wwPDB EM Validation Summary Report

Nov 15, 2022 – 01:24 AM JST

PDB ID	:	6JO5
EMDB ID	:	EMD-9853
Title	:	Structure of the green algal photosystem I supercomplex with light-harvesting complex I
Authors	:	Suga, M.; Miyazaki, N.; Takahashi, Y.
Deposited on	:	2019-03-20
Resolution	:	2.90 Å(reported)

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

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

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

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

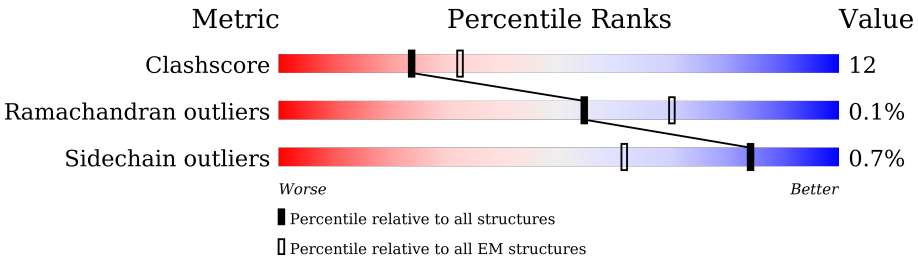
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 2.90 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	751	83% 15%
2	B	755	84% 13%
3	C	81	85% 14%
4	D	161	75% 14% 11%
5	E	73	74% 10% 16%
6	F	165	85% 15%
7	G	94	60% 13% 28%
8	I	106	31% 65%

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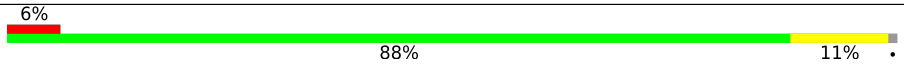
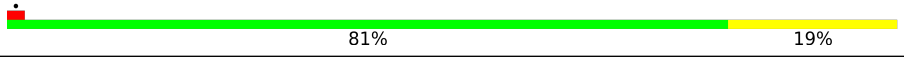
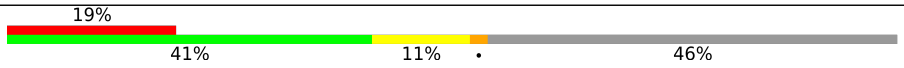
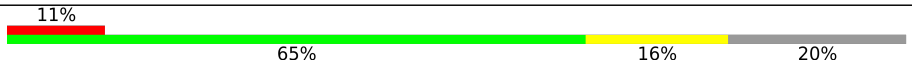
Mol	Chain	Length	Quality of chain
9	J	41	
10	K	87	
11	L	156	
12	1	194	
12	Z	194	
13	3	268	
14	7	215	
15	8	217	
16	4	236	
17	5	229	
18	6	232	
19	2	221	
20	9	189	

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
21	CL0	A	801	X	-	-	-
22	CLA	1	602	X	-	-	-
22	CLA	1	603	X	-	-	-
22	CLA	1	604	X	-	-	-
22	CLA	1	606	X	-	-	-
22	CLA	1	608	X	-	-	-
22	CLA	1	609	X	-	-	-
22	CLA	1	610	X	-	-	-
22	CLA	1	611	X	-	-	-
22	CLA	1	612	X	-	-	-
22	CLA	1	613	X	-	-	-
22	CLA	1	614	X	-	-	-
22	CLA	1	616	X	-	-	-
22	CLA	2	601	X	-	-	-
22	CLA	2	603	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	2	606	X	-	-	-
22	CLA	2	609	X	-	-	-
22	CLA	2	612	X	-	-	-
22	CLA	3	602	X	-	-	-
22	CLA	3	603	X	-	-	-
22	CLA	3	604	X	-	-	-
22	CLA	3	606	X	-	-	-
22	CLA	3	607	X	-	-	-
22	CLA	3	609	X	-	-	-
22	CLA	3	610	X	-	-	-
22	CLA	3	611	X	-	-	-
22	CLA	3	612	X	-	-	-
22	CLA	3	617	X	-	-	-
22	CLA	3	620	X	-	-	-
22	CLA	4	601	X	-	-	-
22	CLA	4	603	X	-	-	-
22	CLA	4	609	X	-	-	-
22	CLA	4	610	X	-	-	-
22	CLA	4	611	X	-	-	-
22	CLA	4	612	X	-	-	-
22	CLA	4	614	X	-	-	-
22	CLA	4	616	X	-	-	-
22	CLA	5	601	X	-	-	-
22	CLA	5	603	X	-	-	-
22	CLA	5	606	X	-	-	-
22	CLA	5	609	X	-	-	-
22	CLA	5	610	X	-	-	-
22	CLA	5	611	X	-	-	-
22	CLA	5	612	X	-	-	-
22	CLA	5	613	X	-	-	-
22	CLA	5	616	X	-	-	-
22	CLA	5	617	X	-	-	-
22	CLA	5	621	X	-	-	-
22	CLA	6	601	X	-	-	-
22	CLA	6	602	X	-	-	-
22	CLA	6	603	X	-	-	-
22	CLA	6	604	X	-	-	-
22	CLA	6	609	X	-	-	-
22	CLA	6	610	X	-	-	-
22	CLA	6	611	X	-	-	-
22	CLA	6	612	X	-	-	-
22	CLA	6	613	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	6	614	X	-	-	-
22	CLA	6	616	X	-	-	-
22	CLA	6	617	X	-	-	-
22	CLA	6	622	X	-	-	-
22	CLA	7	601	X	-	-	-
22	CLA	7	602	X	-	-	-
22	CLA	7	603	X	-	-	-
22	CLA	7	604	X	-	-	-
22	CLA	7	606	X	-	-	-
22	CLA	7	609	X	-	-	-
22	CLA	7	610	X	-	-	-
22	CLA	7	611	X	-	-	-
22	CLA	7	612	X	-	-	-
22	CLA	7	614	X	-	-	-
22	CLA	7	616	X	-	-	-
22	CLA	7	620	X	-	-	-
22	CLA	8	601	X	-	-	-
22	CLA	8	602	X	-	-	-
22	CLA	8	603	X	-	-	-
22	CLA	8	604	X	-	-	-
22	CLA	8	606	X	-	-	-
22	CLA	8	608	X	-	-	-
22	CLA	8	609	X	-	-	-
22	CLA	8	610	X	-	-	-
22	CLA	8	611	X	-	-	-
22	CLA	8	612	X	-	-	-
22	CLA	8	614	X	-	-	-
22	CLA	8	616	X	-	-	-
22	CLA	9	601	X	-	-	-
22	CLA	9	602	X	-	-	-
22	CLA	9	603	X	-	-	-
22	CLA	9	609	X	-	-	-
22	CLA	9	611	X	-	-	-
22	CLA	9	612	X	-	-	-
22	CLA	9	613	X	-	-	-
22	CLA	A	802	X	-	X	-
22	CLA	A	803	X	-	-	-
22	CLA	A	804	X	-	-	-
22	CLA	A	805	X	-	X	-
22	CLA	A	806	X	-	-	-
22	CLA	A	807	X	-	-	-
22	CLA	A	808	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	A	809	X	-	-	-
22	CLA	A	811	X	-	-	-
22	CLA	A	812	X	-	-	-
22	CLA	A	813	X	-	-	-
22	CLA	A	814	X	-	-	-
22	CLA	A	815	X	-	X	-
22	CLA	A	816	X	-	-	-
22	CLA	A	817	X	-	-	-
22	CLA	A	819	X	-	-	-
22	CLA	A	820	X	-	-	-
22	CLA	A	821	X	-	-	-
22	CLA	A	822	X	-	-	-
22	CLA	A	824	X	-	-	-
22	CLA	A	826	X	-	-	-
22	CLA	A	827	X	-	-	-
22	CLA	A	828	X	-	-	-
22	CLA	A	829	X	-	-	-
22	CLA	A	830	X	-	-	-
22	CLA	A	831	X	-	-	-
22	CLA	A	832	X	-	-	-
22	CLA	A	833	X	-	-	-
22	CLA	A	834	X	-	-	-
22	CLA	A	835	X	-	X	-
22	CLA	A	837	X	-	-	-
22	CLA	A	838	X	-	-	-
22	CLA	A	839	X	-	-	-
22	CLA	A	840	X	-	-	-
22	CLA	A	841	X	-	-	-
22	CLA	A	842	X	-	-	-
22	CLA	A	843	X	-	-	-
22	CLA	A	845	X	-	-	-
22	CLA	A	854	X	-	-	-
22	CLA	B	802	X	-	-	-
22	CLA	B	803	X	-	-	-
22	CLA	B	804	X	-	-	-
22	CLA	B	805	X	-	-	-
22	CLA	B	806	X	-	-	-
22	CLA	B	807	X	-	-	-
22	CLA	B	808	X	-	-	-
22	CLA	B	809	X	-	-	-
22	CLA	B	810	X	-	-	-
22	CLA	B	811	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	B	812	X	-	-	-
22	CLA	B	813	X	-	-	-
22	CLA	B	814	X	-	-	-
22	CLA	B	815	X	-	-	-
22	CLA	B	816	X	-	-	-
22	CLA	B	817	X	-	-	-
22	CLA	B	818	X	-	-	-
22	CLA	B	819	X	-	-	-
22	CLA	B	820	X	-	-	-
22	CLA	B	823	X	-	-	-
22	CLA	B	824	X	-	-	-
22	CLA	B	825	X	-	-	-
22	CLA	B	826	X	-	-	-
22	CLA	B	827	X	-	-	-
22	CLA	B	828	X	-	-	-
22	CLA	B	829	X	-	-	-
22	CLA	B	831	X	-	-	-
22	CLA	B	832	X	-	-	-
22	CLA	B	833	X	-	-	-
22	CLA	B	834	X	-	-	-
22	CLA	B	835	X	-	-	-
22	CLA	B	836	X	-	-	-
22	CLA	B	837	X	-	-	-
22	CLA	B	838	X	-	-	-
22	CLA	B	839	X	-	-	-
22	CLA	B	841	X	-	-	-
22	CLA	B	852	X	-	-	-
22	CLA	F	301	X	-	-	-
22	CLA	F	303	X	-	-	-
22	CLA	F	304	X	-	-	-
22	CLA	G	203	X	-	-	-
22	CLA	G	204	X	-	-	-
22	CLA	J	3002	X	-	-	-
22	CLA	K	4003	X	-	-	-
22	CLA	Z	603	X	-	-	-
22	CLA	Z	604	X	-	-	-
22	CLA	Z	606	X	-	-	-
22	CLA	Z	608	X	-	-	-
22	CLA	Z	609	X	-	-	-
22	CLA	Z	610	X	-	-	-
22	CLA	Z	611	X	-	-	-
22	CLA	Z	612	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	Z	613	X	-	-	-
22	CLA	Z	614	X	-	-	-
22	CLA	Z	616	X	-	-	-
25	BCR	4	621	-	-	X	-
29	CHL	1	601	X	-	-	-
29	CHL	1	607	X	-	-	-
29	CHL	3	608	X	-	-	-
29	CHL	4	606	X	-	-	-
29	CHL	4	607	X	-	-	-
29	CHL	4	608	X	-	-	-
29	CHL	4	618	X	-	-	-
29	CHL	5	607	X	-	-	-
29	CHL	5	608	X	-	-	-
29	CHL	5	618	X	-	-	-
29	CHL	6	606	X	-	-	-
29	CHL	6	607	X	-	-	-
29	CHL	6	608	X	-	-	-
29	CHL	6	618	X	-	-	-
29	CHL	7	607	X	-	-	-
29	CHL	8	607	X	-	-	-
29	CHL	9	606	X	-	-	-
29	CHL	9	607	X	-	-	-
29	CHL	Z	601	X	-	-	-
29	CHL	Z	607	X	-	-	-

2 Entry composition (i)

There are 30 unique types of molecules in this entry. The entry contains 48476 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	738	5800	3793	989	996	22	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	732	5822	3824	978	1002	18	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	HIS	-	insertion	UNP P09144
B	-15	HIS	-	insertion	UNP P09144
B	-14	HIS	-	insertion	UNP P09144
B	-13	HIS	-	insertion	UNP P09144
B	-12	HIS	-	insertion	UNP P09144
B	-11	HIS	-	insertion	UNP P09144
B	-10	HIS	-	insertion	UNP P09144
B	-9	HIS	-	insertion	UNP P09144
B	-8	HIS	-	insertion	UNP P09144
B	-7	HIS	-	insertion	UNP P09144
B	-6	HIS	-	insertion	UNP P09144
B	-5	HIS	-	insertion	UNP P09144
B	-4	HIS	-	insertion	UNP P09144
B	-3	HIS	-	insertion	UNP P09144
B	-2	HIS	-	insertion	UNP P09144
B	-1	HIS	-	insertion	UNP P09144
B	0	HIS	-	insertion	UNP P09144
B	1	HIS	-	insertion	UNP P09144
B	2	HIS	-	insertion	UNP P09144
B	3	HIS	-	insertion	UNP P09144

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			600	369	103	116	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	144	Total	C	N	O	S	0	0
			1132	725	200	200	7		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	61	Total	C	N	O	0	0
			480	306	85	89		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	165	Total	C	N	O	S	0	0
			1265	817	213	232	3		

- Molecule 7 is a protein called Photosystem I reaction center subunit V, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	68	Total	C	N	O	0	0
			503	327	87	89		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	37	Total	C	N	O	S	0	0
			281	195	39	46	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	39	Total	C	N	O	S	0	0
			320	219	45	55	1		

- Molecule 10 is a protein called Photosystem I reaction center subunit psaK, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	45	Total	C	N	O	S	0	0
			297	190	49	56	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	118	Total	C	N	O	S	0	0
			853	561	136	153	3		

- Molecule 12 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	1	194	Total	C	N	O	S	0	0
			1444	941	240	260	3		
12	Z	192	Total	C	N	O	S	0	0
			1436	937	238	258	3		

- Molecule 13 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	3	202	Total	C	N	O	S	0	0
			1555	1018	252	277	8		

- Molecule 14 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	7	212	Total	C	N	O	S	0	0
			1644	1069	273	296	6		

- Molecule 15 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	8	217	Total	C	N	O	S	0	0
			1649	1073	280	292	4		

- Molecule 16 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	4	203	Total	C	N	O	S	0	0
			1570	1029	254	282	5		

- Molecule 17 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	5	223	1744	1137	291	308	8	0	0

- Molecule 18 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	6	229	1765	1164	292	303	6	0	0

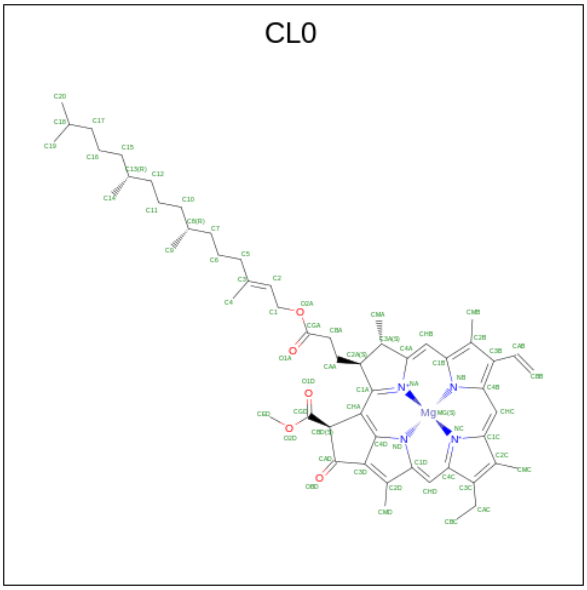
- Molecule 19 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	2	119	838	535	147	151	5	0	0

- Molecule 20 is a protein called Chlorophyll a-b binding protein, chloroplastic.

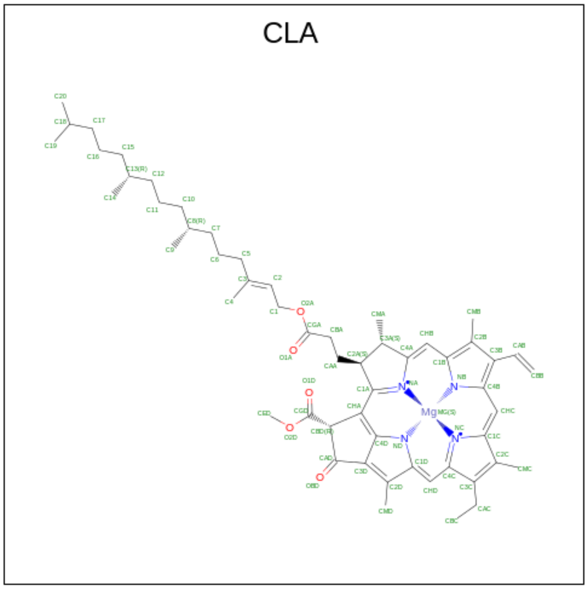
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	9	152	1180	766	195	213	6	0	0

- Molecule 21 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



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

- Molecule 22 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	A	1	2689	2249	44	176	220	0
22	A	1	2689	2249	44	176	220	0
22	A	1	2689	2249	44	176	220	0
22	A	1	2689	2249	44	176	220	0
22	A	1	2689	2249	44	176	220	0
22	A	1	2689	2249	44	176	220	0
22	A	1	2689	2249	44	176	220	0
22	A	1	2689	2249	44	176	220	0
22	A	1	2689	2249	44	176	220	0
22	A	1	2689	2249	44	176	220	0
22	A	1	2689	2249	44	176	220	0
22	A	1	2689	2249	44	176	220	0
22	A	1	2689	2249	44	176	220	0

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Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total 2689	C 2249	Mg 44	N 176	O 220	0
22	A	1	Total 2689	C 2249	Mg 44	N 176	O 220	0
22	A	1	Total 2689	C 2249	Mg 44	N 176	O 220	0
22	A	1	Total 2689	C 2249	Mg 44	N 176	O 220	0
22	A	1	Total 2689	C 2249	Mg 44	N 176	O 220	0
22	A	1	Total 2689	C 2249	Mg 44	N 176	O 220	0
22	A	1	Total 2689	C 2249	Mg 44	N 176	O 220	0
22	A	1	Total 2689	C 2249	Mg 44	N 176	O 220	0
22	A	1	Total 2689	C 2249	Mg 44	N 176	O 220	0
22	A	1	Total 2689	C 2249	Mg 44	N 176	O 220	0
22	A	1	Total 2689	C 2249	Mg 44	N 176	O 220	0
22	A	1	Total 2689	C 2249	Mg 44	N 176	O 220	0
22	A	1	Total 2689	C 2249	Mg 44	N 176	O 220	0
22	A	1	Total 2689	C 2249	Mg 44	N 176	O 220	0
22	A	1	Total 2689	C 2249	Mg 44	N 176	O 220	0
22	A	1	Total 2689	C 2249	Mg 44	N 176	O 220	0
22	A	1	Total 2689	C 2249	Mg 44	N 176	O 220	0
22	A	1	Total 2689	C 2249	Mg 44	N 176	O 220	0
22	A	1	Total 2689	C 2249	Mg 44	N 176	O 220	0
22	A	1	Total 2689	C 2249	Mg 44	N 176	O 220	0
22	A	1	Total 2689	C 2249	Mg 44	N 176	O 220	0

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Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total 2689	C 2249	Mg 44	N 176	O 220	0
22	A	1	Total 2689	C 2249	Mg 44	N 176	O 220	0
22	A	1	Total 2689	C 2249	Mg 44	N 176	O 220	0
22	A	1	Total 2689	C 2249	Mg 44	N 176	O 220	0
22	A	1	Total 2689	C 2249	Mg 44	N 176	O 220	0
22	A	1	Total 2689	C 2249	Mg 44	N 176	O 220	0
22	A	1	Total 2689	C 2249	Mg 44	N 176	O 220	0
22	A	1	Total 2689	C 2249	Mg 44	N 176	O 220	0
22	A	1	Total 2689	C 2249	Mg 44	N 176	O 220	0
22	A	1	Total 2689	C 2249	Mg 44	N 176	O 220	0
22	B	1	Total 2480	C 2070	Mg 41	N 164	O 205	0
22	B	1	Total 2480	C 2070	Mg 41	N 164	O 205	0
22	B	1	Total 2480	C 2070	Mg 41	N 164	O 205	0
22	B	1	Total 2480	C 2070	Mg 41	N 164	O 205	0
22	B	1	Total 2480	C 2070	Mg 41	N 164	O 205	0
22	B	1	Total 2480	C 2070	Mg 41	N 164	O 205	0
22	B	1	Total 2480	C 2070	Mg 41	N 164	O 205	0
22	B	1	Total 2480	C 2070	Mg 41	N 164	O 205	0
22	B	1	Total 2480	C 2070	Mg 41	N 164	O 205	0
22	B	1	Total 2480	C 2070	Mg 41	N 164	O 205	0
22	B	1	Total 2480	C 2070	Mg 41	N 164	O 205	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	B	1	2480	2070	41	164	205	0
22	B	1	2480	2070	41	164	205	0
22	B	1	2480	2070	41	164	205	0
22	B	1	2480	2070	41	164	205	0
22	B	1	2480	2070	41	164	205	0
22	B	1	2480	2070	41	164	205	0
22	B	1	2480	2070	41	164	205	0
22	B	1	2480	2070	41	164	205	0
22	B	1	2480	2070	41	164	205	0
22	B	1	2480	2070	41	164	205	0
22	B	1	2480	2070	41	164	205	0
22	B	1	2480	2070	41	164	205	0
22	B	1	2480	2070	41	164	205	0
22	B	1	2480	2070	41	164	205	0
22	B	1	2480	2070	41	164	205	0
22	B	1	2480	2070	41	164	205	0
22	B	1	2480	2070	41	164	205	0
22	B	1	2480	2070	41	164	205	0
22	B	1	2480	2070	41	164	205	0
22	B	1	2480	2070	41	164	205	0
22	B	1	2480	2070	41	164	205	0

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Mol	Chain	Residues	Atoms	AltConf
22	B	1	Total C Mg N O 2480 2070 41 164 205	0
22	B	1	Total C Mg N O 2480 2070 41 164 205	0
22	B	1	Total C Mg N O 2480 2070 41 164 205	0
22	B	1	Total C Mg N O 2480 2070 41 164 205	0
22	B	1	Total C Mg N O 2480 2070 41 164 205	0
22	B	1	Total C Mg N O 2480 2070 41 164 205	0
22	B	1	Total C Mg N O 2480 2070 41 164 205	0
22	B	1	Total C Mg N O 2480 2070 41 164 205	0
22	B	1	Total C Mg N O 2480 2070 41 164 205	0
22	F	1	Total C Mg N O 175 145 3 12 15	0
22	F	1	Total C Mg N O 175 145 3 12 15	0
22	F	1	Total C Mg N O 175 145 3 12 15	0
22	G	1	Total C Mg N O 96 76 2 8 10	0
22	G	1	Total C Mg N O 96 76 2 8 10	0
22	J	1	Total C Mg N O 42 34 1 4 3	0
22	K	1	Total C Mg N O 91 71 2 8 10	0
22	K	1	Total C Mg N O 91 71 2 8 10	0
22	L	1	Total C Mg N O 115 95 2 8 10	0
22	L	1	Total C Mg N O 115 95 2 8 10	0
22	1	1	Total C Mg N O 722 602 12 48 60	0
22	1	1	Total C Mg N O 722 602 12 48 60	0

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Mol	Chain	Residues	Atoms	AltConf
22	1	1	Total C Mg N O 722 602 12 48 60	0
22	1	1	Total C Mg N O 722 602 12 48 60	0
22	1	1	Total C Mg N O 722 602 12 48 60	0
22	1	1	Total C Mg N O 722 602 12 48 60	0
22	1	1	Total C Mg N O 722 602 12 48 60	0
22	1	1	Total C Mg N O 722 602 12 48 60	0
22	1	1	Total C Mg N O 722 602 12 48 60	0
22	1	1	Total C Mg N O 722 602 12 48 60	0
22	1	1	Total C Mg N O 722 602 12 48 60	0
22	1	1	Total C Mg N O 722 602 12 48 60	0
22	3	1	Total C Mg N O 696 570 13 52 61	0
22	3	1	Total C Mg N O 696 570 13 52 61	0
22	3	1	Total C Mg N O 696 570 13 52 61	0
22	3	1	Total C Mg N O 696 570 13 52 61	0
22	3	1	Total C Mg N O 696 570 13 52 61	0
22	3	1	Total C Mg N O 696 570 13 52 61	0
22	3	1	Total C Mg N O 696 570 13 52 61	0
22	3	1	Total C Mg N O 696 570 13 52 61	0
22	3	1	Total C Mg N O 696 570 13 52 61	0
22	3	1	Total C Mg N O 696 570 13 52 61	0
22	3	1	Total C Mg N O 696 570 13 52 61	0

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Mol	Chain	Residues	Atoms	AltConf
22	3	1	Total C Mg N O 696 570 13 52 61	0
22	3	1	Total C Mg N O 696 570 13 52 61	0
22	7	1	Total C Mg N O 741 607 14 56 64	0
22	7	1	Total C Mg N O 741 607 14 56 64	0
22	7	1	Total C Mg N O 741 607 14 56 64	0
22	7	1	Total C Mg N O 741 607 14 56 64	0
22	7	1	Total C Mg N O 741 607 14 56 64	0
22	7	1	Total C Mg N O 741 607 14 56 64	0
22	7	1	Total C Mg N O 741 607 14 56 64	0
22	7	1	Total C Mg N O 741 607 14 56 64	0
22	7	1	Total C Mg N O 741 607 14 56 64	0
22	7	1	Total C Mg N O 741 607 14 56 64	0
22	7	1	Total C Mg N O 741 607 14 56 64	0
22	7	1	Total C Mg N O 741 607 14 56 64	0
22	7	1	Total C Mg N O 741 607 14 56 64	0
22	7	1	Total C Mg N O 741 607 14 56 64	0
22	8	1	Total C Mg N O 680 552 13 52 63	0
22	8	1	Total C Mg N O 680 552 13 52 63	0
22	8	1	Total C Mg N O 680 552 13 52 63	0
22	8	1	Total C Mg N O 680 552 13 52 63	0
22	8	1	Total C Mg N O 680 552 13 52 63	0

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Mol	Chain	Residues	Atoms					AltConf
22	8	1	Total 680	C 552	Mg 13	N 52	O 63	0
22	8	1	Total 680	C 552	Mg 13	N 52	O 63	0
22	8	1	Total 680	C 552	Mg 13	N 52	O 63	0
22	8	1	Total 680	C 552	Mg 13	N 52	O 63	0
22	8	1	Total 680	C 552	Mg 13	N 52	O 63	0
22	8	1	Total 680	C 552	Mg 13	N 52	O 63	0
22	8	1	Total 680	C 552	Mg 13	N 52	O 63	0
22	8	1	Total 680	C 552	Mg 13	N 52	O 63	0
22	Z	1	Total 714	C 594	Mg 12	N 48	O 60	0
22	Z	1	Total 714	C 594	Mg 12	N 48	O 60	0
22	Z	1	Total 714	C 594	Mg 12	N 48	O 60	0
22	Z	1	Total 714	C 594	Mg 12	N 48	O 60	0
22	Z	1	Total 714	C 594	Mg 12	N 48	O 60	0
22	Z	1	Total 714	C 594	Mg 12	N 48	O 60	0
22	Z	1	Total 714	C 594	Mg 12	N 48	O 60	0
22	Z	1	Total 714	C 594	Mg 12	N 48	O 60	0
22	Z	1	Total 714	C 594	Mg 12	N 48	O 60	0
22	Z	1	Total 714	C 594	Mg 12	N 48	O 60	0
22	Z	1	Total 714	C 594	Mg 12	N 48	O 60	0
22	Z	1	Total 714	C 594	Mg 12	N 48	O 60	0
22	4	1	Total 576	C 468	Mg 11	N 44	O 53	0

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Mol	Chain	Residues	Atoms					AltConf
22	4	1	Total 576	C 468	Mg 11	N 44	O 53	0
22	4	1	Total 576	C 468	Mg 11	N 44	O 53	0
22	4	1	Total 576	C 468	Mg 11	N 44	O 53	0
22	4	1	Total 576	C 468	Mg 11	N 44	O 53	0
22	4	1	Total 576	C 468	Mg 11	N 44	O 53	0
22	4	1	Total 576	C 468	Mg 11	N 44	O 53	0
22	4	1	Total 576	C 468	Mg 11	N 44	O 53	0
22	4	1	Total 576	C 468	Mg 11	N 44	O 53	0
22	4	1	Total 576	C 468	Mg 11	N 44	O 53	0
22	4	1	Total 576	C 468	Mg 11	N 44	O 53	0
22	5	1	Total 737	C 597	Mg 14	N 56	O 70	0
22	5	1	Total 737	C 597	Mg 14	N 56	O 70	0
22	5	1	Total 737	C 597	Mg 14	N 56	O 70	0
22	5	1	Total 737	C 597	Mg 14	N 56	O 70	0
22	5	1	Total 737	C 597	Mg 14	N 56	O 70	0
22	5	1	Total 737	C 597	Mg 14	N 56	O 70	0
22	5	1	Total 737	C 597	Mg 14	N 56	O 70	0
22	5	1	Total 737	C 597	Mg 14	N 56	O 70	0
22	5	1	Total 737	C 597	Mg 14	N 56	O 70	0
22	5	1	Total 737	C 597	Mg 14	N 56	O 70	0
22	5	1	Total 737	C 597	Mg 14	N 56	O 70	0

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Mol	Chain	Residues	Atoms	AltConf
22	5	1	Total C Mg N O 737 597 14 56 70	0
22	5	1	Total C Mg N O 737 597 14 56 70	0
22	5	1	Total C Mg N O 737 597 14 56 70	0
22	6	1	Total C Mg N O 696 566 13 52 65	0
22	6	1	Total C Mg N O 696 566 13 52 65	0
22	6	1	Total C Mg N O 696 566 13 52 65	0
22	6	1	Total C Mg N O 696 566 13 52 65	0
22	6	1	Total C Mg N O 696 566 13 52 65	0
22	6	1	Total C Mg N O 696 566 13 52 65	0
22	6	1	Total C Mg N O 696 566 13 52 65	0
22	6	1	Total C Mg N O 696 566 13 52 65	0
22	6	1	Total C Mg N O 696 566 13 52 65	0
22	6	1	Total C Mg N O 696 566 13 52 65	0
22	6	1	Total C Mg N O 696 566 13 52 65	0
22	6	1	Total C Mg N O 696 566 13 52 65	0
22	6	1	Total C Mg N O 696 566 13 52 65	0
22	2	1	Total C Mg N O 540 432 11 44 53	0
22	2	1	Total C Mg N O 540 432 11 44 53	0
22	2	1	Total C Mg N O 540 432 11 44 53	0
22	2	1	Total C Mg N O 540 432 11 44 53	0
22	2	1	Total C Mg N O 540 432 11 44 53	0

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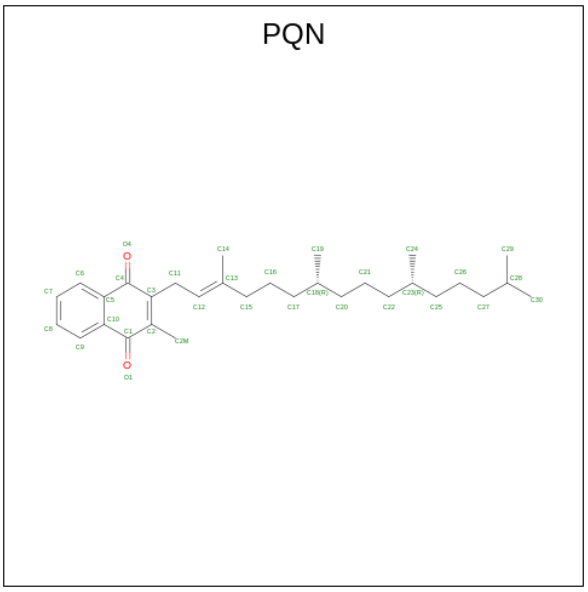
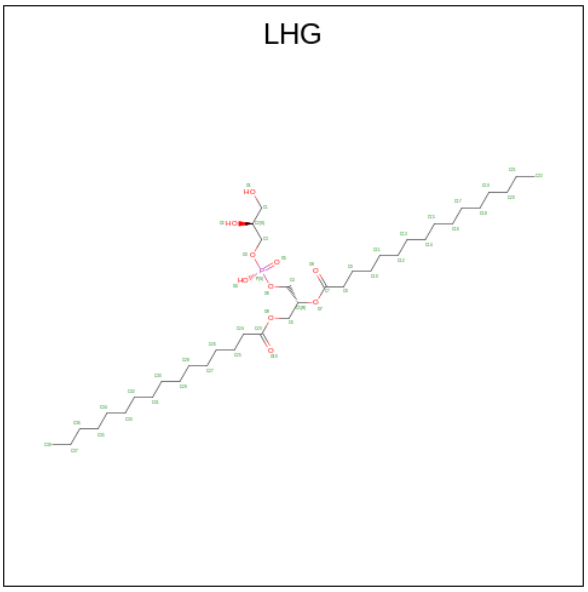
Mol	Chain	Residues	Atoms					AltConf
22	2	1	Total 540	C 432	Mg 11	N 44	O 53	0
22	2	1	Total 540	C 432	Mg 11	N 44	O 53	0
22	2	1	Total 540	C 432	Mg 11	N 44	O 53	0
22	2	1	Total 540	C 432	Mg 11	N 44	O 53	0
22	2	1	Total 540	C 432	Mg 11	N 44	O 53	0
22	2	1	Total 540	C 432	Mg 11	N 44	O 53	0
22	9	1	Total 514	C 414	Mg 10	N 40	O 50	0
22	9	1	Total 514	C 414	Mg 10	N 40	O 50	0
22	9	1	Total 514	C 414	Mg 10	N 40	O 50	0
22	9	1	Total 514	C 414	Mg 10	N 40	O 50	0
22	9	1	Total 514	C 414	Mg 10	N 40	O 50	0
22	9	1	Total 514	C 414	Mg 10	N 40	O 50	0
22	9	1	Total 514	C 414	Mg 10	N 40	O 50	0
22	9	1	Total 514	C 414	Mg 10	N 40	O 50	0
22	9	1	Total 514	C 414	Mg 10	N 40	O 50	0
22	9	1	Total 514	C 414	Mg 10	N 40	O 50	0

- Molecule 23 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



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

- Molecule 24 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
24	A	1	Total	C	O	P	0
			117	84	30	3	

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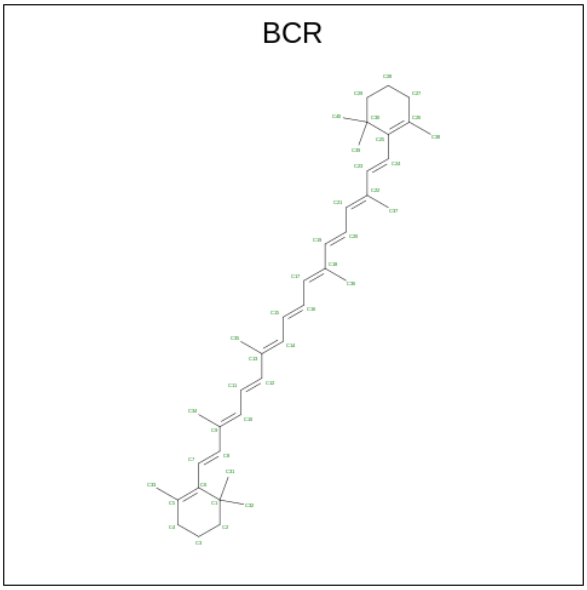
Mol	Chain	Residues	Atoms				AltConf
24	A	1	Total	C	O	P	0
			117	84	30	3	
24	A	1	Total	C	O	P	0
			117	84	30	3	
24	B	1	Total	C	O	P	0
			23	12	10	1	
24	1	1	Total	C	O	P	0
			43	32	10	1	
24	7	1	Total	C	O	P	0
			37	26	10	1	
24	8	1	Total	C	O	P	0
			37	26	10	1	
24	Z	1	Total	C	O	P	0
			43	32	10	1	
24	4	1	Total	C	O	P	0
			81	59	20	2	
24	4	1	Total	C	O	P	0
			81	59	20	2	
24	5	1	Total	C	O	P	0
			37	26	10	1	
24	6	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 25 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	AltConf
25	A	1	Total C 240 240	0
25	A	1	Total C 240 240	0
25	A	1	Total C 240 240	0
25	A	1	Total C 240 240	0
25	A	1	Total C 240 240	0
25	A	1	Total C 240 240	0
25	B	1	Total C 280 280	0
25	B	1	Total C 280 280	0
25	B	1	Total C 280 280	0
25	B	1	Total C 280 280	0
25	B	1	Total C 280 280	0
25	B	1	Total C 280 280	0
25	B	1	Total C 280 280	0
25	F	1	Total C 40 40	0
25	G	1	Total C 40 40	0
25	I	1	Total C 40 40	0
25	J	1	Total C 40 40	0
25	K	1	Total C 80 80	0
25	K	1	Total C 80 80	0
25	L	1	Total C 80 80	0
25	L	1	Total C 80 80	0
25	3	1	Total C 120 120	0

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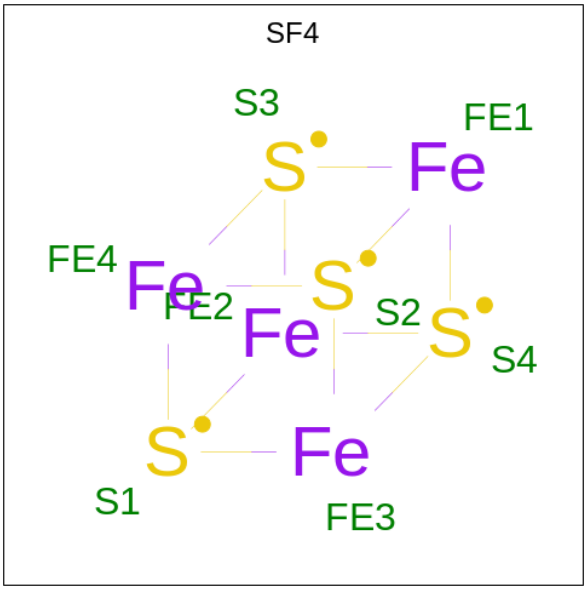
Mol	Chain	Residues	Atoms	AltConf
25	3	1	Total C 120 120	0
25	3	1	Total C 120 120	0
25	7	1	Total C 80 80	0
25	7	1	Total C 80 80	0
25	8	1	Total C 40 40	0
25	4	1	Total C 40 40	0
25	5	1	Total C 80 80	0
25	5	1	Total C 80 80	0
25	6	1	Total C 80 80	0
25	6	1	Total C 80 80	0

- Molecule 26 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

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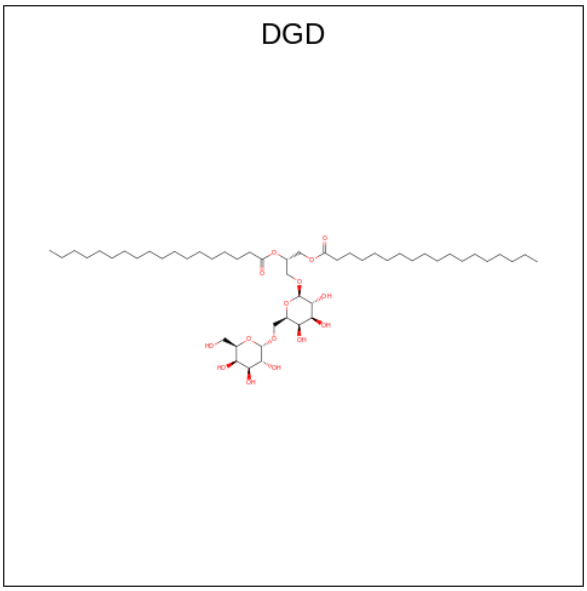
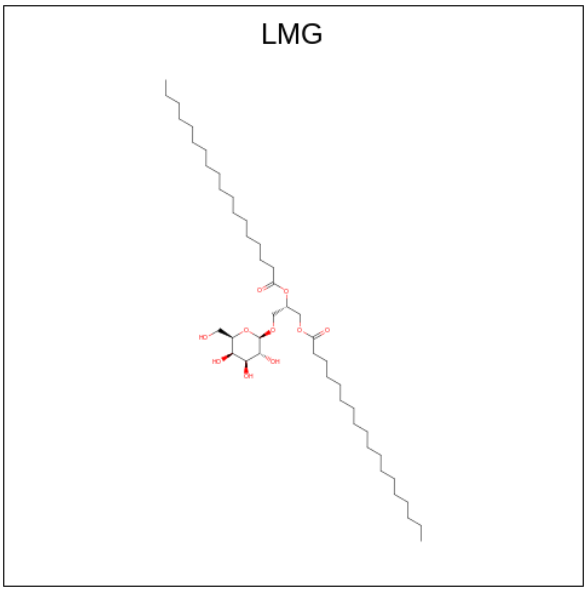
Mol	Chain	Residues	Atoms			AltConf
26	C	1	Total	Fe	S	0
			16	8	8	
26	C	1	Total	Fe	S	0
			16	8	8	

- Molecule 27 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



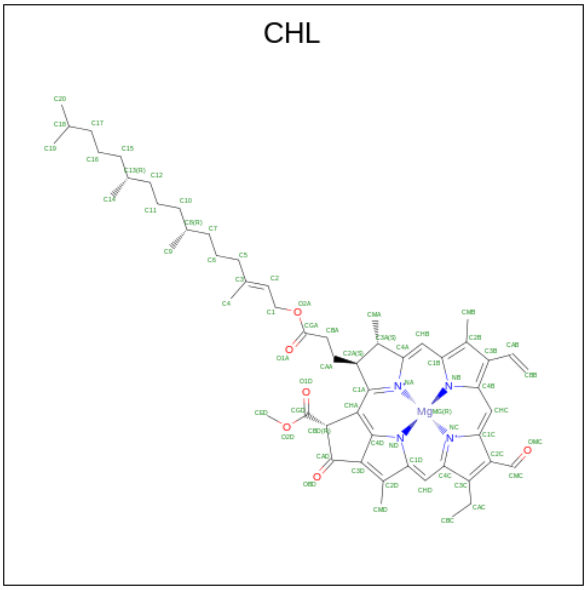
Mol	Chain	Residues	Atoms			AltConf
27	B	1	Total	C	O	0
			66	51	15	

- Molecule 28 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
28	J	1	Total 35	C 25	O 10	0
28	9	1	Total 44	C 34	O 10	0

- Molecule 29 is CHLOROPHYLL B (three-letter code: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
29	1	1	Total 101	C 79	Mg 2	N 8	O 12	0
29	1	1	Total 101	C 79	Mg 2	N 8	O 12	0

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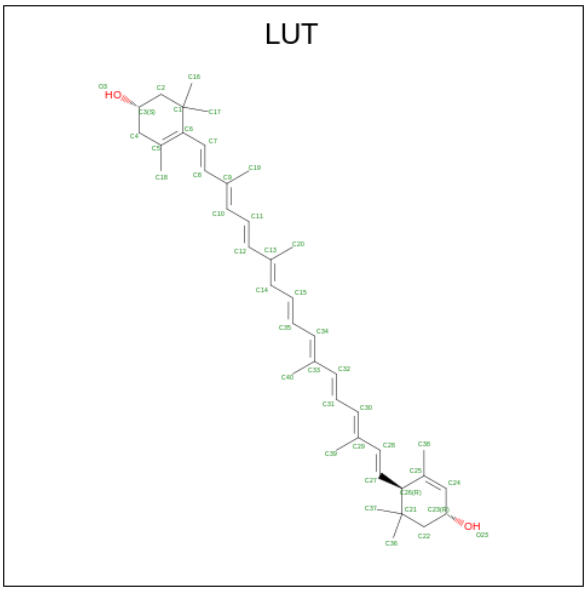
Mol	Chain	Residues	Atoms					AltConf
29	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
29	7	1	Total	C	Mg	N	O	0
			54	43	1	4	6	
29	8	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
29	Z	1	Total	C	Mg	N	O	0
			101	79	2	8	12	
29	Z	1	Total	C	Mg	N	O	0
			101	79	2	8	12	
29	4	1	Total	C	Mg	N	O	0
			201	159	4	16	22	
29	4	1	Total	C	Mg	N	O	0
			201	159	4	16	22	
29	4	1	Total	C	Mg	N	O	0
			201	159	4	16	22	
29	4	1	Total	C	Mg	N	O	0
			201	159	4	16	22	
29	5	1	Total	C	Mg	N	O	0
			145	114	3	12	16	
29	5	1	Total	C	Mg	N	O	0
			145	114	3	12	16	
29	5	1	Total	C	Mg	N	O	0
			145	114	3	12	16	
29	6	1	Total	C	Mg	N	O	0
			206	164	4	16	22	
29	6	1	Total	C	Mg	N	O	0
			206	164	4	16	22	
29	6	1	Total	C	Mg	N	O	0
			206	164	4	16	22	
29	6	1	Total	C	Mg	N	O	0
			206	164	4	16	22	
29	9	1	Total	C	Mg	N	O	0
			93	73	2	8	10	
29	9	1	Total	C	Mg	N	O	0
			93	73	2	8	10	

- Molecule 30 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3 ,3'-DIOL (three-letter code: LUT) (formula: $C_{40}H_{56}O_2$).



Mol	Chain	Residues	Atoms			AltConf
30	1	1	Total	C	O	0
			126	120	6	
30	1	1	Total	C	O	0
			126	120	6	
30	1	1	Total	C	O	0
			126	120	6	
30	3	1	Total	C	O	0
			84	80	4	
30	3	1	Total	C	O	0
			84	80	4	
30	7	1	Total	C	O	0
			84	80	4	
30	7	1	Total	C	O	0
			84	80	4	
30	8	1	Total	C	O	0
			84	80	4	
30	8	1	Total	C	O	0
			84	80	4	
30	Z	1	Total	C	O	0
			126	120	6	
30	Z	1	Total	C	O	0
			126	120	6	
30	Z	1	Total	C	O	0
			126	120	6	
30	4	1	Total	C	O	0
			84	80	4	
30	4	1	Total	C	O	0
			84	80	4	

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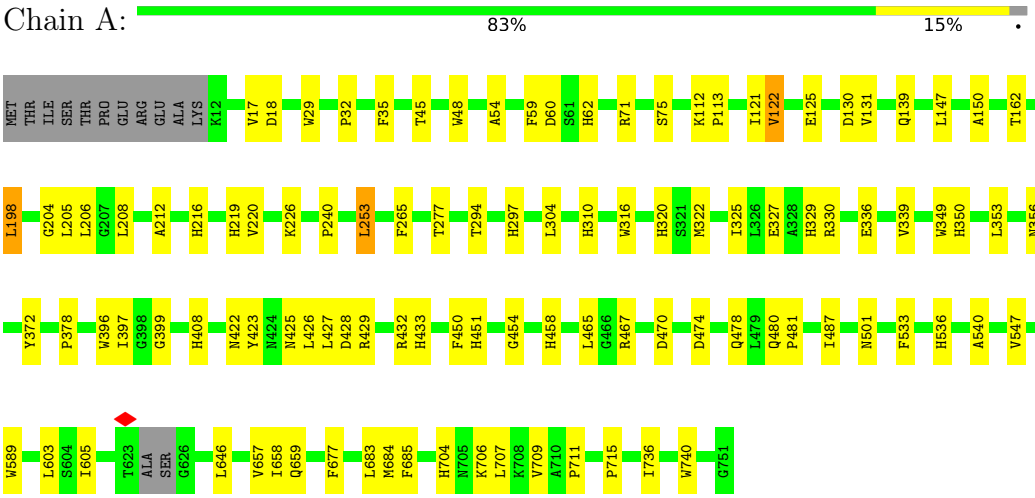
Mol	Chain	Residues	Atoms			AltConf
30	5	1	Total	C	O	0
			84	80	4	
30	5	1	Total	C	O	0
			84	80	4	
30	6	1	Total	C	O	0
			84	80	4	
30	6	1	Total	C	O	0
			84	80	4	
30	2	1	Total	C	O	0
			84	80	4	
30	2	1	Total	C	O	0
			84	80	4	
30	9	1	Total	C	O	0
			84	80	4	
30	9	1	Total	C	O	0
			84	80	4	

3 Residue-property plots

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

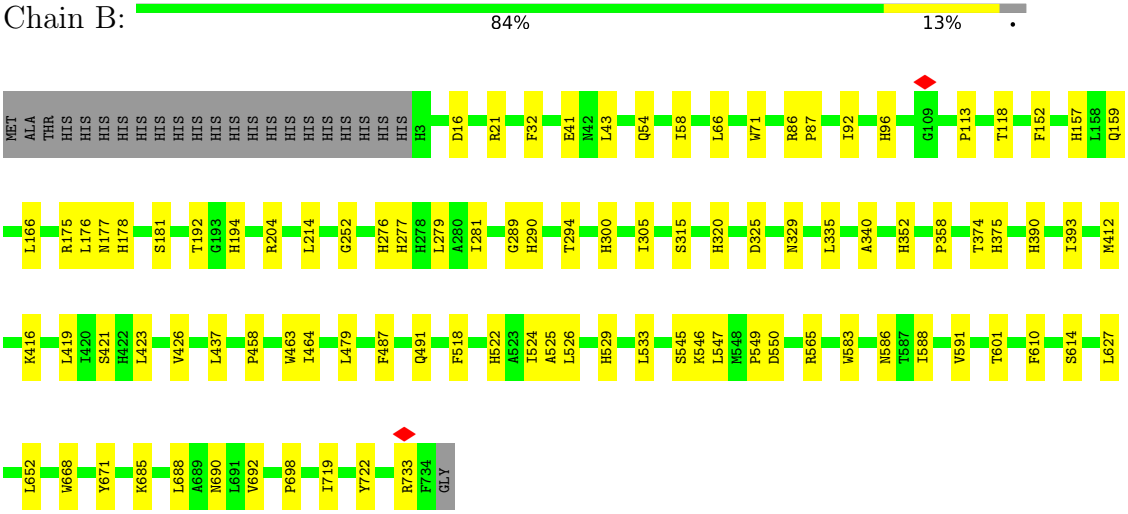
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain A:



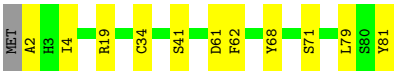
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain B:



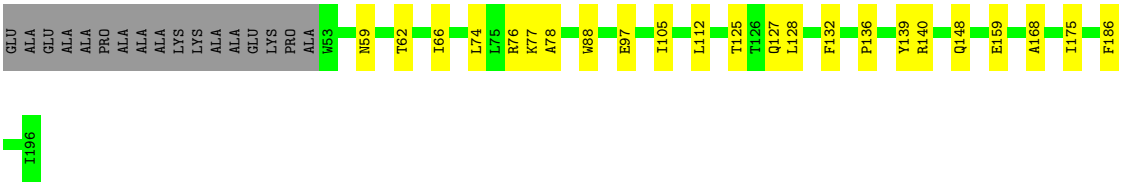
• Molecule 3: Photosystem I iron-sulfur center

Chain C:



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

Chain D:

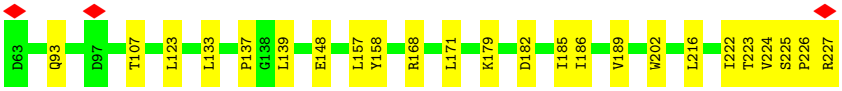


• Molecule 5: Photosystem I reaction center subunit IV, chloroplastic

Chain E:

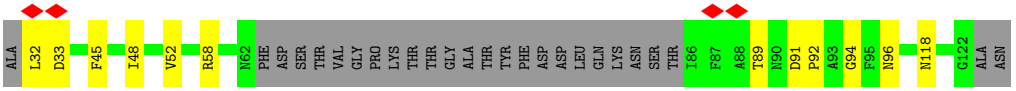
• Molecule 6: Photosystem I reaction center subunit F, Photosystem I reaction center subunit III, chloroplastic

Chain F:



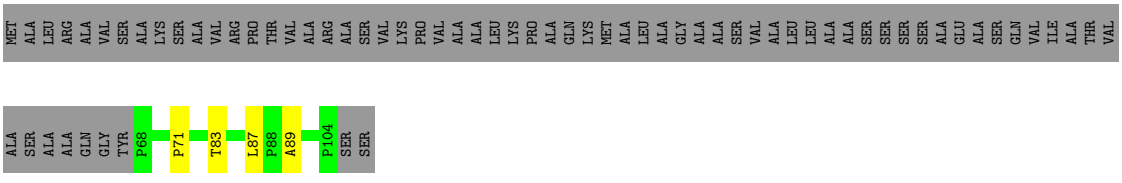
• Molecule 7: Photosystem I reaction center subunit V, chloroplastic

Chain G:



• Molecule 8: Photosystem I reaction center subunit VIII

Chain I:

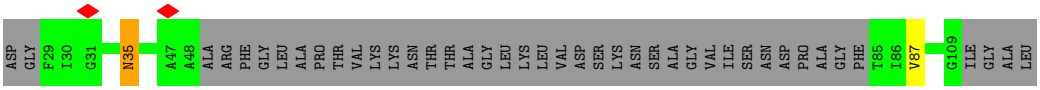


• Molecule 9: Photosystem I reaction center subunit IX

Chain J:

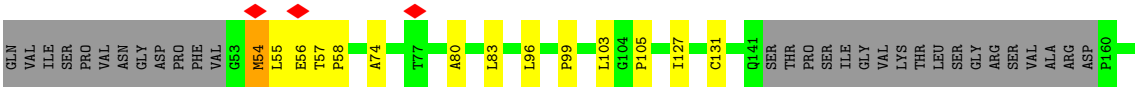
• Molecule 10: Photosystem I reaction center subunit psaK, chloroplastic

Chain K:



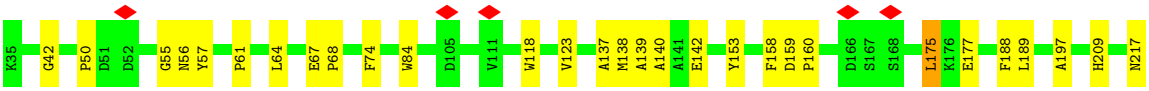
• Molecule 11: Photosystem I reaction center subunit XI

Chain L:



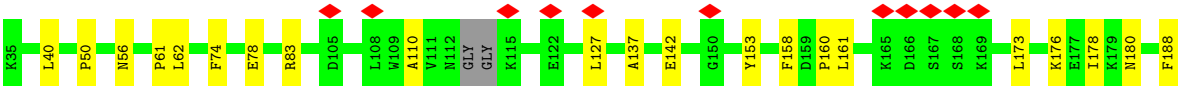
• Molecule 12: Chlorophyll a-b binding protein, chloroplastic

Chain 1:



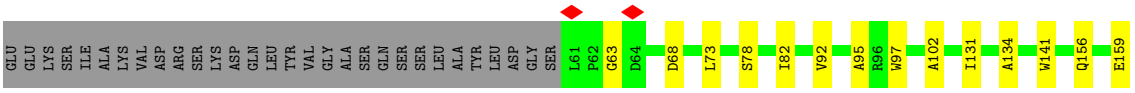
• Molecule 12: Chlorophyll a-b binding protein, chloroplastic

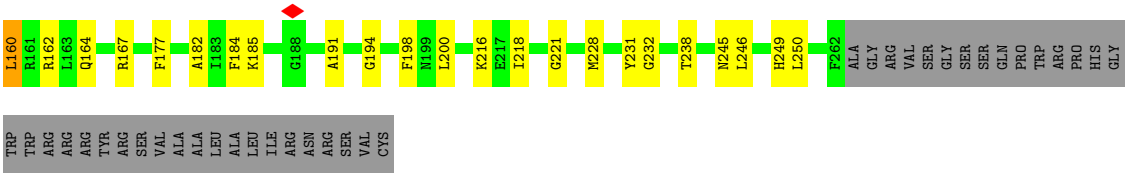
Chain Z:



• Molecule 13: Chlorophyll a-b binding protein, chloroplastic

Chain 3:



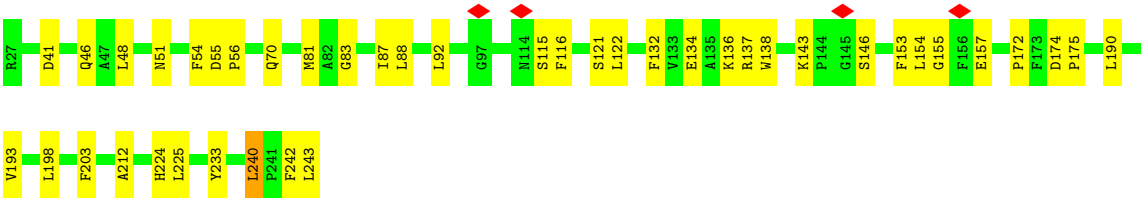


• Molecule 14: Chlorophyll a-b binding protein, chloroplastic

Chain 7:

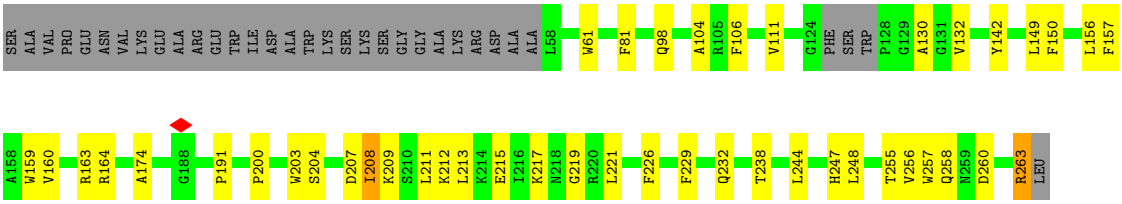
• Molecule 15: Chlorophyll a-b binding protein, chloroplastic

Chain 8:



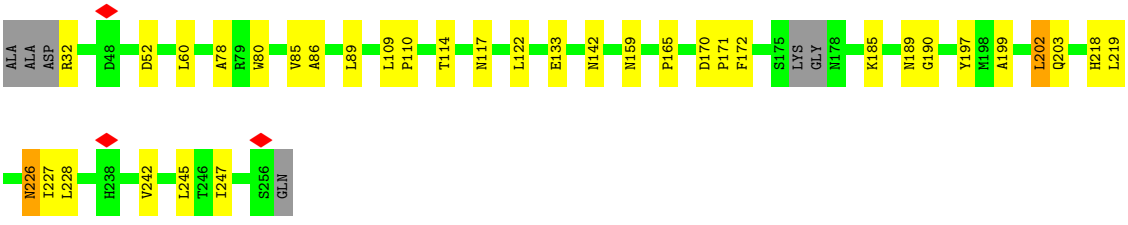
• Molecule 16: Chlorophyll a-b binding protein, chloroplastic

Chain 4:



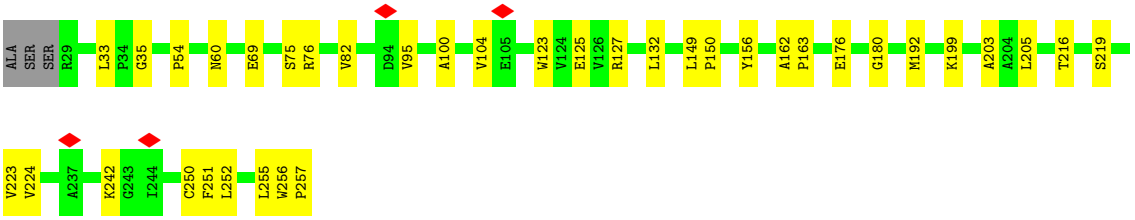
• Molecule 17: Chlorophyll a-b binding protein, chloroplastic

Chain 5:



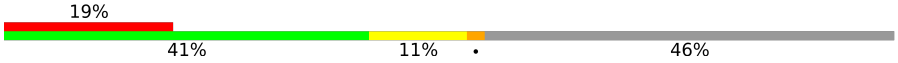
• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

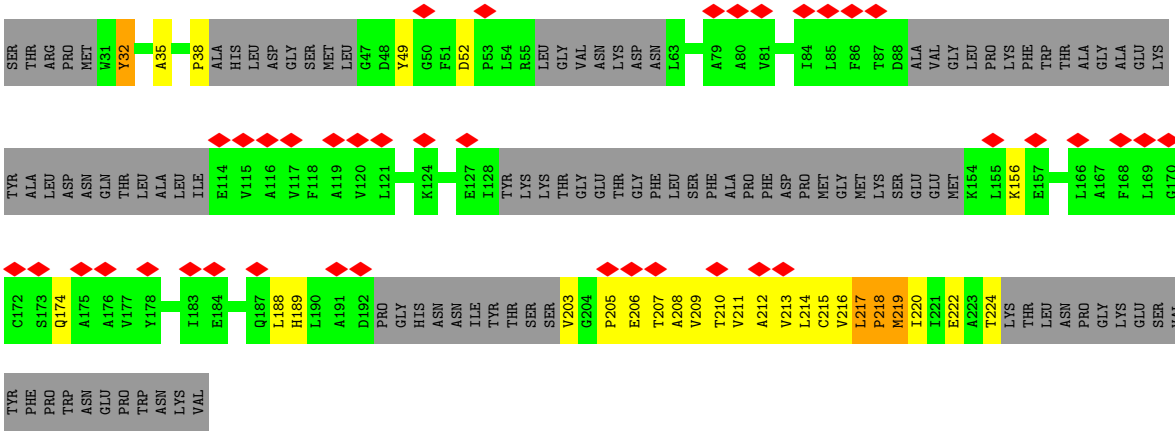
Chain 6:



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

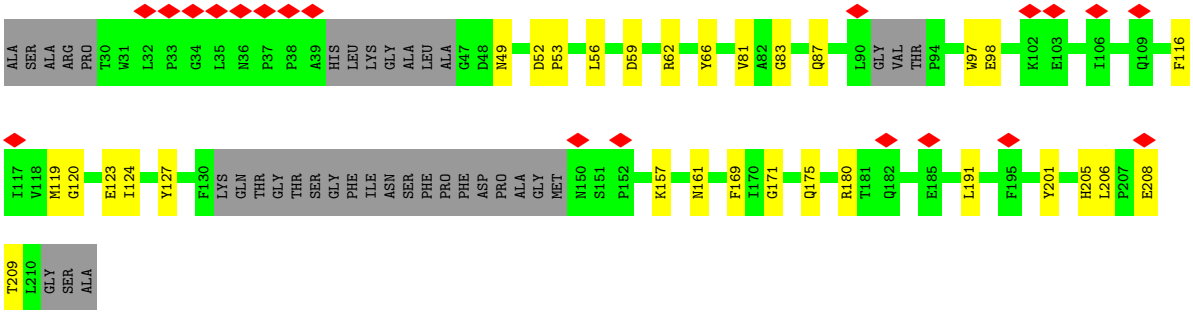
Chain 2:





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

Chain 9:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	338867	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.498	Depositor
Minimum map value	-0.258	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	358.4, 358.4, 358.4	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.12, 1.12, 1.12	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.37	0/5995	0.61	4/8172 (0.0%)
2	B	0.36	0/6035	0.57	1/8240 (0.0%)
3	C	0.36	0/610	0.61	0/826
4	D	0.36	0/1160	0.55	0/1567
5	E	0.33	0/490	0.47	0/667
6	F	0.33	0/1291	0.58	0/1747
7	G	0.29	0/513	0.51	0/696
8	I	0.34	0/293	0.60	0/406
9	J	0.35	0/331	0.55	0/454
10	K	0.28	0/297	0.54	0/401
11	L	0.33	0/874	0.59	0/1194
12	1	0.31	0/1490	0.52	1/2028 (0.0%)
12	Z	0.31	0/1481	0.55	0/2015
13	3	0.36	0/1601	0.57	1/2173 (0.0%)
14	7	0.34	0/1696	0.55	0/2303
15	8	0.34	0/1700	0.67	3/2315 (0.1%)
16	4	0.33	0/1621	0.59	3/2209 (0.1%)
17	5	0.31	0/1798	0.52	0/2450
18	6	0.30	0/1827	0.54	0/2497
19	2	0.36	0/851	0.63	2/1154 (0.2%)
20	9	0.32	0/1211	0.56	0/1643
All	All	0.34	0/33165	0.58	15/45157 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
14	7	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	2

There are no bond length outliers.

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	2	217	LEU	C-N-CD	8.65	146.56	128.40
16	4	164	ARG	NE-CZ-NH1	8.33	124.47	120.30
1	A	198	LEU	CA-CB-CG	7.99	133.68	115.30
15	8	137	ARG	NE-CZ-NH1	7.33	123.97	120.30
19	2	218	PRO	CA-N-CD	-6.93	101.79	111.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	7	150	PHE	Peptide
2	B	668	TRP	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5800	0	5646	111	0
2	B	5822	0	5574	97	0
3	C	600	0	581	9	0
4	D	1132	0	1150	16	0
5	E	480	0	476	6	0
6	F	1265	0	1301	52	0
7	G	503	0	496	7	0
8	I	281	0	292	5	0
9	J	320	0	322	7	0
10	K	297	0	319	2	0
11	L	853	0	864	25	0
12	1	1444	0	1395	26	0
12	Z	1436	0	1388	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	3	1555	0	1522	30	0
14	7	1644	0	1582	23	0
15	8	1649	0	1628	36	0
16	4	1570	0	1526	72	0
17	5	1744	0	1715	39	0
18	6	1765	0	1767	38	0
19	2	838	0	767	65	0
20	9	1180	0	1160	35	0
21	A	65	0	72	3	0
22	1	722	0	735	34	0
22	2	540	0	426	19	0
22	3	696	0	630	26	0
22	4	576	0	490	42	0
22	5	737	0	632	34	0
22	6	696	0	620	44	0
22	7	741	0	658	32	0
22	8	680	0	592	24	0
22	9	514	0	426	19	0
22	A	2689	0	2796	204	0
22	B	2480	0	2545	122	0
22	F	175	0	177	8	0
22	G	96	0	72	0	0
22	J	42	0	31	1	0
22	K	91	0	66	2	0
22	L	115	0	111	1	0
22	Z	714	0	714	24	0
23	A	33	0	46	4	0
23	B	33	0	46	1	0
24	1	43	0	56	2	0
24	4	81	0	106	3	0
24	5	37	0	44	0	0
24	6	49	0	74	19	0
24	7	37	0	44	0	0
24	8	37	0	44	1	0
24	A	117	0	153	5	0
24	B	23	0	16	0	0
24	Z	43	0	56	1	0
25	3	120	0	163	15	0
25	4	40	0	56	39	0
25	5	80	0	112	12	0
25	6	80	0	110	11	0
25	7	80	0	112	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	8	40	0	56	6	0
25	A	240	0	336	25	0
25	B	280	0	392	29	0
25	F	40	0	56	15	0
25	G	40	0	56	3	0
25	I	40	0	56	1	0
25	J	40	0	56	2	0
25	K	80	0	112	6	0
25	L	80	0	112	9	0
26	A	8	0	0	0	0
26	C	16	0	0	0	0
27	B	66	0	96	1	0
28	9	44	0	61	1	0
28	J	35	0	40	0	0
29	1	101	0	74	4	0
29	3	66	0	70	5	0
29	4	201	0	150	25	0
29	5	145	0	101	6	0
29	6	206	0	159	11	0
29	7	54	0	43	1	0
29	8	56	0	47	0	0
29	9	93	0	64	1	0
29	Z	101	0	73	1	0
30	1	126	0	168	14	0
30	2	84	0	112	6	0
30	3	84	0	112	7	0
30	4	84	0	112	16	0
30	5	84	0	112	20	0
30	6	84	0	112	7	0
30	7	84	0	112	8	0
30	8	84	0	112	13	0
30	9	84	0	112	8	0
30	Z	126	0	168	10	0
All	All	48476	0	47944	1162	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 1162 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)
16:4:257:TRP:CD1	22:4:616:CLA:CBB	1.75	1.60
19:2:32:TYR:CE2	19:2:35:ALA:HB2	1.37	1.59
22:A:802:CLA:C19	22:A:842:CLA:C4	1.79	1.53
19:2:32:TYR:CD2	19:2:35:ALA:HB2	1.41	1.50
1:A:198:LEU:HD23	1:A:322:MET:CE	1.43	1.48

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	734/751 (98%)	713 (97%)	20 (3%)	1 (0%)	51 82
2	B	730/755 (97%)	708 (97%)	22 (3%)	0	100 100
3	C	78/81 (96%)	74 (95%)	4 (5%)	0	100 100
4	D	142/161 (88%)	135 (95%)	7 (5%)	0	100 100
5	E	59/73 (81%)	55 (93%)	4 (7%)	0	100 100
6	F	163/165 (99%)	155 (95%)	8 (5%)	0	100 100
7	G	64/94 (68%)	64 (100%)	0	0	100 100
8	I	35/106 (33%)	34 (97%)	1 (3%)	0	100 100
9	J	37/41 (90%)	35 (95%)	2 (5%)	0	100 100
10	K	41/87 (47%)	41 (100%)	0	0	100 100
11	L	114/156 (73%)	108 (95%)	5 (4%)	1 (1%)	17 48
12	1	192/194 (99%)	186 (97%)	6 (3%)	0	100 100
12	Z	188/194 (97%)	181 (96%)	7 (4%)	0	100 100
13	3	200/268 (75%)	191 (96%)	9 (4%)	0	100 100
14	7	210/215 (98%)	200 (95%)	10 (5%)	0	100 100
15	8	215/217 (99%)	206 (96%)	9 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
16	4	199/236 (84%)	187 (94%)	11 (6%)	1 (0%)	29 61
17	5	219/229 (96%)	201 (92%)	18 (8%)	0	100 100
18	6	227/232 (98%)	216 (95%)	11 (5%)	0	100 100
19	2	107/221 (48%)	107 (100%)	0	0	100 100
20	9	144/189 (76%)	136 (94%)	8 (6%)	0	100 100
All	All	4098/4665 (88%)	3933 (96%)	162 (4%)	3 (0%)	54 82

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	L	187	VAL
16	4	208	ILE
1	A	122	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	599/610 (98%)	593 (99%)	6 (1%)	76 92
2	B	596/617 (97%)	595 (100%)	1 (0%)	93 98
3	C	69/70 (99%)	69 (100%)	0	100 100
4	D	121/129 (94%)	119 (98%)	2 (2%)	60 86
5	E	52/62 (84%)	52 (100%)	0	100 100
6	F	127/127 (100%)	126 (99%)	1 (1%)	81 94
7	G	48/69 (70%)	47 (98%)	1 (2%)	53 81
8	I	31/76 (41%)	31 (100%)	0	100 100
9	J	35/37 (95%)	35 (100%)	0	100 100
10	K	30/60 (50%)	29 (97%)	1 (3%)	38 72
11	L	85/119 (71%)	84 (99%)	1 (1%)	71 91
12	1	137/137 (100%)	136 (99%)	1 (1%)	84 95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	Z	137/137 (100%)	137 (100%)	0	100	100
13	3	155/209 (74%)	154 (99%)	1 (1%)	86	96
14	7	164/164 (100%)	163 (99%)	1 (1%)	86	96
15	8	163/163 (100%)	162 (99%)	1 (1%)	86	96
16	4	159/185 (86%)	158 (99%)	1 (1%)	86	96
17	5	181/184 (98%)	178 (98%)	3 (2%)	60	86
18	6	183/185 (99%)	182 (100%)	1 (0%)	88	96
19	2	70/178 (39%)	68 (97%)	2 (3%)	42	76
20	9	118/143 (82%)	118 (100%)	0	100	100
All	All	3260/3661 (89%)	3236 (99%)	24 (1%)	84	95

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	3	160	LEU
16	4	263	ARG
15	8	51	ASN
17	5	117	ASN
2	B	479	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
16	4	175	ASN
18	6	60	ASN
20	9	87	GLN
18	6	130	GLN
4	D	127	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

