wwPDB EM Validation Summary Report (i)

Sep 15, 2026 – 02:07 AM JST

PDB ID	:	8WEY / pdb_00008wey
EMDB ID	:	EMD-37480
Title	:	PSI-LHCI of the red alga Cyanidium caldarium RK-1 (NIES-2137)
Authors	:	Kato, K.; Hamaguchi, T.; Nakajima, Y.; Kawakami, K.; Yonekura, K.; Shen, J.R.; Nagao, R.
Deposited on	:	2023-09-19
Resolution	:	1.92 Å(reported)
Based on initial model	:	.

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:

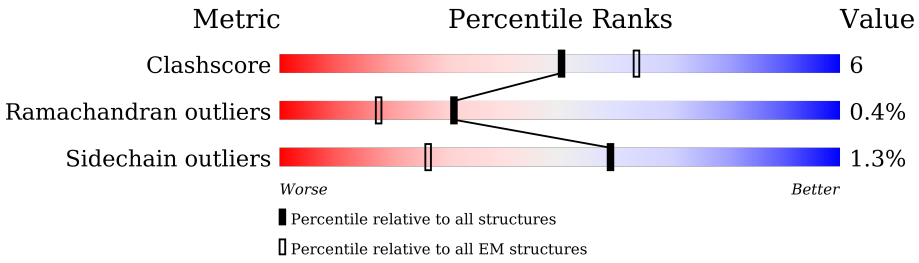
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using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

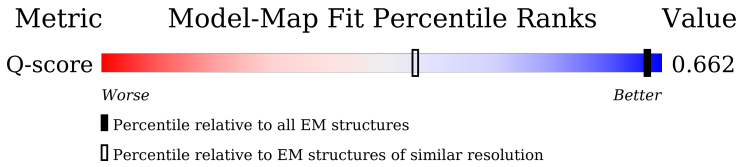
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.92 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.





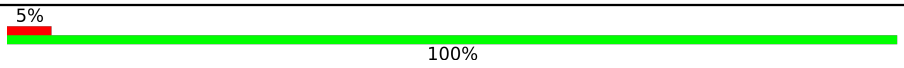
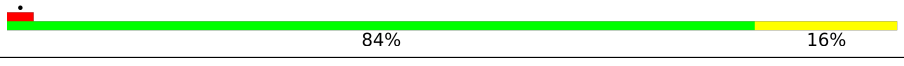
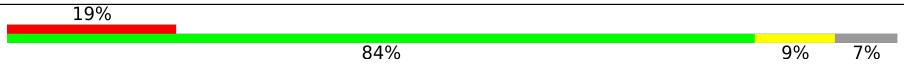
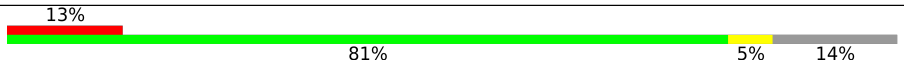
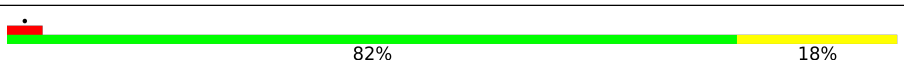
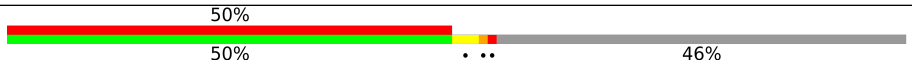
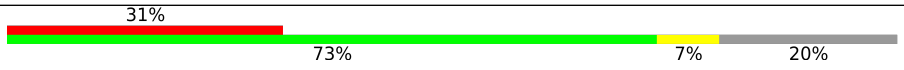
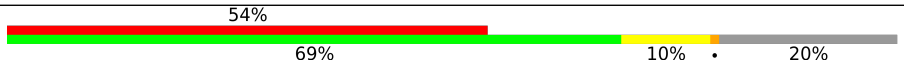
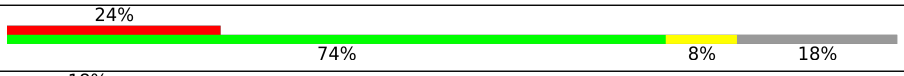
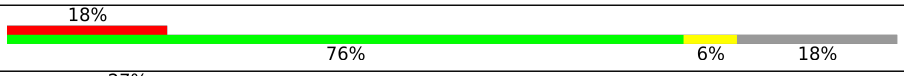
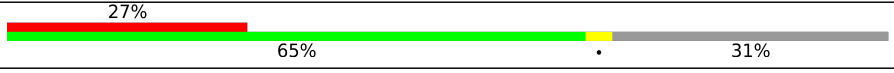
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1227 (1.42 - 2.42)

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

Mol	Chain	Length	Quality of chain
1	A	748	90% 9%
2	B	732	91% 9%
3	C	81	96%
4	D	139	81% 16%

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Mol	Chain	Length	Quality of chain
5	E	61	
6	F	178	
7	I	32	
8	J	38	
9	K	68	
10	L	141	
11	M	28	
12	O	155	
13	1	214	
13	4	214	
14	2	222	
14	5	222	
15	3	219	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	5X6	1	312	-	X	-	-
25	5X6	1	313	-	X	-	-
25	5X6	1	314	-	X	-	-
25	5X6	1	315	-	X	-	-
25	5X6	1	316	-	X	-	-
25	5X6	2	317	-	X	-	-
25	5X6	2	318	-	X	-	-
25	5X6	2	319	-	X	-	-
25	5X6	2	320	-	X	-	-
25	5X6	2	321	-	X	-	-
25	5X6	3	316	-	X	-	-
25	5X6	3	317	-	X	-	-
25	5X6	3	318	-	X	-	-
25	5X6	4	312	-	X	-	-
25	5X6	4	313	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	5X6	4	314	-	X	-	-
25	5X6	5	301	-	X	-	-
25	5X6	5	315	-	X	-	-
25	5X6	5	316	-	X	-	-
25	5X6	5	317	-	X	-	-
25	5X6	5	318	-	X	-	-
25	5X6	F	205	-	X	-	-
25	5X6	J	105	-	X	-	-

2 Entry composition (i)

There are 26 unique types of molecules in this entry. The entry contains 36163 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	741	5794	3784	996	987	27	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	730	5818	3829	981	990	18	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	80	598	367	104	115	12	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	117	938	594	165	176	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	61	491	321	77	92	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	158	1296	829	225	238	4	0	0

- Molecule 7 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	32	Total	C	N	O	S	0	0
			238	163	33	40	2		

- Molecule 8 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	38	Total	C	N	O	S	0	0
			313	214	46	52	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	63	Total	C	N	O	S	0	0
			454	294	75	83	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	121	Total	C	N	O	S	0	0
			923	610	146	164	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	28	Total	C	N	O	S	0	0
			208	138	32	35	3		

- Molecule 12 is a protein called Photosystem I subunit O.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	O	83	Total	C	N	O	0	0
			634	432	97	105		

- Molecule 13 is a protein called Lhcr1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	1	172	Total	C	N	O	S	0	0
			1365	892	228	235	10		
13	4	172	Total	C	N	O	S	0	0
			1365	892	228	235	10		

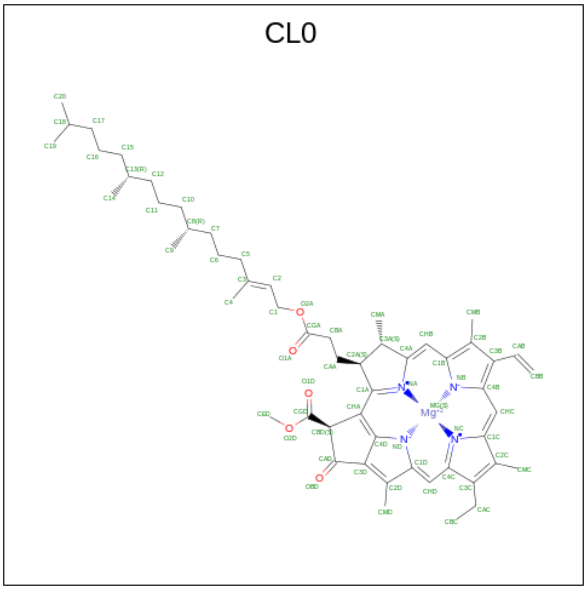
- Molecule 14 is a protein called Lhcr2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	2	183	Total	C	N	O	S	0	0
			1428	926	243	250	9		
14	5	183	Total	C	N	O	S	0	0
			1428	926	243	250	9		

- Molecule 15 is a protein called Lhcr3.

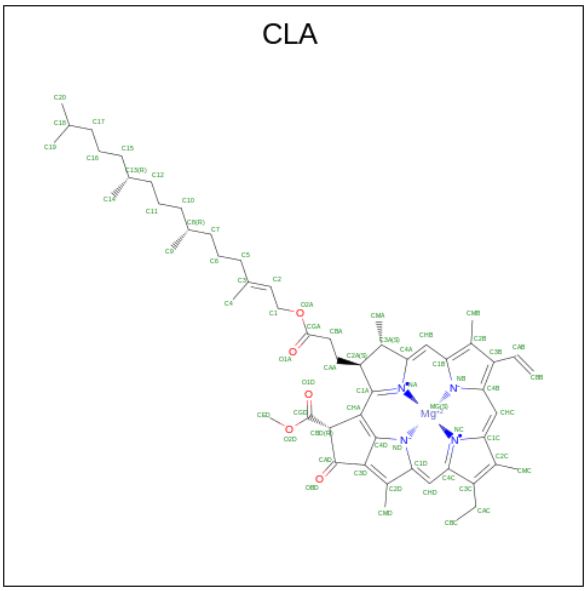
Mol	Chain	Residues	Atoms					AltConf	Trace
15	3	151	Total	C	N	O	S	0	0
			1169	759	198	206	6		

- Molecule 16 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



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

- Molecule 17 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
17	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	A	1	Total 54	C 44	Mg 1	N 4	O 5	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	A	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	A	1	Total 62	C 52	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
17	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
17	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	F	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	J	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	K	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	K	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	L	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
17	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	L	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	O	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	O	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	O	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	1	1	Total	C	Mg	N	O	0
			59	49	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
17	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	2	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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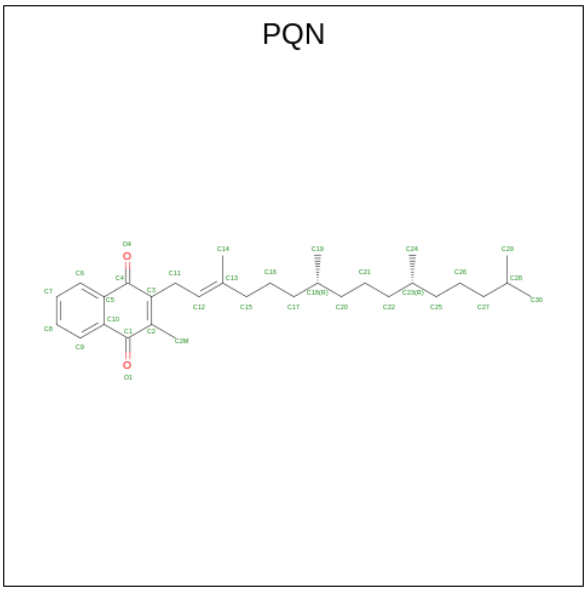
Mol	Chain	Residues	Atoms					AltConf
17	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	3	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
17	4	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
17	4	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
17	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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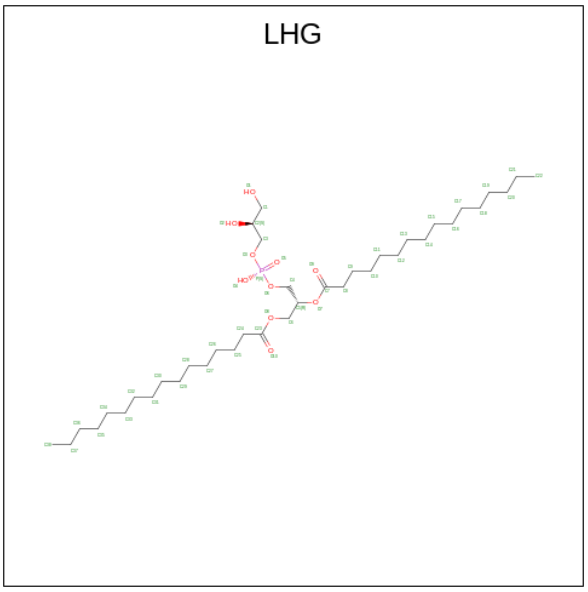
Mol	Chain	Residues	Atoms					AltConf
17	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	5	1	Total 41	C 33	Mg 1	N 4	O 3	0
17	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	5	1	Total 44	C 36	Mg 1	N 4	O 3	0

- Molecule 18 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



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

- Molecule 19 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



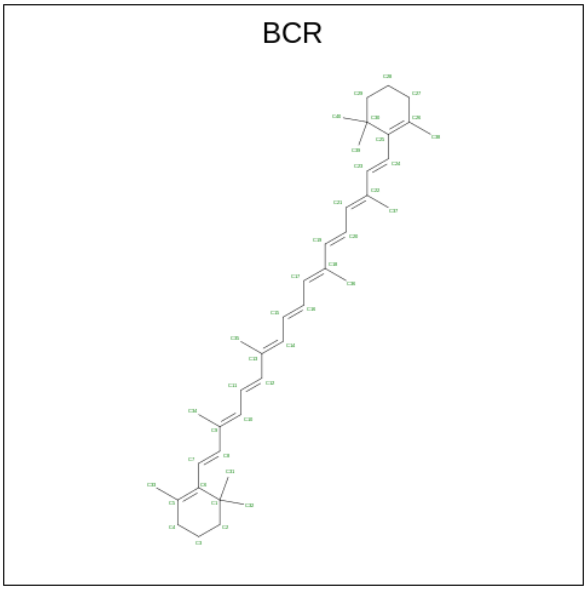
Mol	Chain	Residues	Atoms				AltConf
19	A	1	Total	C	O	P	0
			49	38	10	1	

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Mol	Chain	Residues	Atoms				AltConf
19	A	1	Total	C	O	P	0
			40	29	10	1	
19	J	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 20 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



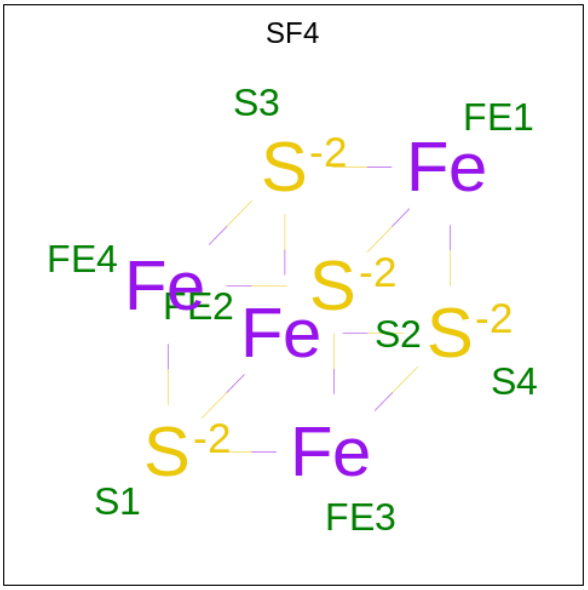
Mol	Chain	Residues	Atoms		AltConf
20	A	1	Total	C	0
			40	40	
20	A	1	Total	C	0
			40	40	
20	A	1	Total	C	0
			40	40	
20	A	1	Total	C	0
			40	40	
20	A	1	Total	C	0
			40	40	
20	B	1	Total	C	0
			40	40	
20	B	1	Total	C	0
			40	40	
20	B	1	Total	C	0
			40	40	
20	B	1	Total	C	0
			40	40	

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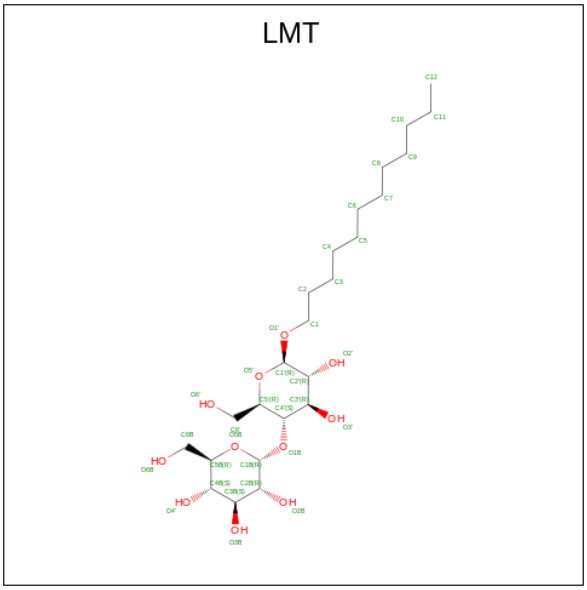
Mol	Chain	Residues	Atoms	AltConf
20	B	1	Total C 40 40	0
20	B	1	Total C 40 40	0
20	B	1	Total C 40 40	0
20	I	1	Total C 40 40	0
20	J	1	Total C 40 40	0
20	K	1	Total C 40 40	0
20	L	1	Total C 40 40	0
20	L	1	Total C 40 40	0
20	L	1	Total C 40 40	0
20	M	1	Total C 40 40	0
20	O	1	Total C 40 40	0

- Molecule 21 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 22 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).

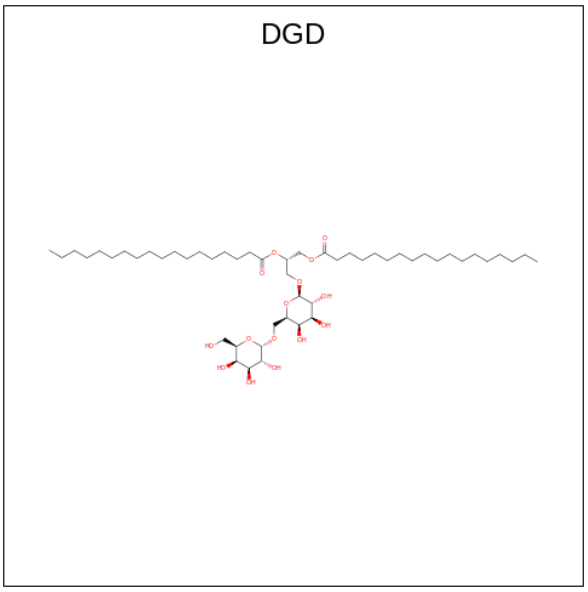


Mol	Chain	Residues	Atoms	AltConf
22	A	1	Total C O 35 24 11	0
22	B	1	Total C O 35 24 11	0
22	B	1	Total C O 35 24 11	0
22	B	1	Total C O 35 24 11	0
22	F	1	Total C O 35 24 11	0
22	L	1	Total C O 35 24 11	0
22	3	1	Total C O 35 24 11	0

- Molecule 23 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

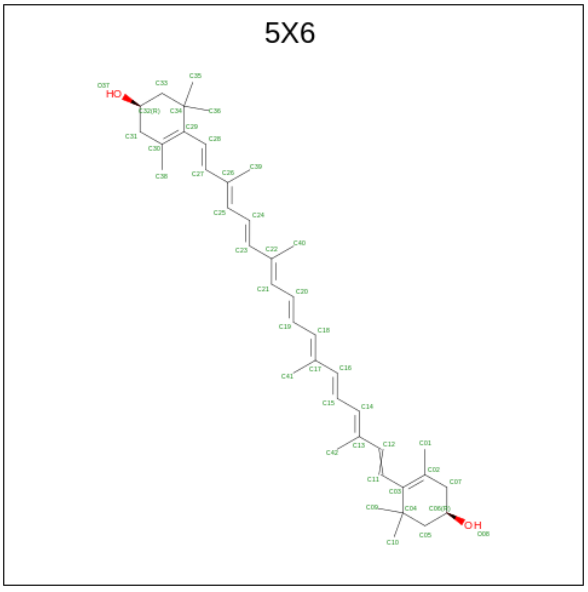
Mol	Chain	Residues	Atoms	AltConf
23	A	4	Total C 48 48	0
23	B	5	Total C 54 54	0
23	F	1	Total C 9 9	0
23	I	1	Total C 12 12	0
23	J	1	Total C 13 13	0
23	K	1	Total C 13 13	0
23	L	1	Total C 13 13	0
23	O	1	Total C 6 6	0
23	1	1	Total C 8 8	0
23	2	3	Total C 32 32	0
23	3	3	Total C 37 37	0
23	4	2	Total C 24 24	0
23	5	1	Total C 8 8	0

- Molecule 24 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



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

- Molecule 25 is Zeaxanthin (CCD ID: 5X6) (formula: $C_{40}H_{56}O_2$).



Mol	Chain	Residues	Atoms			AltConf
25	F	1	Total	C	O	0
			42	40	2	
25	J	1	Total	C	O	0
			42	40	2	
25	1	1	Total	C	O	0
			42	40	2	

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Mol	Chain	Residues	Atoms	AltConf
25	1	1	Total C O 42 40 2	0
25	1	1	Total C O 42 40 2	0
25	1	1	Total C O 42 40 2	0
25	1	1	Total C O 42 40 2	0
25	2	1	Total C O 42 40 2	0
25	2	1	Total C O 42 40 2	0
25	2	1	Total C O 42 40 2	0
25	2	1	Total C O 42 40 2	0
25	2	1	Total C O 42 40 2	0
25	3	1	Total C O 42 40 2	0
25	3	1	Total C O 42 40 2	0
25	3	1	Total C O 42 40 2	0
25	4	1	Total C O 42 40 2	0
25	4	1	Total C O 42 40 2	0
25	4	1	Total C O 42 40 2	0
25	5	1	Total C O 42 40 2	0
25	5	1	Total C O 42 40 2	0
25	5	1	Total C O 42 40 2	0
25	5	1	Total C O 42 40 2	0
25	5	1	Total C O 42 40 2	0

- Molecule 26 is water.

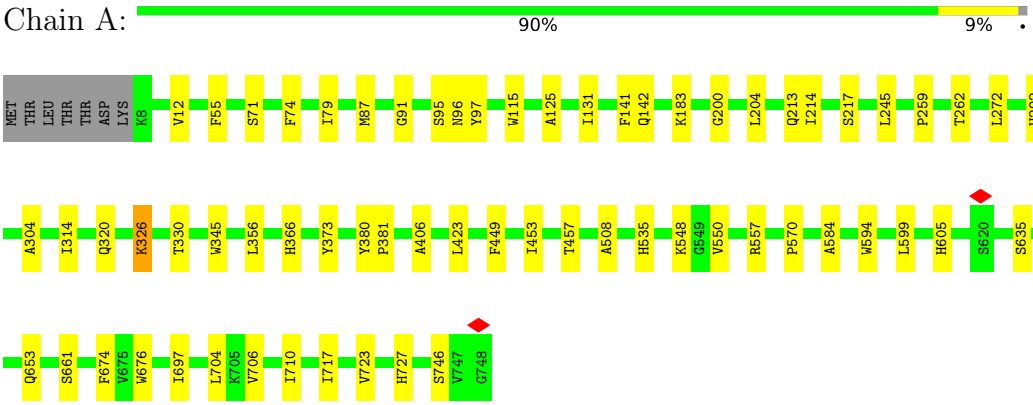
Mol	Chain	Residues	Atoms	AltConf
26	A	203	Total O 203 203	0
26	B	220	Total O 220 220	0
26	C	41	Total O 41 41	0
26	D	18	Total O 18 18	0
26	E	23	Total O 23 23	0
26	F	22	Total O 22 22	0
26	I	2	Total O 2 2	0
26	J	7	Total O 7 7	0
26	K	2	Total O 2 2	0
26	L	7	Total O 7 7	0
26	M	2	Total O 2 2	0
26	1	3	Total O 3 3	0
26	3	1	Total O 1 1	0
26	4	3	Total O 3 3	0
26	5	6	Total O 6 6	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.

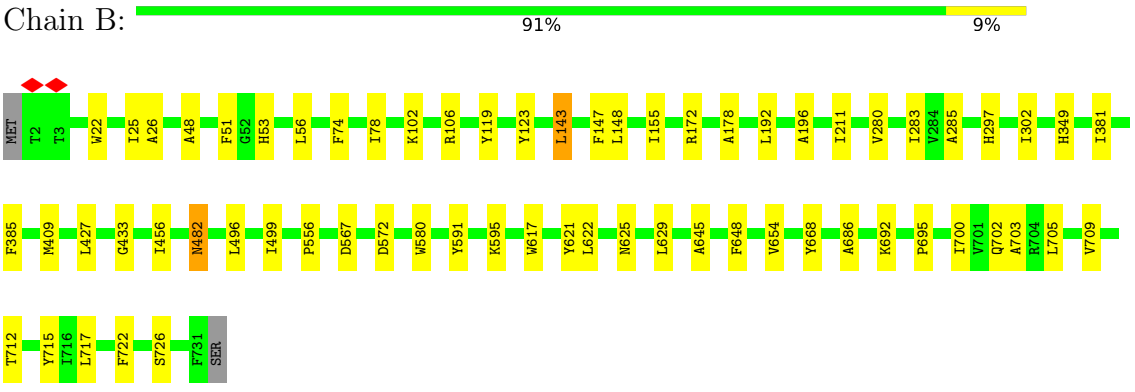
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain A:



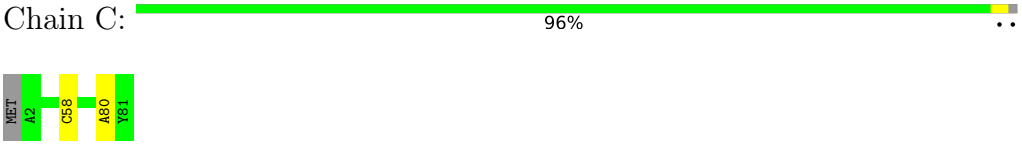
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain B:



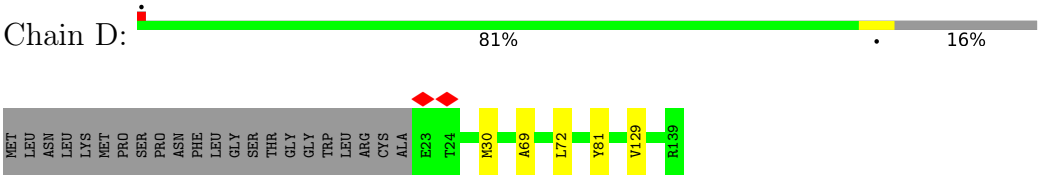
• Molecule 3: Photosystem I iron-sulfur center

Chain C:



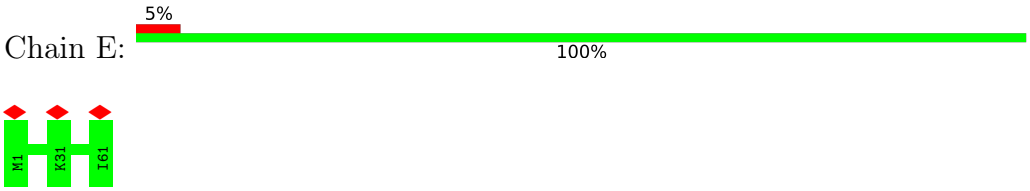
• Molecule 4: Photosystem I reaction center subunit II

Chain D:



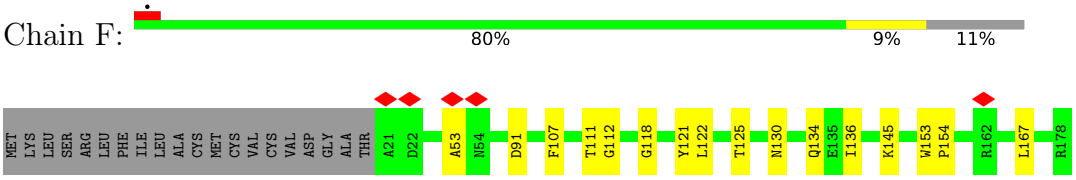
• Molecule 5: Photosystem I reaction center subunit IV

Chain E:



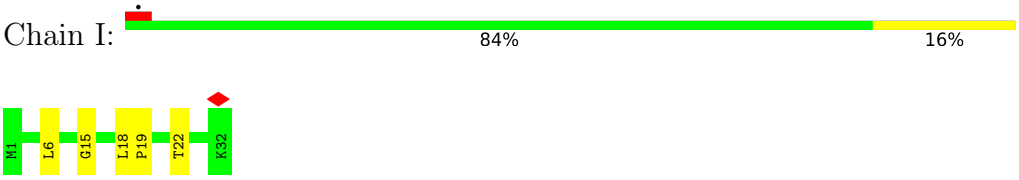
• Molecule 6: Photosystem I reaction center subunit III

Chain F:



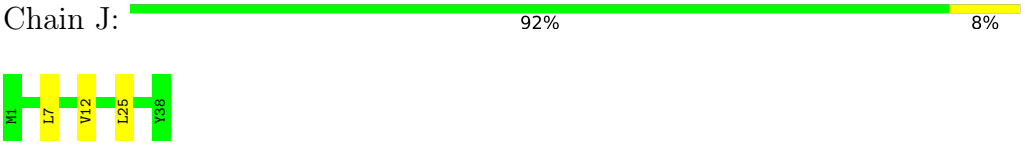
• Molecule 7: Photosystem I reaction center subunit VIII

Chain I:



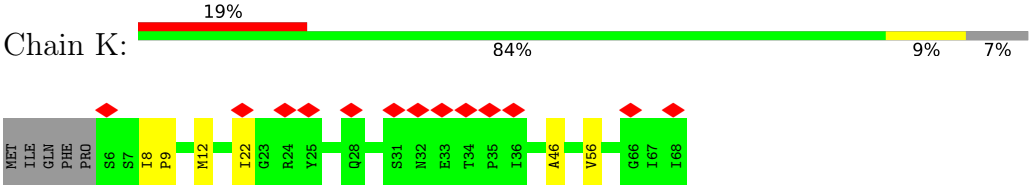
• Molecule 8: Photosystem I reaction center subunit IX

Chain J:



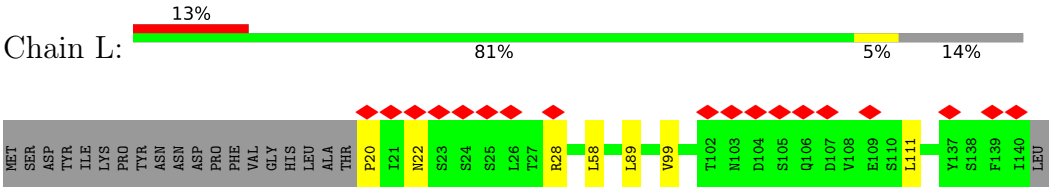
• Molecule 9: Photosystem I reaction center subunit X

Chain K:



• Molecule 10: Photosystem I reaction center subunit XI

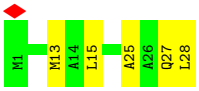
Chain L:



• Molecule 11: Photosystem I reaction center subunit XII

Chain M:

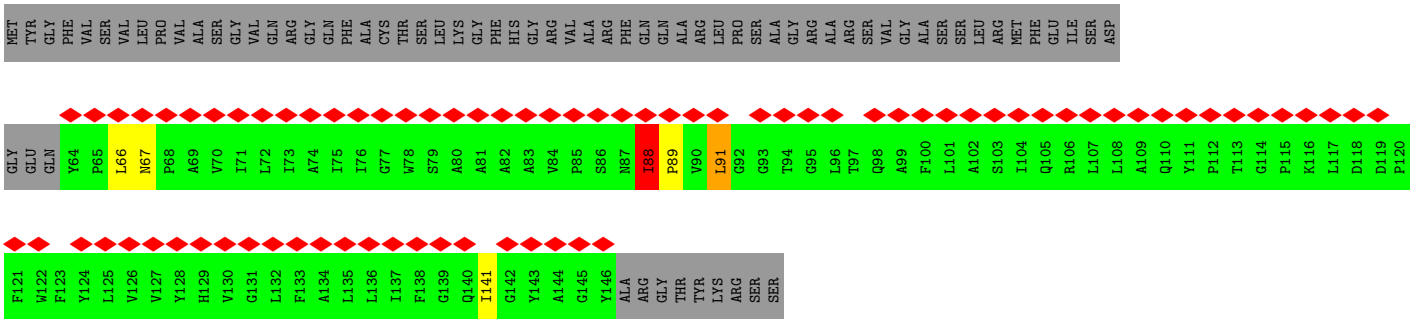




• Molecule 12: Photosystem I subunit O

Chain O:

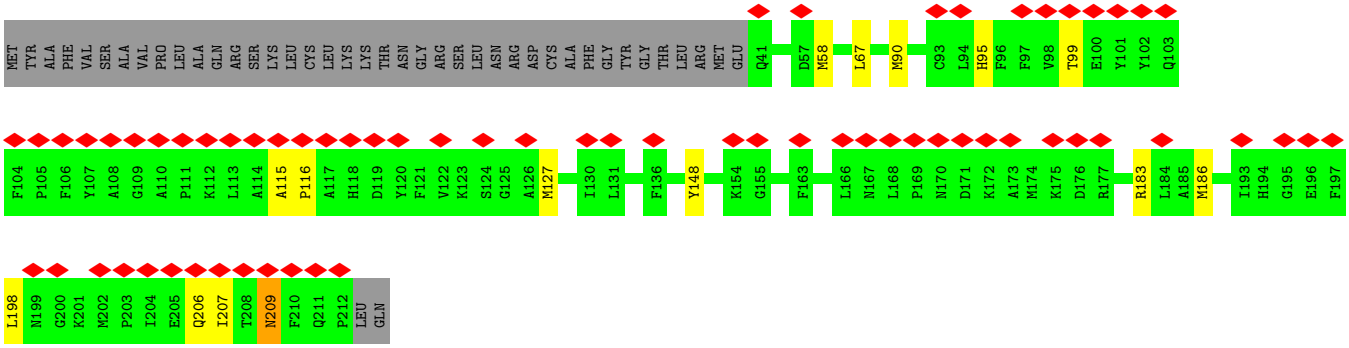




• Molecule 13: Lhcr1

Chain 1:

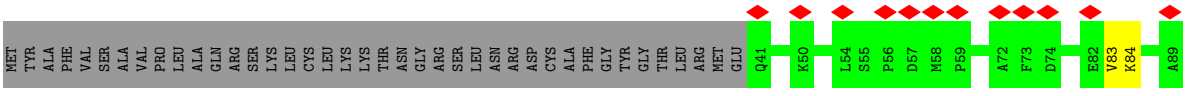


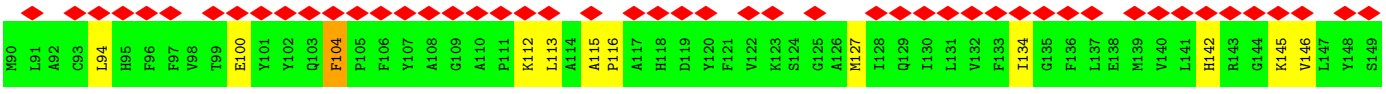


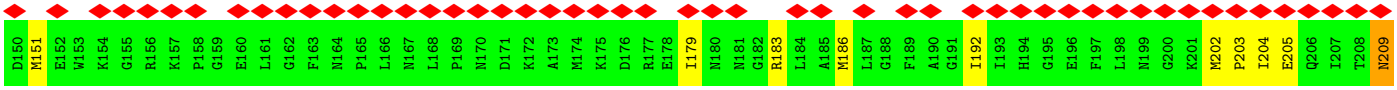
• Molecule 13: Lhcr1

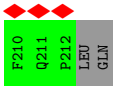
Chain 4:







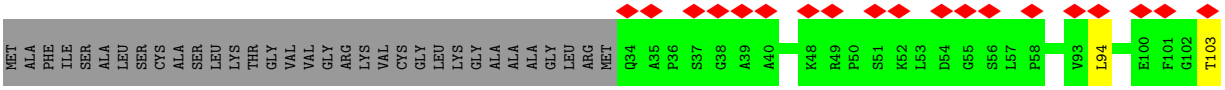


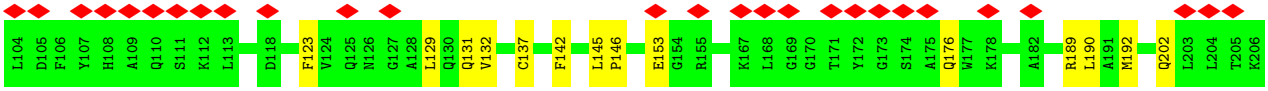


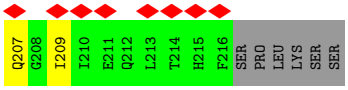
• Molecule 14: Lhcr2

Chain 2:





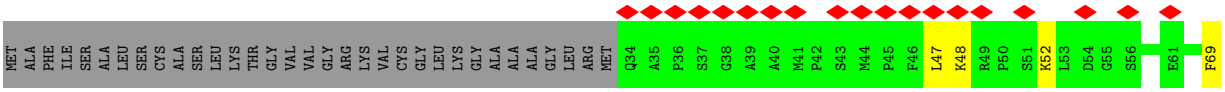


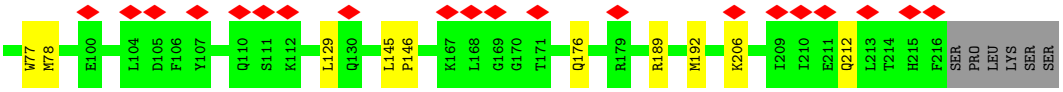


• Molecule 14: Lhcr2

Chain 5:





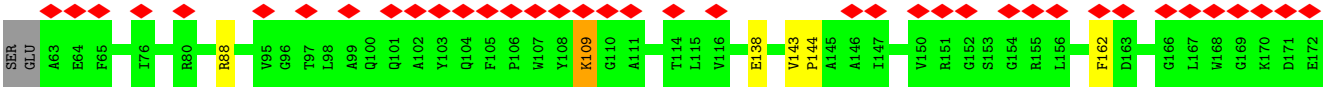


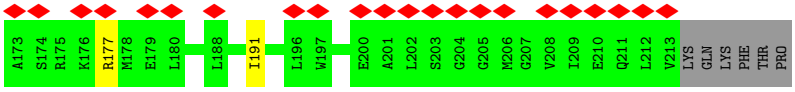
• Molecule 15: Lhcr3

Chain 3:









4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	228449	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	39.8	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.289	Depositor
Minimum map value	-0.106	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.016	Depositor
Map size (Å)	202.752, 202.752, 202.752	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.792, 0.792, 0.792	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, PQN, CL0, LHG, UNL, LMT, 5X6, CLA, BCR, DGD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.92	0/5979	1.43	0/8148
2	B	0.90	0/6027	1.45	0/8236
3	C	0.91	0/608	1.32	0/822
4	D	0.95	0/957	1.31	0/1292
5	E	0.99	0/500	1.26	0/676
6	F	0.95	0/1329	1.52	0/1799
7	I	1.02	0/243	1.52	0/332
8	J	0.88	0/322	1.39	0/439
9	K	1.05	0/459	1.76	2/627 (0.3%)
10	L	0.99	0/945	1.69	0/1281
11	M	1.00	0/209	1.71	0/283
12	O	1.06	0/656	1.65	0/903
13	1	1.01	0/1407	1.58	0/1903
13	4	1.02	0/1407	1.59	0/1903
14	2	1.00	0/1467	1.65	2/1980 (0.1%)
14	5	0.99	0/1467	1.64	0/1980
15	3	1.02	0/1199	1.67	0/1627
All	All	0.96	0/25181	1.51	4/34231 (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
12	O	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	K	22	ILE	CA-C-N	5.29	125.85	119.98
9	K	22	ILE	C-N-CA	5.29	125.85	119.98
14	2	207	GLN	CA-C-N	5.05	124.90	120.10
14	2	207	GLN	C-N-CA	5.05	124.90	120.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	O	88	ILE	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5794	0	5722	55	0
2	B	5818	0	5649	60	0
3	C	598	0	576	2	0
4	D	938	0	933	4	0
5	E	491	0	509	0	0
6	F	1296	0	1263	14	0
7	I	238	0	265	6	0
8	J	313	0	327	2	0
9	K	454	0	490	3	0
10	L	923	0	939	2	0
11	M	208	0	230	5	0
12	O	634	0	644	2	0
13	1	1365	0	1351	12	0
13	4	1365	0	1351	13	0
14	2	1428	0	1406	17	0
14	5	1428	0	1406	5	0
15	3	1169	0	1172	6	0
16	A	65	0	72	1	0
17	1	540	0	442	17	0
17	2	618	0	494	23	0
17	3	530	0	423	13	0
17	4	418	0	321	14	0
17	5	680	0	619	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	A	2664	0	2743	71	0
17	B	2513	0	2633	98	0
17	F	86	0	62	5	0
17	J	42	0	31	1	0
17	K	97	0	80	3	0
17	L	172	0	164	2	0
17	O	136	0	101	4	0
18	A	33	0	46	1	0
18	B	33	0	46	2	0
19	A	89	0	127	1	0
19	J	49	0	74	1	0
20	A	200	0	280	13	0
20	B	280	0	392	8	0
20	I	40	0	56	0	0
20	J	40	0	56	3	0
20	K	40	0	56	1	0
20	L	120	0	168	4	0
20	M	40	0	56	3	0
20	O	40	0	56	0	0
21	A	8	0	0	0	0
21	C	16	0	0	1	0
22	3	35	0	46	0	0
22	A	35	0	46	0	0
22	B	105	0	138	0	0
22	F	35	0	46	0	0
22	L	35	0	46	0	0
23	1	8	0	0	0	0
23	2	32	0	0	0	0
23	3	37	0	0	0	0
23	4	24	0	0	0	0
23	5	8	0	0	0	0
23	A	48	0	0	0	0
23	B	54	0	0	0	0
23	F	9	0	0	0	0
23	I	12	0	0	0	0
23	J	13	0	0	0	0
23	K	13	0	0	0	0
23	L	13	0	0	0	0
23	O	6	0	0	0	0
24	B	66	0	96	3	0
25	1	210	0	0	2	0
25	2	210	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	3	126	0	0	2	0
25	4	126	0	0	0	0
25	5	210	0	0	2	0
25	F	42	0	0	0	0
25	J	42	0	0	0	0
26	1	3	0	0	0	0
26	3	1	0	0	0	0
26	4	3	0	0	0	0
26	5	6	0	0	0	0
26	A	203	0	0	1	0
26	B	220	0	0	1	0
26	C	41	0	0	0	0
26	D	18	0	0	0	0
26	E	23	0	0	0	0
26	F	22	0	0	0	0
26	I	2	0	0	0	0
26	J	7	0	0	0	0
26	K	2	0	0	0	0
26	L	7	0	0	0	0
26	M	2	0	0	0	0
All	All	36163	0	34249	390	0

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

The worst 5 of 390 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)
14:2:190:LEU:HD21	17:2:313:CLA:HBC3	1.66	0.77
14:2:132:VAL:CG2	17:2:309:CLA:HBC1	2.17	0.74
14:2:129:LEU:HD22	17:2:309:CLA:HBC3	1.69	0.74
1:A:535:HIS:HE1	1:A:605:HIS:HD2	1.37	0.72
17:K:103:CLA:HMC3	20:K:104:BCR:H332	1.72	0.71

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	739/748 (99%)	716 (97%)	22 (3%)	1 (0%)	48 40
2	B	728/732 (100%)	712 (98%)	16 (2%)	0	100 100
3	C	78/81 (96%)	76 (97%)	2 (3%)	0	100 100
4	D	115/139 (83%)	112 (97%)	3 (3%)	0	100 100
5	E	59/61 (97%)	55 (93%)	4 (7%)	0	100 100
6	F	156/178 (88%)	153 (98%)	2 (1%)	1 (1%)	21 10
7	I	30/32 (94%)	29 (97%)	1 (3%)	0	100 100
8	J	36/38 (95%)	35 (97%)	1 (3%)	0	100 100
9	K	61/68 (90%)	58 (95%)	3 (5%)	0	100 100
10	L	119/141 (84%)	113 (95%)	5 (4%)	1 (1%)	16 6
11	M	26/28 (93%)	26 (100%)	0	0	100 100
12	O	81/155 (52%)	70 (86%)	7 (9%)	4 (5%)	1 0
13	1	170/214 (79%)	149 (88%)	19 (11%)	2 (1%)	10 3
13	4	170/214 (79%)	150 (88%)	17 (10%)	3 (2%)	6 1
14	2	181/222 (82%)	171 (94%)	10 (6%)	0	100 100
14	5	181/222 (82%)	171 (94%)	10 (6%)	0	100 100
15	3	149/219 (68%)	137 (92%)	11 (7%)	1 (1%)	18 9
All	All	3079/3492 (88%)	2933 (95%)	133 (4%)	13 (0%)	31 19

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	1	99	THR
12	O	88	ILE
1	A	508	ALA
6	F	53	ALA
10	L	22	ASN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	601/608 (99%)	598 (100%)	3 (0%)	81 80
2	B	596/598 (100%)	591 (99%)	5 (1%)	73 71
3	C	66/67 (98%)	66 (100%)	0	100 100
4	D	98/116 (84%)	97 (99%)	1 (1%)	68 64
5	E	57/57 (100%)	57 (100%)	0	100 100
6	F	136/153 (89%)	135 (99%)	1 (1%)	76 73
7	I	27/27 (100%)	27 (100%)	0	100 100
8	J	34/34 (100%)	34 (100%)	0	100 100
9	K	51/56 (91%)	51 (100%)	0	100 100
10	L	96/114 (84%)	92 (96%)	4 (4%)	26 11
11	M	22/22 (100%)	20 (91%)	2 (9%)	9 1
12	O	63/118 (53%)	61 (97%)	2 (3%)	34 18
13	1	143/178 (80%)	142 (99%)	1 (1%)	76 73
13	4	143/178 (80%)	137 (96%)	6 (4%)	26 11
14	2	146/174 (84%)	144 (99%)	2 (1%)	59 50
14	5	146/174 (84%)	140 (96%)	6 (4%)	27 12
15	3	117/171 (68%)	116 (99%)	1 (1%)	70 67
All	All	2542/2845 (89%)	2508 (99%)	34 (1%)	59 53

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	5	47	LEU
14	5	48	LYS
14	5	206	LYS
10	L	99	VAL
10	L	28	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36

such sidechains are listed below:

Mol	Chain	Res	Type
14	2	201	GLN
14	5	201	GLN
14	2	212	GLN
13	4	180	ASN
2	B	489	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 238 ligands modelled in this entry, 25 are unknown - leaving 213 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
17	CLA	B	801	-	69,73,73	1.83	18 (26%)	83,113,113	2.47	25 (30%)
16	CL0	A	801	1	69,73,73	1.85	18 (26%)	83,113,113	2.71	31 (37%)
17	CLA	L	203	10	69,73,73	1.99	20 (28%)	83,113,113	2.66	26 (31%)
17	CLA	B	837	2	69,73,73	1.92	20 (28%)	83,113,113	2.82	32 (38%)
17	CLA	B	829	2	69,73,73	1.88	20 (28%)	83,113,113	2.80	28 (33%)
17	CLA	B	826	26	69,73,73	1.87	20 (28%)	83,113,113	2.77	29 (34%)
17	CLA	5	310	-	45,49,73	2.55	20 (44%)	54,84,113	3.37	26 (48%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	CLA	B	838	2	51,55,73	2.24	19 (37%)	61,91,113	3.32	27 (44%)
25	5X6	1	314	-	43,43,43	5.91	23 (53%)	58,60,60	4.67	34 (58%)
20	BCR	B	844	-	41,41,41	1.60	8 (19%)	56,56,56	1.32	5 (8%)
25	5X6	1	316	-	43,43,43	6.01	23 (53%)	58,60,60	4.31	29 (50%)
17	CLA	A	830	1	60,64,73	2.06	20 (33%)	72,102,113	2.92	29 (40%)
22	LMT	B	850	-	36,36,36	0.41	0	47,47,47	0.67	0
25	5X6	4	314	-	43,43,43	6.09	24 (55%)	58,60,60	4.61	33 (56%)
17	CLA	5	311	14	49,53,73	2.50	21 (42%)	59,89,113	3.17	26 (44%)
21	SF4	C	102	3	0,12,12	-	-	-		
17	CLA	A	855	26	65,69,73	1.96	19 (29%)	78,108,113	2.91	27 (34%)
17	CLA	B	833	2	69,73,73	1.82	18 (26%)	83,113,113	2.89	31 (37%)
17	CLA	K	103	9	46,50,73	2.34	20 (43%)	55,85,113	3.23	28 (50%)
17	CLA	A	812	1	69,73,73	1.92	18 (26%)	83,113,113	2.84	24 (28%)
17	CLA	A	856	1	69,73,73	1.83	20 (28%)	83,113,113	2.78	28 (33%)
17	CLA	3	313	15	46,50,73	2.49	20 (43%)	55,85,113	3.28	26 (47%)
17	CLA	3	308	-	49,53,73	2.46	20 (40%)	59,89,113	3.11	25 (42%)
25	5X6	3	318	-	43,43,43	6.05	25 (58%)	58,60,60	4.43	30 (51%)
17	CLA	1	309	13	49,53,73	2.47	20 (40%)	59,89,113	3.21	26 (44%)
17	CLA	3	309	15	49,53,73	2.46	20 (40%)	59,89,113	3.25	26 (44%)
20	BCR	L	201	-	41,41,41	1.56	10 (24%)	56,56,56	1.52	8 (14%)
17	CLA	5	304	14	69,73,73	2.01	19 (27%)	83,113,113	2.77	29 (34%)
17	CLA	4	309	-	45,49,73	2.54	20 (44%)	54,84,113	3.34	27 (50%)
17	CLA	B	822	2	50,54,73	2.34	19 (38%)	60,90,113	3.32	27 (45%)
17	CLA	2	313	14	46,50,73	2.52	19 (41%)	55,85,113	3.31	27 (49%)
17	CLA	A	824	26	59,63,73	1.93	19 (32%)	71,101,113	3.18	31 (43%)
20	BCR	A	845	-	41,41,41	1.55	11 (26%)	56,56,56	1.44	9 (16%)
17	CLA	1	301	13	49,53,73	2.44	20 (40%)	59,89,113	3.02	25 (42%)
20	BCR	B	847	-	41,41,41	1.55	9 (21%)	56,56,56	1.42	9 (16%)
21	SF4	A	847	2,1	0,12,12	-	-	-		
17	CLA	B	857	2	62,66,73	2.00	18 (29%)	74,104,113	3.08	29 (39%)
22	LMT	3	301	-	36,36,36	0.48	0	47,47,47	0.52	0
18	PQN	B	842	-	34,34,34	1.45	2 (5%)	42,45,45	1.12	3 (7%)
20	BCR	J	104	-	41,41,41	1.58	9 (21%)	56,56,56	1.36	8 (14%)
22	LMT	B	851	-	36,36,36	0.45	0	47,47,47	0.54	0
17	CLA	A	803	1	69,73,73	1.91	21 (30%)	83,113,113	2.81	27 (32%)
17	CLA	5	313	14	49,53,73	2.43	20 (40%)	59,89,113	3.12	30 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	CLA	A	823	26	69,73,73	1.90	21 (30%)	83,113,113	2.80	28 (33%)
17	CLA	2	314	14	49,53,73	2.50	20 (40%)	59,89,113	3.22	27 (45%)
20	BCR	I	101	-	41,41,41	1.55	10 (24%)	56,56,56	1.37	9 (16%)
20	BCR	B	845	-	41,41,41	1.62	9 (21%)	56,56,56	1.41	8 (14%)
20	BCR	B	803	-	41,41,41	1.61	7 (17%)	56,56,56	1.67	10 (17%)
17	CLA	O	204	12	54,58,73	2.39	20 (37%)	65,95,113	3.21	30 (46%)
25	5X6	J	105	-	43,43,43	5.34	23 (53%)	58,60,60	4.97	28 (48%)
17	CLA	B	806	2	69,73,73	1.91	20 (28%)	83,113,113	2.85	29 (34%)
17	CLA	2	310	14	49,53,73	2.50	19 (38%)	59,89,113	3.16	26 (44%)
17	CLA	4	307	13	49,53,73	2.44	20 (40%)	59,89,113	3.16	31 (52%)
17	CLA	1	305	13	49,53,73	2.54	21 (42%)	59,89,113	3.12	25 (42%)
17	CLA	A	826	1	69,73,73	1.93	21 (30%)	83,113,113	2.78	28 (33%)
25	5X6	1	312	-	43,43,43	6.04	24 (55%)	58,60,60	4.32	30 (51%)
17	CLA	B	817	2	59,63,73	2.13	18 (30%)	71,101,113	3.09	28 (39%)
17	CLA	A	828	1	69,73,73	1.83	17 (24%)	83,113,113	2.83	27 (32%)
17	CLA	B	823	2	47,51,73	2.37	20 (42%)	56,86,113	3.25	25 (44%)
17	CLA	5	305	14	69,73,73	2.14	20 (28%)	83,113,113	3.07	37 (44%)
20	BCR	A	844	-	41,41,41	1.59	9 (21%)	56,56,56	1.42	8 (14%)
20	BCR	B	846	-	41,41,41	1.82	7 (17%)	56,56,56	1.70	10 (17%)
17	CLA	5	314	-	47,52,73	2.44	20 (42%)	58,87,113	3.17	27 (46%)
25	5X6	F	205	-	43,43,43	5.20	25 (58%)	58,60,60	5.49	33 (56%)
22	LMT	F	201	-	36,36,36	0.49	0	47,47,47	0.55	0
19	LHG	A	842	17	39,39,48	0.28	0	42,45,54	0.37	0
17	CLA	B	828	2	69,73,73	1.82	20 (28%)	83,113,113	2.82	31 (37%)
17	CLA	B	818	2	63,67,73	1.98	20 (31%)	75,105,113	2.99	30 (40%)
17	CLA	B	809	2	69,73,73	1.83	19 (27%)	83,113,113	2.87	32 (38%)
25	5X6	1	315	-	43,43,43	6.05	23 (53%)	58,60,60	4.73	31 (53%)
17	CLA	5	303	14	69,73,73	2.09	20 (28%)	83,113,113	2.84	32 (38%)
17	CLA	B	819	2	64,68,73	1.94	19 (29%)	77,107,113	3.05	31 (40%)
22	LMT	L	207	-	36,36,36	0.44	0	47,47,47	0.55	0
25	5X6	2	321	-	43,43,43	5.96	23 (53%)	58,60,60	4.85	30 (51%)
17	CLA	A	825	1	69,73,73	1.89	20 (28%)	83,113,113	2.84	30 (36%)
17	CLA	A	835	1	55,59,73	2.17	21 (38%)	66,96,113	2.96	27 (40%)
17	CLA	1	306	13	59,63,73	2.22	21 (35%)	71,101,113	2.80	32 (45%)
17	CLA	3	311	15	56,60,73	2.33	19 (33%)	67,97,113	3.17	27 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	CLA	B	834	26	69,73,73	1.95	17 (24%)	83,113,113	2.78	31 (37%)
22	LMT	A	848	-	36,36,36	0.50	0	47,47,47	1.09	4 (8%)
17	CLA	A	805	1	54,58,73	2.18	19 (35%)	65,95,113	3.15	28 (43%)
17	CLA	A	822	1	59,63,73	2.07	18 (30%)	71,101,113	3.11	23 (32%)
17	CLA	B	832	2	69,73,73	1.96	20 (28%)	83,113,113	2.70	27 (32%)
17	CLA	B	835	26	49,53,73	2.35	18 (36%)	59,89,113	3.13	29 (49%)
25	5X6	5	317	-	43,43,43	6.12	24 (55%)	58,60,60	4.60	32 (55%)
25	5X6	4	312	-	43,43,43	6.03	23 (53%)	58,60,60	4.49	28 (48%)
17	CLA	B	810	2	69,73,73	1.92	17 (24%)	83,113,113	2.63	28 (33%)
20	BCR	L	205	-	41,41,41	1.68	8 (19%)	56,56,56	1.31	6 (10%)
17	CLA	F	203	26	49,53,73	2.28	20 (40%)	59,89,113	3.03	25 (42%)
25	5X6	5	316	-	43,43,43	5.70	24 (55%)	58,60,60	4.64	27 (46%)
17	CLA	4	304	13	63,67,73	2.21	19 (30%)	75,105,113	2.98	32 (42%)
17	CLA	A	814	26	49,53,73	2.39	20 (40%)	59,89,113	3.16	25 (42%)
17	CLA	B	821	2	49,53,73	2.34	20 (40%)	59,89,113	3.21	28 (47%)
17	CLA	4	311	-	49,53,73	2.49	21 (42%)	59,89,113	3.26	26 (44%)
25	5X6	5	315	-	43,43,43	5.93	24 (55%)	58,60,60	4.76	31 (53%)
25	5X6	2	318	-	43,43,43	5.90	24 (55%)	58,60,60	4.38	29 (50%)
20	BCR	B	848	-	41,41,41	1.61	8 (19%)	56,56,56	1.52	9 (16%)
17	CLA	B	820	26	69,73,73	2.03	19 (27%)	83,113,113	2.64	28 (33%)
20	BCR	M	101	-	41,41,41	1.87	6 (14%)	56,56,56	1.63	11 (19%)
25	5X6	2	320	-	43,43,43	6.03	25 (58%)	58,60,60	4.30	32 (55%)
20	BCR	A	857	-	41,41,41	1.58	10 (24%)	56,56,56	1.43	7 (12%)
17	CLA	A	831	1	69,73,73	1.92	19 (27%)	83,113,113	2.75	29 (34%)
20	BCR	A	846	-	41,41,41	1.57	10 (24%)	56,56,56	1.32	8 (14%)
17	CLA	O	205	-	49,53,73	2.51	21 (42%)	59,89,113	3.20	28 (47%)
17	CLA	O	203	-	45,49,73	2.53	20 (44%)	54,84,113	3.35	28 (51%)
25	5X6	1	313	-	43,43,43	6.02	24 (55%)	58,60,60	4.63	33 (56%)
24	DGD	B	849	-	67,67,67	0.88	2 (2%)	81,81,81	0.88	4 (4%)
17	CLA	1	303	13	59,63,73	2.26	18 (30%)	71,101,113	2.99	28 (39%)
17	CLA	A	836	1	60,64,73	2.09	21 (35%)	72,102,113	2.92	28 (38%)
17	CLA	3	305	15	67,71,73	2.13	19 (28%)	80,110,113	2.87	30 (37%)
17	CLA	A	818	1	69,73,73	1.98	20 (28%)	83,113,113	2.79	33 (39%)
17	CLA	2	312	-	45,49,73	2.52	20 (44%)	54,84,113	3.40	28 (51%)
25	5X6	4	313	-	43,43,43	6.17	24 (55%)	58,60,60	4.05	31 (53%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	CLA	A	827	1	69,73,73	1.87	18 (26%)	83,113,113	2.74	26 (31%)
17	CLA	1	302	13	63,67,73	2.11	19 (30%)	75,105,113	2.76	28 (37%)
17	CLA	1	304	13	49,53,73	2.48	20 (40%)	59,89,113	3.30	27 (45%)
17	CLA	2	304	14	49,53,73	2.45	21 (42%)	59,89,113	3.25	28 (47%)
17	CLA	A	815	1	66,70,73	1.98	19 (28%)	79,109,113	2.79	27 (34%)
17	CLA	3	314	-	50,54,73	2.46	20 (40%)	60,90,113	3.19	29 (48%)
20	BCR	K	104	-	41,41,41	1.78	8 (19%)	56,56,56	1.66	12 (21%)
17	CLA	L	204	26	54,58,73	2.36	19 (35%)	65,95,113	3.00	29 (44%)
17	CLA	A	853	26	69,73,73	1.82	20 (28%)	83,113,113	2.86	30 (36%)
17	CLA	3	310	15	49,53,73	2.42	19 (38%)	59,89,113	3.24	28 (47%)
17	CLA	2	305	14	69,73,73	2.09	19 (27%)	83,113,113	2.83	30 (36%)
17	CLA	B	836	2	64,68,73	1.95	19 (29%)	77,107,113	2.82	29 (37%)
17	CLA	B	816	2	69,73,73	1.97	19 (27%)	83,113,113	2.75	28 (33%)
19	LHG	J	102	-	48,48,48	0.27	0	51,54,54	0.36	0
17	CLA	A	832	1	69,73,73	1.89	19 (27%)	83,113,113	2.78	30 (36%)
17	CLA	A	834	1	69,73,73	2.00	21 (30%)	83,113,113	2.73	31 (37%)
25	5X6	3	317	-	43,43,43	6.00	23 (53%)	58,60,60	4.32	28 (48%)
21	SF4	C	101	3	0,12,12	-	-	-		
17	CLA	B	815	2	69,73,73	1.94	20 (28%)	83,113,113	2.74	26 (31%)
17	CLA	5	307	14	49,53,73	2.32	21 (42%)	59,89,113	3.31	27 (45%)
17	CLA	B	840	2	69,73,73	1.82	19 (27%)	83,113,113	2.87	29 (34%)
25	5X6	5	318	-	43,43,43	5.97	24 (55%)	58,60,60	4.77	34 (58%)
17	CLA	A	811	1	69,73,73	1.88	20 (28%)	83,113,113	2.72	29 (34%)
17	CLA	A	839	26	69,73,73	1.93	20 (28%)	83,113,113	2.80	27 (32%)
17	CLA	5	308	14	69,73,73	2.09	21 (30%)	83,113,113	2.79	31 (37%)
17	CLA	5	302	14	49,53,73	2.51	21 (42%)	59,89,113	3.19	25 (42%)
25	5X6	2	317	-	43,43,43	6.11	24 (55%)	58,60,60	4.29	30 (51%)
17	CLA	B	807	2	69,73,73	1.85	20 (28%)	83,113,113	2.74	30 (36%)
17	CLA	A	802	17,1	59,63,73	2.06	16 (27%)	71,101,113	2.97	29 (40%)
17	CLA	B	805	2	69,73,73	1.91	20 (28%)	83,113,113	4.12	38 (45%)
17	CLA	A	813	1	46,50,73	2.33	19 (41%)	55,85,113	3.31	27 (49%)
17	CLA	B	825	26	69,73,73	1.88	21 (30%)	83,113,113	2.70	28 (33%)
19	LHG	A	841	-	48,48,48	0.31	0	51,54,54	0.36	0
17	CLA	3	307	-	59,63,73	2.30	20 (33%)	71,101,113	3.09	30 (42%)
17	CLA	B	841	-	69,73,73	2.01	19 (27%)	83,113,113	2.80	28 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	BCR	B	843	-	41,41,41	1.78	6 (14%)	56,56,56	1.41	9 (16%)
17	CLA	A	821	1	55,59,73	2.18	19 (34%)	66,96,113	3.14	29 (43%)
17	CLA	B	811	2	69,73,73	1.91	19 (27%)	83,113,113	2.69	28 (33%)
17	CLA	B	839	26	69,73,73	1.90	19 (27%)	83,113,113	2.78	23 (27%)
17	CLA	1	311	13	49,53,73	2.50	21 (42%)	59,89,113	3.26	28 (47%)
17	CLA	B	824	2	59,63,73	2.17	18 (30%)	71,101,113	3.17	31 (43%)
17	CLA	1	310	-	49,53,73	2.51	20 (40%)	59,89,113	3.23	26 (44%)
17	CLA	2	311	14	59,63,73	2.27	19 (32%)	71,101,113	3.14	29 (40%)
17	CLA	B	802	26	69,73,73	1.78	17 (24%)	83,113,113	2.96	34 (40%)
17	CLA	B	813	2	59,63,73	2.15	21 (35%)	71,101,113	3.00	31 (43%)
17	CLA	2	307	14	59,63,73	2.23	20 (33%)	71,101,113	3.18	32 (45%)
17	CLA	L	202	10	61,65,73	2.16	21 (34%)	73,103,113	2.90	29 (39%)
17	CLA	2	306	14	49,53,73	2.41	20 (40%)	59,89,113	3.16	27 (45%)
25	5X6	3	316	-	43,43,43	6.07	24 (55%)	58,60,60	4.52	30 (51%)
17	CLA	A	837	1	69,73,73	1.86	17 (24%)	83,113,113	2.96	26 (31%)
17	CLA	1	308	-	45,49,73	2.51	19 (42%)	54,84,113	3.32	27 (50%)
17	CLA	F	204	6	45,49,73	2.45	19 (42%)	54,84,113	3.40	28 (51%)
17	CLA	4	303	13	52,56,73	2.39	20 (38%)	62,92,113	3.13	28 (45%)
22	LMT	B	852	-	36,36,36	0.48	0	47,47,47	0.54	0
17	CLA	A	852	-	69,73,73	1.79	20 (28%)	83,113,113	2.57	31 (37%)
17	CLA	A	804	1	69,73,73	1.91	17 (24%)	83,113,113	2.75	29 (34%)
17	CLA	A	859	19	50,54,73	2.32	20 (40%)	60,90,113	3.25	26 (43%)
17	CLA	4	310	-	49,53,73	2.51	21 (42%)	59,89,113	3.18	28 (47%)
18	PQN	A	840	-	34,34,34	1.51	2 (5%)	42,45,45	1.03	2 (4%)
17	CLA	A	820	1	69,73,73	1.97	19 (27%)	83,113,113	2.84	31 (37%)
17	CLA	2	308	14	49,53,73	2.50	21 (42%)	59,89,113	3.16	27 (45%)
17	CLA	3	306	15	49,53,73	2.43	20 (40%)	59,89,113	3.19	30 (50%)
25	5X6	5	301	-	43,43,43	6.07	24 (55%)	58,60,60	4.27	28 (48%)
17	CLA	B	827	2	69,73,73	1.85	21 (30%)	83,113,113	2.78	30 (36%)
17	CLA	5	312	14	49,53,73	2.46	20 (40%)	59,89,113	3.18	27 (45%)
17	CLA	B	814	2	69,73,73	1.90	19 (27%)	83,113,113	2.72	27 (32%)
17	CLA	B	808	2	69,73,73	1.92	17 (24%)	83,113,113	2.91	26 (31%)
17	CLA	1	307	13	64,68,73	2.16	19 (29%)	77,107,113	2.94	29 (37%)
17	CLA	A	808	1	59,63,73	2.11	18 (30%)	71,101,113	3.00	32 (45%)
17	CLA	A	806	1	69,73,73	1.82	17 (24%)	83,113,113	2.85	29 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	CLA	A	816	1	69,73,73	1.88	19 (27%)	83,113,113	2.68	27 (32%)
17	CLA	B	831	2	69,73,73	1.93	20 (28%)	83,113,113	2.75	33 (39%)
17	CLA	B	830	2	69,73,73	1.82	18 (26%)	83,113,113	2.94	29 (34%)
17	CLA	2	309	14	49,53,73	2.41	20 (40%)	59,89,113	3.23	28 (47%)
17	CLA	3	312	-	45,49,73	2.54	20 (44%)	54,84,113	3.37	25 (46%)
17	CLA	5	306	14	49,53,73	2.46	21 (42%)	59,89,113	3.22	27 (45%)
17	CLA	4	308	13	49,53,73	2.48	20 (40%)	59,89,113	3.25	26 (44%)
17	CLA	A	807	1	69,73,73	1.90	20 (28%)	83,113,113	2.94	30 (36%)
17	CLA	A	838	1	69,73,73	1.79	19 (27%)	83,113,113	2.73	32 (38%)
17	CLA	A	854	1	69,73,73	1.86	19 (27%)	83,113,113	2.83	25 (30%)
17	CLA	A	817	1	69,73,73	1.90	17 (24%)	83,113,113	2.81	28 (33%)
17	CLA	4	306	13	49,53,73	2.52	21 (42%)	59,89,113	3.18	26 (44%)
20	BCR	A	843	-	41,41,41	1.65	9 (21%)	56,56,56	1.43	12 (21%)
17	CLA	5	309	14	69,73,73	2.05	19 (27%)	83,113,113	2.88	32 (38%)
17	CLA	B	812	2	69,73,73	2.00	19 (27%)	83,113,113	2.65	29 (34%)
17	CLA	3	315	-	55,59,73	2.36	21 (38%)	66,96,113	3.11	28 (42%)
17	CLA	A	833	1	69,73,73	1.91	17 (24%)	83,113,113	2.67	33 (39%)
17	CLA	A	809	17,1	69,73,73	1.86	21 (30%)	83,113,113	2.76	28 (33%)
25	5X6	2	319	-	43,43,43	6.21	24 (55%)	58,60,60	4.13	29 (50%)
17	CLA	K	102	26	59,63,73	2.21	21 (35%)	71,101,113	2.94	30 (42%)
17	CLA	A	819	26	69,73,73	1.94	17 (24%)	83,113,113	2.68	27 (32%)
17	CLA	2	315	14	49,53,73	2.47	20 (40%)	59,89,113	3.19	26 (44%)
17	CLA	A	829	1	54,58,73	2.17	19 (35%)	65,95,113	3.03	31 (47%)
17	CLA	2	316	-	49,53,73	2.49	21 (42%)	59,89,113	3.23	27 (45%)
17	CLA	A	810	1	58,62,73	2.12	22 (37%)	69,99,113	3.05	28 (40%)
17	CLA	B	804	2	69,73,73	1.86	19 (27%)	83,113,113	2.73	27 (32%)
20	BCR	L	206	-	41,41,41	1.74	7 (17%)	56,56,56	1.48	11 (19%)
17	CLA	4	305	13	49,53,73	2.47	21 (42%)	59,89,113	3.17	27 (45%)
20	BCR	O	202	-	41,41,41	1.72	7 (17%)	56,56,56	1.44	10 (17%)
17	CLA	J	103	8	46,50,73	2.30	19 (41%)	55,85,113	3.22	27 (49%)

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
17	CLA	B	801	-	-	7/39/115/115	-
16	CL0	A	801	1	-	2/39/115/115	-
17	CLA	L	203	10	-	8/39/115/115	-
17	CLA	B	837	2	-	10/39/115/115	-
17	CLA	B	829	2	-	2/39/115/115	-
17	CLA	B	826	26	-	13/39/115/115	-
17	CLA	5	310	-	-	4/10/86/115	-
17	CLA	B	838	2	-	3/18/94/115	-
25	5X6	1	314	-	-	22/29/67/67	0/2/2/2
20	BCR	B	844	-	-	8/29/63/63	0/2/2/2
25	5X6	1	316	-	-	23/29/67/67	0/2/2/2
17	CLA	A	830	1	-	4/29/105/115	-
22	LMT	B	850	-	-	7/21/61/61	0/2/2/2
25	5X6	4	314	-	-	22/29/67/67	0/2/2/2
17	CLA	5	311	14	-	8/15/91/115	-
21	SF4	C	102	3	-	-	0/6/5/5
17	CLA	A	855	26	-	11/35/111/115	-
17	CLA	B	833	2	-	10/39/115/115	-
17	CLA	K	103	9	-	2/12/88/115	-
17	CLA	A	812	1	-	17/39/115/115	-
17	CLA	A	856	1	-	6/39/115/115	-
17	CLA	3	313	15	-	4/12/88/115	-
17	CLA	3	308	-	-	7/15/91/115	-
25	5X6	3	318	-	-	16/29/67/67	0/2/2/2
17	CLA	1	309	13	-	4/15/91/115	-
17	CLA	3	309	15	-	3/15/91/115	-
20	BCR	L	201	-	-	8/29/63/63	0/2/2/2
17	CLA	5	304	14	-	7/39/115/115	-
17	CLA	4	309	-	-	3/10/86/115	-
17	CLA	B	822	2	-	3/17/93/115	-
17	CLA	2	313	14	-	5/12/88/115	-
17	CLA	A	824	26	-	5/27/103/115	-
20	BCR	A	845	-	-	6/29/63/63	0/2/2/2
17	CLA	1	301	13	-	7/15/91/115	-
20	BCR	B	847	-	-	7/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	LMT	3	301	-	-	10/21/61/61	0/2/2/2
17	CLA	B	857	2	-	4/31/107/115	-
21	SF4	A	847	2,1	-	-	0/6/5/5
18	PQN	B	842	-	-	3/23/43/43	0/2/2/2
20	BCR	J	104	-	-	6/29/63/63	0/2/2/2
22	LMT	B	851	-	-	8/21/61/61	0/2/2/2
17	CLA	A	803	1	-	9/39/115/115	-
17	CLA	5	313	14	-	6/15/91/115	-
17	CLA	A	823	26	-	8/39/115/115	-
17	CLA	2	314	14	-	5/15/91/115	-
20	BCR	I	101	-	-	6/29/63/63	0/2/2/2
20	BCR	B	845	-	-	11/29/63/63	0/2/2/2
20	BCR	B	803	-	-	6/29/63/63	0/2/2/2
17	CLA	O	204	12	-	7/21/97/115	-
25	5X6	J	105	-	-	19/29/67/67	0/2/2/2
17	CLA	B	806	2	-	11/39/115/115	-
17	CLA	2	310	14	-	1/15/91/115	-
17	CLA	4	307	13	-	9/15/91/115	-
17	CLA	1	305	13	-	7/15/91/115	-
17	CLA	A	826	1	-	8/39/115/115	-
25	5X6	1	312	-	-	15/29/67/67	0/2/2/2
17	CLA	B	817	2	-	8/27/103/115	-
17	CLA	A	828	1	-	8/39/115/115	-
17	CLA	B	823	2	-	3/13/89/115	-
17	CLA	5	305	14	-	12/39/115/115	-
20	BCR	A	844	-	-	8/29/63/63	0/2/2/2
20	BCR	B	846	-	-	6/29/63/63	0/2/2/2
17	CLA	5	314	-	-	3/12/88/115	-
25	5X6	F	205	-	-	16/29/67/67	0/2/2/2
22	LMT	F	201	-	-	13/21/61/61	0/2/2/2
19	LHG	A	842	17	-	19/44/44/53	-
17	CLA	B	828	2	-	11/39/115/115	-
17	CLA	B	818	2	-	11/32/108/115	-
17	CLA	B	809	2	-	8/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	5X6	1	315	-	-	25/29/67/67	0/2/2/2
17	CLA	5	303	14	-	12/39/115/115	-
17	CLA	B	819	2	-	4/33/109/115	-
22	LMT	L	207	-	-	8/21/61/61	0/2/2/2
25	5X6	2	321	-	-	25/29/67/67	0/2/2/2
17	CLA	A	825	1	-	8/39/115/115	-
17	CLA	A	835	1	-	3/23/99/115	-
17	CLA	1	306	13	-	5/27/103/115	-
17	CLA	3	311	15	-	3/24/100/115	-
17	CLA	B	834	26	-	9/39/115/115	-
22	LMT	A	848	-	-	7/21/61/61	0/2/2/2
17	CLA	A	805	1	-	2/21/97/115	-
17	CLA	A	822	1	-	7/27/103/115	-
17	CLA	B	832	2	-	11/39/115/115	-
17	CLA	B	835	26	-	6/15/91/115	-
25	5X6	5	317	-	-	22/29/67/67	0/2/2/2
25	5X6	4	312	-	-	22/29/67/67	0/2/2/2
17	CLA	B	810	2	-	12/39/115/115	-
20	BCR	L	205	-	-	4/29/63/63	0/2/2/2
17	CLA	F	203	26	-	0/15/91/115	-
25	5X6	5	316	-	-	18/29/67/67	0/2/2/2
17	CLA	4	304	13	-	8/32/108/115	-
17	CLA	A	814	26	-	3/15/91/115	-
17	CLA	B	821	2	-	4/15/91/115	-
17	CLA	4	311	-	-	6/15/91/115	-
25	5X6	5	315	-	-	20/29/67/67	0/2/2/2
25	5X6	2	318	-	-	18/29/67/67	0/2/2/2
20	BCR	B	848	-	-	4/29/63/63	0/2/2/2
17	CLA	B	820	26	-	10/39/115/115	-
20	BCR	M	101	-	-	11/29/63/63	0/2/2/2
25	5X6	2	320	-	-	22/29/67/67	0/2/2/2
20	BCR	A	857	-	-	4/29/63/63	0/2/2/2
17	CLA	A	831	1	-	10/39/115/115	-
20	BCR	A	846	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	O	205	-	-	7/15/91/115	-
17	CLA	O	203	-	-	4/10/86/115	-
25	5X6	1	313	-	-	17/29/67/67	0/2/2/2
24	DGD	B	849	-	-	23/55/95/95	0/2/2/2
17	CLA	1	303	13	-	9/27/103/115	-
17	CLA	A	836	1	-	5/29/105/115	-
17	CLA	3	305	15	-	10/37/113/115	-
17	CLA	A	818	1	-	9/39/115/115	-
17	CLA	2	312	-	-	5/10/86/115	-
25	5X6	4	313	-	-	22/29/67/67	0/2/2/2
17	CLA	A	827	1	-	6/39/115/115	-
17	CLA	1	302	13	-	6/32/108/115	-
17	CLA	1	304	13	-	7/15/91/115	-
17	CLA	2	304	14	-	6/15/91/115	-
17	CLA	A	815	1	-	10/36/112/115	-
17	CLA	3	314	-	-	8/17/93/115	-
20	BCR	K	104	-	-	7/29/63/63	0/2/2/2
17	CLA	L	204	26	-	7/21/97/115	-
17	CLA	A	853	26	-	3/39/115/115	-
17	CLA	3	310	15	-	6/15/91/115	-
17	CLA	2	305	14	-	7/39/115/115	-
17	CLA	B	836	2	-	7/33/109/115	-
17	CLA	B	816	2	-	14/39/115/115	-
19	LHG	J	102	-	-	24/53/53/53	-
17	CLA	A	832	1	-	7/39/115/115	-
17	CLA	A	834	1	-	14/39/115/115	-
25	5X6	3	317	-	-	23/29/67/67	0/2/2/2
21	SF4	C	101	3	-	-	0/6/5/5
17	CLA	B	815	2	-	14/39/115/115	-
17	CLA	5	307	14	-	4/15/91/115	-
17	CLA	B	840	2	-	9/39/115/115	-
25	5X6	5	318	-	-	19/29/67/67	0/2/2/2
17	CLA	A	811	1	-	7/39/115/115	-
17	CLA	A	839	26	-	9/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	5	308	14	-	12/39/115/115	-
17	CLA	5	302	14	-	8/15/91/115	-
25	5X6	2	317	-	-	22/29/67/67	0/2/2/2
17	CLA	B	807	2	-	11/39/115/115	-
17	CLA	A	802	17,1	-	9/27/103/115	-
17	CLA	B	805	2	-	14/39/115/115	-
17	CLA	A	813	1	-	5/12/88/115	-
17	CLA	B	825	26	-	7/39/115/115	-
19	LHG	A	841	-	-	18/53/53/53	-
17	CLA	3	307	-	-	4/27/103/115	-
17	CLA	B	841	-	-	5/39/115/115	-
20	BCR	B	843	-	-	1/29/63/63	0/2/2/2
17	CLA	A	821	1	-	5/23/99/115	-
17	CLA	B	811	2	-	11/39/115/115	-
17	CLA	B	839	26	-	10/39/115/115	-
17	CLA	1	311	13	-	8/15/91/115	-
17	CLA	B	824	2	-	6/27/103/115	-
17	CLA	1	310	-	-	5/15/91/115	-
17	CLA	2	311	14	-	10/27/103/115	-
17	CLA	B	802	26	-	15/39/115/115	-
17	CLA	B	813	2	-	5/27/103/115	-
17	CLA	2	307	14	-	12/27/103/115	-
17	CLA	L	202	10	-	13/30/106/115	-
17	CLA	2	306	14	-	4/15/91/115	-
25	5X6	3	316	-	-	21/29/67/67	0/2/2/2
17	CLA	A	837	1	-	9/39/115/115	-
17	CLA	1	308	-	-	6/10/86/115	-
17	CLA	F	204	6	-	5/10/86/115	-
17	CLA	4	303	13	-	9/19/95/115	-
22	LMT	B	852	-	-	12/21/61/61	0/2/2/2
17	CLA	A	852	-	-	4/39/115/115	-
17	CLA	A	804	1	-	17/39/115/115	-
17	CLA	A	859	19	-	10/17/93/115	-
17	CLA	4	310	-	-	4/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	PQN	A	840	-	-	4/23/43/43	0/2/2/2
17	CLA	A	820	1	-	10/39/115/115	-
17	CLA	2	308	14	-	4/15/91/115	-
17	CLA	3	306	15	-	5/15/91/115	-
25	5X6	5	301	-	-	20/29/67/67	0/2/2/2
17	CLA	B	827	2	-	7/39/115/115	-
17	CLA	5	312	14	-	5/15/91/115	-
17	CLA	B	814	2	-	8/39/115/115	-
17	CLA	B	808	2	-	7/39/115/115	-
17	CLA	1	307	13	-	7/33/109/115	-
17	CLA	A	808	1	-	7/27/103/115	-
17	CLA	A	806	1	-	10/39/115/115	-
17	CLA	A	816	1	-	7/39/115/115	-
17	CLA	B	831	2	-	13/39/115/115	-
17	CLA	B	830	2	-	9/39/115/115	-
17	CLA	2	309	14	-	7/15/91/115	-
17	CLA	3	312	-	-	2/10/86/115	-
17	CLA	5	306	14	-	7/15/91/115	-
17	CLA	4	308	13	-	4/15/91/115	-
17	CLA	A	807	1	-	12/39/115/115	-
17	CLA	A	838	1	-	5/39/115/115	-
17	CLA	A	854	1	-	6/39/115/115	-
17	CLA	A	817	1	-	6/39/115/115	-
17	CLA	4	306	13	-	6/15/91/115	-
20	BCR	A	843	-	-	10/29/63/63	0/2/2/2
17	CLA	5	309	14	-	11/39/115/115	-
17	CLA	B	812	2	-	14/39/115/115	-
17	CLA	3	315	-	-	11/23/99/115	-
17	CLA	A	833	1	-	7/39/115/115	-
17	CLA	A	809	17,1	-	6/39/115/115	-
25	5X6	2	319	-	-	20/29/67/67	0/2/2/2
17	CLA	K	102	26	-	7/27/103/115	-
17	CLA	A	819	26	-	7/39/115/115	-
17	CLA	2	315	14	-	0/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	A	829	1	-	7/21/97/115	-
17	CLA	2	316	-	-	6/15/91/115	-
17	CLA	A	810	1	-	10/26/102/115	-
17	CLA	B	804	2	-	7/39/115/115	-
20	BCR	L	206	-	-	5/29/63/63	0/2/2/2
17	CLA	4	305	13	-	8/15/91/115	-
20	BCR	O	202	-	-	2/29/63/63	0/2/2/2
17	CLA	J	103	8	-	5/12/88/115	-

The worst 5 of 3727 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	2	319	5X6	C18-C17	16.24	1.57	1.35
25	4	313	5X6	C18-C17	15.98	1.57	1.35
25	1	313	5X6	C18-C17	15.87	1.56	1.35
25	5	318	5X6	C18-C17	15.73	1.56	1.35
25	2	320	5X6	C18-C17	15.71	1.56	1.35

The worst 5 of 5264 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	805	CLA	O2A-CGA-O1A	-17.93	78.34	123.59
17	B	805	CLA	O2A-CGA-CBA	16.54	163.81	111.91
25	2	321	5X6	C01-C02-C03	-14.63	108.10	124.53
25	F	205	5X6	C28-C27-C26	-14.17	104.83	126.23
25	1	316	5X6	C01-C02-C03	-13.59	109.26	124.53

There are no chirality outliers.

