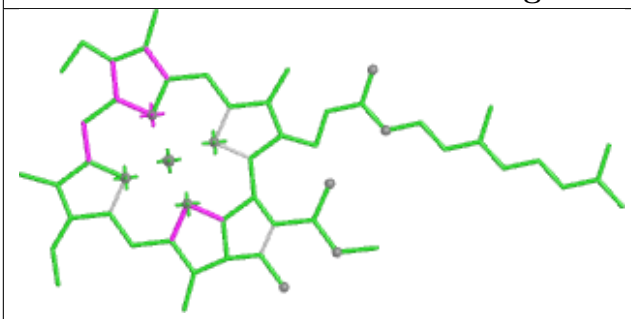


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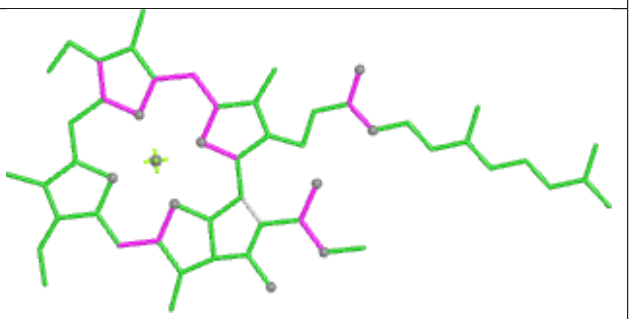


Rings

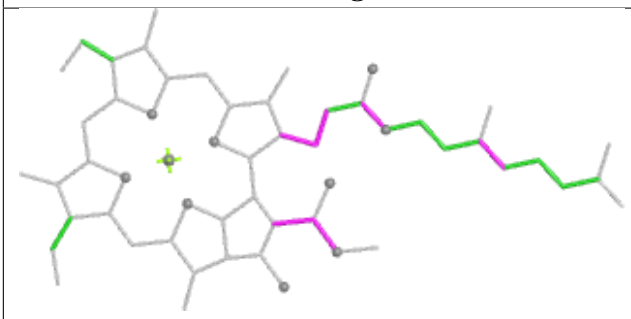
Ligand CLA X 402



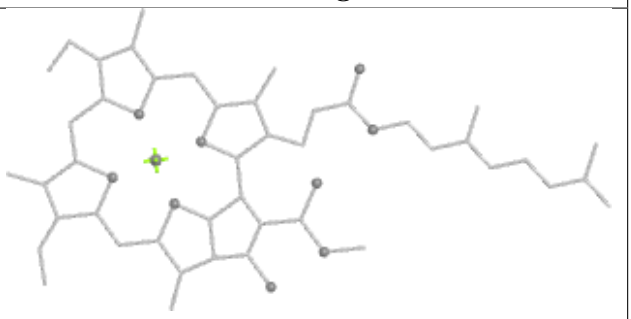
Bond lengths



Bond angles

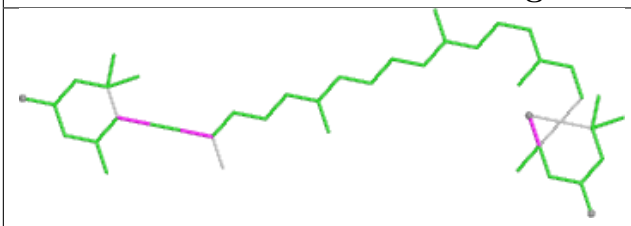


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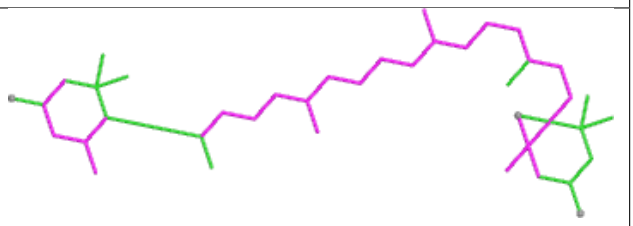


Rings

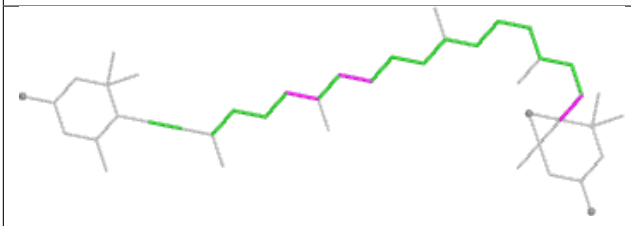
Ligand DD6 P 613



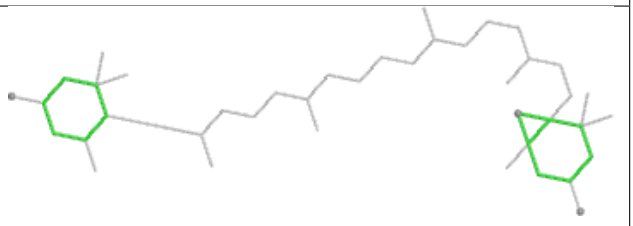
Bond lengths



Bond angles

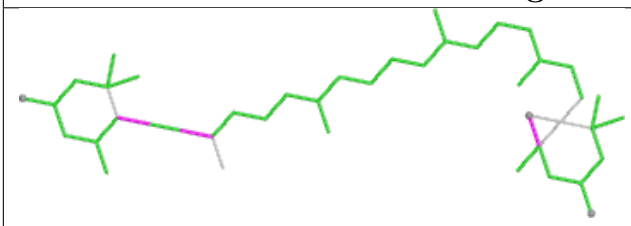


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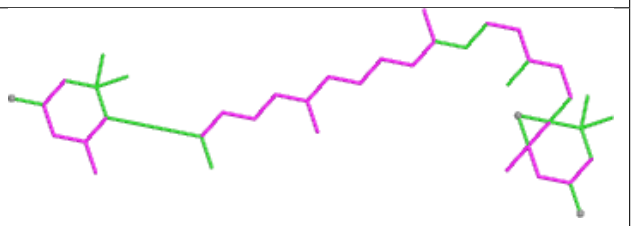


Rings

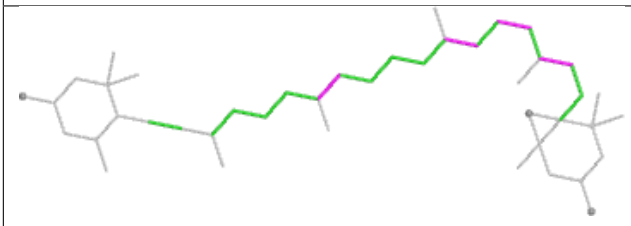
Ligand DD6 F 406



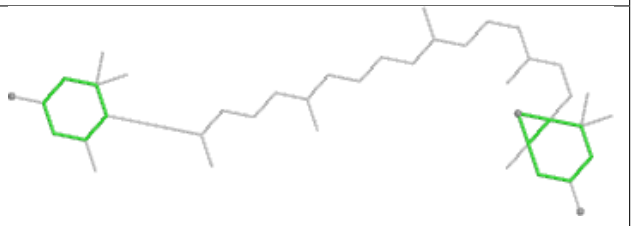
Bond lengths



Bond angles

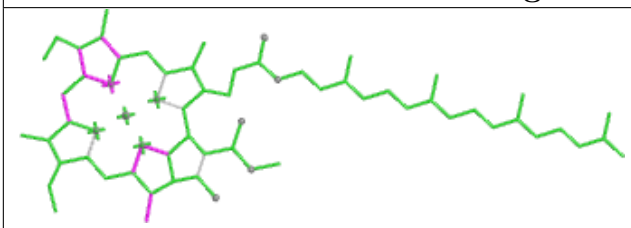


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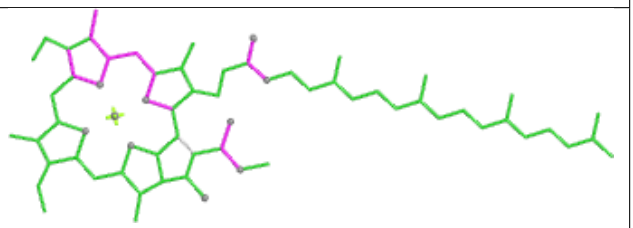


Rings

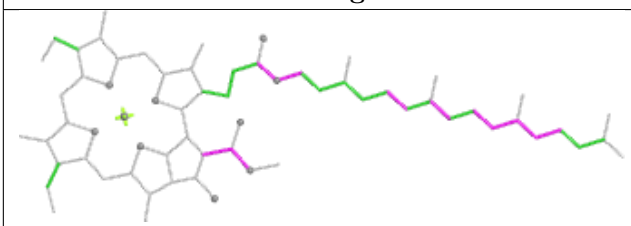
Ligand CLA A 817



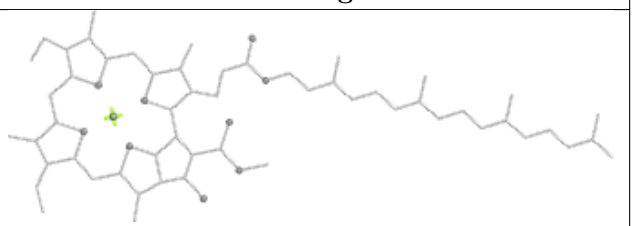
Bond lengths



Bond angles

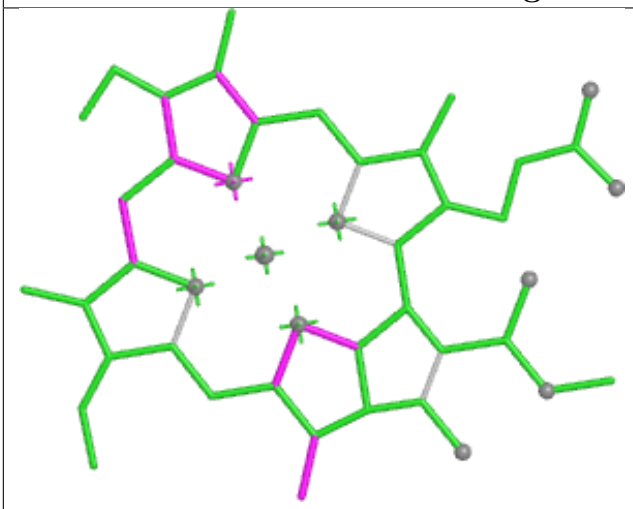


Torsions

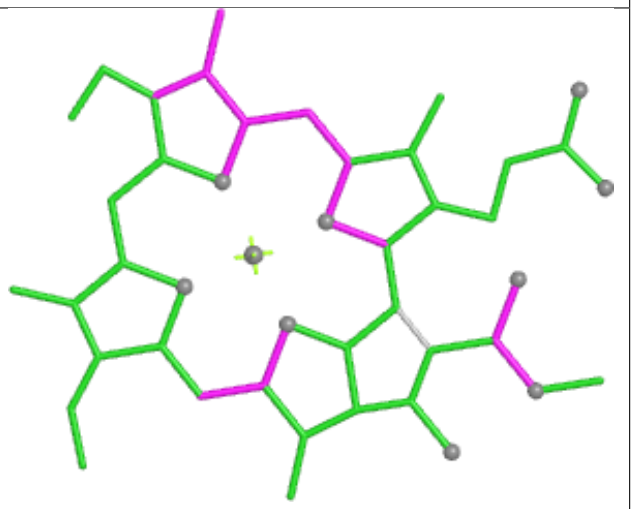


Rings

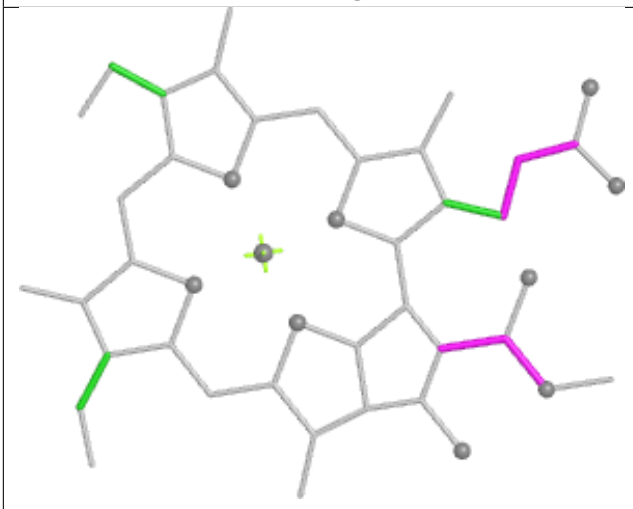
Ligand CLA H 304



Bond lengths



Bond angles

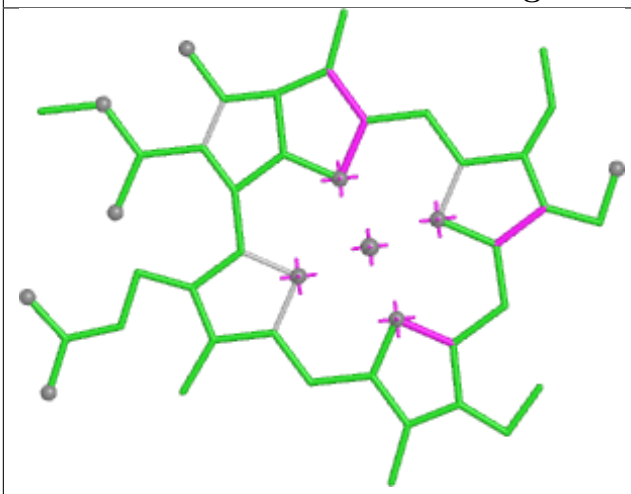


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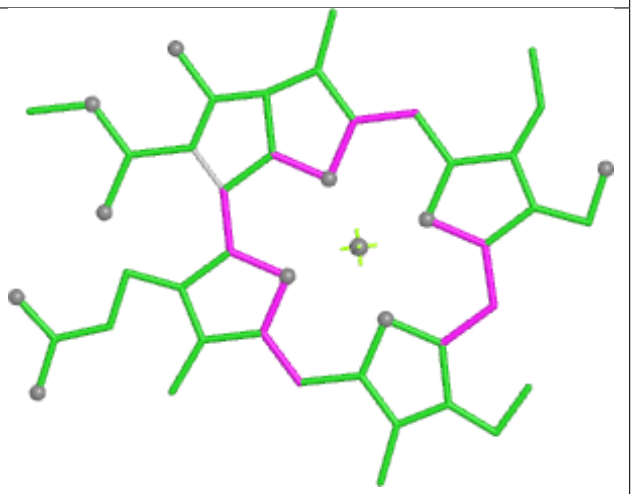


Rings

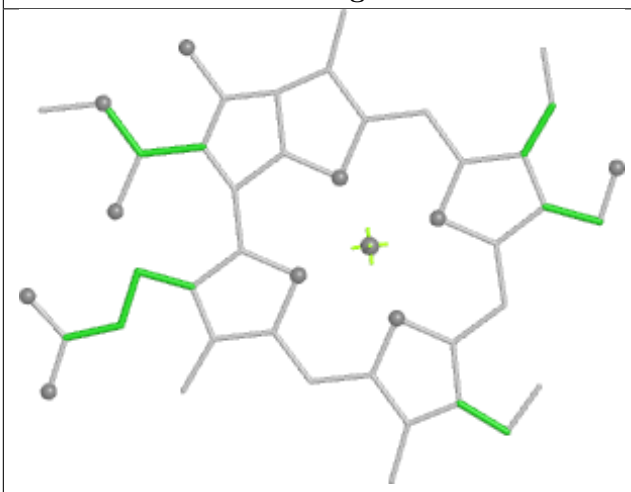
Ligand CHL X 406



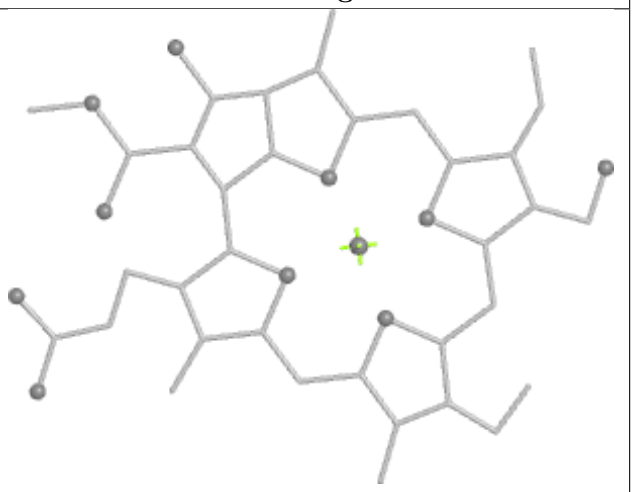
Bond lengths



Bond angles

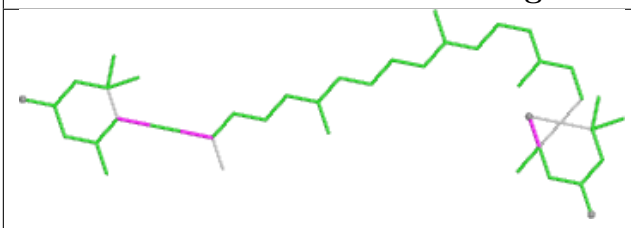


Torsions

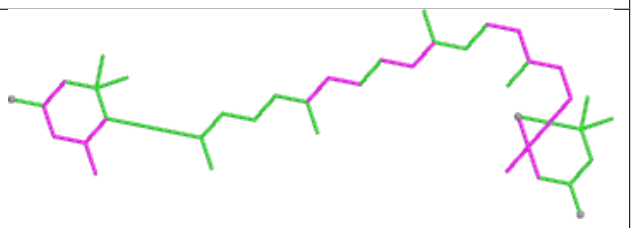


Rings

Ligand DD6 R 612



Bond lengths



Bond angles

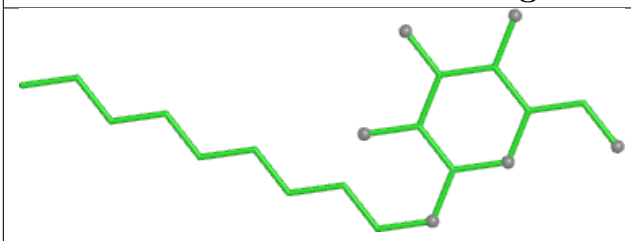


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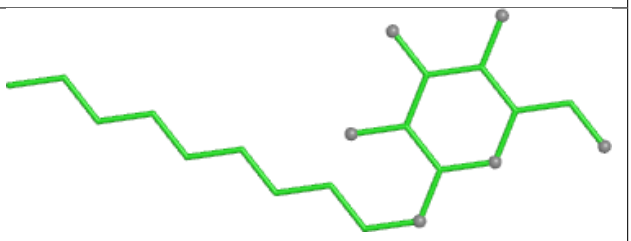


Rings

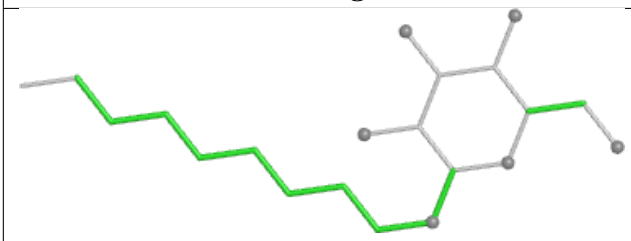
Ligand LMU A 856



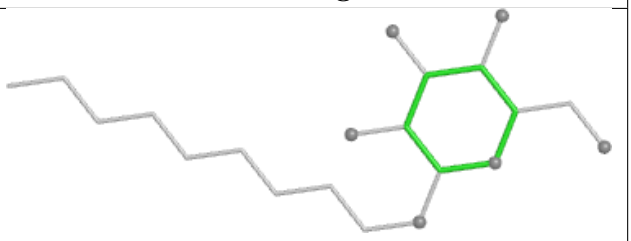
Bond lengths



Bond angles

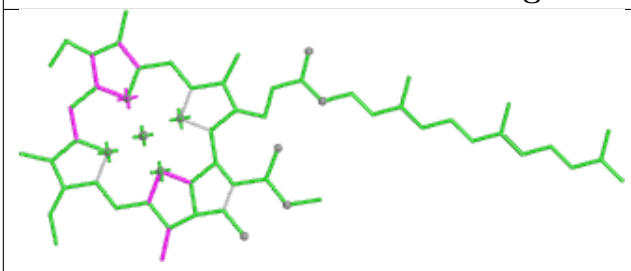


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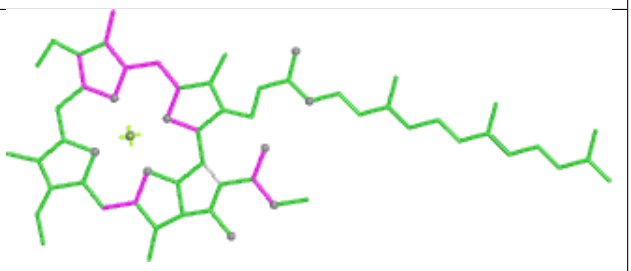


Rings

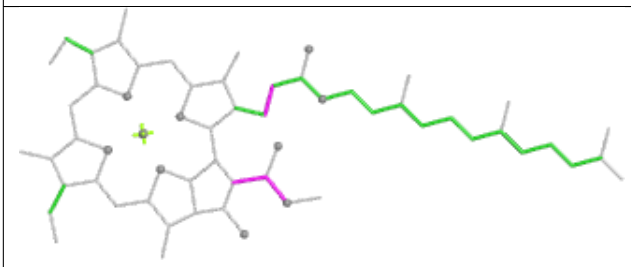
Ligand CLA N 602



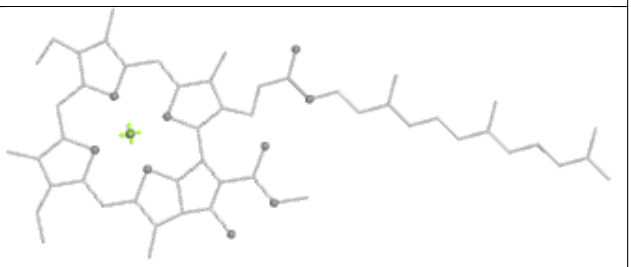
Bond lengths



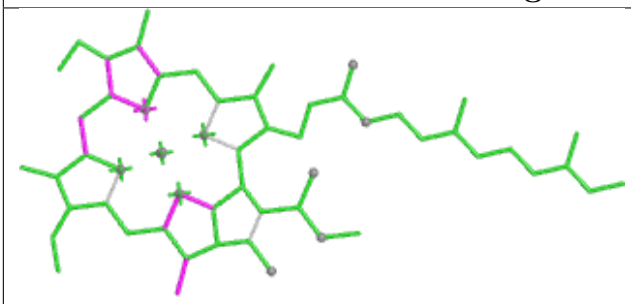
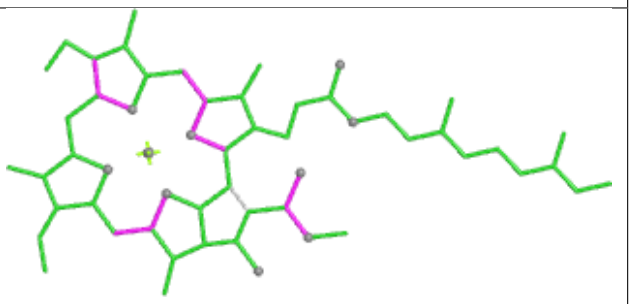
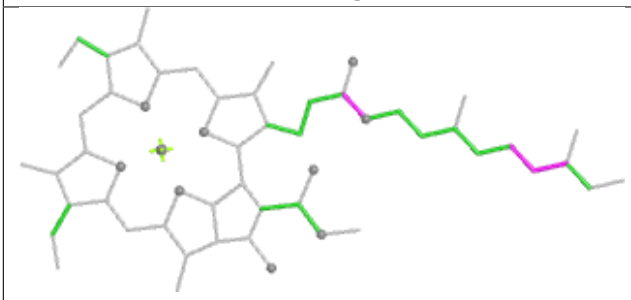
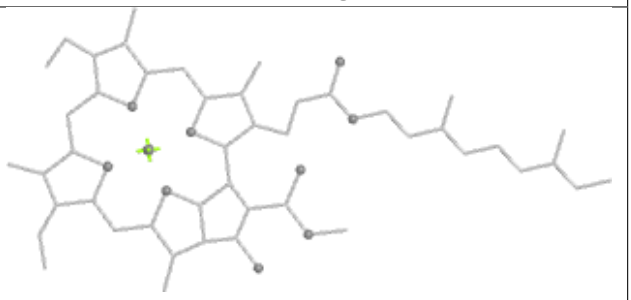
Bond angles

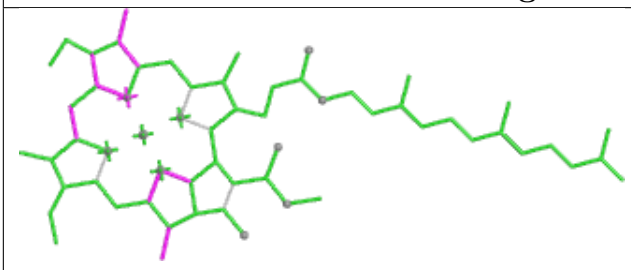
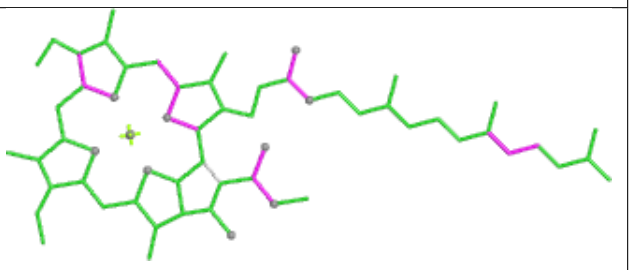
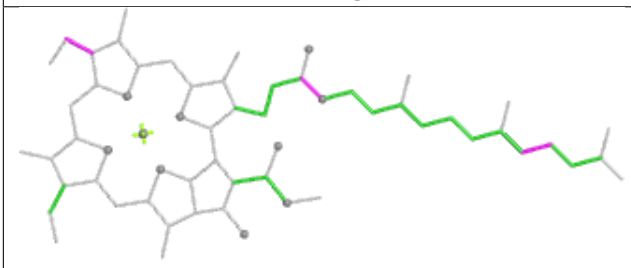
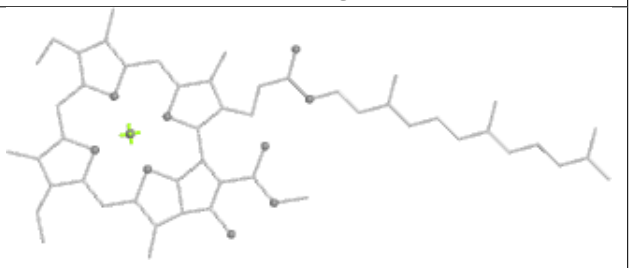


Torsions

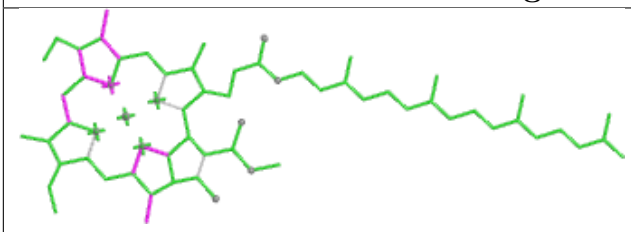


Rings

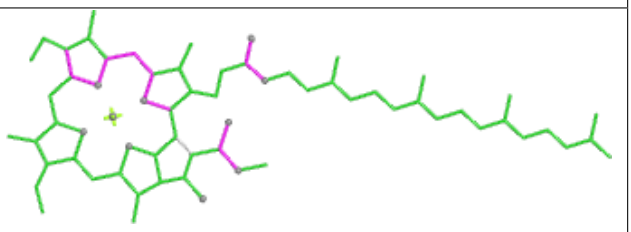
Ligand CLA B 810	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA W 412	
	
Bond lengths	Bond angles
	
Torsions	Rings

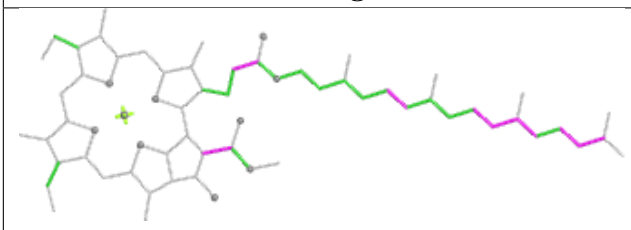
Ligand CLA A 808



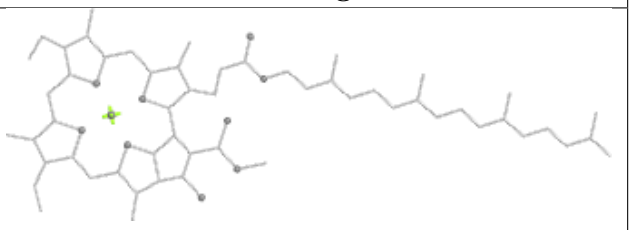
Bond lengths



Bond angles

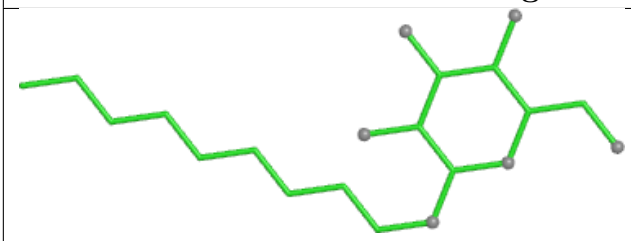


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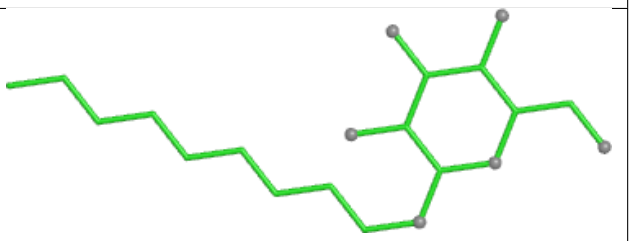


Rings

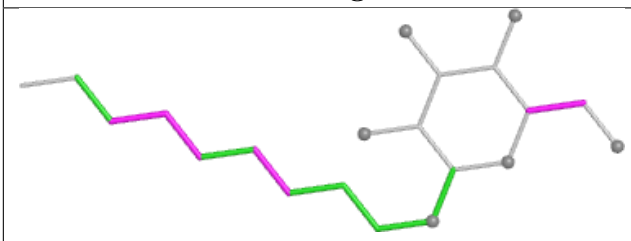
Ligand LMU F 409



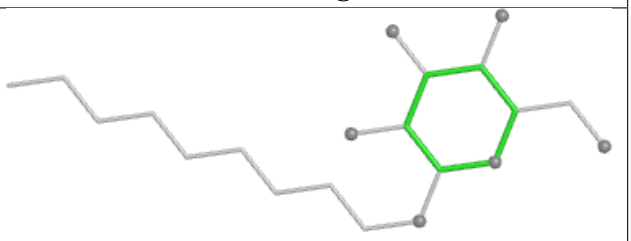
Bond lengths



Bond angles

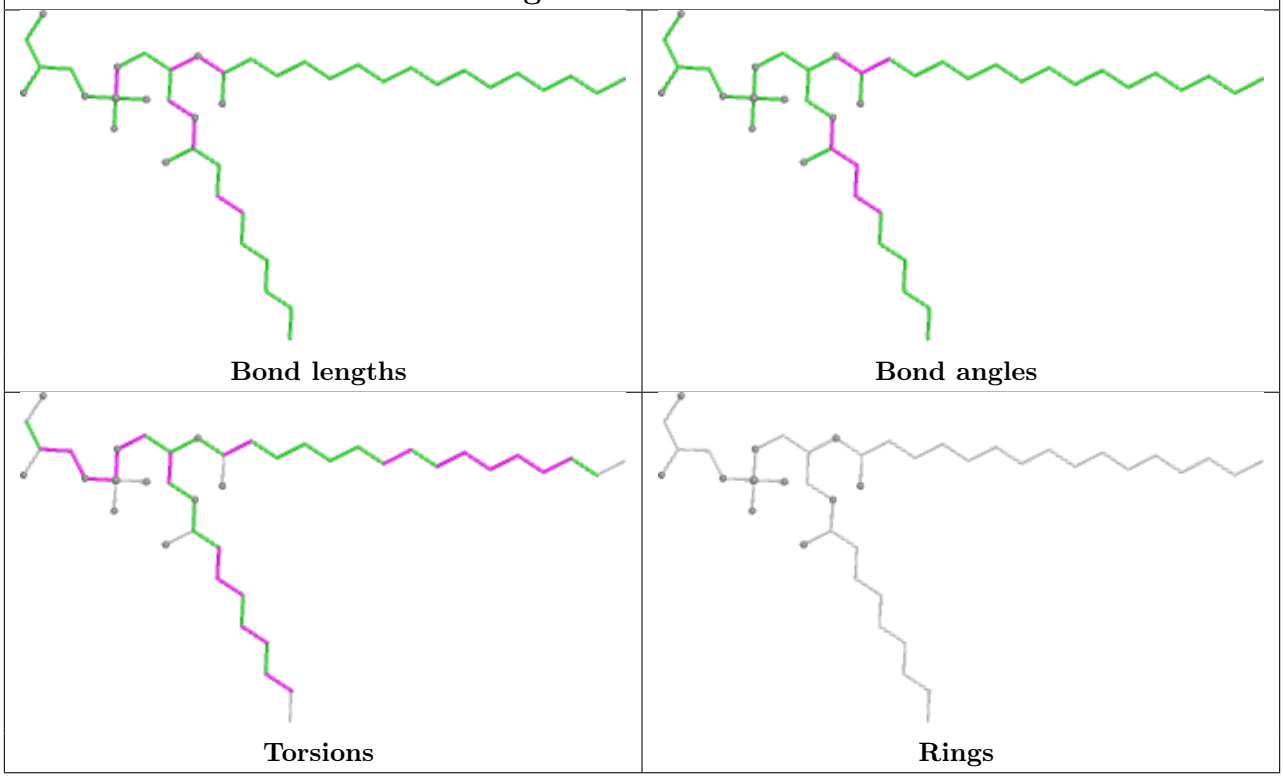


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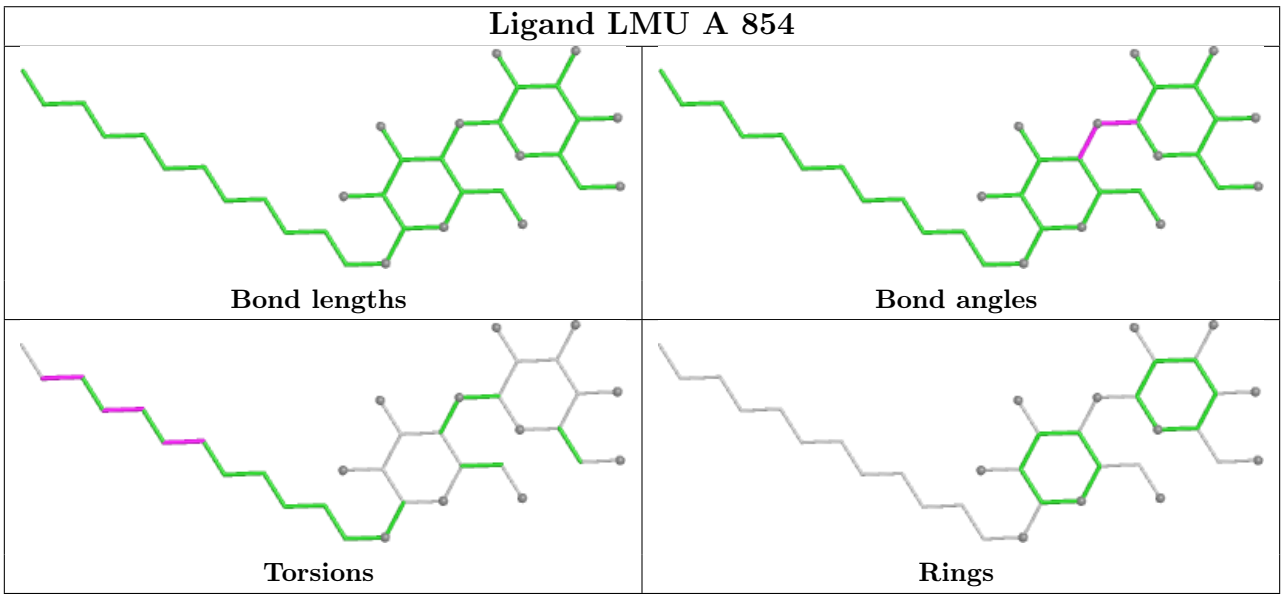


Rings

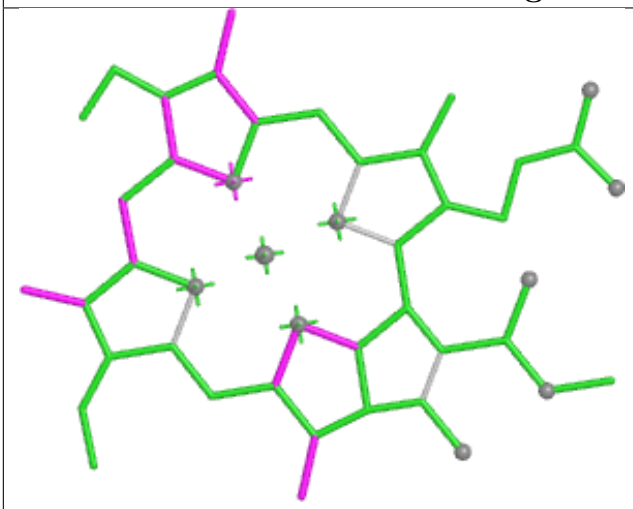
Ligand LHG B 851



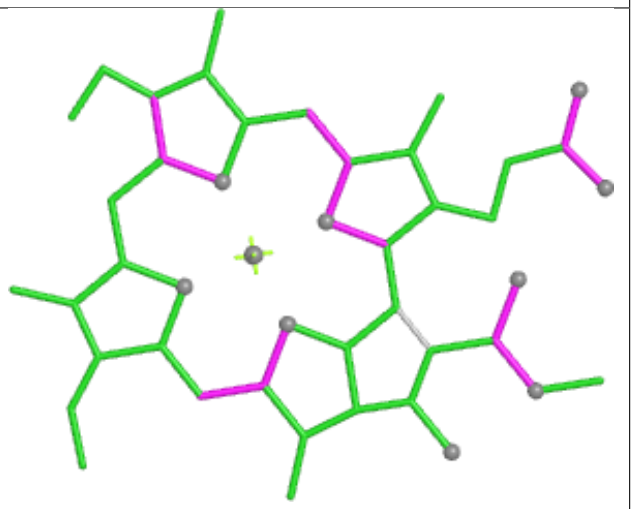
Ligand LMU A 854



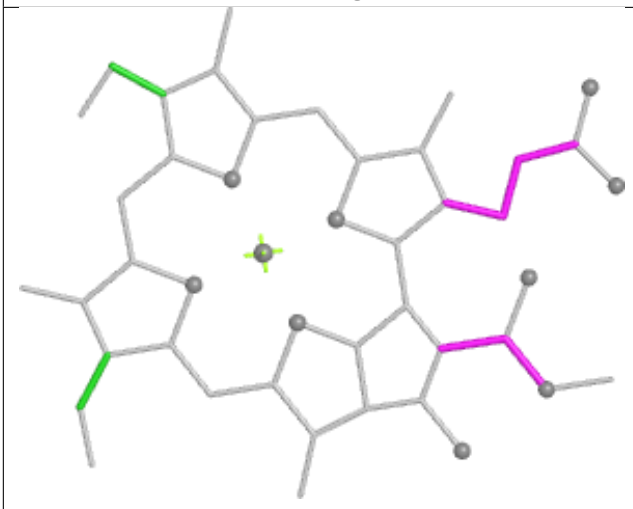
Ligand CLA P 602



Bond lengths



Bond angles

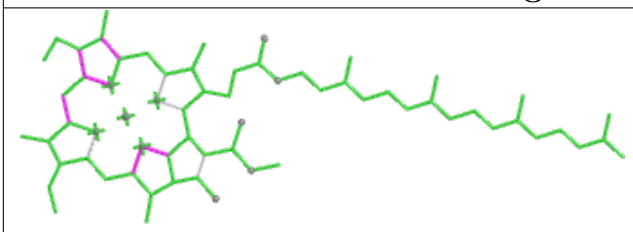


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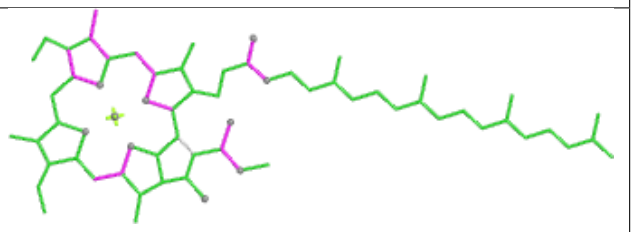


Rings

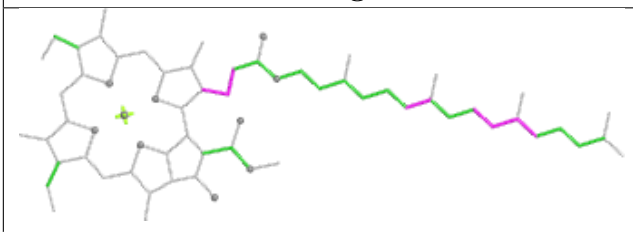
Ligand CLA B 825



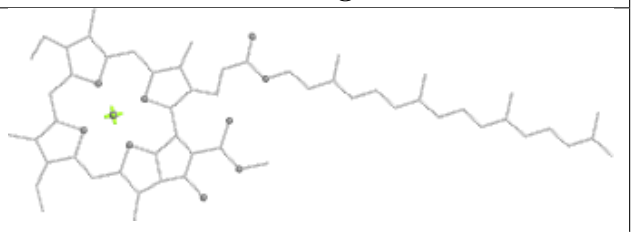
Bond lengths



Bond angles

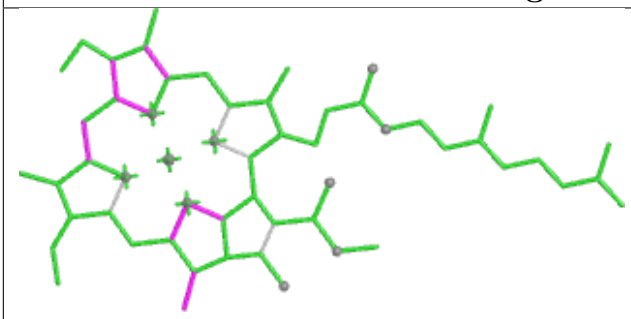


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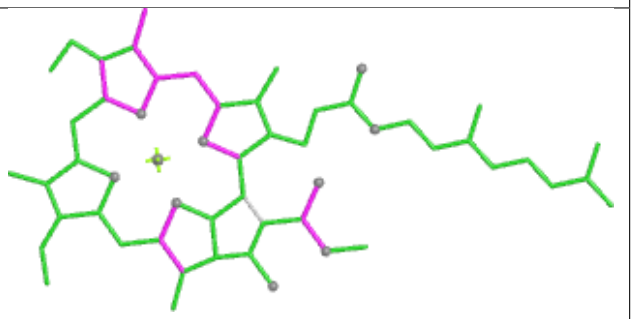


Rings

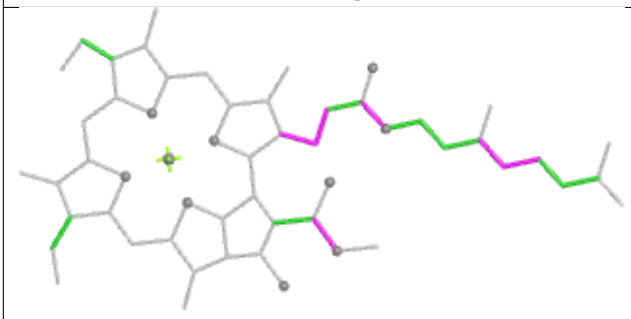
Ligand CLA F 404



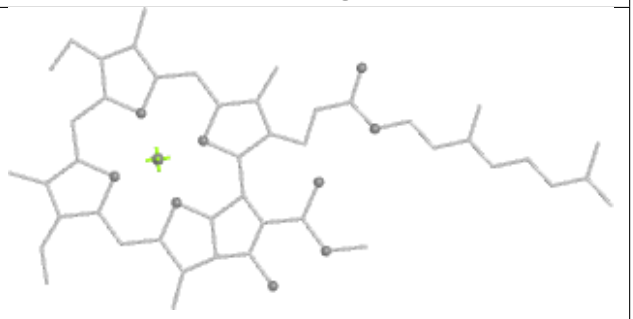
Bond lengths



Bond angles

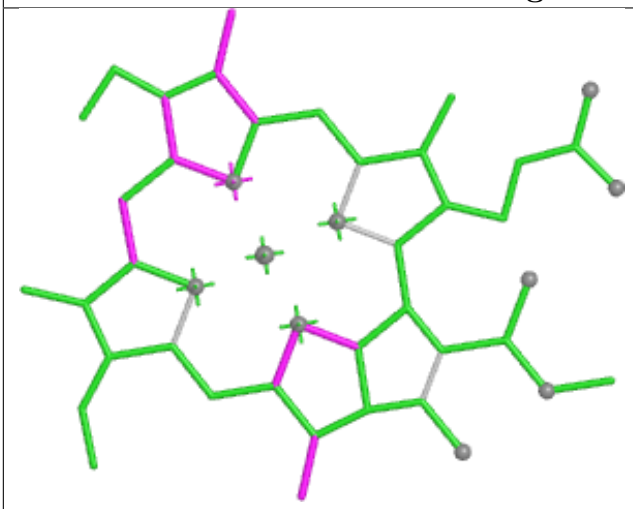


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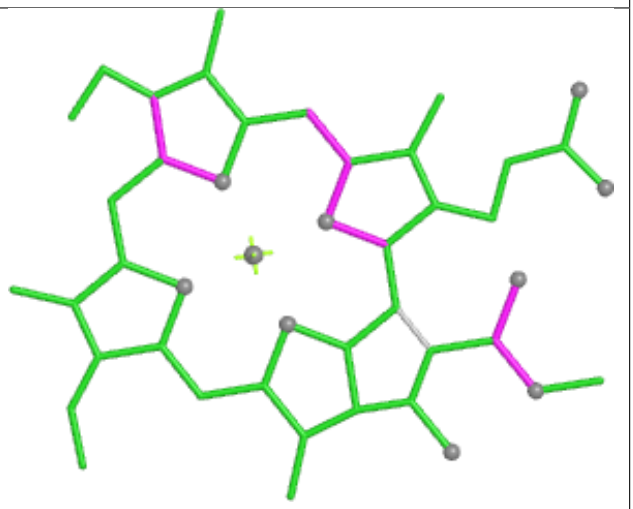


Rings

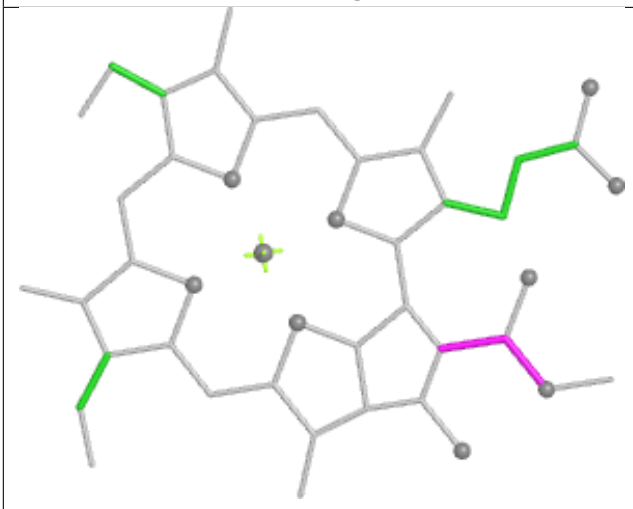
Ligand CLA L 405



Bond lengths



Bond angles

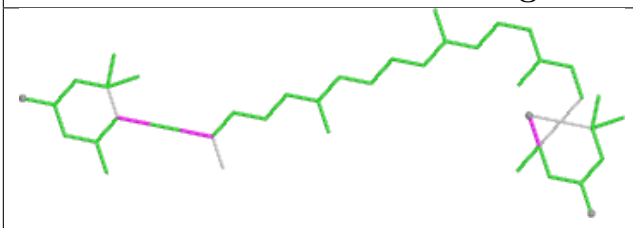


Torsions

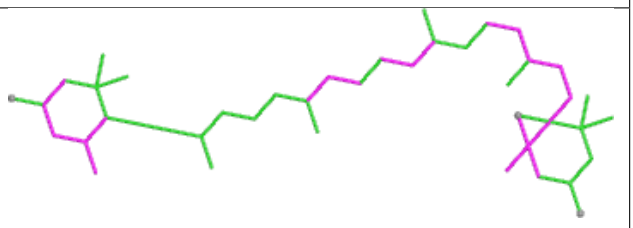


Rings

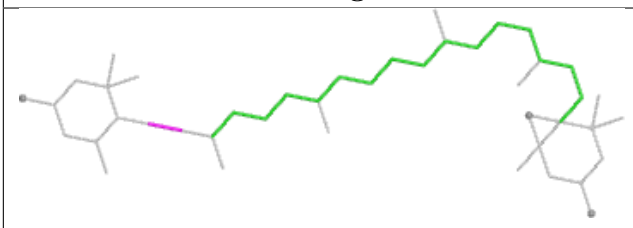
Ligand DD6 W 416



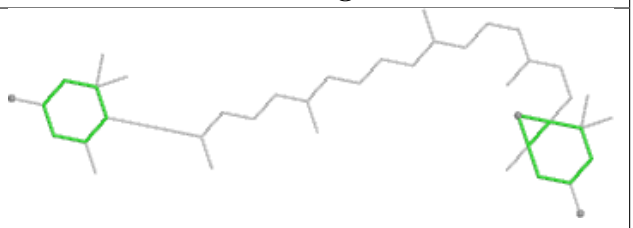
Bond lengths



Bond angles

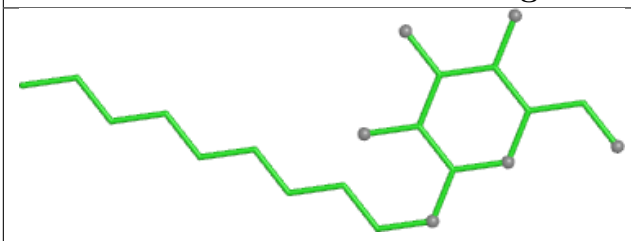


Torsions

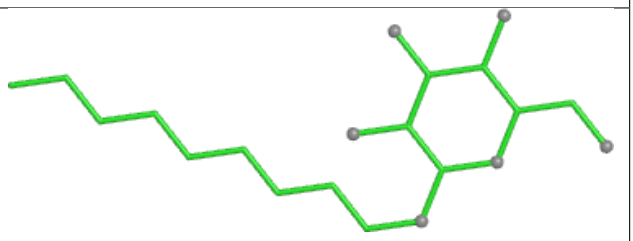


Rings

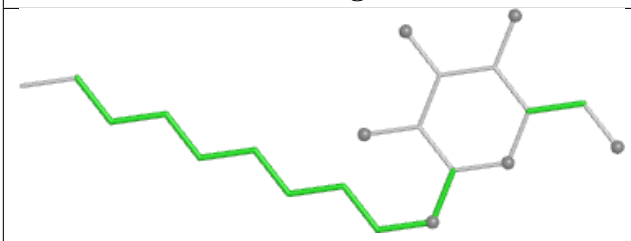
Ligand LMU T 615



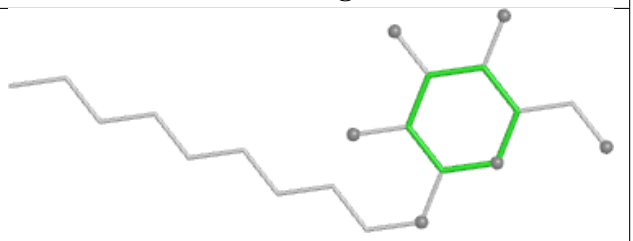
Bond lengths



Bond angles

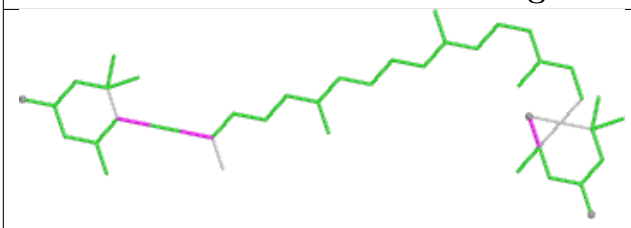


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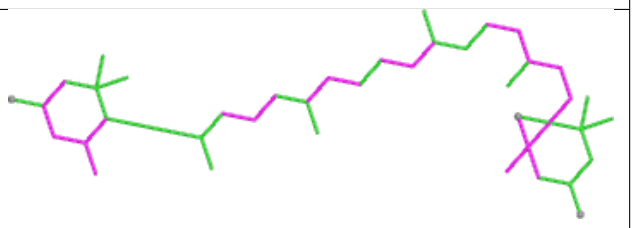


Rings

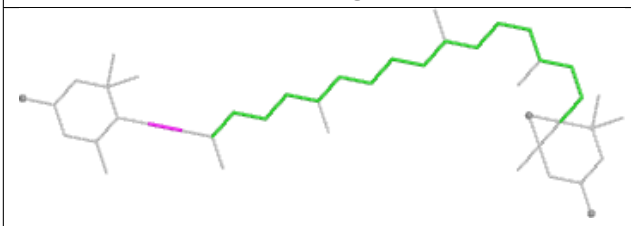
Ligand DD6 S 612



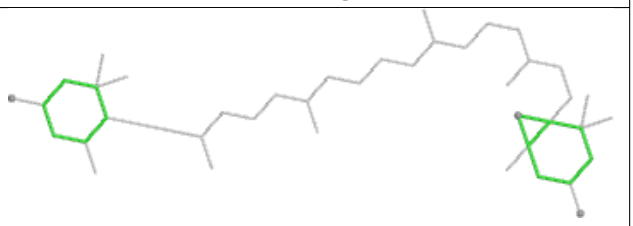
Bond lengths



Bond angles

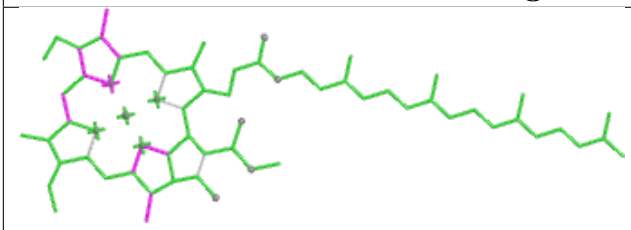


Torsions

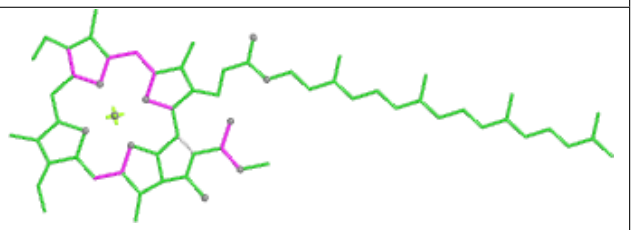


Rings

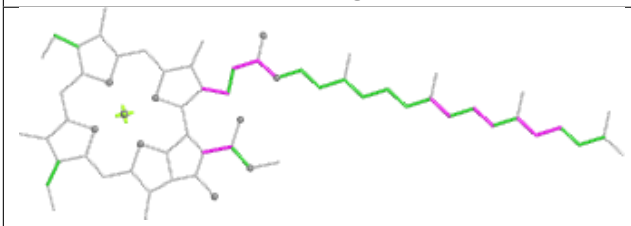
Ligand CLA B 816



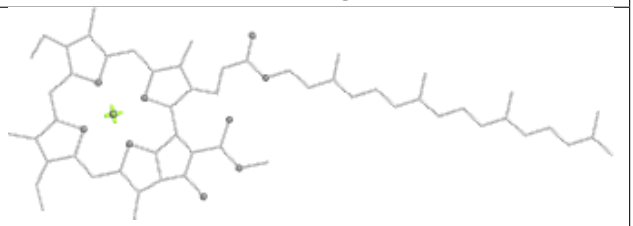
Bond lengths



Bond angles

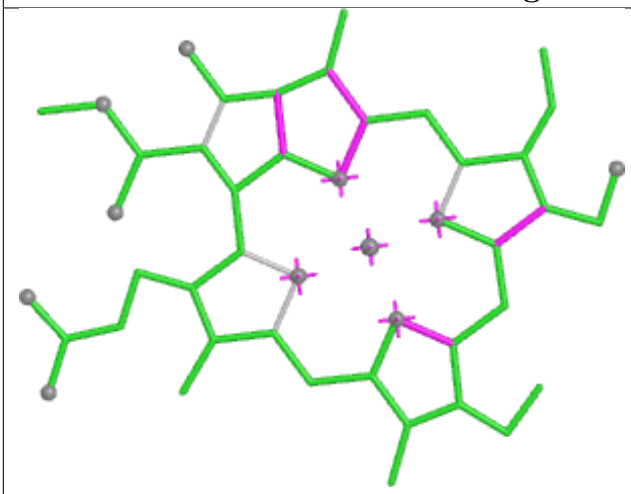


Torsions

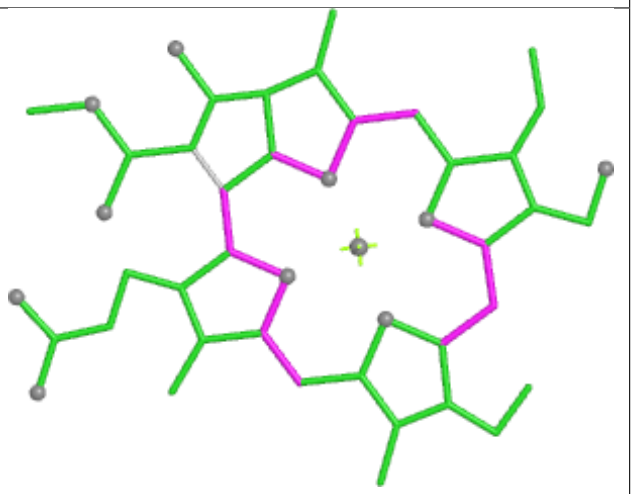


Rings

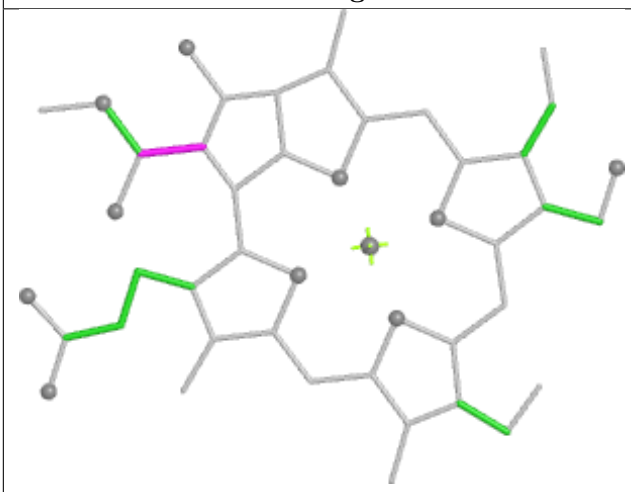
Ligand CHL U 408



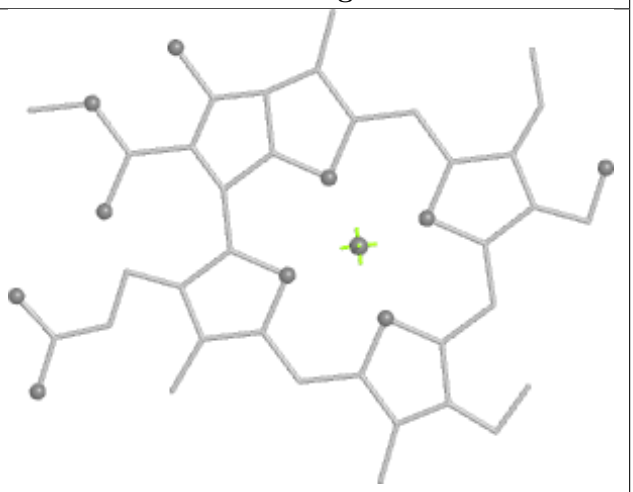
Bond lengths



Bond angles

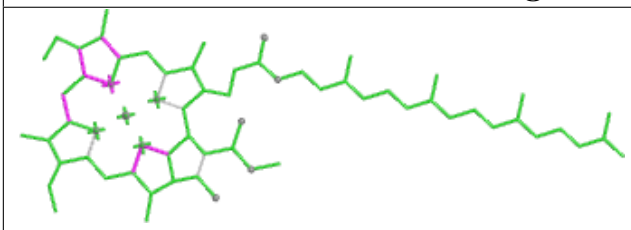


Torsions

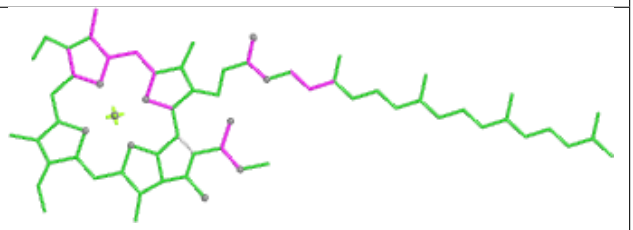


Rings

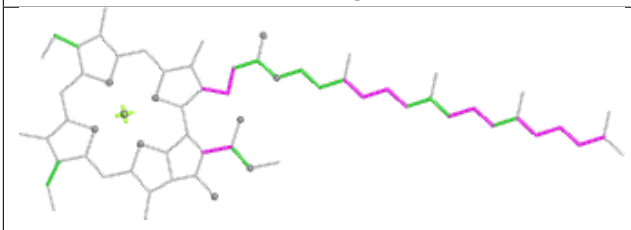
Ligand CLA B 812



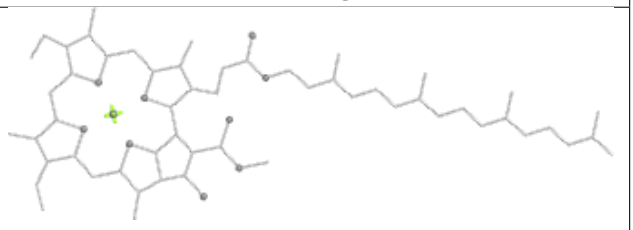
Bond lengths



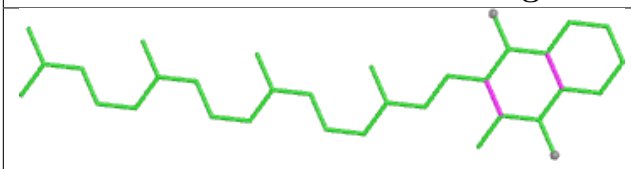
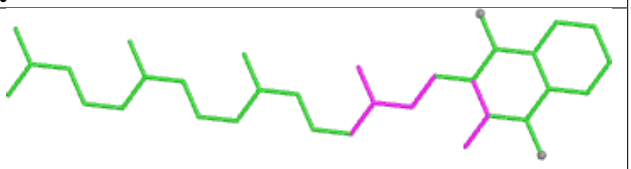
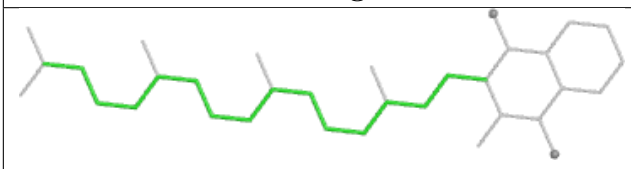
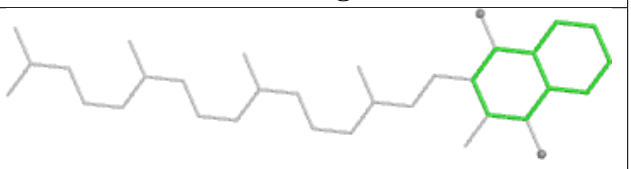
Bond angles

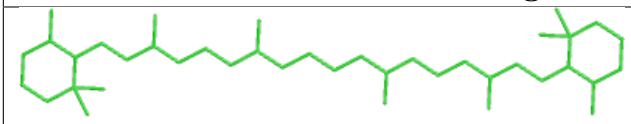
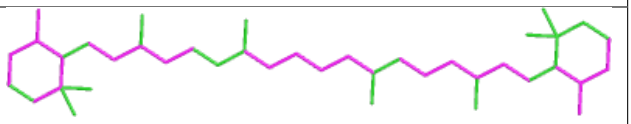
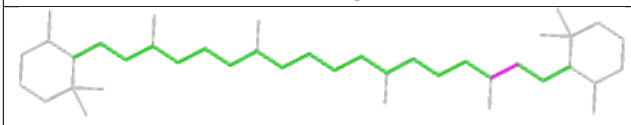
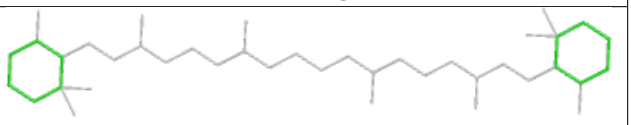


Torsions

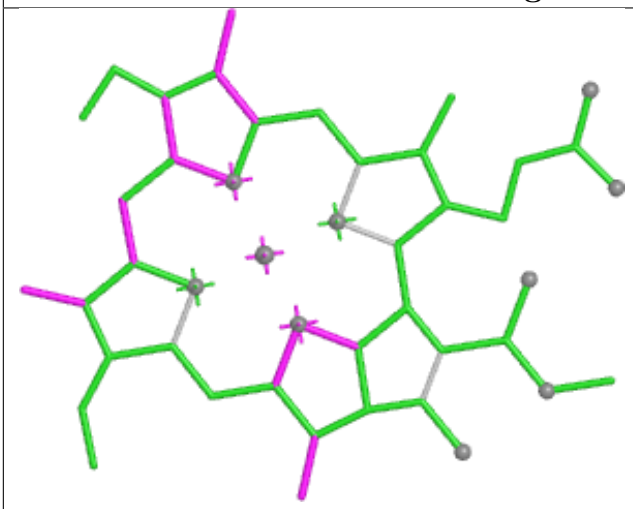


Rings

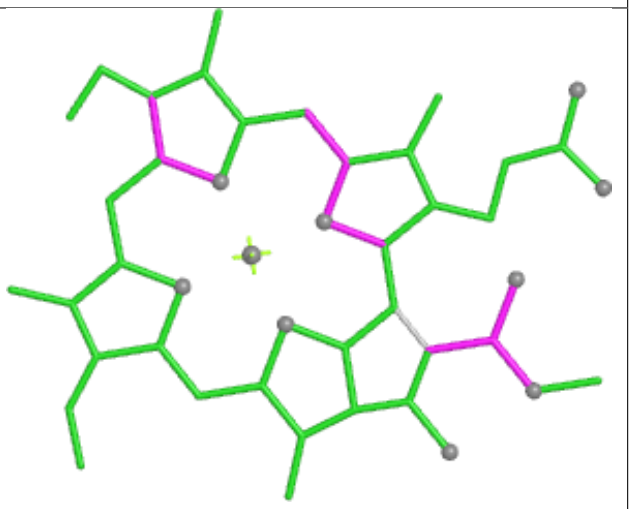
Ligand PQN B 840	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR B 845	
	
