wwPDB EM Validation Summary Report

Aug 5, 2026 – 03:19 AM EDT

PDB ID	:	9MH1 / pdb_00009mh1
EMDB ID	:	EMD-48266
Title	:	Dunaliella tertiolecta PSI-LHCI supercomplex
Authors	:	Liu, H.W.; Khera, R.; Iwai, M.; Merchant, S.S.
Deposited on	:	2024-12-11
Resolution	:	2.10 Å(reported)
Based on initial model	:	6SL5

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

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

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

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

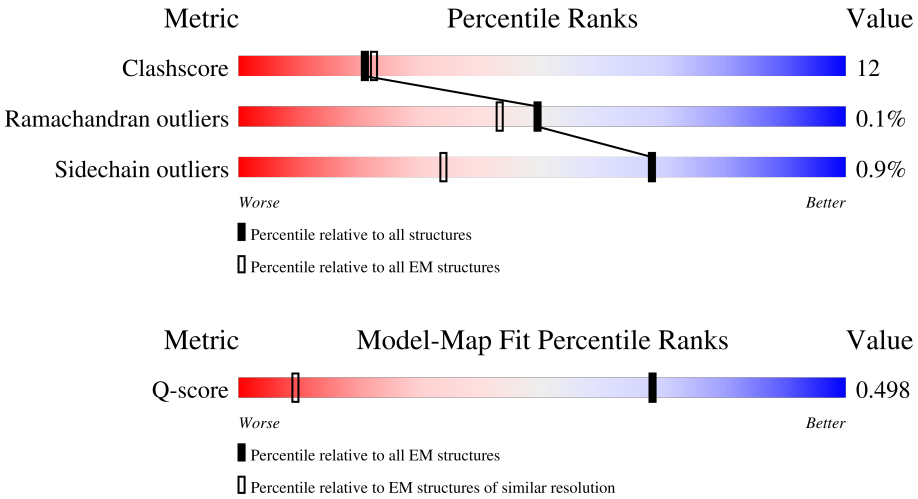
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.10 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	2317 (1.60 - 2.60)

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	1	228	74% 12% 14%
2	3	286	6% 58% 20% 21%
3	7	255	66% 19% 15%
4	8	254	72% 17% 11%

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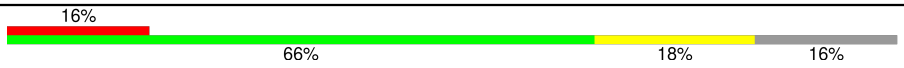
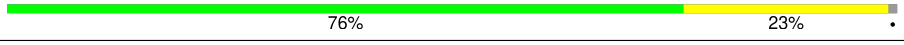
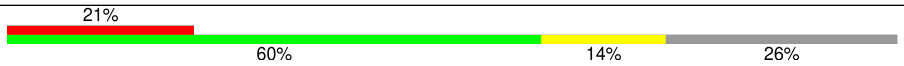
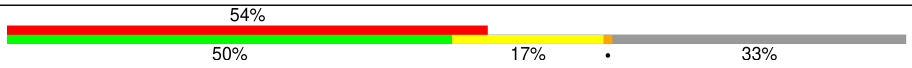
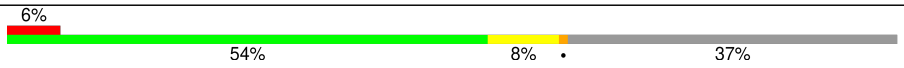
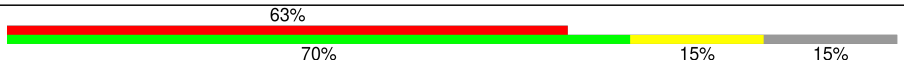
Mol	Chain	Length	Quality of chain
5	9	222	
6	A	751	
7	B	735	
8	C	81	
9	D	193	
10	E	111	
11	F	227	
12	G	141	
13	H	134	
14	I	109	
15	J	41	
16	K	123	
17	L	198	
18	2	261	

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
19	CHL	2	302	X	-	-	-
19	CHL	2	306	X	-	-	-
19	CHL	3	301	X	-	-	-
19	CHL	3	323	X	-	-	-
21	LUT	1	615	X	-	-	-
21	LUT	2	314	X	-	-	-
21	LUT	2	315	X	-	-	-
21	LUT	3	315	X	-	-	-
21	LUT	7	316	X	-	-	-
21	LUT	8	314	X	-	-	-
21	LUT	9	613	X	-	-	-

2 Entry composition (i)

There are 33 unique types of molecules in this entry. The entry contains 41548 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 Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1	197	1505	965	255	278	7	0	0

- Molecule 2 is a protein called LHCA3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	3	226	1719	1120	282	312	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	7	217	1669	1078	281	304	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	8	226	1721	1108	286	320	7	0	0

- Molecule 5 is a protein called LHCA9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	9	187	1453	945	244	259	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	A	740	5808	3795	993	1002	18	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	734	Total	C	N	O	S	0	0
			5814	3816	975	1010	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C	80	Total	C	N	O	S	0	0
			600	370	104	115	11		

- Molecule 9 is a protein called Photosystem I reaction center subunit II, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	143	Total	C	N	O	S	0	0
			1133	727	193	207	6		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
10	E	68	Total	C	N	O	0	0
			540	343	95	102		

- Molecule 11 is a protein called PSAF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	165	Total	C	N	O	S	0	0
			1300	836	225	237	2		

- Molecule 12 is a protein called PSAG1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	G	105	Total	C	N	O	S	0	0
			794	515	134	142	3		

- Molecule 13 is a protein called PSAH1.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	H	47	Total	C	N	O	0	0
			349	223	60	66		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	I	35	Total	C	N	O	S	0	0
			274	191	40	42	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	J	41	Total	C	N	O	S	0	0
			327	223	47	56	1		

- Molecule 16 is a protein called PSI-K.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	K	83	Total	C	N	O	S	0	0
			579	370	101	105	3		

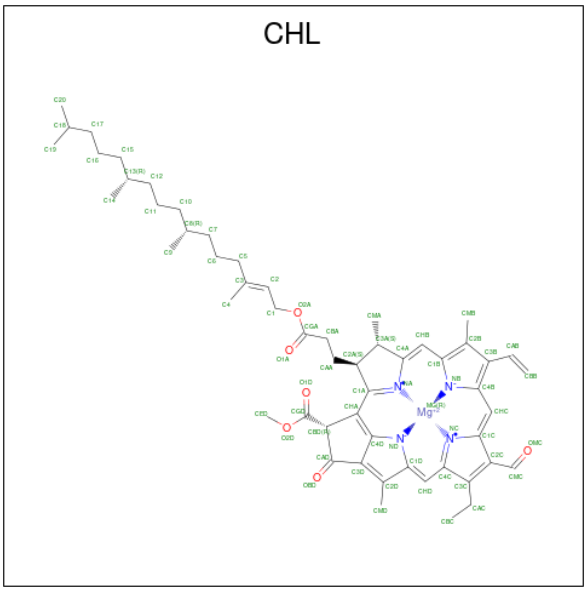
- Molecule 17 is a protein called PSAL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	L	124	Total	C	N	O	S	0	0
			891	580	146	160	5		

- Molecule 18 is a protein called LHCA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	2	222	Total	C	N	O	S	0	0
			1728	1125	284	311	8		

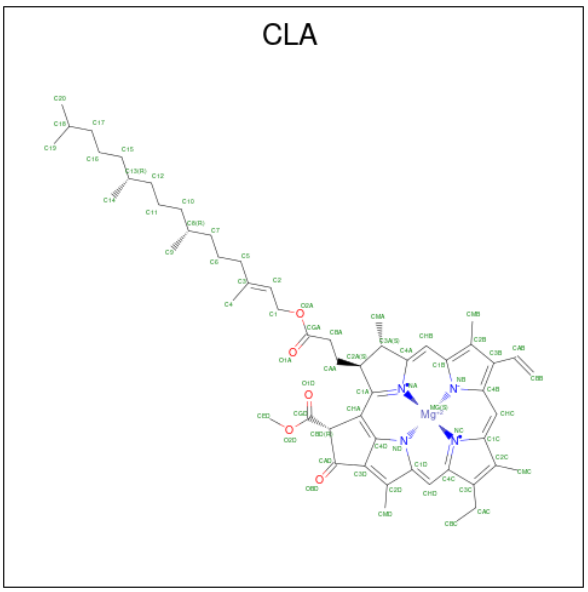
- Molecule 19 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
19	1	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
19	1	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
19	3	1	Total	C	Mg	N	O	0
			62	51	1	4	6	
19	3	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
19	7	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
19	7	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
19	7	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
19	8	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
19	8	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
19	8	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
19	9	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
19	2	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
19	2	1	Total	C	Mg	N	O	0
			47	36	1	4	6	

- Molecule 20 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as

"Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
20	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
20	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
20	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	7	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	7	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	7	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	7	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	7	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	7	1	Total	C	Mg	N	O	0
			52	42	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
20	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	7	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	7	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
20	8	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	8	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
20	8	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	8	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	9	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	9	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	9	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	9	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
20	9	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	9	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	9	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			49	40	1	4	4	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
20	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	F	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
20	F	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	F	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
20	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	G	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
20	G	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	H	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	J	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
20	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	K	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	K	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
20	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	L	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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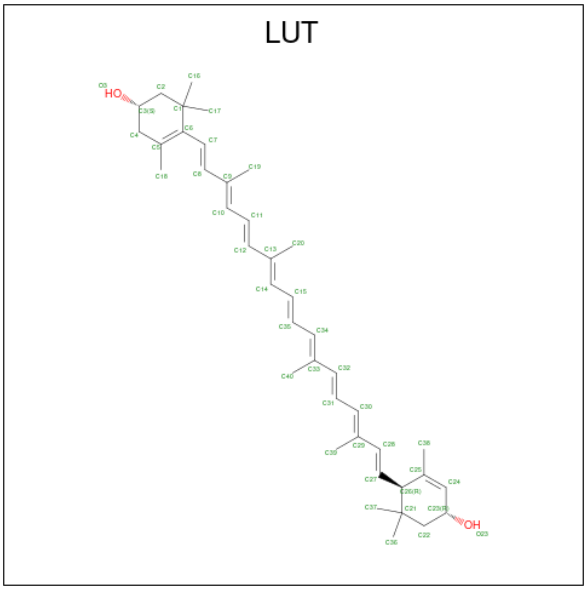
Mol	Chain	Residues	Atoms					AltConf
20	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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



Mol	Chain	Residues	Atoms			AltConf
21	1	1	Total	C	O	0
			42	40	2	
21	3	1	Total	C	O	0
			42	40	2	
21	7	1	Total	C	O	0
			42	40	2	

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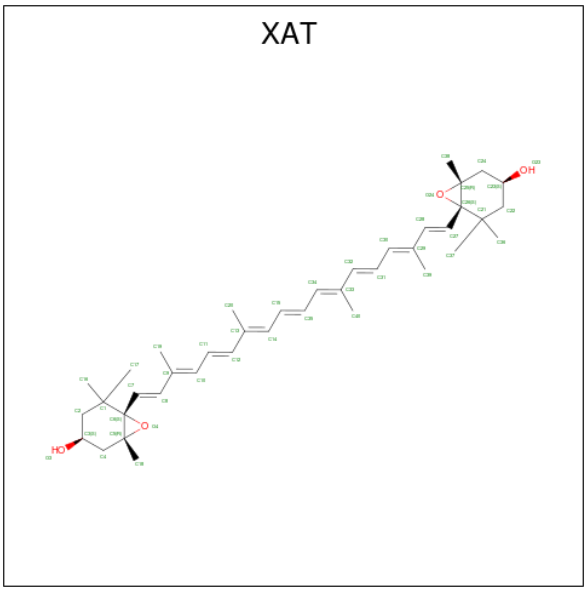
Mol	Chain	Residues	Atoms	AltConf
21	8	1	Total C O 42 40 2	0
21	9	1	Total C O 42 40 2	0
21	2	1	Total C O 42 40 2	0
21	2	1	Total C O 42 40 2	0

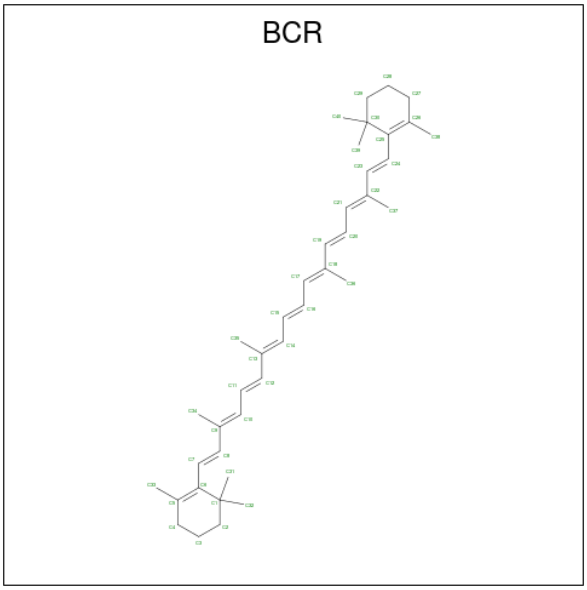
- Molecule 22 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: $C_{40}H_{56}O_4$).



Mol	Chain	Residues	Atoms	AltConf
22	1	1	Total C O 44 40 4	0
22	3	1	Total C O 44 40 4	0
22	7	1	Total C O 44 40 4	0
22	8	1	Total C O 44 40 4	0
22	9	1	Total C O 44 40 4	0
22	9	1	Total C O 44 40 4	0

- Molecule 23 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand

of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
23	1	1	Total C 40 40	0
23	3	1	Total C 40 40	0
23	3	1	Total C 40 40	0
23	3	1	Total C 40 40	0
23	7	1	Total C 40 40	0
23	8	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0

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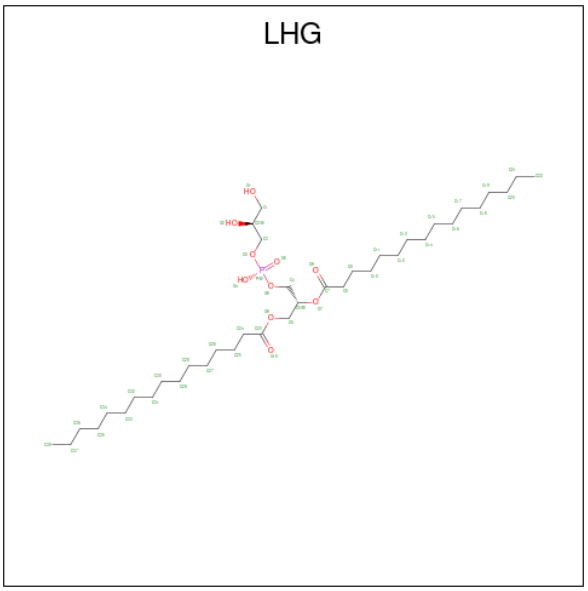
Mol	Chain	Residues	Atoms	AltConf
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 39 39	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	F	1	Total C 40 40	0
23	F	1	Total C 40 40	0
23	G	1	Total C 40 40	0
23	I	1	Total C 40 40	0
23	J	1	Total C 40 40	0
23	J	1	Total C 40 40	0
23	J	1	Total C 40 40	0
23	K	1	Total C 40 40	0
23	K	1	Total C 40 40	0
23	L	1	Total C 40 40	0
23	L	1	Total C 40 40	0

- Molecule 24 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
24	1	1	Total C O P 26 15 10 1	0
24	1	1	Total C O P 46 35 10 1	0
24	7	1	Total C O P 22 11 10 1	0
24	7	1	Total C O P 34 23 10 1	0
24	8	1	Total C O P 29 18 10 1	0
24	8	1	Total C O P 38 27 10 1	0
24	8	1	Total C O P 43 32 10 1	0
24	9	1	Total C O P 36 25 10 1	0
24	A	1	Total C O P 36 25 10 1	0
24	A	1	Total C O P 49 38 10 1	0
24	A	1	Total C O P 28 17 10 1	0
24	A	1	Total C O P 34 25 8 1	0
24	B	1	Total C O P 32 21 10 1	0
24	B	1	Total C O P 30 19 10 1	0

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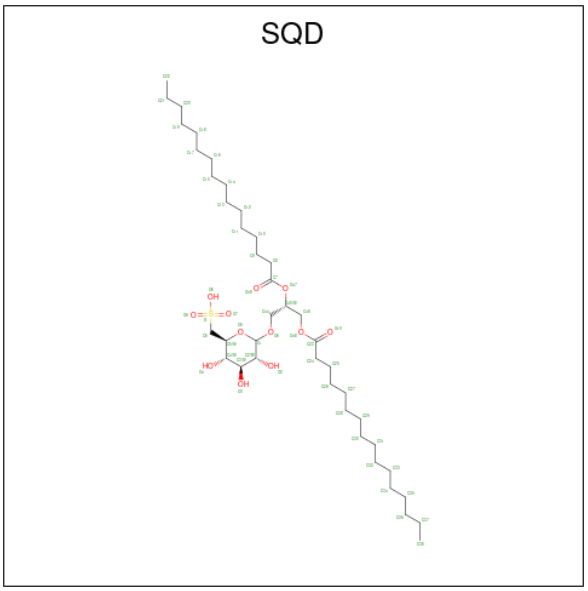
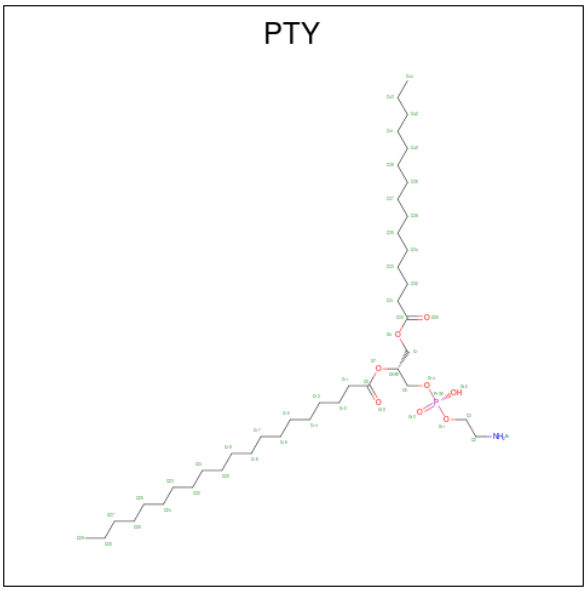
Mol	Chain	Residues	Atoms				AltConf
24	I	1	Total	C	O	P	0
			28	17	10	1	
24	2	1	Total	C	O	P	0
			25	16	8	1	

- Molecule 25 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$) (labeled as "Ligand of Interest" by depositor).



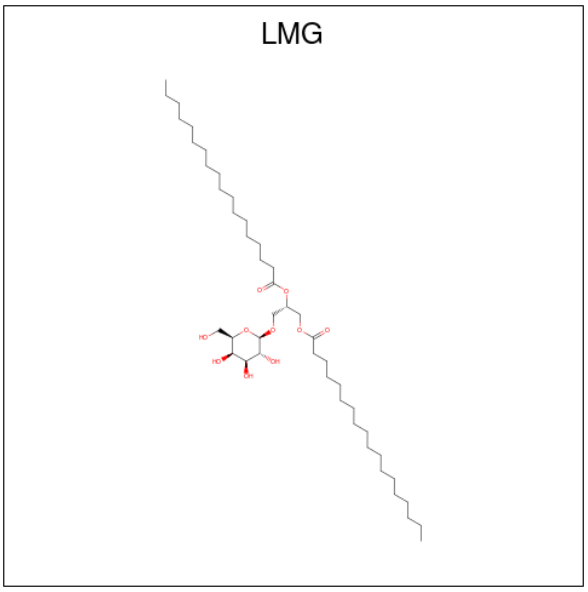
Mol	Chain	Residues	Atoms				AltConf
25	1	1	Total	C	O	S	0
			38	25	12	1	
25	3	1	Total	C	O	S	0
			35	22	12	1	
25	3	1	Total	C	O	S	0
			41	28	12	1	
25	7	1	Total	C	O	S	0
			39	26	12	1	
25	B	1	Total	C	O	S	0
			31	18	12	1	
25	F	1	Total	C	O	S	0
			39	26	12	1	

- Molecule 26 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: $C_{40}H_{80}NO_8P$) (labeled as "Ligand of Interest" by depositor).



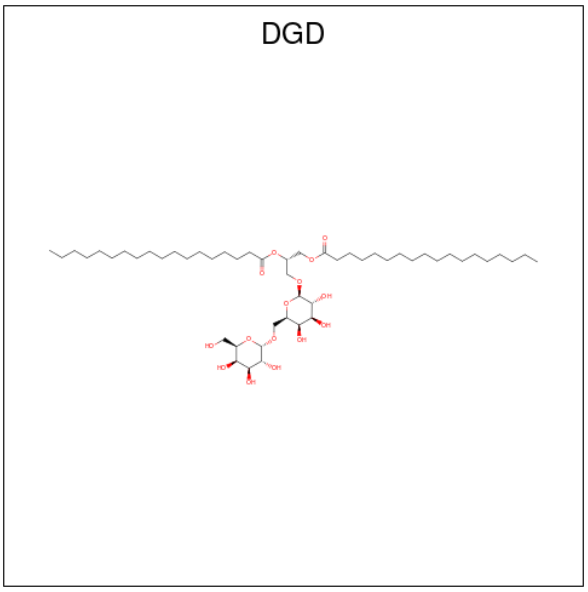
Mol	Chain	Residues	Atoms	AltConf
26	3	1	Total C N O P 50 40 1 8 1	0
26	7	1	Total C O P 15 6 8 1	0
26	B	1	Total C N O P 27 17 1 8 1	0
26	F	1	Total C N O P 29 19 1 8 1	0
26	F	1	Total C N O P 32 22 1 8 1	0
26	F	1	Total C N O P 31 21 1 8 1	0

- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



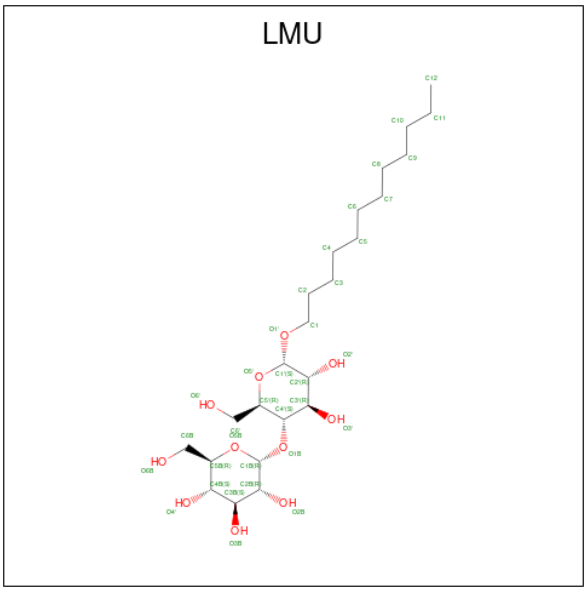
Mol	Chain	Residues	Atoms			AltConf
27	7	1	Total 50	C 40	O 10	0
27	7	1	Total 30	C 20	O 10	0
27	A	1	Total 32	C 22	O 10	0
27	G	1	Total 43	C 34	O 9	0
27	J	1	Total 29	C 19	O 10	0

- Molecule 28 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
28	7	1	Total 39	C 24	O 15	0
28	B	1	Total 61	C 46	O 15	0

- Molecule 29 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
29	7	1	Total 32	C 21	O 11	0

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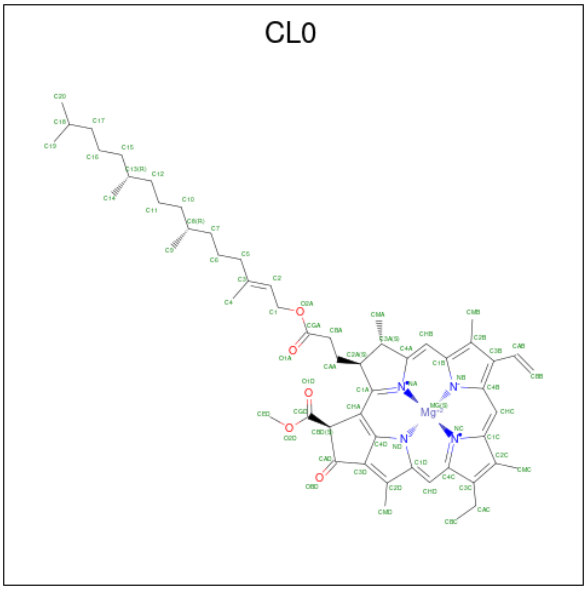
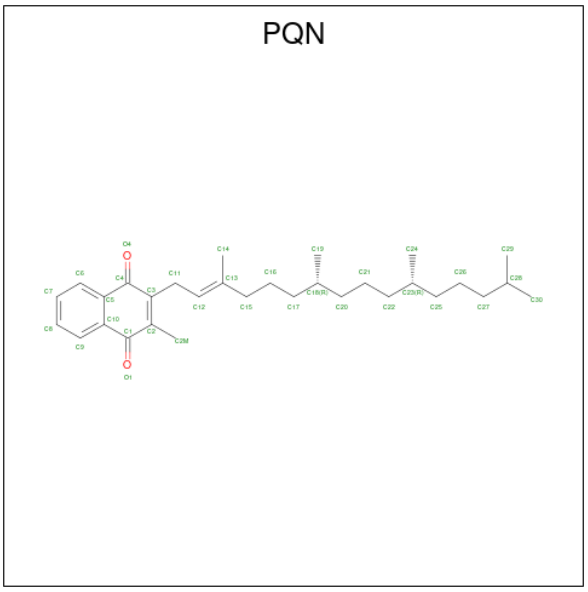
Mol	Chain	Residues	Atoms	AltConf
29	8	1	Total C O 33 22 11	0
29	8	1	Total C O 35 24 11	0
29	9	1	Total C O 29 18 11	0
29	A	1	Total C O 35 24 11	0
29	F	1	Total C O 32 21 11	0

- Molecule 30 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



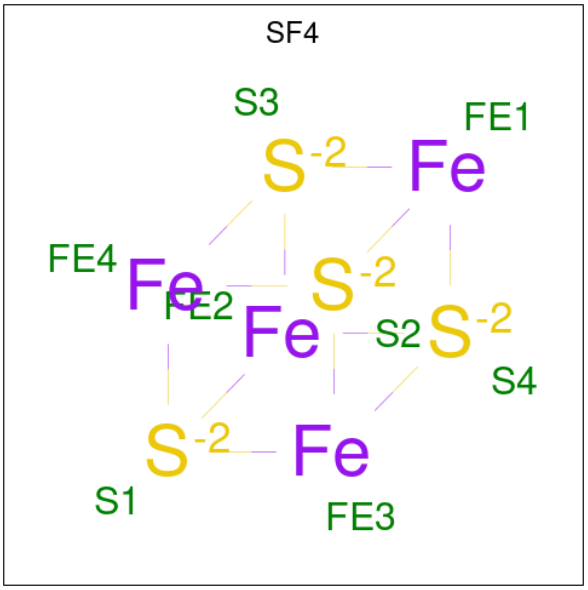
Mol	Chain	Residues	Atoms	AltConf
30	A	1	Total C Mg N O 65 55 1 4 5	0

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



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

- Molecule 32 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

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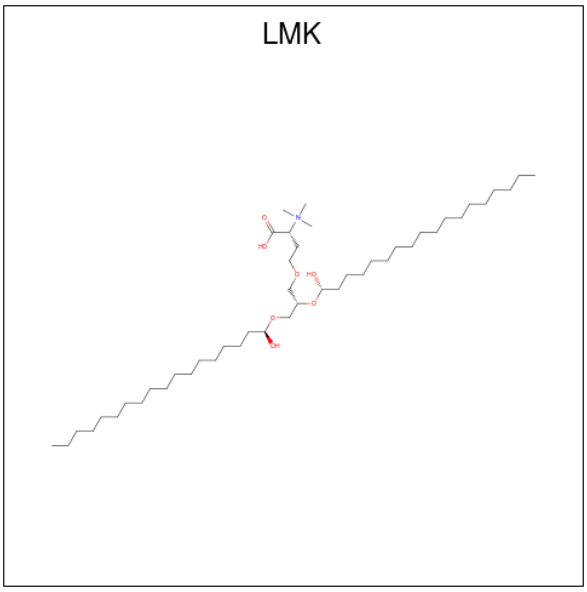
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
32	C	1	8	4	4	0

- Molecule 33 is trimethyl-[(2 {R})-1-oxidanyl-1-oxidanylidene-4-[(2 {S})-2-[(1 {S})-1-oxidanyloctadecoxy]-3-[(1 {R})-1-oxidanyloctadecoxy]propoxy]butan-2-yl]azanium (CCD ID: LMK) (formula: $C_{46}H_{94}NO_7$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
33	J	1	35	27	1	7	0

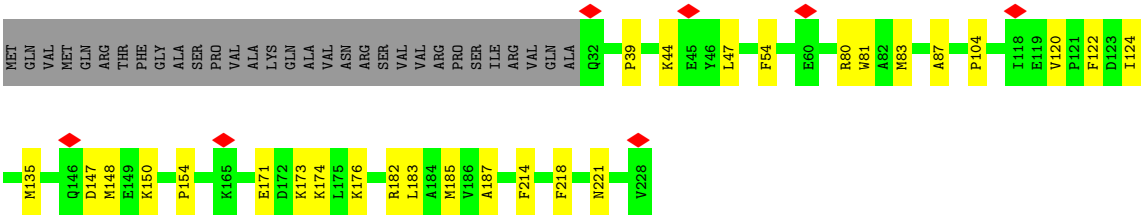
3 Residue-property plots (i)

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: Chlorophyll a-b binding protein, chloroplastic

Chain 1:

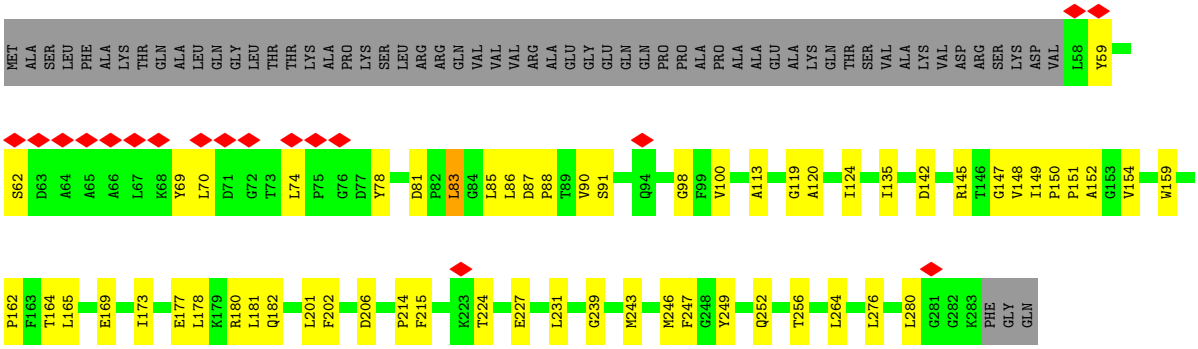




• Molecule 2: LHCA3

Chain 3:

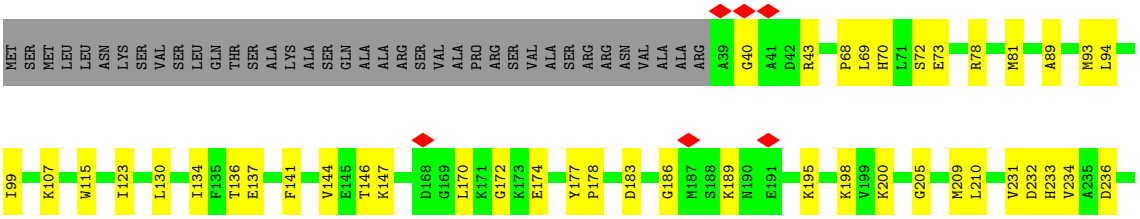


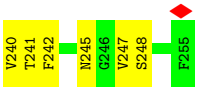


• Molecule 3: Chlorophyll a-b binding protein, chloroplastic

Chain 7:



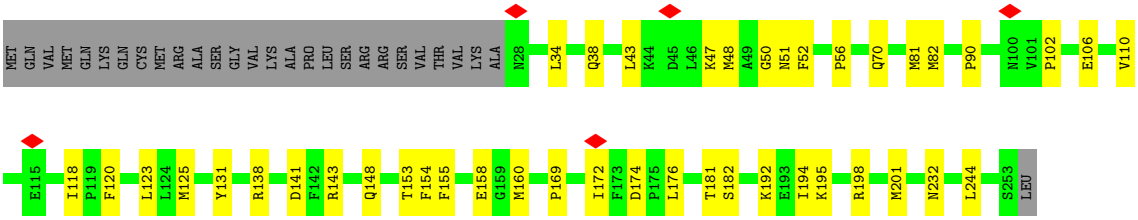




• Molecule 4: Chlorophyll a-b binding protein, chloroplastic

Chain 8:

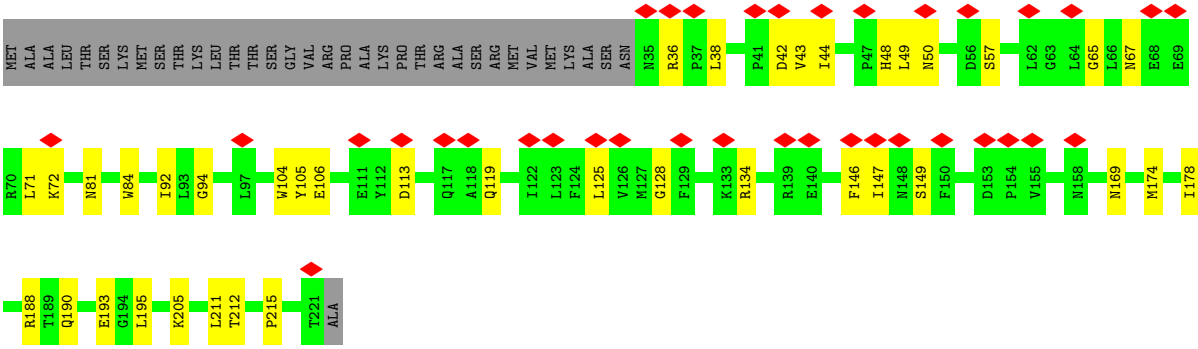




• Molecule 5: LHCA9

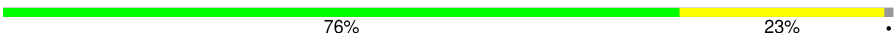
Chain 9:

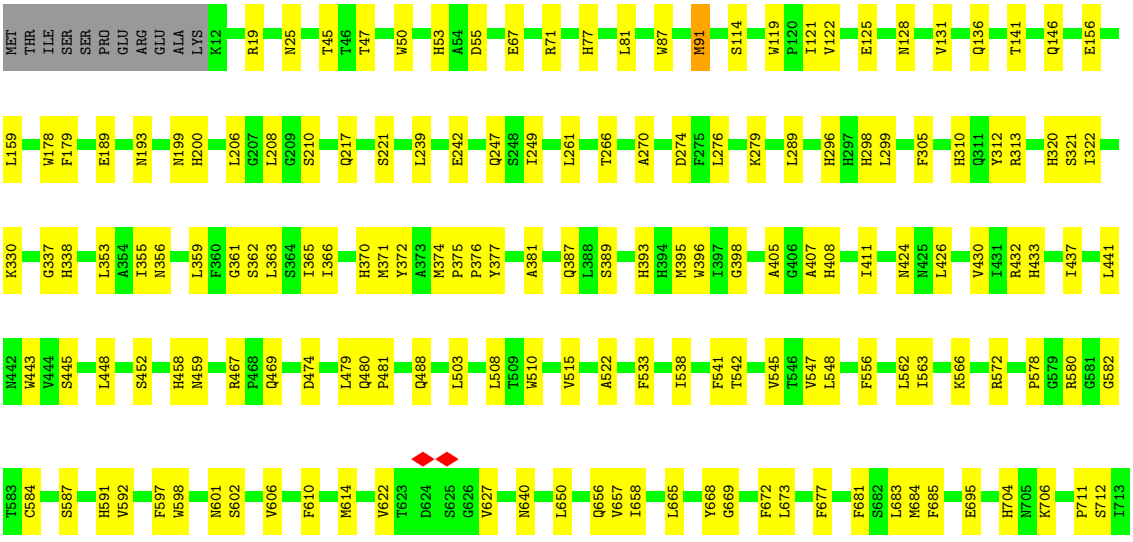




• Molecule 6: Photosystem I P700 chlorophyll a apoprotein A1

Chain A:



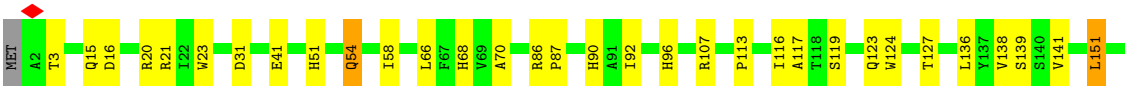




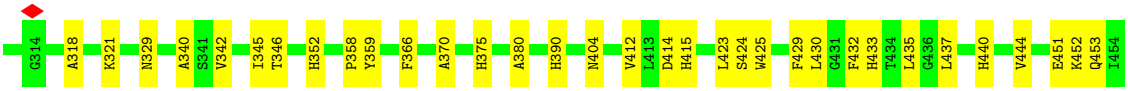
• Molecule 7: Photosystem I P700 chlorophyll a apoprotein A2

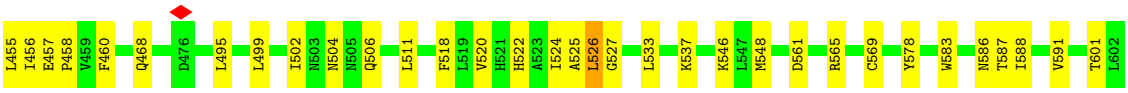
Chain B:









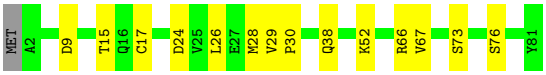




• Molecule 8: Photosystem I iron-sulfur center

Chain C:

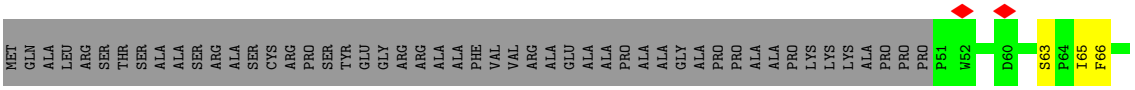


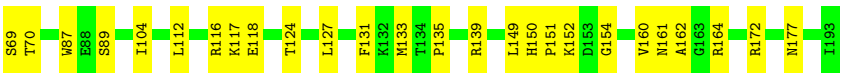


• Molecule 9: Photosystem I reaction center subunit II, chloroplastic

Chain D:



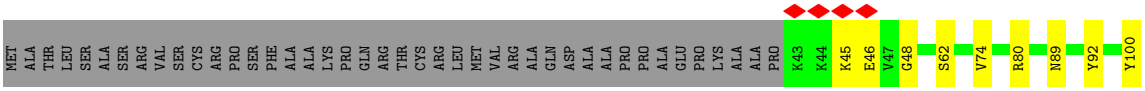


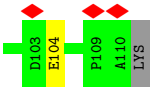


• Molecule 10: Photosystem I reaction center subunit IV

Chain E:



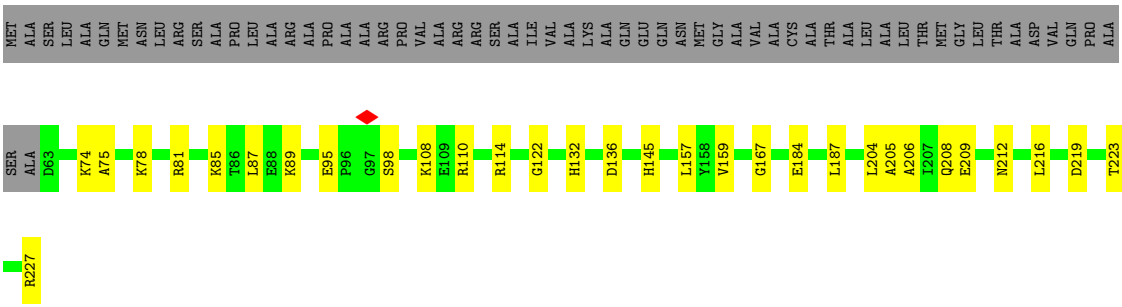




• Molecule 11: PSAF1

Chain F:

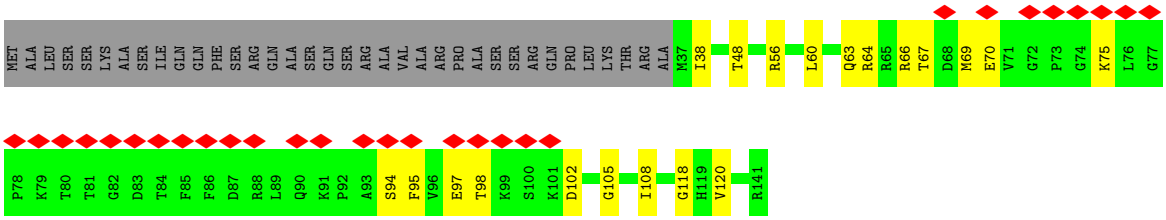




• Molecule 12: PSAG1

Chain G:

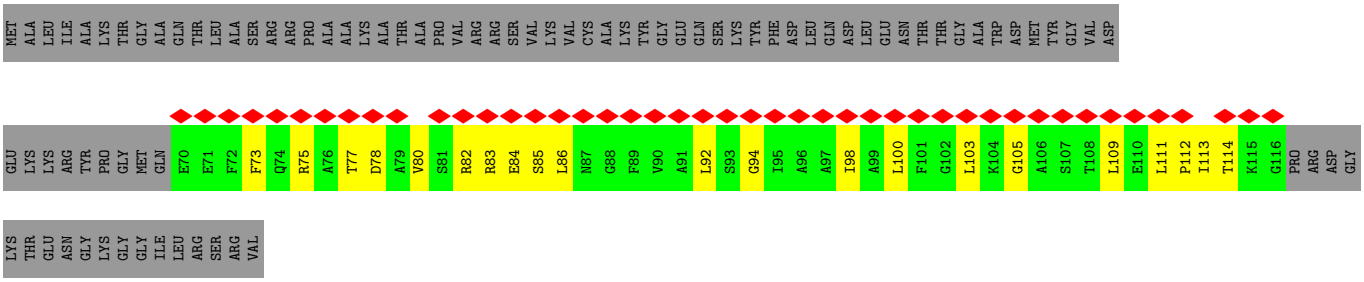




• Molecule 13: PSAH1

Chain H:

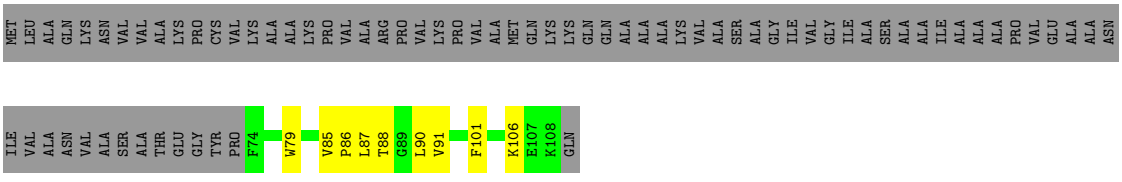




• Molecule 14: Photosystem I reaction center subunit VIII

Chain I:

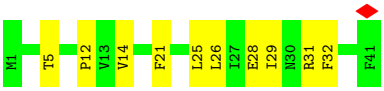




• Molecule 15: Photosystem I reaction center subunit IX

Chain J:

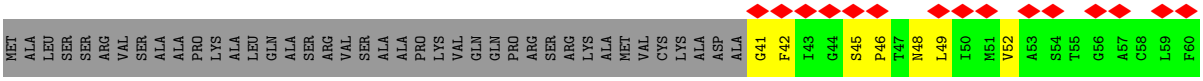




• Molecule 16: PSI-K

Chain K:



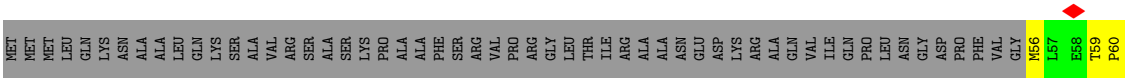


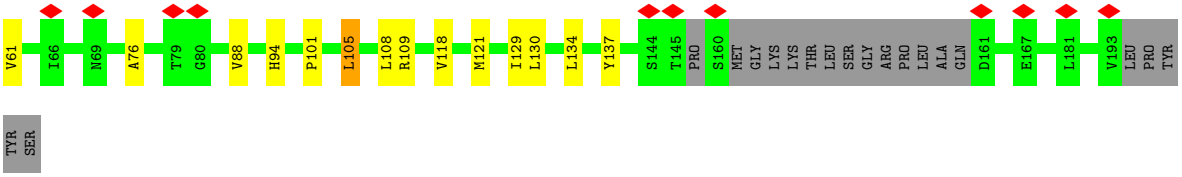


• Molecule 17: PSAL1

Chain L:



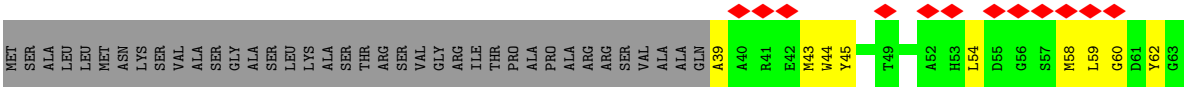


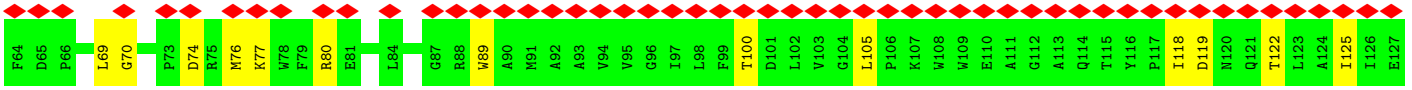


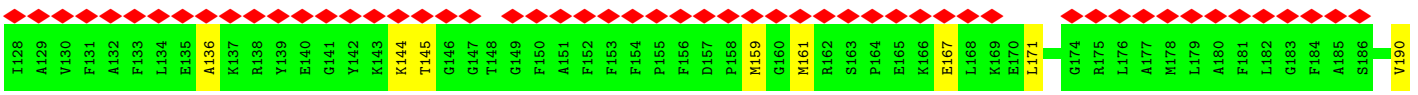
• Molecule 18: LHCA2

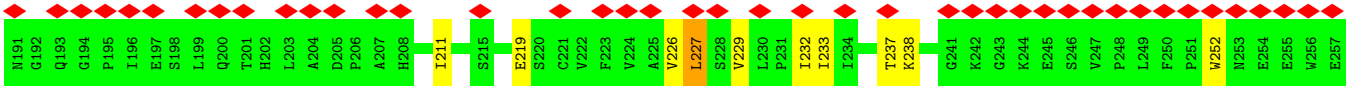
Chain 2:












K258
V259
A260
LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	126839	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.091	Depositor
Minimum map value	-0.019	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0172	Depositor
Map size (Å)	503.99997, 503.99997, 503.99997	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PTY, XAT, PQN, LMK, LMU, CHL, DGD, CL0, LMG, SF4, SQD, LHG, BCR, LUT, CLA

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	1	0.18	0/1544	0.38	0/2093
2	3	0.16	0/1768	0.40	0/2402
3	7	0.15	0/1722	0.39	0/2339
4	8	0.17	0/1770	0.37	0/2401
5	9	0.20	0/1496	0.46	0/2038
6	A	0.14	0/6004	0.33	0/8190
7	B	0.14	0/6026	0.35	1/8235 (0.0%)
8	C	0.12	0/610	0.33	0/828
9	D	0.14	0/1163	0.40	0/1571
10	E	0.10	0/552	0.28	0/750
11	F	0.17	0/1329	0.42	0/1797
12	G	0.17	0/814	0.41	0/1100
13	H	0.18	0/353	0.45	0/474
14	I	0.23	0/286	0.57	0/394
15	J	0.16	0/338	0.43	0/461
16	K	0.22	0/587	0.54	0/795
17	L	0.15	0/911	0.35	0/1244
18	2	0.16	0/1779	0.40	0/2417
All	All	0.16	0/29052	0.38	1/39529 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	54	GLN	CA-CB-CG	6.45	127.00	114.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1505	0	1468	25	0
2	3	1719	0	1676	60	0
3	7	1669	0	1612	42	0
4	8	1721	0	1661	35	0
5	9	1453	0	1437	34	0
6	A	5808	0	5638	135	0
7	B	5814	0	5556	141	0
8	C	600	0	582	10	0
9	D	1133	0	1138	23	0
10	E	540	0	539	7	0
11	F	1300	0	1322	25	0
12	G	794	0	796	20	0
13	H	349	0	357	18	0
14	I	274	0	282	8	0
15	J	327	0	328	9	0
16	K	579	0	608	19	0
17	L	891	0	908	22	0
18	2	1728	0	1697	59	0
19	1	94	0	62	7	0
19	2	108	0	88	10	0
19	3	123	0	115	22	0
19	7	141	0	95	12	0
19	8	145	0	95	18	0
19	9	47	0	30	2	0
20	1	604	0	486	28	0
20	2	517	0	381	20	0
20	3	769	0	649	36	0
20	7	595	0	533	22	0
20	8	606	0	552	29	0
20	9	563	0	462	29	0
20	A	2475	0	2517	137	0
20	B	2260	0	2330	140	0
20	F	217	0	197	11	0
20	G	203	0	170	17	0
20	H	60	0	57	2	0
20	J	49	0	39	2	0
20	K	193	0	151	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	L	245	0	249	11	0
21	1	42	0	56	7	0
21	2	84	0	112	2	0
21	3	42	0	56	2	0
21	7	42	0	56	2	0
21	8	42	0	56	4	0
21	9	42	0	56	2	0
22	1	44	0	56	0	0
22	3	44	0	56	7	0
22	7	44	0	56	4	0
22	8	44	0	54	1	0
22	9	88	0	112	2	0
23	1	40	0	56	5	0
23	3	120	0	168	18	0
23	7	40	0	56	3	0
23	8	40	0	56	10	0
23	A	200	0	280	22	0
23	B	279	0	388	23	0
23	F	80	0	112	10	0
23	G	40	0	56	1	0
23	I	40	0	53	1	0
23	J	120	0	168	15	0
23	K	80	0	112	6	0
23	L	80	0	110	5	0
24	1	72	0	87	6	0
24	2	25	0	23	1	0
24	7	56	0	52	6	0
24	8	110	0	132	3	0
24	9	36	0	45	0	0
24	A	147	0	181	8	0
24	B	62	0	63	1	0
24	I	28	0	26	2	0
25	1	38	0	40	2	0
25	3	76	0	78	3	0
25	7	39	0	42	1	0
25	B	31	0	25	0	0
25	F	39	0	42	3	0
26	3	50	0	79	1	0
26	7	15	0	5	1	0
26	B	27	0	27	0	0
26	F	92	0	99	3	0
27	7	80	0	102	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	A	32	0	34	2	0
27	G	43	0	55	6	0
27	J	29	0	28	0	0
28	7	39	0	36	0	0
28	B	61	0	83	9	0
29	7	32	0	37	0	0
29	8	68	0	85	5	0
29	9	29	0	30	0	0
29	A	35	0	45	2	0
29	F	32	0	37	0	0
30	A	65	0	72	10	0
31	A	33	0	46	3	0
31	B	33	0	46	8	0
32	A	8	0	0	1	0
32	C	16	0	0	1	0
33	J	35	0	0	0	0
All	All	41548	0	40986	992	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

The worst 5 of 992 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)
20:9:607:CLA:CMB	18:2:232:ILE:HD13	1.11	1.58
20:9:607:CLA:HMB1	18:2:232:ILE:CD1	0.97	1.43
20:9:607:CLA:HMB1	18:2:232:ILE:CG1	1.58	1.31
18:2:161:MET:HG2	20:2:308:CLA:O1A	1.31	1.31
20:9:607:CLA:CMB	18:2:232:ILE:CD1	1.84	1.19

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	1	195/228 (86%)	185 (95%)	10 (5%)	0	100 100
2	3	224/286 (78%)	212 (95%)	12 (5%)	0	100 100
3	7	215/255 (84%)	206 (96%)	9 (4%)	0	100 100
4	8	224/254 (88%)	221 (99%)	3 (1%)	0	100 100
5	9	185/222 (83%)	173 (94%)	12 (6%)	0	100 100
6	A	738/751 (98%)	711 (96%)	27 (4%)	0	100 100
7	B	732/735 (100%)	710 (97%)	22 (3%)	0	100 100
8	C	78/81 (96%)	75 (96%)	3 (4%)	0	100 100
9	D	141/193 (73%)	129 (92%)	12 (8%)	0	100 100
10	E	66/111 (60%)	64 (97%)	2 (3%)	0	100 100
11	F	163/227 (72%)	155 (95%)	8 (5%)	0	100 100
12	G	103/141 (73%)	97 (94%)	5 (5%)	1 (1%)	12 9
13	H	45/134 (34%)	42 (93%)	3 (7%)	0	100 100
14	I	33/109 (30%)	33 (100%)	0	0	100 100
15	J	39/41 (95%)	36 (92%)	3 (8%)	0	100 100
16	K	81/123 (66%)	65 (80%)	14 (17%)	2 (2%)	4 1
17	L	120/198 (61%)	117 (98%)	3 (2%)	0	100 100
18	2	220/261 (84%)	211 (96%)	8 (4%)	1 (0%)	24 22
All	All	3602/4350 (83%)	3442 (96%)	156 (4%)	4 (0%)	49 50

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	K	74	ALA
16	K	66	LEU
18	2	118	ILE
12	G	38	ILE

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	1	153/179 (86%)	153 (100%)	0	100 100
2	3	170/217 (78%)	169 (99%)	1 (1%)	78 86
3	7	171/201 (85%)	171 (100%)	0	100 100
4	8	173/197 (88%)	171 (99%)	2 (1%)	63 72
5	9	152/180 (84%)	149 (98%)	3 (2%)	48 56
6	A	599/609 (98%)	594 (99%)	5 (1%)	73 81
7	B	595/596 (100%)	586 (98%)	9 (2%)	57 65
8	C	68/69 (99%)	66 (97%)	2 (3%)	37 42
9	D	123/156 (79%)	122 (99%)	1 (1%)	73 81
10	E	60/93 (64%)	60 (100%)	0	100 100
11	F	136/177 (77%)	136 (100%)	0	100 100
12	G	82/111 (74%)	81 (99%)	1 (1%)	63 72
13	H	35/103 (34%)	35 (100%)	0	100 100
14	I	28/77 (36%)	28 (100%)	0	100 100
15	J	36/36 (100%)	35 (97%)	1 (3%)	38 43
16	K	58/88 (66%)	58 (100%)	0	100 100
17	L	91/150 (61%)	90 (99%)	1 (1%)	65 74
18	2	176/205 (86%)	175 (99%)	1 (1%)	78 86
All	All	2906/3444 (84%)	2879 (99%)	27 (1%)	68 78

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	B	283	VAL
7	B	569	CYS
15	J	5	THR
7	B	526	LEU
7	B	578	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
6	A	421	ASN

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Mol	Chain	Res	Type
6	A	659	GLN
14	I	105	GLN
6	A	637	GLN
7	B	11	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)

270 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
19	CHL	3	323	-	65,69,74	1.19	3 (4%)	73,108,114	2.14	11 (15%)
23	BCR	B	843	-	41,41,41	0.22	0	56,56,56	0.40	0
20	CLA	9	612	5	50,54,73	1.34	7 (14%)	59,90,113	1.22	4 (6%)
24	LHG	B	849	-	29,29,48	0.40	0	32,35,54	0.42	0
20	CLA	A	5010	-	55,59,73	1.30	7 (12%)	64,96,113	1.33	6 (9%)
20	CLA	A	5023	6	54,58,73	1.30	7 (12%)	64,95,113	1.43	7 (10%)
20	CLA	L	205	17	54,58,73	1.28	7 (12%)	64,95,113	1.26	6 (9%)
21	LUT	1	615	-	42,43,43	0.19	0	51,60,60	1.43	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	XAT	3	316	-	41,47,47	0.14	0	54,74,74	0.81	2 (3%)
20	CLA	B	806	7	52,56,73	1.31	6 (11%)	61,92,113	1.29	8 (13%)
21	LUT	3	315	-	42,43,43	0.31	0	51,60,60	0.38	0
20	CLA	A	5018	6	64,68,73	1.18	8 (12%)	76,107,113	1.20	4 (5%)
19	CHL	9	606	5	51,55,74	1.39	4 (7%)	56,91,114	2.03	11 (19%)
20	CLA	B	804	7	69,73,73	1.18	9 (13%)	82,113,113	1.03	4 (4%)
23	BCR	3	319	-	41,41,41	1.38	8 (19%)	56,56,56	1.53	12 (21%)
23	BCR	8	316	-	41,41,41	0.16	0	56,56,56	0.40	0
23	BCR	B	846	-	41,41,41	0.13	0	56,56,56	0.37	0
20	CLA	A	5034	6	69,73,73	1.15	7 (10%)	82,113,113	1.21	6 (7%)
20	CLA	A	5015	6	59,63,73	1.24	7 (11%)	70,101,113	1.33	6 (8%)
27	LMG	J	103	-	29,29,55	0.20	0	37,37,63	0.14	0
20	CLA	B	817	-	64,68,73	1.23	9 (14%)	76,107,113	1.26	4 (5%)
19	CHL	1	601	-	51,55,74	1.39	3 (5%)	56,91,114	1.65	12 (21%)
20	CLA	8	302	20,4	69,73,73	1.18	8 (11%)	82,113,113	1.25	5 (6%)
20	CLA	8	311	4	69,73,73	1.19	8 (11%)	82,113,113	1.14	5 (6%)
20	CLA	A	5019	6	59,63,73	1.29	9 (15%)	70,101,113	1.26	5 (7%)
20	CLA	B	816	-	59,63,73	1.25	7 (11%)	70,101,113	1.27	7 (10%)
20	CLA	2	303	18	54,58,73	1.35	9 (16%)	64,95,113	1.34	8 (12%)
20	CLA	2	304	-	54,58,73	1.27	7 (12%)	64,95,113	1.19	6 (9%)
25	SQD	B	850	7	29,31,54	0.21	0	39,42,65	0.25	0
20	CLA	A	5044	-	69,73,73	1.16	7 (10%)	82,113,113	1.21	8 (9%)
20	CLA	3	309	2	50,54,73	1.32	7 (14%)	59,90,113	1.23	4 (6%)
29	LMU	F	305	-	33,33,36	0.16	0	44,44,47	0.48	0
32	SF4	C	102	8	0,12,12	-	-	-		
20	CLA	8	321	20,11,4	50,54,73	1.37	7 (14%)	59,90,113	1.40	6 (10%)
26	PTY	F	310	11,26	30,30,49	0.56	0	33,35,54	0.55	0
20	CLA	8	312	4	50,54,73	1.34	7 (14%)	59,90,113	1.34	4 (6%)
20	CLA	7	303	3	64,68,73	1.20	8 (12%)	76,107,113	1.10	5 (6%)
20	CLA	7	304	3	59,63,73	1.28	8 (13%)	70,101,113	1.23	5 (7%)
20	CLA	9	601	5	50,54,73	1.32	6 (12%)	59,90,113	1.20	5 (8%)
20	CLA	9	611	-	59,63,73	1.26	8 (13%)	70,101,113	1.33	5 (7%)
20	CLA	L	202	17	69,73,73	1.16	7 (10%)	82,113,113	1.13	5 (6%)
23	BCR	J	102	-	41,41,41	0.24	0	56,56,56	0.93	4 (7%)
20	CLA	B	840	-	69,73,73	1.15	7 (10%)	82,113,113	1.10	5 (6%)
20	CLA	B	828	-	69,73,73	1.20	9 (13%)	82,113,113	1.18	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	CLA	A	5028	6	69,73,73	1.18	9 (13%)	82,113,113	1.27	5 (6%)
20	CLA	B	824	-	69,73,73	1.16	8 (11%)	82,113,113	1.29	7 (8%)
20	CLA	B	810	7	69,73,73	1.13	9 (13%)	82,113,113	1.14	6 (7%)
23	BCR	F	309	-	41,41,41	0.17	0	56,56,56	0.40	0
20	CLA	3	308	2	59,63,73	1.24	7 (11%)	70,101,113	1.12	5 (7%)
19	CHL	8	306	4	55,59,74	1.52	3 (5%)	61,96,114	2.02	11 (18%)
24	LHG	1	618	20,1	25,25,48	0.41	0	28,31,54	0.40	0
27	LMG	7	324	3	30,30,55	0.24	0	38,38,63	0.24	0
28	DGD	7	321	-	40,40,67	0.24	0	54,54,81	0.34	0
20	CLA	2	301	18	50,54,73	1.31	7 (14%)	59,90,113	1.22	4 (6%)
20	CLA	B	815	20	69,73,73	1.12	8 (11%)	82,113,113	1.13	5 (6%)
20	CLA	K	4002	-	49,53,73	1.40	6 (12%)	58,89,113	1.35	4 (6%)
20	CLA	3	310	2	50,54,73	1.36	9 (18%)	59,90,113	1.43	4 (6%)
20	CLA	A	5039	6	59,63,73	1.24	8 (13%)	70,101,113	1.22	6 (8%)
20	CLA	A	5017	-	59,63,73	1.26	7 (11%)	70,101,113	1.33	5 (7%)
20	CLA	B	809	7	69,73,73	1.13	7 (10%)	82,113,113	1.17	5 (6%)
20	CLA	1	611	1	50,54,73	1.37	8 (16%)	59,90,113	1.41	7 (11%)
20	CLA	B	839	7	69,73,73	1.15	6 (8%)	82,113,113	1.10	6 (7%)
20	CLA	A	5027	-	60,64,73	1.34	10 (16%)	71,102,113	1.23	6 (8%)
20	CLA	3	314	25,2	50,54,73	1.35	7 (14%)	59,90,113	1.29	4 (6%)
20	CLA	A	5031	6	69,73,73	1.14	6 (8%)	82,113,113	1.20	5 (6%)
20	CLA	L	204	17	69,73,73	1.13	7 (10%)	82,113,113	1.07	5 (6%)
20	CLA	A	5007	20,6	69,73,73	1.13	7 (10%)	82,113,113	1.08	5 (6%)
22	XAT	8	315	4	41,47,47	0.16	0	54,74,74	0.83	1 (1%)
19	CHL	2	306	-	51,55,74	1.03	4 (7%)	56,91,114	2.07	15 (26%)
23	BCR	B	847	-	41,41,41	0.17	0	56,56,56	0.56	2 (3%)
27	LMG	G	206	-	43,43,55	0.19	0	51,51,63	0.18	0
27	LMG	A	5001	-	32,32,55	0.20	0	40,40,63	0.31	0
25	SQD	3	320	-	33,35,54	0.27	0	43,46,65	0.39	0
20	CLA	A	5037	6	54,58,73	1.29	7 (12%)	64,95,113	1.26	7 (10%)
20	CLA	8	309	24	64,68,73	1.23	9 (14%)	76,107,113	1.21	5 (6%)
20	CLA	2	307	18	50,54,73	1.35	7 (14%)	59,90,113	1.21	4 (6%)
20	CLA	2	313	-	54,58,73	1.28	7 (12%)	64,95,113	1.32	6 (9%)
25	SQD	7	322	-	37,39,54	0.23	0	47,50,65	0.24	0
20	CLA	A	5012	6	69,73,73	1.15	7 (10%)	82,113,113	1.04	5 (6%)
24	LHG	2	316	-	24,24,48	0.55	0	27,29,54	0.84	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	CLA	1	607	-	54,58,73	1.30	7 (12%)	64,95,113	1.24	6 (9%)
20	CLA	2	312	18	46,52,73	1.37	6 (13%)	53,87,113	1.33	4 (7%)
20	CLA	B	818	7	69,73,73	1.13	8 (11%)	82,113,113	1.14	4 (4%)
20	CLA	7	315	3	49,53,73	1.37	7 (14%)	58,89,113	1.35	4 (6%)
20	CLA	A	5004	-	69,73,73	1.17	8 (11%)	82,113,113	1.11	7 (8%)
20	CLA	7	313	3	69,73,73	1.23	8 (11%)	82,113,113	1.21	5 (6%)
20	CLA	B	805	7	69,73,73	1.08	9 (13%)	82,113,113	1.24	9 (10%)
29	LMU	7	325	-	33,33,36	0.13	0	44,44,47	0.15	0
23	BCR	A	5049	-	41,41,41	0.27	0	56,56,56	1.03	5 (8%)
20	CLA	A	5026	-	69,73,73	1.18	8 (11%)	82,113,113	1.32	4 (4%)
32	SF4	A	5046	6,7	0,12,12	-	-	-		
20	CLA	A	5020	6	69,73,73	1.14	7 (10%)	82,113,113	1.18	7 (8%)
20	CLA	A	5033	6	59,63,73	1.25	7 (11%)	70,101,113	1.22	5 (7%)
24	LHG	I	4002	-	27,27,48	0.38	0	30,33,54	0.36	0
20	CLA	A	5021	6	54,58,73	1.30	8 (14%)	64,95,113	1.25	6 (9%)
20	CLA	2	309	-	49,53,73	1.37	7 (14%)	58,89,113	1.29	4 (6%)
20	CLA	1	603	1	59,63,73	1.27	8 (13%)	70,101,113	1.25	5 (7%)
20	CLA	7	312	3	56,60,73	1.29	9 (16%)	65,97,113	1.38	6 (9%)
26	PTY	7	302	-	14,14,49	1.11	2 (14%)	15,18,54	1.70	2 (13%)
20	CLA	9	609	5,24	50,54,73	1.32	7 (14%)	59,90,113	1.25	4 (6%)
23	BCR	G	205	-	41,41,41	0.21	0	56,56,56	0.49	0
20	CLA	9	605	5	49,53,73	1.39	7 (14%)	58,89,113	1.46	4 (6%)
31	PQN	A	5045	-	34,34,34	0.27	0	43,45,45	0.56	1 (2%)
29	LMU	9	616	5	30,30,36	0.19	0	41,41,47	0.86	2 (4%)
20	CLA	3	304	-	50,54,73	1.33	8 (16%)	59,90,113	1.24	4 (6%)
20	CLA	A	5040	-	64,68,73	1.20	7 (10%)	76,107,113	1.14	4 (5%)
23	BCR	1	617	-	41,41,41	0.18	0	56,56,56	0.26	0
20	CLA	7	309	3	50,54,73	1.32	7 (14%)	59,90,113	1.30	4 (6%)
20	CLA	A	5025	24,6	64,68,73	1.21	8 (12%)	76,107,113	1.20	4 (5%)
23	BCR	B	844	-	41,41,41	0.34	0	56,56,56	1.11	6 (10%)
20	CLA	1	608	1	50,54,73	1.32	7 (14%)	59,90,113	1.31	5 (8%)
26	PTY	F	302	-	31,31,49	0.56	0	34,36,54	0.46	0
20	CLA	9	604	5	54,58,73	1.30	7 (12%)	64,95,113	1.19	5 (7%)
20	CLA	1	612	24	64,68,73	1.23	7 (10%)	76,107,113	1.21	4 (5%)
20	CLA	B	833	7	64,68,73	1.20	7 (10%)	76,107,113	1.28	4 (5%)
20	CLA	2	305	-	49,53,73	1.37	7 (14%)	58,89,113	1.28	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	CLA	A	5016	6	69,73,73	1.14	7 (10%)	82,113,113	1.17	6 (7%)
21	LUT	7	316	-	42,43,43	0.35	0	51,60,60	0.53	1 (1%)
23	BCR	A	5050	-	41,41,41	0.13	0	56,56,56	0.39	0
20	CLA	G	204	20,19	49,53,73	1.50	9 (18%)	58,89,113	1.40	5 (8%)
20	CLA	1	604	-	54,58,73	1.26	7 (12%)	64,95,113	1.28	7 (10%)
20	CLA	A	5006	6	69,73,73	1.14	8 (11%)	82,113,113	1.22	6 (7%)
25	SQD	3	322	20,3,2	39,41,54	0.22	0	49,52,65	0.26	0
23	BCR	J	105	-	41,41,41	0.15	0	56,56,56	0.27	0
20	CLA	A	5008	6	69,73,73	1.12	7 (10%)	82,113,113	1.12	6 (7%)
20	CLA	9	610	5	54,58,73	1.36	8 (14%)	64,95,113	1.39	7 (10%)
20	CLA	3	307	2	69,73,73	1.15	7 (10%)	82,113,113	1.14	6 (7%)
22	XAT	9	615	-	41,47,47	0.18	0	54,74,74	0.79	3 (5%)
20	CLA	A	5014	-	69,73,73	1.14	8 (11%)	82,113,113	1.26	6 (7%)
29	LMU	8	322	-	36,36,36	0.12	0	47,47,47	0.20	0
20	CLA	F	303	11,7	69,73,73	1.22	8 (11%)	82,113,113	1.53	13 (15%)
20	CLA	A	5042	6	64,68,73	1.22	9 (14%)	76,107,113	1.22	6 (7%)
29	LMU	A	5053	33	36,36,36	0.13	0	47,47,47	0.15	0
33	LMK	J	101	29	34,34,53	0.42	0	34,41,60	0.52	1 (2%)
19	CHL	7	307	-	51,55,74	1.10	3 (5%)	56,91,114	2.39	12 (21%)
20	CLA	9	607	5	64,68,73	1.19	7 (10%)	76,107,113	1.10	4 (5%)
19	CHL	8	305	4	51,55,74	1.34	3 (5%)	56,91,114	2.36	9 (16%)
20	CLA	K	4004	16	49,53,73	1.42	9 (18%)	58,89,113	1.38	4 (6%)
20	CLA	1	609	1	59,63,73	1.25	8 (13%)	70,101,113	1.19	4 (5%)
20	CLA	B	822	7	69,73,73	1.13	7 (10%)	82,113,113	1.20	5 (6%)
23	BCR	L	203	23	41,41,41	0.14	0	56,56,56	0.25	0
24	LHG	8	317	20	28,28,48	0.38	0	31,34,54	0.34	0
21	LUT	8	314	-	42,43,43	0.27	0	51,60,60	0.42	0
20	CLA	3	324	6,2	59,63,73	1.23	7 (11%)	70,101,113	1.24	5 (7%)
20	CLA	B	821	-	59,63,73	1.26	7 (11%)	70,101,113	1.26	5 (7%)
20	CLA	A	5041	6	69,73,73	1.14	8 (11%)	82,113,113	1.18	6 (7%)
25	SQD	1	619	-	36,38,54	0.27	0	46,49,65	0.52	1 (2%)
20	CLA	B	820	-	69,73,73	1.18	9 (13%)	82,113,113	1.31	5 (6%)
24	LHG	9	617	20	35,35,48	0.35	0	38,41,54	0.36	0
20	CLA	F	308	11	49,53,73	1.37	7 (14%)	58,89,113	1.33	4 (6%)
23	BCR	J	106	-	41,41,41	0.17	0	56,56,56	0.36	0
23	BCR	K	4001	-	41,41,41	0.18	0	56,56,56	0.35	0
20	CLA	B	829	7	69,73,73	1.16	6 (8%)	82,113,113	1.16	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	CLA	9	602	5	64,68,73	1.18	6 (9%)	76,107,113	1.11	7 (9%)
20	CLA	A	5036	6	68,72,73	1.17	8 (11%)	80,111,113	1.22	4 (5%)
20	CLA	3	302	2	69,73,73	1.16	8 (11%)	82,113,113	1.20	5 (6%)
20	CLA	8	310	4	50,54,73	1.38	9 (18%)	59,90,113	1.43	5 (8%)
20	CLA	B	813	7	50,54,73	1.35	8 (16%)	59,90,113	1.27	4 (6%)
20	CLA	B	811	7	69,73,73	1.15	8 (11%)	82,113,113	1.21	5 (6%)
20	CLA	3	305	2	54,58,73	1.28	7 (12%)	64,95,113	1.29	7 (10%)
19	CHL	8	304	20,4	51,55,74	2.04	3 (5%)	56,91,114	2.59	14 (25%)
20	CLA	8	307	4	51,55,73	1.63	11 (21%)	60,91,113	1.82	11 (18%)
24	LHG	A	5002	-	35,35,48	0.36	0	38,41,54	0.40	0
22	XAT	7	317	-	41,47,47	0.17	0	54,74,74	0.86	3 (5%)
21	LUT	2	315	-	42,43,43	0.20	0	51,60,60	0.74	2 (3%)
20	CLA	3	312	2	50,54,73	1.33	7 (14%)	59,90,113	1.21	4 (6%)
20	CLA	8	313	4	50,54,73	1.36	8 (16%)	59,90,113	1.24	4 (6%)
23	BCR	B	803	-	41,41,41	0.26	0	56,56,56	0.63	1 (1%)
20	CLA	7	323	3,4	51,55,73	1.35	8 (15%)	60,91,113	1.30	6 (10%)
20	CLA	A	5013	20,6	69,73,73	1.16	7 (10%)	82,113,113	1.13	5 (6%)
20	CLA	B	825	-	69,73,73	1.18	9 (13%)	82,113,113	1.09	5 (6%)
20	CLA	B	823	7	59,63,73	1.23	8 (13%)	70,101,113	1.13	6 (8%)
20	CLA	B	826	7	69,73,73	1.19	9 (13%)	82,113,113	1.24	6 (7%)
20	CLA	2	310	18	50,54,73	1.37	7 (14%)	59,90,113	1.43	6 (10%)
20	CLA	8	308	4	64,68,73	1.18	7 (10%)	76,107,113	1.08	4 (5%)
21	LUT	2	314	-	42,43,43	0.29	0	51,60,60	1.04	3 (5%)
24	LHG	8	320	4	42,42,48	0.31	0	45,48,54	0.30	0
20	CLA	8	301	4	64,68,73	1.18	7 (10%)	76,107,113	1.16	6 (7%)
20	CLA	A	5022	-	69,73,73	1.14	8 (11%)	82,113,113	1.17	4 (4%)
23	BCR	B	842	-	41,41,41	0.19	0	56,56,56	0.33	0
20	CLA	K	4005	-	52,56,73	1.40	8 (15%)	61,92,113	1.40	5 (8%)
20	CLA	A	5038	6	54,58,73	1.33	8 (14%)	64,95,113	1.36	6 (9%)
28	DGD	B	848	-	62,62,67	0.18	0	76,76,81	0.19	0
20	CLA	7	310	3	69,73,73	1.14	7 (10%)	82,113,113	1.09	5 (6%)
27	LMG	7	301	-	50,50,55	0.18	0	58,58,63	0.15	0
20	CLA	7	311	24	64,68,73	1.23	9 (14%)	76,107,113	1.22	6 (7%)
21	LUT	9	613	-	42,43,43	0.26	0	51,60,60	0.30	0
23	BCR	7	318	-	41,41,41	0.14	0	56,56,56	0.38	0
20	CLA	1	605	-	49,53,73	1.37	8 (16%)	58,89,113	1.41	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	CLA	B	827	7	69,73,73	1.12	6 (8%)	82,113,113	1.15	5 (6%)
26	PTY	3	321	-	49,49,49	0.44	0	52,54,54	0.78	2 (3%)
20	CLA	1	602	1	59,63,73	1.26	7 (11%)	70,101,113	1.28	6 (8%)
20	CLA	7	305	-	54,58,73	1.33	8 (14%)	64,95,113	1.34	6 (9%)
20	CLA	A	5030	-	69,73,73	1.17	8 (11%)	82,113,113	1.26	6 (7%)
20	CLA	A	5043	24	53,57,73	1.29	7 (13%)	62,93,113	1.27	5 (8%)
20	CLA	B	831	7	64,68,73	1.20	8 (12%)	76,107,113	1.21	5 (6%)
20	CLA	F	307	-	51,55,73	1.32	7 (13%)	60,91,113	1.25	5 (8%)
29	LMU	8	318	-	34,34,36	0.13	0	45,45,47	0.14	0
20	CLA	9	603	-	59,63,73	1.28	8 (13%)	70,101,113	1.37	5 (7%)
20	CLA	F	306	-	64,68,73	1.18	7 (10%)	76,107,113	1.12	5 (6%)
24	LHG	8	319	-	37,37,48	0.33	0	40,43,54	0.31	0
20	CLA	1	613	1	54,58,73	1.33	8 (14%)	64,95,113	1.38	5 (7%)
20	CLA	H	201	13,18	64,68,73	1.37	8 (12%)	76,107,113	1.22	7 (9%)
20	CLA	2	311	18	54,58,73	1.31	6 (11%)	64,95,113	1.35	6 (9%)
23	BCR	L	206	-	41,41,41	0.17	0	56,56,56	0.48	0
23	BCR	I	4001	23	41,41,41	0.17	0	56,56,56	0.29	0
20	CLA	B	838	-	59,63,73	1.32	9 (15%)	70,101,113	1.28	5 (7%)
20	CLA	3	313	-	46,50,73	1.39	8 (17%)	53,85,113	1.24	4 (7%)
23	BCR	A	5047	-	41,41,41	0.29	0	56,56,56	0.54	0
20	CLA	B	837	7	59,63,73	1.21	7 (11%)	70,101,113	1.28	6 (8%)
20	CLA	8	303	19	69,73,73	1.18	9 (13%)	82,113,113	1.06	4 (4%)
20	CLA	B	807	-	69,73,73	1.12	7 (10%)	82,113,113	1.17	8 (9%)
25	SQD	F	311	-	37,39,54	0.26	0	47,50,65	0.49	1 (2%)
20	CLA	3	311	-	59,63,73	1.24	7 (11%)	70,101,113	1.26	5 (7%)
20	CLA	1	610	24	50,54,73	1.33	6 (12%)	59,90,113	1.23	4 (6%)
24	LHG	A	5054	20	27,27,48	0.42	0	30,33,54	0.49	0
20	CLA	G	203	12	50,54,73	1.36	7 (14%)	59,90,113	1.30	4 (6%)
20	CLA	L	201	17,7	69,73,73	1.14	7 (10%)	82,113,113	1.22	6 (7%)
23	BCR	A	5051	-	41,41,41	0.14	0	56,56,56	0.25	0
20	CLA	B	808	7	69,73,73	1.97	9 (13%)	82,113,113	1.11	8 (9%)
20	CLA	3	325	6,2	59,63,73	1.26	7 (11%)	70,101,113	1.25	4 (5%)
23	BCR	A	5048	-	41,41,41	0.17	0	56,56,56	0.24	0
24	LHG	7	320	20,3	33,33,48	0.34	0	36,39,54	0.33	0
24	LHG	B	801	7	31,31,48	0.36	0	34,37,54	0.33	0
20	CLA	A	5011	6	69,73,73	1.14	7 (10%)	82,113,113	1.12	4 (4%)
23	BCR	3	317	-	41,41,41	0.16	0	56,56,56	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	CHL	2	302	18	65,69,74	1.07	3 (4%)	73,108,114	1.87	11 (15%)
20	CLA	B	819	7	69,73,73	1.14	6 (8%)	82,113,113	1.19	5 (6%)
19	CHL	7	306	-	50,54,74	1.26	4 (8%)	55,90,114	2.10	9 (16%)
31	PQN	B	841	-	34,34,34	0.29	0	43,45,45	0.55	1 (2%)
20	CLA	B	812	20,7	59,63,73	1.25	7 (11%)	70,101,113	1.22	4 (5%)
20	CLA	3	306	-	55,59,73	1.28	7 (12%)	64,96,113	1.26	6 (9%)
20	CLA	B	830	7	69,73,73	1.17	7 (10%)	82,113,113	1.19	6 (7%)
23	BCR	B	845	-	40,40,41	0.17	0	54,54,56	0.48	1 (1%)
20	CLA	B	834	20	54,58,73	1.30	7 (12%)	64,95,113	1.32	7 (10%)
20	CLA	A	5009	6	69,73,73	1.17	8 (11%)	82,113,113	1.28	6 (7%)
20	CLA	2	308	18	49,53,73	1.36	7 (14%)	58,89,113	1.23	6 (10%)
22	XAT	9	614	-	41,47,47	0.14	0	54,74,74	0.75	3 (5%)
20	CLA	A	5035	6	69,73,73	1.15	7 (10%)	82,113,113	1.16	4 (4%)
23	BCR	K	4006	-	41,41,41	0.17	0	56,56,56	0.32	0
30	CL0	A	5003	6	69,73,73	1.06	4 (5%)	82,113,113	1.82	9 (10%)
20	CLA	B	836	7	64,68,73	1.17	7 (10%)	76,107,113	1.14	6 (7%)
20	CLA	3	303	-	50,54,73	1.35	7 (14%)	59,90,113	1.34	4 (6%)
24	LHG	7	319	-	21,21,48	0.41	0	24,27,54	0.45	0
24	LHG	1	620	-	45,45,48	0.31	0	48,51,54	0.34	0
26	PTY	B	802	-	26,26,49	0.61	0	29,31,54	0.50	0
20	CLA	B	832	7	69,73,73	1.15	8 (11%)	82,113,113	1.13	5 (6%)
20	CLA	A	5024	6	64,68,73	1.19	7 (10%)	76,107,113	1.10	5 (6%)
20	CLA	A	5029	6	69,73,73	1.12	8 (11%)	82,113,113	1.14	6 (7%)
20	CLA	A	5032	6	54,58,73	1.40	9 (16%)	64,95,113	1.30	6 (9%)
19	CHL	7	308	3	52,56,74	1.37	3 (5%)	57,92,114	1.91	11 (19%)
23	BCR	3	318	-	41,41,41	0.14	0	56,56,56	0.34	0
23	BCR	F	304	-	41,41,41	0.17	0	56,56,56	0.30	0
20	CLA	B	814	7	69,73,73	1.18	8 (11%)	82,113,113	1.20	5 (6%)
19	CHL	3	301	2	66,70,74	1.13	3 (4%)	74,109,114	1.92	12 (16%)
20	CLA	G	202	12	51,55,73	1.34	8 (15%)	60,91,113	1.39	5 (8%)
20	CLA	7	314	3	54,58,73	1.31	7 (12%)	64,95,113	1.29	6 (9%)
20	CLA	G	201	7,12	69,73,73	1.17	7 (10%)	82,113,113	1.08	4 (4%)
20	CLA	J	104	15	53,57,73	1.29	7 (13%)	61,93,113	1.31	4 (6%)
24	LHG	A	5052	-	48,48,48	0.29	0	51,54,54	0.28	0
19	CHL	1	606	20	51,55,74	1.47	3 (5%)	56,91,114	1.96	11 (19%)
24	LHG	A	5055	-	33,33,48	0.45	0	36,38,54	0.65	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	PTY	F	301	26	28,28,49	0.59	0	31,33,54	0.50	0
20	CLA	B	835	7	55,59,73	1.30	7 (12%)	64,96,113	1.44	4 (6%)
22	XAT	1	616	-	41,47,47	0.14	0	54,74,74	0.84	2 (3%)
32	SF4	C	101	8	0,12,12	-	-	-		
20	CLA	1	614	1	50,54,73	1.35	6 (12%)	59,90,113	1.34	4 (6%)
20	CLA	A	5005	-	69,73,73	1.18	8 (11%)	82,113,113	1.11	4 (4%)
20	CLA	K	4003	-	59,63,73	1.26	6 (10%)	70,101,113	1.19	5 (7%)
20	CLA	9	608	5	54,58,73	1.29	8 (14%)	64,95,113	1.20	5 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CHL	3	323	-	1/1/14/21	16/35/111/117	-
23	BCR	B	843	-	-	0/29/63/63	0/2/2/2
20	CLA	9	612	5	-	8/17/93/115	-
24	LHG	B	849	-	-	8/34/34/53	-
20	CLA	A	5010	-	-	4/23/99/115	-
20	CLA	A	5023	6	-	7/21/97/115	-
21	LUT	1	615	-	3/3/12/27	8/29/67/67	0/2/2/2
20	CLA	L	205	17	-	8/21/97/115	-
22	XAT	3	316	-	-	3/31/93/93	0/4/4/4
21	LUT	3	315	-	3/3/12/27	2/29/67/67	0/2/2/2
20	CLA	B	806	7	-	9/19/95/115	-
20	CLA	A	5018	6	-	11/33/109/115	-
19	CHL	9	606	5	-	11/19/95/117	-
20	CLA	B	804	7	-	19/39/115/115	-
23	BCR	3	319	-	-	23/29/63/63	0/2/2/2
23	BCR	8	316	-	-	2/29/63/63	0/2/2/2
23	BCR	B	846	-	-	0/29/63/63	0/2/2/2
20	CLA	A	5034	6	-	4/39/115/115	-
20	CLA	A	5015	6	-	10/27/103/115	-
27	LMG	J	103	-	-	3/24/44/70	0/1/1/1
20	CLA	B	817	-	-	9/33/109/115	-
19	CHL	1	601	-	-	6/19/95/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	8	302	20,4	-	13/39/115/115	-
20	CLA	8	311	4	-	19/39/115/115	-
20	CLA	A	5019	6	-	11/27/103/115	-
20	CLA	B	816	-	-	10/27/103/115	-
20	CLA	2	303	18	-	6/21/97/115	-
20	CLA	2	304	-	-	10/21/97/115	-
25	SQD	B	850	7	-	10/25/45/69	0/1/1/1
20	CLA	A	5044	-	-	10/39/115/115	-
20	CLA	3	309	2	-	10/17/93/115	-
29	LMU	F	305	-	-	7/18/58/61	0/2/2/2
32	SF4	C	102	8	-	-	0/6/5/5
20	CLA	8	321	20,11,4	-	11/17/93/115	-
26	PTY	F	310	11,26	-	13/34/34/53	-
20	CLA	8	312	4	-	9/17/93/115	-
20	CLA	7	303	3	-	13/33/109/115	-
20	CLA	7	304	3	-	4/27/103/115	-
20	CLA	9	601	5	-	11/17/93/115	-
20	CLA	9	611	-	-	7/27/103/115	-
20	CLA	L	202	17	-	16/39/115/115	-
23	BCR	J	102	-	-	8/29/63/63	0/2/2/2
20	CLA	B	840	-	-	11/39/115/115	-
20	CLA	B	828	-	-	18/39/115/115	-
20	CLA	A	5028	6	-	17/39/115/115	-
20	CLA	B	824	-	-	12/39/115/115	-
20	CLA	B	810	7	-	13/39/115/115	-
23	BCR	F	309	-	-	4/29/63/63	0/2/2/2
20	CLA	3	308	2	-	10/27/103/115	-
19	CHL	8	306	4	-	8/23/99/117	-
24	LHG	1	618	20,1	-	5/30/30/53	-
27	LMG	7	324	3	-	10/25/45/70	0/1/1/1
28	DGD	7	321	-	-	8/28/68/95	0/2/2/2
20	CLA	2	301	18	-	6/17/93/115	-
20	CLA	B	815	20	-	10/39/115/115	-
20	CLA	K	4002	-	-	8/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	3	310	2	-	7/17/93/115	-
20	CLA	A	5039	6	-	5/27/103/115	-
20	CLA	A	5017	-	-	13/27/103/115	-
20	CLA	B	809	7	-	16/39/115/115	-
20	CLA	1	611	1	-	8/17/93/115	-
20	CLA	B	839	7	-	10/39/115/115	-
20	CLA	A	5027	-	-	10/29/105/115	-
20	CLA	3	314	25,2	-	7/17/93/115	-
20	CLA	A	5031	6	-	9/39/115/115	-
20	CLA	L	204	17	-	12/39/115/115	-
20	CLA	A	5007	20,6	-	10/39/115/115	-
22	XAT	8	315	4	-	1/31/93/93	0/4/4/4
19	CHL	2	306	-	1/1/11/21	7/19/95/117	-
23	BCR	B	847	-	-	5/29/63/63	0/2/2/2
27	LMG	G	206	-	-	6/37/57/70	0/1/1/1
27	LMG	A	5001	-	-	6/26/46/70	0/1/1/1
25	SQD	3	320	-	-	4/30/50/69	0/1/1/1
20	CLA	A	5037	6	-	9/21/97/115	-
20	CLA	8	309	24	-	12/33/109/115	-
20	CLA	2	307	18	-	11/17/93/115	-
20	CLA	2	313	-	-	7/21/97/115	-
25	SQD	7	322	-	-	4/34/54/69	0/1/1/1
20	CLA	A	5012	6	-	12/39/115/115	-
24	LHG	2	316	-	-	4/26/26/53	-
20	CLA	1	607	-	-	9/21/97/115	-
20	CLA	2	312	18	-	7/15/91/115	-
20	CLA	B	818	7	-	17/39/115/115	-
20	CLA	7	315	3	-	6/15/91/115	-
20	CLA	A	5004	-	-	15/39/115/115	-
20	CLA	7	313	3	-	13/39/115/115	-
20	CLA	B	805	7	-	14/39/115/115	-
29	LMU	7	325	-	-	4/18/58/61	0/2/2/2
23	BCR	A	5049	-	-	4/29/63/63	0/2/2/2
20	CLA	A	5026	-	-	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	SF4	A	5046	6,7	-	-	0/6/5/5
20	CLA	A	5020	6	-	15/39/115/115	-
20	CLA	A	5033	6	-	3/27/103/115	-
24	LHG	I	4002	-	-	6/32/32/53	-
20	CLA	A	5021	6	-	8/21/97/115	-
20	CLA	2	309	-	-	4/15/91/115	-
20	CLA	1	603	1	-	13/27/103/115	-
20	CLA	7	312	3	-	7/24/100/115	-
26	PTY	7	302	-	-	8/14/14/53	-
20	CLA	9	609	5,24	-	10/17/93/115	-
23	BCR	G	205	-	-	6/29/63/63	0/2/2/2
20	CLA	9	605	5	-	6/15/91/115	-
31	PQN	A	5045	-	-	2/23/43/43	0/2/2/2
29	LMU	9	616	5	-	5/15/55/61	0/2/2/2
20	CLA	3	304	-	-	6/17/93/115	-
20	CLA	A	5040	-	-	9/33/109/115	-
23	BCR	1	617	-	-	0/29/63/63	0/2/2/2
20	CLA	7	309	3	-	6/17/93/115	-
20	CLA	A	5025	24,6	-	13/33/109/115	-
23	BCR	B	844	-	-	10/29/63/63	0/2/2/2
20	CLA	1	608	1	-	8/17/93/115	-
26	PTY	F	302	-	-	16/35/35/53	-
20	CLA	9	604	5	-	6/21/97/115	-
20	CLA	1	612	24	-	13/33/109/115	-
20	CLA	B	833	7	-	12/33/109/115	-
20	CLA	2	305	-	-	8/15/91/115	-
20	CLA	A	5016	6	-	15/39/115/115	-
21	LUT	7	316	-	3/3/12/27	2/29/67/67	0/2/2/2
23	BCR	A	5050	-	-	3/29/63/63	0/2/2/2
20	CLA	G	204	20,19	-	7/15/91/115	-
20	CLA	1	604	-	-	7/21/97/115	-
20	CLA	A	5006	6	-	16/39/115/115	-
25	SQD	3	322	20,3,2	-	14/36/56/69	0/1/1/1
23	BCR	J	105	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	A	5008	6	-	11/39/115/115	-
20	CLA	9	610	5	-	12/21/97/115	-
20	CLA	3	307	2	-	15/39/115/115	-
22	XAT	9	615	-	-	5/31/93/93	0/4/4/4
20	CLA	A	5014	-	-	13/39/115/115	-
29	LMU	8	322	-	-	6/21/61/61	0/2/2/2
20	CLA	F	303	11,7	-	12/39/115/115	-
20	CLA	A	5042	6	-	8/33/109/115	-
29	LMU	A	5053	33	-	3/21/61/61	0/2/2/2
33	LMK	J	101	29	-	5/41/41/60	-
19	CHL	7	307	-	-	7/19/95/117	-
20	CLA	9	607	5	-	15/33/109/115	-
19	CHL	8	305	4	-	4/19/95/117	-
20	CLA	K	4004	16	-	8/15/91/115	-
20	CLA	1	609	1	-	8/27/103/115	-
20	CLA	B	822	7	-	15/39/115/115	-
23	BCR	L	203	23	-	4/29/63/63	0/2/2/2
24	LHG	8	317	20	-	5/33/33/53	-
21	LUT	8	314	-	3/3/12/27	2/29/67/67	0/2/2/2
20	CLA	3	324	6,2	-	12/27/103/115	-
20	CLA	B	821	-	-	10/27/103/115	-
20	CLA	A	5041	6	-	8/39/115/115	-
25	SQD	1	619	-	-	14/33/53/69	0/1/1/1
20	CLA	B	820	-	-	13/39/115/115	-
24	LHG	9	617	20	-	15/40/40/53	-
20	CLA	F	308	11	-	5/15/91/115	-
23	BCR	J	106	-	-	2/29/63/63	0/2/2/2
23	BCR	K	4001	-	-	4/29/63/63	0/2/2/2
20	CLA	B	829	7	-	16/39/115/115	-
20	CLA	9	602	5	-	11/33/109/115	-
20	CLA	A	5036	6	-	8/39/115/115	-
20	CLA	3	302	2	-	12/39/115/115	-
20	CLA	8	310	4	-	9/17/93/115	-
20	CLA	B	813	7	-	4/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	B	811	7	-	9/39/115/115	-
20	CLA	3	305	2	-	5/21/97/115	-
19	CHL	8	304	20,4	-	7/19/95/117	-
20	CLA	8	307	4	-	8/18/94/115	-
24	LHG	A	5002	-	-	10/40/40/53	-
22	XAT	7	317	-	-	3/31/93/93	0/4/4/4
21	LUT	2	315	-	3/3/12/27	12/29/67/67	0/2/2/2
20	CLA	3	312	2	-	9/17/93/115	-
20	CLA	8	313	4	-	7/17/93/115	-
23	BCR	B	803	-	-	3/29/63/63	0/2/2/2
20	CLA	7	323	3,4	-	10/18/94/115	-
20	CLA	A	5013	20,6	-	13/39/115/115	-
20	CLA	B	825	-	-	11/39/115/115	-
20	CLA	B	823	7	-	12/27/103/115	-
20	CLA	B	826	7	-	11/39/115/115	-
20	CLA	2	310	18	-	10/17/93/115	-
21	LUT	2	314	-	3/3/12/27	4/29/67/67	0/2/2/2
20	CLA	8	308	4	-	13/33/109/115	-
24	LHG	8	320	4	-	6/47/47/53	-
20	CLA	8	301	4	-	11/33/109/115	-
20	CLA	A	5022	-	-	8/39/115/115	-
23	BCR	B	842	-	-	2/29/63/63	0/2/2/2
20	CLA	K	4005	-	-	11/19/95/115	-
20	CLA	A	5038	6	-	5/21/97/115	-
28	DGD	B	848	-	-	12/50/90/95	0/2/2/2
20	CLA	7	310	3	-	16/39/115/115	-
27	LMG	7	301	-	-	10/45/65/70	0/1/1/1
20	CLA	7	311	24	-	10/33/109/115	-
21	LUT	9	613	-	3/3/12/27	2/29/67/67	0/2/2/2
23	BCR	7	318	-	-	2/29/63/63	0/2/2/2
20	CLA	1	605	-	-	6/15/91/115	-
20	CLA	B	827	7	-	10/39/115/115	-
26	PTY	3	321	-	-	24/53/53/53	-
20	CLA	1	602	1	-	13/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	7	305	-	-	6/21/97/115	-
20	CLA	A	5030	-	-	14/39/115/115	-
20	CLA	A	5043	24	-	7/19/95/115	-
20	CLA	B	831	7	-	10/33/109/115	-
20	CLA	F	307	-	-	7/18/94/115	-
29	LMU	8	318	-	-	2/19/59/61	0/2/2/2
20	CLA	9	603	-	-	12/27/103/115	-
20	CLA	F	306	-	-	12/33/109/115	-
24	LHG	8	319	-	-	8/42/42/53	-
20	CLA	1	613	1	-	8/21/97/115	-
20	CLA	H	201	13,18	-	19/33/109/115	-
20	CLA	2	311	18	-	10/21/97/115	-
23	BCR	L	206	-	-	6/29/63/63	0/2/2/2
23	BCR	I	4001	23	-	4/29/63/63	0/2/2/2
20	CLA	B	838	-	-	7/27/103/115	-
20	CLA	3	313	-	-	2/12/88/115	-
23	BCR	A	5047	-	-	5/29/63/63	0/2/2/2
20	CLA	B	837	7	-	3/27/103/115	-
20	CLA	8	303	19	-	15/39/115/115	-
20	CLA	B	807	-	-	12/39/115/115	-
25	SQD	F	311	-	-	6/34/54/69	0/1/1/1
20	CLA	3	311	-	-	10/27/103/115	-
20	CLA	1	610	24	-	9/17/93/115	-
24	LHG	A	5054	20	-	9/32/32/53	-
20	CLA	G	203	12	-	8/17/93/115	-
20	CLA	L	201	17,7	-	15/39/115/115	-
23	BCR	A	5051	-	-	4/29/63/63	0/2/2/2
20	CLA	B	808	7	-	13/39/115/115	-
20	CLA	3	325	6,2	-	6/27/103/115	-
23	BCR	A	5048	-	-	0/29/63/63	0/2/2/2
24	LHG	7	320	20,3	-	9/38/38/53	-
24	LHG	B	801	7	-	8/36/36/53	-
20	CLA	A	5011	6	-	13/39/115/115	-
23	BCR	3	317	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CHL	2	302	18	1/1/14/21	18/35/111/117	-
20	CLA	B	819	7	-	13/39/115/115	-
19	CHL	7	306	-	-	2/17/93/117	-
31	PQN	B	841	-	-	5/23/43/43	0/2/2/2
20	CLA	B	812	20,7	-	6/27/103/115	-
20	CLA	3	306	-	-	8/23/99/115	-
20	CLA	B	830	7	-	16/39/115/115	-
23	BCR	B	845	-	-	2/27/61/63	0/2/2/2
20	CLA	B	834	20	-	13/21/97/115	-
20	CLA	A	5009	6	-	16/39/115/115	-
20	CLA	2	308	18	-	5/15/91/115	-
22	XAT	9	614	-	-	0/31/93/93	0/4/4/4
20	CLA	A	5035	6	-	17/39/115/115	-
23	BCR	K	4006	-	-	4/29/63/63	0/2/2/2
30	CL0	A	5003	6	-	21/39/115/115	-
20	CLA	B	836	7	-	6/33/109/115	-
20	CLA	3	303	-	-	6/17/93/115	-
24	LHG	7	319	-	-	7/25/25/53	-
24	LHG	1	620	-	-	13/50/50/53	-
26	PTY	B	802	-	-	12/30/30/53	-
20	CLA	B	832	7	-	14/39/115/115	-
20	CLA	A	5024	6	-	16/33/109/115	-
20	CLA	A	5029	6	-	18/39/115/115	-
20	CLA	A	5032	6	-	4/21/97/115	-
19	CHL	7	308	3	-	6/20/96/117	-
23	BCR	3	318	-	-	3/29/63/63	0/2/2/2
23	BCR	F	304	-	-	0/29/63/63	0/2/2/2
20	CLA	B	814	7	-	17/39/115/115	-
19	CHL	3	301	2	1/1/14/21	22/37/113/117	-
20	CLA	G	202	12	-	7/18/94/115	-
20	CLA	7	314	3	-	7/21/97/115	-
20	CLA	G	201	7,12	-	15/39/115/115	-
20	CLA	J	104	15	-	6/20/96/115	-
24	LHG	A	5052	-	-	12/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CHL	1	606	20	-	12/19/95/117	-
24	LHG	A	5055	-	-	4/35/35/53	-
26	PTY	F	301	26	-	14/32/32/53	-
20	CLA	B	835	7	-	5/23/99/115	-
22	XAT	1	616	-	-	2/31/93/93	0/4/4/4
32	SF4	C	101	8	-	-	0/6/5/5
20	CLA	1	614	1	-	10/17/93/115	-
20	CLA	A	5005	-	-	6/39/115/115	-
20	CLA	K	4003	-	-	13/27/103/115	-
20	CLA	9	608	5	-	8/21/97/115	-

The worst 5 of 1313 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	808	CLA	MG-NA	11.87	2.34	2.06
19	8	304	CHL	MG-NC	11.84	2.34	2.06
19	1	606	CHL	MG-NA	8.23	2.25	2.06
19	8	306	CHL	MG-NA	7.43	2.23	2.06
19	8	304	CHL	MG-NA	7.10	2.23	2.06

The worst 5 of 1117 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	8	304	CHL	C4A-NA-C1A	15.46	113.73	106.68
19	7	307	CHL	C4A-NA-C1A	14.62	113.35	106.68
19	3	323	CHL	C4A-NA-C1A	14.54	113.31	106.68
19	8	305	CHL	C4A-NA-C1A	14.54	113.31	106.68
30	A	5003	CL0	C4A-NA-C1A	12.73	112.49	106.68

5 of 25 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	3	301	CHL	C8
19	3	323	CHL	C8
19	2	302	CHL	C8
19	2	306	CHL	C3A
21	1	615	LUT	C23

5 of 2371 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	1	601	CHL	C3A-C2A-CAA-CBA
19	1	601	CHL	CHA-CBD-CGD-O1D
19	1	601	CHL	CHA-CBD-CGD-O2D
19	1	601	CHL	CBD-CGD-O2D-CED
19	1	606	CHL	C1C-C2C-CMC-OMC

There are no ring outliers.