5 of 1869 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	A	804	CLA	C11-C10-C8-C9
17	A	808	CLA	C2-C3-C5-C6
17	A	808	CLA	C4-C3-C5-C6
17	A	813	CLA	C1A-C2A-CAA-CBA
17	A	816	CLA	C3A-C2A-CAA-CBA

There are no ring outliers.

167 monomers are involved in 299 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	B	801	CLA	1	0
16	A	801	CL0	1	0
17	B	837	CLA	5	0
17	B	829	CLA	2	0
17	B	826	CLA	4	0
17	5	310	CLA	1	0
17	B	838	CLA	2	0
25	1	314	5X6	1	0
20	B	844	BCR	2	0
17	5	311	CLA	1	0
21	C	102	SF4	1	0
17	A	855	CLA	2	0
17	B	833	CLA	2	0
17	K	103	CLA	2	0
17	3	313	CLA	1	0
17	3	308	CLA	1	0
17	1	309	CLA	1	0
17	3	309	CLA	1	0
20	L	201	BCR	2	0
17	5	304	CLA	2	0
17	4	309	CLA	1	0
17	B	822	CLA	1	0
17	2	313	CLA	3	0
20	A	845	BCR	2	0
17	1	301	CLA	1	0
20	B	847	BCR	2	0
17	B	857	CLA	2	0
18	B	842	PQN	2	0
20	J	104	BCR	3	0
17	A	803	CLA	3	0
17	5	313	CLA	4	0
17	A	823	CLA	2	0
17	2	314	CLA	1	0
20	B	845	BCR	1	0
20	B	803	BCR	1	0
17	O	204	CLA	2	0
17	B	806	CLA	1	0
17	2	310	CLA	1	0
17	4	307	CLA	6	0
17	1	305	CLA	2	0
17	A	826	CLA	2	0
25	1	312	5X6	1	0
17	B	817	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	B	823	CLA	4	0
17	5	305	CLA	3	0
20	A	844	BCR	3	0
17	5	314	CLA	1	0
19	A	842	LHG	1	0
17	B	828	CLA	5	0
17	B	818	CLA	4	0
17	5	303	CLA	1	0
17	A	825	CLA	1	0
17	A	835	CLA	1	0
17	1	306	CLA	1	0
17	3	311	CLA	1	0
17	B	834	CLA	3	0
17	A	805	CLA	1	0
17	A	822	CLA	1	0
17	B	832	CLA	1	0
17	B	835	CLA	2	0
17	B	810	CLA	4	0
20	L	205	BCR	1	0
17	F	203	CLA	3	0
17	A	814	CLA	1	0
17	B	821	CLA	1	0
17	4	311	CLA	1	0
20	B	848	BCR	1	0
17	B	820	CLA	3	0
20	M	101	BCR	3	0
20	A	857	BCR	2	0
17	A	831	CLA	2	0
20	A	846	BCR	4	0
17	O	205	CLA	1	0
17	O	203	CLA	2	0
24	B	849	DGD	3	0
17	1	303	CLA	1	0
17	A	836	CLA	1	0
17	3	305	CLA	2	0
17	A	818	CLA	2	0
17	2	312	CLA	1	0
17	A	827	CLA	1	0
17	1	302	CLA	3	0
17	1	304	CLA	2	0
17	2	304	CLA	2	0
17	A	815	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	3	314	CLA	1	0
20	K	104	BCR	1	0
17	L	204	CLA	1	0
17	A	853	CLA	4	0
17	B	836	CLA	6	0
17	B	816	CLA	2	0
19	J	102	LHG	1	0
17	A	832	CLA	2	0
17	A	834	CLA	2	0
25	3	317	5X6	2	0
17	B	815	CLA	1	0
17	5	307	CLA	2	0
17	B	840	CLA	3	0
25	5	318	5X6	2	0
17	A	811	CLA	3	0
17	A	839	CLA	2	0
17	5	308	CLA	2	0
17	5	302	CLA	1	0
17	B	807	CLA	6	0
17	A	802	CLA	1	0
17	B	805	CLA	3	0
17	A	813	CLA	2	0
17	B	825	CLA	2	0
17	3	307	CLA	1	0
17	B	841	CLA	6	0
20	B	843	BCR	1	0
17	A	821	CLA	1	0
17	B	811	CLA	3	0
17	B	839	CLA	5	0
17	1	311	CLA	1	0
17	B	824	CLA	3	0
17	1	310	CLA	3	0
17	B	802	CLA	6	0
17	B	813	CLA	4	0
17	2	307	CLA	7	0
17	L	202	CLA	1	0
17	A	837	CLA	1	0
17	1	308	CLA	1	0
17	F	204	CLA	2	0
17	4	303	CLA	1	0
17	A	852	CLA	2	0
17	A	804	CLA	2	0

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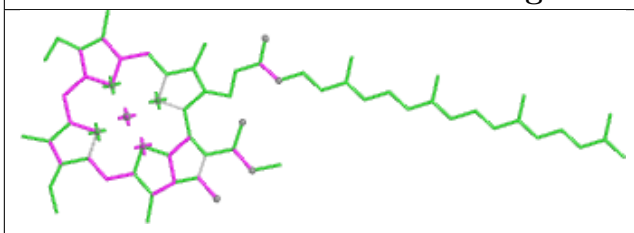
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	A	859	CLA	5	0
17	4	310	CLA	1	0
18	A	840	PQN	1	0
17	A	820	CLA	1	0
17	2	308	CLA	1	0
17	3	306	CLA	2	0
17	B	827	CLA	1	0
17	5	312	CLA	1	0
17	B	814	CLA	1	0
17	B	808	CLA	2	0
17	1	307	CLA	2	0
17	A	808	CLA	1	0
17	A	816	CLA	7	0
17	B	831	CLA	3	0
17	B	830	CLA	3	0
17	2	309	CLA	5	0
17	3	312	CLA	2	0
17	5	306	CLA	1	0
17	4	308	CLA	1	0
17	A	807	CLA	2	0
17	A	838	CLA	1	0
17	A	854	CLA	4	0
17	A	817	CLA	1	0
17	4	306	CLA	2	0
20	A	843	BCR	3	0
17	5	309	CLA	1	0
17	B	812	CLA	4	0
17	3	315	CLA	1	0
17	A	833	CLA	1	0
17	A	809	CLA	2	0
17	K	102	CLA	1	0
17	A	819	CLA	5	0
17	2	315	CLA	1	0
17	A	829	CLA	1	0
17	2	316	CLA	1	0
17	A	810	CLA	2	0
17	B	804	CLA	3	0
20	L	206	BCR	1	0
17	4	305	CLA	1	0
17	J	103	CLA	1	0

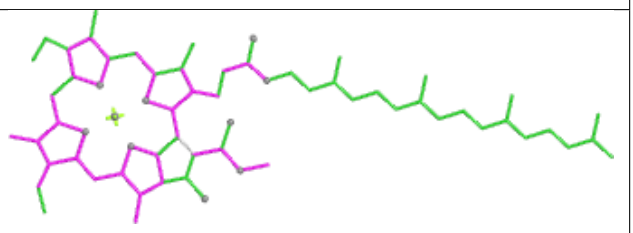
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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

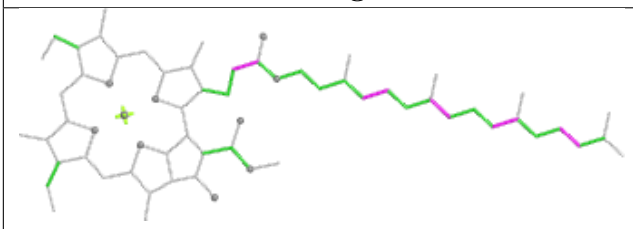
Ligand CLA B 801



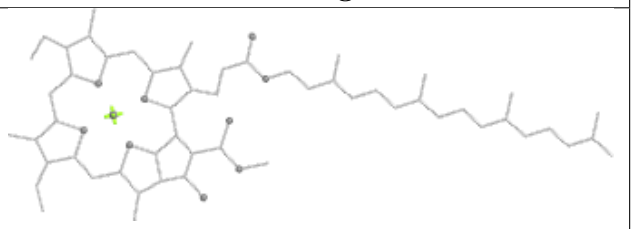
Bond lengths



Bond angles

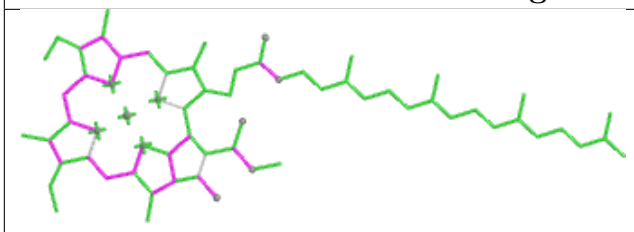


Torsions

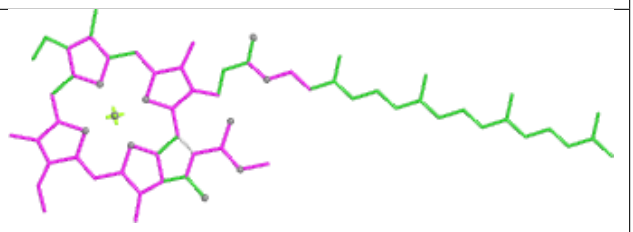


Rings

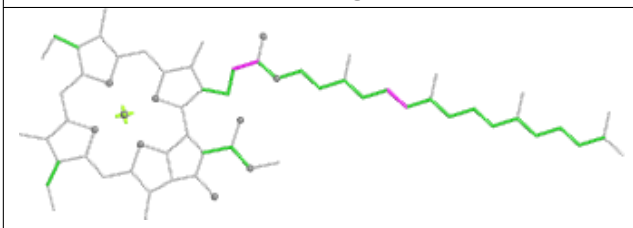
Ligand CL0 A 801



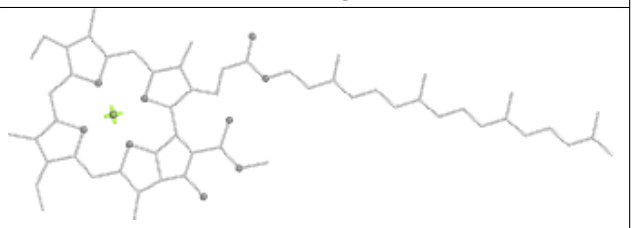
Bond lengths



Bond angles

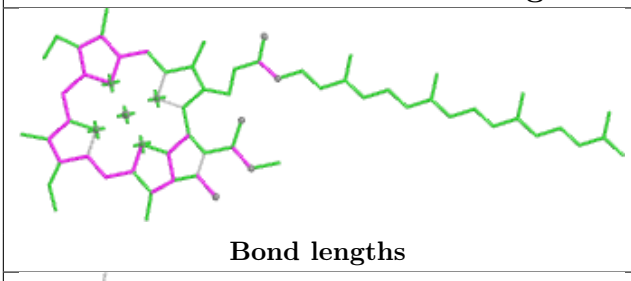


Torsions

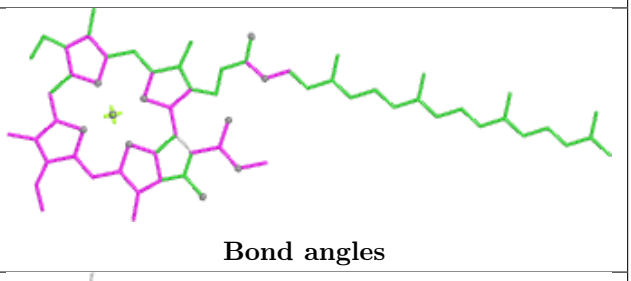


Rings

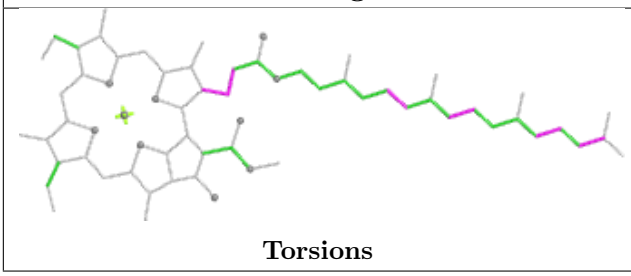
Ligand CLA L 203



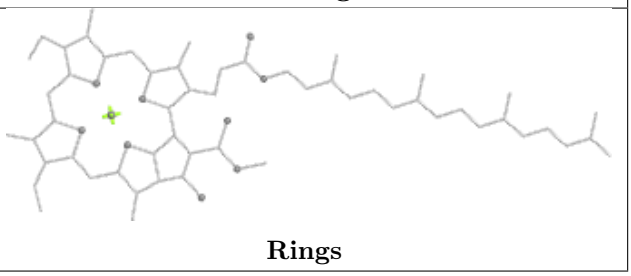
Bond lengths



Bond angles

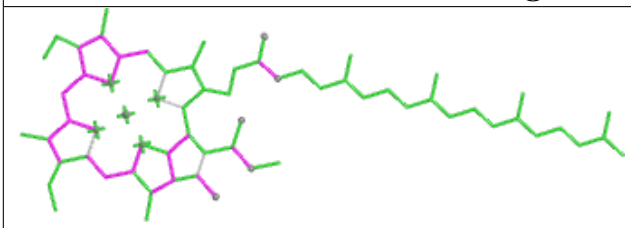


Torsions

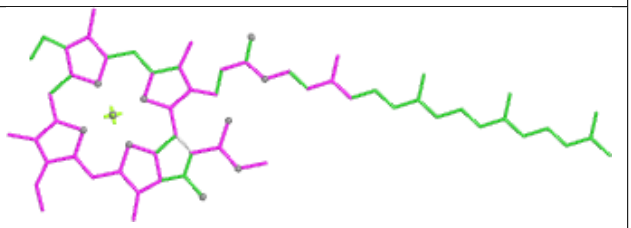


Rings

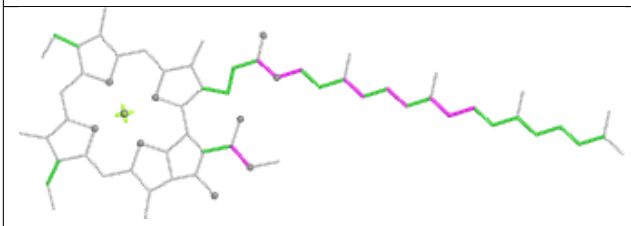
Ligand CLA B 837



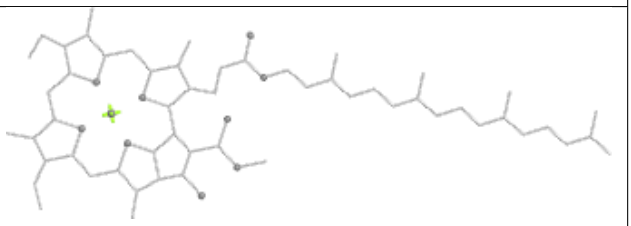
Bond lengths



Bond angles

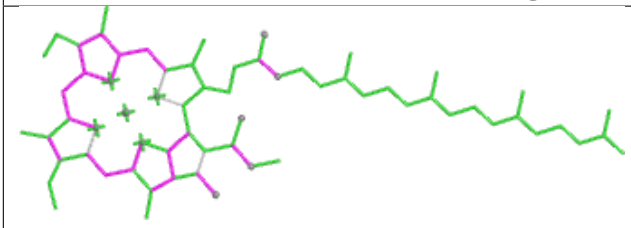


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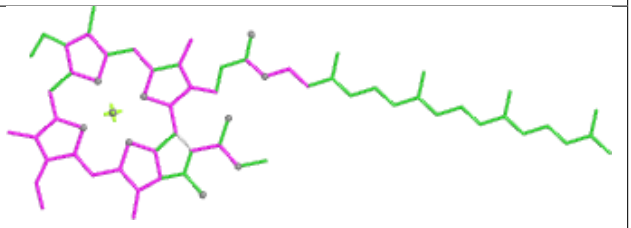


Rings

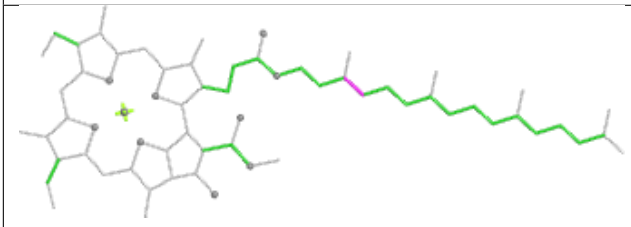
Ligand CLA B 829



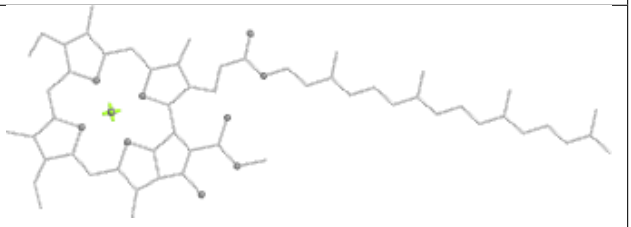
Bond lengths



Bond angles

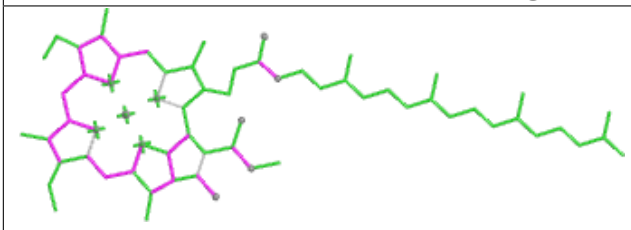


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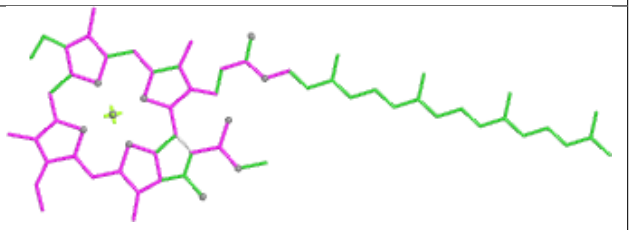


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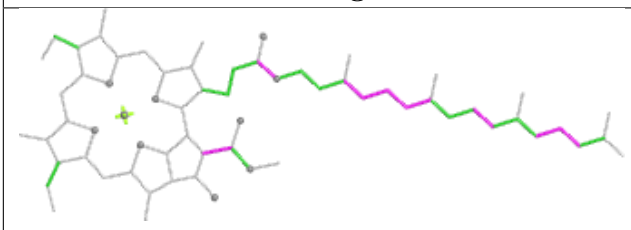
Ligand CLA B 826



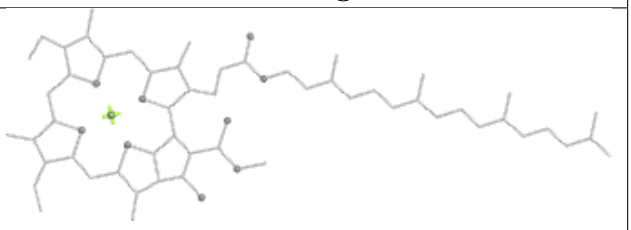
Bond lengths



Bond angles

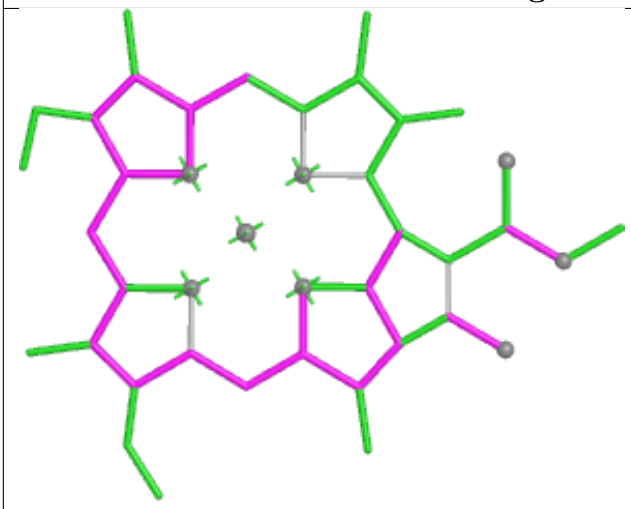


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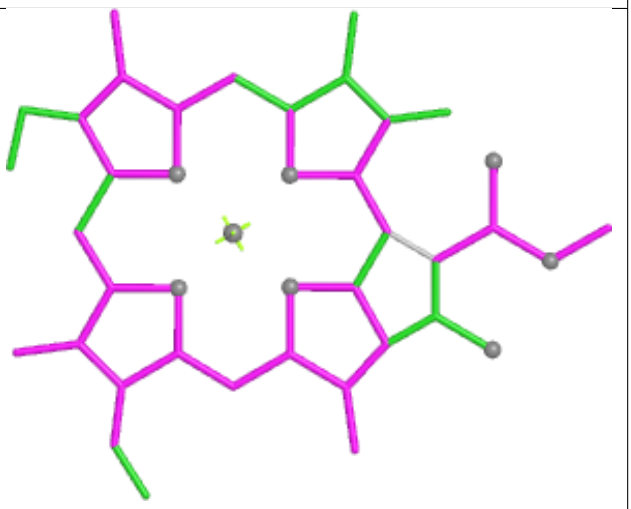


Rings

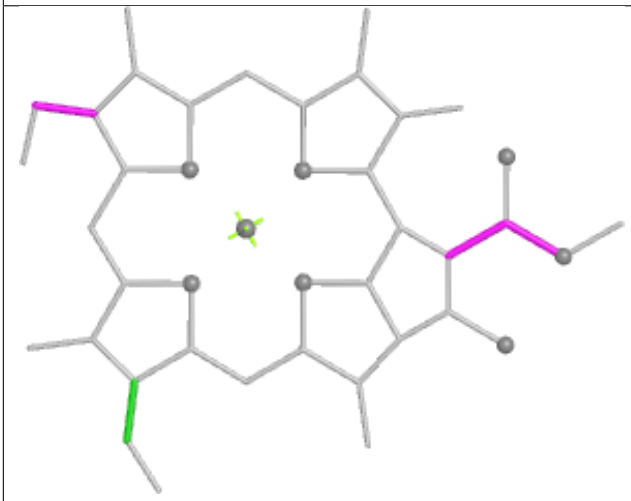
Ligand CLA 5 310



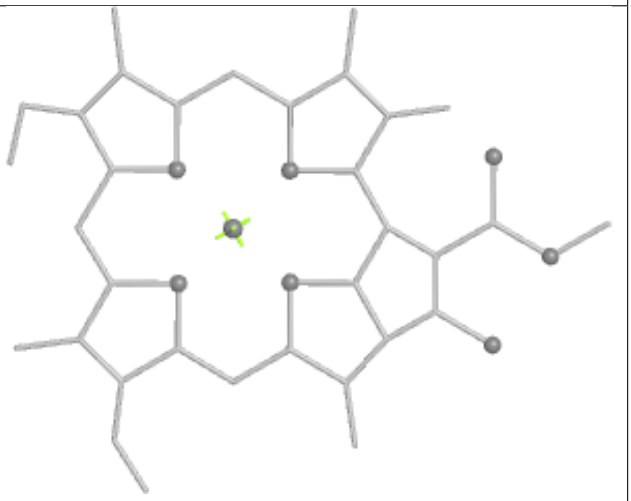
Bond lengths



Bond angles

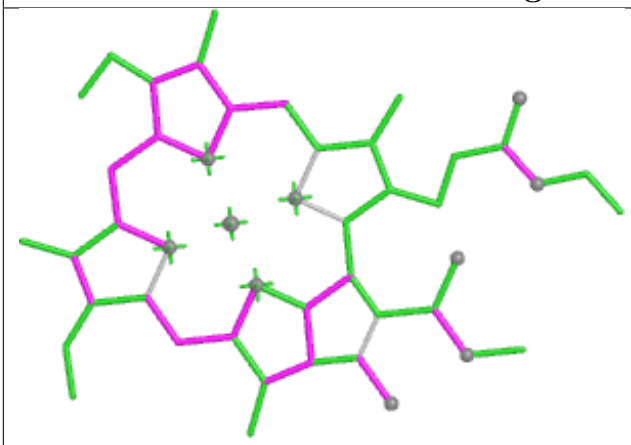


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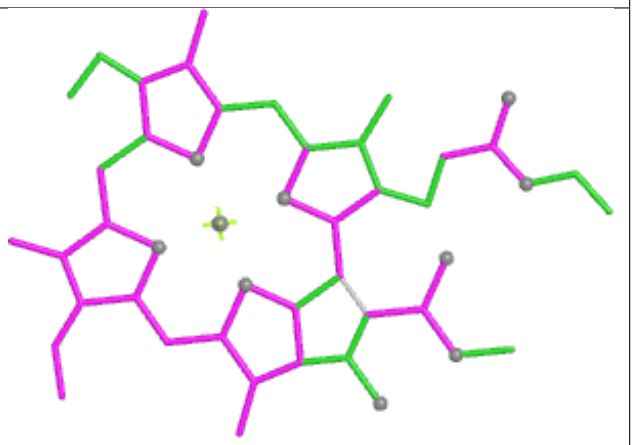


Rings

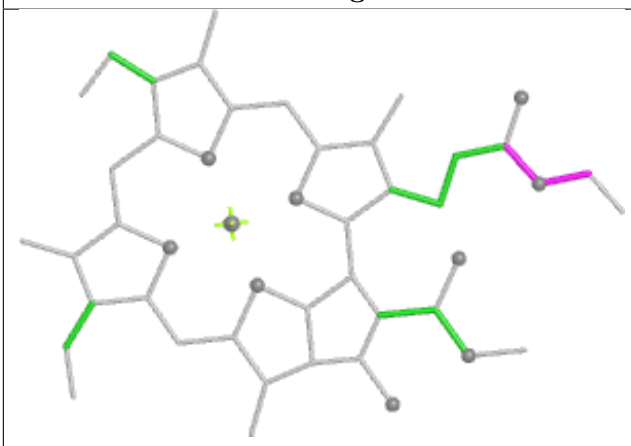
Ligand CLA B 838



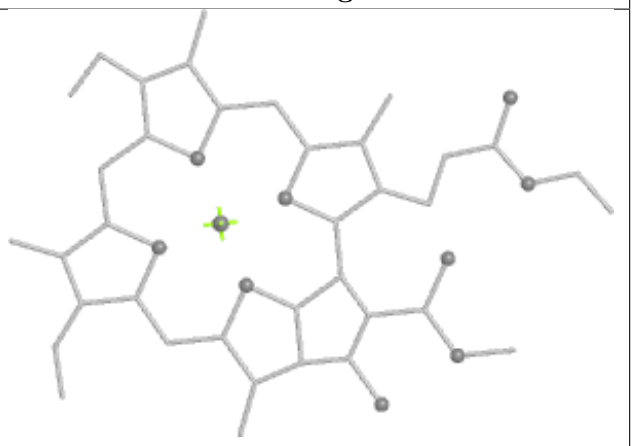
Bond lengths



Bond angles

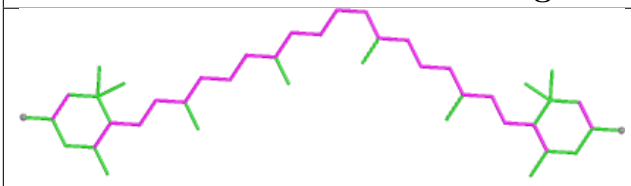


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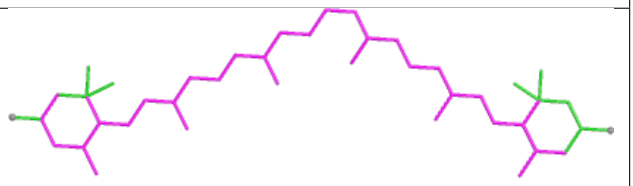


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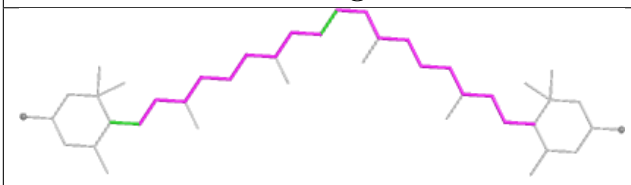
Ligand 5X6 1 314



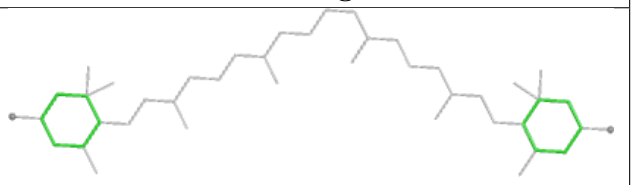
Bond lengths



Bond angles

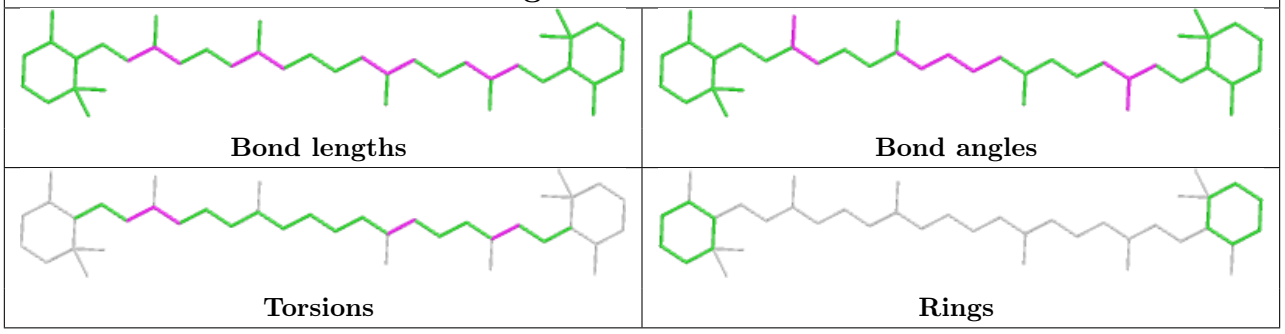


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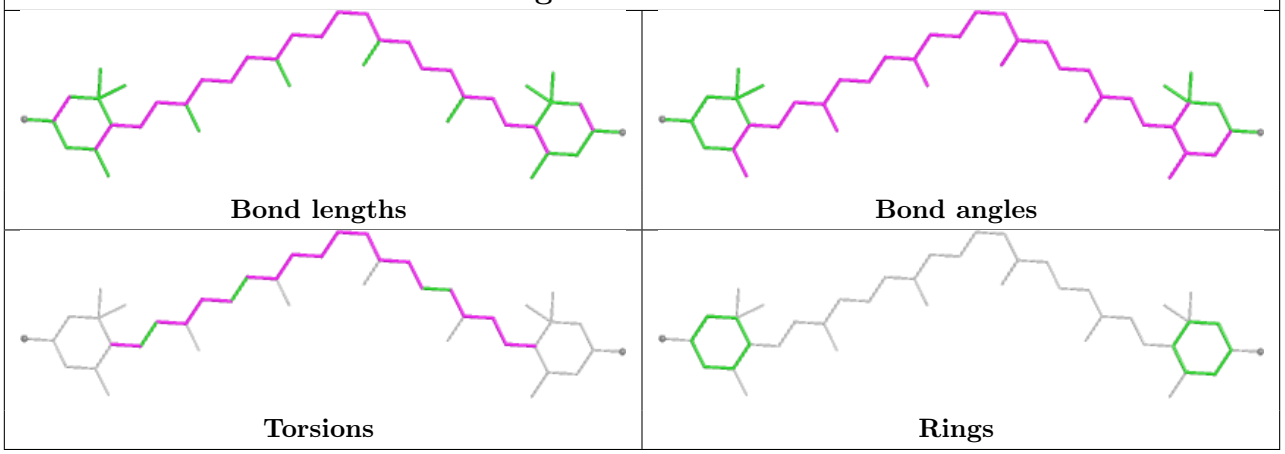


Rings

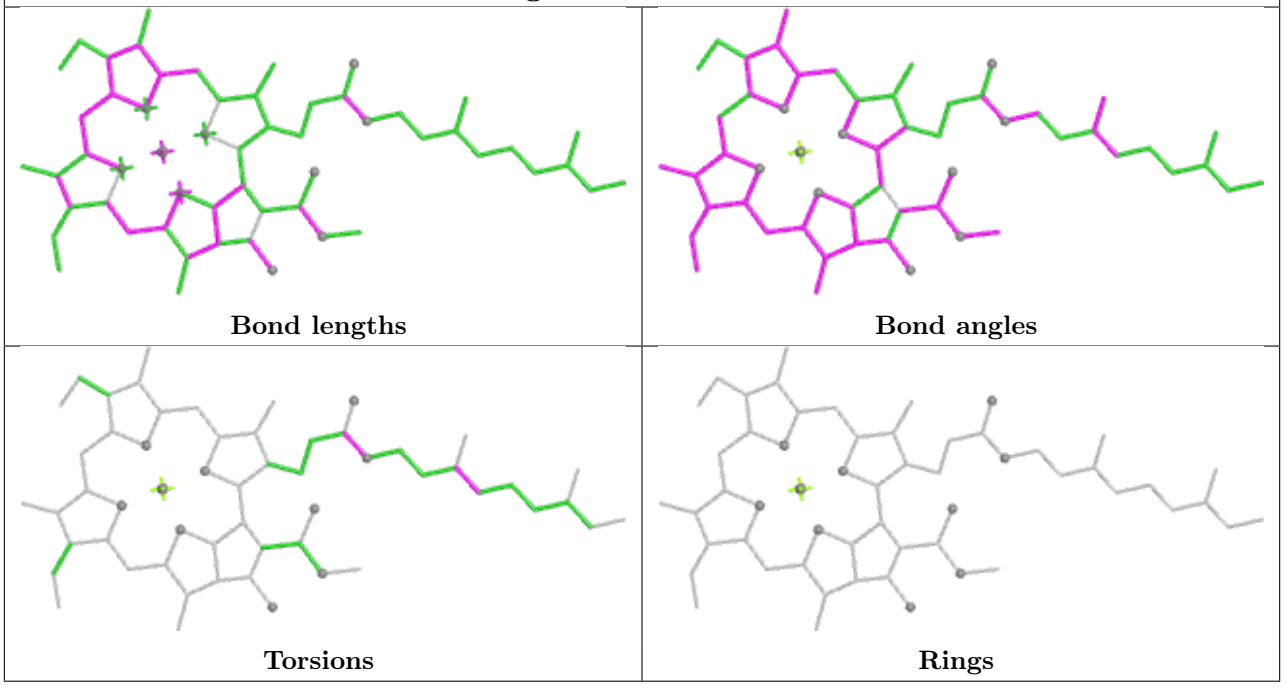
Ligand BCR B 844



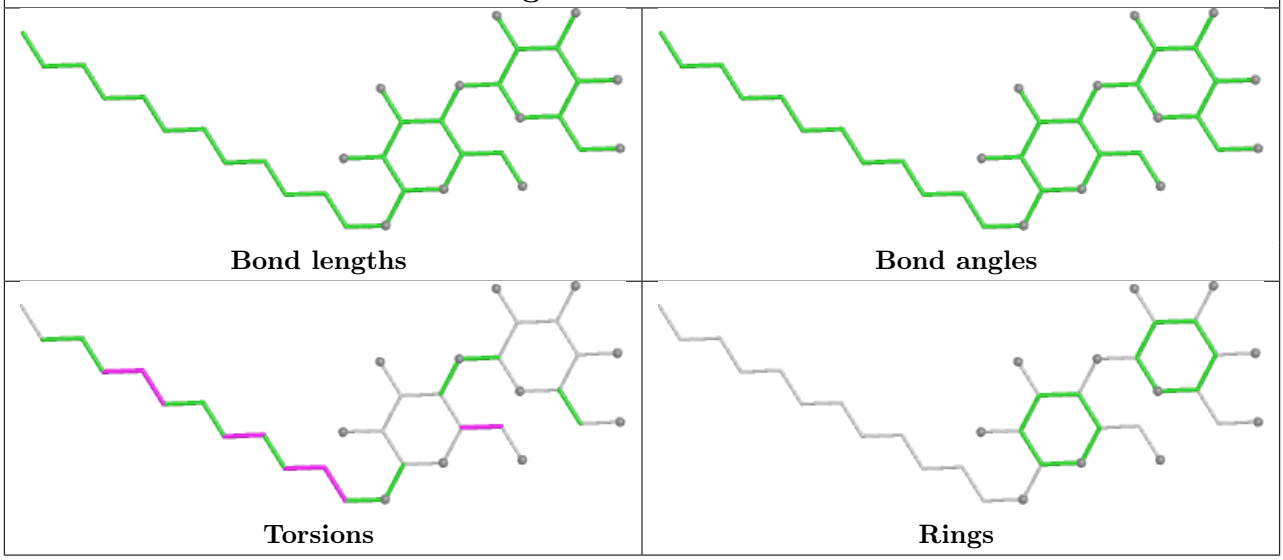
Ligand 5X6 1 316



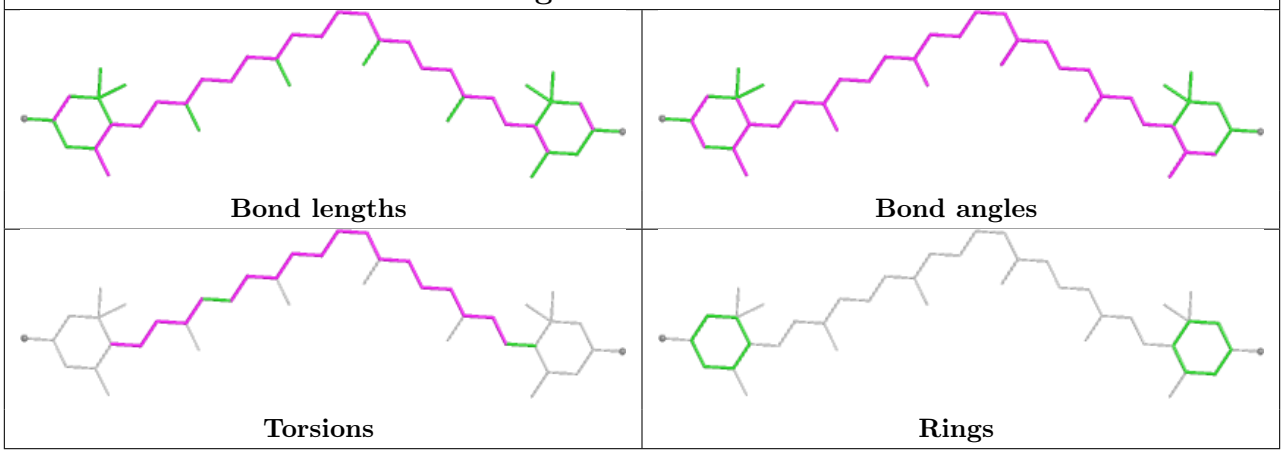
Ligand CLA A 830



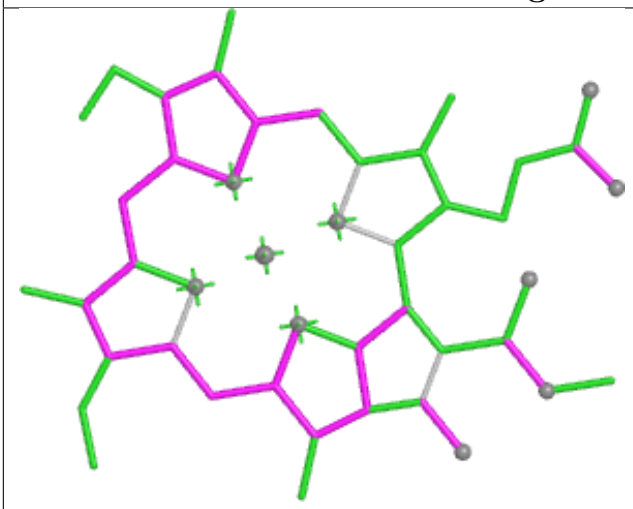
Ligand LMT B 850



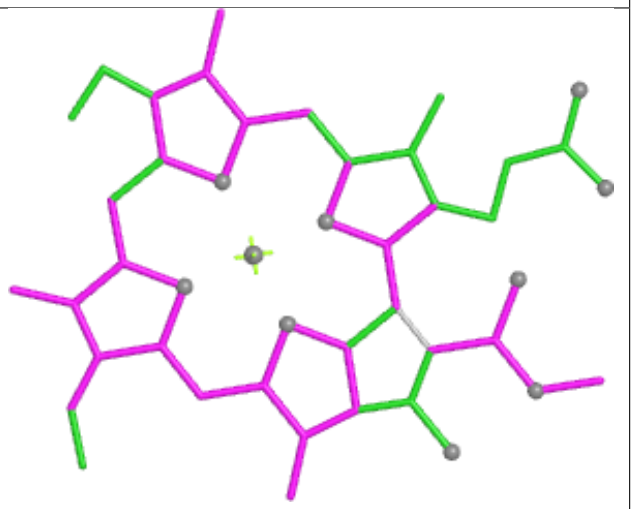
Ligand 5X6 4 314



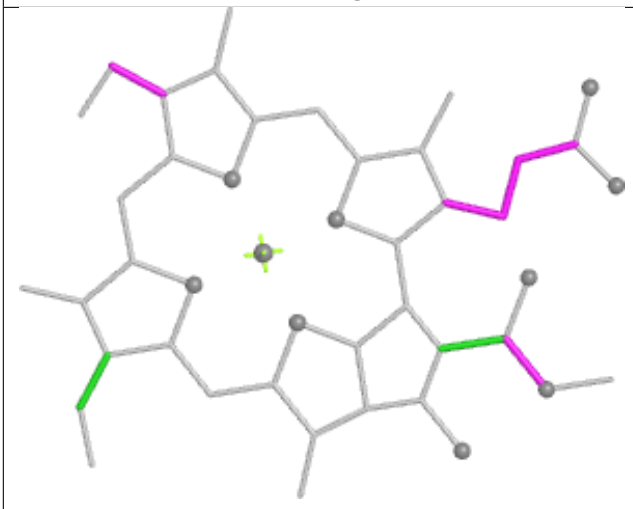
Ligand CLA 5 311



Bond lengths



Bond angles

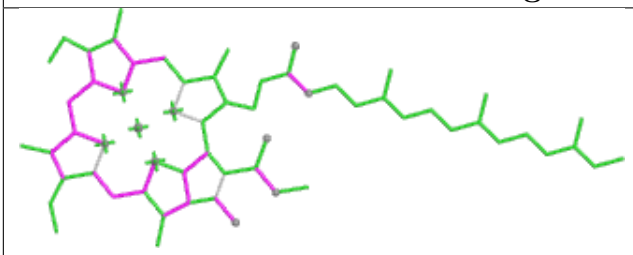


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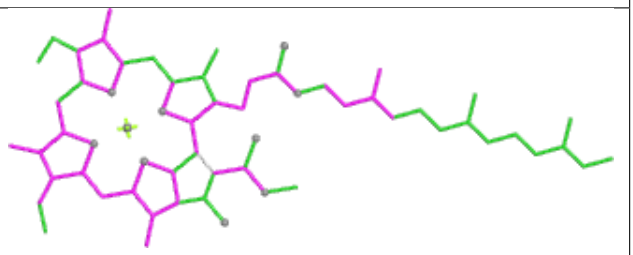


Rings

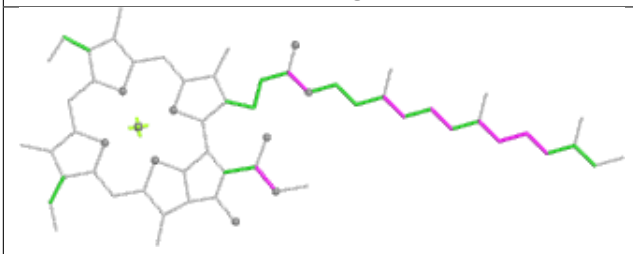
Ligand CLA A 855



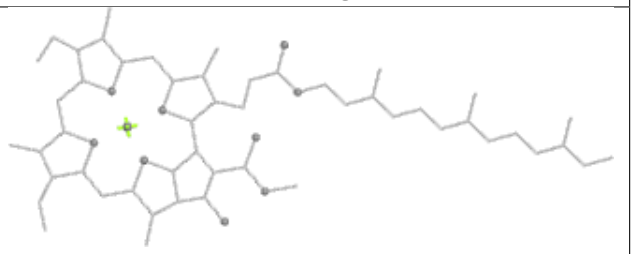
Bond lengths



Bond angles

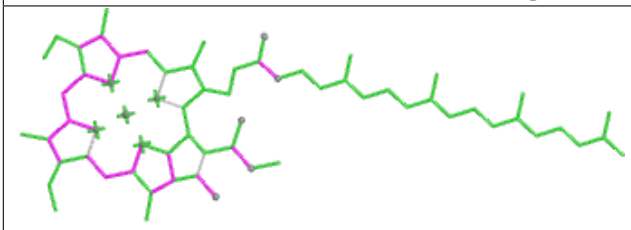


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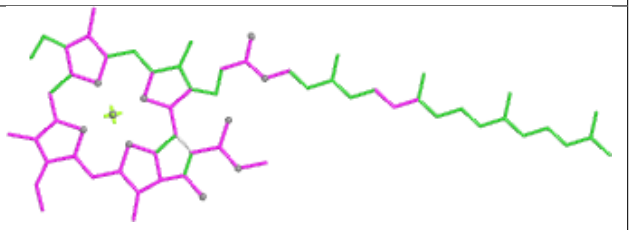


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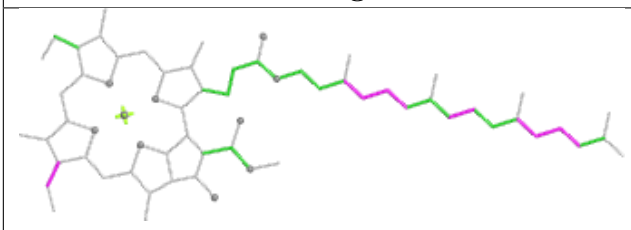
Ligand CLA B 833



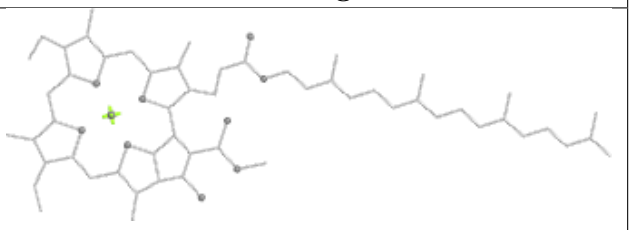
Bond lengths



Bond angles



Torsions



Rings

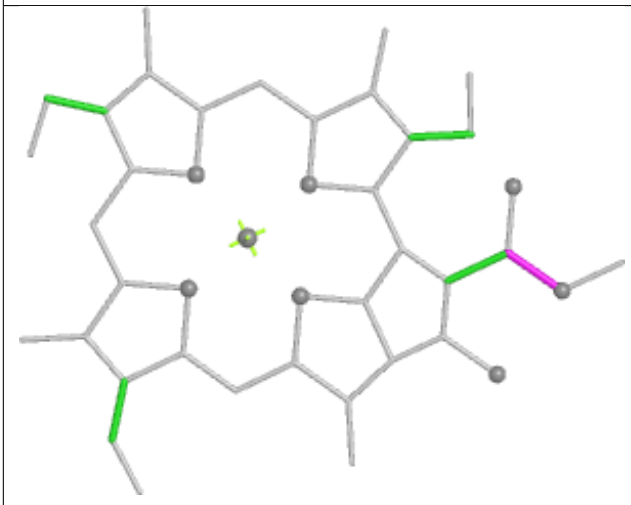
Ligand CLA K 103



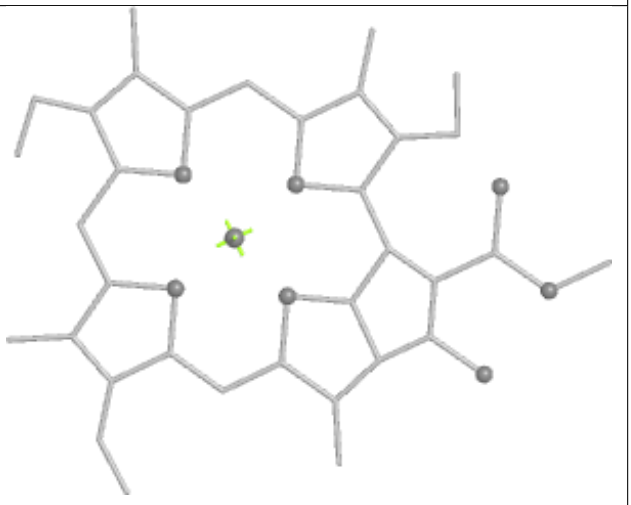
Bond lengths



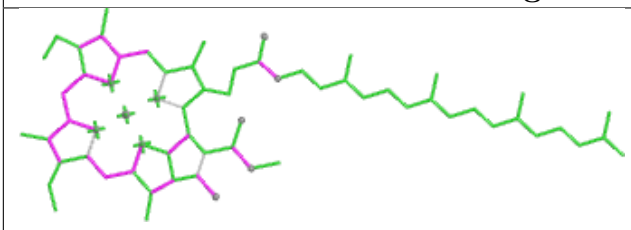
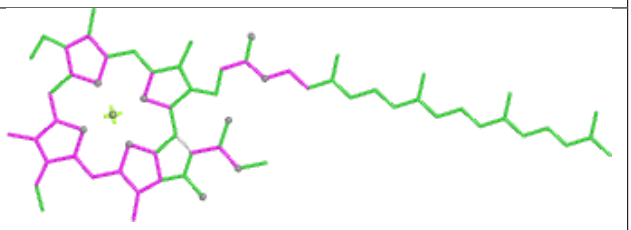
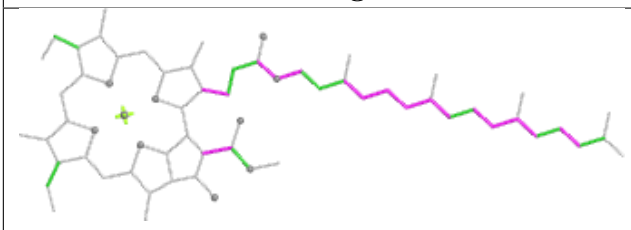
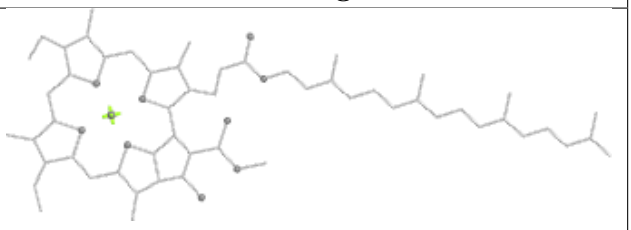
Bond angles

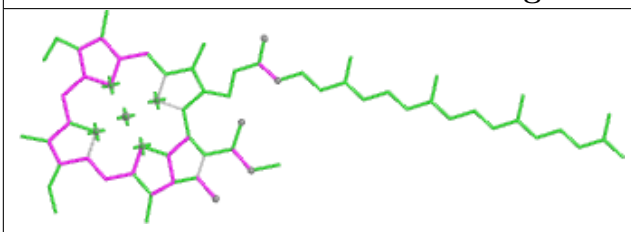
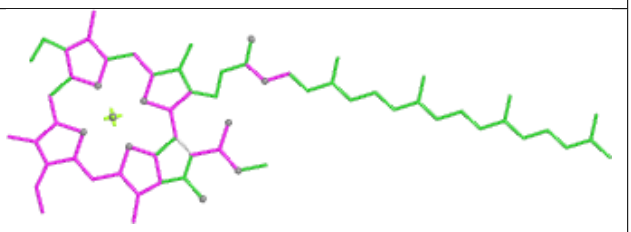
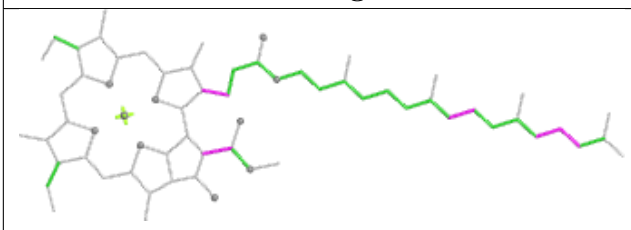
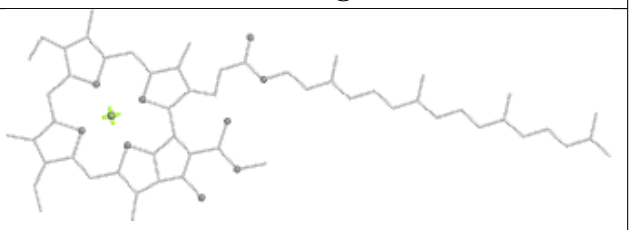


Torsions

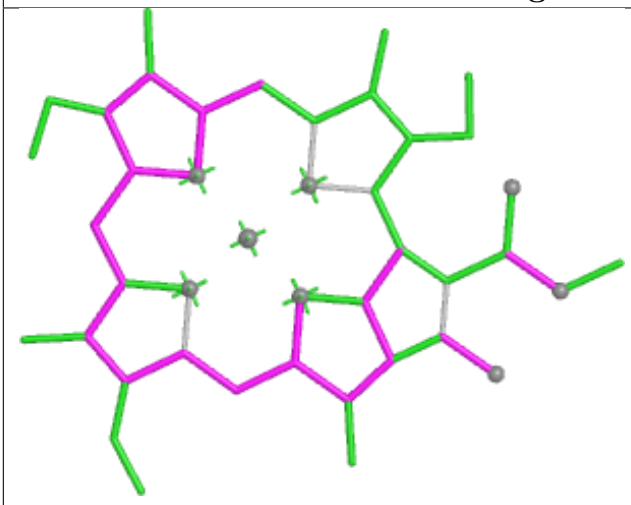


Rings

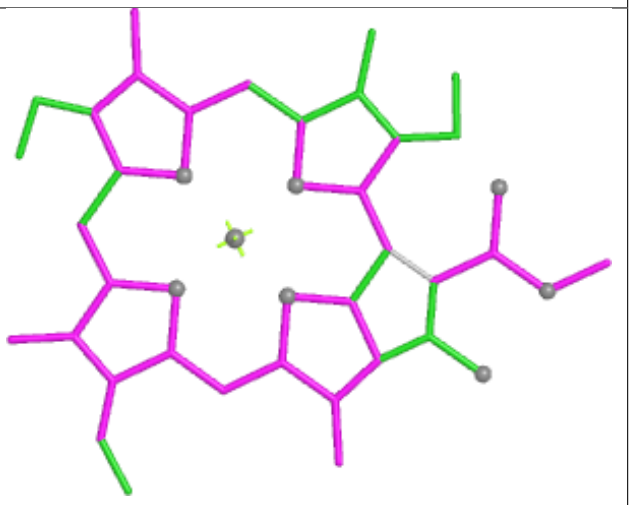
Ligand CLA A 812	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 856	
	
Bond lengths	Bond angles
	
Torsions	Rings

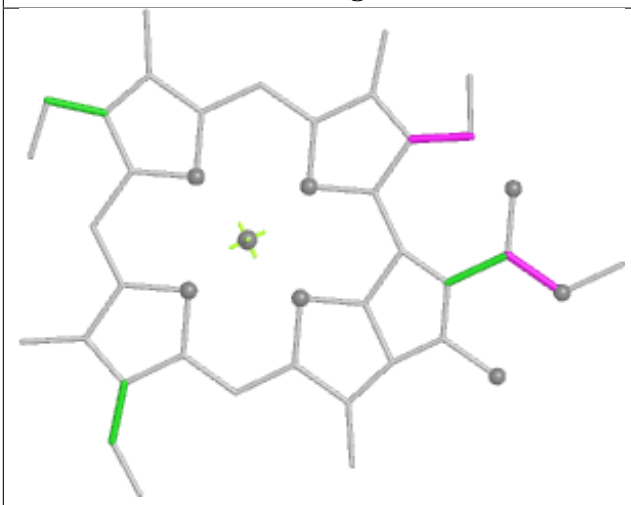
Ligand CLA 3 313



Bond lengths



Bond angles

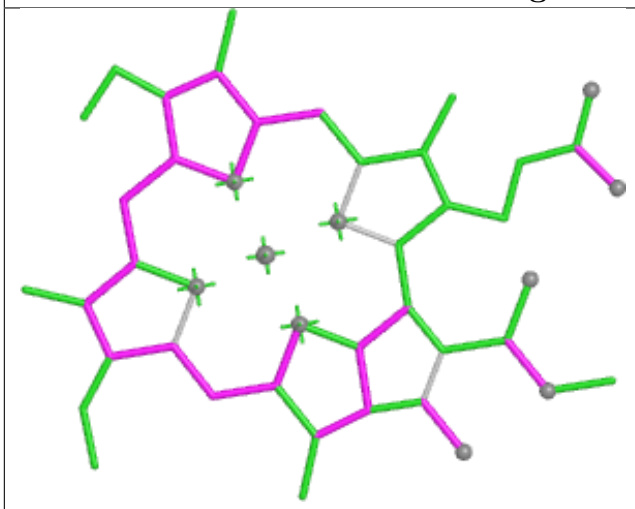


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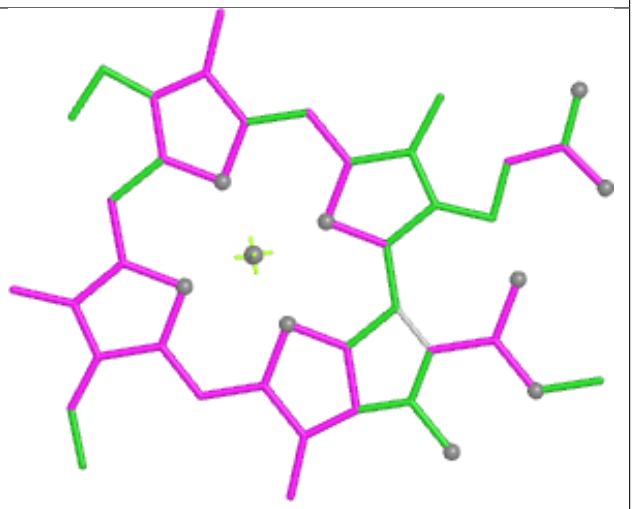


Rings

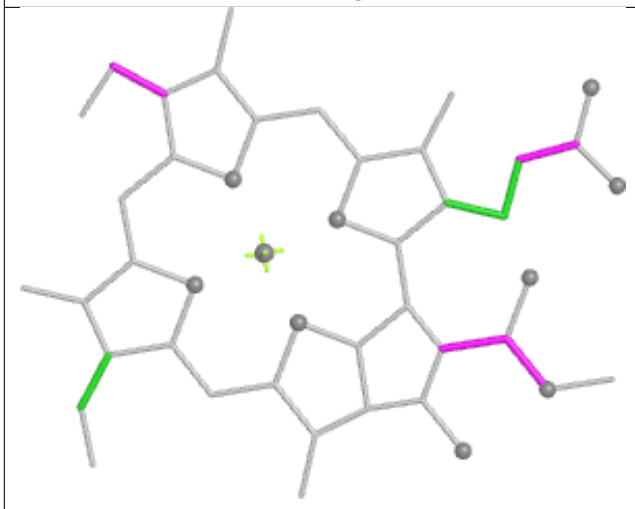
Ligand CLA 3 308



Bond lengths



Bond angles

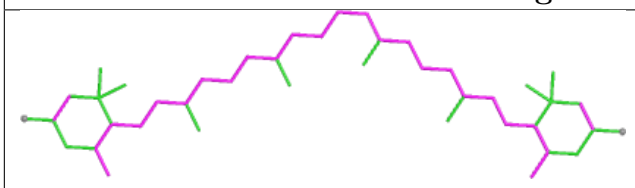


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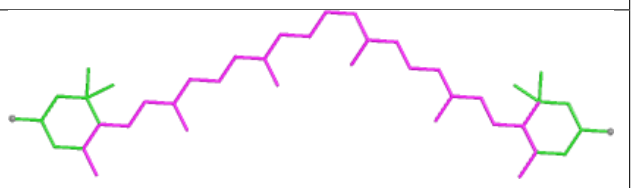


Rings

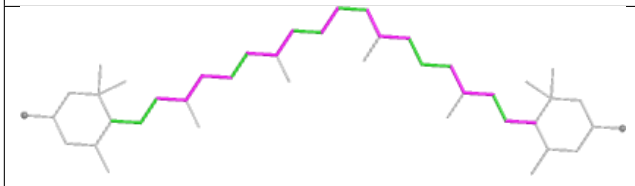
Ligand 5X6 3 318



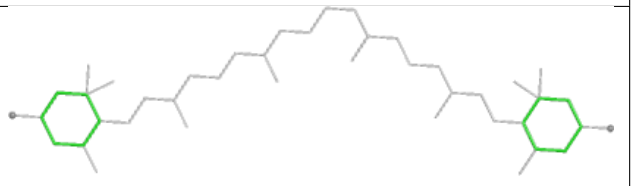
Bond lengths



Bond angles

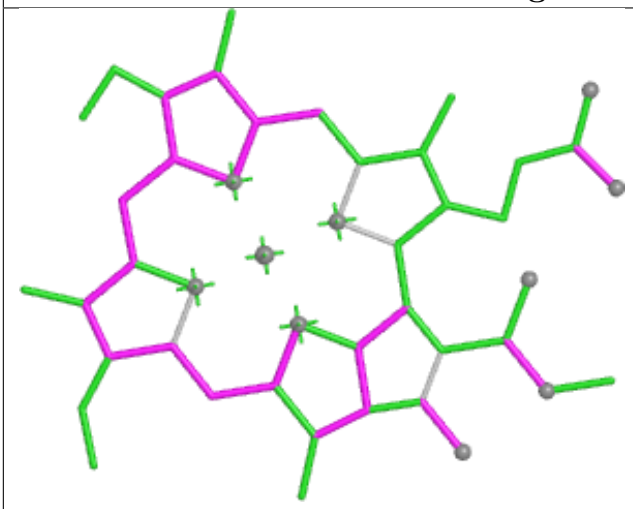


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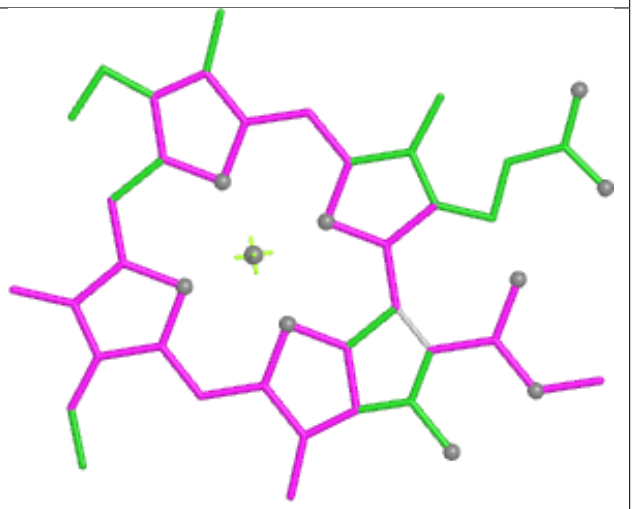


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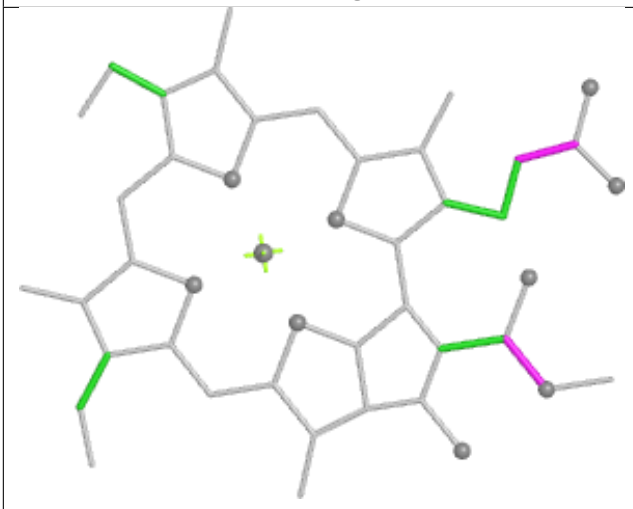
Ligand CLA 1 309



Bond lengths



Bond angles

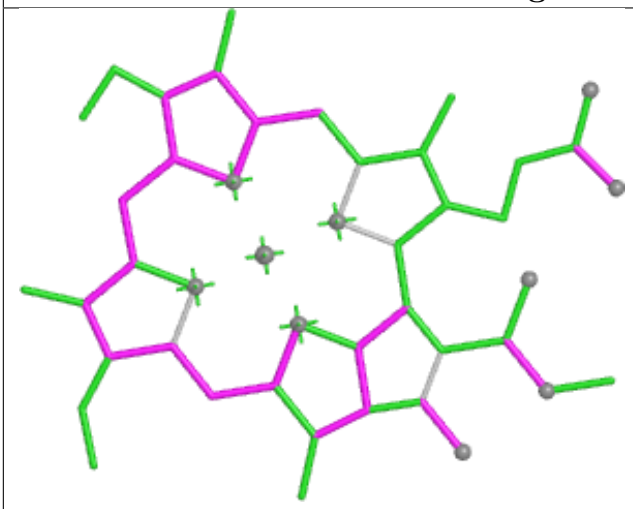


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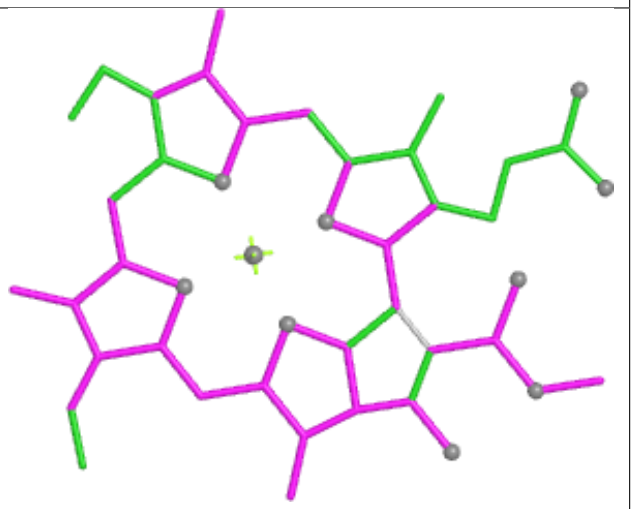


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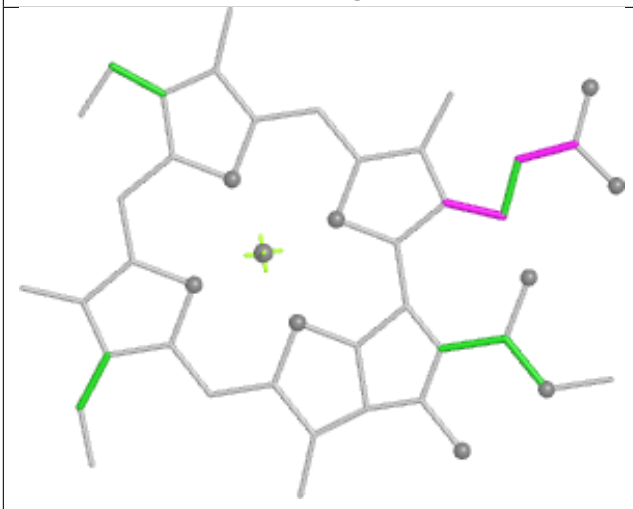
Ligand CLA 3 309



Bond lengths



Bond angles

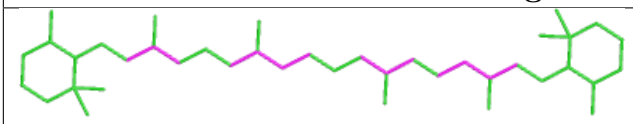


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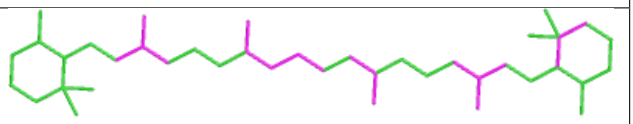


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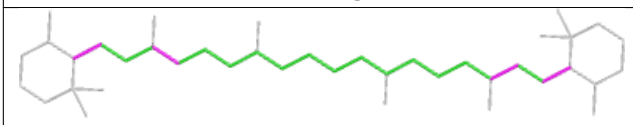
Ligand BCR L 201



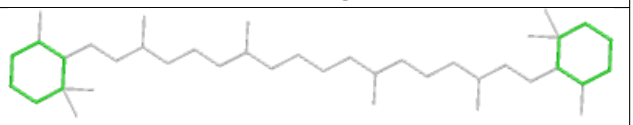
Bond lengths



Bond angles

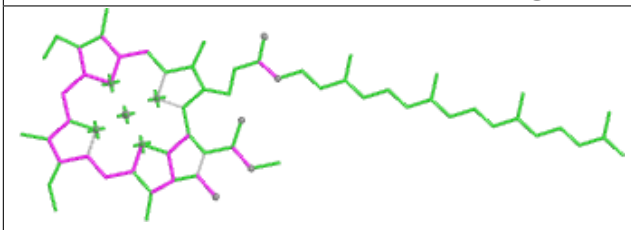


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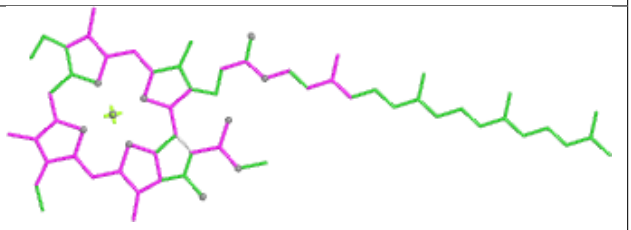


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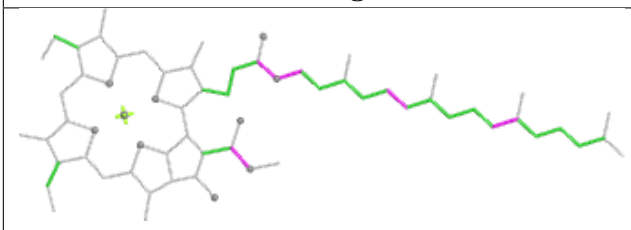
Ligand CLA 5 304



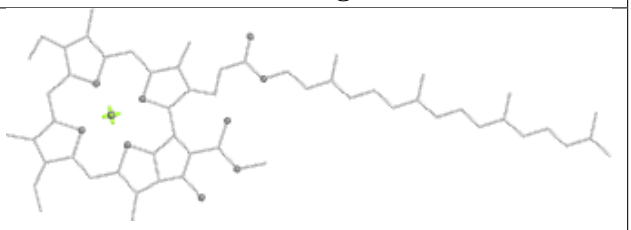
Bond lengths



Bond angles

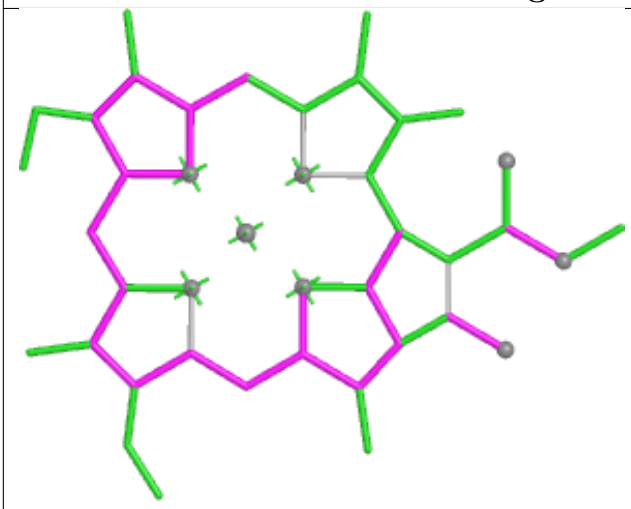


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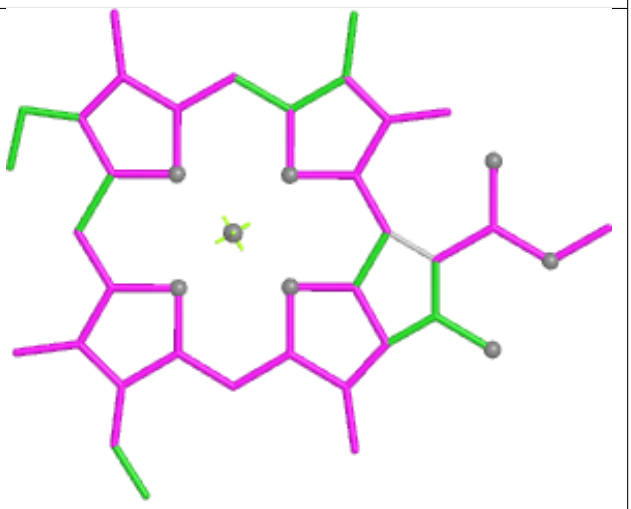


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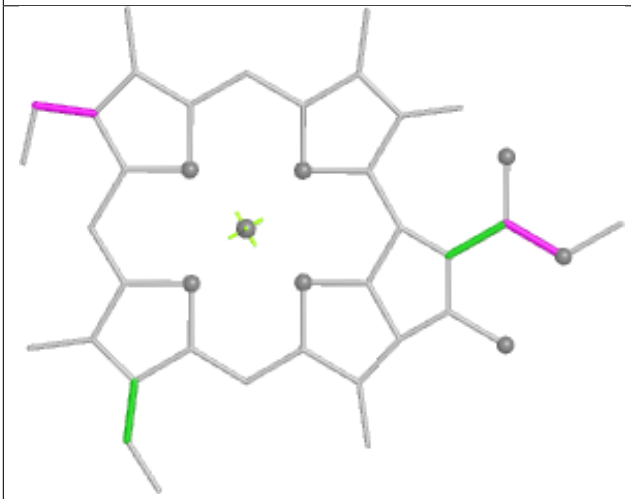
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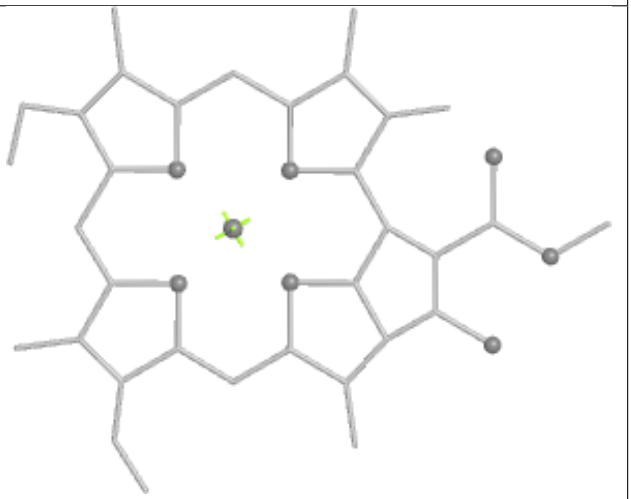
Bond lengths



Bond angles

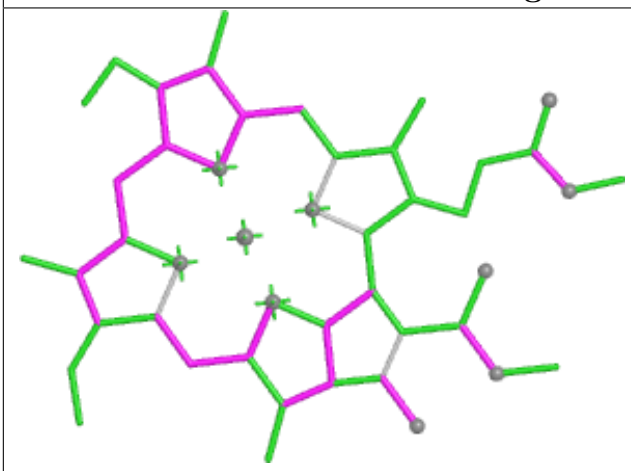


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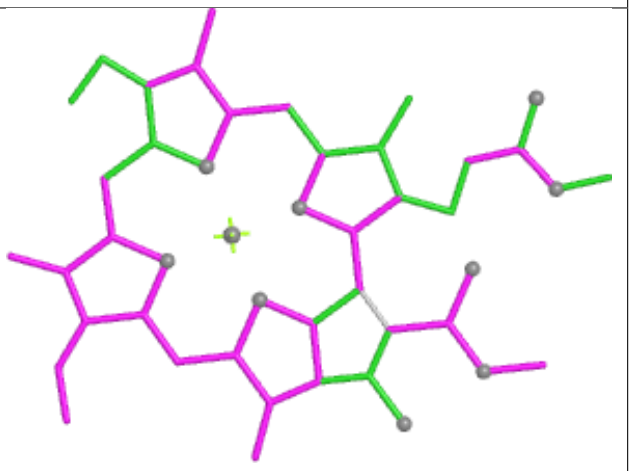


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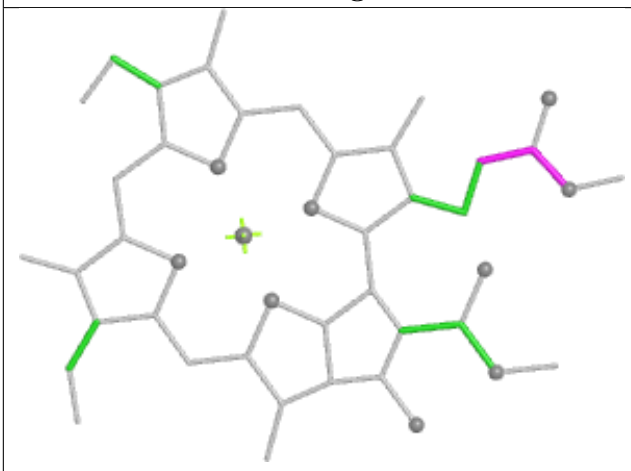
Ligand CLA B 822