Bond lengths	Bond angles
	
Torsions	Rings

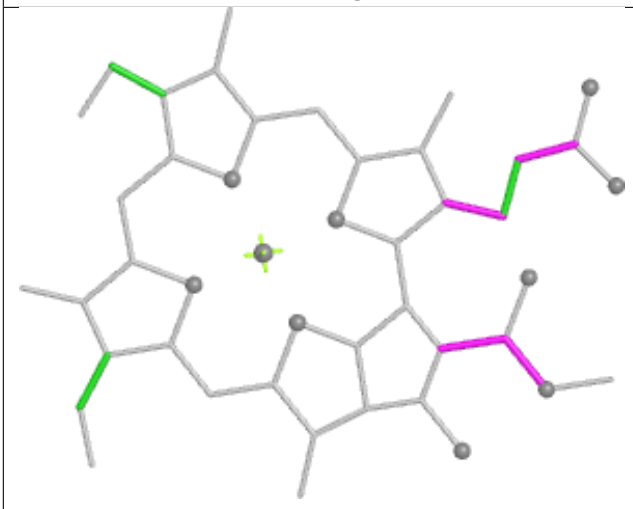
Ligand CLA B 829



Bond lengths



Bond angles

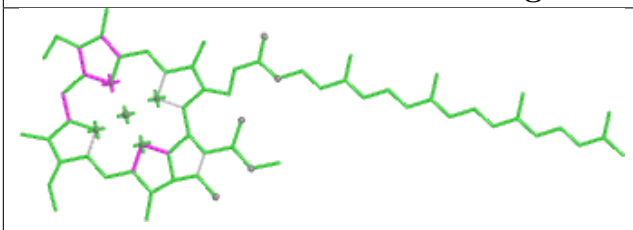


Torsions

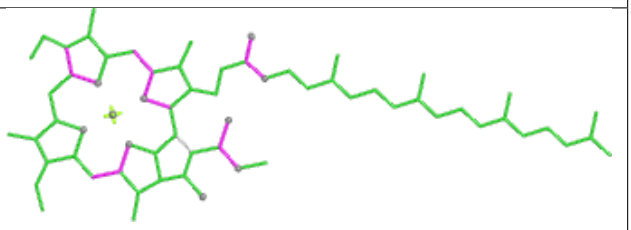


Rings

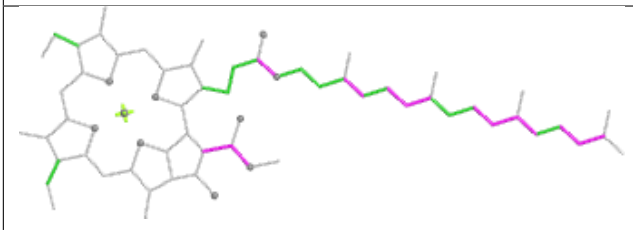
Ligand CLA T 604



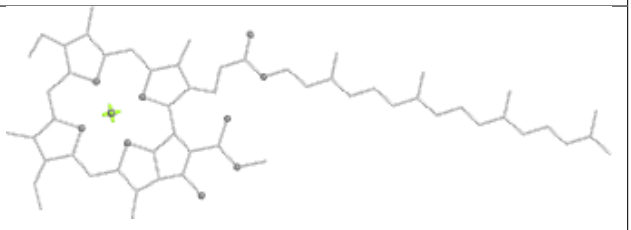
Bond lengths



Bond angles

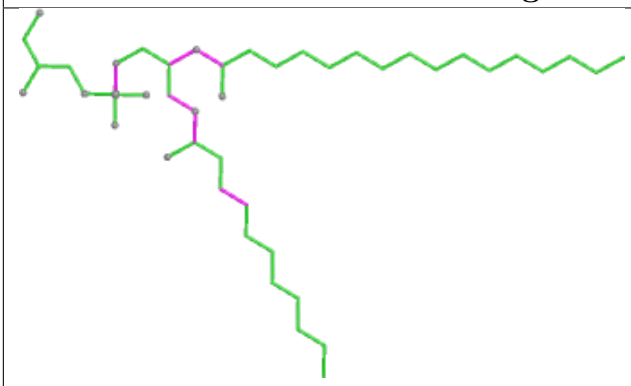


Torsions

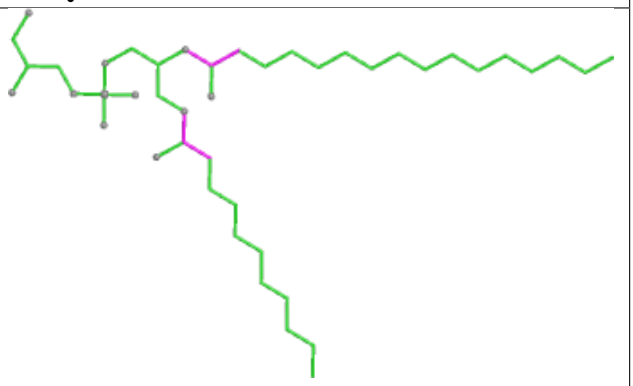


Rings

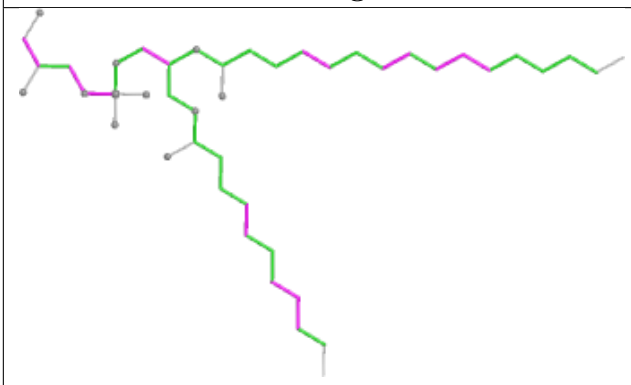
Ligand LHG Q 616



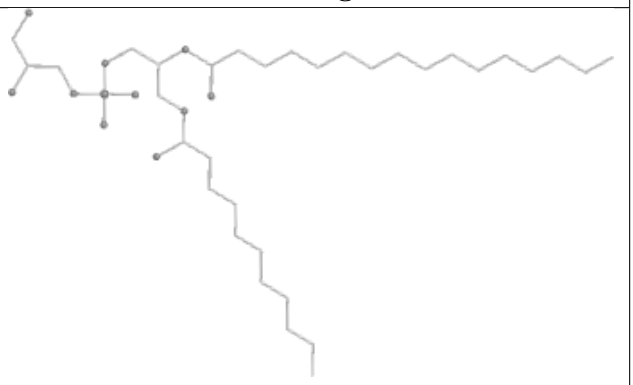
Bond lengths



Bond angles

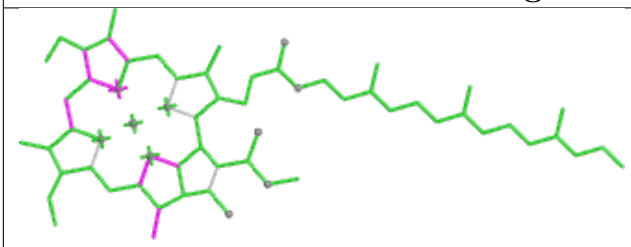


Torsions

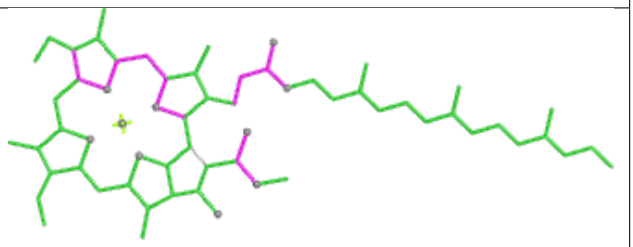


Rings

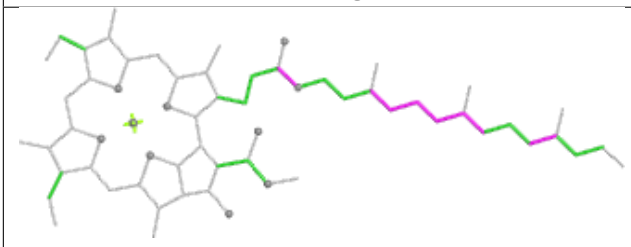
Ligand CLA B 832



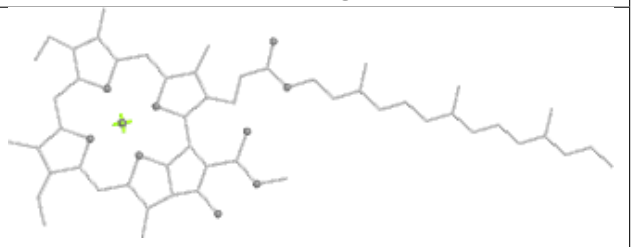
Bond lengths



Bond angles

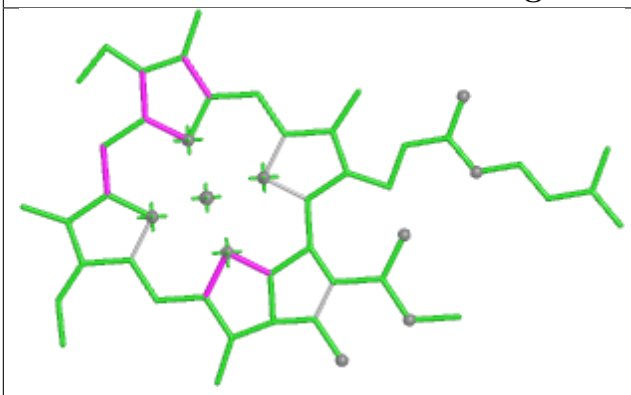


Torsions

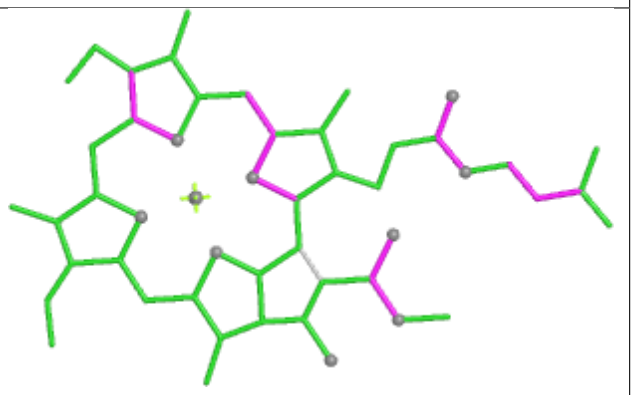


Rings

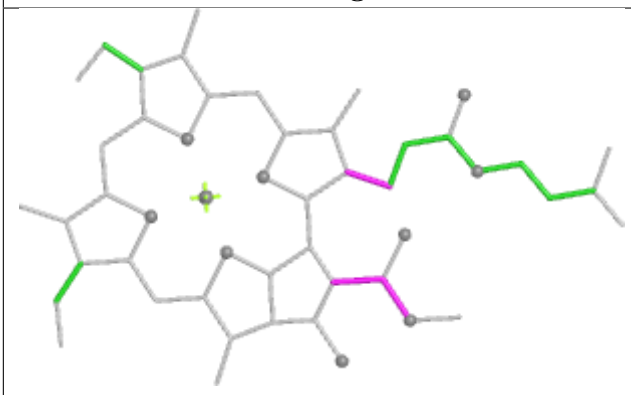
Ligand CLA T 606



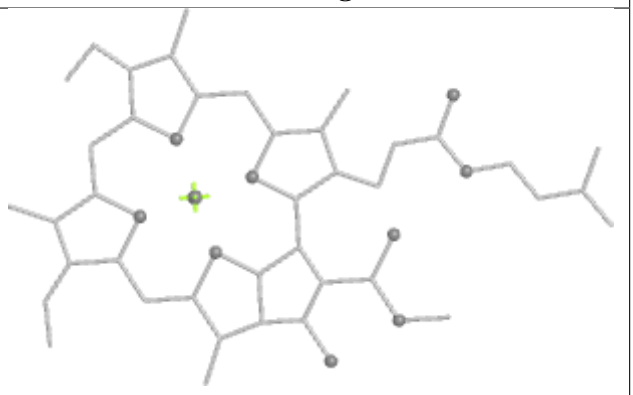
Bond lengths



Bond angles

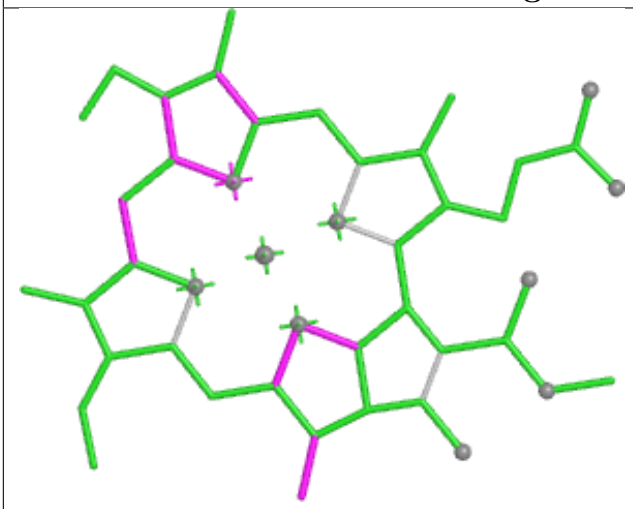


Torsions

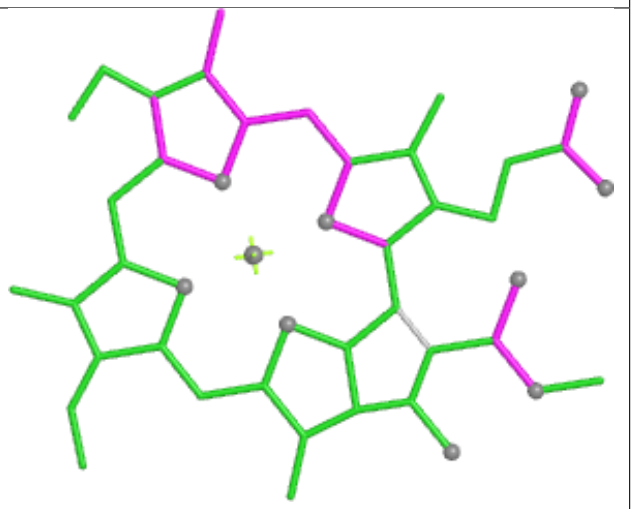


Rings

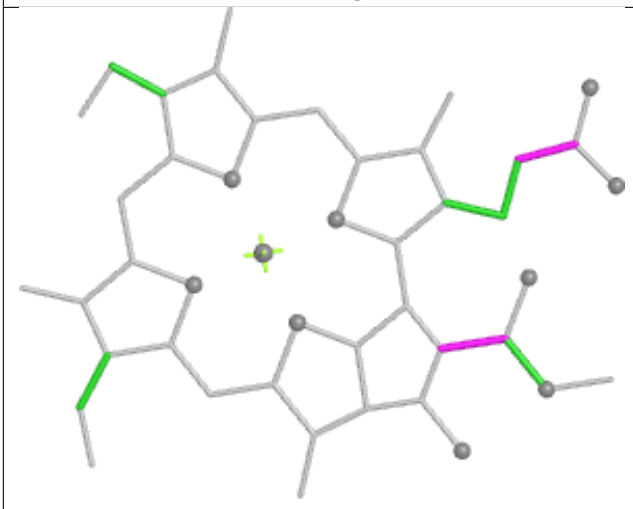
Ligand CLA X 411



Bond lengths



Bond angles

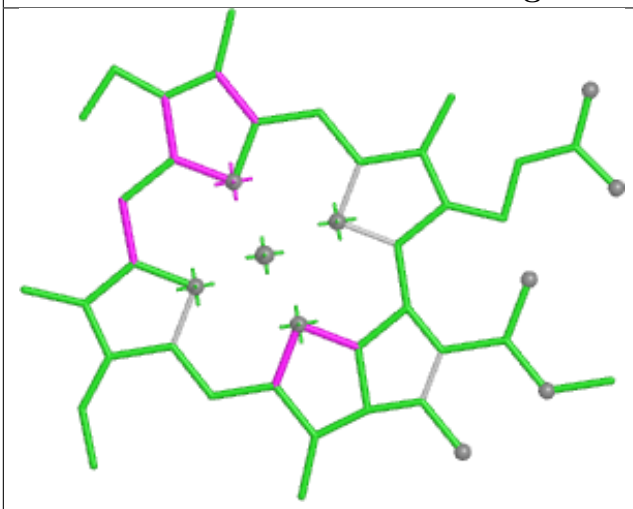


Torsions

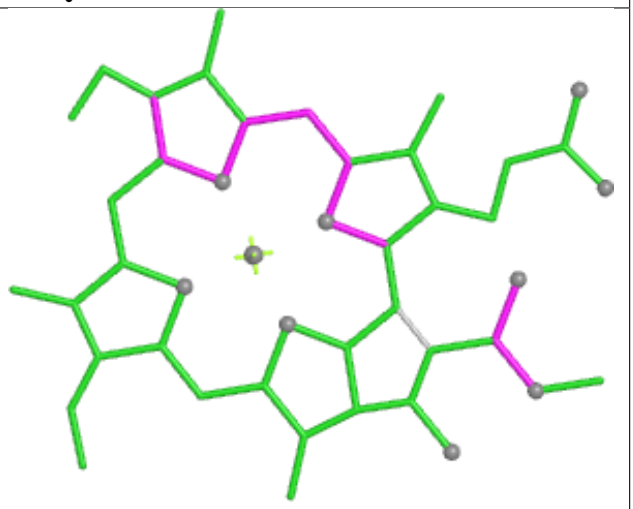


Rings

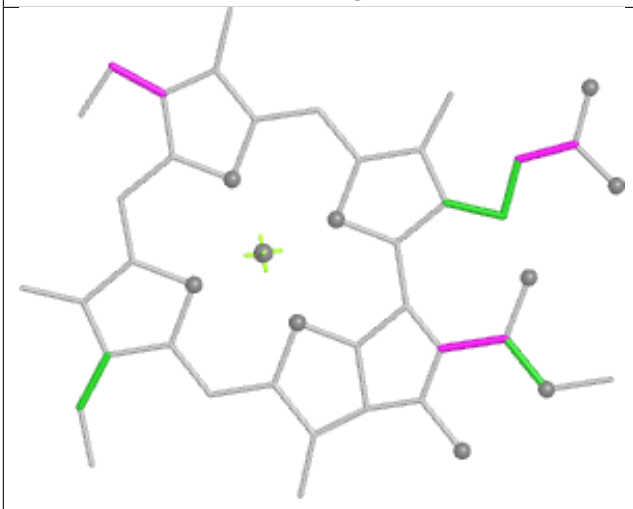
Ligand CLA Q 607



Bond lengths



Bond angles

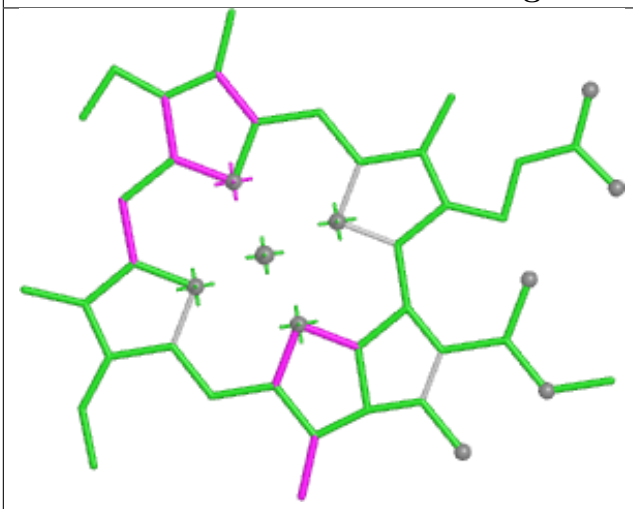


Torsions

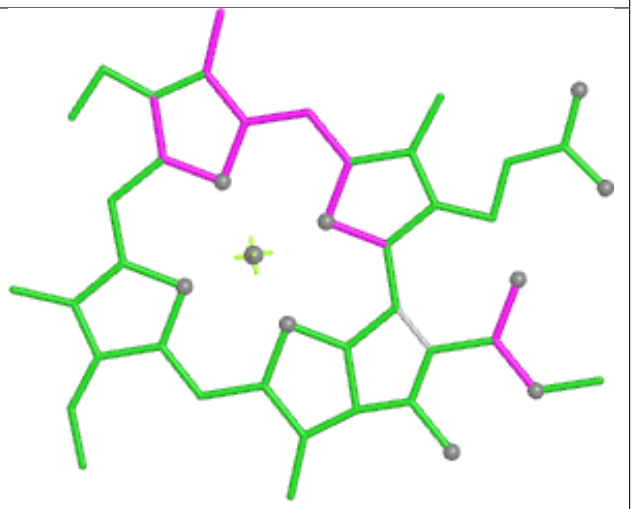


Rings

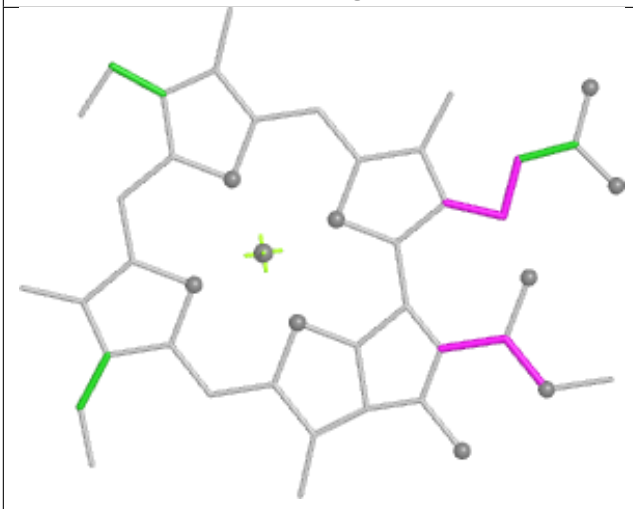
Ligand CLA U 409



Bond lengths



Bond angles

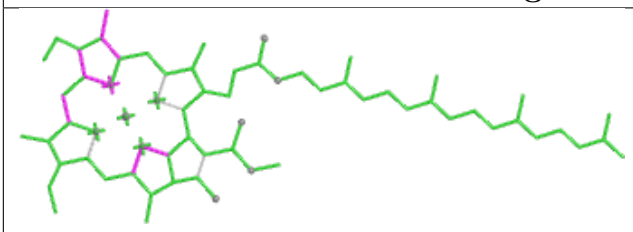


Torsions

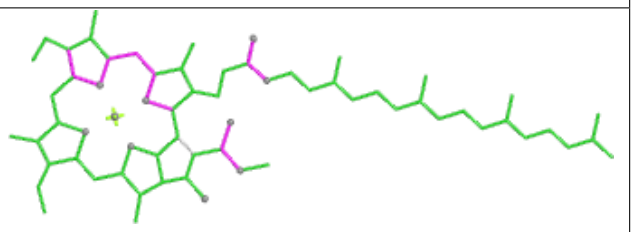


Rings

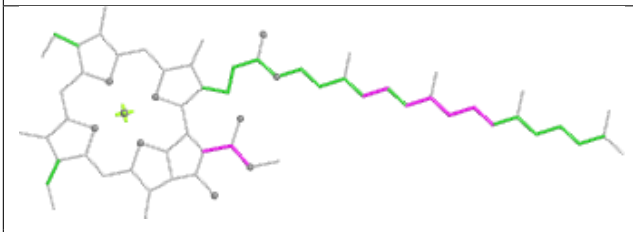
Ligand CLA B 813



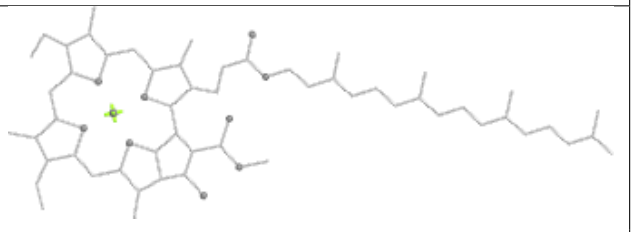
Bond lengths



Bond angles

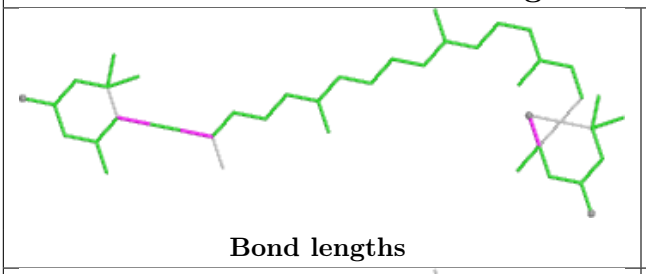


Torsions

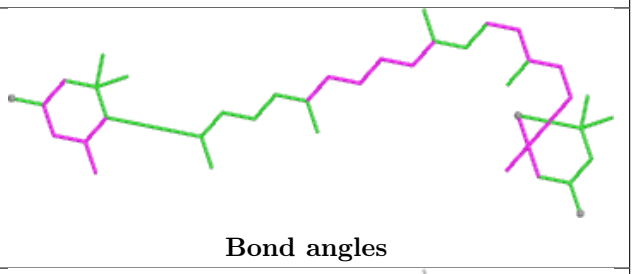


Rings

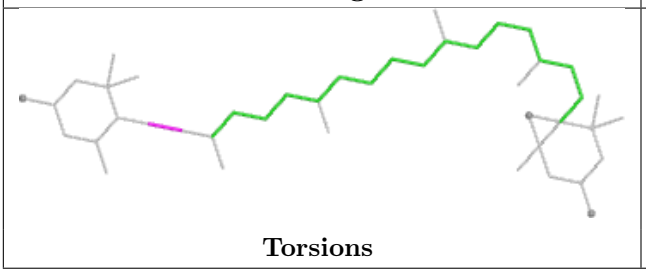
Ligand DD6 V 614



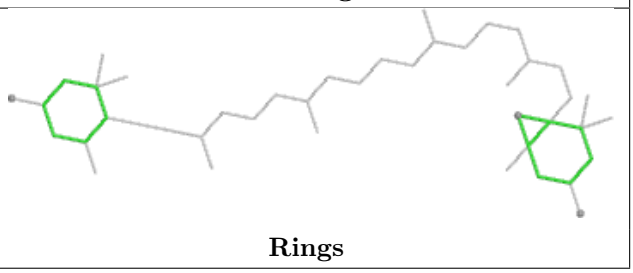
Bond lengths



Bond angles

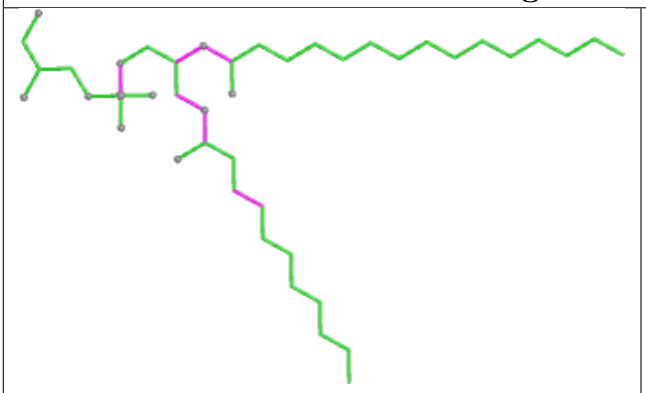


Torsions

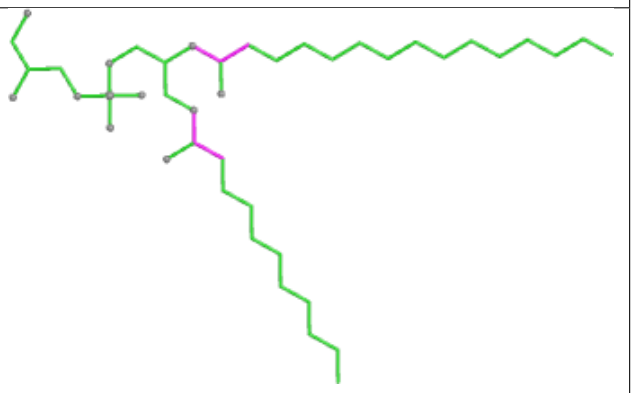


Rings

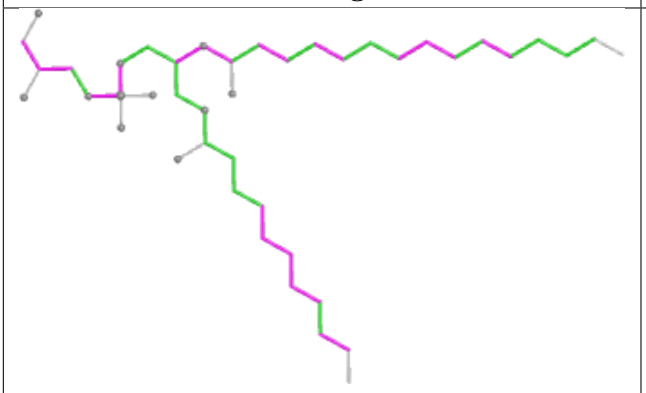
Ligand LHG N 616



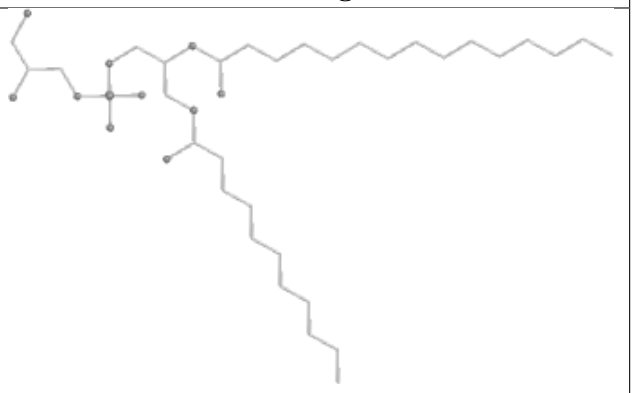
Bond lengths



Bond angles

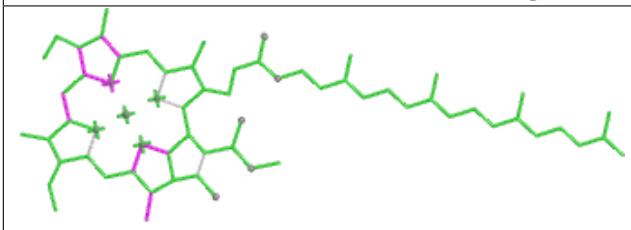


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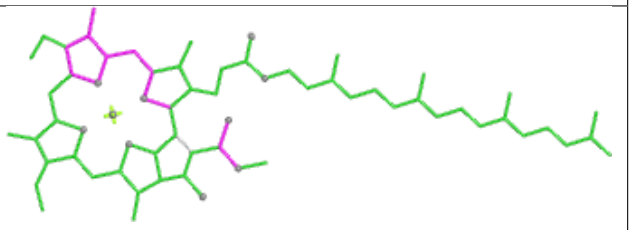


Rings

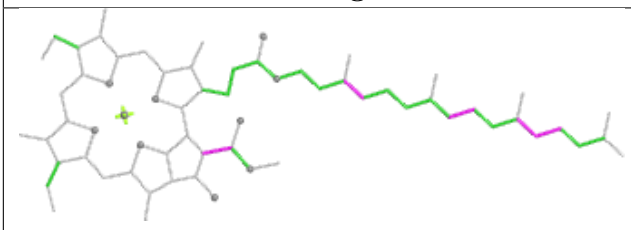
Ligand CLA B 834



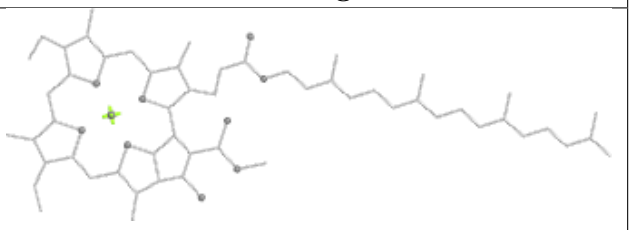
Bond lengths



Bond angles

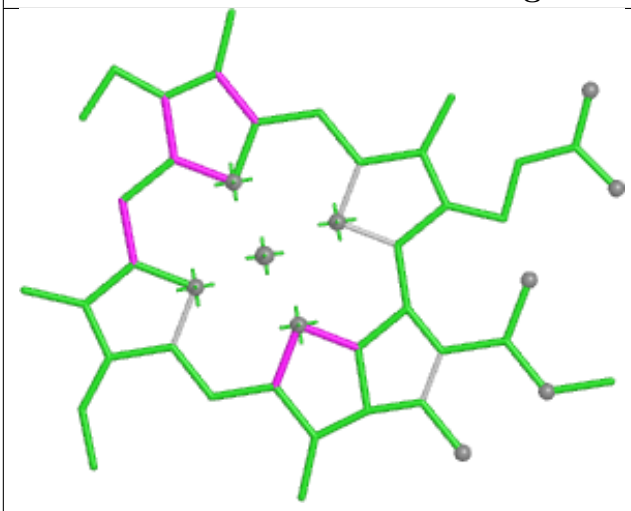


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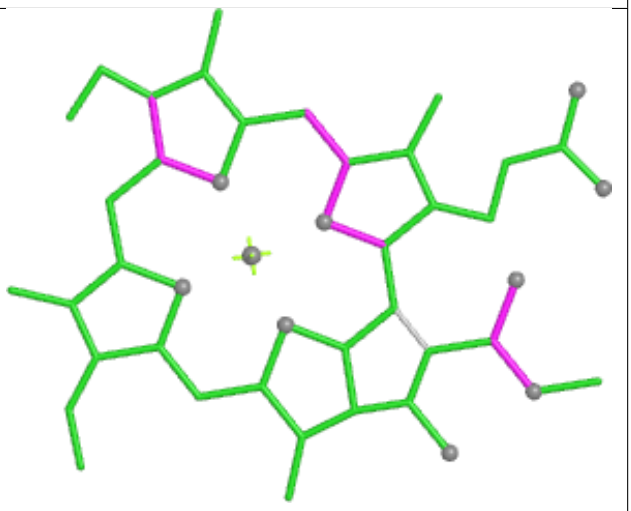


Rings

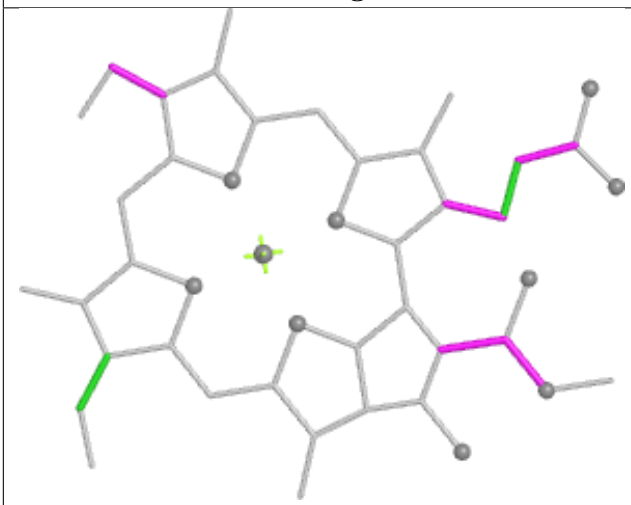
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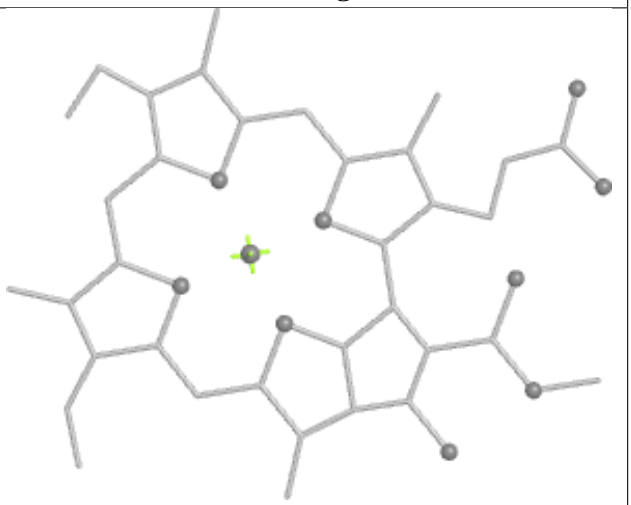
Bond lengths



Bond angles

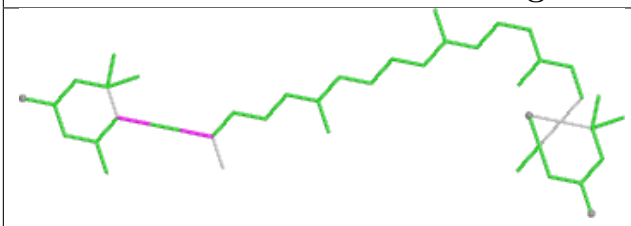


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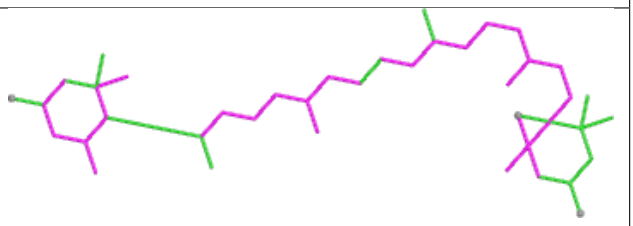


Rings

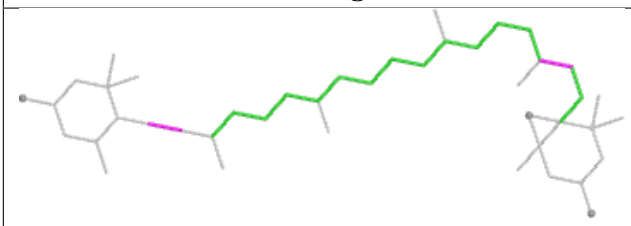
Ligand DD6 L 415



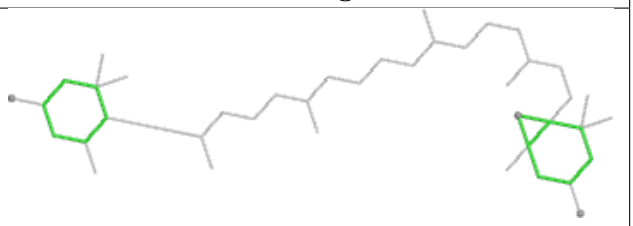
Bond lengths



Bond angles

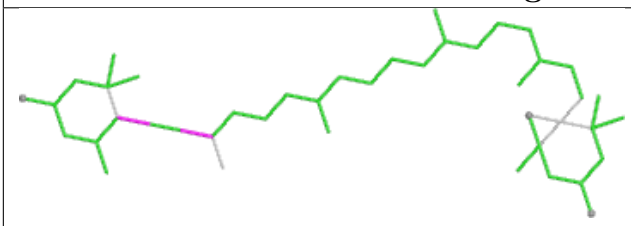


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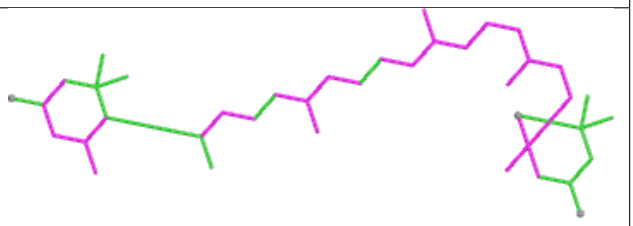


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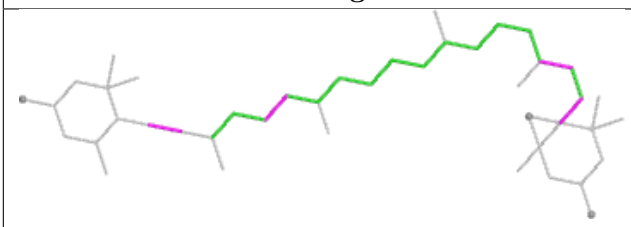
Ligand DD6 A 858



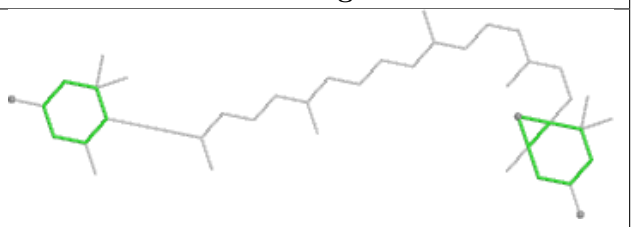
Bond lengths



Bond angles

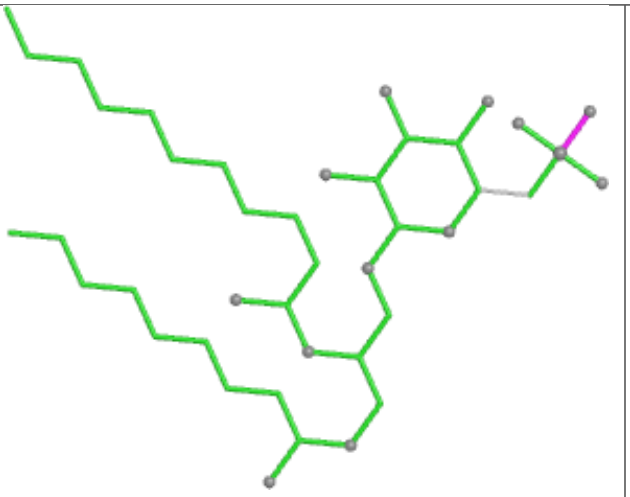


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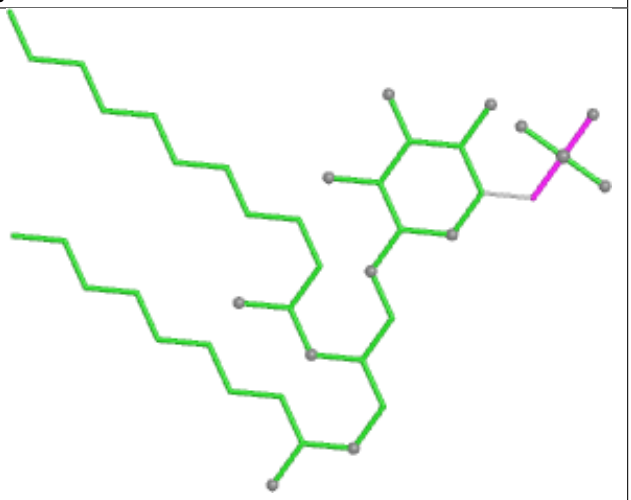


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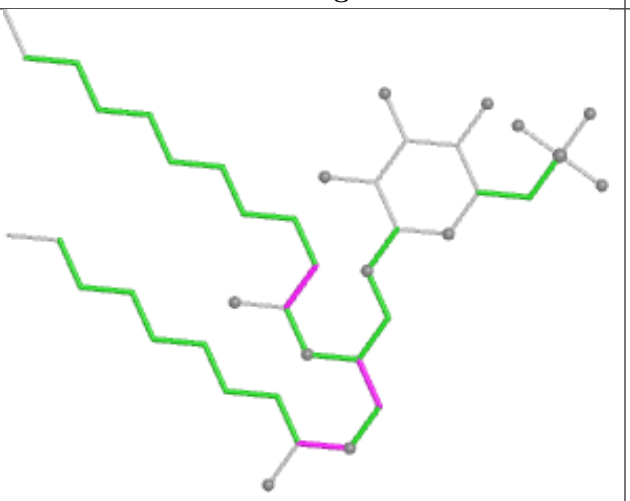
Ligand SQD O 302



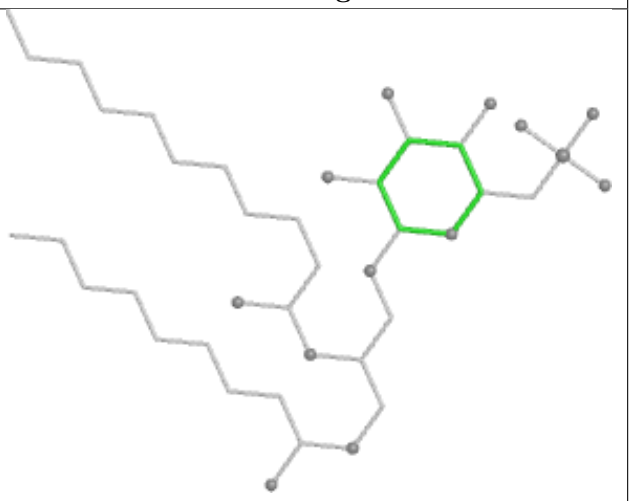
Bond lengths



Bond angles

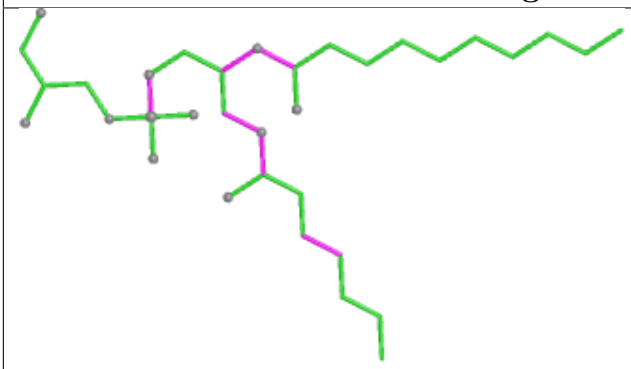


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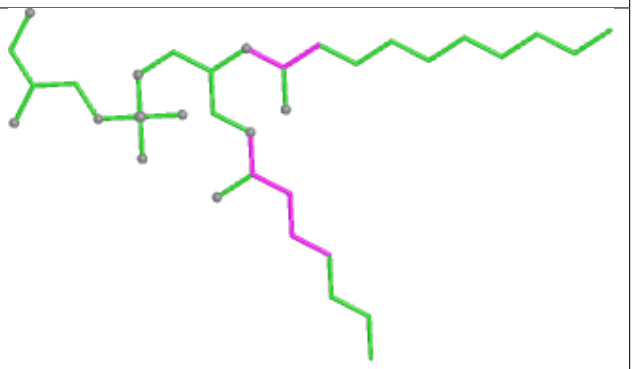


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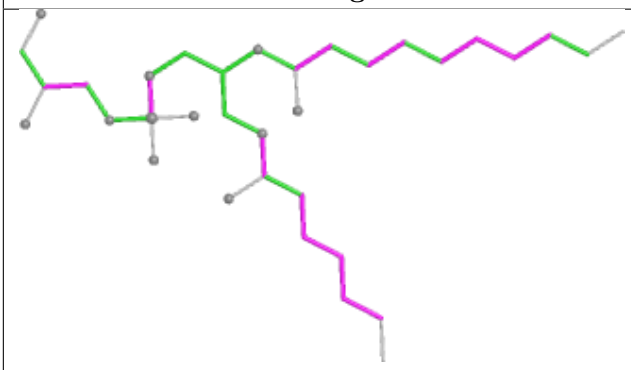
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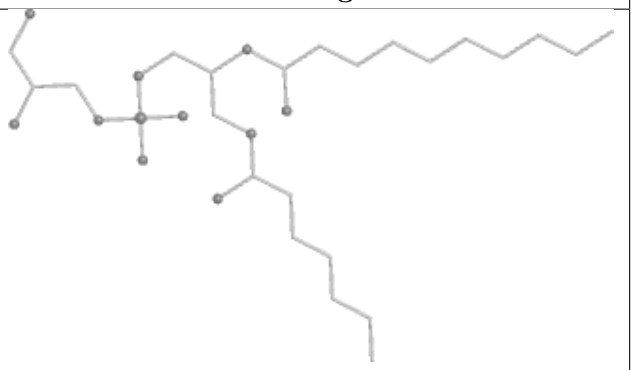
Bond lengths



Bond angles

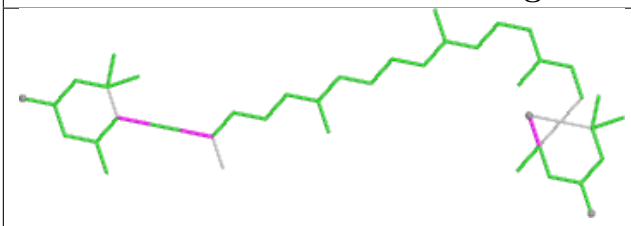


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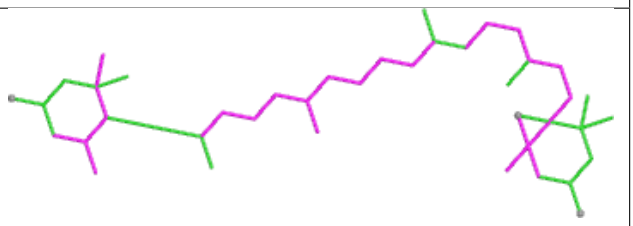


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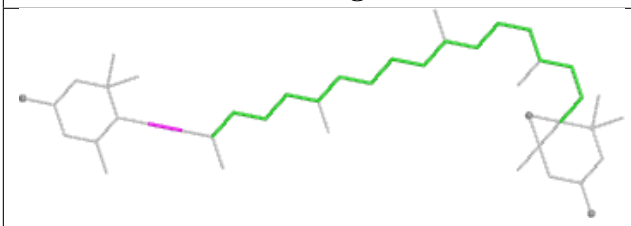
Ligand DD6 G 613



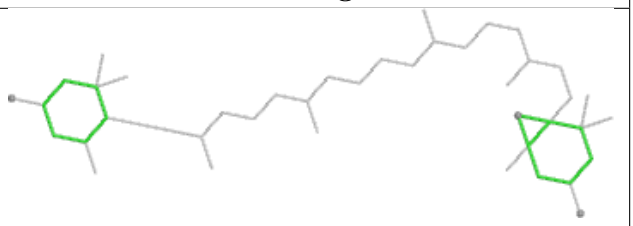
Bond lengths



Bond angles

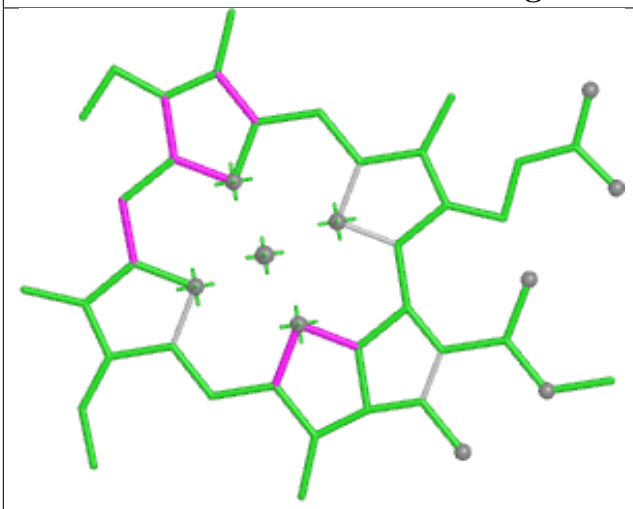


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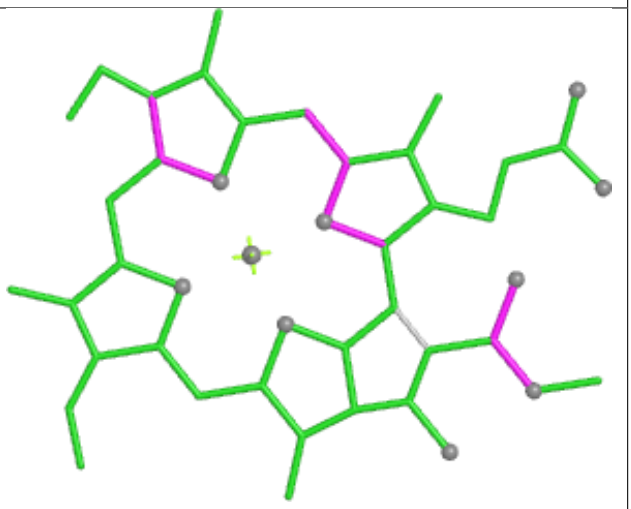


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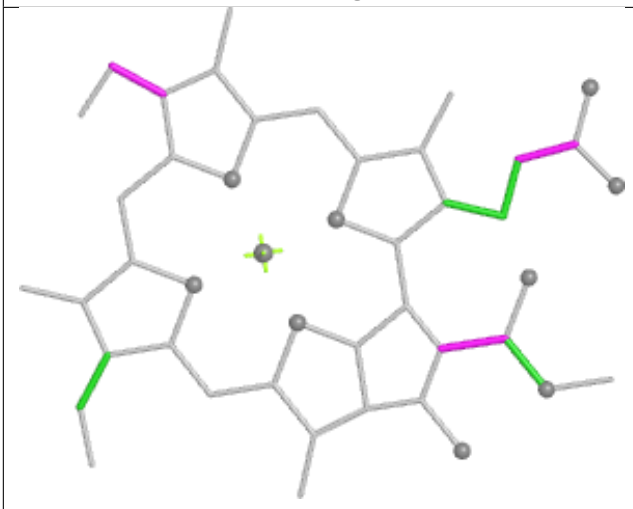
Ligand CLA T 610



Bond lengths



Bond angles

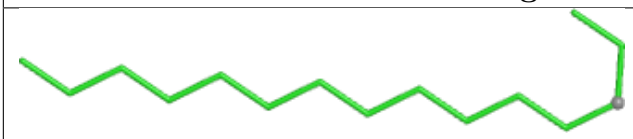


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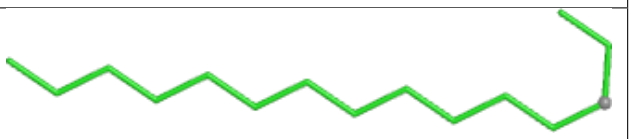


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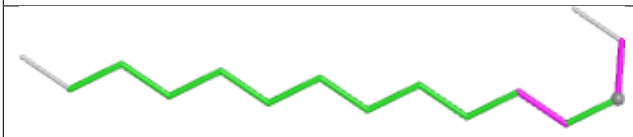
Ligand LMU B 858



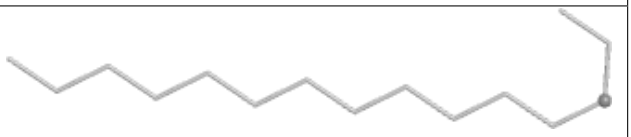
Bond lengths



Bond angles

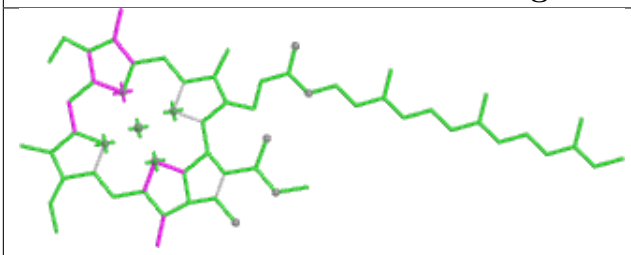


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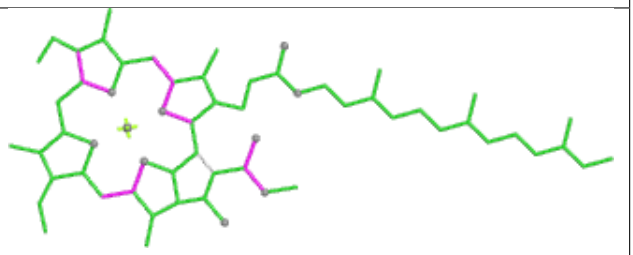


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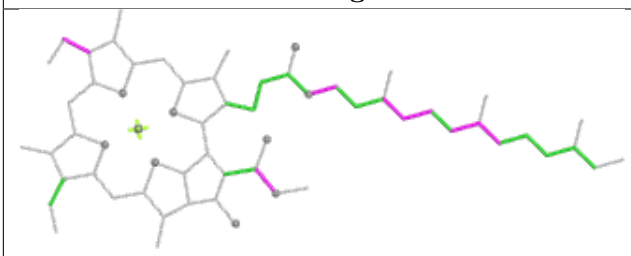
Ligand CLA I 606



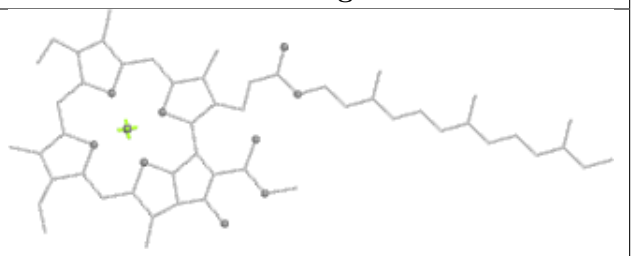
Bond lengths



Bond angles

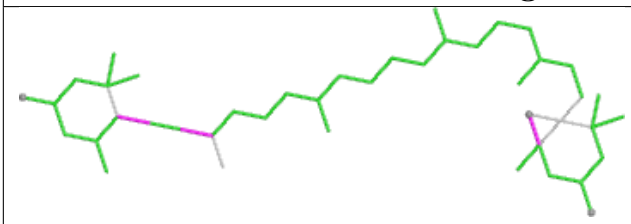


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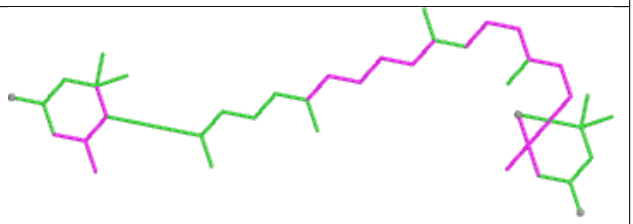


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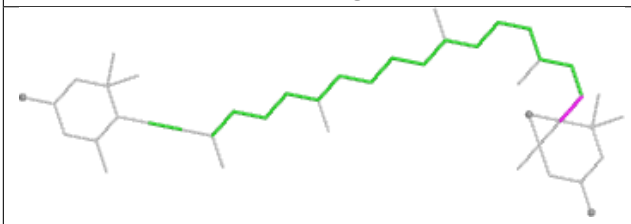
Ligand DD6 W 418



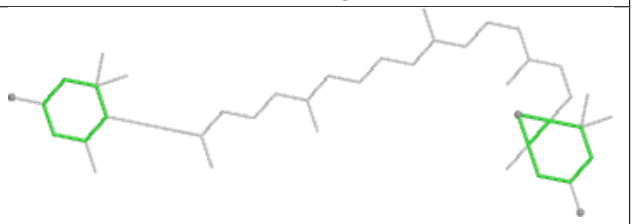
Bond lengths



Bond angles

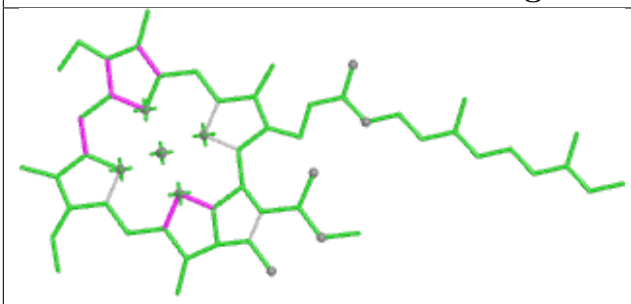


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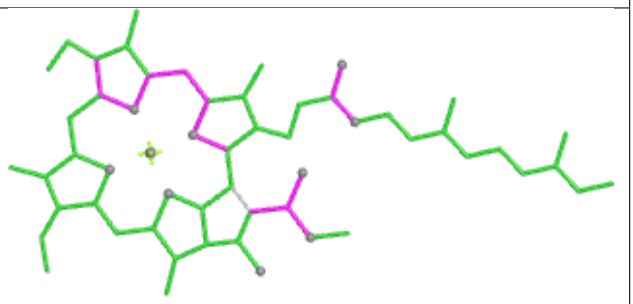


Rings

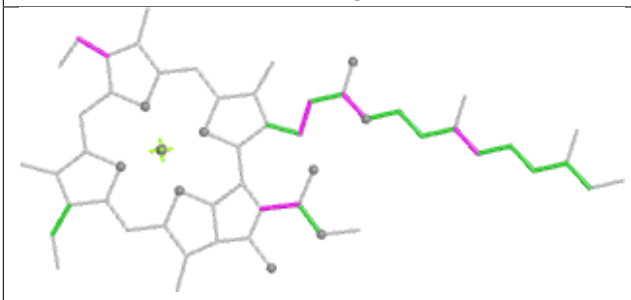
Ligand CLA B 803



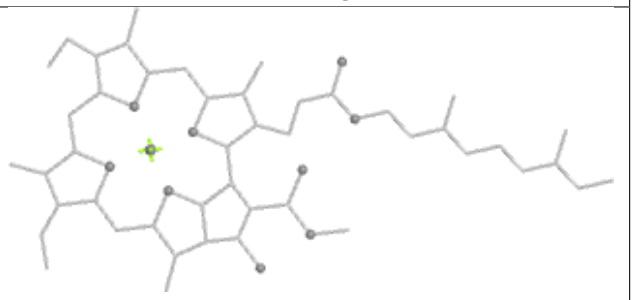
Bond lengths



Bond angles

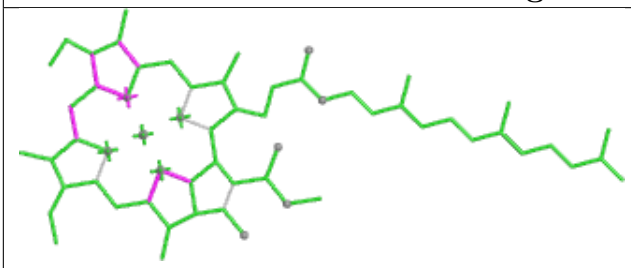


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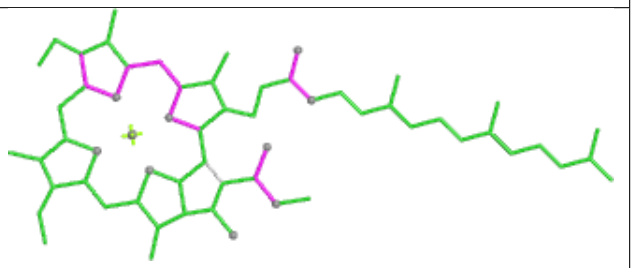


Rings

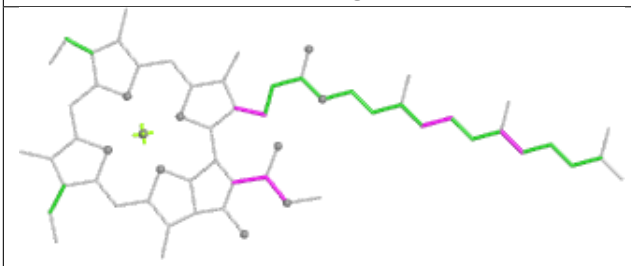
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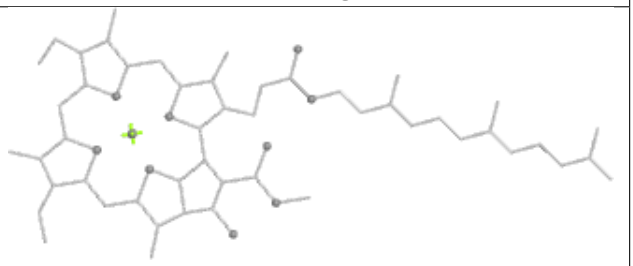
Bond lengths



Bond angles

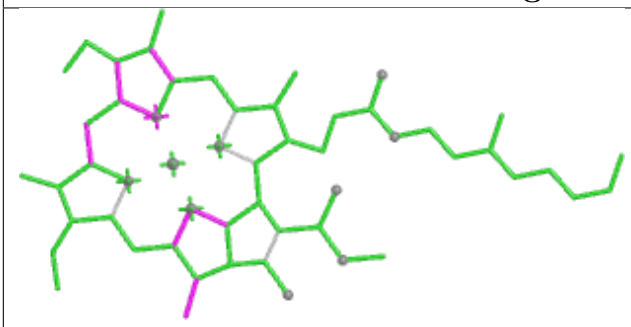


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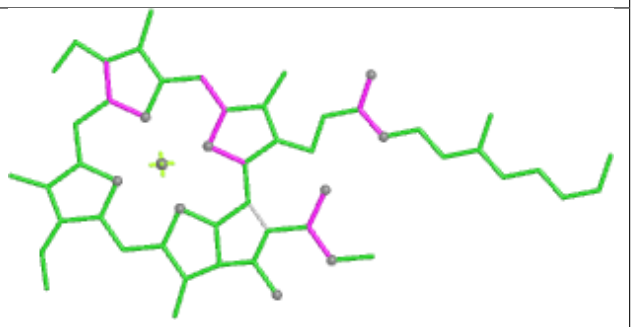


Rings

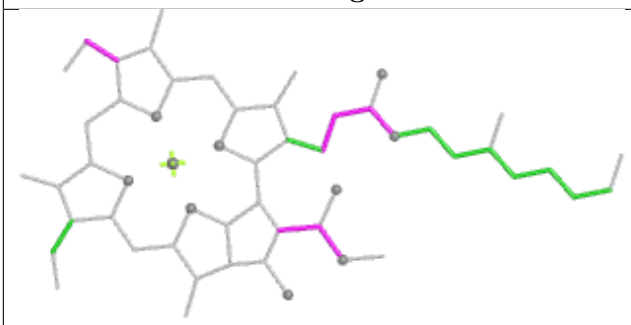
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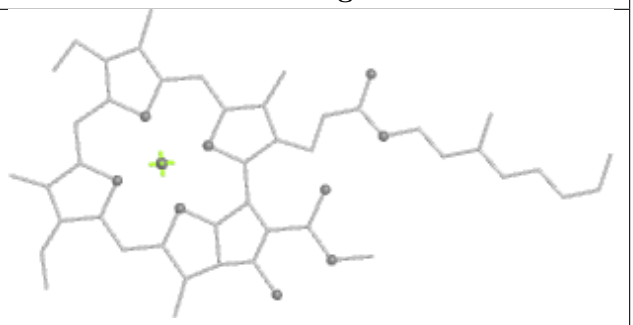
Bond lengths



Bond angles

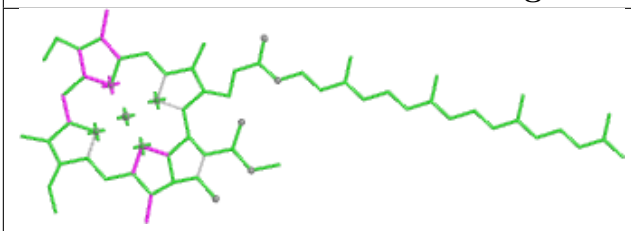


Torsions

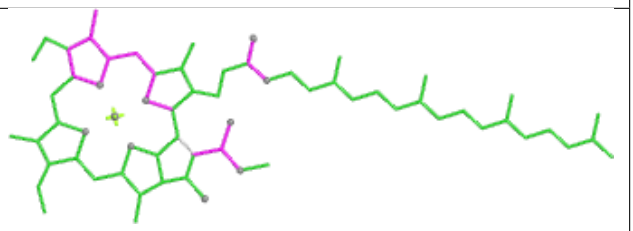


Rings

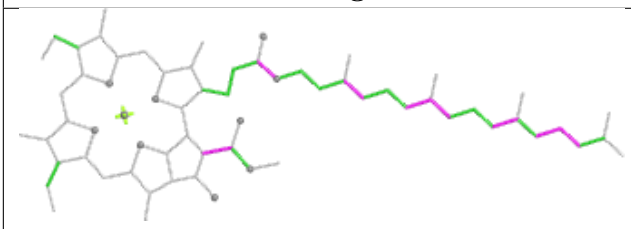
Ligand CLA B 828



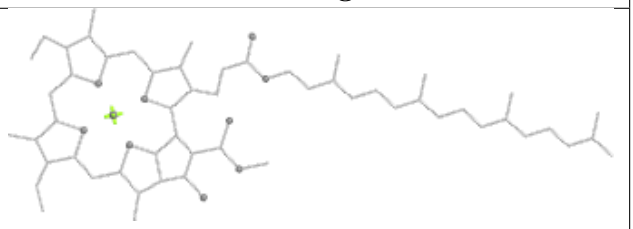
Bond lengths



Bond angles

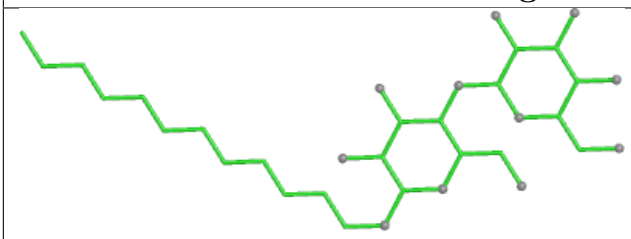


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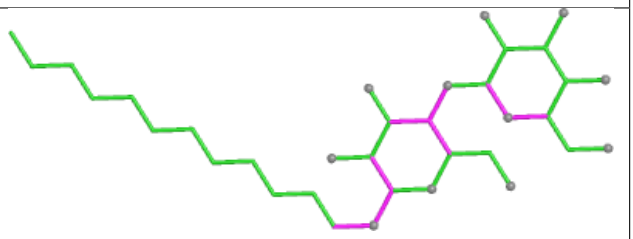


Rings

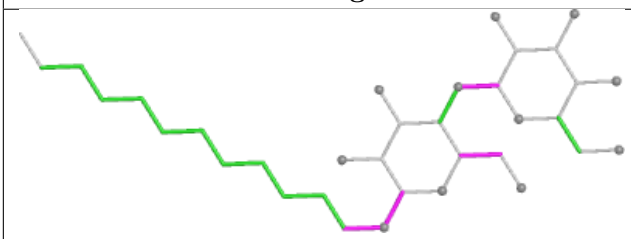
Ligand LMU O 322



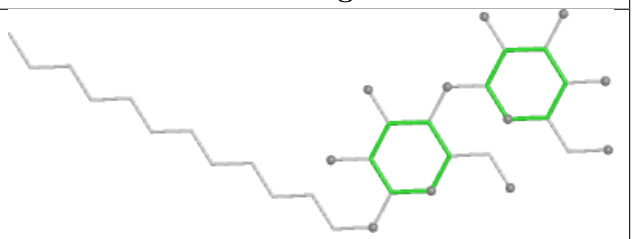
Bond lengths



Bond angles

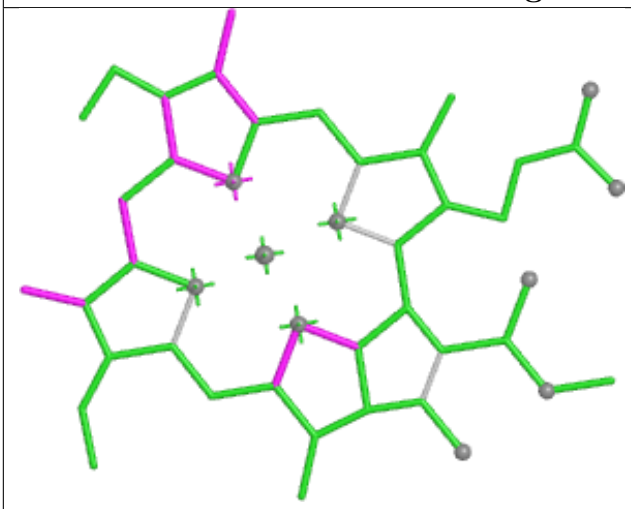


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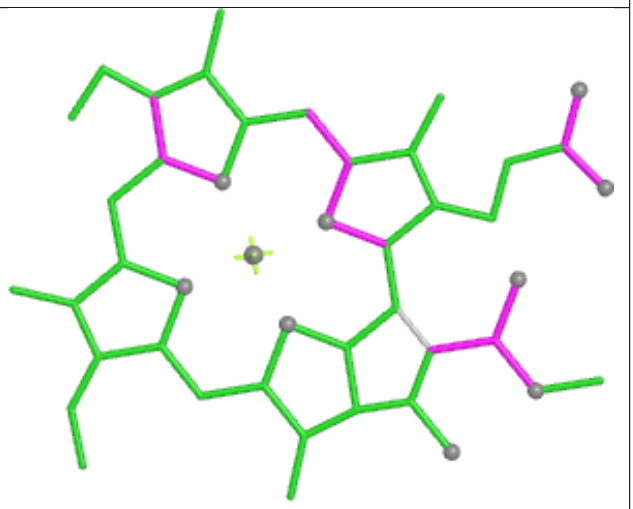


Rings

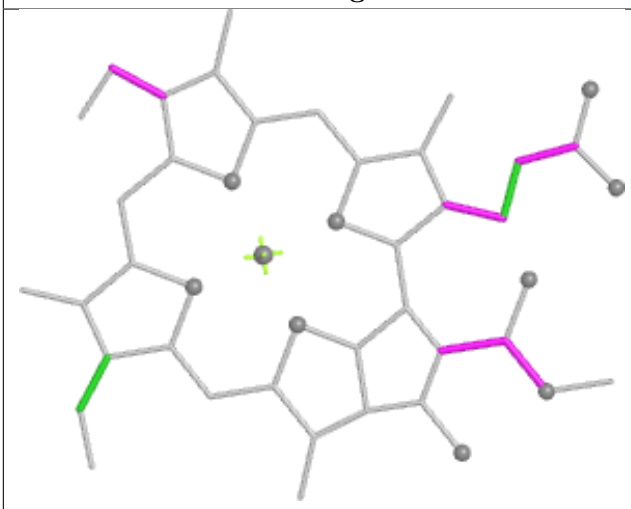
Ligand CLA P 608



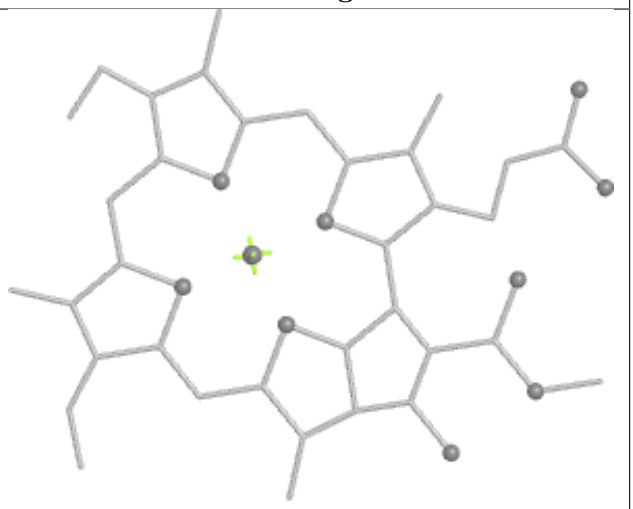
Bond lengths



Bond angles

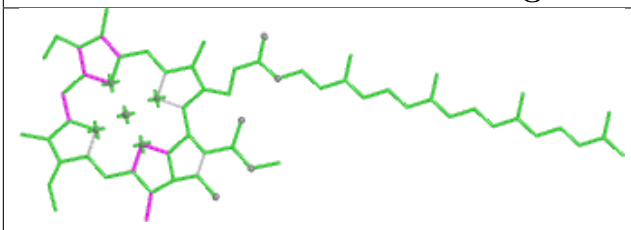


Torsions

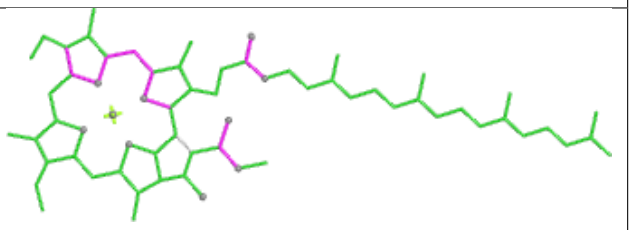


Rings

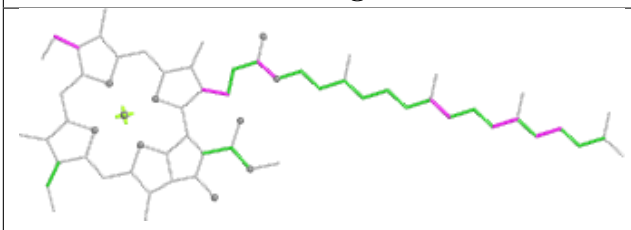
Ligand CLA A 813



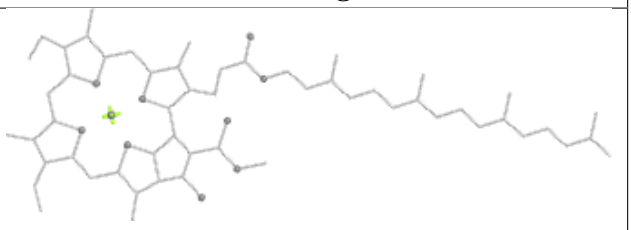
Bond lengths



Bond angles

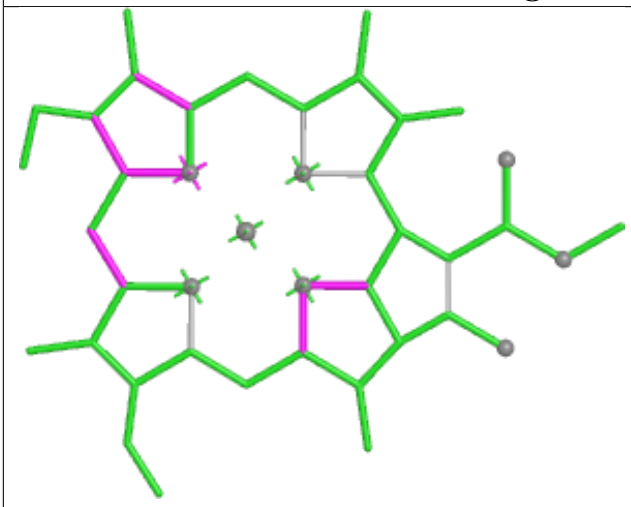


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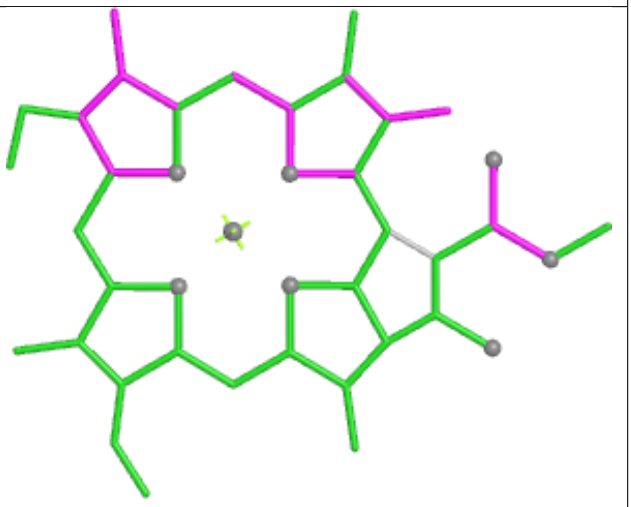


Rings

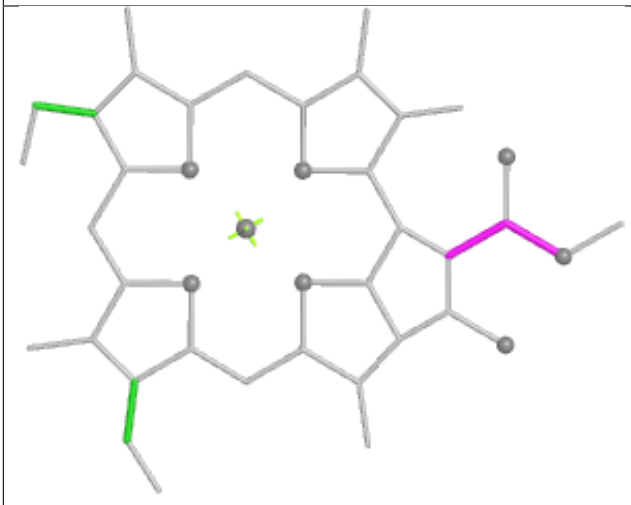
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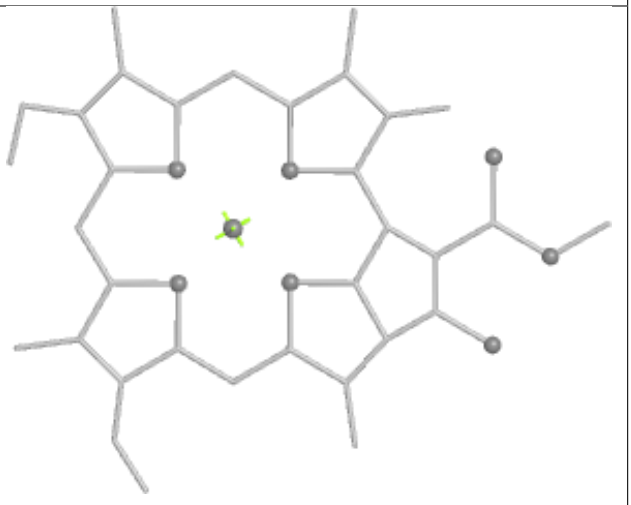
Bond lengths



Bond angles

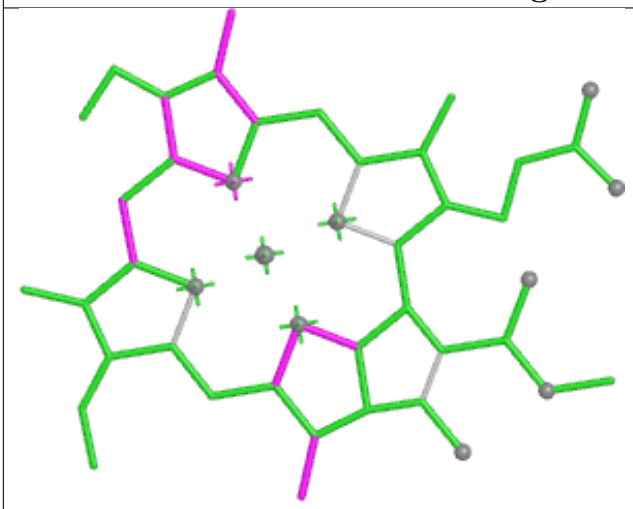


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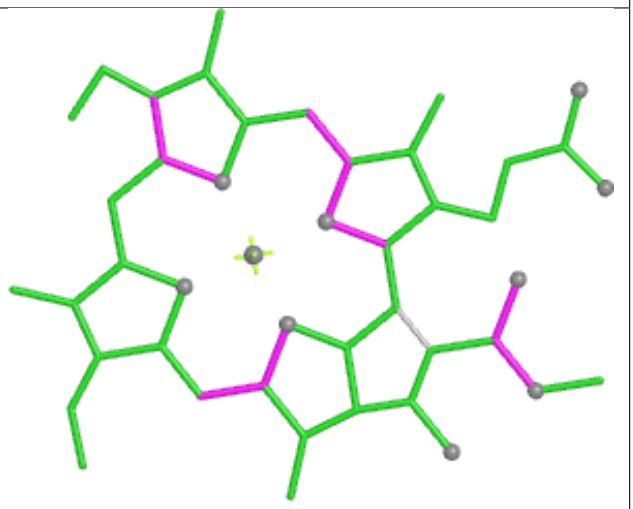


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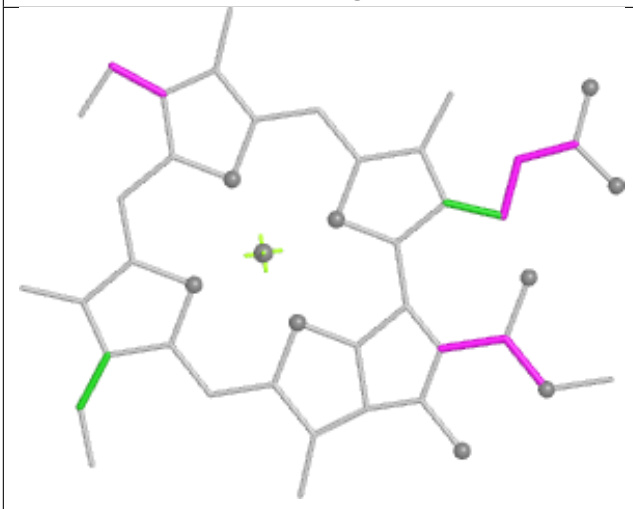
Ligand CLA I 610



Bond lengths



Bond angles

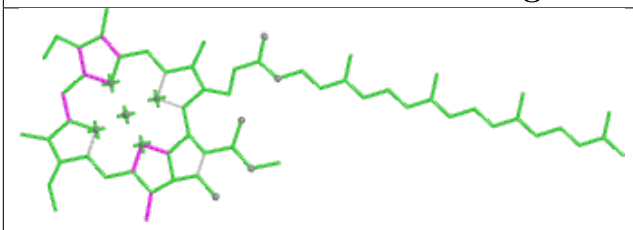


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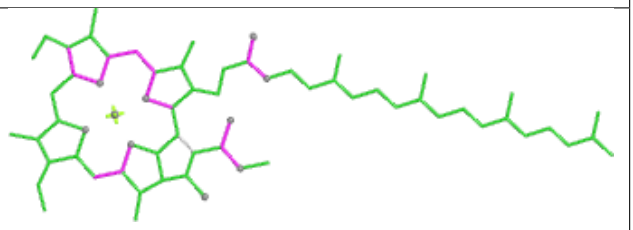


Rings

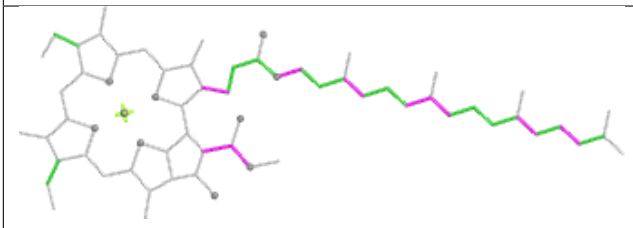
Ligand CLA N 606



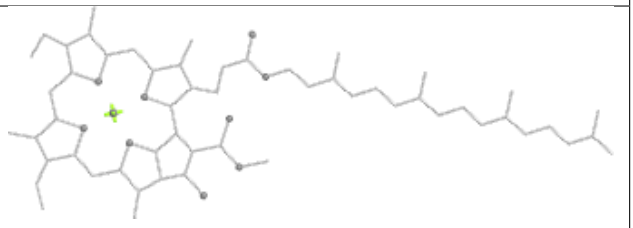
Bond lengths



Bond angles

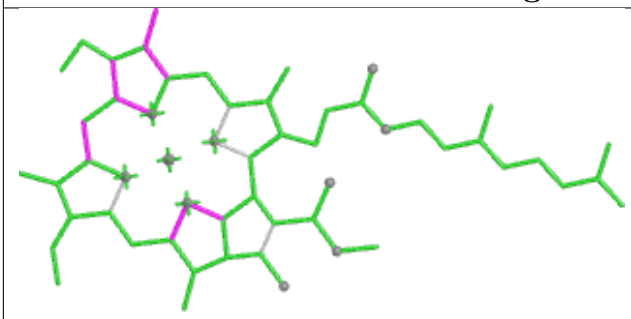


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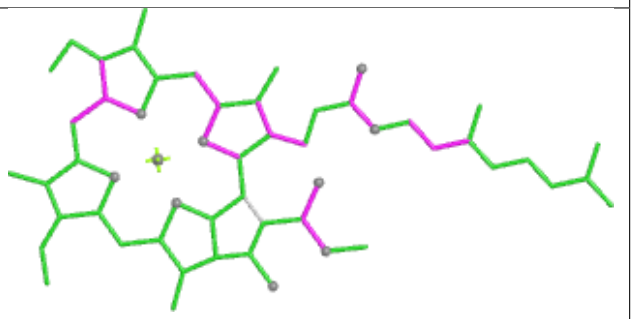


Rings

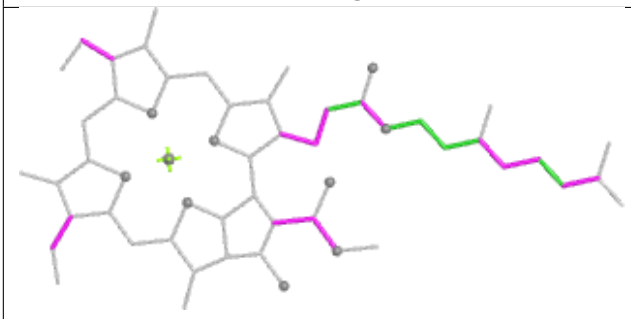
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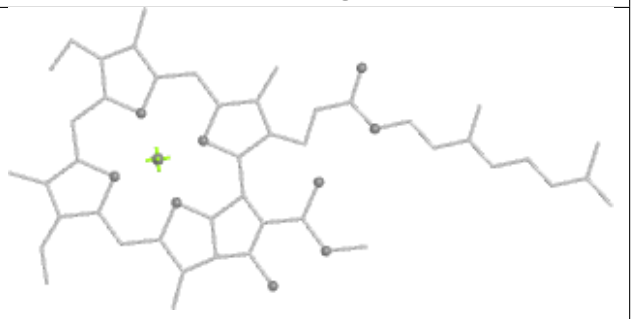
Bond lengths