229 monomers are involved in 645 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	3	323	CHL	9	0
23	B	843	BCR	4	0
24	B	849	LHG	1	0
20	A	5010	CLA	4	0
20	A	5023	CLA	3	0
20	L	205	CLA	1	0
21	1	615	LUT	7	0
22	3	316	XAT	7	0
20	B	806	CLA	2	0
21	3	315	LUT	2	0
20	A	5018	CLA	5	0
19	9	606	CHL	2	0
20	B	804	CLA	5	0
23	3	319	BCR	10	0
23	8	316	BCR	10	0
23	B	846	BCR	3	0
20	A	5034	CLA	1	0
20	B	817	CLA	2	0
19	1	601	CHL	4	0
20	8	302	CLA	2	0
20	8	311	CLA	1	0
20	A	5019	CLA	2	0
20	B	816	CLA	3	0
20	2	303	CLA	3	0
20	A	5044	CLA	7	0
32	C	102	SF4	1	0
20	8	321	CLA	2	0
20	8	312	CLA	1	0
20	7	303	CLA	5	0
20	7	304	CLA	1	0
20	9	611	CLA	3	0
20	L	202	CLA	2	0
23	J	102	BCR	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	B	840	CLA	4	0
20	B	828	CLA	5	0
20	A	5028	CLA	4	0
20	B	824	CLA	5	0
20	B	810	CLA	6	0
23	F	309	BCR	6	0
20	3	308	CLA	1	0
19	8	306	CHL	5	0
24	1	618	LHG	3	0
27	7	324	LMG	2	0
20	2	301	CLA	1	0
20	B	815	CLA	3	0
20	K	4002	CLA	2	0
20	A	5017	CLA	2	0
20	B	809	CLA	4	0
20	1	611	CLA	3	0
20	B	839	CLA	9	0
20	A	5027	CLA	2	0
20	3	314	CLA	2	0
20	A	5031	CLA	3	0
20	L	204	CLA	4	0
20	A	5007	CLA	2	0
22	8	315	XAT	1	0
19	2	306	CHL	5	0
23	B	847	BCR	4	0
27	G	206	LMG	6	0
27	A	5001	LMG	2	0
25	3	320	SQD	1	0
20	8	309	CLA	4	0
20	2	307	CLA	1	0
20	2	313	CLA	1	0
25	7	322	SQD	1	0
20	A	5012	CLA	5	0
24	2	316	LHG	1	0
20	1	607	CLA	3	0
20	B	818	CLA	1	0
20	A	5004	CLA	7	0
20	7	313	CLA	5	0
20	B	805	CLA	12	0
23	A	5049	BCR	5	0
20	A	5026	CLA	4	0
32	A	5046	SF4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	5020	CLA	6	0
20	A	5033	CLA	5	0
24	I	4002	LHG	2	0
20	A	5021	CLA	3	0
20	1	603	CLA	1	0
20	7	312	CLA	1	0
26	7	302	PTY	1	0
23	G	205	BCR	1	0
31	A	5045	PQN	3	0
20	3	304	CLA	1	0
20	A	5040	CLA	5	0
23	1	617	BCR	5	0
20	A	5025	CLA	5	0
23	B	844	BCR	5	0
20	1	608	CLA	4	0
26	F	302	PTY	1	0
20	9	604	CLA	1	0
20	1	612	CLA	5	0
20	B	833	CLA	2	0
20	2	305	CLA	1	0
20	A	5016	CLA	7	0
21	7	316	LUT	2	0
23	A	5050	BCR	4	0
20	G	204	CLA	5	0
20	1	604	CLA	1	0
20	A	5006	CLA	3	0
25	3	322	SQD	2	0
23	J	105	BCR	3	0
20	A	5008	CLA	1	0
20	3	307	CLA	8	0
22	9	615	XAT	1	0
20	A	5014	CLA	4	0
29	8	322	LMU	4	0
20	F	303	CLA	3	0
20	A	5042	CLA	6	0
29	A	5053	LMU	2	0
19	7	307	CHL	7	0
20	9	607	CLA	19	0
19	8	305	CHL	7	0
20	K	4004	CLA	3	0
20	1	609	CLA	2	0
20	B	822	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	L	203	BCR	2	0
24	8	317	LHG	1	0
21	8	314	LUT	4	0
20	3	324	CLA	2	0
20	B	821	CLA	2	0
20	A	5041	CLA	7	0
25	1	619	SQD	2	0
20	B	820	CLA	4	0
23	J	106	BCR	3	0
23	K	4001	BCR	3	0
20	B	829	CLA	5	0
20	9	602	CLA	2	0
20	A	5036	CLA	3	0
20	3	302	CLA	6	0
20	8	310	CLA	2	0
20	B	811	CLA	4	0
20	3	305	CLA	4	0
19	8	304	CHL	9	0
20	8	307	CLA	3	0
24	A	5002	LHG	2	0
22	7	317	XAT	4	0
21	2	315	LUT	2	0
23	B	803	BCR	4	0
20	7	323	CLA	2	0
20	A	5013	CLA	3	0
20	B	825	CLA	5	0
20	B	823	CLA	3	0
20	B	826	CLA	8	0
20	8	308	CLA	3	0
20	8	301	CLA	6	0
20	A	5022	CLA	1	0
23	B	842	BCR	1	0
20	K	4005	CLA	4	0
28	B	848	DGD	9	0
20	7	310	CLA	3	0
27	7	301	LMG	5	0
20	7	311	CLA	1	0
21	9	613	LUT	2	0
23	7	318	BCR	3	0
20	1	605	CLA	7	0
20	B	827	CLA	6	0
26	3	321	PTY	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	1	602	CLA	1	0
20	7	305	CLA	2	0
20	A	5030	CLA	4	0
20	A	5043	CLA	3	0
20	B	831	CLA	6	0
20	F	307	CLA	6	0
29	8	318	LMU	1	0
20	9	603	CLA	4	0
20	F	306	CLA	2	0
24	8	319	LHG	2	0
20	H	201	CLA	2	0
20	2	311	CLA	8	0
23	L	206	BCR	3	0
23	I	4001	BCR	1	0
20	B	838	CLA	2	0
20	3	313	CLA	2	0
23	A	5047	BCR	5	0
20	B	837	CLA	1	0
20	8	303	CLA	6	0
20	B	807	CLA	8	0
25	F	311	SQD	3	0
20	3	311	CLA	4	0
20	1	610	CLA	3	0
24	A	5054	LHG	2	0
20	G	203	CLA	8	0
20	L	201	CLA	4	0
23	A	5051	BCR	4	0
20	B	808	CLA	5	0
20	3	325	CLA	2	0
23	A	5048	BCR	4	0
24	7	320	LHG	5	0
20	A	5011	CLA	6	0
23	3	317	BCR	1	0
19	2	302	CHL	5	0
20	B	819	CLA	6	0
19	7	306	CHL	5	0
31	B	841	PQN	8	0
20	B	812	CLA	3	0
20	3	306	CLA	5	0
20	B	830	CLA	2	0
23	B	845	BCR	2	0
20	B	834	CLA	2	0

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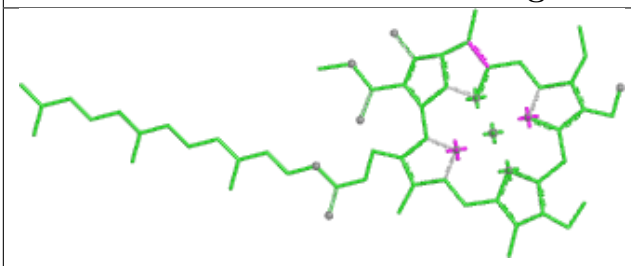
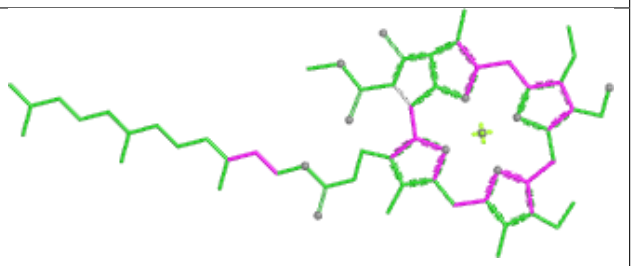
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	5009	CLA	1	0
20	2	308	CLA	5	0
22	9	614	XAT	1	0
20	A	5035	CLA	6	0
23	K	4006	BCR	3	0
30	A	5003	CL0	10	0
20	B	836	CLA	5	0
24	7	319	LHG	1	0
24	1	620	LHG	3	0
20	B	832	CLA	8	0
20	A	5029	CLA	8	0
20	A	5032	CLA	3	0
19	7	308	CHL	3	0
23	3	318	BCR	7	0
23	F	304	BCR	4	0
20	B	814	CLA	8	0
19	3	301	CHL	13	0
20	7	314	CLA	2	0
20	G	201	CLA	4	0
20	J	104	CLA	2	0
24	A	5052	LHG	2	0
19	1	606	CHL	3	0
24	A	5055	LHG	2	0
26	F	301	PTY	2	0
20	B	835	CLA	1	0
20	1	614	CLA	1	0
20	A	5005	CLA	13	0
20	9	608	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.

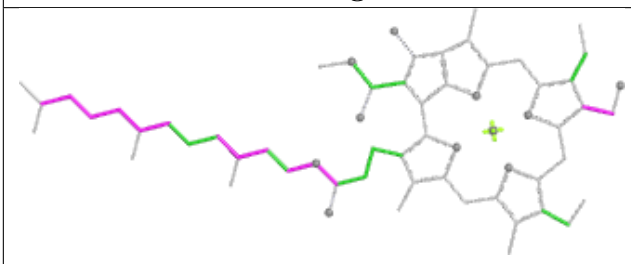
Ligand CHL 3 323



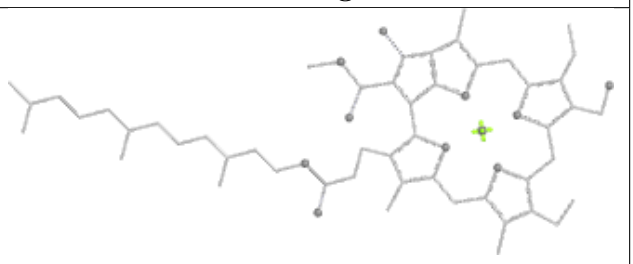
Bond lengths



Bond angles

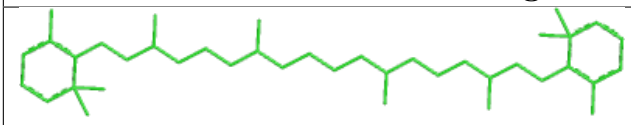


Torsions

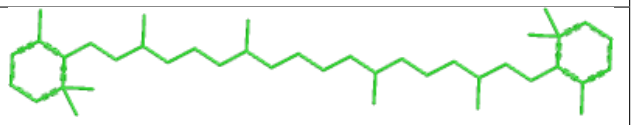


Rings

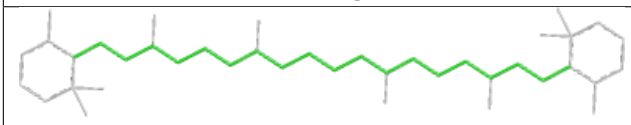
Ligand BCR B 843



Bond lengths



Bond angles



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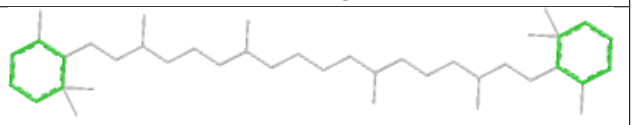
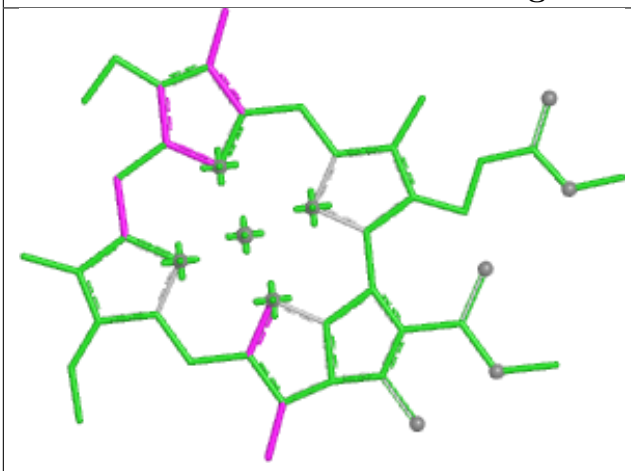
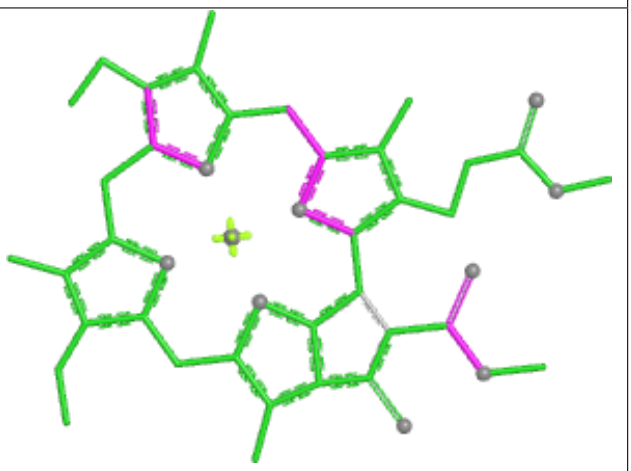


Rings

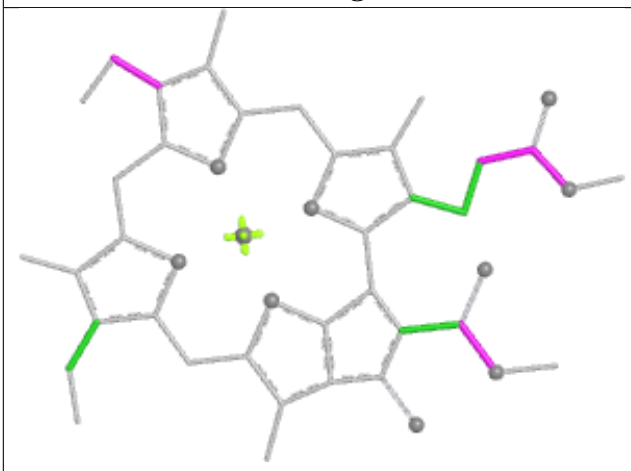
Ligand CLA 9 612



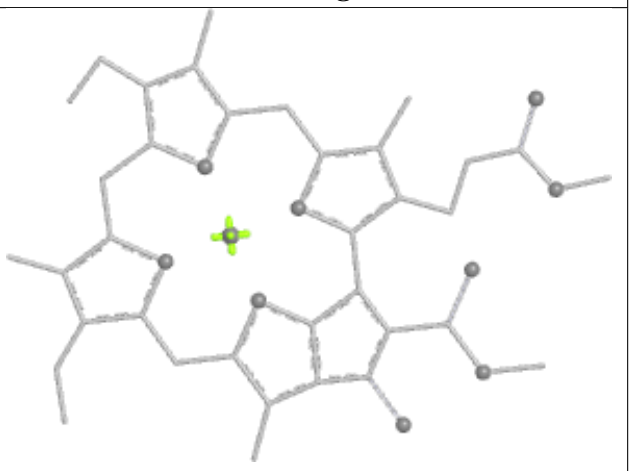
Bond lengths



Bond angles

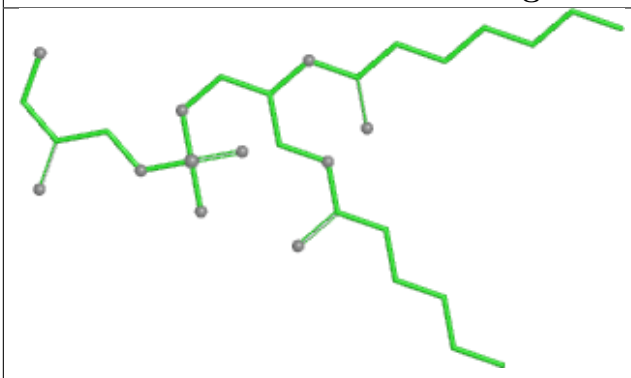


Torsions

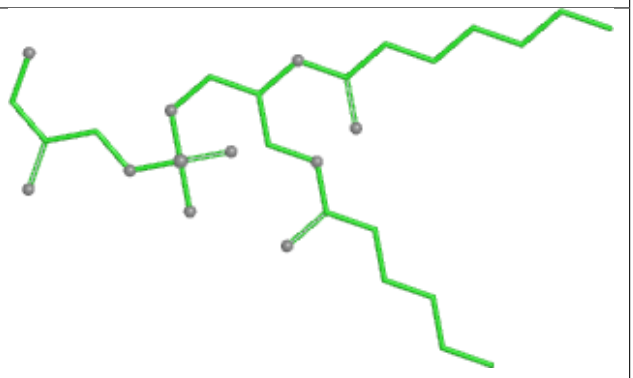


Rings

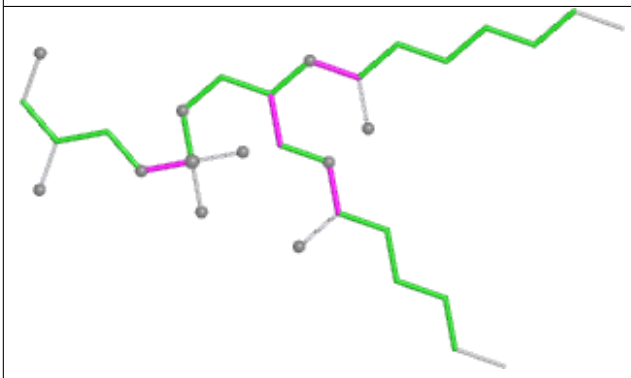
Ligand LHG B 849



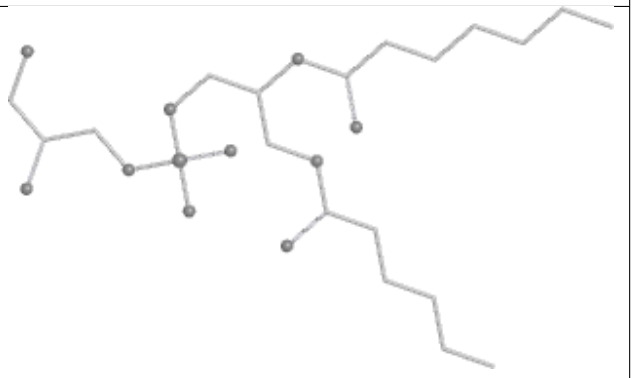
Bond lengths



Bond angles

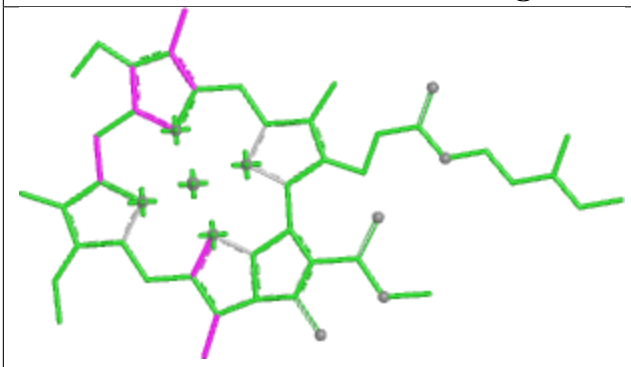


Torsions

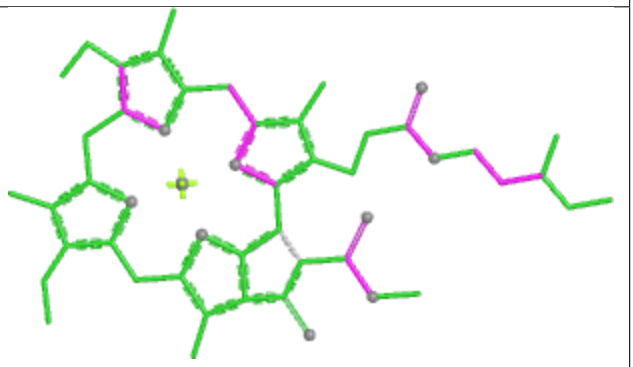


Rings

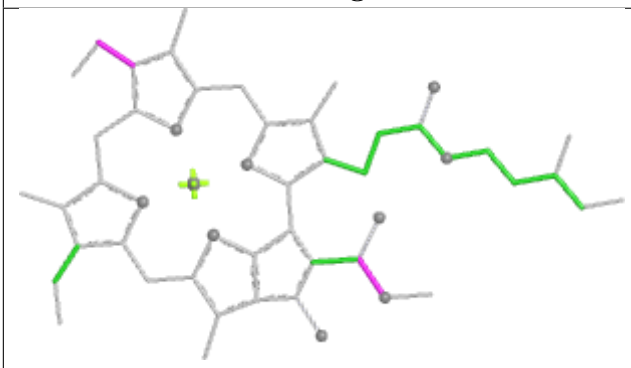
Ligand CLA A 5010



Bond lengths



Bond angles



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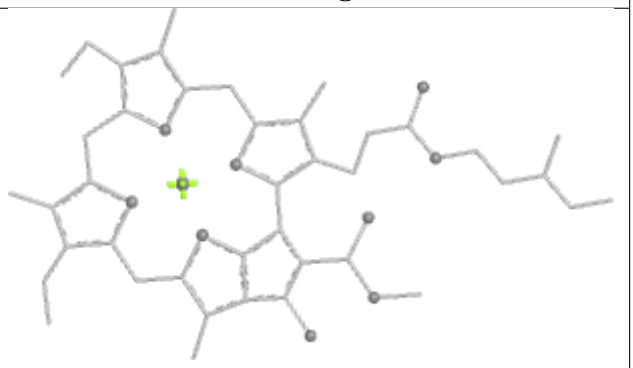
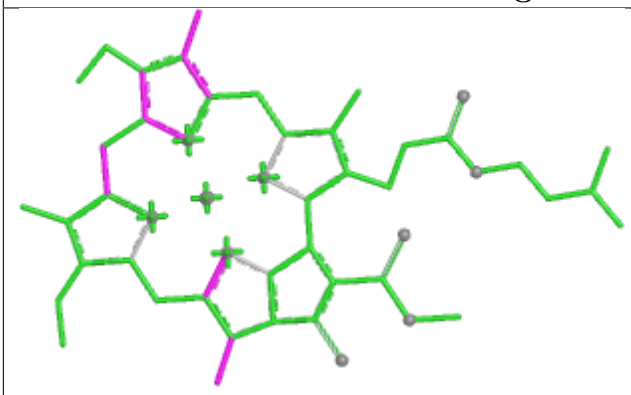
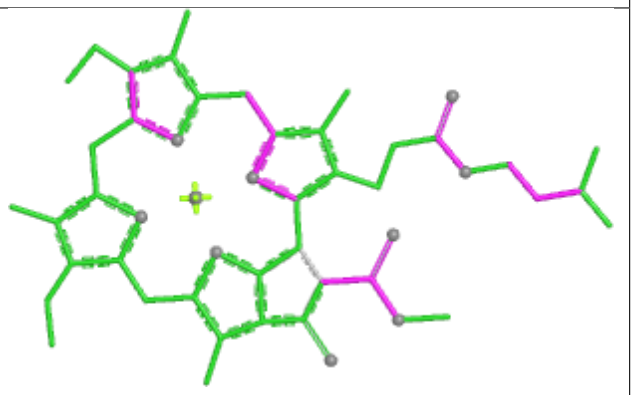


Rings

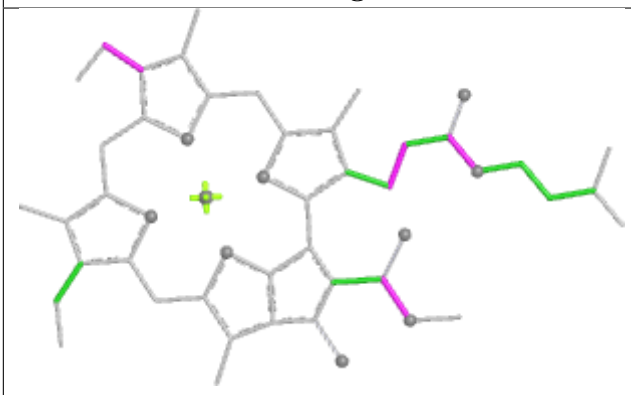
Ligand CLA A 5023



Bond lengths



Bond angles



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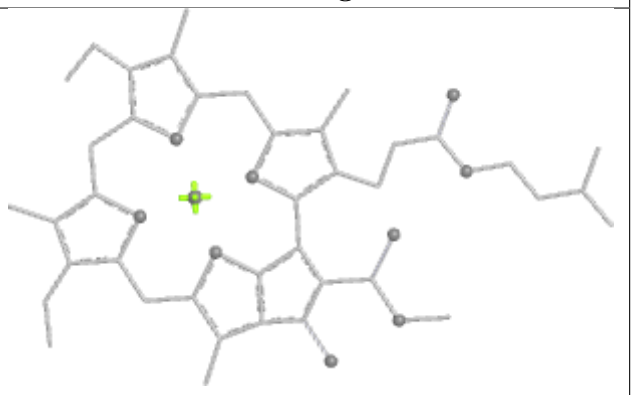
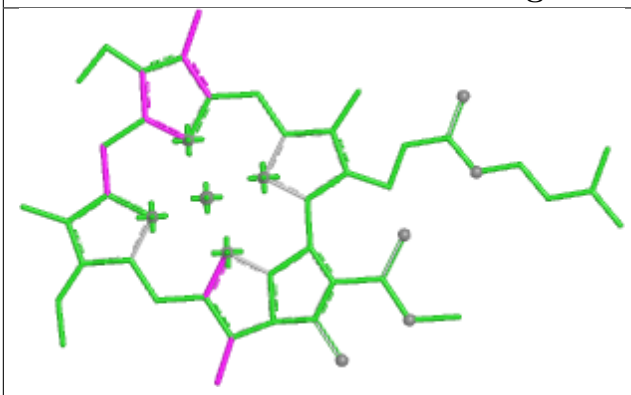


Rings

Ligand CLA L 205



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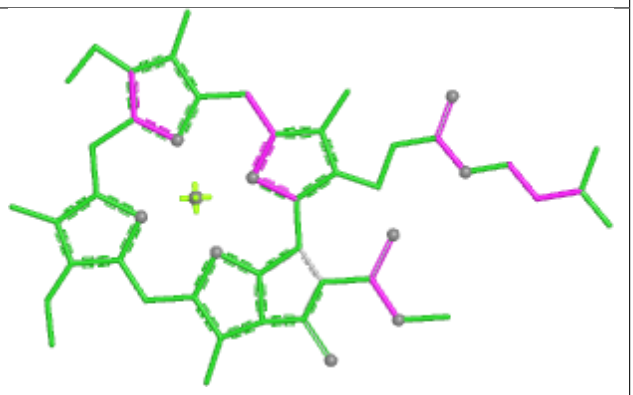
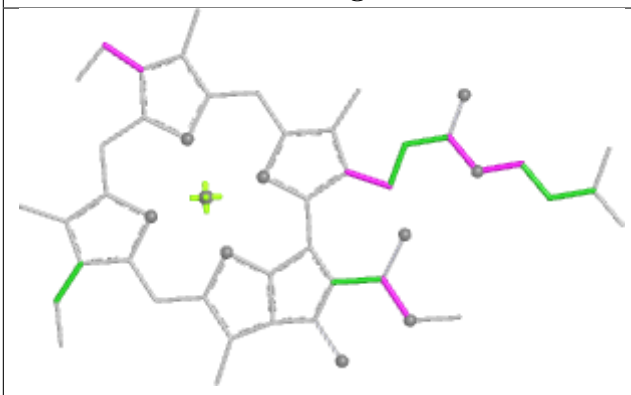


Bond angles



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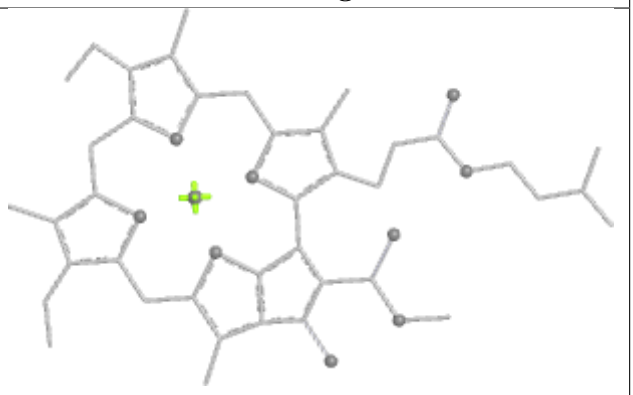
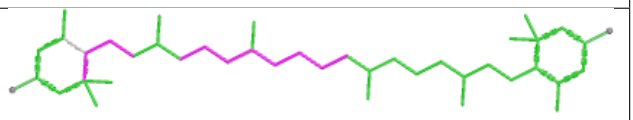


Rings

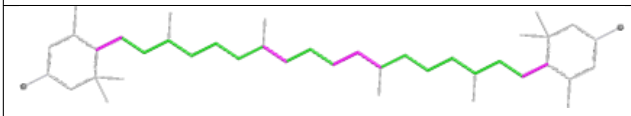
Ligand LUT 1 615



Bond lengths



Bond angles



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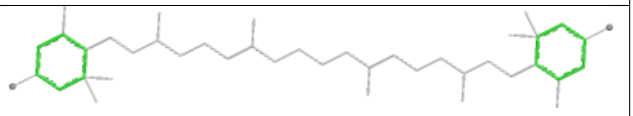
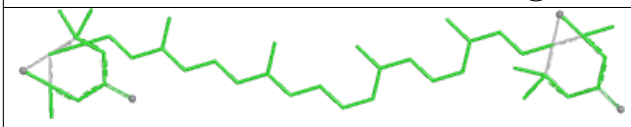


Rings

Ligand XAT 3 316



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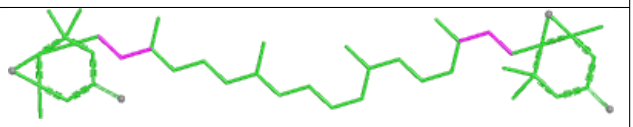
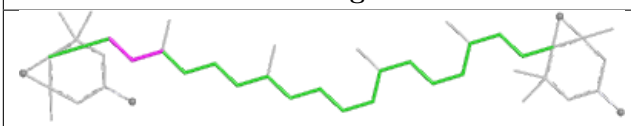


Bond angles



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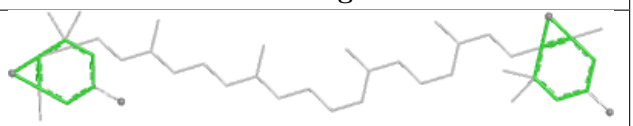
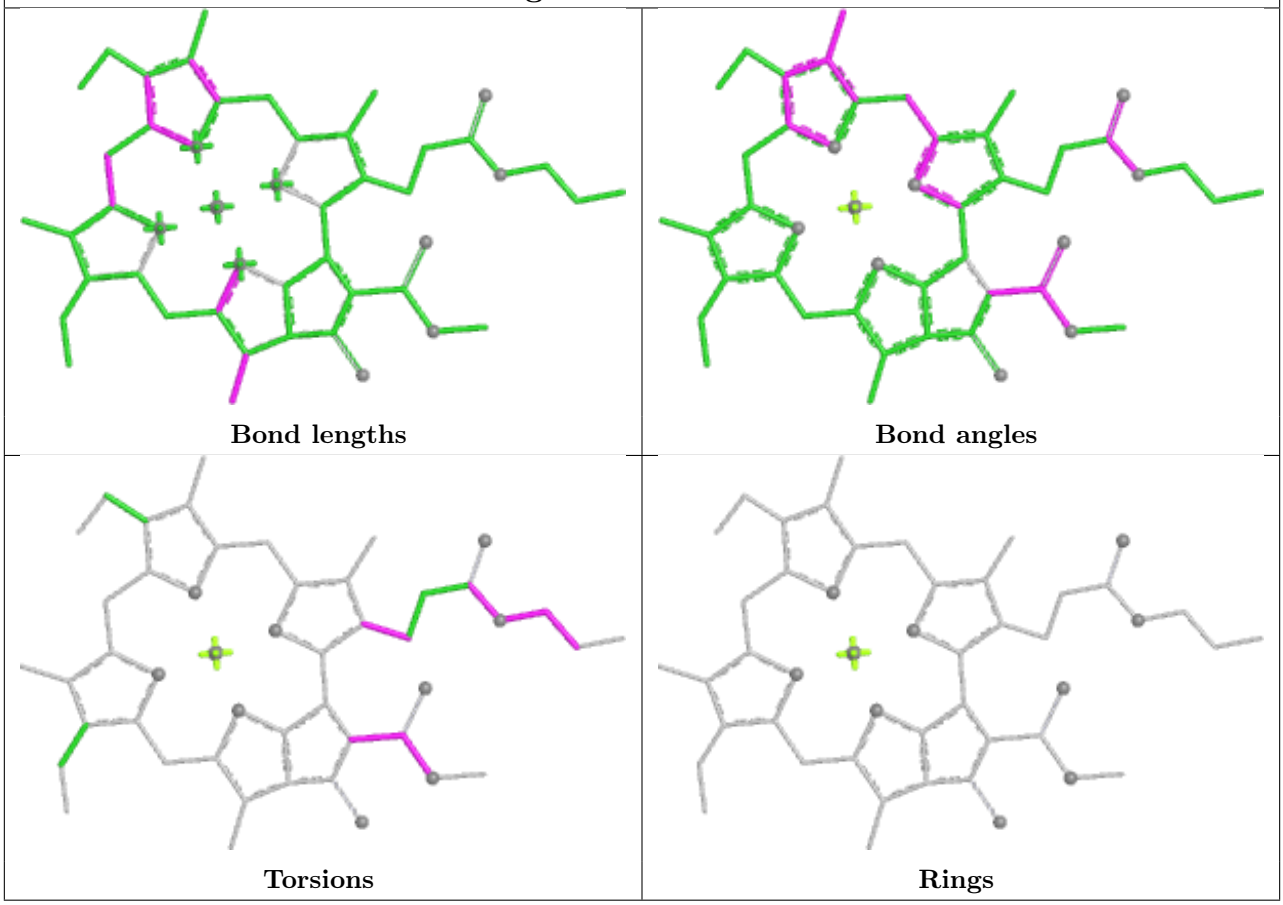


Rings

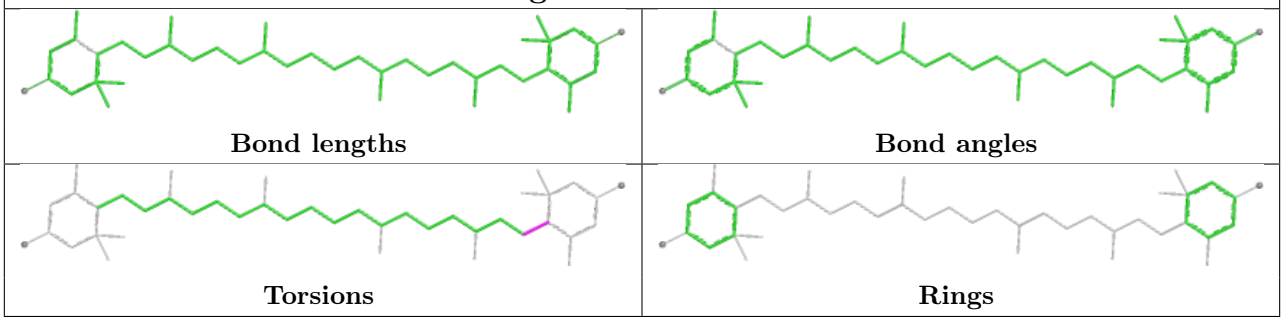
Ligand CLA B 806



Bond lengths | Bond angles

Torsions | Rings

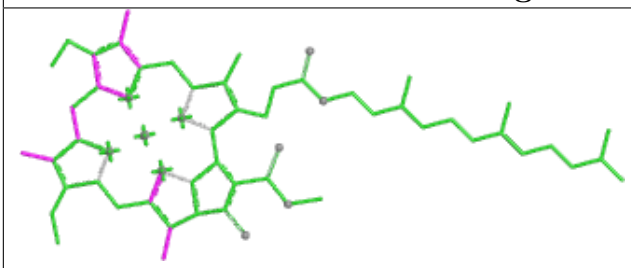
Ligand LUT 3 315



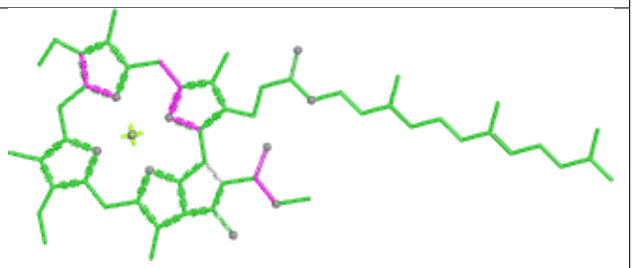
Bond lengths | Bond angles

Torsions | Rings

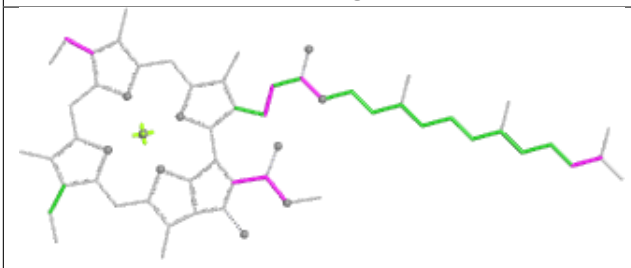
Ligand CLA A 5018



Bond lengths



Bond angles



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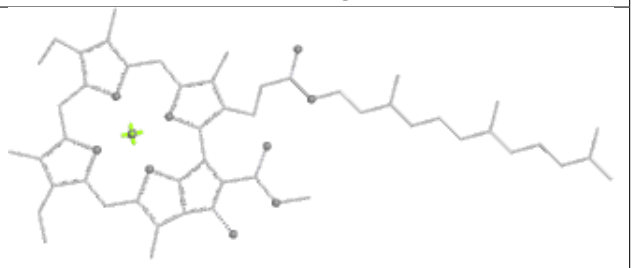
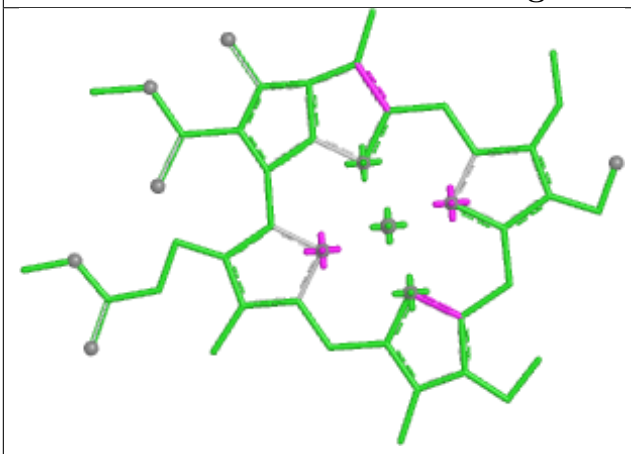
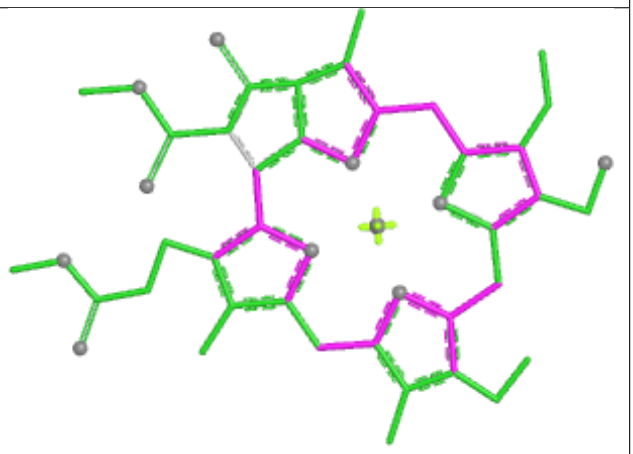


Rings

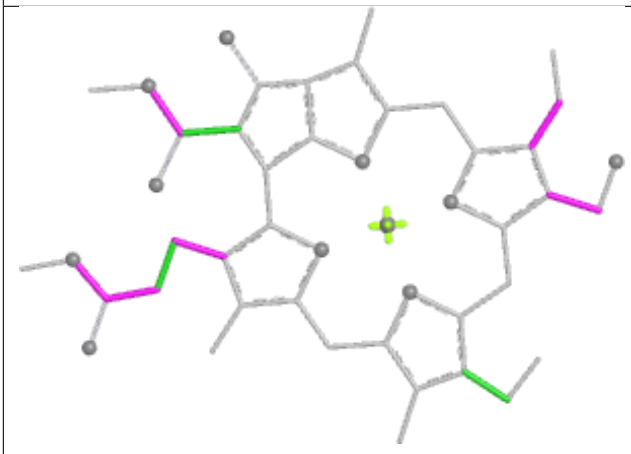
Ligand CHL 9 606



Bond lengths



Bond angles



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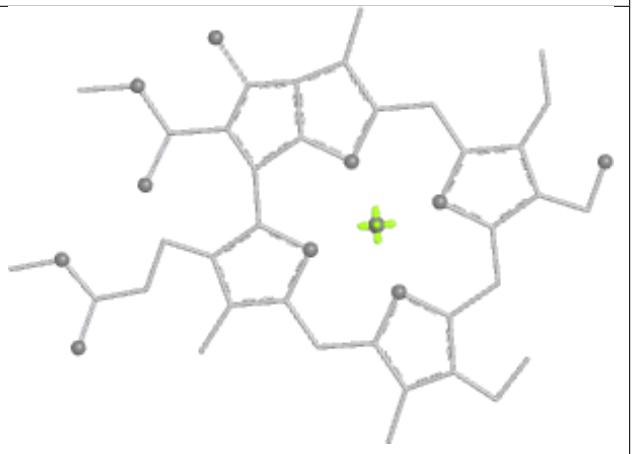
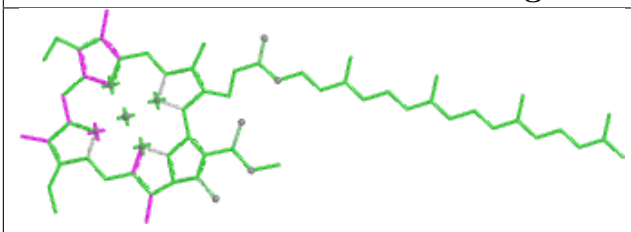
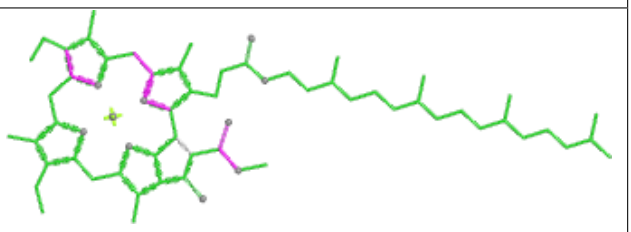
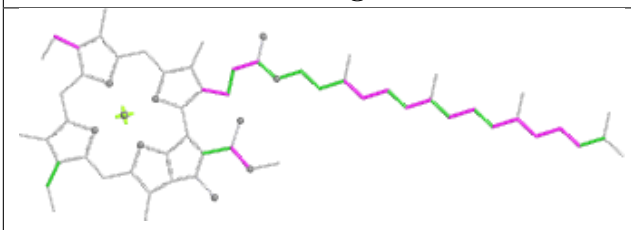


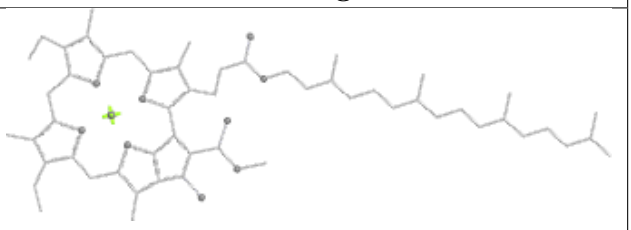
Rings

Ligand CLA B 804

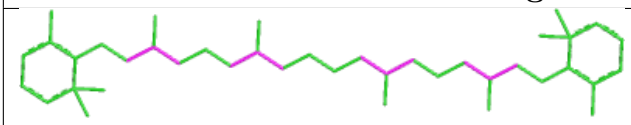

Bond lengths


Bond angles

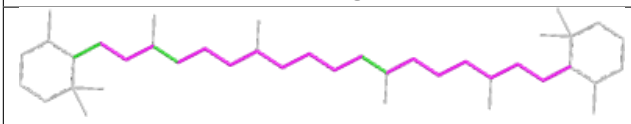

Torsions


Rings

Ligand BCR 3 319


Bond lengths


Bond angles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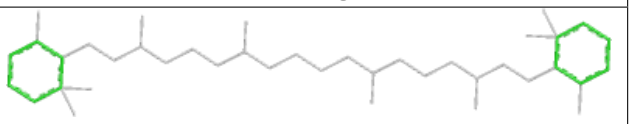
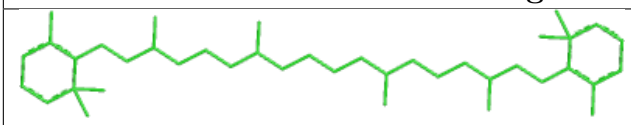

Rings

Ligand BCR 8 316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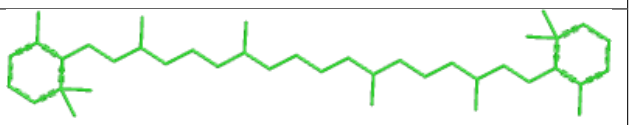
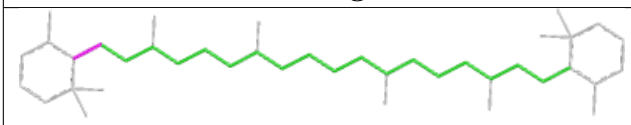

Bond angles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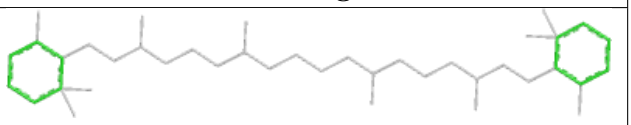
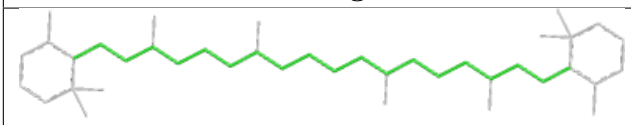

Rings

Ligand BCR B 846


Bond lengths


Bond angles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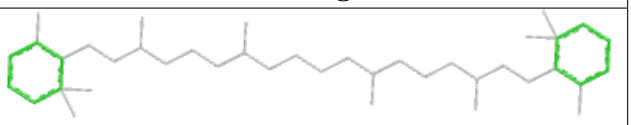
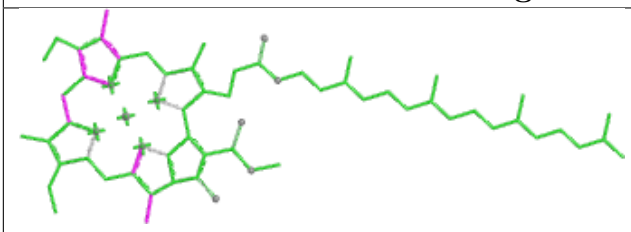
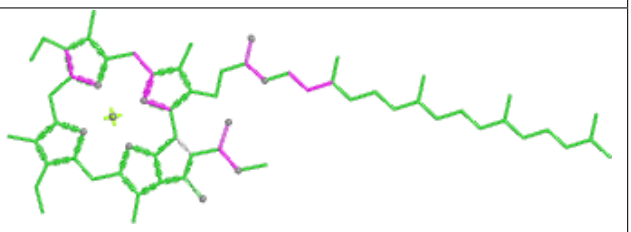

Rings

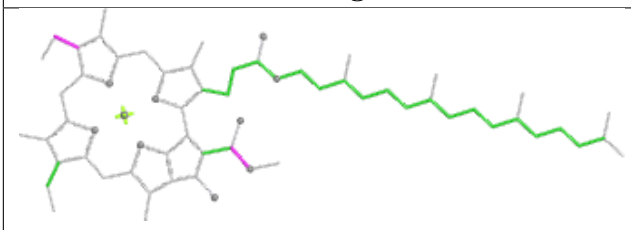
Ligand CLA A 5034



Bond lengths



Bond angles



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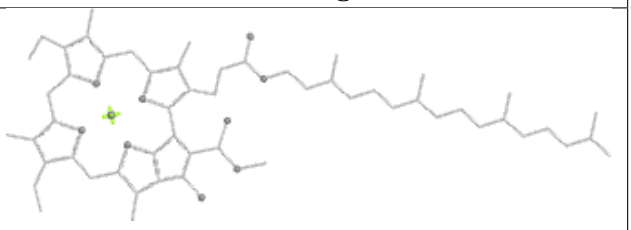
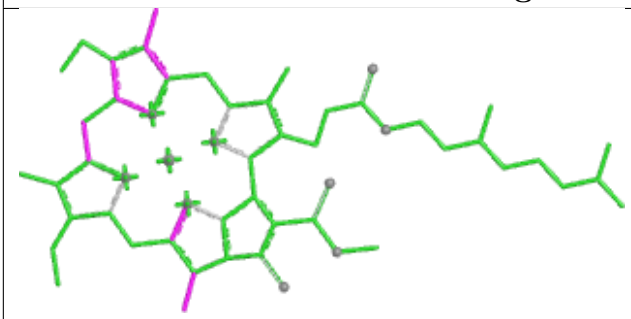
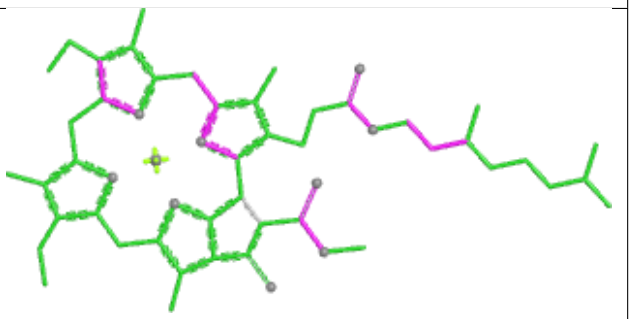


Rings

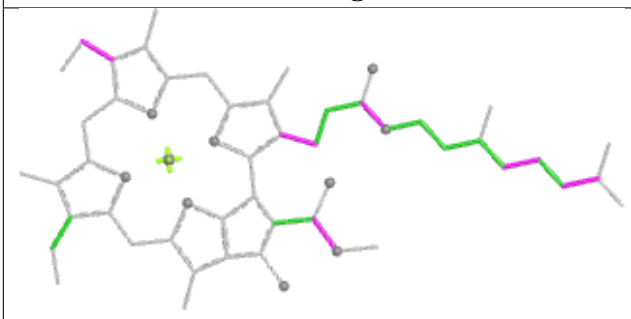
Ligand CLA A 5015



Bond lengths



Bond angles



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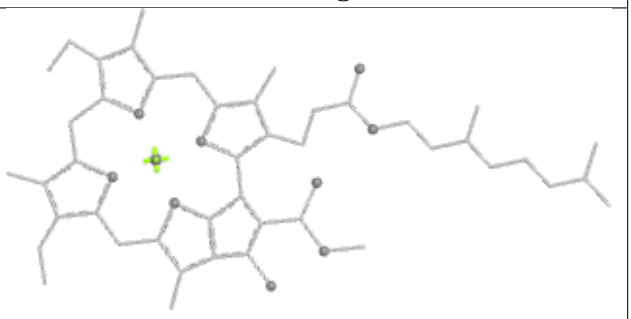
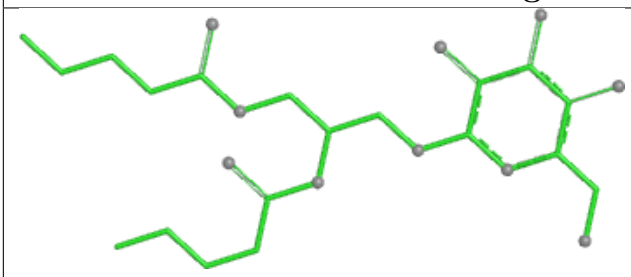
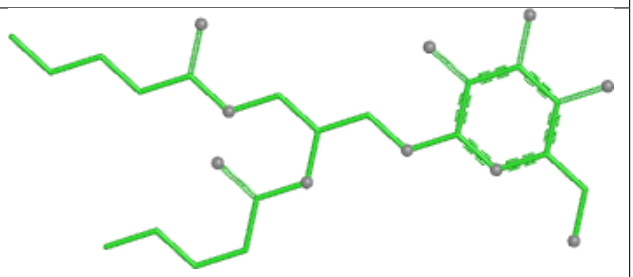


Rings

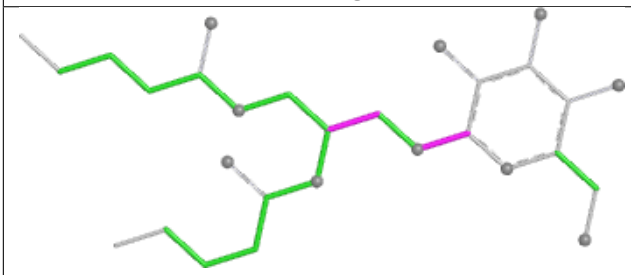
Ligand LMG J 103



Bond lengths



Bond angles



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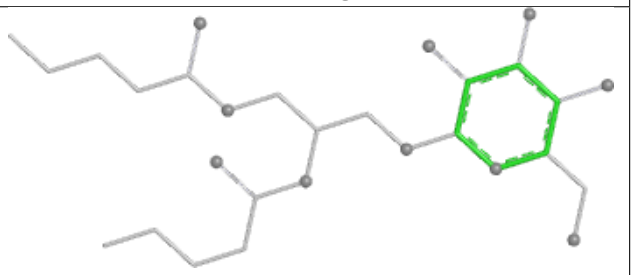
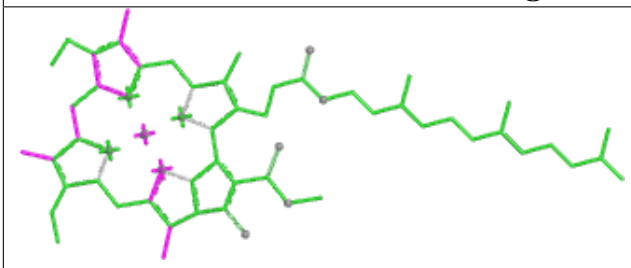
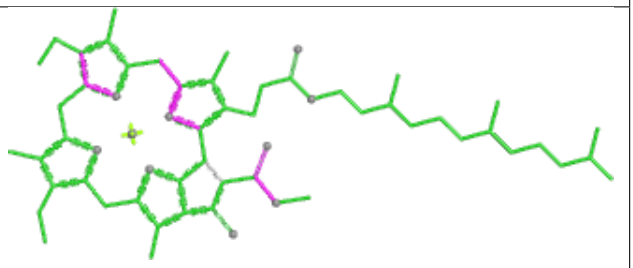


Rings

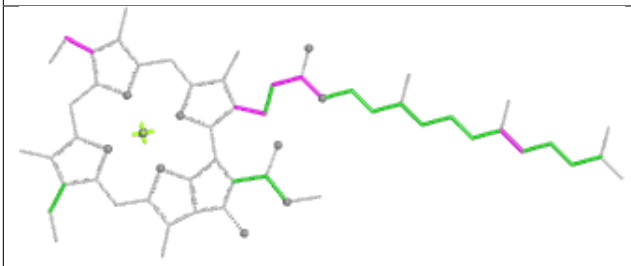
Ligand CLA B 817



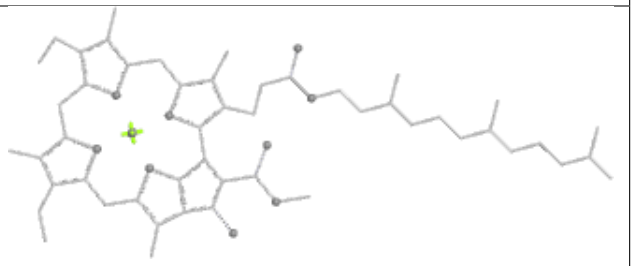
Bond lengths



Bond angles

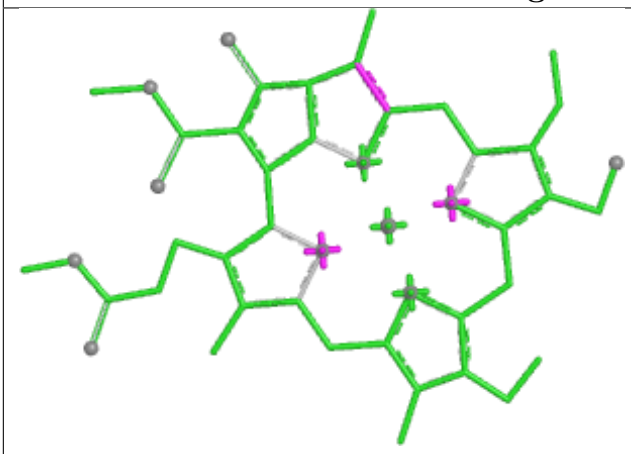


Torsions

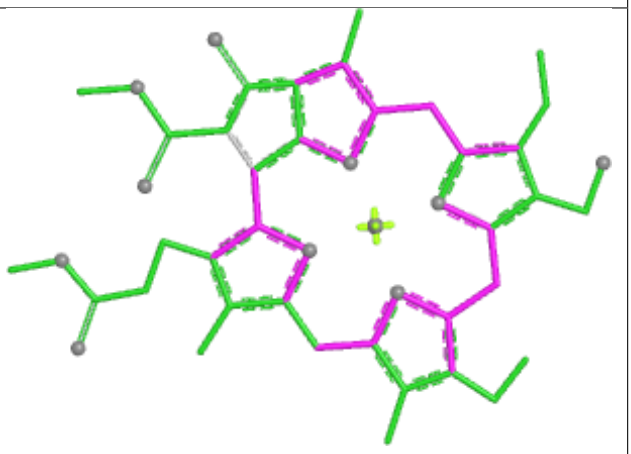


Rings

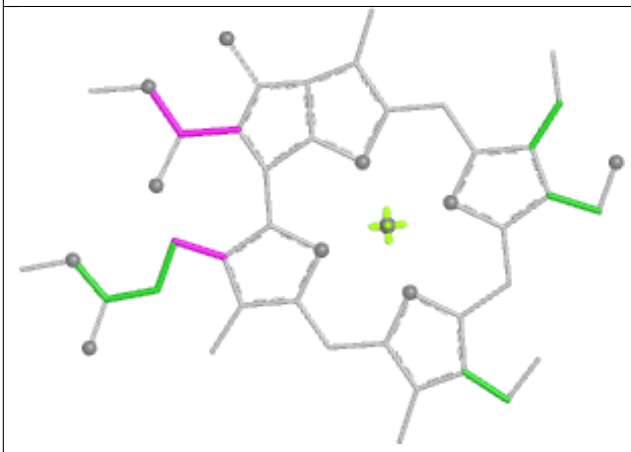
Ligand CHL 1 601



Bond lengths



Bond angles



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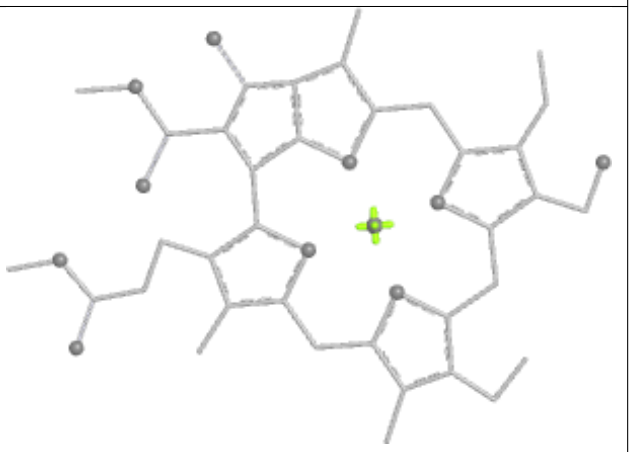
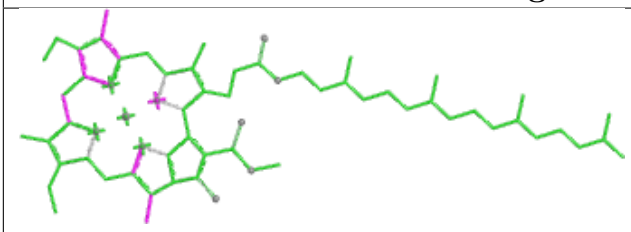


Rings

Ligand CLA 8 302



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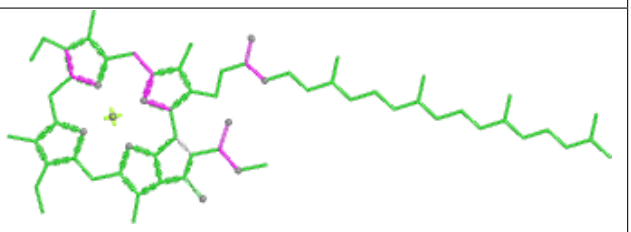

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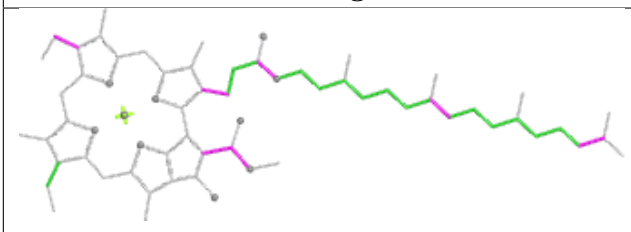

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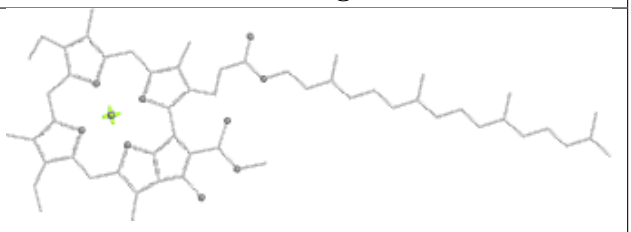

Rings

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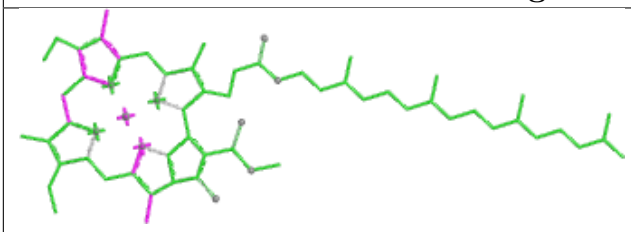
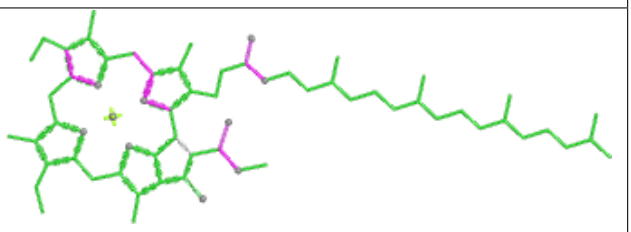
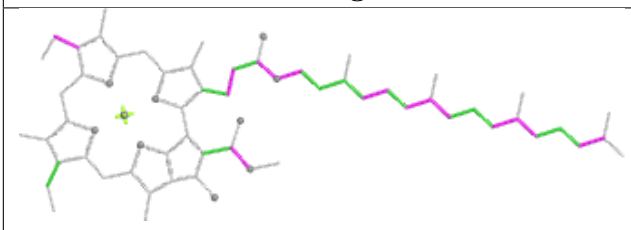
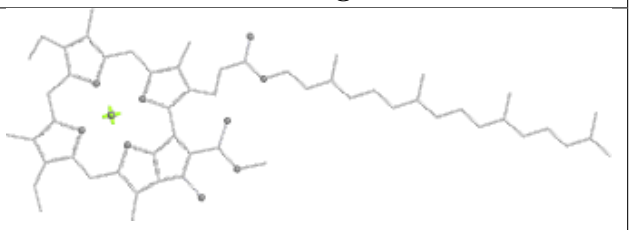
 Bond lengths	 Bond angles
 Torsions	 Rings

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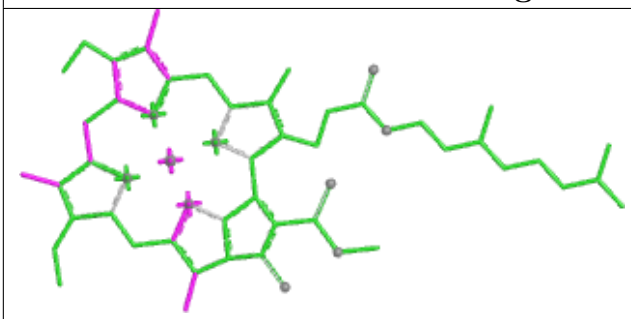
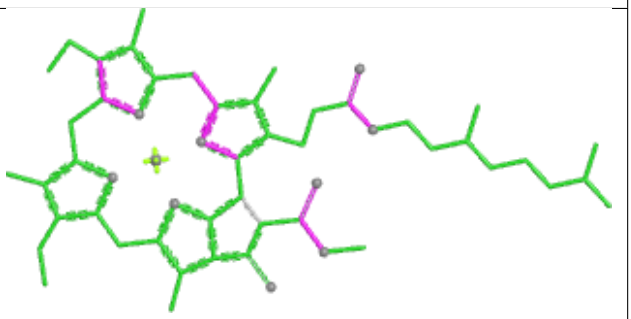
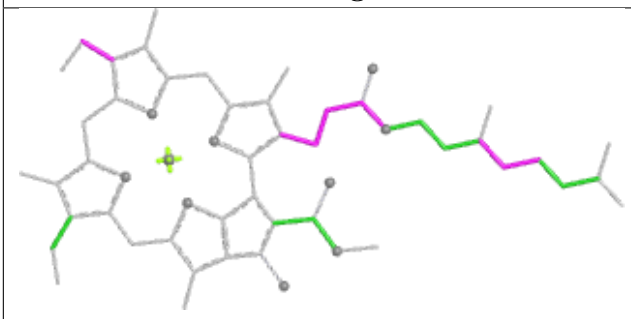
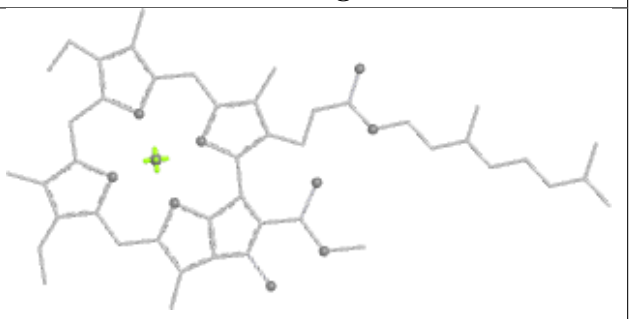
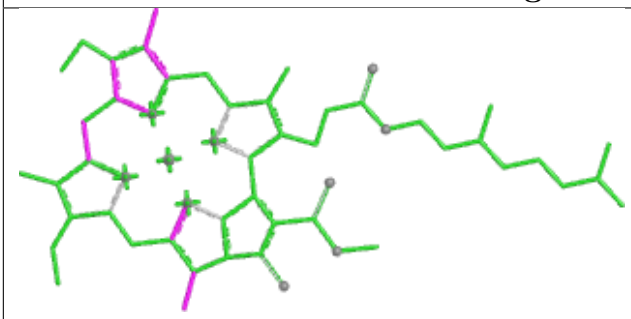
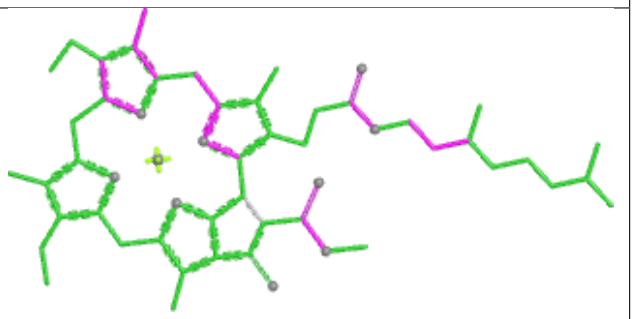
 Bond lengths	 Bond angles
 Torsions	 Rings

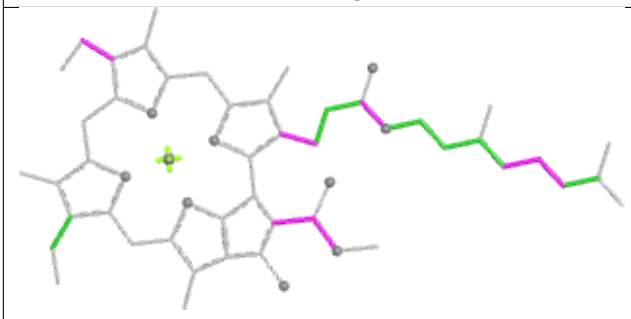
Ligand CLA B 816



Bond lengths



Bond angles



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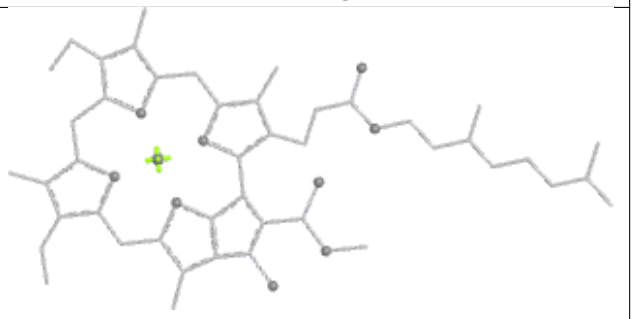
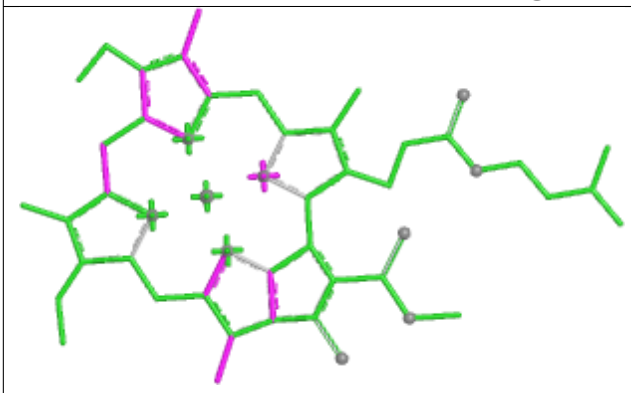


Rings

Ligand CLA 2 303



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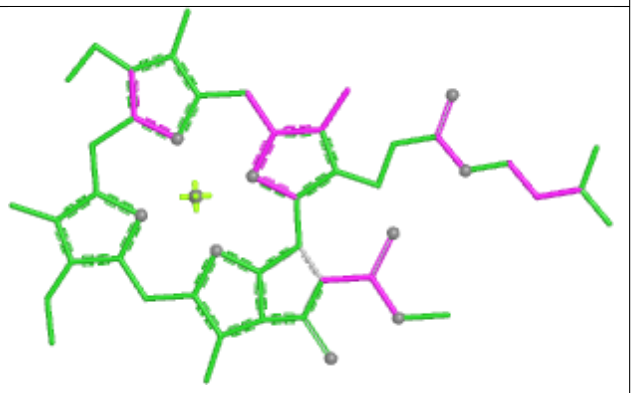

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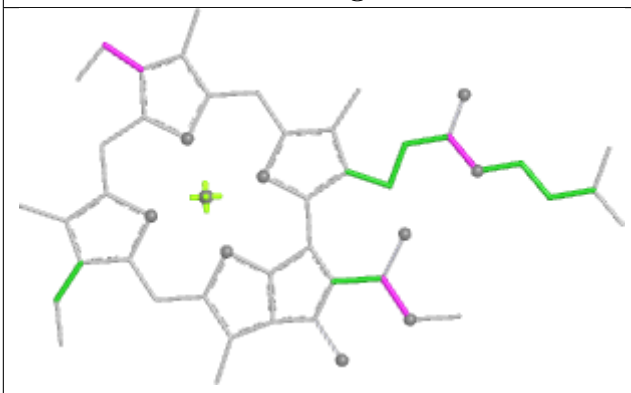

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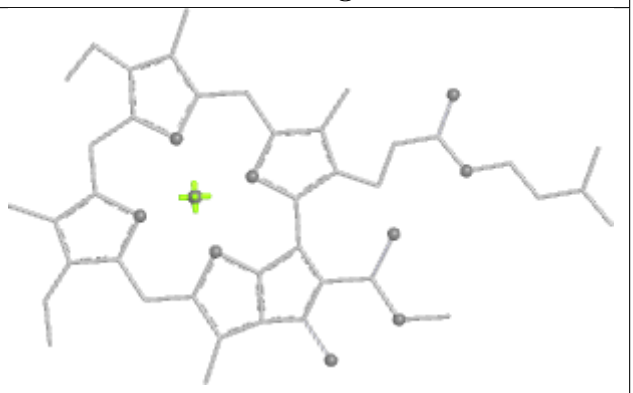

Rings

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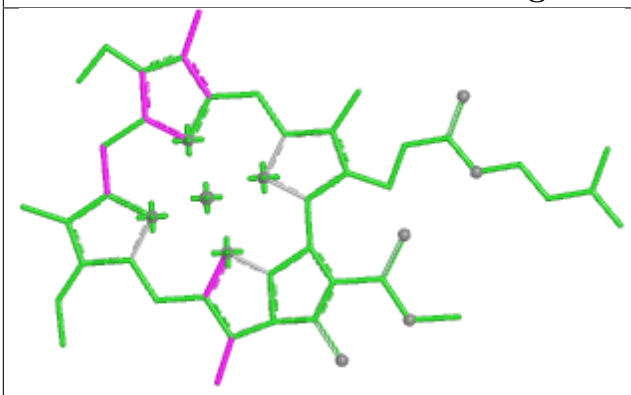

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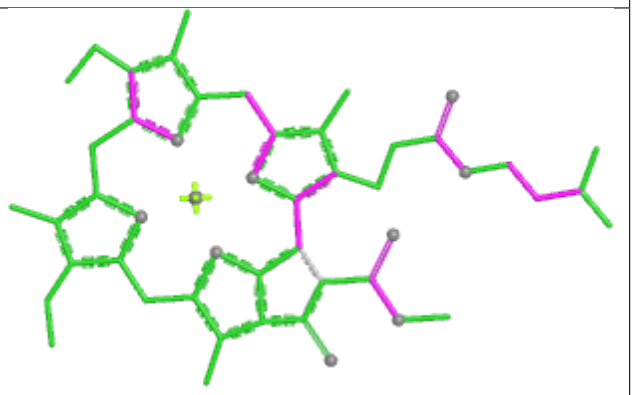

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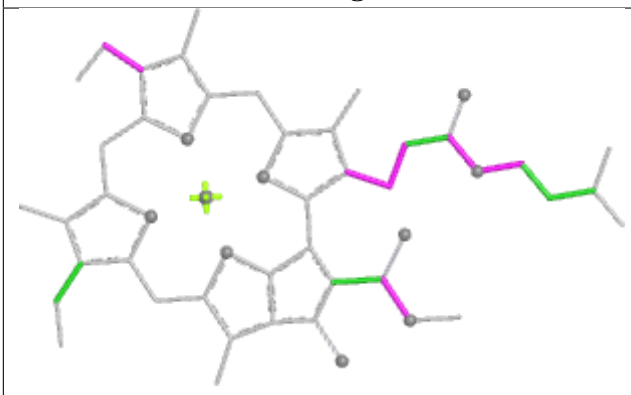

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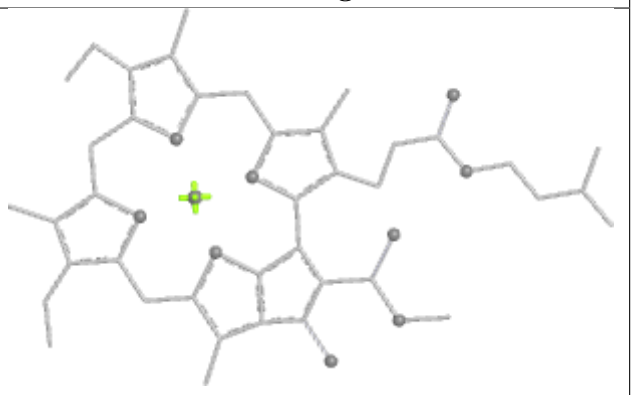
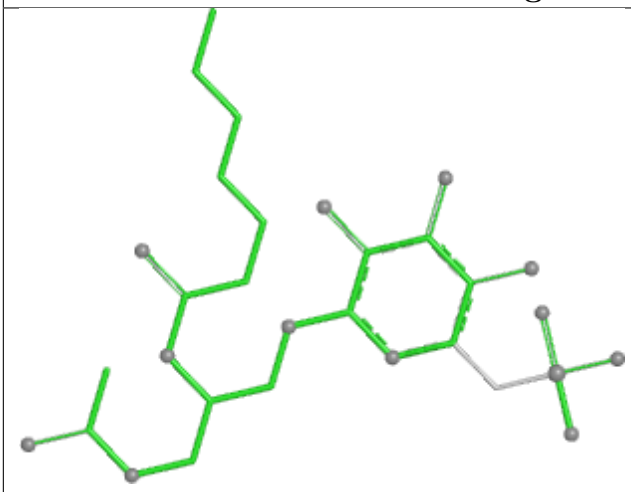


Rings

Ligand SQD B 850



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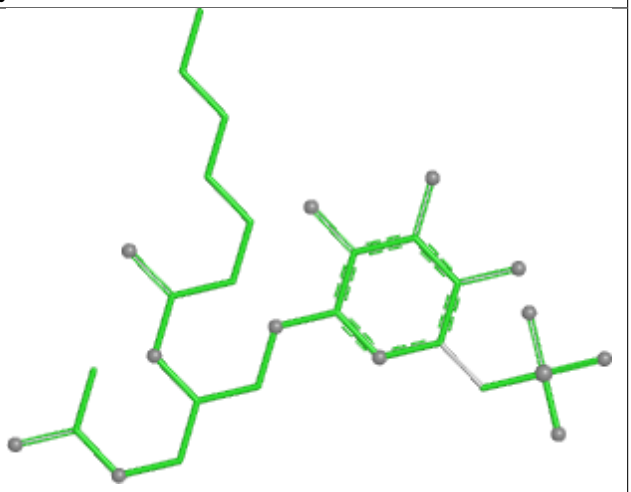
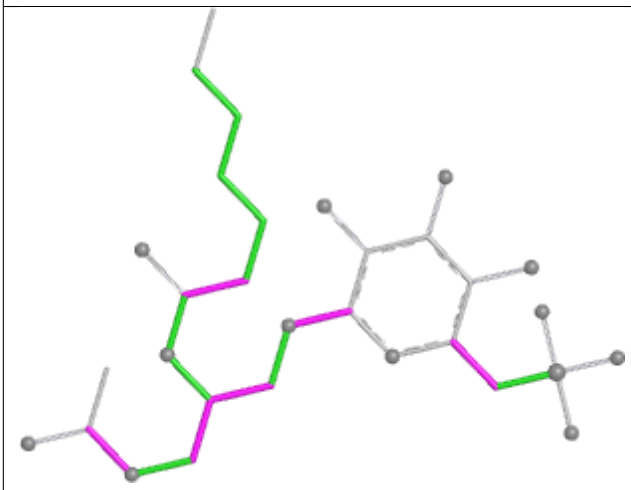


Bond angles



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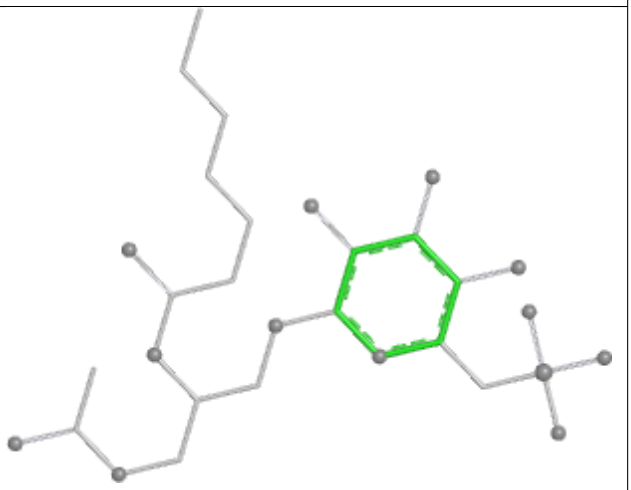
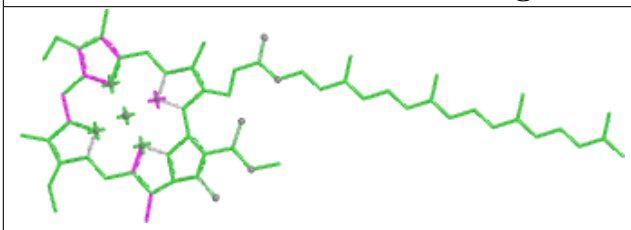


Rings

Ligand CLA A 5044



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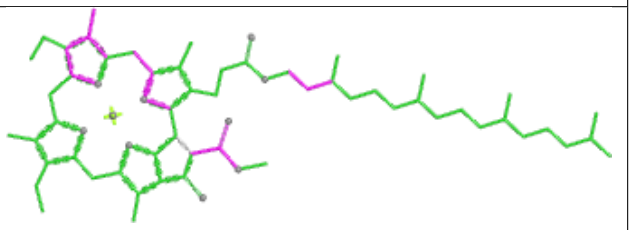

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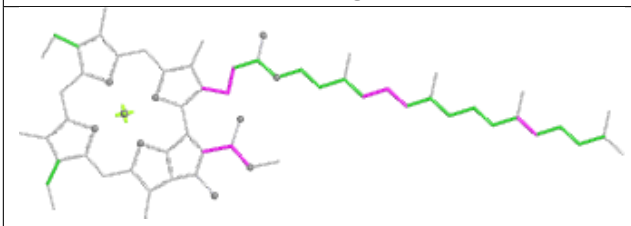

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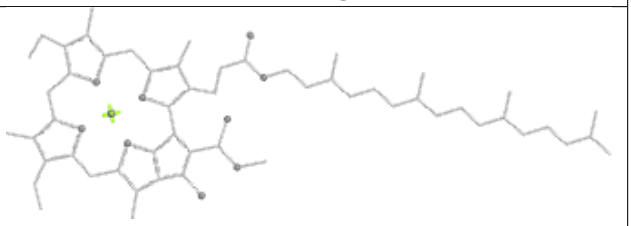
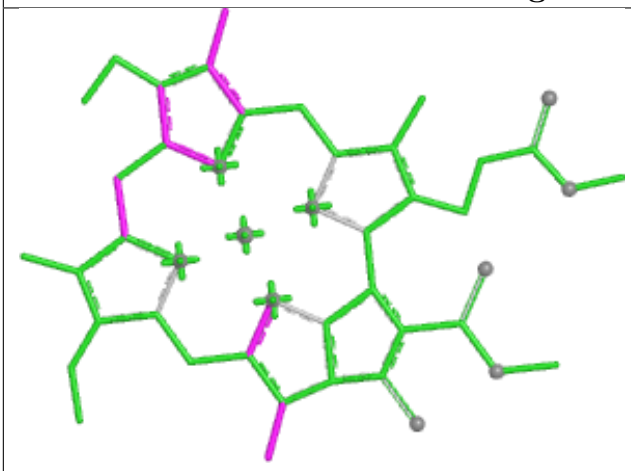


Rings

Ligand CLA 3 309



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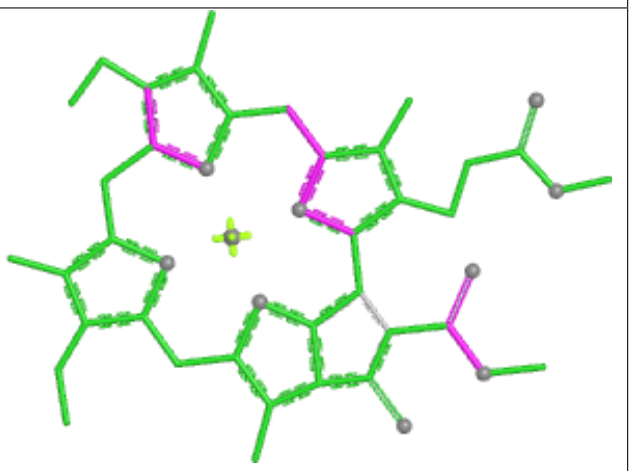

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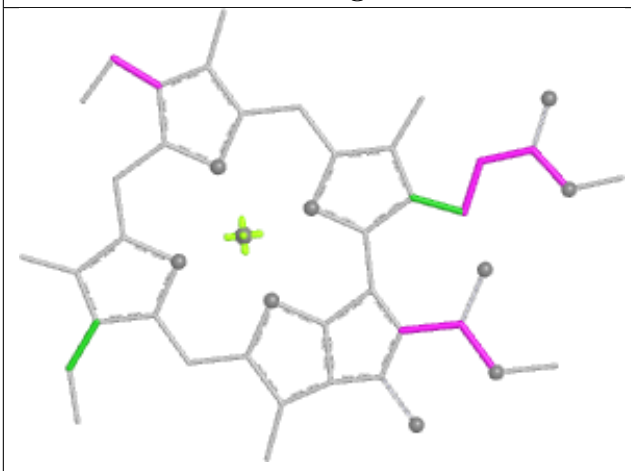

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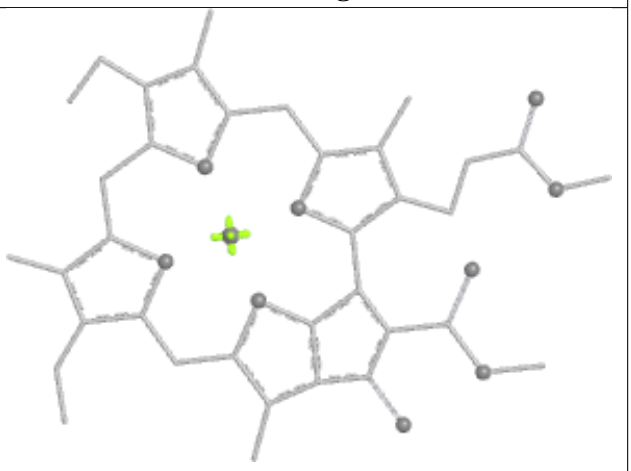
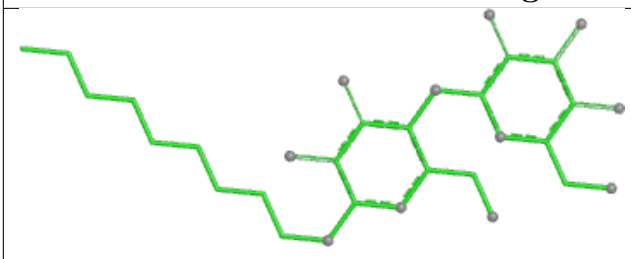


Rings

Ligand LMU F 305



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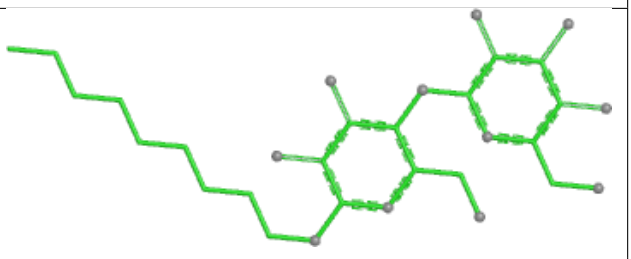

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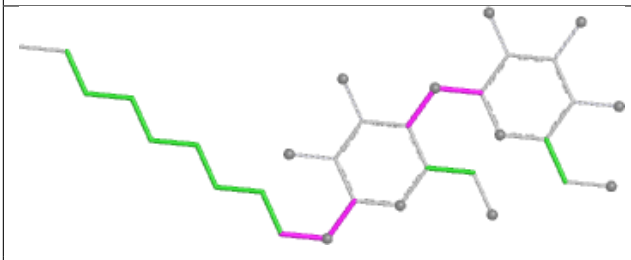

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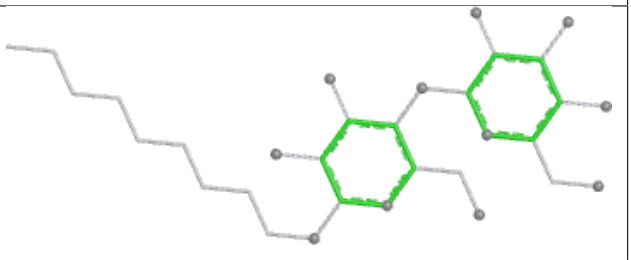
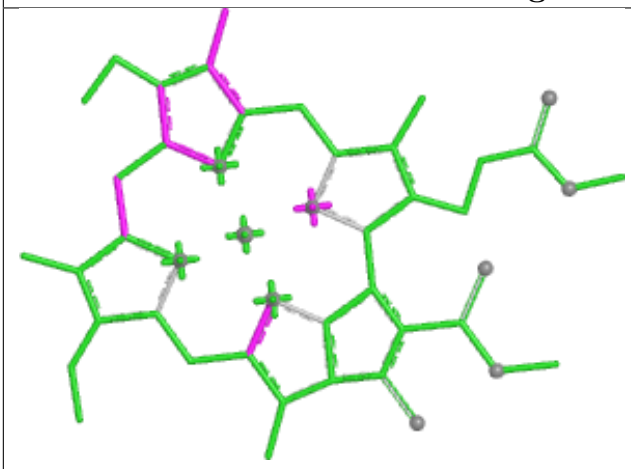


Rings

Ligand CLA 8 321



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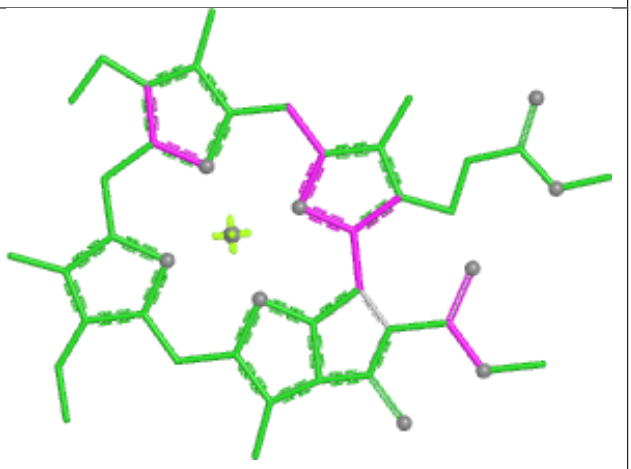
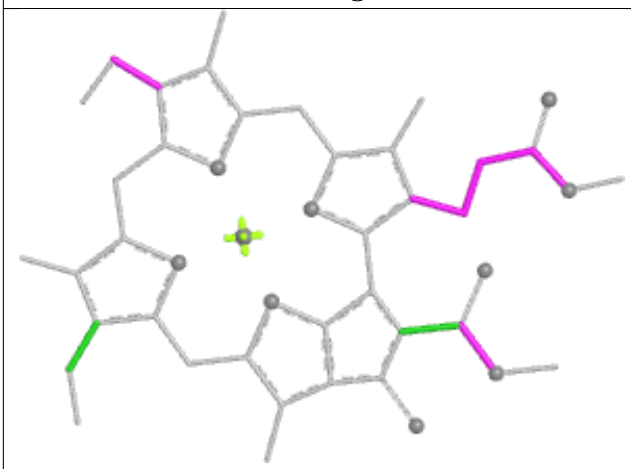


Bond angles



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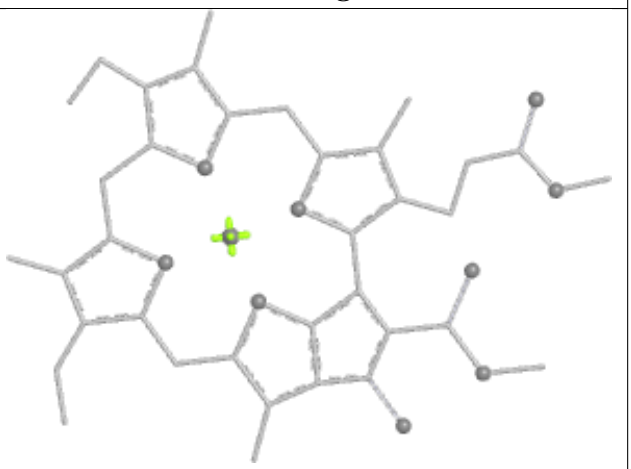
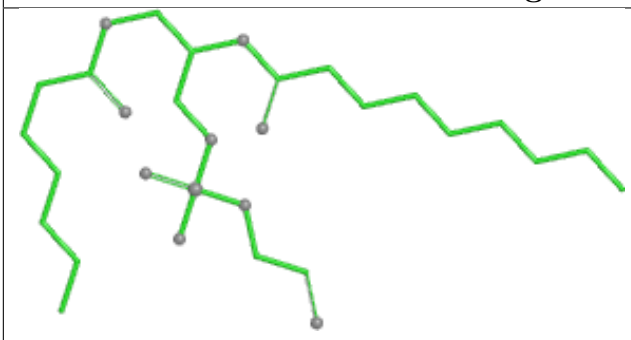


Rings

Ligand PTY F 310



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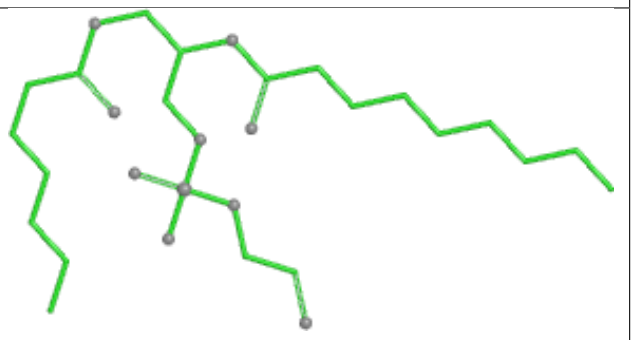
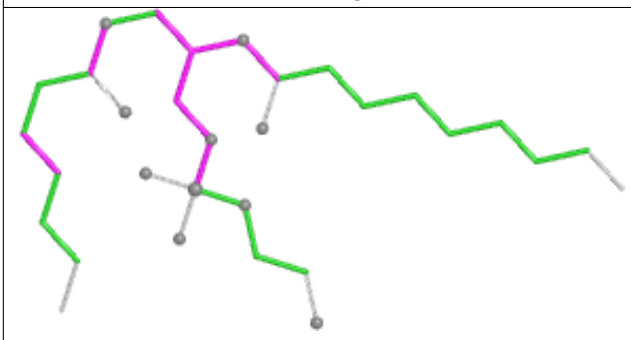


Bond angles



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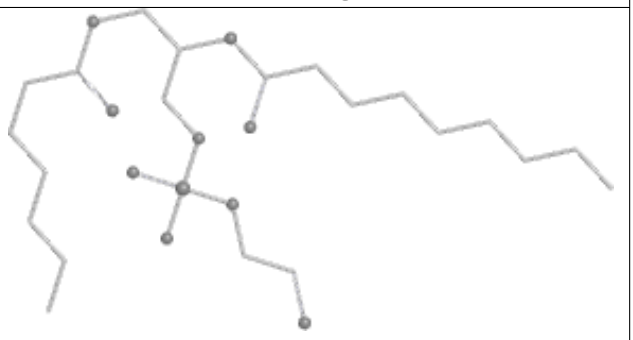
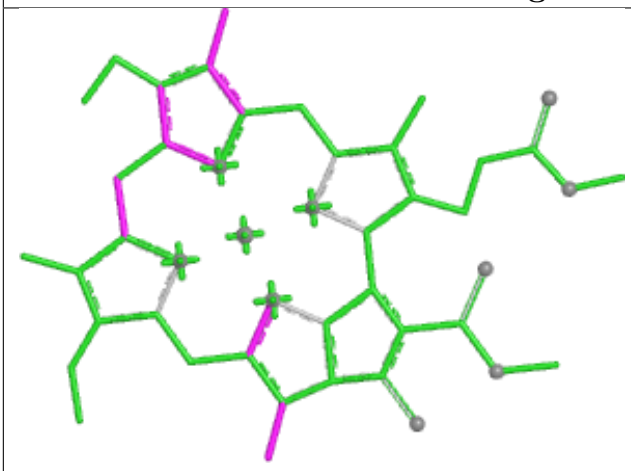
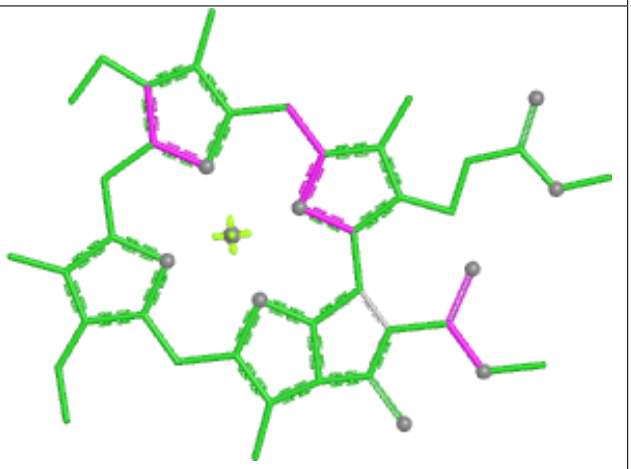


Rings

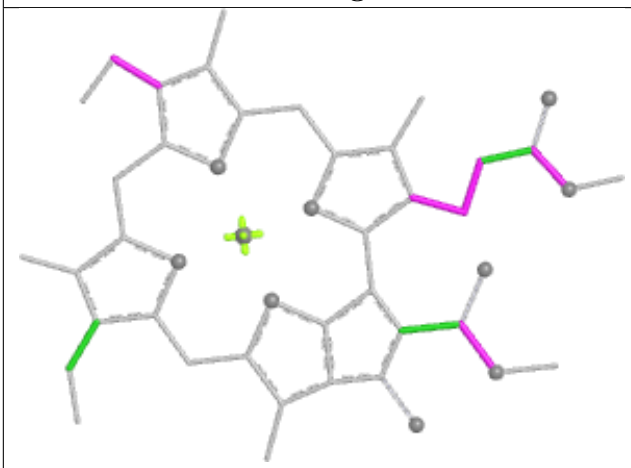
Ligand CLA 8 312



Bond lengths



Bond angles



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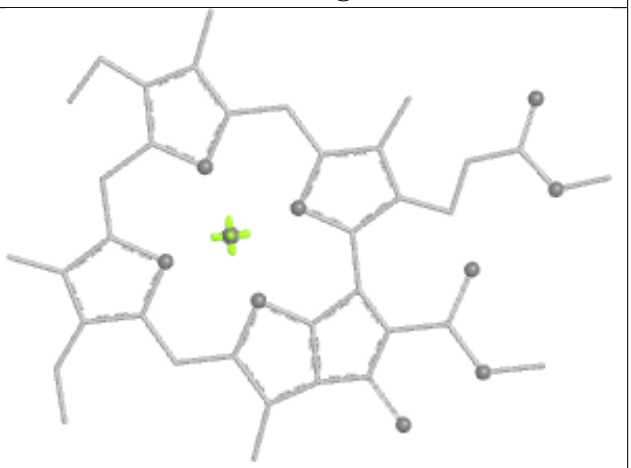
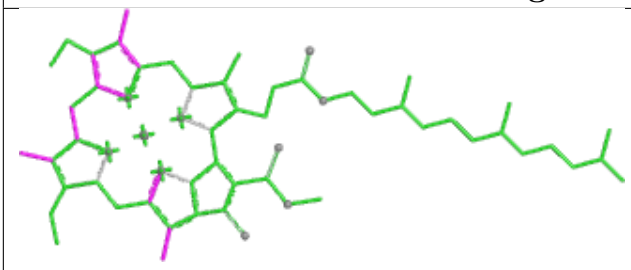
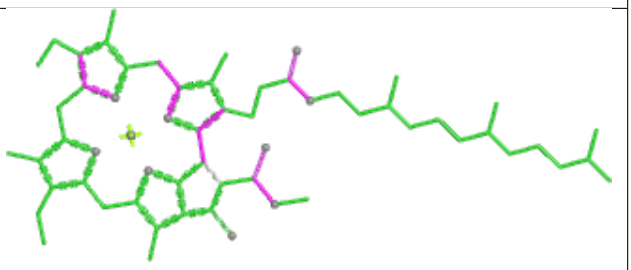


Rings

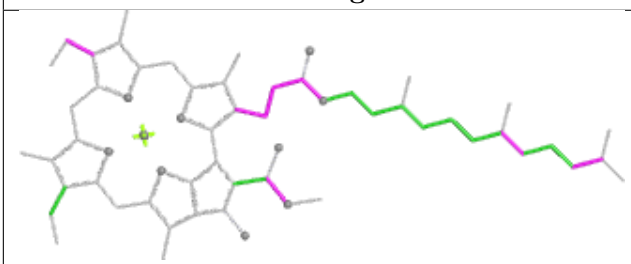
Ligand CLA 7 303



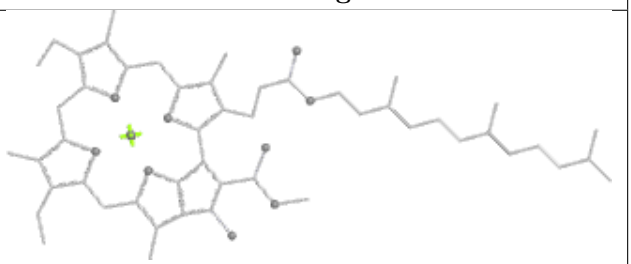
Bond lengths



Bond angles

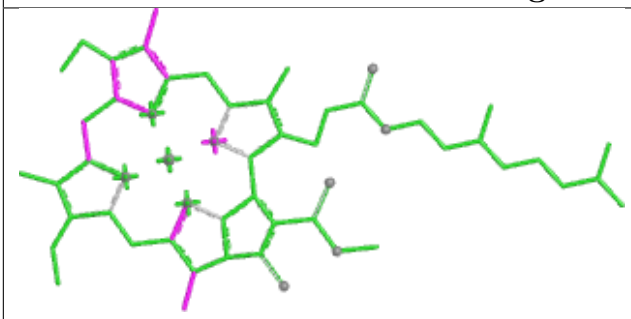


Torsions

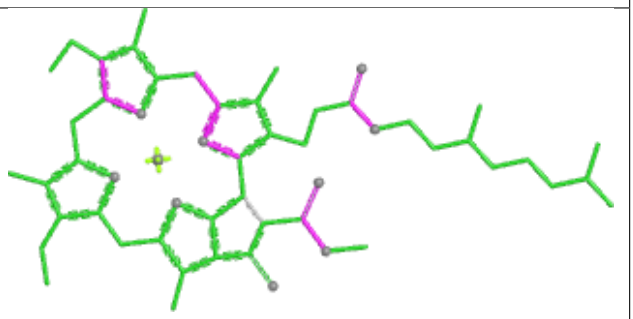


Rings

Ligand CLA 7 304



Bond lengths



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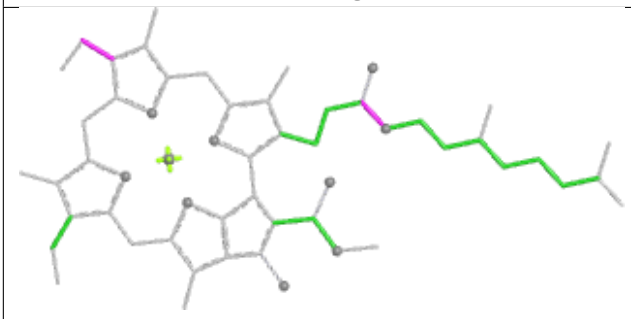

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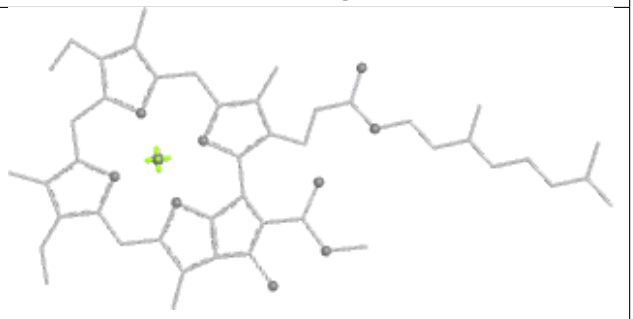
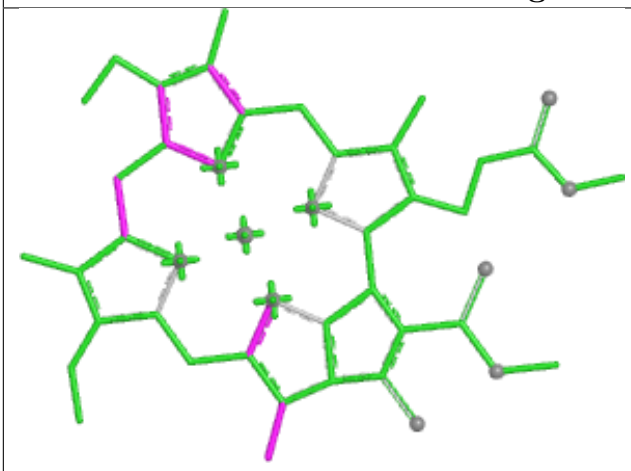


Rings

Ligand CLA 9 601



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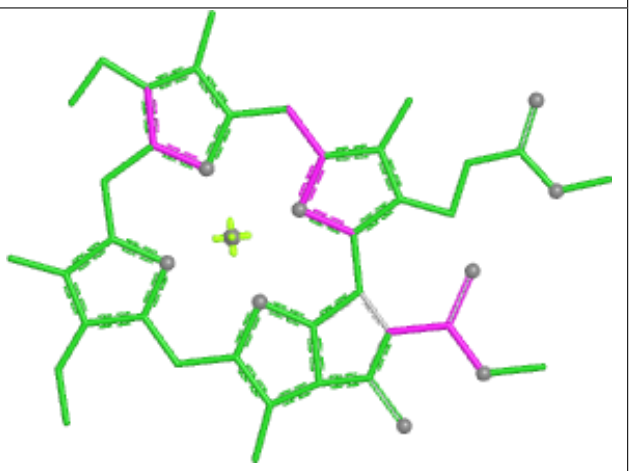

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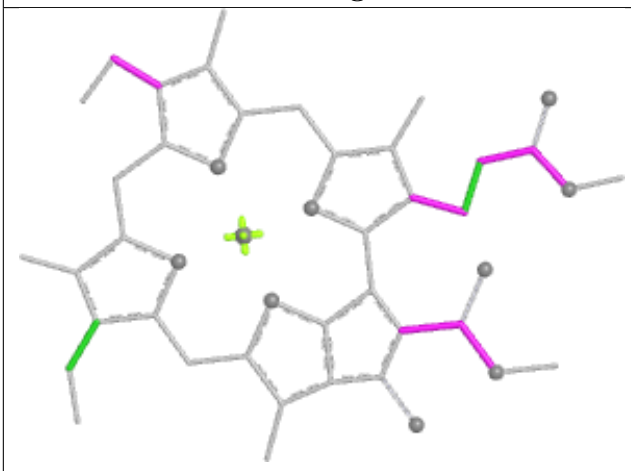