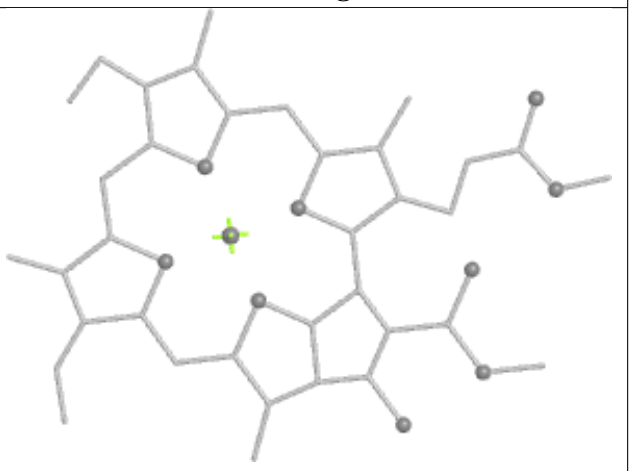
Bond lengths



Bond angles

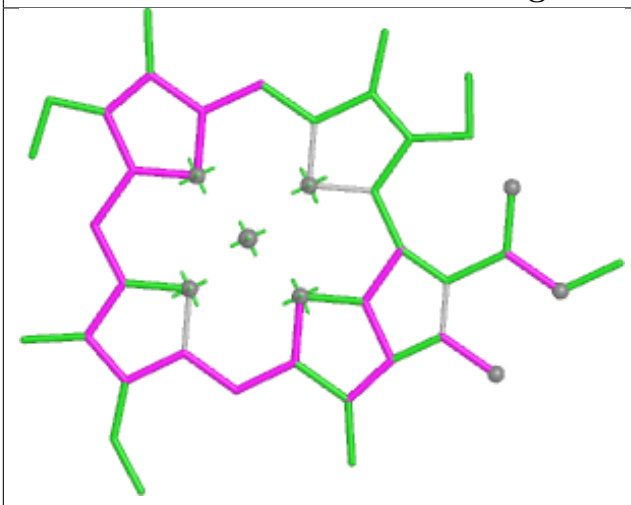


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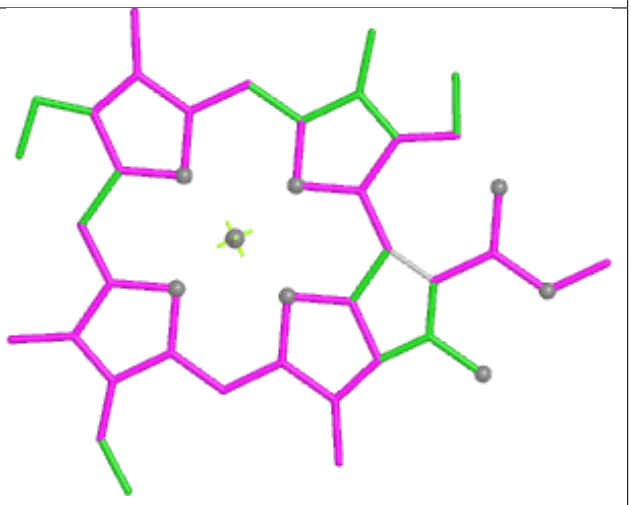


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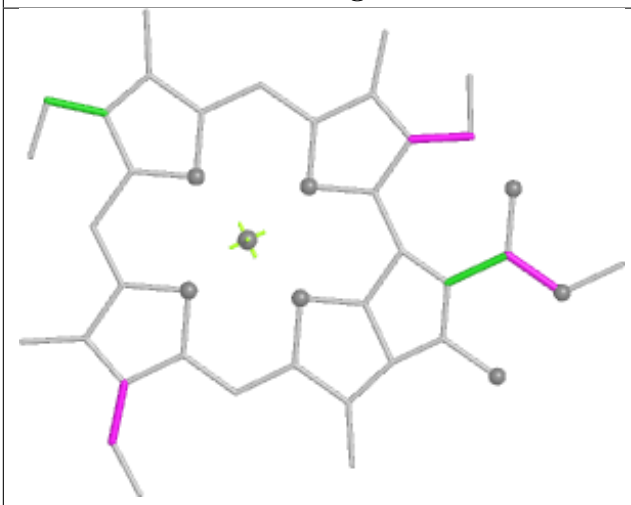
Ligand CLA 2 313



Bond lengths



Bond angles

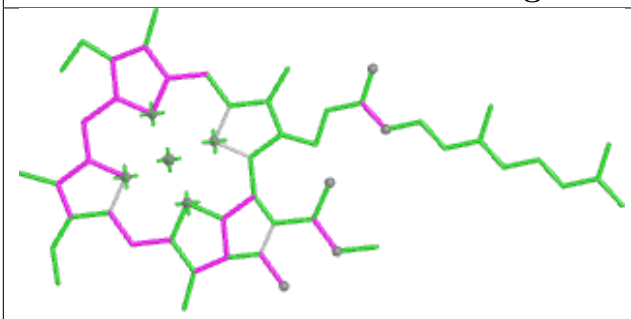


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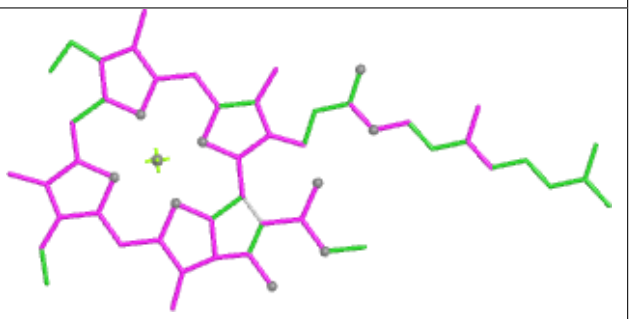


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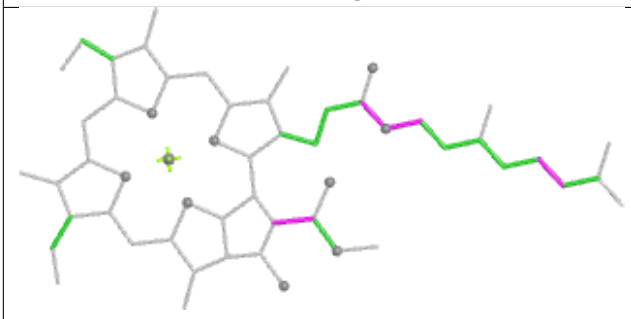
Ligand CLA A 824



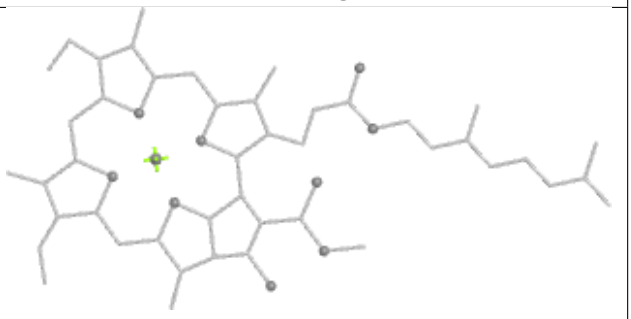
Bond lengths



Bond angles

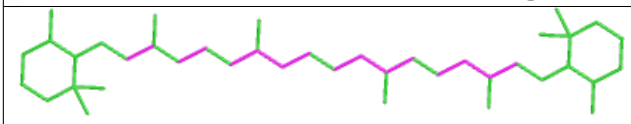


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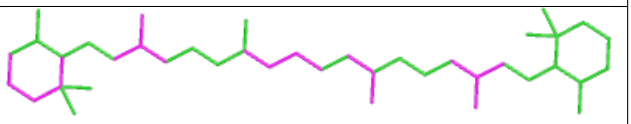


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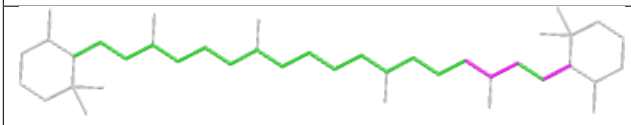
Ligand BCR A 845



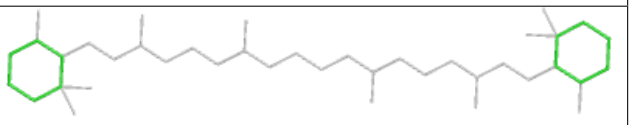
Bond lengths



Bond angles

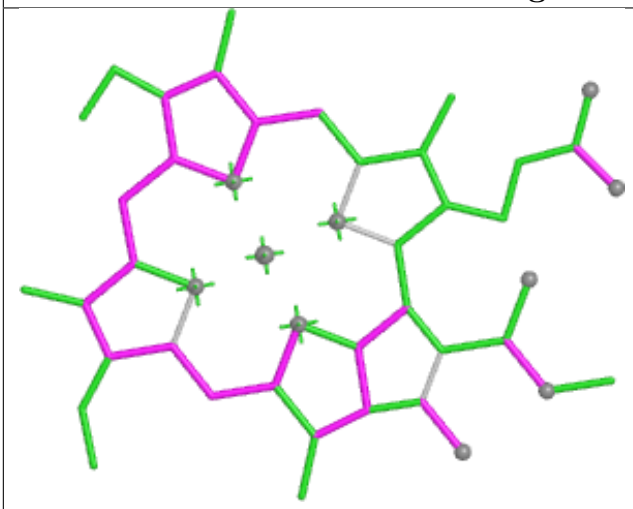


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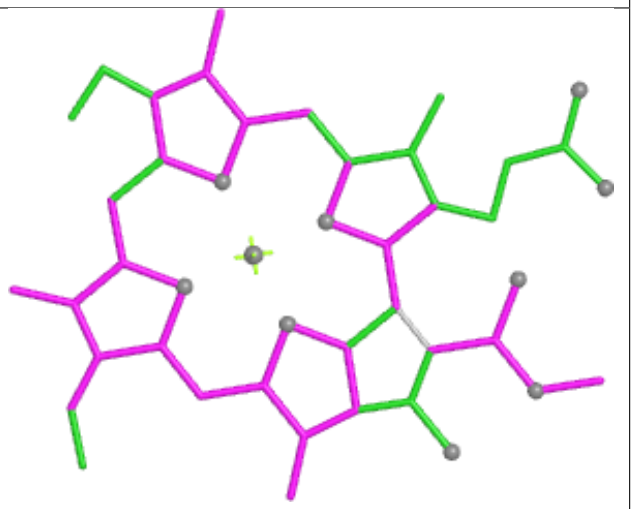


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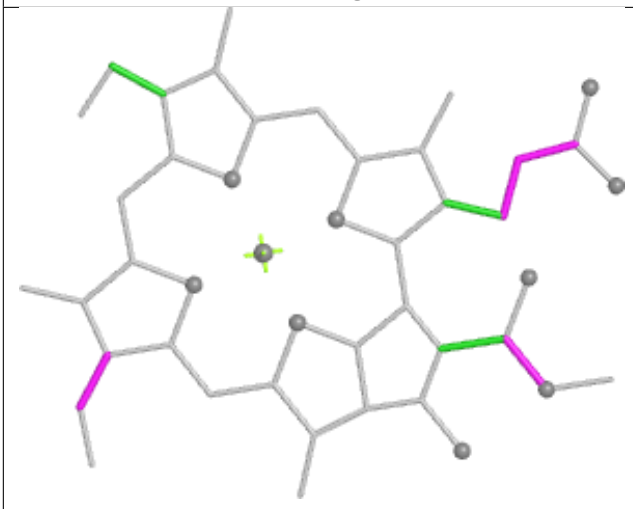
Ligand CLA 1 301



Bond lengths



Bond angles

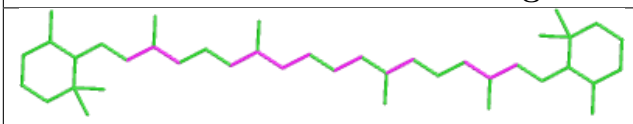


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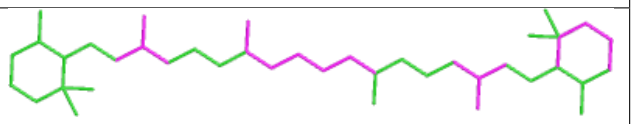


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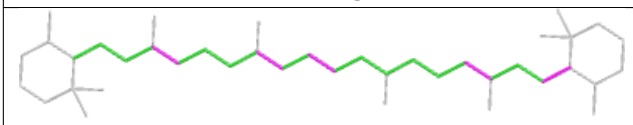
Ligand BCR B 847



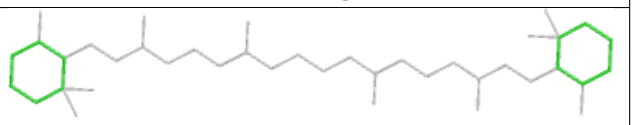
Bond lengths



Bond angles

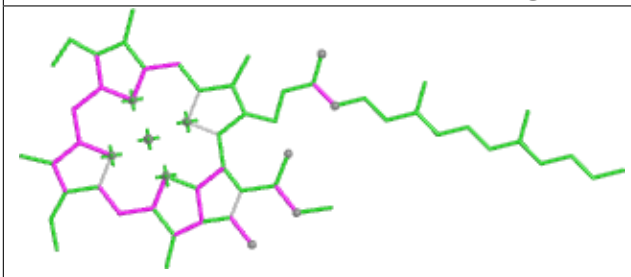


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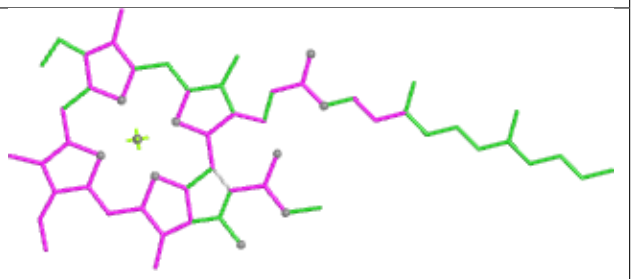


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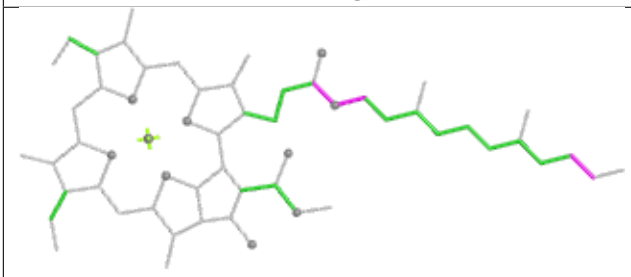
Ligand CLA B 857



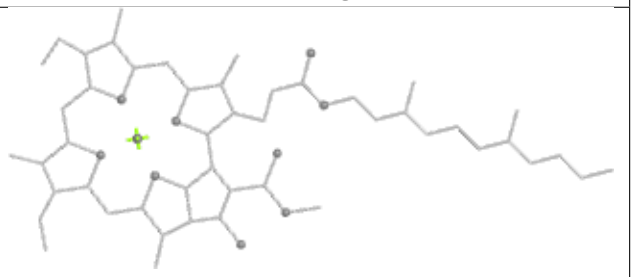
Bond lengths



Bond angles

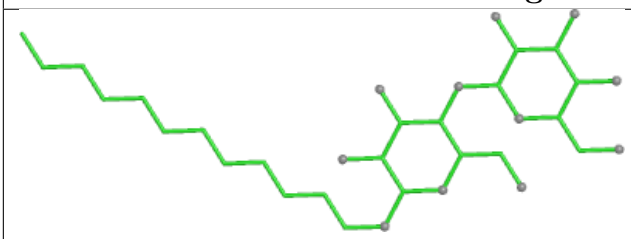


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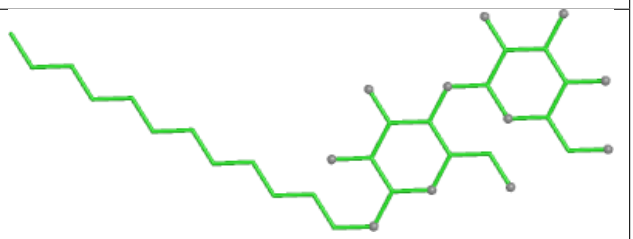


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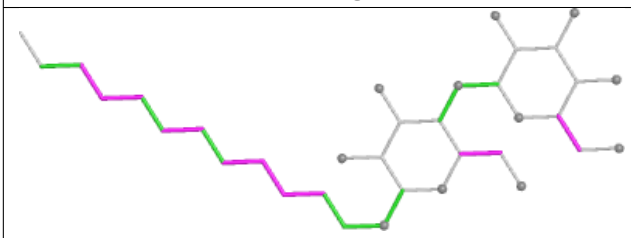
Ligand LMT 3 301



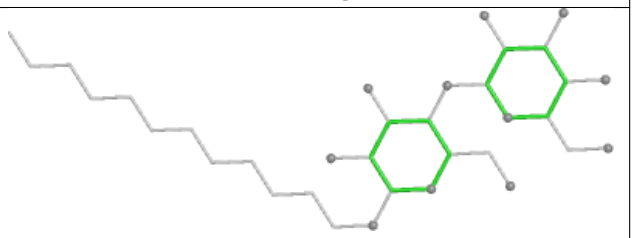
Bond lengths



Bond angles

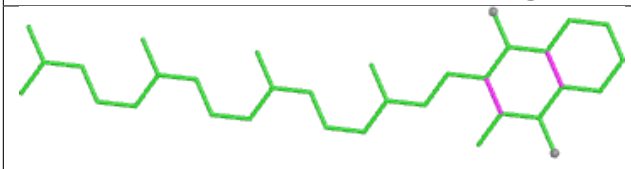


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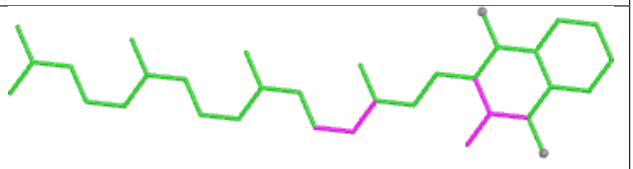


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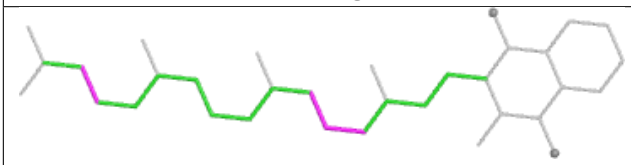
Ligand PQN B 842



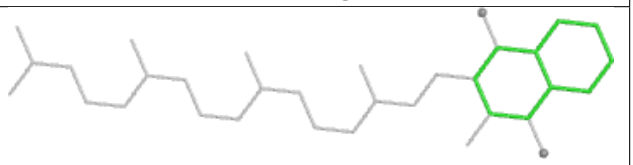
Bond lengths



Bond angles



Torsions

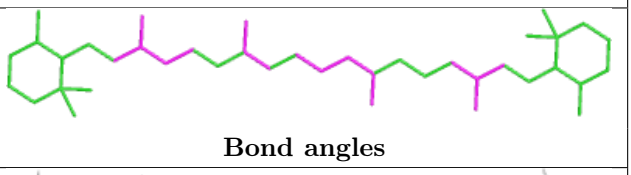


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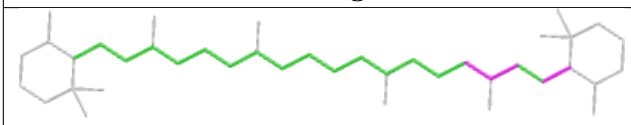
Ligand BCR J 104



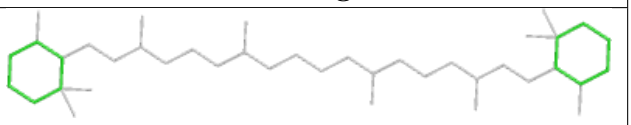
Bond lengths



Bond angles

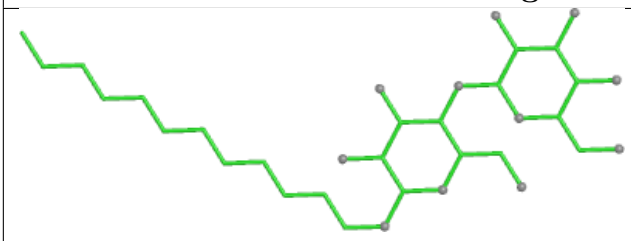


Torsions

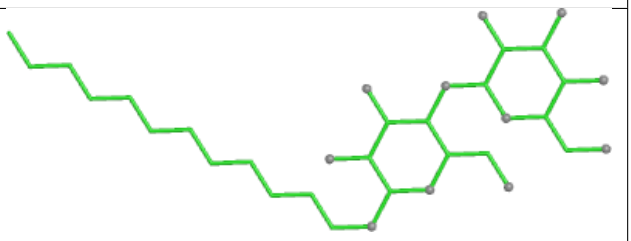


Rings

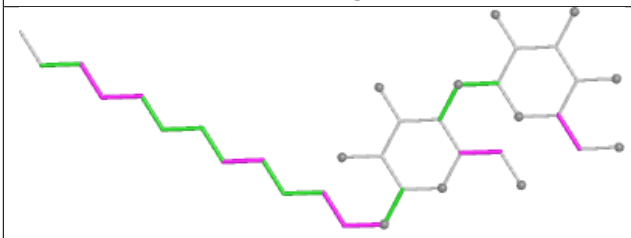
Ligand LMT B 851



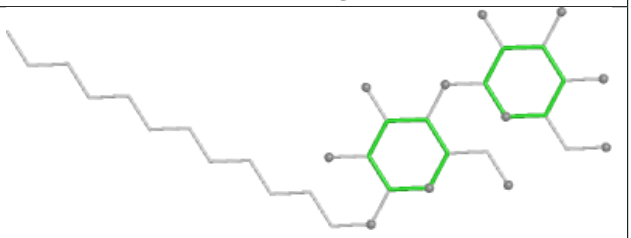
Bond lengths



Bond angles

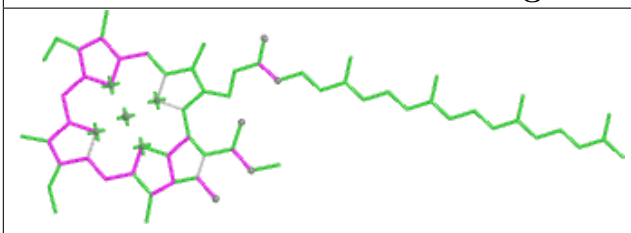


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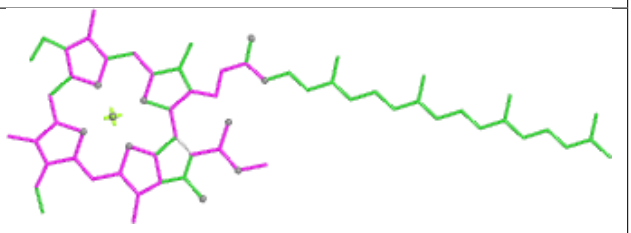


Rings

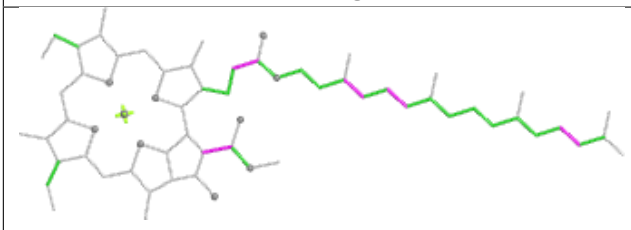
Ligand CLA A 803



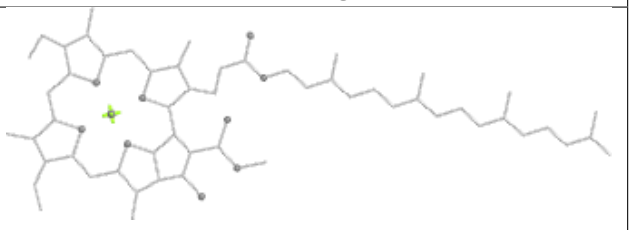
Bond lengths



Bond angles

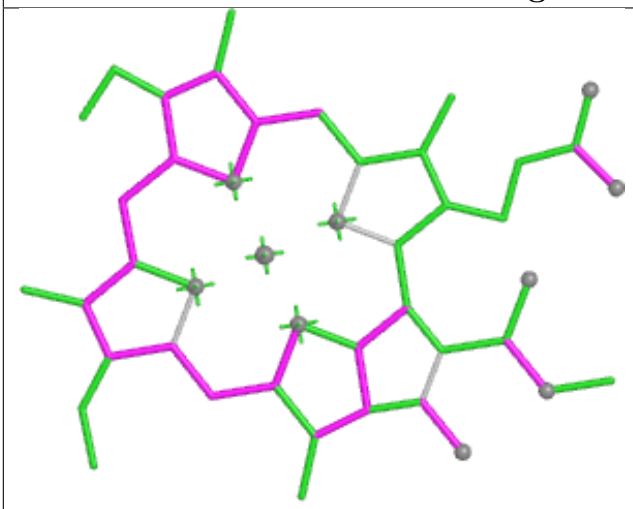


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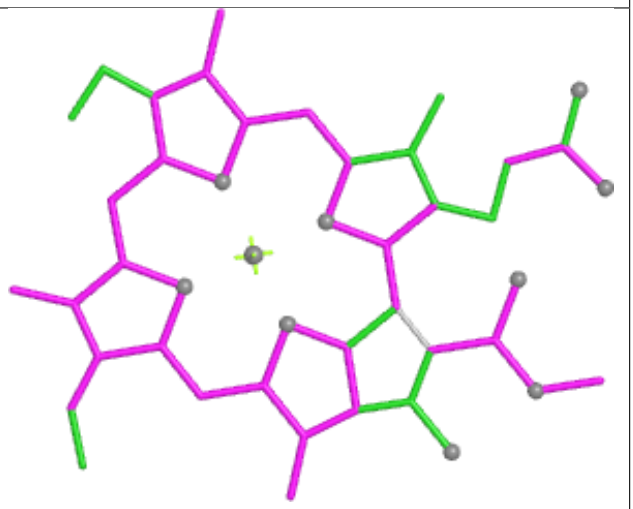


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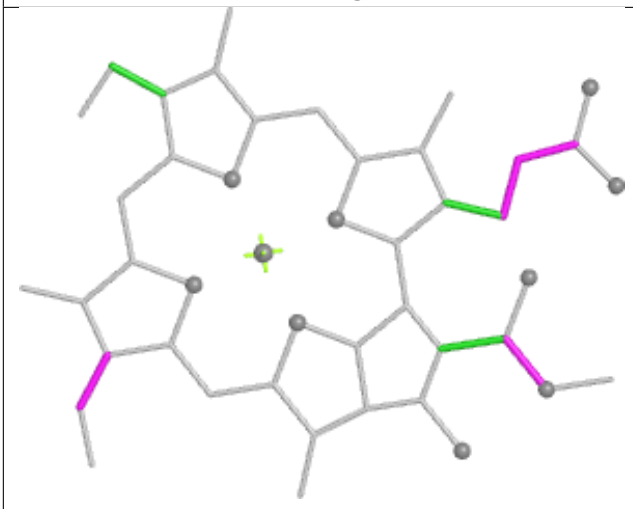
Ligand CLA 5 313



Bond lengths



Bond angles

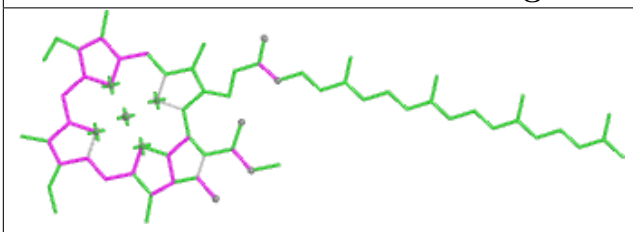


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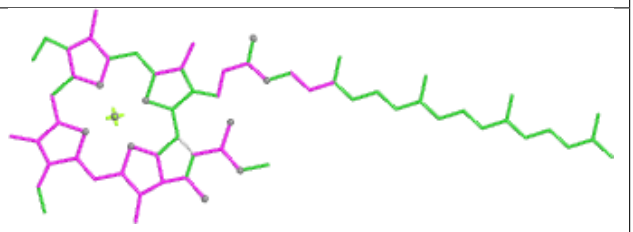


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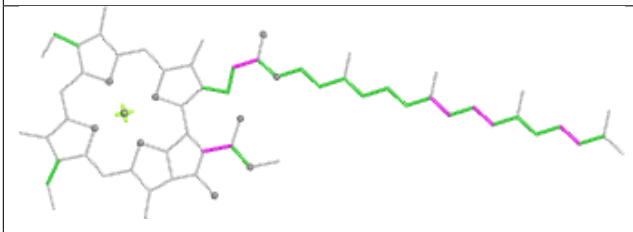
Ligand CLA A 823



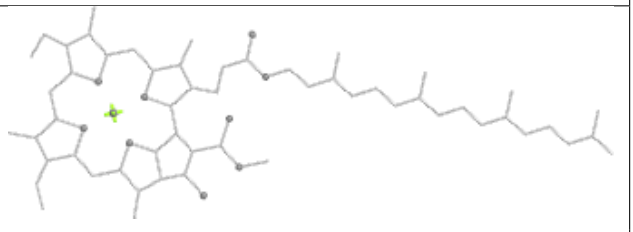
Bond lengths



Bond angles

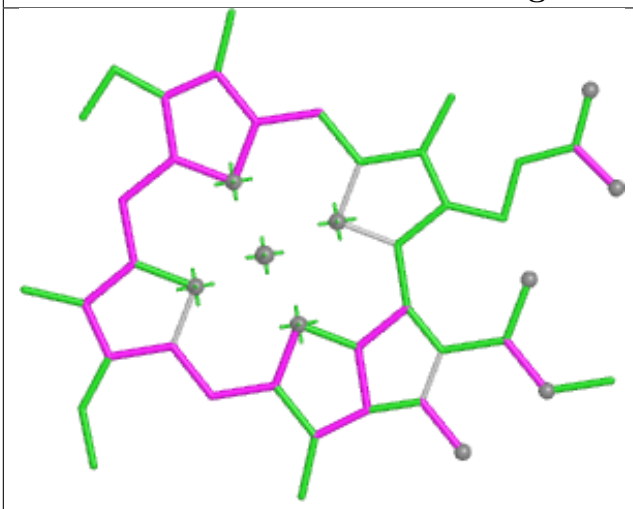


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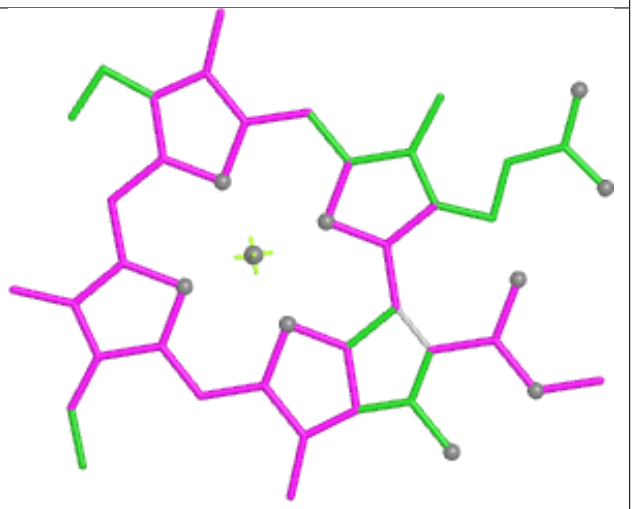


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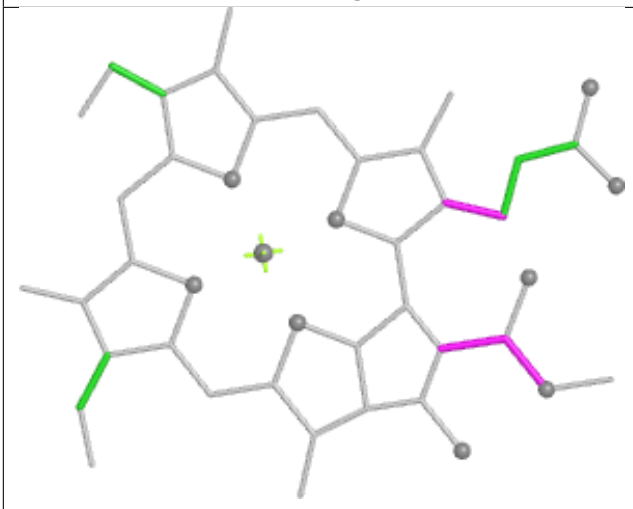
Ligand CLA 2 314



Bond lengths



Bond angles

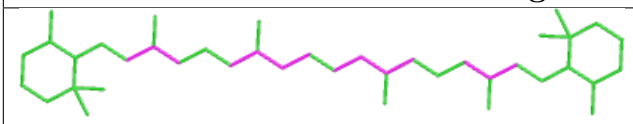


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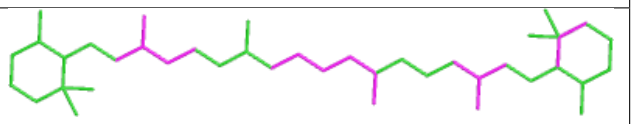


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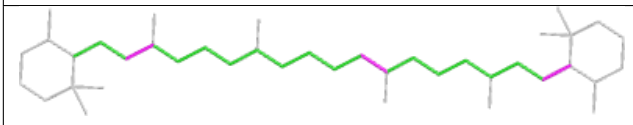
Ligand BCR I 101



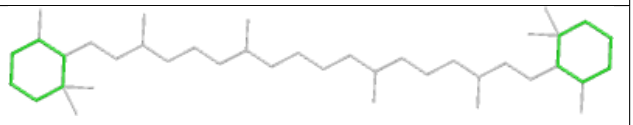
Bond lengths



Bond angles



Torsions

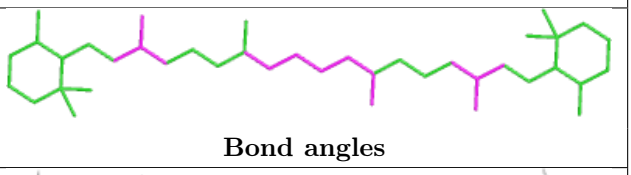


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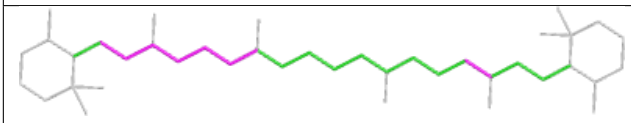
Ligand BCR B 845



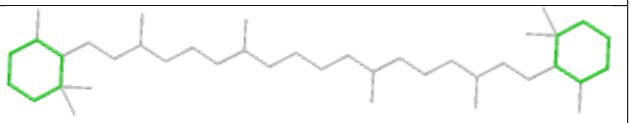
Bond lengths



Bond angles

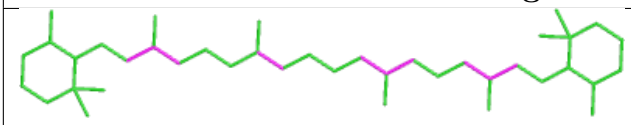


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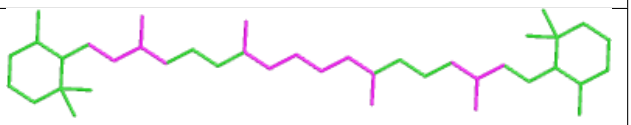


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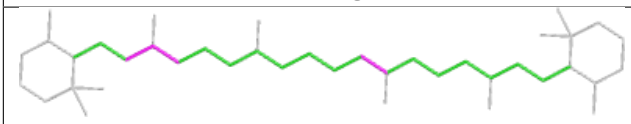
Ligand BCR B 803



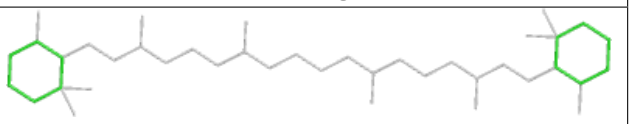
Bond lengths



Bond angles

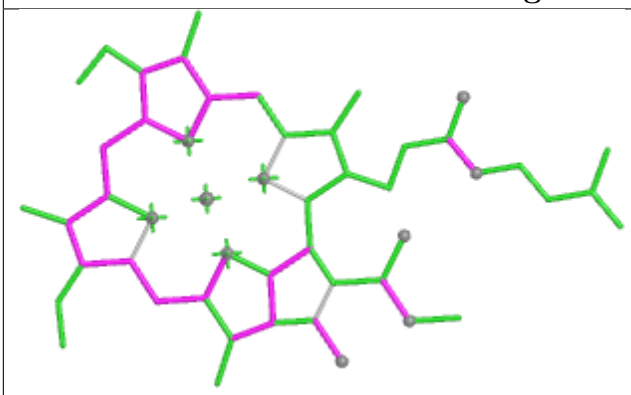


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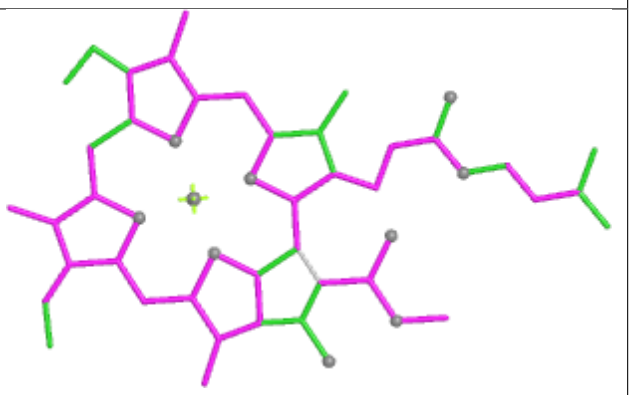


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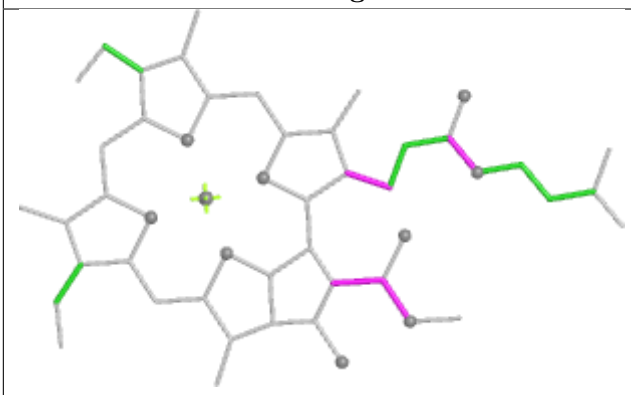
Ligand CLA O 204



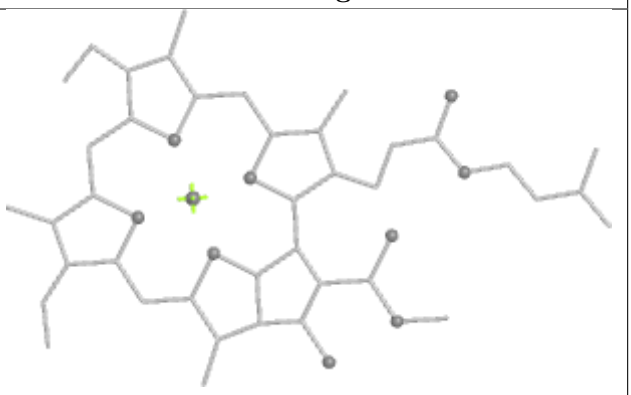
Bond lengths



Bond angles

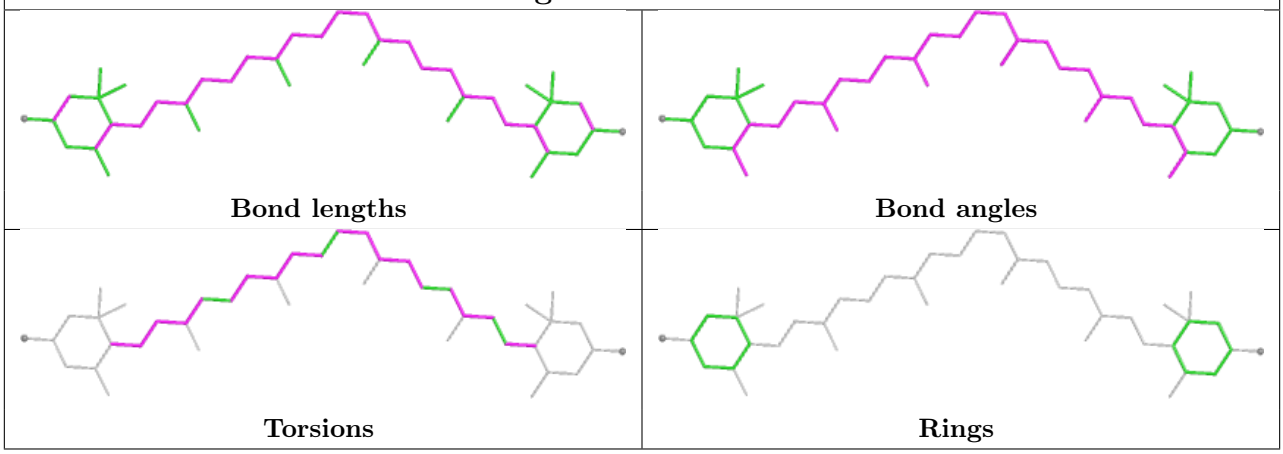


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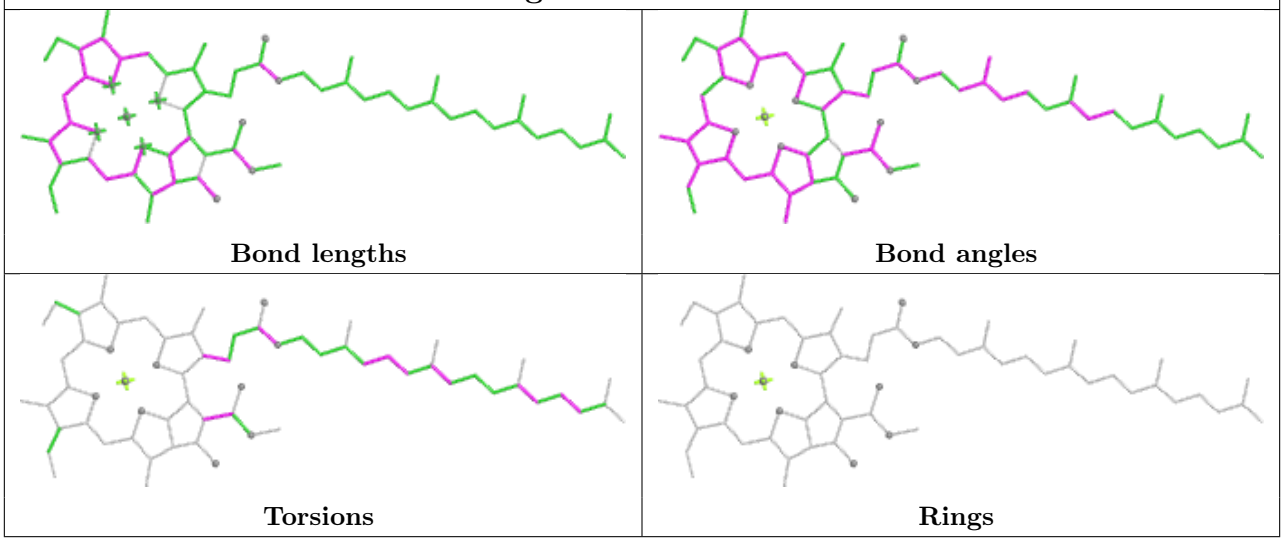


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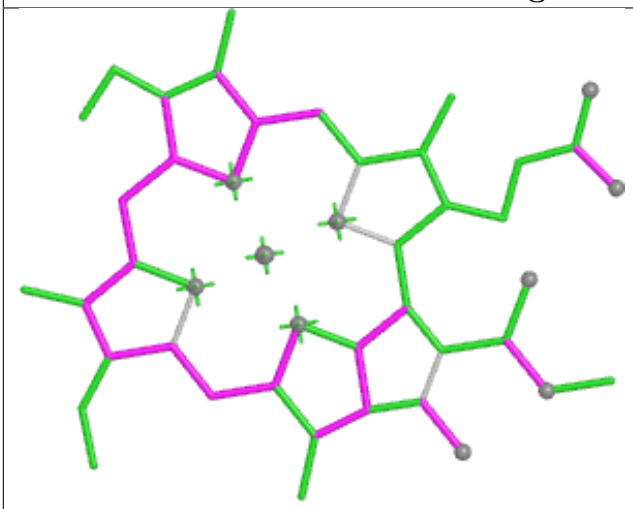
Ligand 5X6 J 105



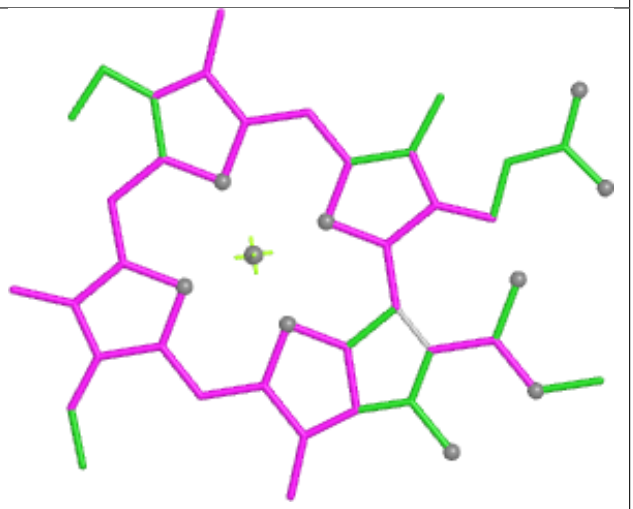
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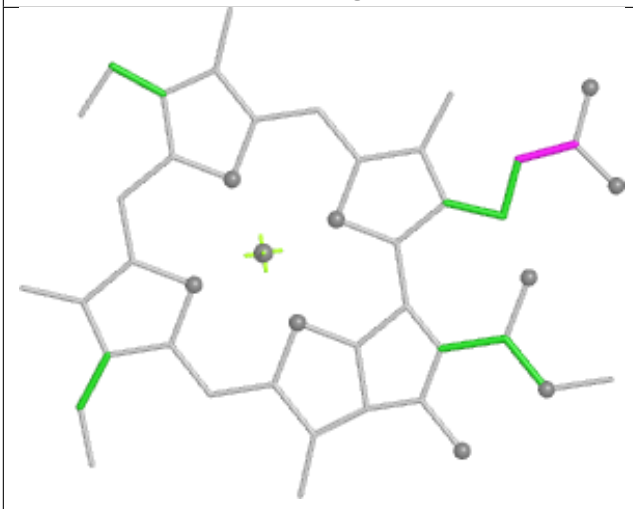
Ligand CLA 2 310



Bond lengths



Bond angles

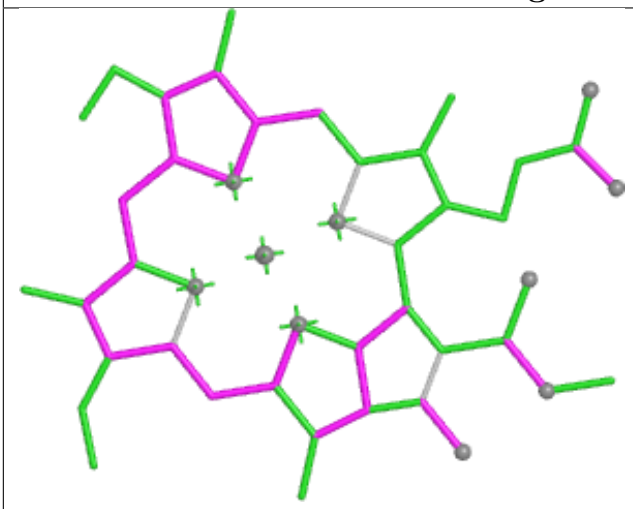


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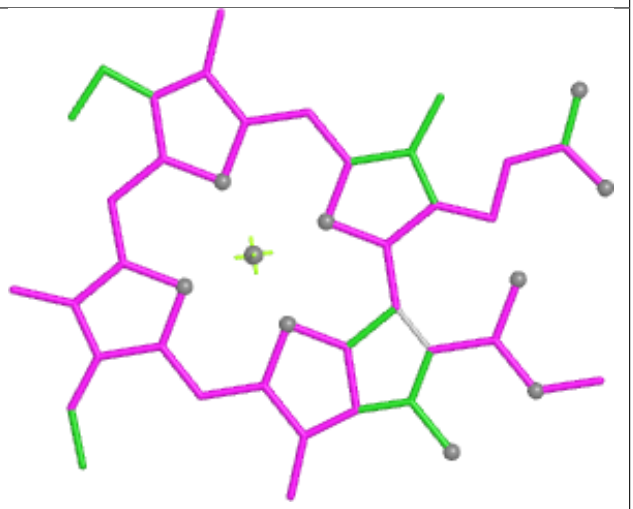


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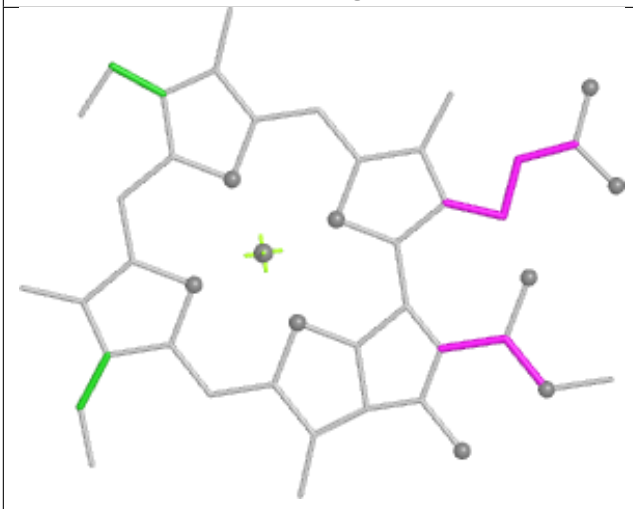
Ligand CLA 4 307



Bond lengths



Bond angles

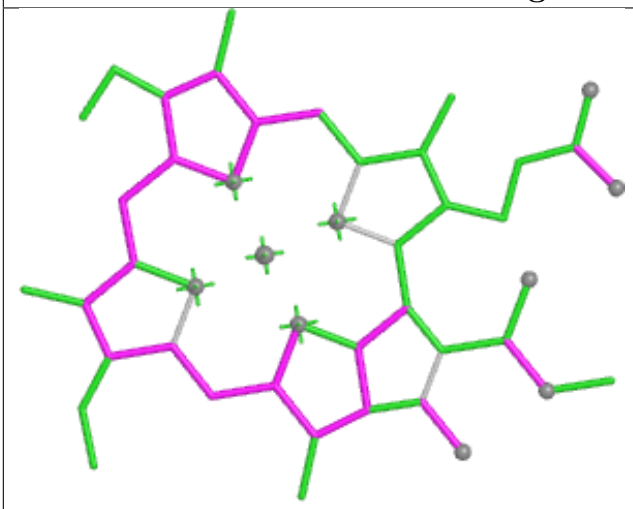


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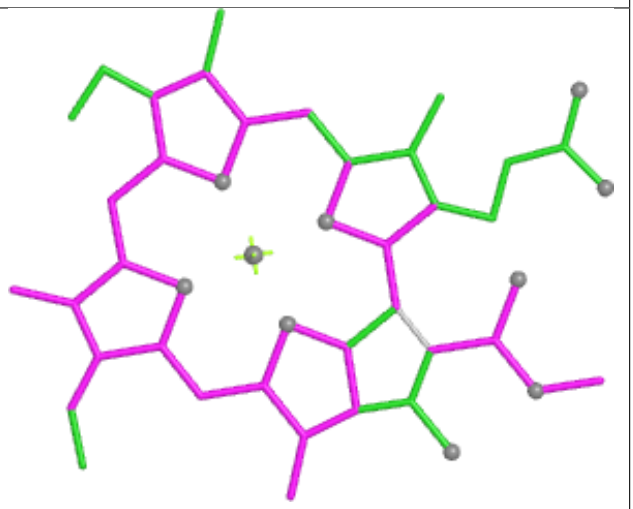


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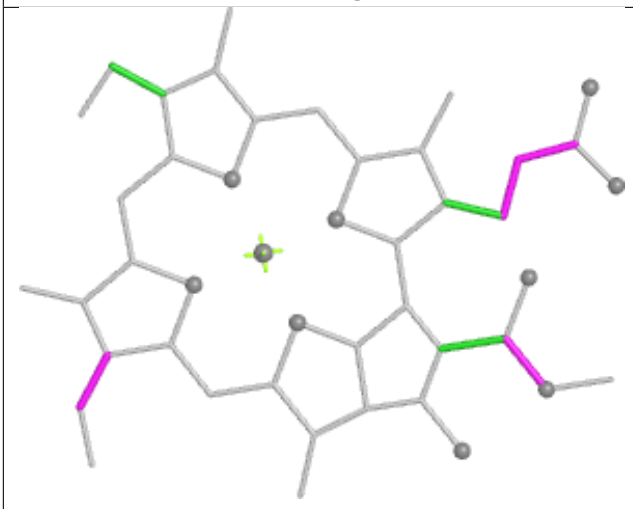
Ligand CLA 1 305



Bond lengths



Bond angles

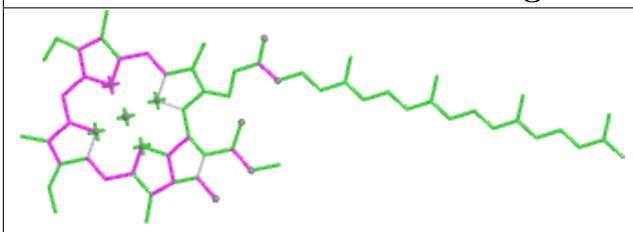


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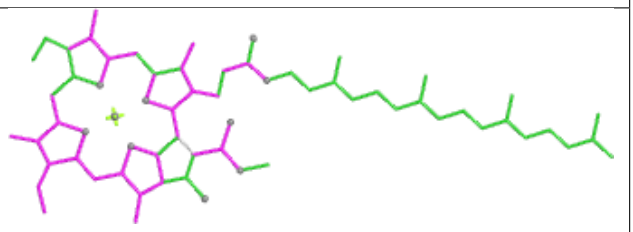


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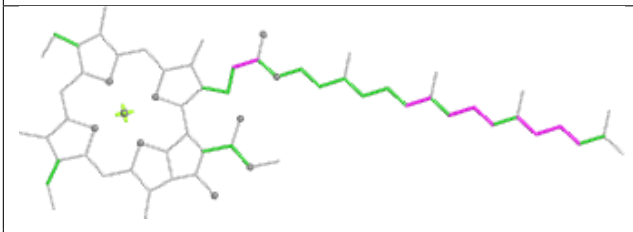
Ligand CLA A 826



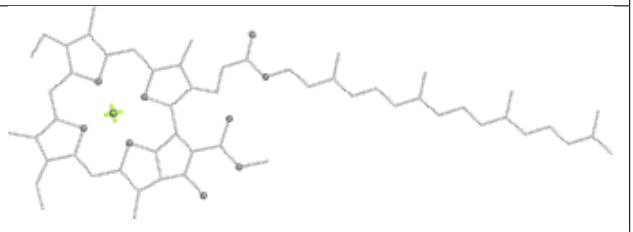
Bond lengths



Bond angles

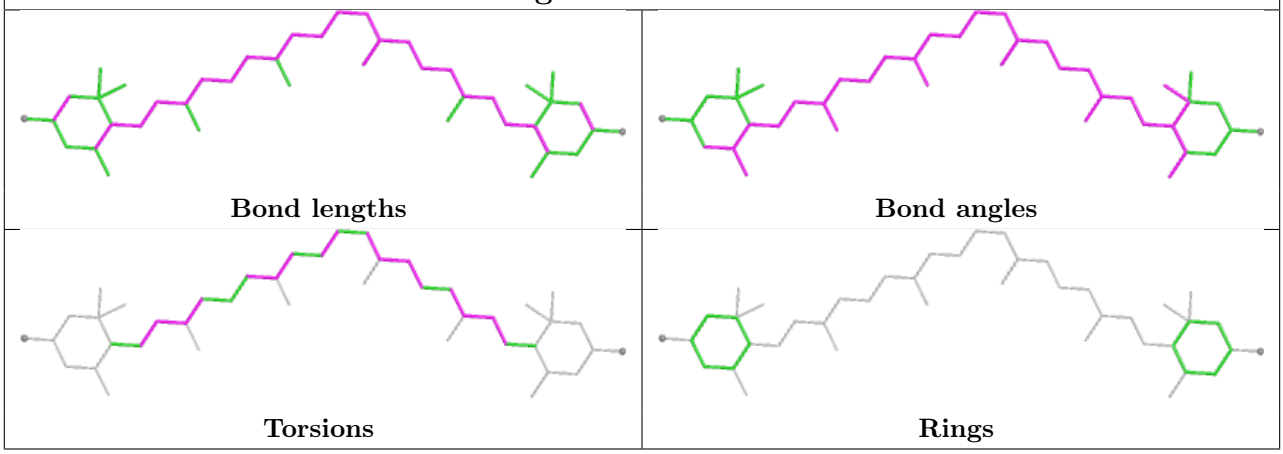


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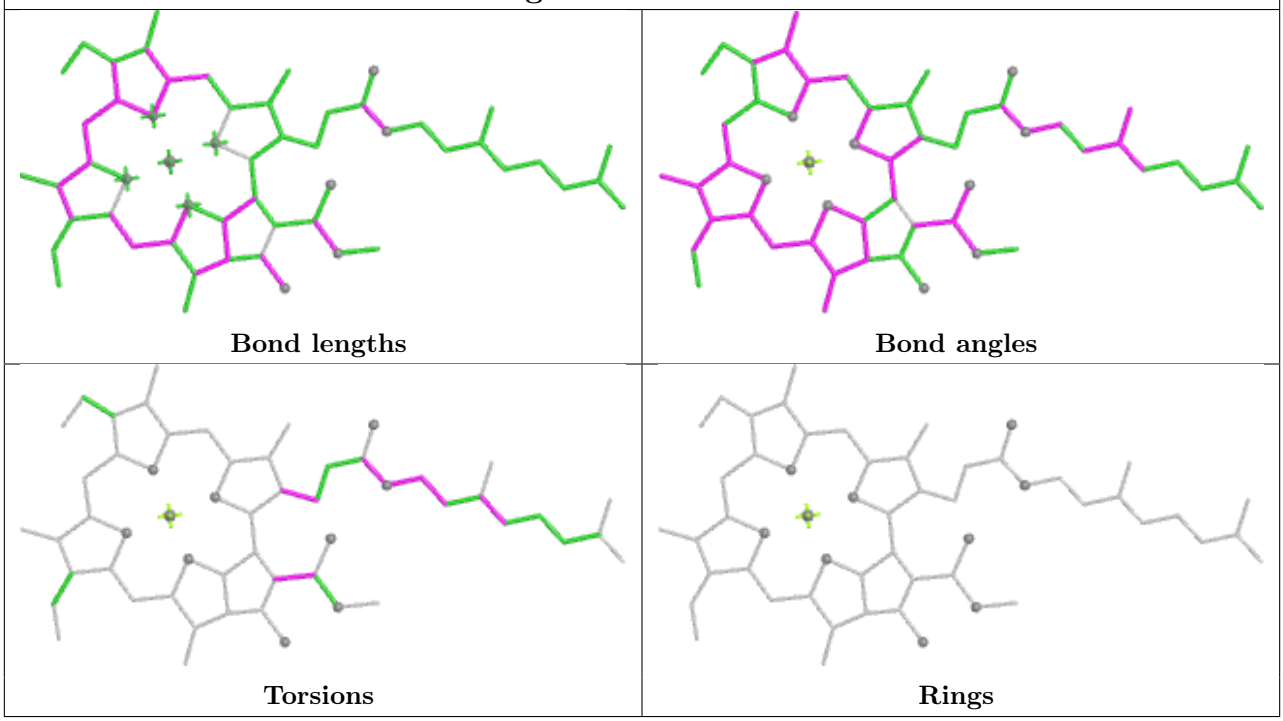


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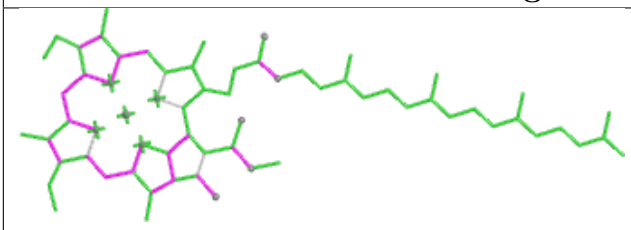
Ligand 5X6 1 312



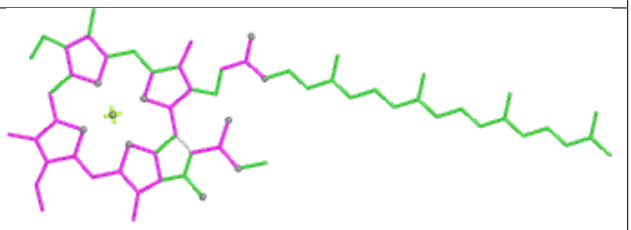
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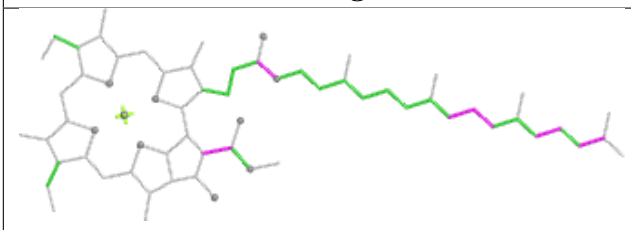
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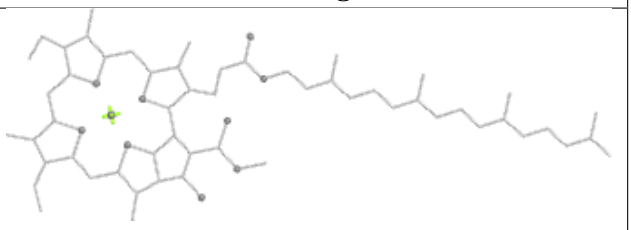
Bond lengths



Bond angles

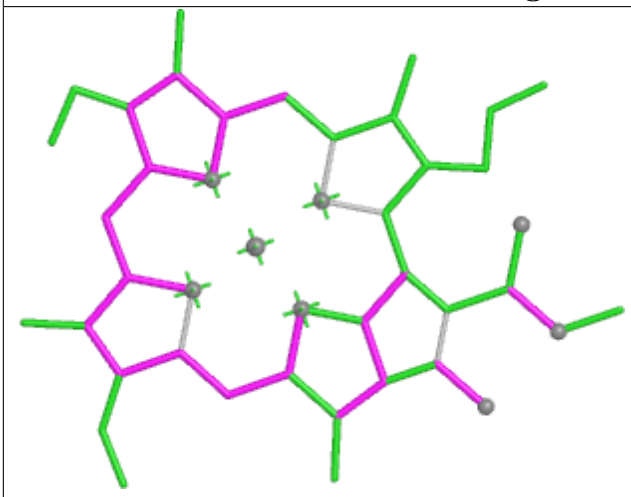


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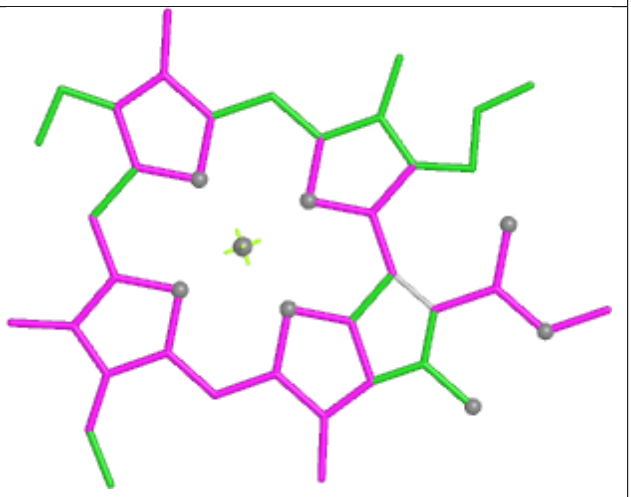


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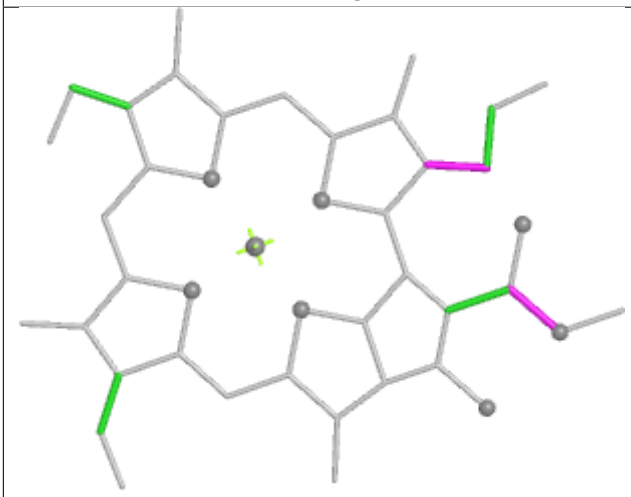
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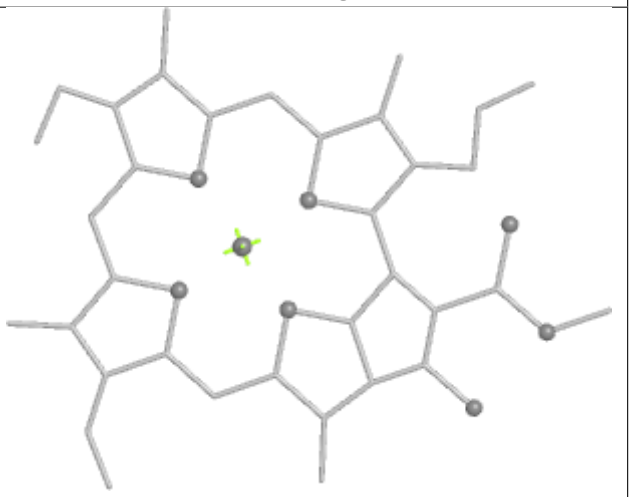
Bond lengths



Bond angles

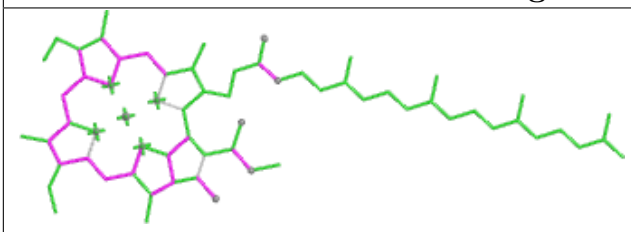


Torsions

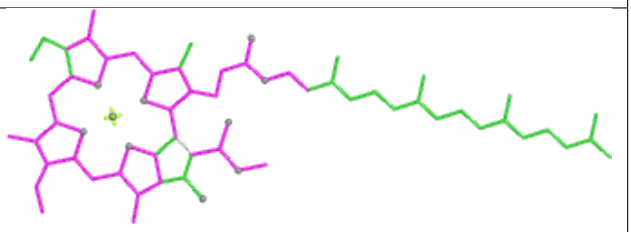


Rings

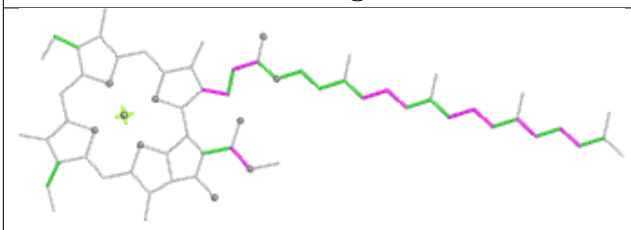
Ligand CLA 5 305



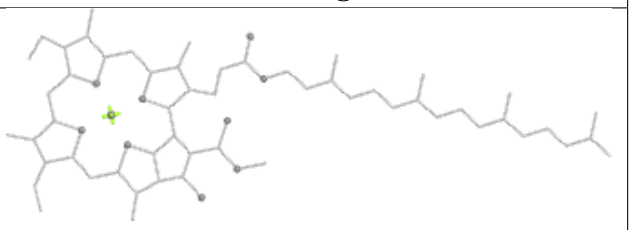
Bond lengths



Bond angles

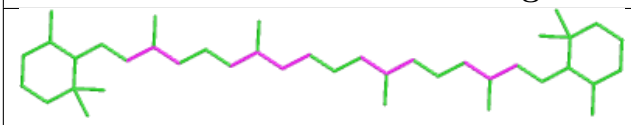


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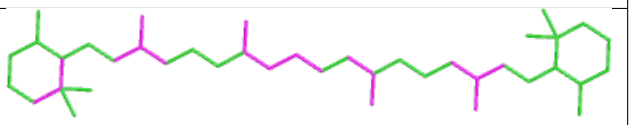


Rings

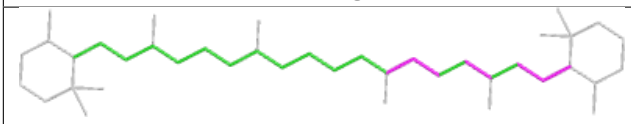
Ligand BCR A 844



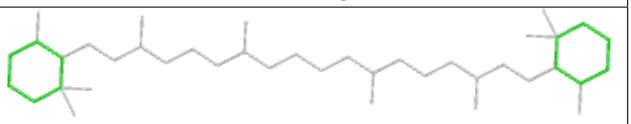
Bond lengths



Bond angles

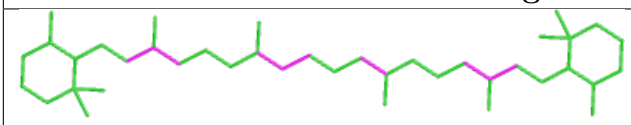


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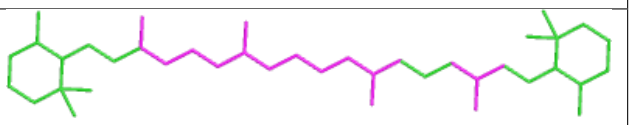


Rings

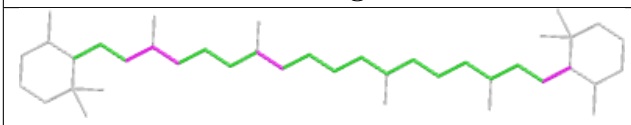
Ligand BCR B 846



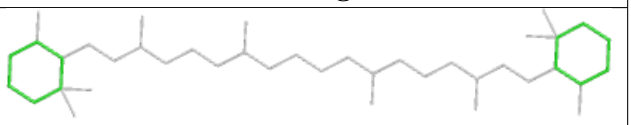
Bond lengths



Bond angles

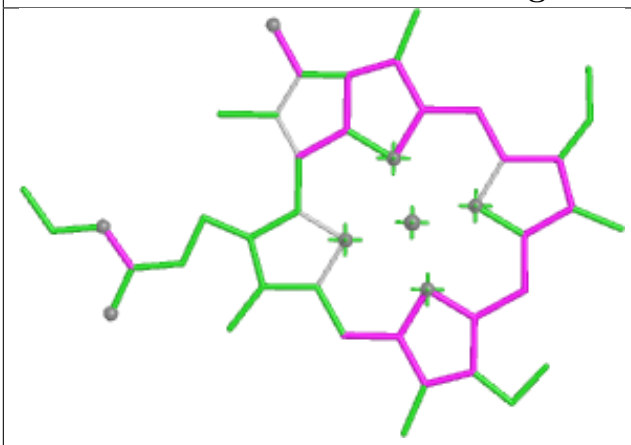


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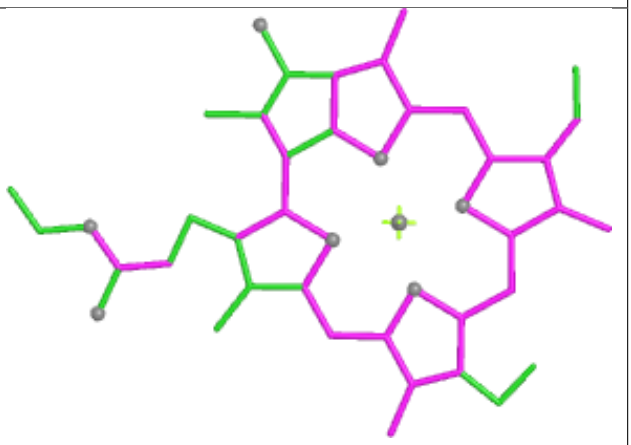


Rings

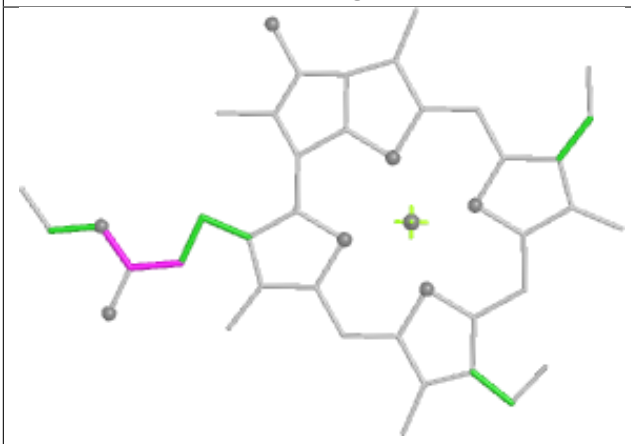
Ligand CLA 5 314



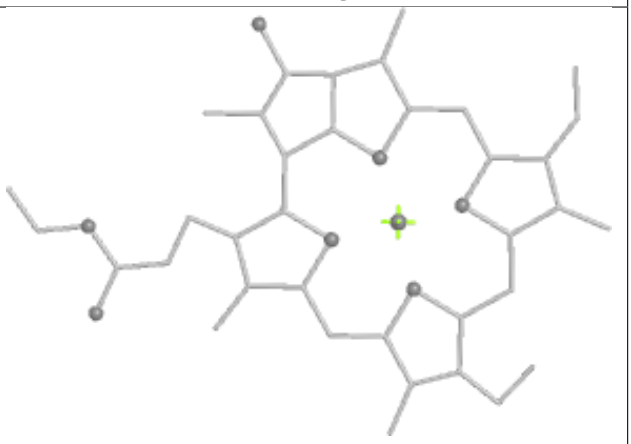
Bond lengths



Bond angles

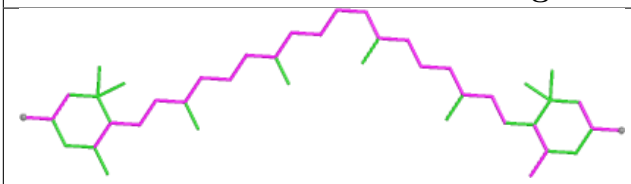


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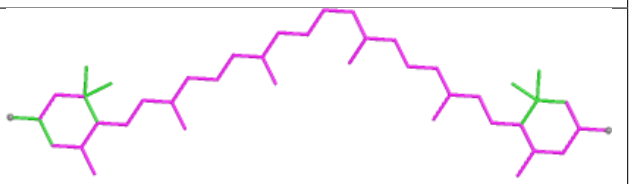


Rings

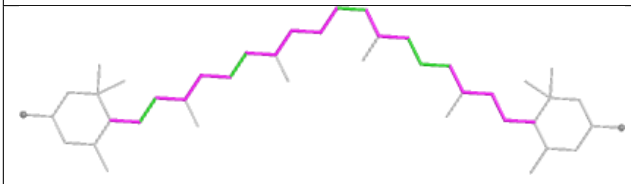
Ligand 5X6 F 205



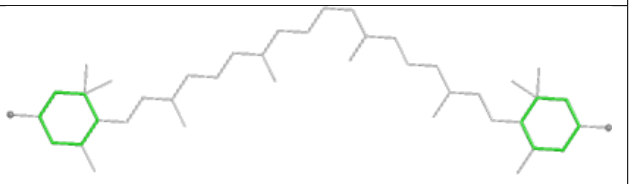
Bond lengths



Bond angles

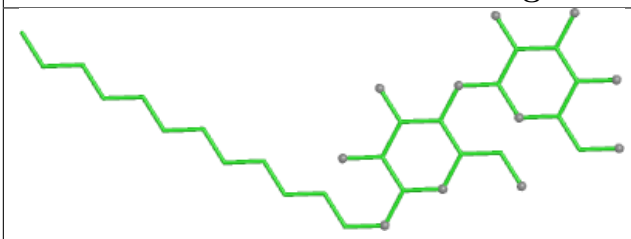


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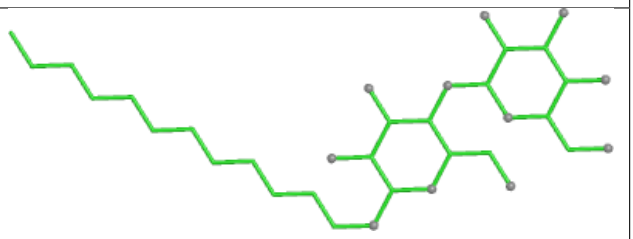


Rings

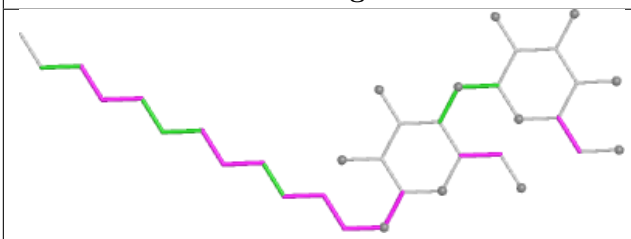
Ligand LMT F 201



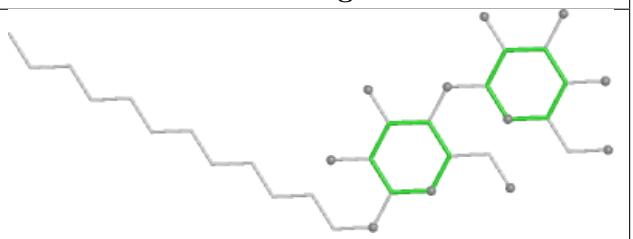
Bond lengths



Bond angles

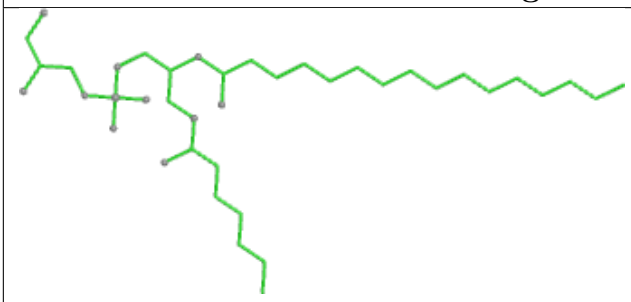


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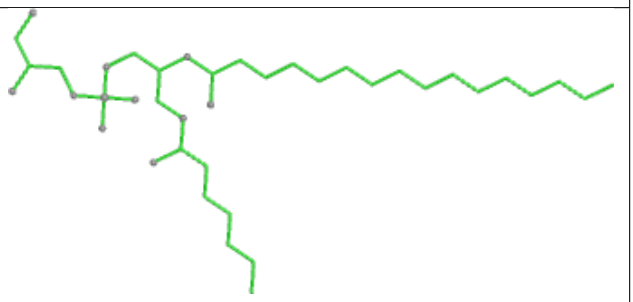


Rings

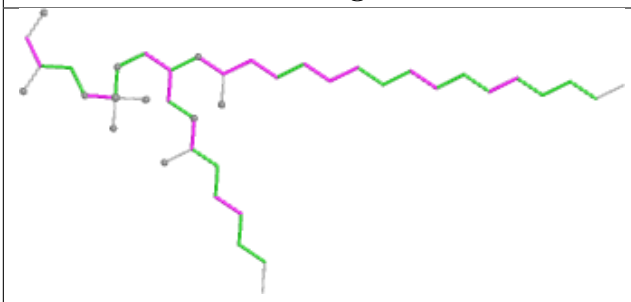
Ligand LHG A 842



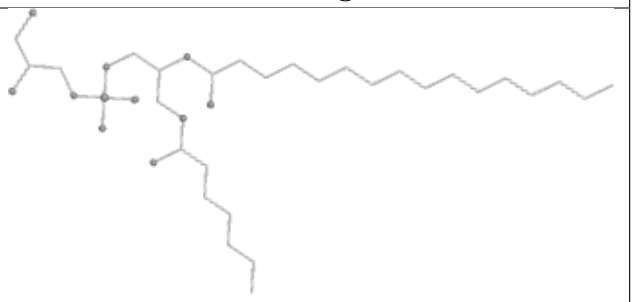
Bond lengths



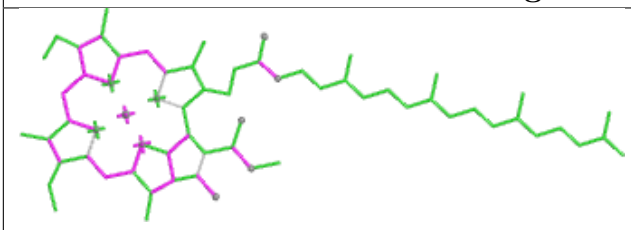
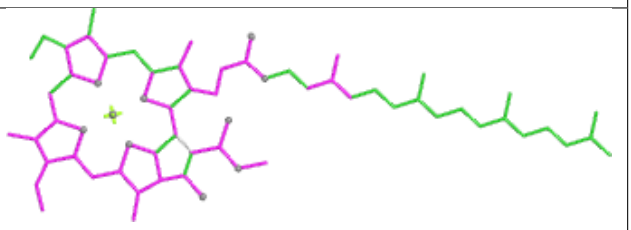
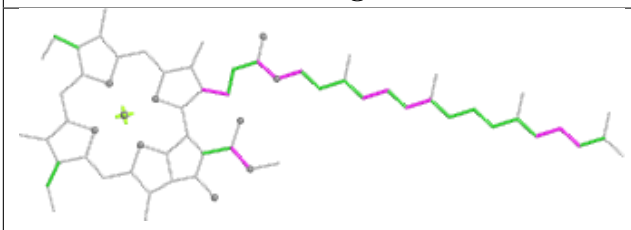
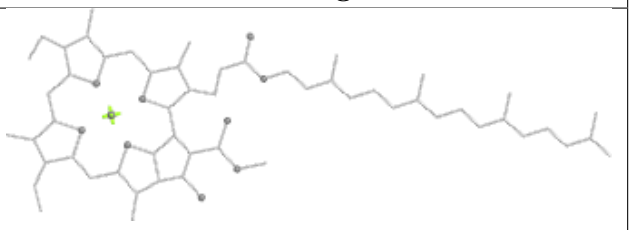
Bond angles