Bond angles

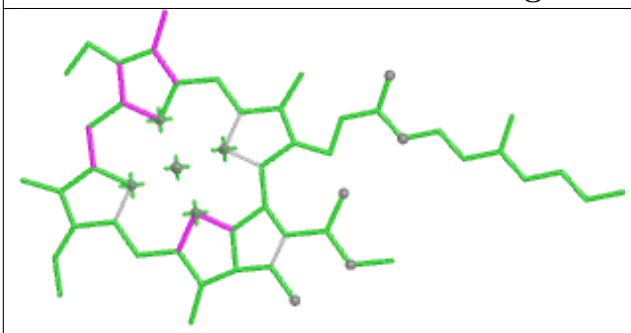


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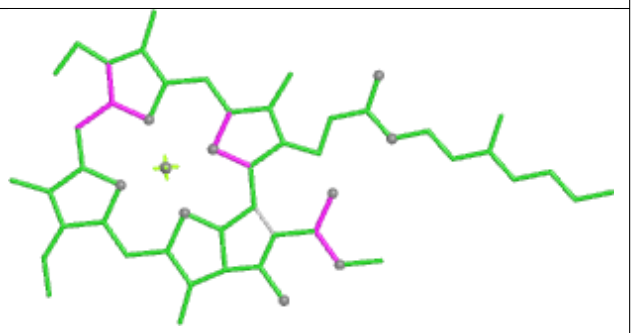


Rings

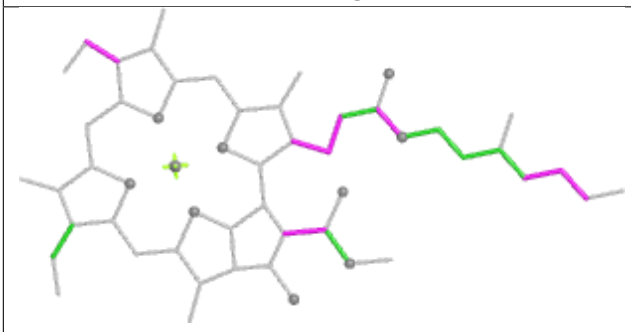
Ligand CLA B 819



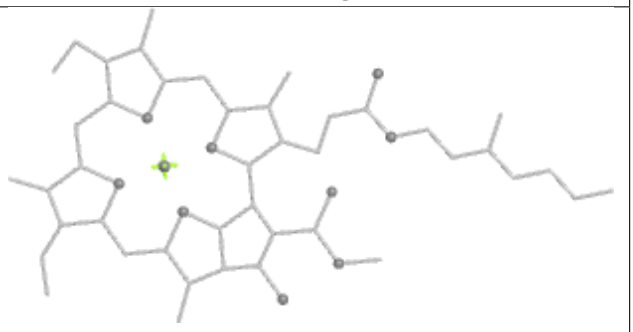
Bond lengths



Bond angles

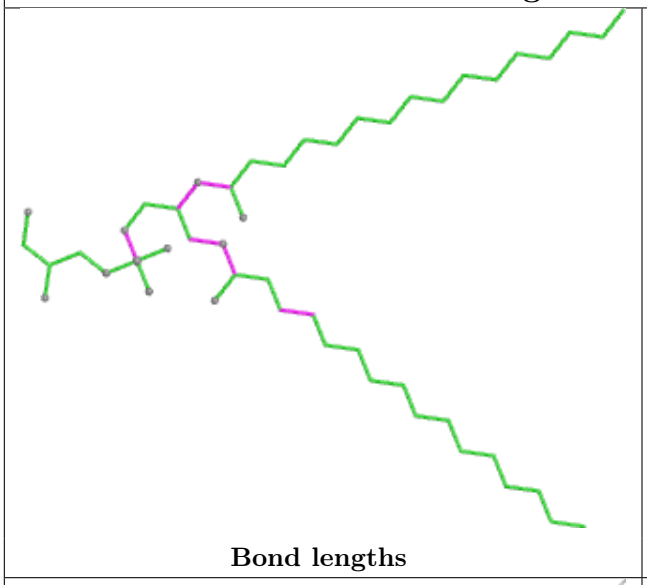


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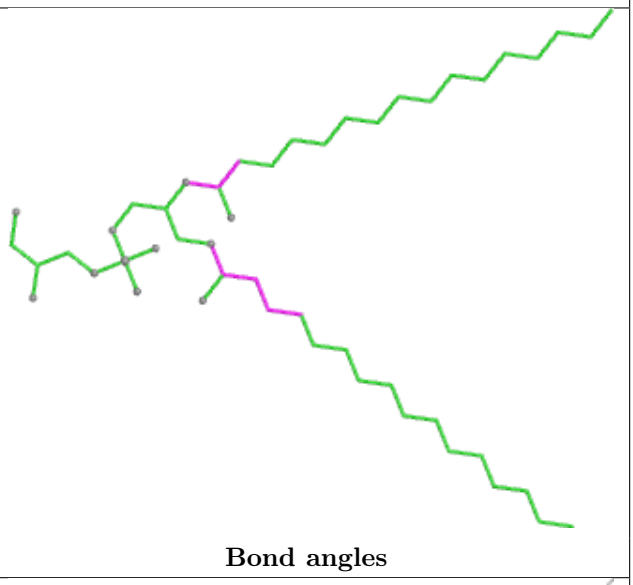


Rings

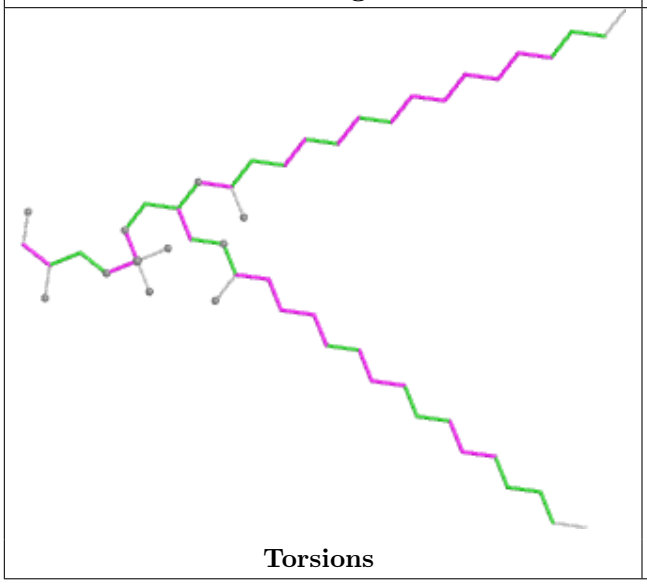
Ligand LHG A 845



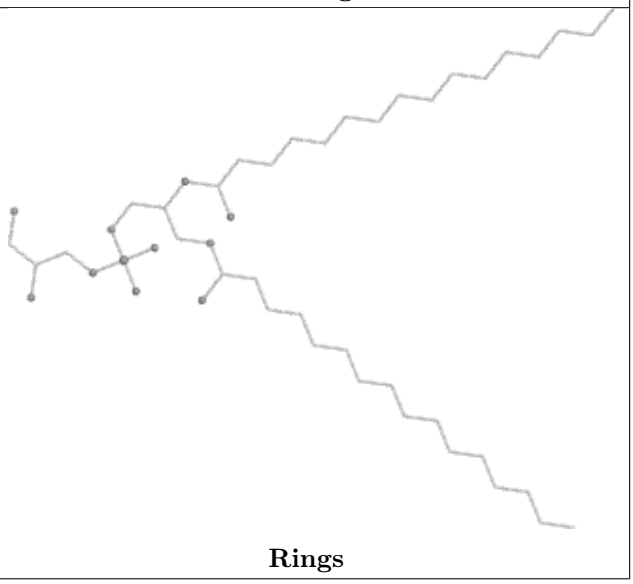
Bond lengths



Bond angles

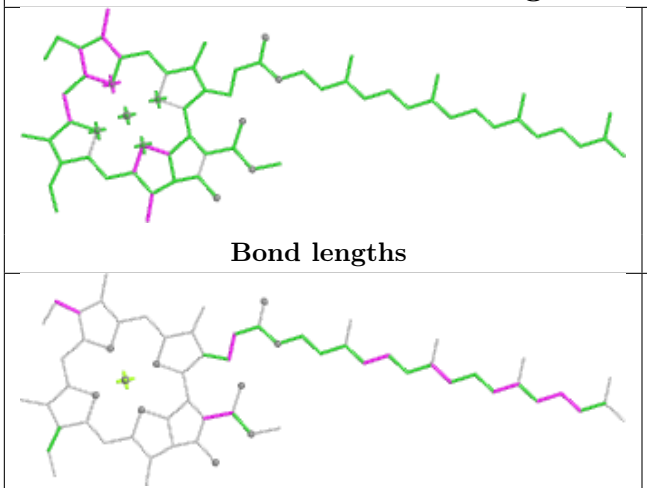


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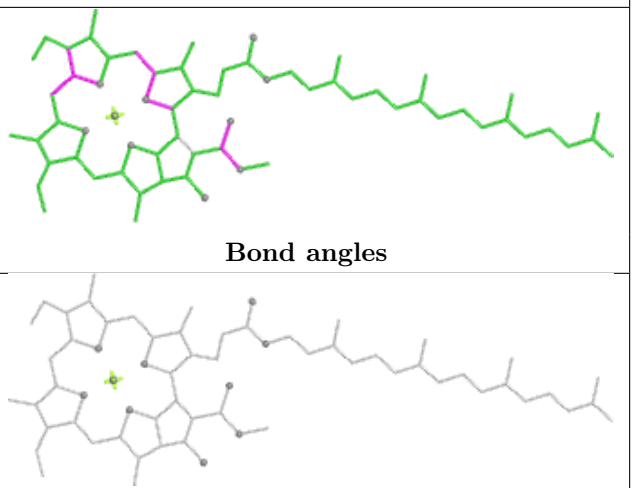


Rings

Ligand CLA A 841



Bond lengths

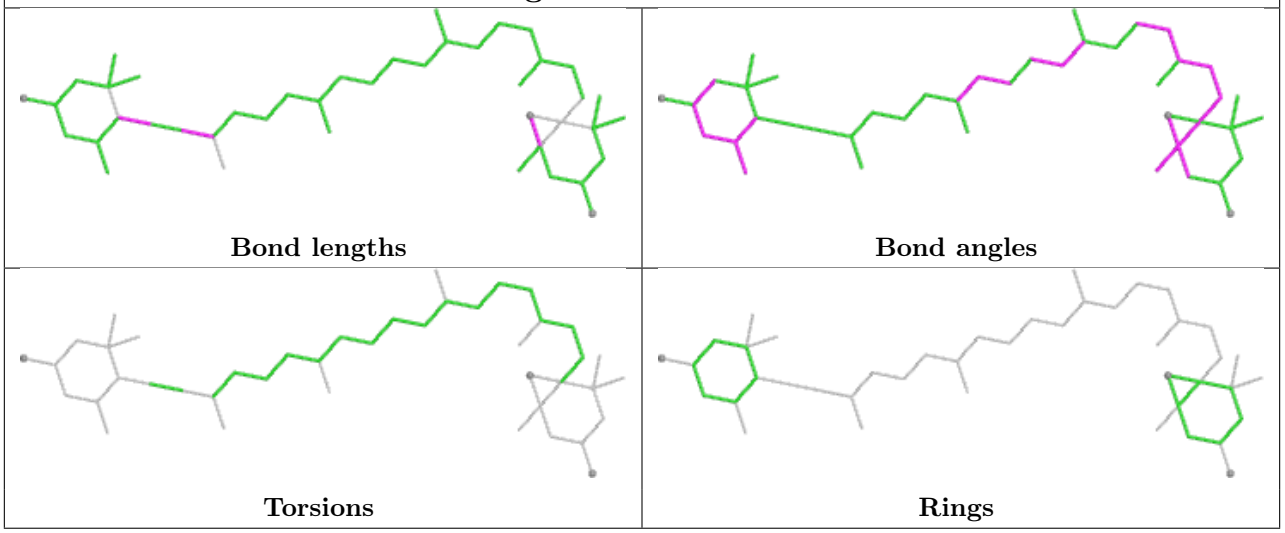


Bond angles

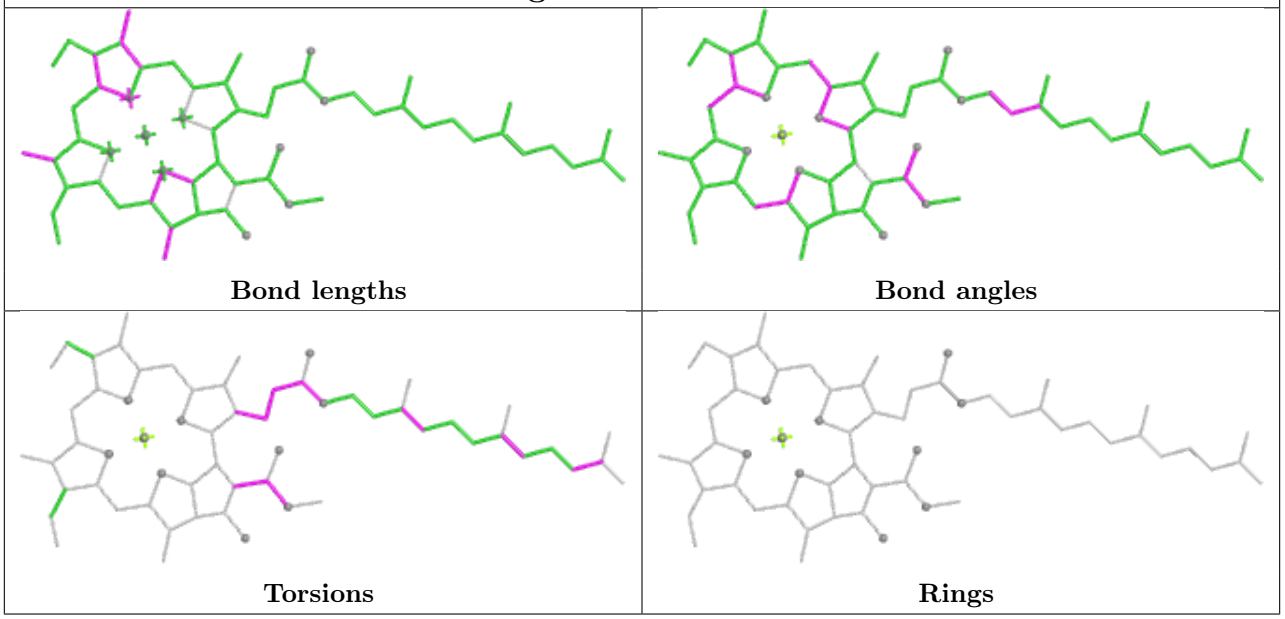
Torsions

Rings

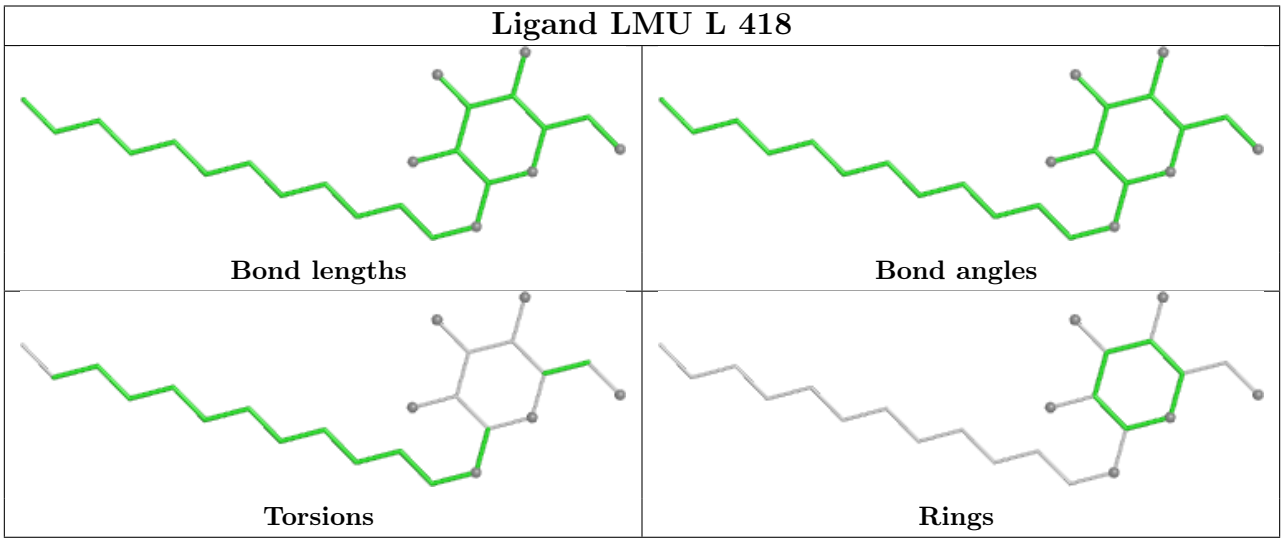
Ligand DD6 G 612



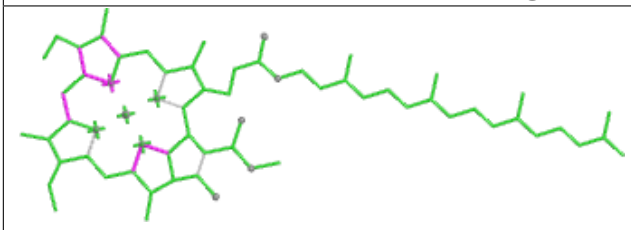
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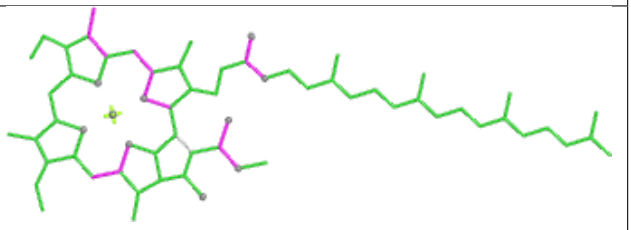
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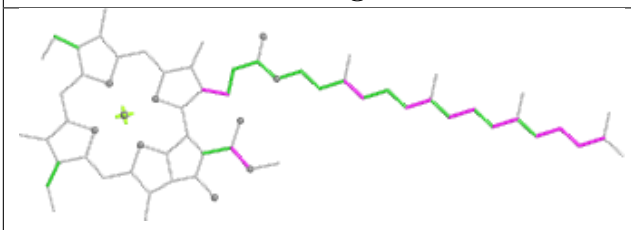
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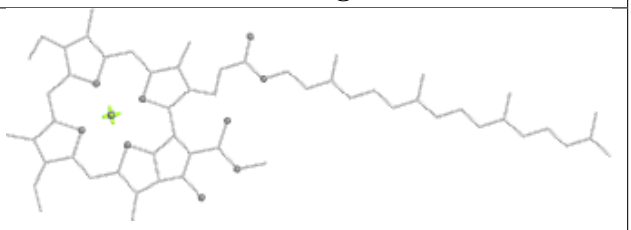
Bond lengths



Bond angles



Torsions

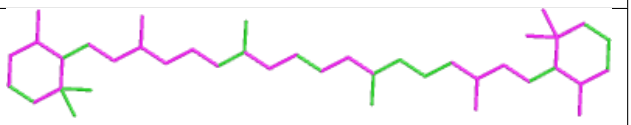


Rings

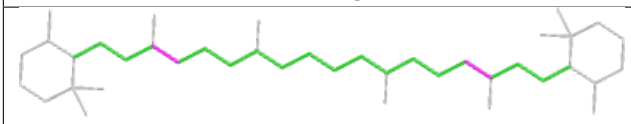
Ligand BCR B 843



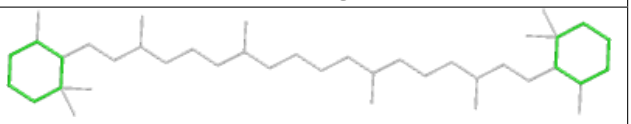
Bond lengths



Bond angles

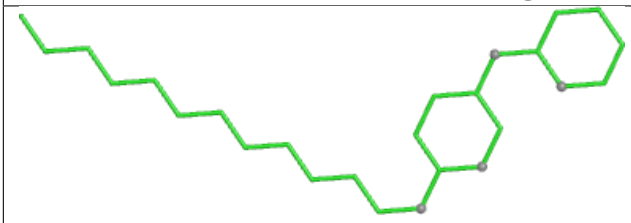


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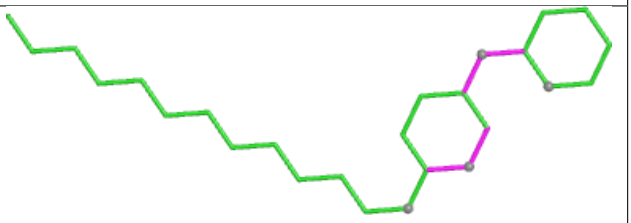


Rings

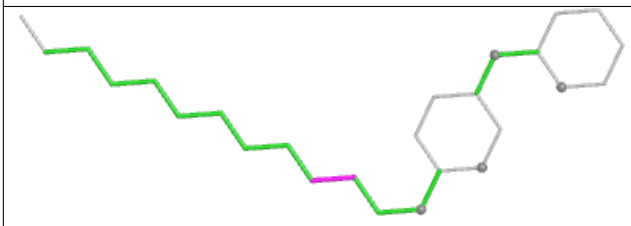
Ligand LMU O 320



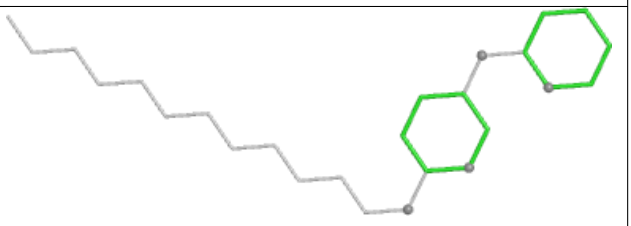
Bond lengths



Bond angles

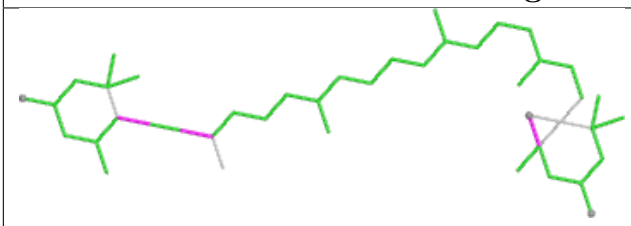


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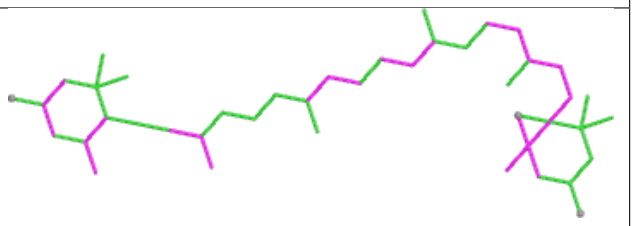


Rings

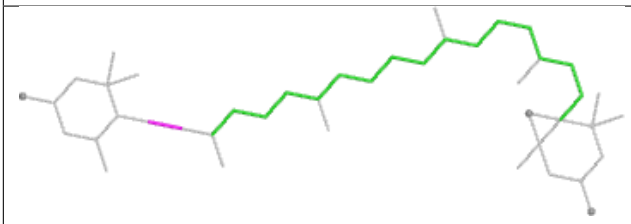
Ligand DD6 U 416



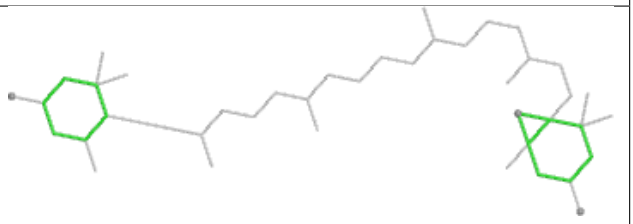
Bond lengths



Bond angles

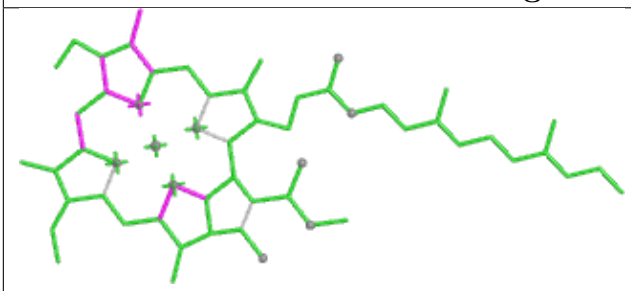


Torsions

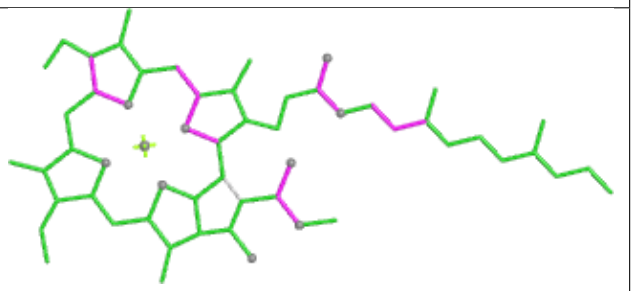


Rings

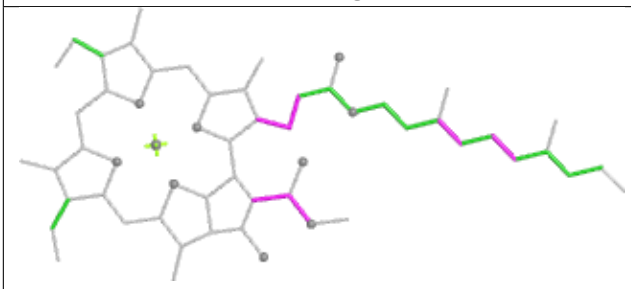
Ligand CLA V 609



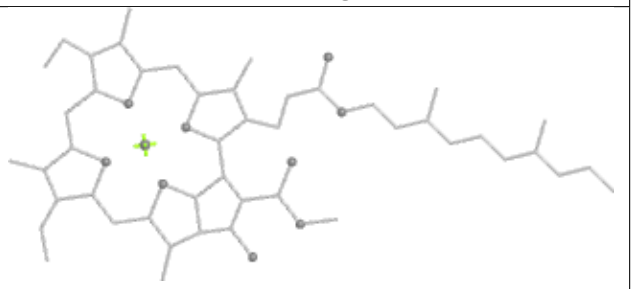
Bond lengths



Bond angles

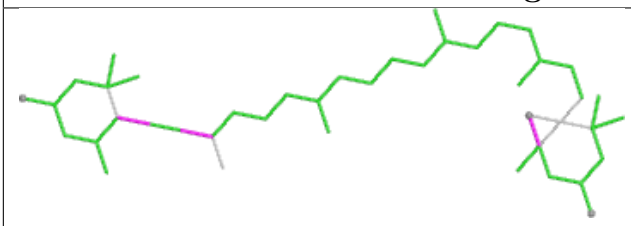


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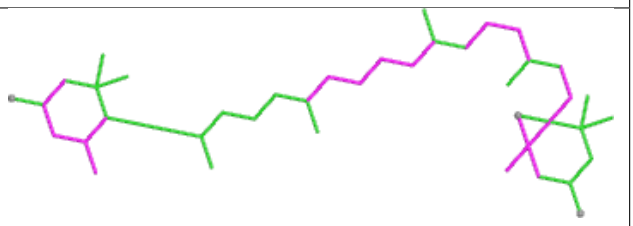


Rings

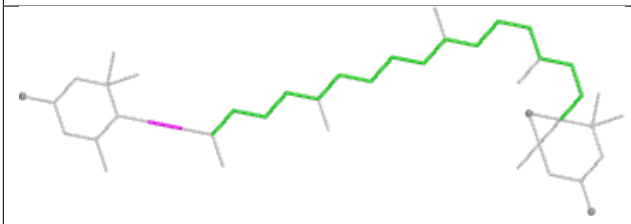
Ligand DD6 H 315



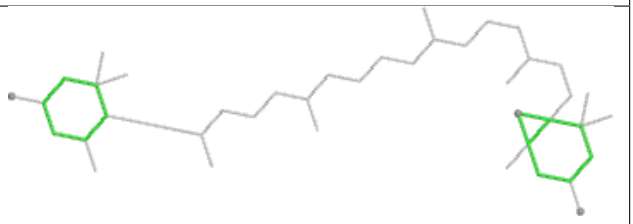
Bond lengths



Bond angles

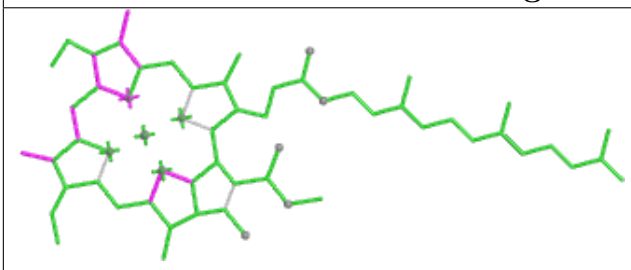


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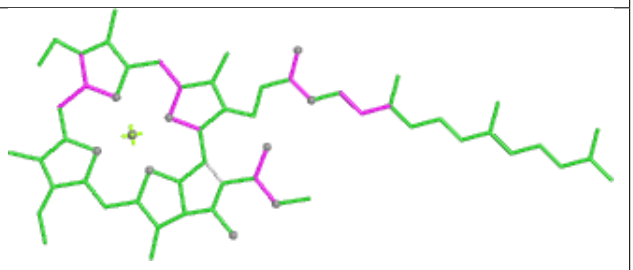


Rings

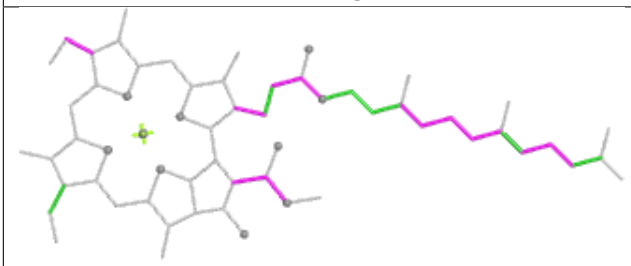
Ligand CLA R 607



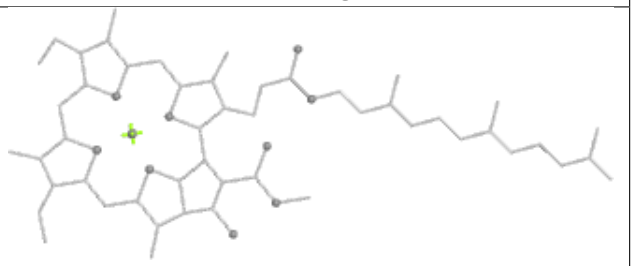
Bond lengths



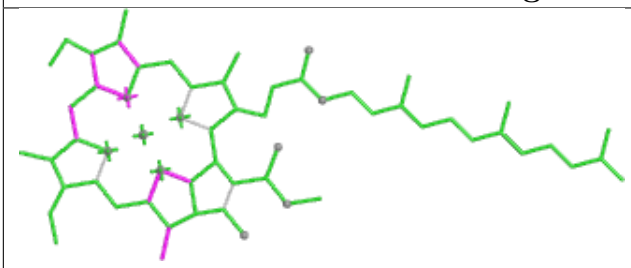
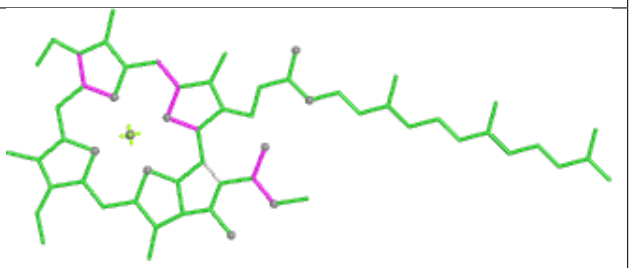
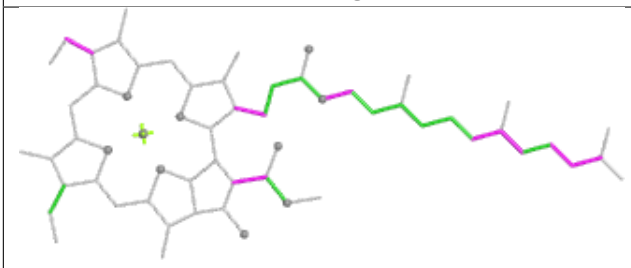
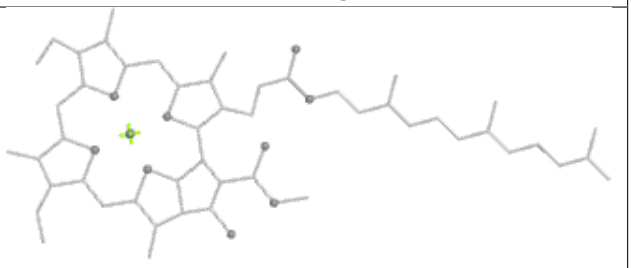
Bond angles

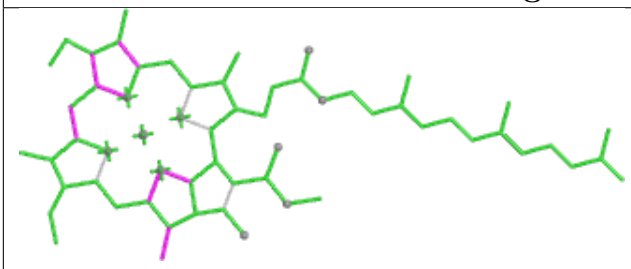
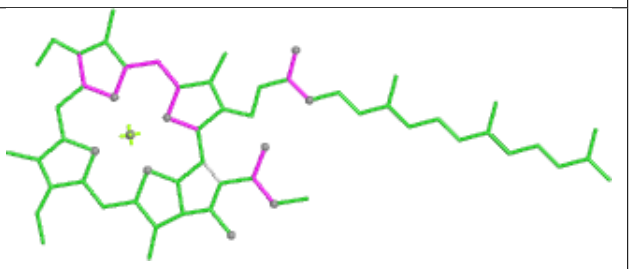
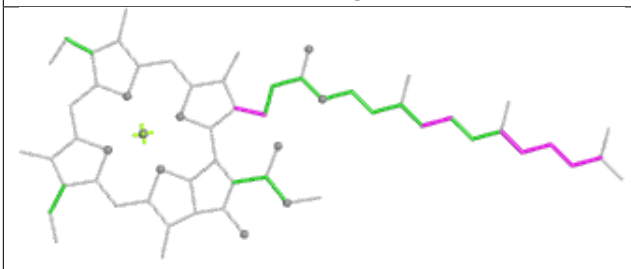
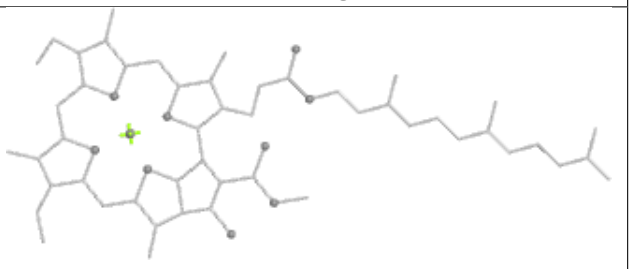


Torsions

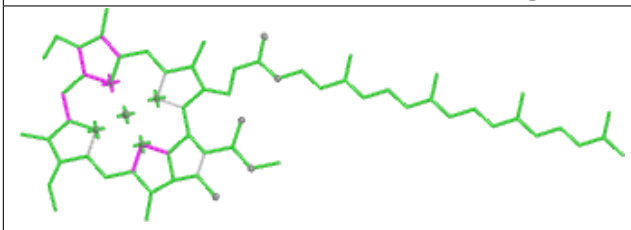


Rings

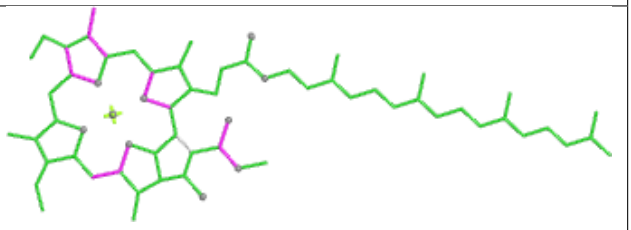
Ligand CLA K 609	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA X 404	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

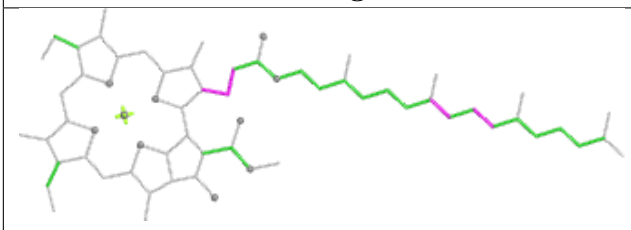
Ligand CLA A 804



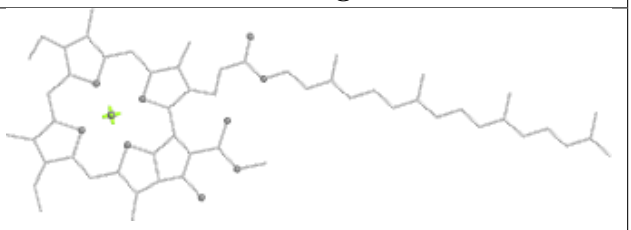
Bond lengths



Bond angles

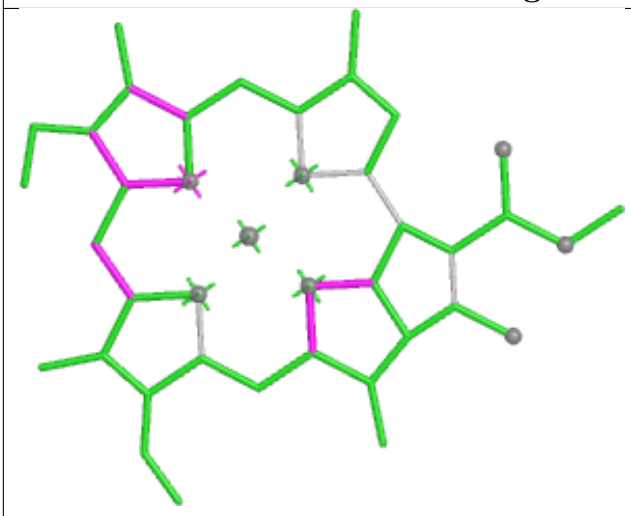


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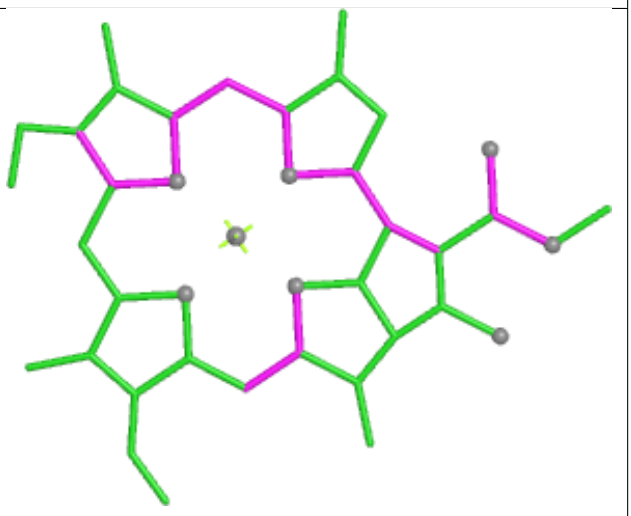


Rings

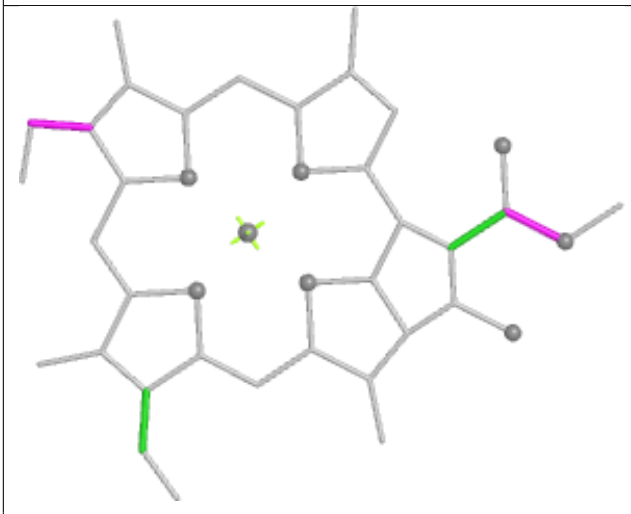
Ligand CLA N 611



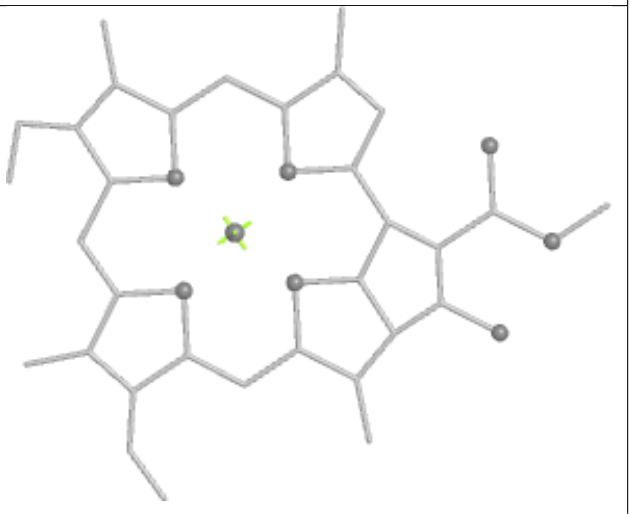
Bond lengths



Bond angles

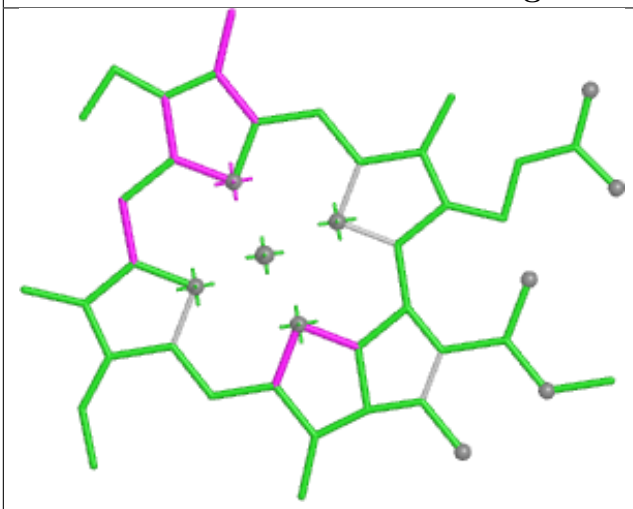


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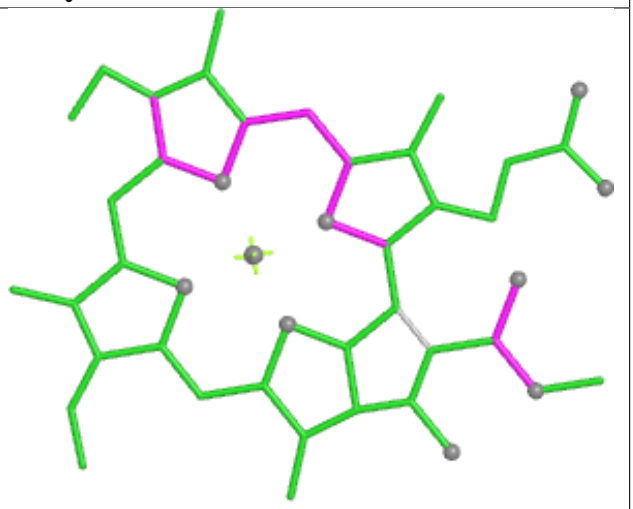


Rings

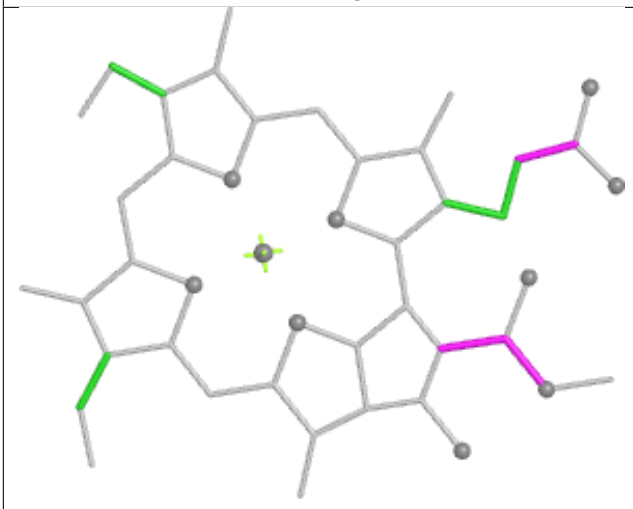
Ligand CLA Q 606



Bond lengths



Bond angles

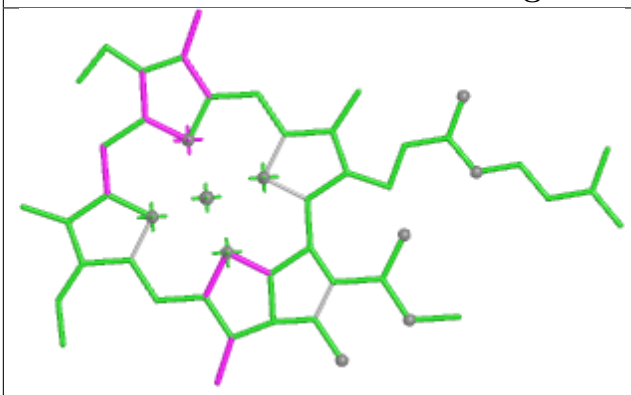


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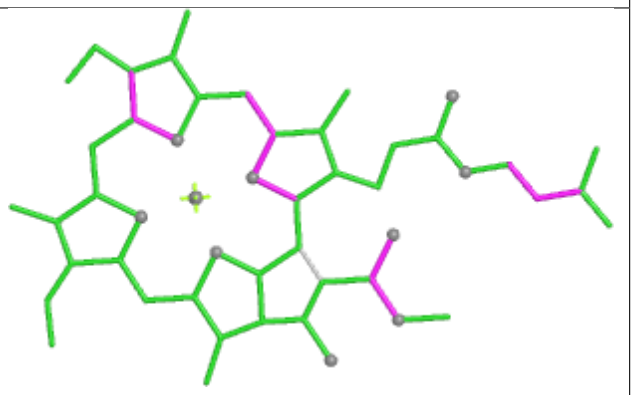


Rings

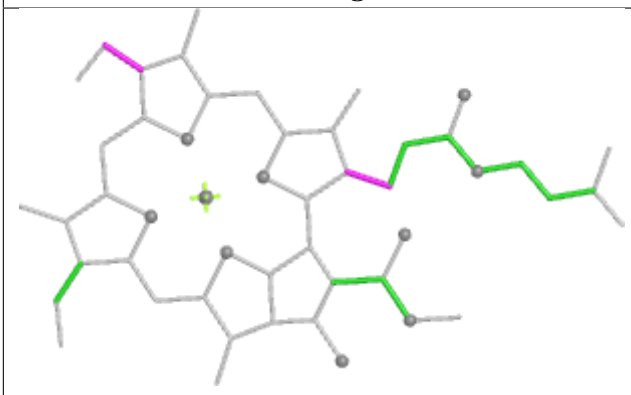
Ligand CLA O 309



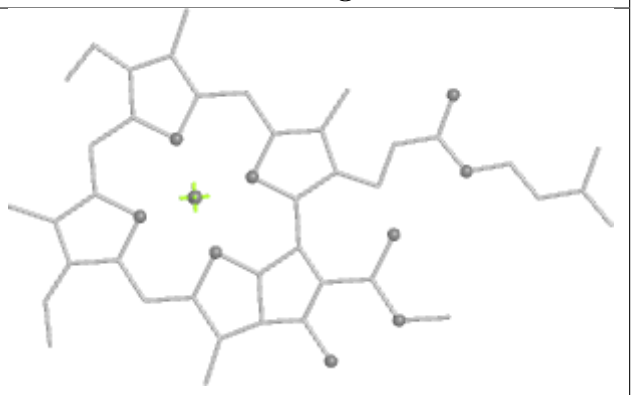
Bond lengths



Bond angles

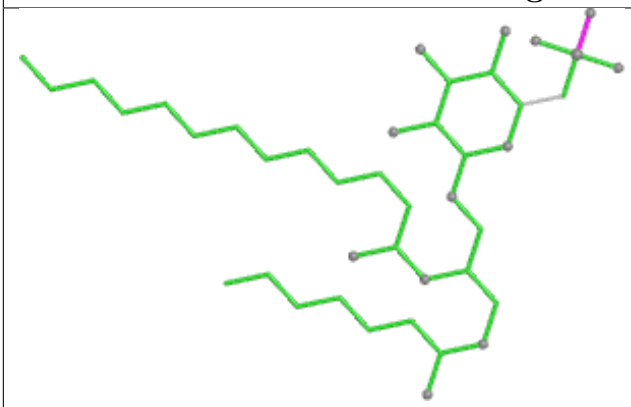


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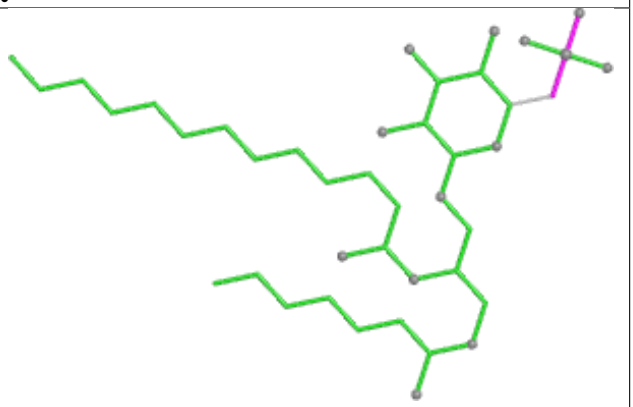


Rings

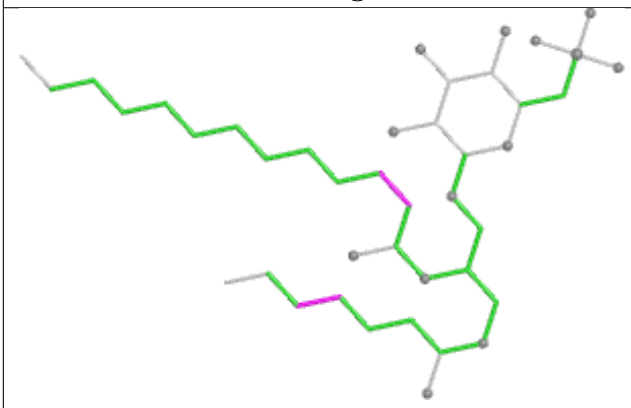
Ligand SQD F 407



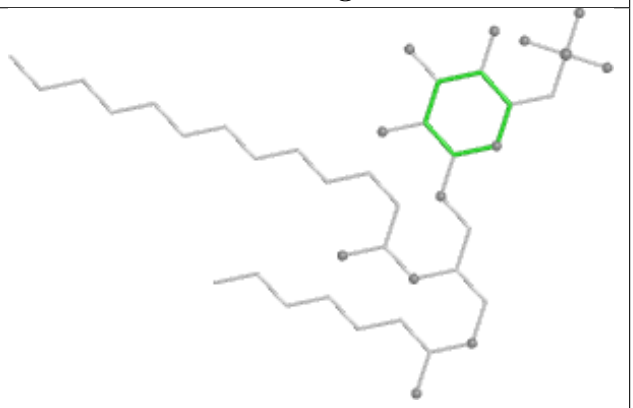
Bond lengths



Bond angles

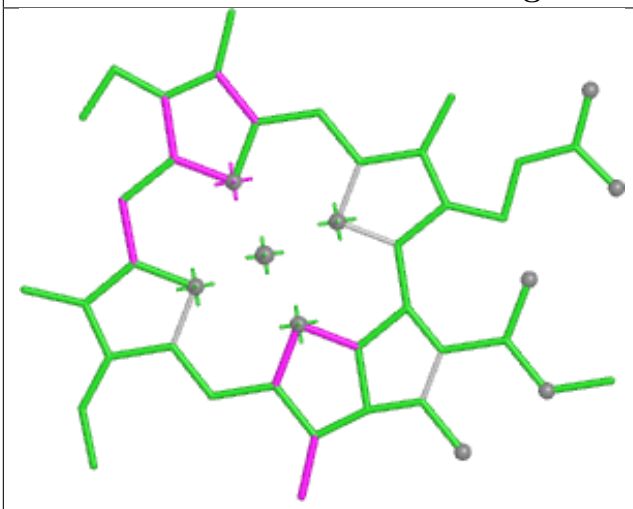


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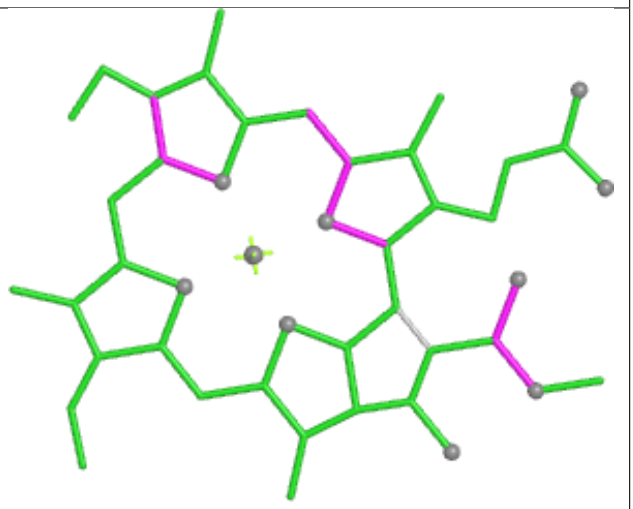


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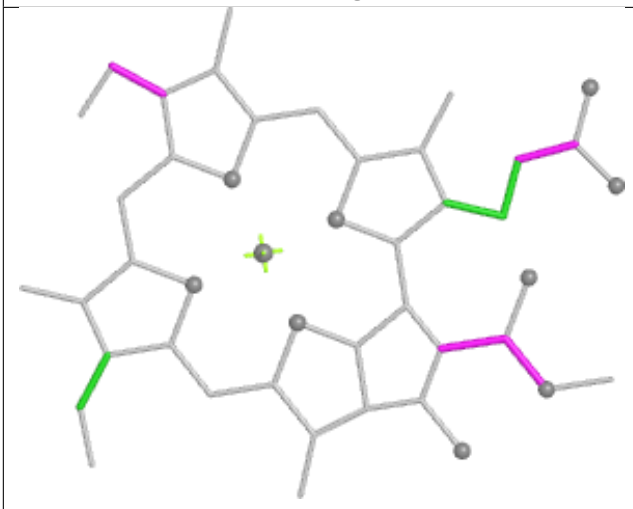
Ligand CLA N 608



Bond lengths



Bond angles

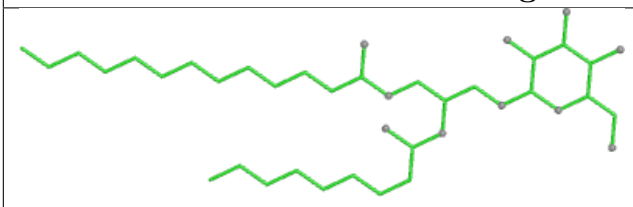


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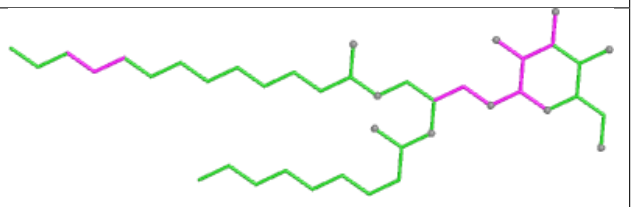


Rings

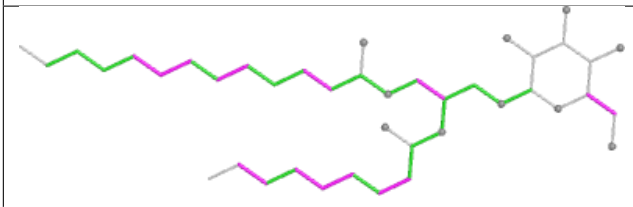
Ligand LMG A 855



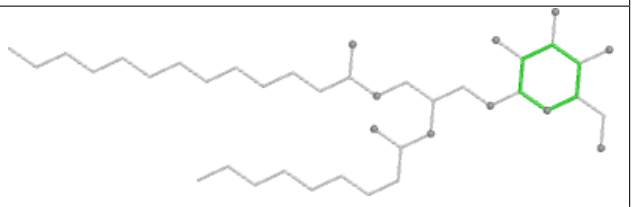
Bond lengths



Bond angles

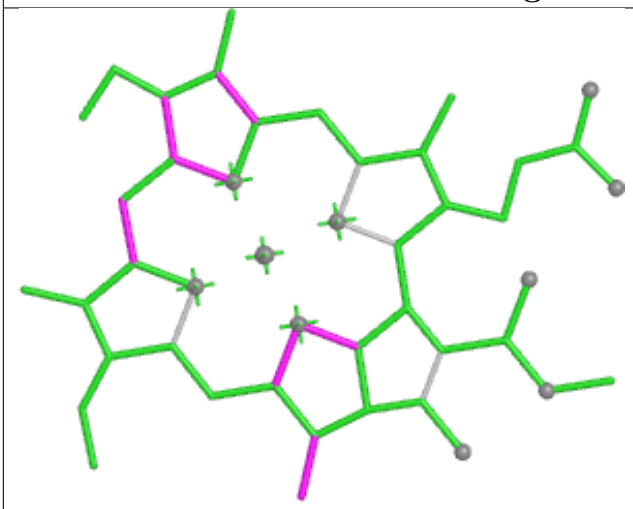


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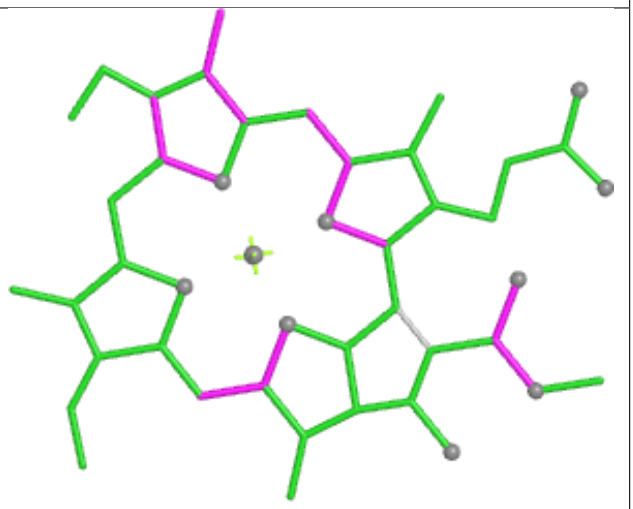


Rings

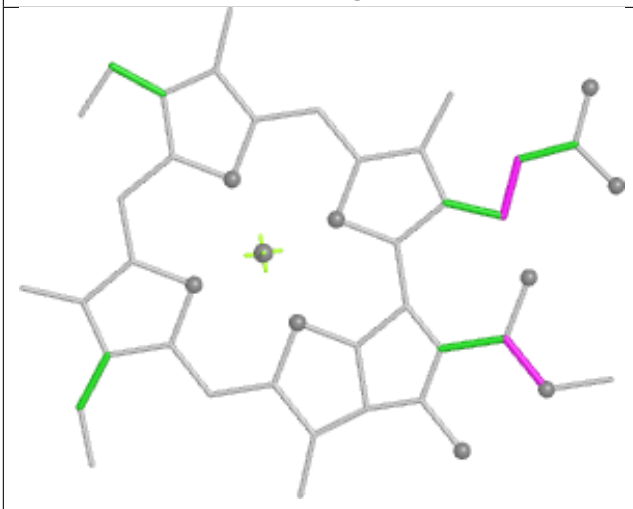
Ligand CLA V 607



Bond lengths



Bond angles

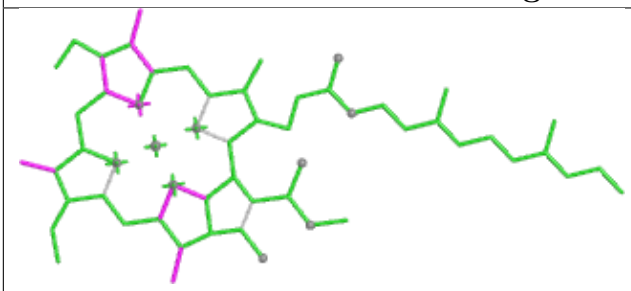


Torsions

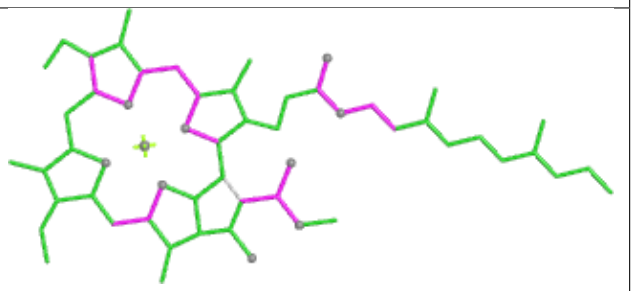


Rings

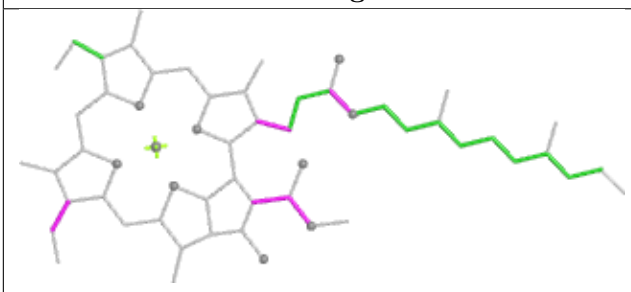
Ligand CLA K 607



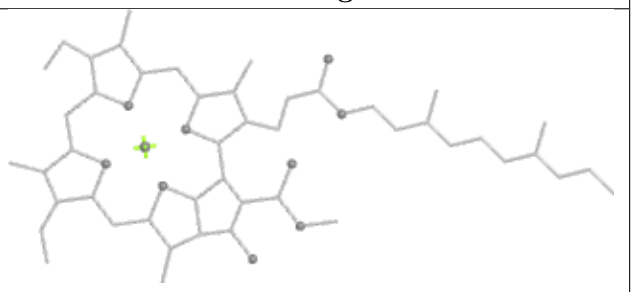
Bond lengths



Bond angles

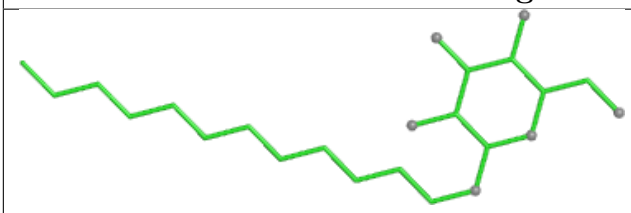


Torsions

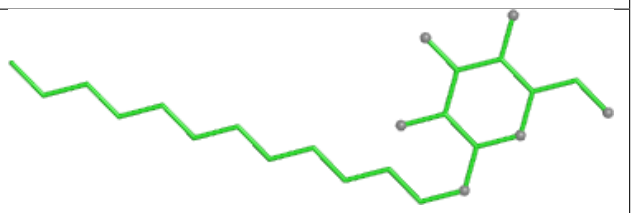


Rings

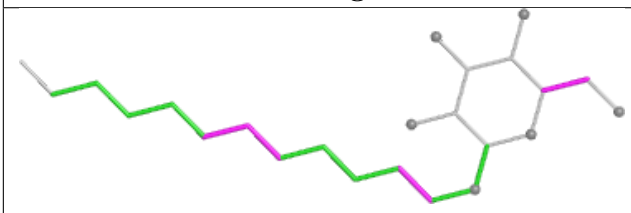
Ligand LMU M 102



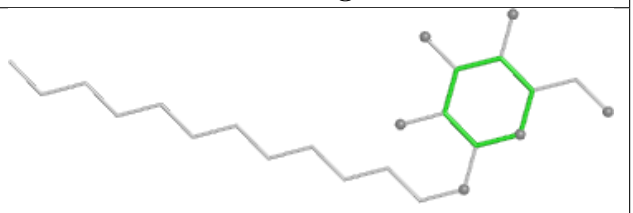
Bond lengths



Bond angles



Torsions



Rings

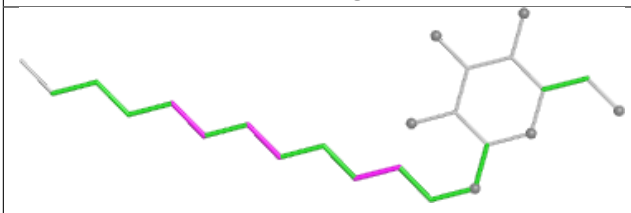
Ligand LMU B 854



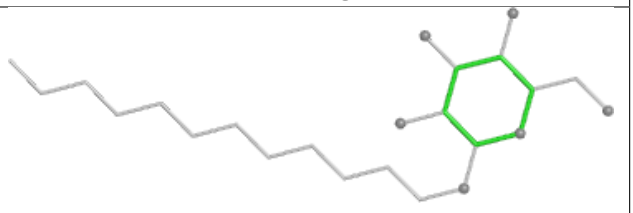
Bond lengths



Bond angles

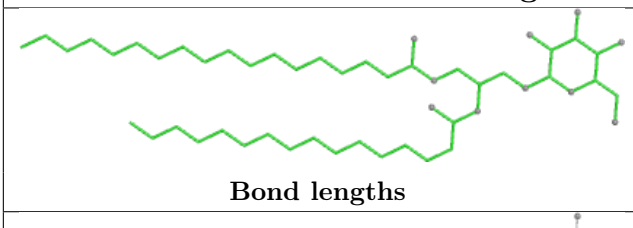


Torsions

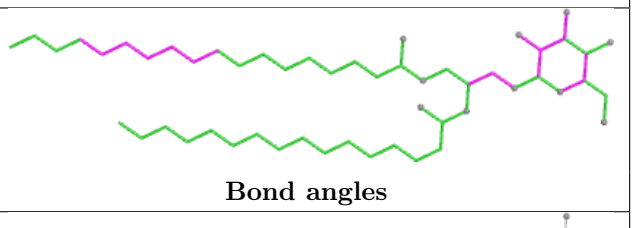


Rings

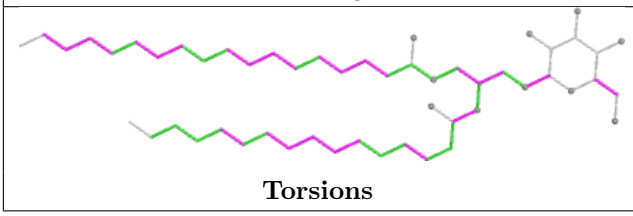
Ligand LMG B 856



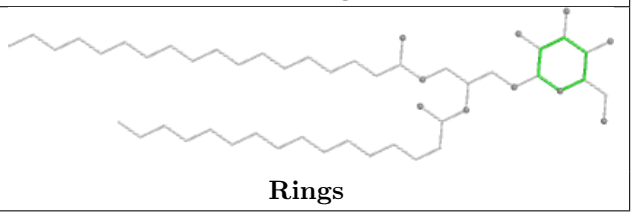
Bond lengths



Bond angles



Torsions



Rings

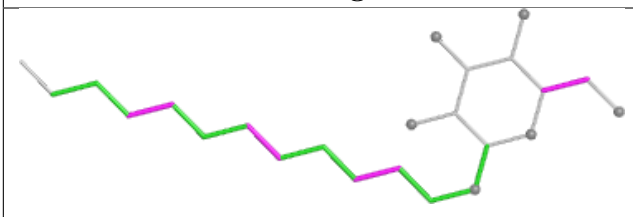
Ligand LMU W 421



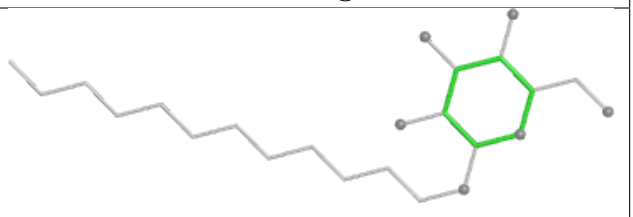
Bond lengths



Bond angles

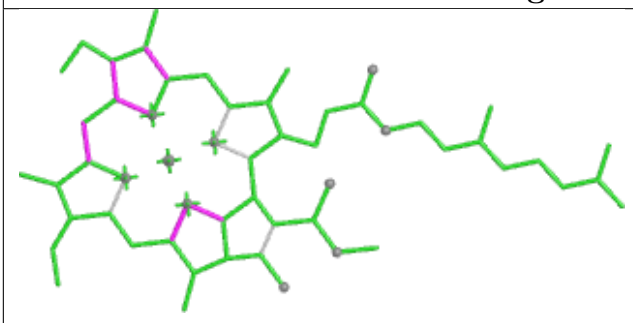


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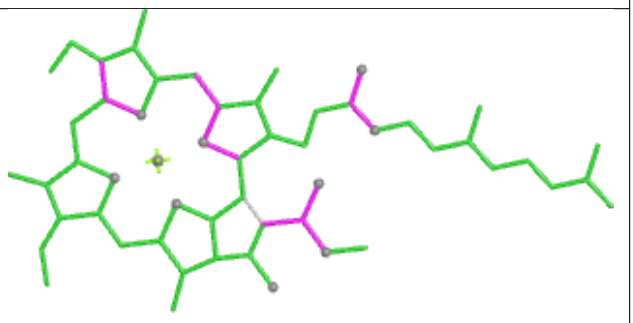


Rings

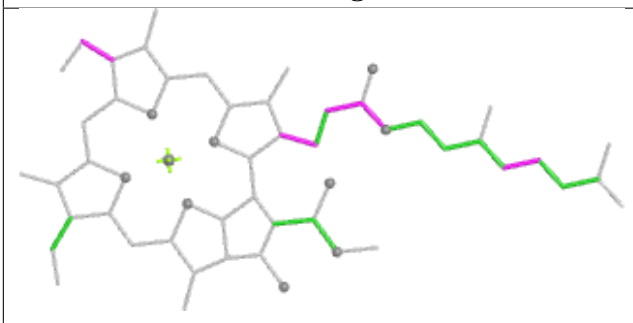
Ligand CLA S 609



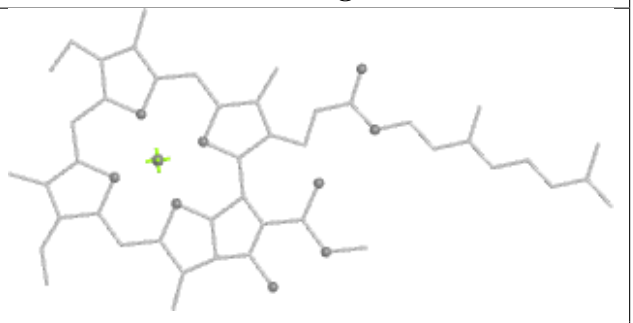
Bond lengths



Bond angles

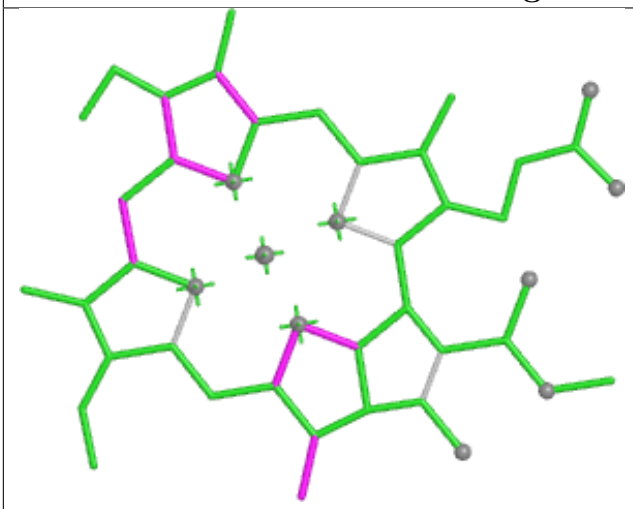


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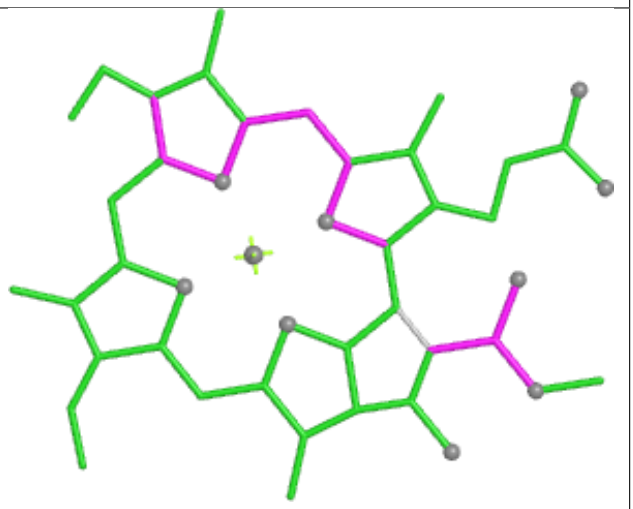


Rings

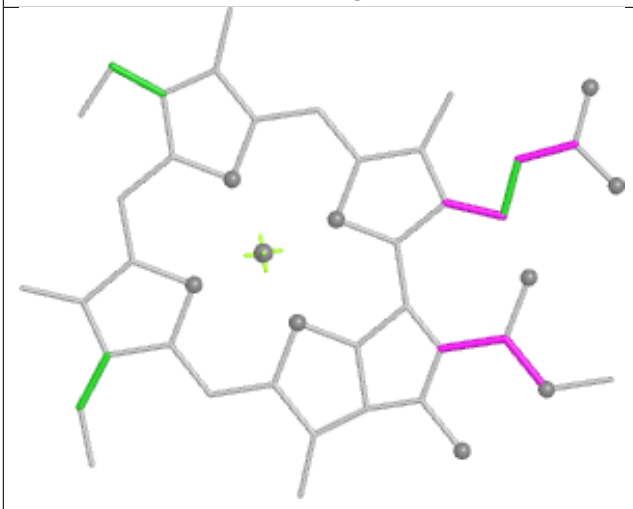
Ligand CLA U 403



Bond lengths



Bond angles

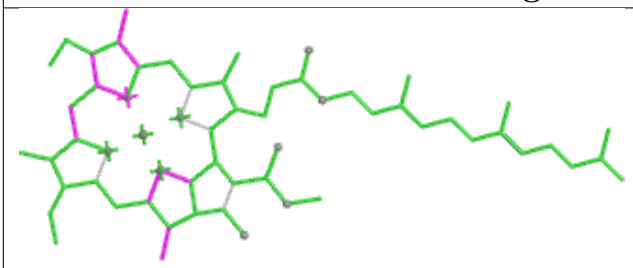


Torsions

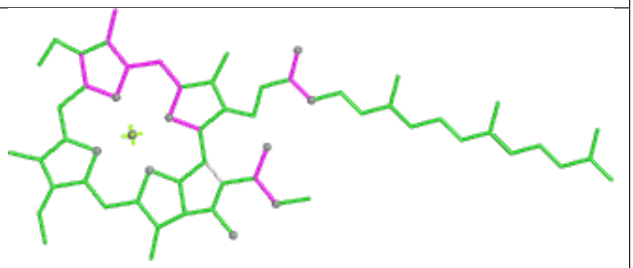


Rings

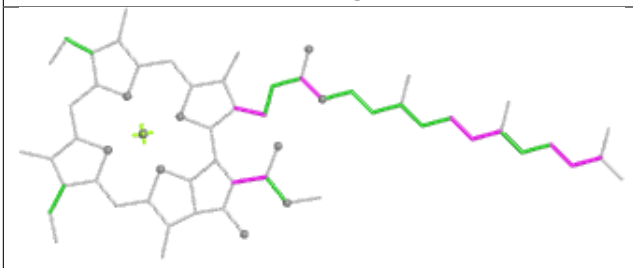
Ligand CLA K 602



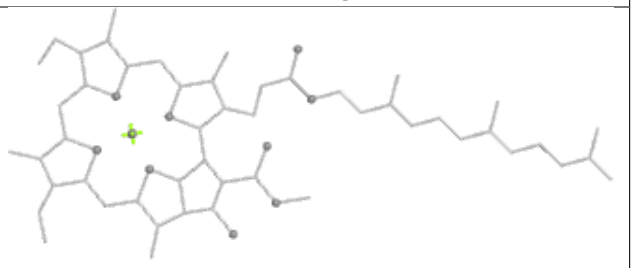
Bond lengths



Bond angles

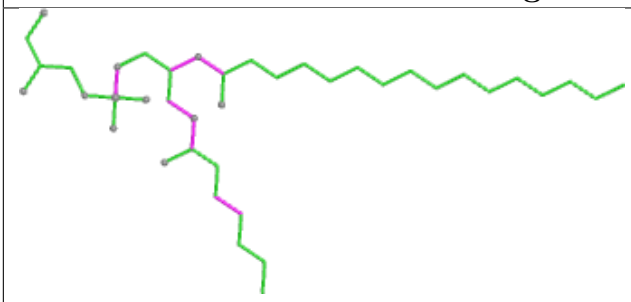


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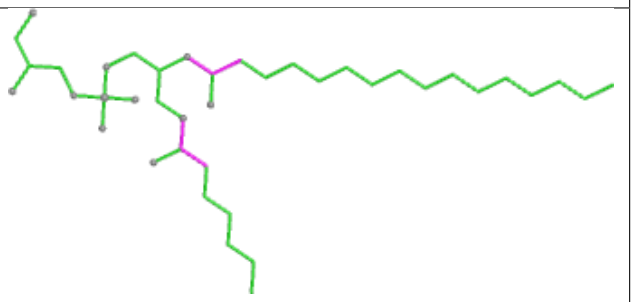