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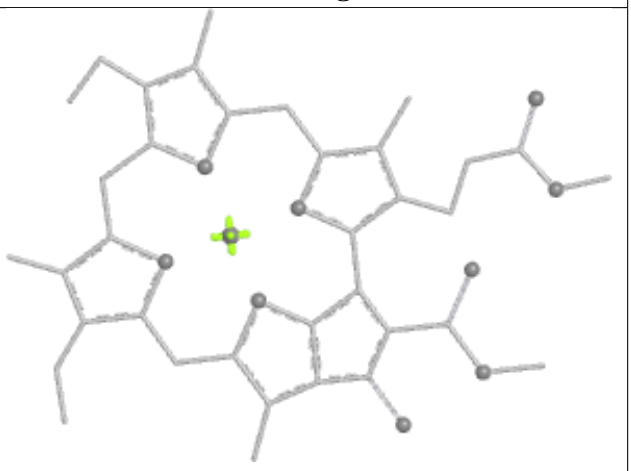
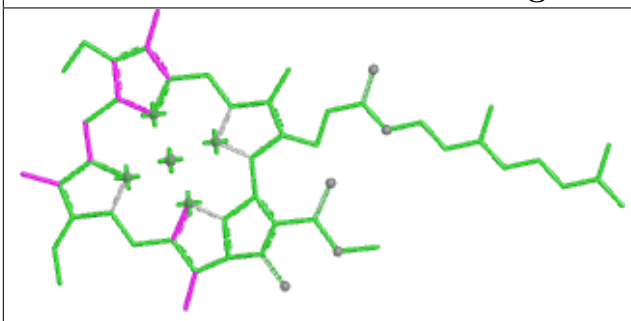


Rings

Ligand CLA 9 611



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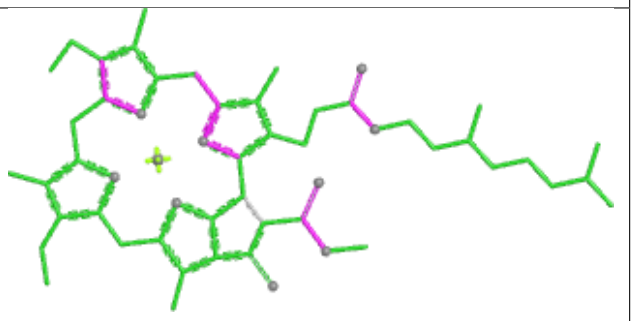
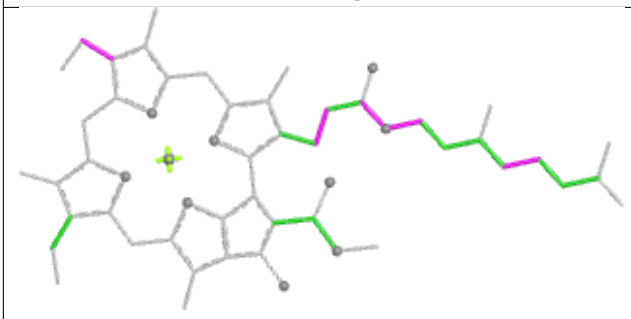


Bond angles



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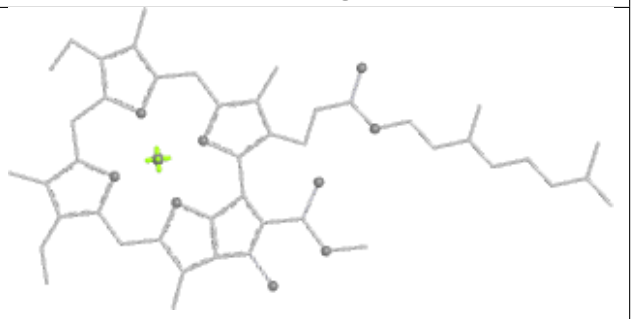
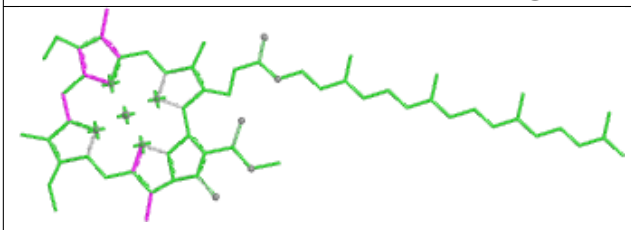


Rings

Ligand CLA L 202



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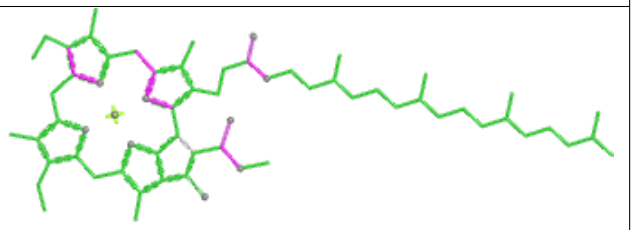
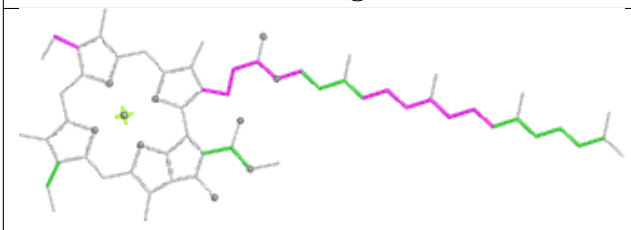


Bond angles



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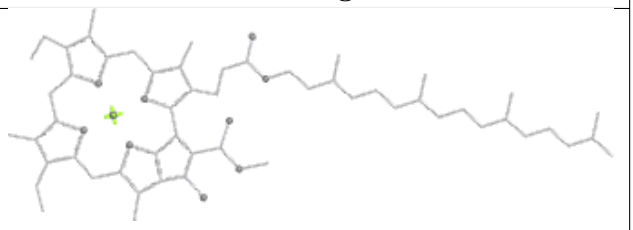
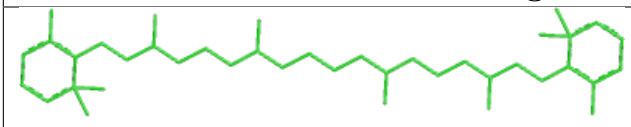


Rings

Ligand BCR J 102



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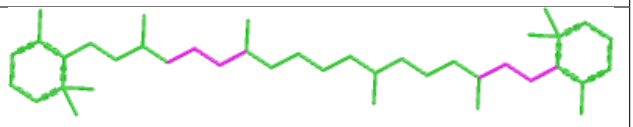

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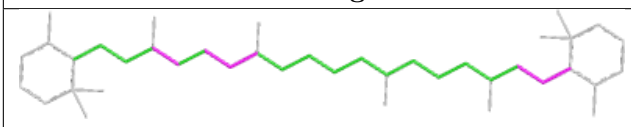

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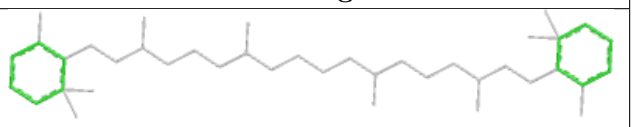
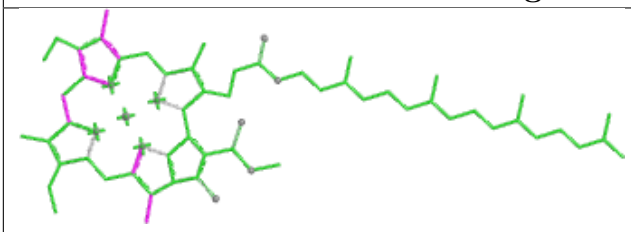


Rings

Ligand CLA B 840



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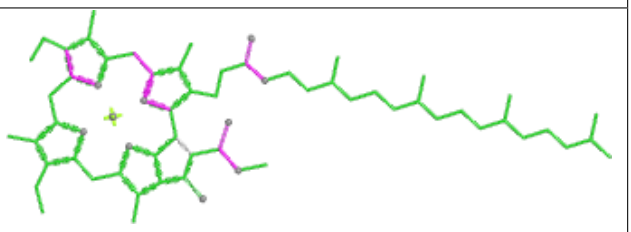
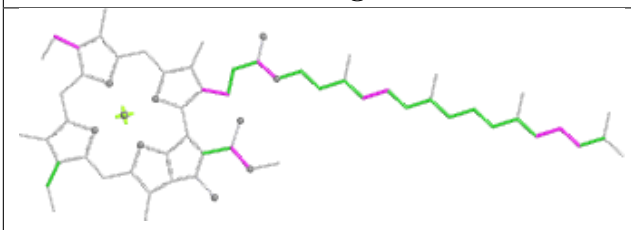


Bond angles



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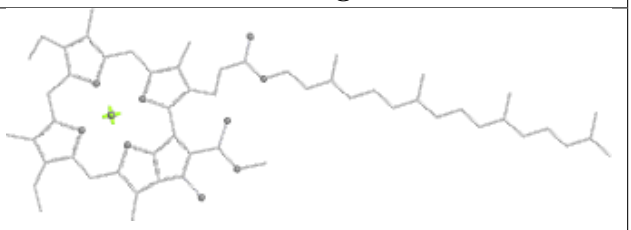
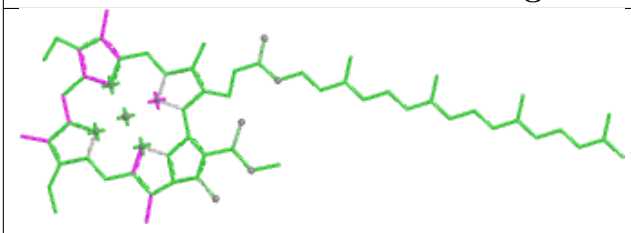


Rings

Ligand CLA B 828



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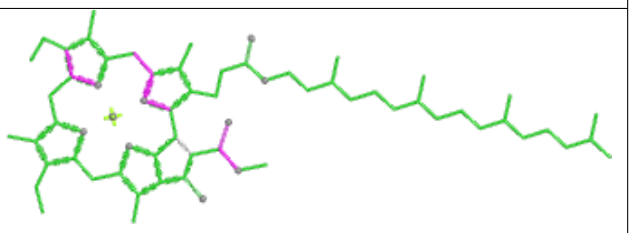

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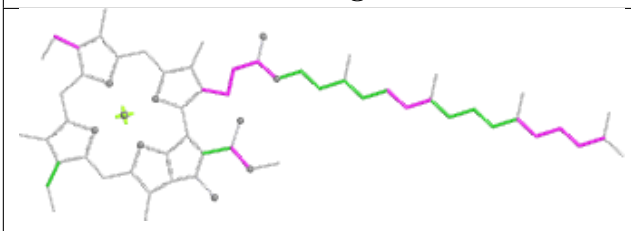

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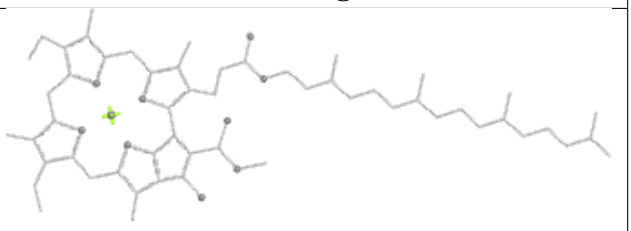
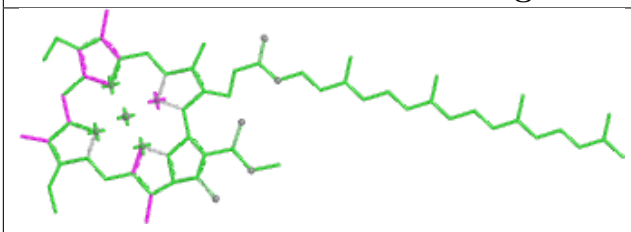


Rings

Ligand CLA A 5028



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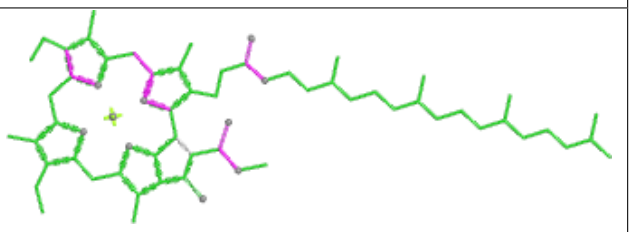
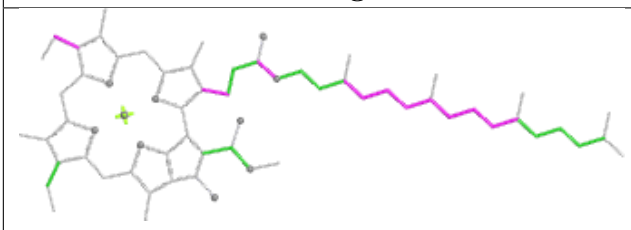


Bond angles



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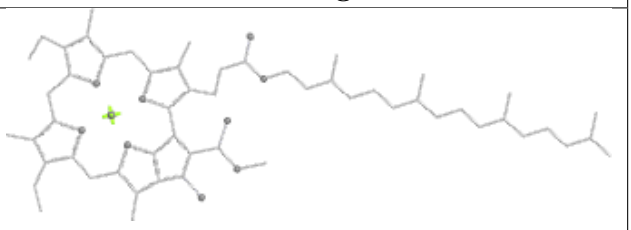
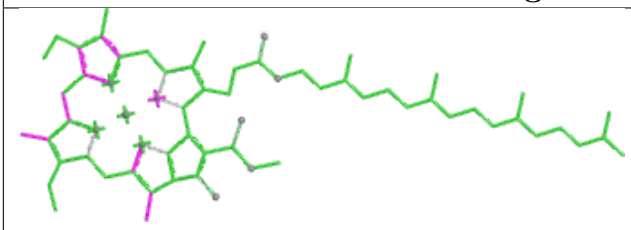


Rings

Ligand CLA B 824



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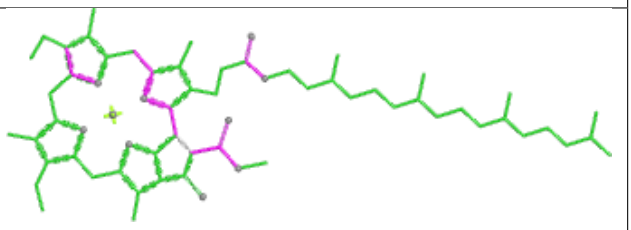
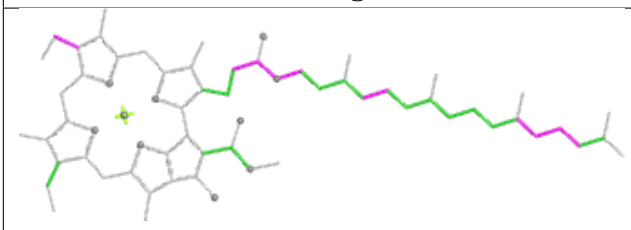


Bond angles



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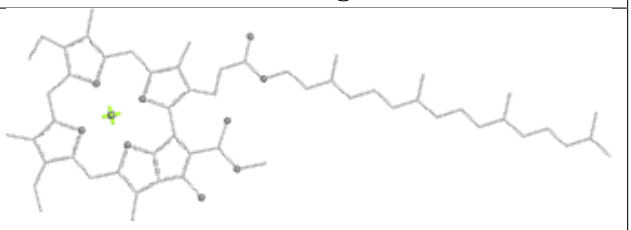
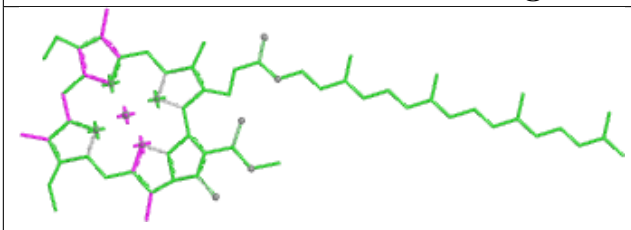


Rings

Ligand CLA B 810



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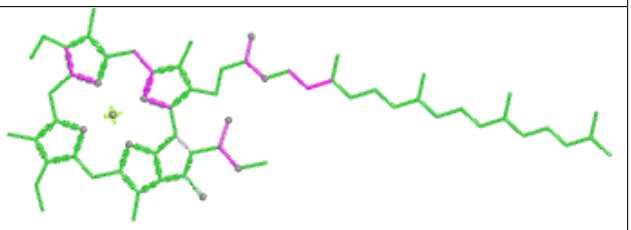
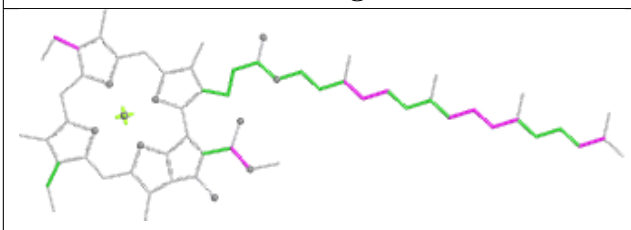


Bond angles



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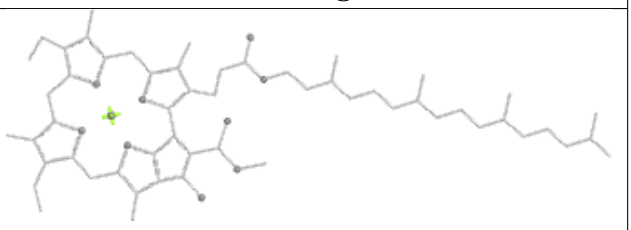
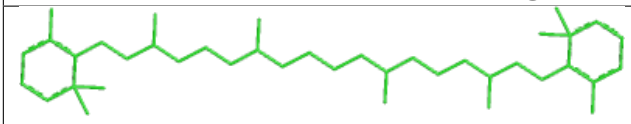


Rings

Ligand BCR F 309



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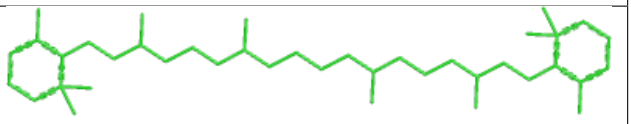
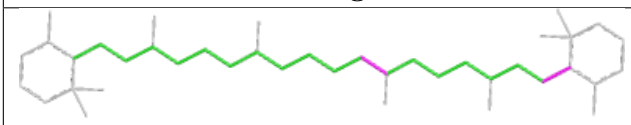


Bond angles



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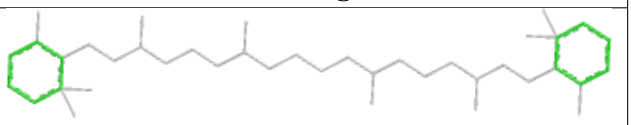
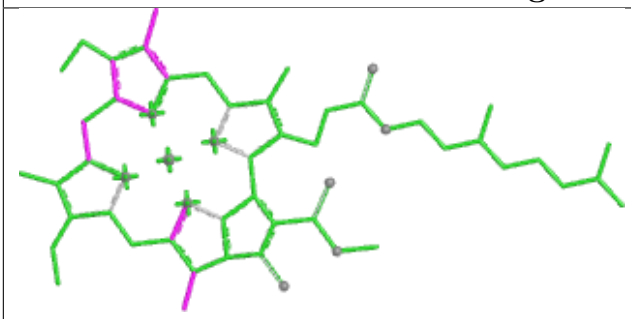


Rings

Ligand CLA 3 308



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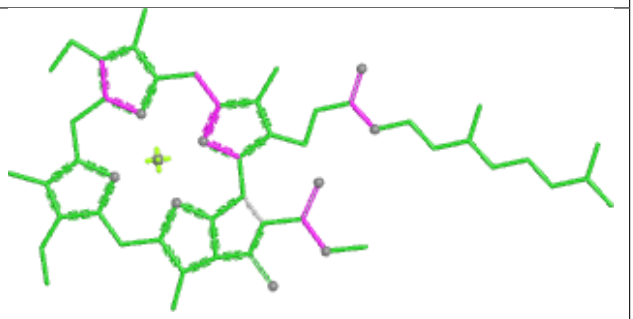
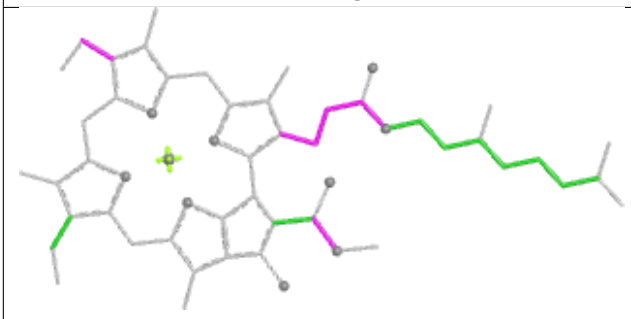


Bond angles



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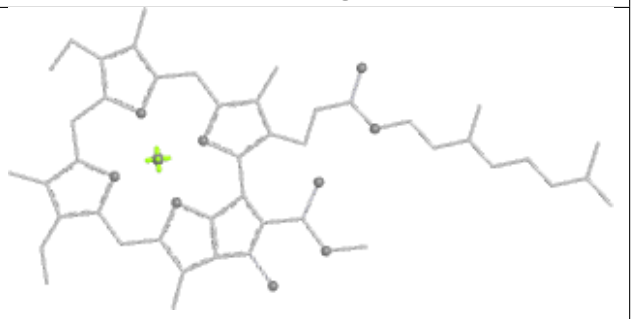
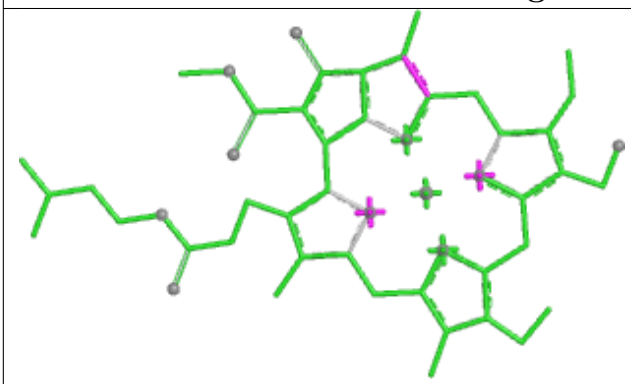


Rings

Ligand CHL 8 306



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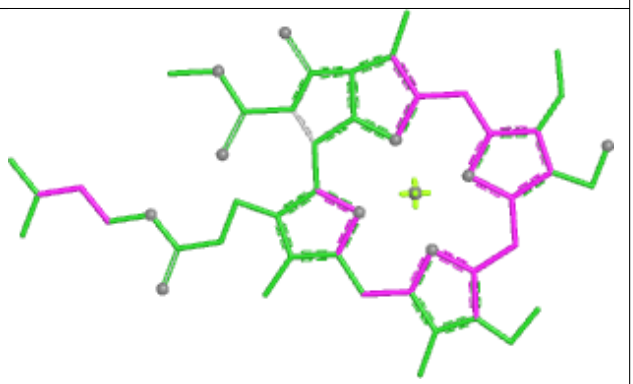
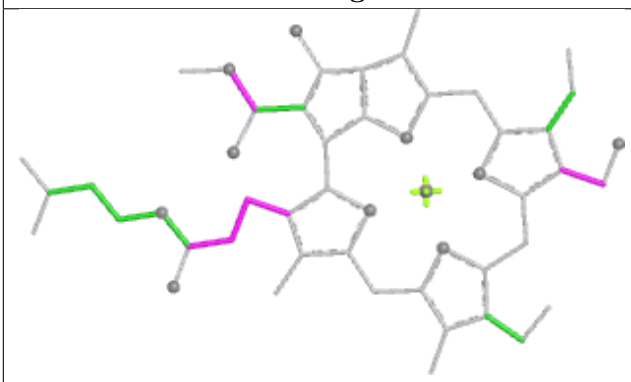


Bond angles



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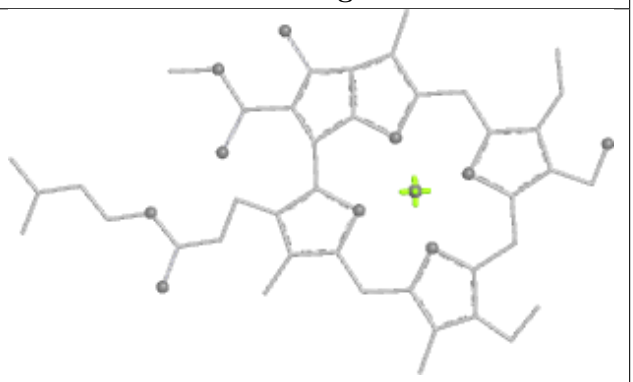
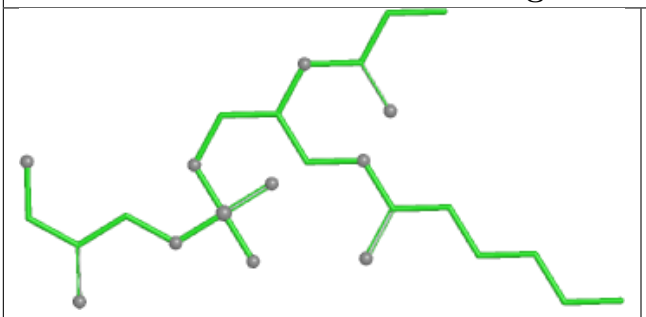
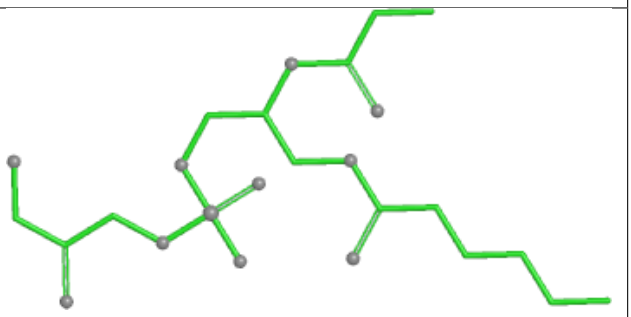


Rings

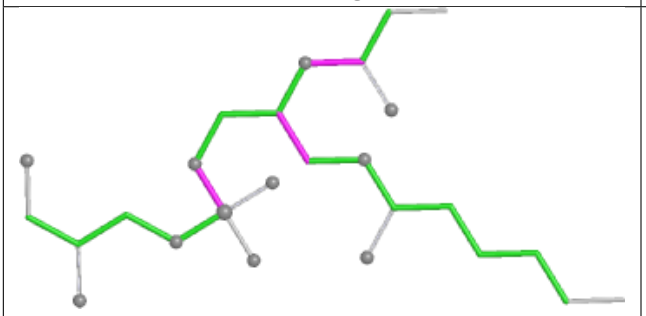
Ligand LHG 1 618



Bond lengths



Bond angles



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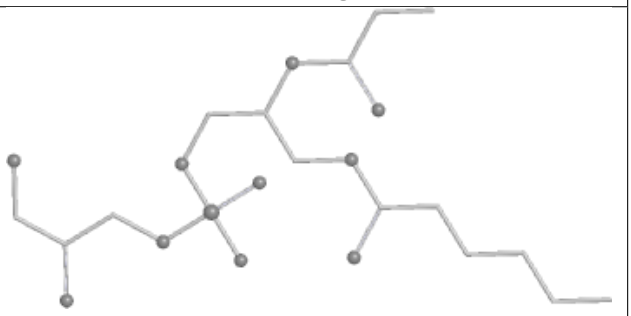
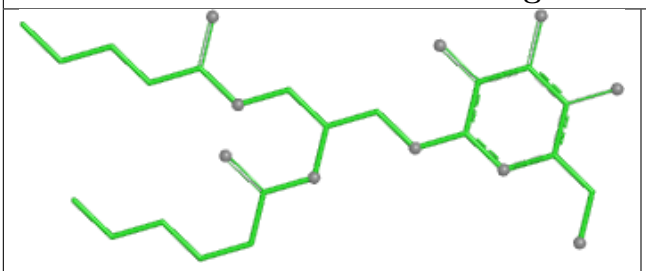
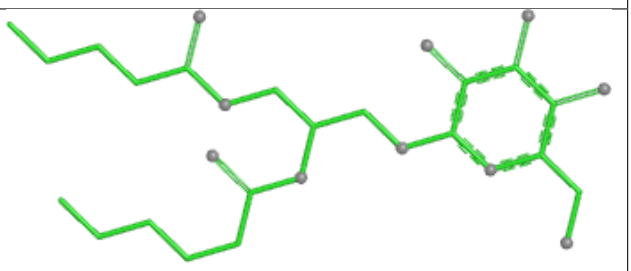


Rings

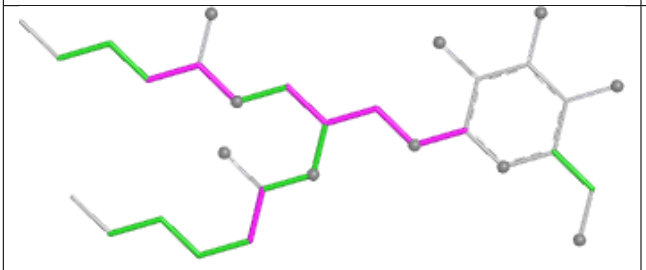
Ligand LMG 7 324



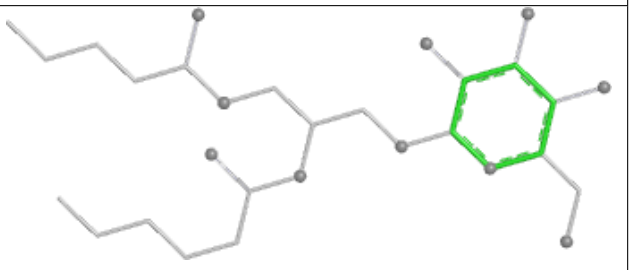
Bond lengths



Bond angles

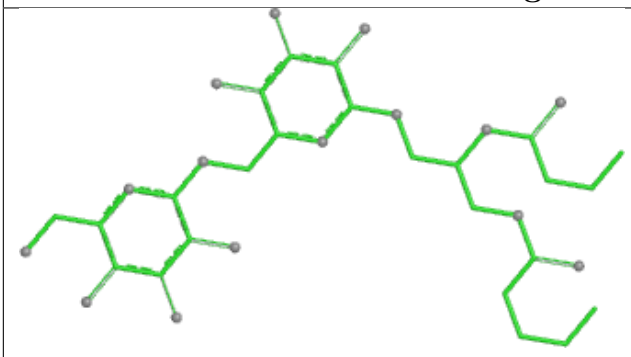


Torsions



Rings

Ligand DGD 7 321



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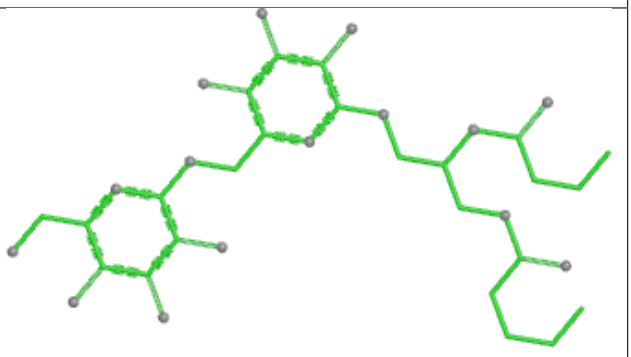

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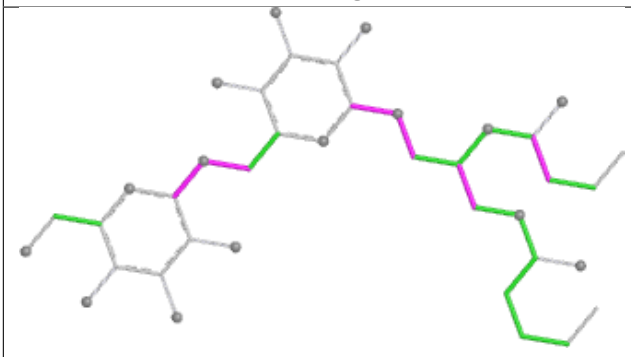

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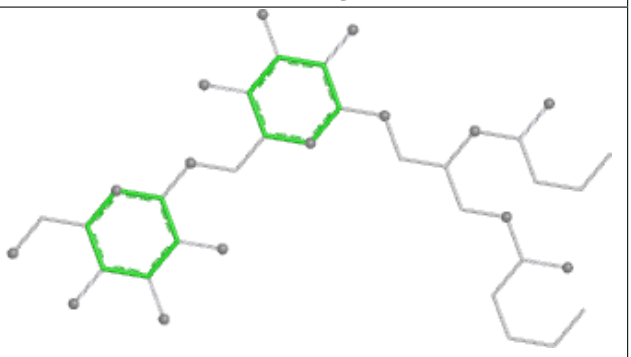
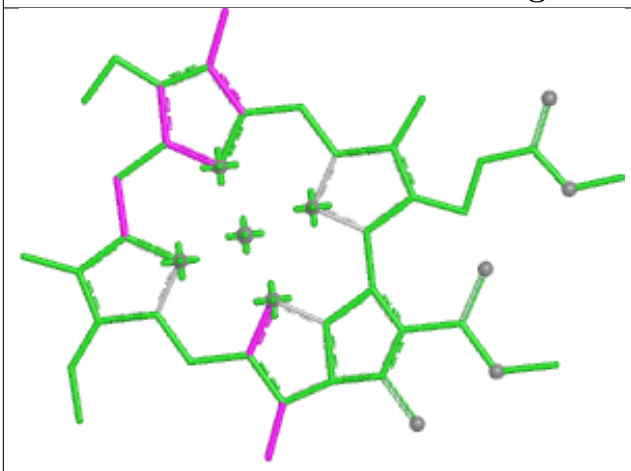


Rings

Ligand CLA 2 301



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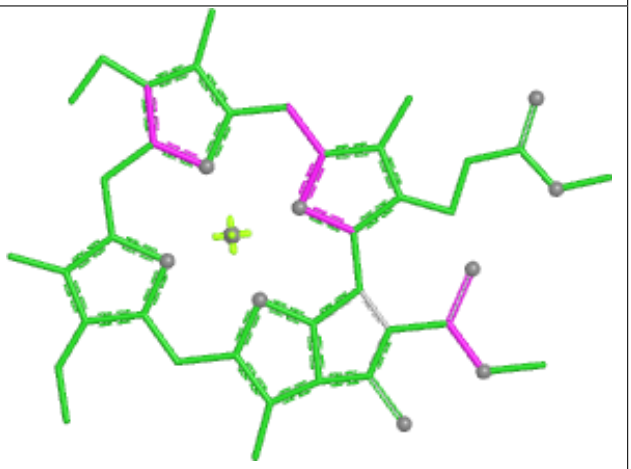
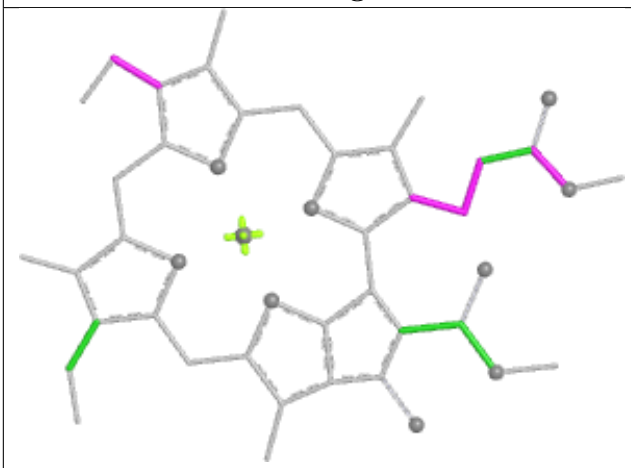


Bond angles



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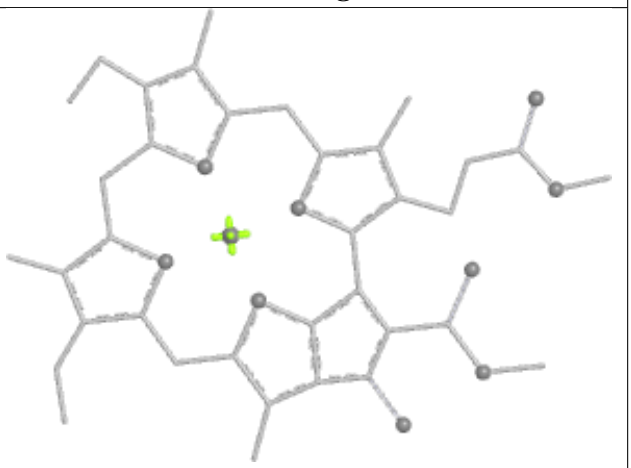
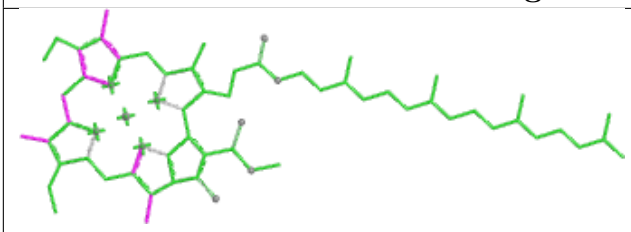


Rings

Ligand CLA B 815



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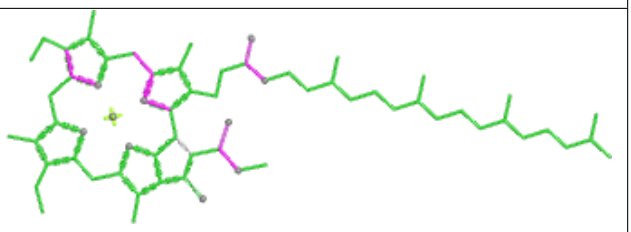

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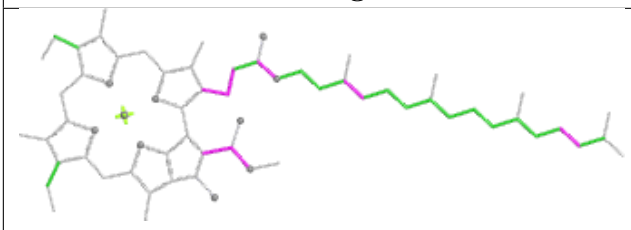

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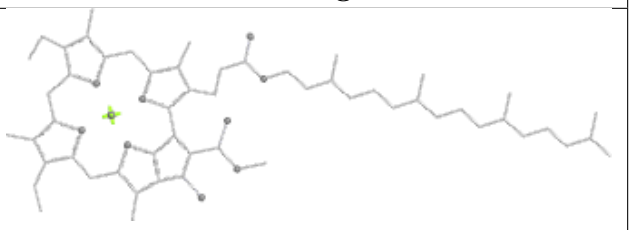
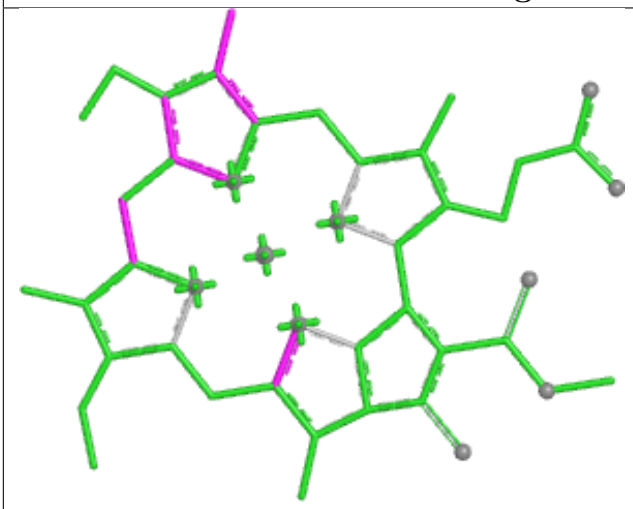


Rings

Ligand CLA K 4002



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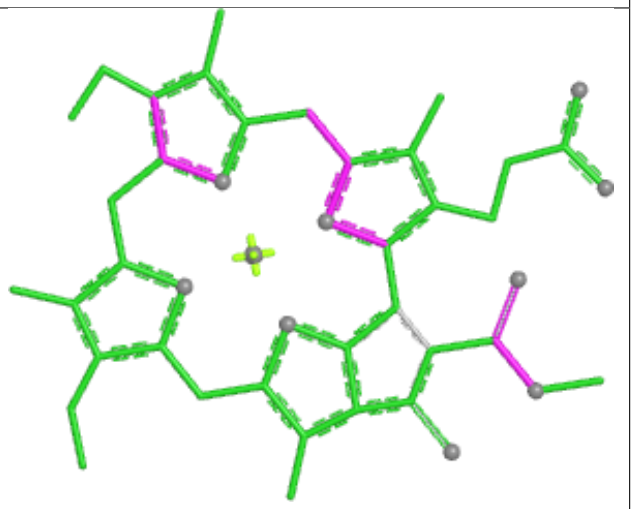

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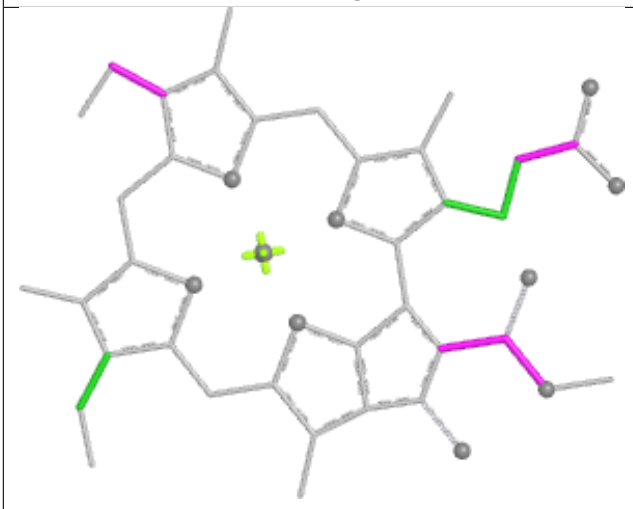
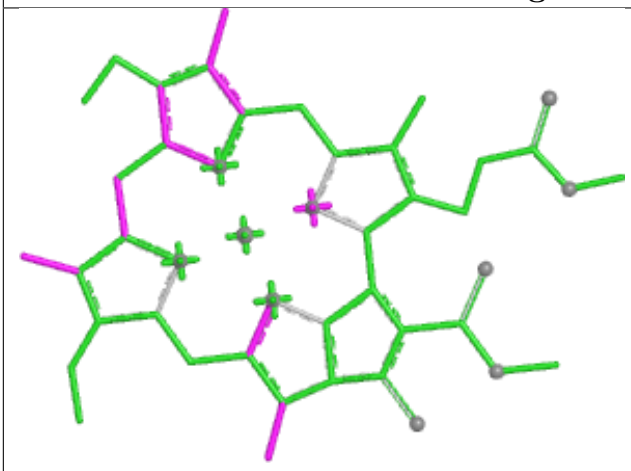


Torsions



Rings

Ligand CLA 3 310



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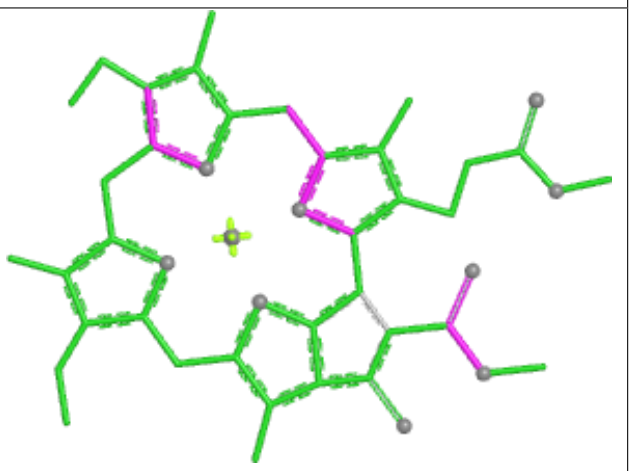

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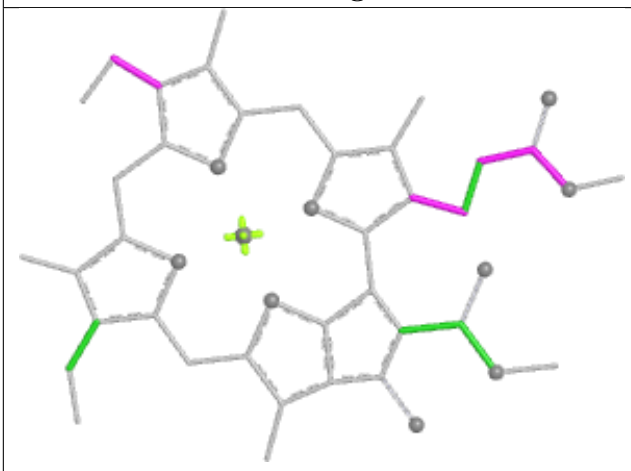

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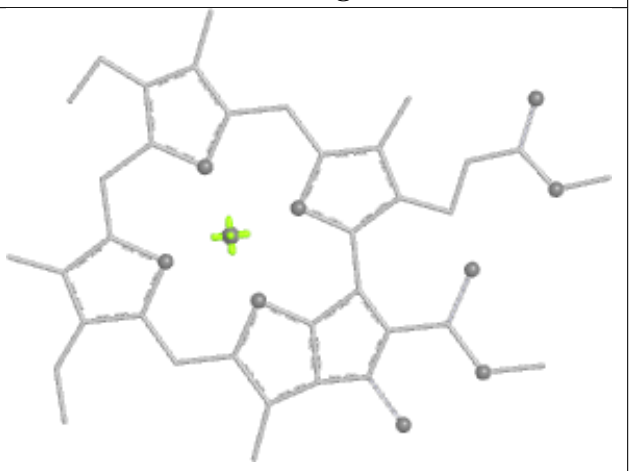
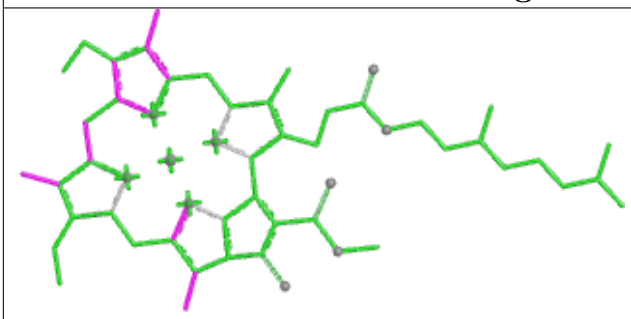
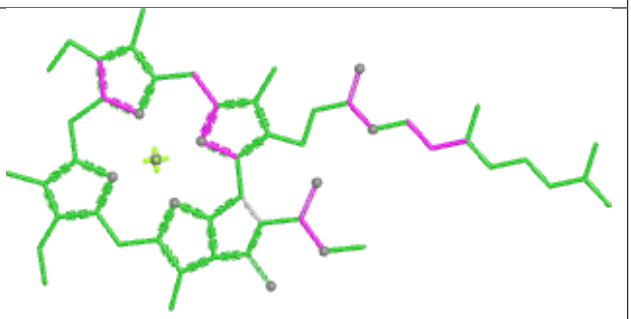
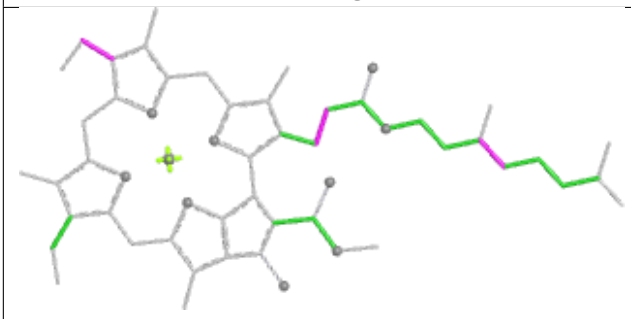
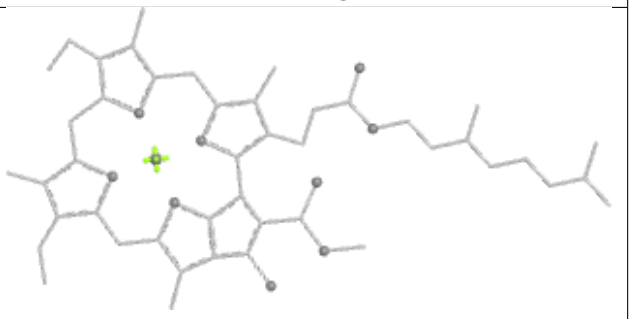


Rings

Ligand CLA A 5039	
 Bond lengths	 Bond angles
 Torsions	 Rings

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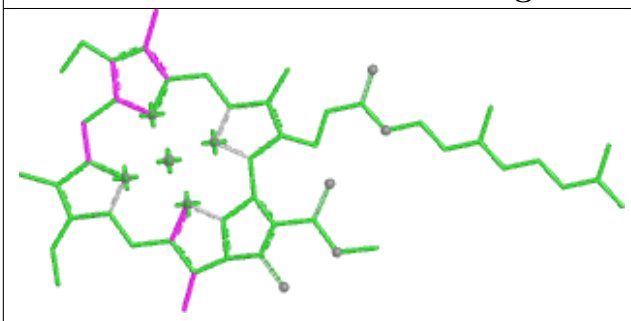
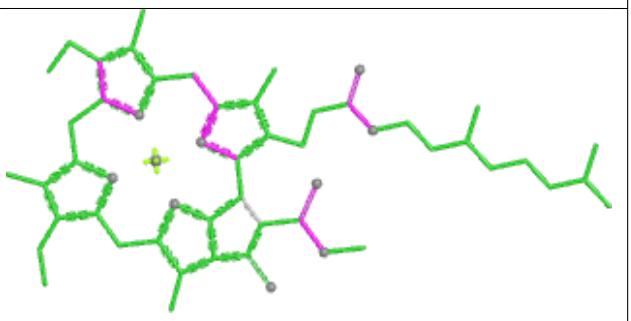
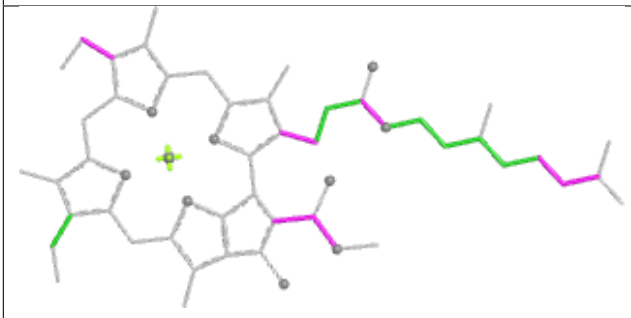
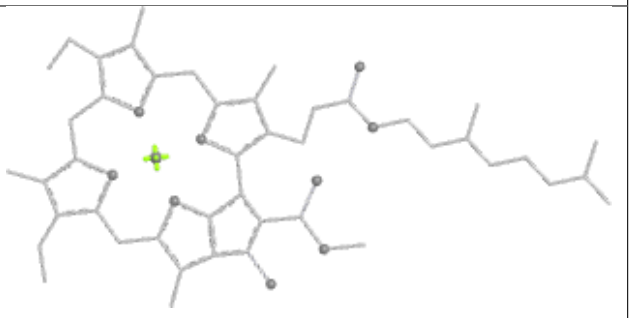
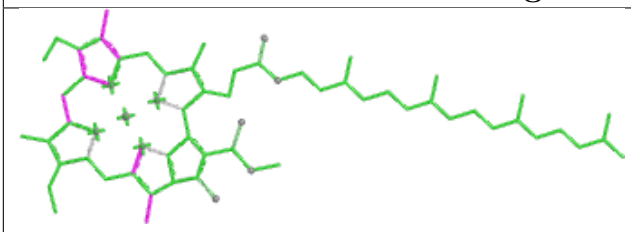
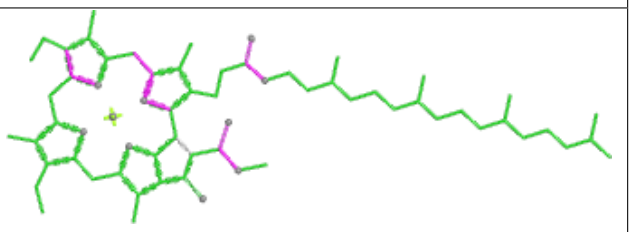
 Bond lengths	 Bond angles
 Torsions	 Rings

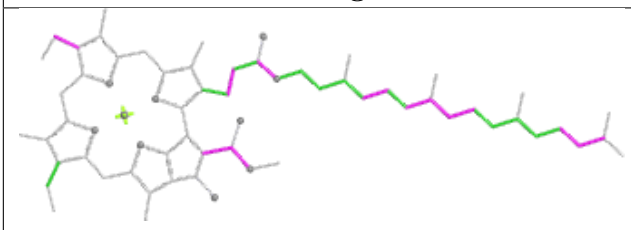
Ligand CLA B 809



Bond lengths



Bond angles



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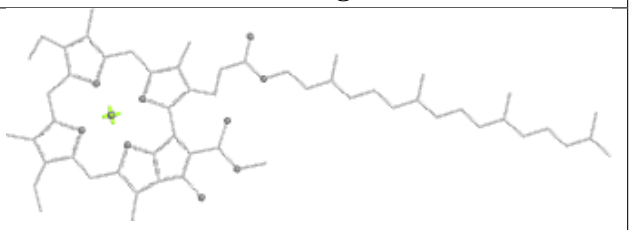
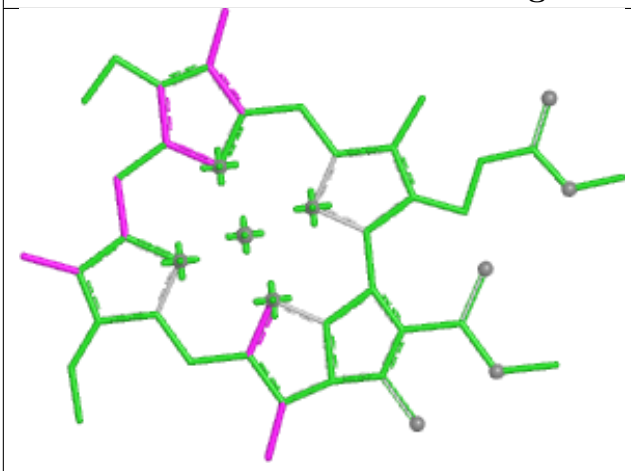


Rings

Ligand CLA 1 611



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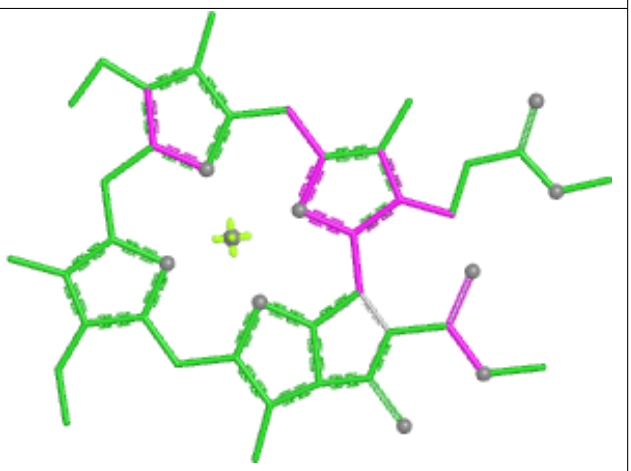
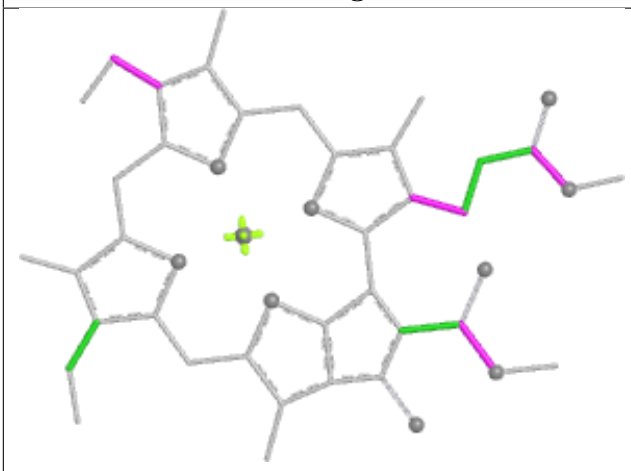


Bond angles



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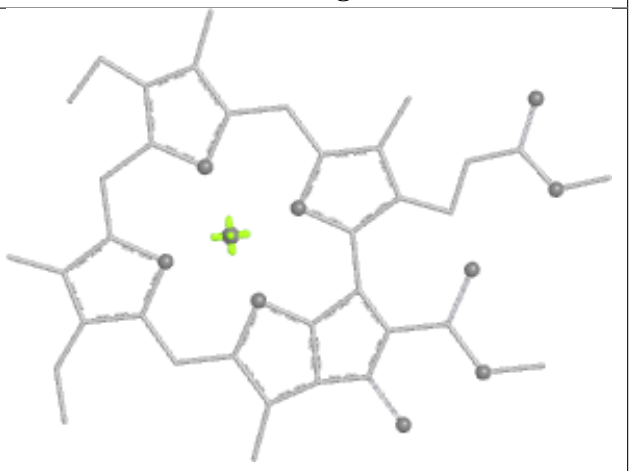
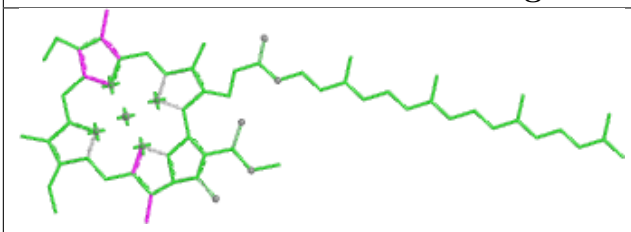


Rings

Ligand CLA B 839



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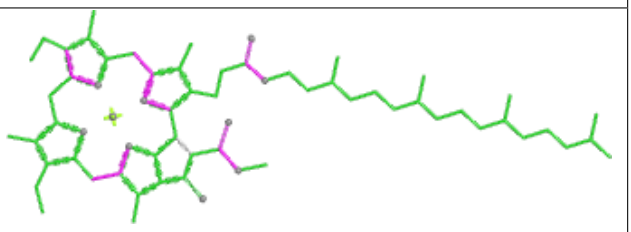
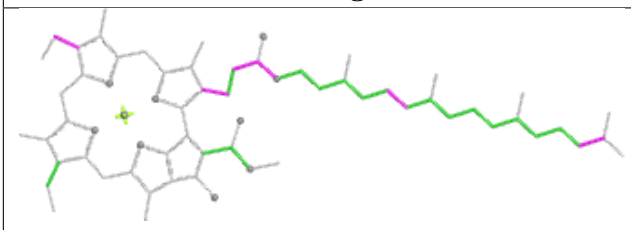


Bond angles



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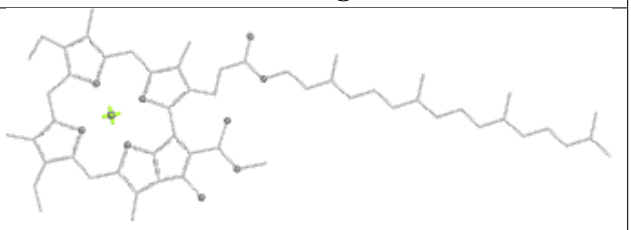
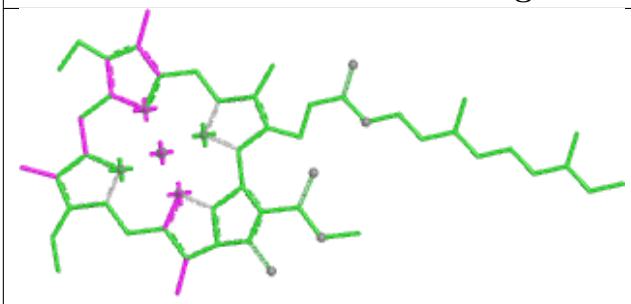


Rings

Ligand CLA A 5027



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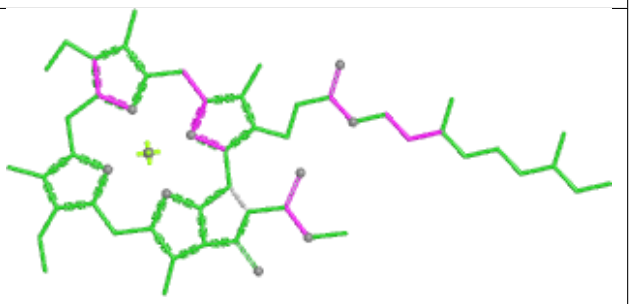
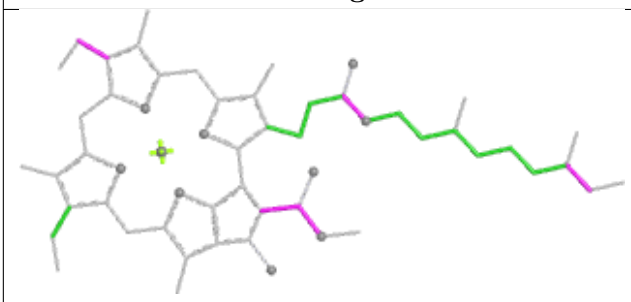


Bond angles



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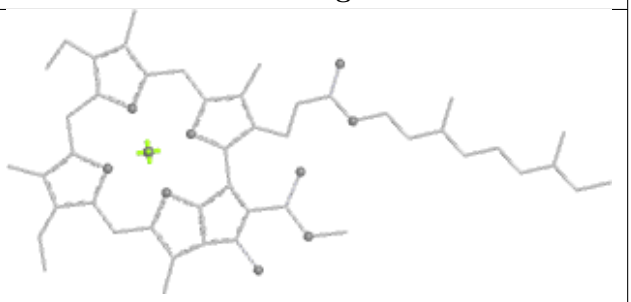
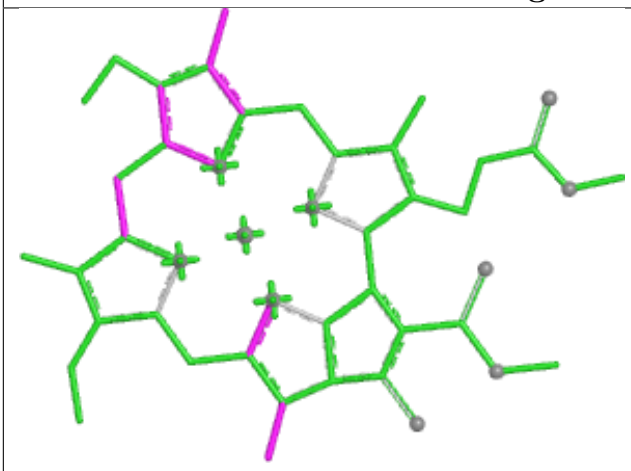


Rings

Ligand CLA 3 314



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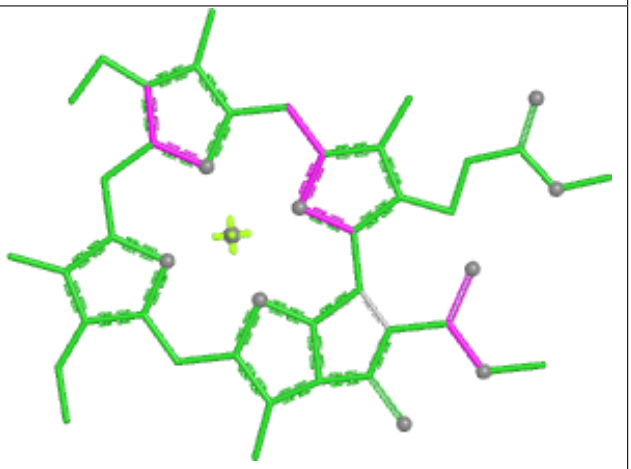
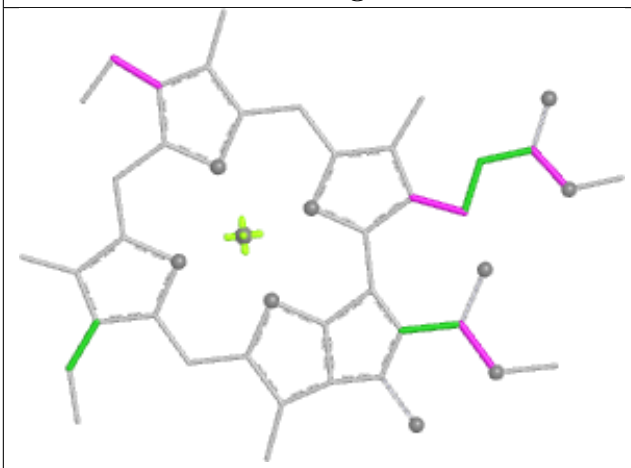


Bond angles



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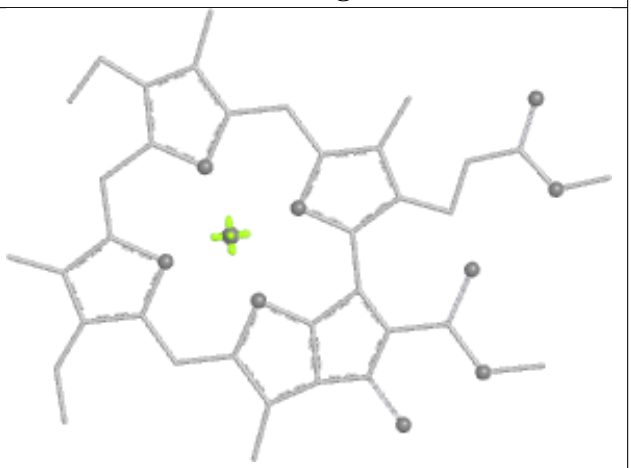
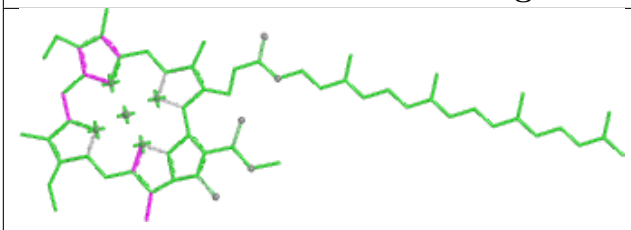


Rings

Ligand CLA A 5031



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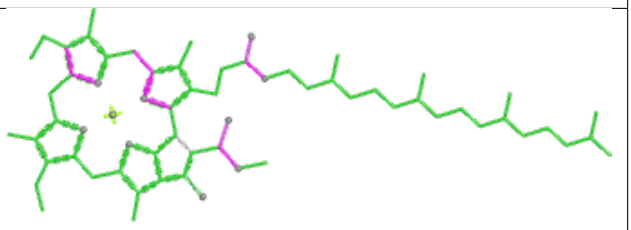
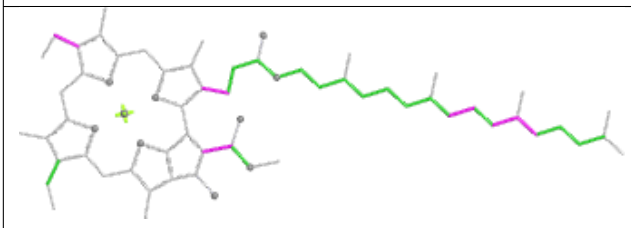


Bond angles



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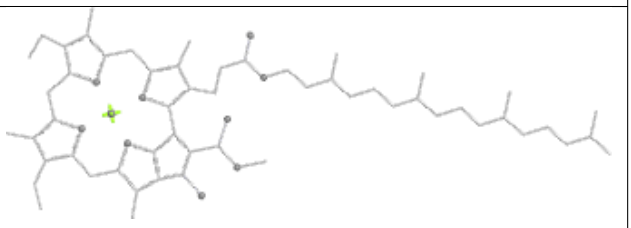
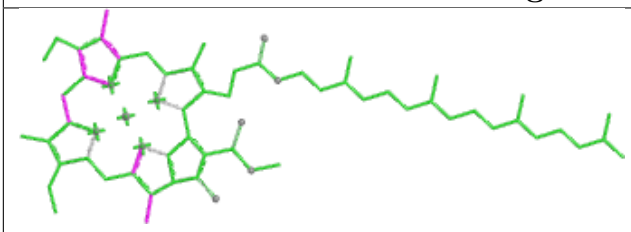


Rings

Ligand CLA L 204



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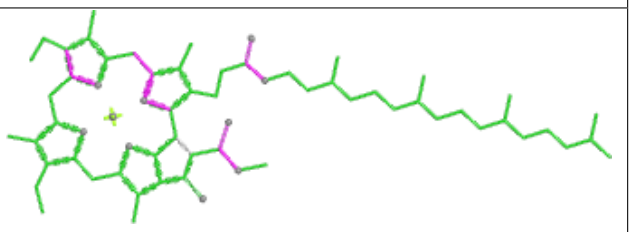
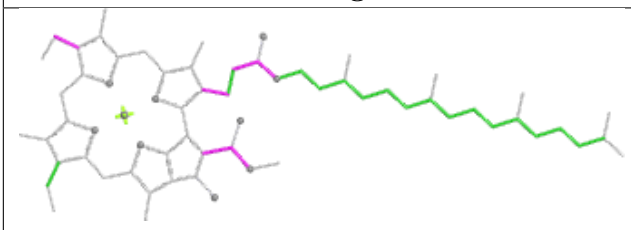


Bond angles



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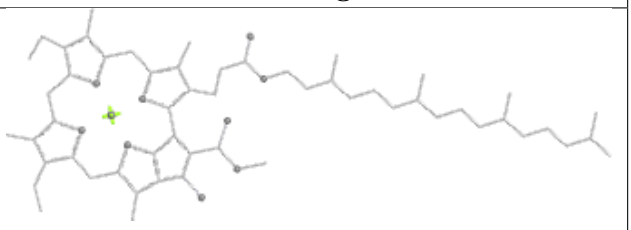
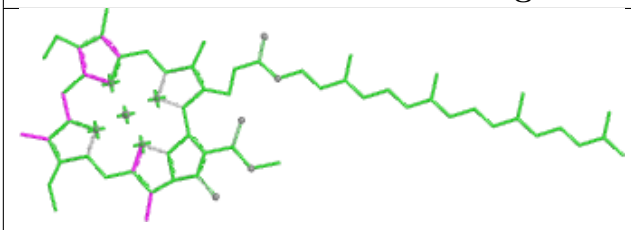


Rings

Ligand CLA A 5007



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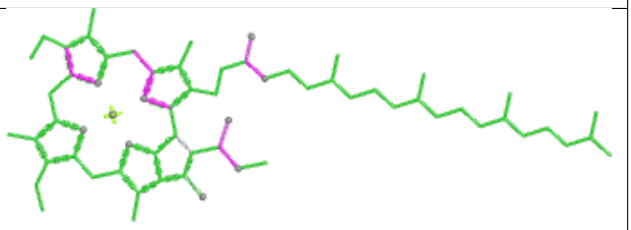

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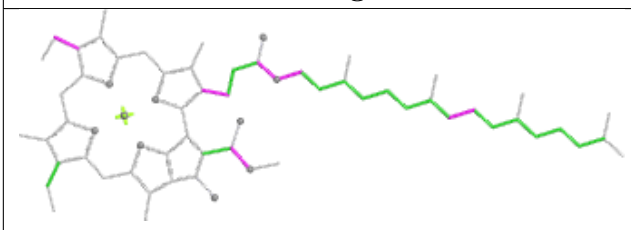
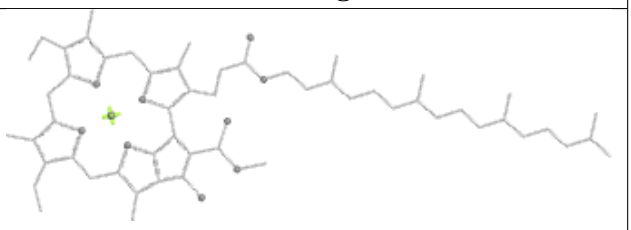
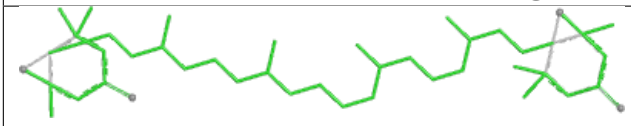


Torsions



Rings

Ligand XAT 8 315



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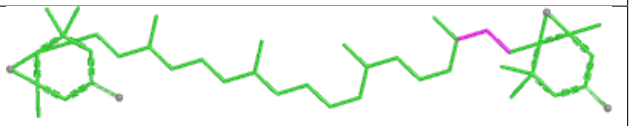

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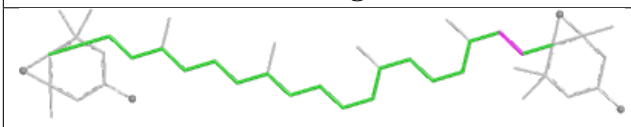

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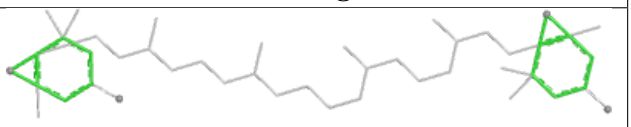
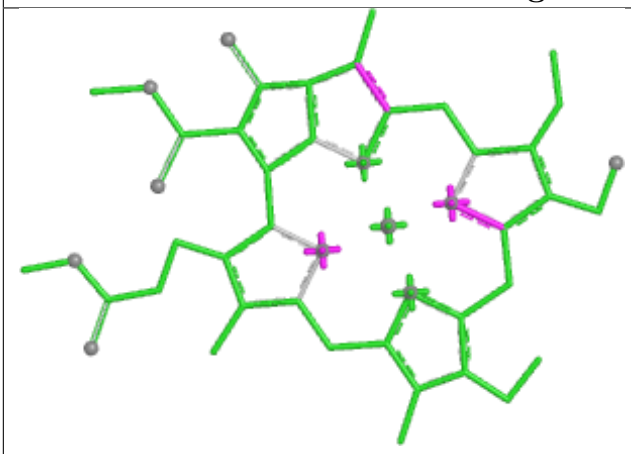


Rings

Ligand CHL 2 306



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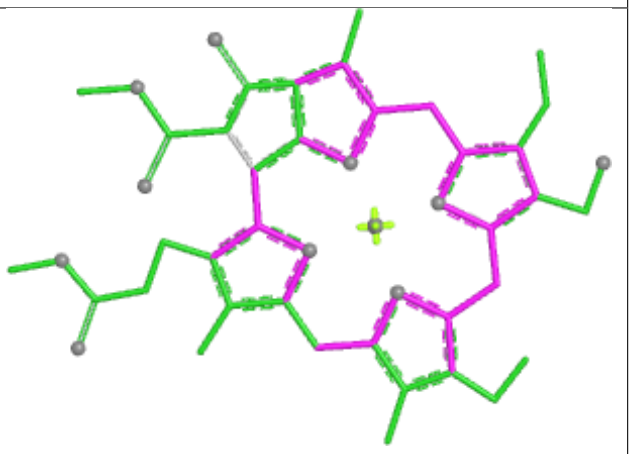

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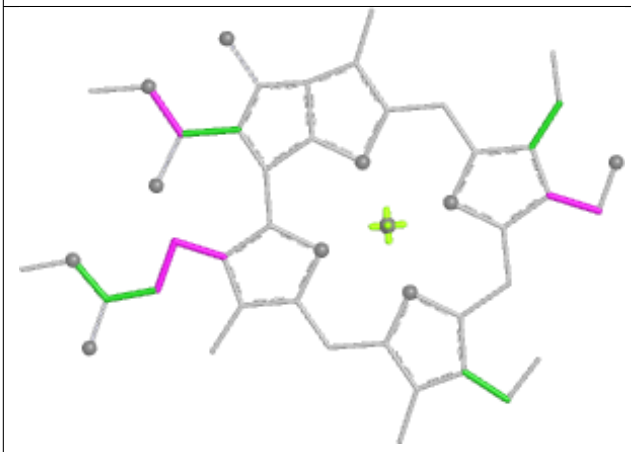

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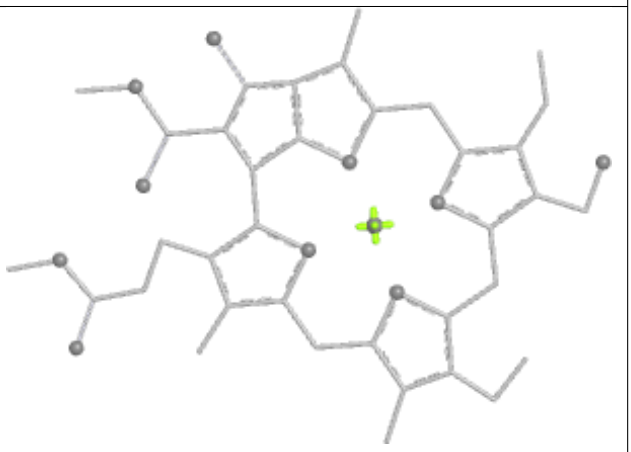
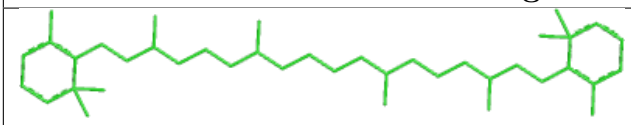


Rings

Ligand BCR B 847



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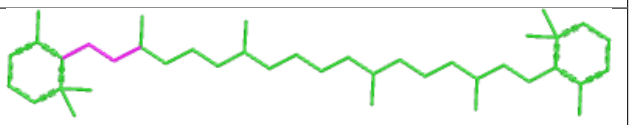

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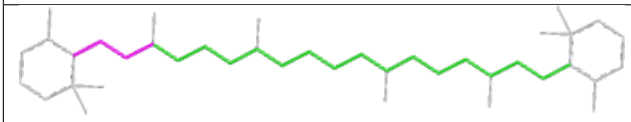

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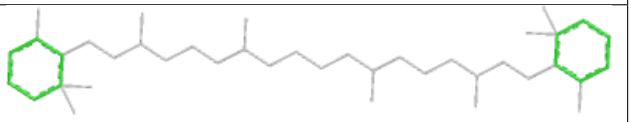
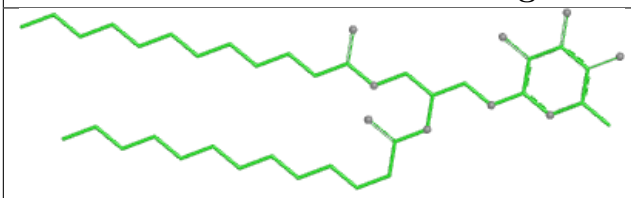


Rings

Ligand LMG G 206



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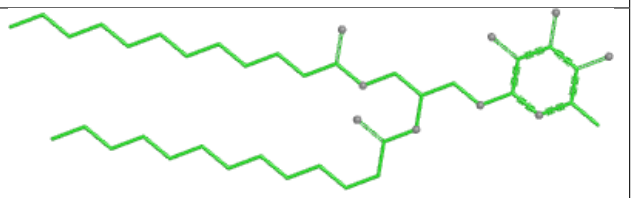

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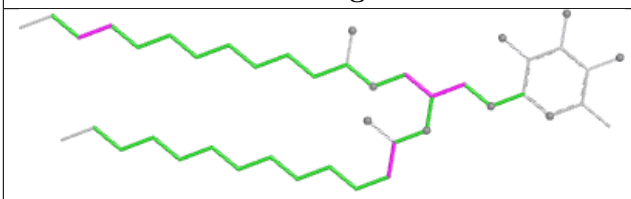

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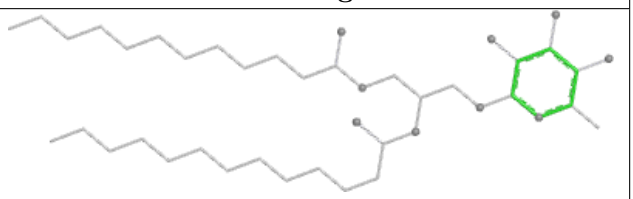
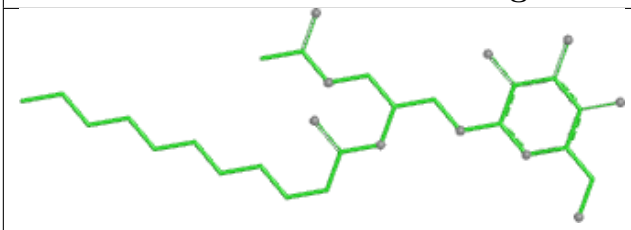


Rings

Ligand LMG A 5001



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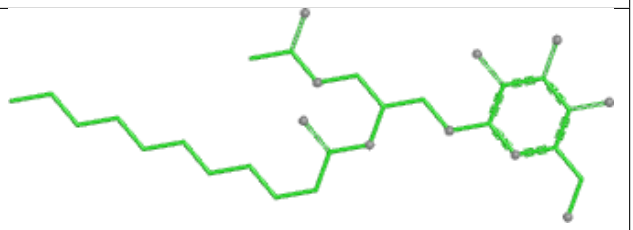

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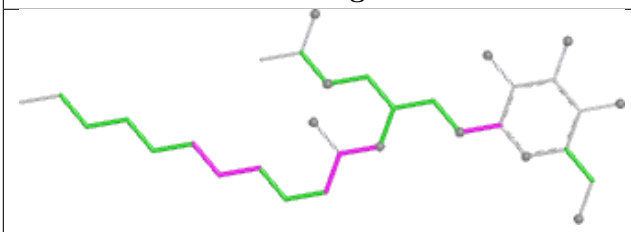

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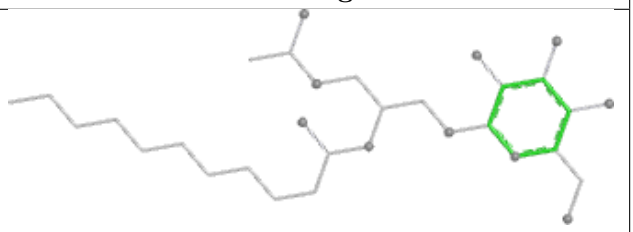
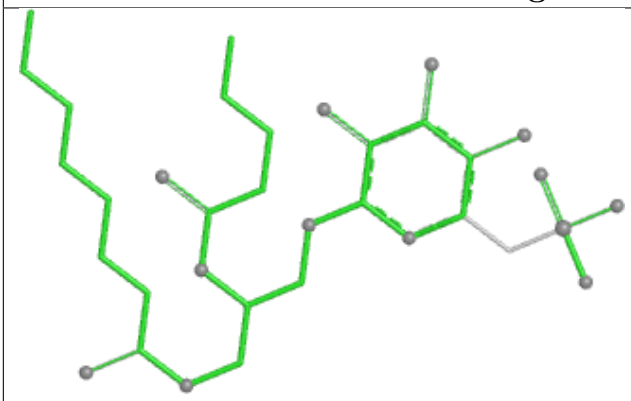


Rings

Ligand SQD 3 320



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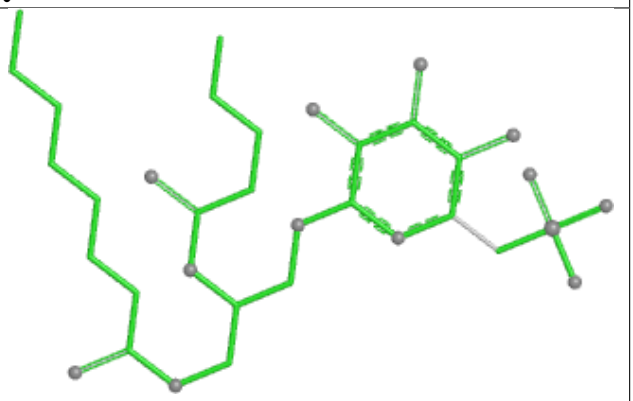

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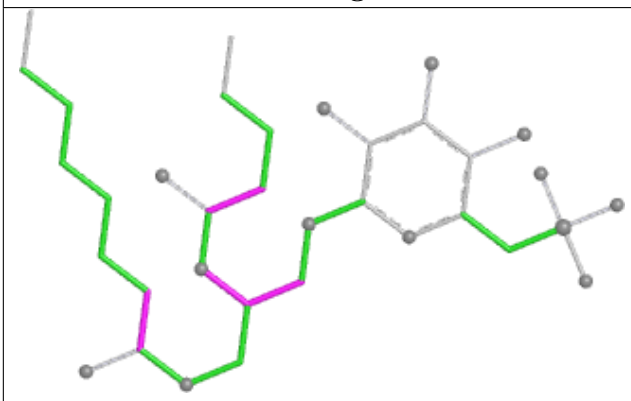

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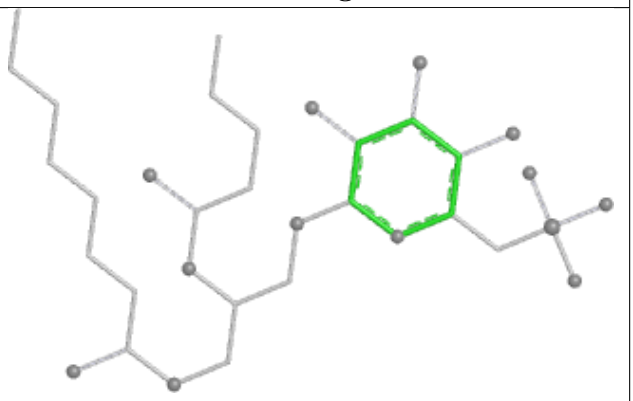
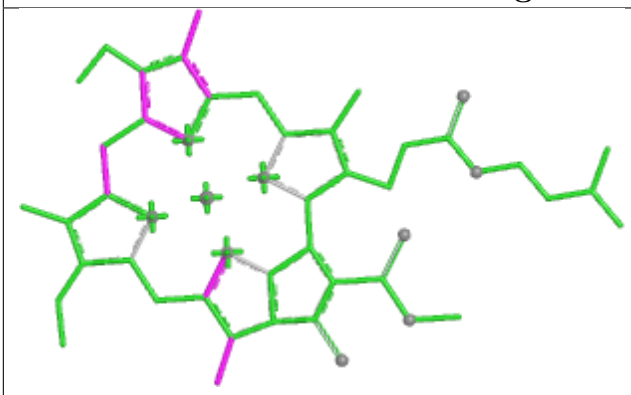


Rings

Ligand CLA A 5037



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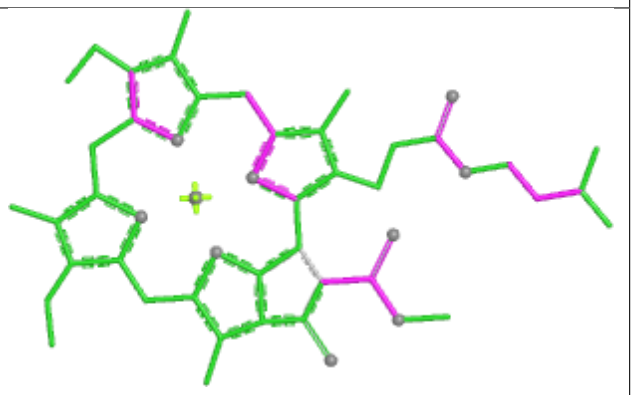

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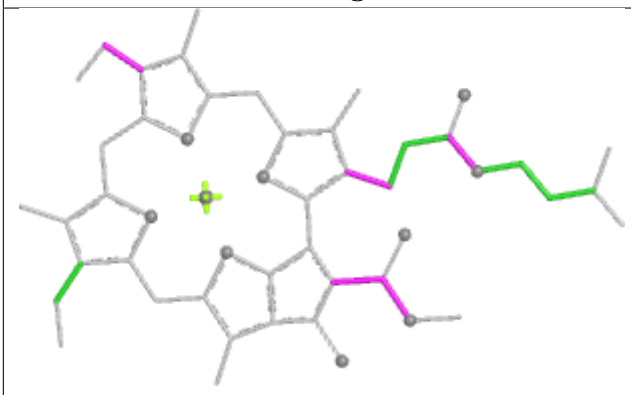

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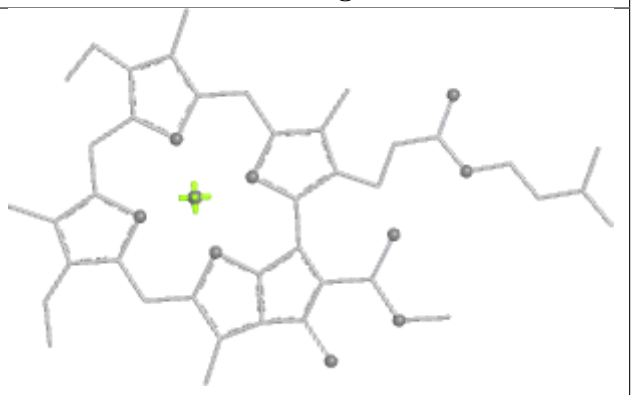
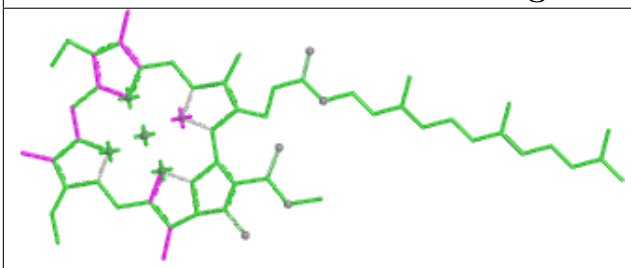


Rings

Ligand CLA 8 309



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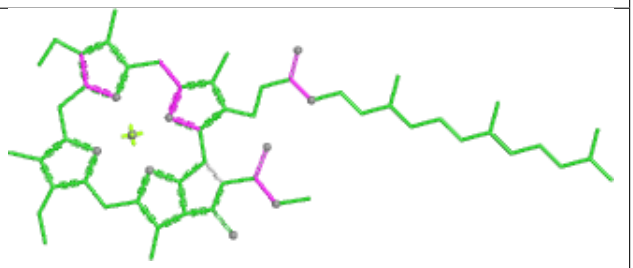

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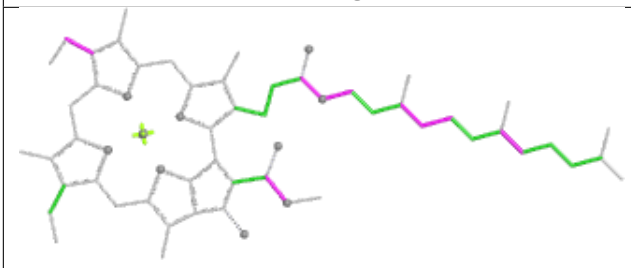

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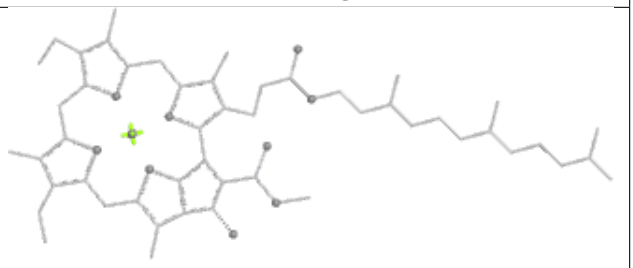
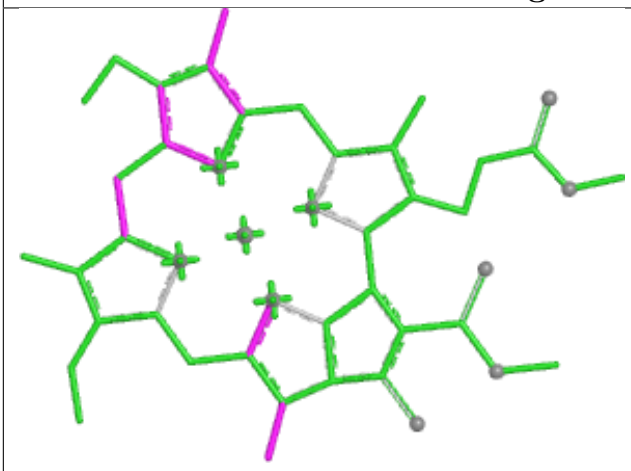


Rings

Ligand CLA 2 307



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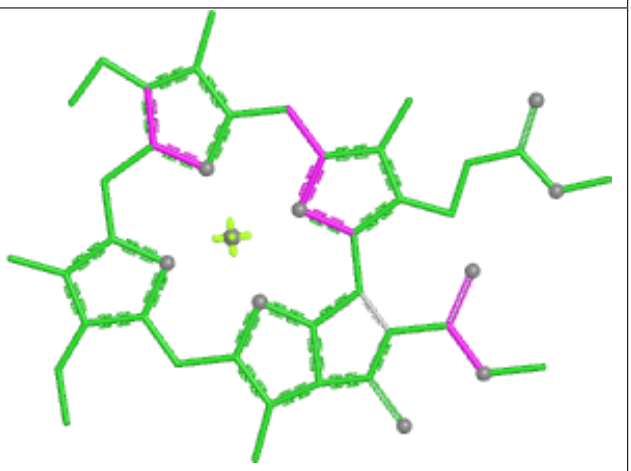

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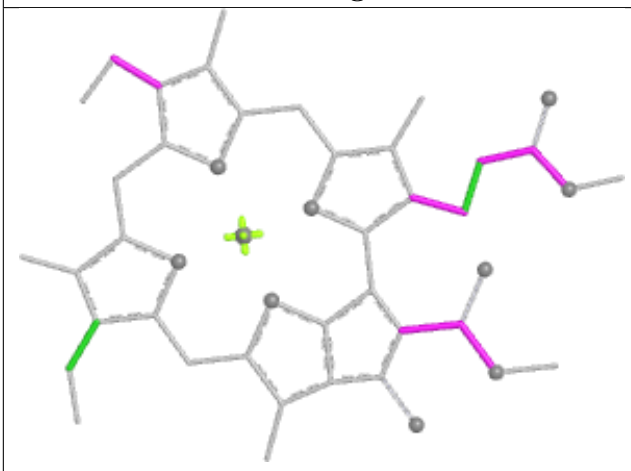

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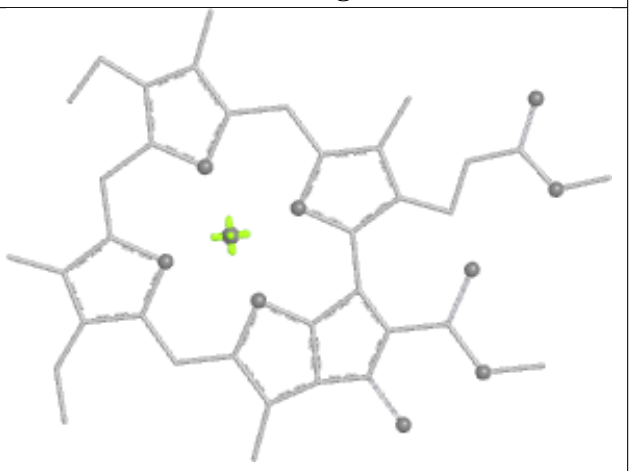

Rings

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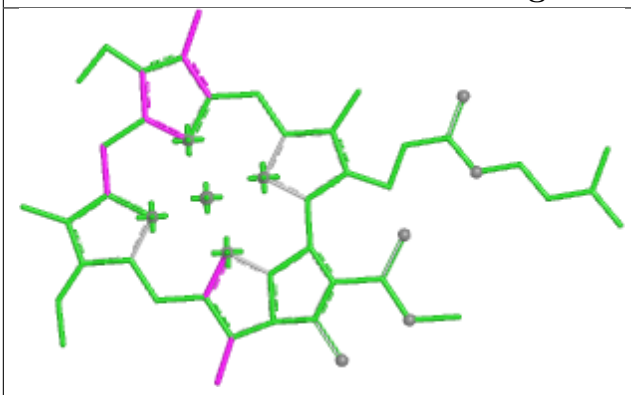

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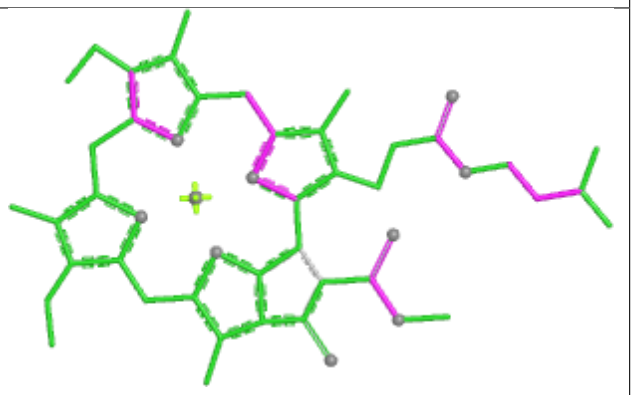

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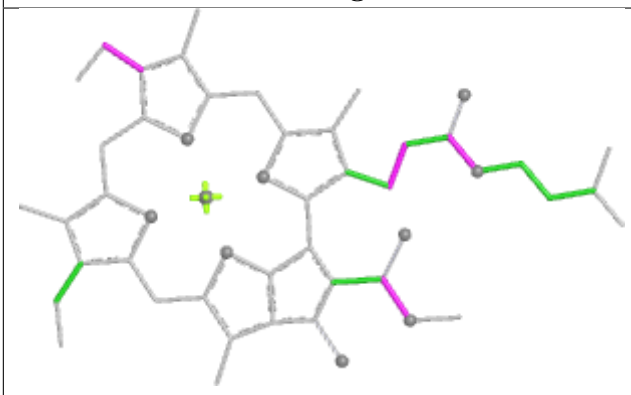

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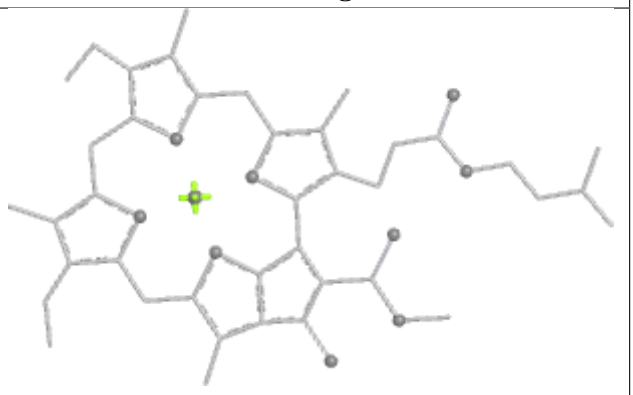
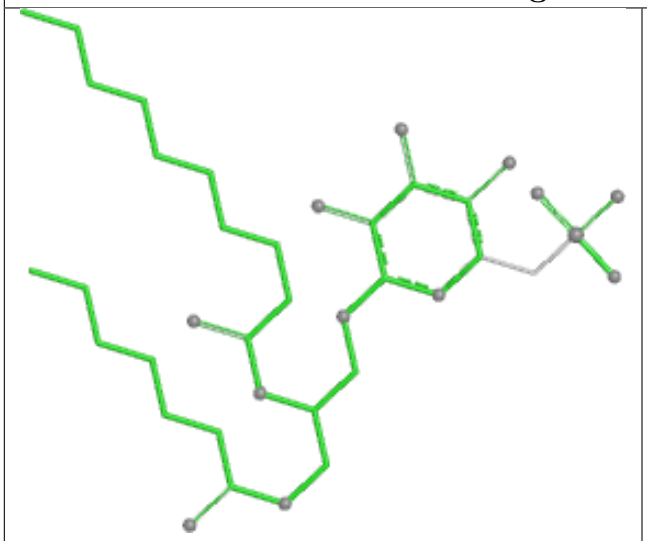


Rings

Ligand SQD 7 322



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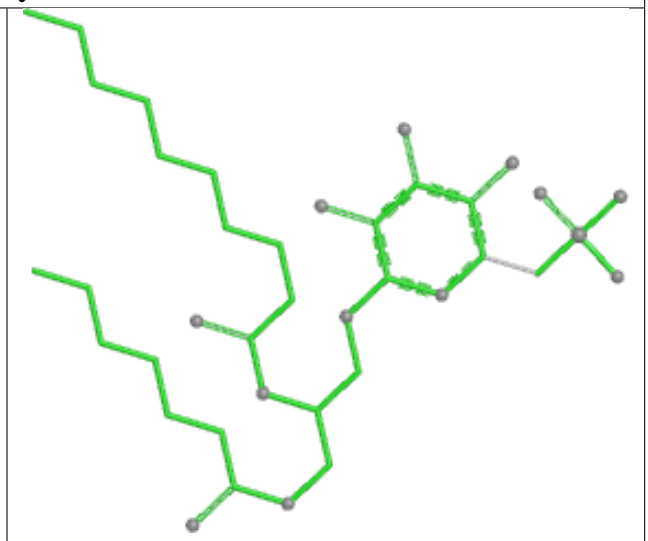

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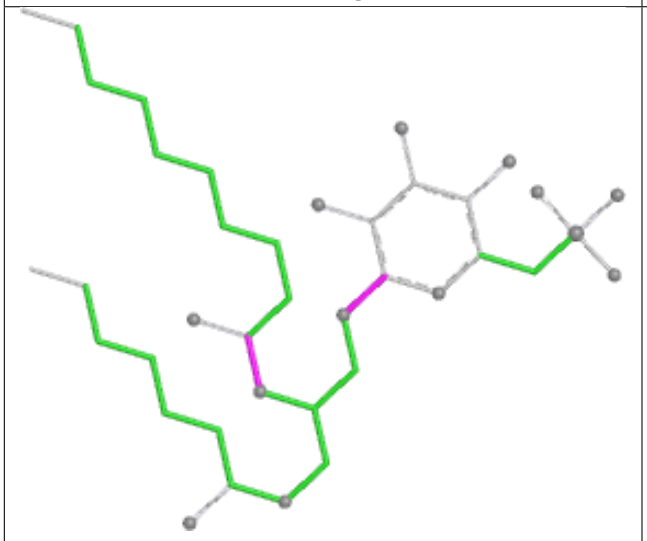

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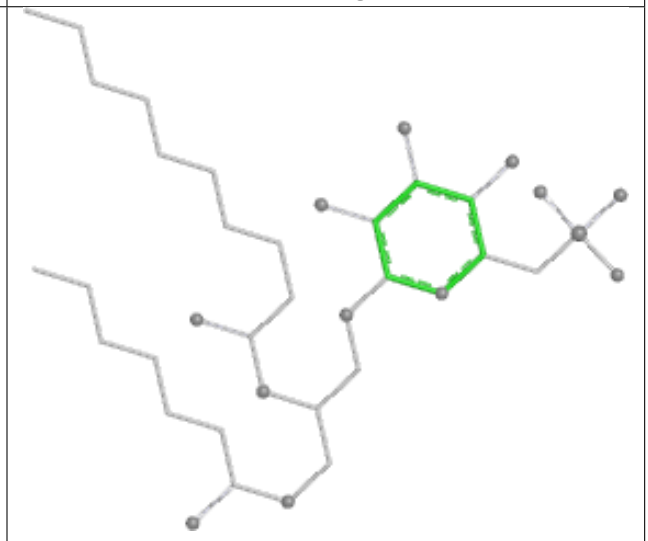
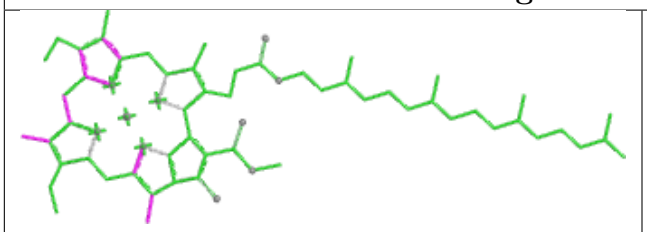


Rings

Ligand CLA A 5012



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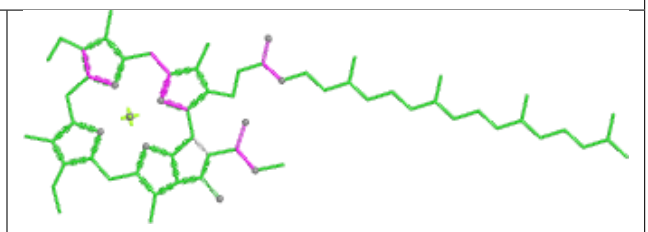

