wwPDB EM Validation Summary Report (i)

Nov 2, 2026 – 07:15 PM JST

PDB ID	:	9XLV / pdb_00009xlv
EMDB ID	:	EMD-67007
Title	:	Cryo-EM structure of a PSI supercomplex in the leaves of Hevea brasiliensis
Authors	:	Wang, M.; Yang, Y.; Li, Z.H.; Wang, W.D.; Wang, X.C.
Deposited on	:	2025-11-08
Resolution	:	2.70 Å(reported)

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

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

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

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

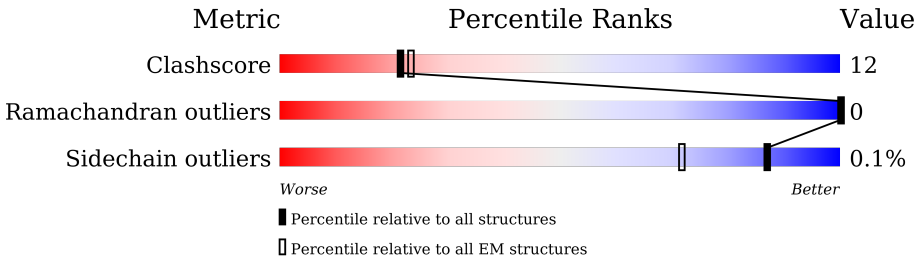
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

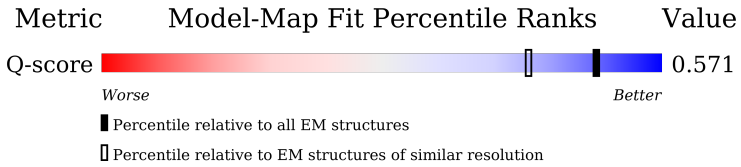
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10327 (2.20 - 3.20)

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

Mol	Chain	Length	Quality of chain
1	L	162	81% 17% ••
2	1	195	83% 17%
3	2	203	84% 16%
4	3	216	81% 19%

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Mol	Chain	Length	Quality of chain
5	4	195	77% 23%
6	A	742	78% 22%
7	B	733	81% 19%
8	C	80	70% 30%
9	D	139	81% 19%
10	E	64	89% 11%
11	F	152	67% 33%
12	G	94	80% 20%
13	H	93	86% 14%
14	I	32	84% 16%
15	J	39	77% 23%
16	K	81	90% 10%
17	O	88	81% 19%

2 Entry composition (i)

There are 29 unique types of molecules in this entry. The entry contains 37231 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 PsaL.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	L	162	1210	798	191	219	2	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	61	ASP	GLU	conflict	UNP A0ABQ9LPG4
L	73	ASP	GLU	conflict	UNP A0ABQ9LPG4

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	195	1530	996	256	273	5	0	0

- Molecule 3 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	203	1591	1043	259	284	5	0	0

- Molecule 4 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	3	216	1662	1086	266	304	6	0	0

- Molecule 5 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	4	195	1546	1013	252	278	3	0	0

- Molecule 6 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	742	Total	C	N	O	S	0	0
			5839	3825	993	1003	18		

- Molecule 7 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	733	Total	C	N	O	S	0	0
			5851	3841	998	999	13		

- Molecule 8 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C	80	Total	C	N	O	S	0	0
			617	381	107	118	11		

- Molecule 9 is a protein called PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	139	Total	C	N	O	S	0	0
			1111	713	199	195	4		

- Molecule 10 is a protein called PsaE.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	E	64	Total	C	N	O	0	0
			518	330	91	97		

- Molecule 11 is a protein called Photosystem I reaction center subunit III.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	152	Total	C	N	O	S	0	0
			1206	782	209	212	3		

- Molecule 12 is a protein called PsaG.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	G	94	Total	C	N	O	S	0	0
			724	474	118	130	2		

- Molecule 13 is a protein called PsaH.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	H	93	Total	C	N	O	0	0
			710	466	112	132		

- Molecule 14 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	I	32	Total	C	N	O	S	0	0
			244	165	38	40	1		

- Molecule 15 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	J	39	Total	C	N	O	S	0	0
			313	210	48	54	1		

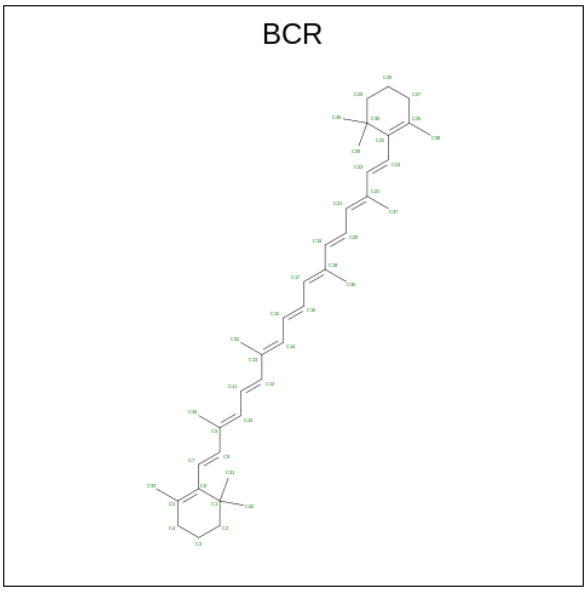
- Molecule 16 is a protein called PSI-K.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	K	81	Total	C	N	O	S	0	0
			569	360	99	107	3		

- Molecule 17 is a protein called PsaO.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	88	Total	C	N	O	S	0	0
			713	478	113	121	1		

- Molecule 18 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



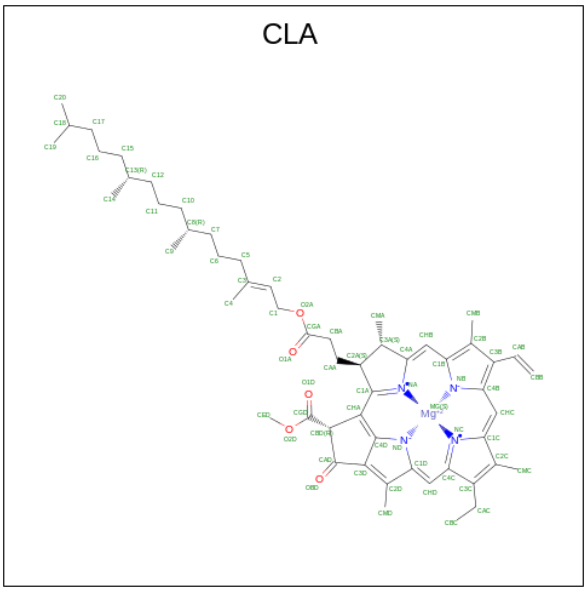
Mol	Chain	Residues	Atoms	AltConf
18	L	1	Total C 40 40	0
18	L	1	Total C 40 40	0
18	L	1	Total C 40 40	0
18	1	1	Total C 40 40	0
18	2	1	Total C 40 40	0
18	3	1	Total C 40 40	0
18	4	1	Total C 40 40	0
18	A	1	Total C 40 40	0
18	A	1	Total C 40 40	0
18	A	1	Total C 40 40	0
18	A	1	Total C 40 40	0
18	A	1	Total C 40 40	0
18	B	1	Total C 40 40	0
18	B	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
18	B	1	Total C 40 40	0
18	B	1	Total C 40 40	0
18	B	1	Total C 40 40	0
18	F	1	Total C 40 40	0
18	F	1	Total C 40 40	0
18	F	1	Total C 40 40	0
18	G	1	Total C 40 40	0
18	G	1	Total C 40 40	0
18	I	1	Total C 40 40	0
18	J	1	Total C 40 40	0
18	J	1	Total C 40 40	0
18	K	1	Total C 40 40	0
18	K	1	Total C 40 40	0
18	O	1	Total C 40 40	0
18	O	1	Total C 40 40	0

- Molecule 19 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
19	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	L	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
19	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
19	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
19	2	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
19	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
19	3	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
19	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
19	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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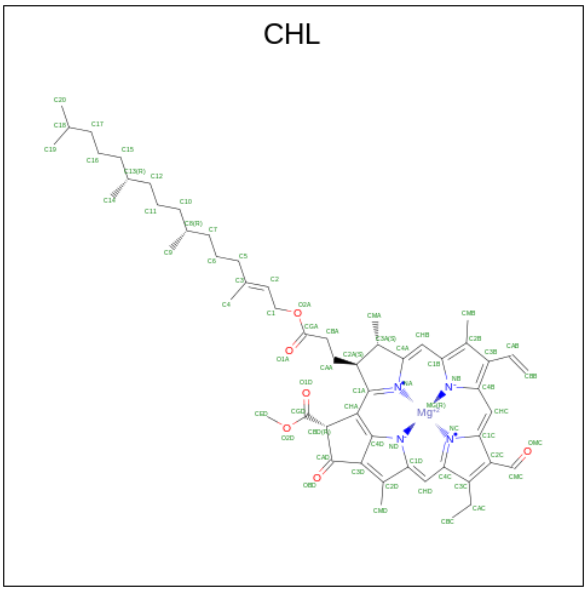
Mol	Chain	Residues	Atoms					AltConf
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	F	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	G	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
19	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	G	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	J	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
19	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	K	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
19	O	1	Total 52	C 42	Mg 1	N 4	O 5	0
19	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	O	1	Total 52	C 42	Mg 1	N 4	O 5	0
19	O	1	Total 45	C 35	Mg 1	N 4	O 5	0

- Molecule 20 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



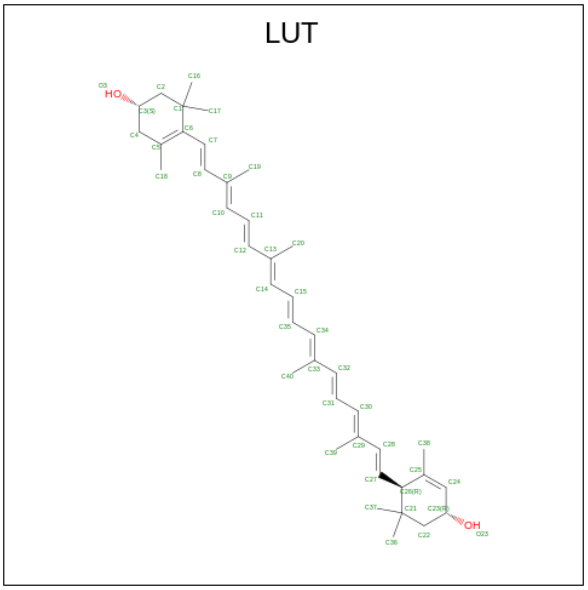
Mol	Chain	Residues	Atoms					AltConf
20	1	1	Total 48	C 37	Mg 1	N 4	O 6	0
20	1	1	Total 61	C 50	Mg 1	N 4	O 6	0
20	2	1	Total 43	C 34	Mg 1	N 4	O 4	0
20	2	1	Total 48	C 37	Mg 1	N 4	O 6	0
20	2	1	Total 51	C 40	Mg 1	N 4	O 6	0
20	2	1	Total 43	C 34	Mg 1	N 4	O 4	0
20	2	1	Total 56	C 45	Mg 1	N 4	O 6	0

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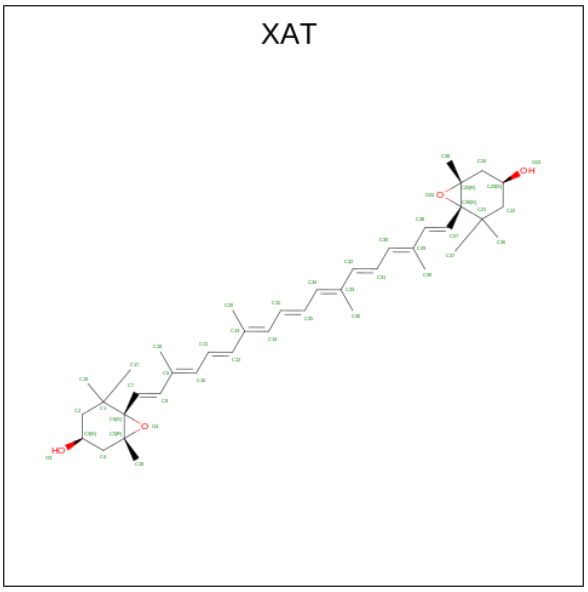
Mol	Chain	Residues	Atoms					AltConf
20	3	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
20	4	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
20	4	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
20	4	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
20	4	1	Total	C	Mg	N	O	0
			43	34	1	4	4	

- Molecule 21 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3 ,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$).



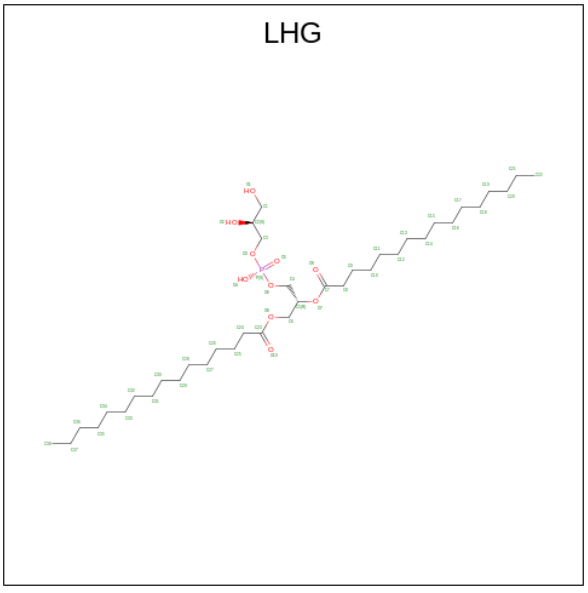
Mol	Chain	Residues	Atoms			AltConf
21	1	1	Total	C	O	0
			42	40	2	
21	2	1	Total	C	O	0
			42	40	2	
21	3	1	Total	C	O	0
			42	40	2	
21	4	1	Total	C	O	0
			42	40	2	

- Molecule 22 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: $C_{40}H_{56}O_4$).



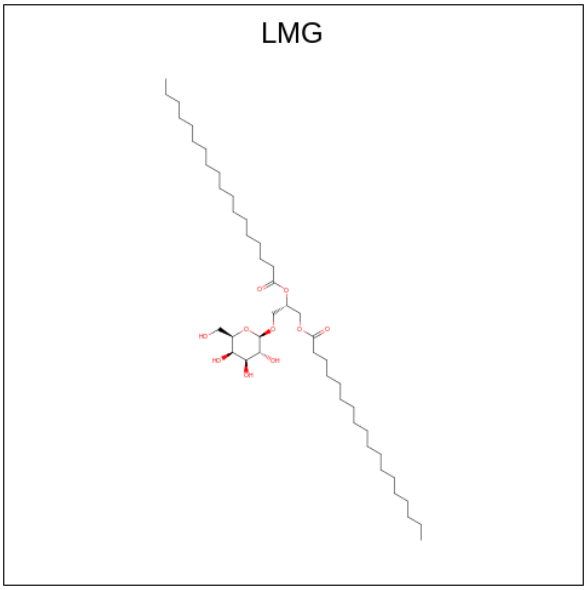
Mol	Chain	Residues	Atoms			AltConf
22	1	1	Total	C	O	0
			44	40	4	
22	2	1	Total	C	O	0
			44	40	4	
22	3	1	Total	C	O	0
			44	40	4	
22	4	1	Total	C	O	0
			44	40	4	

- Molecule 23 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
23	1	1	Total	C	O	P	0
			49	38	10	1	
23	1	1	Total	C	O	P	0
			23	12	10	1	
23	1	1	Total	C	O	P	0
			49	38	10	1	
23	2	1	Total	C	O	P	0
			37	26	10	1	
23	2	1	Total	C	O	P	0
			49	38	10	1	
23	4	1	Total	C	O	P	0
			49	38	10	1	
23	4	1	Total	C	O	P	0
			40	29	10	1	
23	A	1	Total	C	O	P	0
			49	38	10	1	
23	A	1	Total	C	O	P	0
			27	16	10	1	

- Molecule 24 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



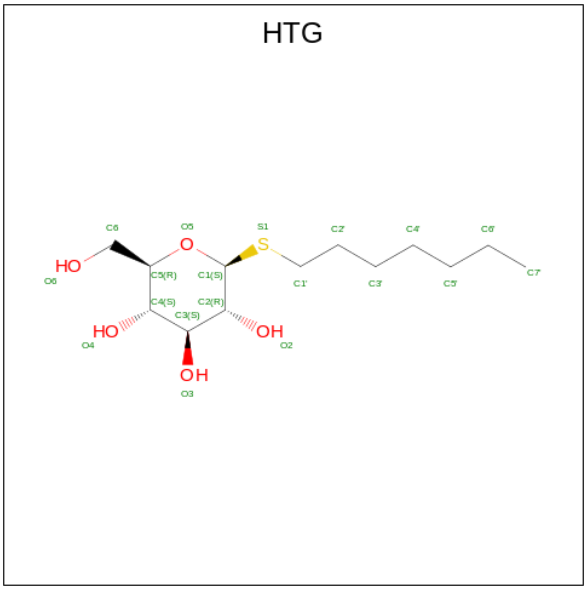
Mol	Chain	Residues	Atoms			AltConf
24	4	1	Total	C	O	0
			50	40	10	
24	B	1	Total	C	O	0
			44	34	10	

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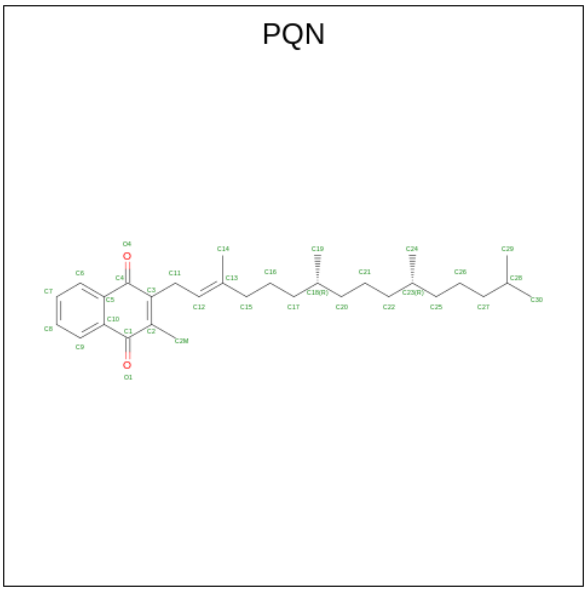
Mol	Chain	Residues	Atoms	AltConf
24	F	1	Total C O 40 30 10	0
24	G	1	Total C O 40 30 10	0
24	J	1	Total C O 51 41 10	0

- Molecule 25 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula: $C_{13}H_{26}O_5S$).



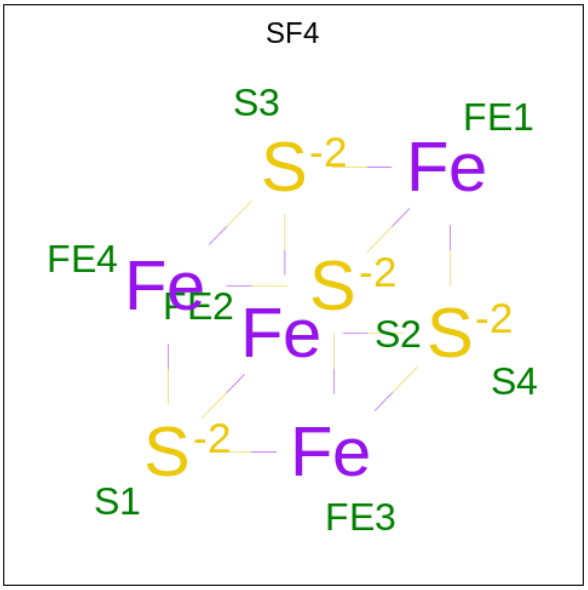
Mol	Chain	Residues	Atoms	AltConf
25	4	1	Total C O S 19 13 5 1	0
25	B	1	Total C O S 19 13 5 1	0
25	F	1	Total C O S 19 13 5 1	0
25	F	1	Total C O S 19 13 5 1	0
25	F	1	Total C O S 19 13 5 1	0
25	F	1	Total C O S 19 13 5 1	0

- Molecule 26 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



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

- Molecule 27 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



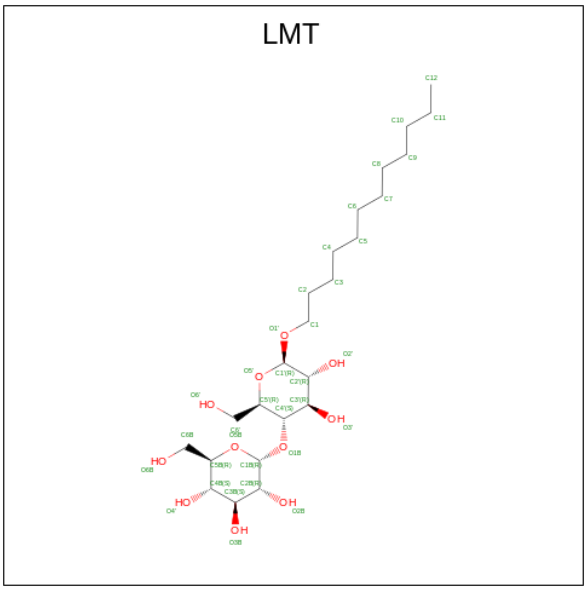
Mol	Chain	Residues	Atoms	AltConf
27	A	1	Total Fe S 8 4 4	0
27	C	1	Total Fe S 8 4 4	0

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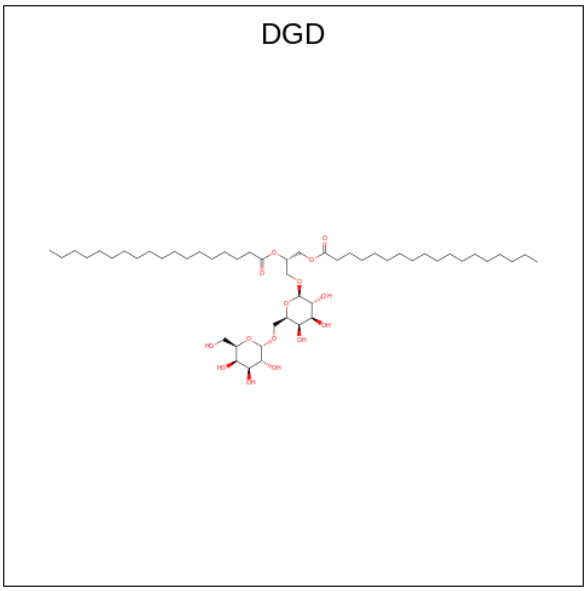
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
27	C	1	8	4	4	0

- Molecule 28 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
28	A	1	35	24	11	0

- Molecule 29 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
29	B	1	66	51	15	0

3 Residue-property plots (i)

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

• Molecule 1: PsaL

Chain L:

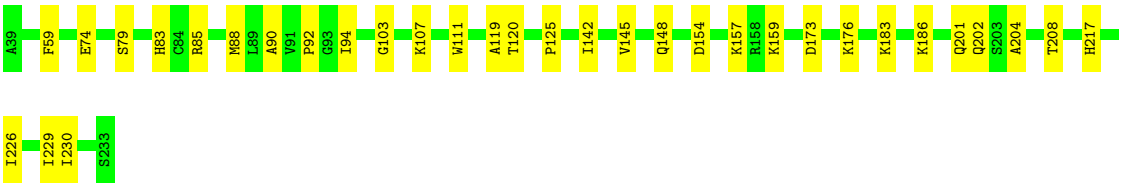




• Molecule 2: Chlorophyll a-b binding protein, chloroplastic

Chain 1:

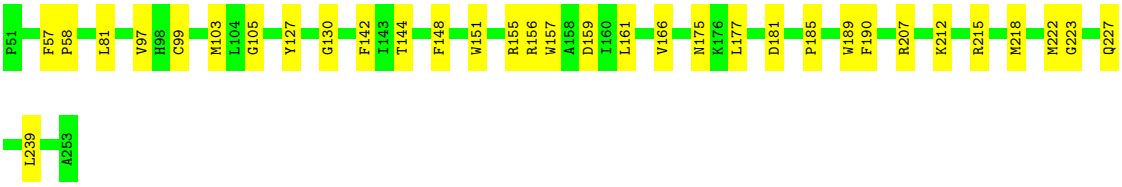




• Molecule 3: Chlorophyll a-b binding protein, chloroplastic

Chain 2:

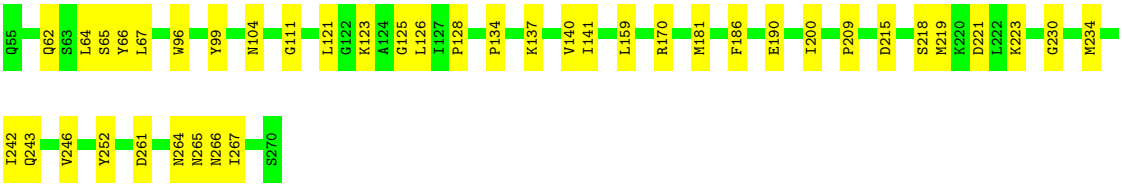




• Molecule 4: Chlorophyll a-b binding protein, chloroplastic

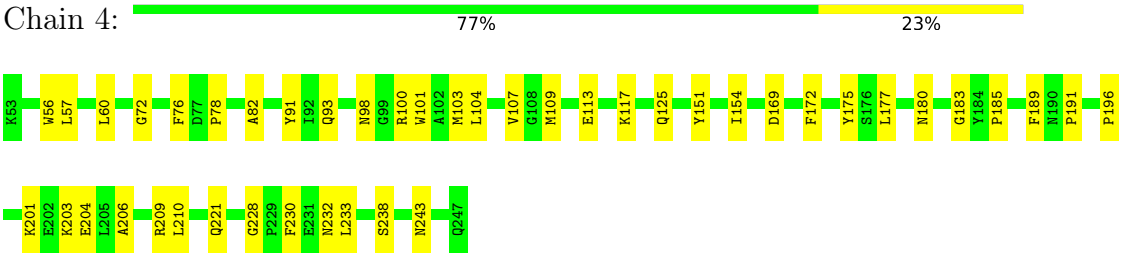
Chain 3:





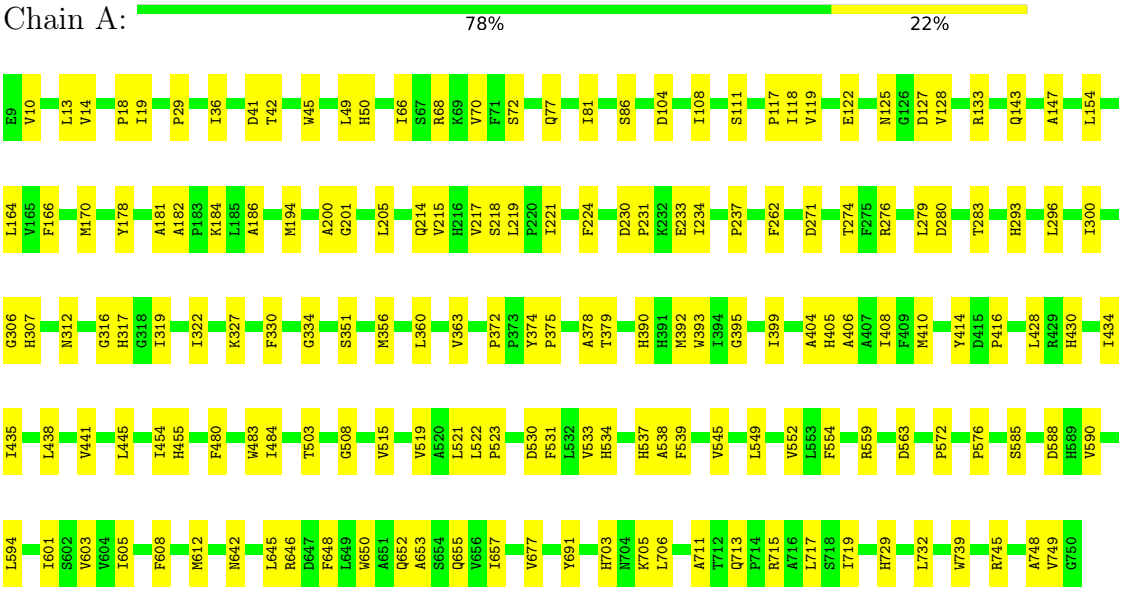
• Molecule 5: Chlorophyll a-b binding protein, chloroplastic

Chain 4:



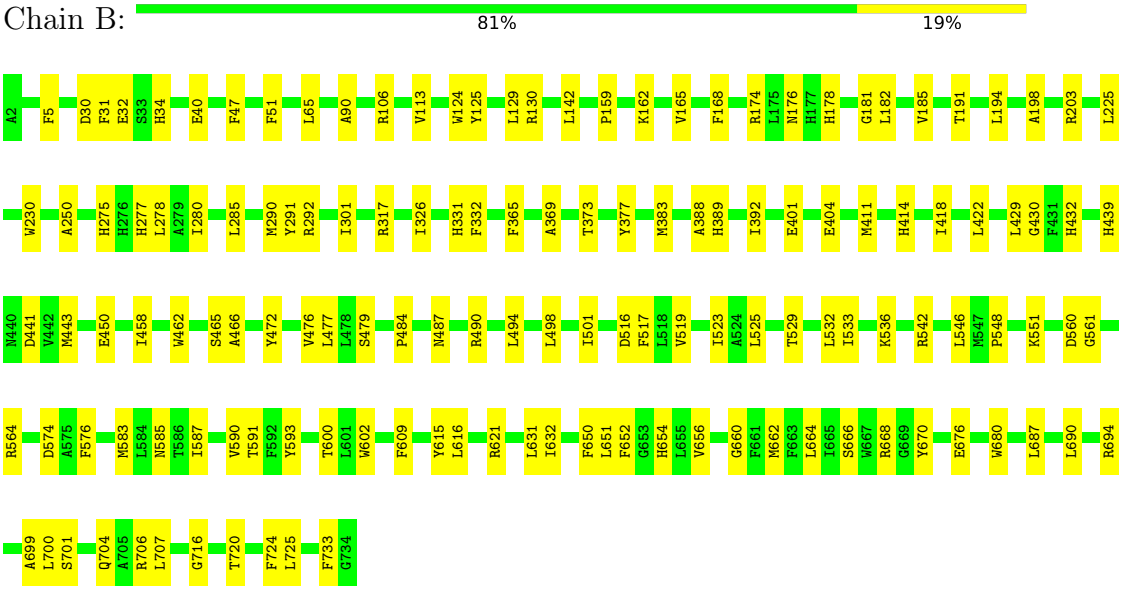
• Molecule 6: Photosystem I P700 chlorophyll a apoprotein A1

Chain A:



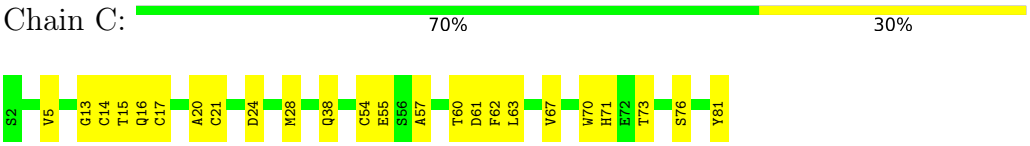
• Molecule 7: Photosystem I P700 chlorophyll a apoprotein A2

Chain B:



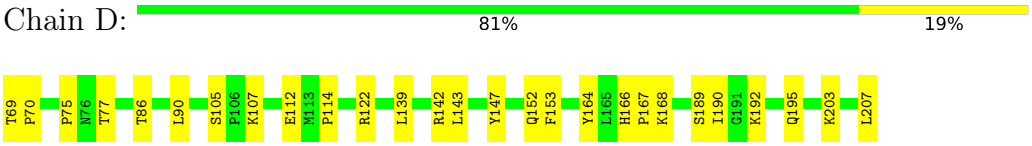
• Molecule 8: Photosystem I iron-sulfur center

Chain C:



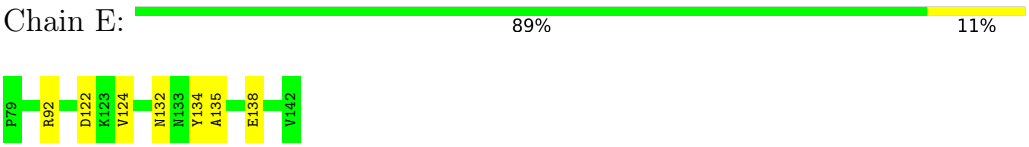
• Molecule 9: PsaD

Chain D:



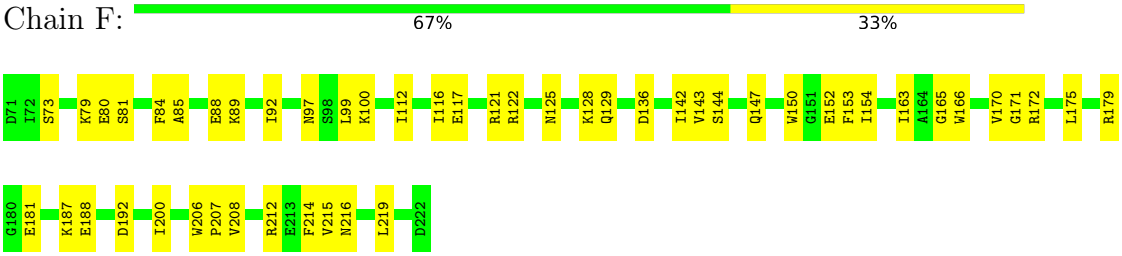
• Molecule 10: PsaE

Chain E:



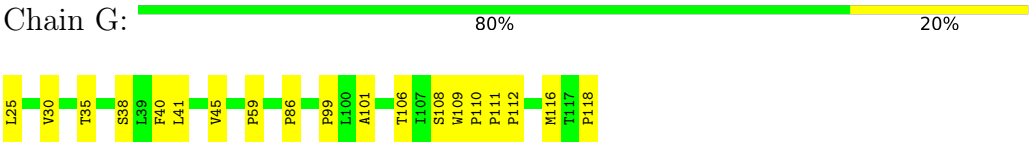
• Molecule 11: Photosystem I reaction center subunit III

Chain F:



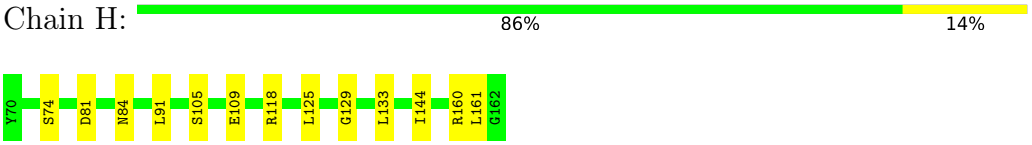
• Molecule 12: PsaG

Chain G:



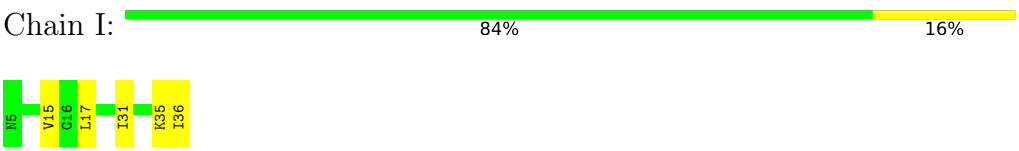
• Molecule 13: PsaH

Chain H:



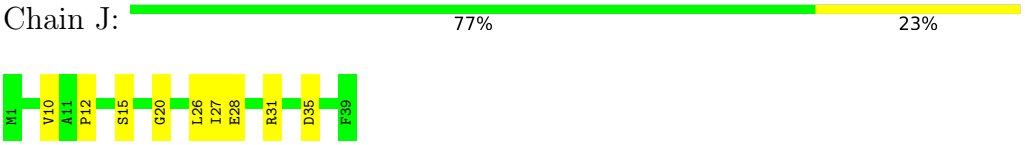
• Molecule 14: Photosystem I reaction center subunit VIII

Chain I:



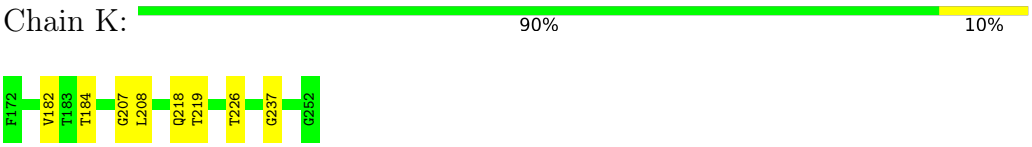
• Molecule 15: Photosystem I reaction center subunit IX

Chain J:



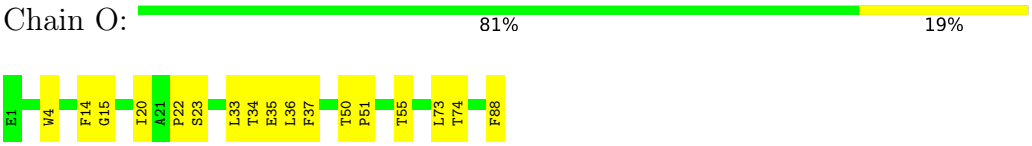
• Molecule 16: PSI-K

Chain K:



• Molecule 17: PsaO

Chain O:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	618810	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI MORGAGNI	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.724	Depositor
Minimum map value	-0.427	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.0418	Depositor
Map size (Å)	532.48, 532.48, 532.48	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, DGD, PQN, LMT, HTG, LUT, CLA, XAT, BCR, LMG, SF4, CHL

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	L	0.36	1/1244 (0.1%)	0.54	3/1700 (0.2%)
2	1	0.13	0/1582	0.27	0/2156
3	2	0.14	0/1650	0.31	0/2257
4	3	0.13	0/1712	0.30	0/2327
5	4	0.13	0/1597	0.27	0/2180
6	A	0.15	0/6037	0.27	0/8236
7	B	0.15	0/6063	0.28	0/8280
8	C	0.18	0/630	0.44	0/853
9	D	0.15	0/1140	0.34	0/1538
10	E	0.11	0/529	0.21	0/716
11	F	0.15	0/1235	0.30	0/1665
12	G	0.18	0/744	0.38	0/1018
13	H	0.17	0/731	0.28	0/993
14	I	0.20	0/249	0.32	0/339
15	J	0.12	0/321	0.26	0/435
16	K	0.10	0/576	0.28	0/777
17	O	0.13	0/741	0.36	0/1012
All	All	0.16	1/26781 (0.0%)	0.31	3/36482 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	209	VAL	C-O	-9.51	1.12	1.24

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	209	VAL	O-C-N	-11.85	107.76	122.57
1	L	73	ASP	CA-C-N	5.41	136.33	120.97
1	L	73	ASP	C-N-CA	5.41	136.33	120.97

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	209	VAL	Mainchain

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	L	1210	0	1219	27	0
2	1	1530	0	1501	25	0
3	2	1591	0	1537	35	0
4	3	1662	0	1633	33	0
5	4	1546	0	1504	45	0
6	A	5839	0	5691	128	0
7	B	5851	0	5636	111	0
8	C	617	0	593	21	0
9	D	1111	0	1129	19	0
10	E	518	0	519	6	0
11	F	1206	0	1235	40	0
12	G	724	0	730	23	0
13	H	710	0	710	12	0
14	I	244	0	267	4	0
15	J	313	0	324	8	0
16	K	569	0	592	6	0
17	O	713	0	697	15	0
18	1	40	0	56	5	0
18	2	40	0	56	6	0
18	3	40	0	56	5	0
18	4	40	0	56	5	0
18	A	200	0	280	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	B	200	0	280	14	0
18	F	120	0	168	12	0
18	G	80	0	112	3	0
18	I	40	0	56	3	0
18	J	80	0	112	4	0
18	K	80	0	112	7	0
18	L	120	0	168	6	0
18	O	80	0	112	7	0
19	1	672	0	636	45	0
19	2	487	0	447	18	0
19	3	587	0	466	22	0
19	4	586	0	509	44	0
19	A	2690	0	2803	129	0
19	B	2493	0	2570	111	0
19	F	100	0	82	4	0
19	G	137	0	101	4	0
19	J	42	0	31	0	0
19	K	105	0	92	6	0
19	L	180	0	183	10	0
19	O	194	0	152	9	0
20	1	109	0	90	8	0
20	2	241	0	169	24	0
20	3	47	0	31	3	0
20	4	201	0	150	16	0
21	1	42	0	56	4	0
21	2	42	0	56	4	0
21	3	42	0	56	5	0
21	4	42	0	56	3	0
22	1	44	0	56	2	0
22	2	44	0	56	2	0
22	3	44	0	56	2	0
22	4	44	0	56	5	0
23	1	121	0	164	15	0
23	2	86	0	118	10	0
23	4	89	0	127	9	0
23	A	76	0	98	3	0
24	4	50	0	73	8	0
24	B	44	0	58	3	0
24	F	40	0	50	1	0
24	G	40	0	53	1	0
24	J	51	0	72	2	0
25	4	19	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	B	19	0	26	1	0
25	F	76	0	104	9	0
26	A	33	0	46	4	0
26	B	33	0	46	1	0
27	A	8	0	0	0	0
27	C	16	0	0	1	0
28	A	35	0	46	2	0
29	B	66	0	96	7	0
All	All	37231	0	37304	871	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 12.

The worst 5 of 871 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)
19:3:303:CLA:HBB1	18:3:315:BCR:H24C	1.41	1.01
4:3:128:PRO:HD3	19:3:316:CLA:HAA1	1.46	0.97
6:A:531:PHE:HA	19:A:835:CLA:HED1	1.51	0.91
19:4:309:CLA:H11	19:4:311:CLA:HAB	1.57	0.86
17:O:14:PHE:HB3	19:O:103:CLA:HBC1	1.58	0.86

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	L	160/162 (99%)	152 (95%)	8 (5%)	0	100	100
2	1	193/195 (99%)	181 (94%)	12 (6%)	0	100	100
3	2	201/203 (99%)	198 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	3	214/216 (99%)	206 (96%)	8 (4%)	0	100	100
5	4	193/195 (99%)	177 (92%)	16 (8%)	0	100	100
6	A	740/742 (100%)	721 (97%)	19 (3%)	0	100	100
7	B	731/733 (100%)	710 (97%)	21 (3%)	0	100	100
8	C	78/80 (98%)	74 (95%)	4 (5%)	0	100	100
9	D	137/139 (99%)	124 (90%)	13 (10%)	0	100	100
10	E	62/64 (97%)	61 (98%)	1 (2%)	0	100	100
11	F	150/152 (99%)	147 (98%)	3 (2%)	0	100	100
12	G	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
13	H	91/93 (98%)	86 (94%)	5 (6%)	0	100	100
14	I	30/32 (94%)	30 (100%)	0	0	100	100
15	J	37/39 (95%)	37 (100%)	0	0	100	100
16	K	79/81 (98%)	79 (100%)	0	0	100	100
17	O	86/88 (98%)	76 (88%)	10 (12%)	0	100	100
All	All	3274/3308 (99%)	3147 (96%)	127 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	L	126/126 (100%)	124 (98%)	2 (2%)	55	80
2	1	159/159 (100%)	159 (100%)	0	100	100
3	2	165/165 (100%)	165 (100%)	0	100	100
4	3	169/169 (100%)	169 (100%)	0	100	100
5	4	164/164 (100%)	164 (100%)	0	100	100
6	A	601/601 (100%)	601 (100%)	0	100	100
7	B	596/596 (100%)	596 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	C	71/71 (100%)	71 (100%)	0	100 100
9	D	119/119 (100%)	118 (99%)	1 (1%)	73 88
10	E	57/57 (100%)	57 (100%)	0	100 100
11	F	126/126 (100%)	126 (100%)	0	100 100
12	G	80/80 (100%)	80 (100%)	0	100 100
13	H	75/75 (100%)	75 (100%)	0	100 100
14	I	28/28 (100%)	28 (100%)	0	100 100
15	J	34/34 (100%)	34 (100%)	0	100 100
16	K	58/58 (100%)	58 (100%)	0	100 100
17	O	75/75 (100%)	75 (100%)	0	100 100
All	All	2703/2703 (100%)	2700 (100%)	3 (0%)	87 96

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	209	VAL
1	L	210	LEU
9	D	152	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
6	A	485	GLN
16	K	178	ASN
7	B	98	GLN
11	F	149	HIS
7	B	64	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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)

220 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	$\#\|Z\| > 2$
19	CLA	B	831	7	64,68,73	1.24	7 (10%)	77,107,113	0.91	3 (3%)
19	CLA	A	853	6	69,73,73	1.21	7 (10%)	83,113,113	0.93	3 (3%)
19	CLA	A	822	6	59,63,73	1.25	7 (11%)	71,101,113	1.03	4 (5%)
19	CLA	3	311	4	49,53,73	1.40	6 (12%)	59,89,113	1.12	5 (8%)
19	CLA	A	811	-	69,73,73	1.19	7 (10%)	83,113,113	0.98	4 (4%)
19	CLA	4	312	-	60,64,73	1.26	7 (11%)	72,102,113	1.06	5 (6%)
19	CLA	B	810	7	69,73,73	1.19	7 (10%)	83,113,113	0.94	4 (4%)
19	CLA	B	825	-	69,73,73	1.17	7 (10%)	83,113,113	0.94	4 (4%)
20	CHL	4	305	5	60,64,74	1.24	8 (13%)	68,102,114	1.12	5 (7%)
19	CLA	1	309	23	69,73,73	1.18	6 (8%)	83,113,113	0.83	3 (3%)
21	LUT	2	314	-	42,43,43	1.62	8 (19%)	51,60,60	1.61	10 (19%)
19	CLA	B	814	7	69,73,73	1.25	8 (11%)	83,113,113	0.98	4 (4%)
19	CLA	B	820	7	54,58,73	1.37	7 (12%)	65,95,113	1.04	3 (4%)
19	CLA	A	828	6	69,73,73	1.30	8 (11%)	83,113,113	0.95	3 (3%)
23	LHG	4	322	-	39,39,48	0.33	0	42,45,54	0.35	0
19	CLA	3	304	-	46,50,73	1.43	6 (13%)	55,85,113	1.14	4 (7%)
23	LHG	2	318	-	48,48,48	0.28	0	51,54,54	0.34	0
20	CHL	3	306	-	51,55,74	1.27	6 (11%)	57,91,114	1.18	6 (10%)
19	CLA	B	816	7	59,63,73	1.28	7 (11%)	71,101,113	1.07	5 (7%)
19	CLA	4	308	5	54,58,73	1.35	6 (11%)	65,95,113	1.01	4 (6%)
26	PQN	A	841	-	34,34,34	0.34	0	42,45,45	0.56	1 (2%)
19	CLA	A	837	6	69,73,73	1.19	6 (8%)	83,113,113	0.91	3 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	CLA	B	828	-	69,73,73	1.22	7 (10%)	83,113,113	0.89	3 (3%)
19	CLA	B	822	7	59,63,73	1.25	7 (11%)	71,101,113	1.05	4 (5%)
20	CHL	2	306	-	55,59,74	1.23	7 (12%)	62,96,114	1.13	5 (8%)
19	CLA	A	803	6	69,73,73	1.19	7 (10%)	83,113,113	0.98	4 (4%)
19	CLA	B	819	-	69,73,73	1.19	7 (10%)	83,113,113	0.93	4 (4%)
19	CLA	A	835	6	69,73,73	1.19	7 (10%)	83,113,113	1.02	5 (6%)
19	CLA	1	312	2	59,63,73	1.29	6 (10%)	71,101,113	0.97	3 (4%)
18	BCR	2	316	-	41,41,41	1.68	8 (19%)	56,56,56	1.67	12 (21%)
21	LUT	1	314	-	42,43,43	1.59	8 (19%)	51,60,60	1.56	10 (19%)
19	CLA	A	814	-	49,53,73	1.42	7 (14%)	59,89,113	1.09	3 (5%)
19	CLA	A	817	6	69,73,73	1.20	7 (10%)	83,113,113	0.95	4 (4%)
19	CLA	3	303	-	49,53,73	1.41	6 (12%)	59,89,113	1.09	4 (6%)
18	BCR	G	201	-	41,41,41	1.71	8 (19%)	56,56,56	1.63	11 (19%)
22	XAT	2	315	-	39,47,47	1.69	8 (20%)	54,74,74	1.72	10 (18%)
18	BCR	A	846	-	41,41,41	1.69	8 (19%)	56,56,56	1.52	10 (17%)
19	CLA	B	823	7	64,68,73	1.23	6 (9%)	77,107,113	0.97	3 (3%)
18	BCR	A	848	-	41,41,41	1.71	8 (19%)	56,56,56	1.53	10 (17%)
23	LHG	A	843	19	26,26,48	0.37	0	29,32,54	0.43	0
19	CLA	B	802	7	69,73,73	1.17	7 (10%)	83,113,113	0.89	3 (3%)
20	CHL	4	306	-	55,59,74	1.26	7 (12%)	62,96,114	1.12	5 (8%)
18	BCR	J	104	-	41,41,41	1.70	8 (19%)	56,56,56	1.61	11 (19%)
19	CLA	B	808	7	69,73,73	1.20	7 (10%)	83,113,113	0.94	4 (4%)
19	CLA	B	813	7	69,73,73	1.20	7 (10%)	83,113,113	0.96	3 (3%)
19	CLA	A	821	6	55,59,73	1.31	7 (12%)	66,96,113	1.14	5 (7%)
19	CLA	2	310	3	56,60,73	1.32	8 (14%)	67,97,113	1.12	7 (10%)
19	CLA	4	303	5	64,68,73	1.28	8 (12%)	77,107,113	1.02	5 (6%)
20	CHL	4	315	5	47,51,74	1.41	8 (17%)	52,86,114	1.15	4 (7%)
25	HTG	F	310	-	19,19,19	0.19	0	23,24,24	0.40	0
18	BCR	O	105	-	41,41,41	1.70	8 (19%)	56,56,56	1.57	10 (17%)
19	CLA	1	308	2	64,68,73	1.19	7 (10%)	77,107,113	1.03	4 (5%)
18	BCR	B	844	-	41,41,41	1.69	8 (19%)	56,56,56	1.63	12 (21%)
18	BCR	3	315	-	41,41,41	1.69	8 (19%)	56,56,56	1.60	11 (19%)
19	CLA	K	302	-	49,53,73	1.41	7 (14%)	59,89,113	1.14	5 (8%)
23	LHG	1	319	19	22,22,48	0.33	0	25,28,54	0.46	0
23	LHG	1	320	-	48,48,48	0.29	0	51,54,54	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	BCR	B	842	-	41,41,41	1.70	8 (19%)	56,56,56	1.56	11 (19%)
18	BCR	F	304	-	41,41,41	1.67	8 (19%)	56,56,56	1.61	11 (19%)
19	CLA	B	801	-	69,73,73	1.19	7 (10%)	83,113,113	0.93	4 (4%)
20	CHL	4	307	-	55,59,74	1.24	7 (12%)	62,96,114	1.13	6 (9%)
28	LMT	A	851	-	36,36,36	0.18	0	47,47,47	0.31	0
19	CLA	1	313	2	50,54,73	1.33	6 (12%)	60,90,113	1.06	3 (5%)
19	CLA	B	812	7	59,63,73	1.28	7 (11%)	71,101,113	1.05	5 (7%)
19	CLA	A	829	6	54,58,73	1.34	7 (12%)	65,95,113	1.02	3 (4%)
19	CLA	F	306	-	49,53,73	1.39	6 (12%)	59,89,113	1.11	4 (6%)
19	CLA	4	304	-	54,58,73	1.29	6 (11%)	65,95,113	1.05	4 (6%)
19	CLA	B	826	7	69,73,73	1.22	8 (11%)	83,113,113	0.89	4 (4%)
19	CLA	O	101	23	56,60,73	1.34	6 (10%)	67,97,113	0.95	3 (4%)
19	CLA	G	204	-	54,58,73	1.35	7 (12%)	65,95,113	0.94	3 (4%)
19	CLA	A	809	6	69,73,73	1.19	7 (10%)	83,113,113	1.04	4 (4%)
19	CLA	B	850	7	69,73,73	1.21	7 (10%)	83,113,113	1.08	5 (6%)
19	CLA	A	816	6	69,73,73	1.17	7 (10%)	83,113,113	0.99	5 (6%)
18	BCR	K	301	-	41,41,41	1.71	8 (19%)	56,56,56	1.66	11 (19%)
19	CLA	4	311	19,5	56,60,73	1.32	7 (12%)	67,97,113	1.17	7 (10%)
19	CLA	F	307	11	59,63,73	1.27	7 (11%)	71,101,113	0.98	3 (4%)
19	CLA	1	301	2	69,73,73	1.16	6 (8%)	83,113,113	1.02	5 (6%)
18	BCR	A	844	-	41,41,41	1.66	8 (19%)	56,56,56	1.64	12 (21%)
19	CLA	3	307	4	54,58,73	1.39	7 (12%)	65,95,113	0.99	3 (4%)
19	CLA	B	832	7	62,66,73	1.31	8 (12%)	74,104,113	1.10	6 (8%)
19	CLA	4	301	-	50,54,73	1.41	7 (14%)	60,90,113	1.05	3 (5%)
19	CLA	A	818	6	69,73,73	1.22	7 (10%)	83,113,113	0.96	4 (4%)
20	CHL	2	304	-	47,51,74	1.34	6 (12%)	52,86,114	1.19	6 (11%)
20	CHL	2	319	3	57,61,74	1.23	6 (10%)	64,98,114	1.10	5 (7%)
19	CLA	B	838	-	69,73,73	1.18	7 (10%)	83,113,113	0.98	5 (6%)
18	BCR	4	318	-	41,41,41	1.70	8 (19%)	56,56,56	1.71	12 (21%)
19	CLA	O	104	-	49,53,73	1.36	6 (12%)	59,89,113	1.23	5 (8%)
19	CLA	2	307	3	54,58,73	1.37	7 (12%)	65,95,113	1.22	6 (9%)
21	LUT	4	316	-	42,43,43	1.64	8 (19%)	51,60,60	1.68	10 (19%)
20	CHL	2	313	-	47,51,74	1.34	7 (14%)	52,86,114	1.30	8 (15%)
19	CLA	G	203	-	45,49,73	1.45	6 (13%)	54,84,113	1.22	4 (7%)
19	CLA	1	306	-	50,54,73	1.38	7 (14%)	60,90,113	1.10	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	CLA	B	804	7	49,53,73	1.44	8 (16%)	59,89,113	1.10	4 (6%)
19	CLA	4	310	19	64,68,73	1.31	8 (12%)	77,107,113	1.06	9 (11%)
19	CLA	A	820	6	53,57,73	1.37	8 (15%)	62,93,113	1.09	3 (4%)
20	CHL	1	305	2	52,56,74	1.25	6 (11%)	58,92,114	1.23	5 (8%)
19	CLA	A	838	-	69,73,73	1.20	6 (8%)	83,113,113	0.93	3 (3%)
18	BCR	F	302	-	41,41,41	1.72	8 (19%)	56,56,56	1.68	11 (19%)
19	CLA	3	305	4	51,55,73	1.36	7 (13%)	61,91,113	1.03	3 (4%)
19	CLA	B	835	7	64,68,73	1.29	8 (12%)	77,107,113	0.93	3 (3%)
19	CLA	2	309	23	45,49,73	1.50	6 (13%)	54,84,113	1.08	3 (5%)
19	CLA	A	850	-	69,73,73	1.20	7 (10%)	83,113,113	0.92	4 (4%)
19	CLA	2	311	-	69,73,73	1.19	6 (8%)	83,113,113	1.03	6 (7%)
23	LHG	2	317	19	36,36,48	0.33	0	39,42,54	0.35	0
19	CLA	O	102	17	49,53,73	1.35	6 (12%)	59,89,113	1.19	5 (8%)
19	CLA	B	836	7	69,73,73	1.16	7 (10%)	83,113,113	1.01	4 (4%)
19	CLA	3	308	4	54,58,73	1.29	7 (12%)	65,95,113	1.10	5 (7%)
19	CLA	A	839	6	69,73,73	1.20	7 (10%)	83,113,113	0.97	3 (3%)
22	XAT	3	314	-	39,47,47	1.70	8 (20%)	54,74,74	1.75	10 (18%)
24	LMG	J	101	-	51,51,55	0.24	0	59,59,63	0.31	0
25	HTG	F	301	-	19,19,19	0.25	0	23,24,24	0.55	0
25	HTG	4	321	-	19,19,19	0.23	0	23,24,24	0.36	0
19	CLA	A	819	-	69,73,73	1.19	7 (10%)	83,113,113	0.91	4 (4%)
19	CLA	B	805	7	69,73,73	1.19	7 (10%)	83,113,113	0.92	3 (3%)
19	CLA	A	804	6	69,73,73	1.20	8 (11%)	83,113,113	0.89	3 (3%)
18	BCR	L	301	-	41,41,41	1.66	8 (19%)	56,56,56	1.47	9 (16%)
19	CLA	B	821	7	69,73,73	1.24	8 (11%)	83,113,113	0.96	4 (4%)
18	BCR	A	845	-	41,41,41	1.63	8 (19%)	56,56,56	1.51	10 (17%)
19	CLA	3	309	4	56,60,73	1.33	7 (12%)	67,97,113	1.01	4 (5%)
19	CLA	A	823	-	69,73,73	1.21	8 (11%)	83,113,113	0.88	3 (3%)
19	CLA	A	802	6	59,63,73	1.28	7 (11%)	71,101,113	1.01	4 (5%)
25	HTG	B	848	-	19,19,19	0.27	0	23,24,24	0.60	0
19	CLA	A	826	6	69,73,73	1.16	6 (8%)	83,113,113	0.97	5 (6%)
19	CLA	A	808	6	69,73,73	1.16	7 (10%)	83,113,113	1.01	4 (4%)
19	CLA	A	801	6	69,73,73	1.19	7 (10%)	83,113,113	0.93	4 (4%)
19	CLA	K	303	-	64,68,73	1.23	7 (10%)	77,107,113	0.96	4 (5%)
19	CLA	B	818	7	64,68,73	1.26	7 (10%)	77,107,113	1.00	4 (5%)
19	CLA	1	311	-	64,68,73	1.24	6 (9%)	77,107,113	1.02	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	CLA	1	303	-	55,59,73	1.32	7 (12%)	66,96,113	1.03	4 (6%)
19	CLA	2	302	3	55,59,73	1.32	7 (12%)	66,96,113	1.05	4 (6%)
19	CLA	4	309	5	64,68,73	1.24	7 (10%)	77,107,113	1.15	6 (7%)
19	CLA	A	830	6	69,73,73	1.20	7 (10%)	83,113,113	0.97	4 (4%)
19	CLA	B	809	7	69,73,73	1.25	7 (10%)	83,113,113	0.94	4 (4%)
19	CLA	3	312	4	50,54,73	1.38	7 (14%)	60,90,113	1.08	4 (6%)
19	CLA	A	832	6	54,58,73	1.32	6 (11%)	65,95,113	1.00	3 (4%)
19	CLA	B	806	7	69,73,73	1.22	6 (8%)	83,113,113	0.89	3 (3%)
18	BCR	F	308	-	41,41,41	1.64	8 (19%)	56,56,56	1.49	10 (17%)
19	CLA	B	840	23	69,73,73	1.18	6 (8%)	83,113,113	0.90	3 (3%)
19	CLA	A	810	6	58,62,73	1.31	7 (12%)	69,99,113	1.02	4 (5%)
18	BCR	B	845	-	41,41,41	1.67	8 (19%)	56,56,56	1.52	10 (17%)
19	CLA	L	304	-	54,58,73	1.38	7 (12%)	65,95,113	1.00	3 (4%)
19	CLA	A	825	6	69,73,73	1.22	8 (11%)	83,113,113	0.91	4 (4%)
19	CLA	G	205	12	50,54,73	1.36	7 (14%)	60,90,113	1.17	5 (8%)
19	CLA	B	817	7	63,67,73	1.21	6 (9%)	75,105,113	1.06	5 (6%)
19	CLA	A	833	6	49,53,73	1.40	7 (14%)	59,89,113	1.18	5 (8%)
19	CLA	A	805	-	69,73,73	1.20	7 (10%)	83,113,113	0.95	4 (4%)
20	CHL	1	318	2	65,69,74	1.08	6 (9%)	74,108,114	0.98	5 (6%)
19	CLA	3	310	4	59,63,73	1.29	7 (11%)	71,101,113	1.03	5 (7%)
18	BCR	1	316	-	41,41,41	1.73	8 (19%)	56,56,56	1.79	14 (25%)
19	CLA	1	304	2	46,50,73	1.48	8 (17%)	55,85,113	1.11	3 (5%)
19	CLA	B	837	7	51,55,73	1.35	7 (13%)	61,91,113	1.09	4 (6%)
29	DGD	B	847	-	67,67,67	0.80	2 (2%)	81,81,81	1.09	5 (6%)
27	SF4	C	102	8	0,12,12	-	-	-		
25	HTG	F	303	-	19,19,19	0.22	0	23,24,24	0.50	0
27	SF4	A	849	7,6	0,12,12	-	-	-		
19	CLA	A	836	6	69,73,73	1.15	7 (10%)	83,113,113	1.09	7 (8%)
23	LHG	A	842	-	48,48,48	0.30	0	51,54,54	0.36	0
19	CLA	B	807	7	69,73,73	1.20	7 (10%)	83,113,113	0.91	3 (3%)
19	CLA	A	812	6	59,63,73	1.34	8 (13%)	71,101,113	1.12	6 (8%)
19	CLA	A	827	6	69,73,73	1.21	7 (10%)	83,113,113	0.90	3 (3%)
22	XAT	4	317	-	39,47,47	1.76	8 (20%)	54,74,74	1.89	13 (24%)
22	XAT	1	315	-	39,47,47	1.64	8 (20%)	54,74,74	1.66	10 (18%)
18	BCR	O	106	-	41,41,41	1.70	8 (19%)	56,56,56	1.70	12 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	CLA	B	830	7	54,58,73	1.31	7 (12%)	65,95,113	1.02	4 (6%)
24	LMG	F	309	-	40,40,55	0.27	0	48,48,63	0.33	0
19	CLA	B	833	7	69,73,73	1.14	6 (8%)	83,113,113	1.03	4 (4%)
19	CLA	3	301	4	64,68,73	1.21	7 (10%)	77,107,113	1.01	5 (6%)
19	CLA	1	302	2	69,73,73	1.18	7 (10%)	83,113,113	0.91	4 (4%)
19	CLA	B	824	-	69,73,73	1.19	7 (10%)	83,113,113	0.96	4 (4%)
19	CLA	A	813	-	54,58,73	1.33	7 (12%)	65,95,113	1.11	5 (7%)
19	CLA	B	815	-	59,63,73	1.28	7 (11%)	71,101,113	1.06	5 (7%)
18	BCR	G	206	-	41,41,41	1.67	8 (19%)	56,56,56	1.62	11 (19%)
19	CLA	3	316	-	49,53,73	1.39	7 (14%)	59,89,113	1.05	4 (6%)
18	BCR	A	847	-	41,41,41	1.66	8 (19%)	56,56,56	1.50	9 (16%)
19	CLA	L	302	1	69,73,73	1.21	7 (10%)	83,113,113	1.00	6 (7%)
19	CLA	1	307	2	69,73,73	1.20	7 (10%)	83,113,113	0.94	5 (6%)
27	SF4	C	101	8	0,12,12	-	-	-		
19	CLA	3	302	4	54,58,73	1.36	8 (14%)	65,95,113	1.02	4 (6%)
18	BCR	J	103	-	41,41,41	1.67	8 (19%)	56,56,56	1.61	11 (19%)
19	CLA	L	303	1	69,73,73	1.18	7 (10%)	83,113,113	0.94	4 (4%)
19	CLA	2	308	3	64,68,73	1.21	8 (12%)	77,107,113	1.11	7 (9%)
19	CLA	B	834	-	49,53,73	1.37	7 (14%)	59,89,113	1.14	5 (8%)
19	CLA	B	803	-	69,73,73	1.19	7 (10%)	83,113,113	1.01	5 (6%)
24	LMG	G	202	-	40,40,55	0.22	0	48,48,63	0.23	0
18	BCR	L	306	-	41,41,41	1.65	8 (19%)	56,56,56	1.45	9 (16%)
19	CLA	A	806	6	69,73,73	1.18	7 (10%)	83,113,113	0.94	4 (4%)
19	CLA	A	831	6	69,73,73	1.23	8 (11%)	83,113,113	1.01	4 (4%)
19	CLA	2	303	-	64,68,73	1.25	7 (10%)	77,107,113	0.97	4 (5%)
24	LMG	4	319	-	50,50,55	0.25	0	58,58,63	0.32	0
19	CLA	J	102	15	46,50,73	1.44	7 (15%)	55,85,113	1.19	5 (9%)
18	BCR	I	101	-	41,41,41	1.69	8 (19%)	56,56,56	1.65	12 (21%)
23	LHG	4	320	-	48,48,48	0.28	0	51,54,54	0.33	0
18	BCR	K	304	-	41,41,41	1.69	8 (19%)	56,56,56	1.73	12 (21%)
23	LHG	1	317	19	48,48,48	0.29	0	51,54,54	0.41	0
19	CLA	4	302	5	64,68,73	1.22	8 (12%)	77,107,113	1.03	5 (6%)
25	HTG	F	305	-	19,19,19	0.33	0	23,24,24	0.48	0
19	CLA	O	103	-	56,60,73	1.26	6 (10%)	67,97,113	1.05	4 (5%)
18	BCR	B	843	-	41,41,41	1.70	8 (19%)	56,56,56	1.61	11 (19%)
19	CLA	4	313	5	49,53,73	1.39	6 (12%)	59,89,113	1.13	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	CHL	2	305	-	52,56,74	1.26	6 (11%)	58,92,114	1.05	3 (5%)
24	LMG	B	849	-	44,44,55	0.23	0	52,52,63	0.31	0
18	BCR	L	305	-	41,41,41	1.69	8 (19%)	56,56,56	1.65	11 (19%)
19	CLA	A	807	6	69,73,73	1.19	7 (10%)	83,113,113	0.95	3 (3%)
19	CLA	A	852	-	69,73,73	1.19	7 (10%)	83,113,113	0.95	4 (4%)
19	CLA	A	854	6	69,73,73	1.17	7 (10%)	83,113,113	0.99	5 (6%)
19	CLA	B	811	7	58,62,73	1.33	8 (13%)	73,100,113	1.09	4 (5%)
19	CLA	1	310	2	56,60,73	1.31	6 (10%)	67,97,113	1.03	4 (5%)
19	CLA	A	824	-	69,73,73	1.18	6 (8%)	83,113,113	0.89	3 (3%)
19	CLA	2	301	3	69,73,73	1.16	6 (8%)	83,113,113	0.94	4 (4%)
19	CLA	4	314	5	51,55,73	1.36	6 (11%)	61,91,113	1.08	4 (6%)
21	LUT	3	313	-	42,43,43	1.64	8 (19%)	51,60,60	1.63	10 (19%)
19	CLA	2	312	3	47,51,73	1.45	7 (14%)	56,86,113	1.18	5 (8%)
19	CLA	B	827	7	69,73,73	1.18	7 (10%)	83,113,113	1.05	5 (6%)
19	CLA	A	815	6	69,73,73	1.20	7 (10%)	83,113,113	0.89	3 (3%)
19	CLA	B	829	7	69,73,73	1.21	7 (10%)	83,113,113	1.03	4 (4%)
19	CLA	B	839	7	69,73,73	1.19	6 (8%)	83,113,113	0.97	4 (4%)
19	CLA	A	840	-	69,73,73	1.21	8 (11%)	83,113,113	0.89	3 (3%)
26	PQN	B	841	-	34,34,34	0.37	0	42,45,45	0.61	1 (2%)
18	BCR	B	846	-	41,41,41	1.66	8 (19%)	56,56,56	1.48	10 (17%)
19	CLA	A	834	6	55,59,73	1.39	8 (14%)	66,96,113	0.98	3 (4%)

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
19	CLA	B	831	7	-	14/33/109/115	-
19	CLA	A	853	6	-	14/39/115/115	-
19	CLA	A	822	6	-	11/27/103/115	-
19	CLA	3	311	4	-	9/15/91/115	-
19	CLA	A	811	-	-	24/39/115/115	-
19	CLA	4	312	-	-	9/29/105/115	-
19	CLA	B	810	7	-	16/39/115/115	-
19	CLA	B	825	-	-	21/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CHL	4	305	5	-	16/29/105/117	-
19	CLA	1	309	23	-	23/39/115/115	-
21	LUT	2	314	-	-	11/29/67/67	0/2/2/2
19	CLA	B	814	7	-	19/39/115/115	-
19	CLA	B	820	7	-	13/21/97/115	-
19	CLA	A	828	6	-	19/39/115/115	-
23	LHG	4	322	-	-	28/44/44/53	-
19	CLA	3	304	-	-	6/12/88/115	-
23	LHG	2	318	-	-	30/53/53/53	-
20	CHL	3	306	-	-	11/19/95/117	-
19	CLA	B	816	7	-	14/27/103/115	-
19	CLA	4	308	5	-	10/21/97/115	-
26	PQN	A	841	-	-	3/23/43/43	0/2/2/2
19	CLA	A	837	6	-	21/39/115/115	-
19	CLA	B	828	-	-	20/39/115/115	-
19	CLA	B	822	7	-	13/27/103/115	-
20	CHL	2	306	-	-	11/23/99/117	-
19	CLA	A	803	6	-	11/39/115/115	-
19	CLA	B	819	-	-	17/39/115/115	-
19	CLA	A	835	6	-	14/39/115/115	-
19	CLA	1	312	2	-	19/27/103/115	-
18	BCR	2	316	-	-	24/29/63/63	0/2/2/2
21	LUT	1	314	-	-	13/29/67/67	0/2/2/2
19	CLA	A	814	-	-	8/15/91/115	-
19	CLA	A	817	6	-	14/39/115/115	-
19	CLA	3	303	-	-	5/15/91/115	-
18	BCR	G	201	-	-	15/29/63/63	0/2/2/2
22	XAT	2	315	-	-	10/31/93/93	0/4/4/4
18	BCR	A	846	-	-	8/29/63/63	0/2/2/2
19	CLA	B	823	7	-	20/33/109/115	-
18	BCR	A	848	-	-	21/29/63/63	0/2/2/2
23	LHG	A	843	19	-	15/31/31/53	-
19	CLA	B	802	7	-	16/39/115/115	-
20	CHL	4	306	-	-	12/23/99/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	BCR	J	104	-	-	20/29/63/63	0/2/2/2
19	CLA	B	808	7	-	12/39/115/115	-
19	CLA	B	813	7	-	18/39/115/115	-
19	CLA	A	821	6	-	13/23/99/115	-
19	CLA	2	310	3	-	13/24/100/115	-
19	CLA	4	303	5	-	17/33/109/115	-
20	CHL	4	315	5	-	10/14/90/117	-
25	HTG	F	310	-	-	4/10/30/30	0/1/1/1
18	BCR	O	105	-	-	22/29/63/63	0/2/2/2
19	CLA	1	308	2	-	13/33/109/115	-
18	BCR	B	844	-	-	13/29/63/63	0/2/2/2
18	BCR	3	315	-	-	17/29/63/63	0/2/2/2
19	CLA	K	302	-	-	10/15/91/115	-
23	LHG	1	319	19	-	8/26/26/53	-
23	LHG	1	320	-	-	36/53/53/53	-
18	BCR	B	842	-	-	14/29/63/63	0/2/2/2
18	BCR	F	304	-	-	18/29/63/63	0/2/2/2
19	CLA	B	801	-	-	9/39/115/115	-
20	CHL	4	307	-	-	11/23/99/117	-
28	LMT	A	851	-	-	13/21/61/61	0/2/2/2
19	CLA	1	313	2	-	8/17/93/115	-
19	CLA	B	812	7	-	9/27/103/115	-
19	CLA	A	829	6	-	13/21/97/115	-
19	CLA	F	306	-	-	3/15/91/115	-
19	CLA	4	304	-	-	12/21/97/115	-
19	CLA	B	826	7	-	10/39/115/115	-
19	CLA	O	101	23	-	12/24/100/115	-
19	CLA	G	204	-	-	6/21/97/115	-
19	CLA	A	809	6	-	14/39/115/115	-
19	CLA	B	850	7	-	12/39/115/115	-
19	CLA	A	816	6	-	22/39/115/115	-
18	BCR	K	301	-	-	17/29/63/63	0/2/2/2
19	CLA	4	311	19,5	-	13/24/100/115	-
19	CLA	F	307	11	-	10/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	1	301	2	-	15/39/115/115	-
18	BCR	A	844	-	-	19/29/63/63	0/2/2/2
19	CLA	3	307	4	-	10/21/97/115	-
19	CLA	B	832	7	-	14/31/107/115	-
19	CLA	4	301	-	-	4/17/93/115	-
19	CLA	A	818	6	-	20/39/115/115	-
20	CHL	2	304	-	-	5/14/90/117	-
20	CHL	2	319	3	-	15/26/102/117	-
19	CLA	B	838	-	-	14/39/115/115	-
18	BCR	4	318	-	-	16/29/63/63	0/2/2/2
19	CLA	O	104	-	-	10/15/91/115	-
19	CLA	2	307	3	-	6/21/97/115	-
21	LUT	4	316	-	-	15/29/67/67	0/2/2/2
20	CHL	2	313	-	-	8/14/90/117	-
19	CLA	G	203	-	-	6/10/86/115	-
19	CLA	1	306	-	-	10/17/93/115	-
19	CLA	B	804	7	-	5/15/91/115	-
19	CLA	4	310	19	-	19/33/109/115	-
19	CLA	A	820	6	-	12/20/96/115	-
20	CHL	1	305	2	-	16/20/96/117	-
19	CLA	A	838	-	-	24/39/115/115	-
18	BCR	F	302	-	-	18/29/63/63	0/2/2/2
19	CLA	3	305	4	-	7/18/94/115	-
19	CLA	B	835	7	-	14/33/109/115	-
19	CLA	2	309	23	-	4/10/86/115	-
19	CLA	A	850	-	-	17/39/115/115	-
19	CLA	2	311	-	-	15/39/115/115	-
23	LHG	2	317	19	-	22/41/41/53	-
19	CLA	O	102	17	-	9/15/91/115	-
19	CLA	B	836	7	-	12/39/115/115	-
19	CLA	3	308	4	-	11/21/97/115	-
19	CLA	A	839	6	-	20/39/115/115	-
22	XAT	3	314	-	-	6/31/93/93	0/4/4/4
24	LMG	J	101	-	-	26/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	HTG	F	301	-	-	8/10/30/30	0/1/1/1
25	HTG	4	321	-	-	7/10/30/30	0/1/1/1
19	CLA	A	819	-	-	9/39/115/115	-
19	CLA	B	805	7	-	12/39/115/115	-
19	CLA	A	804	6	-	15/39/115/115	-
18	BCR	L	301	-	-	16/29/63/63	0/2/2/2
19	CLA	B	821	7	-	19/39/115/115	-
18	BCR	A	845	-	-	20/29/63/63	0/2/2/2
19	CLA	3	309	4	-	3/24/100/115	-
19	CLA	A	823	-	-	9/39/115/115	-
19	CLA	A	802	6	-	7/27/103/115	-
25	HTG	B	848	-	-	5/10/30/30	0/1/1/1
19	CLA	A	826	6	-	15/39/115/115	-
19	CLA	A	808	6	-	22/39/115/115	-
19	CLA	A	801	6	-	12/39/115/115	-
19	CLA	K	303	-	-	17/33/109/115	-
19	CLA	B	818	7	-	17/33/109/115	-
19	CLA	1	311	-	-	14/33/109/115	-
19	CLA	1	303	-	-	7/23/99/115	-
19	CLA	2	302	3	-	8/23/99/115	-
19	CLA	4	309	5	-	14/33/109/115	-
19	CLA	A	830	6	-	19/39/115/115	-
19	CLA	B	809	7	-	18/39/115/115	-
19	CLA	3	312	4	-	2/17/93/115	-
19	CLA	A	832	6	-	8/21/97/115	-
19	CLA	B	806	7	-	22/39/115/115	-
18	BCR	F	308	-	-	13/29/63/63	0/2/2/2
19	CLA	B	840	23	-	11/39/115/115	-
19	CLA	A	810	6	-	4/26/102/115	-
18	BCR	B	845	-	-	13/29/63/63	0/2/2/2
19	CLA	L	304	-	-	8/21/97/115	-
19	CLA	A	825	6	-	12/39/115/115	-
19	CLA	G	205	12	-	4/17/93/115	-
19	CLA	B	817	7	-	11/32/108/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	833	6	-	7/15/91/115	-
19	CLA	A	805	-	-	17/39/115/115	-
20	CHL	1	318	2	-	15/35/111/117	-
19	CLA	3	310	4	-	13/27/103/115	-
18	BCR	1	316	-	-	22/29/63/63	0/2/2/2
19	CLA	1	304	2	-	5/12/88/115	-
19	CLA	B	837	7	-	5/18/94/115	-
29	DGD	B	847	-	-	26/55/95/95	0/2/2/2
27	SF4	C	102	8	-	-	0/6/5/5
25	HTG	F	303	-	-	6/10/30/30	0/1/1/1
27	SF4	A	849	7,6	-	-	0/6/5/5
19	CLA	A	836	6	-	14/39/115/115	-
23	LHG	A	842	-	-	27/53/53/53	-
19	CLA	B	807	7	-	12/39/115/115	-
19	CLA	A	812	6	-	10/27/103/115	-
19	CLA	A	827	6	-	18/39/115/115	-
22	XAT	4	317	-	-	8/31/93/93	0/4/4/4
22	XAT	1	315	-	-	12/31/93/93	0/4/4/4
18	BCR	O	106	-	-	20/29/63/63	0/2/2/2
19	CLA	B	830	7	-	10/21/97/115	-
24	LMG	F	309	-	-	11/35/55/70	0/1/1/1
19	CLA	B	833	7	-	22/39/115/115	-
19	CLA	3	301	4	-	16/33/109/115	-
19	CLA	1	302	2	-	27/39/115/115	-
19	CLA	B	824	-	-	11/39/115/115	-
19	CLA	A	813	-	-	11/21/97/115	-
19	CLA	B	815	-	-	12/27/103/115	-
18	BCR	G	206	-	-	21/29/63/63	0/2/2/2
19	CLA	3	316	-	-	6/15/91/115	-
18	BCR	A	847	-	-	16/29/63/63	0/2/2/2
19	CLA	L	302	1	-	20/39/115/115	-
19	CLA	1	307	2	-	23/39/115/115	-
27	SF4	C	101	8	-	-	0/6/5/5
19	CLA	3	302	4	-	6/21/97/115	-
18	BCR	J	103	-	-	19/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	L	303	1	-	17/39/115/115	-
19	CLA	2	308	3	-	7/33/109/115	-
19	CLA	B	834	-	-	2/15/91/115	-
19	CLA	B	803	-	-	11/39/115/115	-
24	LMG	G	202	-	-	17/35/55/70	0/1/1/1
18	BCR	L	306	-	-	12/29/63/63	0/2/2/2
19	CLA	A	806	6	-	19/39/115/115	-
19	CLA	A	831	6	-	18/39/115/115	-
19	CLA	2	303	-	-	22/33/109/115	-
24	LMG	4	319	-	-	27/45/65/70	0/1/1/1
19	CLA	J	102	15	-	6/12/88/115	-
18	BCR	I	101	-	-	14/29/63/63	0/2/2/2
23	LHG	4	320	-	-	35/53/53/53	-
18	BCR	K	304	-	-	22/29/63/63	0/2/2/2
23	LHG	1	317	19	-	30/53/53/53	-
19	CLA	4	302	5	-	14/33/109/115	-
25	HTG	F	305	-	-	5/10/30/30	0/1/1/1
19	CLA	O	103	-	-	11/24/100/115	-
18	BCR	B	843	-	-	17/29/63/63	0/2/2/2
19	CLA	4	313	5	-	10/15/91/115	-
20	CHL	2	305	-	-	12/20/96/117	-
24	LMG	B	849	-	-	20/39/59/70	0/1/1/1
18	BCR	L	305	-	-	14/29/63/63	0/2/2/2
19	CLA	A	807	6	-	18/39/115/115	-
19	CLA	A	852	-	-	8/39/115/115	-
19	CLA	A	854	6	-	18/39/115/115	-
19	CLA	B	811	7	-	14/25/101/115	-
19	CLA	1	310	2	-	15/24/100/115	-
19	CLA	A	824	-	-	17/39/115/115	-
19	CLA	2	301	3	-	18/39/115/115	-
19	CLA	4	314	5	-	6/18/94/115	-
21	LUT	3	313	-	-	20/29/67/67	0/2/2/2
19	CLA	2	312	3	-	2/13/89/115	-
19	CLA	B	827	7	-	22/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	815	6	-	19/39/115/115	-
19	CLA	B	829	7	-	16/39/115/115	-
19	CLA	B	839	7	-	20/39/115/115	-
19	CLA	A	840	-	-	22/39/115/115	-
26	PQN	B	841	-	-	2/23/43/43	0/2/2/2
18	BCR	B	846	-	-	16/29/63/63	0/2/2/2
19	CLA	A	834	6	-	10/23/99/115	-

The worst 5 of 1376 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	4	310	CLA	C1C-C2C	-4.95	1.35	1.44
19	B	817	CLA	C1C-C2C	-4.77	1.35	1.44
19	4	309	CLA	C4C-C3C	-4.76	1.36	1.45
19	A	814	CLA	C4C-C3C	-4.76	1.36	1.45
19	3	312	CLA	C4C-C3C	-4.76	1.36	1.45

The worst 5 of 1066 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	4	309	CLA	CHD-C1D-ND	-5.25	119.63	124.45
20	1	305	CHL	CHD-C1D-ND	-5.09	119.77	124.45
29	B	847	DGD	O2G-C1B-C2B	4.97	122.20	111.50
19	O	104	CLA	CHD-C1D-ND	-4.71	120.13	124.45
19	2	307	CLA	C4D-CHA-C1A	4.62	126.87	121.25

There are no chirality outliers.

5 of 3018 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	L	301	BCR	C14-C15-C16-C17
18	L	301	BCR	C16-C17-C18-C19
18	L	301	BCR	C16-C17-C18-C36
18	L	301	BCR	C17-C18-C19-C20
18	L	301	BCR	C36-C18-C19-C20

There are no ring outliers.