313 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	CLA	3	607	13	60,68,73	2.13	18 (30%)	70,107,113	2.82	28 (40%)
25	BCR	G	205	-	41,41,41	0.72	0	56,56,56	1.50	7 (12%)
22	CLA	G	204	7	46,54,73	2.46	17 (36%)	53,90,113	3.13	24 (45%)
22	CLA	A	825	1	55,63,73	2.18	15 (27%)	64,101,113	2.90	26 (40%)
22	CLA	3	609	13	50,58,73	2.32	17 (34%)	58,95,113	3.03	26 (44%)
22	CLA	1	613	-	65,73,73	2.00	17 (26%)	76,113,113	2.61	25 (32%)
22	CLA	B	806	2	65,73,73	2.01	15 (23%)	76,113,113	2.73	29 (38%)
22	CLA	7	610	14	60,68,73	2.09	14 (23%)	70,107,113	2.86	28 (40%)
25	BCR	6	623	-	41,41,41	0.65	0	56,56,56	1.98	18 (32%)
25	BCR	K	4001	-	41,41,41	0.69	0	56,56,56	2.00	15 (26%)
29	CHL	1	601	12	53,61,74	2.20	18 (33%)	57,98,114	3.36	27 (47%)
22	CLA	7	611	24	41,49,73	2.50	19 (46%)	47,84,113	3.41	26 (55%)
22	CLA	4	614	16	45,53,73	2.44	17 (37%)	52,89,113	3.14	25 (48%)
22	CLA	1	602	12	65,73,73	1.99	15 (23%)	76,113,113	2.67	28 (36%)
22	CLA	A	832	1	50,58,73	2.27	16 (32%)	58,95,113	3.00	27 (46%)
25	BCR	J	3003	-	41,41,41	0.74	0	56,56,56	1.74	13 (23%)
24	LHG	Z	620	22	42,42,48	0.99	2 (4%)	45,48,54	1.06	2 (4%)
22	CLA	4	611	24	55,63,73	2.25	18 (32%)	64,101,113	2.83	28 (43%)
24	LHG	4	623	-	31,31,48	1.14	2 (6%)	34,37,54	1.14	3 (8%)
25	BCR	B	847	-	41,41,41	0.76	0	56,56,56	1.71	14 (25%)
22	CLA	3	613	13	55,63,73	2.18	17 (30%)	64,101,113	2.77	24 (37%)
29	CHL	6	607	-	56,64,74	2.14	18 (32%)	61,102,114	3.10	29 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	5	616	17	46,54,73	2.40	18 (39%)	53,90,113	3.07	26 (49%)
22	CLA	A	835	1	65,73,73	2.09	17 (26%)	76,113,113	2.75	26 (34%)
22	CLA	Z	604	-	57,65,73	2.18	17 (29%)	66,103,113	2.82	26 (39%)
22	CLA	A	809	1	65,73,73	2.02	17 (26%)	76,113,113	2.80	29 (38%)
22	CLA	Z	606	-	52,60,73	2.31	18 (34%)	60,97,113	3.05	28 (46%)
22	CLA	4	613	16	56,64,73	2.18	15 (26%)	65,102,113	2.89	28 (43%)
22	CLA	5	606	-	55,63,73	2.24	17 (30%)	64,101,113	2.92	26 (40%)
25	BCR	L	201	-	41,41,41	0.72	0	56,56,56	1.73	12 (21%)
22	CLA	2	603	19	46,54,73	2.43	16 (34%)	53,90,113	3.24	25 (47%)
22	CLA	5	611	24	55,63,73	2.24	17 (30%)	64,101,113	2.91	27 (42%)
24	LHG	6	619	22	48,48,48	0.94	2 (4%)	51,54,54	0.98	2 (3%)
22	CLA	A	823	1	49,57,73	2.33	17 (34%)	55,93,113	3.14	23 (41%)
22	CLA	3	612	13	46,54,73	2.39	17 (36%)	53,90,113	3.26	24 (45%)
22	CLA	A	824	1	51,59,73	2.27	18 (35%)	59,96,113	3.07	25 (42%)
22	CLA	2	612	19	52,60,73	2.30	16 (30%)	60,97,113	3.01	26 (43%)
22	CLA	B	812	2	65,73,73	2.02	18 (27%)	76,113,113	2.72	26 (34%)
24	LHG	5	623	22	36,36,48	1.07	2 (5%)	39,42,54	1.10	3 (7%)
22	CLA	4	612	16	52,60,73	2.25	18 (34%)	60,97,113	3.10	27 (45%)
30	LUT	8	618	-	42,43,43	0.79	0	51,60,60	1.56	11 (21%)
22	CLA	3	602	13	60,68,73	2.15	18 (30%)	70,107,113	2.87	31 (44%)
30	LUT	7	622	-	42,43,43	0.75	0	51,60,60	1.49	10 (19%)
25	BCR	7	623	-	41,41,41	0.78	1 (2%)	56,56,56	1.93	15 (26%)
29	CHL	6	608	-	51,59,74	2.21	17 (33%)	55,96,114	3.41	26 (47%)
30	LUT	6	621	-	42,43,43	0.73	0	51,60,60	1.62	11 (21%)
22	CLA	B	828	2	65,73,73	2.01	16 (24%)	76,113,113	2.58	27 (35%)
22	CLA	B	837	2	65,73,73	1.97	16 (24%)	76,113,113	2.83	28 (36%)
22	CLA	A	804	1	65,73,73	1.96	16 (24%)	76,113,113	2.81	30 (39%)
25	BCR	B	846	-	41,41,41	0.76	0	56,56,56	2.01	15 (26%)
22	CLA	A	810	1	65,73,73	1.98	17 (26%)	76,113,113	2.74	30 (39%)
25	BCR	5	622	-	41,41,41	0.66	0	56,56,56	1.87	15 (26%)
29	CHL	5	618	17	43,51,74	2.40	17 (39%)	45,86,114	3.62	22 (48%)
22	CLA	9	603	20	46,54,73	2.42	17 (36%)	53,90,113	3.29	26 (49%)
29	CHL	5	607	-	51,59,74	2.25	17 (33%)	55,96,114	3.29	25 (45%)
22	CLA	J	3002	9	42,50,73	2.46	15 (35%)	48,85,113	3.32	24 (50%)
22	CLA	B	808	2	65,73,73	2.02	17 (26%)	76,113,113	2.72	27 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	A	842	1	65,73,73	1.99	16 (24%)	76,113,113	2.80	27 (35%)
22	CLA	A	821	1	45,53,73	2.41	16 (35%)	52,89,113	3.12	25 (48%)
25	BCR	B	801	-	41,41,41	0.72	0	56,56,56	1.97	14 (25%)
22	CLA	5	613	17	56,64,73	2.17	16 (28%)	65,102,113	2.79	24 (36%)
22	CLA	B	833	2	58,66,73	2.15	16 (27%)	67,104,113	2.95	28 (41%)
25	BCR	B	848	-	41,41,41	0.73	0	56,56,56	1.53	10 (17%)
21	CL0	A	801	1	65,73,73	1.93	15 (23%)	76,113,113	2.81	30 (39%)
22	CLA	4	610	16	60,68,73	2.11	16 (26%)	70,107,113	2.81	30 (42%)
25	BCR	K	4004	-	41,41,41	0.70	0	56,56,56	1.74	14 (25%)
22	CLA	9	609	-	50,58,73	2.32	16 (32%)	58,95,113	3.06	27 (46%)
29	CHL	9	607	-	51,59,74	2.30	17 (33%)	55,96,114	3.17	24 (43%)
22	CLA	A	803	-	65,73,73	2.02	17 (26%)	76,113,113	2.88	29 (38%)
22	CLA	B	823	2	60,68,73	2.11	16 (26%)	70,107,113	2.68	28 (40%)
22	CLA	7	601	14	65,73,73	2.02	17 (26%)	76,113,113	2.77	26 (34%)
22	CLA	7	603	14	46,54,73	2.40	17 (36%)	53,90,113	3.28	24 (45%)
29	CHL	8	607	-	56,64,74	2.12	17 (30%)	61,102,114	3.10	24 (39%)
22	CLA	B	824	-	65,73,73	1.99	16 (24%)	76,113,113	2.65	28 (36%)
26	SF4	C	101	3	0,12,12	-	-	-		
22	CLA	B	852	-	65,73,73	2.07	17 (26%)	76,113,113	2.60	27 (35%)
22	CLA	6	602	18	65,73,73	2.02	14 (21%)	76,113,113	2.74	26 (34%)
30	LUT	5	620	-	42,43,43	0.78	0	51,60,60	1.72	14 (27%)
30	LUT	2	617	-	42,43,43	0.72	0	51,60,60	1.79	12 (23%)
22	CLA	9	614	20	45,53,73	2.49	16 (35%)	52,89,113	3.23	27 (51%)
22	CLA	A	802	-	65,73,73	2.09	17 (26%)	76,113,113	2.72	29 (38%)
22	CLA	B	830	2	50,58,73	2.28	16 (32%)	58,95,113	3.14	27 (46%)
22	CLA	5	604	17	50,58,73	2.33	15 (30%)	58,95,113	2.98	27 (46%)
22	CLA	8	614	15	55,63,73	2.23	17 (30%)	64,101,113	2.86	29 (45%)
22	CLA	A	819	1	65,73,73	2.02	16 (24%)	76,113,113	2.70	27 (35%)
22	CLA	B	826	2	65,73,73	1.98	15 (23%)	76,113,113	2.75	29 (38%)
22	CLA	7	616	14	46,54,73	2.46	18 (39%)	53,90,113	3.24	24 (45%)
29	CHL	5	608	-	51,59,74	2.20	16 (31%)	55,96,114	3.17	25 (45%)
30	LUT	4	620	-	42,43,43	0.73	0	51,60,60	1.50	10 (19%)
22	CLA	9	610	20	60,68,73	2.15	16 (26%)	70,107,113	2.84	27 (38%)
22	CLA	6	617	18	46,54,73	2.41	17 (36%)	53,90,113	3.13	25 (47%)
22	CLA	4	602	16	60,68,73	2.11	17 (28%)	70,107,113	2.79	27 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	3	606	-	42,50,73	2.45	15 (35%)	48,85,113	3.28	23 (47%)
22	CLA	7	608	-	50,58,73	2.28	16 (32%)	58,95,113	3.12	25 (43%)
25	BCR	6	625	-	41,41,41	0.67	0	56,56,56	2.05	16 (28%)
22	CLA	8	603	15	45,53,73	2.41	18 (40%)	52,89,113	3.21	24 (46%)
22	CLA	B	816	2	55,63,73	2.15	15 (27%)	64,101,113	3.07	26 (40%)
22	CLA	A	808	1	65,73,73	2.02	17 (26%)	76,113,113	2.80	28 (36%)
22	CLA	2	613	19	50,58,73	2.39	16 (32%)	58,95,113	3.10	30 (51%)
22	CLA	8	616	15	46,54,73	2.41	17 (36%)	53,90,113	3.01	24 (45%)
22	CLA	3	610	13	65,73,73	1.99	15 (23%)	76,113,113	2.81	31 (40%)
22	CLA	B	811	2	54,62,73	2.14	16 (29%)	67,100,113	3.03	32 (47%)
22	CLA	A	806	1	65,73,73	2.01	15 (23%)	76,113,113	2.72	25 (32%)
25	BCR	A	848	-	41,41,41	0.71	0	56,56,56	1.76	15 (26%)
22	CLA	A	854	-	65,73,73	2.02	15 (23%)	76,113,113	2.81	28 (36%)
22	CLA	9	612	-	52,60,73	2.32	16 (30%)	60,97,113	3.00	27 (45%)
25	BCR	4	621	-	41,41,41	0.70	0	56,56,56	2.00	18 (32%)
22	CLA	8	611	24	46,54,73	2.42	17 (36%)	53,90,113	3.13	26 (49%)
29	CHL	7	607	-	54,62,74	2.20	17 (31%)	58,99,114	3.03	23 (39%)
22	CLA	7	606	-	42,50,73	2.41	15 (35%)	48,85,113	3.48	24 (50%)
30	LUT	9	617	-	42,43,43	0.75	0	51,60,60	1.60	13 (25%)
22	CLA	F	303	-	45,53,73	2.42	17 (37%)	52,89,113	3.21	22 (42%)
22	CLA	A	817	-	57,65,73	2.15	17 (29%)	66,103,113	2.94	26 (39%)
22	CLA	A	818	1	65,73,73	1.96	15 (23%)	76,113,113	2.85	26 (34%)
22	CLA	1	603	12	65,73,73	2.01	16 (24%)	76,113,113	2.76	27 (35%)
25	BCR	B	845	-	41,41,41	0.73	0	56,56,56	1.84	15 (26%)
22	CLA	5	602	17	65,73,73	2.00	15 (23%)	76,113,113	2.77	26 (34%)
22	CLA	8	609	15	46,54,73	2.42	16 (34%)	53,90,113	3.04	26 (49%)
22	CLA	Z	611	24	65,73,73	2.07	17 (26%)	76,113,113	2.65	26 (34%)
22	CLA	5	621	-	46,54,73	2.44	18 (39%)	53,90,113	2.96	25 (47%)
22	CLA	6	609	18	50,58,73	2.33	17 (34%)	58,95,113	3.04	26 (44%)
22	CLA	2	609	19	50,58,73	2.40	17 (34%)	58,95,113	3.05	29 (50%)
29	CHL	4	618	16	43,51,74	2.38	17 (39%)	45,86,114	3.57	22 (48%)
22	CLA	7	614	14	43,51,73	2.43	16 (37%)	49,86,113	3.35	26 (53%)
22	CLA	A	822	-	65,73,73	1.99	16 (24%)	76,113,113	2.57	26 (34%)
22	CLA	2	610	19	60,68,73	2.18	16 (26%)	70,107,113	2.86	27 (38%)
29	CHL	3	608	-	66,74,74	1.89	16 (24%)	73,114,114	2.86	24 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	LHG	1	620	22	42,42,48	0.99	2 (4%)	45,48,54	1.10	3 (6%)
22	CLA	8	606	-	42,50,73	2.46	17 (40%)	48,85,113	3.25	22 (45%)
30	LUT	3	621	-	42,43,43	0.77	0	51,60,60	1.52	13 (25%)
22	CLA	B	840	2	65,73,73	2.06	16 (24%)	76,113,113	2.82	25 (32%)
25	BCR	5	625	-	41,41,41	0.71	0	56,56,56	2.25	15 (26%)
22	CLA	Z	603	12	57,65,73	2.19	16 (28%)	66,103,113	2.94	31 (46%)
25	BCR	A	852	-	41,41,41	0.72	0	56,56,56	1.89	13 (23%)
25	BCR	8	619	-	41,41,41	0.71	0	56,56,56	1.83	15 (26%)
24	LHG	A	855	-	29,29,48	1.20	2 (6%)	32,35,54	1.17	3 (9%)
30	LUT	9	616	-	42,43,43	0.73	0	51,60,60	1.52	11 (21%)
22	CLA	9	604	20	50,58,73	2.39	17 (34%)	58,95,113	3.07	27 (46%)
25	BCR	A	849	-	41,41,41	0.78	0	56,56,56	1.80	17 (30%)
22	CLA	6	603	18	46,54,73	2.38	16 (34%)	53,90,113	3.23	26 (49%)
22	CLA	A	820	1	65,73,73	2.01	17 (26%)	76,113,113	2.79	29 (38%)
22	CLA	5	617	17	46,54,73	2.36	17 (36%)	53,90,113	4.43	25 (47%)
22	CLA	A	830	1	65,73,73	1.95	16 (24%)	76,113,113	2.63	26 (34%)
22	CLA	A	816	1	65,73,73	2.08	17 (26%)	76,113,113	2.68	26 (34%)
22	CLA	B	841	24	65,73,73	2.09	17 (26%)	76,113,113	2.78	28 (36%)
22	CLA	7	613	14	65,73,73	1.99	16 (24%)	76,113,113	2.65	23 (30%)
22	CLA	A	826	-	65,73,73	1.99	17 (26%)	76,113,113	2.71	26 (34%)
23	PQN	B	842	-	34,34,34	1.56	2 (5%)	42,45,45	0.94	2 (4%)
22	CLA	A	827	-	65,73,73	2.02	15 (23%)	76,113,113	2.70	27 (35%)
22	CLA	1	611	24	65,73,73	2.06	17 (26%)	76,113,113	2.65	25 (32%)
22	CLA	B	815	2	57,65,73	2.14	15 (26%)	66,103,113	2.92	27 (40%)
22	CLA	B	832	2	65,73,73	1.97	15 (23%)	76,113,113	2.76	27 (35%)
22	CLA	A	807	1	65,73,73	2.03	17 (26%)	76,113,113	2.74	25 (32%)
30	LUT	8	617	-	42,43,43	0.77	0	51,60,60	1.70	13 (25%)
22	CLA	3	603	13	65,73,73	1.98	17 (26%)	76,113,113	2.69	26 (34%)
28	LMG	J	3001	-	35,35,55	0.94	2 (5%)	43,43,63	1.23	5 (11%)
22	CLA	B	825	-	65,73,73	2.01	16 (24%)	76,113,113	2.65	28 (36%)
22	CLA	Z	609	12	65,73,73	2.07	16 (24%)	76,113,113	2.67	27 (35%)
22	CLA	A	836	1	50,58,73	2.33	18 (36%)	58,95,113	3.05	29 (50%)
22	CLA	A	811	1	65,73,73	2.00	15 (23%)	76,113,113	2.73	28 (36%)
22	CLA	A	833	1	65,73,73	2.05	16 (24%)	76,113,113	2.67	27 (35%)
22	CLA	3	614	13	45,53,73	2.49	16 (35%)	52,89,113	3.25	24 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	9	601	20	46,54,73	2.47	16 (34%)	53,90,113	3.14	24 (45%)
22	CLA	8	610	15	60,68,73	2.10	16 (26%)	70,107,113	2.85	31 (44%)
22	CLA	A	831	1	65,73,73	1.99	16 (24%)	76,113,113	2.77	29 (38%)
24	LHG	B	851	22	22,22,48	1.15	2 (9%)	25,28,54	1.24	2 (8%)
29	CHL	9	606	-	42,50,74	2.38	16 (38%)	44,85,114	3.67	23 (52%)
22	CLA	Z	608	-	65,73,73	2.04	17 (26%)	76,113,113	2.69	26 (34%)
23	PQN	A	844	-	34,34,34	1.52	2 (5%)	42,45,45	1.04	2 (4%)
22	CLA	4	609	16	50,58,73	2.30	16 (32%)	58,95,113	3.04	28 (48%)
29	CHL	4	607	-	51,59,74	2.26	16 (31%)	55,96,114	3.33	25 (45%)
22	CLA	B	818	2	60,68,73	2.09	16 (26%)	70,107,113	2.79	32 (45%)
22	CLA	6	604	-	65,73,73	2.05	18 (27%)	76,113,113	2.64	27 (35%)
22	CLA	7	612	14	52,60,73	2.25	16 (30%)	60,97,113	3.06	26 (43%)
22	CLA	4	604	-	50,58,73	2.34	16 (32%)	58,95,113	3.03	27 (46%)
22	CLA	7	604	-	56,64,73	2.16	17 (30%)	65,102,113	3.03	26 (40%)
24	LHG	A	846	-	48,48,48	0.91	2 (4%)	51,54,54	1.01	3 (5%)
22	CLA	1	612	12	52,60,73	2.26	16 (30%)	60,97,113	2.99	28 (46%)
22	CLA	1	608	-	65,73,73	2.01	16 (24%)	76,113,113	2.71	27 (35%)
22	CLA	B	820	2	56,64,73	2.24	16 (28%)	65,102,113	2.92	27 (41%)
22	CLA	8	604	-	46,54,73	2.39	17 (36%)	53,90,113	3.10	24 (45%)
22	CLA	2	614	-	45,53,73	2.51	16 (35%)	52,89,113	3.21	24 (46%)
30	LUT	1	617	-	42,43,43	0.75	0	51,60,60	1.69	13 (25%)
22	CLA	Z	610	12	60,68,73	2.09	15 (25%)	70,107,113	2.92	28 (40%)
22	CLA	B	822	2	59,67,73	2.12	17 (28%)	68,105,113	2.86	28 (41%)
24	LHG	7	625	22	36,36,48	1.02	2 (5%)	39,42,54	1.13	3 (7%)
22	CLA	5	603	17	46,54,73	2.38	17 (36%)	53,90,113	3.18	26 (49%)
22	CLA	9	611	-	55,63,73	2.27	16 (29%)	64,101,113	2.87	27 (42%)
25	BCR	A	856	-	41,41,41	0.74	0	56,56,56	1.77	13 (23%)
22	CLA	K	4003	10	46,54,73	2.43	15 (32%)	53,90,113	3.16	23 (43%)
22	CLA	6	610	-	60,68,73	2.14	16 (26%)	70,107,113	2.82	30 (42%)
22	CLA	5	612	17	52,60,73	2.26	17 (32%)	60,97,113	3.02	27 (45%)
22	CLA	Z	612	12	52,60,73	2.27	17 (32%)	60,97,113	3.07	26 (43%)
30	LUT	1	618	-	42,43,43	0.74	0	51,60,60	1.58	12 (23%)
22	CLA	B	813	2	65,73,73	2.00	16 (24%)	76,113,113	2.73	30 (39%)
26	SF4	A	853	2,1	0,12,12	-	-	-		
22	CLA	B	807	2	65,73,73	2.04	16 (24%)	76,113,113	2.74	27 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	LMG	9	620	-	44,44,55	0.85	2 (4%)	52,52,63	1.23	2 (3%)
22	CLA	2	601	19	46,54,73	2.45	16 (34%)	53,90,113	3.14	25 (47%)
22	CLA	4	601	16	61,69,73	2.08	16 (26%)	71,108,113	2.80	27 (38%)
25	BCR	B	843	-	41,41,41	0.72	0	56,56,56	1.56	8 (14%)
29	CHL	4	608	-	51,59,74	2.17	16 (31%)	55,96,114	3.26	24 (43%)
25	BCR	7	624	-	41,41,41	0.67	0	56,56,56	1.75	12 (21%)
22	CLA	A	845	24	52,60,73	2.29	16 (30%)	60,97,113	3.07	23 (38%)
29	CHL	4	606	-	56,64,74	2.12	17 (30%)	61,102,114	3.05	24 (39%)
22	CLA	3	611	-	41,49,73	2.55	16 (39%)	47,84,113	3.30	25 (53%)
22	CLA	8	601	15	65,73,73	2.03	18 (27%)	76,113,113	2.69	28 (36%)
30	LUT	Z	617	-	42,43,43	0.77	0	51,60,60	1.69	15 (29%)
27	DGD	B	850	-	67,67,67	0.80	2 (2%)	81,81,81	1.03	4 (4%)
30	LUT	4	619	-	42,43,43	0.71	0	51,60,60	1.67	11 (21%)
22	CLA	B	831	2	49,57,73	2.29	15 (30%)	55,93,113	3.11	22 (40%)
24	LHG	A	847	22	37,37,48	1.06	2 (5%)	40,43,54	1.26	4 (10%)
22	CLA	6	614	18	45,53,73	2.44	16 (35%)	52,89,113	3.31	26 (50%)
22	CLA	B	803	-	65,73,73	1.93	17 (26%)	76,113,113	2.59	26 (34%)
22	CLA	Z	616	12	46,54,73	2.44	17 (36%)	53,90,113	3.09	24 (45%)
22	CLA	B	810	2	65,73,73	2.05	17 (26%)	76,113,113	2.74	25 (32%)
22	CLA	B	838	2	47,55,73	2.35	17 (36%)	54,91,113	3.15	24 (44%)
22	CLA	B	827	2	65,73,73	2.00	17 (26%)	76,113,113	2.70	28 (36%)
22	CLA	A	814	1	65,73,73	2.00	17 (26%)	76,113,113	2.78	26 (34%)
22	CLA	F	301	-	65,73,73	2.02	16 (24%)	76,113,113	2.78	29 (38%)
30	LUT	Z	618	-	42,43,43	0.71	0	51,60,60	1.58	12 (23%)
29	CHL	Z	601	12	53,61,74	2.26	17 (32%)	57,98,114	3.26	22 (38%)
22	CLA	Z	602	12	65,73,73	2.00	18 (27%)	76,113,113	2.73	28 (36%)
22	CLA	A	812	1	65,73,73	1.99	18 (27%)	76,113,113	2.85	25 (32%)
25	BCR	3	719	-	41,41,41	0.69	0	56,56,56	1.64	13 (23%)
22	CLA	4	616	16	41,49,73	2.56	15 (36%)	47,84,113	3.46	25 (53%)
22	CLA	1	609	12	65,73,73	2.05	17 (26%)	76,113,113	2.73	26 (34%)
22	CLA	9	613	-	50,58,73	2.35	17 (34%)	58,95,113	3.00	27 (46%)
22	CLA	3	620	-	56,64,73	2.19	17 (30%)	65,102,113	2.88	26 (40%)
30	LUT	6	624	-	42,43,43	0.72	0	51,60,60	1.44	8 (15%)
22	CLA	6	611	24	55,63,73	2.24	18 (32%)	64,101,113	2.82	26 (40%)
25	BCR	B	844	-	41,41,41	0.71	0	56,56,56	1.75	11 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	B	834	2	65,73,73	2.07	15 (23%)	76,113,113	2.72	30 (39%)
22	CLA	3	617	13	46,54,73	2.41	16 (34%)	53,90,113	3.14	25 (47%)
25	BCR	A	851	-	41,41,41	0.81	2 (4%)	56,56,56	1.83	12 (21%)
22	CLA	A	828	1	65,73,73	1.98	17 (26%)	76,113,113	2.83	23 (30%)
22	CLA	A	840	1	65,73,73	1.98	18 (27%)	76,113,113	2.83	27 (35%)
22	CLA	A	805	1	55,63,73	2.22	17 (30%)	64,101,113	2.94	26 (40%)
25	BCR	I	172	-	41,41,41	0.67	0	56,56,56	1.97	15 (26%)
22	CLA	B	817	2	59,67,73	2.09	16 (27%)	68,105,113	2.83	26 (38%)
22	CLA	A	839	1	65,73,73	2.00	16 (24%)	76,113,113	2.77	27 (35%)
22	CLA	7	620	-	60,68,73	2.15	16 (26%)	70,107,113	2.79	28 (40%)
22	CLA	A	829	1	65,73,73	1.96	16 (24%)	76,113,113	2.73	29 (38%)
22	CLA	5	614	17	45,53,73	2.45	16 (35%)	52,89,113	3.30	26 (50%)
22	CLA	8	613	15	65,73,73	2.03	16 (24%)	76,113,113	2.60	25 (32%)
22	CLA	6	612	18	52,60,73	2.26	17 (32%)	60,97,113	3.00	25 (41%)
22	CLA	Z	614	12	65,73,73	2.07	16 (24%)	76,113,113	2.71	28 (36%)
24	LHG	4	622	22	48,48,48	0.96	2 (4%)	51,54,54	1.09	3 (5%)
22	CLA	K	4002	-	45,53,73	2.49	17 (37%)	52,89,113	3.18	26 (50%)
22	CLA	8	612	15	52,60,73	2.26	16 (30%)	60,97,113	3.00	29 (48%)
22	CLA	Z	613	-	65,73,73	2.04	15 (23%)	76,113,113	2.63	27 (35%)
22	CLA	1	616	12	46,54,73	2.42	17 (36%)	53,90,113	3.01	25 (47%)
22	CLA	A	813	1	54,62,73	2.22	16 (29%)	62,99,113	2.95	26 (41%)
30	LUT	5	624	-	42,43,43	0.77	0	51,60,60	1.54	11 (21%)
22	CLA	G	203	7	50,58,73	2.33	17 (34%)	58,95,113	3.19	28 (48%)
22	CLA	B	804	2	45,53,73	2.40	16 (35%)	52,89,113	3.29	27 (51%)
22	CLA	3	604	-	65,73,73	2.01	15 (23%)	76,113,113	2.67	25 (32%)
22	CLA	L	203	11	65,73,73	1.97	18 (27%)	76,113,113	2.77	26 (34%)
25	BCR	A	850	-	41,41,41	0.70	0	56,56,56	1.90	12 (21%)
22	CLA	6	601	18	65,73,73	2.02	16 (24%)	76,113,113	2.75	27 (35%)
22	CLA	7	602	14	65,73,73	2.02	16 (24%)	76,113,113	2.80	28 (36%)
22	CLA	6	616	18	46,54,73	2.45	17 (36%)	53,90,113	3.19	28 (52%)
29	CHL	Z	607	-	48,56,74	2.34	18 (37%)	51,92,114	3.20	23 (45%)
22	CLA	2	602	19	45,53,73	2.49	16 (35%)	52,89,113	3.19	24 (46%)
29	CHL	1	607	-	48,56,74	2.34	18 (37%)	51,92,114	3.13	20 (39%)
29	CHL	6	606	-	56,64,74	2.16	17 (30%)	61,102,114	3.15	25 (40%)
22	CLA	2	607	-	50,58,73	2.39	16 (32%)	58,95,113	3.07	27 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	5	609	17	50,58,73	2.32	17 (34%)	58,95,113	3.10	27 (46%)
22	CLA	B	821	2	46,54,73	2.41	17 (36%)	53,90,113	3.14	23 (43%)
22	CLA	L	204	-	50,58,73	2.36	16 (32%)	58,95,113	3.08	25 (43%)
22	CLA	A	834	1	65,73,73	2.02	17 (26%)	76,113,113	2.79	29 (38%)
22	CLA	B	814	2	60,68,73	2.09	16 (26%)	70,107,113	2.76	29 (41%)
22	CLA	1	610	12	60,68,73	2.10	15 (25%)	70,107,113	2.90	31 (44%)
22	CLA	6	622	18	45,53,73	2.42	17 (37%)	52,89,113	3.20	25 (48%)
22	CLA	5	610	17	60,68,73	2.11	16 (26%)	70,107,113	2.85	30 (42%)
22	CLA	B	805	2	65,73,73	1.99	16 (24%)	76,113,113	2.79	26 (34%)
22	CLA	8	608	-	50,58,73	2.25	16 (32%)	58,95,113	3.14	25 (43%)
25	BCR	3	718	-	41,41,41	0.74	0	56,56,56	1.90	17 (30%)
22	CLA	1	604	-	57,65,73	2.18	17 (29%)	66,103,113	2.82	29 (43%)
22	CLA	1	606	-	52,60,73	2.28	17 (32%)	60,97,113	2.99	27 (45%)
22	CLA	8	602	15	62,70,73	2.02	15 (24%)	72,109,113	2.87	28 (38%)
25	BCR	F	305	-	41,41,41	0.69	0	56,56,56	1.88	13 (23%)
22	CLA	B	829	2	65,73,73	2.05	17 (26%)	76,113,113	2.86	30 (39%)
22	CLA	2	611	-	55,63,73	2.27	16 (29%)	64,101,113	2.88	28 (43%)
26	SF4	C	102	3	0,12,12	-	-	-		
24	LHG	8	620	22	36,36,48	1.02	2 (5%)	39,42,54	1.14	5 (12%)
22	CLA	B	836	2	60,68,73	2.13	17 (28%)	70,107,113	2.89	29 (41%)
22	CLA	1	614	12	65,73,73	2.05	17 (26%)	76,113,113	2.77	25 (32%)
22	CLA	A	841	1	65,73,73	2.01	17 (26%)	76,113,113	2.79	28 (36%)
29	CHL	6	618	18	43,51,74	2.36	15 (34%)	45,86,114	3.52	23 (51%)
30	LUT	7	621	-	42,43,43	0.73	0	51,60,60	1.53	10 (19%)
22	CLA	7	609	14	50,58,73	2.32	16 (32%)	58,95,113	3.11	27 (46%)
22	CLA	B	802	2	65,73,73	1.92	17 (26%)	76,113,113	2.84	27 (35%)
25	BCR	L	205	-	41,41,41	0.71	0	56,56,56	1.60	12 (21%)
30	LUT	3	622	-	42,43,43	0.80	0	51,60,60	1.67	10 (19%)
22	CLA	A	838	1	51,59,73	2.28	16 (31%)	59,96,113	3.13	30 (50%)
22	CLA	F	304	6	65,73,73	2.06	18 (27%)	76,113,113	2.72	25 (32%)
22	CLA	B	835	-	45,53,73	2.45	17 (37%)	52,89,113	3.08	25 (48%)
22	CLA	5	601	17	65,73,73	2.06	17 (26%)	76,113,113	2.72	29 (38%)
22	CLA	B	809	2	65,73,73	1.97	14 (21%)	76,113,113	2.67	28 (36%)
22	CLA	B	819	-	65,73,73	2.02	16 (24%)	76,113,113	2.58	27 (35%)
22	CLA	9	602	20	60,68,73	2.12	15 (25%)	70,107,113	2.83	28 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	BCR	3	717	-	41,41,41	0.75	0	56,56,56	1.87	16 (28%)
22	CLA	4	603	16	46,54,73	2.38	16 (34%)	53,90,113	3.18	25 (47%)
22	CLA	A	837	1	45,53,73	2.49	17 (37%)	52,89,113	3.08	26 (50%)
30	LUT	2	616	-	42,43,43	0.75	0	51,60,60	1.72	15 (29%)
22	CLA	B	839	-	65,73,73	2.05	18 (27%)	76,113,113	2.66	26 (34%)
22	CLA	2	606	-	41,49,73	2.58	16 (39%)	47,84,113	3.36	26 (55%)
30	LUT	Z	619	-	42,43,43	0.71	0	51,60,60	1.76	12 (23%)
30	LUT	1	619	-	42,43,43	0.76	0	51,60,60	1.83	14 (27%)
22	CLA	A	815	1	60,68,73	2.17	17 (28%)	70,107,113	2.88	27 (38%)
22	CLA	A	843	-	65,73,73	2.01	18 (27%)	76,113,113	2.61	27 (35%)
22	CLA	6	613	-	56,64,73	2.22	17 (30%)	65,102,113	2.84	27 (41%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	3	607	13	1/1/14/20	15/31/109/115	-
25	BCR	G	205	-	-	2/29/63/63	0/2/2/2
22	CLA	G	204	7	1/1/11/20	5/15/93/115	-
22	CLA	A	825	1	-	7/25/103/115	-
22	CLA	3	609	13	1/1/12/20	5/19/97/115	-
22	CLA	1	613	-	1/1/15/20	7/37/115/115	-
22	CLA	B	806	2	1/1/15/20	13/37/115/115	-
22	CLA	7	610	14	1/1/14/20	6/31/109/115	-
25	BCR	6	623	-	-	9/29/63/63	0/2/2/2
25	BCR	K	4001	-	-	5/29/63/63	0/2/2/2
29	CHL	1	601	12	3/3/17/26	11/24/122/137	-
22	CLA	7	611	24	1/1/10/20	2/8/86/115	-
22	CLA	4	614	16	1/1/11/20	2/13/91/115	-
22	CLA	1	602	12	1/1/15/20	13/37/115/115	-
22	CLA	A	832	1	1/1/12/20	2/19/97/115	-
25	BCR	J	3003	-	-	8/29/63/63	0/2/2/2
24	LHG	Z	620	22	-	15/47/47/53	-
22	CLA	4	611	24	1/1/13/20	8/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	LHG	4	623	-	-	9/36/36/53	-
25	BCR	B	847	-	-	7/29/63/63	0/2/2/2
22	CLA	3	613	13	-	14/25/103/115	-
29	CHL	6	607	-	2/2/18/26	12/27/125/137	-
22	CLA	5	616	17	1/1/11/20	7/15/93/115	-
22	CLA	A	835	1	1/1/15/20	4/37/115/115	-
22	CLA	Z	604	-	1/1/13/20	9/28/106/115	-
22	CLA	A	809	1	1/1/15/20	17/37/115/115	-
22	CLA	Z	606	-	1/1/12/20	4/22/100/115	-
22	CLA	4	613	16	-	10/27/105/115	-
22	CLA	5	606	-	1/1/13/20	5/25/103/115	-
25	BCR	L	201	-	-	8/29/63/63	0/2/2/2
22	CLA	2	603	19	1/1/11/20	6/15/93/115	-
22	CLA	5	611	24	1/1/13/20	7/25/103/115	-
24	LHG	6	619	22	-	11/53/53/53	-
22	CLA	A	823	1	-	10/18/96/115	-
22	CLA	3	612	13	1/1/11/20	2/15/93/115	-
22	CLA	A	824	1	1/1/12/20	8/21/99/115	-
22	CLA	2	612	19	1/1/12/20	5/22/100/115	-
22	CLA	B	812	2	1/1/15/20	14/37/115/115	-
24	LHG	5	623	22	-	10/41/41/53	-
22	CLA	4	612	16	1/1/12/20	3/22/100/115	-
30	LUT	8	618	-	-	4/29/67/67	0/2/2/2
22	CLA	3	602	13	1/1/14/20	8/31/109/115	-
30	LUT	7	622	-	-	3/29/67/67	0/2/2/2
25	BCR	7	623	-	-	7/29/63/63	0/2/2/2
29	CHL	6	608	-	3/3/17/26	4/21/119/137	-
30	LUT	6	621	-	-	2/29/67/67	0/2/2/2
22	CLA	B	828	2	1/1/15/20	9/37/115/115	-
22	CLA	B	837	2	1/1/15/20	11/37/115/115	-
22	CLA	A	804	1	1/1/15/20	12/37/115/115	-
25	BCR	B	846	-	-	5/29/63/63	0/2/2/2
22	CLA	A	810	1	-	11/37/115/115	-
25	BCR	5	622	-	-	7/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CHL	5	618	17	3/3/15/26	4/12/110/137	-
22	CLA	9	603	20	1/1/11/20	1/15/93/115	-
29	CHL	5	607	-	3/3/17/26	10/21/119/137	-
22	CLA	J	3002	9	1/1/10/20	3/10/88/115	-
22	CLA	B	808	2	1/1/15/20	10/37/115/115	-
22	CLA	A	842	1	1/1/15/20	16/37/115/115	-
22	CLA	A	821	1	1/1/11/20	2/13/91/115	-
25	BCR	B	801	-	-	9/29/63/63	0/2/2/2
22	CLA	5	613	17	1/1/13/20	8/27/105/115	-
22	CLA	B	833	2	1/1/13/20	8/29/107/115	-
25	BCR	B	848	-	-	3/29/63/63	0/2/2/2
21	CL0	A	801	1	2/2/20/25	6/37/135/135	-
22	CLA	4	610	16	1/1/14/20	9/31/109/115	-
25	BCR	K	4004	-	-	5/29/63/63	0/2/2/2
22	CLA	9	609	-	1/1/12/20	0/19/97/115	-
29	CHL	9	607	-	3/3/17/26	7/21/119/137	-
22	CLA	A	803	-	1/1/15/20	4/37/115/115	-
22	CLA	B	823	2	1/1/14/20	8/31/109/115	-
22	CLA	7	601	14	1/1/15/20	16/37/115/115	-
22	CLA	7	603	14	1/1/11/20	2/15/93/115	-
29	CHL	8	607	-	3/3/18/26	11/27/125/137	-
22	CLA	B	824	-	1/1/15/20	9/37/115/115	-
26	SF4	C	101	3	-	-	0/6/5/5
22	CLA	B	852	-	1/1/15/20	5/37/115/115	-
22	CLA	6	602	18	1/1/15/20	13/37/115/115	-
30	LUT	5	620	-	-	0/29/67/67	0/2/2/2
30	LUT	2	617	-	-	3/29/67/67	0/2/2/2
22	CLA	9	614	20	-	4/13/91/115	-
22	CLA	A	802	-	1/1/15/20	5/37/115/115	-
22	CLA	B	830	2	-	3/19/97/115	-
22	CLA	5	604	17	-	5/19/97/115	-
22	CLA	8	614	15	1/1/13/20	6/25/103/115	-
22	CLA	A	819	1	1/1/15/20	12/37/115/115	-
22	CLA	B	826	2	1/1/15/20	9/37/115/115	-
22	CLA	7	616	14	1/1/11/20	5/15/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CHL	5	608	-	3/3/17/26	8/21/119/137	-
30	LUT	4	620	-	-	3/29/67/67	0/2/2/2
22	CLA	9	610	20	-	4/31/109/115	-
22	CLA	6	617	18	1/1/11/20	3/15/93/115	-
22	CLA	4	602	16	-	12/31/109/115	-
22	CLA	3	606	-	1/1/10/20	0/10/88/115	-
22	CLA	7	608	-	-	3/19/97/115	-
25	BCR	6	625	-	-	9/29/63/63	0/2/2/2
22	CLA	8	603	15	1/1/11/20	2/13/91/115	-
22	CLA	B	816	2	1/1/13/20	8/25/103/115	-
22	CLA	A	808	1	1/1/15/20	10/37/115/115	-
22	CLA	2	613	19	-	3/19/97/115	-
22	CLA	8	616	15	1/1/11/20	2/15/93/115	-
22	CLA	3	610	13	1/1/15/20	14/37/115/115	-
22	CLA	B	811	2	1/1/13/20	5/25/101/115	-
22	CLA	A	806	1	1/1/15/20	16/37/115/115	-
25	BCR	A	848	-	-	4/29/63/63	0/2/2/2
22	CLA	A	854	-	1/1/15/20	12/37/115/115	-
22	CLA	9	612	-	1/1/12/20	4/22/100/115	-
25	BCR	4	621	-	-	3/29/63/63	0/2/2/2
22	CLA	8	611	24	1/1/11/20	3/15/93/115	-
29	CHL	7	607	-	3/3/17/26	9/25/123/137	-
22	CLA	7	606	-	1/1/10/20	7/10/88/115	-
30	LUT	9	617	-	-	2/29/67/67	0/2/2/2
22	CLA	F	303	-	1/1/11/20	4/13/91/115	-
22	CLA	A	817	-	1/1/13/20	6/28/106/115	-
22	CLA	A	818	1	-	14/37/115/115	-
22	CLA	1	603	12	1/1/15/20	8/37/115/115	-
25	BCR	B	845	-	-	10/29/63/63	0/2/2/2
22	CLA	5	602	17	-	10/37/115/115	-
22	CLA	8	609	15	1/1/11/20	3/15/93/115	-
22	CLA	Z	611	24	1/1/15/20	16/37/115/115	-
22	CLA	5	621	-	1/1/11/20	3/15/93/115	-
22	CLA	6	609	18	1/1/12/20	4/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	2	609	19	1/1/12/20	4/19/97/115	-
29	CHL	4	618	16	3/3/15/26	4/12/110/137	-
22	CLA	7	614	14	1/1/10/20	2/11/89/115	-
22	CLA	A	822	-	1/1/15/20	13/37/115/115	-
22	CLA	2	610	19	-	11/31/109/115	-
29	CHL	3	608	-	3/3/20/26	22/39/137/137	-
24	LHG	1	620	22	-	14/47/47/53	-
22	CLA	8	606	-	1/1/10/20	4/10/88/115	-
30	LUT	3	621	-	-	5/29/67/67	0/2/2/2
22	CLA	B	840	2	-	6/37/115/115	-
25	BCR	5	625	-	-	7/29/63/63	0/2/2/2
22	CLA	Z	603	12	1/1/13/20	9/28/106/115	-
25	BCR	A	852	-	-	7/29/63/63	0/2/2/2
25	BCR	8	619	-	-	6/29/63/63	0/2/2/2
24	LHG	A	855	-	-	10/34/34/53	-
30	LUT	9	616	-	-	2/29/67/67	0/2/2/2
22	CLA	9	604	20	-	6/19/97/115	-
25	BCR	A	849	-	-	3/29/63/63	0/2/2/2
22	CLA	6	603	18	1/1/11/20	1/15/93/115	-
22	CLA	A	820	1	1/1/15/20	14/37/115/115	-
22	CLA	5	617	17	1/1/11/20	4/15/93/115	-
22	CLA	A	830	1	1/1/15/20	8/37/115/115	-
22	CLA	A	816	1	1/1/15/20	10/37/115/115	-
22	CLA	B	841	24	1/1/15/20	5/37/115/115	-
22	CLA	7	613	14	-	10/37/115/115	-
22	CLA	A	826	-	1/1/15/20	16/37/115/115	-
23	PQN	B	842	-	-	4/23/43/43	0/2/2/2
22	CLA	A	827	-	1/1/15/20	6/37/115/115	-
22	CLA	1	611	24	1/1/15/20	10/37/115/115	-
22	CLA	B	815	2	1/1/13/20	6/28/106/115	-
22	CLA	B	832	2	1/1/15/20	9/37/115/115	-
22	CLA	A	807	1	1/1/15/20	18/37/115/115	-
30	LUT	8	617	-	-	2/29/67/67	0/2/2/2
22	CLA	3	603	13	1/1/15/20	7/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LMG	J	3001	-	-	12/30/50/70	0/1/1/1
22	CLA	B	825	-	1/1/15/20	7/37/115/115	-
22	CLA	Z	609	12	1/1/15/20	4/37/115/115	-
22	CLA	A	836	1	-	2/19/97/115	-
22	CLA	A	811	1	1/1/15/20	8/37/115/115	-
22	CLA	A	833	1	1/1/15/20	10/37/115/115	-
22	CLA	3	614	13	-	2/13/91/115	-
22	CLA	9	601	20	1/1/11/20	6/15/93/115	-
22	CLA	8	610	15	1/1/14/20	12/31/109/115	-
22	CLA	A	831	1	1/1/15/20	14/37/115/115	-
24	LHG	B	851	22	-	12/26/26/53	-
29	CHL	9	606	-	3/3/15/26	4/10/108/137	-
22	CLA	Z	608	-	1/1/15/20	17/37/115/115	-
23	PQN	A	844	-	-	12/23/43/43	0/2/2/2
22	CLA	4	609	16	1/1/12/20	7/19/97/115	-
29	CHL	4	607	-	3/3/17/26	7/21/119/137	-
22	CLA	B	818	2	1/1/14/20	12/31/109/115	-
22	CLA	6	604	-	1/1/15/20	11/37/115/115	-
22	CLA	7	612	14	1/1/12/20	7/22/100/115	-
22	CLA	4	604	-	-	4/19/97/115	-
22	CLA	7	604	-	1/1/13/20	9/27/105/115	-
24	LHG	A	846	-	-	16/53/53/53	-
22	CLA	1	612	12	1/1/12/20	8/22/100/115	-
22	CLA	1	608	-	1/1/15/20	11/37/115/115	-
22	CLA	B	820	2	1/1/13/20	6/27/105/115	-
22	CLA	8	604	-	1/1/11/20	3/15/93/115	-
22	CLA	2	614	-	-	2/13/91/115	-
30	LUT	1	617	-	-	2/29/67/67	0/2/2/2
22	CLA	Z	610	12	1/1/14/20	14/31/109/115	-
22	CLA	B	822	2	-	8/30/108/115	-
24	LHG	7	625	22	-	10/41/41/53	-
22	CLA	5	603	17	1/1/11/20	1/15/93/115	-
22	CLA	9	611	-	1/1/13/20	10/25/103/115	-
25	BCR	A	856	-	-	7/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	K	4003	10	1/1/11/20	3/15/93/115	-
22	CLA	6	610	-	1/1/14/20	9/31/109/115	-
22	CLA	5	612	17	1/1/12/20	3/22/100/115	-
22	CLA	Z	612	12	1/1/12/20	6/22/100/115	-
30	LUT	1	618	-	-	3/29/67/67	0/2/2/2
22	CLA	B	813	2	1/1/15/20	13/37/115/115	-
26	SF4	A	853	2,1	-	-	0/6/5/5
22	CLA	B	807	2	1/1/15/20	11/37/115/115	-
28	LMG	9	620	-	-	16/39/59/70	0/1/1/1
22	CLA	2	601	19	1/1/11/20	7/15/93/115	-
22	CLA	4	601	16	1/1/14/20	11/33/111/115	-
25	BCR	B	843	-	-	10/29/63/63	0/2/2/2
29	CHL	4	608	-	3/3/17/26	6/21/119/137	-
25	BCR	7	624	-	-	4/29/63/63	0/2/2/2
22	CLA	A	845	24	1/1/12/20	15/22/100/115	-
22	CLA	3	611	-	1/1/10/20	2/8/86/115	-
22	CLA	8	601	15	1/1/15/20	13/37/115/115	-
29	CHL	4	606	-	3/3/18/26	3/27/125/137	-
30	LUT	Z	617	-	-	4/29/67/67	0/2/2/2
27	DGD	B	850	-	-	17/55/95/95	0/2/2/2
30	LUT	4	619	-	-	2/29/67/67	0/2/2/2
22	CLA	B	831	2	1/1/11/20	5/18/96/115	-
24	LHG	A	847	22	-	14/42/42/53	-
22	CLA	6	614	18	1/1/11/20	4/13/91/115	-
22	CLA	B	803	-	1/1/15/20	6/37/115/115	-
22	CLA	Z	616	12	1/1/11/20	4/15/93/115	-
22	CLA	B	810	2	1/1/15/20	11/37/115/115	-
22	CLA	B	838	2	1/1/11/20	4/16/94/115	-
22	CLA	B	827	2	1/1/15/20	16/37/115/115	-
22	CLA	A	814	1	1/1/15/20	15/37/115/115	-
22	CLA	F	301	-	1/1/15/20	10/37/115/115	-
30	LUT	Z	618	-	-	4/29/67/67	0/2/2/2
29	CHL	Z	601	12	3/3/17/26	11/24/122/137	-
22	CLA	Z	602	12	-	10/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	A	812	1	1/1/15/20	13/37/115/115	-
25	BCR	3	719	-	-	4/29/63/63	0/2/2/2
22	CLA	4	616	16	1/1/10/20	0/8/86/115	-
22	CLA	1	609	12	1/1/15/20	7/37/115/115	-
22	CLA	9	613	-	1/1/12/20	8/19/97/115	-
22	CLA	3	620	-	1/1/13/20	8/27/105/115	-
30	LUT	6	624	-	-	3/29/67/67	0/2/2/2
22	CLA	6	611	24	1/1/13/20	7/25/103/115	-
25	BCR	B	844	-	-	7/29/63/63	0/2/2/2
22	CLA	B	834	2	1/1/15/20	13/37/115/115	-
22	CLA	3	617	13	1/1/11/20	3/15/93/115	-
25	BCR	A	851	-	-	4/29/63/63	0/2/2/2
22	CLA	A	828	1	1/1/15/20	11/37/115/115	-
22	CLA	A	840	1	1/1/15/20	8/37/115/115	-
22	CLA	A	805	1	1/1/13/20	8/25/103/115	-
25	BCR	I	172	-	-	6/29/63/63	0/2/2/2
22	CLA	B	817	2	1/1/13/20	12/30/108/115	-
22	CLA	A	839	1	1/1/15/20	11/37/115/115	-
22	CLA	7	620	-	1/1/14/20	8/31/109/115	-
22	CLA	A	829	1	1/1/15/20	19/37/115/115	-
22	CLA	5	614	17	-	1/13/91/115	-
22	CLA	8	613	15	-	12/37/115/115	-
22	CLA	6	612	18	1/1/12/20	5/22/100/115	-
22	CLA	Z	614	12	1/1/15/20	9/37/115/115	-
24	LHG	4	622	22	-	19/53/53/53	-
22	CLA	K	4002	-	-	6/13/91/115	-
22	CLA	8	612	15	1/1/12/20	6/22/100/115	-
22	CLA	Z	613	-	1/1/15/20	11/37/115/115	-
22	CLA	1	616	12	1/1/11/20	3/15/93/115	-
22	CLA	A	813	1	1/1/12/20	7/24/102/115	-
30	LUT	5	624	-	-	3/29/67/67	0/2/2/2
22	CLA	G	203	7	1/1/12/20	3/19/97/115	-
22	CLA	B	804	2	1/1/11/20	4/13/91/115	-
22	CLA	3	604	-	1/1/15/20	9/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	L	203	11	-	10/37/115/115	-
25	BCR	A	850	-	-	4/29/63/63	0/2/2/2
22	CLA	6	601	18	1/1/15/20	14/37/115/115	-
22	CLA	7	602	14	1/1/15/20	12/37/115/115	-
22	CLA	6	616	18	1/1/11/20	2/15/93/115	-
29	CHL	Z	607	-	3/3/16/26	4/18/116/137	-
22	CLA	2	602	19	-	4/13/91/115	-
29	CHL	1	607	-	3/3/16/26	7/18/116/137	-
29	CHL	6	606	-	3/3/18/26	8/27/125/137	-
22	CLA	2	607	-	-	5/19/97/115	-
22	CLA	5	609	17	1/1/12/20	4/19/97/115	-
22	CLA	B	821	2	-	4/15/93/115	-
22	CLA	L	204	-	-	5/19/97/115	-
22	CLA	A	834	1	1/1/15/20	10/37/115/115	-
22	CLA	B	814	2	1/1/14/20	11/31/109/115	-
22	CLA	1	610	12	1/1/14/20	12/31/109/115	-
22	CLA	6	622	18	1/1/11/20	3/13/91/115	-
22	CLA	5	610	17	1/1/14/20	7/31/109/115	-
22	CLA	B	805	2	1/1/15/20	14/37/115/115	-
22	CLA	8	608	-	1/1/12/20	1/19/97/115	-
25	BCR	3	718	-	-	4/29/63/63	0/2/2/2
22	CLA	1	604	-	1/1/13/20	8/28/106/115	-
22	CLA	1	606	-	1/1/12/20	5/22/100/115	-
22	CLA	8	602	15	1/1/14/20	10/34/112/115	-
25	BCR	F	305	-	-	2/29/63/63	0/2/2/2
22	CLA	B	829	2	1/1/15/20	9/37/115/115	-
22	CLA	2	611	-	-	7/25/103/115	-
26	SF4	C	102	3	-	-	0/6/5/5
24	LHG	8	620	22	-	14/41/41/53	-
22	CLA	B	836	2	1/1/14/20	5/31/109/115	-
22	CLA	1	614	12	1/1/15/20	13/37/115/115	-
22	CLA	A	841	1	1/1/15/20	9/37/115/115	-
29	CHL	6	618	18	3/3/15/26	6/12/110/137	-
30	LUT	7	621	-	-	3/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	7	609	14	1/1/12/20	5/19/97/115	-
22	CLA	B	802	2	1/1/15/20	9/37/115/115	-
25	BCR	L	205	-	-	9/29/63/63	0/2/2/2
30	LUT	3	622	-	-	2/29/67/67	0/2/2/2
22	CLA	A	838	1	1/1/12/20	5/21/99/115	-
22	CLA	F	304	6	1/1/15/20	9/37/115/115	-
22	CLA	B	835	-	1/1/11/20	5/13/91/115	-
22	CLA	5	601	17	1/1/15/20	9/37/115/115	-
22	CLA	B	809	2	1/1/15/20	12/37/115/115	-
22	CLA	B	819	-	1/1/15/20	9/37/115/115	-
22	CLA	9	602	20	1/1/14/20	9/31/109/115	-
25	BCR	3	717	-	-	5/29/63/63	0/2/2/2
22	CLA	4	603	16	1/1/11/20	2/15/93/115	-
22	CLA	A	837	1	1/1/11/20	9/13/91/115	-
30	LUT	2	616	-	-	0/29/67/67	0/2/2/2
22	CLA	B	839	-	1/1/15/20	7/37/115/115	-
22	CLA	2	606	-	1/1/10/20	1/8/86/115	-
30	LUT	Z	619	-	-	4/29/67/67	0/2/2/2
30	LUT	1	619	-	-	2/29/67/67	0/2/2/2
22	CLA	A	815	1	1/1/14/20	11/31/109/115	-
22	CLA	A	843	-	1/1/15/20	17/37/115/115	-
22	CLA	6	613	-	1/1/13/20	4/27/105/115	-

The worst 5 of 3969 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	842	PQN	C3-C2	7.50	1.48	1.35
23	A	844	PQN	C3-C2	7.35	1.48	1.35
22	B	836	CLA	C3B-C2B	6.40	1.49	1.40
22	3	602	CLA	C3B-C2B	6.31	1.49	1.40
22	5	621	CLA	C3B-C2B	6.19	1.49	1.40

The worst 5 of 7074 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	5	617	CLA	O2A-CGA-O1A	-13.94	79.44	123.14
22	5	617	CLA	O2A-CGA-CBA	12.13	160.18	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	6	608	CHL	C4A-NA-C1A	-11.78	101.41	106.71
22	5	617	CLA	O1A-CGA-CBA	-11.02	80.75	123.73
29	Z	601	CHL	C4A-NA-C1A	-10.94	101.79	106.71

5 of 246 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
21	A	801	CL0	ND
21	A	801	CL0	NC
22	A	802	CLA	ND
22	A	803	CLA	ND
22	A	804	CLA	ND

5 of 2298 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A	804	CLA	CHA-CBD-CGD-O1D
22	A	804	CLA	CHA-CBD-CGD-O2D
22	A	804	CLA	CAD-CBD-CGD-O1D
22	A	809	CLA	C3A-C2A-CAA-CBA
22	A	809	CLA	CHA-CBD-CGD-O2D

There are no ring outliers.

274 monomers are involved in 852 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	3	607	CLA	4	0
25	G	205	BCR	3	0
22	A	825	CLA	3	0
22	3	609	CLA	1	0
22	1	613	CLA	2	0
22	B	806	CLA	2	0
22	7	610	CLA	2	0
25	6	623	BCR	8	0
25	K	4001	BCR	5	0
29	1	601	CHL	1	0
22	7	611	CLA	1	0
22	4	614	CLA	4	0
22	1	602	CLA	9	0
22	A	832	CLA	5	0
25	J	3003	BCR	2	0
24	Z	620	LHG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	4	611	CLA	6	0
25	B	847	BCR	4	0
22	3	613	CLA	2	0
29	6	607	CHL	5	0
22	5	616	CLA	1	0
22	A	835	CLA	23	0
22	Z	604	CLA	1	0
22	A	809	CLA	4	0
22	Z	606	CLA	2	0
22	4	613	CLA	3	0
22	5	606	CLA	4	0
25	L	201	BCR	7	0
24	6	619	LHG	19	0
22	A	823	CLA	3	0
22	3	612	CLA	2	0
22	A	824	CLA	1	0
22	2	612	CLA	1	0
22	B	812	CLA	8	0
22	4	612	CLA	1	0
30	8	618	LUT	5	0
22	3	602	CLA	1	0
30	7	622	LUT	2	0
25	7	623	BCR	5	0
29	6	608	CHL	1	0
30	6	621	LUT	4	0
22	B	828	CLA	3	0
22	B	837	CLA	4	0
22	A	804	CLA	2	0
25	B	846	BCR	6	0
25	5	622	BCR	5	0
22	9	603	CLA	1	0
29	5	607	CHL	3	0
22	J	3002	CLA	1	0
22	B	808	CLA	1	0
22	A	842	CLA	10	0
22	A	821	CLA	1	0
25	B	801	BCR	6	0
22	5	613	CLA	3	0
22	B	833	CLA	3	0
25	B	848	BCR	3	0
21	A	801	CL0	3	0
22	4	610	CLA	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	K	4004	BCR	1	0
22	9	609	CLA	11	0
29	9	607	CHL	1	0
22	A	803	CLA	2	0
22	B	823	CLA	4	0
22	7	601	CLA	4	0
22	B	824	CLA	1	0
22	6	602	CLA	1	0
30	5	620	LUT	15	0
30	2	617	LUT	3	0
22	9	614	CLA	2	0
22	A	802	CLA	26	0
22	B	830	CLA	3	0
22	5	604	CLA	2	0
22	8	614	CLA	5	0
22	A	819	CLA	3	0
22	B	826	CLA	2	0
22	7	616	CLA	1	0
29	5	608	CHL	3	0
30	4	620	LUT	4	0
22	9	610	CLA	1	0
22	4	602	CLA	1	0
22	3	606	CLA	3	0
22	7	608	CLA	2	0
25	6	625	BCR	3	0
22	B	816	CLA	5	0
22	A	808	CLA	2	0
22	2	613	CLA	9	0
22	8	616	CLA	1	0
22	3	610	CLA	3	0
22	B	811	CLA	3	0
22	A	806	CLA	5	0
25	A	848	BCR	5	0
22	A	854	CLA	5	0
22	9	612	CLA	1	0
25	4	621	BCR	39	0
29	7	607	CHL	1	0
22	7	606	CLA	2	0
30	9	617	LUT	4	0
22	F	303	CLA	2	0
22	A	817	CLA	5	0
22	A	818	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	1	603	CLA	3	0
25	B	845	BCR	3	0
22	5	602	CLA	4	0
22	8	609	CLA	2	0
22	Z	611	CLA	2	0
22	5	621	CLA	1	0
22	6	609	CLA	2	0
29	4	618	CHL	7	0
22	7	614	CLA	1	0
22	A	822	CLA	2	0
22	2	610	CLA	2	0
29	3	608	CHL	5	0
24	1	620	LHG	2	0
22	8	606	CLA	2	0
30	3	621	LUT	4	0
22	B	840	CLA	4	0
25	5	625	BCR	7	0
22	Z	603	CLA	1	0
25	A	852	BCR	3	0
25	8	619	BCR	6	0
30	9	616	LUT	4	0
25	A	849	BCR	5	0
22	A	820	CLA	4	0
22	5	617	CLA	6	0
22	A	830	CLA	3	0
22	A	816	CLA	7	0
22	B	841	CLA	13	0
22	7	613	CLA	3	0
22	A	826	CLA	2	0
23	B	842	PQN	1	0
22	A	827	CLA	1	0
22	1	611	CLA	1	0
22	B	815	CLA	3	0
22	B	832	CLA	5	0
22	A	807	CLA	9	0
30	8	617	LUT	8	0
22	3	603	CLA	4	0
22	B	825	CLA	5	0
22	Z	609	CLA	1	0
22	A	836	CLA	2	0
22	A	811	CLA	4	0
22	A	833	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	3	614	CLA	3	0
22	8	610	CLA	6	0
22	A	831	CLA	8	0
22	Z	608	CLA	4	0
23	A	844	PQN	4	0
29	4	607	CHL	1	0
22	B	818	CLA	4	0
22	6	604	CLA	4	0
22	7	612	CLA	1	0
22	4	604	CLA	6	0
22	7	604	CLA	1	0
24	A	846	LHG	2	0
22	1	608	CLA	5	0
22	B	820	CLA	15	0
22	8	604	CLA	1	0
30	1	617	LUT	7	0
22	Z	610	CLA	3	0
22	B	822	CLA	1	0
22	5	603	CLA	1	0
22	9	611	CLA	1	0
25	A	856	BCR	5	0
22	K	4003	CLA	2	0
22	6	610	CLA	5	0
22	5	612	CLA	2	0
22	Z	612	CLA	1	0
30	1	618	LUT	5	0
22	B	813	CLA	5	0
22	B	807	CLA	2	0
28	9	620	LMG	1	0
22	2	601	CLA	5	0
22	4	601	CLA	6	0
25	B	843	BCR	5	0
29	4	608	CHL	8	0
25	7	624	BCR	1	0
22	A	845	CLA	1	0
29	4	606	CHL	10	0
22	8	601	CLA	1	0
30	Z	617	LUT	4	0
27	B	850	DGD	1	0
30	4	619	LUT	12	0
22	B	831	CLA	6	0
24	A	847	LHG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	6	614	CLA	2	0
22	B	803	CLA	4	0
22	B	838	CLA	3	0
22	B	827	CLA	4	0
22	A	814	CLA	2	0
22	F	301	CLA	4	0
30	Z	618	LUT	4	0
29	Z	601	CHL	1	0
22	Z	602	CLA	3	0
22	A	812	CLA	15	0
25	3	719	BCR	6	0
22	4	616	CLA	6	0
22	1	609	CLA	2	0
22	9	613	CLA	1	0
22	3	620	CLA	1	0
30	6	624	LUT	3	0
22	6	611	CLA	1	0
25	B	844	BCR	2	0
22	B	834	CLA	1	0
22	3	617	CLA	3	0
25	A	851	BCR	3	0
22	A	828	CLA	1	0
22	A	840	CLA	3	0
22	A	805	CLA	22	0
25	I	172	BCR	1	0
22	B	817	CLA	3	0
22	A	839	CLA	4	0
22	7	620	CLA	12	0
22	A	829	CLA	7	0
22	5	614	CLA	5	0
22	8	613	CLA	3	0
22	6	612	CLA	2	0
22	Z	614	CLA	2	0
24	4	622	LHG	3	0
22	8	612	CLA	1	0
22	Z	613	CLA	5	0
22	1	616	CLA	1	0
22	A	813	CLA	2	0
30	5	624	LUT	5	0
22	3	604	CLA	3	0
22	L	203	CLA	1	0
25	A	850	BCR	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	6	601	CLA	7	0
22	7	602	CLA	2	0
22	6	616	CLA	8	0
22	2	602	CLA	2	0
29	1	607	CHL	3	0
29	6	606	CHL	4	0
22	5	609	CLA	6	0
22	B	821	CLA	1	0
22	A	834	CLA	3	0
22	B	814	CLA	5	0
22	1	610	CLA	5	0
22	6	622	CLA	14	0
22	5	610	CLA	1	0
22	B	805	CLA	5	0
22	8	608	CLA	1	0
25	3	718	BCR	5	0
22	1	604	CLA	1	0
22	1	606	CLA	3	0
22	8	602	CLA	3	0
25	F	305	BCR	15	0
22	B	829	CLA	4	0
22	2	611	CLA	1	0
24	8	620	LHG	1	0
22	B	836	CLA	2	0
22	1	614	CLA	3	0
22	A	841	CLA	11	0
29	6	618	CHL	2	0
30	7	621	LUT	6	0
22	7	609	CLA	3	0
22	B	802	CLA	2	0
25	L	205	BCR	2	0
30	3	622	LUT	3	0
22	A	838	CLA	1	0
22	F	304	CLA	2	0
22	B	835	CLA	2	0
22	5	601	CLA	1	0
22	B	809	CLA	1	0
22	B	819	CLA	2	0
22	9	602	CLA	3	0
25	3	717	BCR	4	0
22	A	837	CLA	1	0
30	2	616	LUT	3	0

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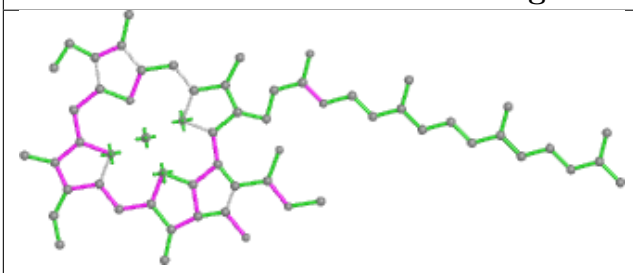
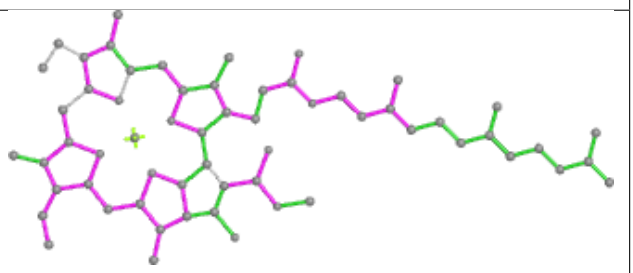
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	839	CLA	4	0
30	Z	619	LUT	2	0
30	1	619	LUT	2	0
22	A	815	CLA	21	0
22	A	843	CLA	7	0
22	6	613	CLA	2	0

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

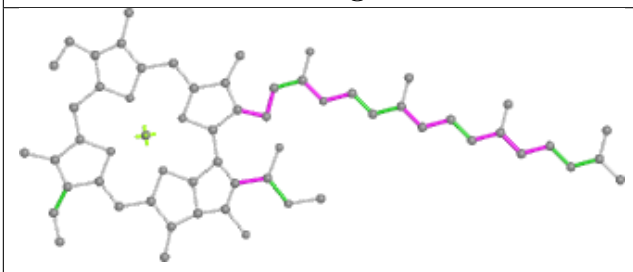
Ligand CLA 3 607



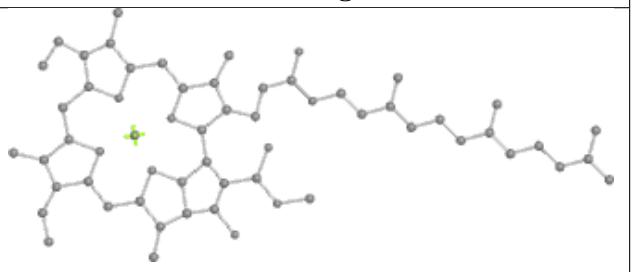
Bond lengths



Bond angles

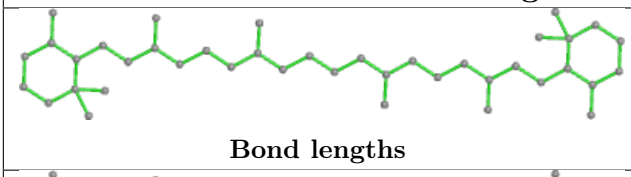


Torsions

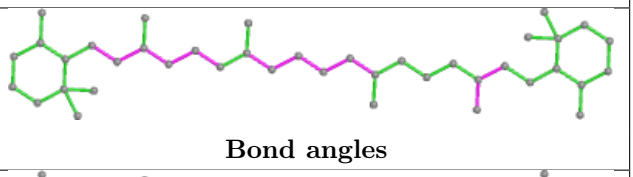


Rings

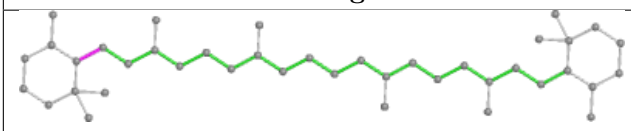
Ligand BCR G 205



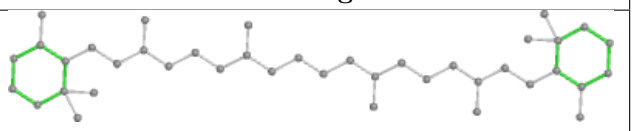
Bond lengths



Bond angles

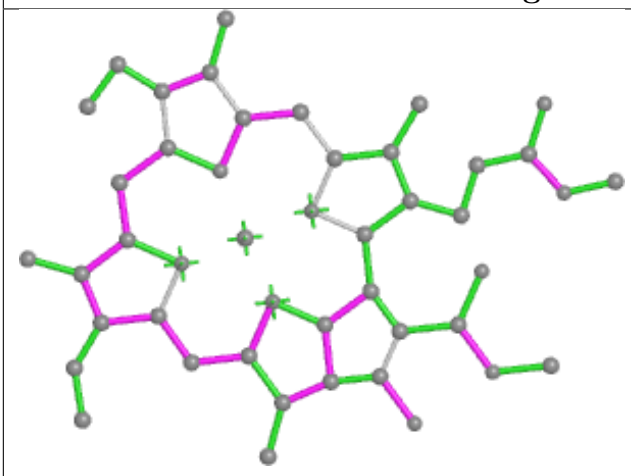


Torsions

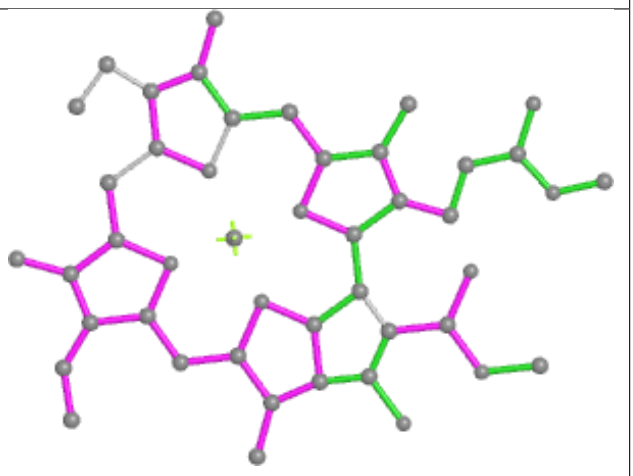


Rings

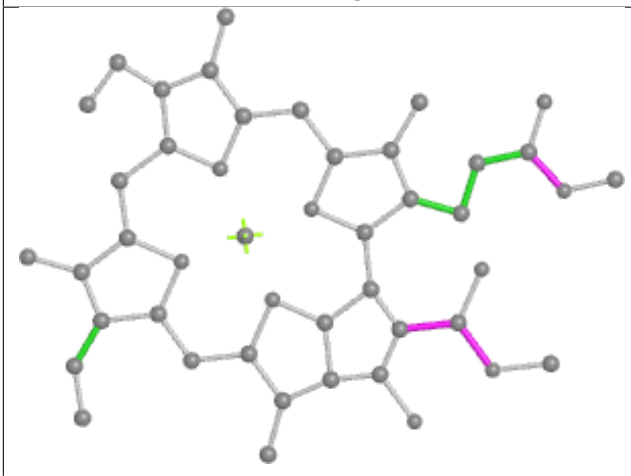
Ligand CLA G 204



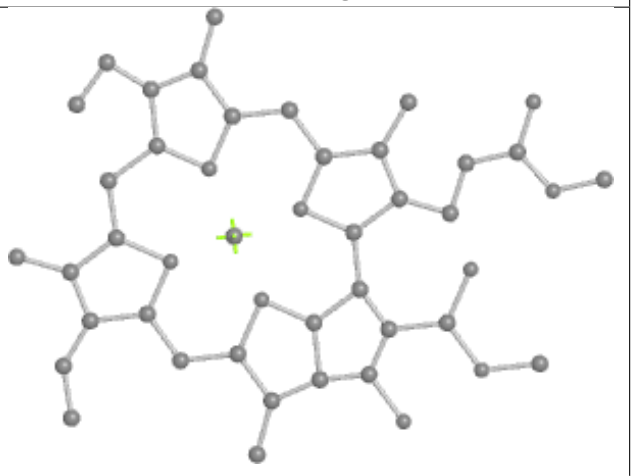
Bond lengths



Bond angles

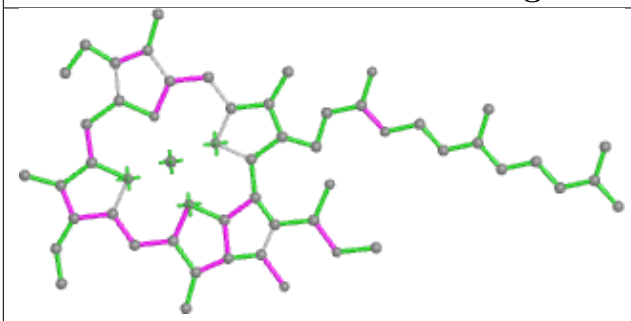


Torsions

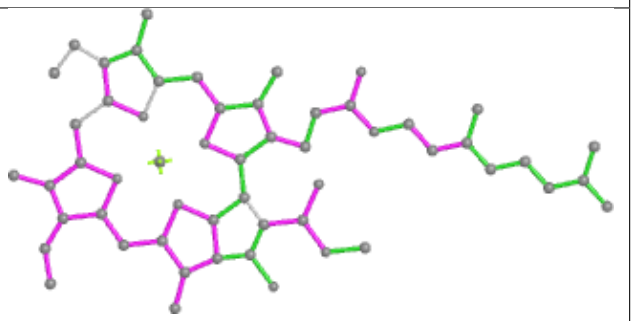


Rings

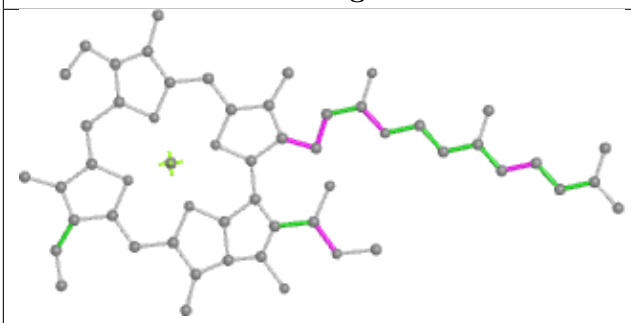
Ligand CLA A 825



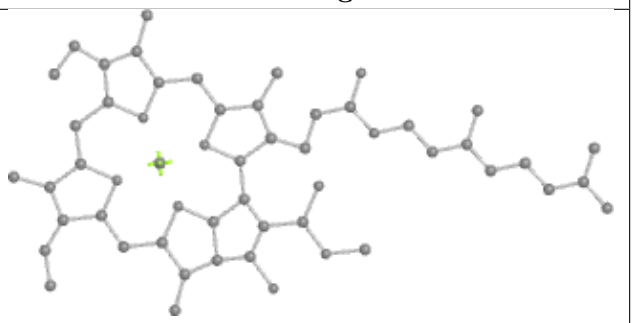
Bond lengths



Bond angles

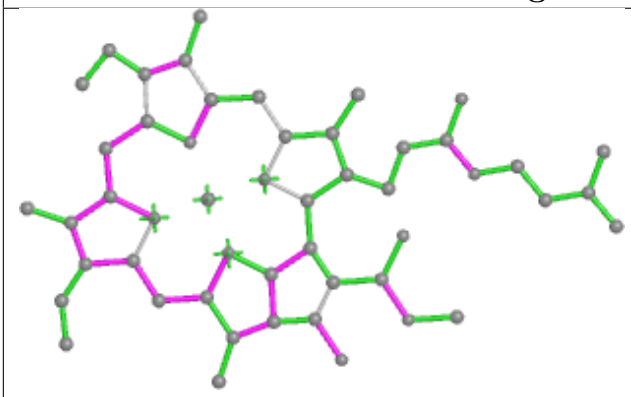


Torsions

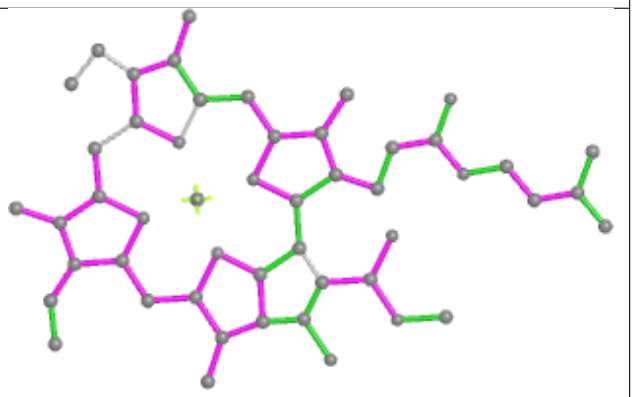


Rings

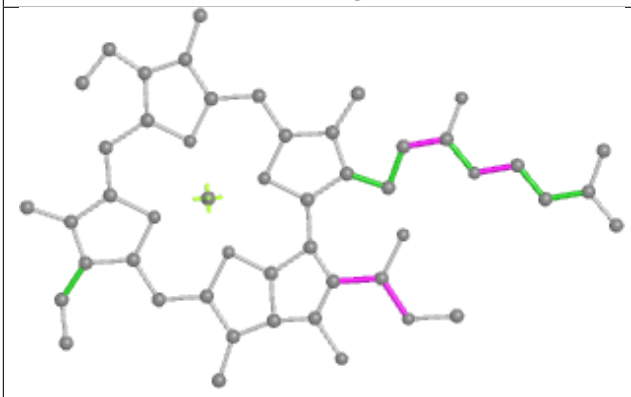
Ligand CLA 3 609



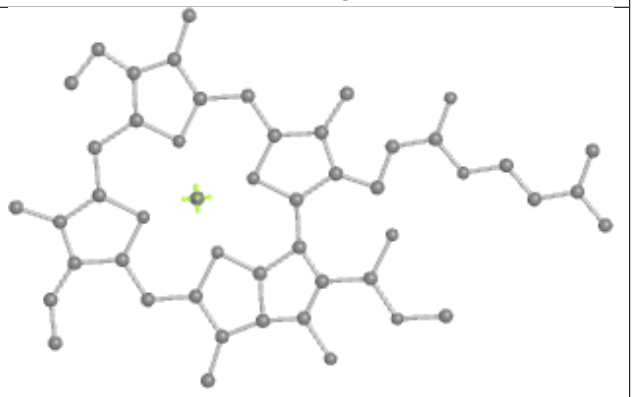
Bond lengths



Bond angles

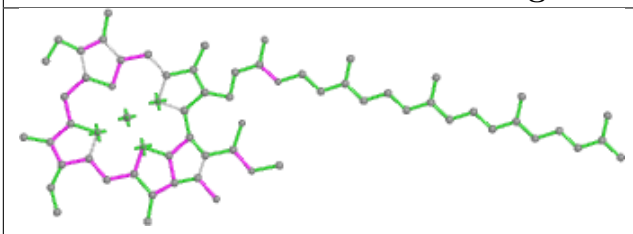


Torsions

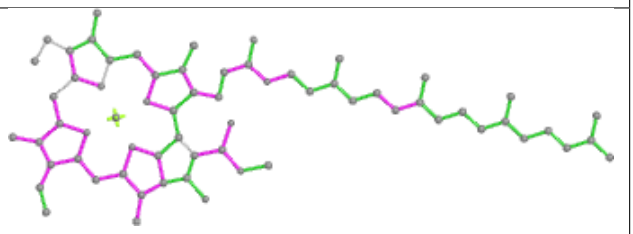


Rings

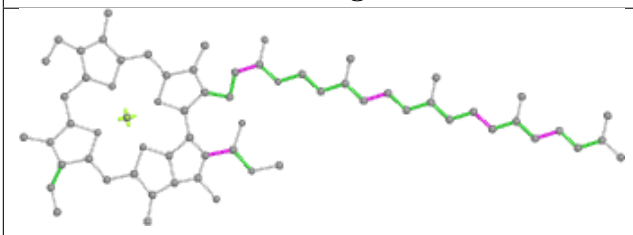
Ligand CLA 1 613



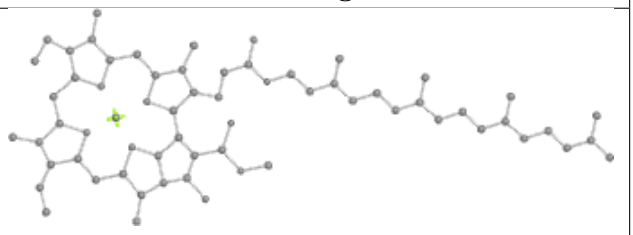
Bond lengths



Bond angles

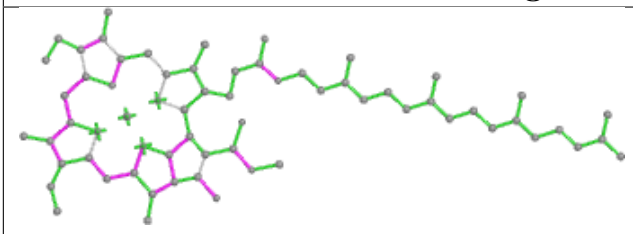


Torsions

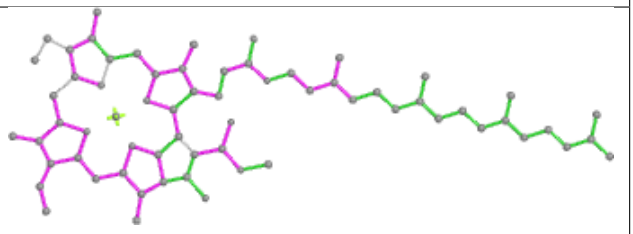


Rings

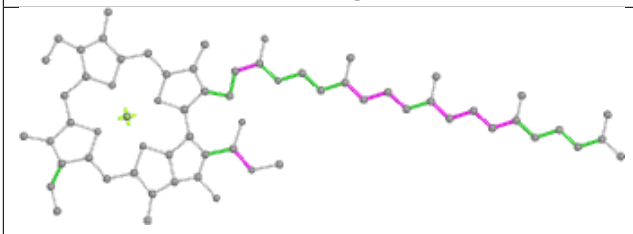
Ligand CLA B 806



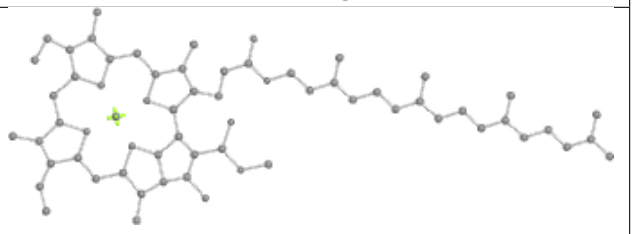
Bond lengths



Bond angles

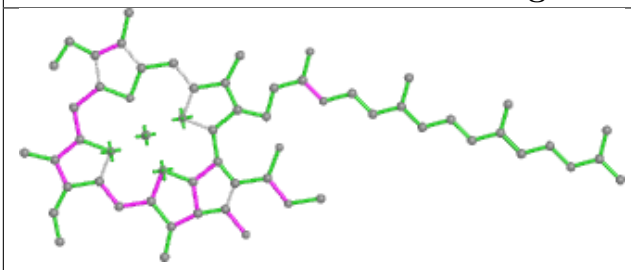


Torsions

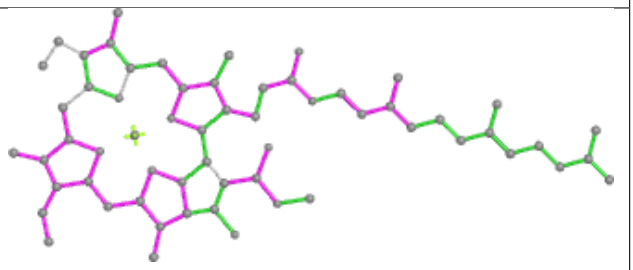


Rings

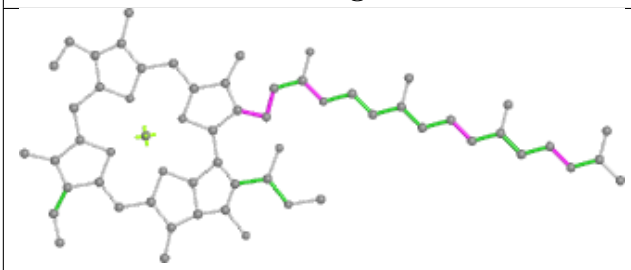
Ligand CLA 7 610



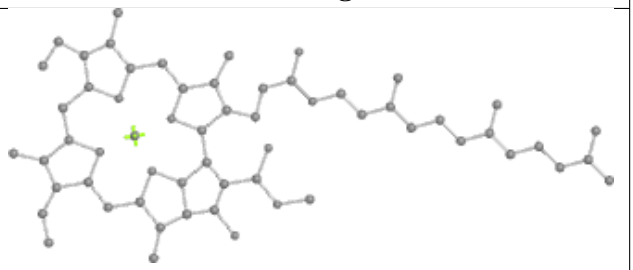
Bond lengths



Bond angles

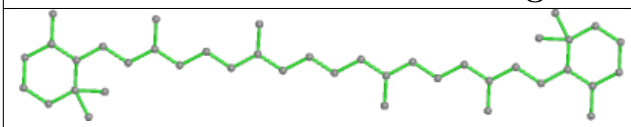


Torsions

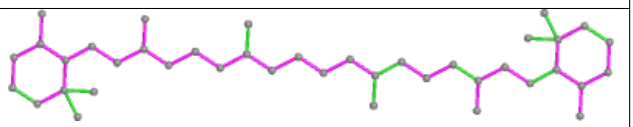


Rings

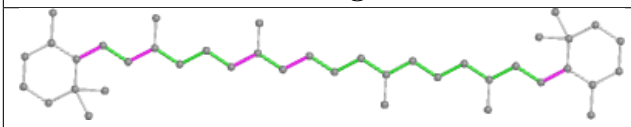
Ligand BCR 6 623



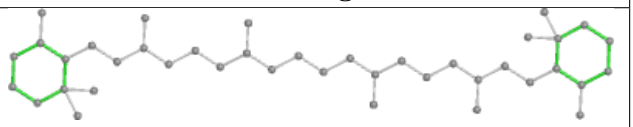
Bond lengths



Bond angles

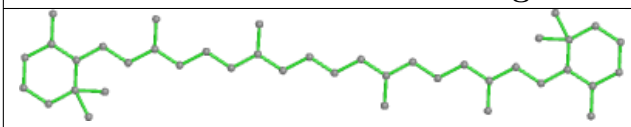


Torsions

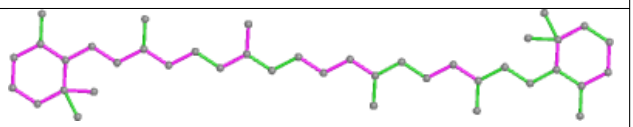


Rings

Ligand BCR K 4001



Bond lengths



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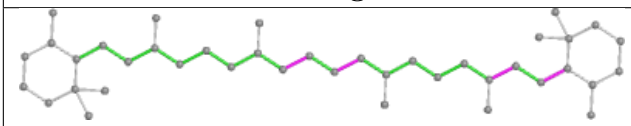
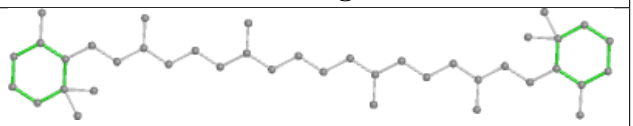
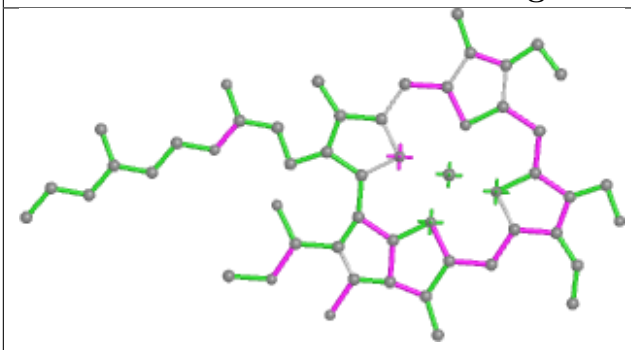


Torsions



Rings

Ligand CHL 1 601



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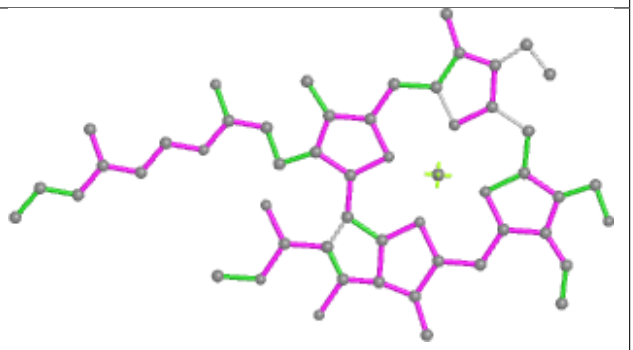
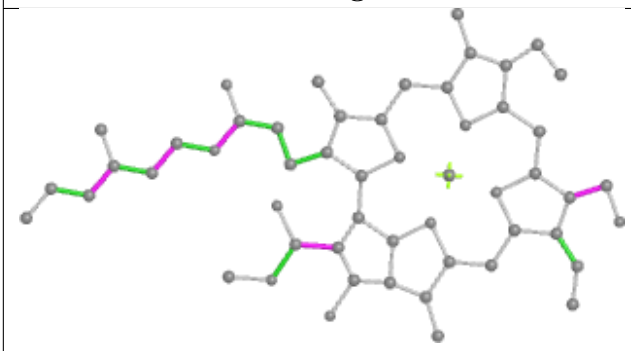


Bond angles



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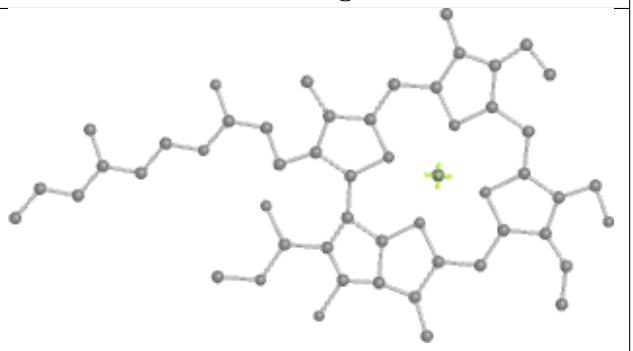
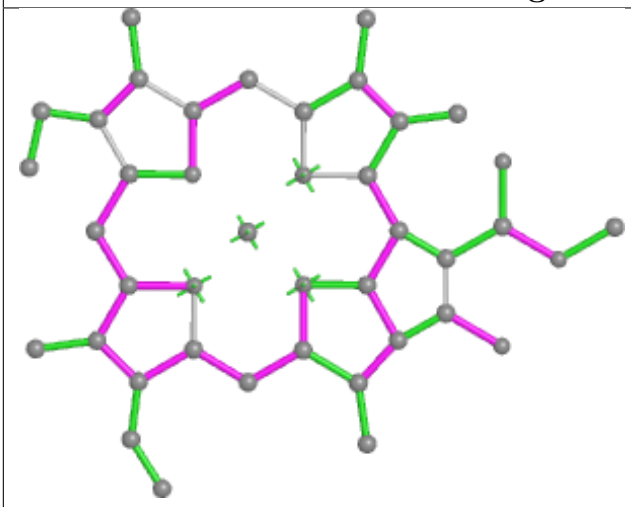


Rings

Ligand CLA 7 611



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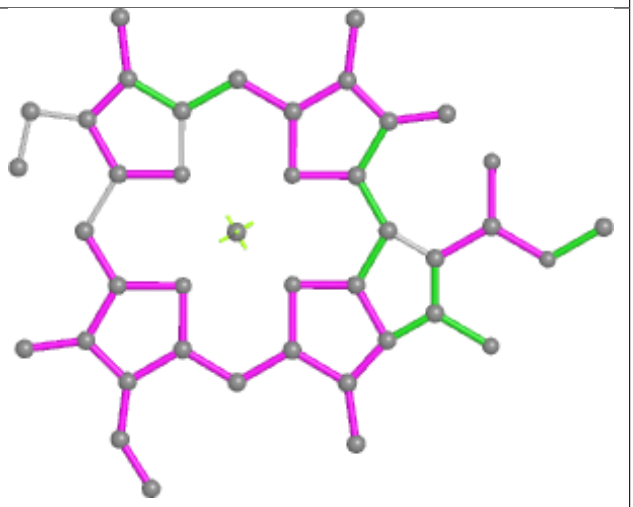
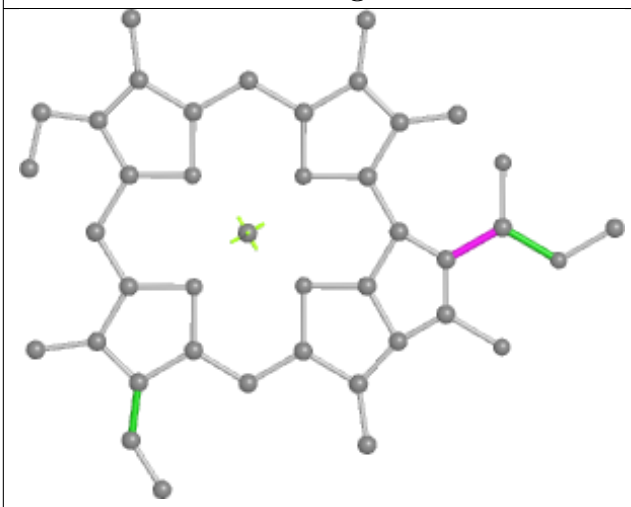


Bond angles



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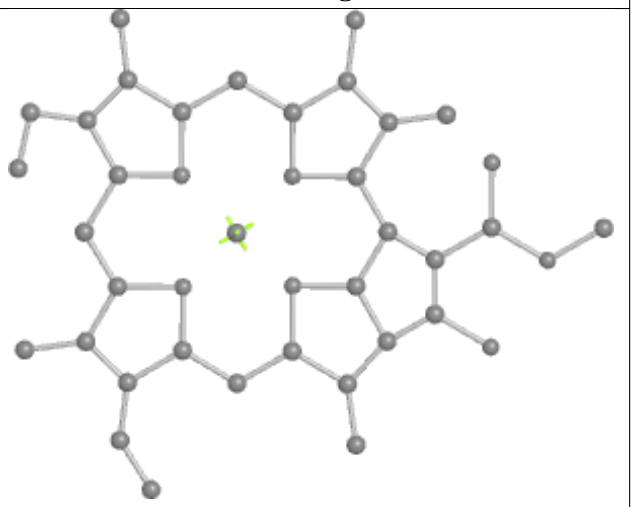
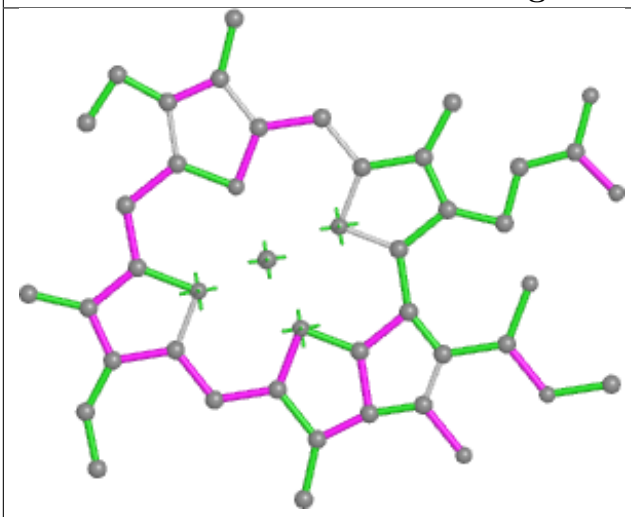


Rings

Ligand CLA 4 614



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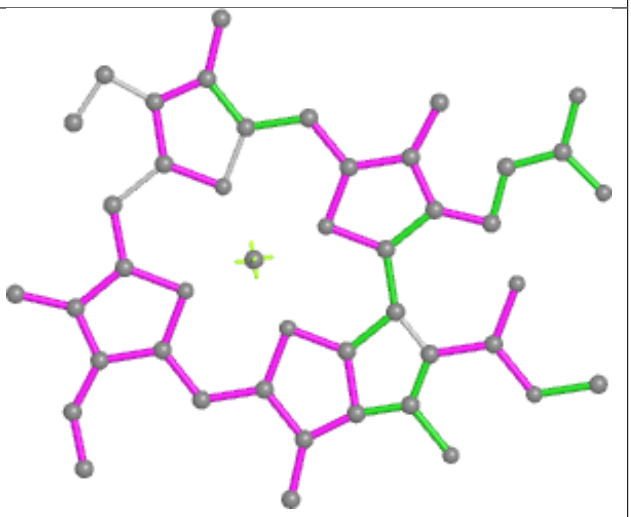

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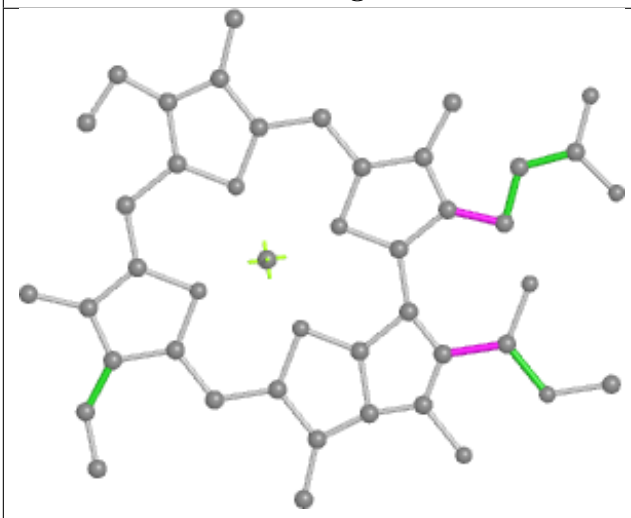

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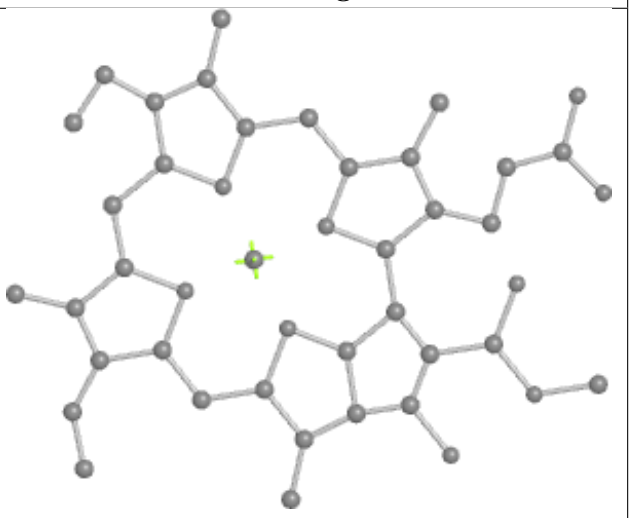
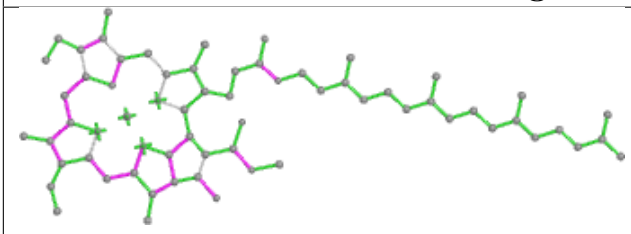


Rings

Ligand CLA 1 602



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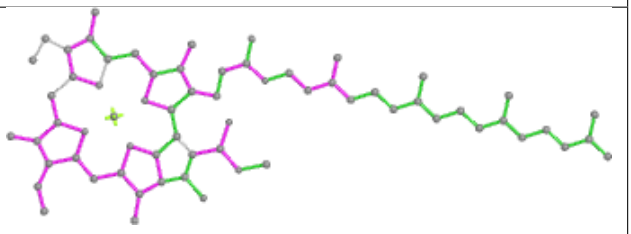
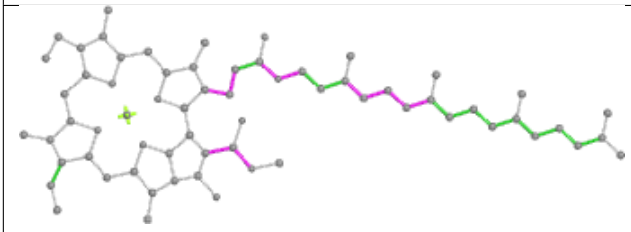


Bond angles



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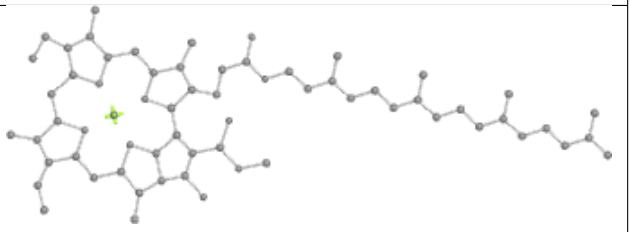
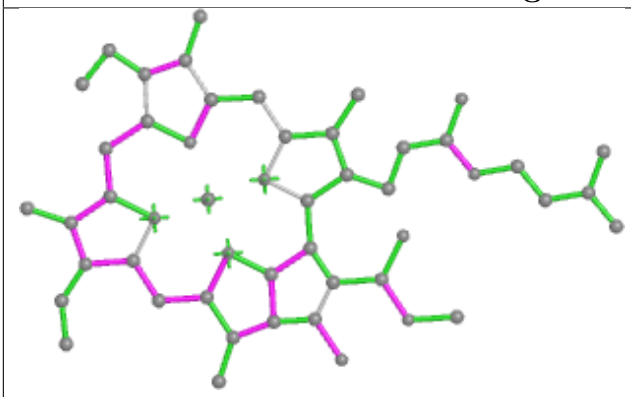


Rings

Ligand CLA A 832



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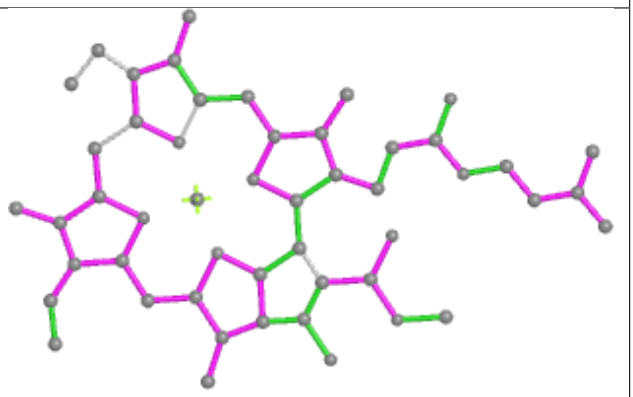
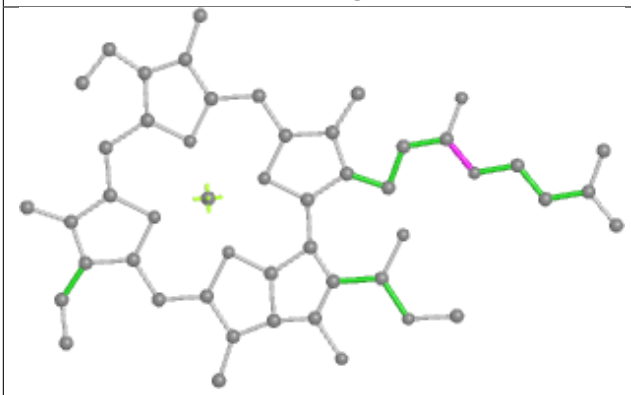


Bond angles



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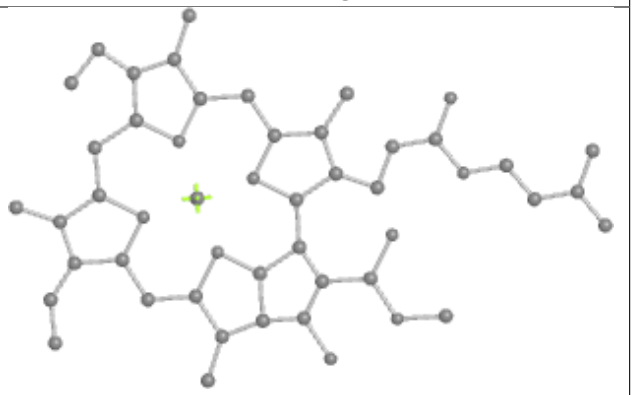
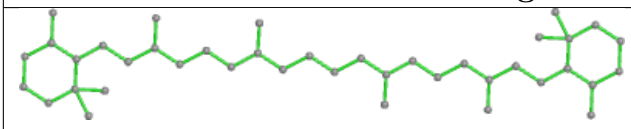
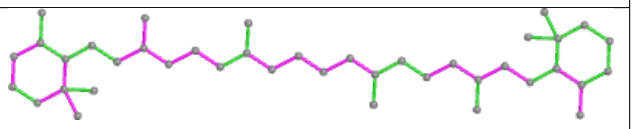


Rings

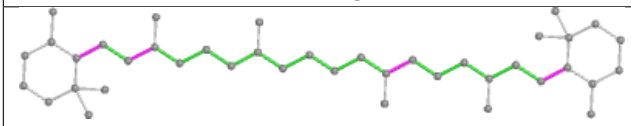
Ligand BCR J 3003



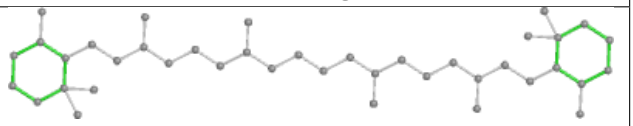
Bond lengths



Bond angles

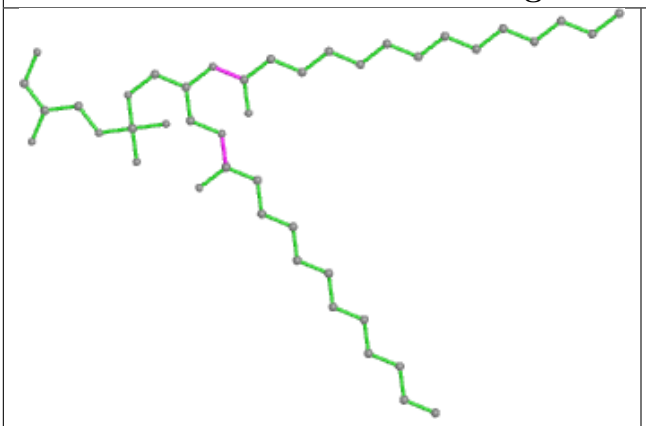


Torsions



Rings

Ligand LHG Z 620



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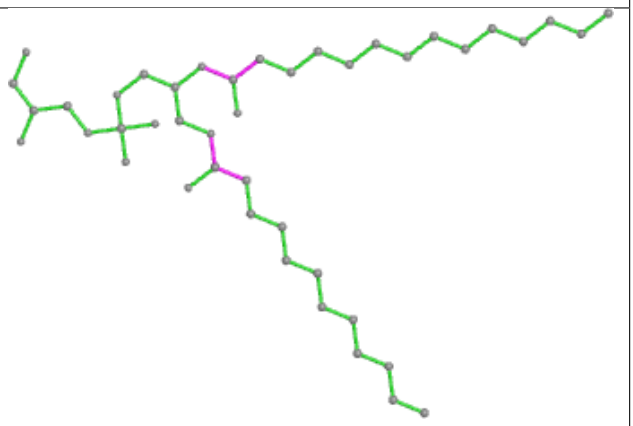
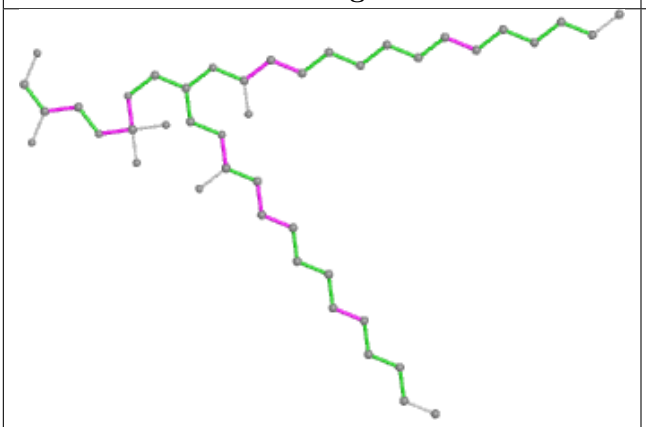
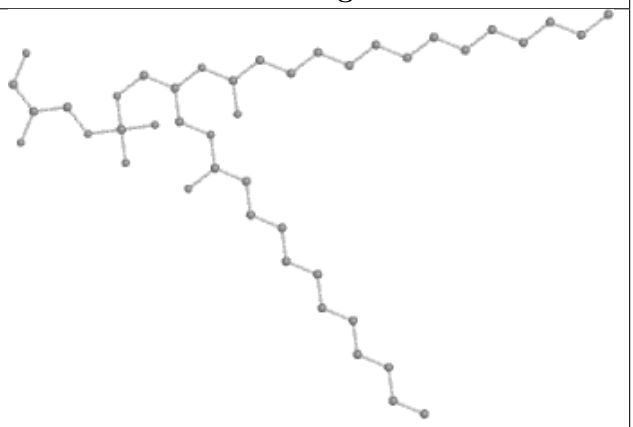


Bond angles

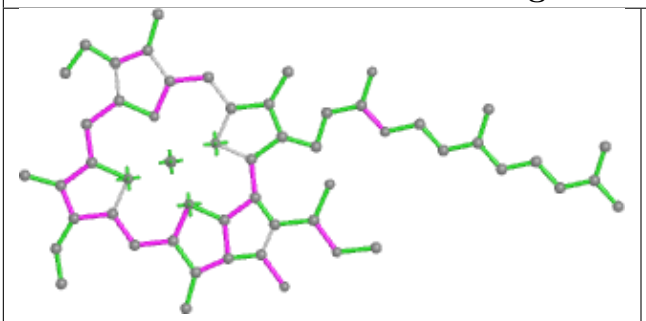


Torsions



Rings

Ligand CLA 4 611



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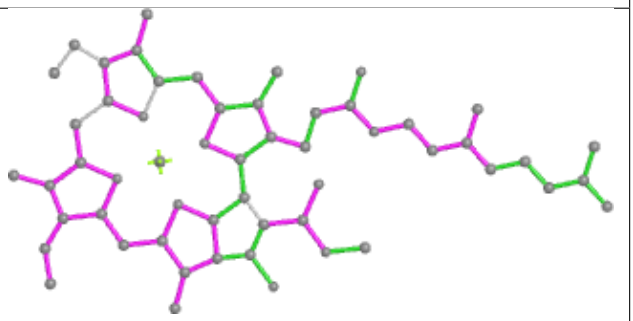
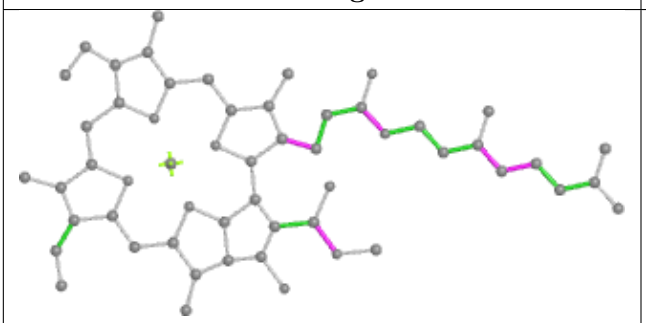
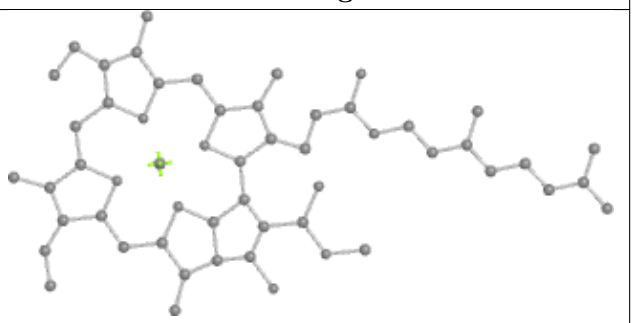


Bond angles

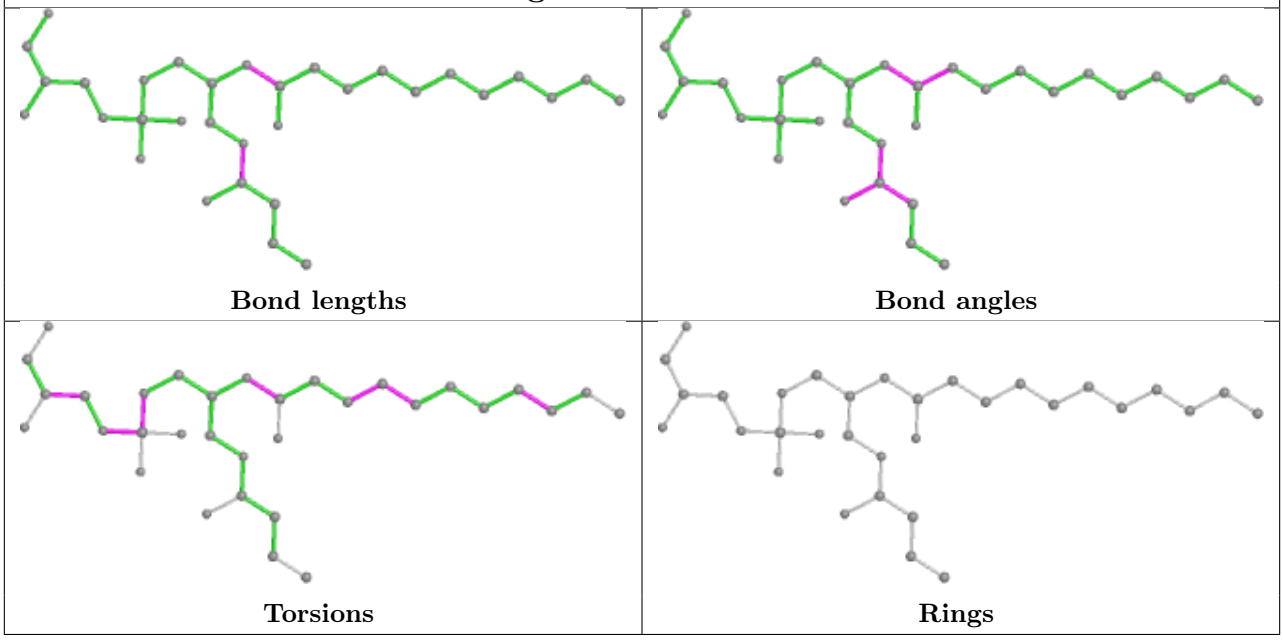


Torsions

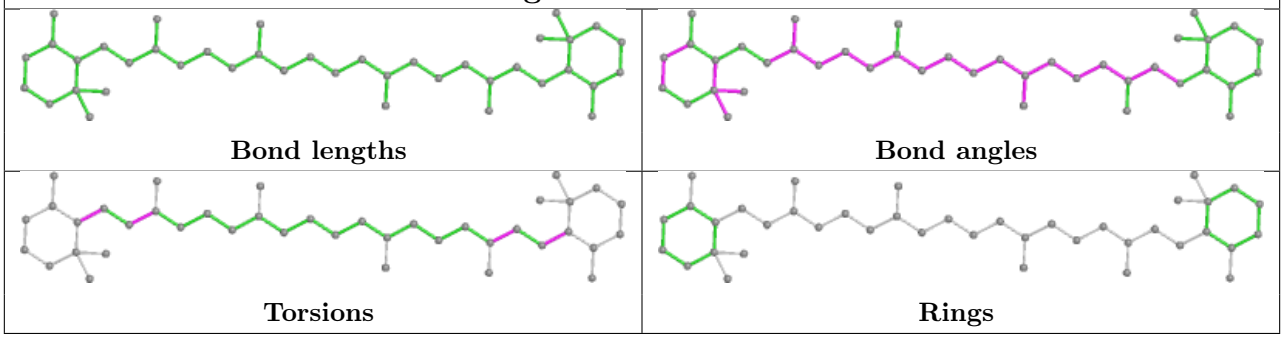


Rings

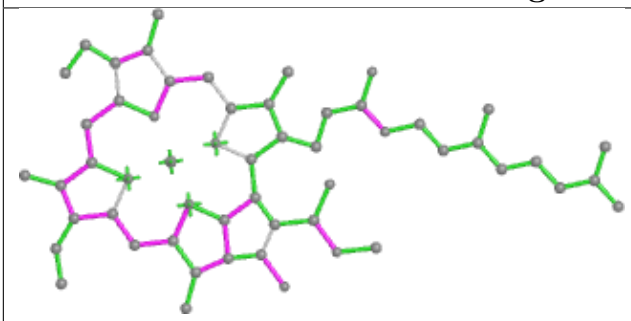
Ligand LHG 4 623



Ligand BCR B 847



Ligand CLA 3 613



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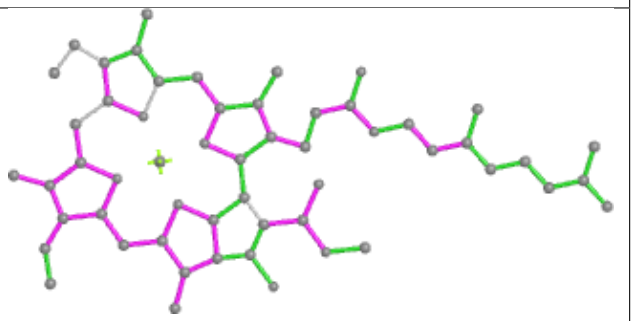
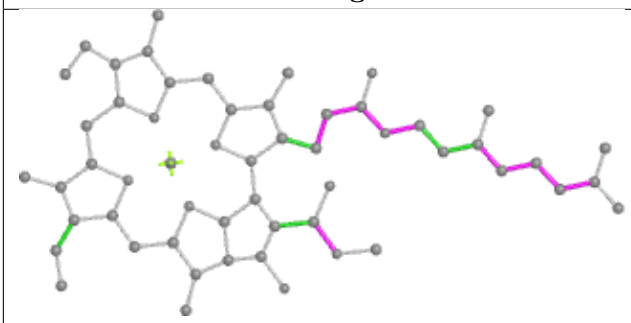
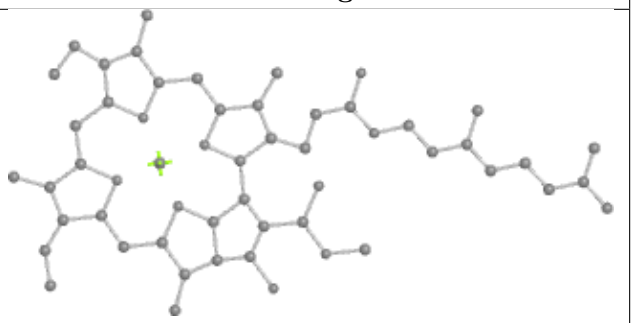


Bond angles

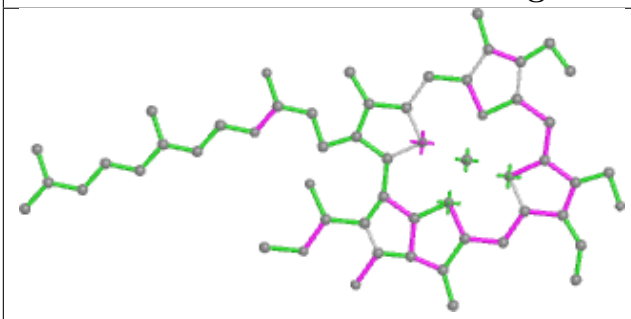


Torsions



Rings

Ligand CHL 6 607



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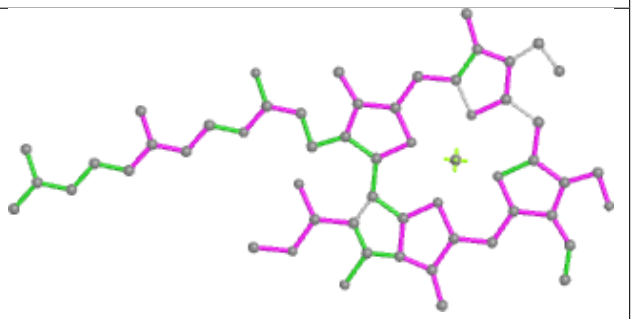
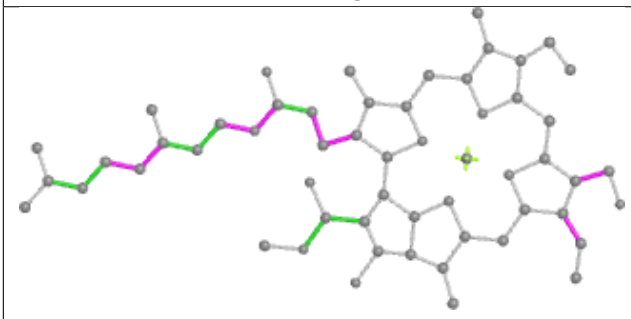