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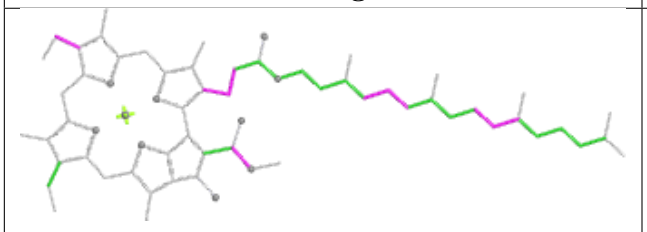

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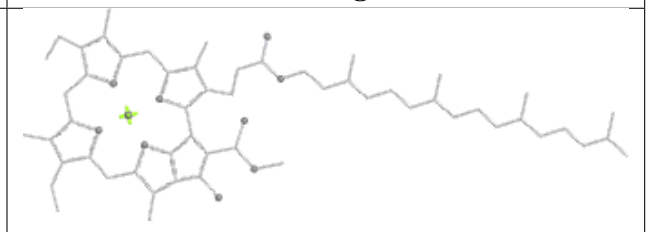
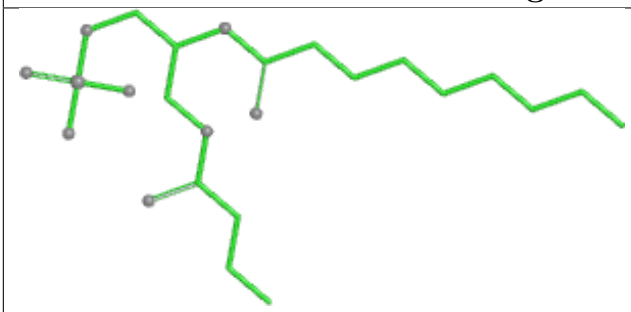


Rings

Ligand LHG 2 316



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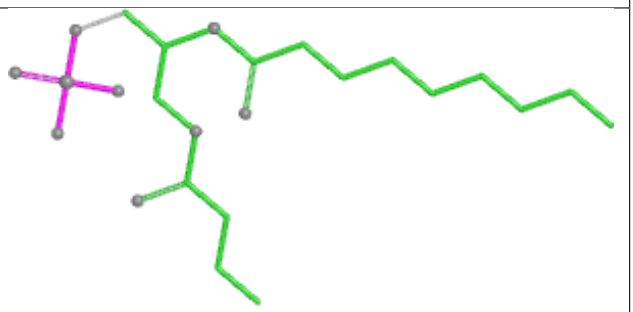
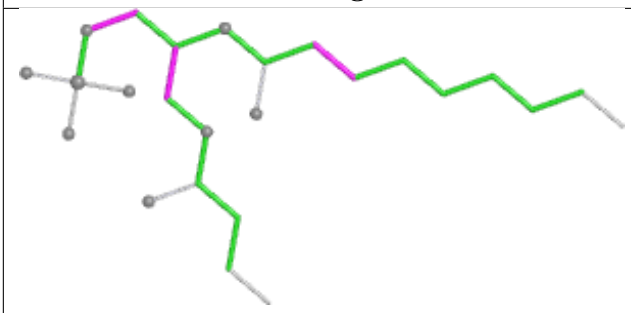


Bond angles



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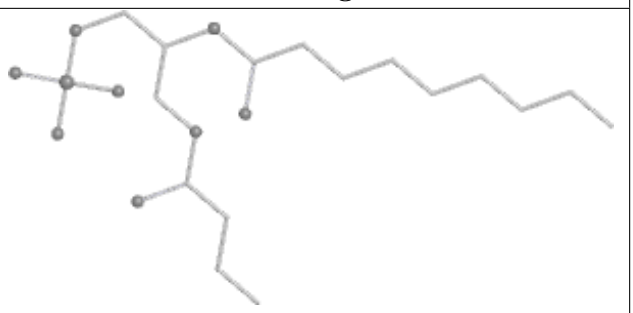
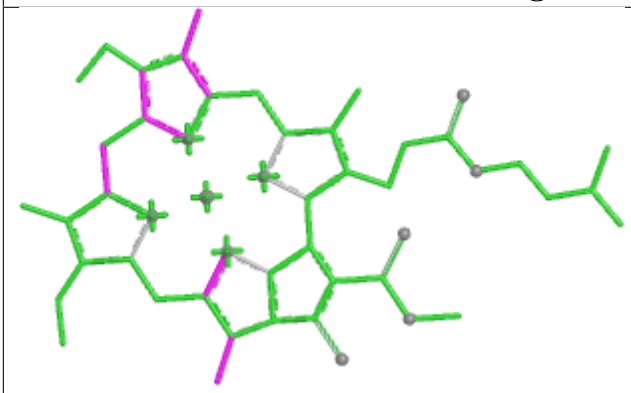


Rings

Ligand CLA 1 607



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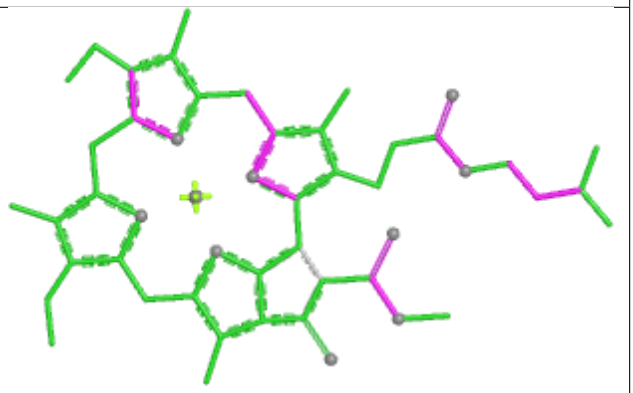
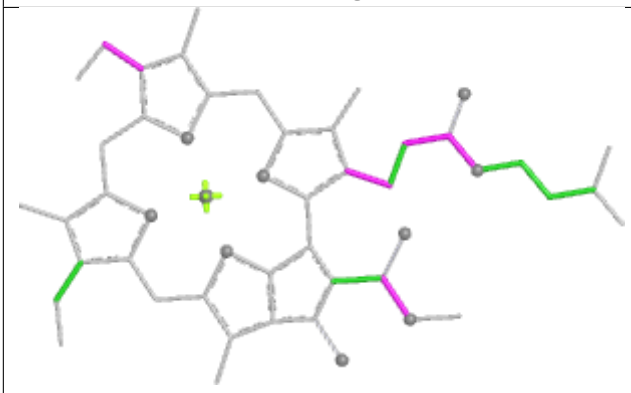
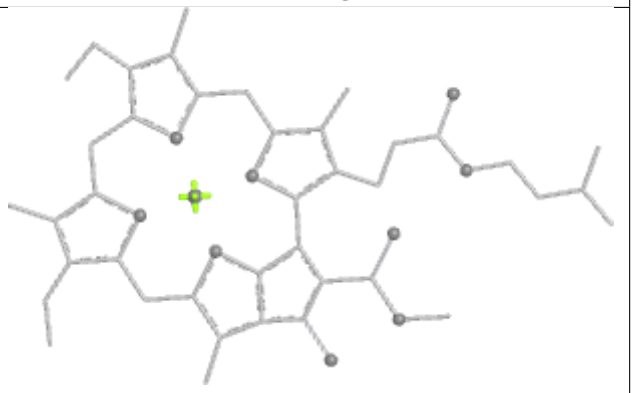


Bond angles

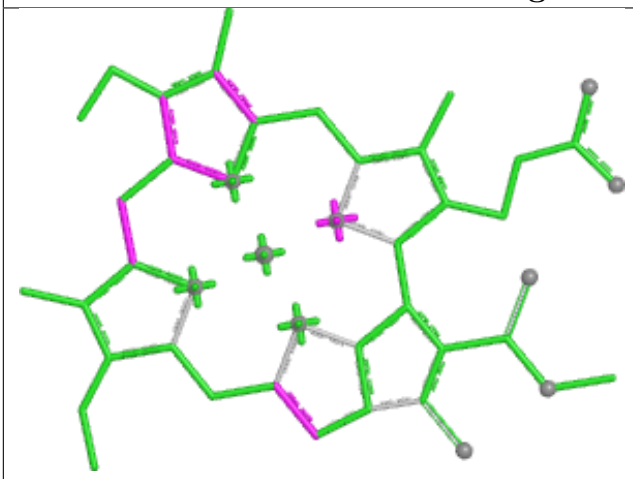


Torsions



Rings

Ligand CLA 2 312



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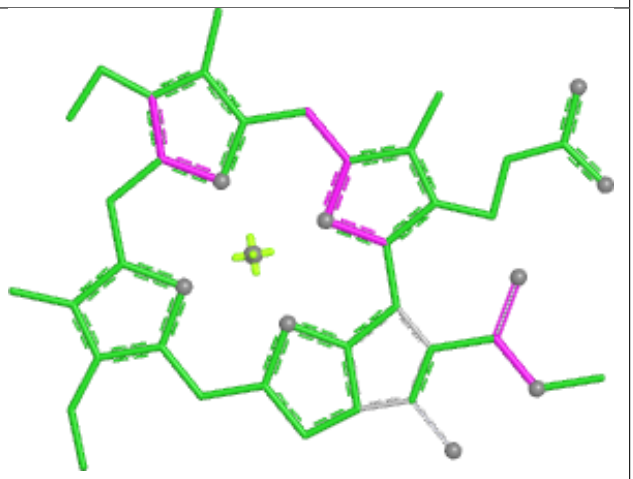
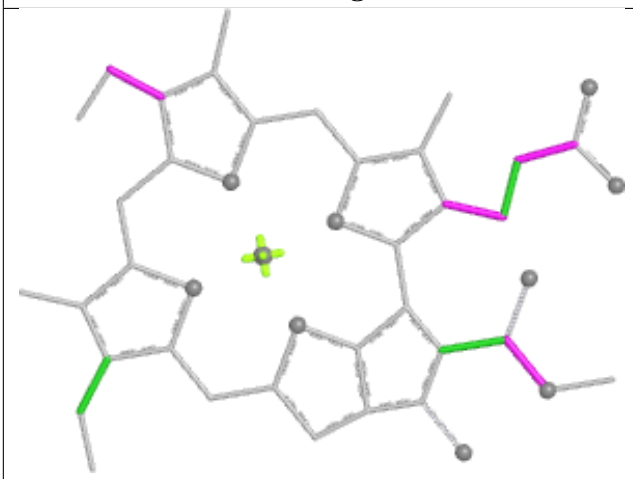


Bond angles

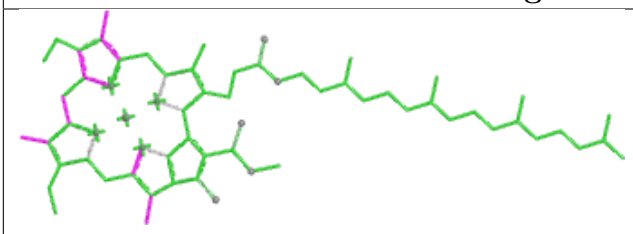


Torsions



Rings

Ligand CLA B 818



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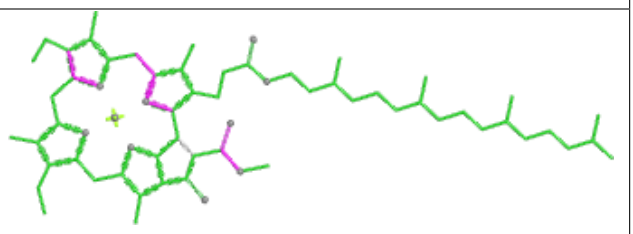

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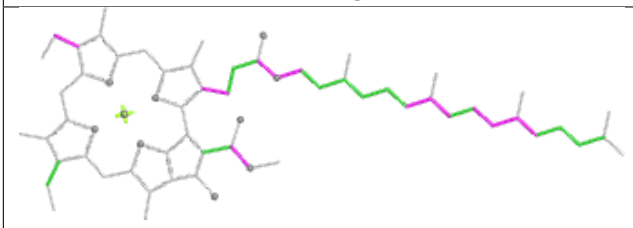

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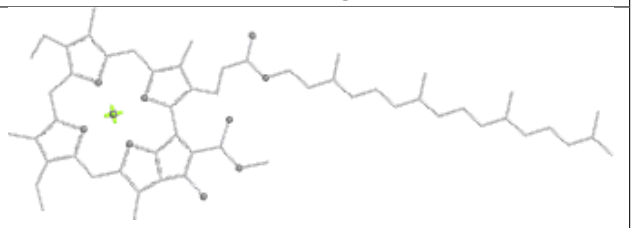
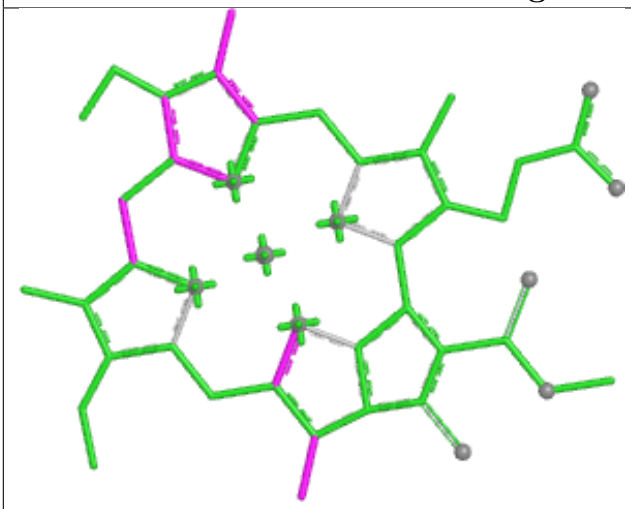


Rings

Ligand CLA 7 315



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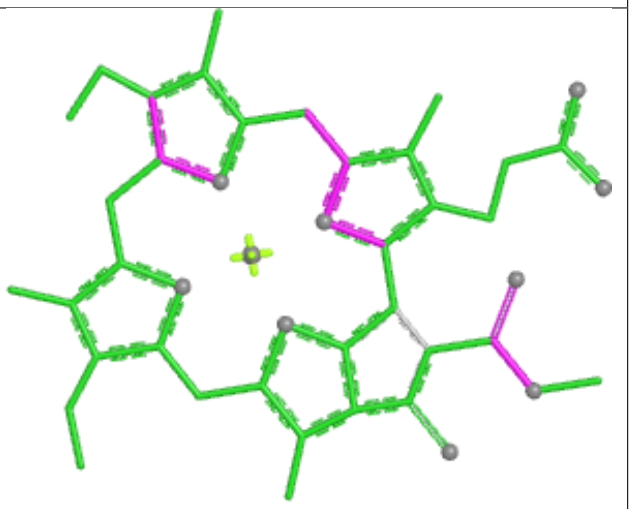
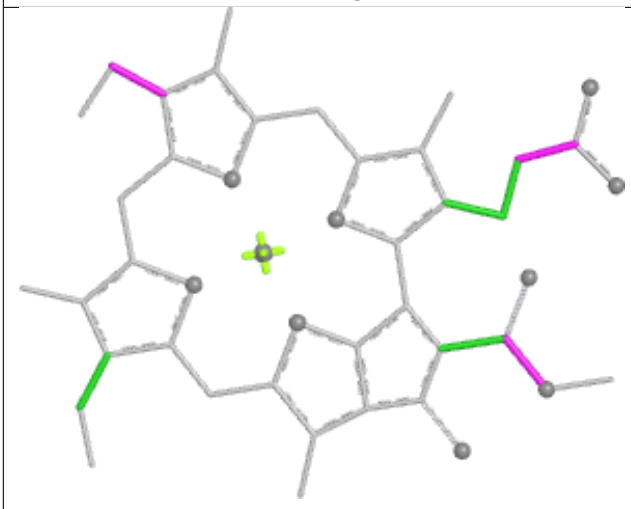


Bond angles

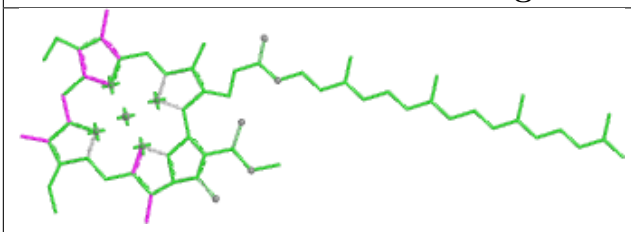


Torsions



Rings

Ligand CLA A 5004



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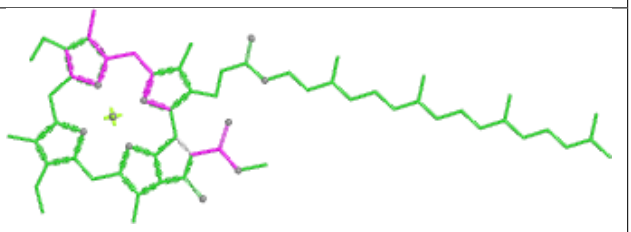
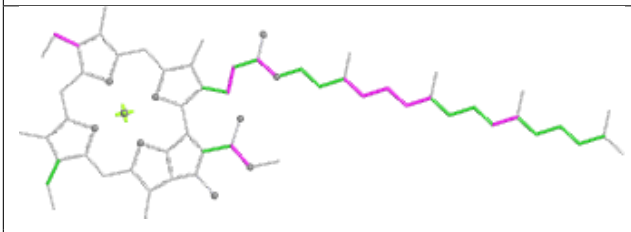


Bond angles



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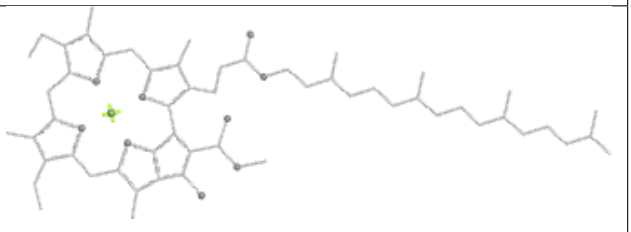
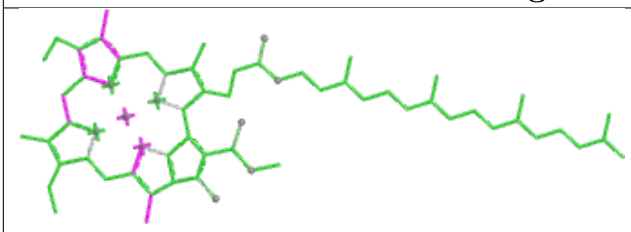


Rings

Ligand CLA 7 313



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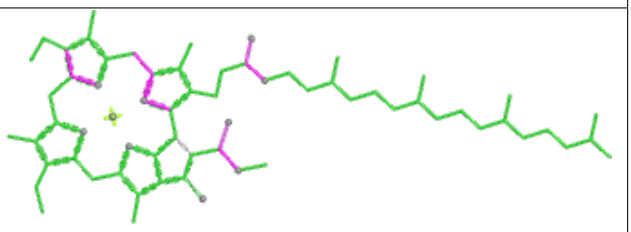

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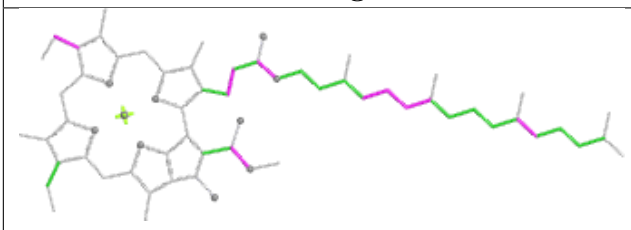

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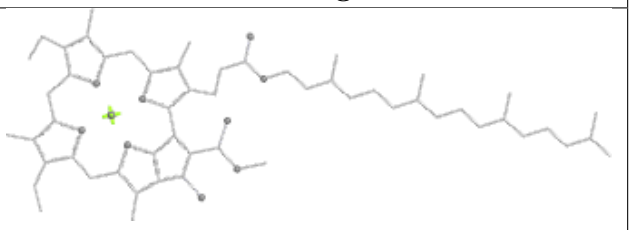
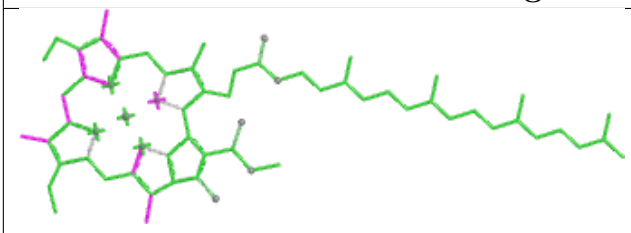


Rings

Ligand CLA B 805



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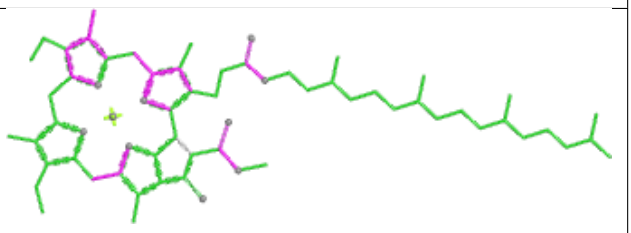

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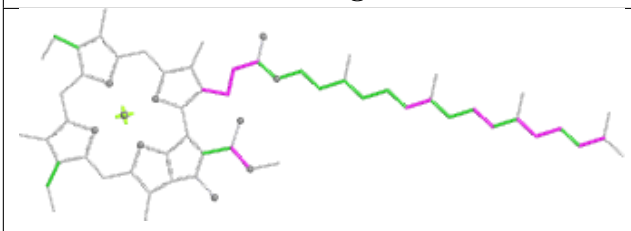

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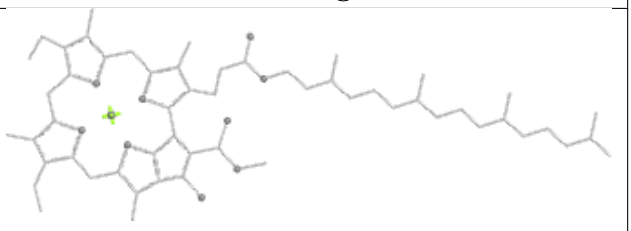
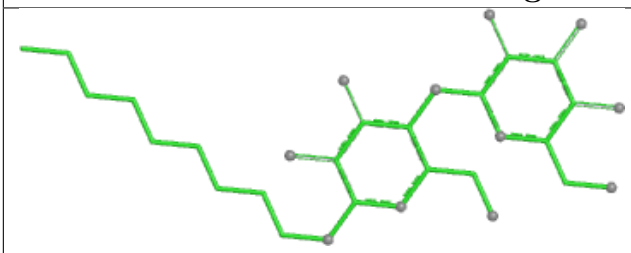


Rings

Ligand LMU 7 325



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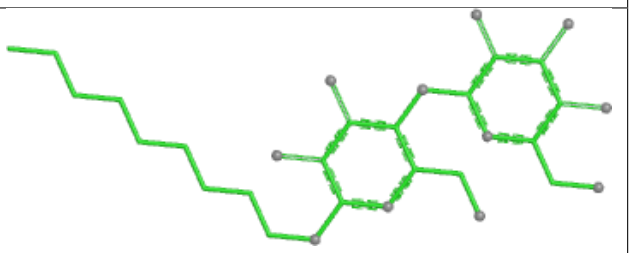
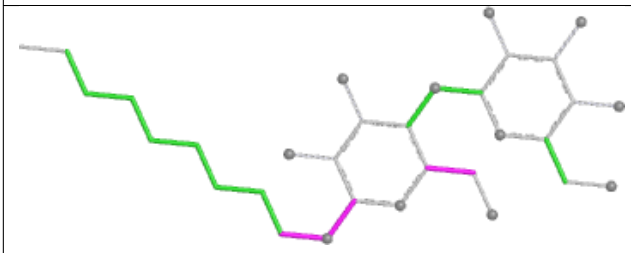


Bond angles



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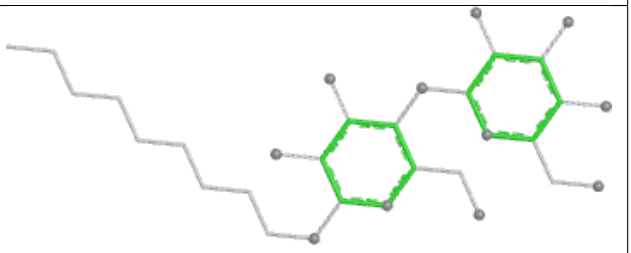
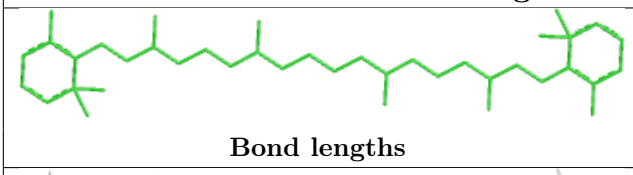


Rings

Ligand BCR A 5049



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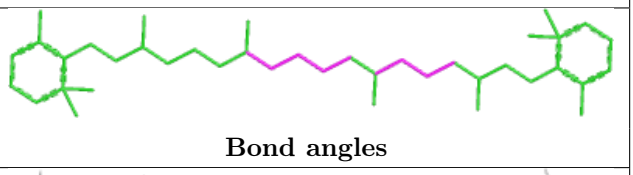

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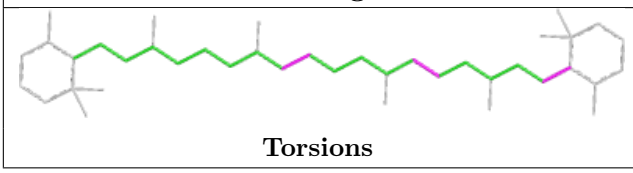

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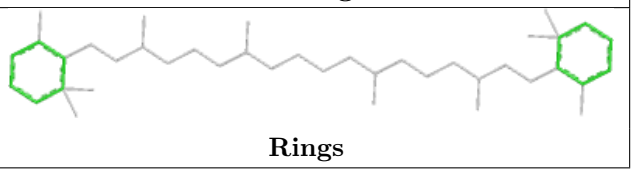
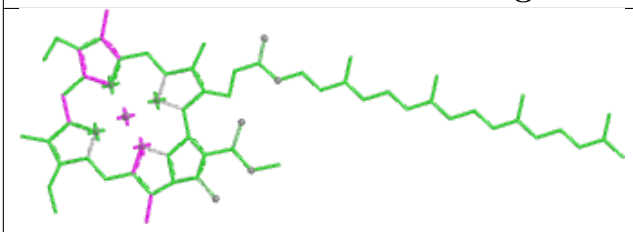


Rings

Ligand CLA A 5026



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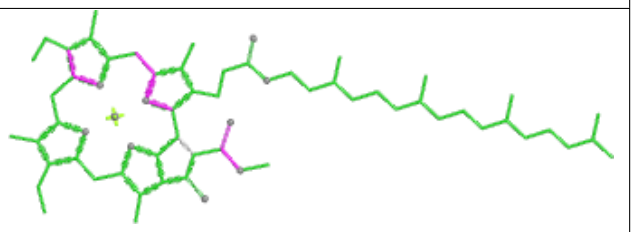
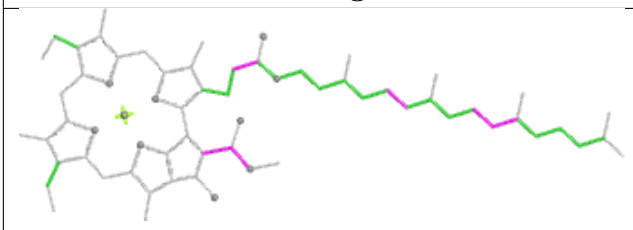


Bond angles



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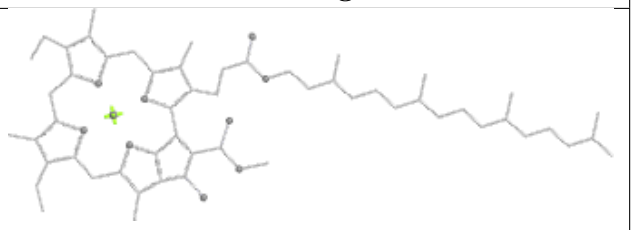
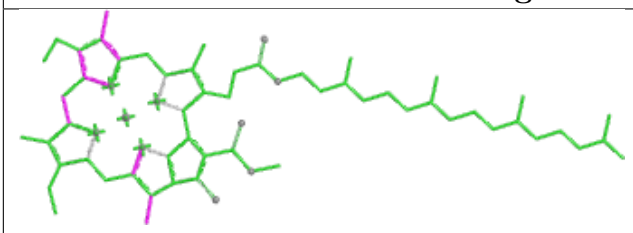


Rings

Ligand CLA A 5020



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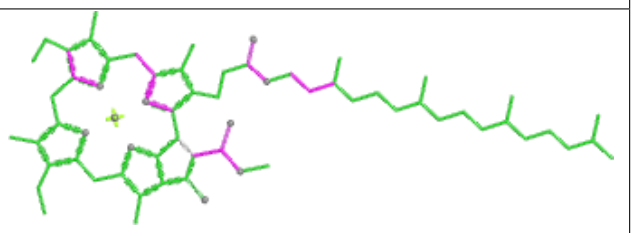

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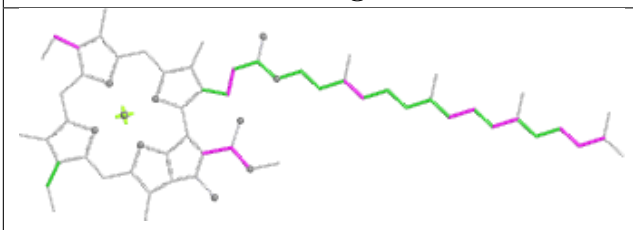

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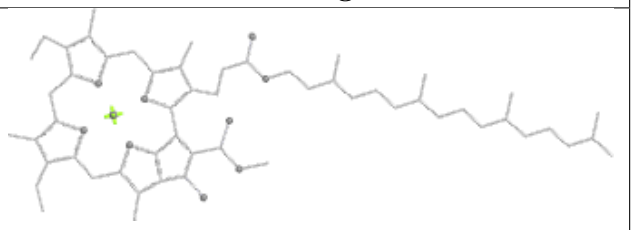
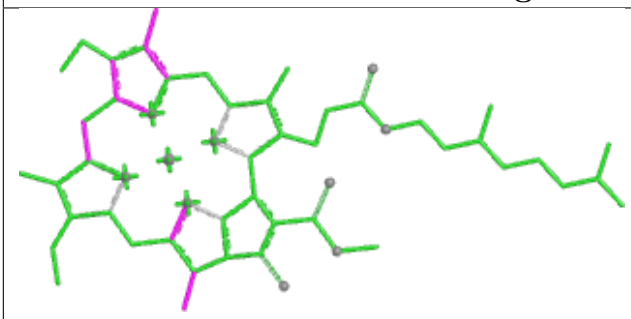


Rings

Ligand CLA A 5033



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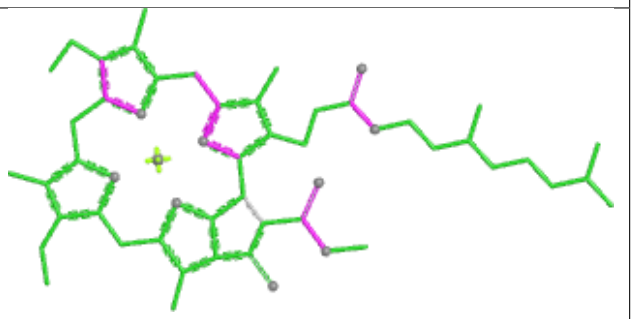

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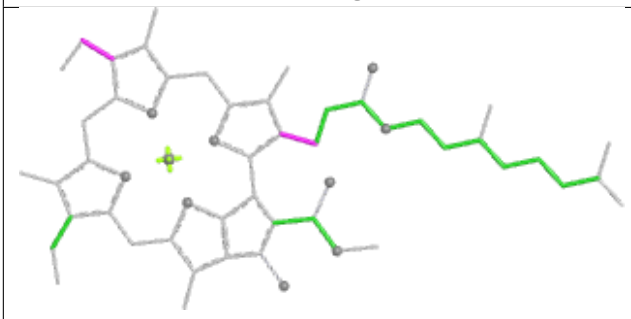

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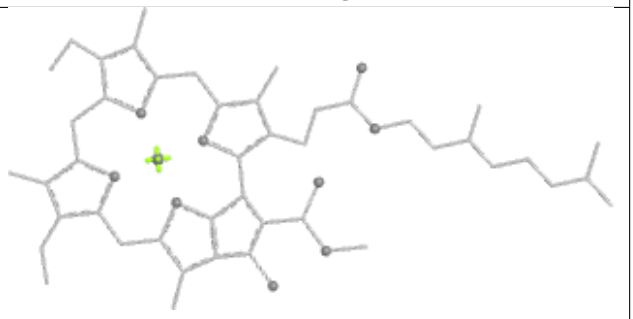
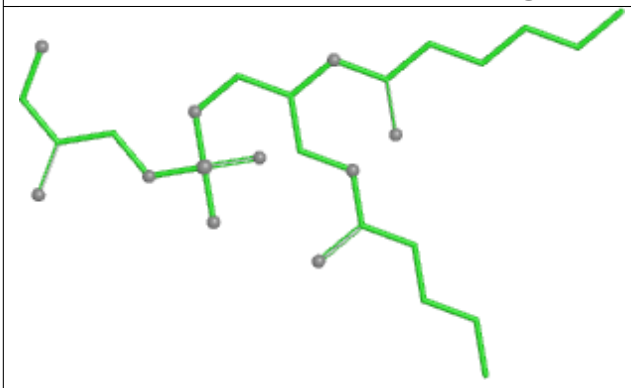


Rings

Ligand LHG I 4002



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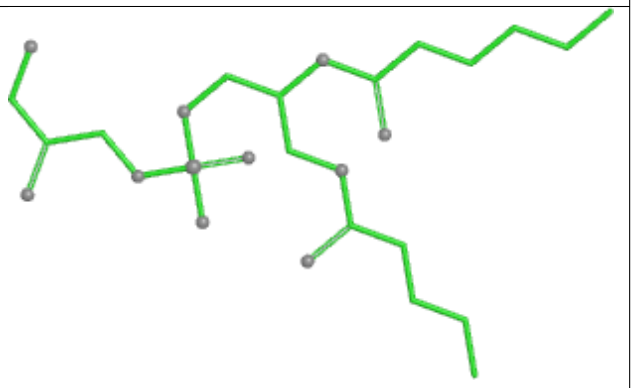
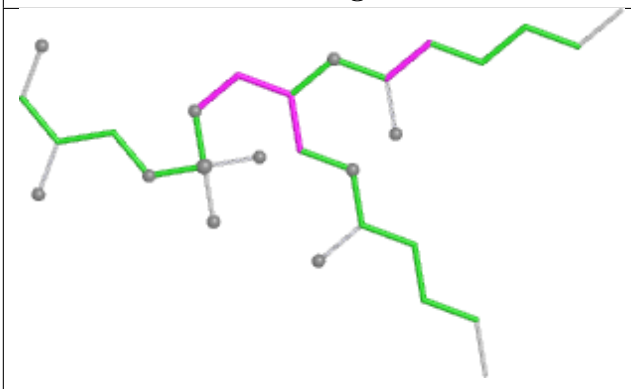


Bond angles



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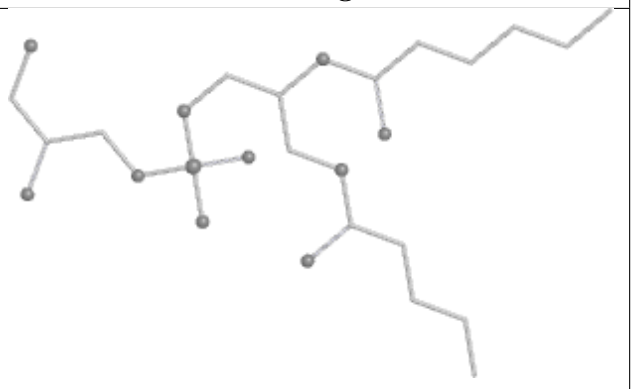
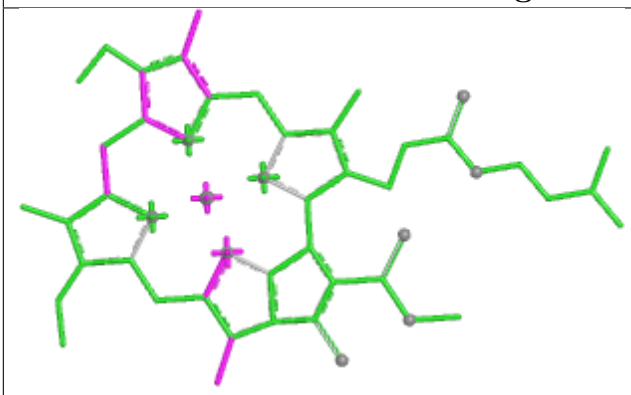


Rings

Ligand CLA A 5021



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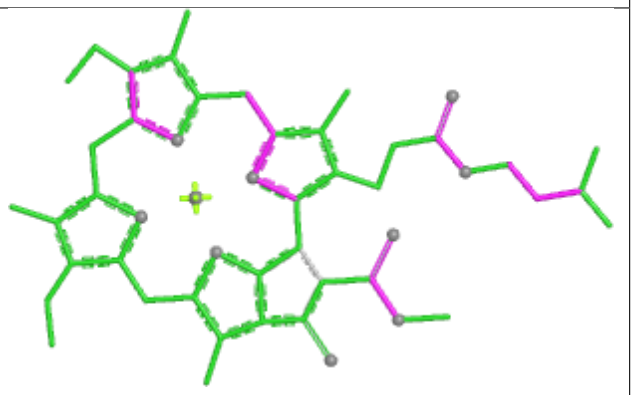
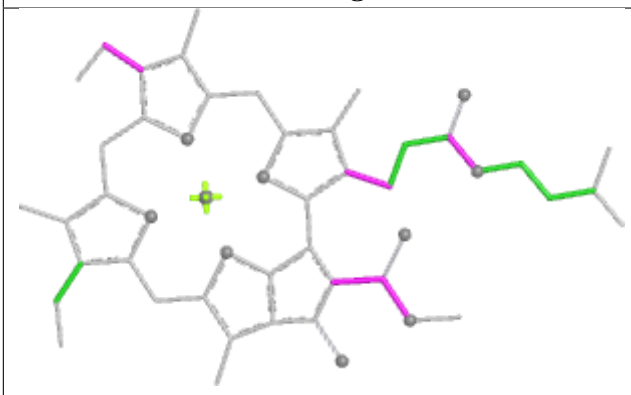


Bond angles



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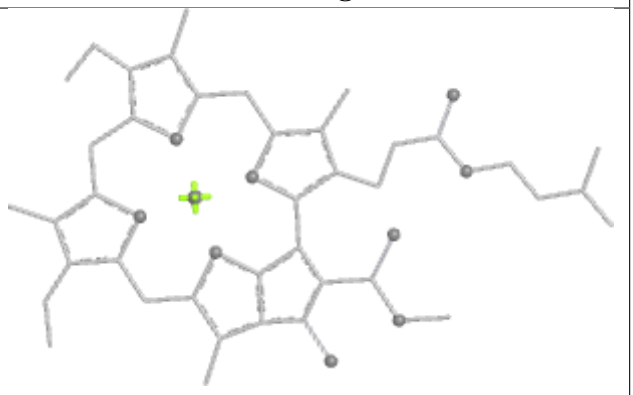
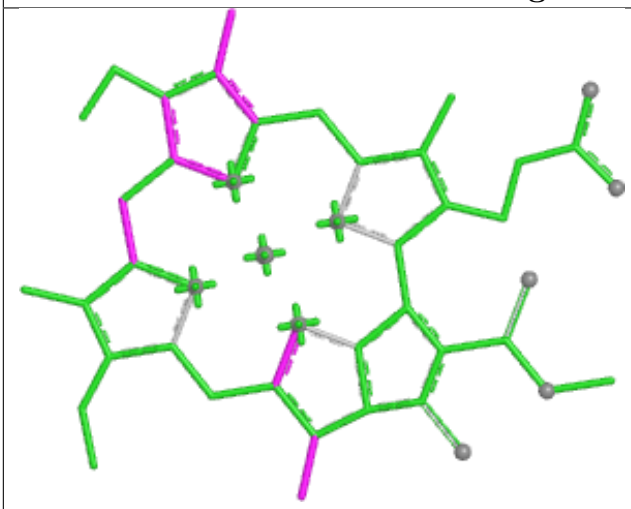


Rings

Ligand CLA 2 309



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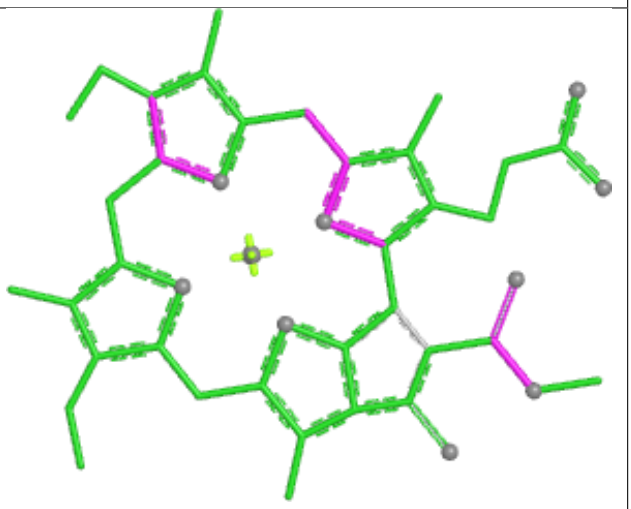
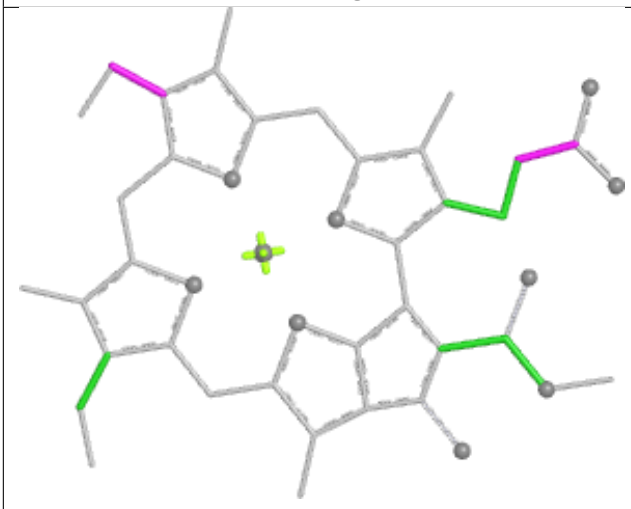


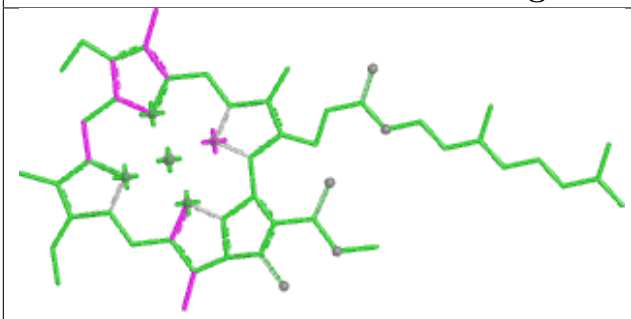
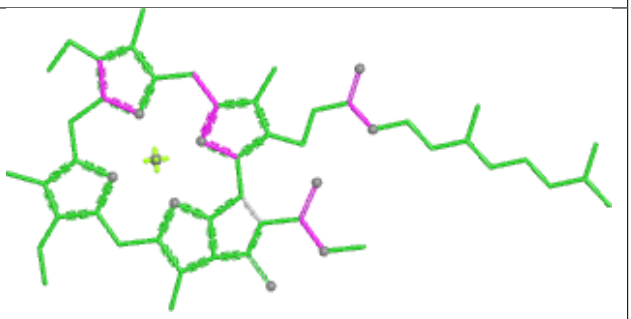
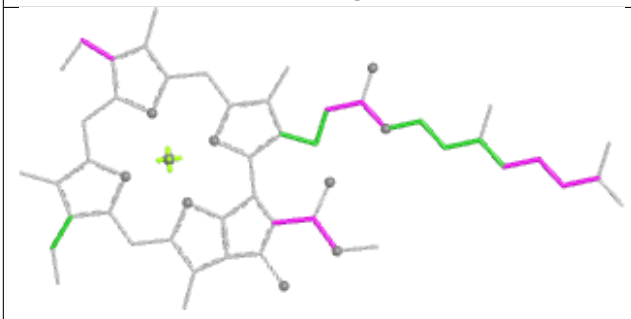
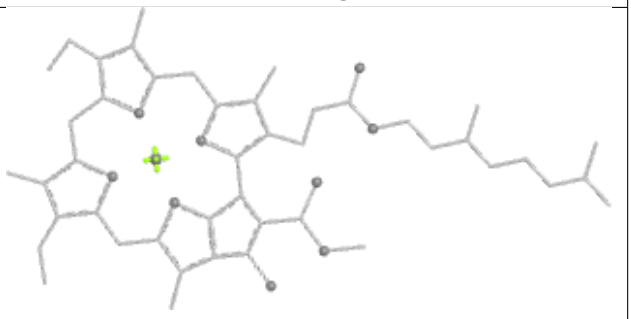
Bond angles

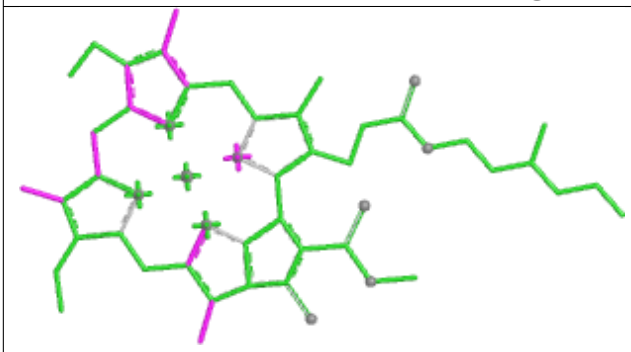
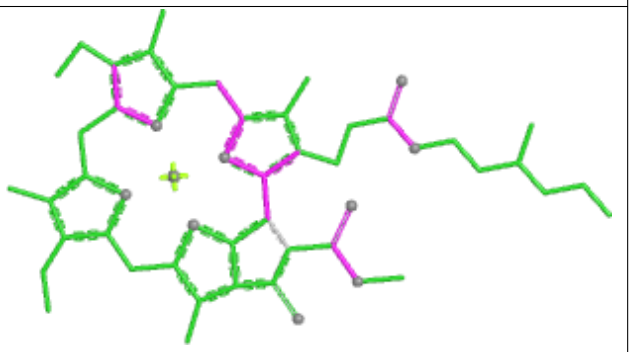
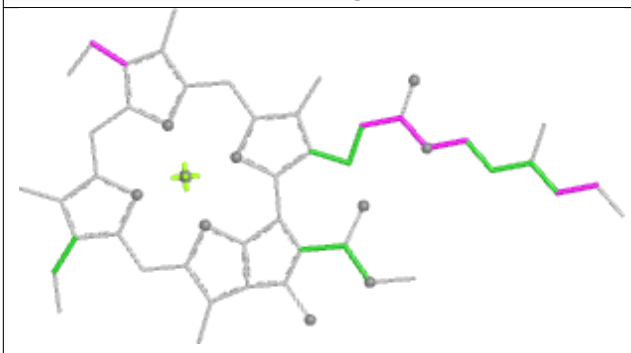
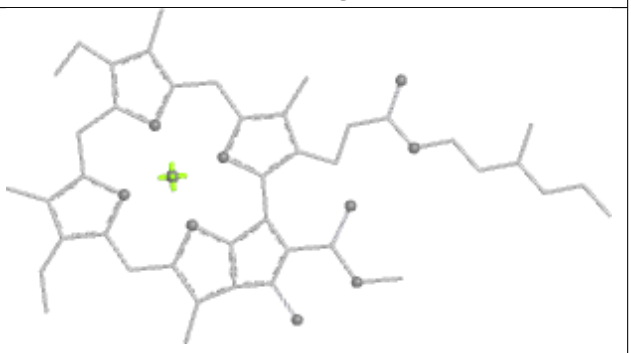


Torsions

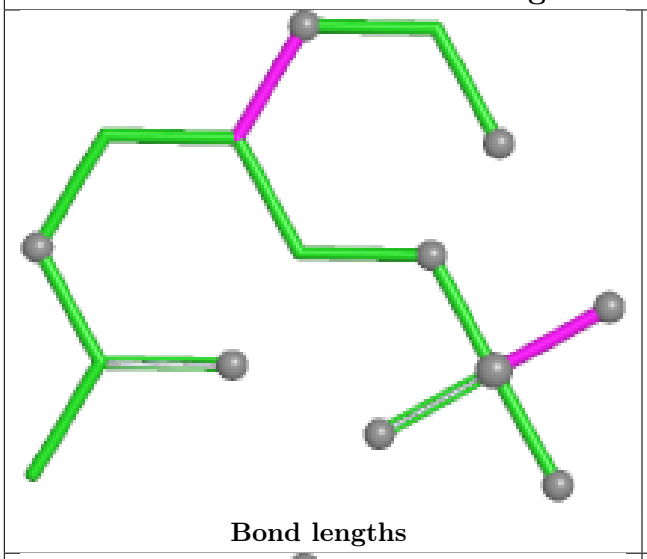


Rings

Ligand CLA 1 603	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 7 312	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PTY 7 302



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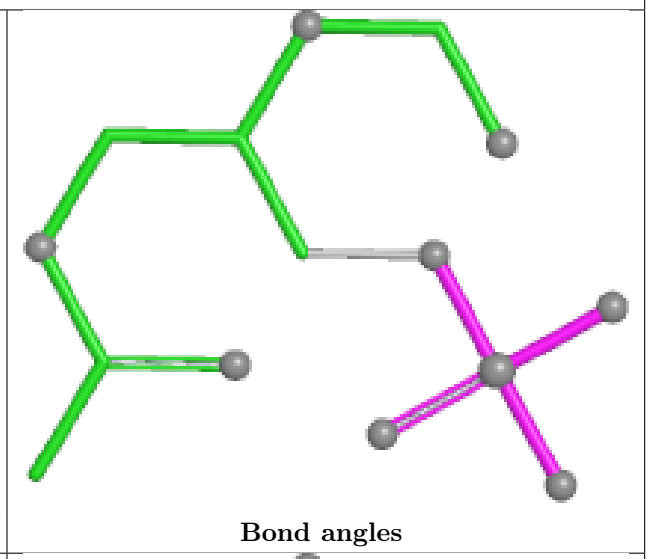

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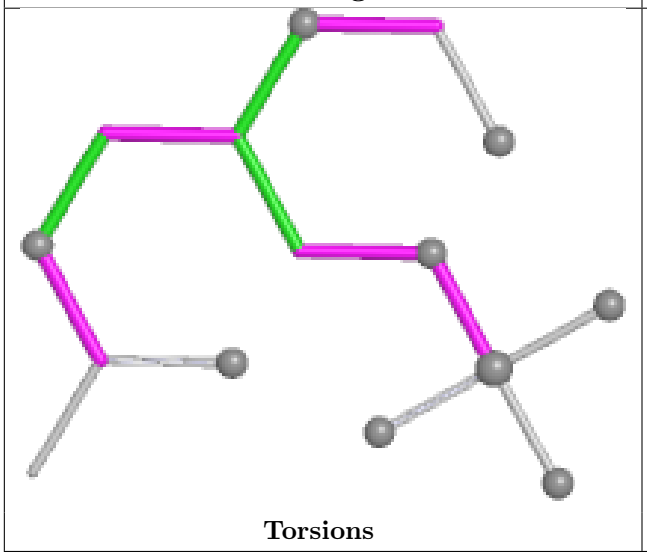

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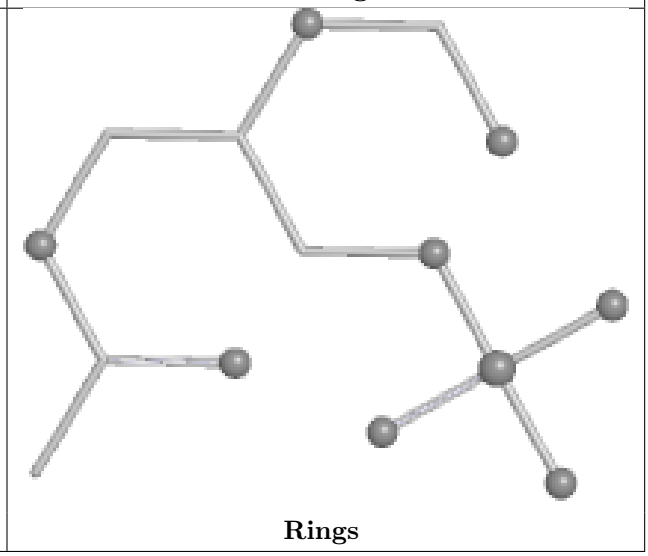
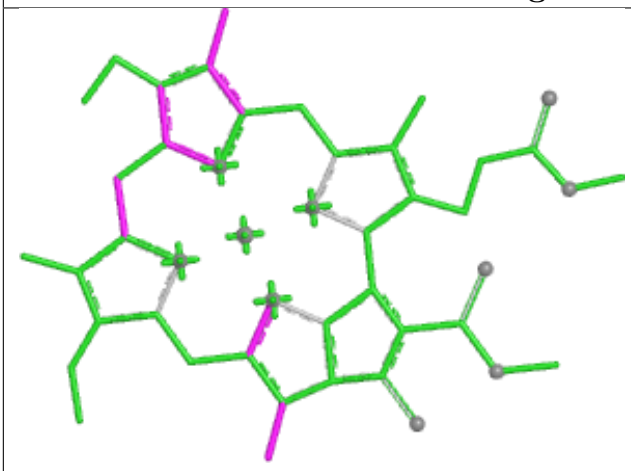


Rings

Ligand CLA 9 609



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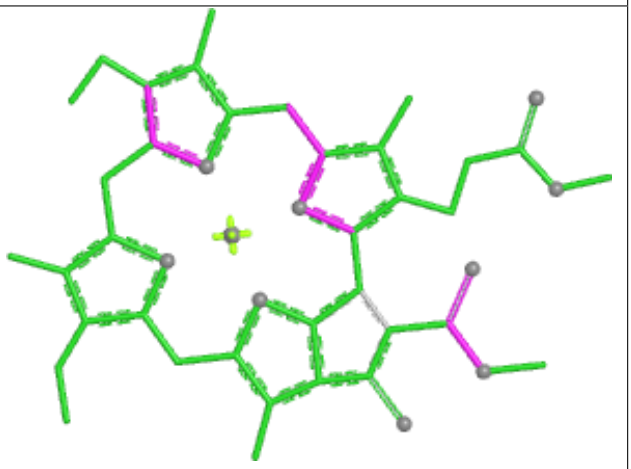
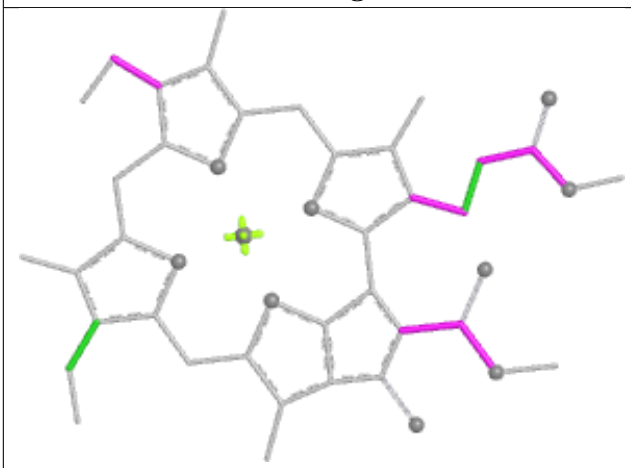


Bond angles



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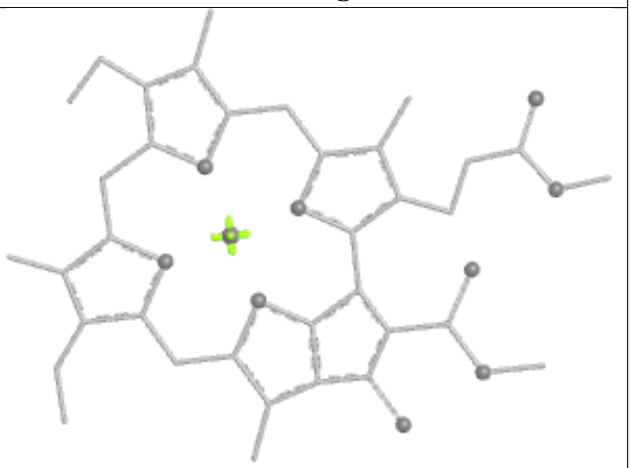


Rings

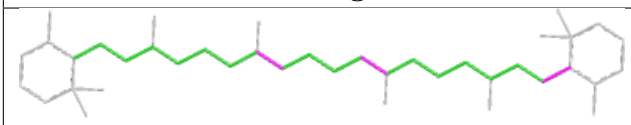
Ligand BCR G 205



Bond lengths



Bond angles



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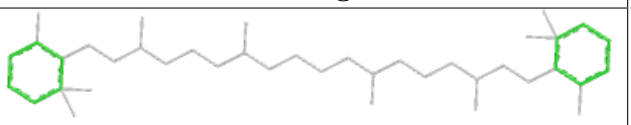
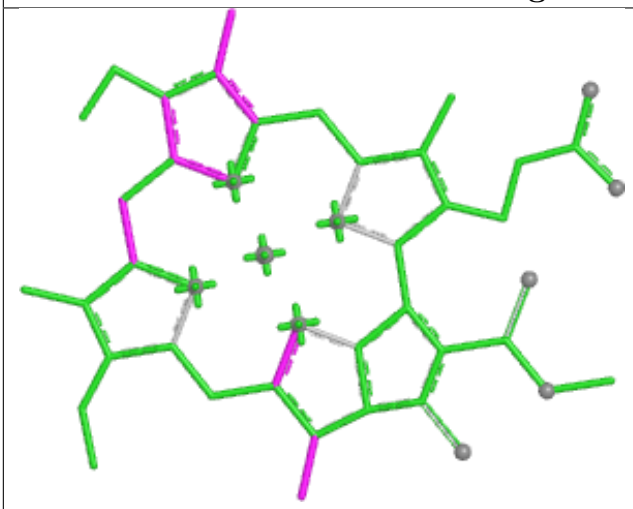


Rings

Ligand CLA 9 605



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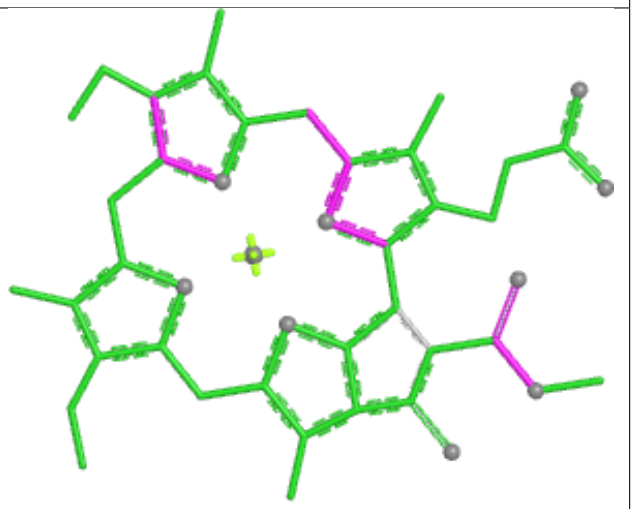

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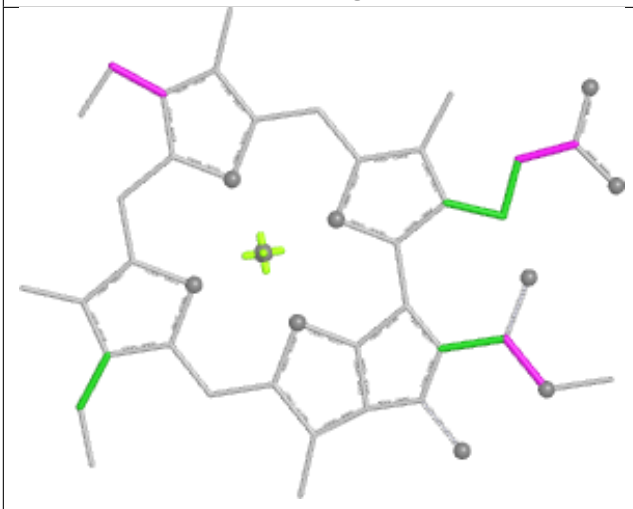
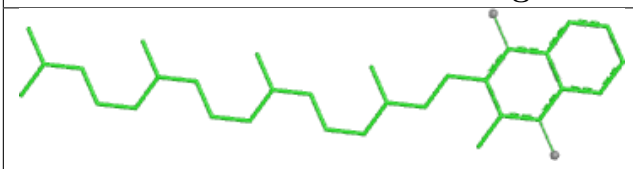


Torsions



Rings

Ligand PQN A 5045



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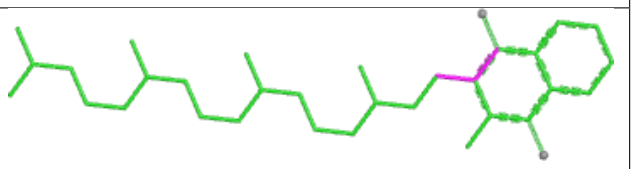
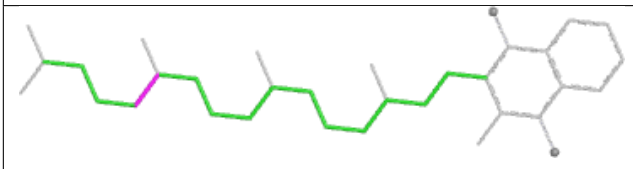


Bond angles



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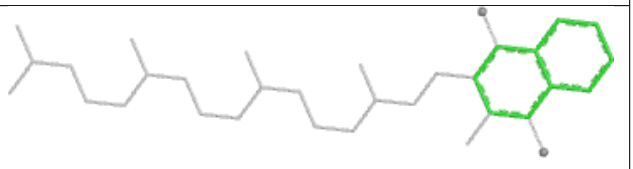
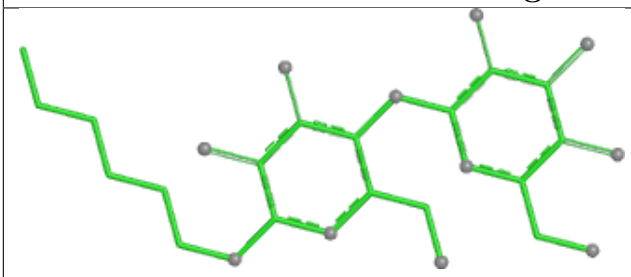


Rings

Ligand LMU 9 616



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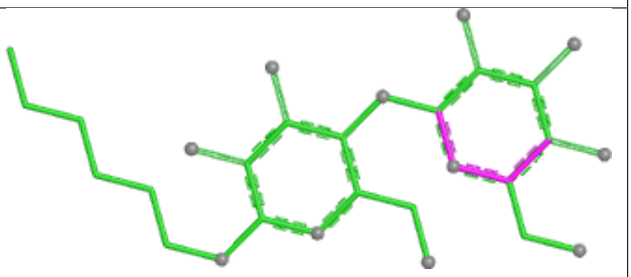
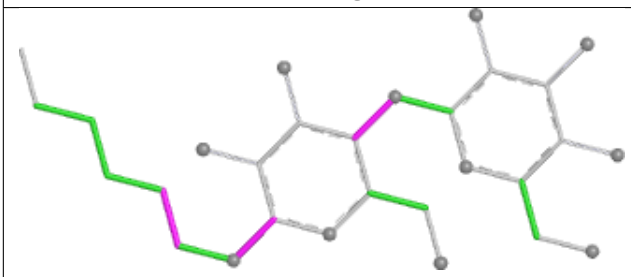


Bond angles



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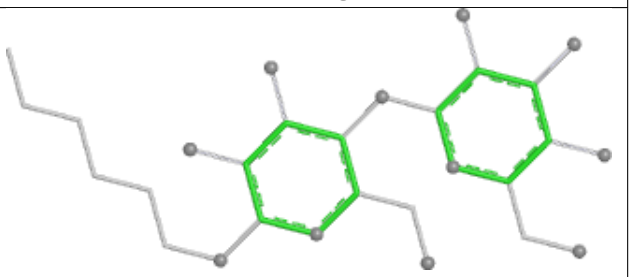
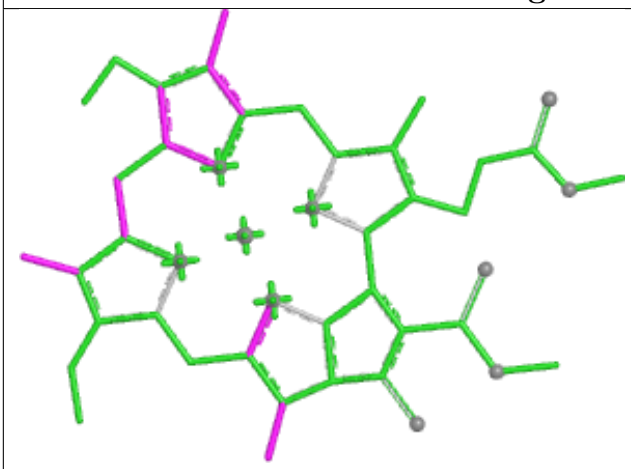


Rings

Ligand CLA 3 304



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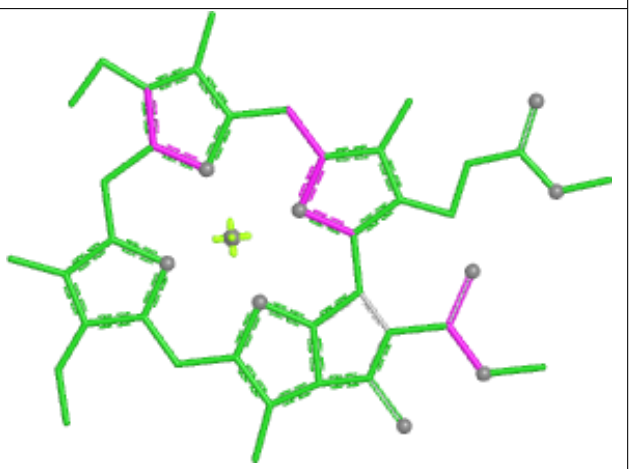

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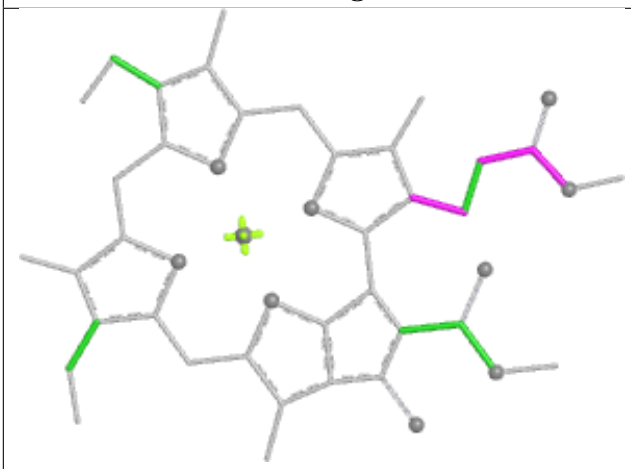

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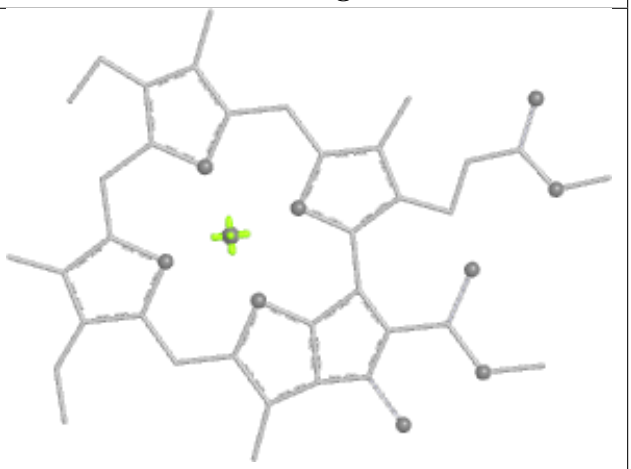
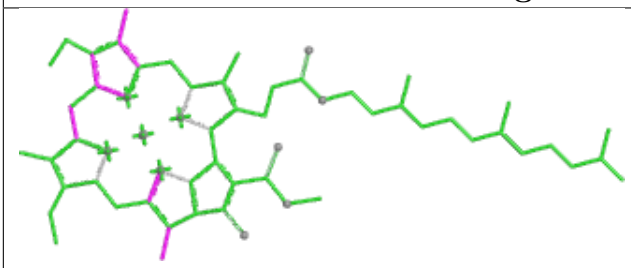


Rings

Ligand CLA A 5040



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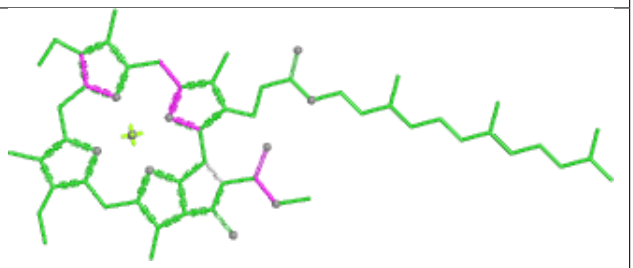
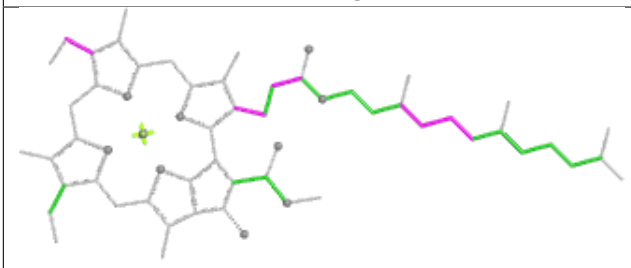


Bond angles



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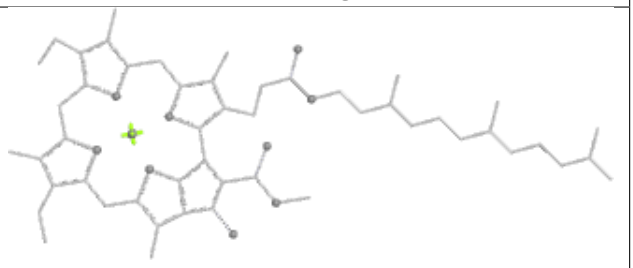
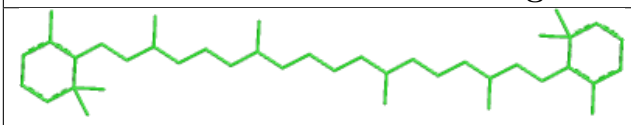


Rings

Ligand BCR 1 617



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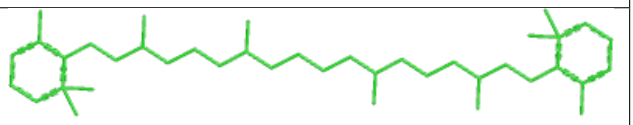
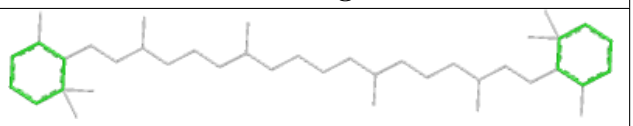


Bond angles

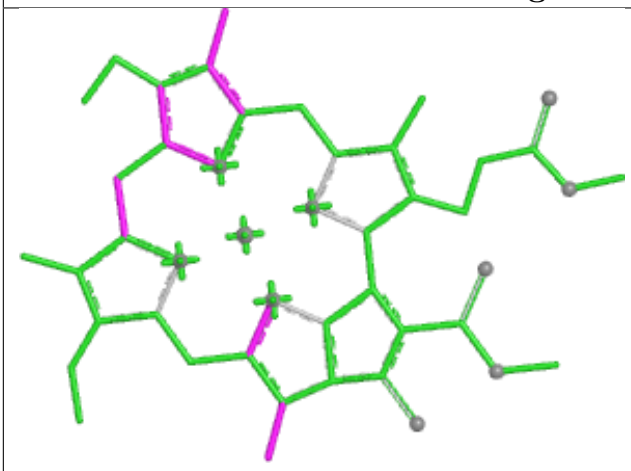


Torsions



Rings

Ligand CLA 7 309



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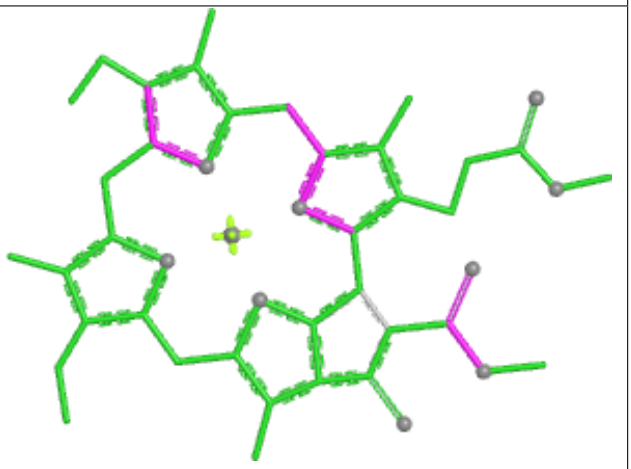

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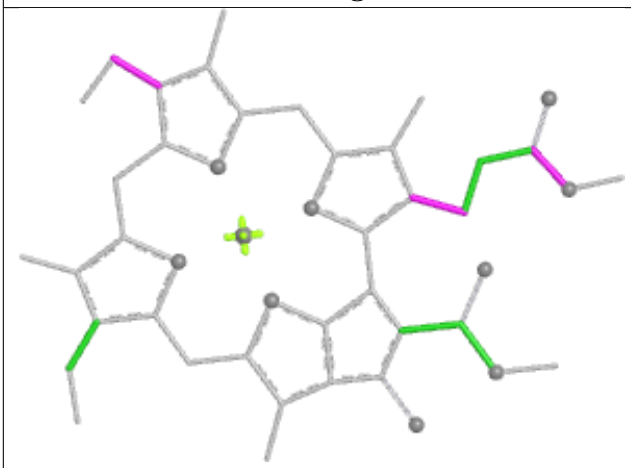

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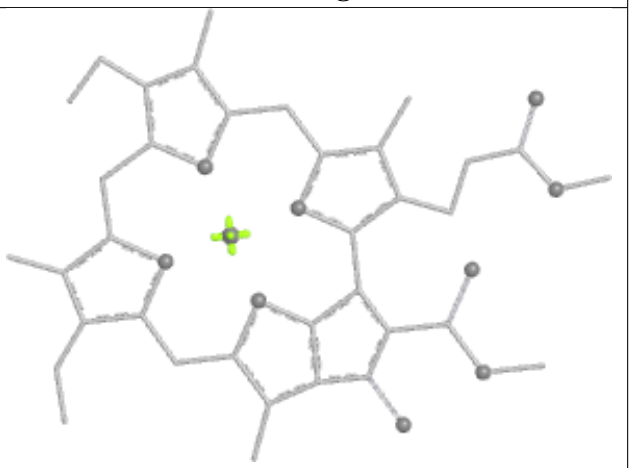
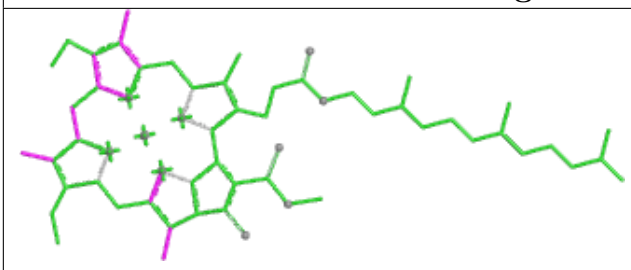


Rings

Ligand CLA A 5025



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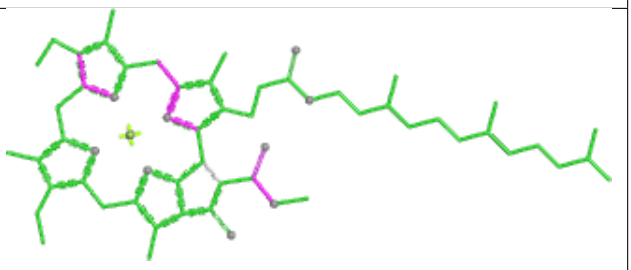
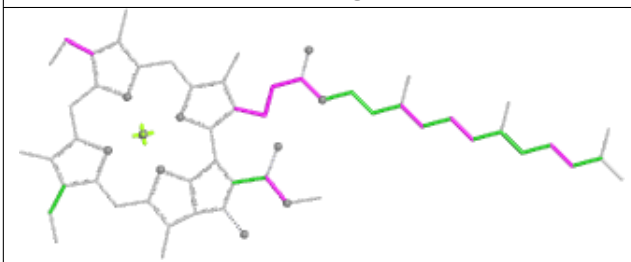


Bond angles



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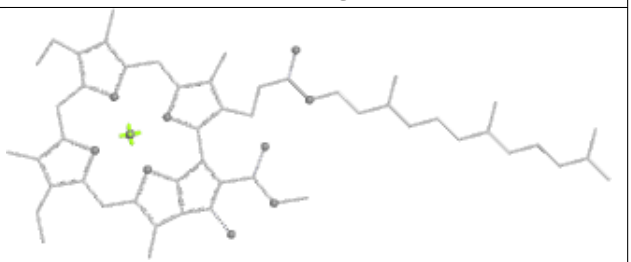
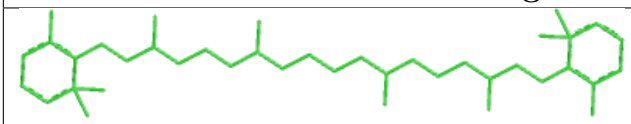


Rings

Ligand BCR B 844



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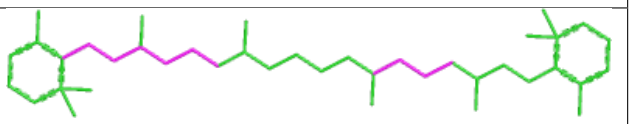
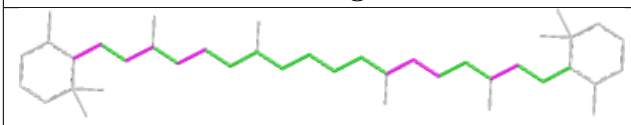


Bond angles



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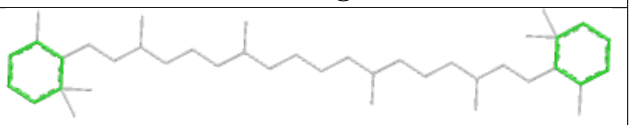
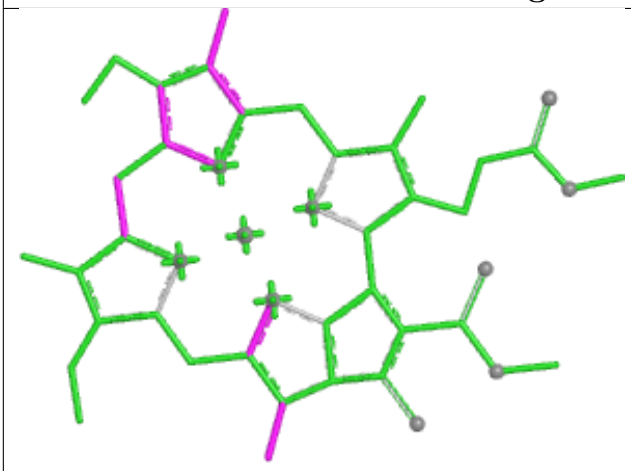


Rings

Ligand CLA 1 608



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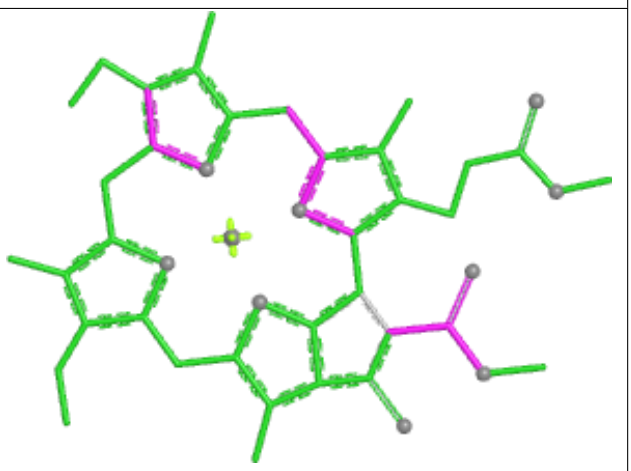
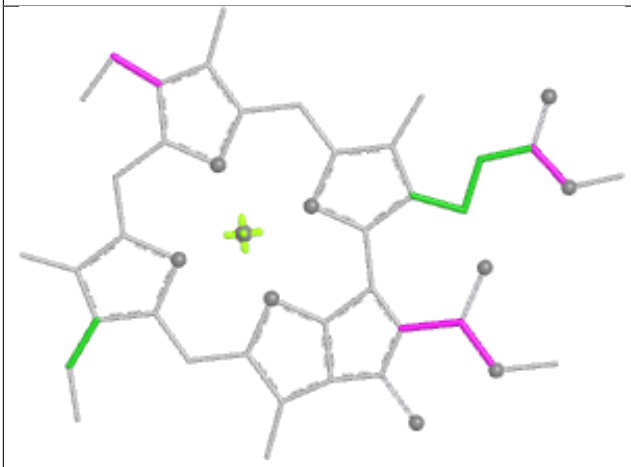


Bond angles



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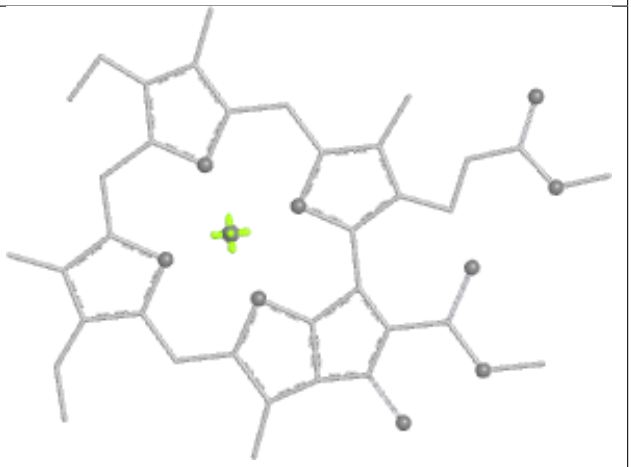
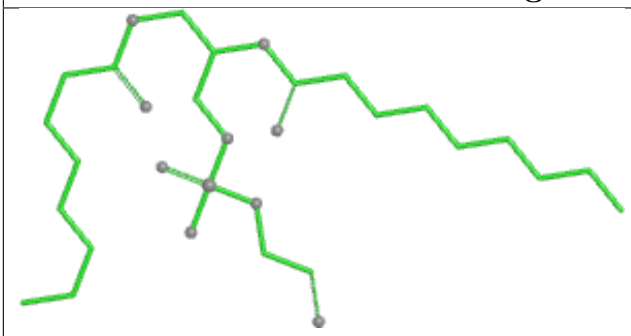


Rings

Ligand PTY F 302



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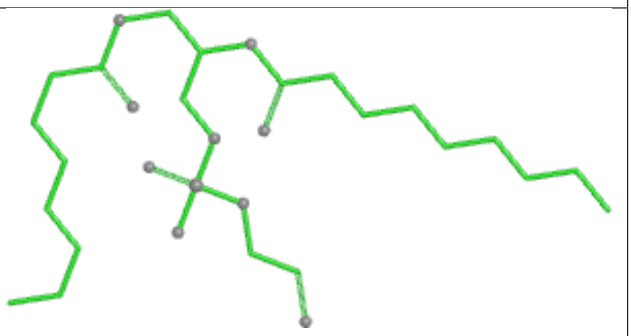
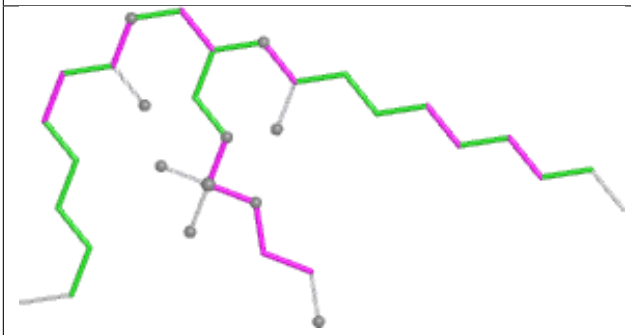


Bond angles



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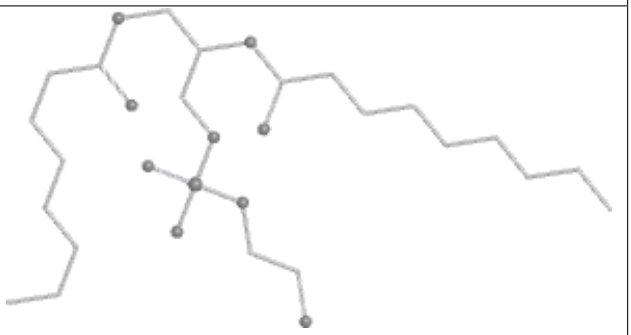
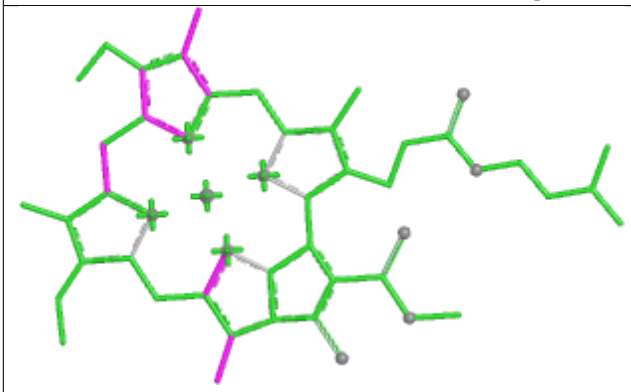
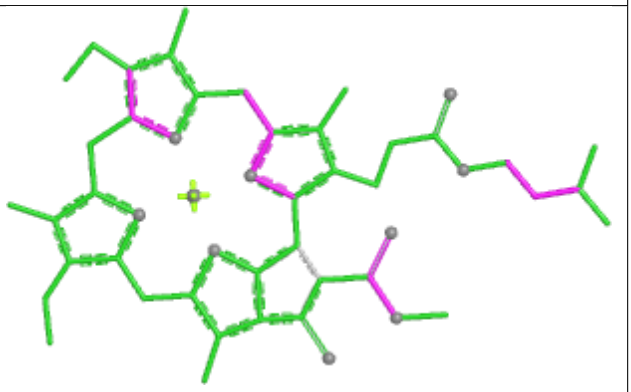


Rings

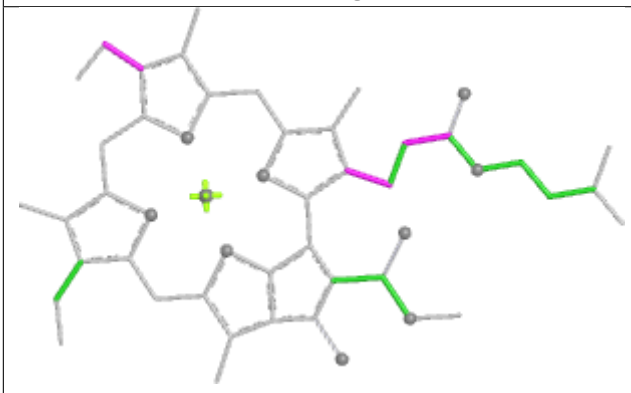
Ligand CLA 9 604



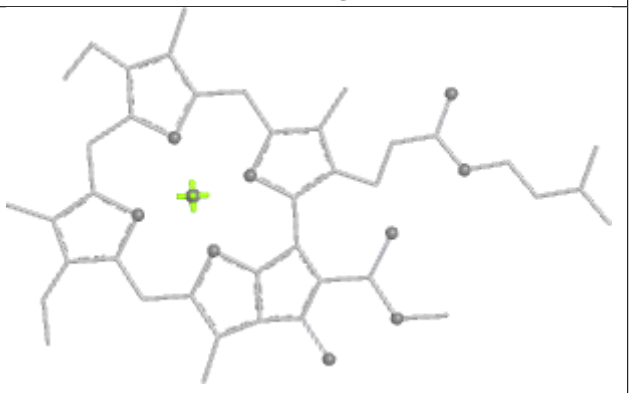
Bond lengths



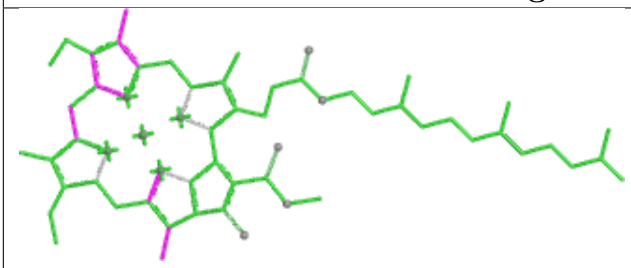
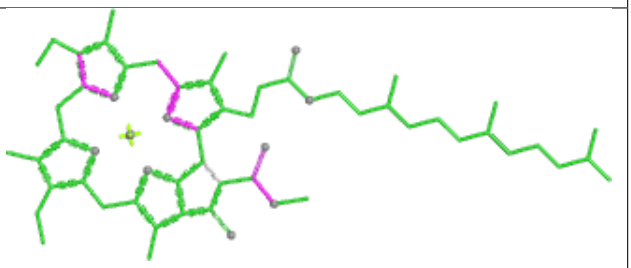
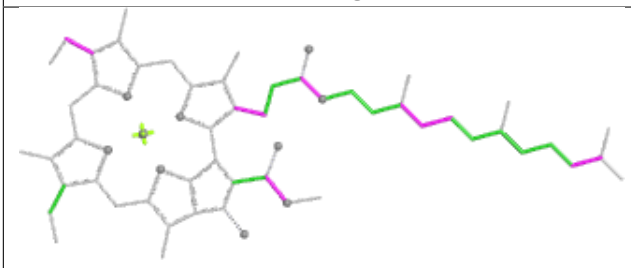
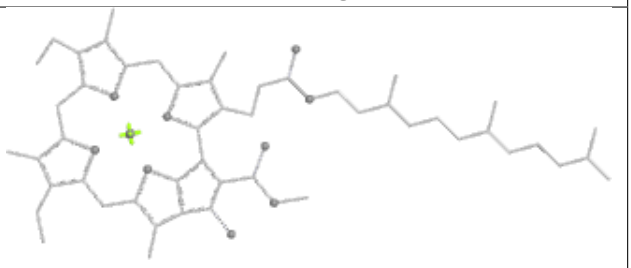
Bond angles



Torsions



Rings

Ligand CLA 1 612	
	
Bond lengths	Bond angles
	
Torsions	Rings

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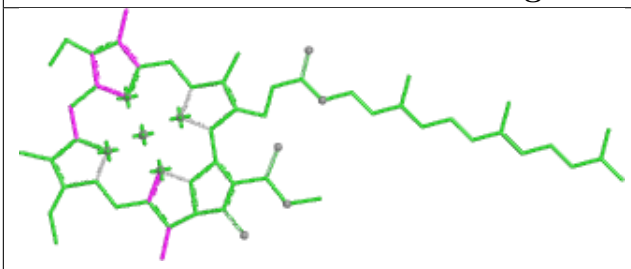
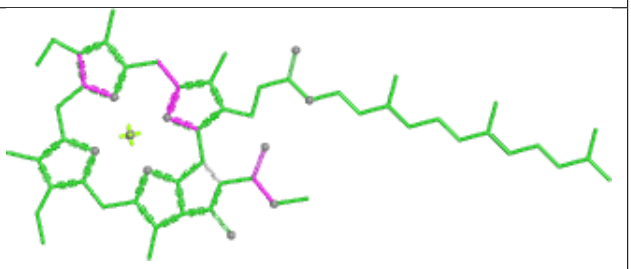
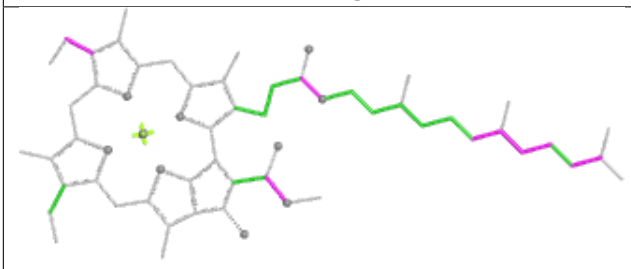
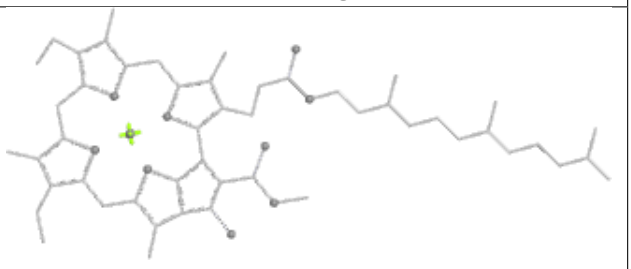
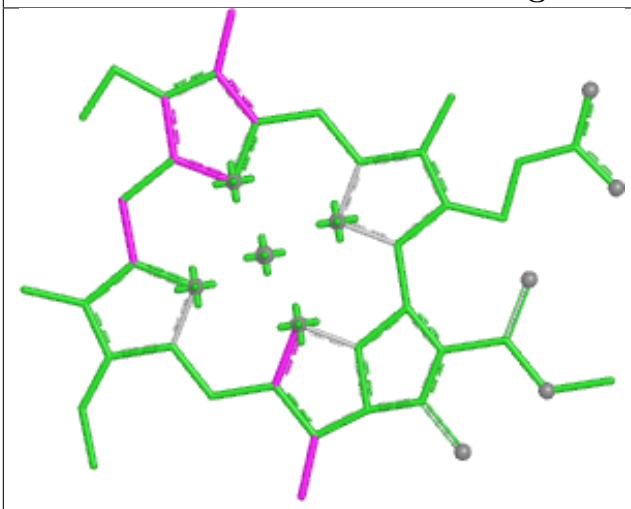
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 2 305



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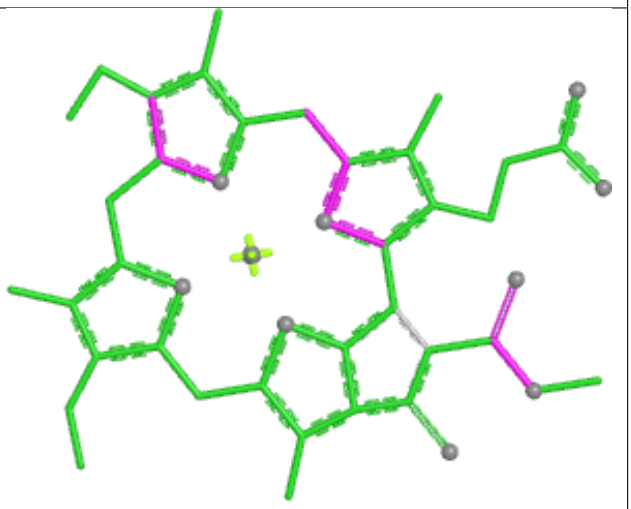
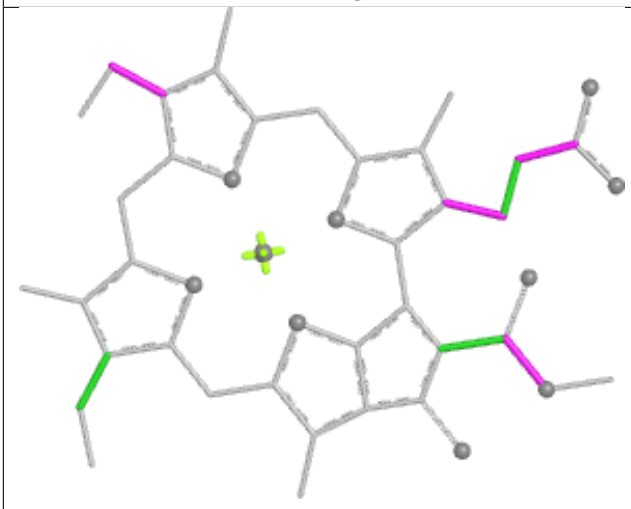


Bond angles

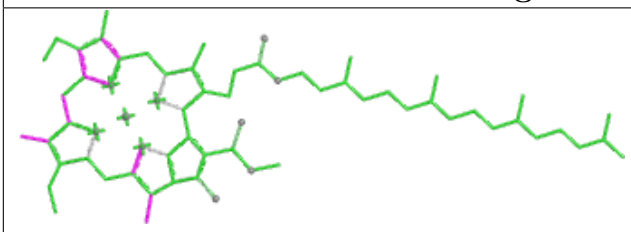


Torsions



Rings

Ligand CLA A 5016



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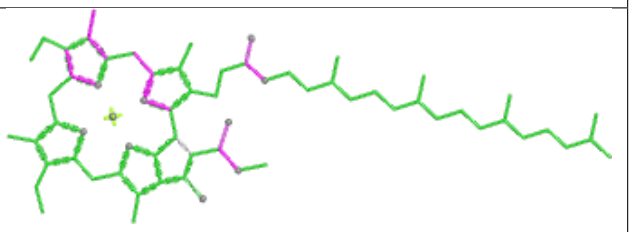

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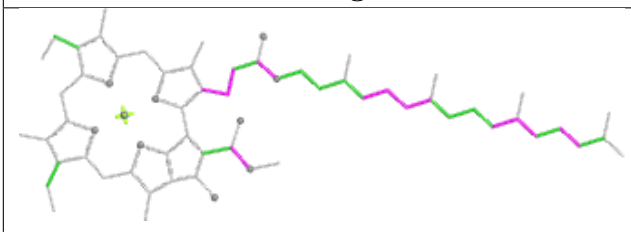

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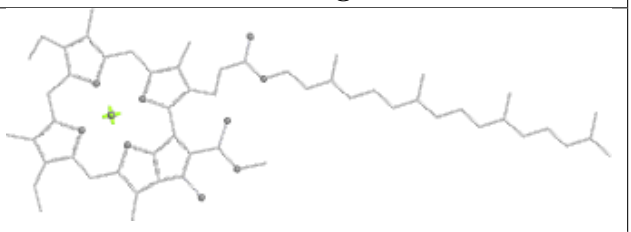
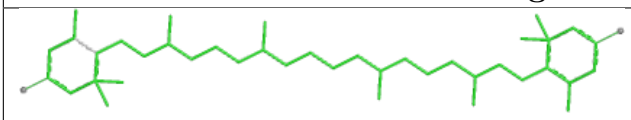
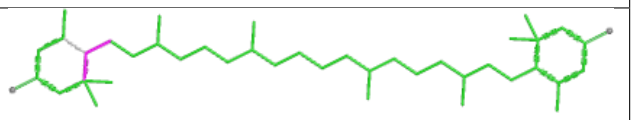
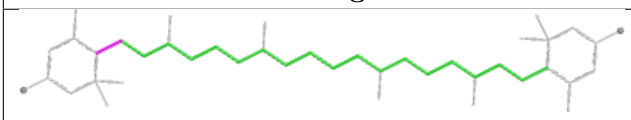
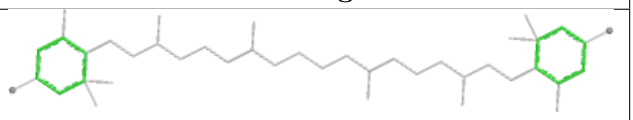


Rings

Ligand LUT 7 316	
	
Bond lengths	Bond angles
	
Torsions	Rings

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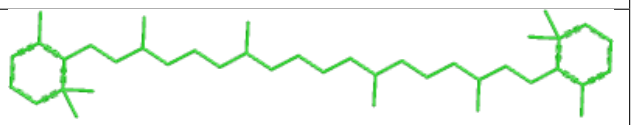
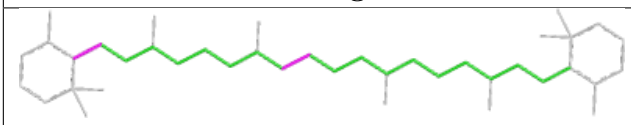
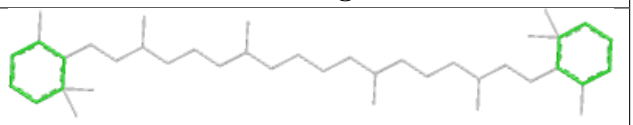
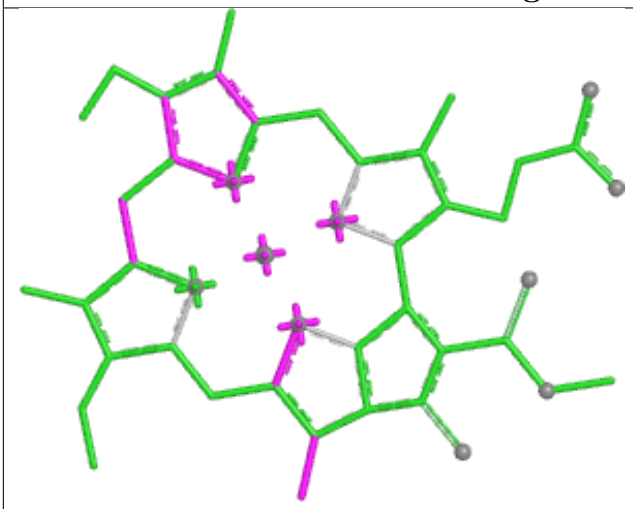
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA G 204



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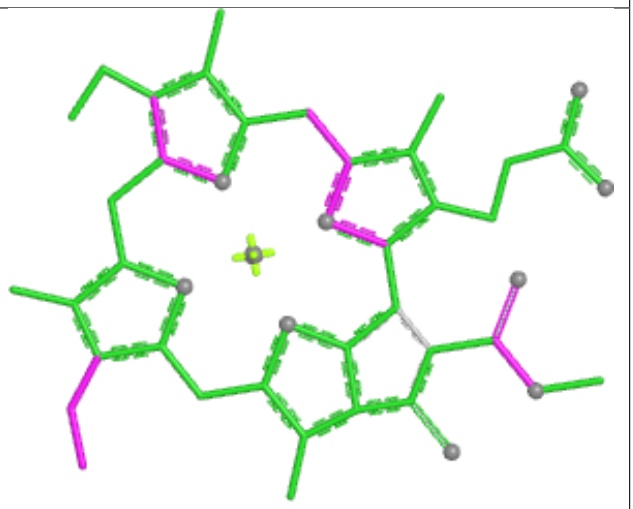

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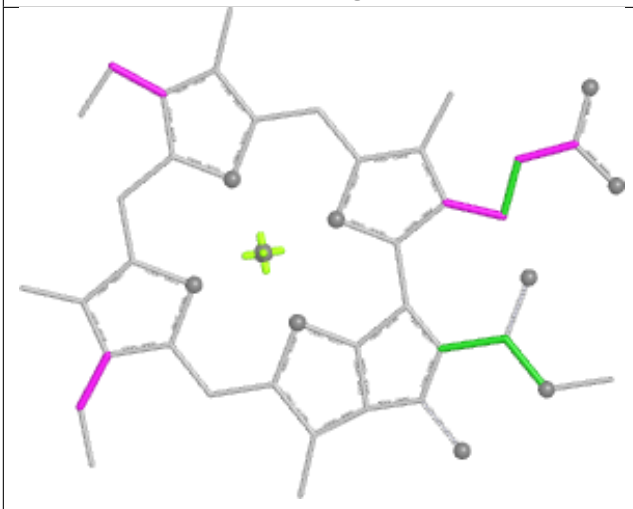
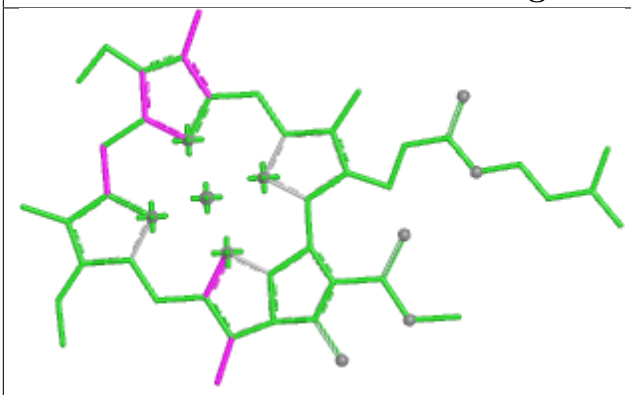