203 monomers are involved in 544 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B	831	CLA	4	0
19	A	853	CLA	3	0
19	A	822	CLA	4	0
19	3	311	CLA	1	0
19	A	811	CLA	6	0
19	4	312	CLA	4	0
19	B	810	CLA	3	0
19	B	825	CLA	2	0
20	4	305	CHL	7	0
19	1	309	CLA	7	0
21	2	314	LUT	4	0
19	B	814	CLA	3	0
19	A	828	CLA	4	0
23	4	322	LHG	7	0
19	3	304	CLA	1	0
23	2	318	LHG	6	0
20	3	306	CHL	3	0
19	B	816	CLA	6	0
19	4	308	CLA	1	0
26	A	841	PQN	4	0
19	A	837	CLA	6	0
19	B	828	CLA	3	0
19	B	822	CLA	5	0
20	2	306	CHL	9	0
19	B	819	CLA	7	0
19	A	835	CLA	6	0
19	1	312	CLA	3	0
18	2	316	BCR	6	0
21	1	314	LUT	4	0
19	A	814	CLA	1	0
19	A	817	CLA	6	0
19	3	303	CLA	2	0
18	G	201	BCR	2	0
22	2	315	XAT	2	0
18	A	846	BCR	2	0
19	B	823	CLA	3	0
18	A	848	BCR	1	0
23	A	843	LHG	2	0
19	B	802	CLA	7	0
20	4	306	CHL	3	0
18	J	104	BCR	1	0
19	B	808	CLA	5	0
19	B	813	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	821	CLA	1	0
19	2	310	CLA	3	0
19	4	303	CLA	4	0
20	4	315	CHL	3	0
25	F	310	HTG	1	0
18	O	105	BCR	2	0
19	1	308	CLA	3	0
18	B	844	BCR	4	0
18	3	315	BCR	5	0
19	K	302	CLA	3	0
23	1	320	LHG	9	0
18	B	842	BCR	2	0
18	F	304	BCR	4	0
19	B	801	CLA	3	0
20	4	307	CHL	6	0
28	A	851	LMT	2	0
19	B	812	CLA	3	0
19	A	829	CLA	1	0
19	F	306	CLA	1	0
19	4	304	CLA	1	0
19	B	826	CLA	6	0
19	O	101	CLA	3	0
19	G	204	CLA	2	0
19	A	809	CLA	4	0
19	B	850	CLA	3	0
19	A	816	CLA	2	0
18	K	301	BCR	5	0
19	4	311	CLA	6	0
19	F	307	CLA	3	0
19	1	301	CLA	2	0
18	A	844	BCR	2	0
19	3	307	CLA	2	0
19	4	301	CLA	5	0
19	A	818	CLA	4	0
20	2	304	CHL	4	0
20	2	319	CHL	4	0
19	B	838	CLA	4	0
18	4	318	BCR	5	0
19	2	307	CLA	1	0
21	4	316	LUT	3	0
20	2	313	CHL	3	0
19	G	203	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	1	306	CLA	2	0
19	B	804	CLA	2	0
19	4	310	CLA	10	0
19	A	820	CLA	4	0
20	1	305	CHL	1	0
19	A	838	CLA	6	0
18	F	302	BCR	5	0
19	3	305	CLA	1	0
19	B	835	CLA	4	0
19	2	309	CLA	1	0
19	A	850	CLA	6	0
19	2	311	CLA	3	0
23	2	317	LHG	4	0
19	O	102	CLA	1	0
19	B	836	CLA	4	0
19	3	308	CLA	4	0
19	A	839	CLA	7	0
22	3	314	XAT	2	0
24	J	101	LMG	2	0
25	F	301	HTG	3	0
19	A	819	CLA	5	0
19	B	805	CLA	1	0
19	A	804	CLA	3	0
18	L	301	BCR	1	0
19	B	821	CLA	4	0
18	A	845	BCR	3	0
19	3	309	CLA	2	0
19	A	823	CLA	2	0
19	A	802	CLA	2	0
25	B	848	HTG	1	0
19	A	826	CLA	6	0
19	A	808	CLA	4	0
19	A	801	CLA	5	0
19	K	303	CLA	3	0
19	B	818	CLA	5	0
19	1	311	CLA	10	0
19	1	303	CLA	2	0
19	2	302	CLA	2	0
19	4	309	CLA	8	0
19	A	830	CLA	1	0
19	B	809	CLA	3	0
19	A	832	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B	806	CLA	3	0
18	F	308	BCR	3	0
19	B	840	CLA	6	0
19	A	810	CLA	1	0
18	B	845	BCR	5	0
19	L	304	CLA	1	0
19	A	825	CLA	2	0
19	G	205	CLA	1	0
19	B	817	CLA	2	0
19	A	805	CLA	2	0
20	1	318	CHL	7	0
19	3	310	CLA	5	0
18	1	316	BCR	5	0
19	1	304	CLA	2	0
29	B	847	DGD	7	0
27	C	102	SF4	1	0
25	F	303	HTG	1	0
19	A	836	CLA	8	0
23	A	842	LHG	1	0
19	B	807	CLA	6	0
19	A	827	CLA	2	0
22	4	317	XAT	5	0
22	1	315	XAT	2	0
18	O	106	BCR	5	0
24	F	309	LMG	1	0
19	B	833	CLA	2	0
19	3	301	CLA	2	0
19	1	302	CLA	8	0
19	B	824	CLA	7	0
19	A	813	CLA	1	0
18	G	206	BCR	2	0
19	3	316	CLA	3	0
18	A	847	BCR	4	0
19	L	302	CLA	5	0
19	1	307	CLA	6	0
19	3	302	CLA	1	0
18	J	103	BCR	3	0
19	L	303	CLA	5	0
19	2	308	CLA	4	0
19	B	834	CLA	3	0
19	B	803	CLA	5	0
24	G	202	LMG	1	0

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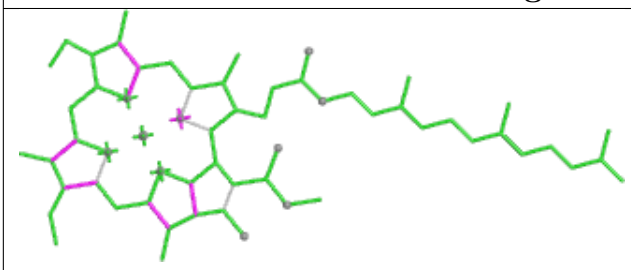
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	L	306	BCR	1	0
19	A	806	CLA	6	0
19	A	831	CLA	4	0
19	2	303	CLA	1	0
24	4	319	LMG	8	0
18	I	101	BCR	3	0
23	4	320	LHG	2	0
18	K	304	BCR	3	0
23	1	317	LHG	6	0
19	4	302	CLA	5	0
25	F	305	HTG	4	0
19	O	103	CLA	5	0
18	B	843	BCR	2	0
19	4	313	CLA	2	0
20	2	305	CHL	5	0
24	B	849	LMG	3	0
18	L	305	BCR	4	0
19	A	852	CLA	3	0
19	A	854	CLA	6	0
19	B	811	CLA	1	0
19	1	310	CLA	3	0
19	A	824	CLA	2	0
19	2	301	CLA	4	0
19	4	314	CLA	2	0
21	3	313	LUT	5	0
19	2	312	CLA	1	0
19	B	827	CLA	3	0
19	A	815	CLA	2	0
19	B	829	CLA	6	0
19	B	839	CLA	2	0
19	A	840	CLA	3	0
26	B	841	PQN	1	0
18	B	846	BCR	2	0
19	A	834	CLA	2	0

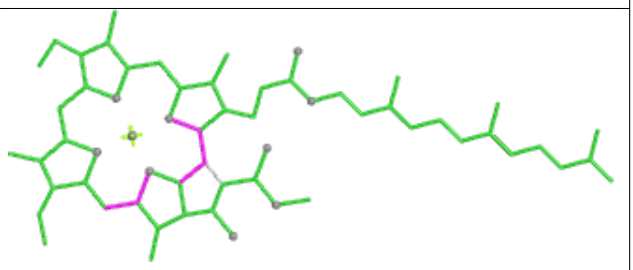
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

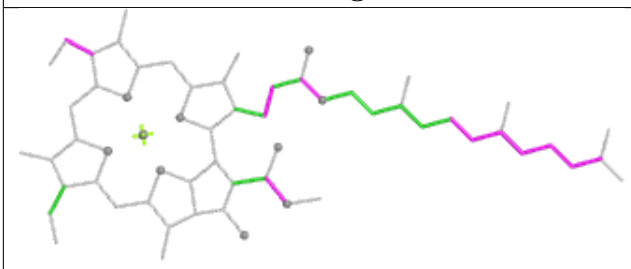
Ligand CLA B 831



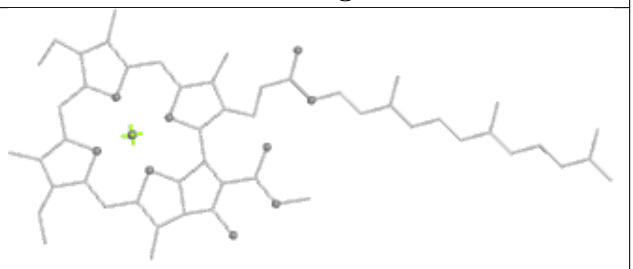
Bond lengths



Bond angles

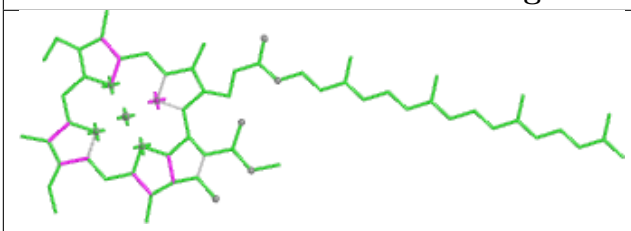


Torsions

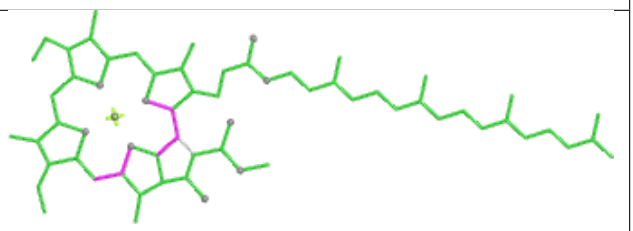


Rings

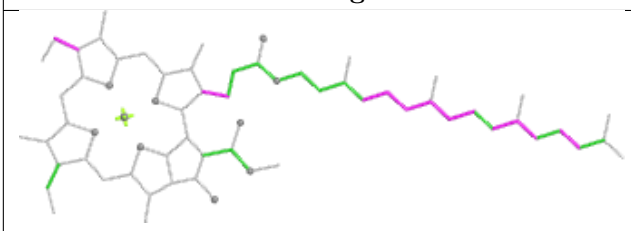
Ligand CLA A 853



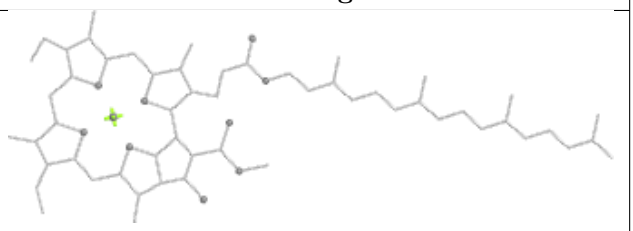
Bond lengths



Bond angles

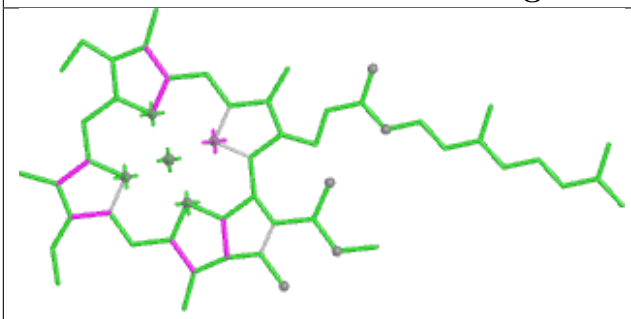


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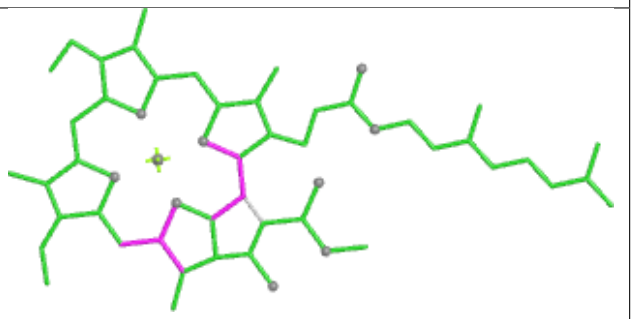


Rings

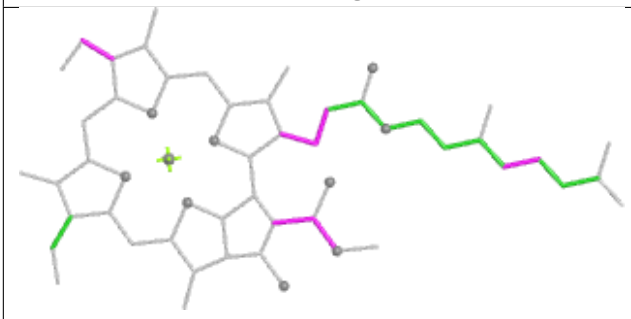
Ligand CLA A 822



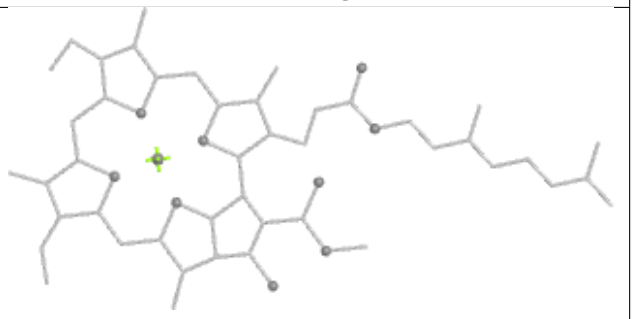
Bond lengths



Bond angles

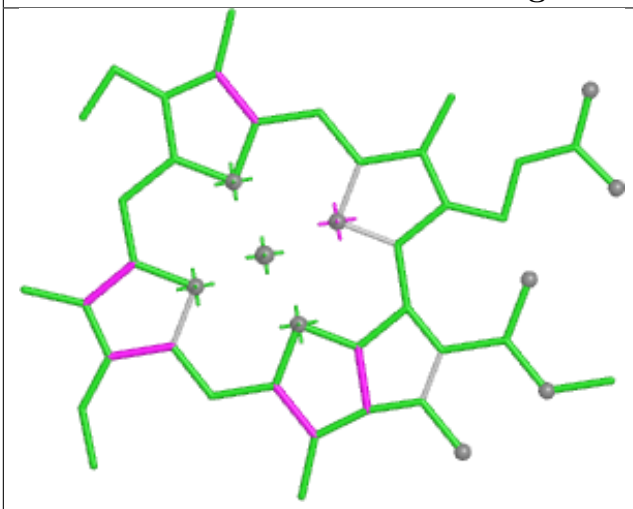


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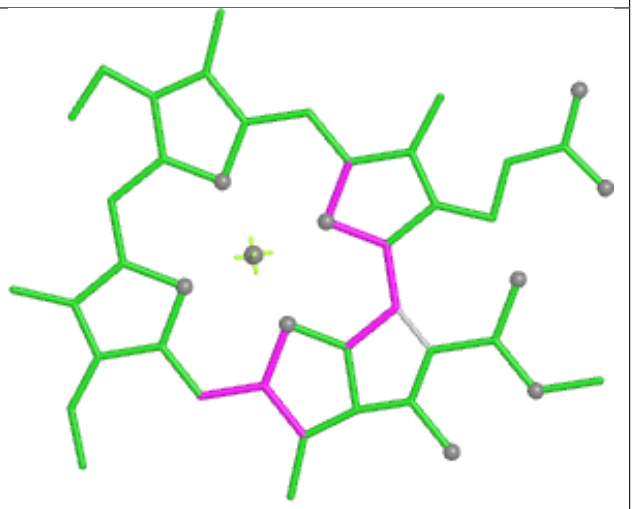


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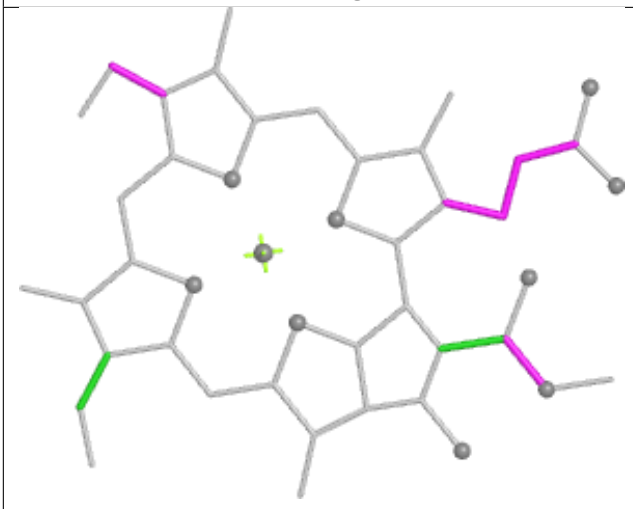
Ligand CLA 3 311



Bond lengths



Bond angles

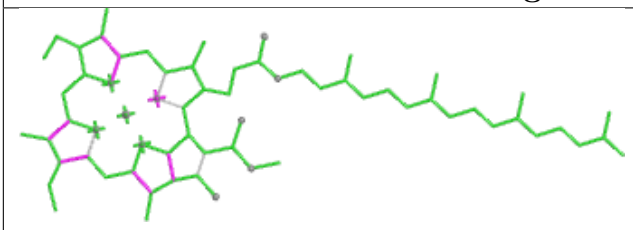


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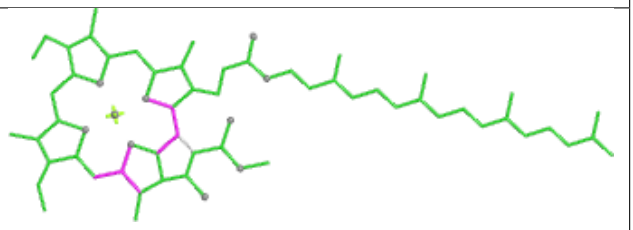


Rings

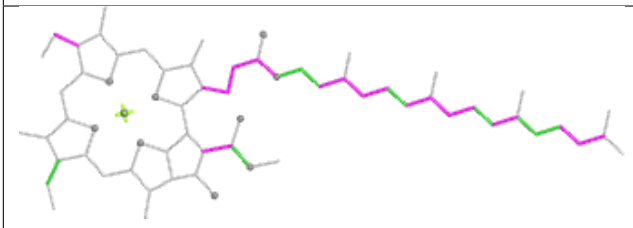
Ligand CLA A 811



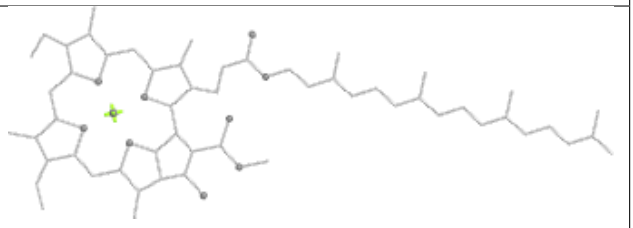
Bond lengths



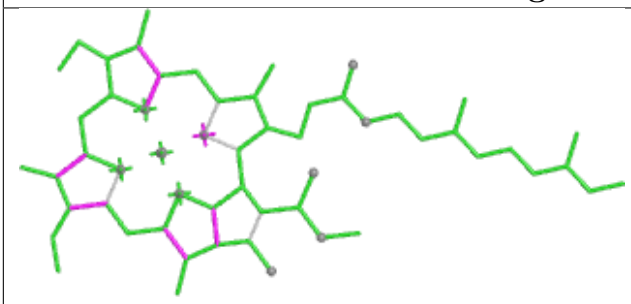
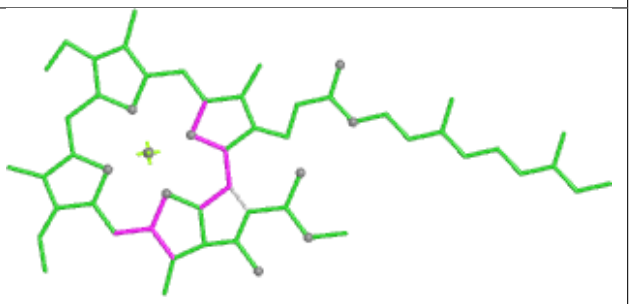
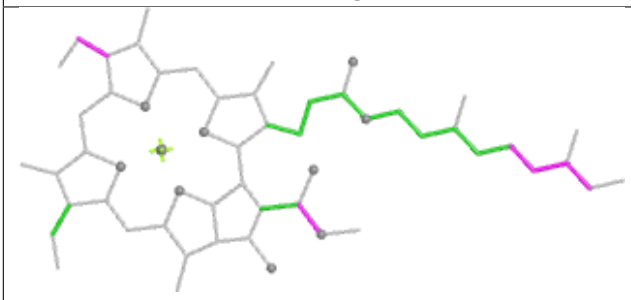
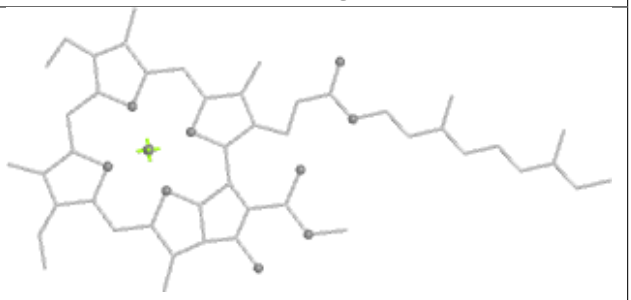
Bond angles

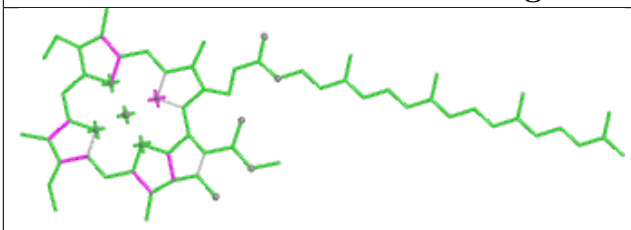
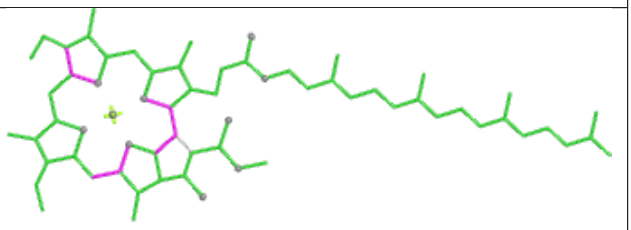
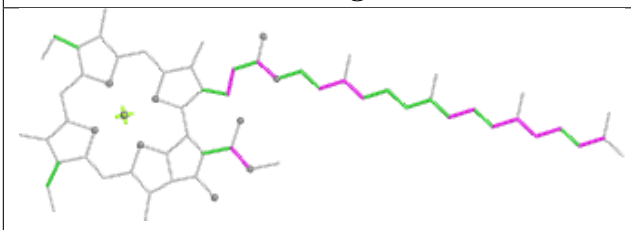
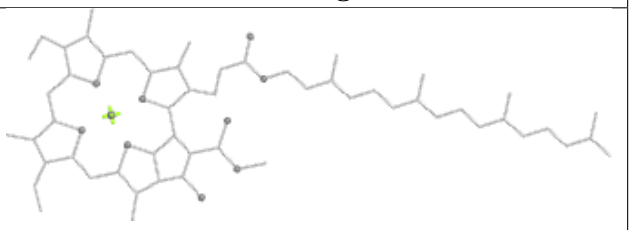


Torsions

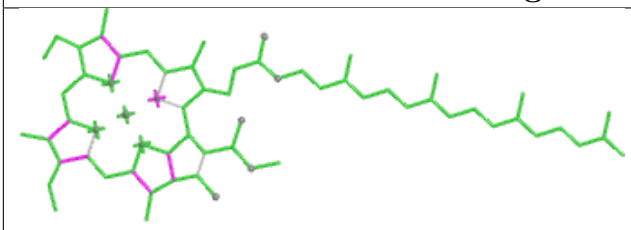


Rings

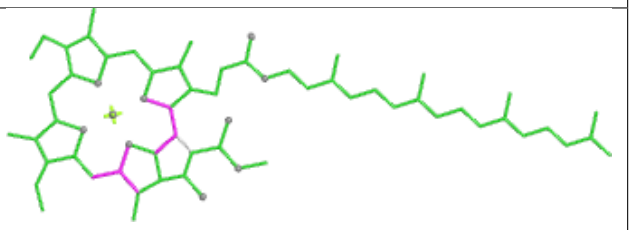
Ligand CLA 4 312	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 810	
	
Bond lengths	Bond angles
	
Torsions	Rings

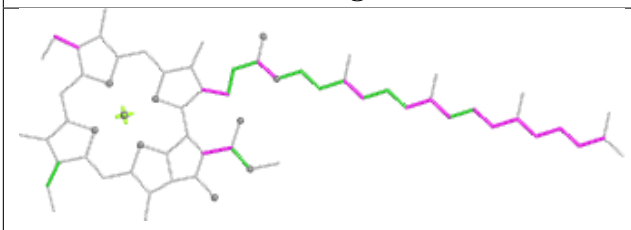
Ligand CLA B 825



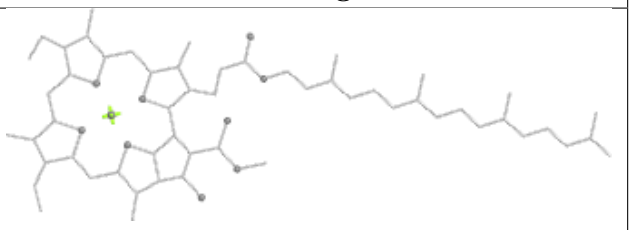
Bond lengths



Bond angles

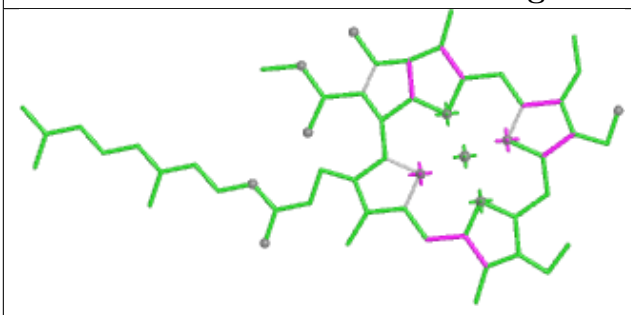


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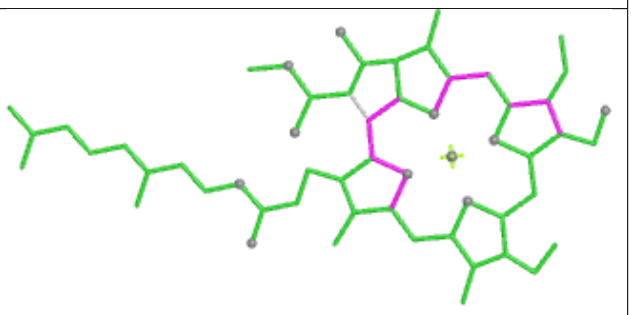


Rings

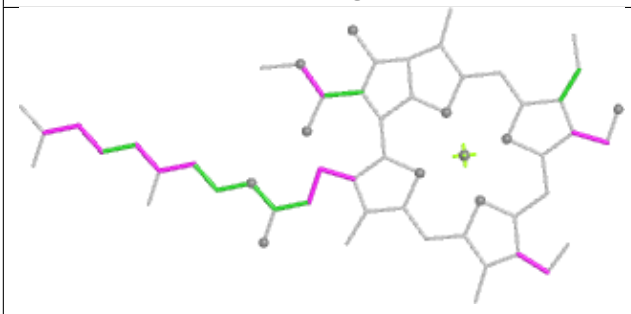
Ligand CHL 4 305



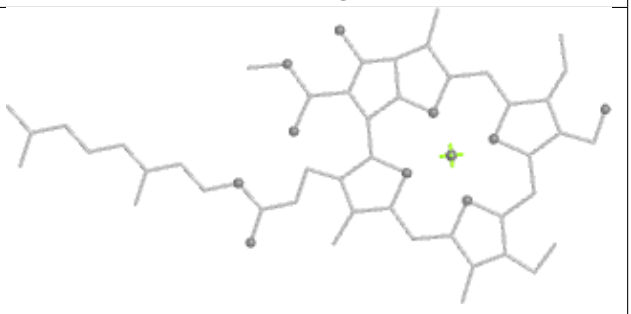
Bond lengths



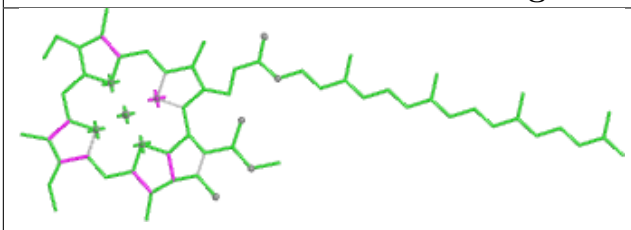
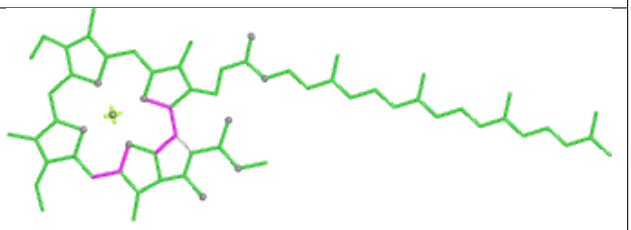
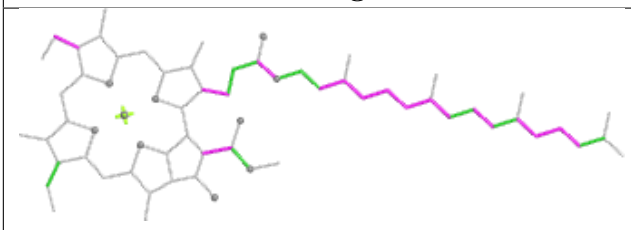
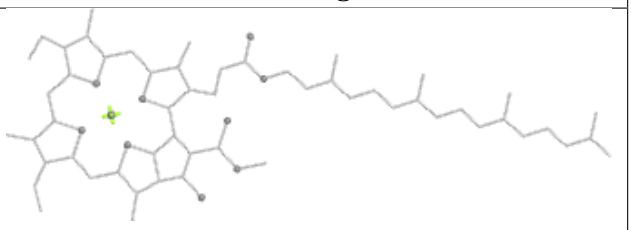
Bond angles

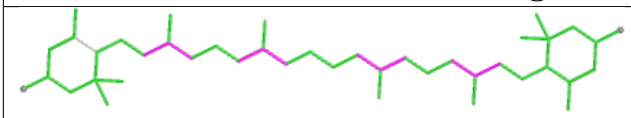
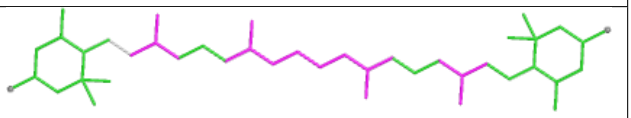
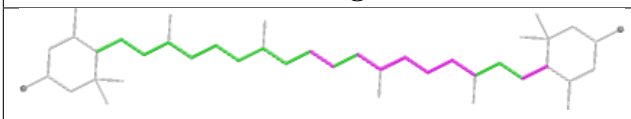
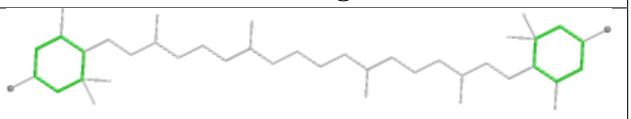


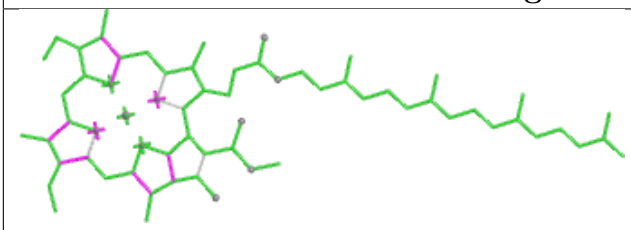
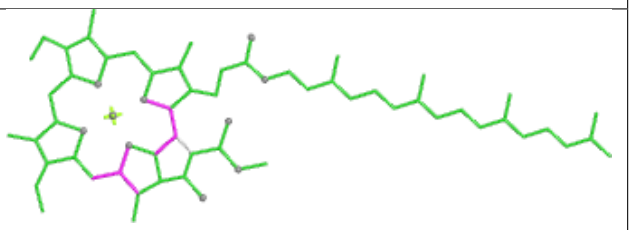
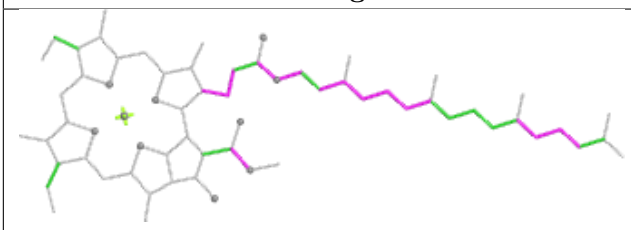
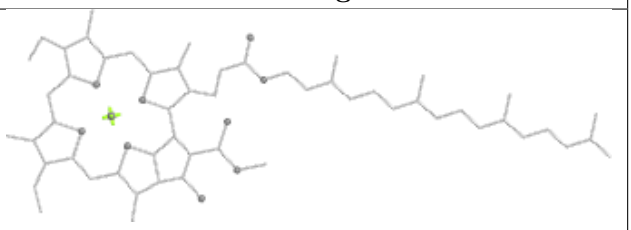
Torsions



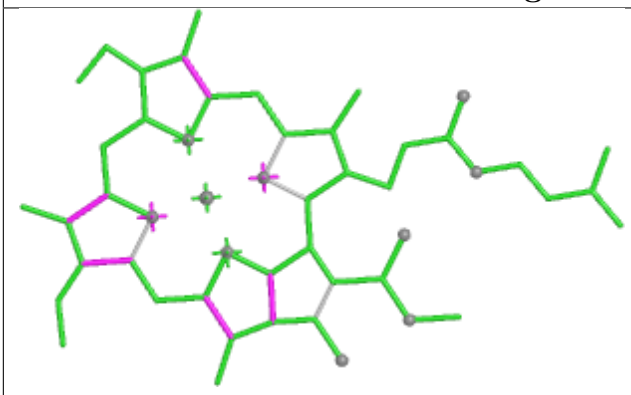
Rings

Ligand CLA 1 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

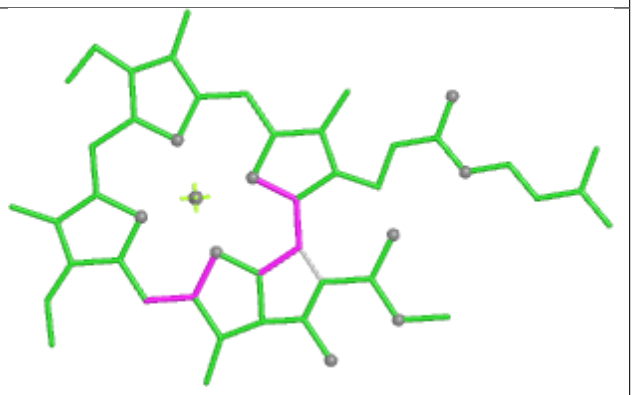
Ligand LUT 2 314	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 814	
 Bond lengths	 Bond angles
 Torsions	 Rings

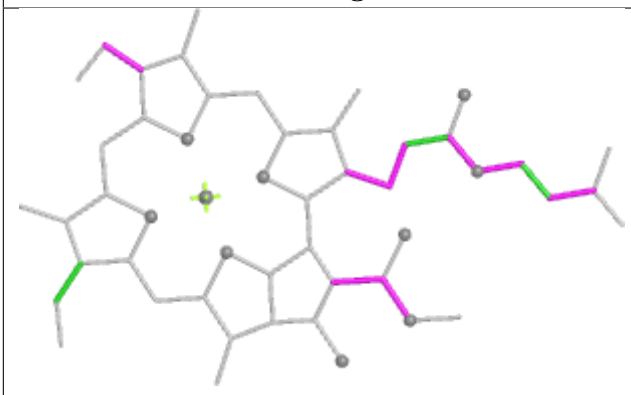
Ligand CLA B 820



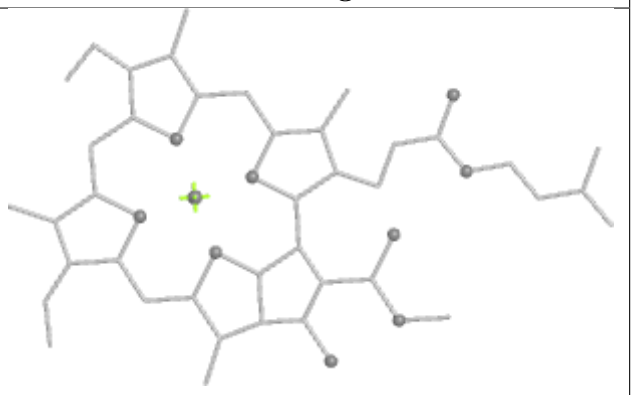
Bond lengths



Bond angles

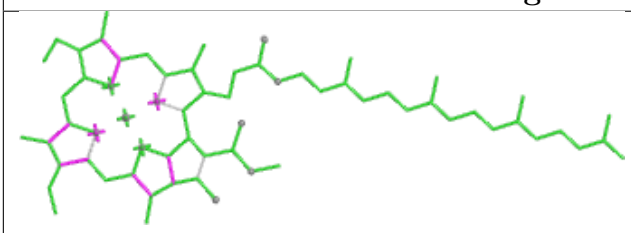


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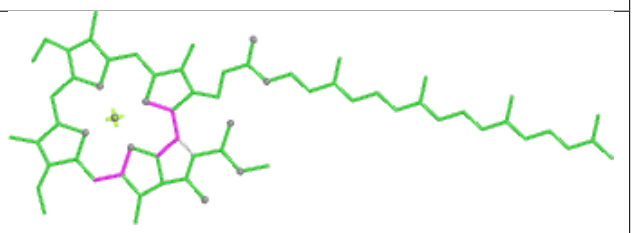


Rings

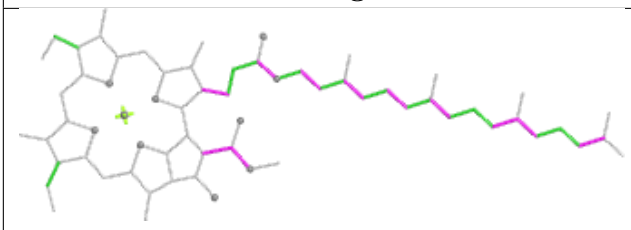
Ligand CLA A 828



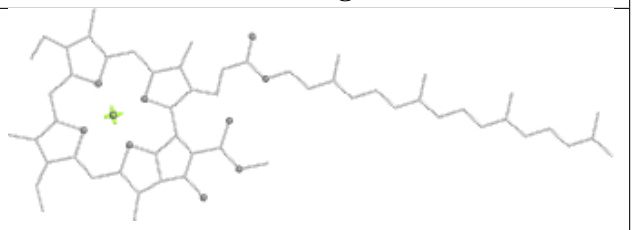
Bond lengths



Bond angles

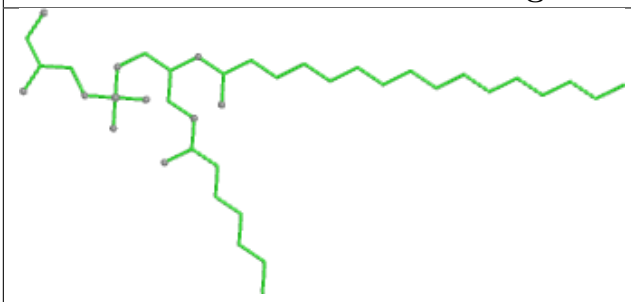


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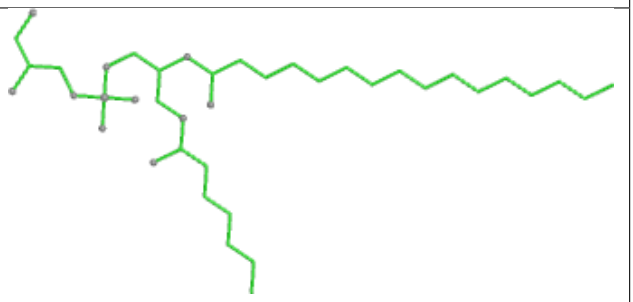


Rings

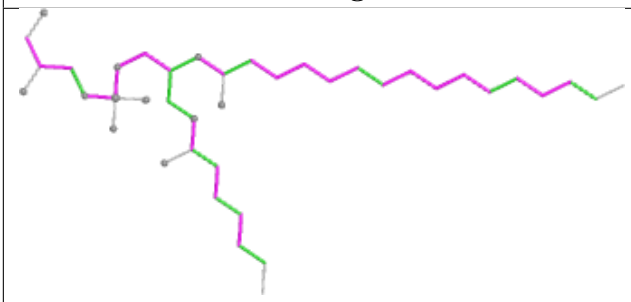
Ligand LHG 4 322



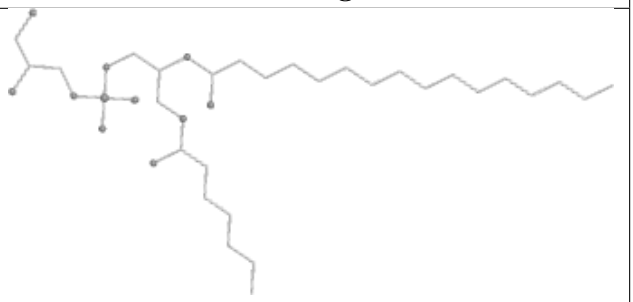
Bond lengths



Bond angles

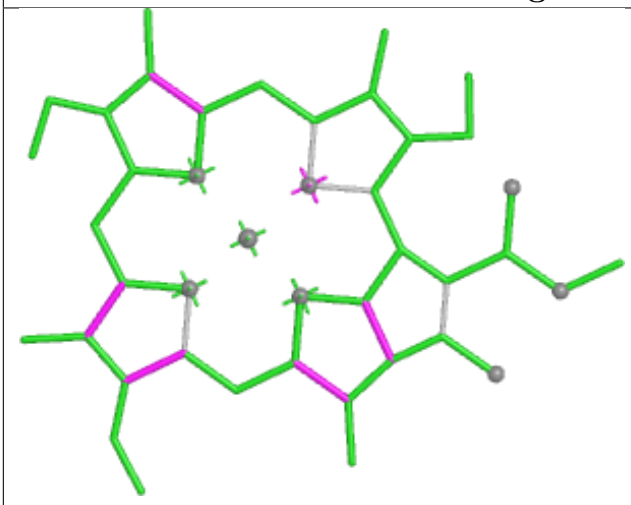


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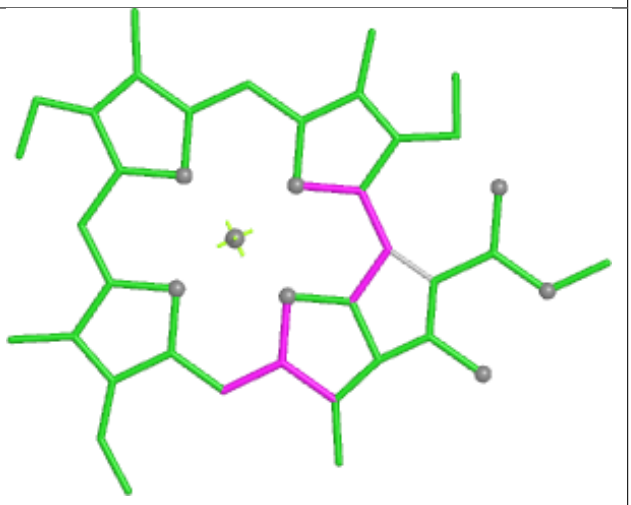


Rings

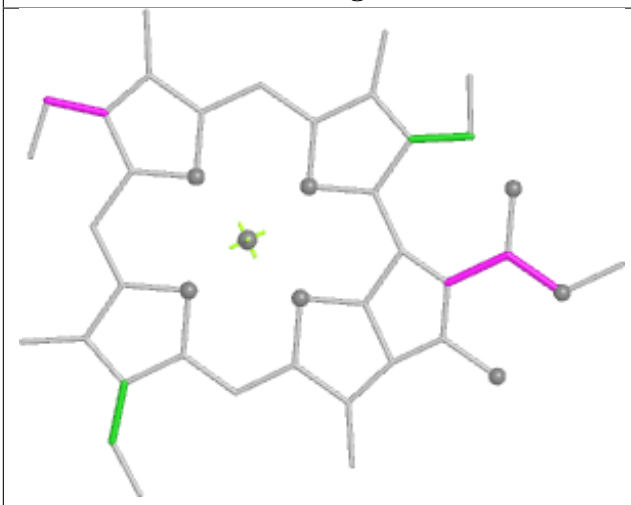
Ligand CLA 3 304



Bond lengths



Bond angles

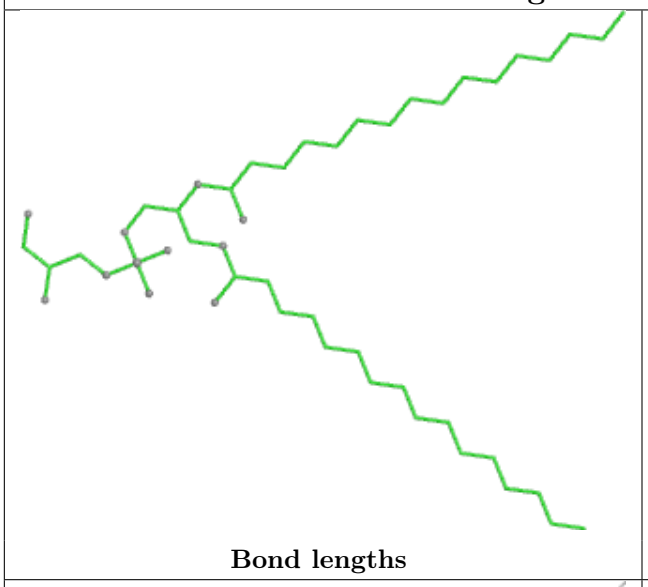


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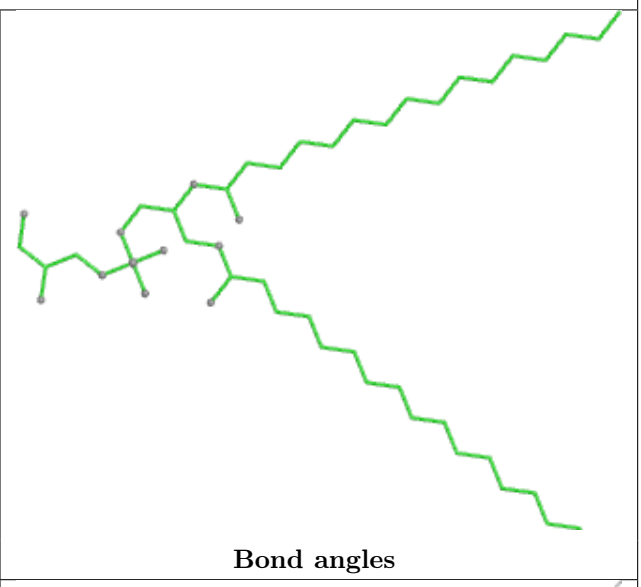


Rings

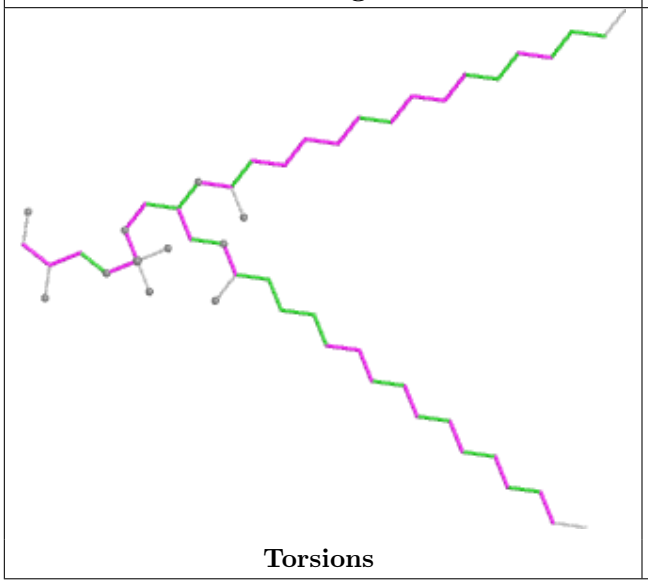
Ligand LHG 2 318



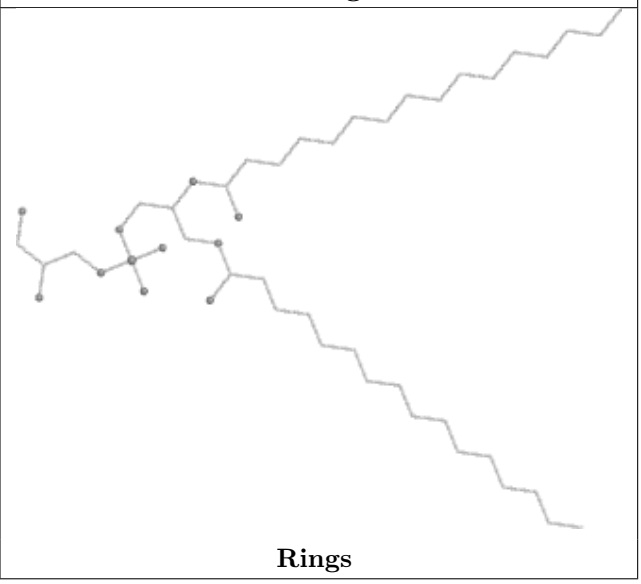
Bond lengths



Bond angles

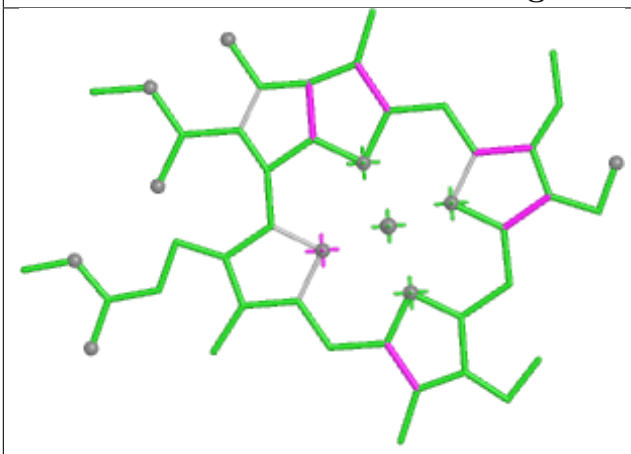


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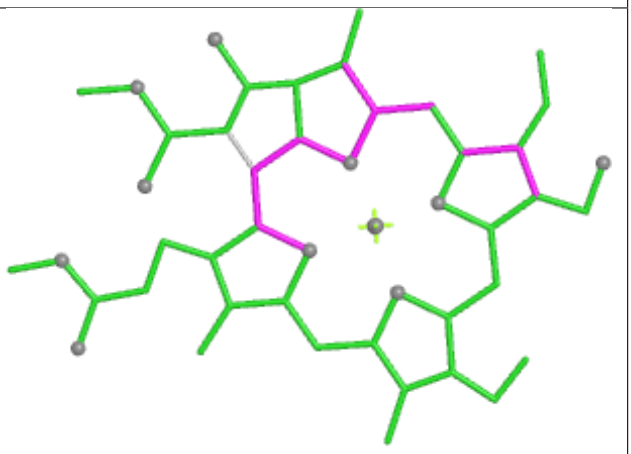


Rings

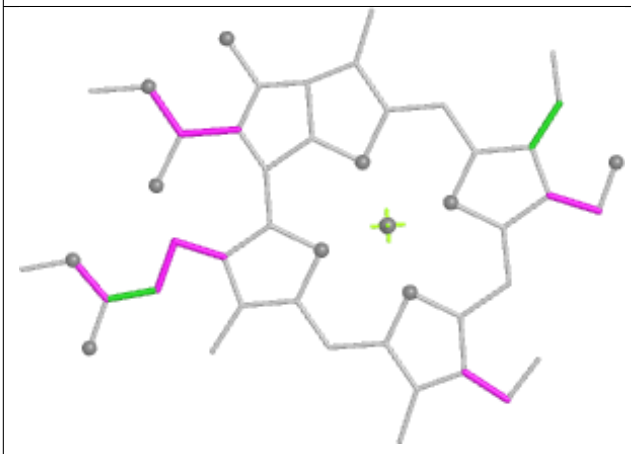
Ligand CHL 3 306



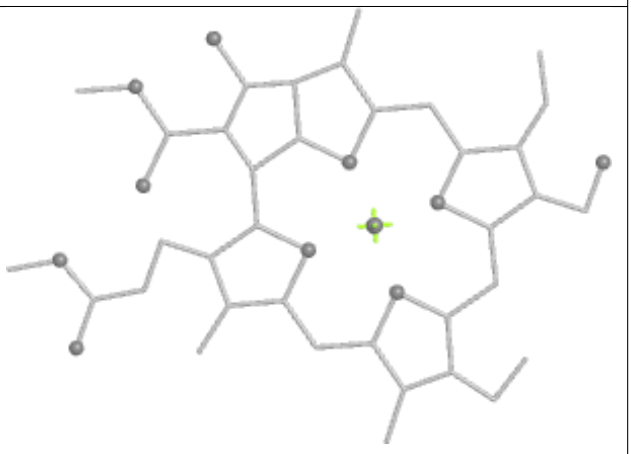
Bond lengths



Bond angles

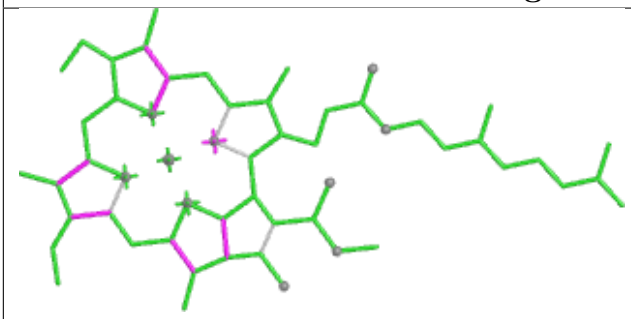


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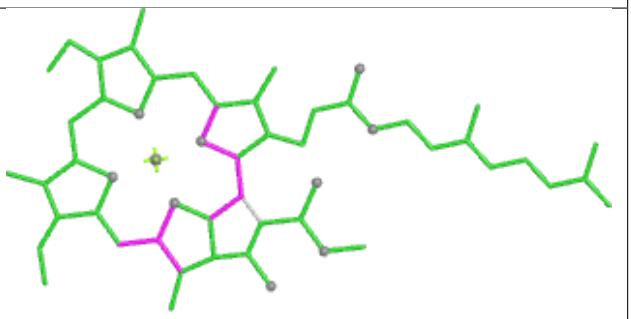


Rings

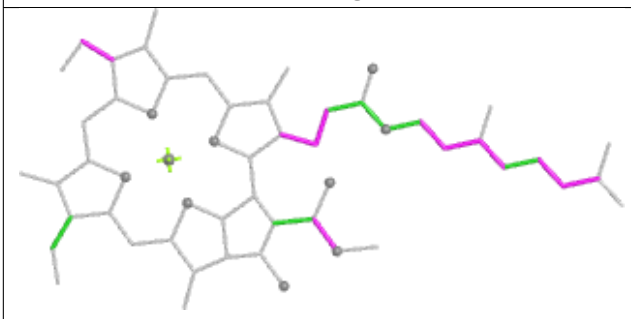
Ligand CLA B 816



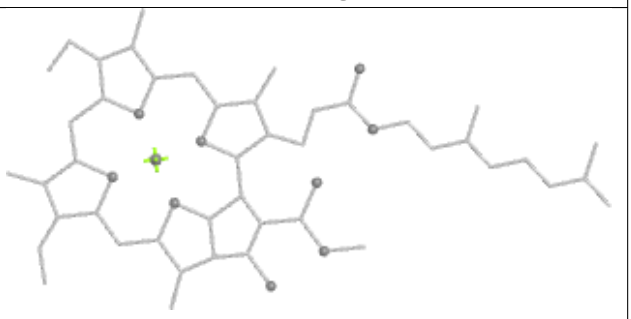
Bond lengths



Bond angles

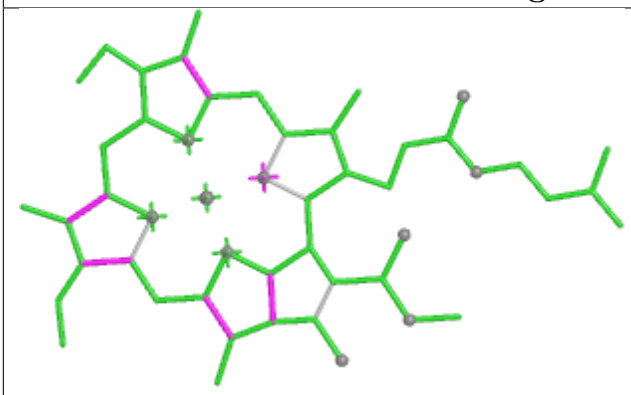


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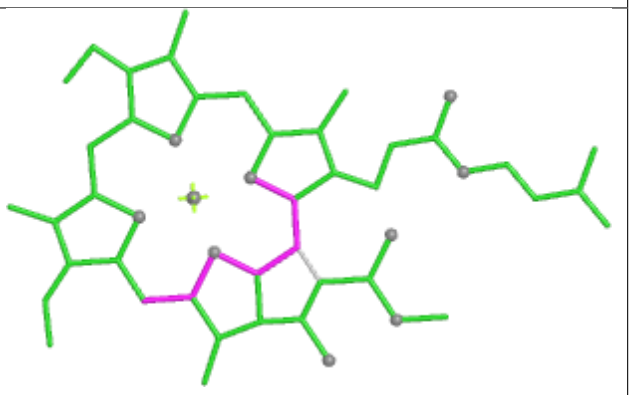


Rings

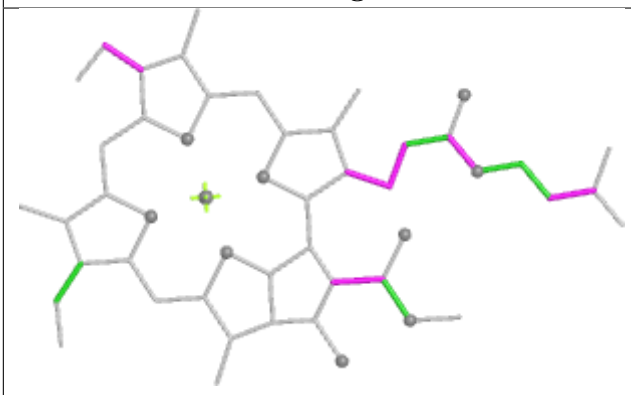
Ligand CLA 4 308



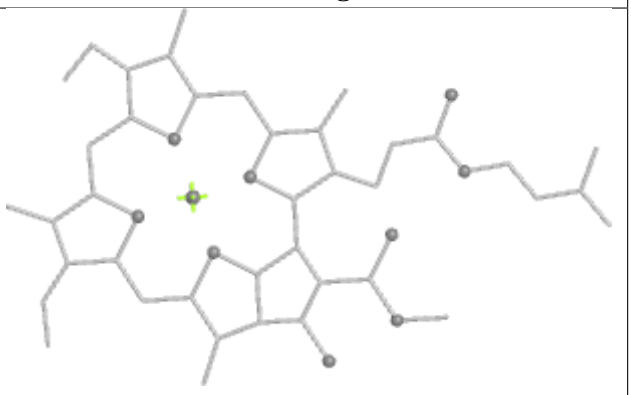
Bond lengths



Bond angles

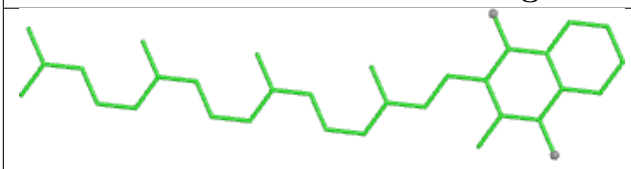


Torsions

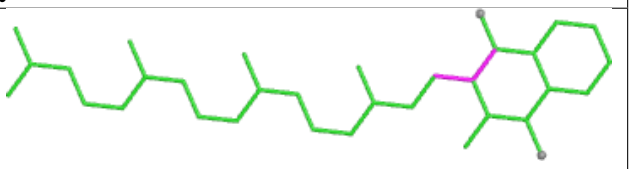


Rings

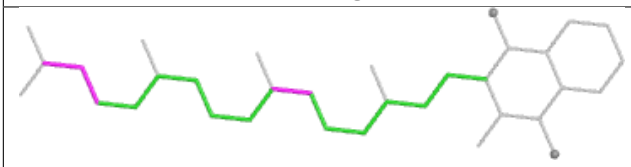
Ligand PQN A 841



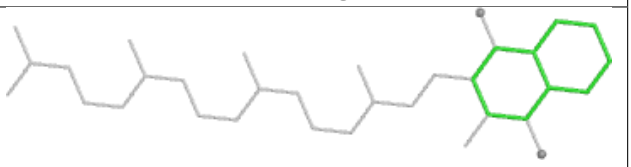
Bond lengths



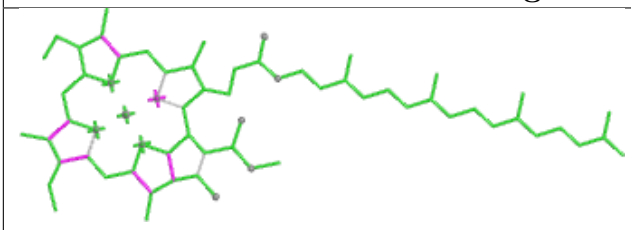
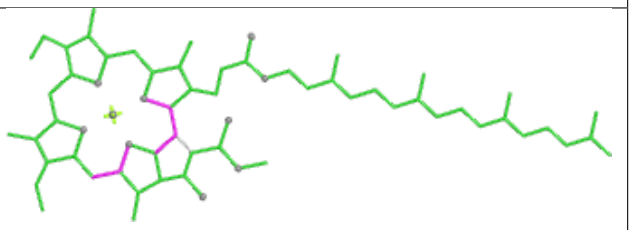
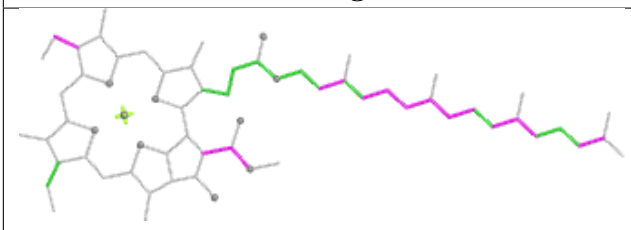
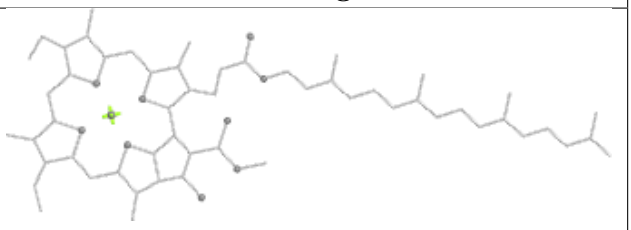
Bond angles

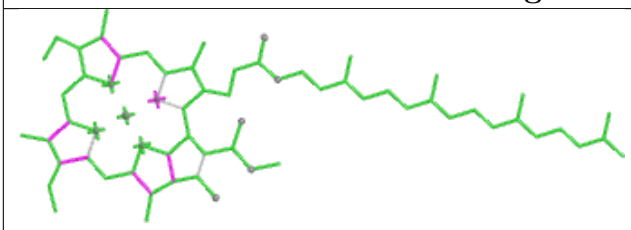
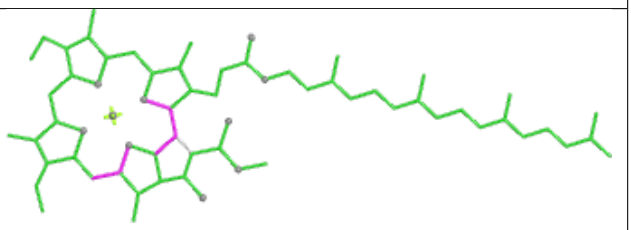
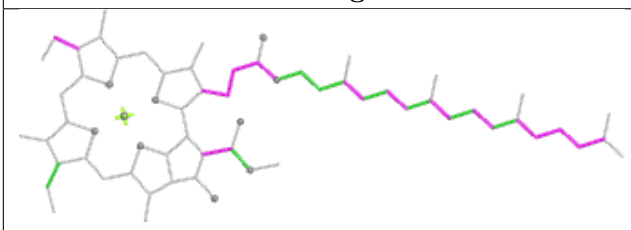
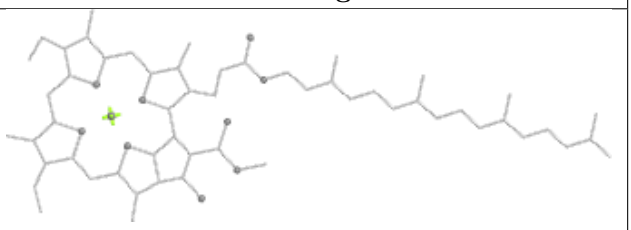


Torsions

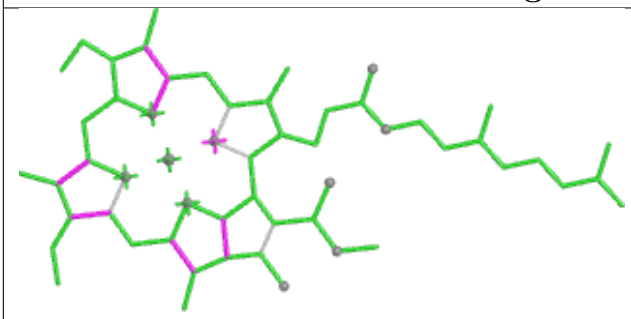


Rings

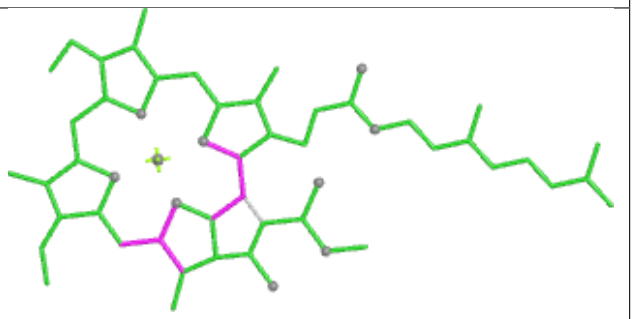
Ligand CLA A 837	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 828	
 Bond lengths	 Bond angles
 Torsions	 Rings

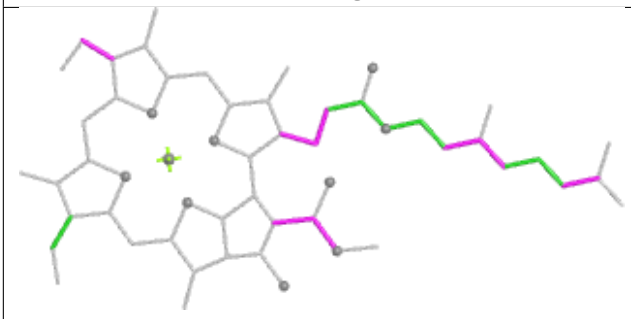
Ligand CLA B 822



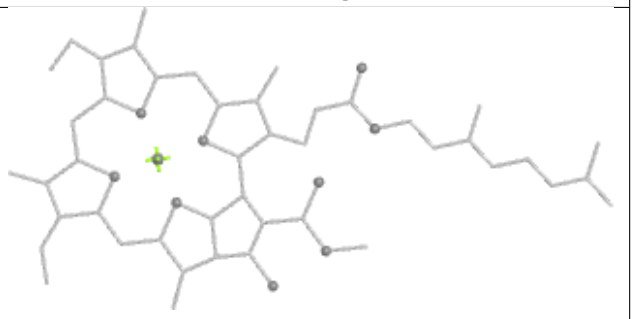
Bond lengths



Bond angles

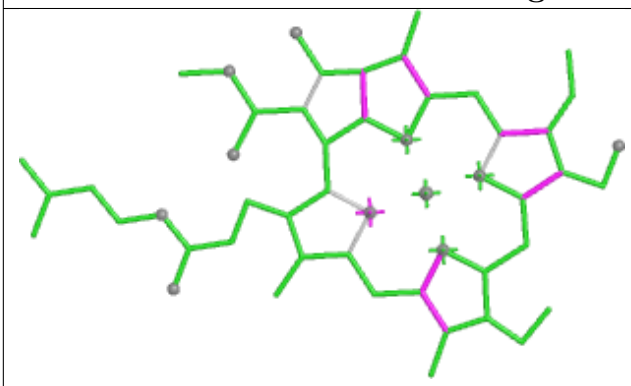


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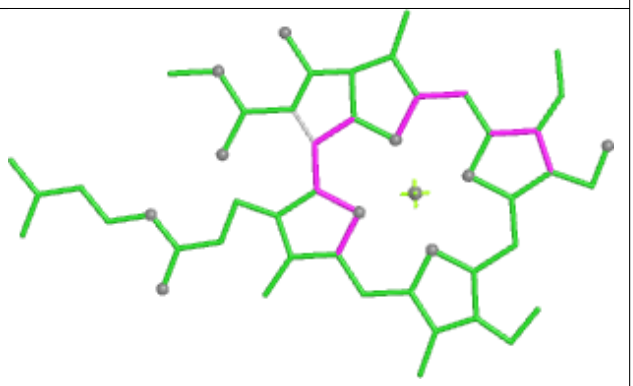


Rings

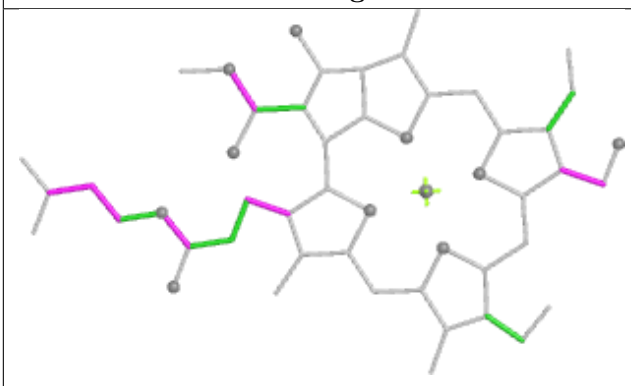
Ligand CHL 2 306



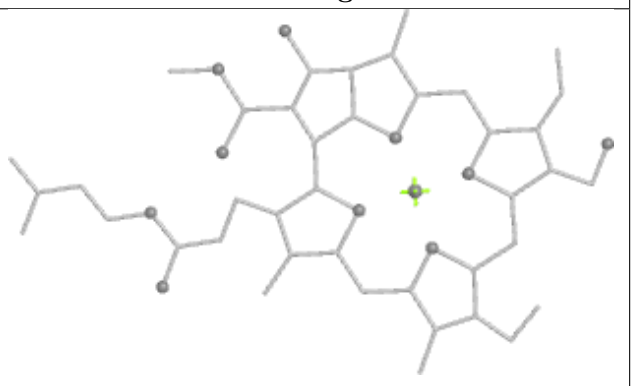
Bond lengths



Bond angles

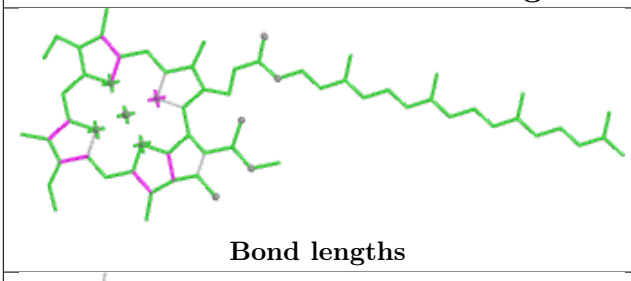


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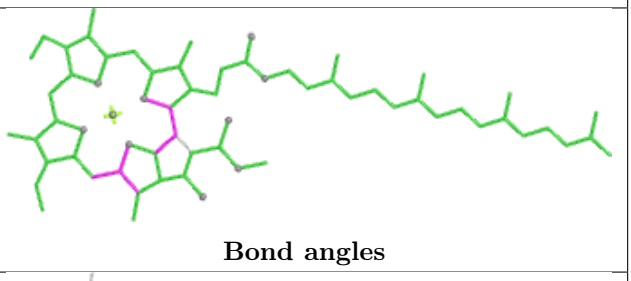


Rings

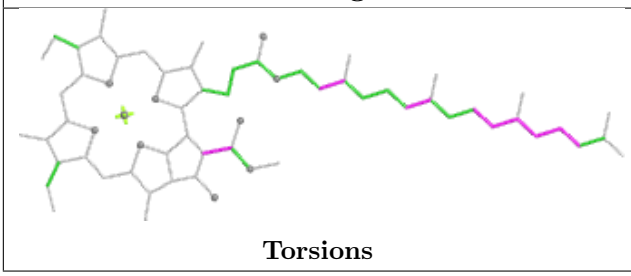
Ligand CLA A 803



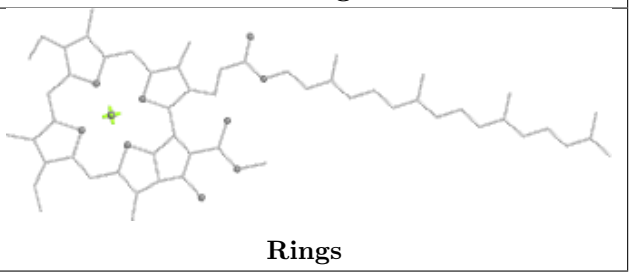
Bond lengths



Bond angles

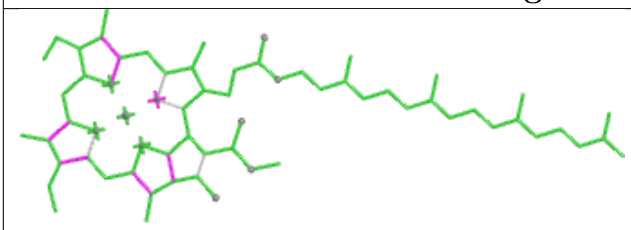


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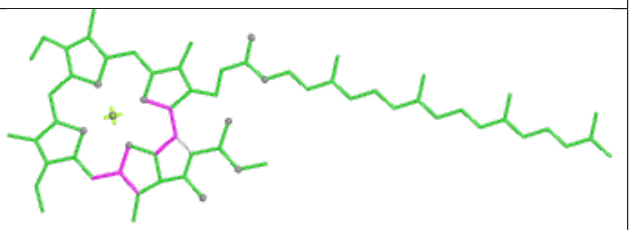


Rings

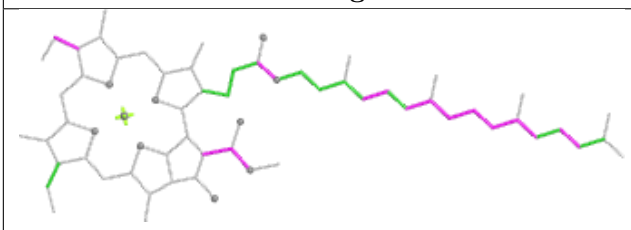
Ligand CLA B 819



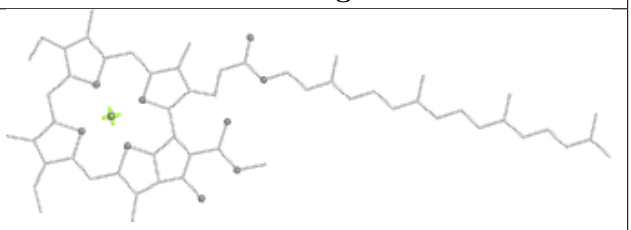
Bond lengths



Bond angles

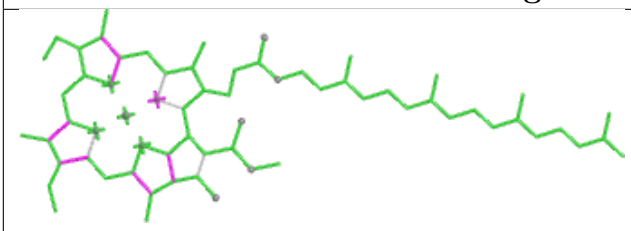


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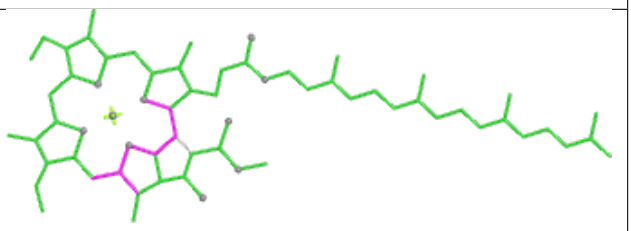


Rings

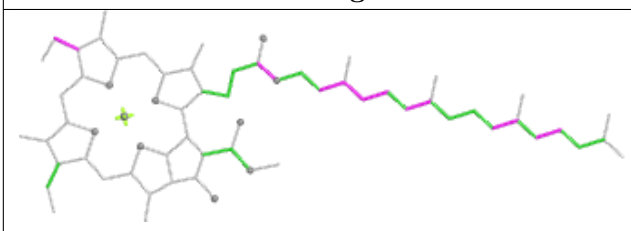
Ligand CLA A 835



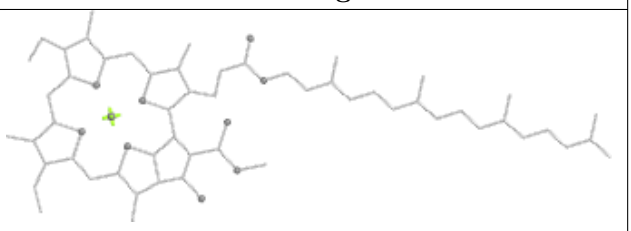
Bond lengths



Bond angles

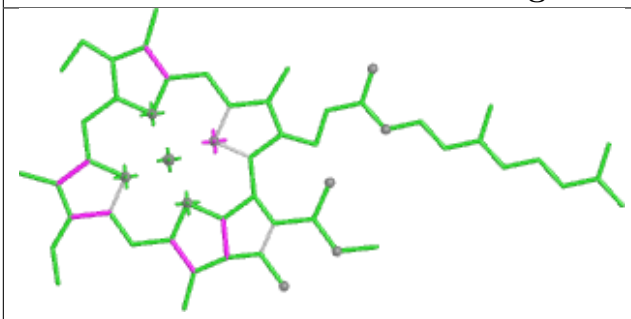


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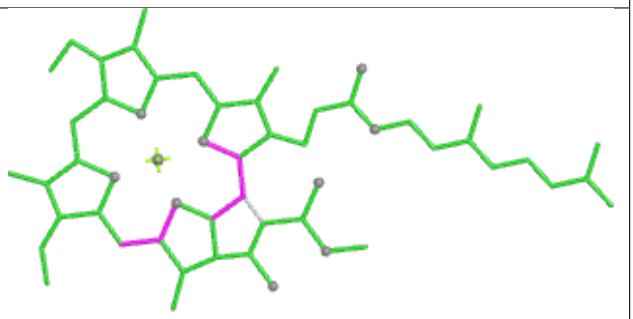


Rings

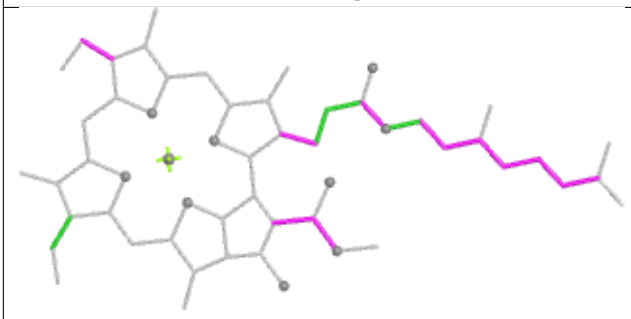
Ligand CLA 1 312



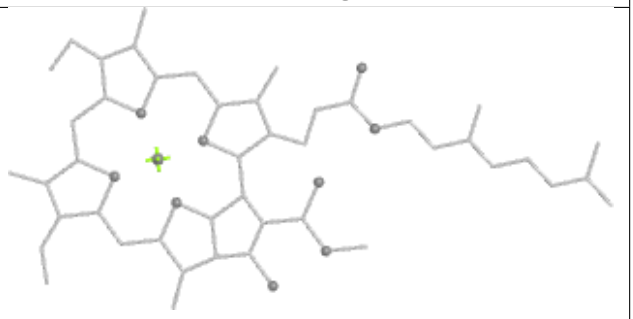
Bond lengths



Bond angles

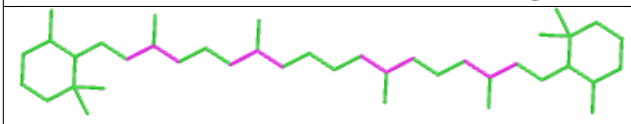


Torsions



Rings

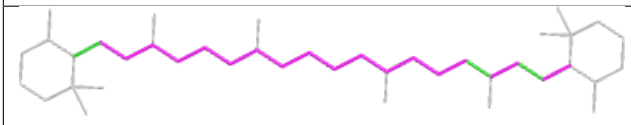
Ligand BCR 2 316



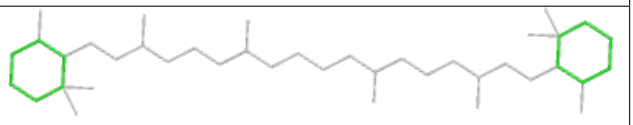
Bond lengths



Bond angles

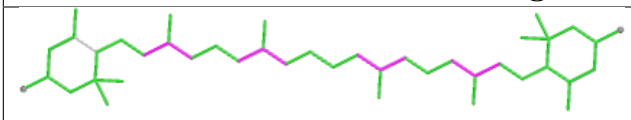


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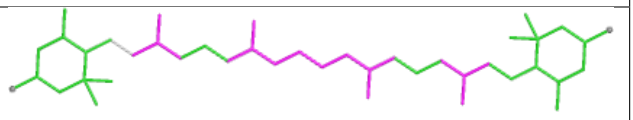