Bond angles



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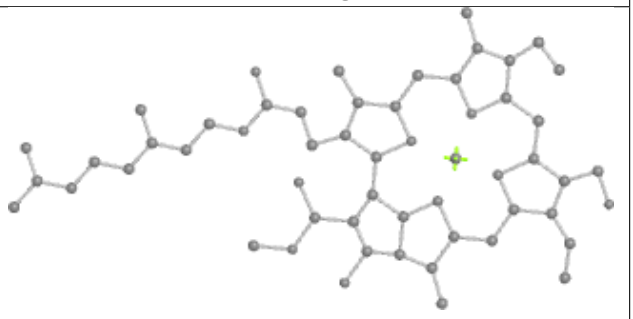
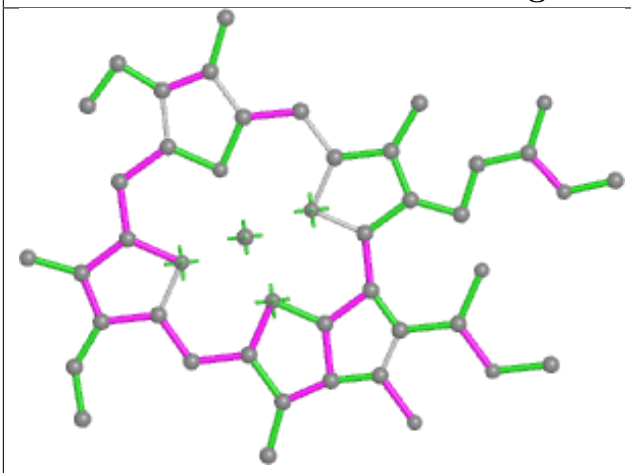
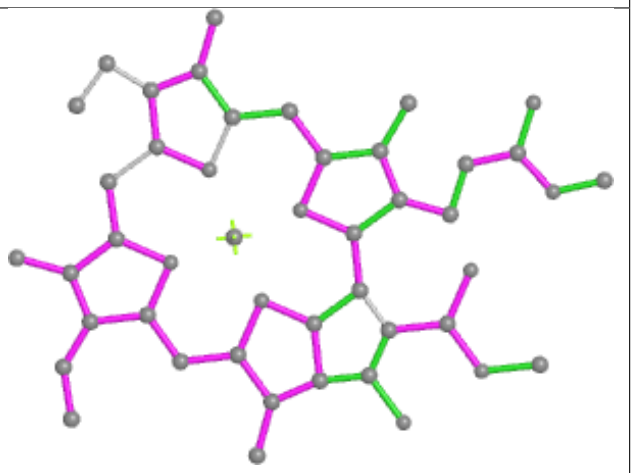


Rings

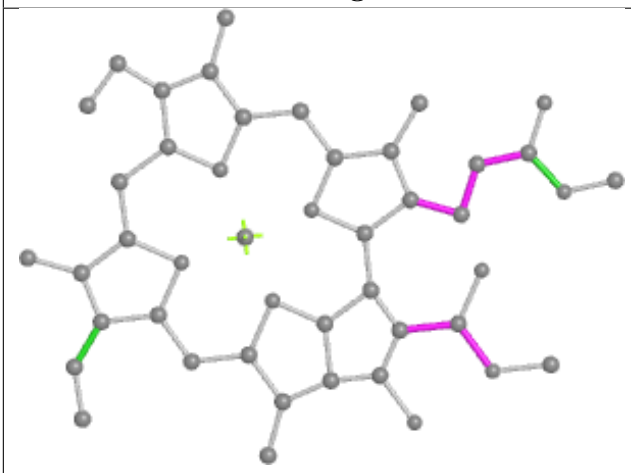
Ligand CLA 5 616



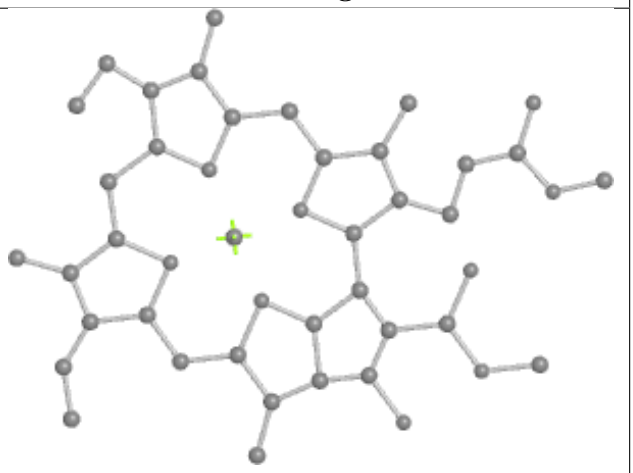
Bond lengths



Bond angles

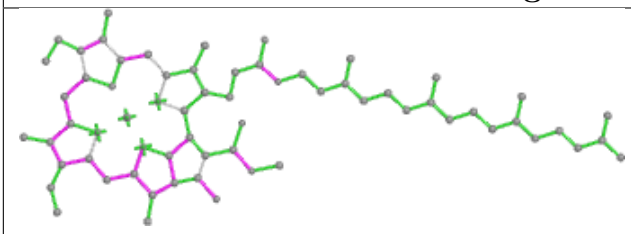


Torsions

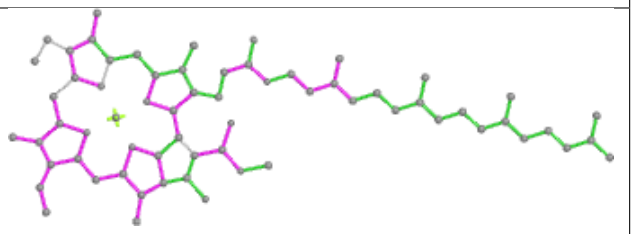


Rings

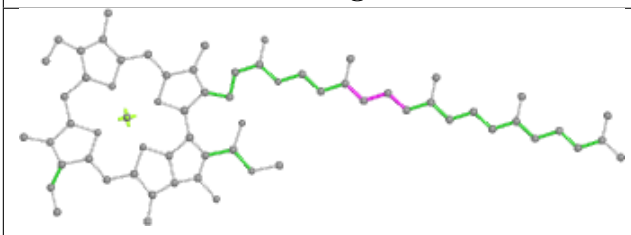
Ligand CLA A 835



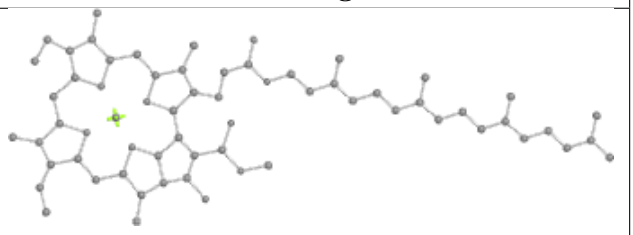
Bond lengths



Bond angles

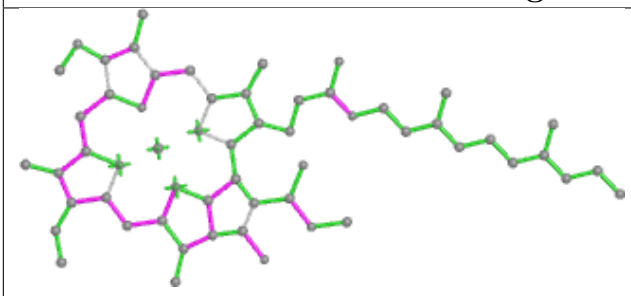


Torsions

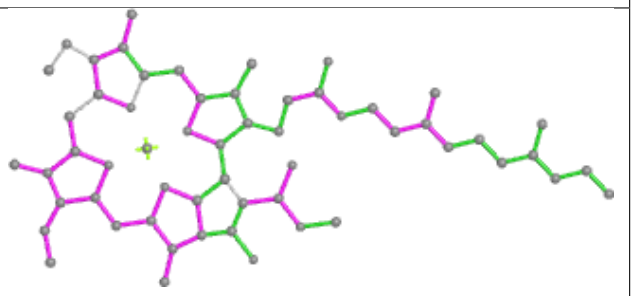


Rings

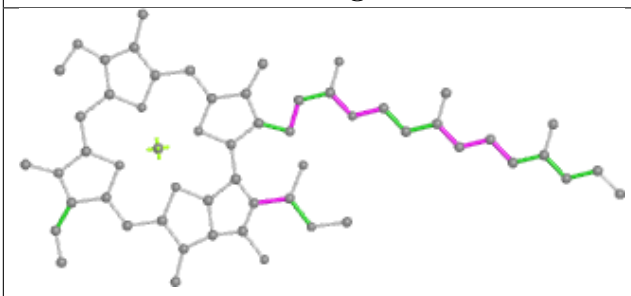
Ligand CLA Z 604



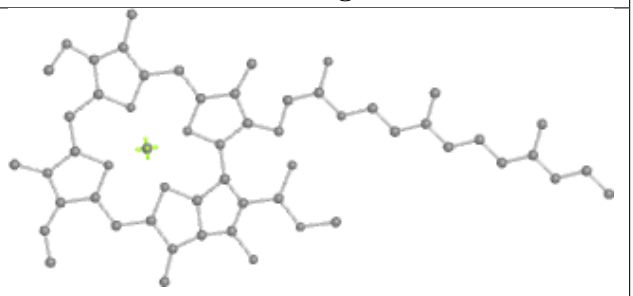
Bond lengths



Bond angles

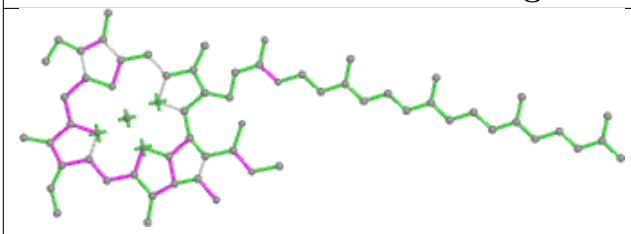


Torsions



Rings

Ligand CLA A 809



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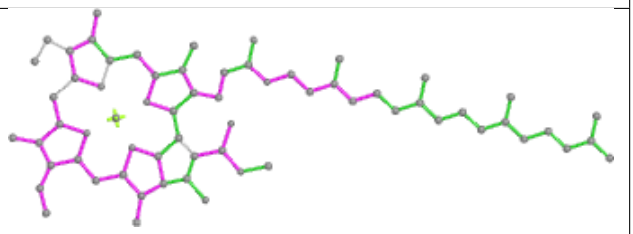
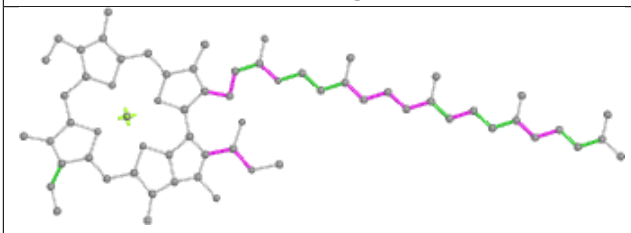
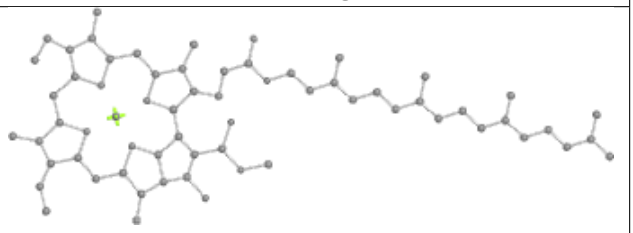


Bond angles

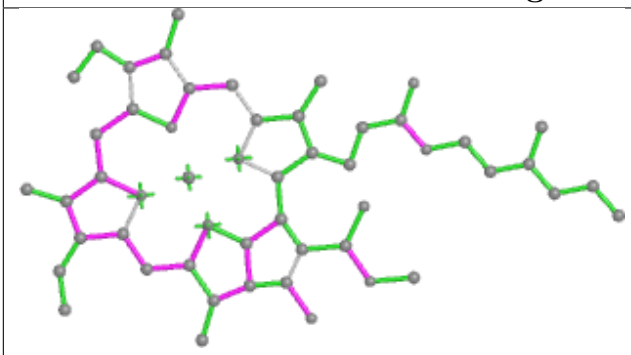


Torsions



Rings

Ligand CLA Z 606



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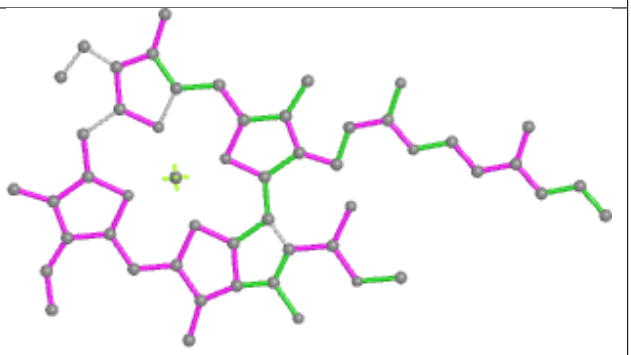
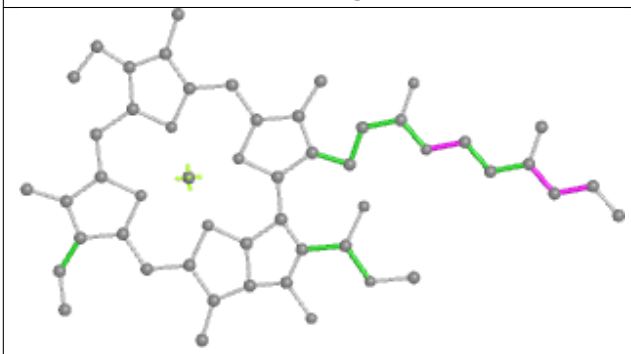
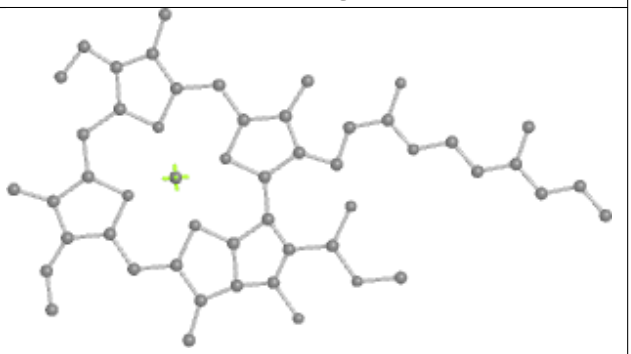


Bond angles

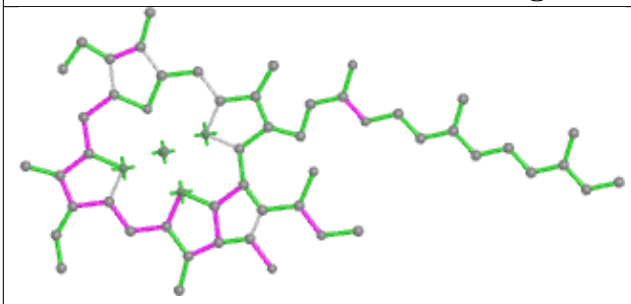


Torsions



Rings

Ligand CLA 4 613



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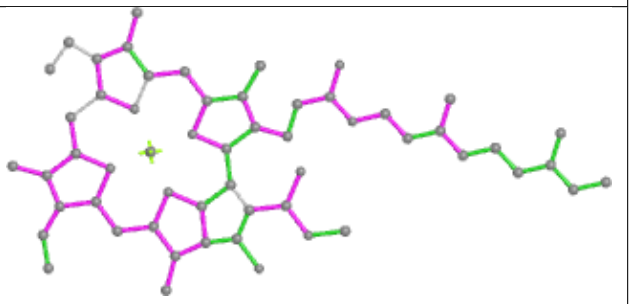
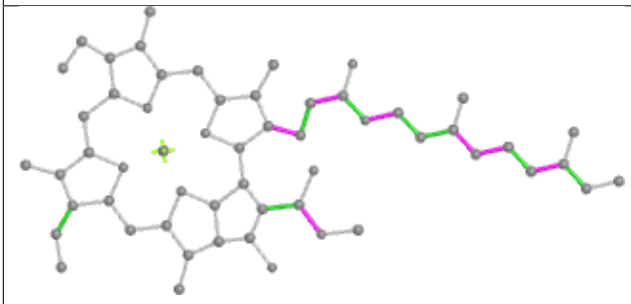


Bond angles



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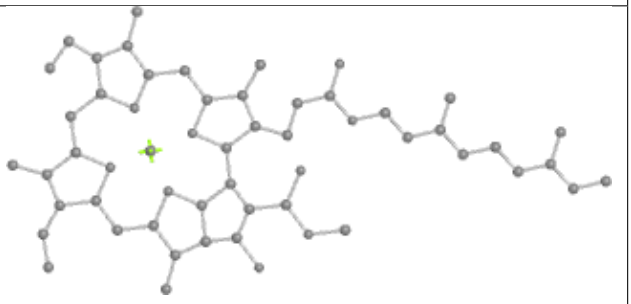
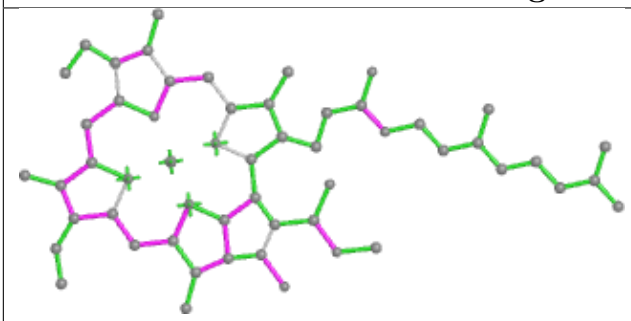


Rings

Ligand CLA 5 606



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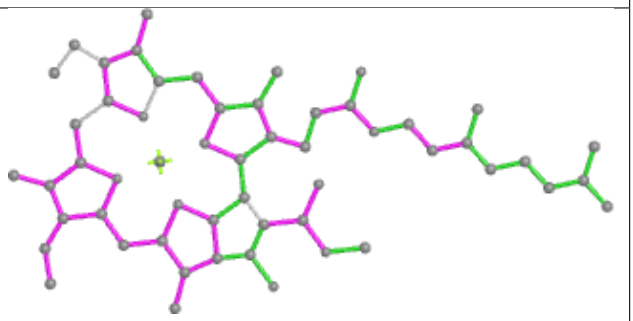
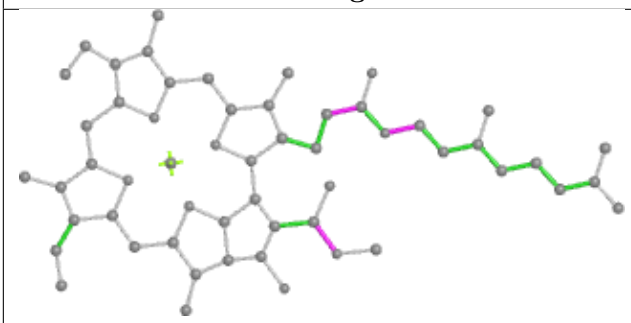


Bond angles



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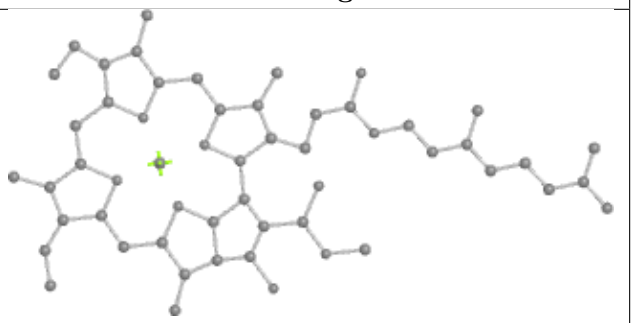
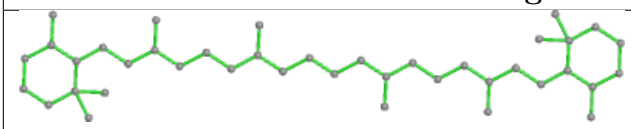


Rings

Ligand BCR L 201



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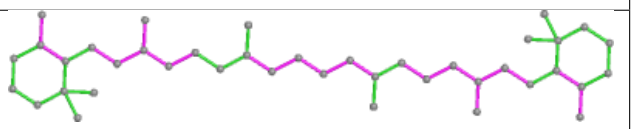
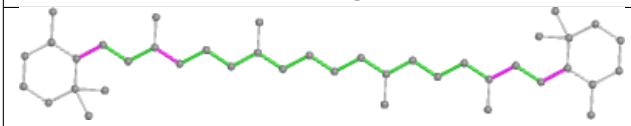


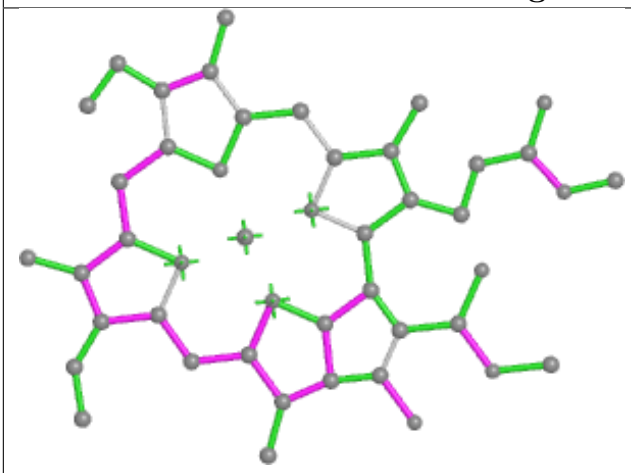
Bond angles



Torsions

Rings

Ligand CLA 2 603



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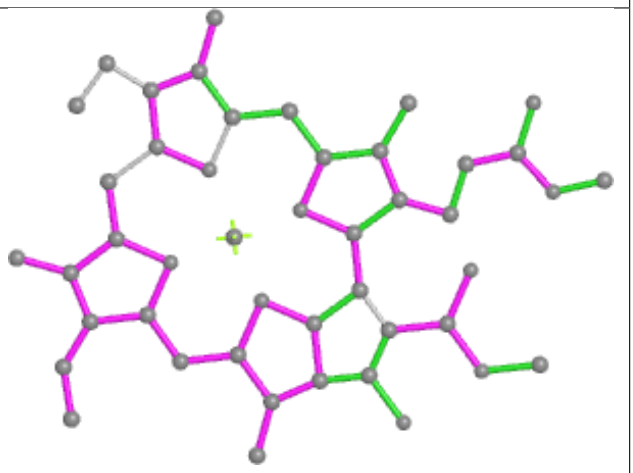
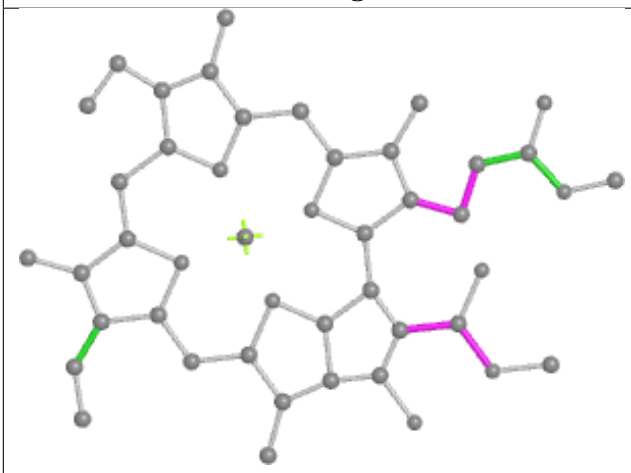


Bond angles



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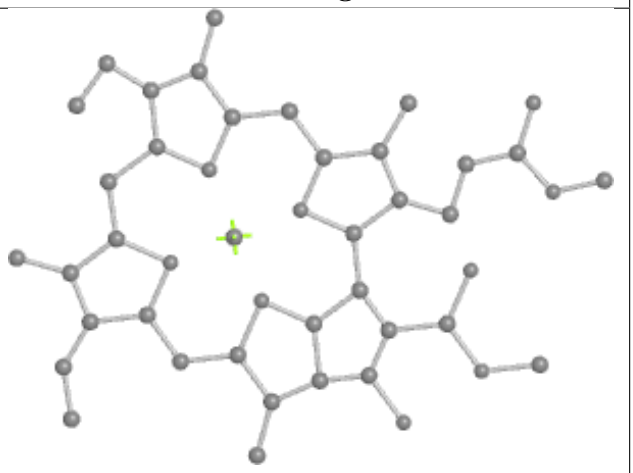
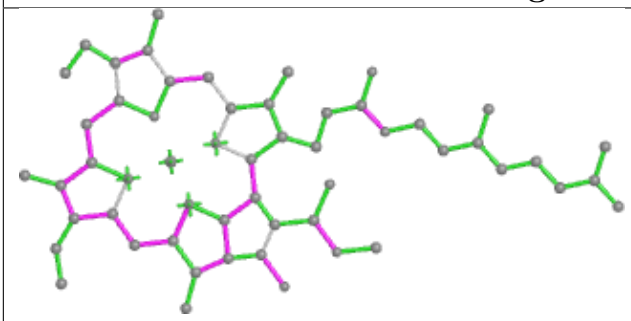


Rings

Ligand CLA 5 611



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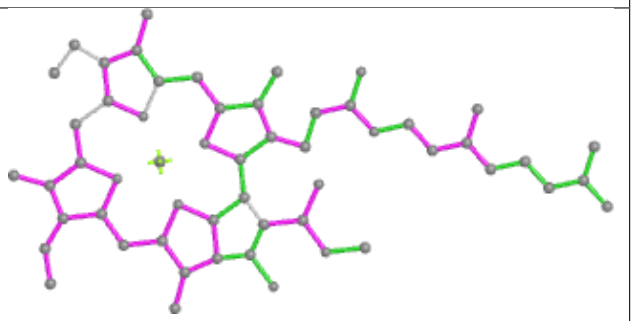
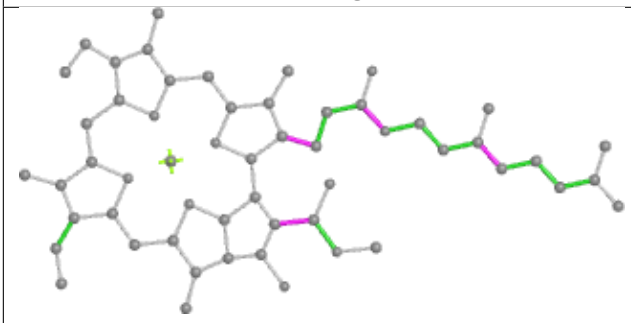


Bond angles



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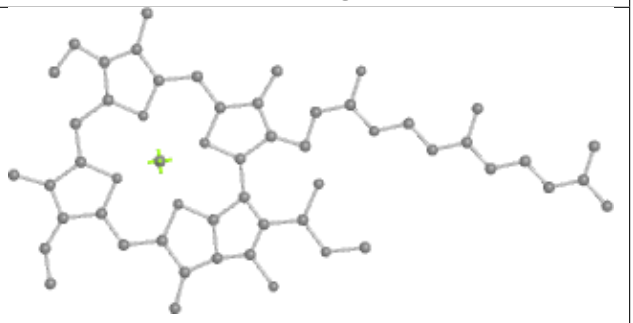
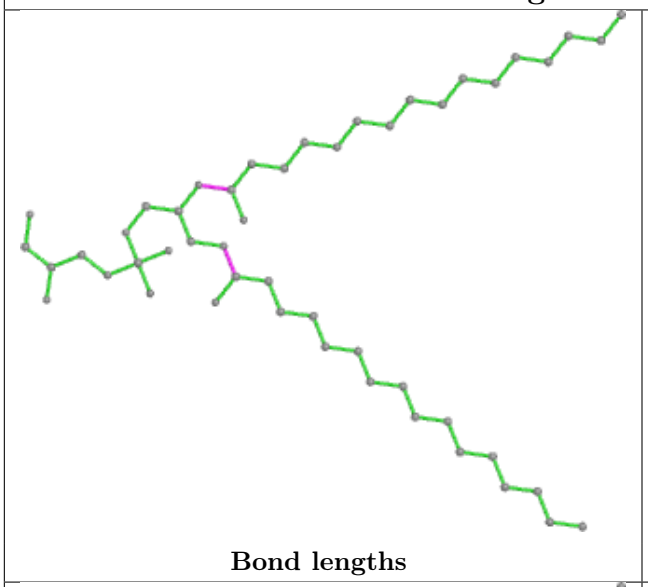


Rings

Ligand LHG 6 619



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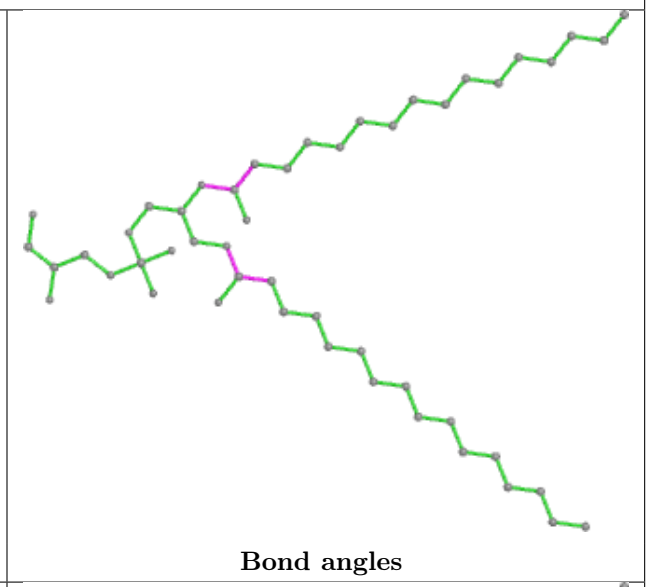
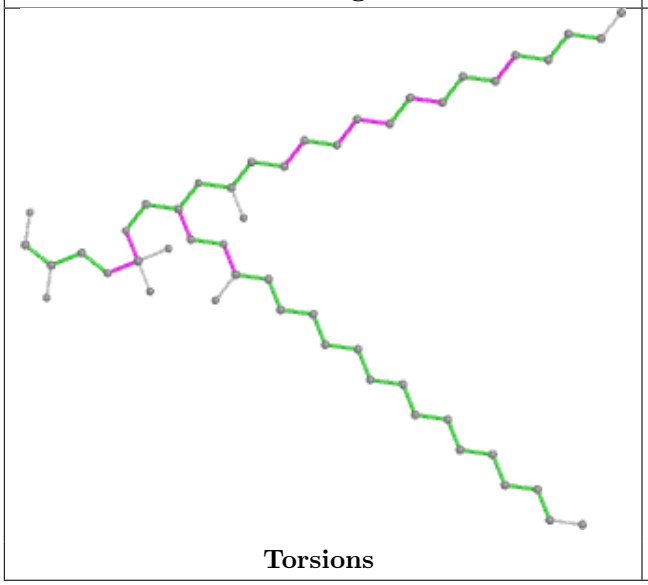
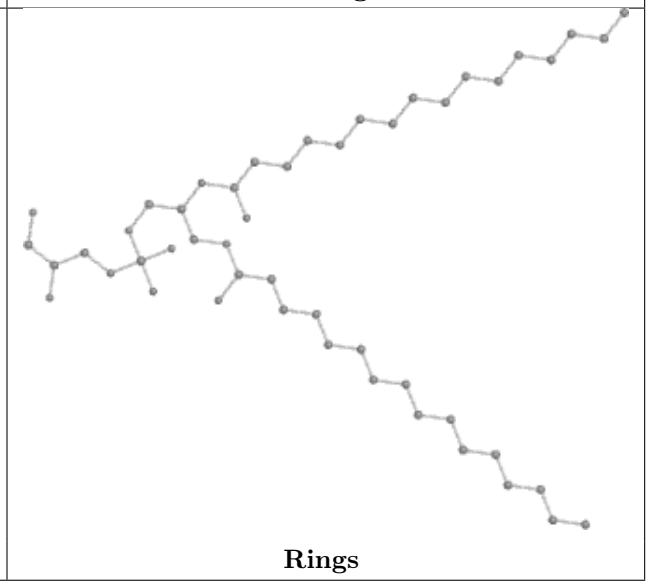


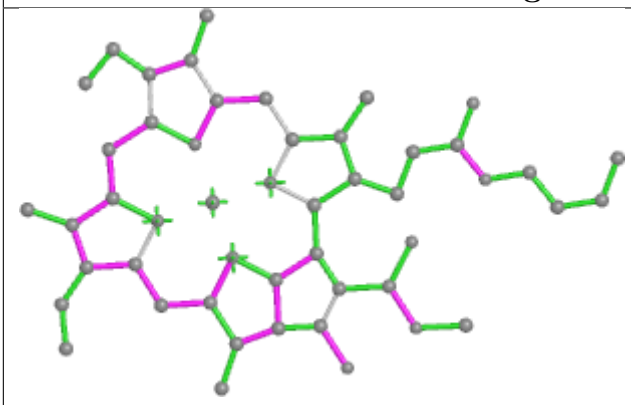
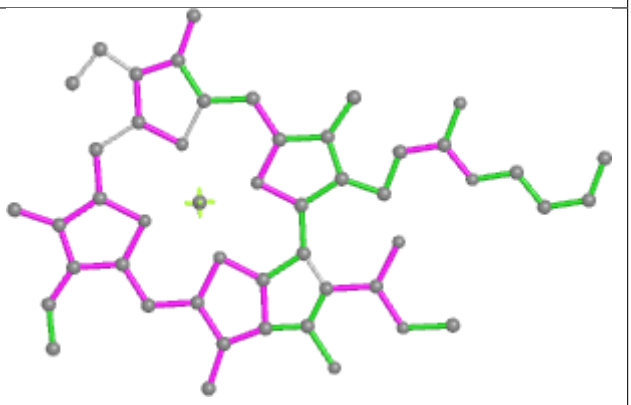
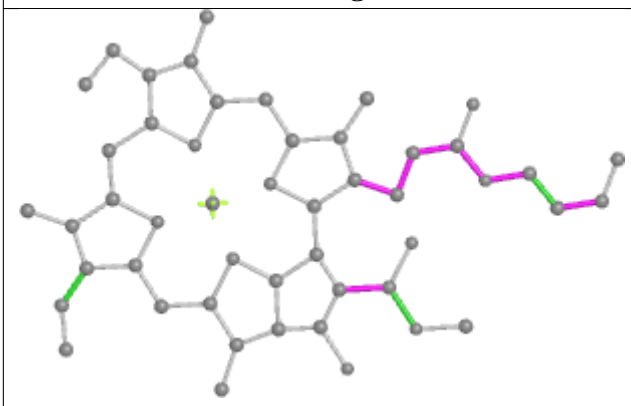
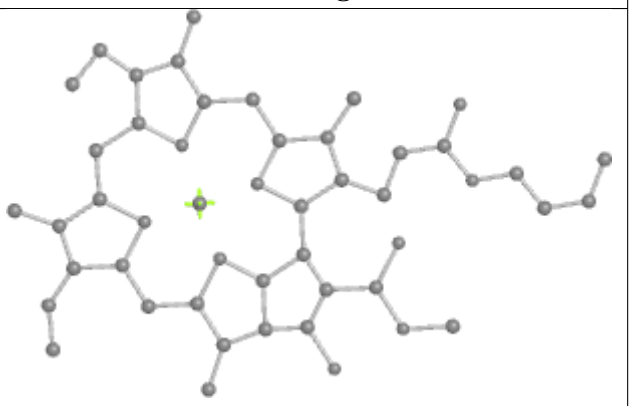
Bond angles



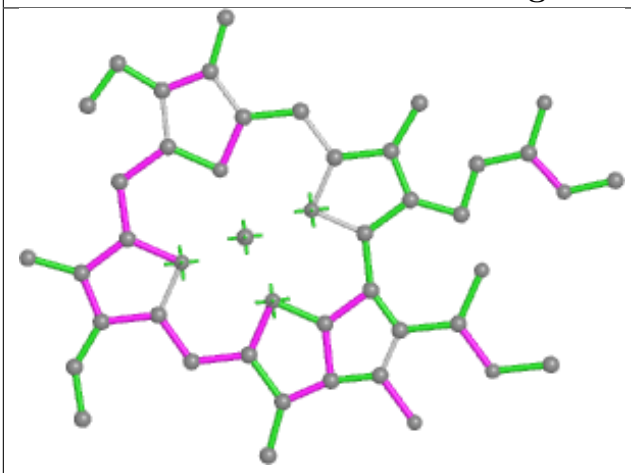
Torsions



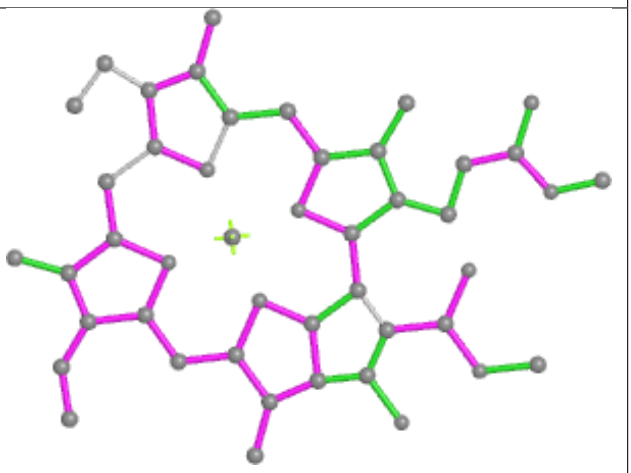
Rings

Ligand CLA A 823	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

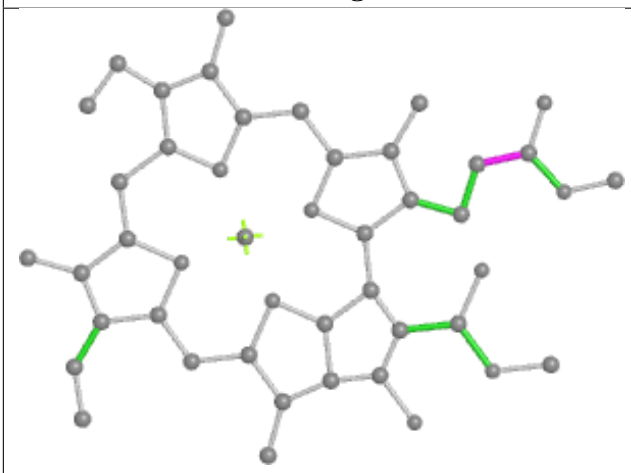
Ligand CLA 3 612



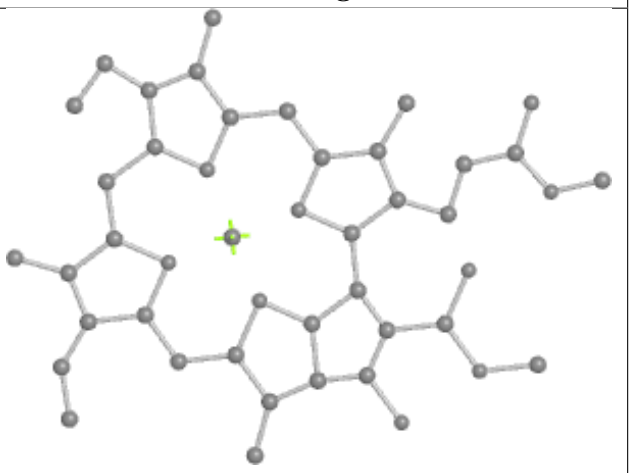
Bond lengths



Bond angles

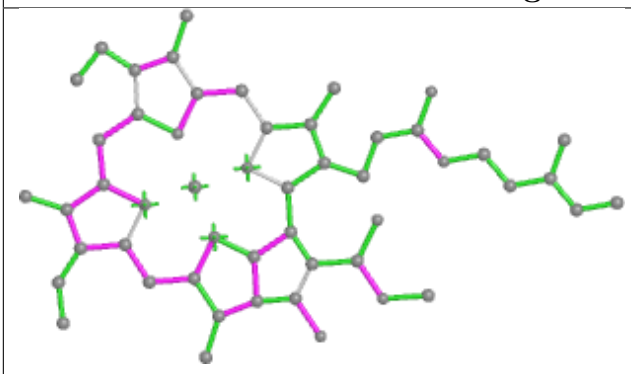


Torsions

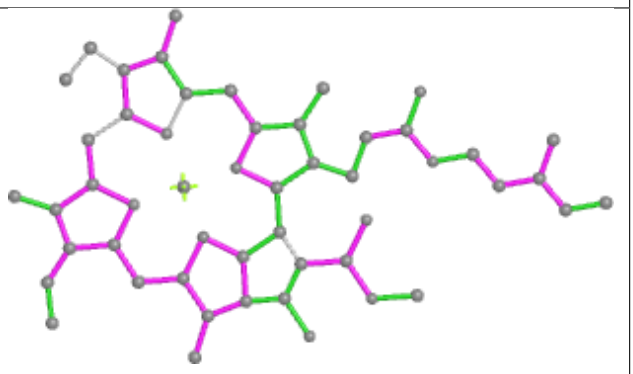


Rings

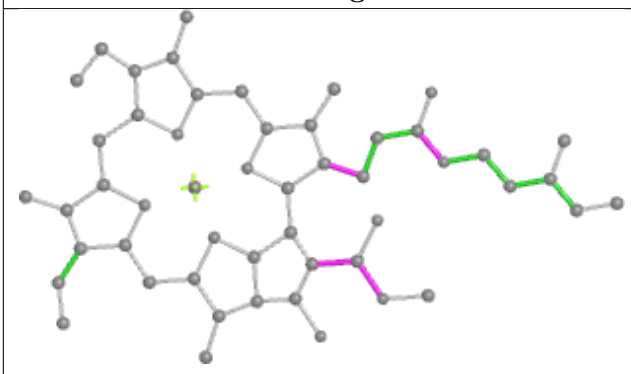
Ligand CLA A 824



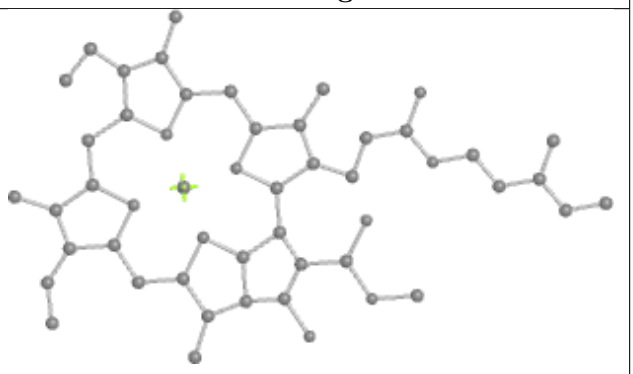
Bond lengths



Bond angles

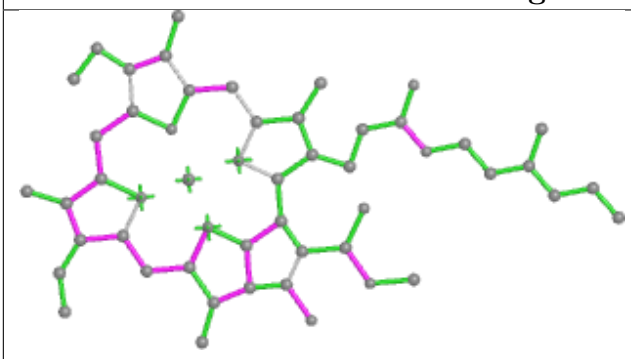


Torsions

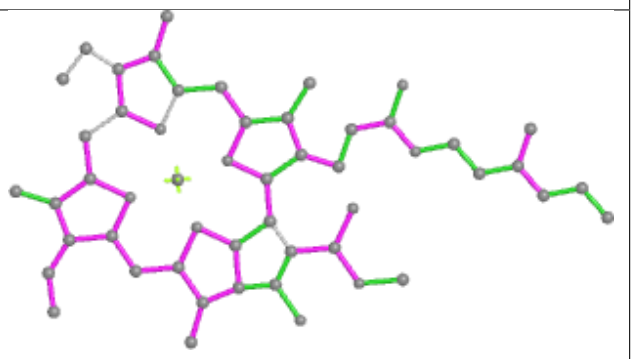


Rings

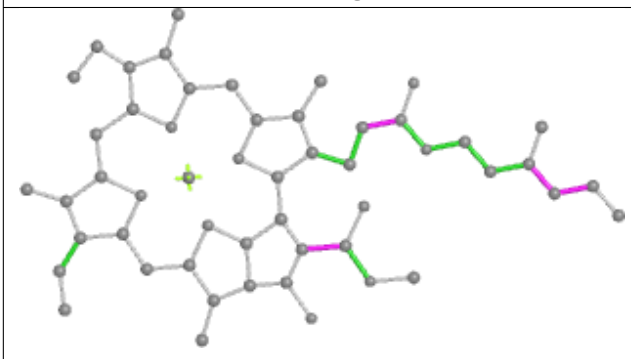
Ligand CLA 2 612



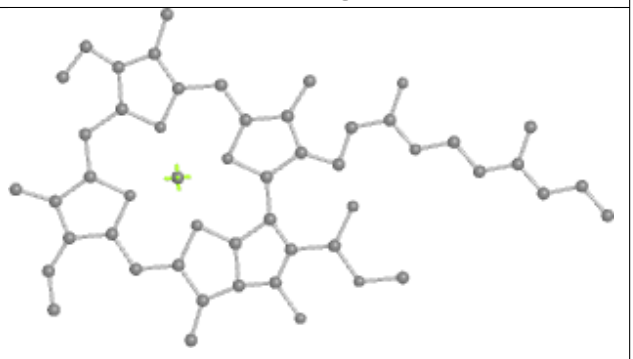
Bond lengths



Bond angles

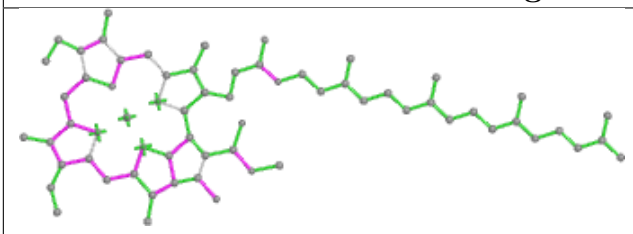


Torsions

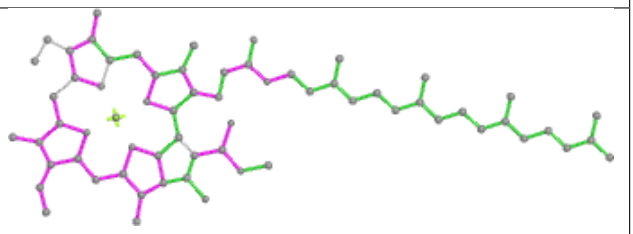


Rings

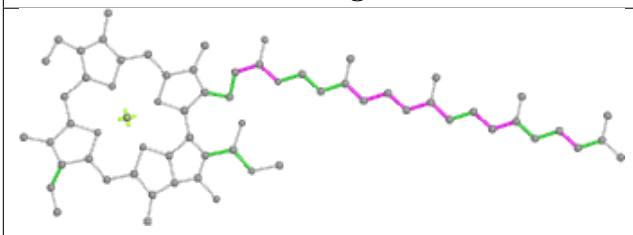
Ligand CLA B 812



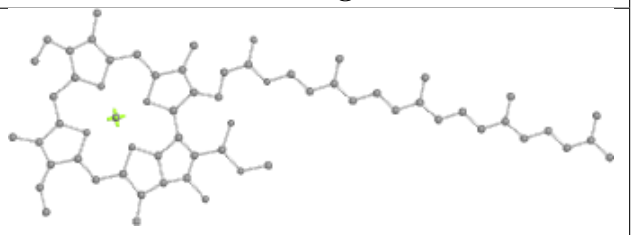
Bond lengths



Bond angles

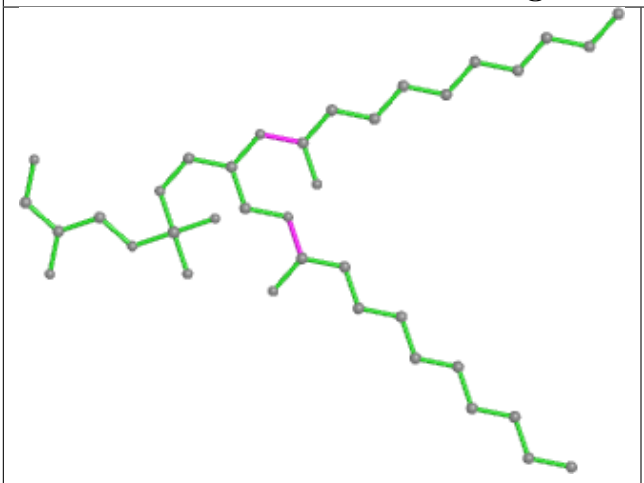


Torsions

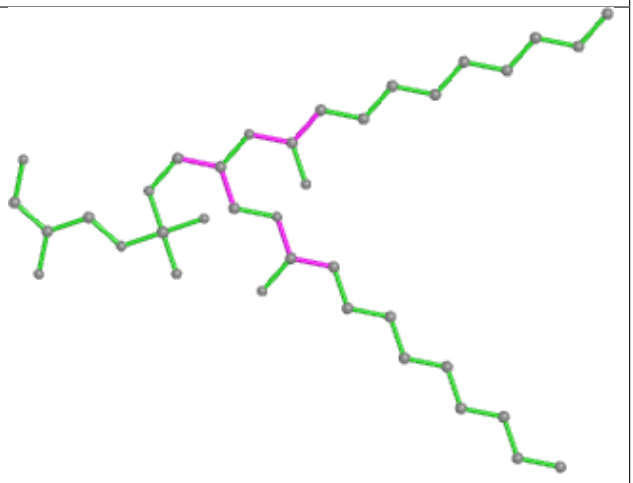


Rings

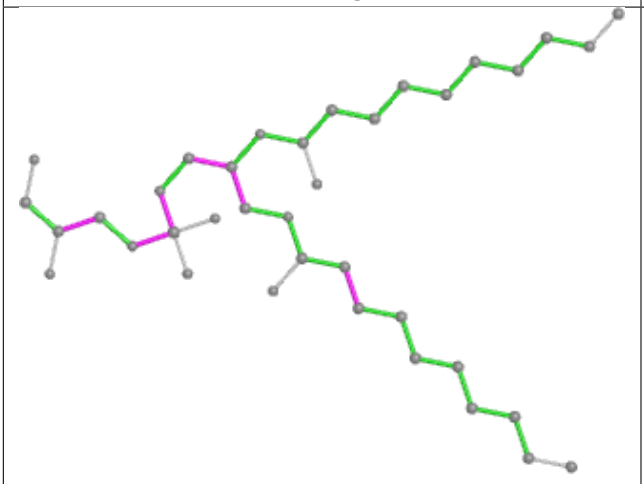
Ligand LHG 5 623



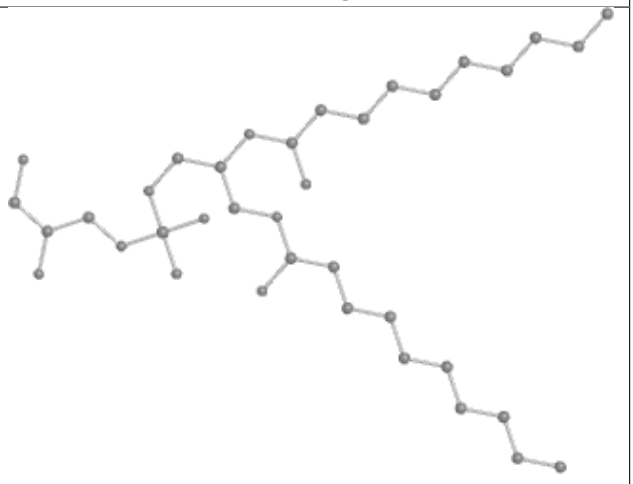
Bond lengths



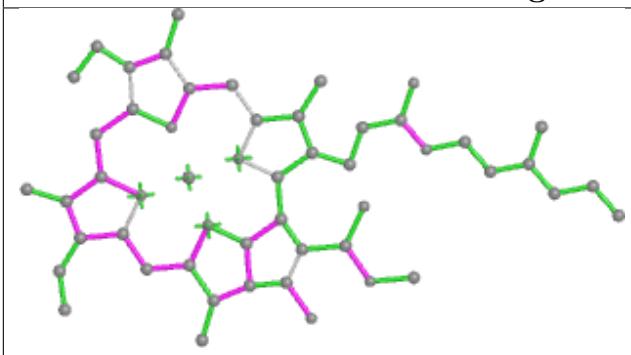
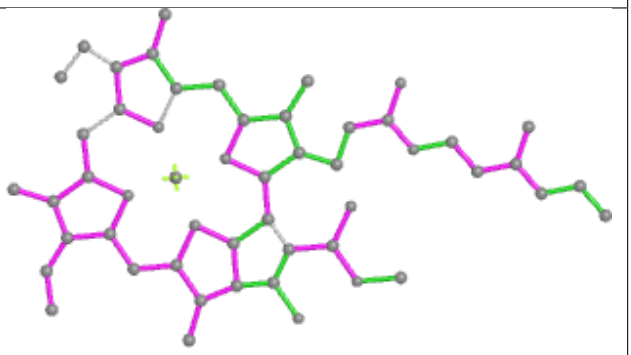
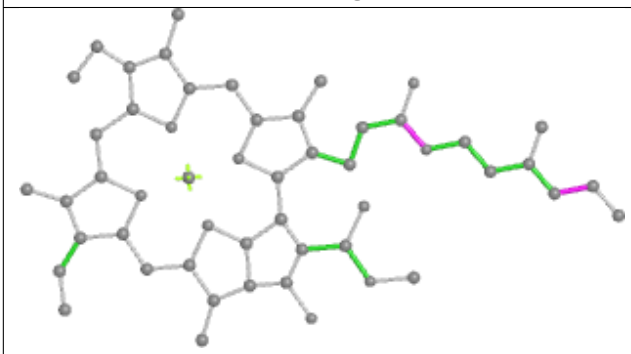
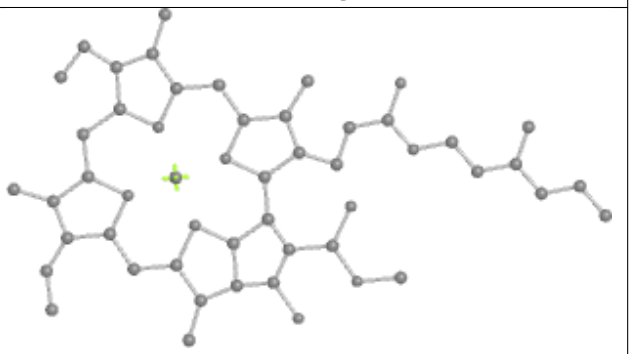
Bond angles

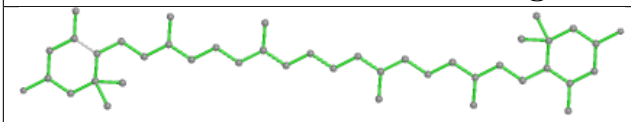
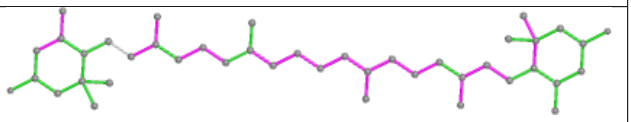
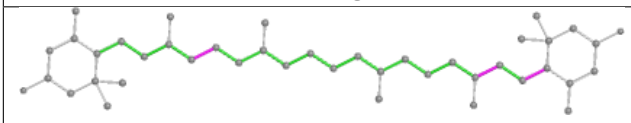
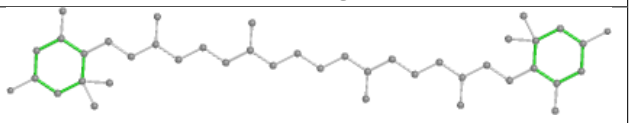


Torsions

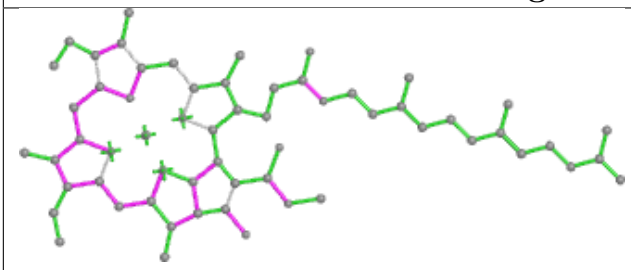


Rings

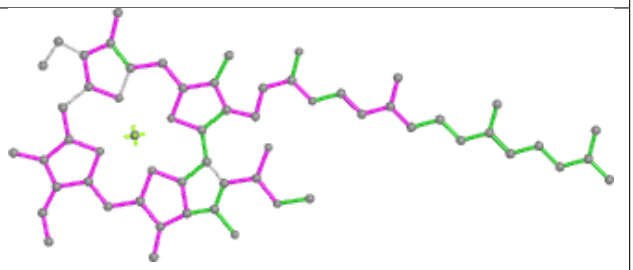
Ligand CLA 4 612	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT 8 618	
	
Bond lengths	Bond angles
	
Torsions	Rings

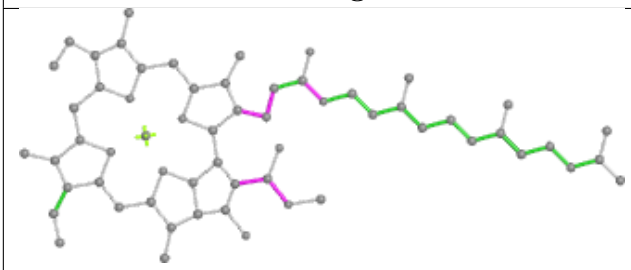
Ligand CLA 3 602



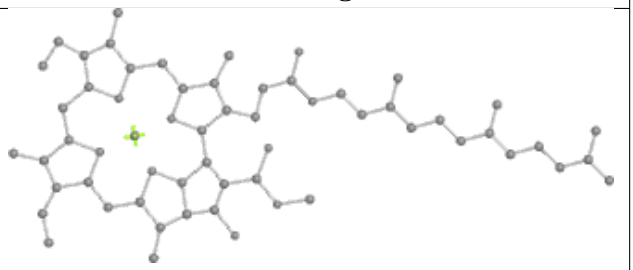
Bond lengths



Bond angles

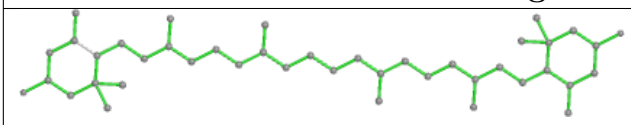


Torsions

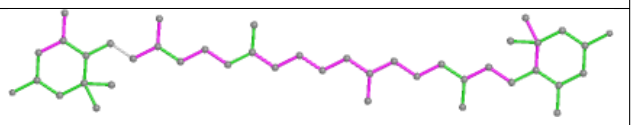


Rings

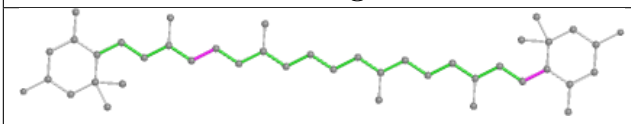
Ligand LUT 7 622



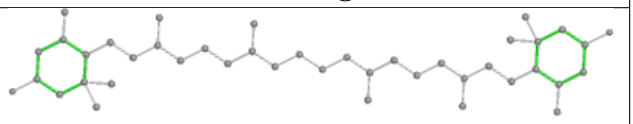
Bond lengths



Bond angles

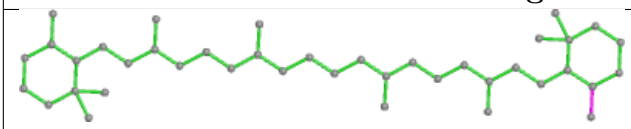


Torsions



Rings

Ligand BCR 7 623



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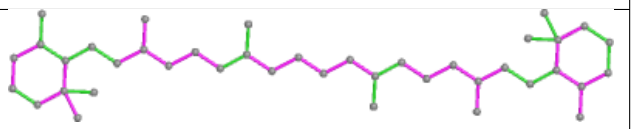
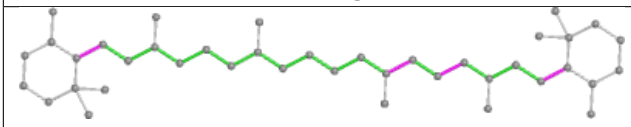
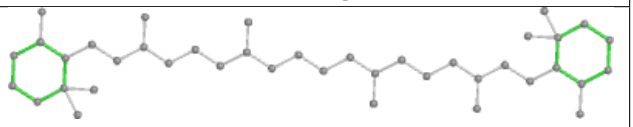


Bond angles

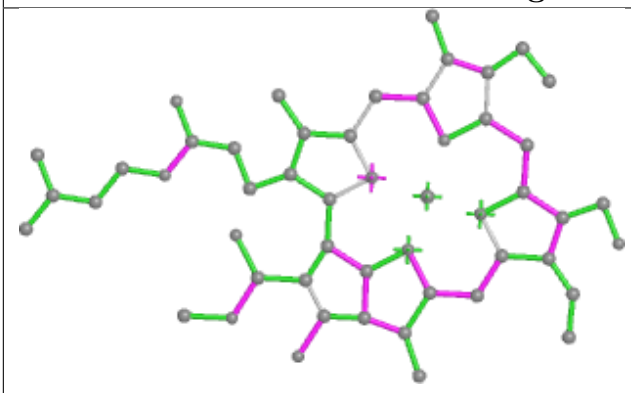


Torsions

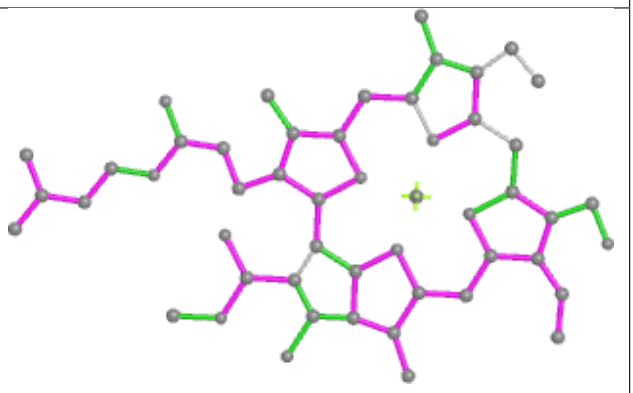


Rings

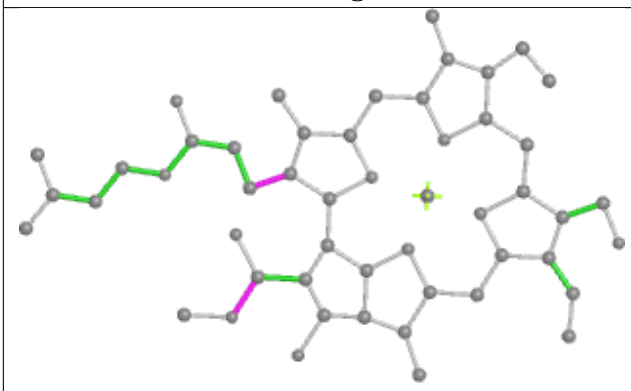
Ligand CHL 6 608



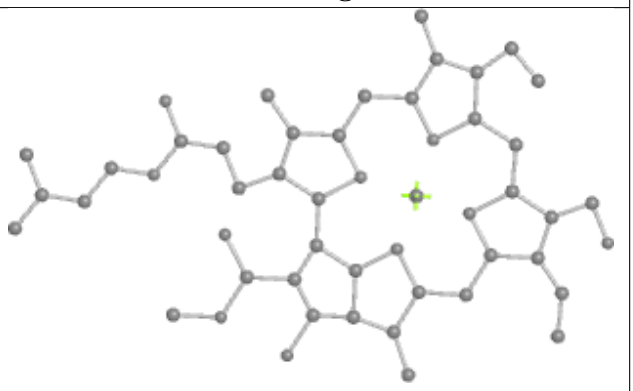
Bond lengths



Bond angles

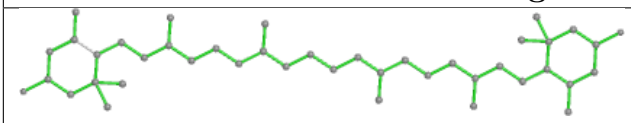


Torsions

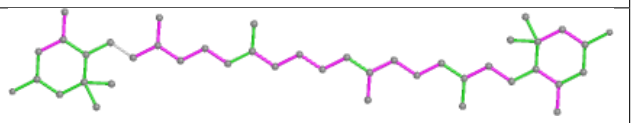


Rings

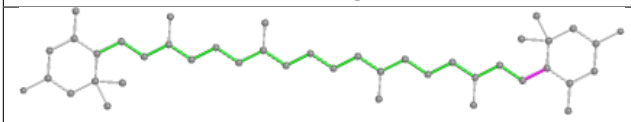
Ligand LUT 6 621



Bond lengths



Bond angles



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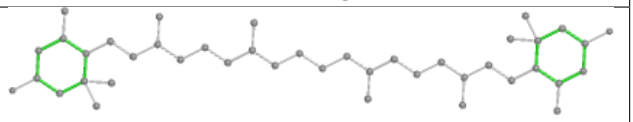
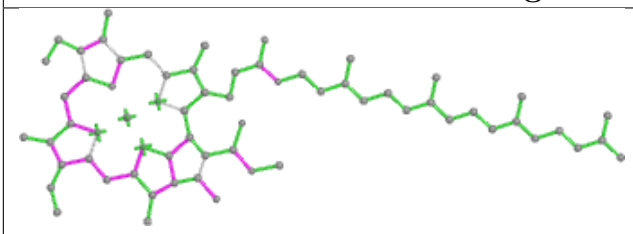
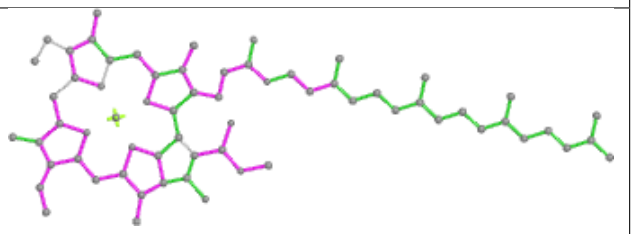


Rings

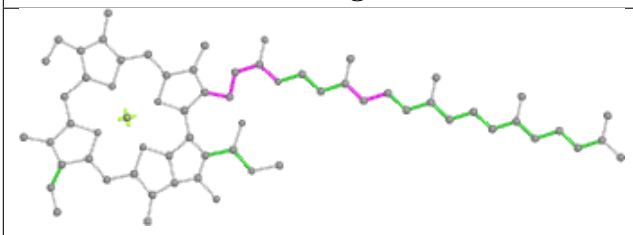
Ligand CLA B 828



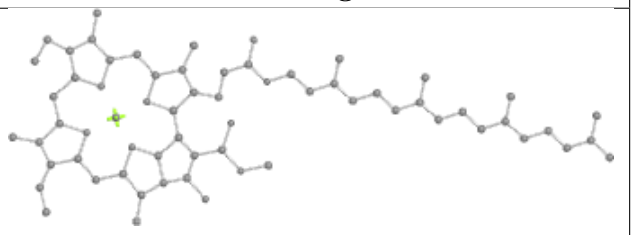
Bond lengths



Bond angles

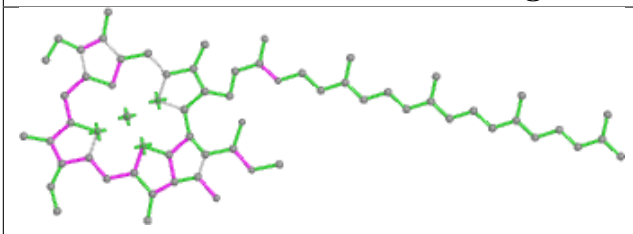


Torsions

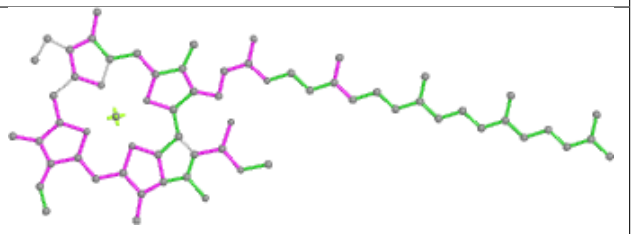


Rings

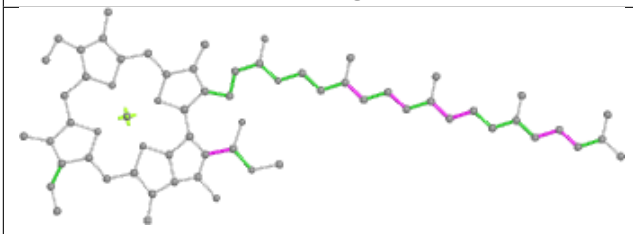
Ligand CLA B 837



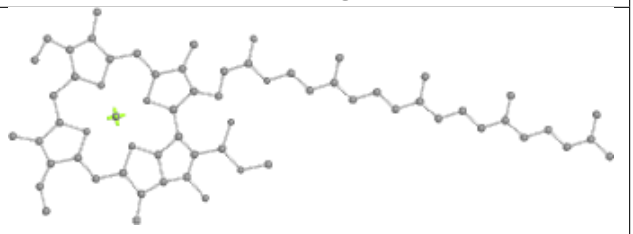
Bond lengths



Bond angles

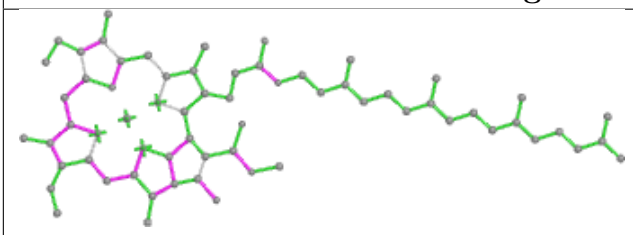


Torsions

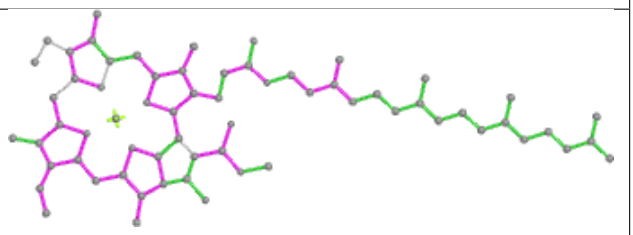


Rings

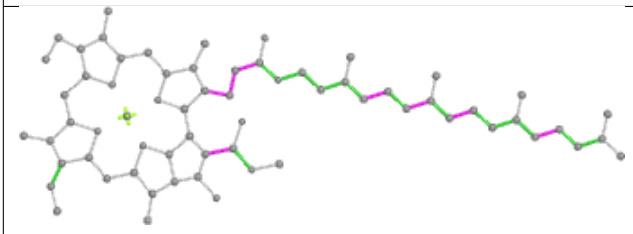
Ligand CLA A 804



Bond lengths



Bond angles



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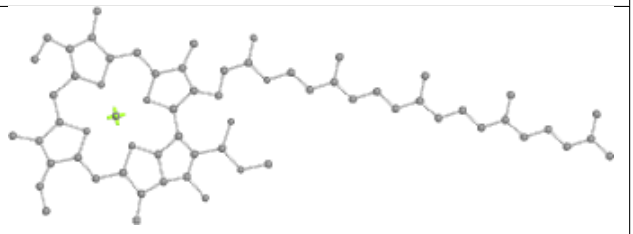
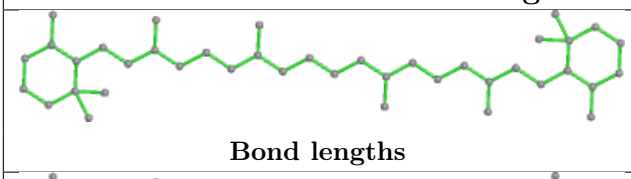
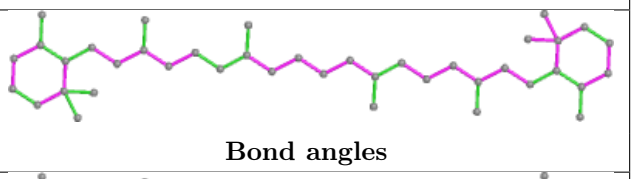


Rings

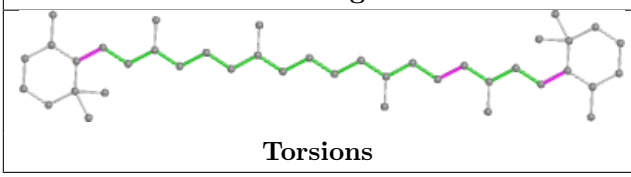
Ligand BCR B 846



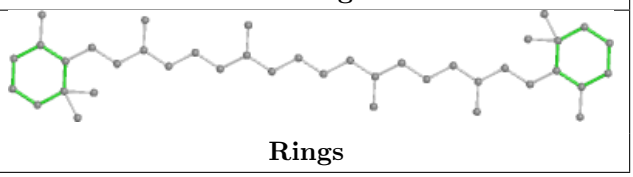
Bond lengths



Bond angles

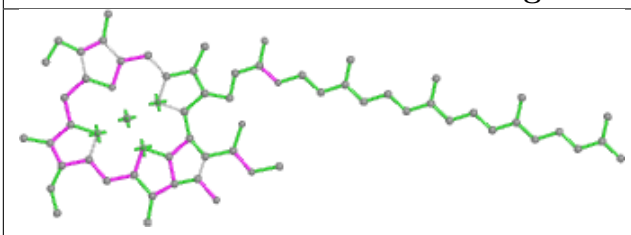


Torsions

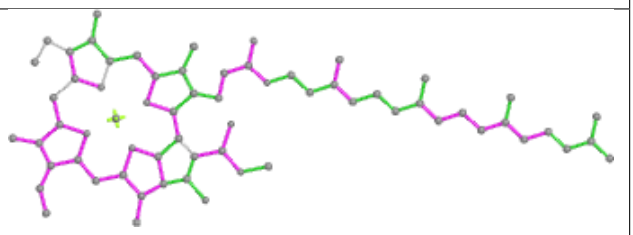


Rings

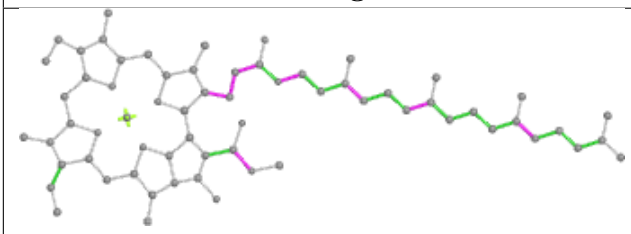
Ligand CLA A 810



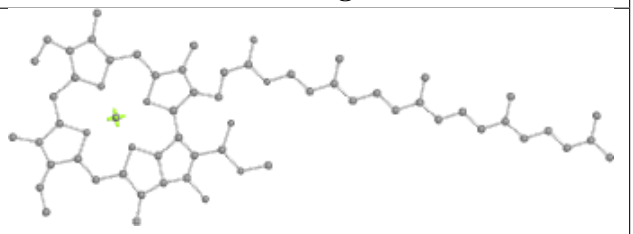
Bond lengths



Bond angles

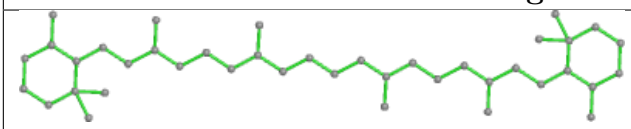


Torsions

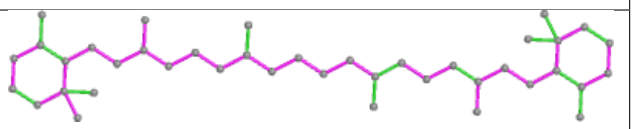


Rings

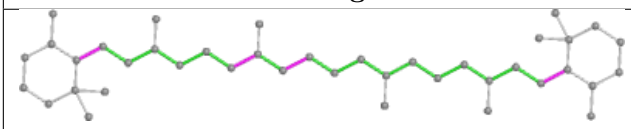
Ligand BCR 5 622



Bond lengths



Bond angles



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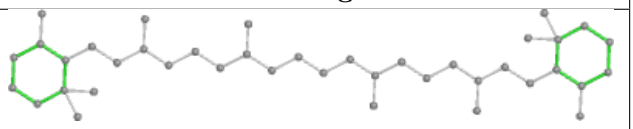
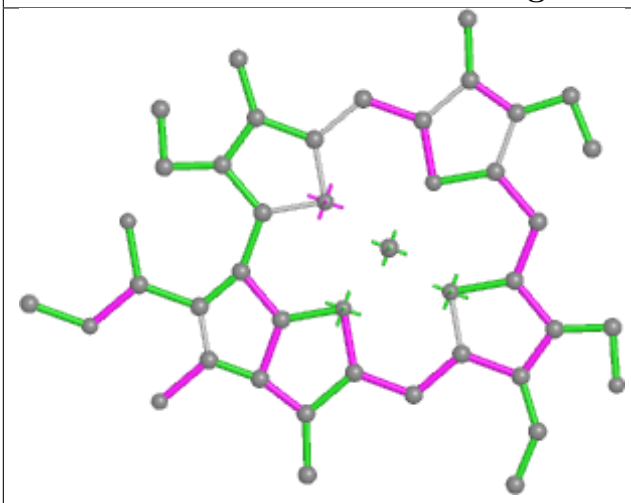
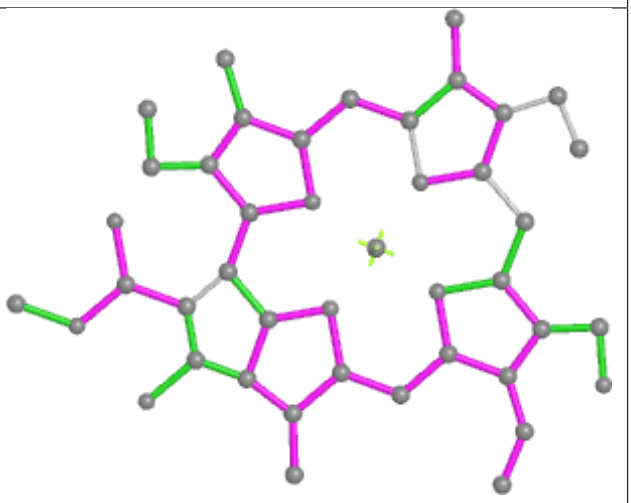


Rings

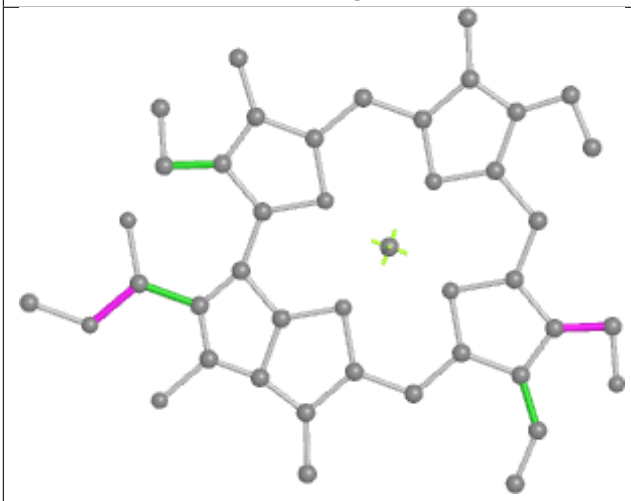
Ligand CHL 5 618



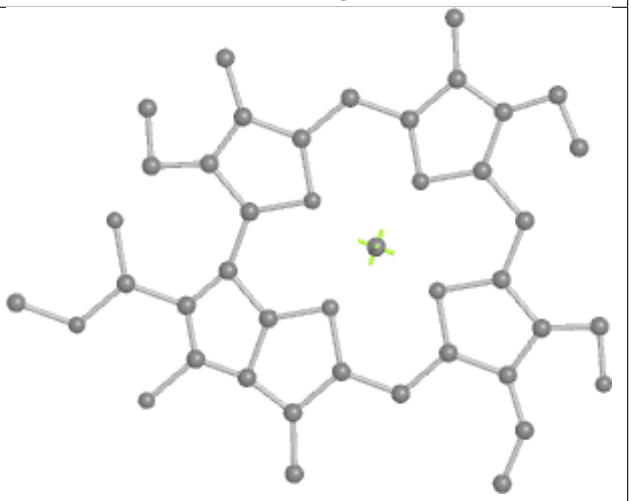
Bond lengths



Bond angles

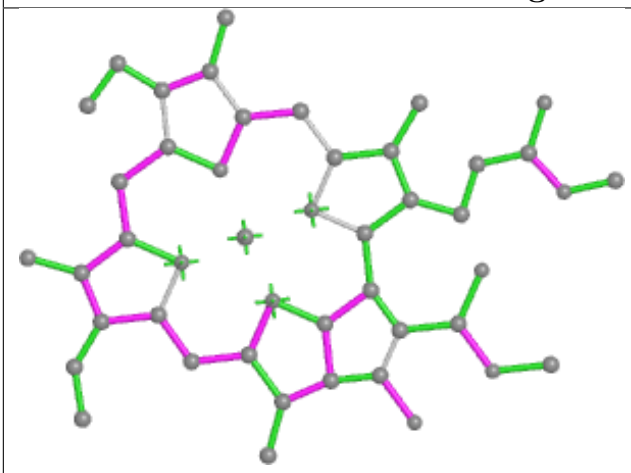


Torsions

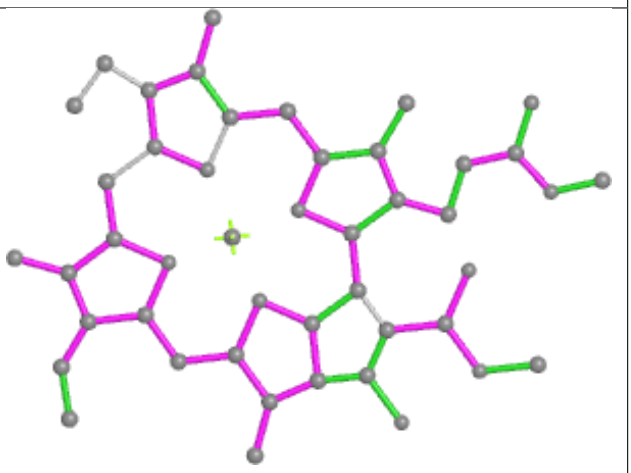


Rings

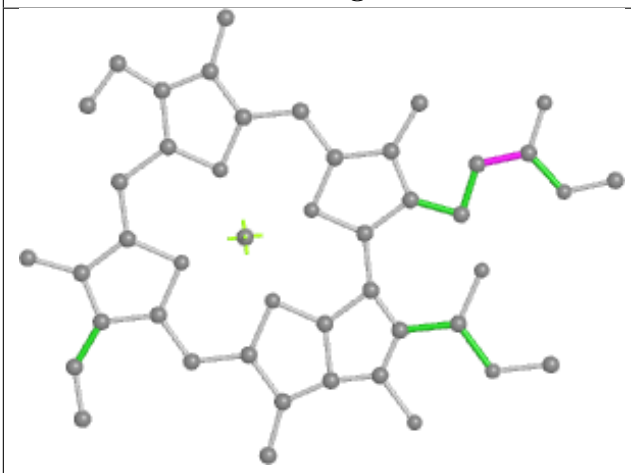
Ligand CLA 9 603



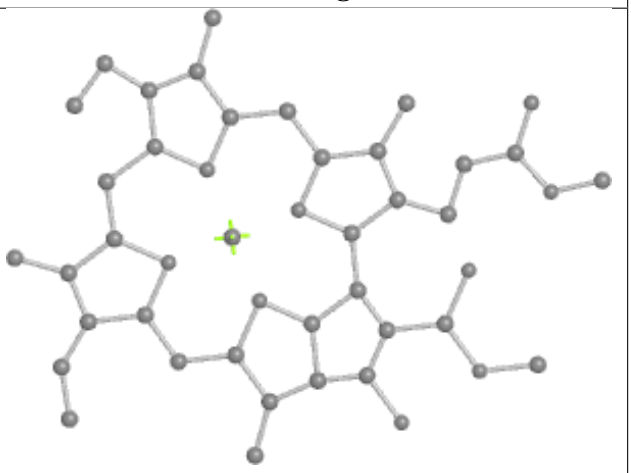
Bond lengths



Bond angles

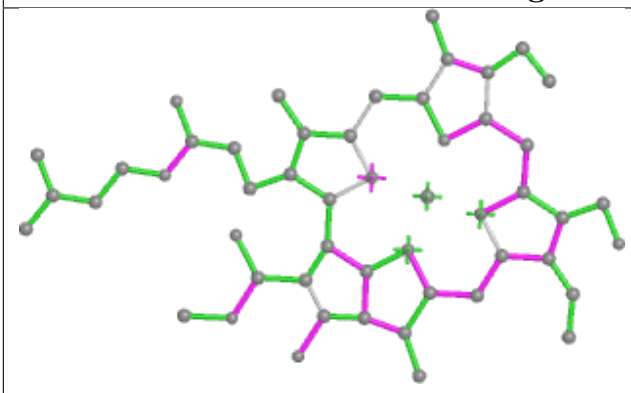


Torsions

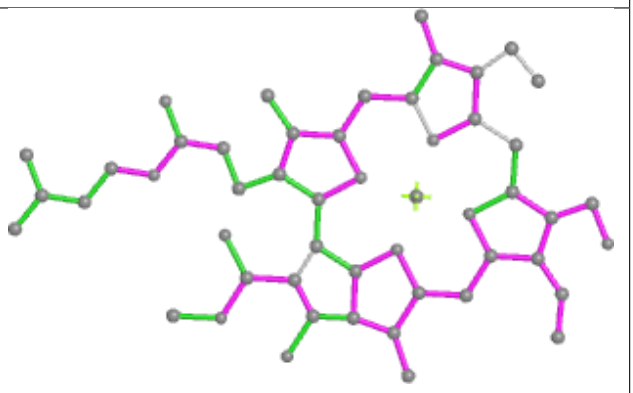


Rings

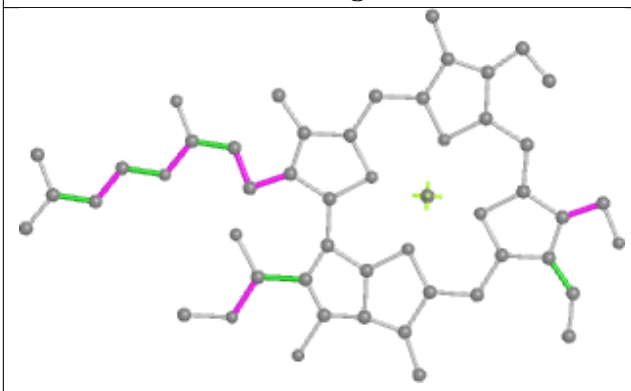
Ligand CHL 5 607



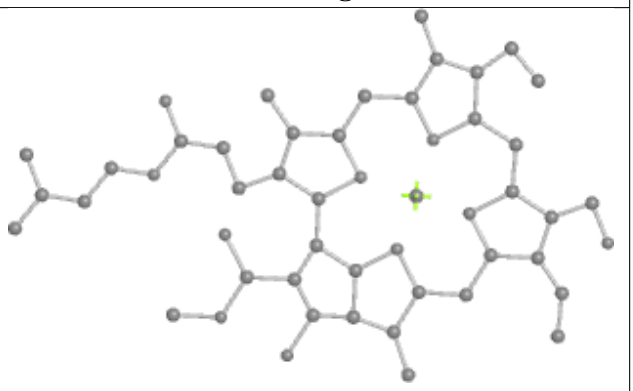
Bond lengths



Bond angles

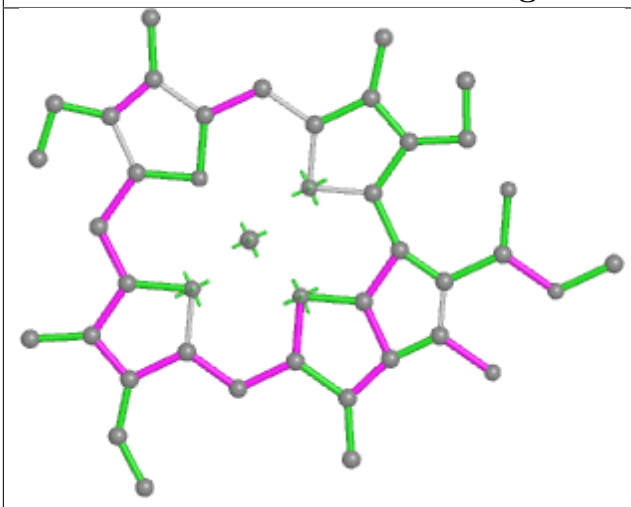


Torsions

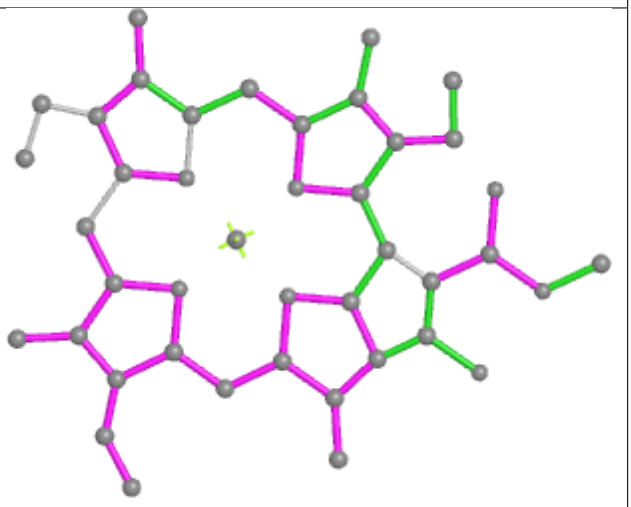


Rings

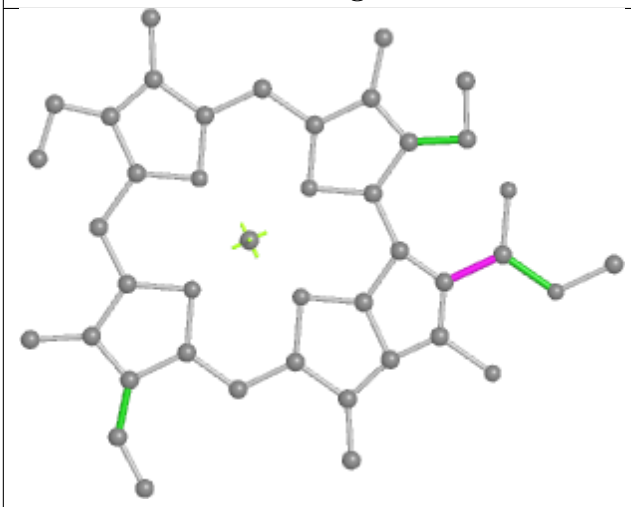
Ligand CLA J 3002



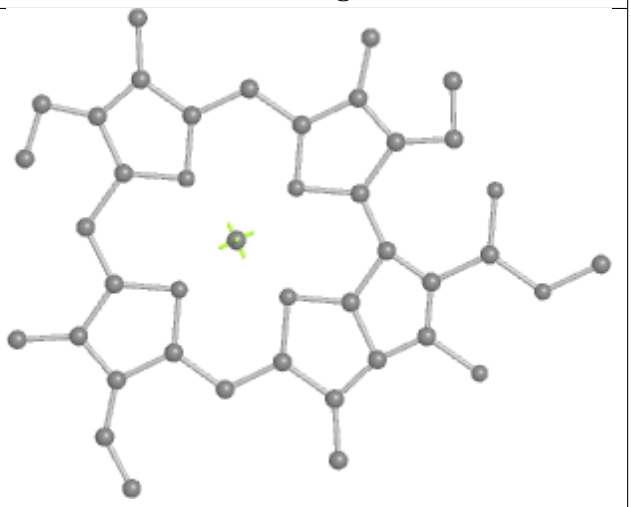
Bond lengths



Bond angles

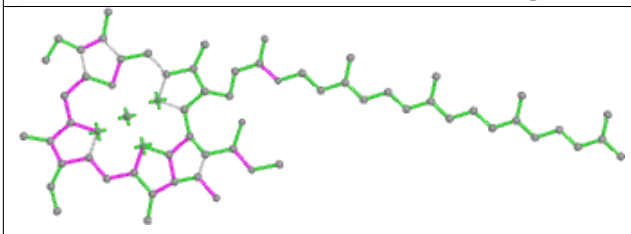


Torsions

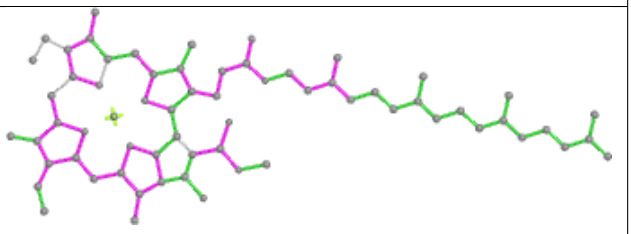


Rings

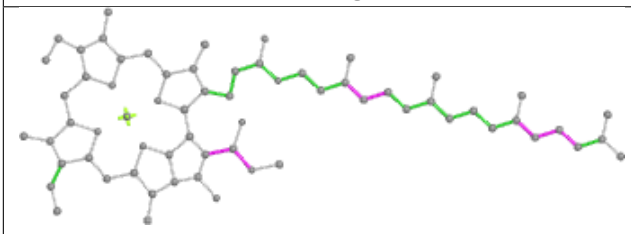
Ligand CLA B 808



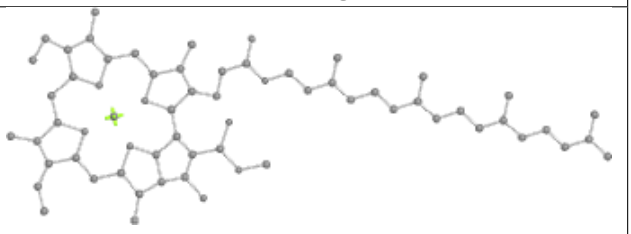
Bond lengths



Bond angles

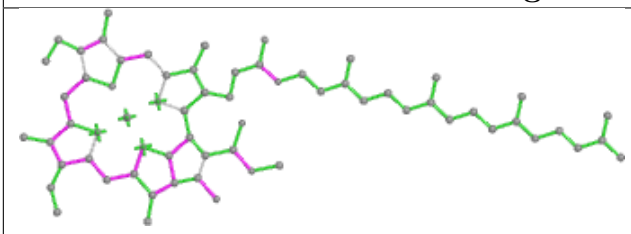


Torsions

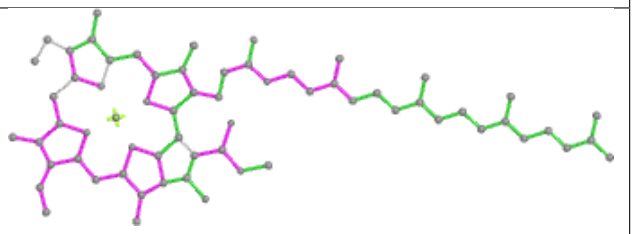


Rings

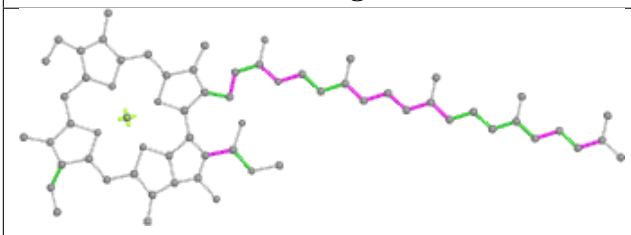
Ligand CLA A 842



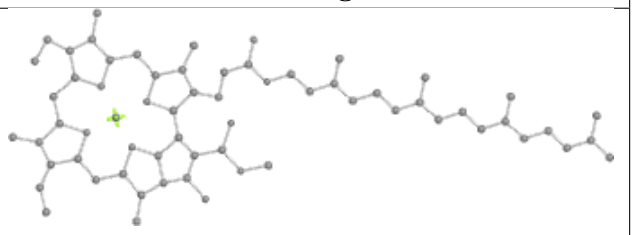
Bond lengths



Bond angles

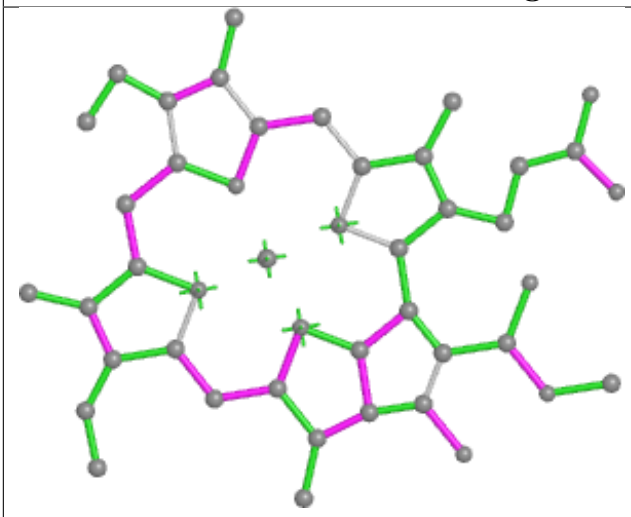


Torsions

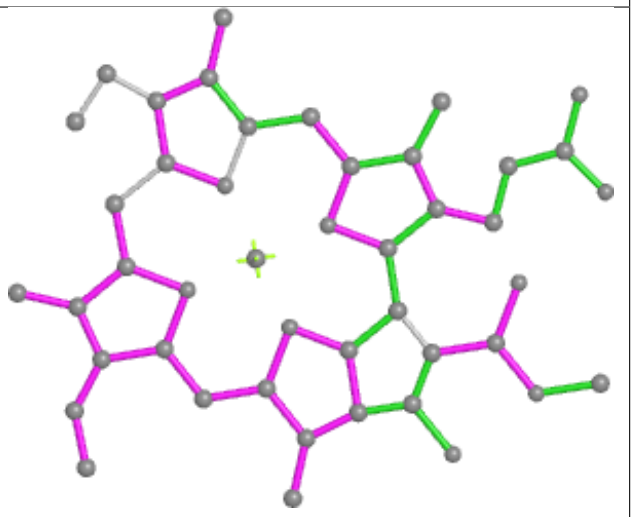


Rings

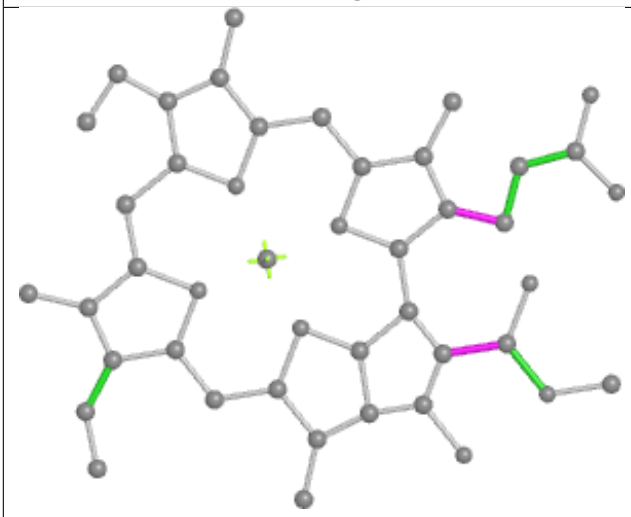
Ligand CLA A 821



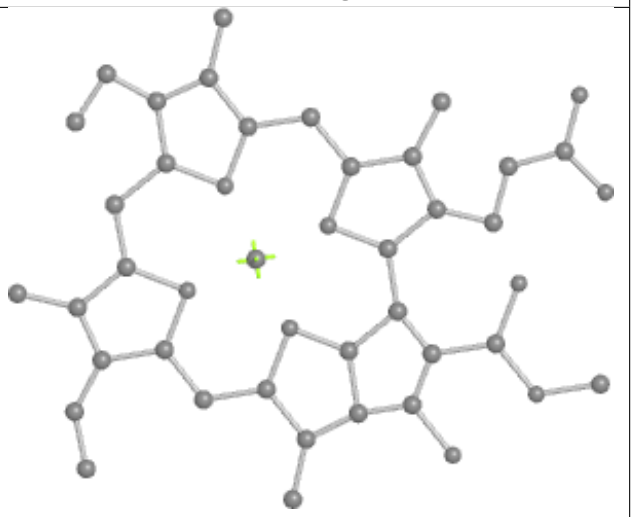
Bond lengths



Bond angles

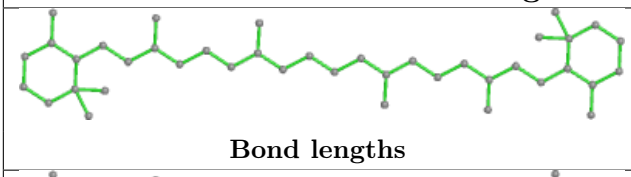


Torsions



Rings

Ligand BCR B 801



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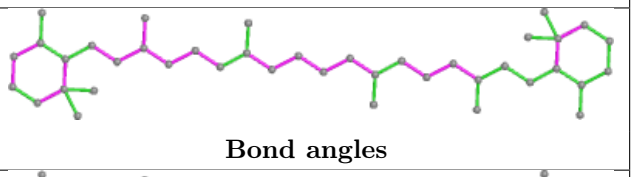
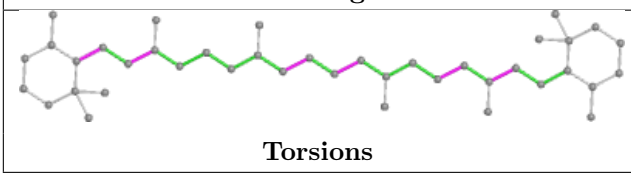
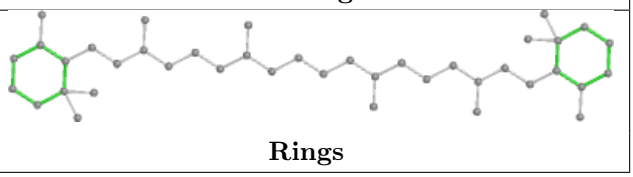