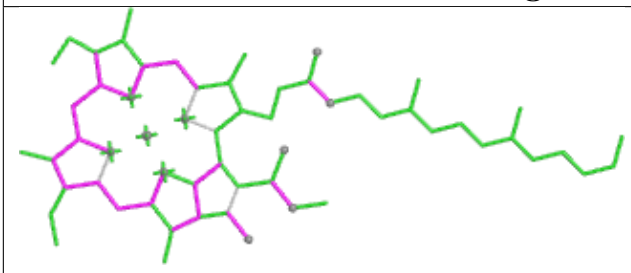
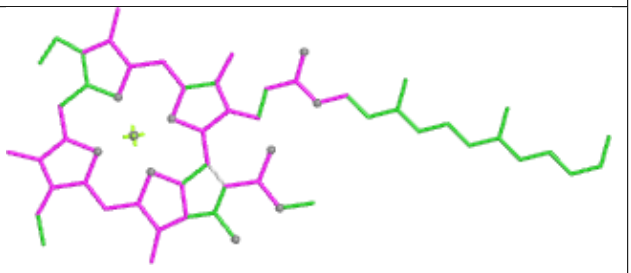
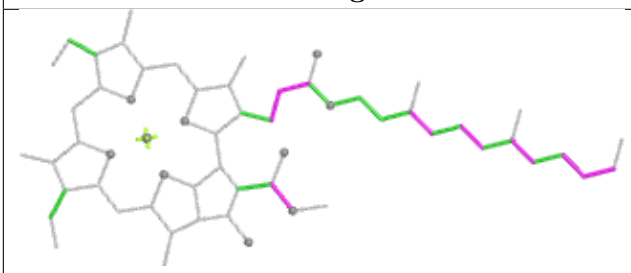
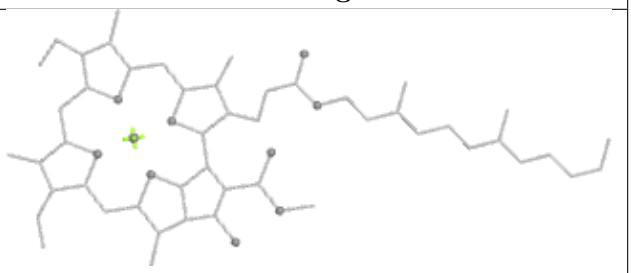


Torsions

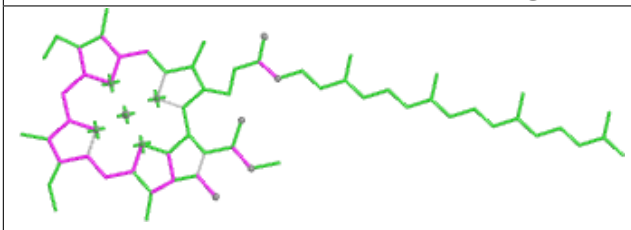


Rings

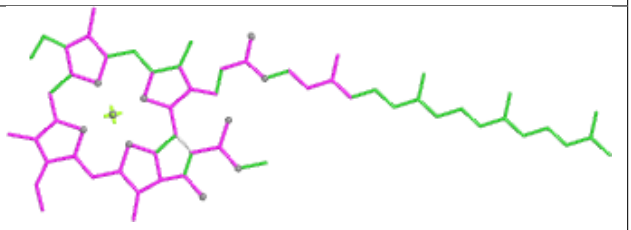
Ligand CLA B 828	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 818	
 Bond lengths	 Bond angles
 Torsions	 Rings

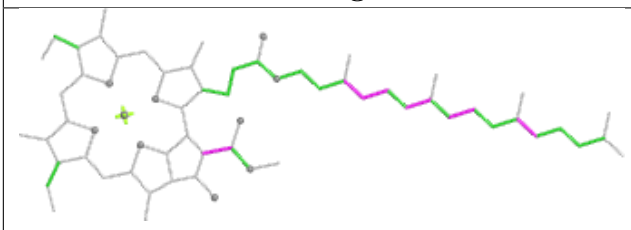
Ligand CLA B 809



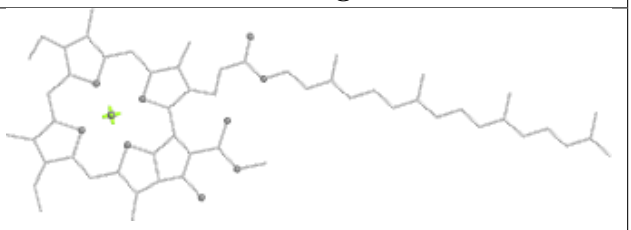
Bond lengths



Bond angles

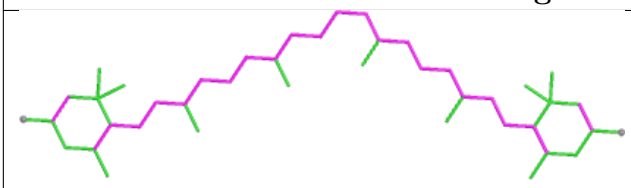


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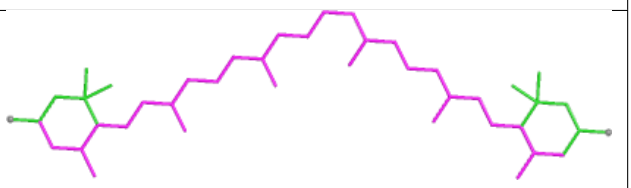


Rings

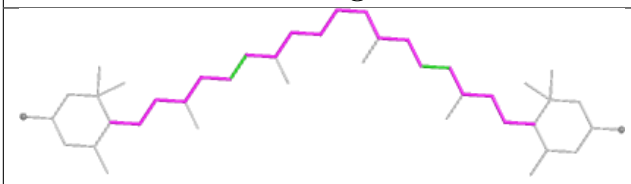
Ligand 5X6 1 315



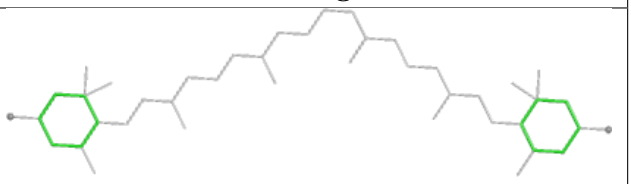
Bond lengths



Bond angles

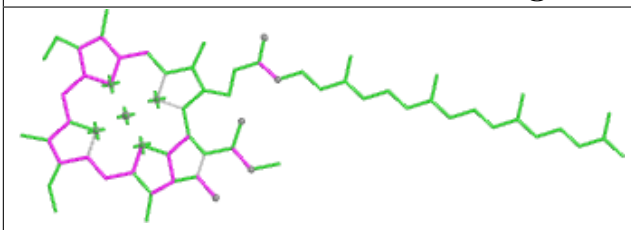


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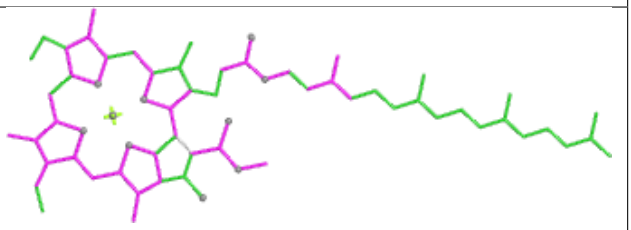


Rings

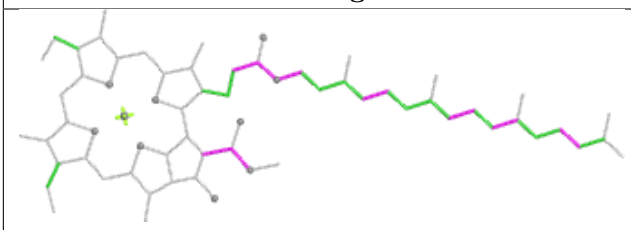
Ligand CLA 5 303



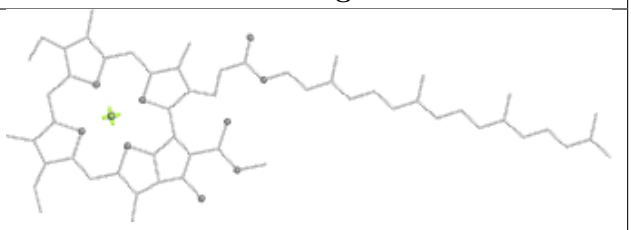
Bond lengths



Bond angles

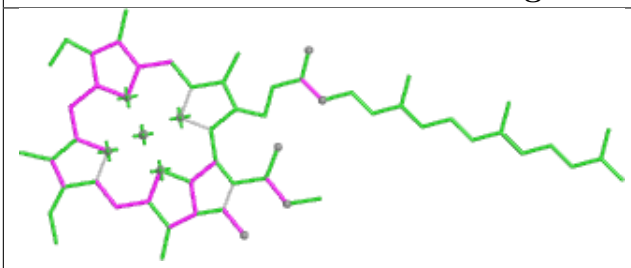


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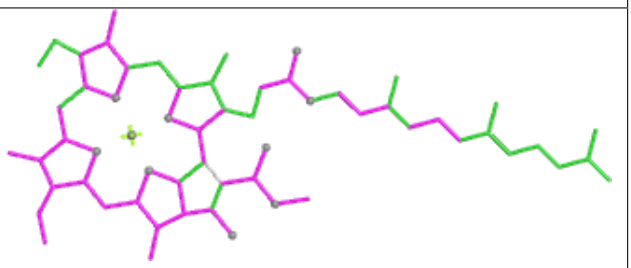


Rings

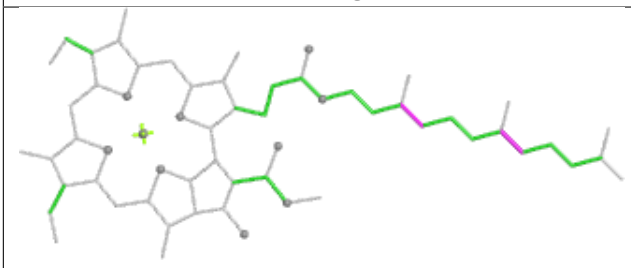
Ligand CLA B 819



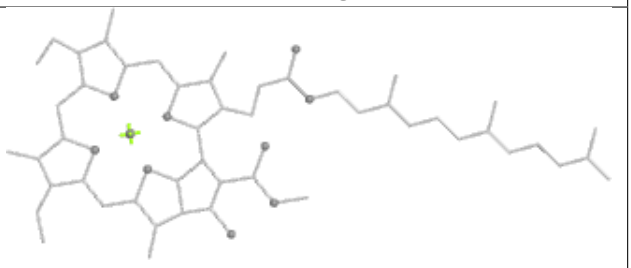
Bond lengths



Bond angles

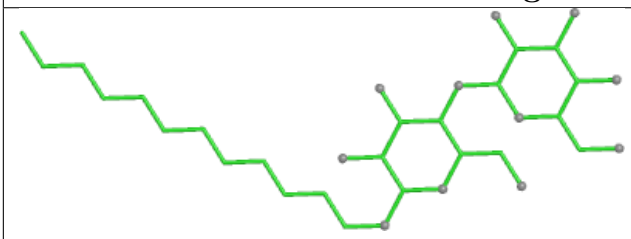


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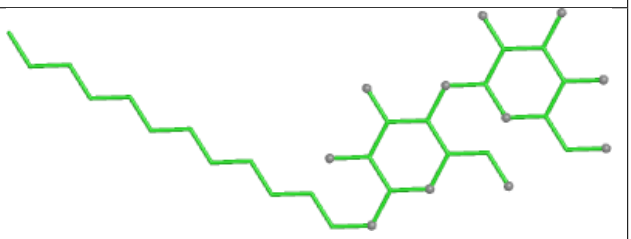


Rings

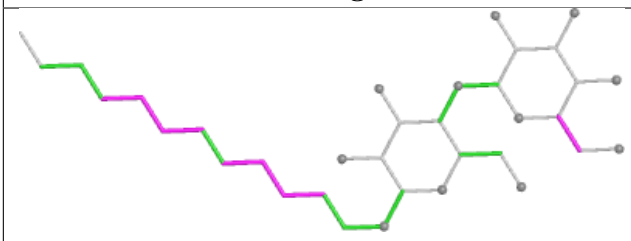
Ligand LMT L 207



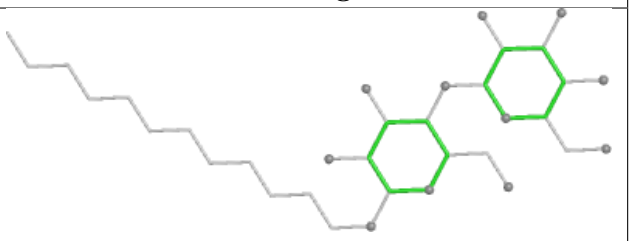
Bond lengths



Bond angles

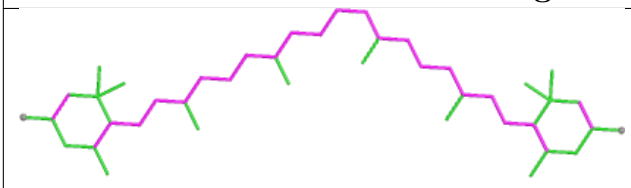


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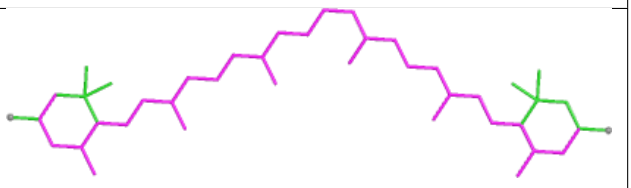


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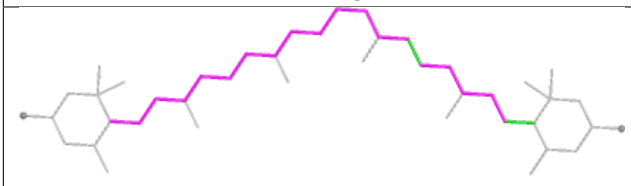
Ligand 5X6 2 321



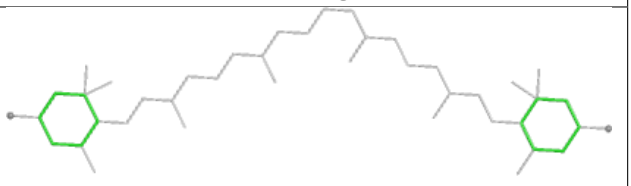
Bond lengths



Bond angles

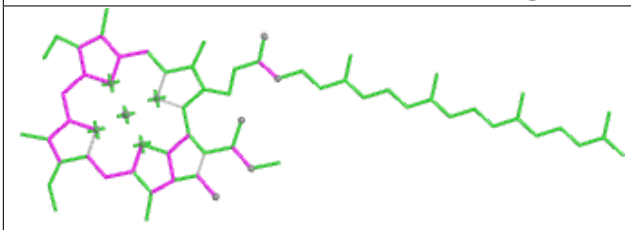


Torsions

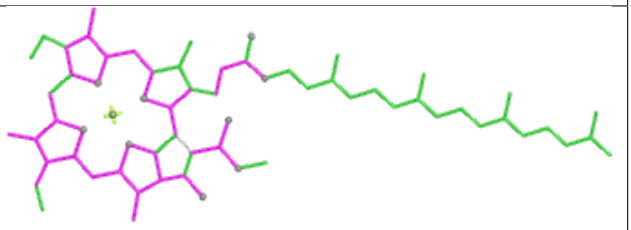


Rings

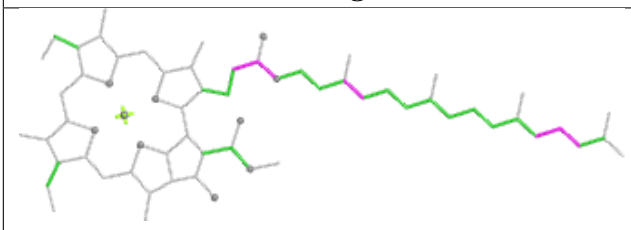
Ligand CLA A 825



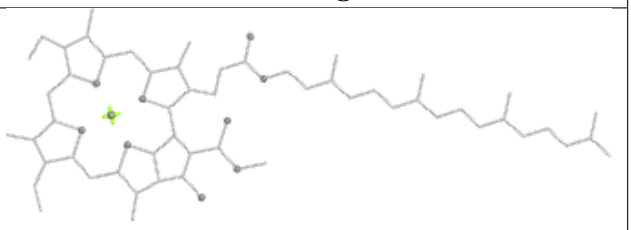
Bond lengths



Bond angles

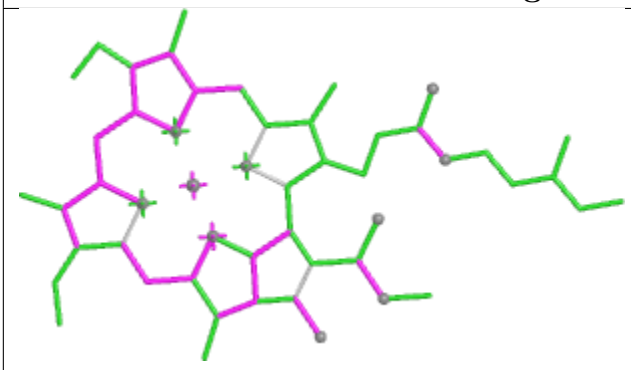


Torsions

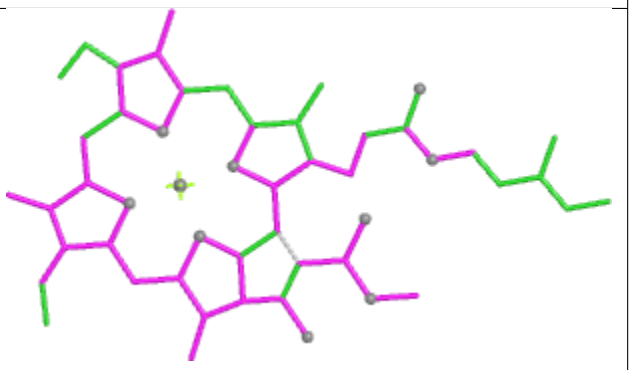


Rings

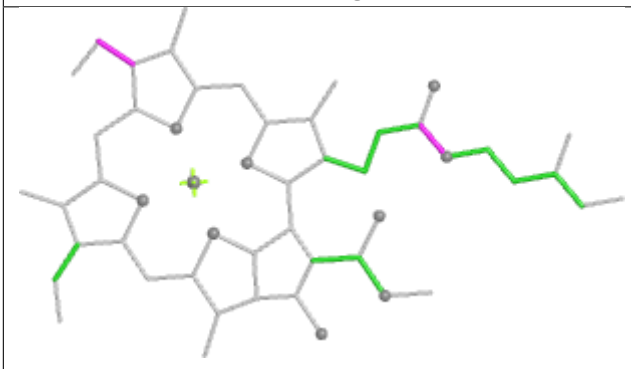
Ligand CLA A 835



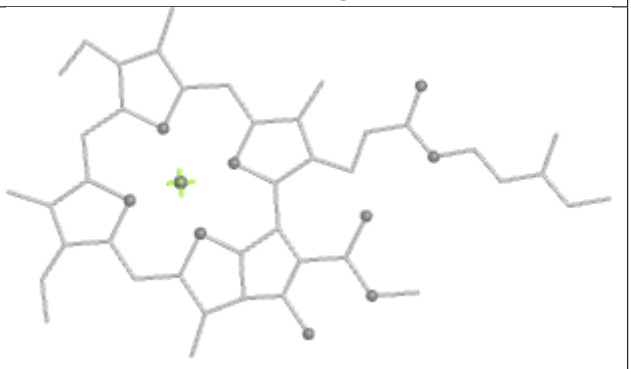
Bond lengths



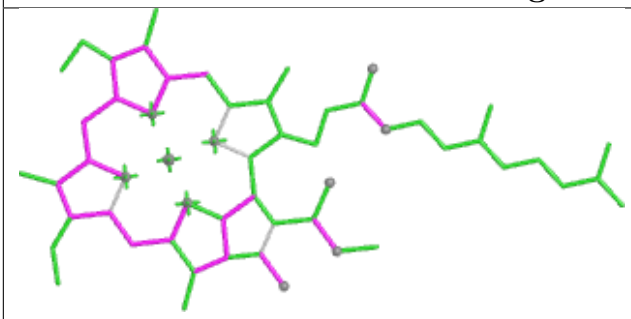
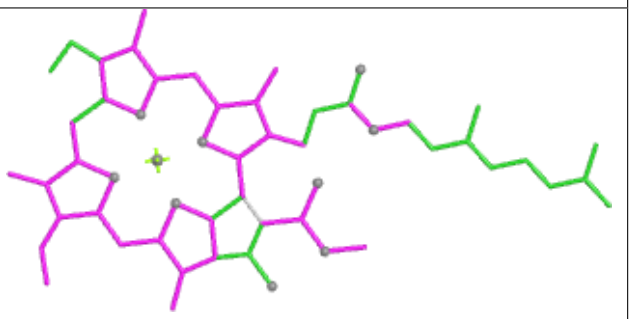
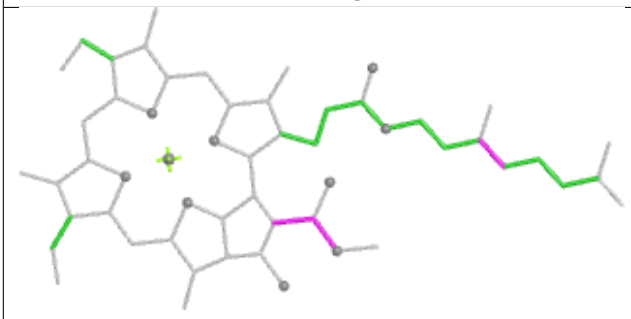
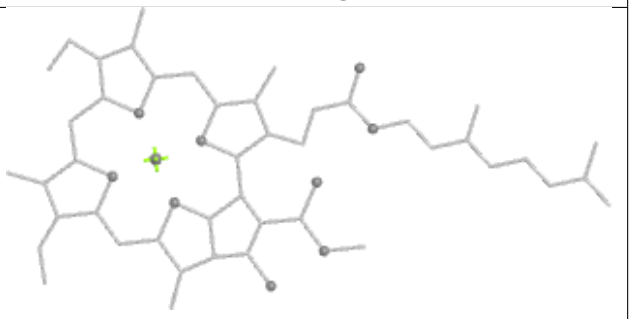
Bond angles

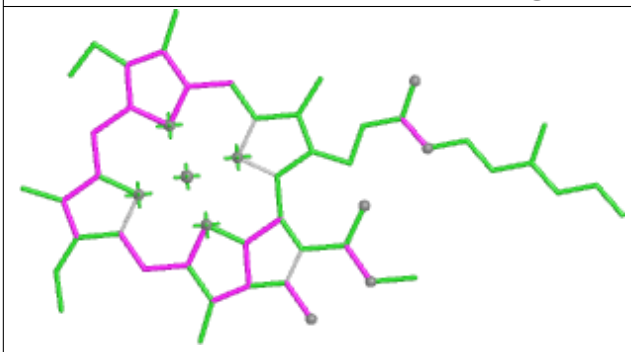
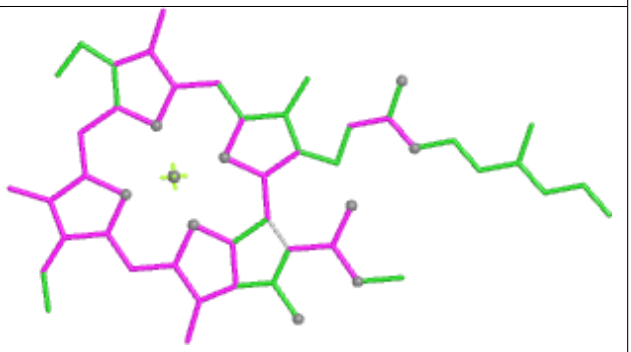
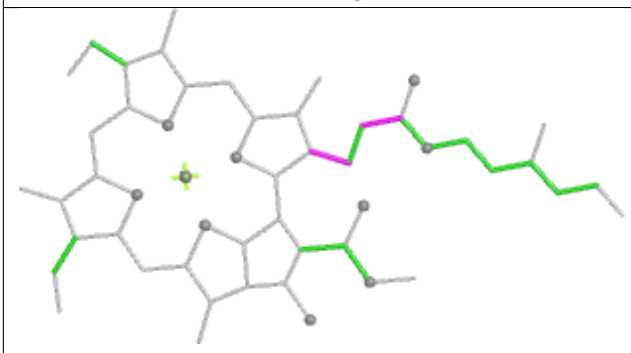
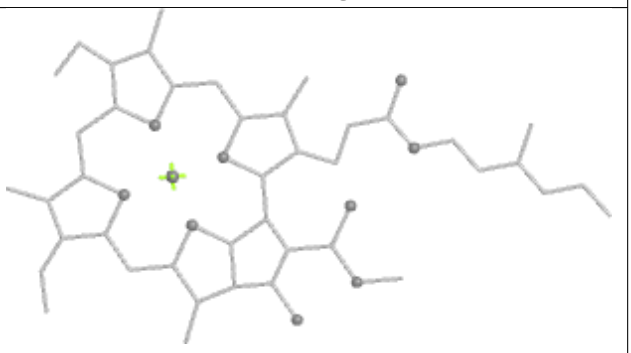


Torsions

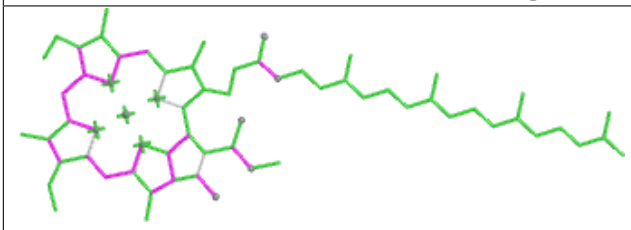


Rings

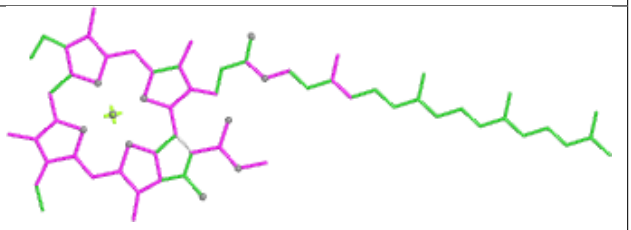
Ligand CLA 1 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 3 311	
 Bond lengths	 Bond angles
 Torsions	 Rings

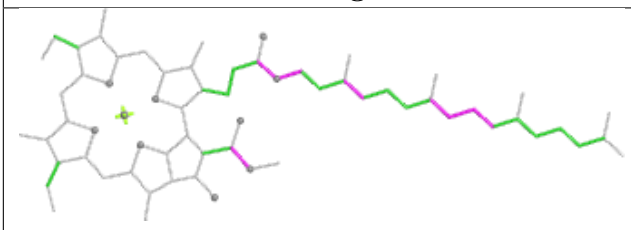
Ligand CLA B 834



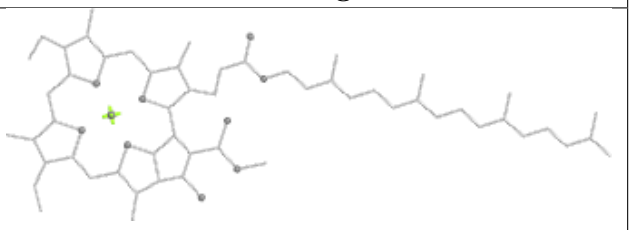
Bond lengths



Bond angles

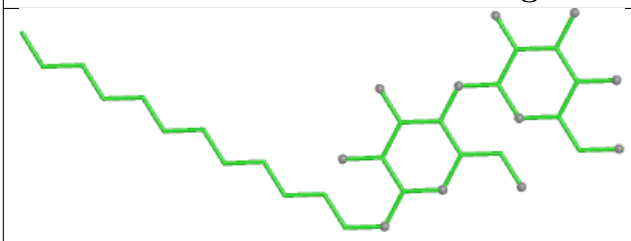


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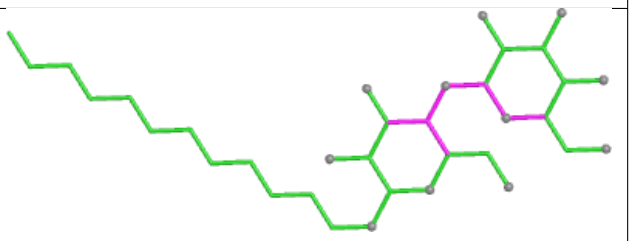


Rings

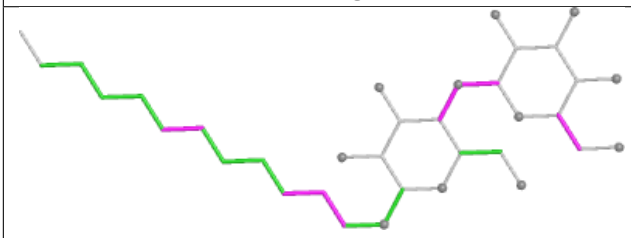
Ligand LMT A 848



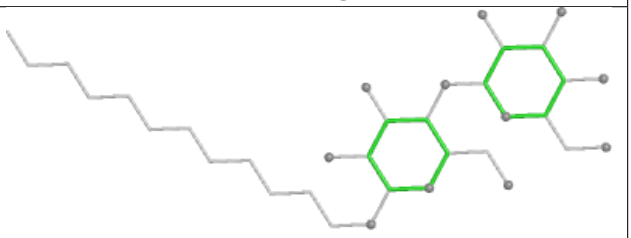
Bond lengths



Bond angles

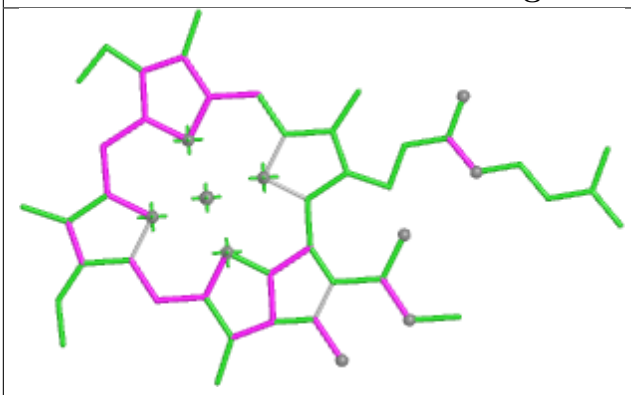


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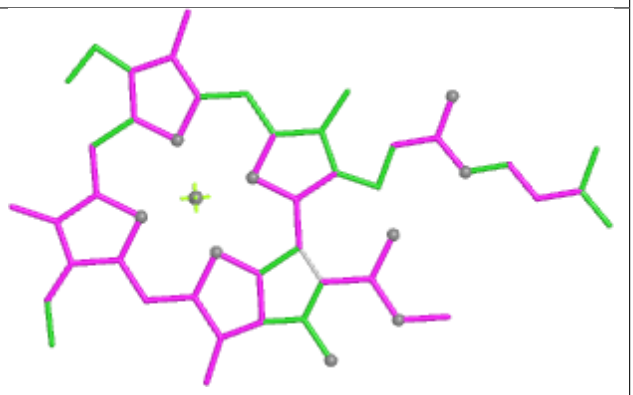


Rings

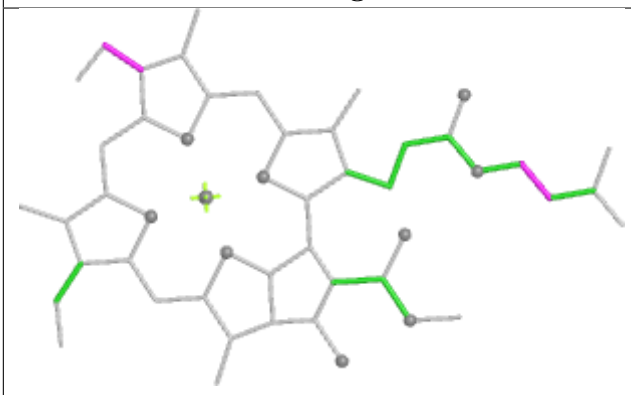
Ligand CLA A 805



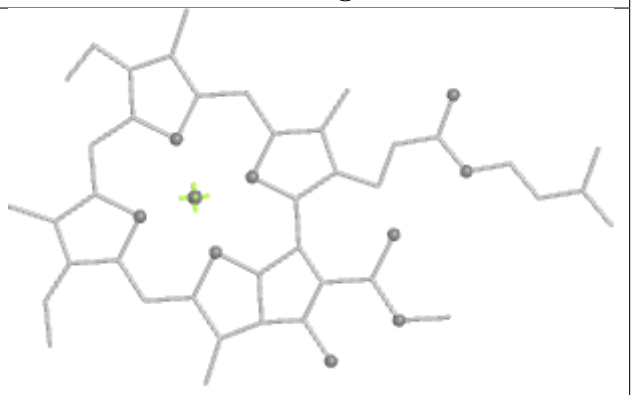
Bond lengths



Bond angles

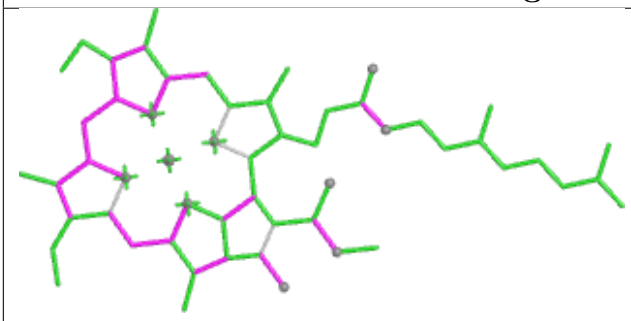


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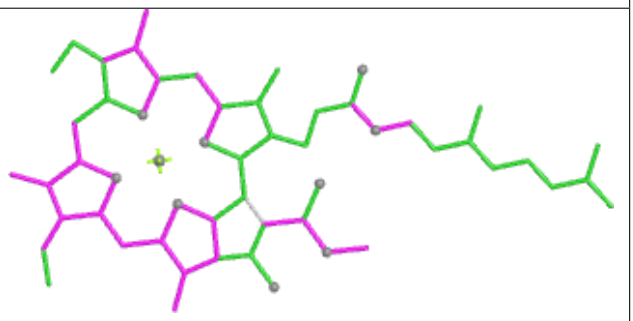


Rings

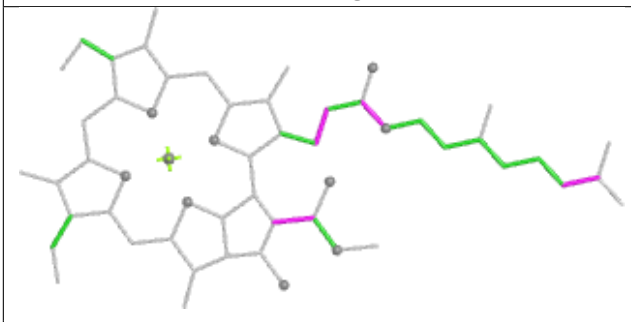
Ligand CLA A 822



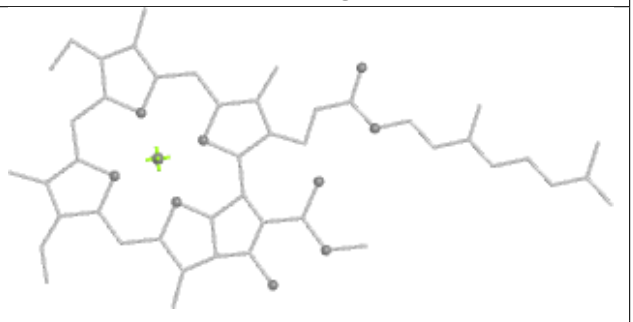
Bond lengths



Bond angles

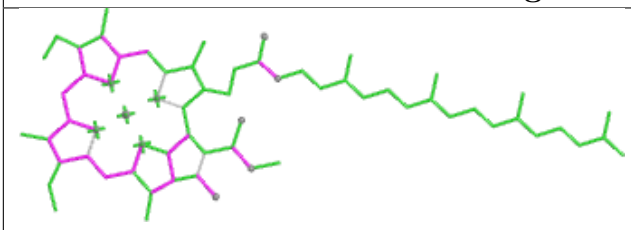


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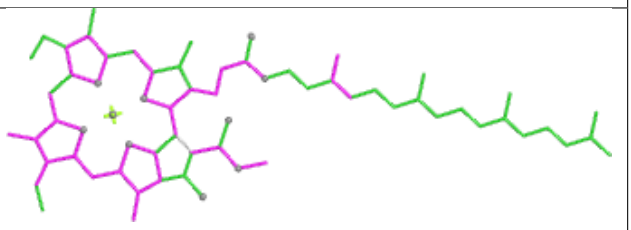


Rings

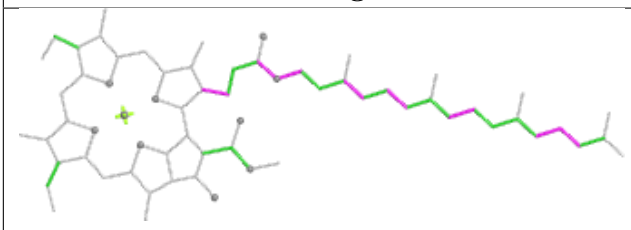
Ligand CLA B 832



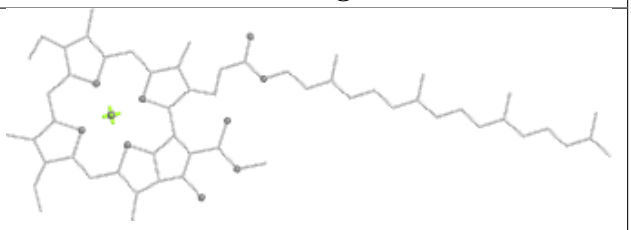
Bond lengths



Bond angles

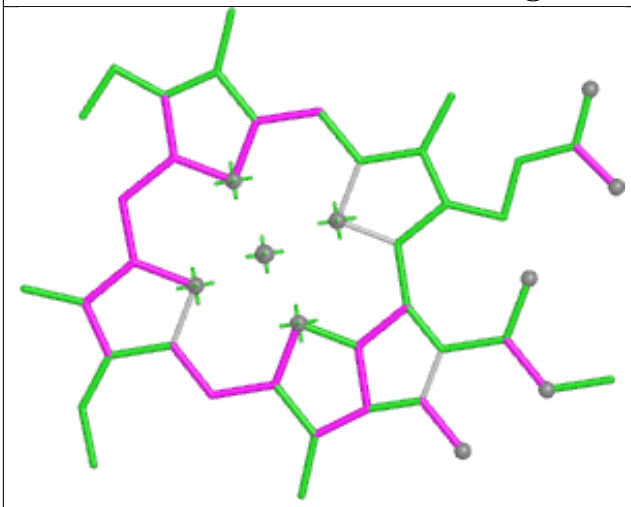


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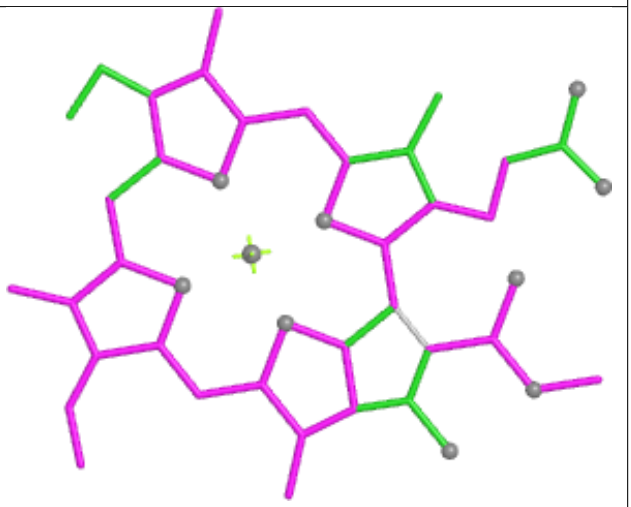


Rings

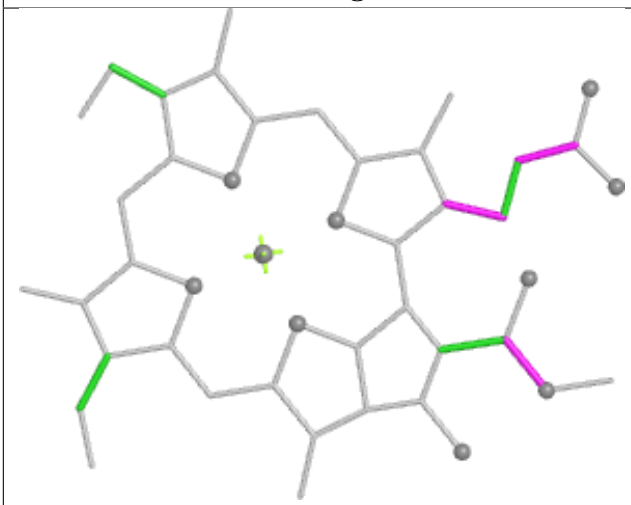
Ligand CLA B 835



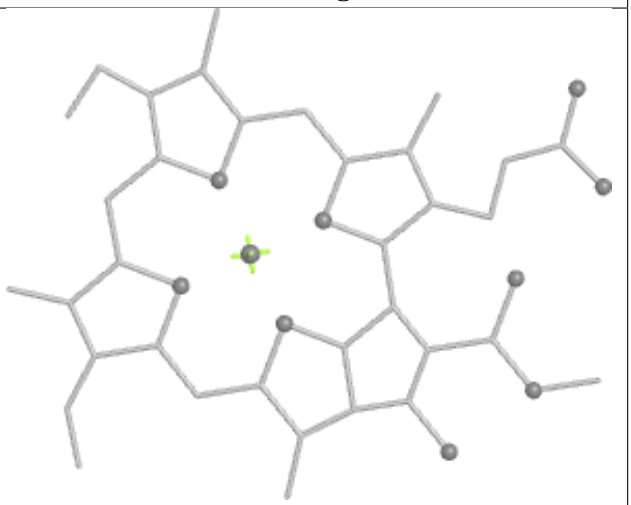
Bond lengths



Bond angles

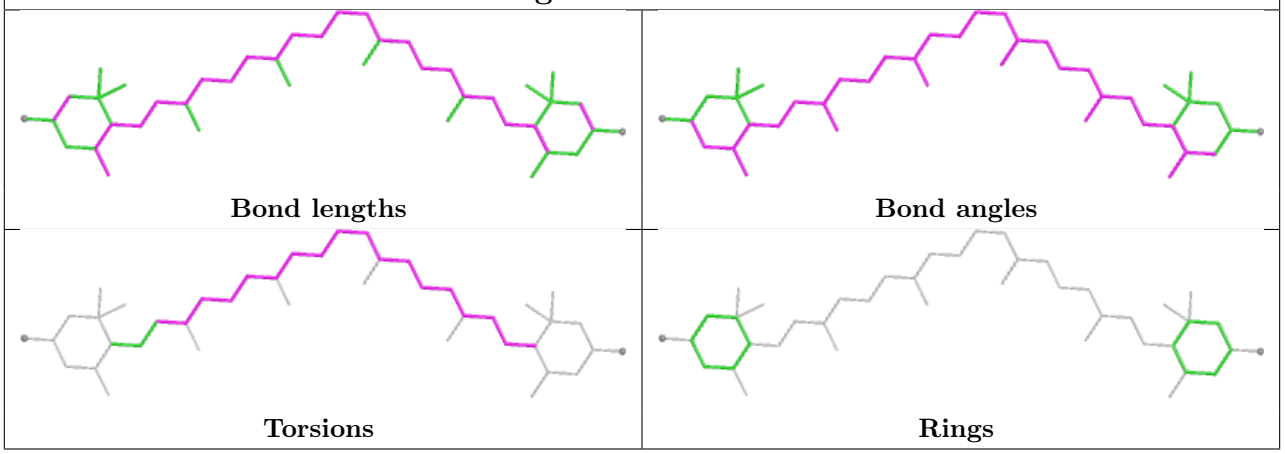


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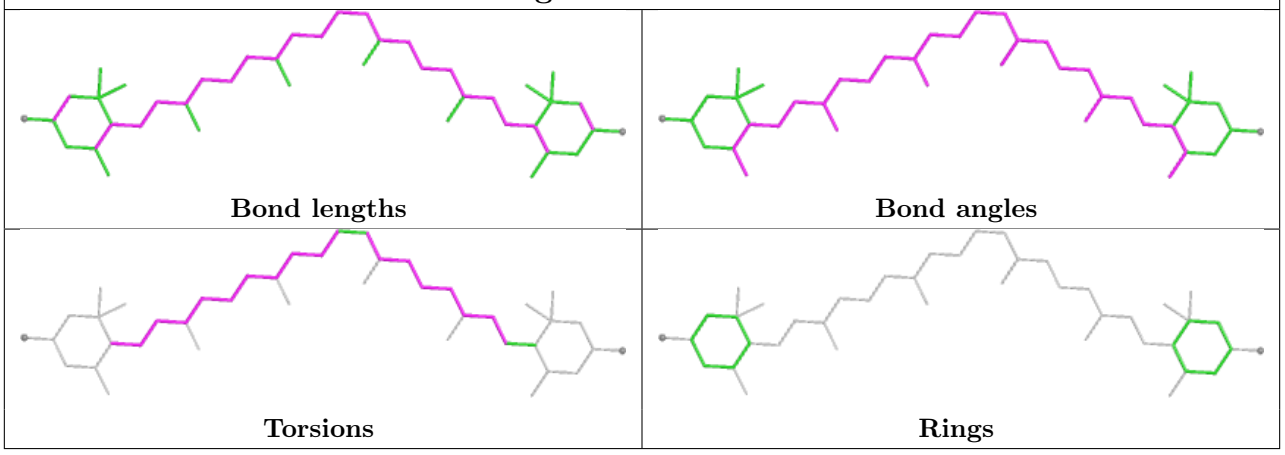


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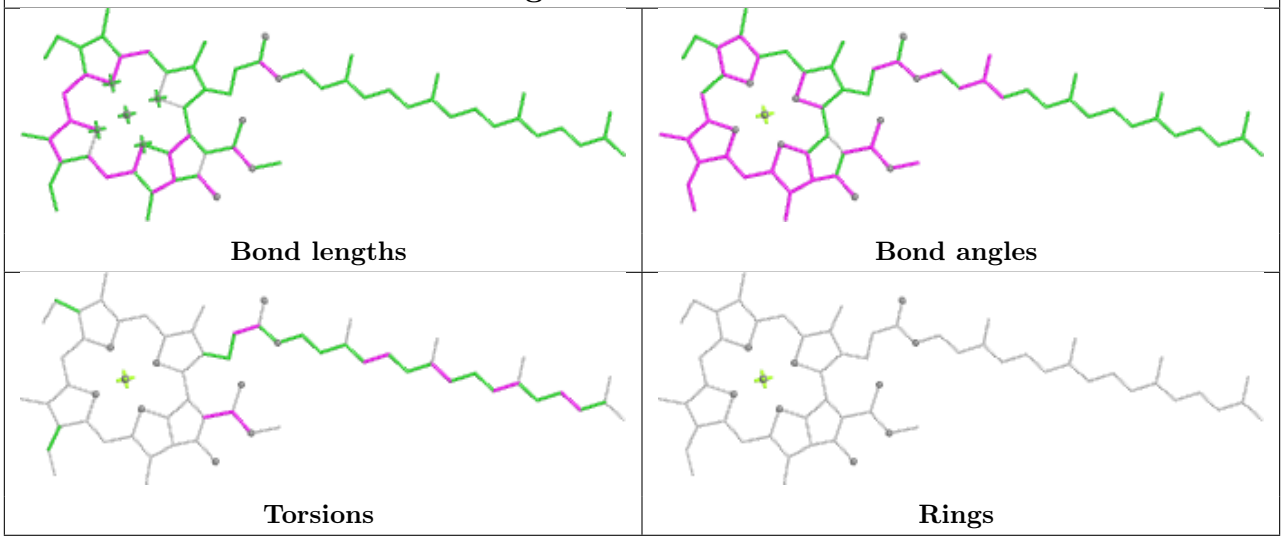
Ligand 5X6 5 317



Ligand 5X6 4 312



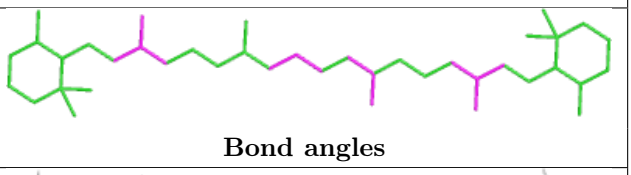
Ligand CLA B 810



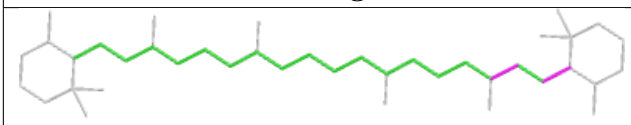
Ligand BCR L 205



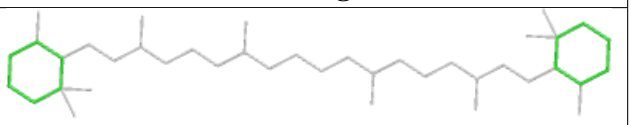
Bond lengths



Bond angles

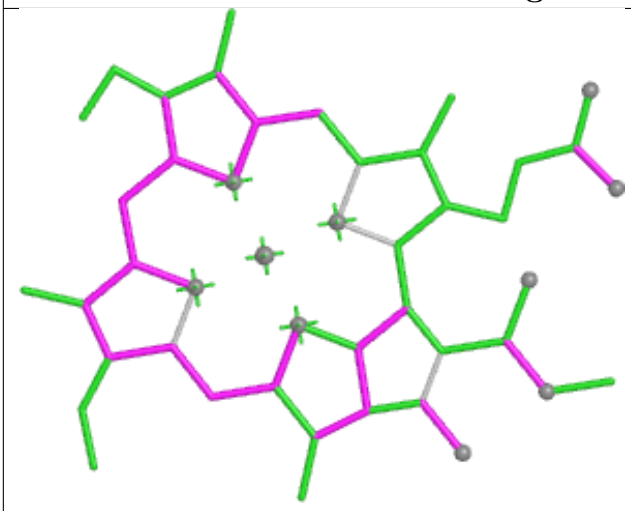


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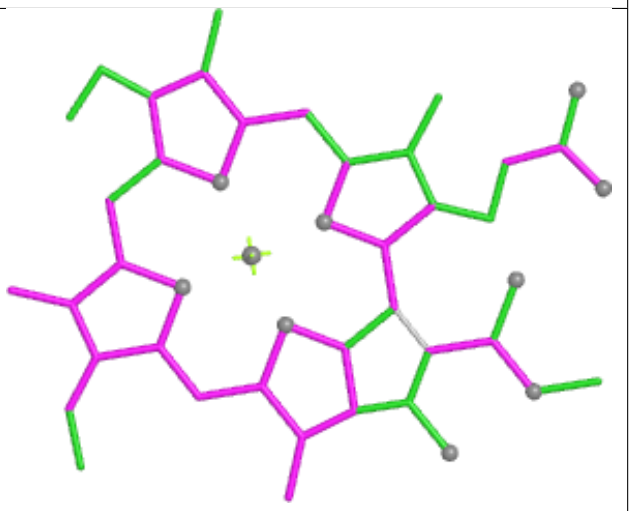


Rings

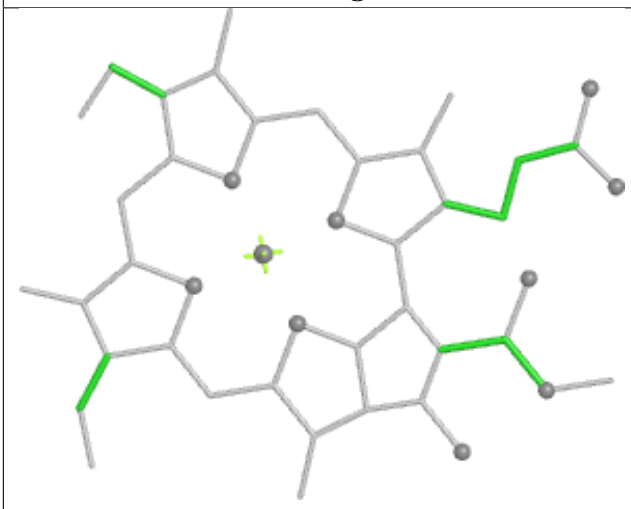
Ligand CLA F 203



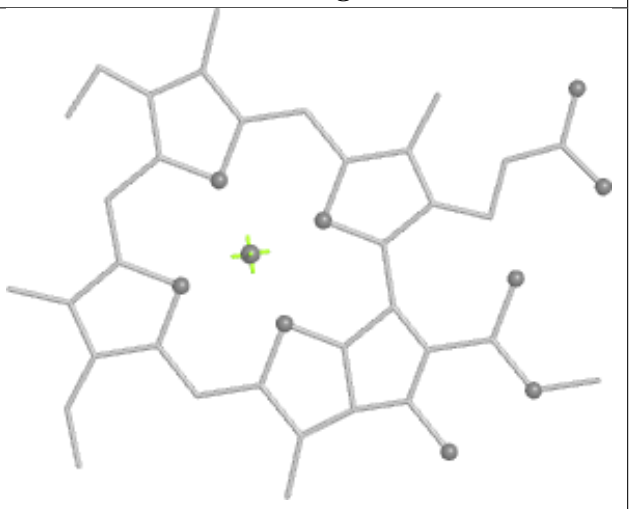
Bond lengths



Bond angles

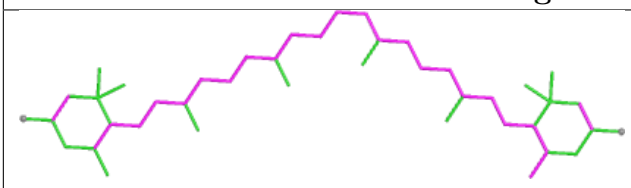


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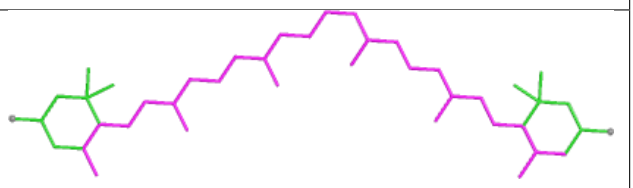


Rings

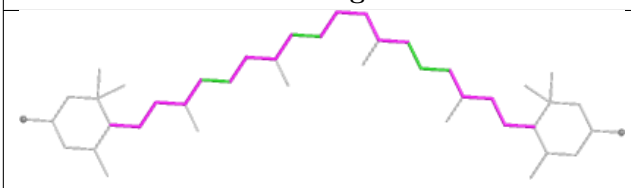
Ligand 5X6 5 316



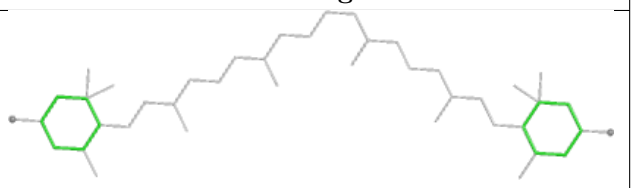
Bond lengths



Bond angles

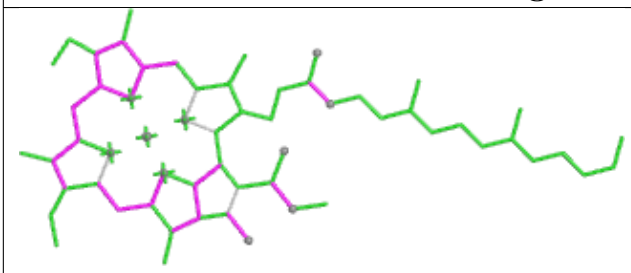


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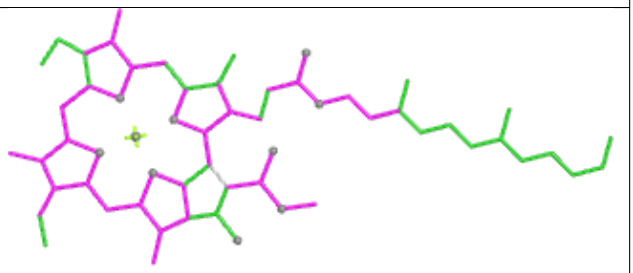


Rings

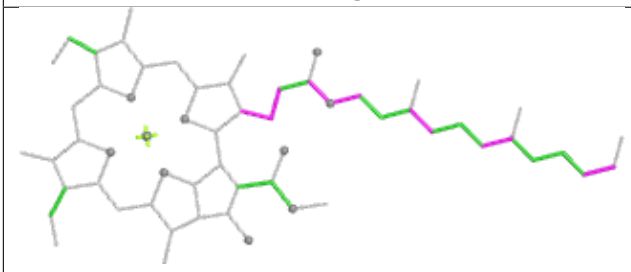
Ligand CLA 4 304



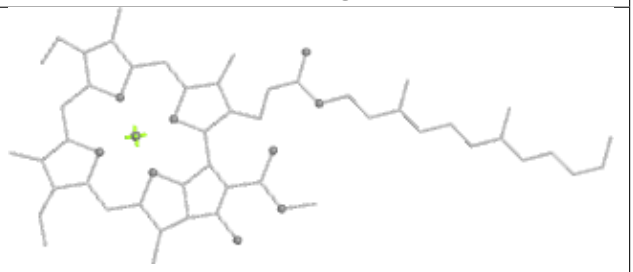
Bond lengths



Bond angles

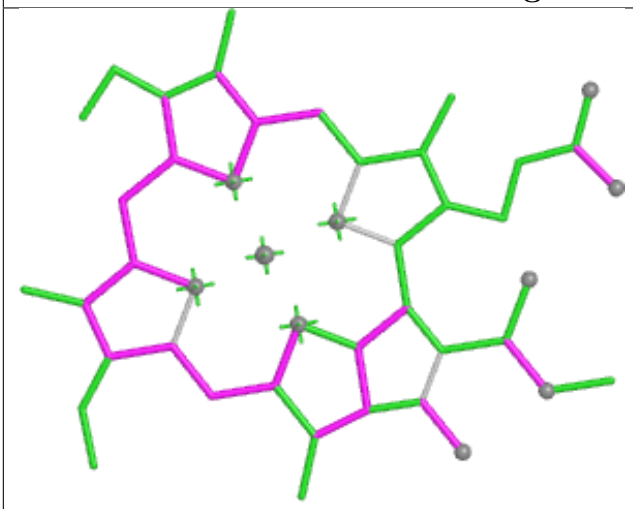


Torsions

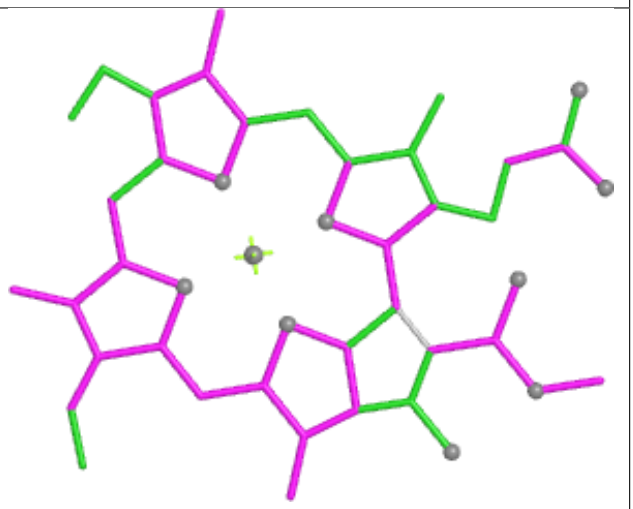


Rings

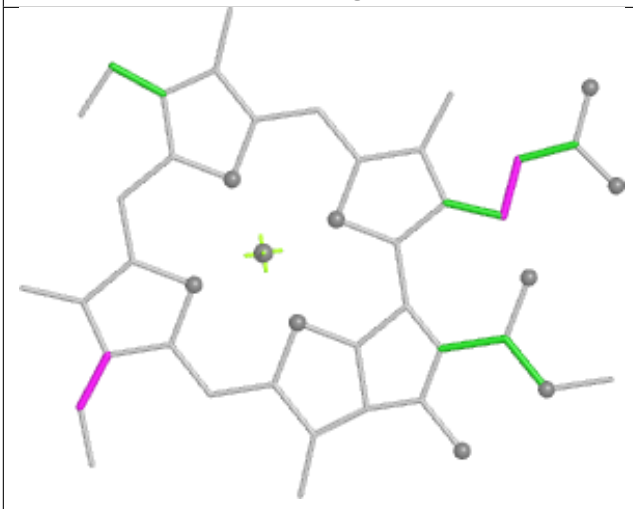
Ligand CLA A 814



Bond lengths



Bond angles

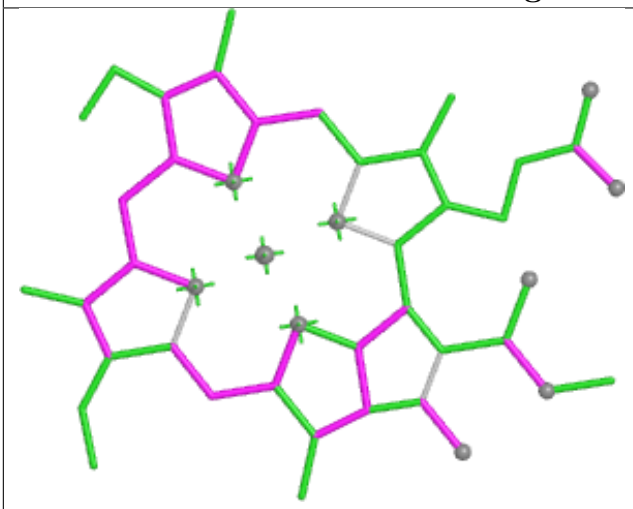


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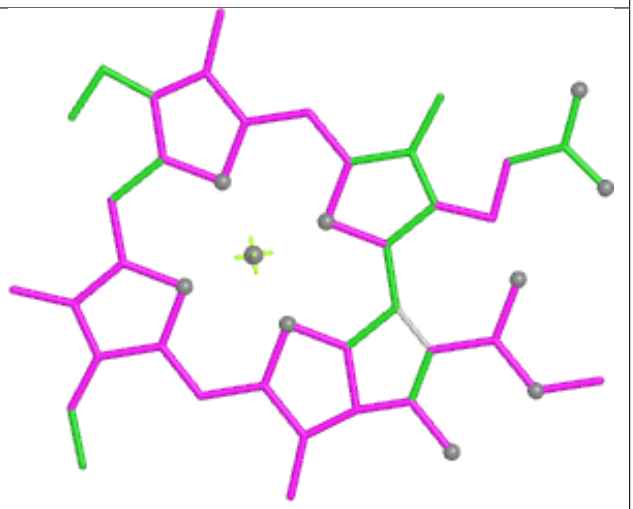


Rings

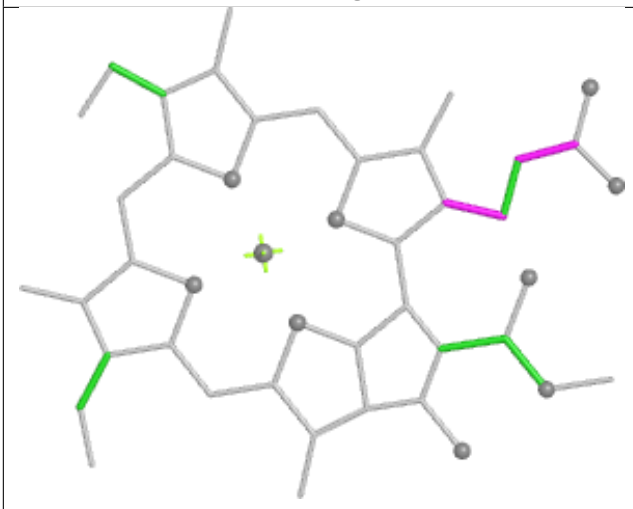
Ligand CLA B 821



Bond lengths



Bond angles

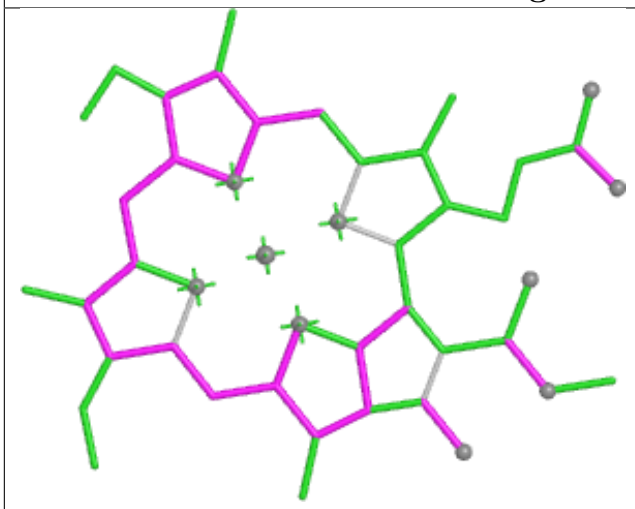


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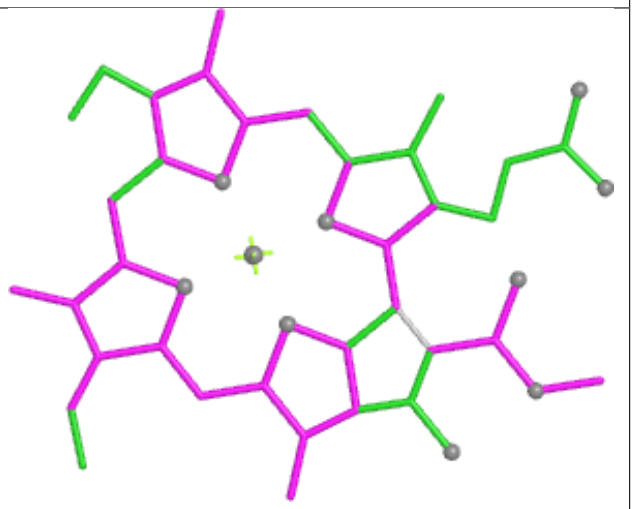


Rings

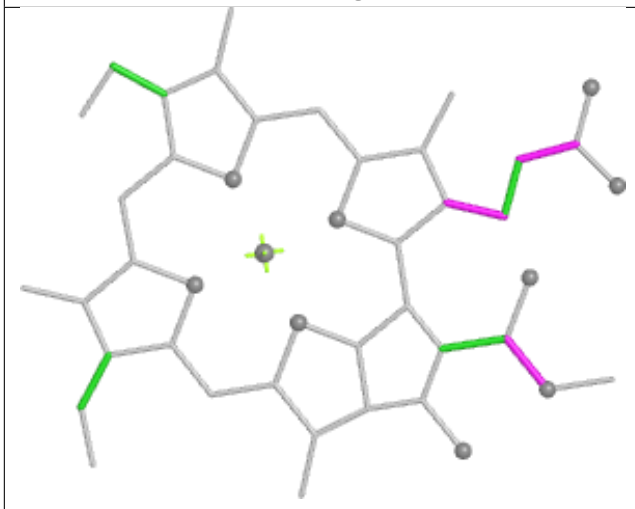
Ligand CLA 4 311



Bond lengths



Bond angles

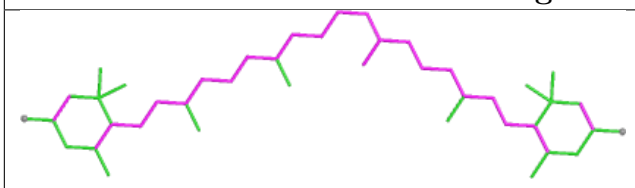


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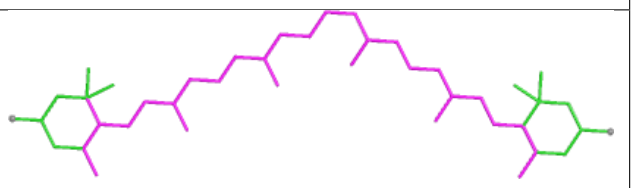


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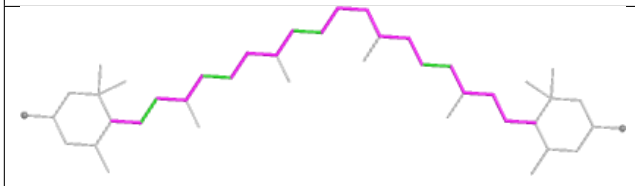
Ligand 5X6 5 315



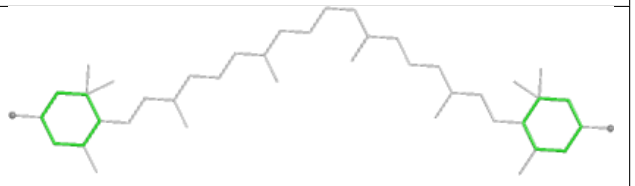
Bond lengths



Bond angles

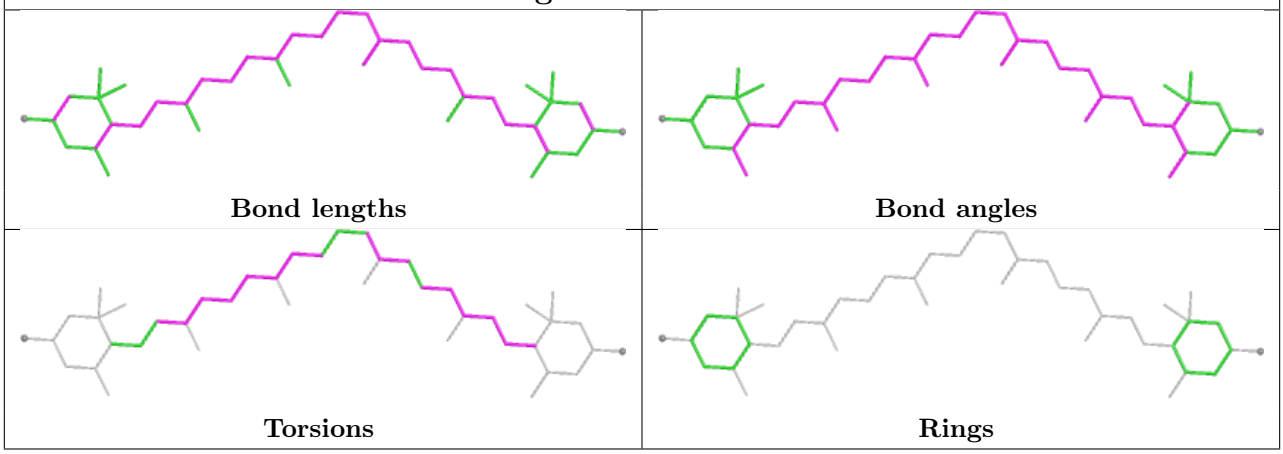


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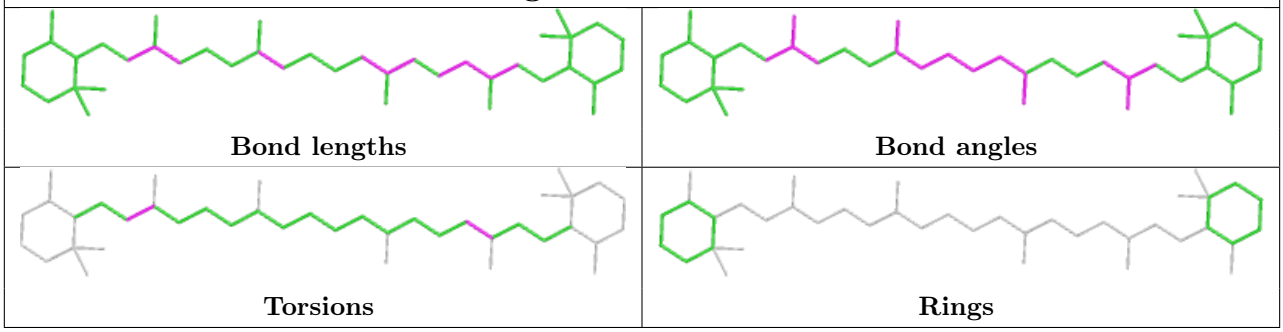


Rings

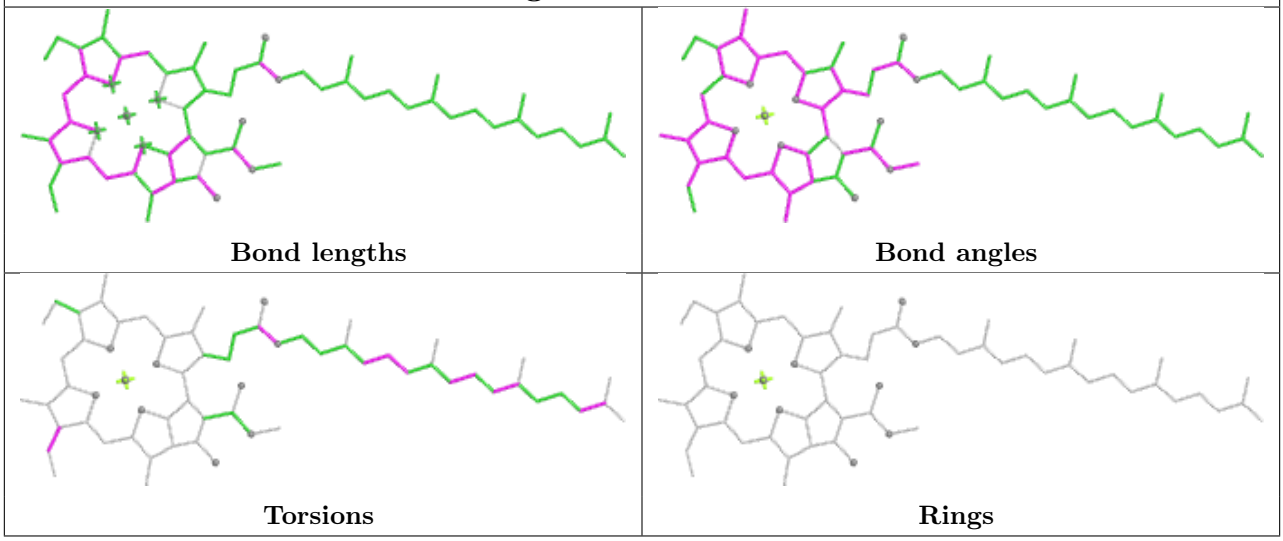
Ligand 5X6 2 318



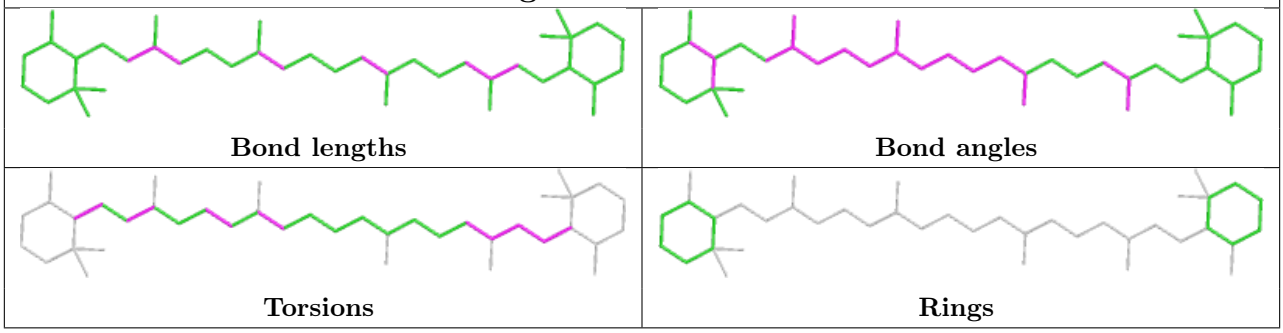
Ligand BCR B 848



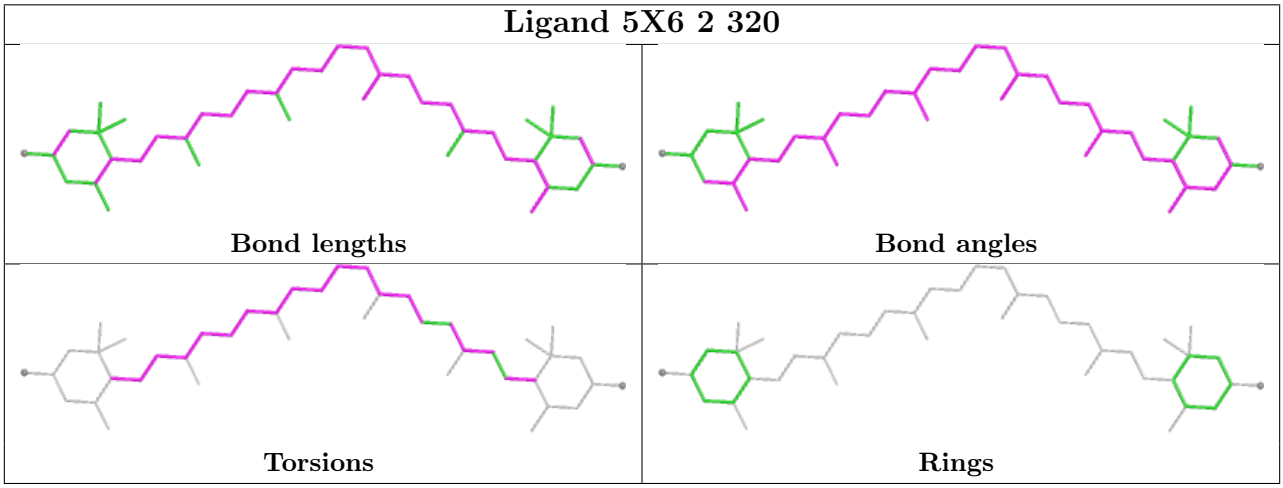
Ligand CLA B 820



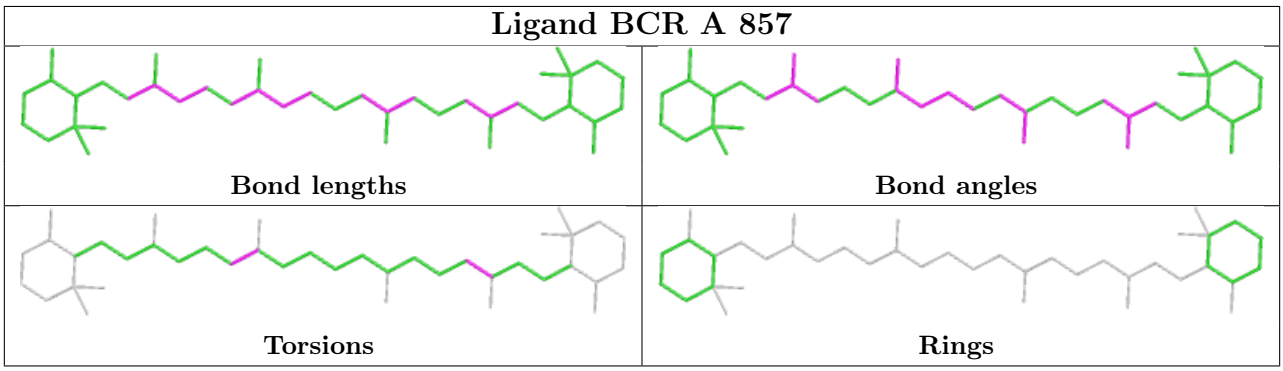
Ligand BCR M 101



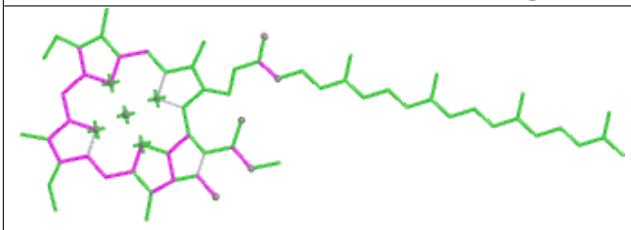
Ligand 5X6 2 320



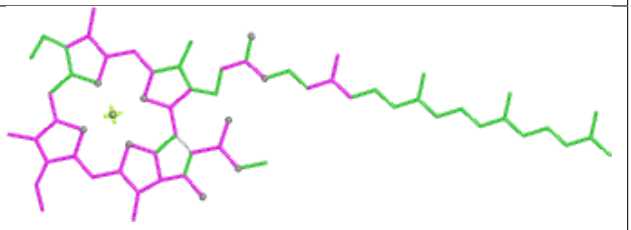
Ligand BCR A 857



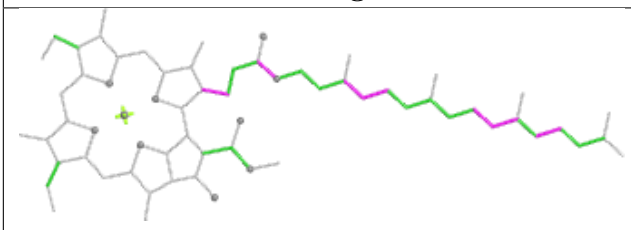
Ligand CLA A 831



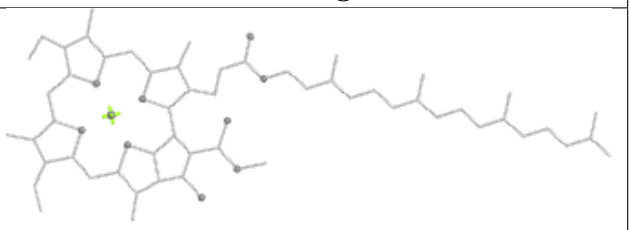
Bond lengths



Bond angles

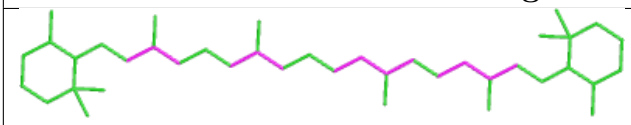


Torsions

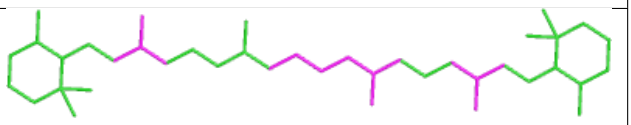


Rings

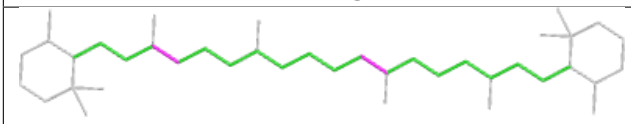
Ligand BCR A 846



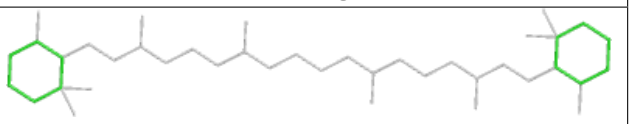
Bond lengths



Bond angles

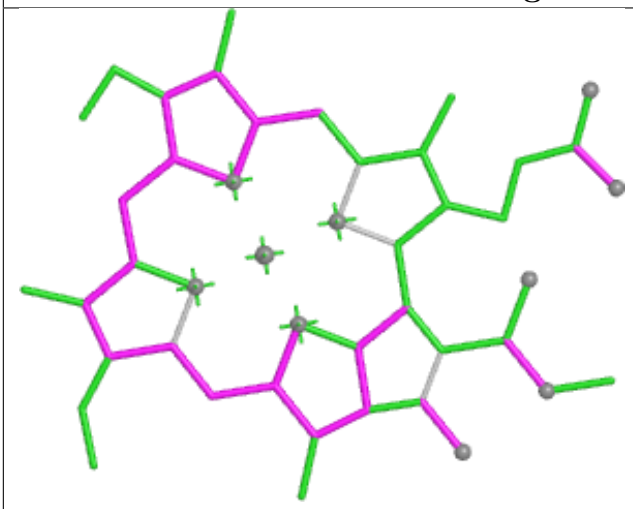


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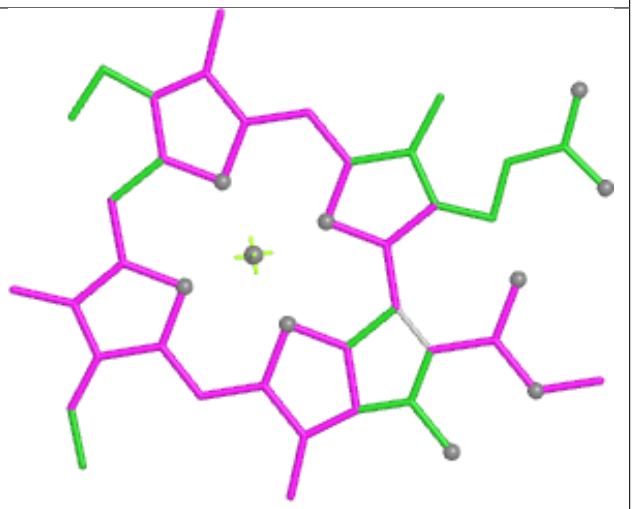