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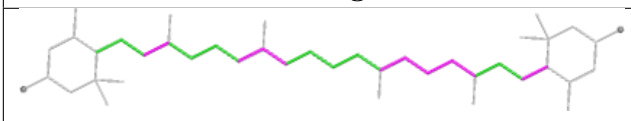
Ligand LUT 1 314



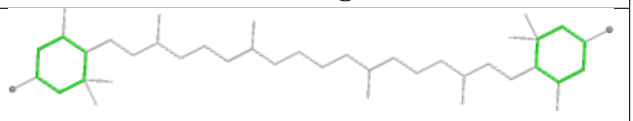
Bond lengths



Bond angles

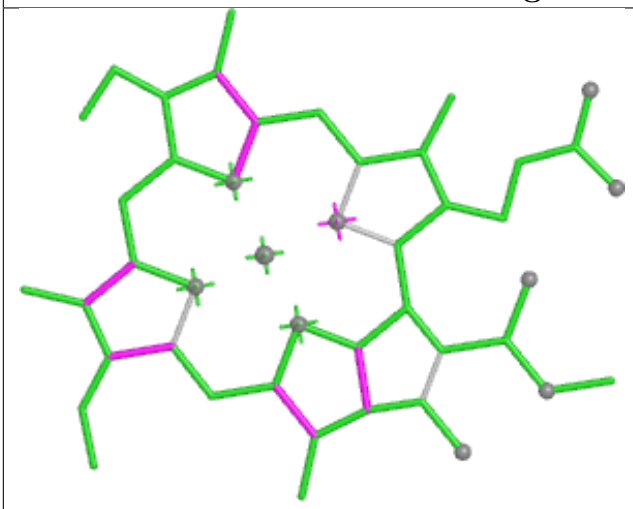


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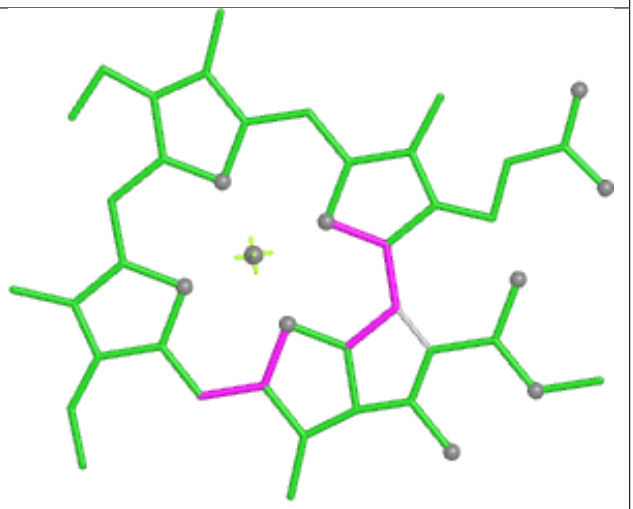


Rings

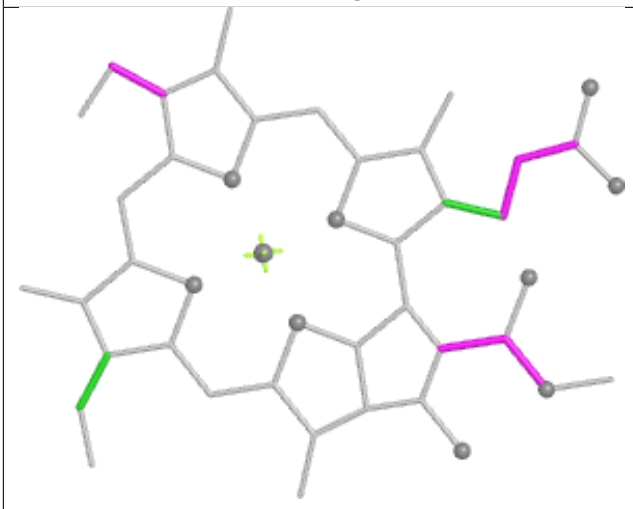
Ligand CLA A 814



Bond lengths



Bond angles

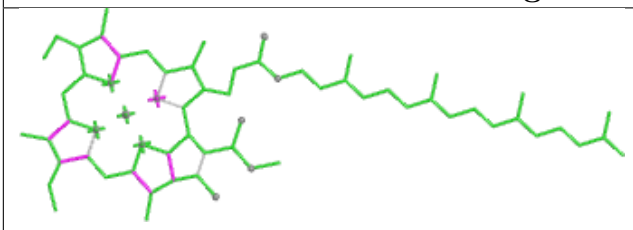


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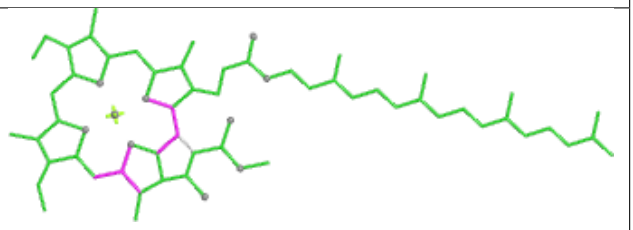


Rings

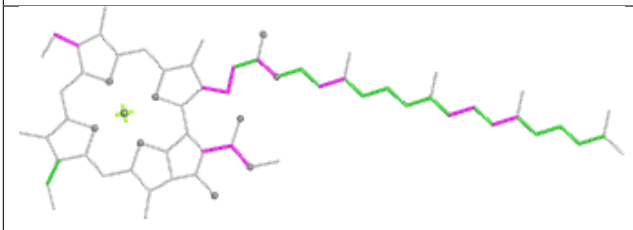
Ligand CLA A 817



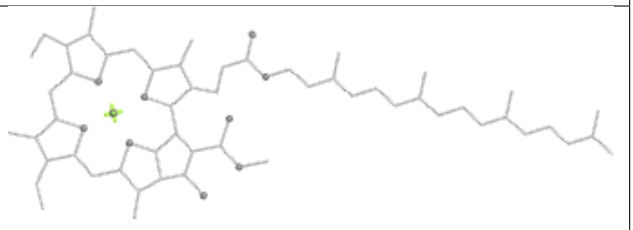
Bond lengths



Bond angles

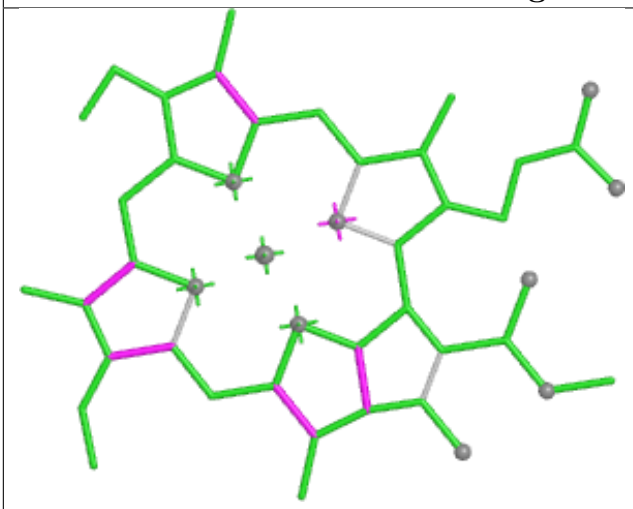


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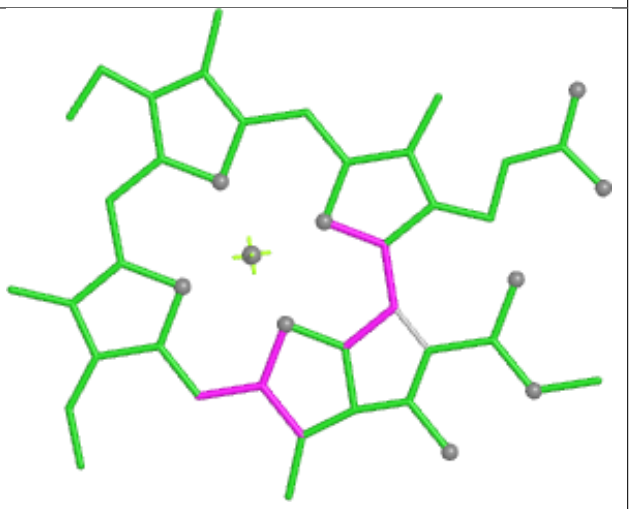


Rings

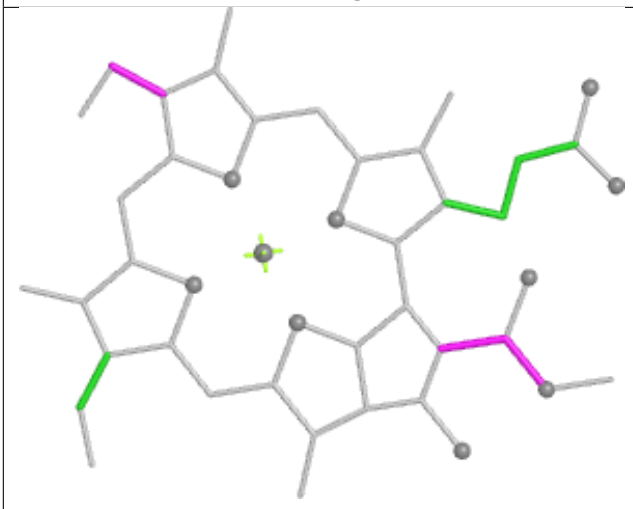
Ligand CLA 3 303



Bond lengths



Bond angles

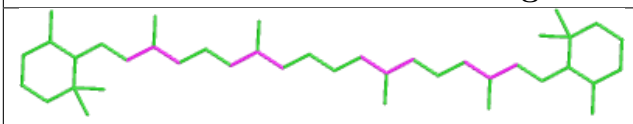


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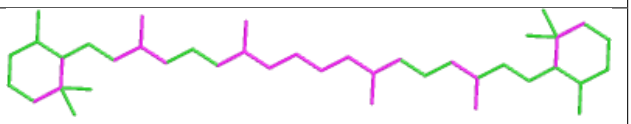


Rings

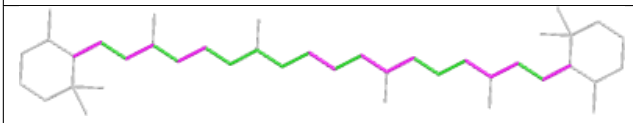
Ligand BCR G 201



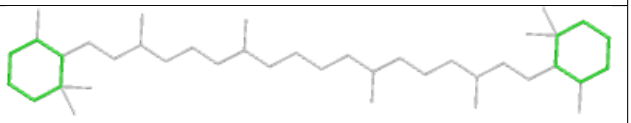
Bond lengths



Bond angles

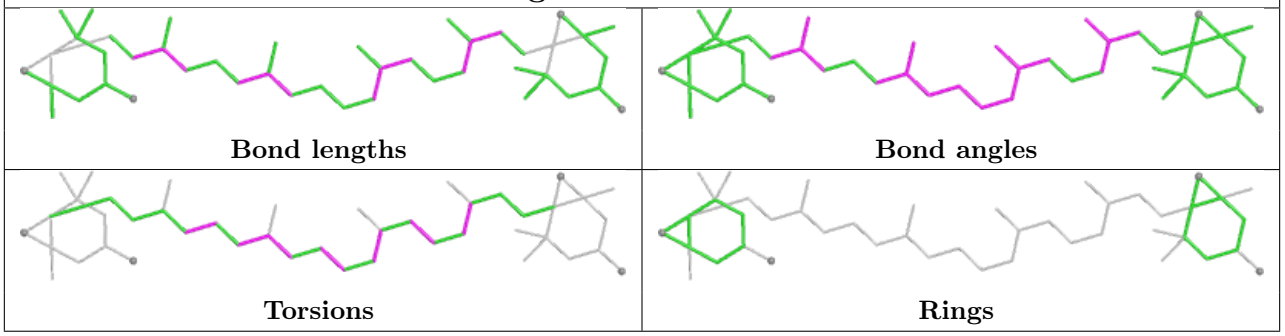


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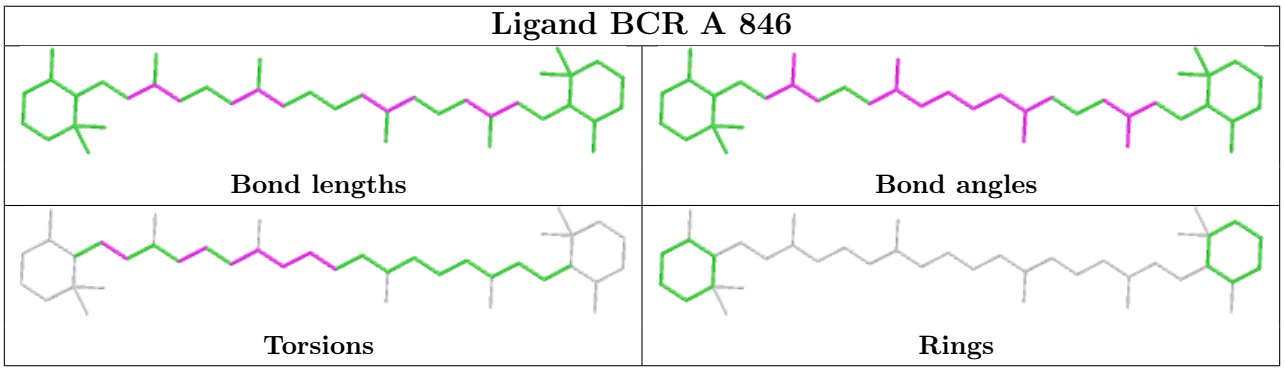


Rings

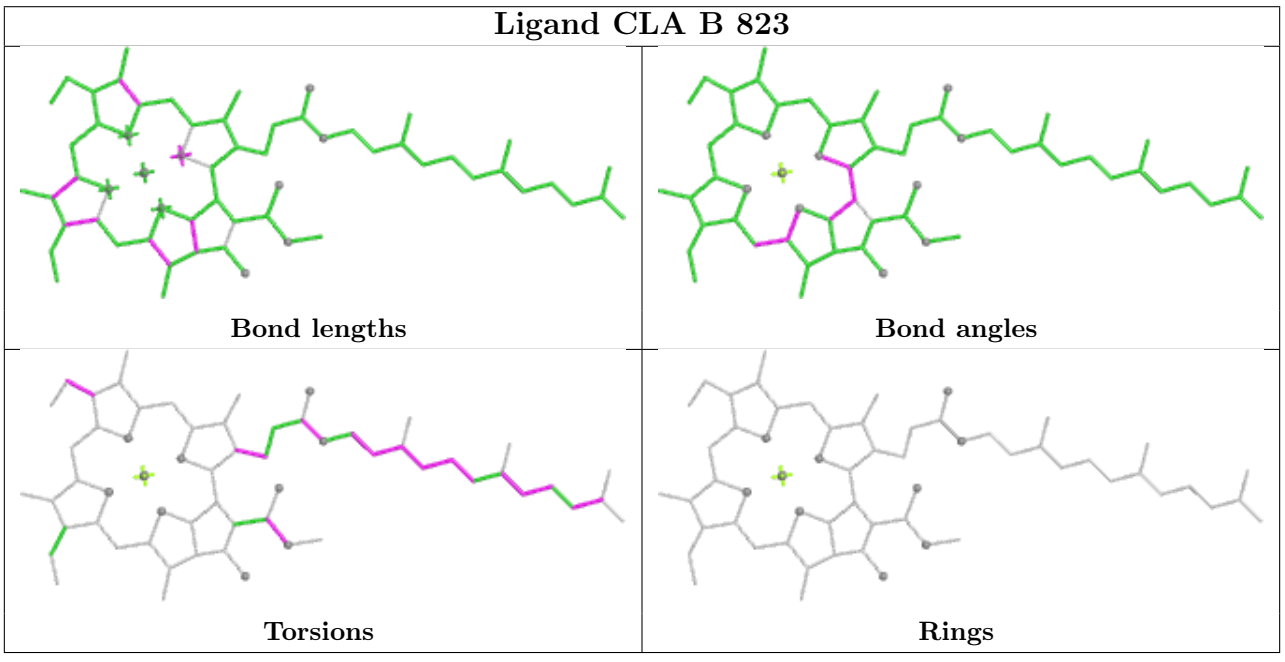
Ligand XAT 2 315



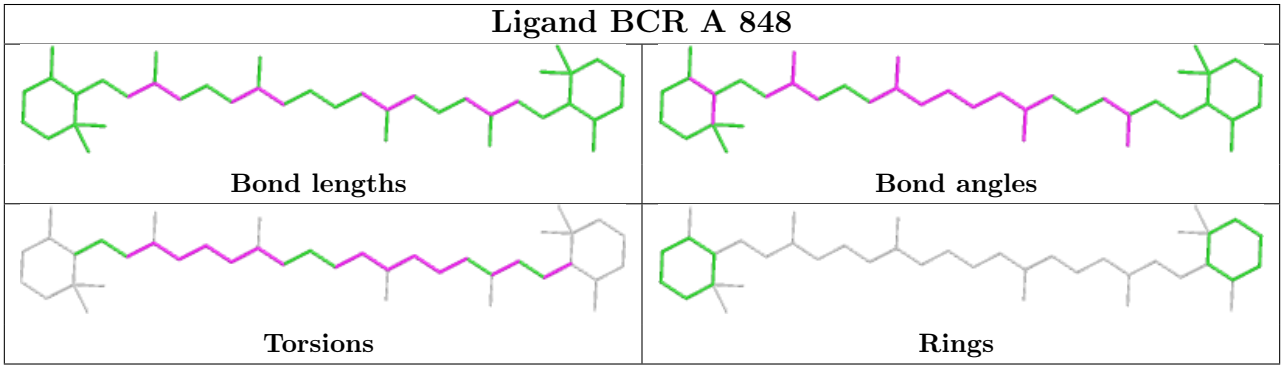
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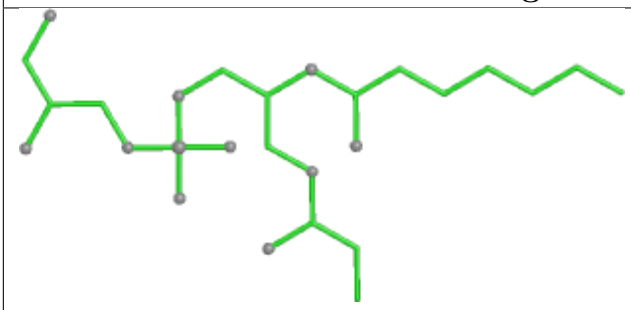
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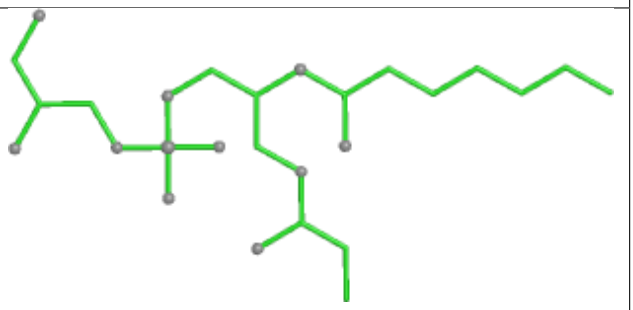
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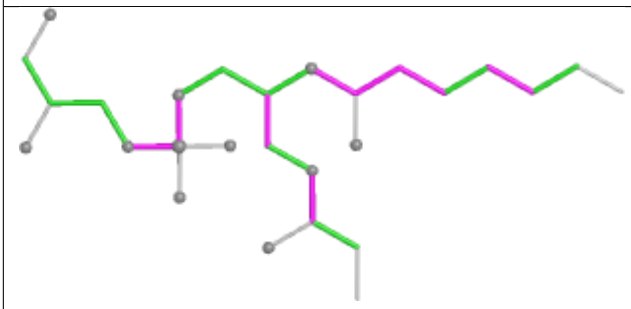
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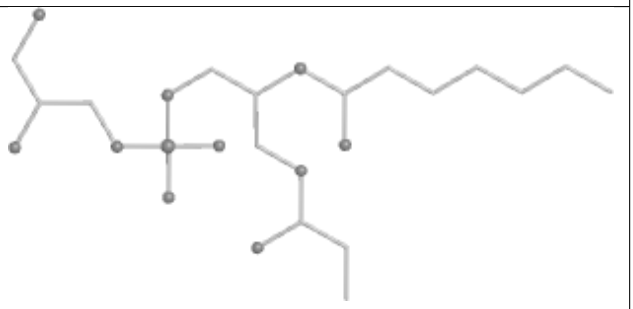
Bond lengths



Bond angles

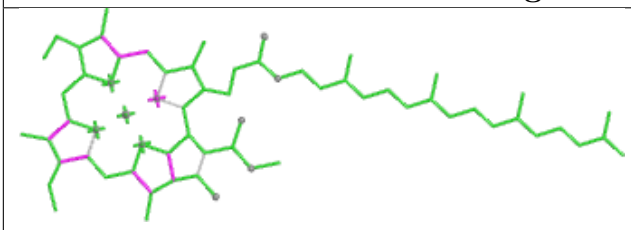


Torsions

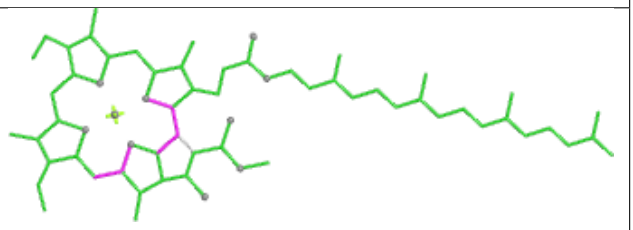


Rings

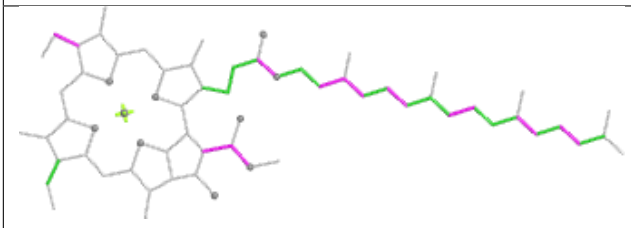
Ligand CLA B 802



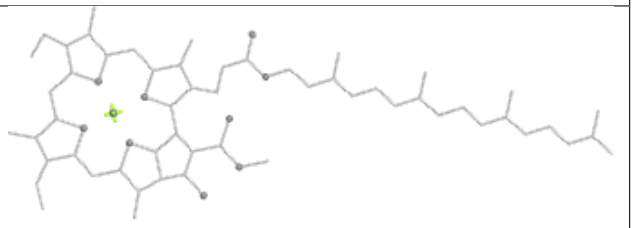
Bond lengths



Bond angles

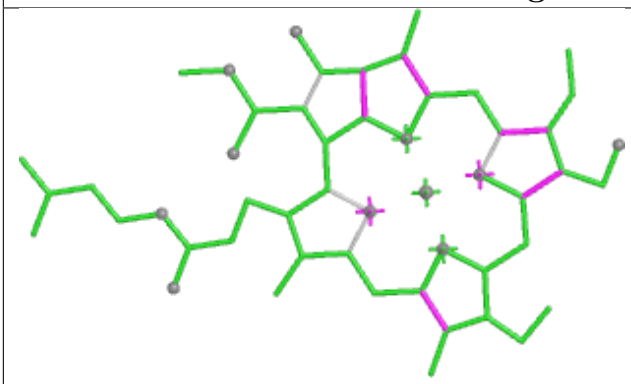


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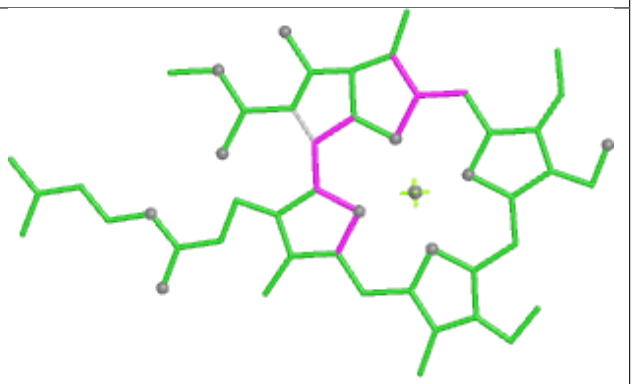


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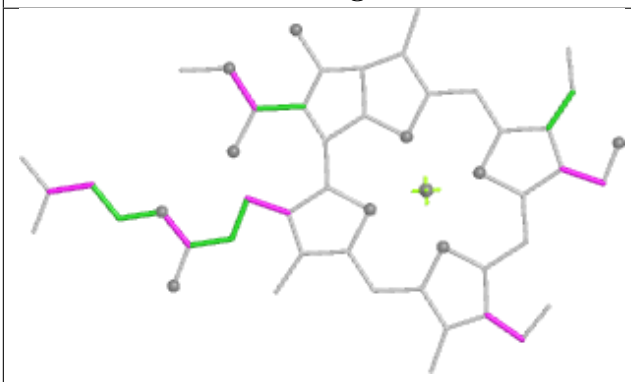
Ligand CHL 4 306



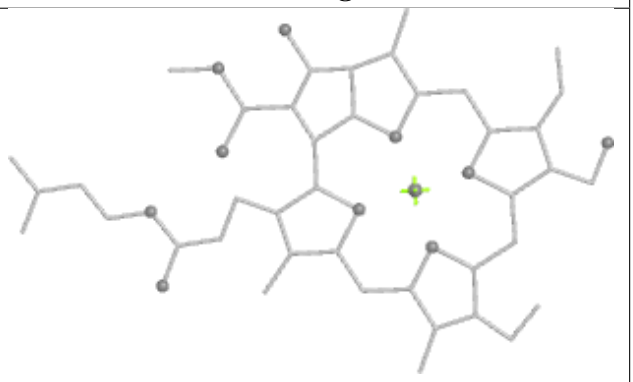
Bond lengths



Bond angles

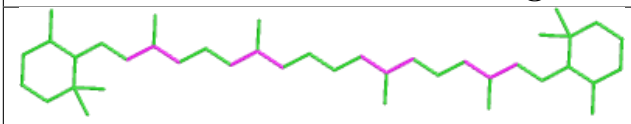


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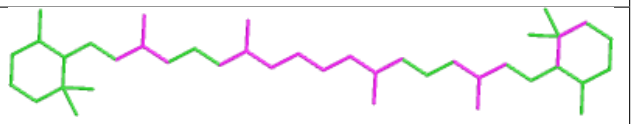


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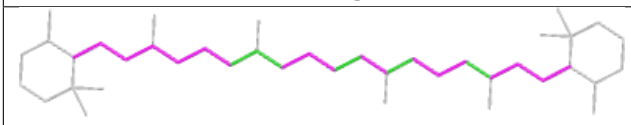
Ligand BCR J 104



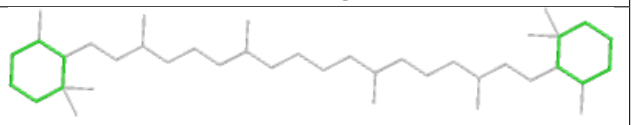
Bond lengths



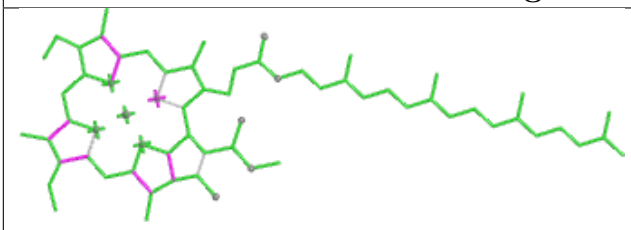
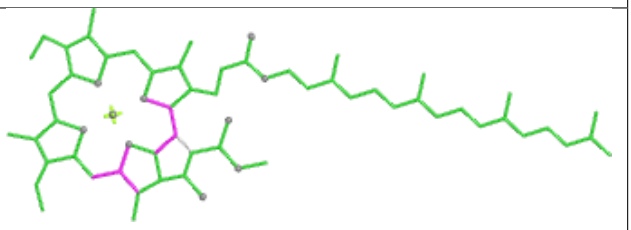
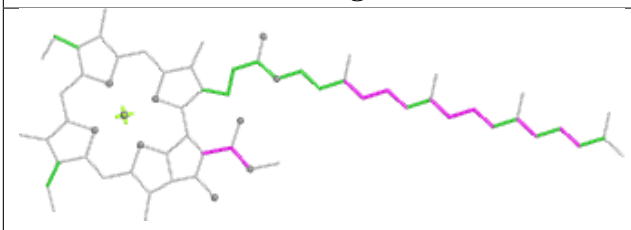
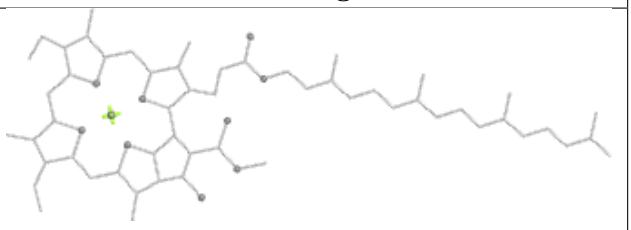
Bond angles

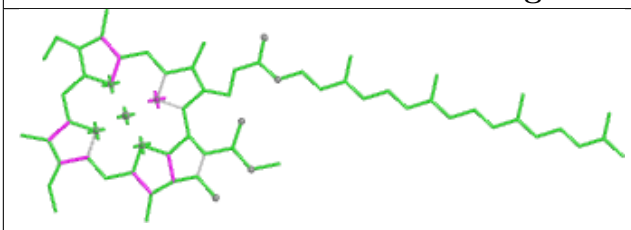
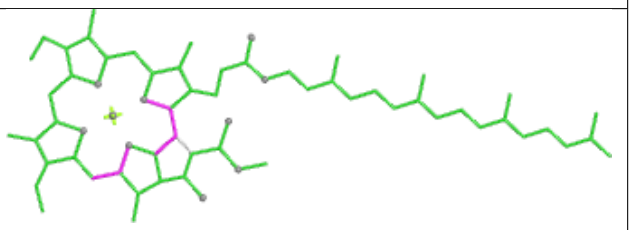
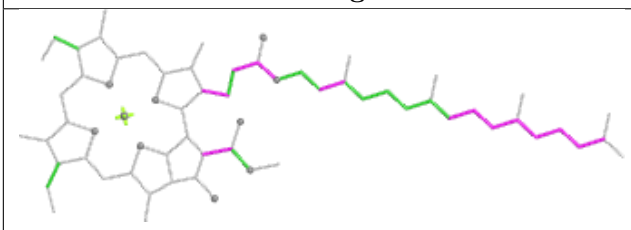
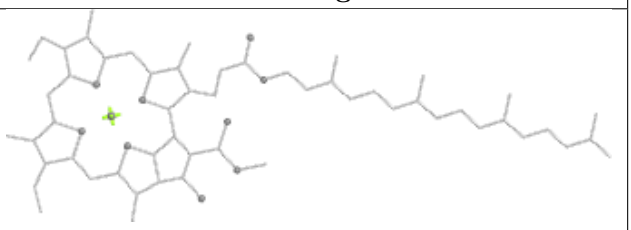


Torsions

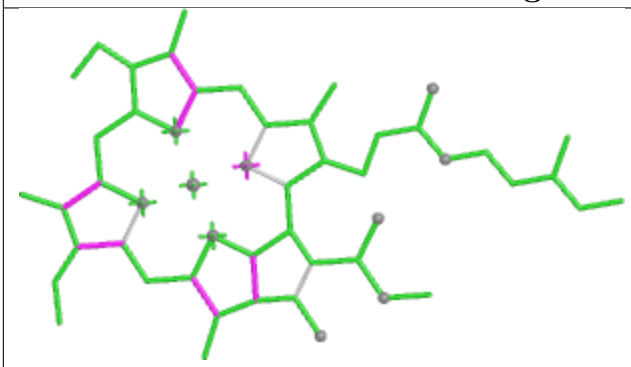


Rings

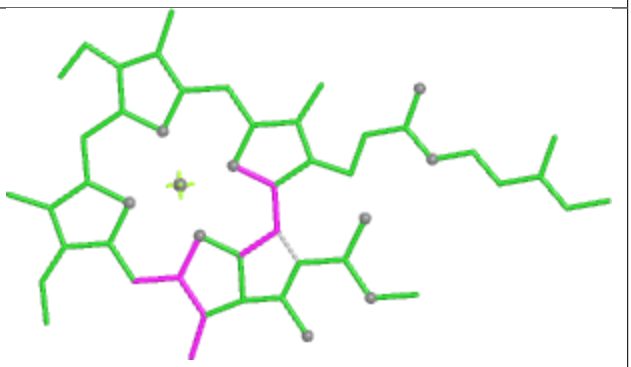
Ligand CLA B 808	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA B 813	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

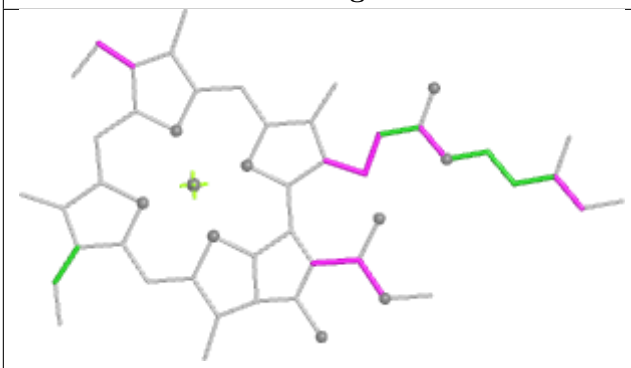
Ligand CLA A 821



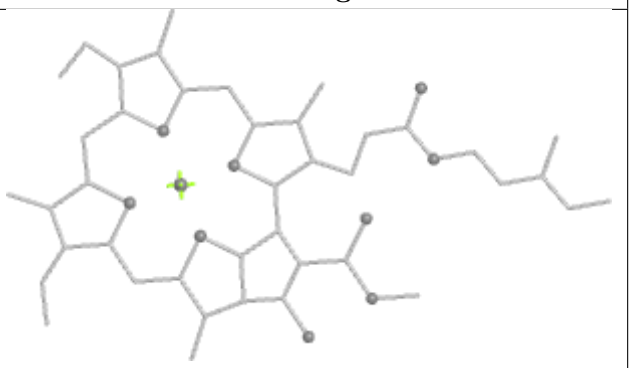
Bond lengths



Bond angles

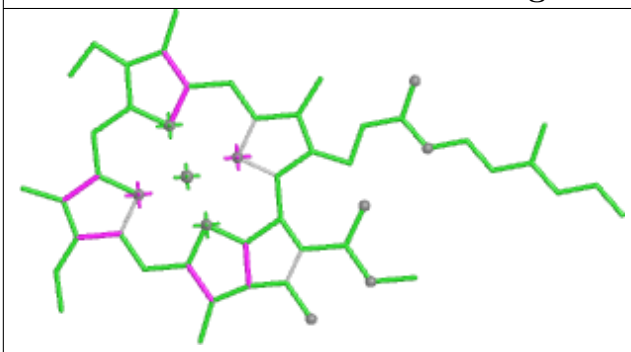


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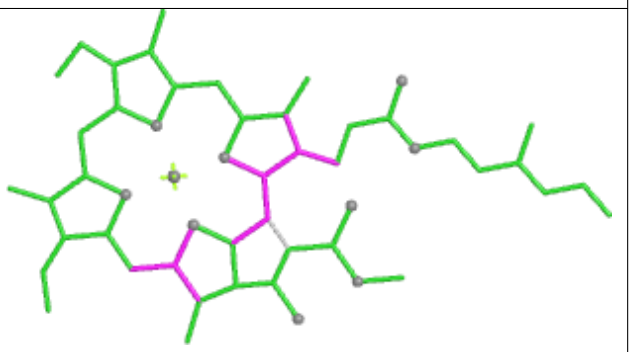


Rings

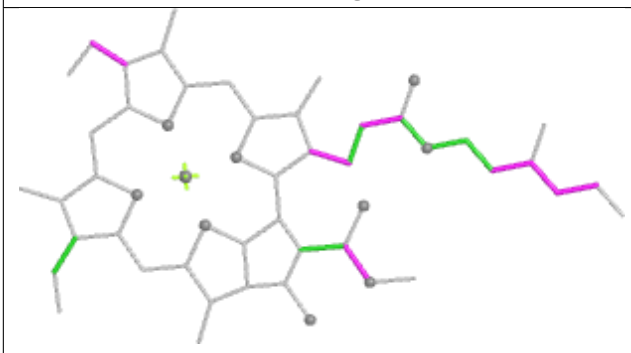
Ligand CLA 2 310



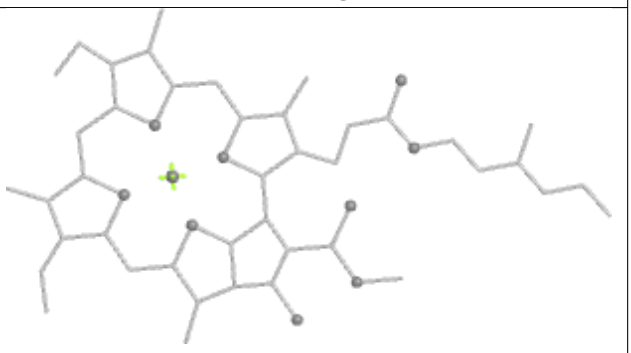
Bond lengths



Bond angles

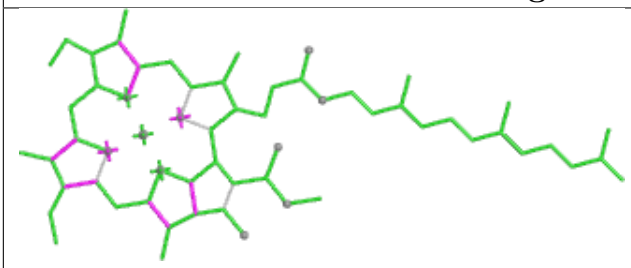


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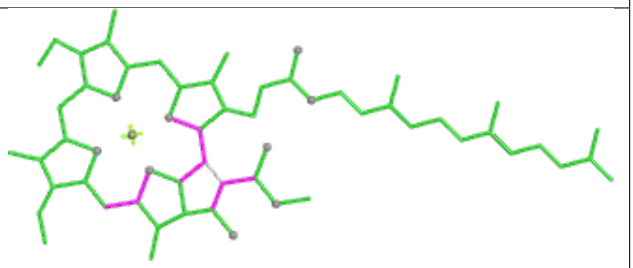


Rings

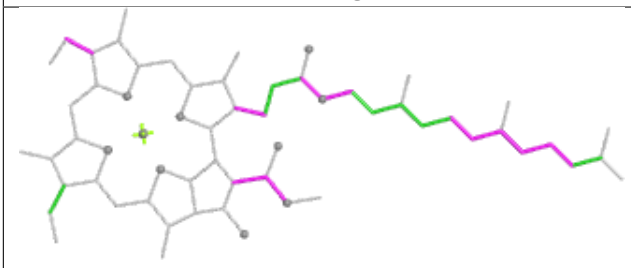
Ligand CLA 4 303



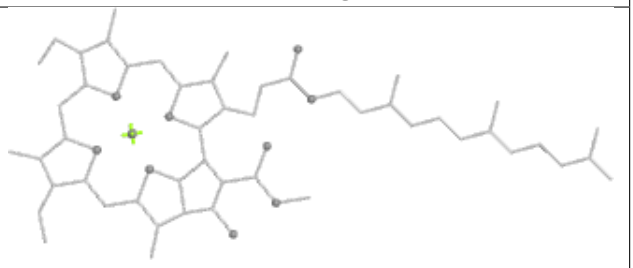
Bond lengths



Bond angles

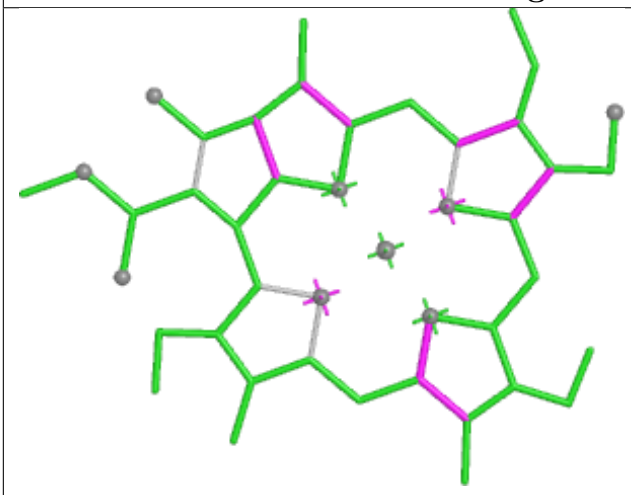


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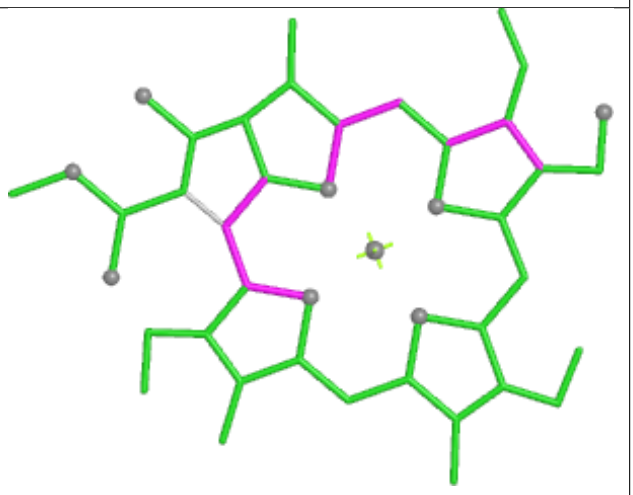


Rings

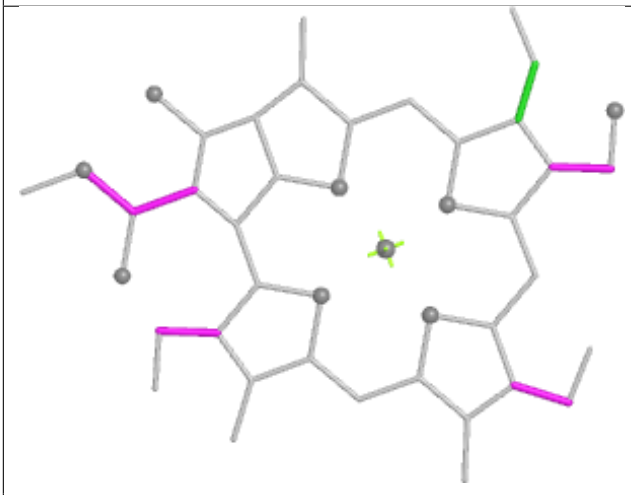
Ligand CHL 4 315



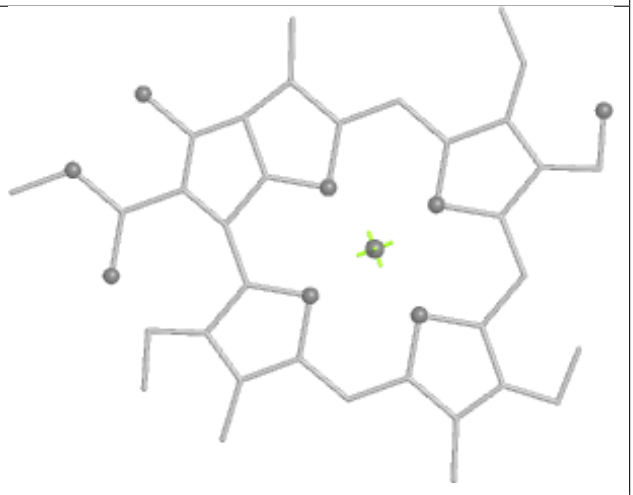
Bond lengths



Bond angles

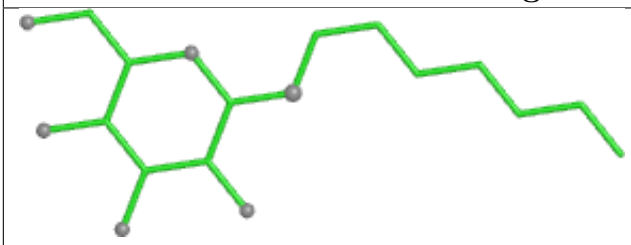


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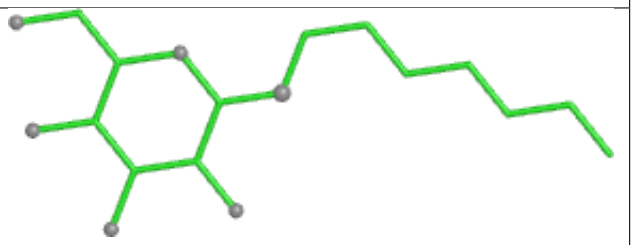


Rings

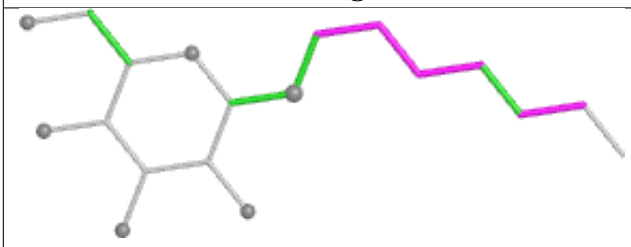
Ligand HTG F 310



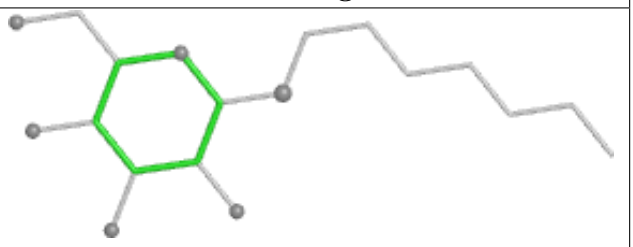
Bond lengths



Bond angles

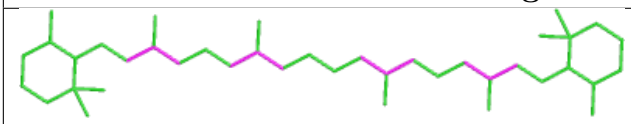


Torsions



Rings

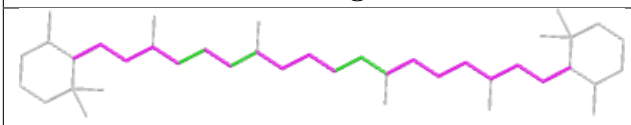
Ligand BCR O 105



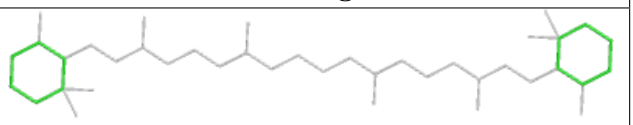
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Bond angles

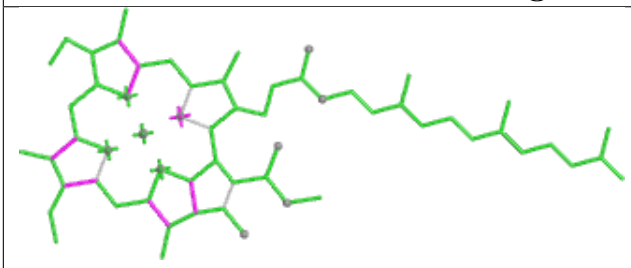


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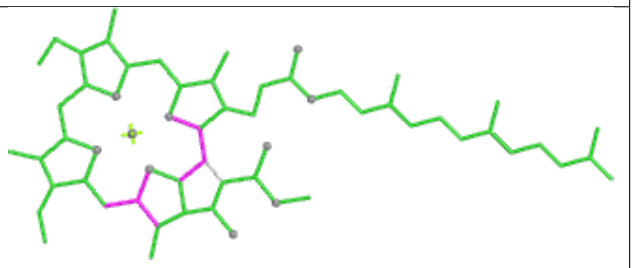


Rings

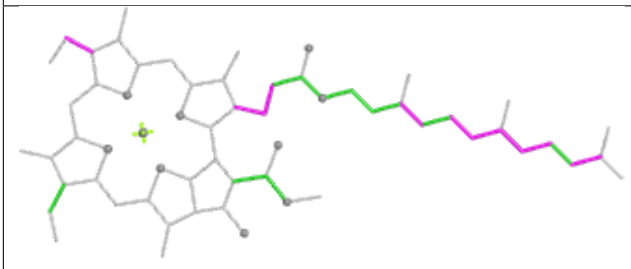
Ligand CLA 1 308



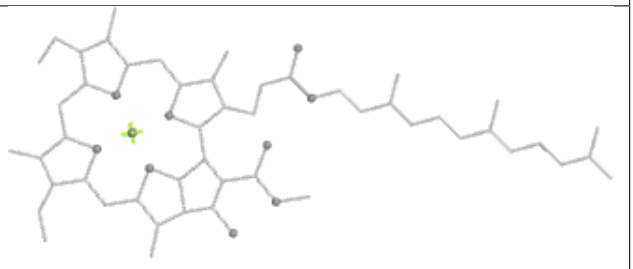
Bond lengths



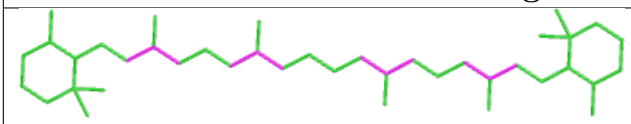
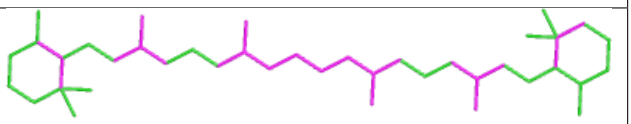
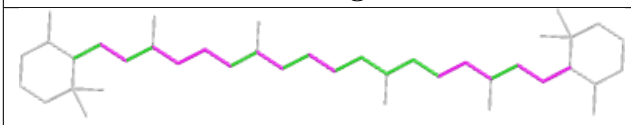
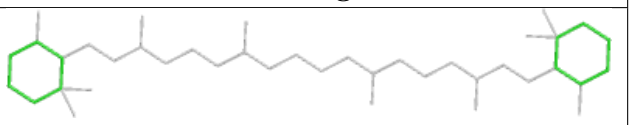
Bond angles

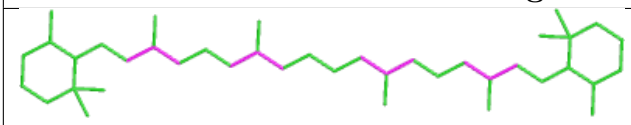
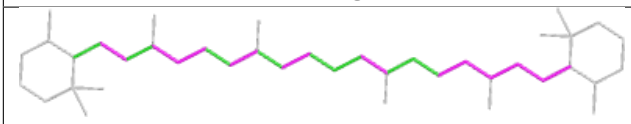
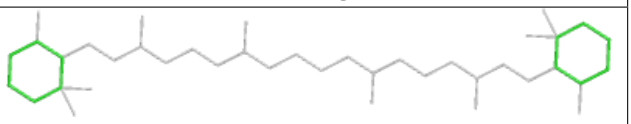


Torsions

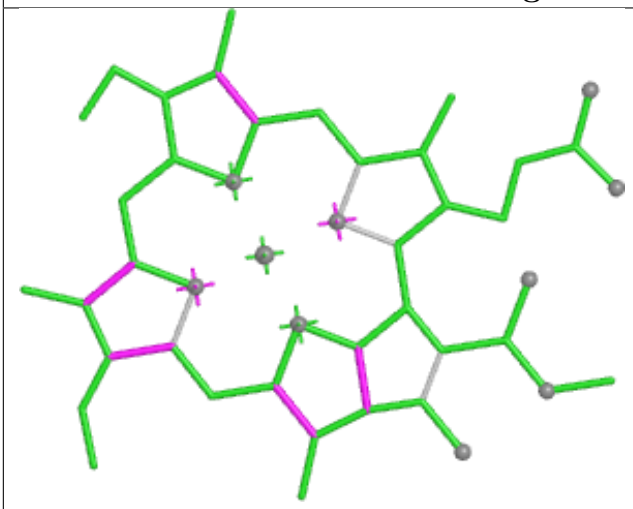


Rings

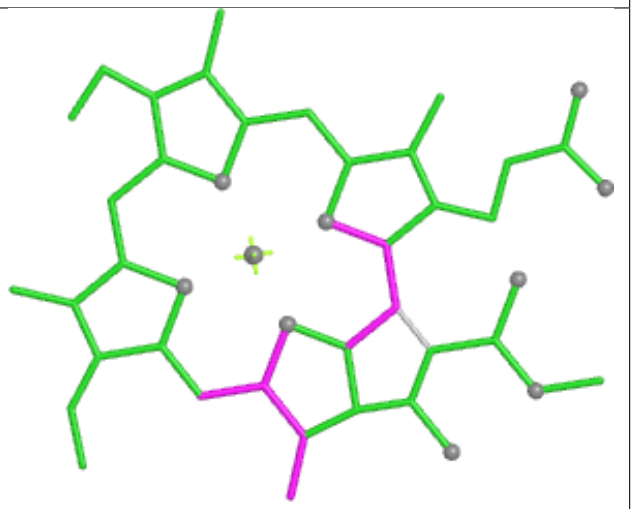
Ligand BCR B 844	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR 3 315	
 Bond lengths	 Bond angles
 Torsions	 Rings

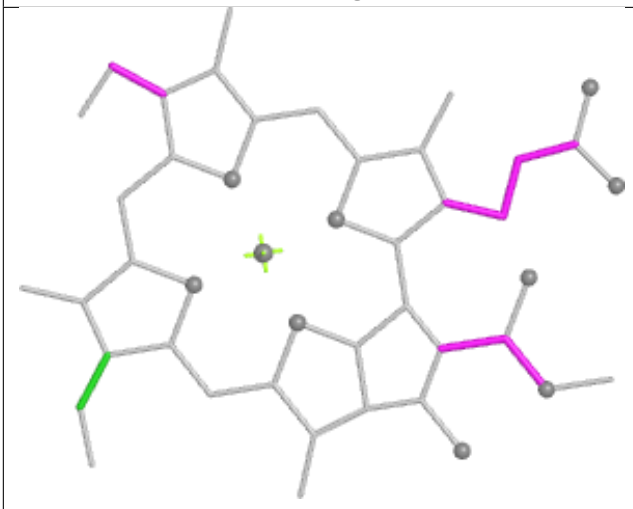
Ligand CLA K 302



Bond lengths



Bond angles

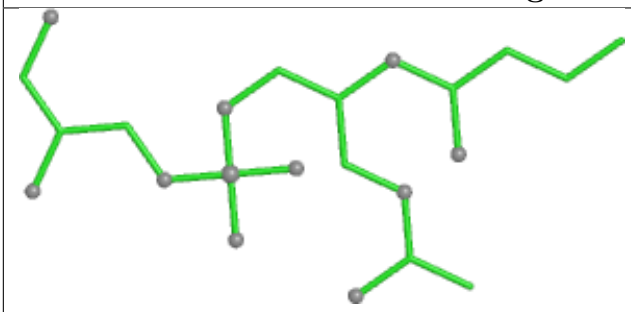


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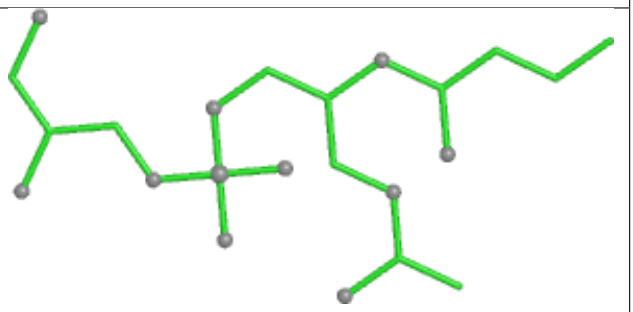


Rings

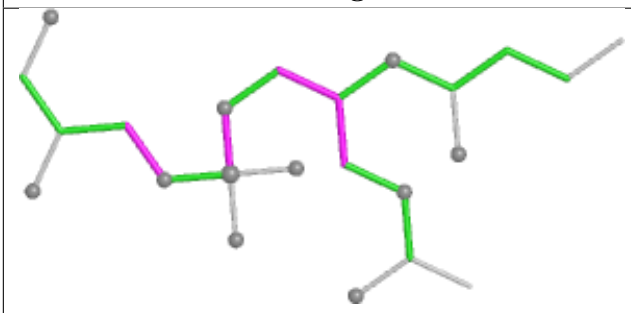
Ligand LHG 1 319



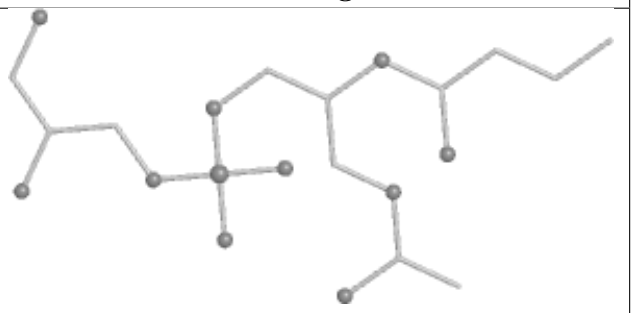
Bond lengths



Bond angles

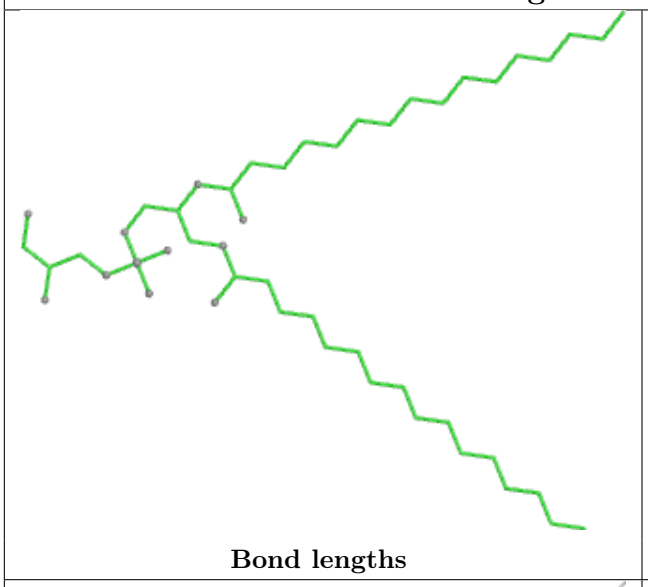


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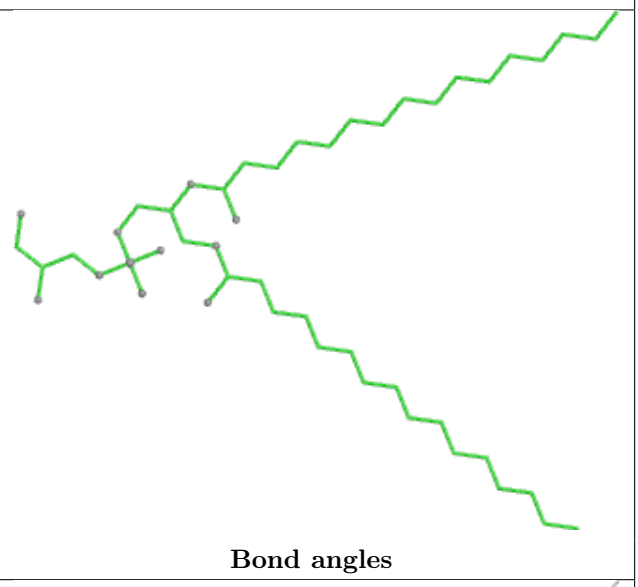


Rings

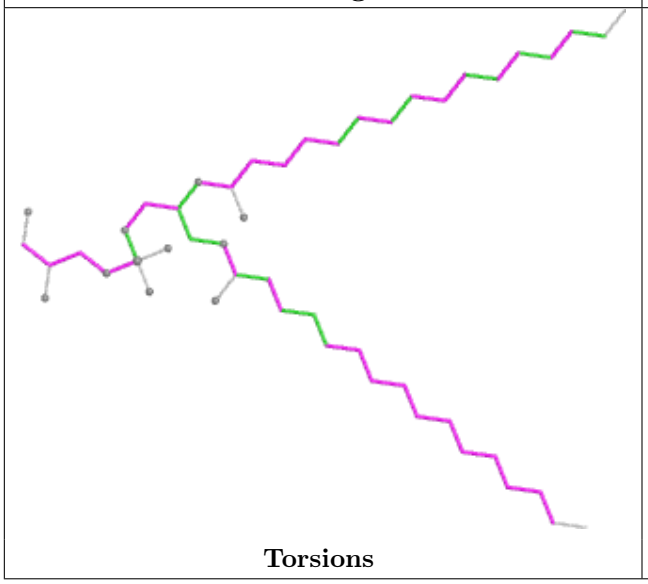
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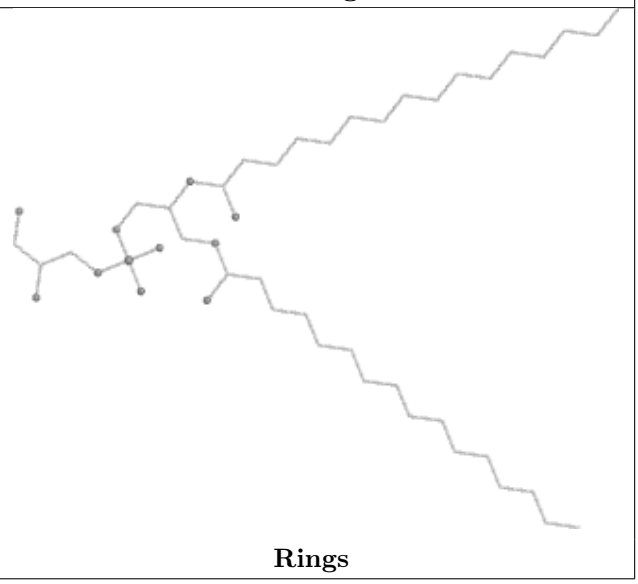
Bond lengths



Bond angles

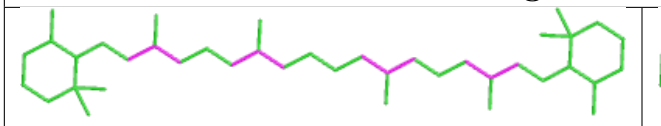


Torsions



Rings

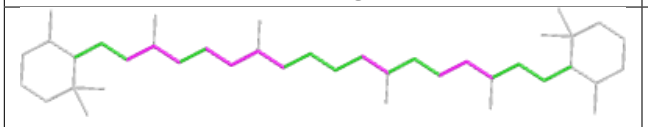
Ligand BCR B 842



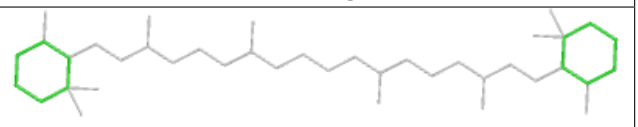
Bond lengths



Bond angles



Torsions

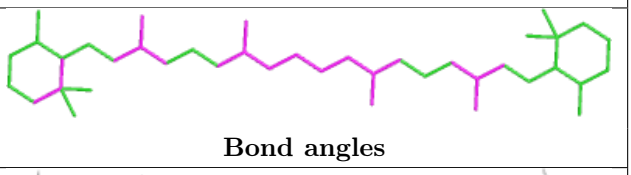


Rings

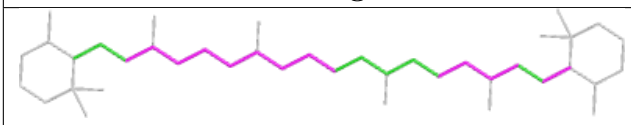
Ligand BCR F 304



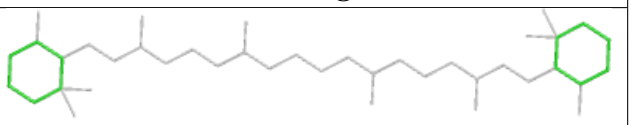
Bond lengths



Bond angles

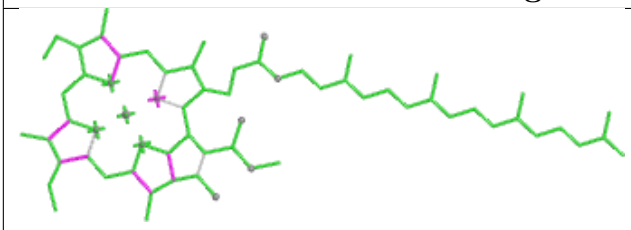


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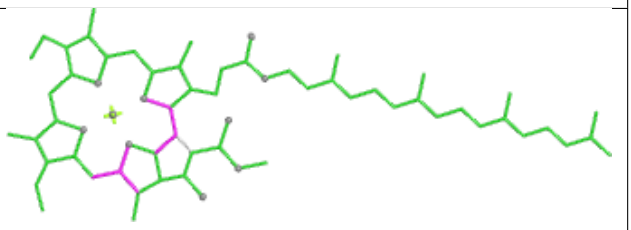


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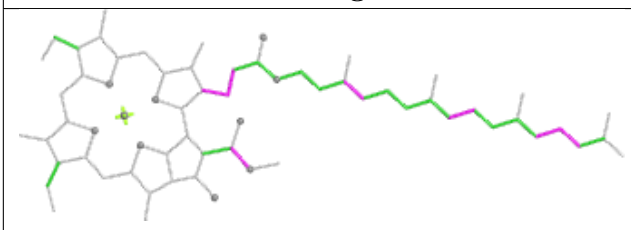
Ligand CLA B 801



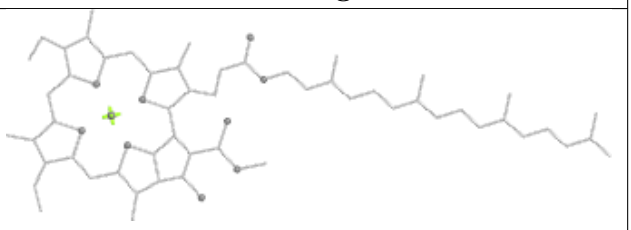
Bond lengths



Bond angles

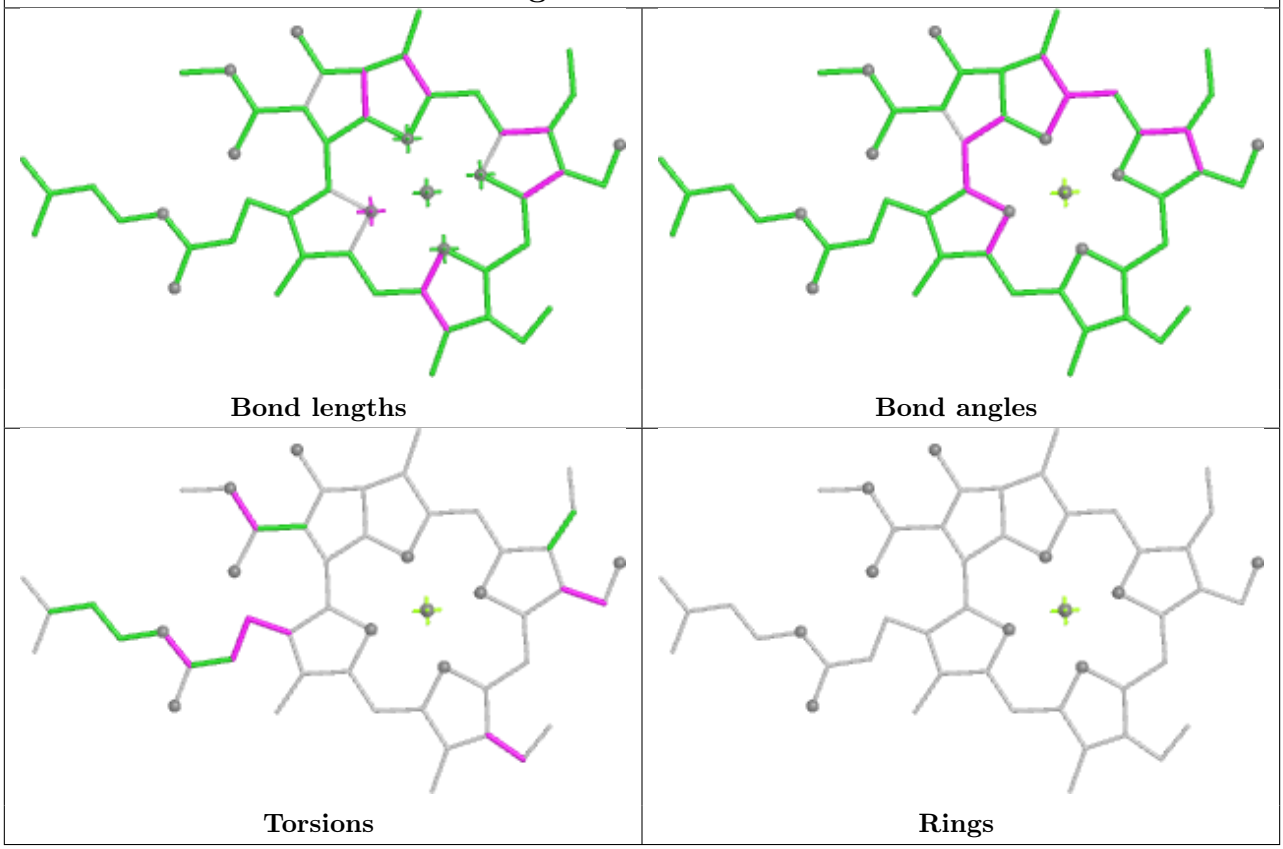


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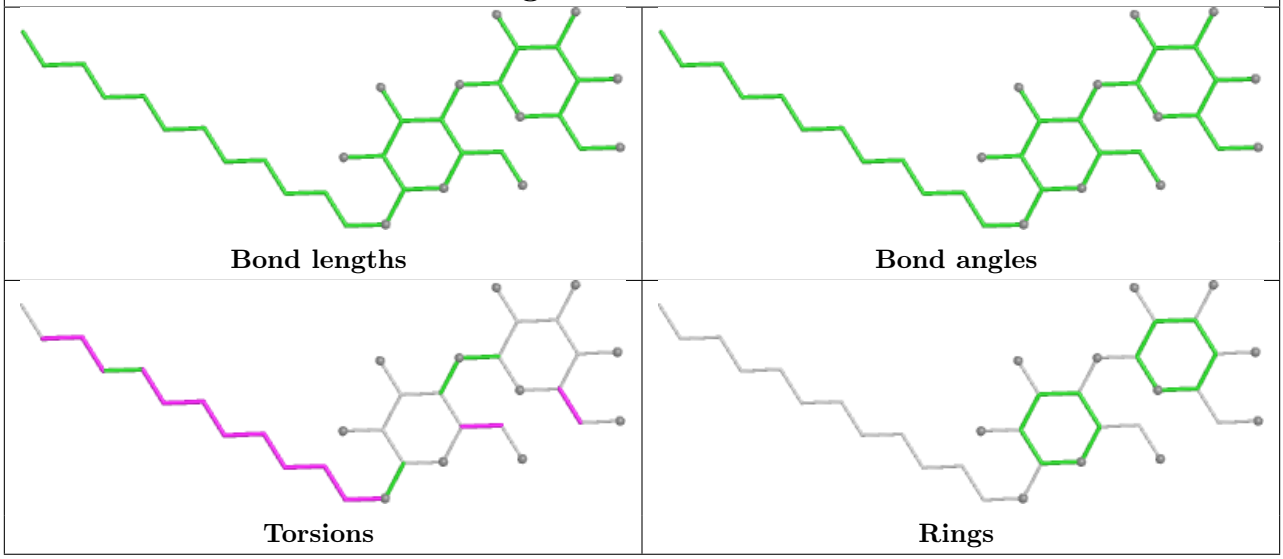


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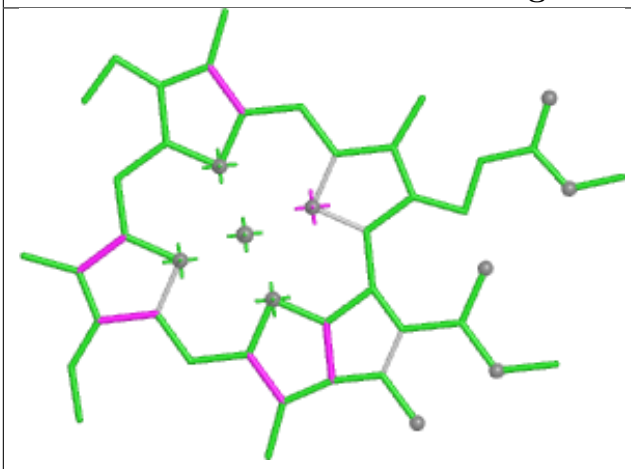
Ligand CHL 4 307



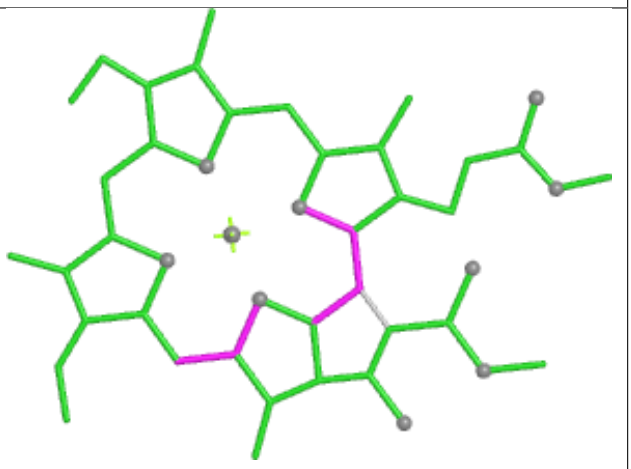
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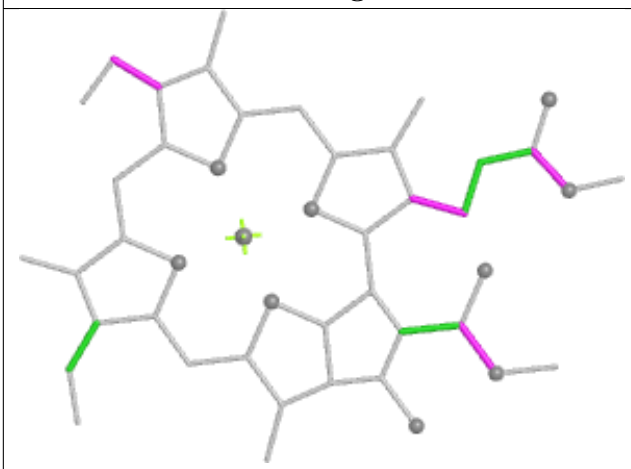
Ligand CLA 1 313



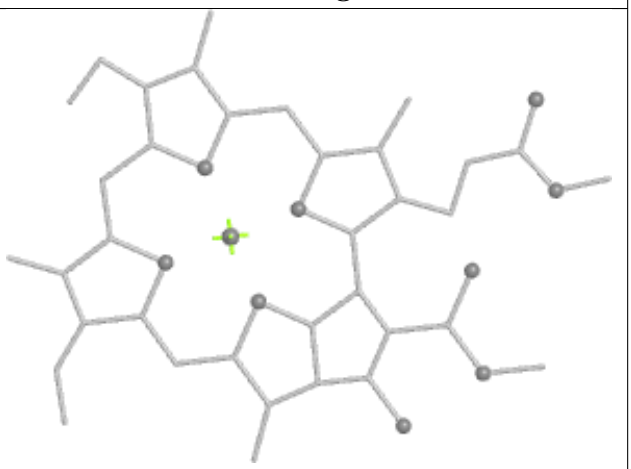
Bond lengths



Bond angles

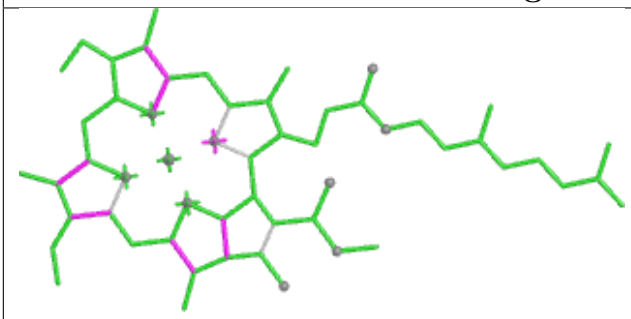


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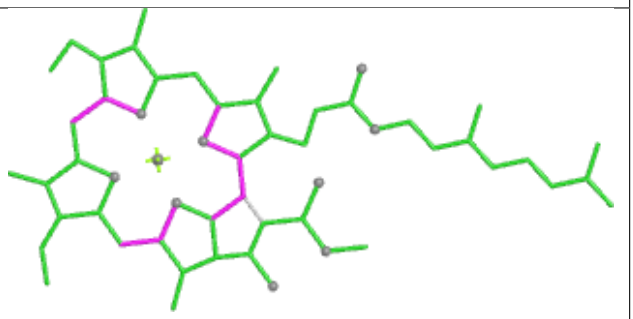


Rings

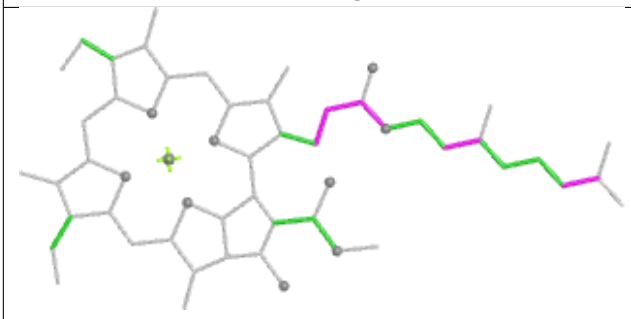
Ligand CLA B 812



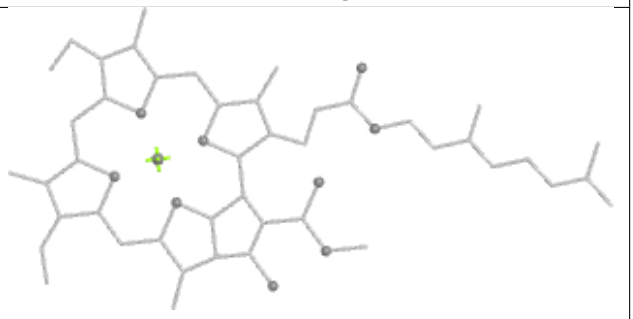
Bond lengths



Bond angles

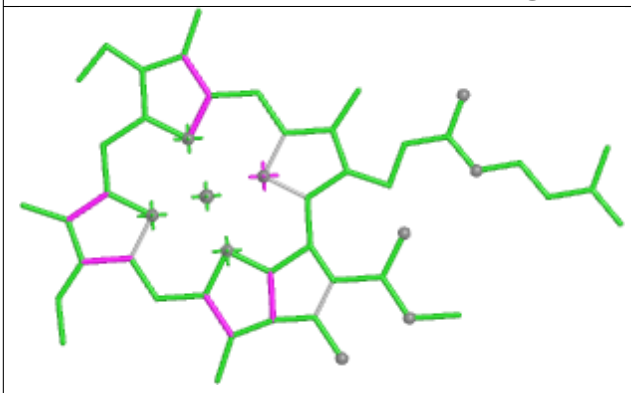


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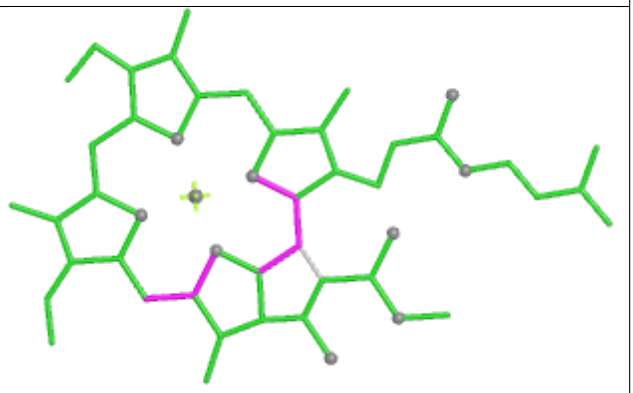


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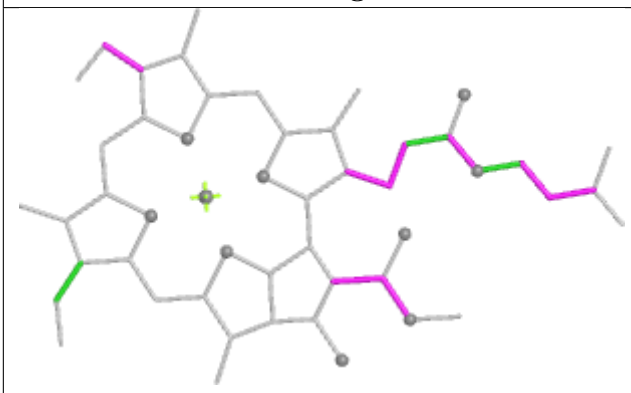
Ligand CLA A 829