Rings

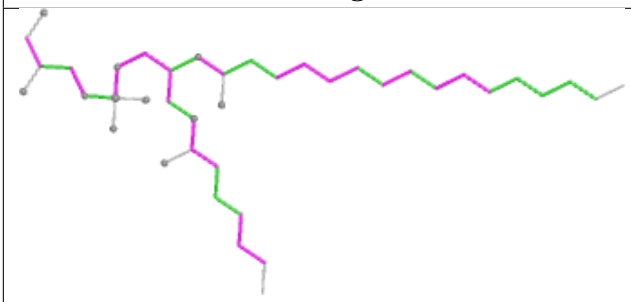
Ligand LHG P 601



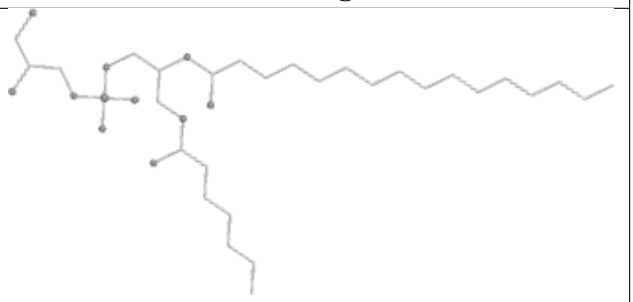
Bond lengths



Bond angles

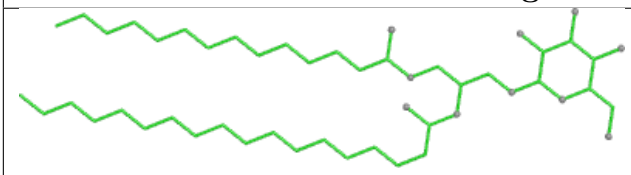


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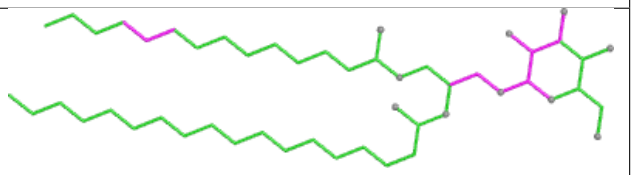


Rings

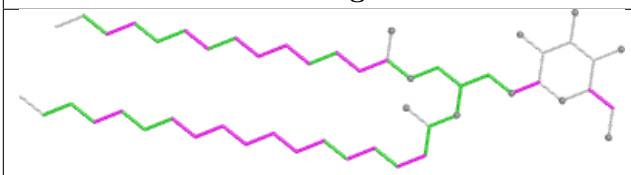
Ligand LMG L 401



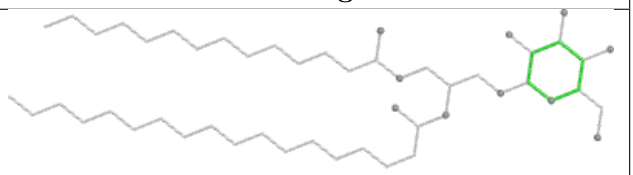
Bond lengths



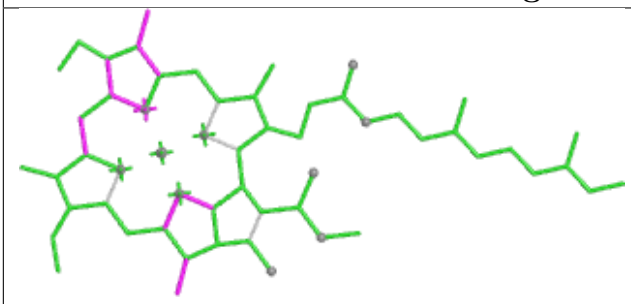
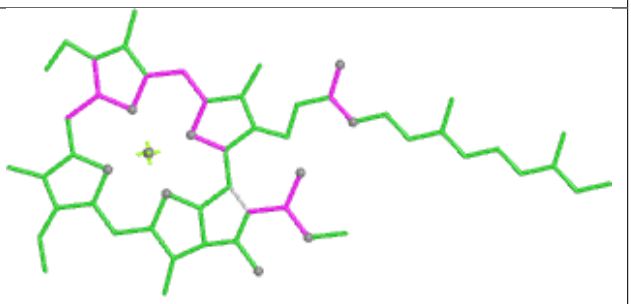
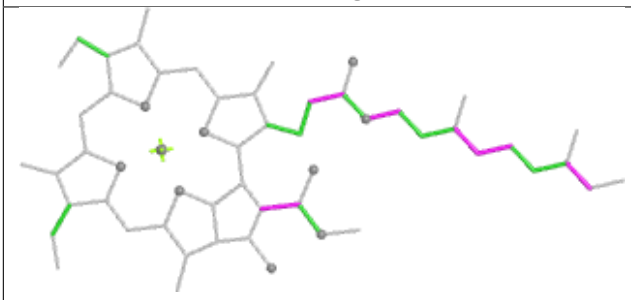
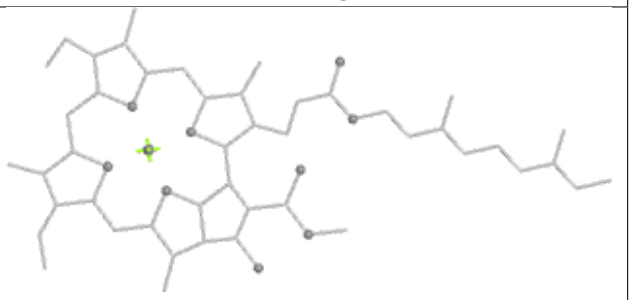
Bond angles

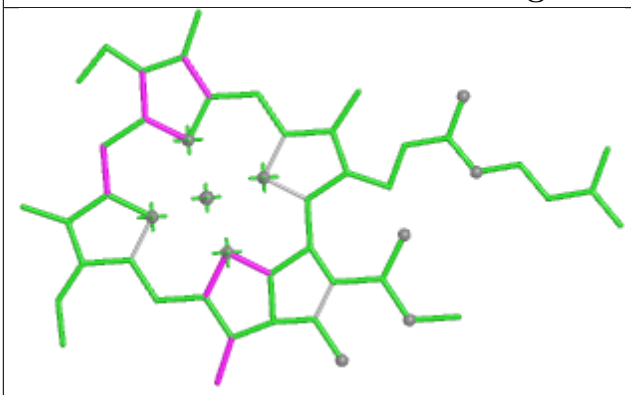
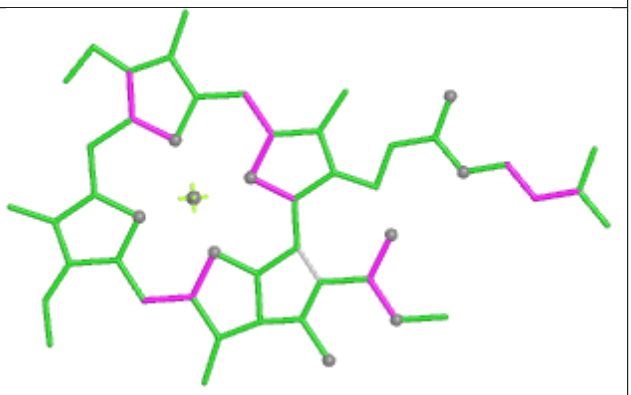
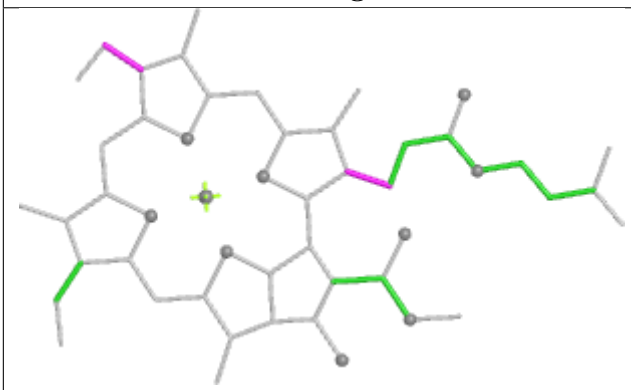
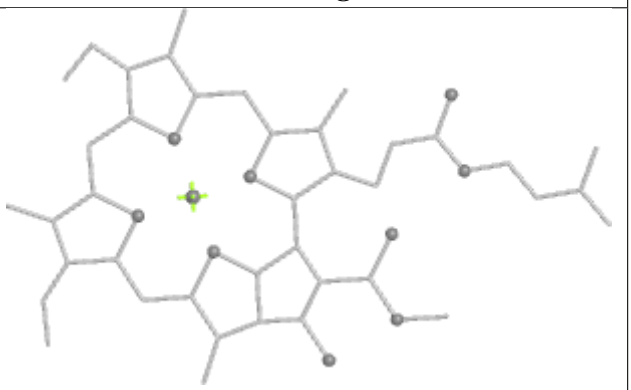


Torsions

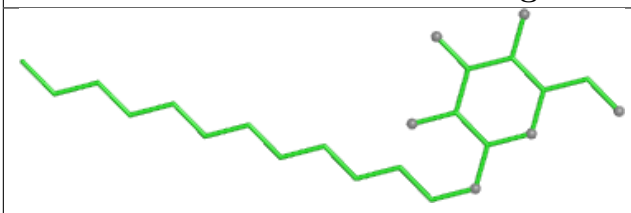


Rings

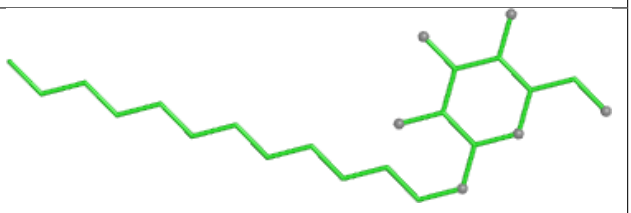
Ligand CLA G 603	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA S 606	
	
Bond lengths	Bond angles
	
Torsions	Rings

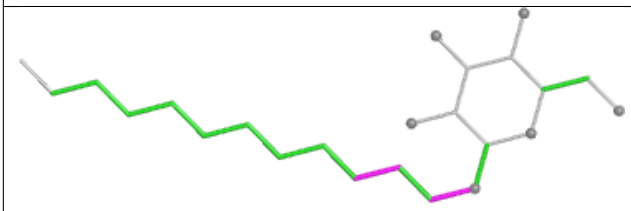
Ligand LMU B 849



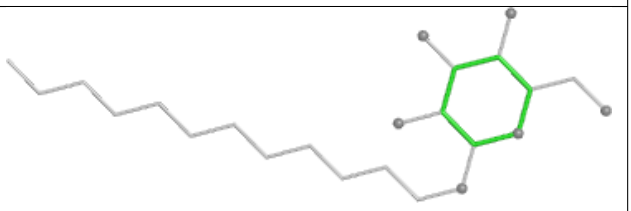
Bond lengths



Bond angles

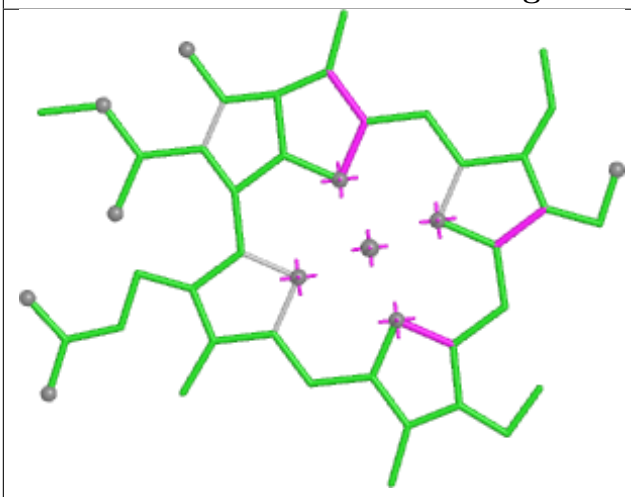


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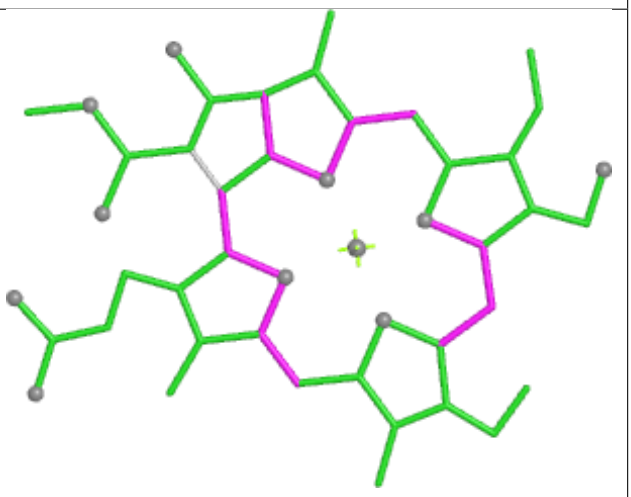


Rings

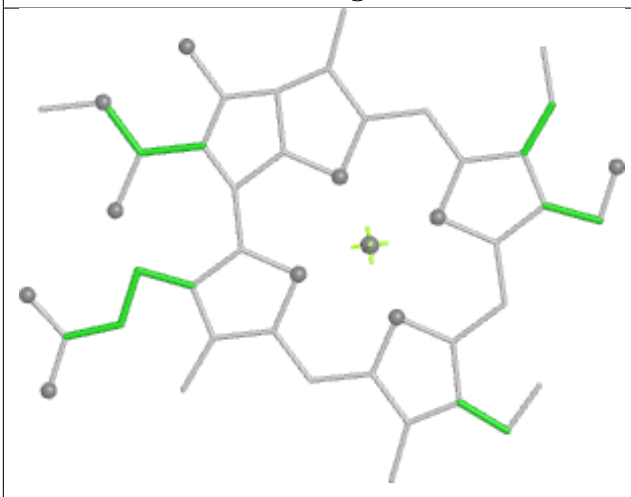
Ligand CHL U 407



Bond lengths



Bond angles

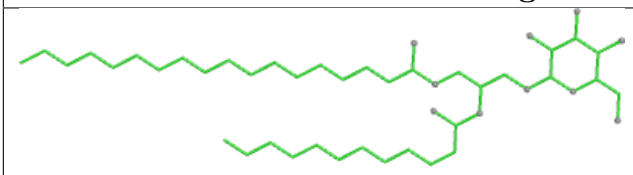


Torsions

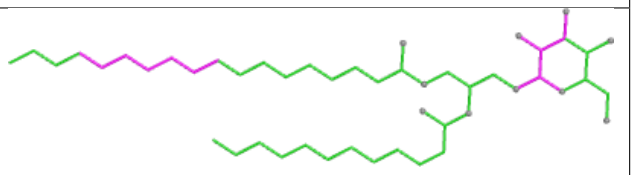


Rings

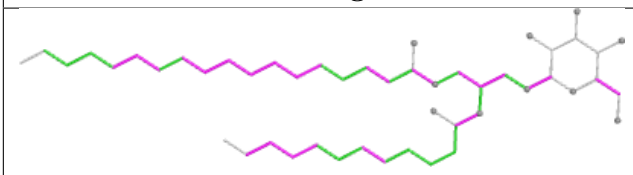
Ligand LMG K 618



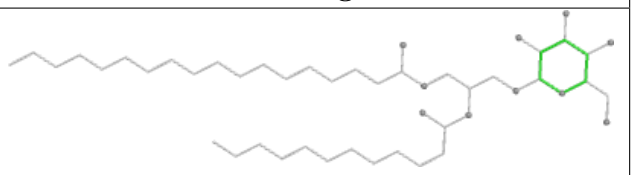
Bond lengths



Bond angles

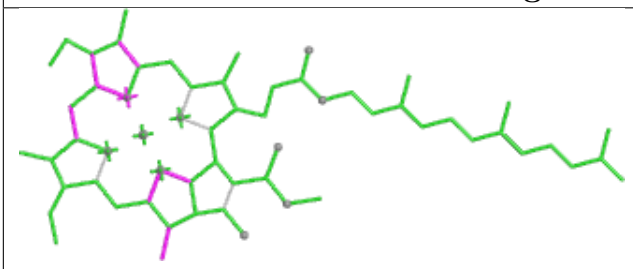


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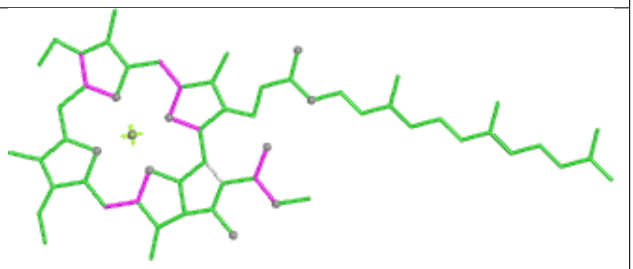


Rings

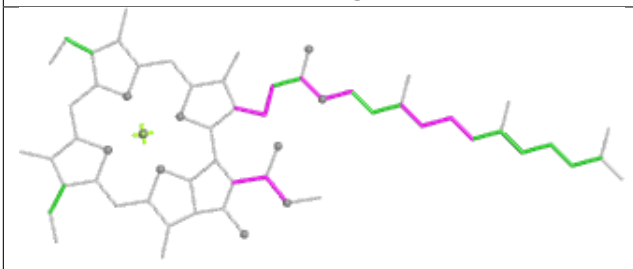
Ligand CLA R 602



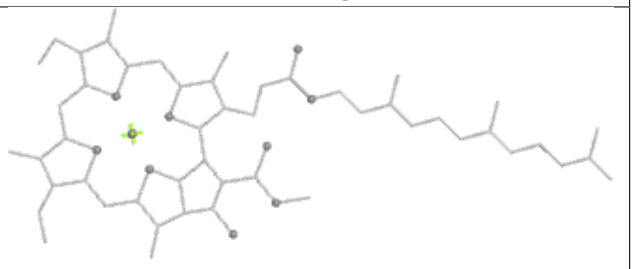
Bond lengths



Bond angles

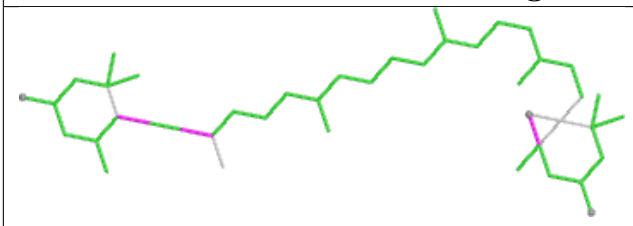


Torsions

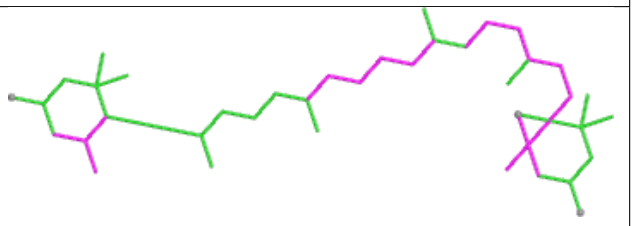


Rings

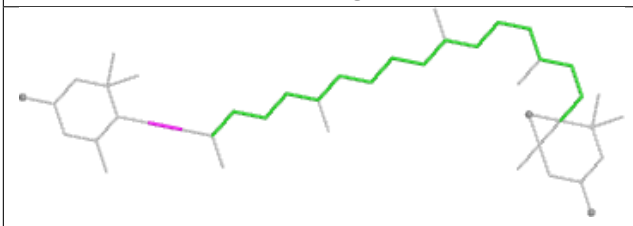
Ligand DD6 T 612



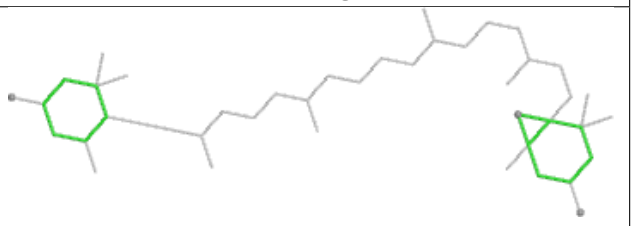
Bond lengths



Bond angles

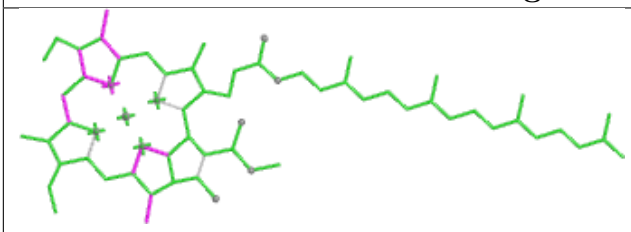


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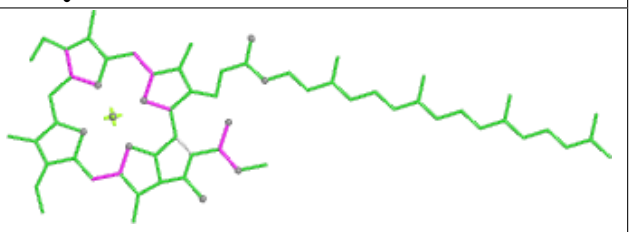


Rings

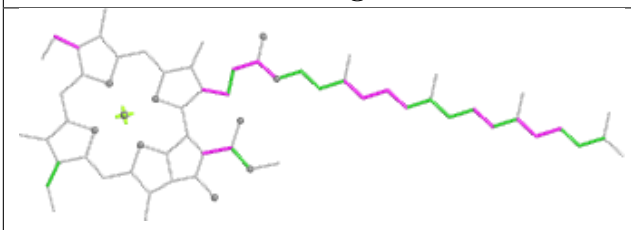
Ligand CLA Q 610



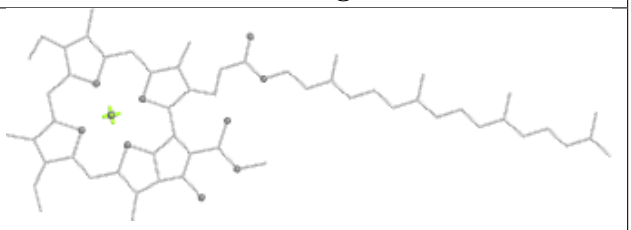
Bond lengths



Bond angles

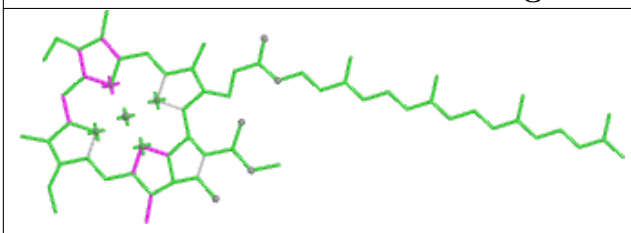


Torsions

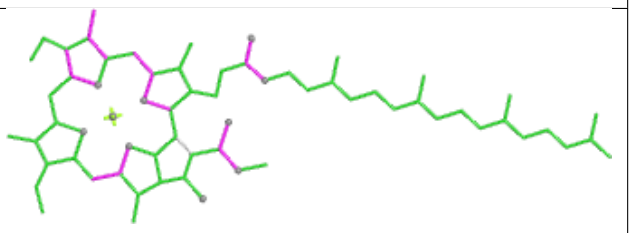


Rings

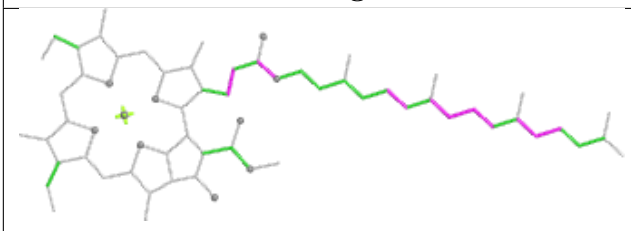
Ligand CLA B 835



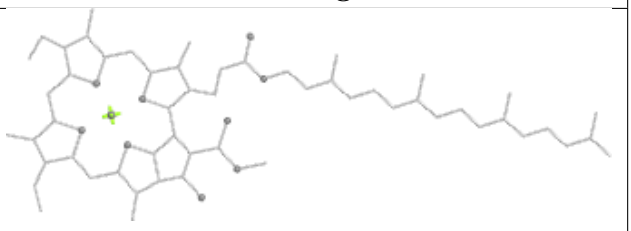
Bond lengths



Bond angles

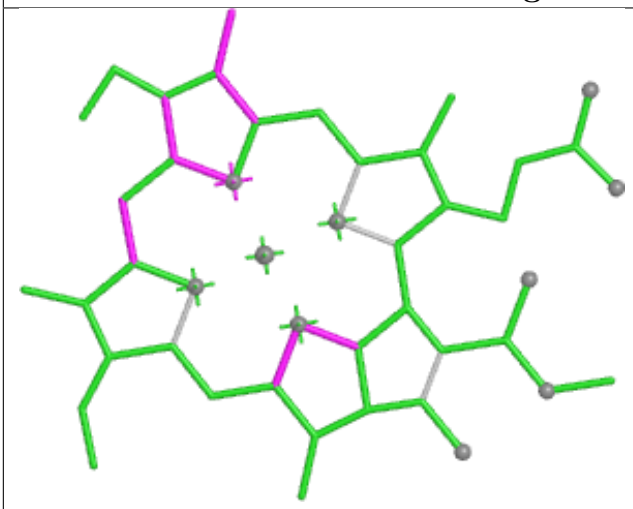


Torsions

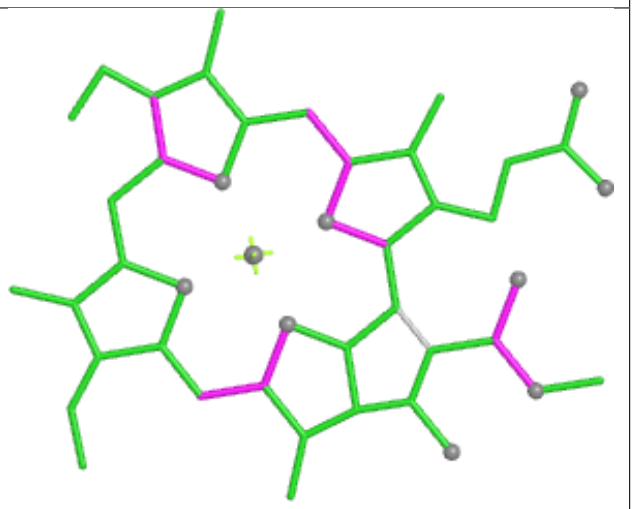


Rings

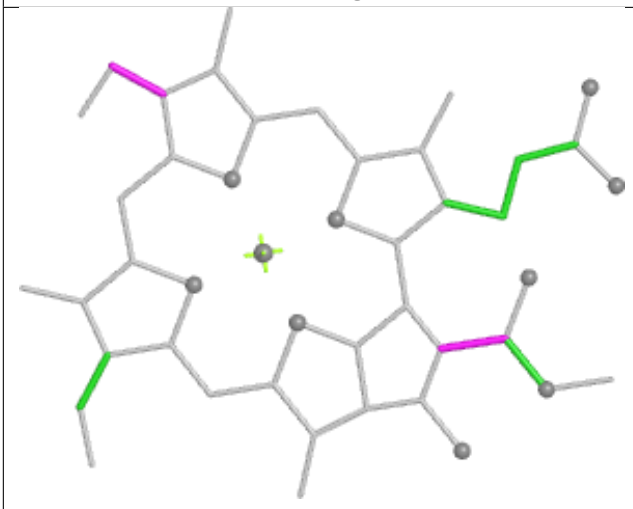
Ligand CLA H 302



Bond lengths



Bond angles

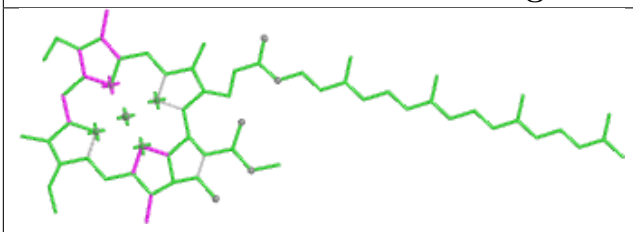


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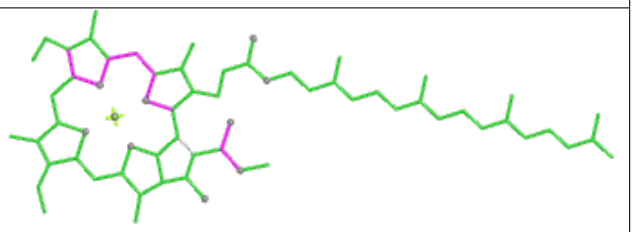


Rings

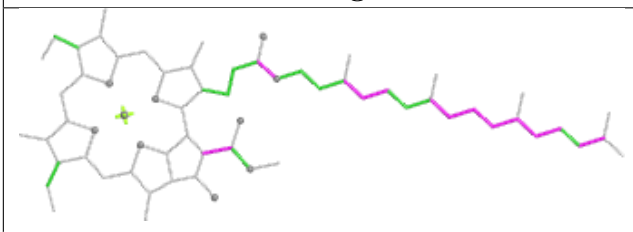
Ligand CLA L 402



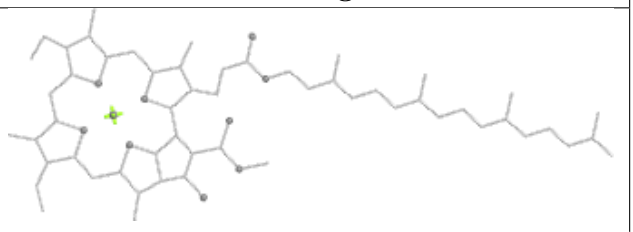
Bond lengths



Bond angles

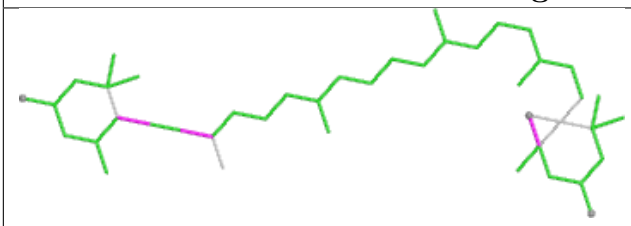


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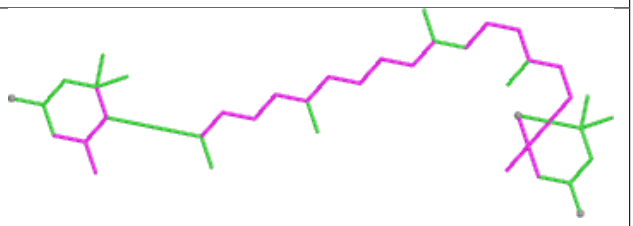


Rings

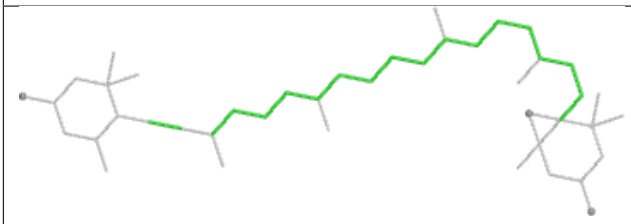
Ligand DD6 I 613



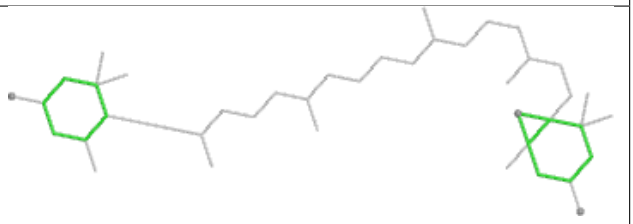
Bond lengths



Bond angles

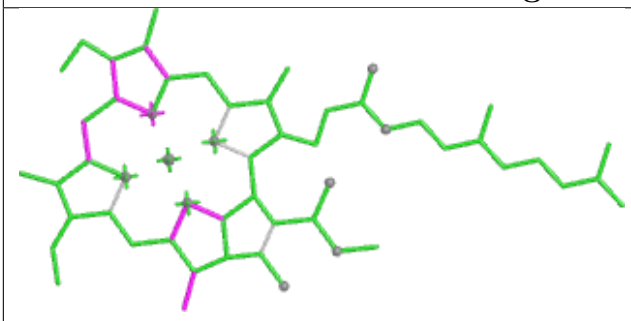


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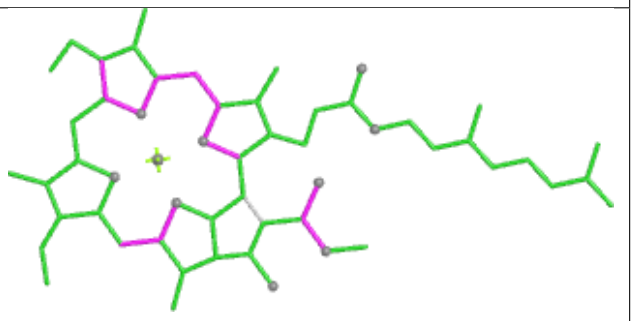


Rings

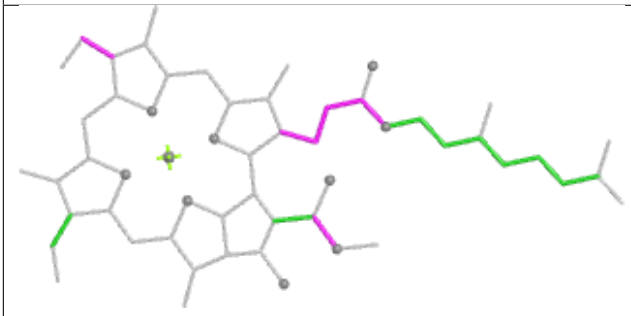
Ligand CLA H 309



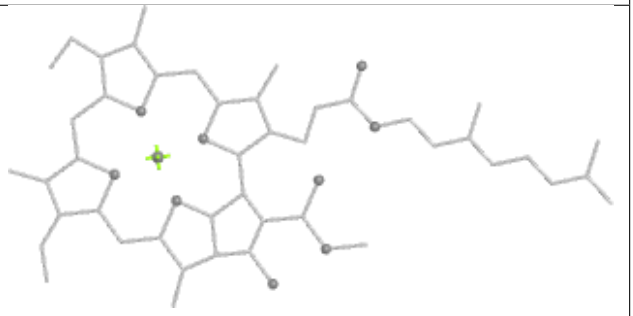
Bond lengths



Bond angles

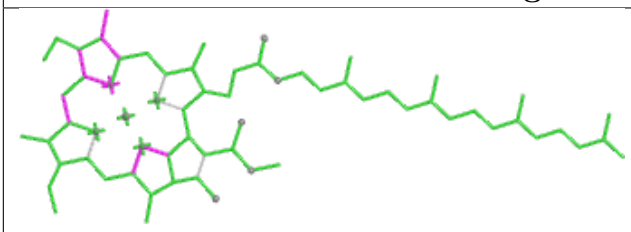


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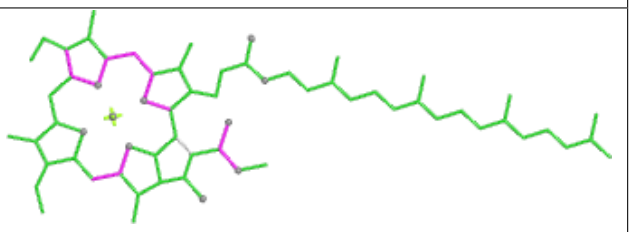


Rings

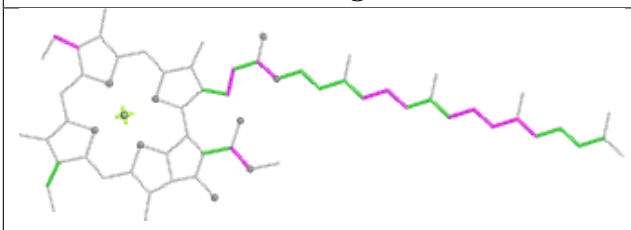
Ligand CLA V 612



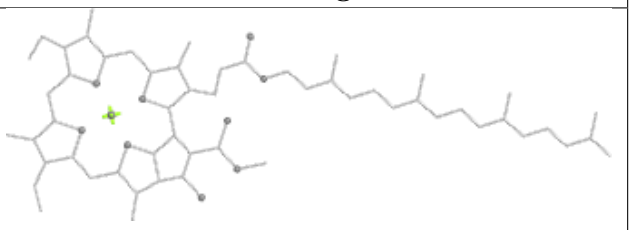
Bond lengths



Bond angles

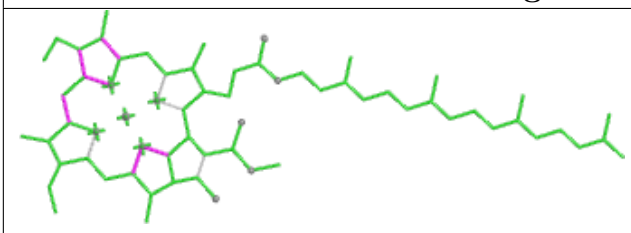


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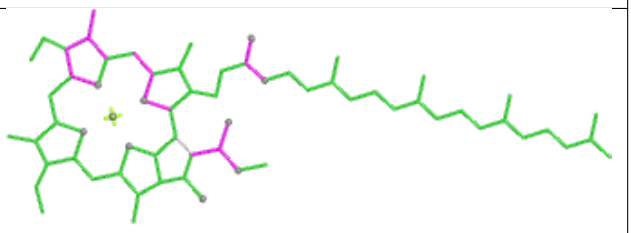


Rings

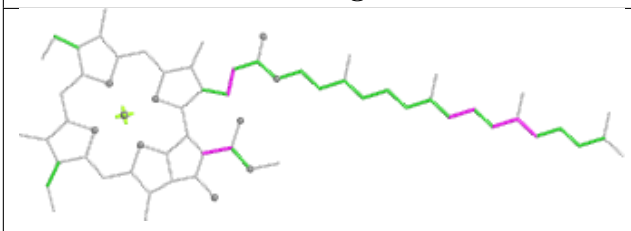
Ligand CLA A 839



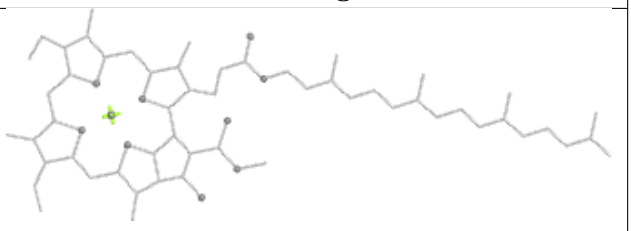
Bond lengths



Bond angles

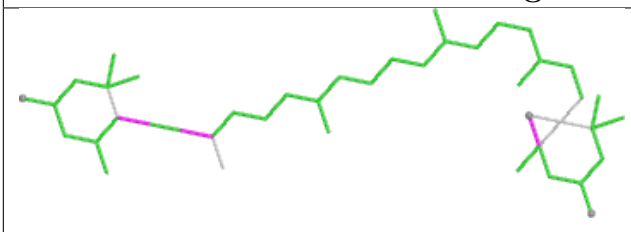


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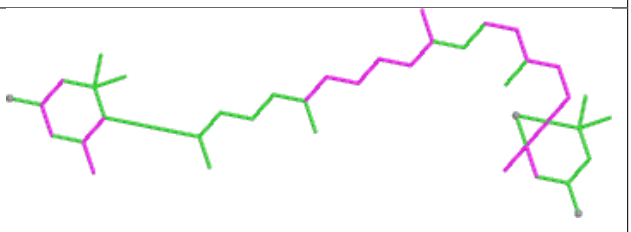


Rings

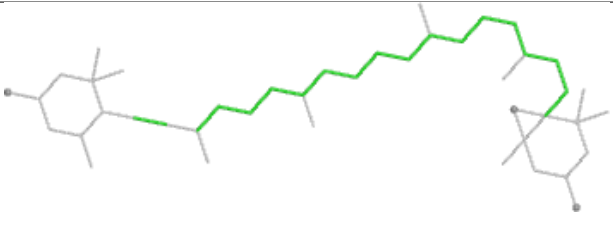
Ligand DD6 X 401



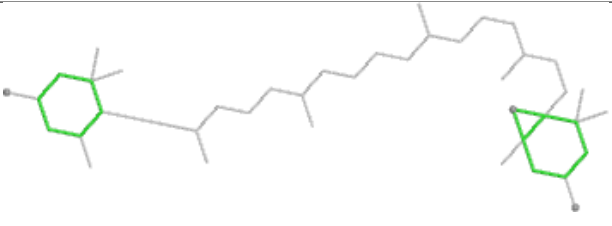
Bond lengths



Bond angles

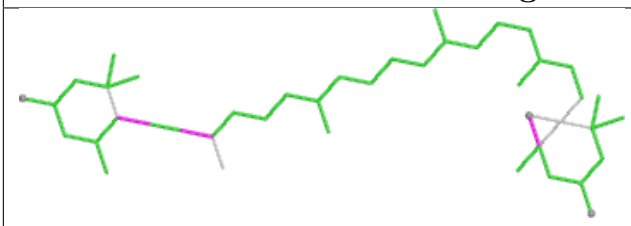


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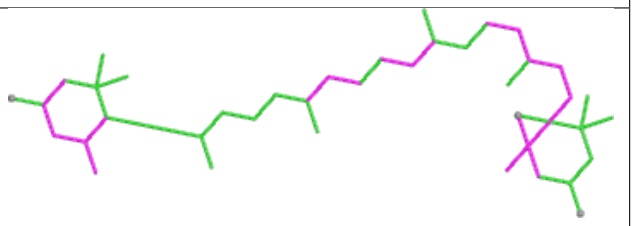


Rings

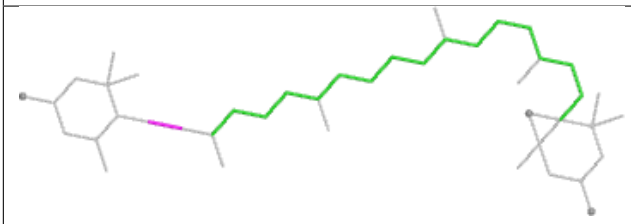
Ligand DD6 W 417



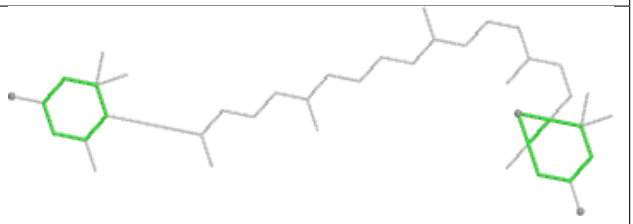
Bond lengths



Bond angles

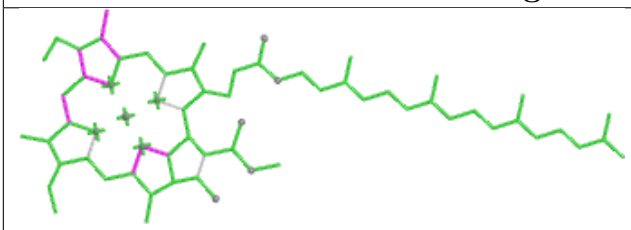


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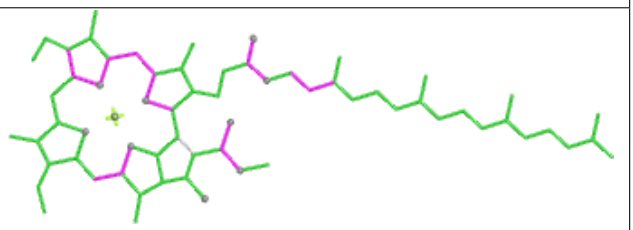


Rings

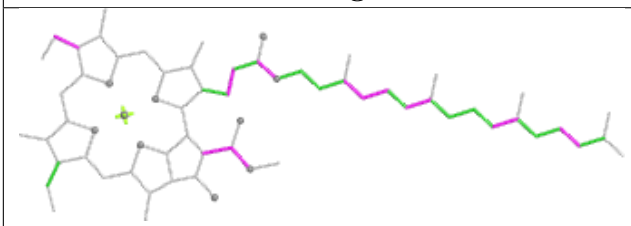
Ligand CLA H 311



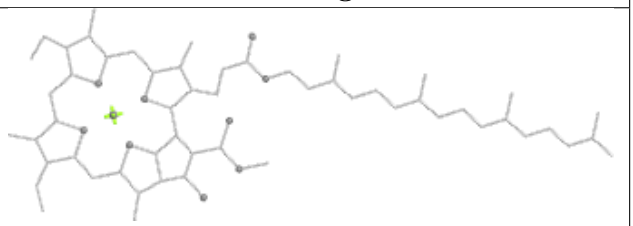
Bond lengths



Bond angles

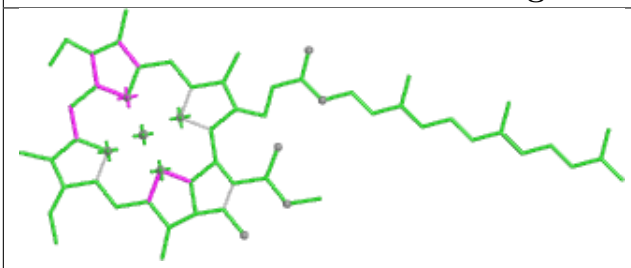


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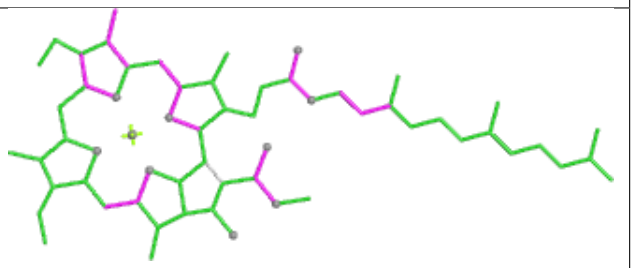


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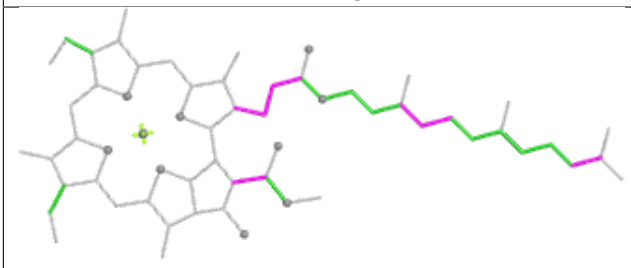
Ligand CLA S 602



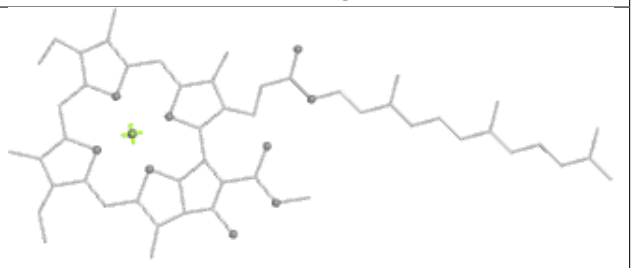
Bond lengths



Bond angles

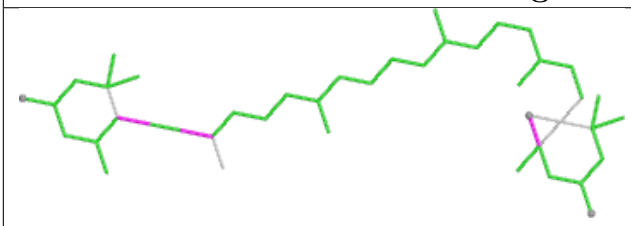


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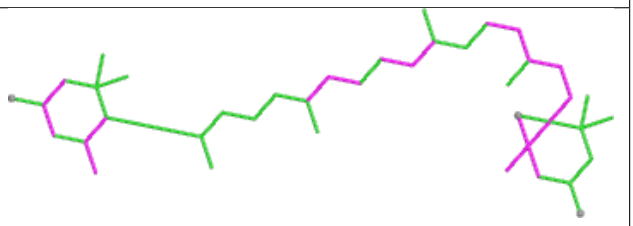


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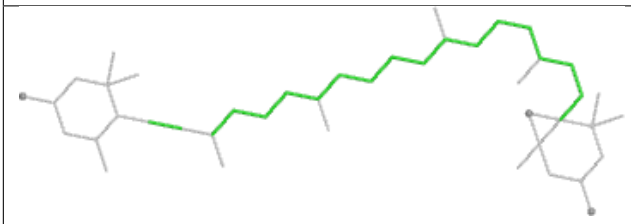
Ligand DD6 I 612



Bond lengths



Bond angles

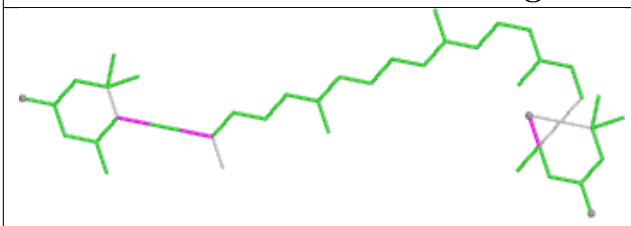


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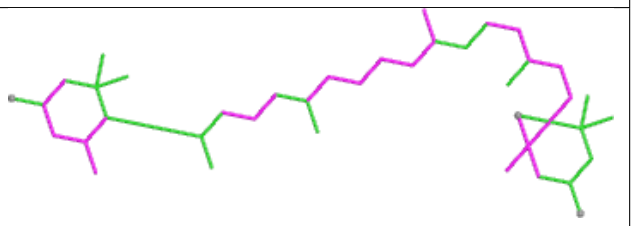


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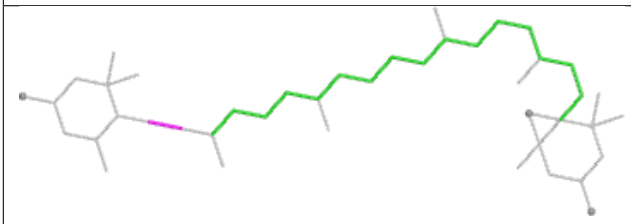
Ligand DD6 A 847



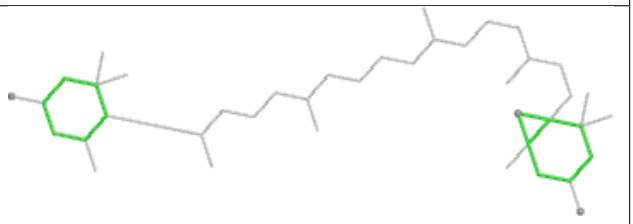
Bond lengths



Bond angles

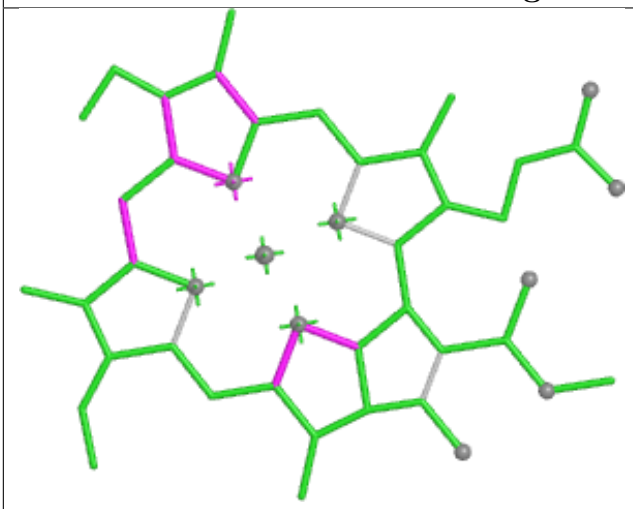


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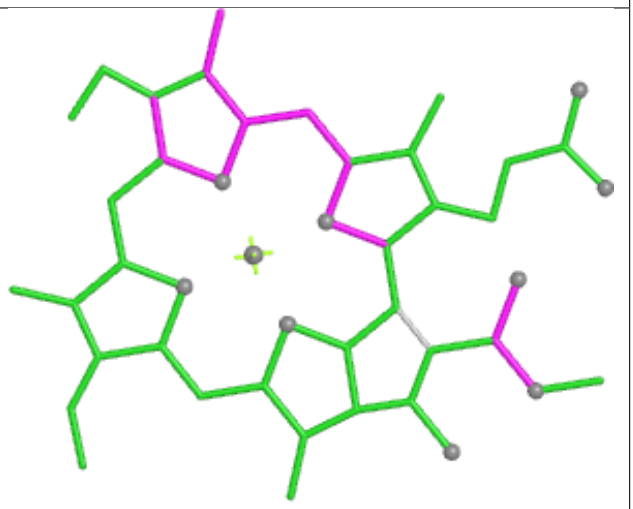


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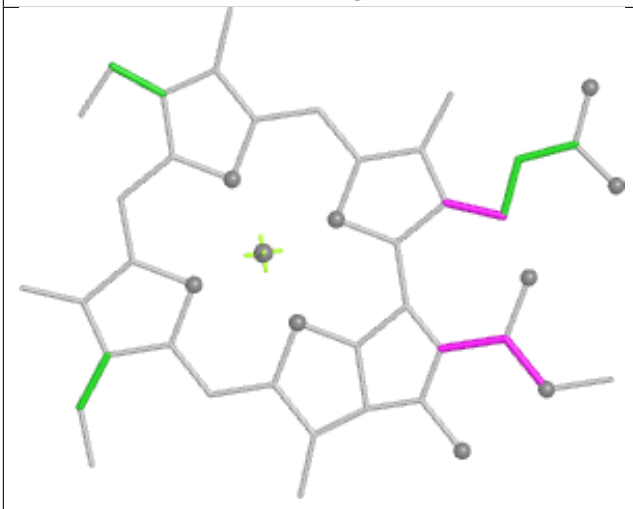
Ligand CLA U 413



Bond lengths



Bond angles

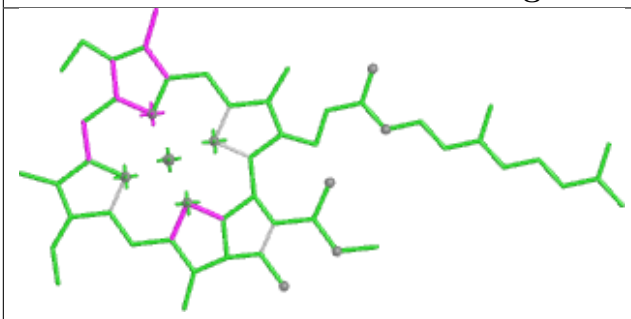


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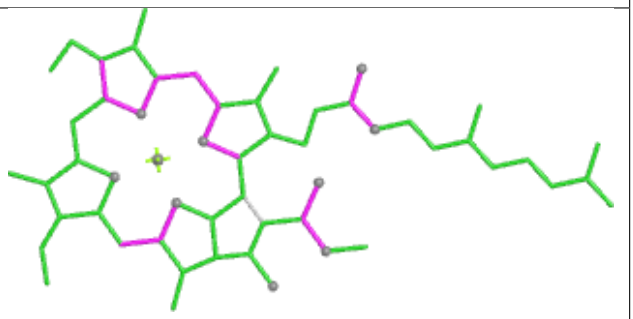


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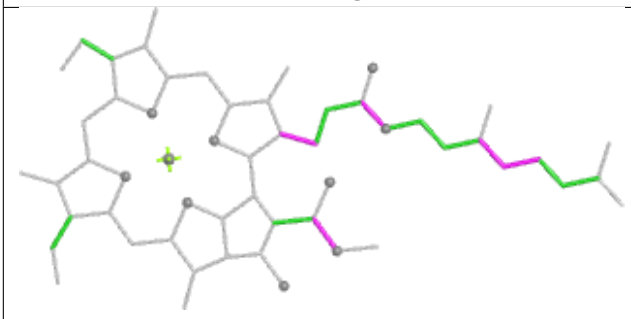
Ligand CLA U 401



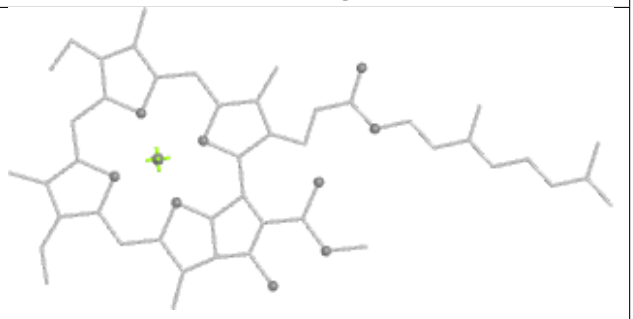
Bond lengths



Bond angles

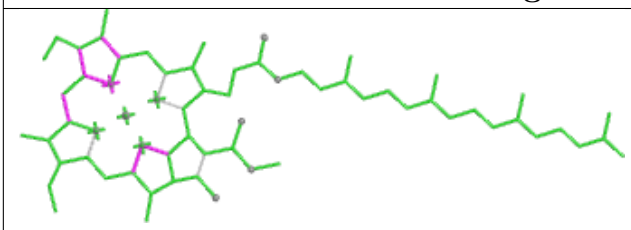


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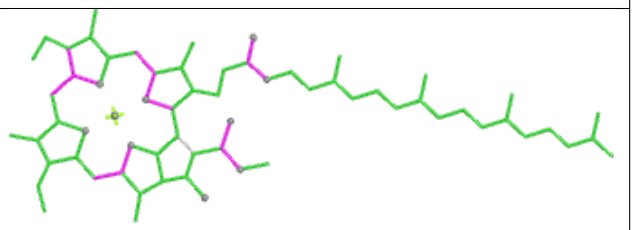


Rings

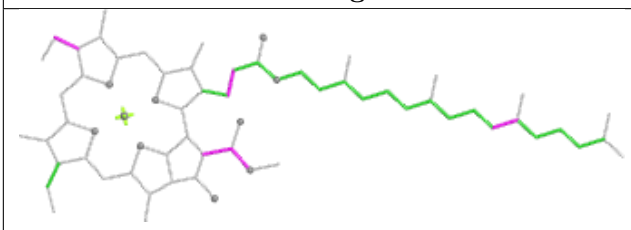
Ligand CLA V 602



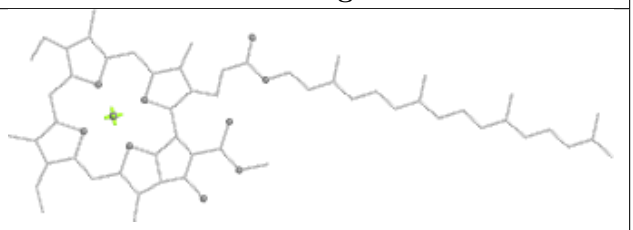
Bond lengths



Bond angles

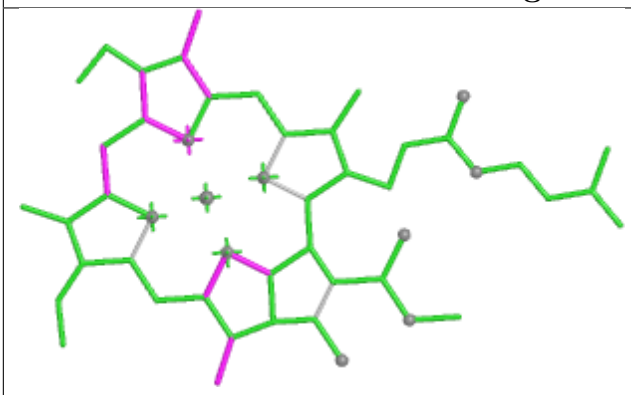


Torsions

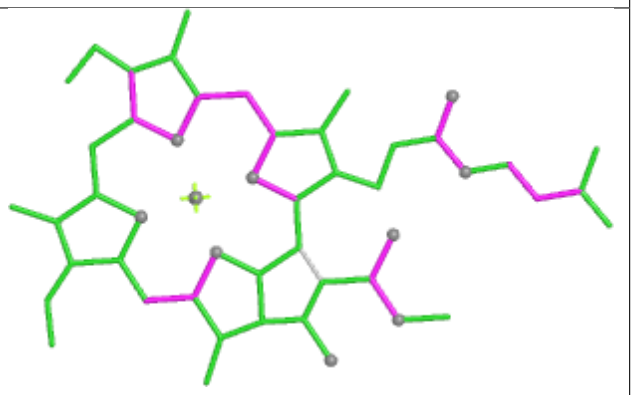


Rings

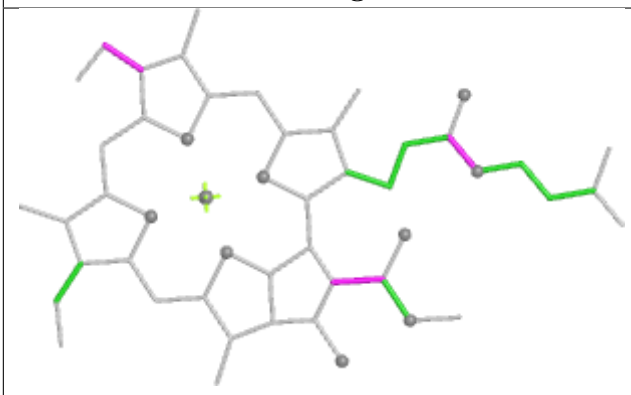
Ligand CLA A 837



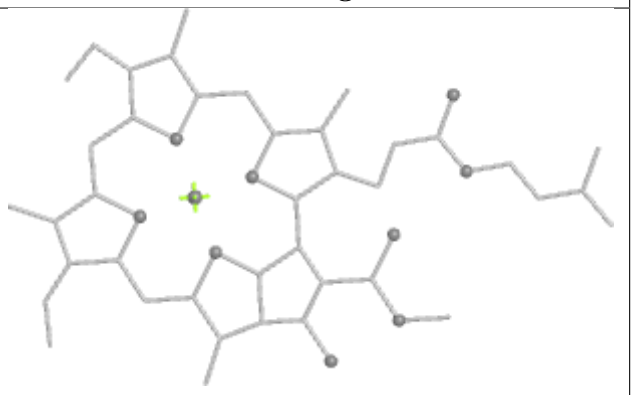
Bond lengths



Bond angles

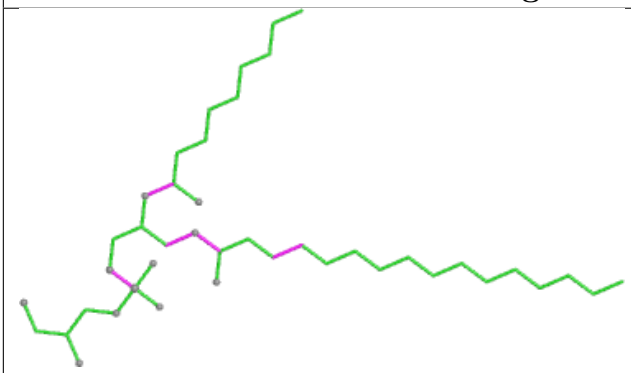


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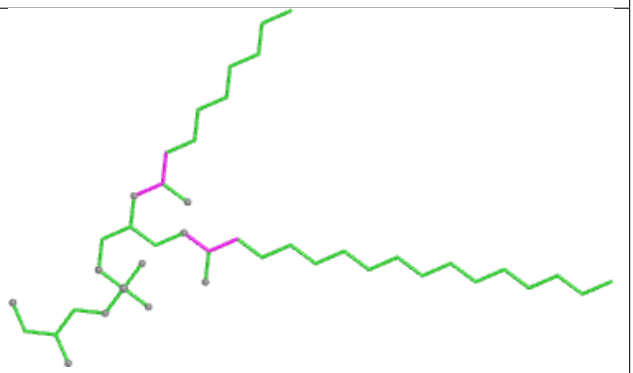


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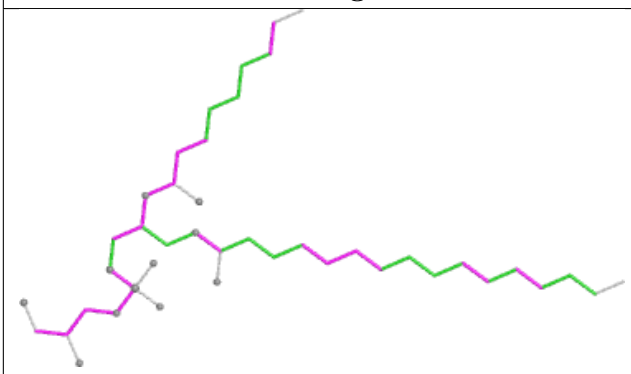
Ligand LHG O 324



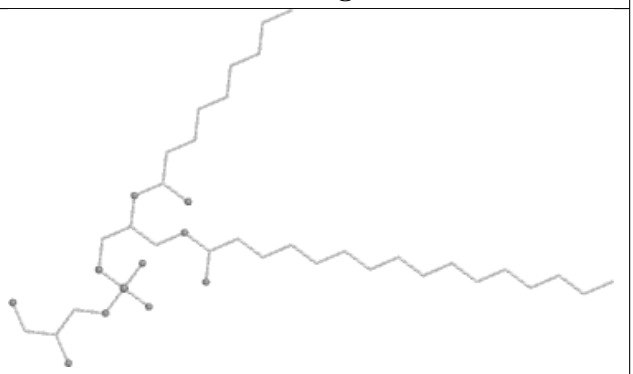
Bond lengths



Bond angles

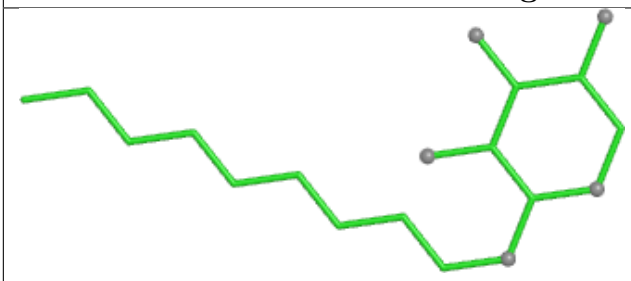


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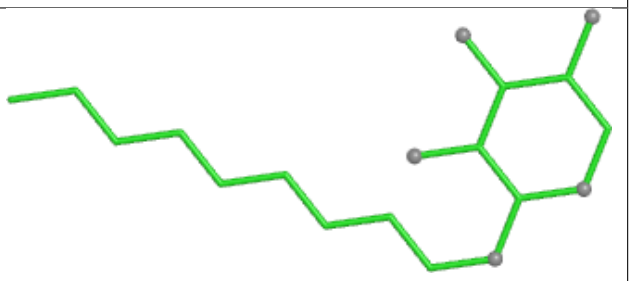


Rings

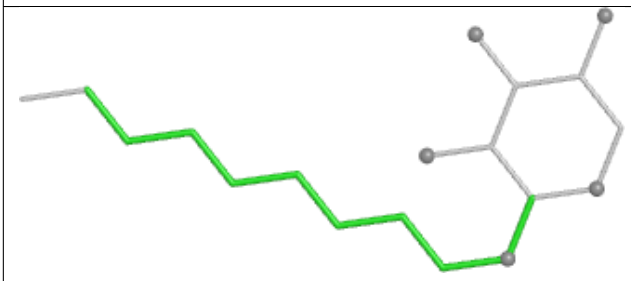
Ligand LMU B 853



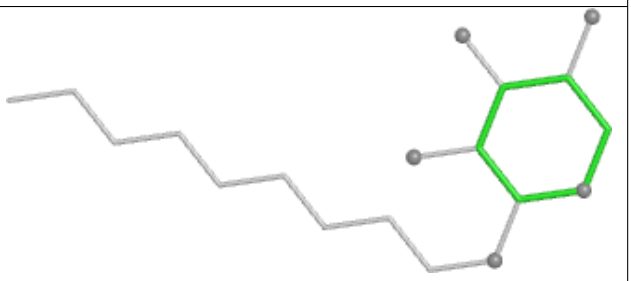
Bond lengths



Bond angles

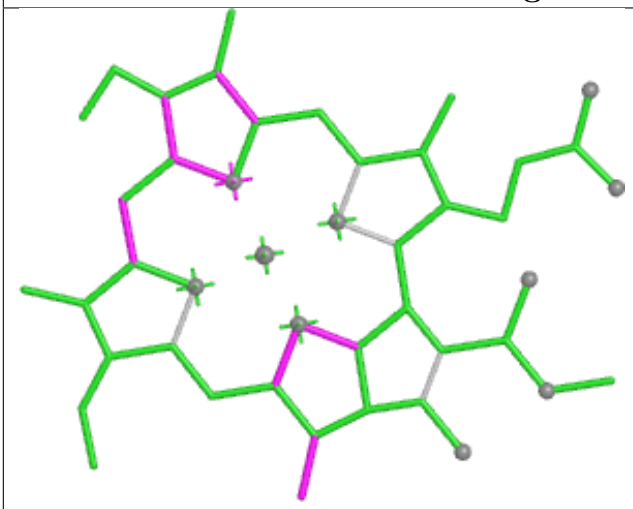


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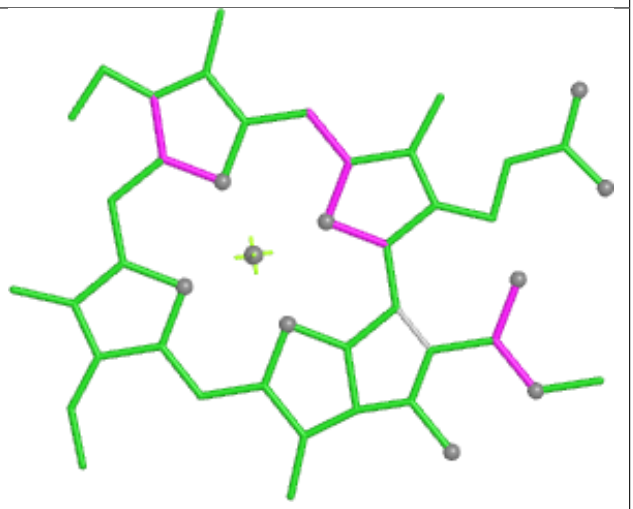


Rings

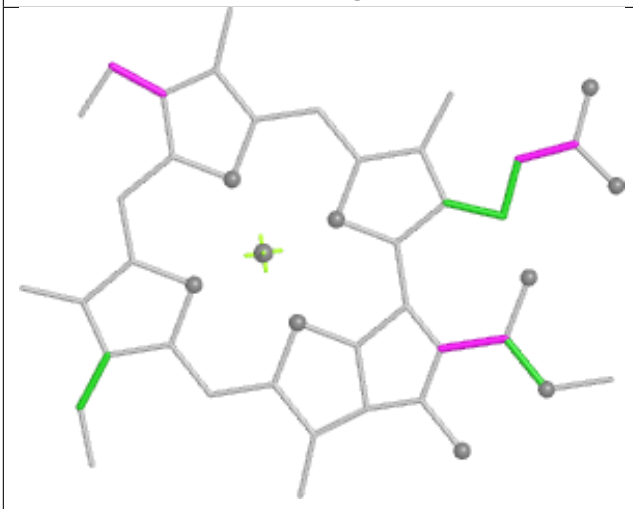
Ligand CLA V 611



Bond lengths



Bond angles

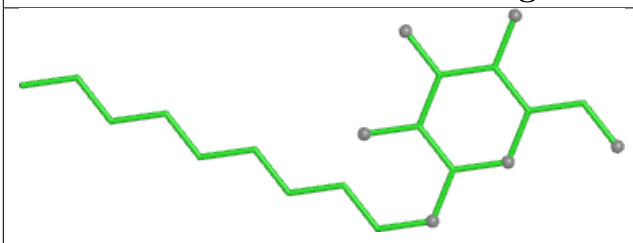


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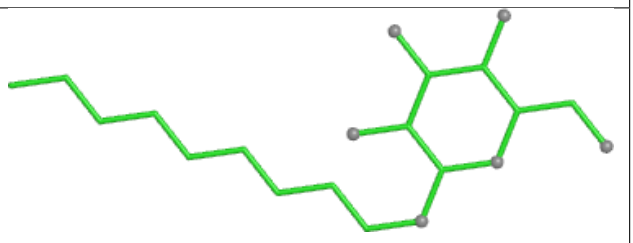


Rings

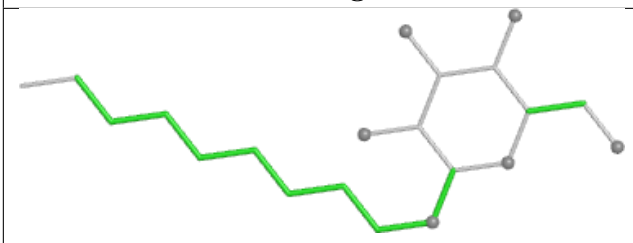
Ligand LMU G 615



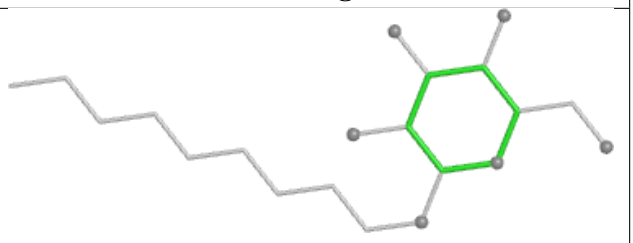
Bond lengths



Bond angles

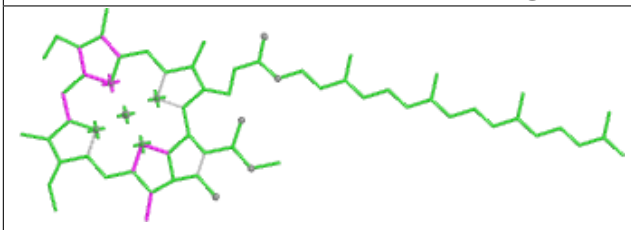


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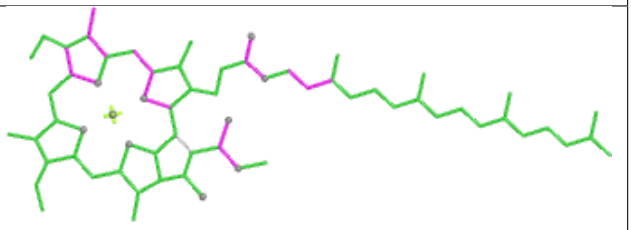


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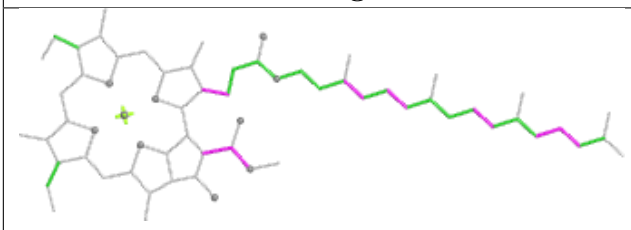
Ligand CLA X 409



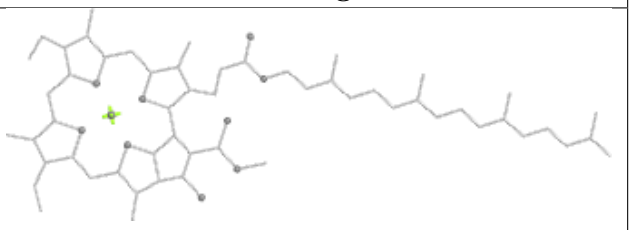
Bond lengths



Bond angles

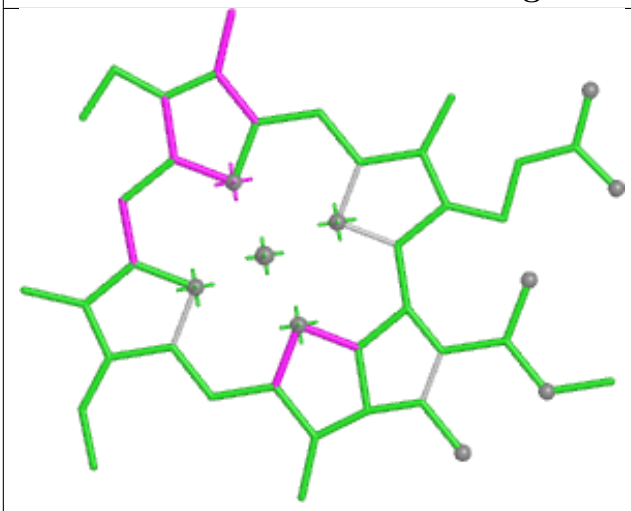


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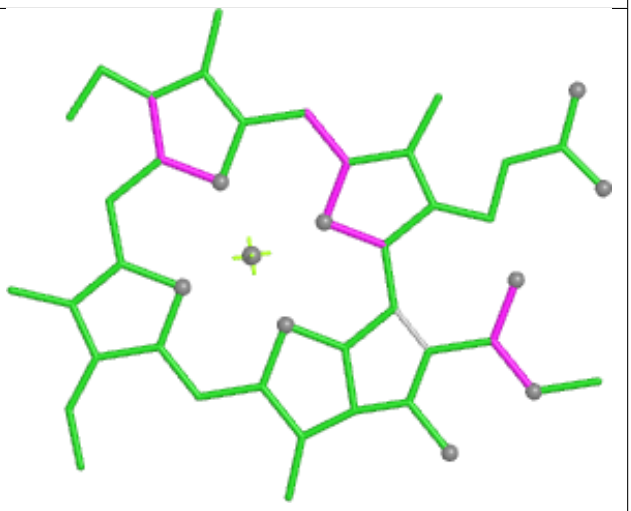