Rings

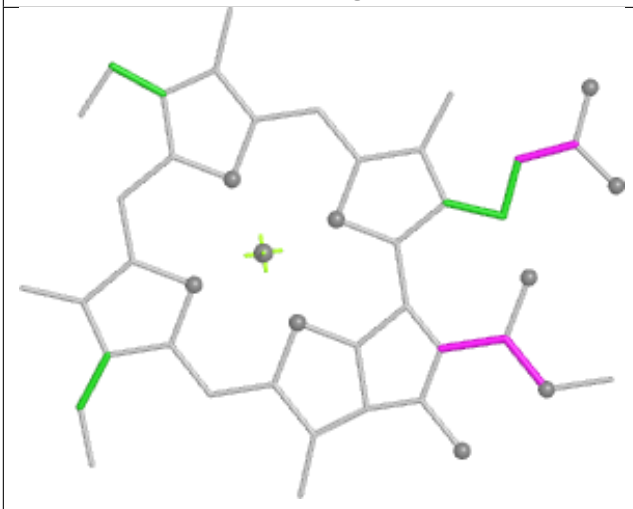
Ligand CLA O 205



Bond lengths



Bond angles

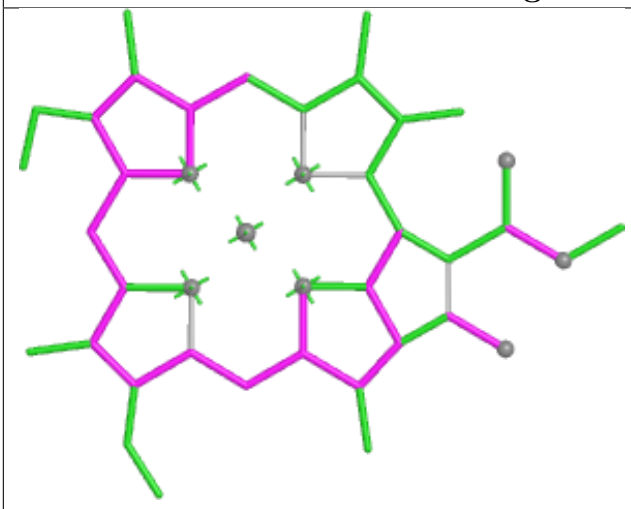


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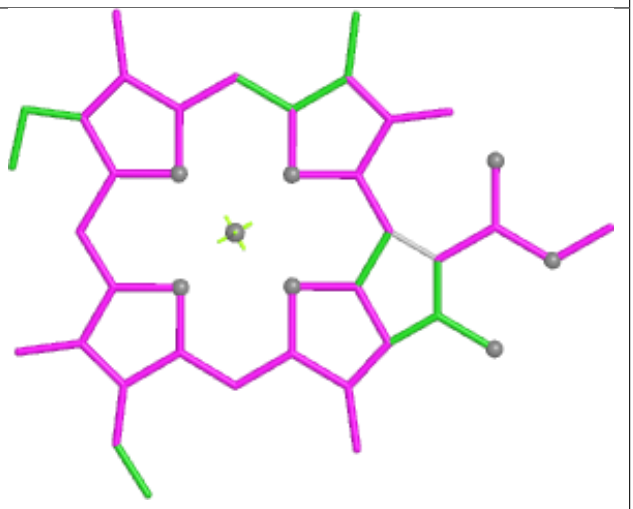


Rings

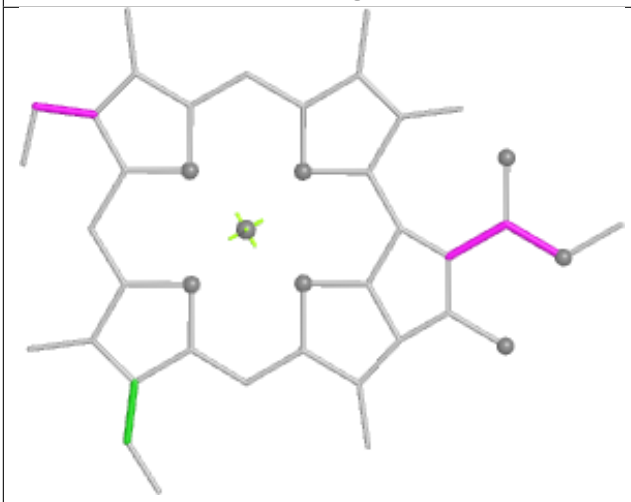
Ligand CLA O 203



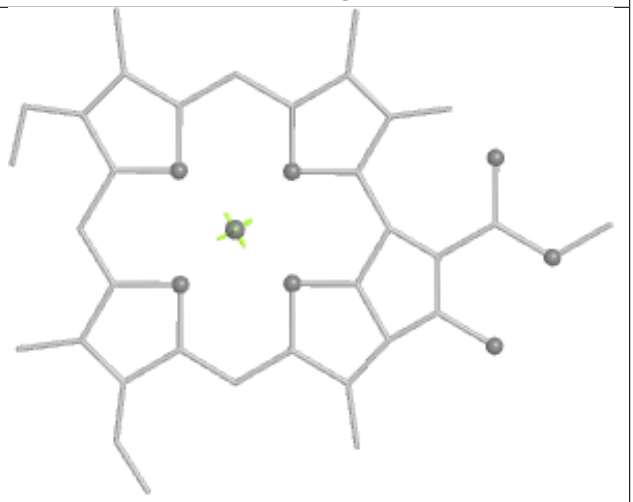
Bond lengths



Bond angles

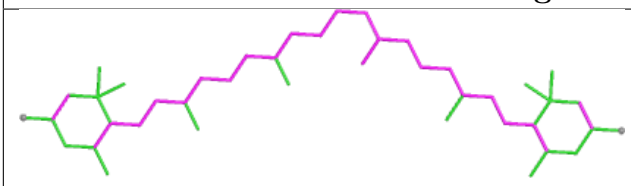


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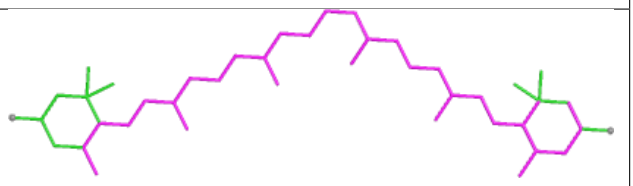


Rings

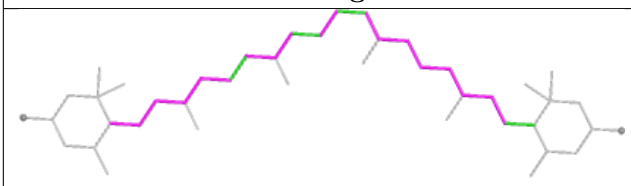
Ligand 5X6 1 313



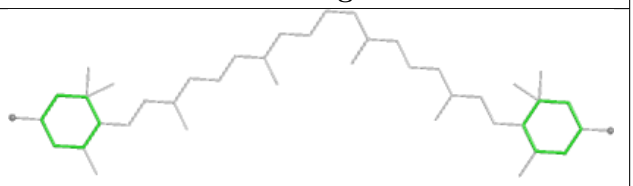
Bond lengths



Bond angles

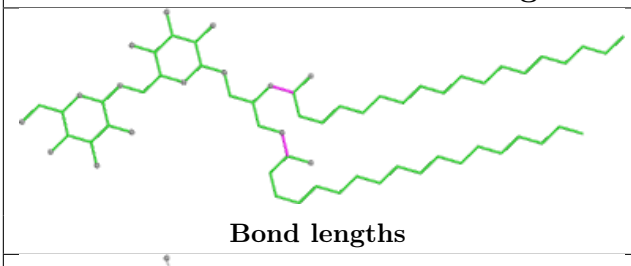


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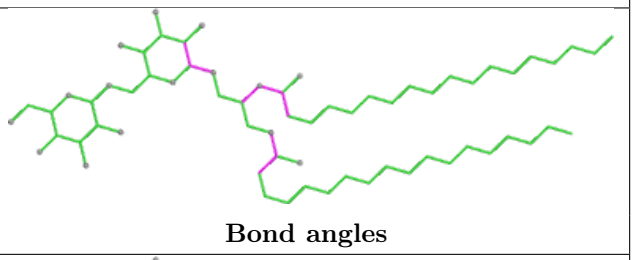


Rings

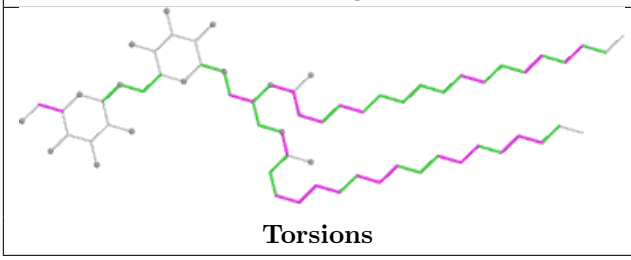
Ligand DGD B 849



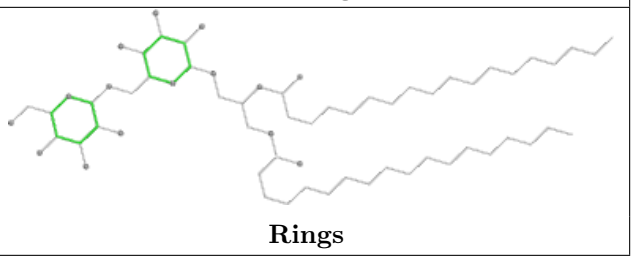
Bond lengths



Bond angles

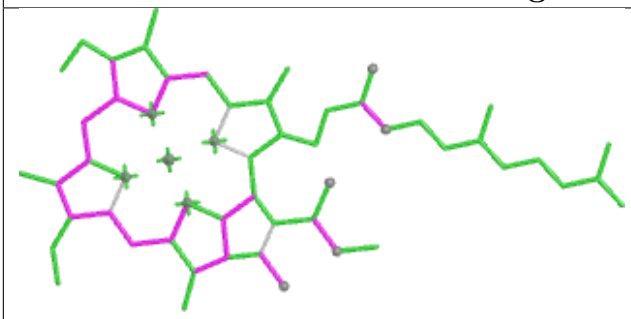


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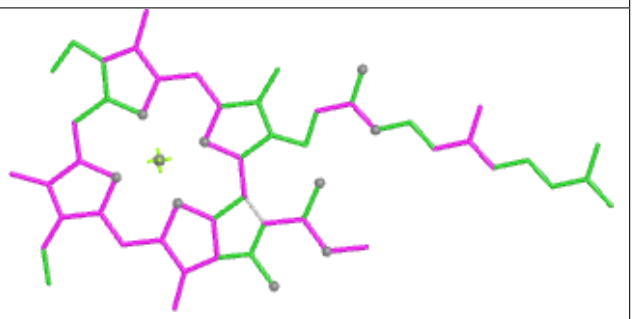


Rings

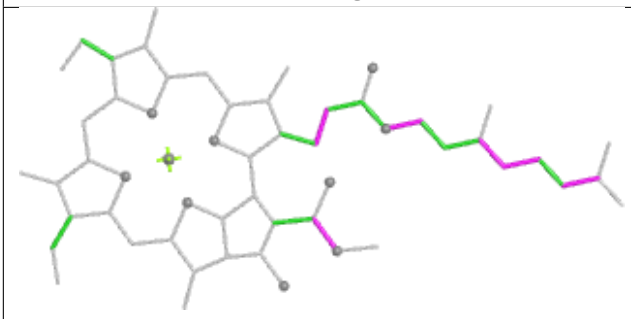
Ligand CLA 1 303



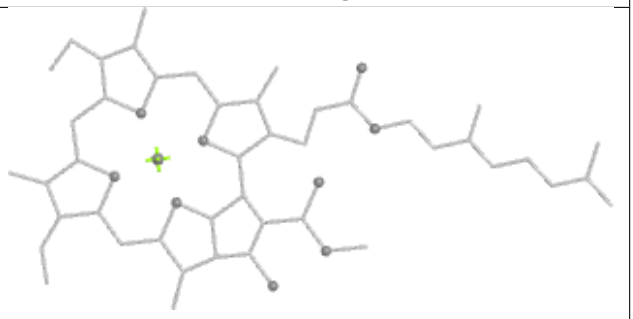
Bond lengths



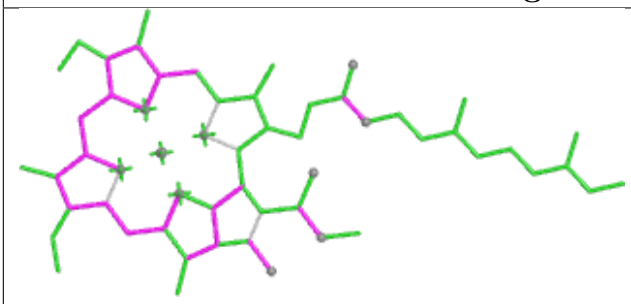
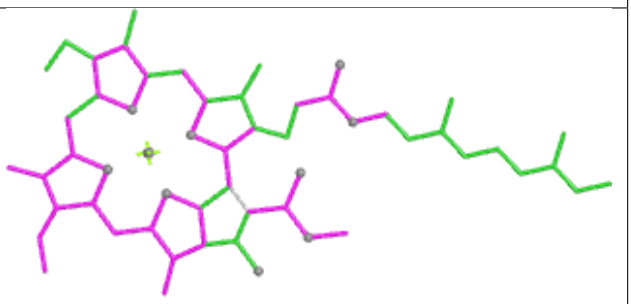
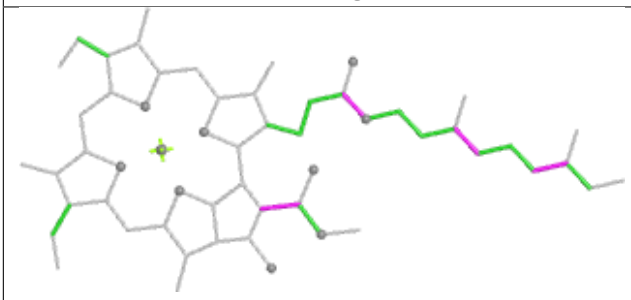
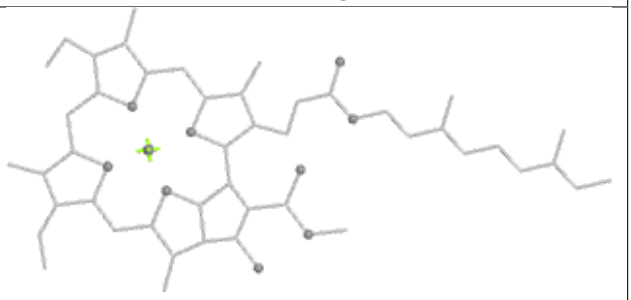
Bond angles

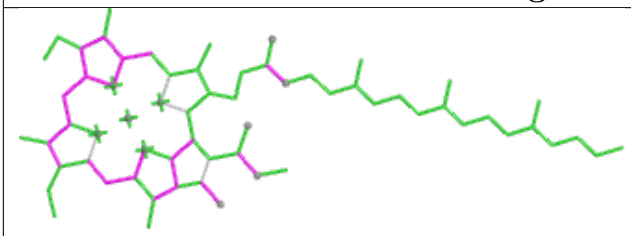
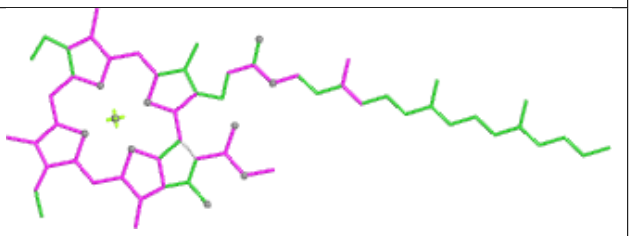
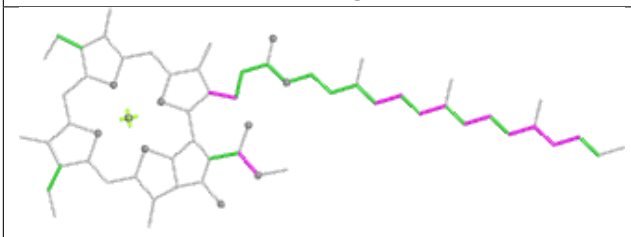
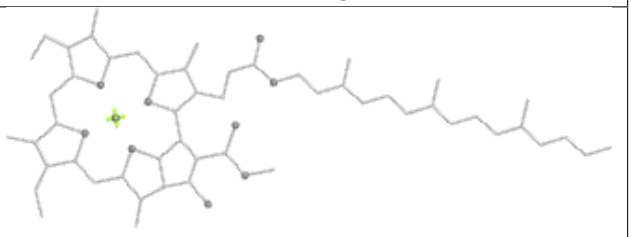


Torsions

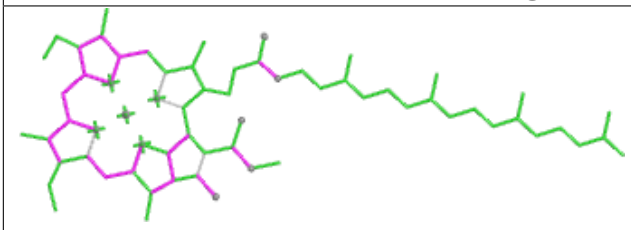


Rings

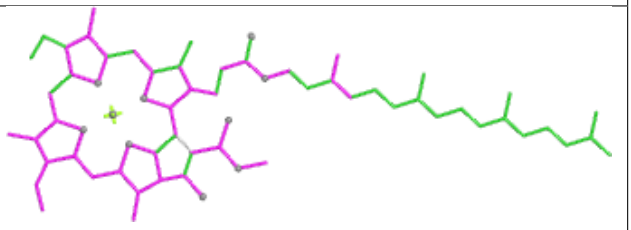
Ligand CLA A 836	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 3 305	
	
Bond lengths	Bond angles
	
Torsions	Rings

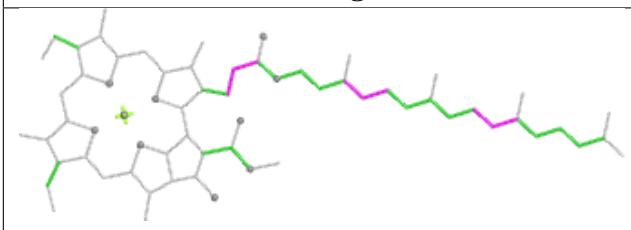
Ligand CLA A 818



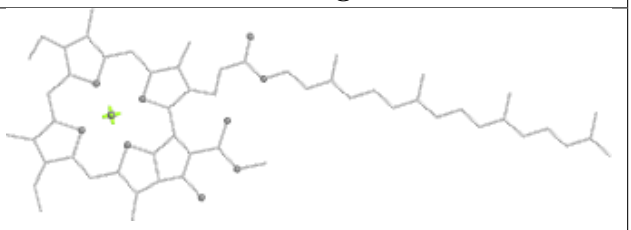
Bond lengths



Bond angles

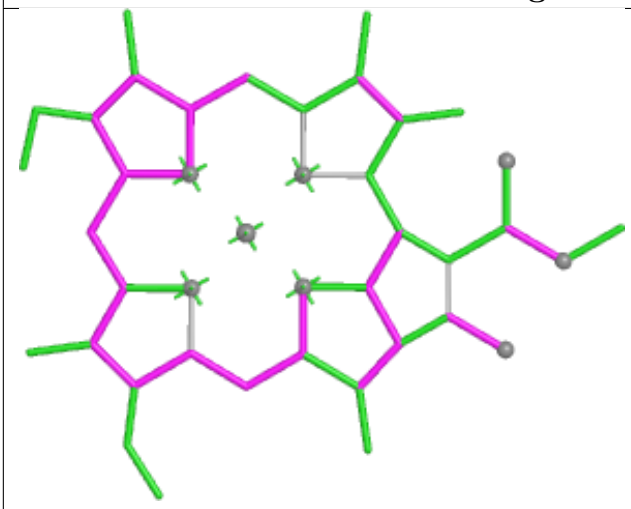


Torsions

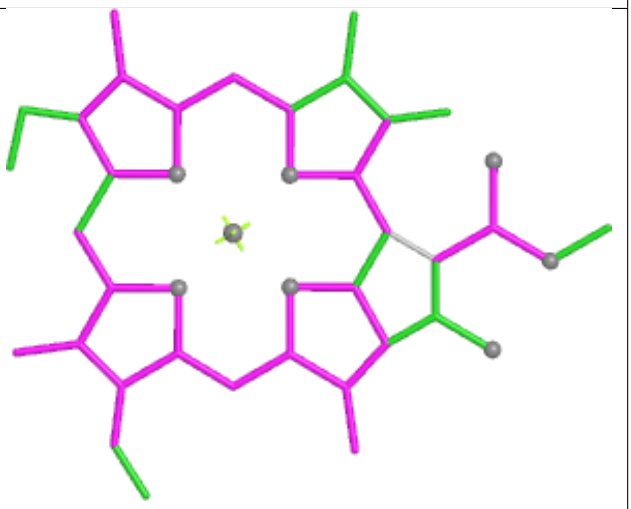


Rings

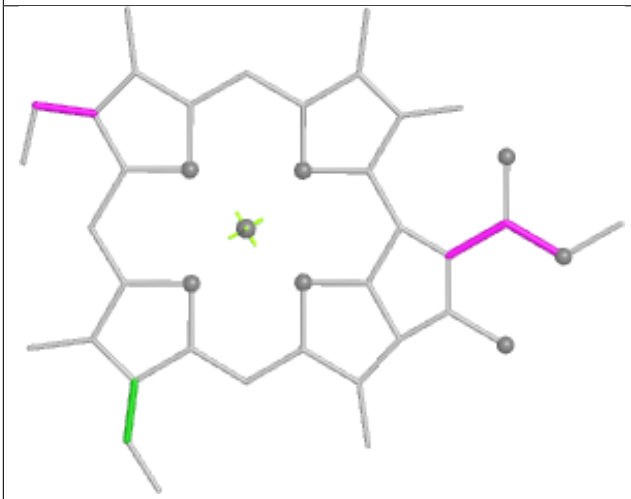
Ligand CLA 2 312



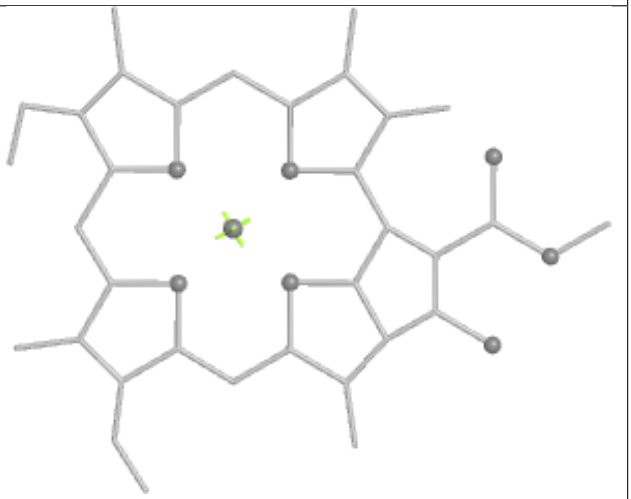
Bond lengths



Bond angles

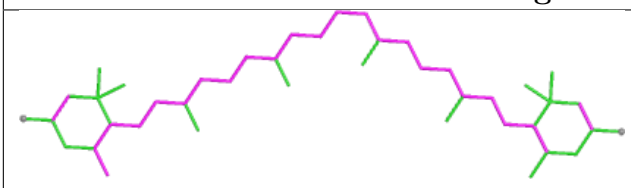


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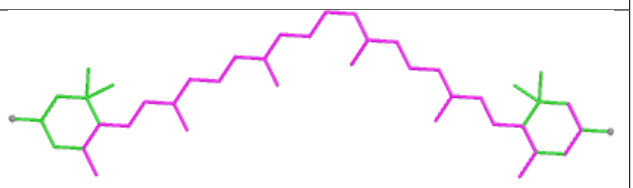


Rings

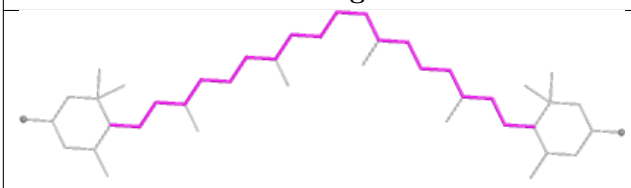
Ligand 5X6 4 313



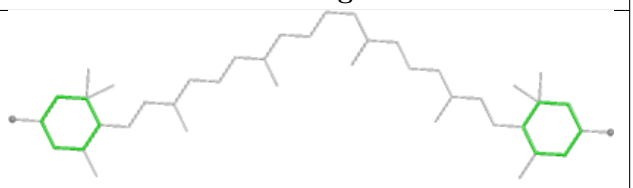
Bond lengths



Bond angles

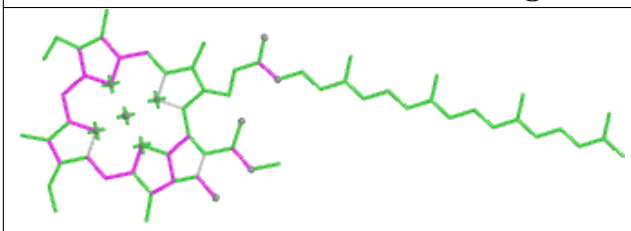


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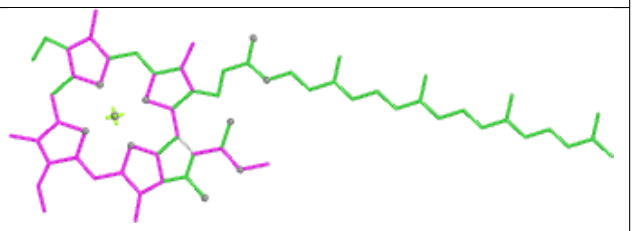


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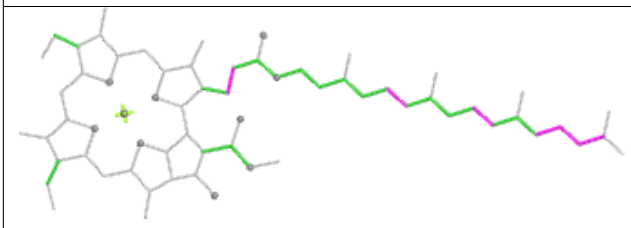
Ligand CLA A 827



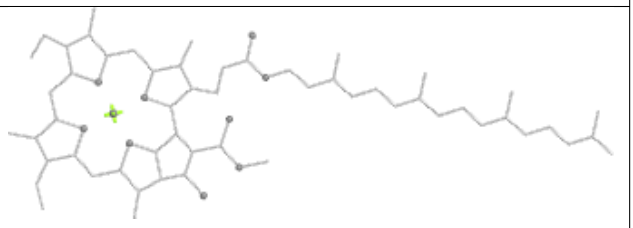
Bond lengths



Bond angles

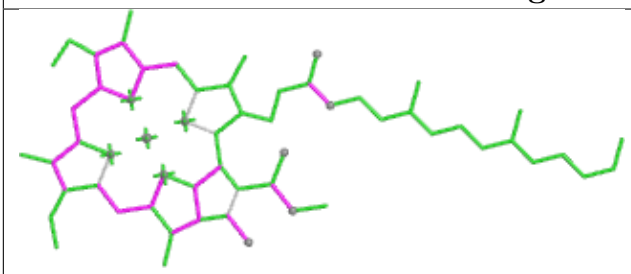


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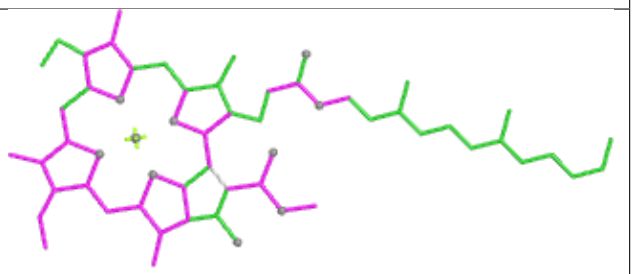


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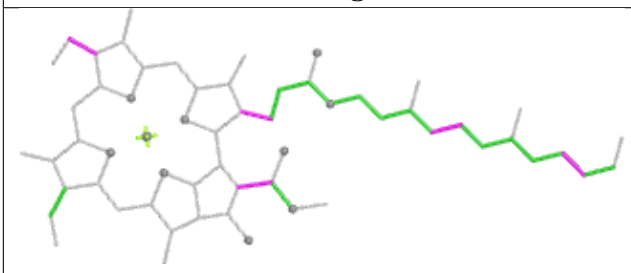
Ligand CLA 1 302



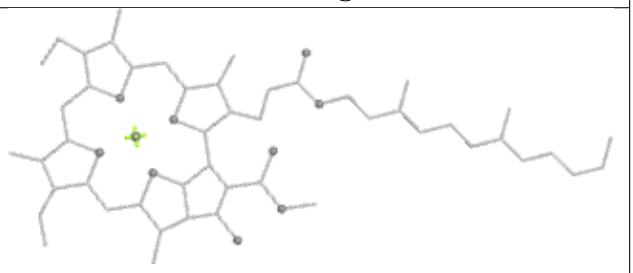
Bond lengths



Bond angles

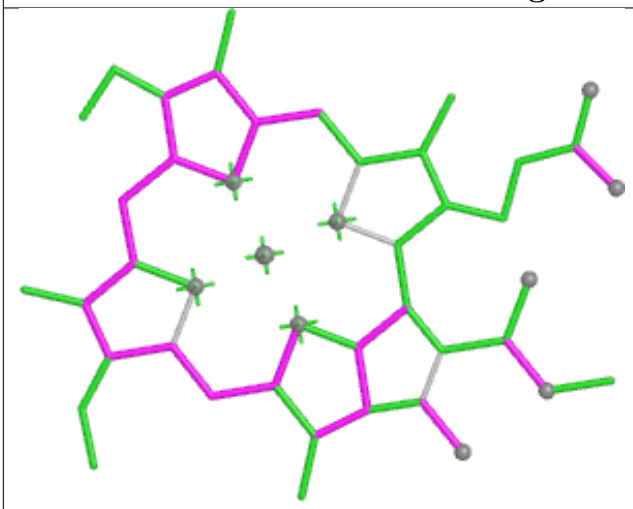


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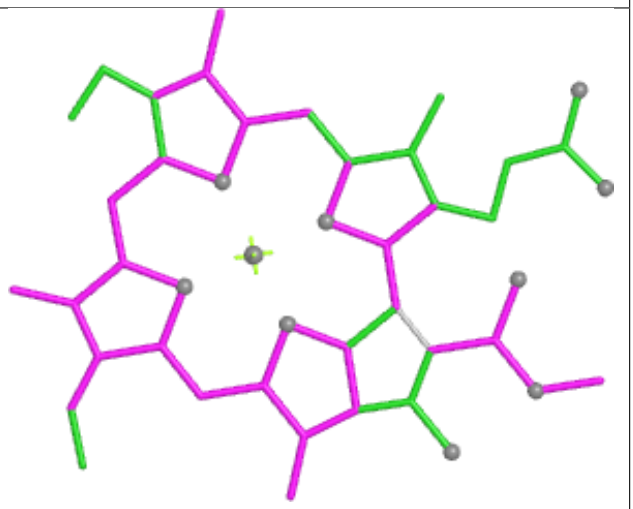


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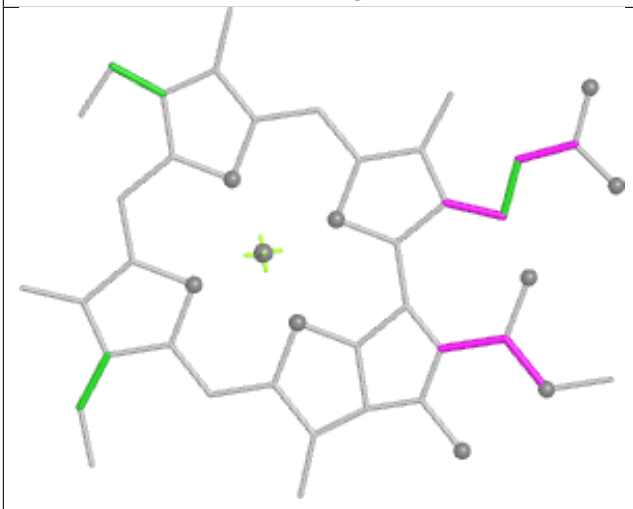
Ligand CLA 1 304



Bond lengths



Bond angles

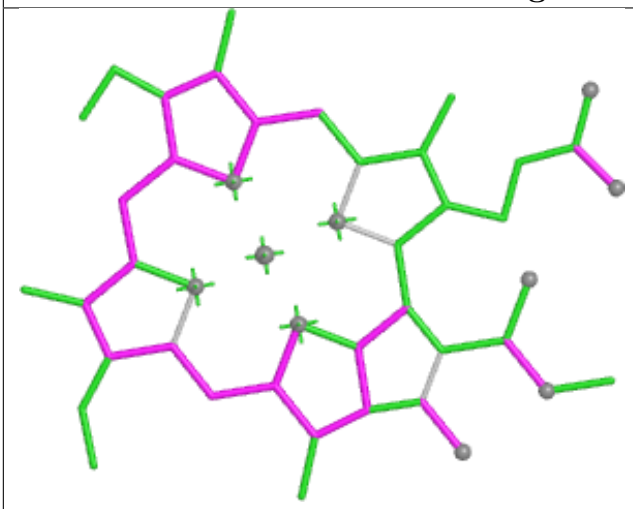


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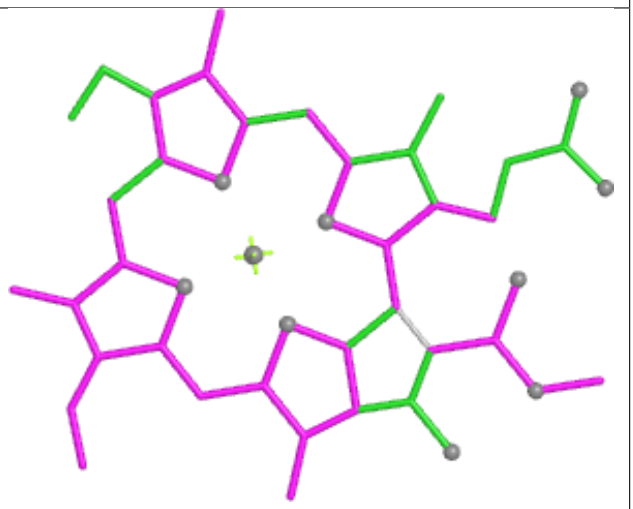


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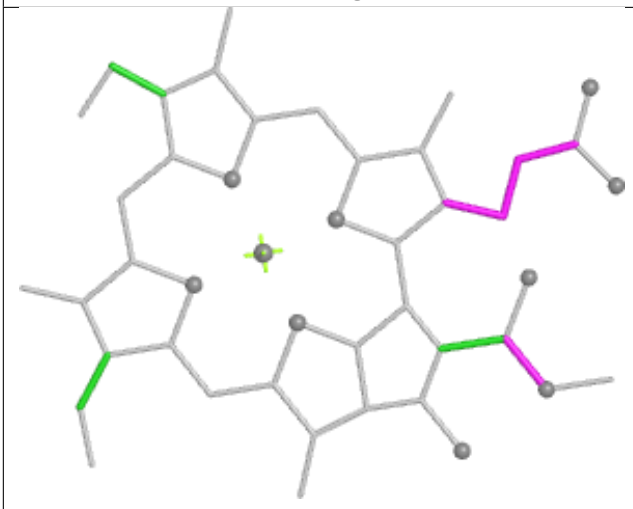
Ligand CLA 2 304



Bond lengths



Bond angles

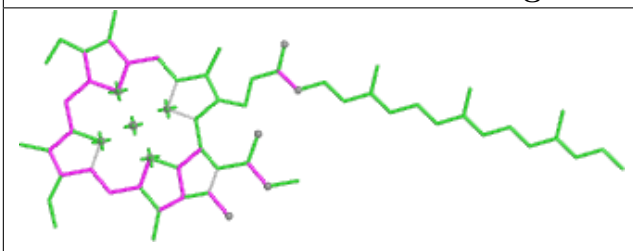


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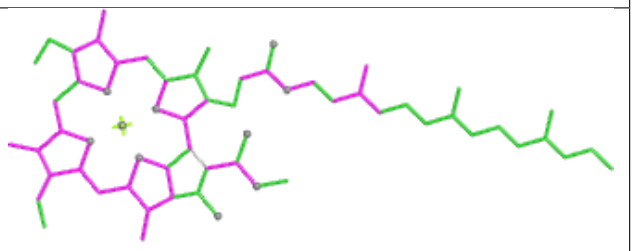


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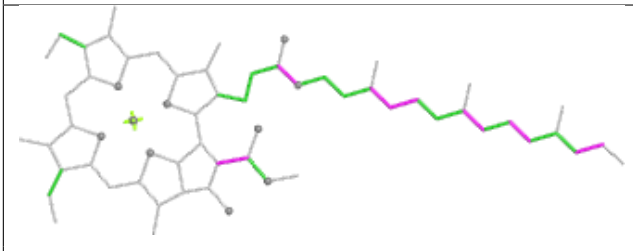
Ligand CLA A 815



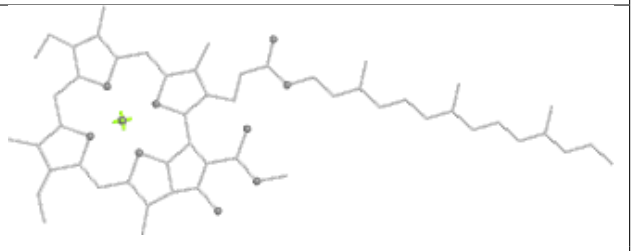
Bond lengths



Bond angles

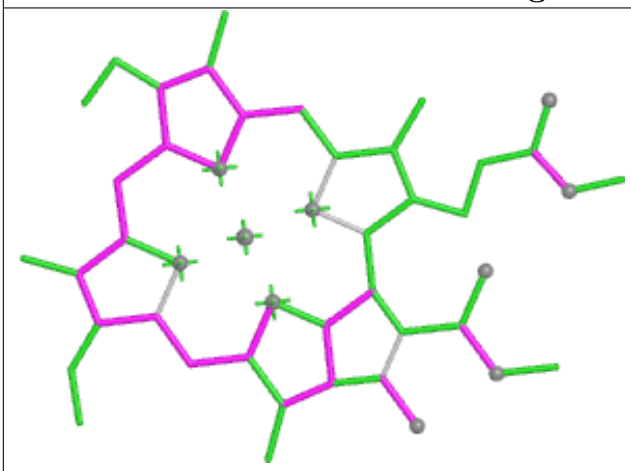


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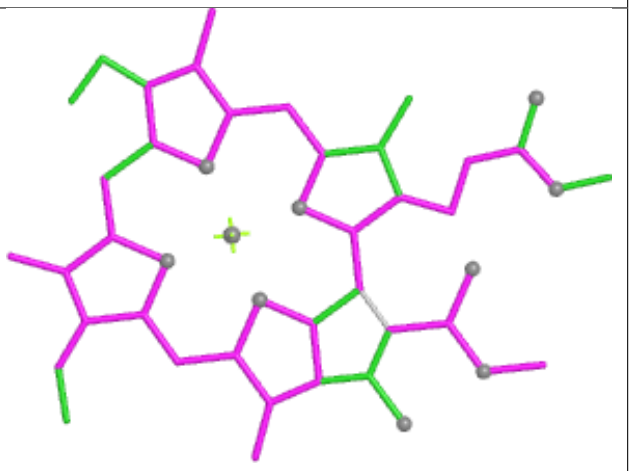


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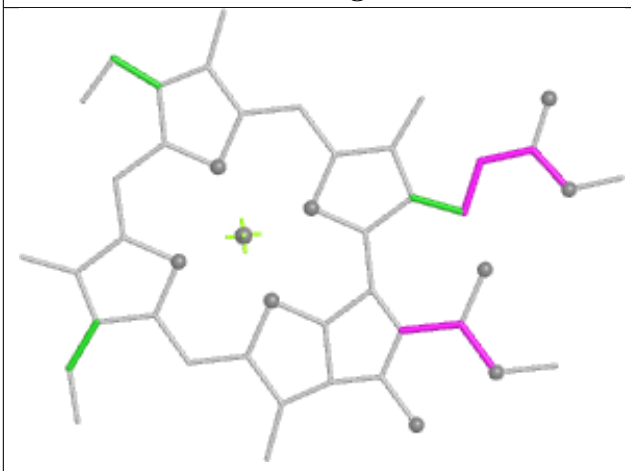
Ligand CLA 3 314



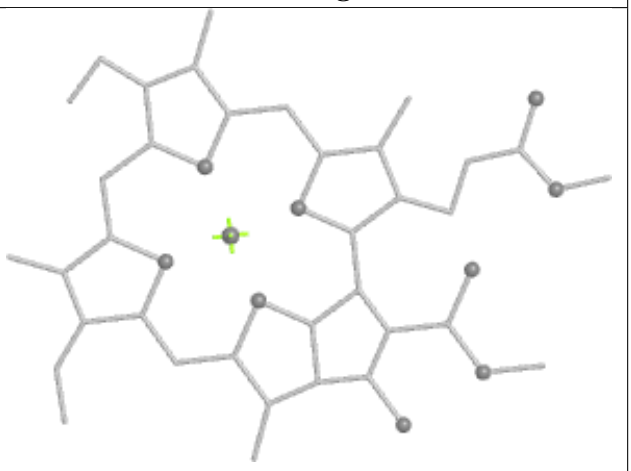
Bond lengths



Bond angles

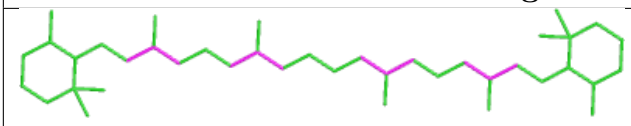


Torsions



Rings

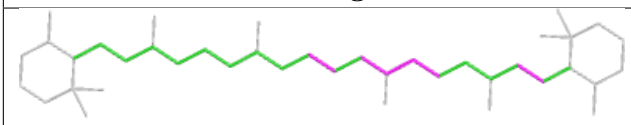
Ligand BCR K 104



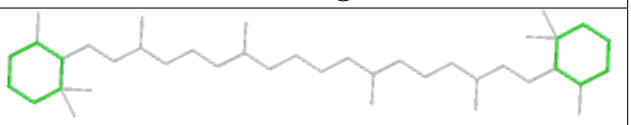
Bond lengths



Bond angles

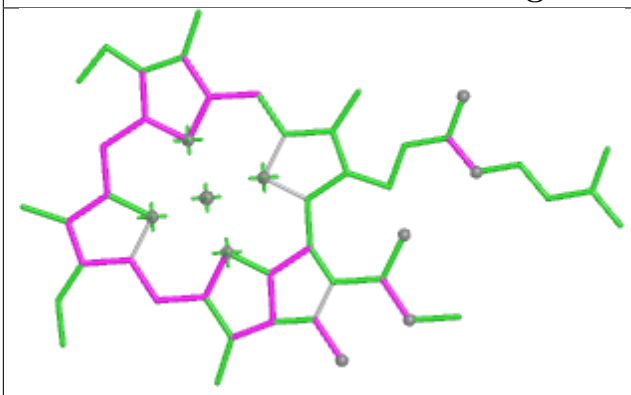


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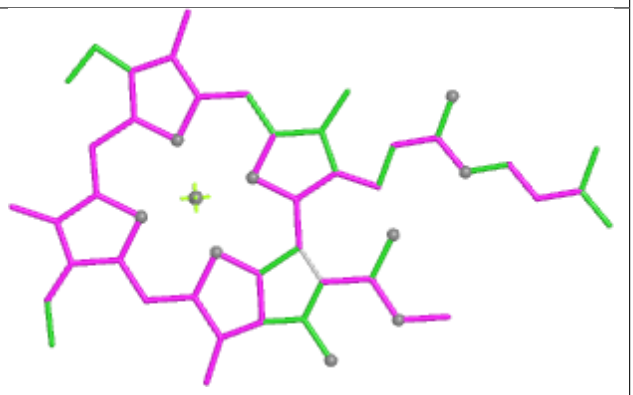


Rings

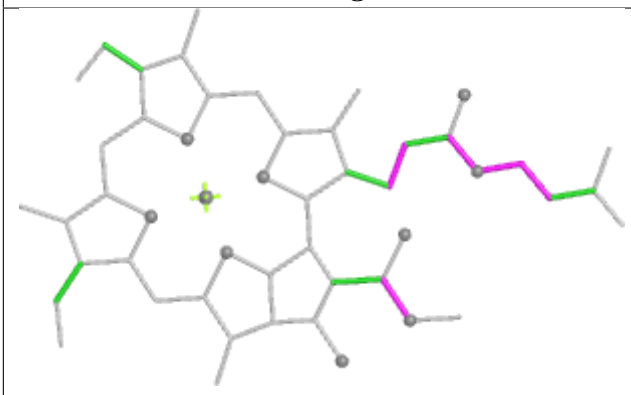
Ligand CLA L 204



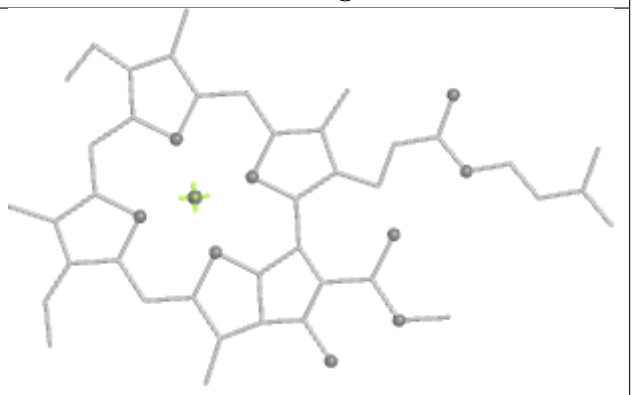
Bond lengths



Bond angles

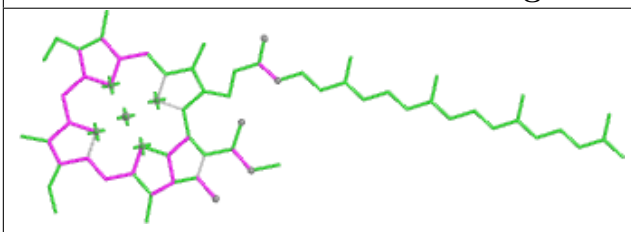


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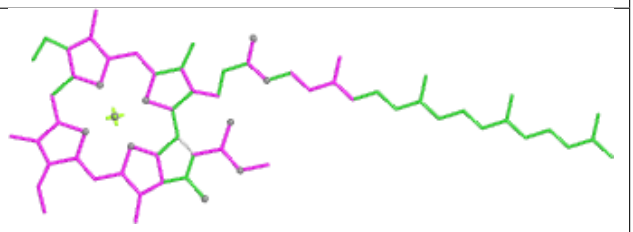


Rings

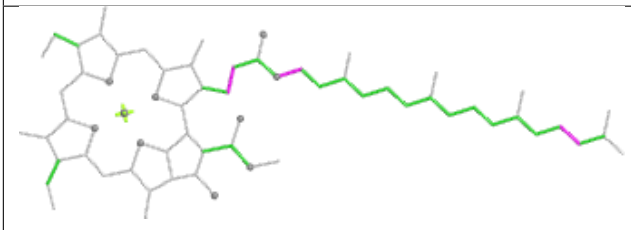
Ligand CLA A 853



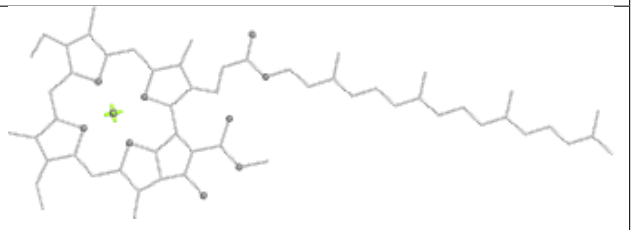
Bond lengths



Bond angles

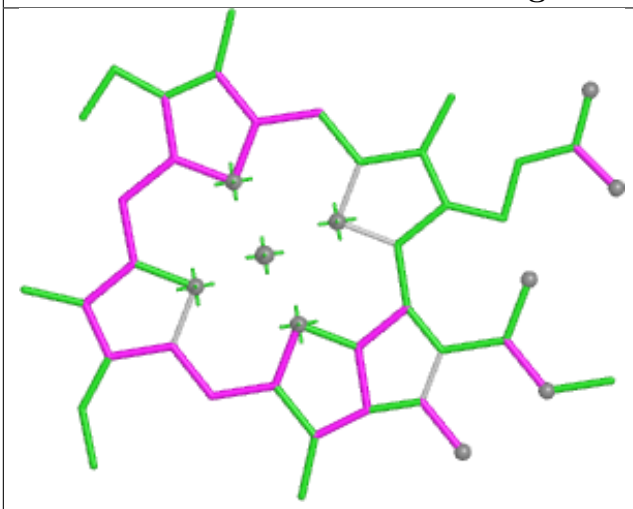


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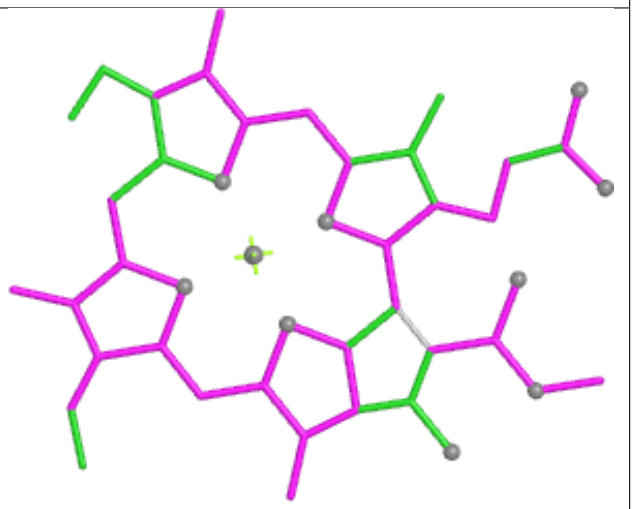


Rings

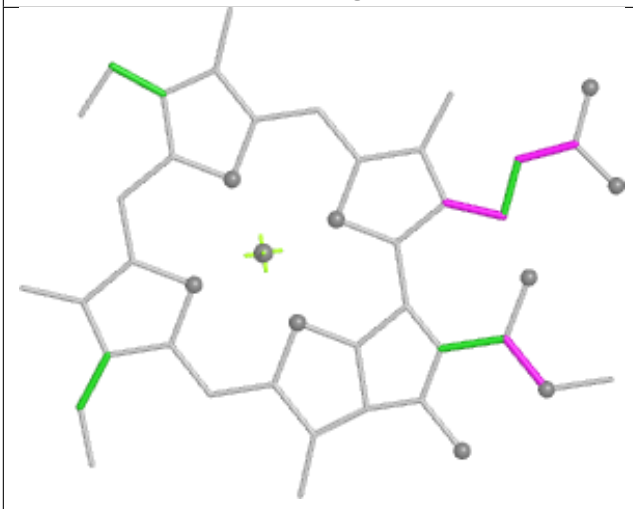
Ligand CLA 3 310



Bond lengths



Bond angles

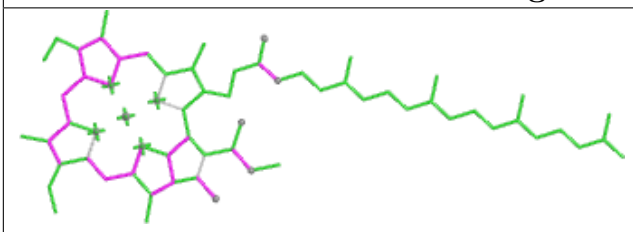


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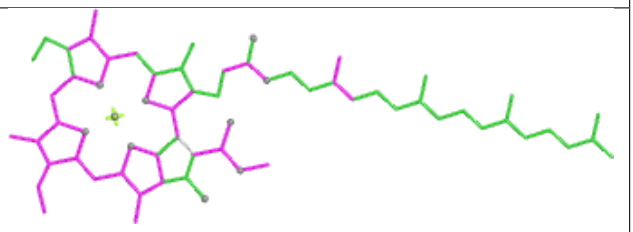


Rings

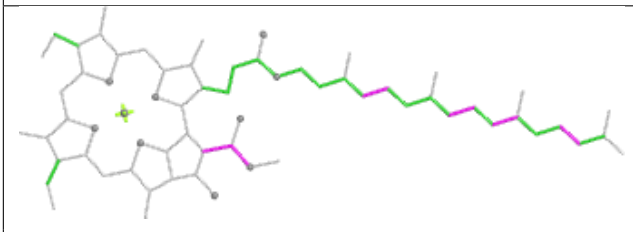
Ligand CLA 2 305



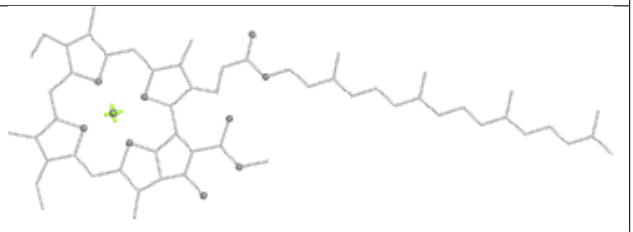
Bond lengths



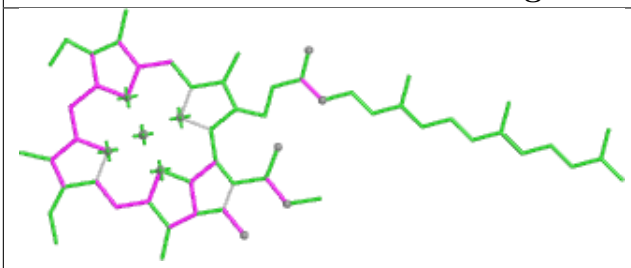
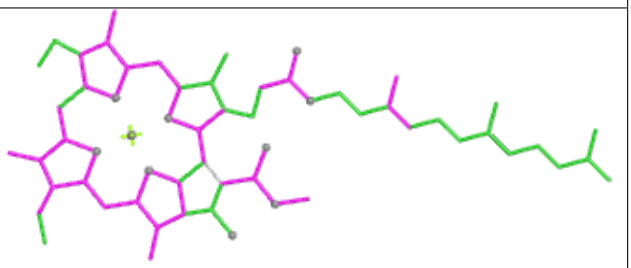
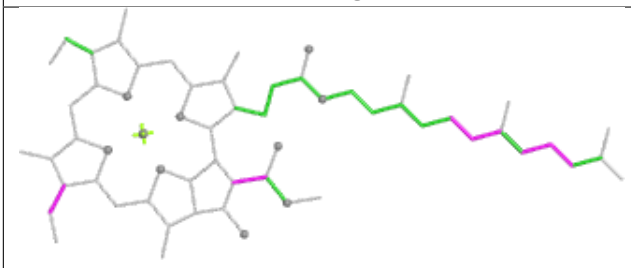
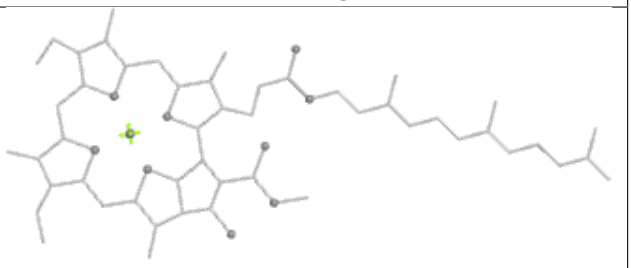
Bond angles

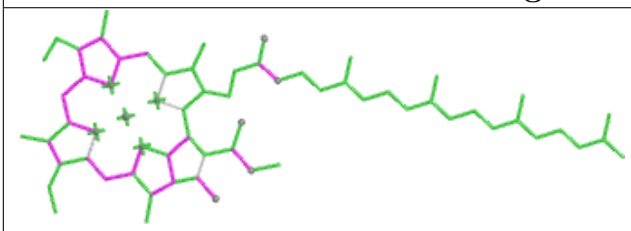
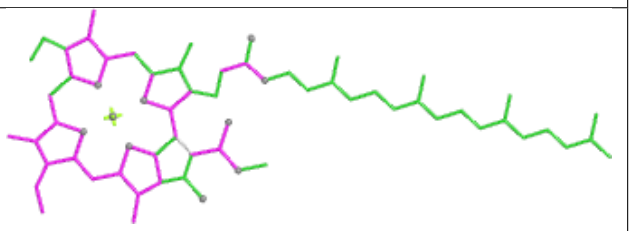
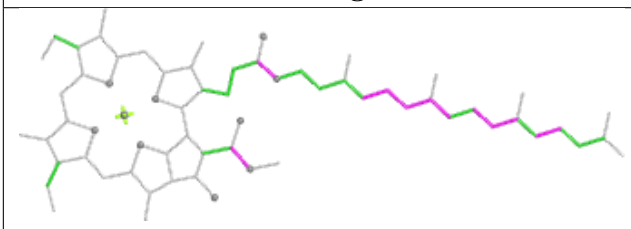
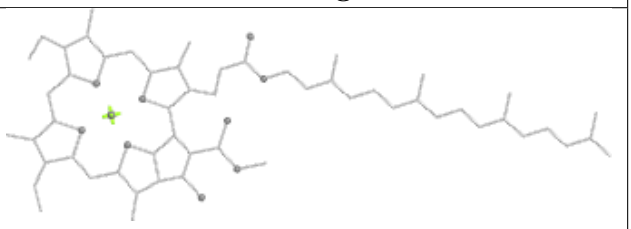


Torsions

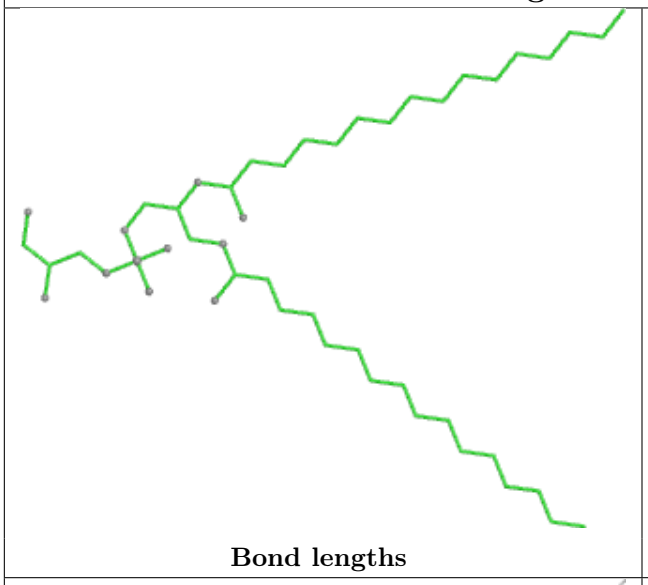


Rings

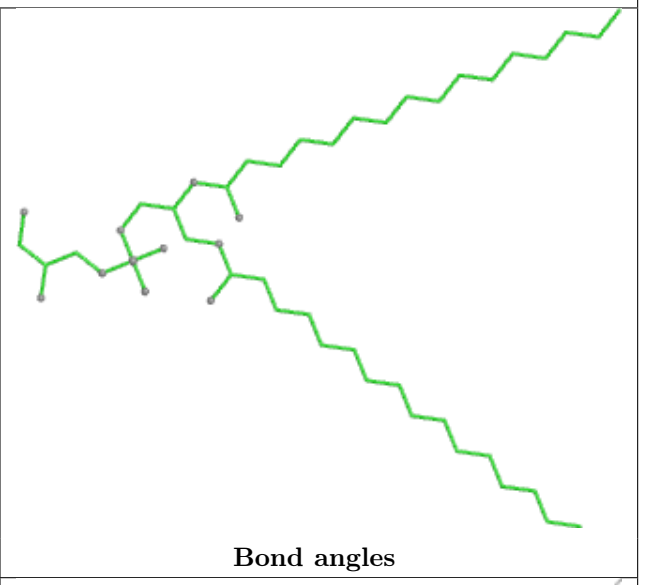
Ligand CLA B 836	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA B 816	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

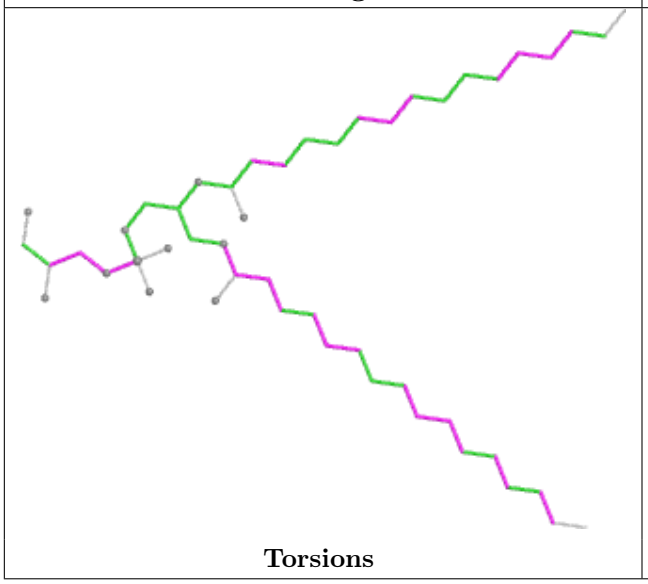
Ligand LHG J 102



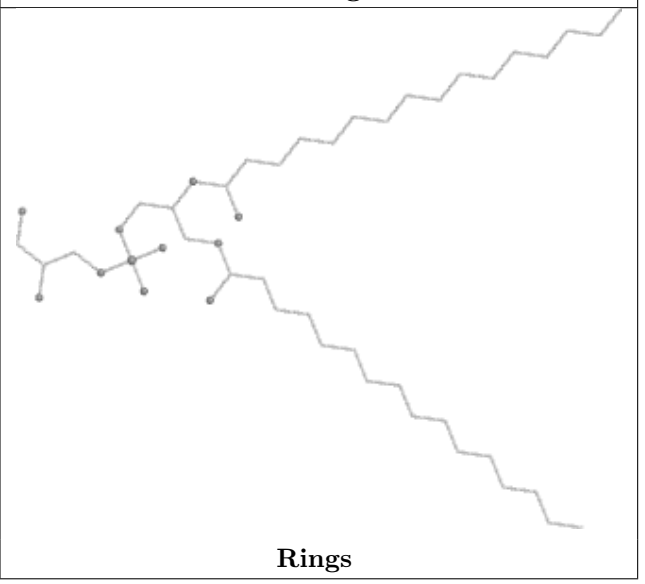
Bond lengths



Bond angles

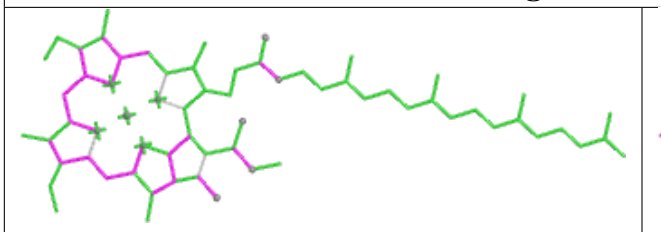


Torsions

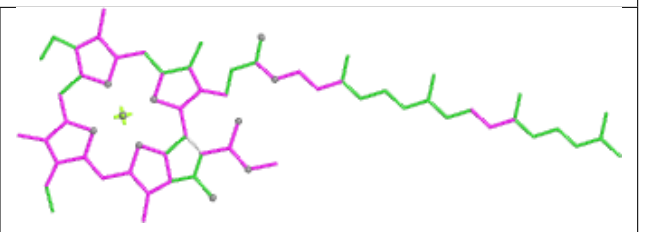


Rings

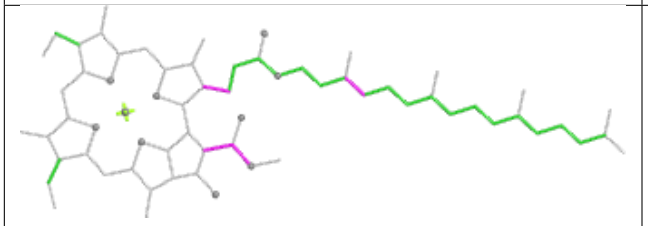
Ligand CLA A 832



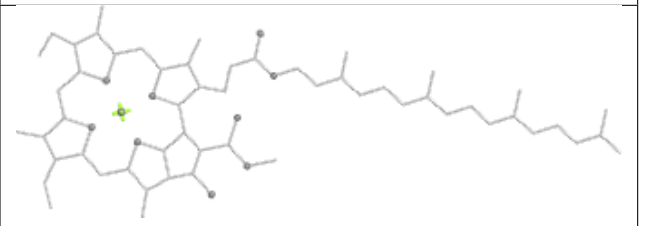
Bond lengths



Bond angles

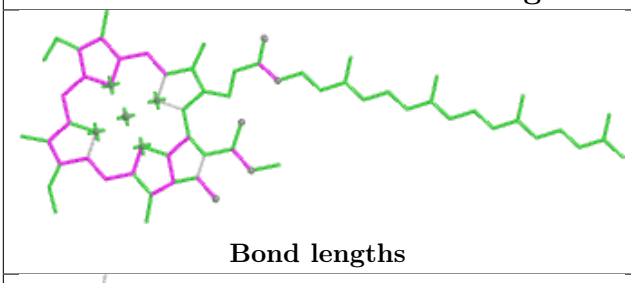


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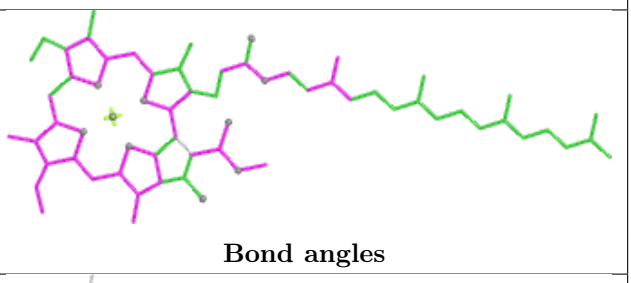


Rings

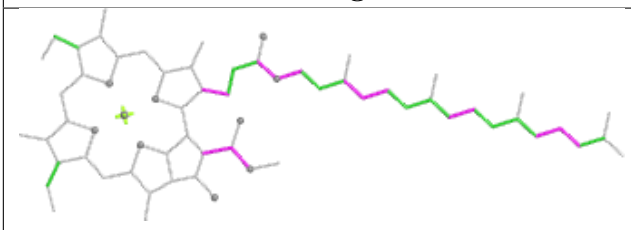
Ligand CLA A 834



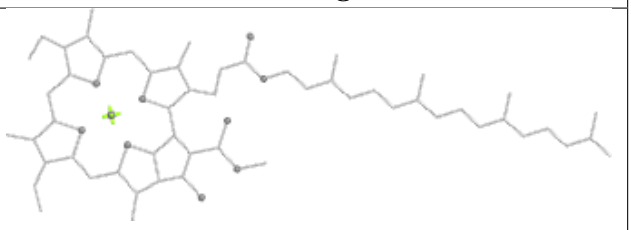
Bond lengths



Bond angles

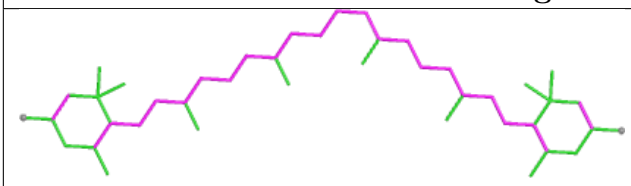


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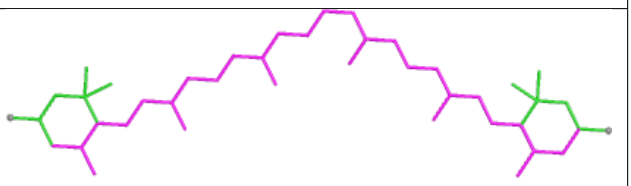


Rings

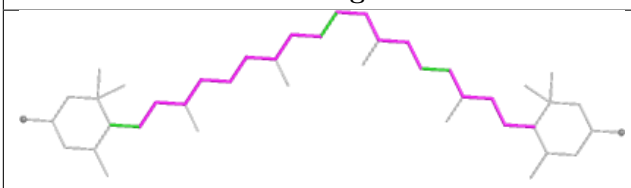
Ligand 5X6 3 317



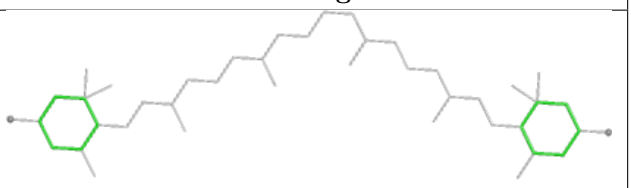
Bond lengths



Bond angles

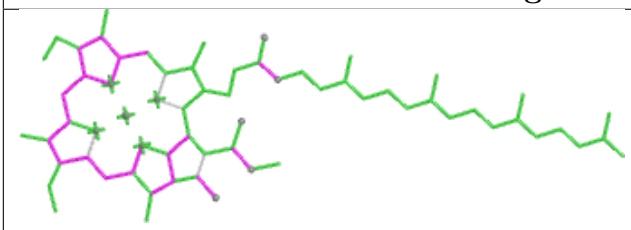


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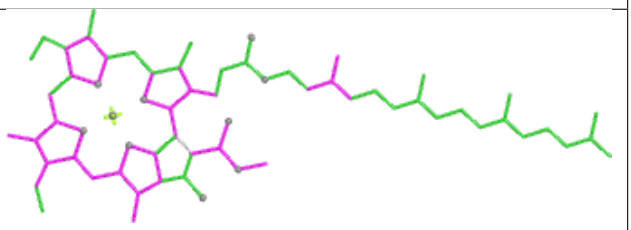


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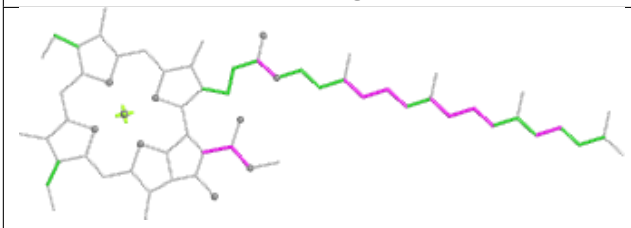
Ligand CLA B 815



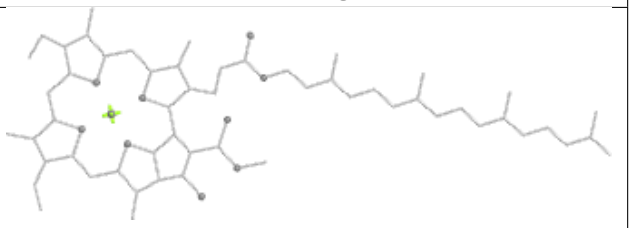
Bond lengths



Bond angles

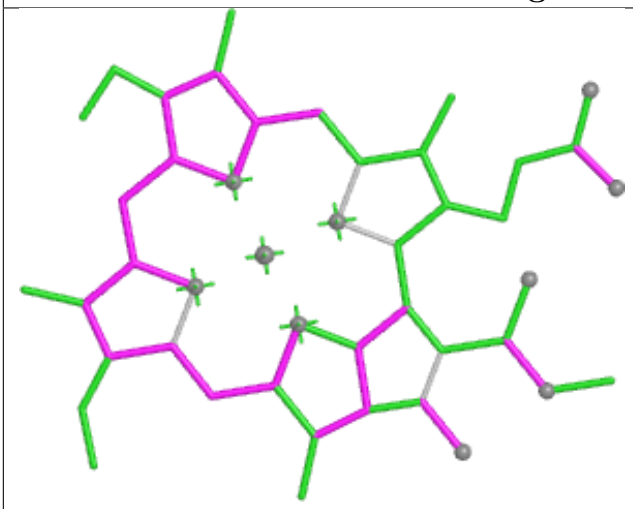


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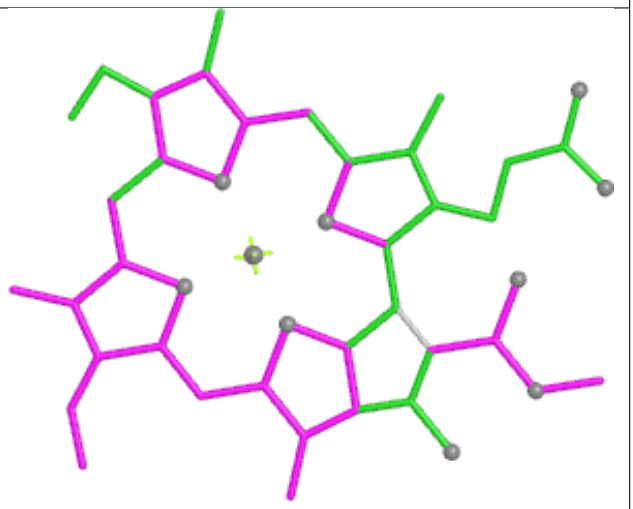


Rings

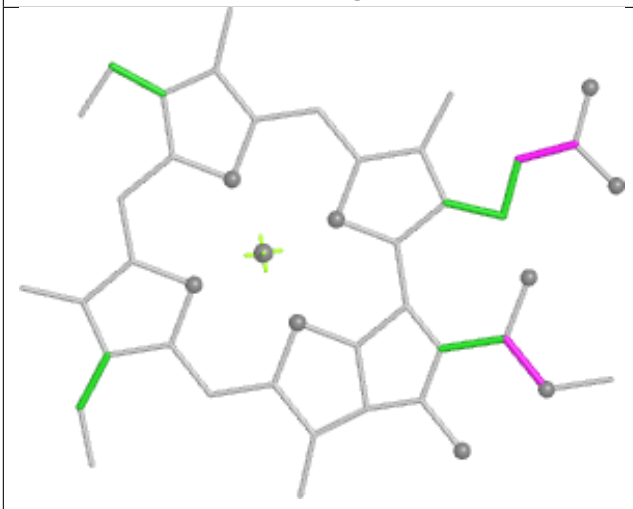
Ligand CLA 5 307



Bond lengths



Bond angles

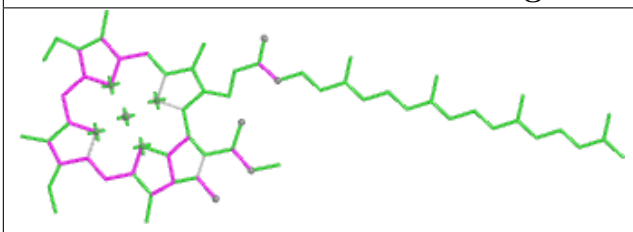


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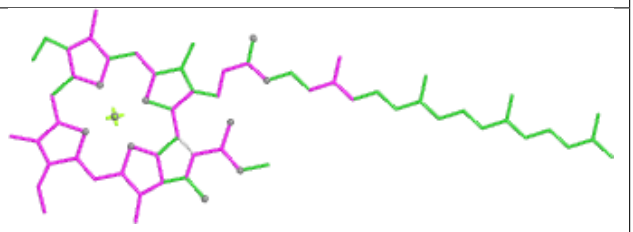


Rings

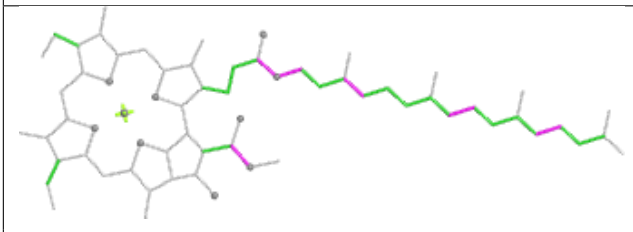
Ligand CLA B 840



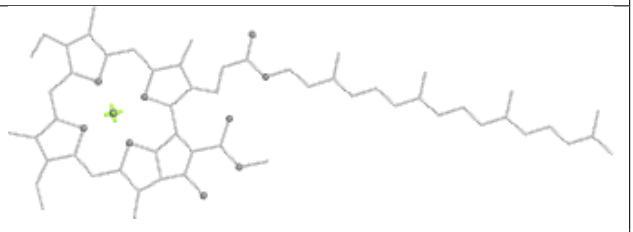
Bond lengths



Bond angles

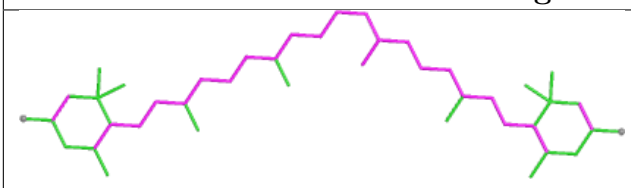


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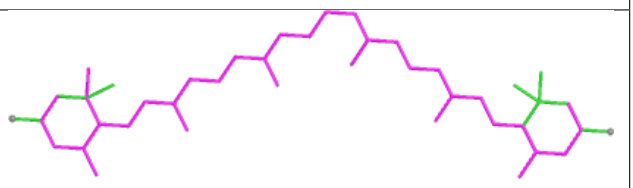


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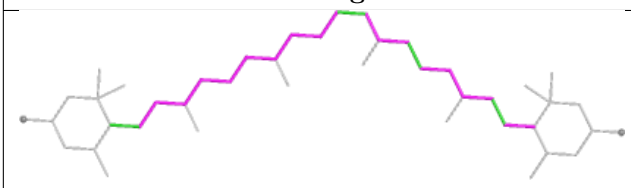
Ligand 5X6 5 318