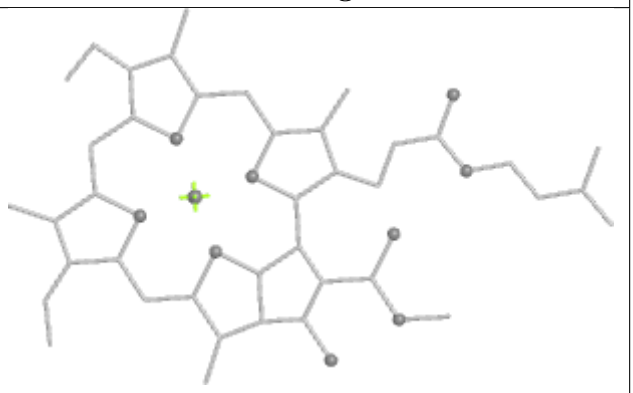
Bond lengths



Bond angles

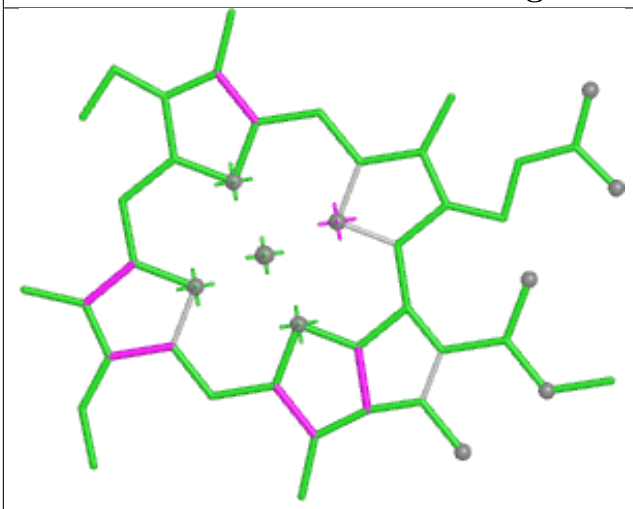


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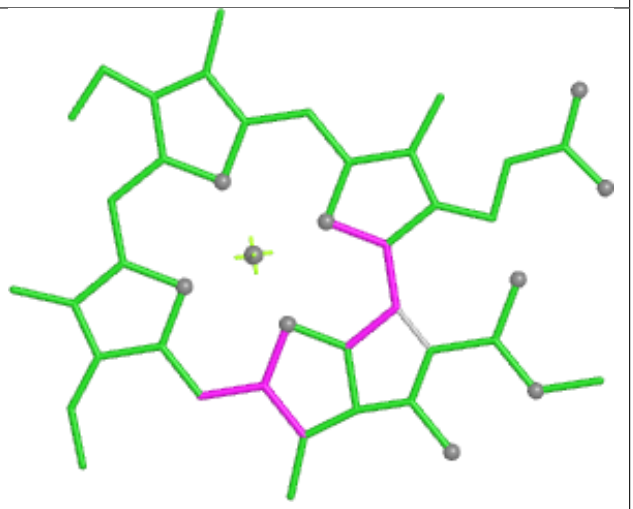


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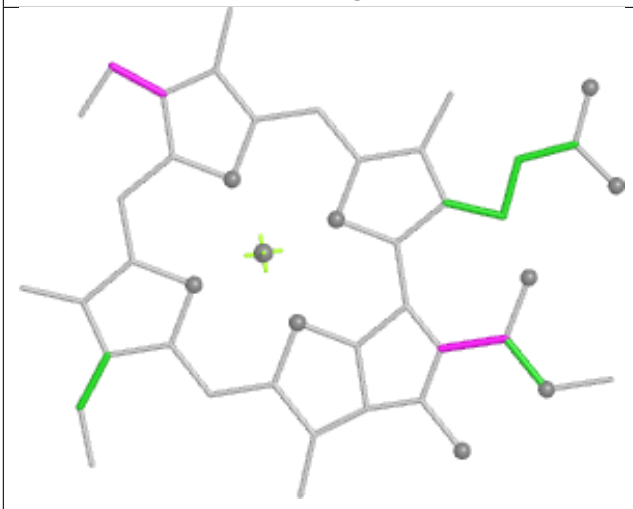
Ligand CLA F 306



Bond lengths



Bond angles

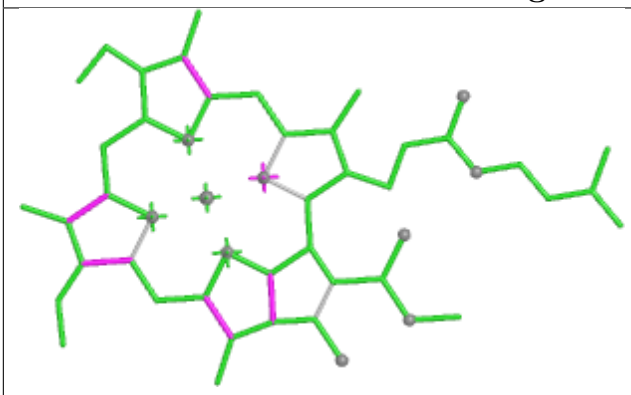


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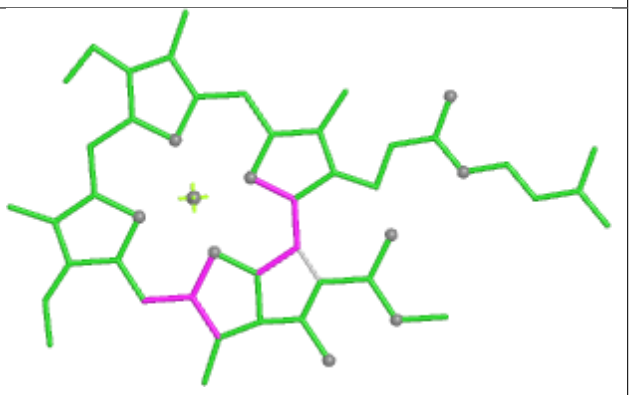


Rings

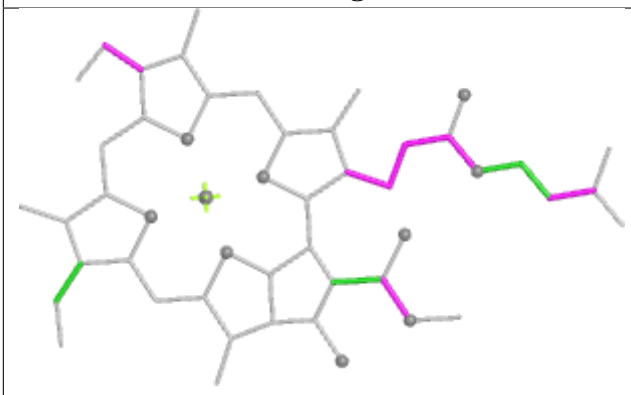
Ligand CLA 4 304



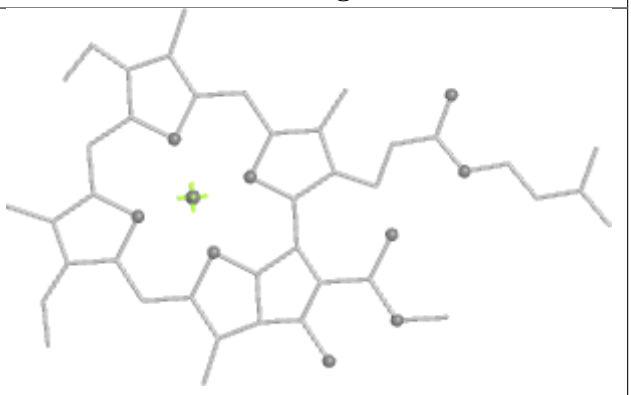
Bond lengths



Bond angles

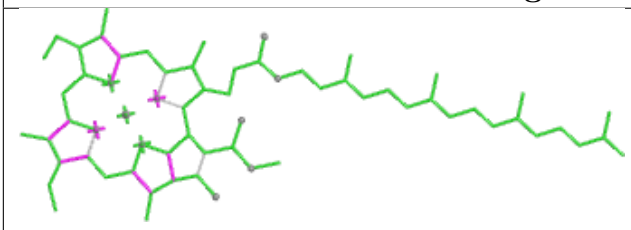


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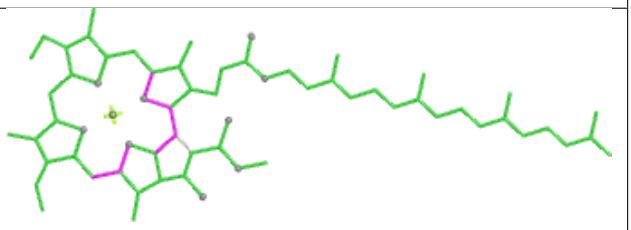


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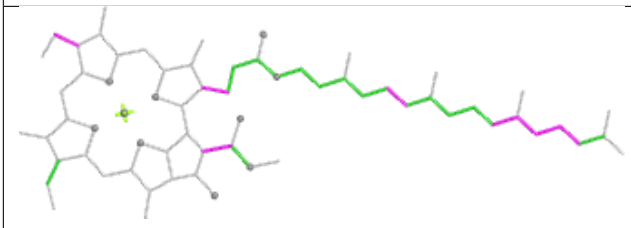
Ligand CLA B 826



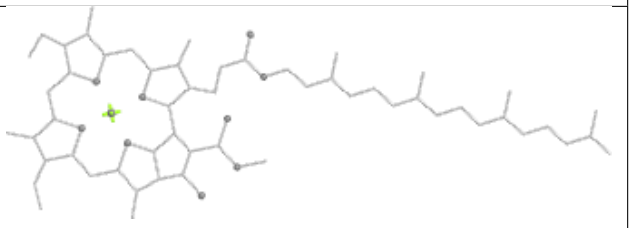
Bond lengths



Bond angles

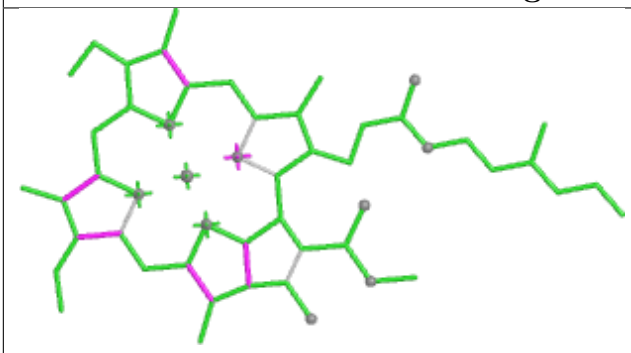


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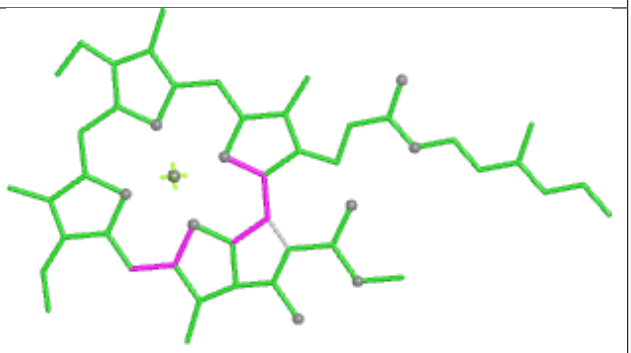


Rings

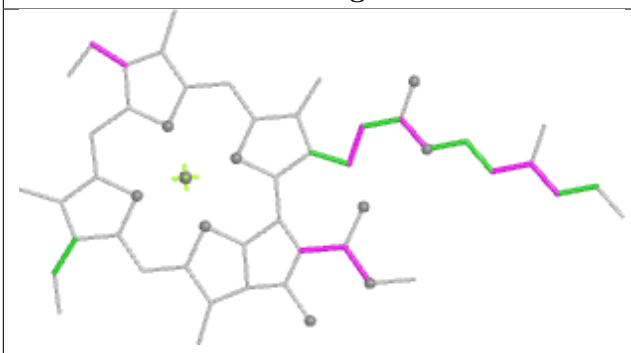
Ligand CLA O 101



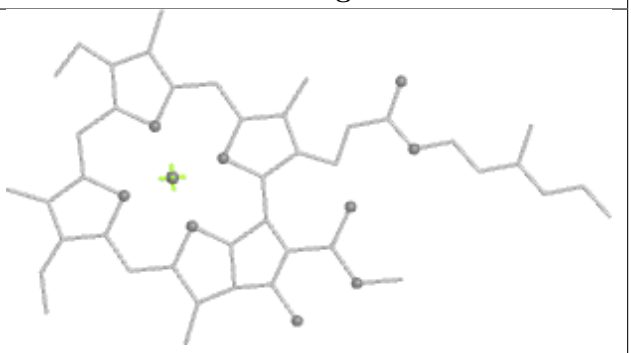
Bond lengths



Bond angles

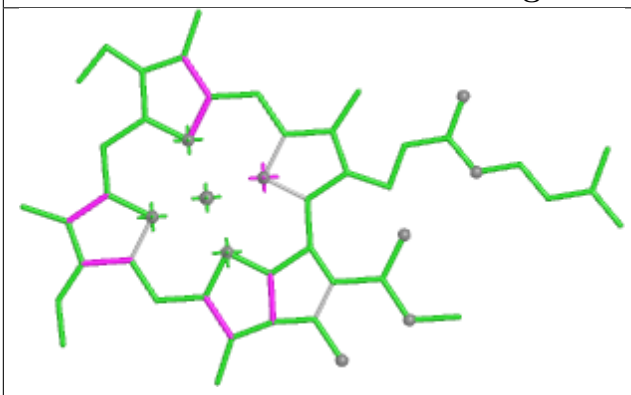


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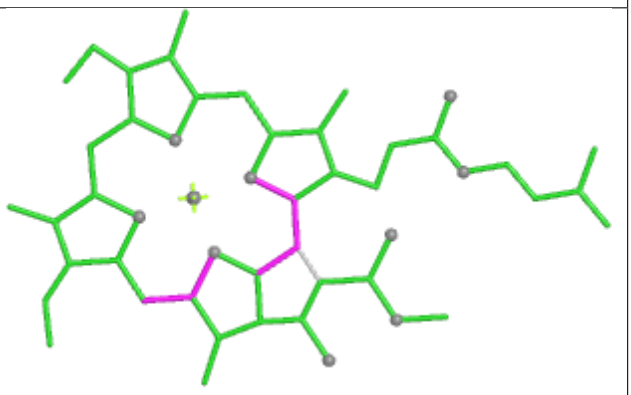


Rings

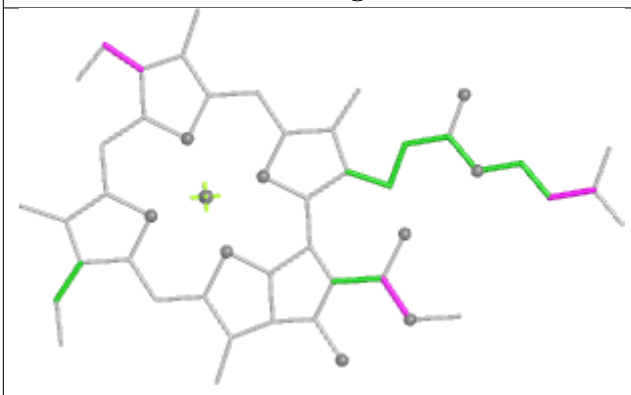
Ligand CLA G 204



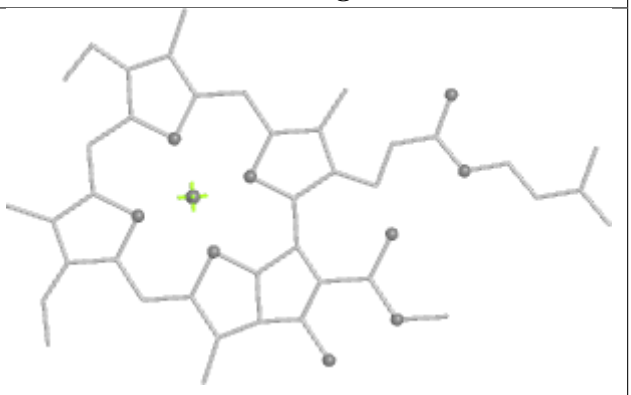
Bond lengths



Bond angles

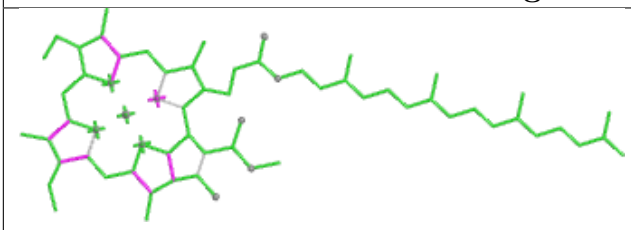


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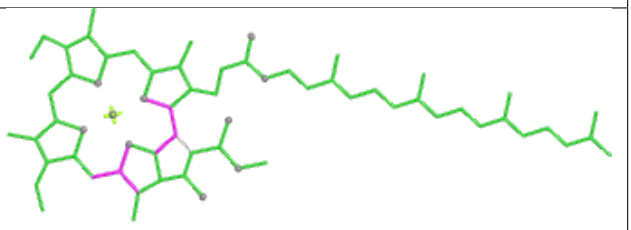


Rings

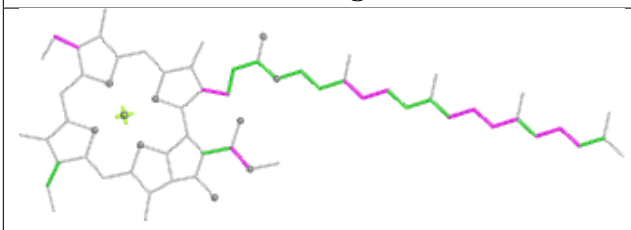
Ligand CLA A 809



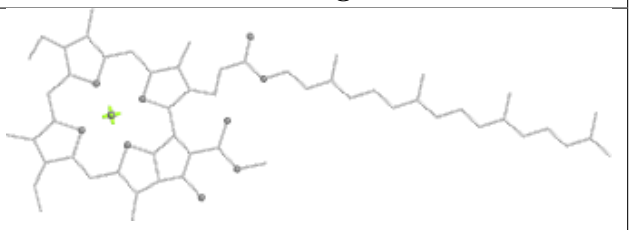
Bond lengths



Bond angles

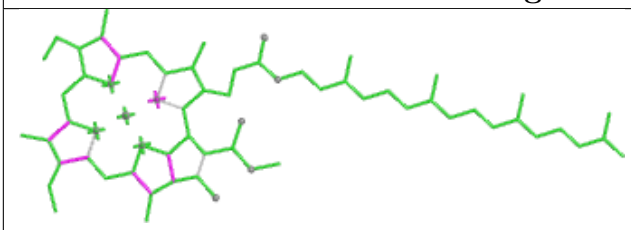


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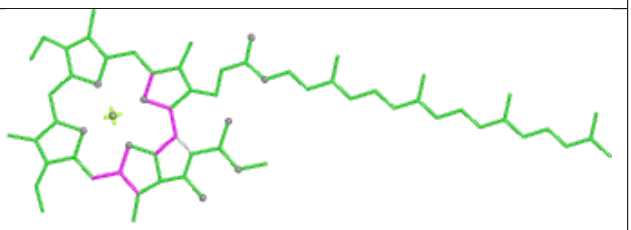


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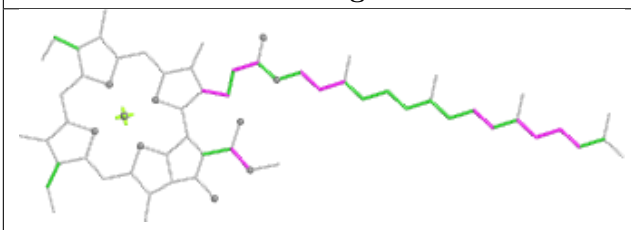
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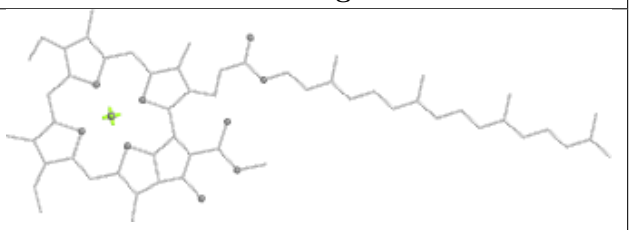
Bond lengths



Bond angles

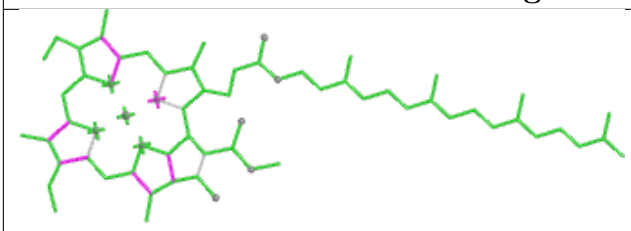


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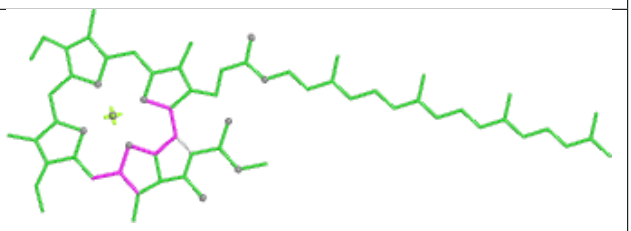


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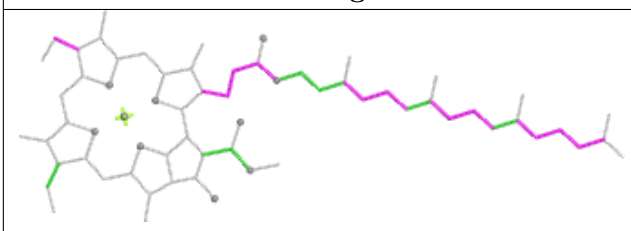
Ligand CLA A 816



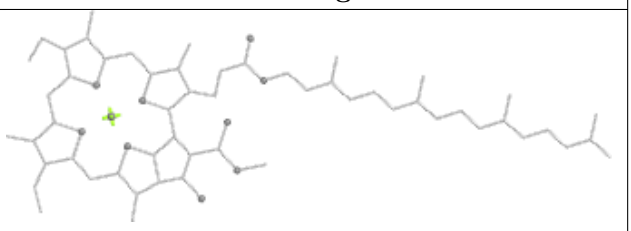
Bond lengths



Bond angles



Torsions

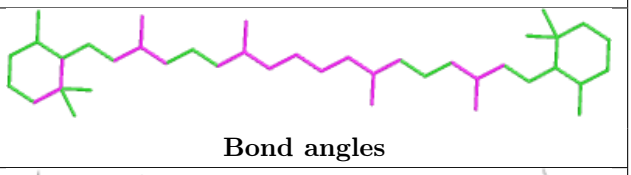


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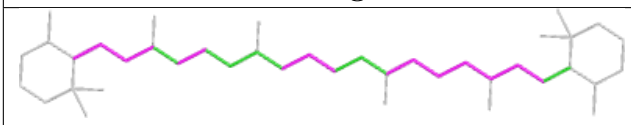
Ligand BCR K 301



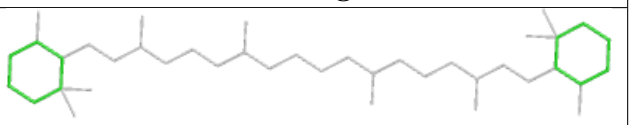
Bond lengths



Bond angles

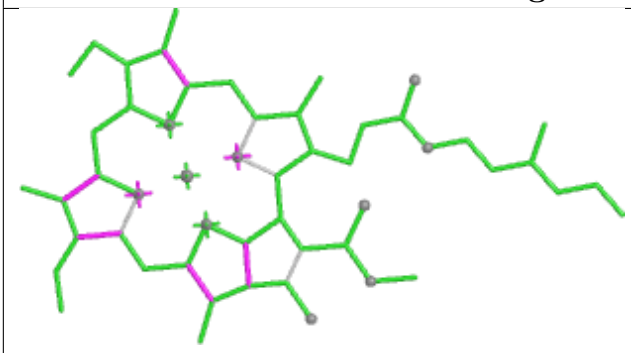


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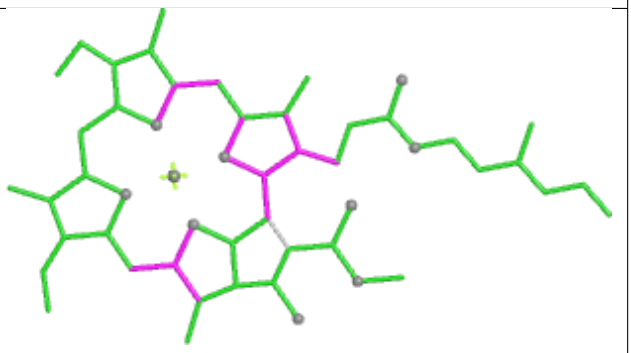


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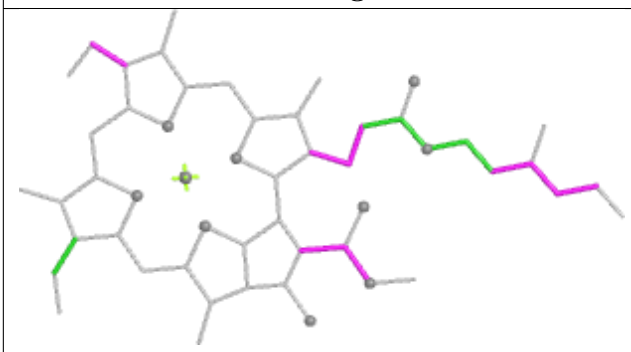
Ligand CLA 4 311



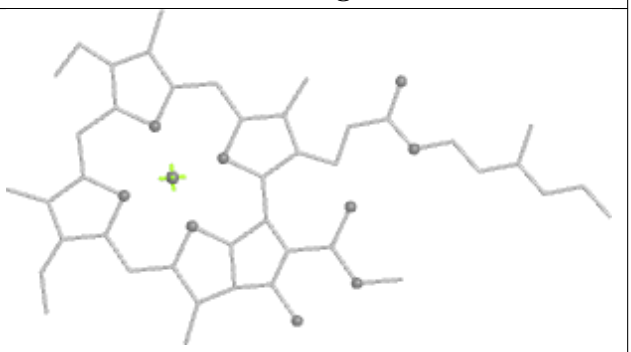
Bond lengths



Bond angles

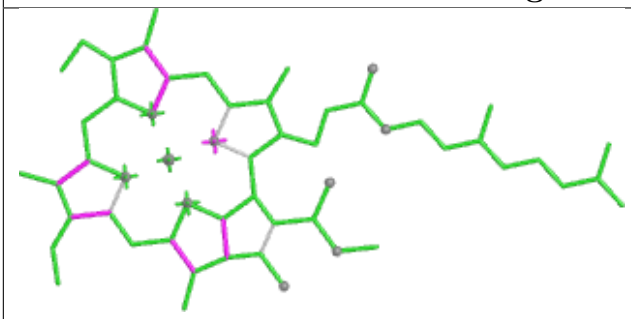


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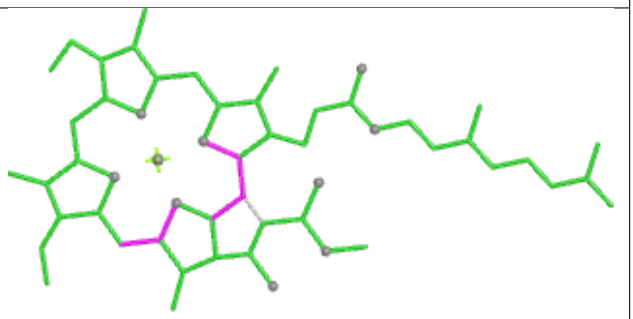


Rings

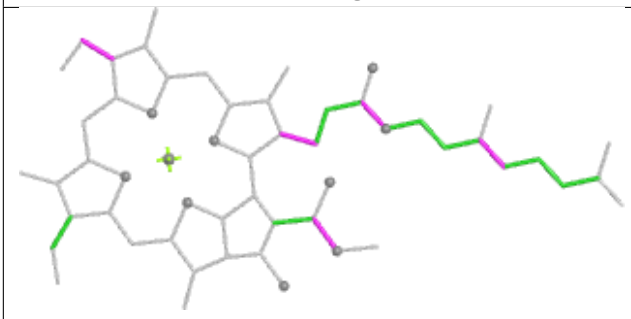
Ligand CLA F 307



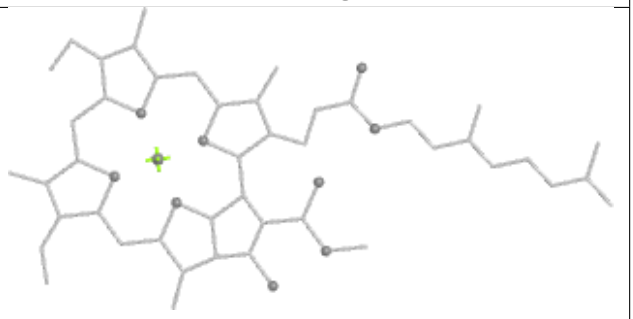
Bond lengths



Bond angles

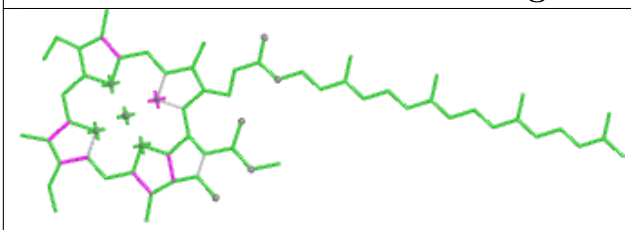


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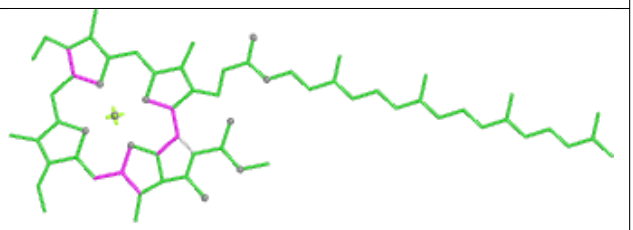


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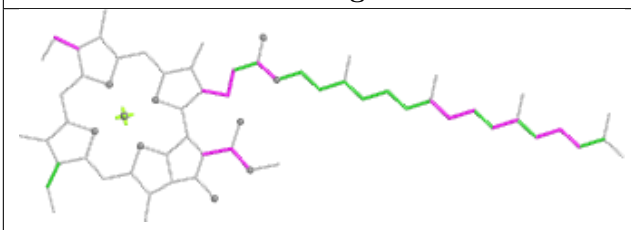
Ligand CLA 1 301



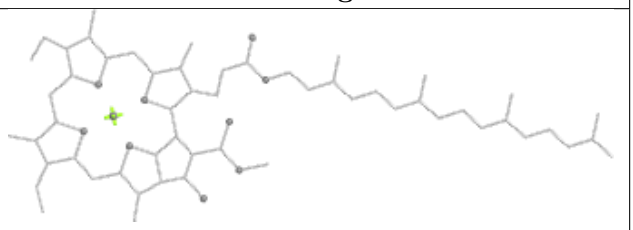
Bond lengths



Bond angles

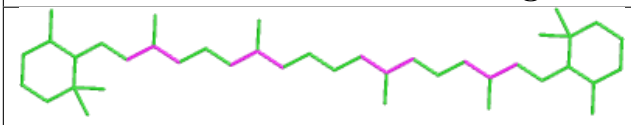


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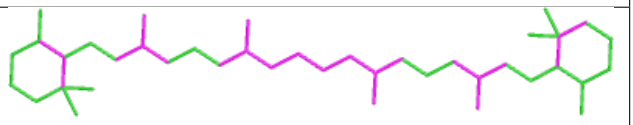


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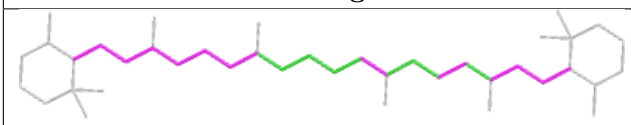
Ligand BCR A 844



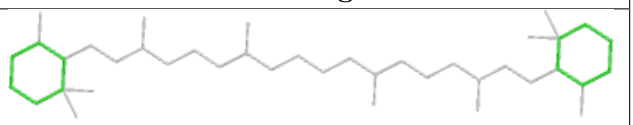
Bond lengths



Bond angles

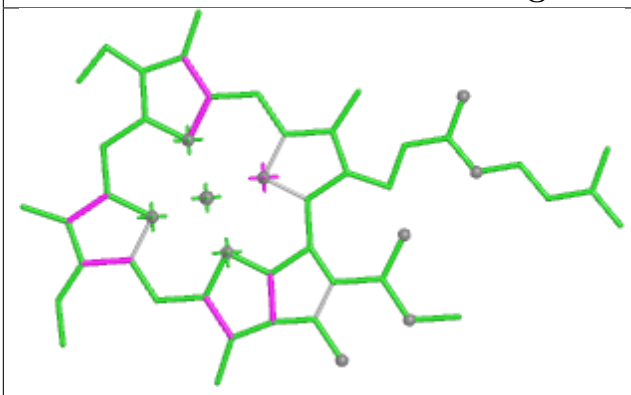


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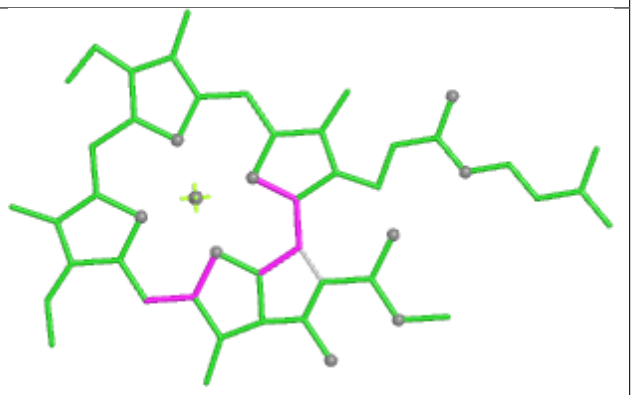


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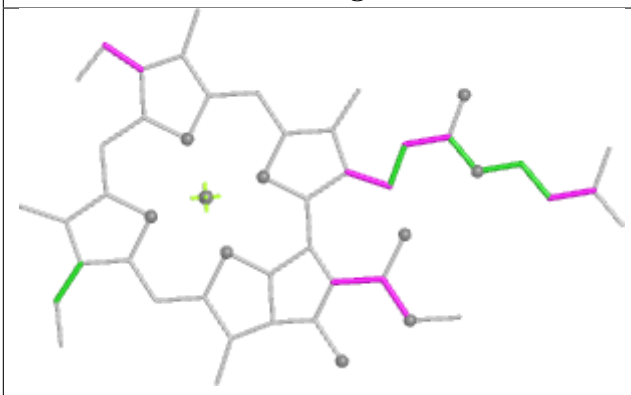
Ligand CLA 3 307



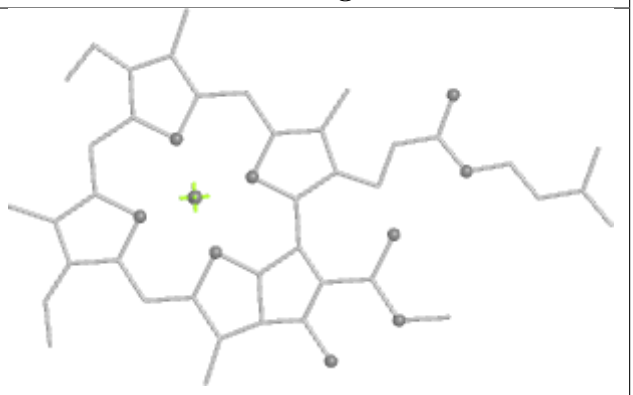
Bond lengths



Bond angles

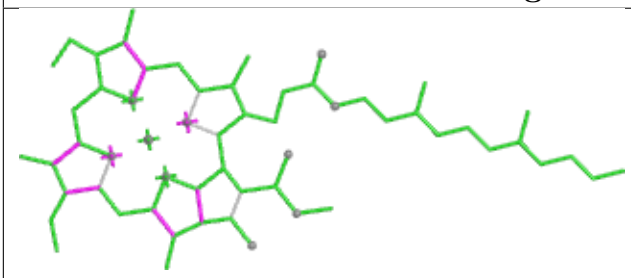


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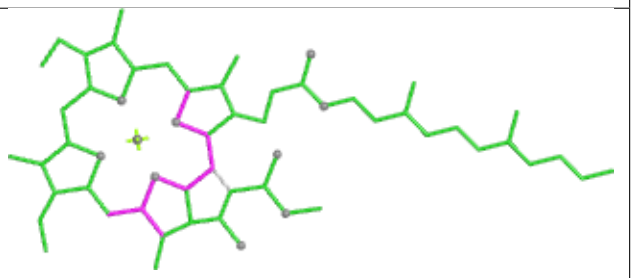


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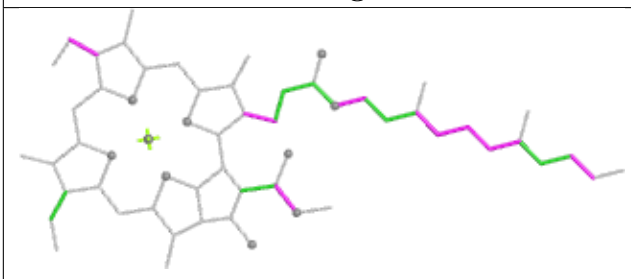
Ligand CLA B 832



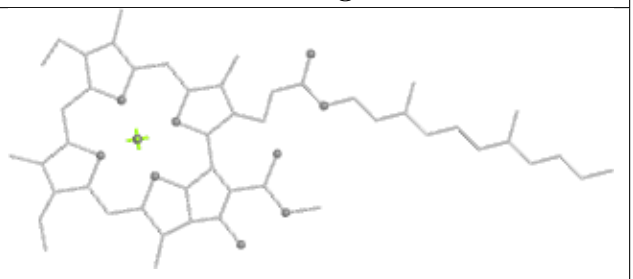
Bond lengths



Bond angles

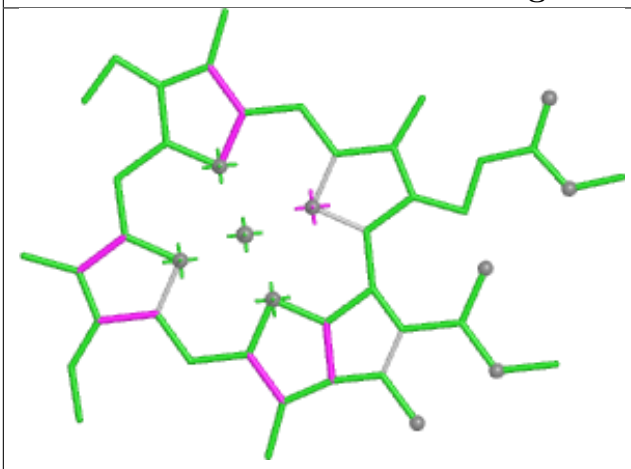


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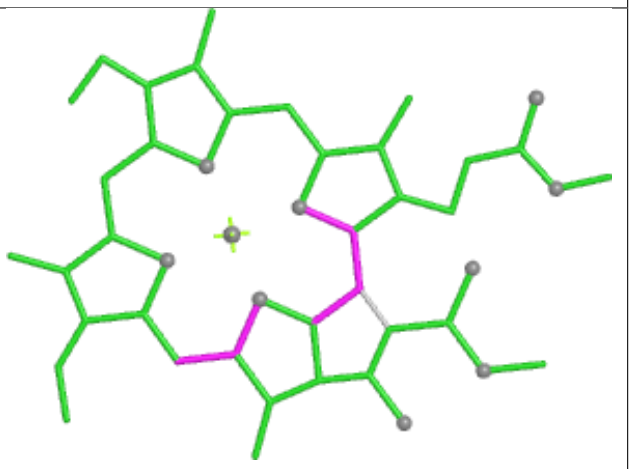


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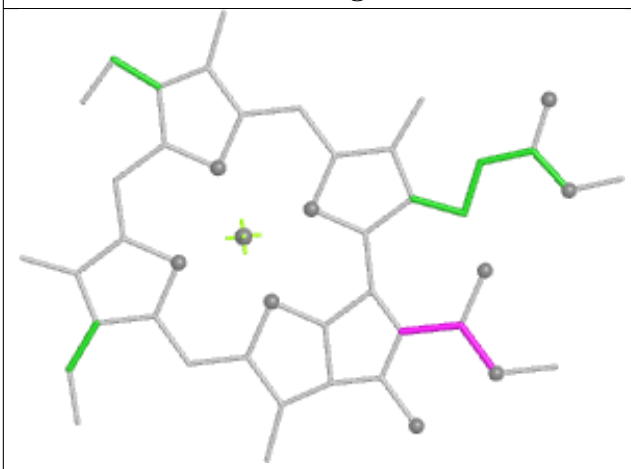
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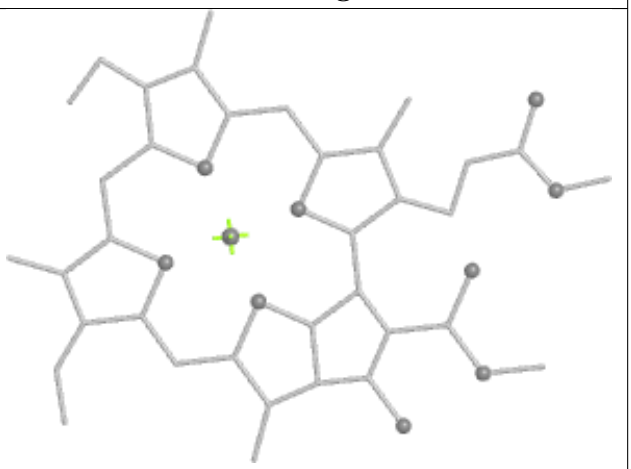
Bond lengths



Bond angles

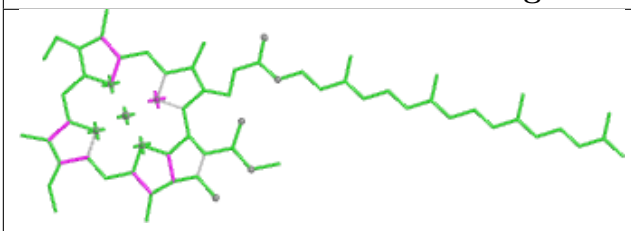


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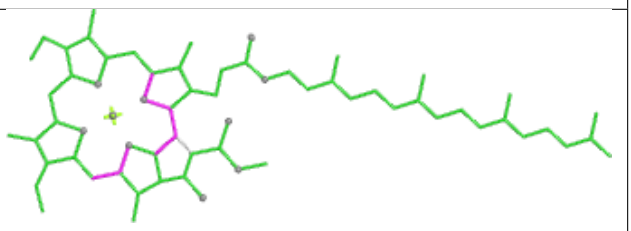


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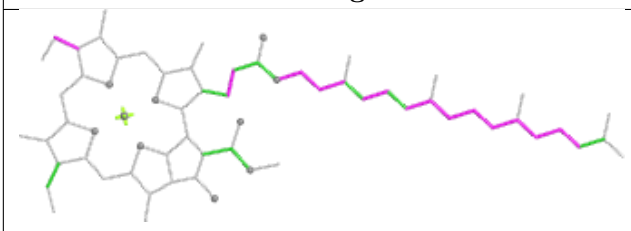
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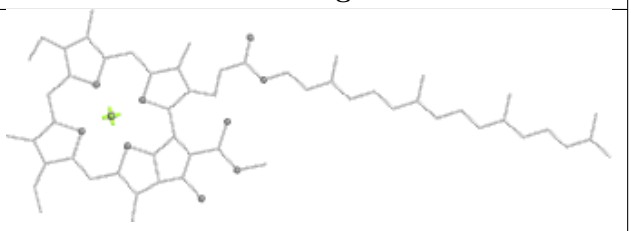
Bond lengths



Bond angles

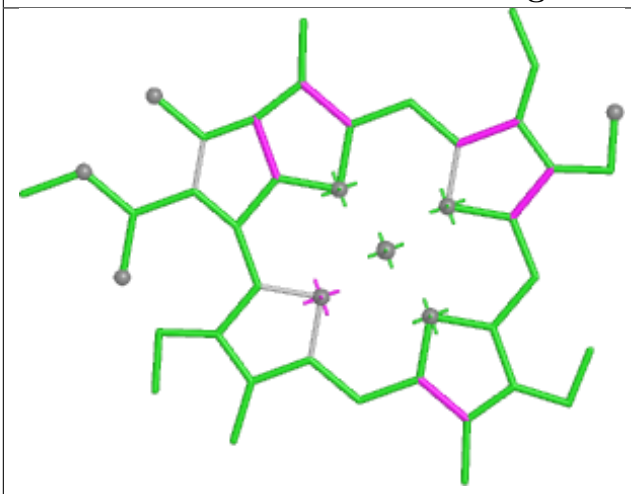


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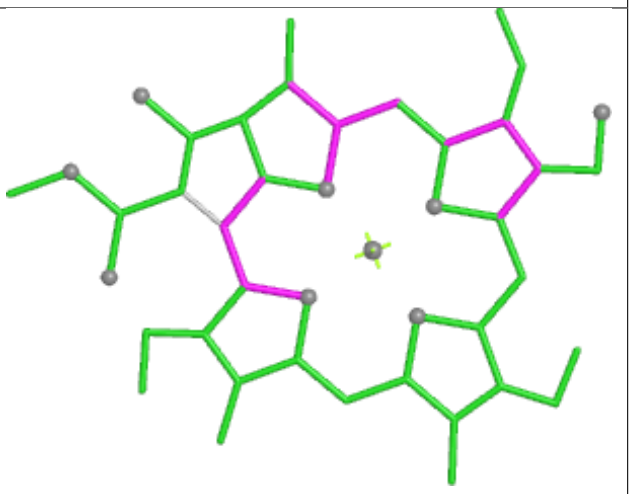


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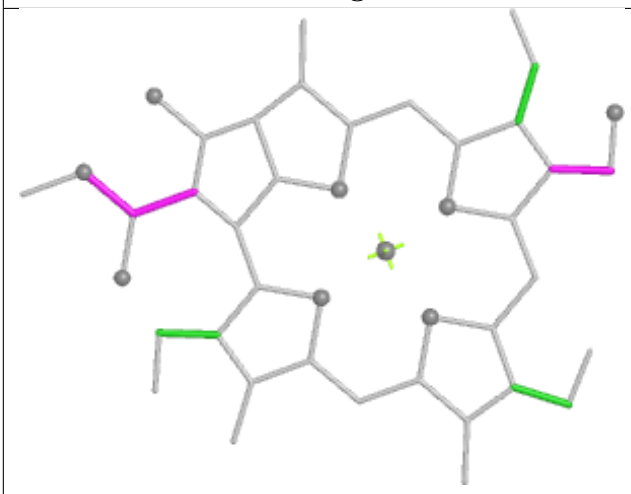
Ligand CHL 2 304



Bond lengths



Bond angles

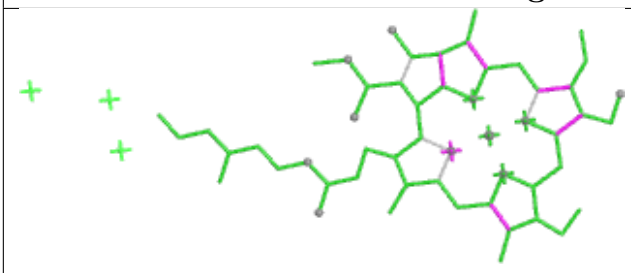


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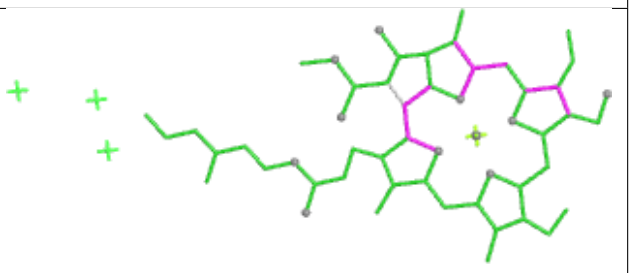


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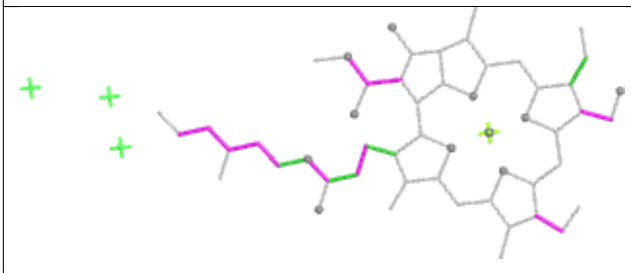
Ligand CHL 2 319



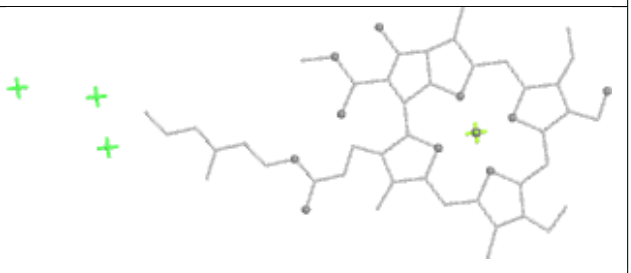
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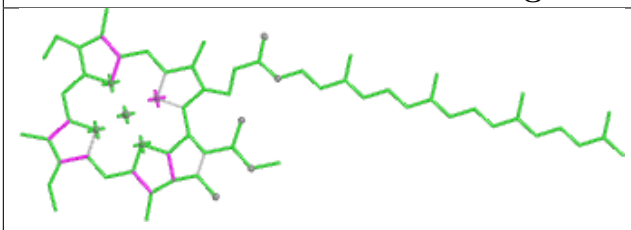
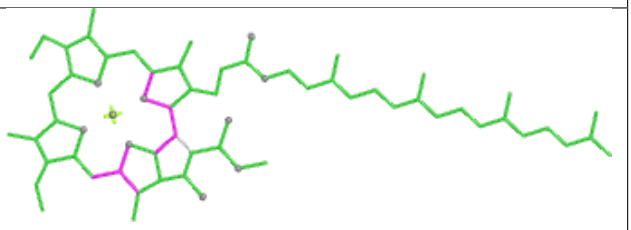
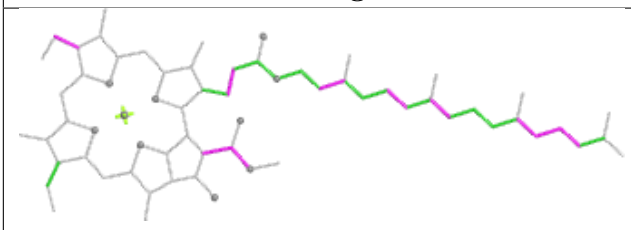
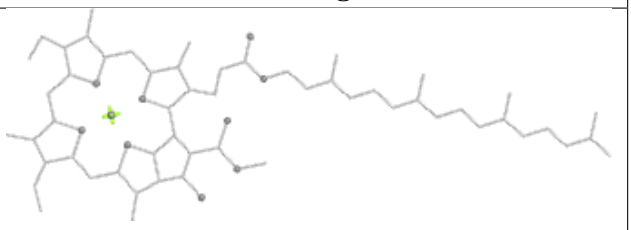
Bond angles

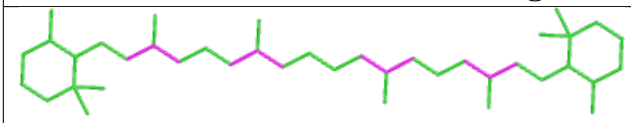
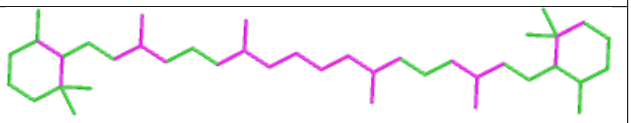
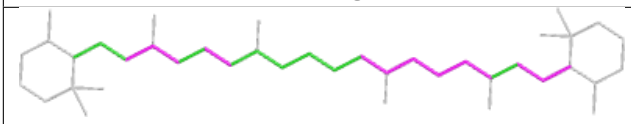
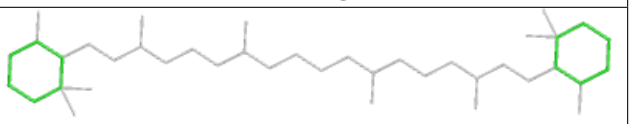


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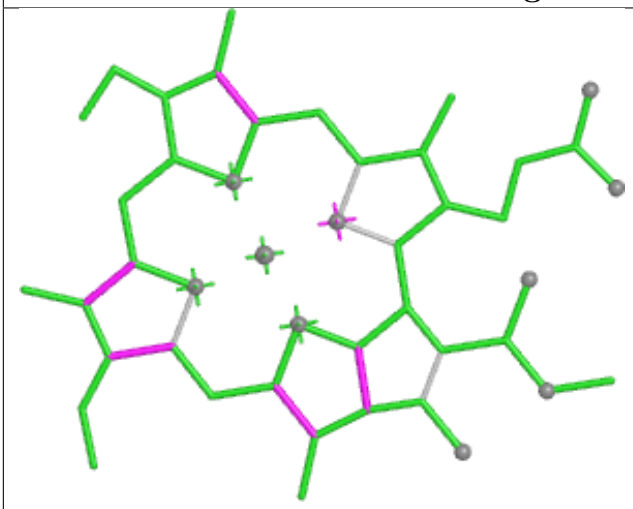


Rings

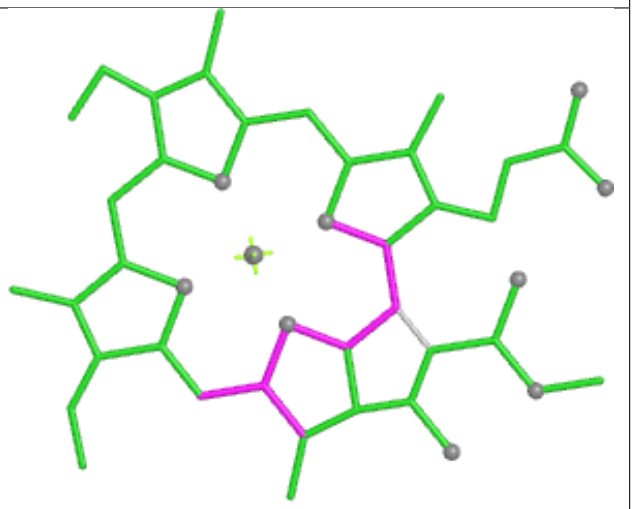
Ligand CLA B 838	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR 4 318	
	
Bond lengths	Bond angles
	
Torsions	Rings

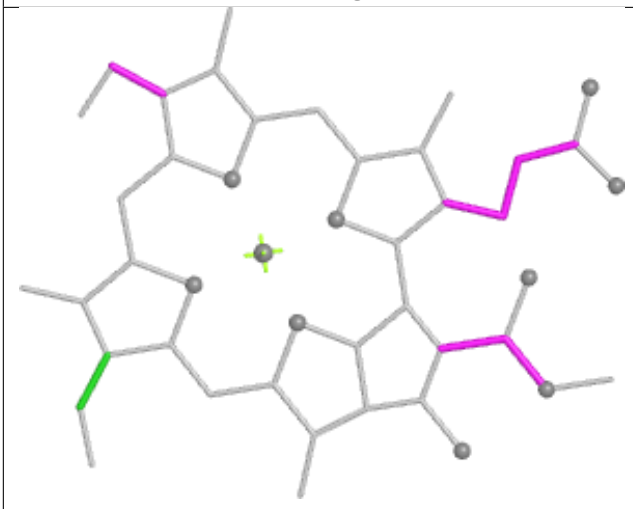
Ligand CLA O 104



Bond lengths



Bond angles

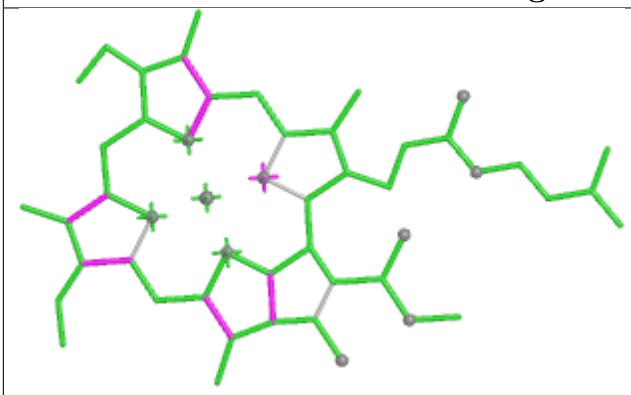


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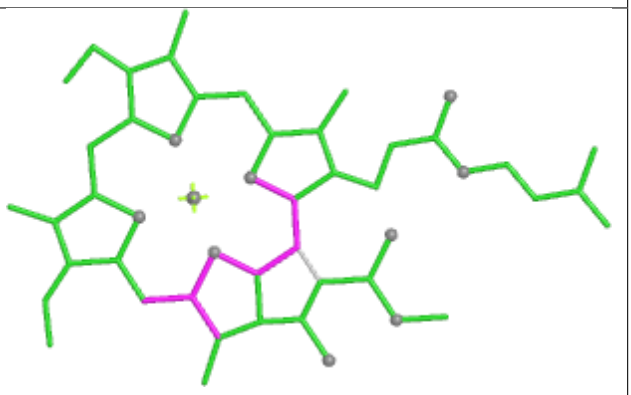


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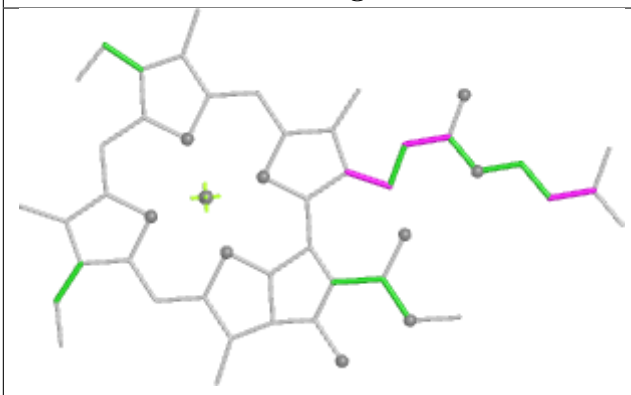
Ligand CLA 2 307



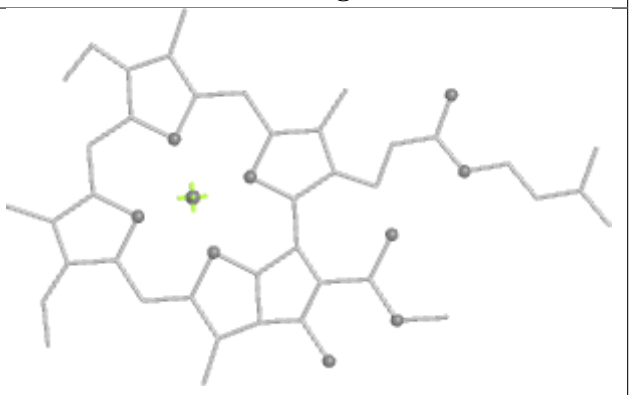
Bond lengths



Bond angles

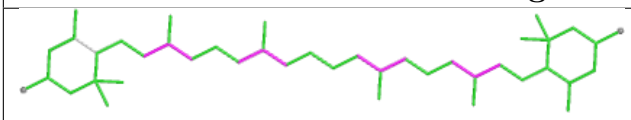


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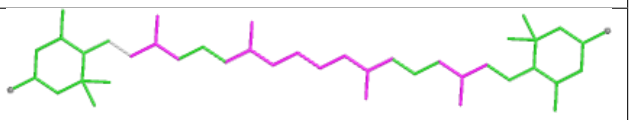


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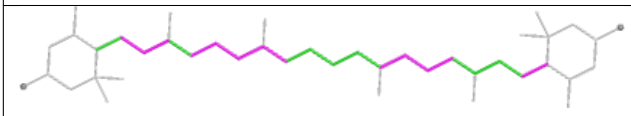
Ligand LUT 4 316



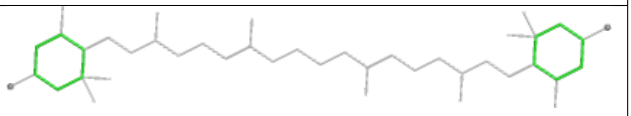
Bond lengths



Bond angles

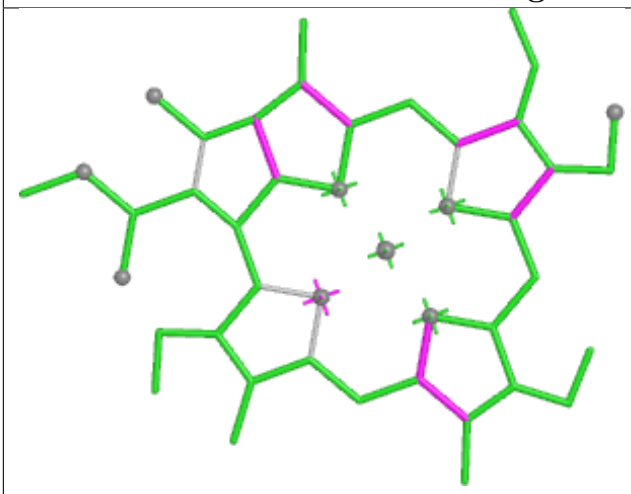


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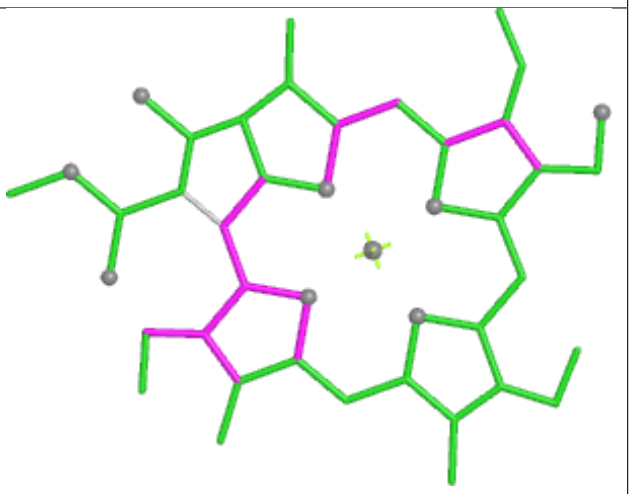


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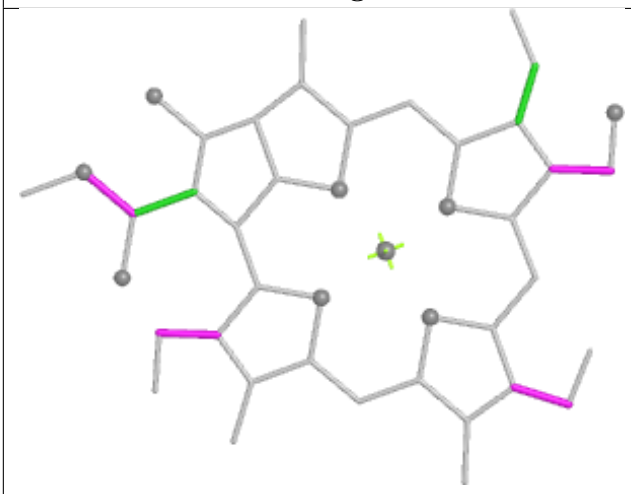
Ligand CHL 2 313



Bond lengths



Bond angles

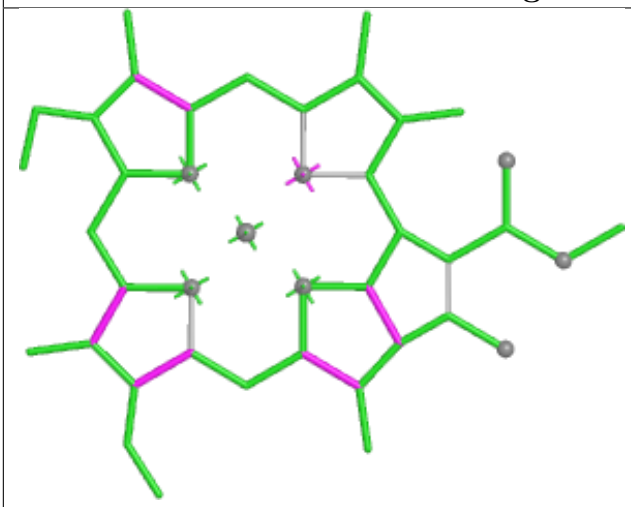


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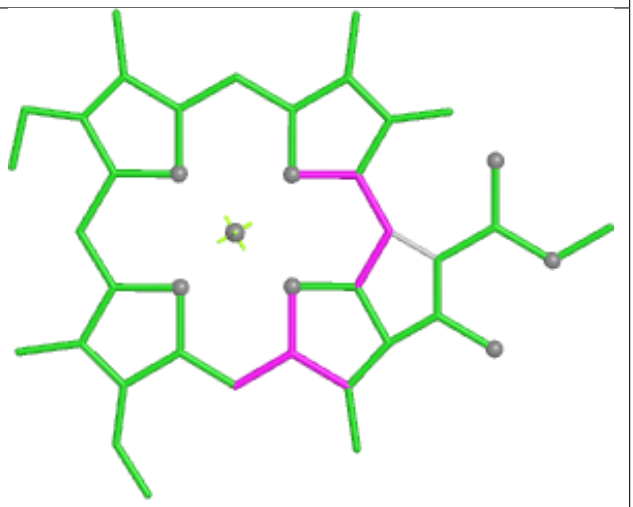


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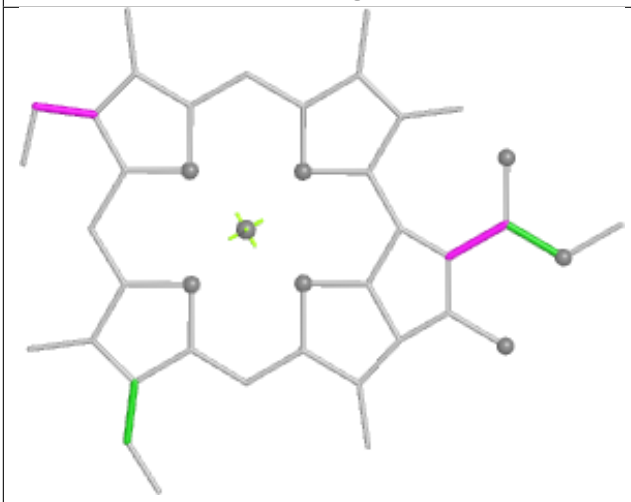
Ligand CLA G 203



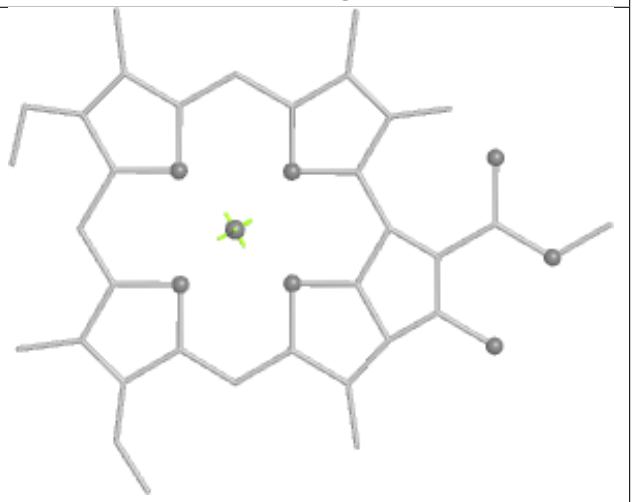
Bond lengths



Bond angles

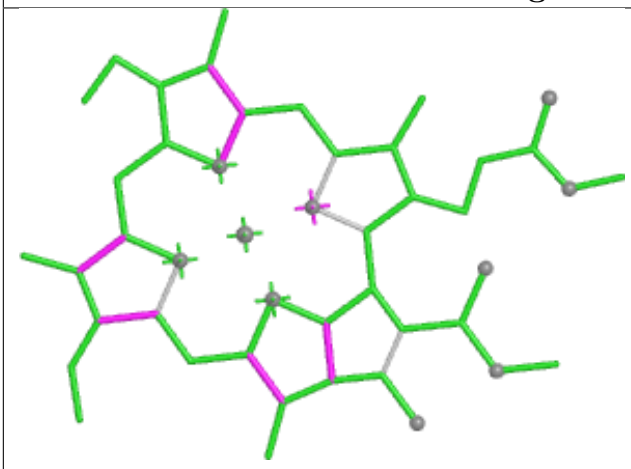


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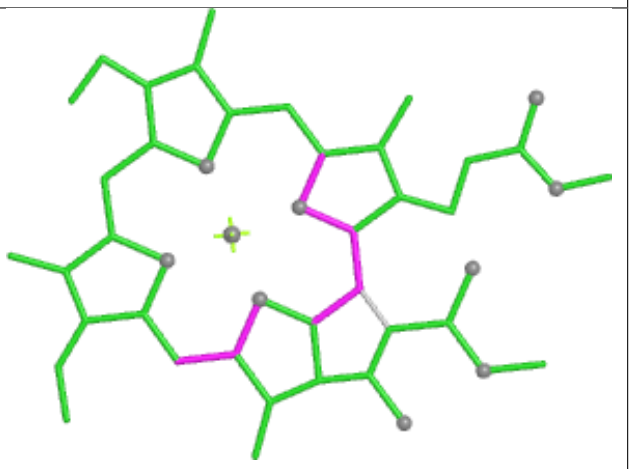


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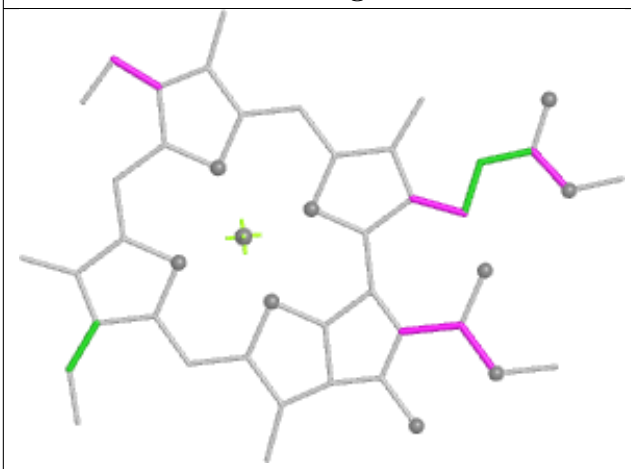
Ligand CLA 1 306



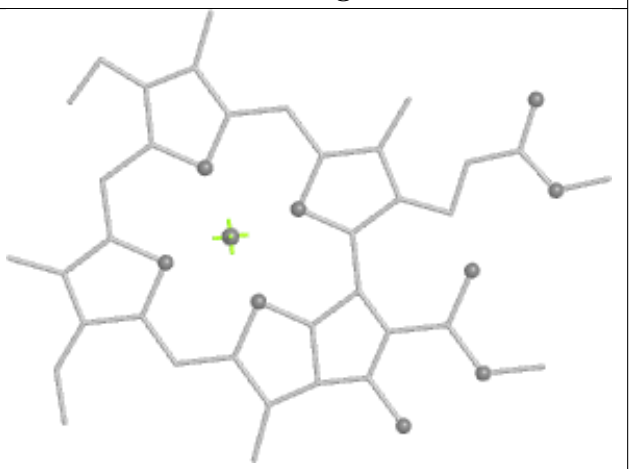
Bond lengths



Bond angles

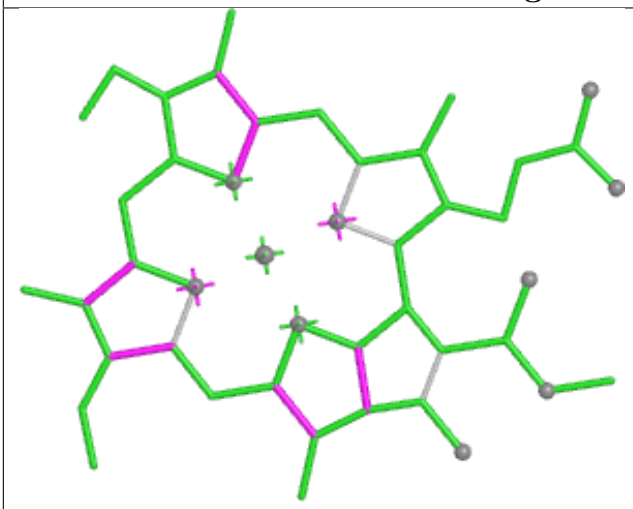


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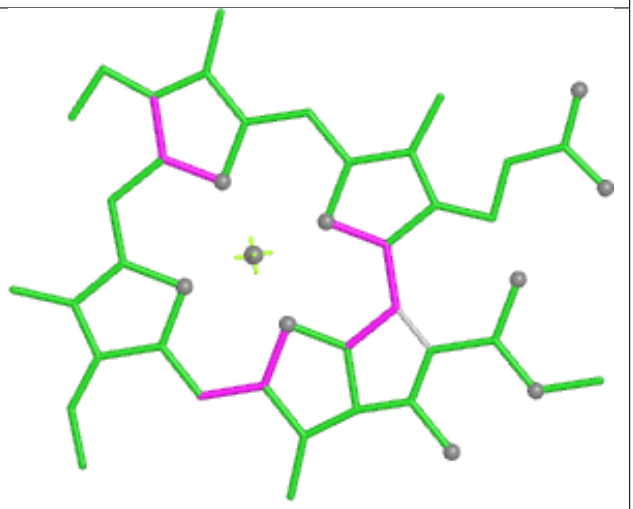


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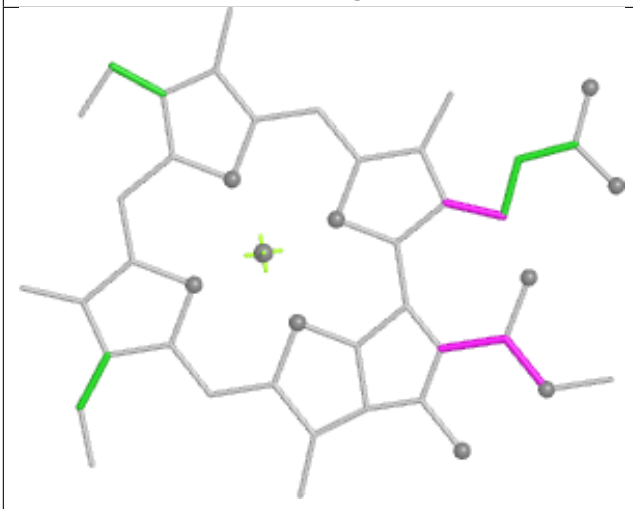
Ligand CLA B 804



Bond lengths



Bond angles

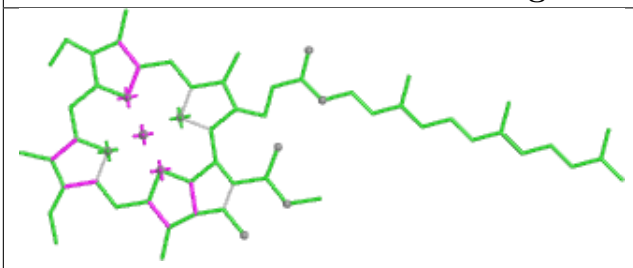


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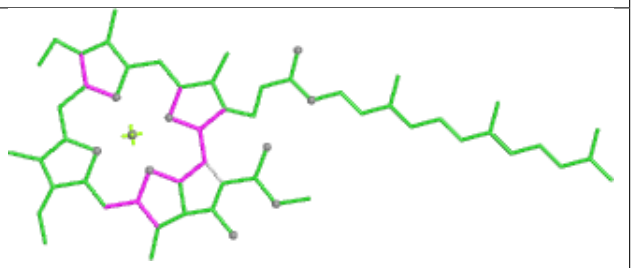


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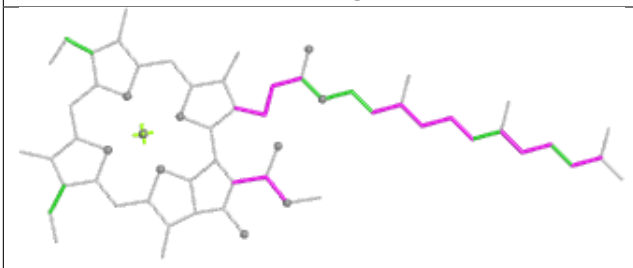
Ligand CLA 4 310



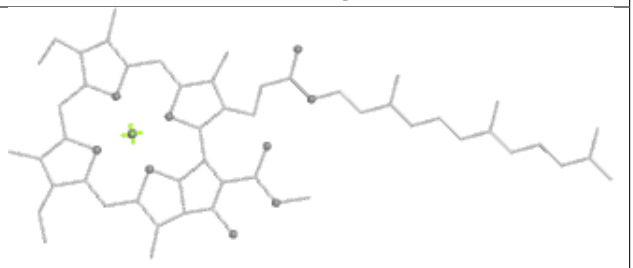
Bond lengths



Bond angles

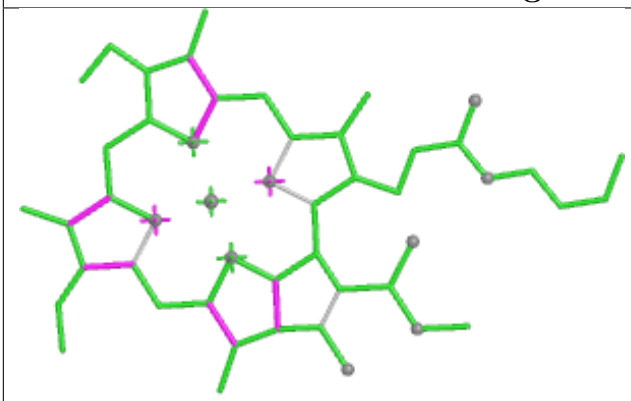


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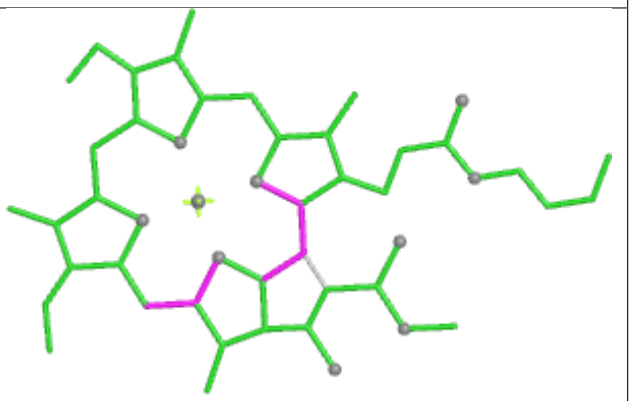


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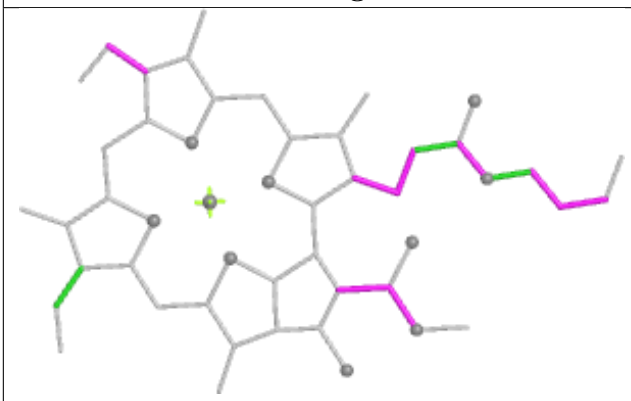
Ligand CLA A 820



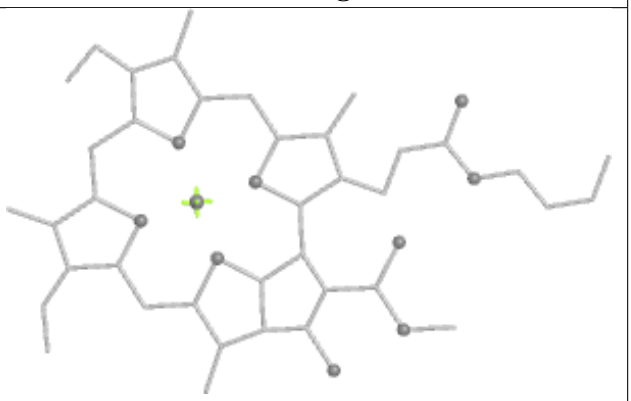
Bond lengths



Bond angles

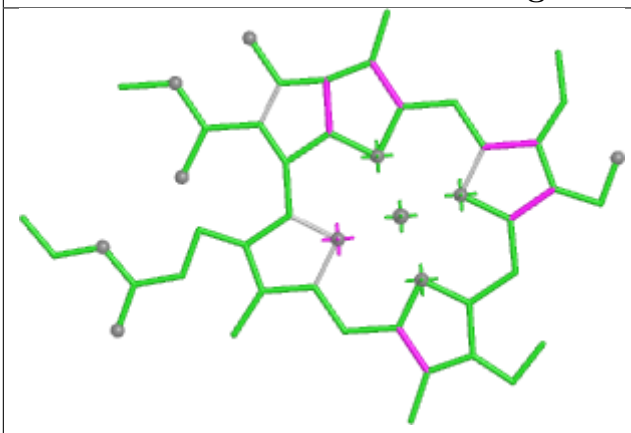


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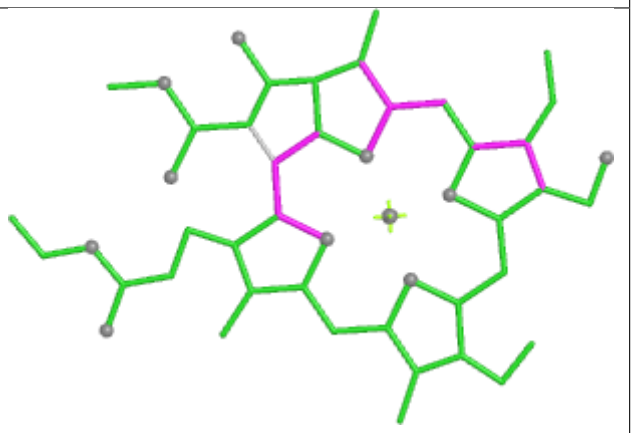


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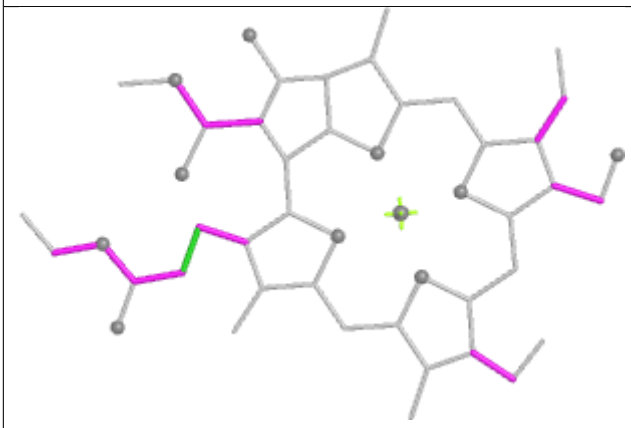
Ligand CHL 1 305