Rings

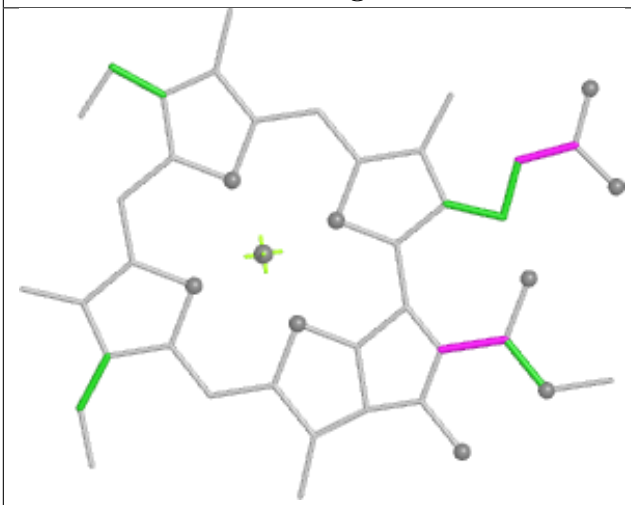
Ligand CLA G 605



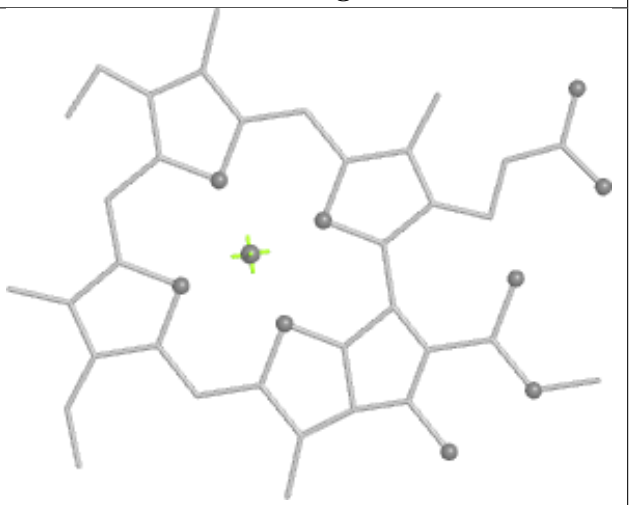
Bond lengths



Bond angles

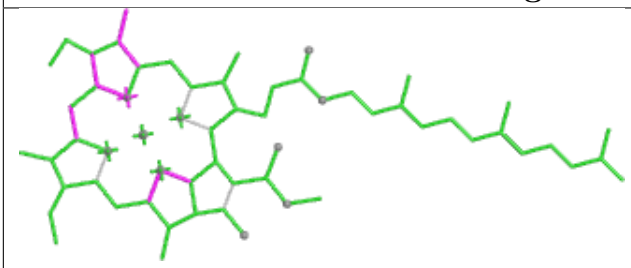


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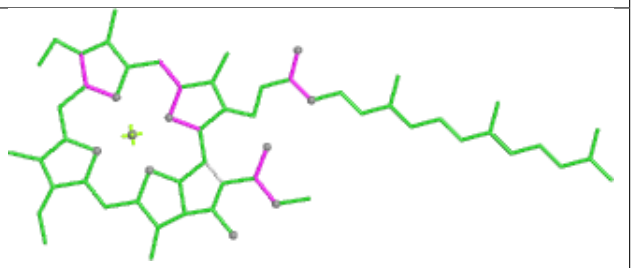


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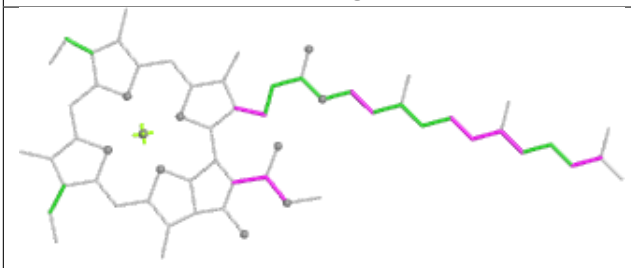
Ligand CLA B 821



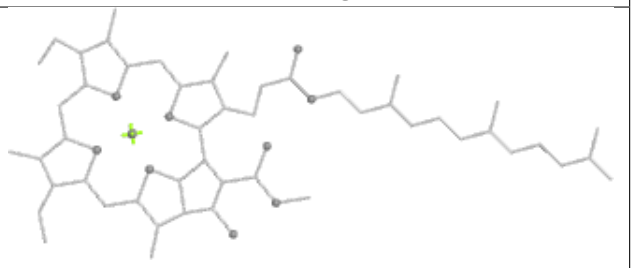
Bond lengths



Bond angles

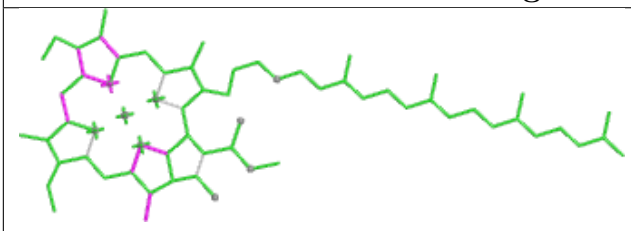


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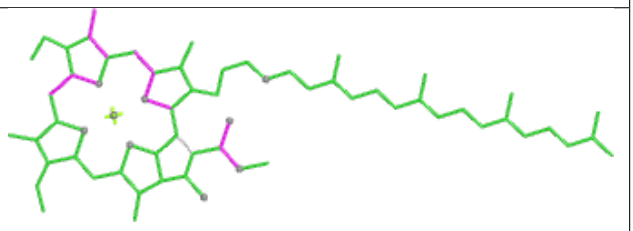


Rings

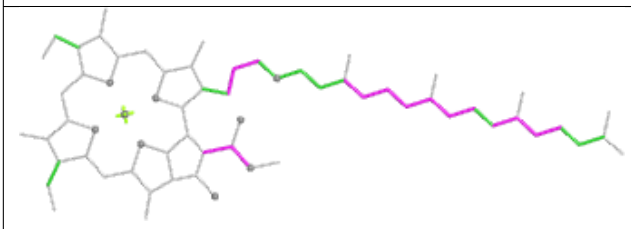
Ligand CLA K 604



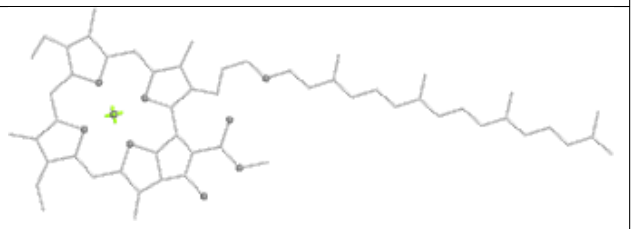
Bond lengths



Bond angles

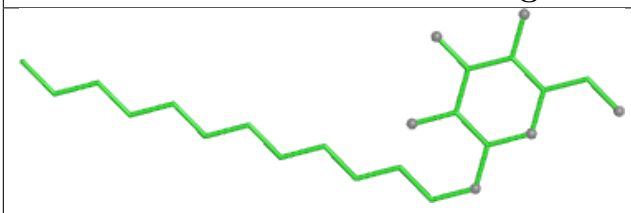


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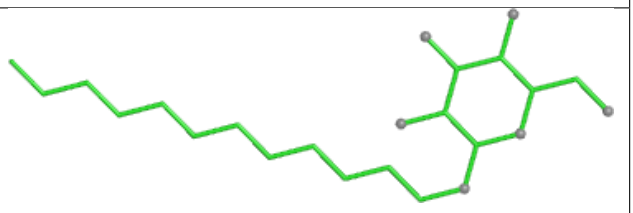


Rings

Ligand LMU T 618



Bond lengths



Bond angles

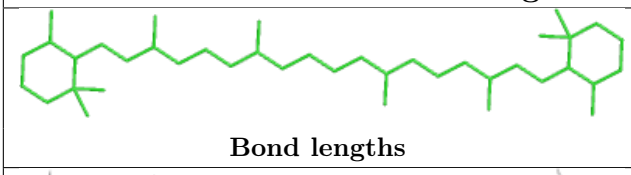


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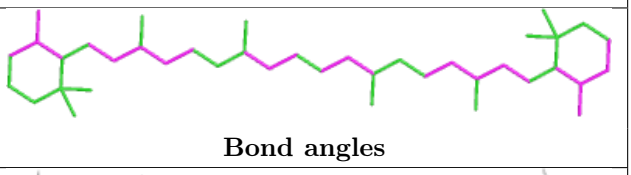


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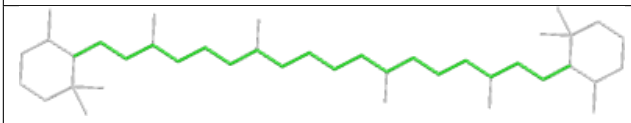
Ligand BCR A 848



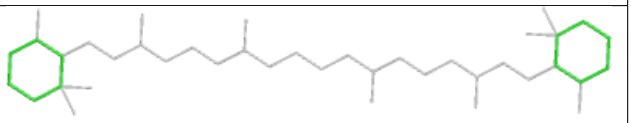
Bond lengths



Bond angles

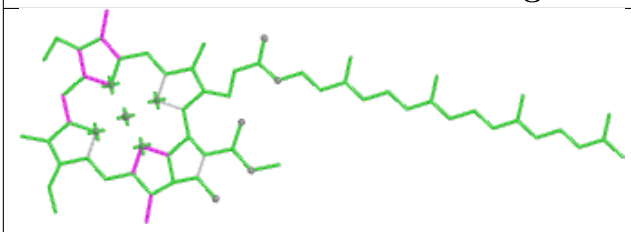


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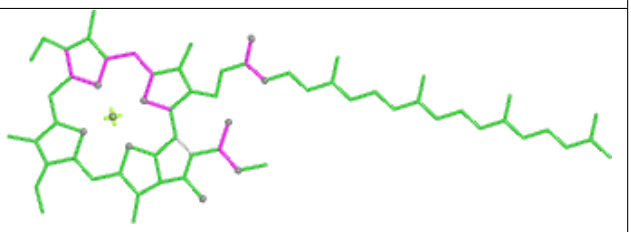


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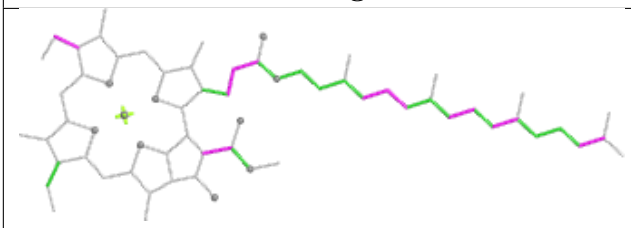
Ligand CLA X 412



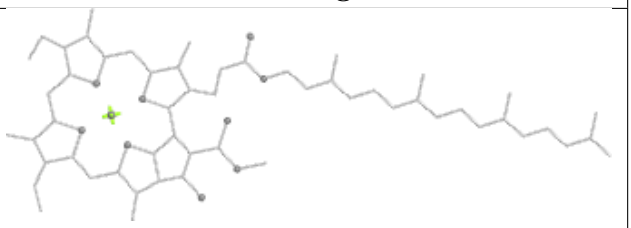
Bond lengths



Bond angles

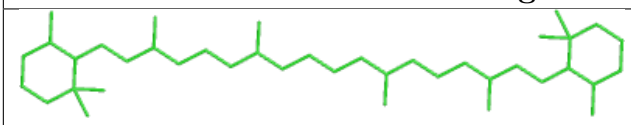


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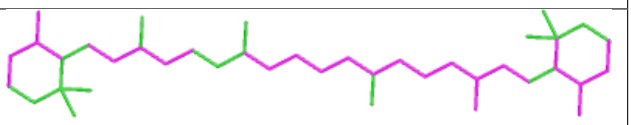


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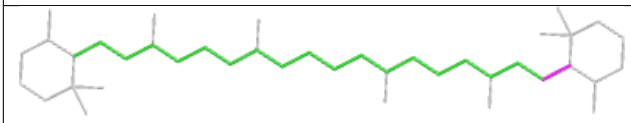
Ligand BCR M 101



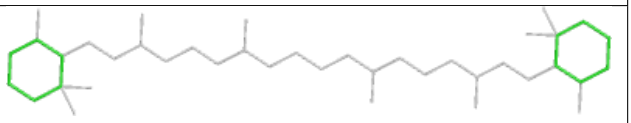
Bond lengths



Bond angles

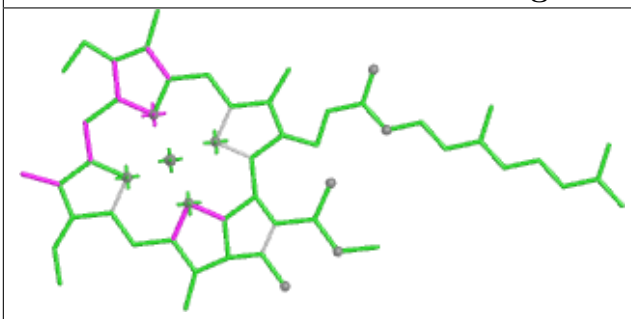


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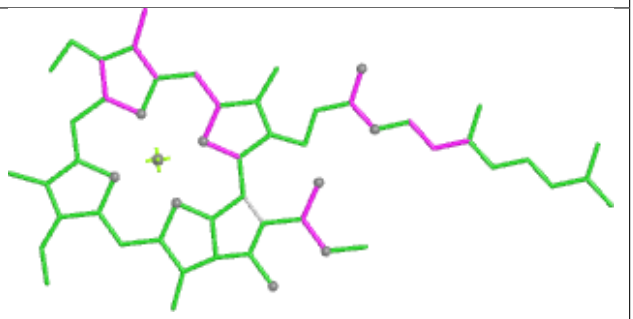


Rings

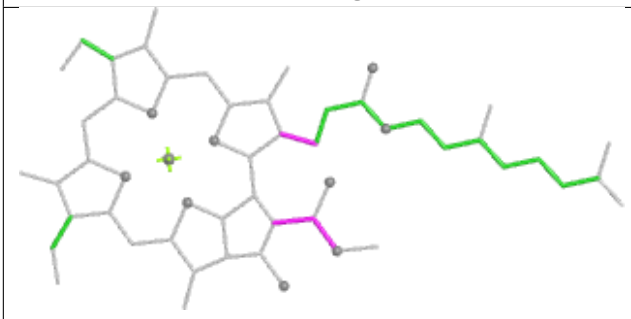
Ligand CLA I 607



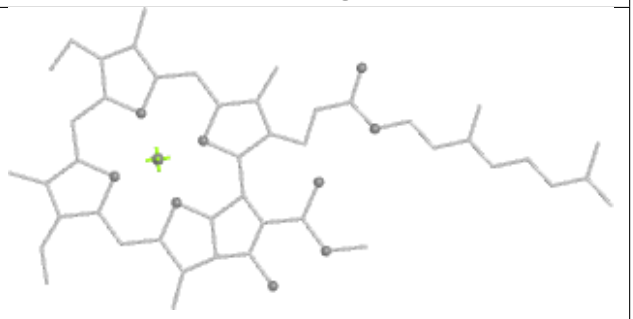
Bond lengths



Bond angles

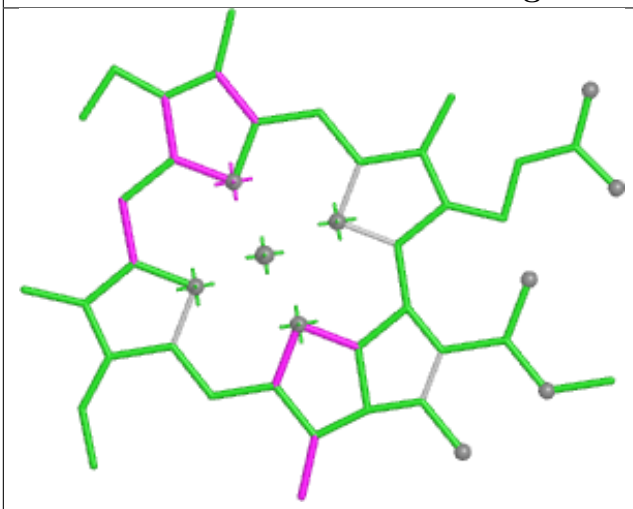


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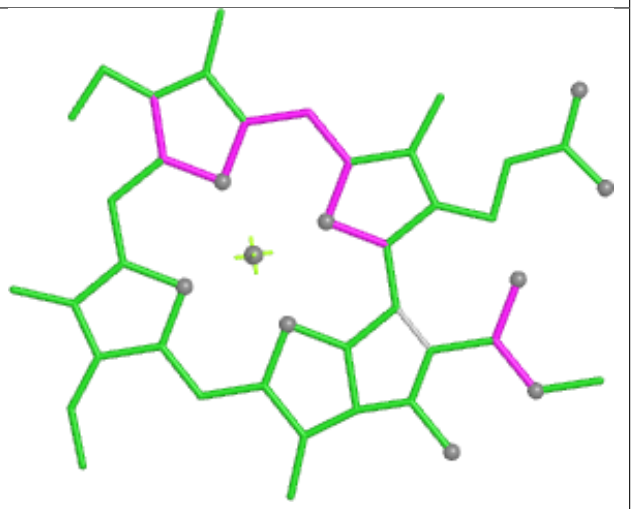


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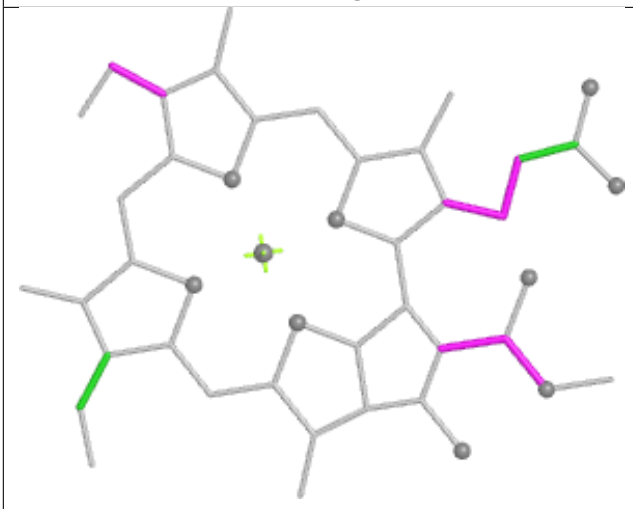
Ligand CLA U 420



Bond lengths



Bond angles

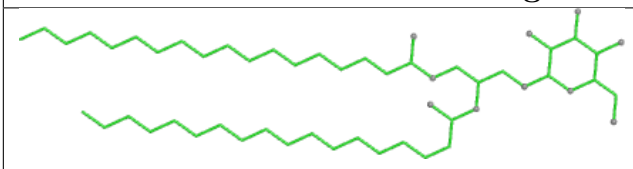


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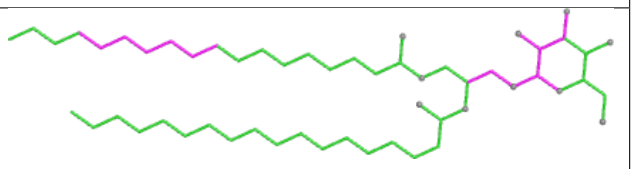


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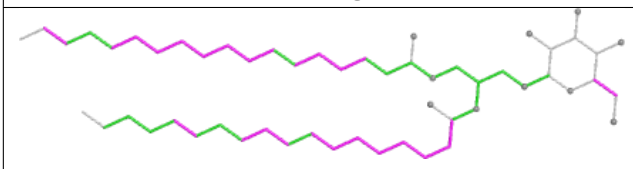
Ligand LMG J 101



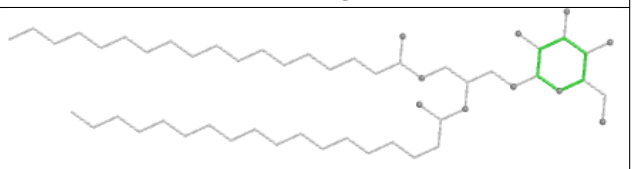
Bond lengths



Bond angles

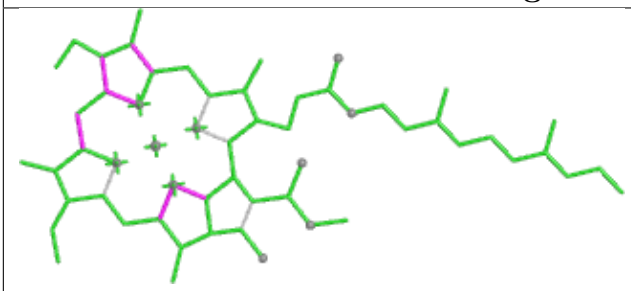


Torsions

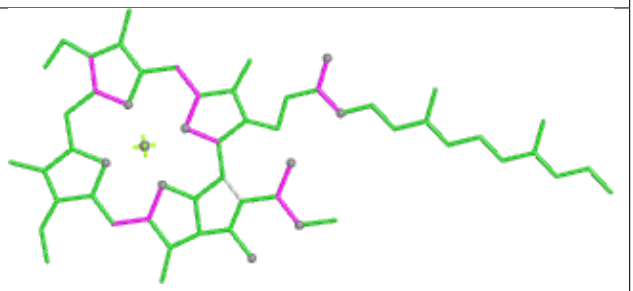


Rings

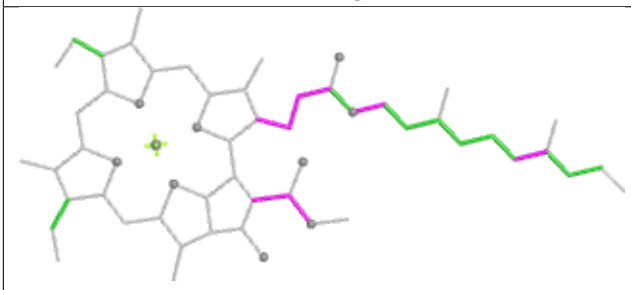
Ligand CLA R 606



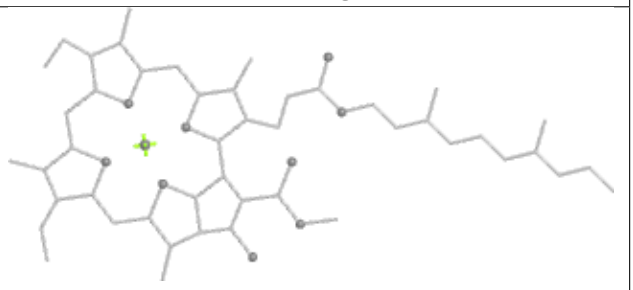
Bond lengths



Bond angles

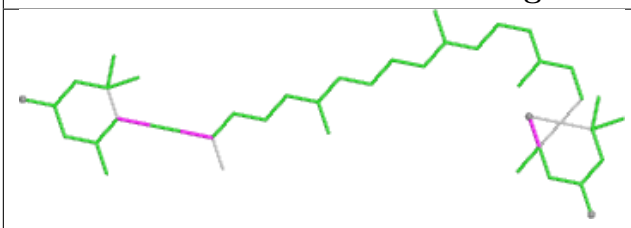


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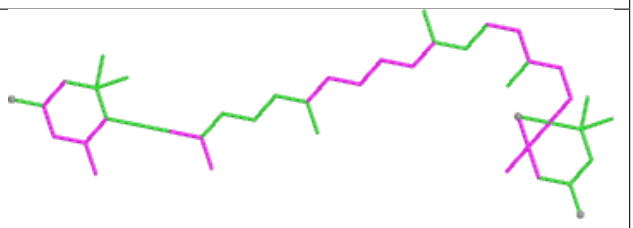


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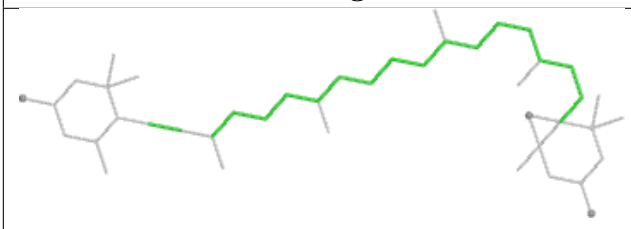
Ligand DD6 N 612



Bond lengths



Bond angles

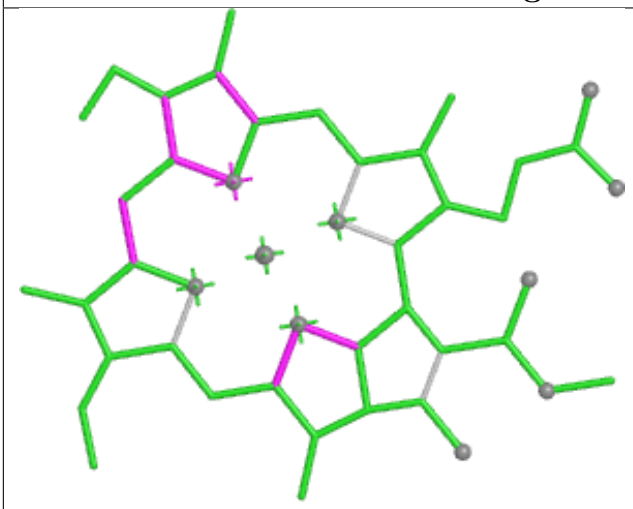


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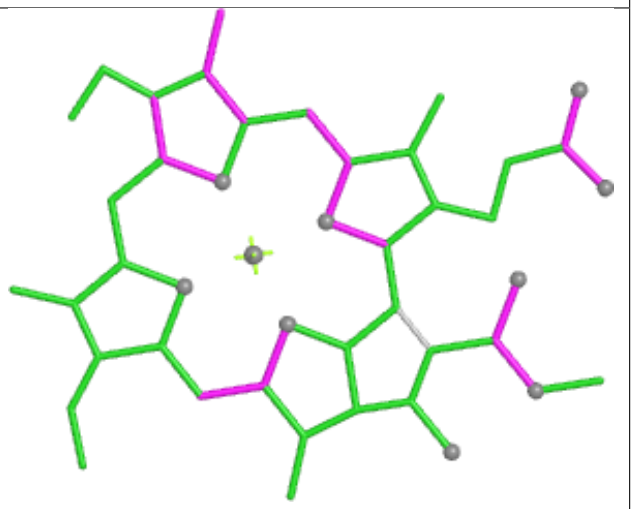


Rings

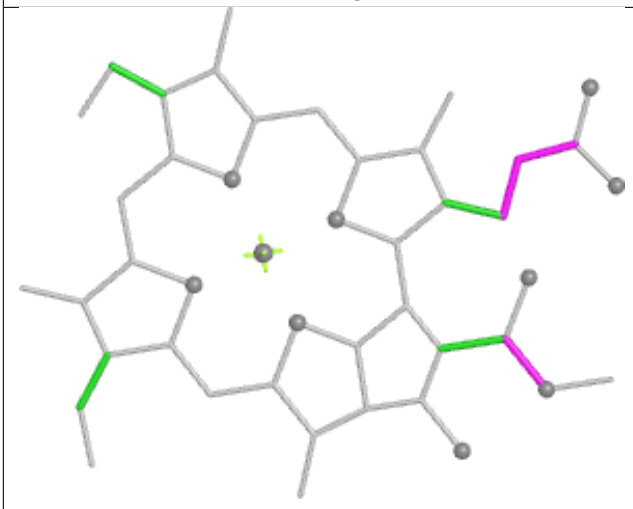
Ligand CLA R 604



Bond lengths



Bond angles

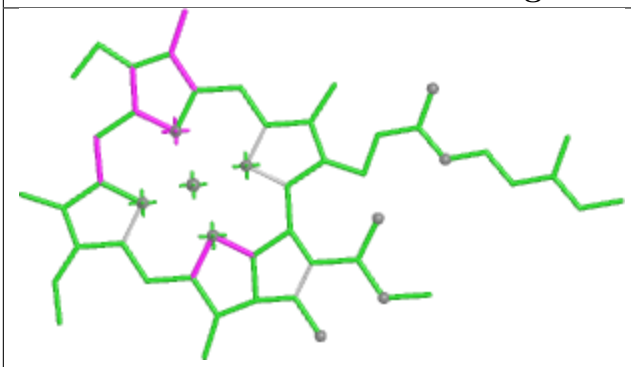


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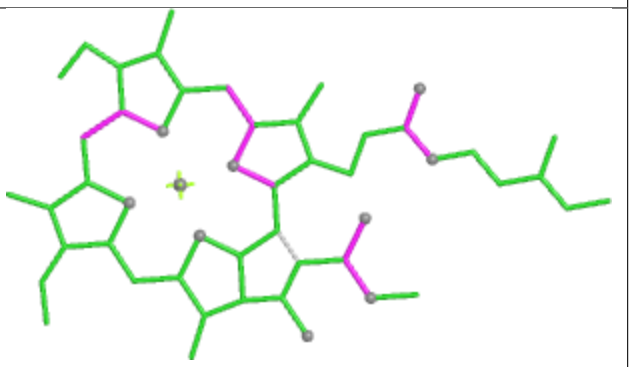


Rings

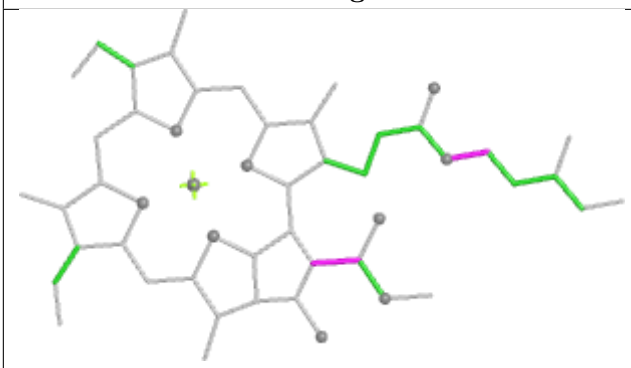
Ligand CLA B 836



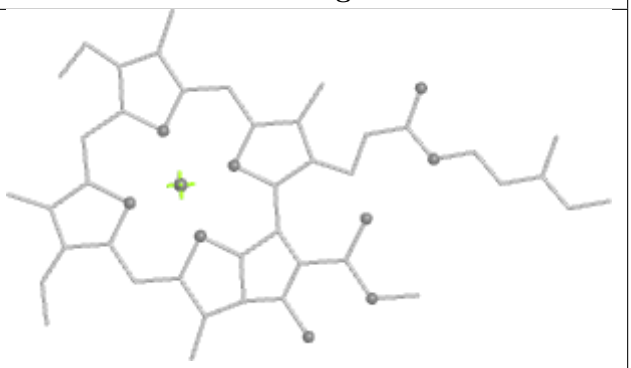
Bond lengths



Bond angles

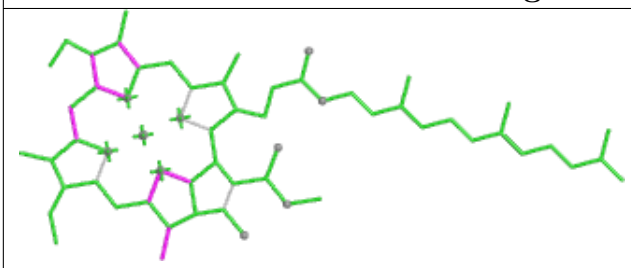


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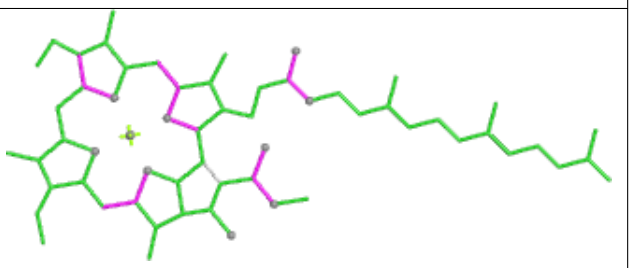


Rings

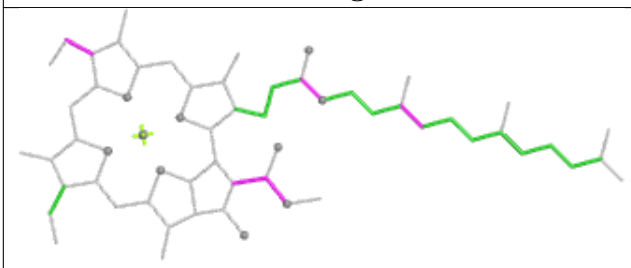
Ligand CLA O 311



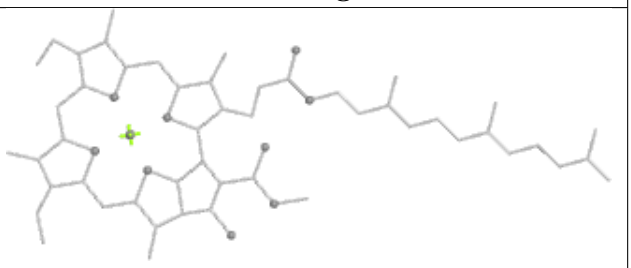
Bond lengths



Bond angles

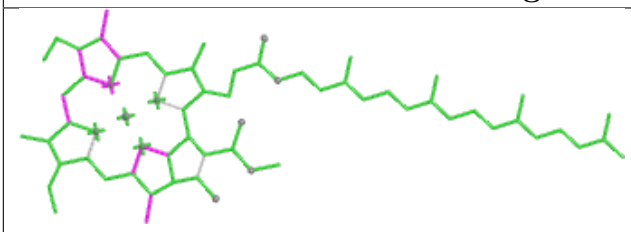


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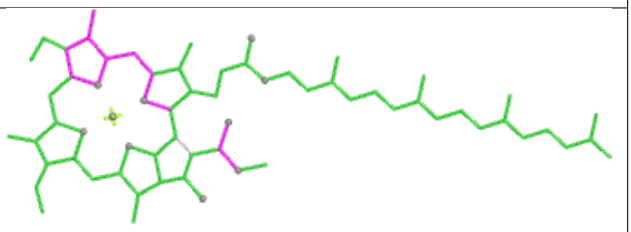


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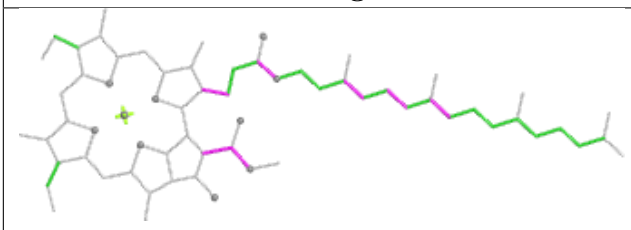
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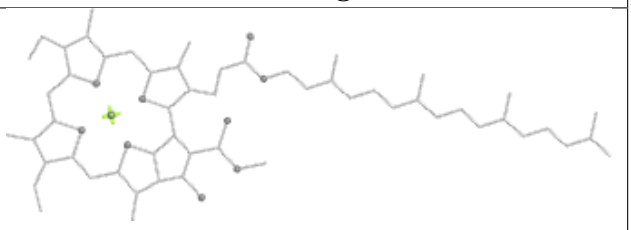
Bond lengths



Bond angles

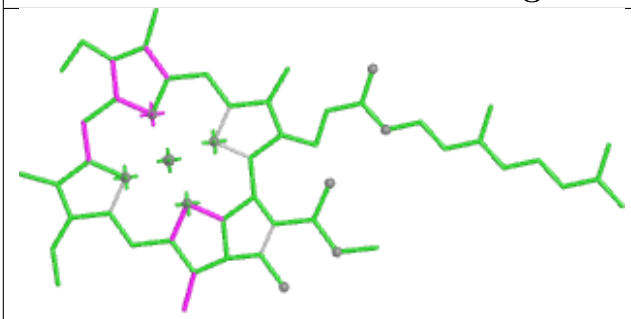


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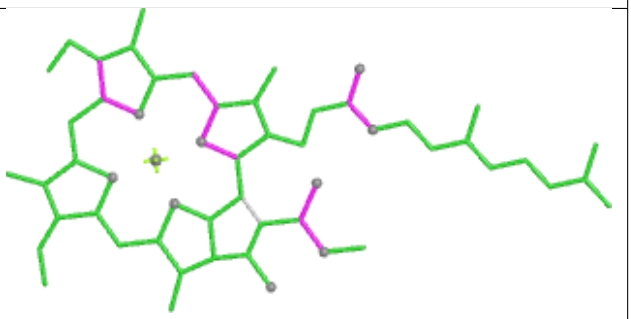


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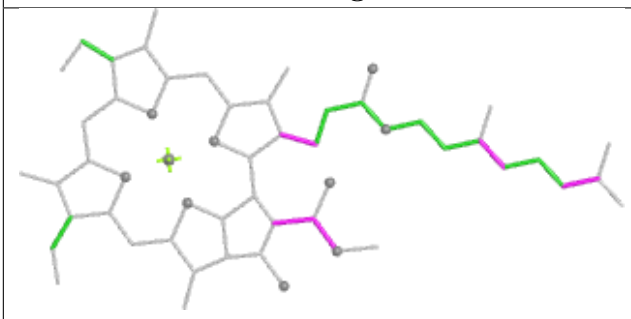
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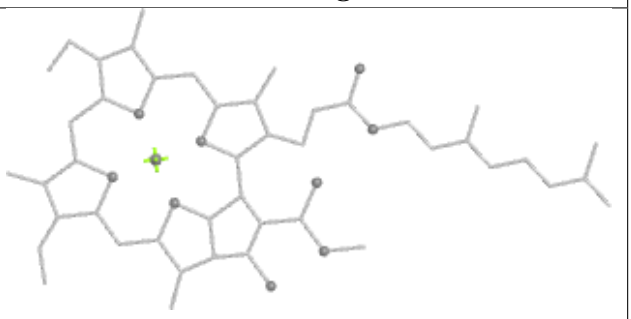
Bond lengths



Bond angles

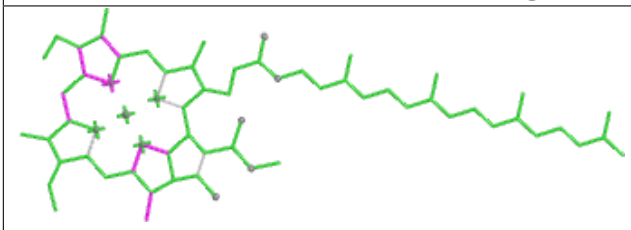


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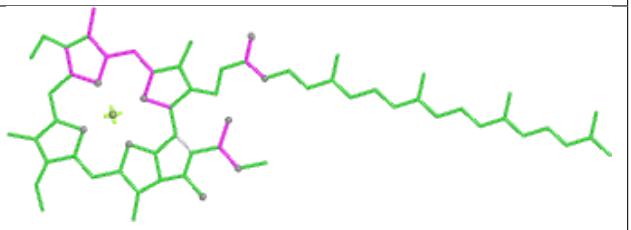


Rings

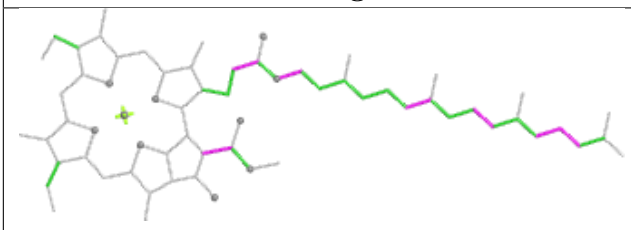
Ligand CLA N 603



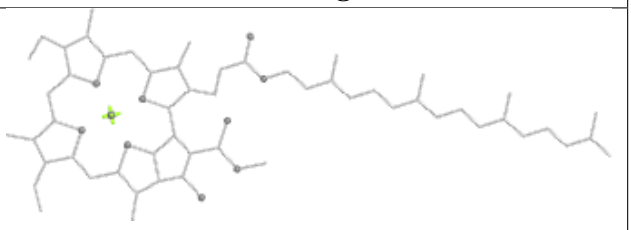
Bond lengths



Bond angles

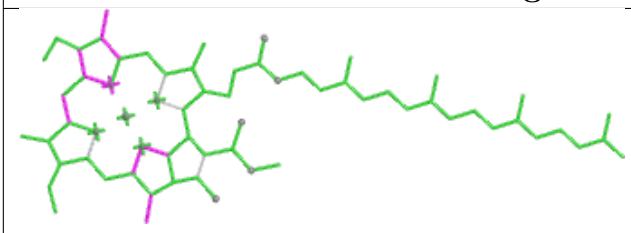


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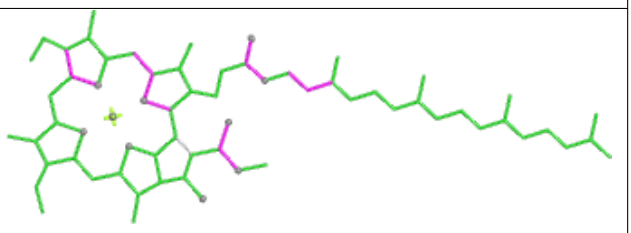


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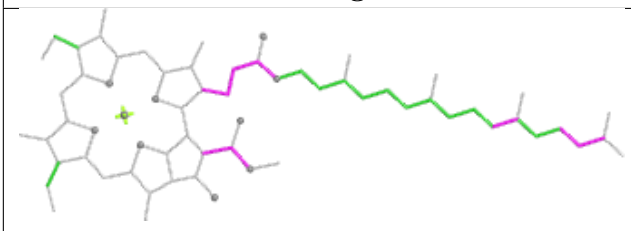
Ligand CLA A 821



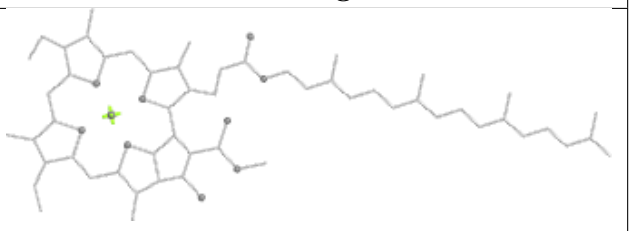
Bond lengths



Bond angles

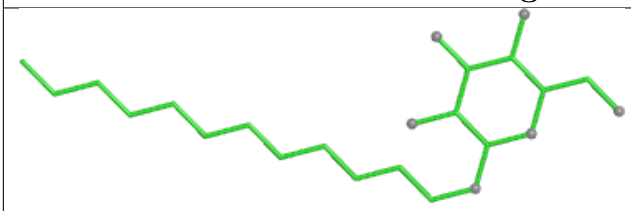


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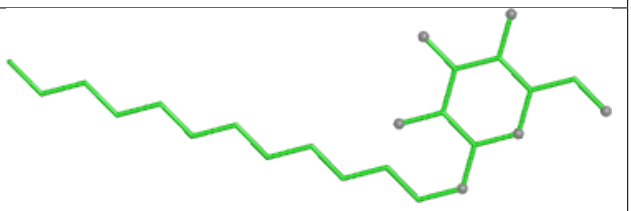


Rings

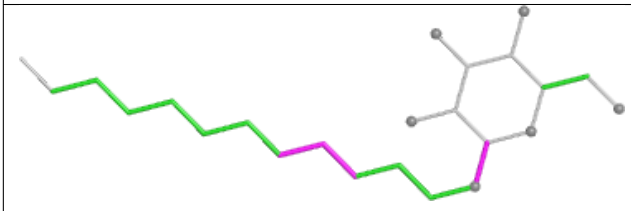
Ligand LMU T 617



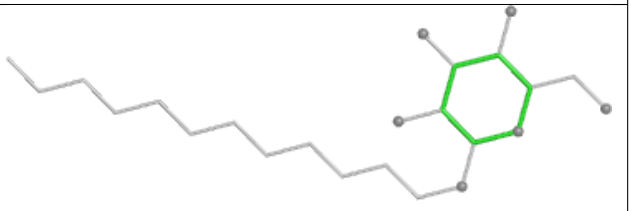
Bond lengths



Bond angles

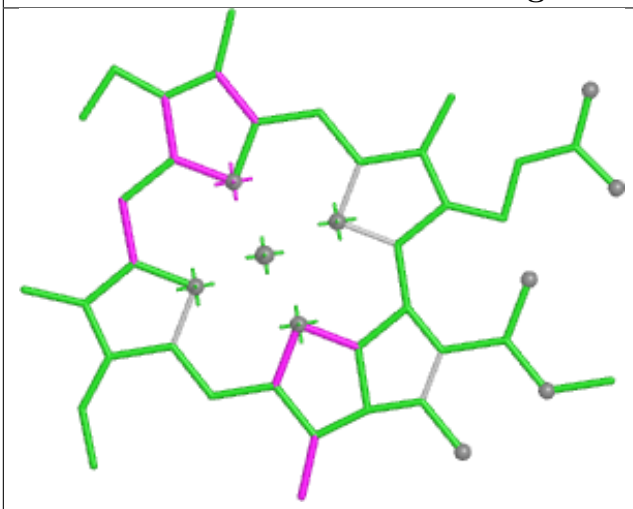


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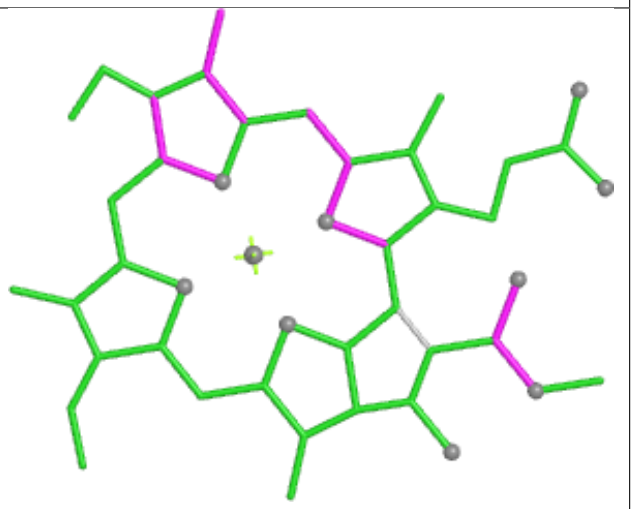


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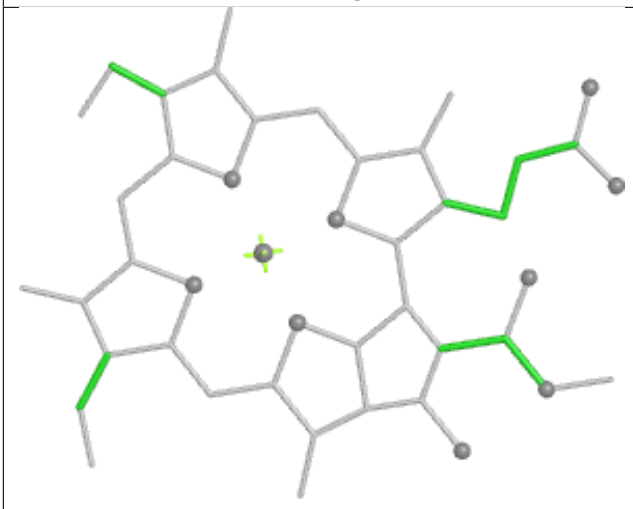
Ligand CLA S 614



Bond lengths



Bond angles

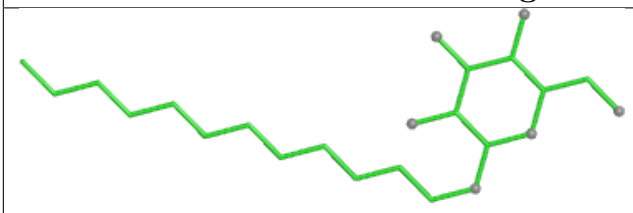


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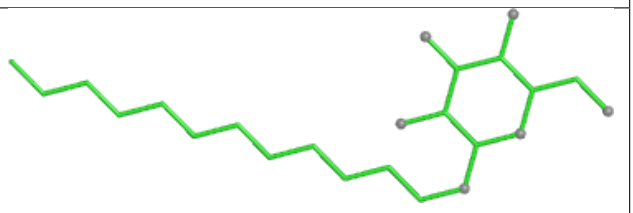


Rings

Ligand LMU A 853



Bond lengths



Bond angles

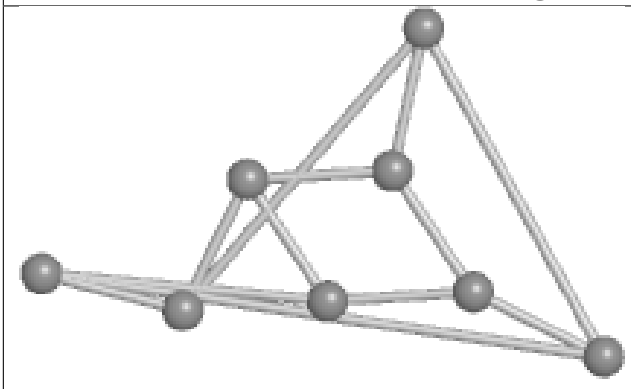


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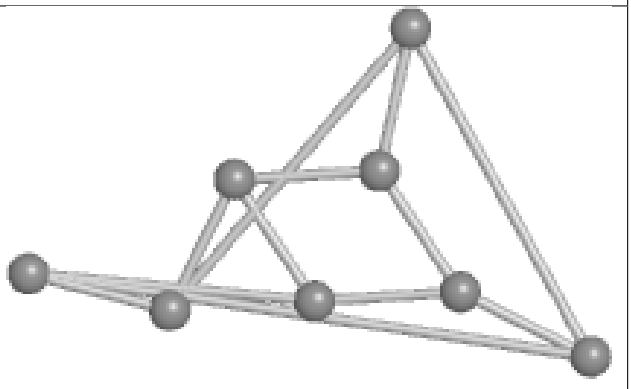


Rings

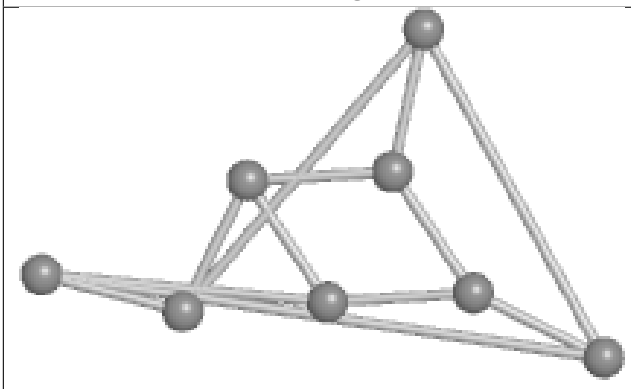
Ligand SF4 C 101



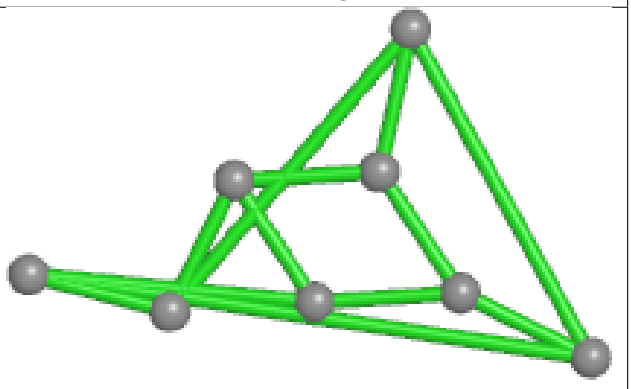
Bond lengths



Bond angles

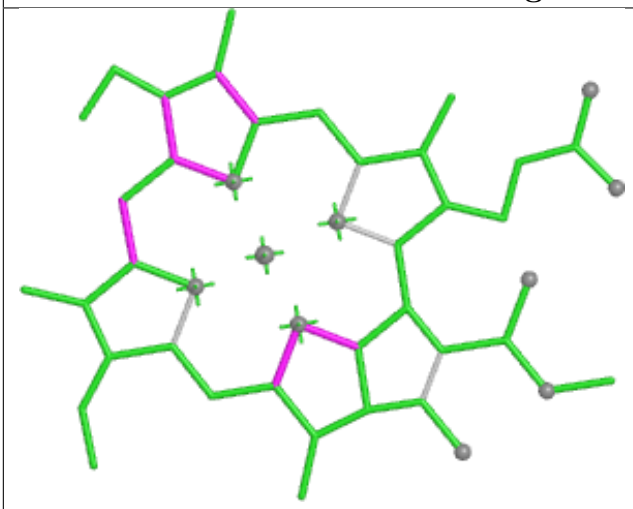


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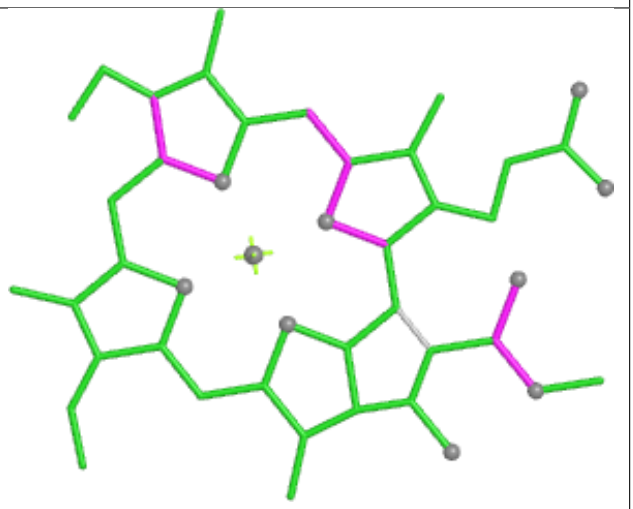


Rings

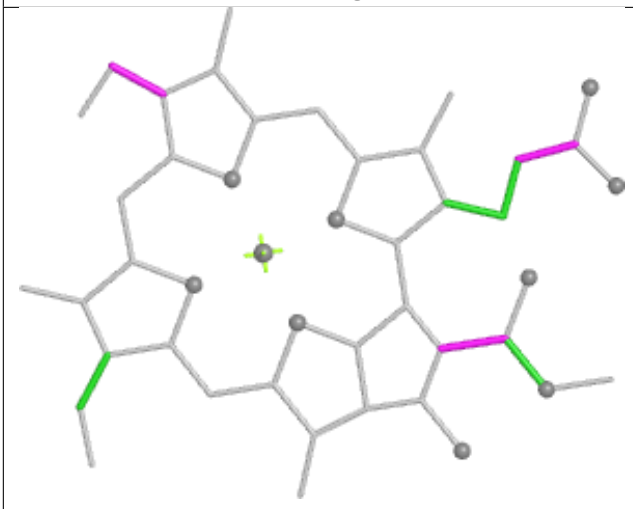
Ligand CLA P 603



Bond lengths



Bond angles

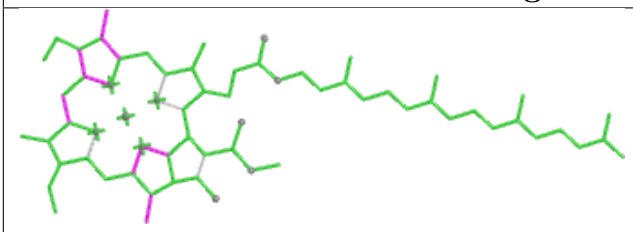


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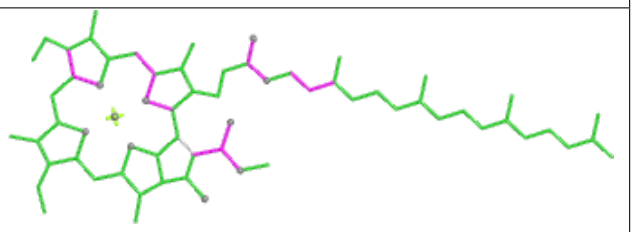


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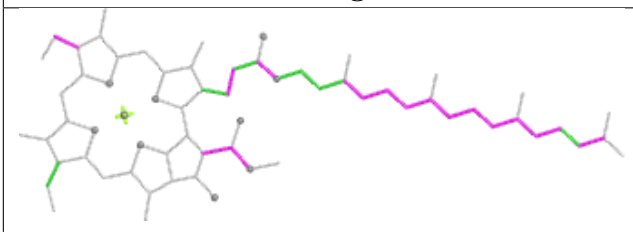
Ligand CLA A 824



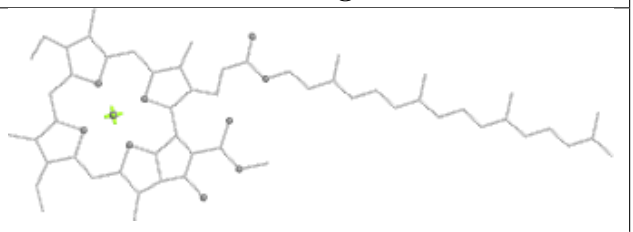
Bond lengths



Bond angles

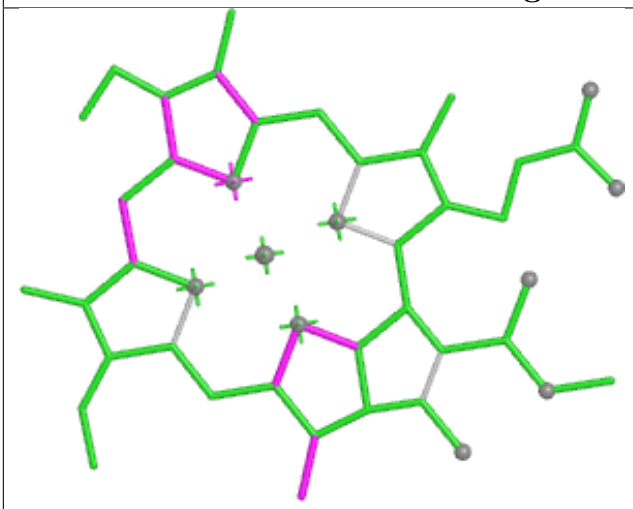


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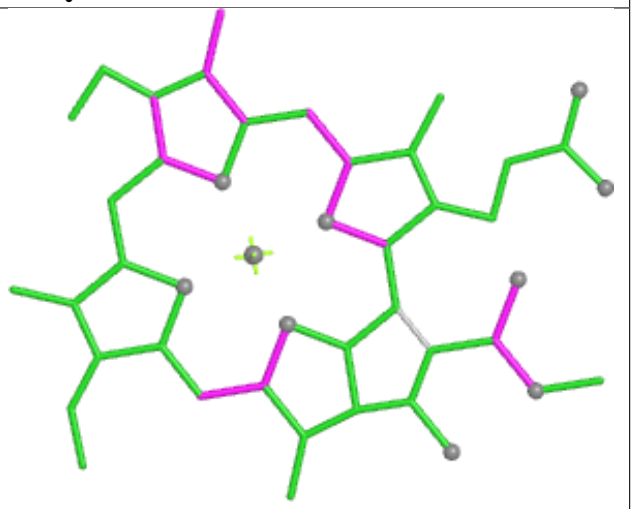


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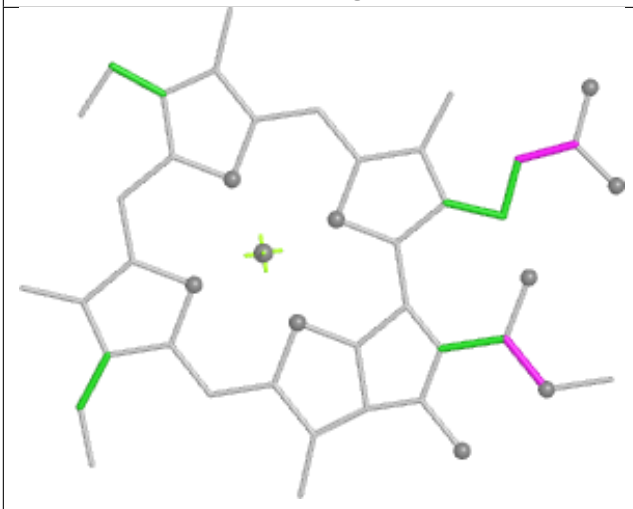
Ligand CLA Q 603



Bond lengths



Bond angles

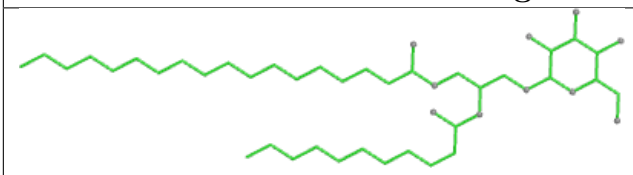


Torsions

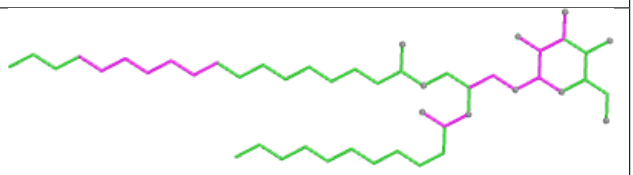


Rings

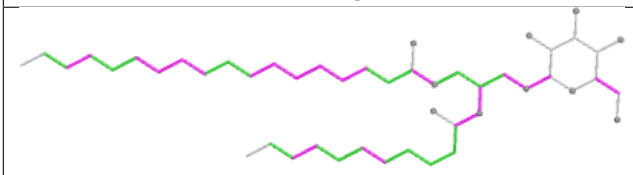
Ligand LMG W 401



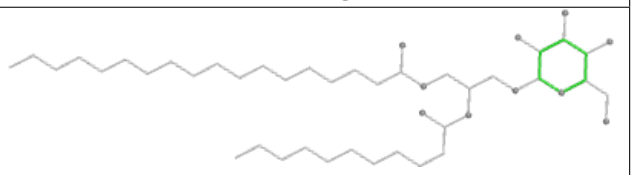
Bond lengths



Bond angles

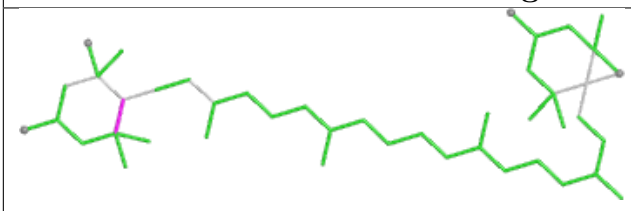


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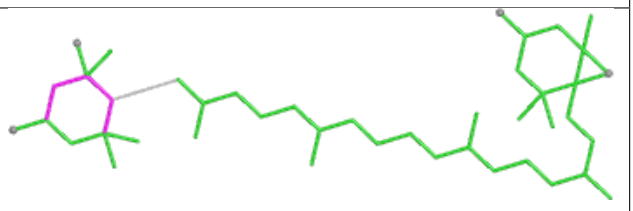


Rings

Ligand NEX U 418



Bond lengths



Bond angles

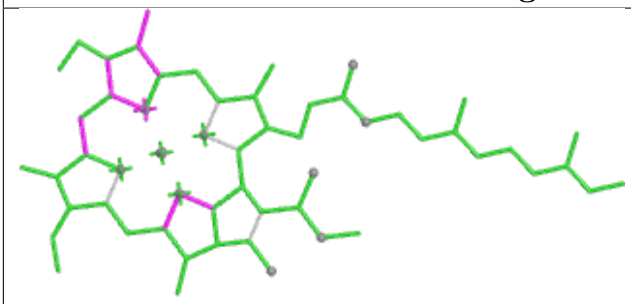


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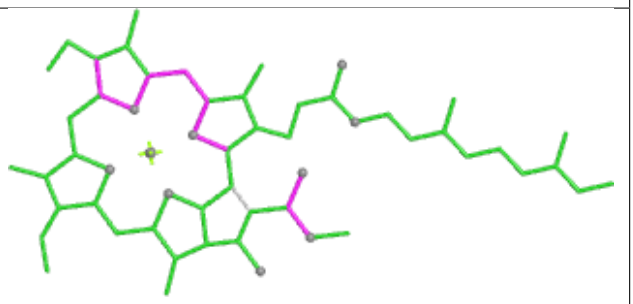


Rings

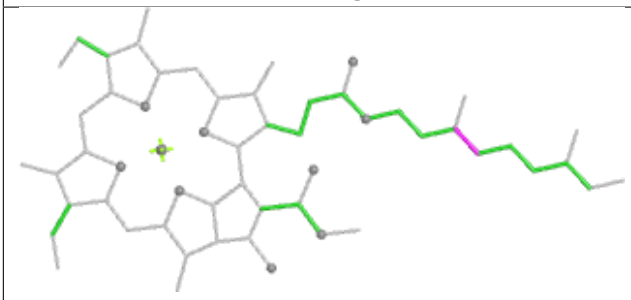
Ligand CLA W 406



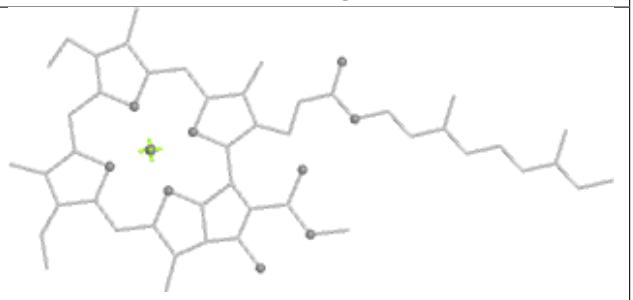
Bond lengths



Bond angles

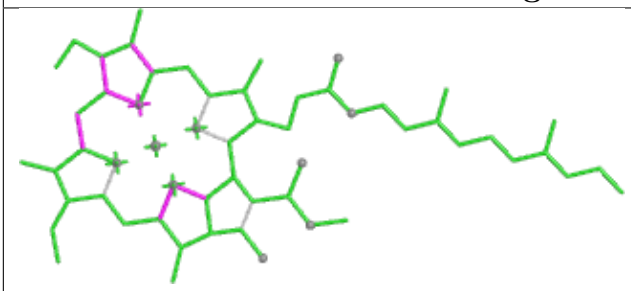


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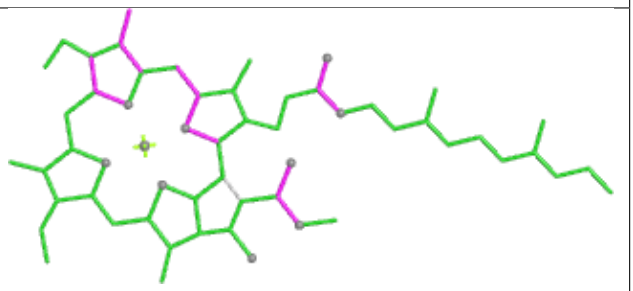


Rings

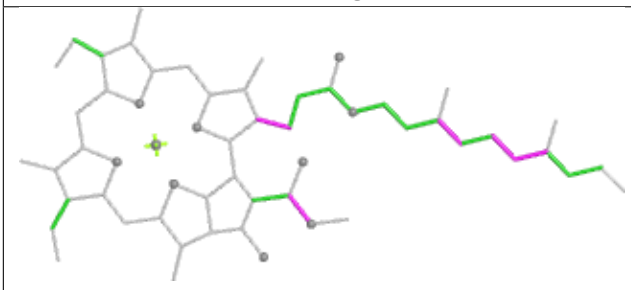
Ligand CLA U 411



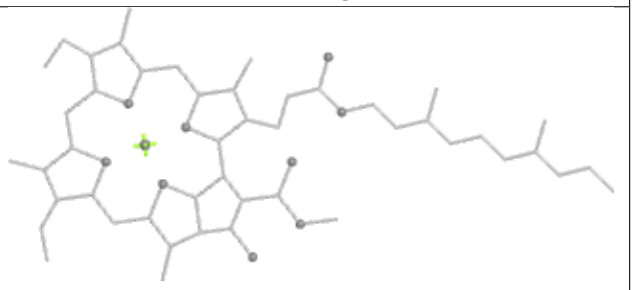
Bond lengths



Bond angles

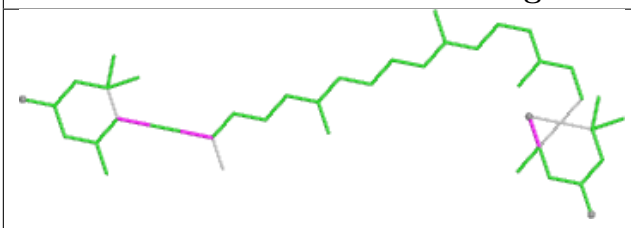


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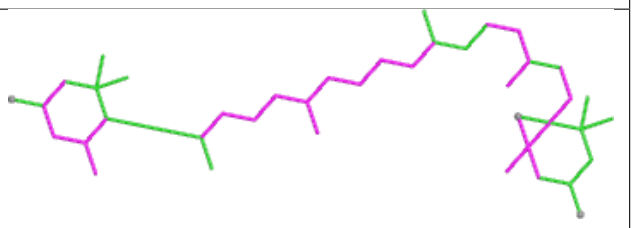


Rings

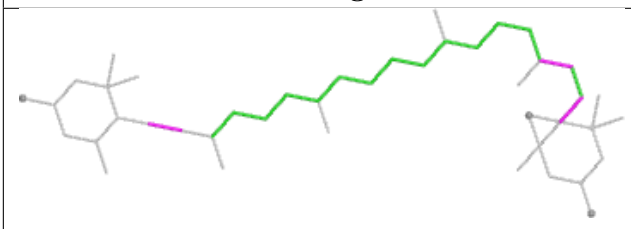
Ligand DD6 N 613



Bond lengths



Bond angles

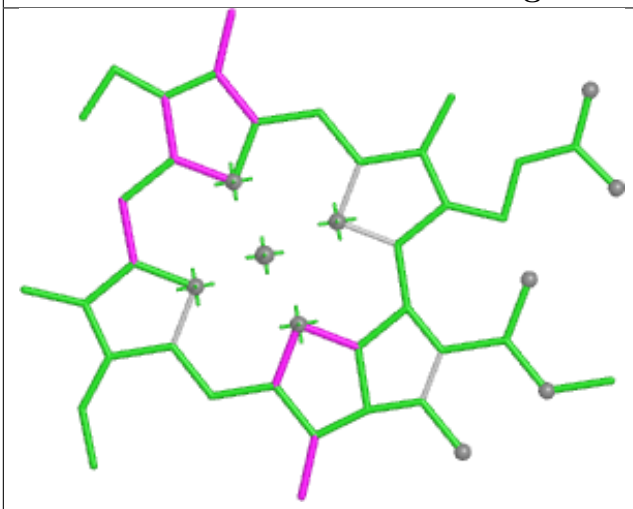


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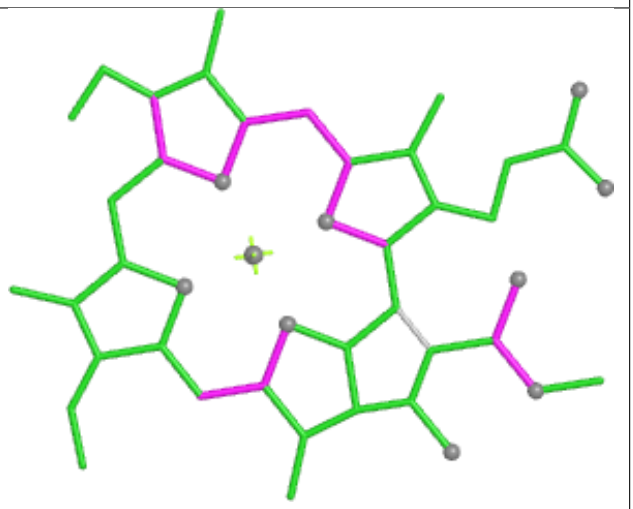


Rings

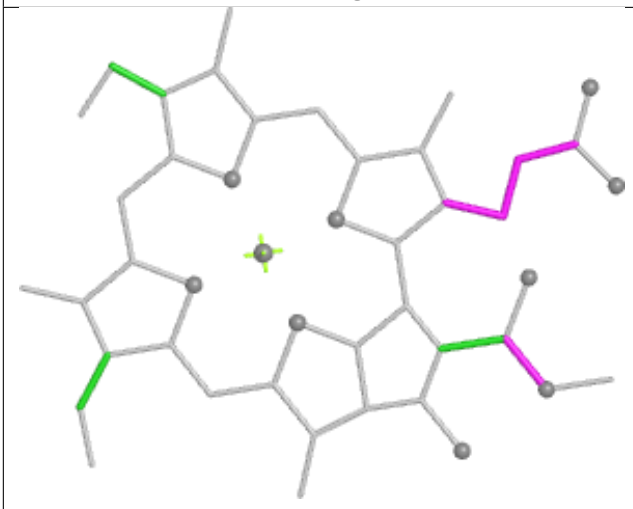
Ligand CLA A 823



Bond lengths



Bond angles

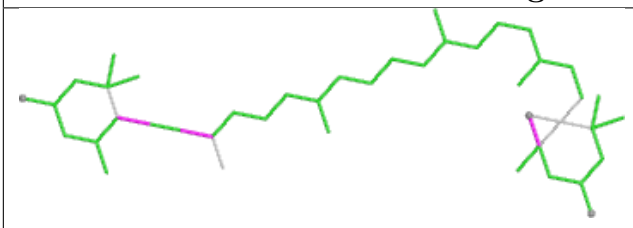


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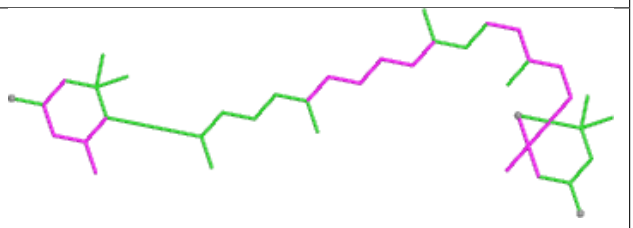


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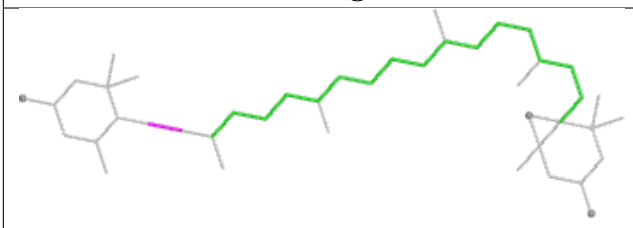
Ligand DD6 L 413



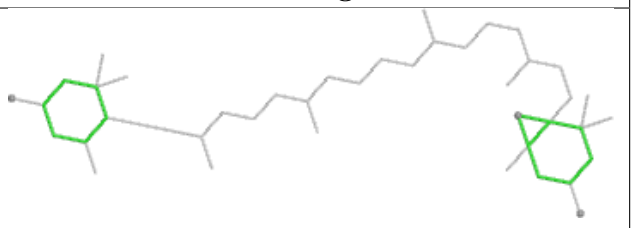
Bond lengths



Bond angles

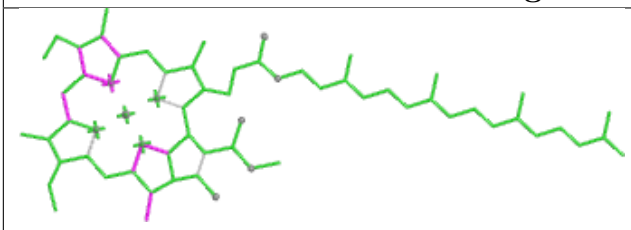


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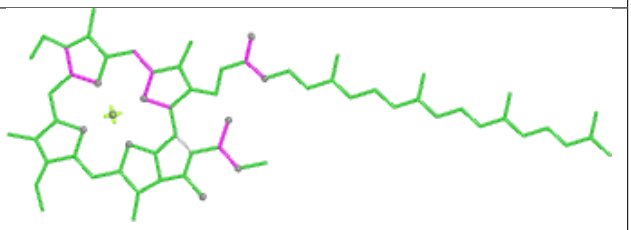


Rings

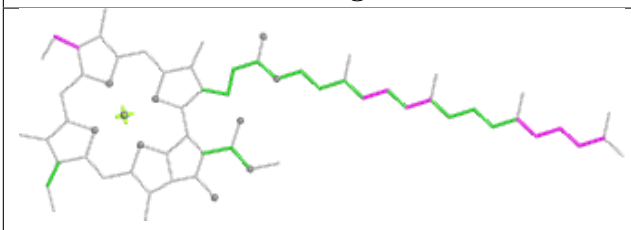
Ligand CLA B 833



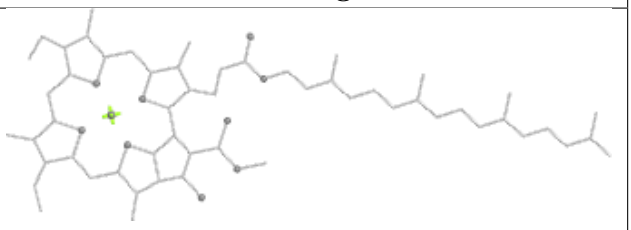
Bond lengths



Bond angles

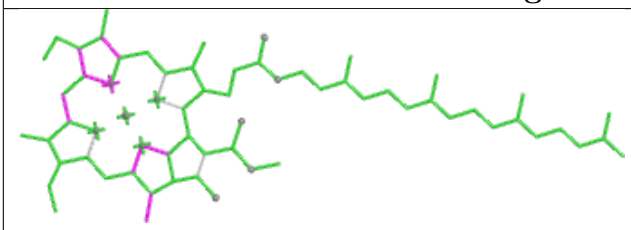


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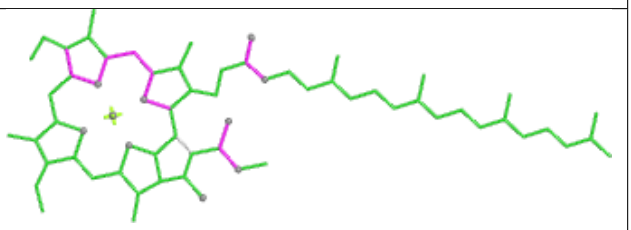


Rings

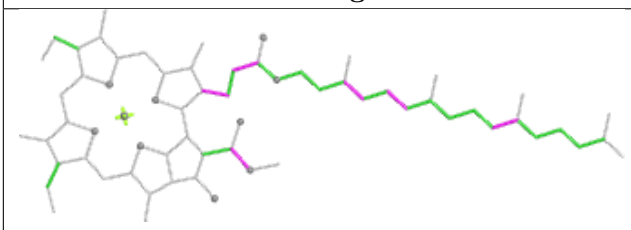
Ligand CLA B 822



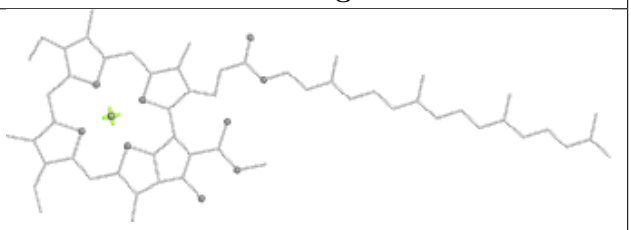
Bond lengths



Bond angles

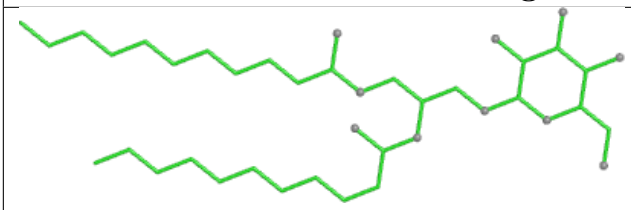


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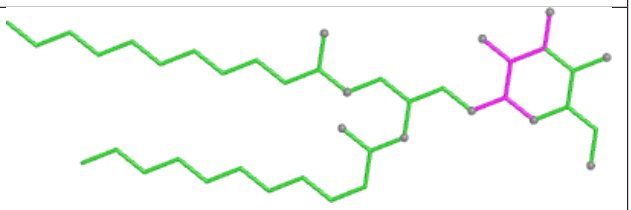