Torsions



Rings

Ligand CLA 1 604



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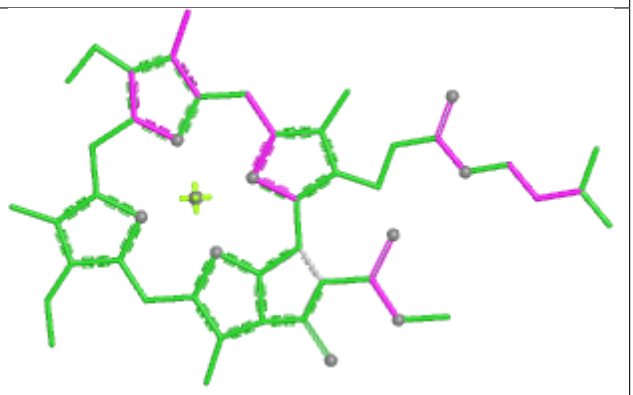

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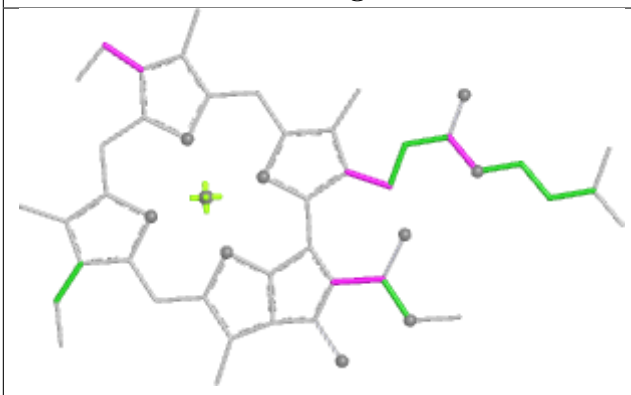

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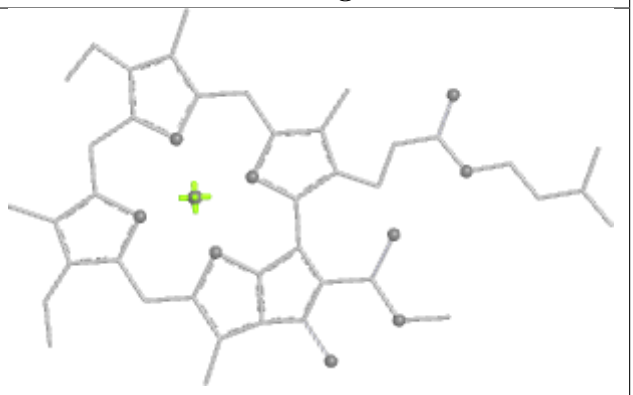
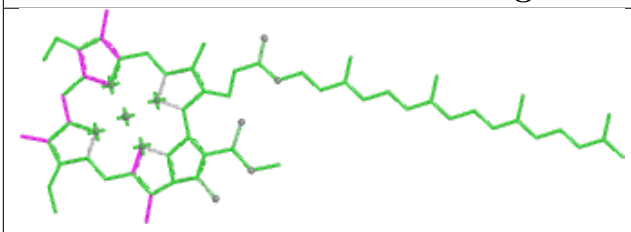


Rings

Ligand CLA A 5006



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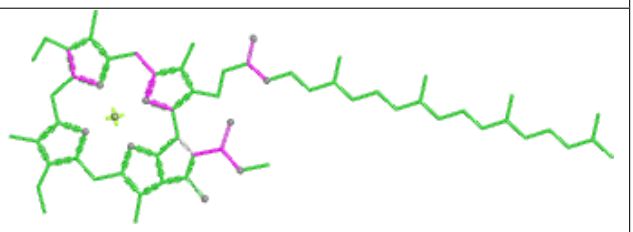
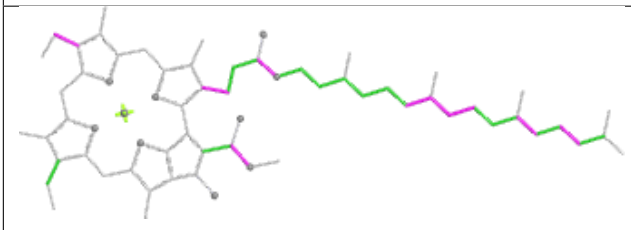


Bond angles



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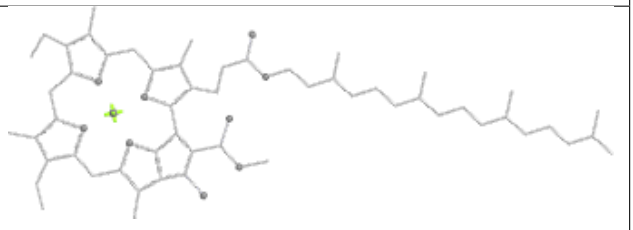
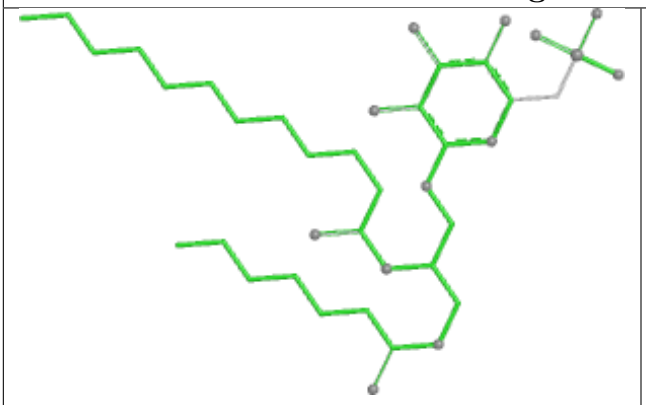


Rings

Ligand SQD 3 322



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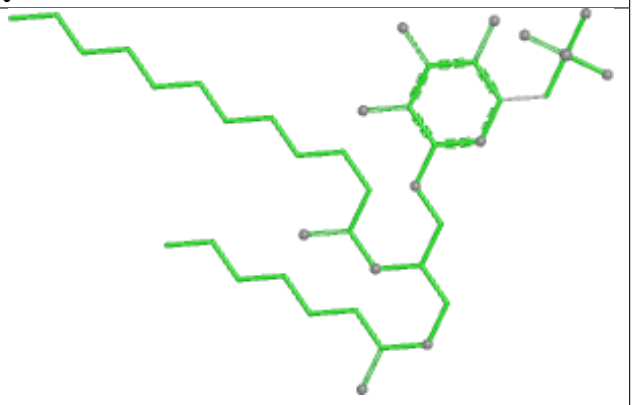
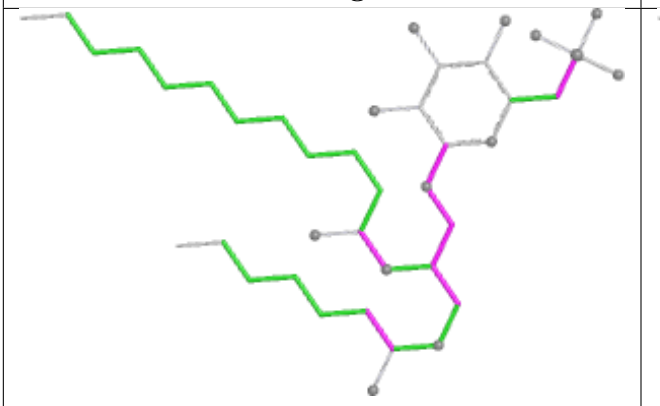


Bond angles



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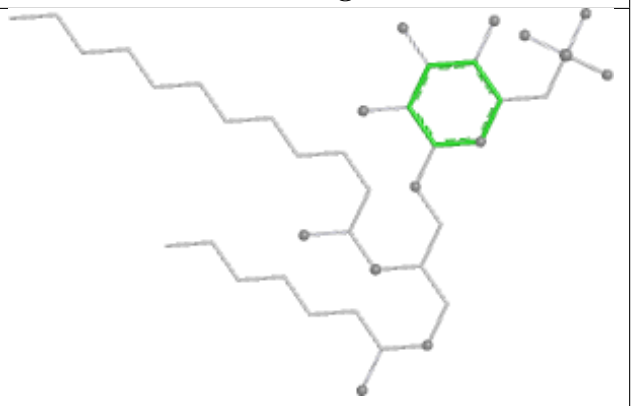


Rings

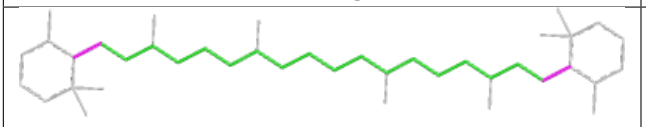
Ligand BCR J 105



Bond lengths



Bond angles



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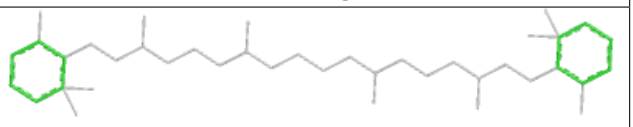
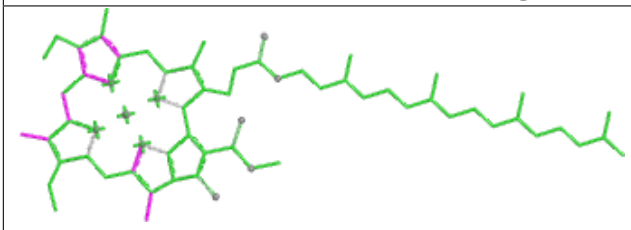
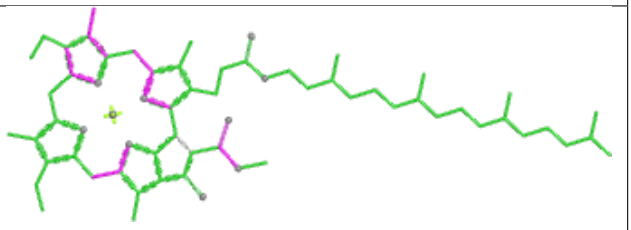


Rings

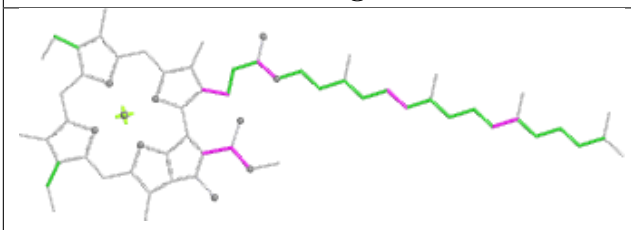
Ligand CLA A 5008



Bond lengths



Bond angles



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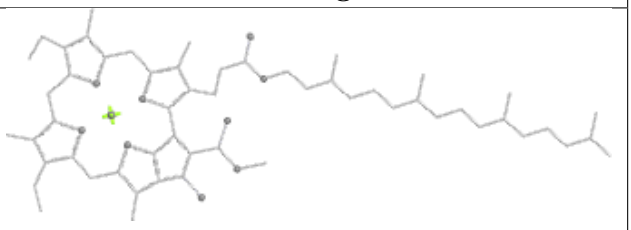
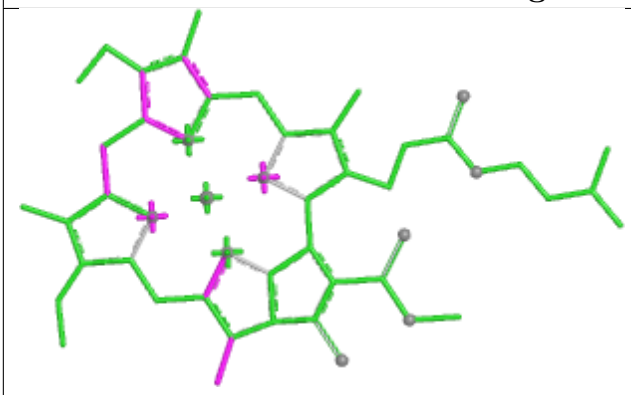


Rings

Ligand CLA 9 610



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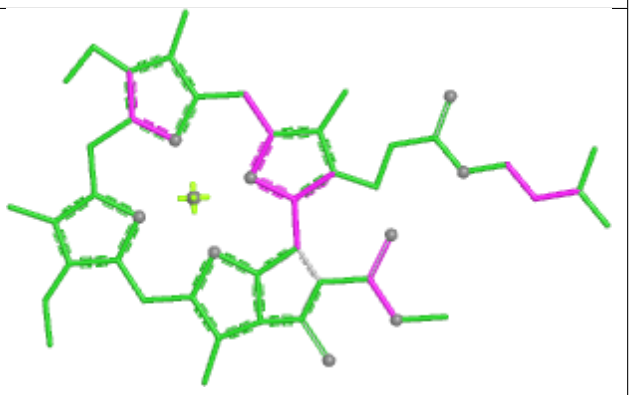
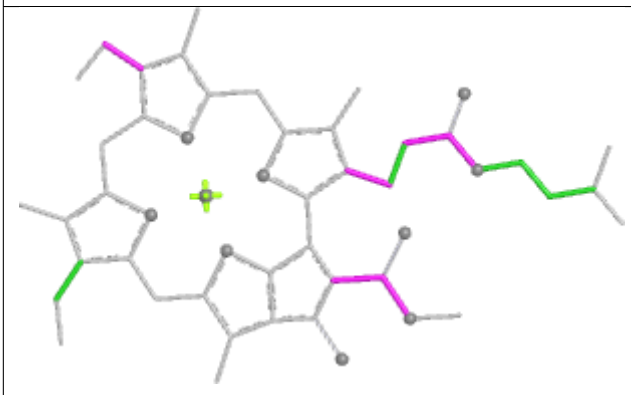


Bond angles



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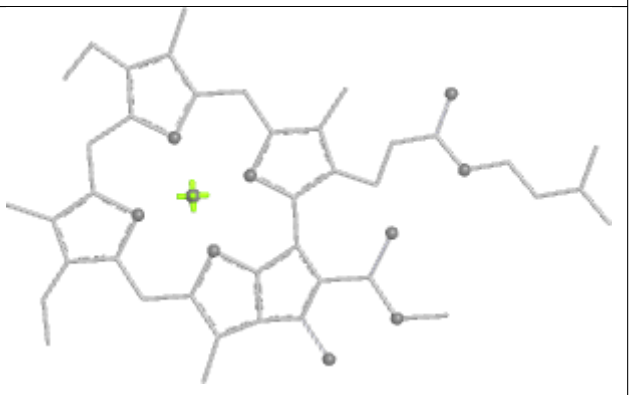
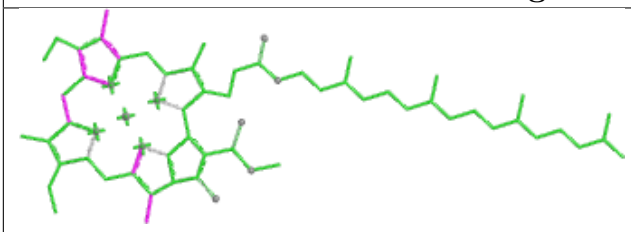


Rings

Ligand CLA 3 307



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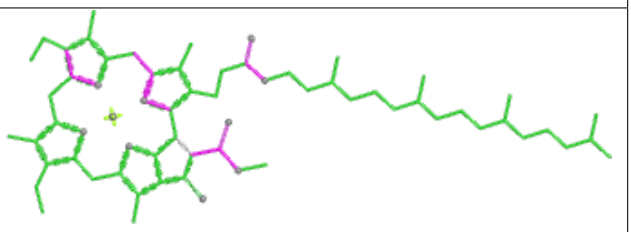
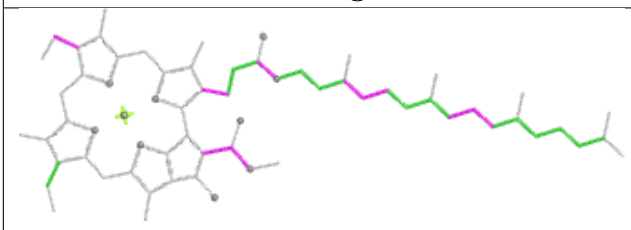


Bond angles



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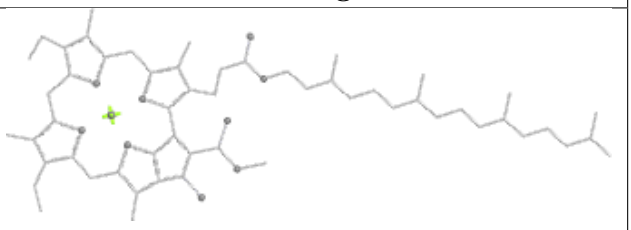
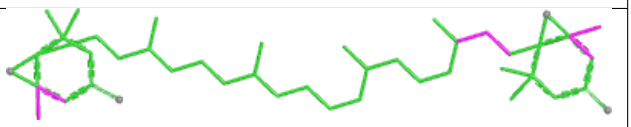


Rings

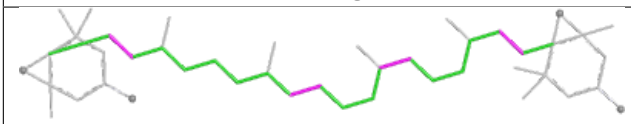
Ligand XAT 9 615



Bond lengths



Bond angles



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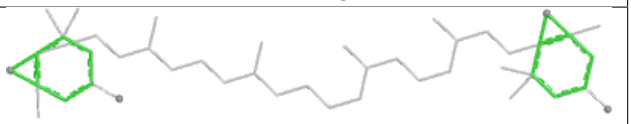
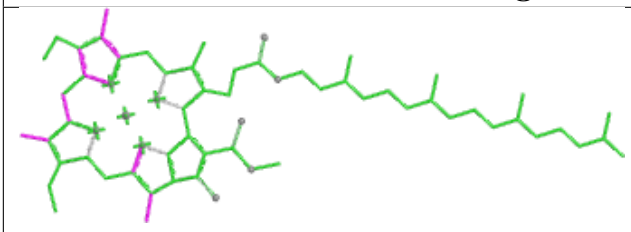


Rings

Ligand CLA A 5014



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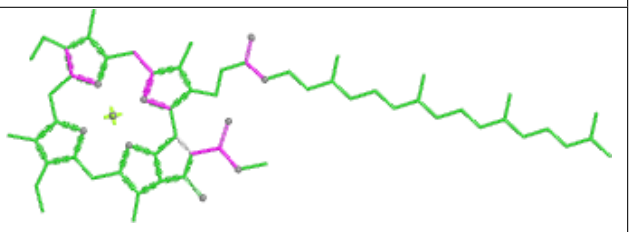
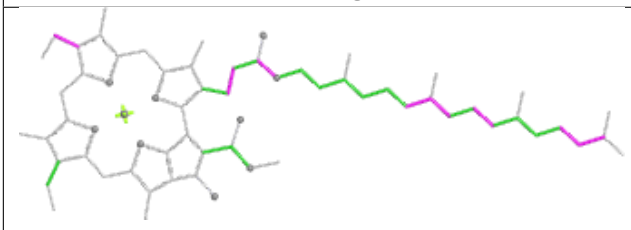
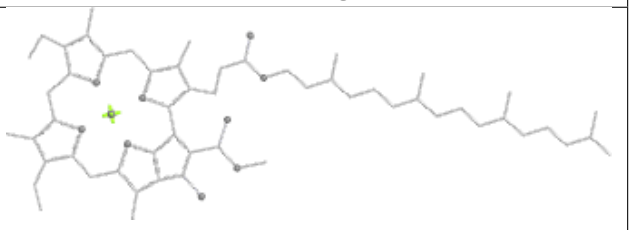


Bond angles

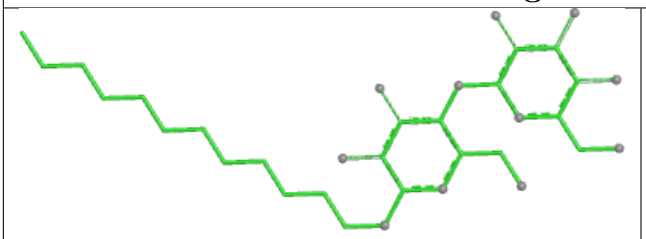


Torsions



Rings

Ligand LMU 8 322



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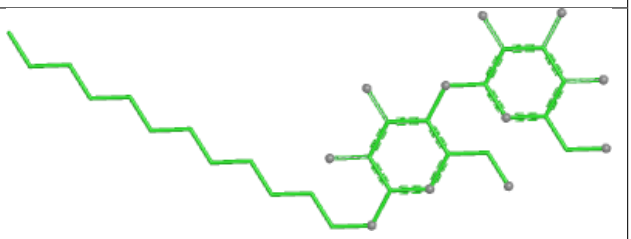
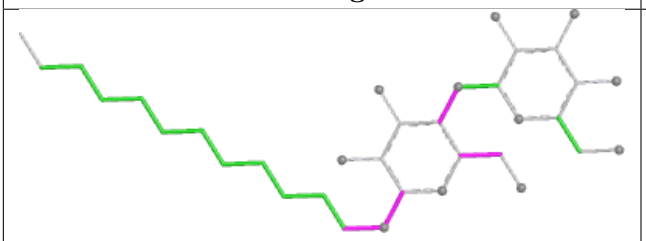


Bond angles



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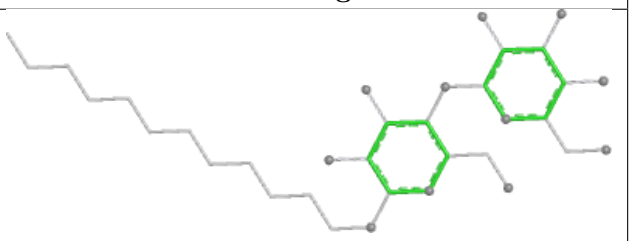
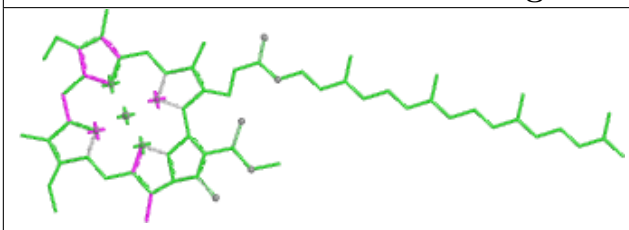


Rings

Ligand CLA F 303



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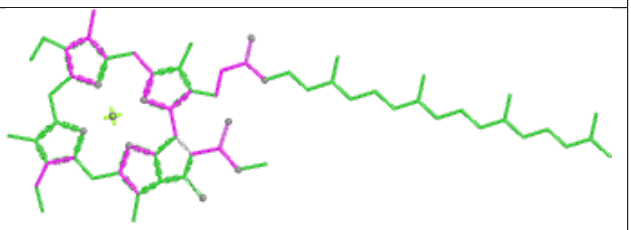

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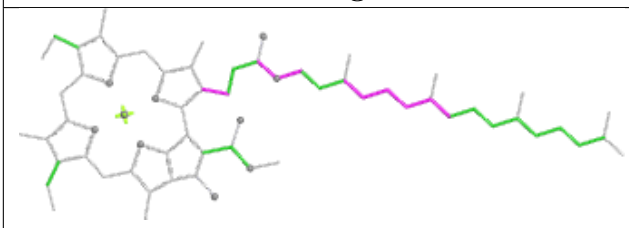

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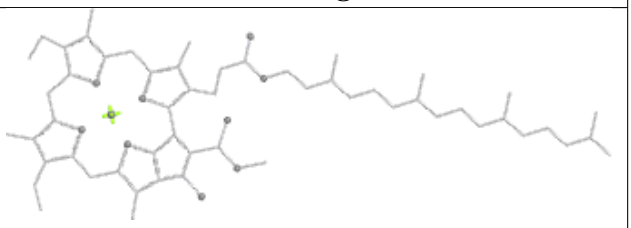
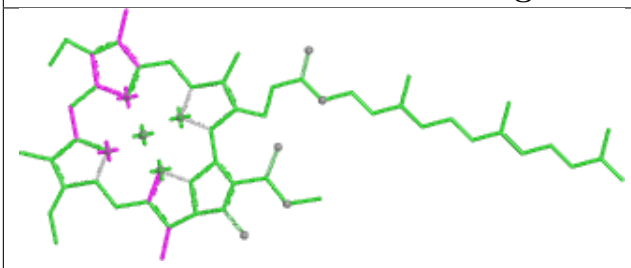


Rings

Ligand CLA A 5042



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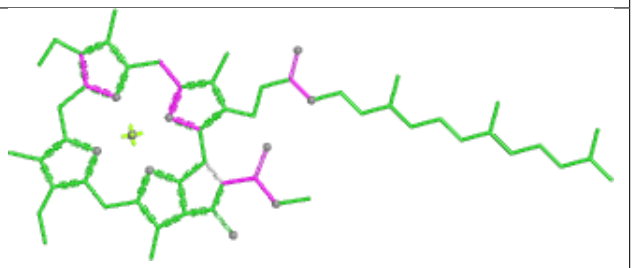

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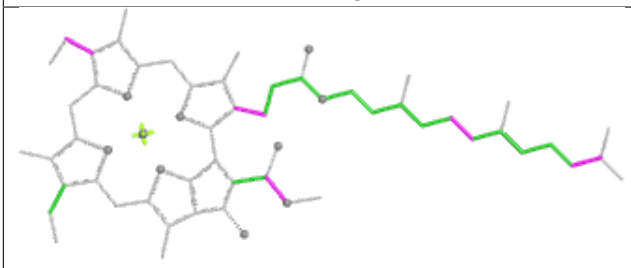

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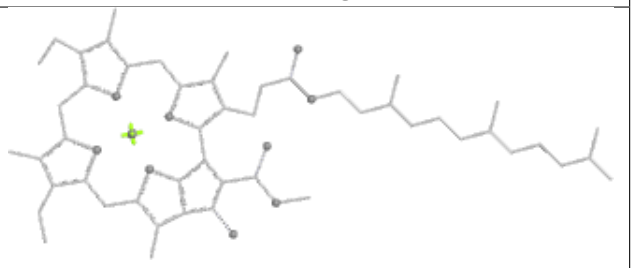
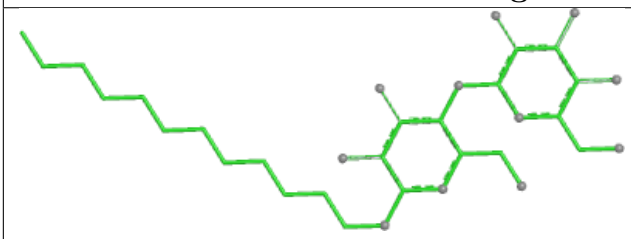


Rings

Ligand LMU A 5053



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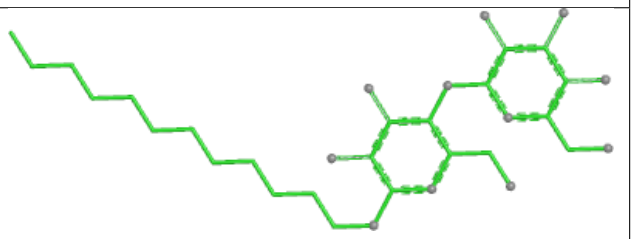

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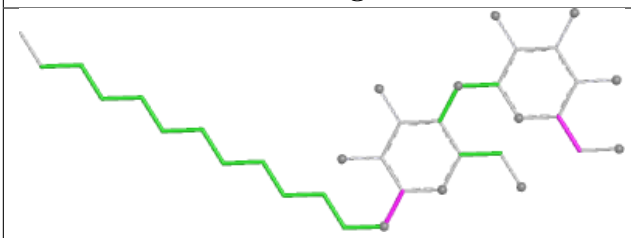

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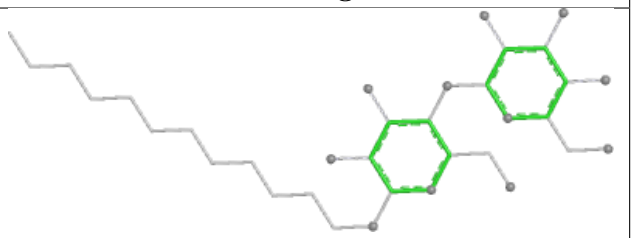
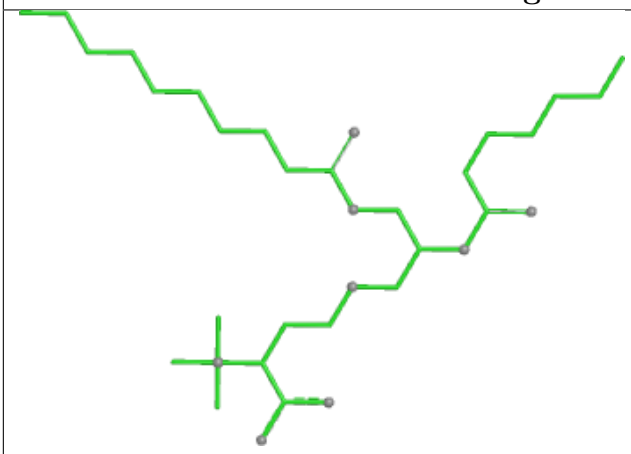


Rings

Ligand LMK J 101



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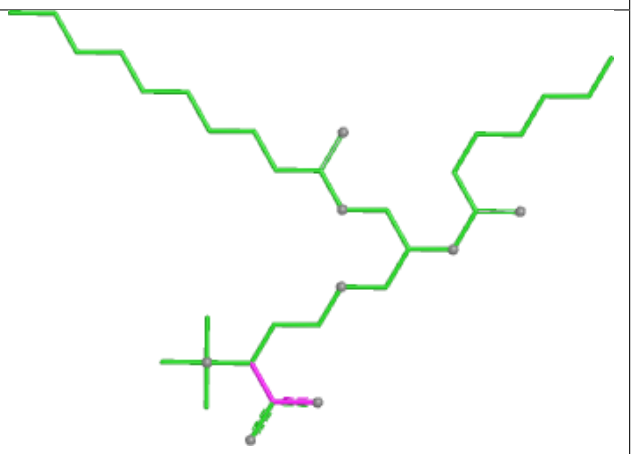

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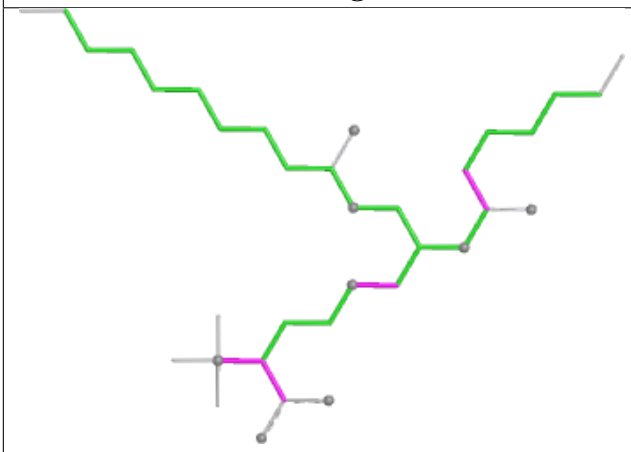

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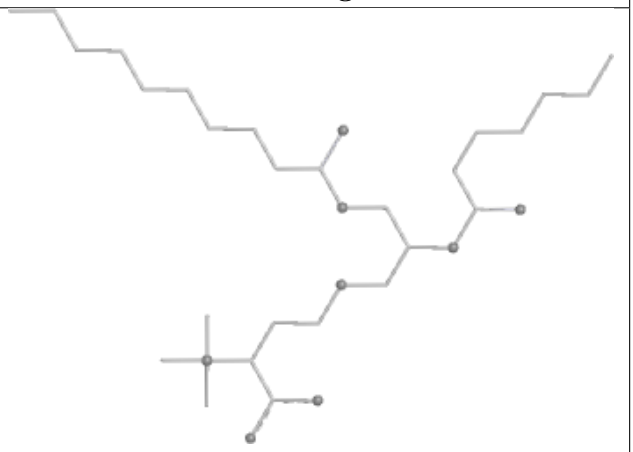
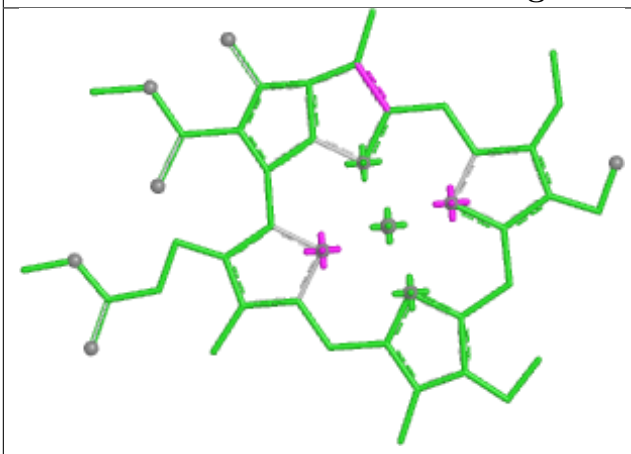


Rings

Ligand CHL 7 307



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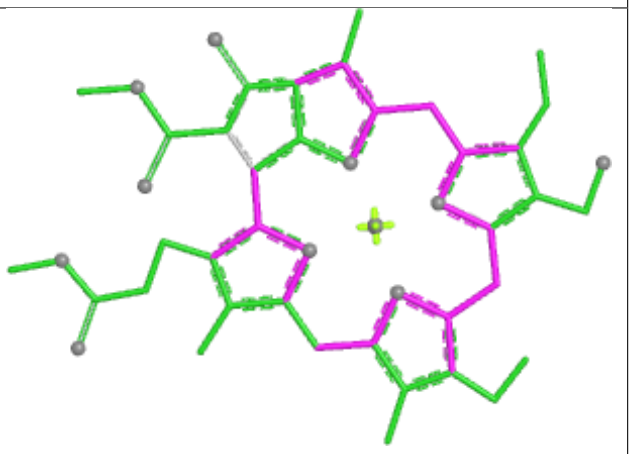
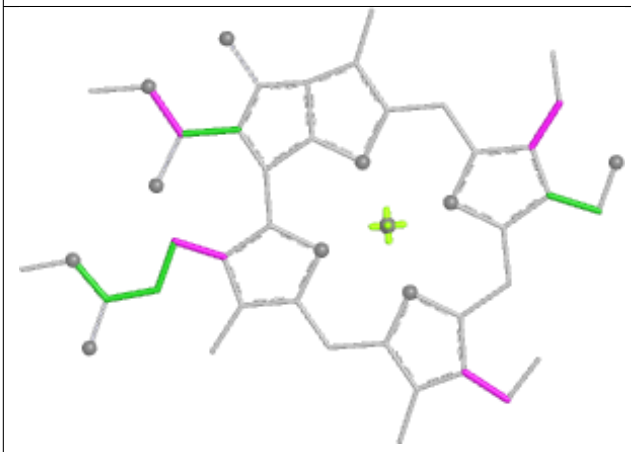


Bond angles



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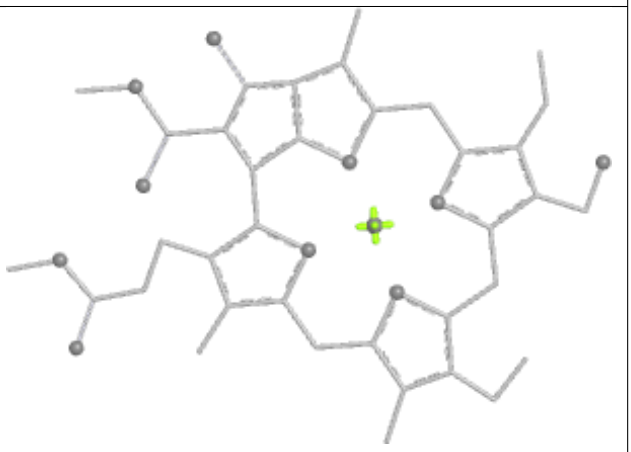
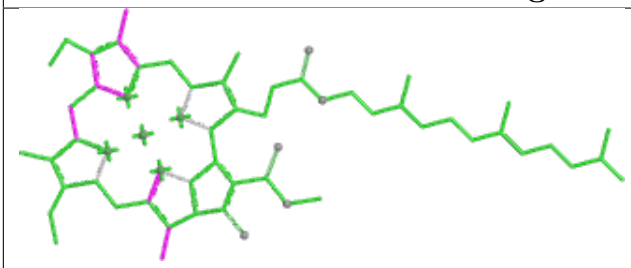


Rings

Ligand CLA 9 607



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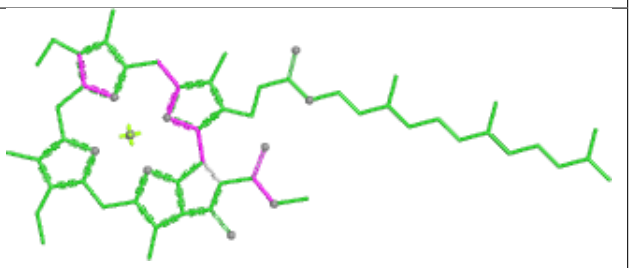

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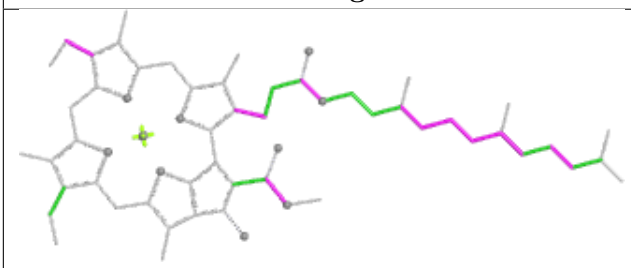

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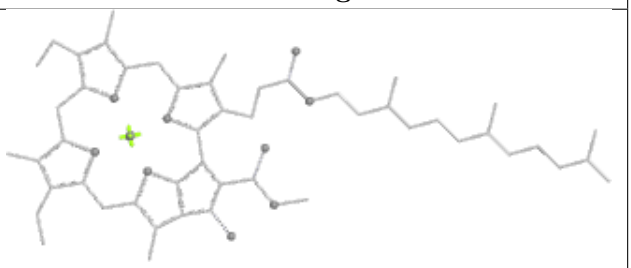
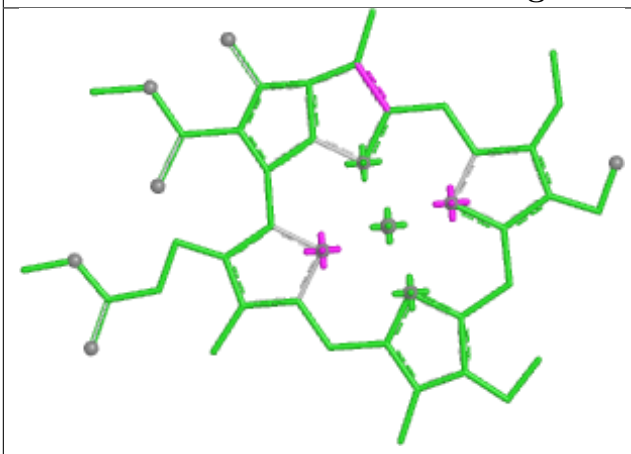


Rings

Ligand CHL 8 305



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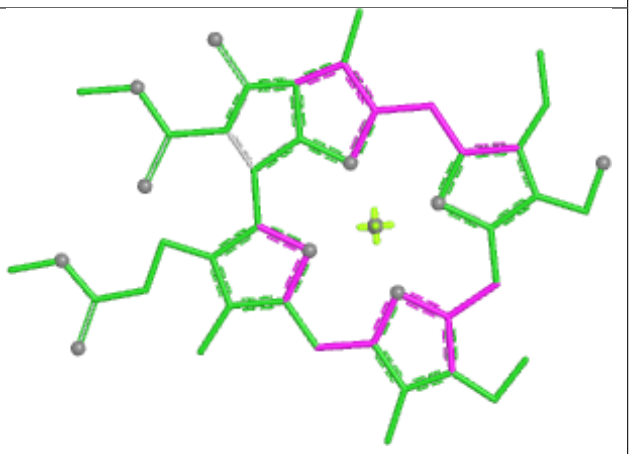
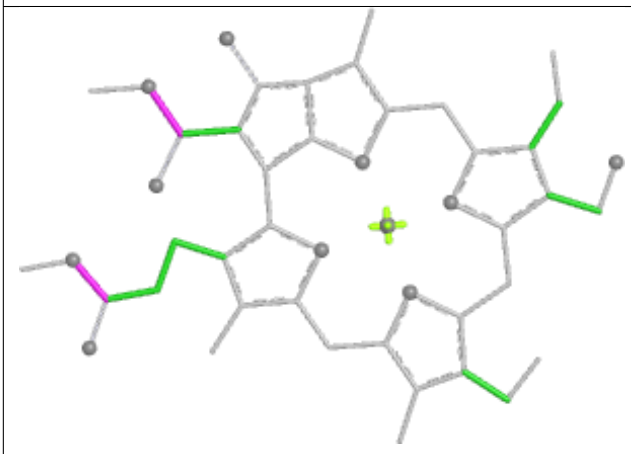


Bond angles



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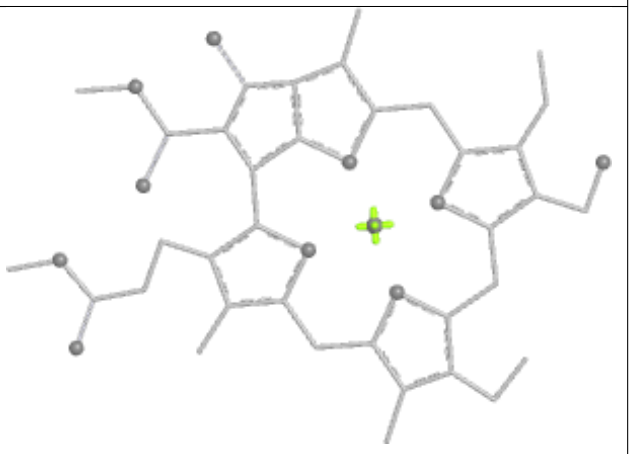
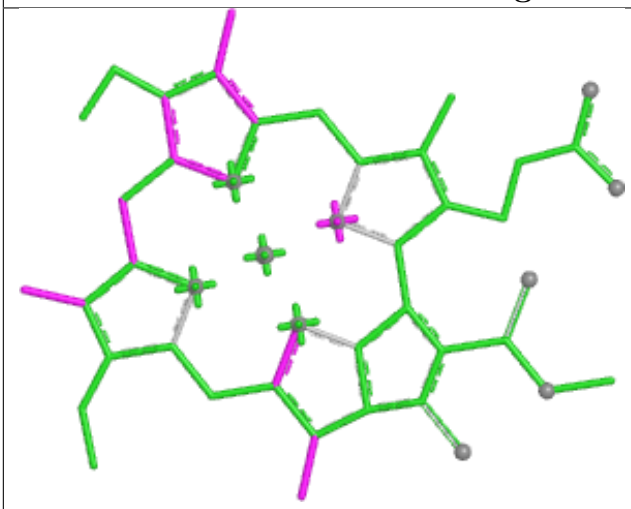


Rings

Ligand CLA K 4004



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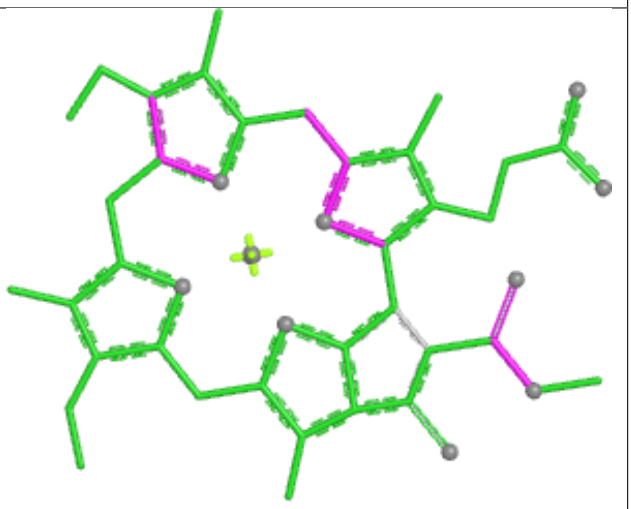
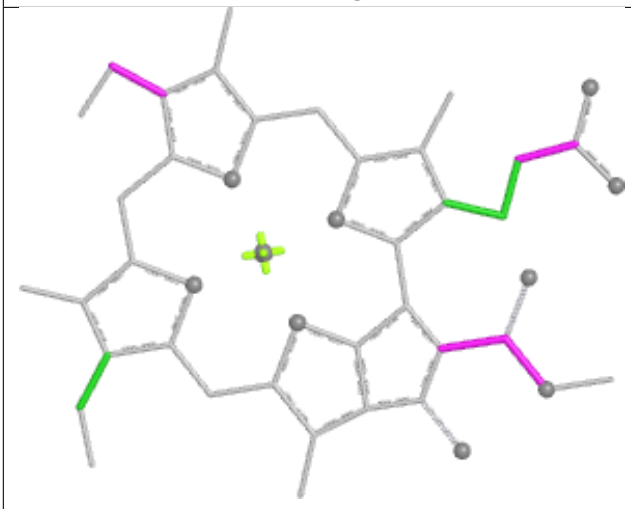


Bond angles

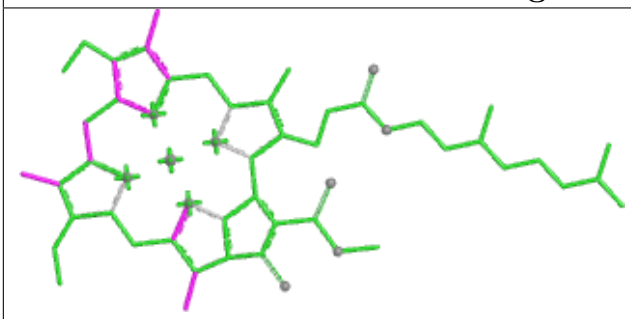


Torsions



Rings

Ligand CLA 1 609



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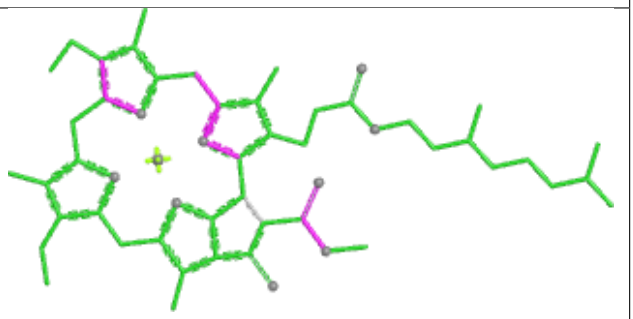

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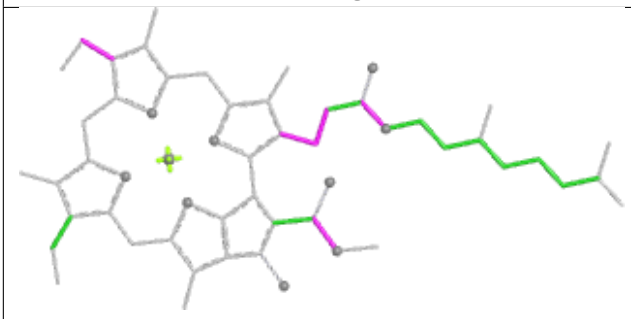

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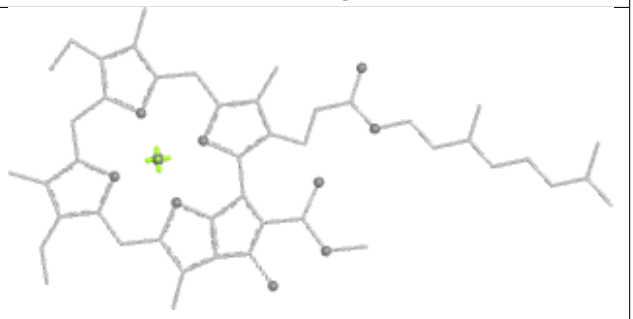
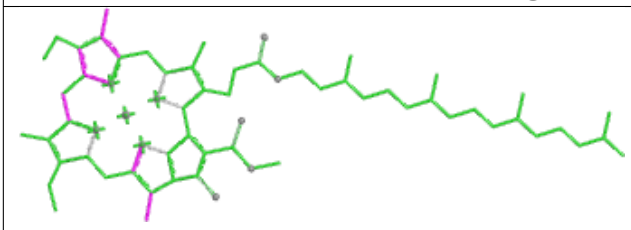


Rings

Ligand CLA B 822



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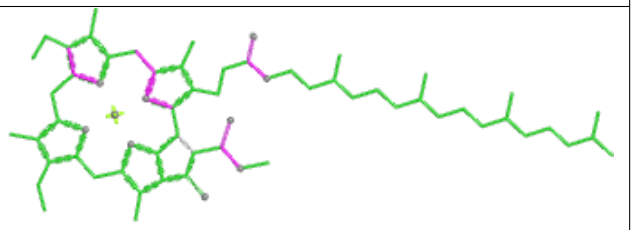
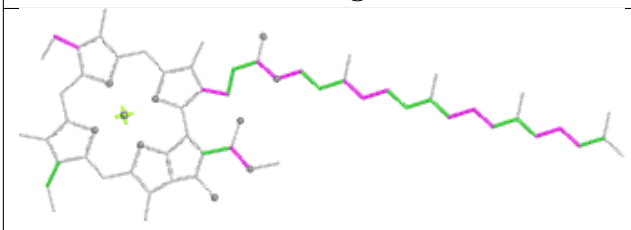


Bond angles



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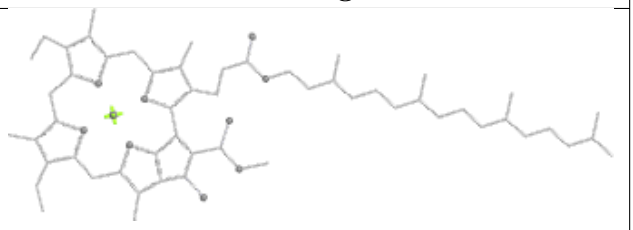
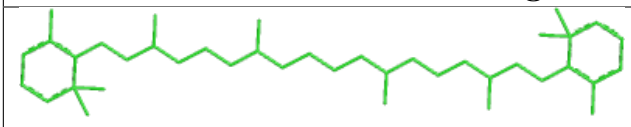


Rings

Ligand BCR L 203



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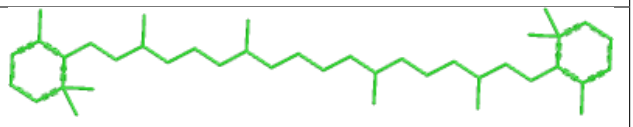
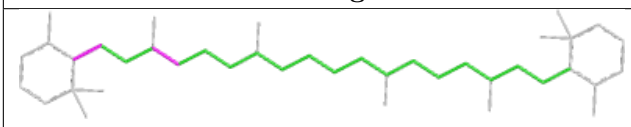


Bond angles



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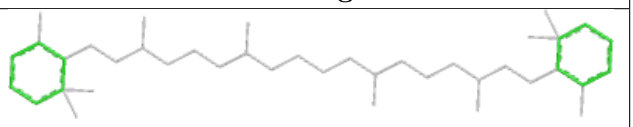
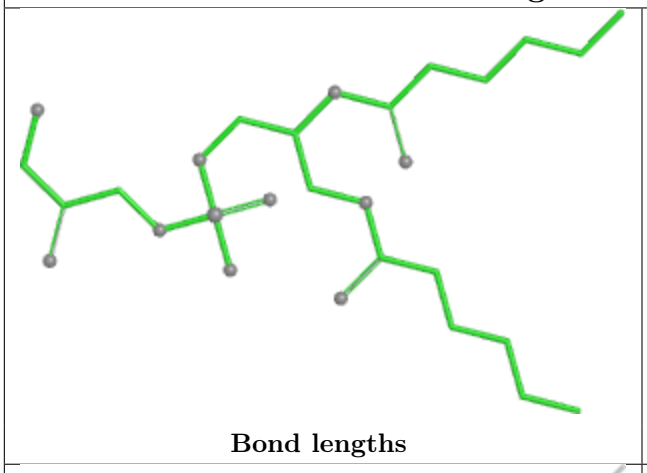


Rings

Ligand LHG 8 317



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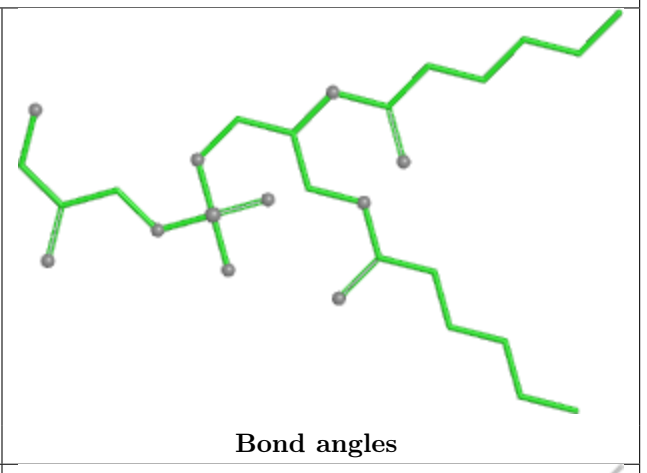
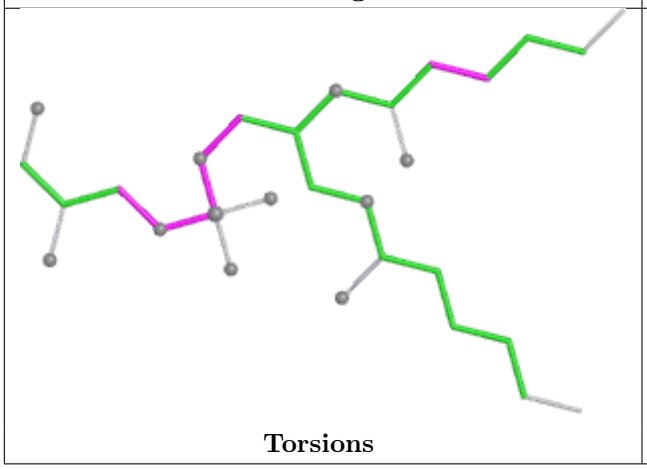


Bond angles



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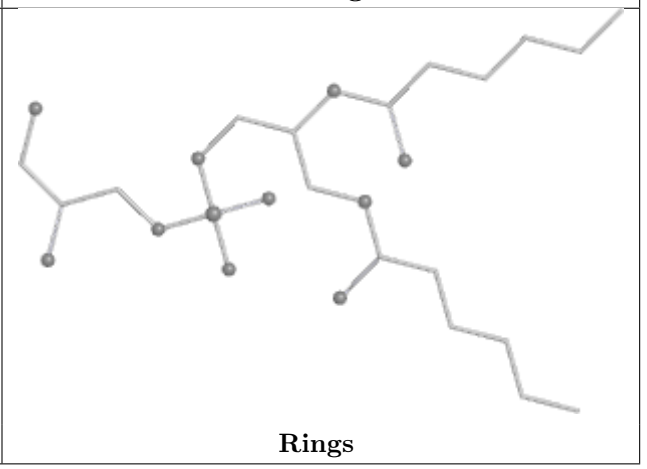


Rings

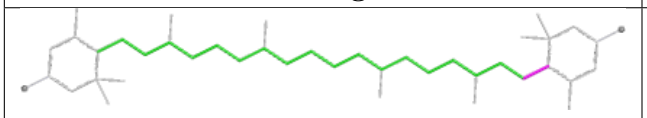
Ligand LUT 8 314



Bond lengths



Bond angles



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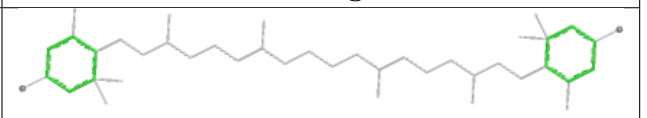
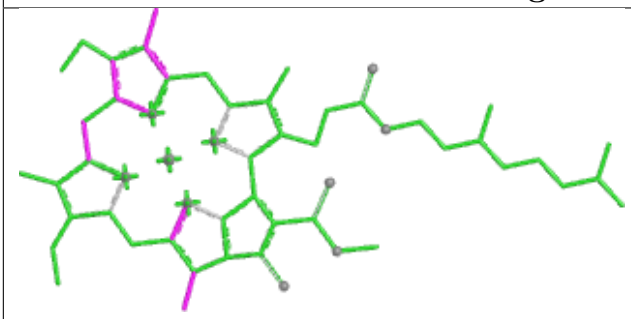
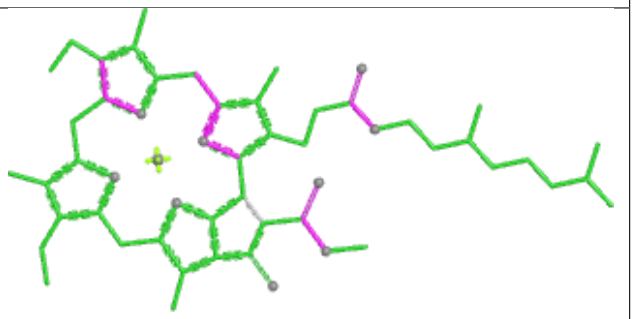


Rings

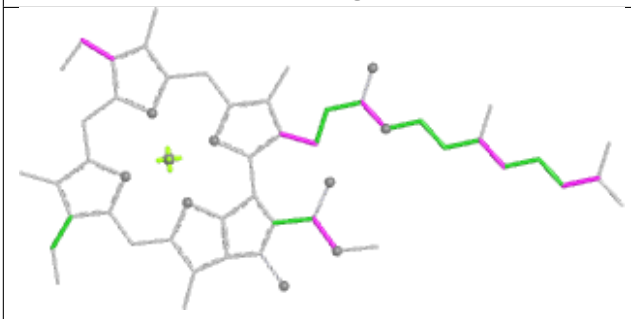
Ligand CLA 3 324



Bond lengths



Bond angles



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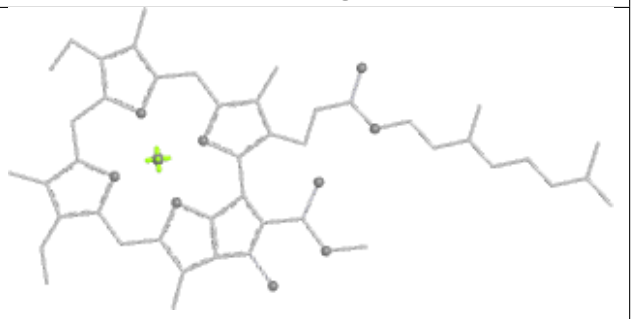
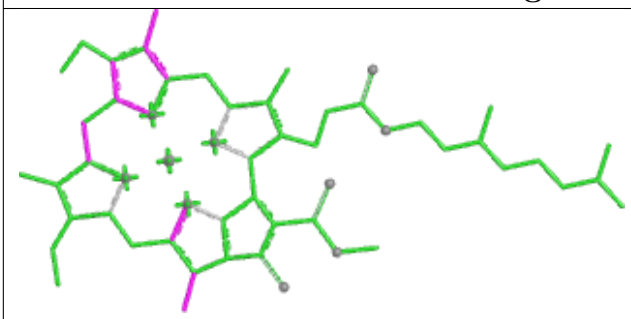
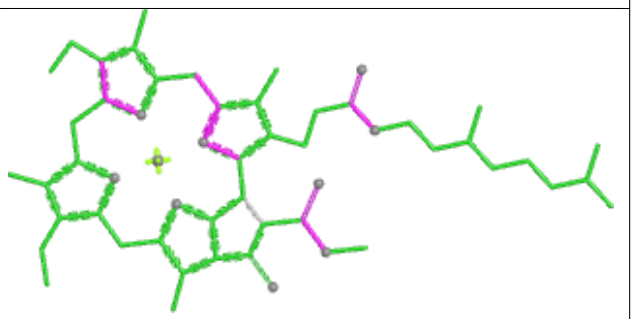


Rings

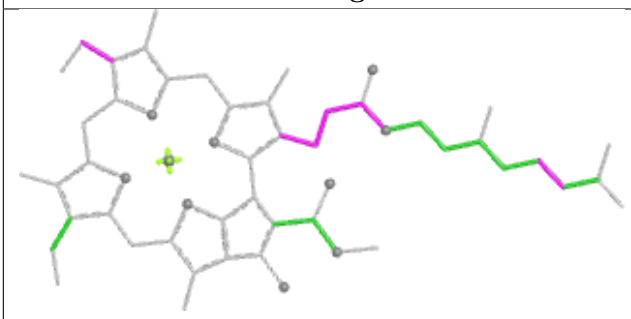
Ligand CLA B 821



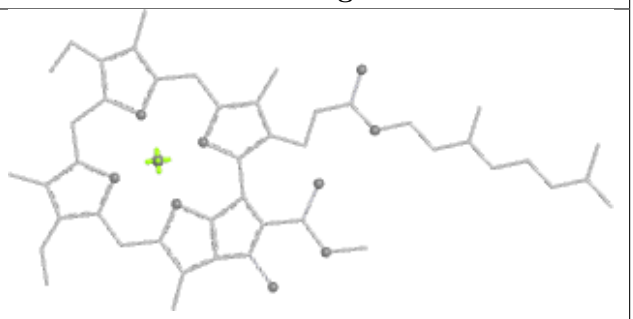
Bond lengths



Bond angles

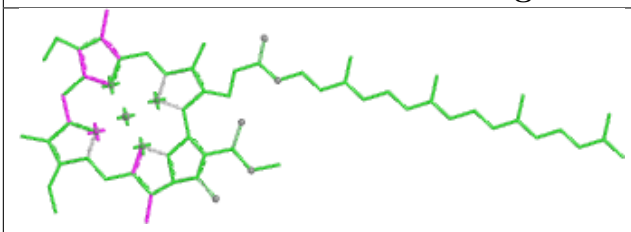


Torsions



Rings

Ligand CLA A 5041



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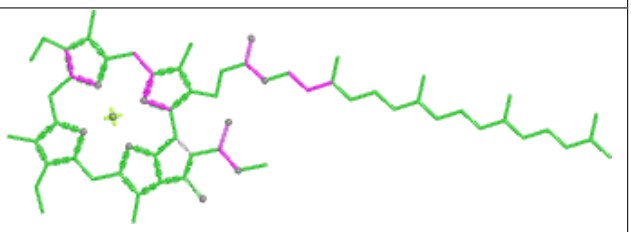

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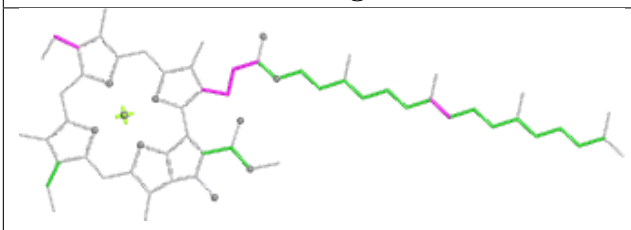

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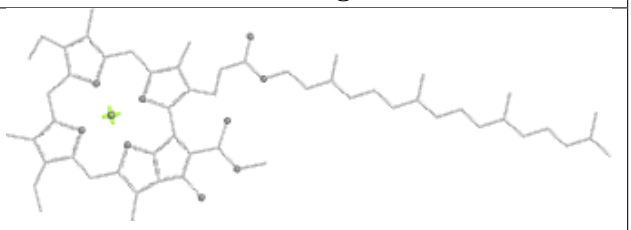
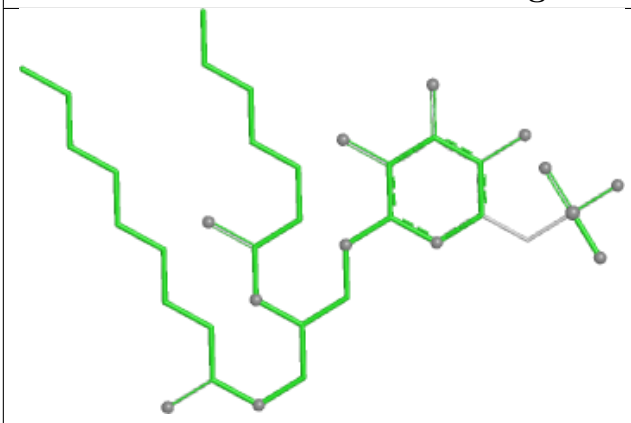


Rings

Ligand SQD 1 619



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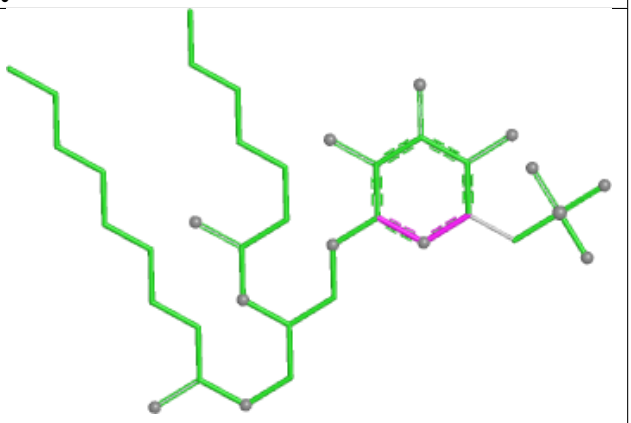

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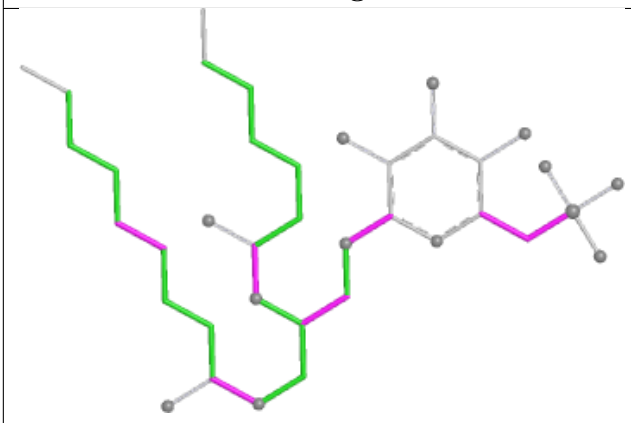

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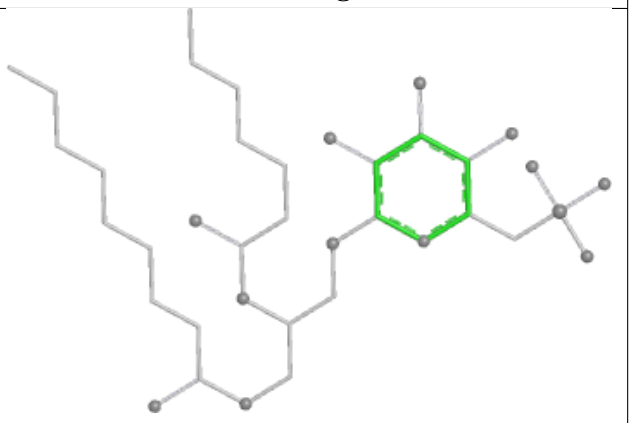
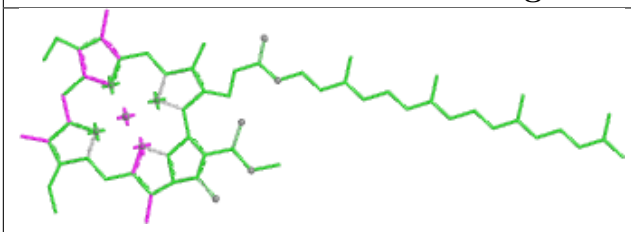


Rings

Ligand CLA B 820



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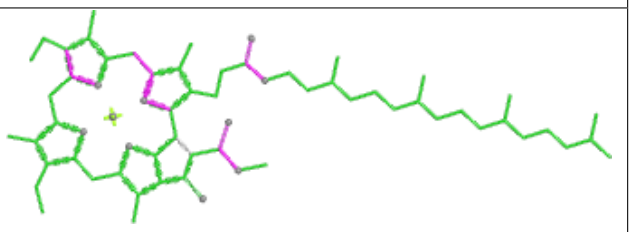

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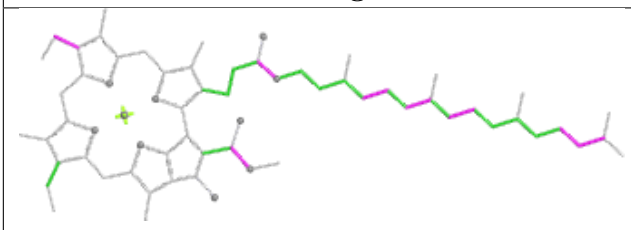

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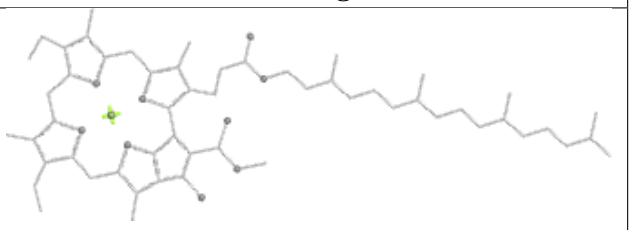
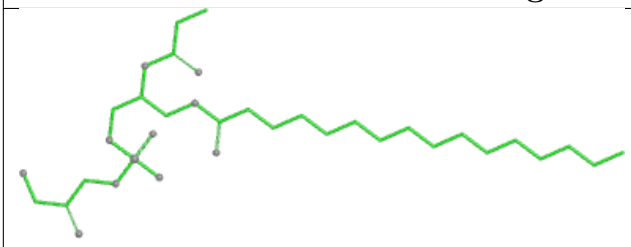


Rings

Ligand LHG 9 617



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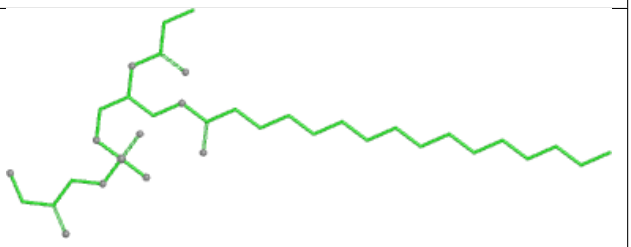

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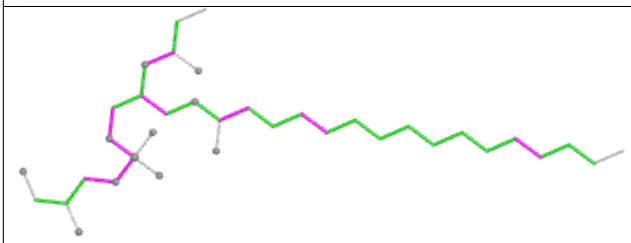

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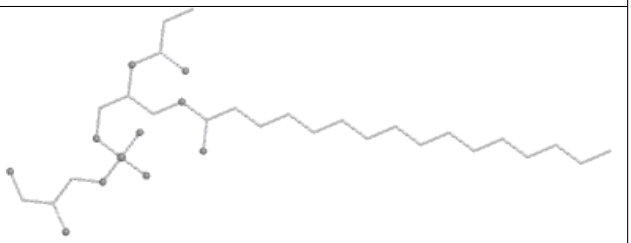
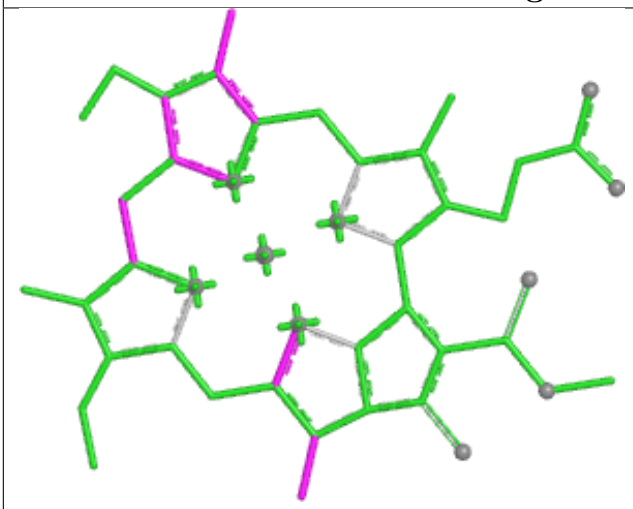


Rings

Ligand CLA F 308



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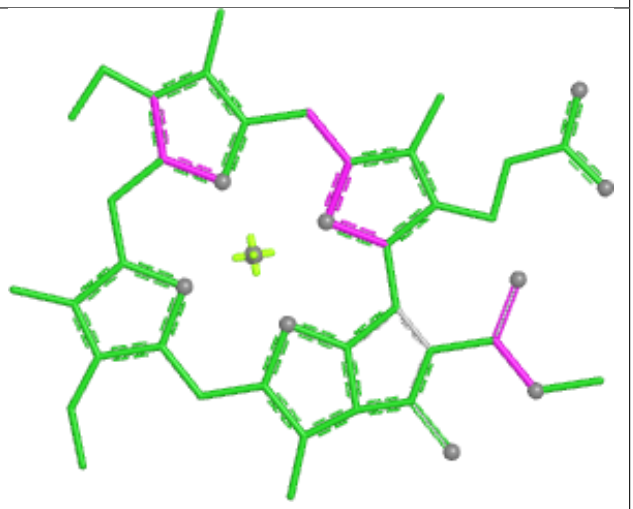

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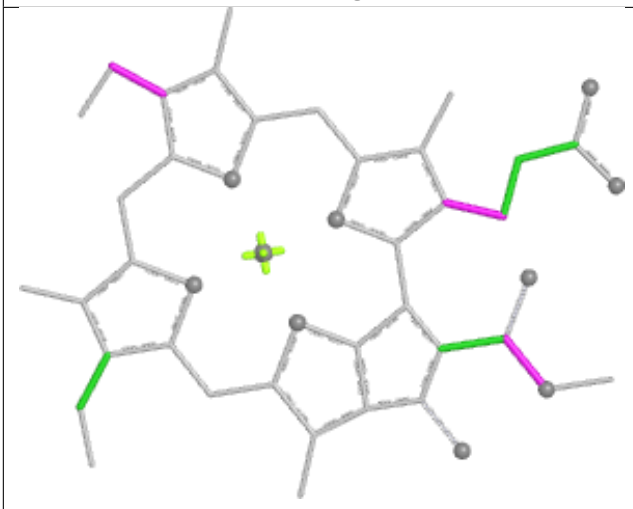
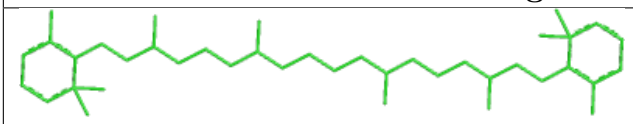


Torsions



Rings

Ligand BCR J 106



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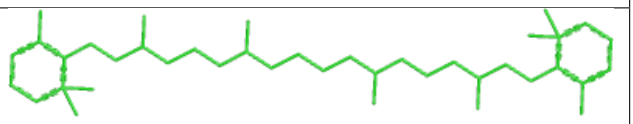

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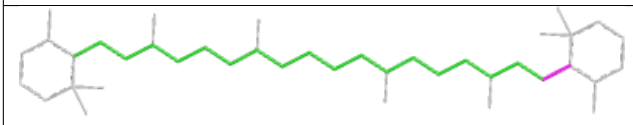

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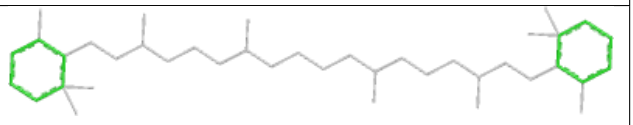
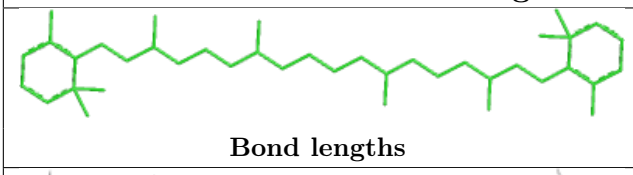


Rings

Ligand BCR K 4001



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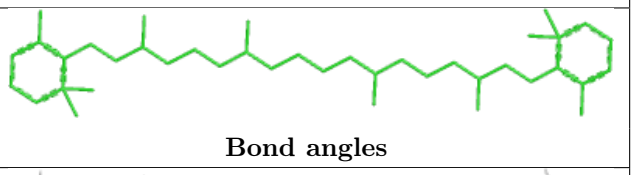

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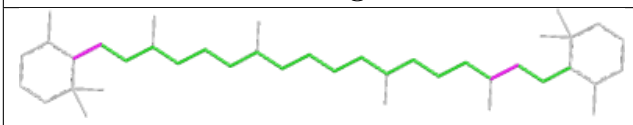

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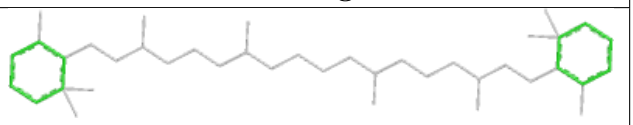
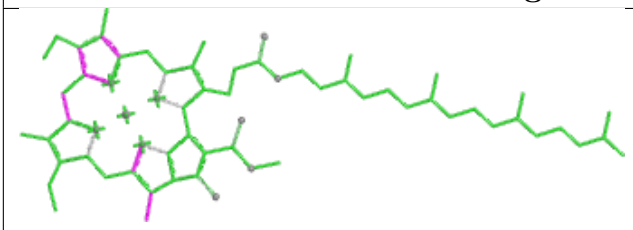


Rings

Ligand CLA B 829



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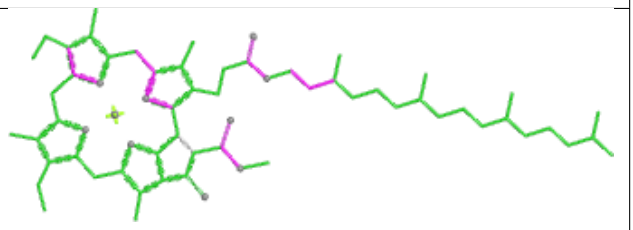
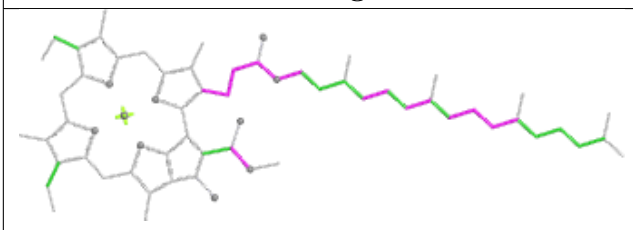


Bond angles



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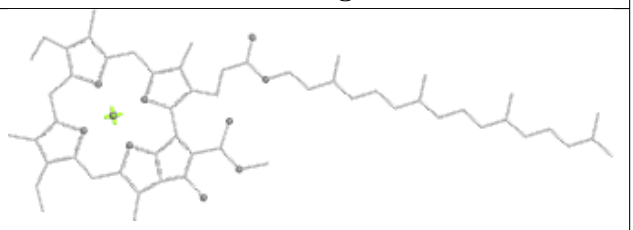
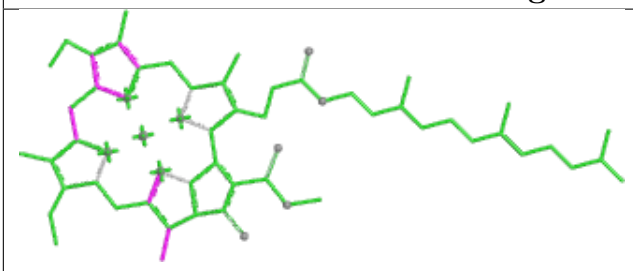


Rings

Ligand CLA 9 602



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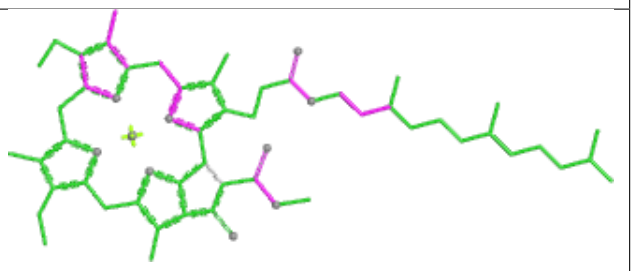

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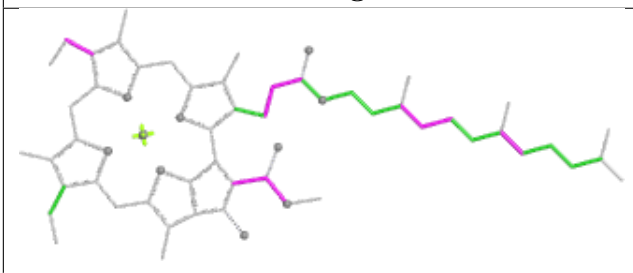

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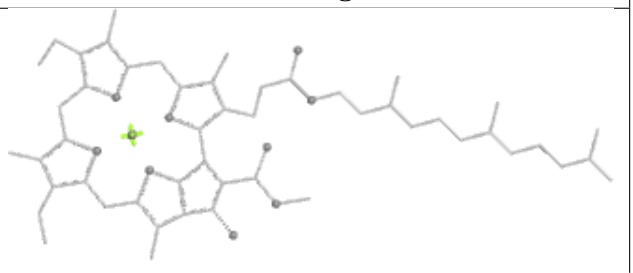
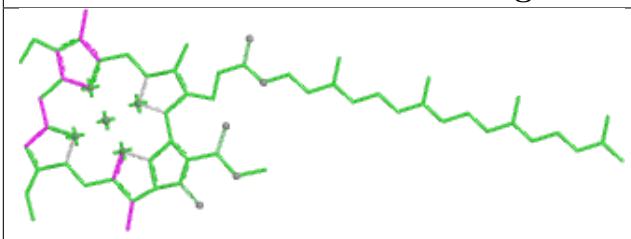


Rings

Ligand CLA A 5036



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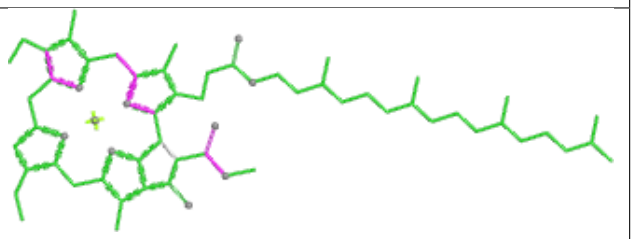

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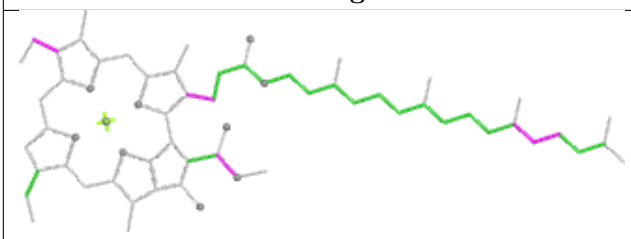

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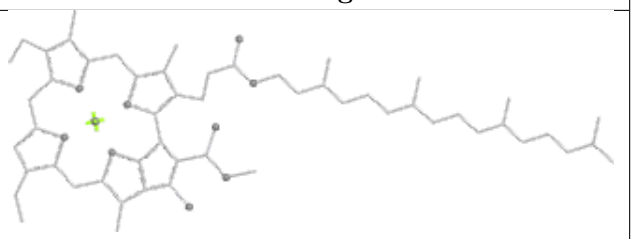
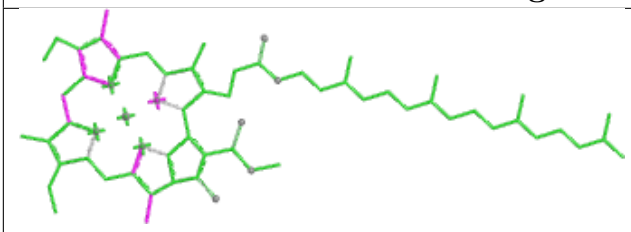


Rings

Ligand CLA 3 302



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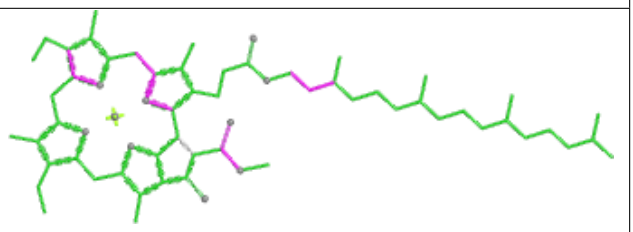

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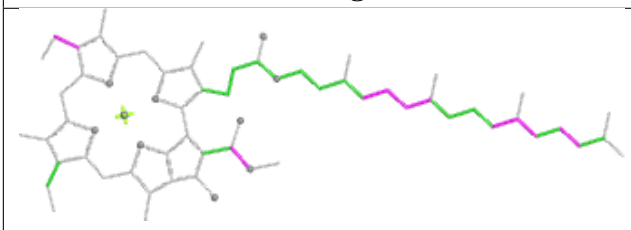

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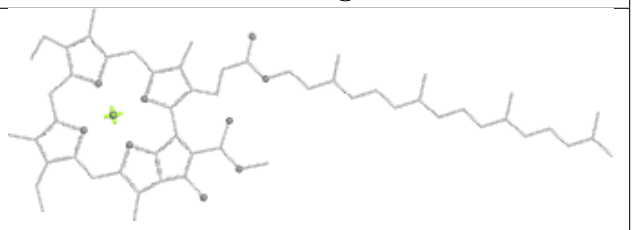
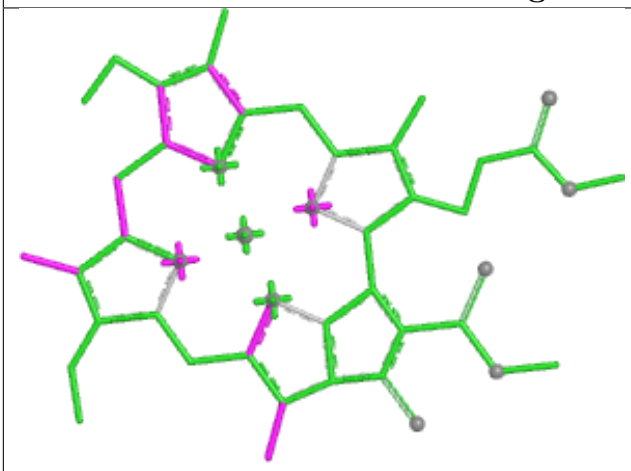


Rings

Ligand CLA 8 310



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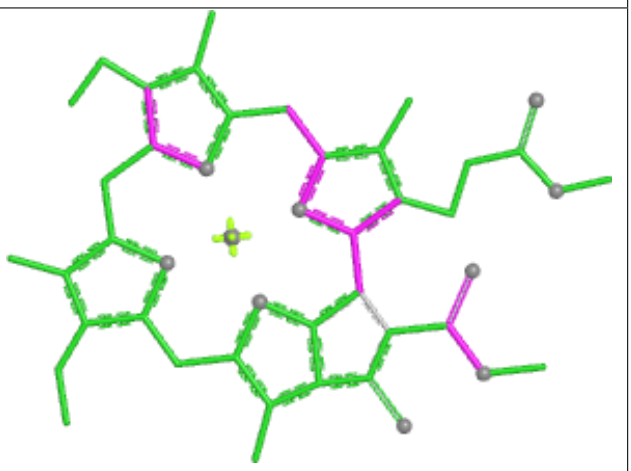
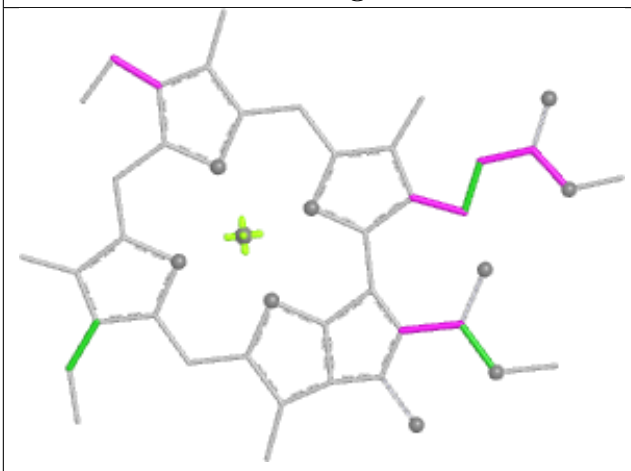


Bond angles



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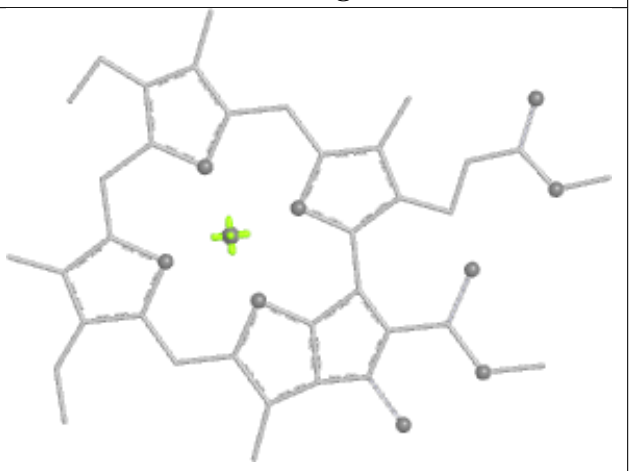
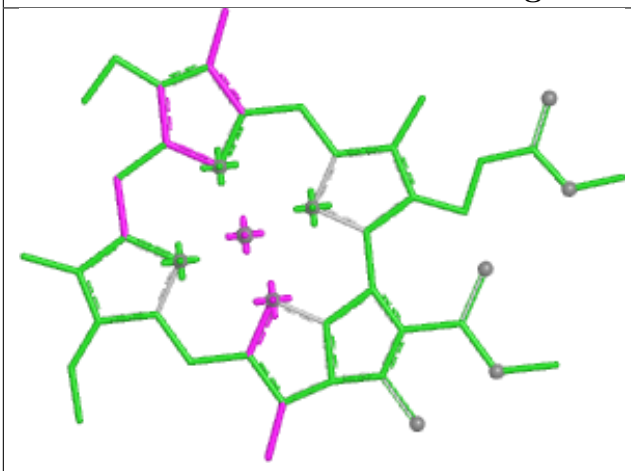


Rings

Ligand CLA B 813



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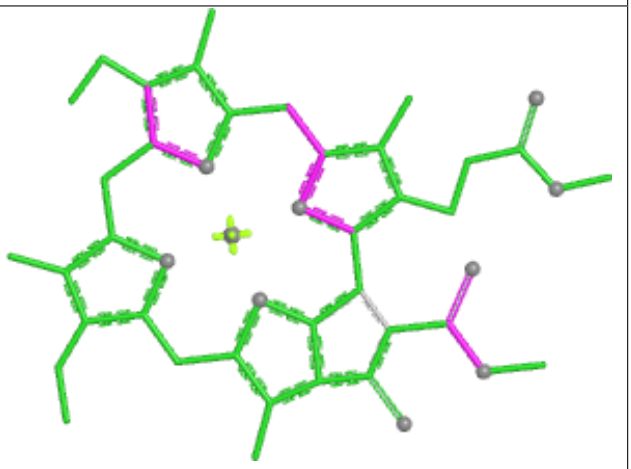
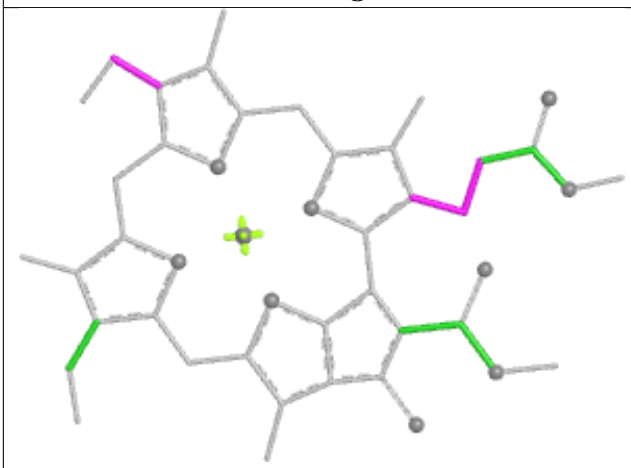


Bond angles



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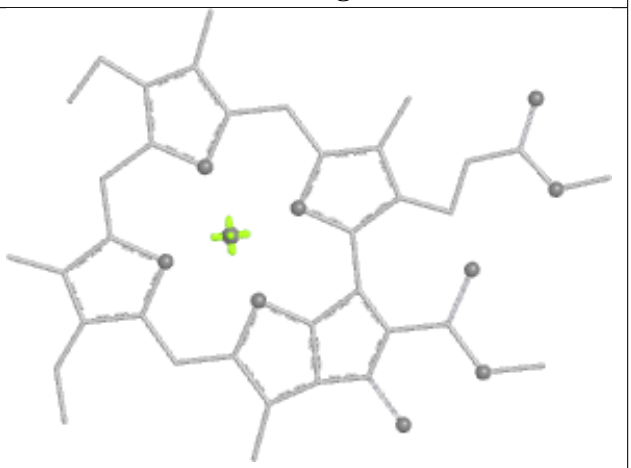
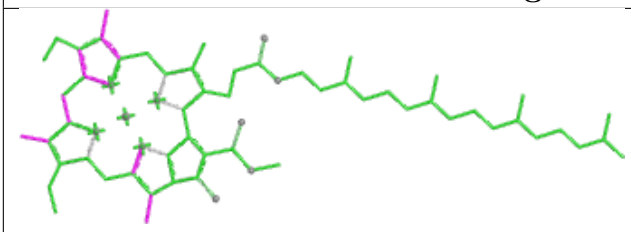


Rings

Ligand CLA B 811



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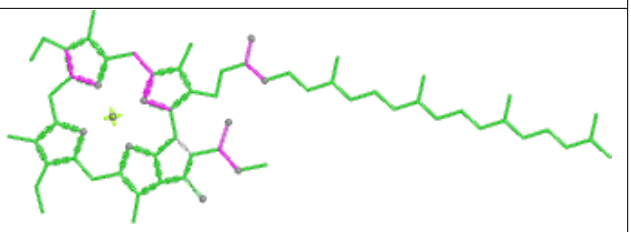
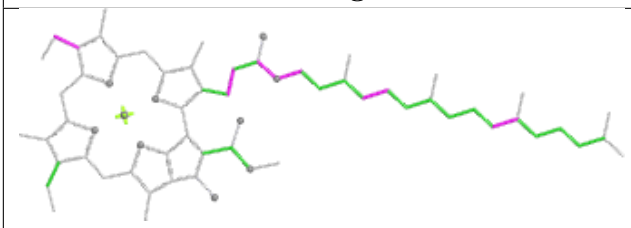


Bond angles



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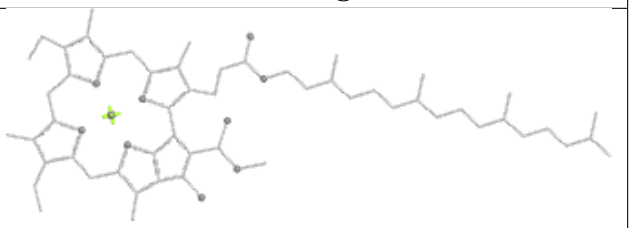
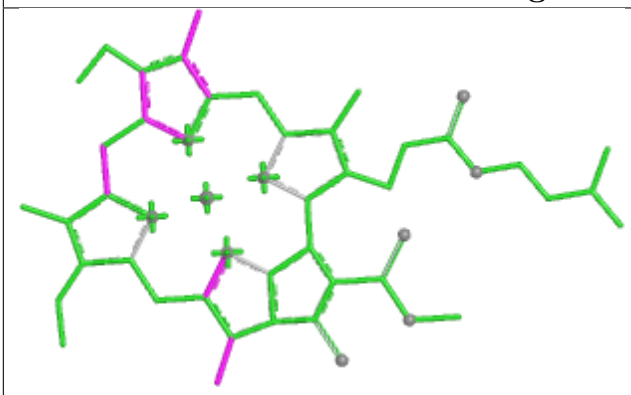
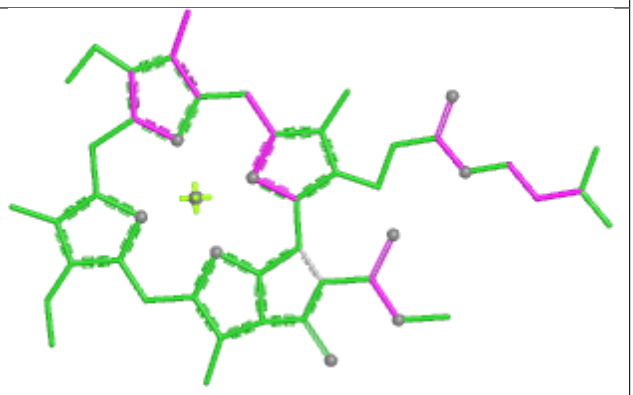


Rings

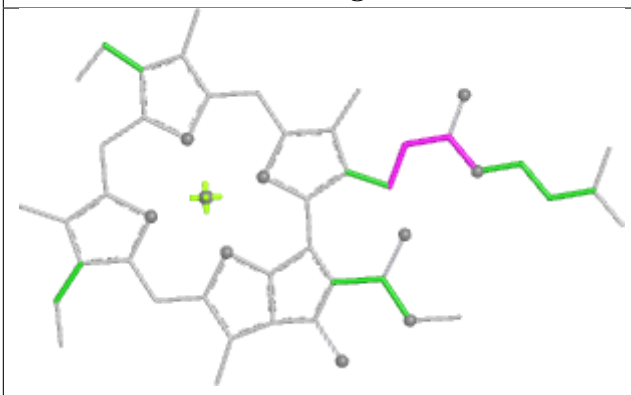
Ligand CLA 3 305



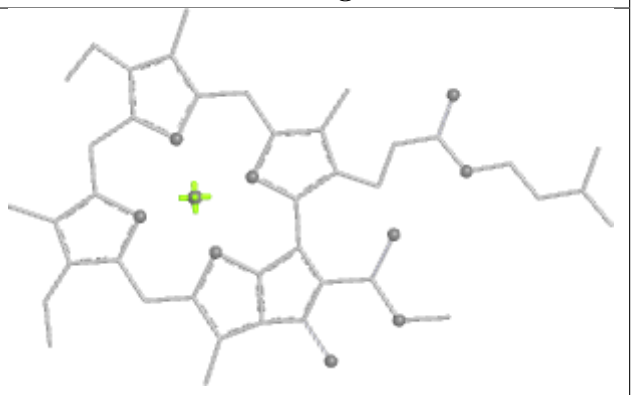
Bond lengths



Bond angles

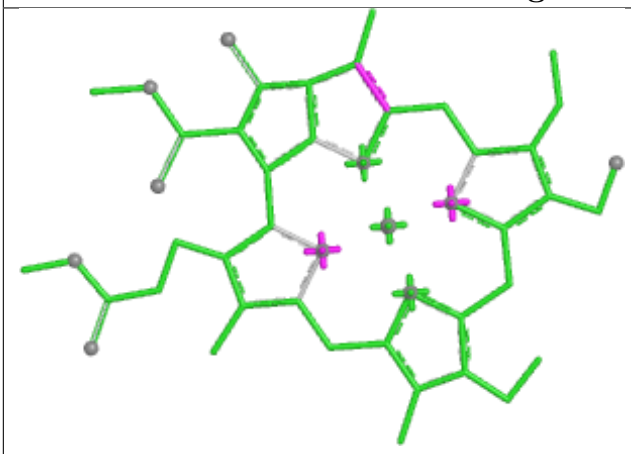


Torsions



Rings

Ligand CHL 8 304



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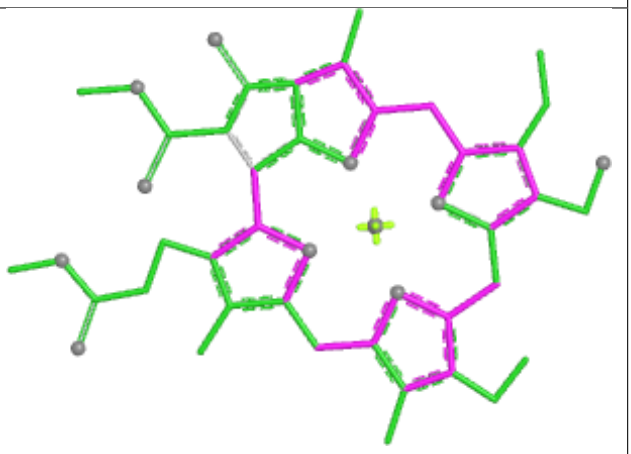

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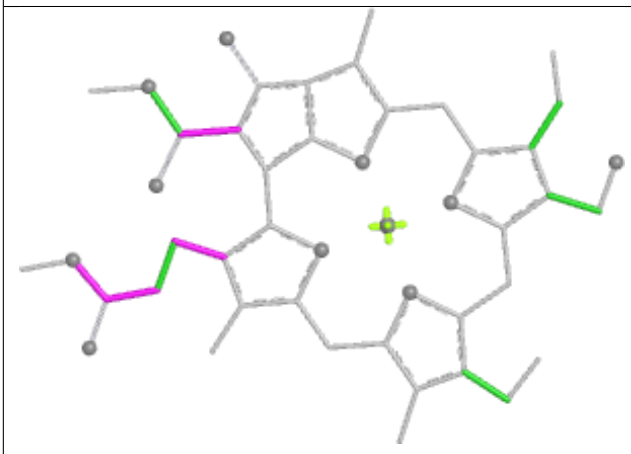

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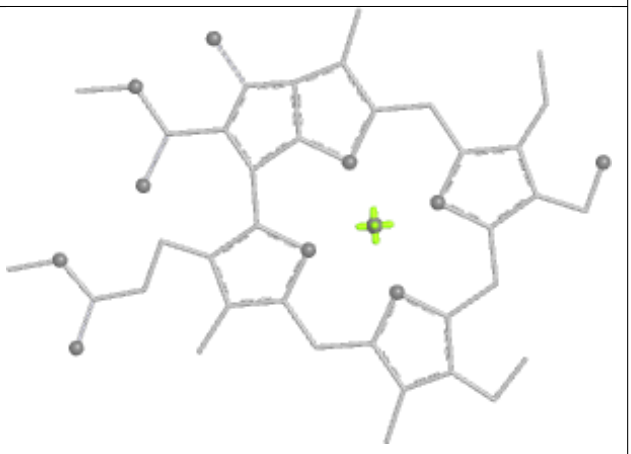
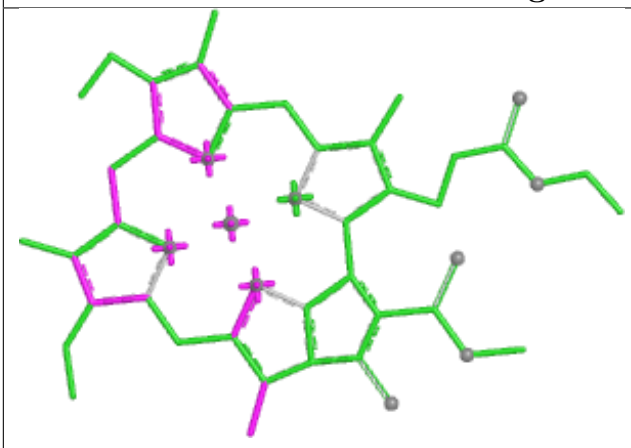


Rings

Ligand CLA 8 307



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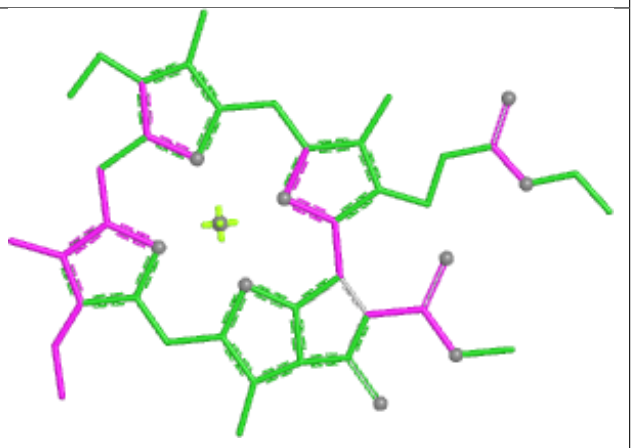