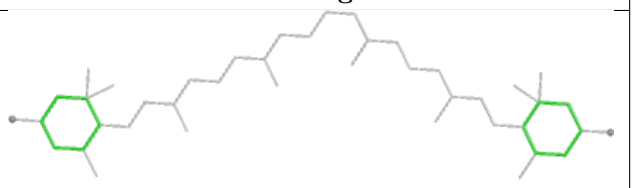
Bond lengths



Bond angles

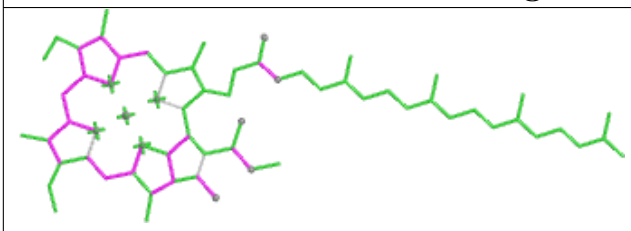


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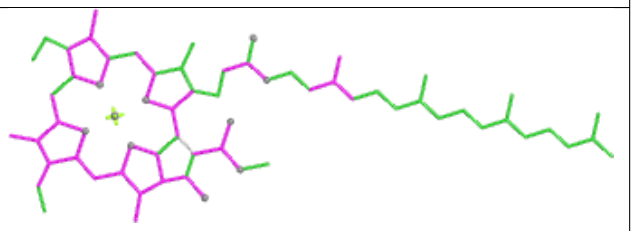


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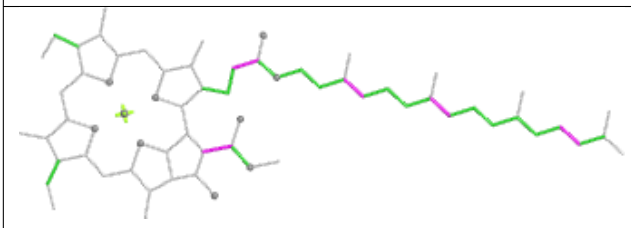
Ligand CLA A 811



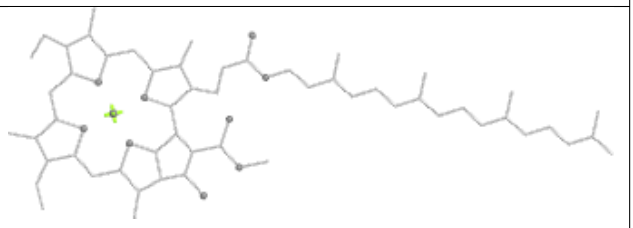
Bond lengths



Bond angles

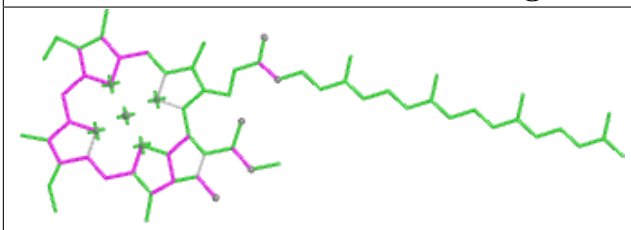


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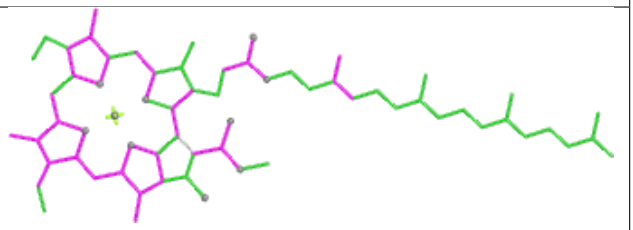


Rings

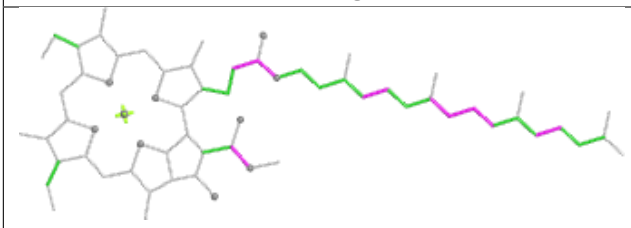
Ligand CLA A 839



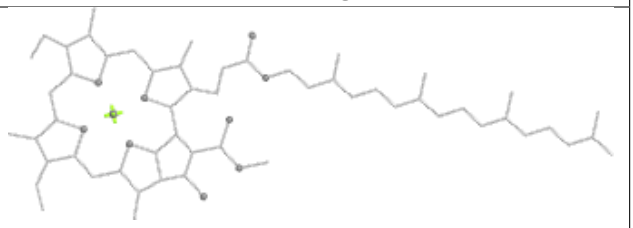
Bond lengths



Bond angles

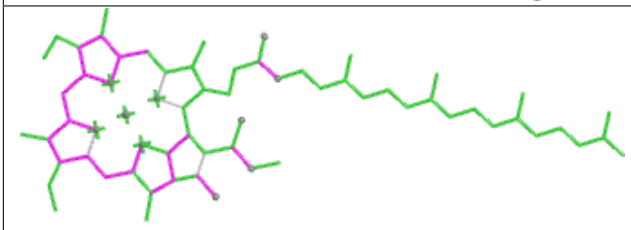


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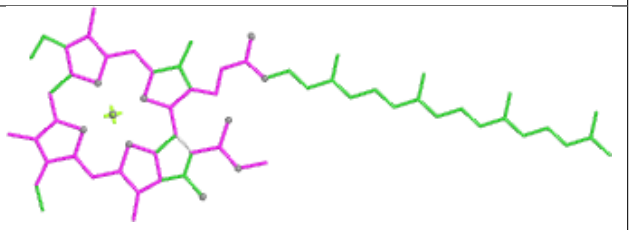


Rings

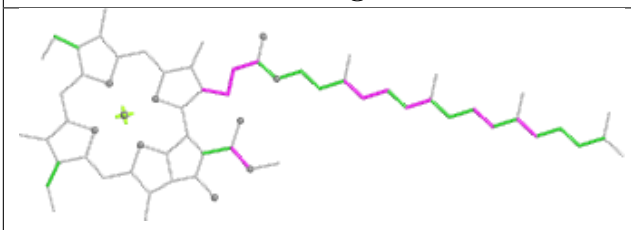
Ligand CLA 5 308



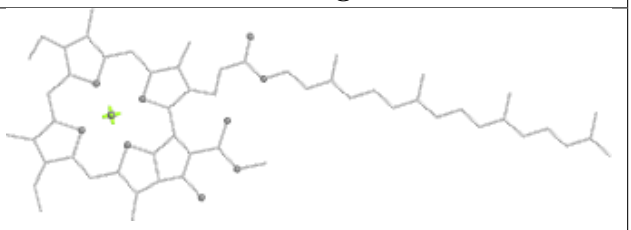
Bond lengths



Bond angles

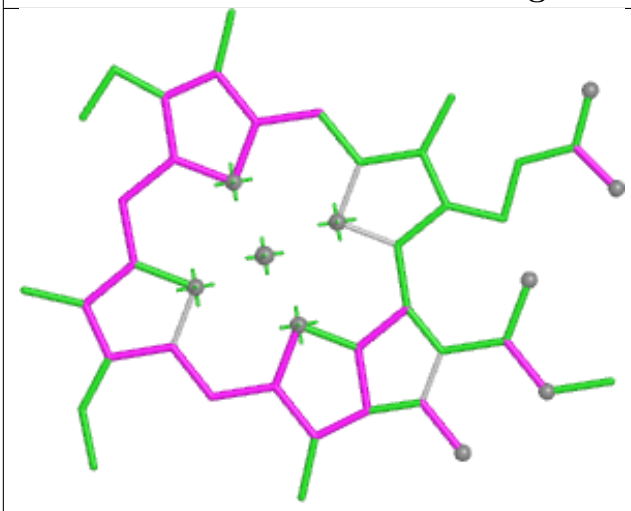


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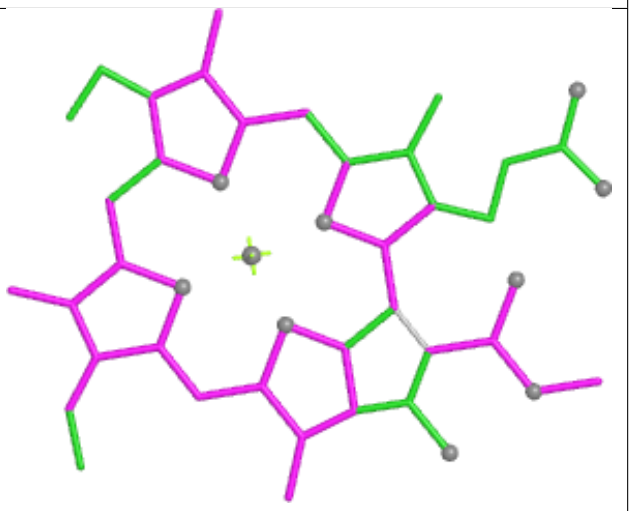


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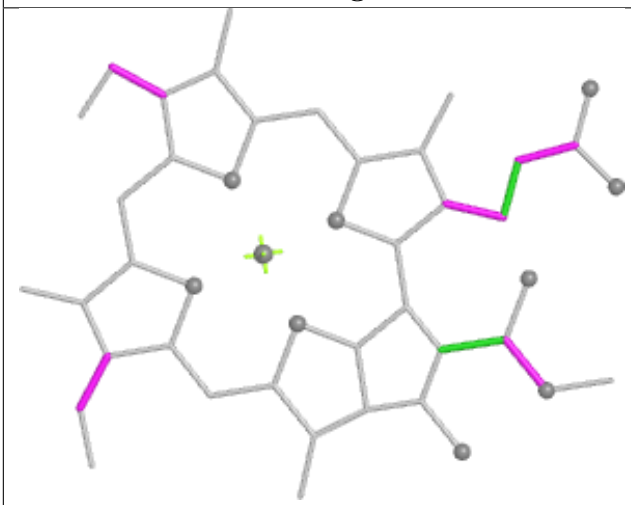
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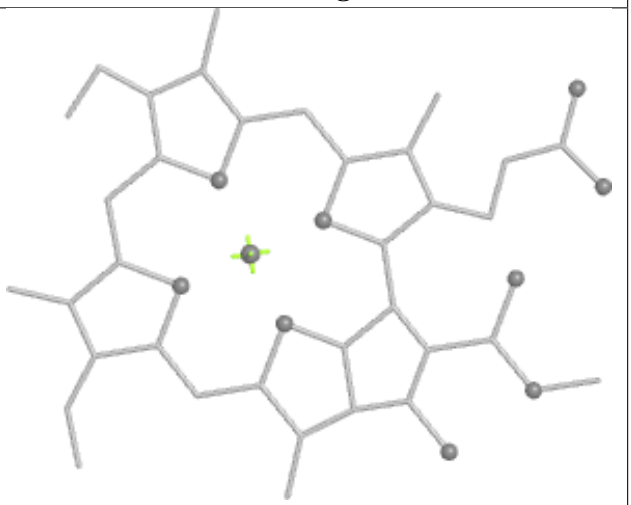
Bond lengths



Bond angles

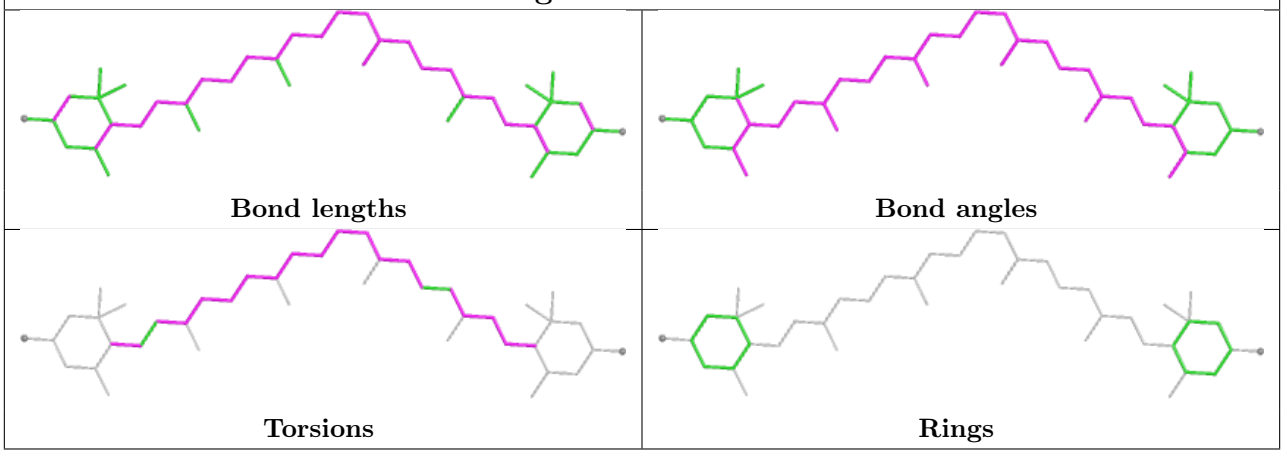


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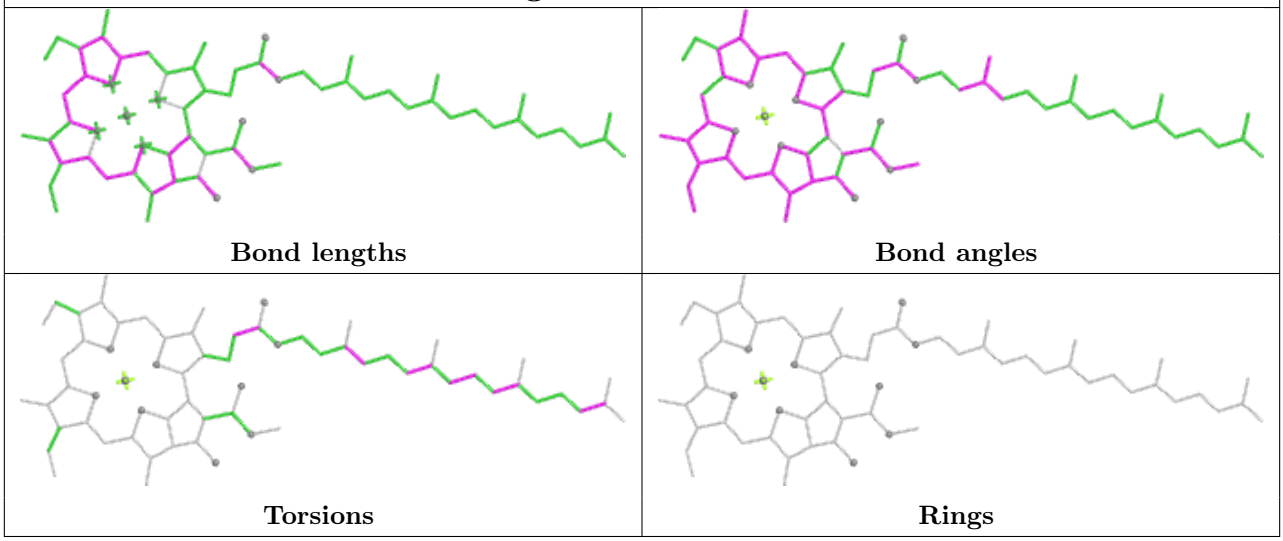


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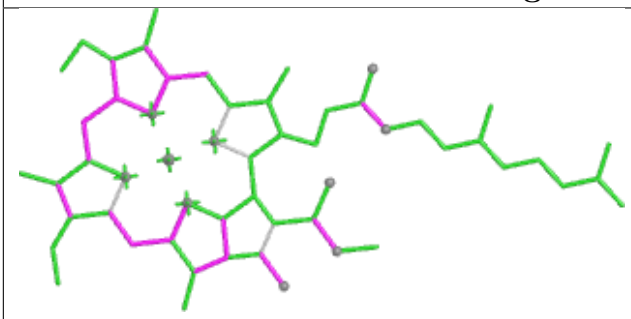
Ligand 5X6 2 317



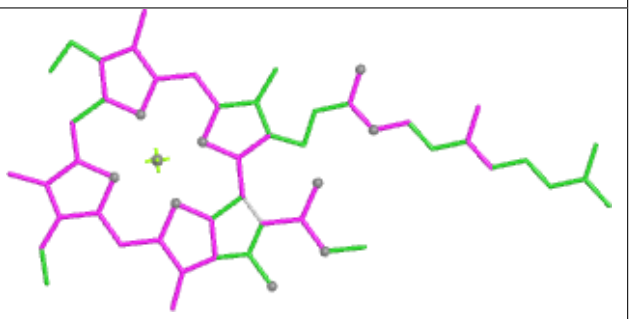
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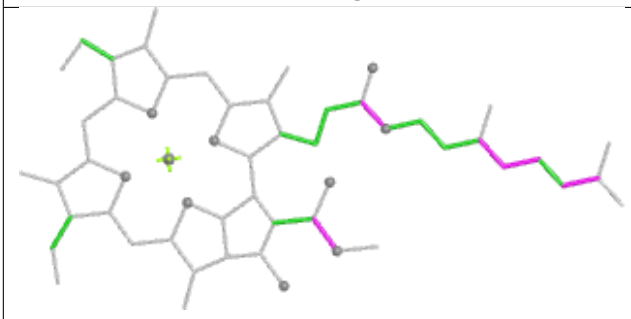
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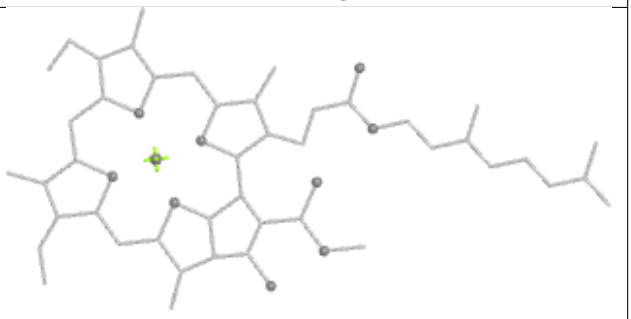
Bond lengths



Bond angles

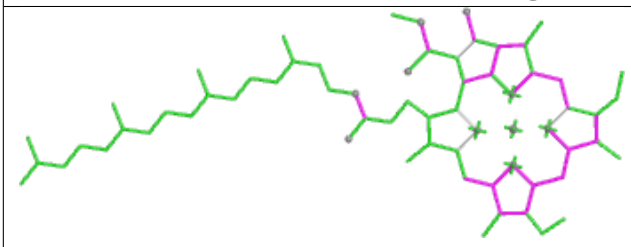


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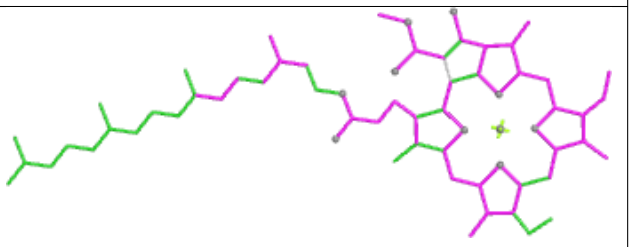


Rings

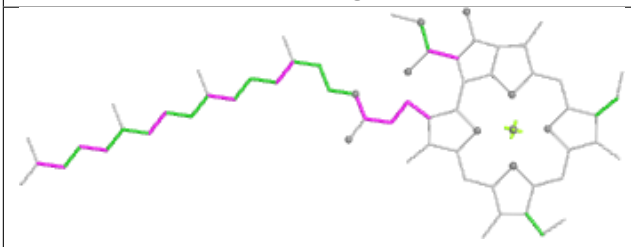
Ligand CLA B 805



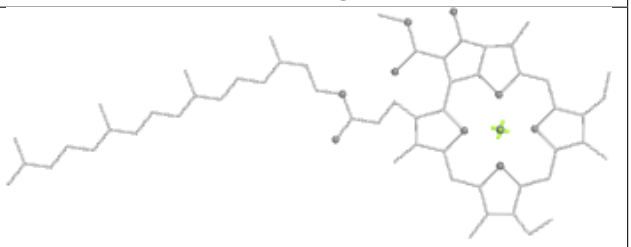
Bond lengths



Bond angles

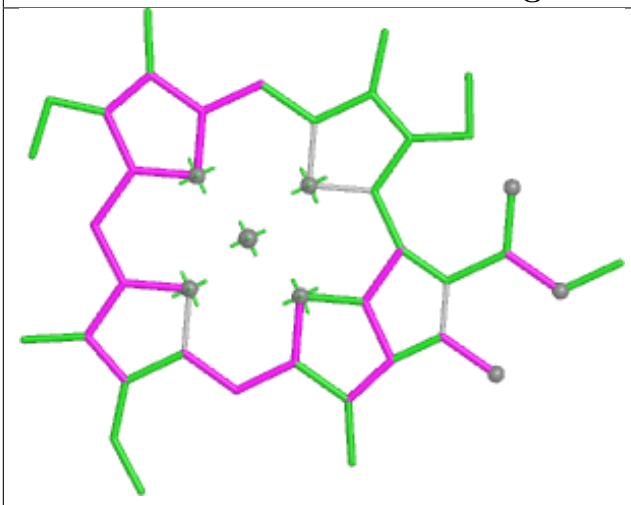


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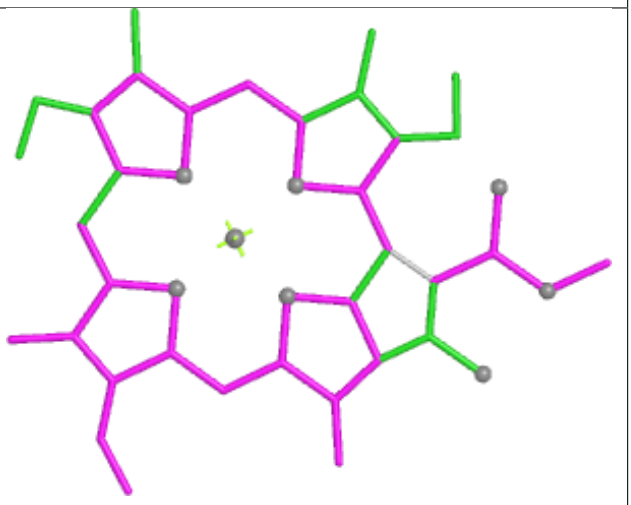


Rings

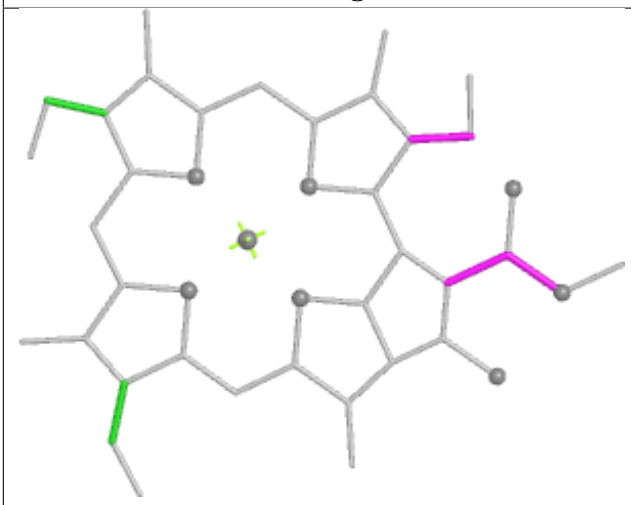
Ligand CLA A 813



Bond lengths



Bond angles

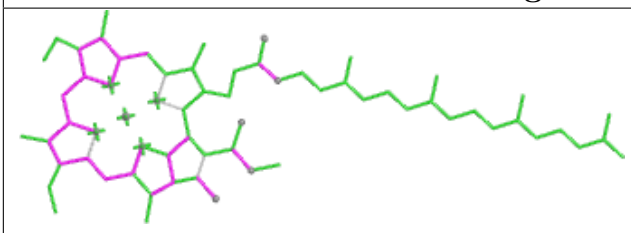


Torsions

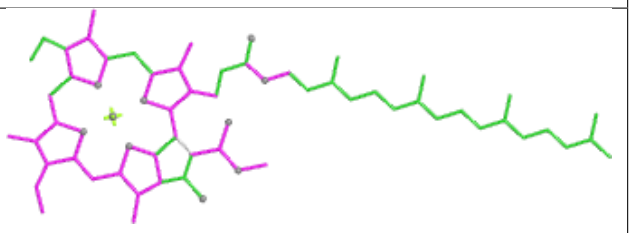


Rings

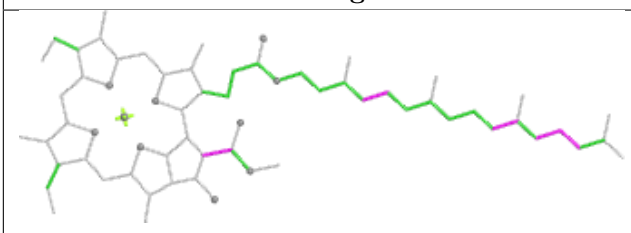
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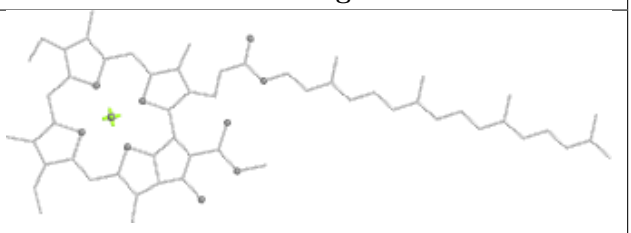
Bond lengths



Bond angles

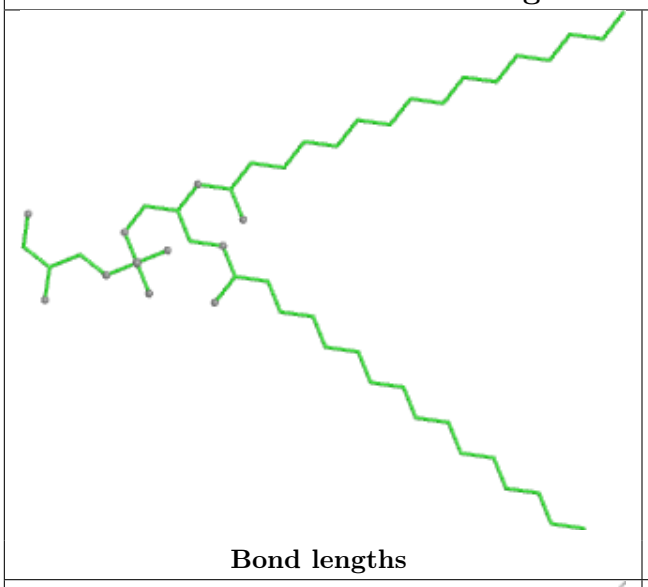


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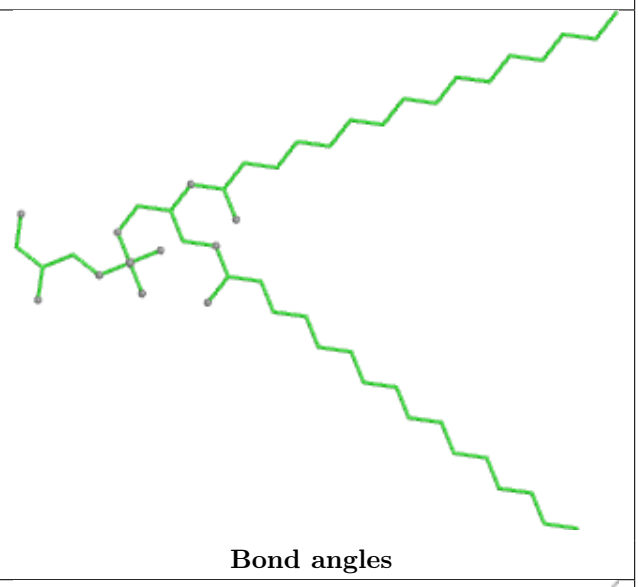


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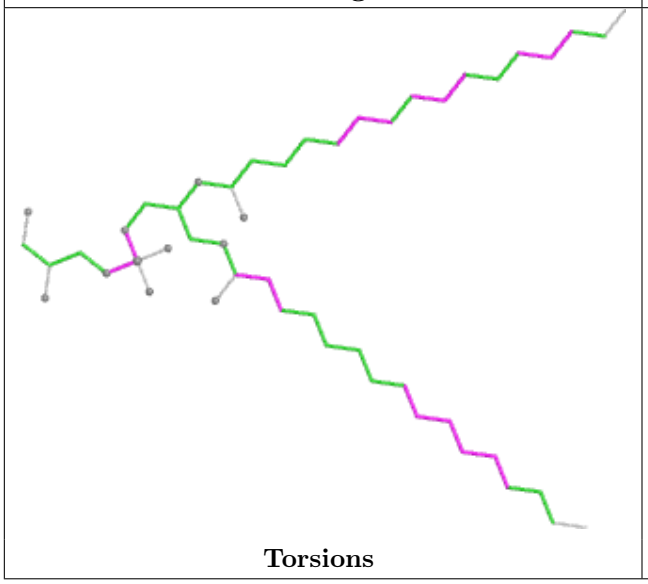
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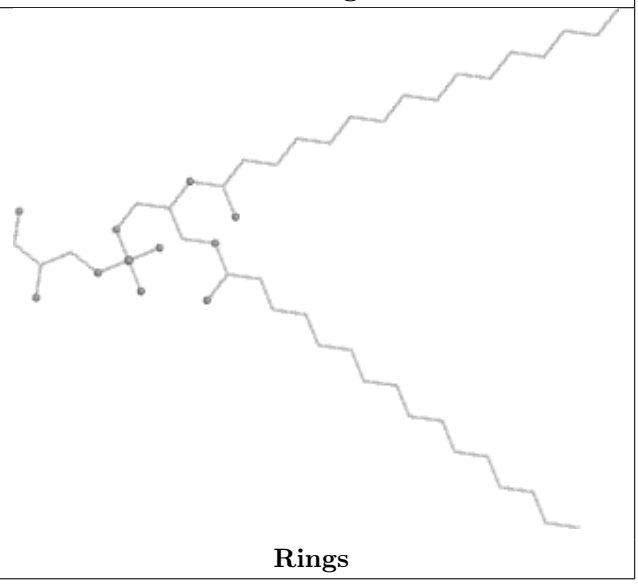
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Bond angles

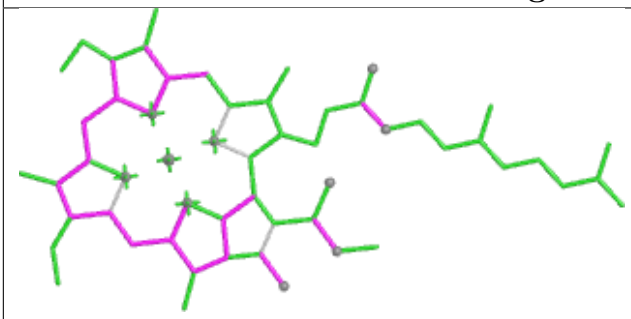


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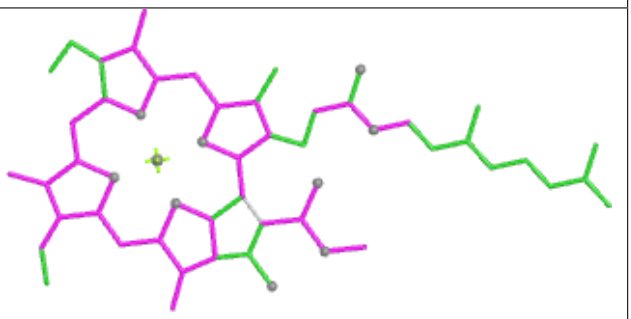


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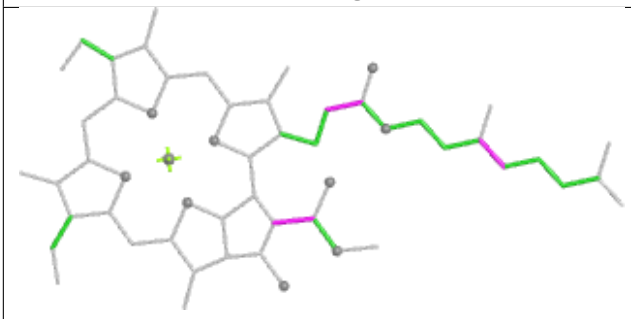
Ligand CLA 3 307



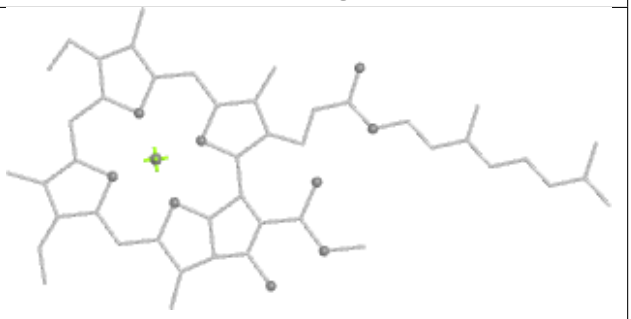
Bond lengths



Bond angles

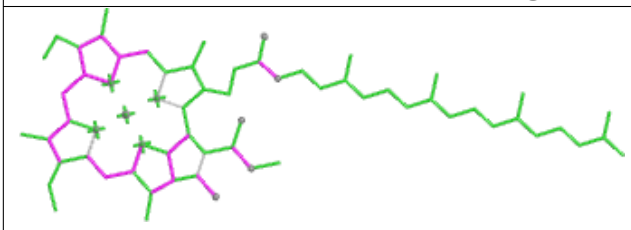


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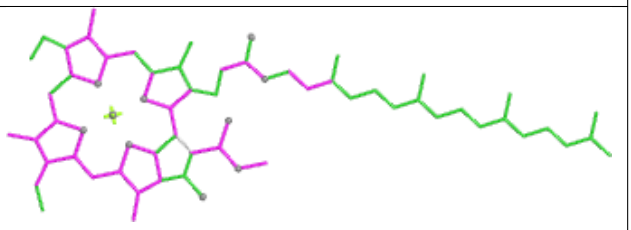


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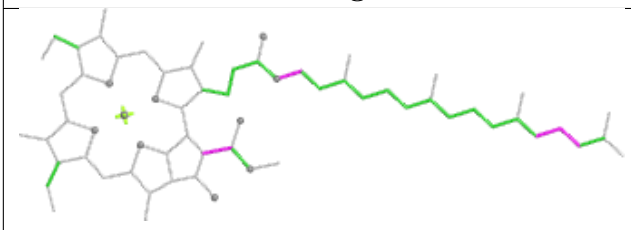
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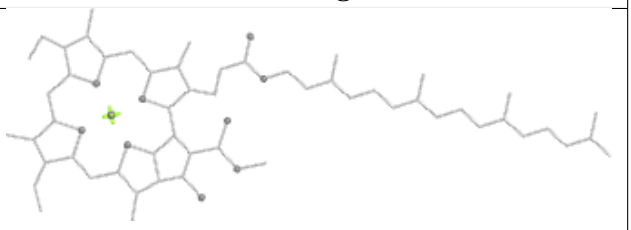
Bond lengths



Bond angles

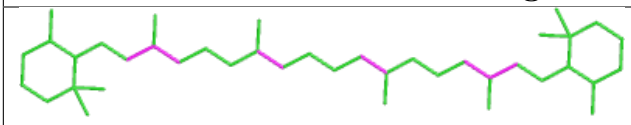


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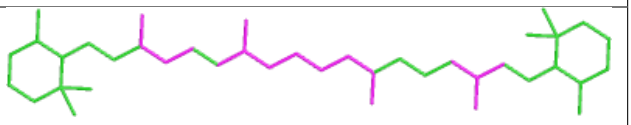


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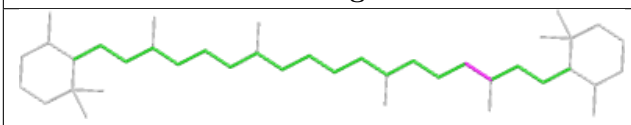
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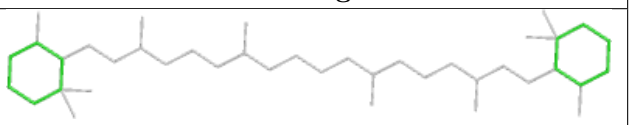
Bond lengths



Bond angles

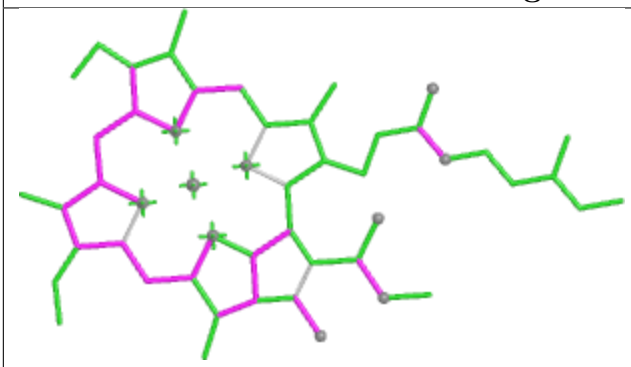


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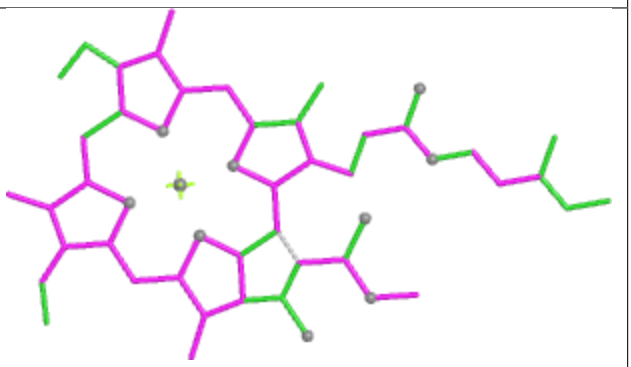


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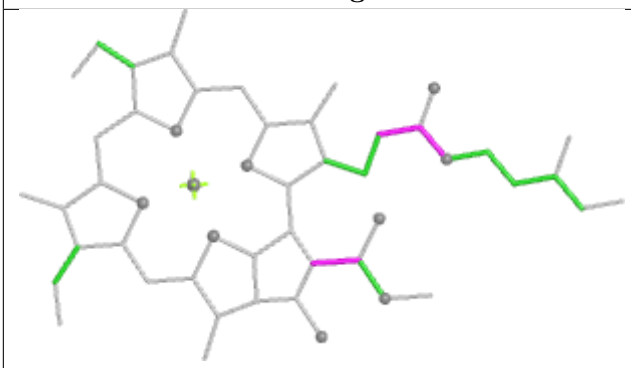
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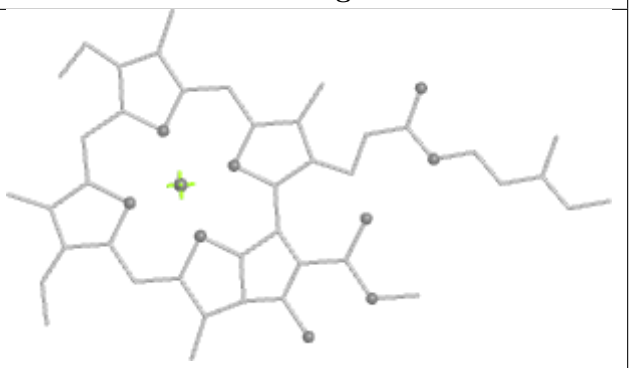
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Bond angles

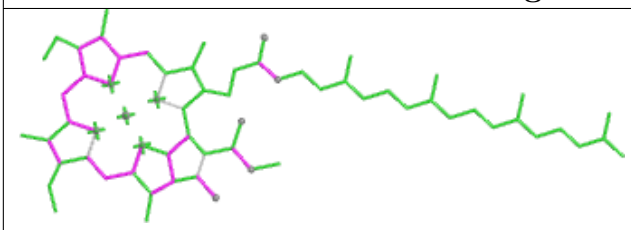


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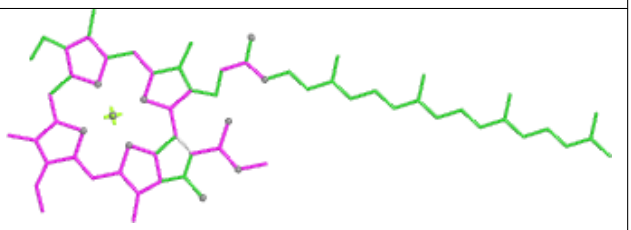


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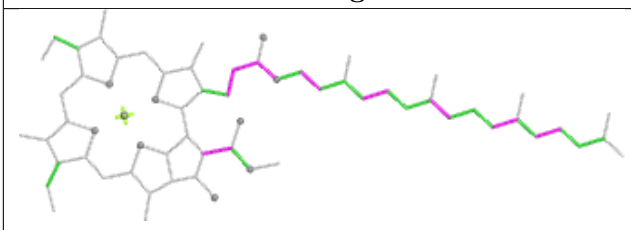
Ligand CLA B 811



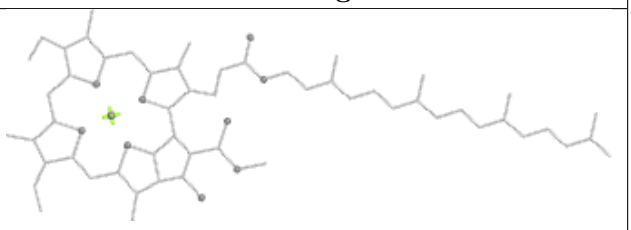
Bond lengths



Bond angles

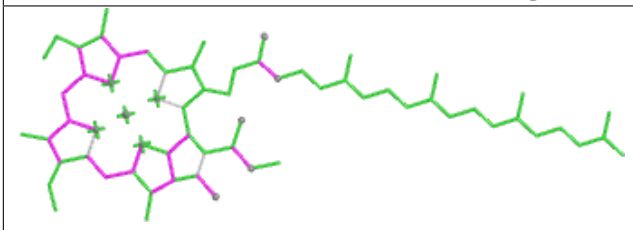


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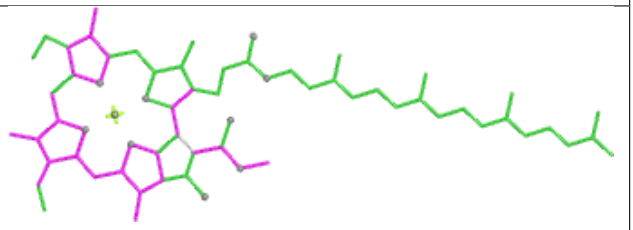


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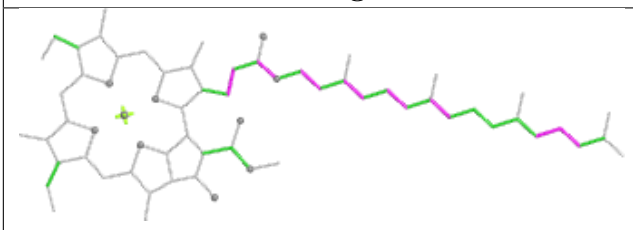
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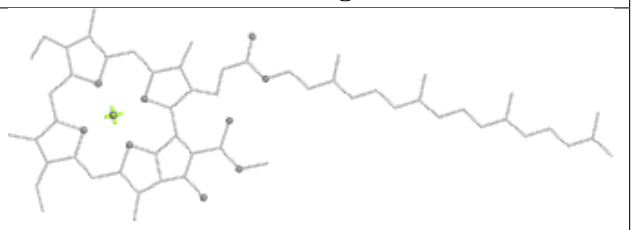
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Bond angles

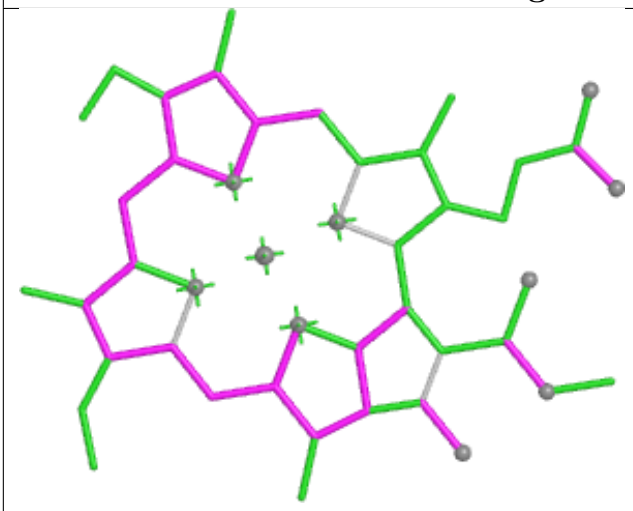


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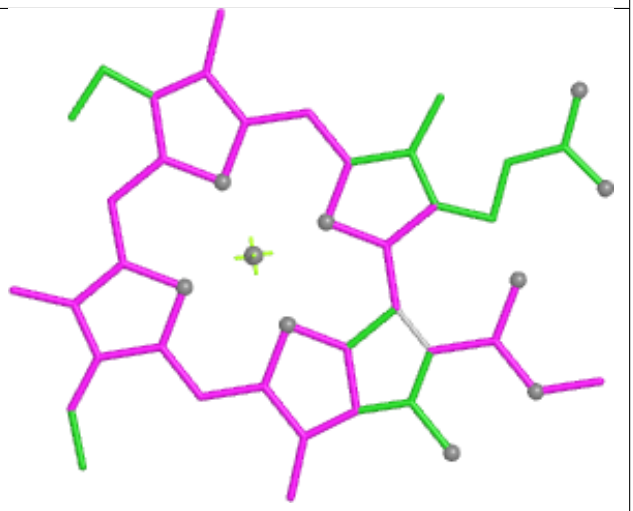


Rings

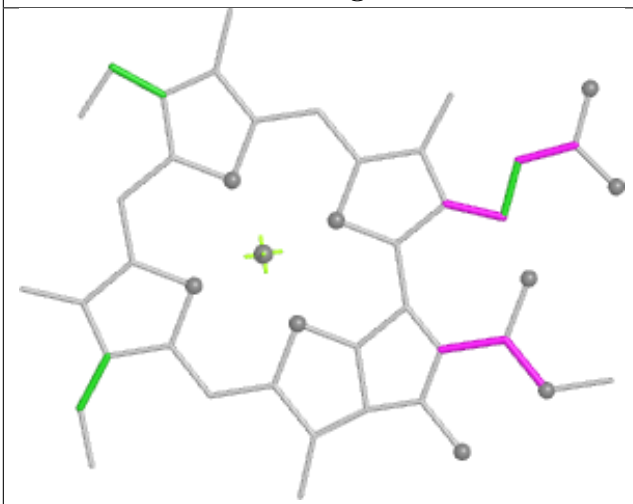
Ligand CLA 1 311



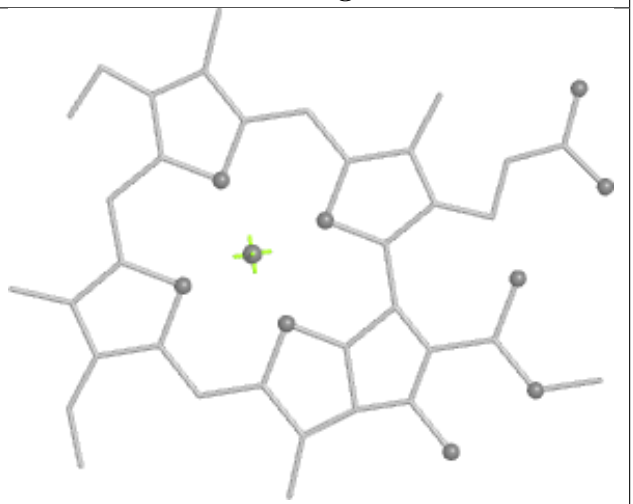
Bond lengths



Bond angles

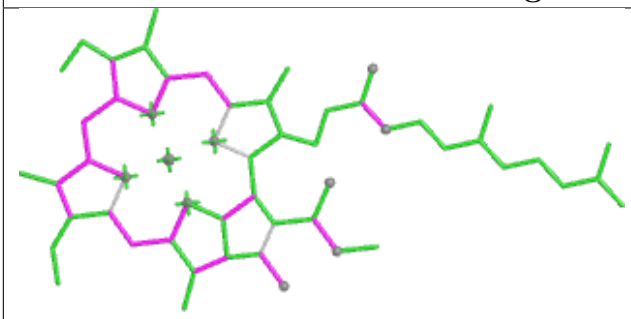


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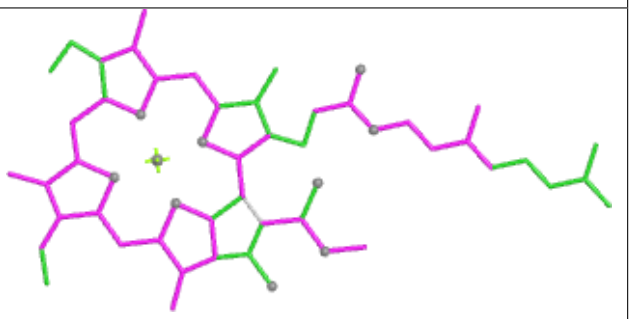


Rings

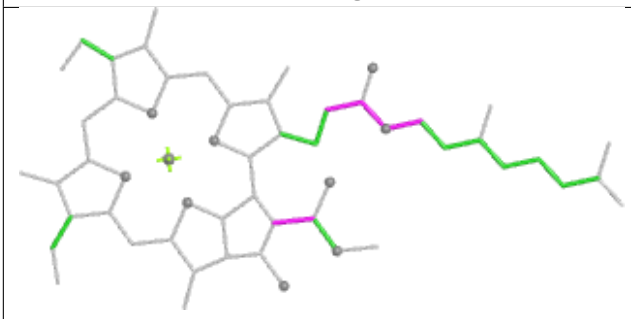
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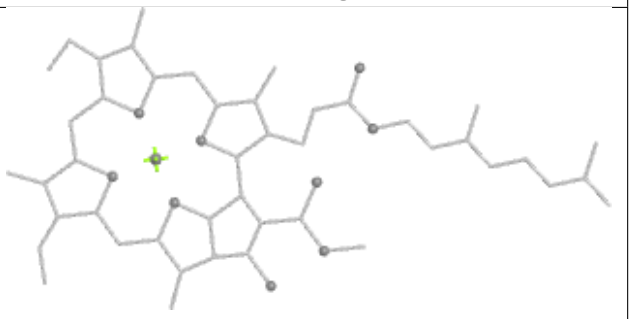
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Bond angles

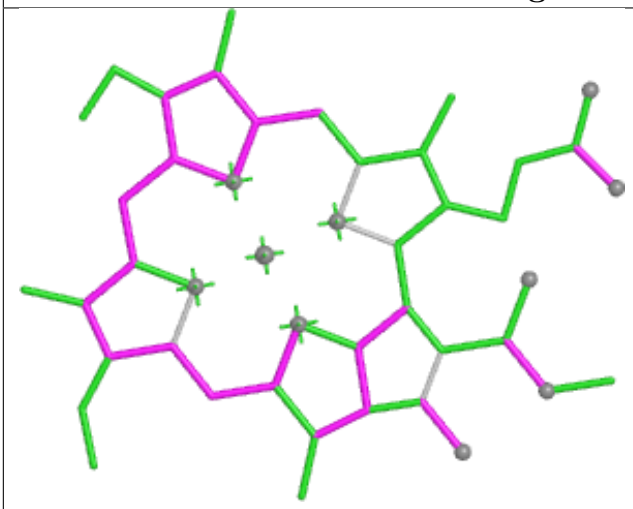


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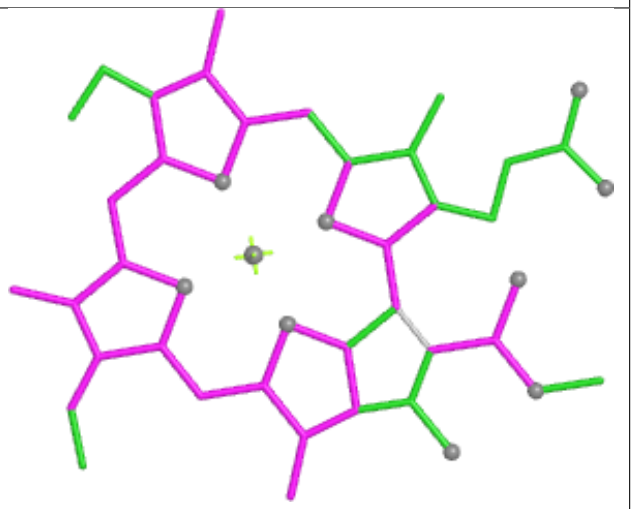


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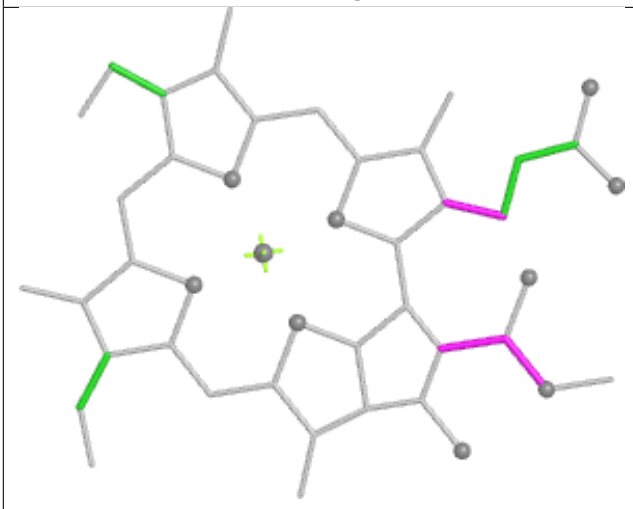
Ligand CLA 1 310



Bond lengths



Bond angles

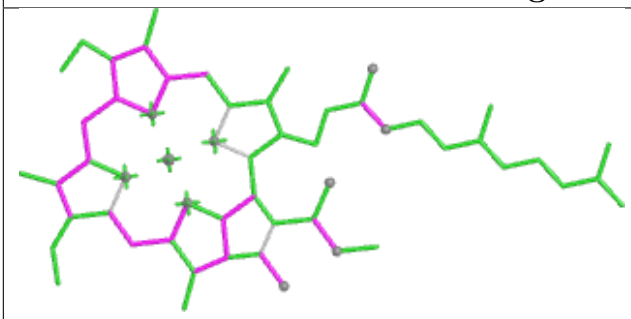


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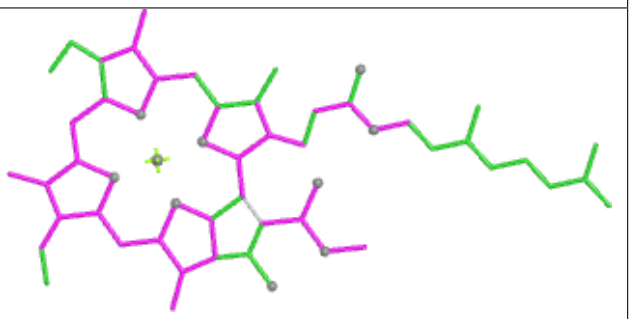


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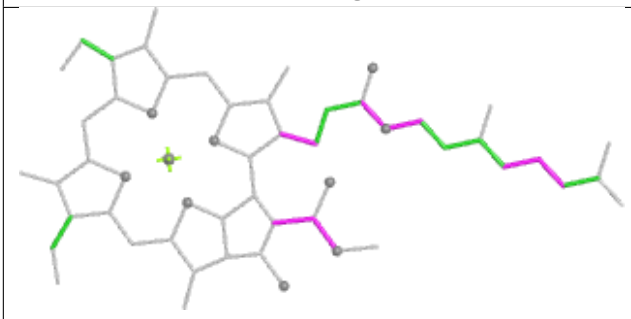
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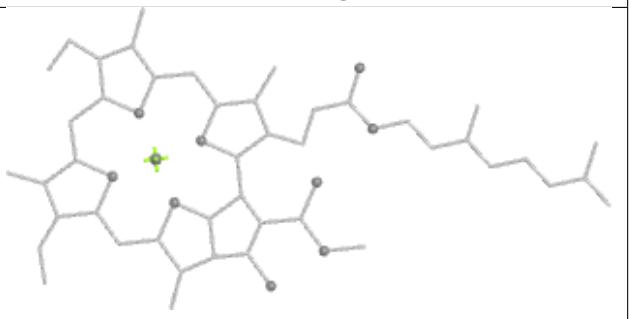
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Bond angles

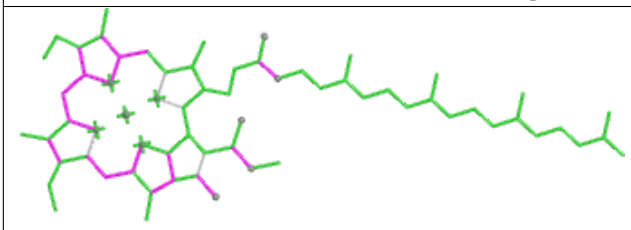


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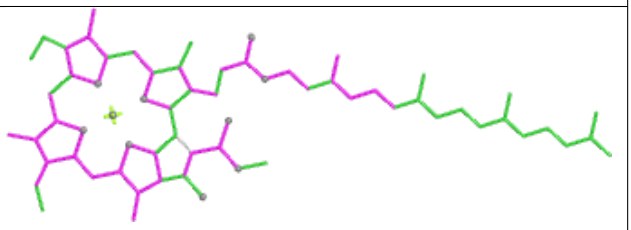


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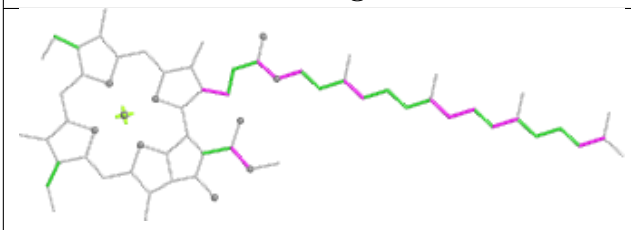
Ligand CLA B 802



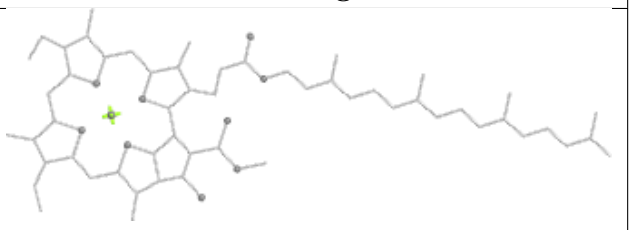
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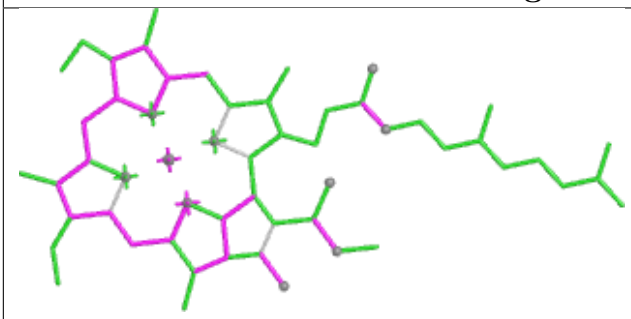
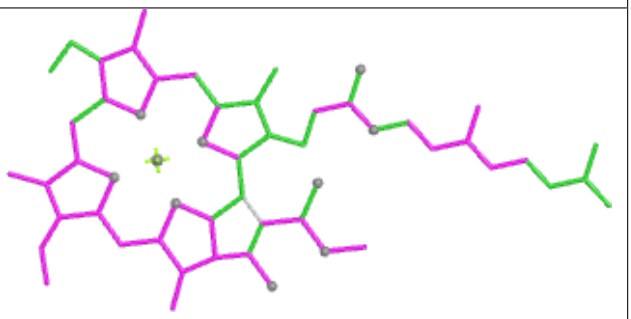
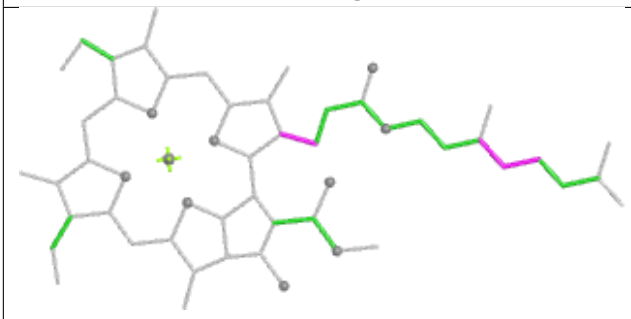
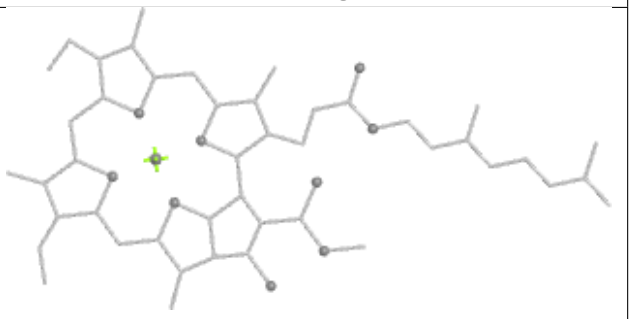
Bond angles

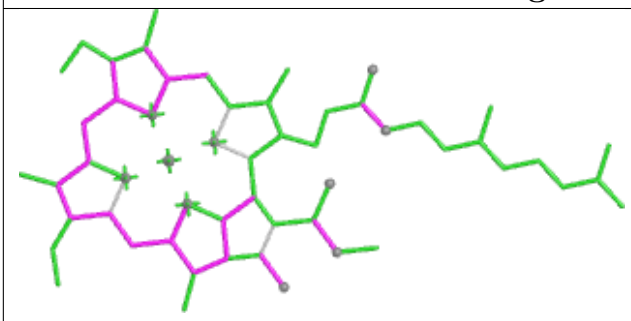
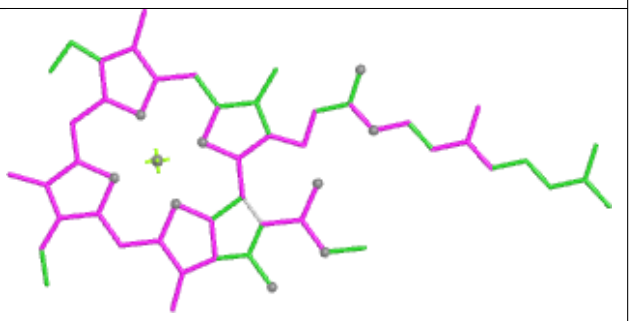
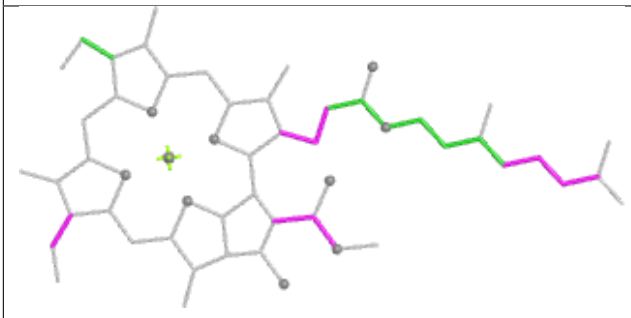
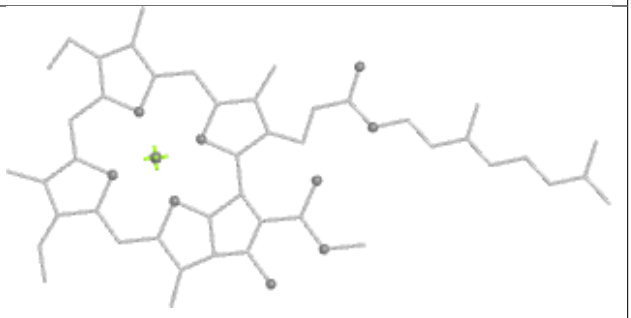


Torsions

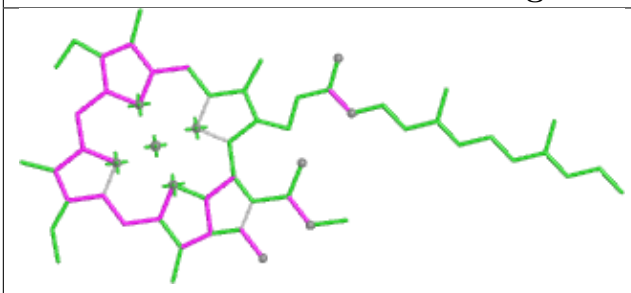


Rings

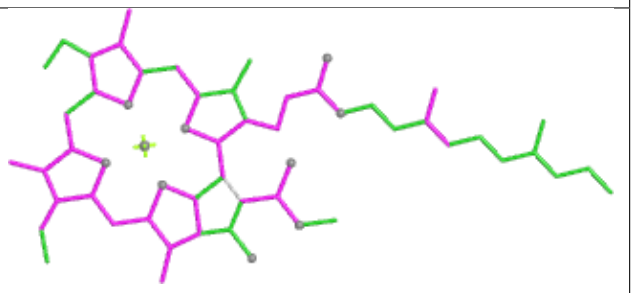
Ligand CLA B 813	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 2 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

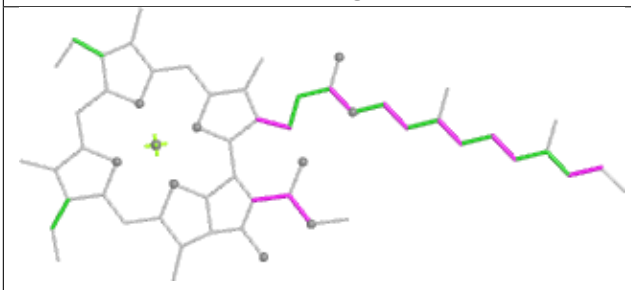
Ligand CLA L 202



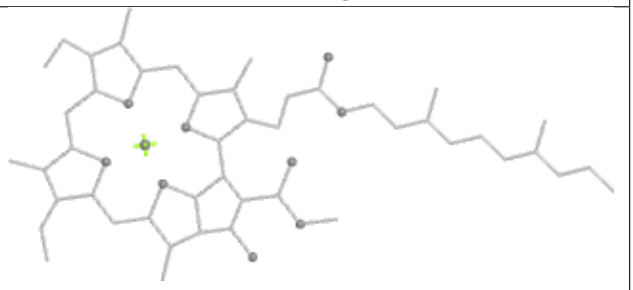
Bond lengths



Bond angles

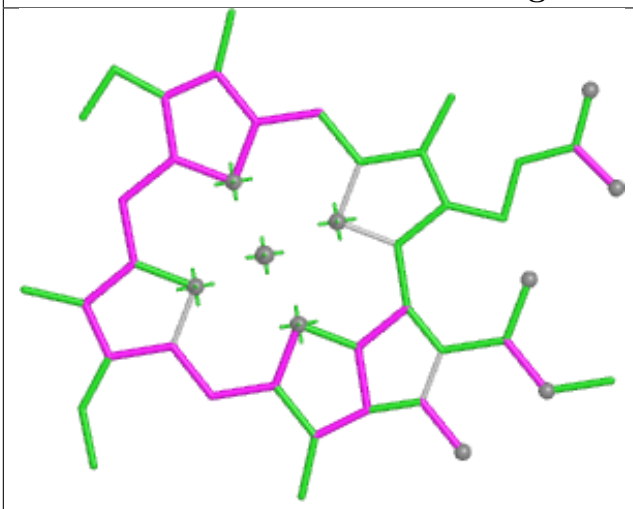


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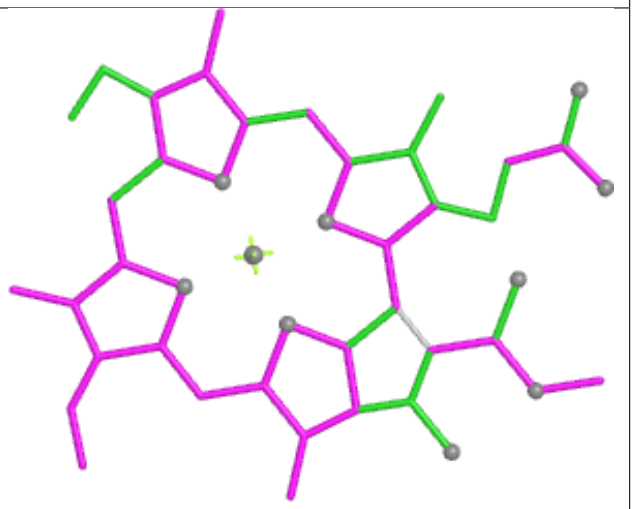


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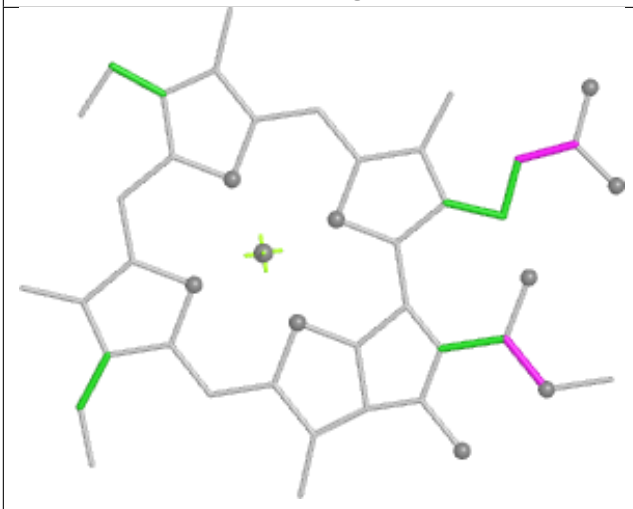
Ligand CLA 2 306



Bond lengths



Bond angles

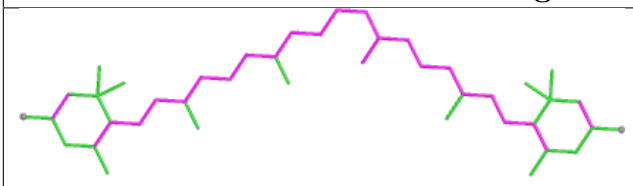


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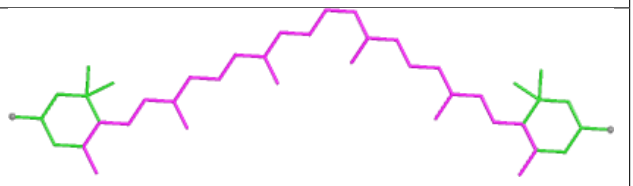


Rings

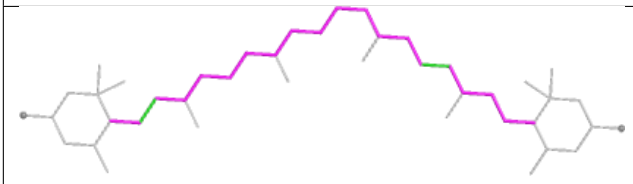
Ligand 5X6 3 316



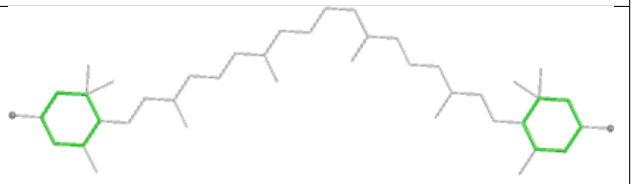
Bond lengths



Bond angles

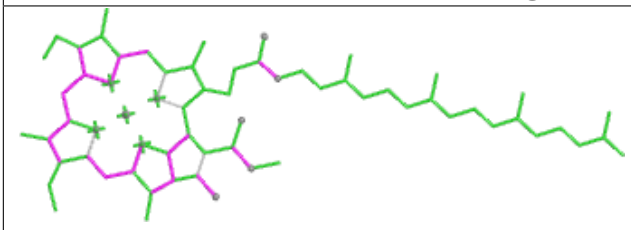


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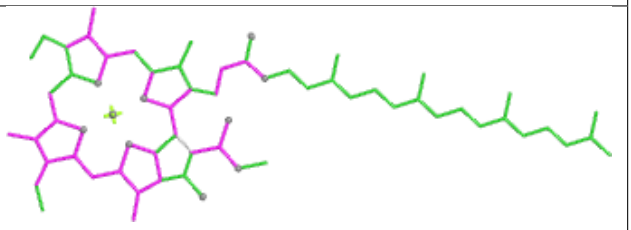


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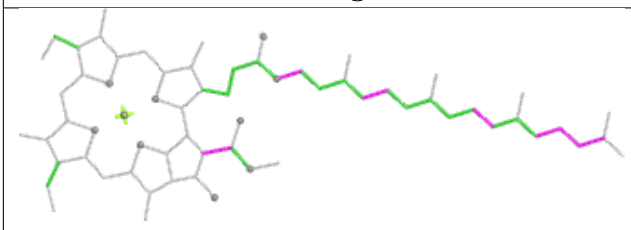
Ligand CLA A 837



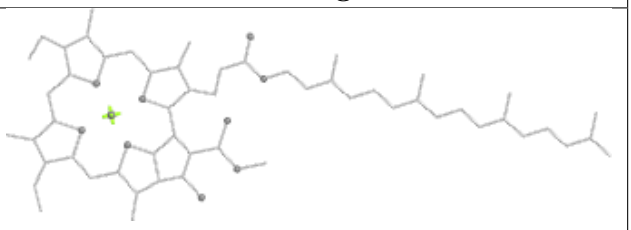
Bond lengths



Bond angles

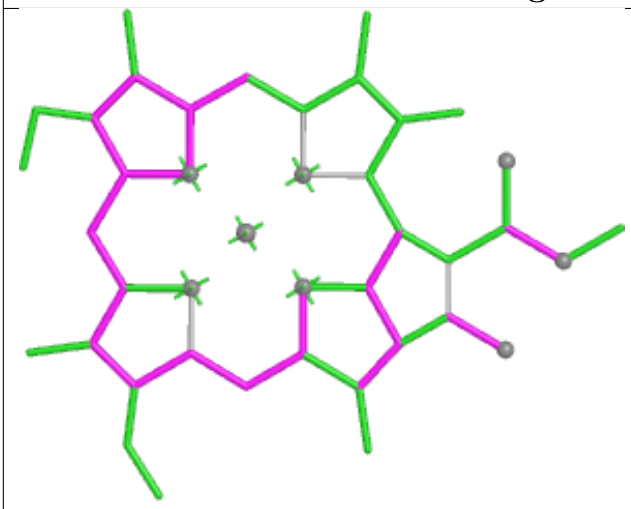


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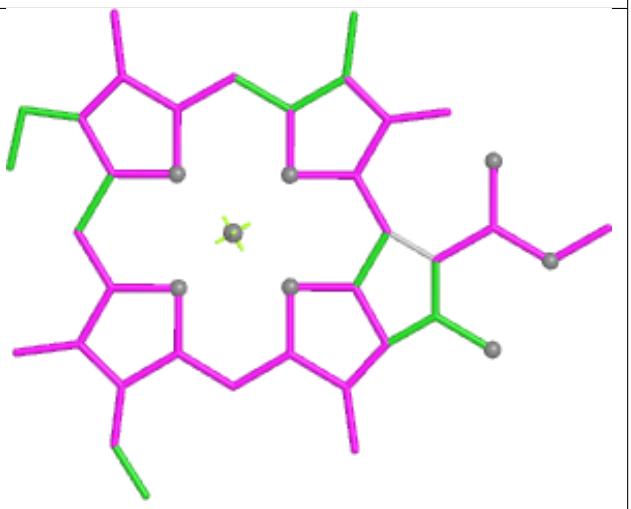


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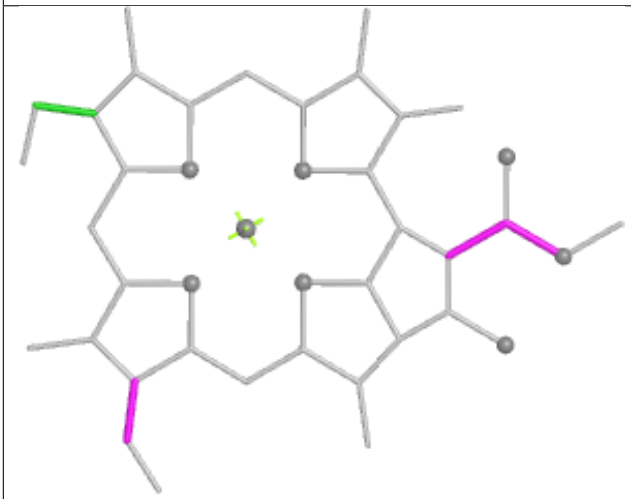
Ligand CLA 1 308



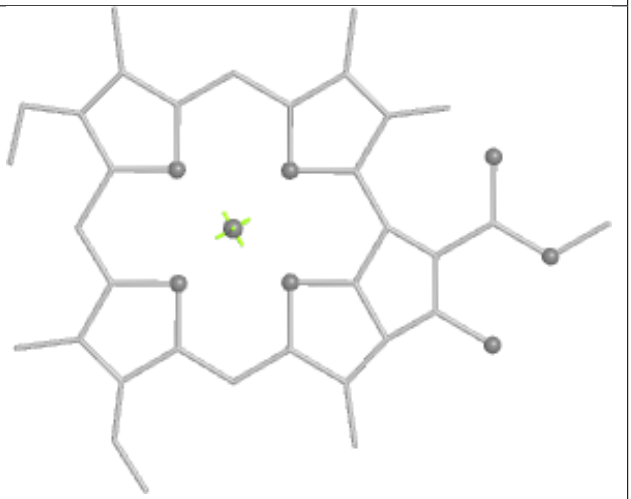
Bond lengths



Bond angles

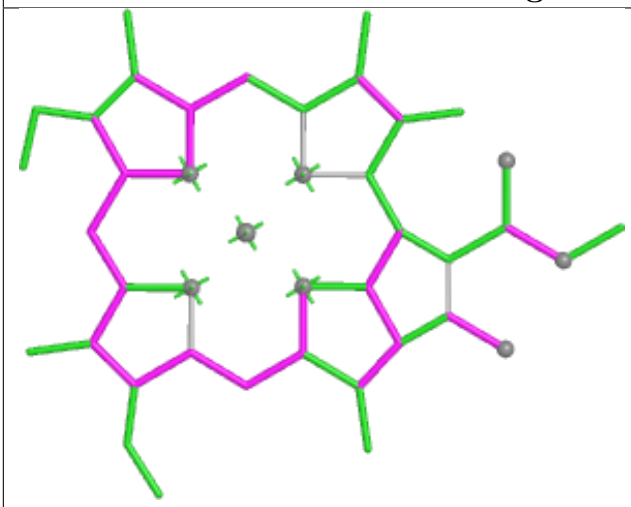


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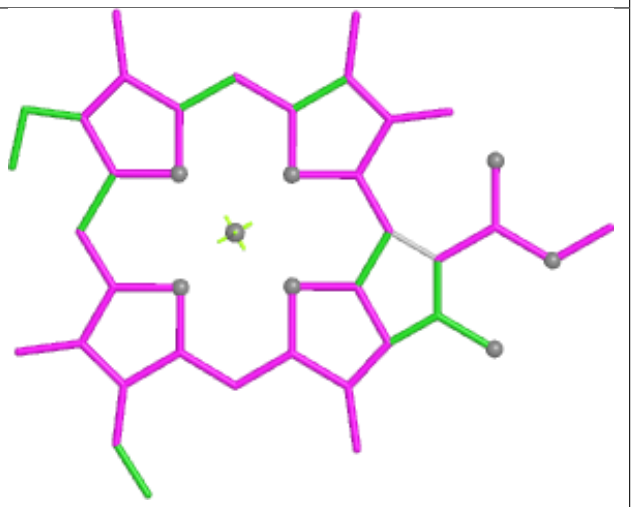


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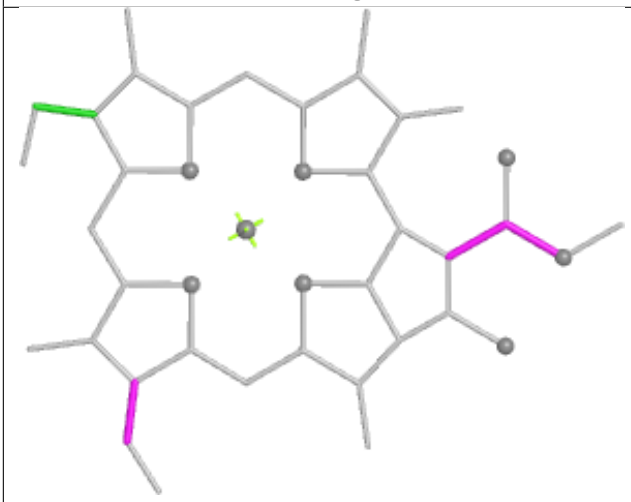
Ligand CLA F 204