Bond angles

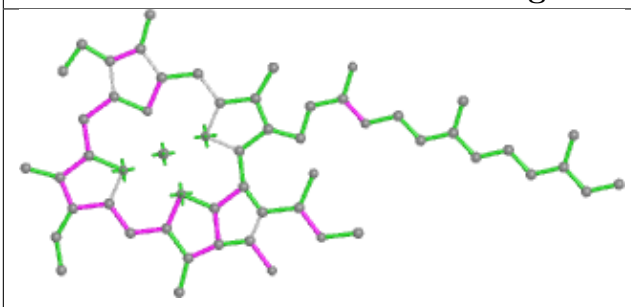


Torsions

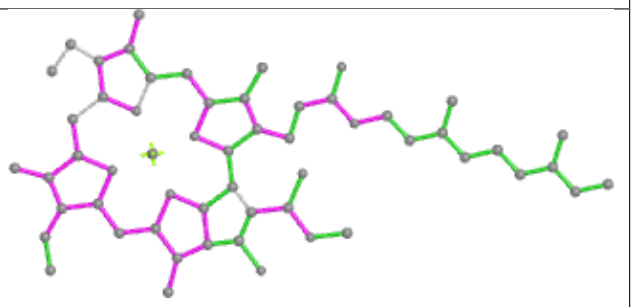


Rings

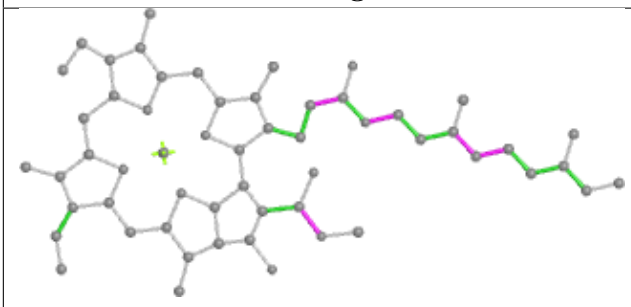
Ligand CLA 5 613



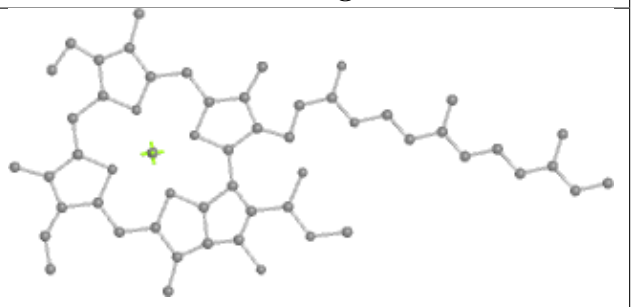
Bond lengths



Bond angles

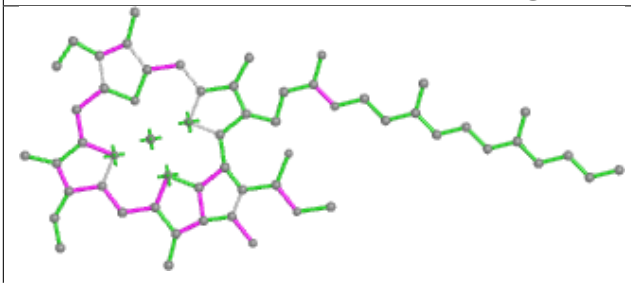


Torsions

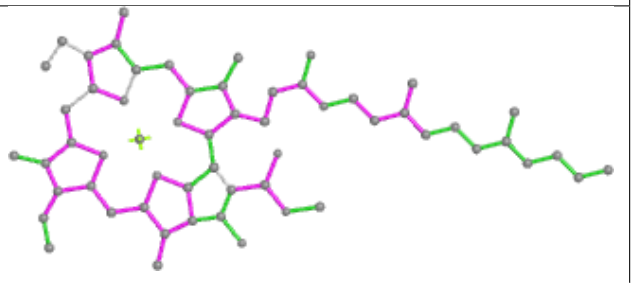


Rings

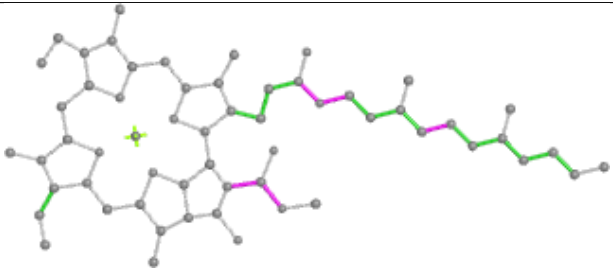
Ligand CLA B 833



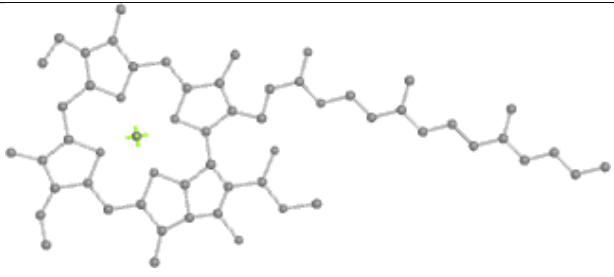
Bond lengths



Bond angles

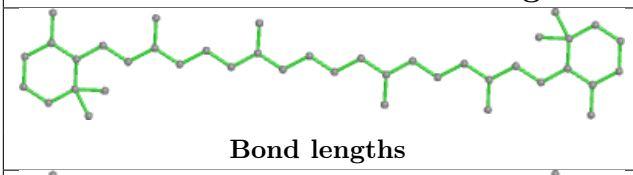


Torsions

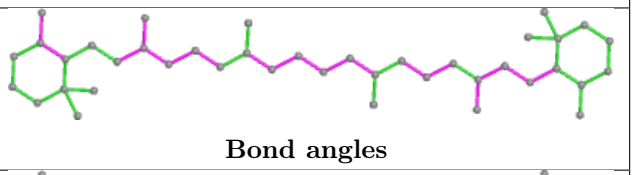


Rings

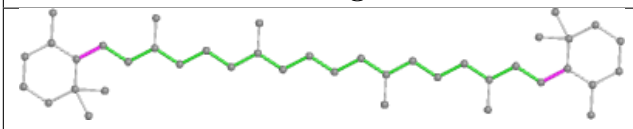
Ligand BCR B 848



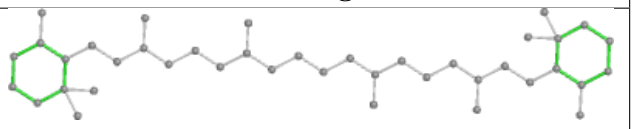
Bond lengths



Bond angles

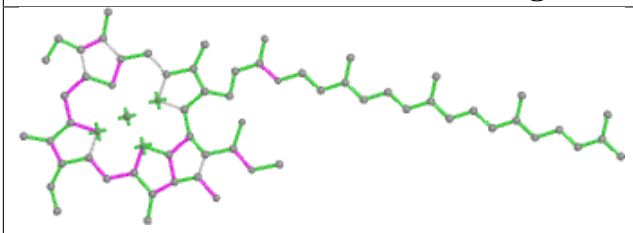


Torsions

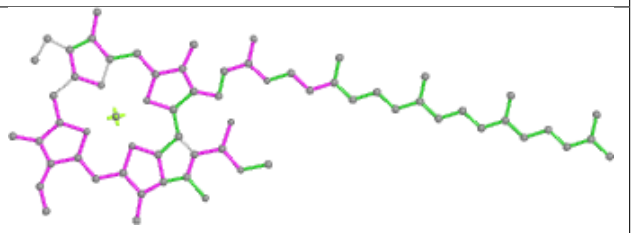


Rings

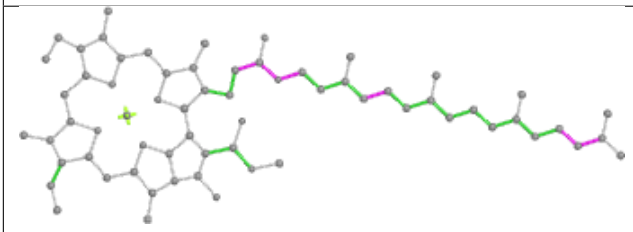
Ligand CL0 A 801



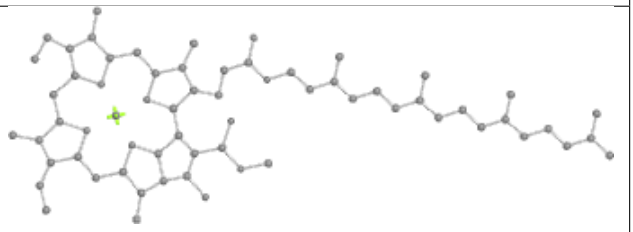
Bond lengths



Bond angles

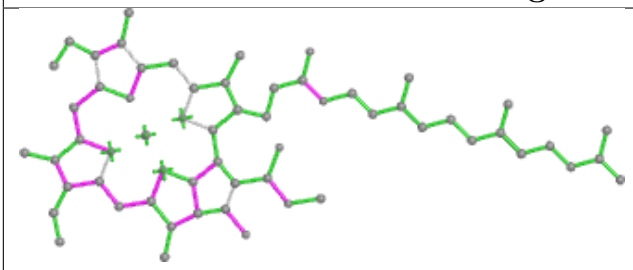


Torsions

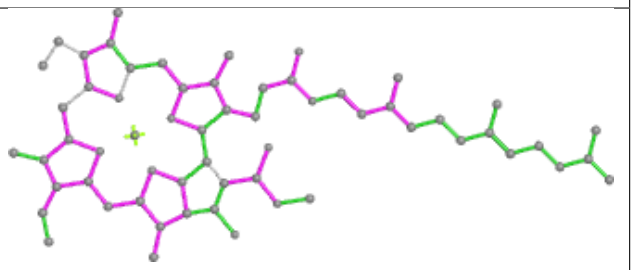


Rings

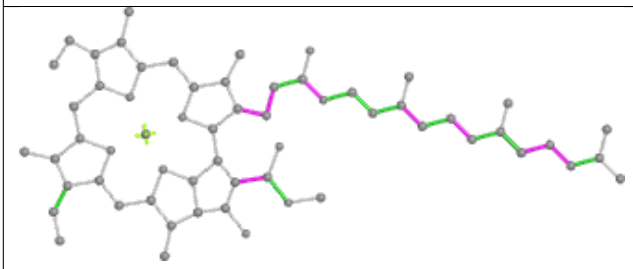
Ligand CLA 4 610



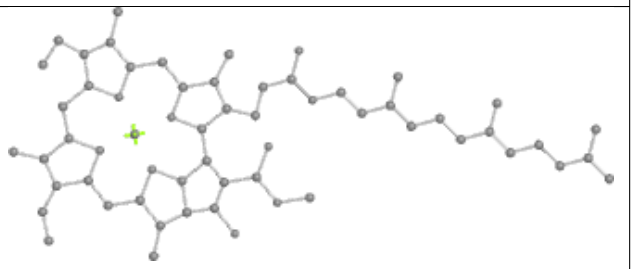
Bond lengths



Bond angles

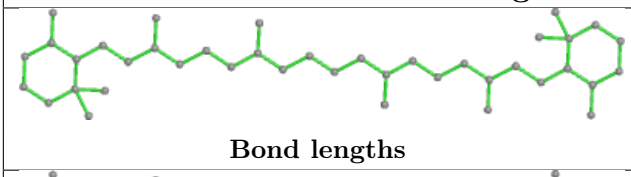


Torsions

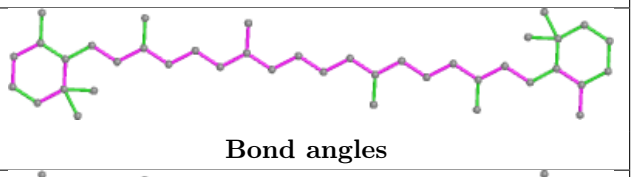


Rings

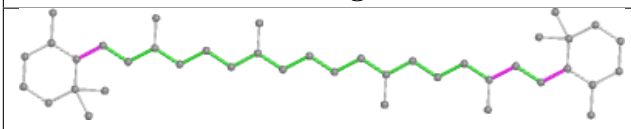
Ligand BCR K 4004



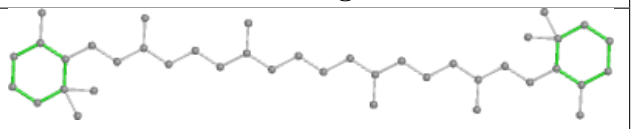
Bond lengths



Bond angles

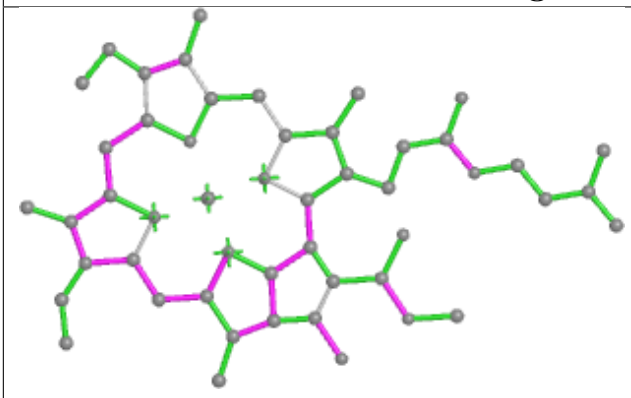


Torsions

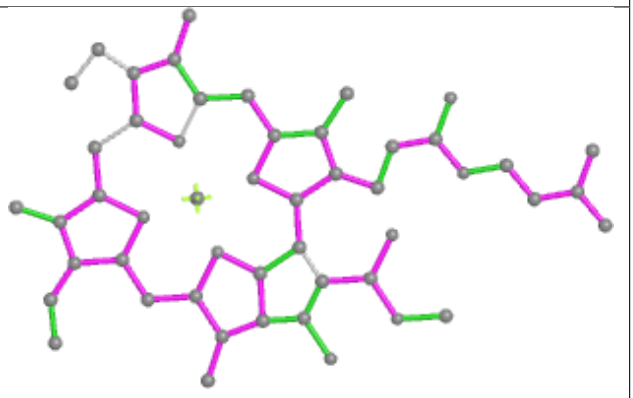


Rings

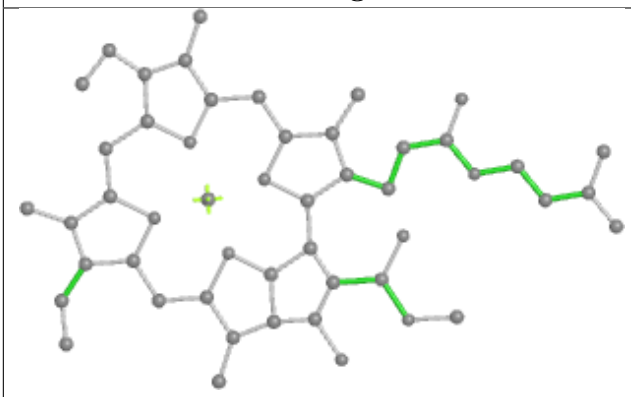
Ligand CLA 9 609



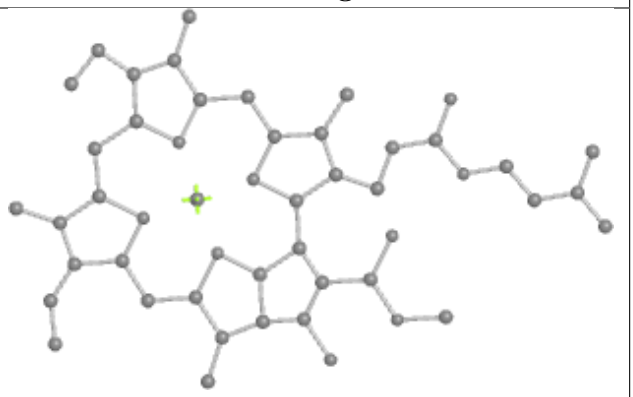
Bond lengths



Bond angles

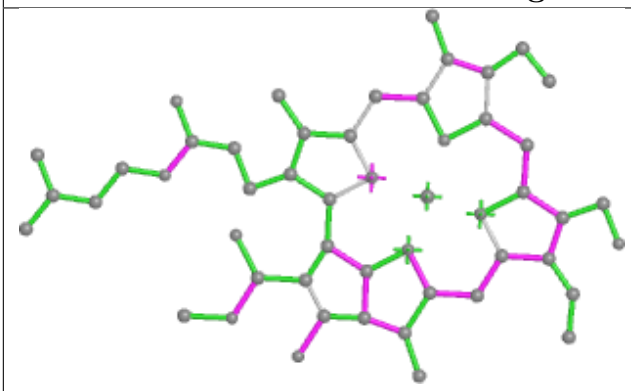


Torsions

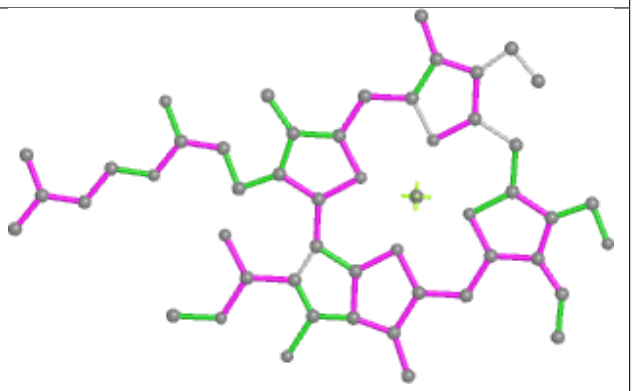


Rings

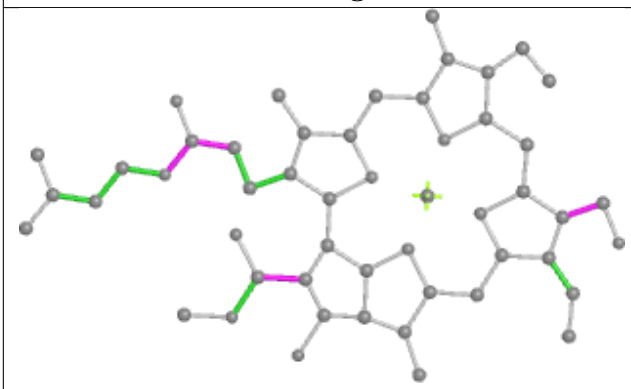
Ligand CHL 9 607



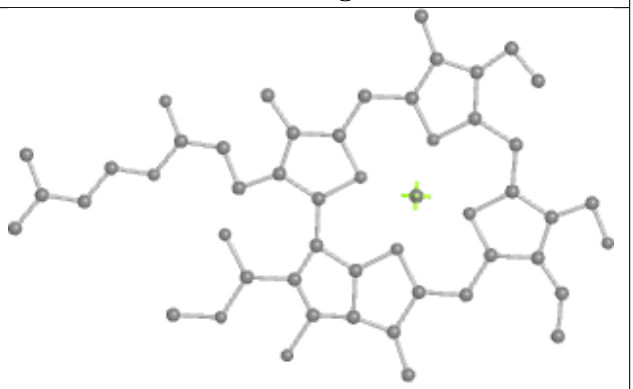
Bond lengths



Bond angles

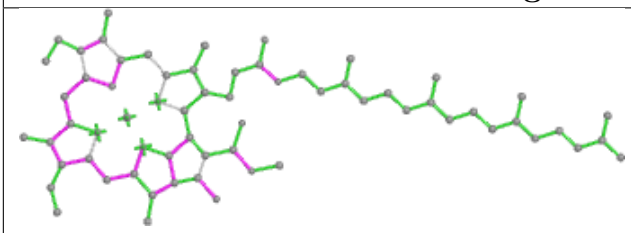


Torsions

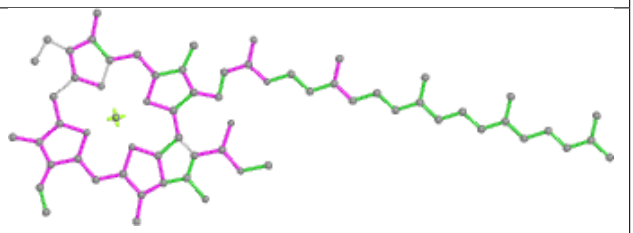


Rings

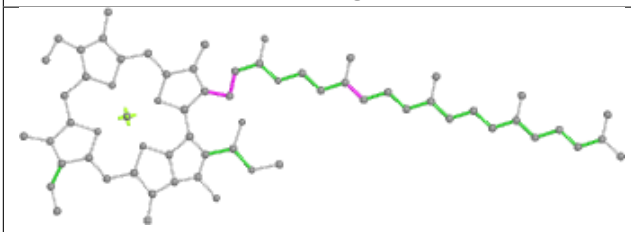
Ligand CLA A 803



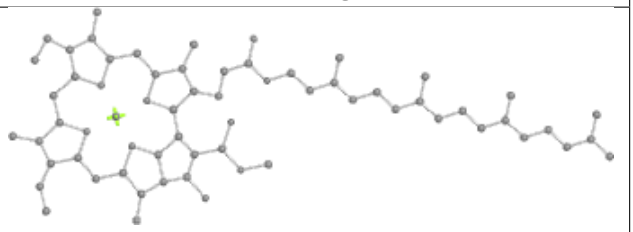
Bond lengths



Bond angles

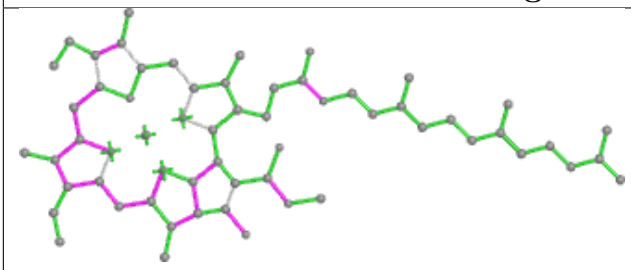


Torsions

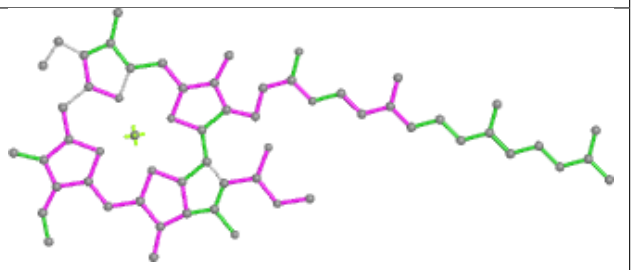


Rings

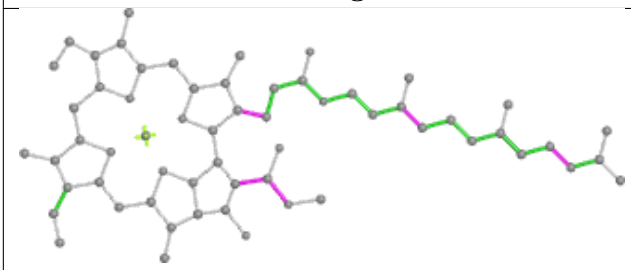
Ligand CLA B 823



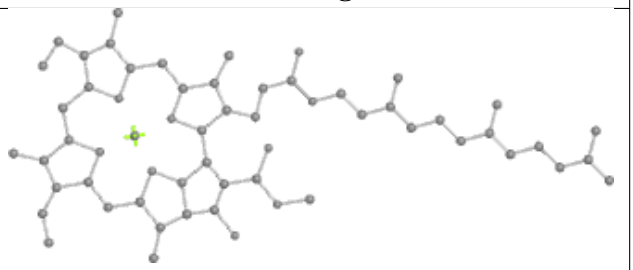
Bond lengths



Bond angles

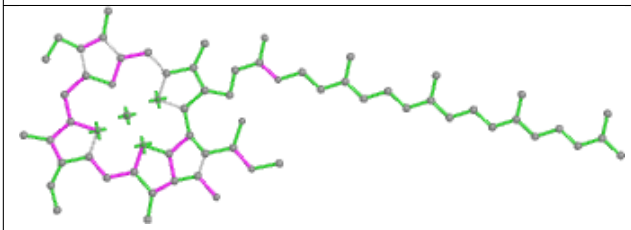


Torsions



Rings

Ligand CLA 7 601



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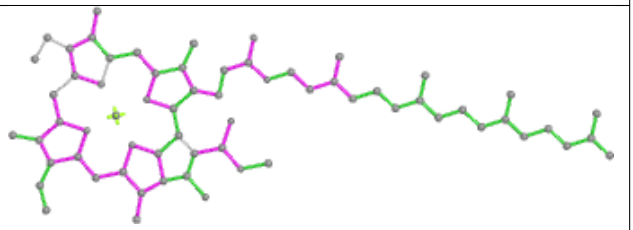
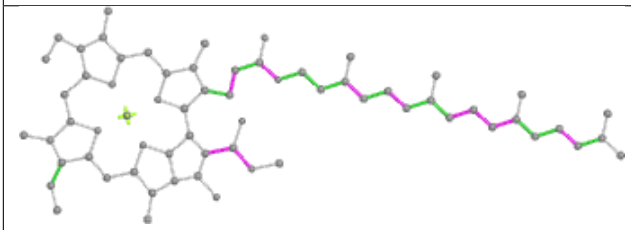
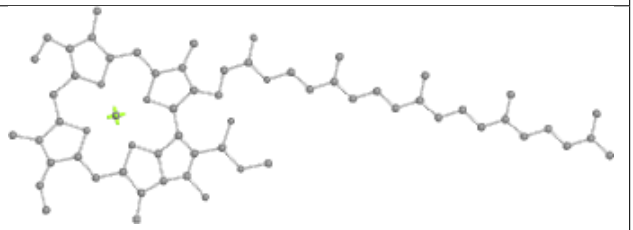


Bond angles

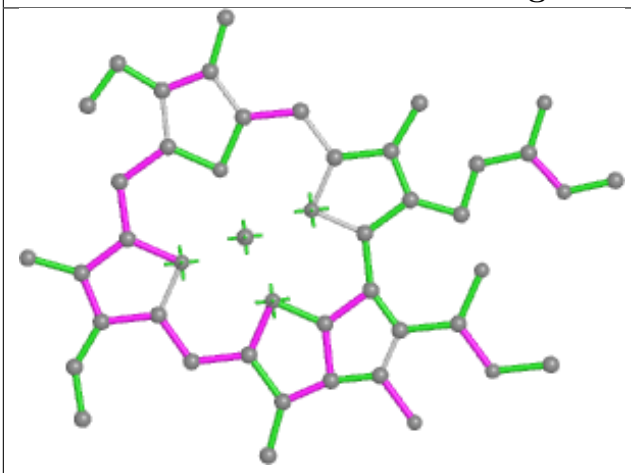


Torsions



Rings

Ligand CLA 7 603



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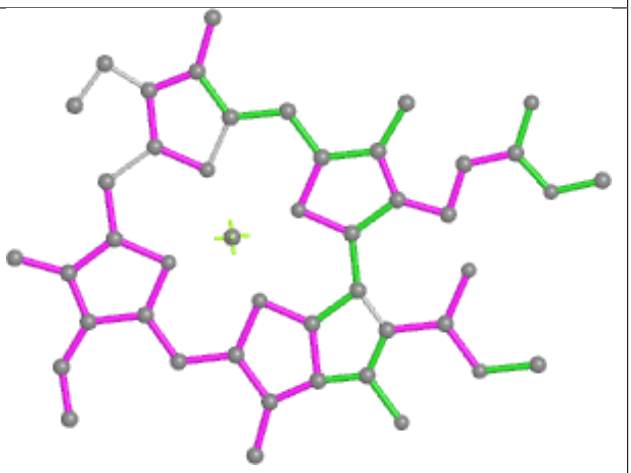
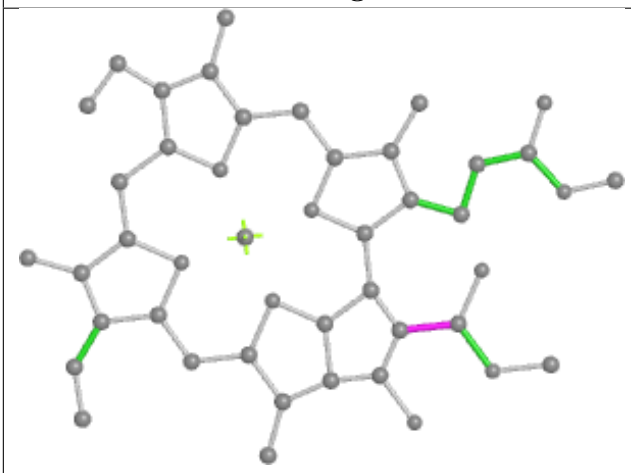
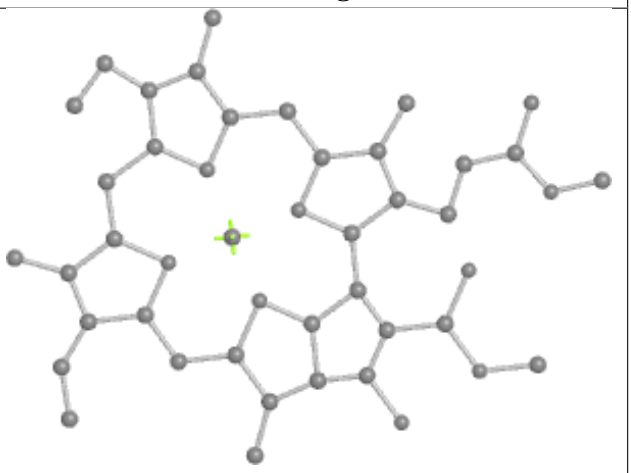


Bond angles

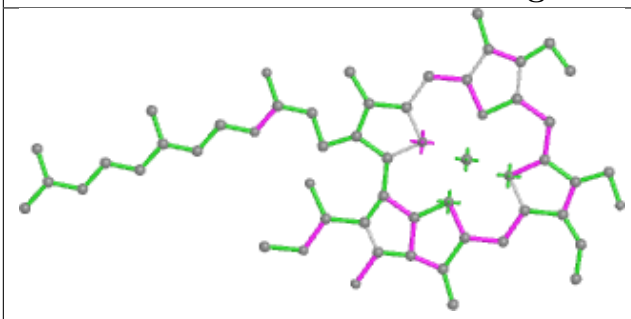


Torsions

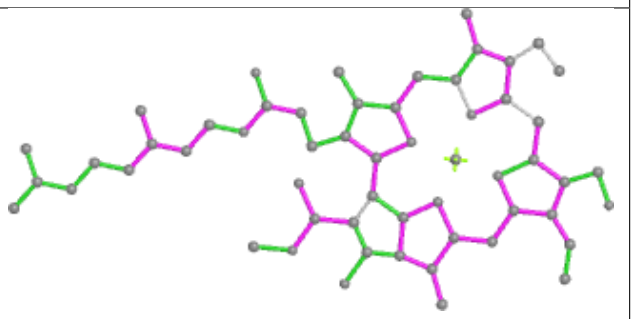


Rings

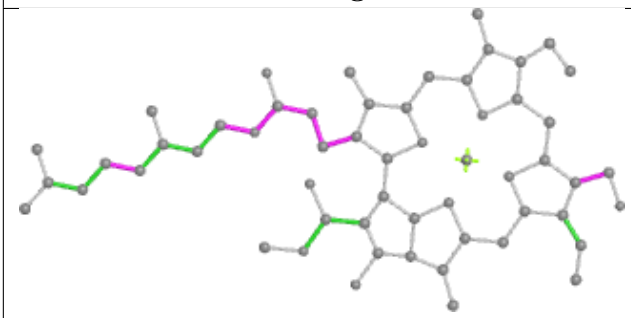
Ligand CHL 8 607



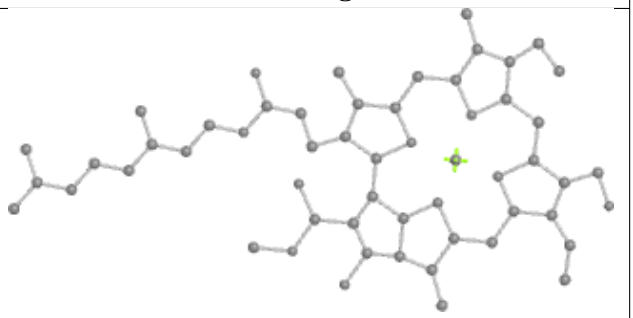
Bond lengths



Bond angles

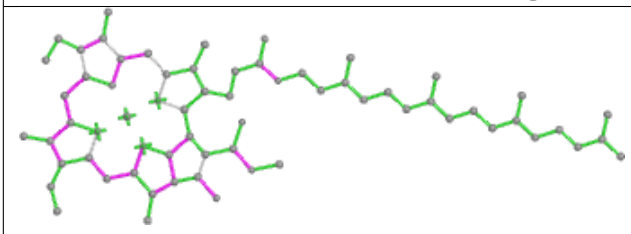


Torsions

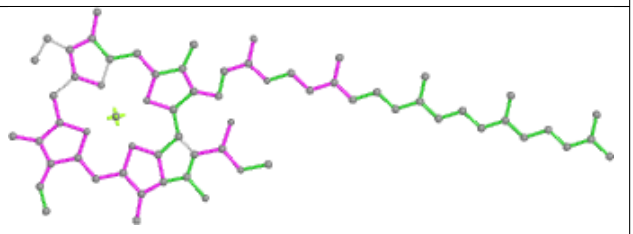


Rings

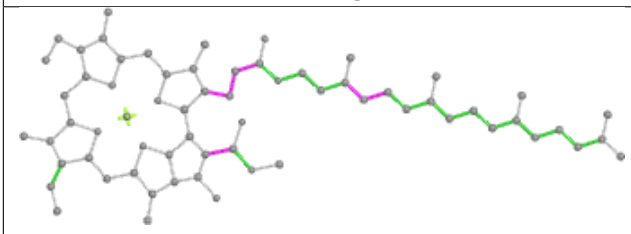
Ligand CLA B 824



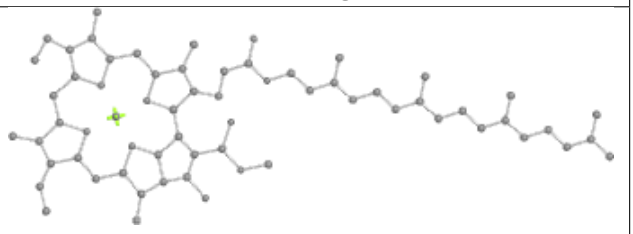
Bond lengths



Bond angles

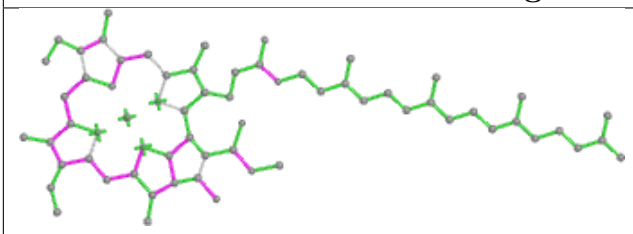


Torsions

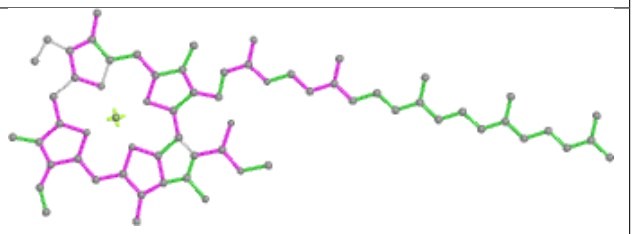


Rings

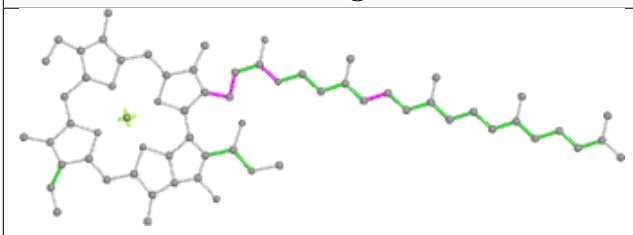
Ligand CLA B 852



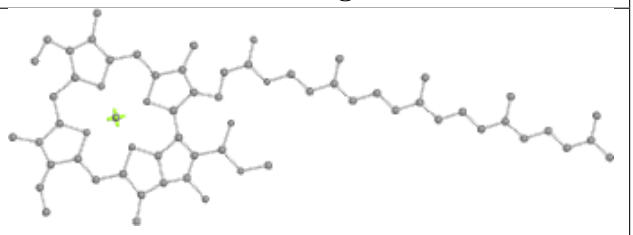
Bond lengths



Bond angles

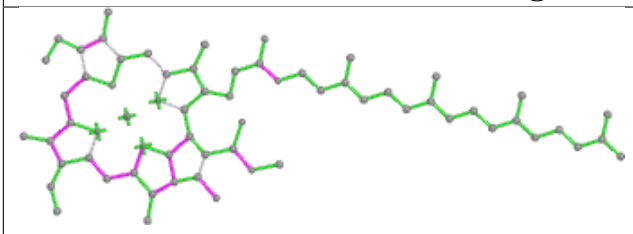


Torsions

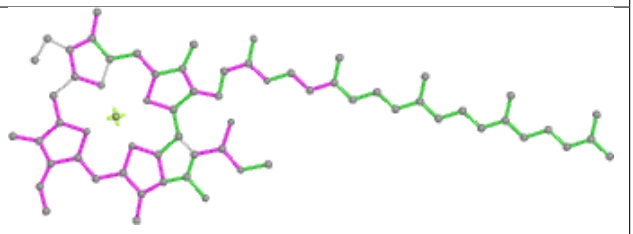


Rings

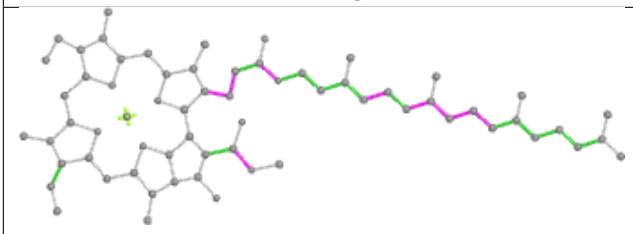
Ligand CLA 6 602



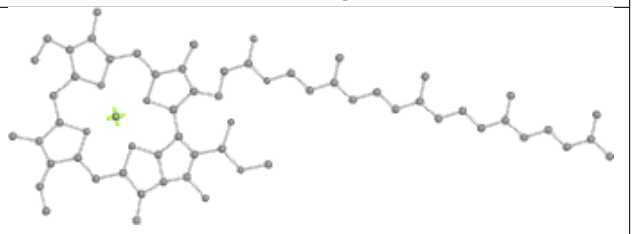
Bond lengths



Bond angles

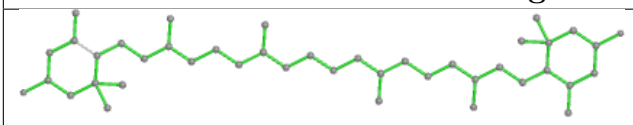


Torsions

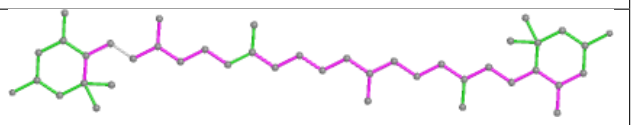


Rings

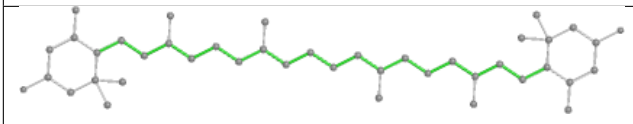
Ligand LUT 5 620



Bond lengths



Bond angles



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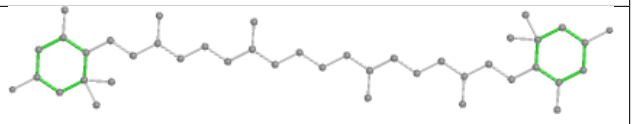
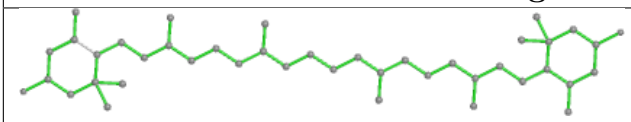
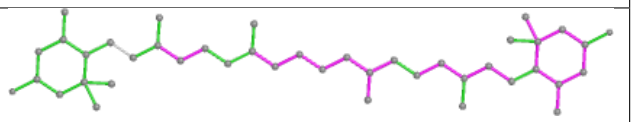


Rings

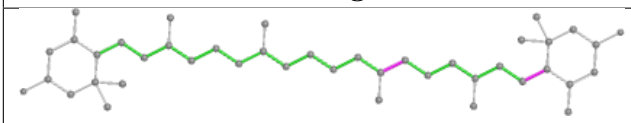
Ligand LUT 2 617



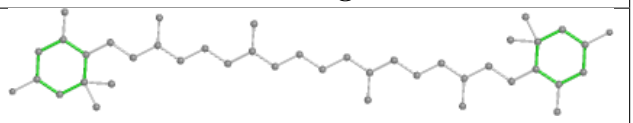
Bond lengths



Bond angles

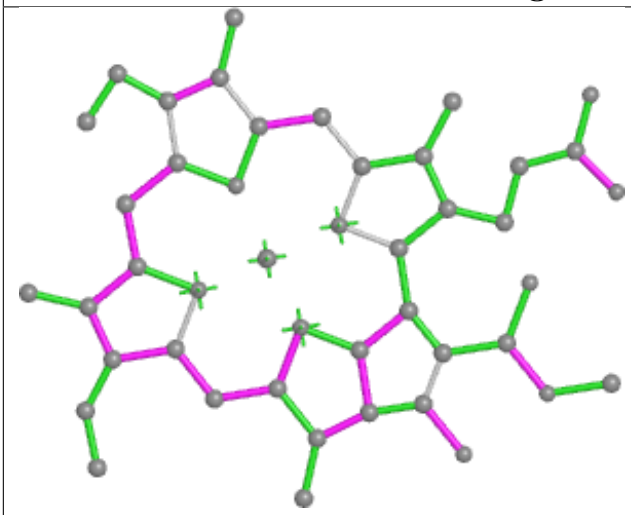


Torsions

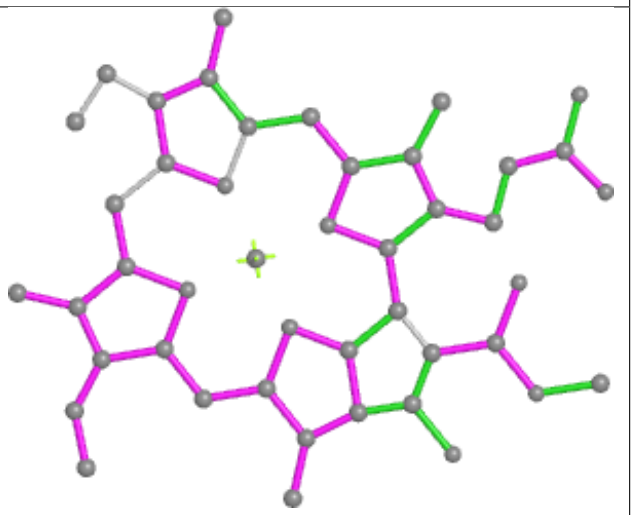


Rings

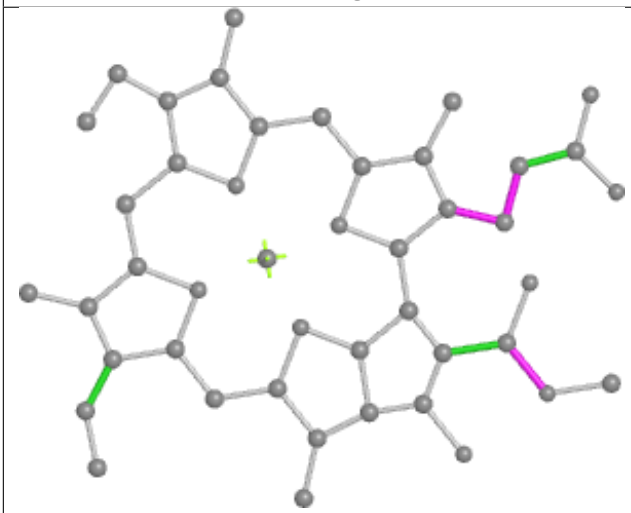
Ligand CLA 9 614



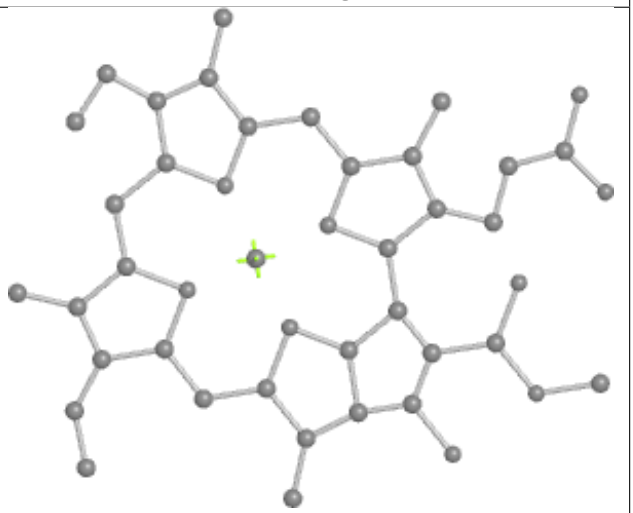
Bond lengths



Bond angles

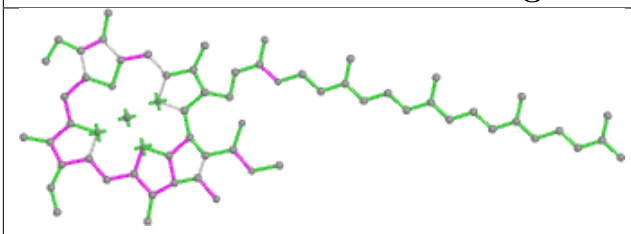


Torsions

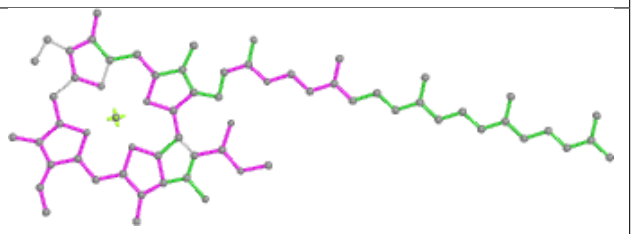


Rings

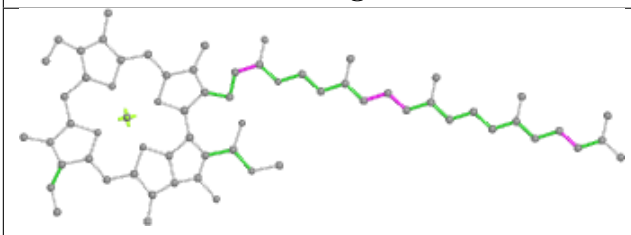
Ligand CLA A 802



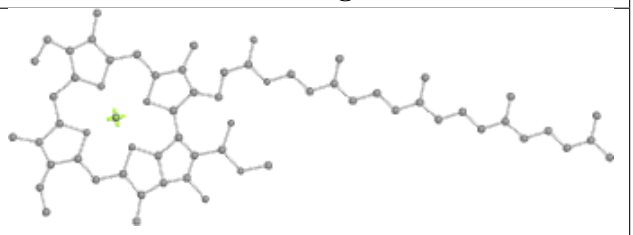
Bond lengths



Bond angles

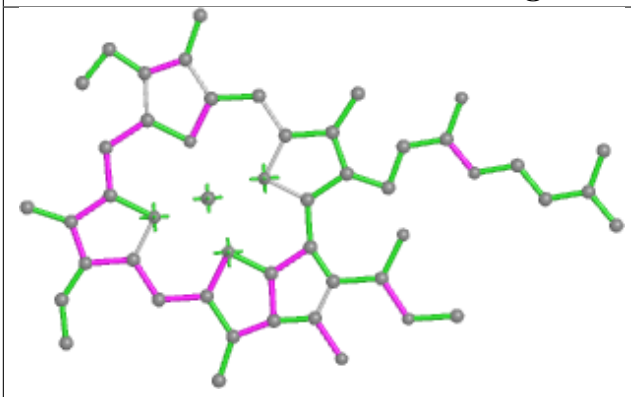


Torsions



Rings

Ligand CLA B 830



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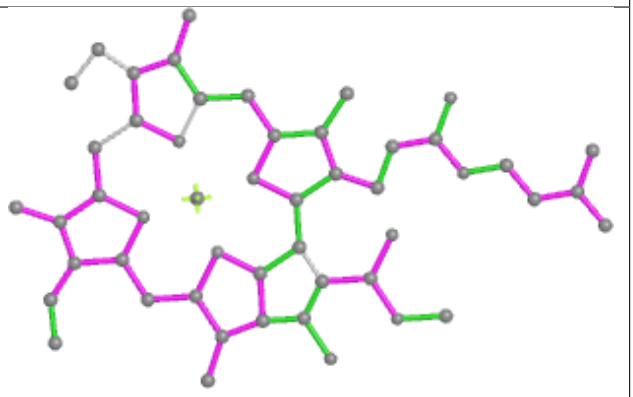
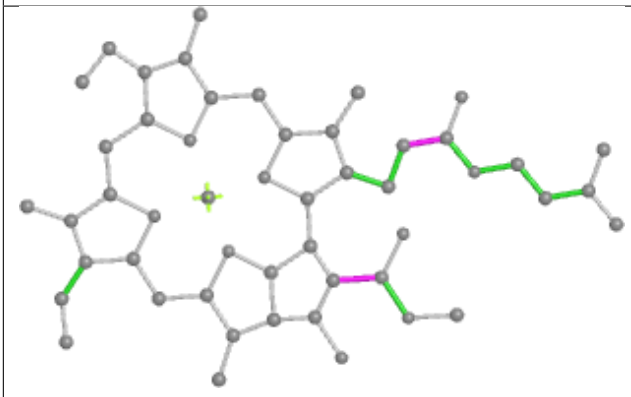
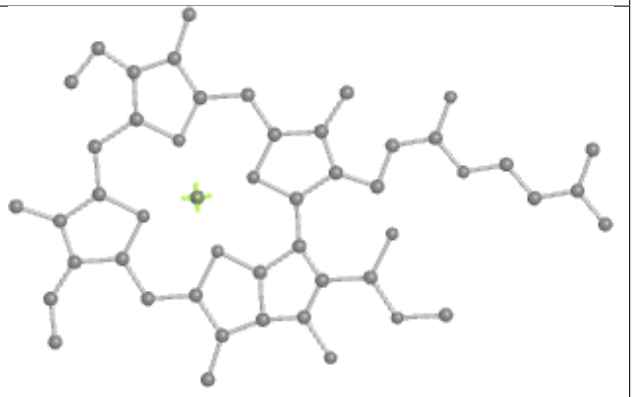


Bond angles

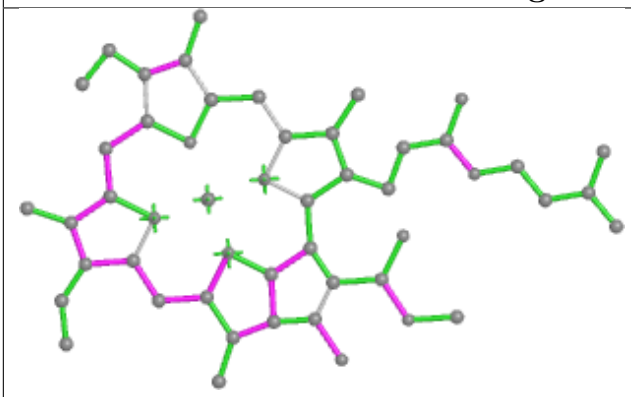


Torsions

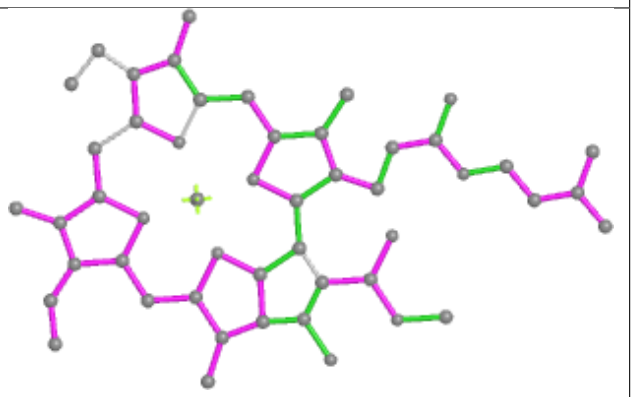


Rings

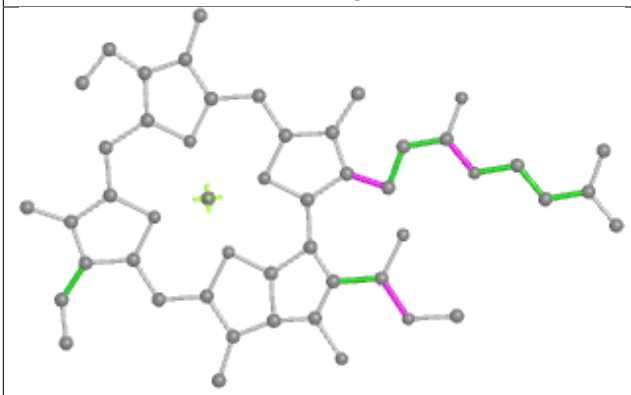
Ligand CLA 5 604



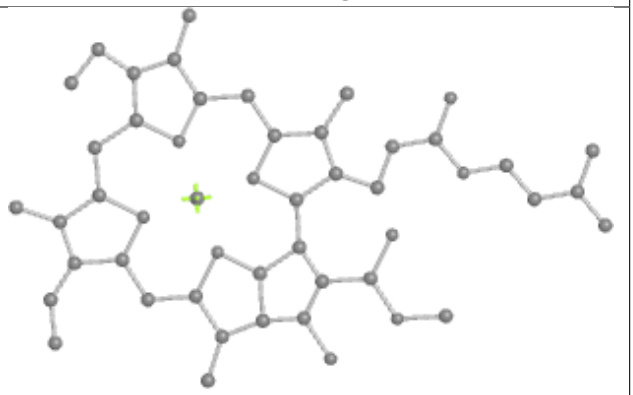
Bond lengths



Bond angles

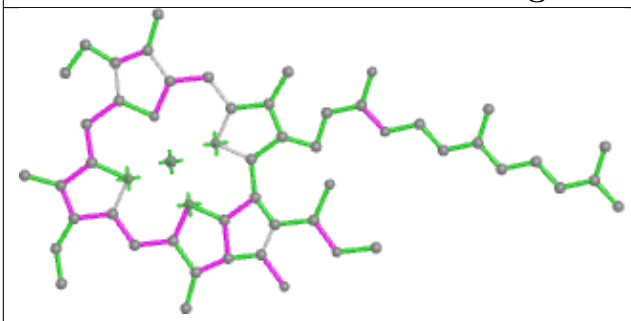


Torsions

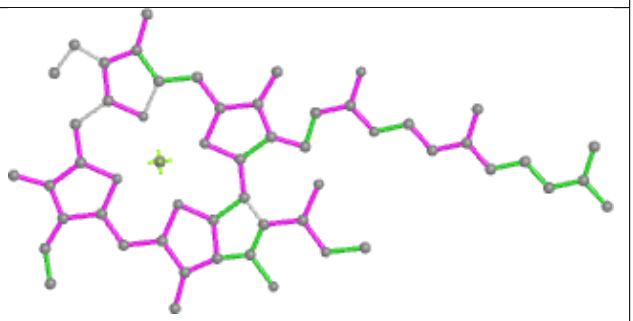


Rings

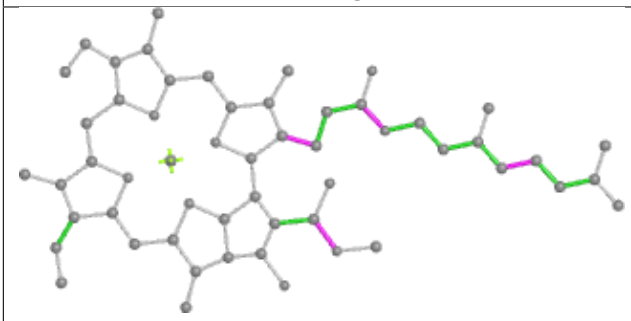
Ligand CLA 8 614



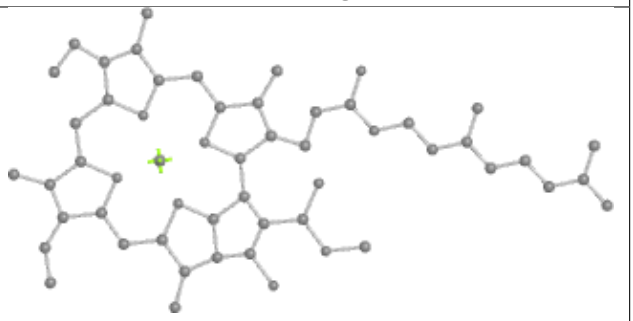
Bond lengths



Bond angles

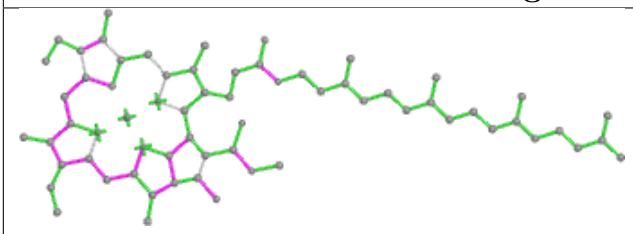


Torsions

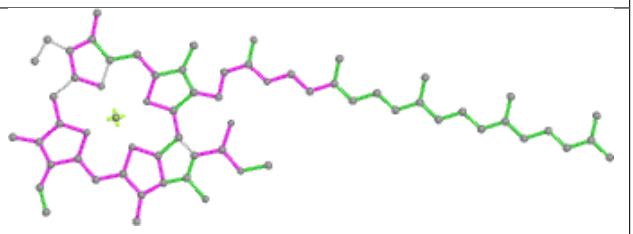


Rings

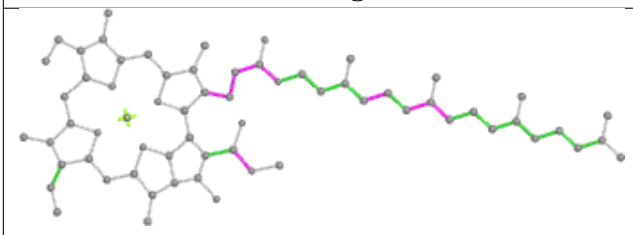
Ligand CLA A 819



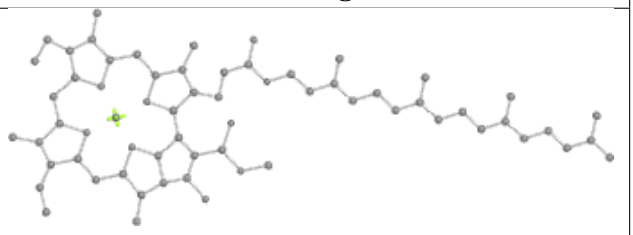
Bond lengths



Bond angles

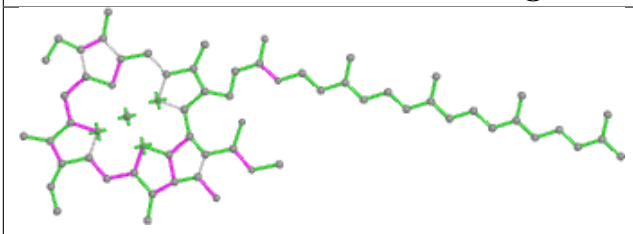


Torsions

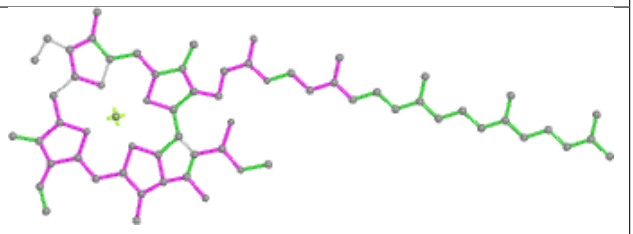


Rings

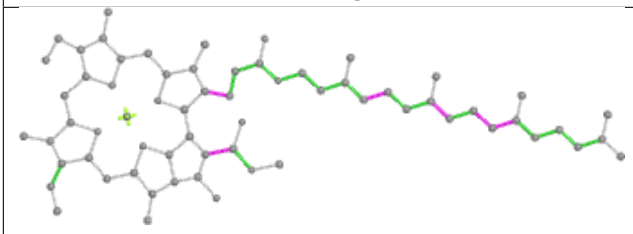
Ligand CLA B 826



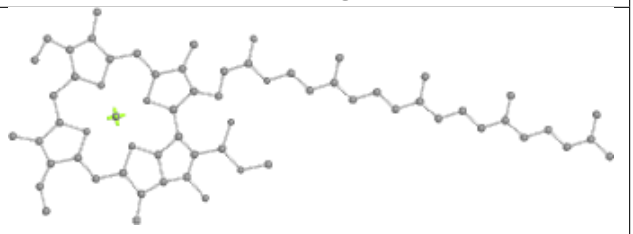
Bond lengths



Bond angles

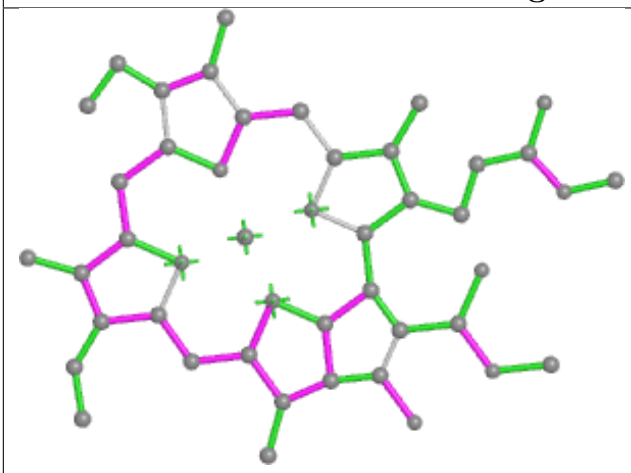


Torsions



Rings

Ligand CLA 7 616



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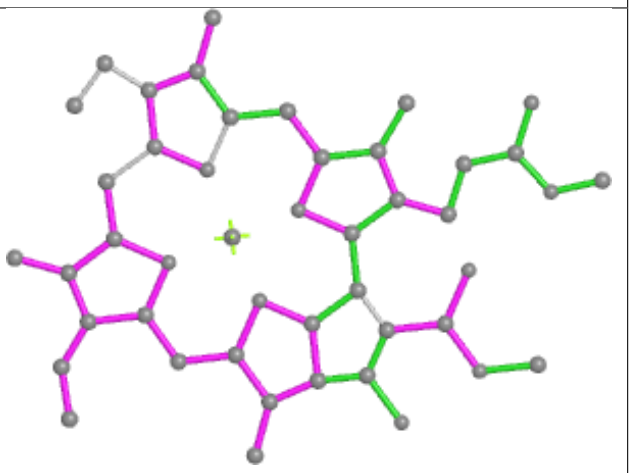
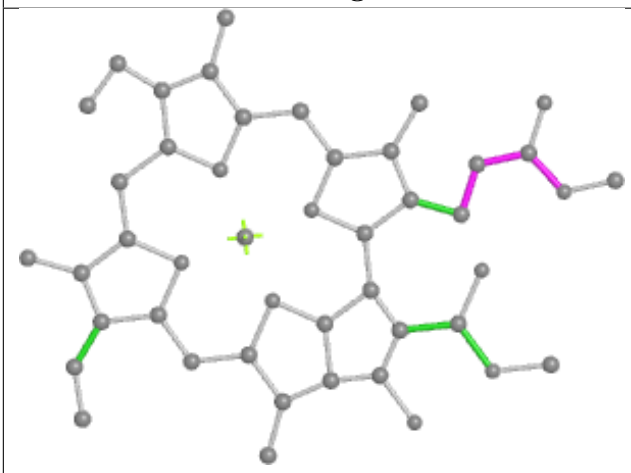


Bond angles



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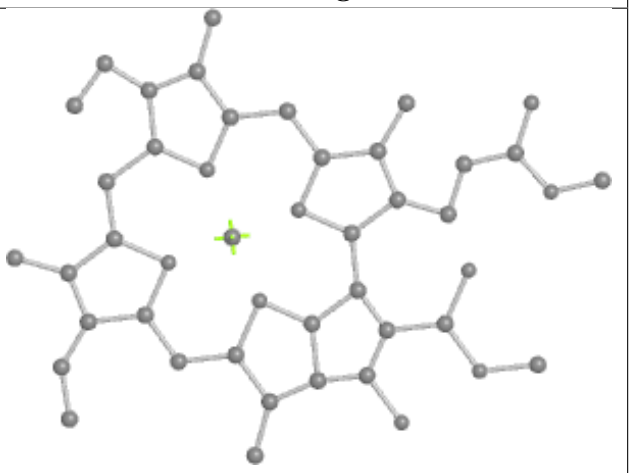
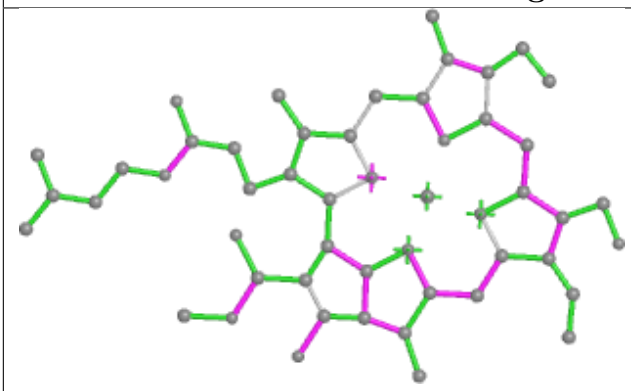


Rings

Ligand CHL 5 608



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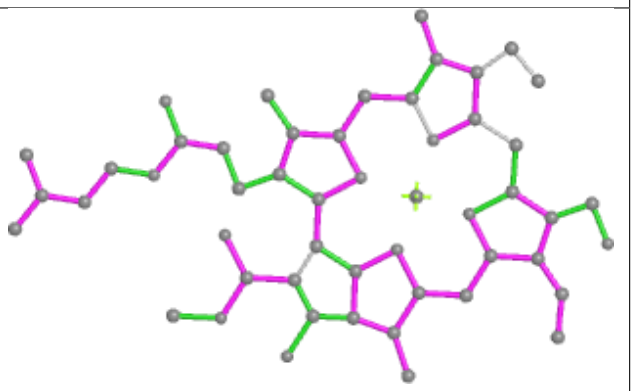
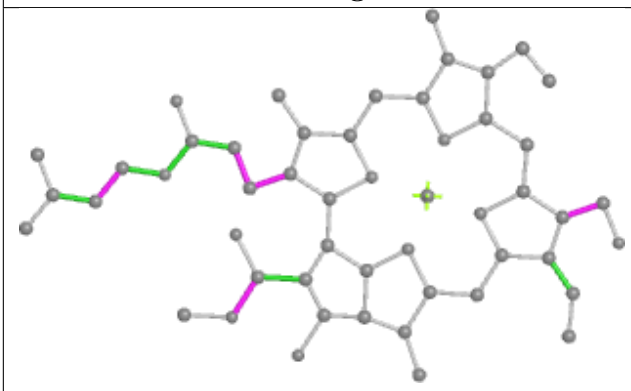
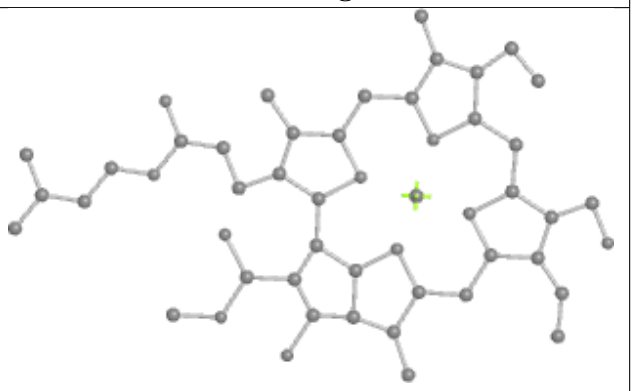


Bond angles

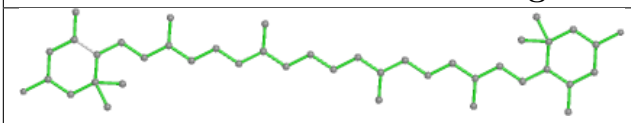


Torsions



Rings

Ligand LUT 4 620



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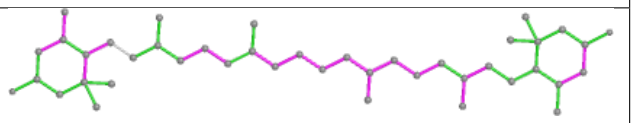
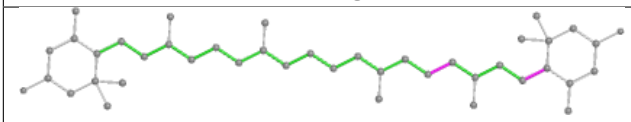
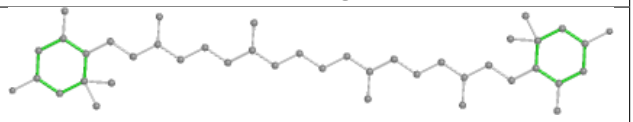


Bond angles

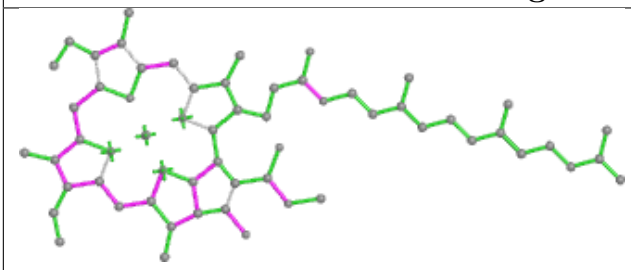


Torsions



Rings

Ligand CLA 9 610



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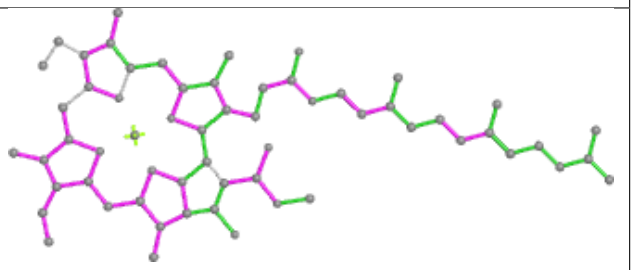
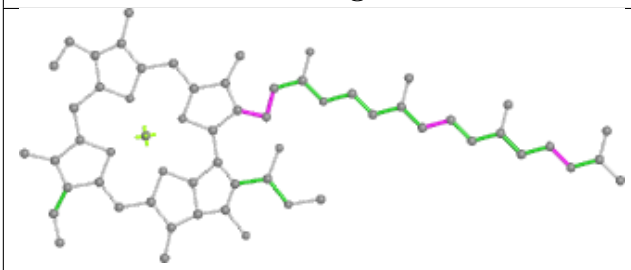
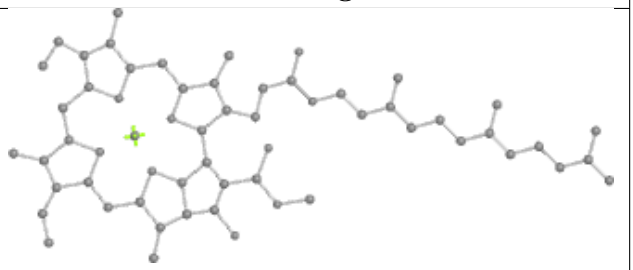


Bond angles

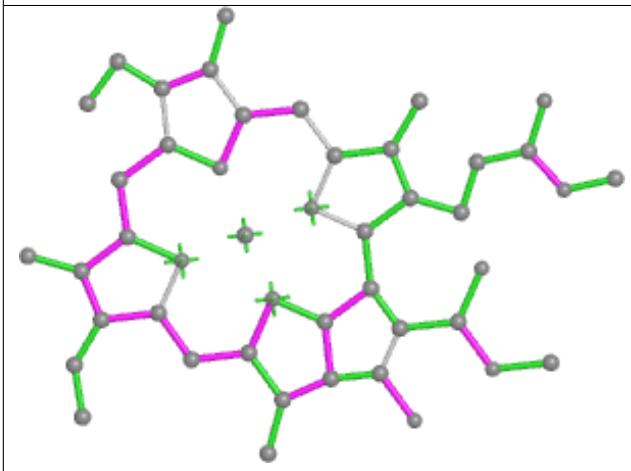


Torsions



Rings

Ligand CLA 6 617



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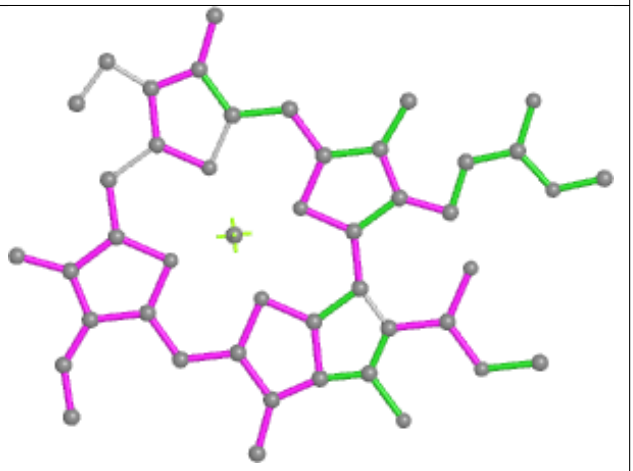
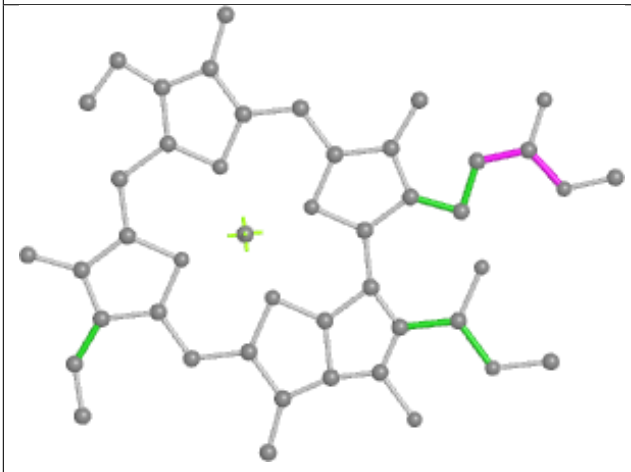


Bond angles



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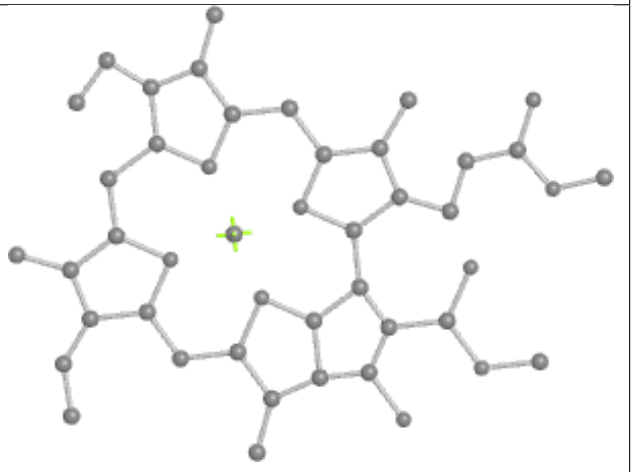
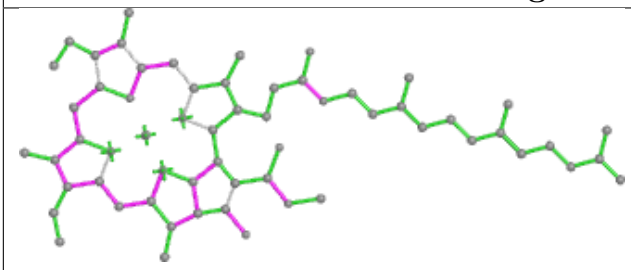
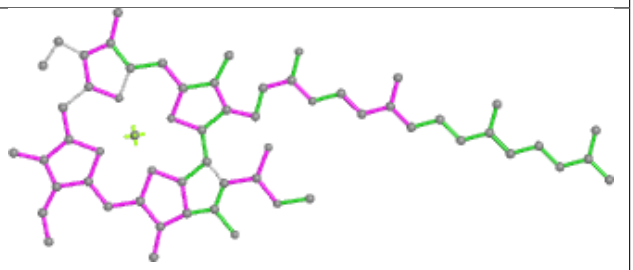


Rings

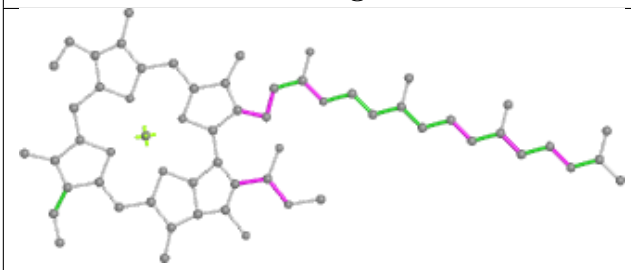
Ligand CLA 4 602



Bond lengths



Bond angles



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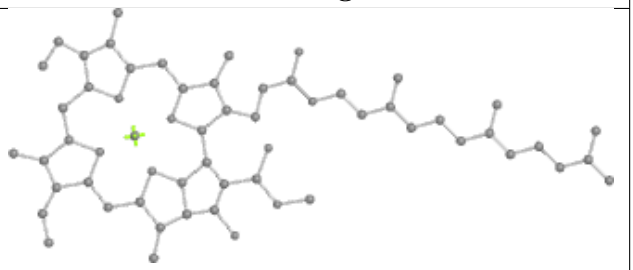
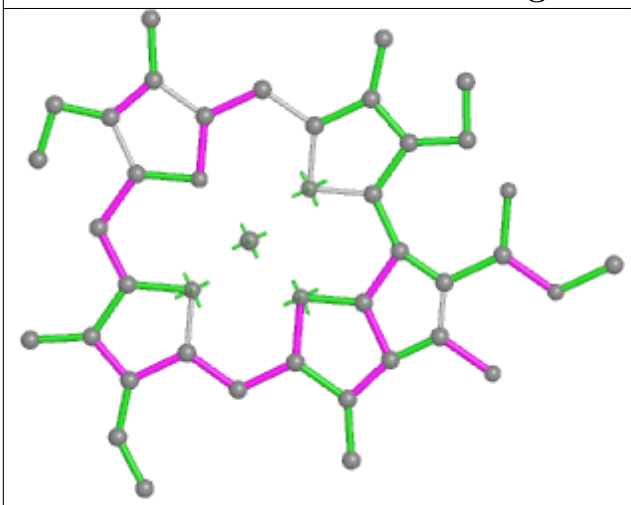
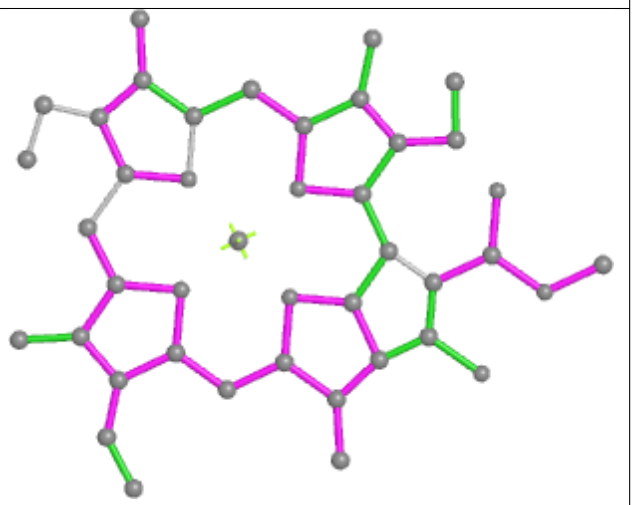


Rings

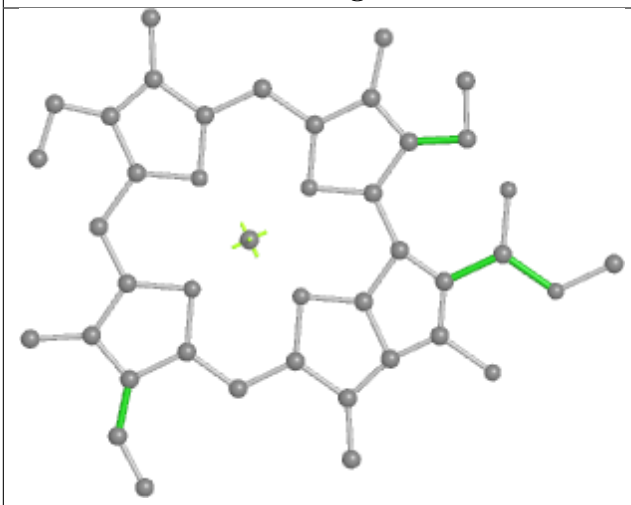
Ligand CLA 3 606



Bond lengths



Bond angles



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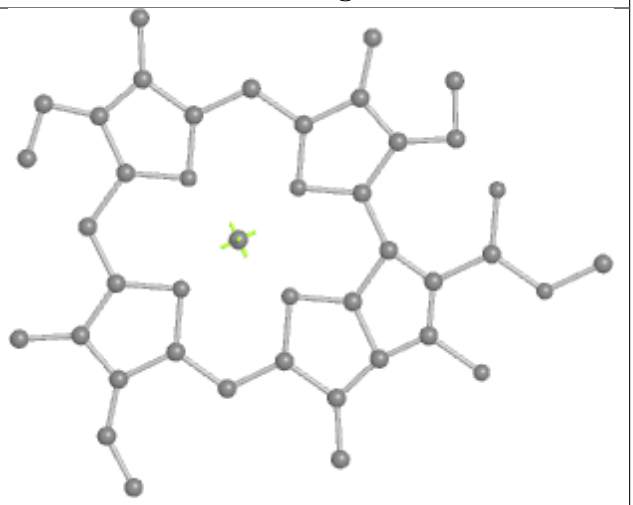
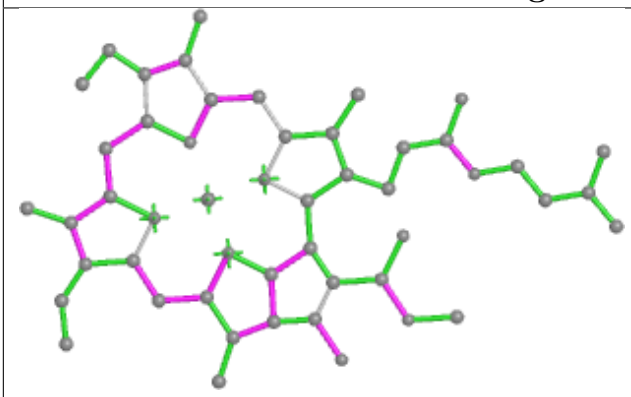


Rings

Ligand CLA 7 608



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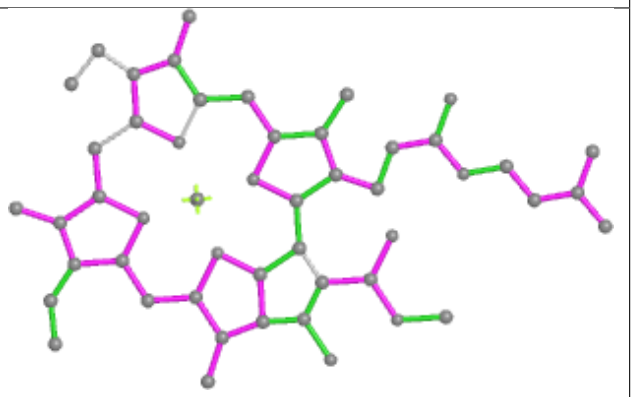
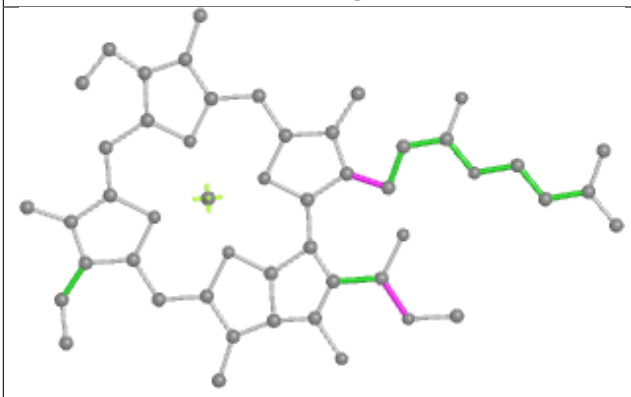
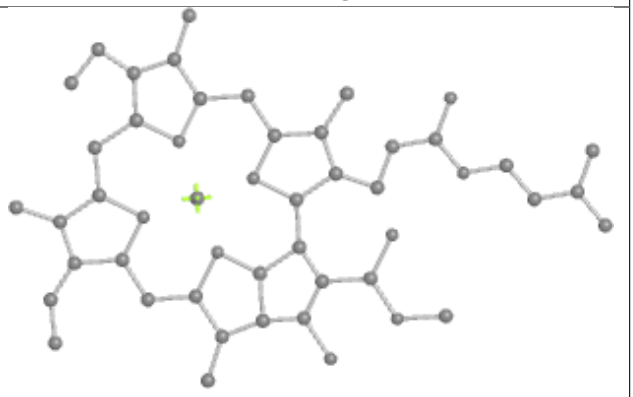


Bond angles

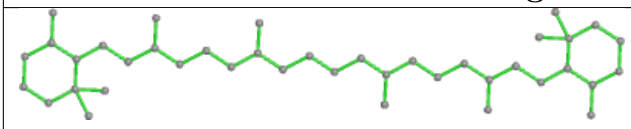


Torsions

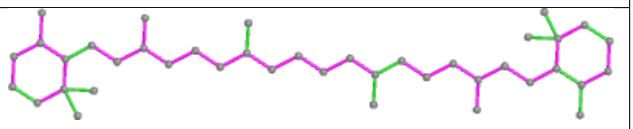


Rings

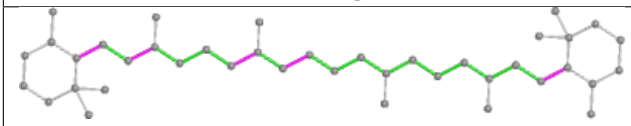
Ligand BCR 6 625



Bond lengths



Bond angles



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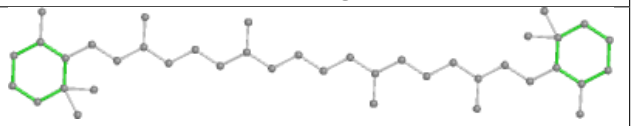
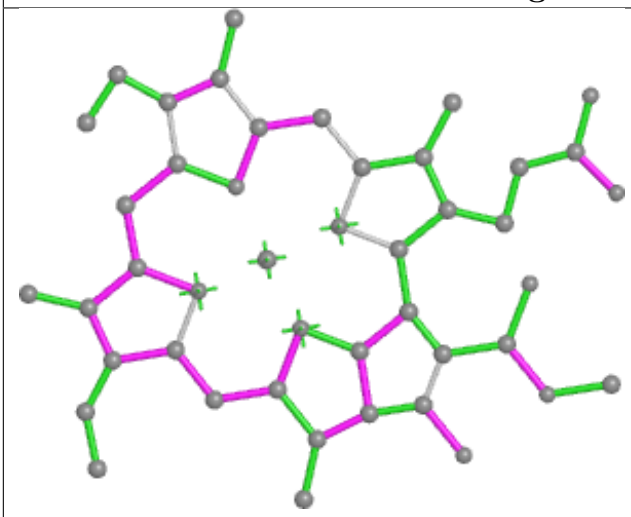
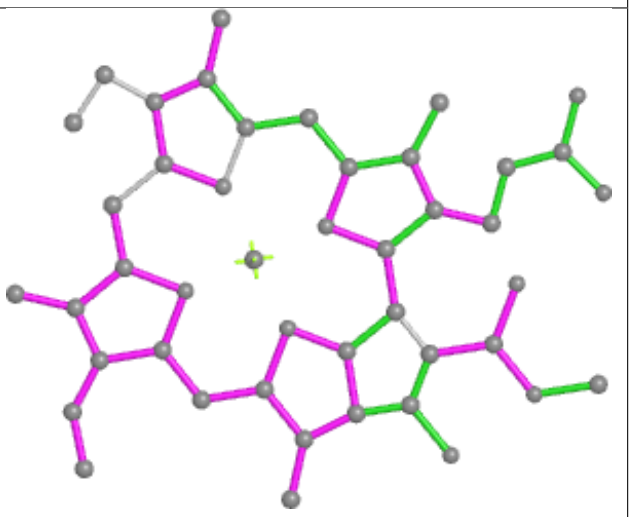