Rings

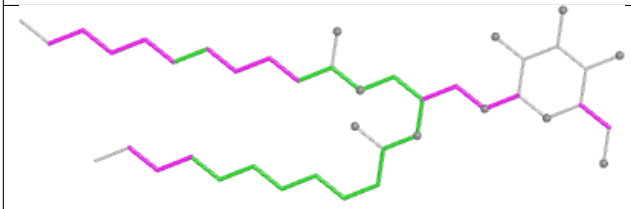
Ligand LMG T 616



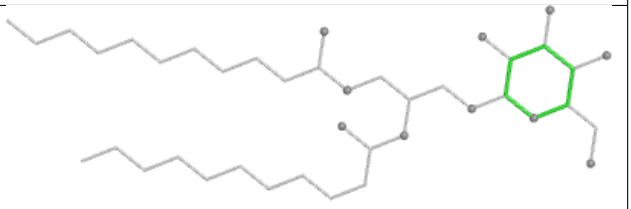
Bond lengths



Bond angles

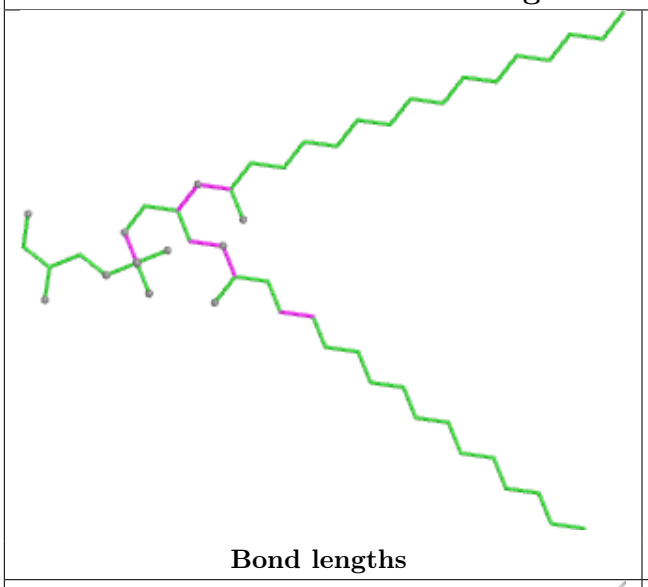


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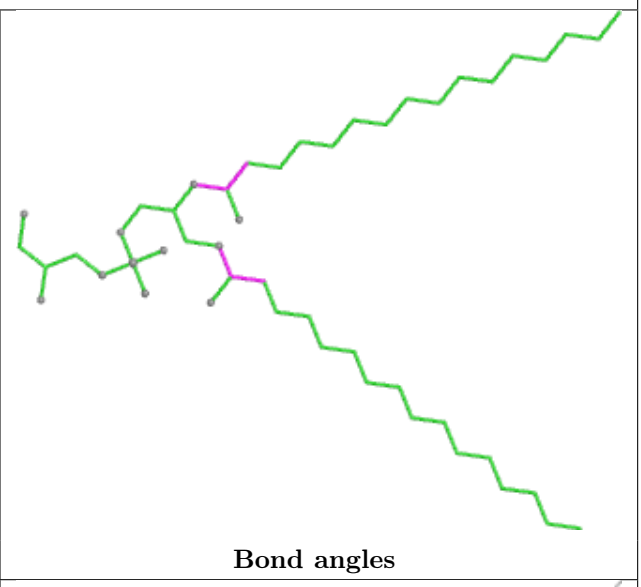


Rings

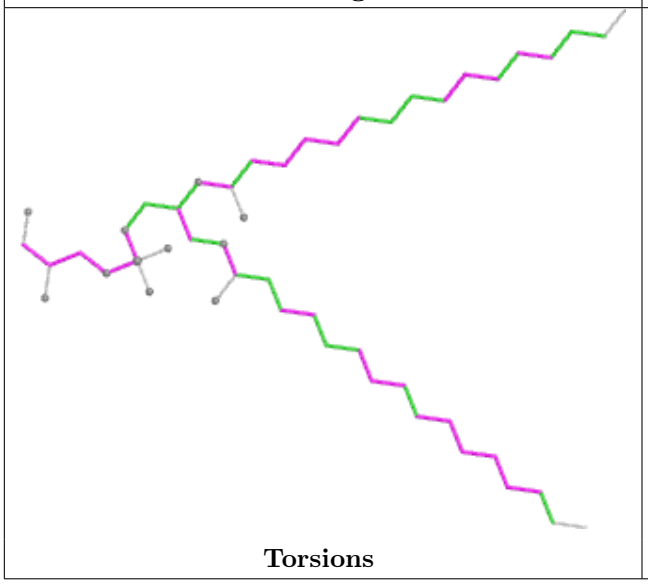
Ligand LHG O 321



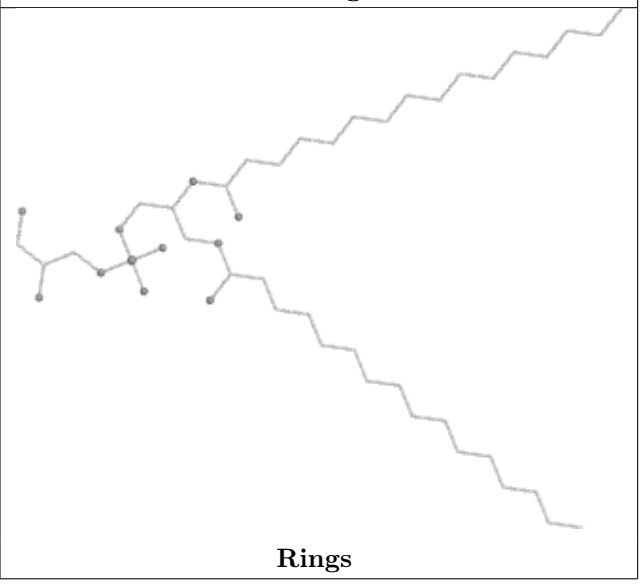
Bond lengths



Bond angles

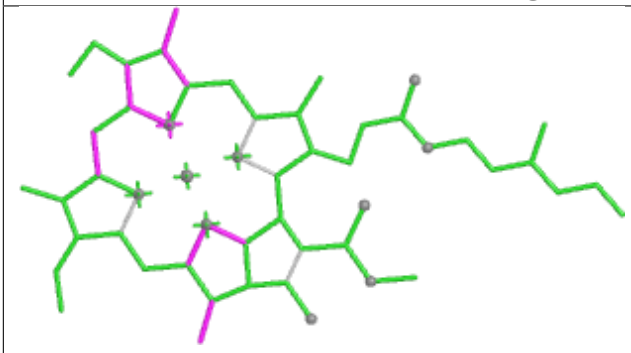


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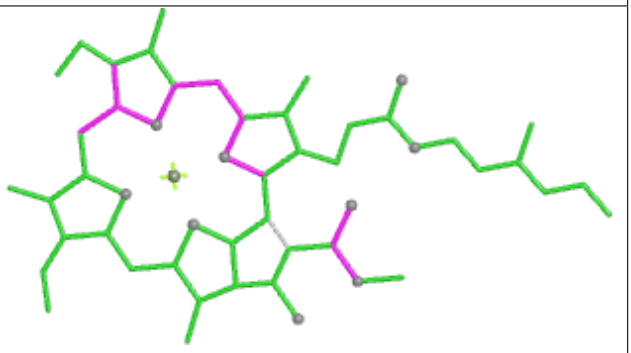


Rings

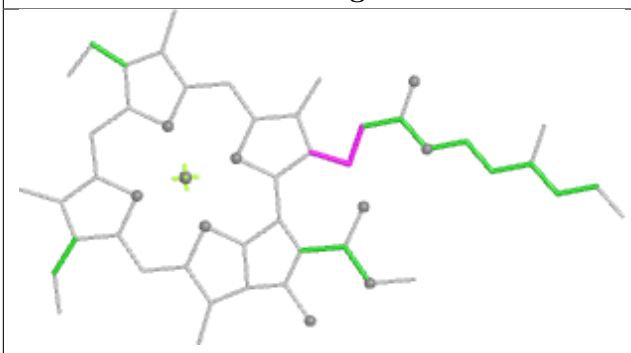
Ligand CLA B 815



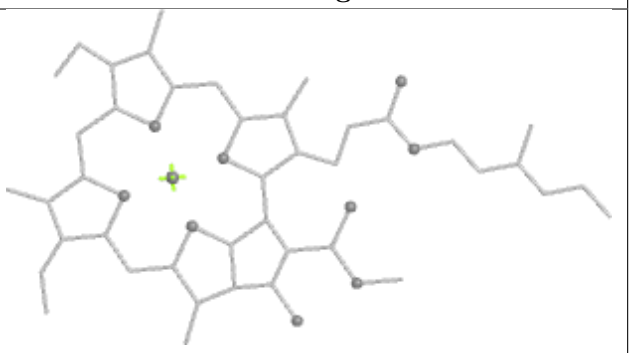
Bond lengths



Bond angles

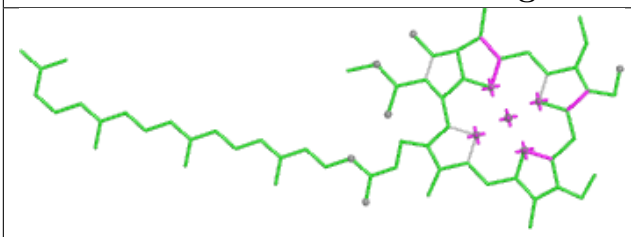


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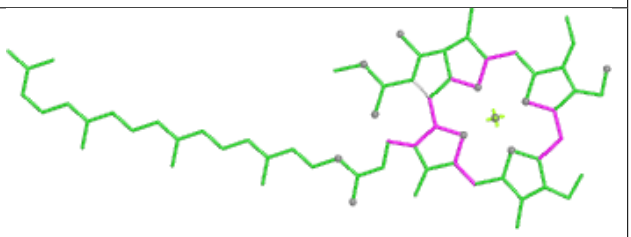


Rings

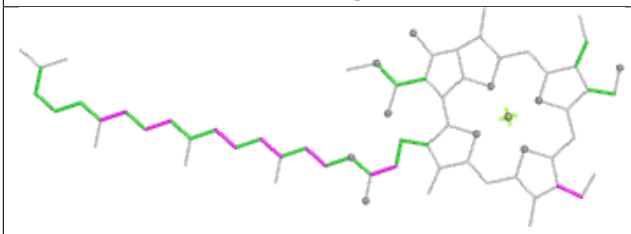
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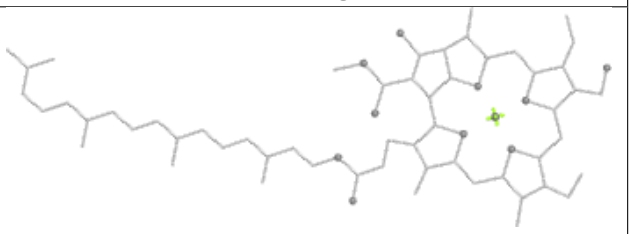
Bond lengths



Bond angles

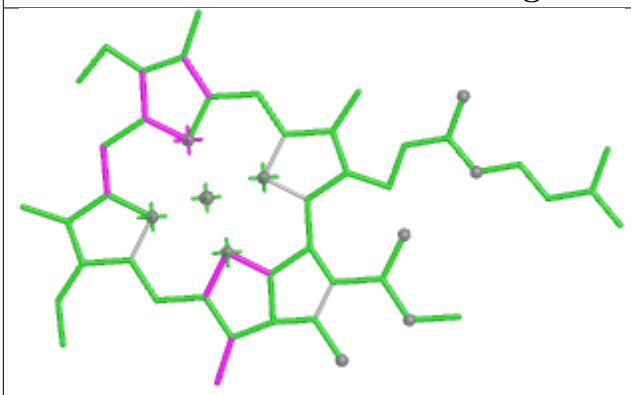


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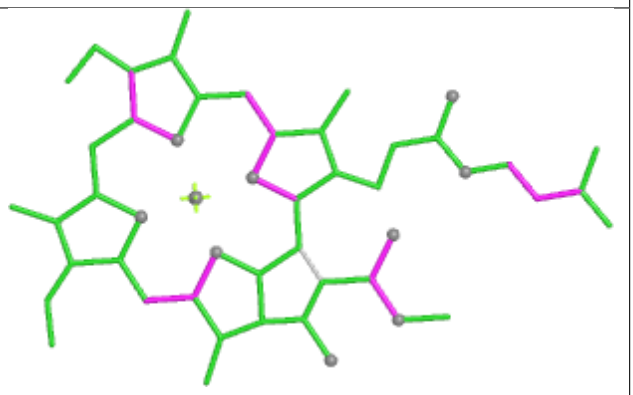


Rings

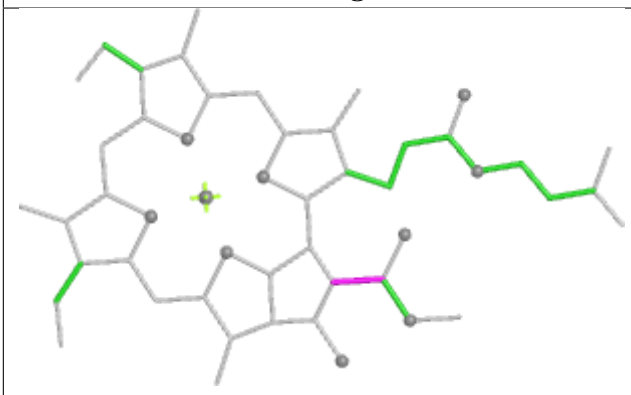
Ligand CLA K 606



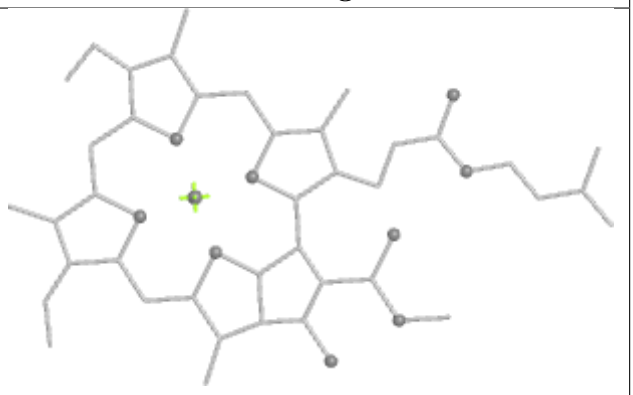
Bond lengths



Bond angles

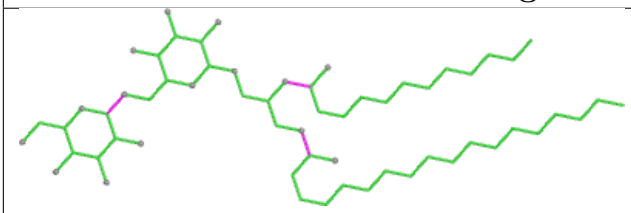


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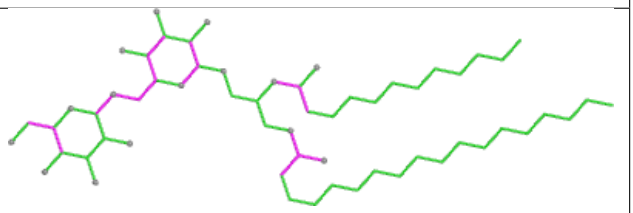


Rings

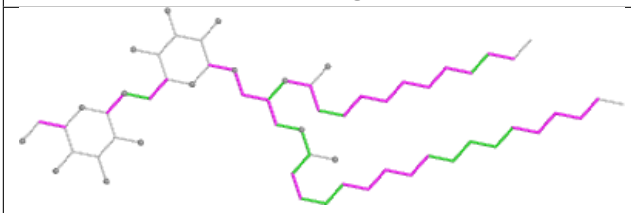
Ligand DGD O 304



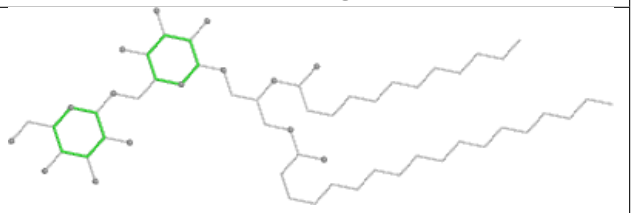
Bond lengths



Bond angles

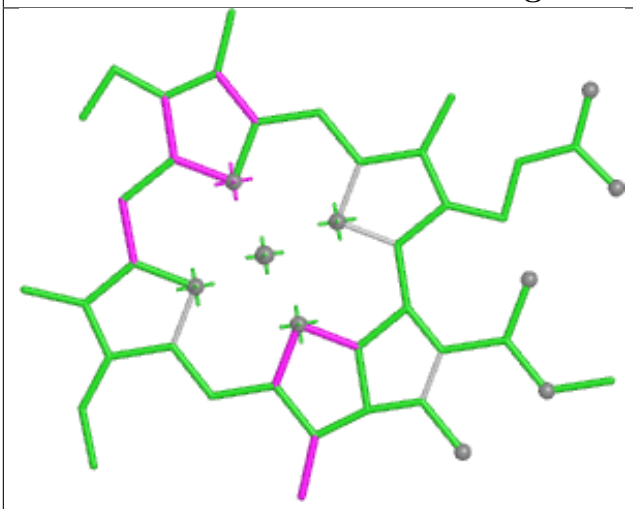


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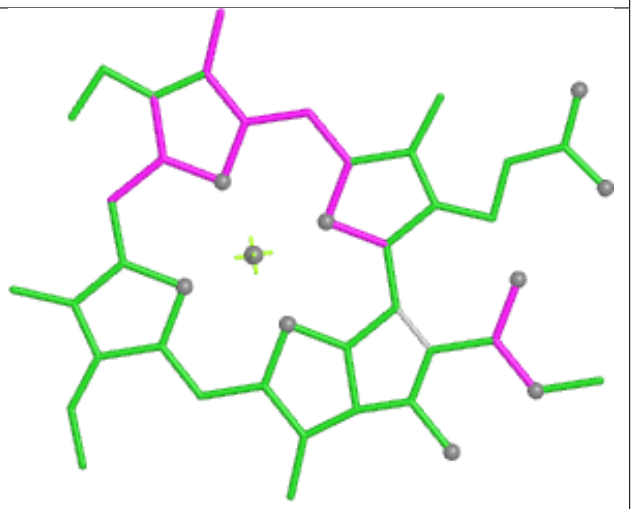


Rings

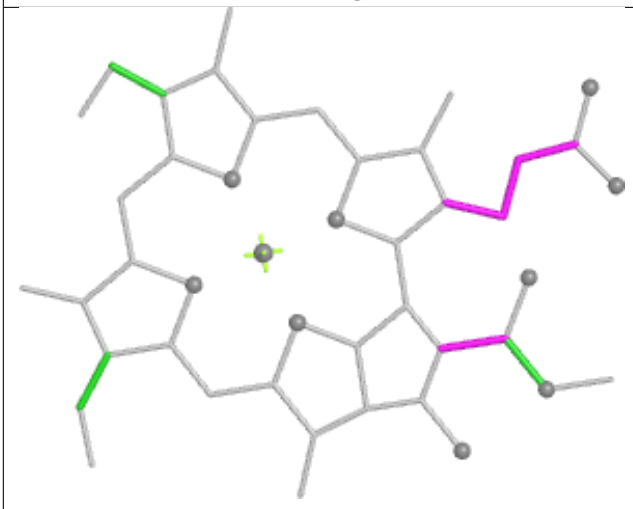
Ligand CLA B 814



Bond lengths



Bond angles

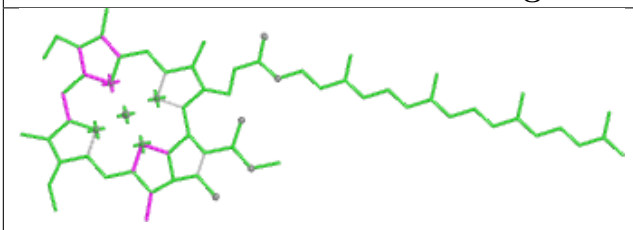


Torsions

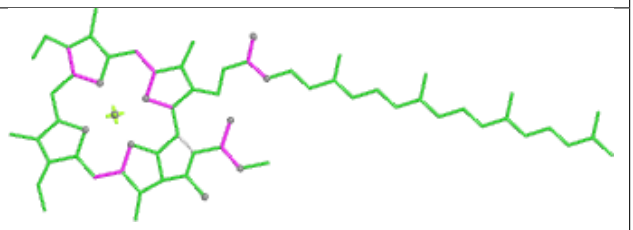


Rings

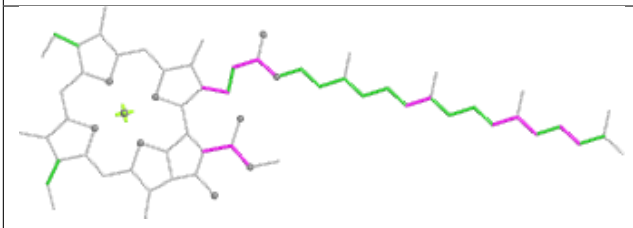
Ligand CLA R 605



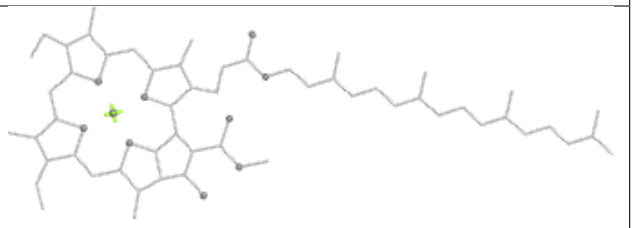
Bond lengths



Bond angles

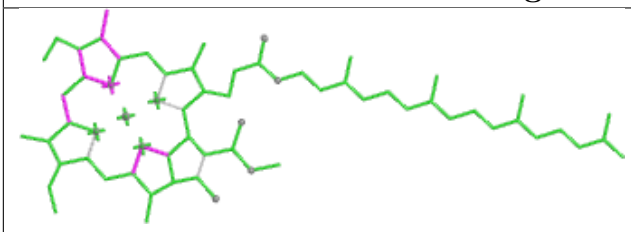


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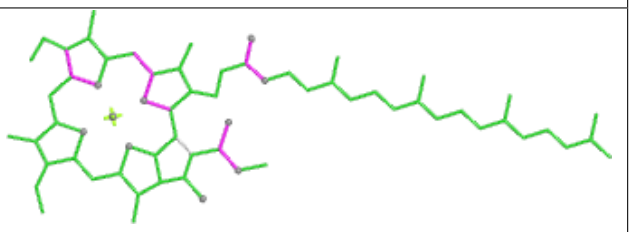


Rings

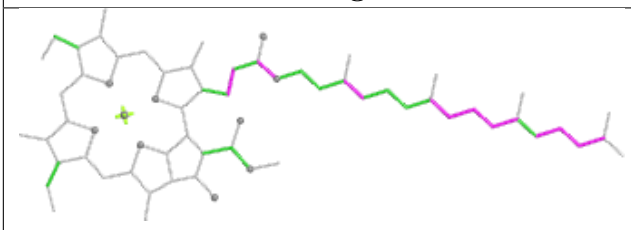
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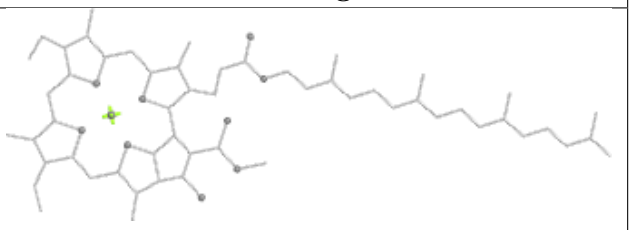
Bond lengths



Bond angles



Torsions

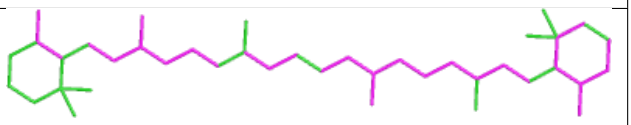


Rings

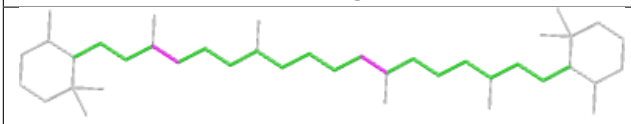
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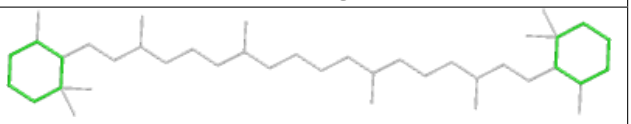
Bond lengths



Bond angles

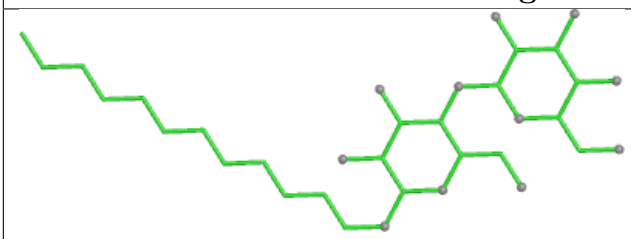


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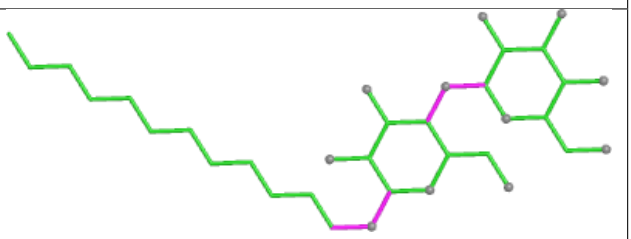


Rings

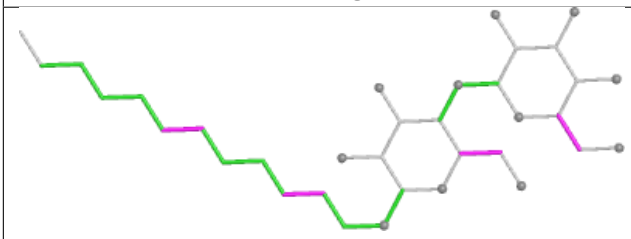
Ligand LMU U 422



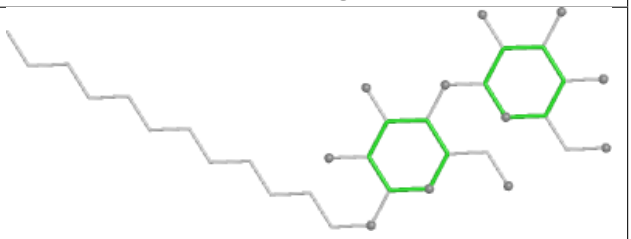
Bond lengths



Bond angles

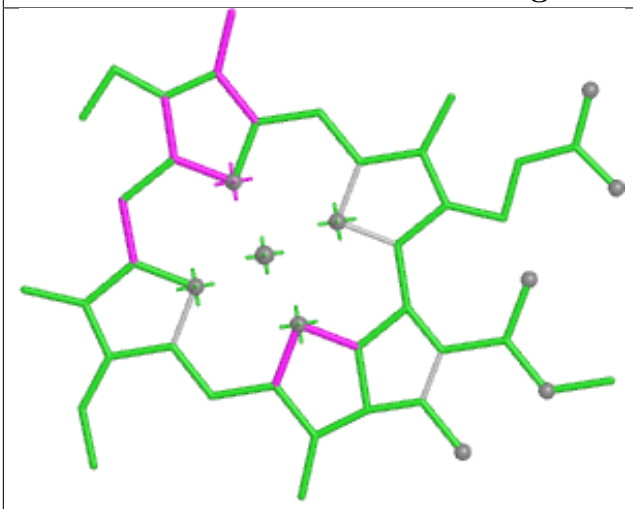


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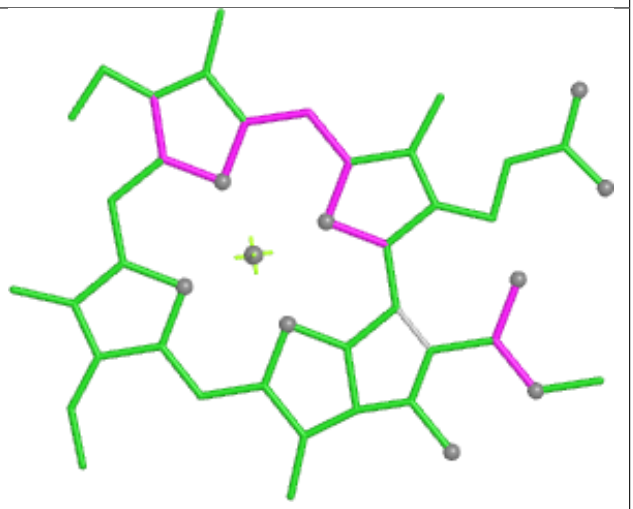


Rings

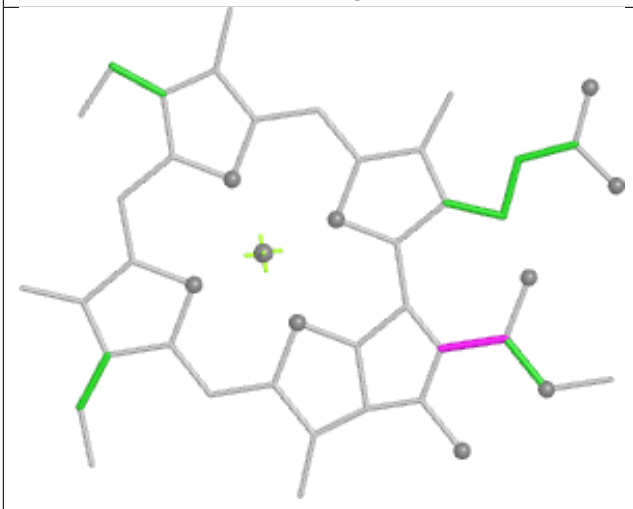
Ligand CLA I 604



Bond lengths



Bond angles

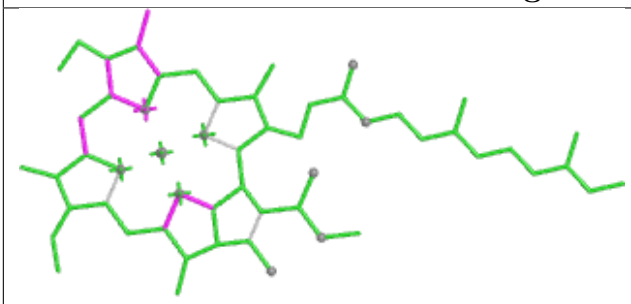


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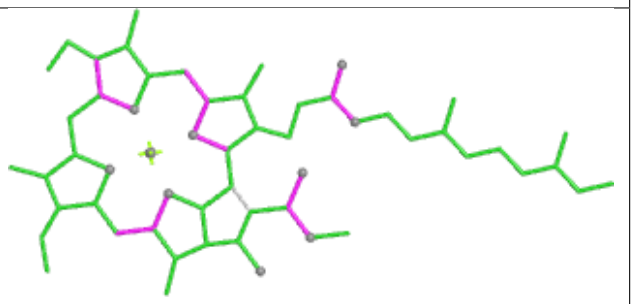


Rings

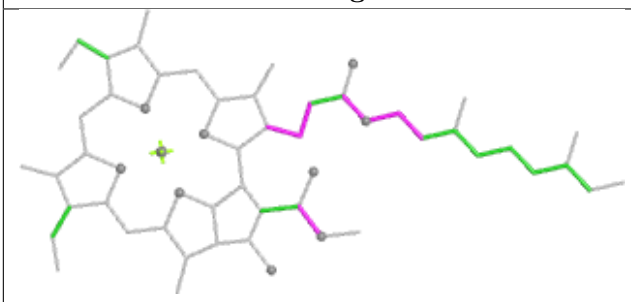
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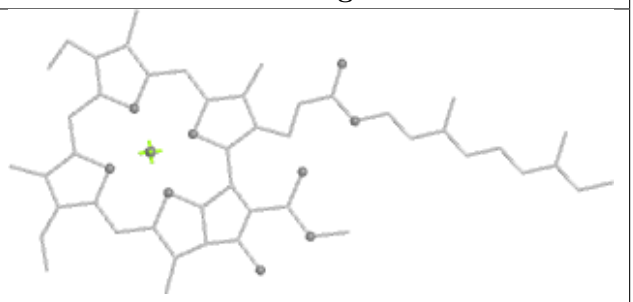
Bond lengths



Bond angles

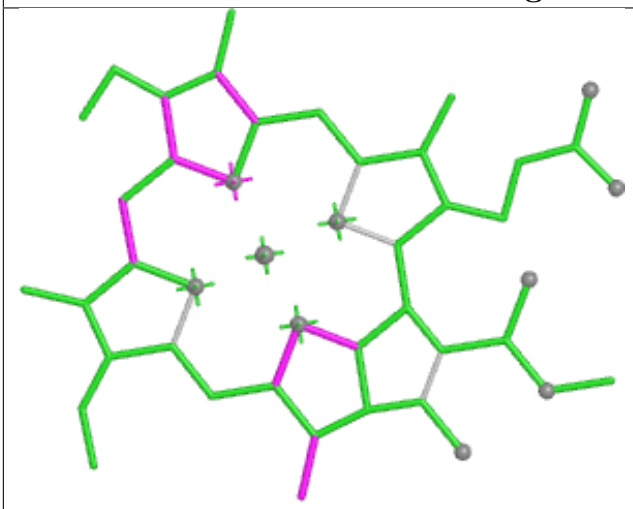


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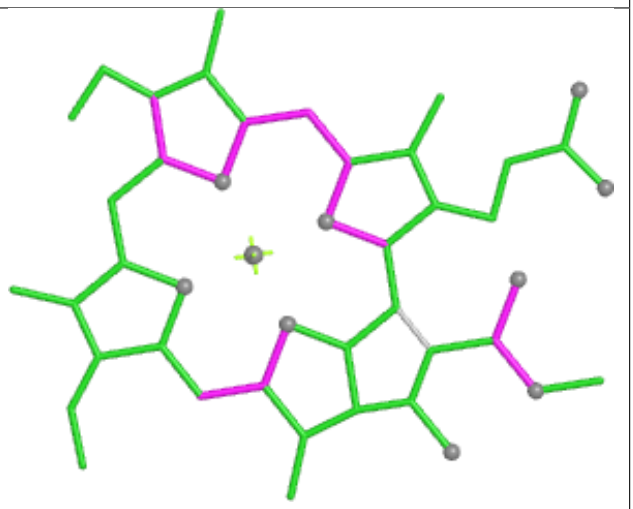


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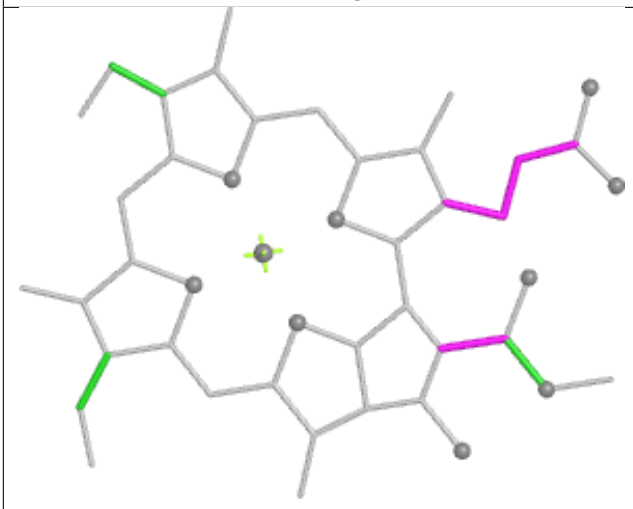
Ligand CLA P 605



Bond lengths



Bond angles

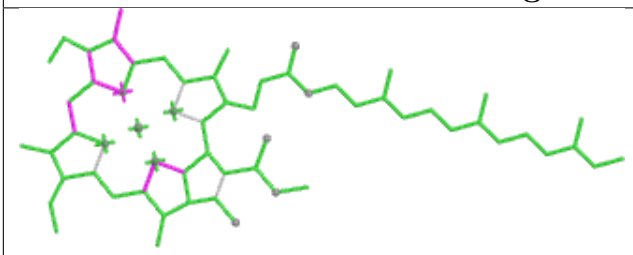


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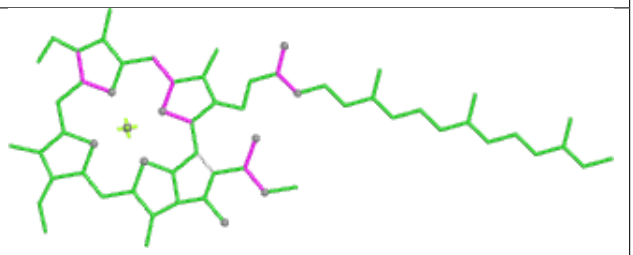


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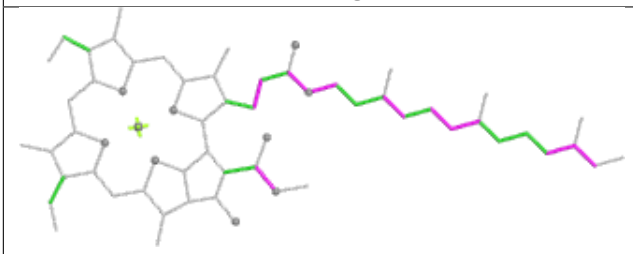
Ligand CLA U 414



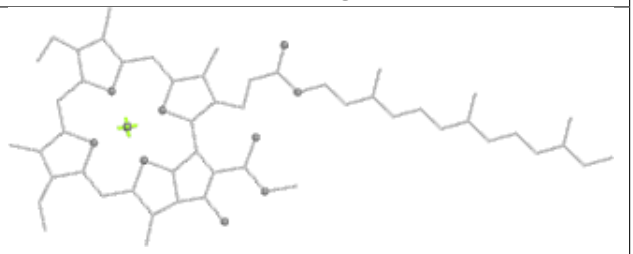
Bond lengths



Bond angles

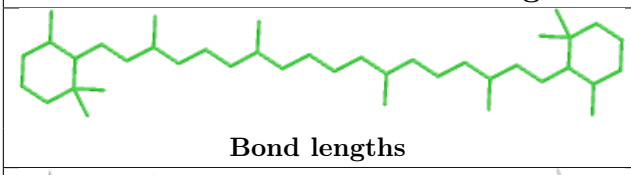


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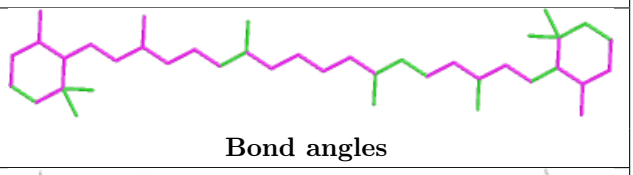


Rings

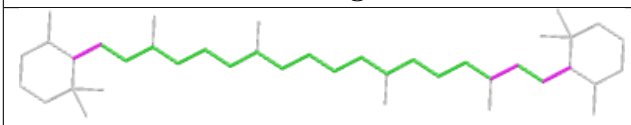
Ligand BCR B 846



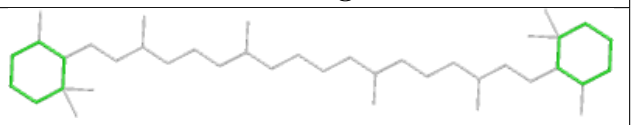
Bond lengths



Bond angles

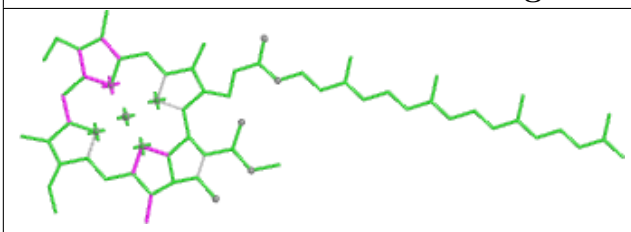


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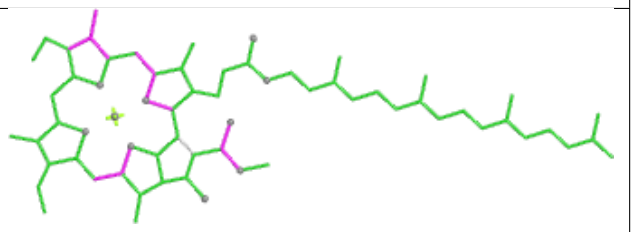


Rings

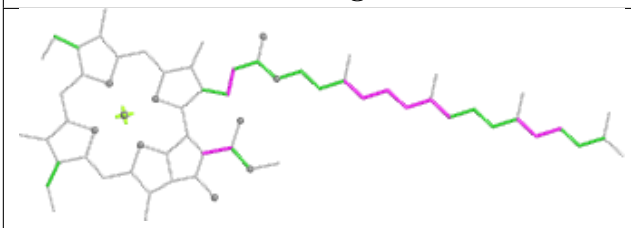
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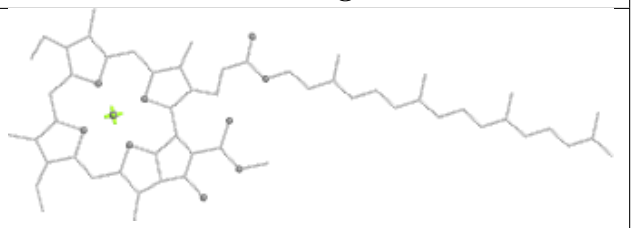
Bond lengths



Bond angles

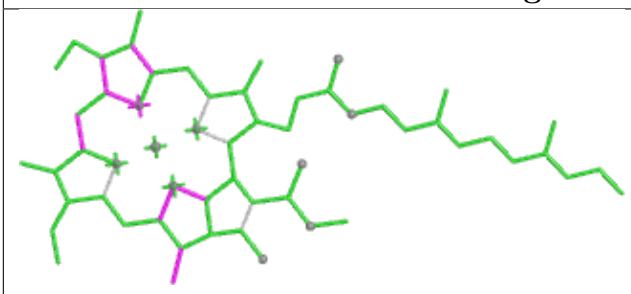


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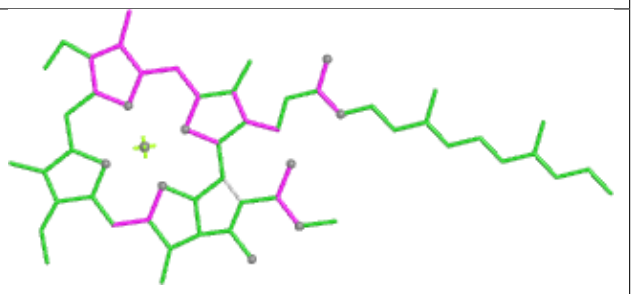


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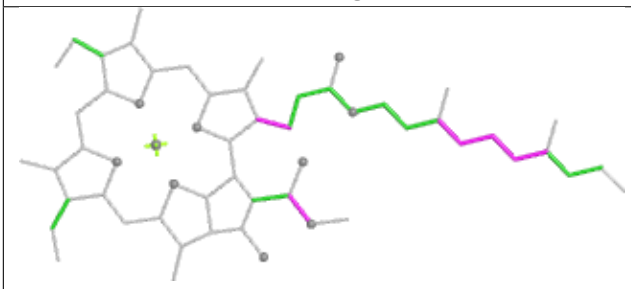
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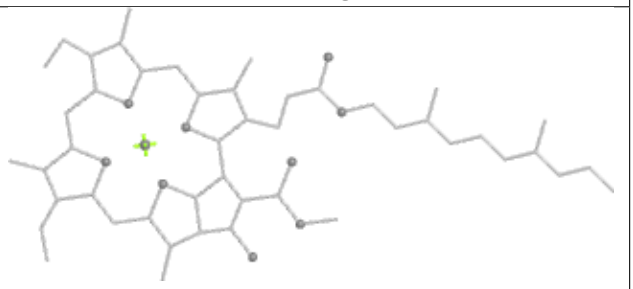
Bond lengths



Bond angles

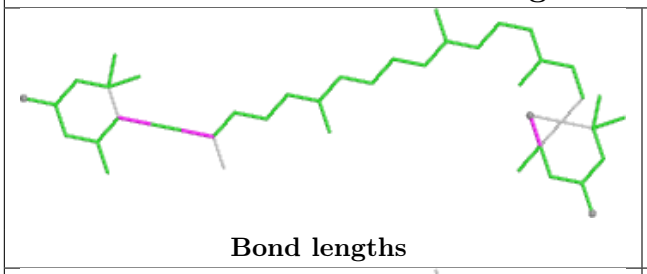


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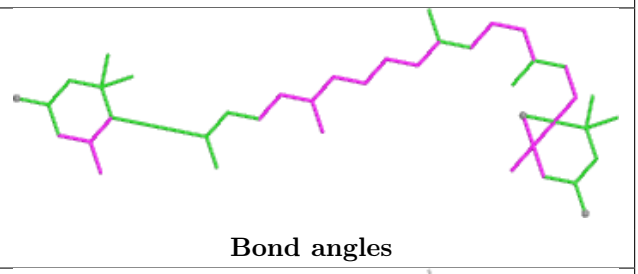


Rings

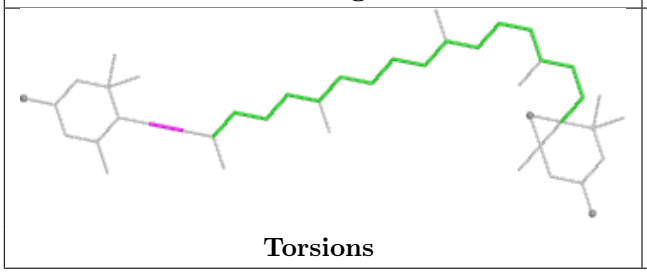
Ligand DD6 S 611



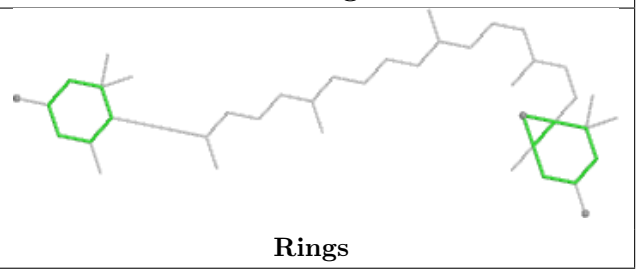
Bond lengths



Bond angles

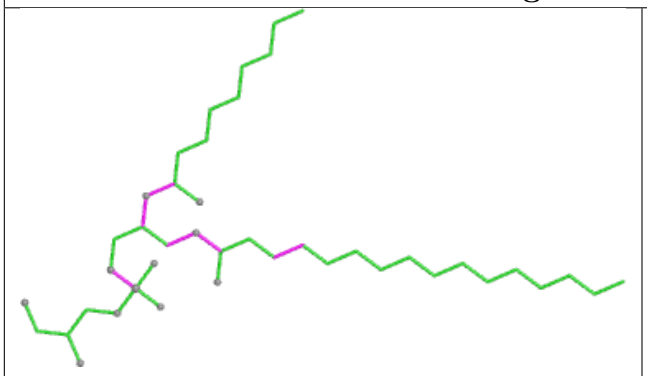


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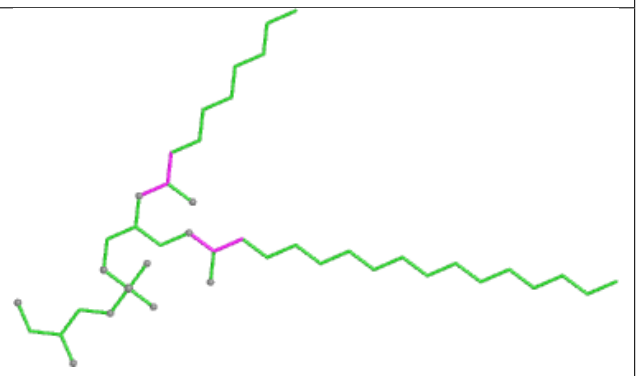


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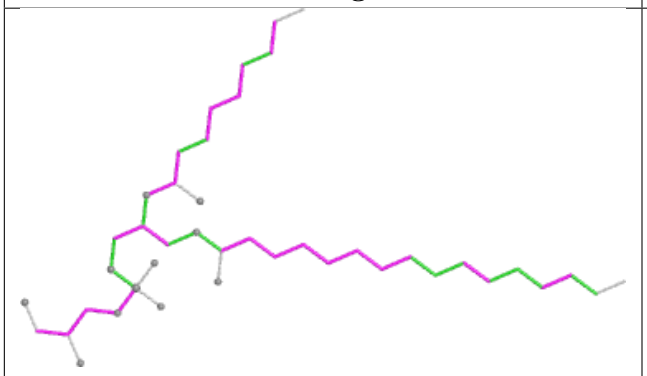
Ligand LHG X 420



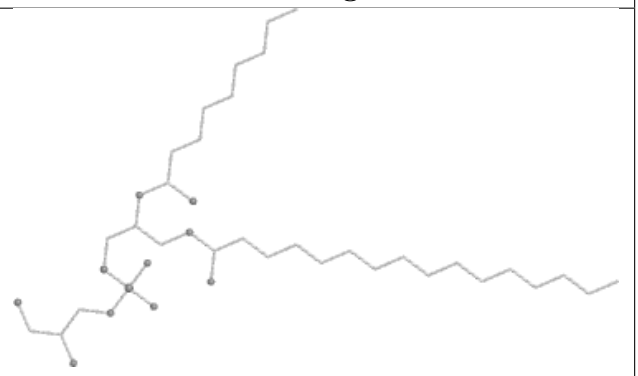
Bond lengths



Bond angles

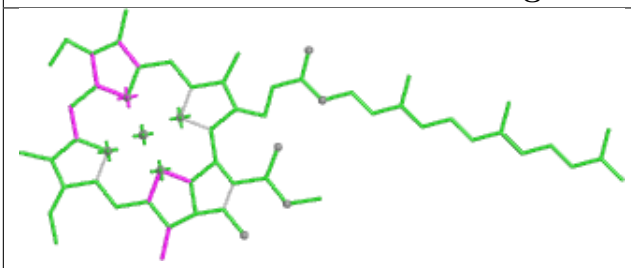


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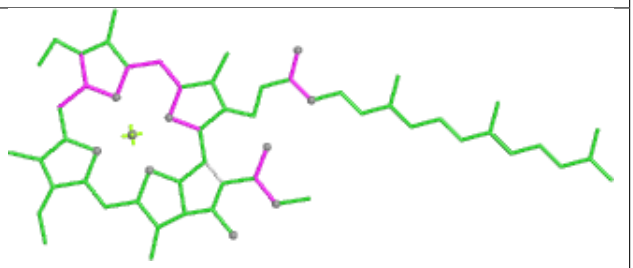


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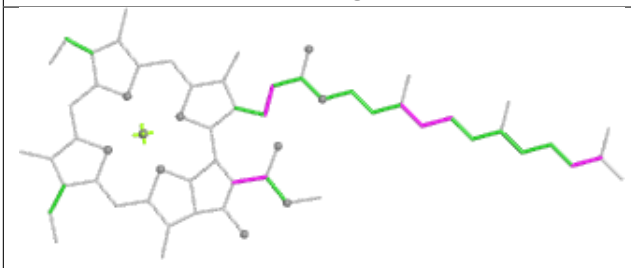
Ligand CLA O 306



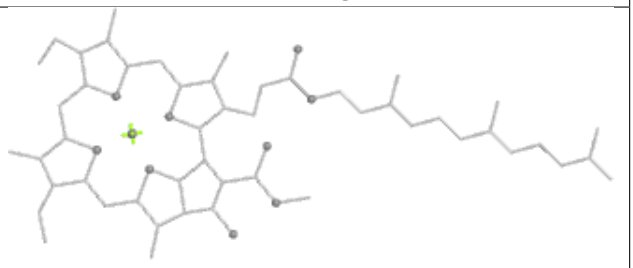
Bond lengths



Bond angles

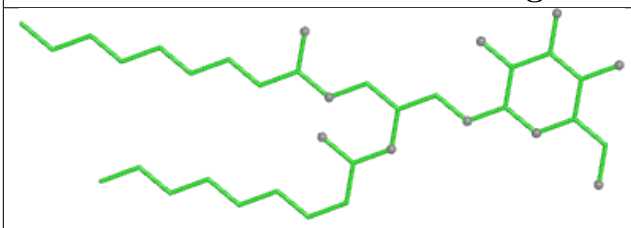


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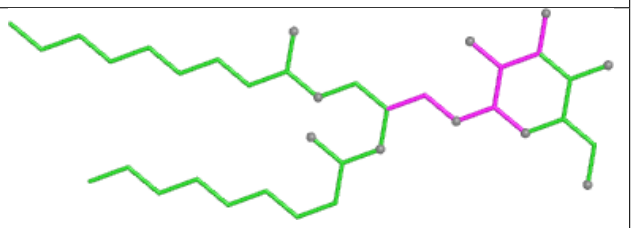


Rings

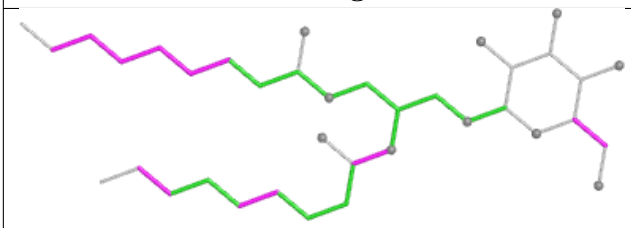
Ligand LMG I 614



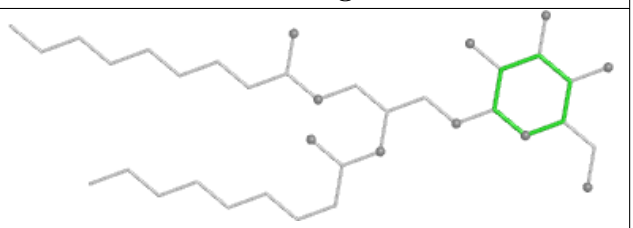
Bond lengths



Bond angles

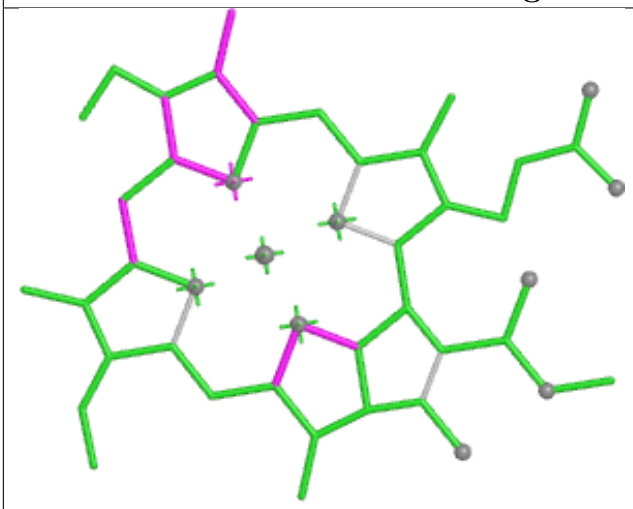


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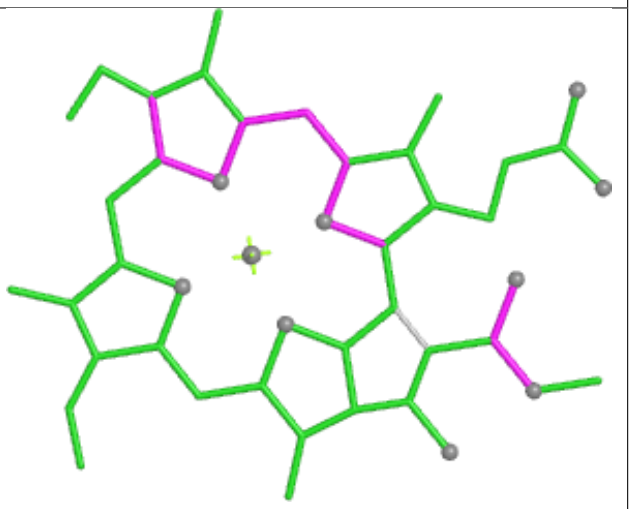


Rings

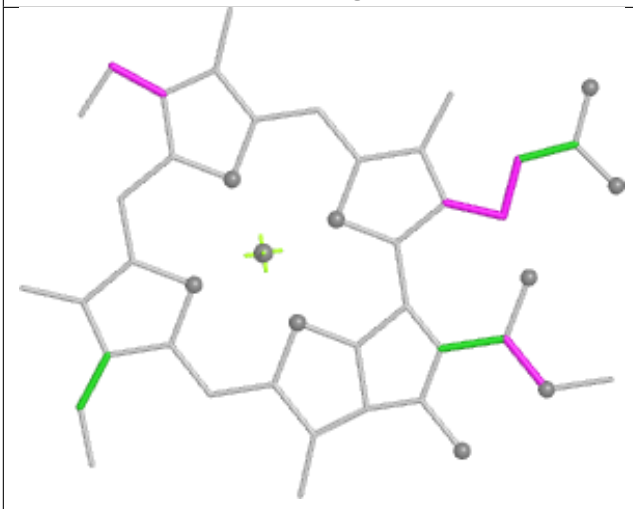
Ligand CLA U 415



Bond lengths



Bond angles

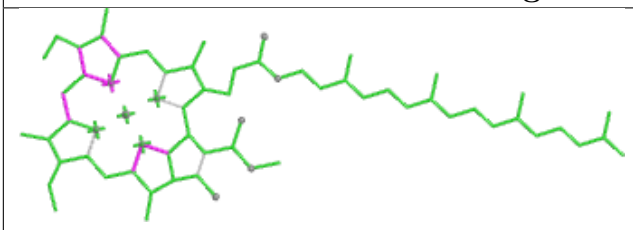


Torsions

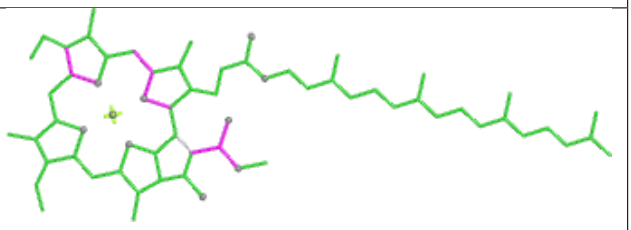


Rings

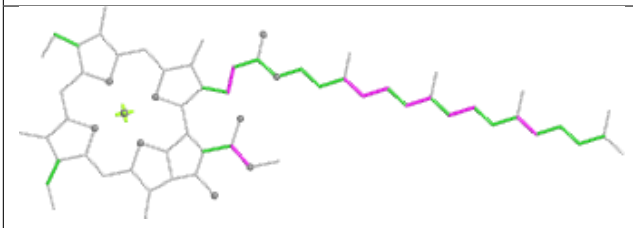
Ligand CLA K 611



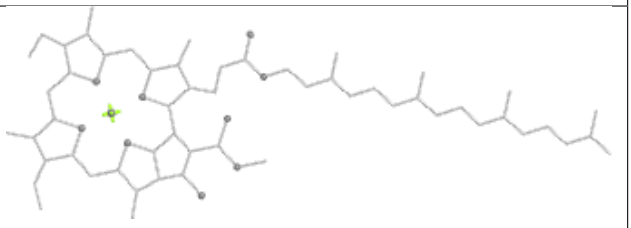
Bond lengths



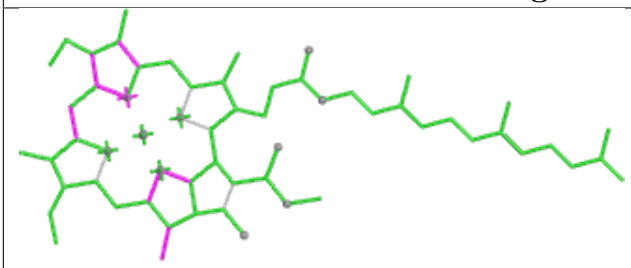
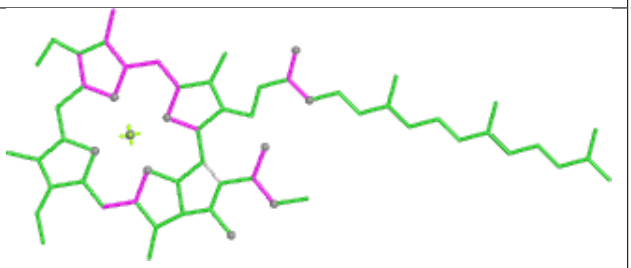
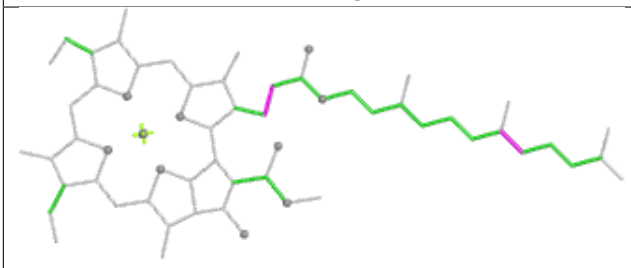
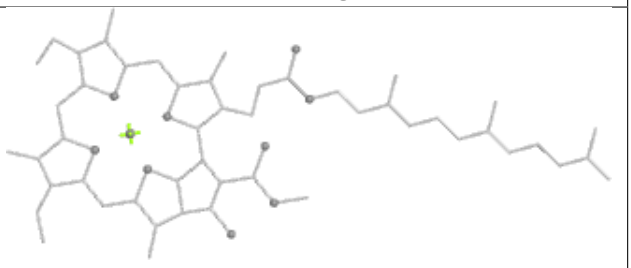
Bond angles

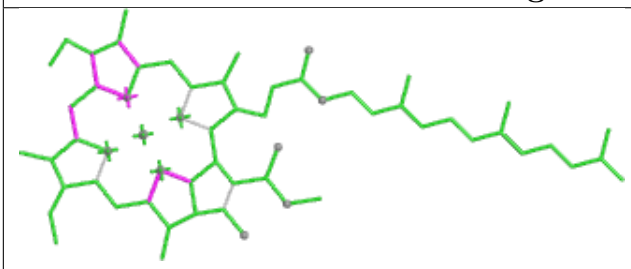
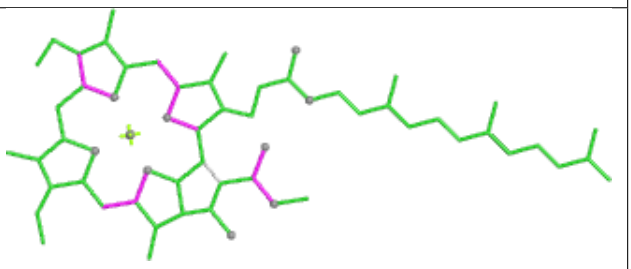
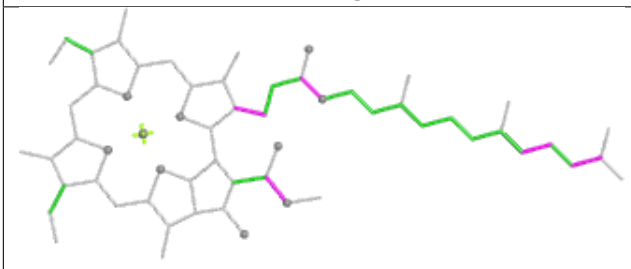
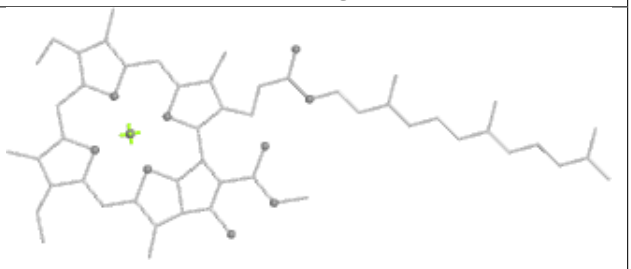


Torsions

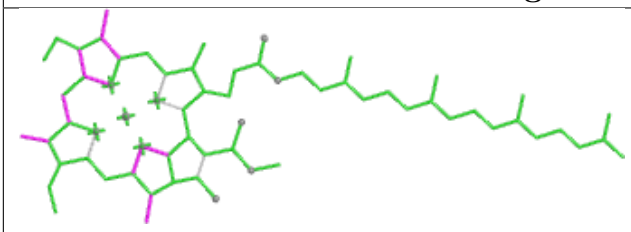


Rings

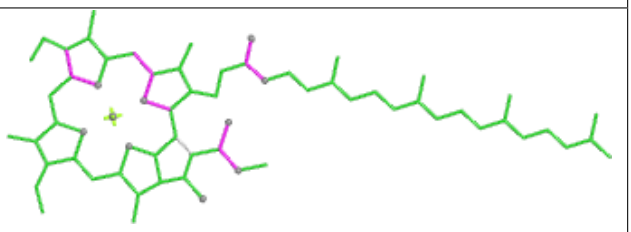
Ligand CLA I 602	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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

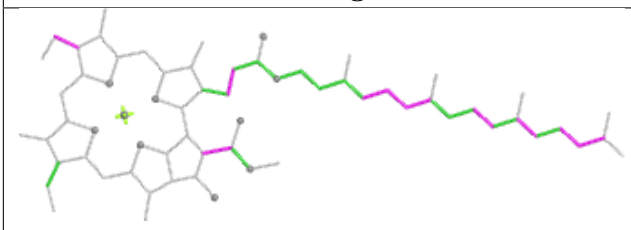
Ligand CLA B 807



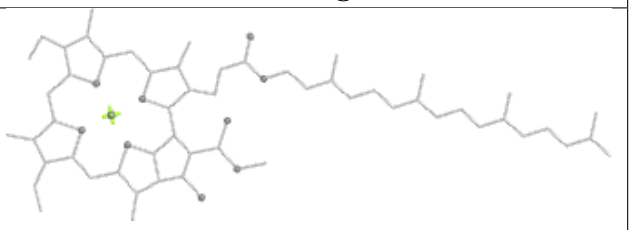
Bond lengths



Bond angles

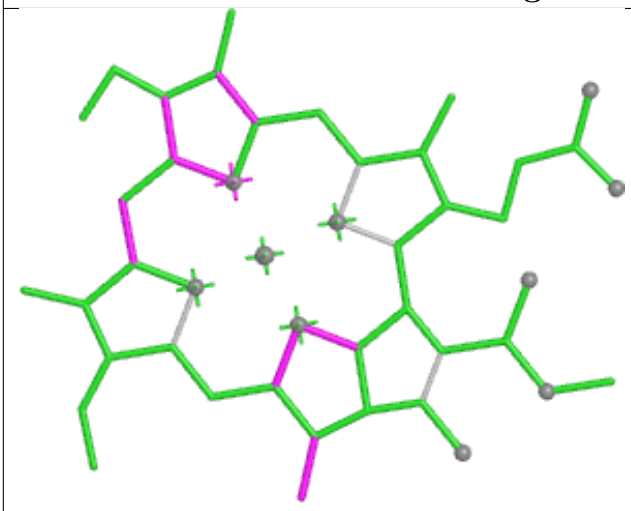


Torsions

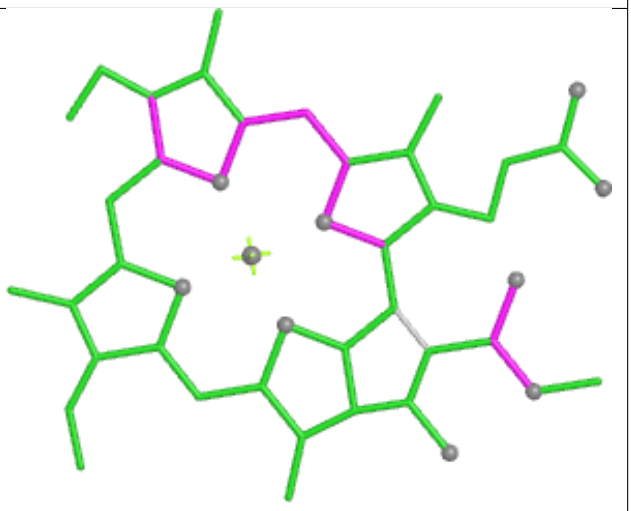


Rings

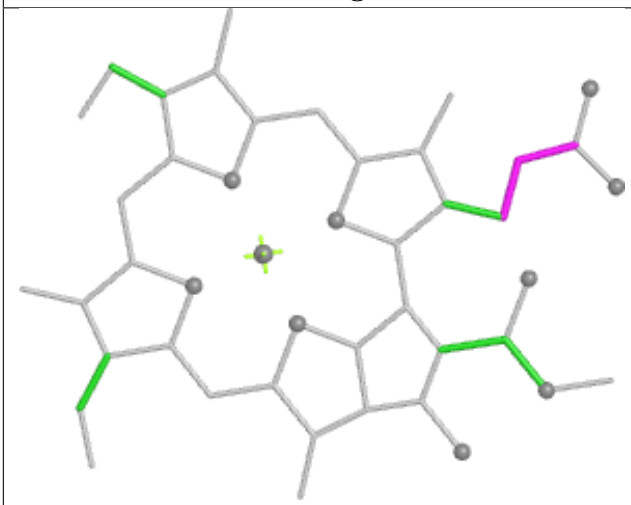
Ligand CLA O 307



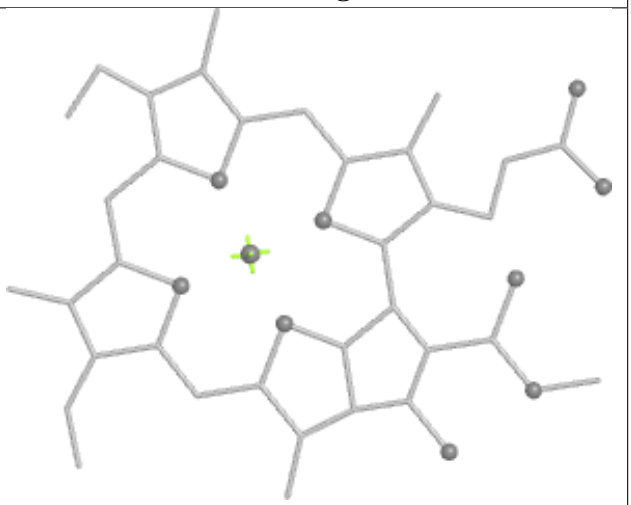
Bond lengths



Bond angles

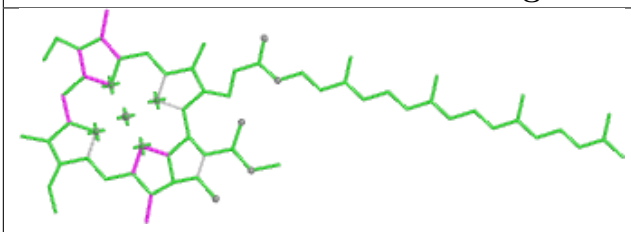


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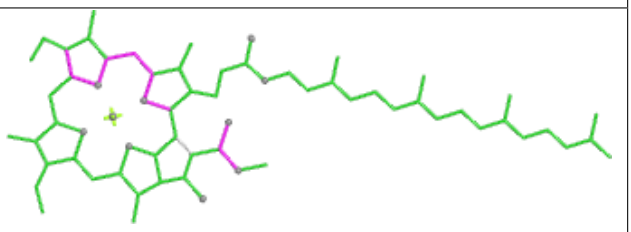


Rings

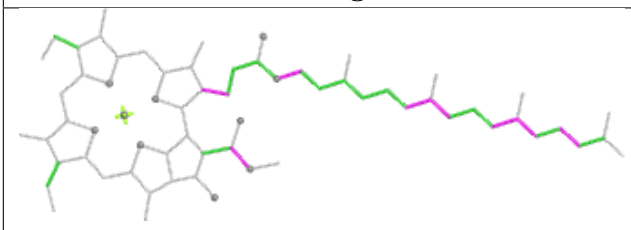
Ligand CLA G 606



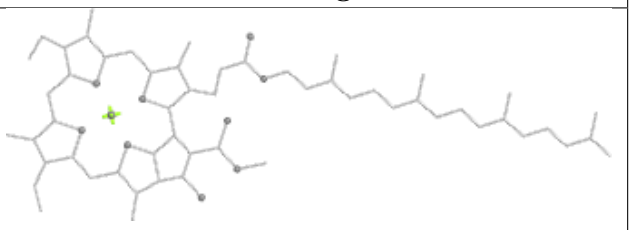
Bond lengths



Bond angles

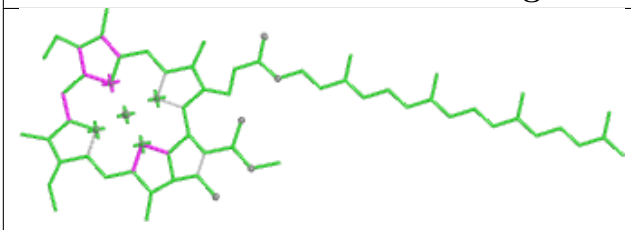


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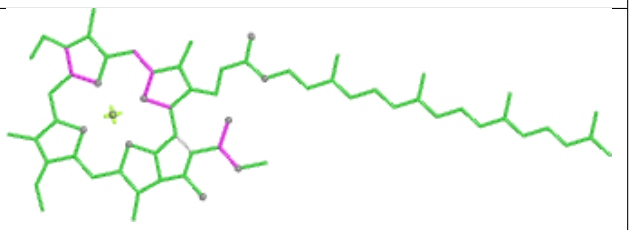


Rings

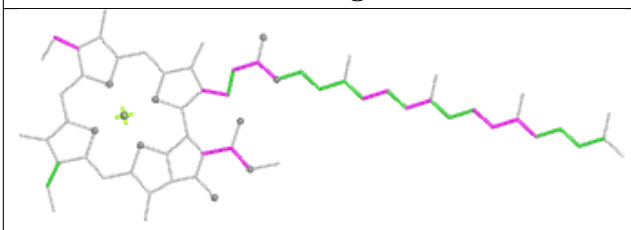
Ligand CLA K 605



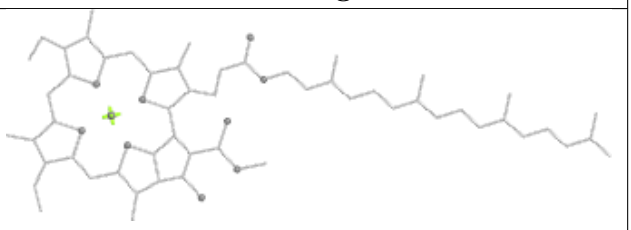
Bond lengths



Bond angles



Torsions

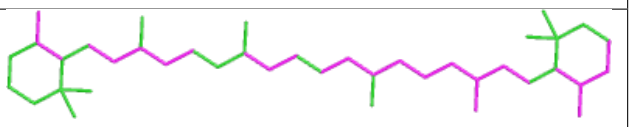


Rings

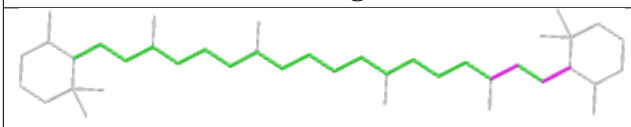
Ligand BCR A 850



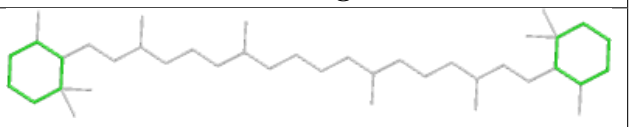
Bond lengths



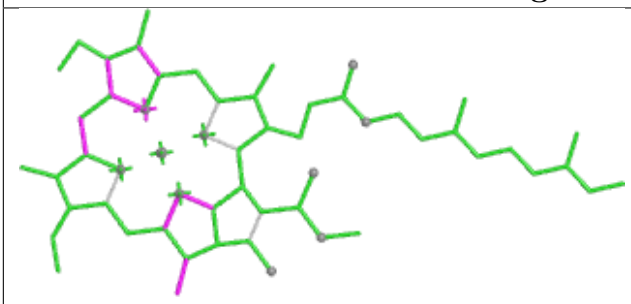
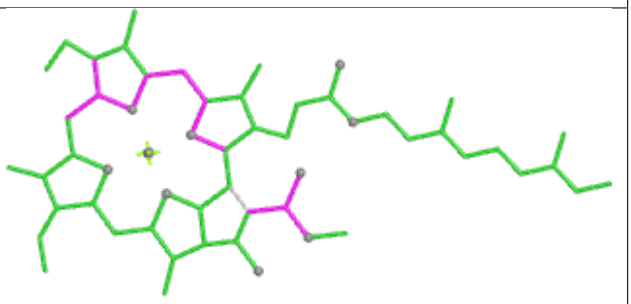
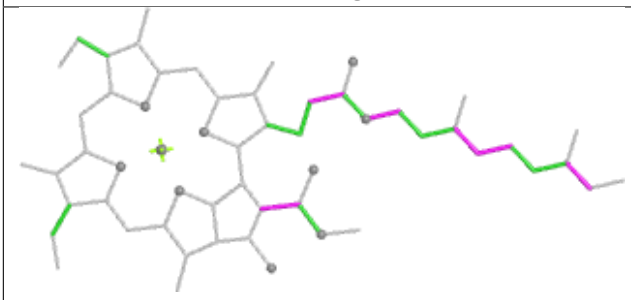
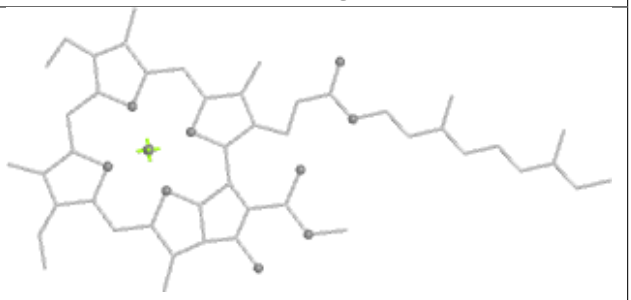
Bond angles