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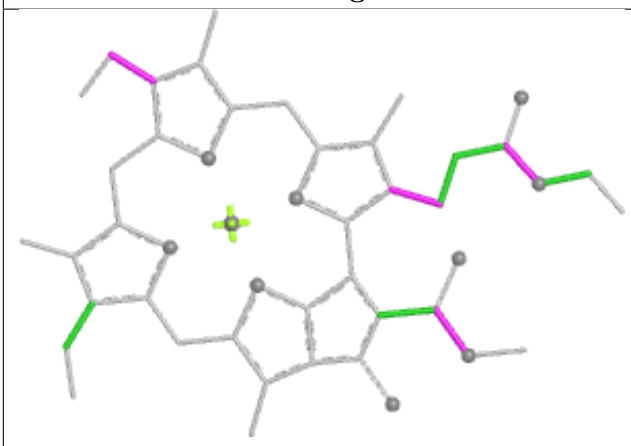

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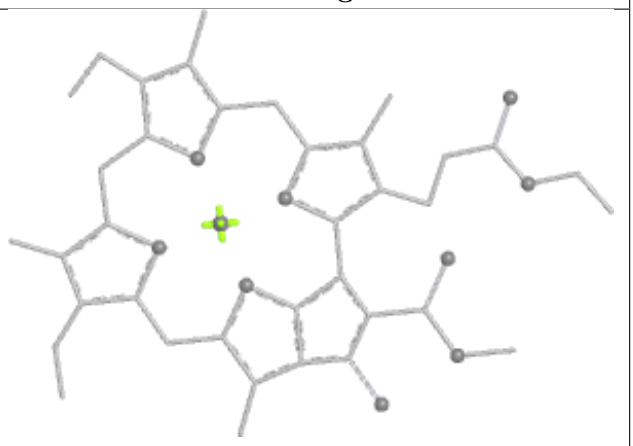
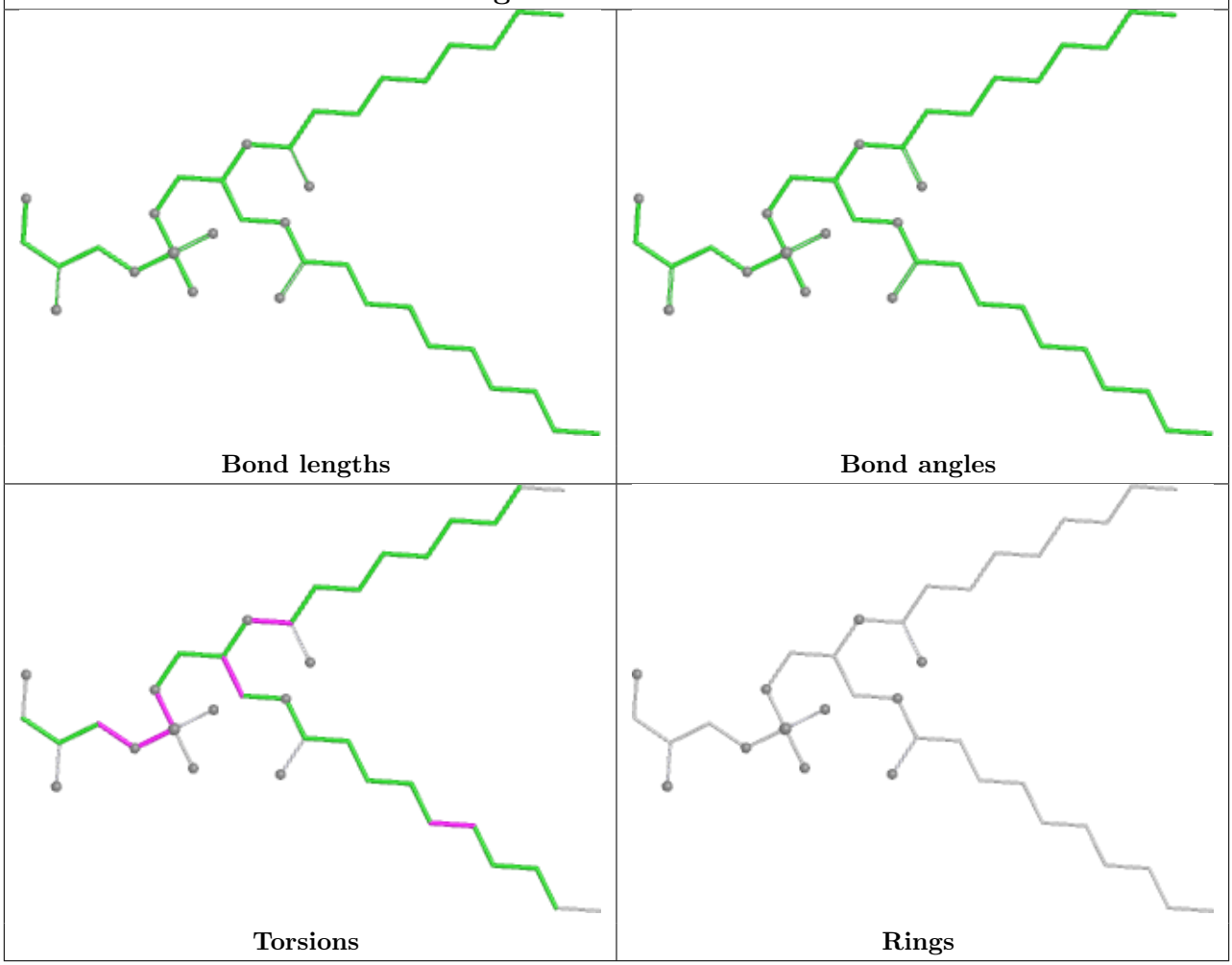
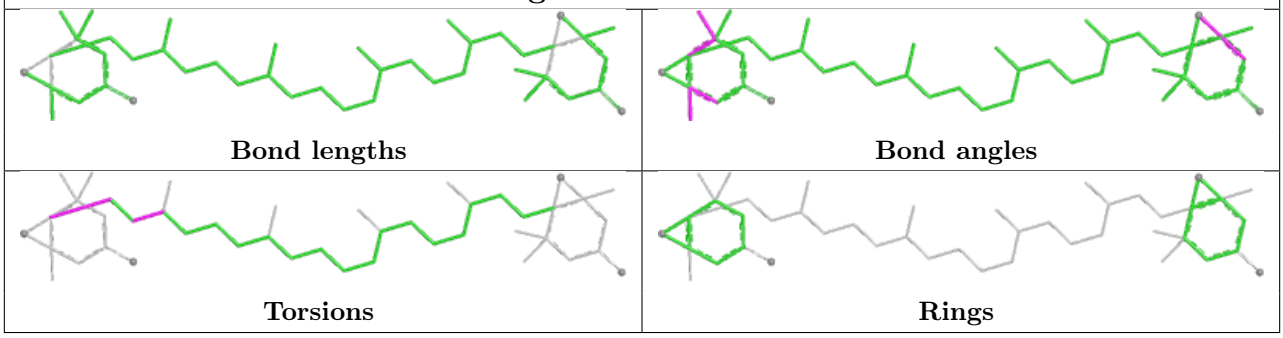


Rings

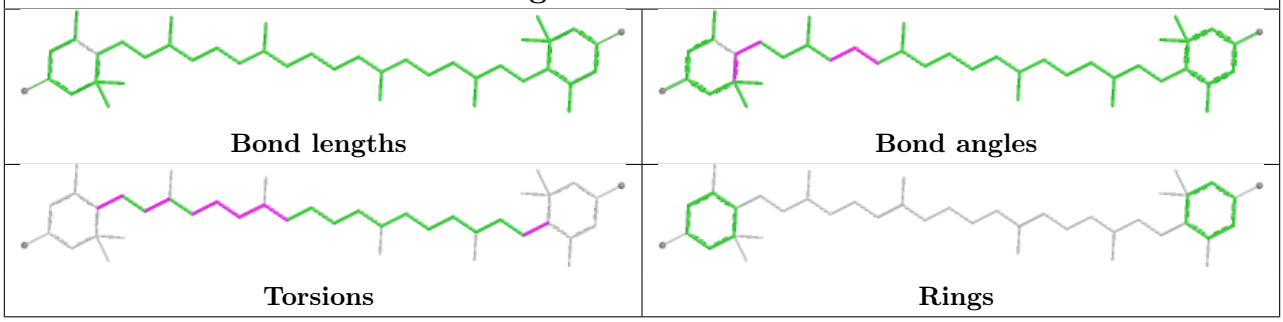
Ligand LHG A 5002



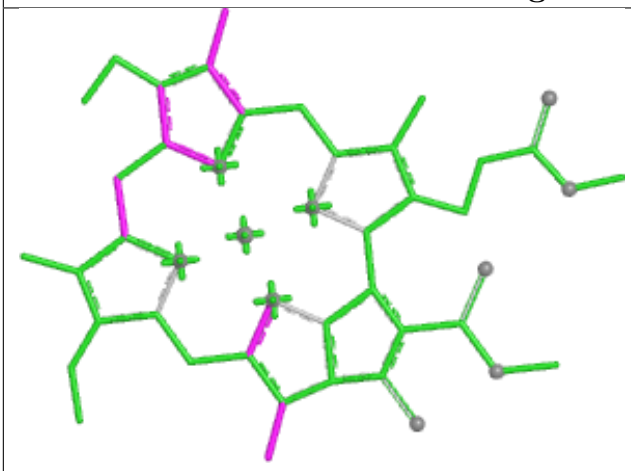
Ligand XAT 7 317



Ligand LUT 2 315



Ligand CLA 3 312



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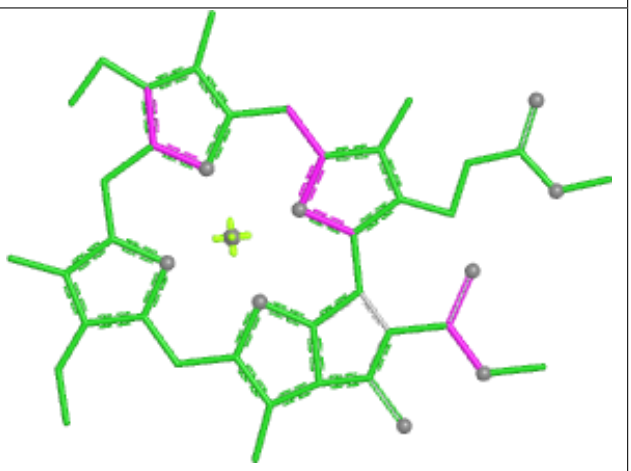
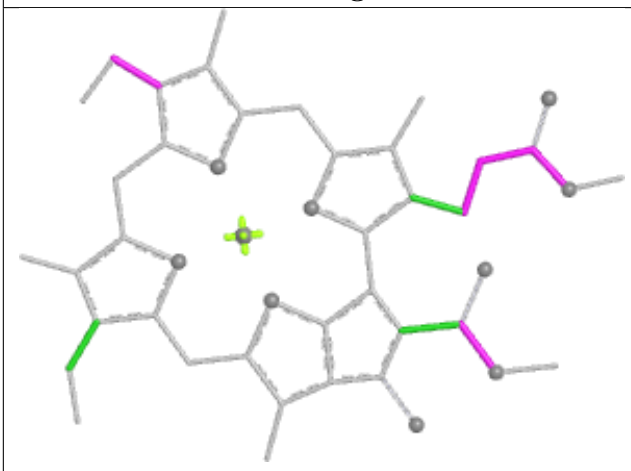


Bond angles



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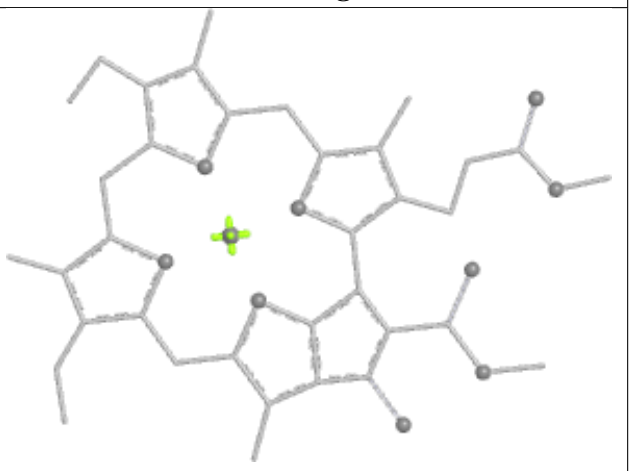
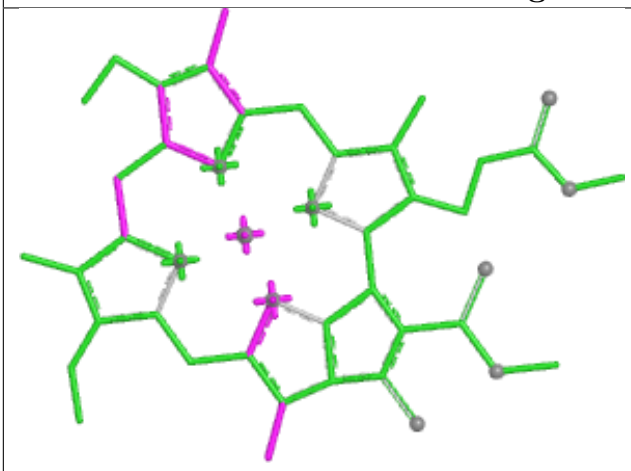


Rings

Ligand CLA 8 313



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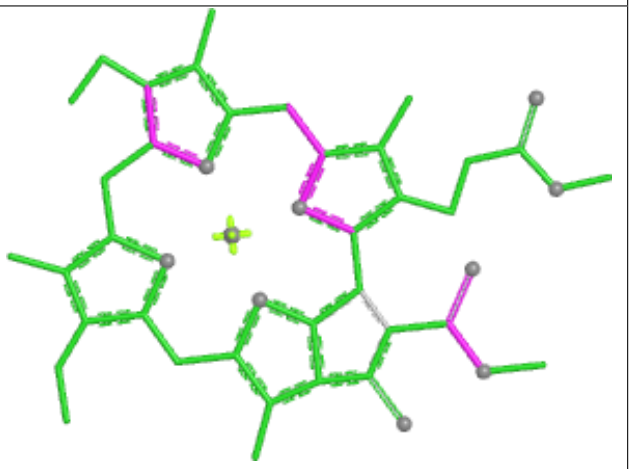

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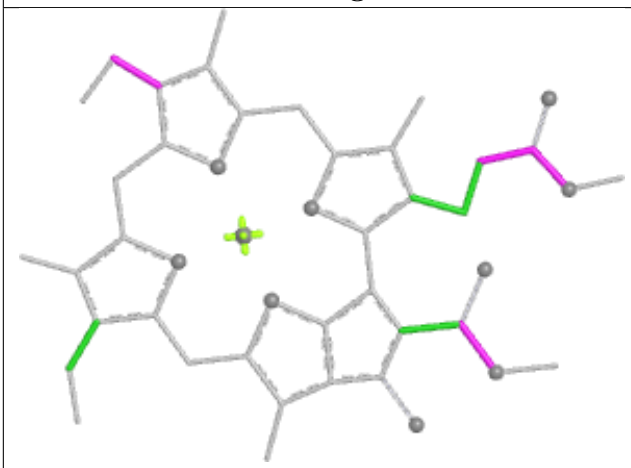

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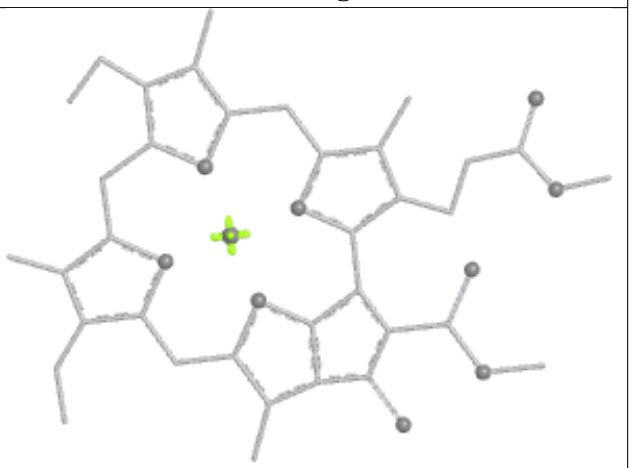
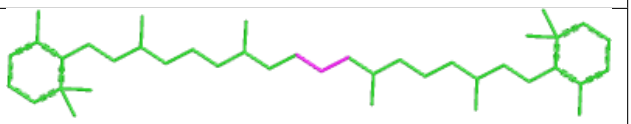


Rings

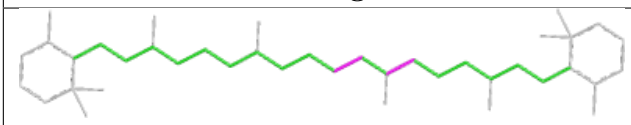
Ligand BCR B 803



Bond lengths



Bond angles



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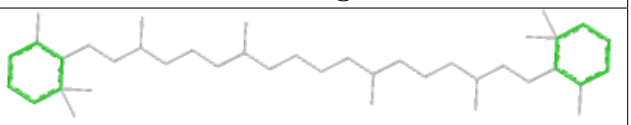
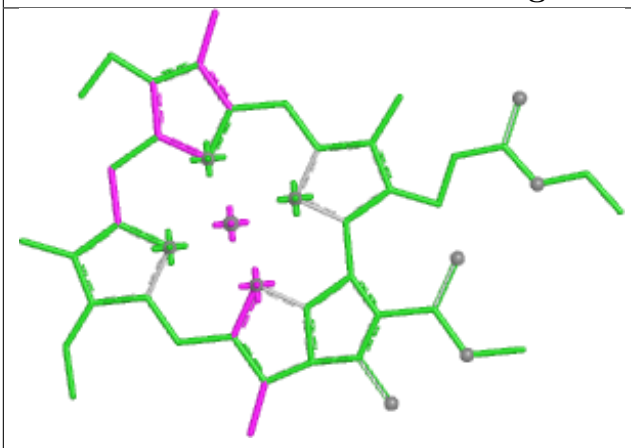


Rings

Ligand CLA 7 323



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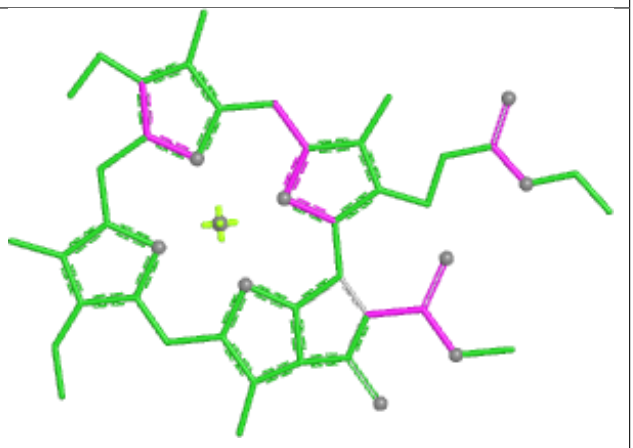

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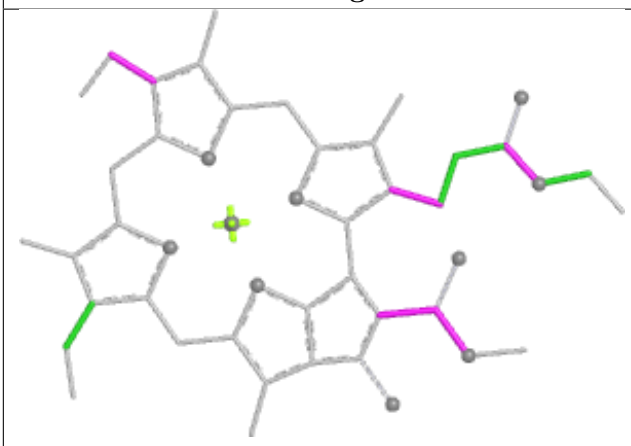

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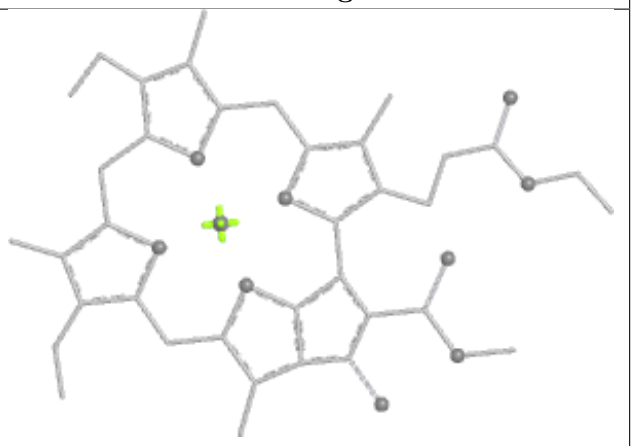
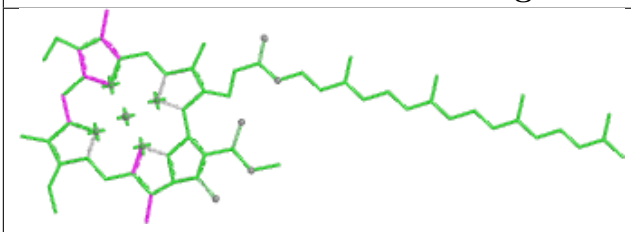


Rings

Ligand CLA A 5013



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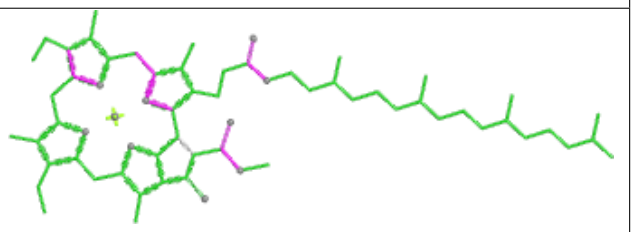
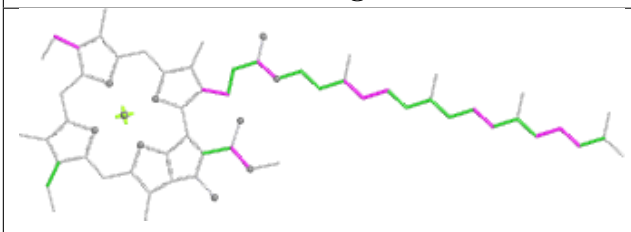


Bond angles



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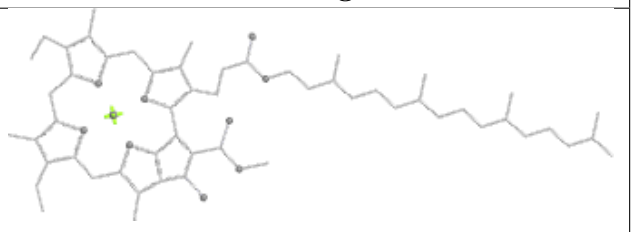
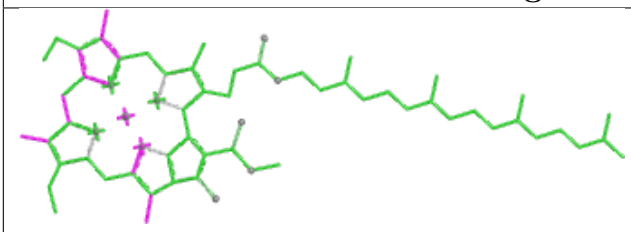
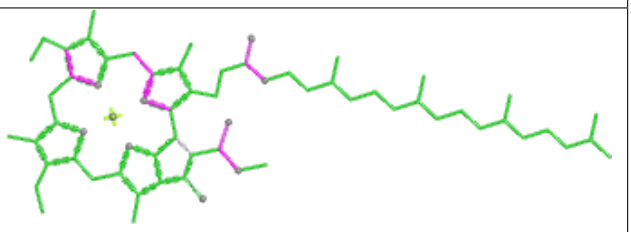
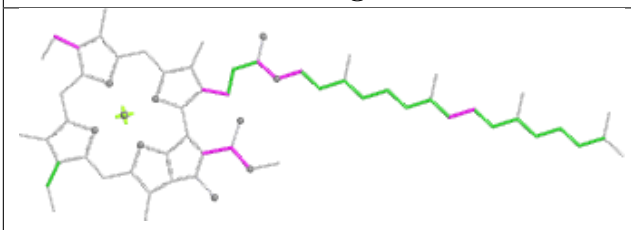
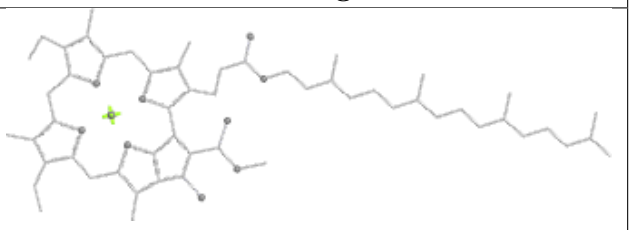


Rings

Ligand CLA B 825	
	
Bond lengths	Bond angles
	
Torsions	Rings

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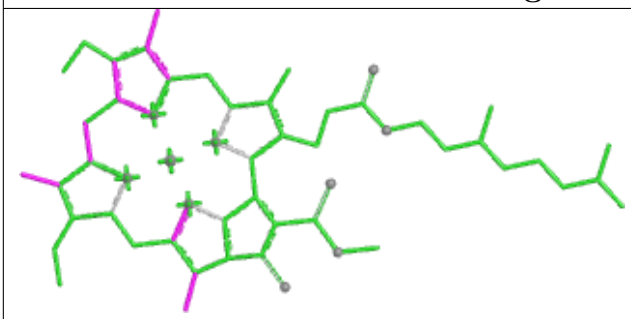
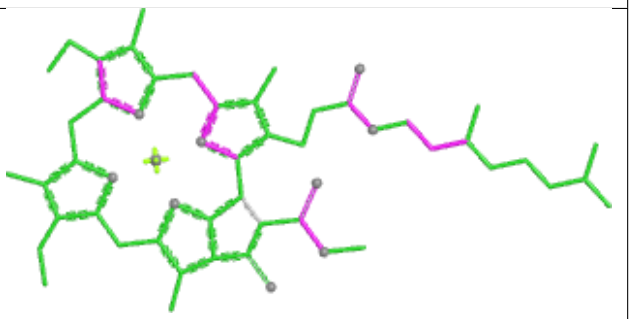
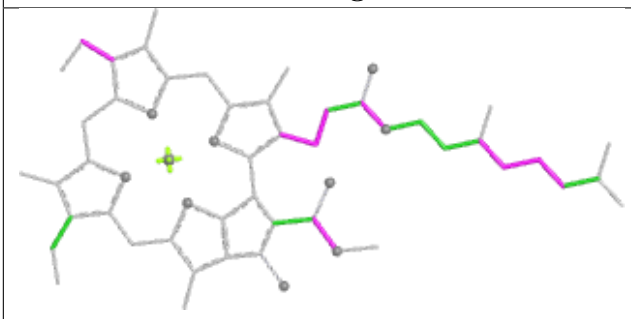
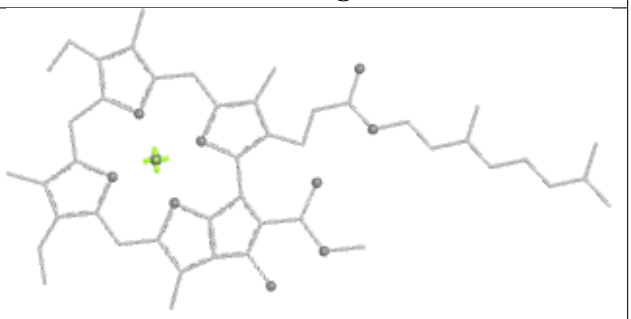
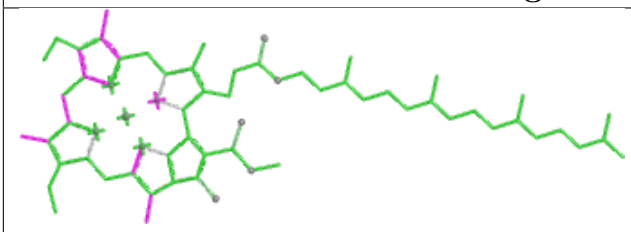
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 826



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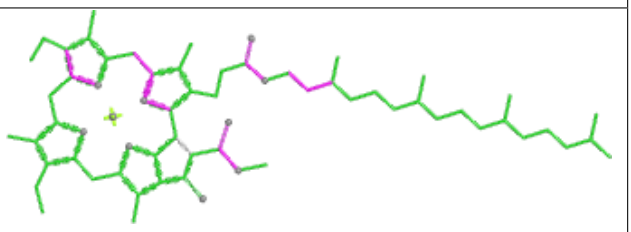

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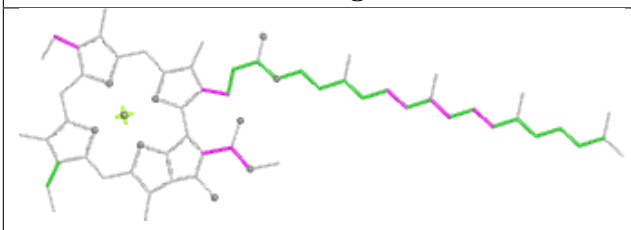

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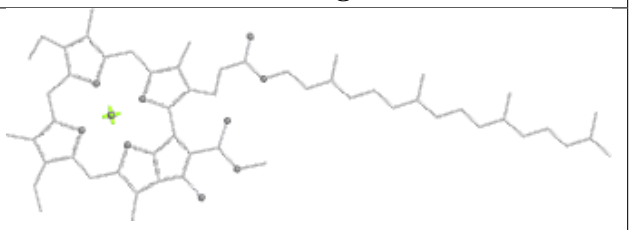
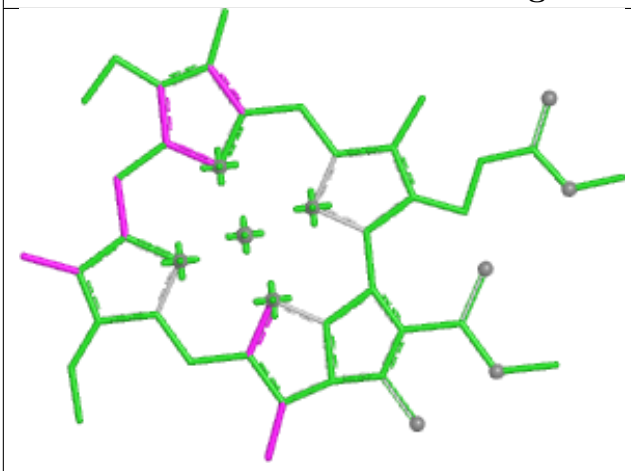


Rings

Ligand CLA 2 310



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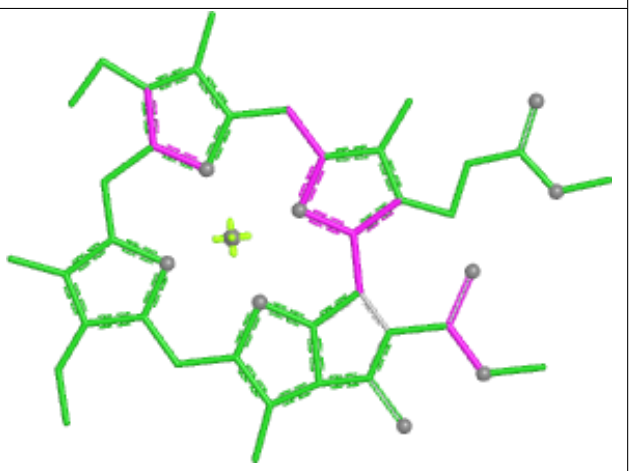
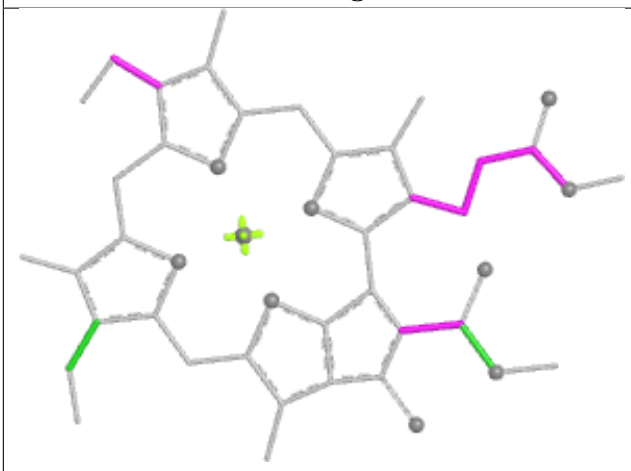


Bond angles



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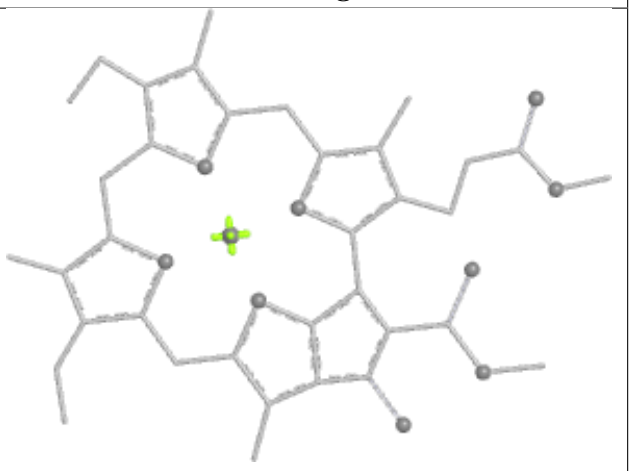
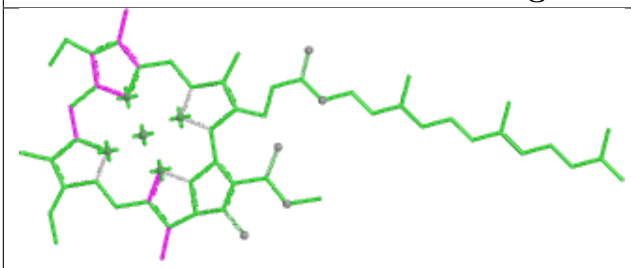
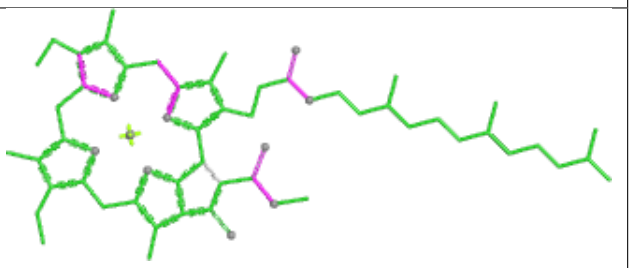
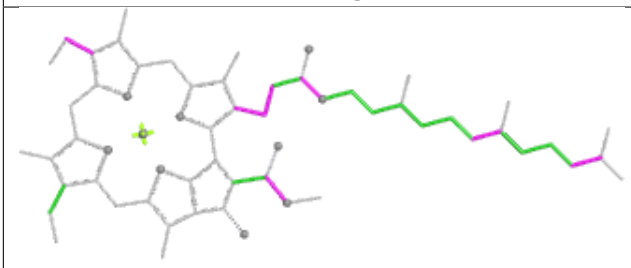
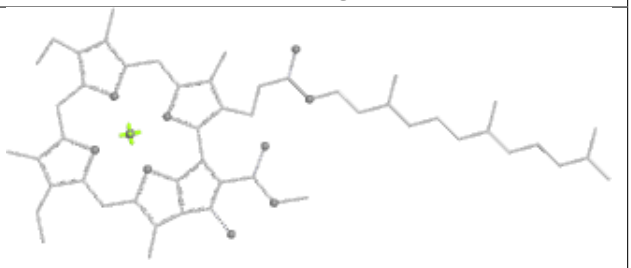


Rings

Ligand CLA 8 308	
	
Bond lengths	Bond angles
	
Torsions	Rings

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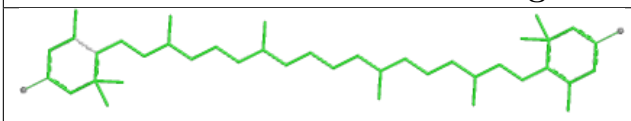
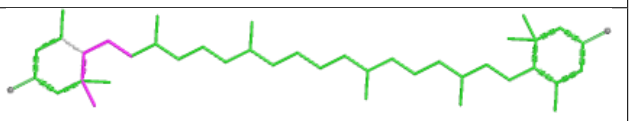
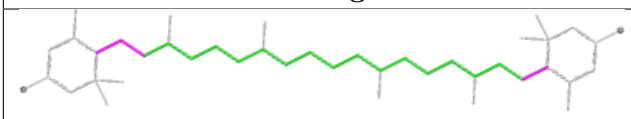
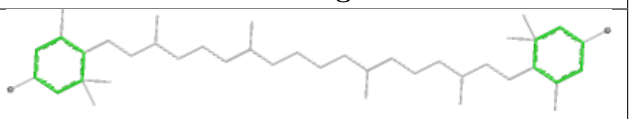
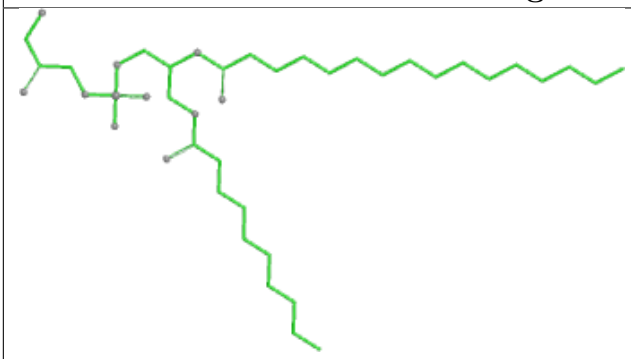
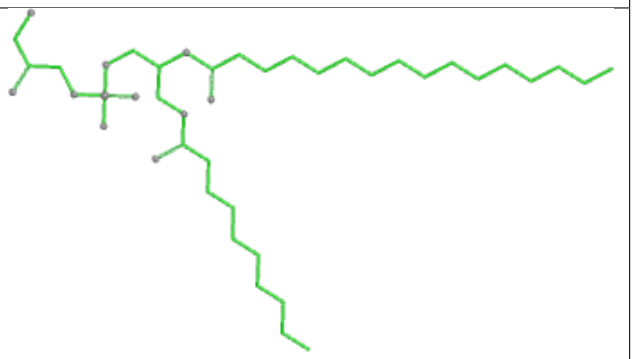
	
Bond lengths	Bond angles
	
Torsions	Rings

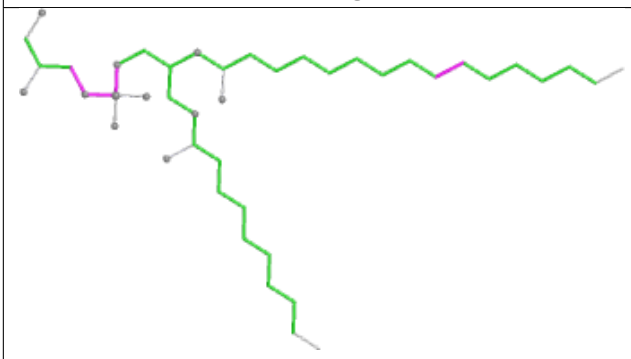
Ligand LHG 8 320



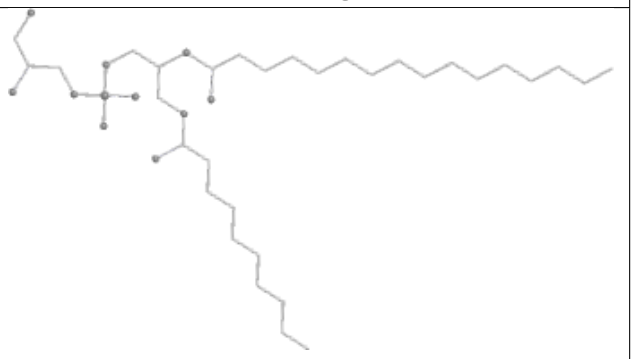
Bond lengths



Bond angles

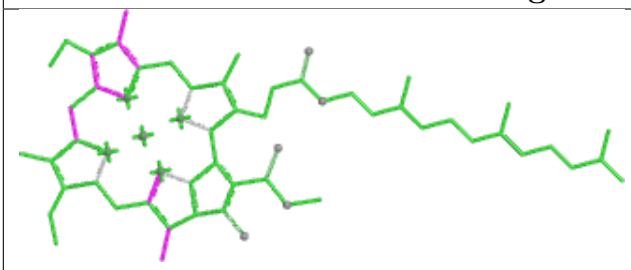


Torsions

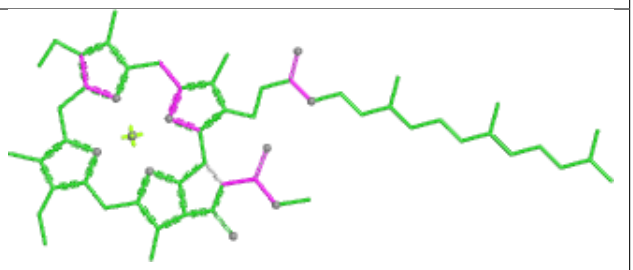


Rings

Ligand CLA 8 301



Bond lengths



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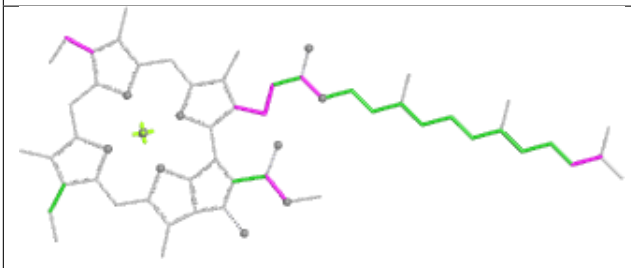

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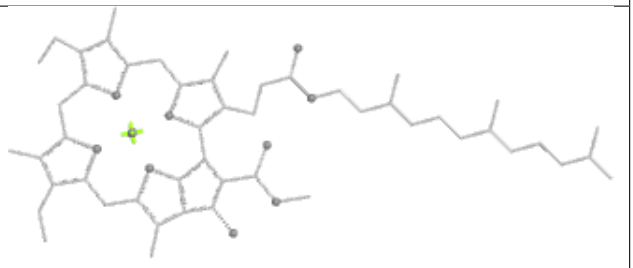
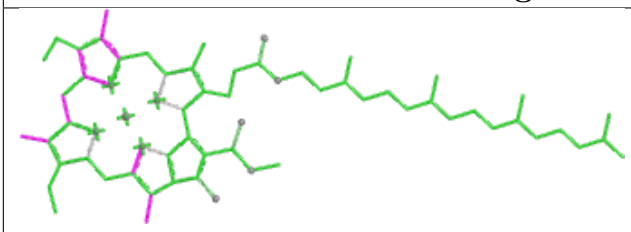


Rings

Ligand CLA A 5022



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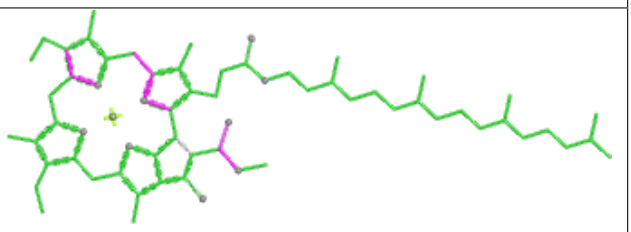
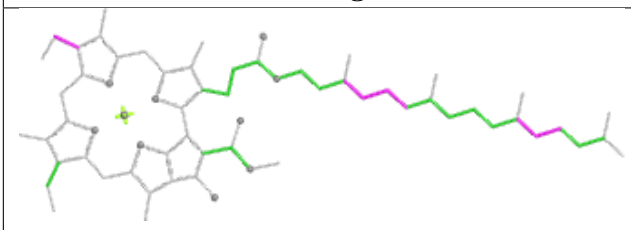


Bond angles



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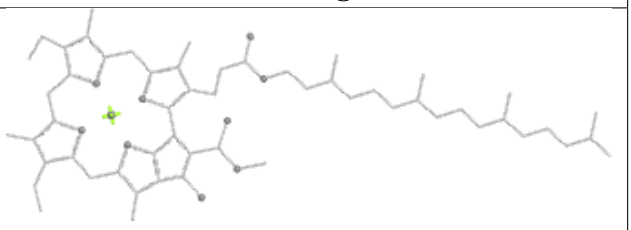
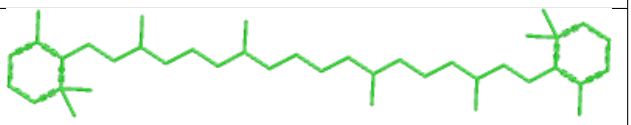


Rings

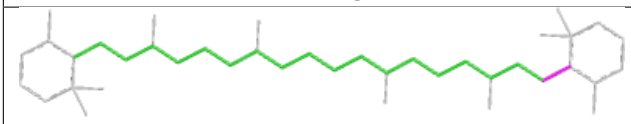
Ligand BCR B 842



Bond lengths



Bond angles



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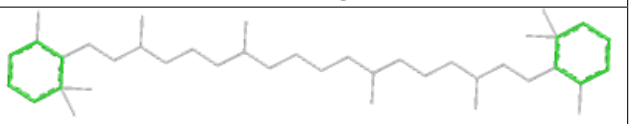
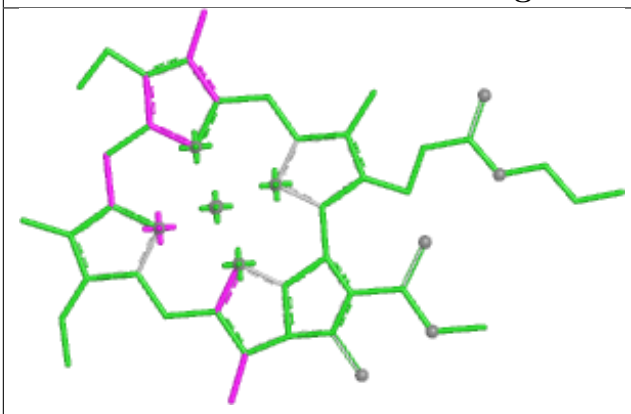
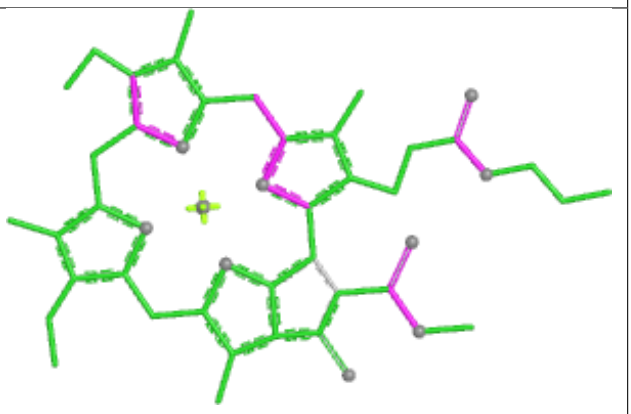


Rings

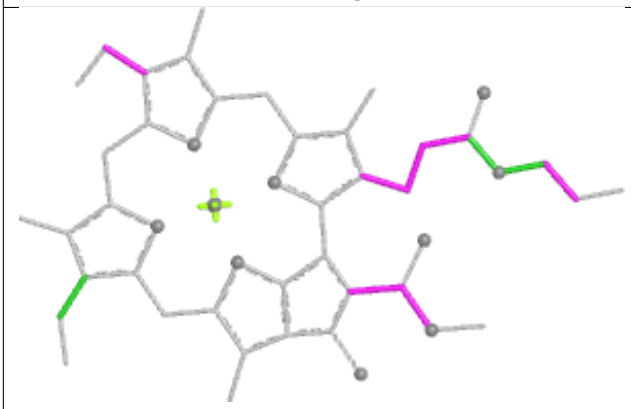
Ligand CLA K 4005



Bond lengths



Bond angles



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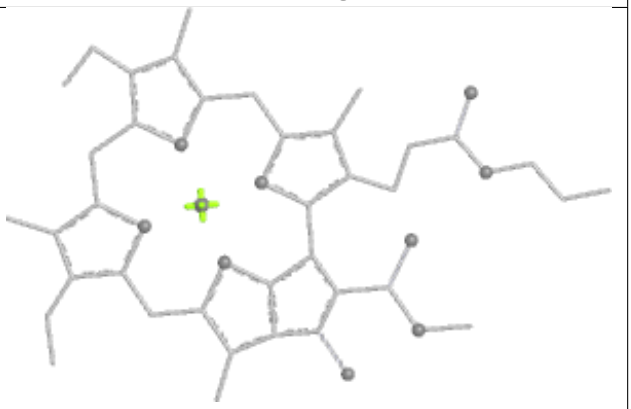
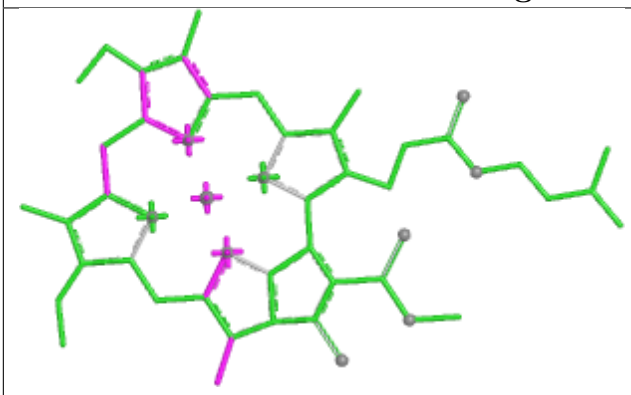


Rings

Ligand CLA A 5038



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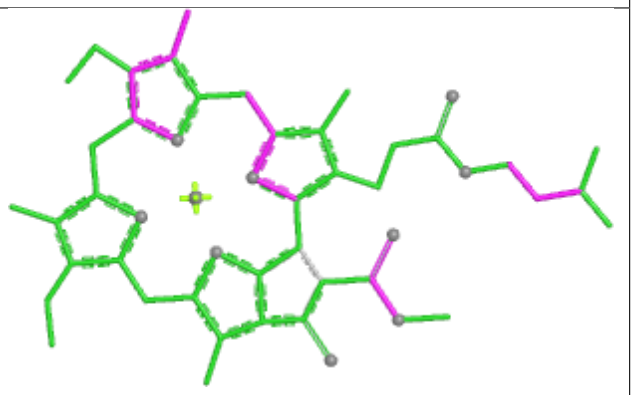

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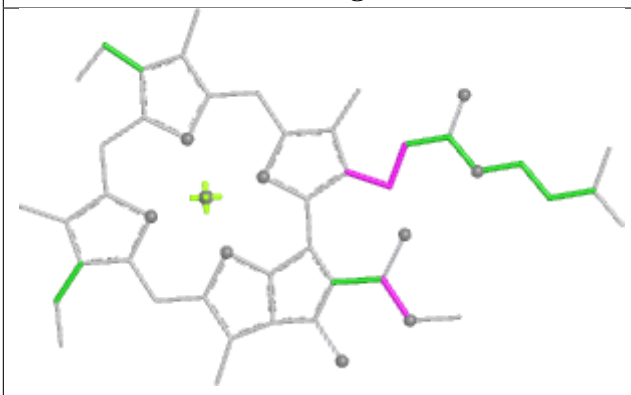

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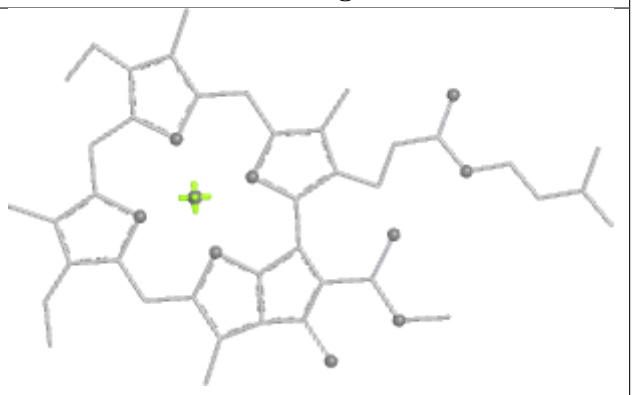
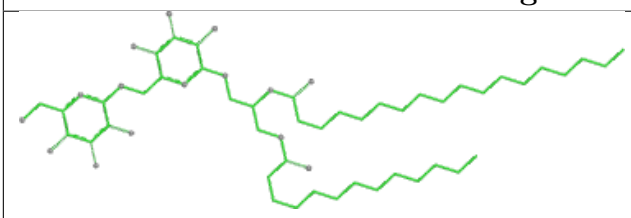


Rings

Ligand DGD B 848



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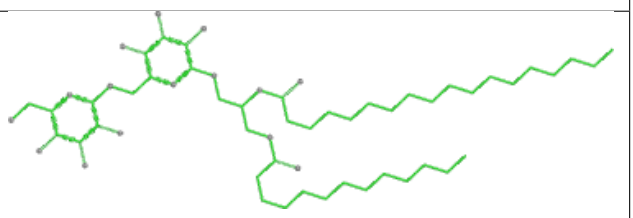
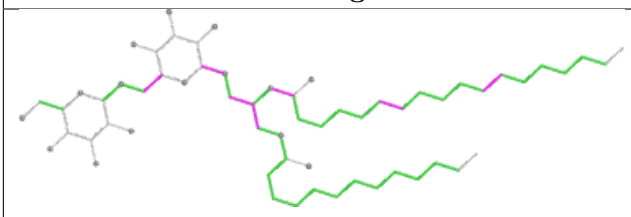


Bond angles



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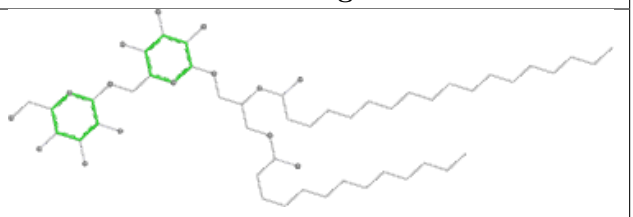
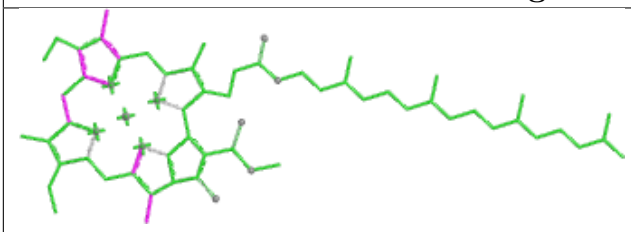


Rings

Ligand CLA 7 310



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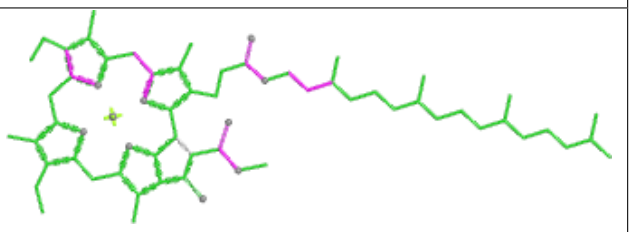
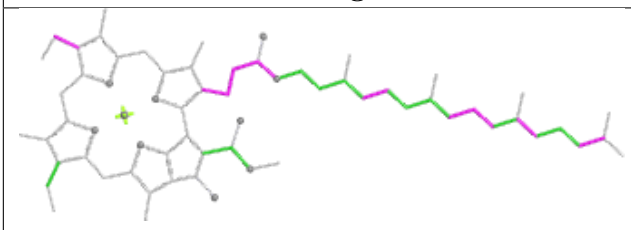


Bond angles



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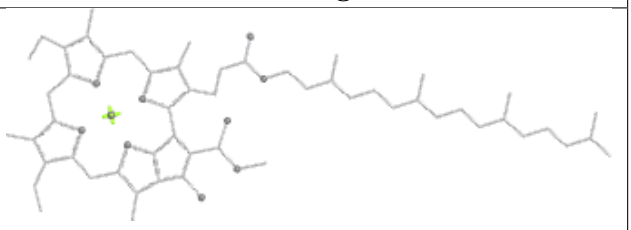
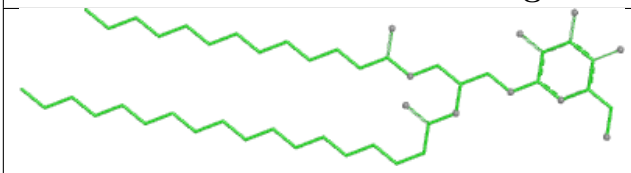


Rings

Ligand LMG 7 301



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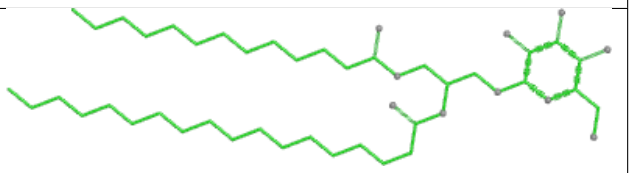

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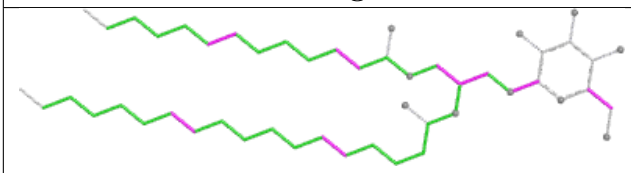

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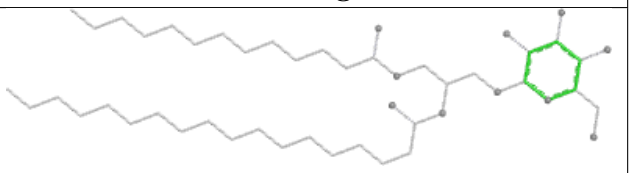
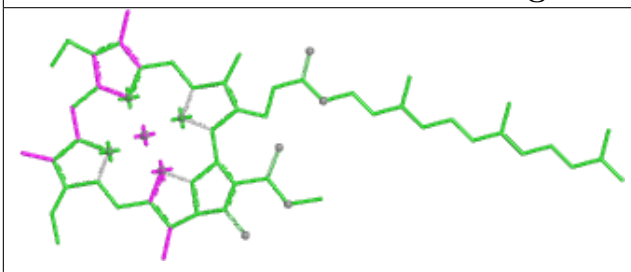


Rings

Ligand CLA 7 311



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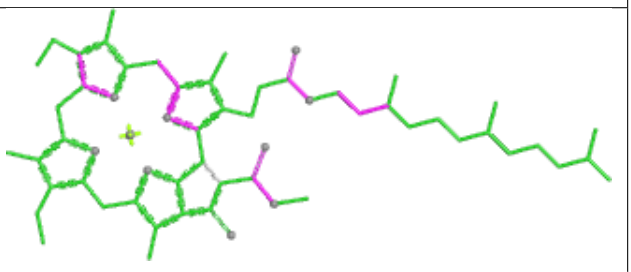

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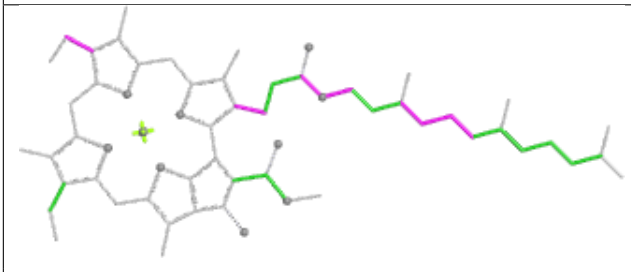

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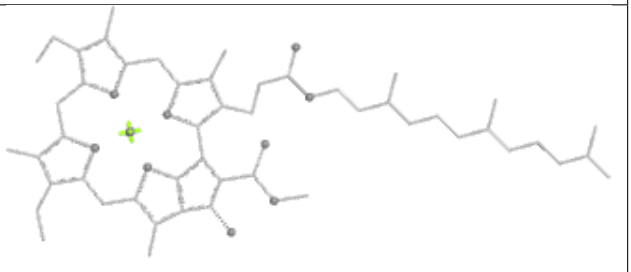
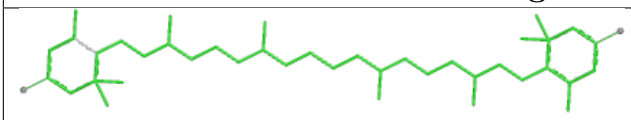


Rings

Ligand LUT 9 613



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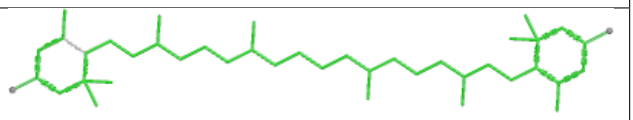
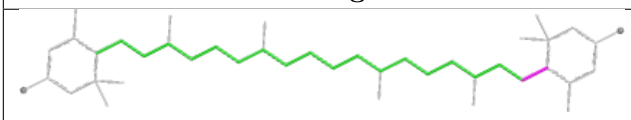


Bond angles



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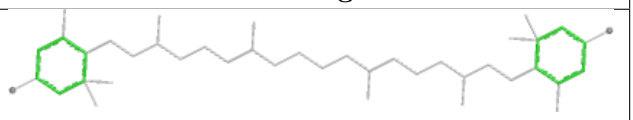
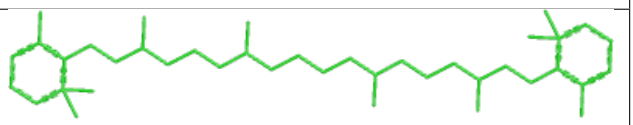


Rings

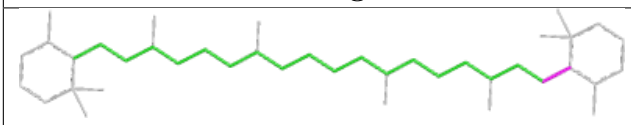
Ligand BCR 7 318



Bond lengths



Bond angles



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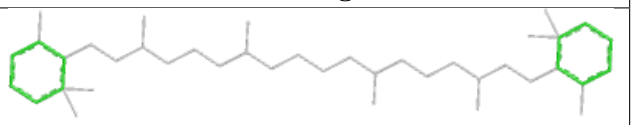
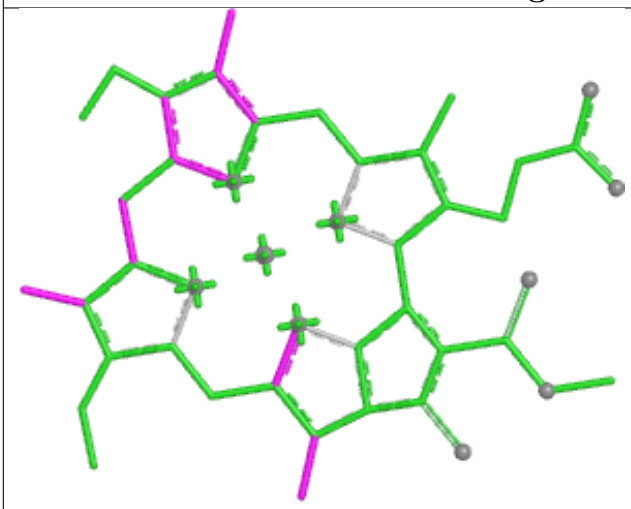


Rings

Ligand CLA 1 605



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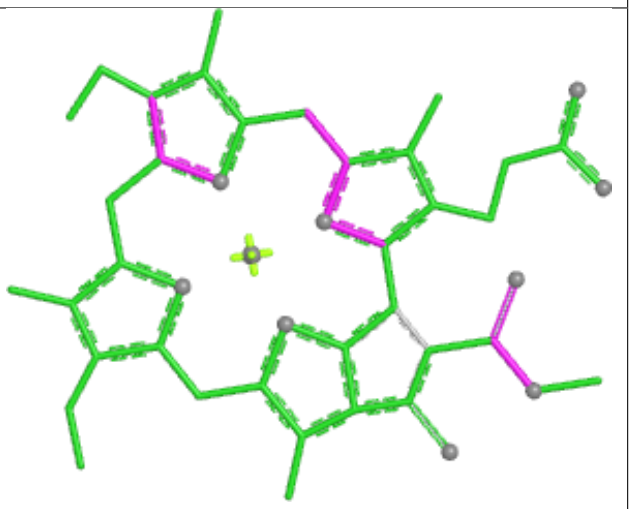
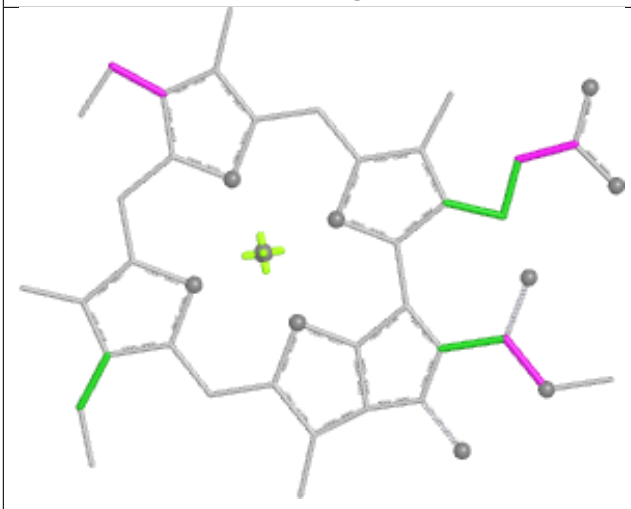


Bond angles

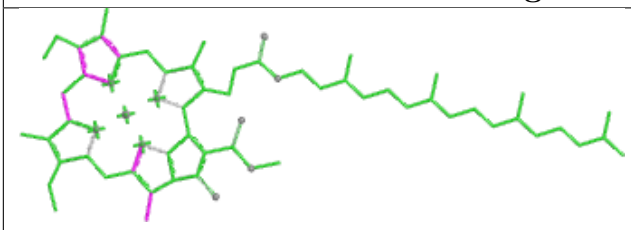


Torsions



Rings

Ligand CLA B 827



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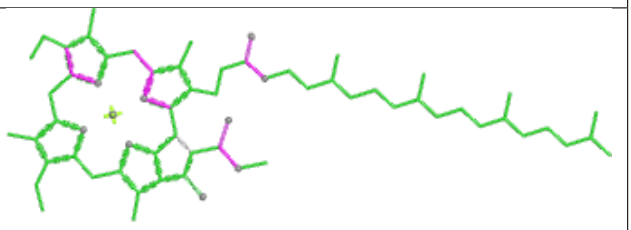
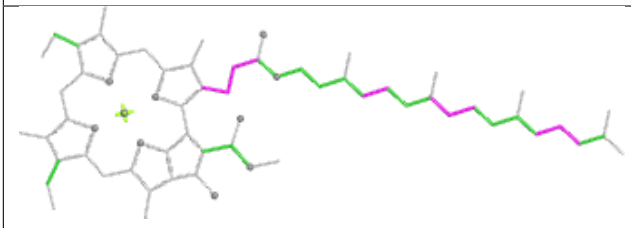


Bond angles



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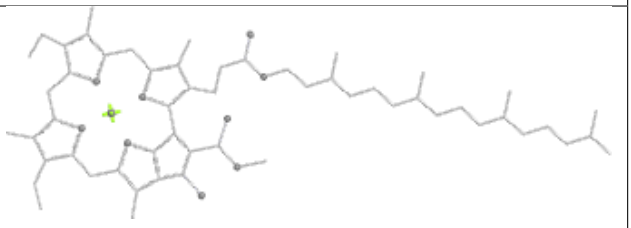
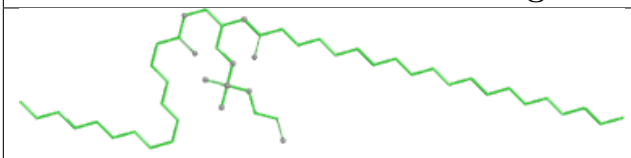
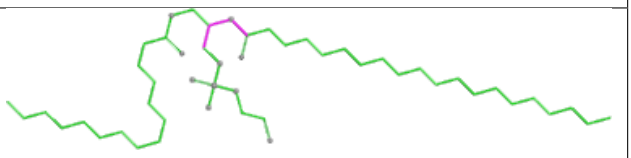
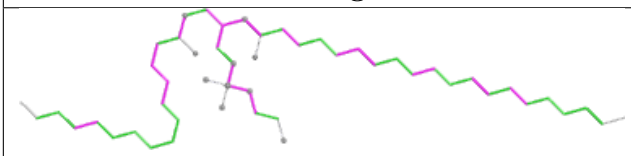
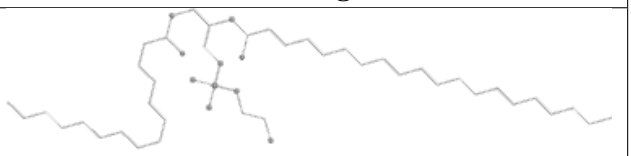


Rings

Ligand PTY 3 321	
 Bond lengths	 Bond angles
 Torsions	 Rings

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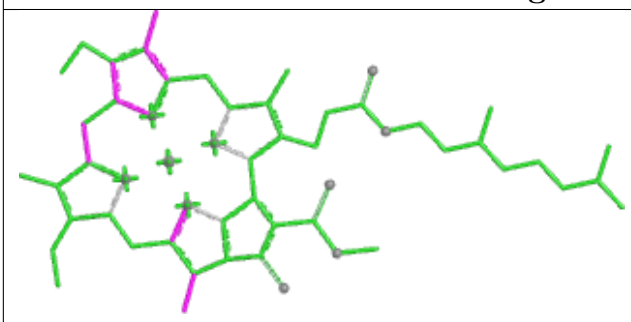
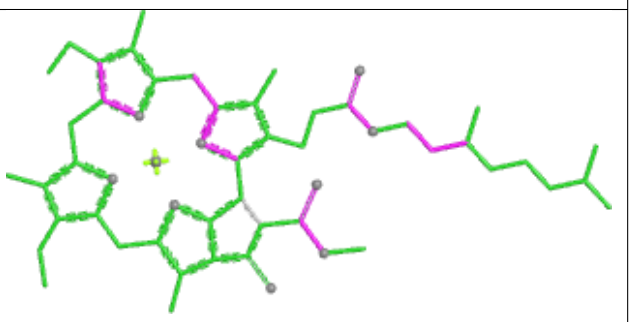
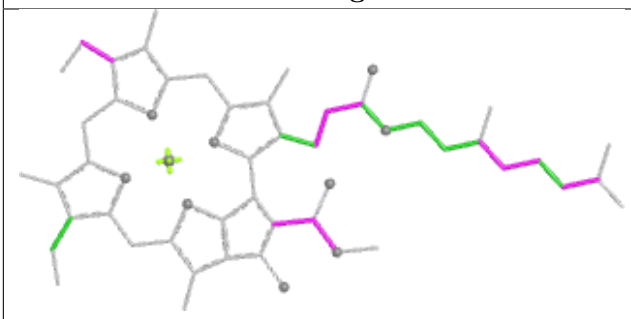
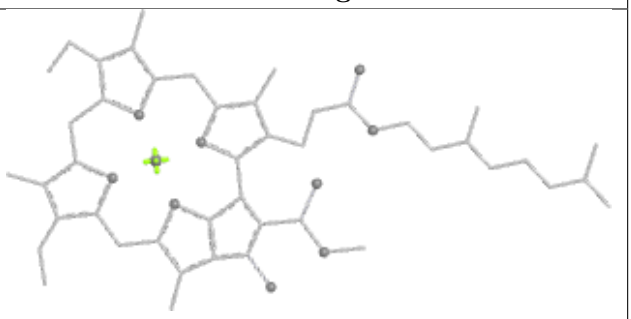
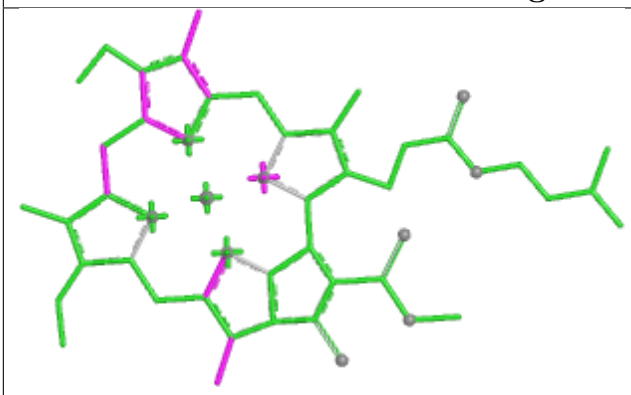
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 7 305



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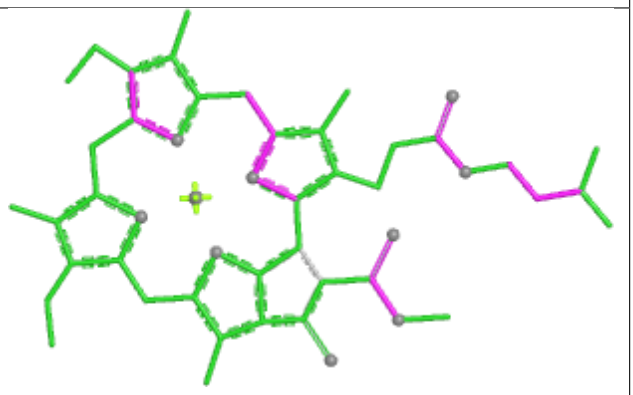

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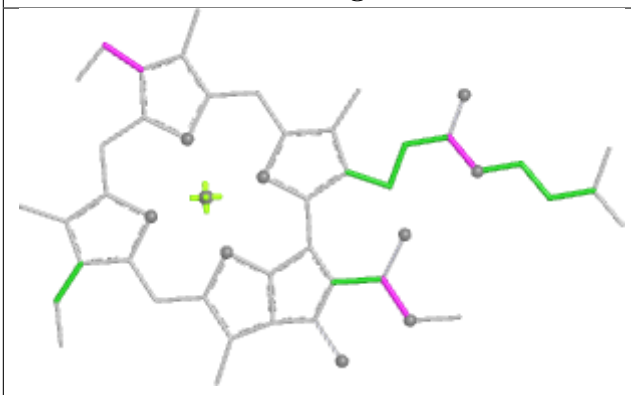

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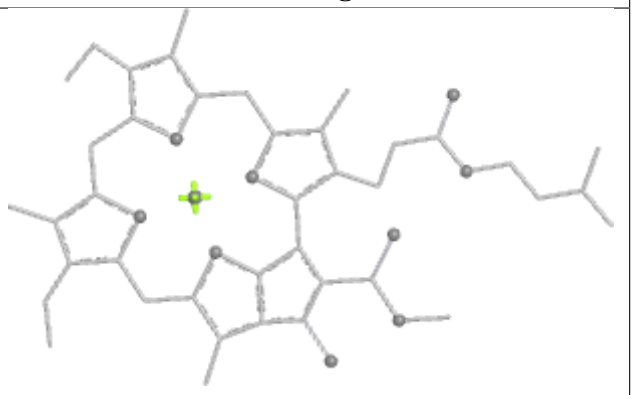
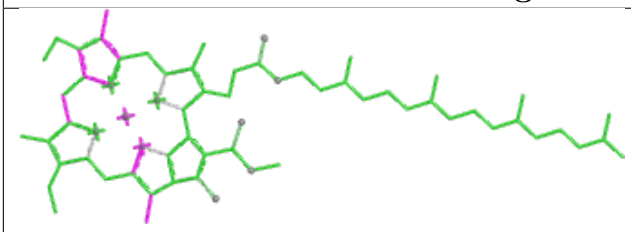


Rings

Ligand CLA A 5030



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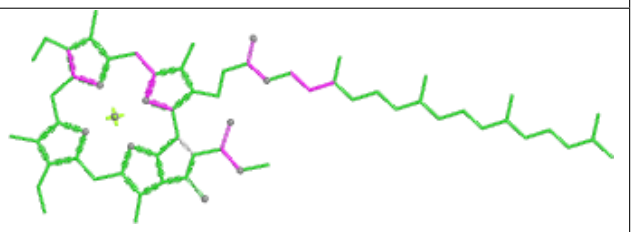

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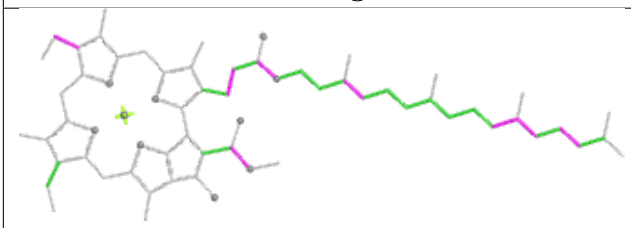

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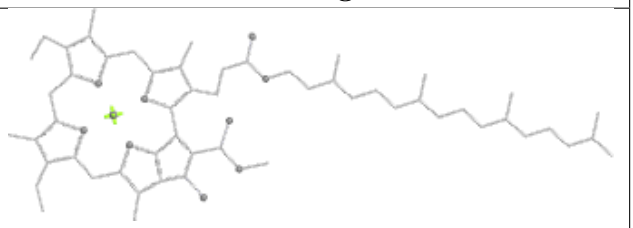

Rings

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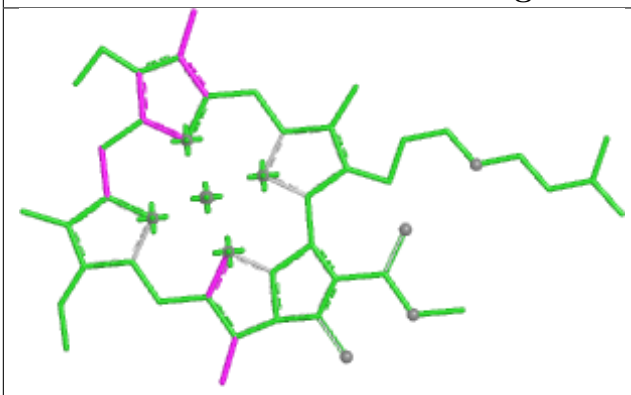

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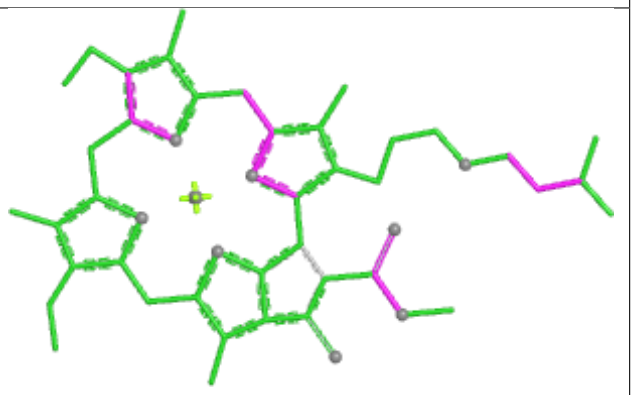

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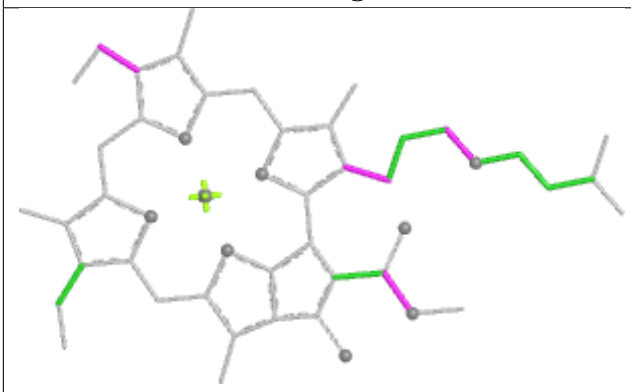

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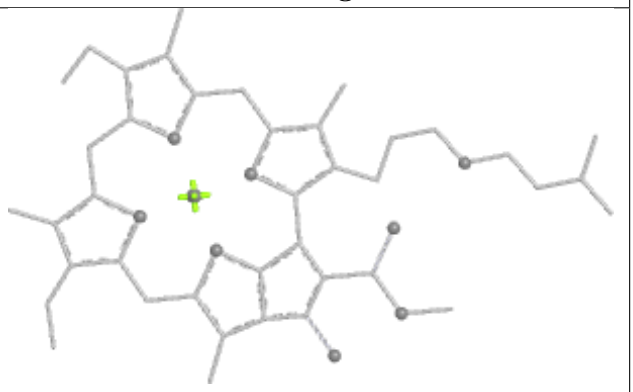
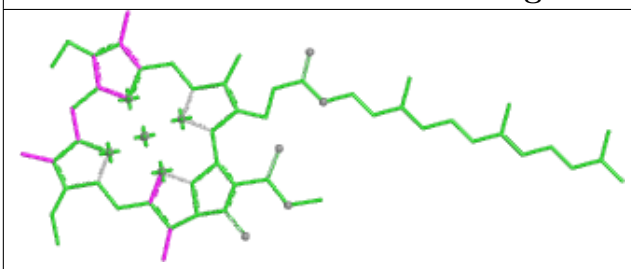


Rings

Ligand CLA B 831



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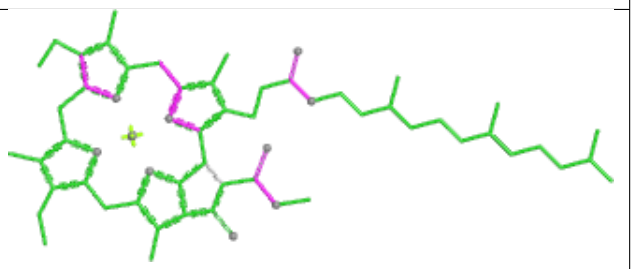

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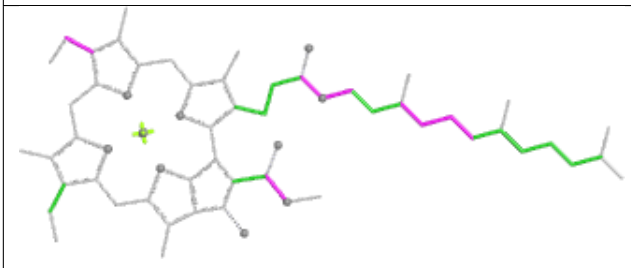

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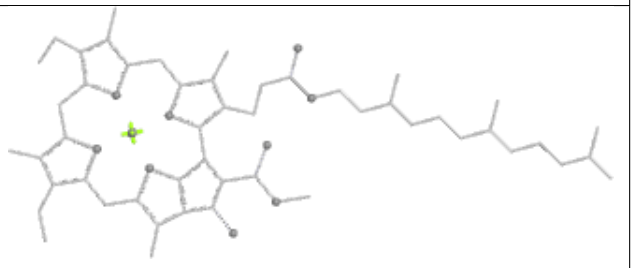
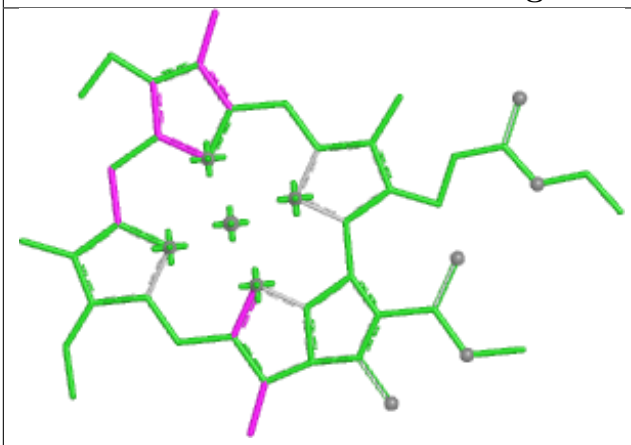


Rings

Ligand CLA F 307



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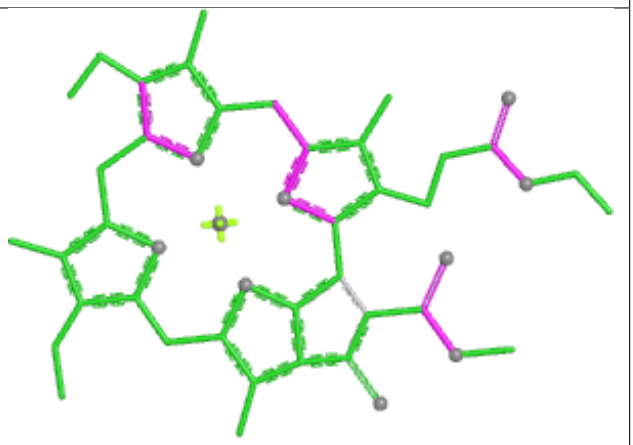

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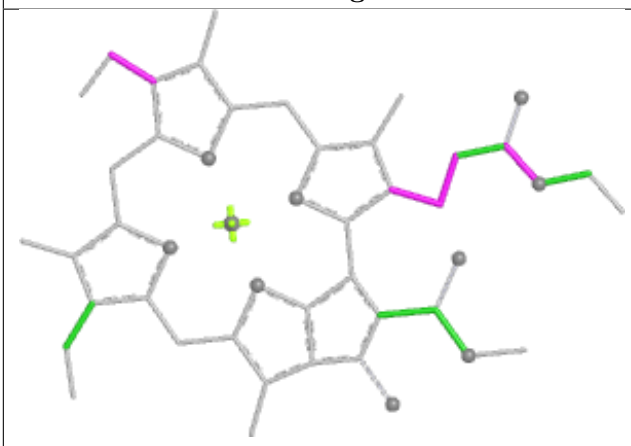

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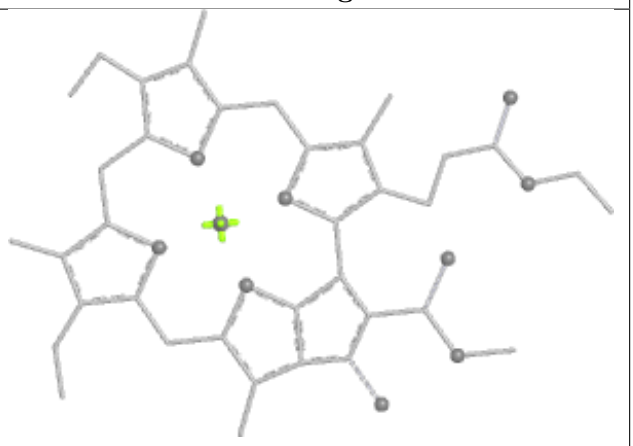
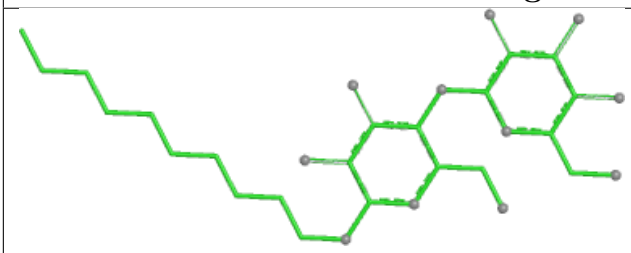


Rings

Ligand LMU 8 318



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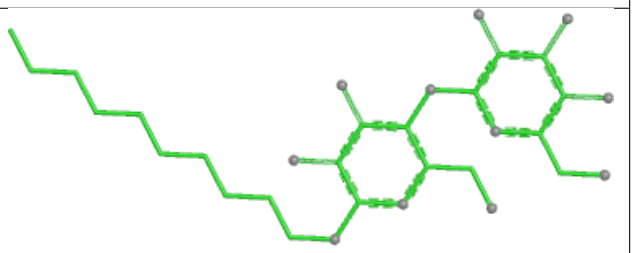

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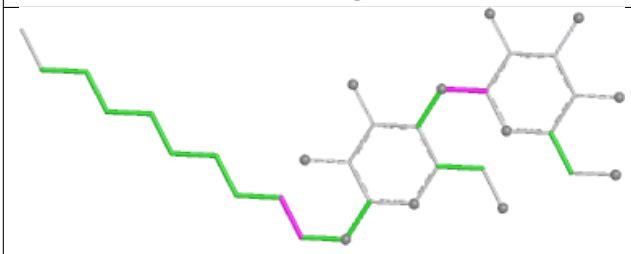

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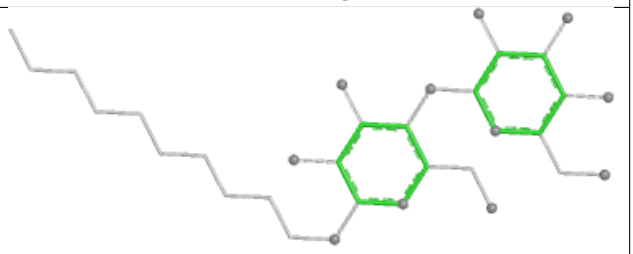

Rings

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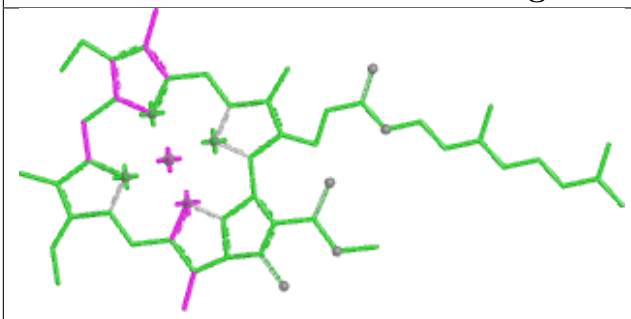	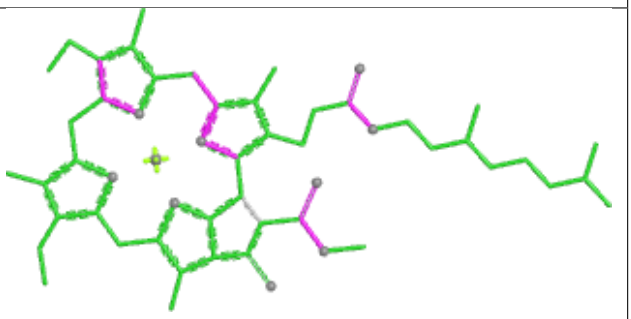
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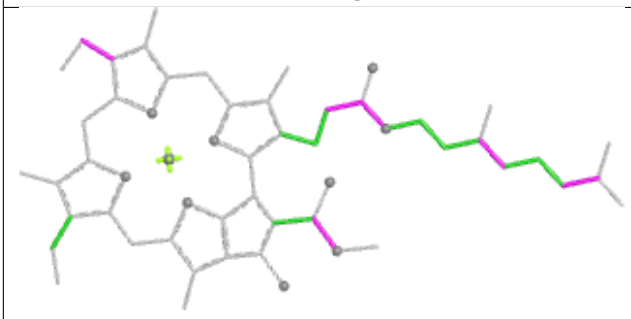	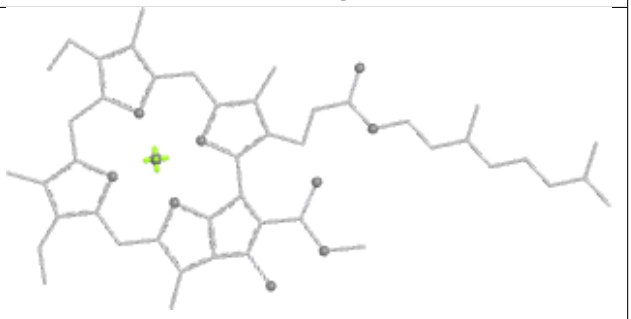
Torsions	Rings

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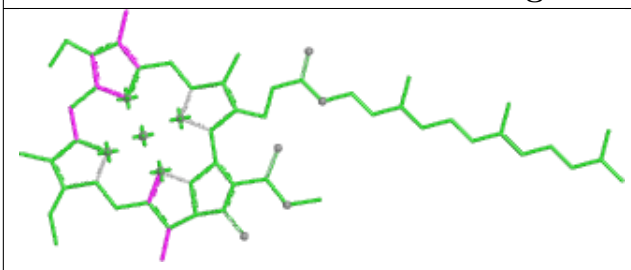	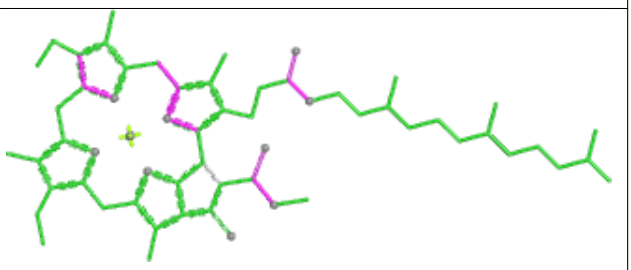
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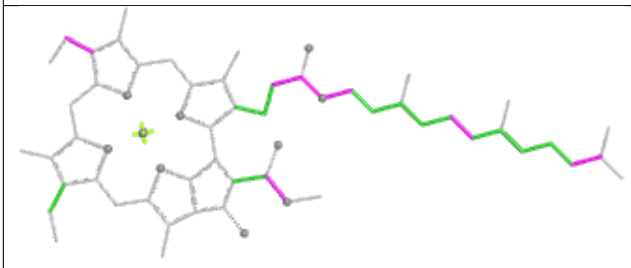
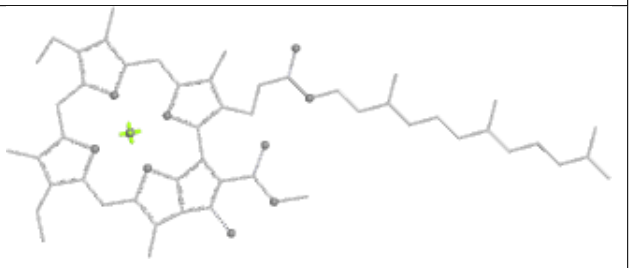
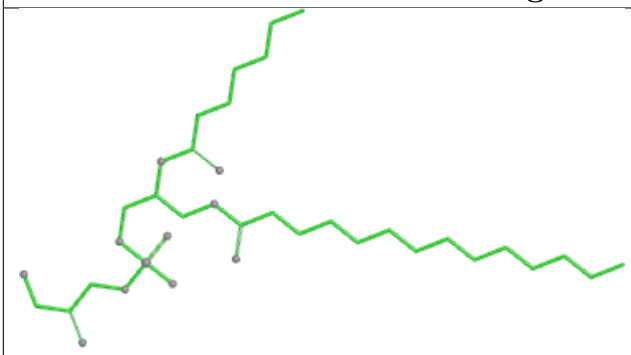
	
Torsions	Rings

Ligand LHG 8 319



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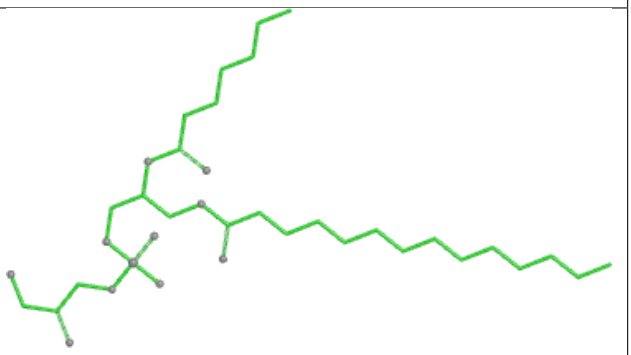

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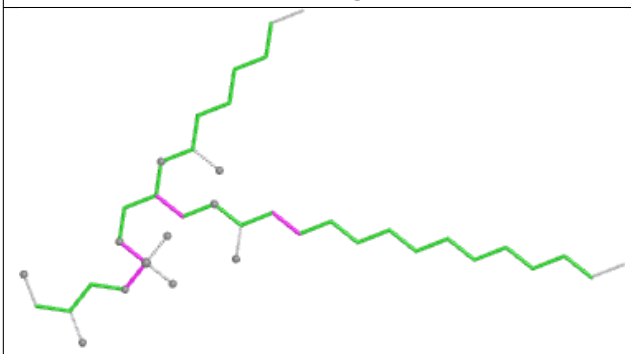

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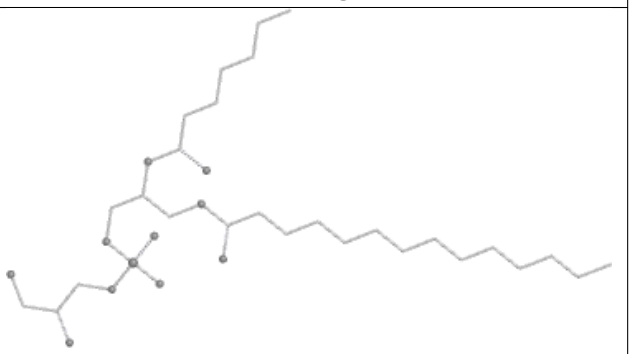
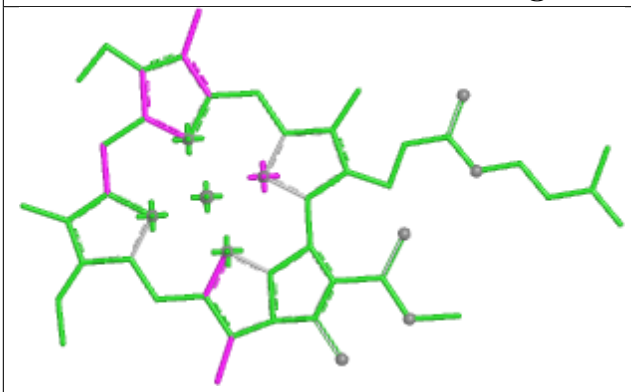


Rings

Ligand CLA 1 613



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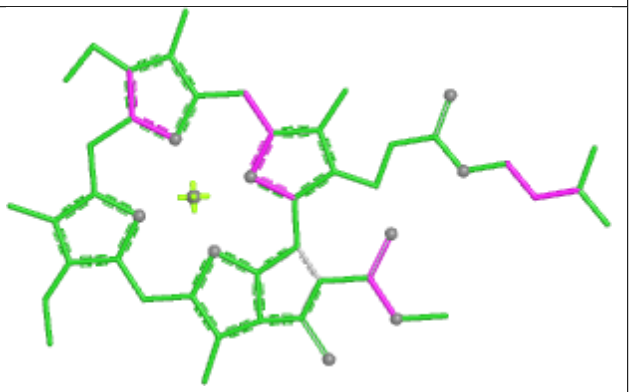

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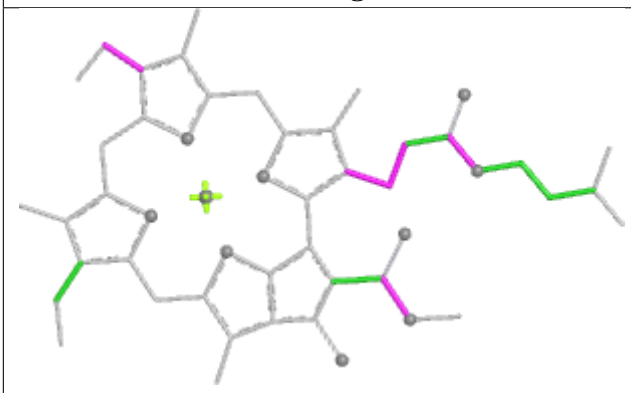

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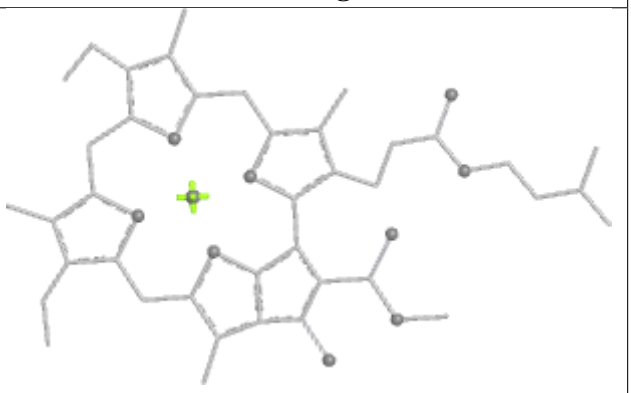
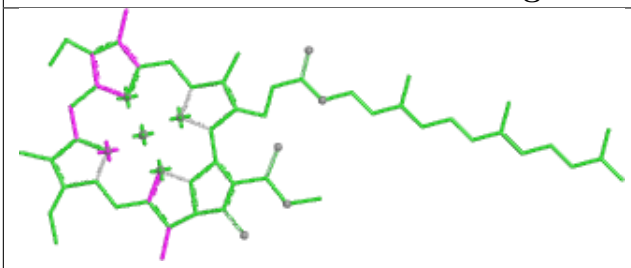


Rings

Ligand CLA H 201



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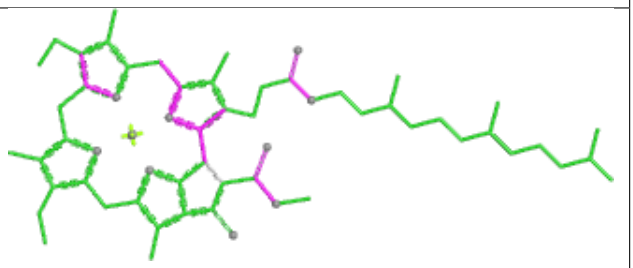
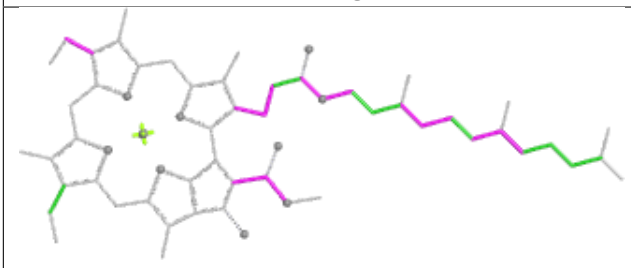


Bond angles



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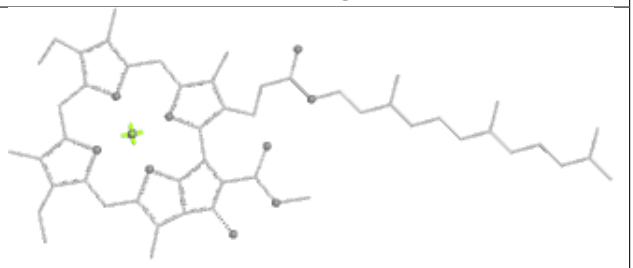
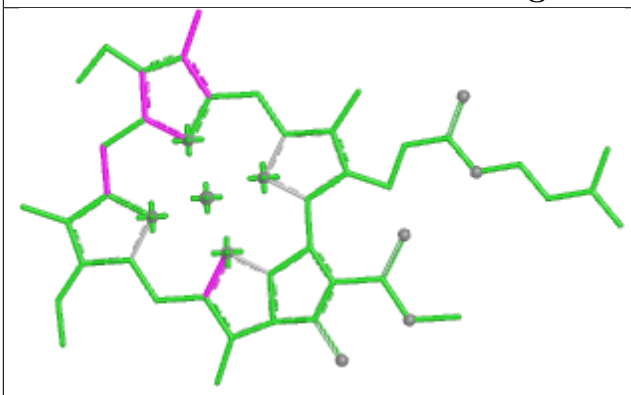


Rings

Ligand CLA 2 311



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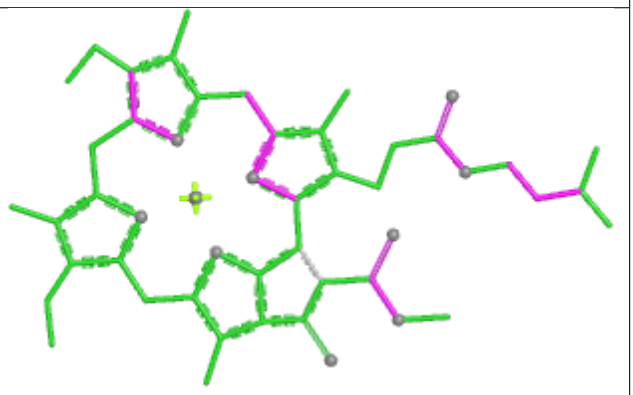