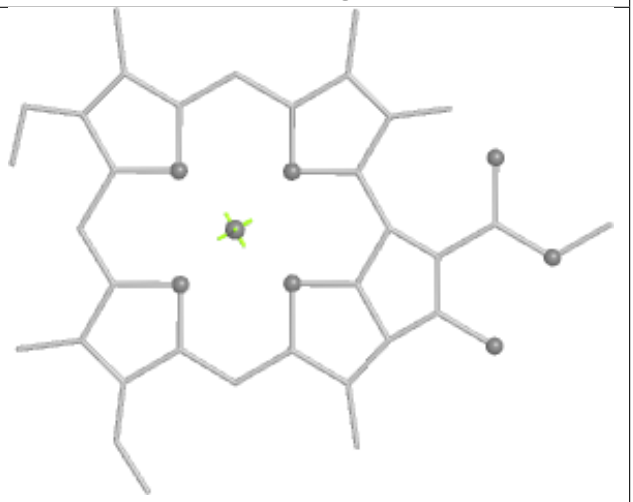
Bond lengths



Bond angles

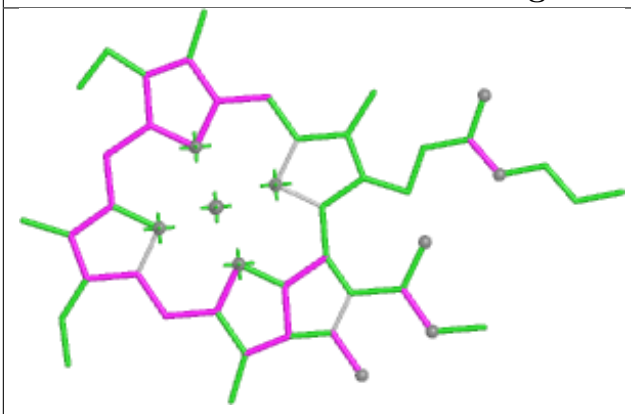


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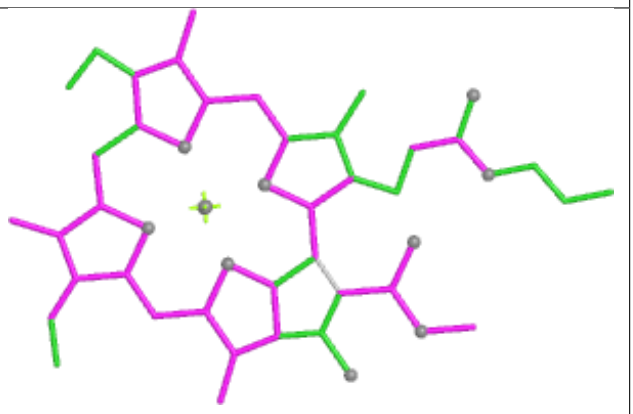


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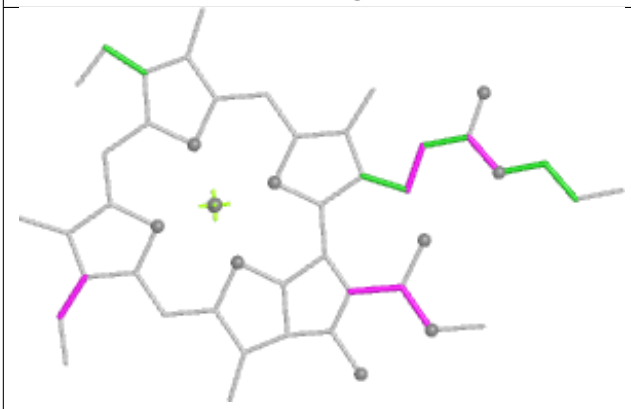
Ligand CLA 4 303



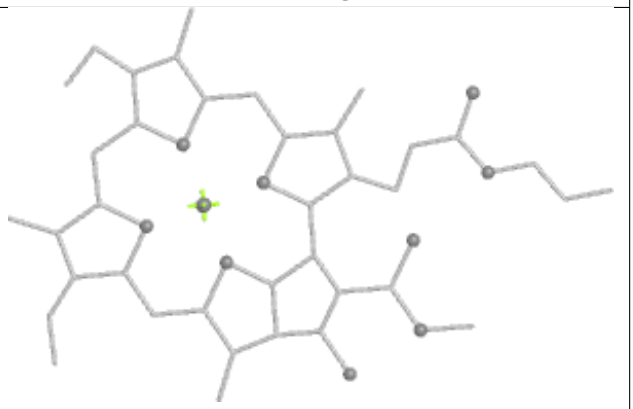
Bond lengths



Bond angles

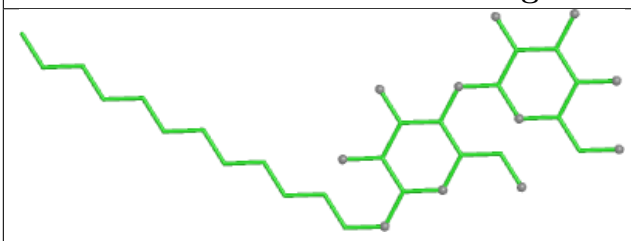


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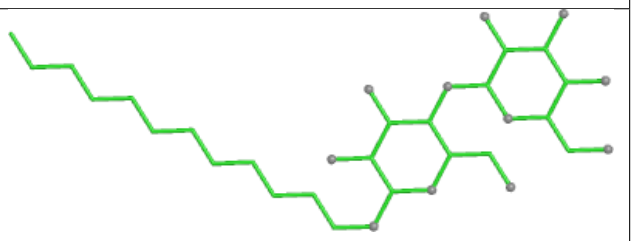


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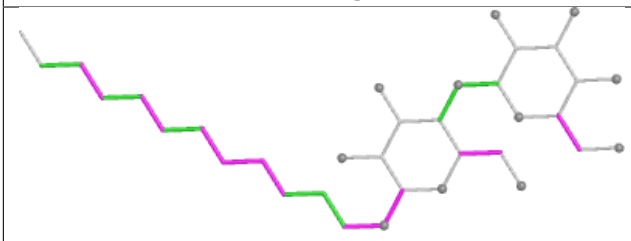
Ligand LMT B 852



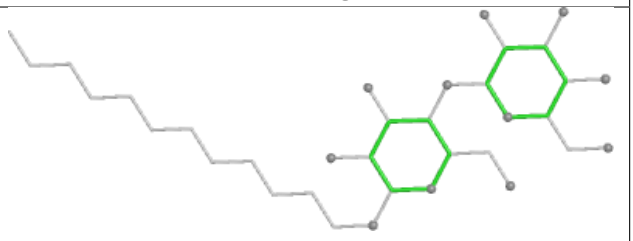
Bond lengths



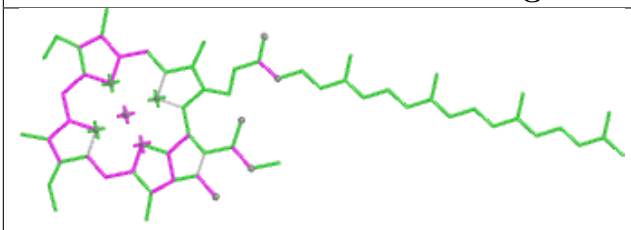
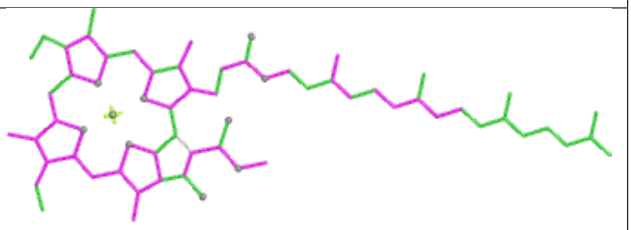
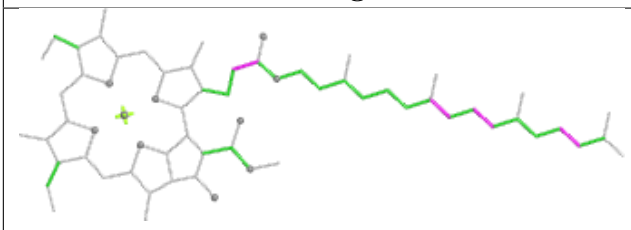
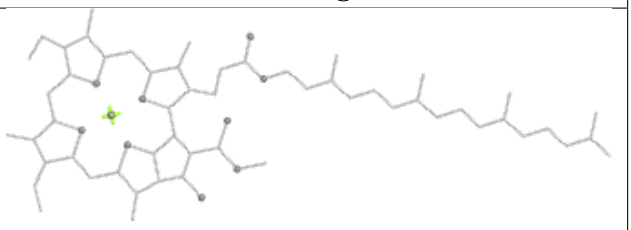
Bond angles

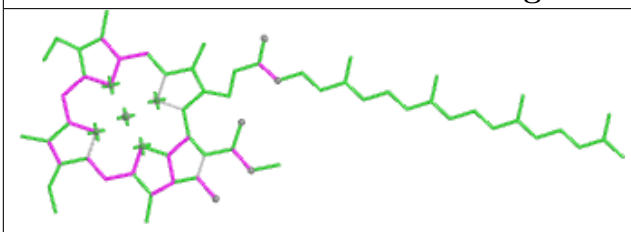
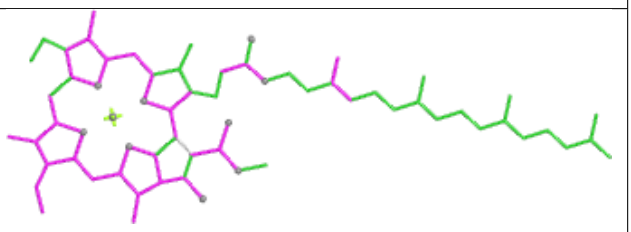
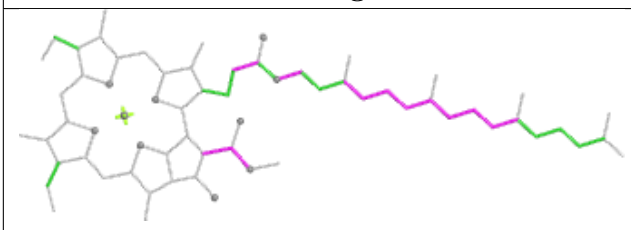
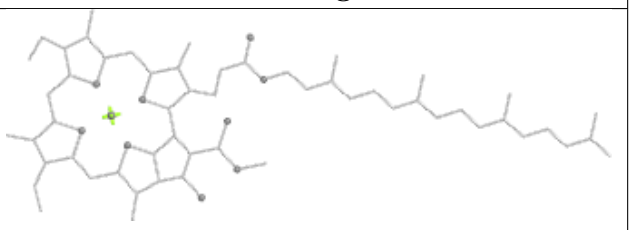


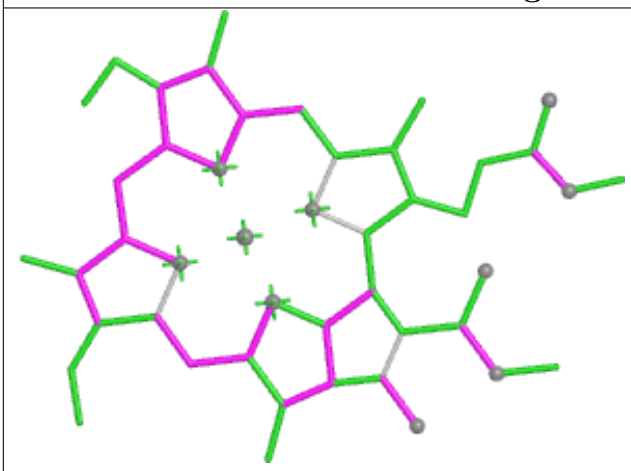
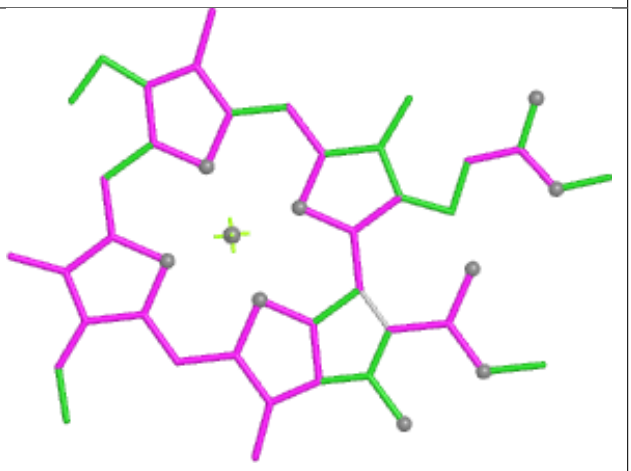
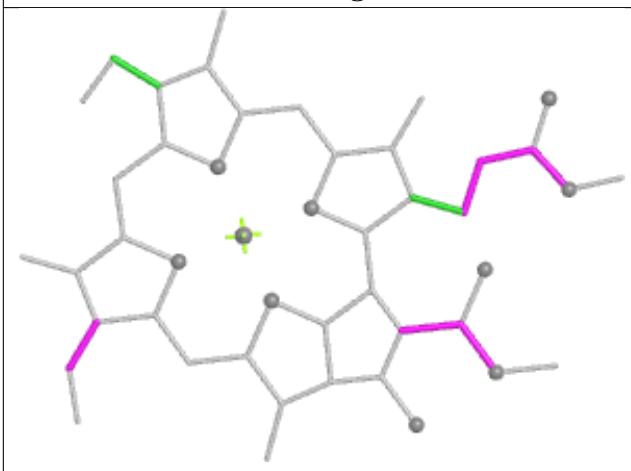
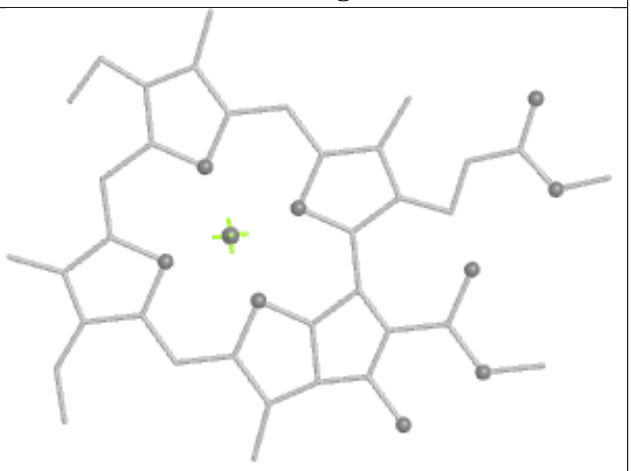
Torsions



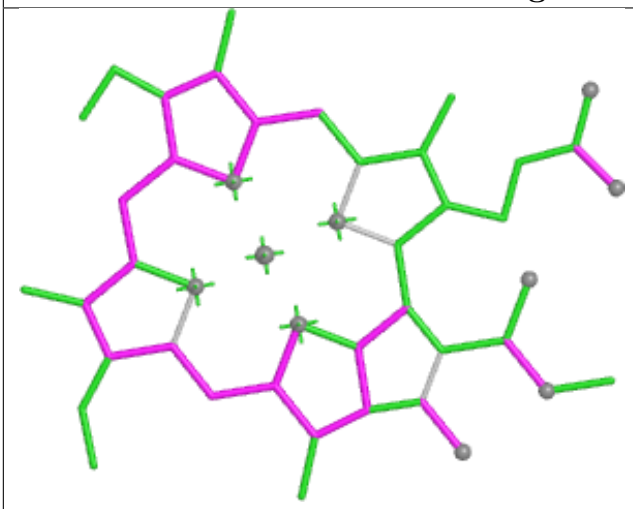
Rings

Ligand CLA A 852	
	
Bond lengths	Bond angles
	
Torsions	Rings

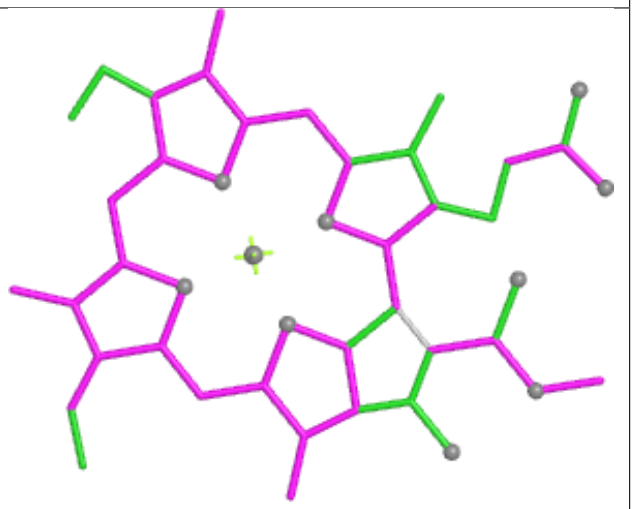
Ligand CLA A 804	
	
Bond lengths	Bond angles
	
Torsions	Rings

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

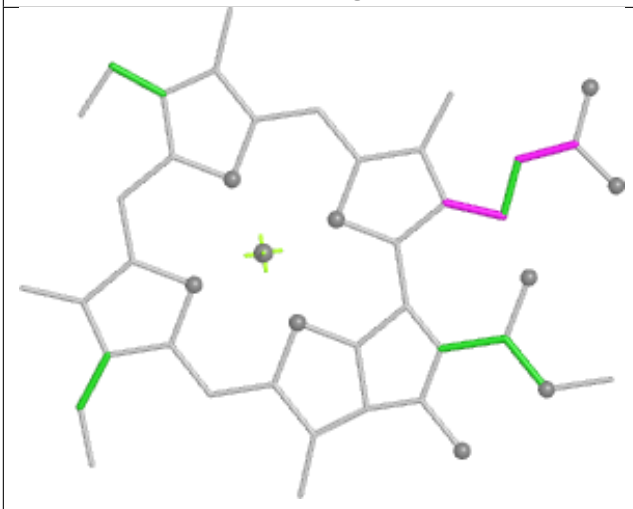
Ligand CLA 4 310



Bond lengths



Bond angles

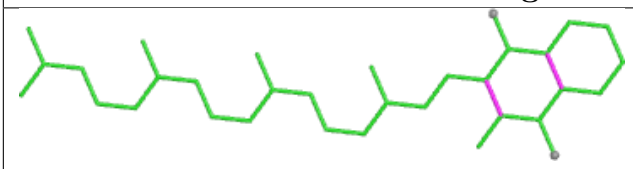


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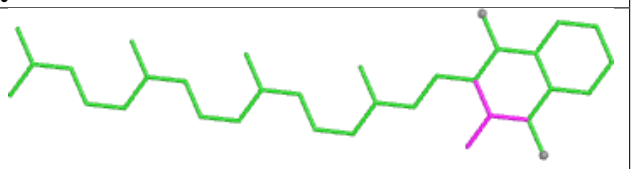


Rings

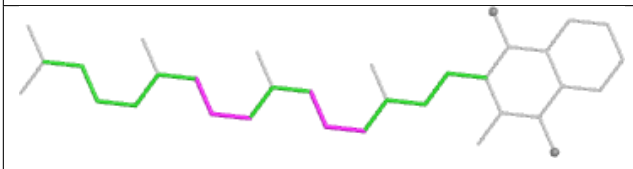
Ligand PQN A 840



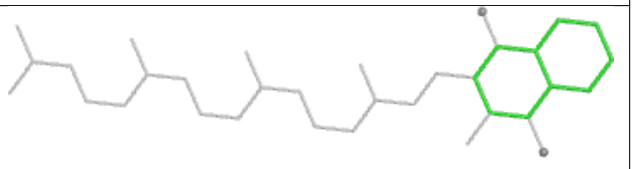
Bond lengths



Bond angles

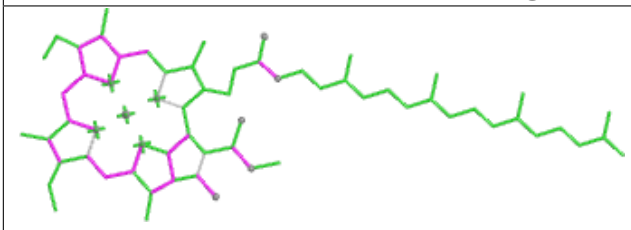


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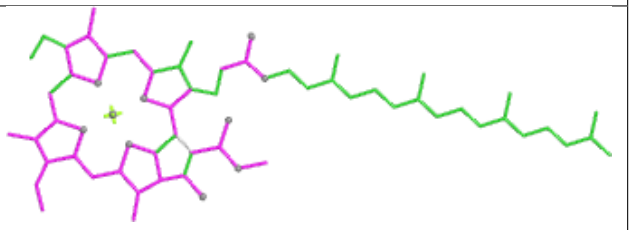


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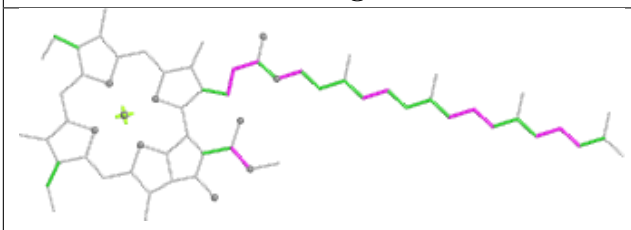
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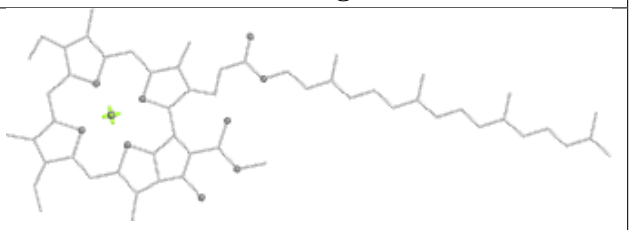
Bond lengths



Bond angles

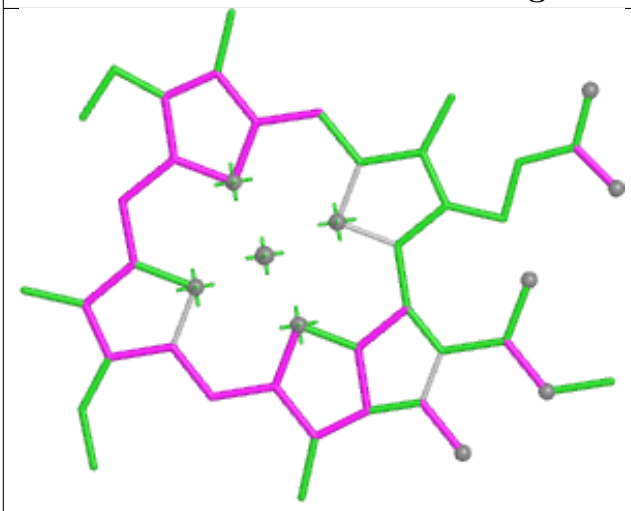


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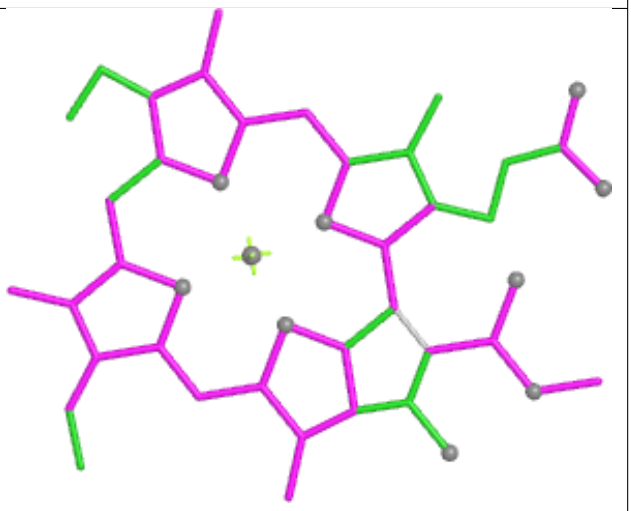


Rings

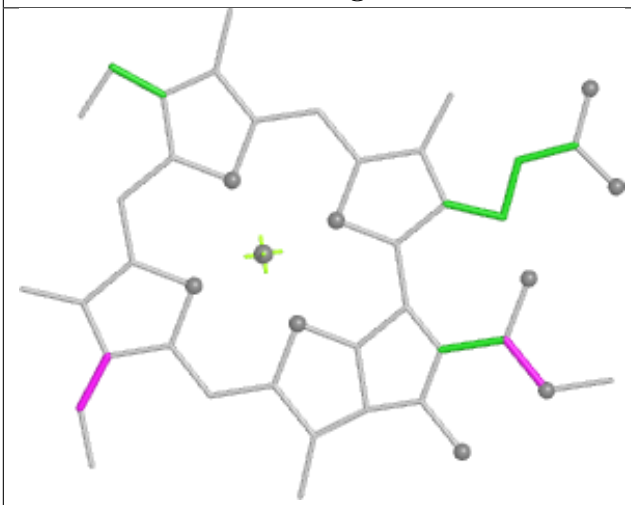
Ligand CLA 2 308



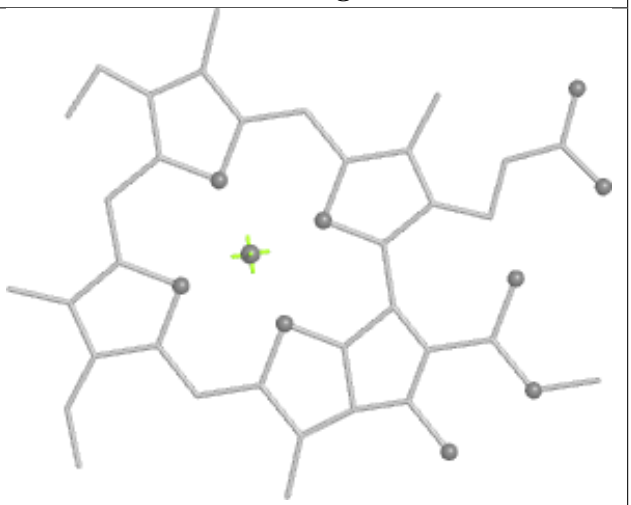
Bond lengths



Bond angles

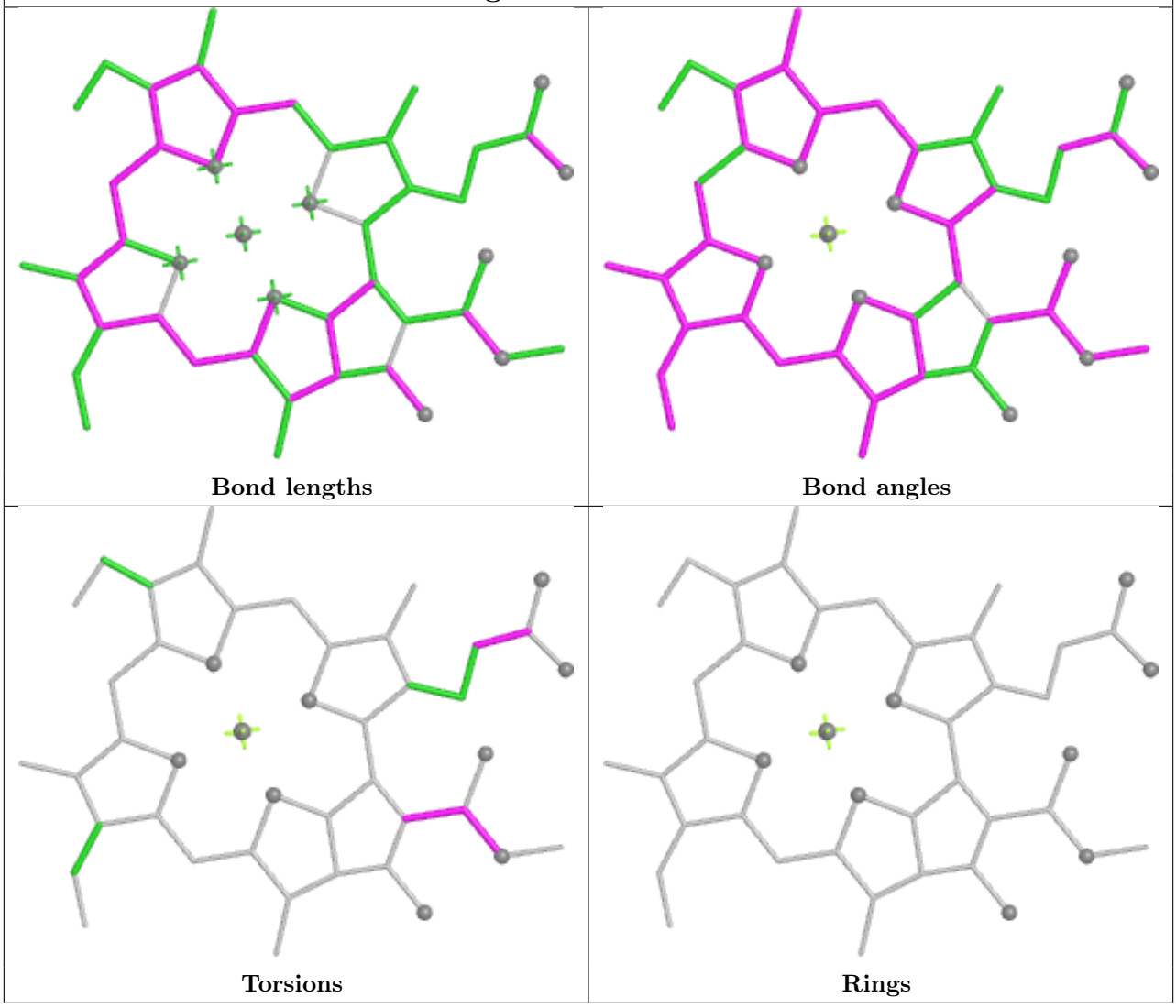


Torsions

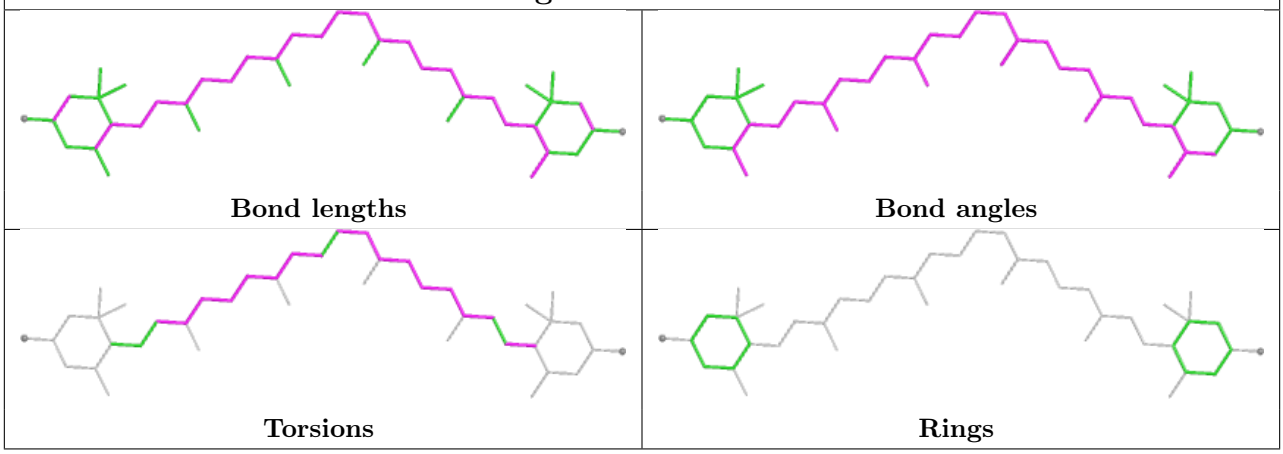


Rings

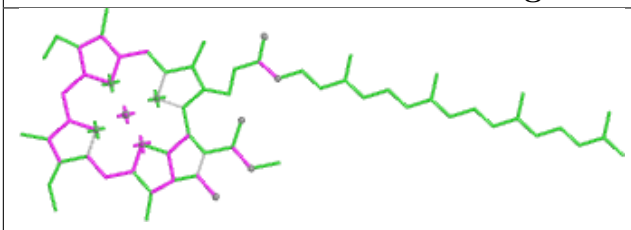
Ligand CLA 3 306



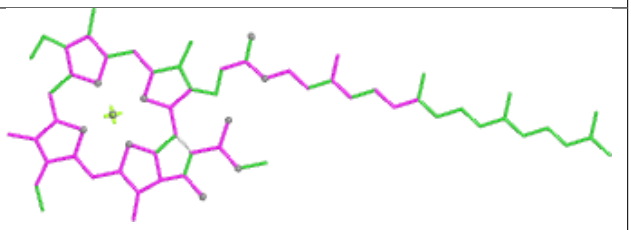
Ligand 5X6 5 301



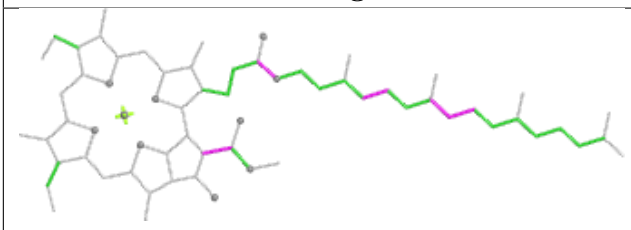
Ligand CLA B 827



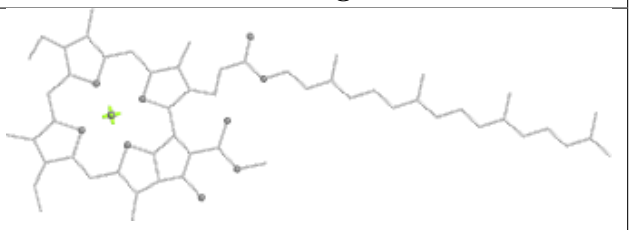
Bond lengths



Bond angles

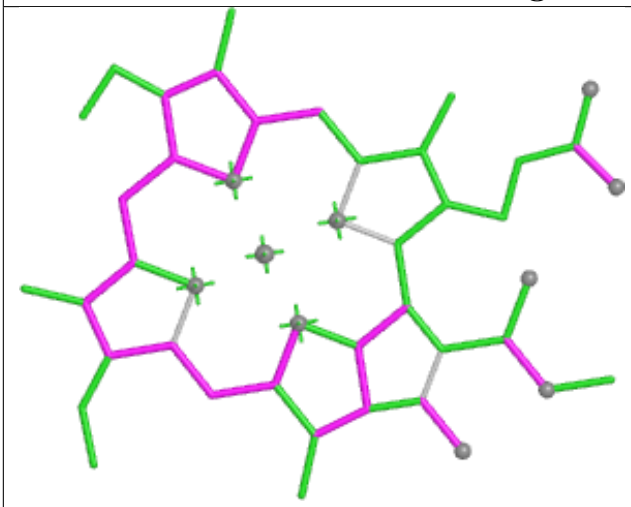


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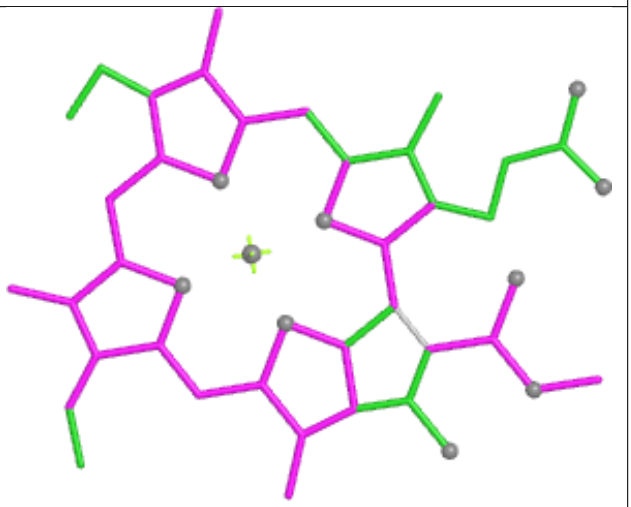


Rings

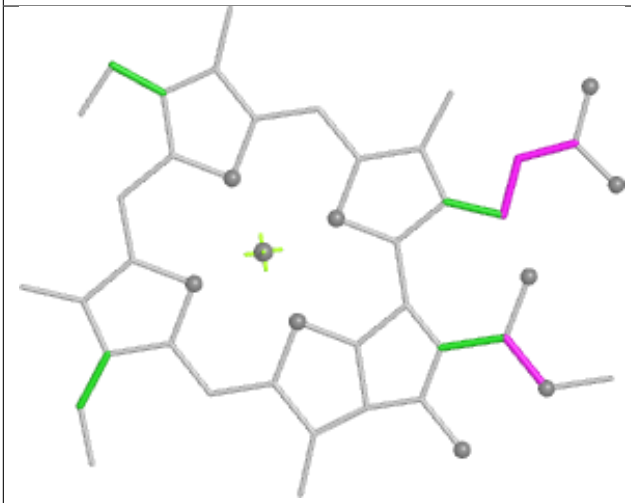
Ligand CLA 5 312



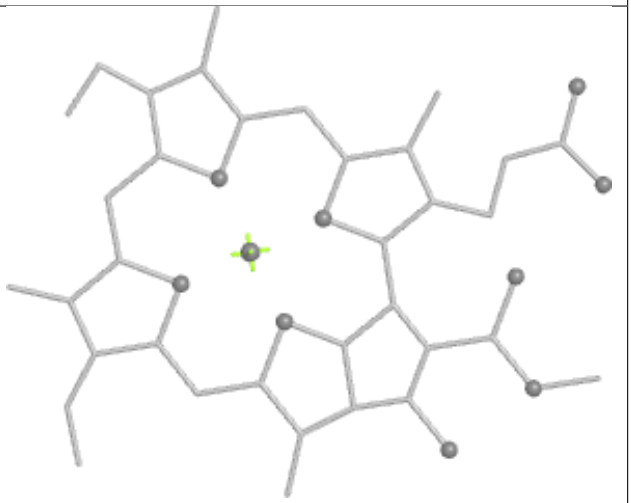
Bond lengths



Bond angles

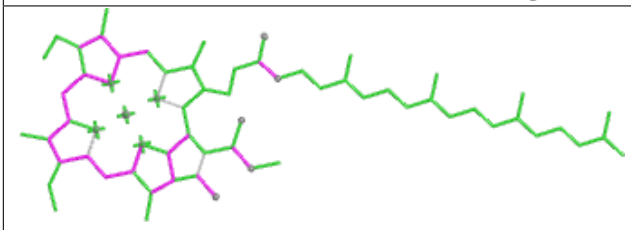


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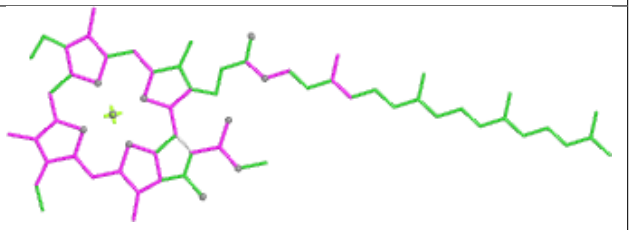


Rings

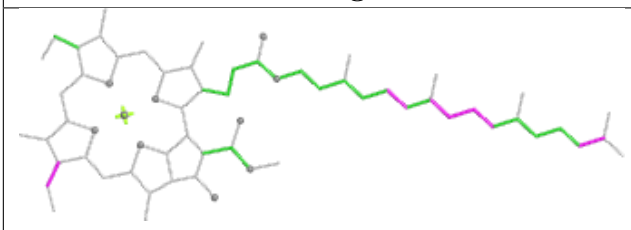
Ligand CLA B 814



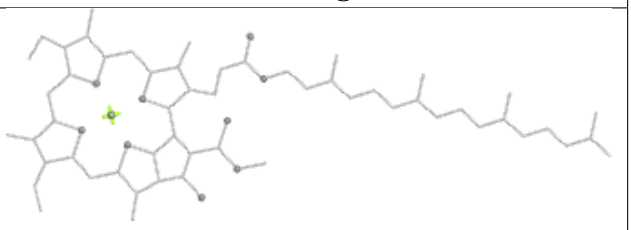
Bond lengths



Bond angles

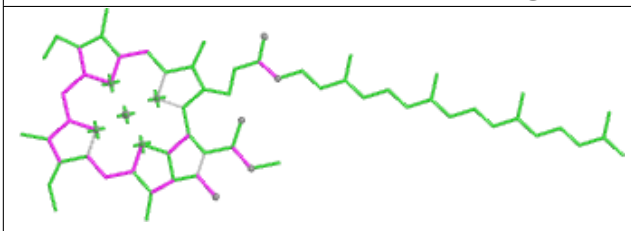


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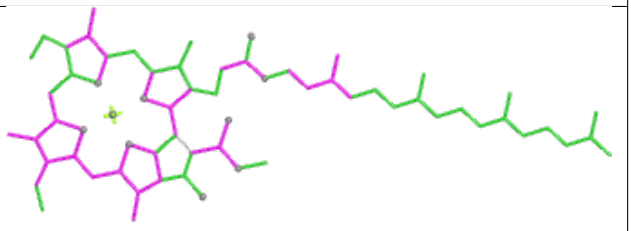


Rings

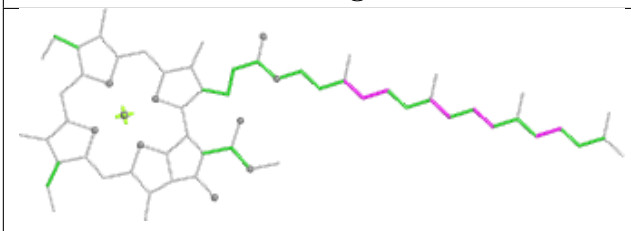
Ligand CLA B 808



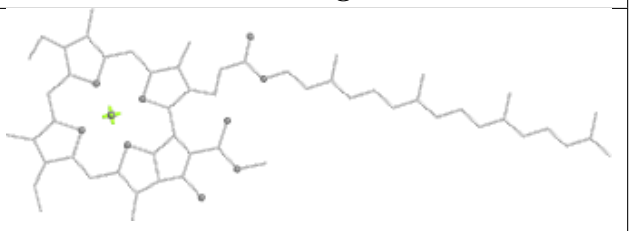
Bond lengths



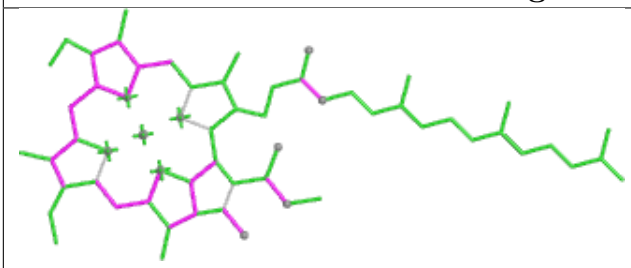
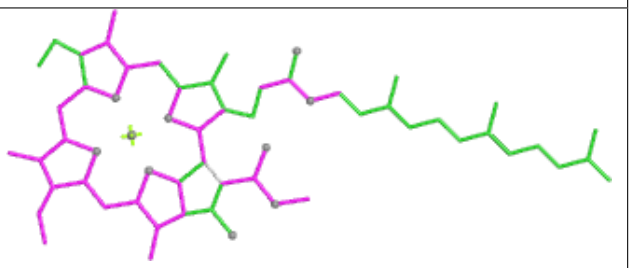
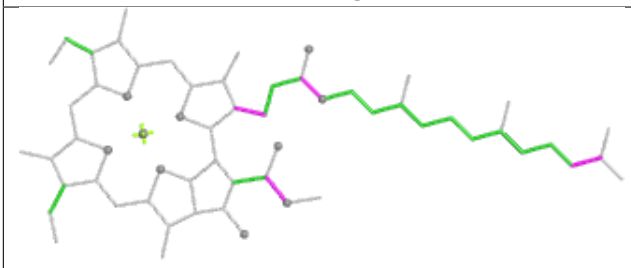
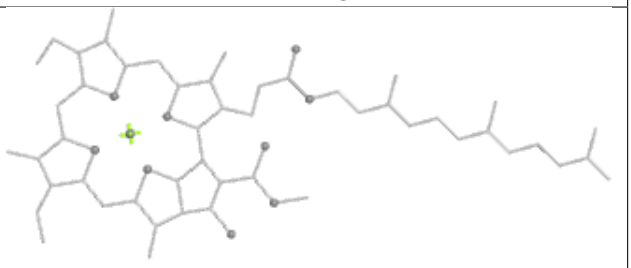
Bond angles

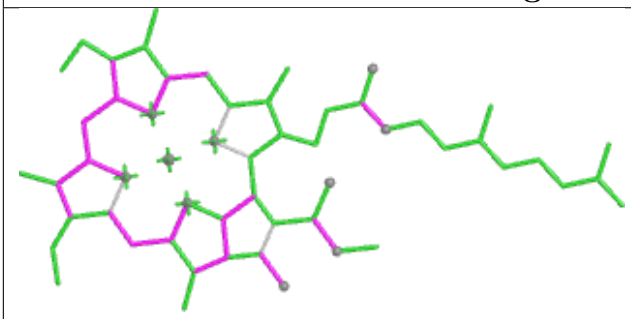
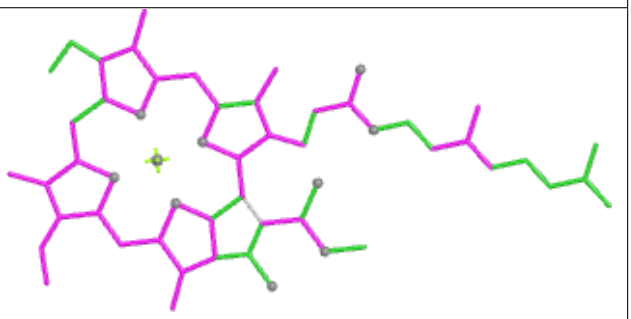
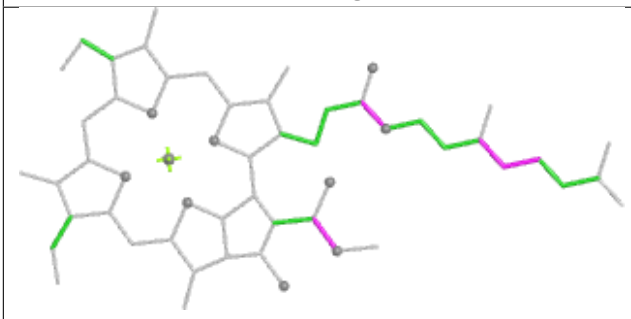
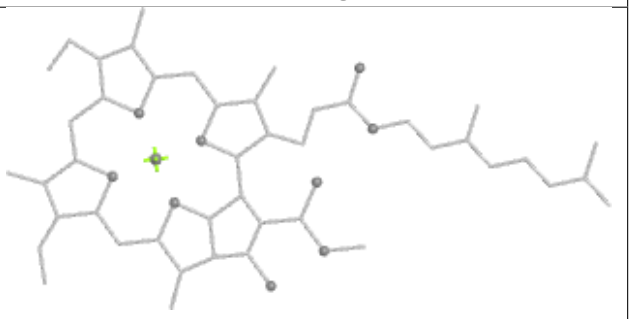


Torsions

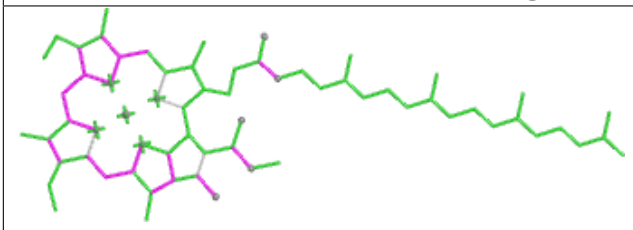


Rings

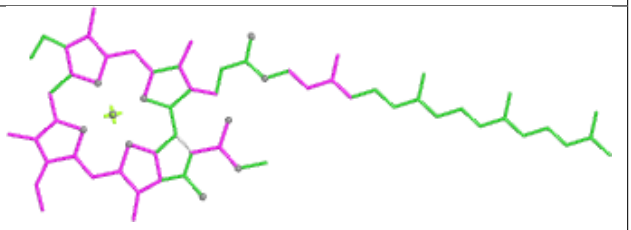
Ligand CLA 1 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 808	
 Bond lengths	 Bond angles
 Torsions	 Rings

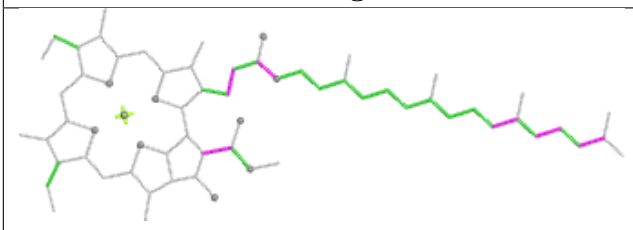
Ligand CLA A 806



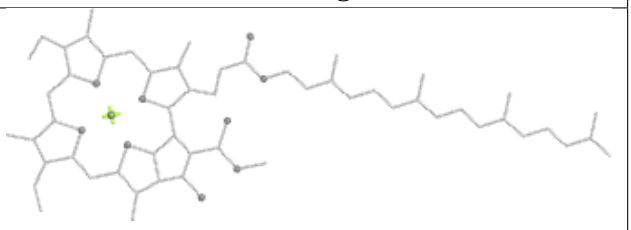
Bond lengths



Bond angles

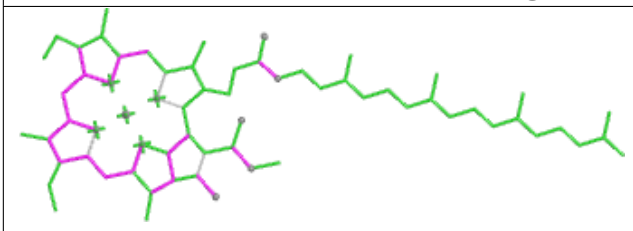


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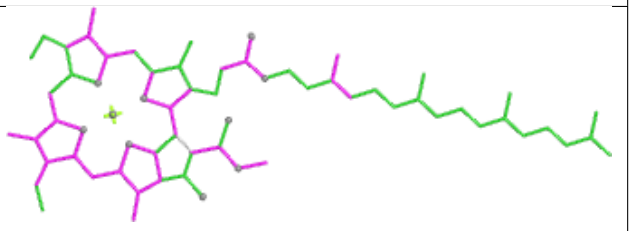


Rings

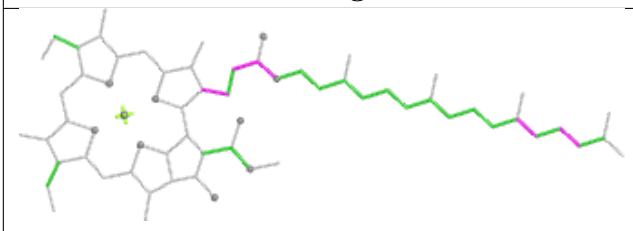
Ligand CLA A 816



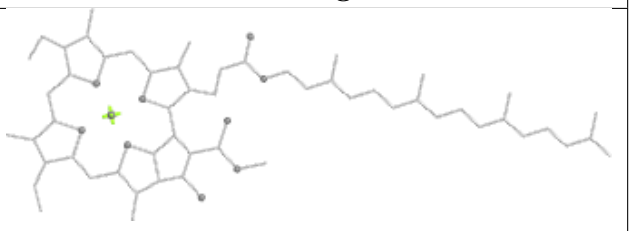
Bond lengths



Bond angles

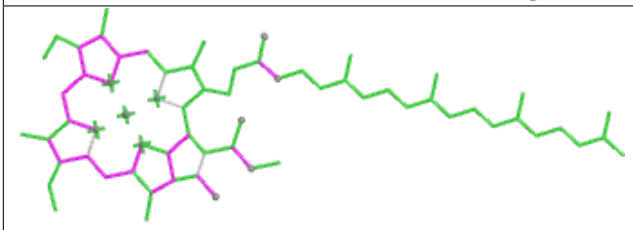


Torsions

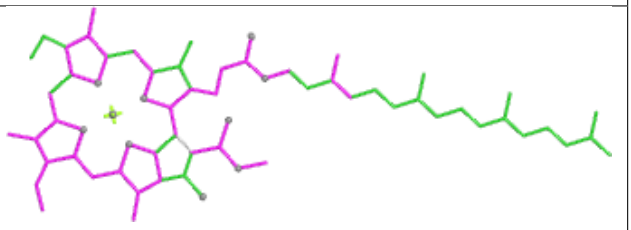


Rings

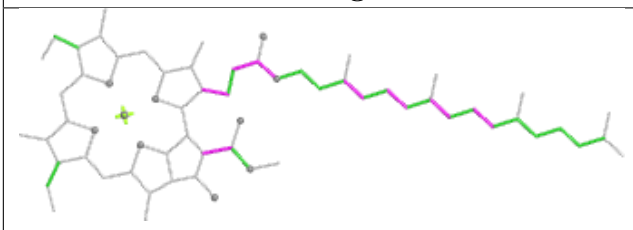
Ligand CLA B 831



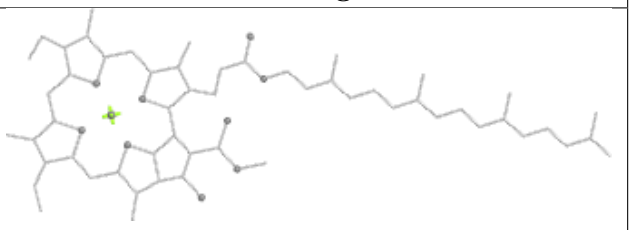
Bond lengths



Bond angles

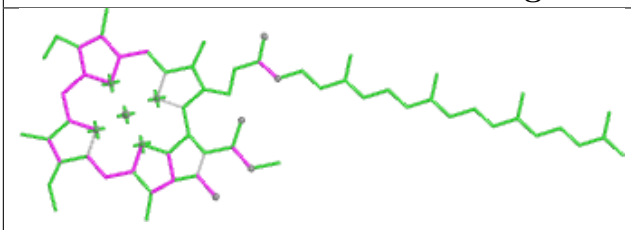


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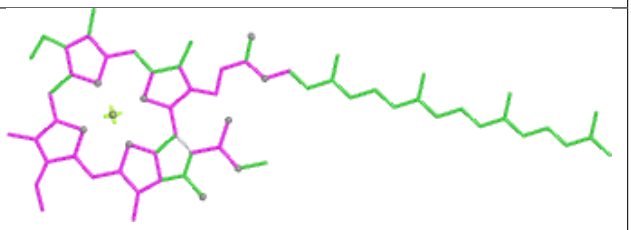


Rings

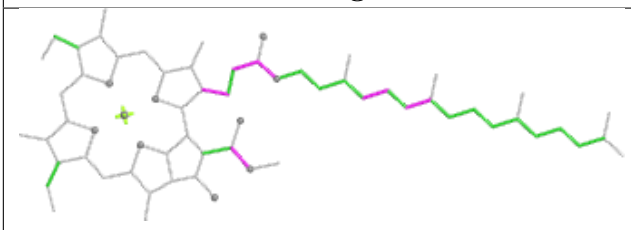
Ligand CLA B 830



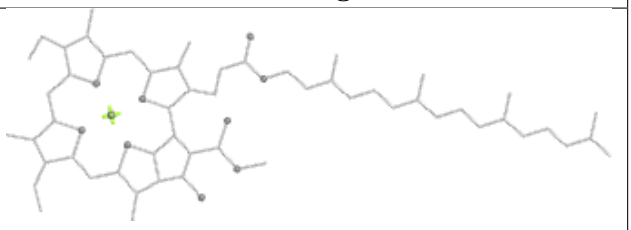
Bond lengths



Bond angles

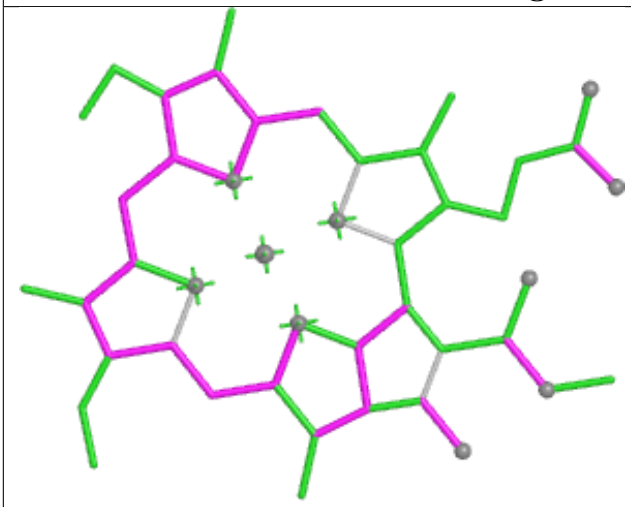


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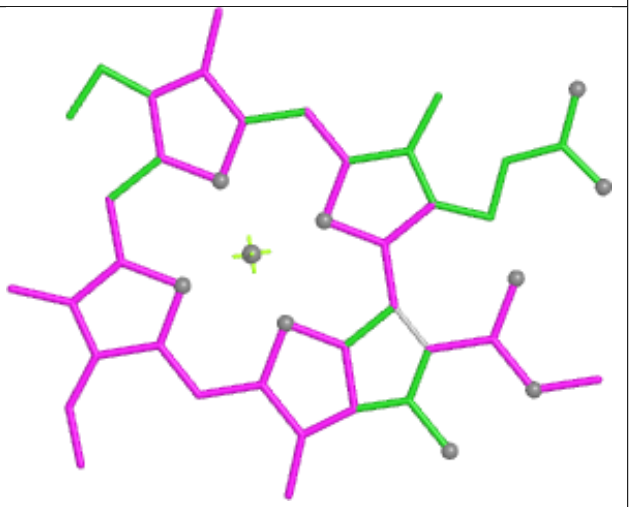


Rings

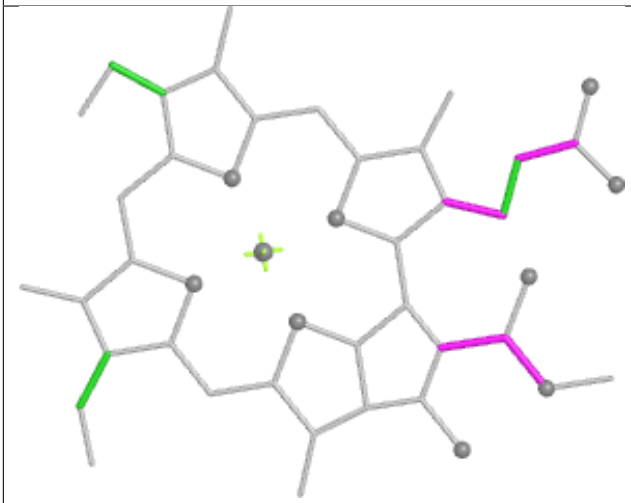
Ligand CLA 2 309



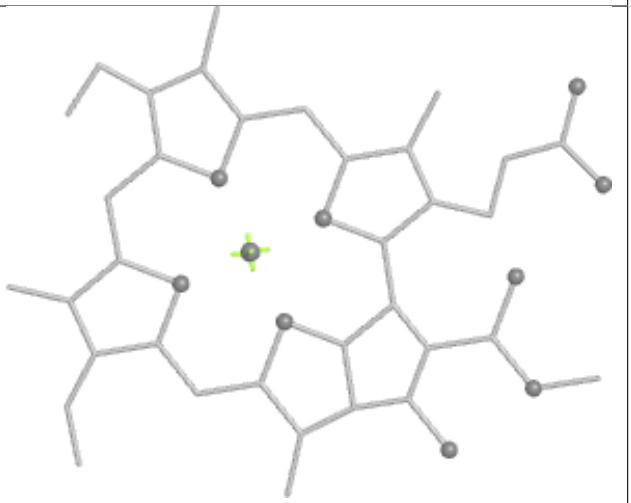
Bond lengths



Bond angles

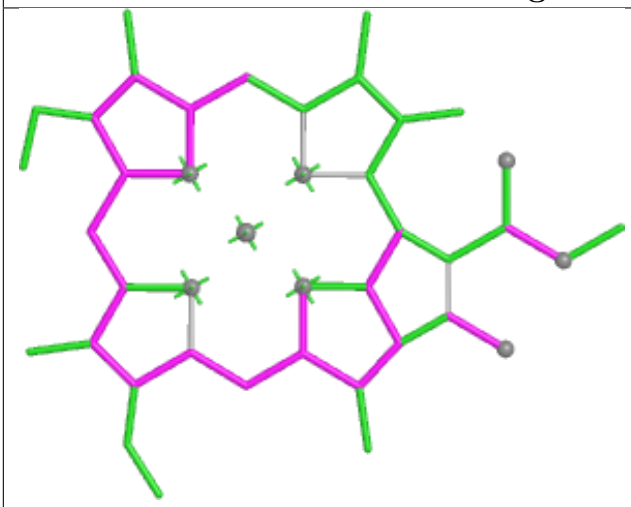


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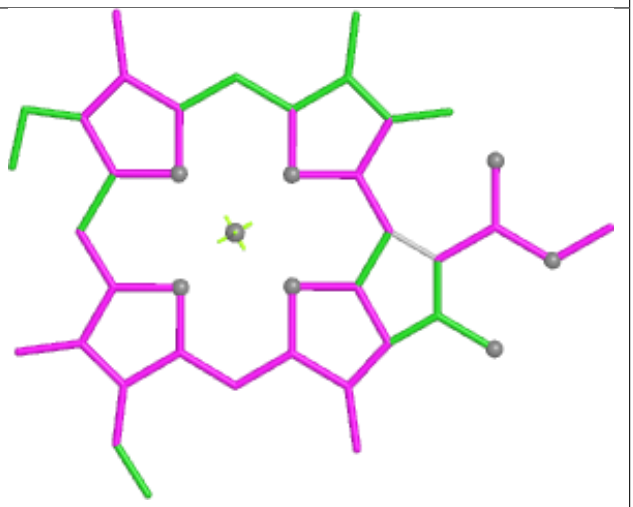


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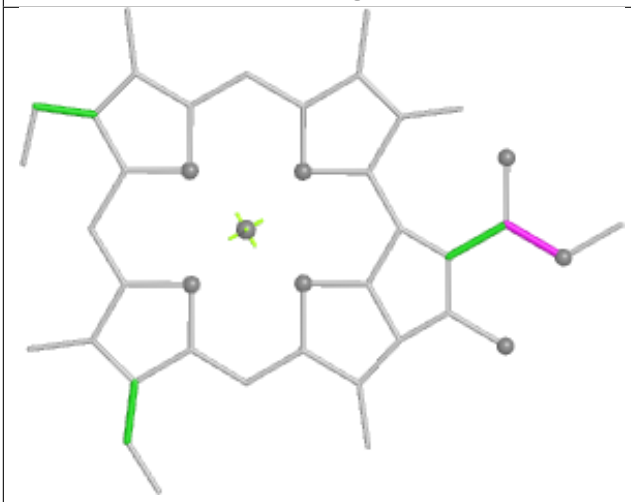
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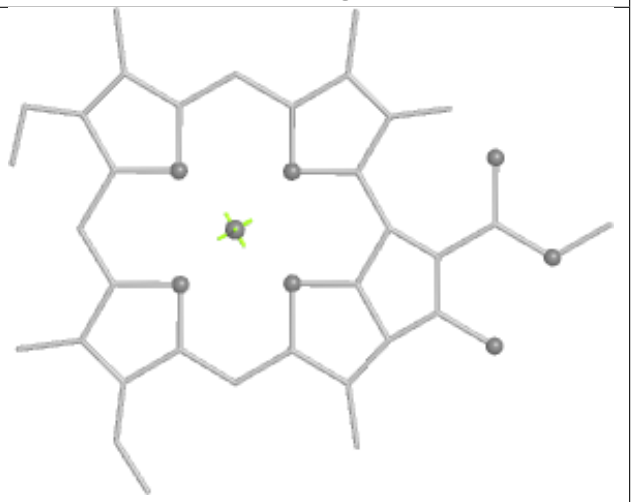
Bond lengths



Bond angles

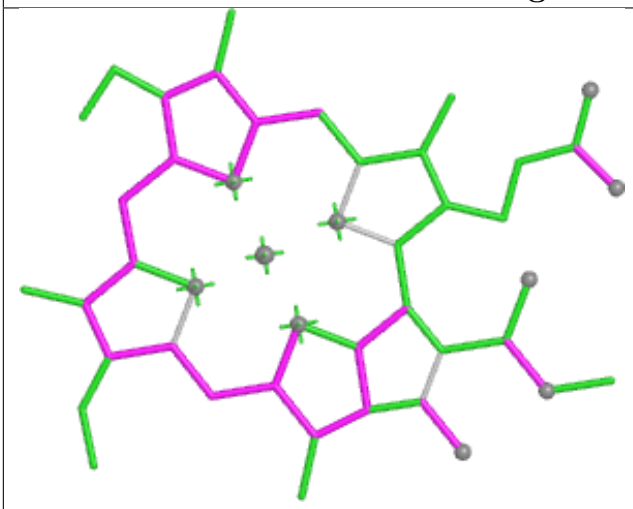


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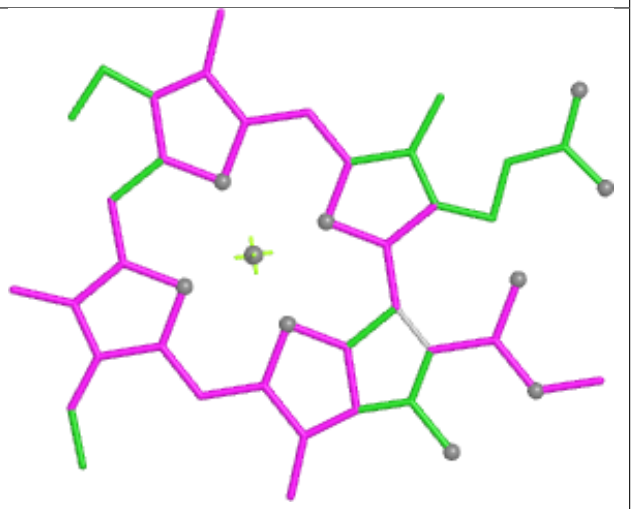


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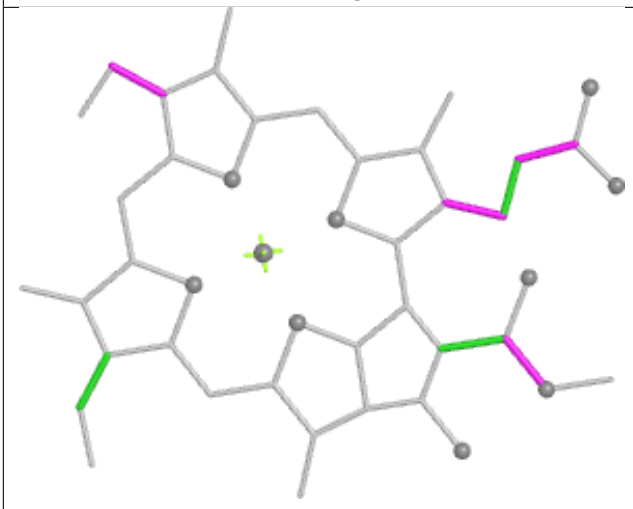
Ligand CLA 5 306



Bond lengths



Bond angles

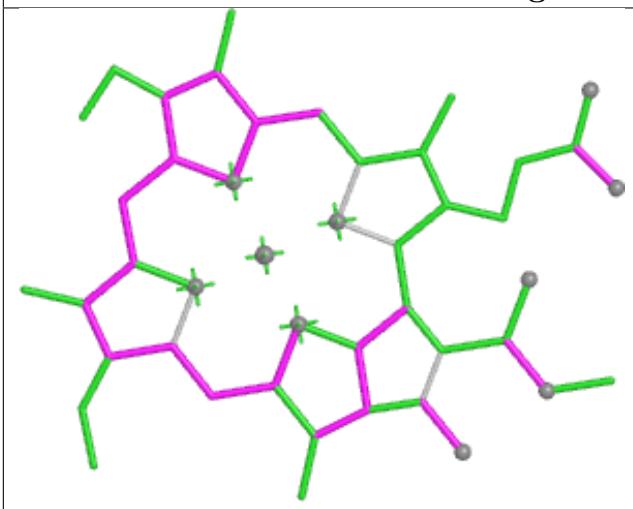


Torsions

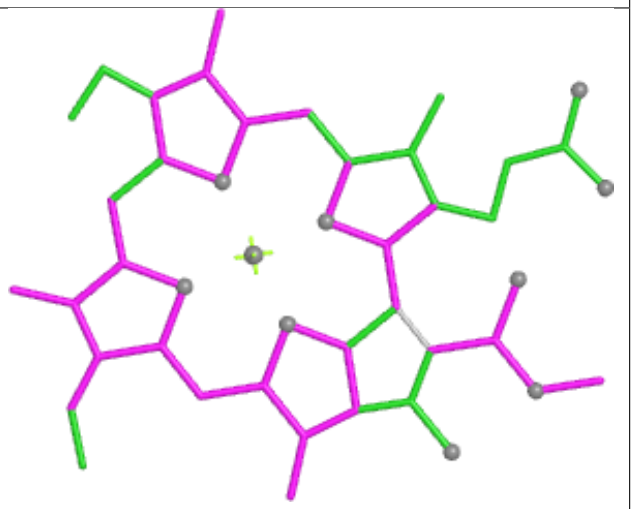


Rings

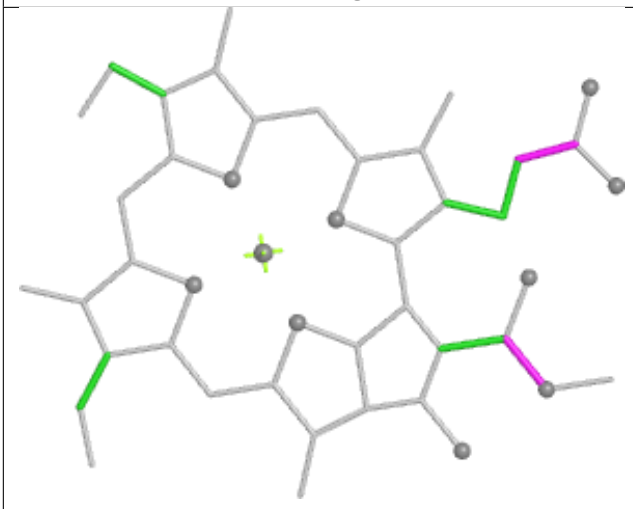
Ligand CLA 4 308



Bond lengths



Bond angles

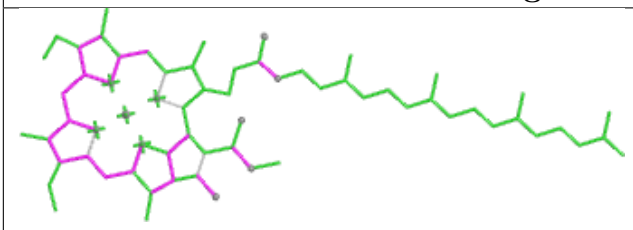


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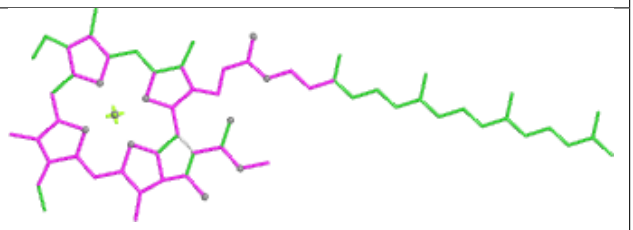


Rings

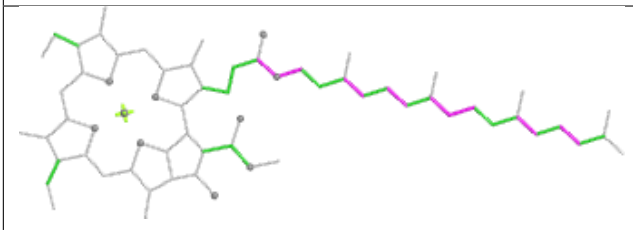
Ligand CLA A 807



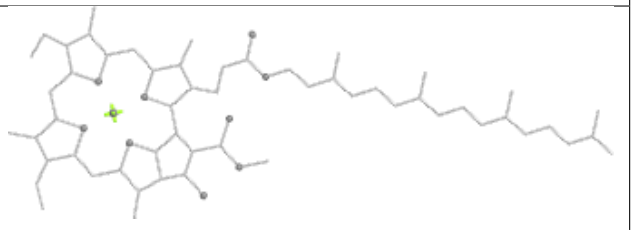
Bond lengths



Bond angles

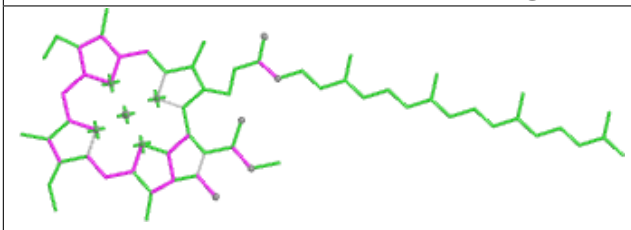


Torsions

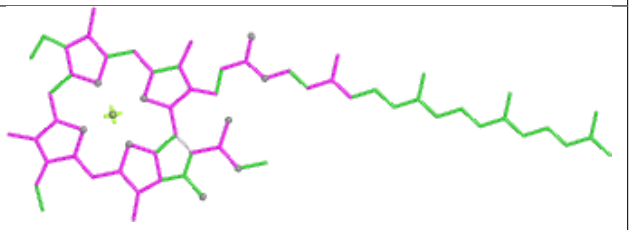


Rings

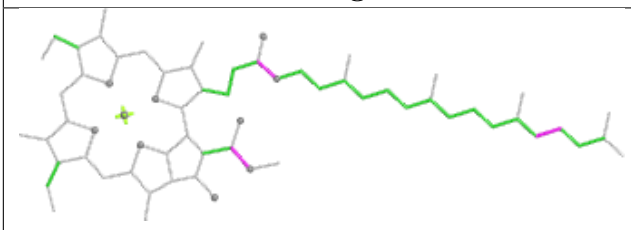
Ligand CLA A 838



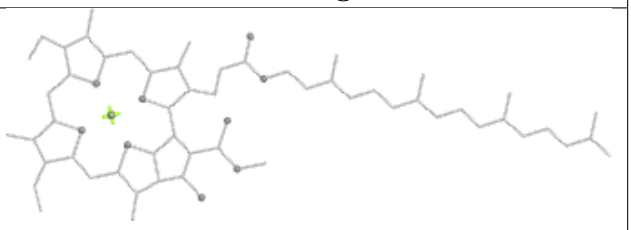
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Bond angles

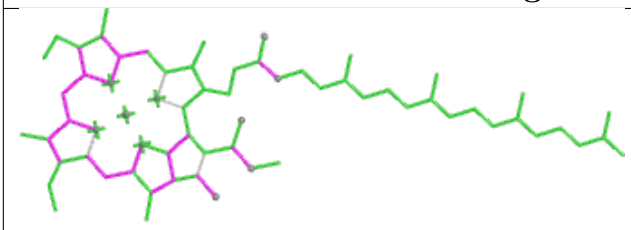


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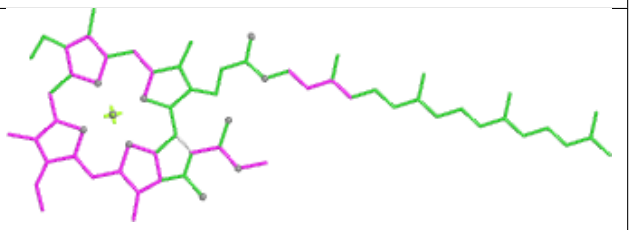


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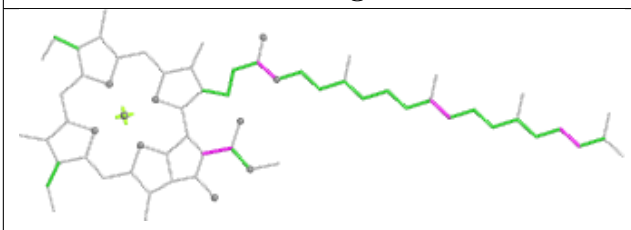
Ligand CLA A 854



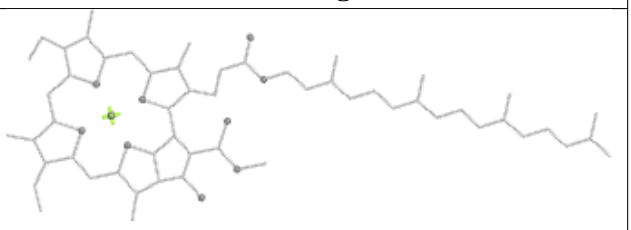
Bond lengths



Bond angles

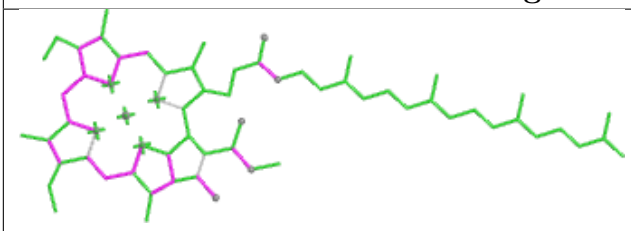


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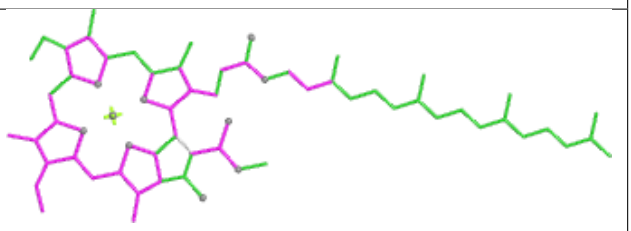


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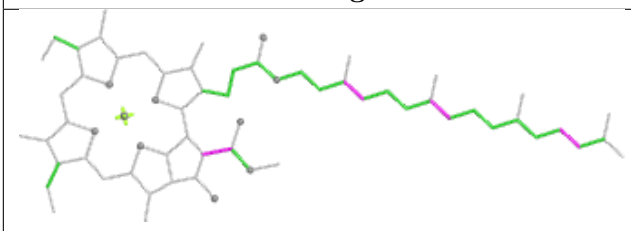
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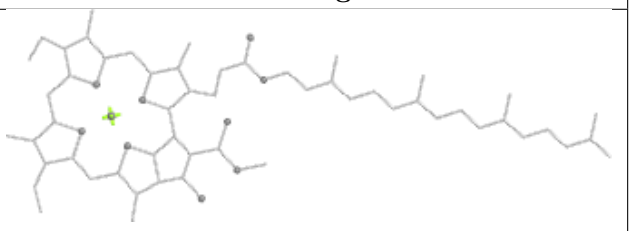
Bond lengths



Bond angles

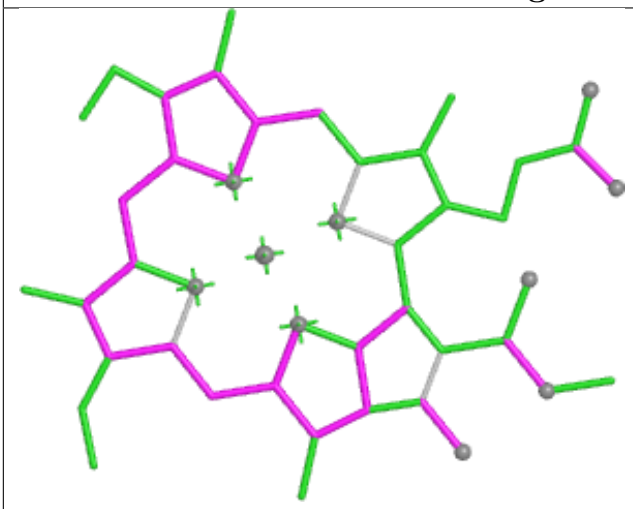


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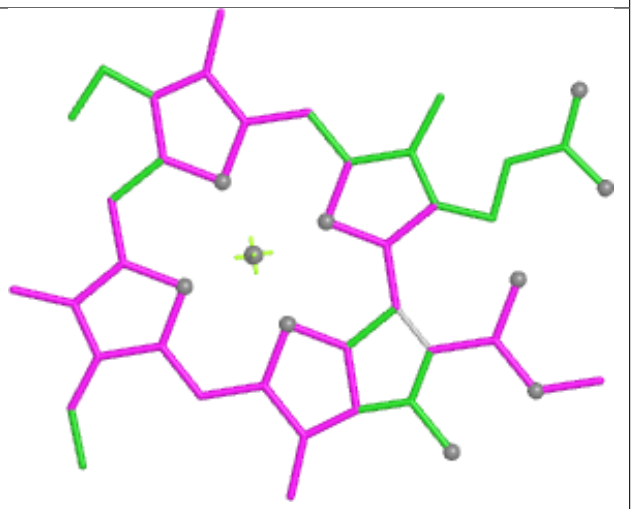


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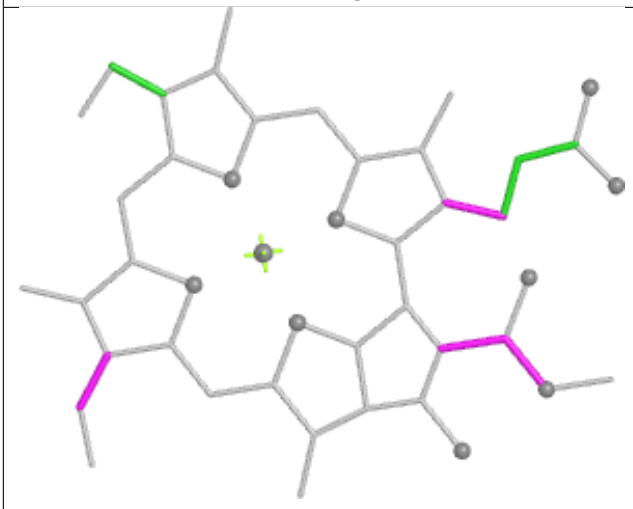
Ligand CLA 4 306



Bond lengths



Bond angles

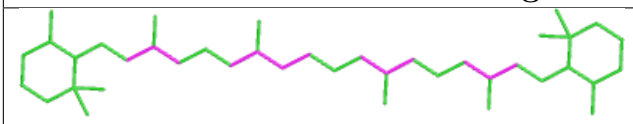


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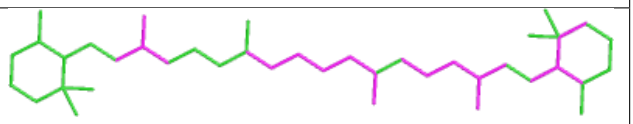