Rings

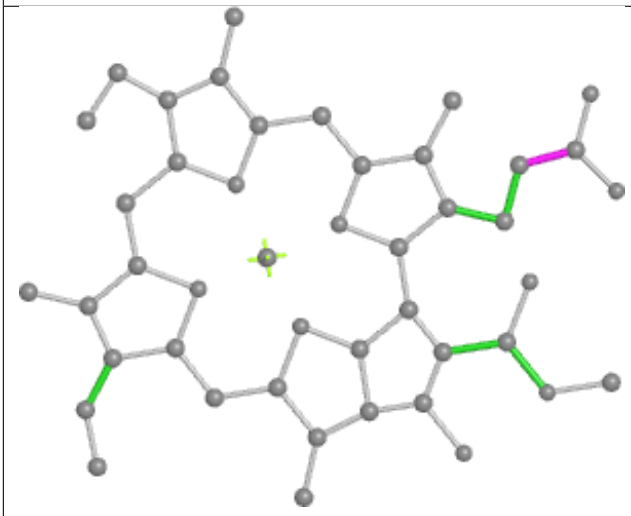
Ligand CLA 8 603



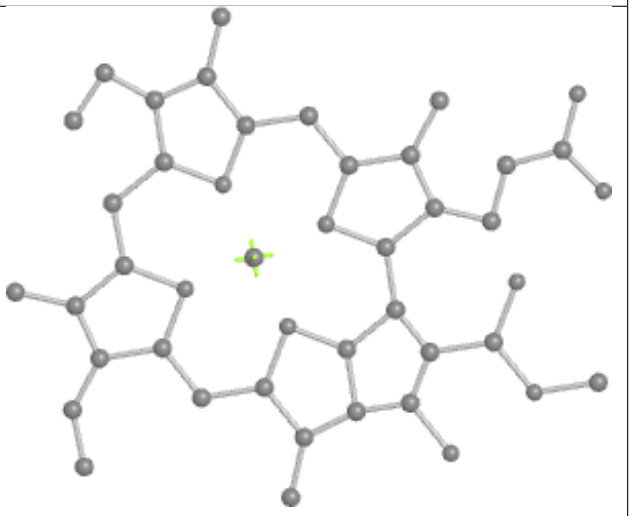
Bond lengths



Bond angles

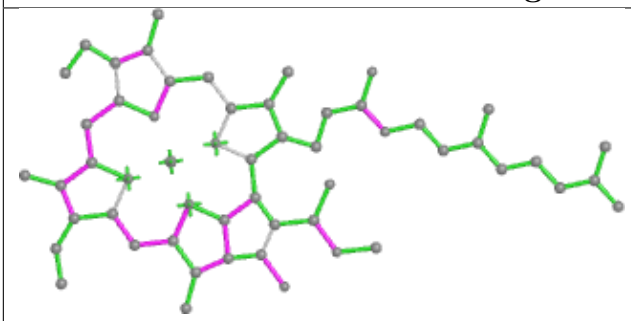


Torsions

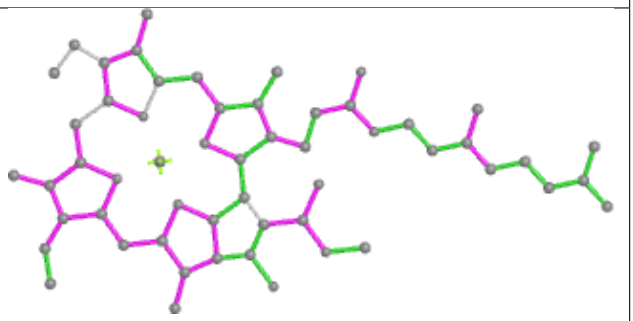


Rings

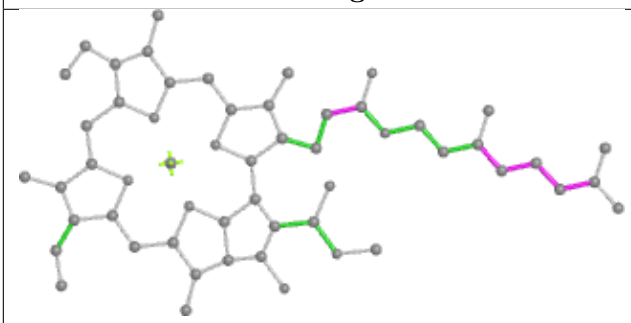
Ligand CLA B 816



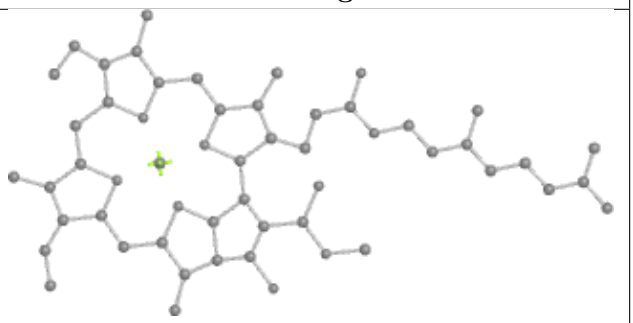
Bond lengths



Bond angles

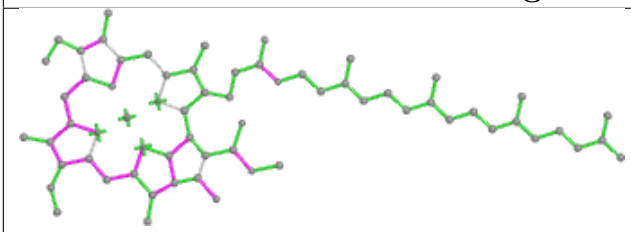


Torsions

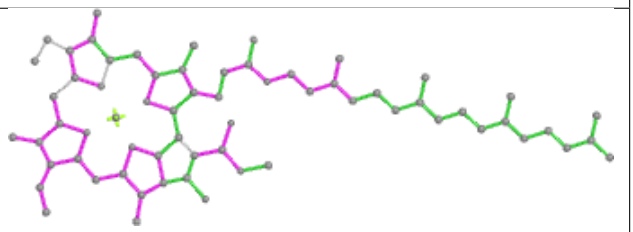


Rings

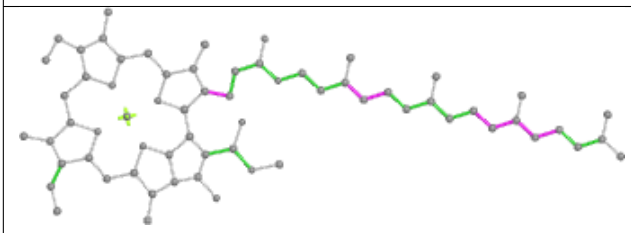
Ligand CLA A 808



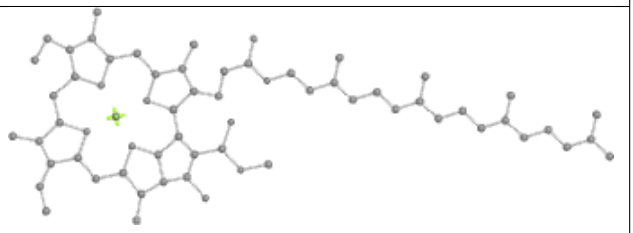
Bond lengths



Bond angles

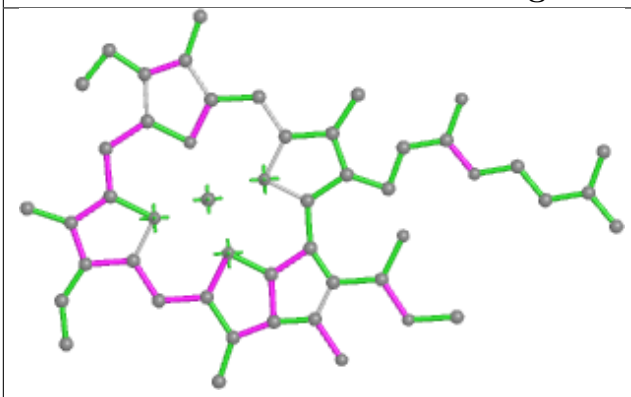


Torsions

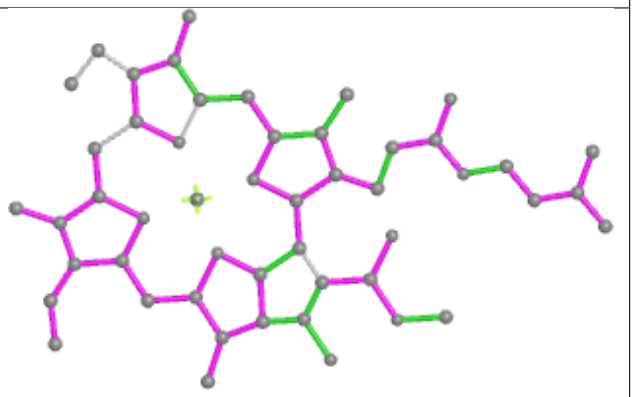


Rings

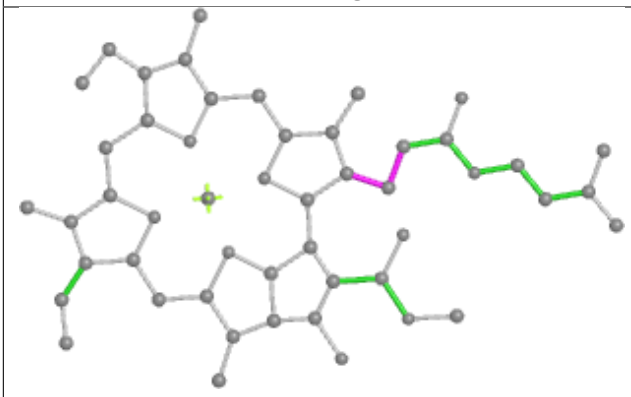
Ligand CLA 2 613



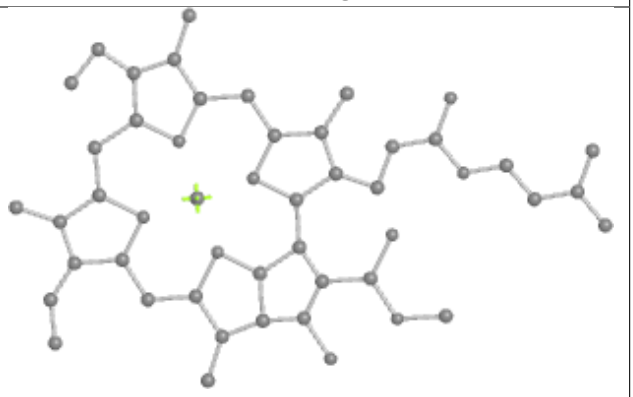
Bond lengths



Bond angles

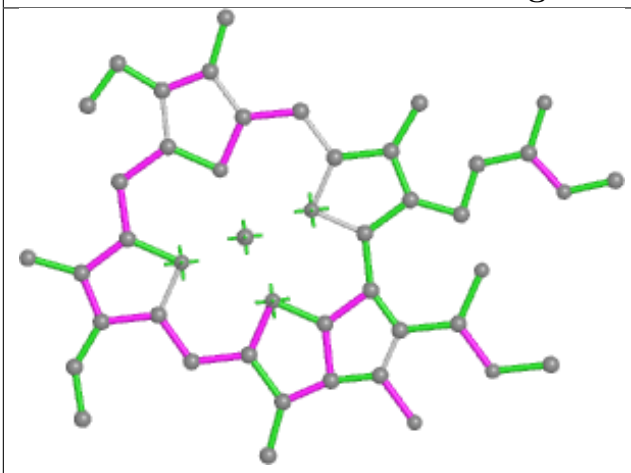


Torsions

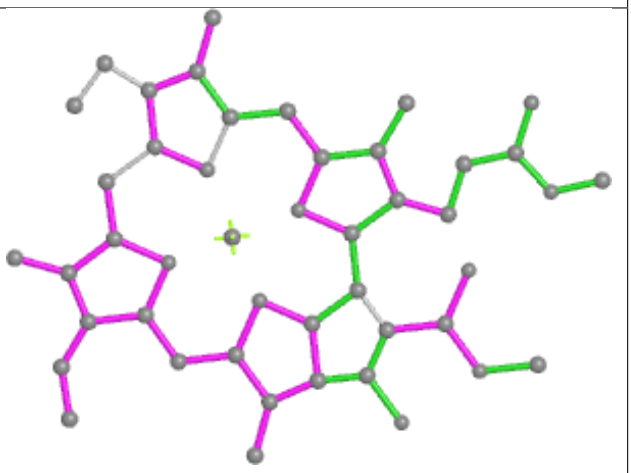


Rings

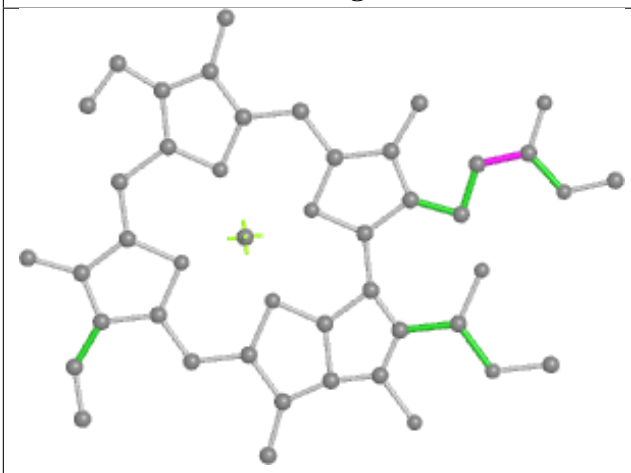
Ligand CLA 8 616



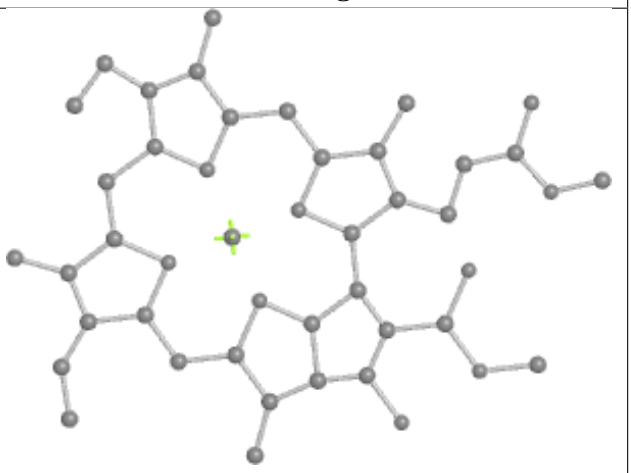
Bond lengths



Bond angles

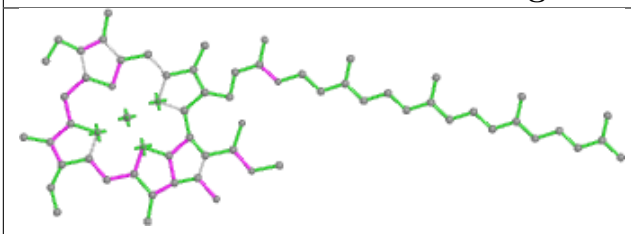


Torsions

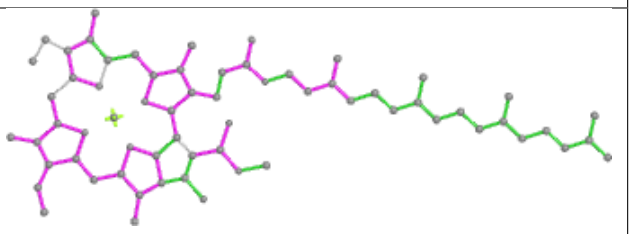


Rings

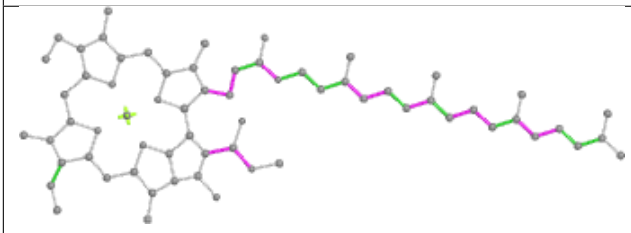
Ligand CLA 3 610



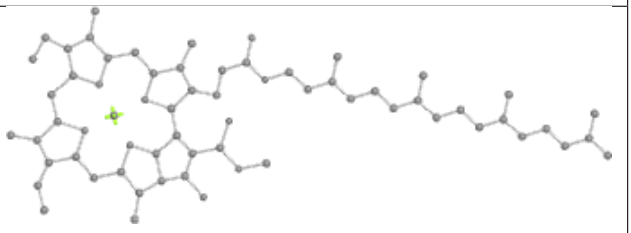
Bond lengths



Bond angles

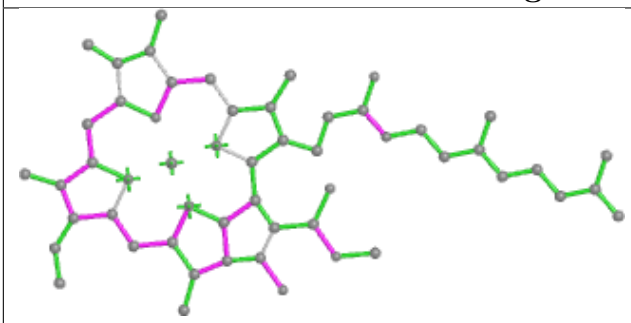


Torsions

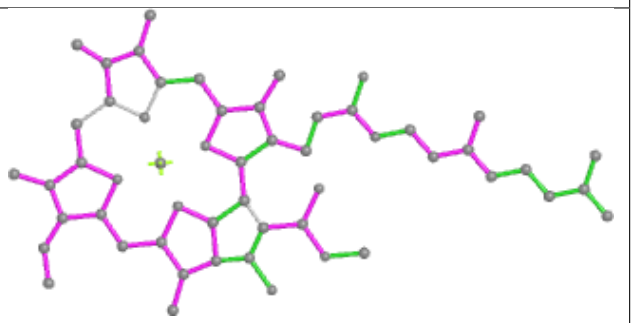


Rings

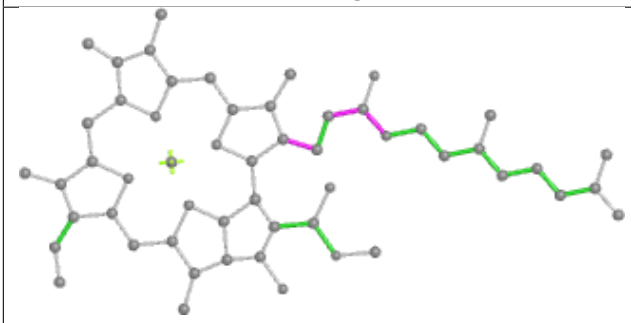
Ligand CLA B 811



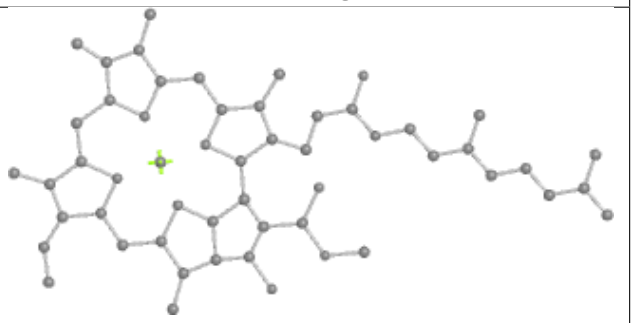
Bond lengths



Bond angles

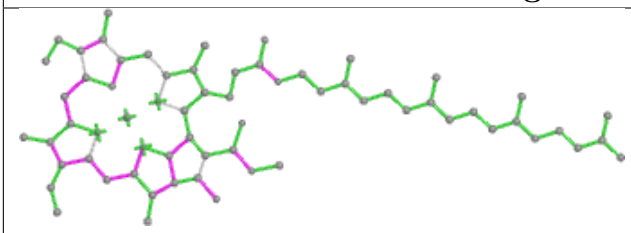


Torsions

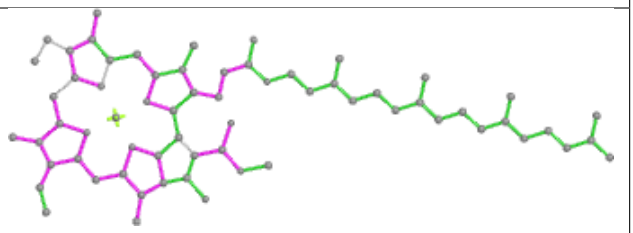


Rings

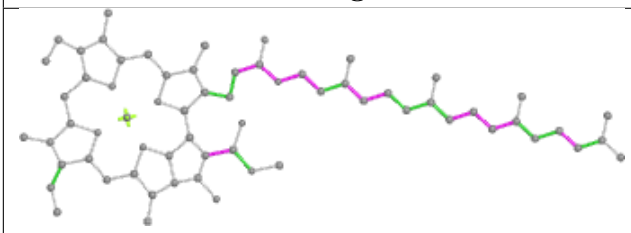
Ligand CLA A 806



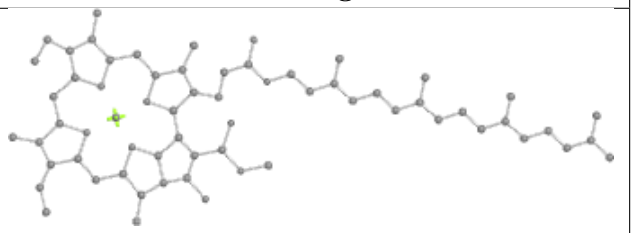
Bond lengths



Bond angles

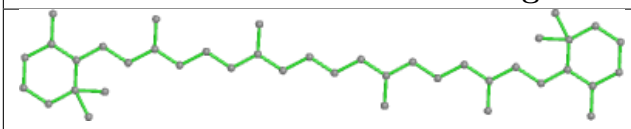


Torsions

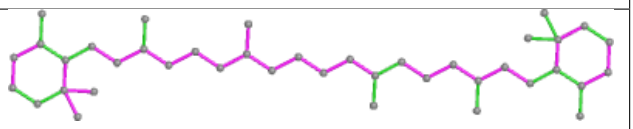


Rings

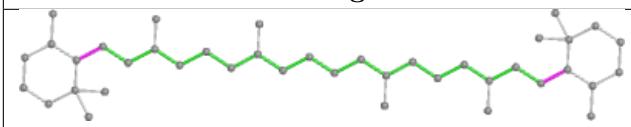
Ligand BCR A 848



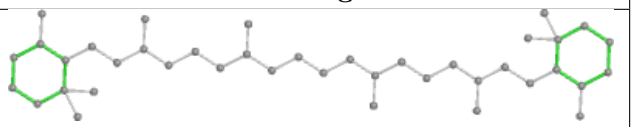
Bond lengths



Bond angles

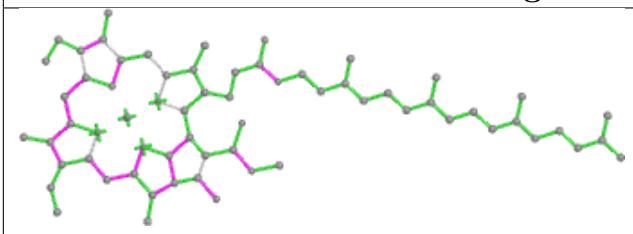


Torsions

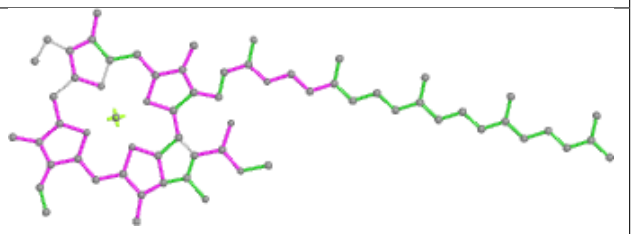


Rings

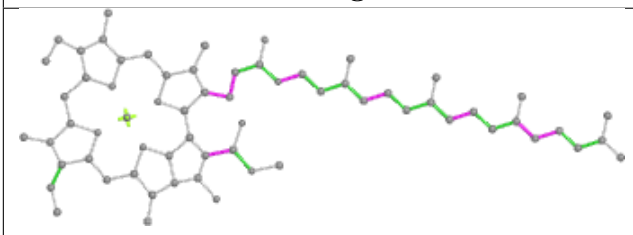
Ligand CLA A 854



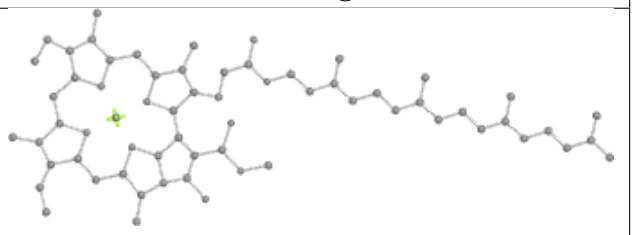
Bond lengths



Bond angles

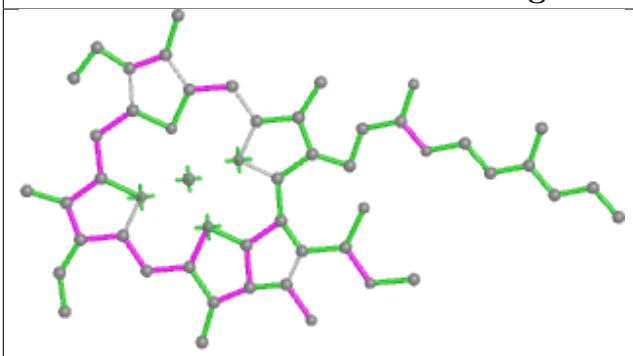


Torsions

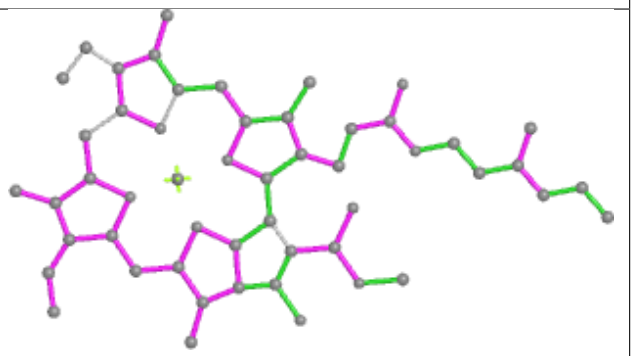


Rings

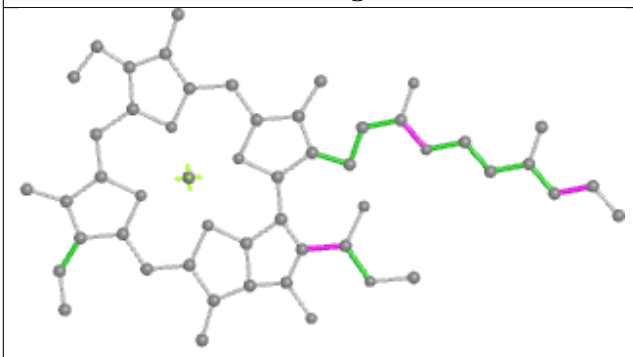
Ligand CLA 9 612



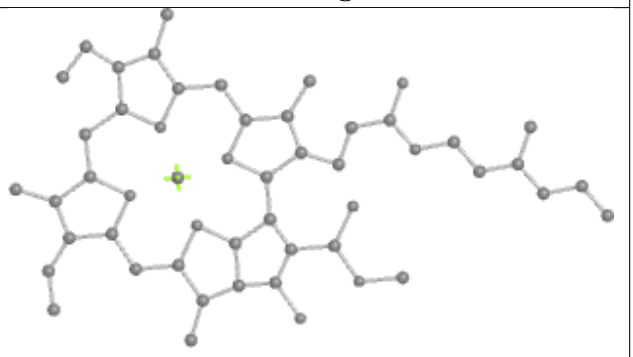
Bond lengths



Bond angles

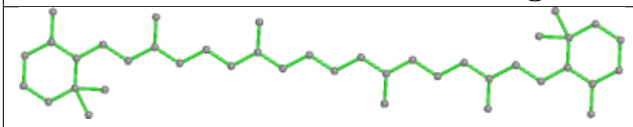


Torsions

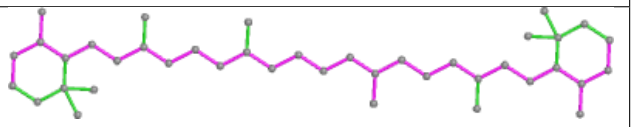


Rings

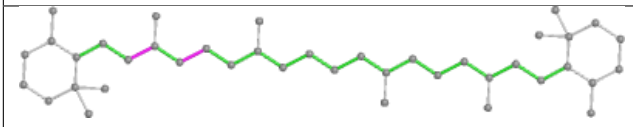
Ligand BCR 4 621



Bond lengths



Bond angles



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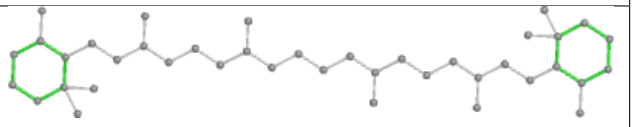
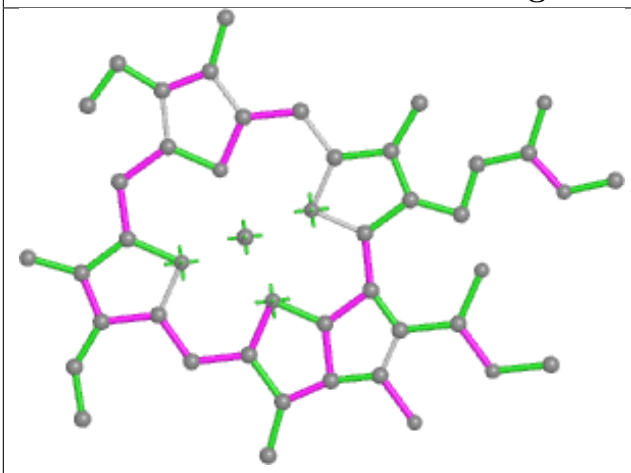
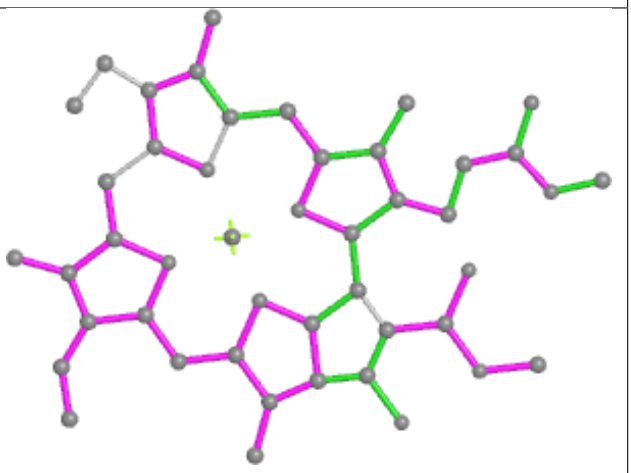


Rings

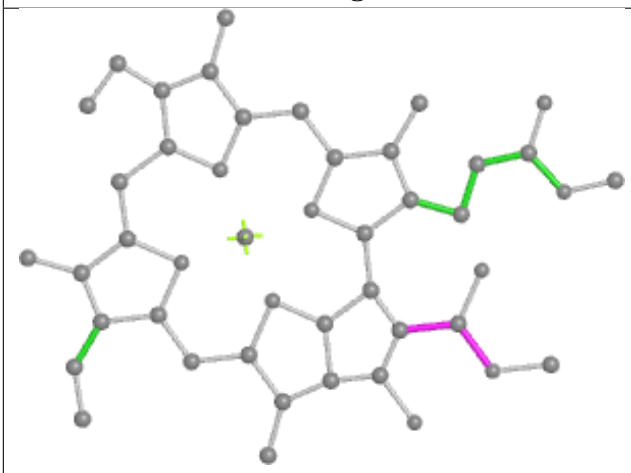
Ligand CLA 8 611



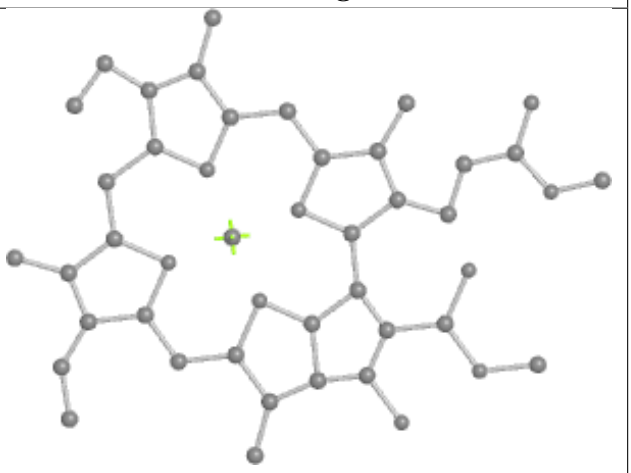
Bond lengths



Bond angles

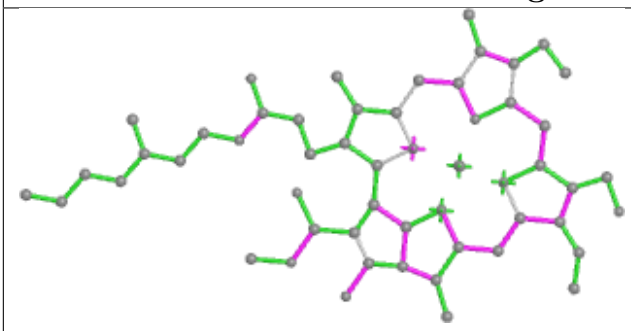


Torsions

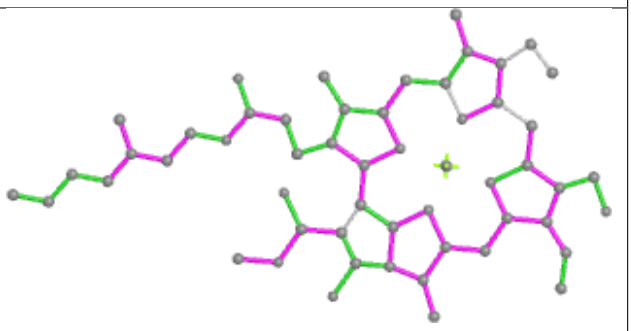


Rings

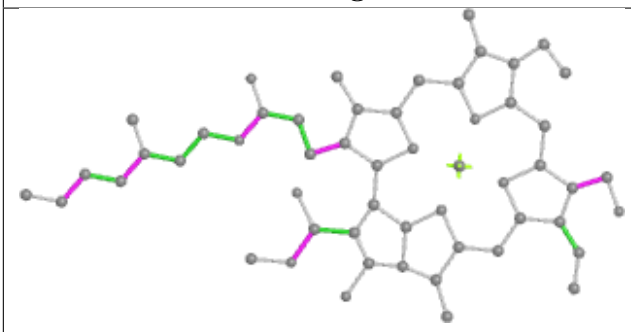
Ligand CHL 7 607



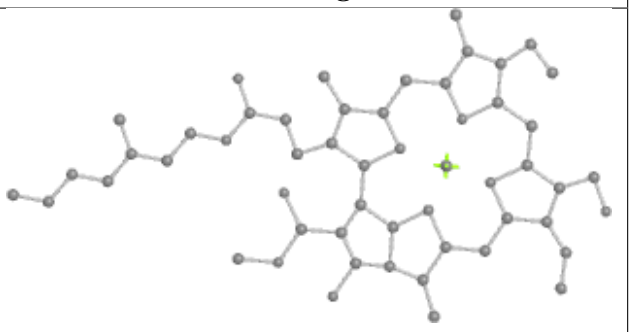
Bond lengths



Bond angles

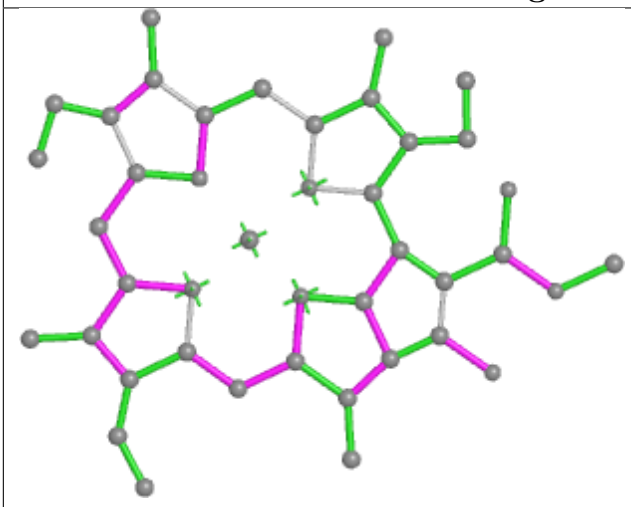


Torsions

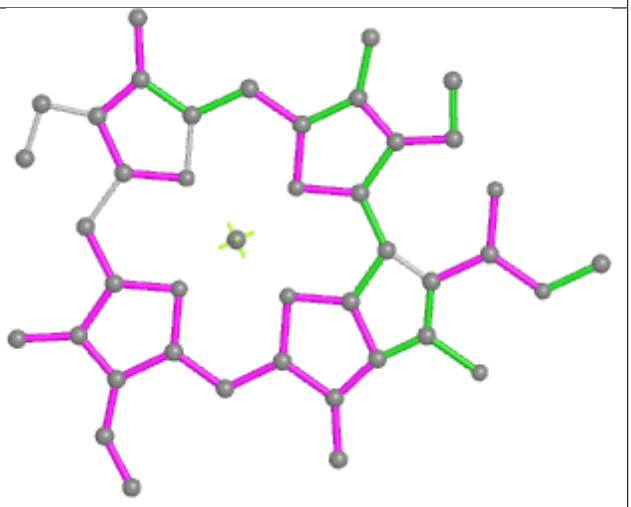


Rings

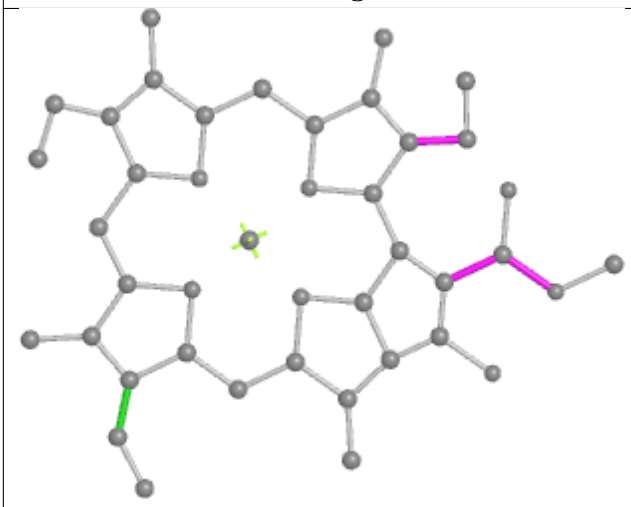
Ligand CLA 7 606



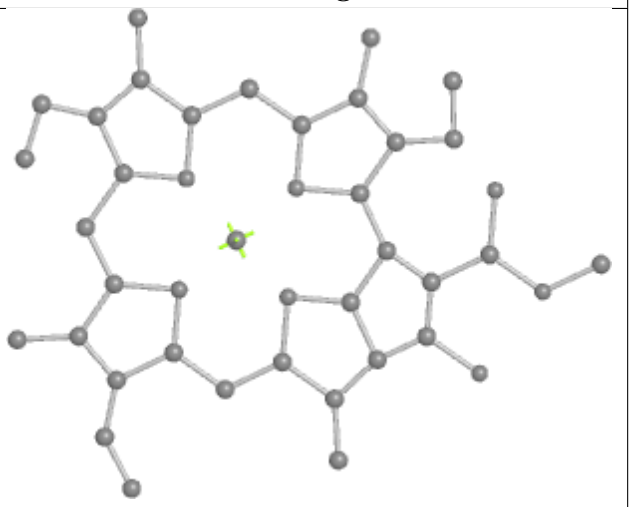
Bond lengths



Bond angles

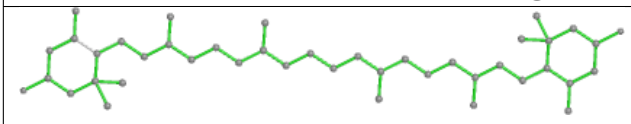


Torsions

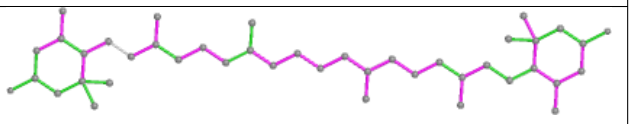


Rings

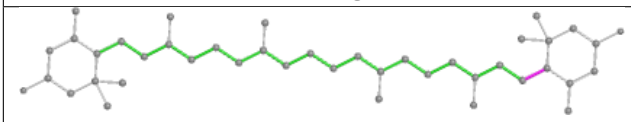
Ligand LUT 9 617



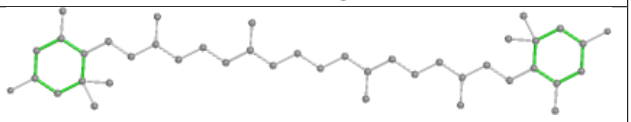
Bond lengths



Bond angles

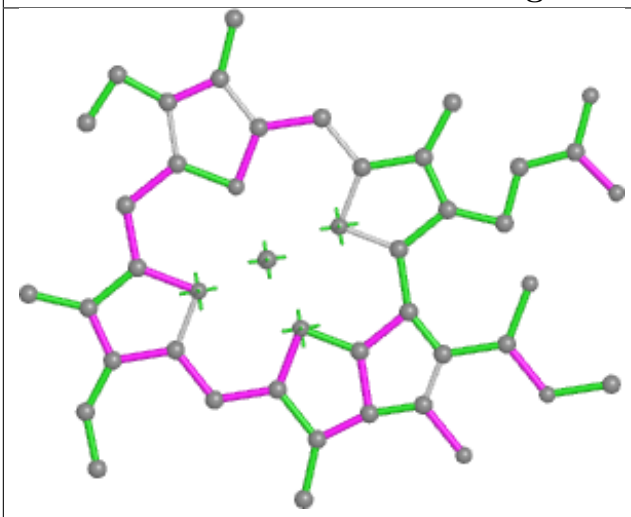


Torsions

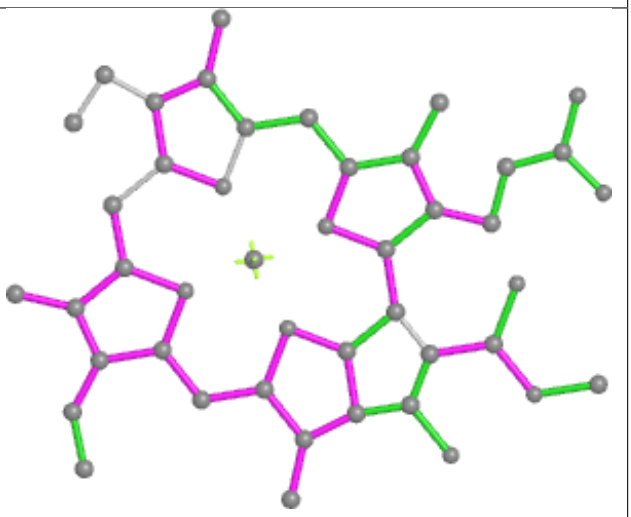


Rings

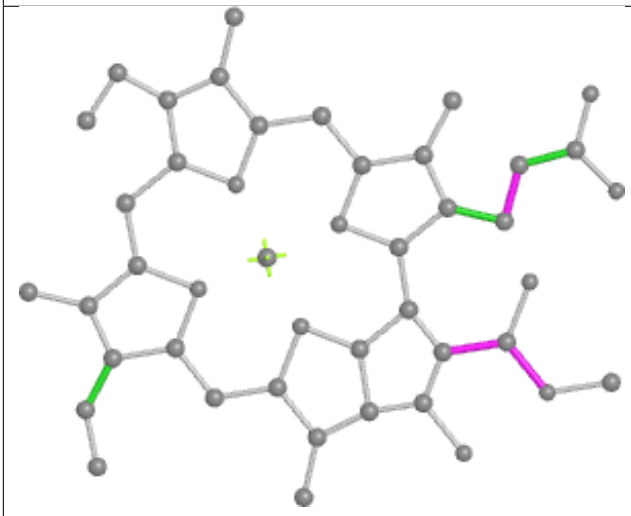
Ligand CLA F 303



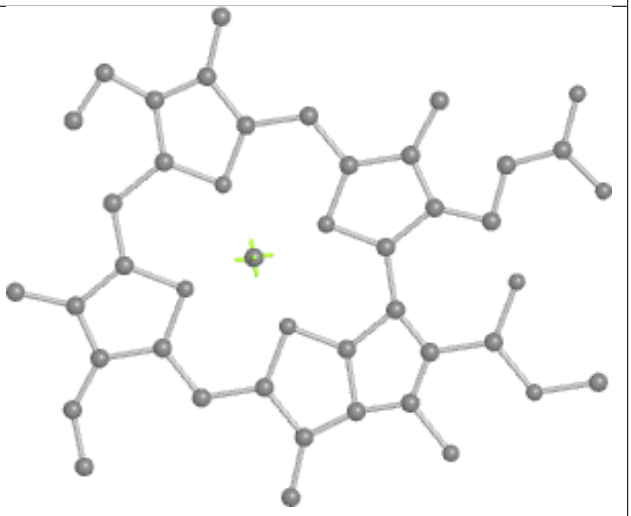
Bond lengths



Bond angles

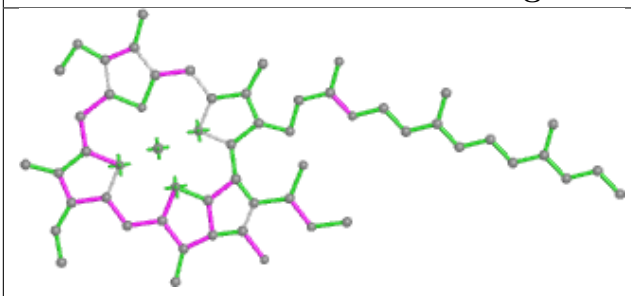


Torsions

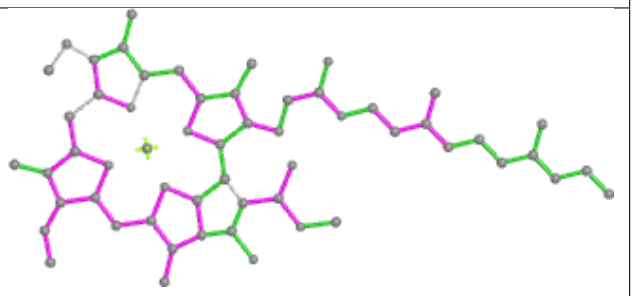


Rings

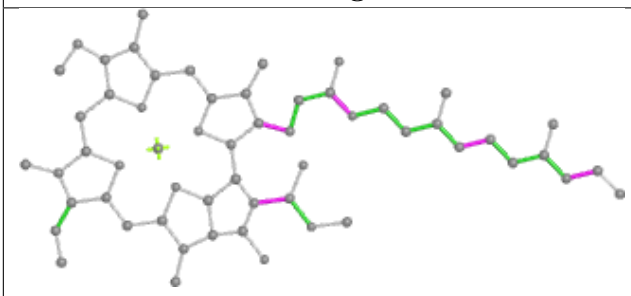
Ligand CLA A 817



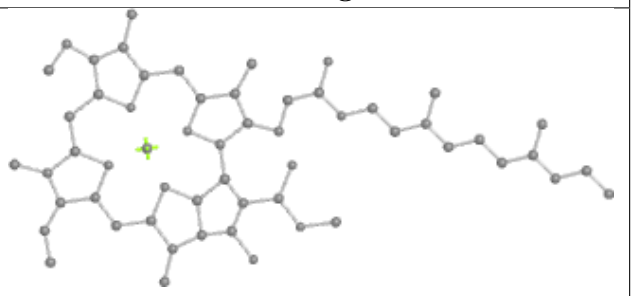
Bond lengths



Bond angles

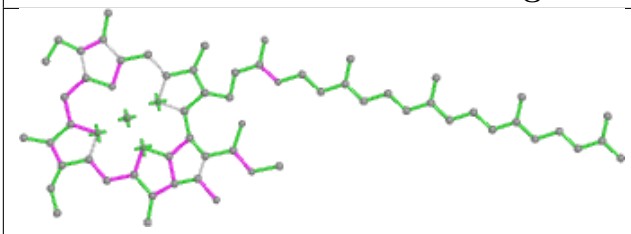


Torsions

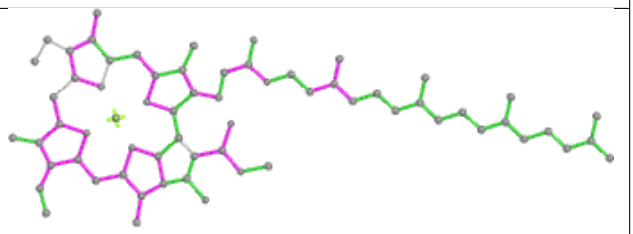


Rings

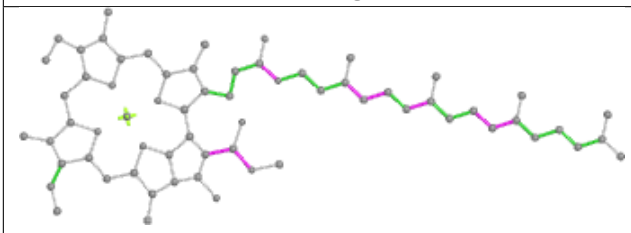
Ligand CLA A 818



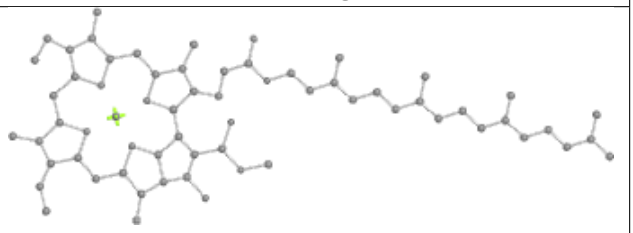
Bond lengths



Bond angles

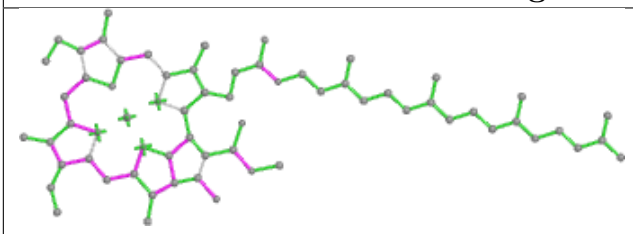


Torsions

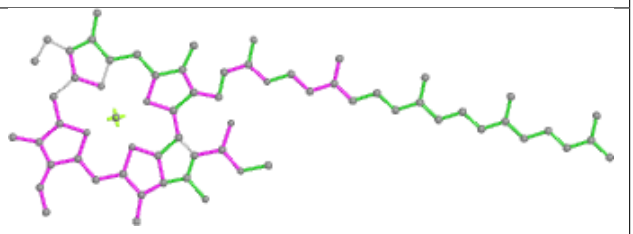


Rings

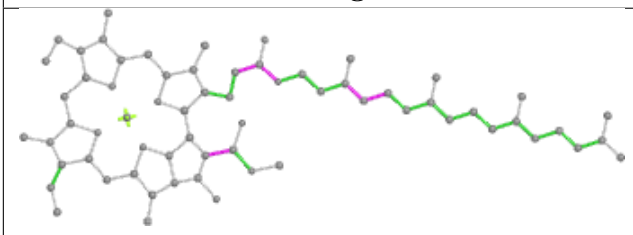
Ligand CLA 1 603



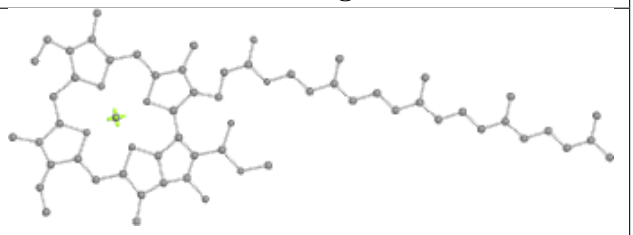
Bond lengths



Bond angles

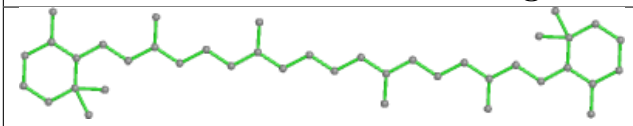


Torsions

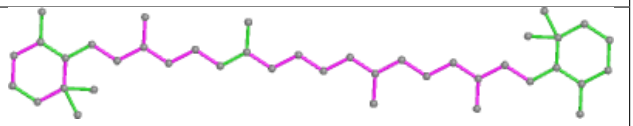


Rings

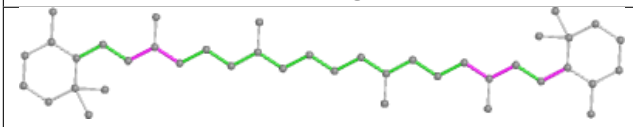
Ligand BCR B 845



Bond lengths



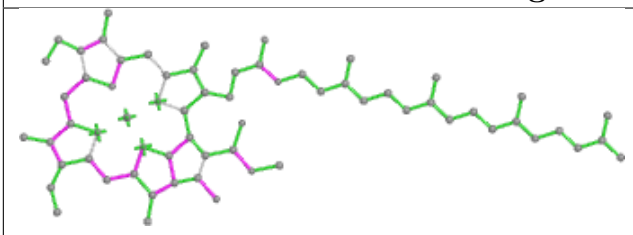
Bond angles



Torsions

Rings

Ligand CLA 5 602



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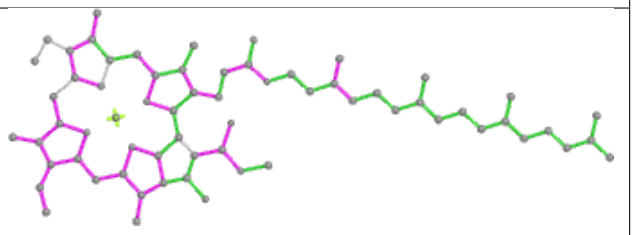

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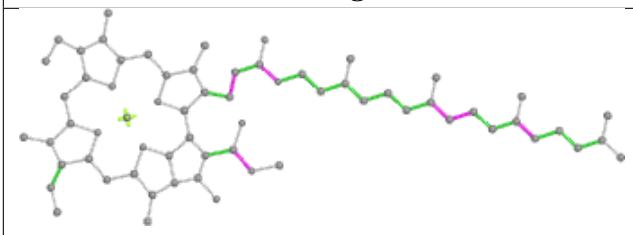

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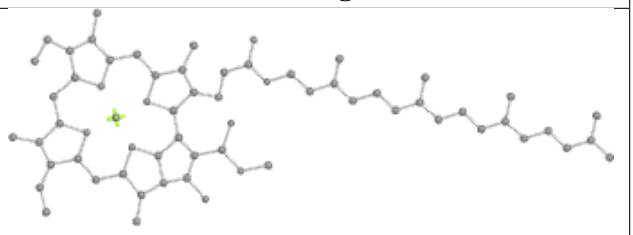
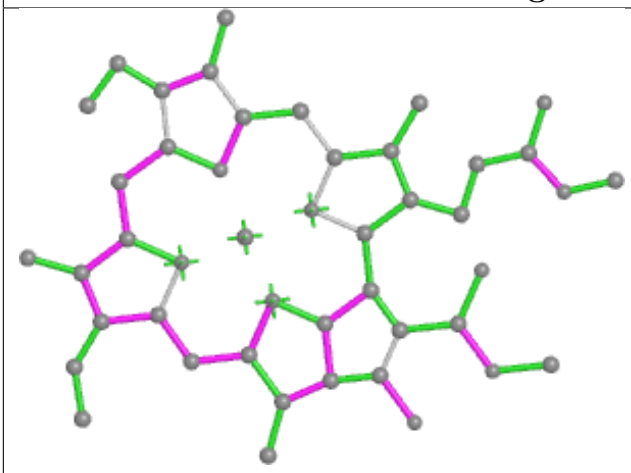


Rings

Ligand CLA 8 609



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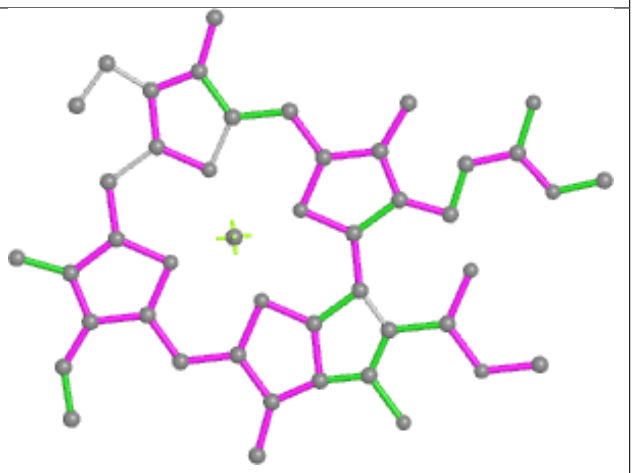

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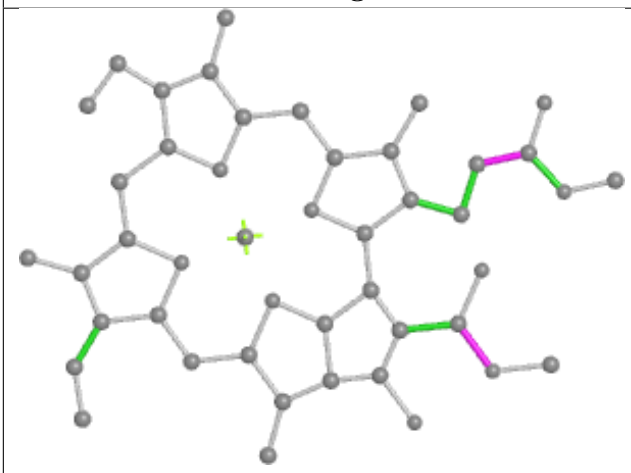

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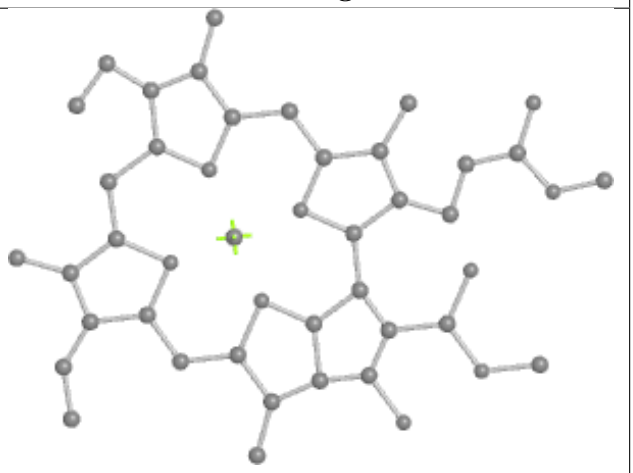
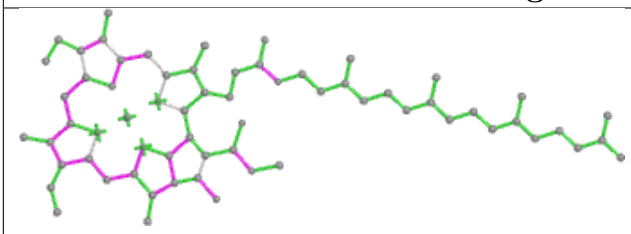


Rings

Ligand CLA Z 611



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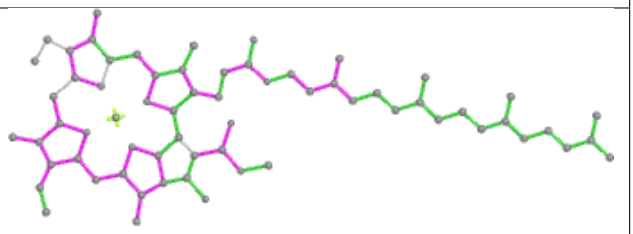

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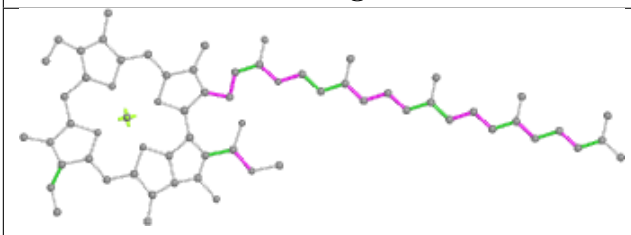

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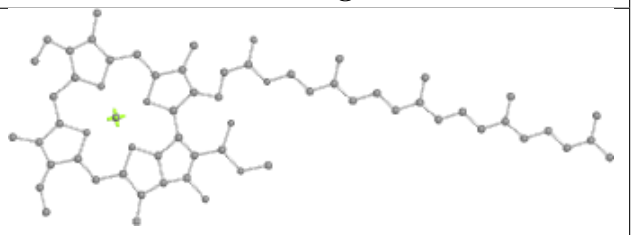
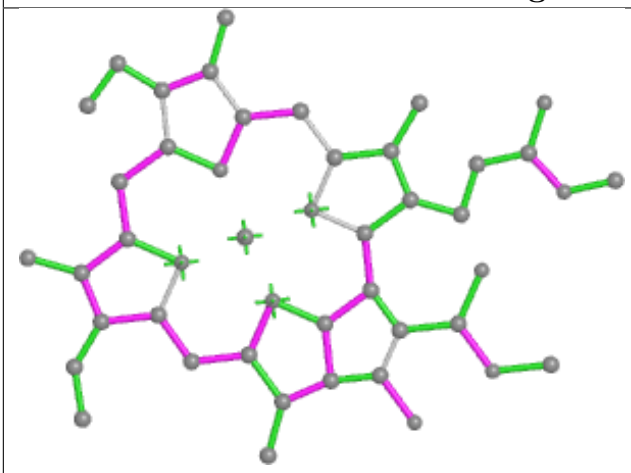


Rings

Ligand CLA 5 621



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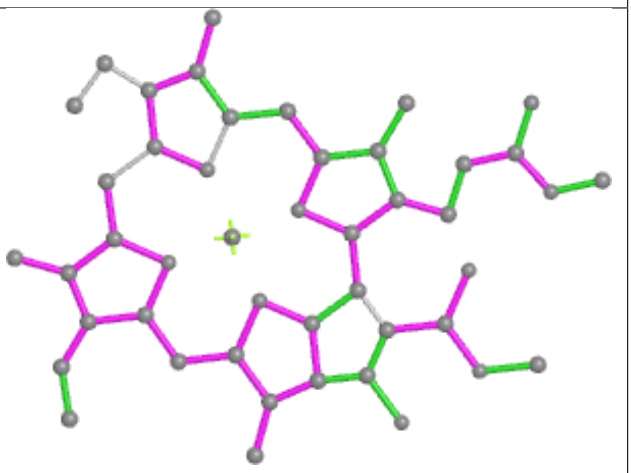
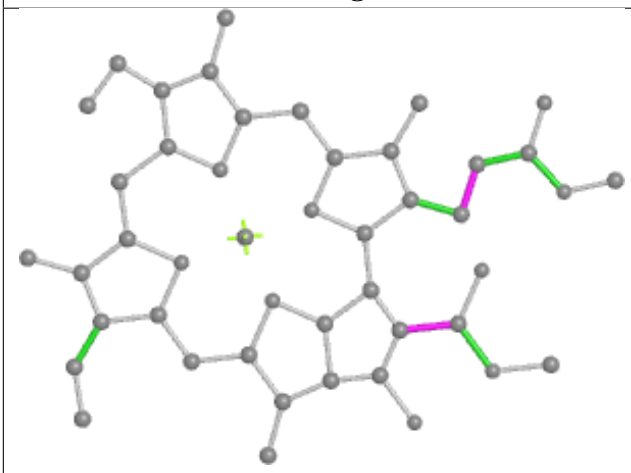
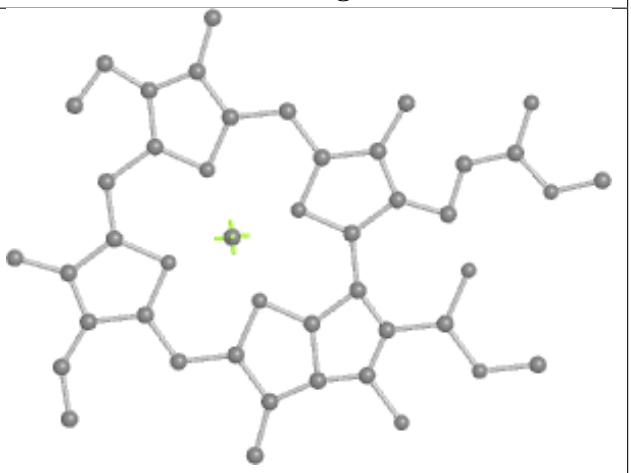


Bond angles

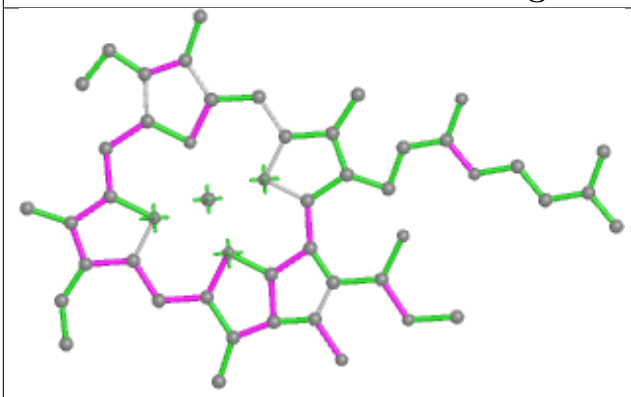


Torsions



Rings

Ligand CLA 6 609



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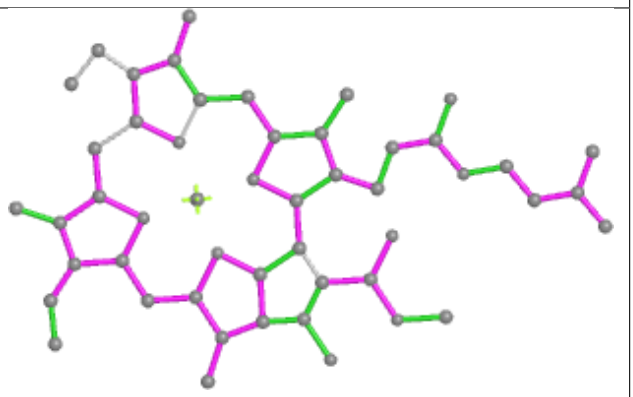
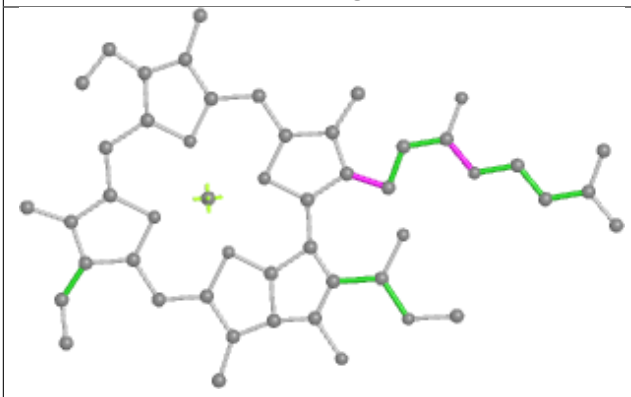


Bond angles



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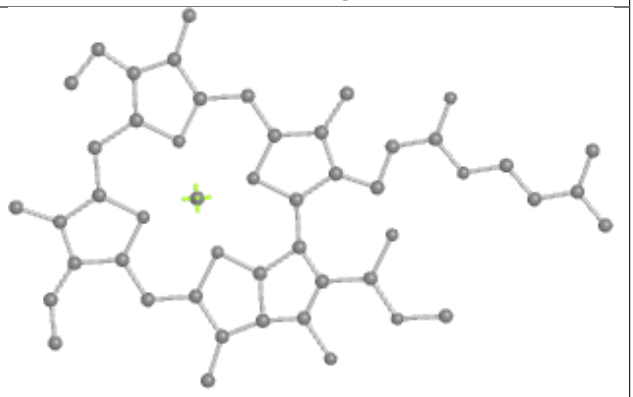
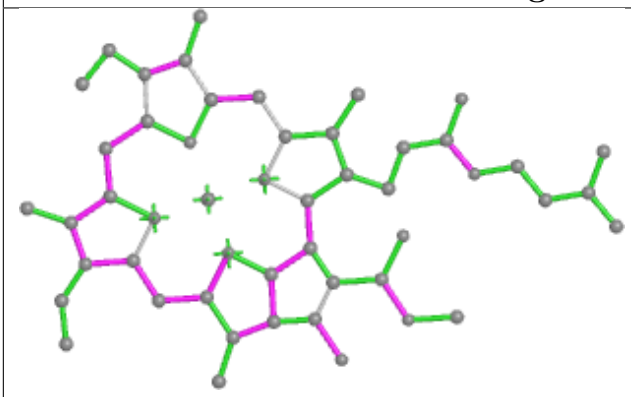


Rings

Ligand CLA 2 609



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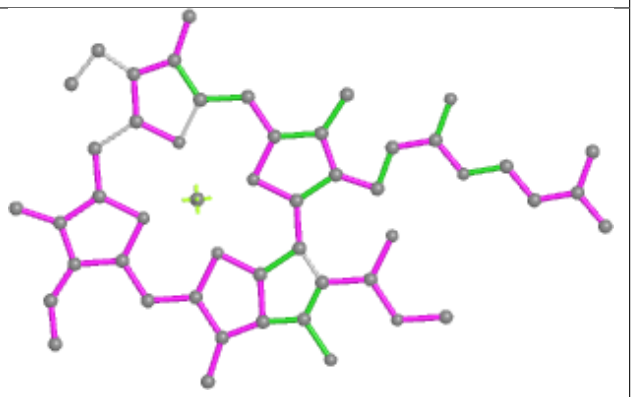
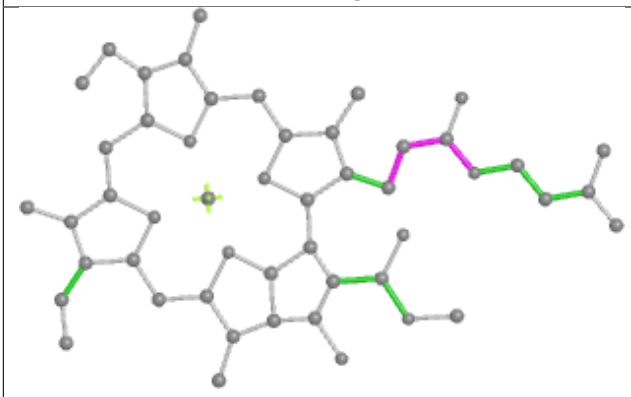


Bond angles



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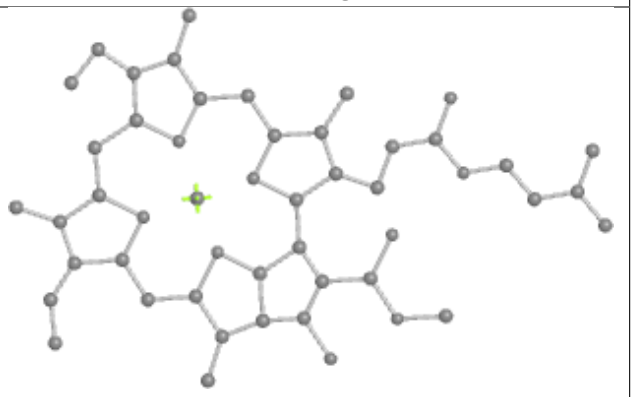
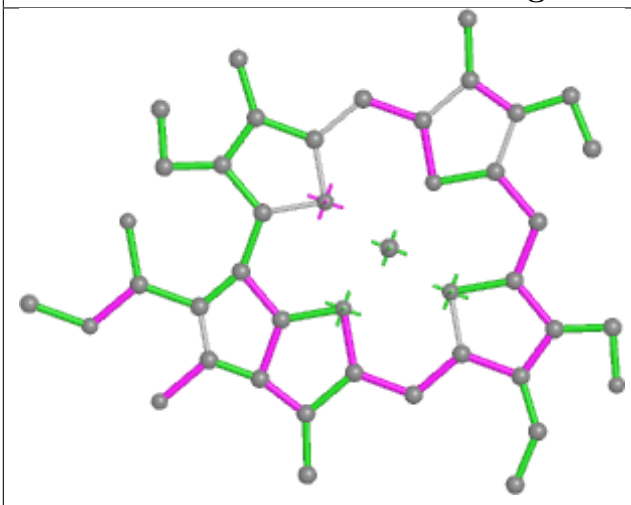


Rings

Ligand CHL 4 618



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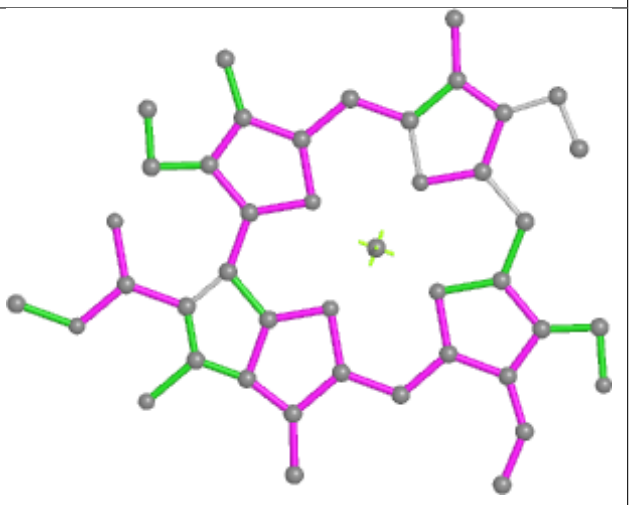
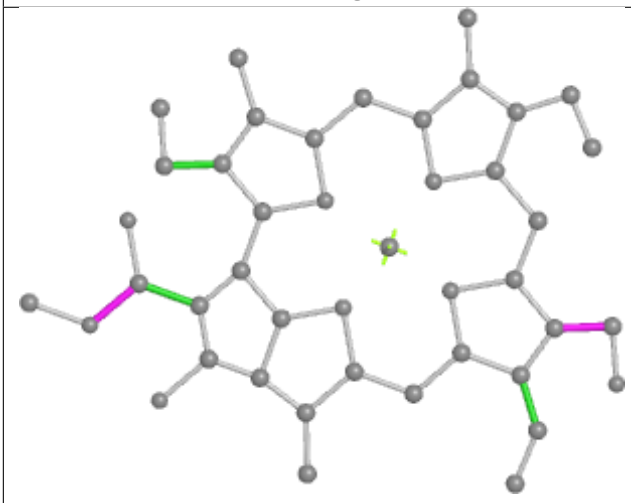


Bond angles



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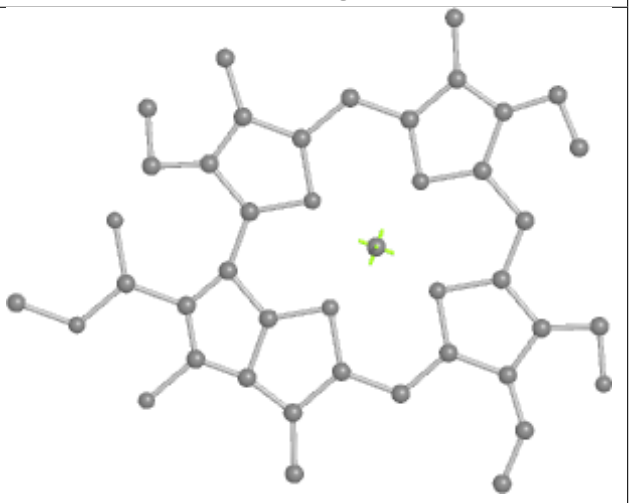
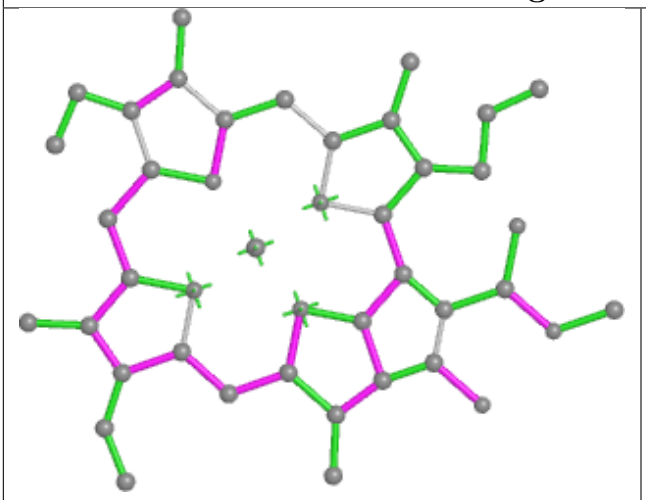


Rings

Ligand CLA 7 614



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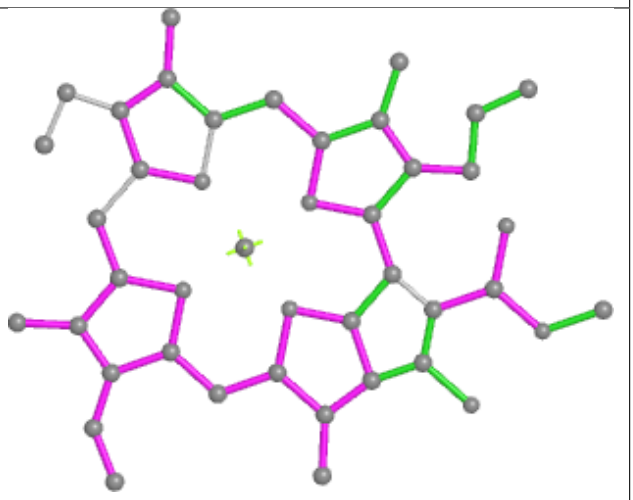
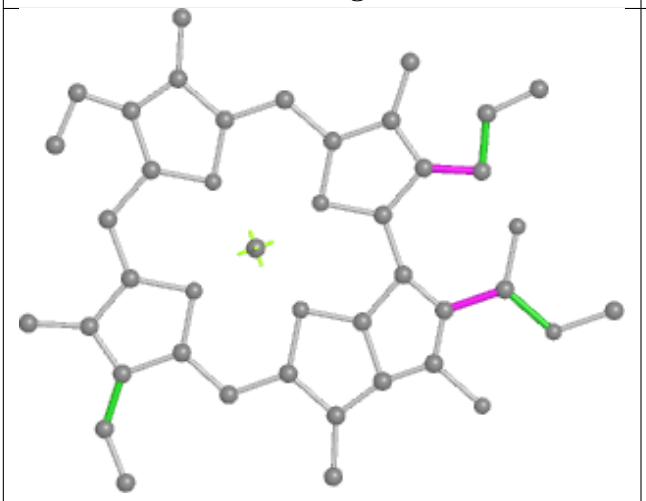


Bond angles



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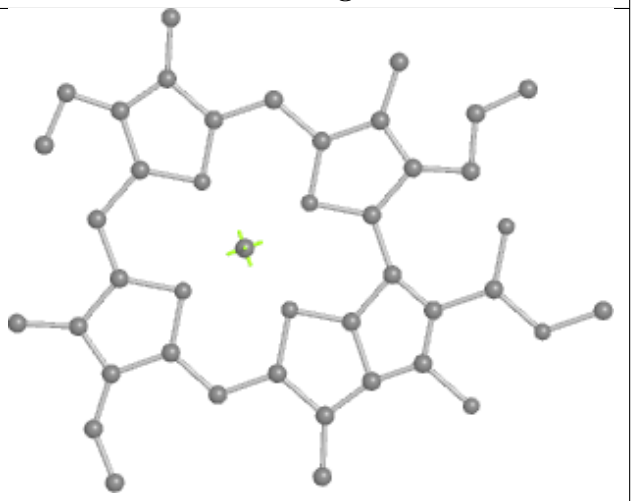
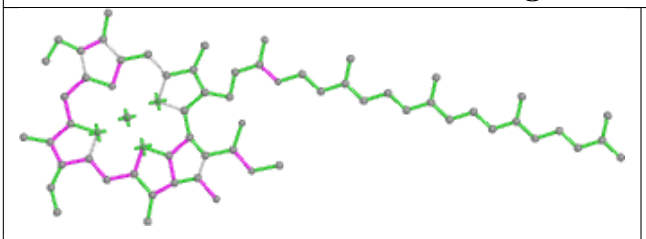


Rings

Ligand CLA A 822



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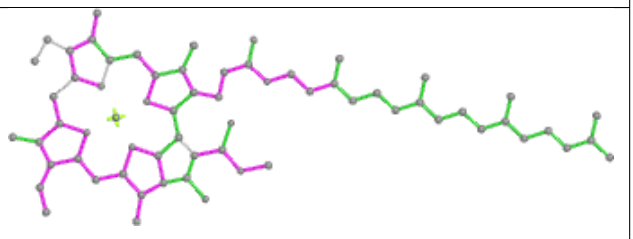
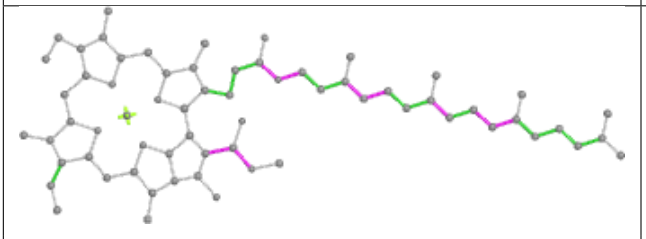
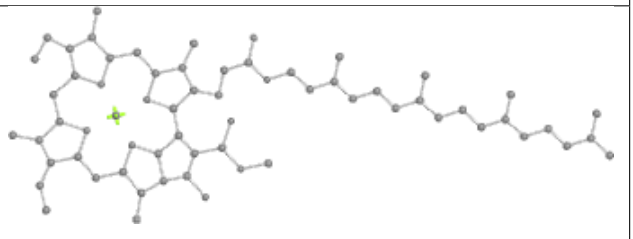


Bond angles

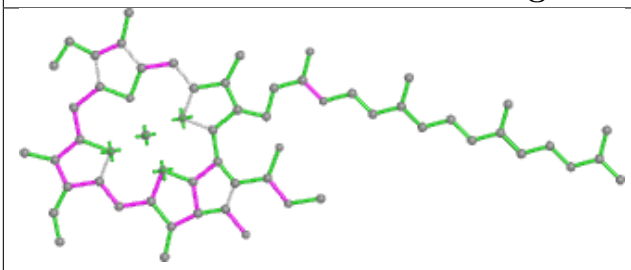


Torsions

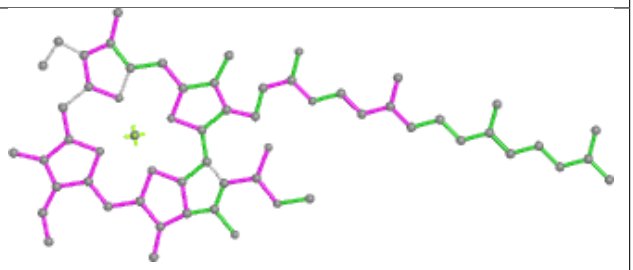


Rings

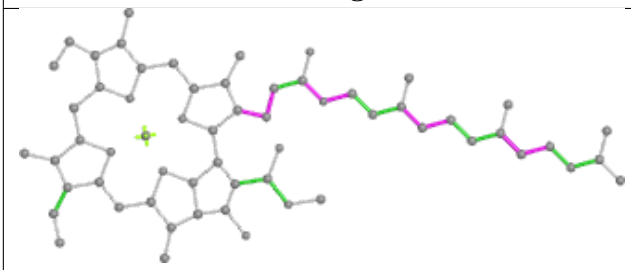
Ligand CLA 2 610



Bond lengths



Bond angles



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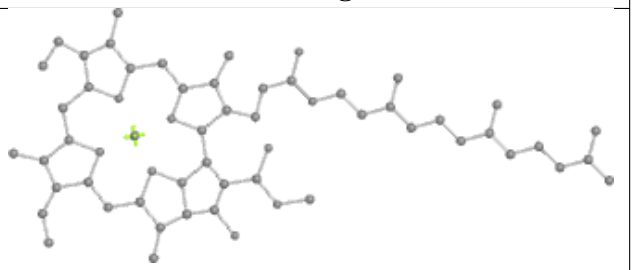
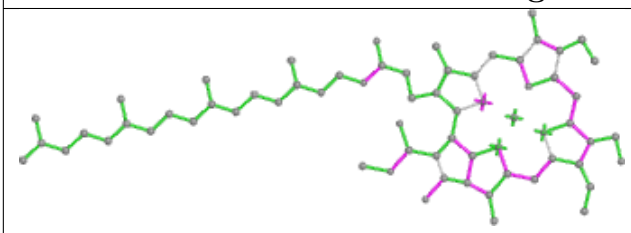


Rings

Ligand CHL 3 608



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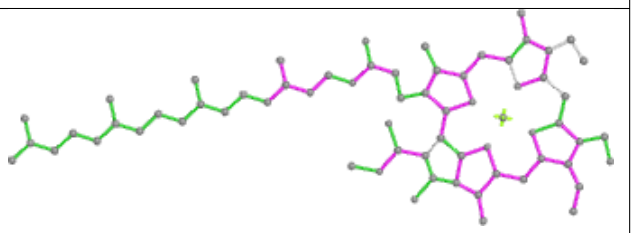
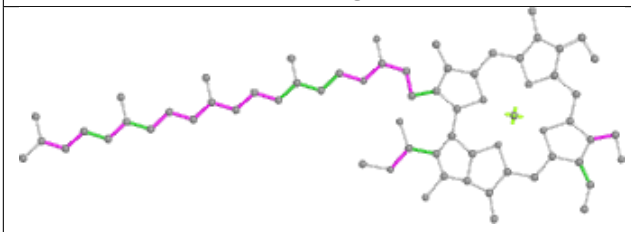


Bond angles



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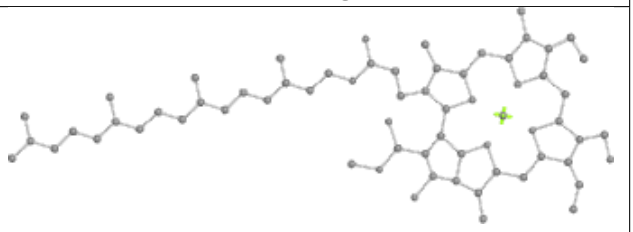
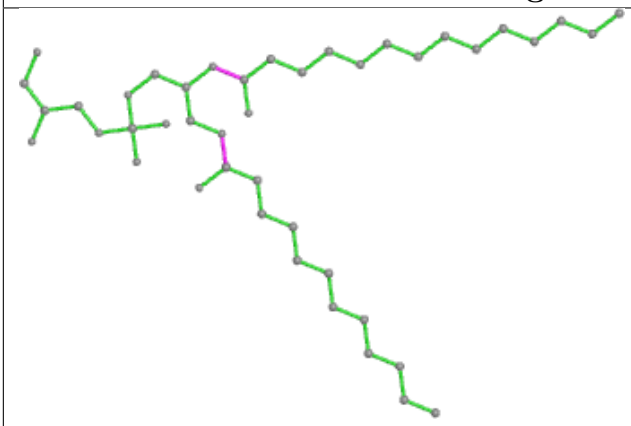


Rings

Ligand LHG 1 620



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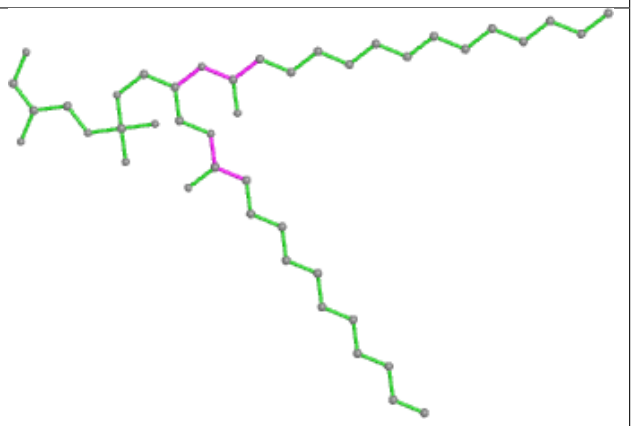
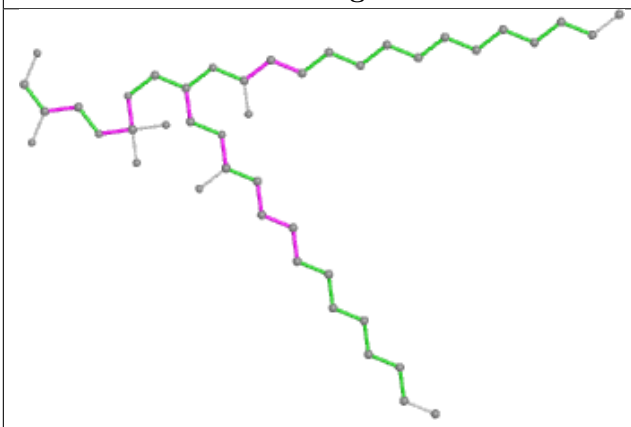


Bond angles



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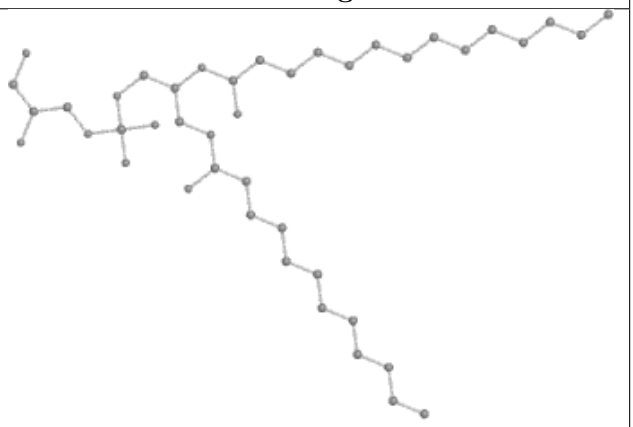
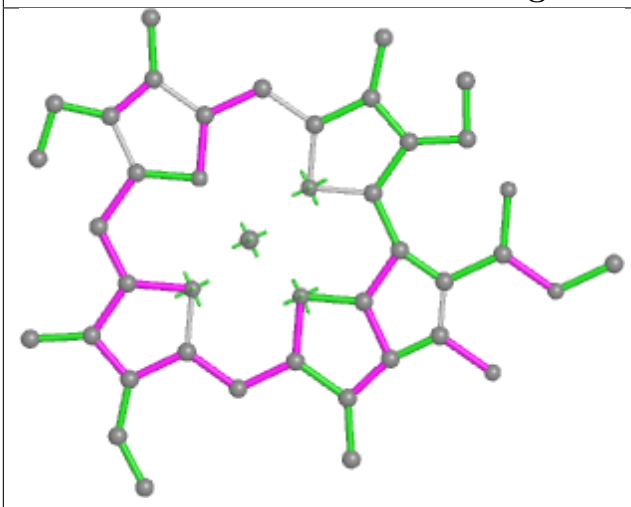
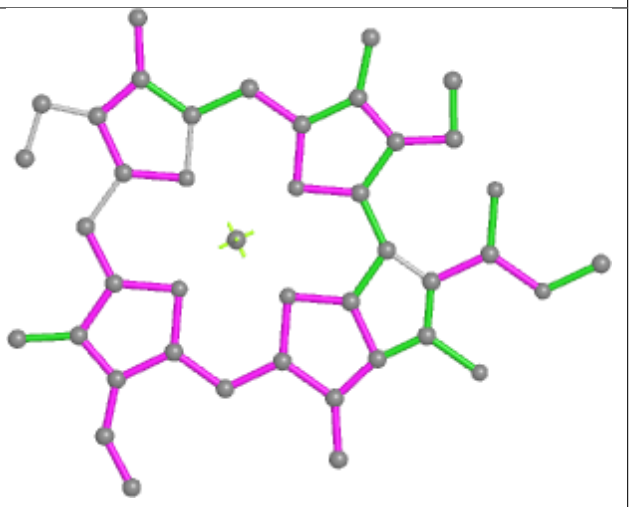


Rings

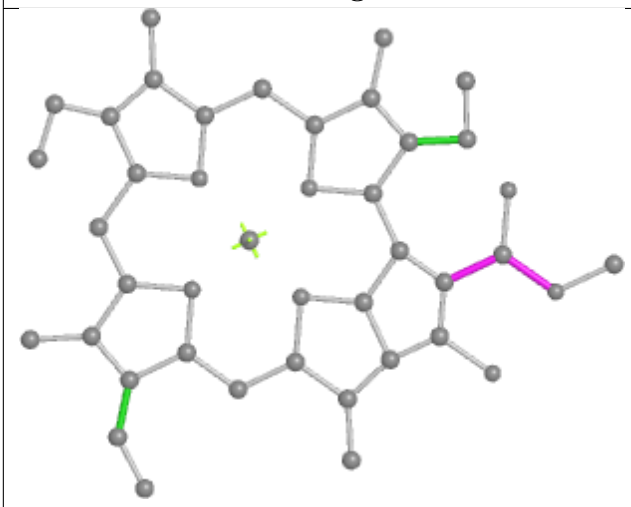
Ligand CLA 8 606



Bond lengths



Bond angles



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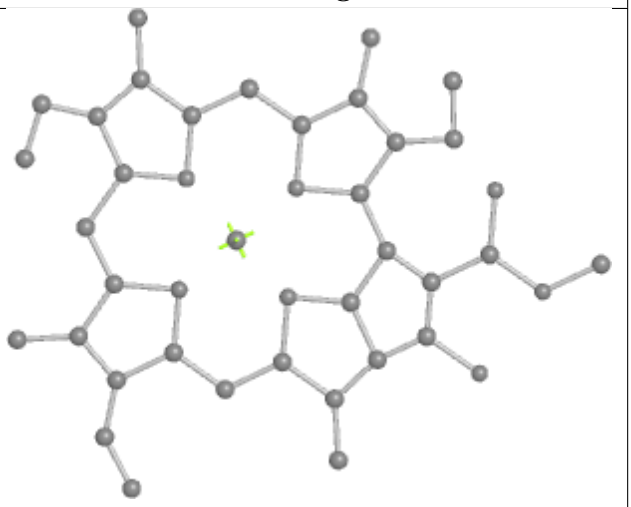
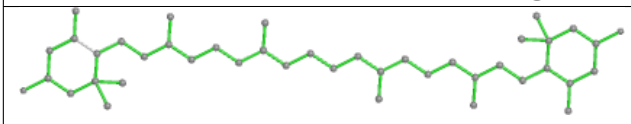


Rings

Ligand LUT 3 621



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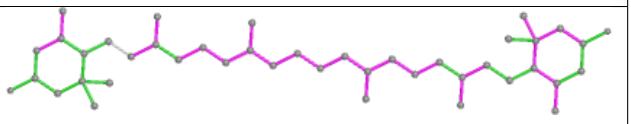
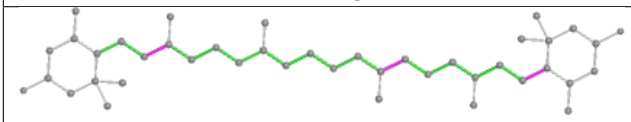


Bond angles



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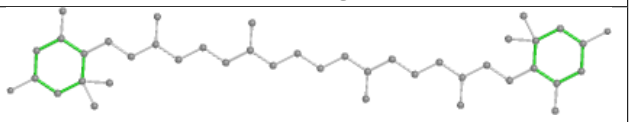
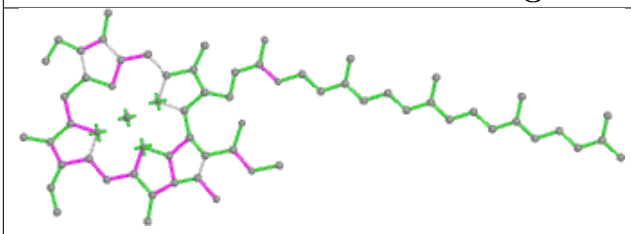


Rings

Ligand CLA B 840



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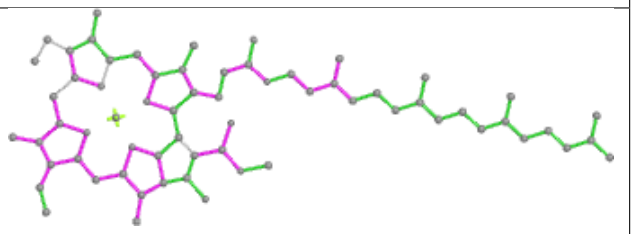
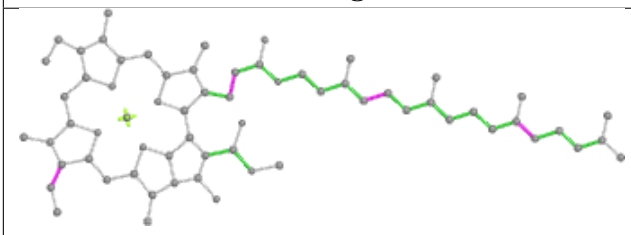
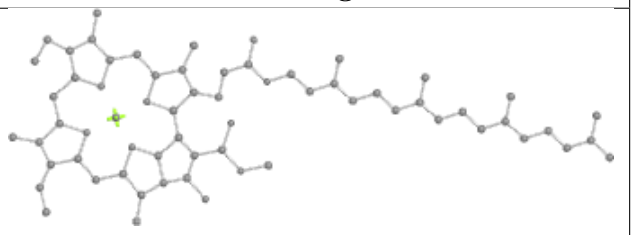