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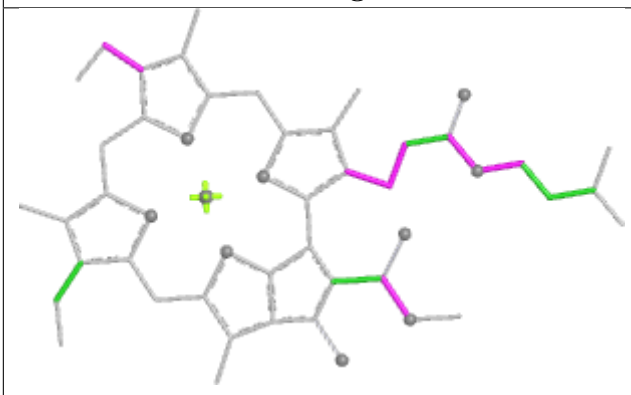

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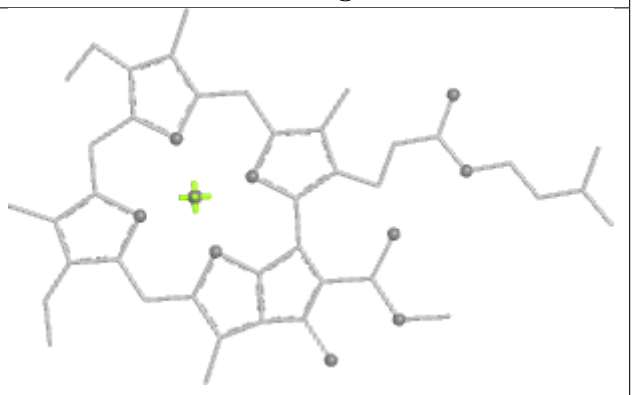
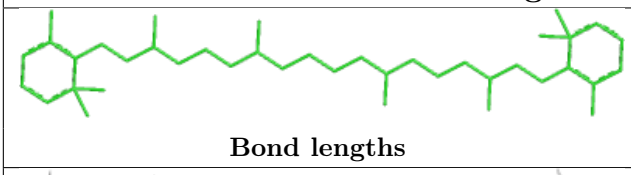


Rings

Ligand BCR L 206



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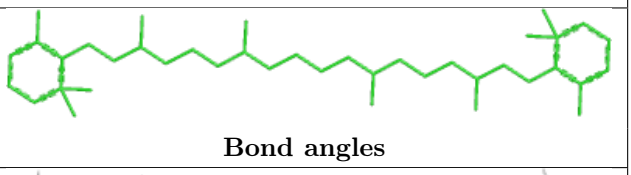

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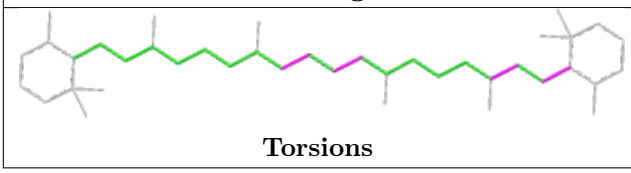

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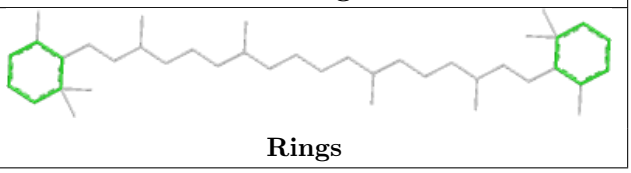
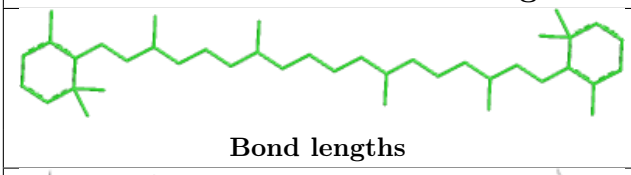
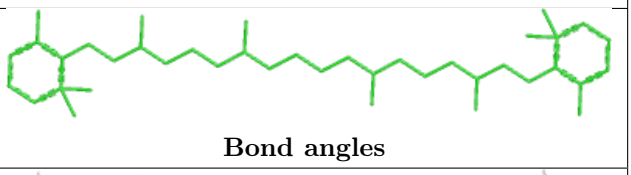


Rings

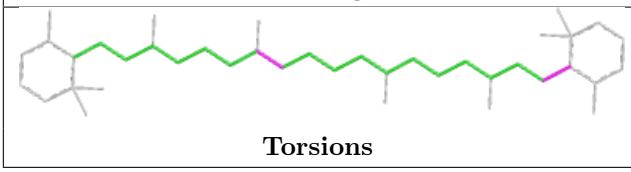
Ligand BCR I 4001



Bond lengths



Bond angles



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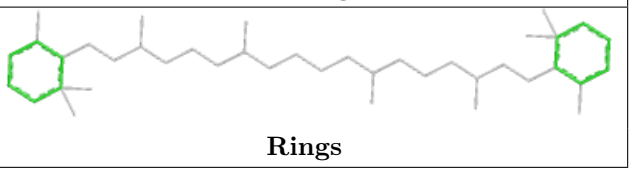
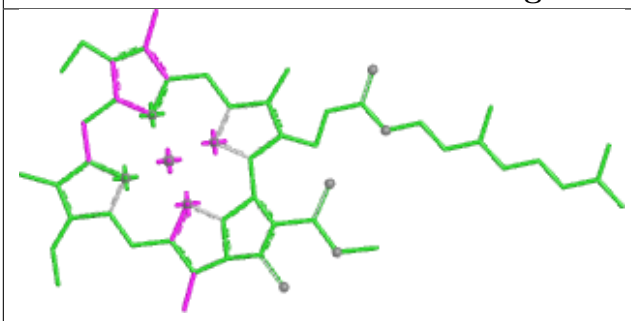
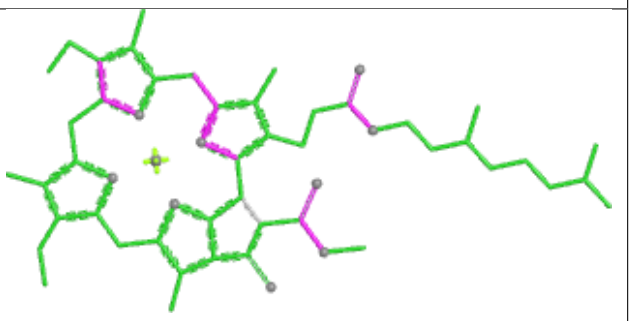


Rings

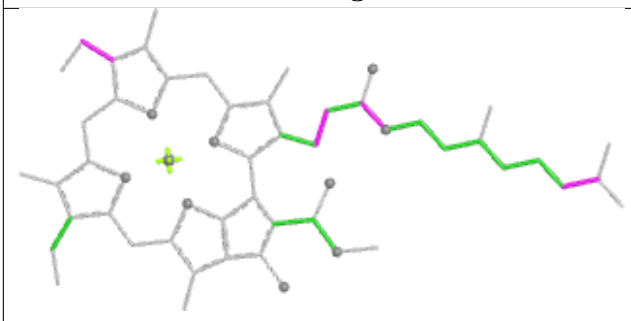
Ligand CLA B 838



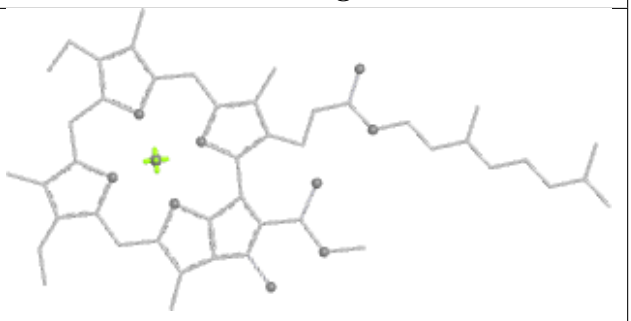
Bond lengths



Bond angles

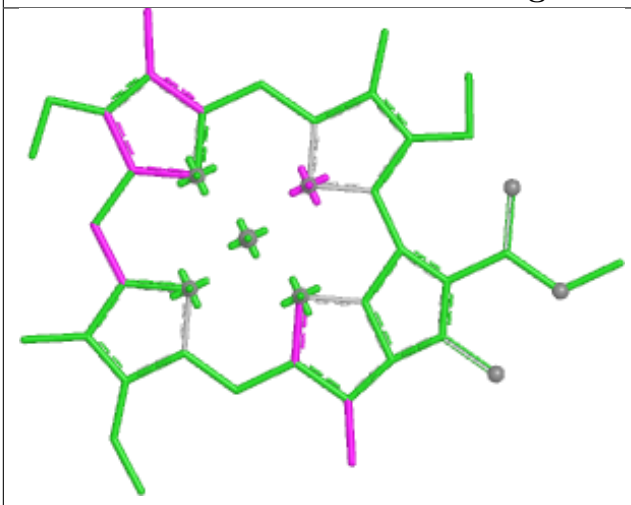


Torsions



Rings

Ligand CLA 3 313



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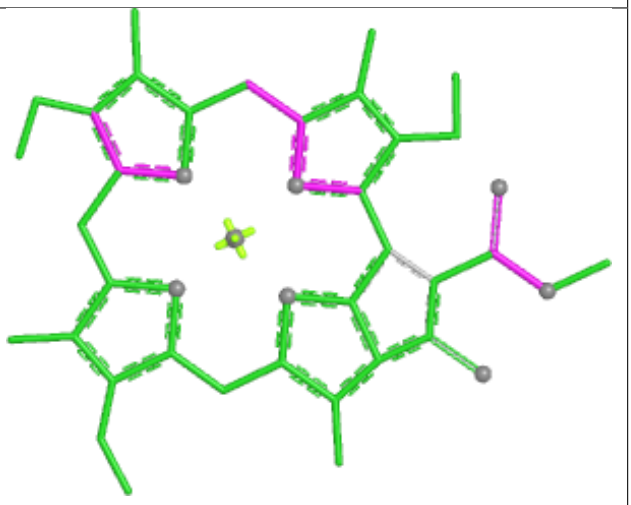


Bond angles



Torsions

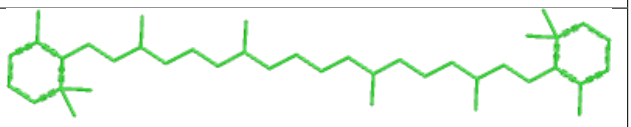


Rings

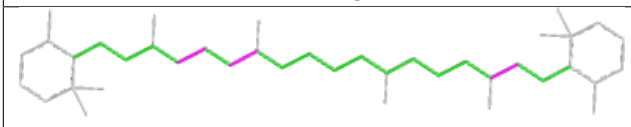
Ligand BCR A 5047



Bond lengths



Bond angles



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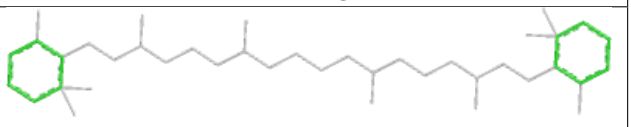
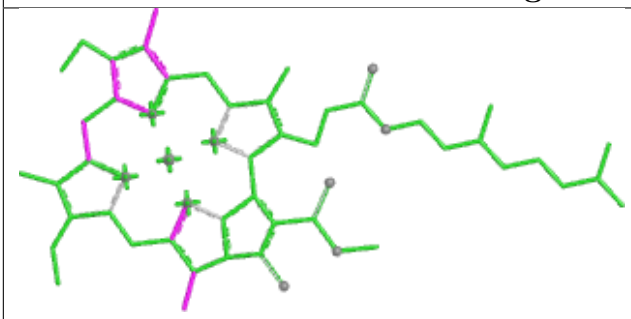


Rings

Ligand CLA B 837



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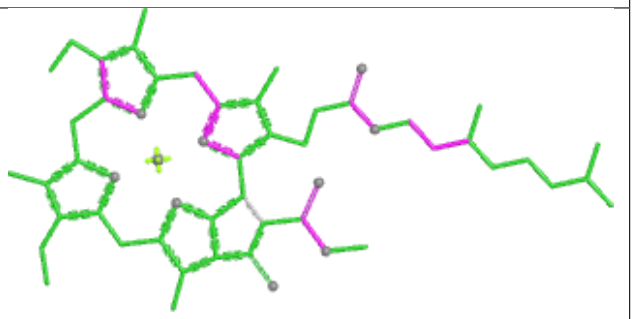

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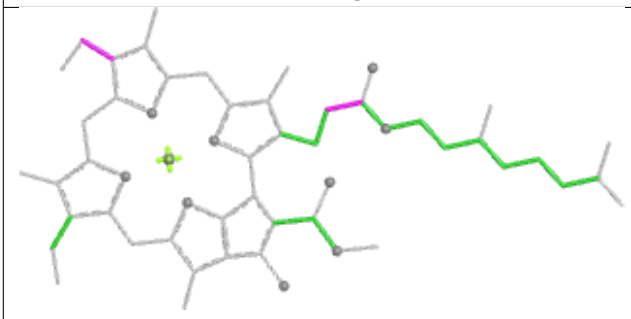

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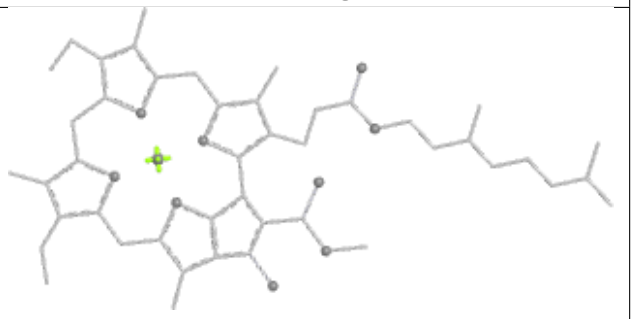
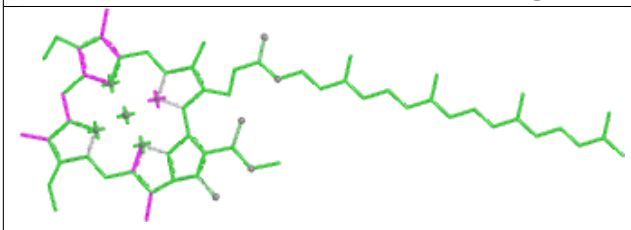


Rings

Ligand CLA 8 303



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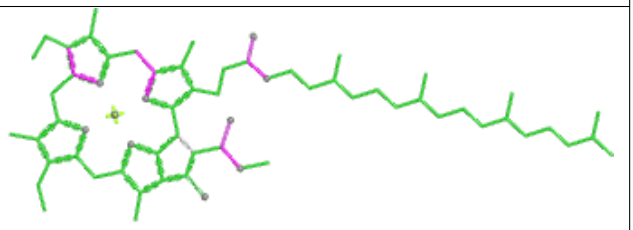
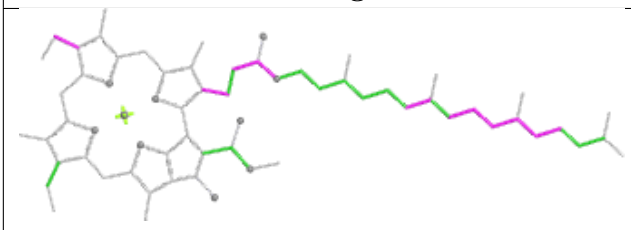


Bond angles



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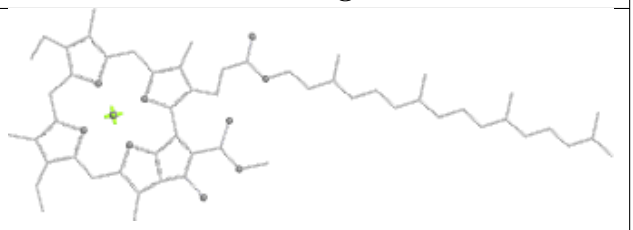
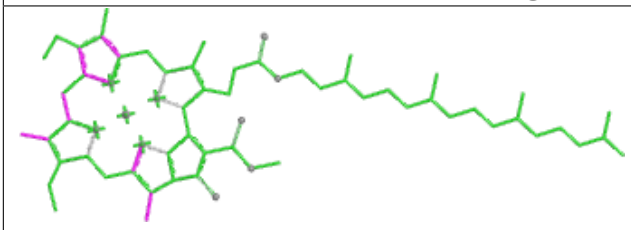


Rings

Ligand CLA B 807



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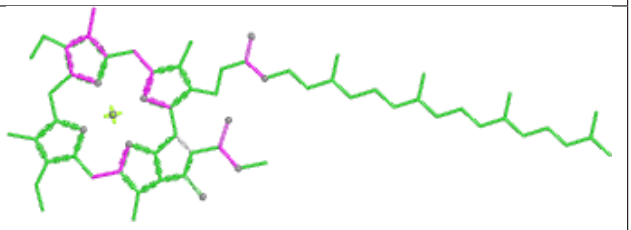
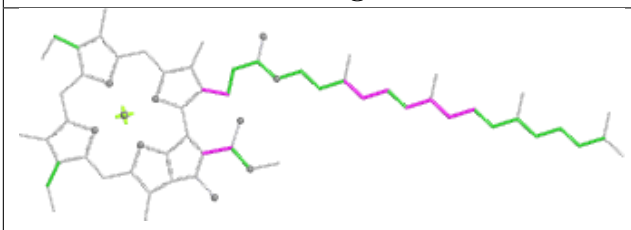


Bond angles



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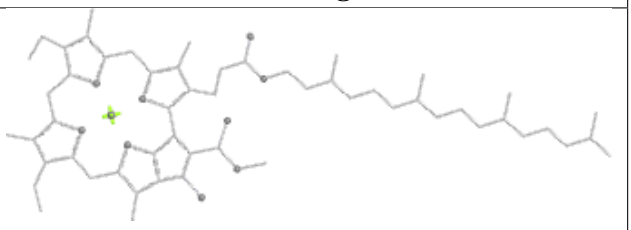
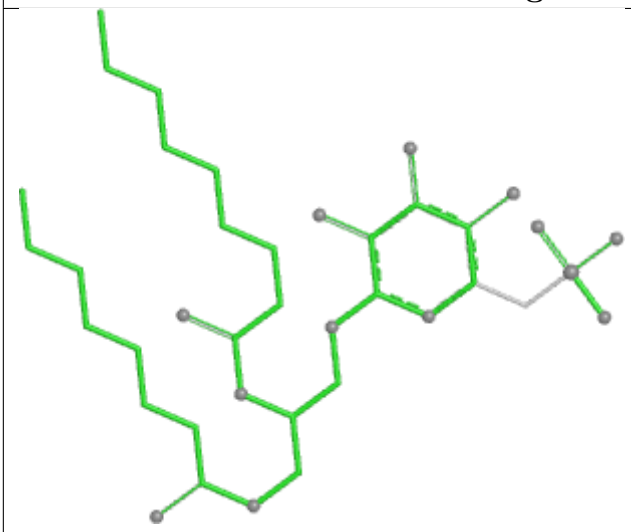


Rings

Ligand SQD F 311



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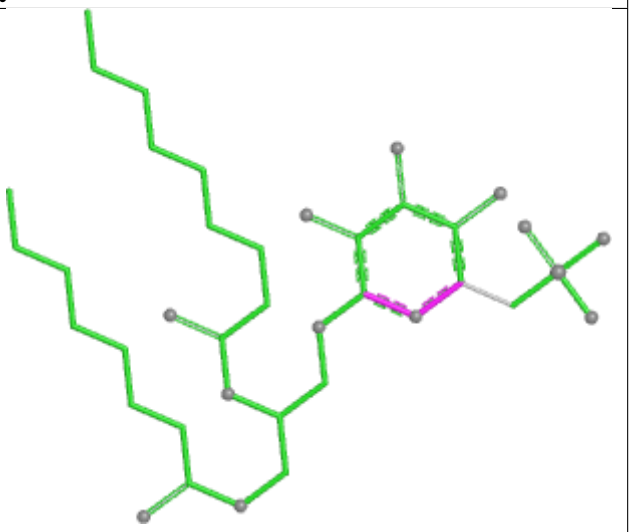
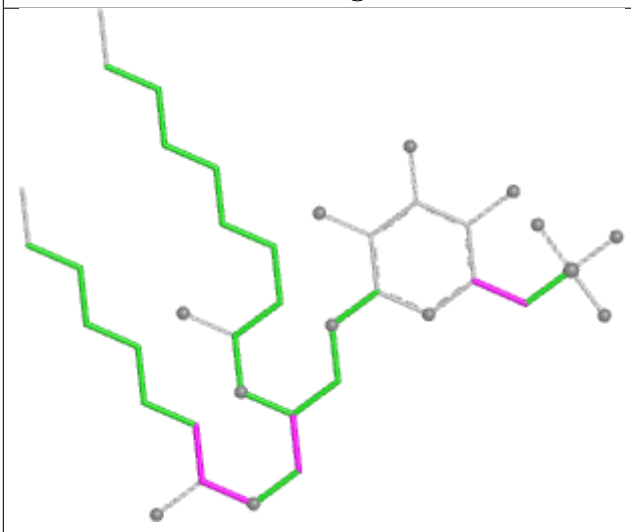


Bond angles



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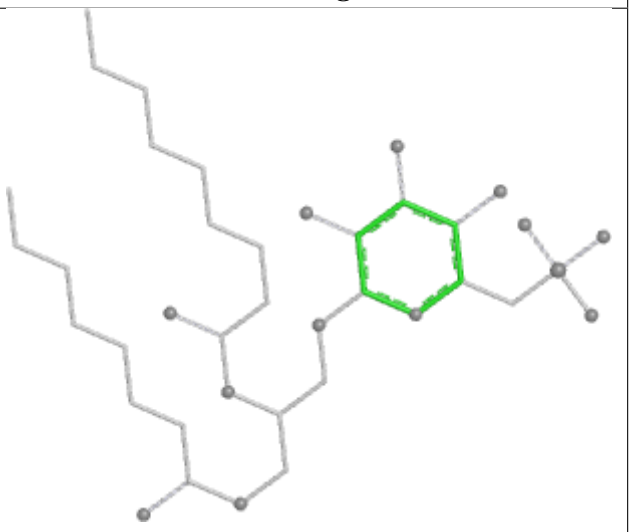
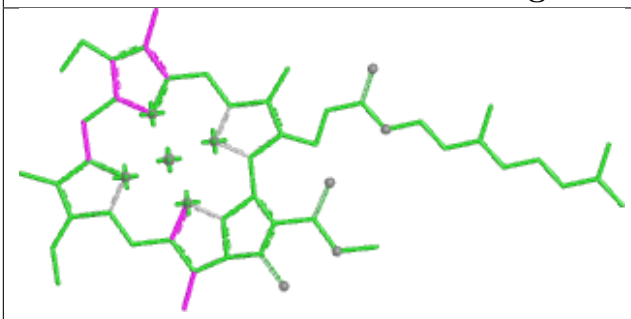


Rings

Ligand CLA 3 311



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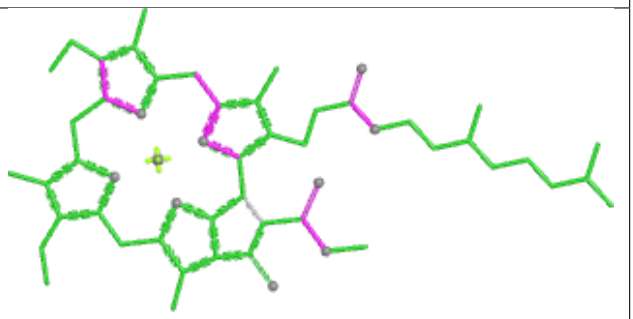
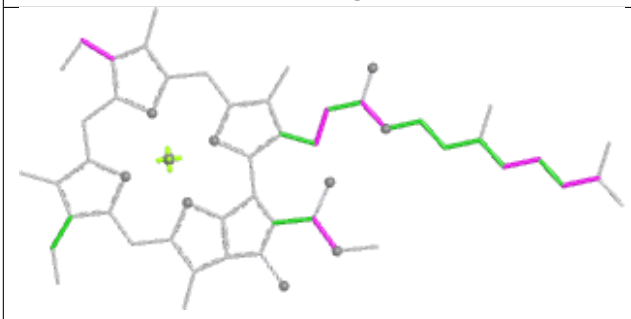


Bond angles



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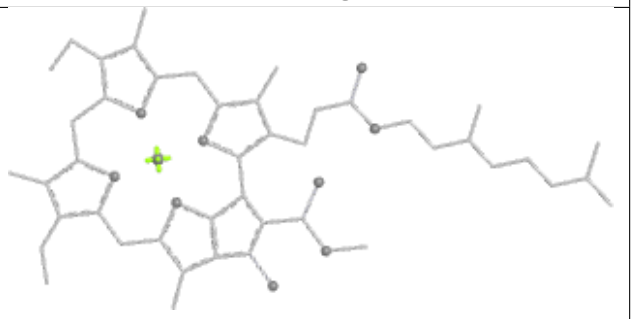
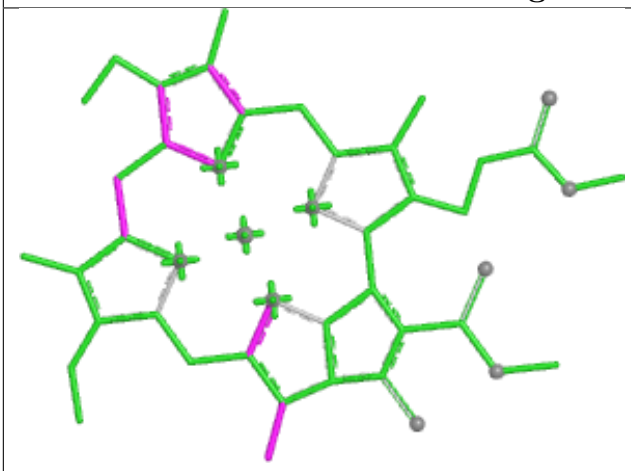
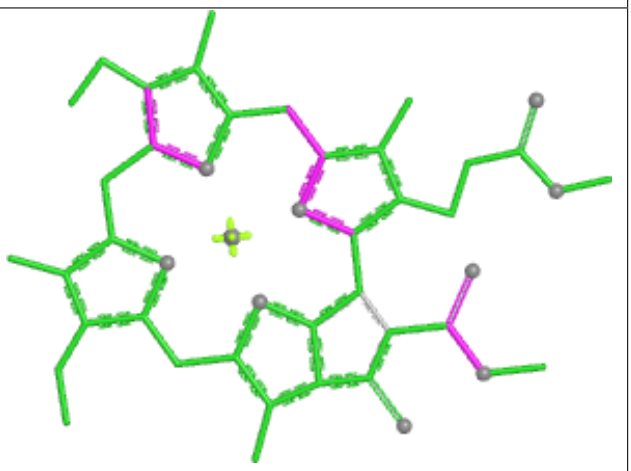


Rings

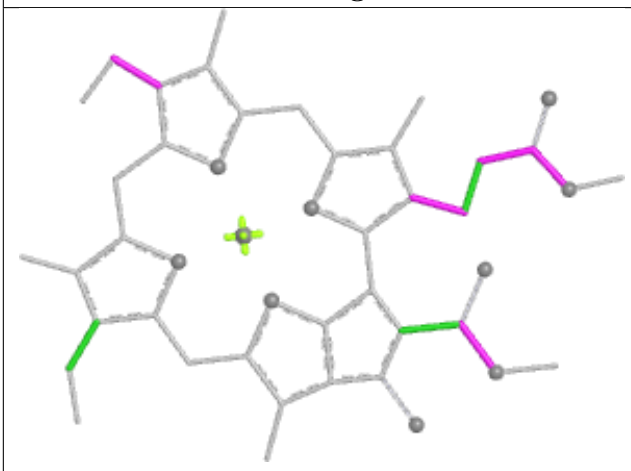
Ligand CLA 1 610



Bond lengths



Bond angles



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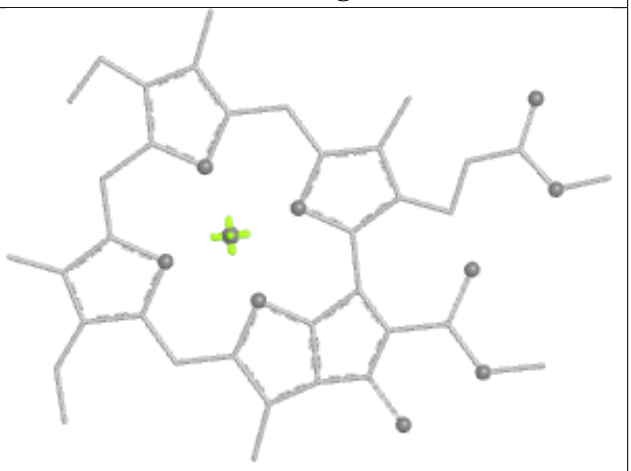
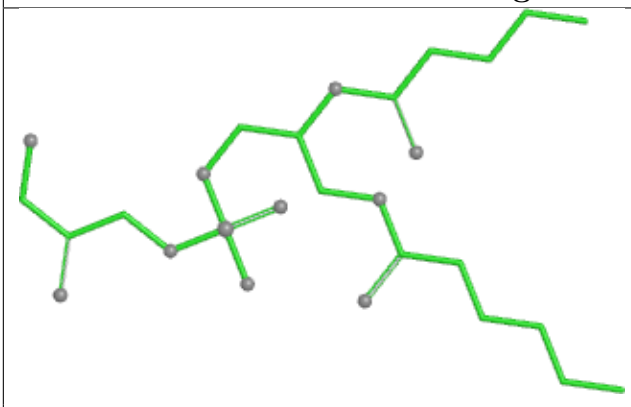


Rings

Ligand LHG A 5054



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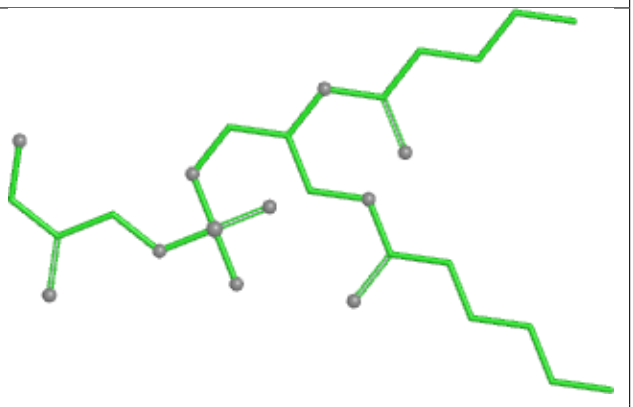
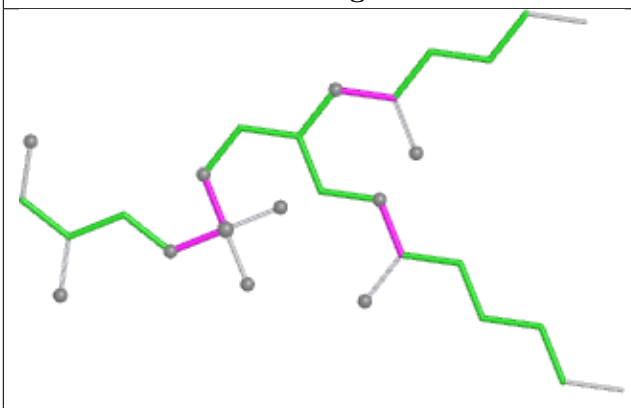


Bond angles



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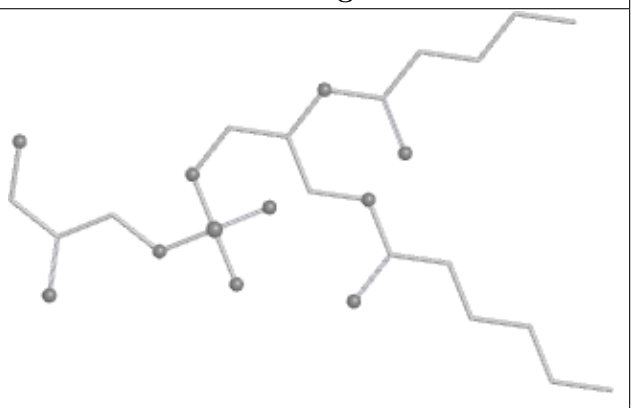
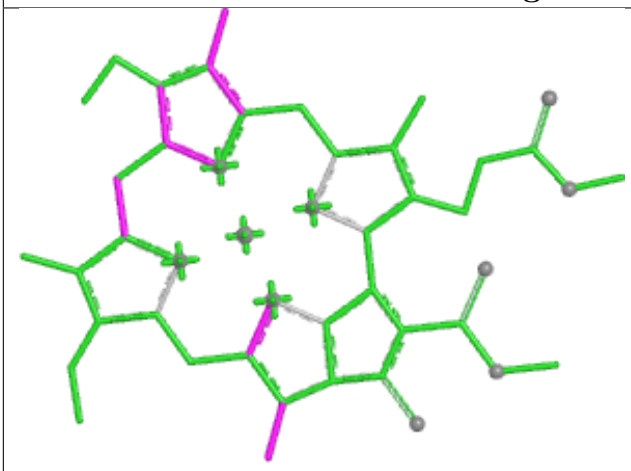


Rings

Ligand CLA G 203



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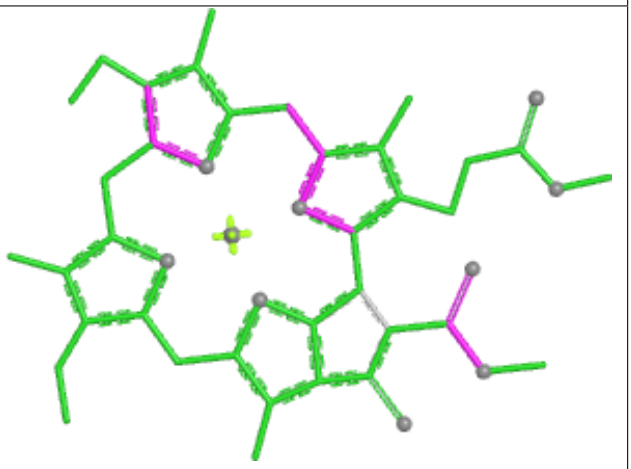
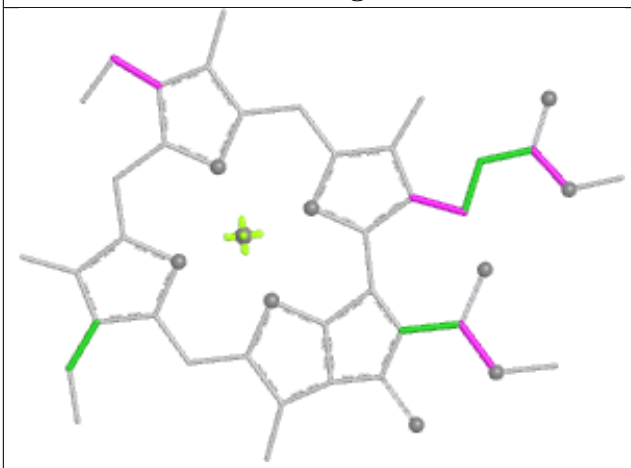


Bond angles



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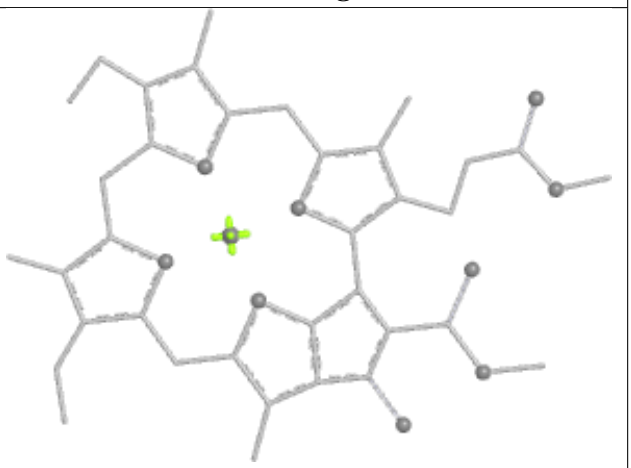
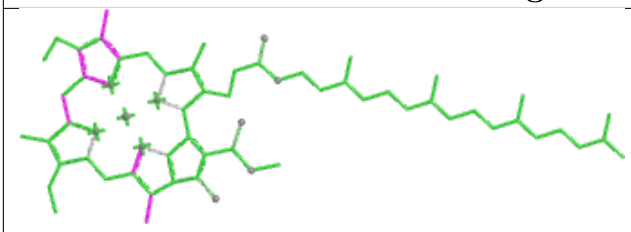
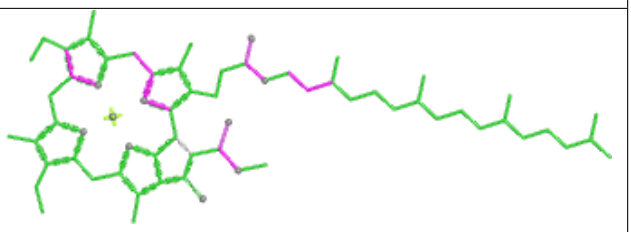


Rings

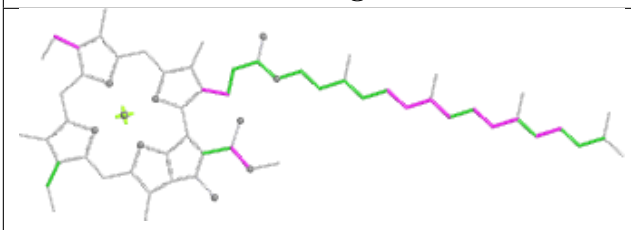
Ligand CLA L 201



Bond lengths



Bond angles



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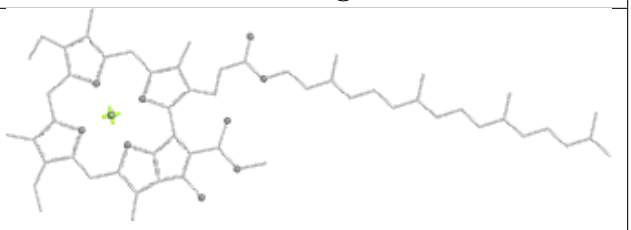
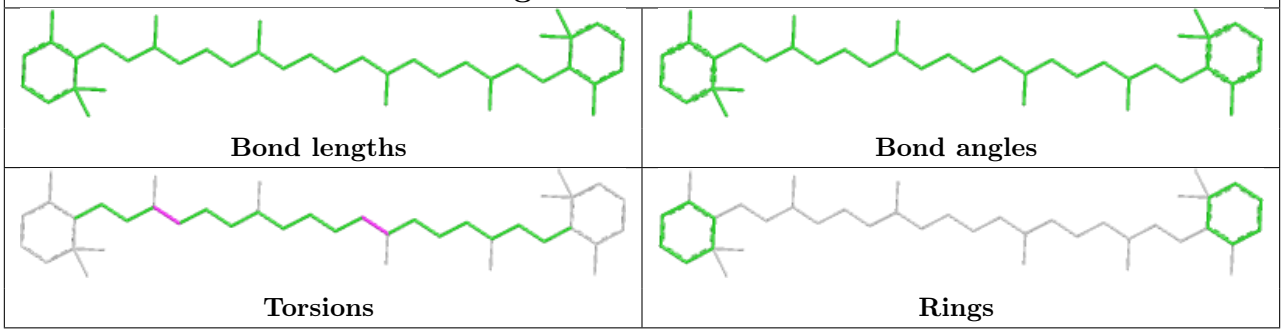
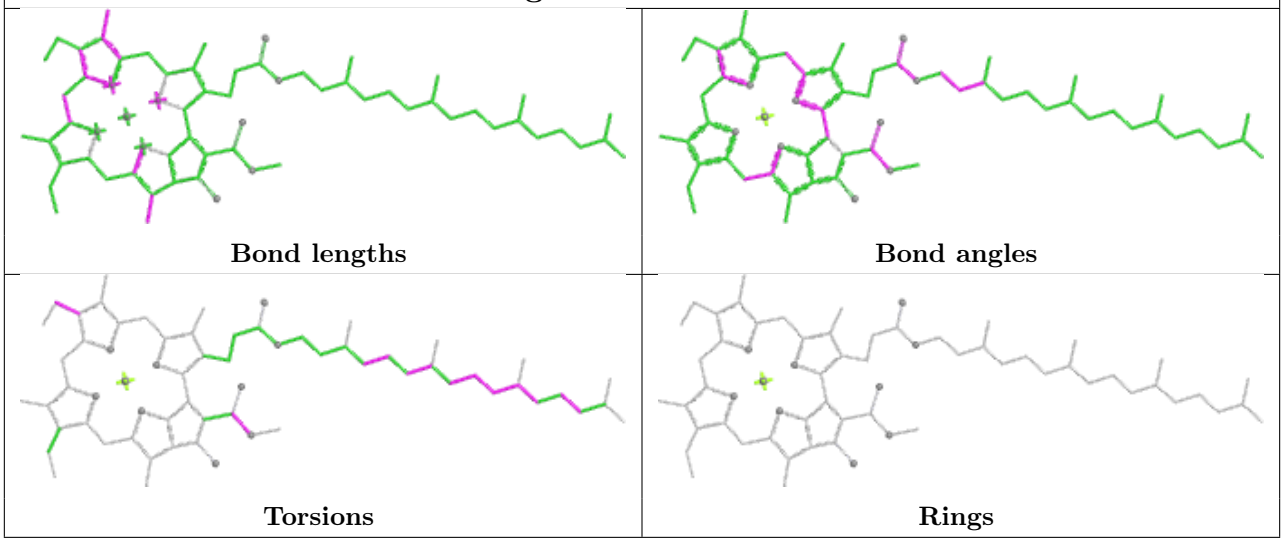


Rings

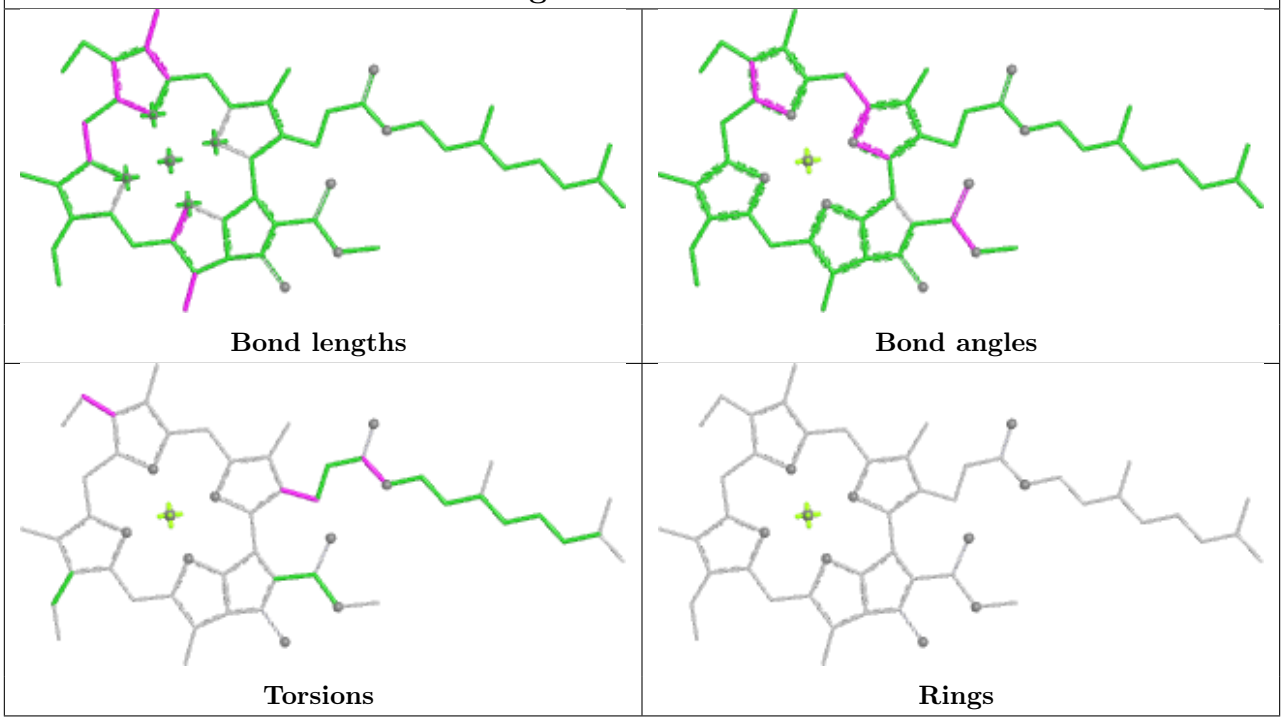
Ligand BCR A 5051



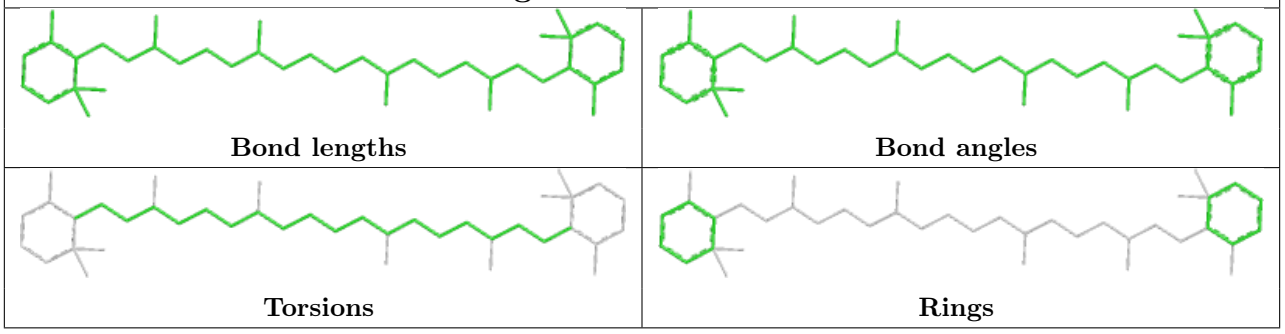
Ligand CLA B 808



Ligand CLA 3 325



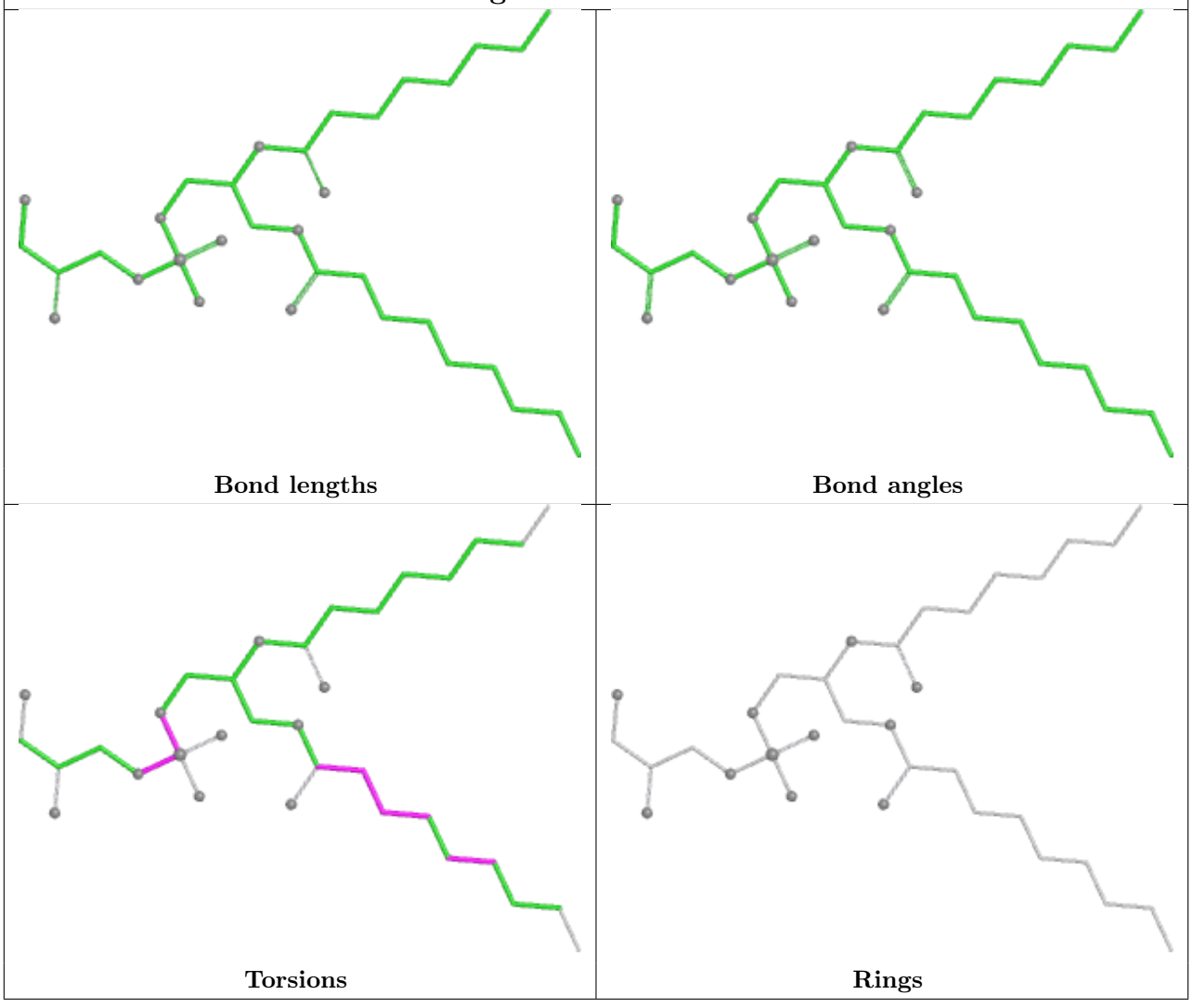
Ligand BCR A 5048



Bond lengths | Bond angles

Torsions | Rings

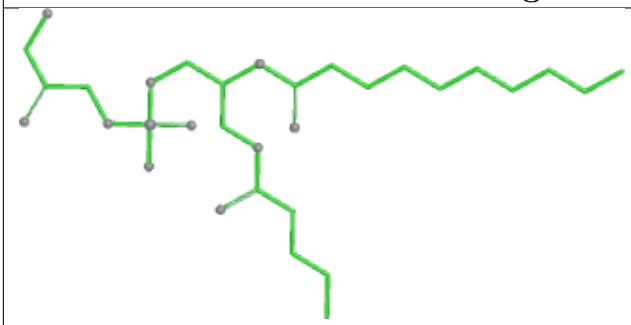
Ligand LHG 7 320



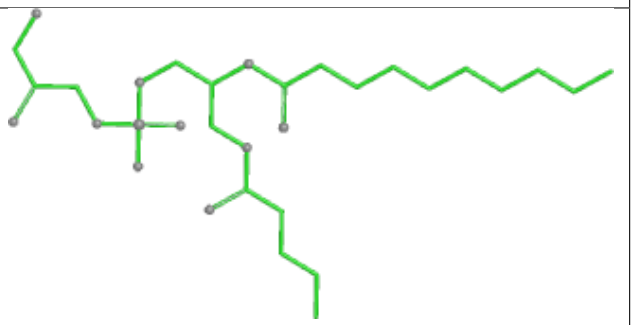
Bond lengths | Bond angles

Torsions | Rings

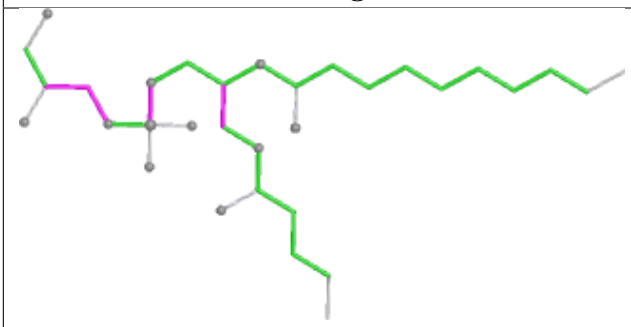
Ligand LHG B 801



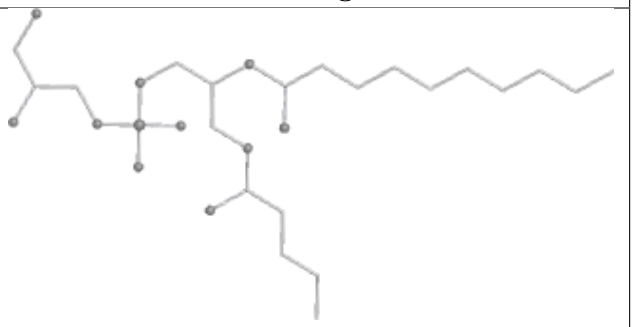
Bond lengths



Bond angles

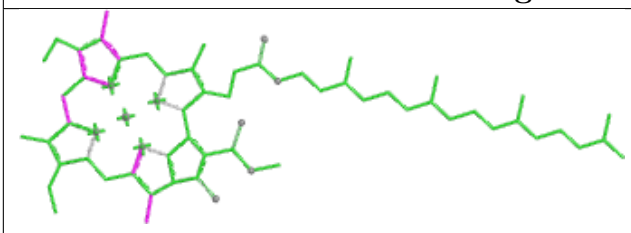


Torsions

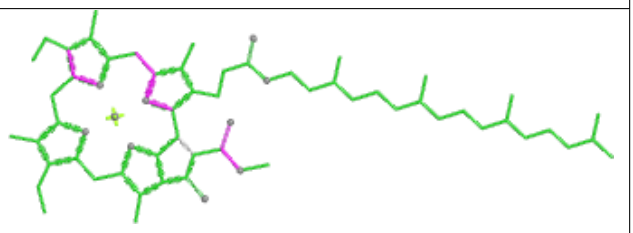


Rings

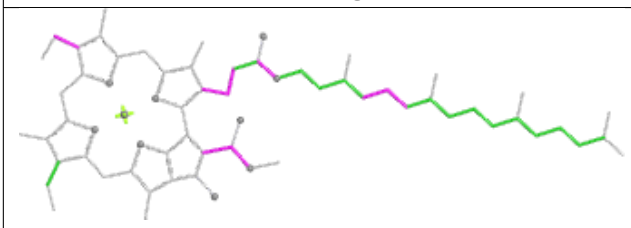
Ligand CLA A 5011



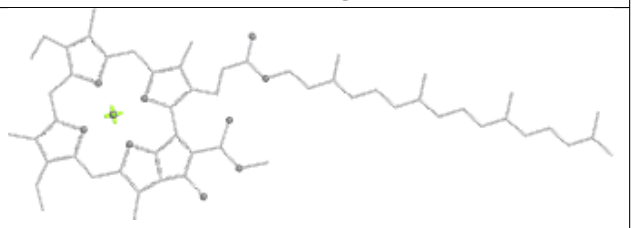
Bond lengths



Bond angles



Torsions

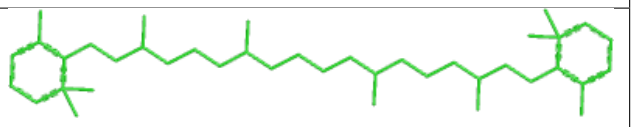


Rings

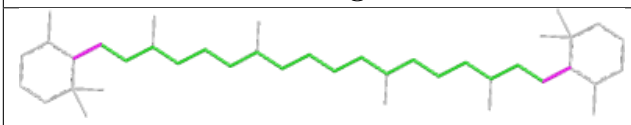
Ligand BCR 3 317



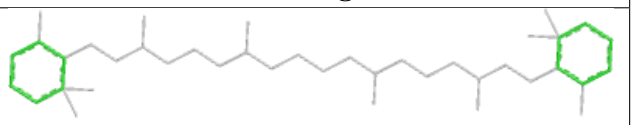
Bond lengths



Bond angles

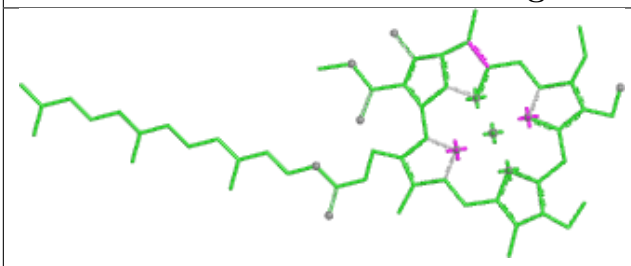


Torsions



Rings

Ligand CHL 2 302



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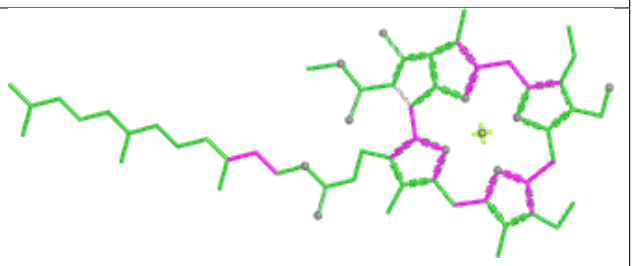
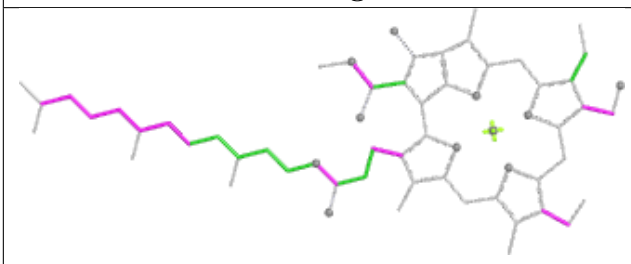


Bond angles



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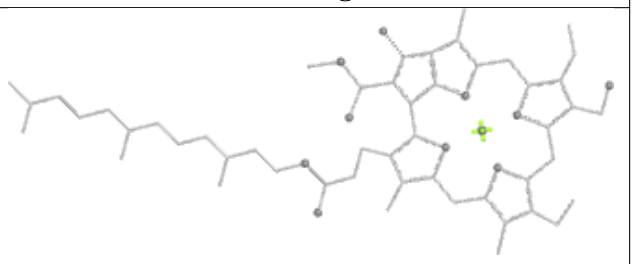
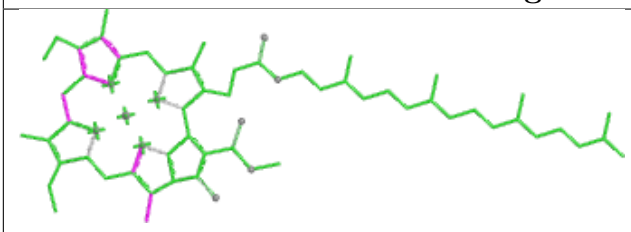
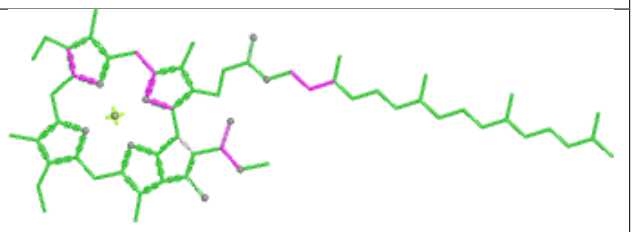


Rings

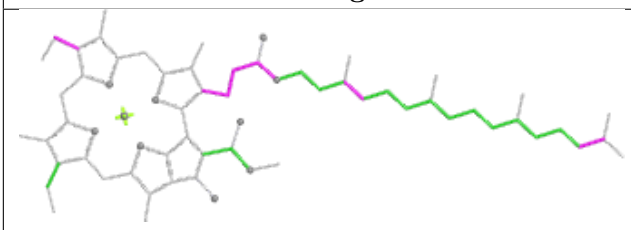
Ligand CLA B 819



Bond lengths



Bond angles



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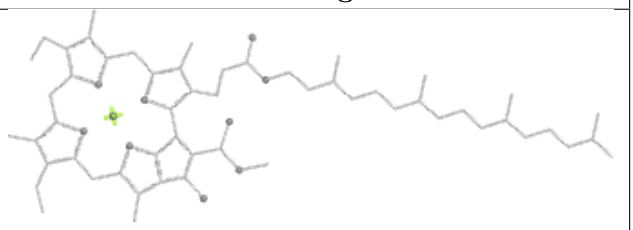
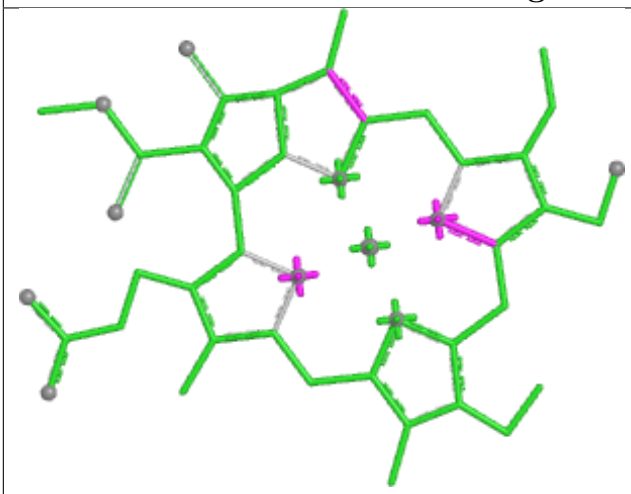


Rings

Ligand CHL 7 306



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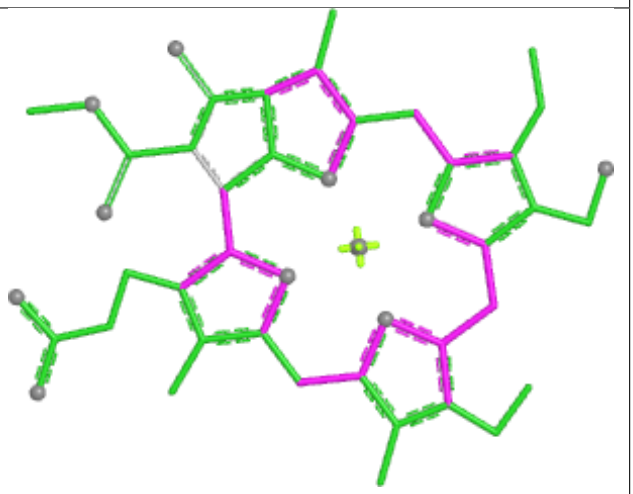

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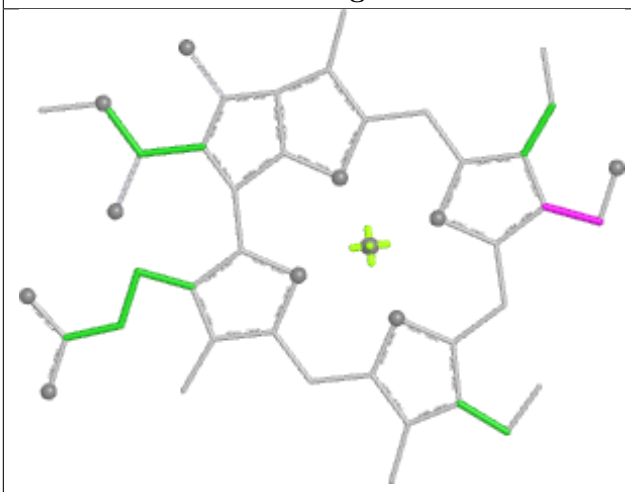
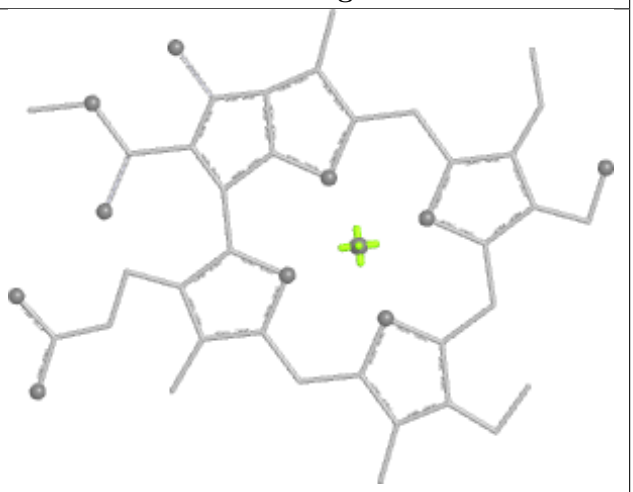
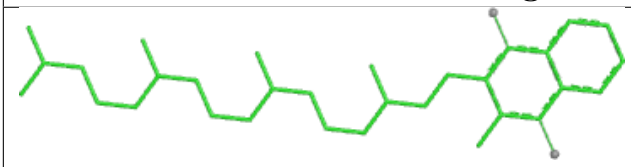


Torsions



Rings

Ligand PQN B 841



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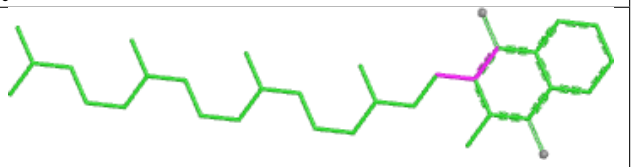
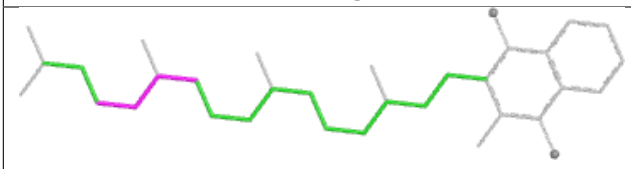


Bond angles



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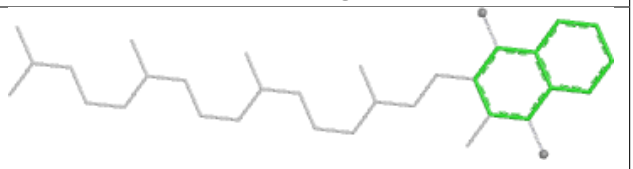
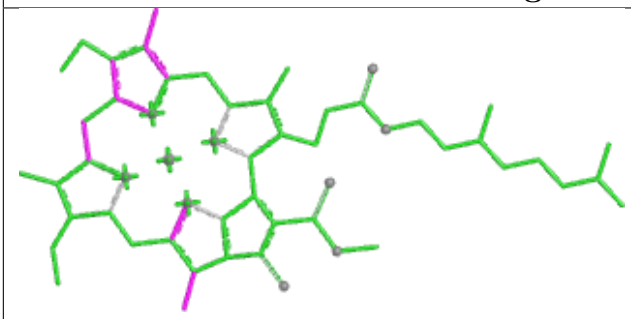


Rings

Ligand CLA B 812



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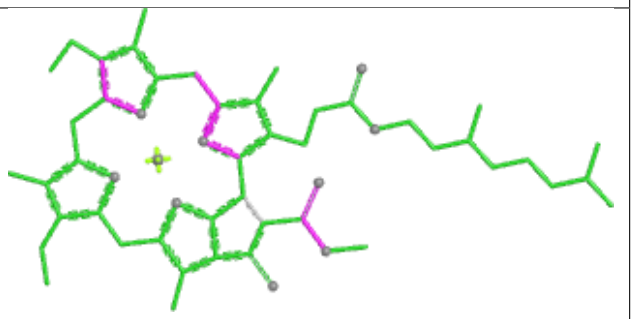

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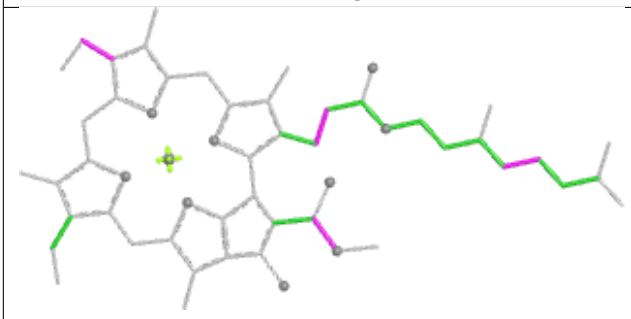

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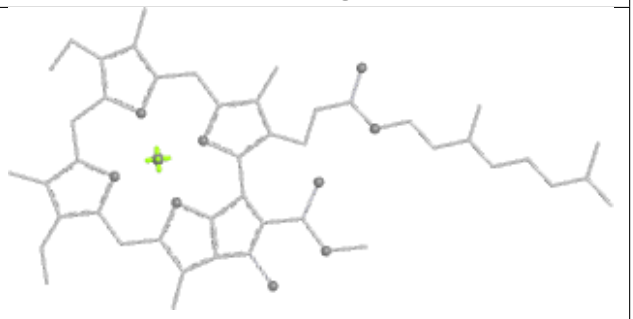
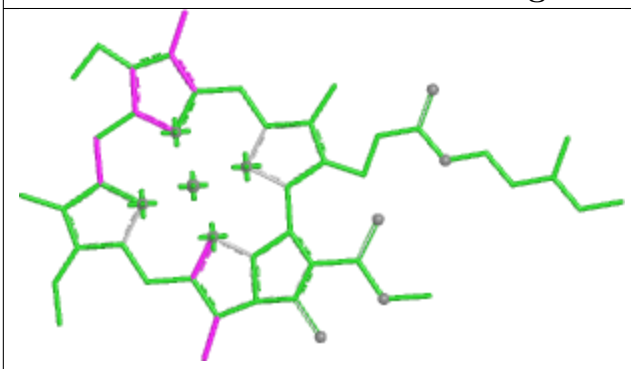


Rings

Ligand CLA 3 306



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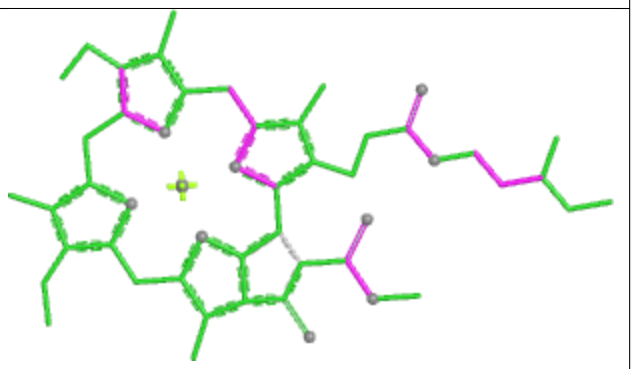
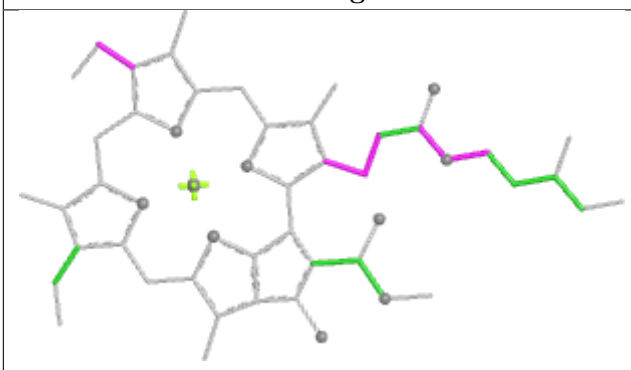


Bond angles



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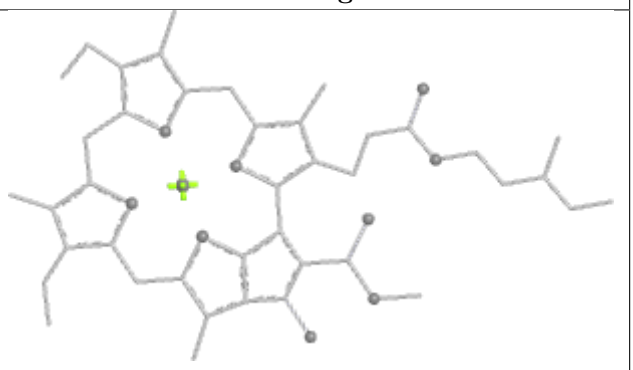
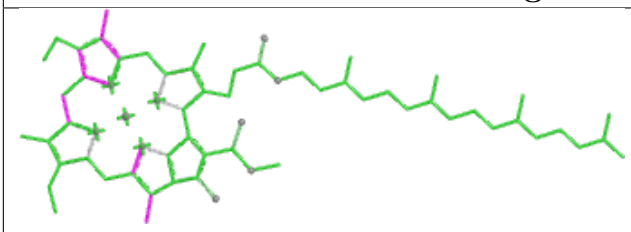


Rings

Ligand CLA B 830



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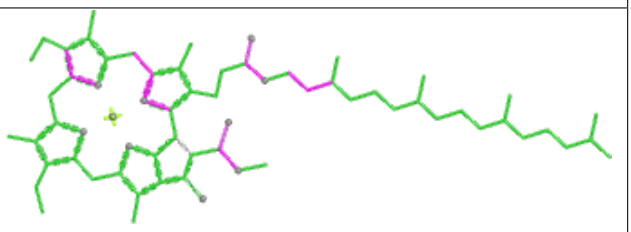
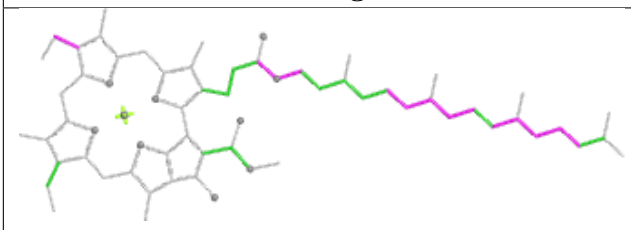


Bond angles



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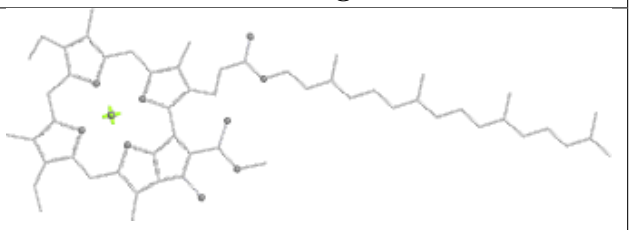


Rings

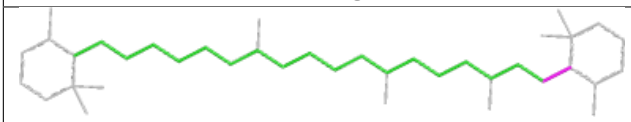
Ligand BCR B 845



Bond lengths



Bond angles



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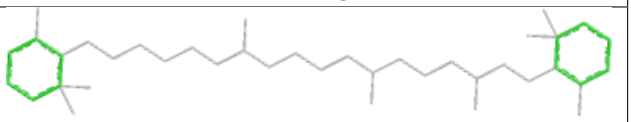
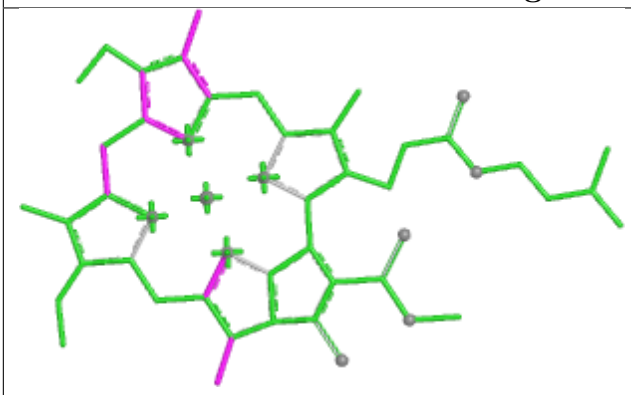
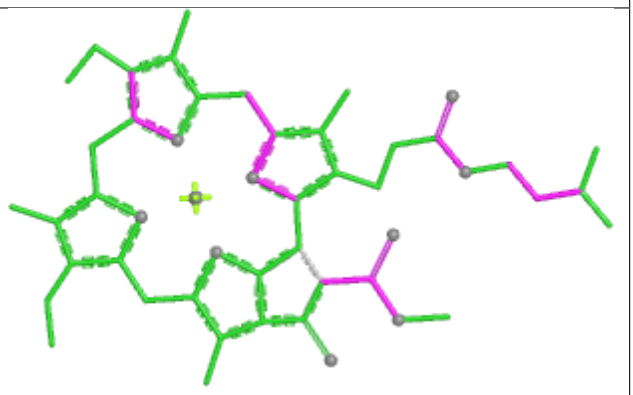


Rings

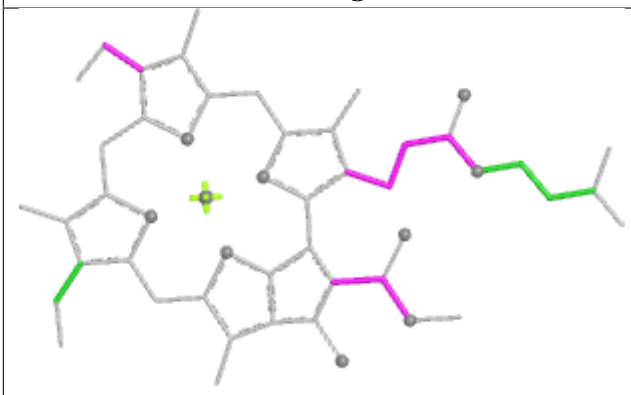
Ligand CLA B 834



Bond lengths



Bond angles



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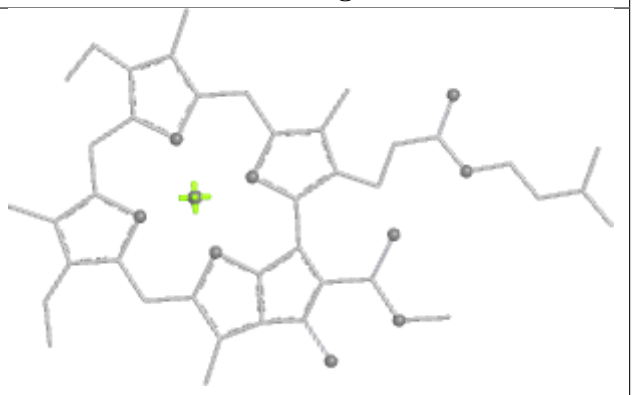
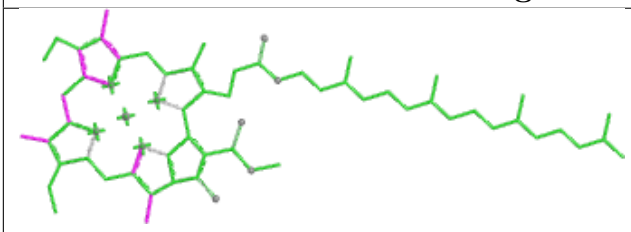


Rings

Ligand CLA A 5009



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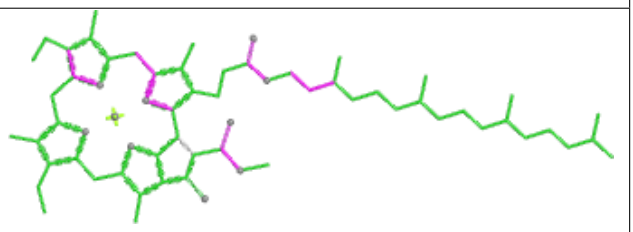
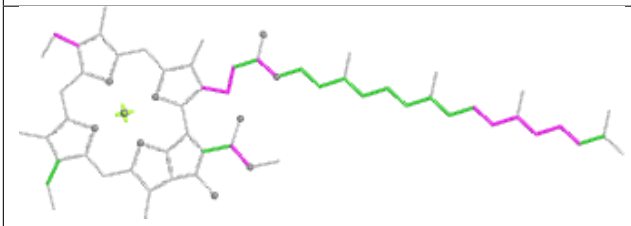


Bond angles



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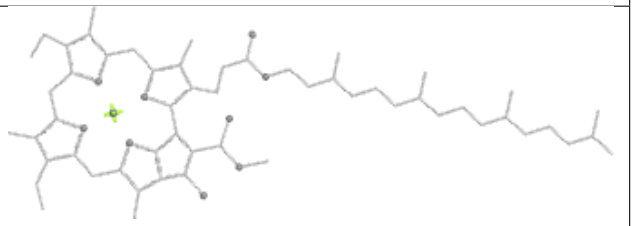
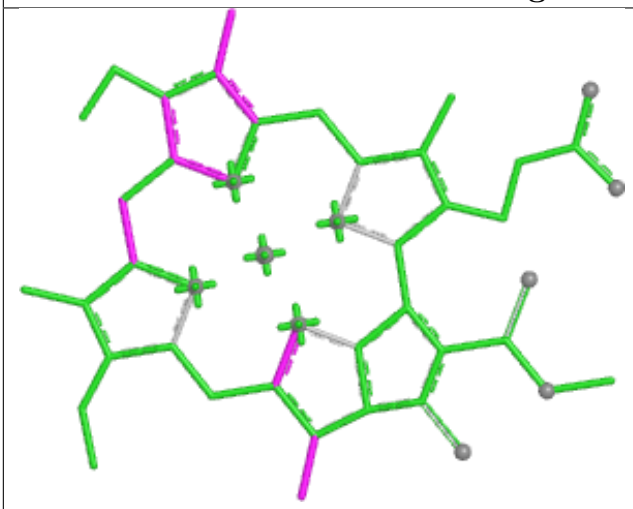


Rings

Ligand CLA 2 308



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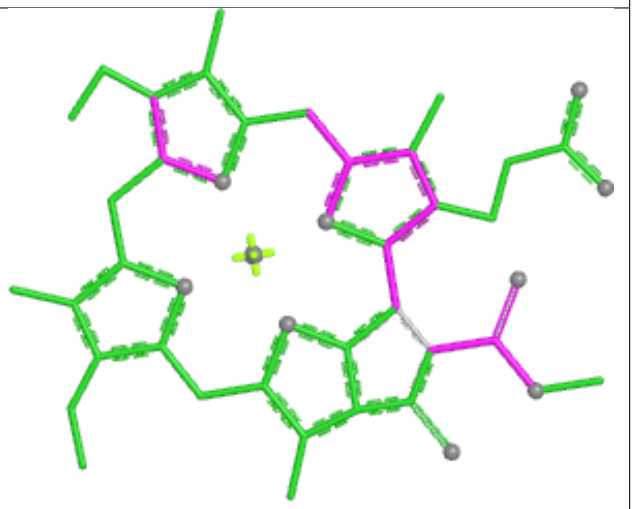
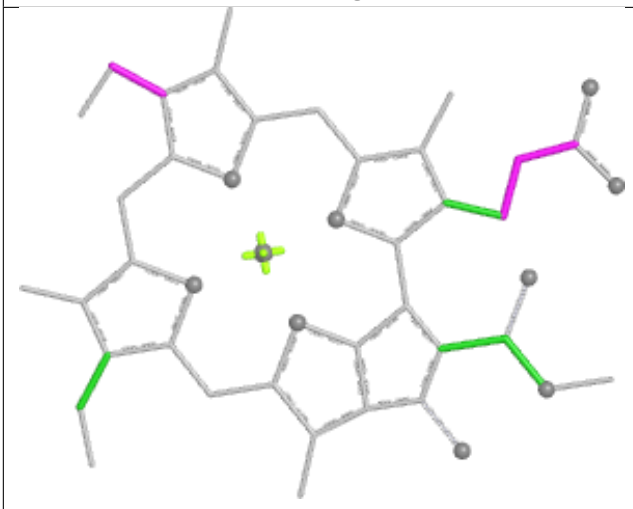


Bond angles

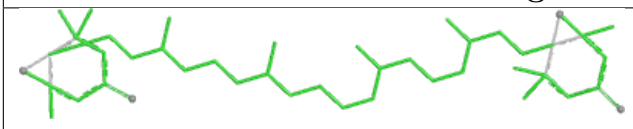


Torsions



Rings

Ligand XAT 9 614



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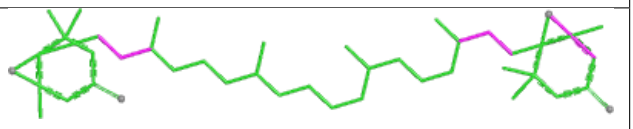
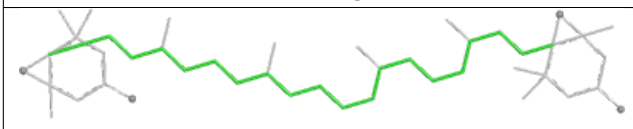
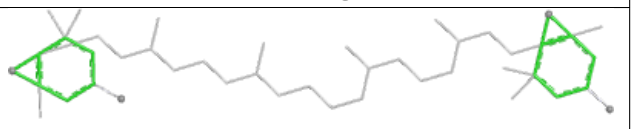


Bond angles

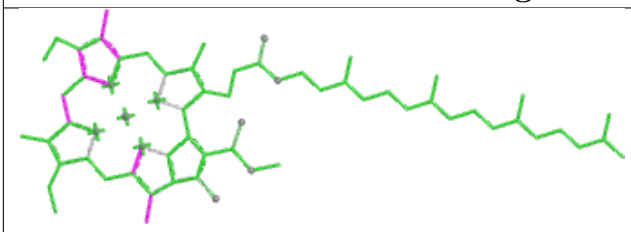


Torsions



Rings

Ligand CLA A 5035



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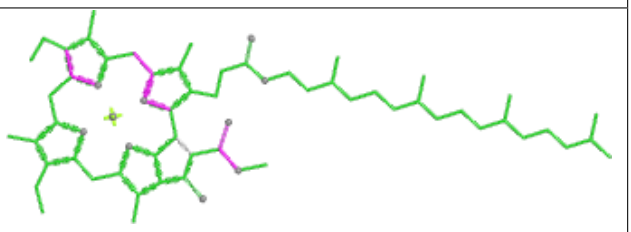
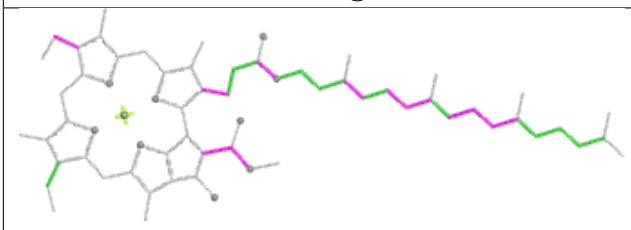


Bond angles



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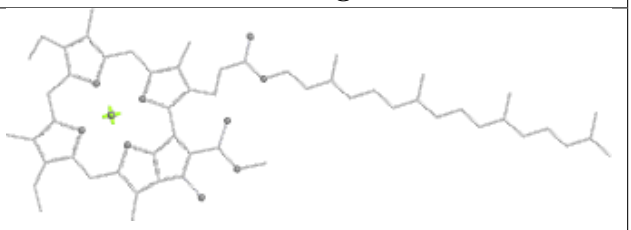
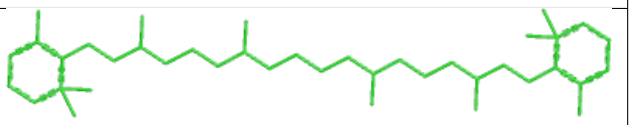


Rings

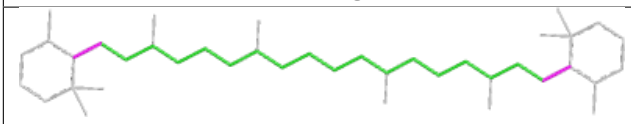
Ligand BCR K 4006



Bond lengths



Bond angles



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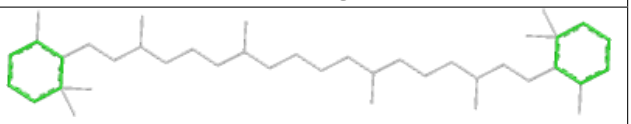
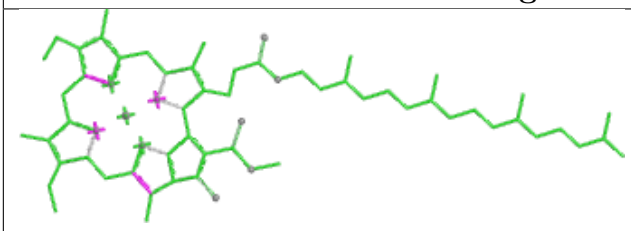
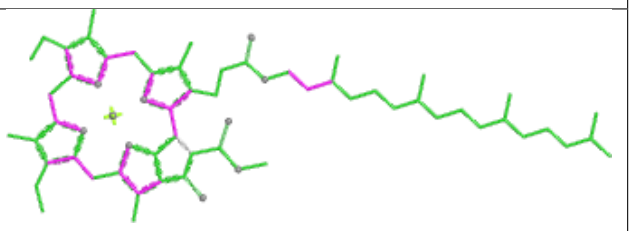


Rings

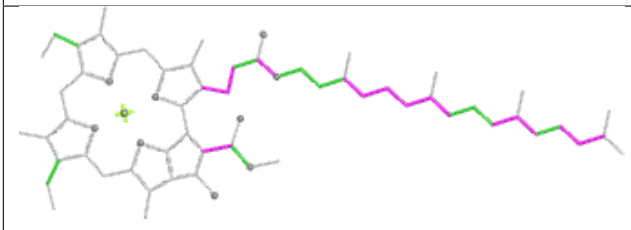
Ligand CL0 A 5003



Bond lengths



Bond angles



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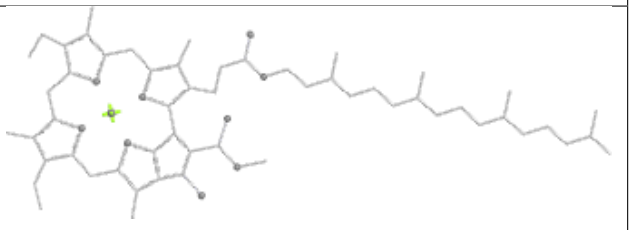
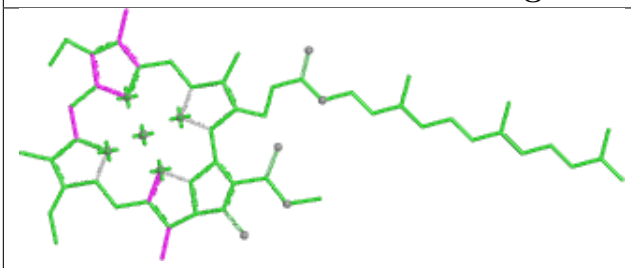
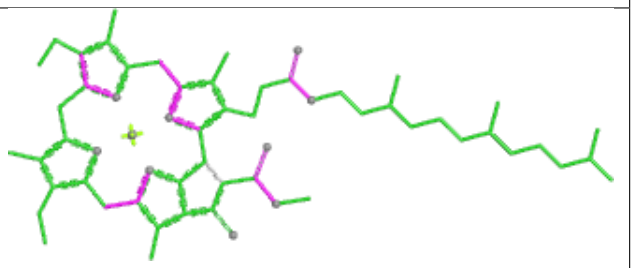


Rings

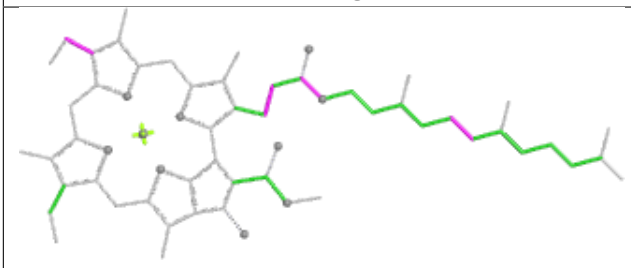
Ligand CLA B 836



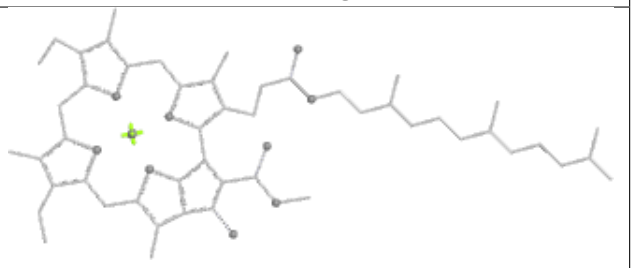
Bond lengths



Bond angles

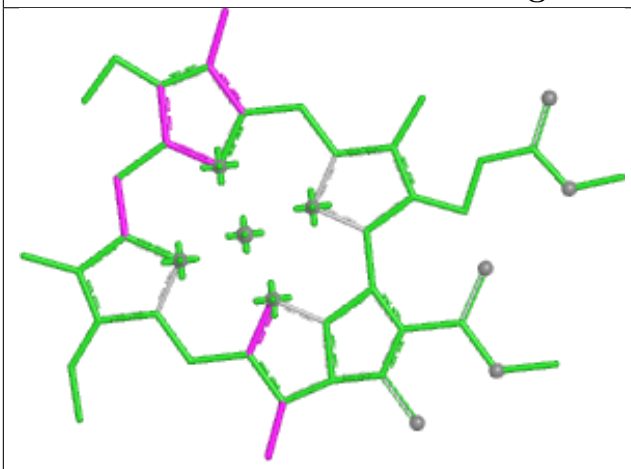


Torsions



Rings

Ligand CLA 3 303



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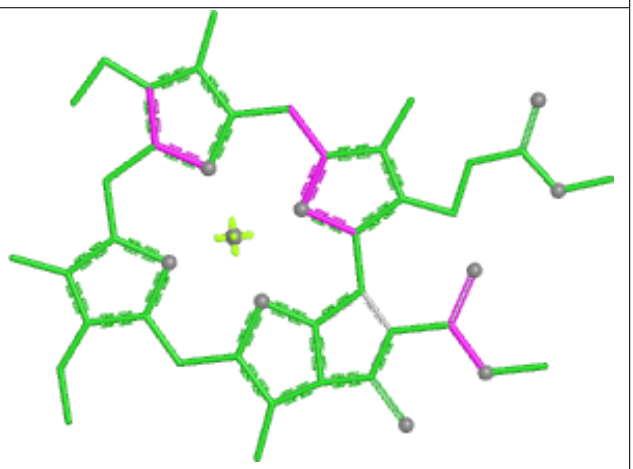

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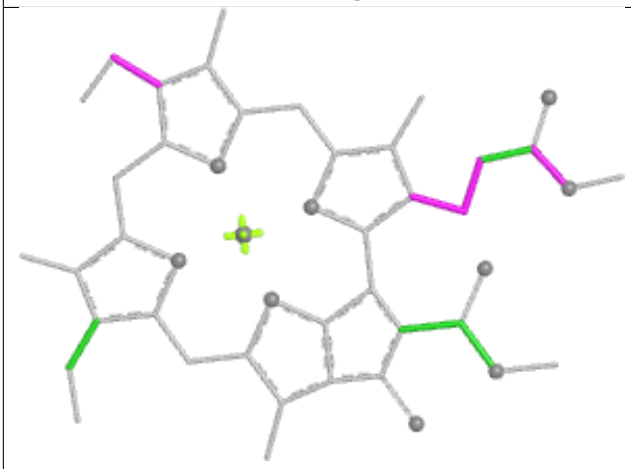

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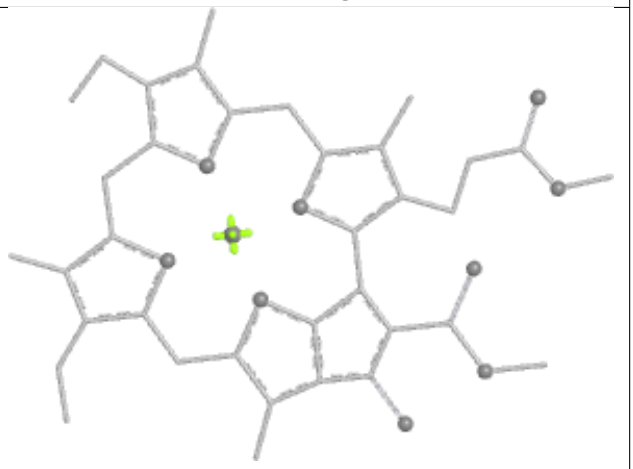
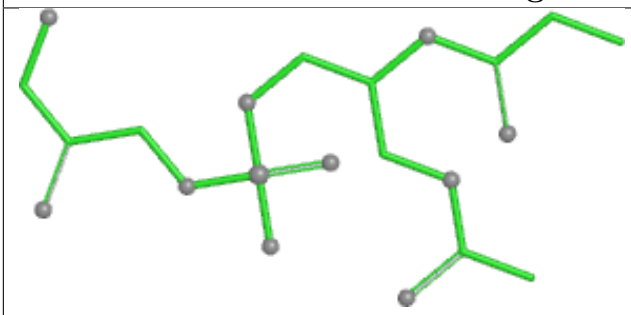


Rings

Ligand LHG 7 319



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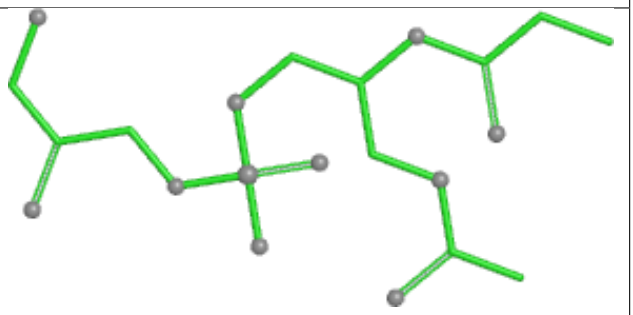
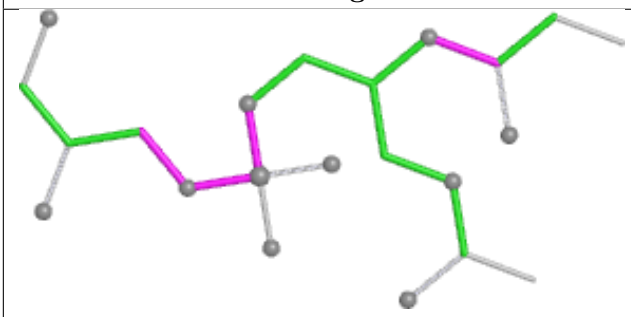


Bond angles



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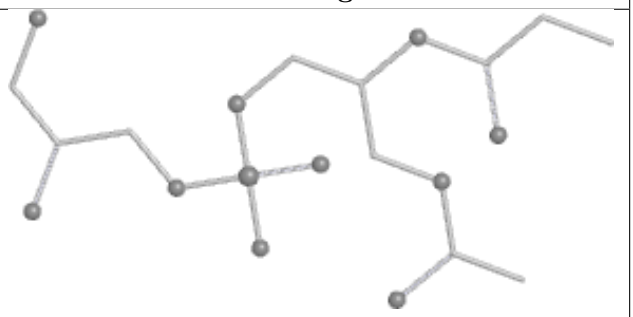
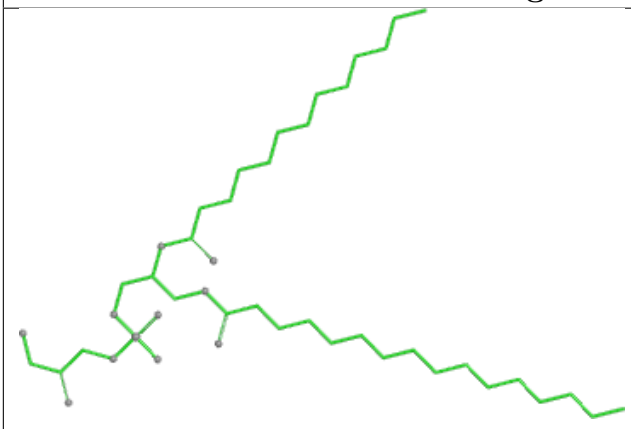


Rings

Ligand LHG 1 620



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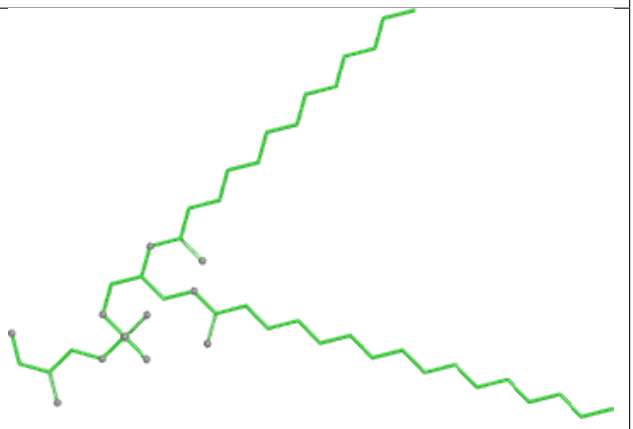
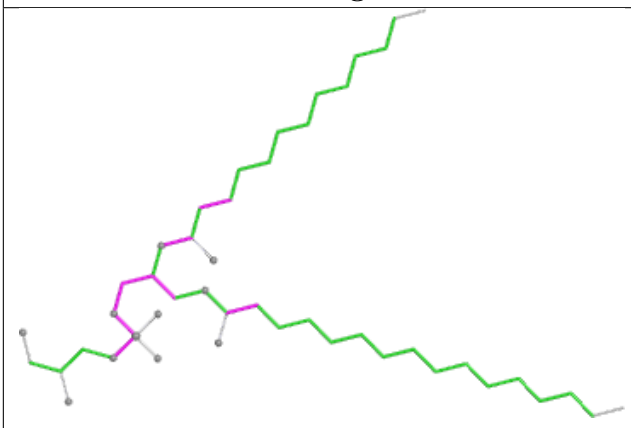


Bond angles



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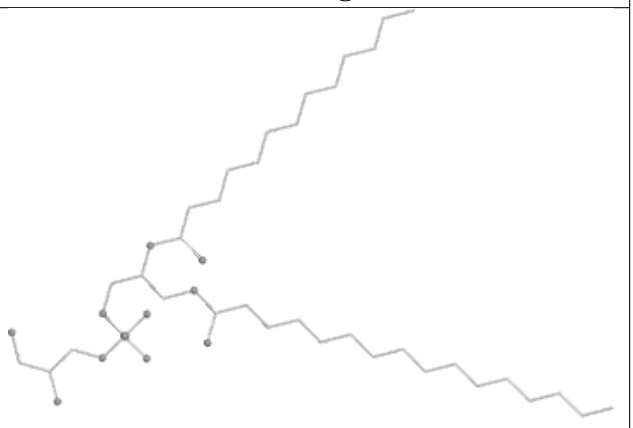
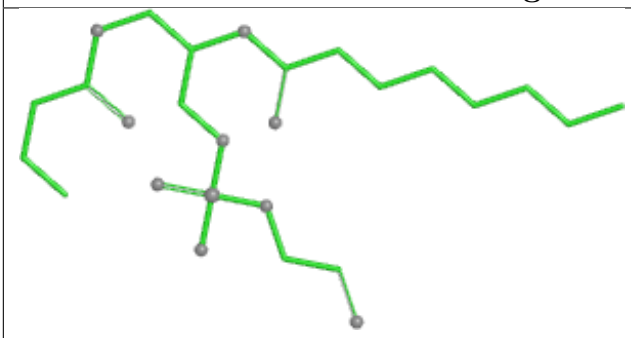
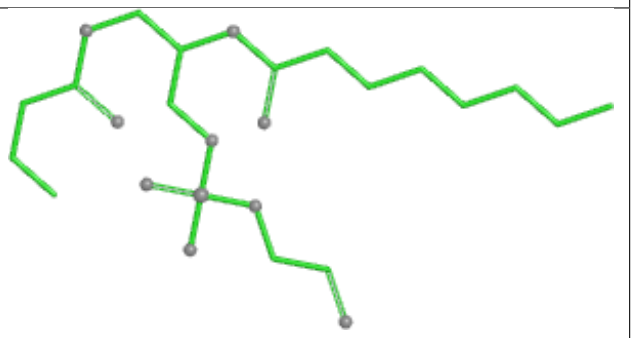


Rings

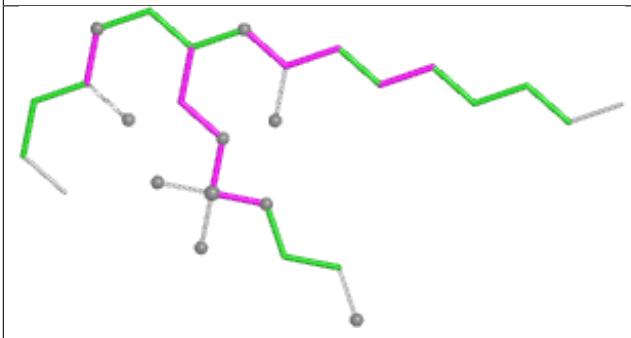
Ligand PTY B 802



Bond lengths



Bond angles



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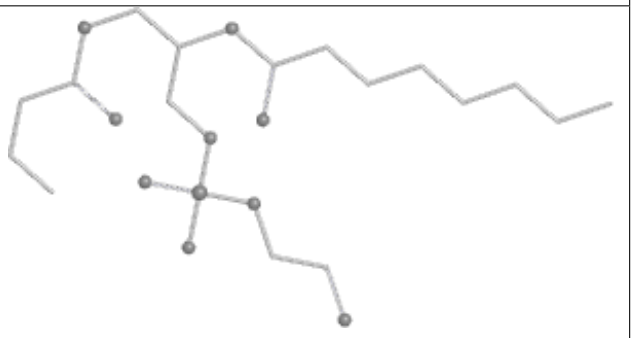
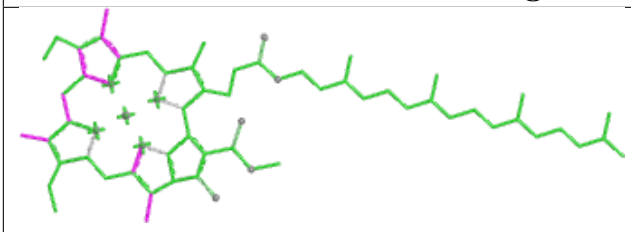