Rings

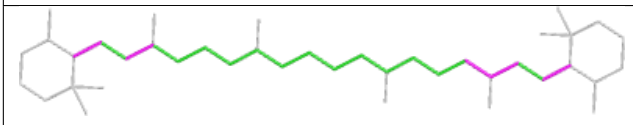
Ligand BCR A 843



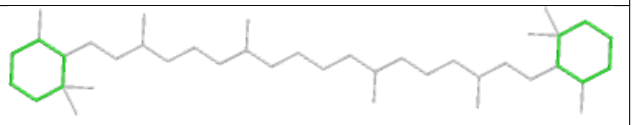
Bond lengths



Bond angles

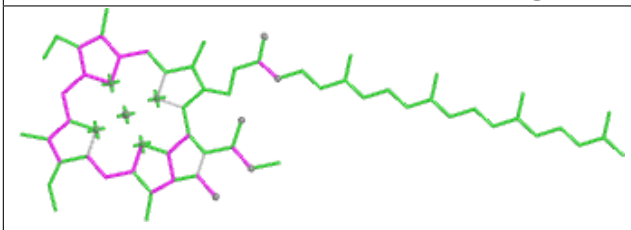


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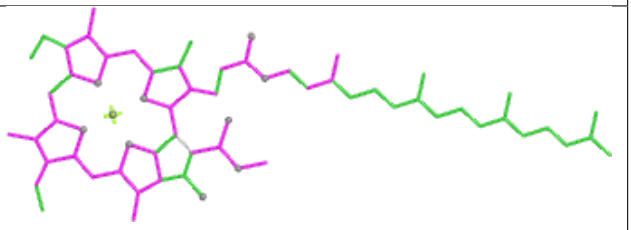


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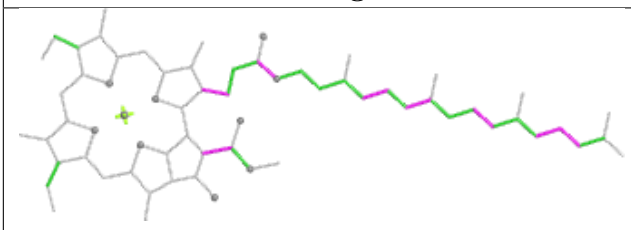
Ligand CLA 5 309



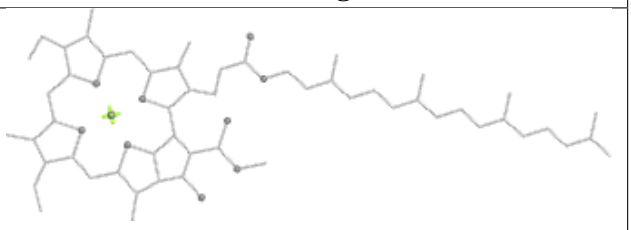
Bond lengths



Bond angles

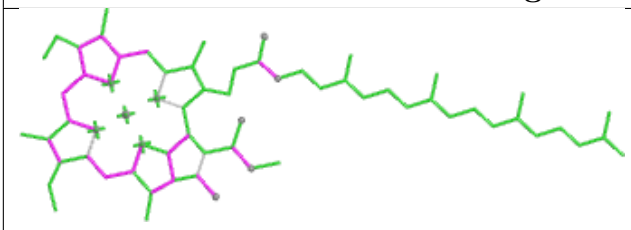


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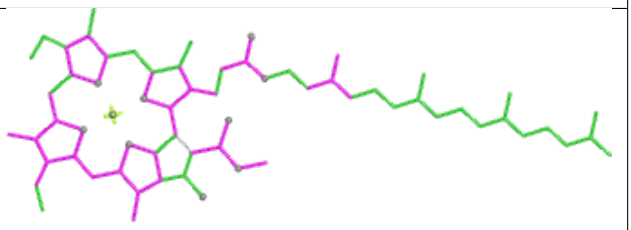


Rings

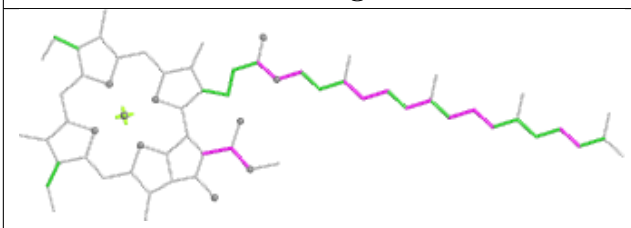
Ligand CLA B 812



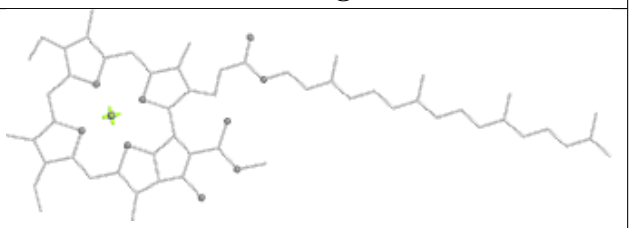
Bond lengths



Bond angles

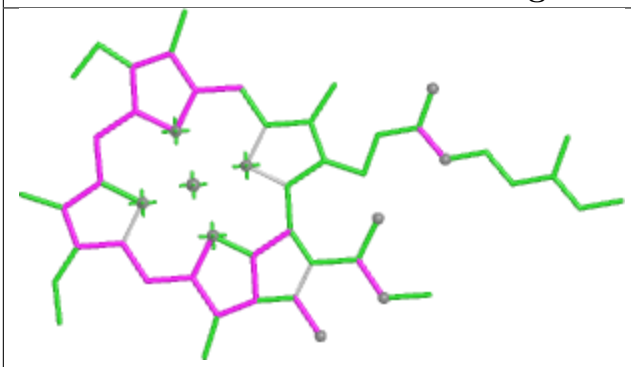


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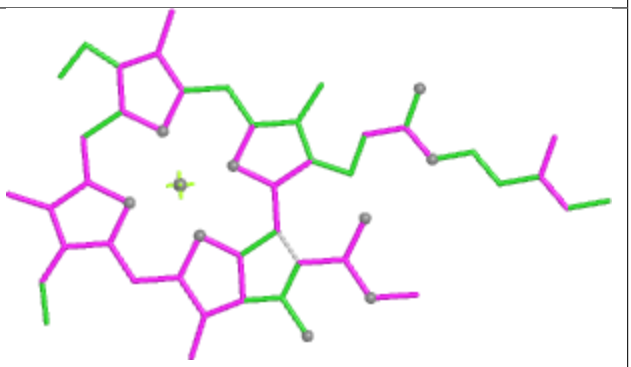


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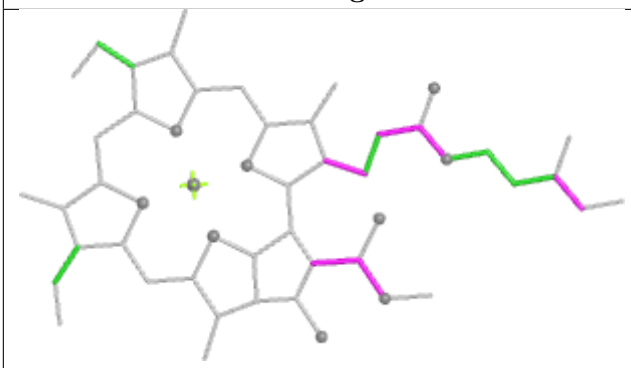
Ligand CLA 3 315



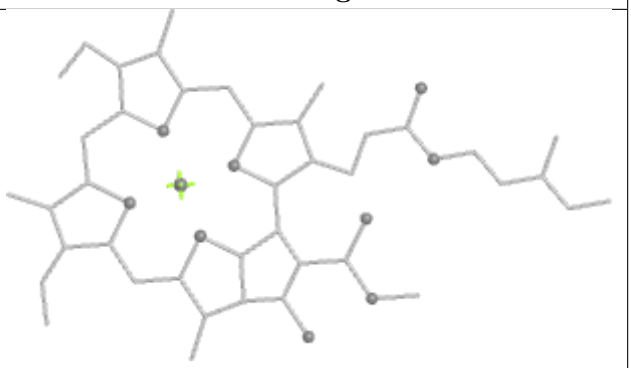
Bond lengths



Bond angles

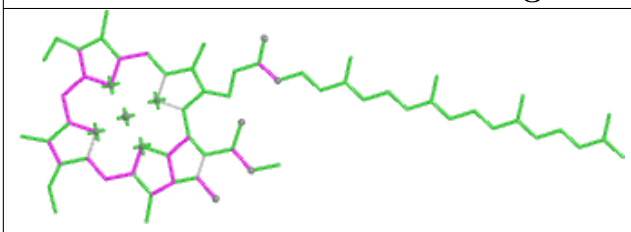


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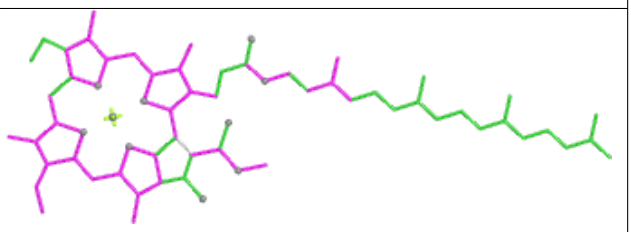


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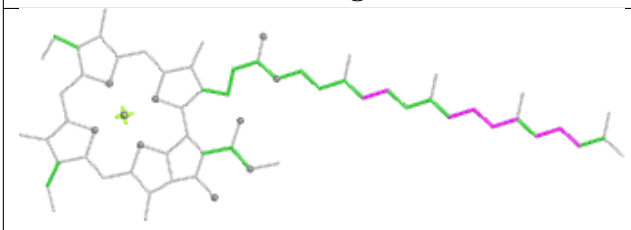
Ligand CLA A 833



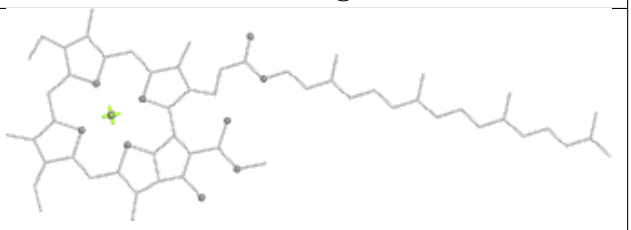
Bond lengths



Bond angles

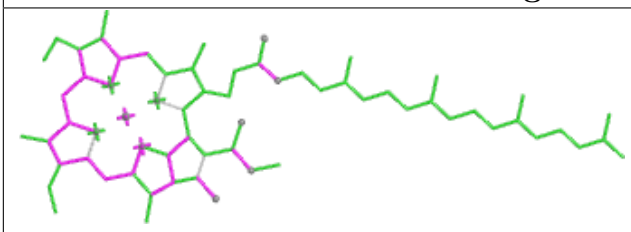


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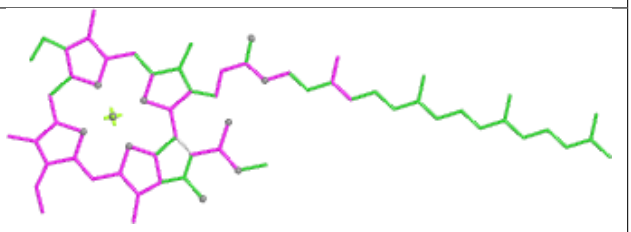


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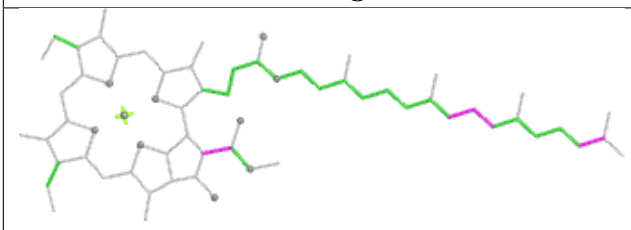
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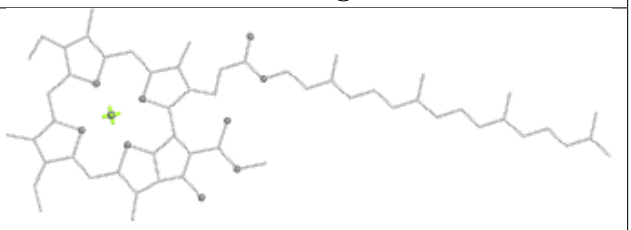
Bond lengths



Bond angles

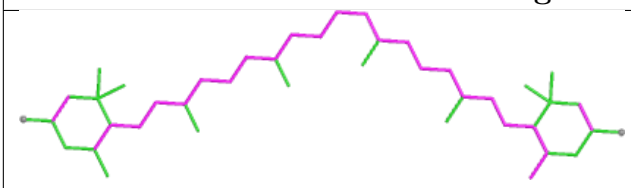


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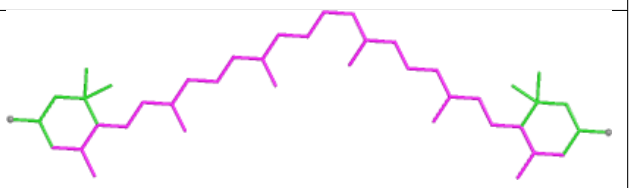


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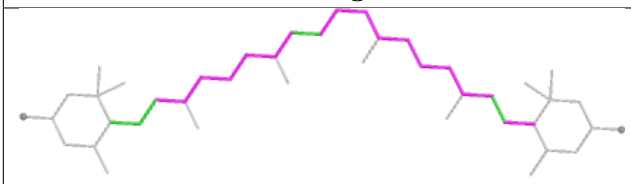
Ligand 5X6 2 319



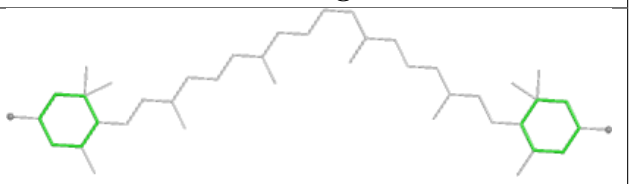
Bond lengths



Bond angles

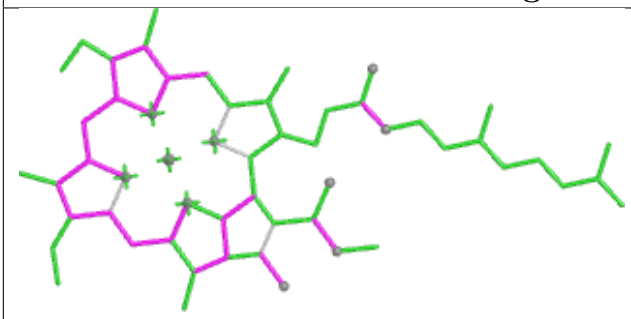


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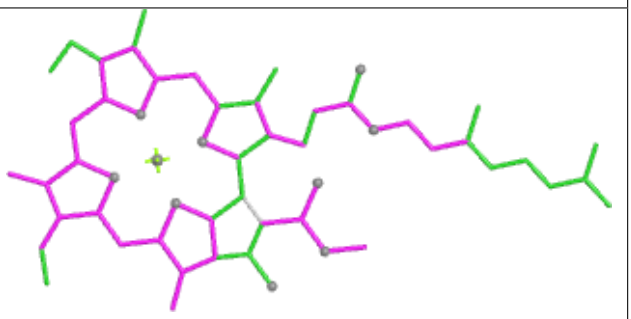


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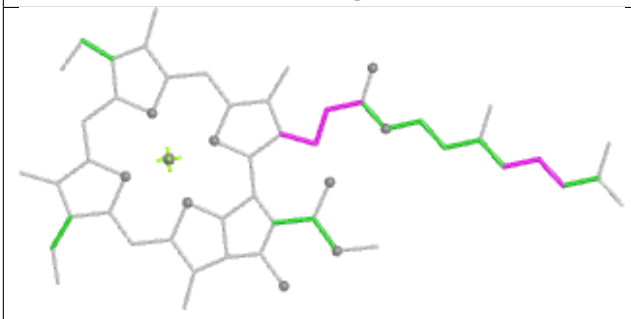
Ligand CLA K 102



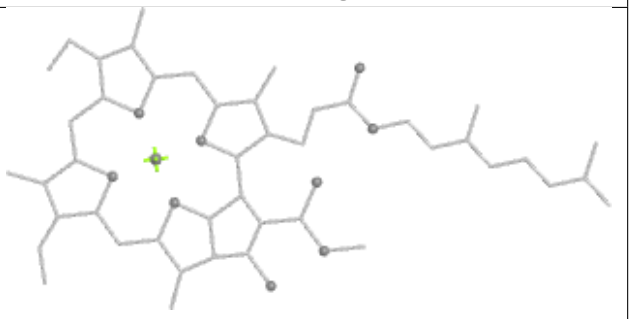
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Bond angles

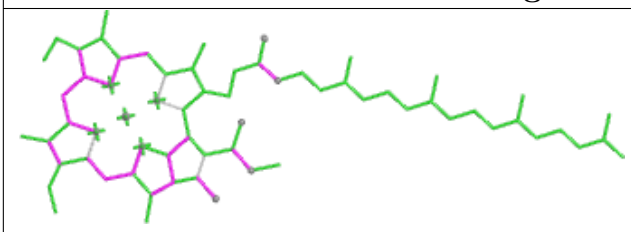


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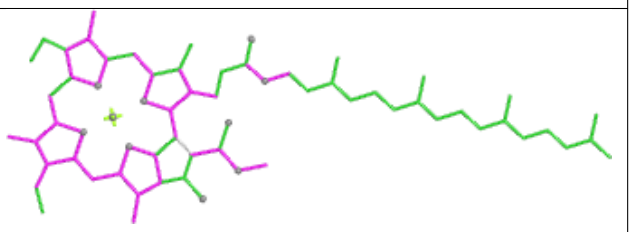


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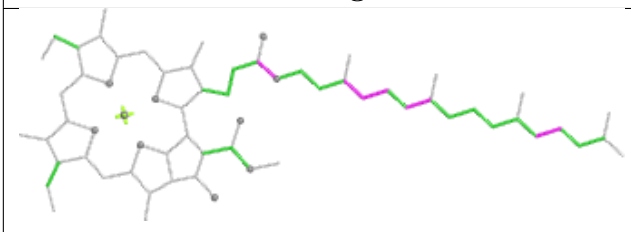
Ligand CLA A 819



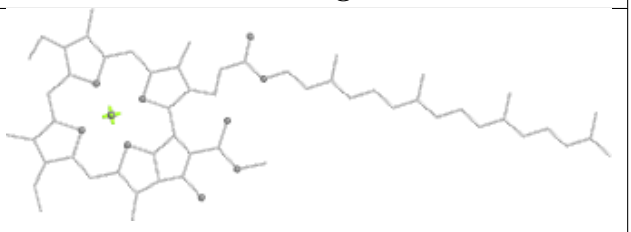
Bond lengths



Bond angles

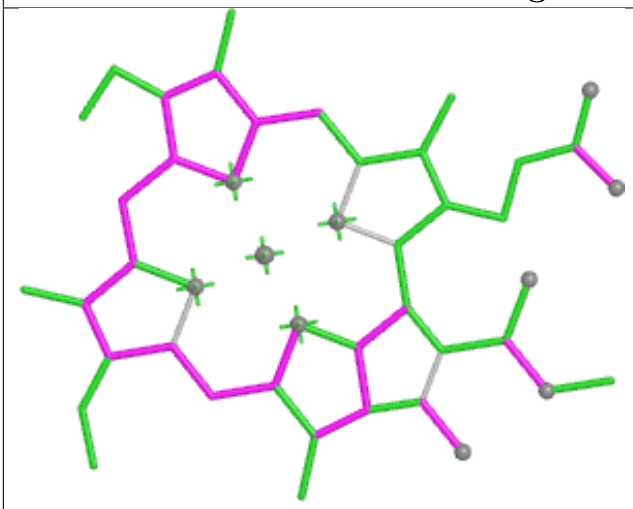


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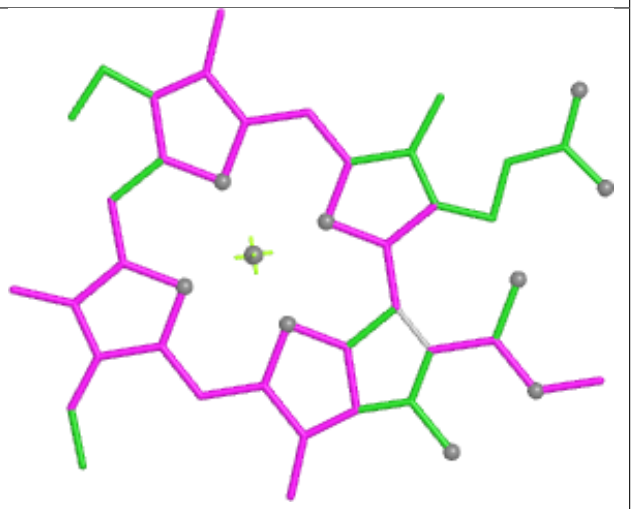


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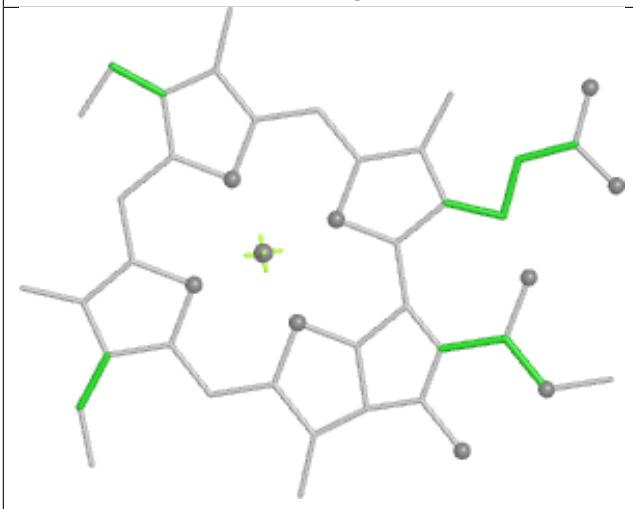
Ligand CLA 2 315



Bond lengths



Bond angles

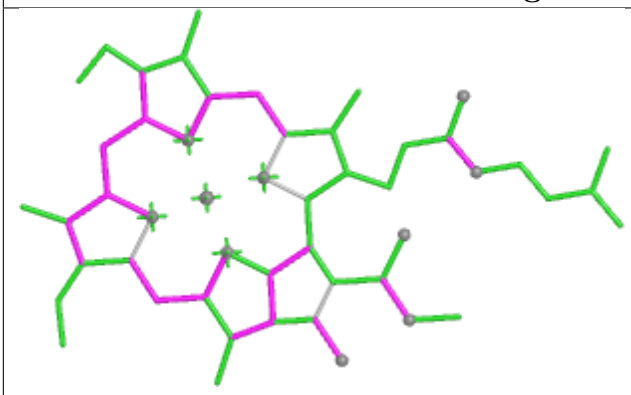


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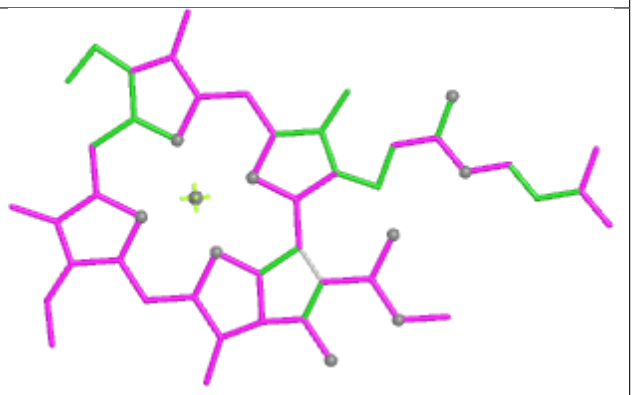


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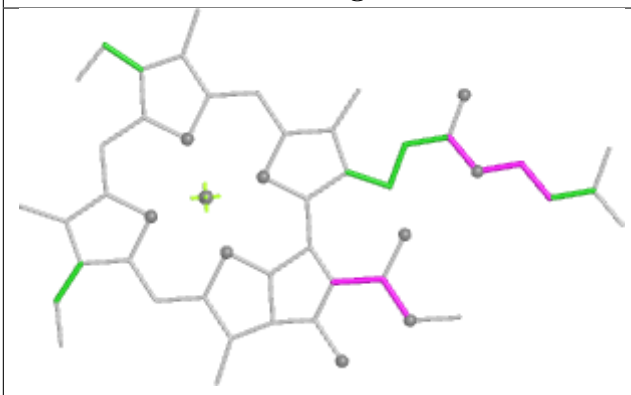
Ligand CLA A 829



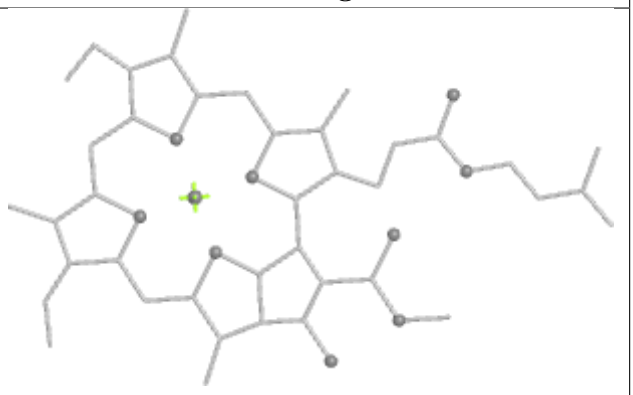
Bond lengths



Bond angles

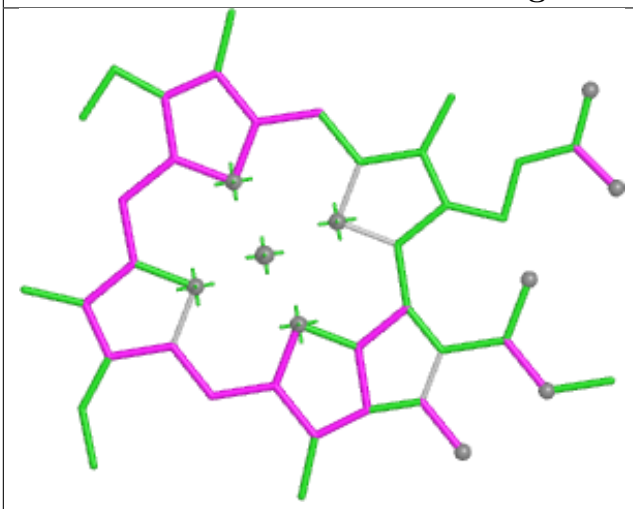


Torsions

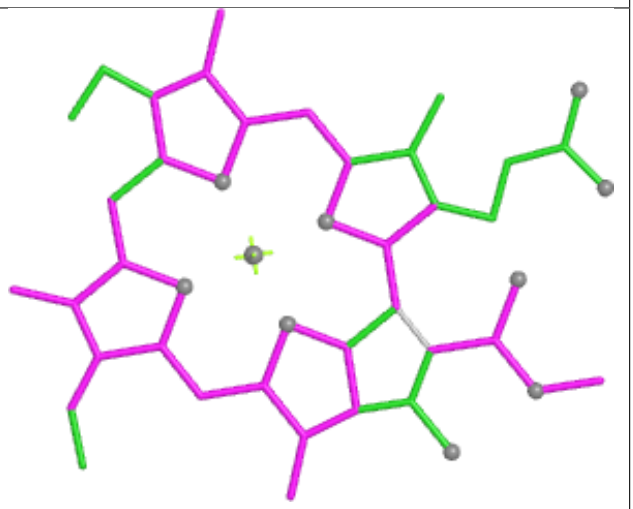


Rings

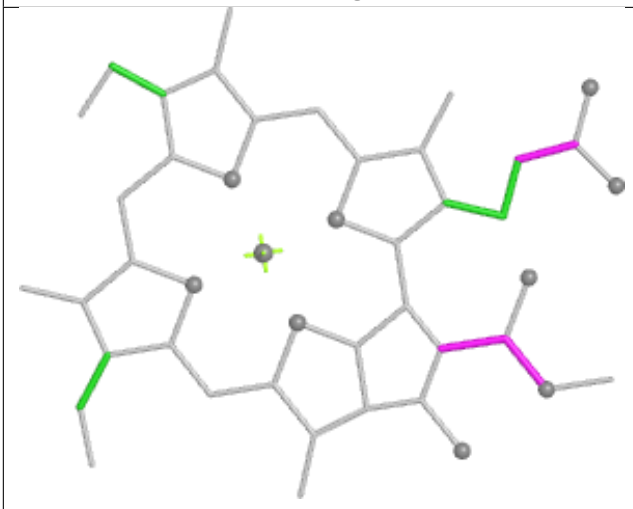
Ligand CLA 2 316



Bond lengths



Bond angles

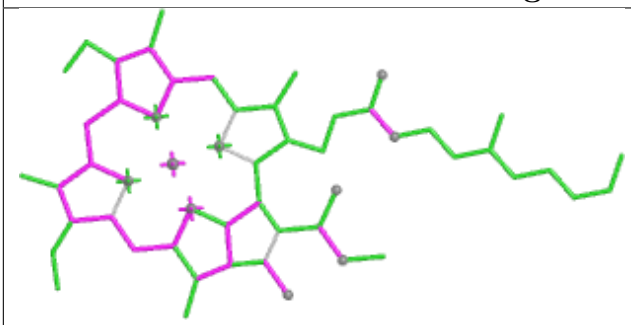


Torsions

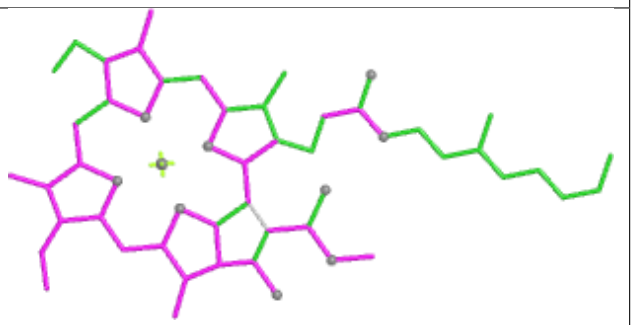


Rings

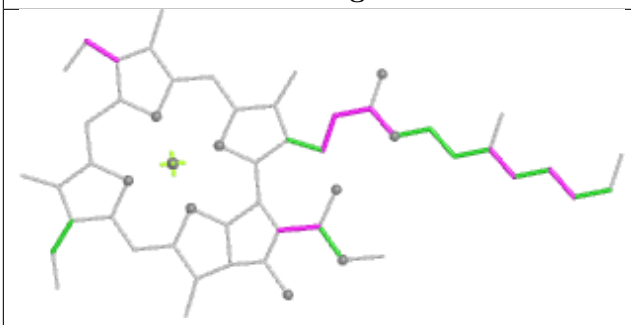
Ligand CLA A 810



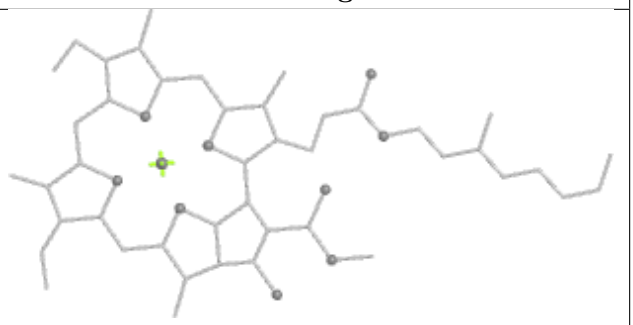
Bond lengths



Bond angles

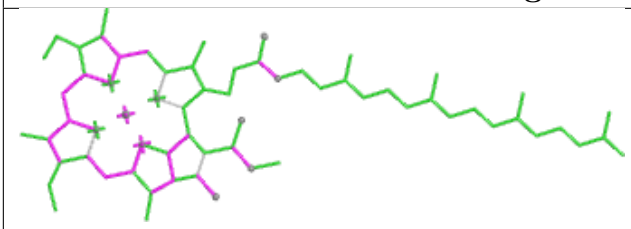


Torsions

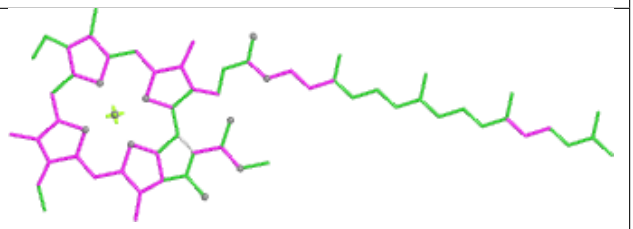


Rings

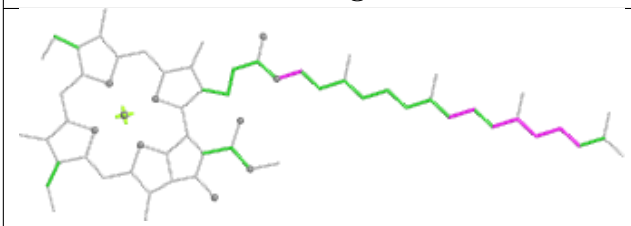
Ligand CLA B 804



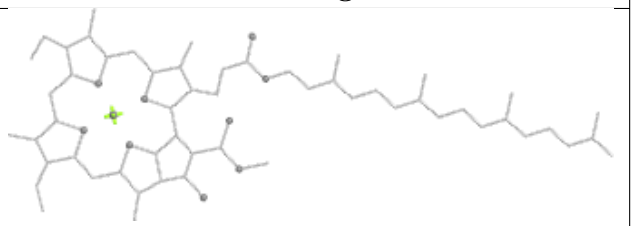
Bond lengths



Bond angles

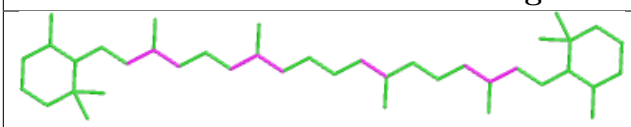


Torsions

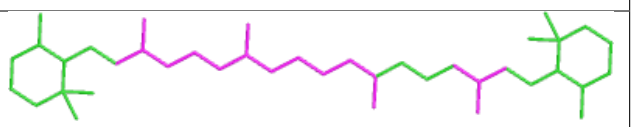


Rings

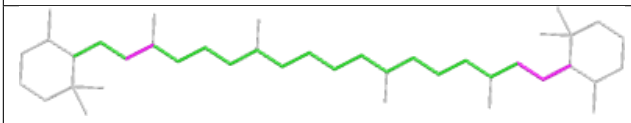
Ligand BCR L 206



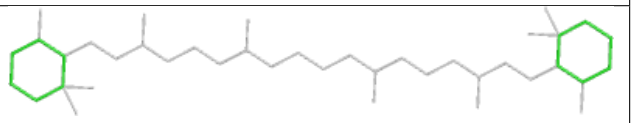
Bond lengths



Bond angles

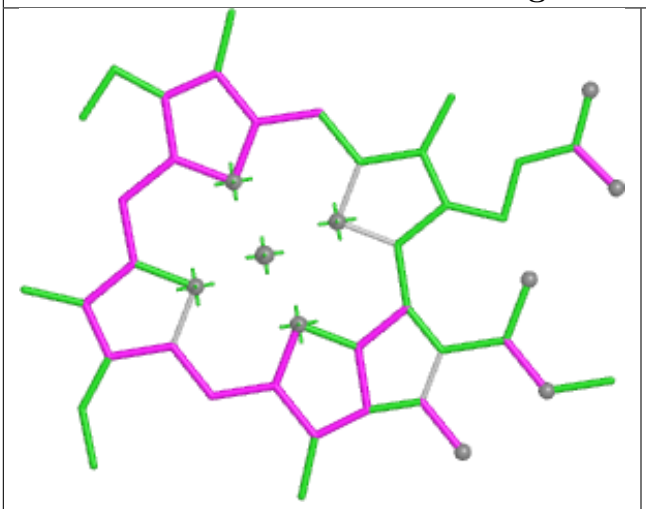


Torsions

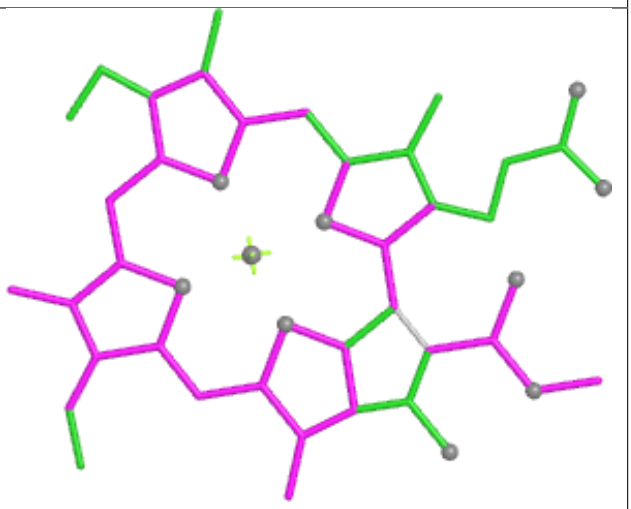


Rings

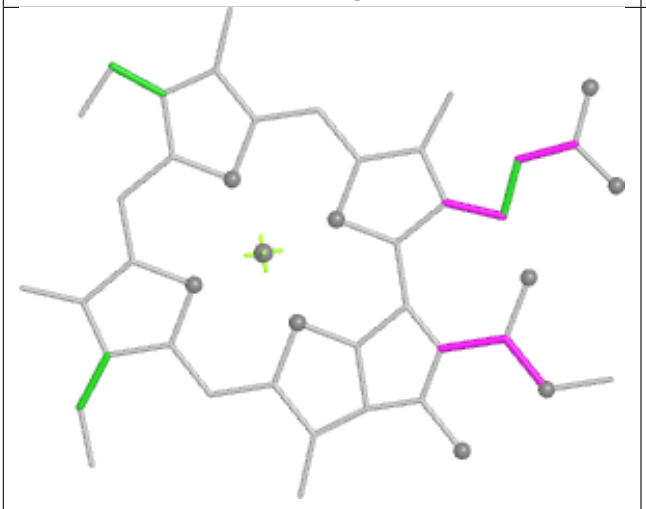
Ligand CLA 4 305



Bond lengths



Bond angles

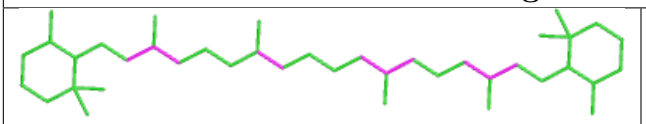


Torsions

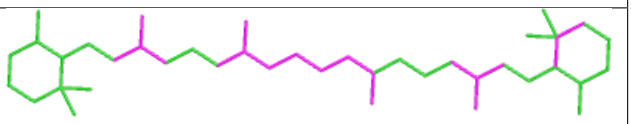


Rings

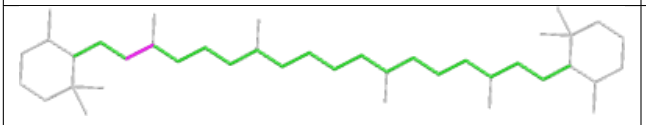
Ligand BCR O 202



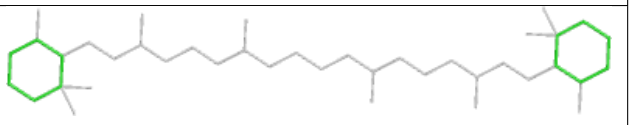
Bond lengths



Bond angles

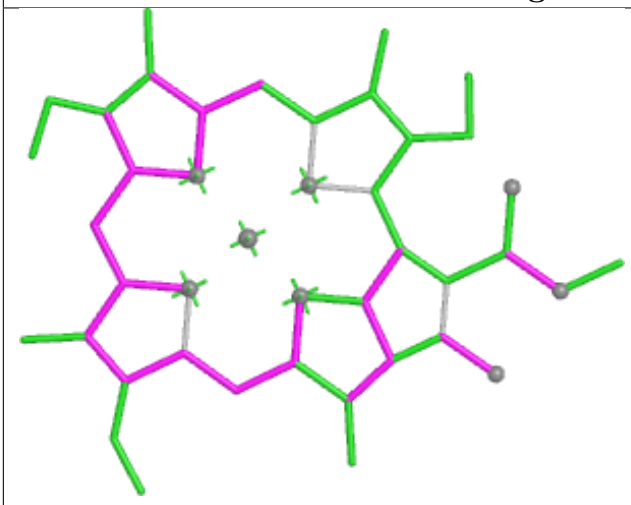


Torsions

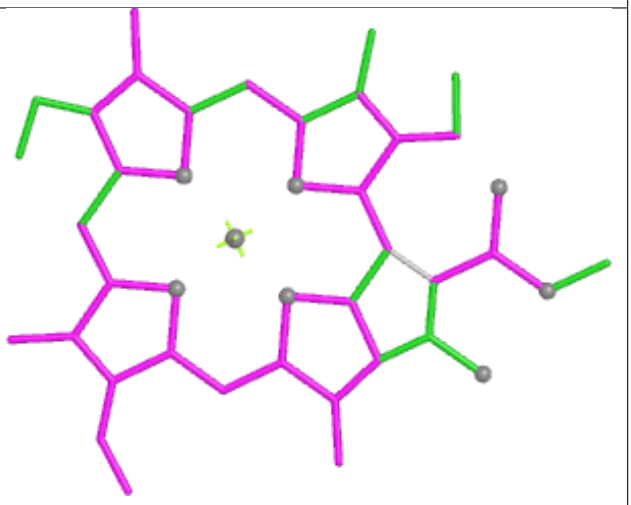


Rings

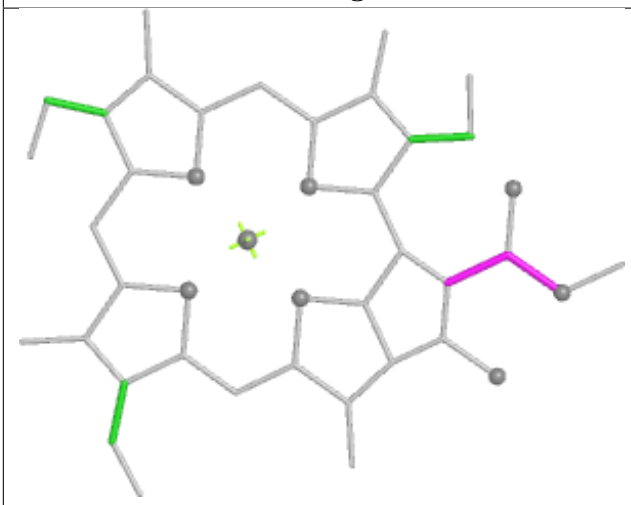
Ligand CLA J 103



Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

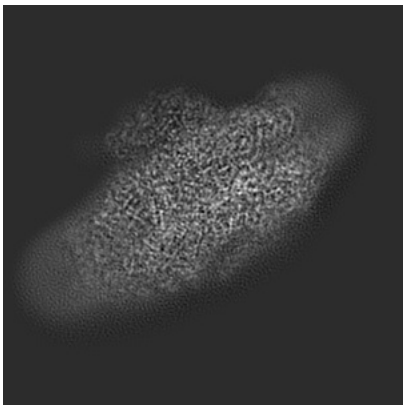
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-37480. These allow visual inspection of the internal detail of the map and identification of artifacts.

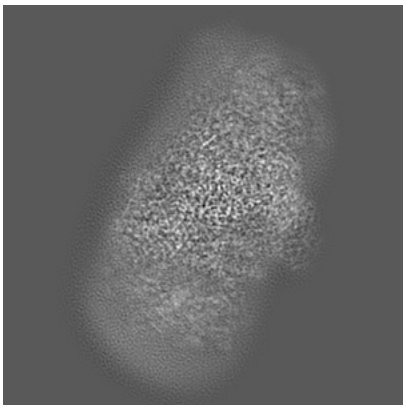
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

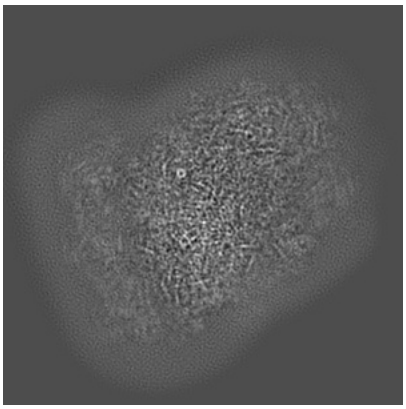
6.1.1 Primary map



X

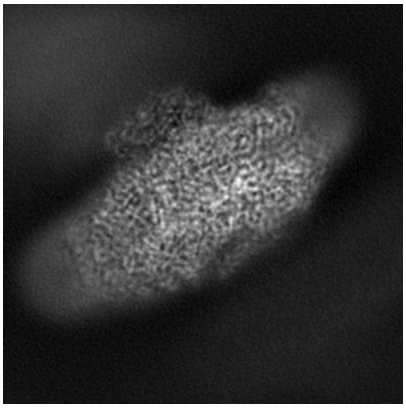


Y

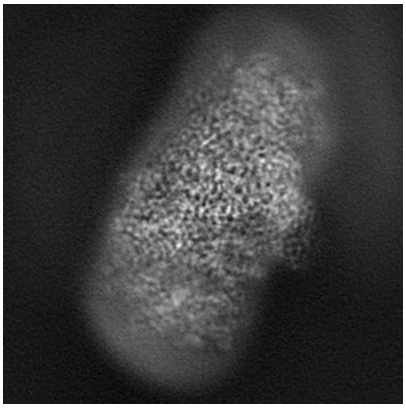


Z

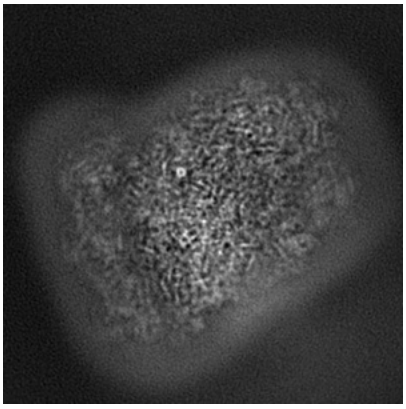
6.1.2 Raw map



X



Y

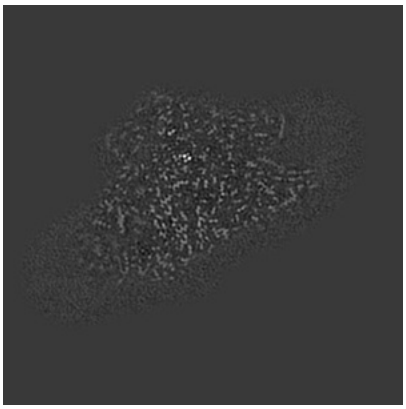


Z

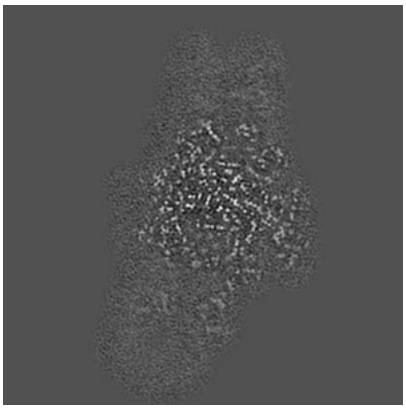
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

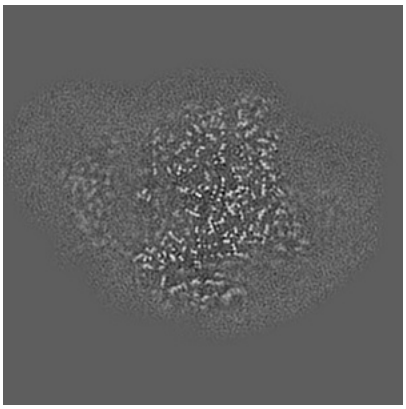
6.2.1 Primary map



X Index: 128

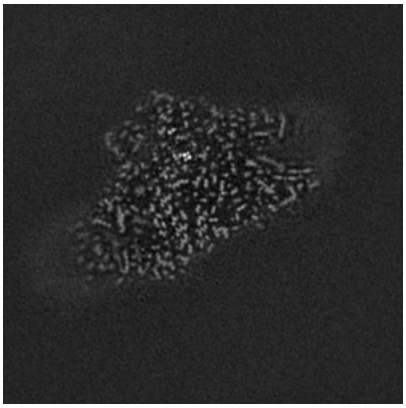


Y Index: 128

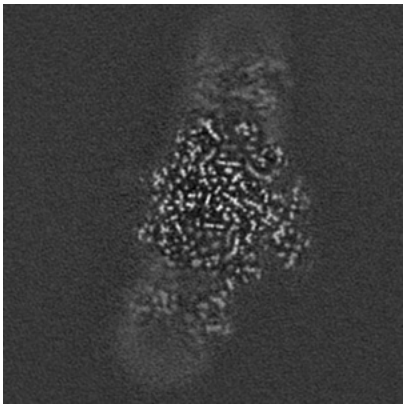


Z Index: 128

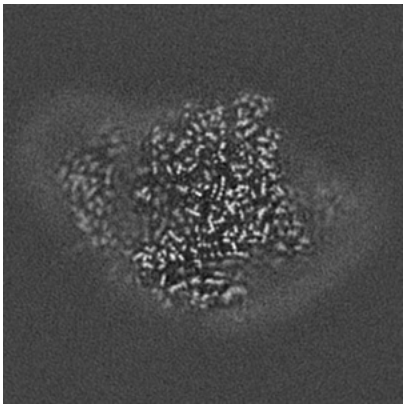
6.2.2 Raw map



X Index: 128



Y Index: 128

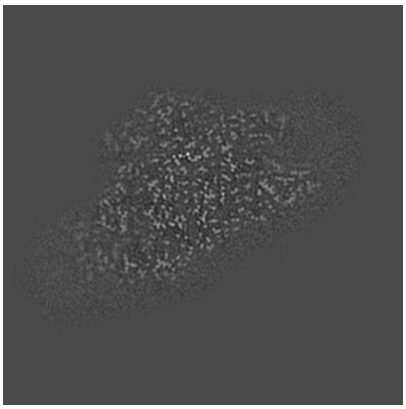


Z Index: 128

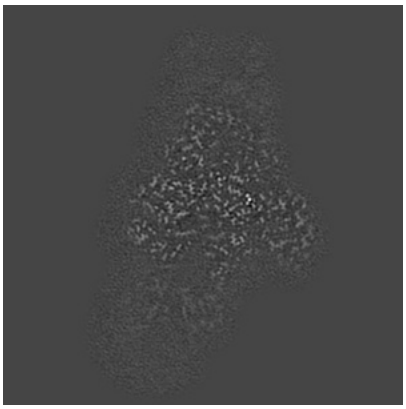
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

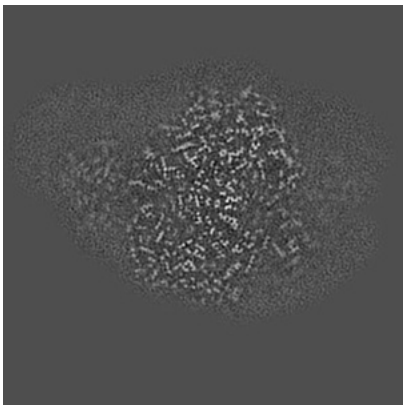
6.3.1 Primary map



X Index: 127

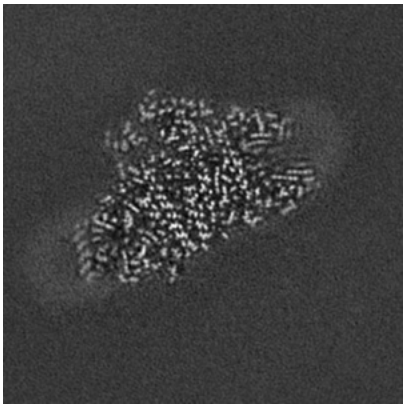


Y Index: 117

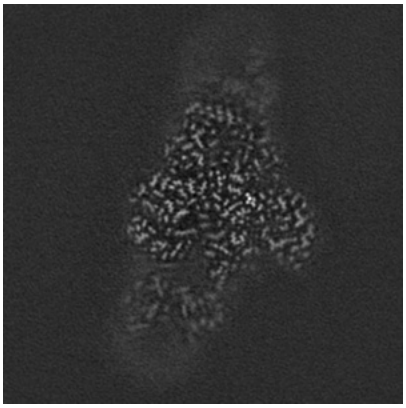


Z Index: 137

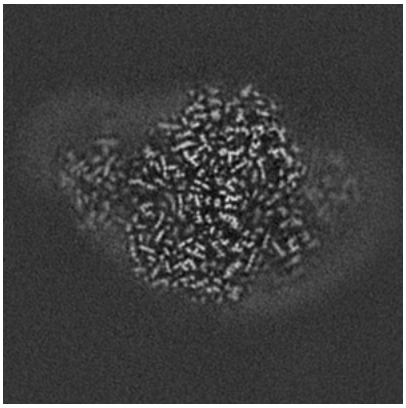
6.3.2 Raw map



X Index: 125



Y Index: 117

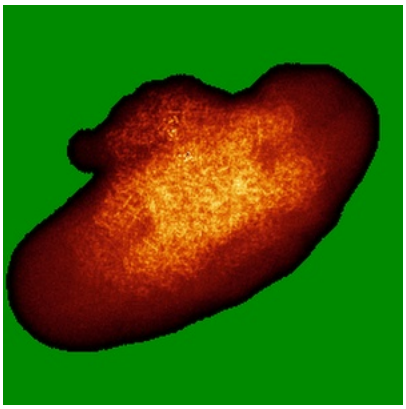


Z Index: 137

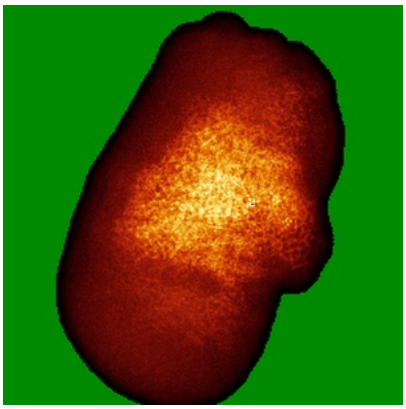
The images above show the largest variance slices of the map in three orthogonal directions.

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

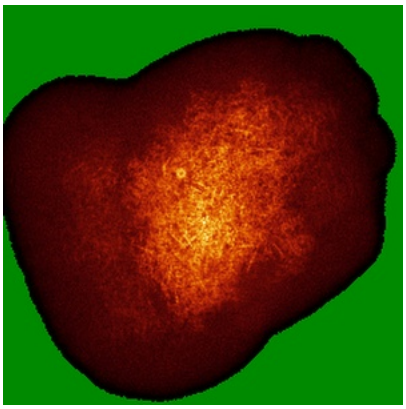
6.4.1 Primary map



X

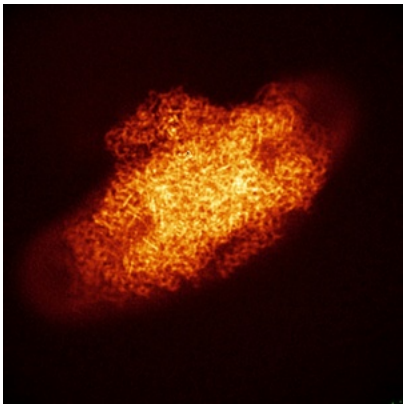


Y

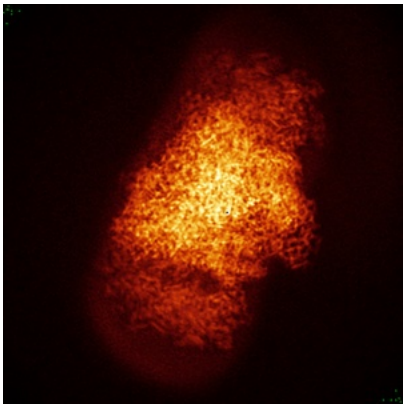


Z

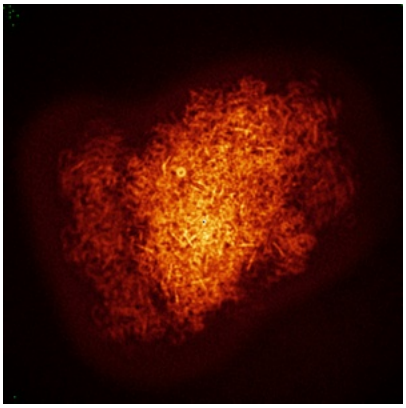
6.4.2 Raw map



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 0.016. 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.

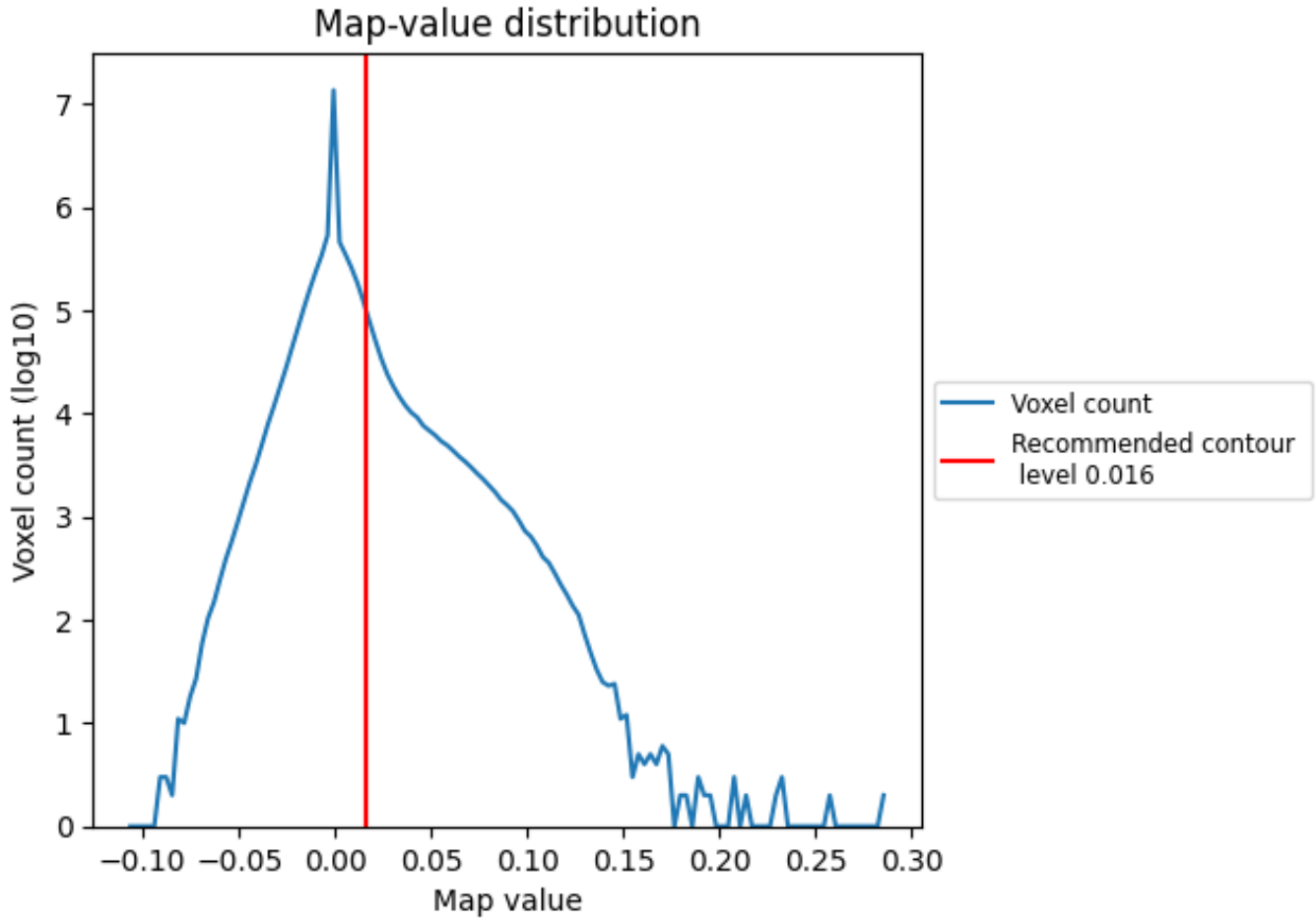
6.6 Mask visualisation (i)

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

7 Map analysis

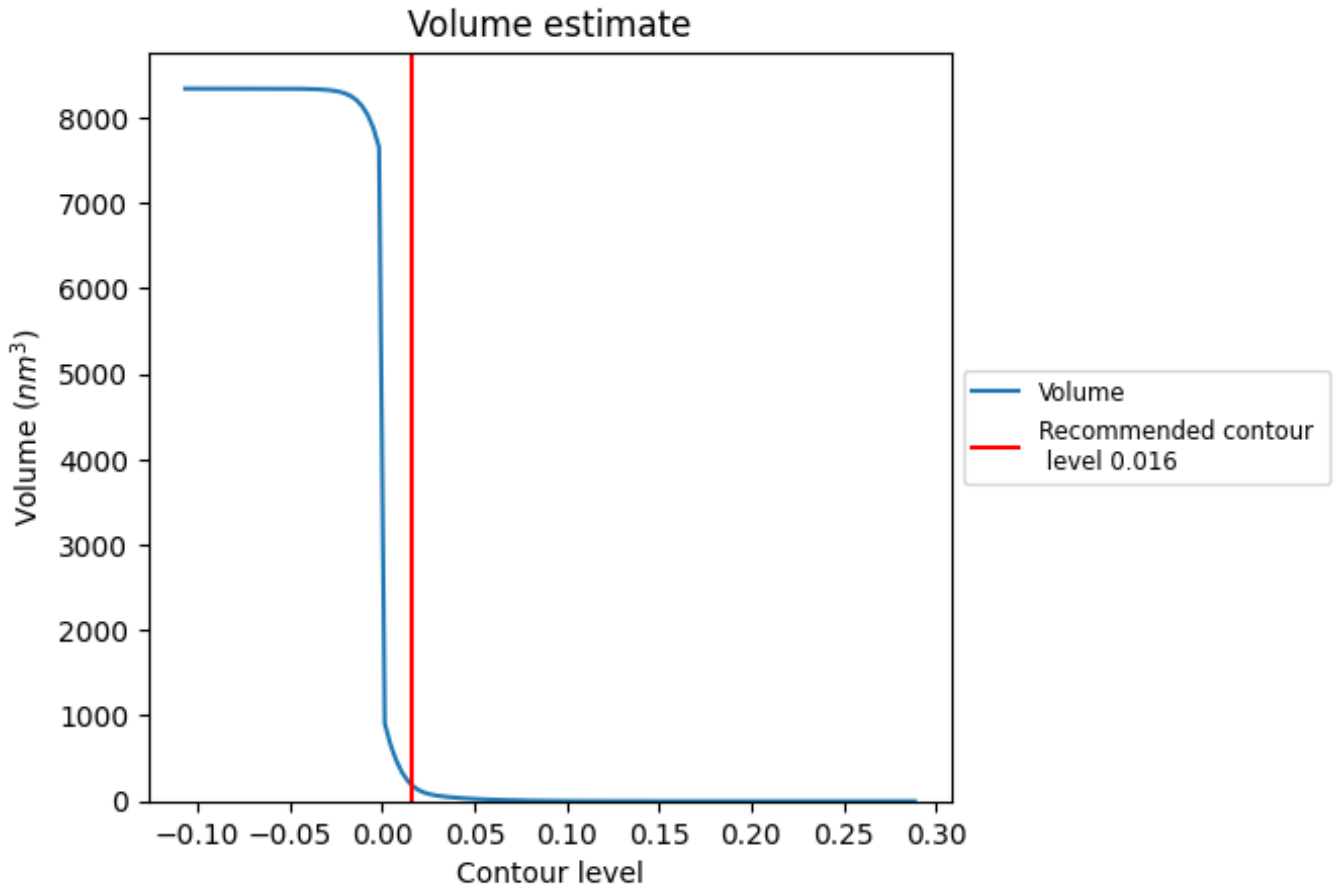
This section contains the results of statistical analysis of the map.

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.

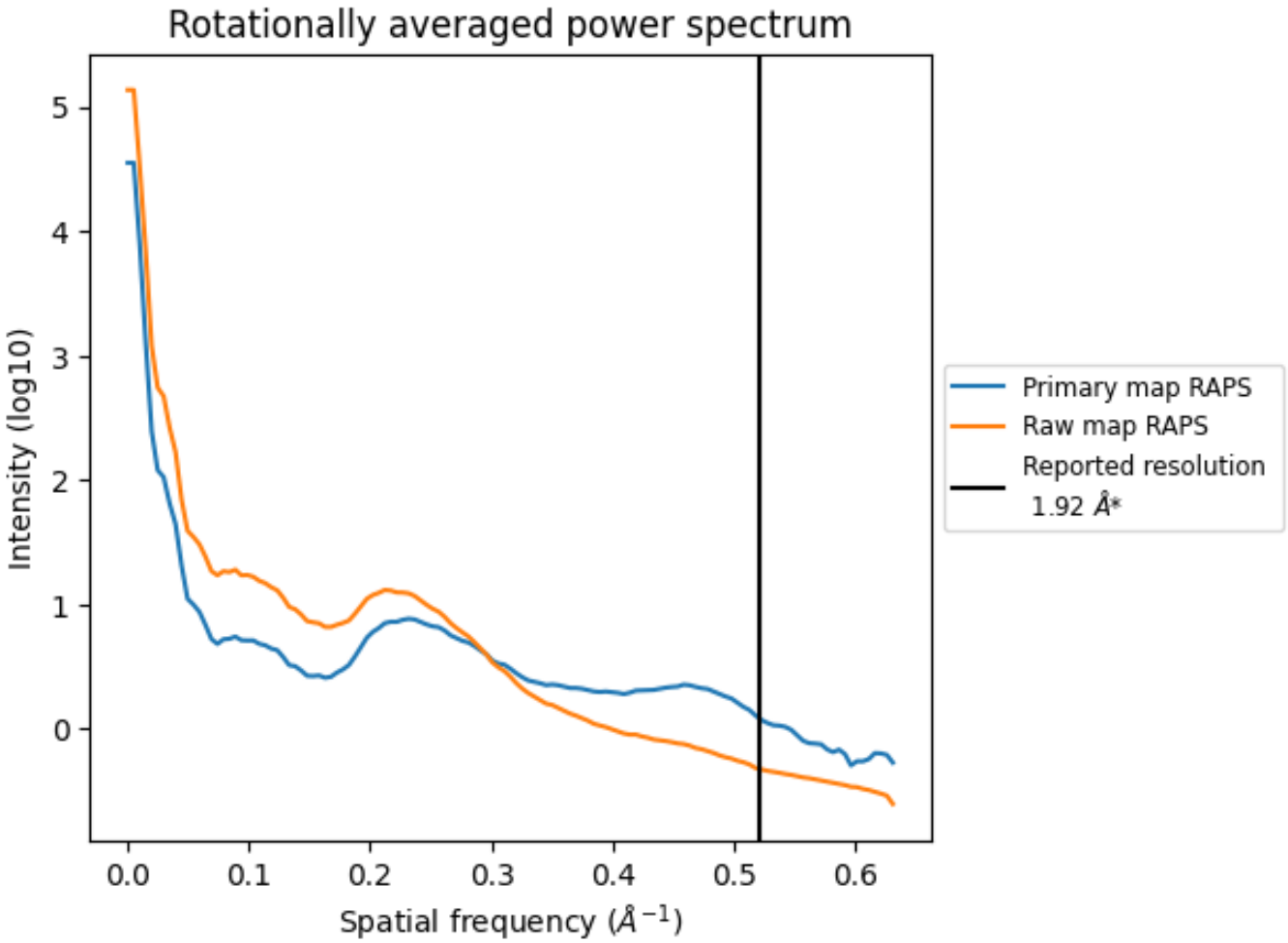
7.2 Volume estimate (i)



The volume at the recommended contour level is 193 nm^3; this corresponds to an approximate mass of 174 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)

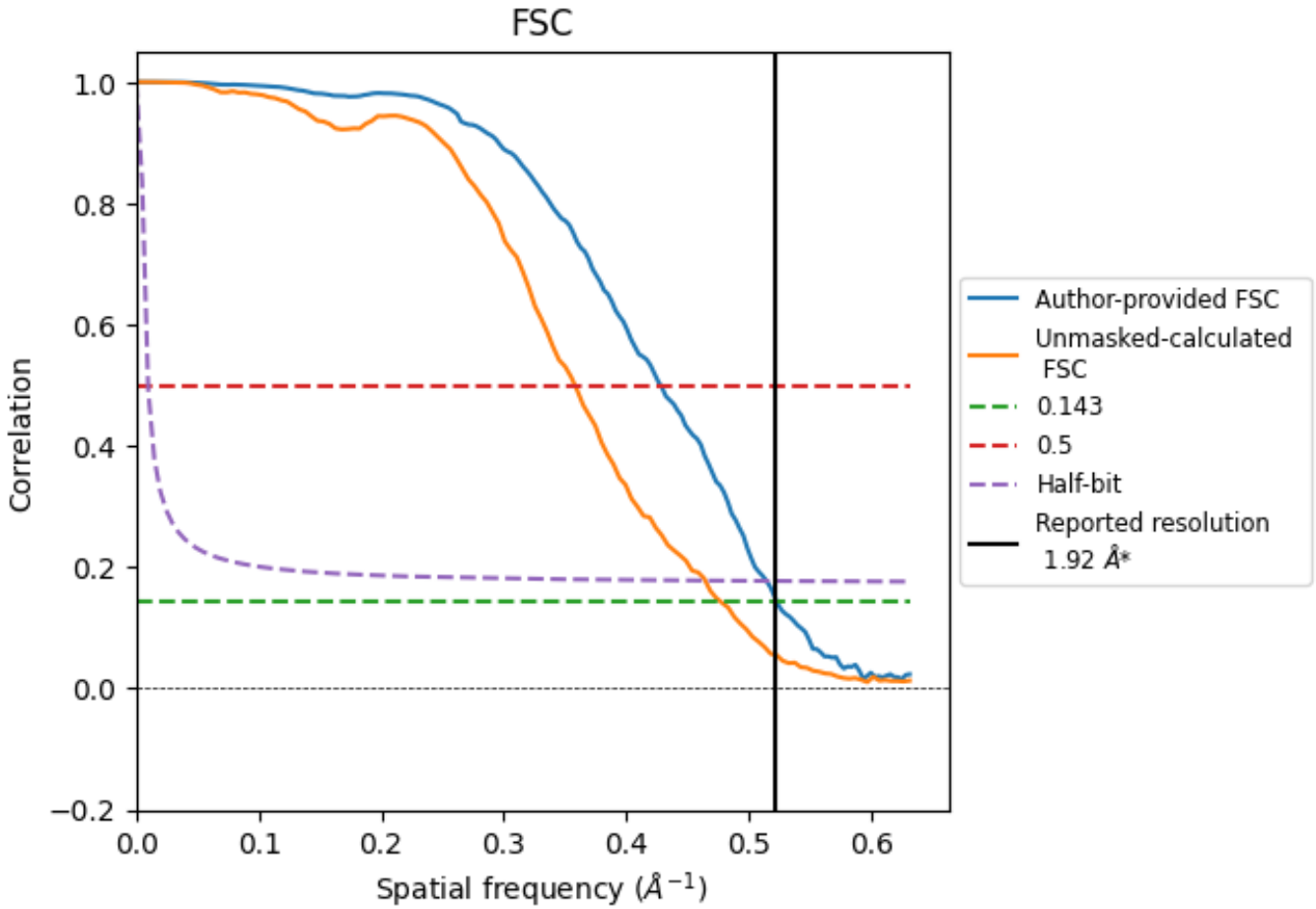


*Reported resolution corresponds to spatial frequency of 0.521 Å^{-1}

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 0.521 Å^{-1}

8.2 Resolution estimates (i)

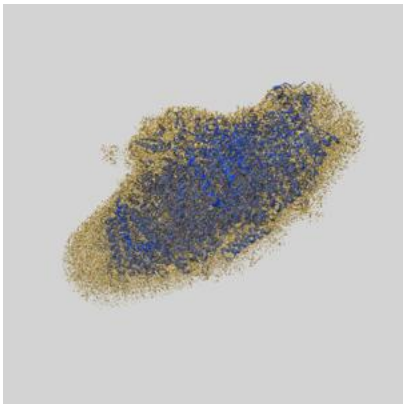
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.92	-	-
Author-provided FSC curve	1.91	2.34	1.94
Unmasked-calculated*	2.10	2.79	2.15

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

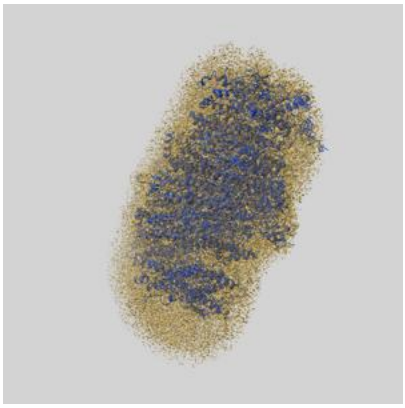
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-37480 and PDB model 8WEY. Per-residue inclusion information can be found in section 3 on page 24.

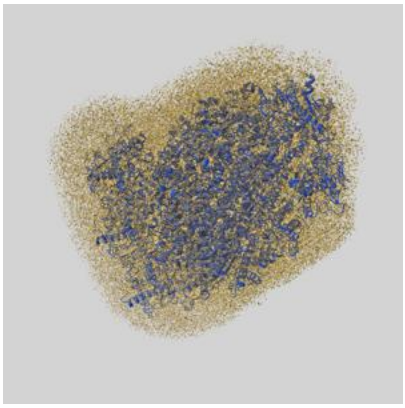
9.1 Map-model overlay



X



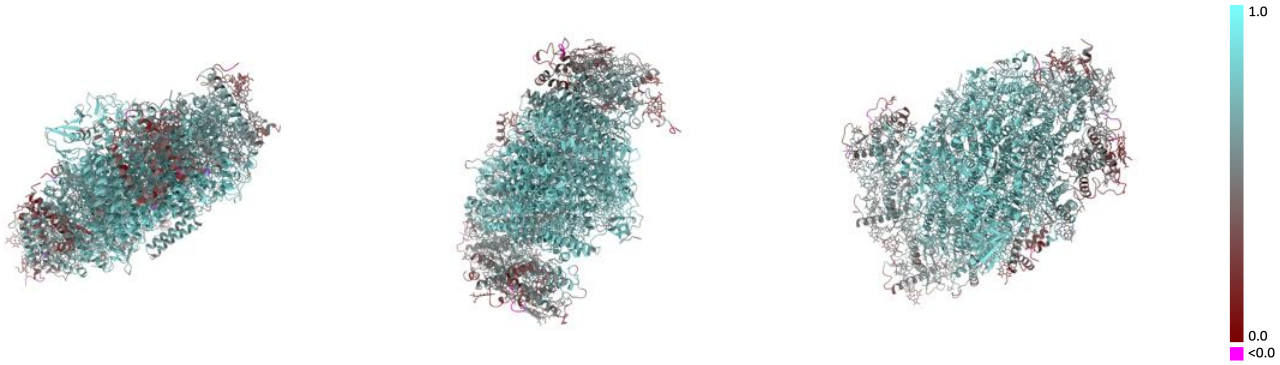
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.016 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

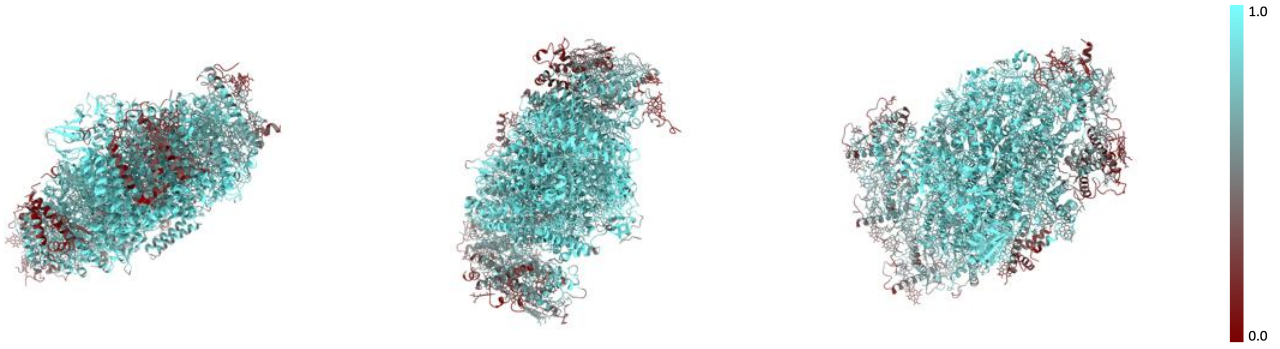
9.2 Q-score mapped to coordinate model



X Y Z

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

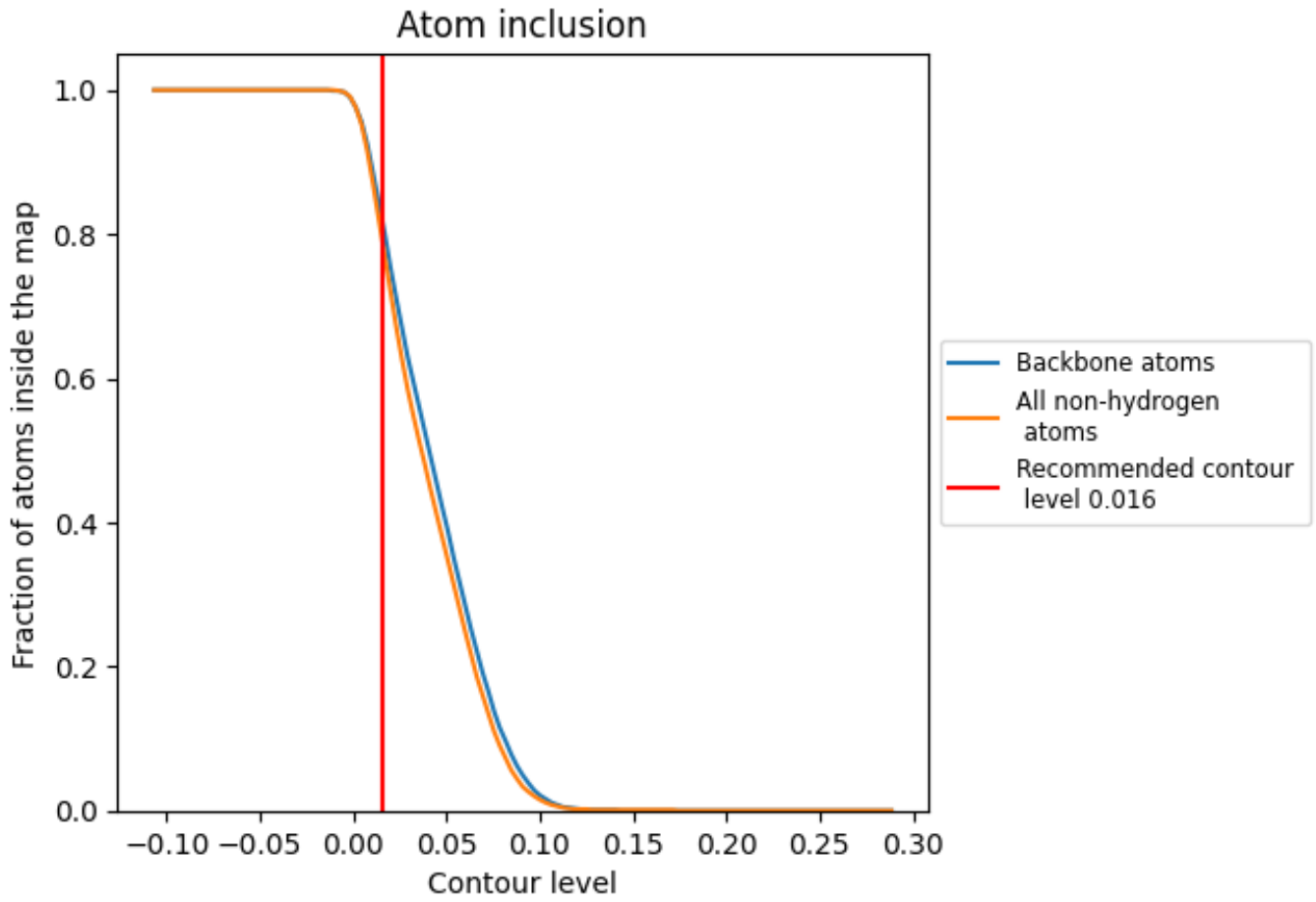
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.016).

9.4 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 78% 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 (0.016) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7850	0.6620
1	0.5470	0.4670
2	0.5650	0.4990
3	0.4990	0.4530
4	0.3480	0.3730
5	0.6250	0.5340
A	0.9480	0.7870
B	0.9320	0.7720
C	0.9780	0.8100
D	0.8930	0.7170
E	0.8800	0.7220
F	0.8730	0.7150
I	0.8930	0.7250
J	0.8960	0.7440
K	0.7180	0.5880
L	0.7930	0.6310
M	0.8300	0.6850
O	0.2150	0.3110