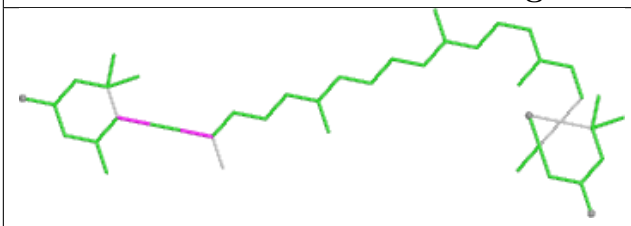
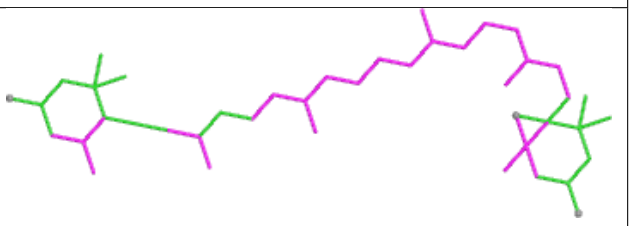
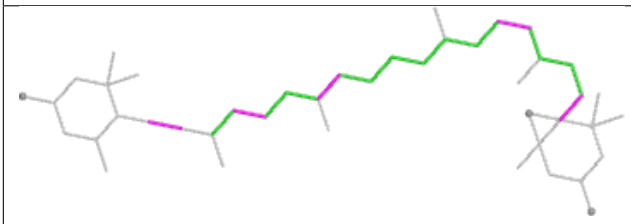
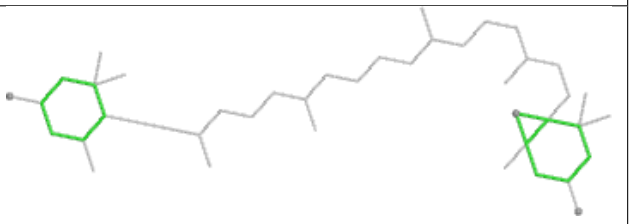


Torsions

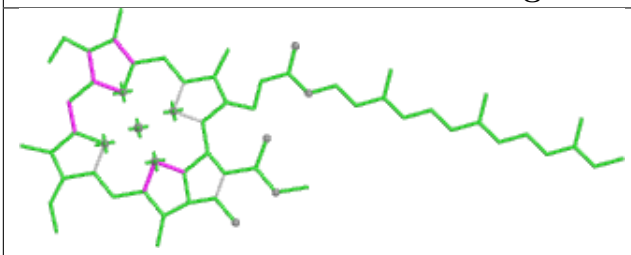


Rings

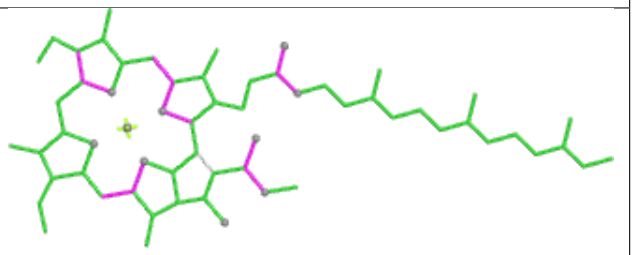
Ligand CLA I 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand DD6 P 612	
 Bond lengths	 Bond angles
 Torsions	 Rings

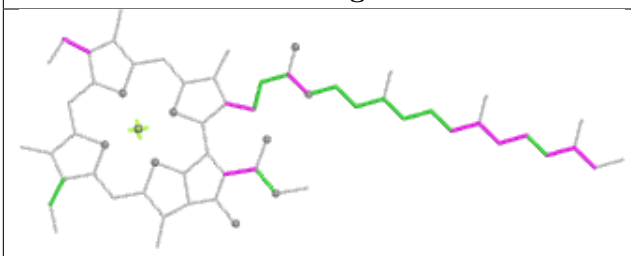
Ligand CLA A 825



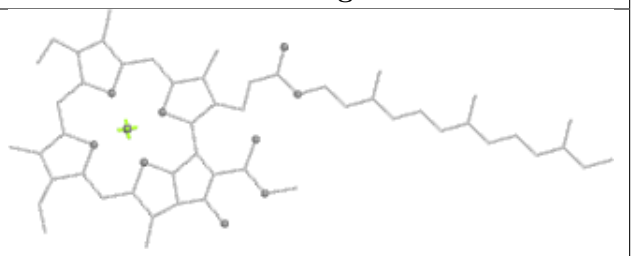
Bond lengths



Bond angles

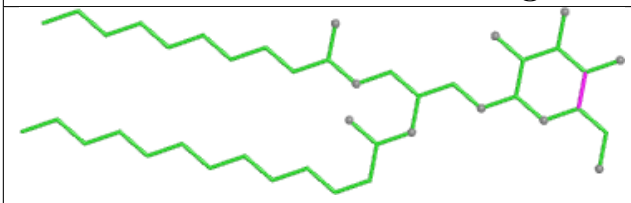


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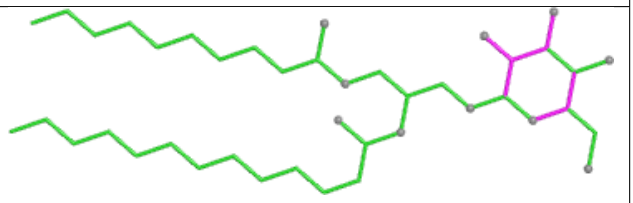


Rings

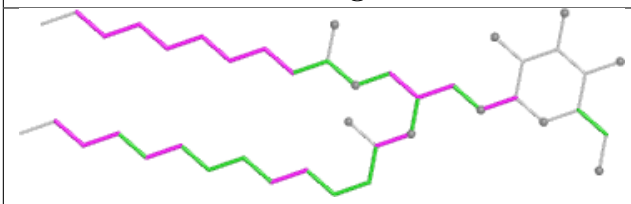
Ligand LMG F 408



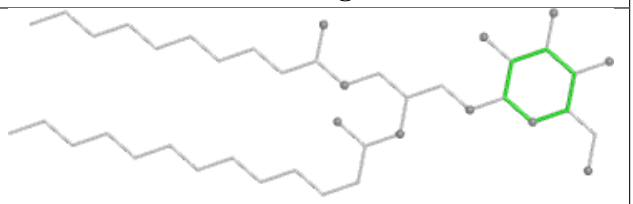
Bond lengths



Bond angles

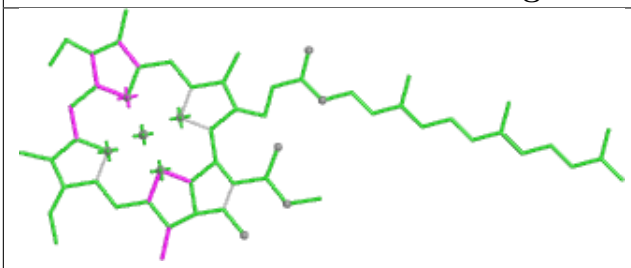


Torsions

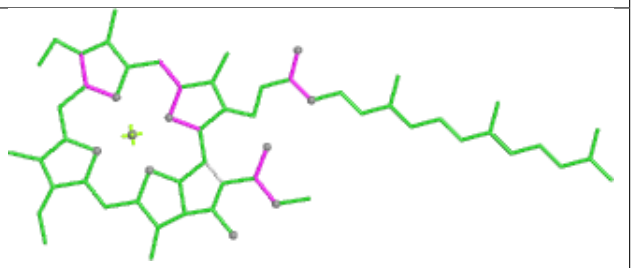


Rings

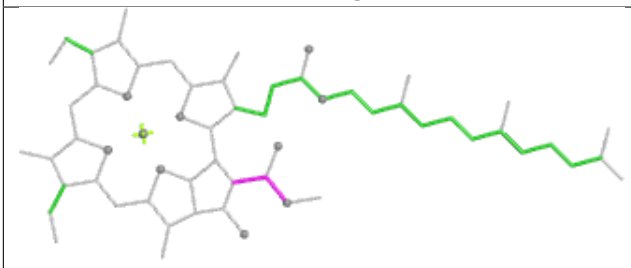
Ligand CLA G 607



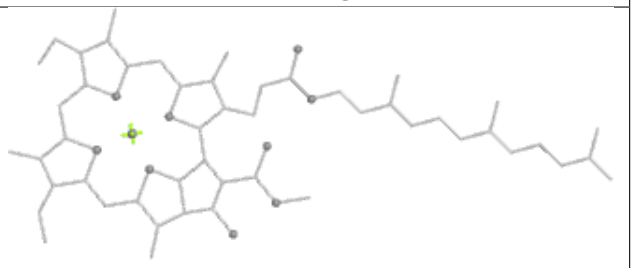
Bond lengths



Bond angles

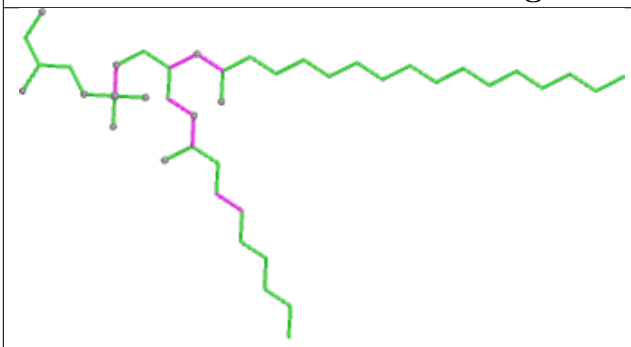


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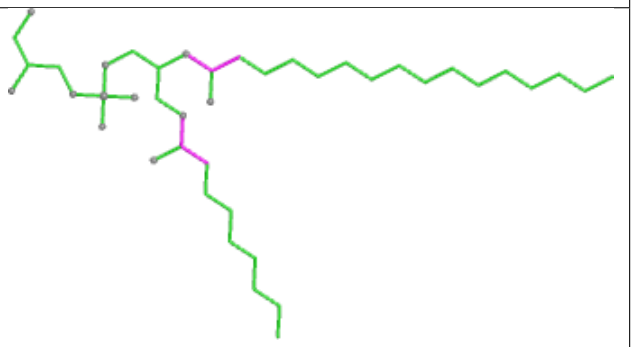


Rings

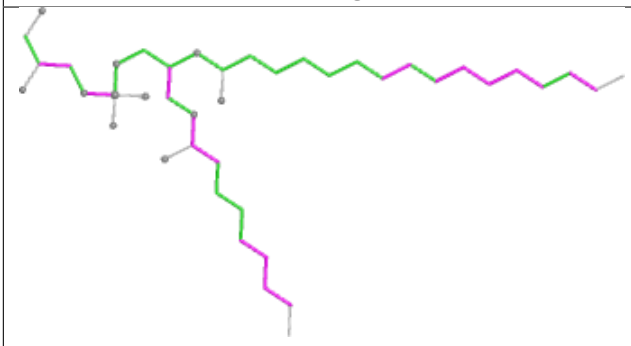
Ligand LHG L 416



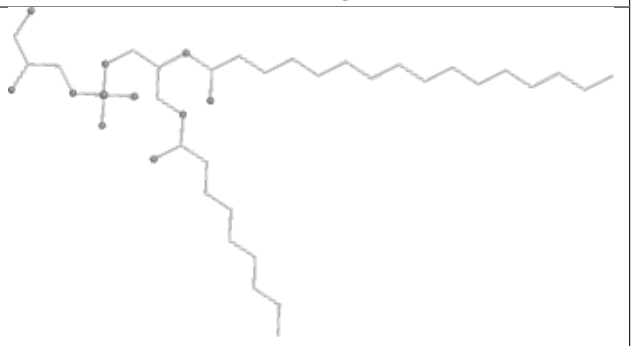
Bond lengths



Bond angles

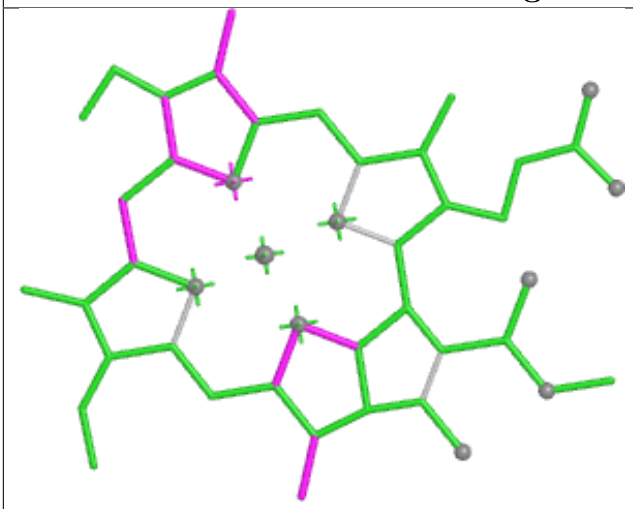


Torsions

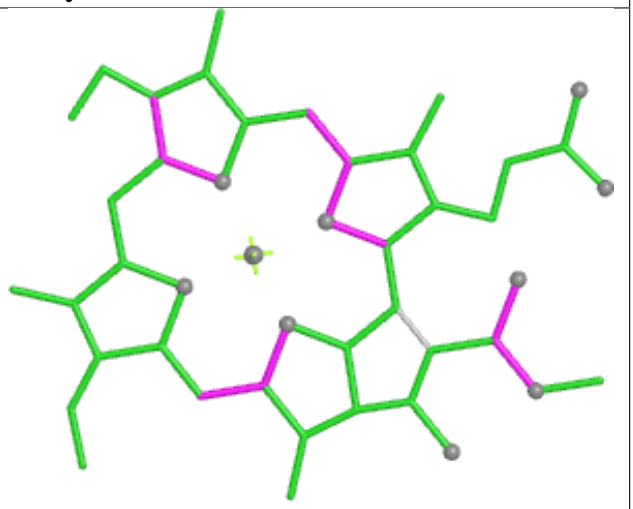


Rings

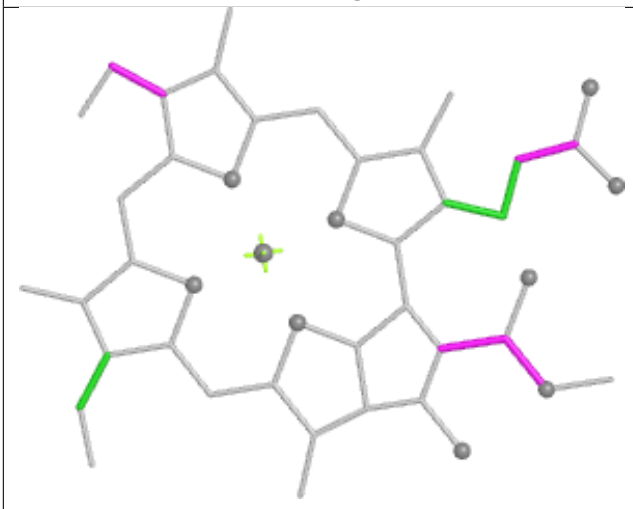
Ligand CLA Q 601



Bond lengths



Bond angles

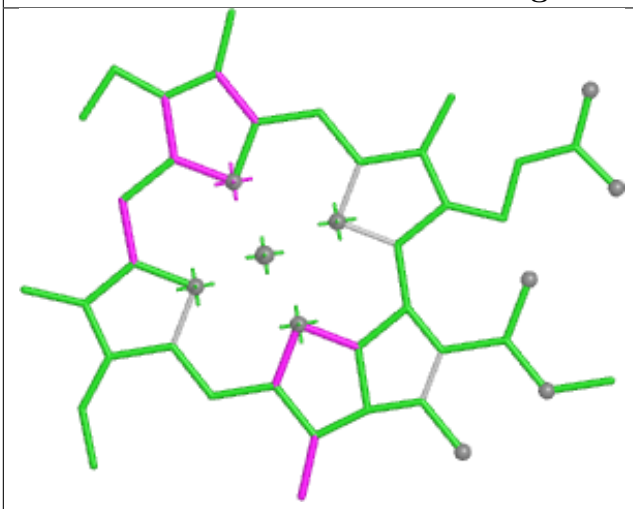


Torsions

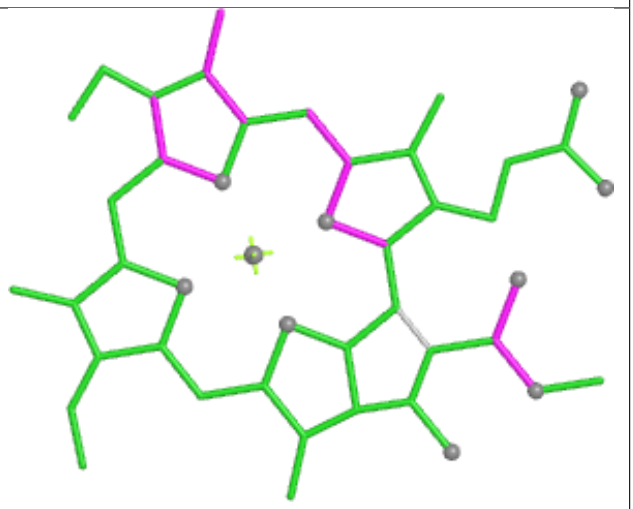


Rings

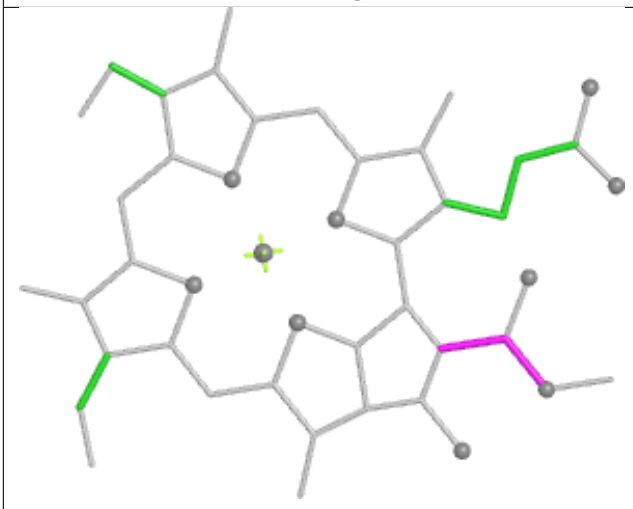
Ligand CLA I 609



Bond lengths



Bond angles

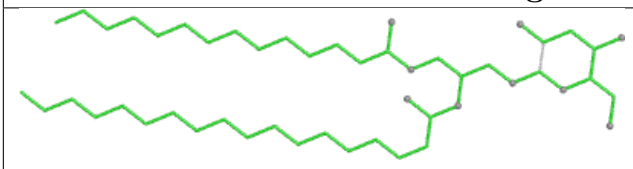


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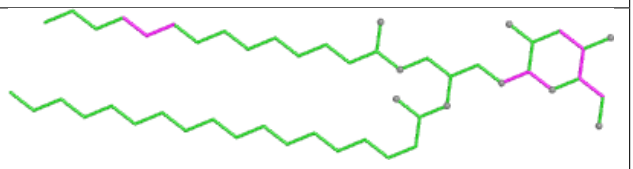


Rings

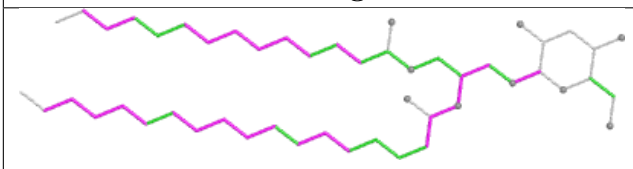
Ligand LMG I 615



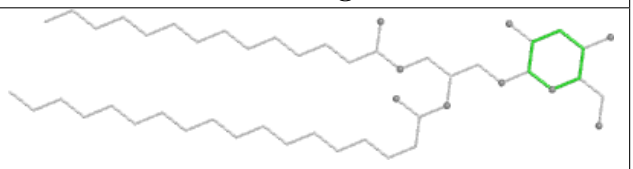
Bond lengths



Bond angles

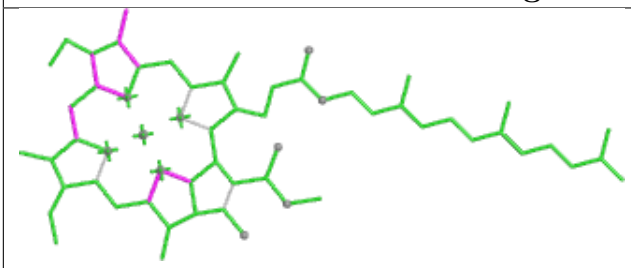


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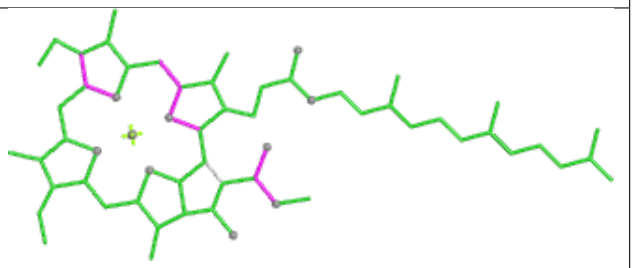


Rings

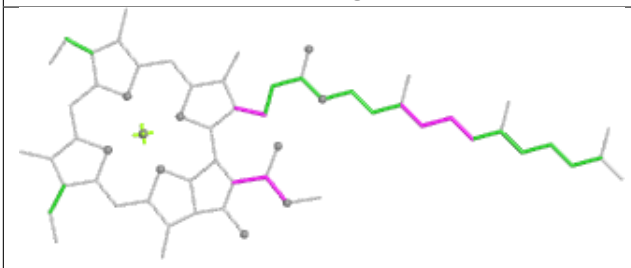
Ligand CLA H 307



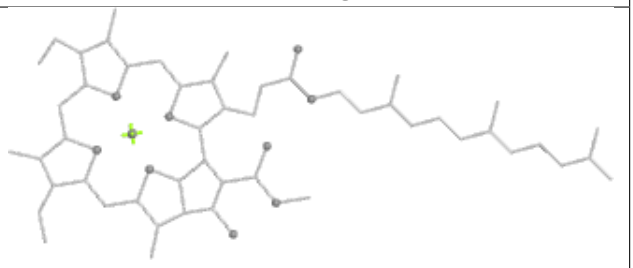
Bond lengths



Bond angles

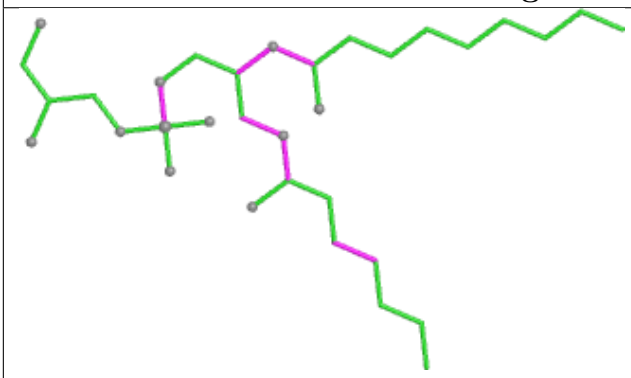


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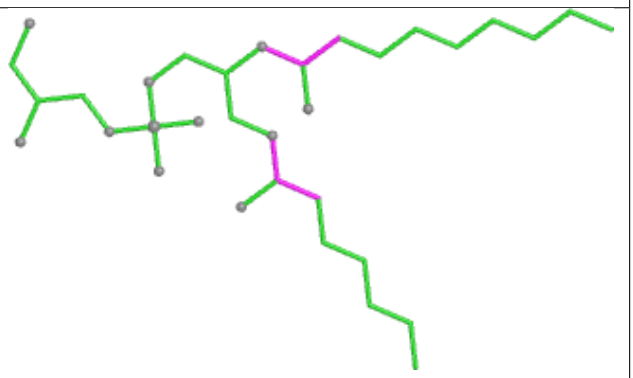


Rings

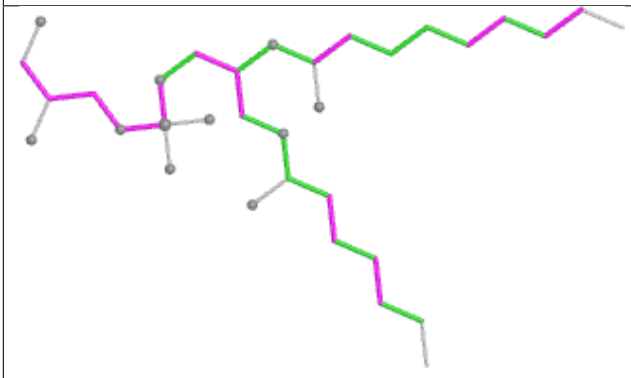
Ligand LHG K 619



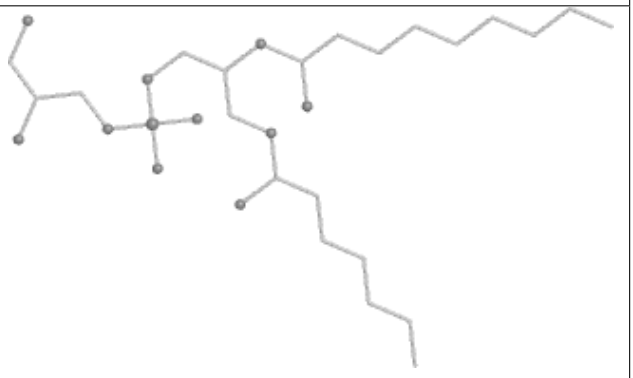
Bond lengths



Bond angles

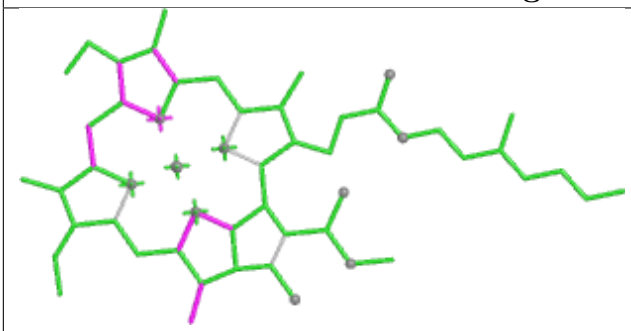


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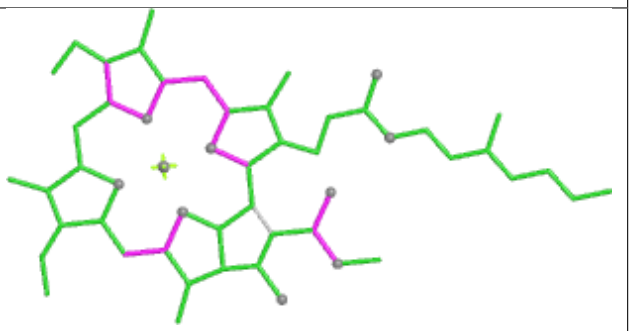


Rings

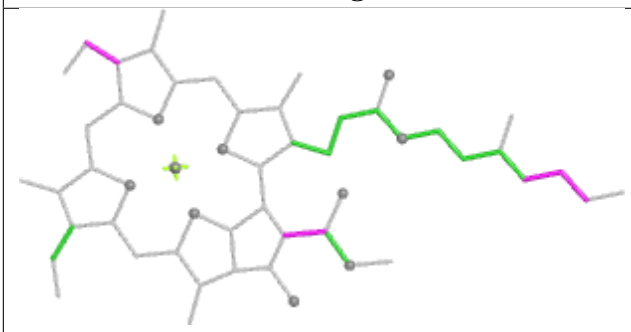
Ligand CLA K 613



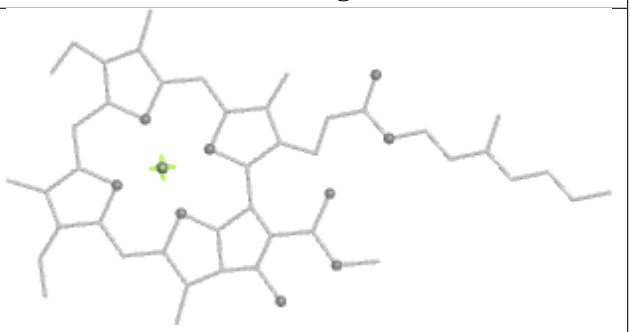
Bond lengths



Bond angles

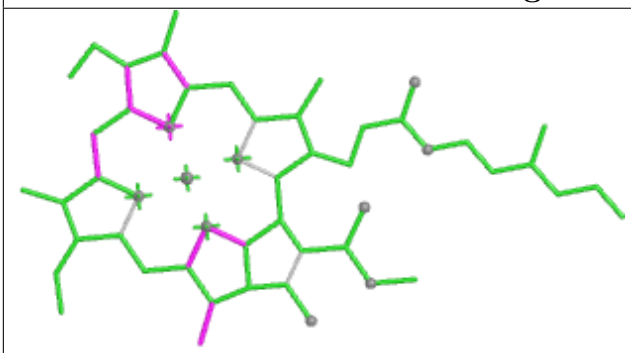


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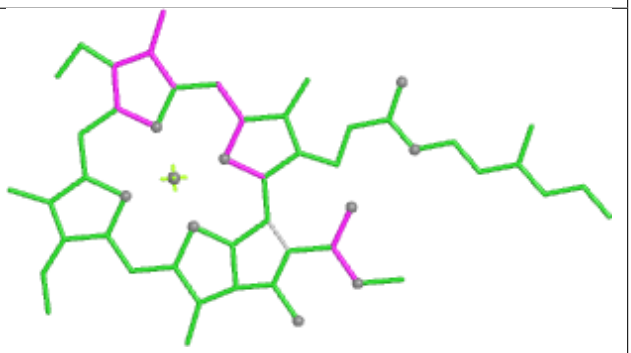


Rings

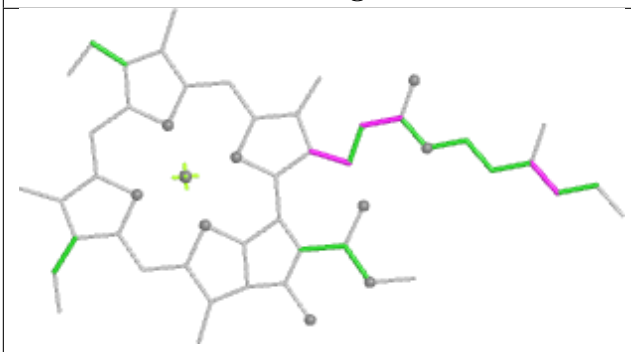
Ligand CLA A 832



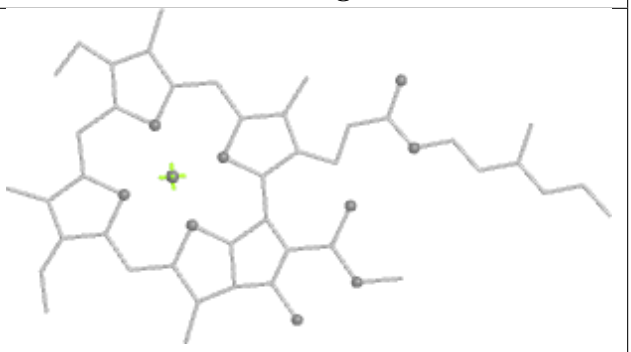
Bond lengths



Bond angles

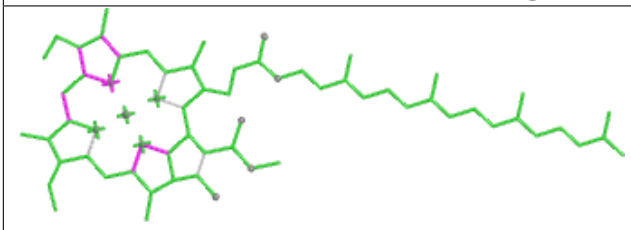


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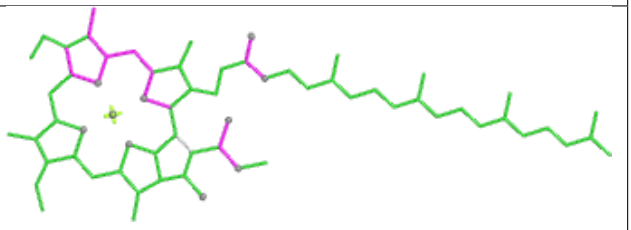


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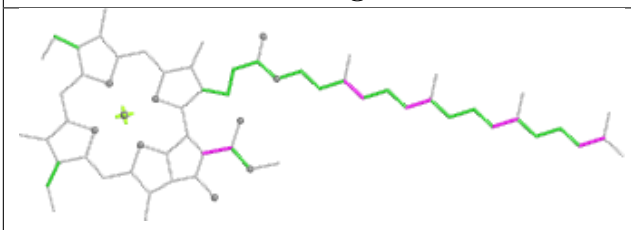
Ligand CLA A 828



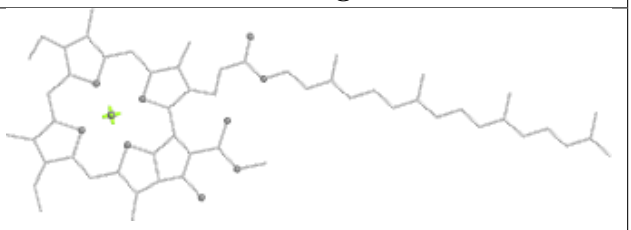
Bond lengths



Bond angles

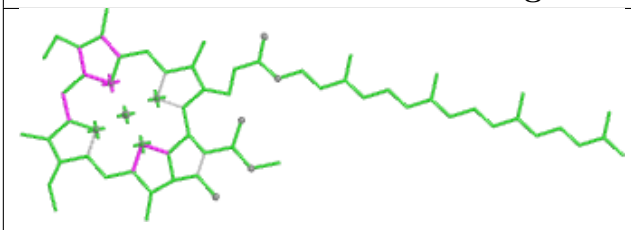


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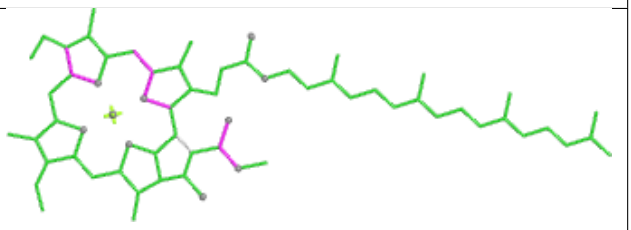


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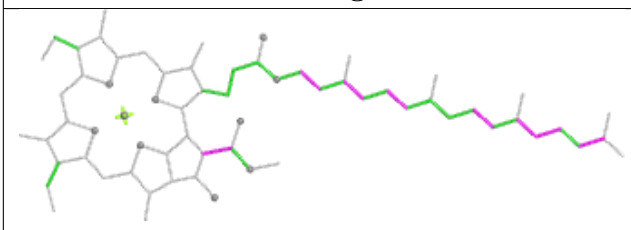
Ligand CLA B 823



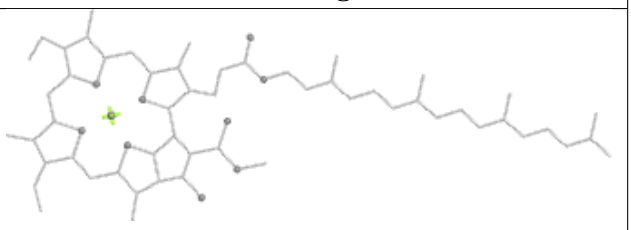
Bond lengths



Bond angles



Torsions

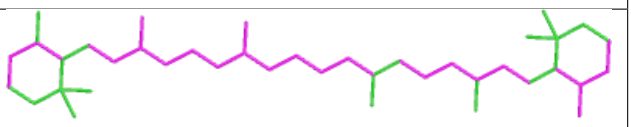


Rings

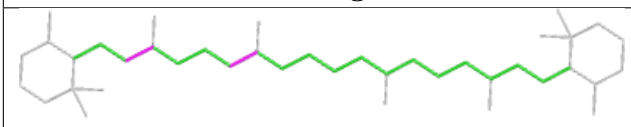
Ligand BCR B 801



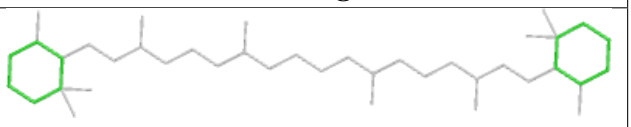
Bond lengths



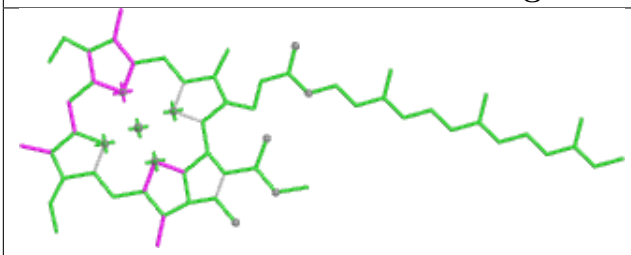
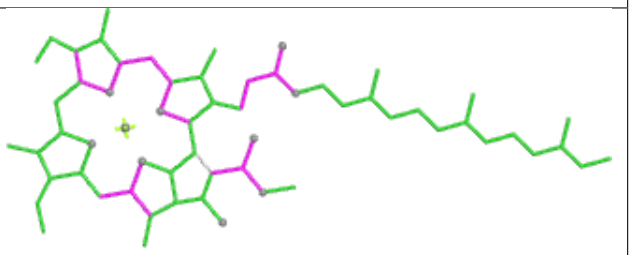
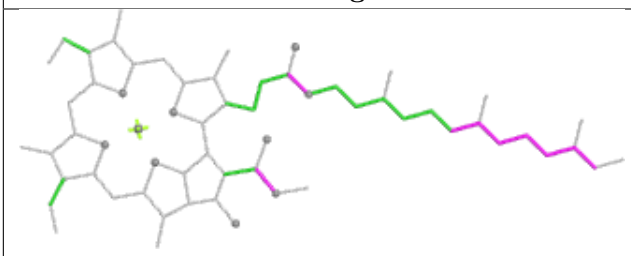
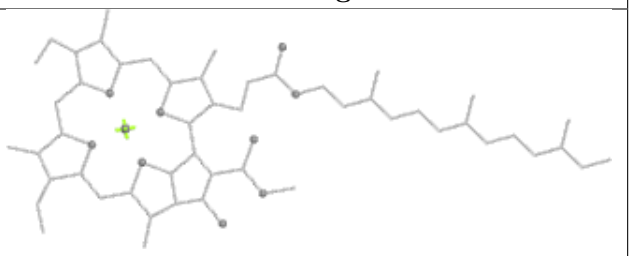
Bond angles

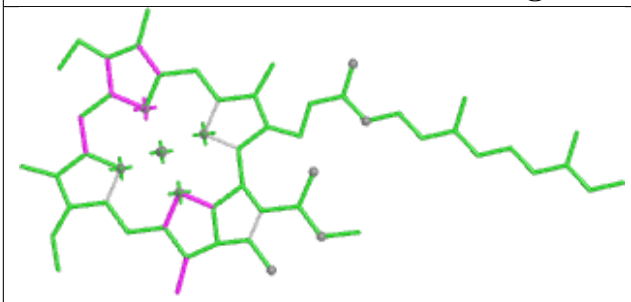
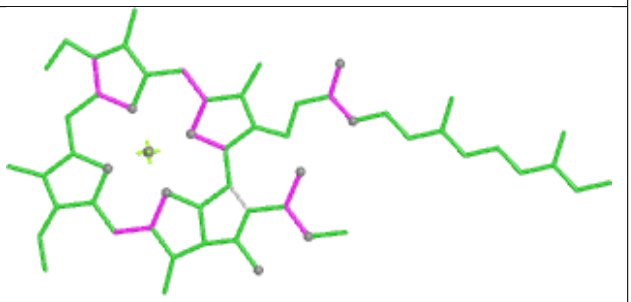
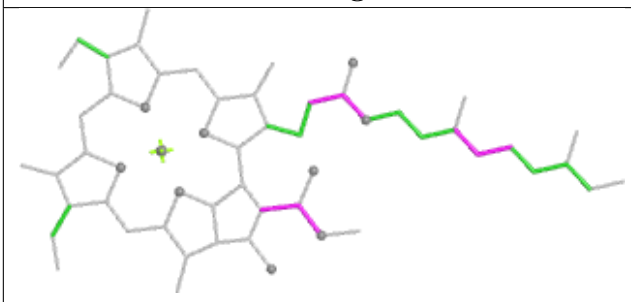
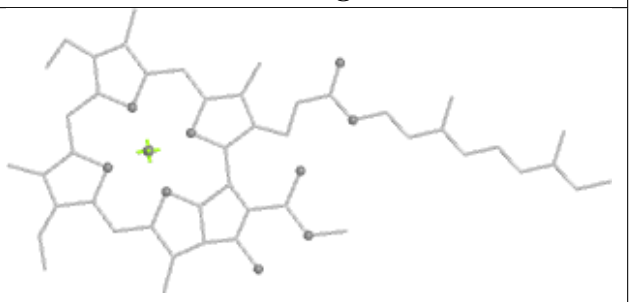


Torsions

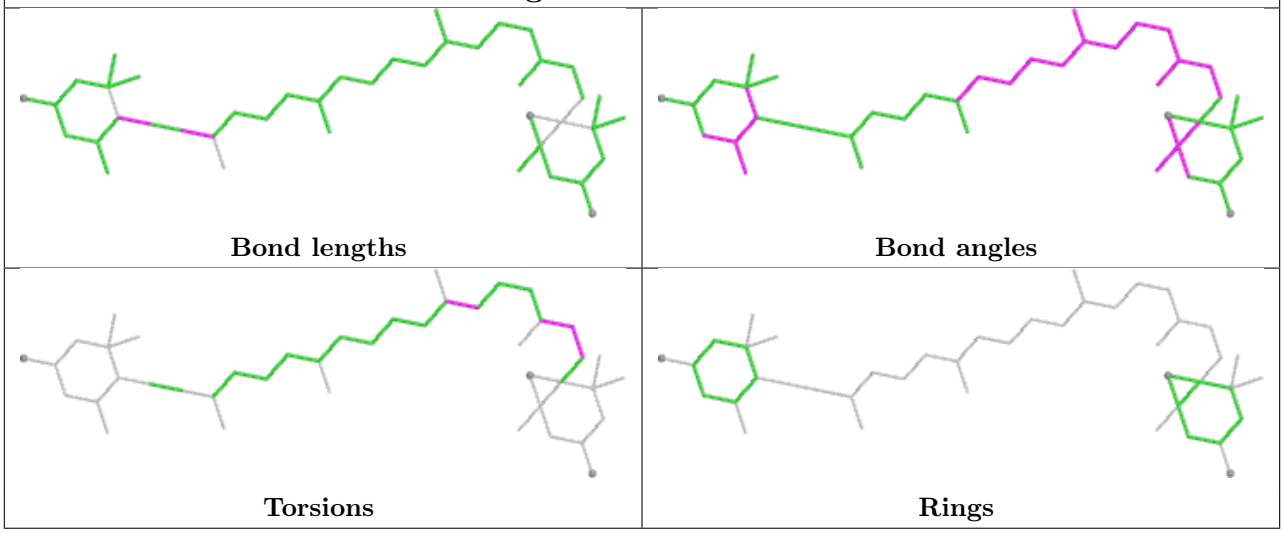


Rings

Ligand CLA A 816	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA L 404	
	
Bond lengths	Bond angles
	
Torsions	Rings

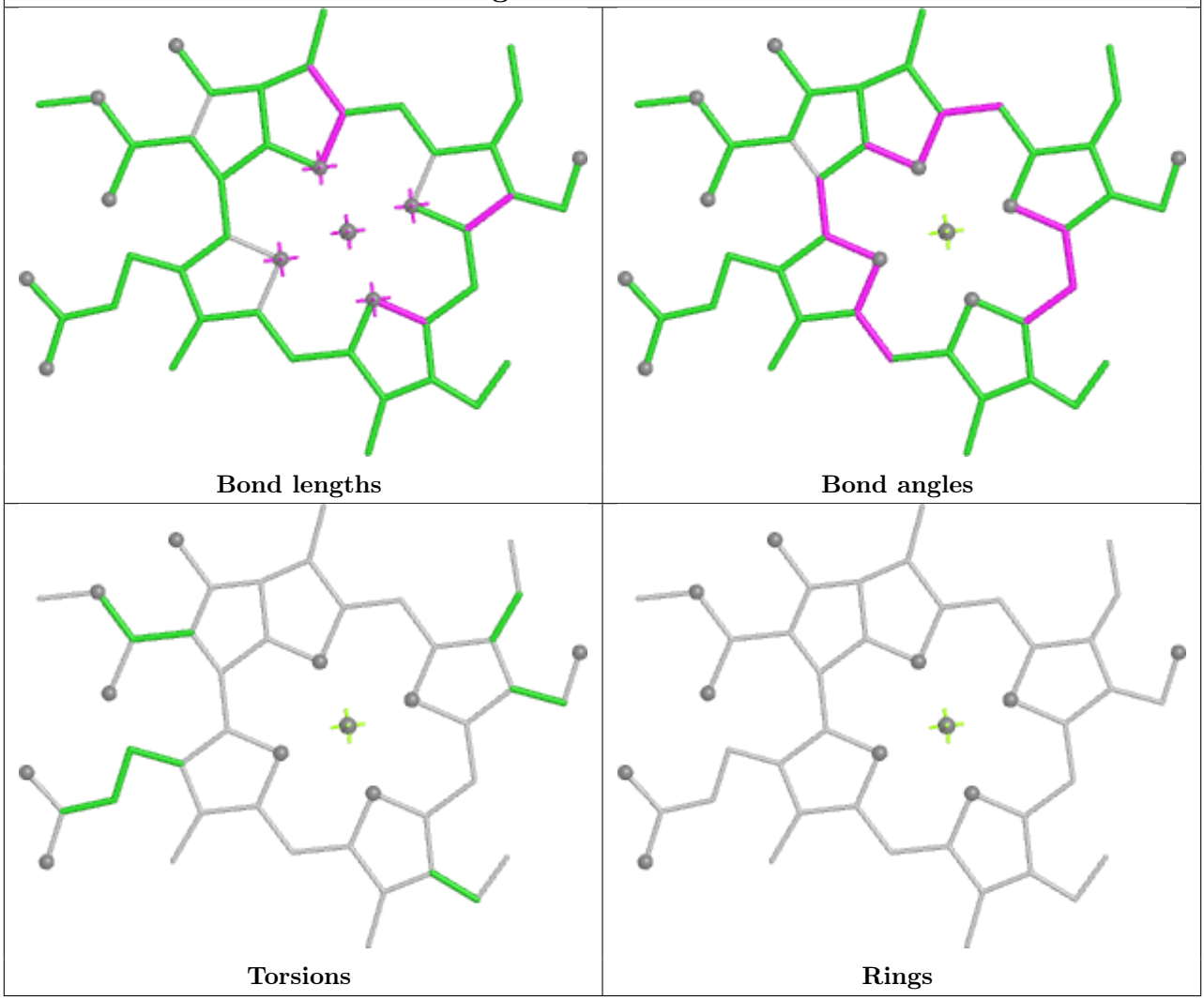
Ligand DD6 X 416



Bond lengths | Bond angles

Torsions | Rings

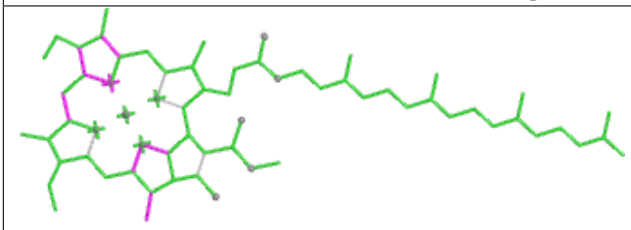
Ligand CHL V 605



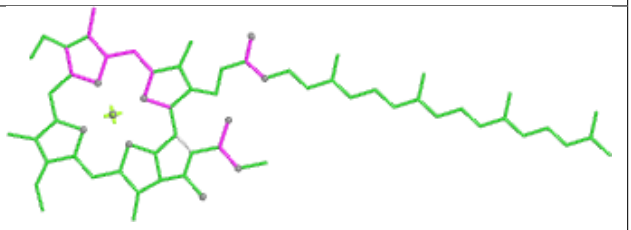
Bond lengths | Bond angles

Torsions | Rings

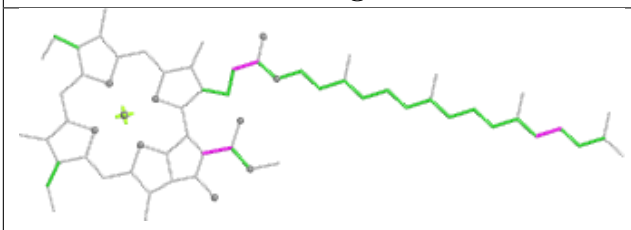
Ligand CLA B 839



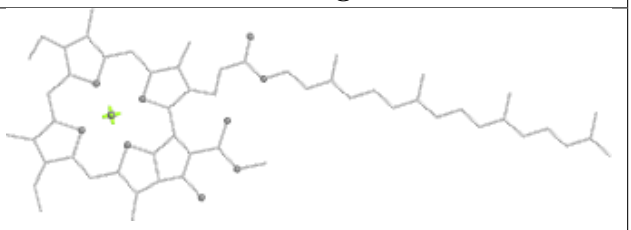
Bond lengths



Bond angles

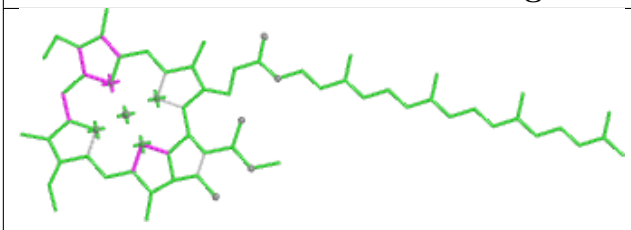


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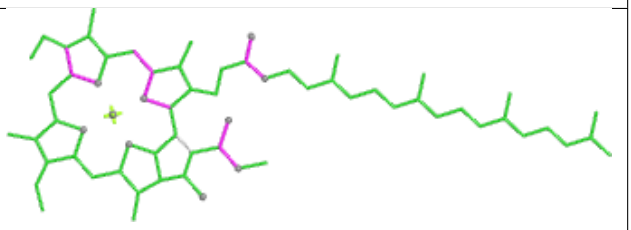


Rings

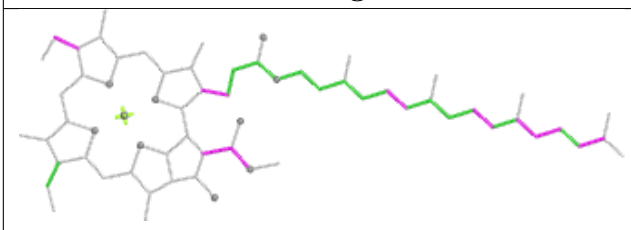
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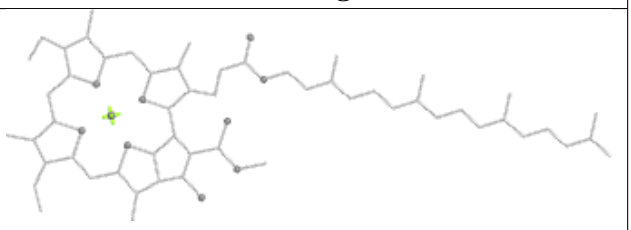
Bond lengths



Bond angles

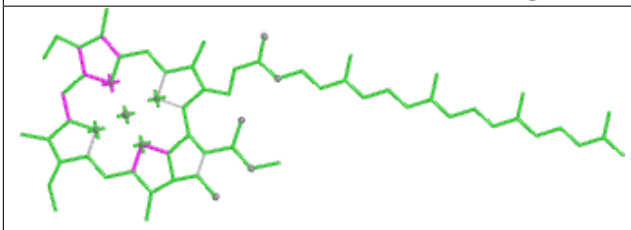


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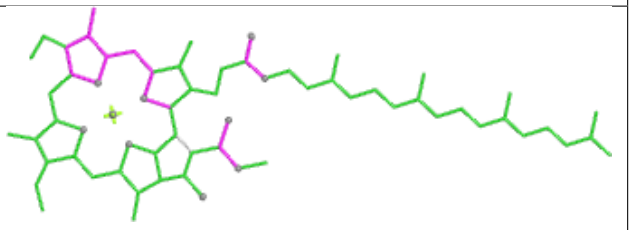


Rings

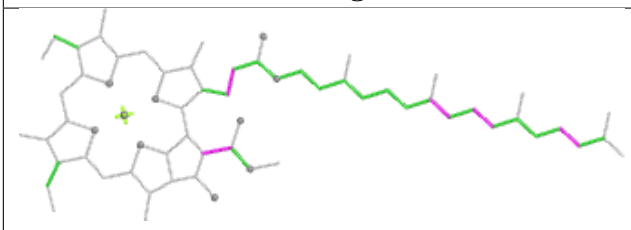
Ligand CLA A 815



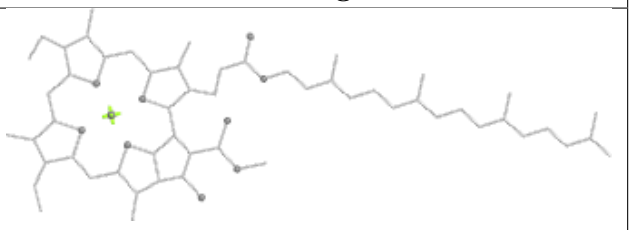
Bond lengths



Bond angles

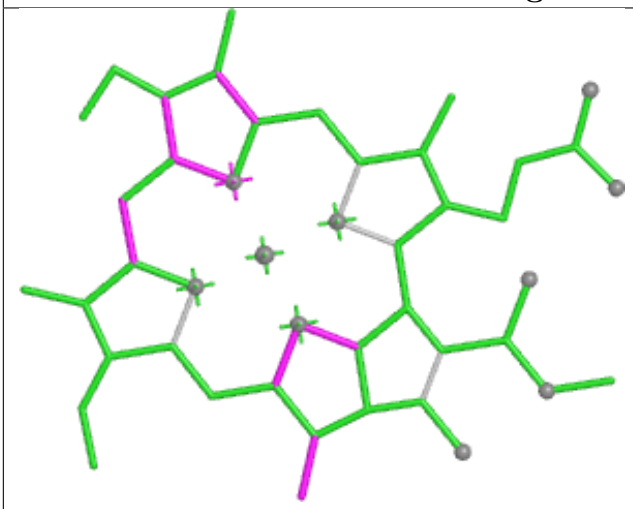


Torsions

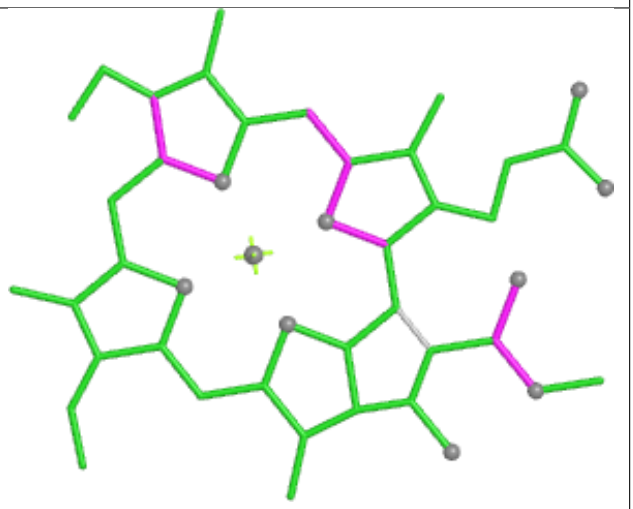


Rings

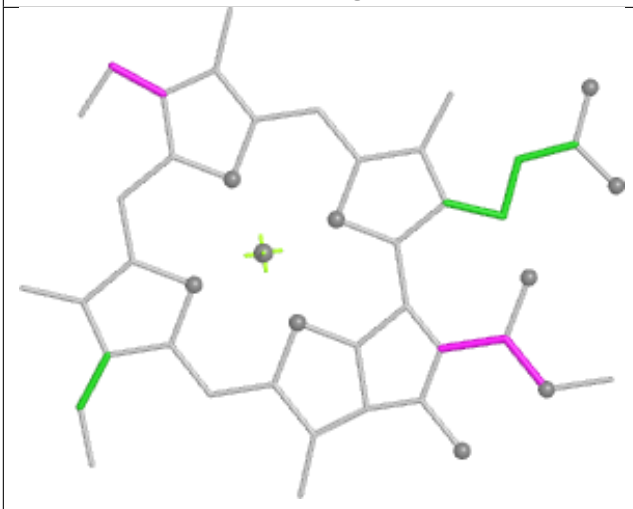
Ligand CLA F 405



Bond lengths



Bond angles

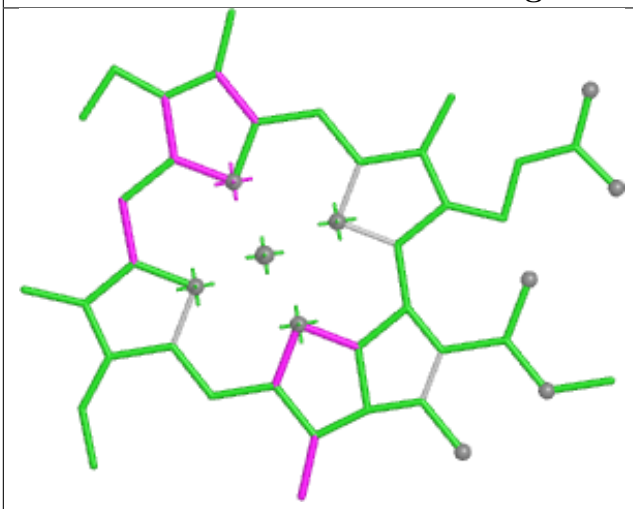


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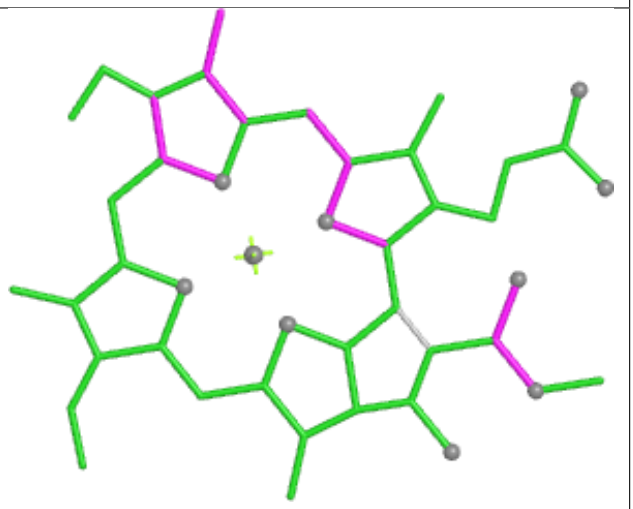


Rings

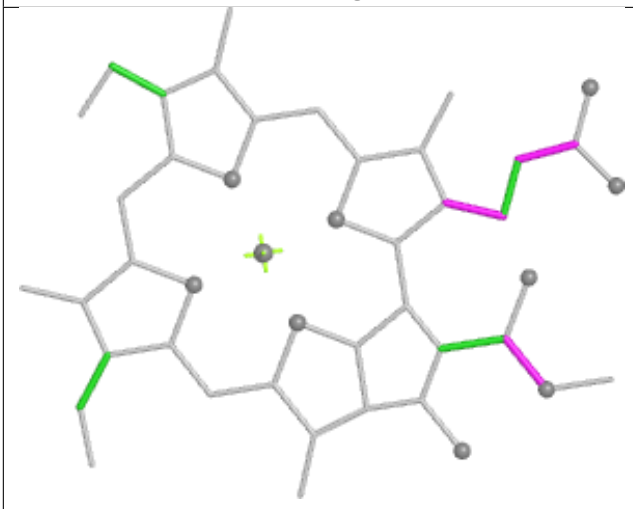
Ligand CLA P 606



Bond lengths



Bond angles

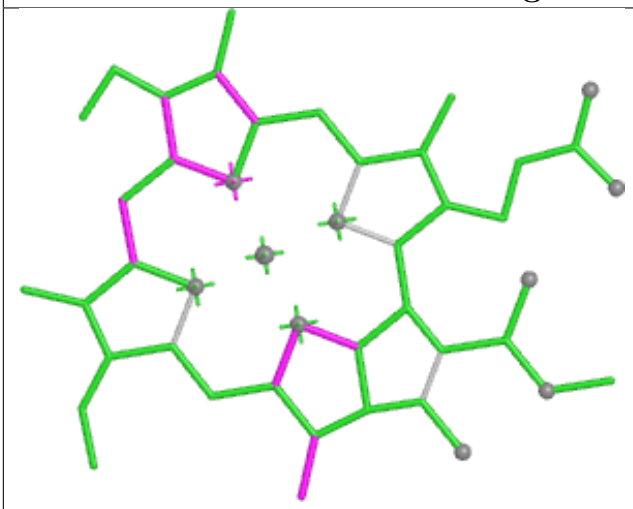


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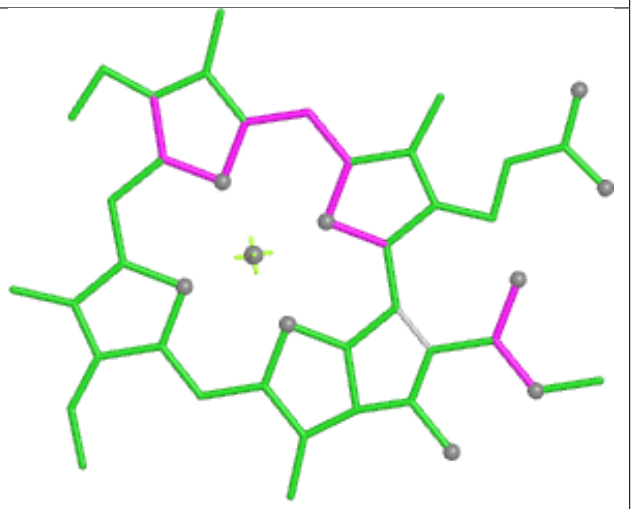


Rings

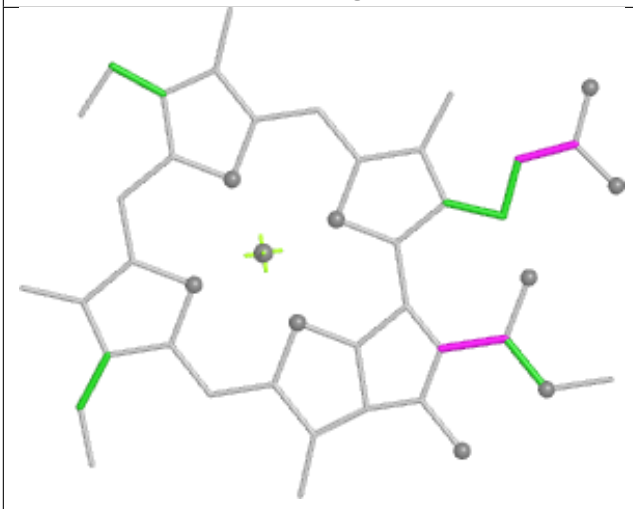
Ligand CLA N 609



Bond lengths



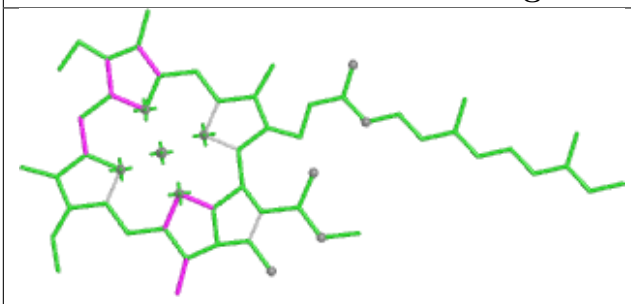
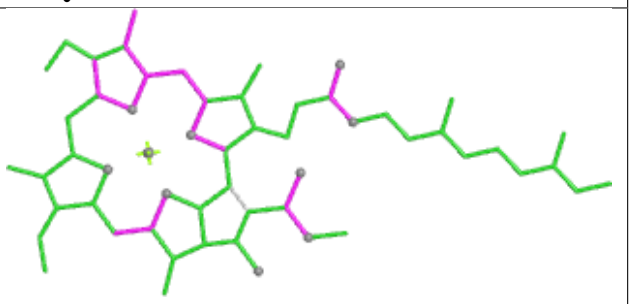
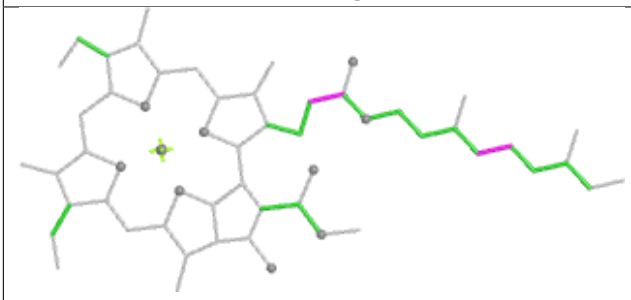
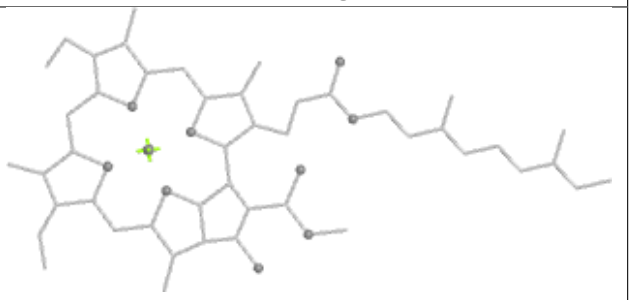
Bond angles

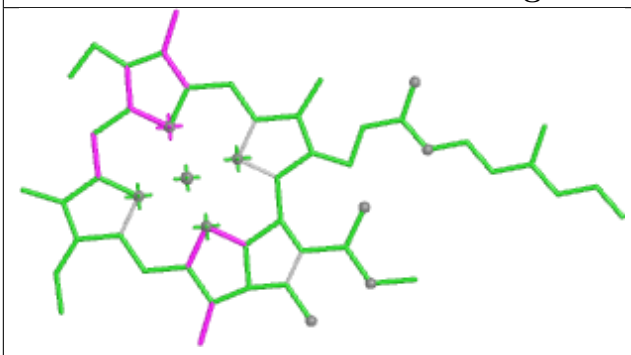
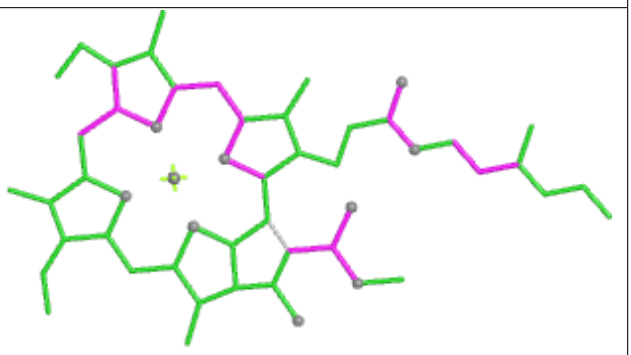
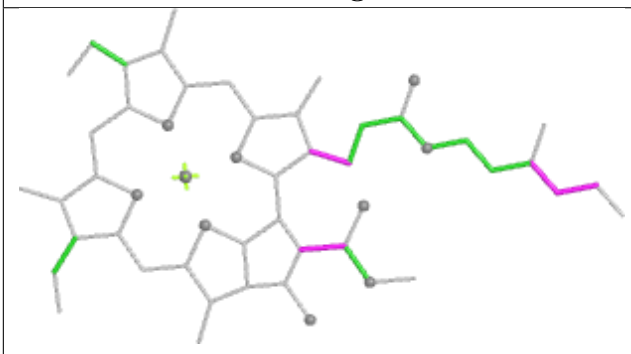
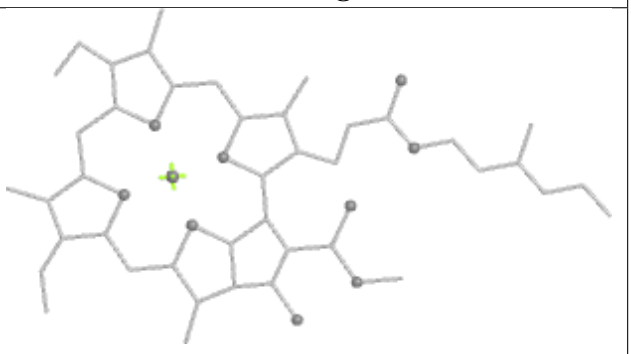


Torsions

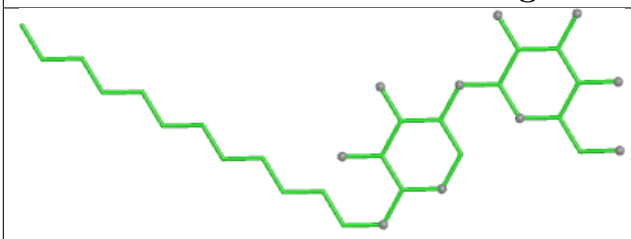


Rings

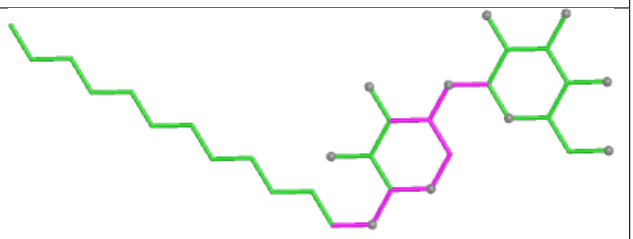
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Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 838	
	
Bond lengths	Bond angles
	
Torsions	Rings

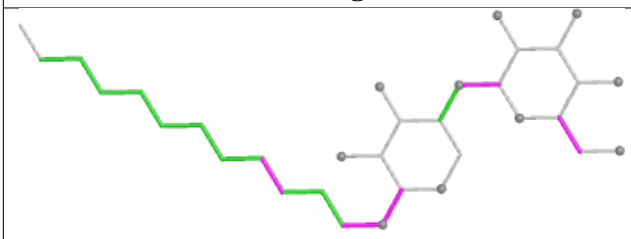
Ligand LMU K 620



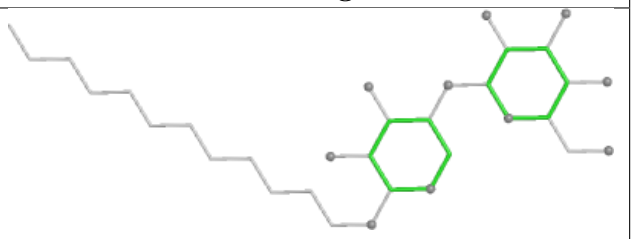
Bond lengths



Bond angles

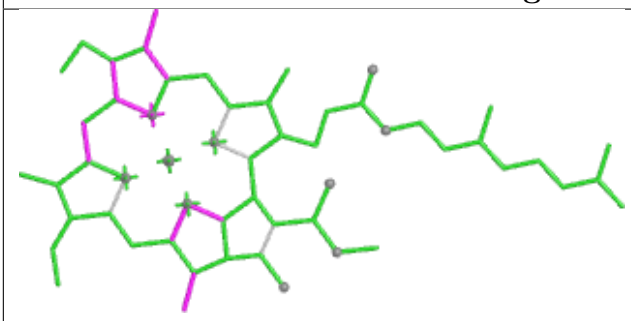


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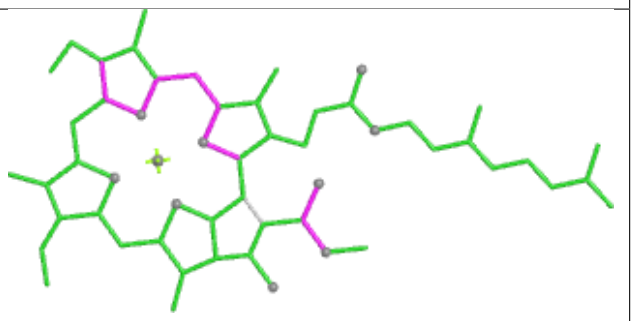


Rings

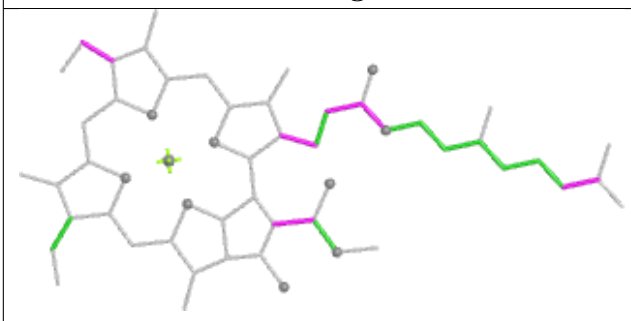
Ligand CLA H 306



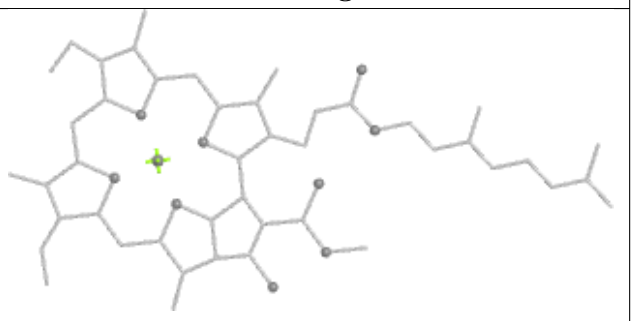
Bond lengths



Bond angles

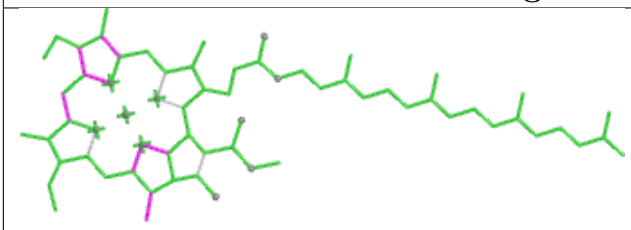


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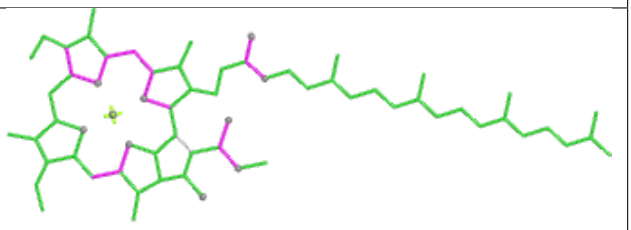


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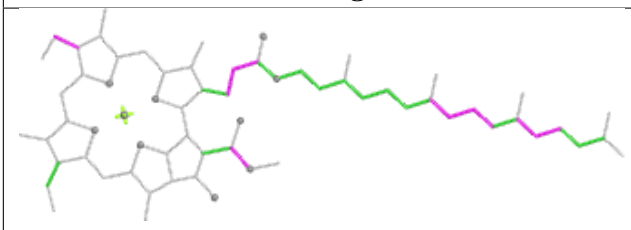
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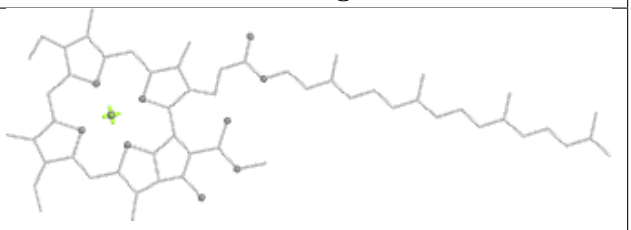
Bond lengths



Bond angles

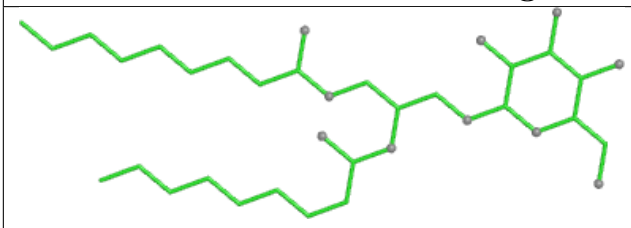


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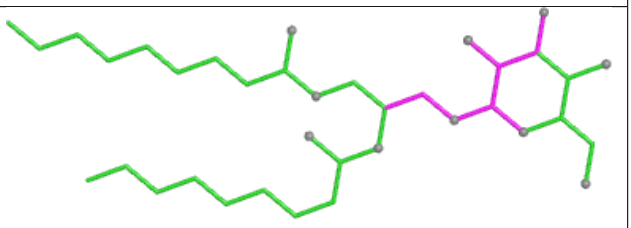


Rings

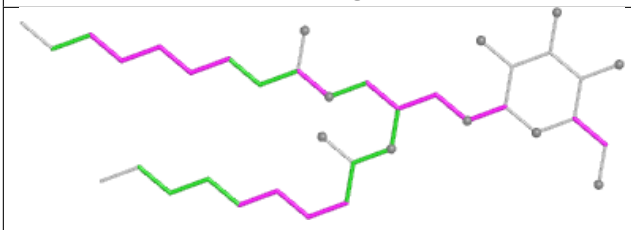
Ligand LMG H 322



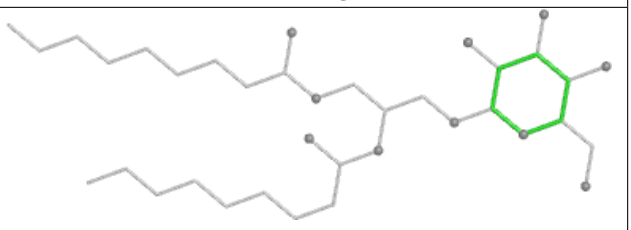
Bond lengths



Bond angles

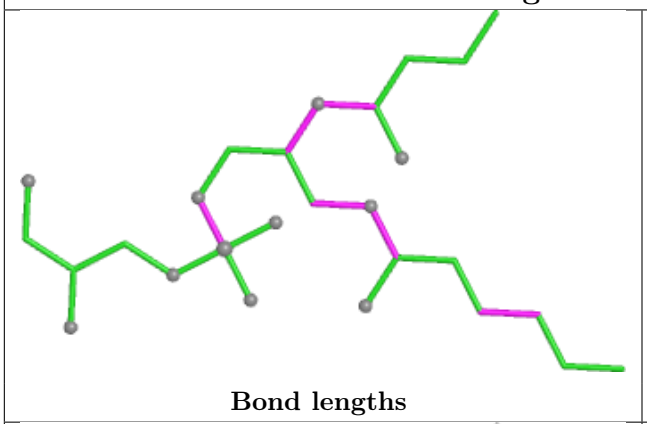


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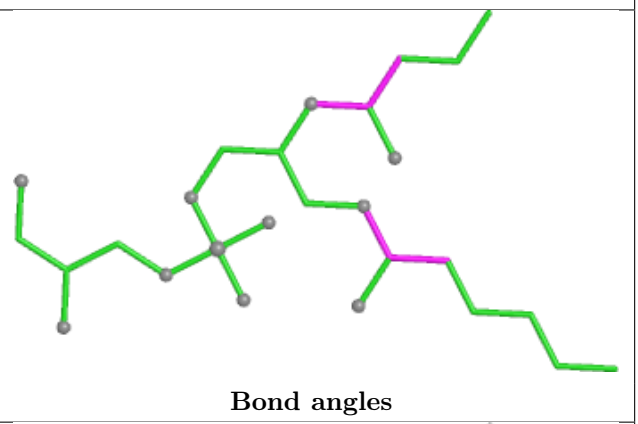