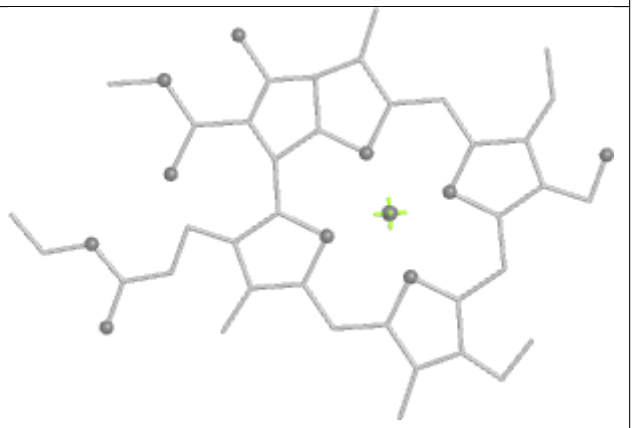
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Bond angles

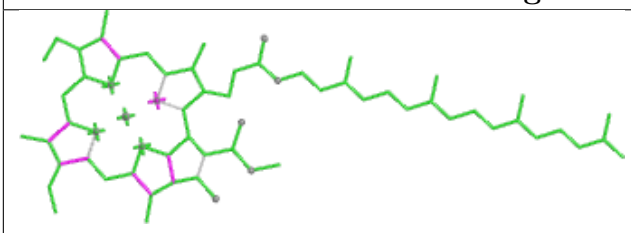


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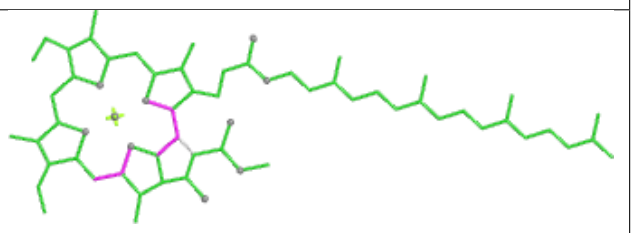


Rings

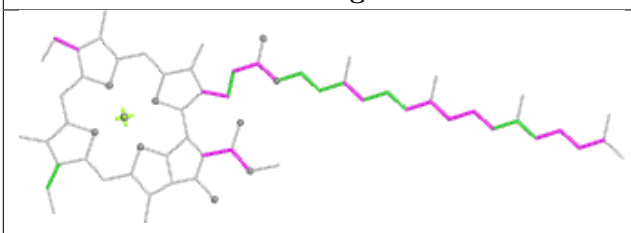
Ligand CLA A 838



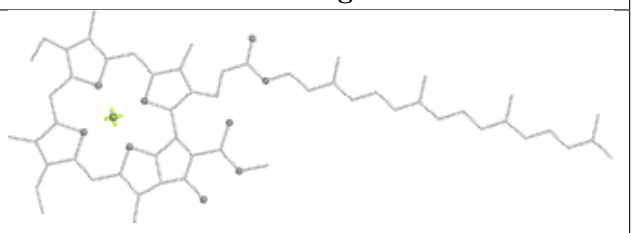
Bond lengths



Bond angles

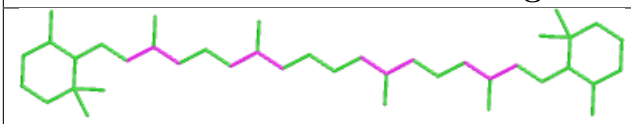


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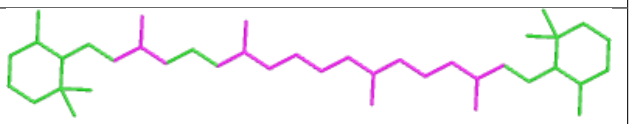


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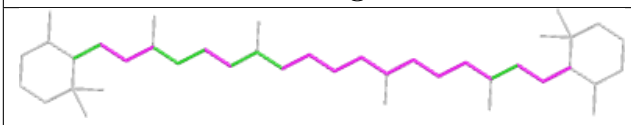
Ligand BCR F 302



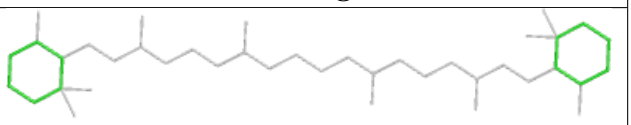
Bond lengths



Bond angles

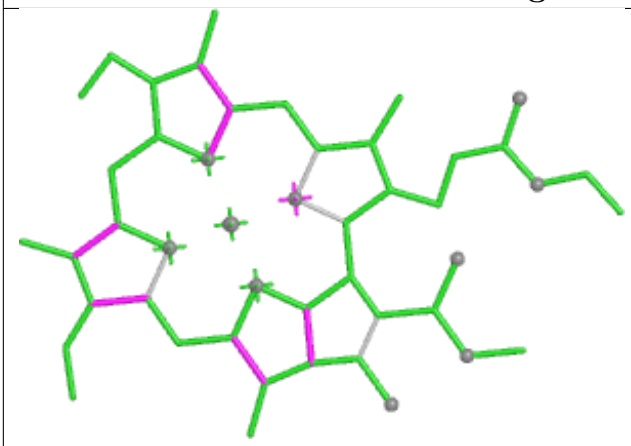


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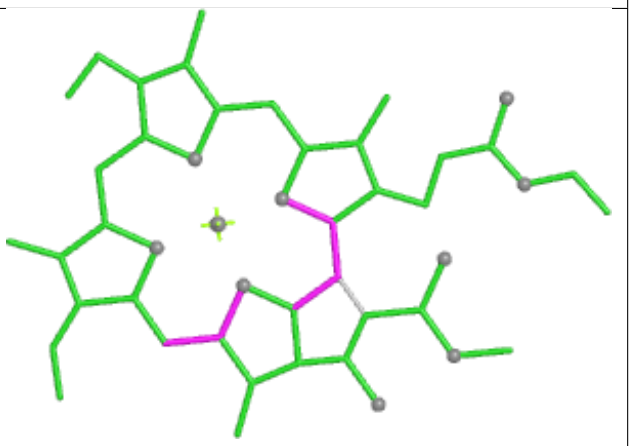


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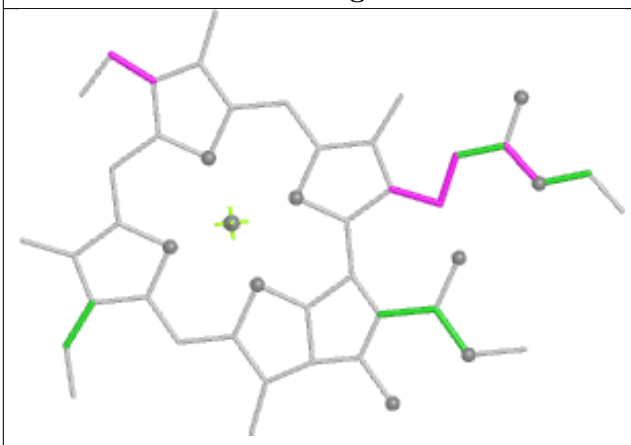
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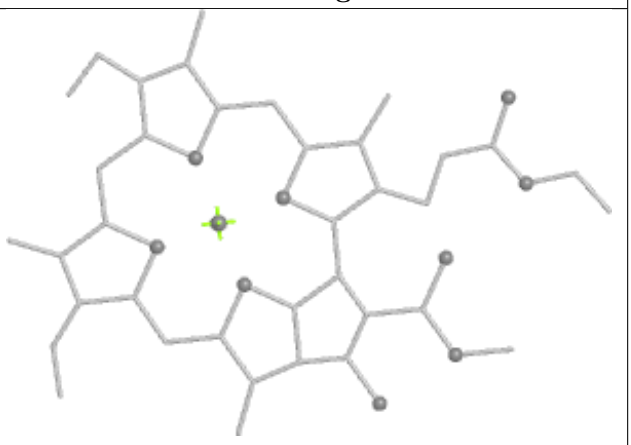
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Bond angles

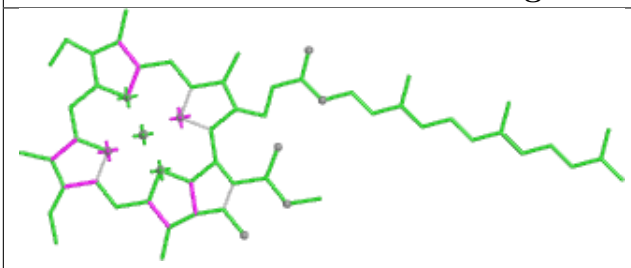


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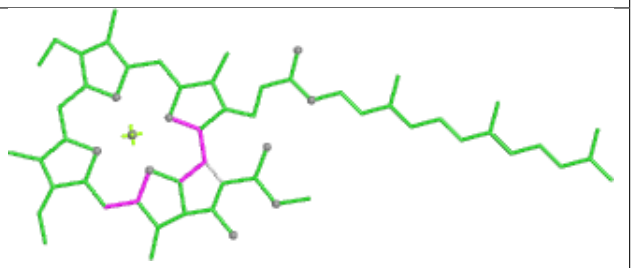


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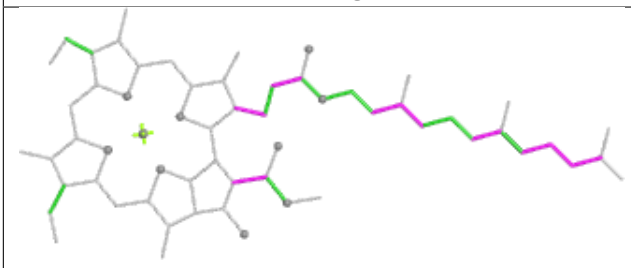
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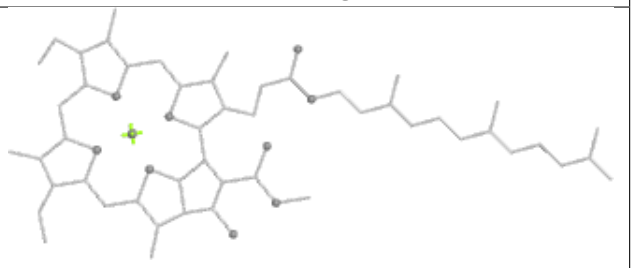
Bond lengths



Bond angles

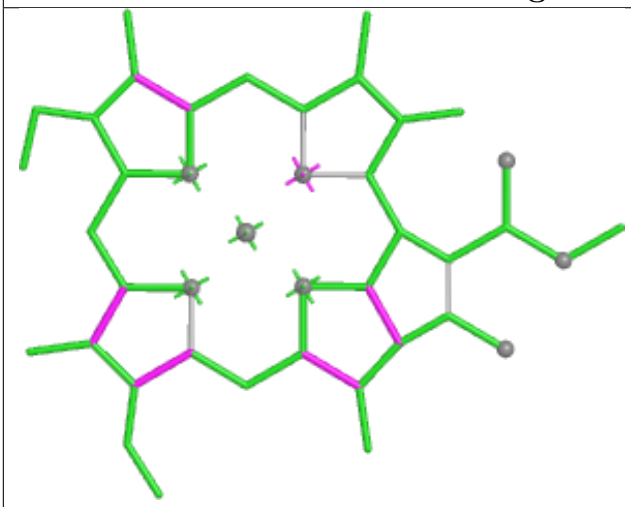


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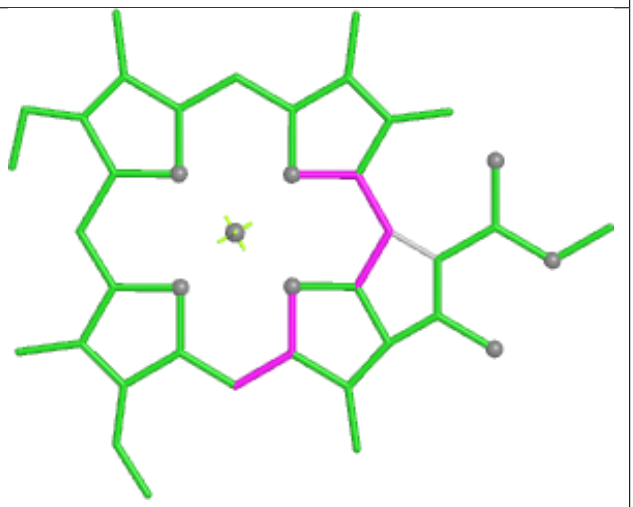


Rings

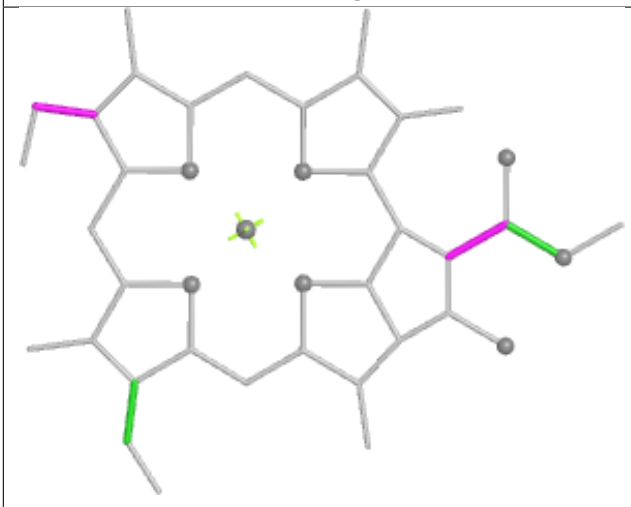
Ligand CLA 2 309



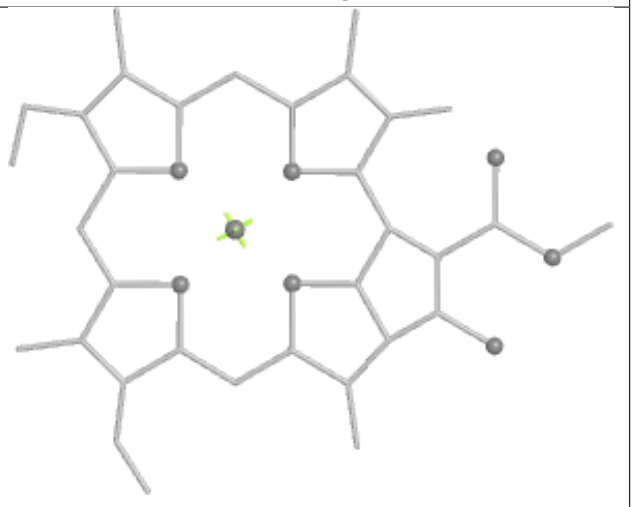
Bond lengths



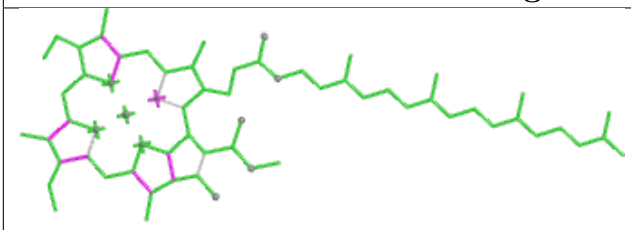
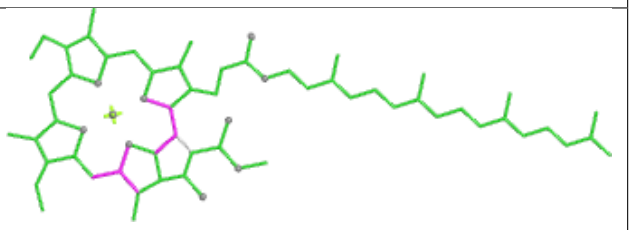
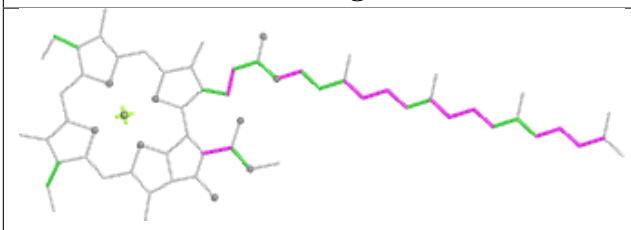
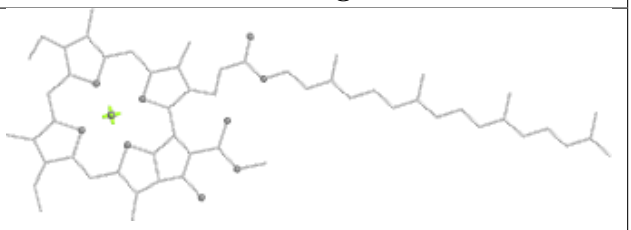
Bond angles

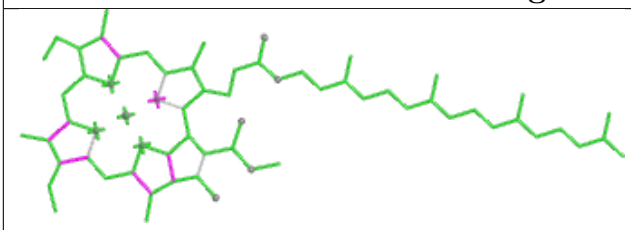
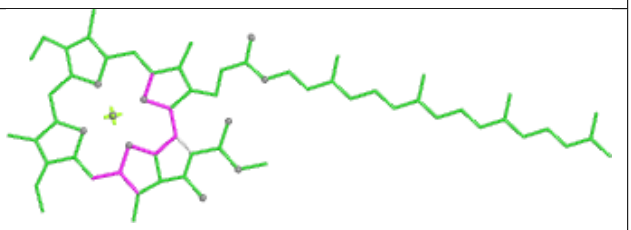
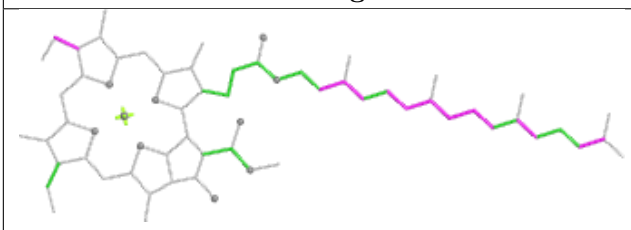
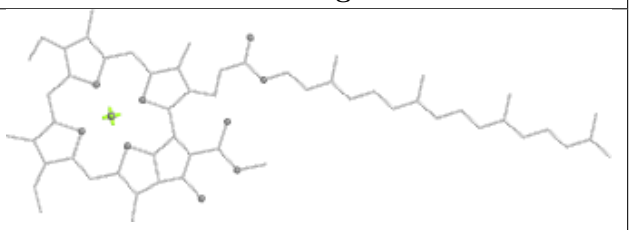


Torsions

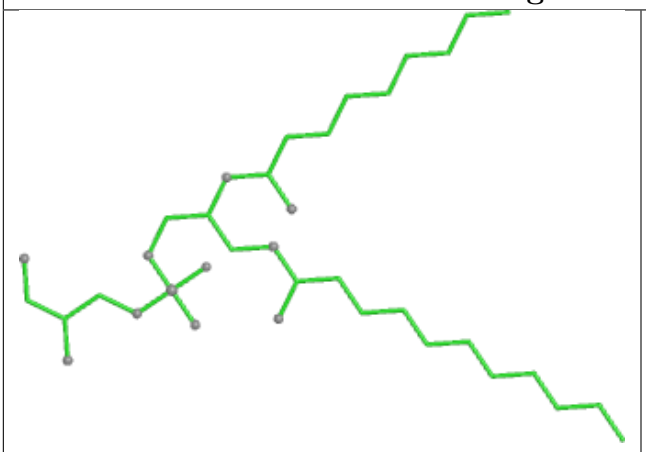


Rings

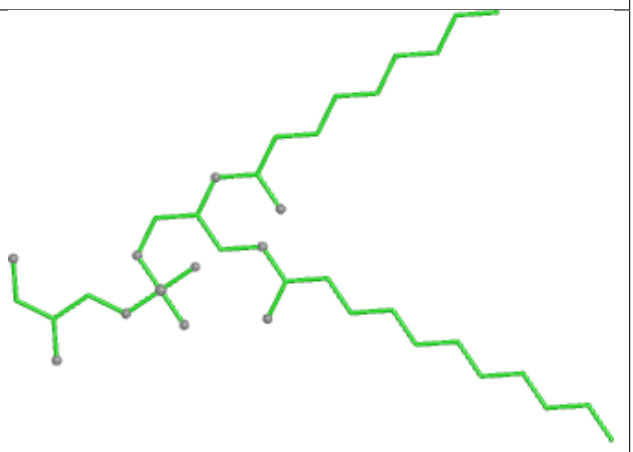
Ligand CLA A 850	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 2 311	
	
Bond lengths	Bond angles
	
Torsions	Rings

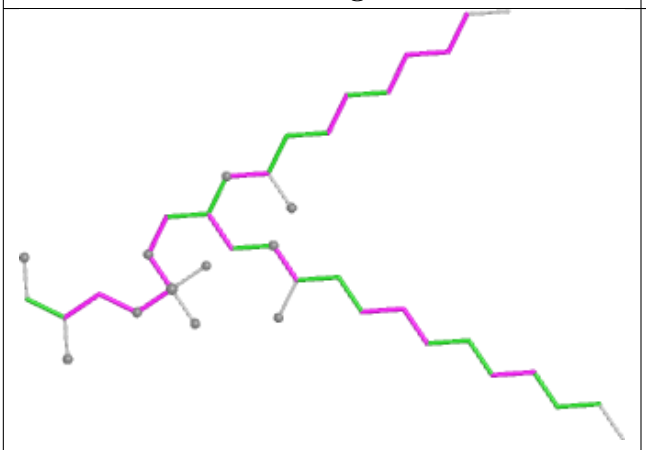
Ligand LHG 2 317



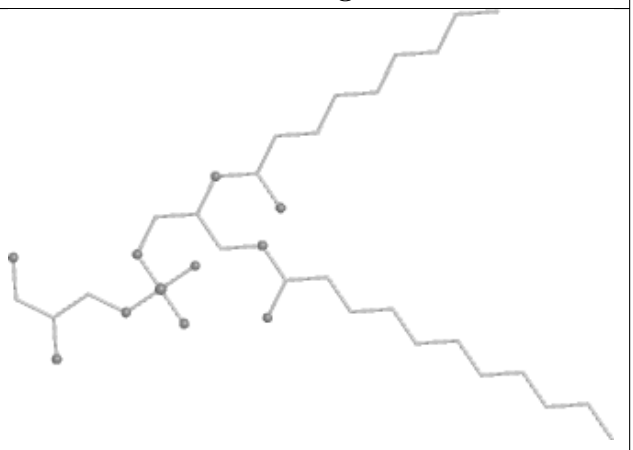
Bond lengths



Bond angles

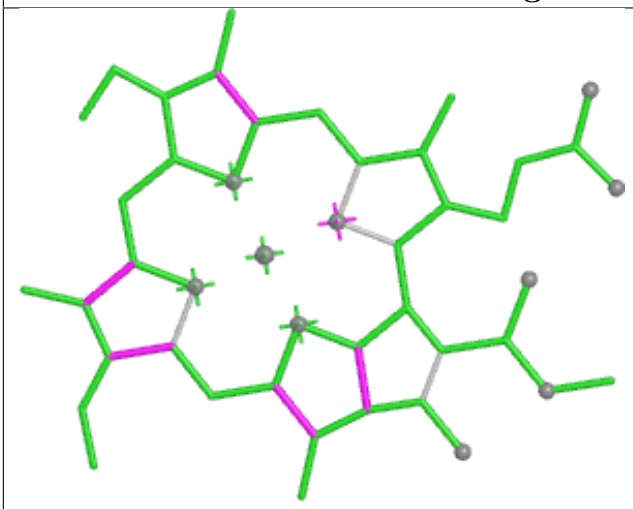


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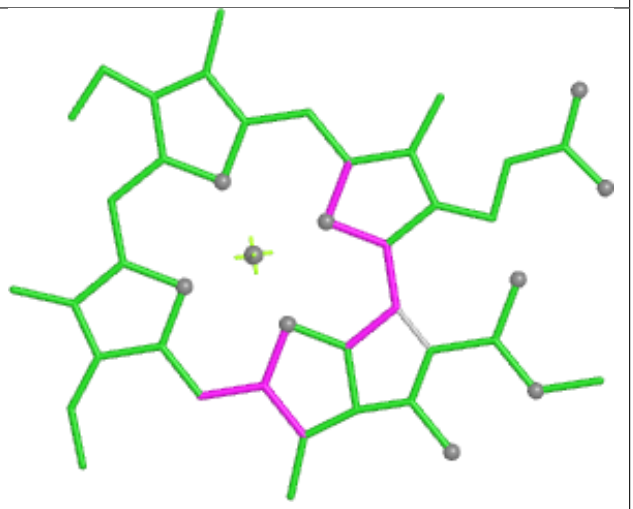


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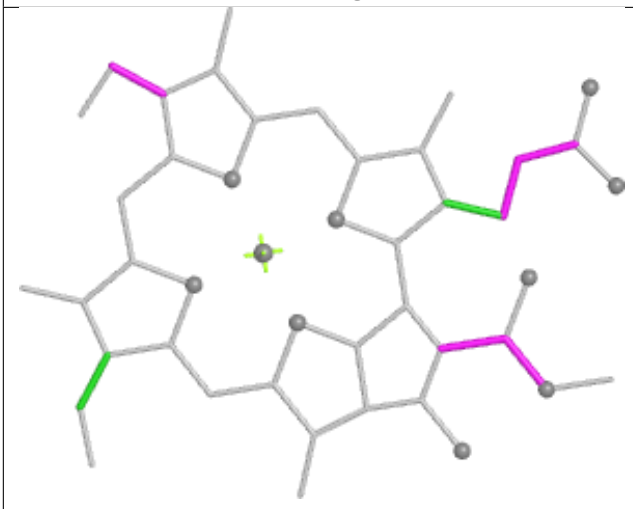
Ligand CLA O 102



Bond lengths



Bond angles

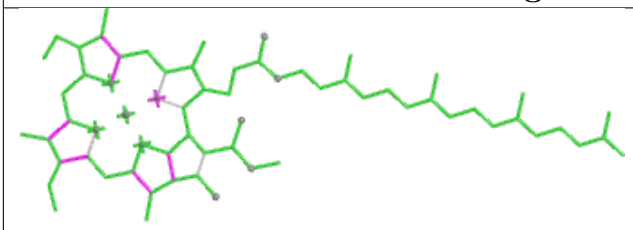


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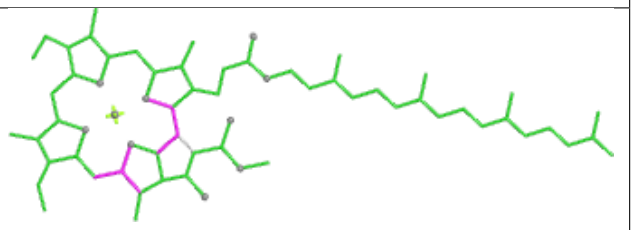


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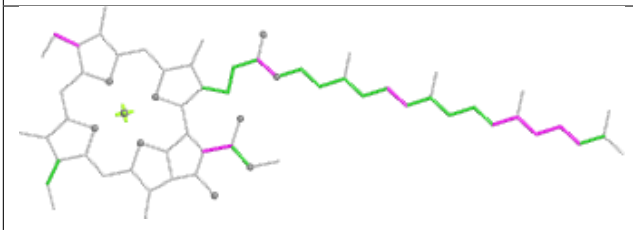
Ligand CLA B 836



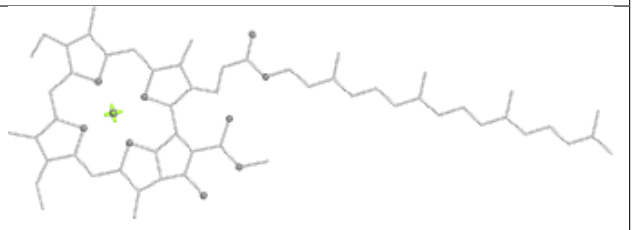
Bond lengths



Bond angles

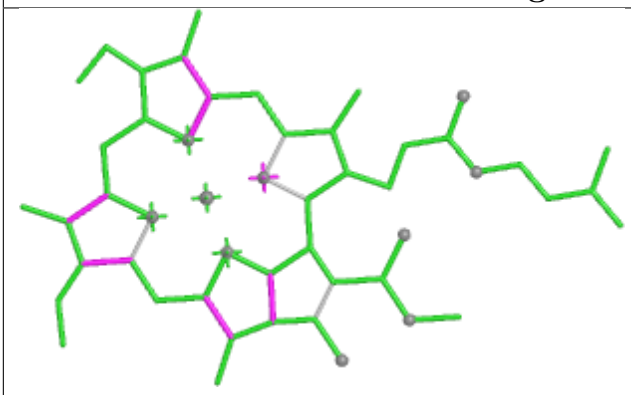


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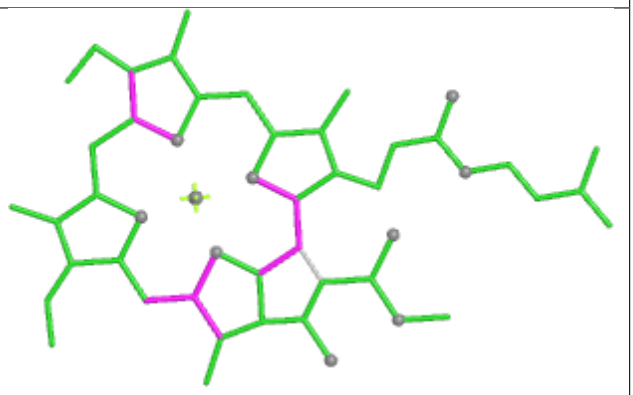


Rings

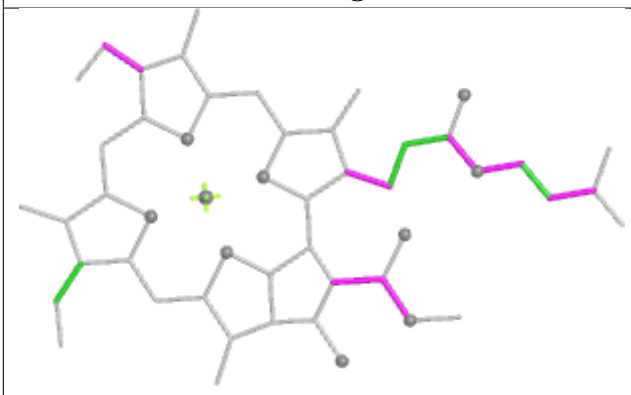
Ligand CLA 3 308



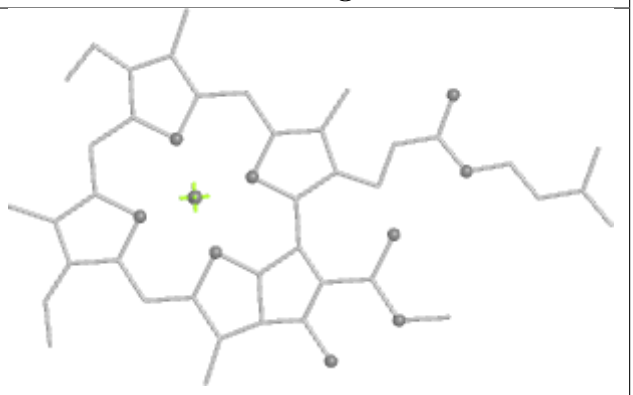
Bond lengths



Bond angles

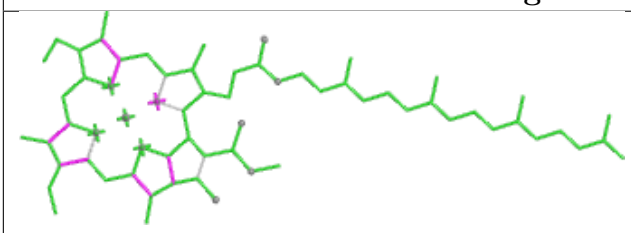


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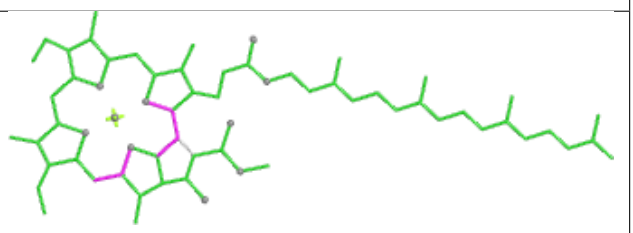


Rings

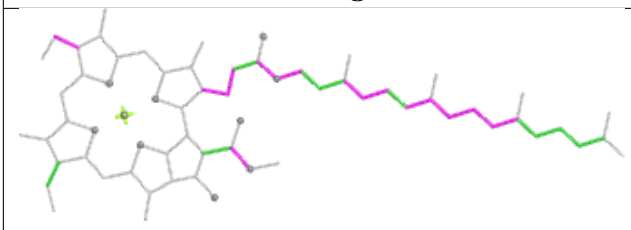
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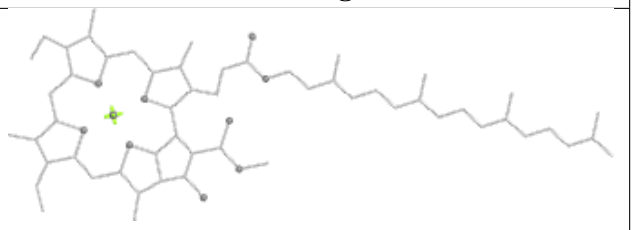
Bond lengths



Bond angles

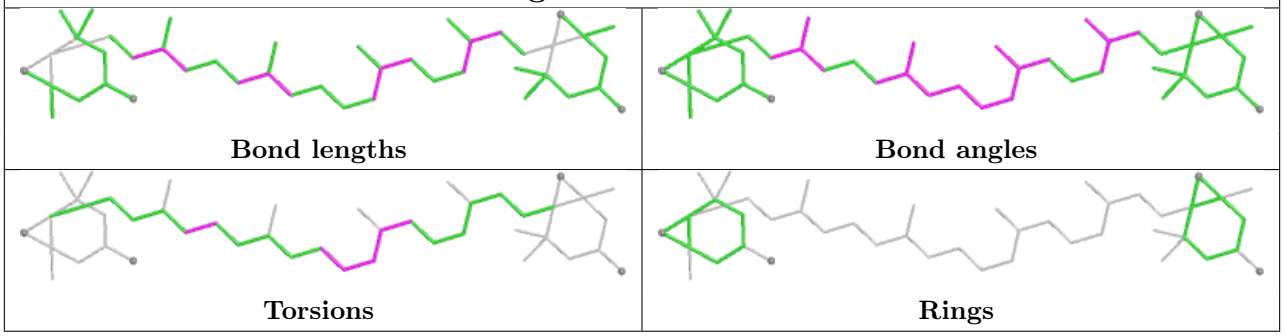


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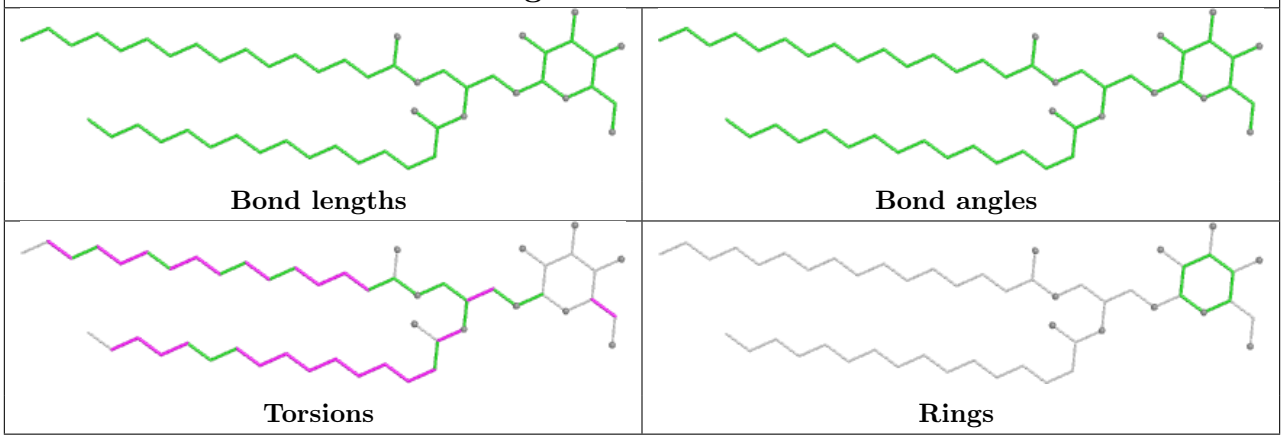


Rings

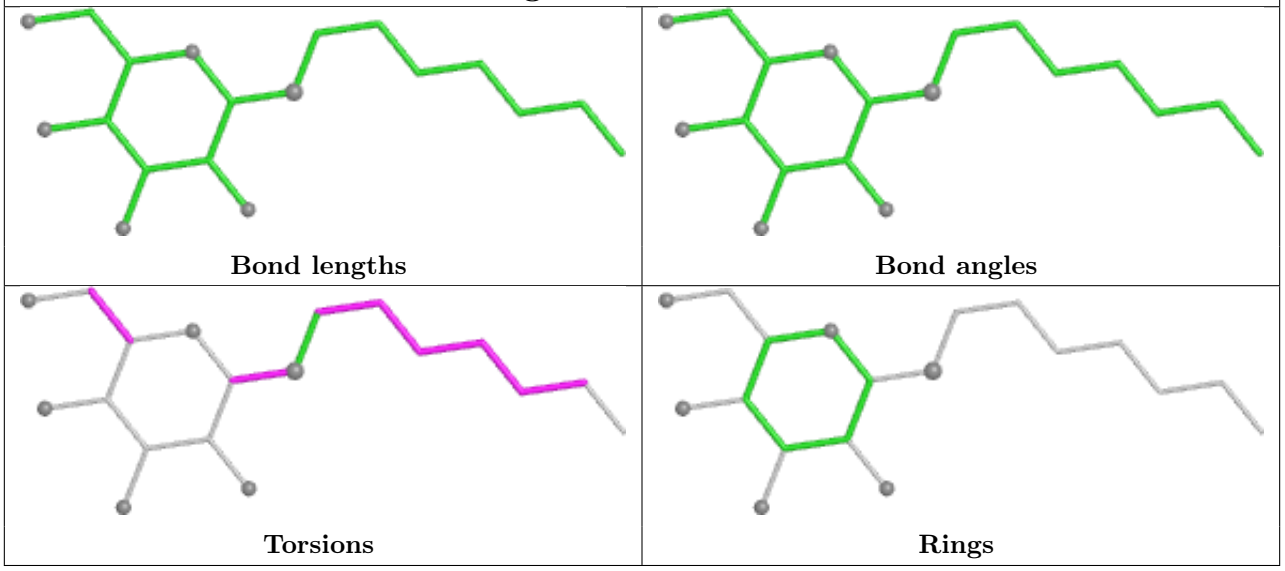
Ligand XAT 3 314



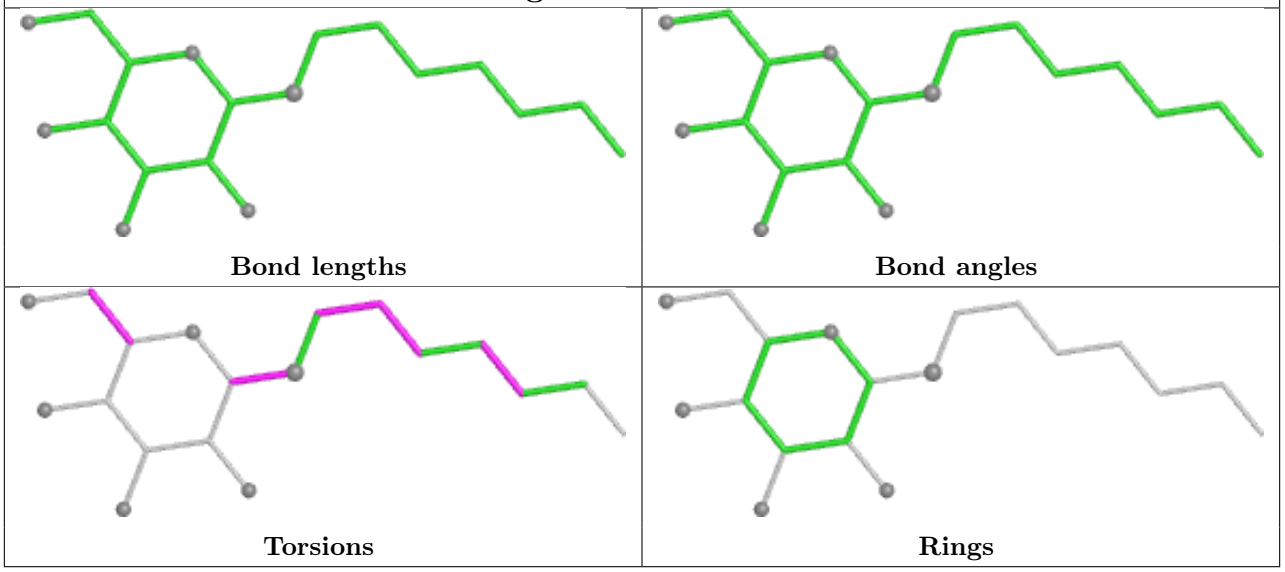
Ligand LMG J 101



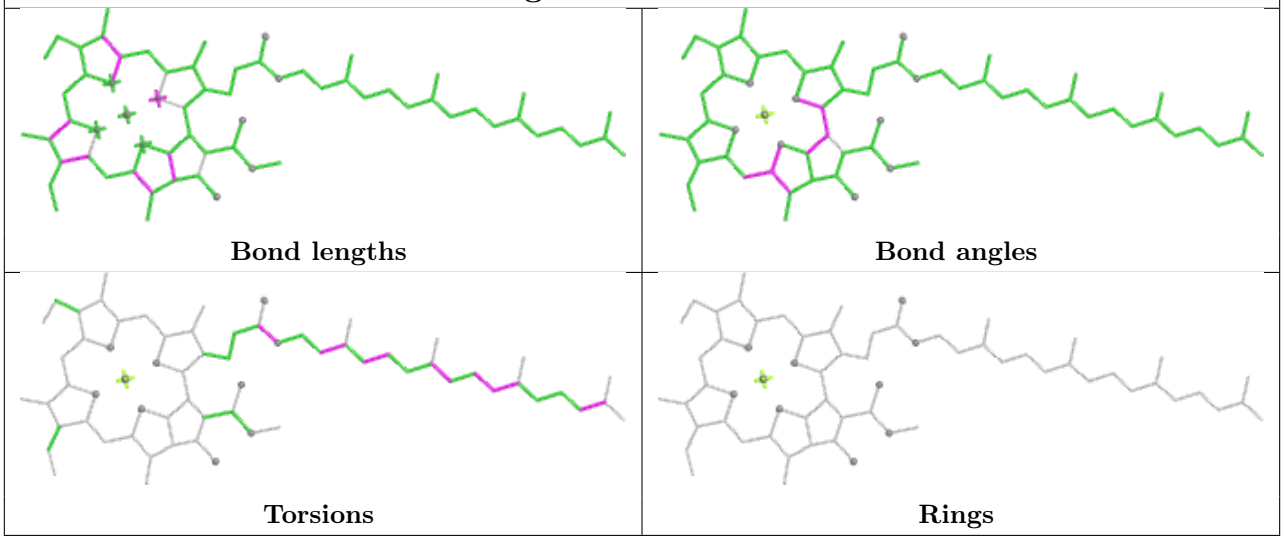
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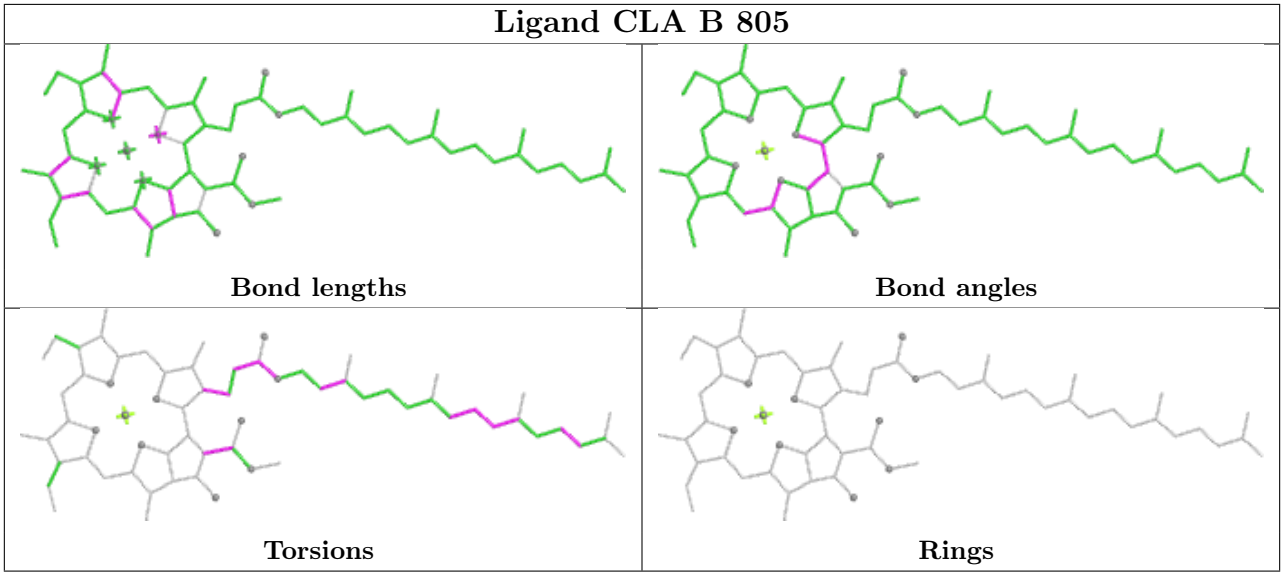
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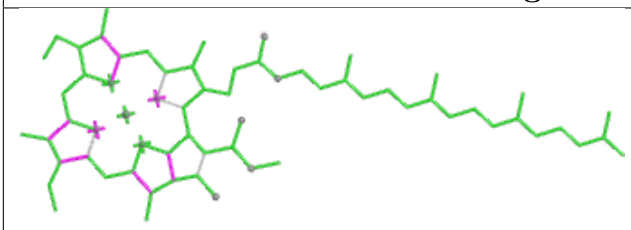
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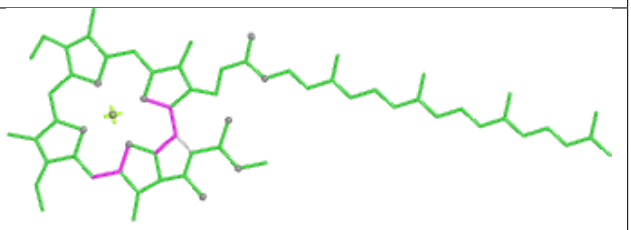
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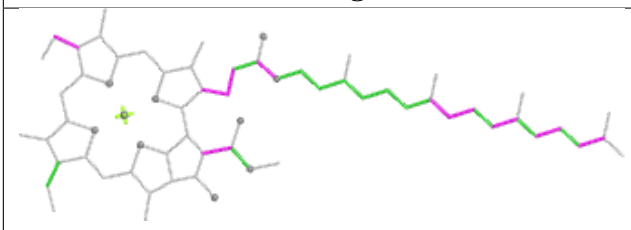
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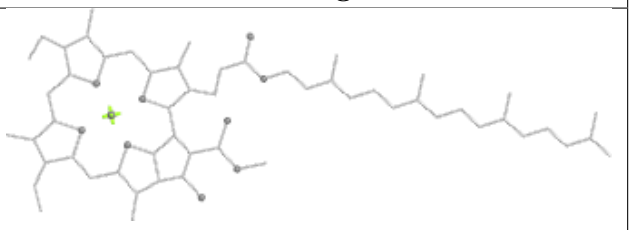
Bond lengths



Bond angles

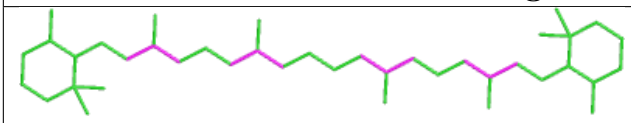


Torsions

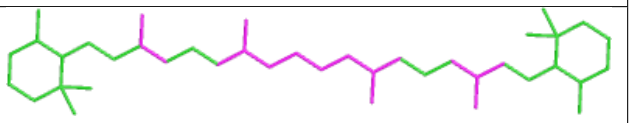


Rings

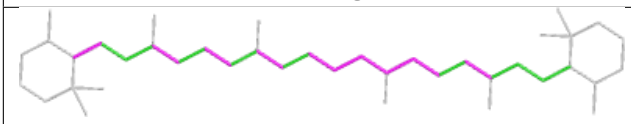
Ligand BCR L 301



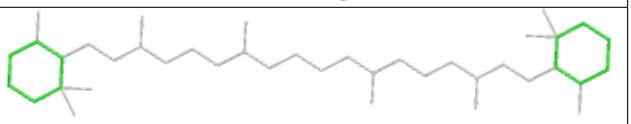
Bond lengths



Bond angles

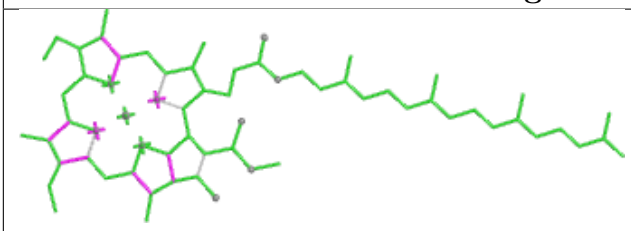


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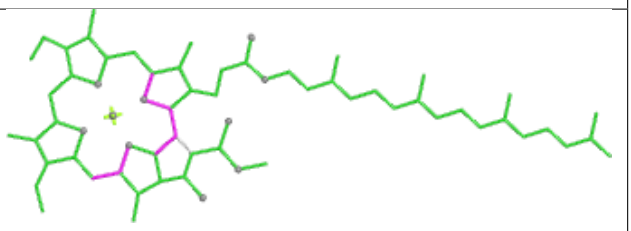


Rings

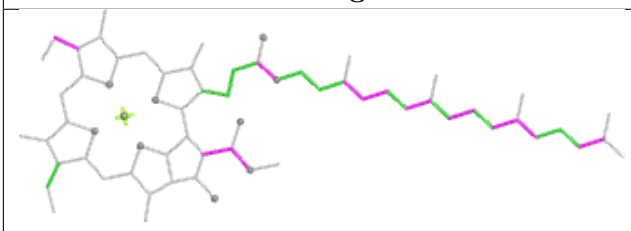
Ligand CLA B 821



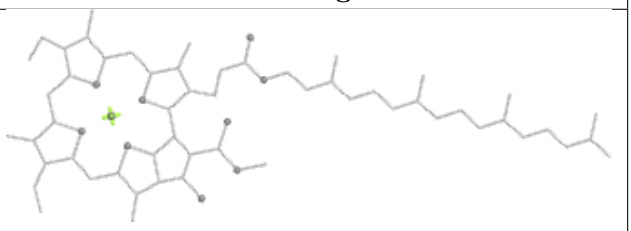
Bond lengths



Bond angles



Torsions

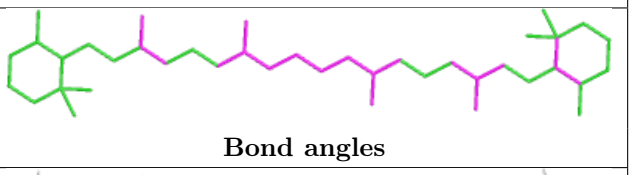


Rings

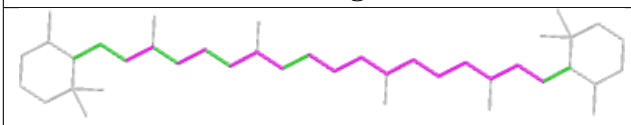
Ligand BCR A 845



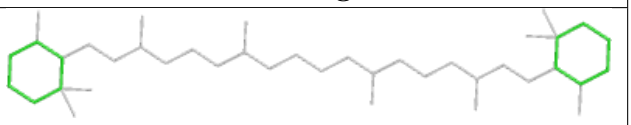
Bond lengths



Bond angles

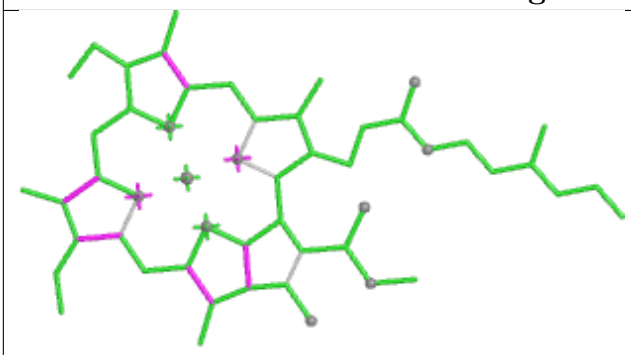


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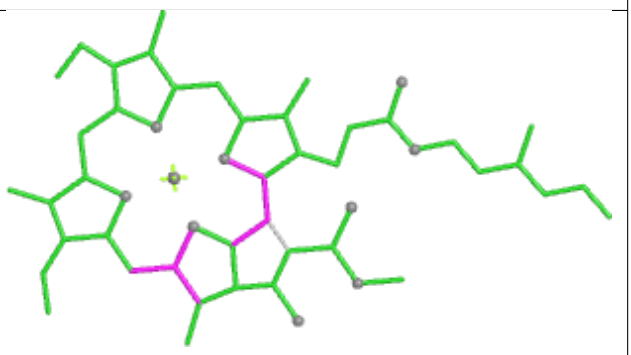


Rings

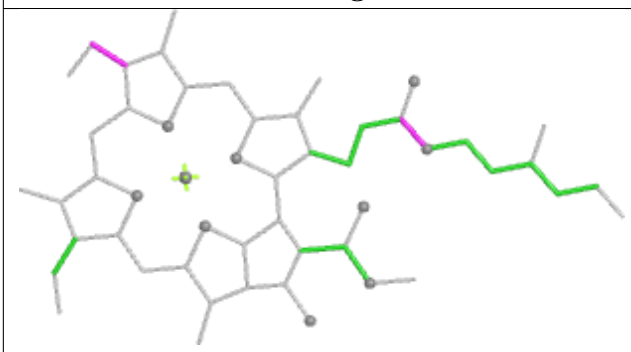
Ligand CLA 3 309



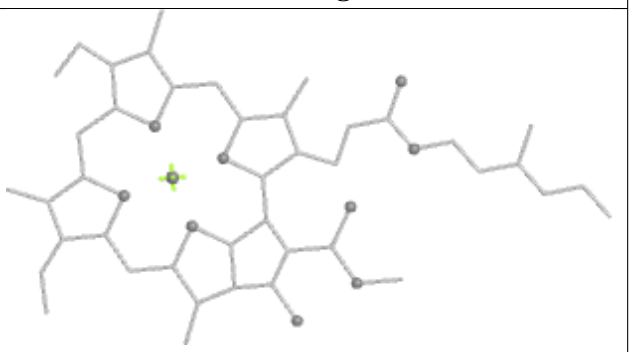
Bond lengths



Bond angles

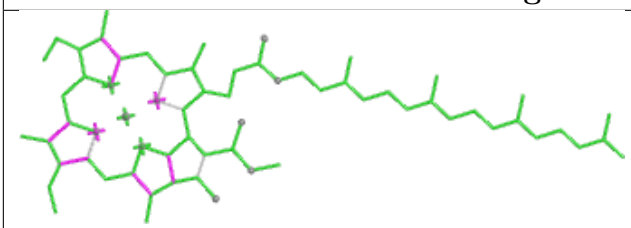


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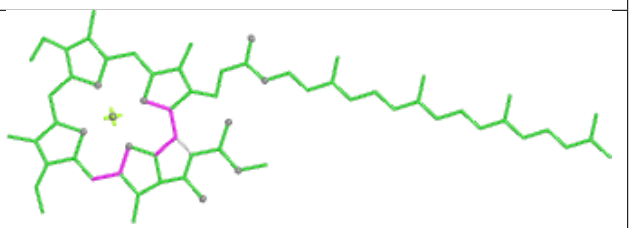


Rings

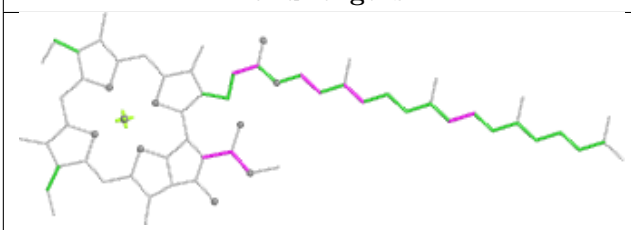
Ligand CLA A 823



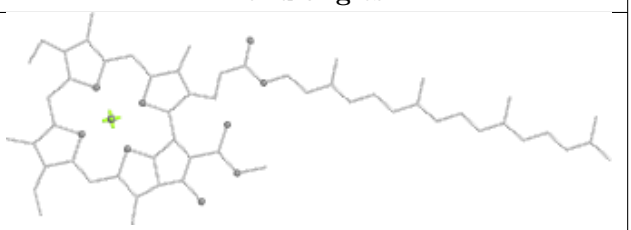
Bond lengths



Bond angles

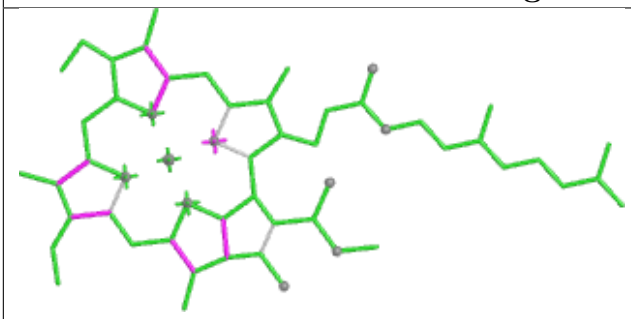


Torsions

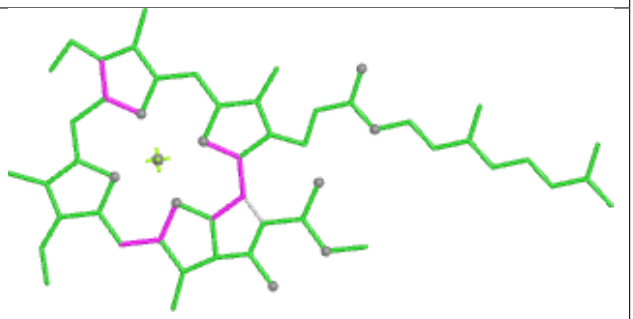


Rings

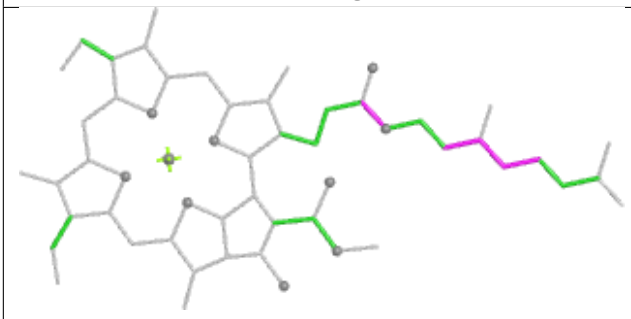
Ligand CLA A 802



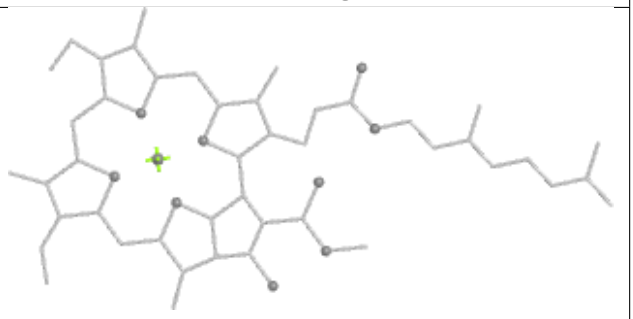
Bond lengths



Bond angles

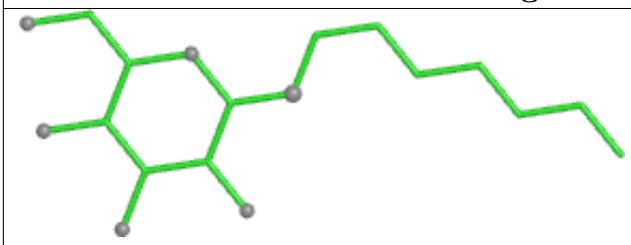


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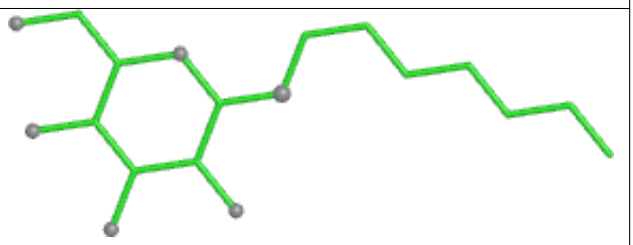


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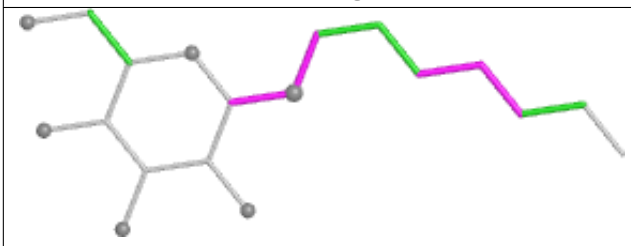
Ligand HTG B 848



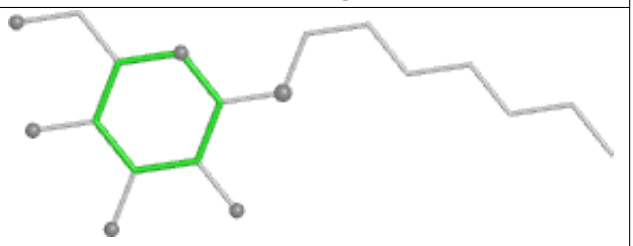
Bond lengths



Bond angles

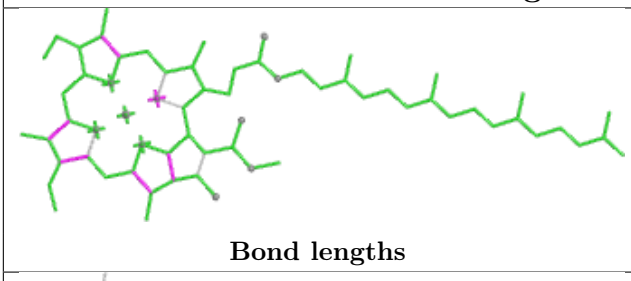


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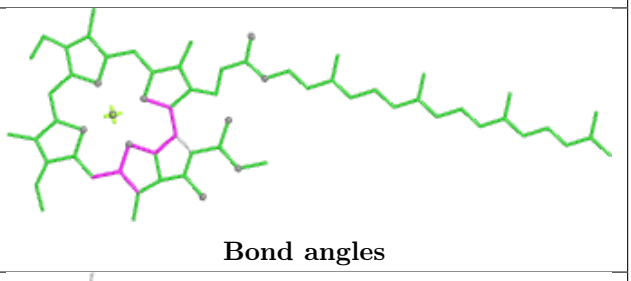


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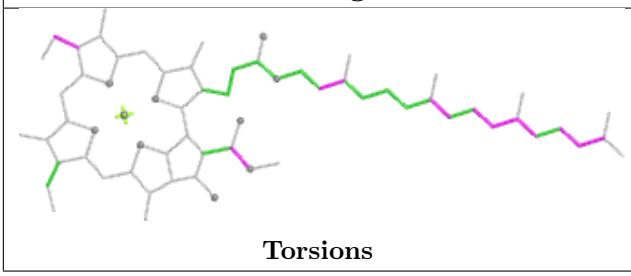
Ligand CLA A 826



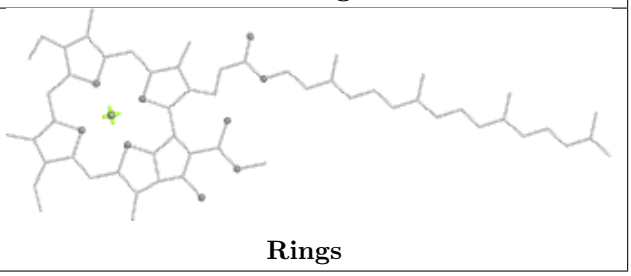
Bond lengths



Bond angles

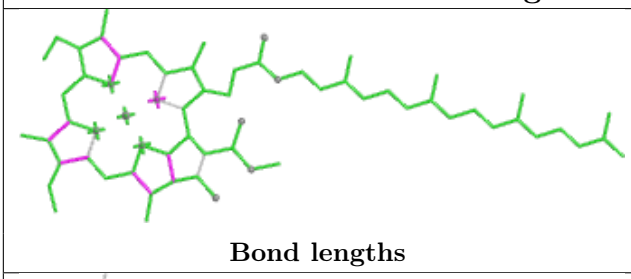


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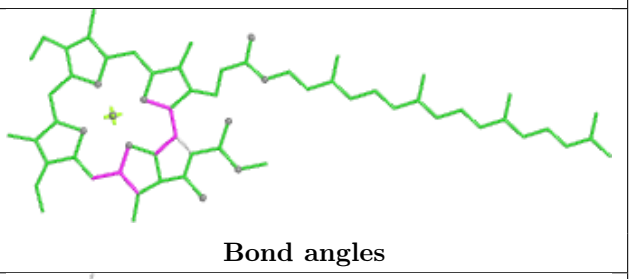


Rings

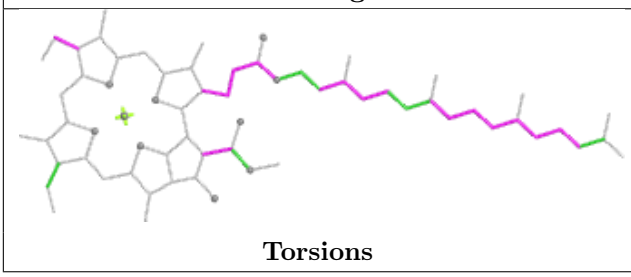
Ligand CLA A 808



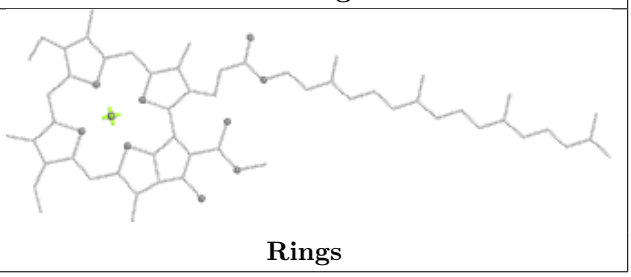
Bond lengths



Bond angles

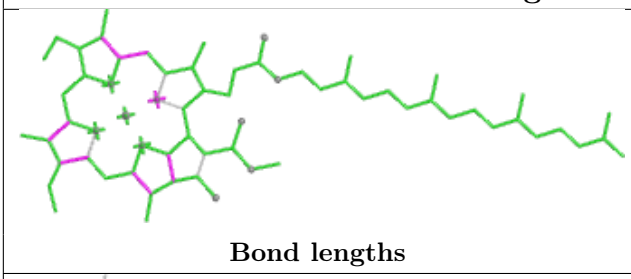


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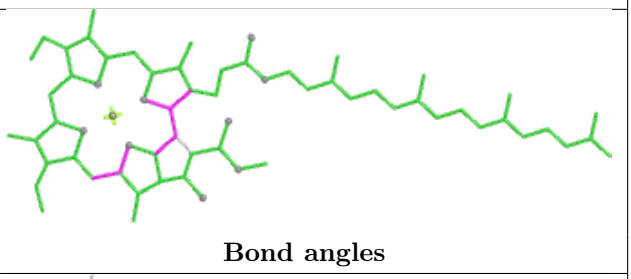


Rings

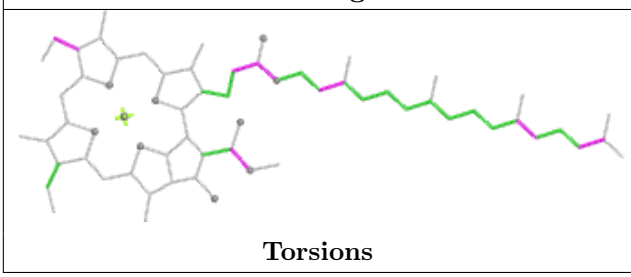
Ligand CLA A 801



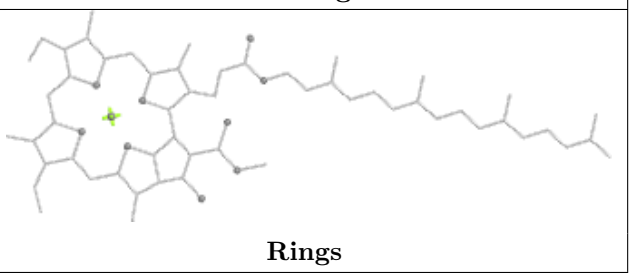
Bond lengths



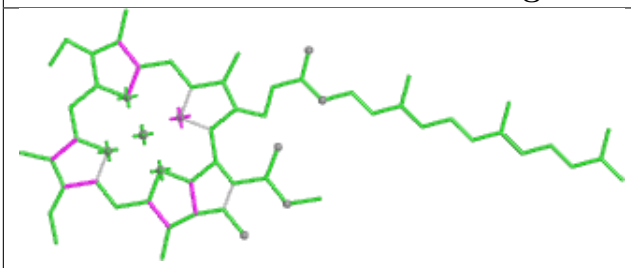
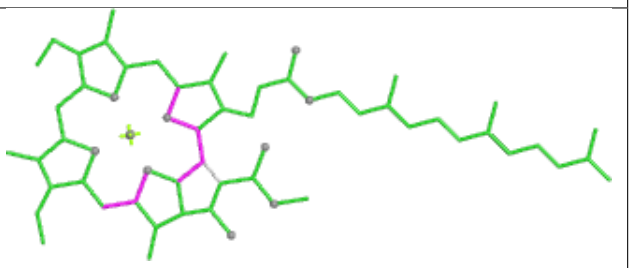
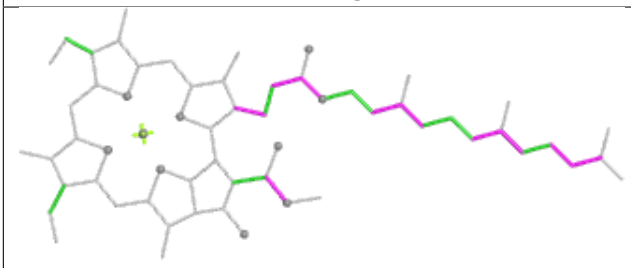
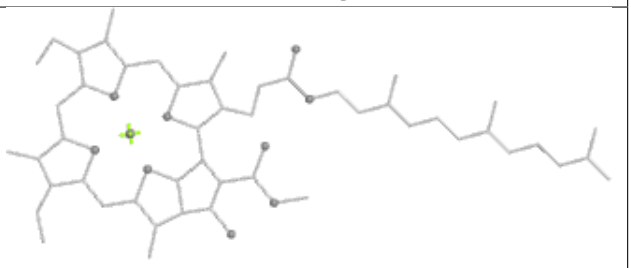
Bond angles

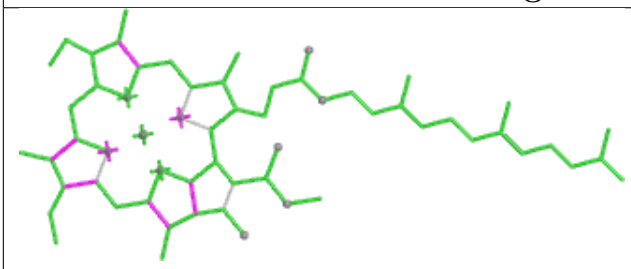
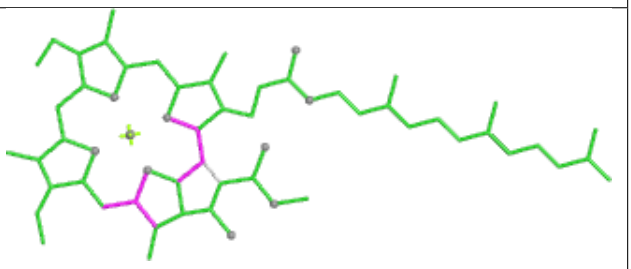
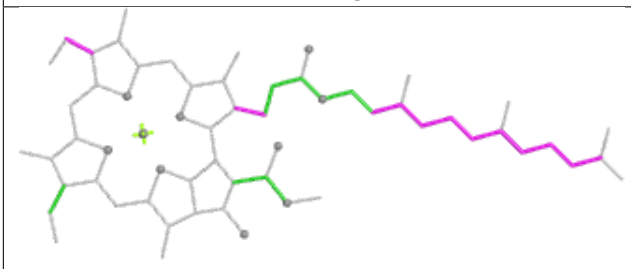
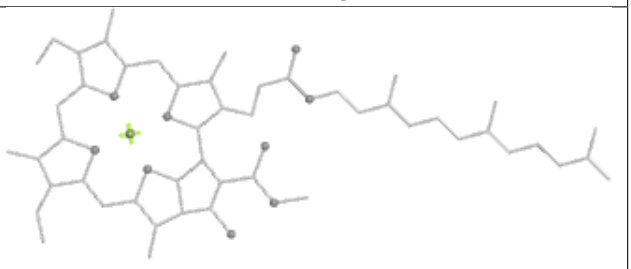


Torsions

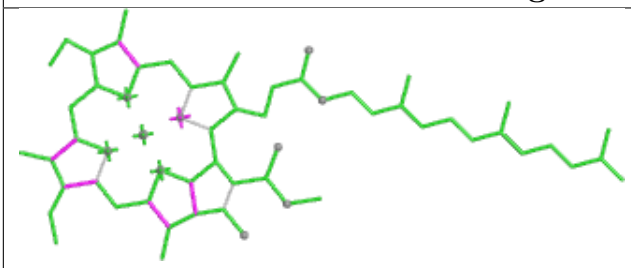


Rings

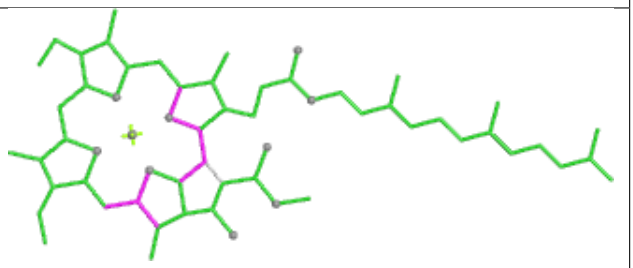
Ligand CLA K 303	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA B 818	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

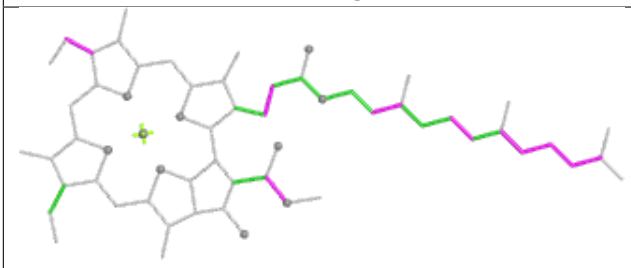
Ligand CLA 1 311



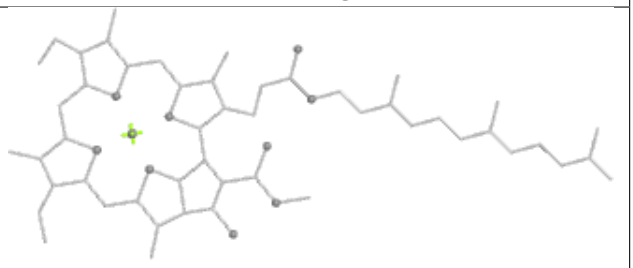
Bond lengths



Bond angles

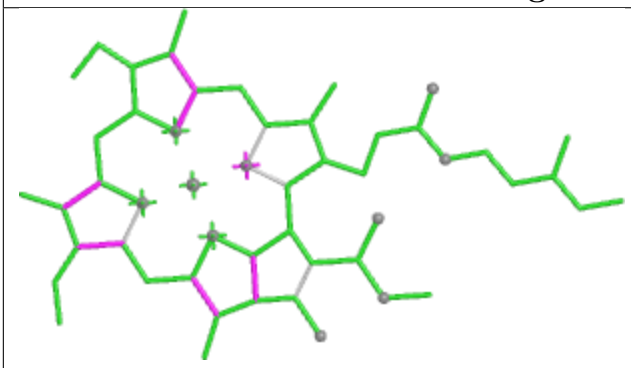


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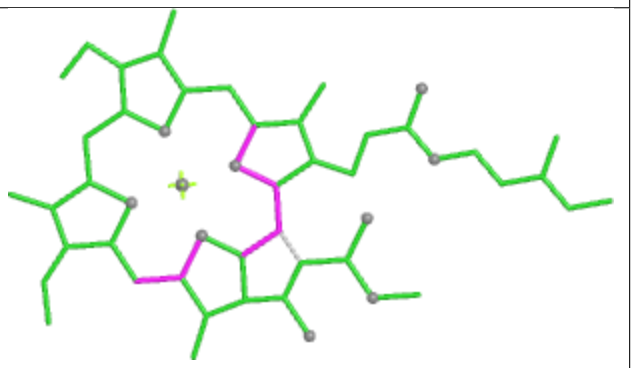


Rings

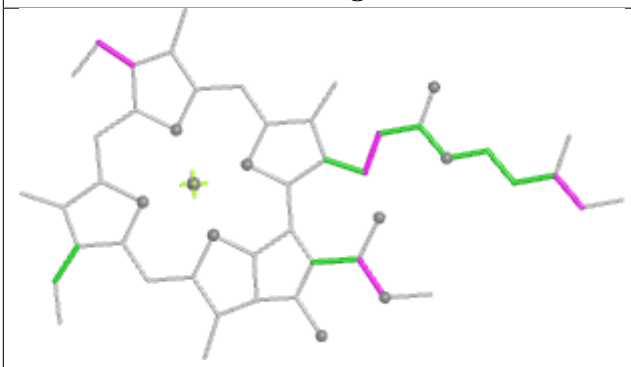
Ligand CLA 1 303



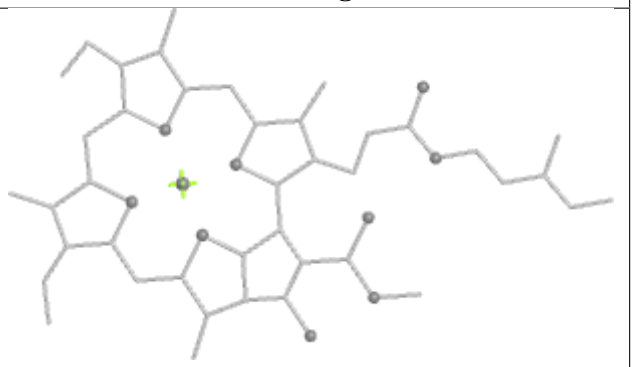
Bond lengths



Bond angles

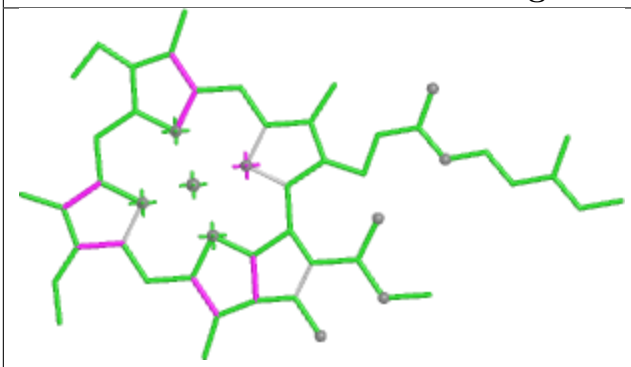


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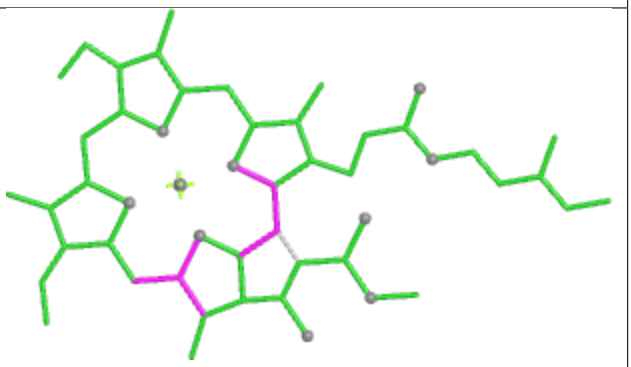