Bond angles

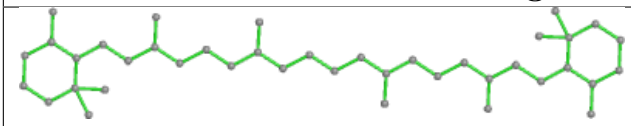


Torsions

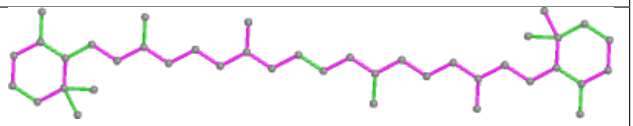


Rings

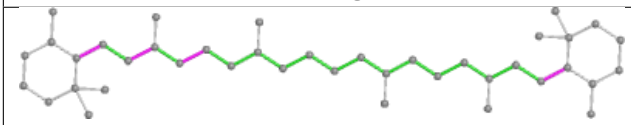
Ligand BCR 5 625



Bond lengths



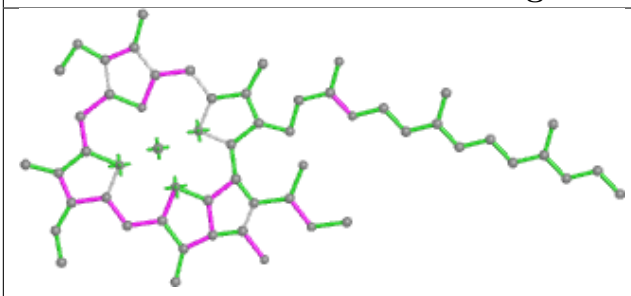
Bond angles



Torsions

Rings

Ligand CLA Z 603



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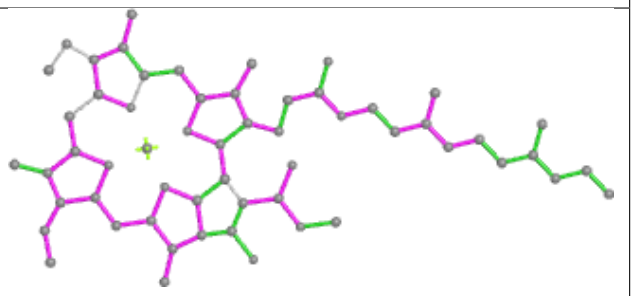
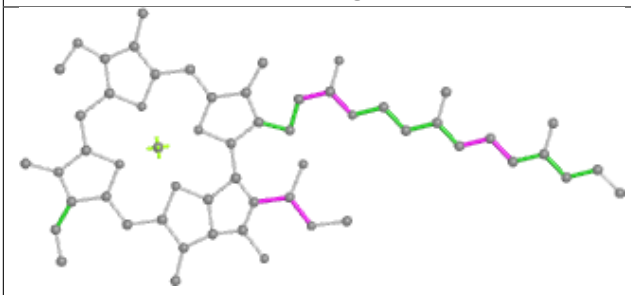
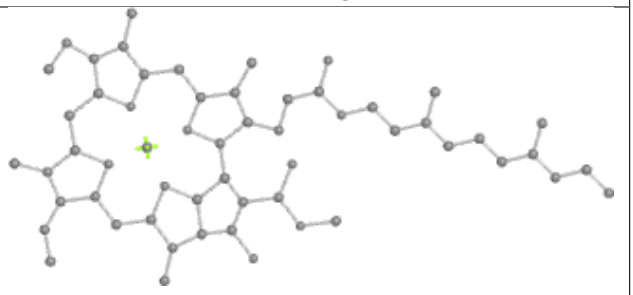


Bond angles

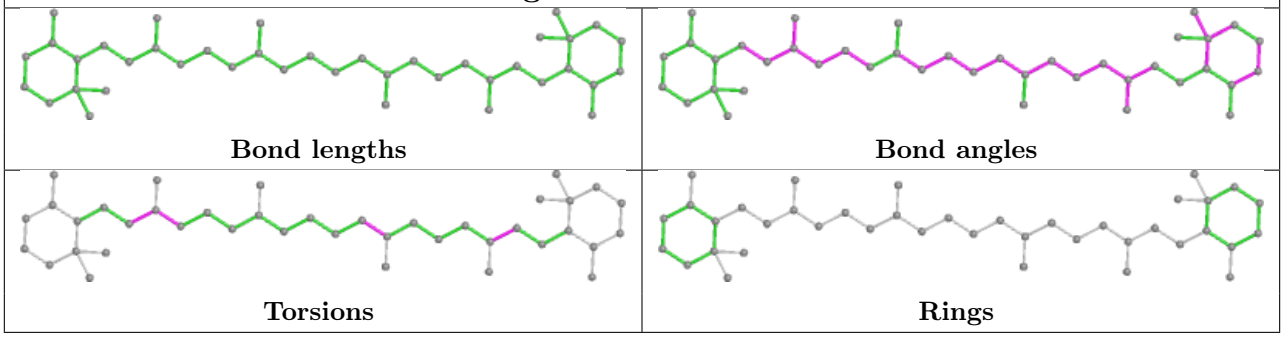


Torsions

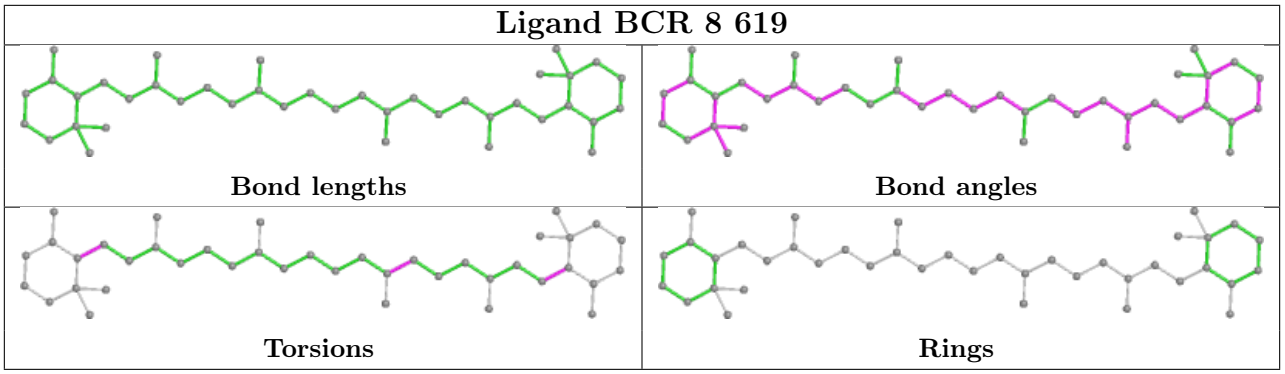


Rings

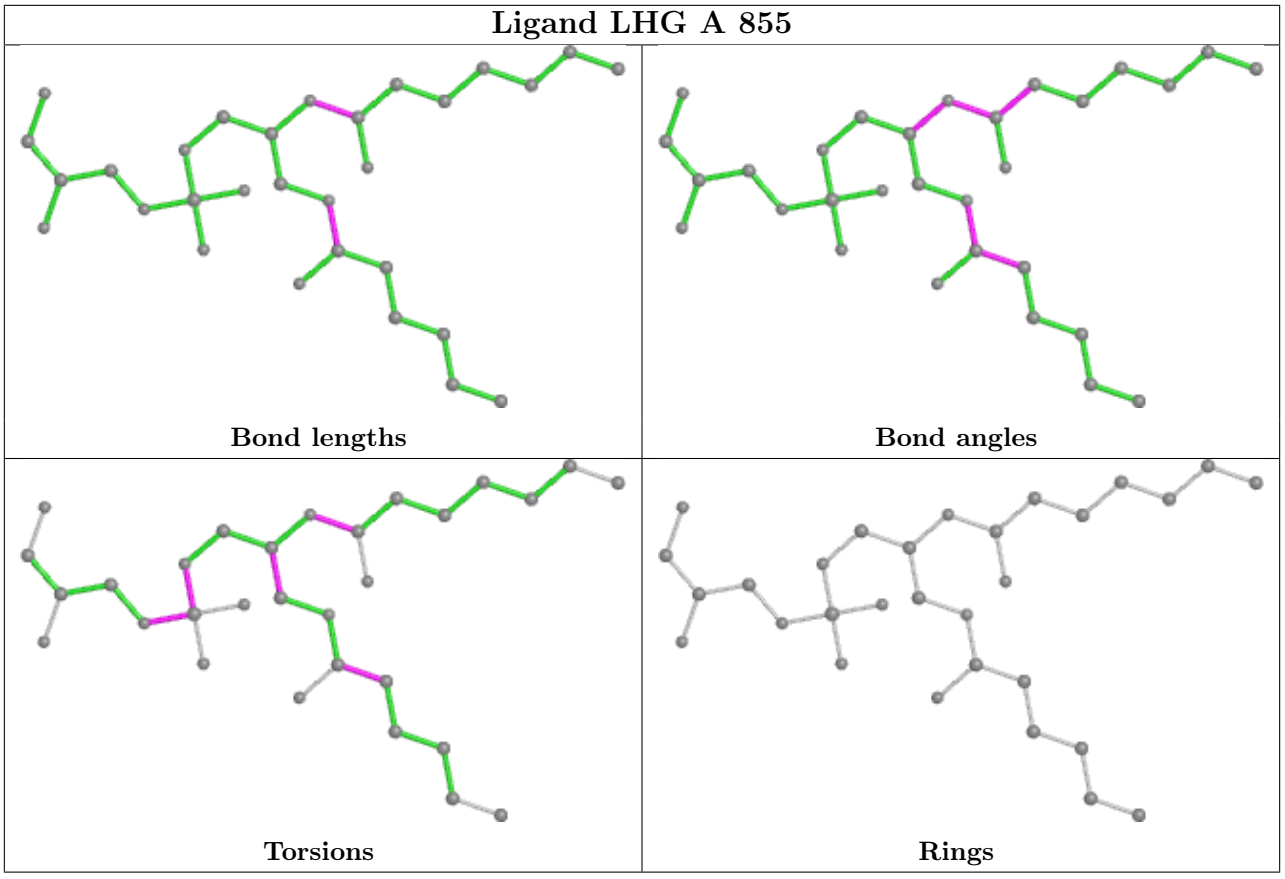
Ligand BCR A 852



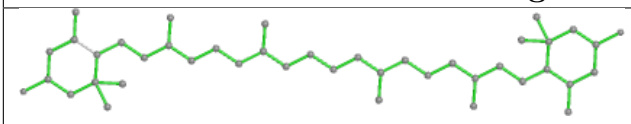
Ligand BCR 8 619



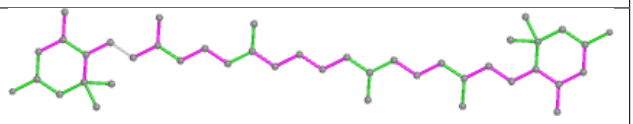
Ligand LHG A 855



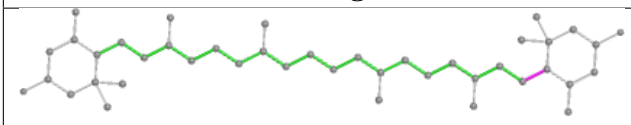
Ligand LUT 9 616



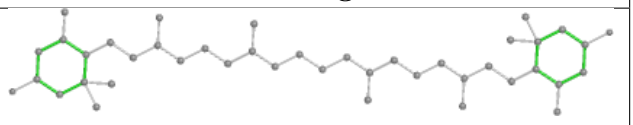
Bond lengths



Bond angles

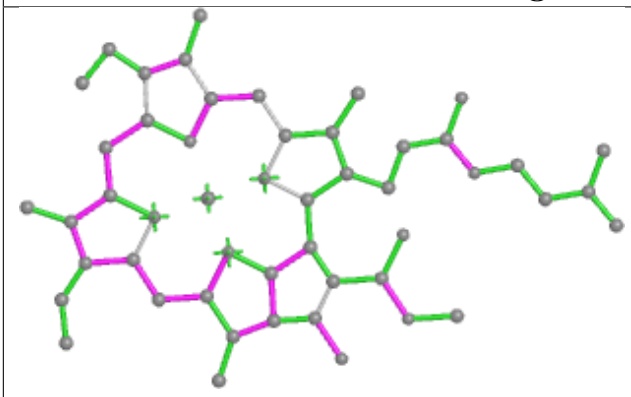


Torsions

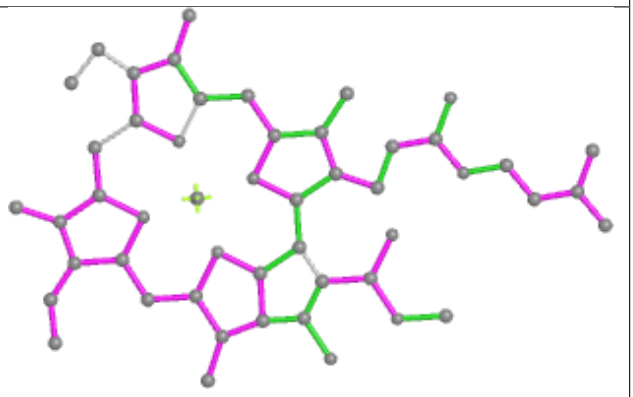


Rings

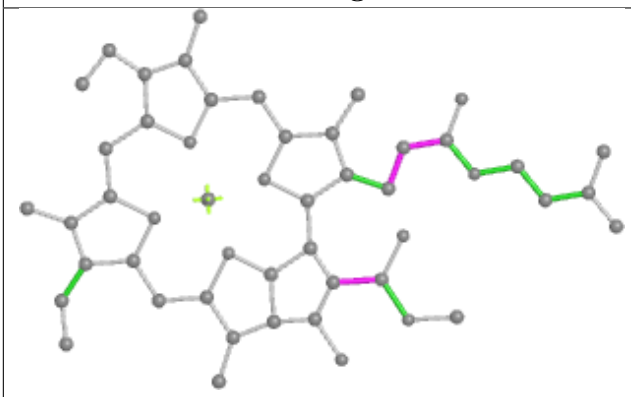
Ligand CLA 9 604



Bond lengths



Bond angles



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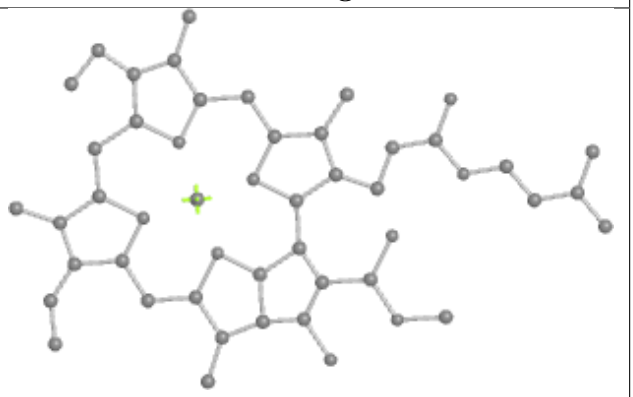
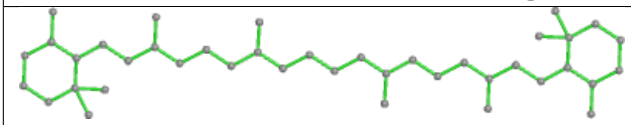
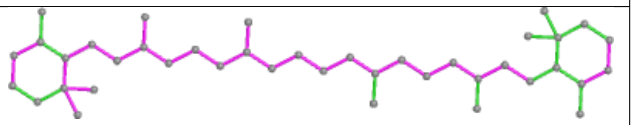


Rings

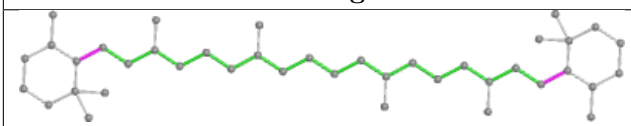
Ligand BCR A 849



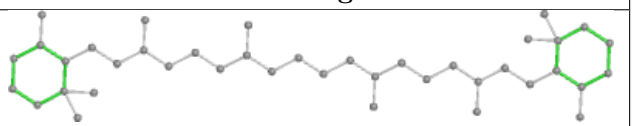
Bond lengths



Bond angles

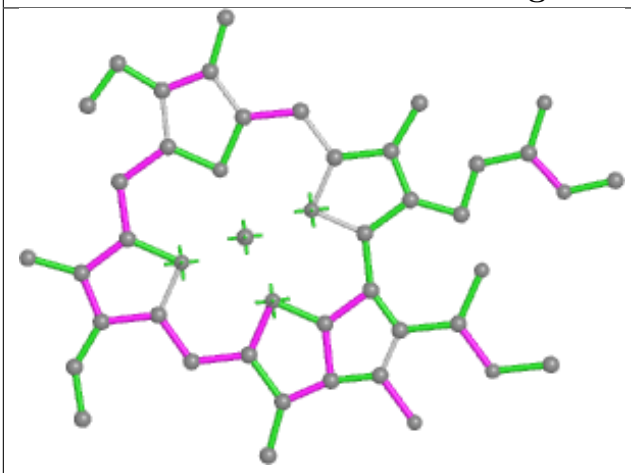


Torsions

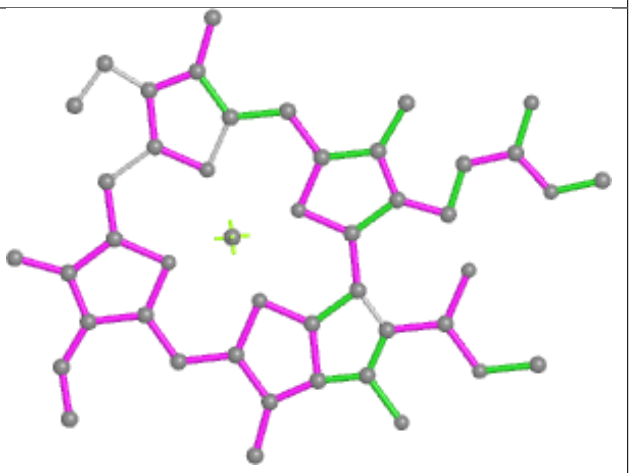


Rings

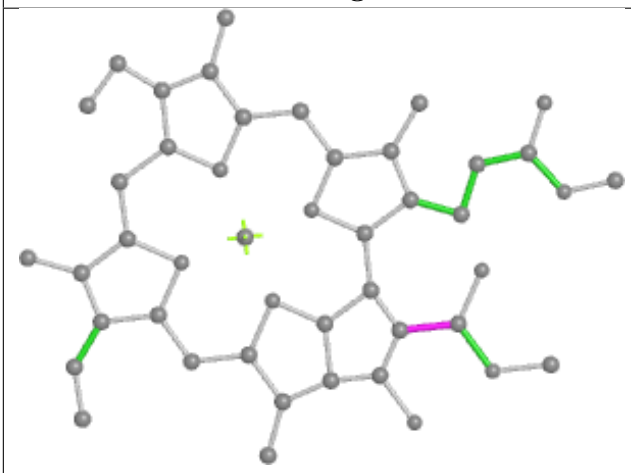
Ligand CLA 6 603



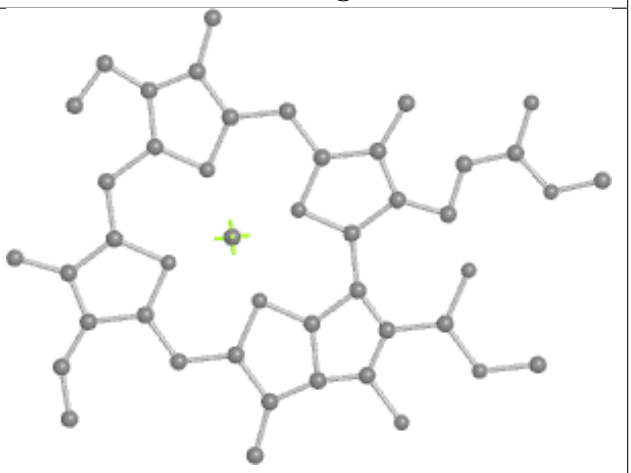
Bond lengths



Bond angles

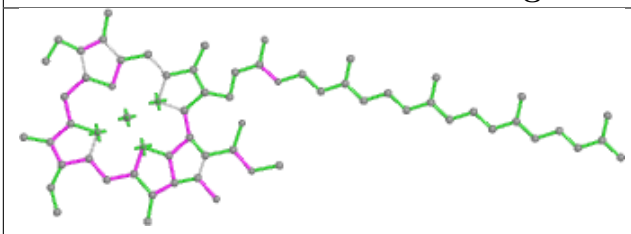


Torsions

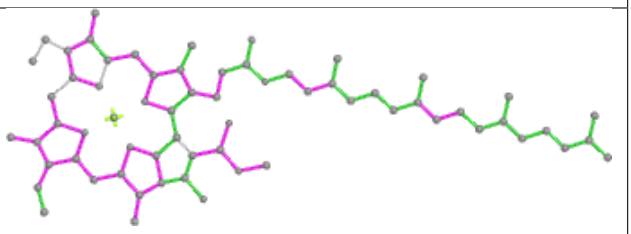


Rings

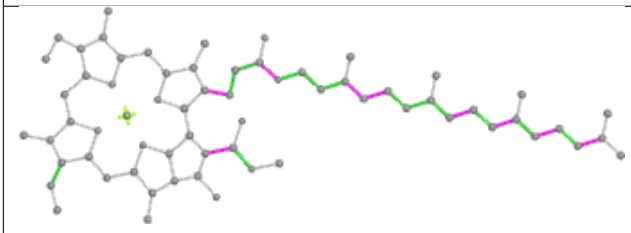
Ligand CLA A 820



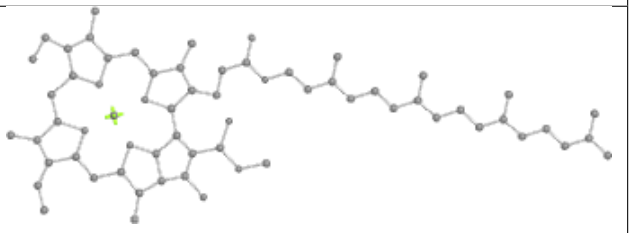
Bond lengths



Bond angles

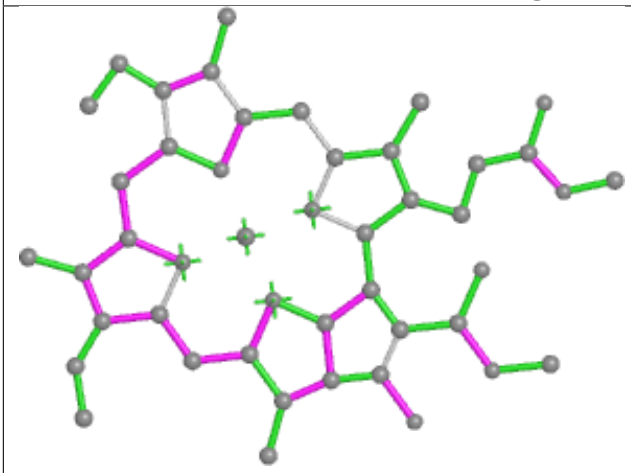


Torsions

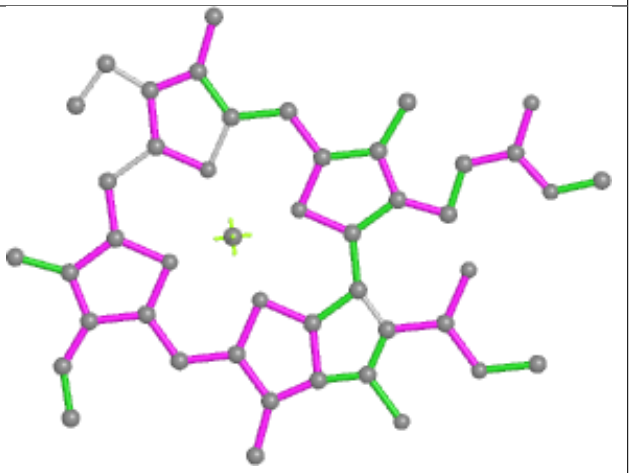


Rings

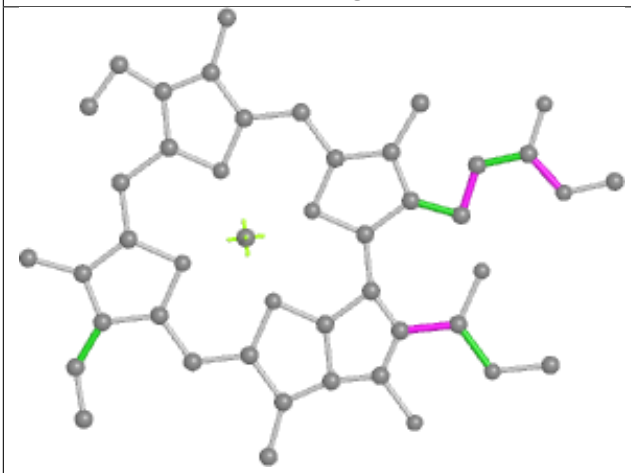
Ligand CLA 5 617



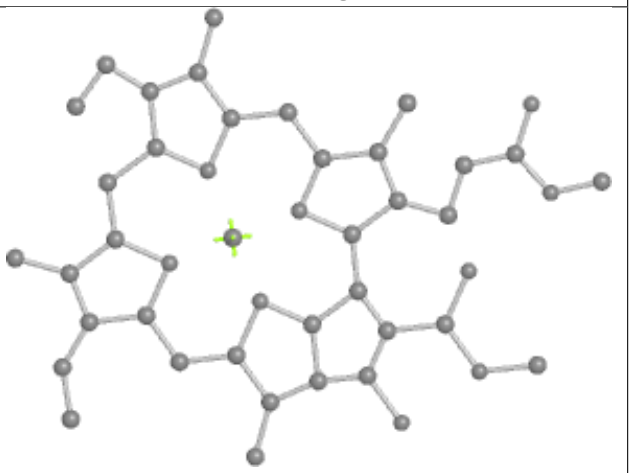
Bond lengths



Bond angles

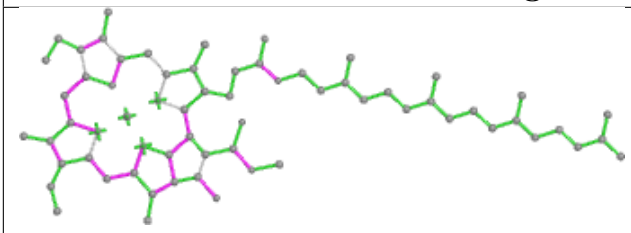


Torsions

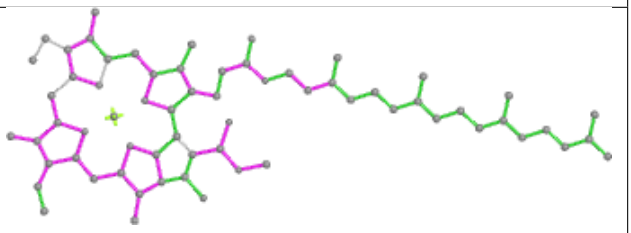


Rings

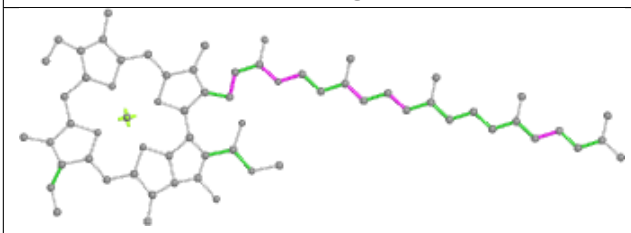
Ligand CLA A 830



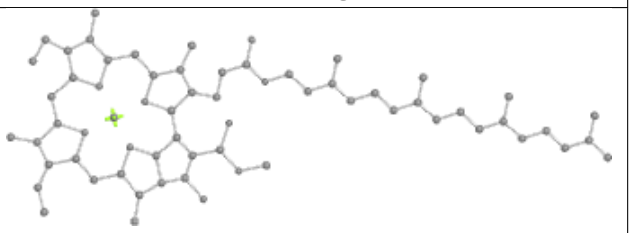
Bond lengths



Bond angles

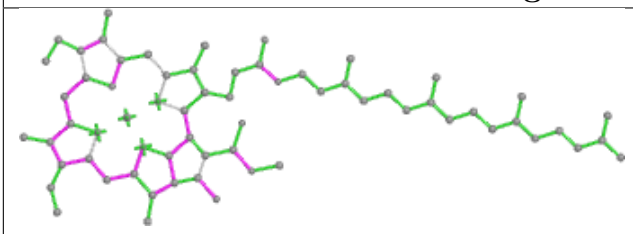


Torsions

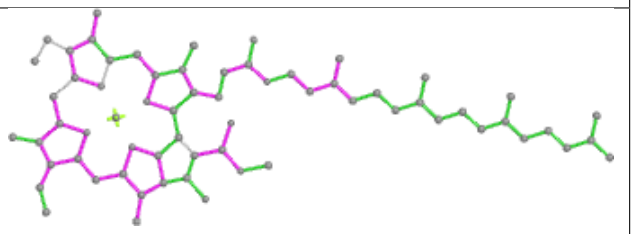


Rings

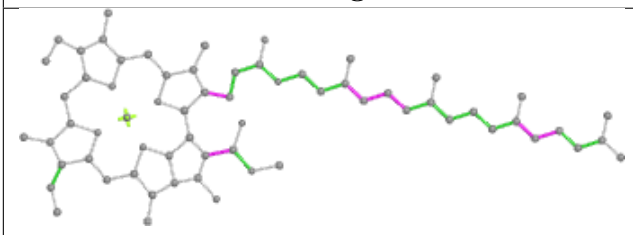
Ligand CLA A 816



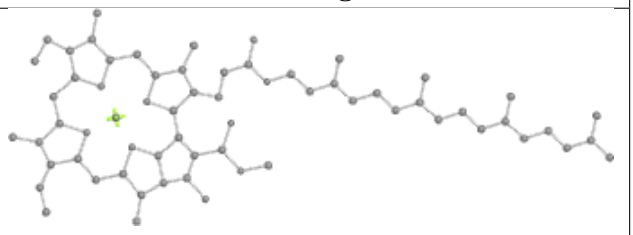
Bond lengths



Bond angles

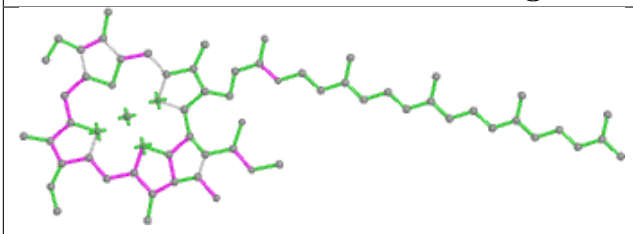


Torsions



Rings

Ligand CLA B 841



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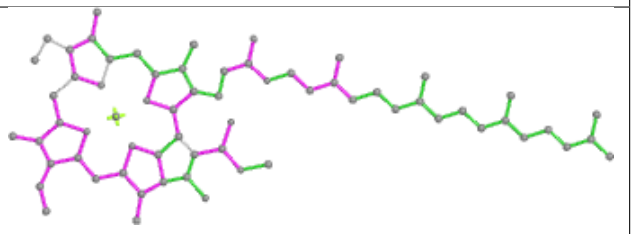
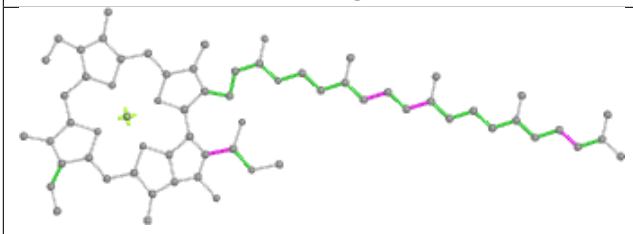


Bond angles



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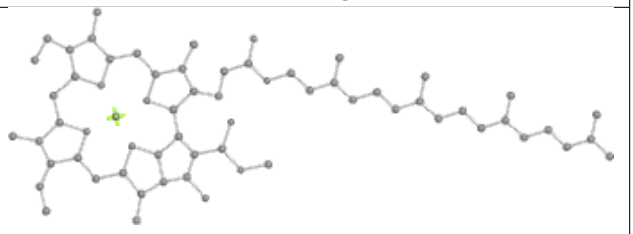
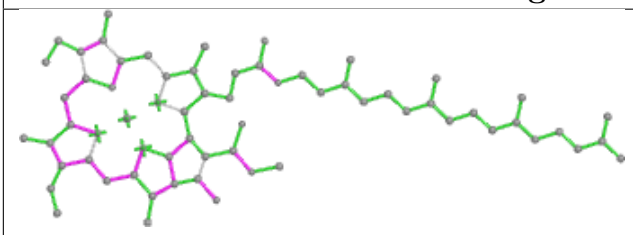
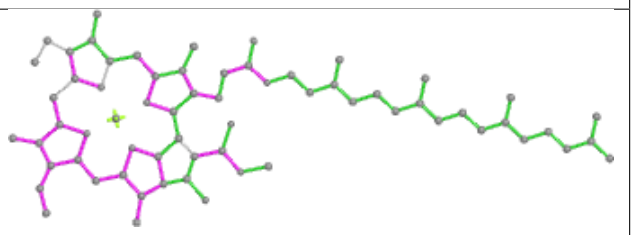


Rings

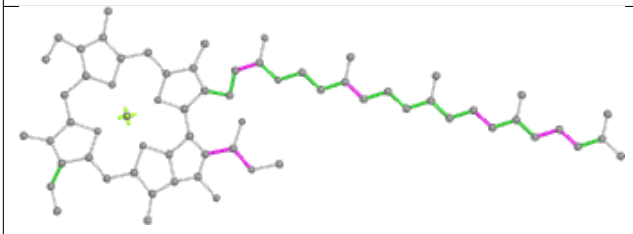
Ligand CLA 7 613



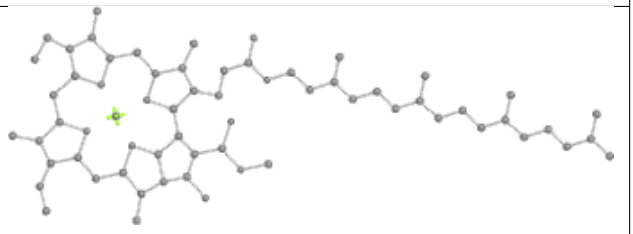
Bond lengths



Bond angles

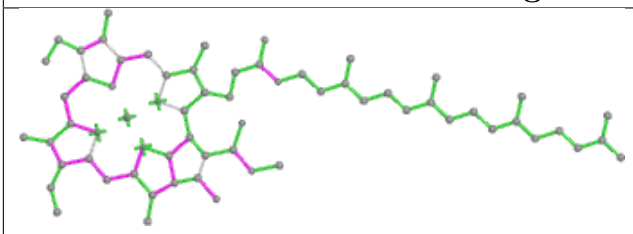


Torsions

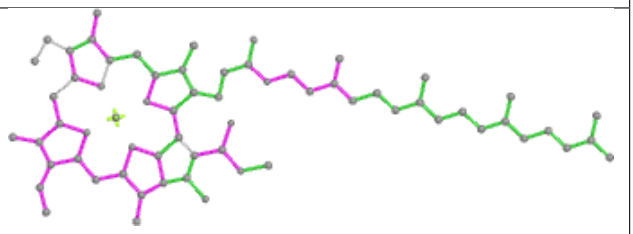


Rings

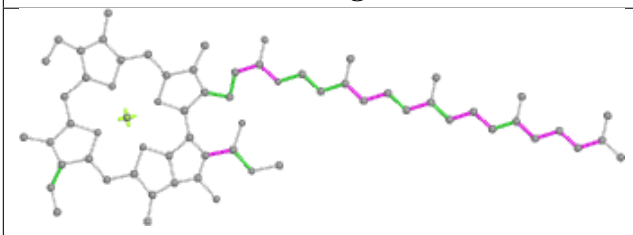
Ligand CLA A 826



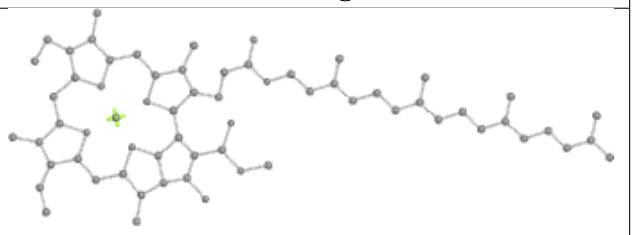
Bond lengths



Bond angles

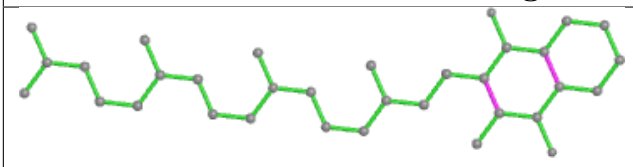


Torsions

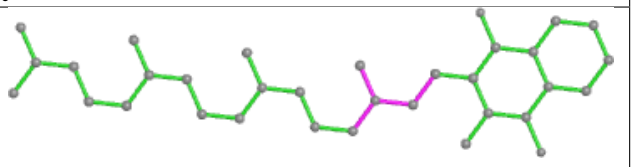


Rings

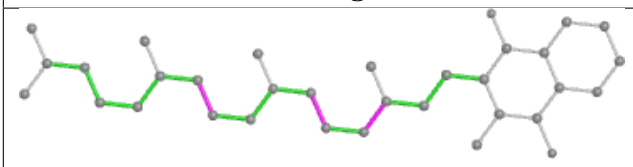
Ligand PQN B 842



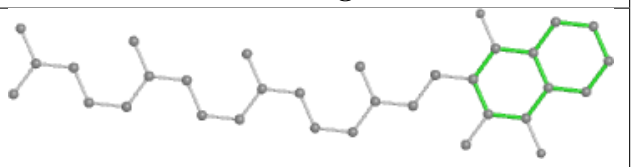
Bond lengths



Bond angles

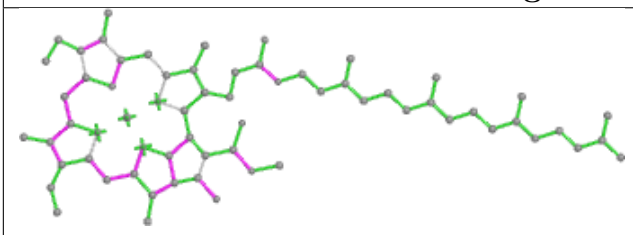


Torsions

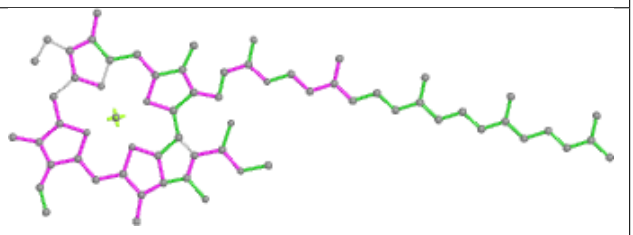


Rings

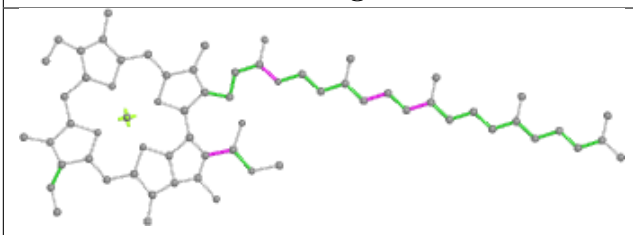
Ligand CLA A 827



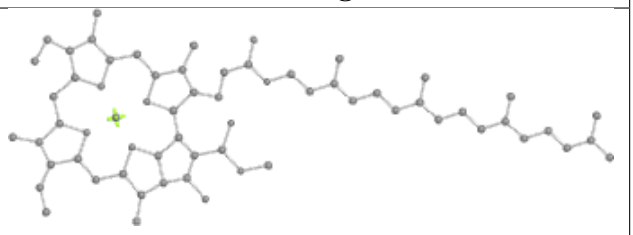
Bond lengths



Bond angles

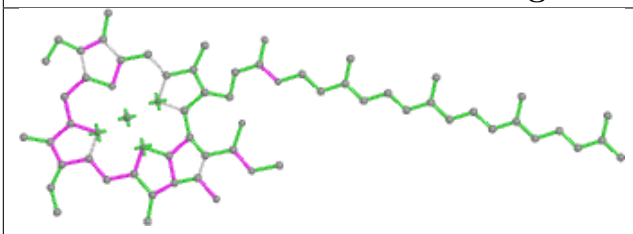


Torsions

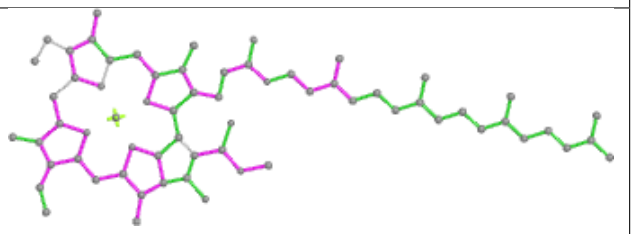


Rings

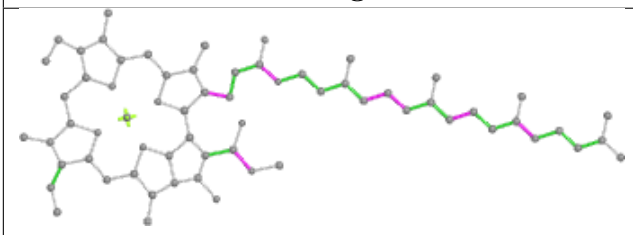
Ligand CLA 1 611



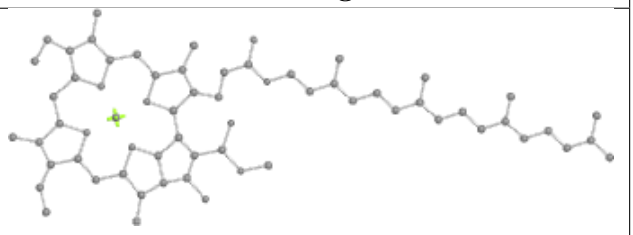
Bond lengths



Bond angles

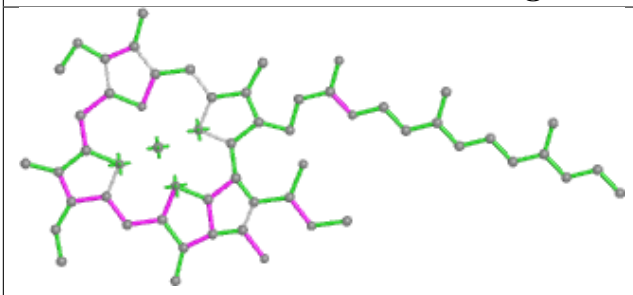


Torsions



Rings

Ligand CLA B 815



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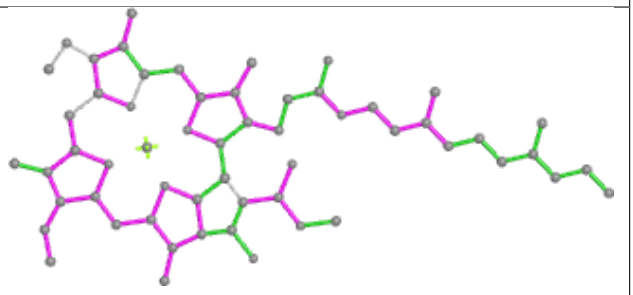
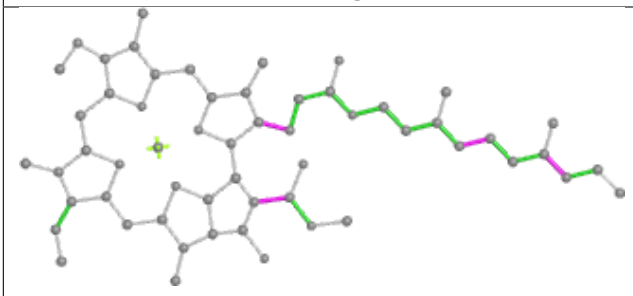
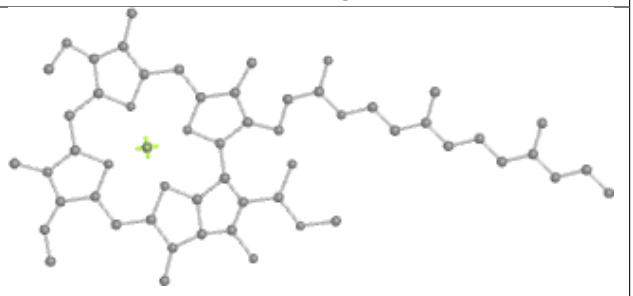


Bond angles

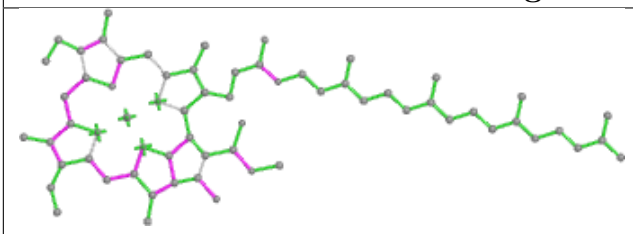


Torsions

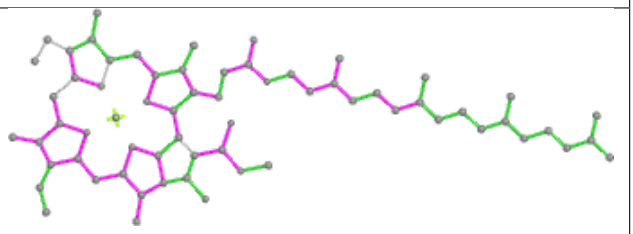


Rings

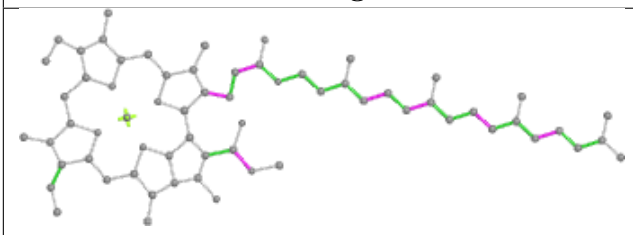
Ligand CLA B 832



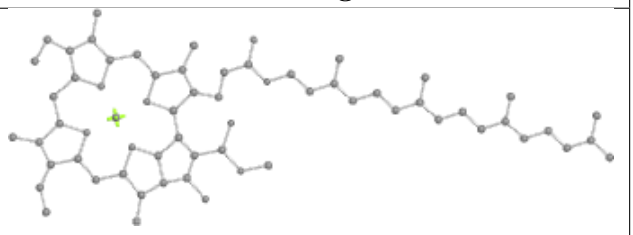
Bond lengths



Bond angles

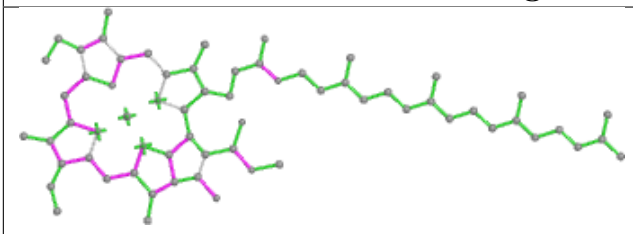


Torsions



Rings

Ligand CLA A 807



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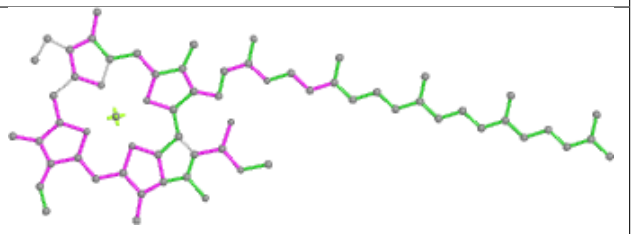
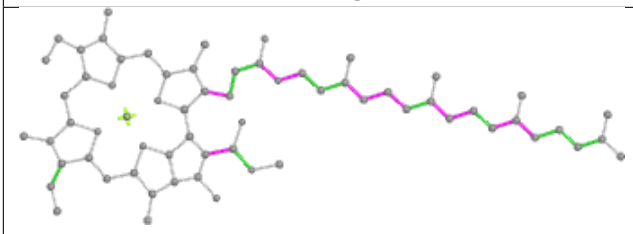
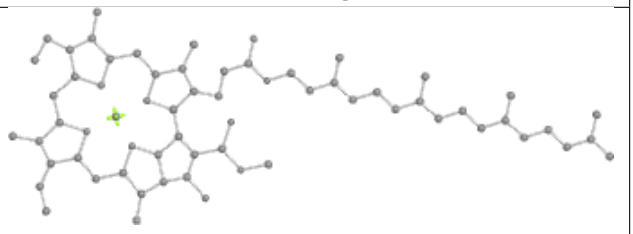


Bond angles

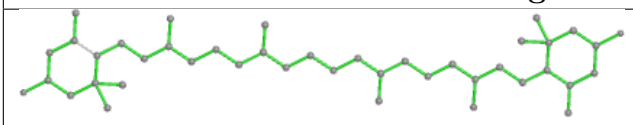


Torsions



Rings

Ligand LUT 8 617



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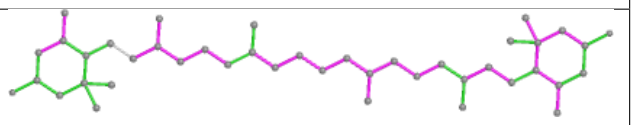
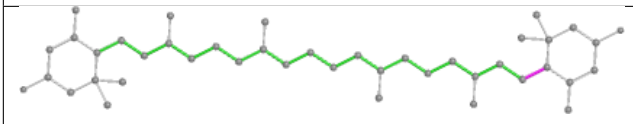


Bond angles



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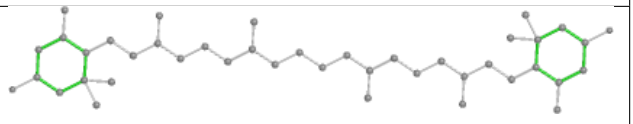
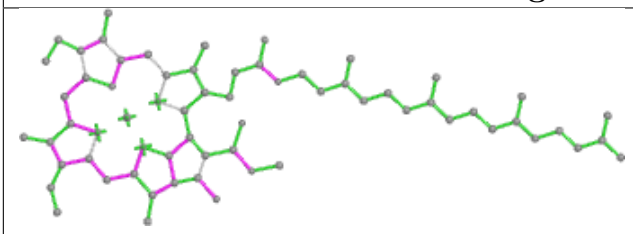


Rings

Ligand CLA 3 603



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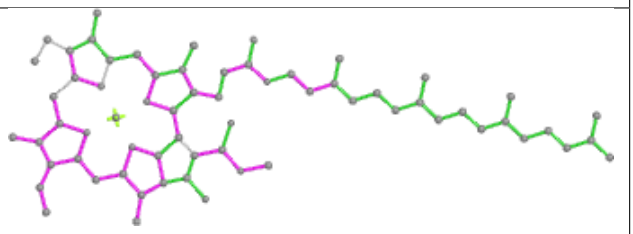
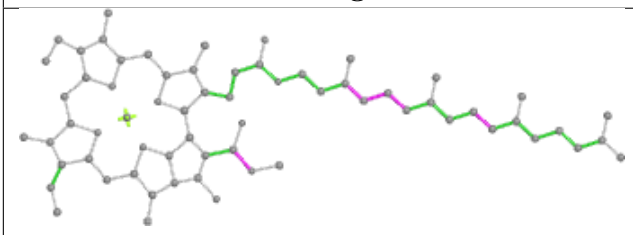


Bond angles



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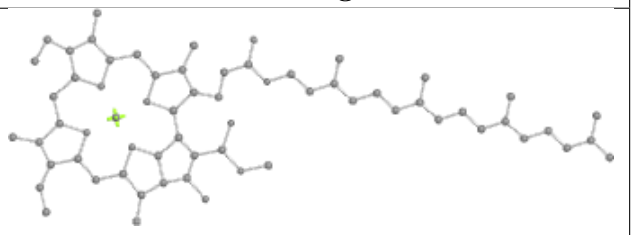
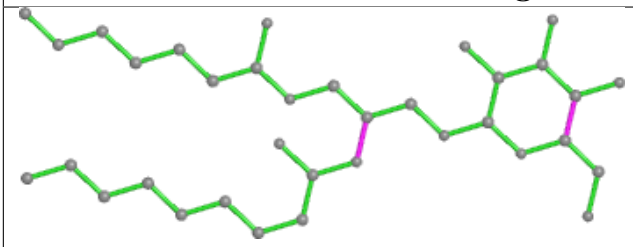
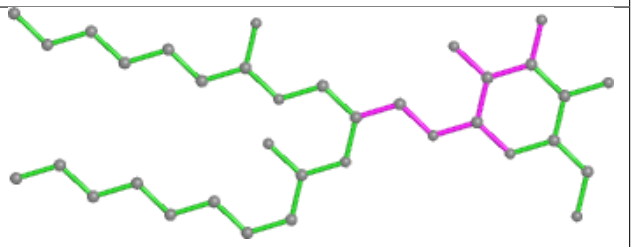


Rings

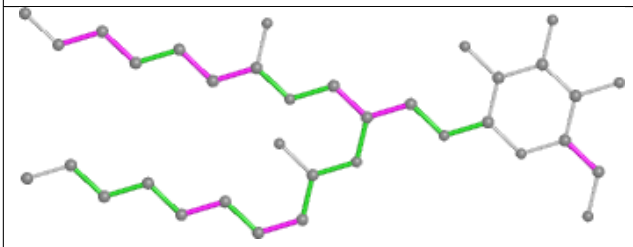
Ligand LMG J 3001



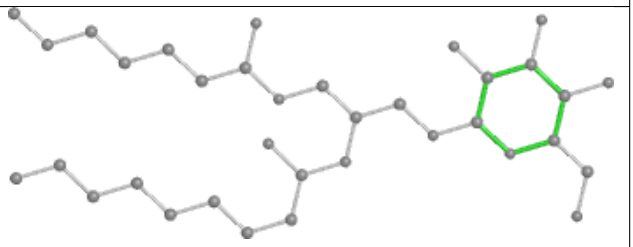
Bond lengths



Bond angles

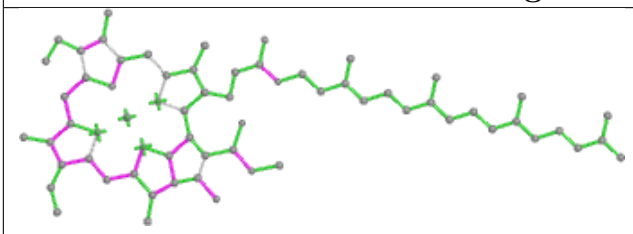


Torsions

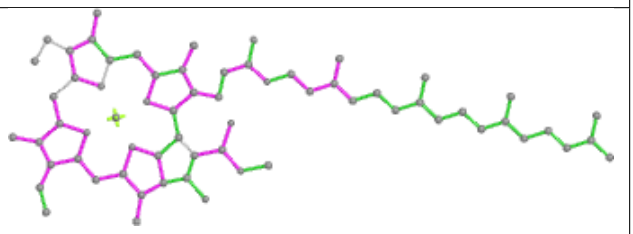


Rings

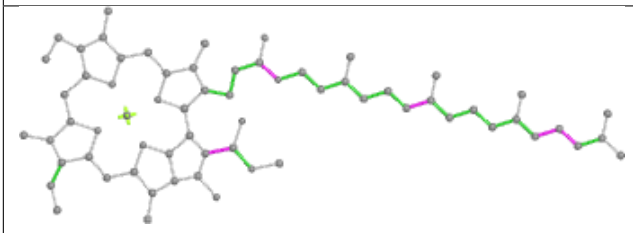
Ligand CLA B 825



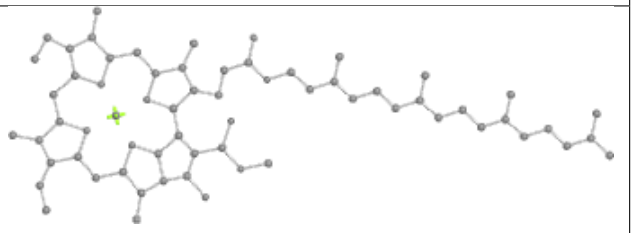
Bond lengths



Bond angles

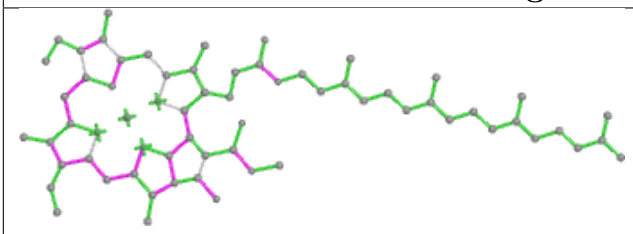


Torsions

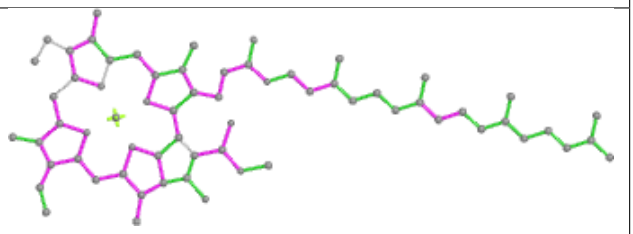


Rings

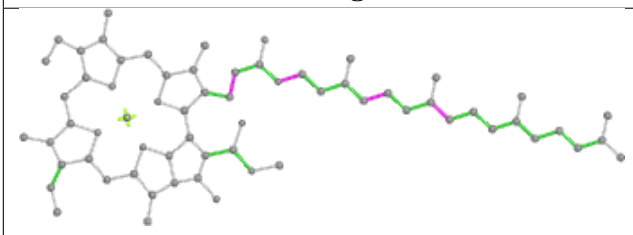
Ligand CLA Z 609



Bond lengths



Bond angles



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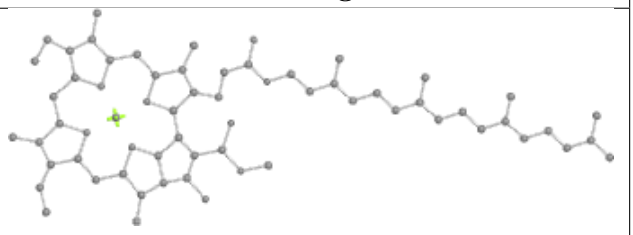
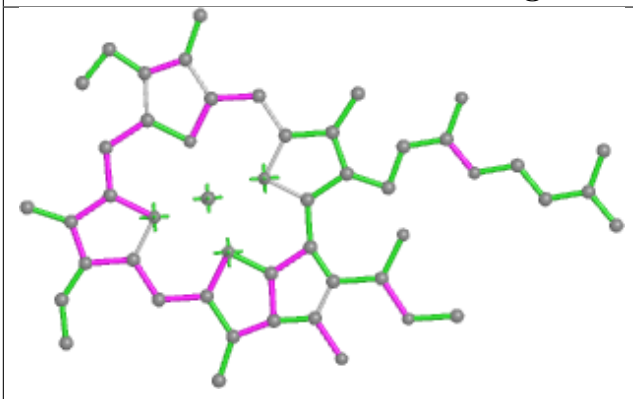


Rings

Ligand CLA A 836



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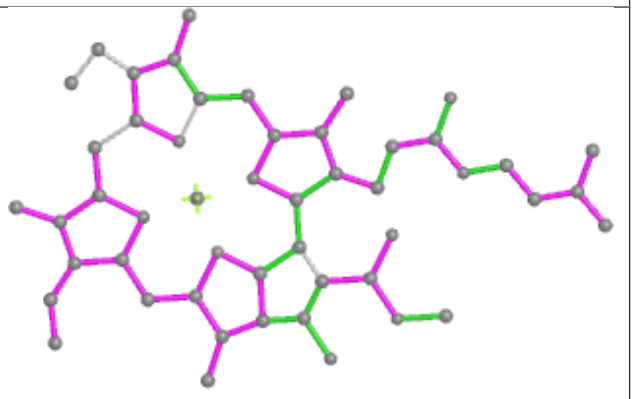

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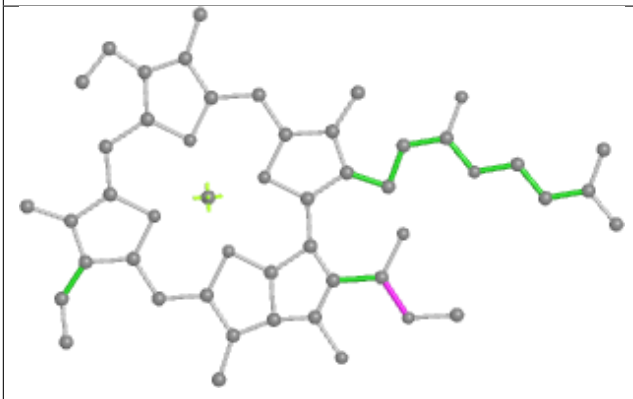

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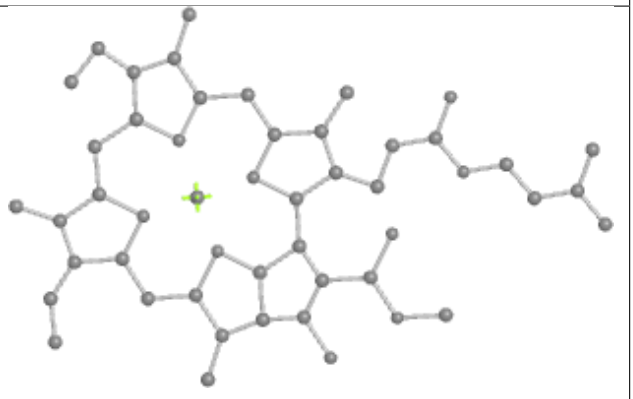
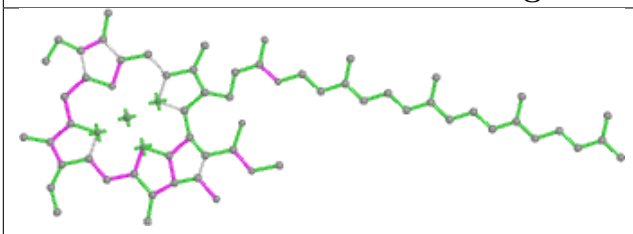
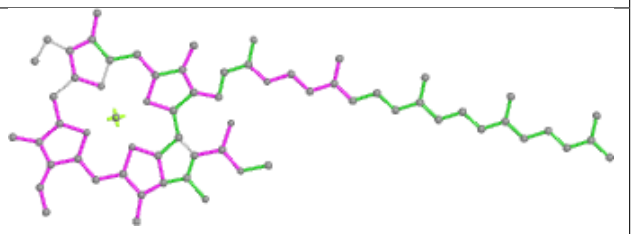


Rings

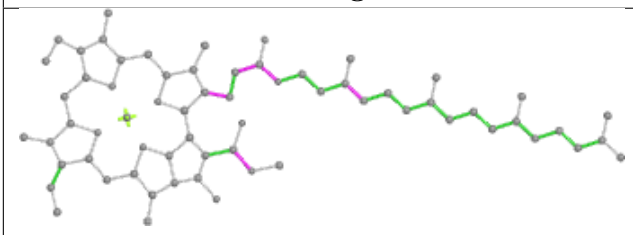
Ligand CLA A 811



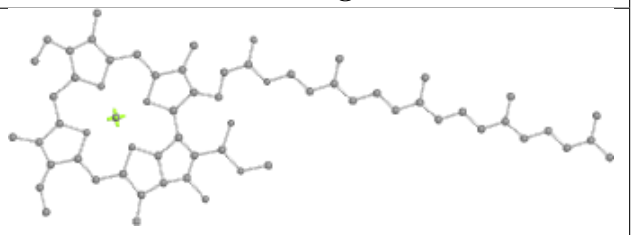
Bond lengths



Bond angles

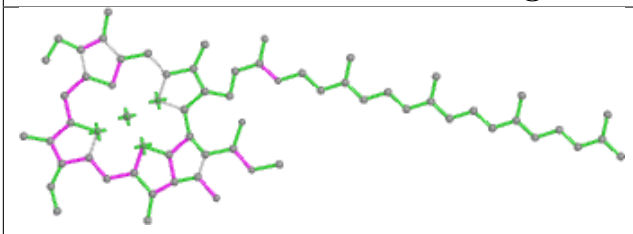


Torsions

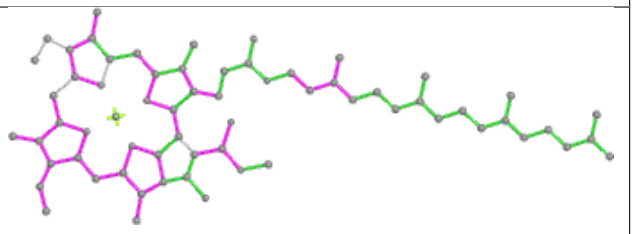


Rings

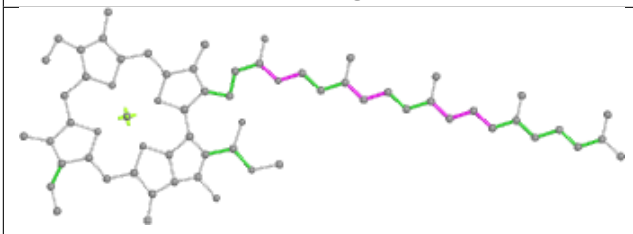
Ligand CLA A 833



Bond lengths



Bond angles



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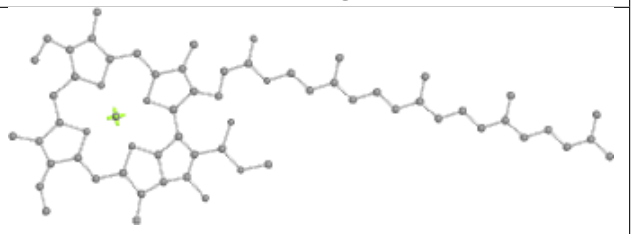
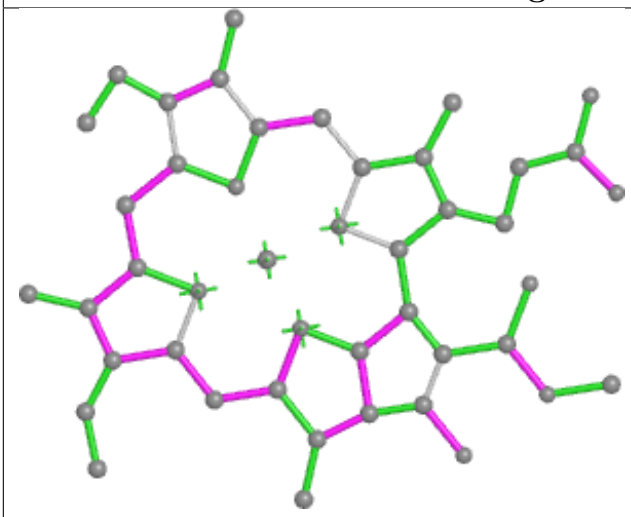
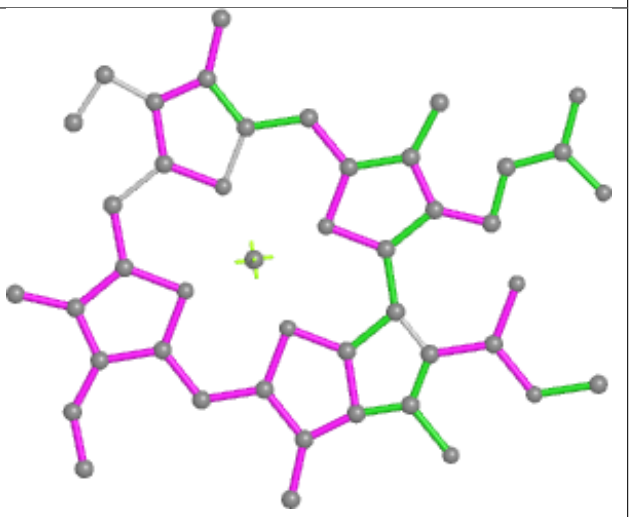


Rings

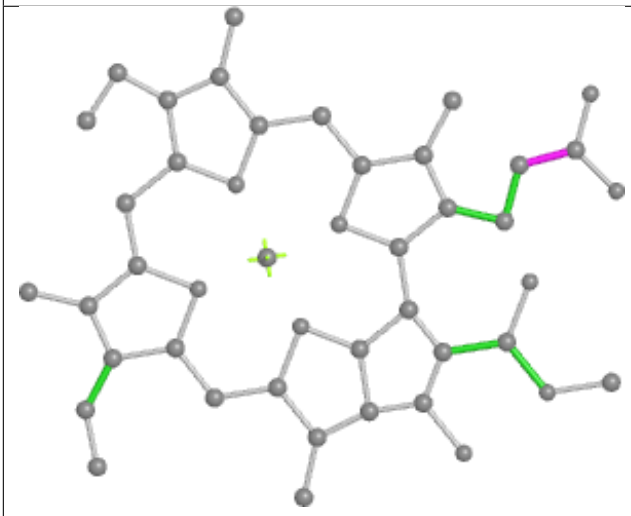
Ligand CLA 3 614



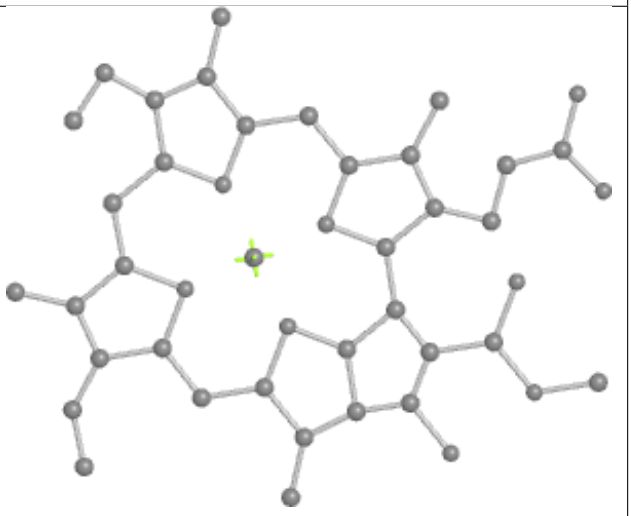
Bond lengths



Bond angles

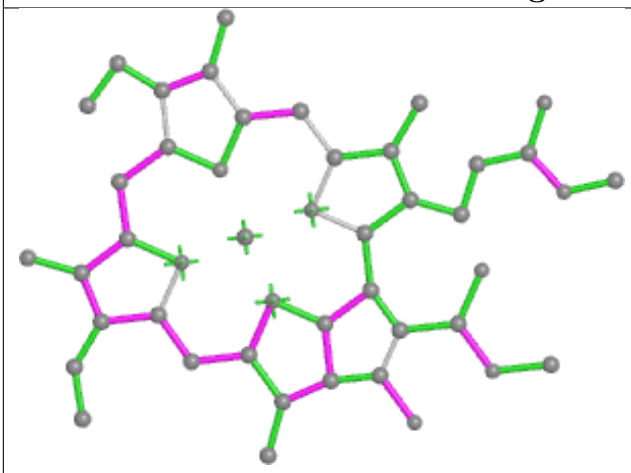


Torsions

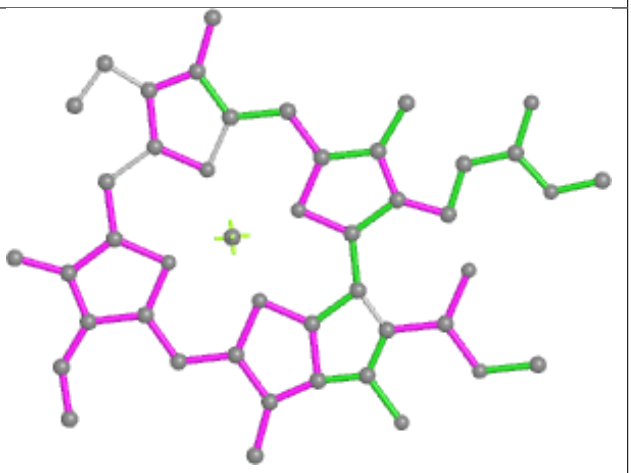


Rings

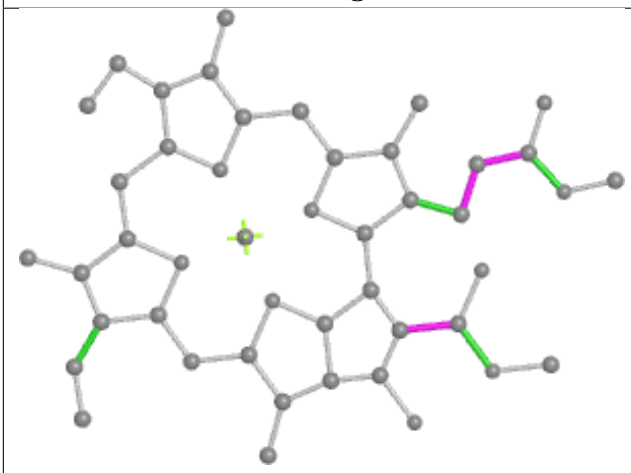
Ligand CLA 9 601



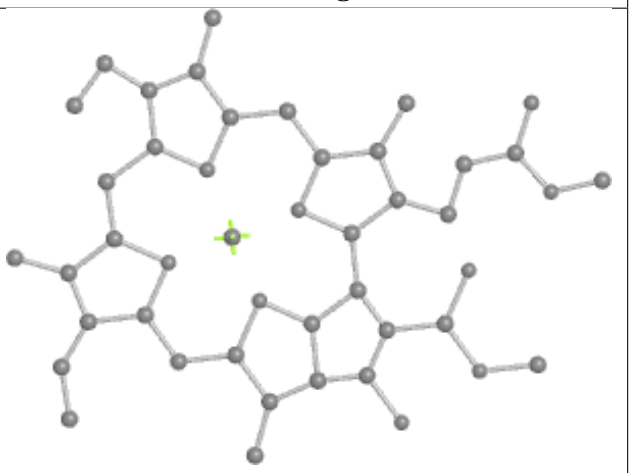
Bond lengths



Bond angles

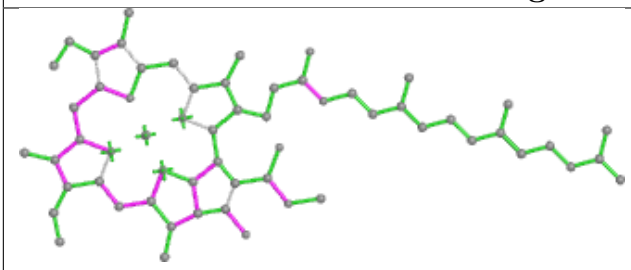


Torsions

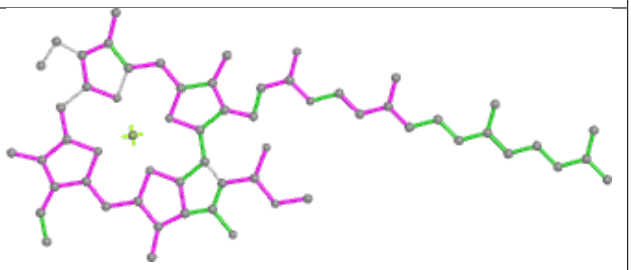


Rings

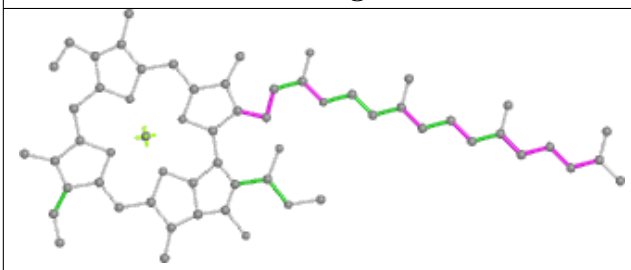
Ligand CLA 8 610



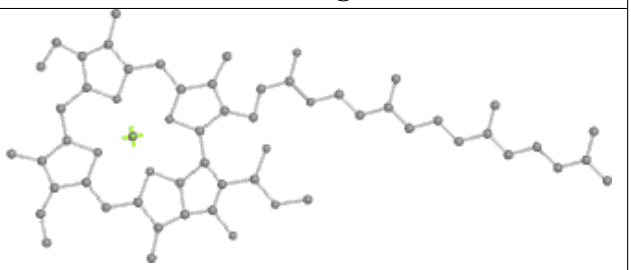
Bond lengths



Bond angles

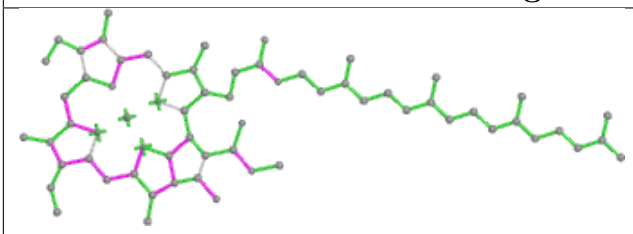


Torsions



Rings

Ligand CLA A 831



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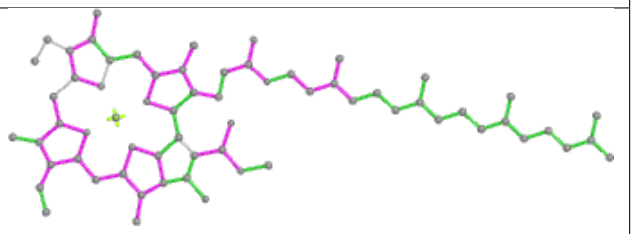
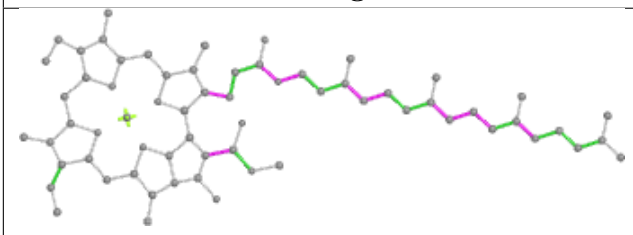
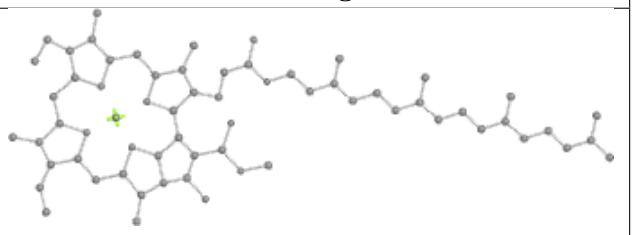


Bond angles

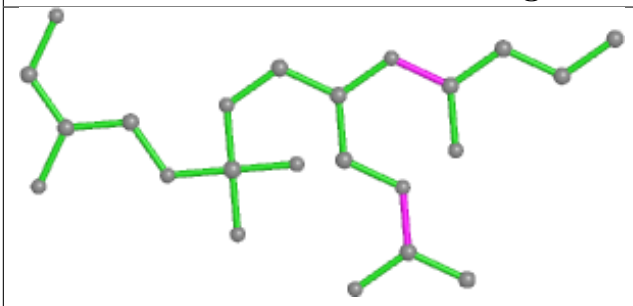


Torsions

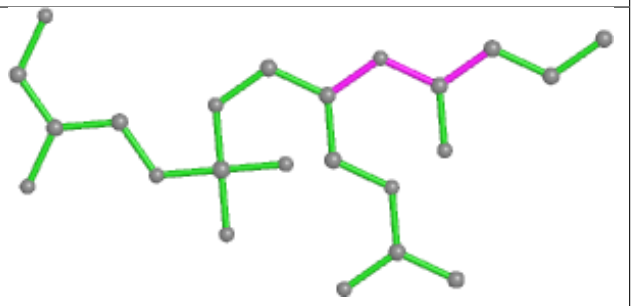


Rings

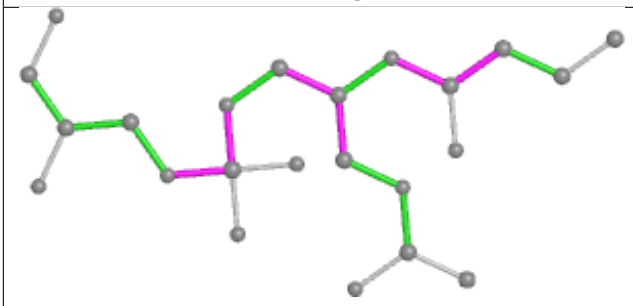
Ligand LHG B 851



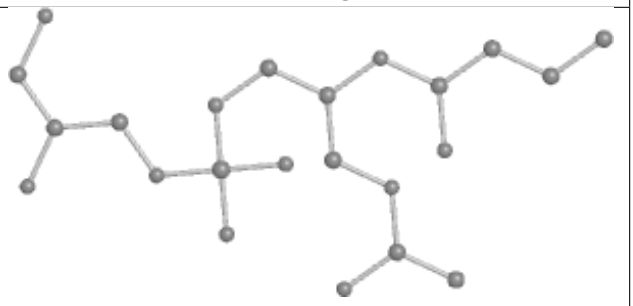
Bond lengths



Bond angles

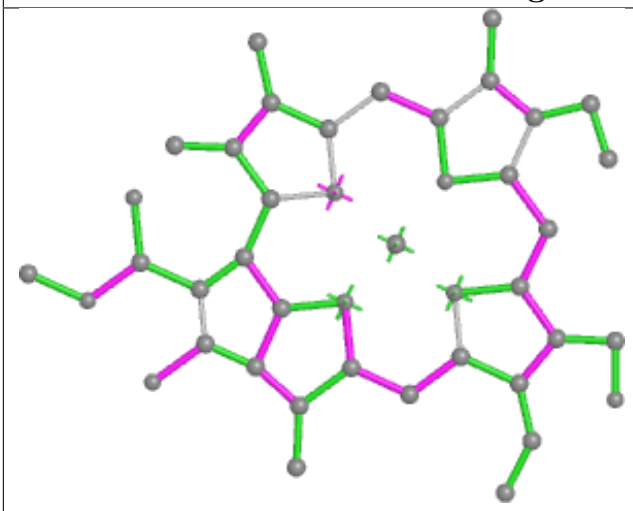


Torsions



Rings

Ligand CHL 9 606



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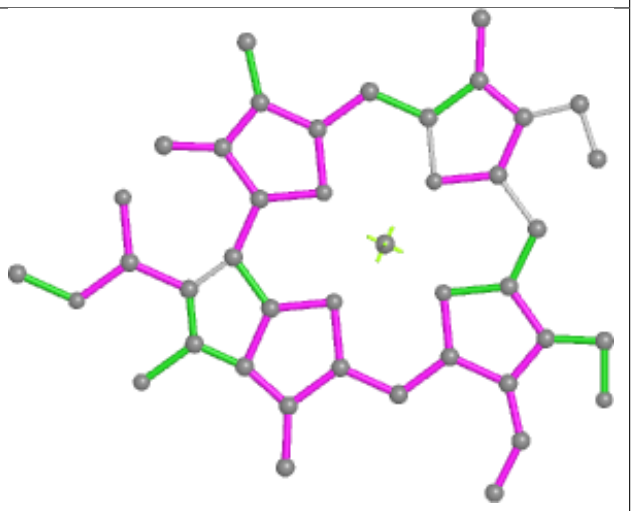
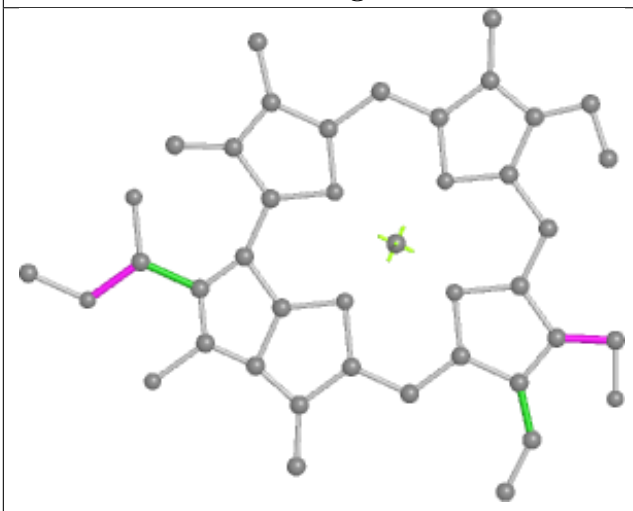
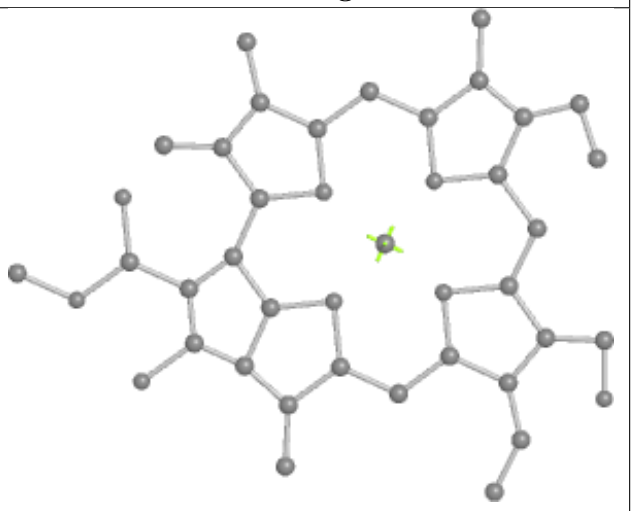


Bond angles

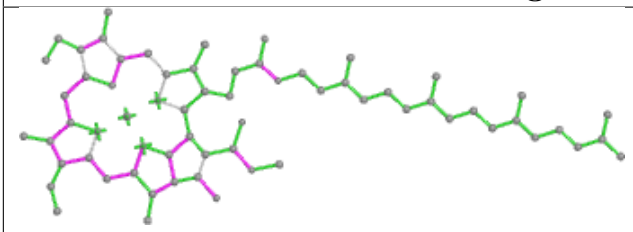


Torsions

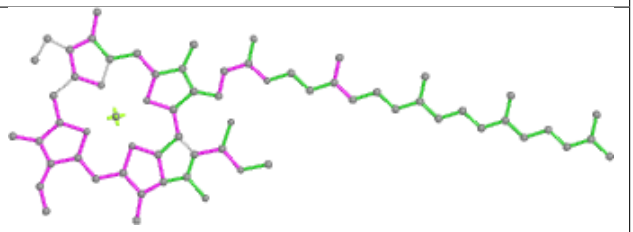


Rings

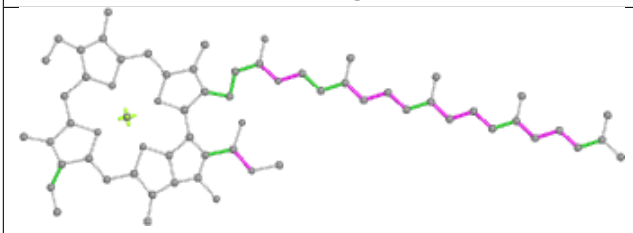
Ligand CLA Z 608



Bond lengths



Bond angles



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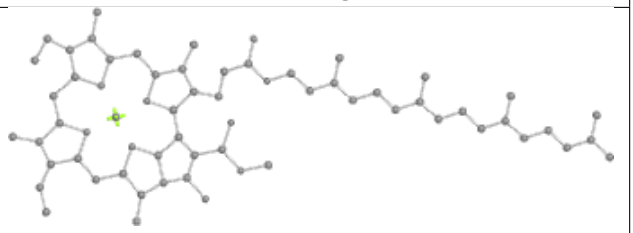
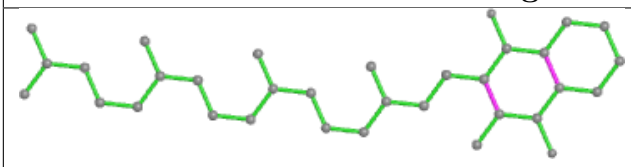


Rings

Ligand PQN A 844



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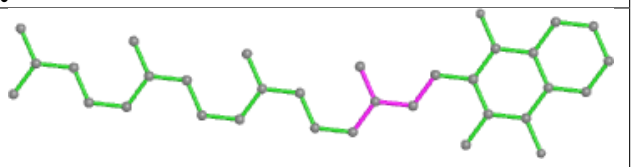
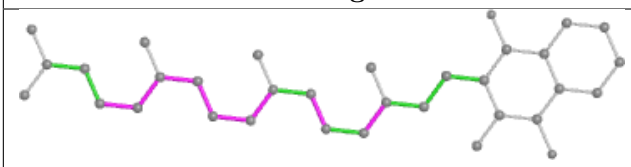


Bond angles



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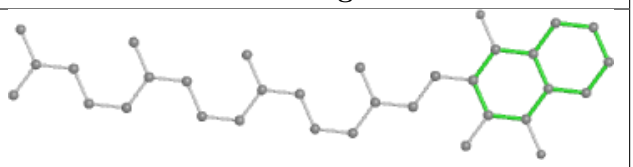
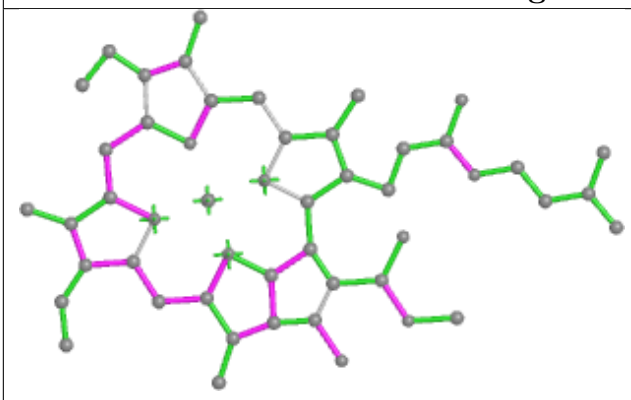


Rings

Ligand CLA 4 609



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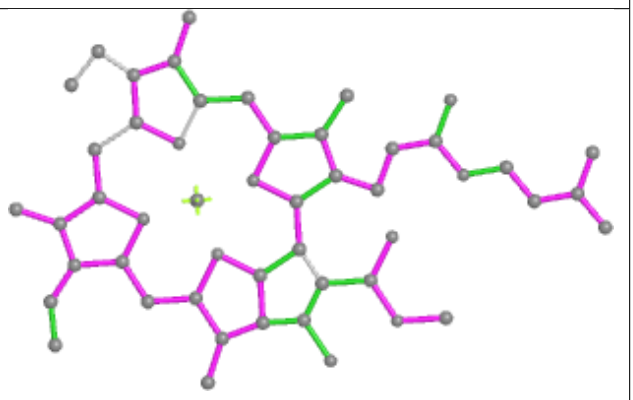
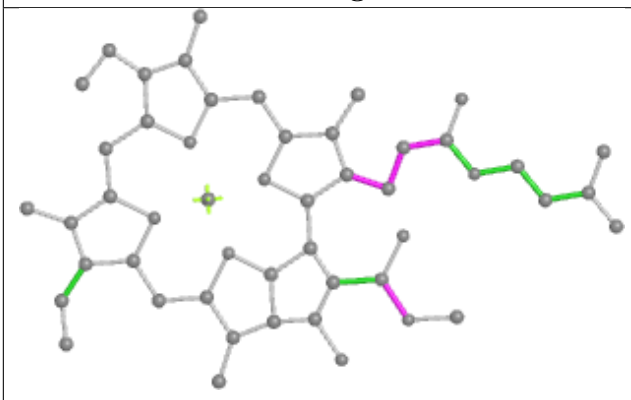


Bond angles



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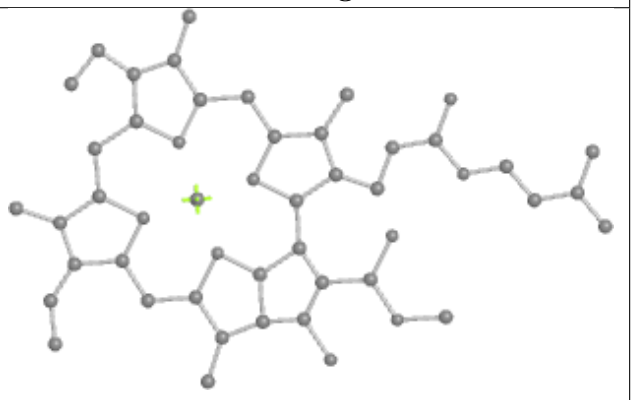
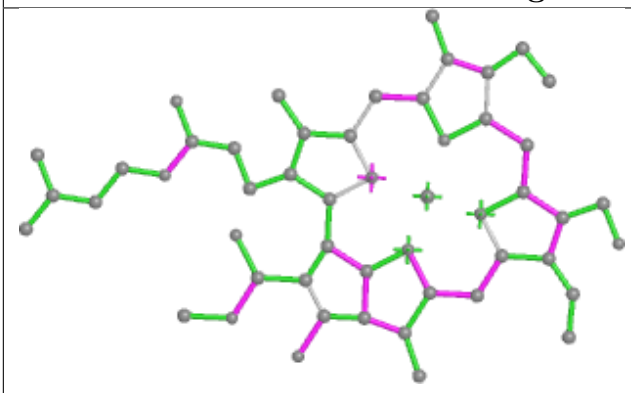
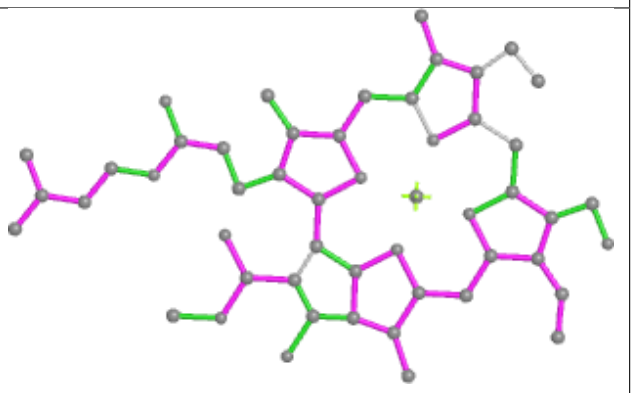


Rings

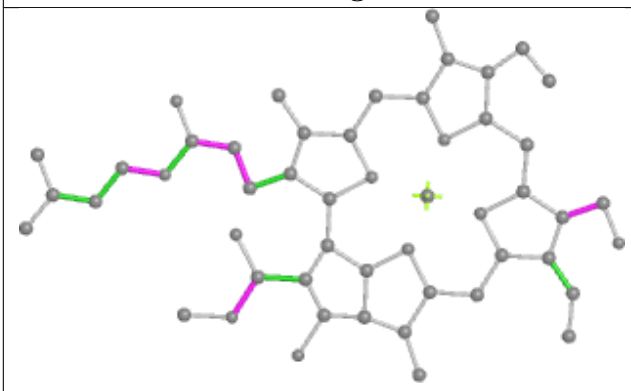
Ligand CHL 4 607



Bond lengths



Bond angles



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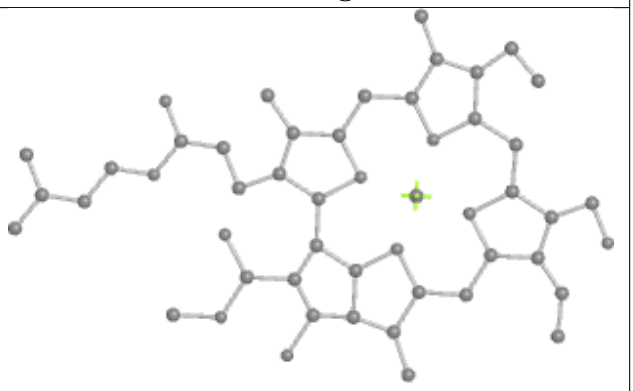
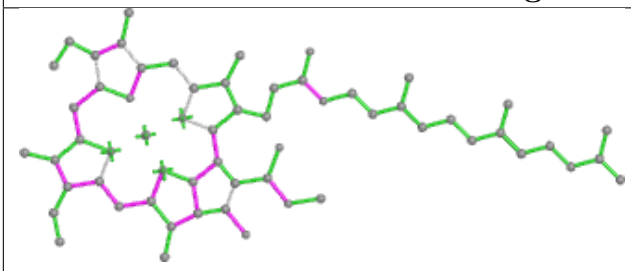
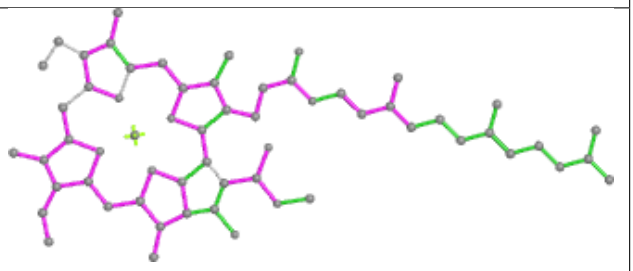