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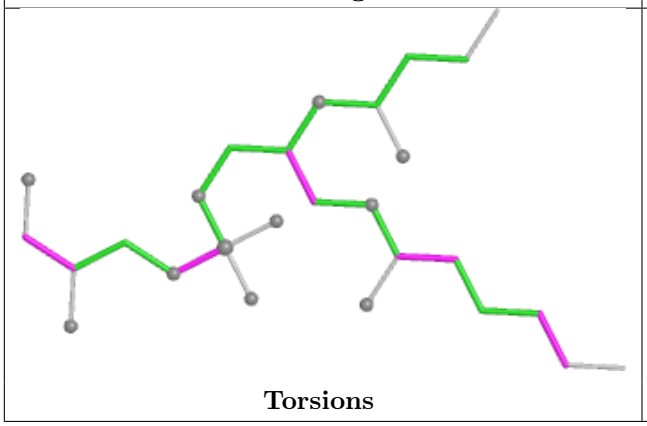
Ligand LHG H 316



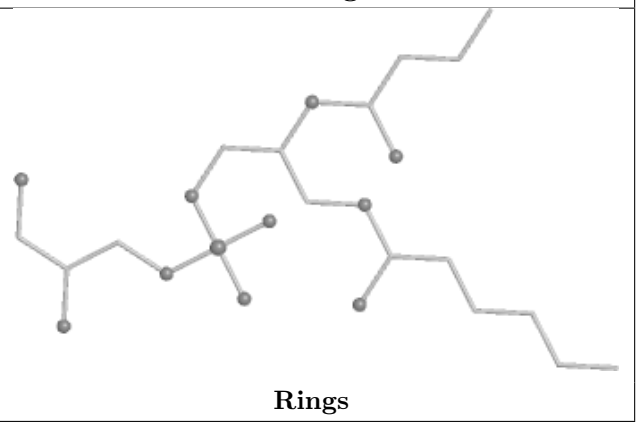
Bond lengths



Bond angles

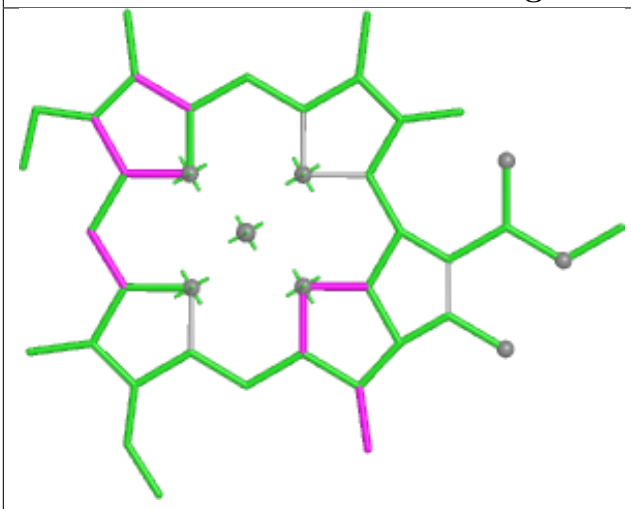


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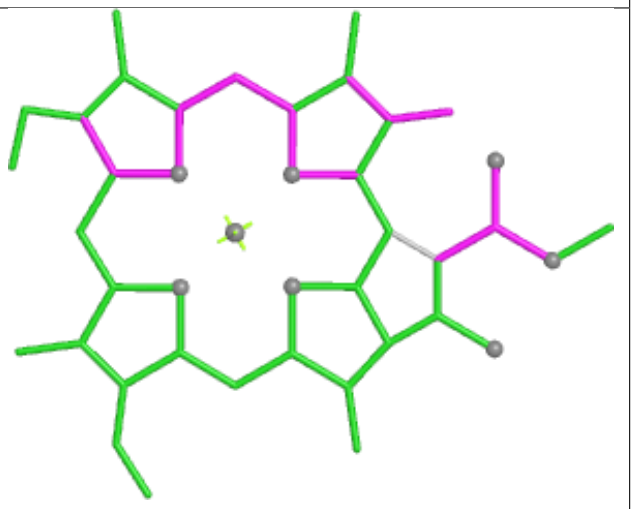


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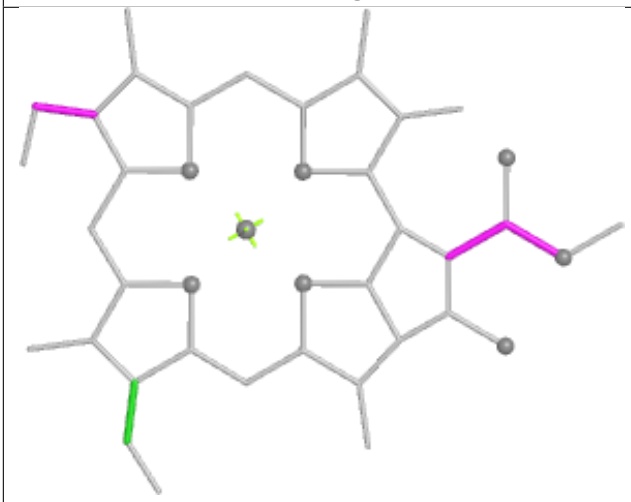
Ligand CLA P 610



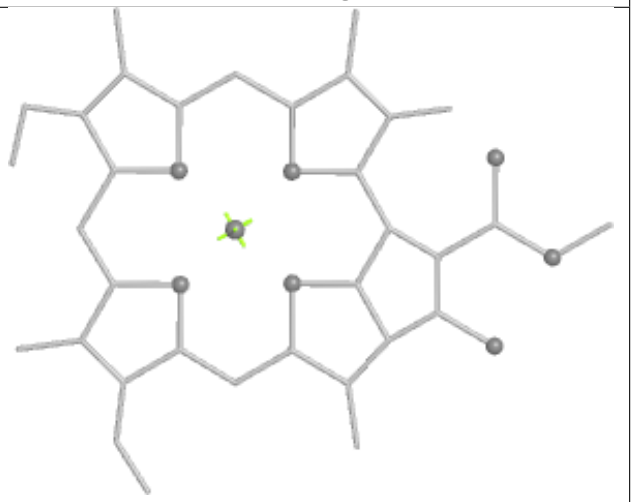
Bond lengths



Bond angles

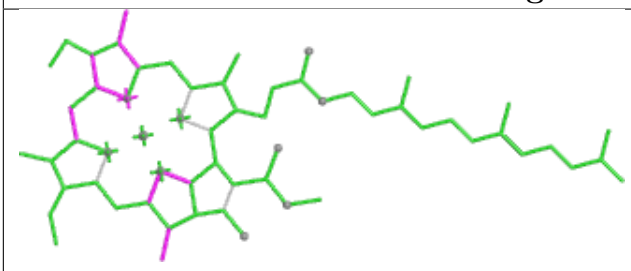


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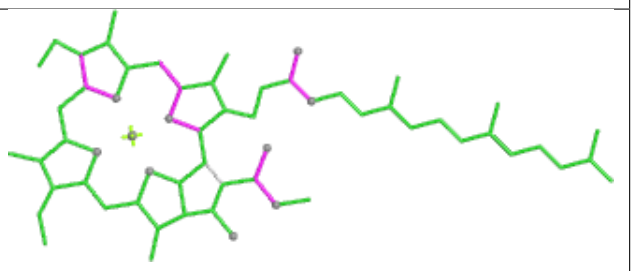


Rings

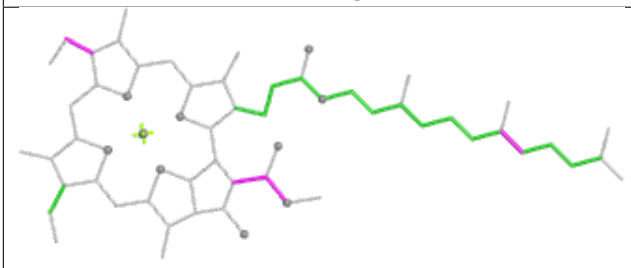
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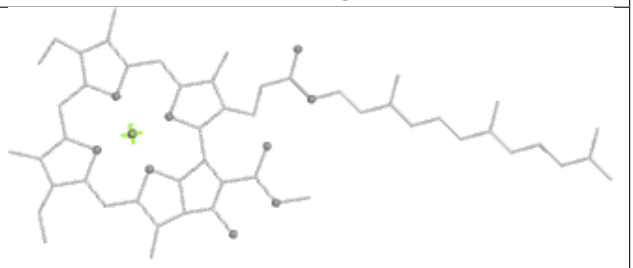
Bond lengths



Bond angles

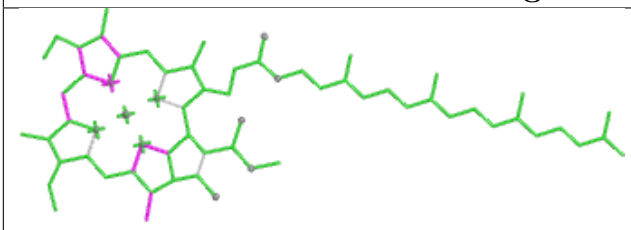


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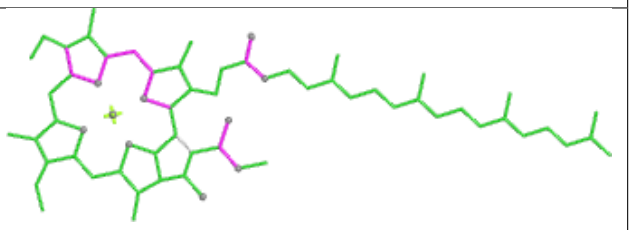


Rings

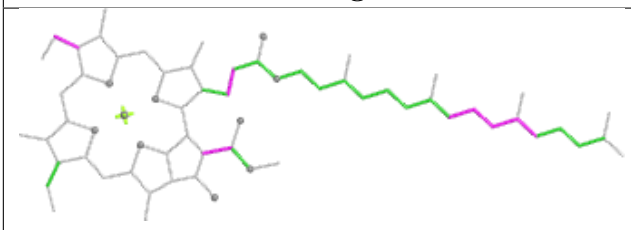
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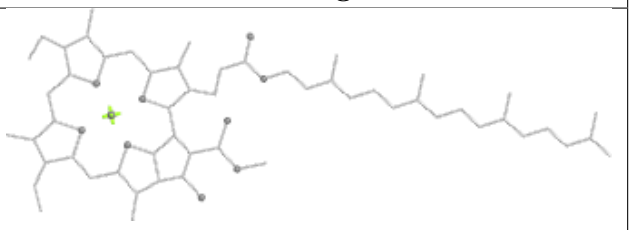
Bond lengths



Bond angles

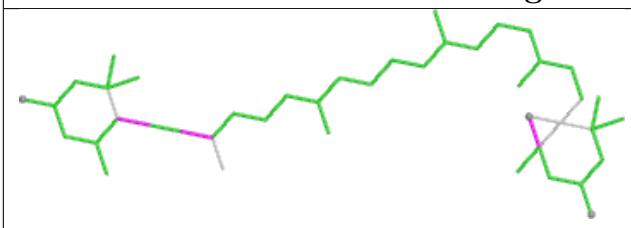


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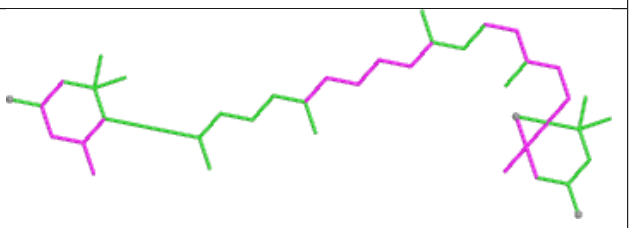


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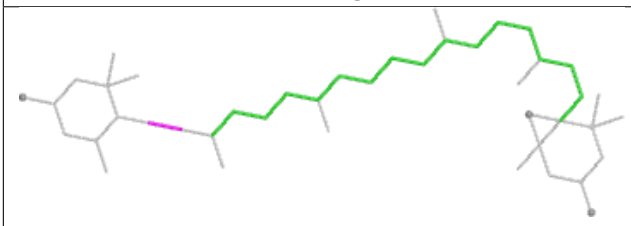
Ligand DD6 O 316



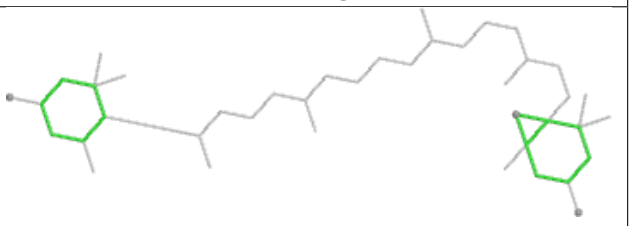
Bond lengths



Bond angles

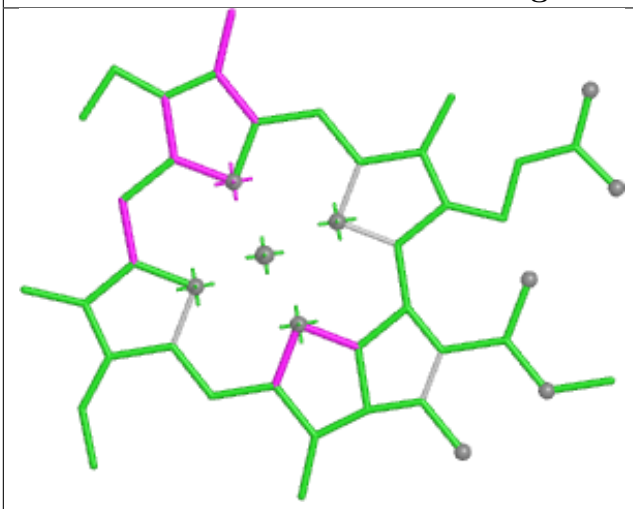


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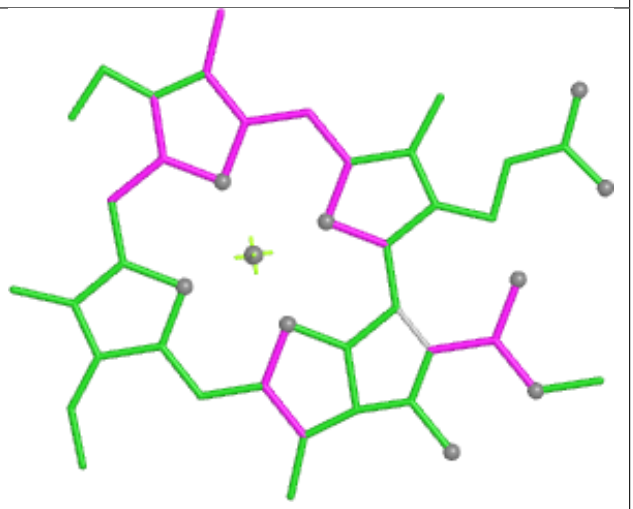


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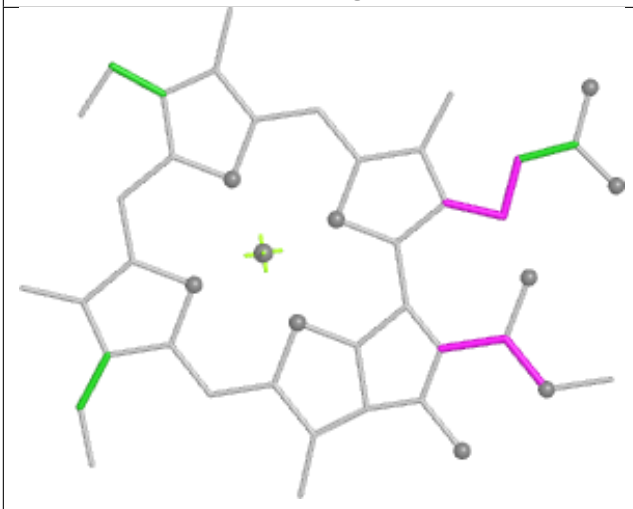
Ligand CLA I 611



Bond lengths



Bond angles

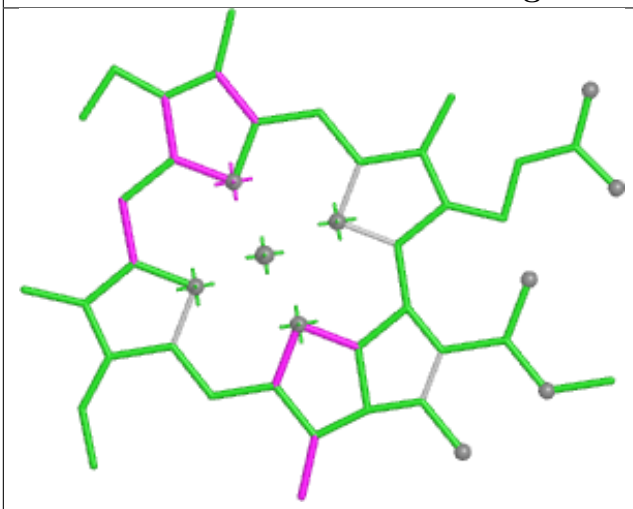


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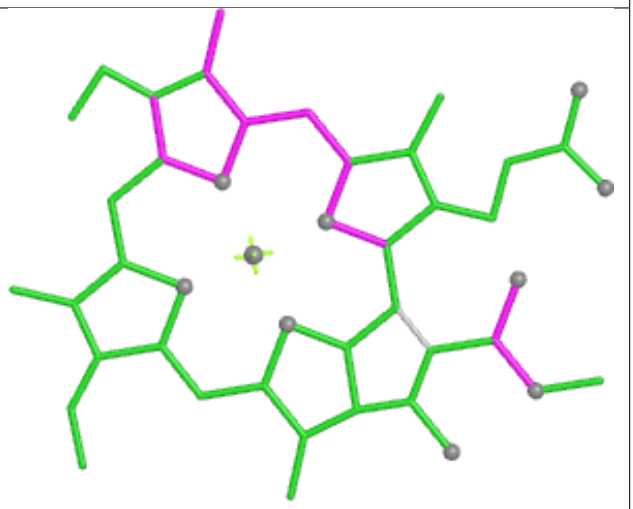


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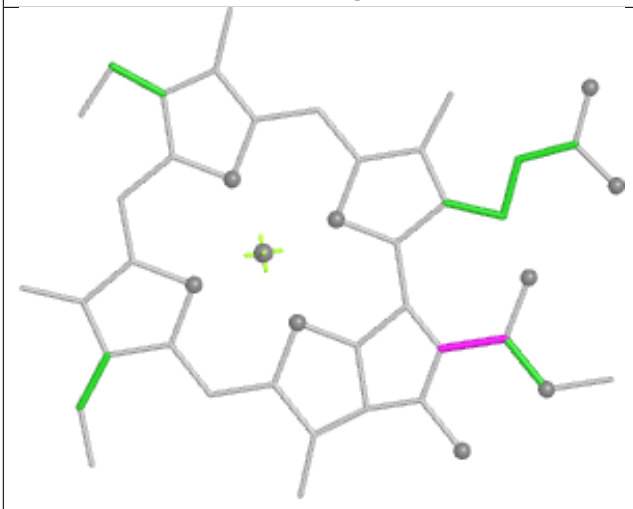
Ligand CLA N 605



Bond lengths



Bond angles

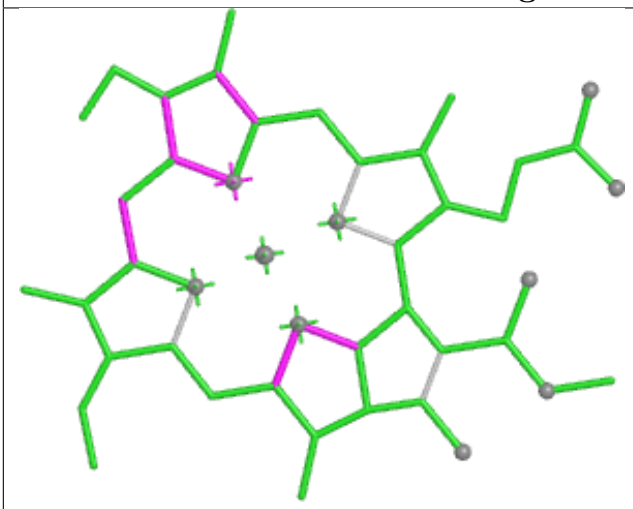


Torsions

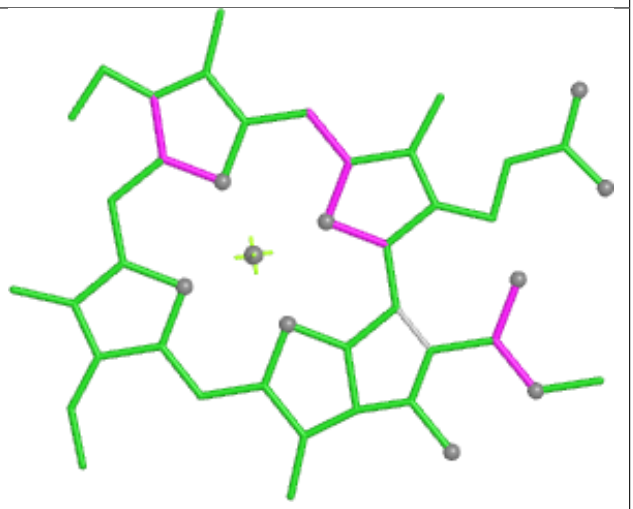


Rings

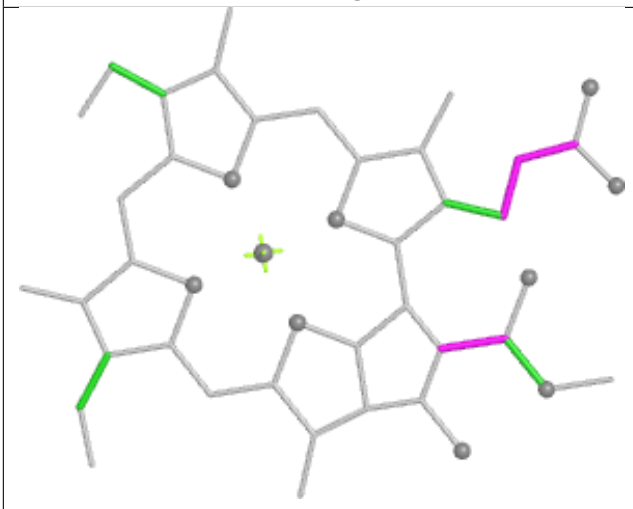
Ligand CLA W 419



Bond lengths



Bond angles

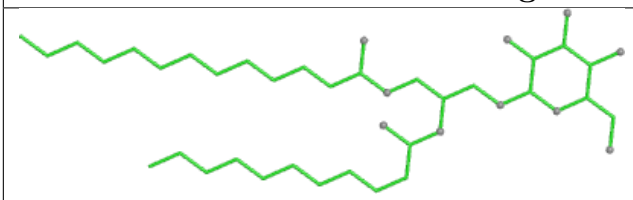


Torsions

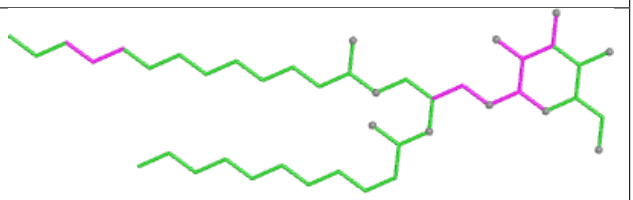


Rings

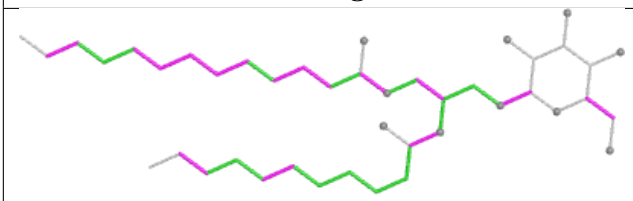
Ligand LMG K 622



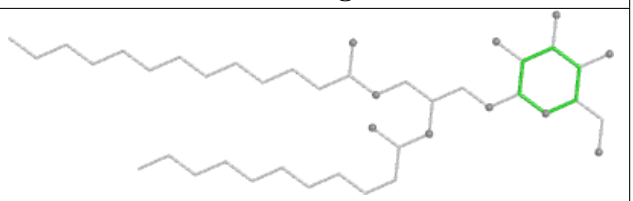
Bond lengths



Bond angles

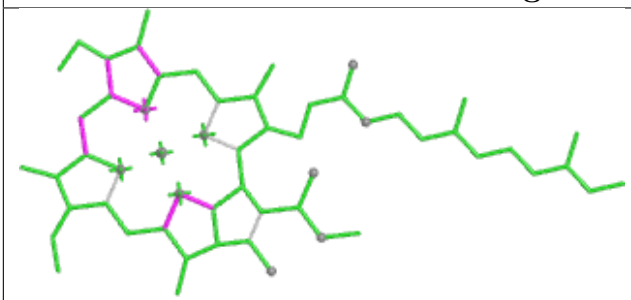


Torsions

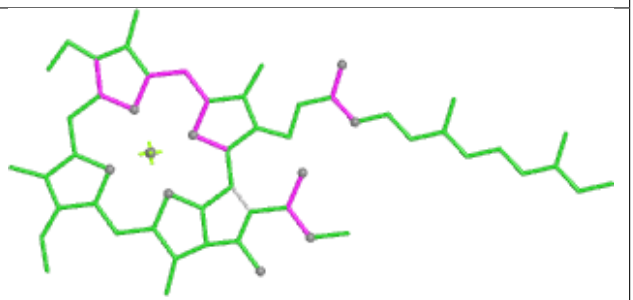


Rings

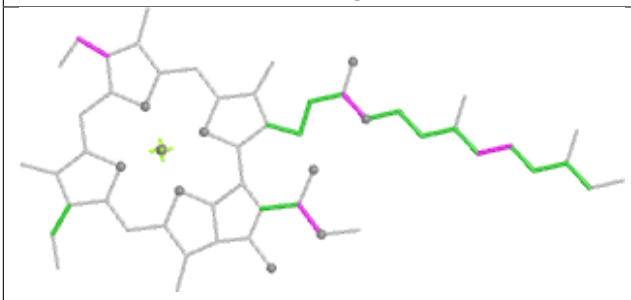
Ligand CLA U 406



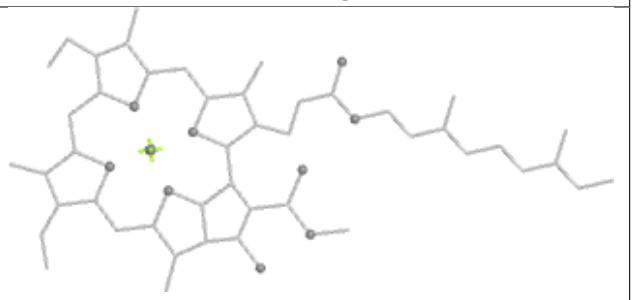
Bond lengths



Bond angles

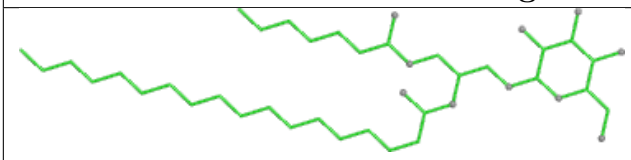


Torsions

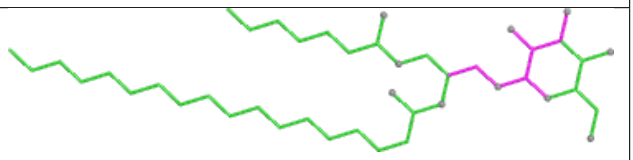


Rings

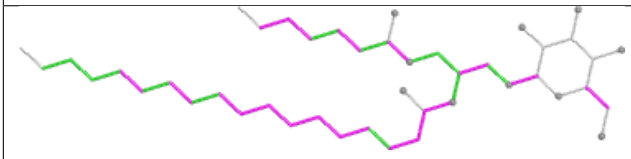
Ligand LMG N 615



Bond lengths



Bond angles

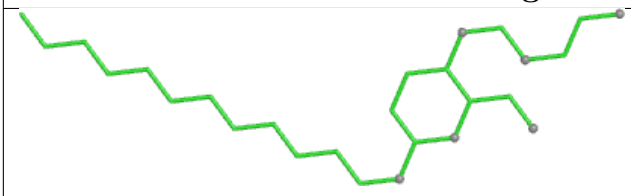


Torsions

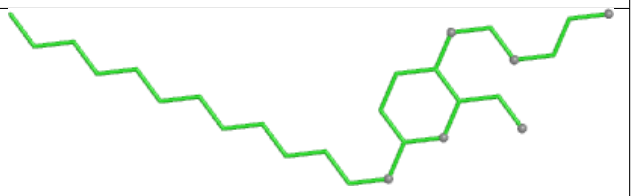


Rings

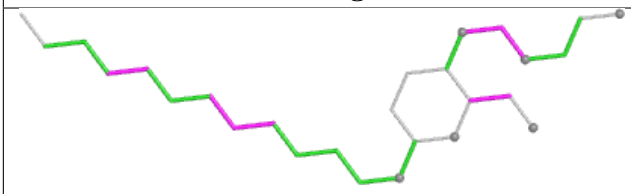
Ligand LMU L 419



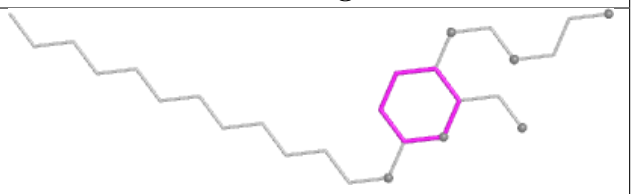
Bond lengths



Bond angles

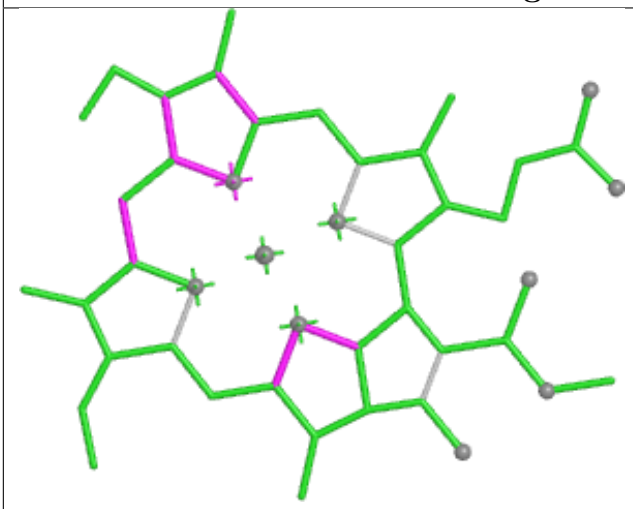


Torsions

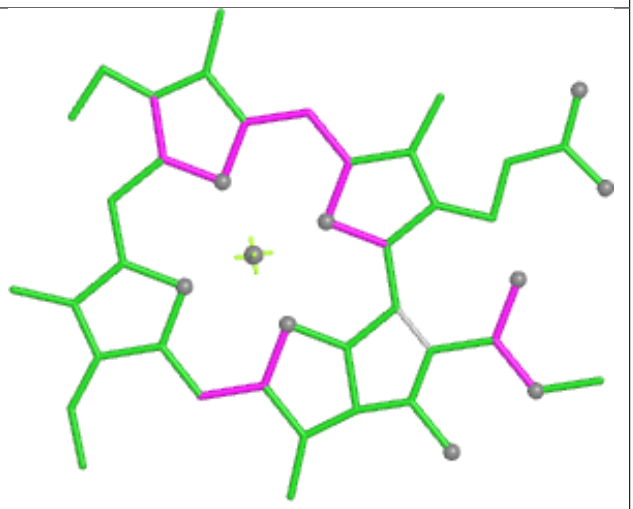


Rings

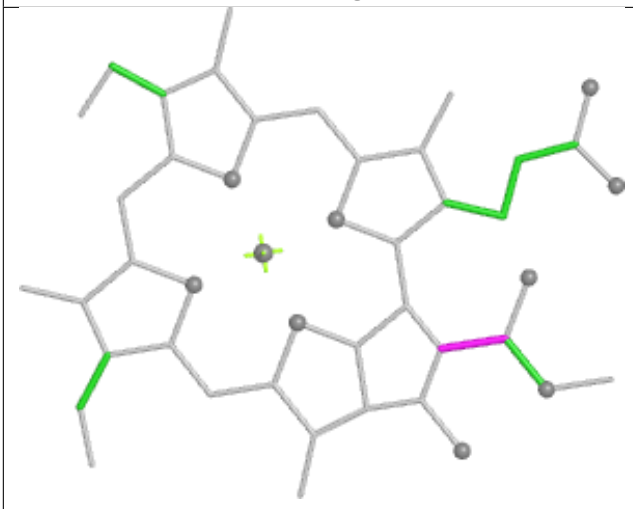
Ligand CLA O 319



Bond lengths



Bond angles

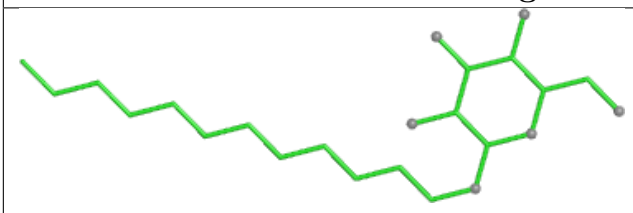


Torsions

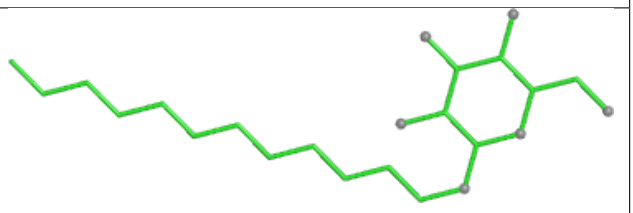


Rings

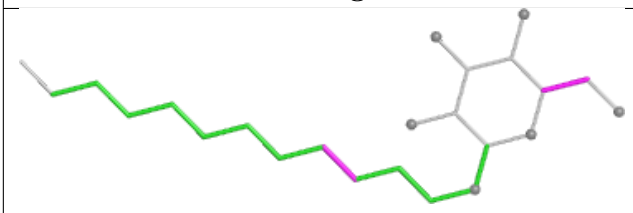
Ligand LMU U 424



Bond lengths



Bond angles

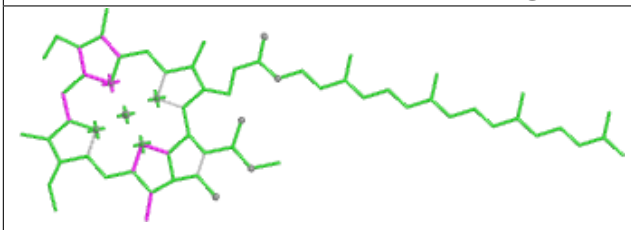


Torsions

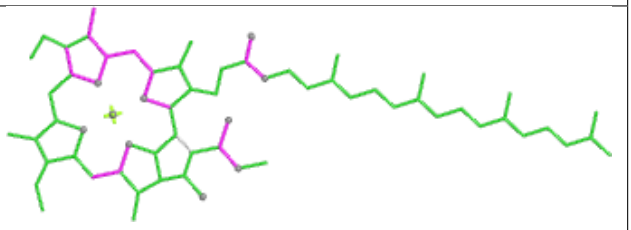


Rings

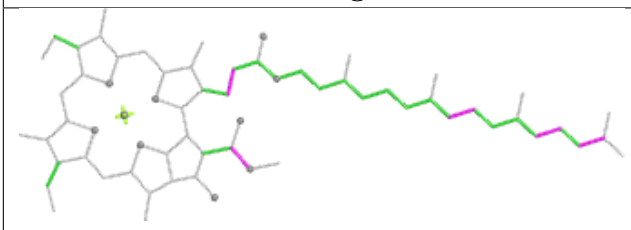
Ligand CLA A 833



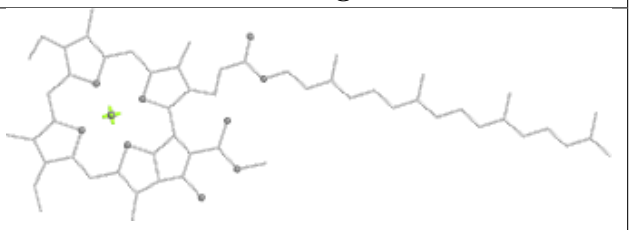
Bond lengths



Bond angles

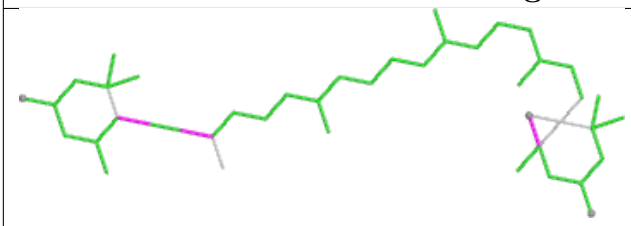


Torsions

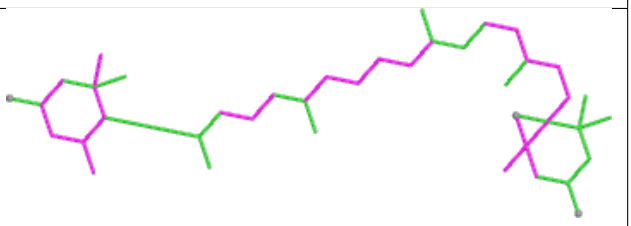


Rings

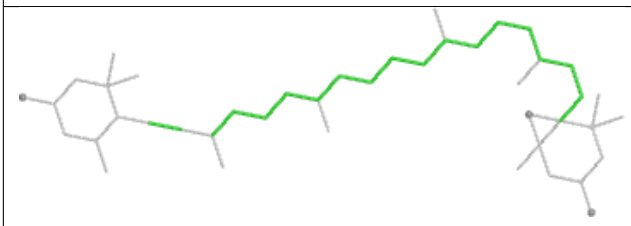
Ligand DD6 K 614



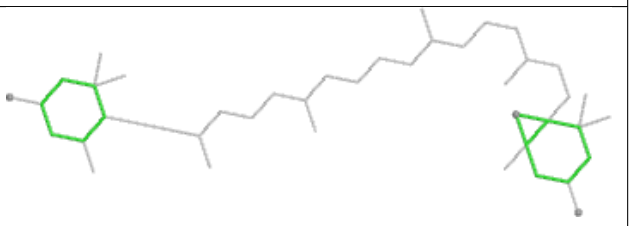
Bond lengths



Bond angles

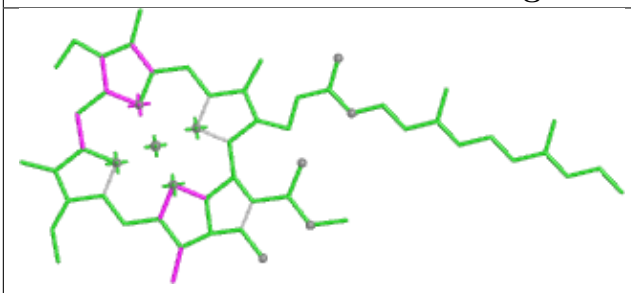


Torsions

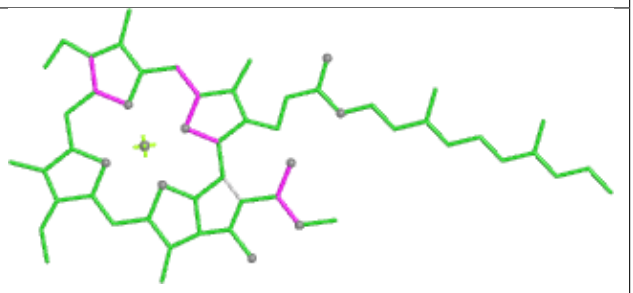


Rings

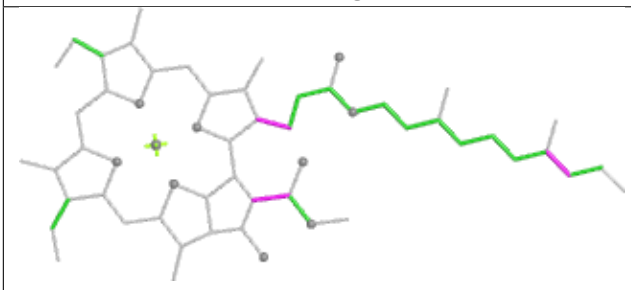
Ligand CLA U 405



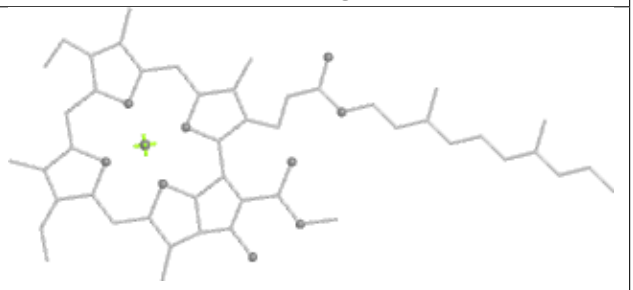
Bond lengths



Bond angles

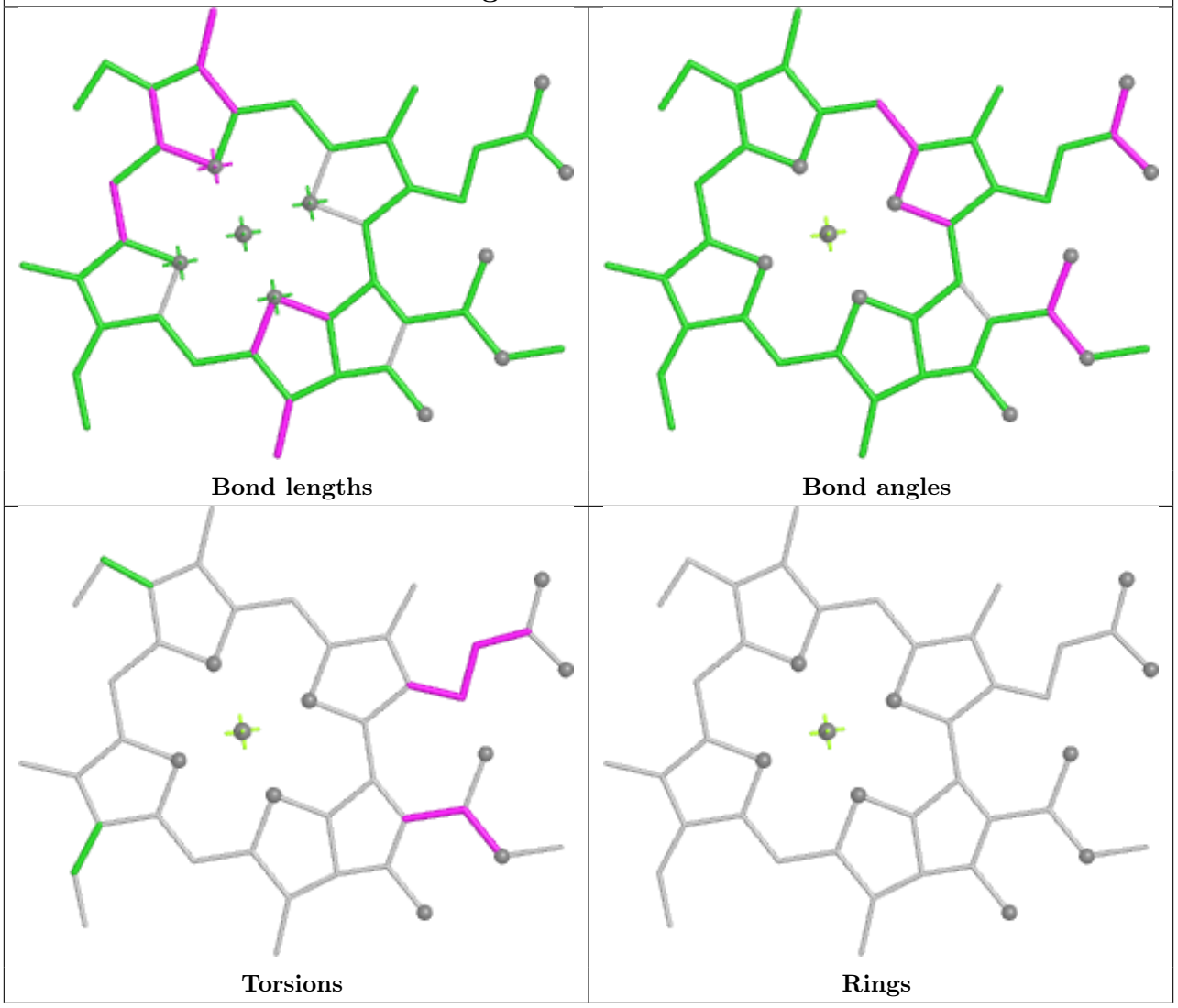


Torsions

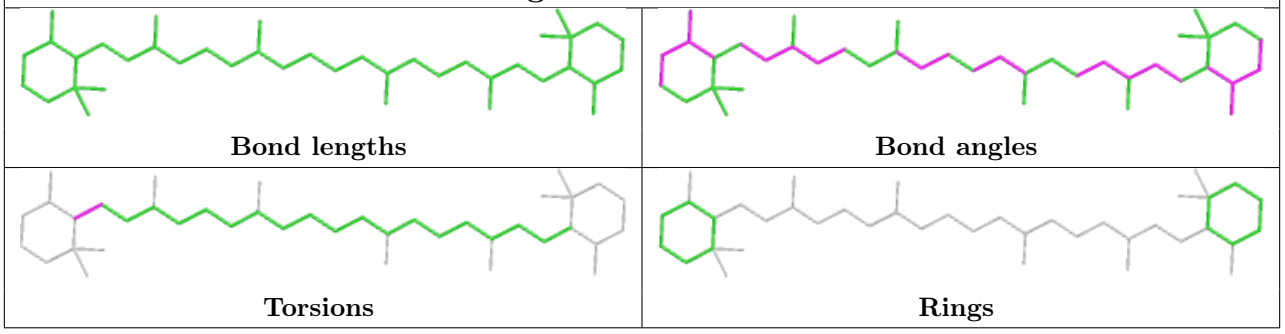


Rings

Ligand CLA P 609



Ligand BCR J 103



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.

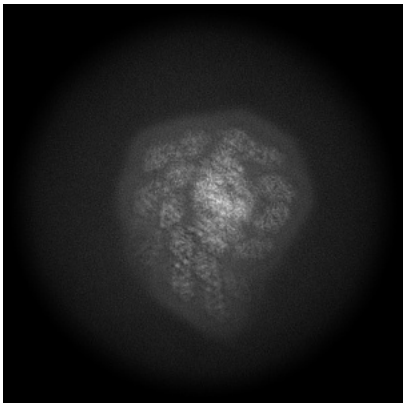
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-63994. These allow visual inspection of the internal detail of the map and identification of artifacts.

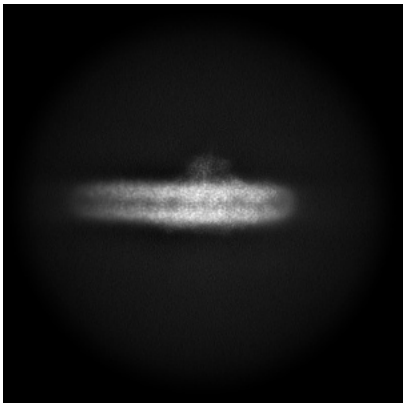
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

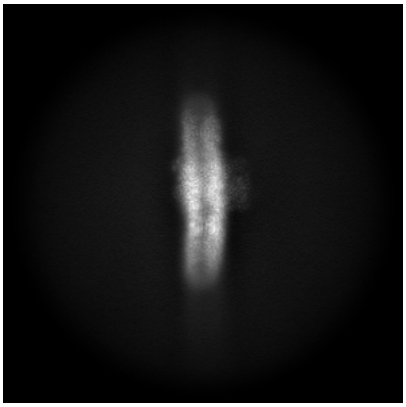
6.1.1 Primary map



X



Y

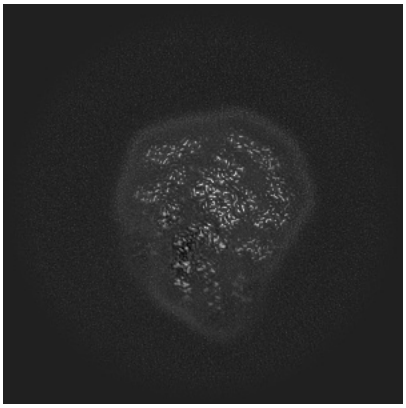


Z

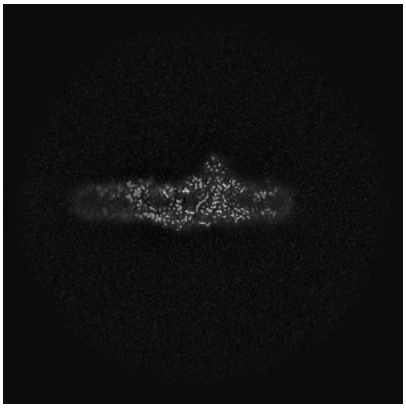
The images above show the map projected in three orthogonal directions.

6.2 Central slices

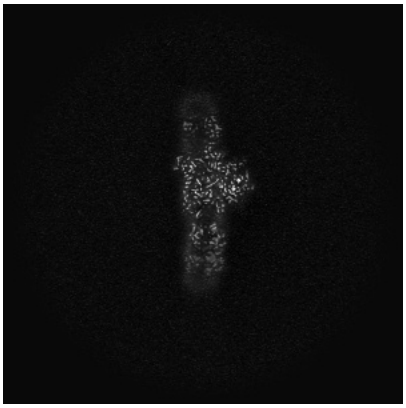
6.2.1 Primary map



X Index: 256



Y Index: 256

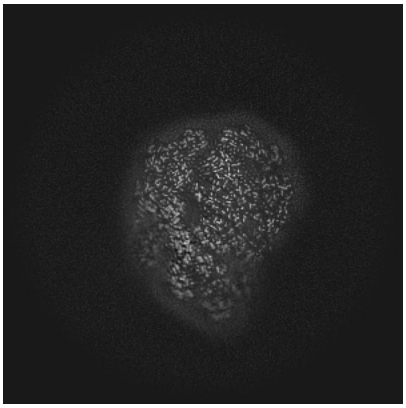


Z Index: 256

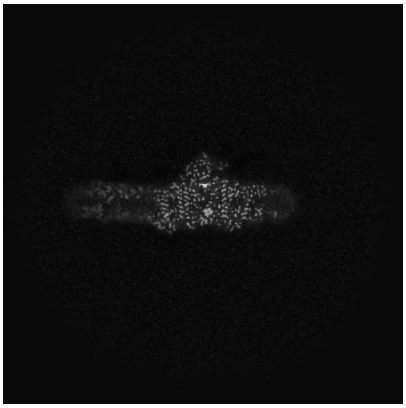
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

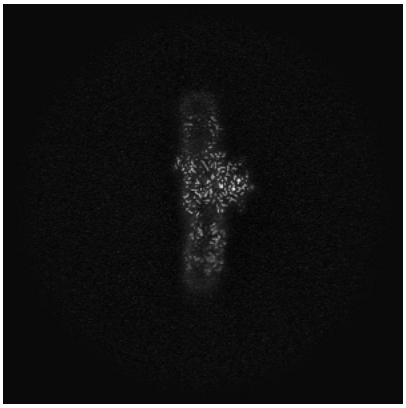
6.3.1 Primary map



X Index: 270



Y Index: 278

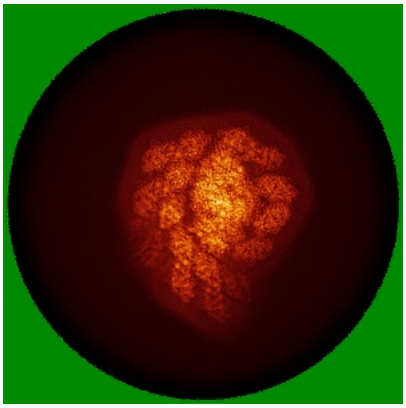


Z Index: 257

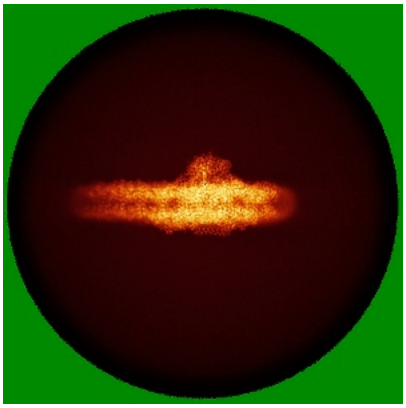
The images above show the largest variance slices of the map in three orthogonal directions.

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

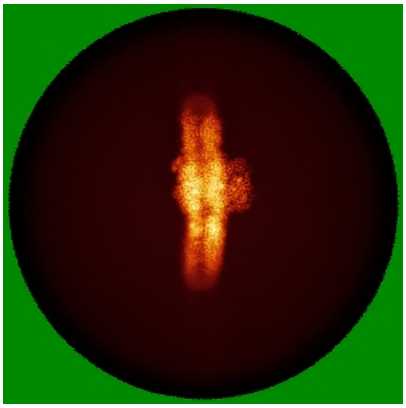
6.4.1 Primary map



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

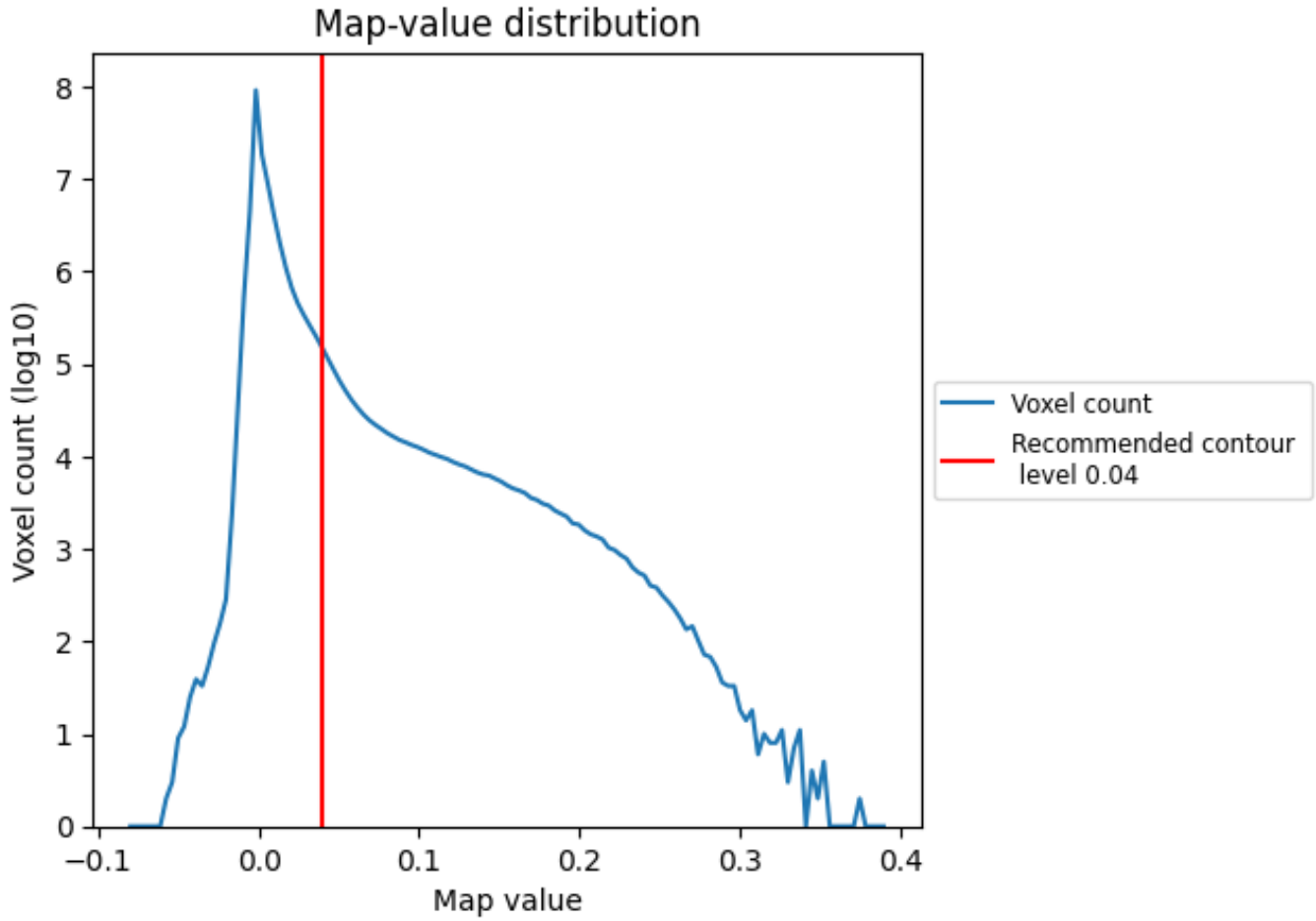
6.6 Mask visualisation (i)

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

7 Map analysis

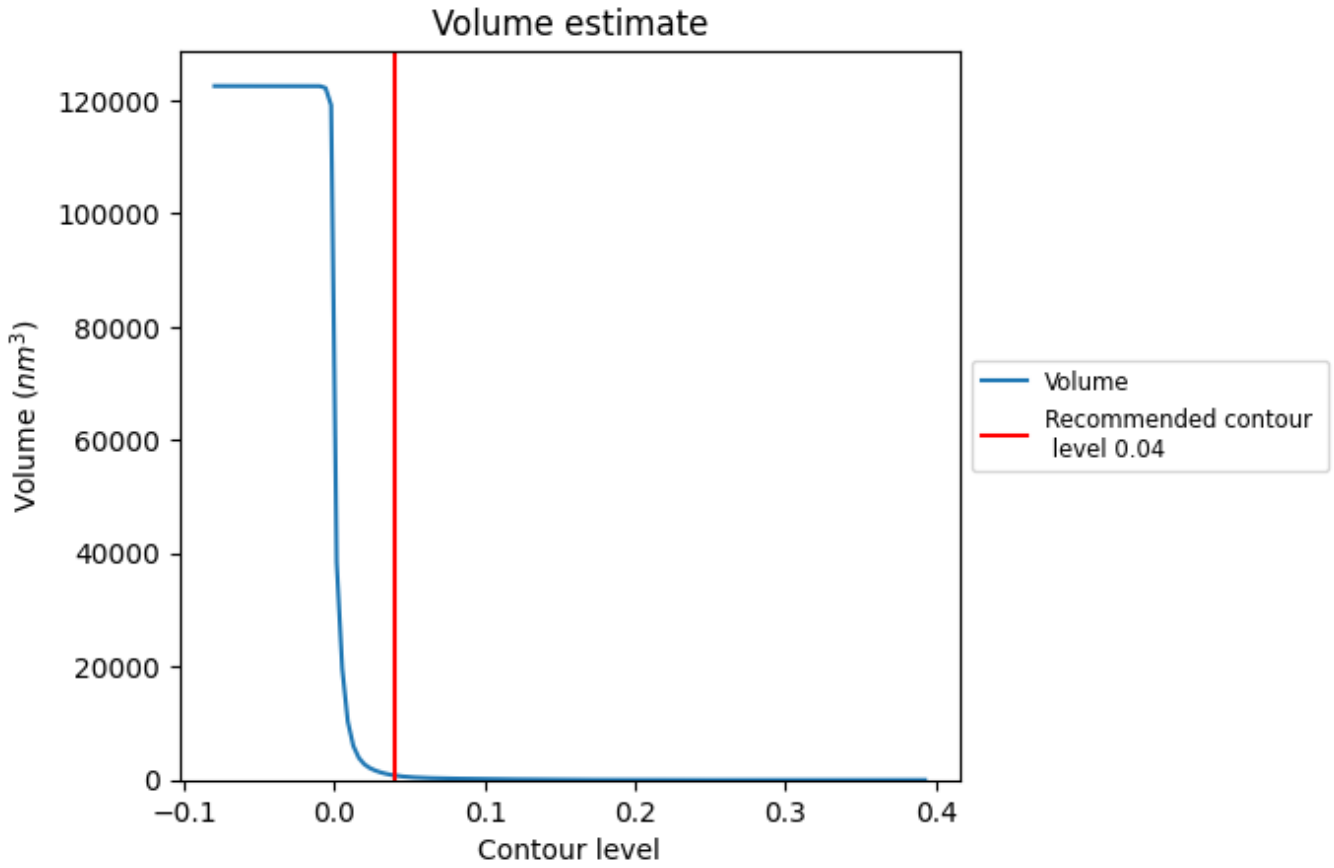
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

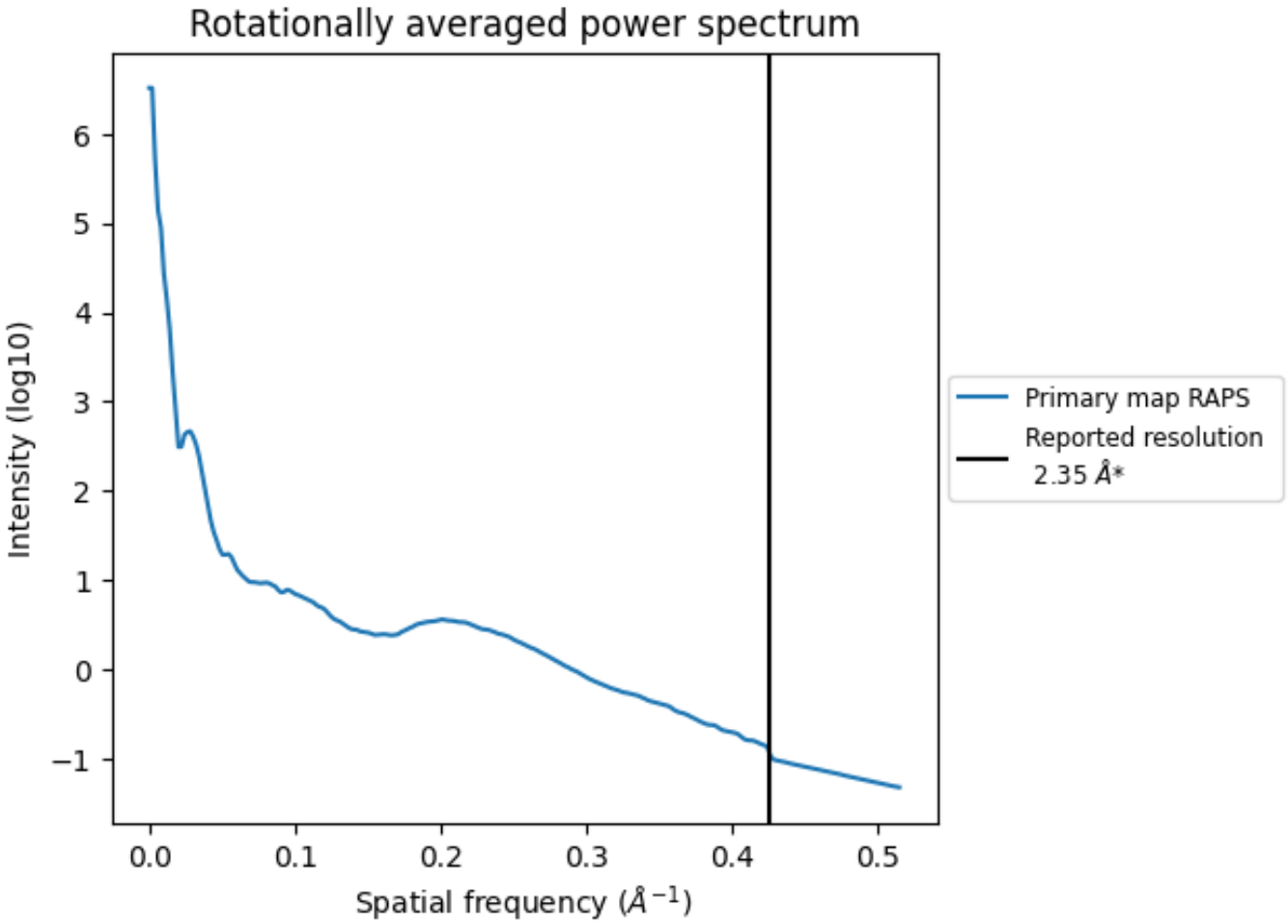
7.2 Volume estimate (i)



The volume at the recommended contour level is 801 nm^3; this corresponds to an approximate mass of 724 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)

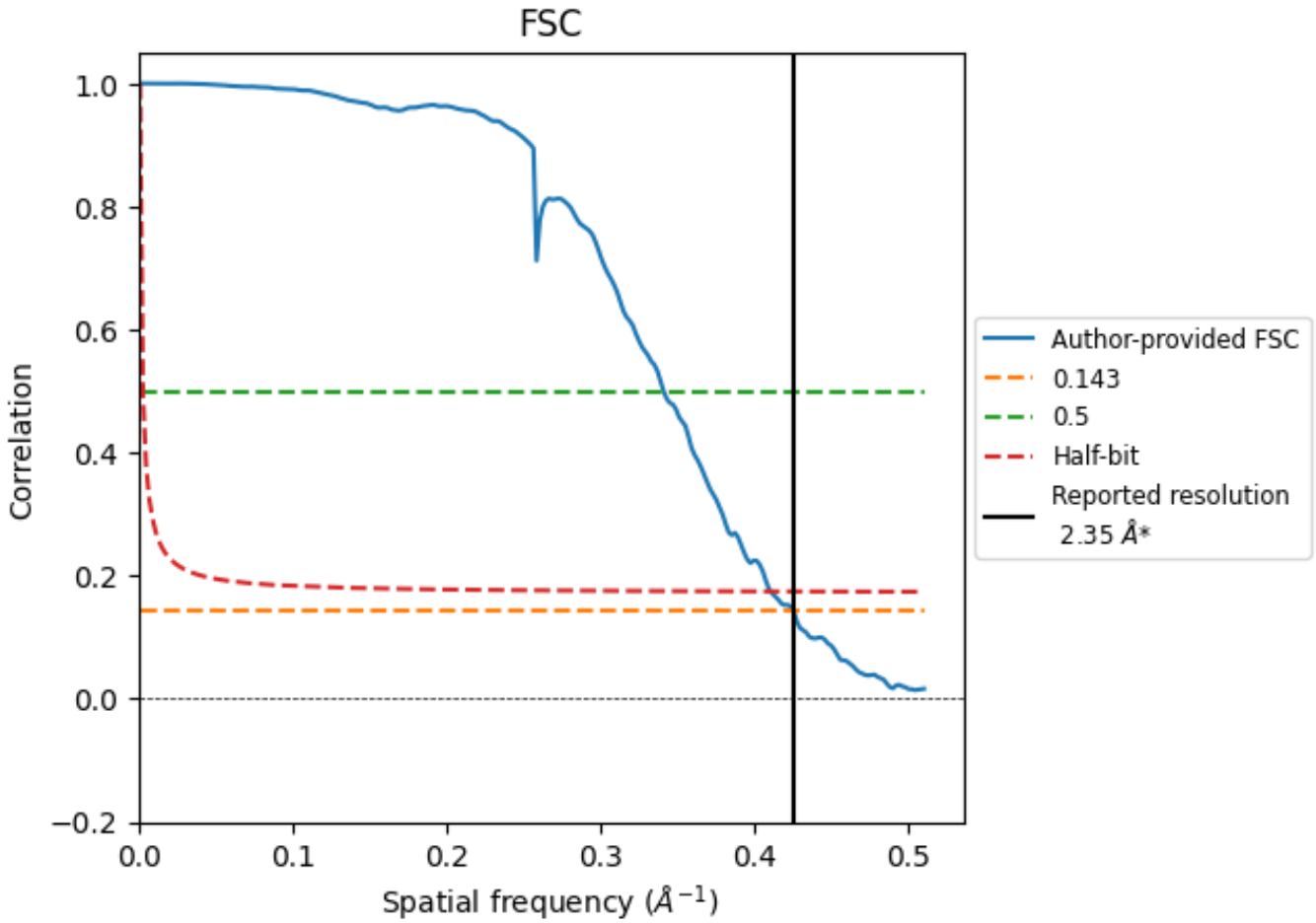


*Reported resolution corresponds to spatial frequency of 0.426 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.426 Å^{-1}

8.2 Resolution estimates (i)

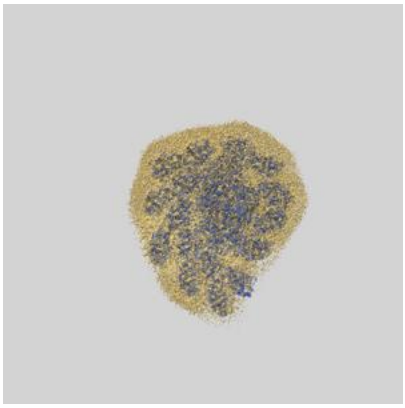
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.35	-	-
Author-provided FSC curve	2.35	2.93	2.43
Unmasked-calculated*	-	-	-

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

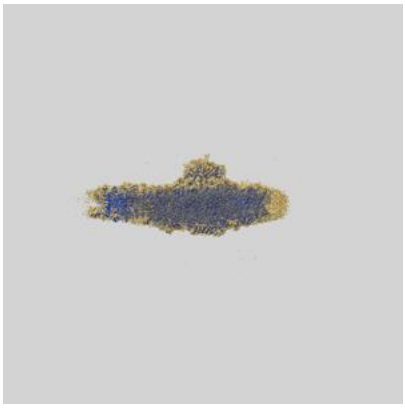
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-63994 and PDB model 9UAS. Per-residue inclusion information can be found in section 3 on page 35.

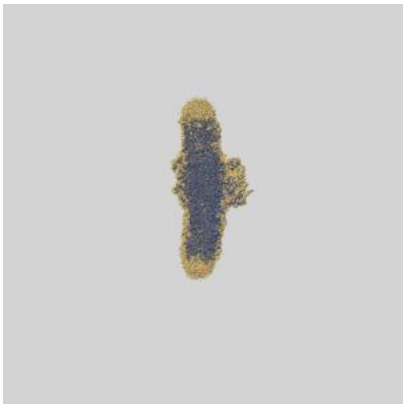
9.1 Map-model overlay



X



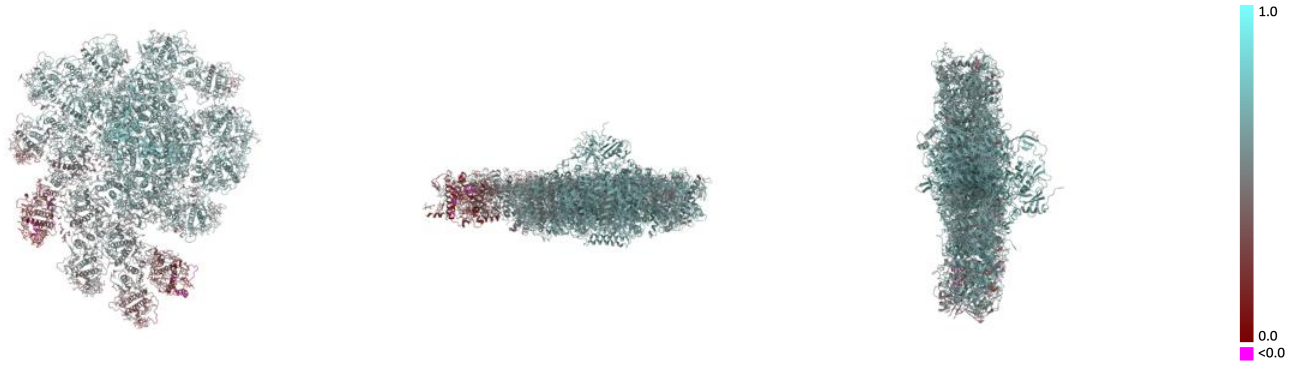
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04 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.

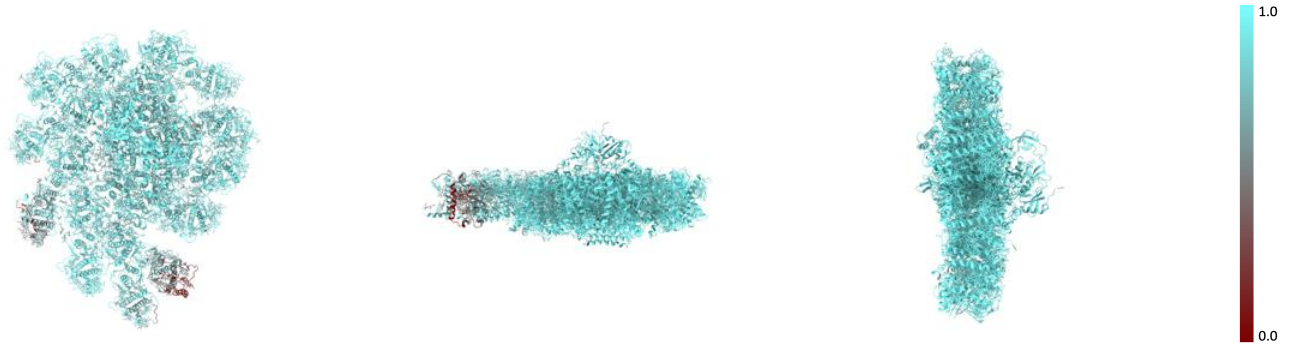
9.2 Q-score mapped to coordinate model



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.

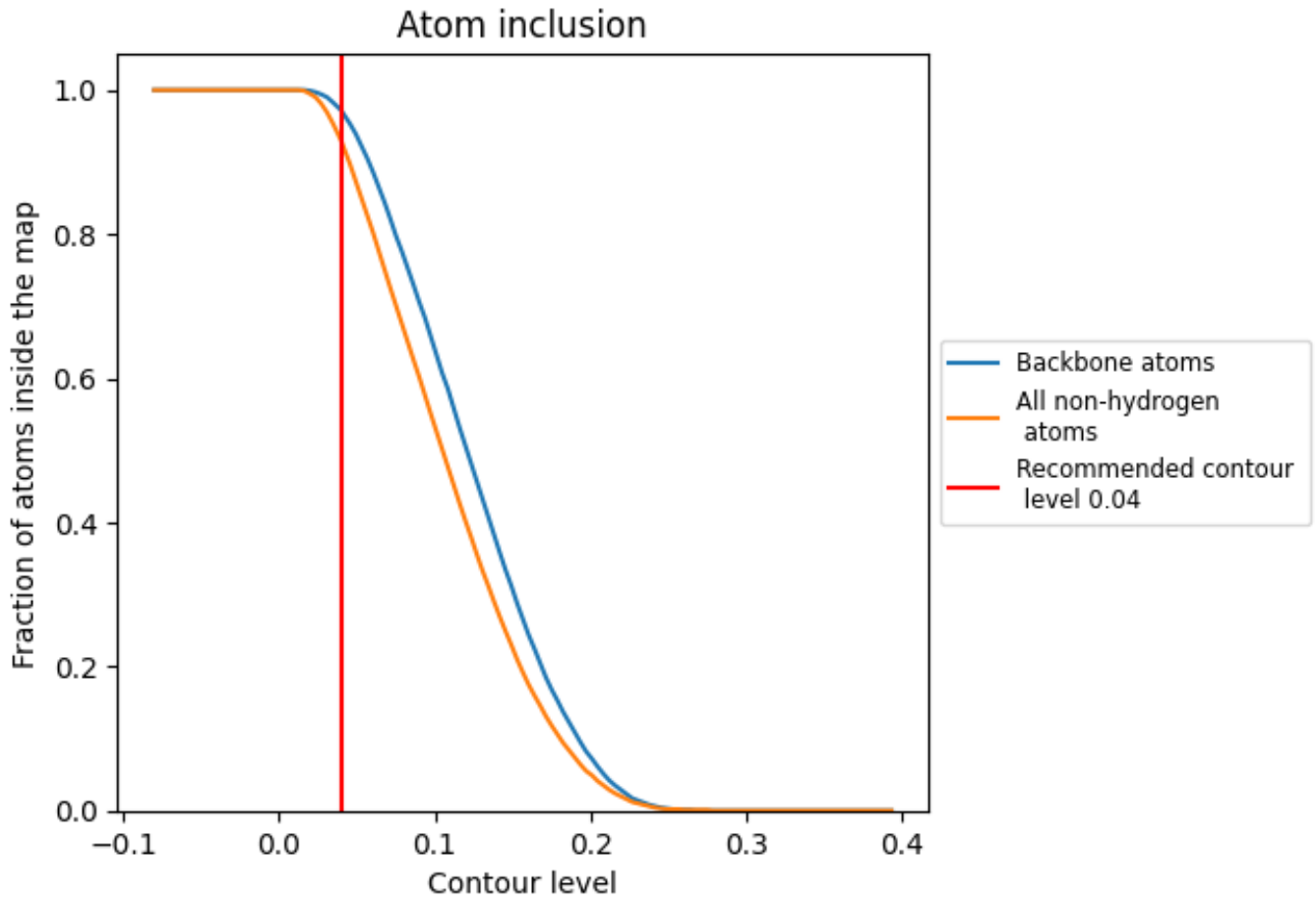
9.3 Atom inclusion mapped to coordinate model



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 (0.04).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 93% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9300	0.5550
A	0.9840	0.6580
B	0.9780	0.6190
C	0.9970	0.6770
D	0.9510	0.6400
E	0.9560	0.6350
F	0.9620	0.6150
G	0.9560	0.5620
H	0.9670	0.5870
I	0.9400	0.4830
J	0.9420	0.6280
K	0.9690	0.6110
L	0.9710	0.5060
M	0.9840	0.5760
N	0.9490	0.4660
O	0.9660	0.4920
P	0.7790	0.3540
Q	0.9570	0.5030
R	0.4970	0.2490
S	0.9380	0.5600
T	0.9500	0.6030
U	0.9200	0.5570
V	0.6770	0.2230
W	0.9550	0.6060
X	0.9420	0.6030