Rings

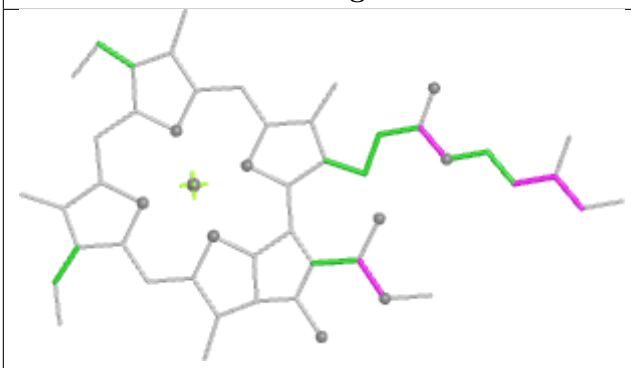
Ligand CLA 2 302



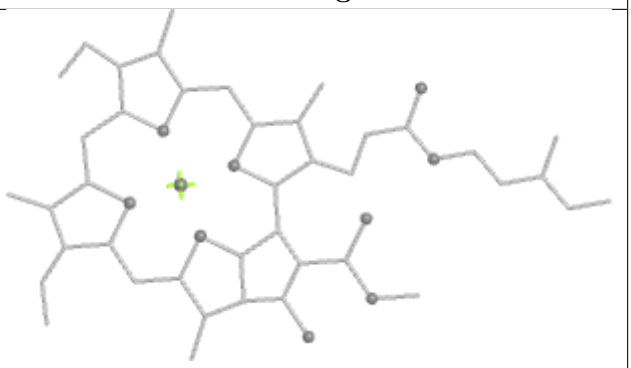
Bond lengths



Bond angles

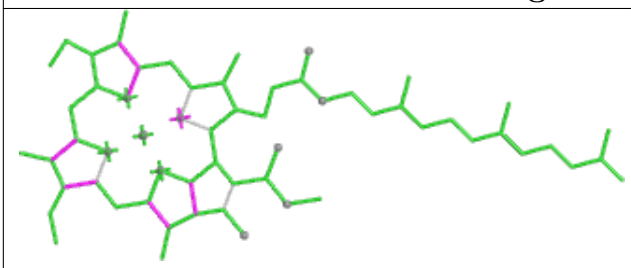


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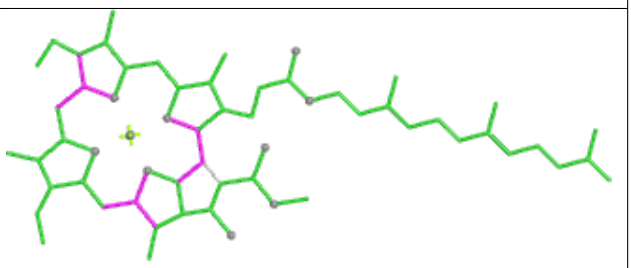


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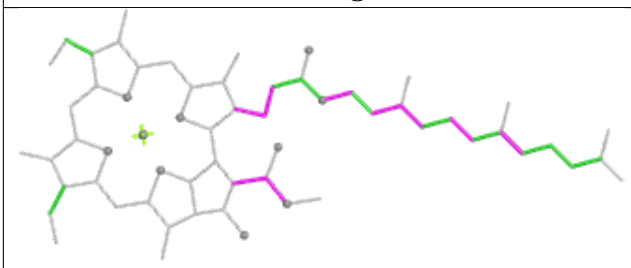
Ligand CLA 4 309



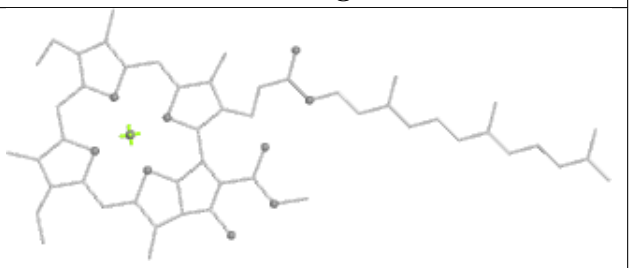
Bond lengths



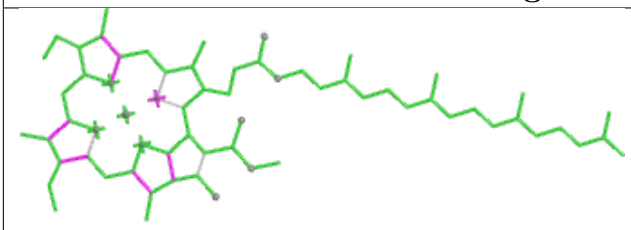
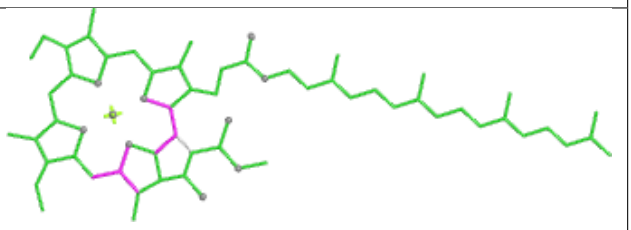
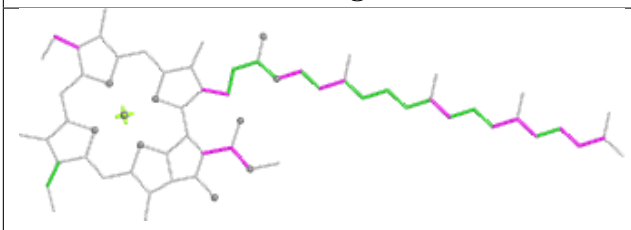
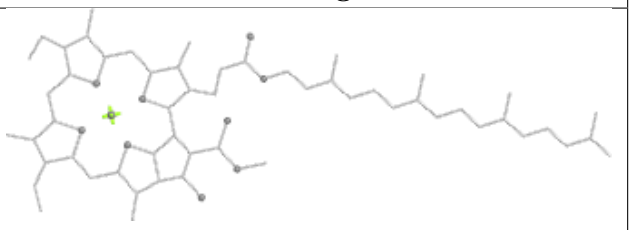
Bond angles

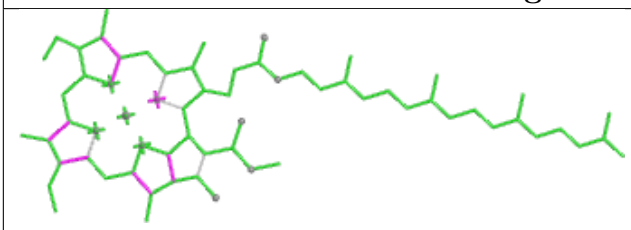
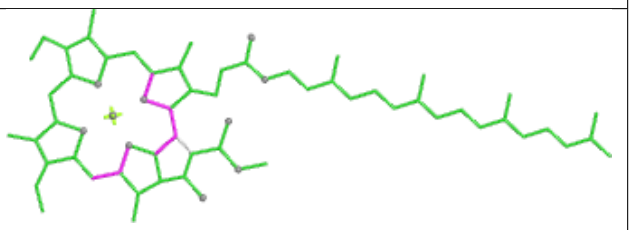
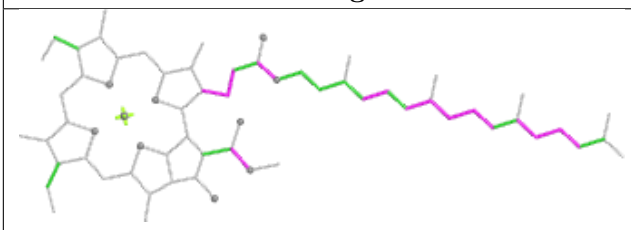
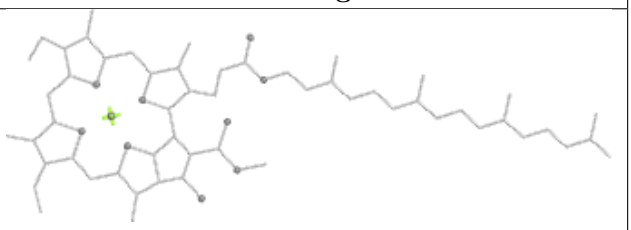


Torsions

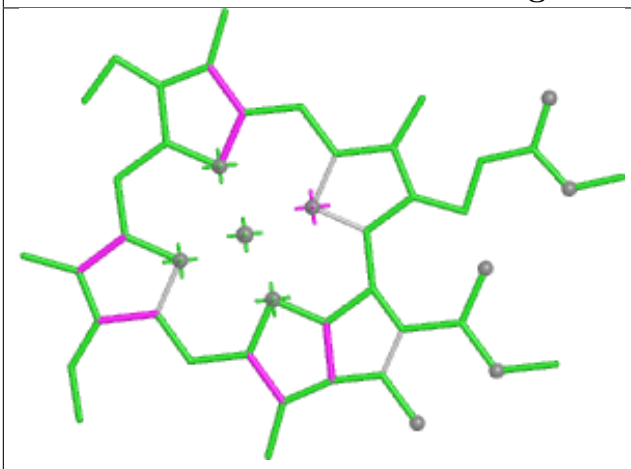


Rings

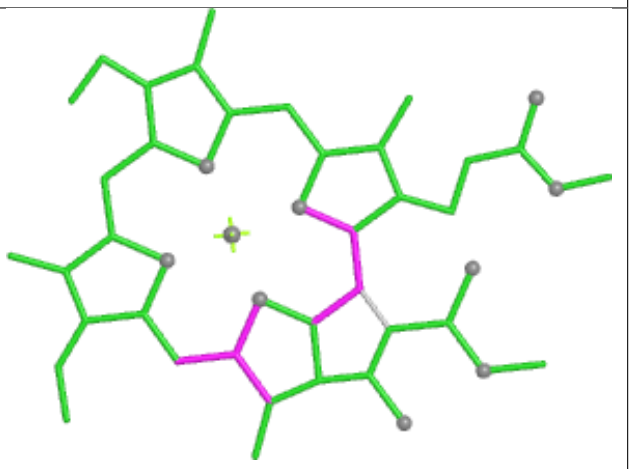
Ligand CLA A 830	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 809	
	
Bond lengths	Bond angles
	
Torsions	Rings

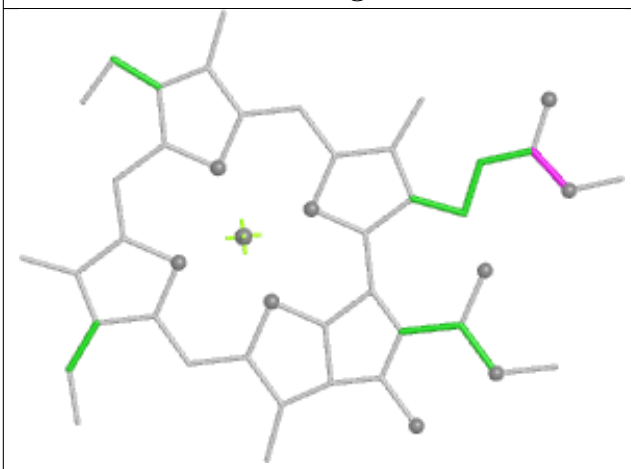
Ligand CLA 3 312



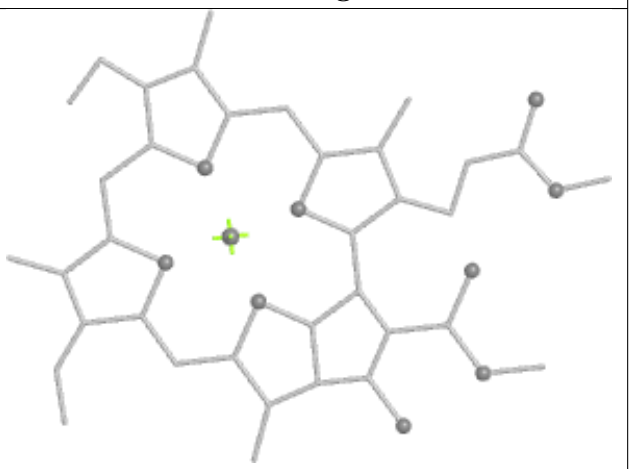
Bond lengths



Bond angles

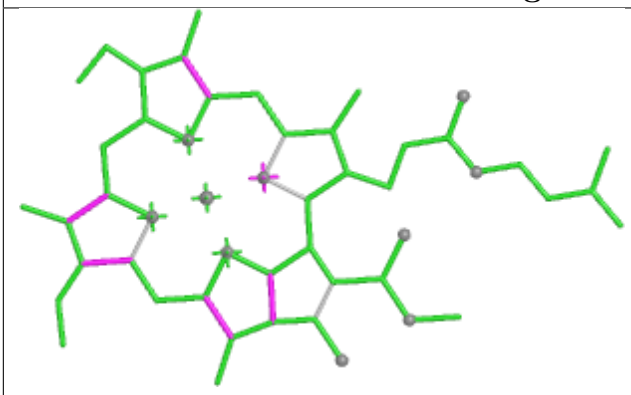


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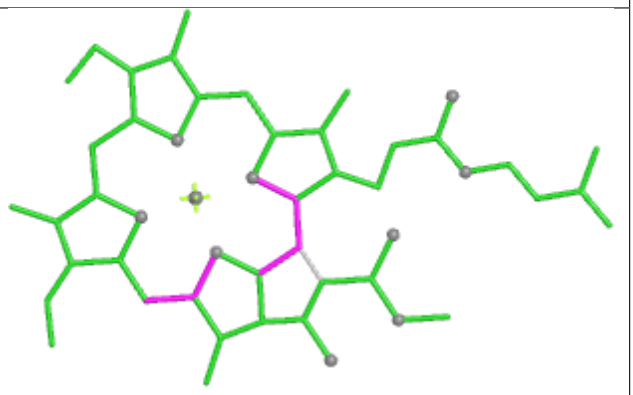


Rings

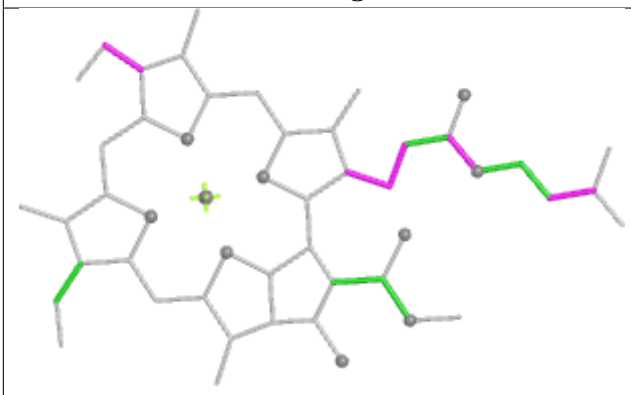
Ligand CLA A 832



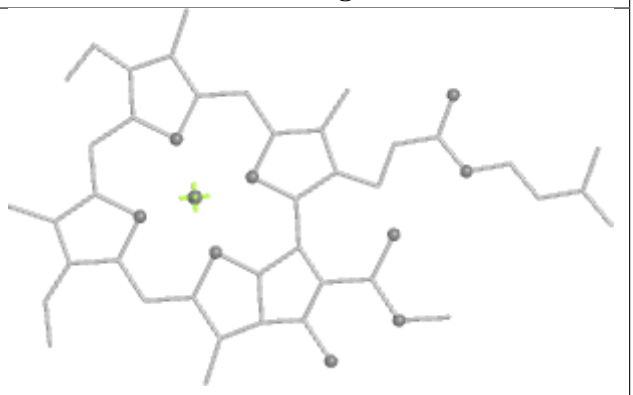
Bond lengths



Bond angles

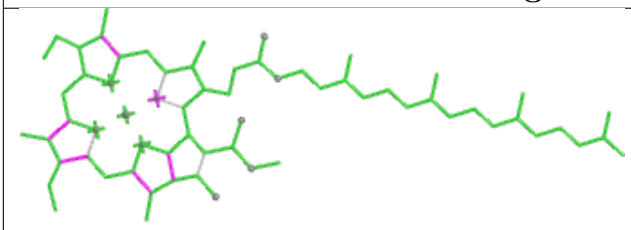


Torsions

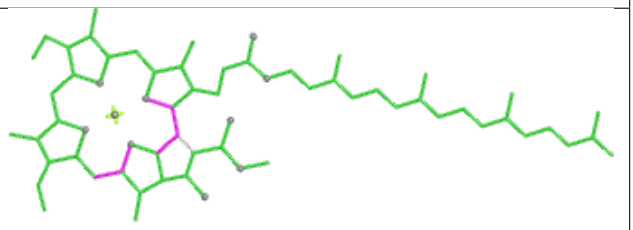


Rings

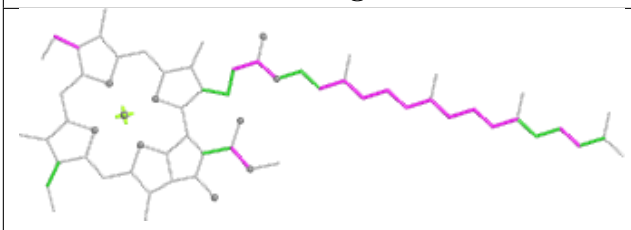
Ligand CLA B 806



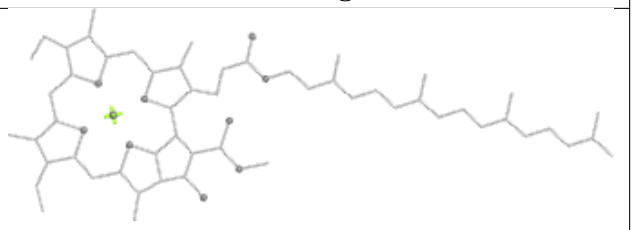
Bond lengths



Bond angles



Torsions

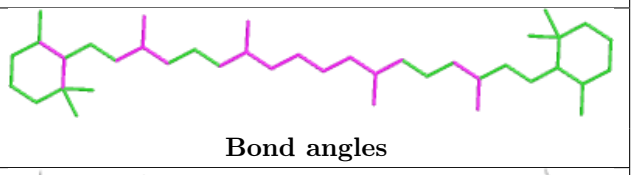


Rings

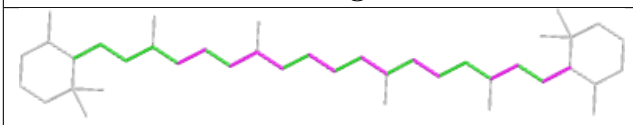
Ligand BCR F 308



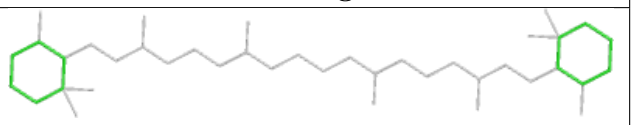
Bond lengths



Bond angles

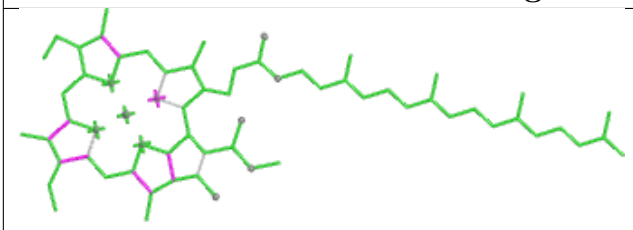


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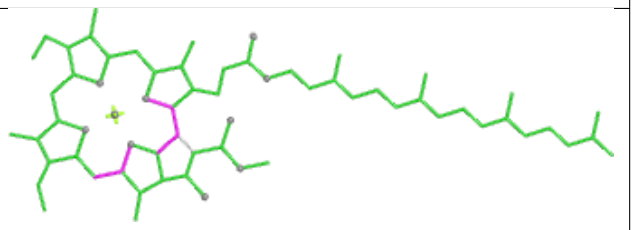


Rings

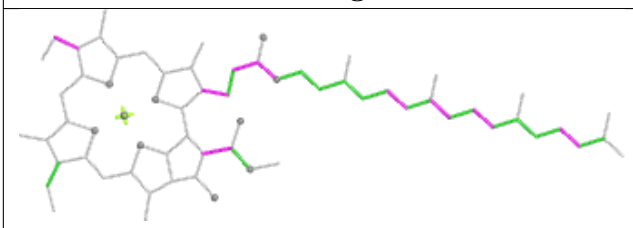
Ligand CLA B 840



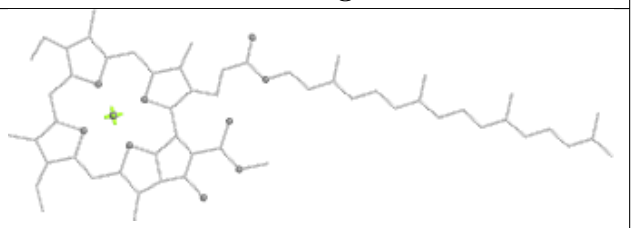
Bond lengths



Bond angles

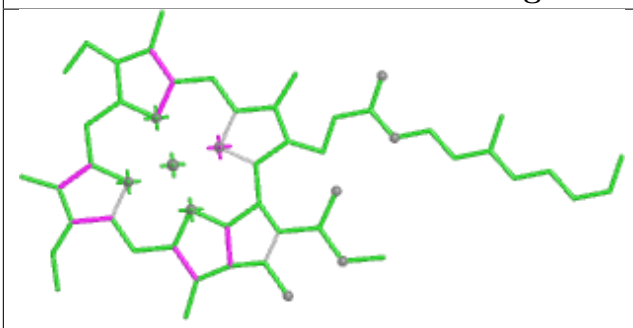


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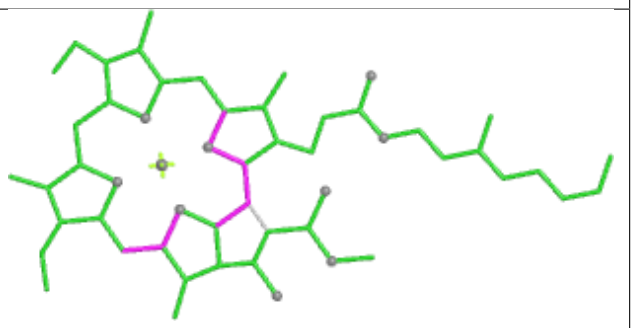


Rings

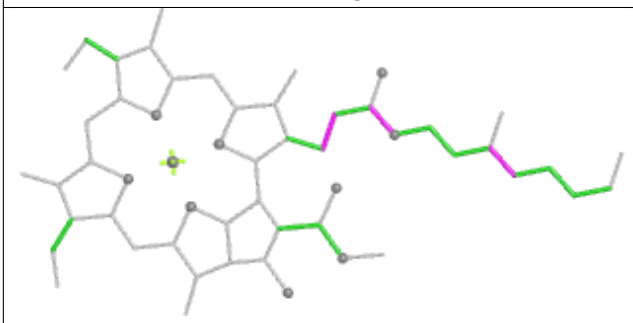
Ligand CLA A 810



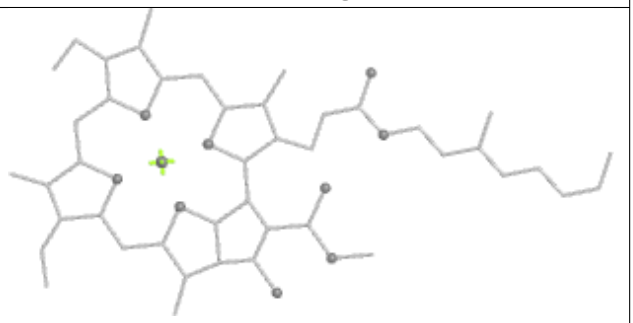
Bond lengths



Bond angles

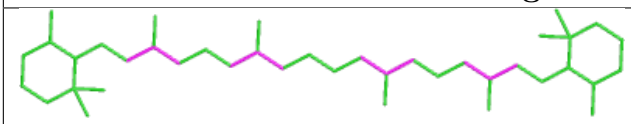


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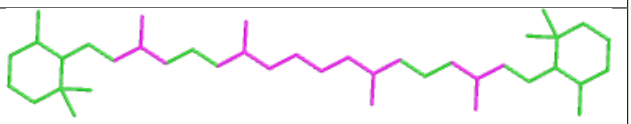


Rings

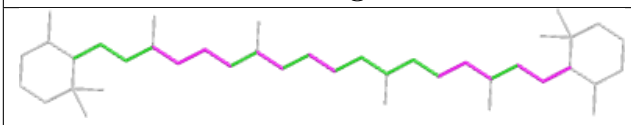
Ligand BCR B 845



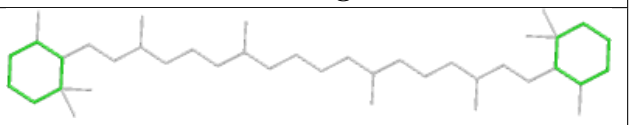
Bond lengths



Bond angles

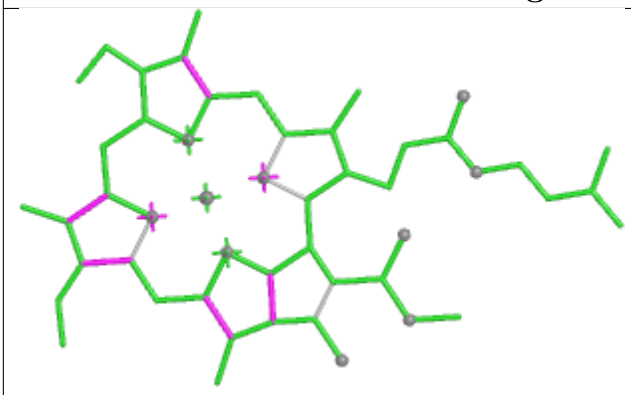


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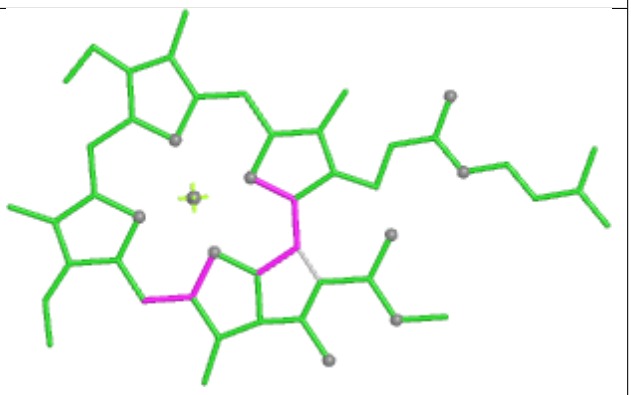


Rings

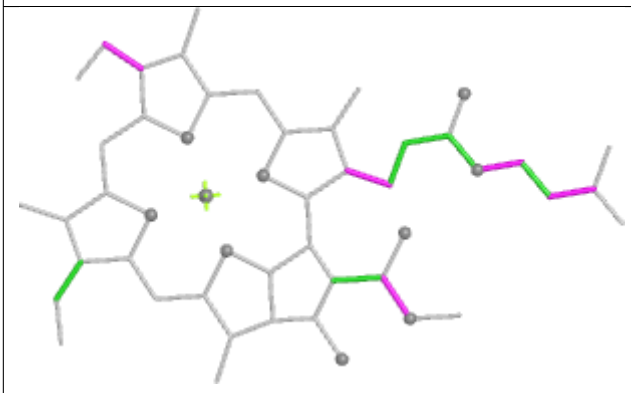
Ligand CLA L 304



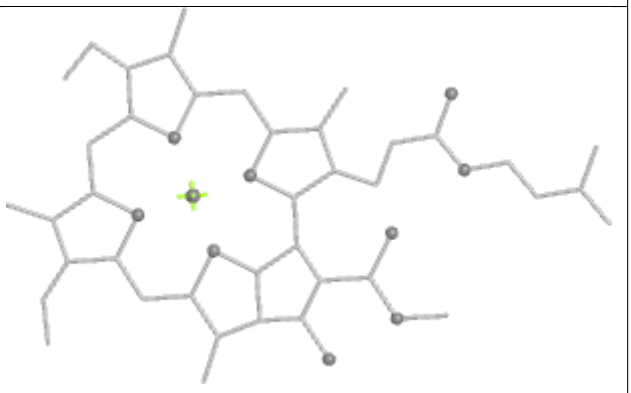
Bond lengths



Bond angles

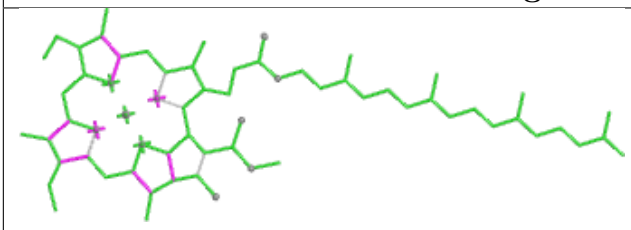


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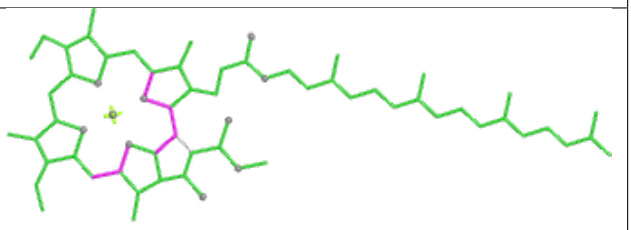


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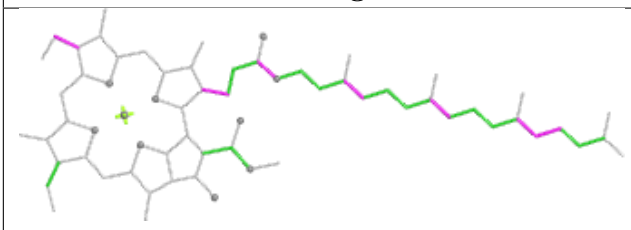
Ligand CLA A 825



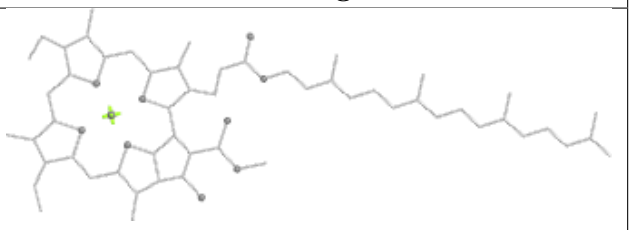
Bond lengths



Bond angles

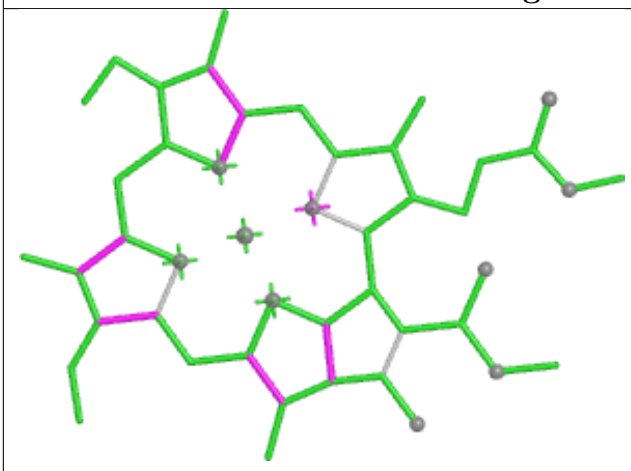


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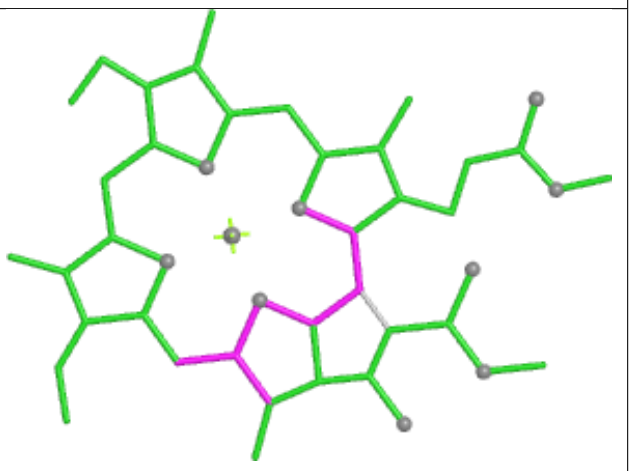


Rings

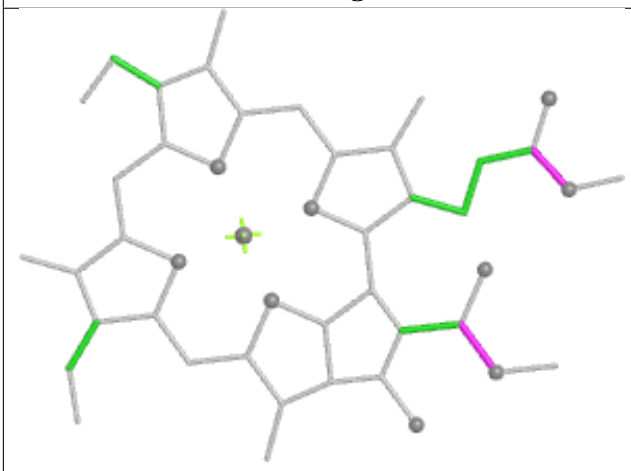
Ligand CLA G 205



Bond lengths



Bond angles

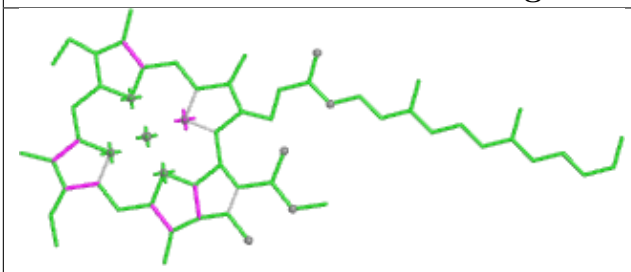


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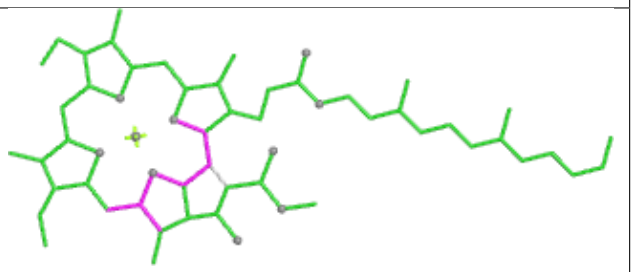


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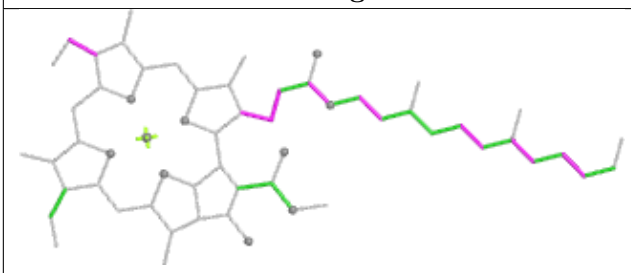
Ligand CLA B 817



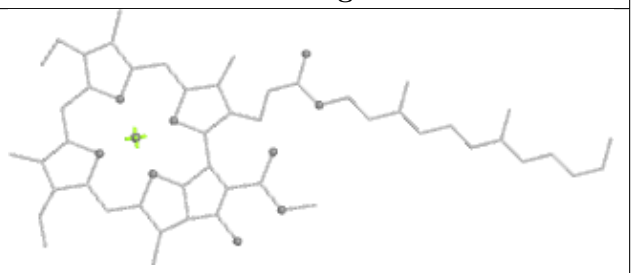
Bond lengths



Bond angles

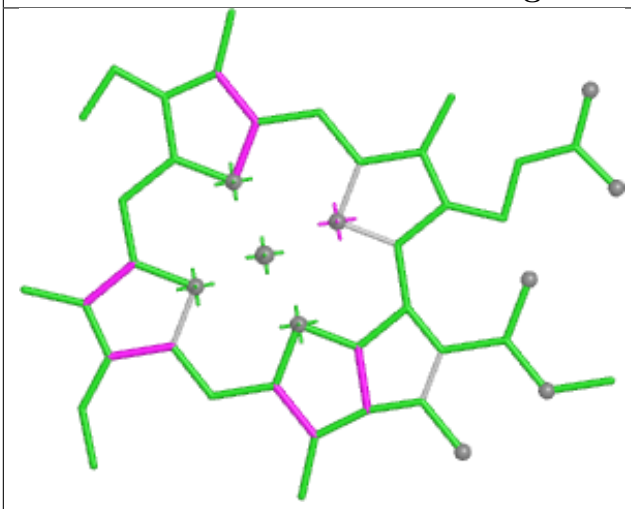


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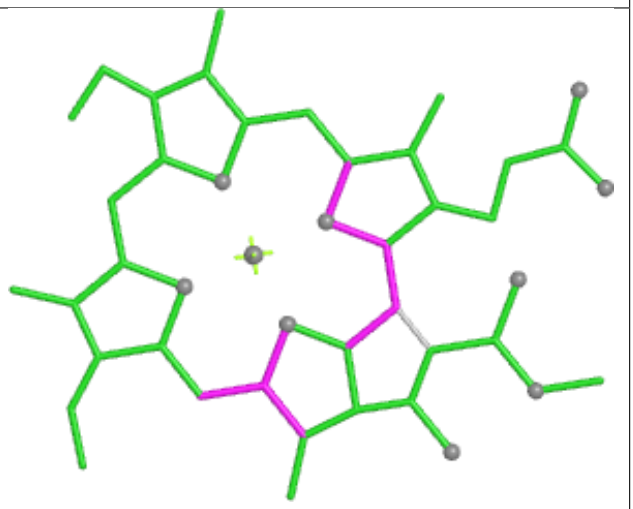


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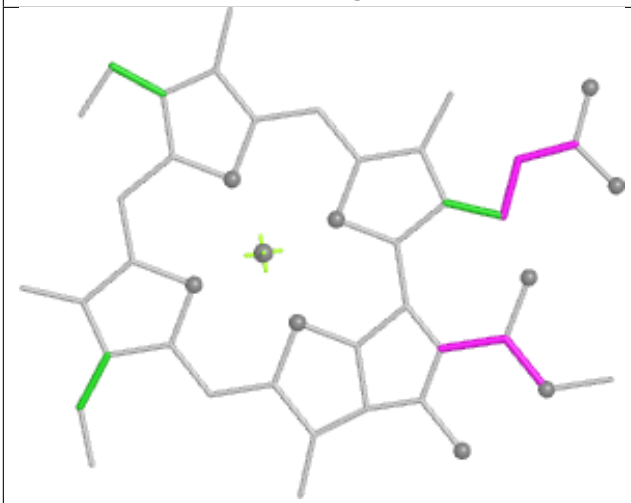
Ligand CLA A 833



Bond lengths



Bond angles

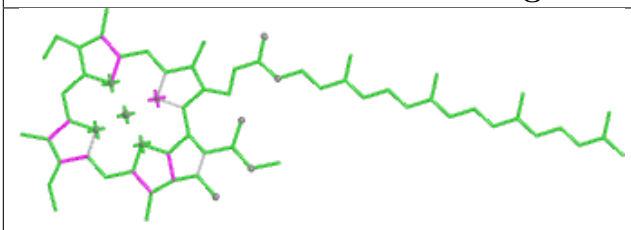


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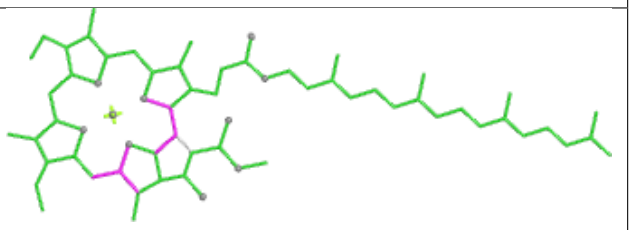


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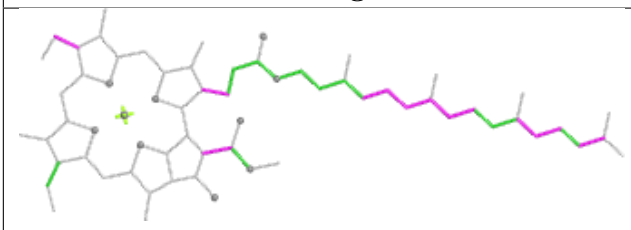
Ligand CLA A 805



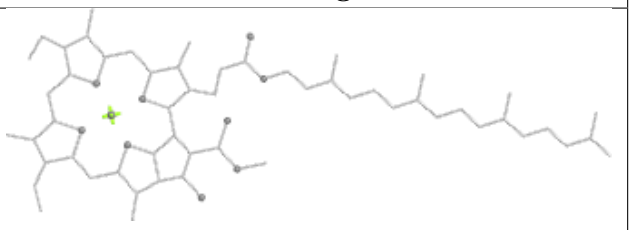
Bond lengths



Bond angles

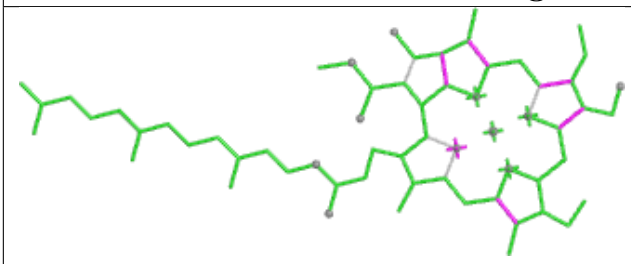


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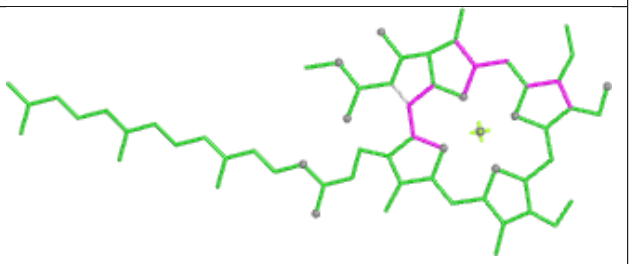


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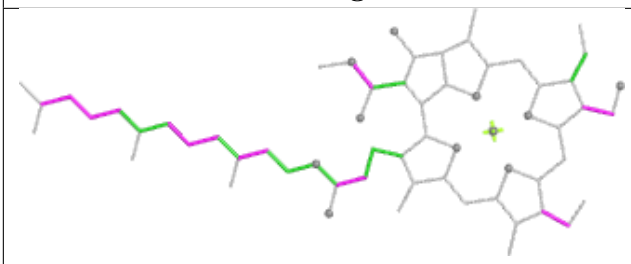
Ligand CHL 1 318



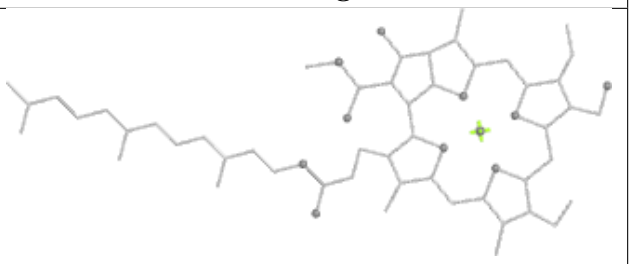
Bond lengths



Bond angles

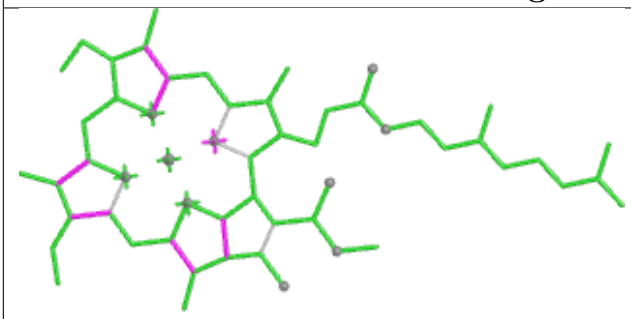


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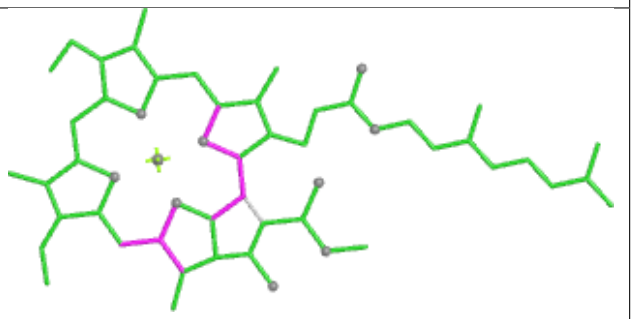


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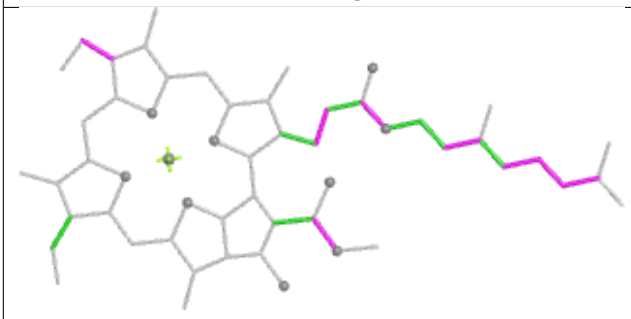
Ligand CLA 3 310



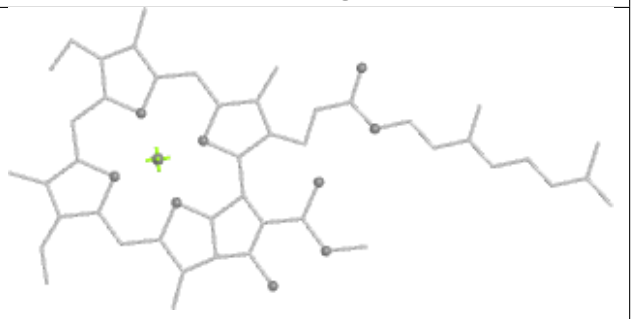
Bond lengths



Bond angles

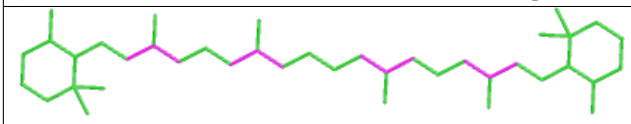


Torsions



Rings

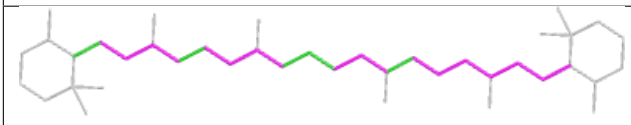
Ligand BCR 1 316



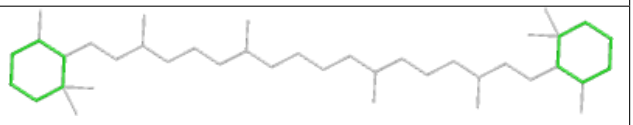
Bond lengths



Bond angles

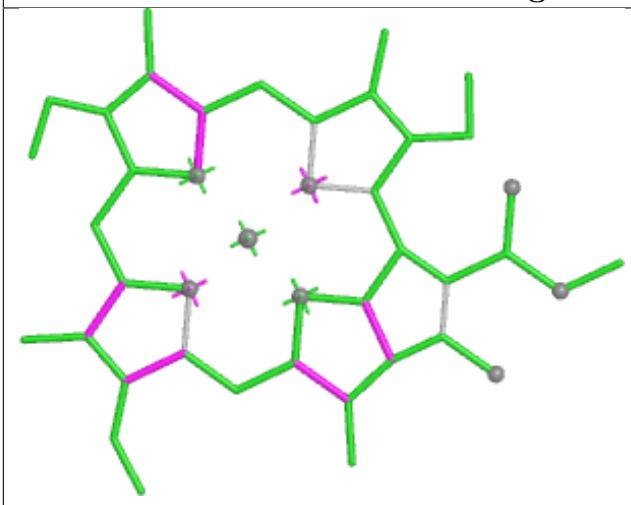


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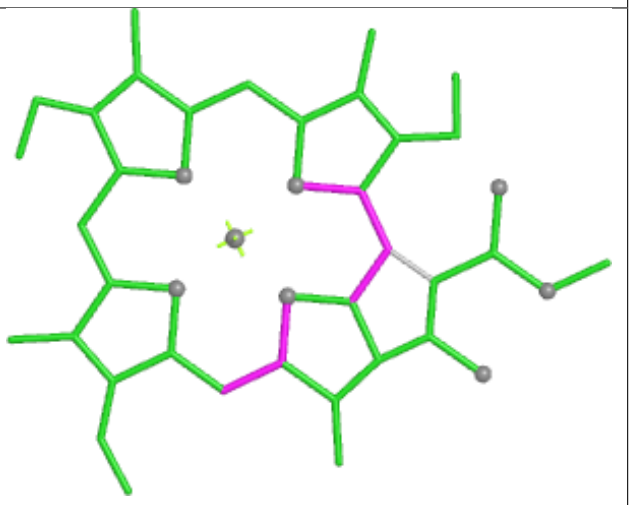


Rings

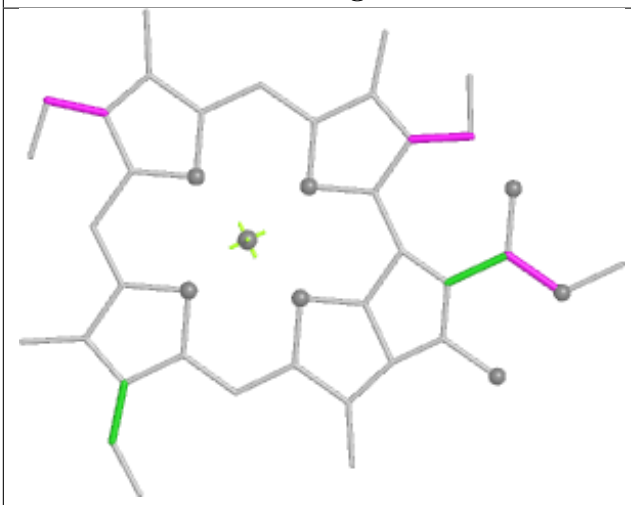
Ligand CLA 1 304



Bond lengths



Bond angles

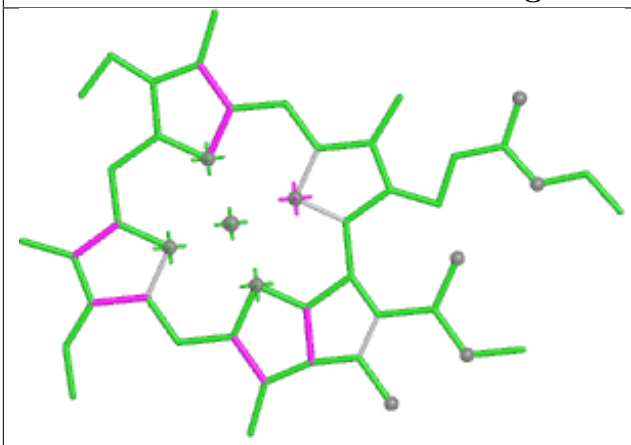


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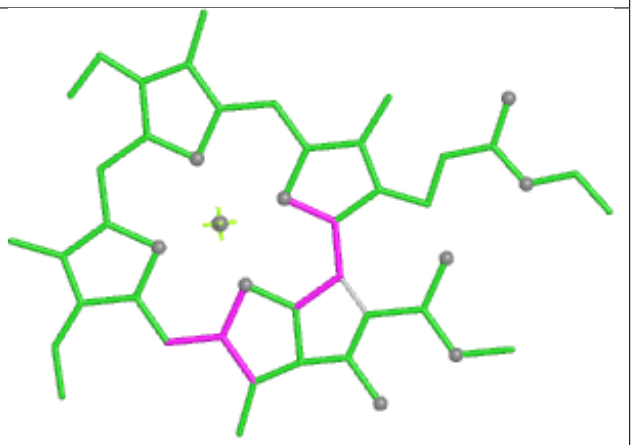


Rings

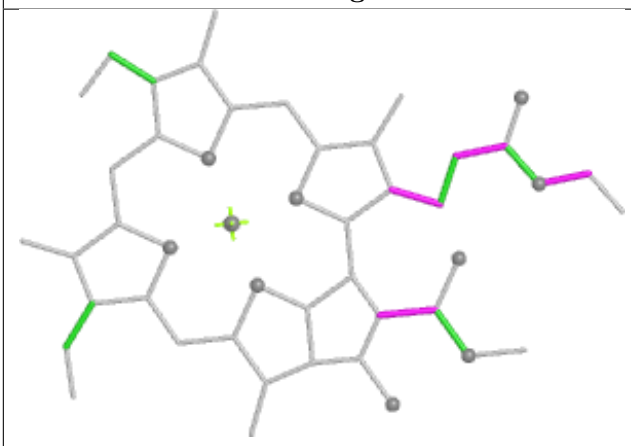
Ligand CLA B 837



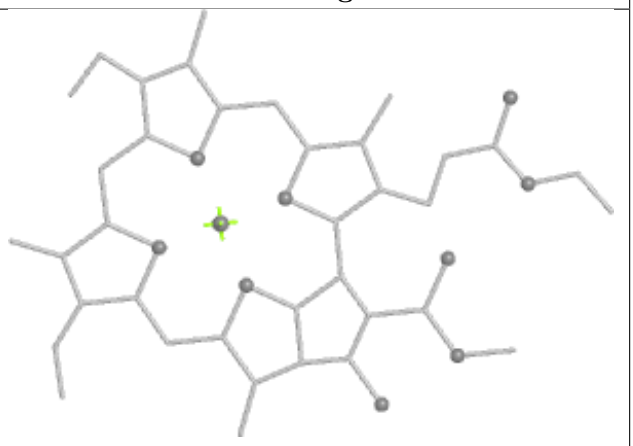
Bond lengths



Bond angles

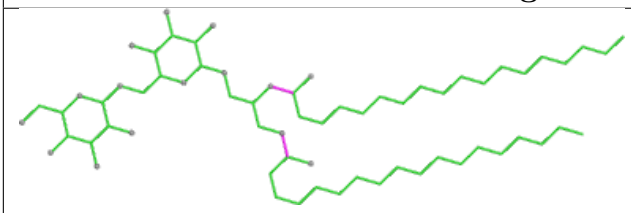


Torsions

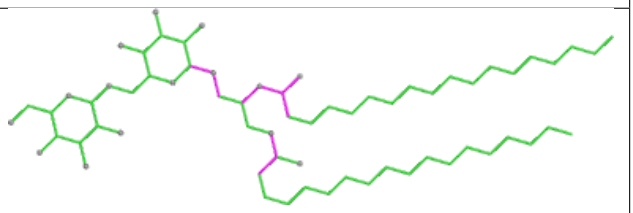


Rings

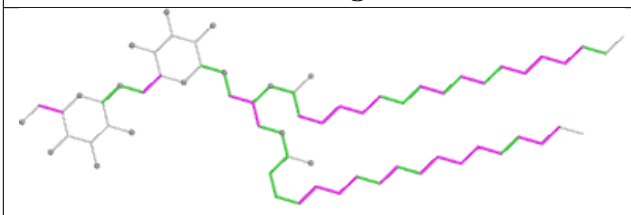
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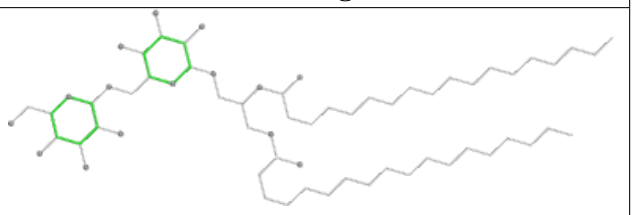
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Bond angles

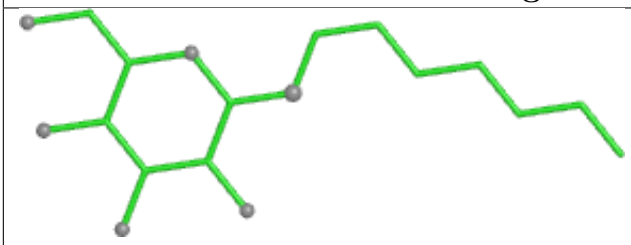


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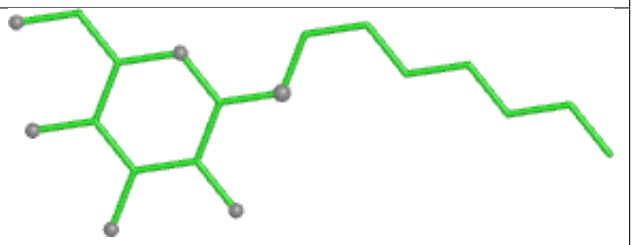


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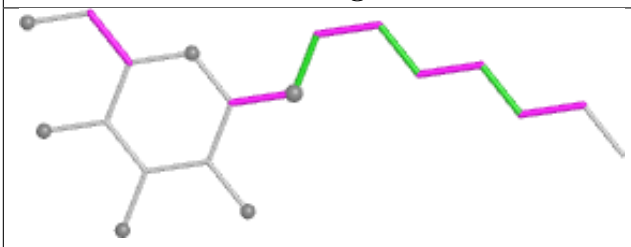
Ligand HTG F 303



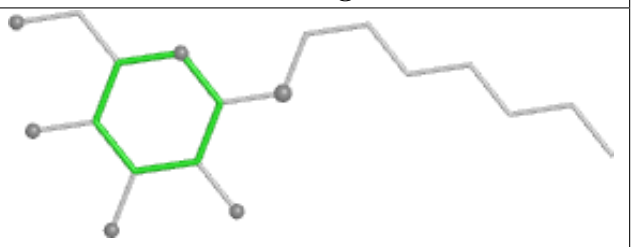
Bond lengths



Bond angles

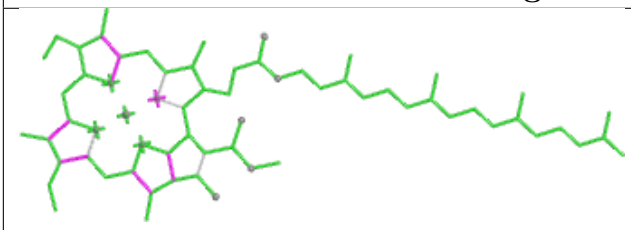


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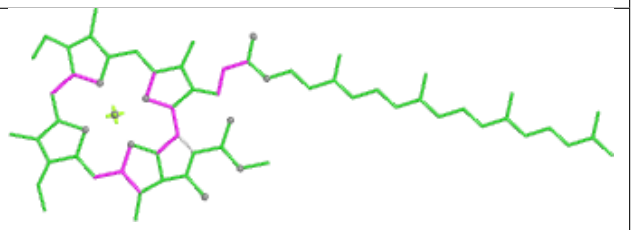


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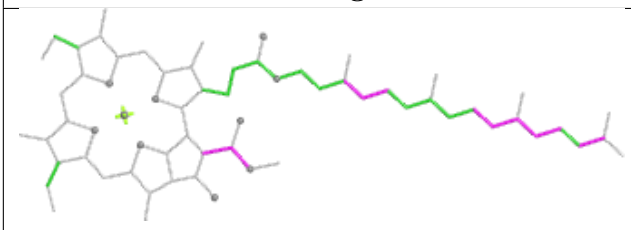
Ligand CLA A 836



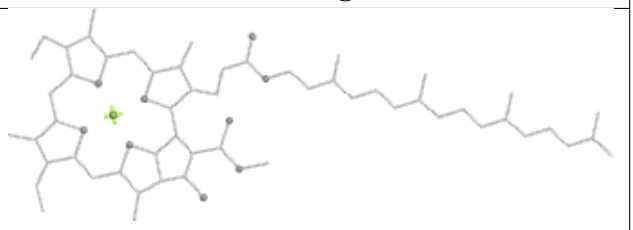
Bond lengths



Bond angles

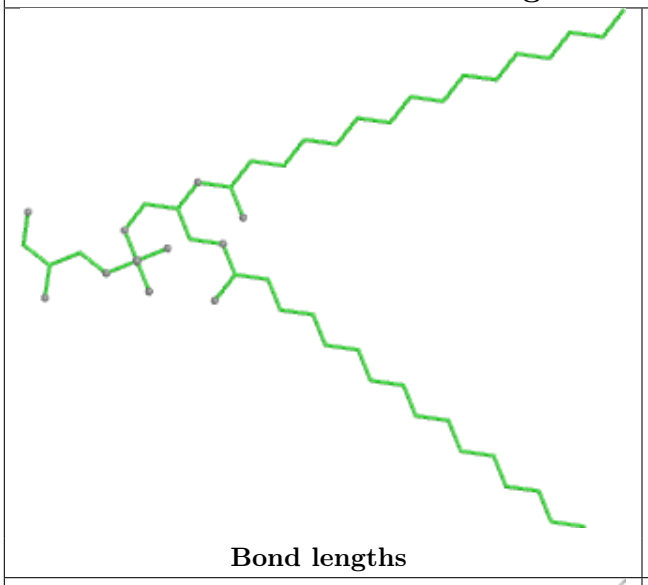


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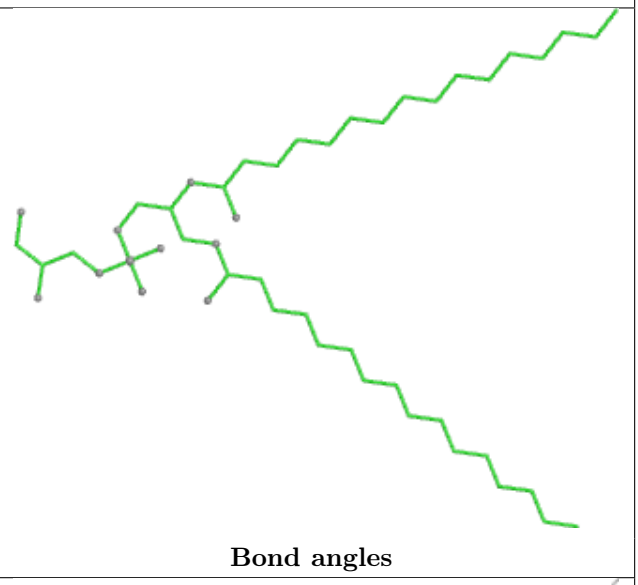


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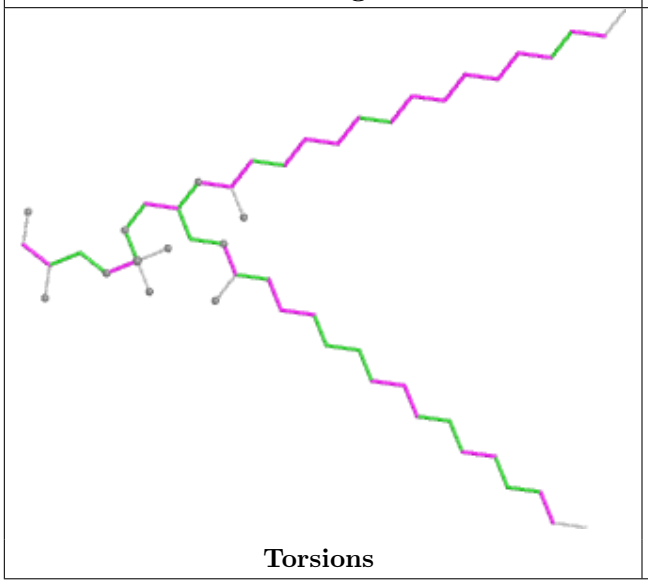
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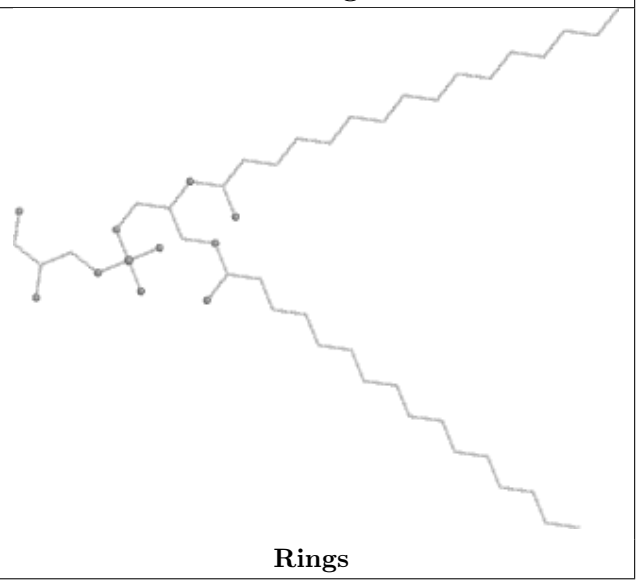
Bond lengths



Bond angles

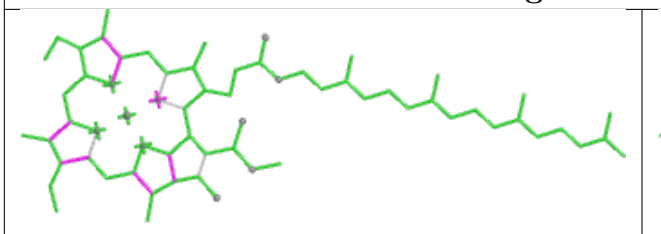


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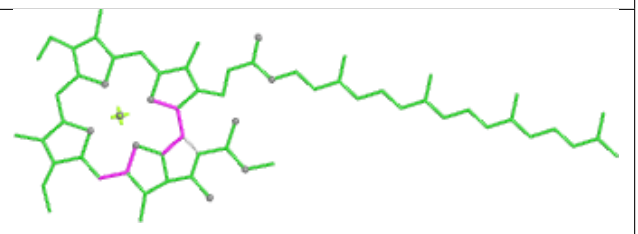


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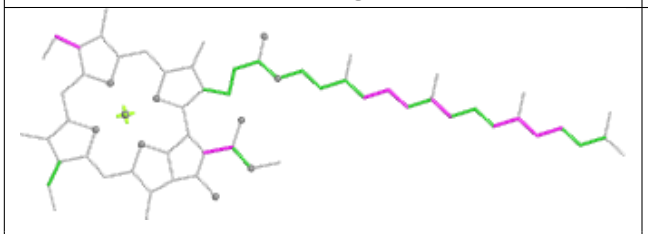
Ligand CLA B 807



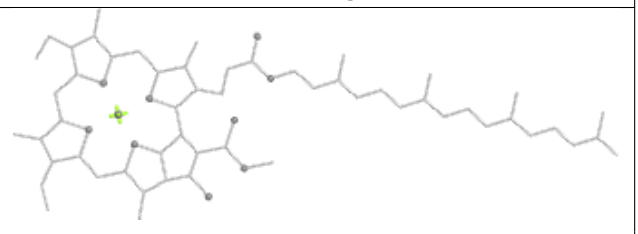
Bond lengths



Bond angles

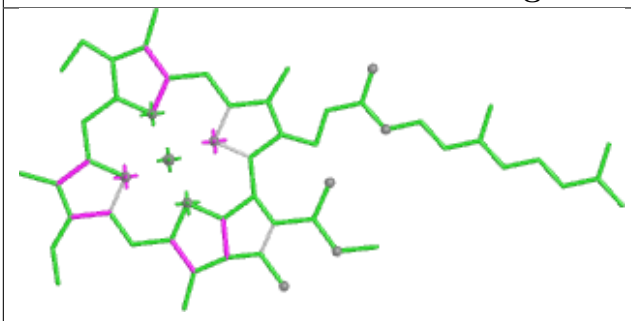


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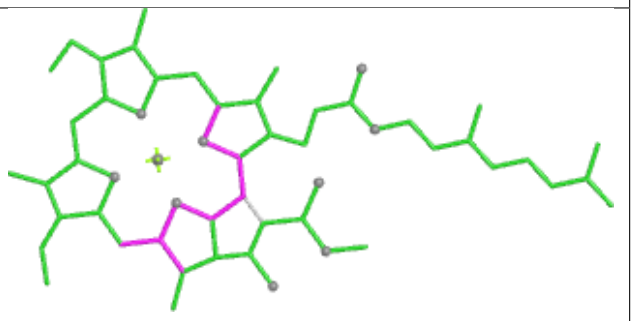


Rings

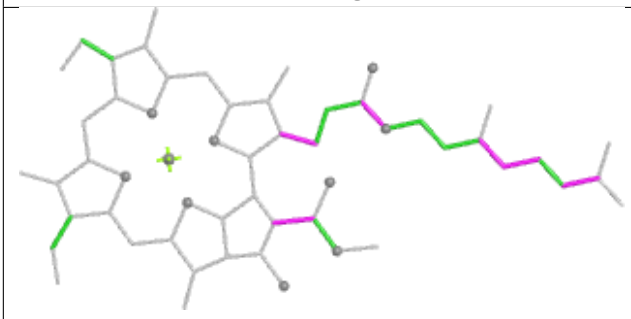
Ligand CLA A 812



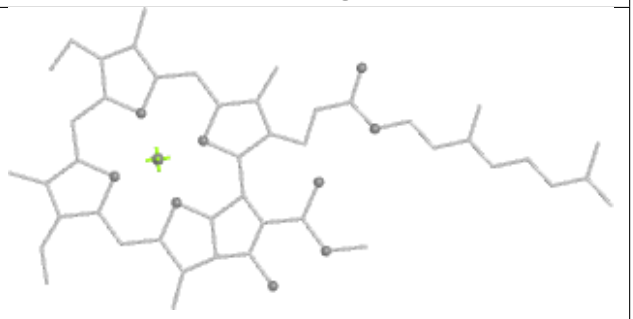
Bond lengths



Bond angles

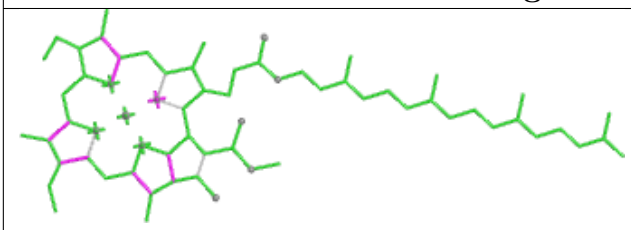


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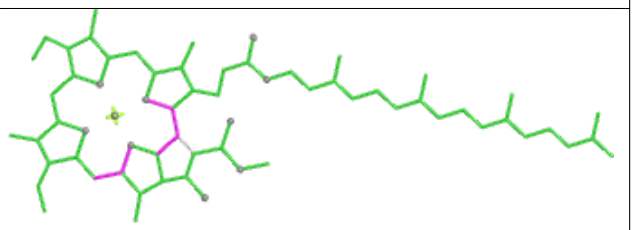


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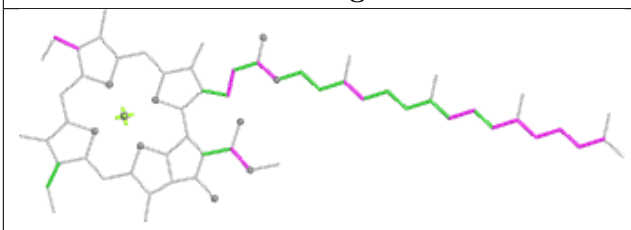
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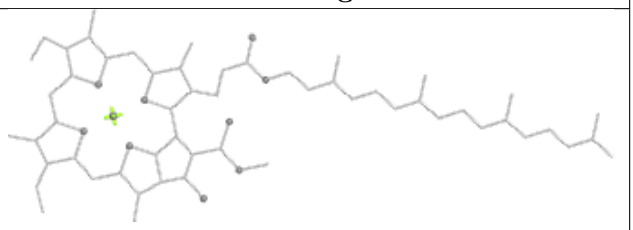
Bond lengths



Bond angles

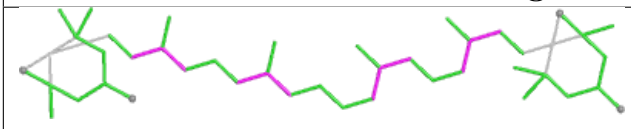


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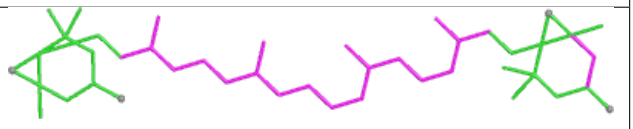


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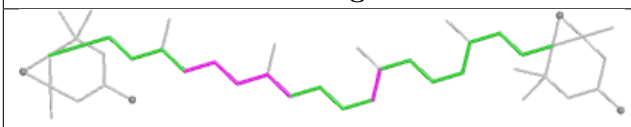
Ligand XAT 4 317



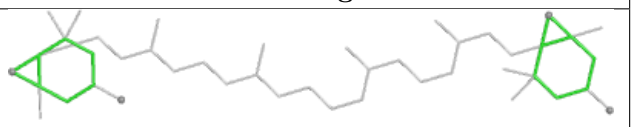
Bond lengths



Bond angles

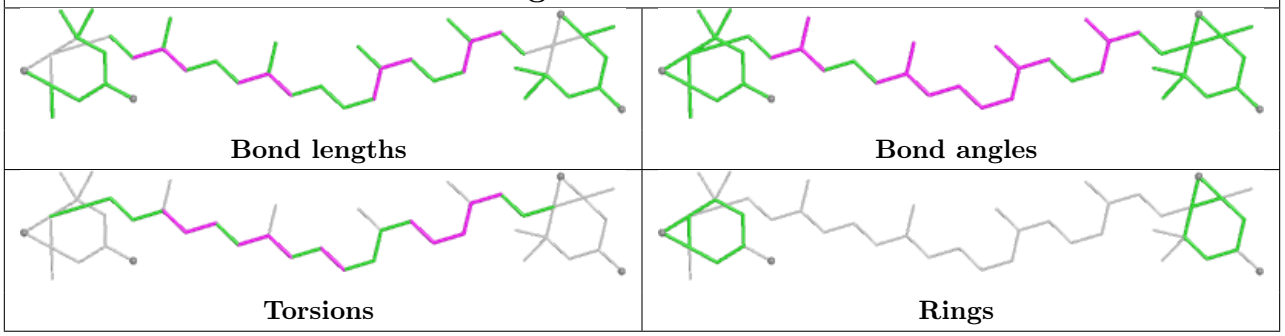


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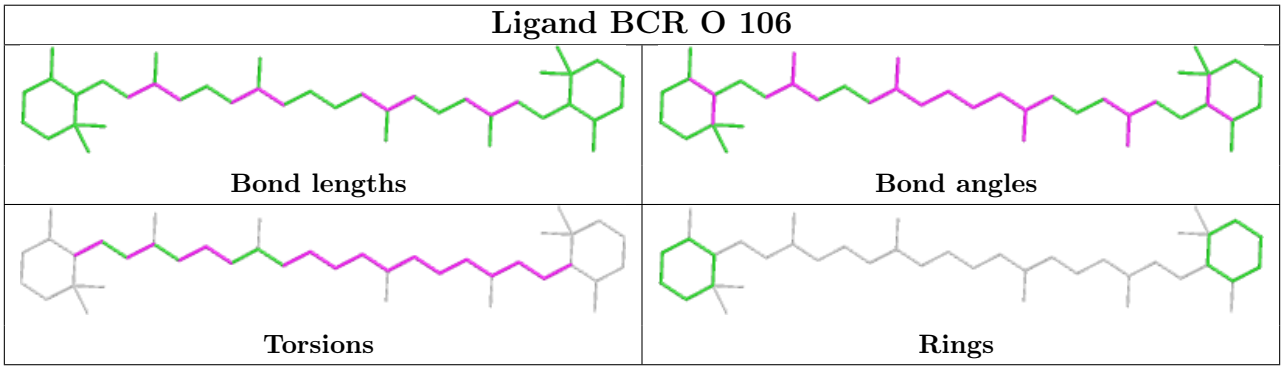


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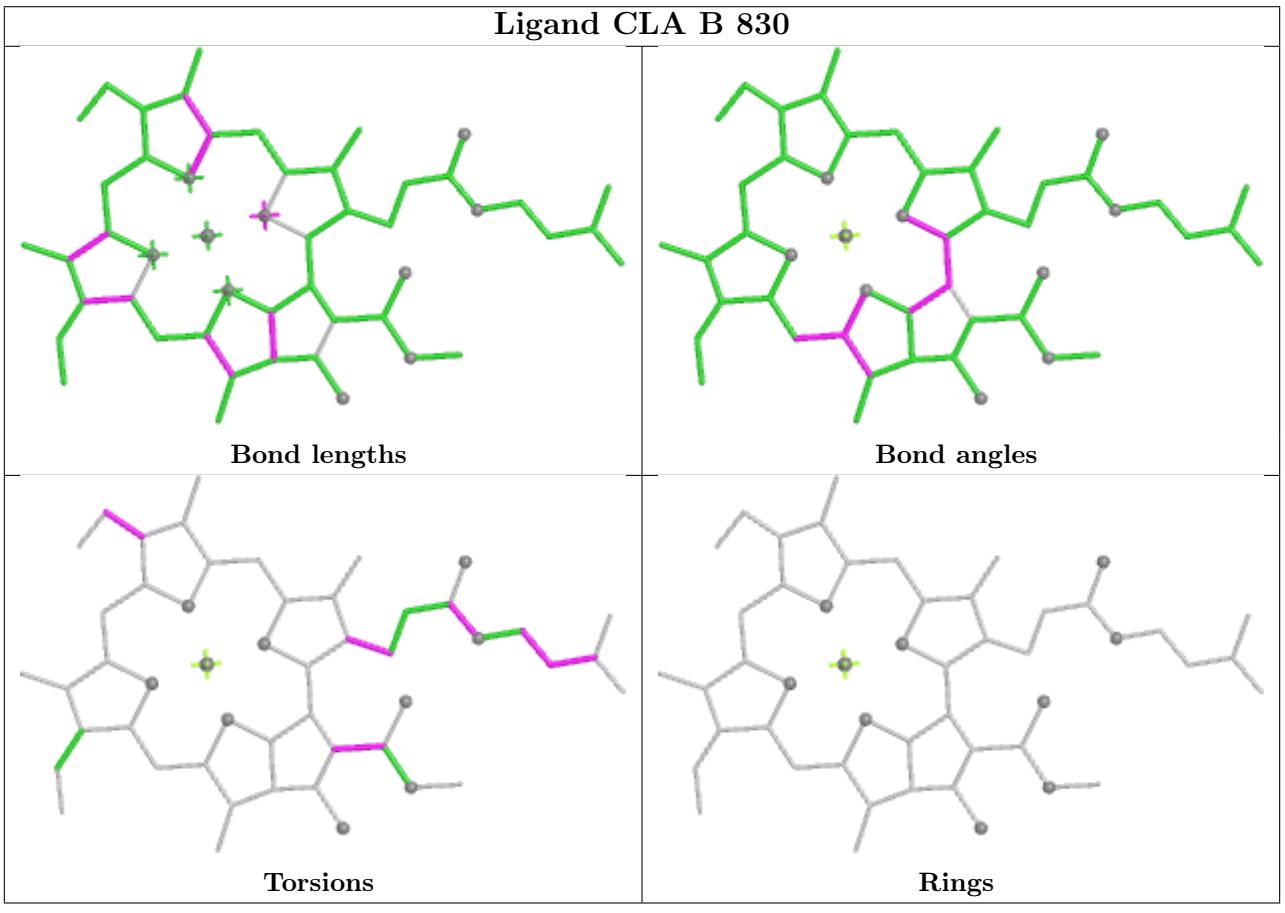
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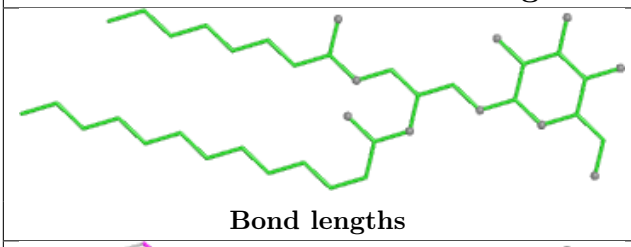
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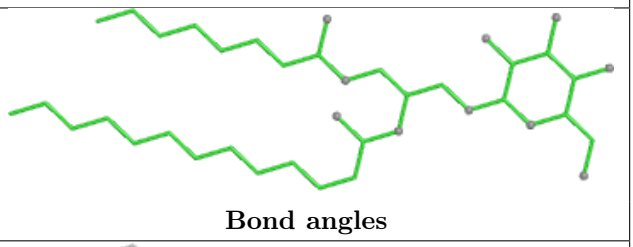


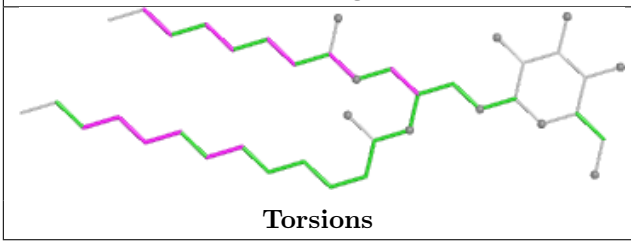
Ligand CLA B 830

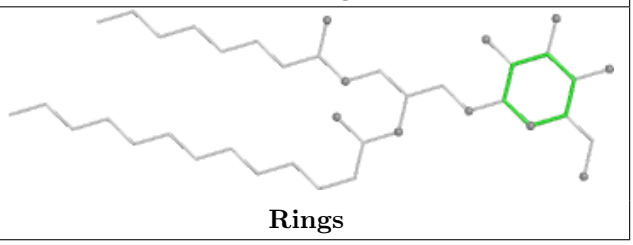


Ligand LMG F 309

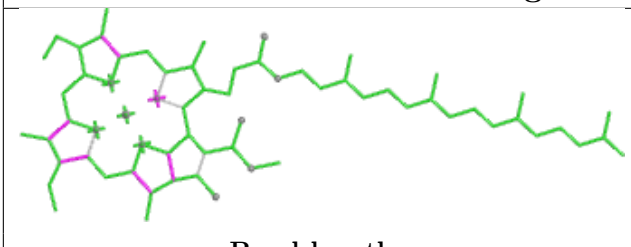

Bond lengths

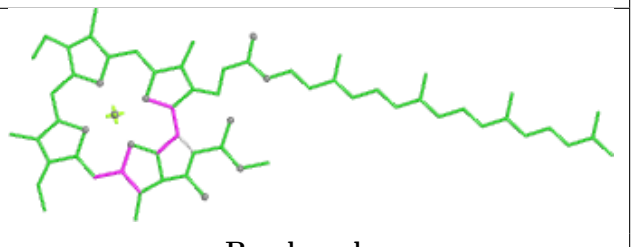

Bond angles

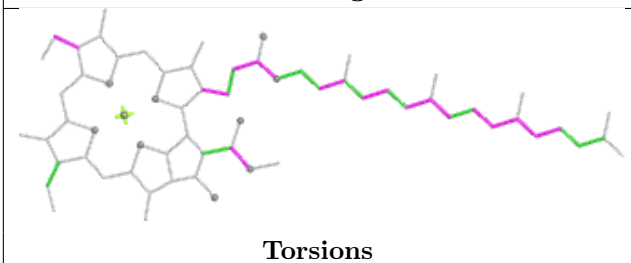

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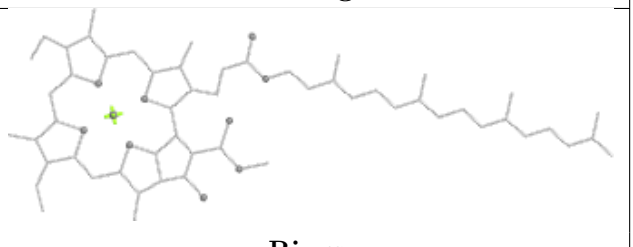