Rings

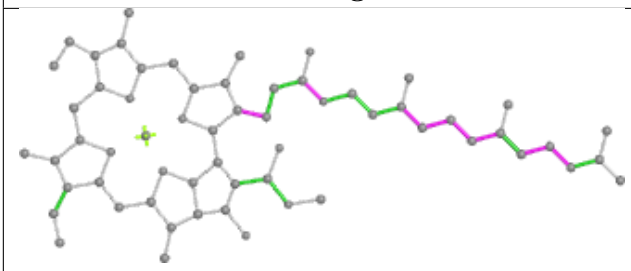
Ligand CLA B 818



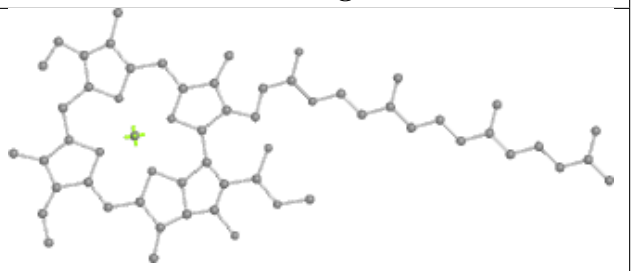
Bond lengths



Bond angles

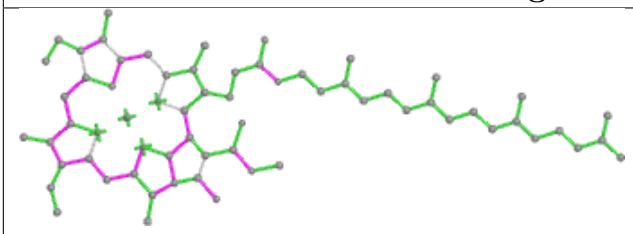


Torsions

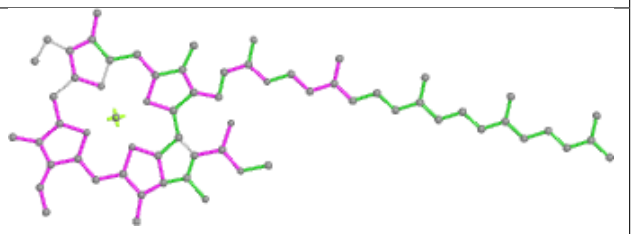


Rings

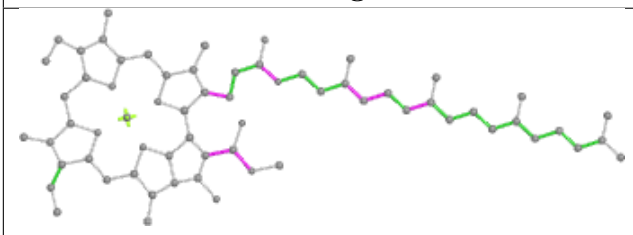
Ligand CLA 6 604



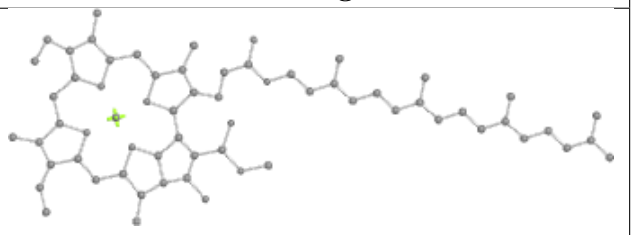
Bond lengths



Bond angles

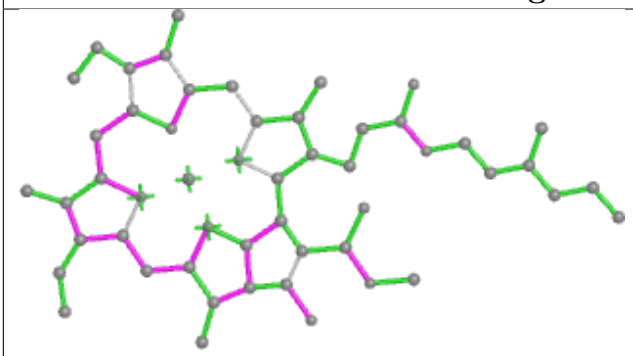


Torsions

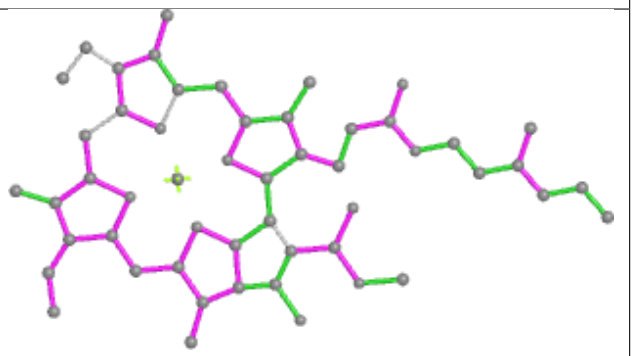


Rings

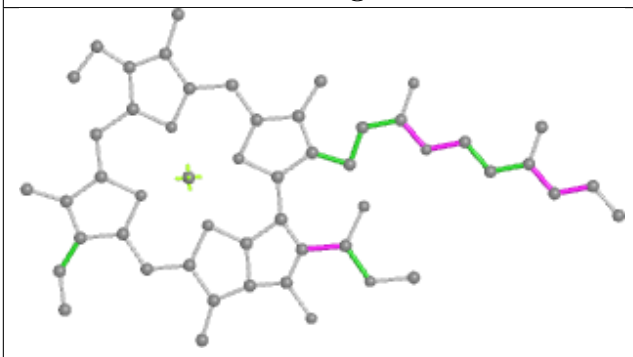
Ligand CLA 7 612



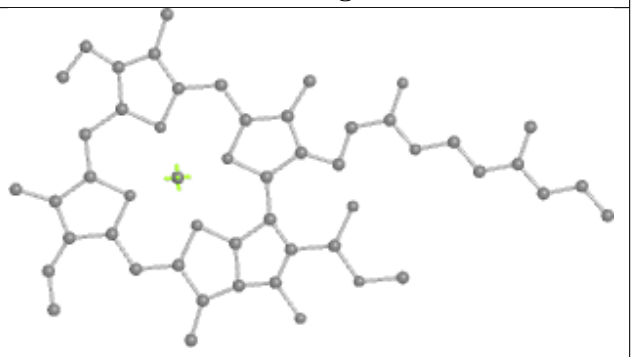
Bond lengths



Bond angles

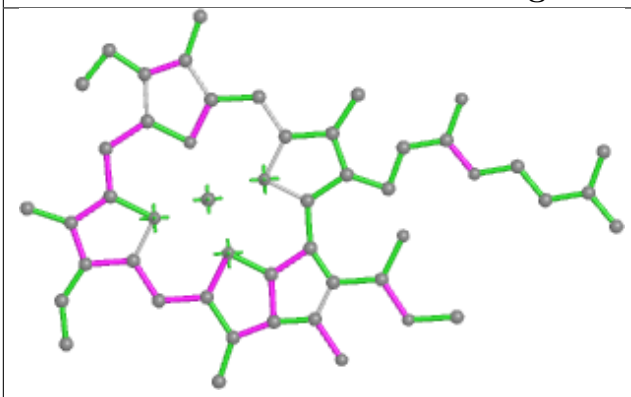


Torsions



Rings

Ligand CLA 4 604



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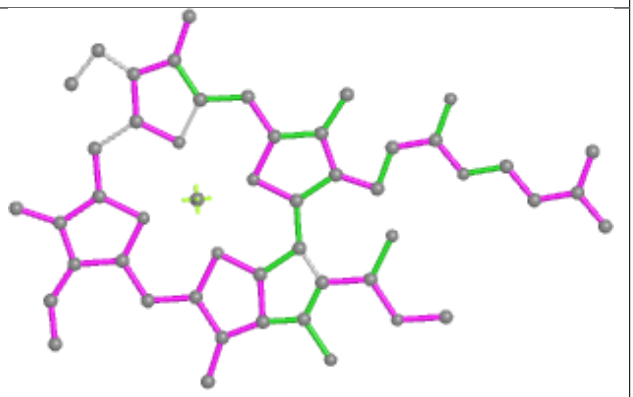
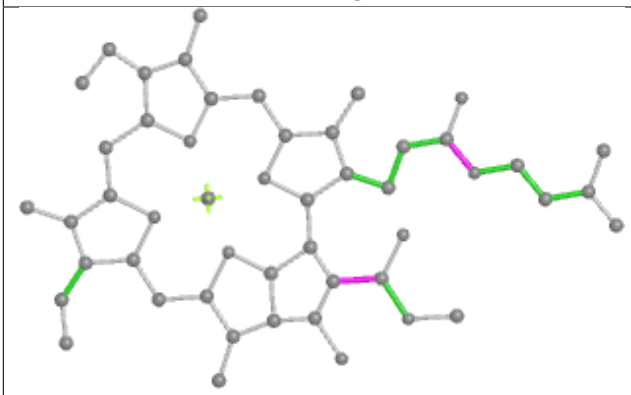


Bond angles



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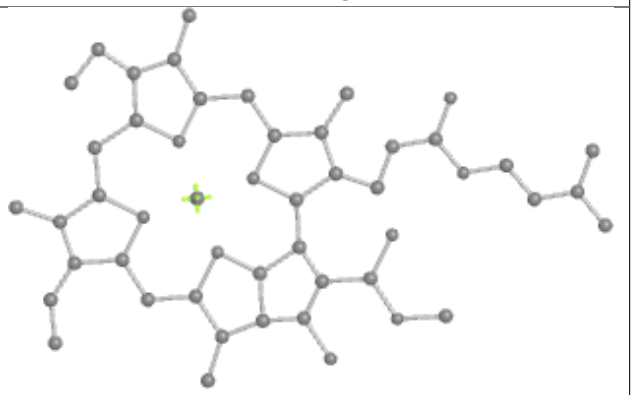
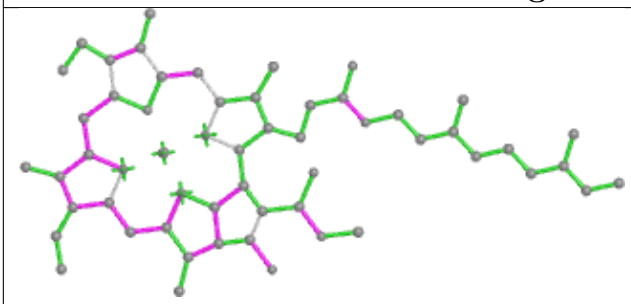


Rings

Ligand CLA 7 604



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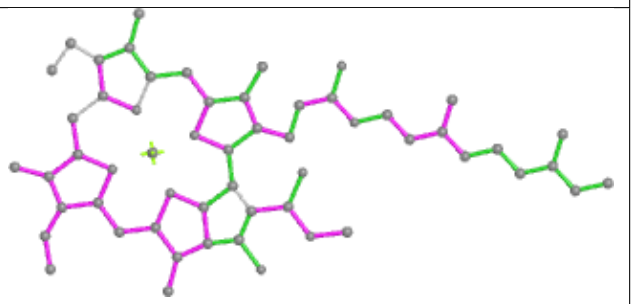
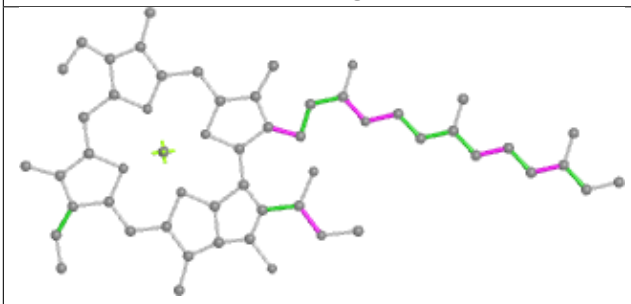


Bond angles



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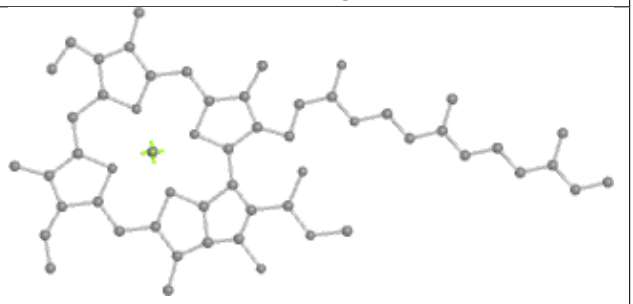
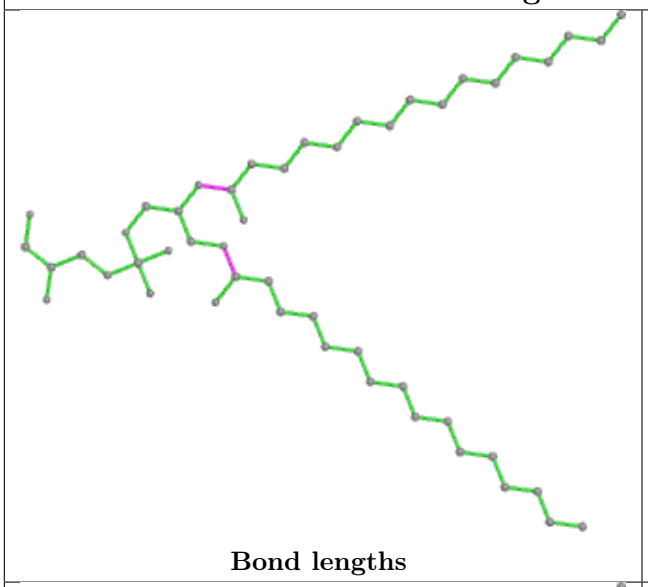
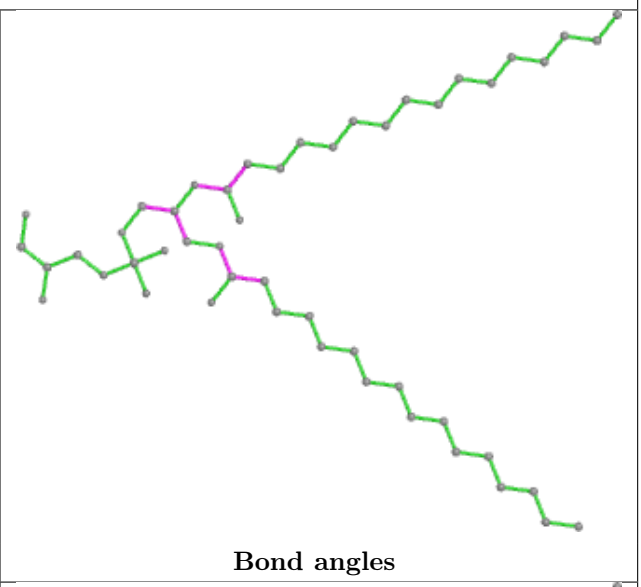


Rings

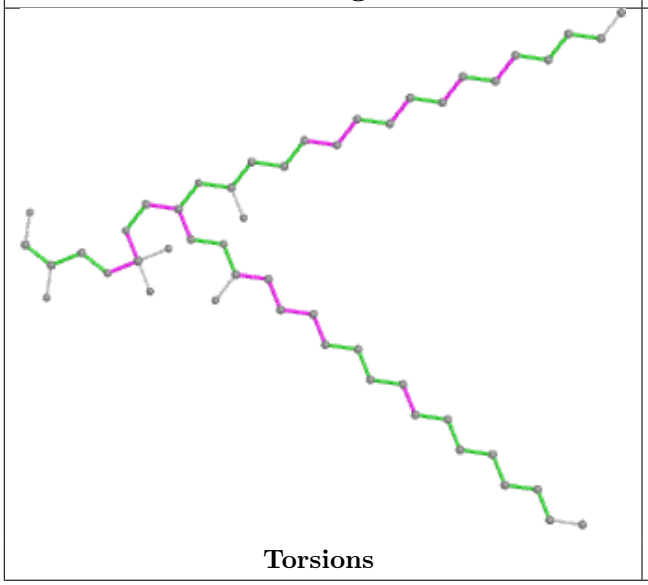
Ligand LHG A 846



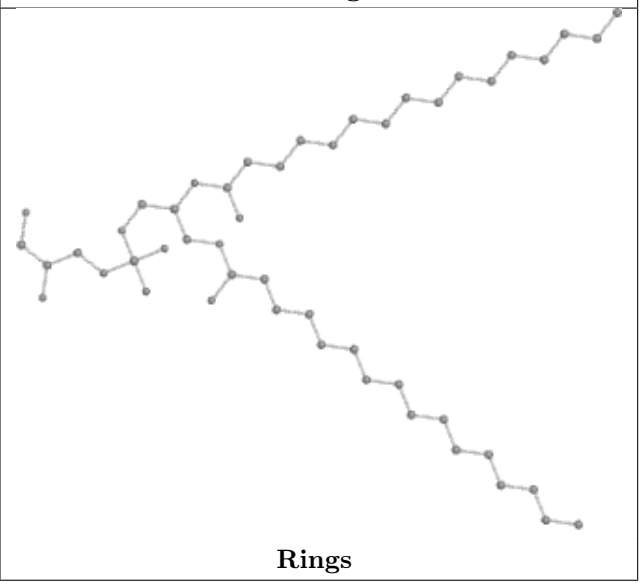
Bond lengths



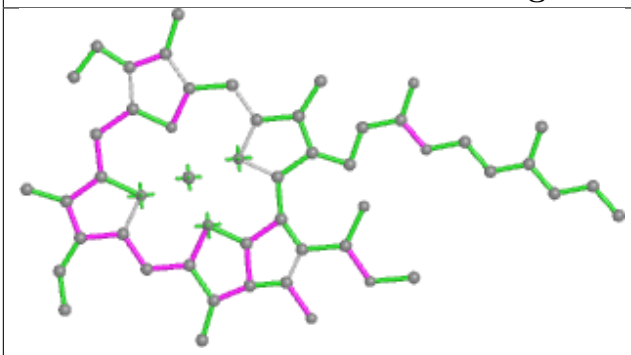
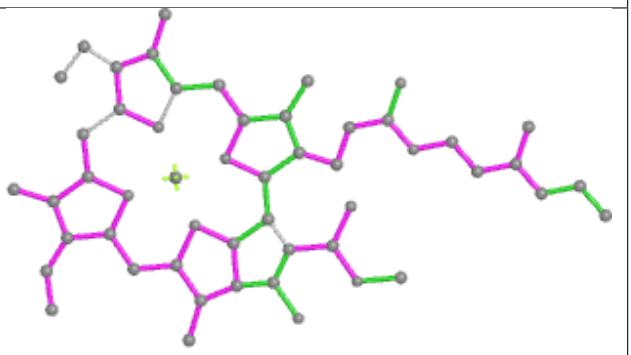
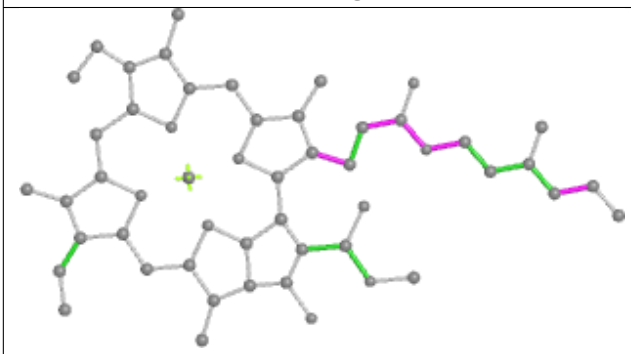
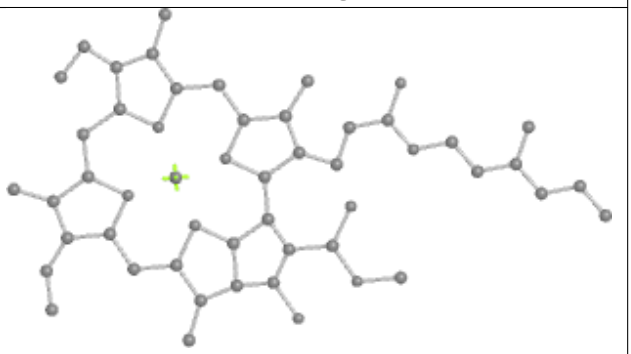
Bond angles

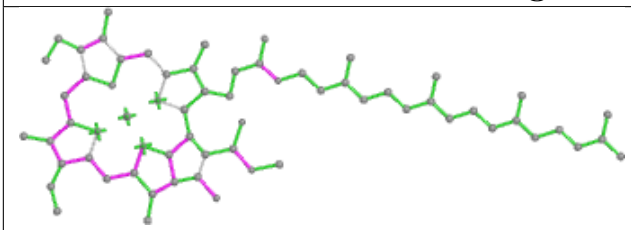
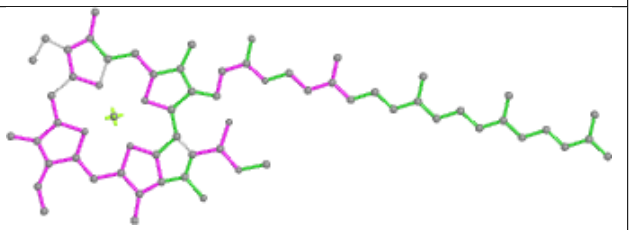
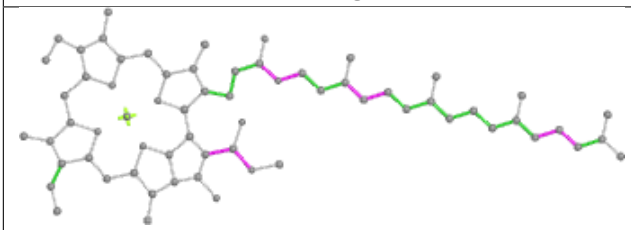
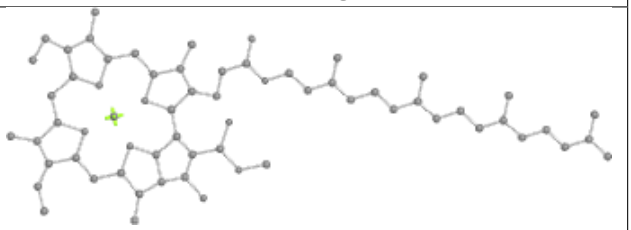


Torsions

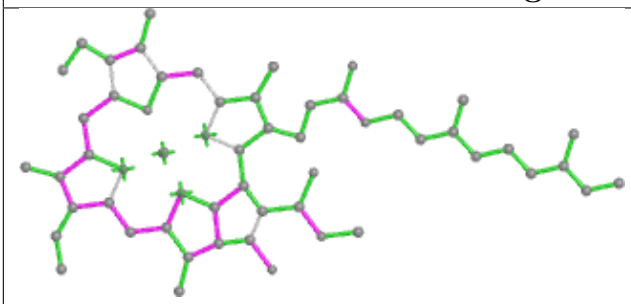


Rings

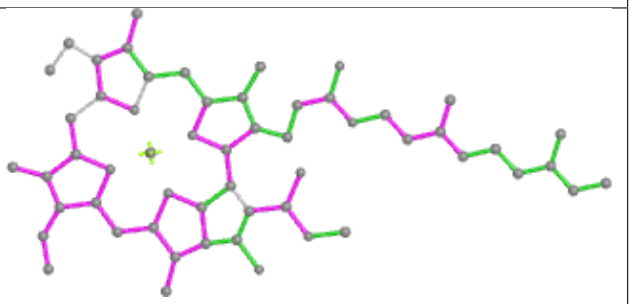
Ligand CLA 1 612	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 1 608	
	
Bond lengths	Bond angles
	
Torsions	Rings

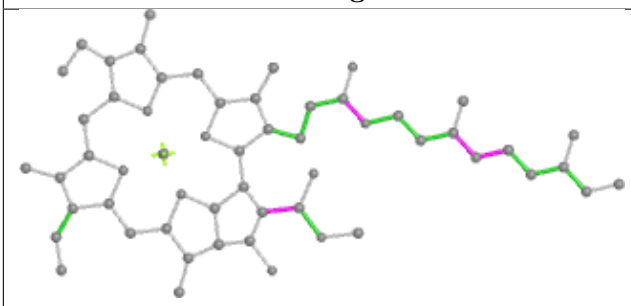
Ligand CLA B 820



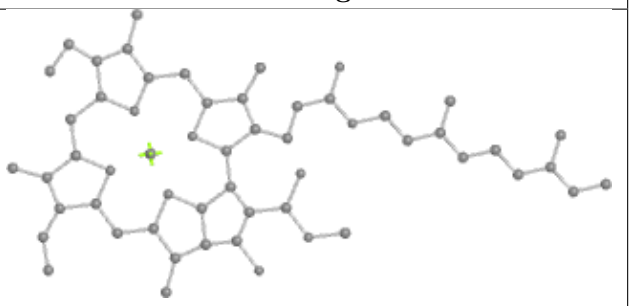
Bond lengths



Bond angles

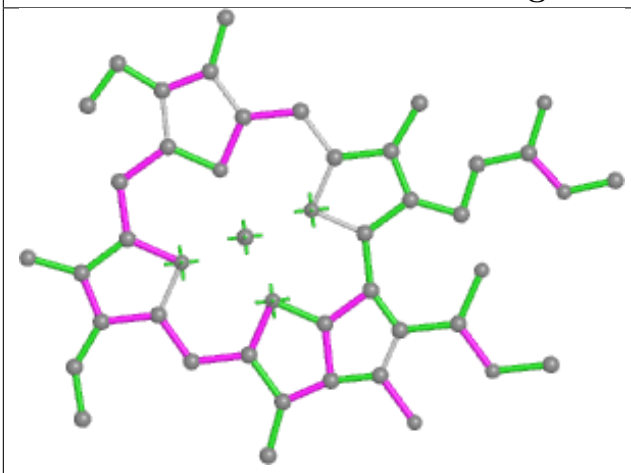


Torsions



Rings

Ligand CLA 8 604



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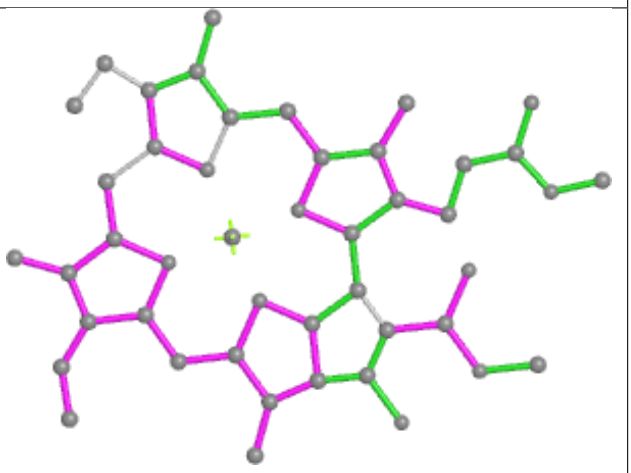

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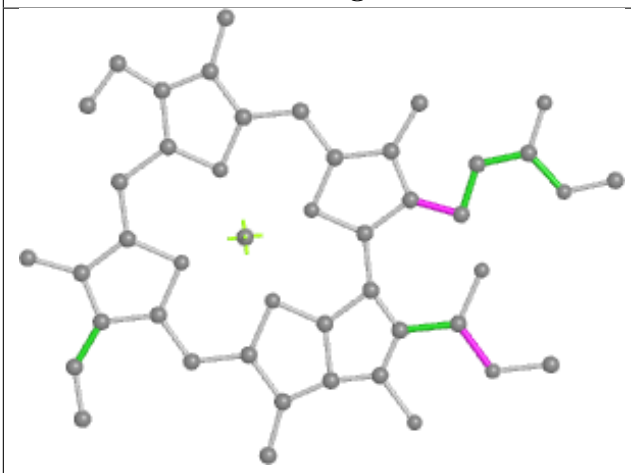

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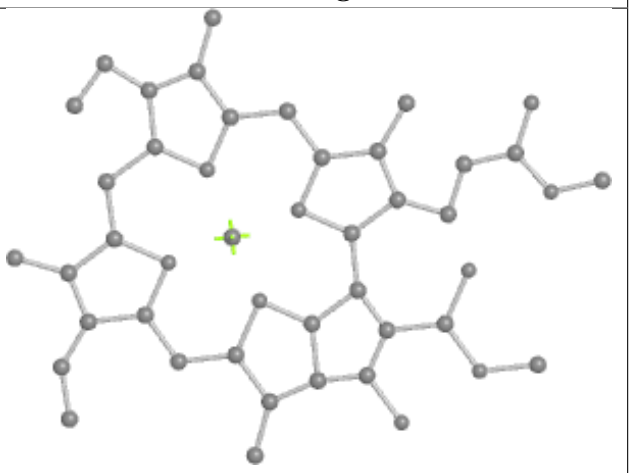
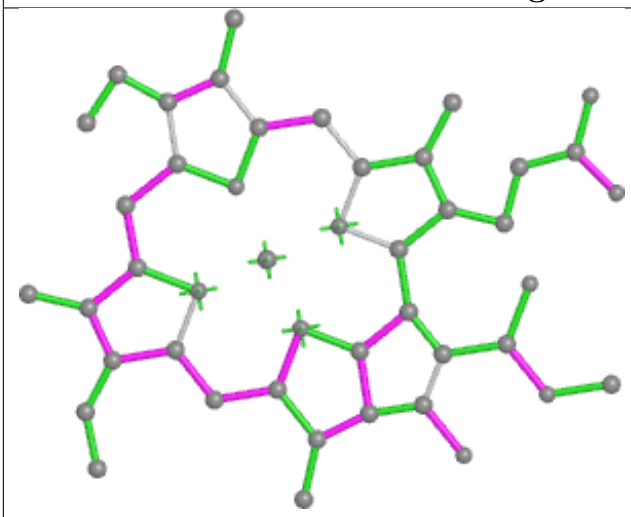
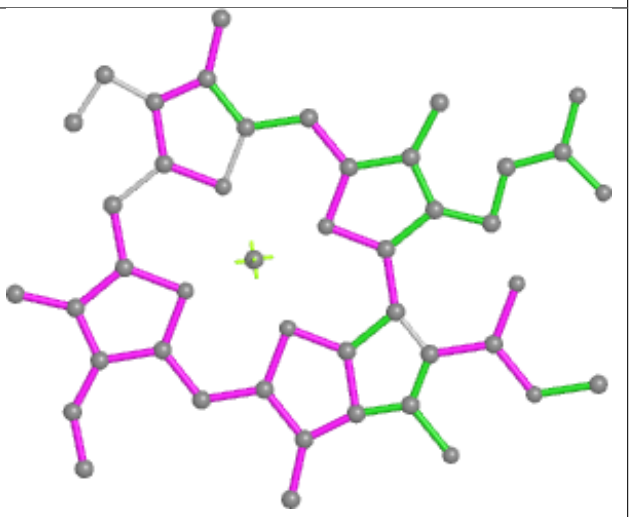


Rings

Ligand CLA 2 614



Bond lengths



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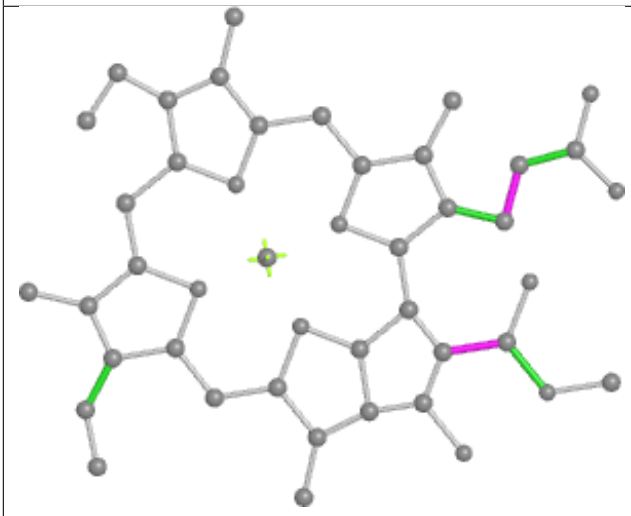

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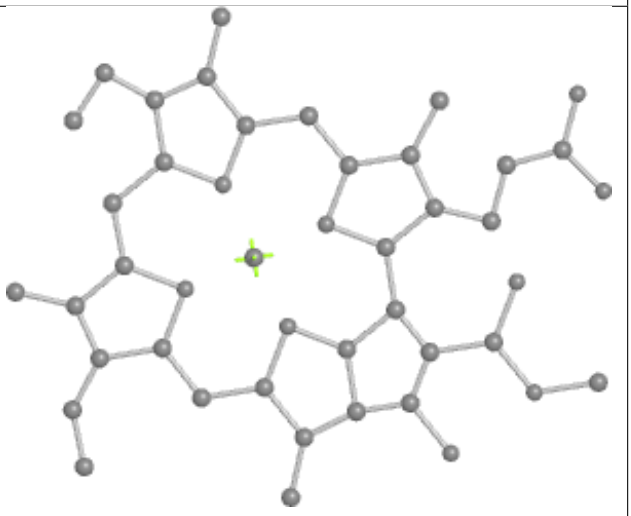
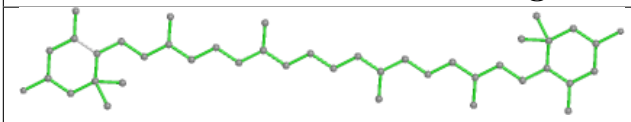


Rings

Ligand LUT 1 617



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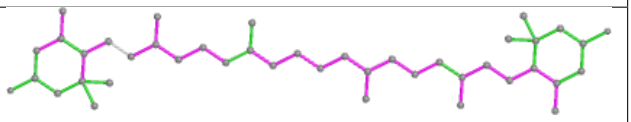
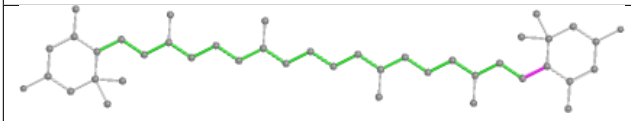


Bond angles



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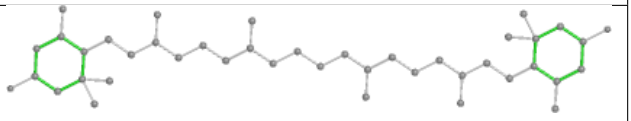

Rings

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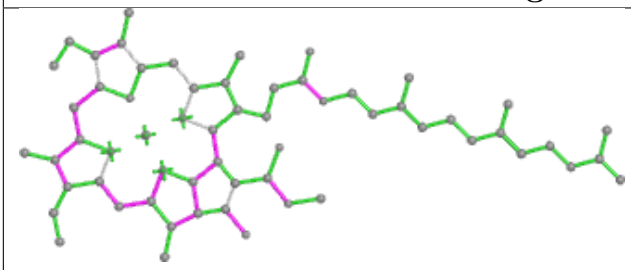

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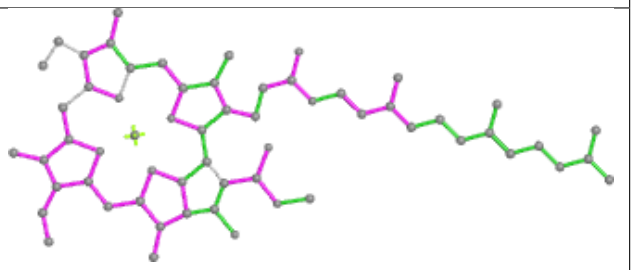
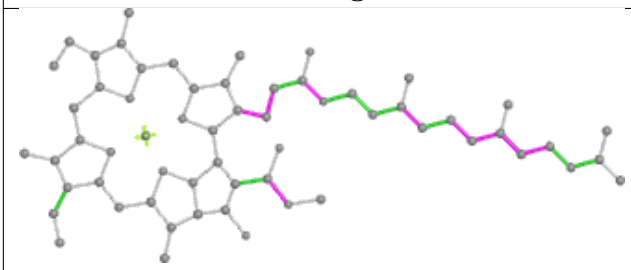


Bond angles



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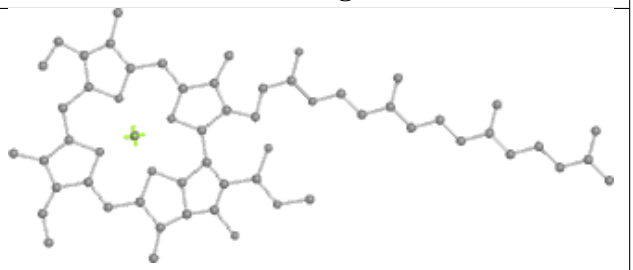
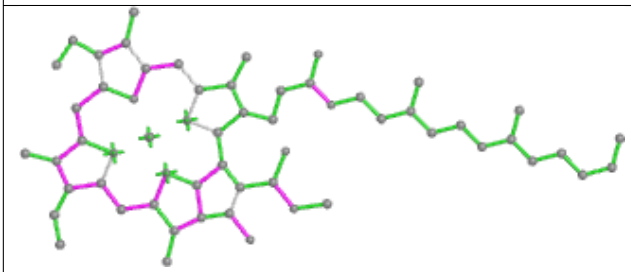


Rings

Ligand CLA B 822



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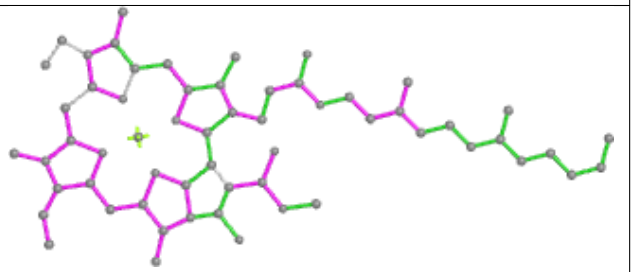

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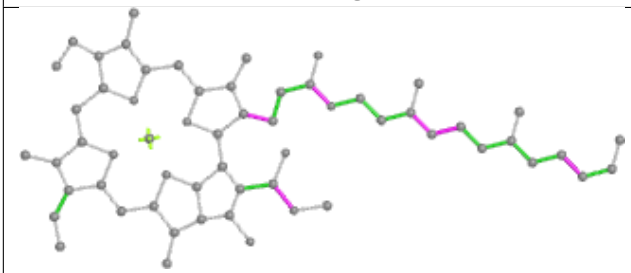

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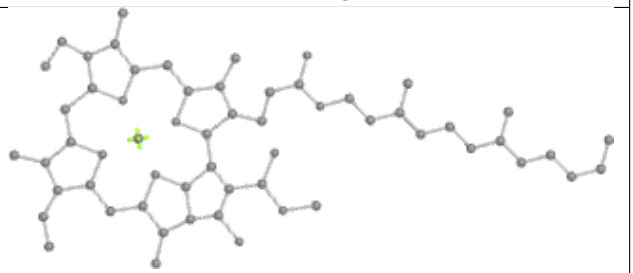
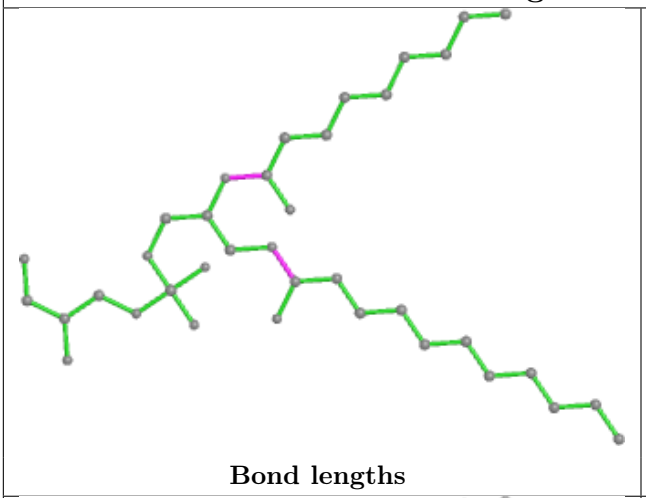


Rings

Ligand LHG 7 625



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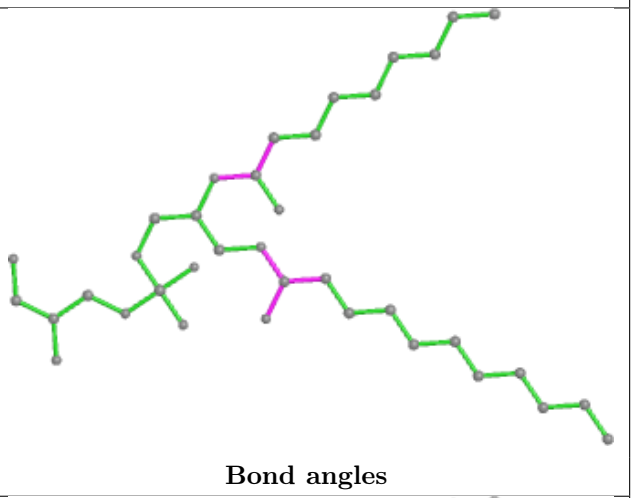

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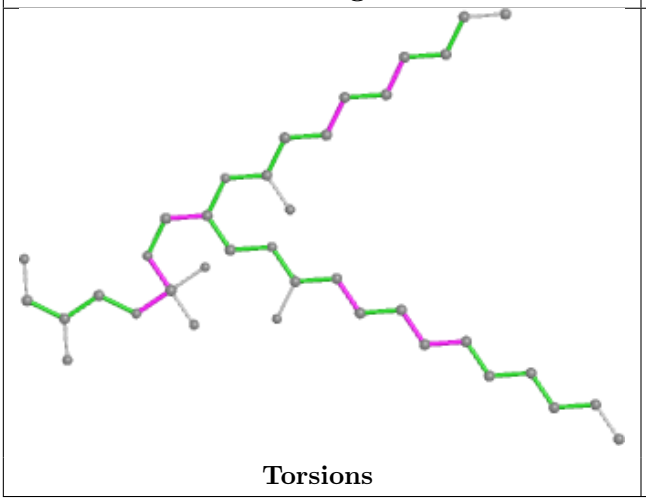

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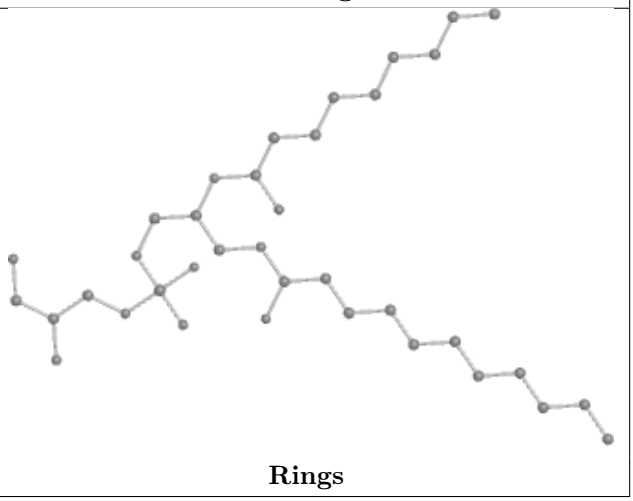
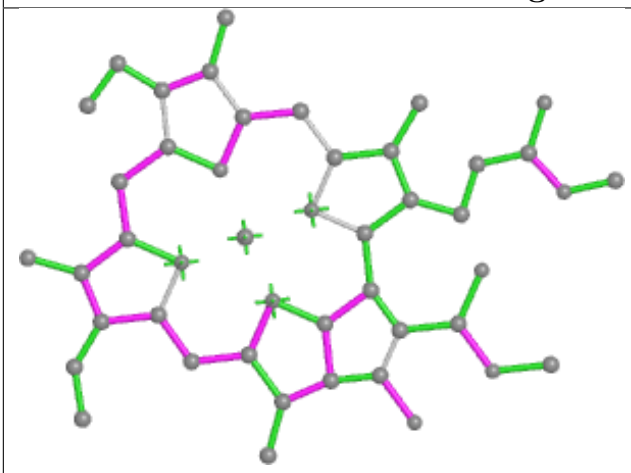
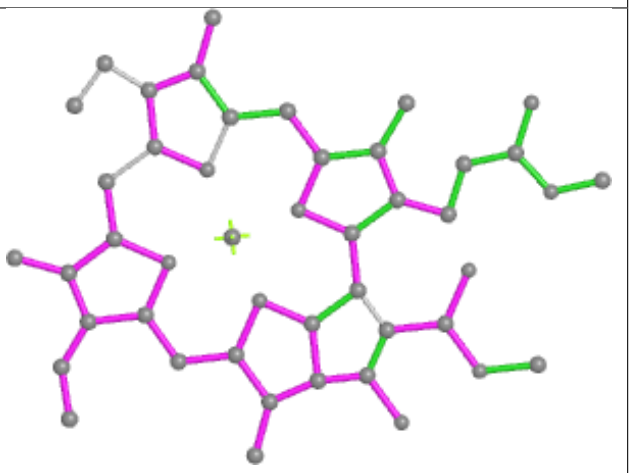


Rings

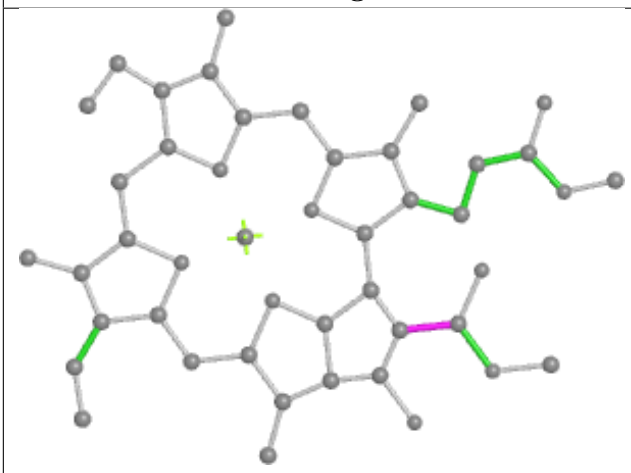
Ligand CLA 5 603



Bond lengths



Bond angles



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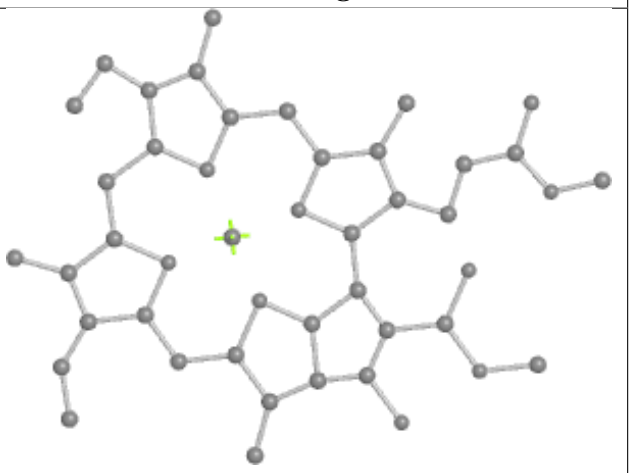
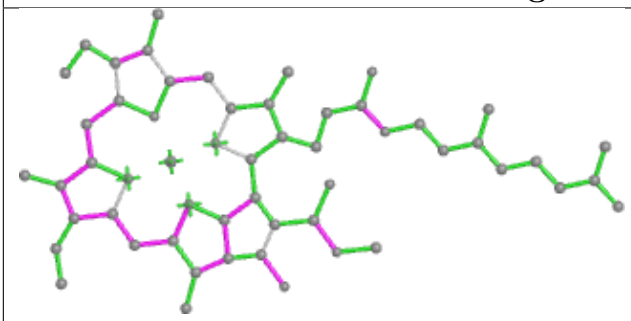


Rings

Ligand CLA 9 611



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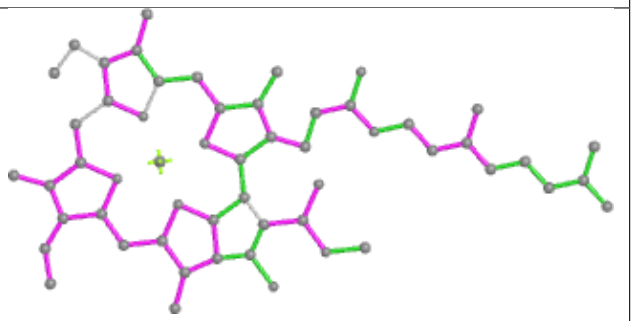
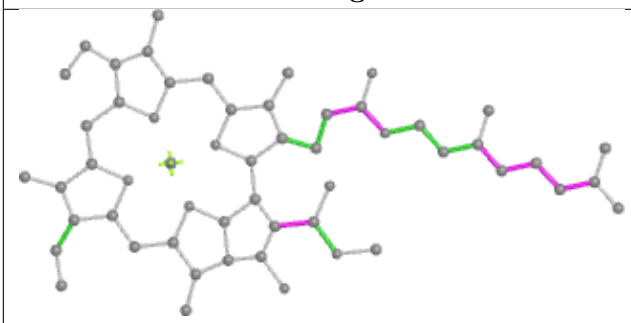


Bond angles



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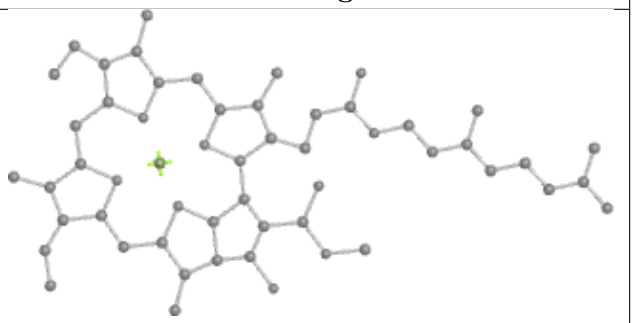
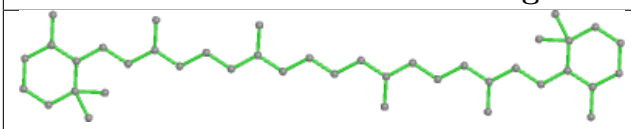


Rings

Ligand BCR A 856



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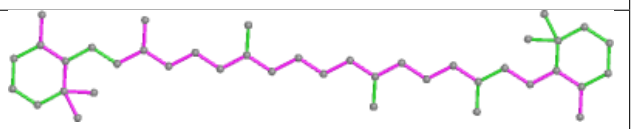
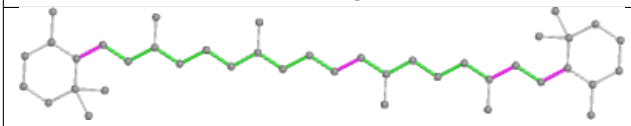


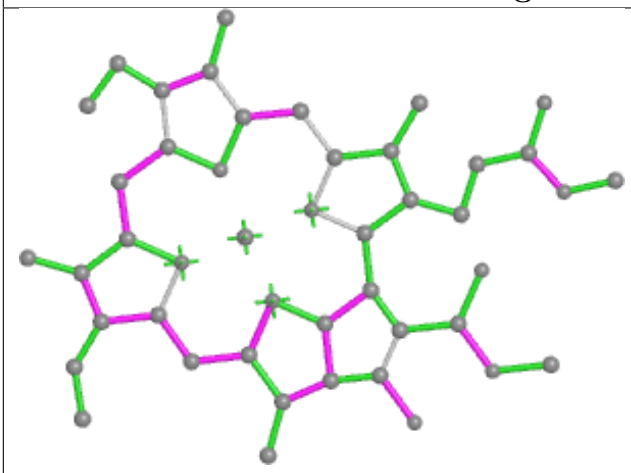
Bond angles



Torsions

Rings

Ligand CLA K 4003



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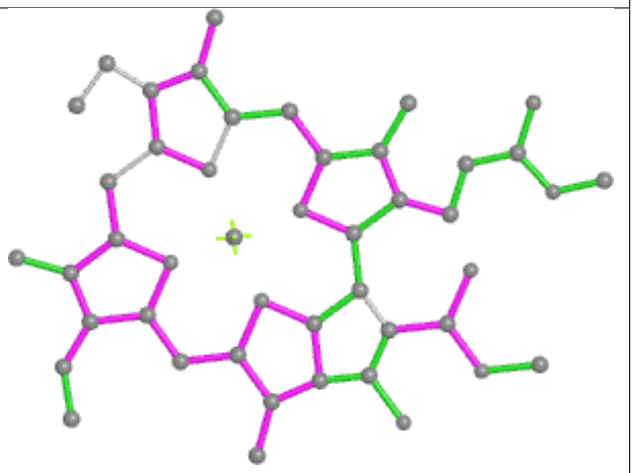
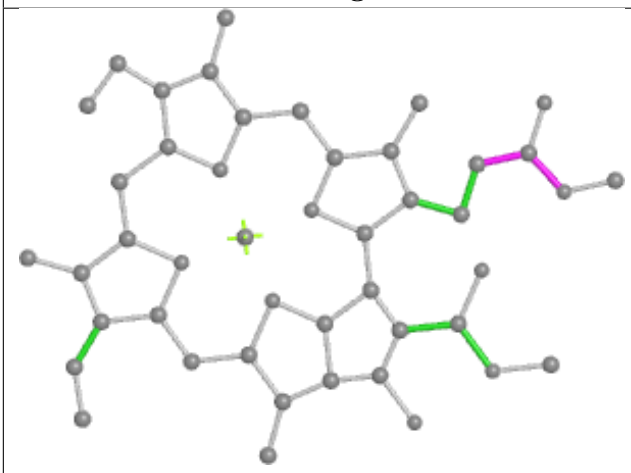


Bond angles



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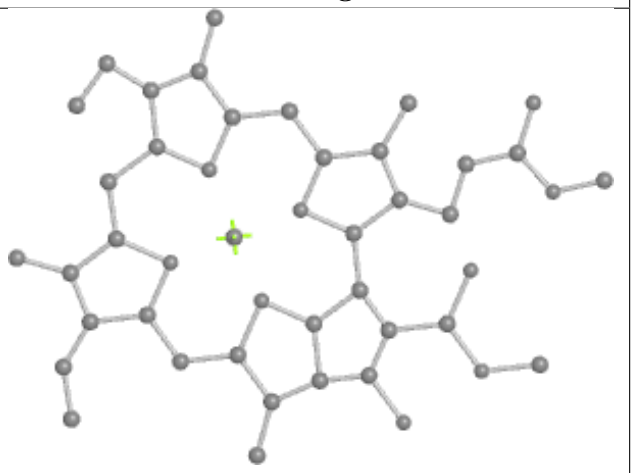
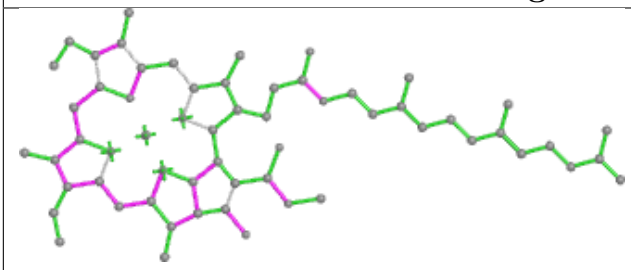


Rings

Ligand CLA 6 610



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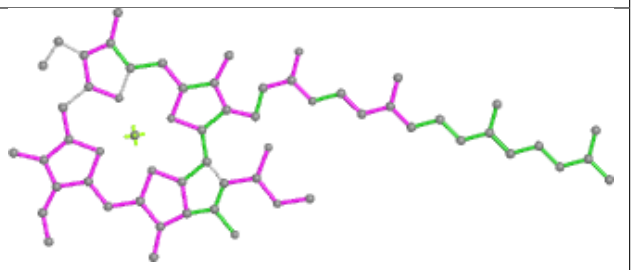
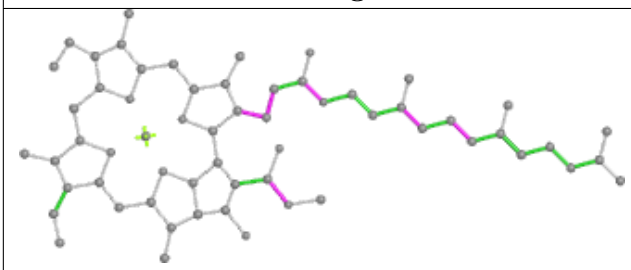


Bond angles



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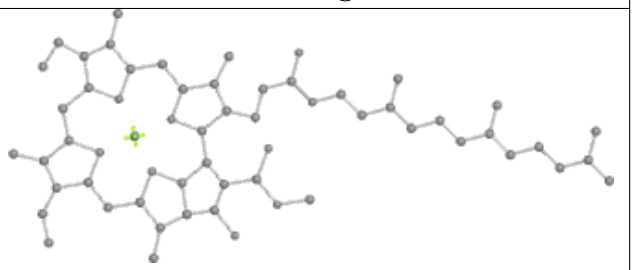

Rings

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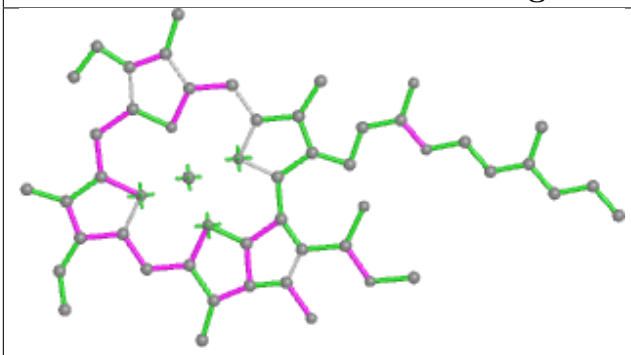

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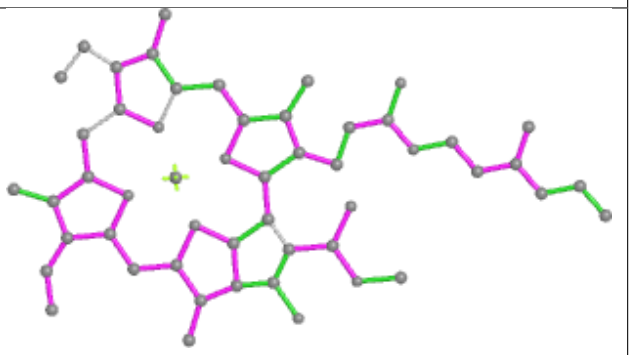
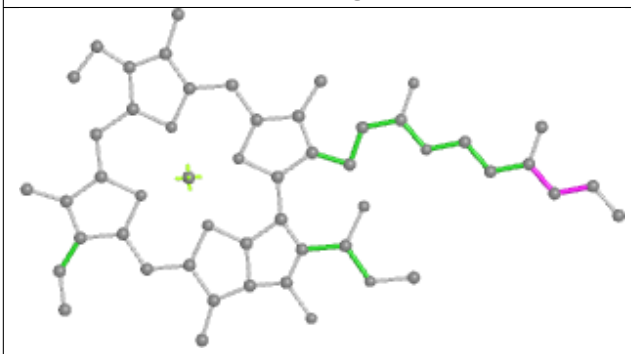


Bond angles



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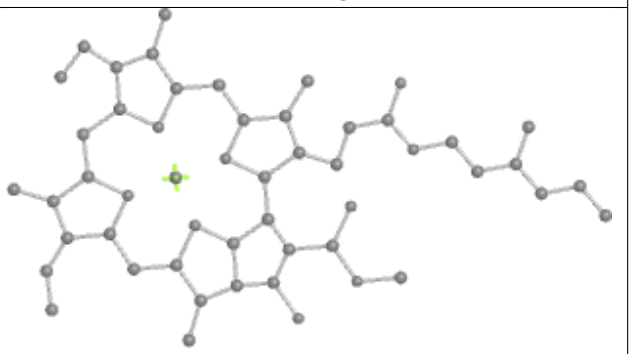
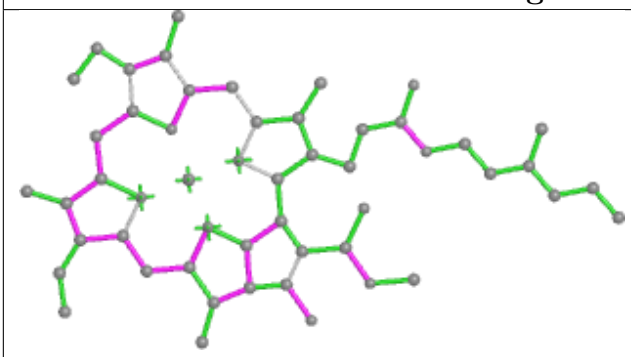
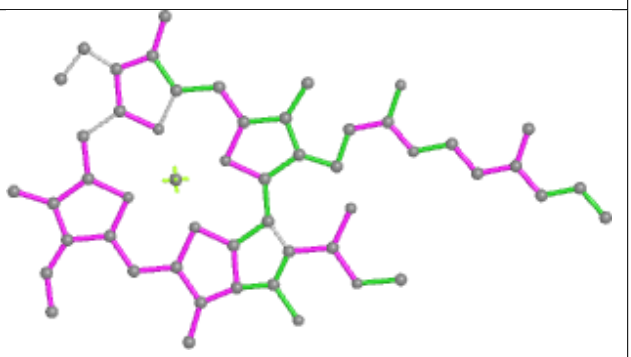


Rings

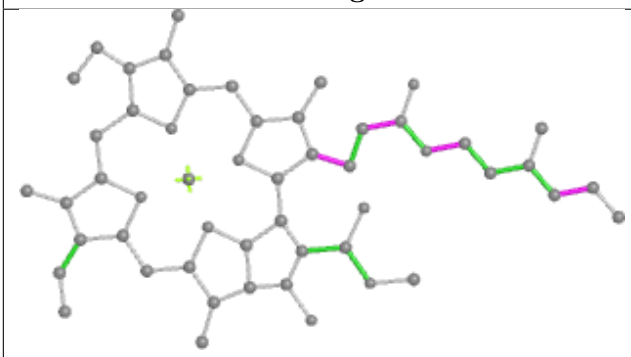
Ligand CLA Z 612



Bond lengths



Bond angles



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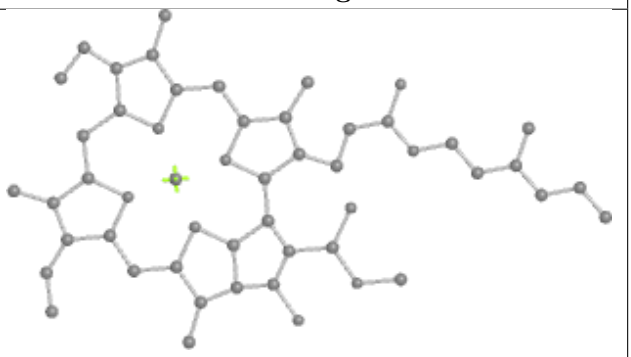
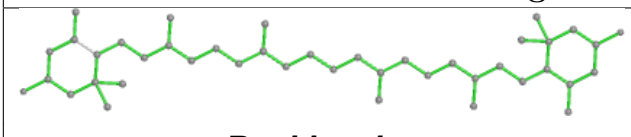
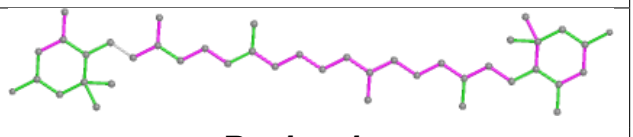


Rings

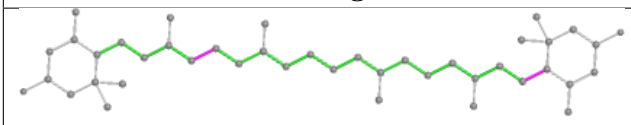
Ligand LUT 1 618



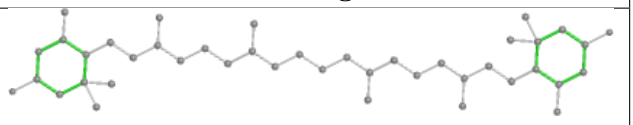
Bond lengths



Bond angles

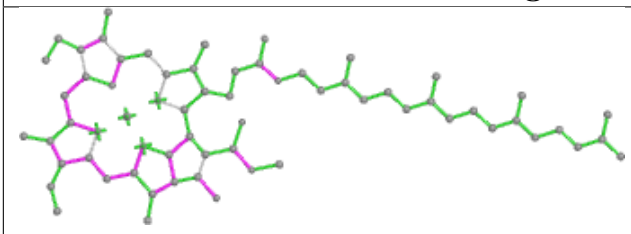


Torsions

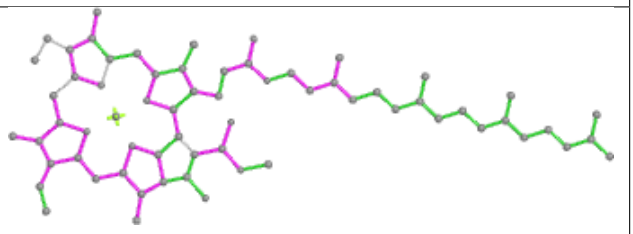


Rings

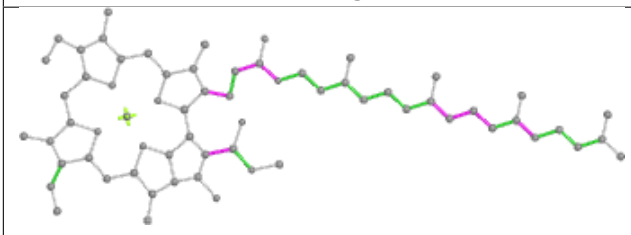
Ligand CLA B 813



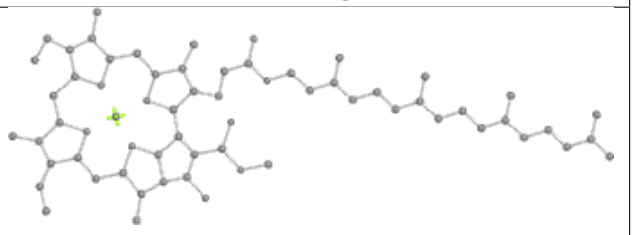
Bond lengths



Bond angles

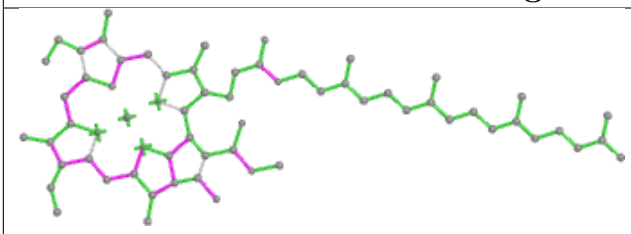


Torsions

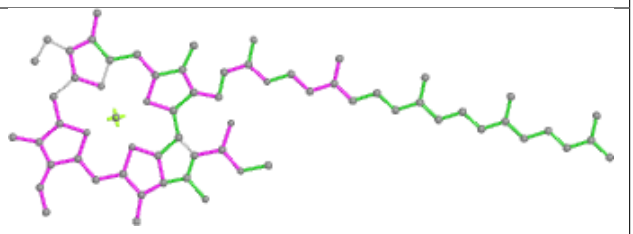


Rings

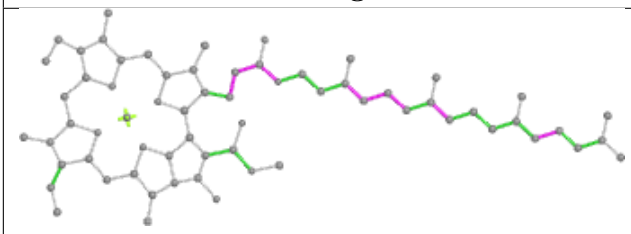
Ligand CLA B 807



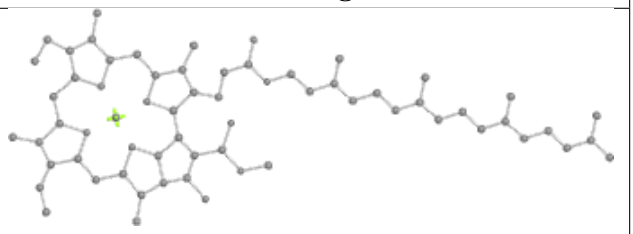
Bond lengths



Bond angles

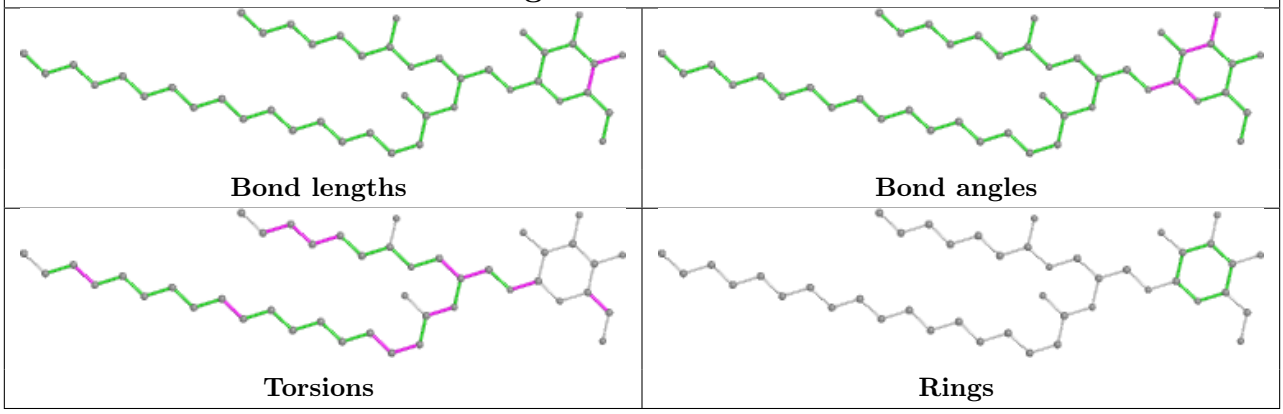


Torsions

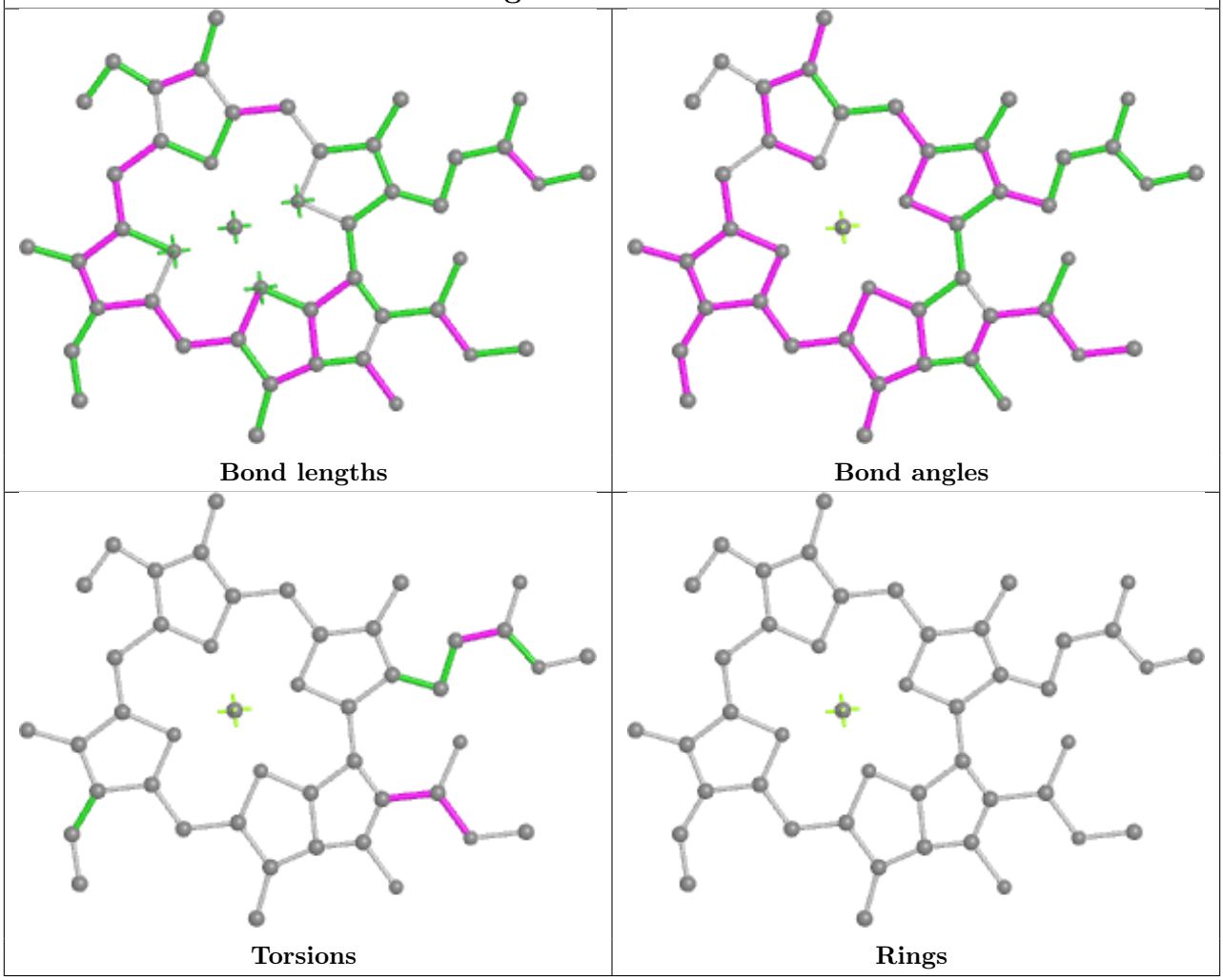


Rings

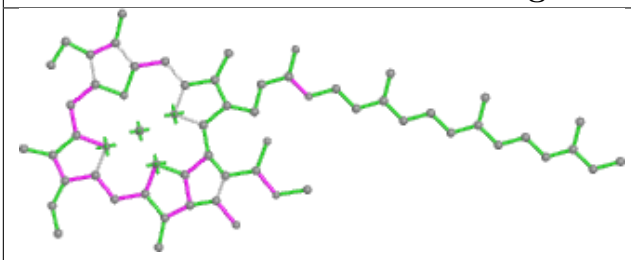
Ligand LMG 9 620



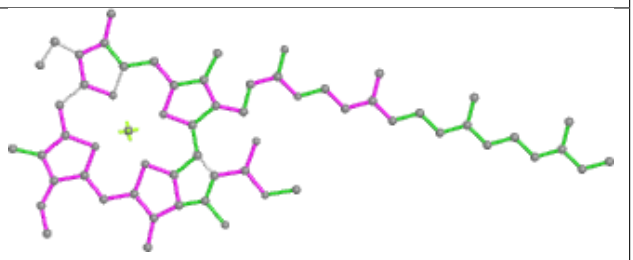
Ligand CLA 2 601



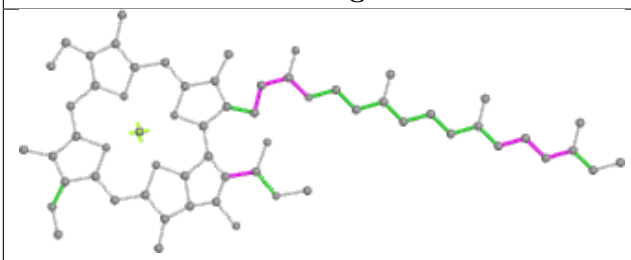
Ligand CLA 4 601



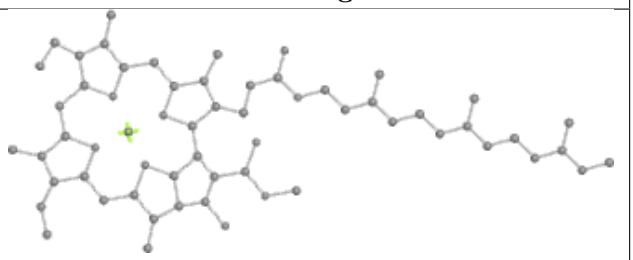
Bond lengths



Bond angles

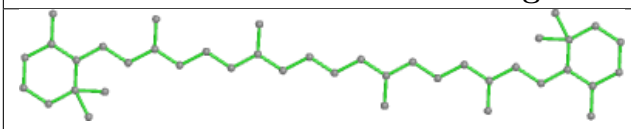


Torsions

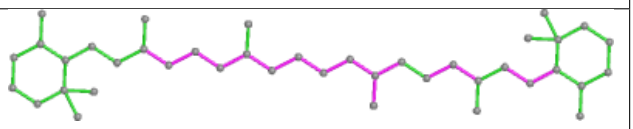


Rings

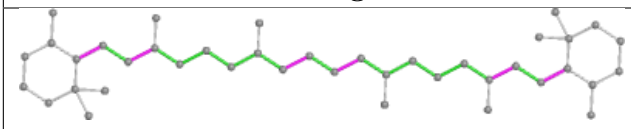
Ligand BCR B 843



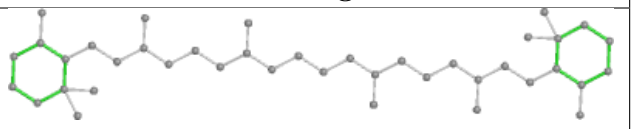
Bond lengths



Bond angles

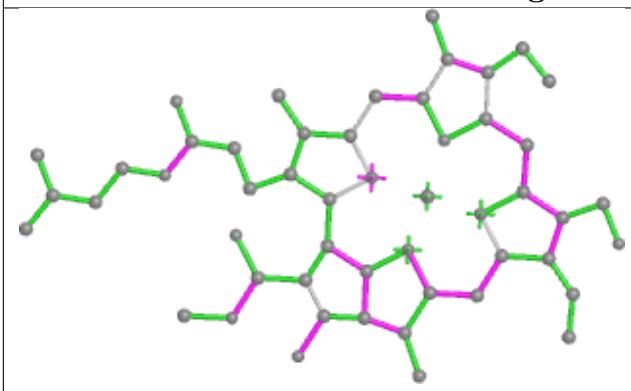


Torsions

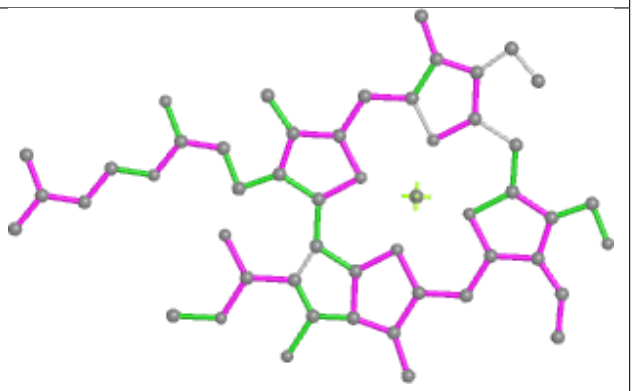


Rings

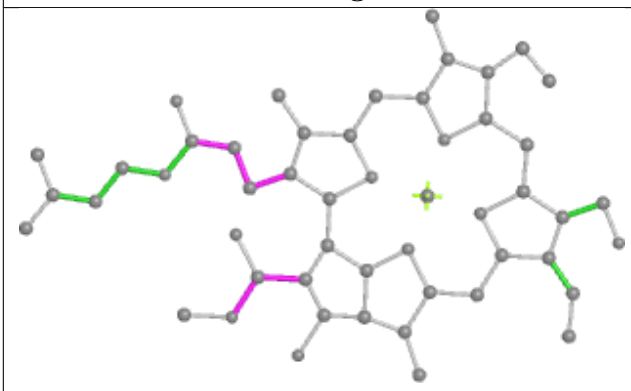
Ligand CHL 4 608



Bond lengths



Bond angles



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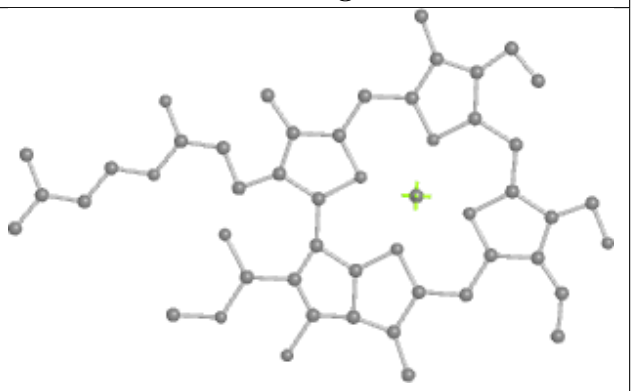
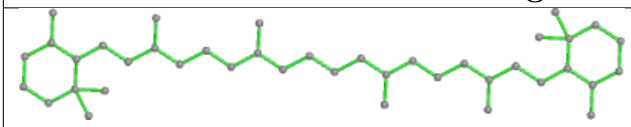
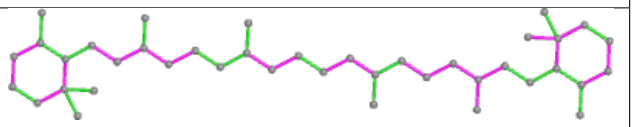