Rings

Ligand CLA B 832



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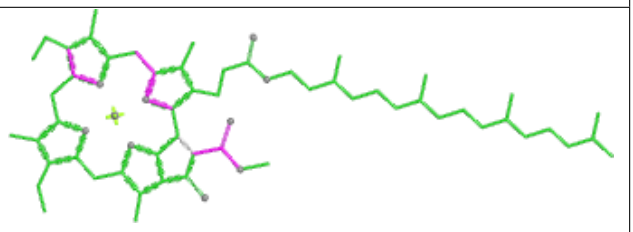
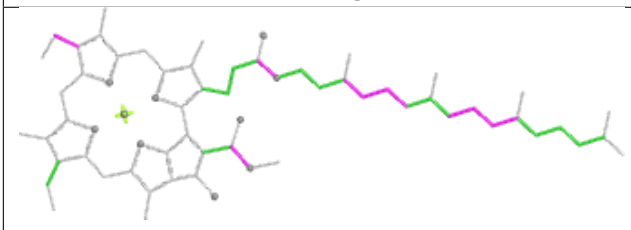


Bond angles



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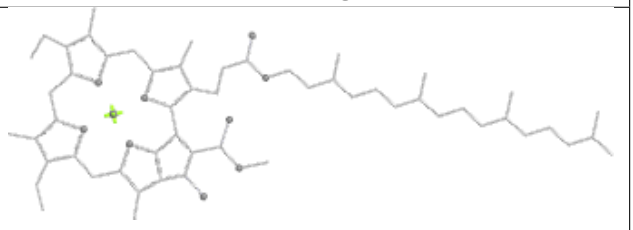
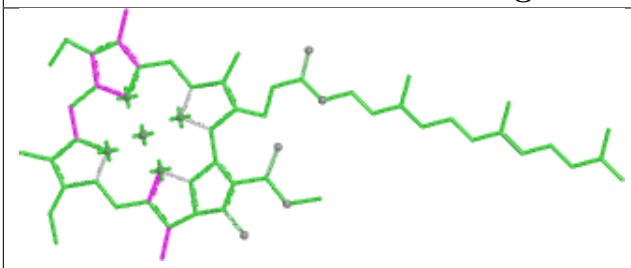
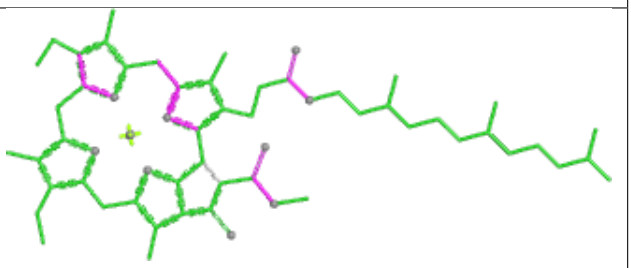
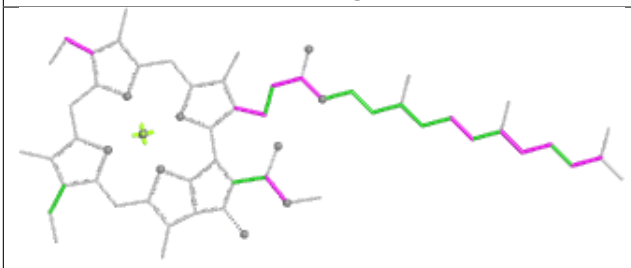
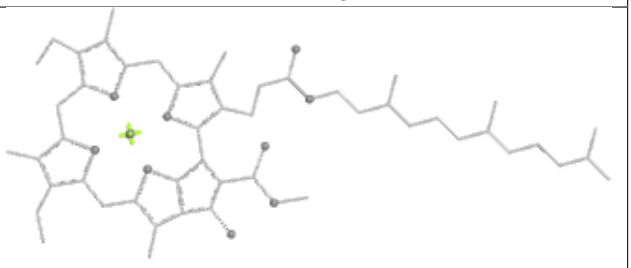


Rings

Ligand CLA A 5024	
 Bond lengths	 Bond angles
 Torsions	 Rings

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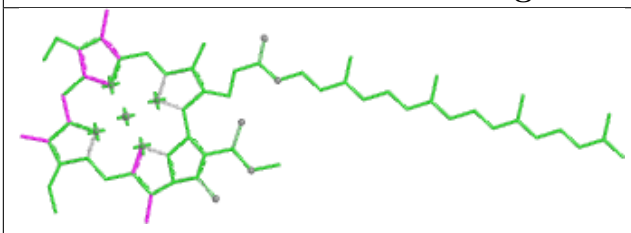
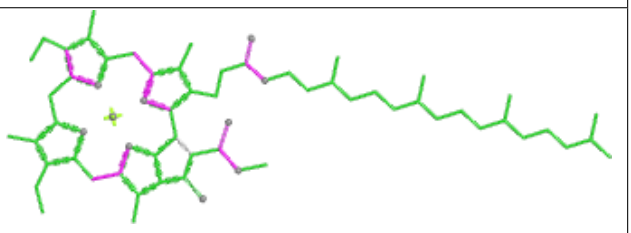
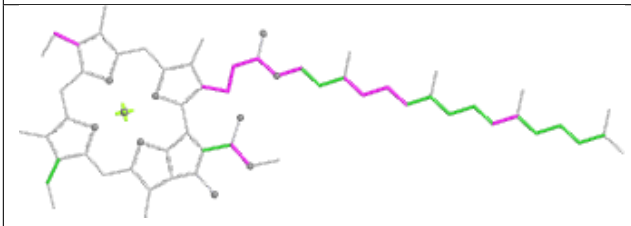
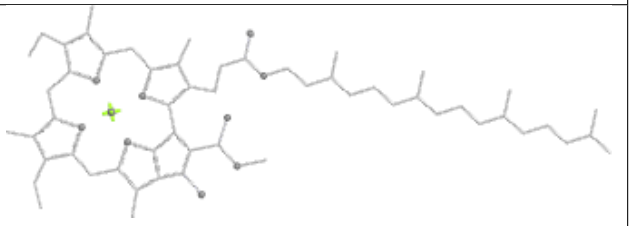
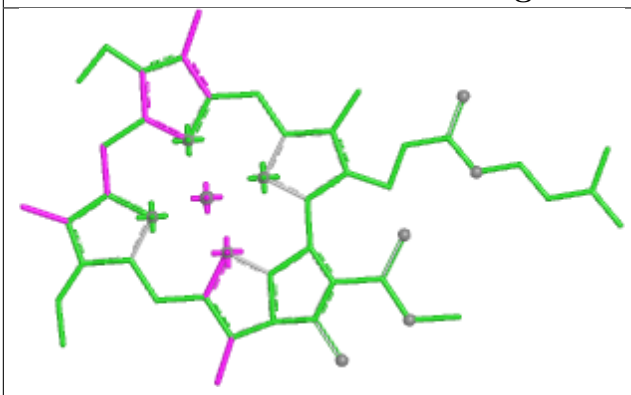
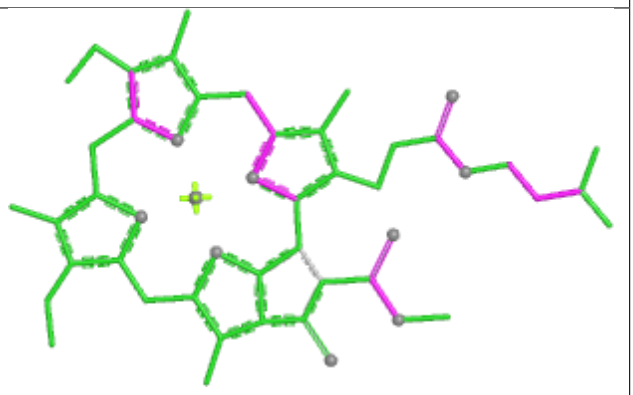
 Bond lengths	 Bond angles
 Torsions	 Rings

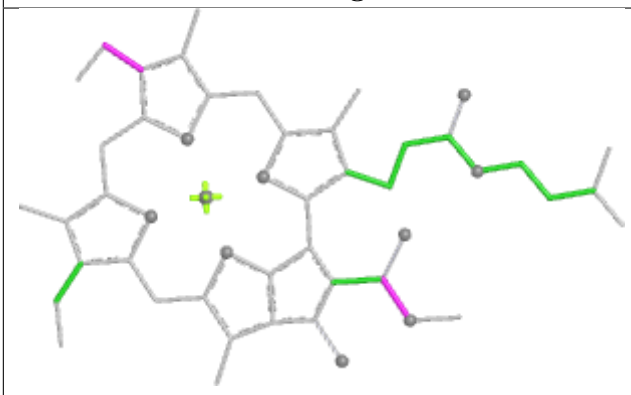
Ligand CLA A 5032



Bond lengths



Bond angles



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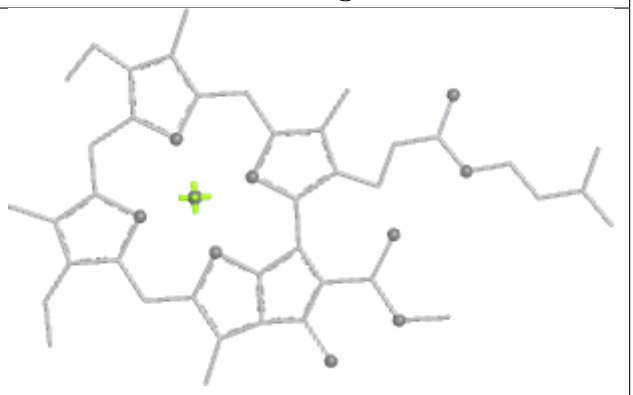
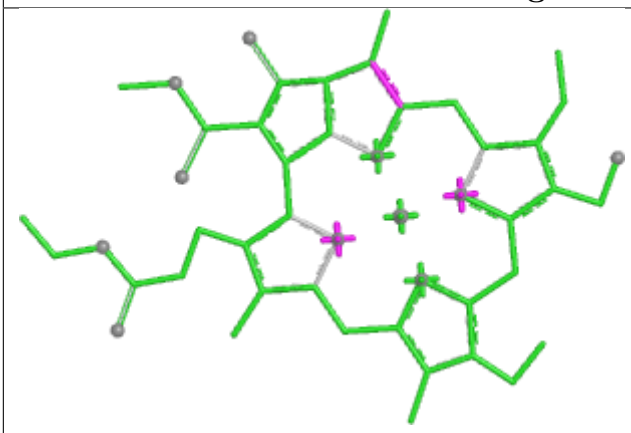


Rings

Ligand CHL 7 308



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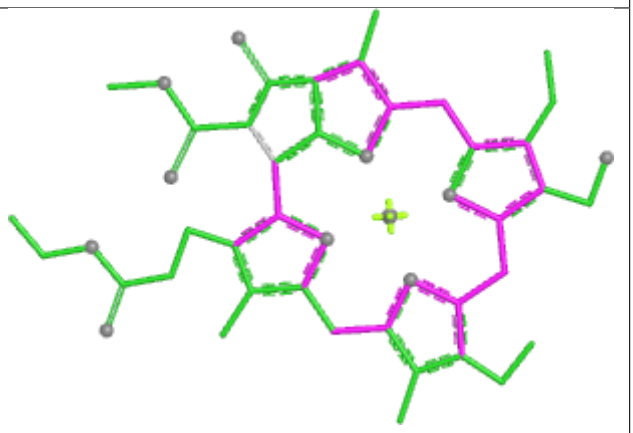
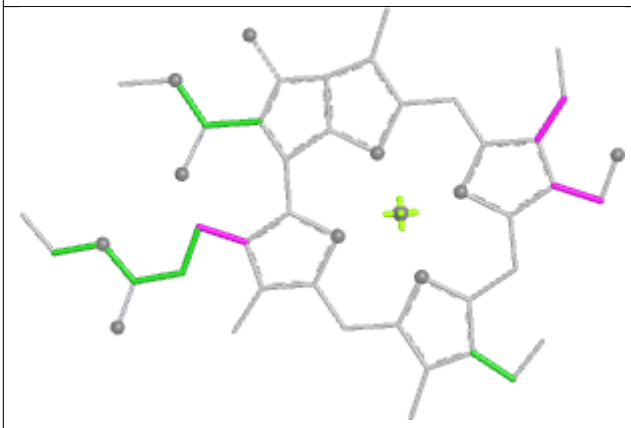


Bond angles

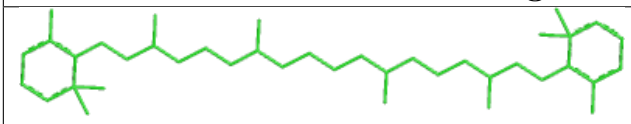


Torsions



Rings

Ligand BCR 3 318



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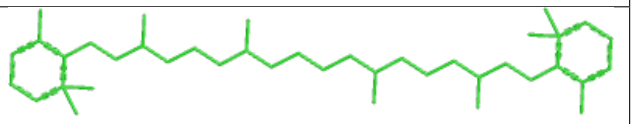
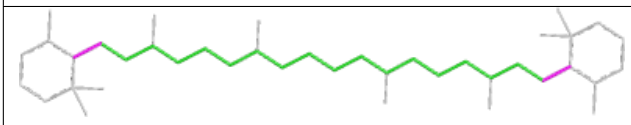


Bond angles



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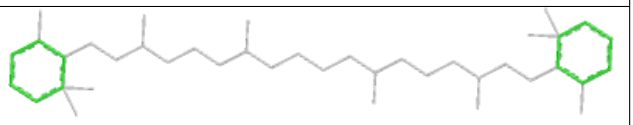


Rings

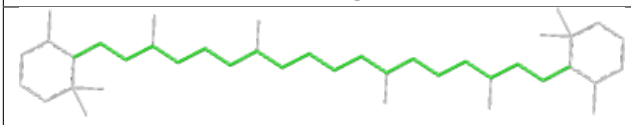
Ligand BCR F 304



Bond lengths



Bond angles



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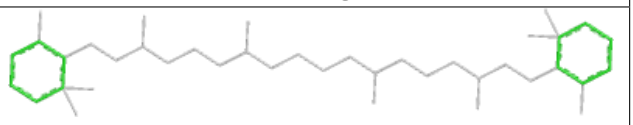
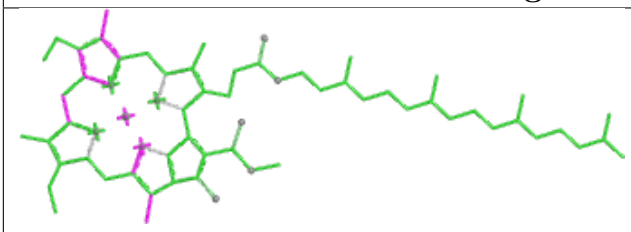
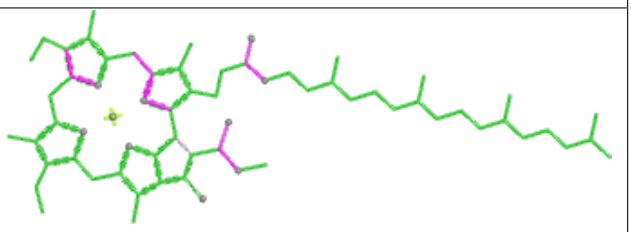


Rings

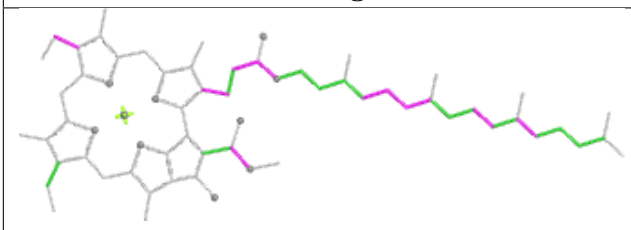
Ligand CLA B 814



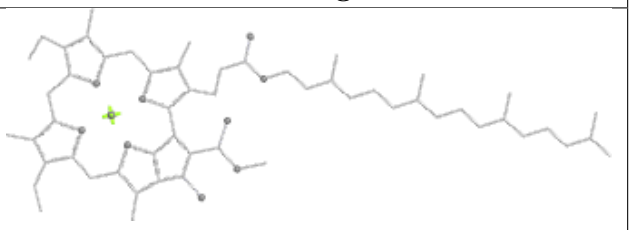
Bond lengths



Bond angles

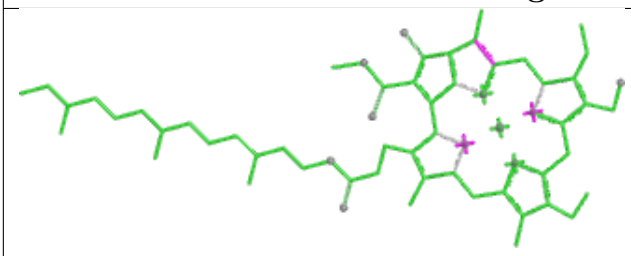


Torsions



Rings

Ligand CHL 3 301



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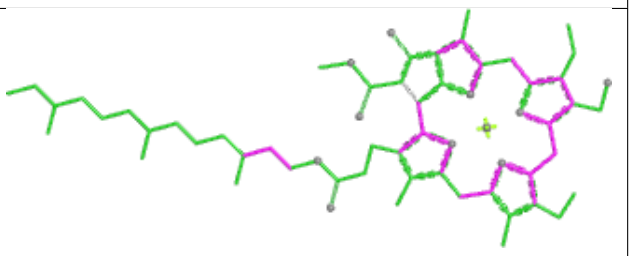
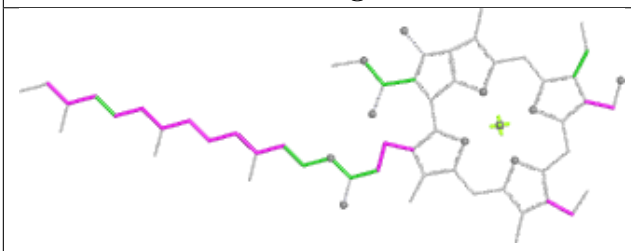


Bond angles



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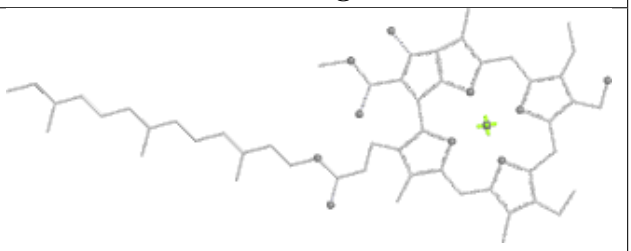
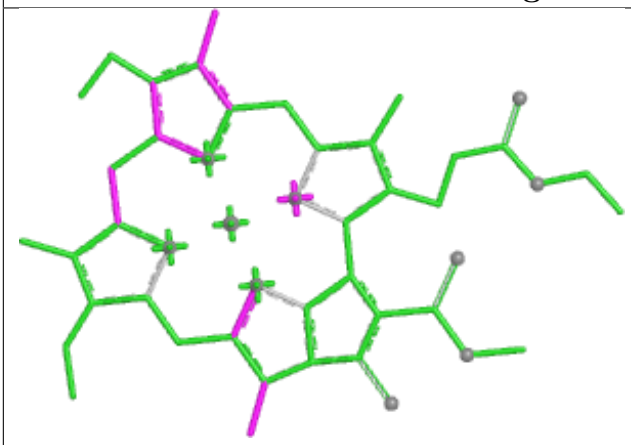
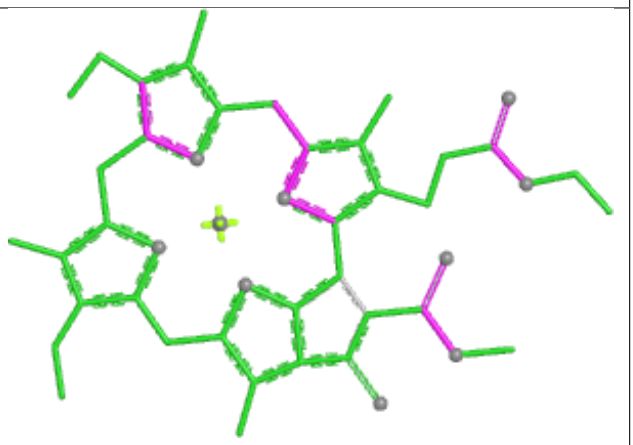


Rings

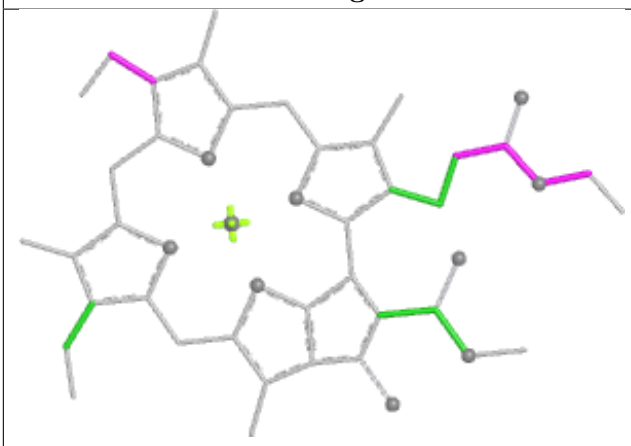
Ligand CLA G 202



Bond lengths



Bond angles



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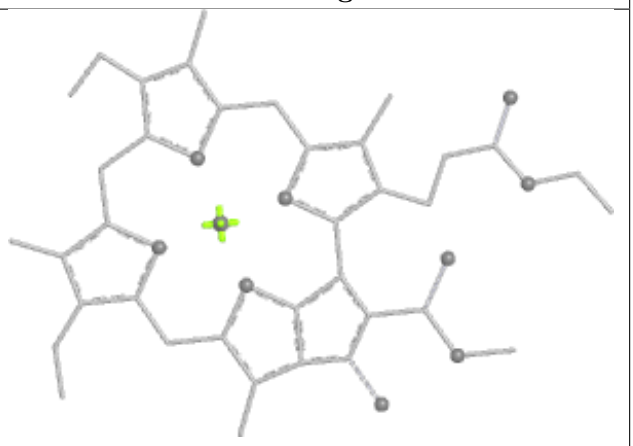
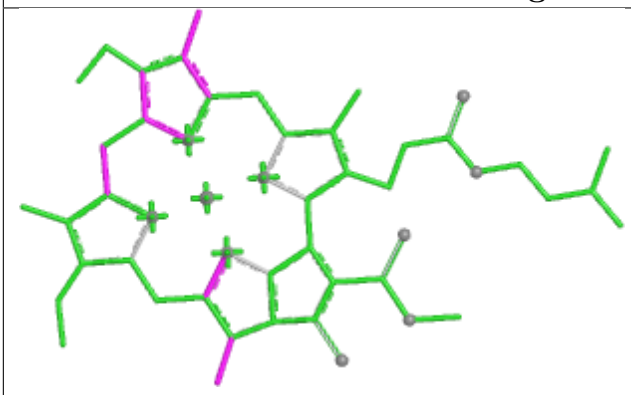
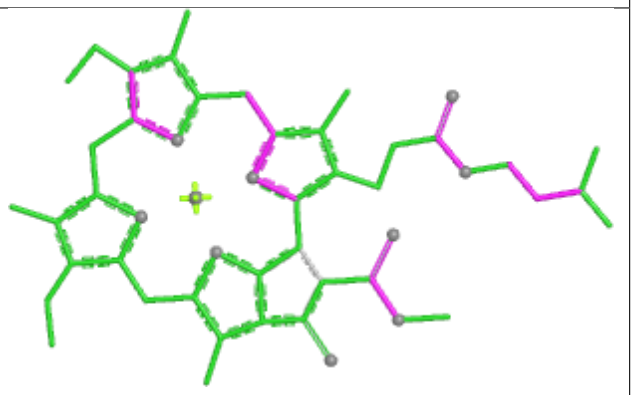


Rings

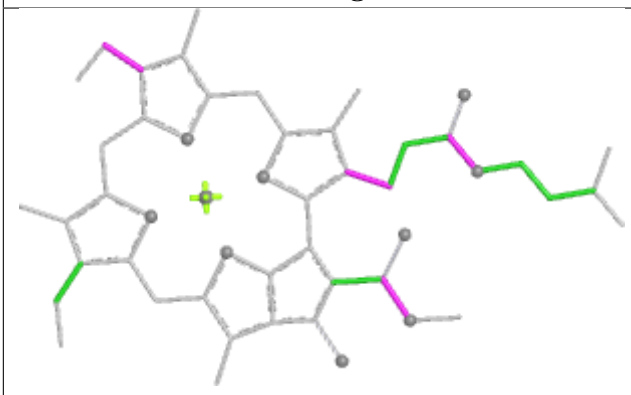
Ligand CLA 7 314



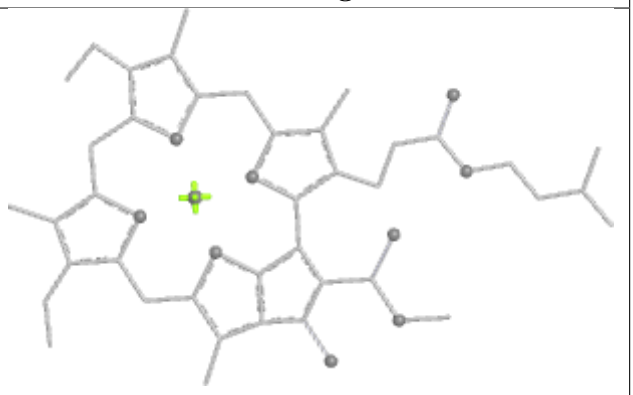
Bond lengths



Bond angles

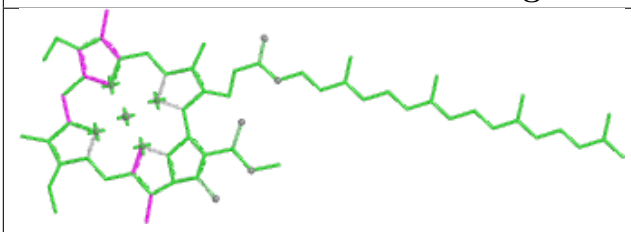


Torsions



Rings

Ligand CLA G 201



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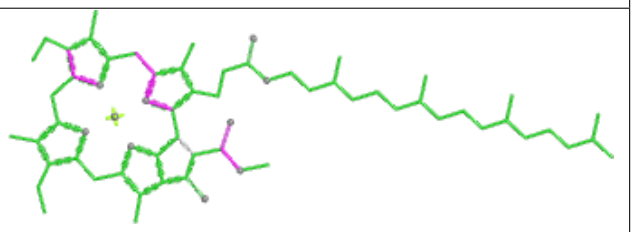
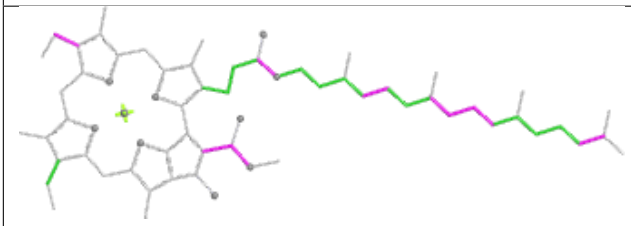


Bond angles



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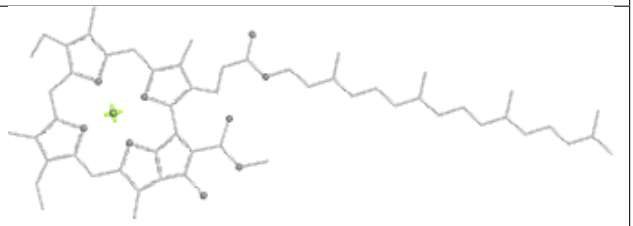
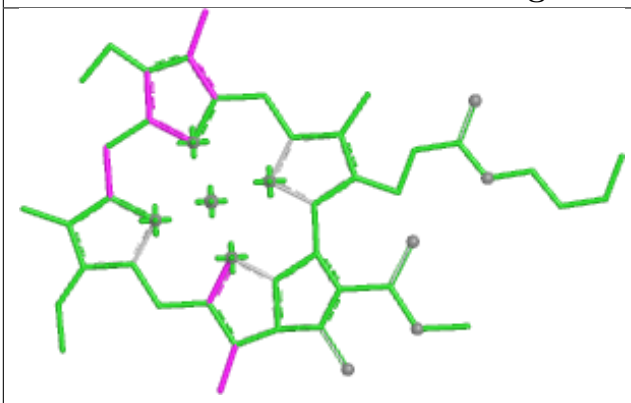


Rings

Ligand CLA J 104



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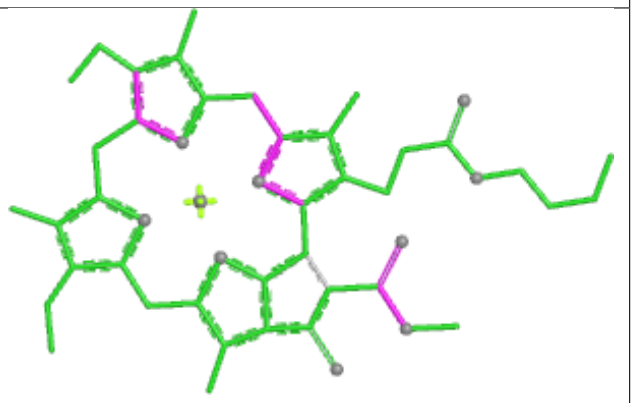
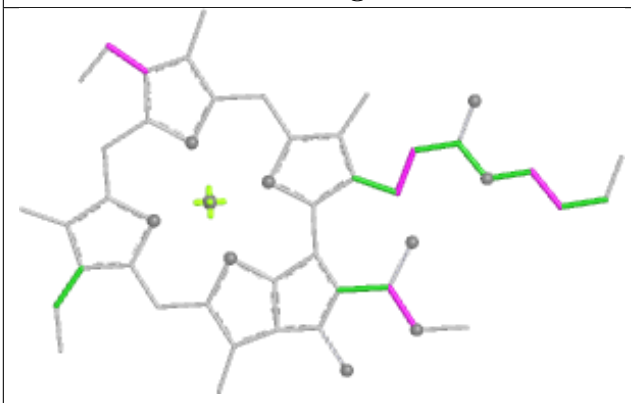


Bond angles



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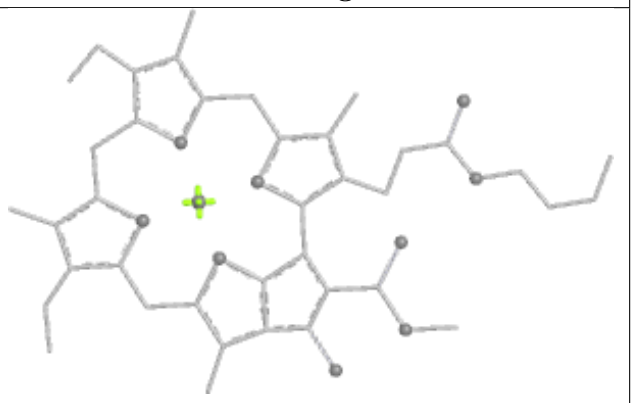
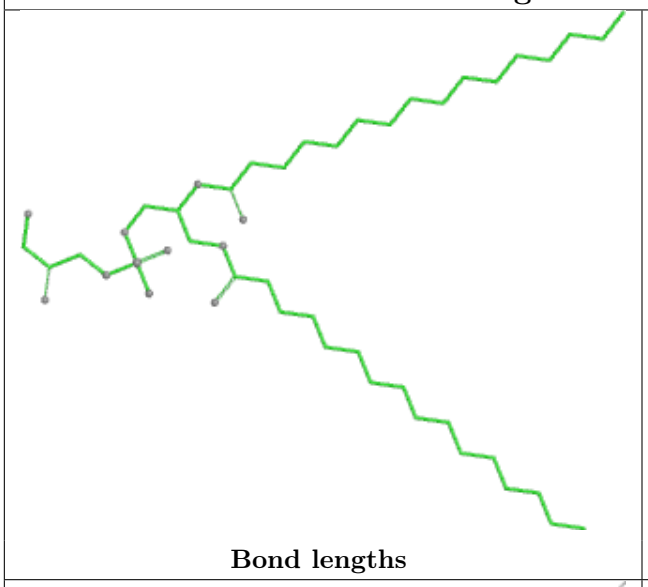


Rings

Ligand LHG A 5052



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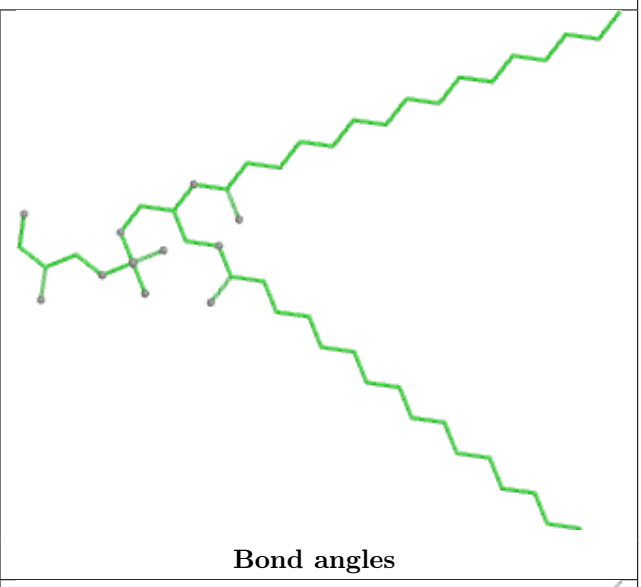
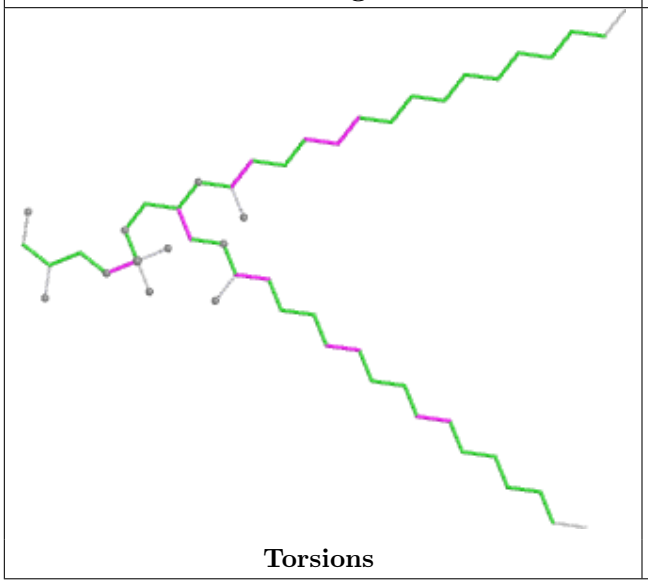


Bond angles



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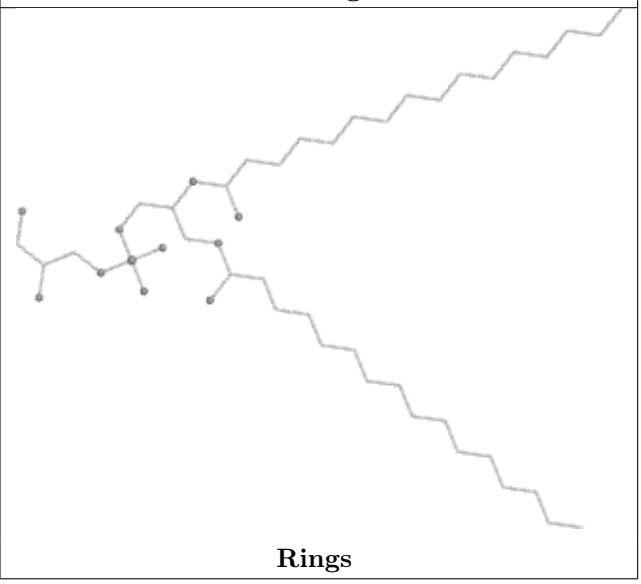
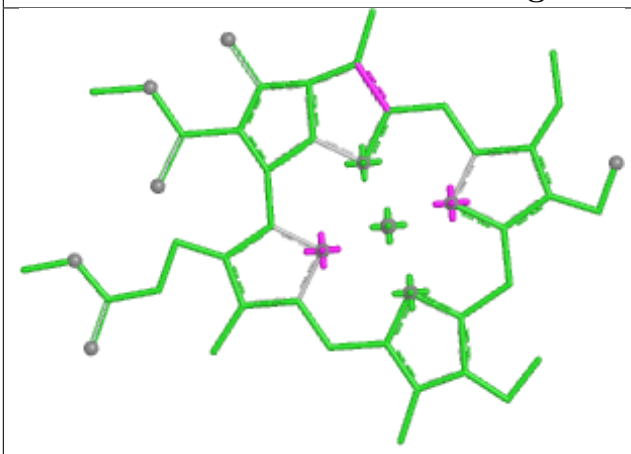


Rings

Ligand CHL 1 606



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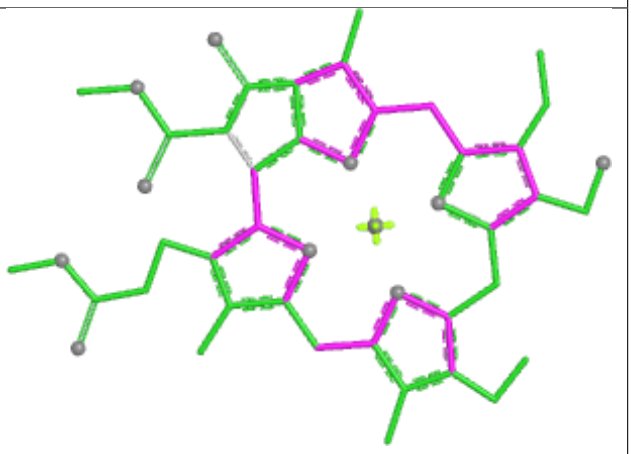
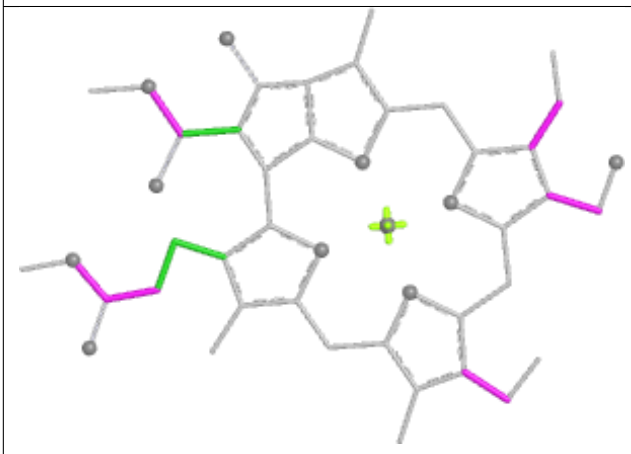


Bond angles



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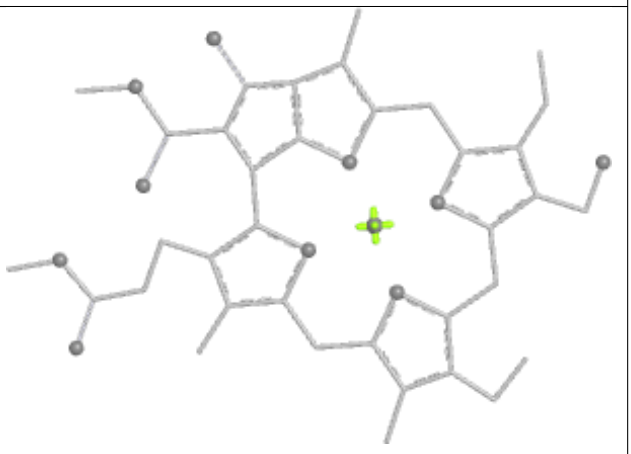
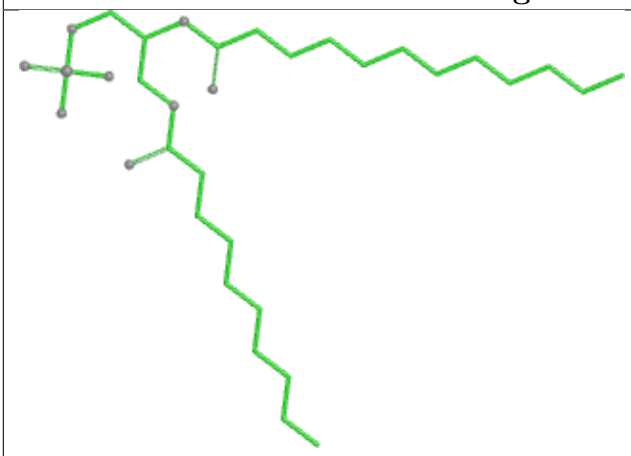


Rings

Ligand LHG A 5055



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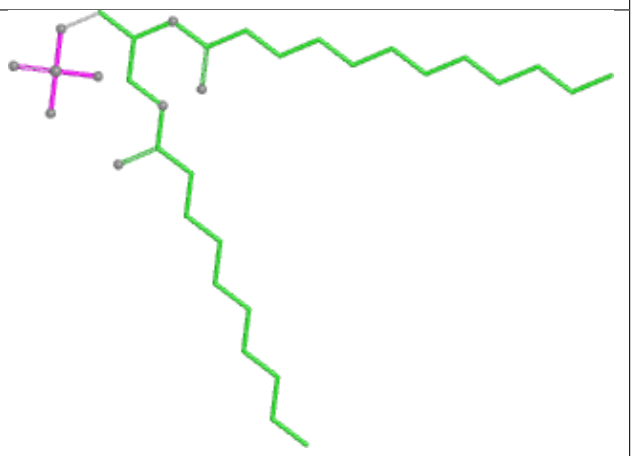
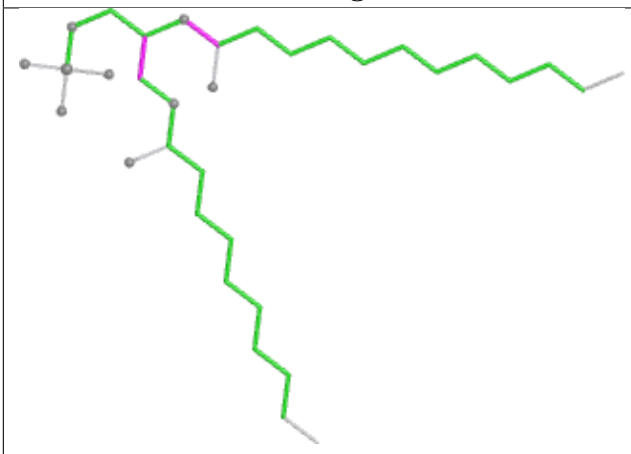


Bond angles



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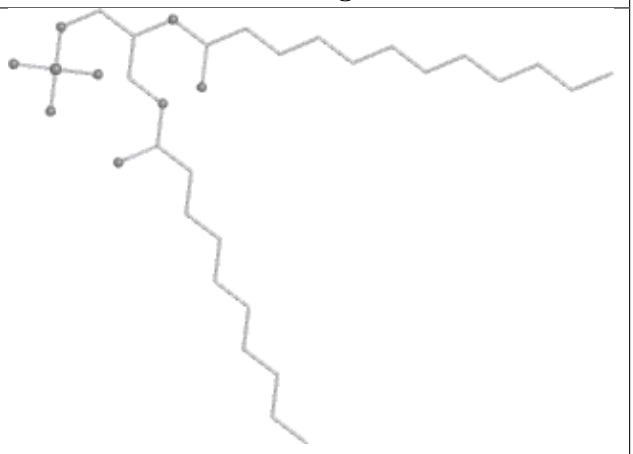
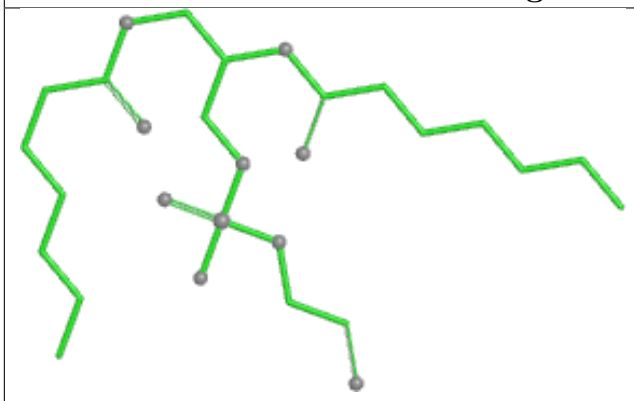


Rings

Ligand PTY F 301



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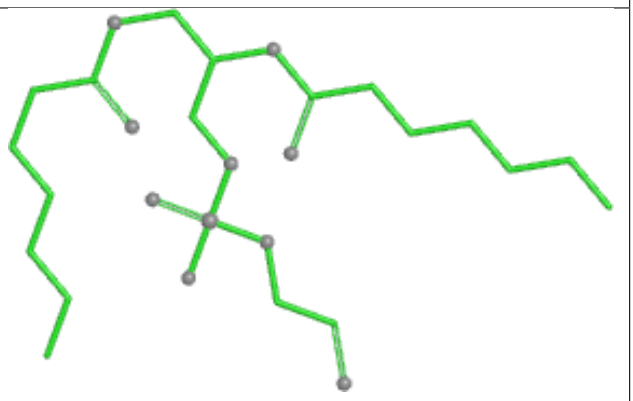
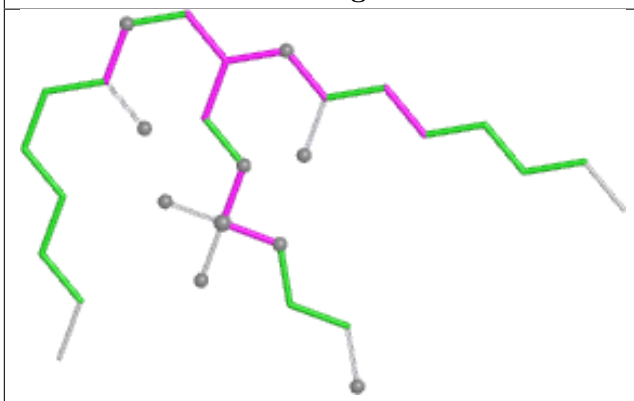


Bond angles



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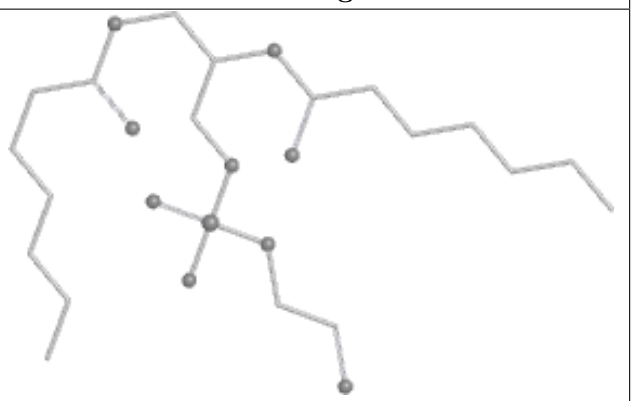
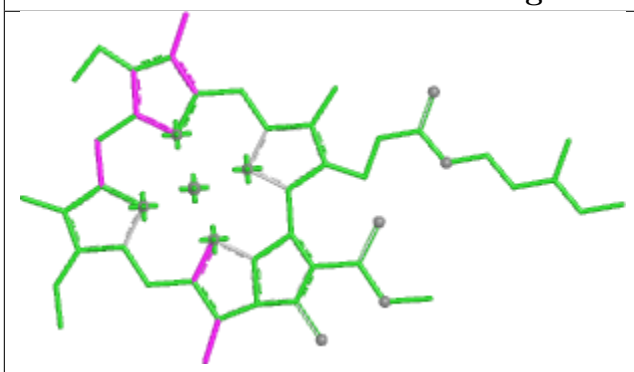


Rings

Ligand CLA B 835



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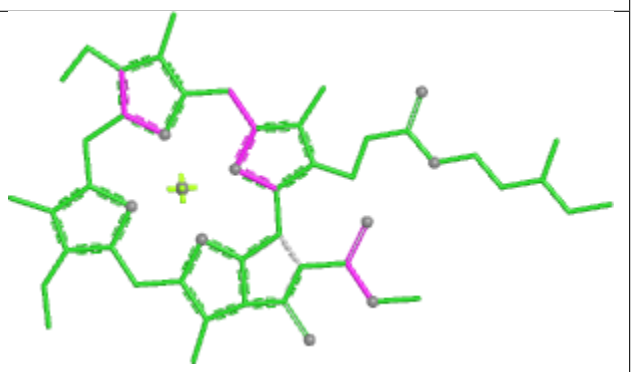
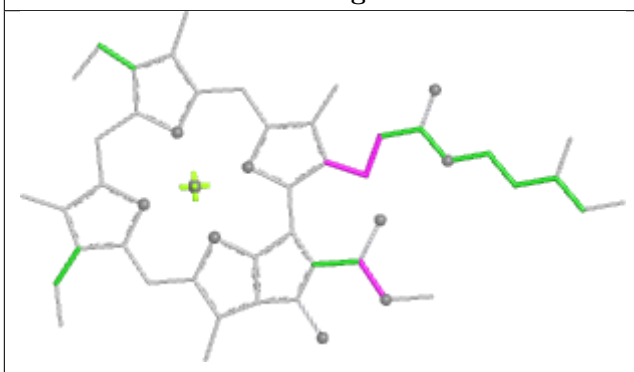


Bond angles



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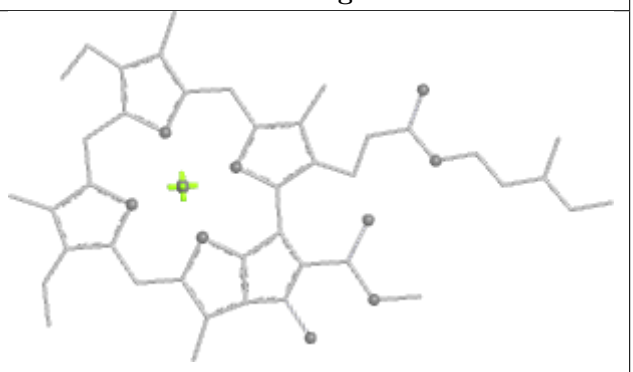
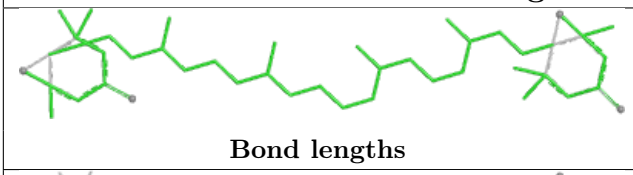


Rings

Ligand XAT 1 616



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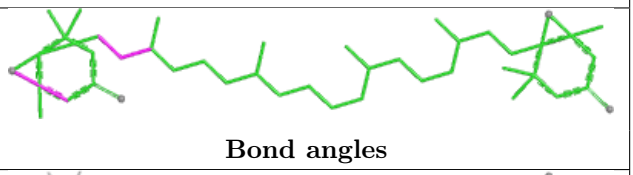
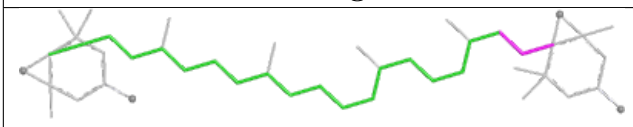


Bond angles



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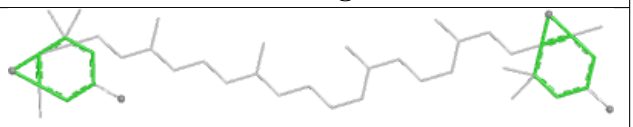
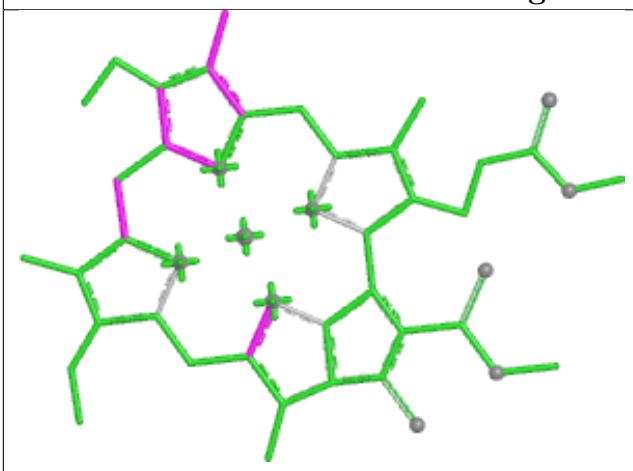


Rings

Ligand CLA 1 614



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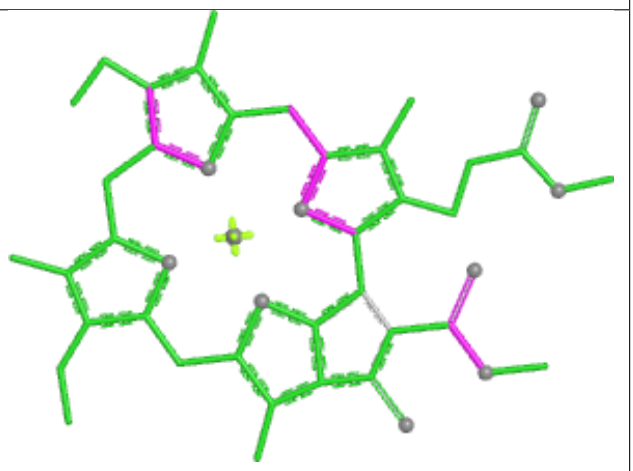
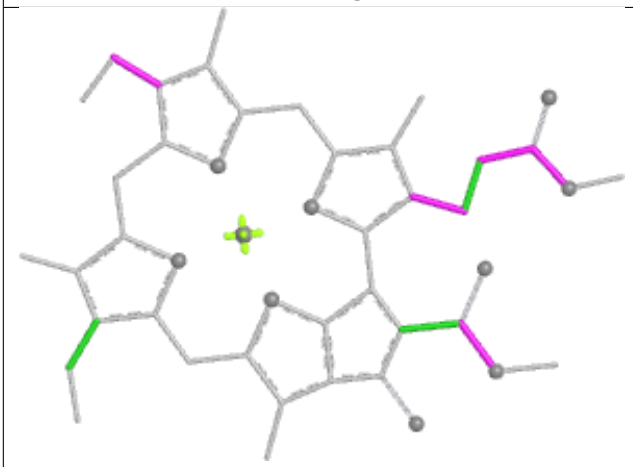


Bond angles



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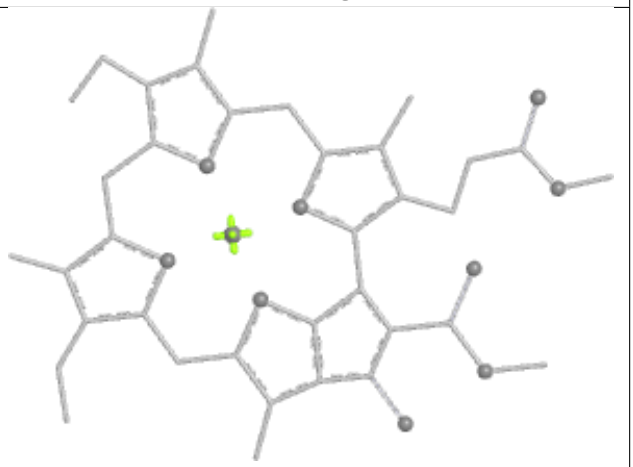
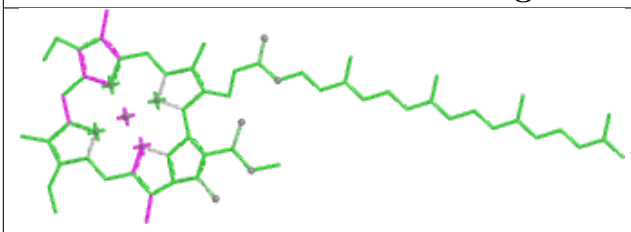
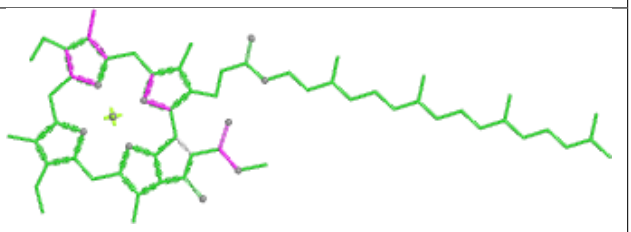


Rings

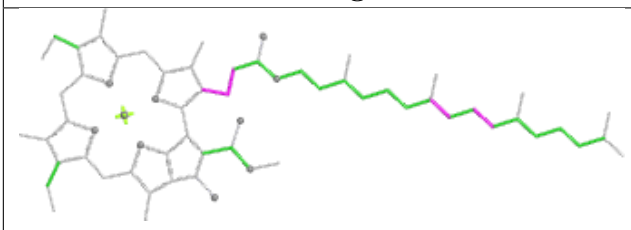
Ligand CLA A 5005



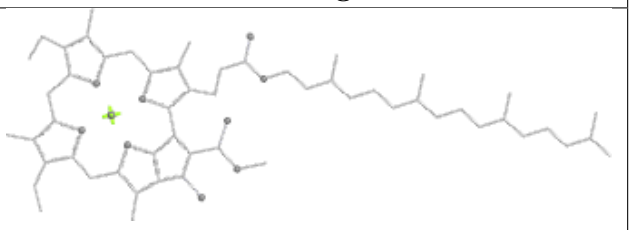
Bond lengths



Bond angles

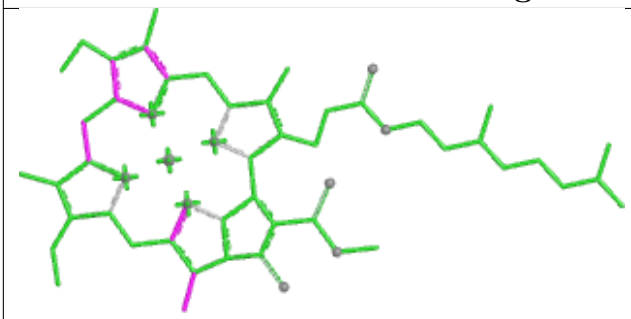


Torsions



Rings

Ligand CLA K 4003



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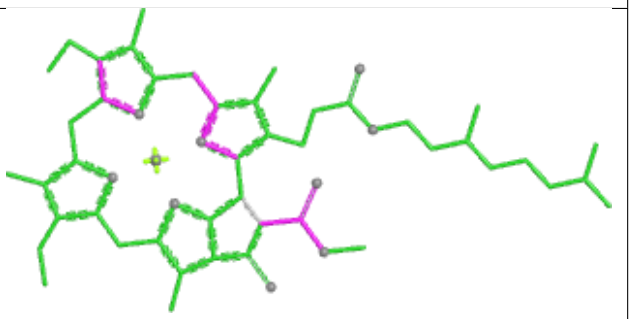
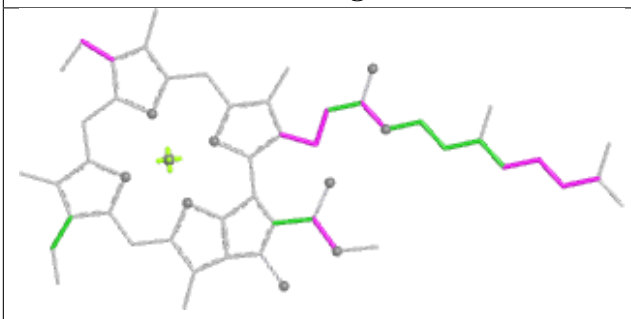


Bond angles



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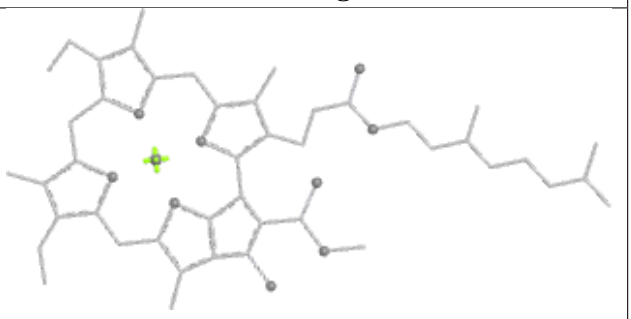
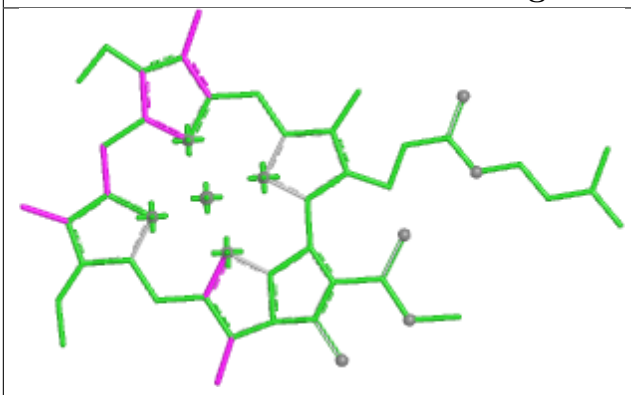


Rings

Ligand CLA 9 608



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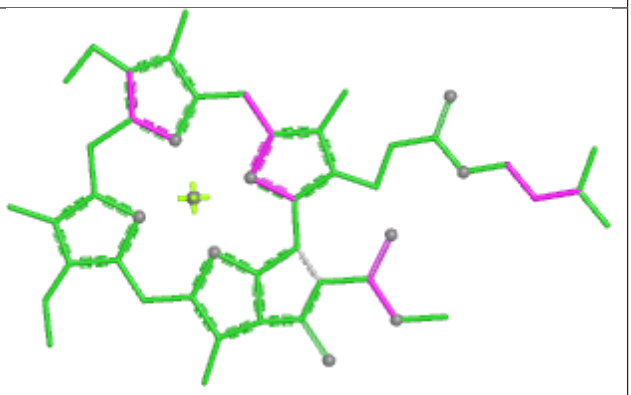
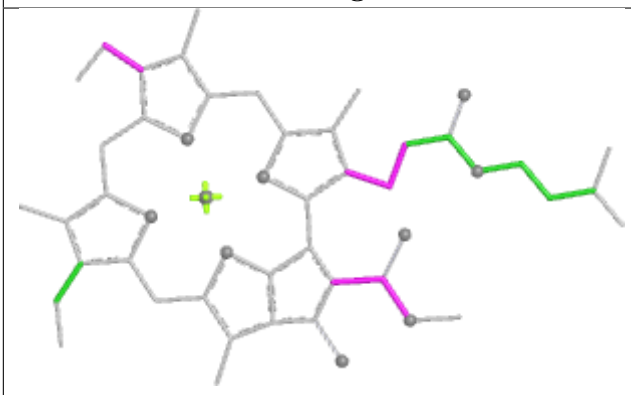


Bond angles



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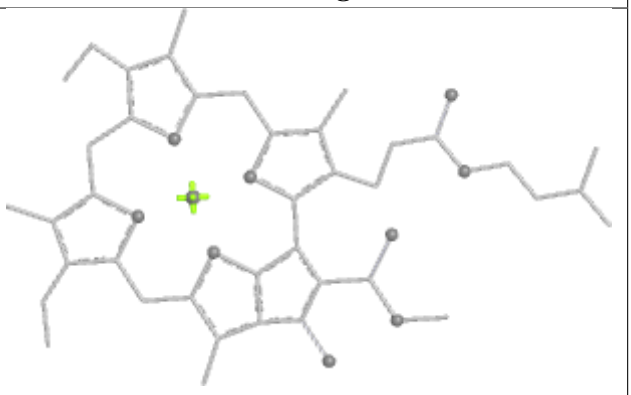


Rings

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.

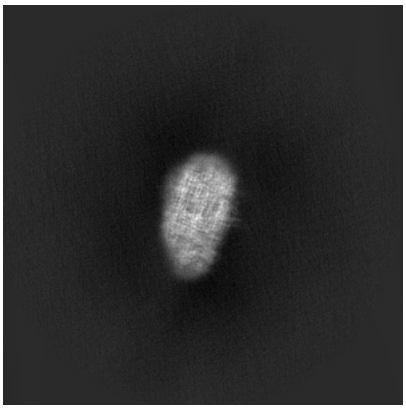
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-48266. These allow visual inspection of the internal detail of the map and identification of artifacts.

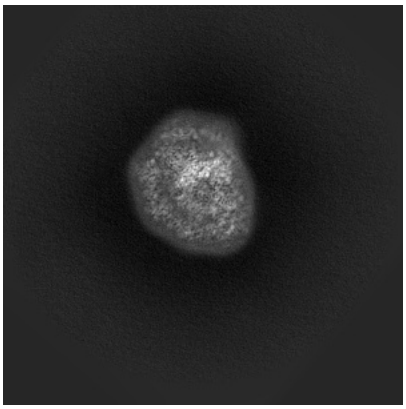
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

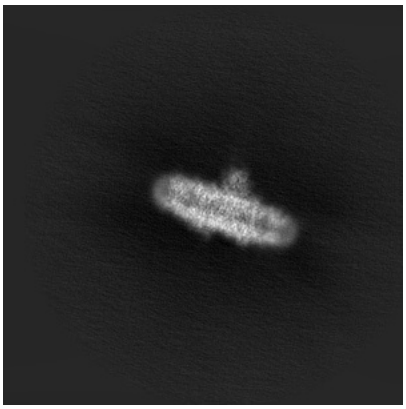
6.1.1 Primary map



X

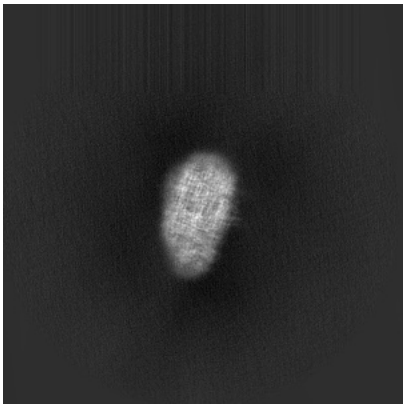


Y



Z

6.1.2 Raw map



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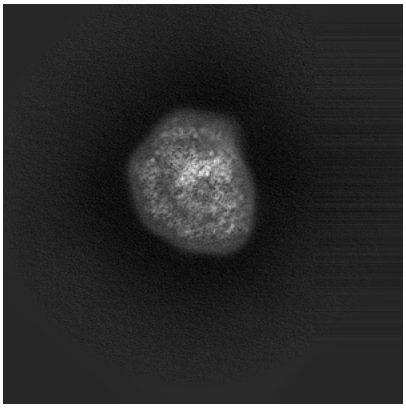

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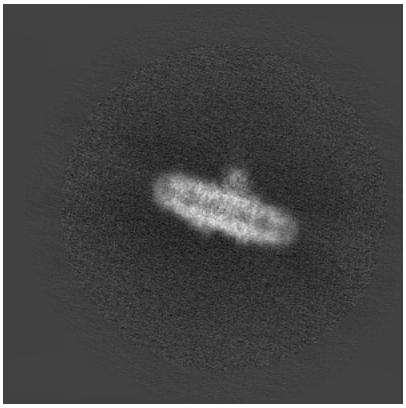
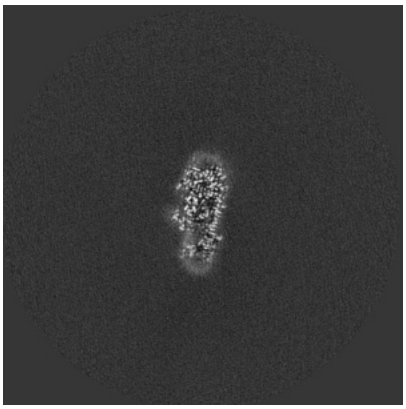


Z

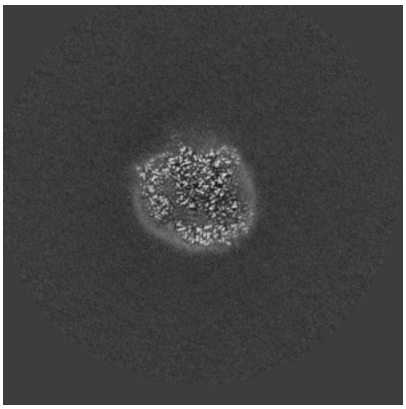
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

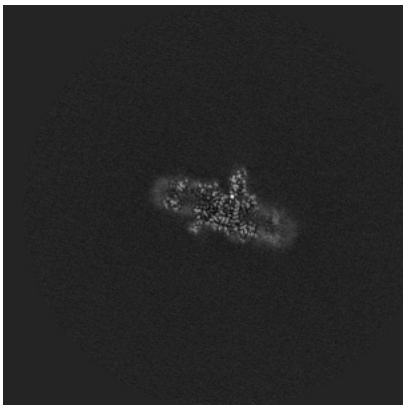
6.2.1 Primary map



X Index: 240

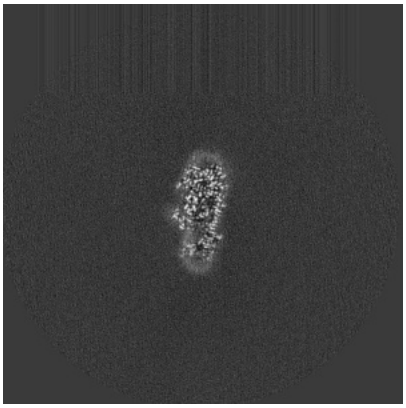


Y Index: 240

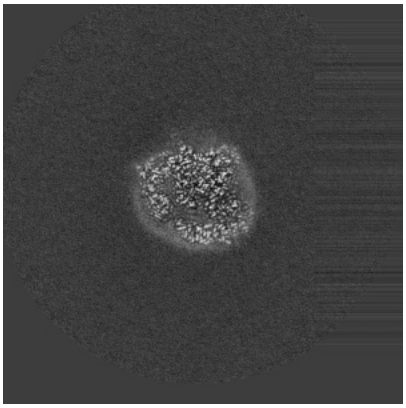


Z Index: 240

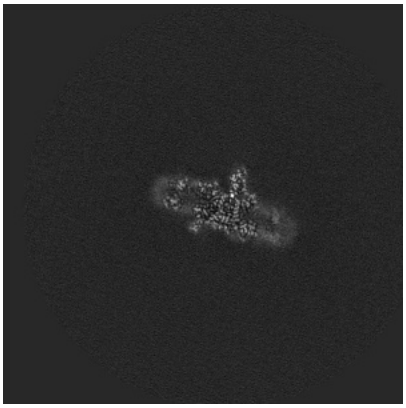
6.2.2 Raw map



X Index: 240



Y Index: 240

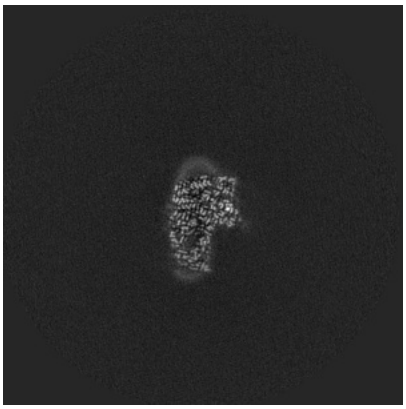


Z Index: 240

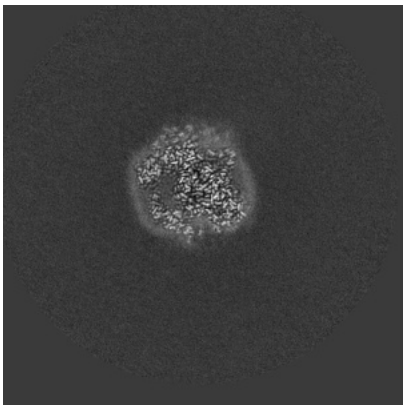
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

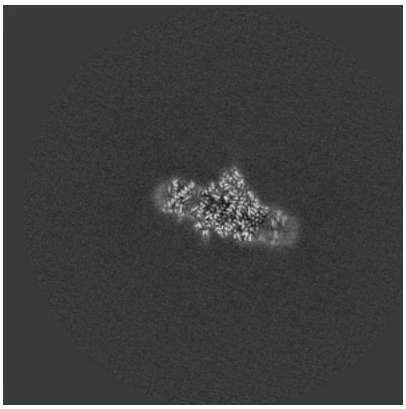
6.3.1 Primary map



X Index: 277

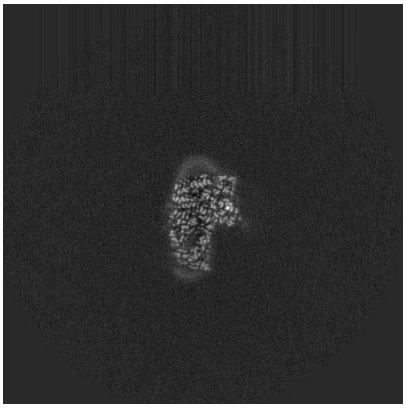


Y Index: 231

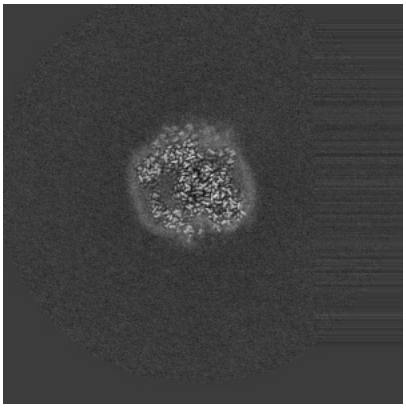


Z Index: 224

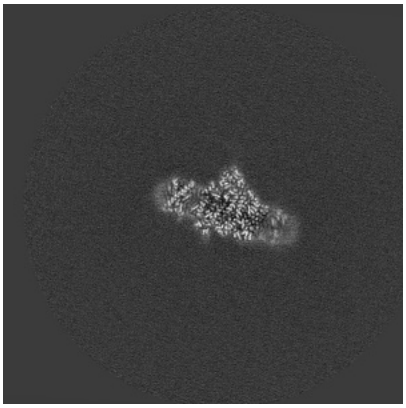
6.3.2 Raw map



X Index: 277



Y Index: 231

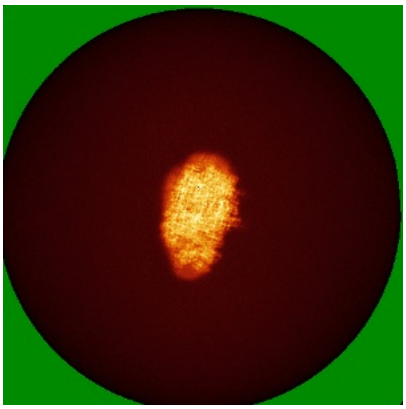


Z Index: 224

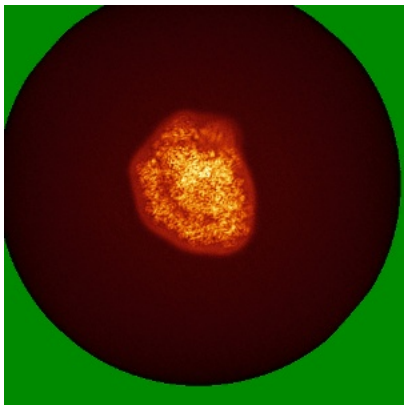
The images above show the largest variance slices of the map in three orthogonal directions.

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

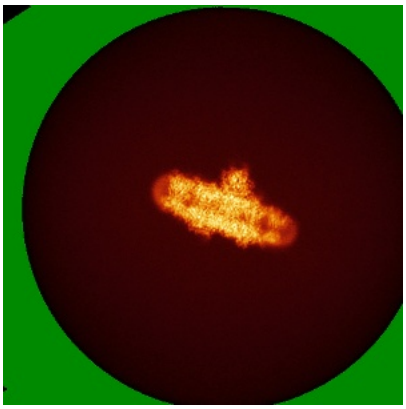
6.4.1 Primary map



X

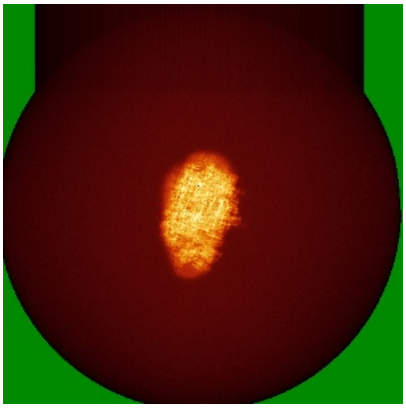


Y

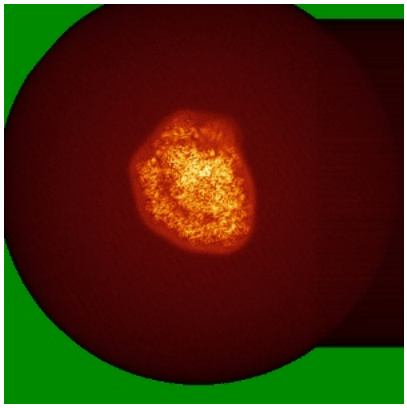


Z

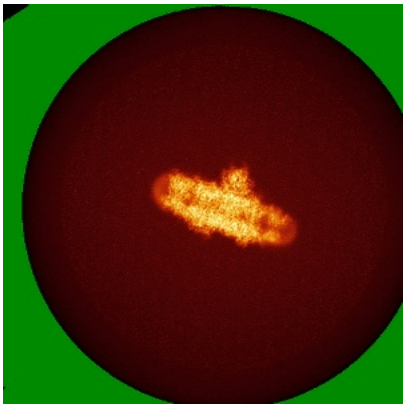
6.4.2 Raw map



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 0.0172. 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.

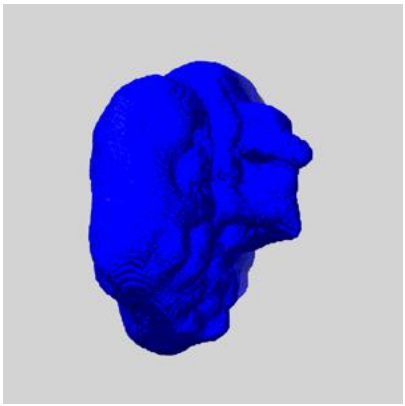
6.6 Mask visualisation

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

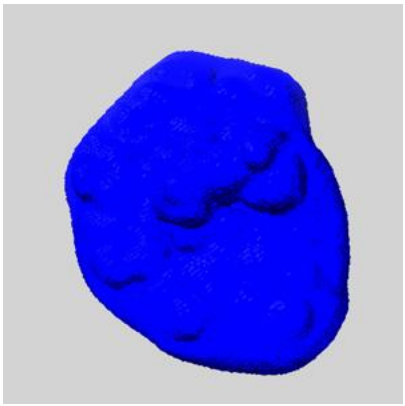
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

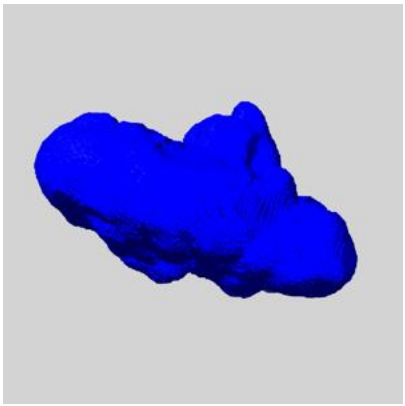
6.6.1 emd_48266_msk_1.map



X



Y

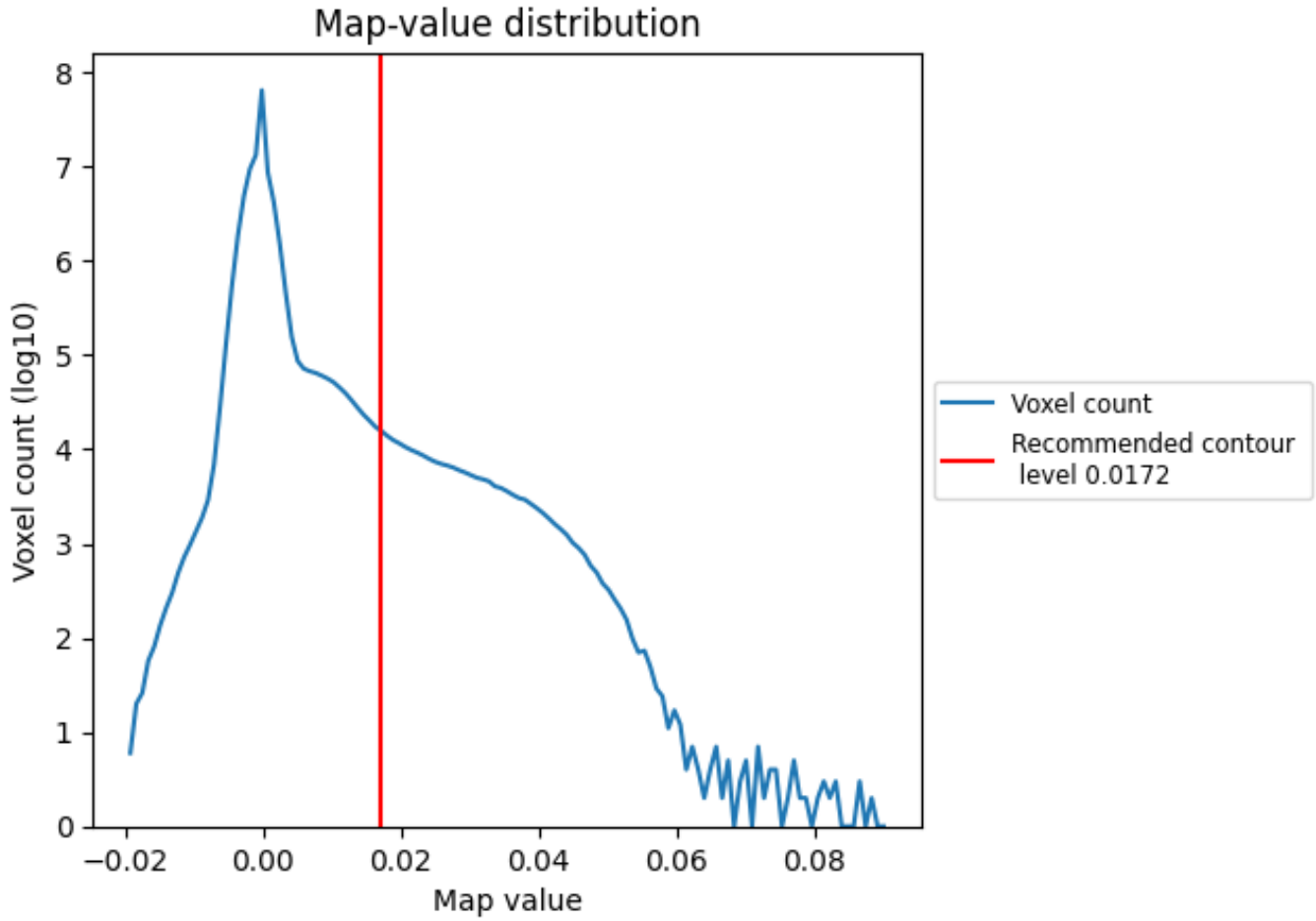


Z

7 Map analysis

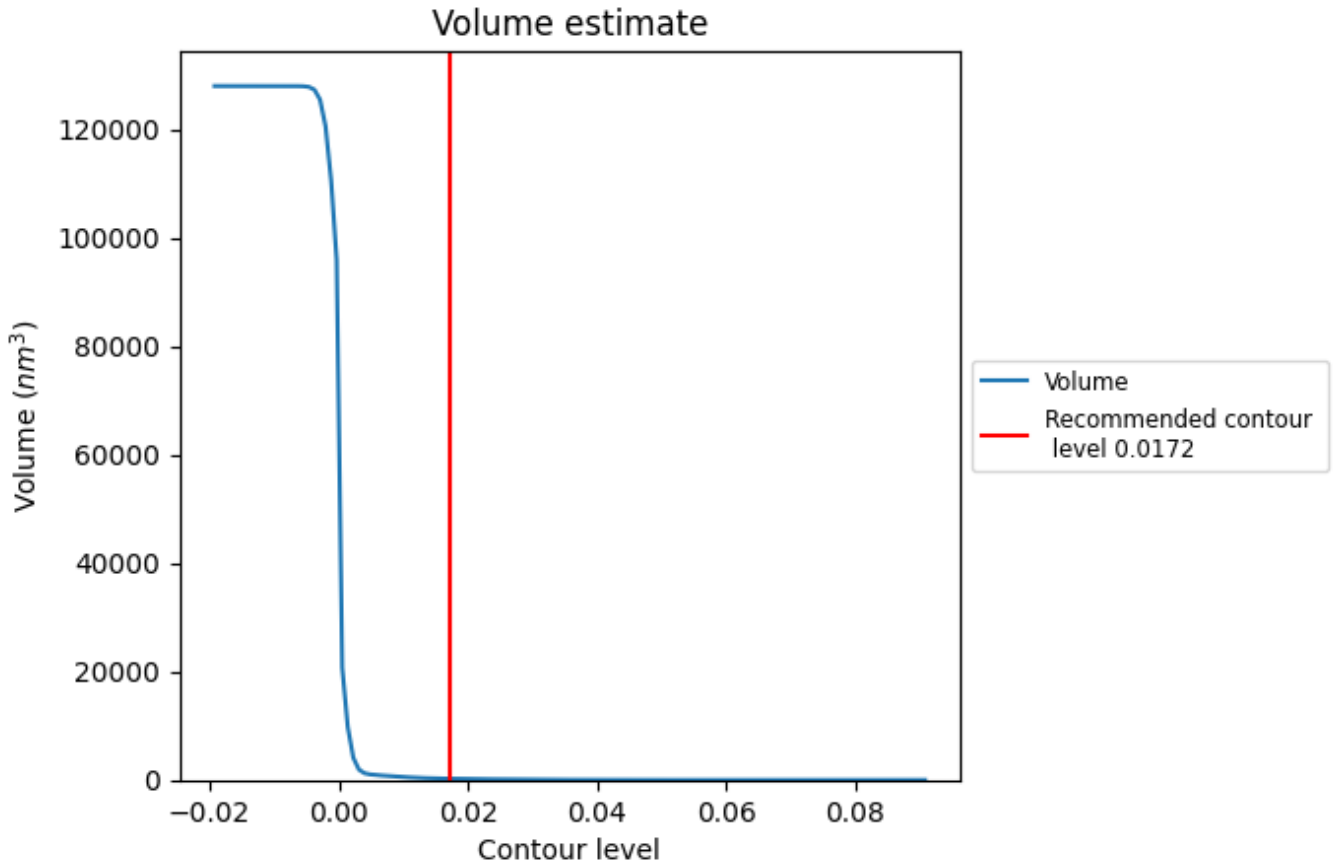
This section contains the results of statistical analysis of the map.

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.

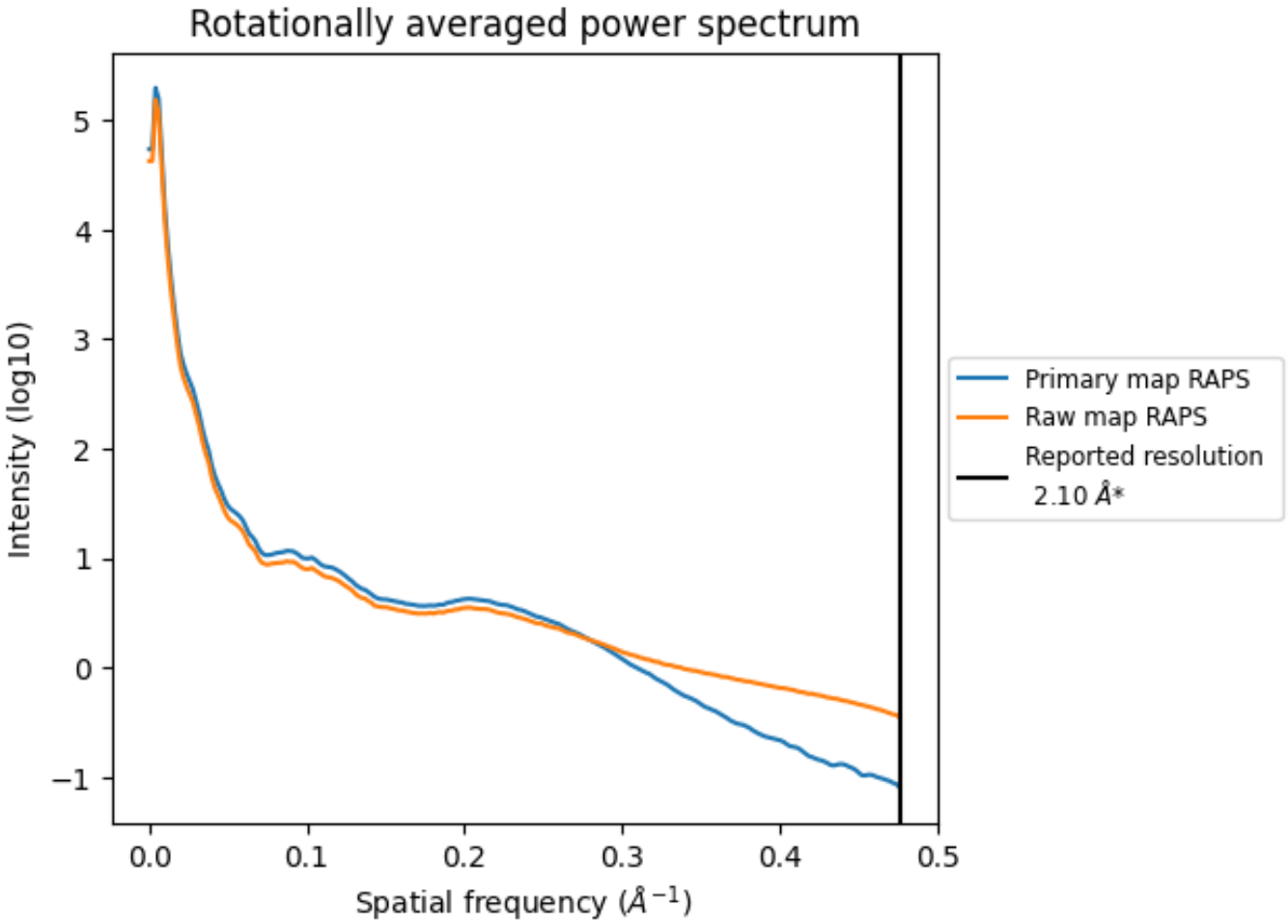
7.2 Volume estimate (i)



The volume at the recommended contour level is 229 nm^3; this corresponds to an approximate mass of 207 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)

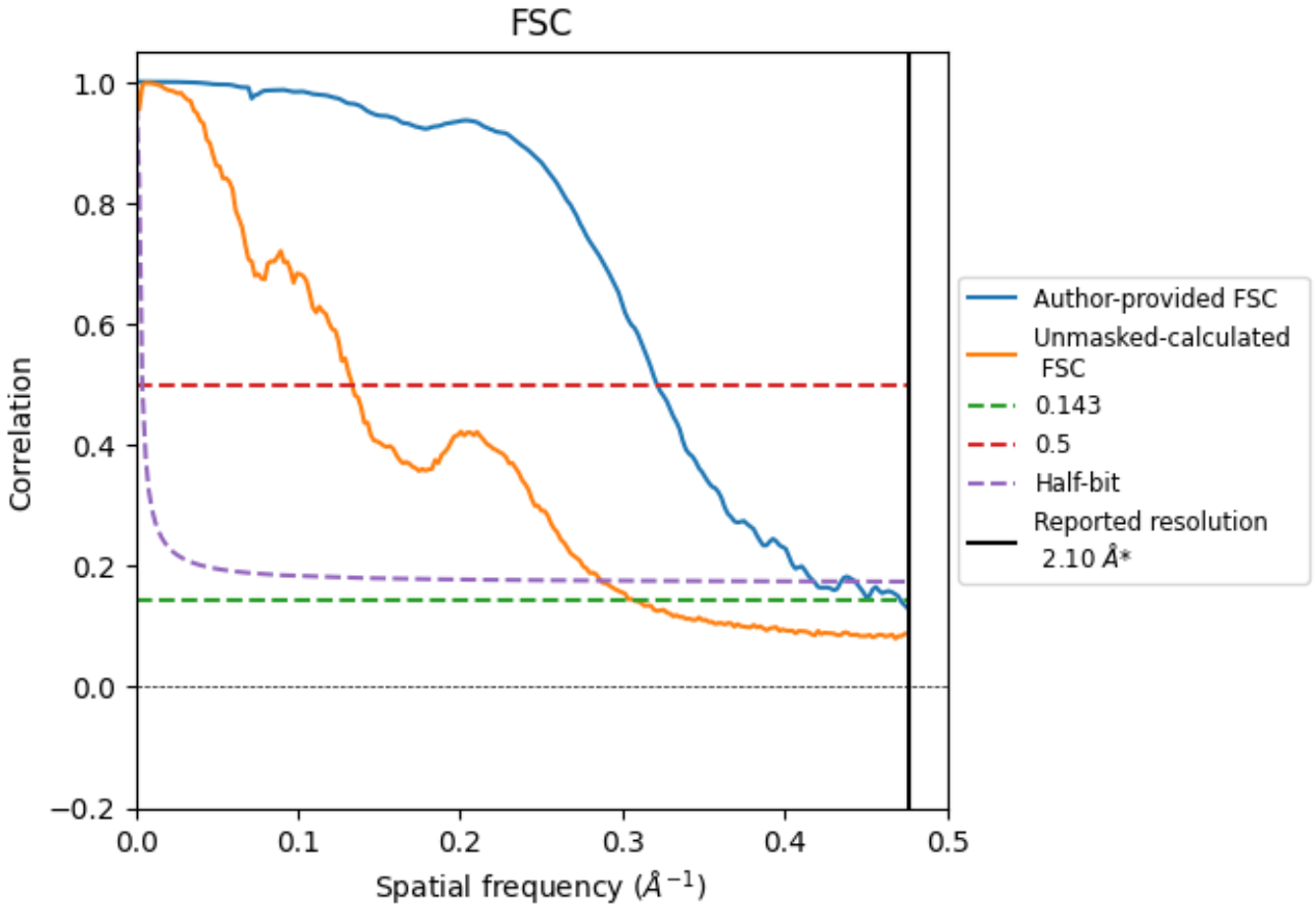


*Reported resolution corresponds to spatial frequency of 0.476 $Å^{-1}$

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 0.476 Å^{-1}

8.2 Resolution estimates (i)

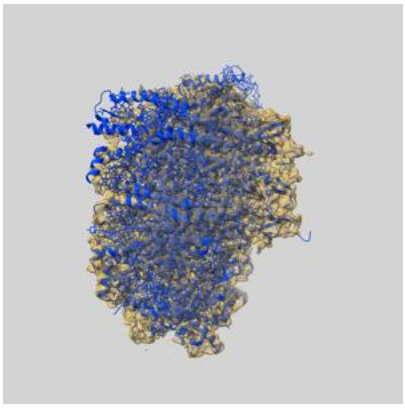
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.10	-	-
Author-provided FSC curve	2.12	3.11	2.39
Unmasked-calculated*	3.26	7.50	3.49

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.26 differs from the reported value 2.1 by more than 10 %

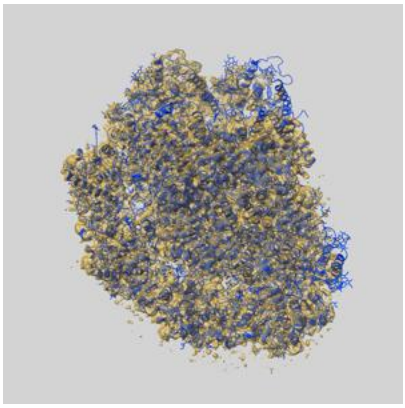
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-48266 and PDB model 9MH1. Per-residue inclusion information can be found in section 3 on page 28.

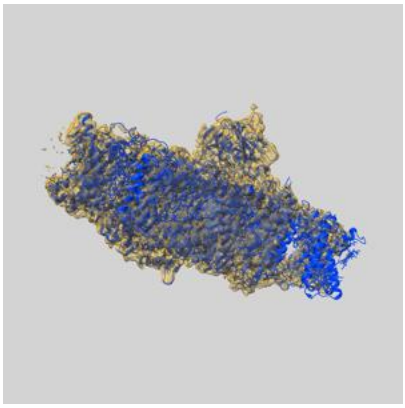
9.1 Map-model overlay



X



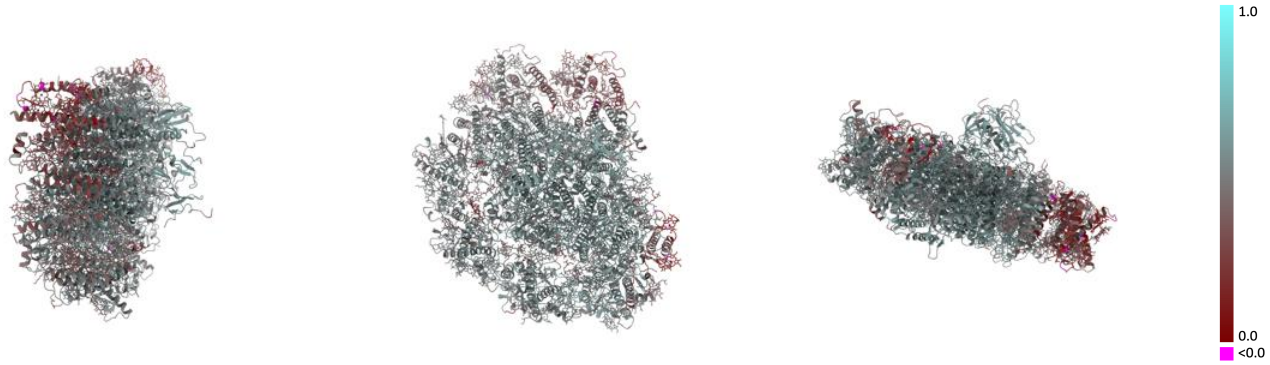
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0172 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.

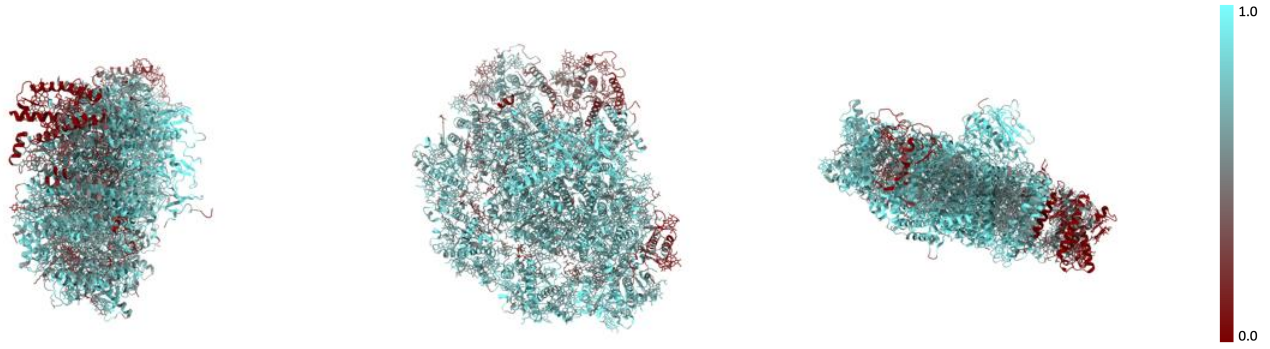
9.2 Q-score mapped to coordinate model



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.

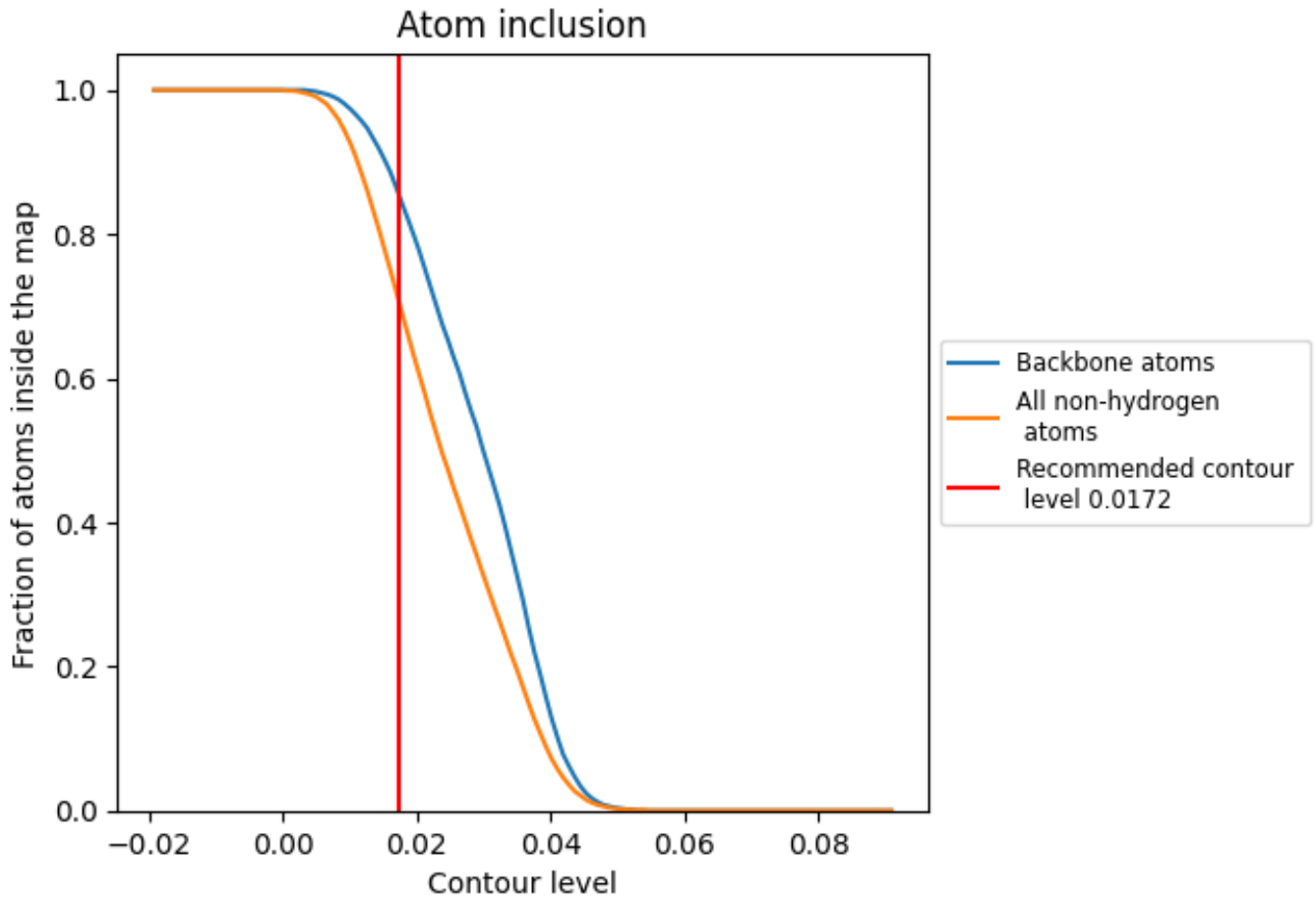
9.3 Atom inclusion mapped to coordinate model



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 (0.0172).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 71% 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 (0.0172) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7100	0.4980
1	0.7310	0.4860
2	0.2090	0.2700
3	0.7210	0.5040
7	0.7580	0.5100
8	0.7130	0.4890
9	0.5830	0.4050
A	0.8190	0.5560
B	0.8060	0.5480
C	0.9350	0.5560
D	0.8560	0.5350
E	0.7870	0.5370
F	0.7380	0.5230
G	0.5650	0.4550
H	0.0980	0.2690
I	0.7050	0.4850
J	0.7390	0.5190
K	0.2050	0.3020
L	0.6460	0.4800