Rings

Ligand CLA B 833

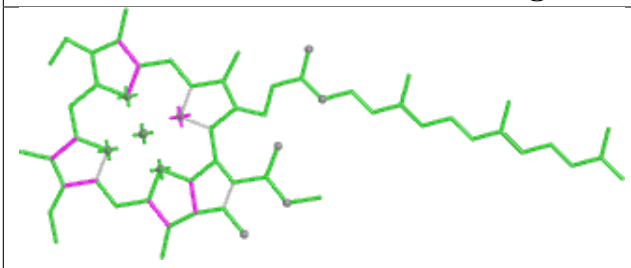

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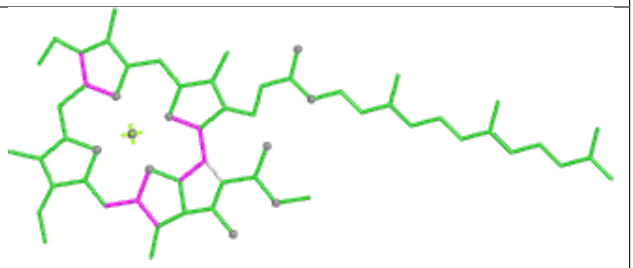

Bond angles

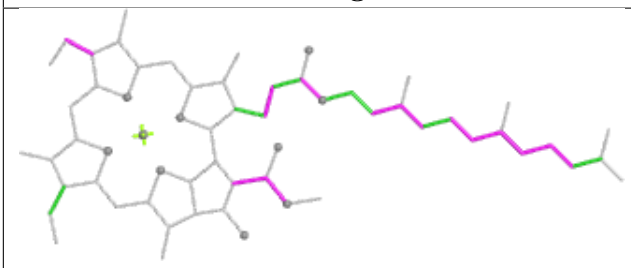

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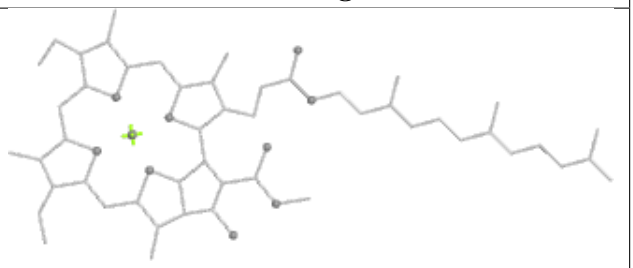

Rings

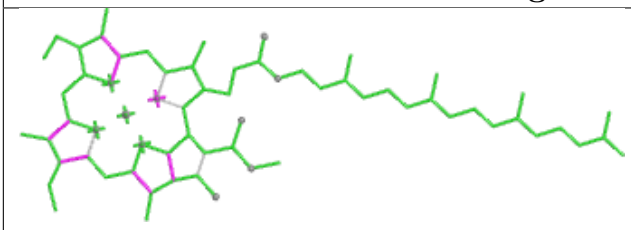
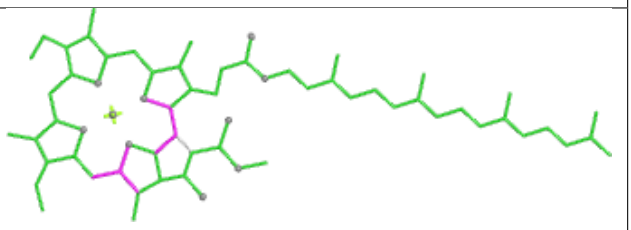
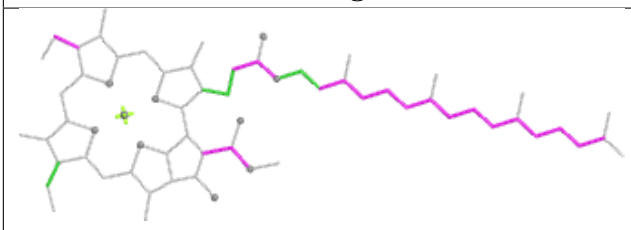
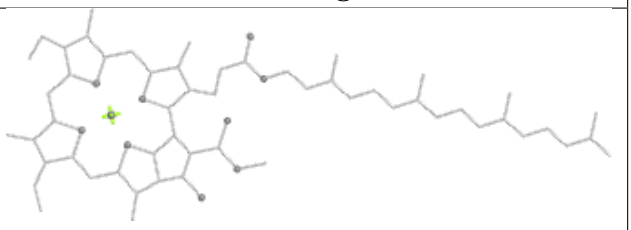
Ligand CLA 3 301

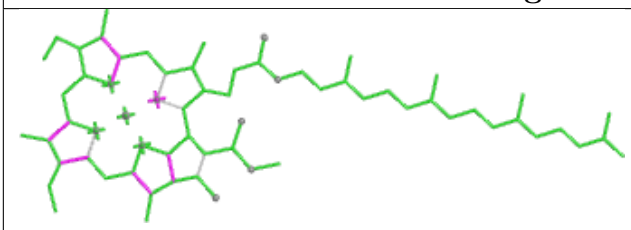
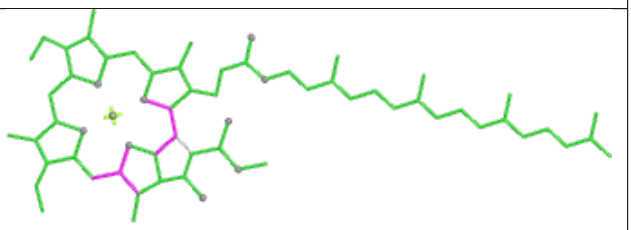
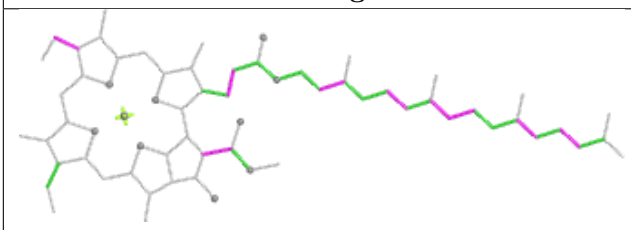
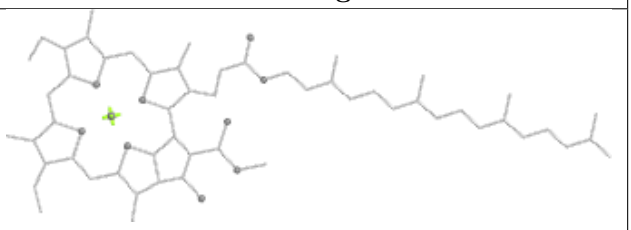

Bond lengths


Bond angles

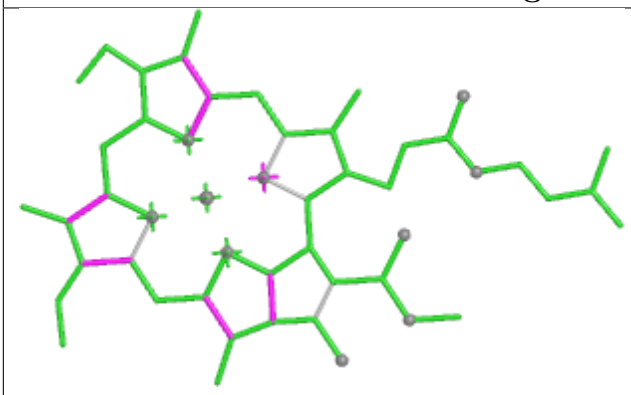

Torsions


Rings

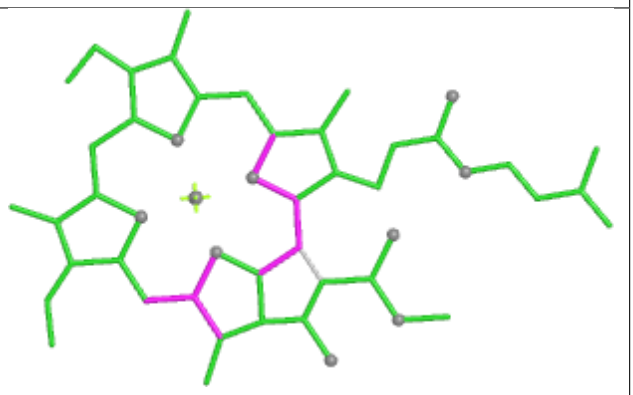
Ligand CLA 1 302	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 824	
	
Bond lengths	Bond angles
	
Torsions	Rings

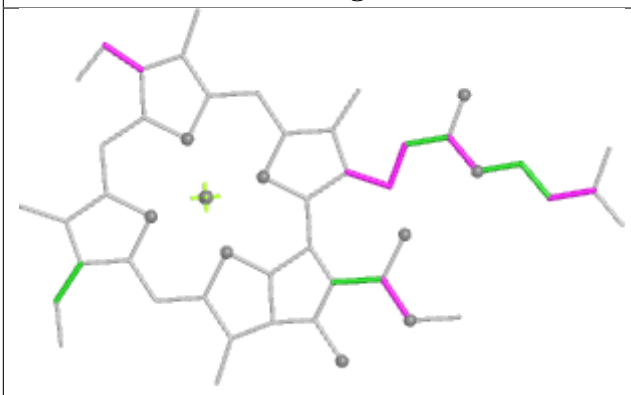
Ligand CLA A 813



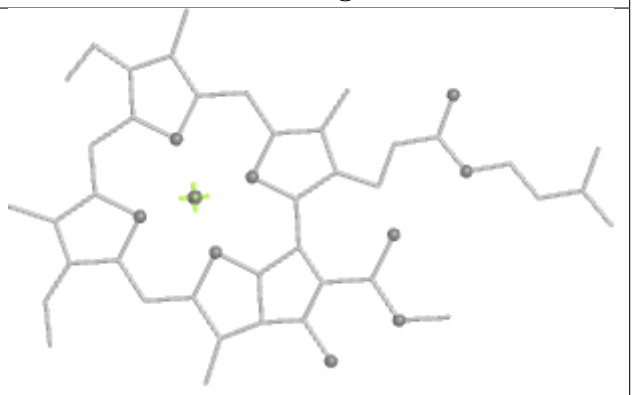
Bond lengths



Bond angles

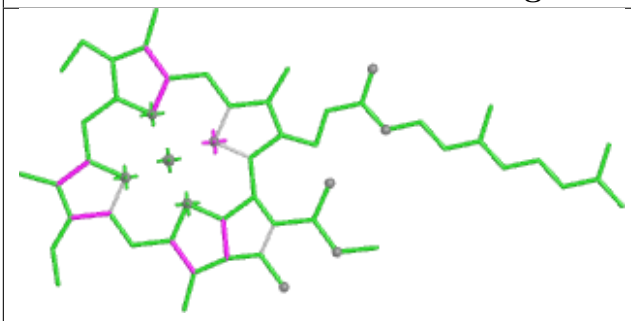


Torsions

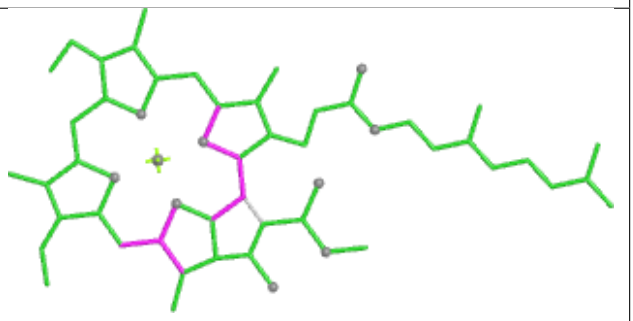


Rings

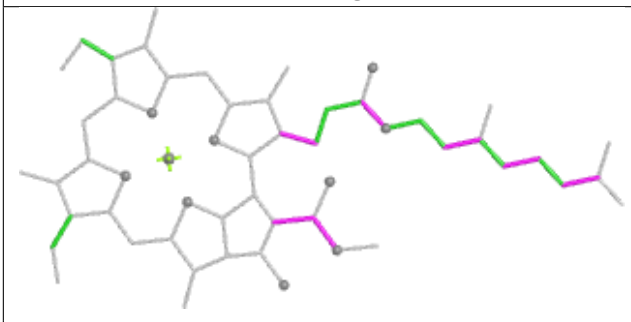
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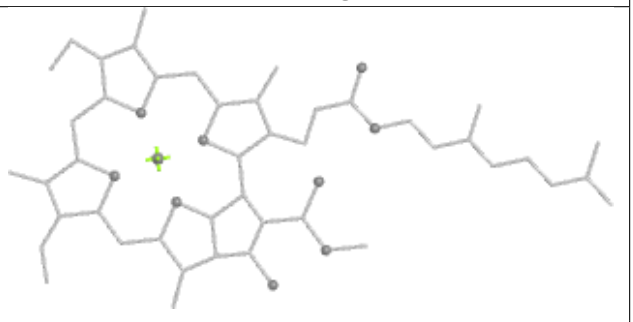
Bond lengths



Bond angles



Torsions

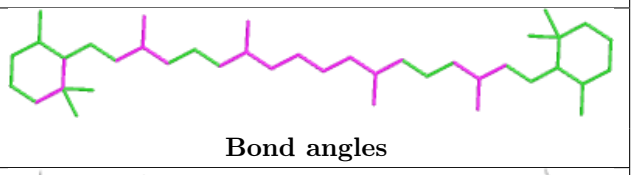


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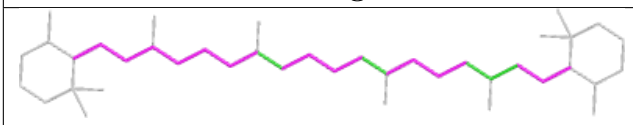
Ligand BCR G 206



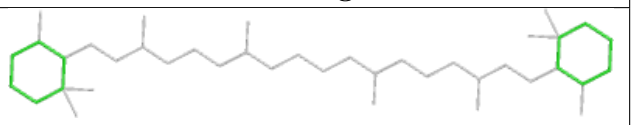
Bond lengths



Bond angles

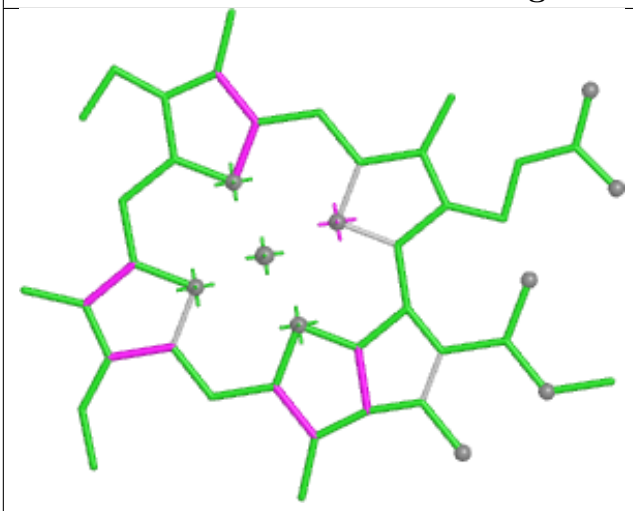


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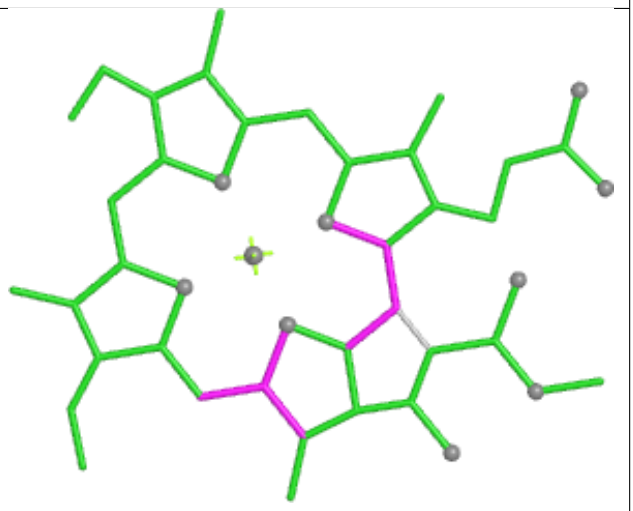


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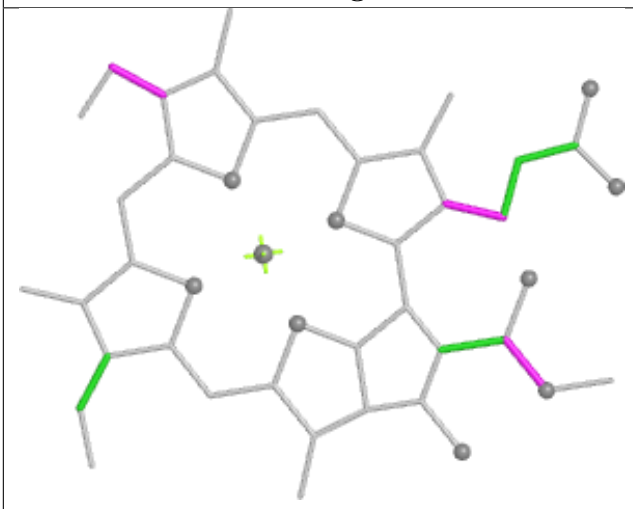
Ligand CLA 3 316



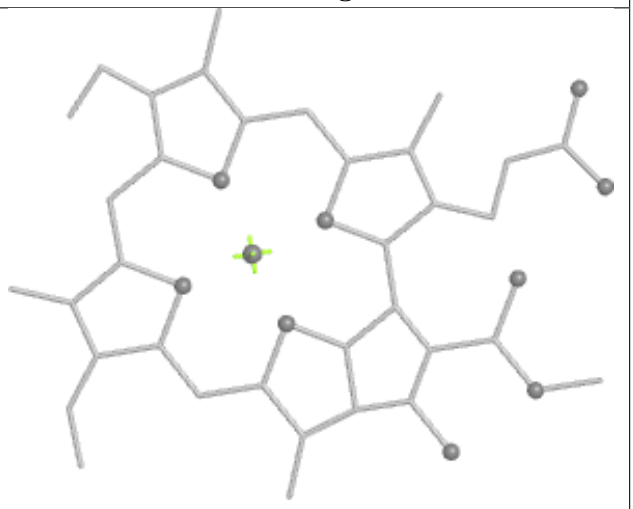
Bond lengths



Bond angles



Torsions

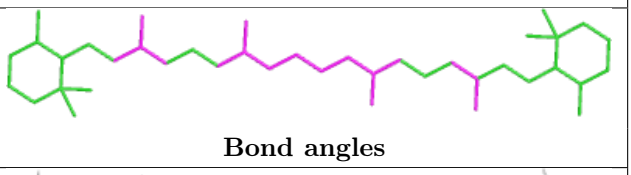


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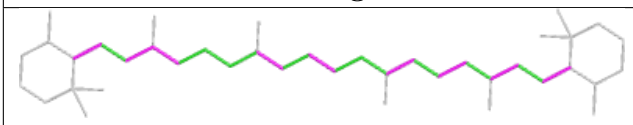
Ligand BCR A 847



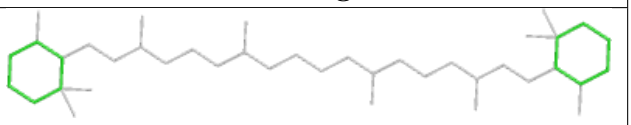
Bond lengths



Bond angles

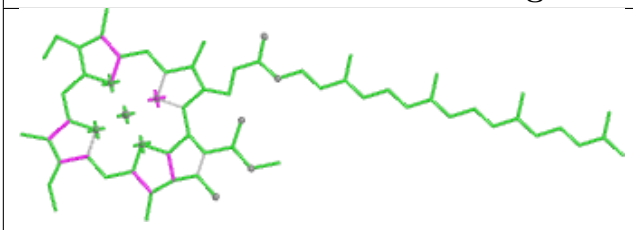


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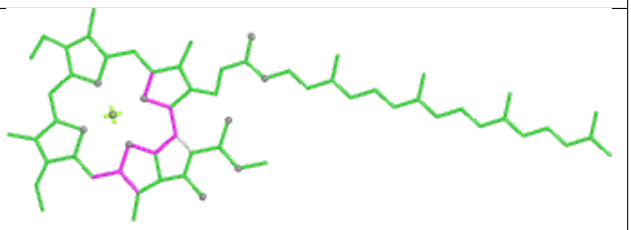


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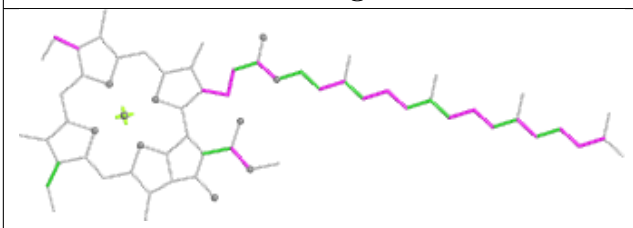
Ligand CLA L 302



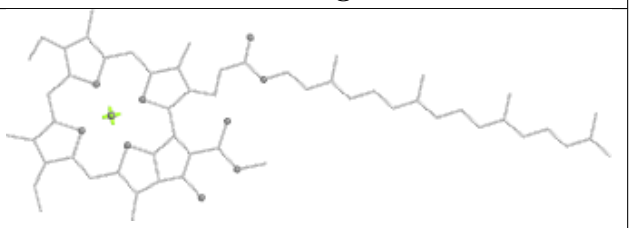
Bond lengths



Bond angles

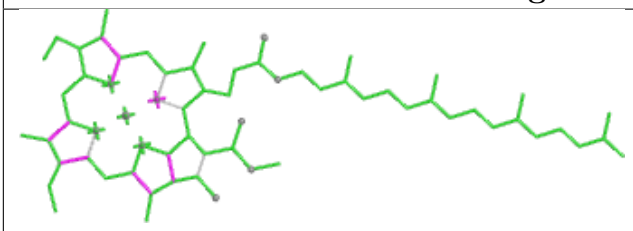


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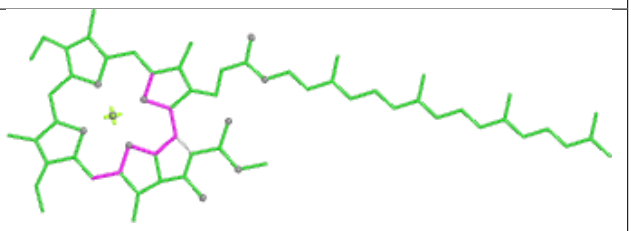


Rings

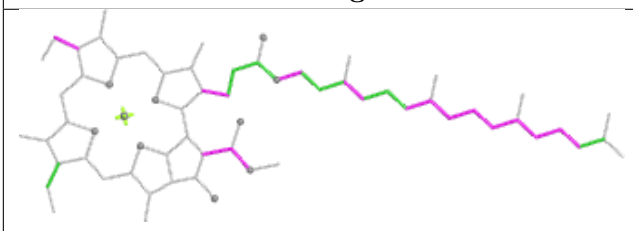
Ligand CLA 1 307



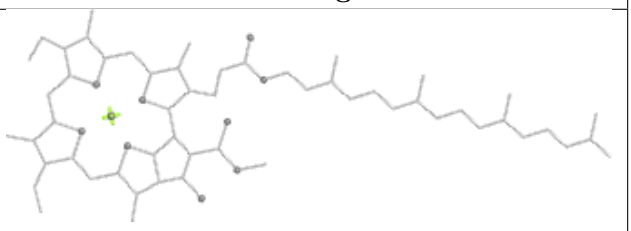
Bond lengths



Bond angles

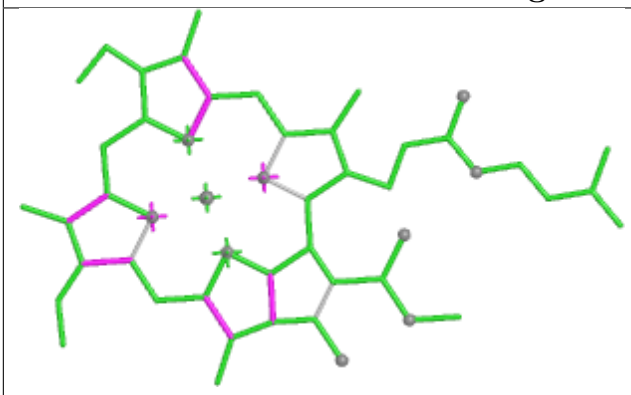


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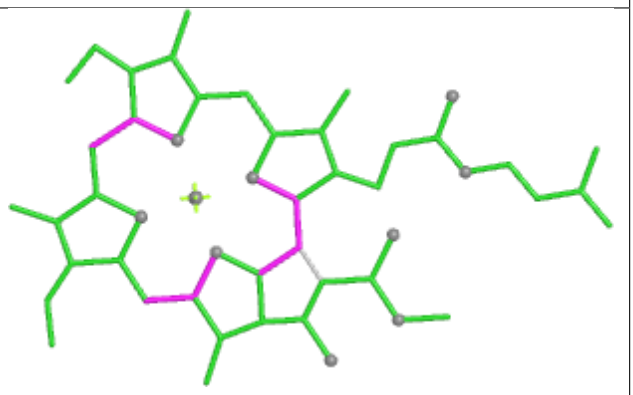


Rings

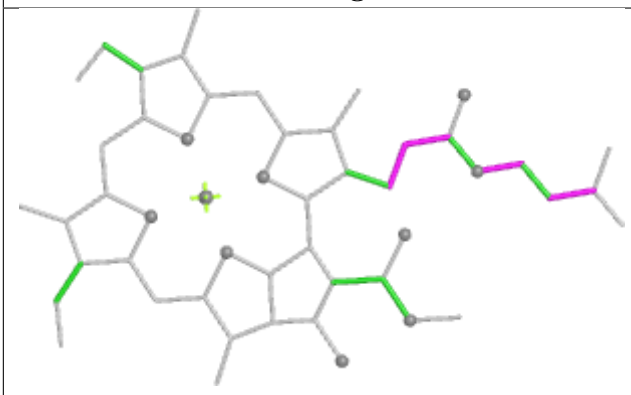
Ligand CLA 3 302



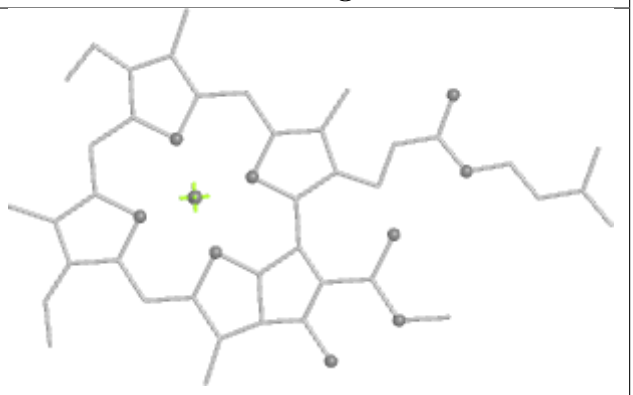
Bond lengths



Bond angles

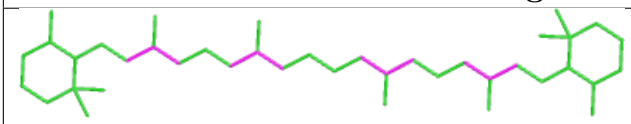


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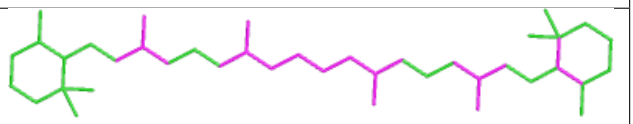


Rings

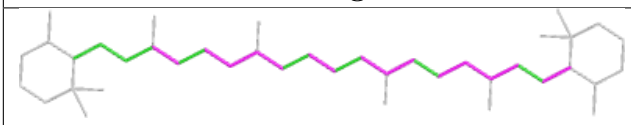
Ligand BCR J 103



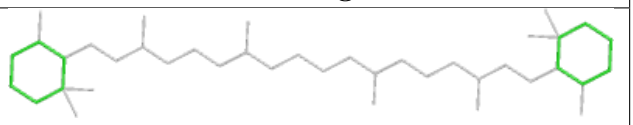
Bond lengths



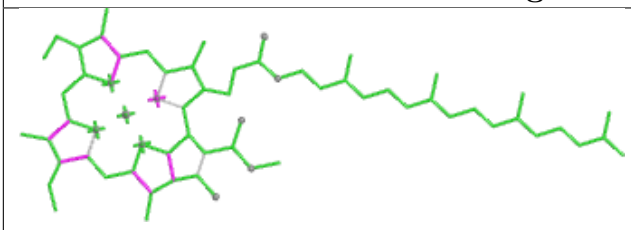
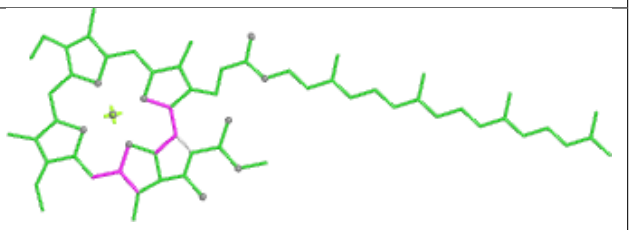
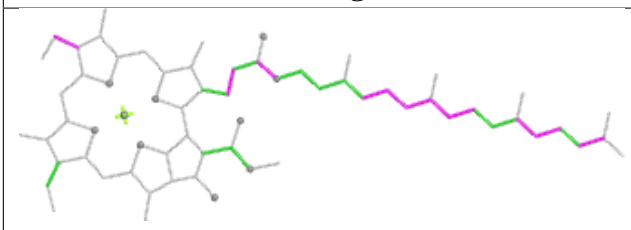
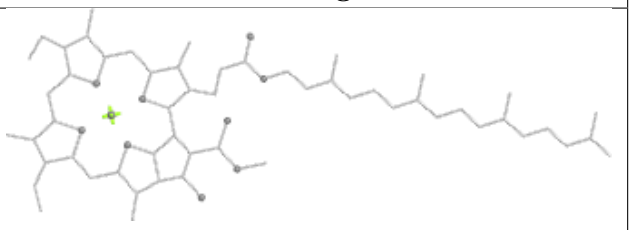
Bond angles

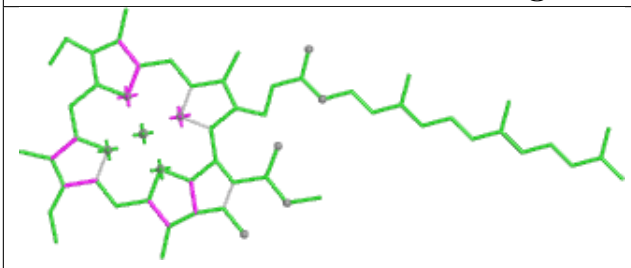
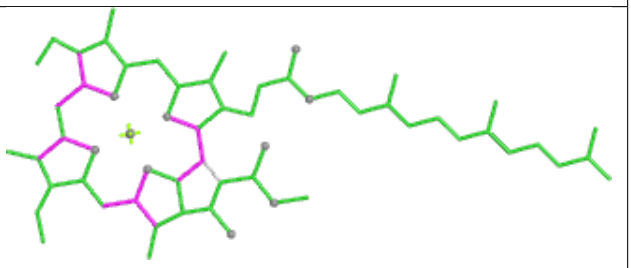
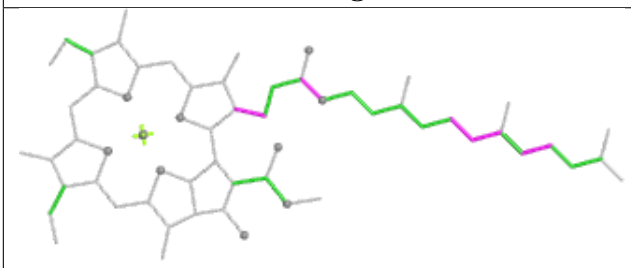
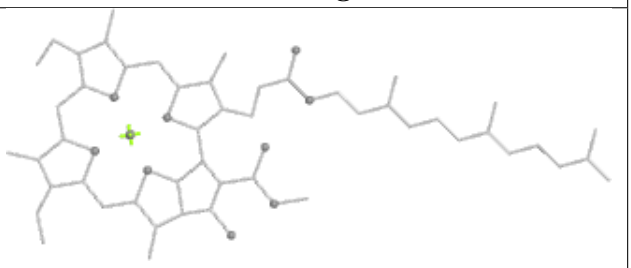


Torsions

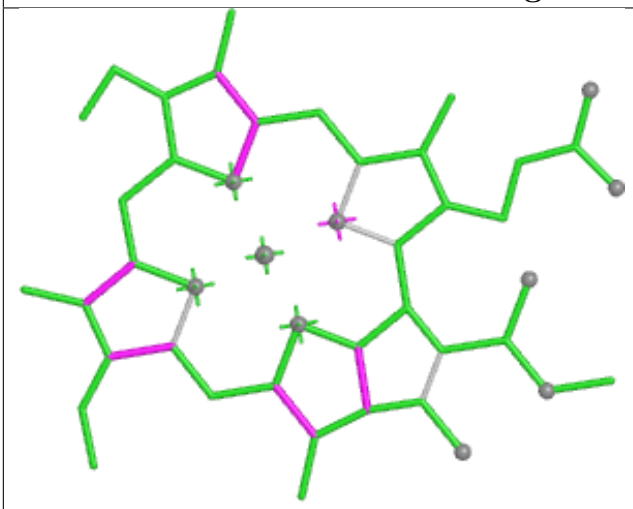


Rings

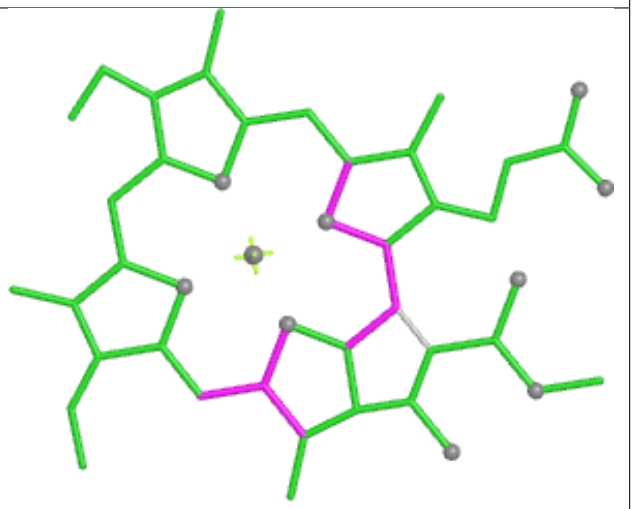
Ligand CLA L 303	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 2 308	
	
Bond lengths	Bond angles
	
Torsions	Rings

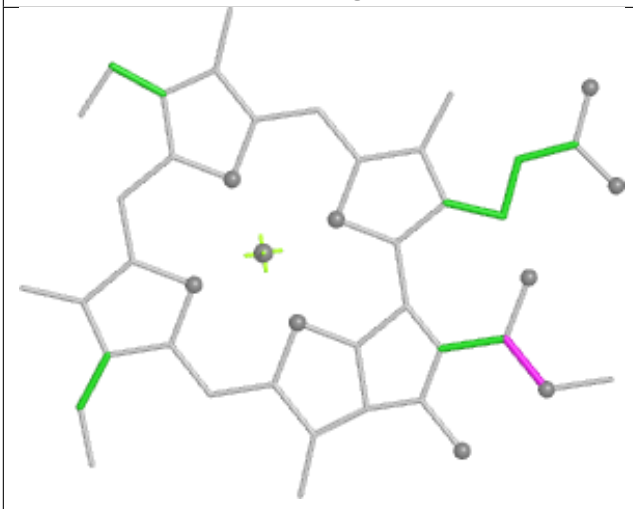
Ligand CLA B 834



Bond lengths



Bond angles

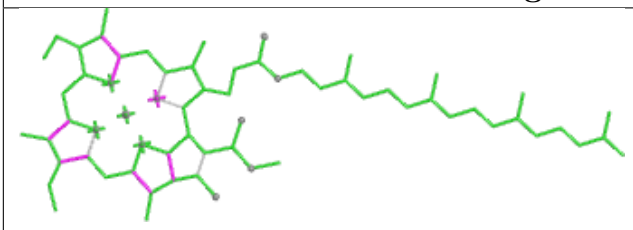


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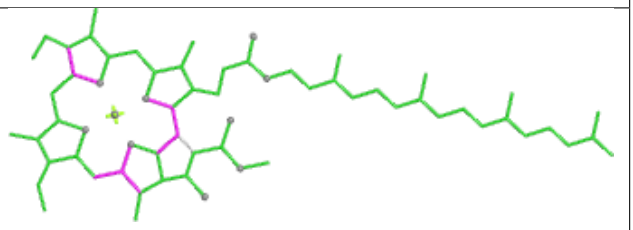


Rings

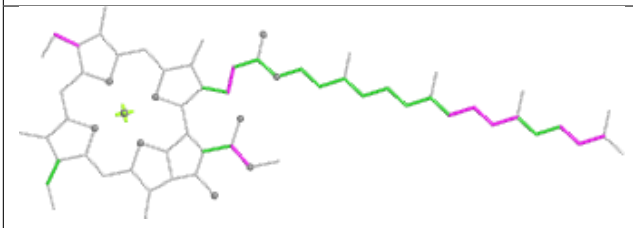
Ligand CLA B 803



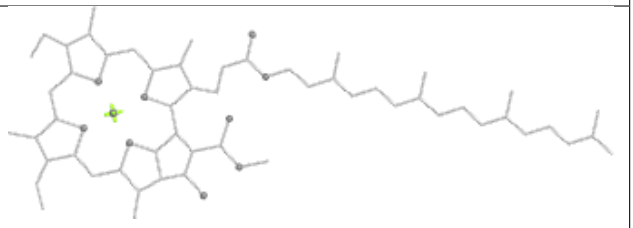
Bond lengths



Bond angles

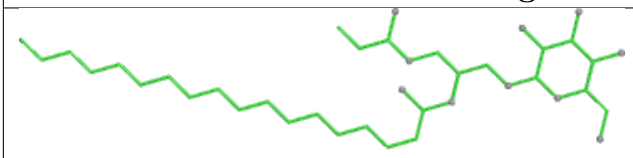


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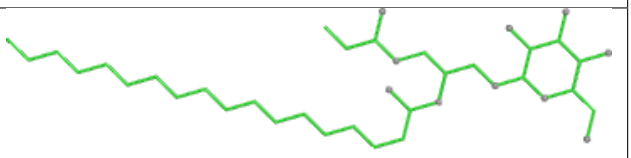


Rings

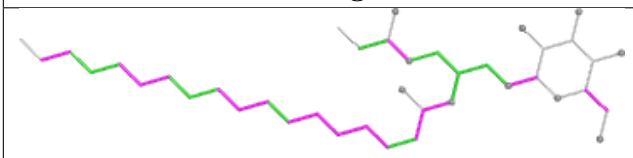
Ligand LMG G 202



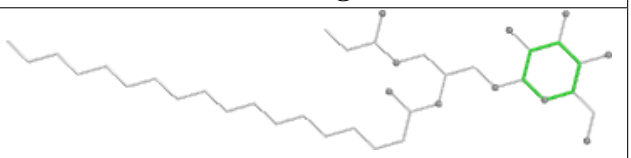
Bond lengths



Bond angles

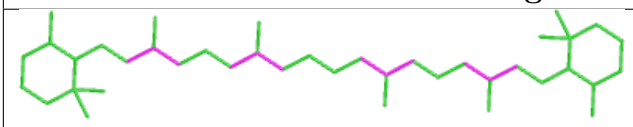


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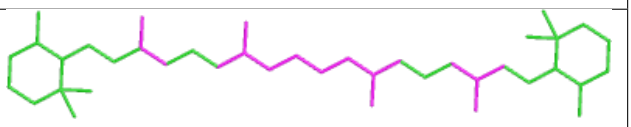


Rings

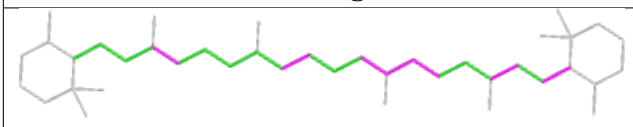
Ligand BCR L 306



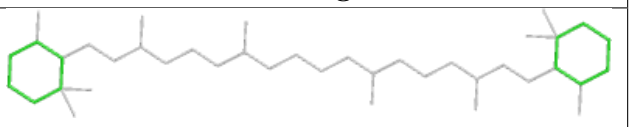
Bond lengths



Bond angles

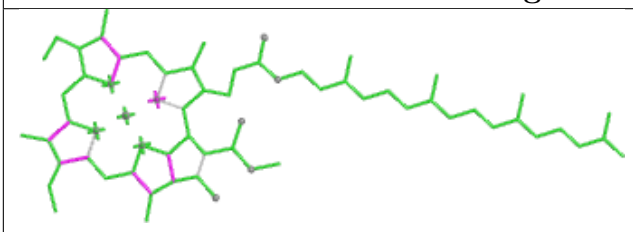


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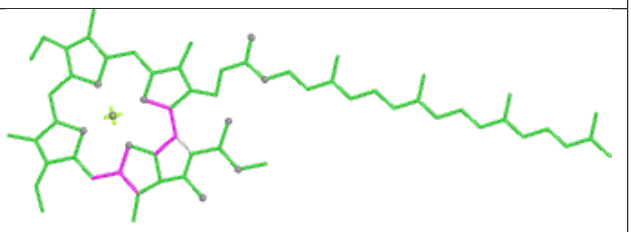


Rings

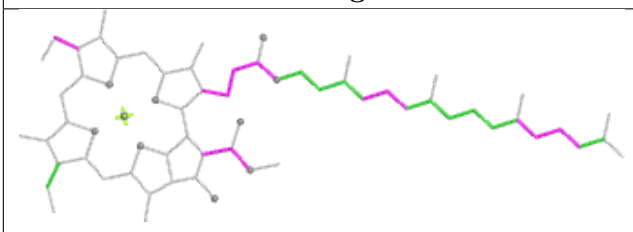
Ligand CLA A 806



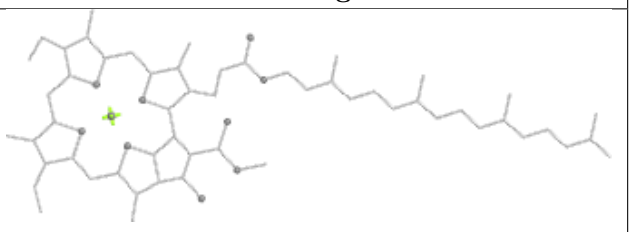
Bond lengths



Bond angles

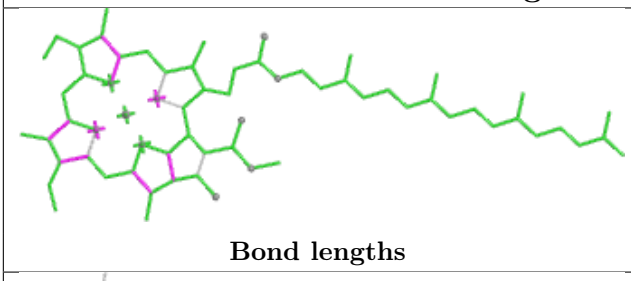


Torsions

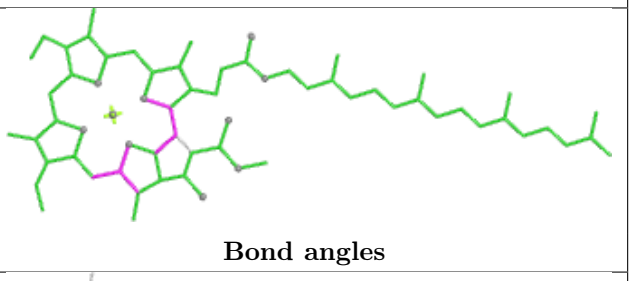


Rings

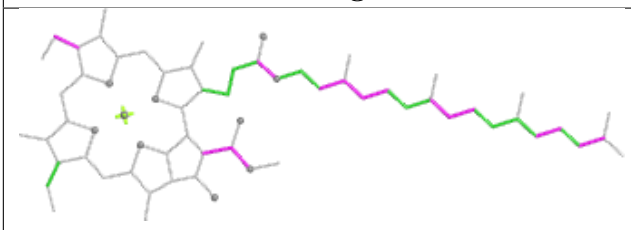
Ligand CLA A 831



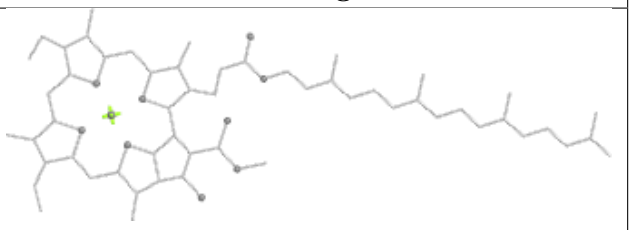
Bond lengths



Bond angles

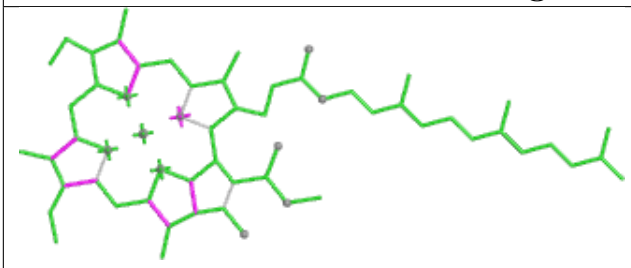


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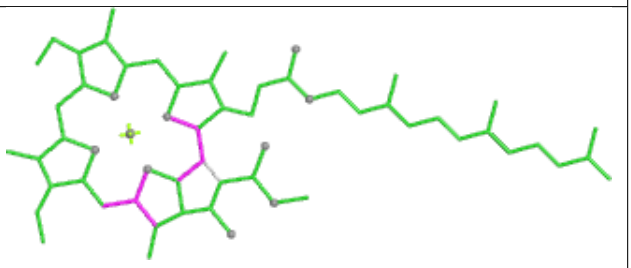


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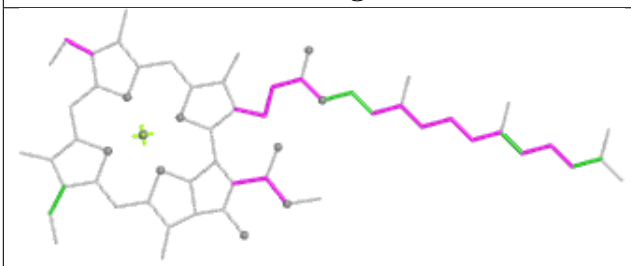
Ligand CLA 2 303



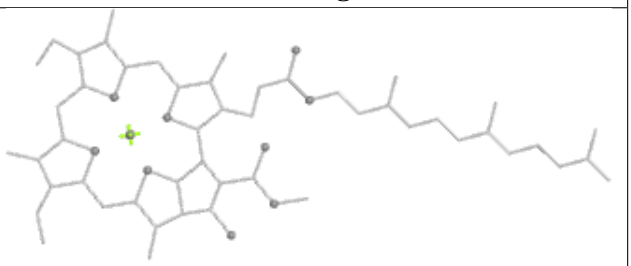
Bond lengths



Bond angles



Torsions

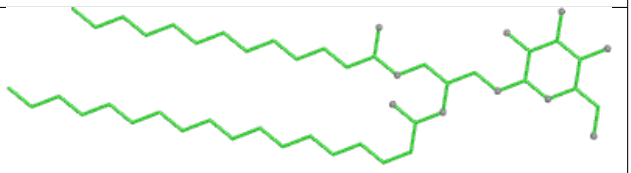


Rings

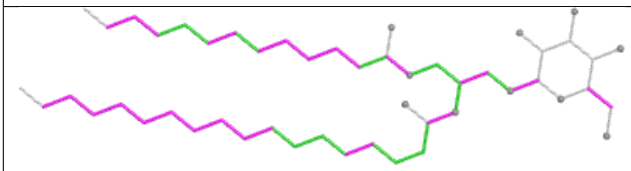
Ligand LMG 4 319



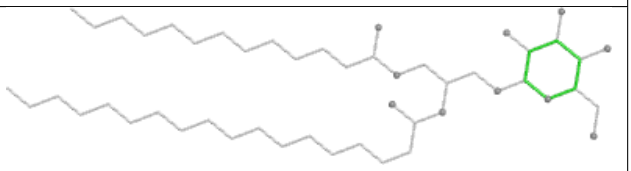
Bond lengths



Bond angles

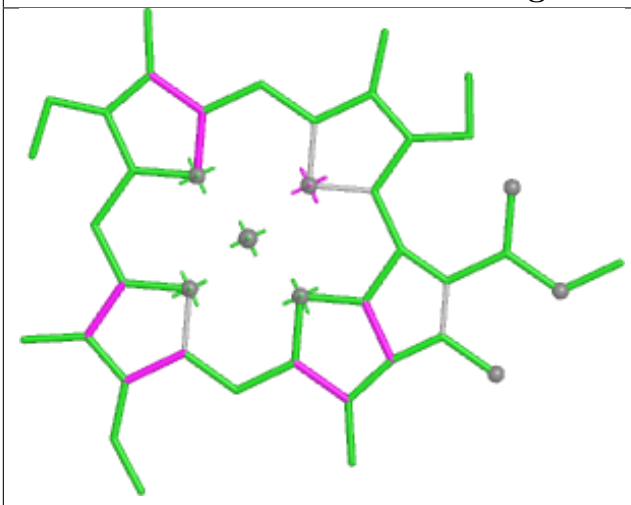


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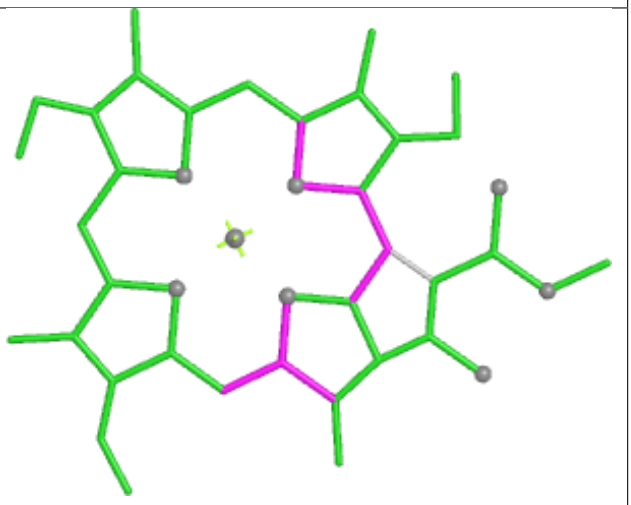


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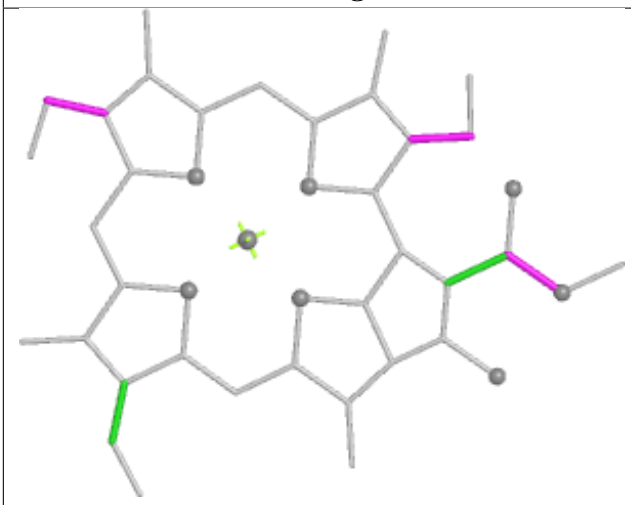
Ligand CLA J 102



Bond lengths



Bond angles

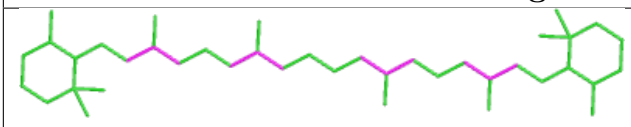


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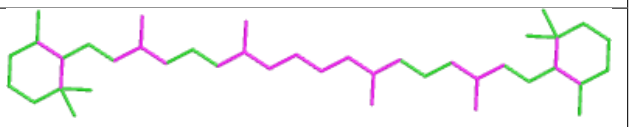


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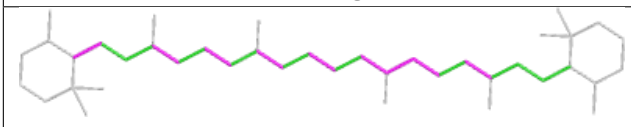
Ligand BCR I 101



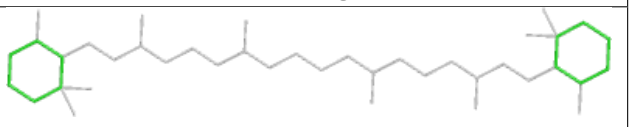
Bond lengths



Bond angles

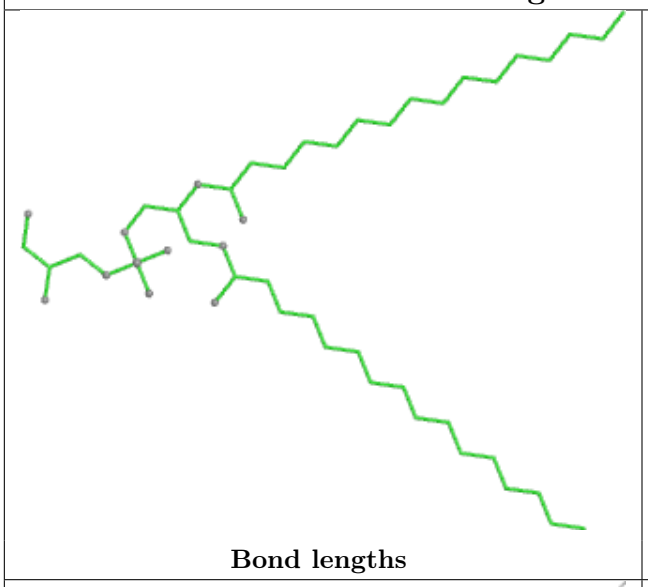


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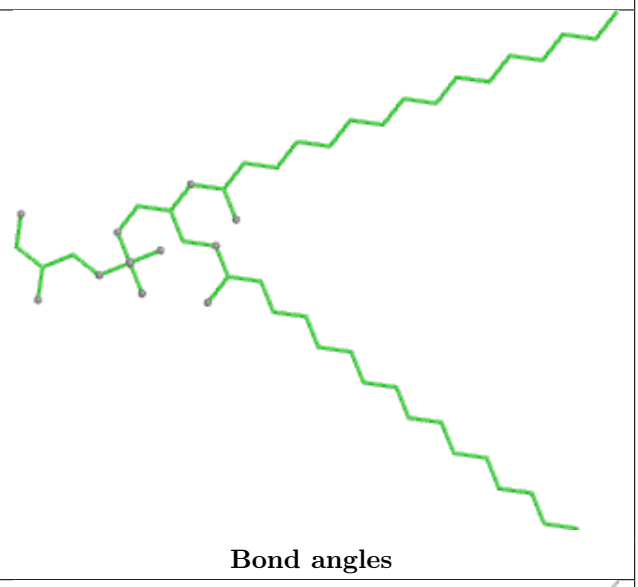


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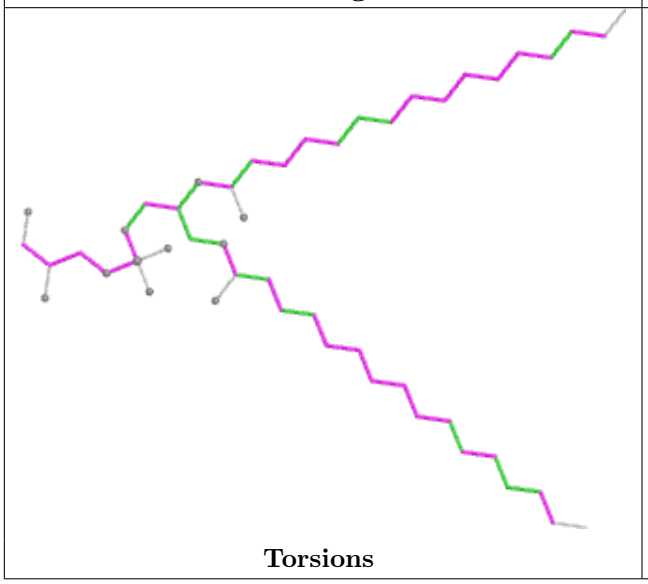
Ligand LHG 4 320



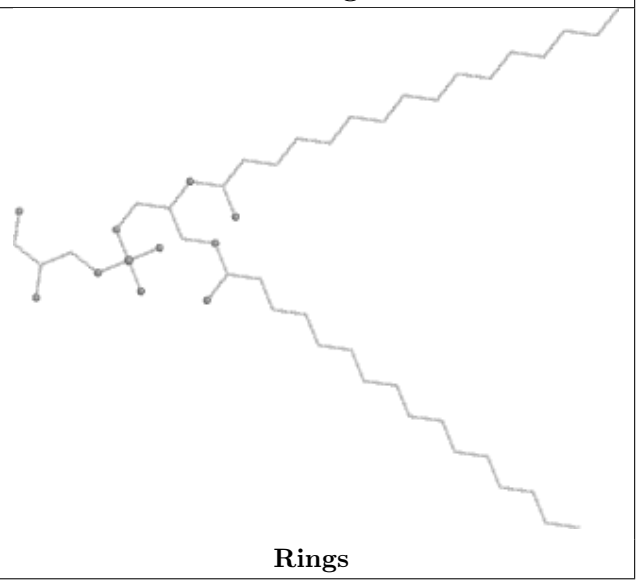
Bond lengths



Bond angles

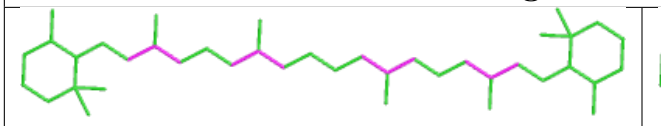


Torsions



Rings

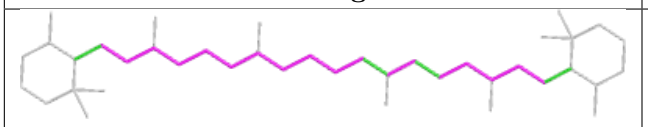
Ligand BCR K 304



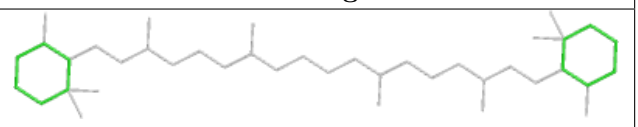
Bond lengths



Bond angles

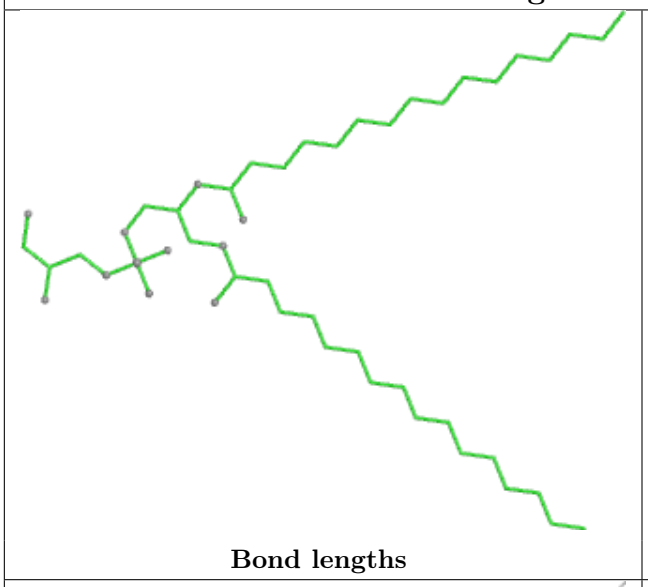


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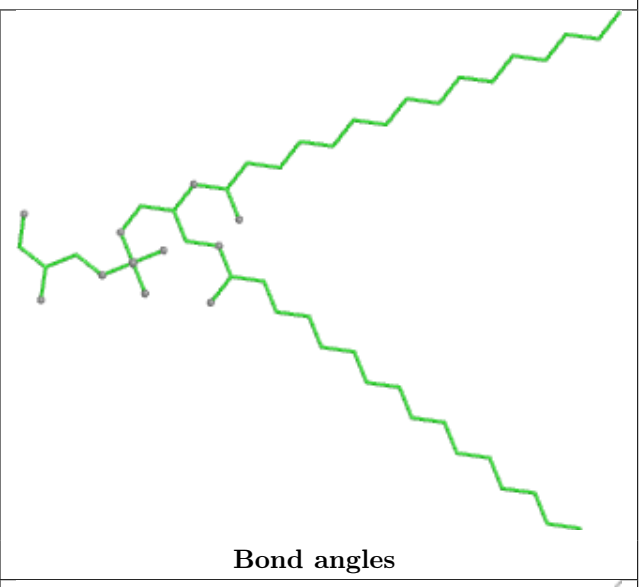


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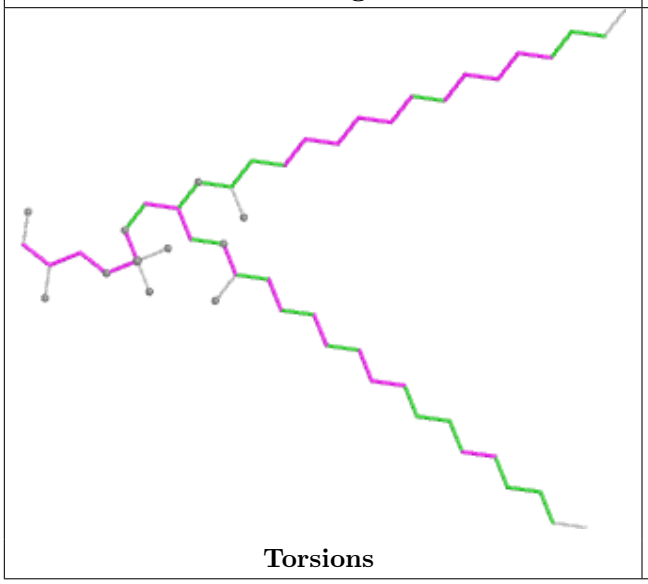
Ligand LHG 1 317



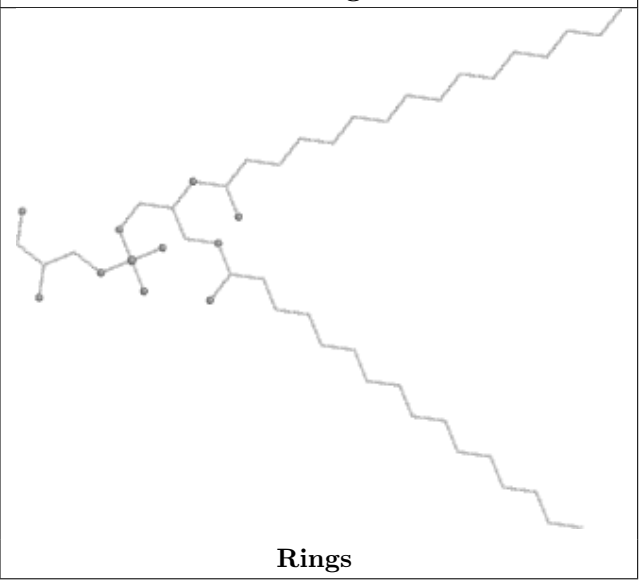
Bond lengths



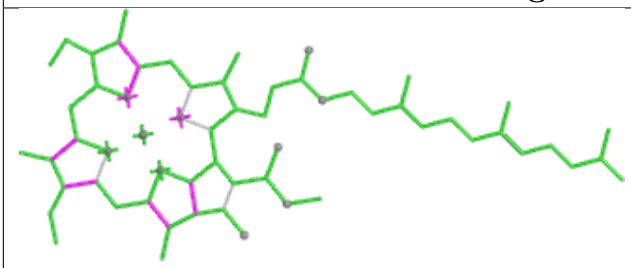
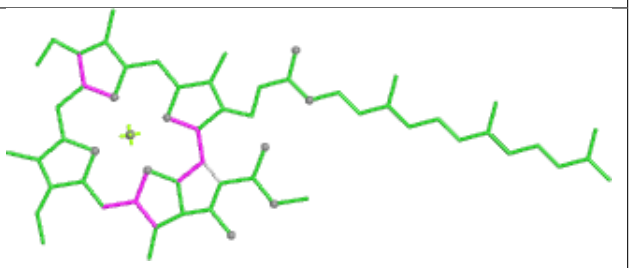
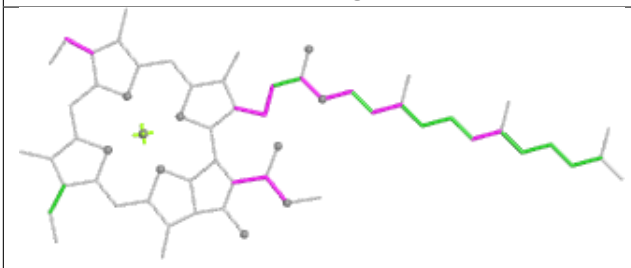
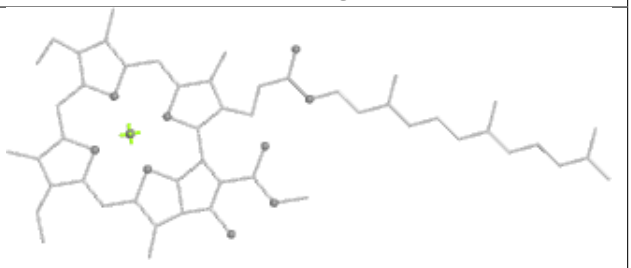
Bond angles

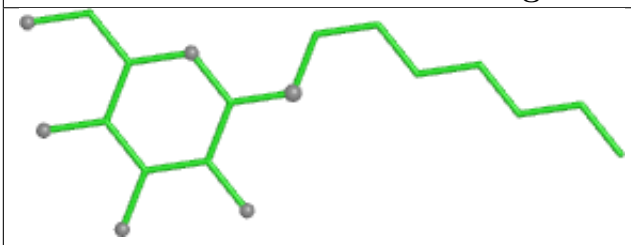
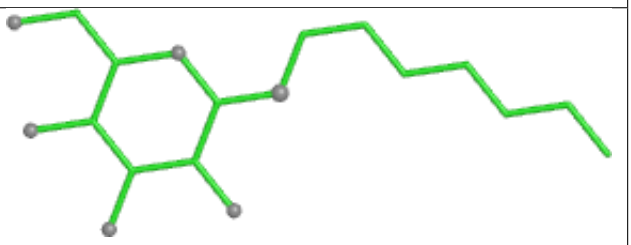
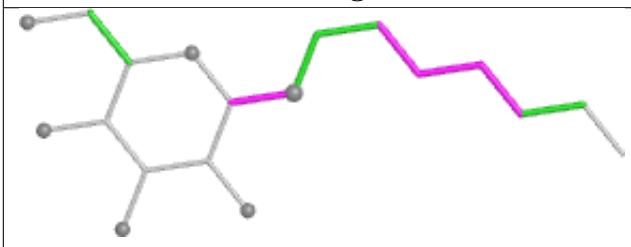
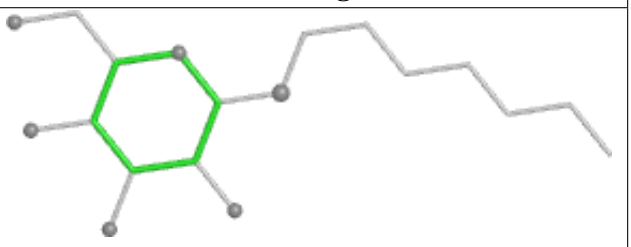


Torsions

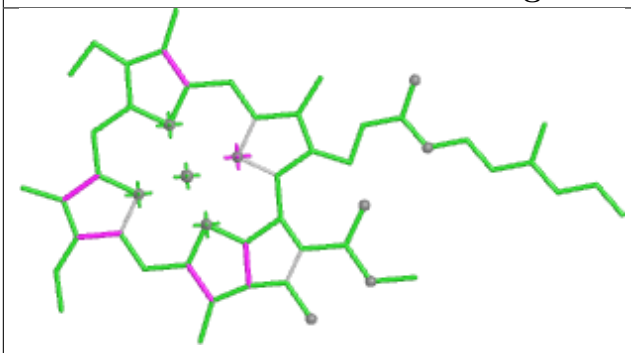


Rings

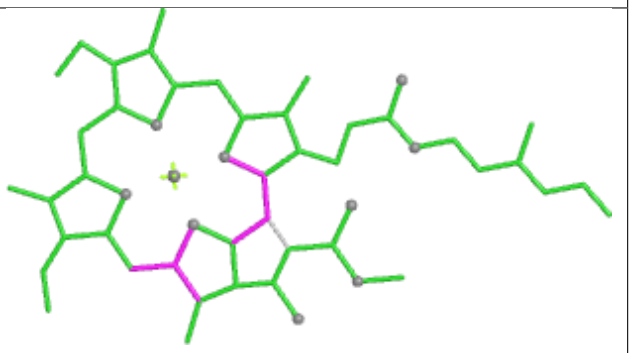
Ligand CLA 4 302	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand HTG F 305	
	
Bond lengths	Bond angles
	
Torsions	Rings

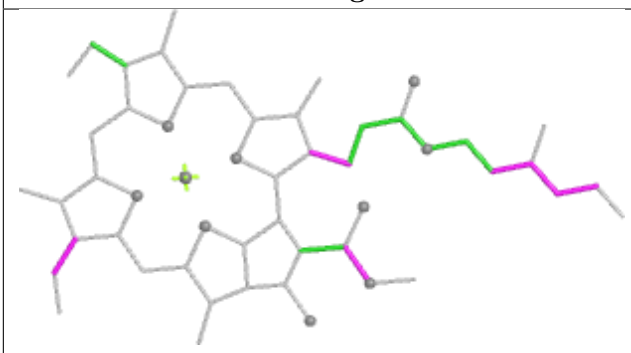
Ligand CLA O 103



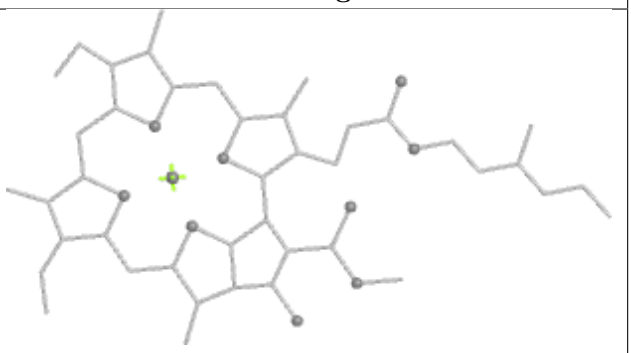
Bond lengths



Bond angles

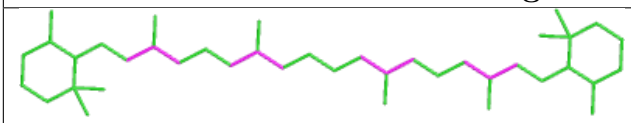


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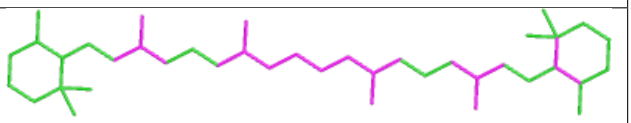


Rings

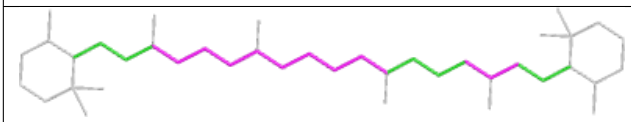
Ligand BCR B 843



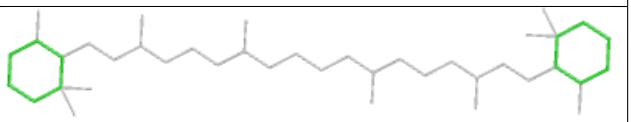
Bond lengths



Bond angles

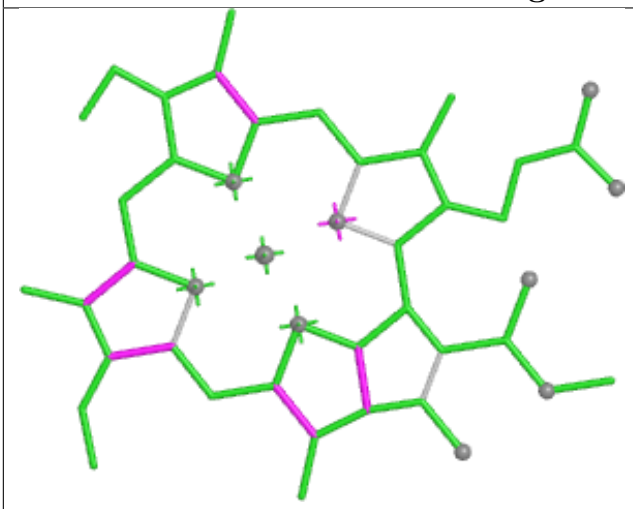


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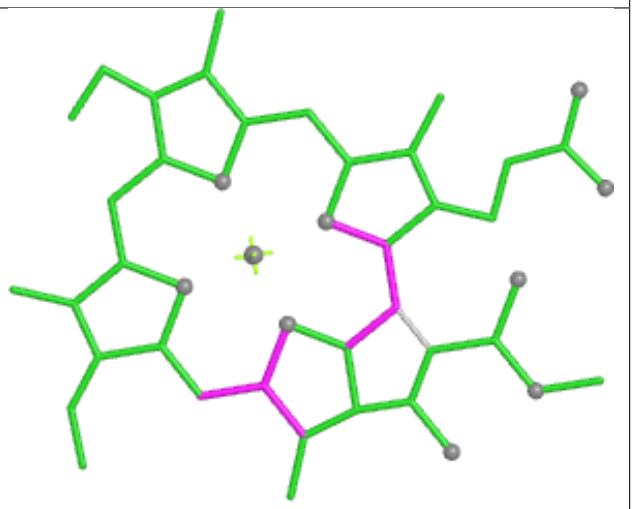


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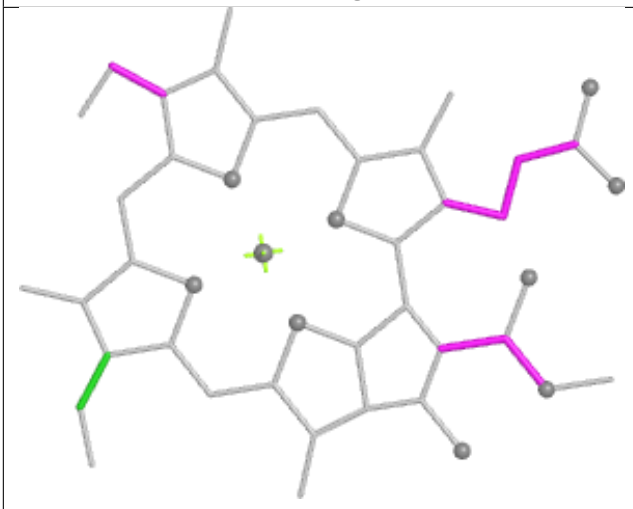
Ligand CLA 4 313



Bond lengths



Bond angles

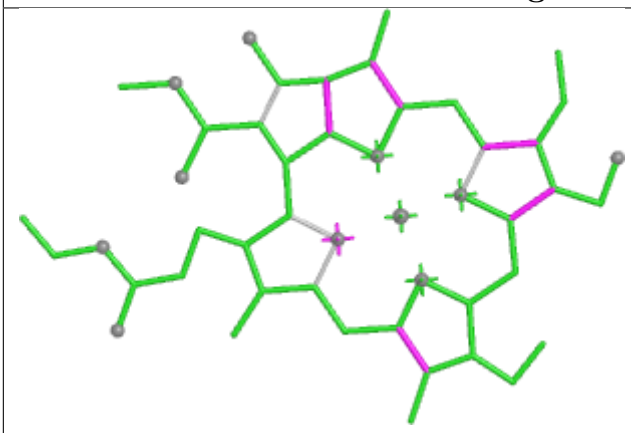


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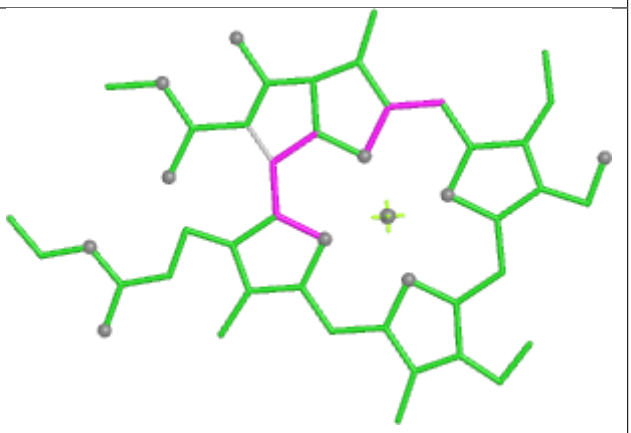


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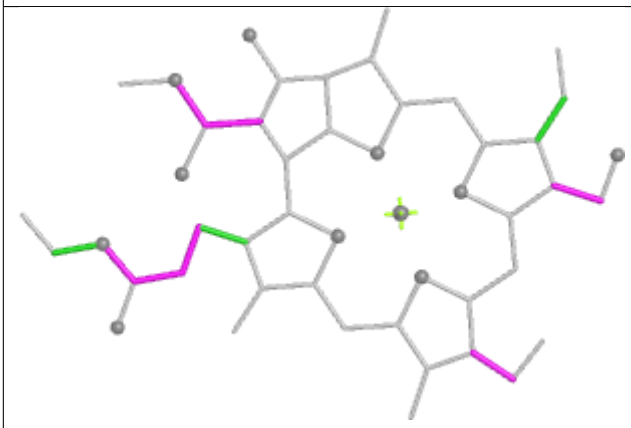
Ligand CHL 2 305



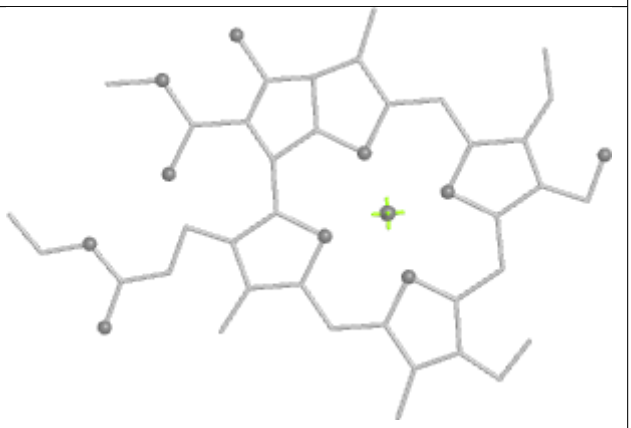
Bond lengths



Bond angles

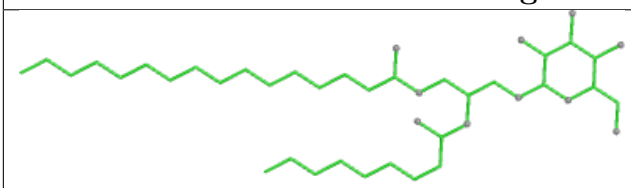


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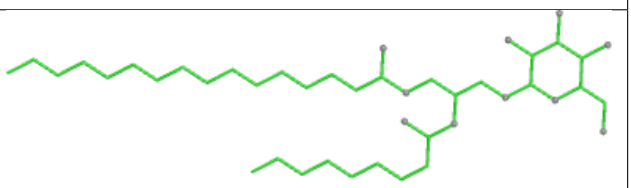


Rings

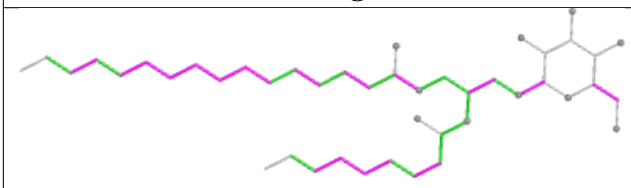
Ligand LMG B 849



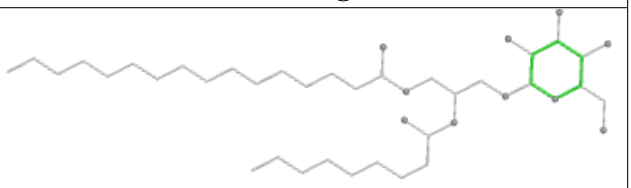
Bond lengths



Bond angles



Torsions

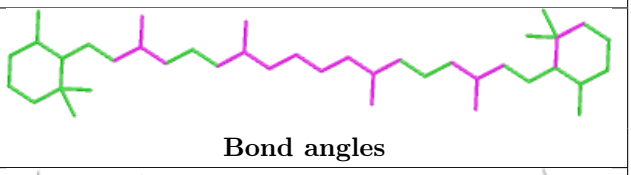


Rings

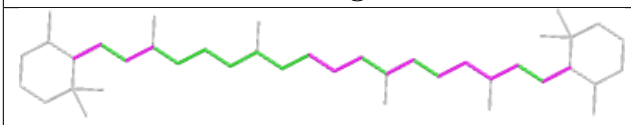
Ligand BCR L 305



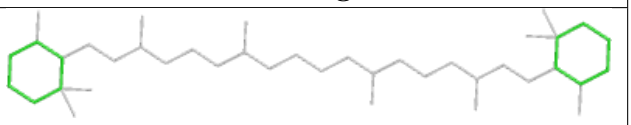
Bond lengths



Bond angles

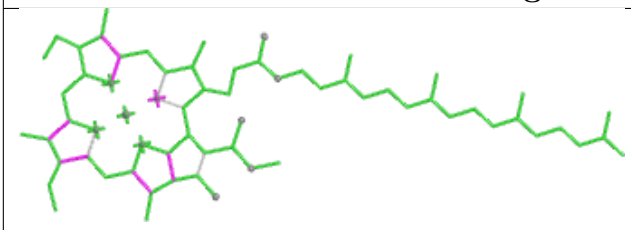


Torsions

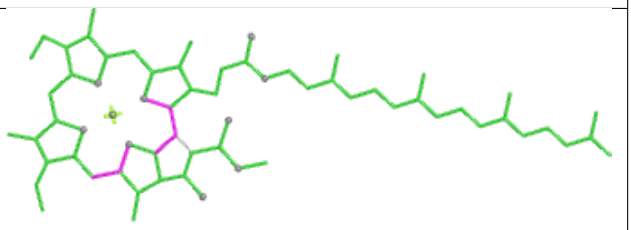


Rings

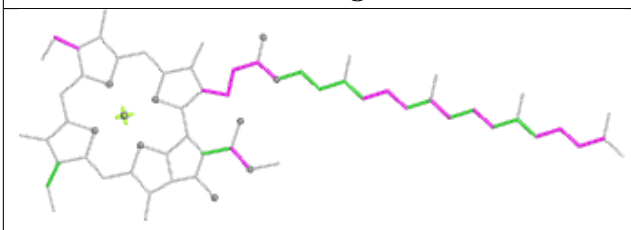
Ligand CLA A 807



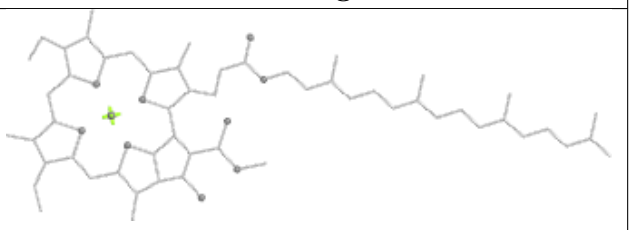
Bond lengths



Bond angles

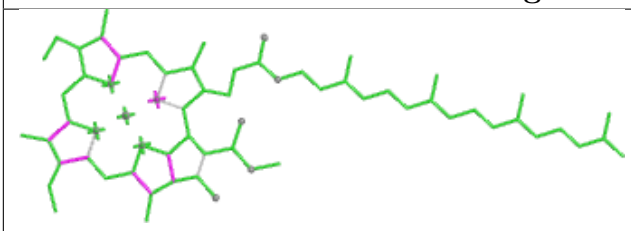


Torsions

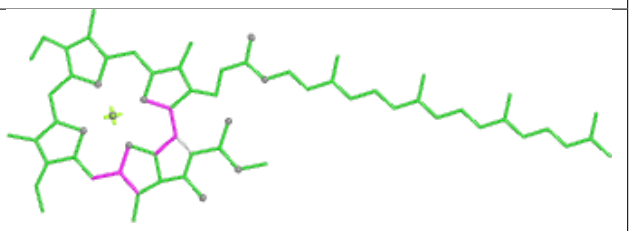


Rings

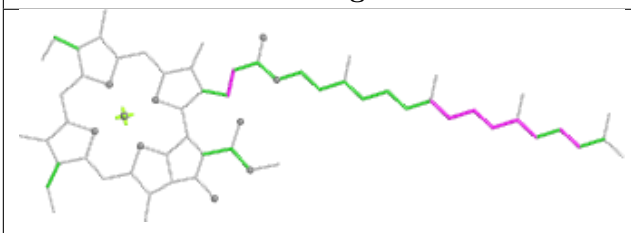
Ligand CLA A 852



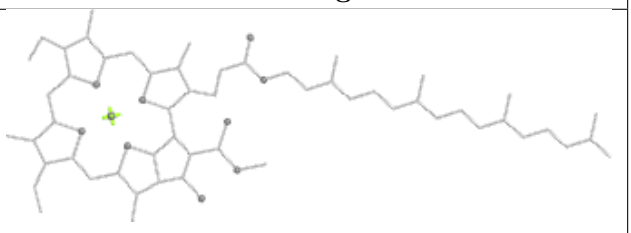
Bond lengths



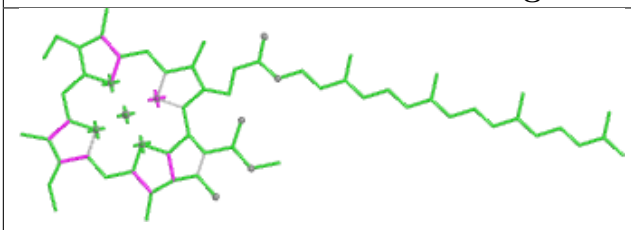
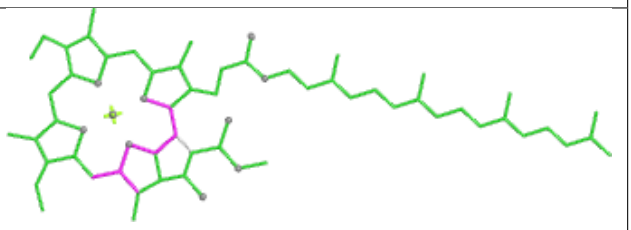
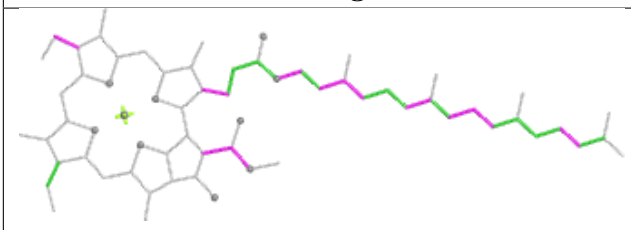
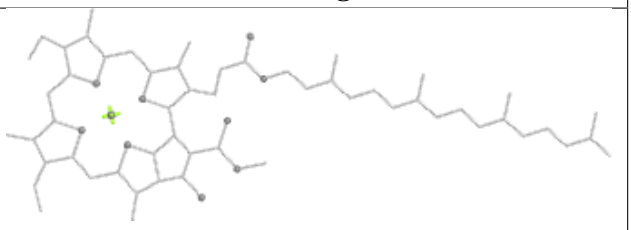
Bond angles

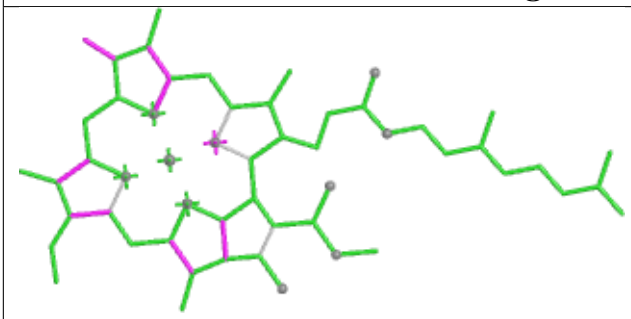
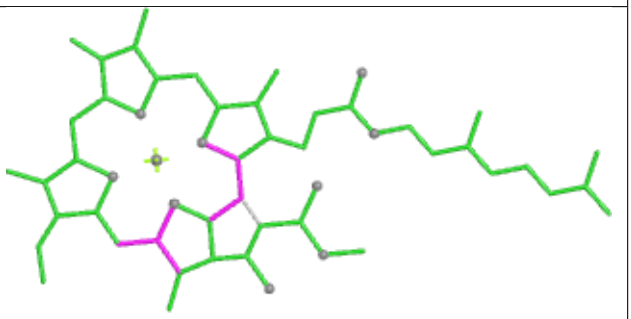
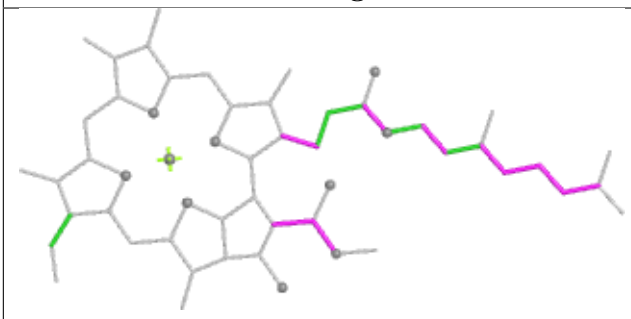
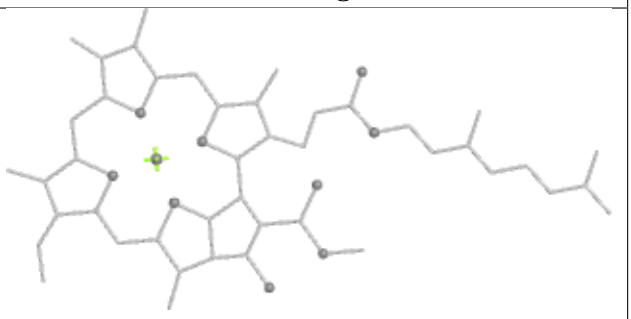


Torsions

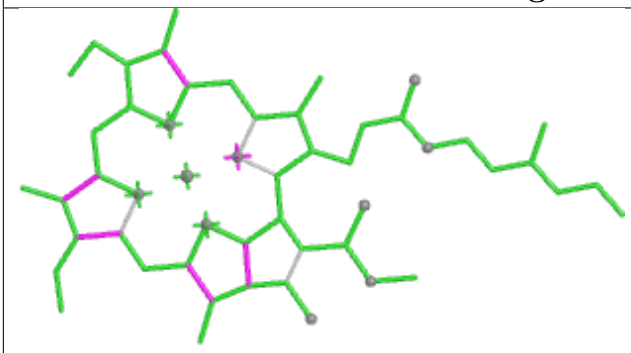


Rings

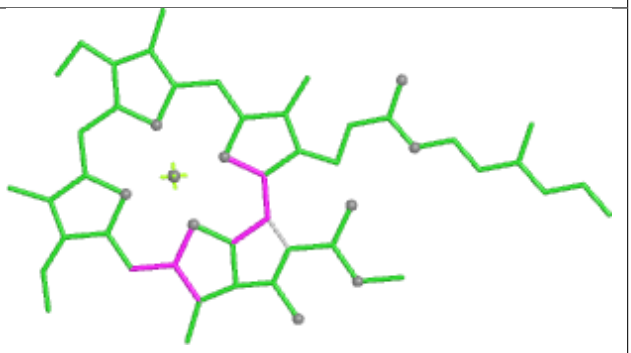
Ligand CLA A 854	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 811	
 Bond lengths	 Bond angles
 Torsions	 Rings

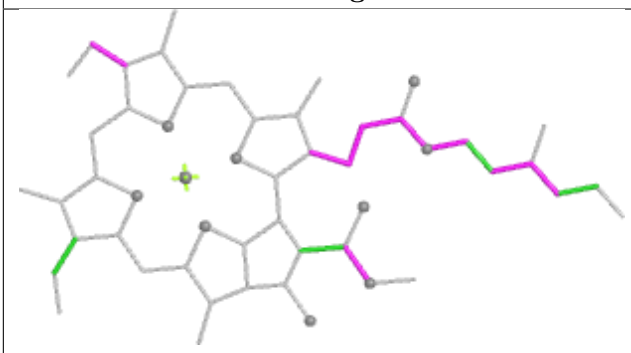
Ligand CLA 1 310



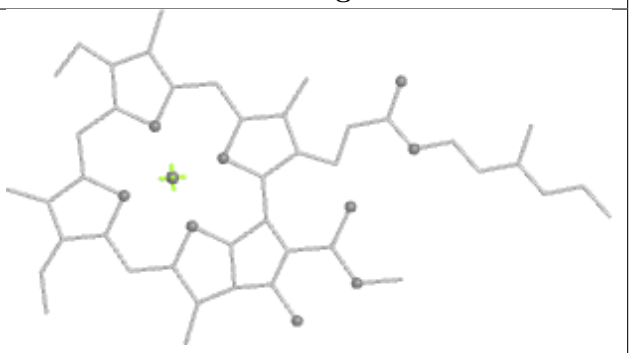
Bond lengths



Bond angles

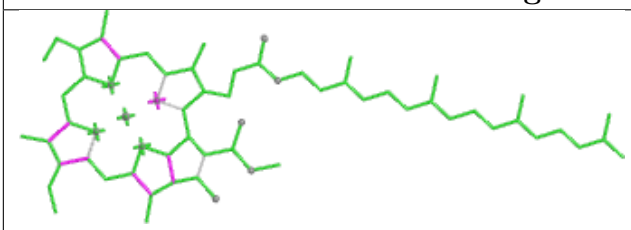


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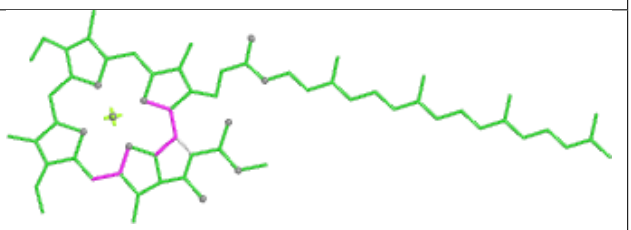


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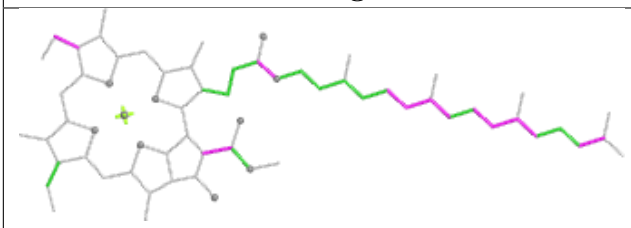
Ligand CLA A 824



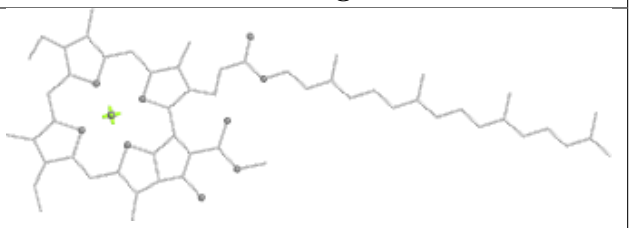
Bond lengths



Bond angles

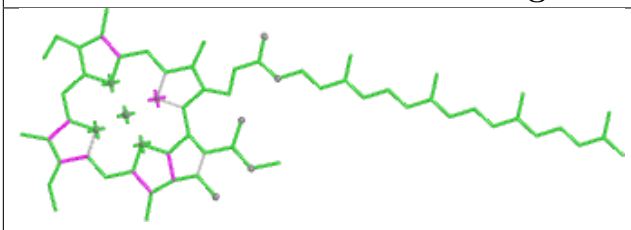


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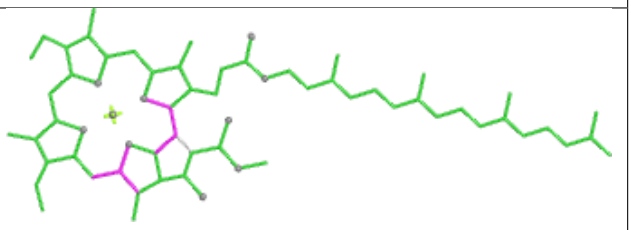


Rings

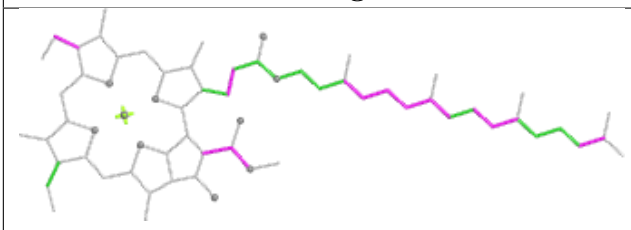
Ligand CLA 2 301



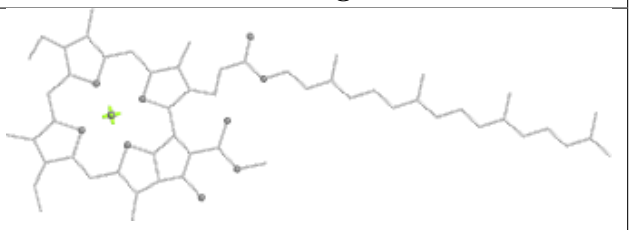
Bond lengths



Bond angles

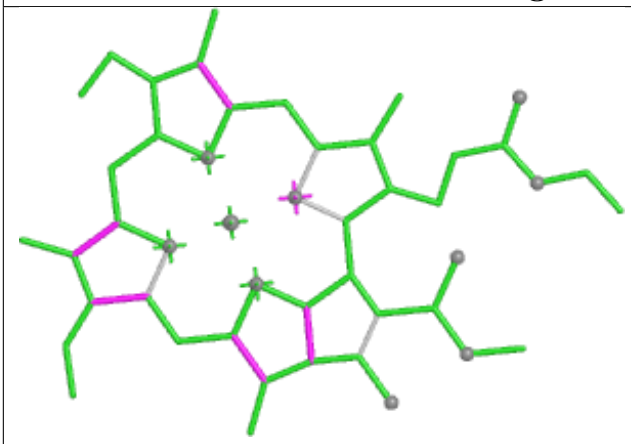


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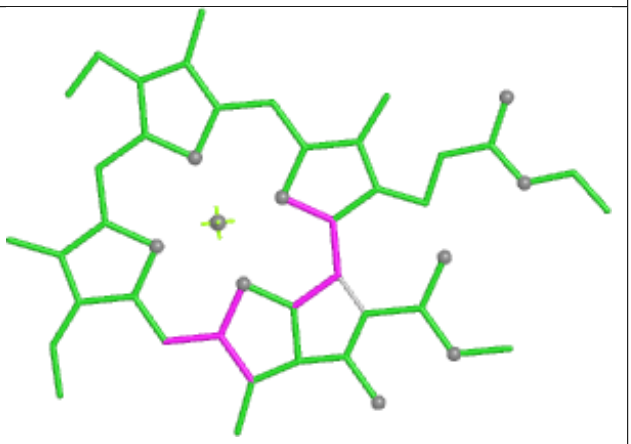


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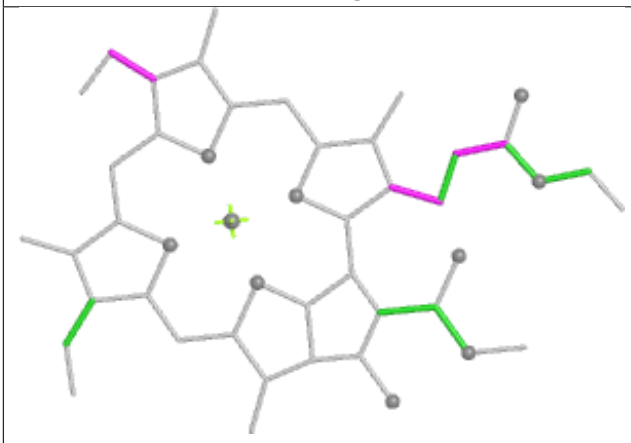
Ligand CLA 4 314



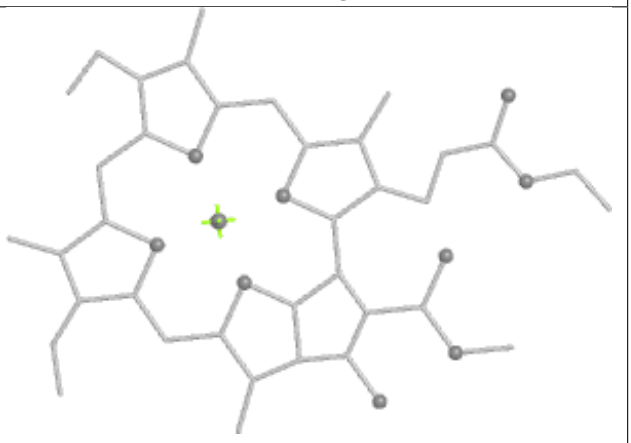
Bond lengths



Bond angles

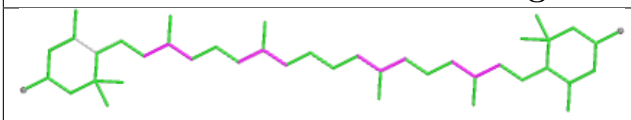


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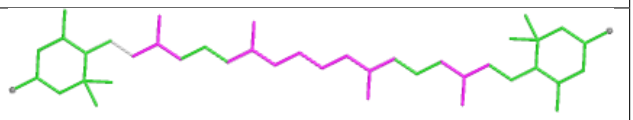


Rings

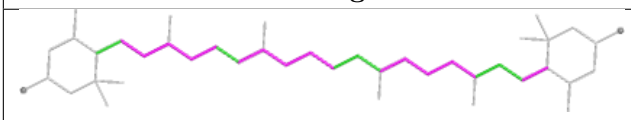
Ligand LUT 3 313



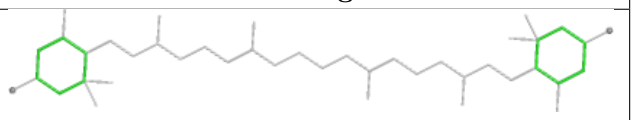
Bond lengths



Bond angles

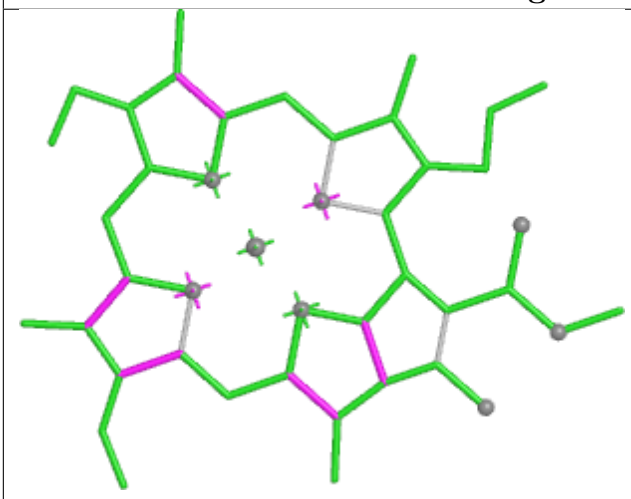


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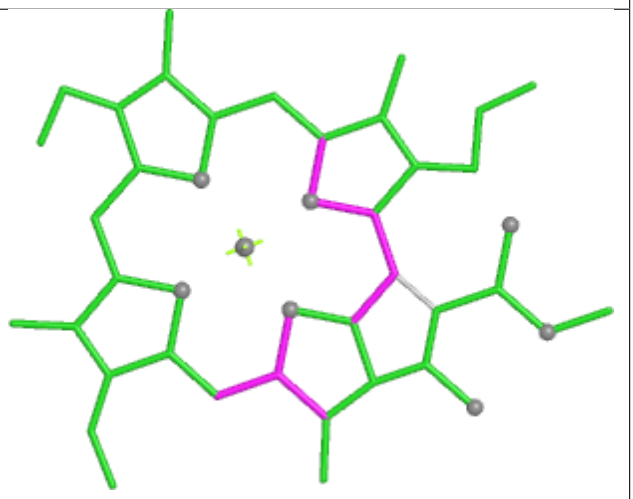


Rings

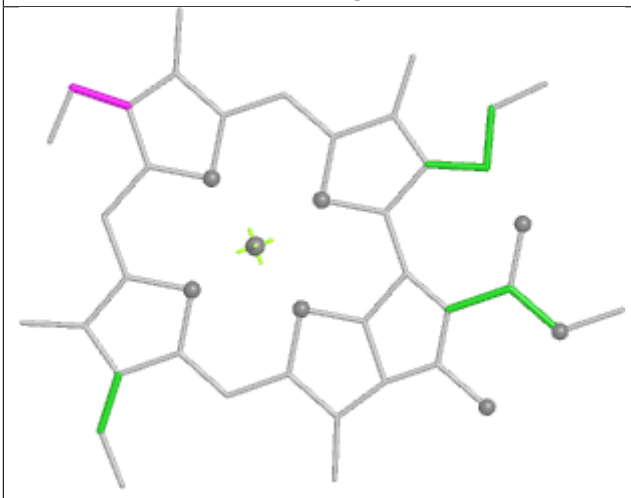
Ligand CLA 2 312



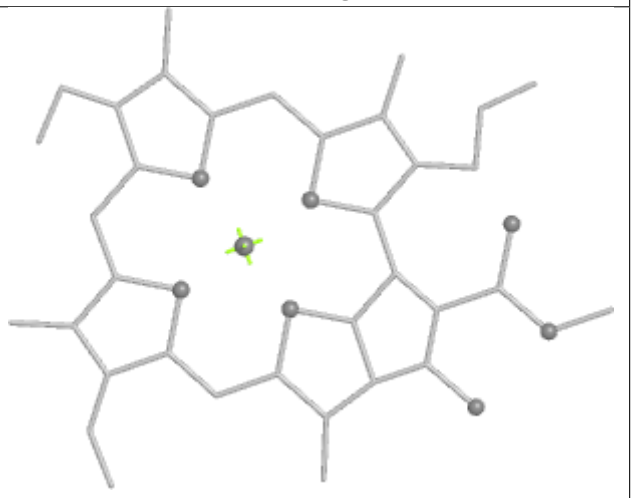
Bond lengths



Bond angles

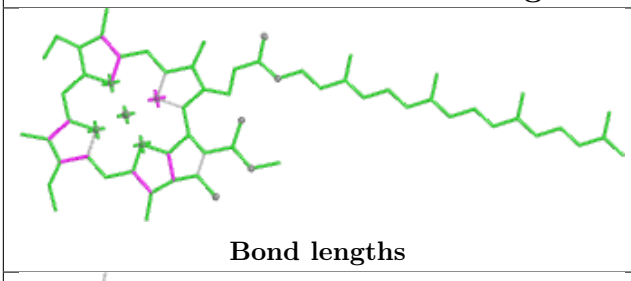


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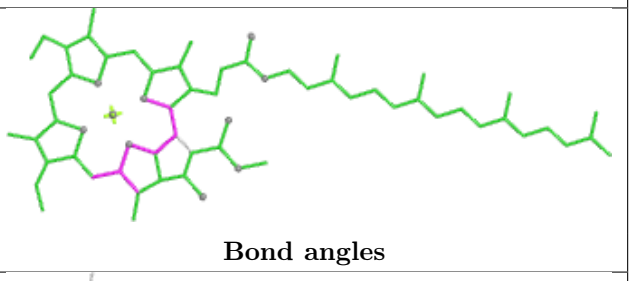


Rings

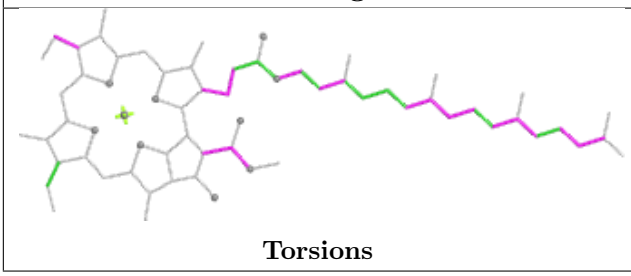
Ligand CLA B 827



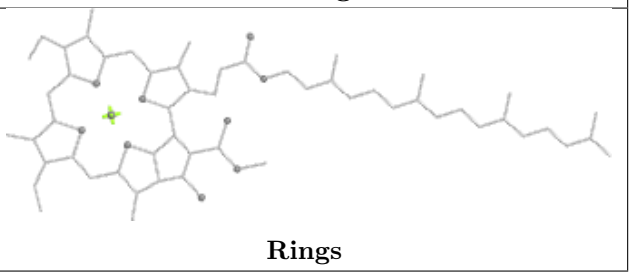
Bond lengths



Bond angles

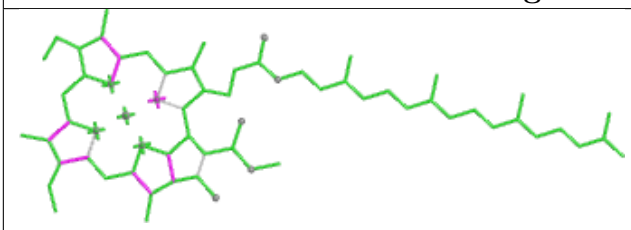


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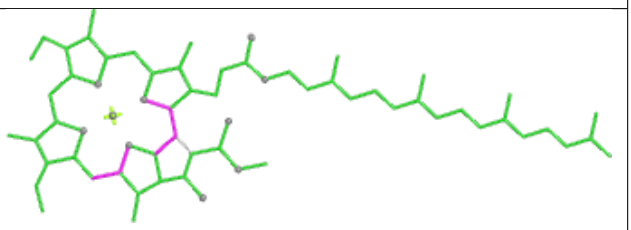


Rings

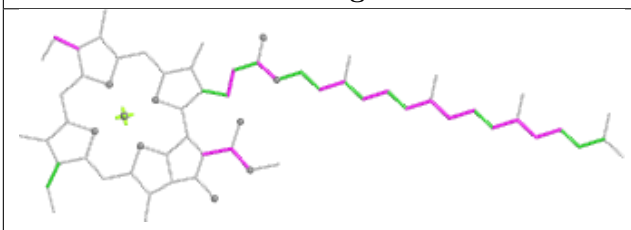
Ligand CLA A 815



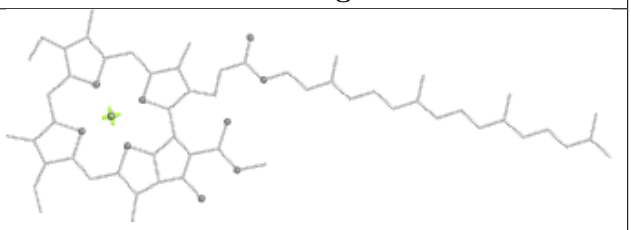
Bond lengths



Bond angles

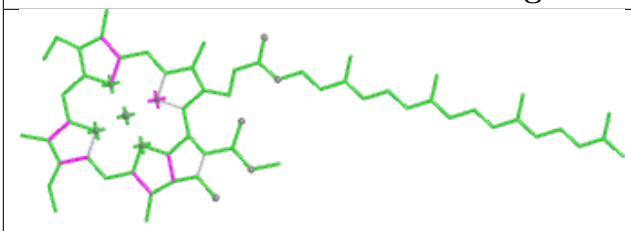


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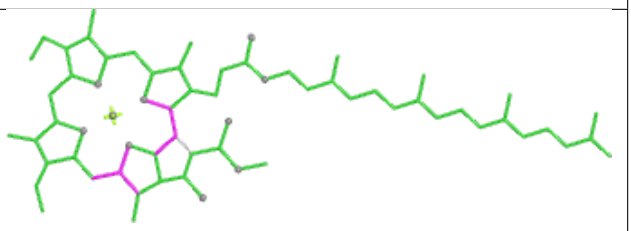


Rings

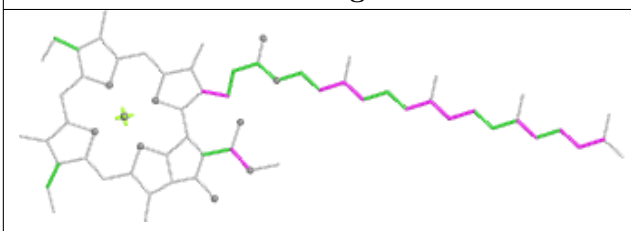
Ligand CLA B 829



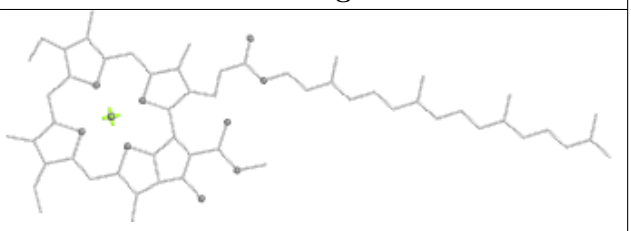
Bond lengths



Bond angles

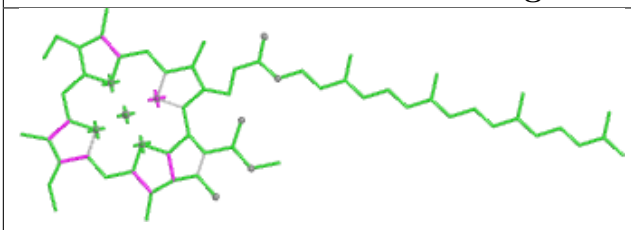


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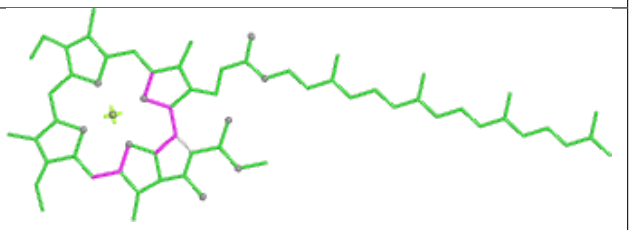


Rings

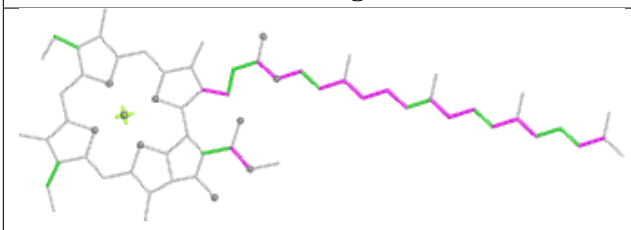
Ligand CLA B 839



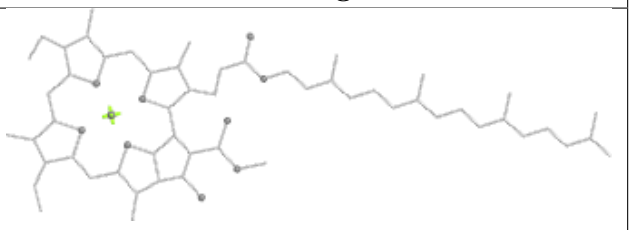
Bond lengths



Bond angles

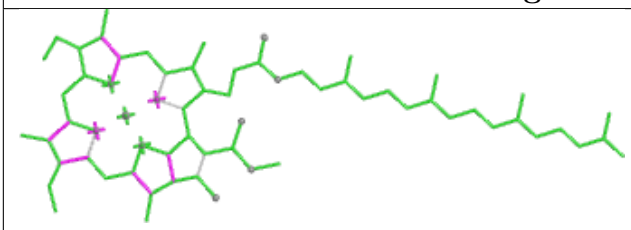


Torsions

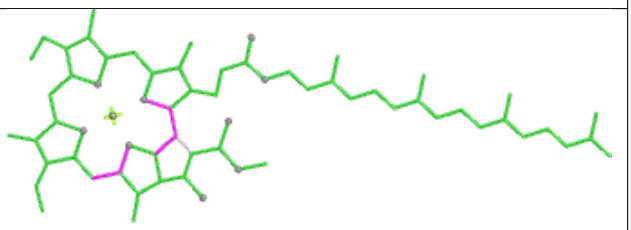


Rings

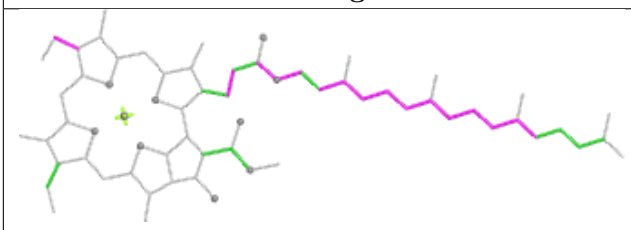
Ligand CLA A 840



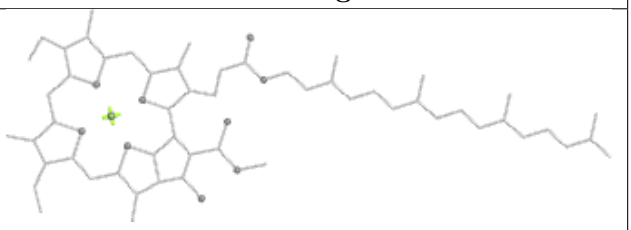
Bond lengths



Bond angles

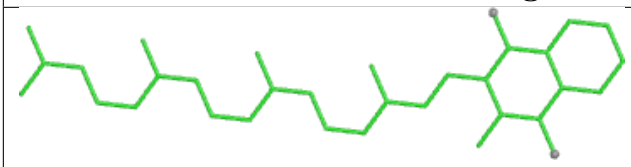


Torsions

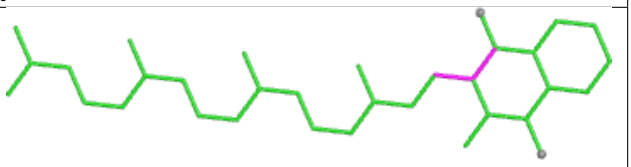


Rings

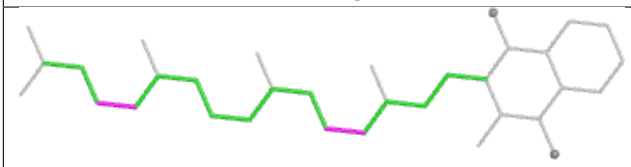
Ligand PQN B 841



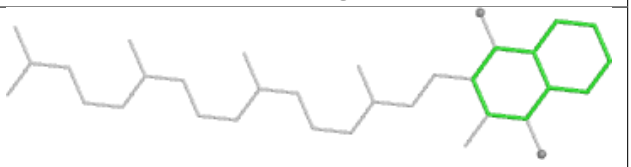
Bond lengths



Bond angles

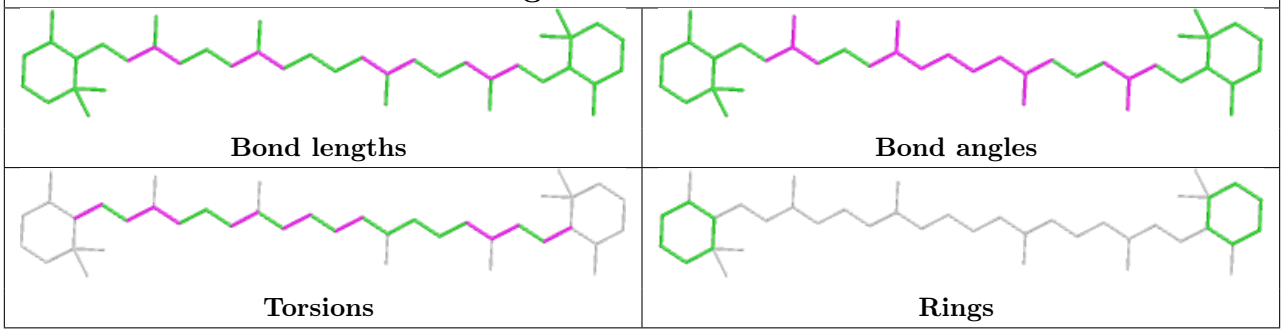


Torsions

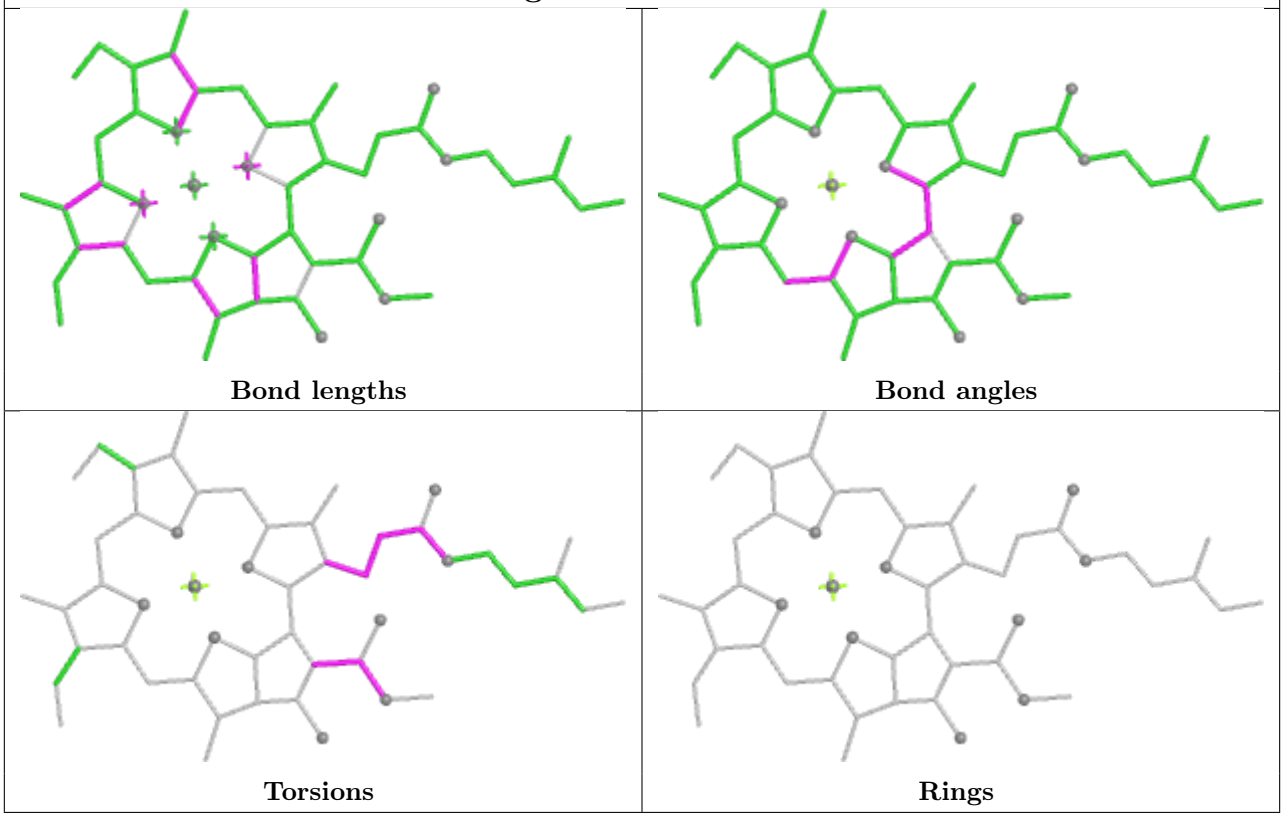


Rings

Ligand BCR B 846



Ligand CLA A 834



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.

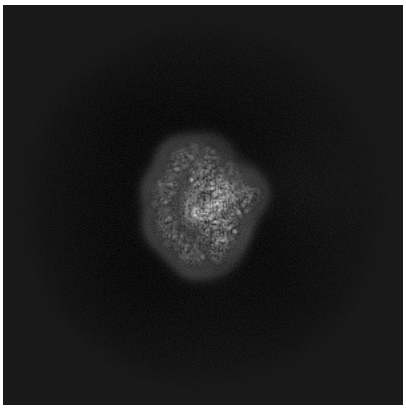
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-67007. These allow visual inspection of the internal detail of the map and identification of artifacts.

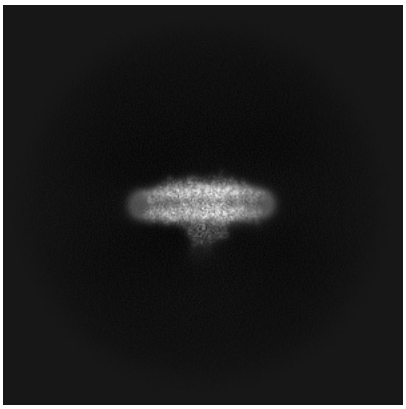
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

6.1.1 Primary map



X

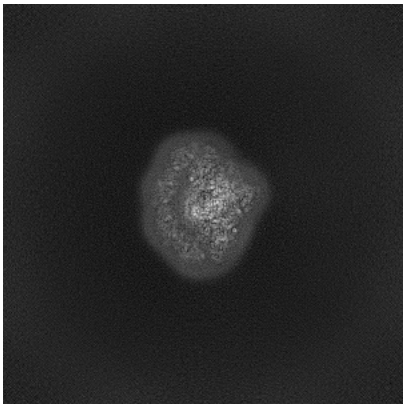


Y

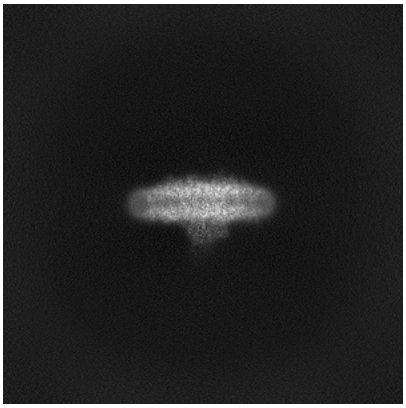


Z

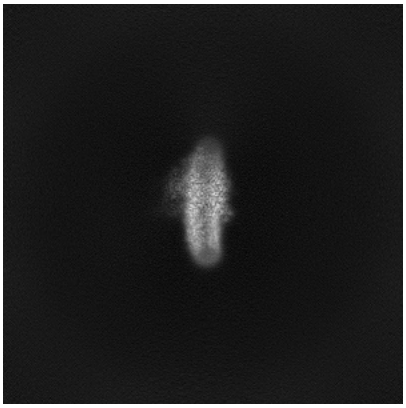
6.1.2 Raw map



X



Y

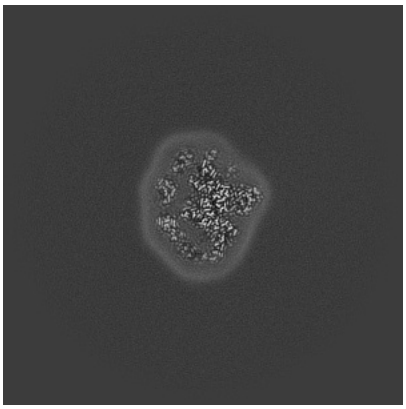


Z

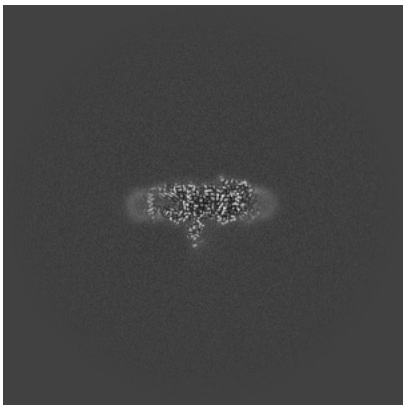
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

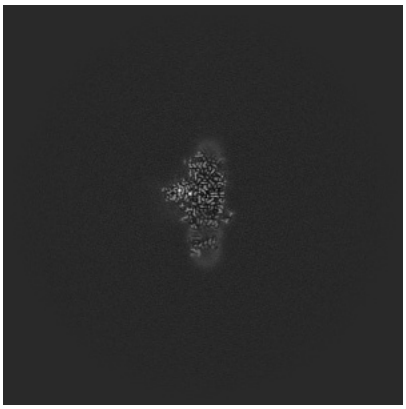
6.2.1 Primary map



X Index: 256

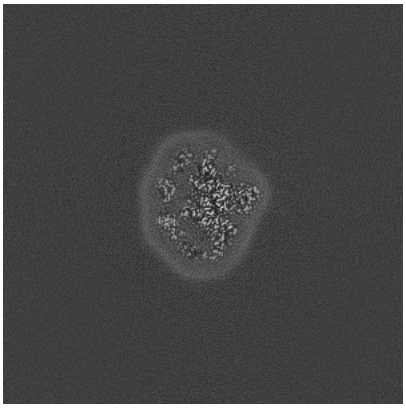


Y Index: 256

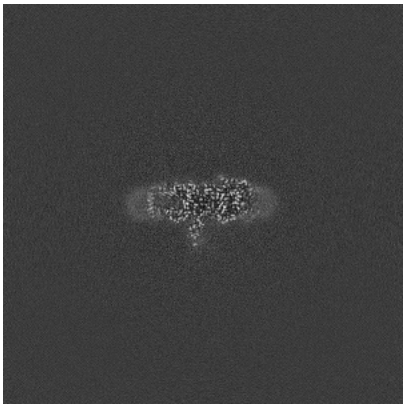


Z Index: 256

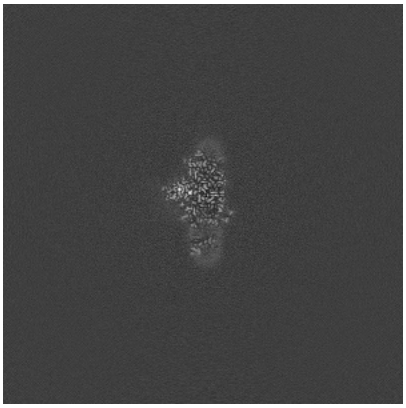
6.2.2 Raw map



X Index: 256



Y Index: 256

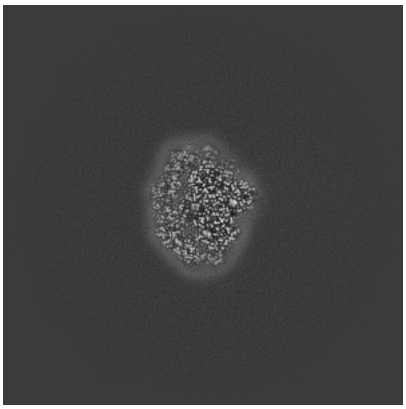


Z Index: 256

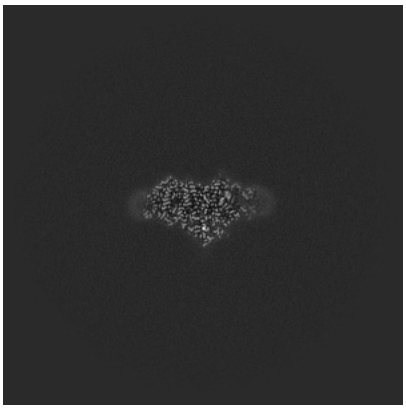
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

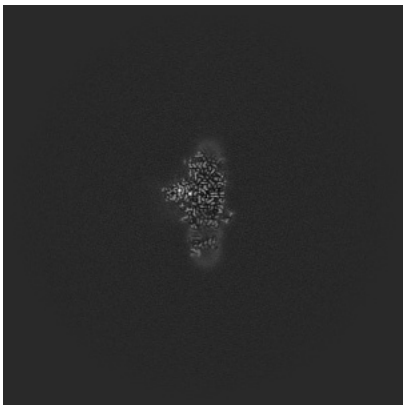
6.3.1 Primary map



X Index: 245

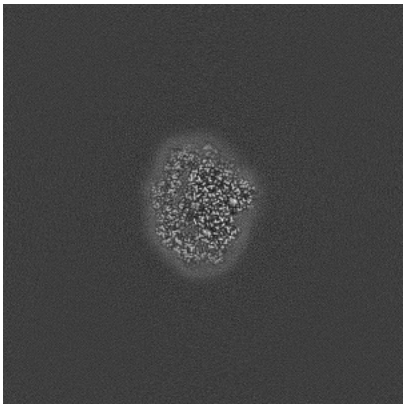


Y Index: 274

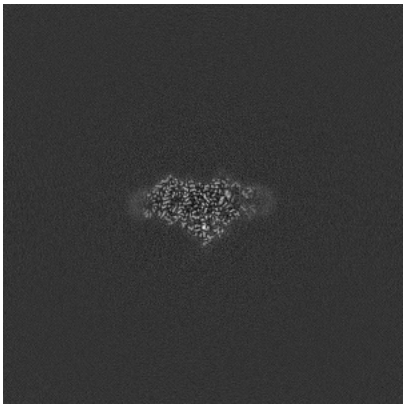


Z Index: 256

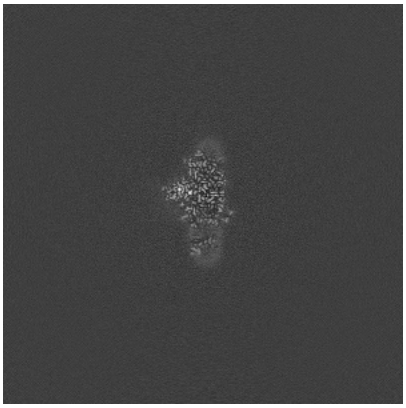
6.3.2 Raw map



X Index: 245



Y Index: 274

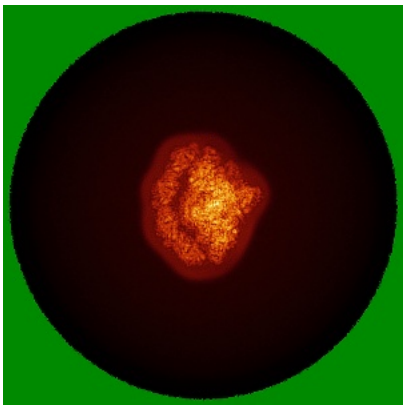


Z Index: 256

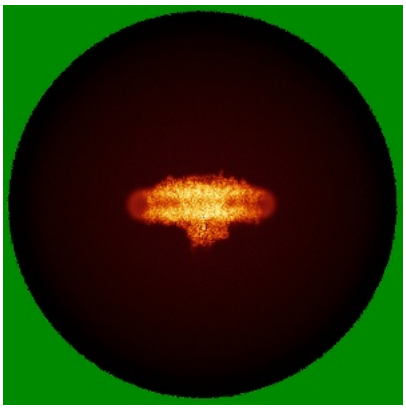
The images above show the largest variance slices of the map in three orthogonal directions.

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

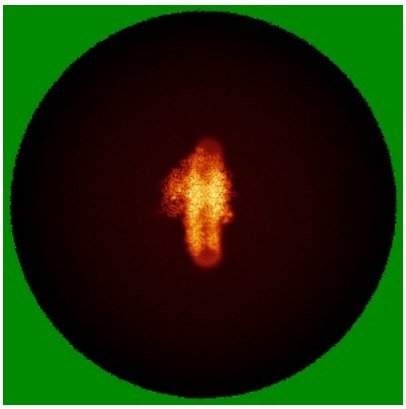
6.4.1 Primary map



X

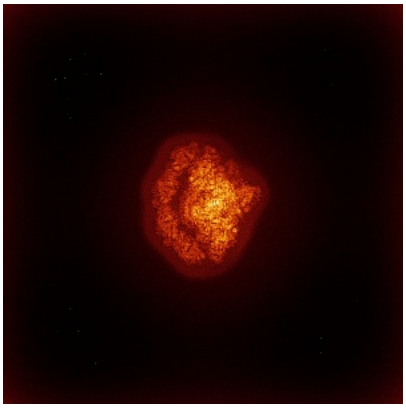


Y

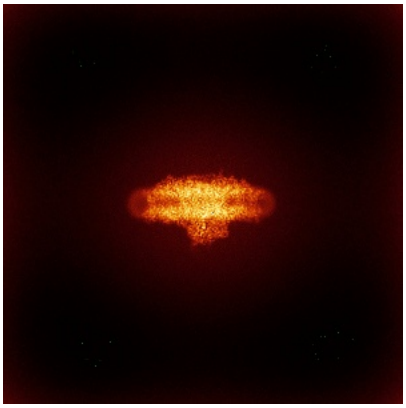


Z

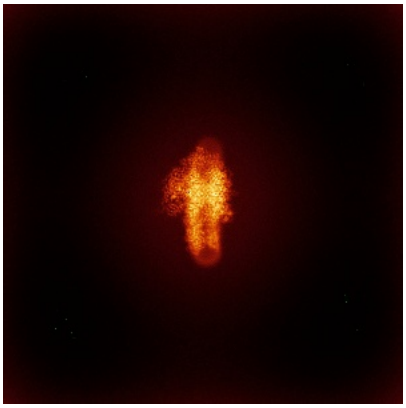
6.4.2 Raw map



X



Y

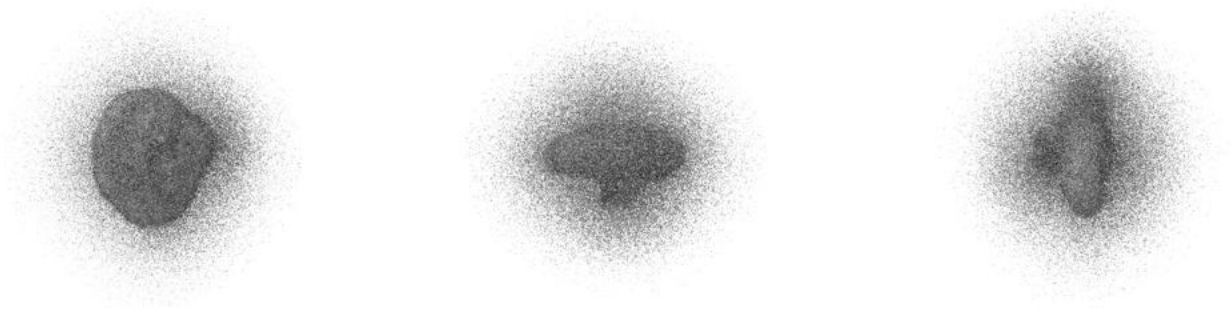


Z

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)

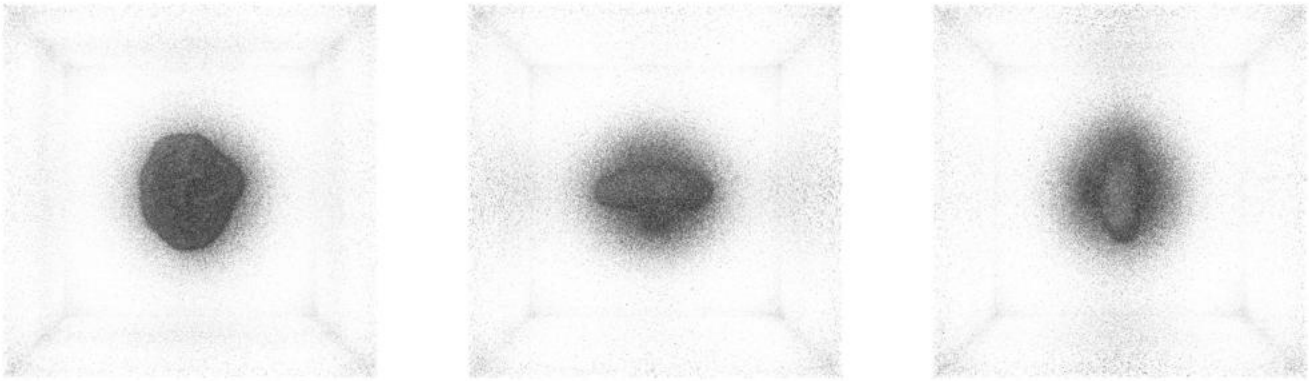
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0418. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

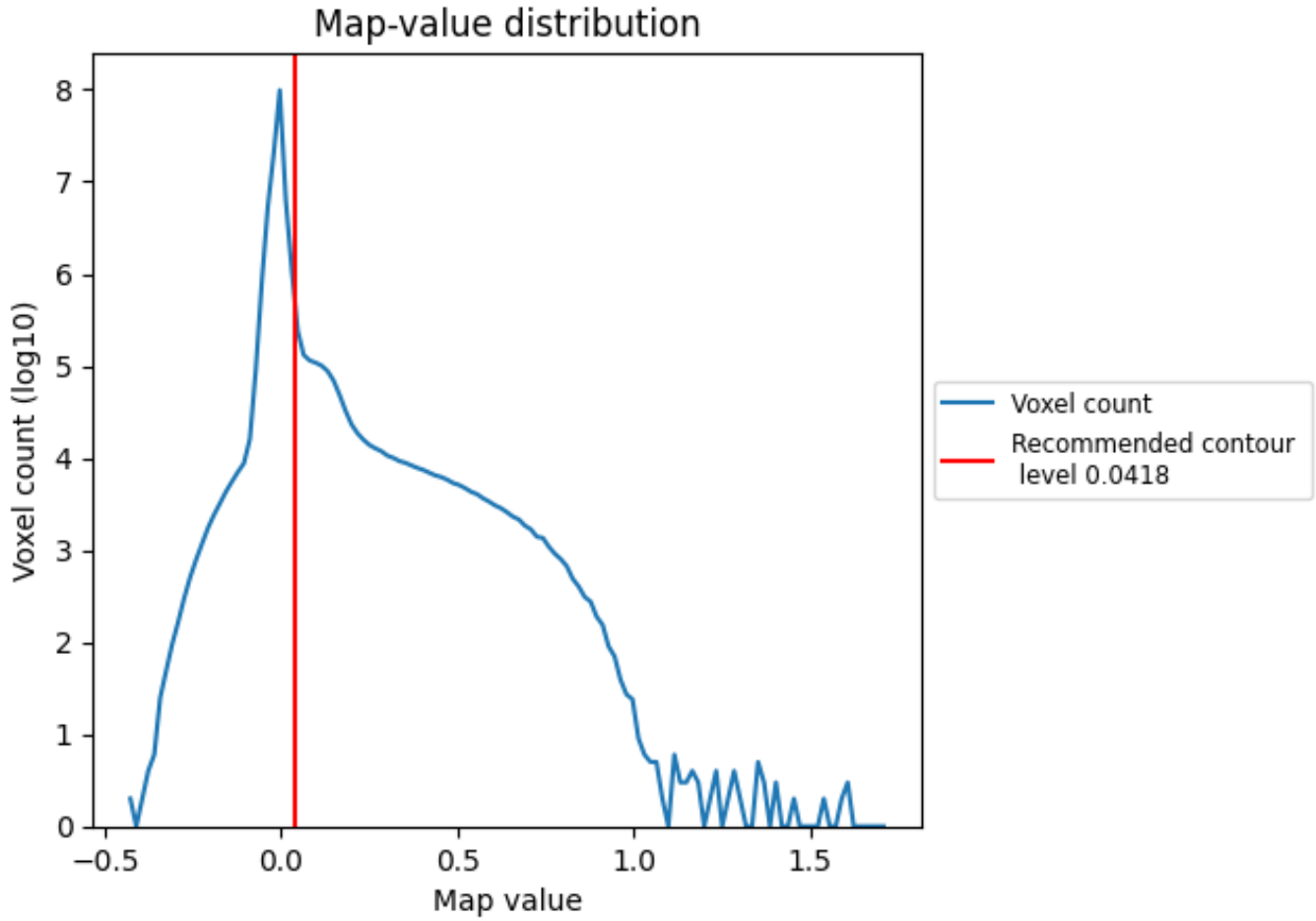
6.6 Mask visualisation (i)

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

7 Map analysis

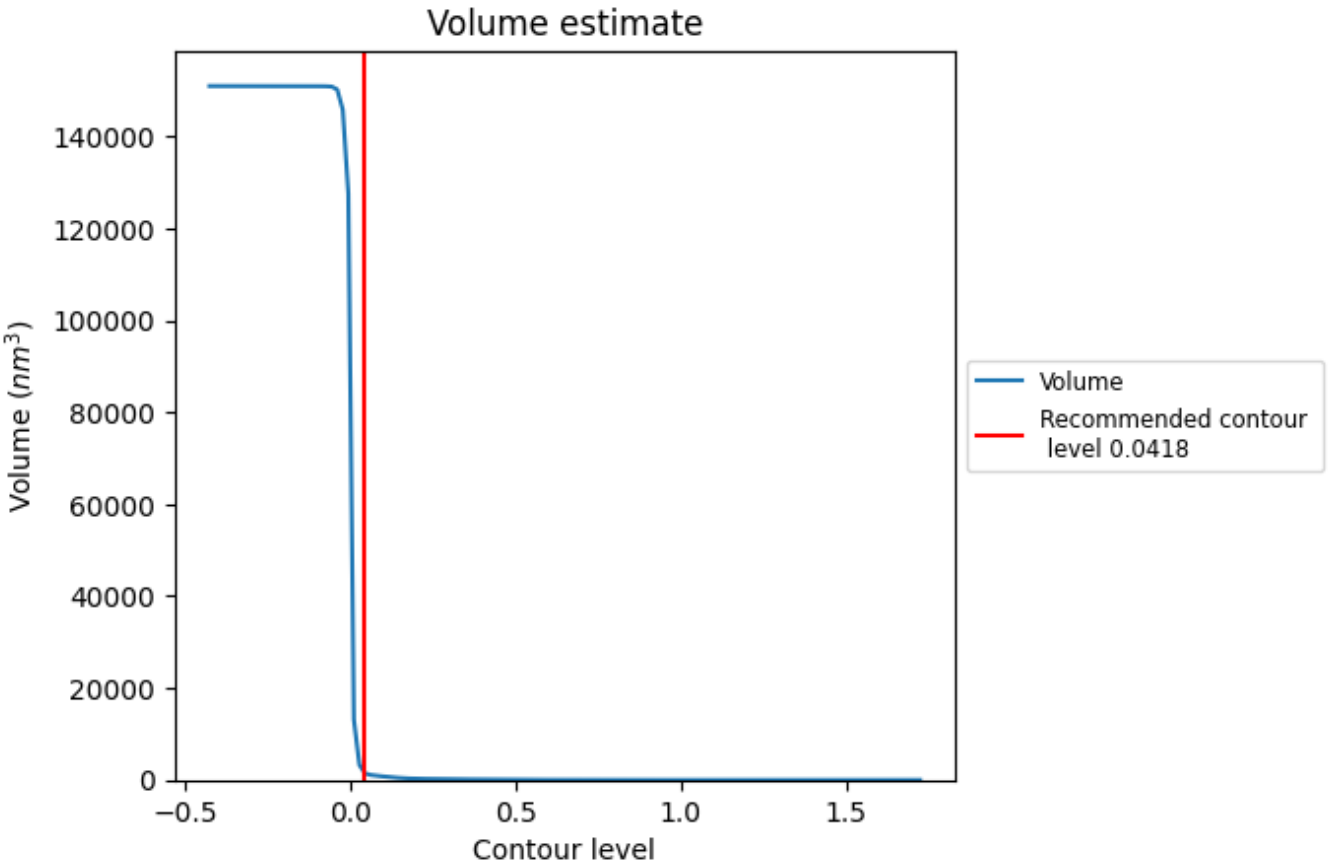
This section contains the results of statistical analysis of the map.

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.

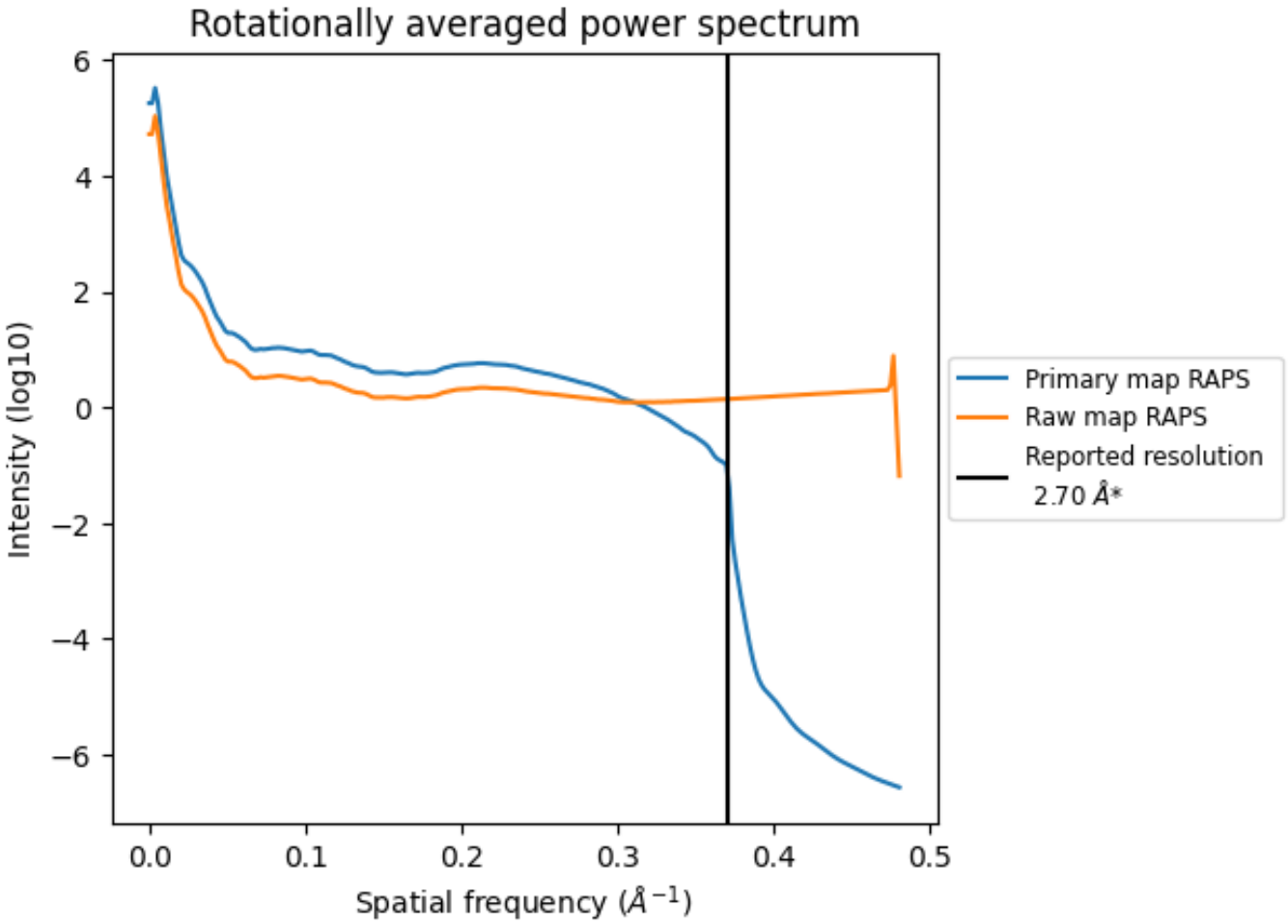
7.2 Volume estimate (i)



The volume at the recommended contour level is 1604 nm^3; this corresponds to an approximate mass of 1449 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

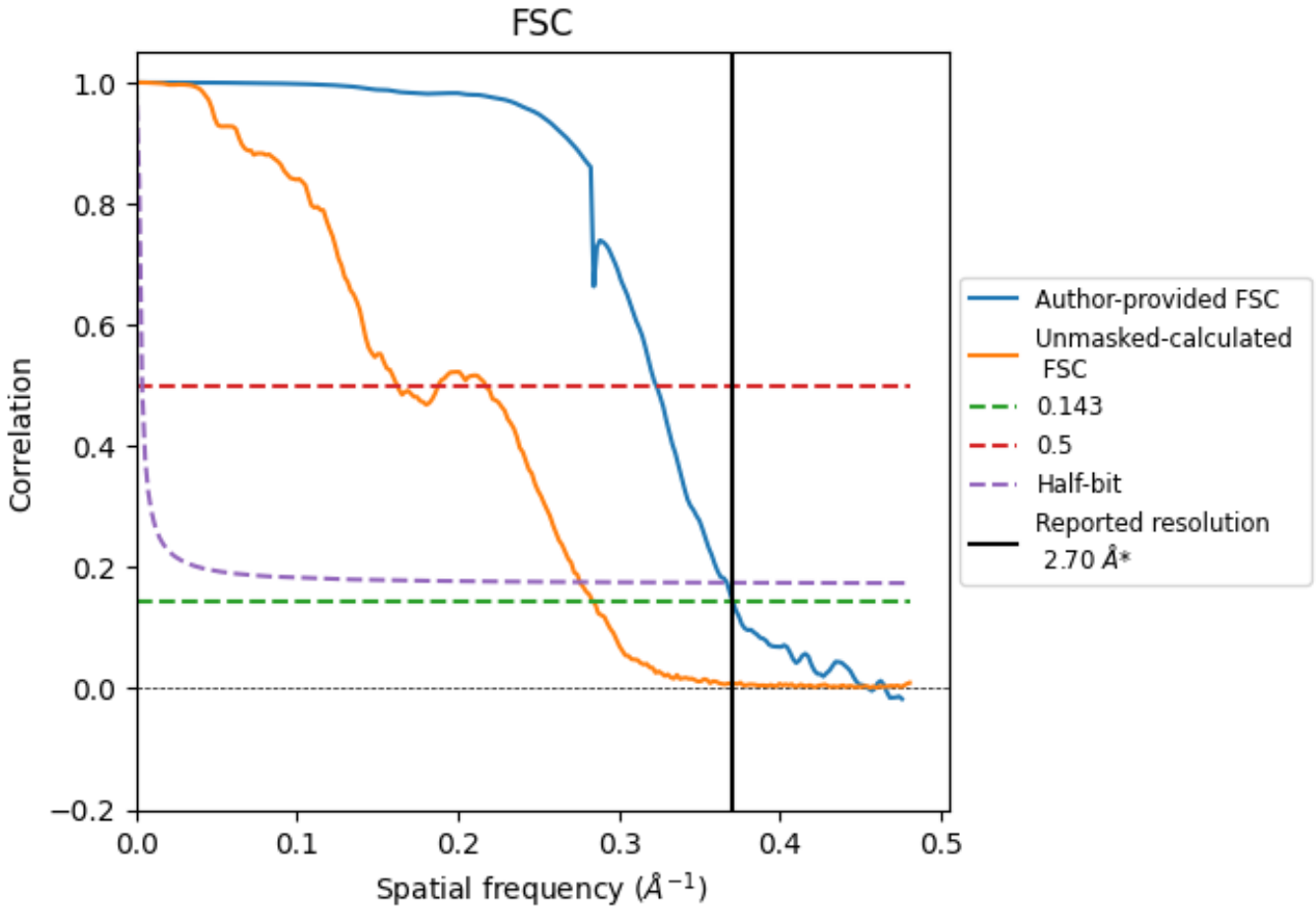


*Reported resolution corresponds to spatial frequency of 0.370 Å^{-1}

8 Fourier-Shell correlation

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 0.370 Å^{-1}

8.2 Resolution estimates (i)

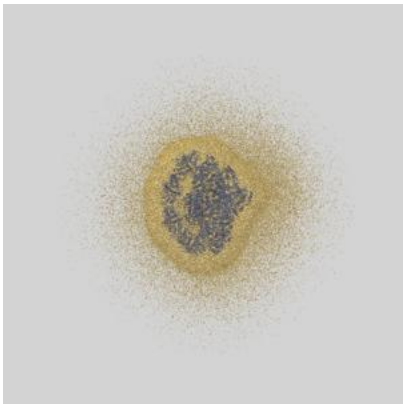
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.70	3.09	2.72
Unmasked-calculated*	3.52	6.17	3.63

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.52 differs from the reported value 2.7 by more than 10 %

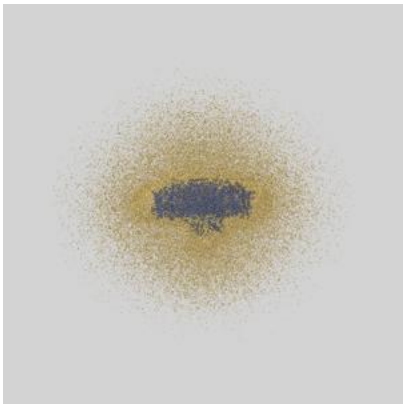
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-67007 and PDB model 9XLV. Per-residue inclusion information can be found in section 3 on page 24.

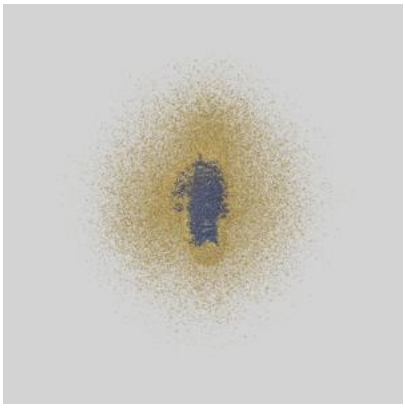
9.1 Map-model overlay



X



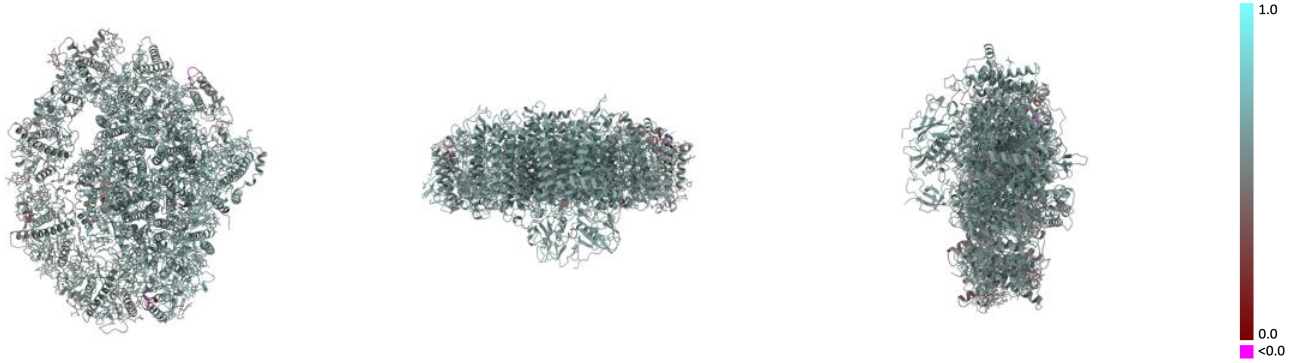
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0418 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

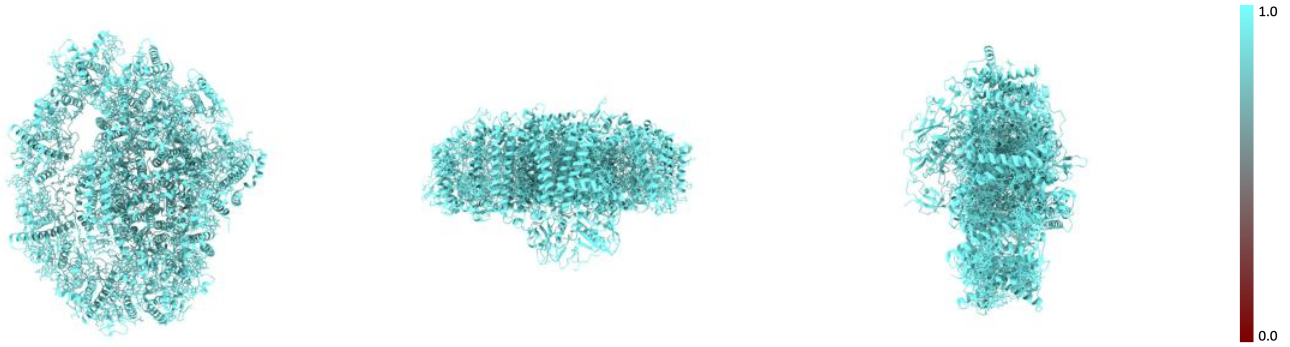
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

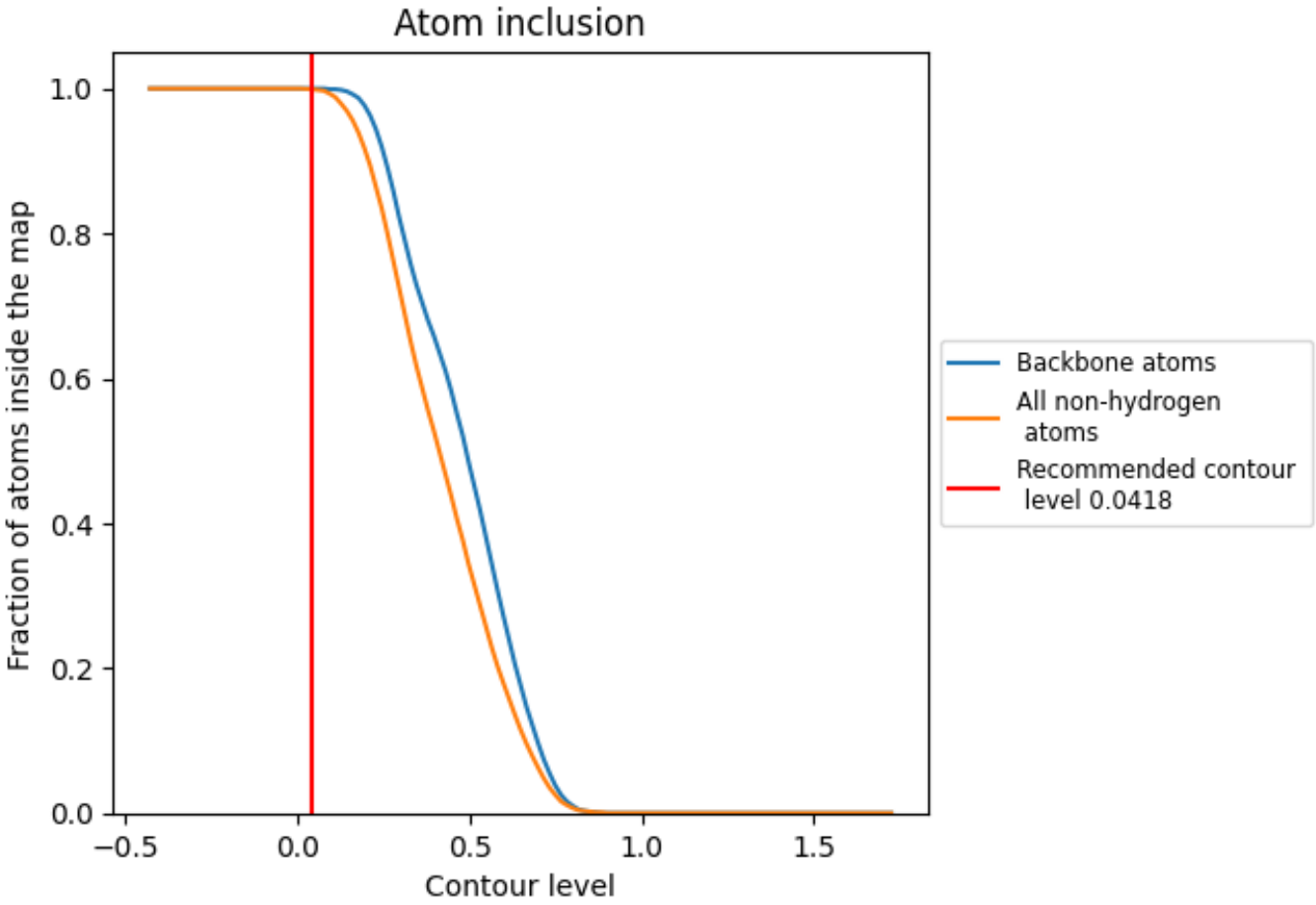
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0418).

9.4 Atom inclusion (i)



At the recommended contour level, 100% of all backbone atoms, 100% 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 (0.0418) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9990	0.5710
1	0.9980	0.5490
2	0.9980	0.5340
3	1.0000	0.5230
4	0.9970	0.5370
A	0.9990	0.5980
B	1.0000	0.6010
C	0.9970	0.5710
D	0.9990	0.5780
E	1.0000	0.5760
F	0.9980	0.5600
G	0.9930	0.5340
H	1.0000	0.5660
I	1.0000	0.5780
J	1.0000	0.5670
K	0.9990	0.5220
L	1.0000	0.5770
O	0.9990	0.4960