Rings

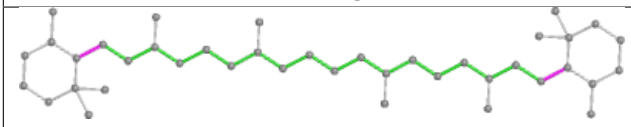
Ligand BCR 7 624



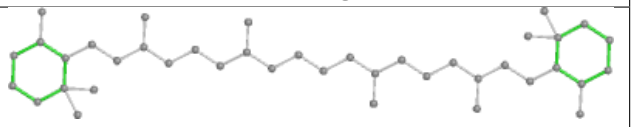
Bond lengths



Bond angles

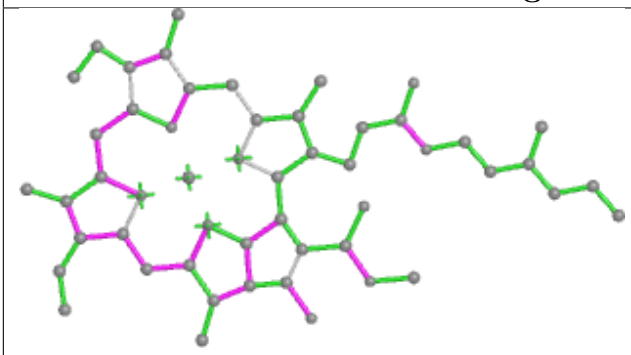


Torsions

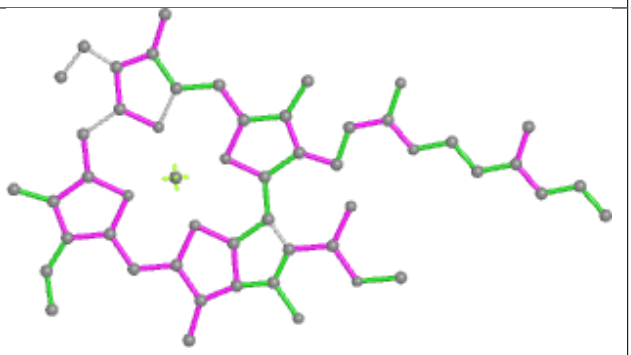


Rings

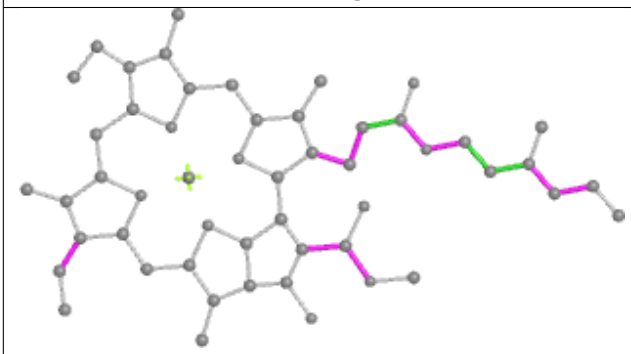
Ligand CLA A 845



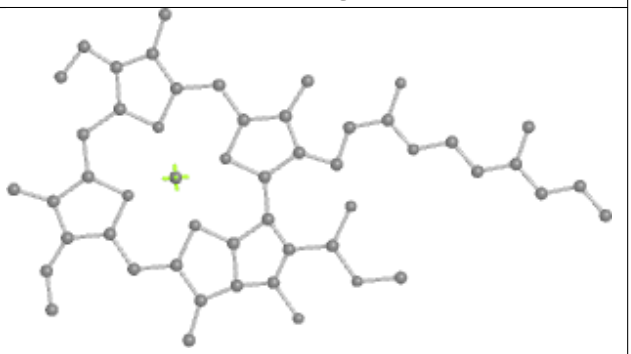
Bond lengths



Bond angles

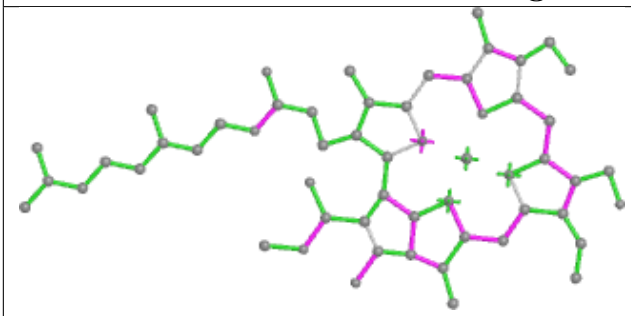


Torsions

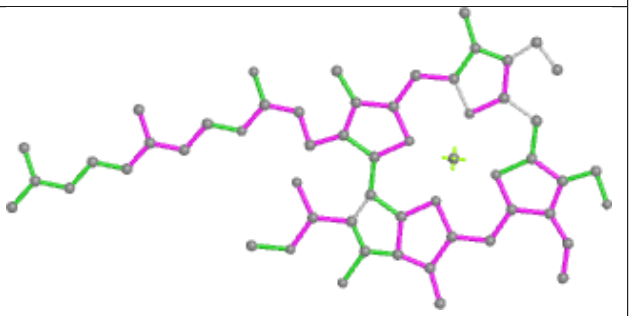


Rings

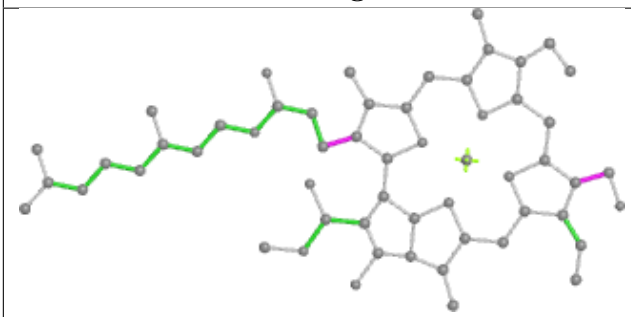
Ligand CHL 4 606



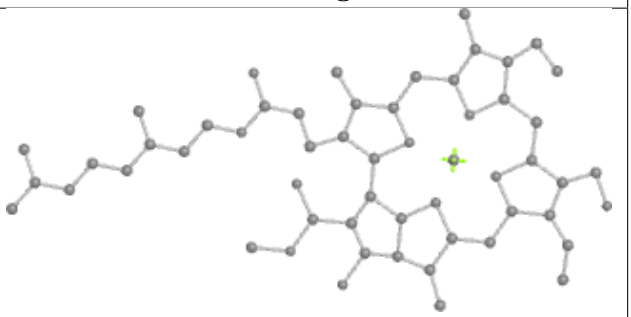
Bond lengths



Bond angles

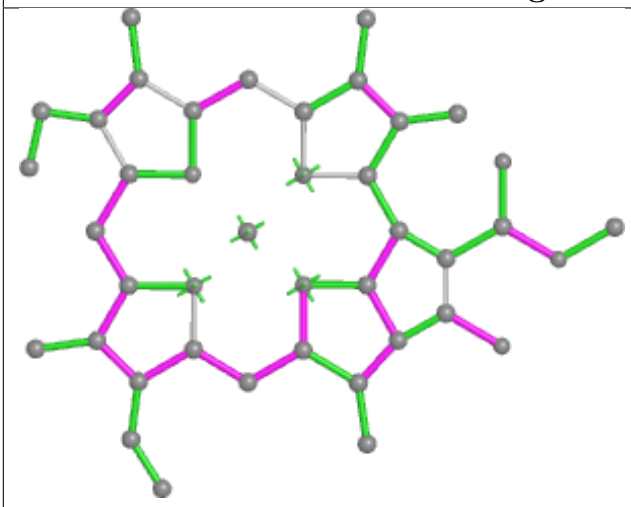


Torsions

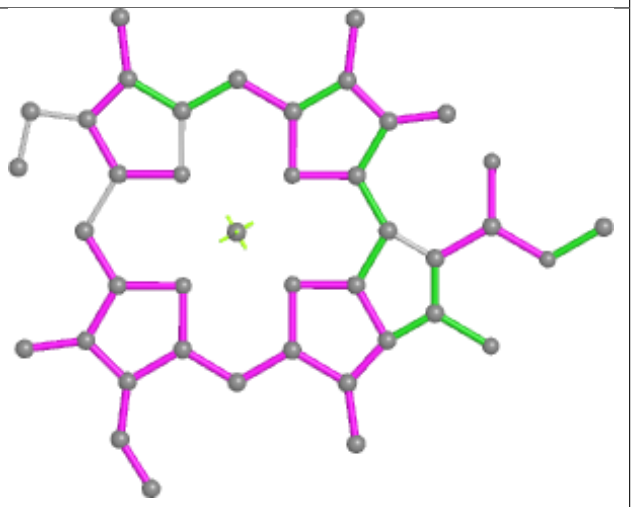


Rings

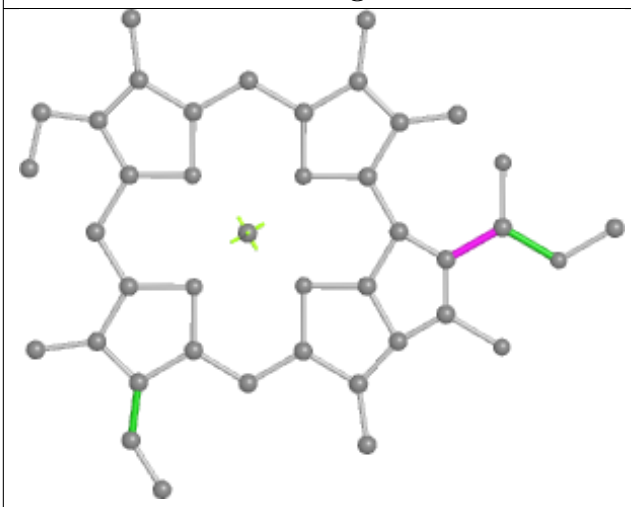
Ligand CLA 3 611



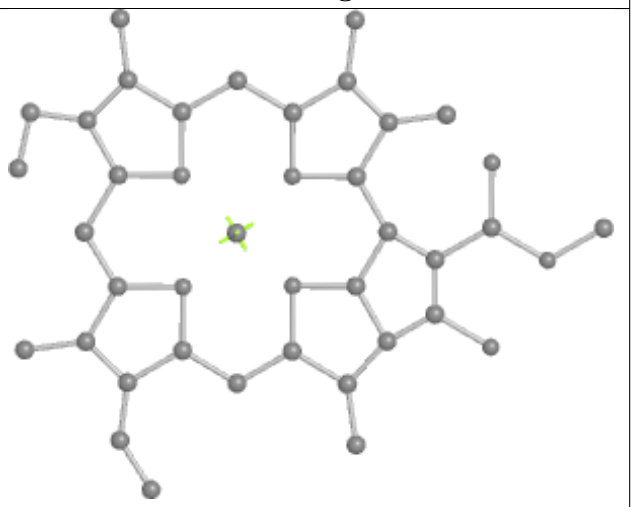
Bond lengths



Bond angles

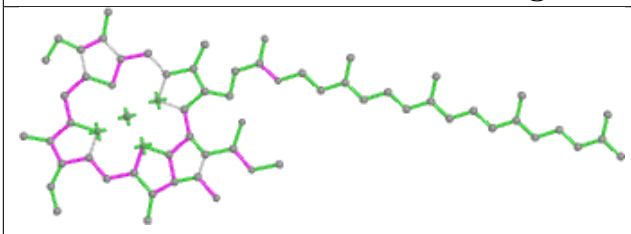


Torsions

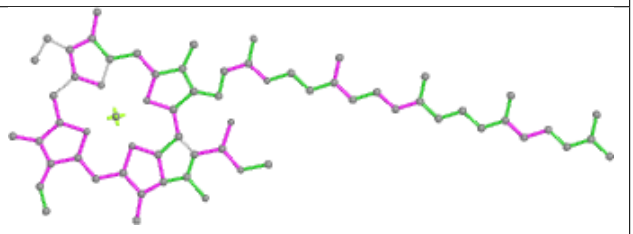


Rings

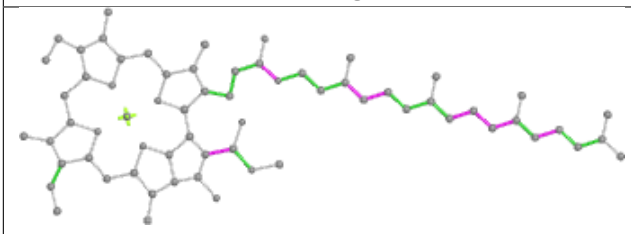
Ligand CLA 8 601



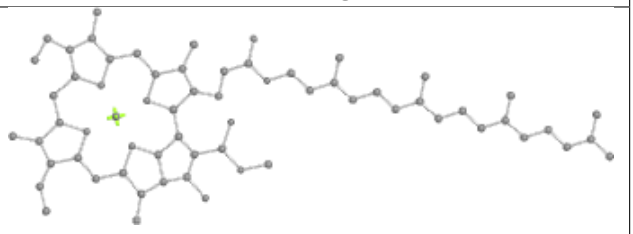
Bond lengths



Bond angles

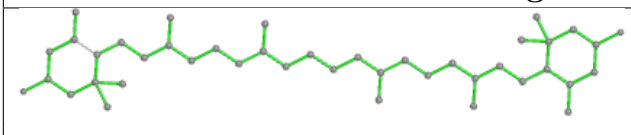


Torsions

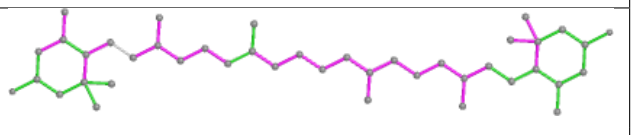


Rings

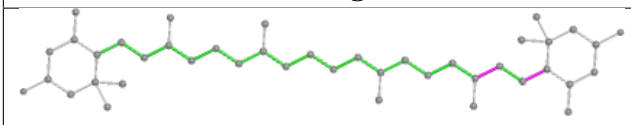
Ligand LUT Z 617



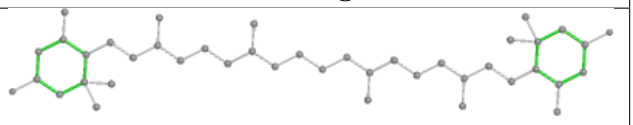
Bond lengths



Bond angles

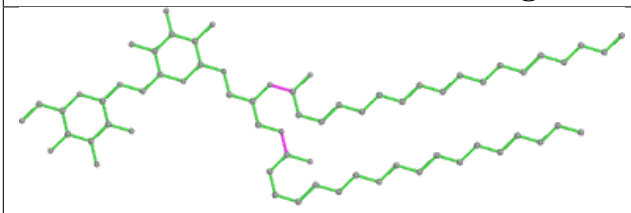


Torsions

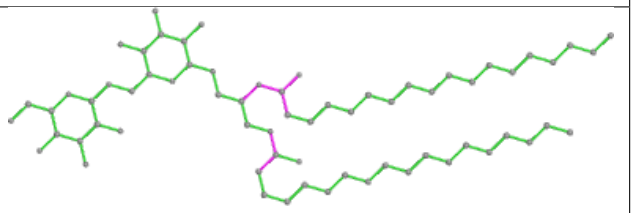


Rings

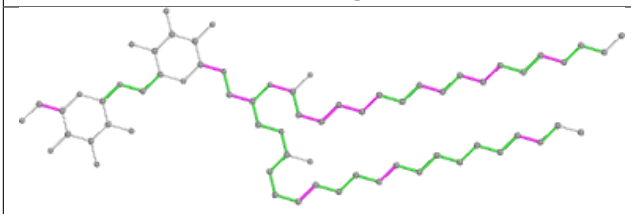
Ligand DGD B 850



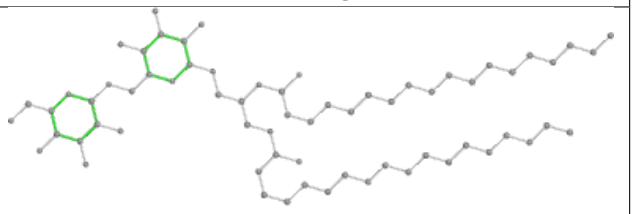
Bond lengths



Bond angles

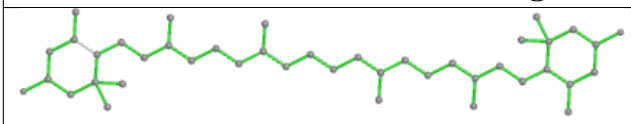


Torsions

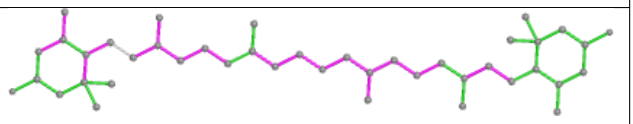


Rings

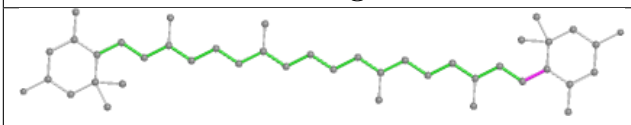
Ligand LUT 4 619



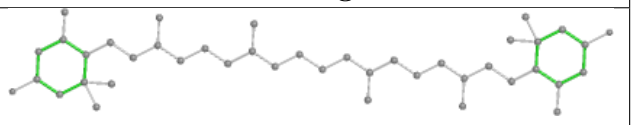
Bond lengths



Bond angles

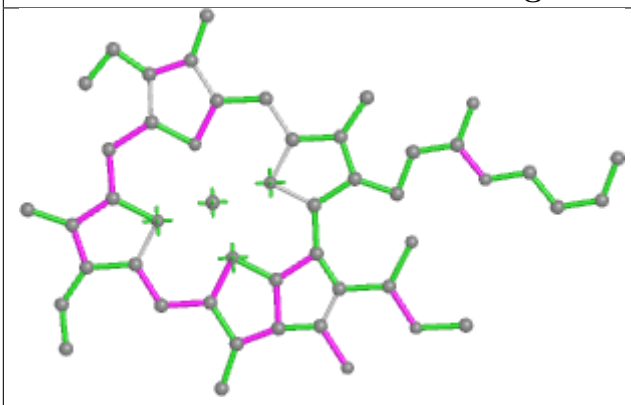


Torsions

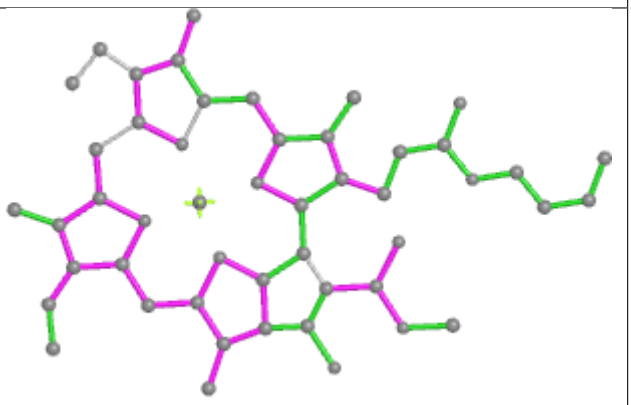


Rings

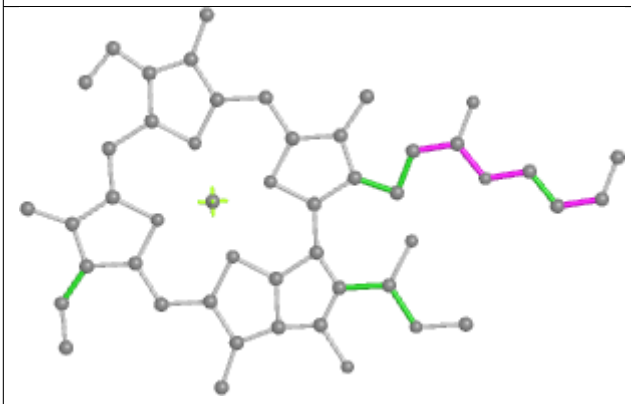
Ligand CLA B 831



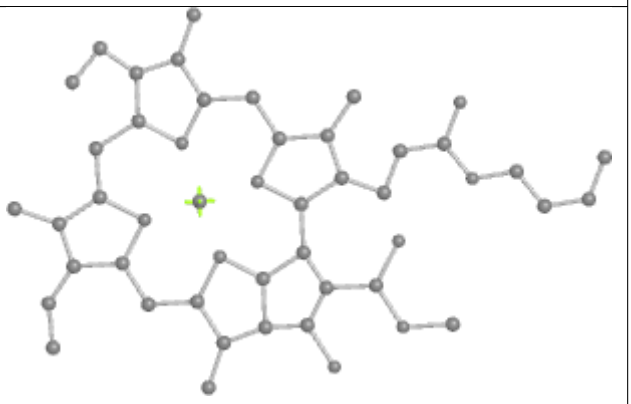
Bond lengths



Bond angles

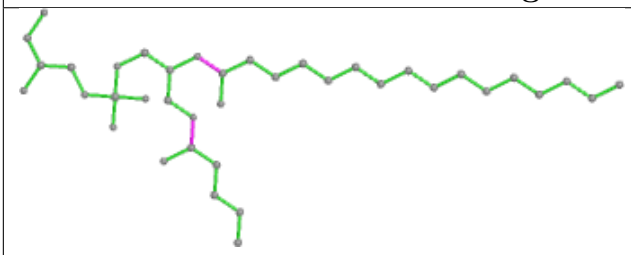


Torsions

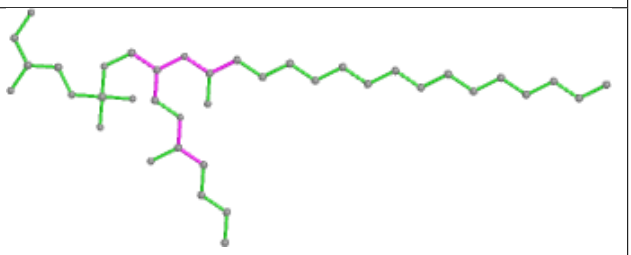


Rings

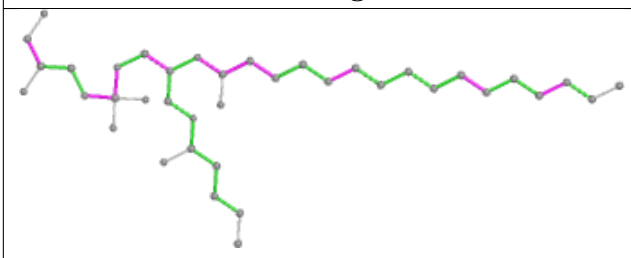
Ligand LHG A 847



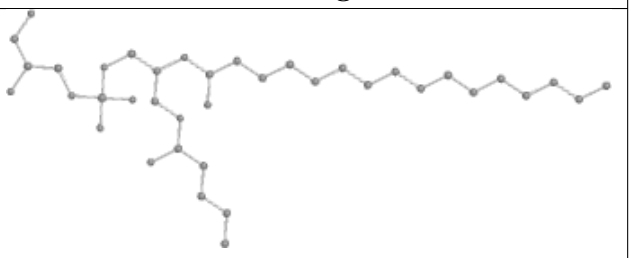
Bond lengths



Bond angles

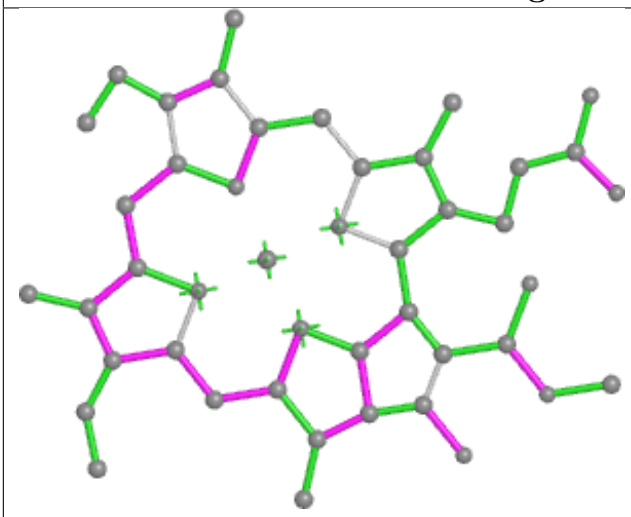


Torsions

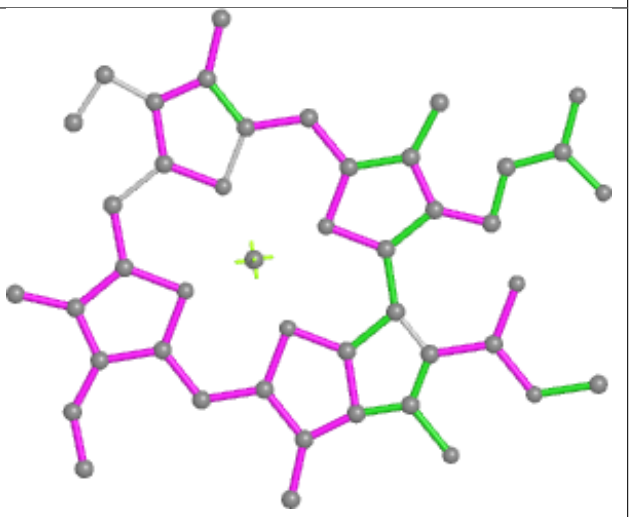


Rings

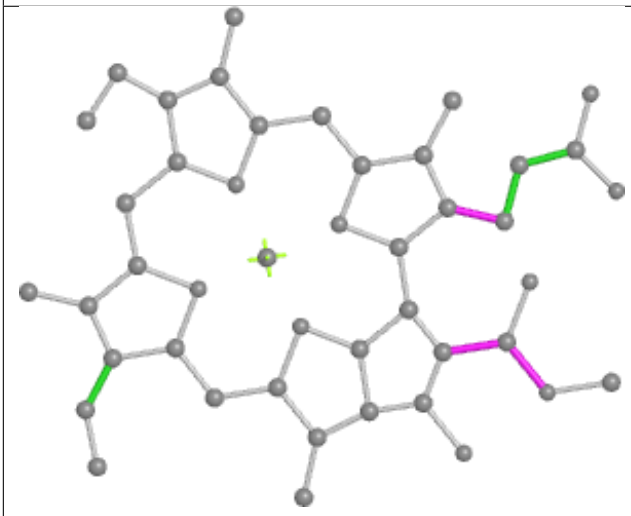
Ligand CLA 6 614



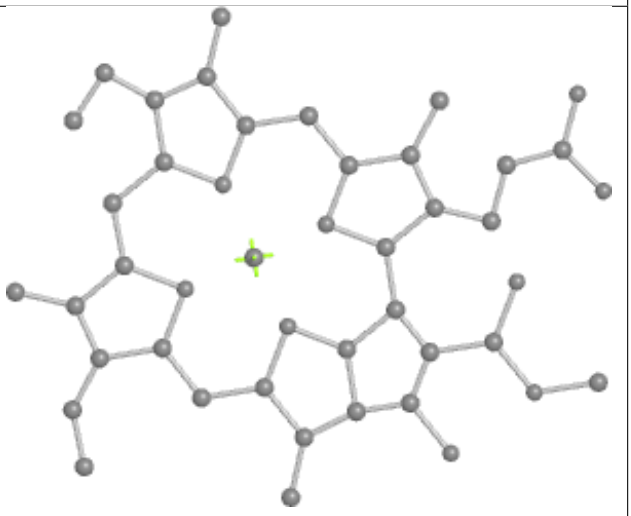
Bond lengths



Bond angles

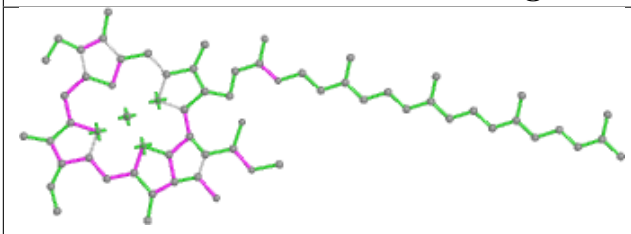


Torsions

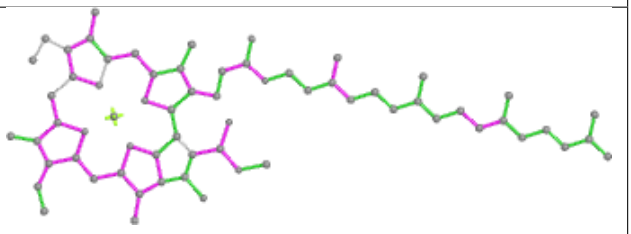


Rings

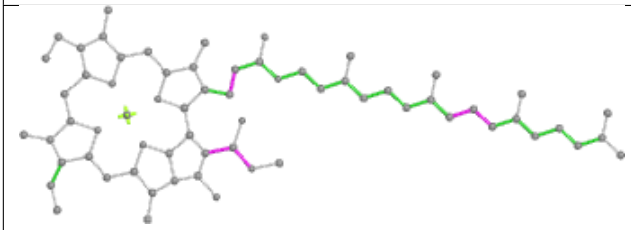
Ligand CLA B 803



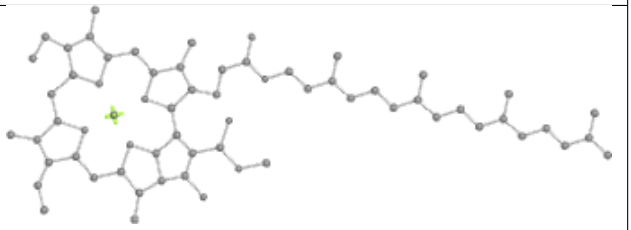
Bond lengths



Bond angles

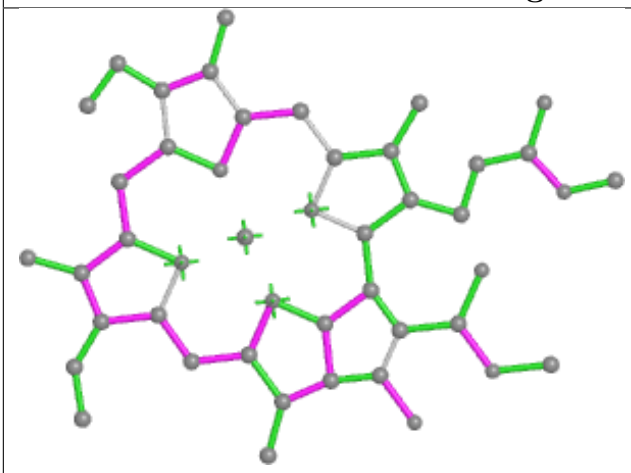


Torsions

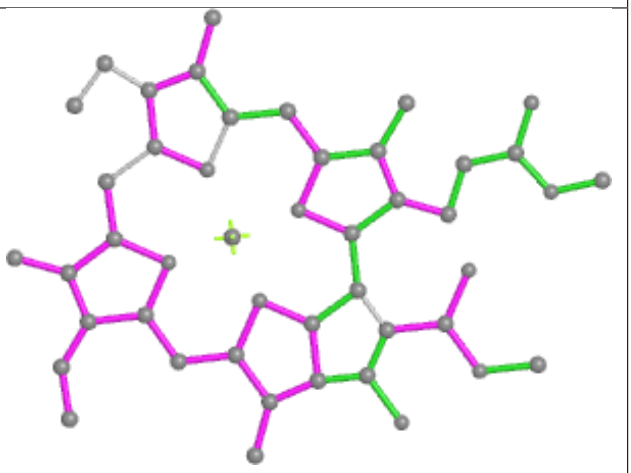


Rings

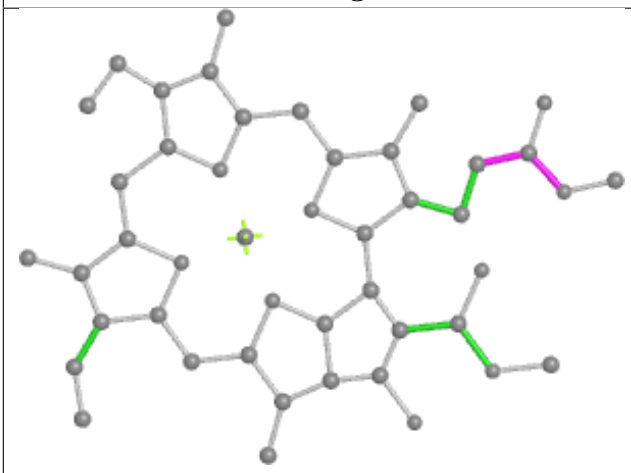
Ligand CLA Z 616



Bond lengths



Bond angles



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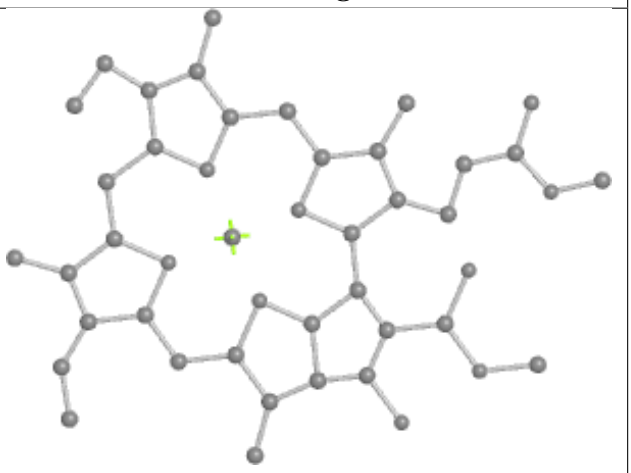
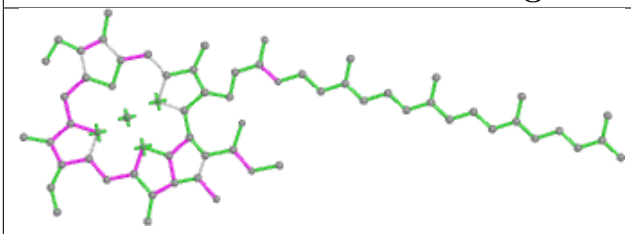
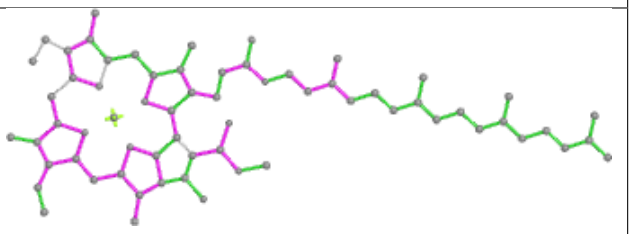


Rings

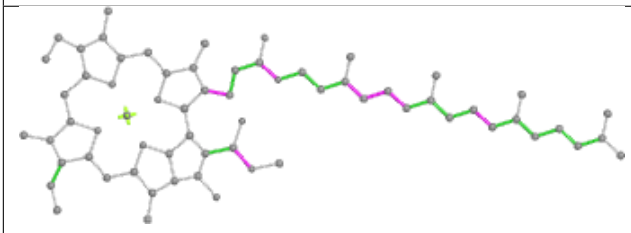
Ligand CLA B 810



Bond lengths



Bond angles



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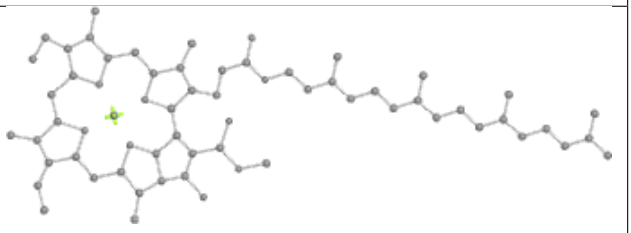
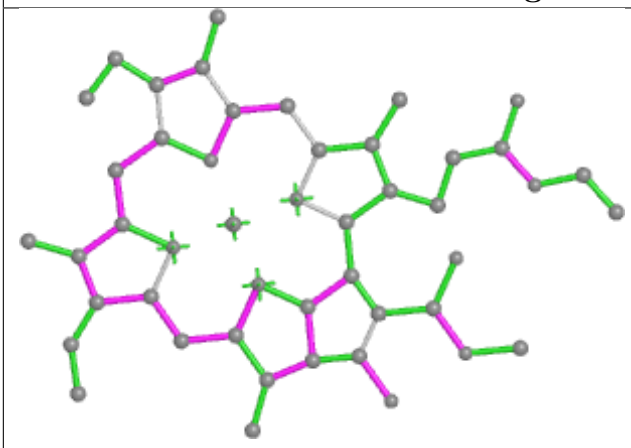


Rings

Ligand CLA B 838



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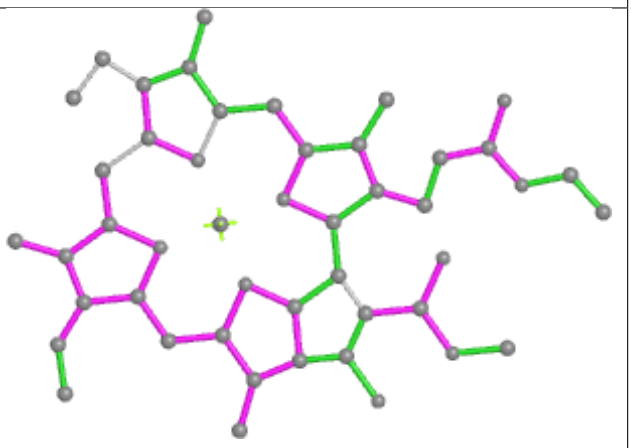
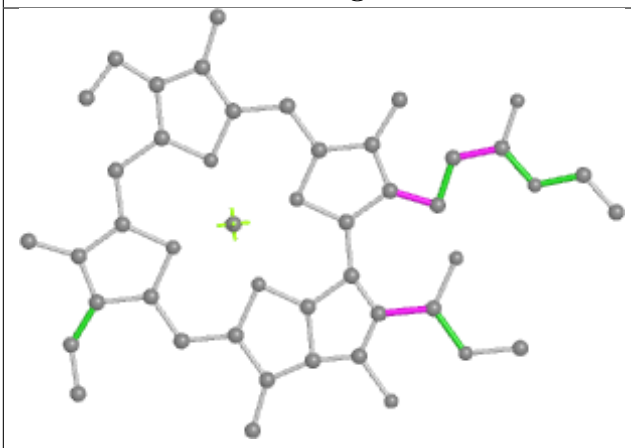


Bond angles



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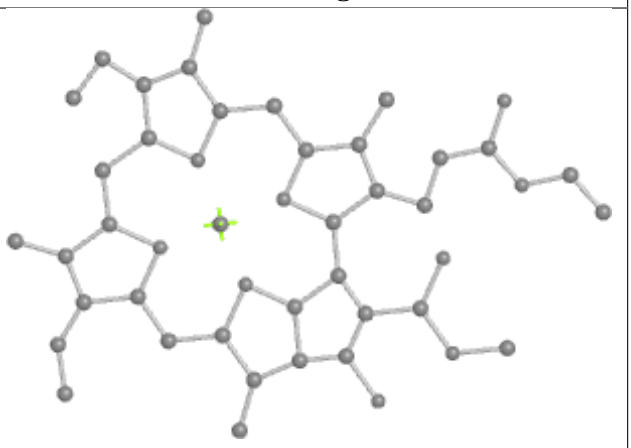
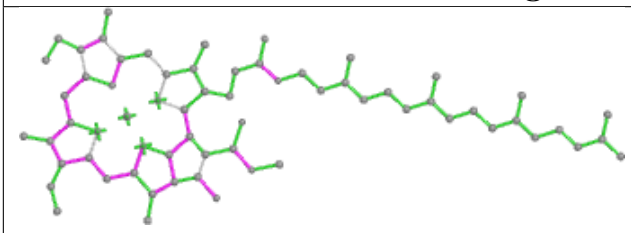
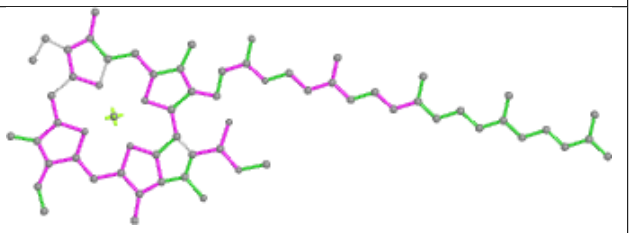


Rings

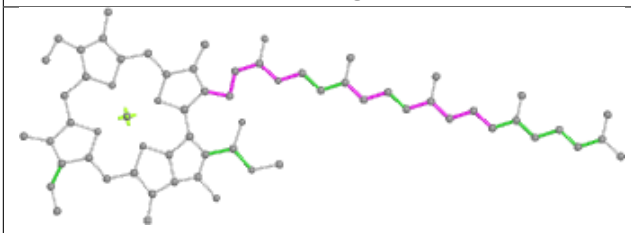
Ligand CLA B 827



Bond lengths



Bond angles



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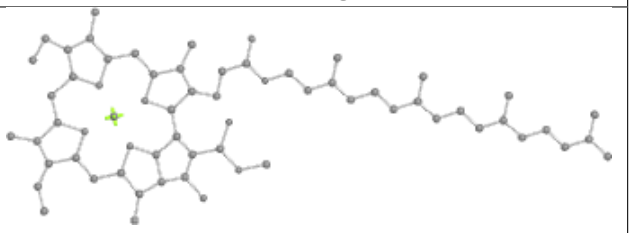
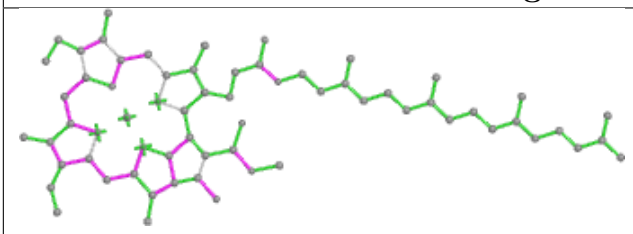
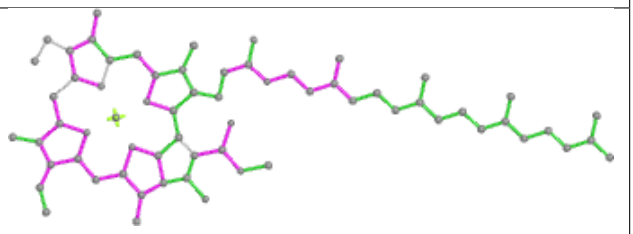


Rings

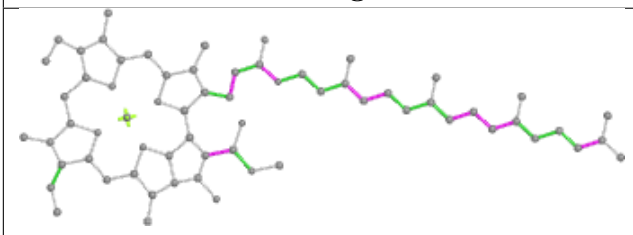
Ligand CLA A 814



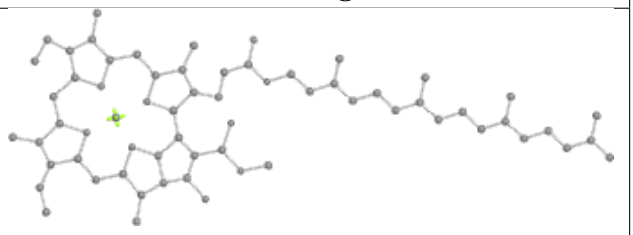
Bond lengths



Bond angles

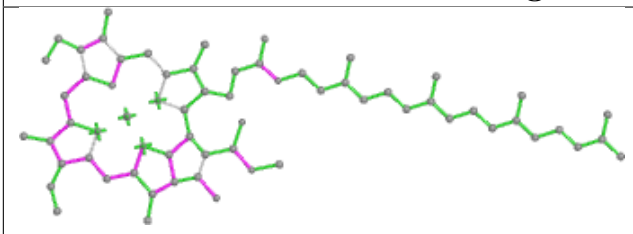


Torsions

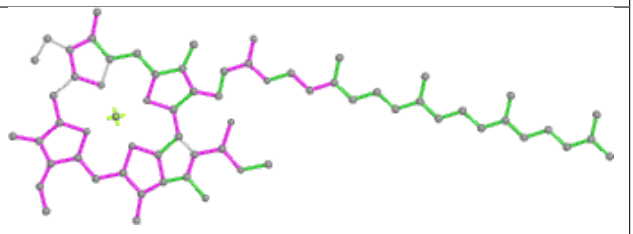


Rings

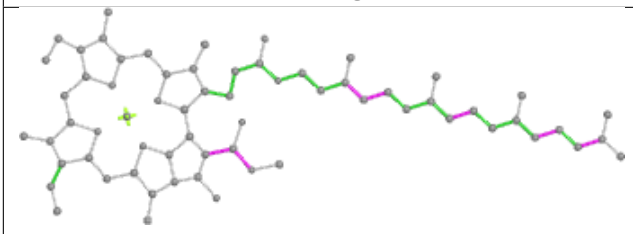
Ligand CLA F 301



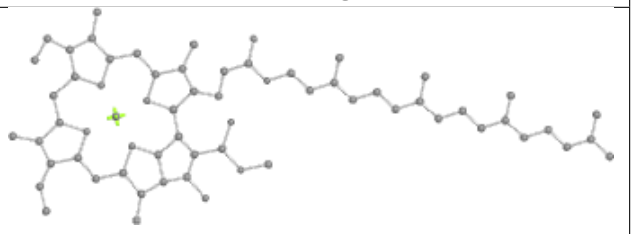
Bond lengths



Bond angles

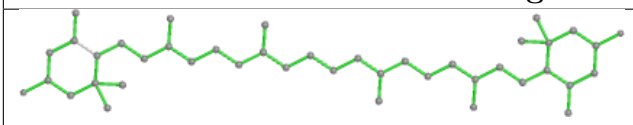


Torsions



Rings

Ligand LUT Z 618



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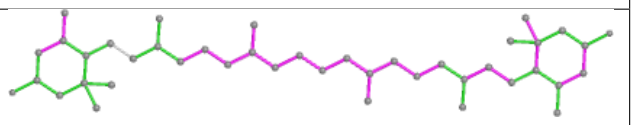
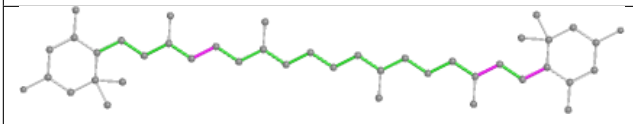
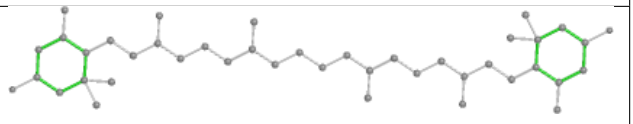


Bond angles

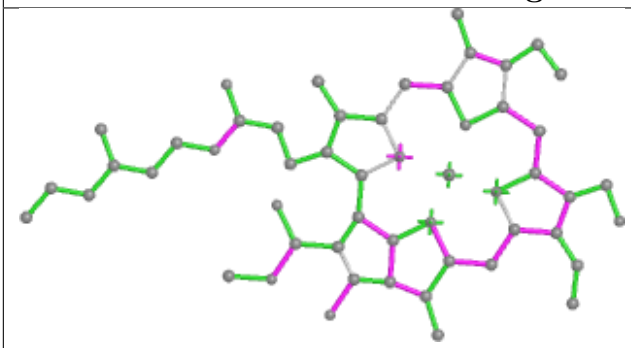


Torsions



Rings

Ligand CHL Z 601



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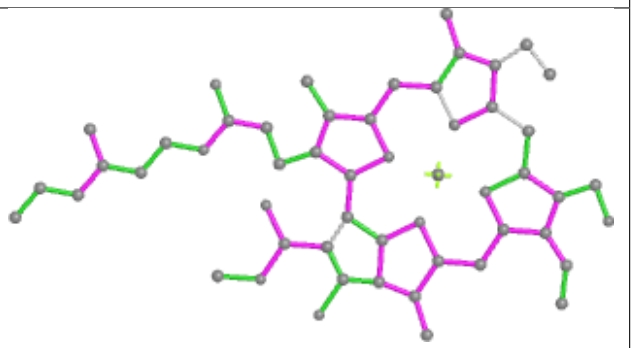
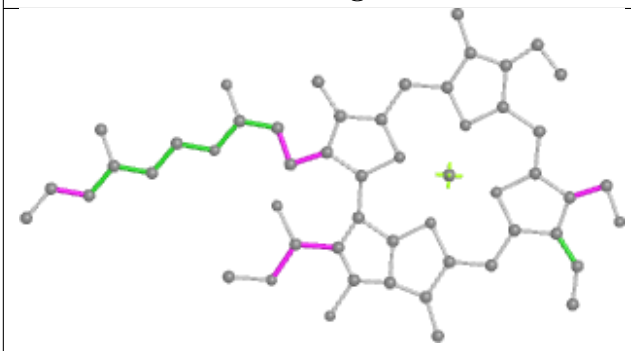
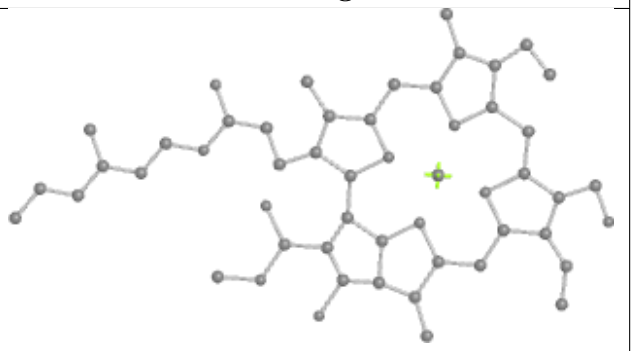


Bond angles

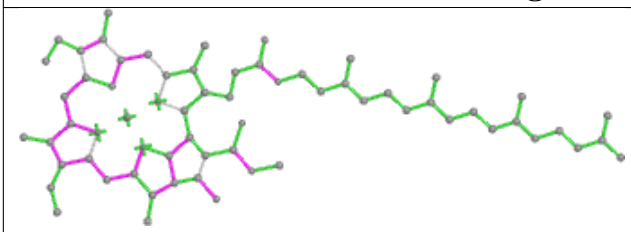


Torsions



Rings

Ligand CLA Z 602



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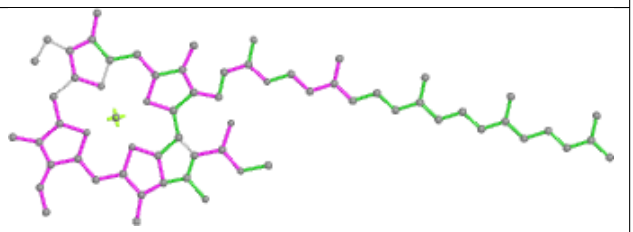
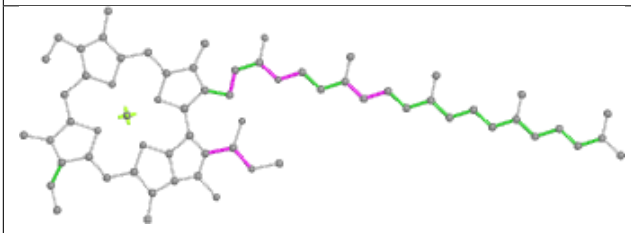
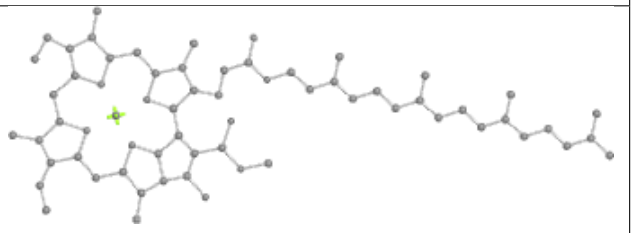


Bond angles

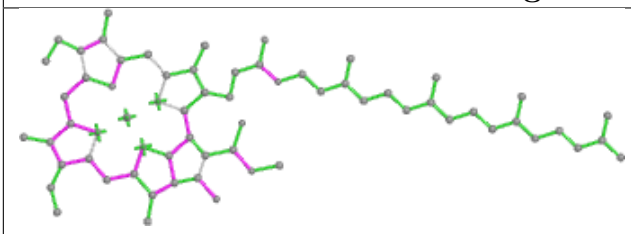


Torsions

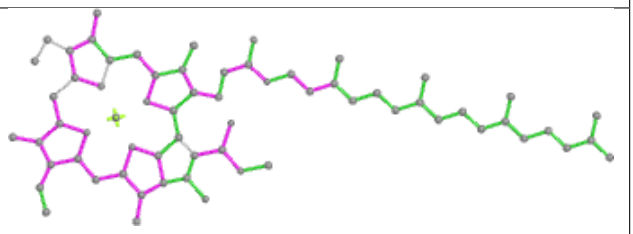


Rings

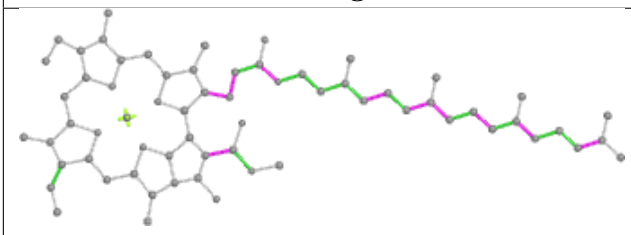
Ligand CLA A 812



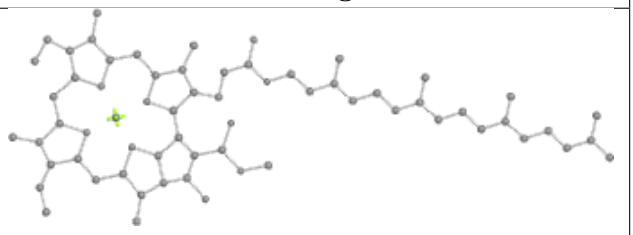
Bond lengths



Bond angles

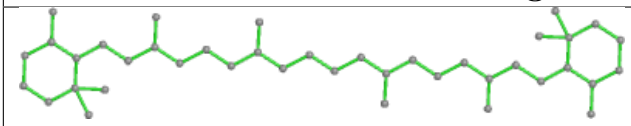


Torsions

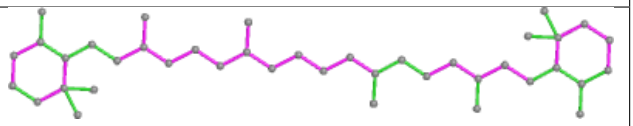


Rings

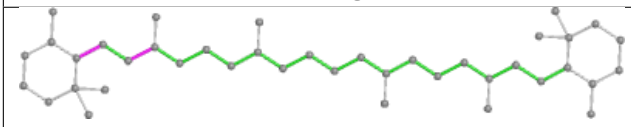
Ligand BCR 3 719



Bond lengths



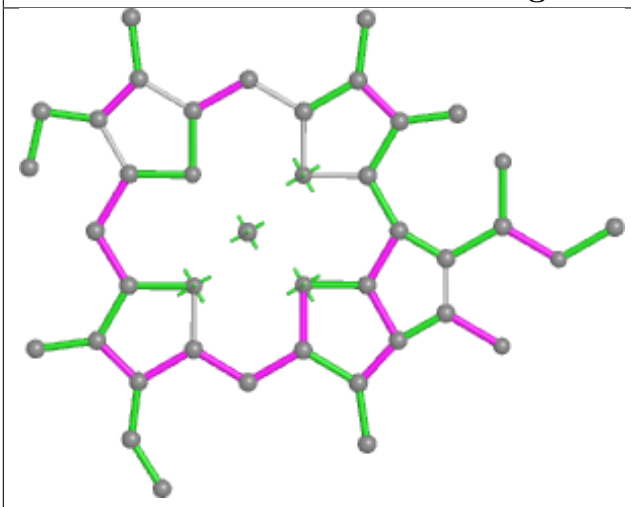
Bond angles



Torsions

Rings

Ligand CLA 4 616



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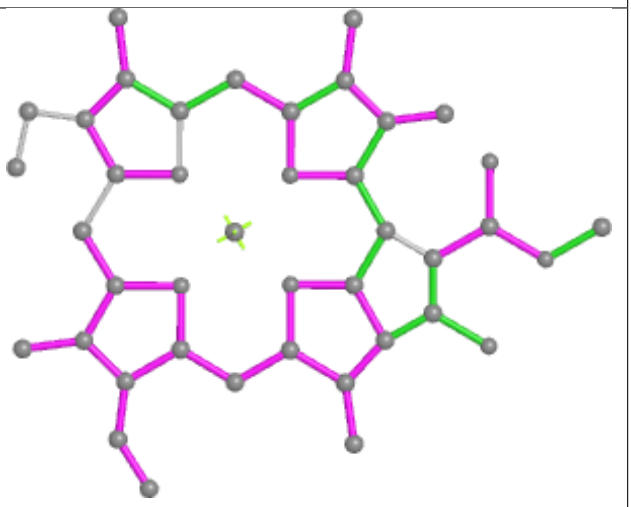
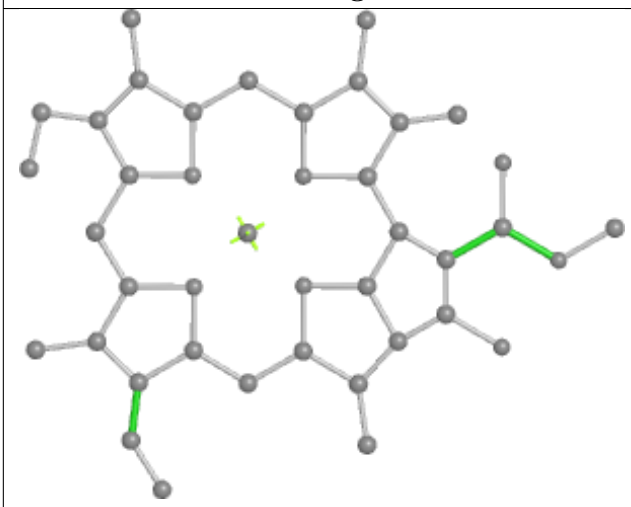
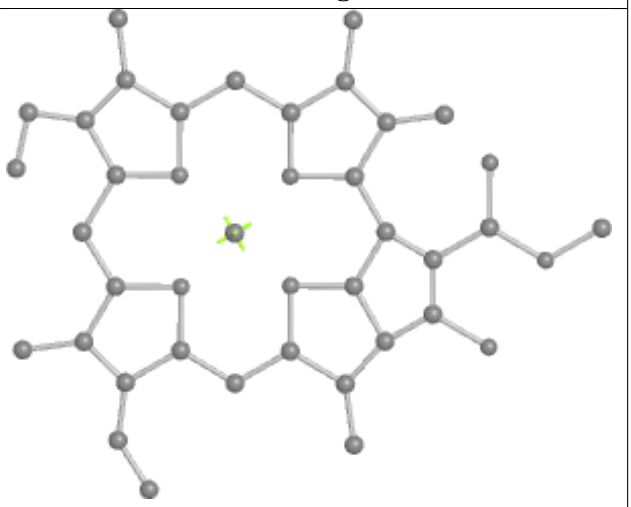


Bond angles

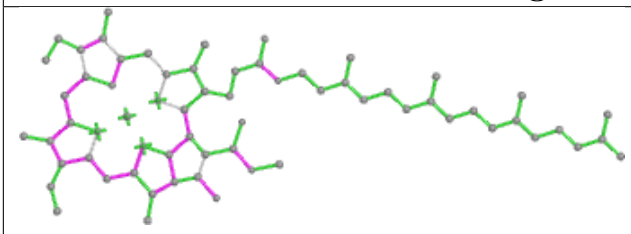


Torsions

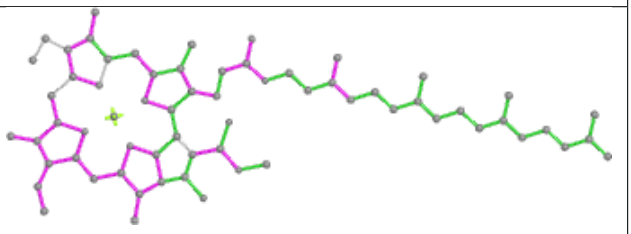


Rings

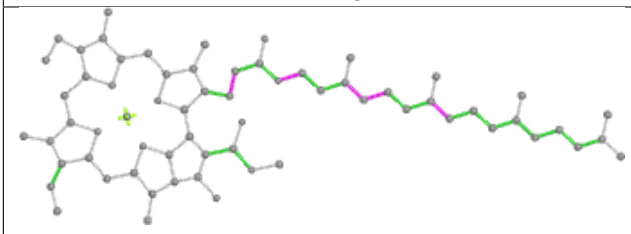
Ligand CLA 1 609



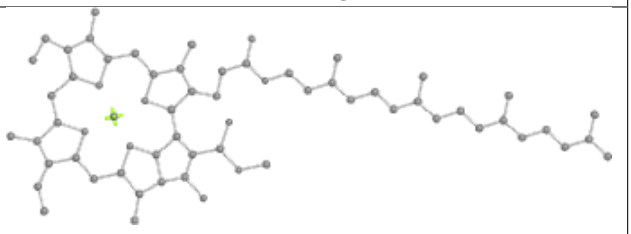
Bond lengths



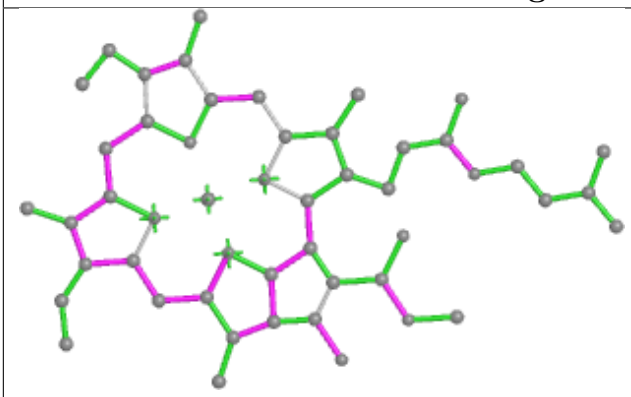
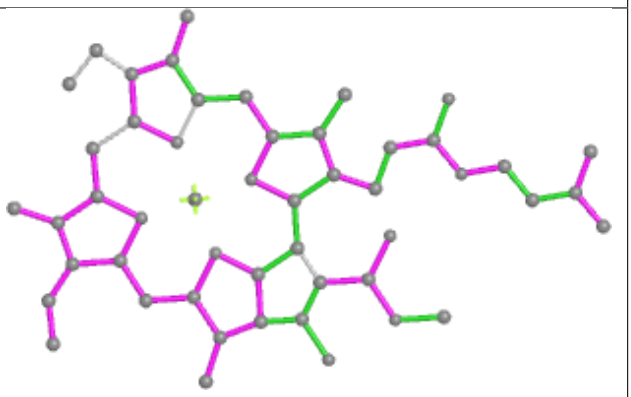
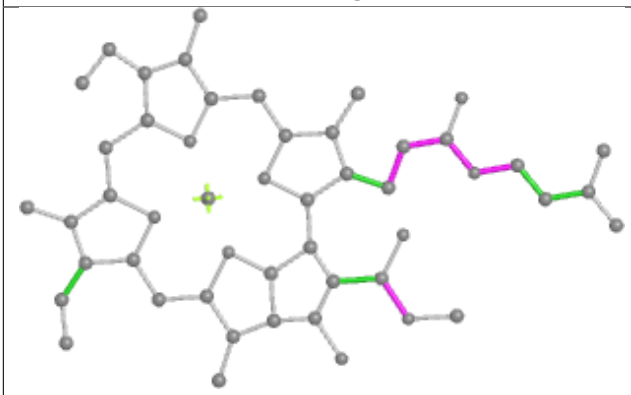
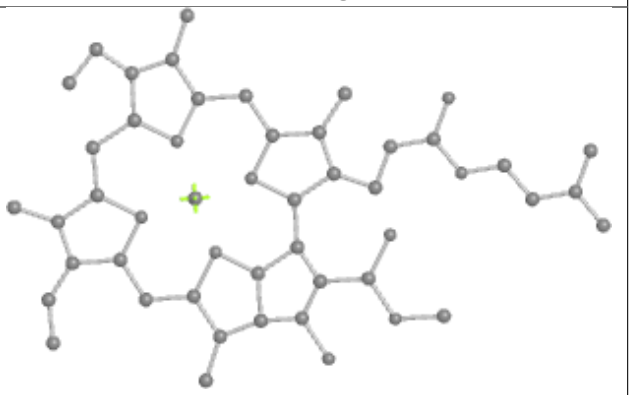
Bond angles

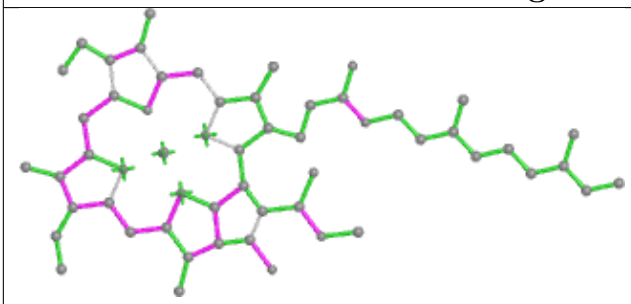
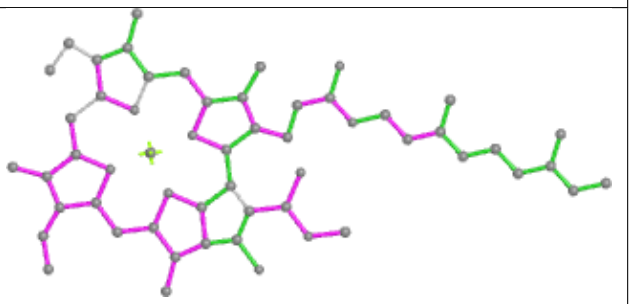
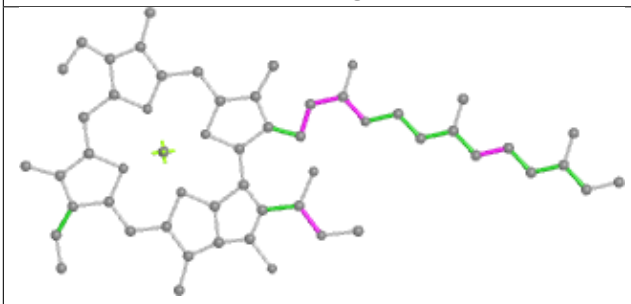
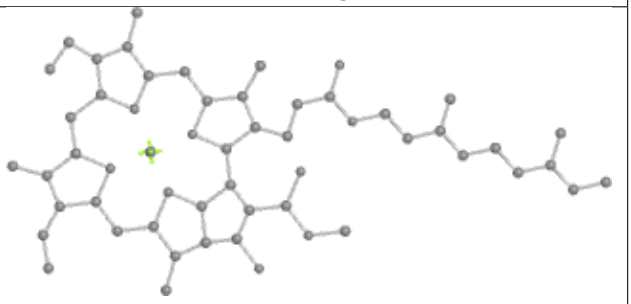


Torsions

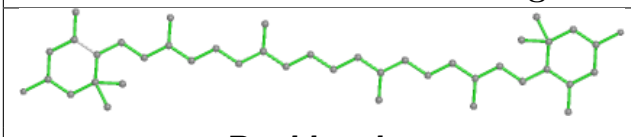


Rings

Ligand CLA 9 613	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 3 620	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LUT 6 624



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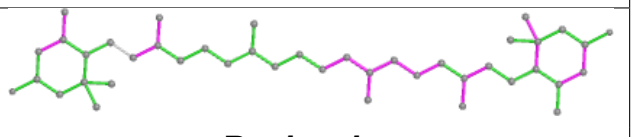
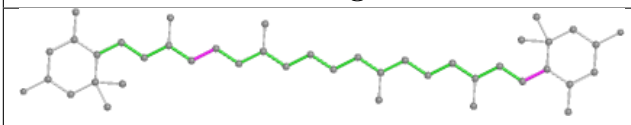


Bond angles



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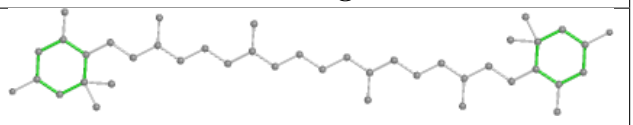
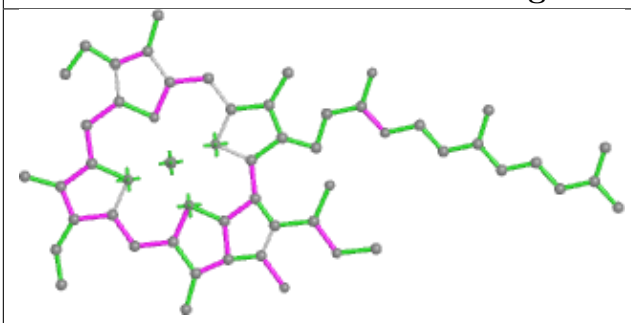


Rings

Ligand CLA 6 611



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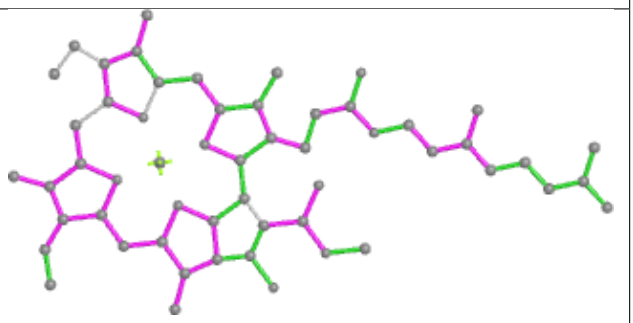
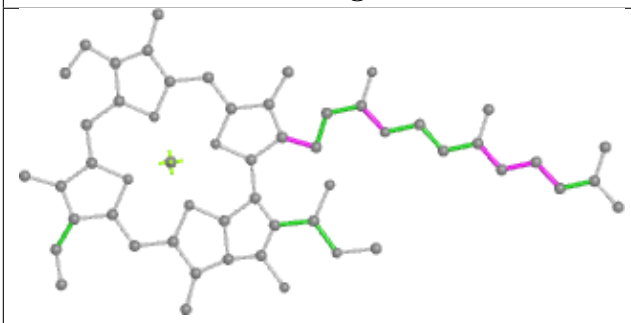


Bond angles



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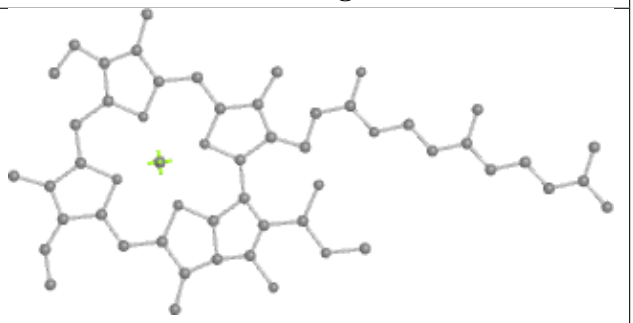
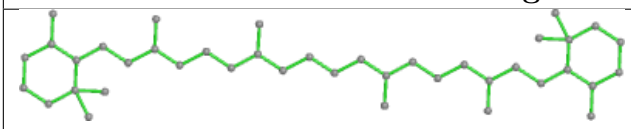
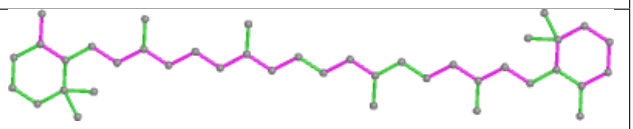


Rings

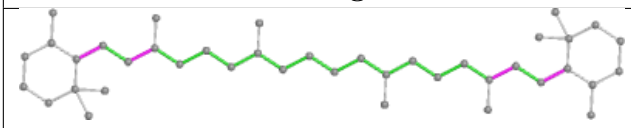
Ligand BCR B 844



Bond lengths



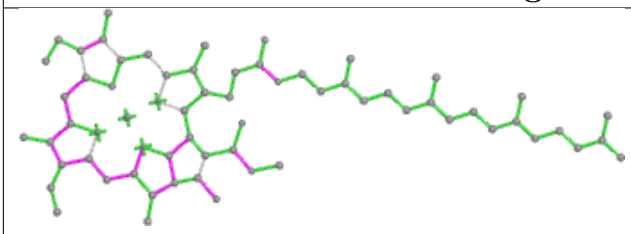
Bond angles



Torsions

Rings

Ligand CLA B 834



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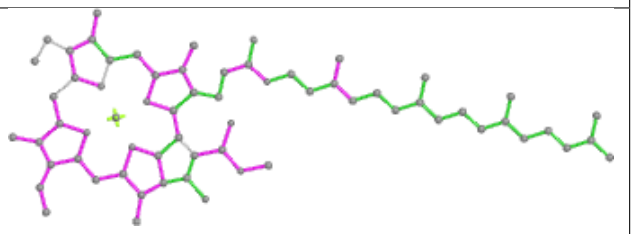
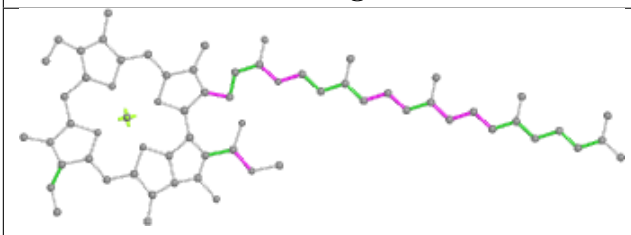


Bond angles



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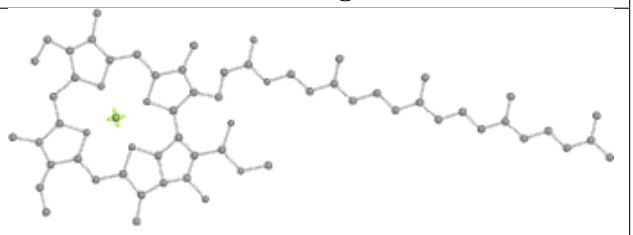
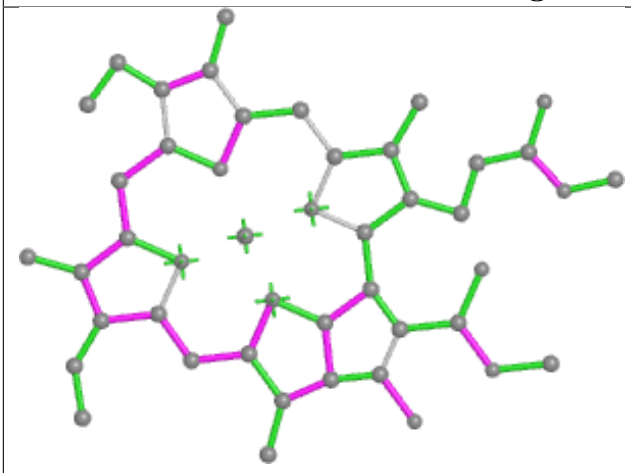


Rings

Ligand CLA 3 617



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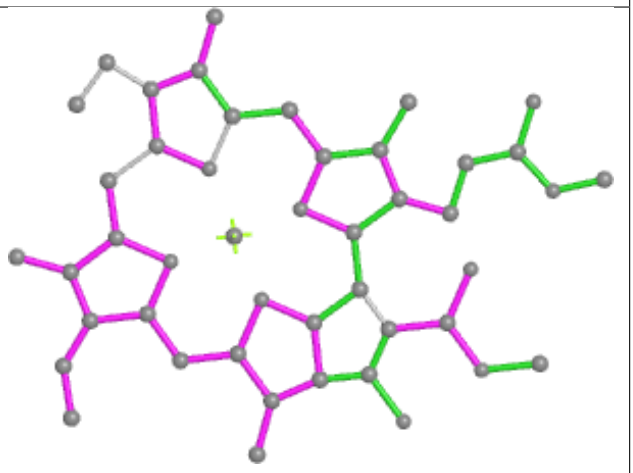
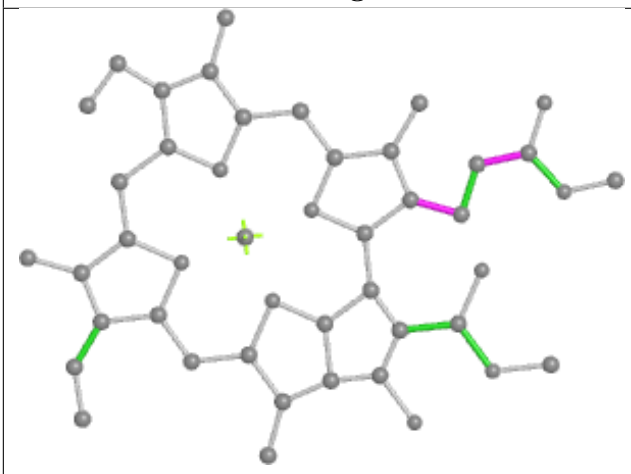


Bond angles



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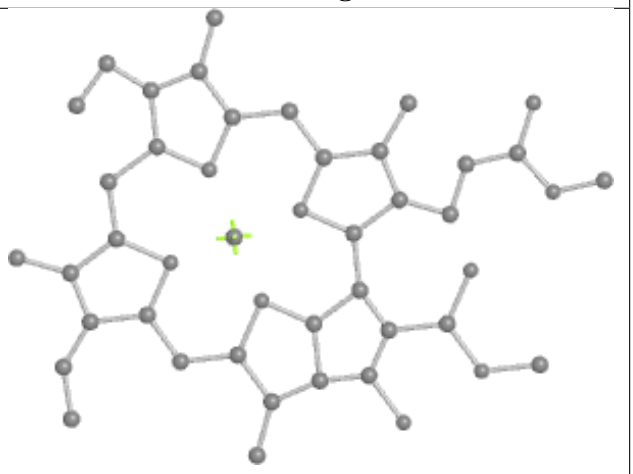
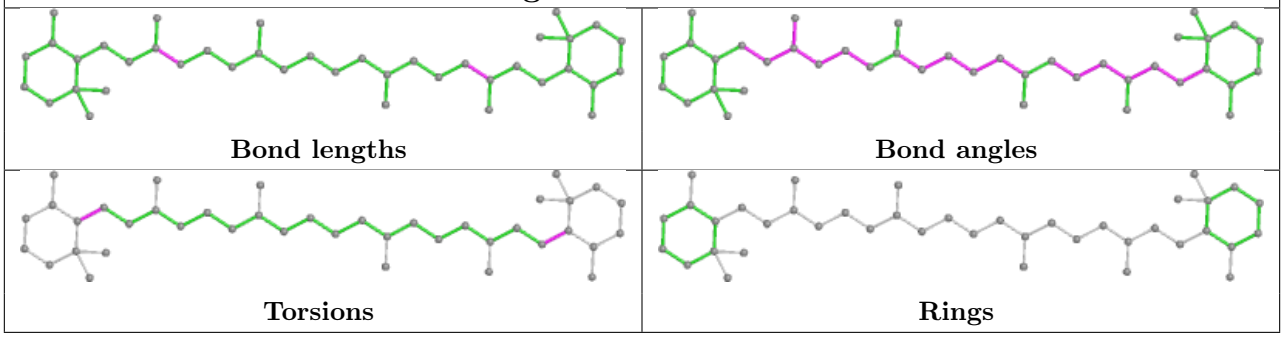
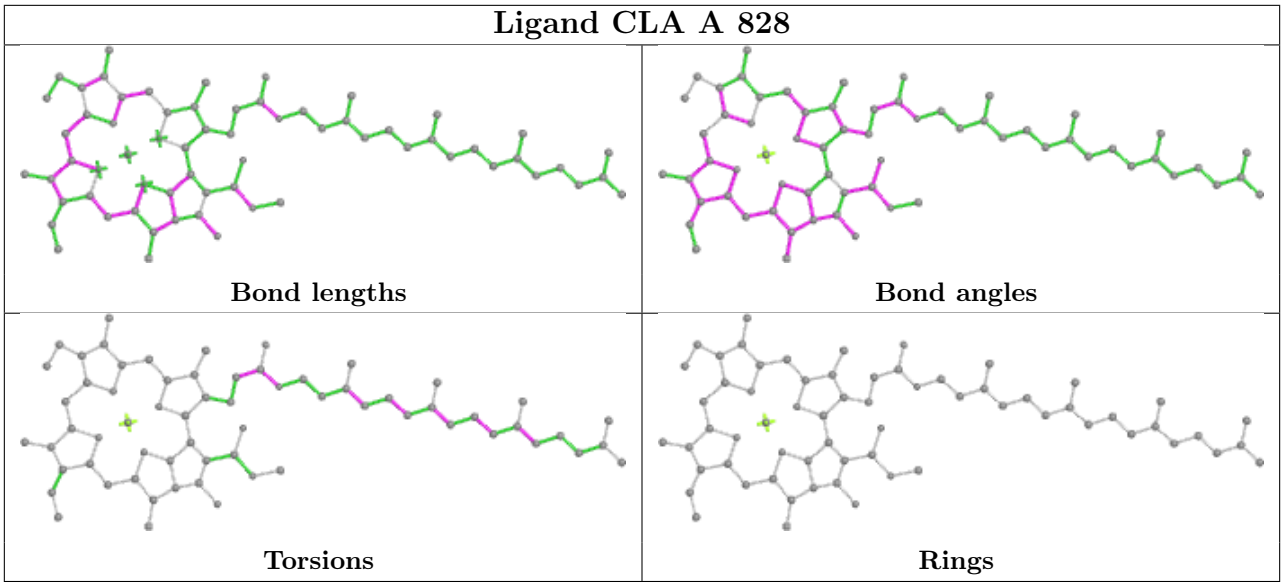


Rings

Ligand BCR A 851



Ligand CLA A 828



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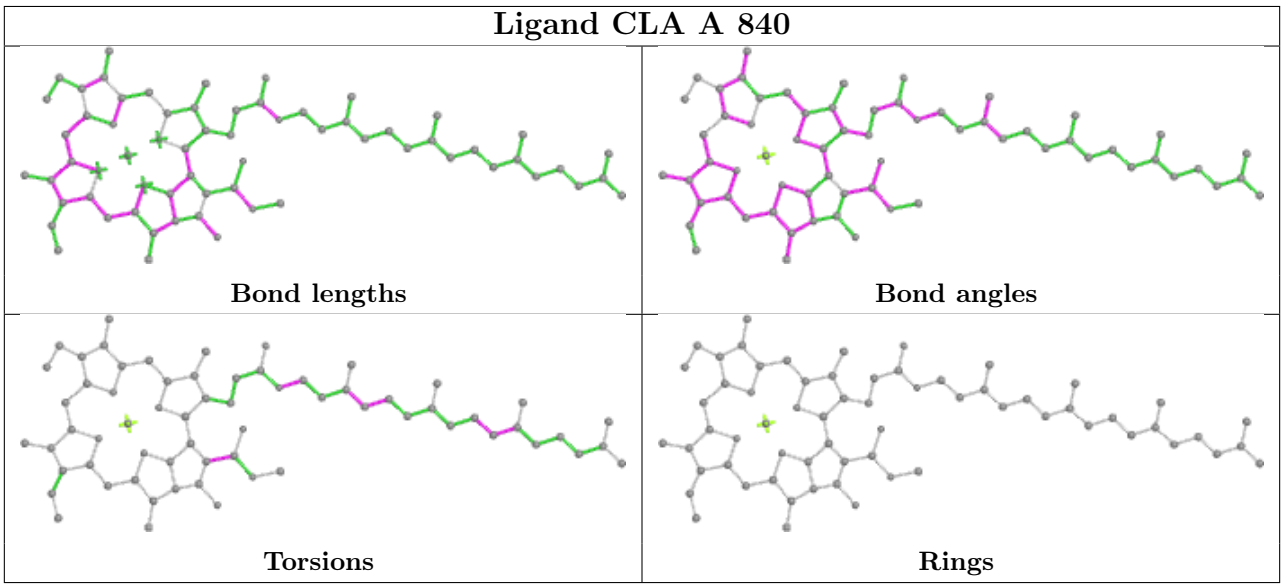

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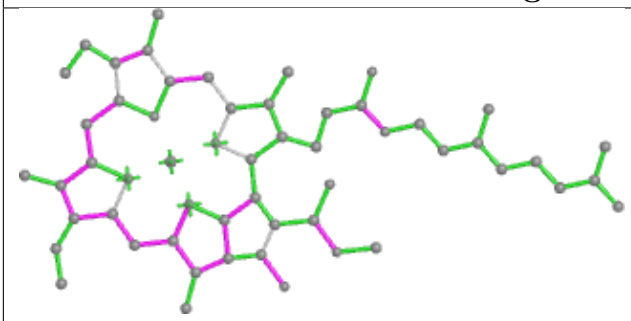
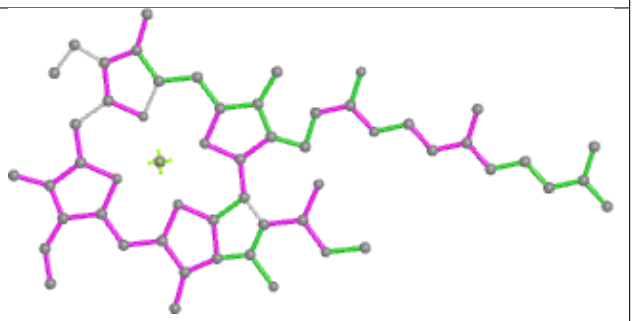
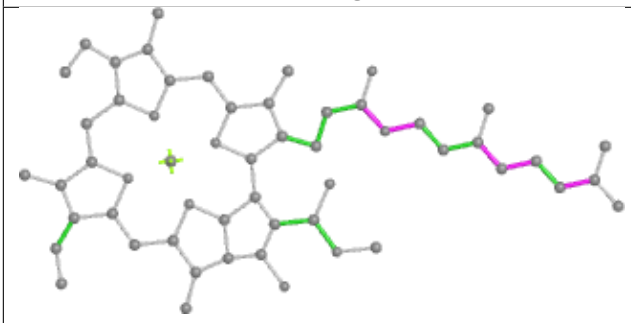


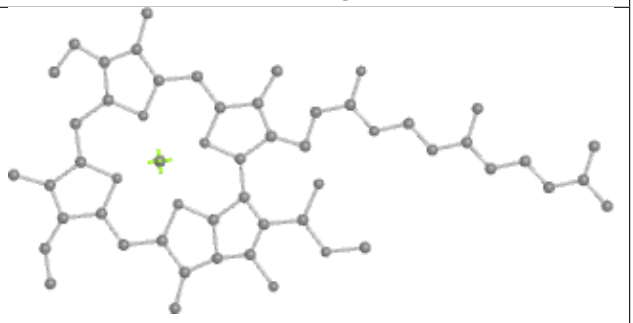
Bond lengths



Bond angles

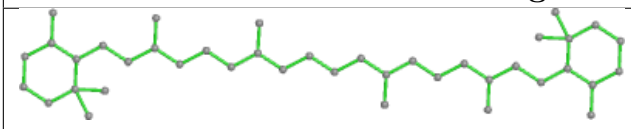


Torsions

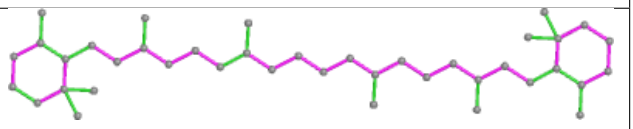


Rings

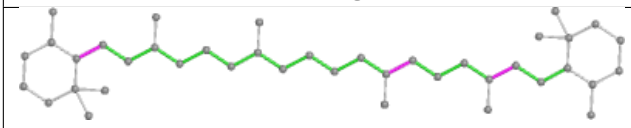
Ligand BCR I 172



Bond lengths



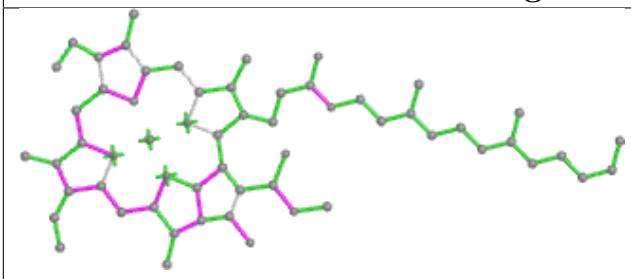
Bond angles



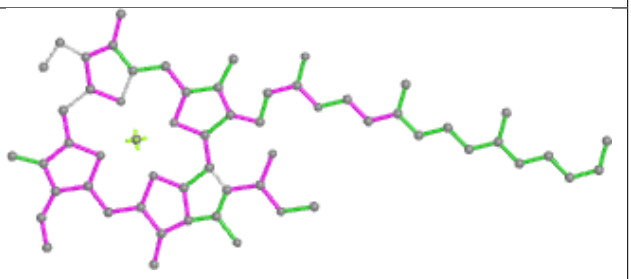
Torsions

Rings

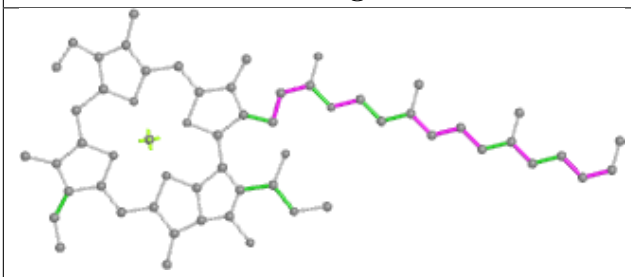
Ligand CLA B 817



Bond lengths



Bond angles



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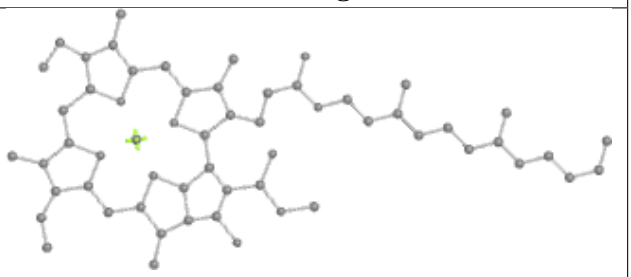
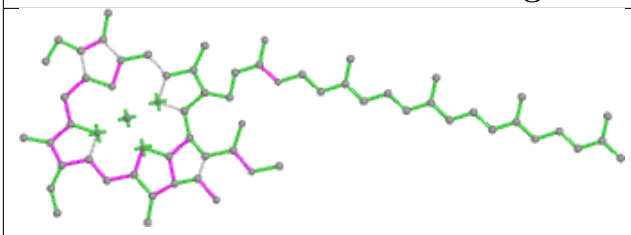
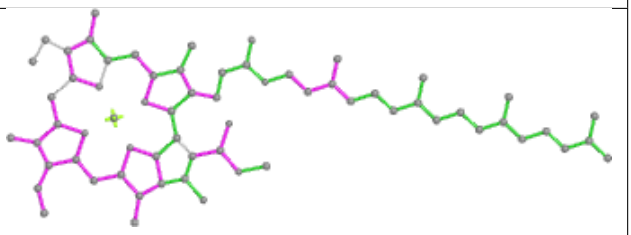


Rings

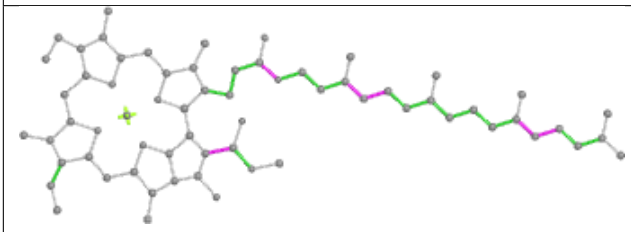
Ligand CLA A 839



Bond lengths



Bond angles



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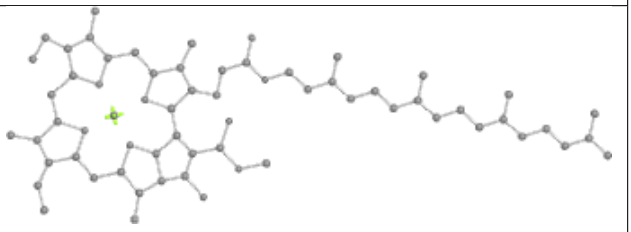
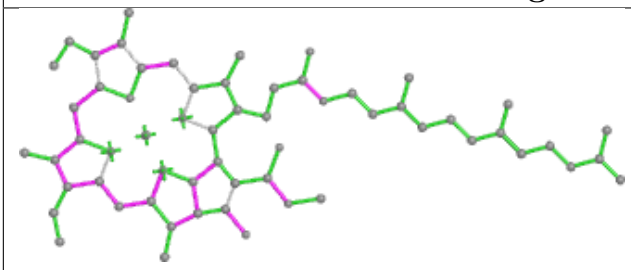
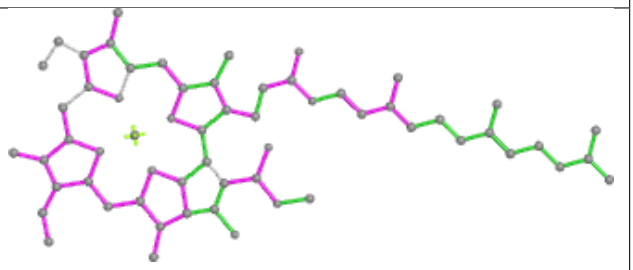
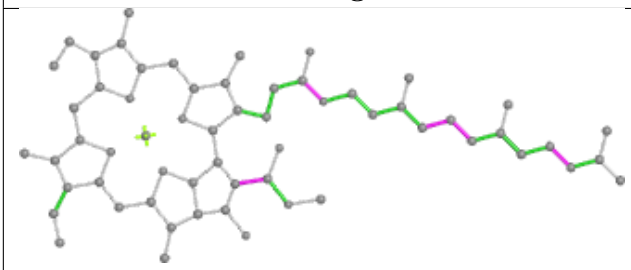
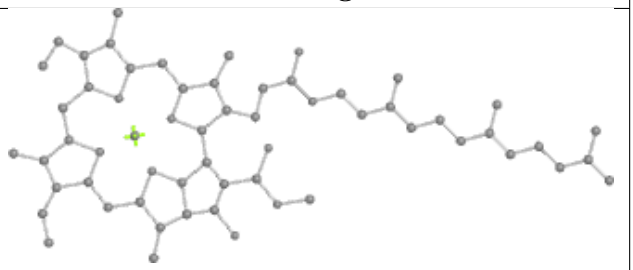
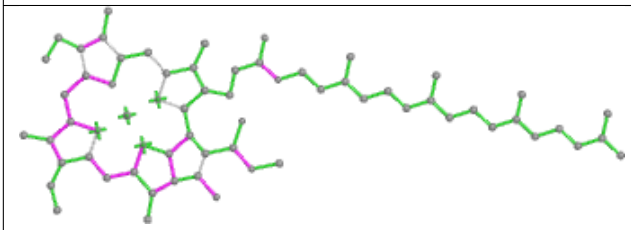
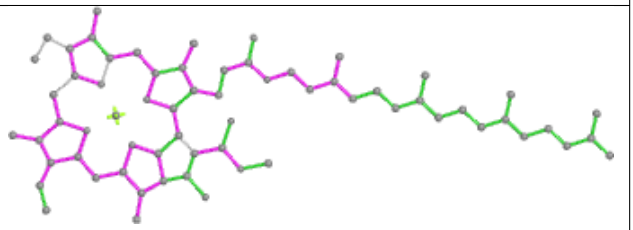
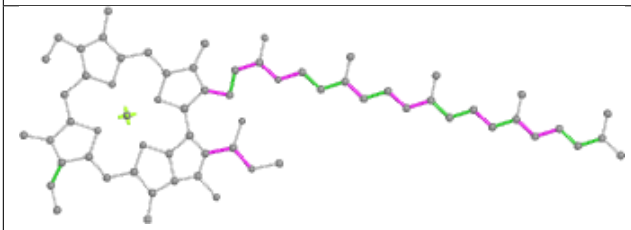
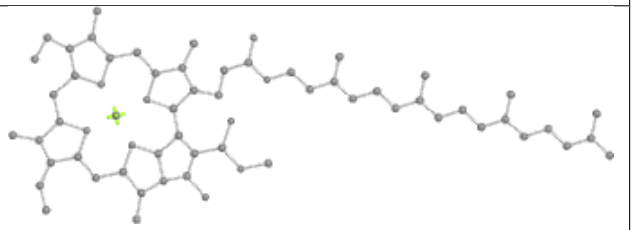
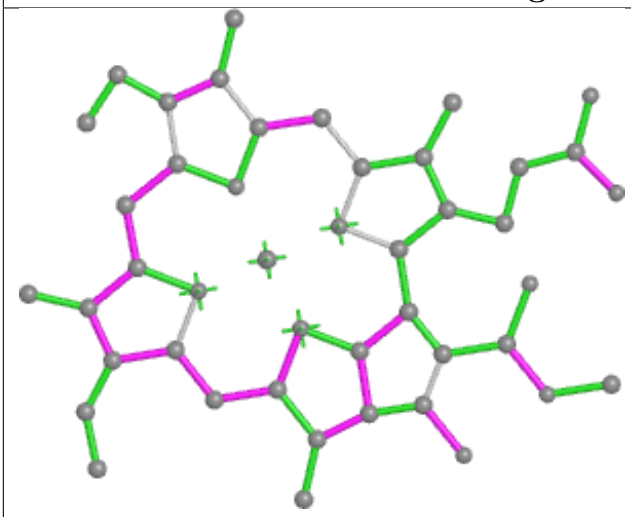


Rings

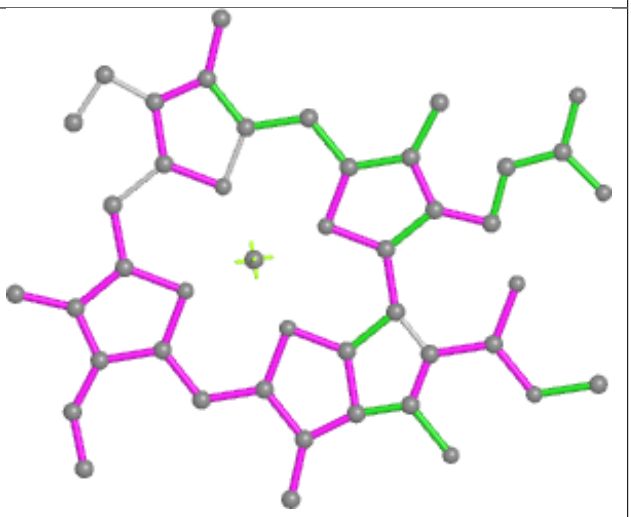
Ligand CLA 7 620	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 829	
 Bond lengths	 Bond angles
 Torsions	 Rings

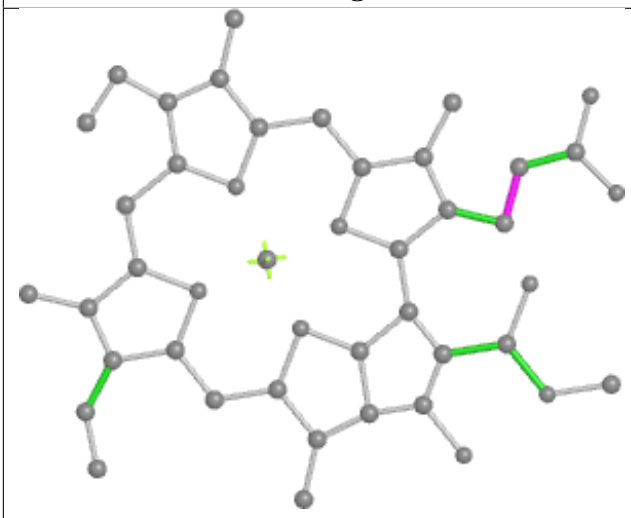
Ligand CLA 5 614



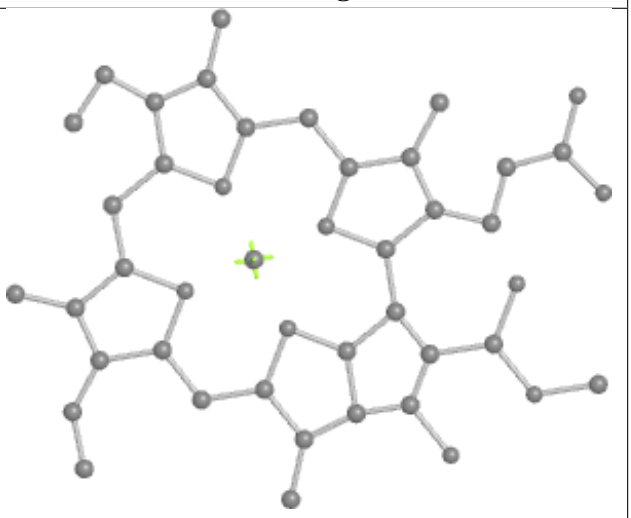
Bond lengths



Bond angles

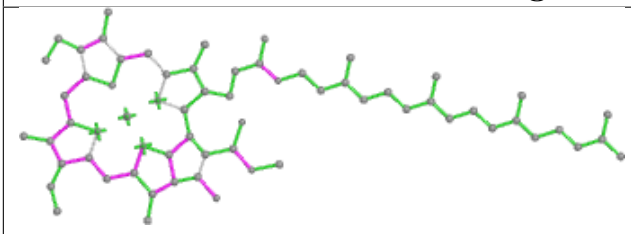


Torsions

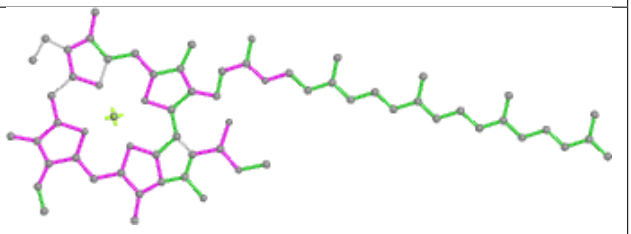


Rings

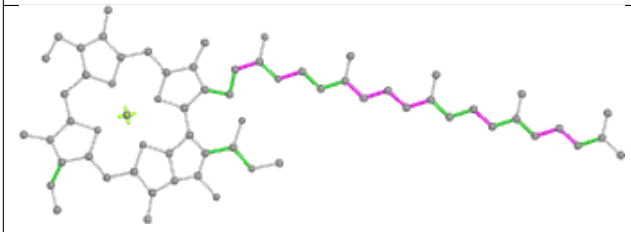
Ligand CLA 8 613



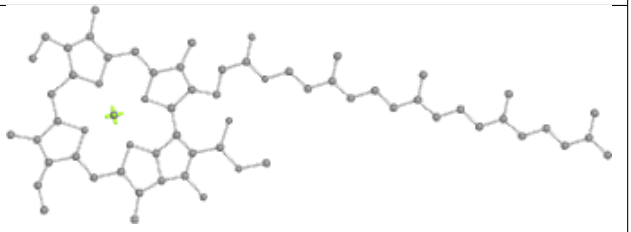
Bond lengths



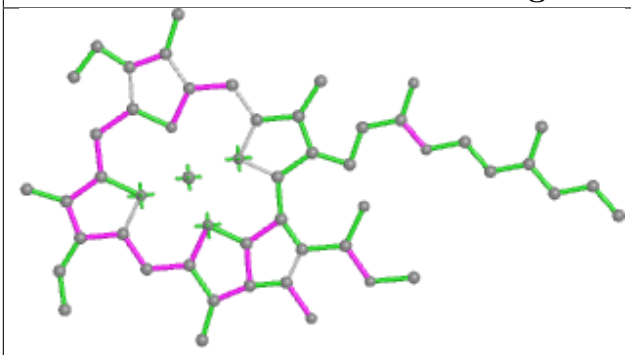
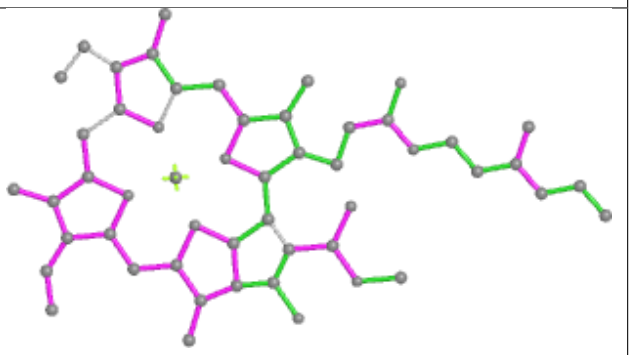
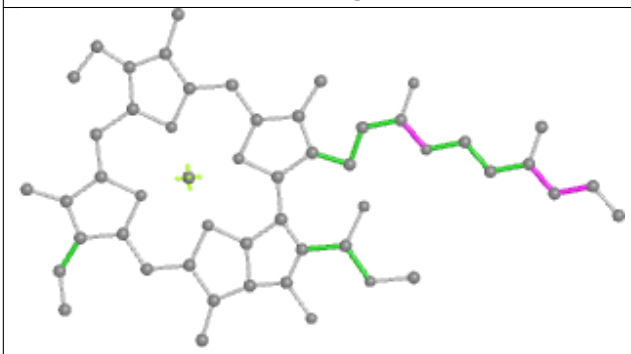
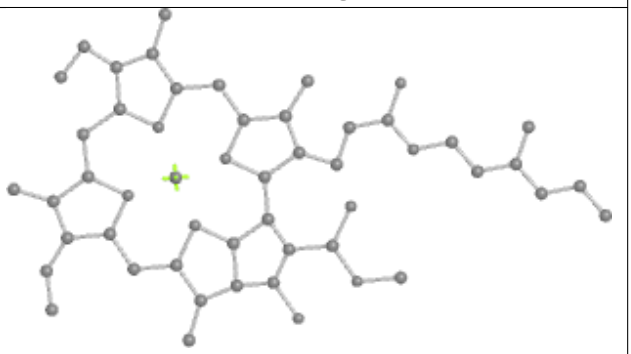
Bond angles



Torsions



Rings

Ligand CLA 6 612	
	
Bond lengths	Bond angles
	
Torsions	Rings

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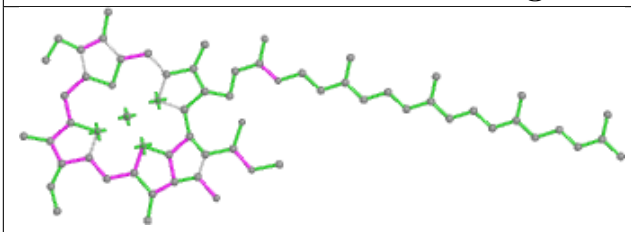
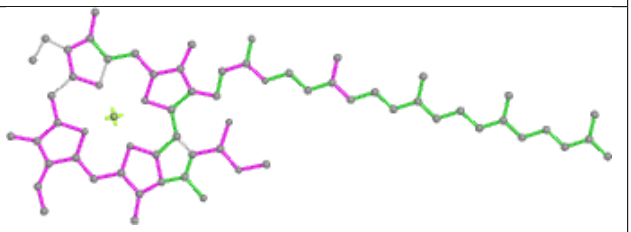
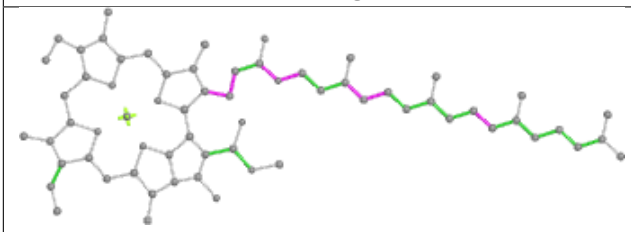
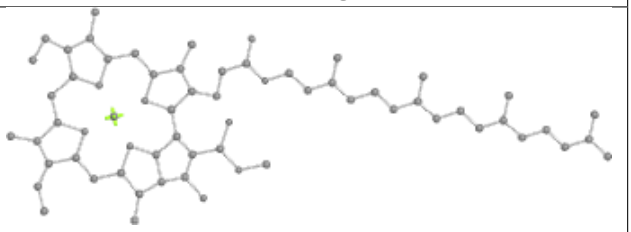
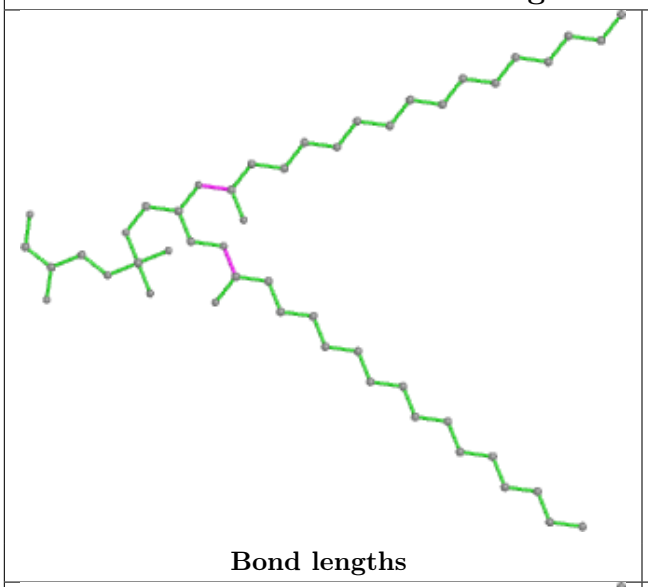
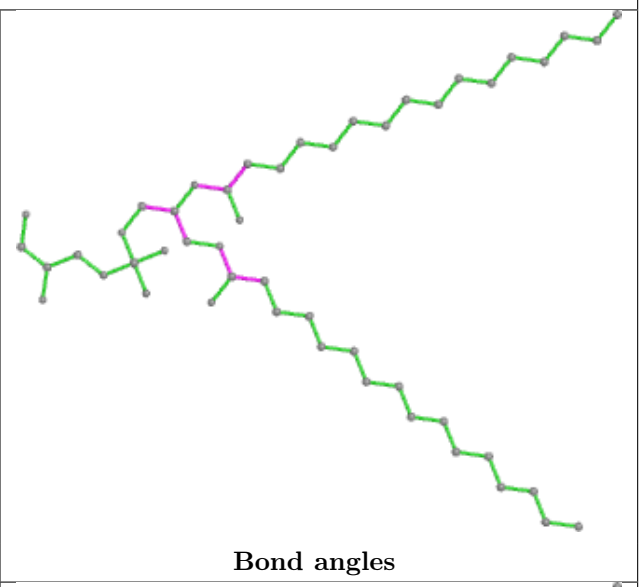
	
Bond lengths	Bond angles
	
Torsions	Rings

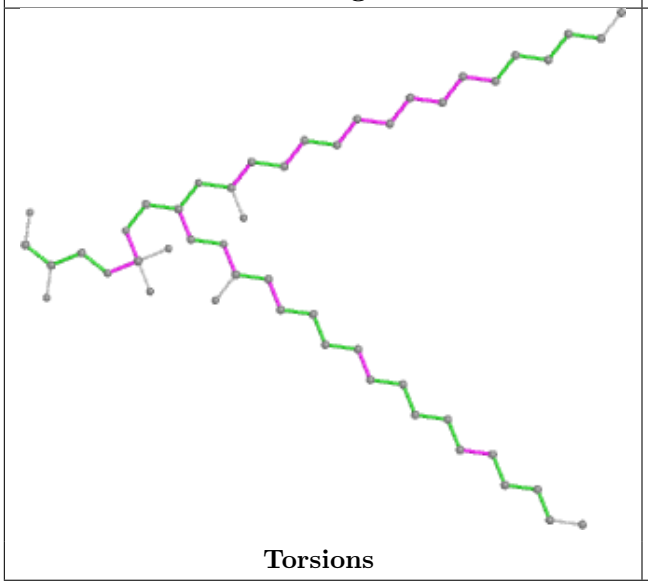
Ligand LHG 4 622



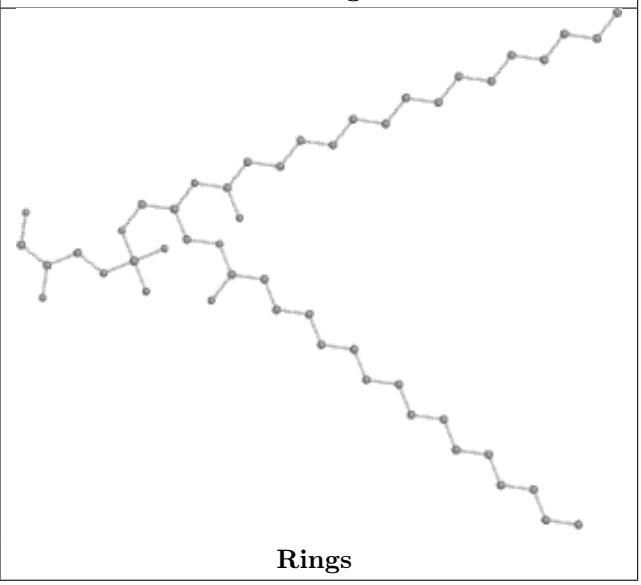
Bond lengths



Bond angles

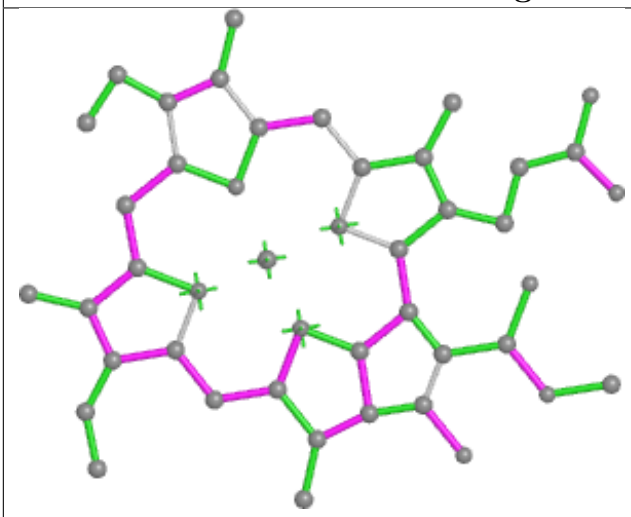


Torsions



Rings

Ligand CLA K 4002



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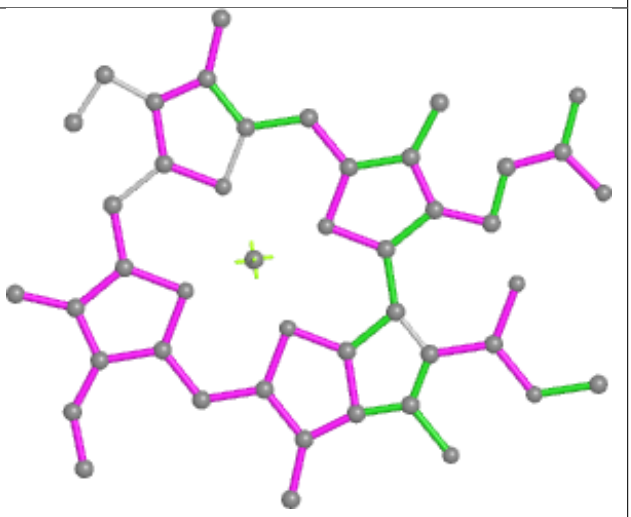
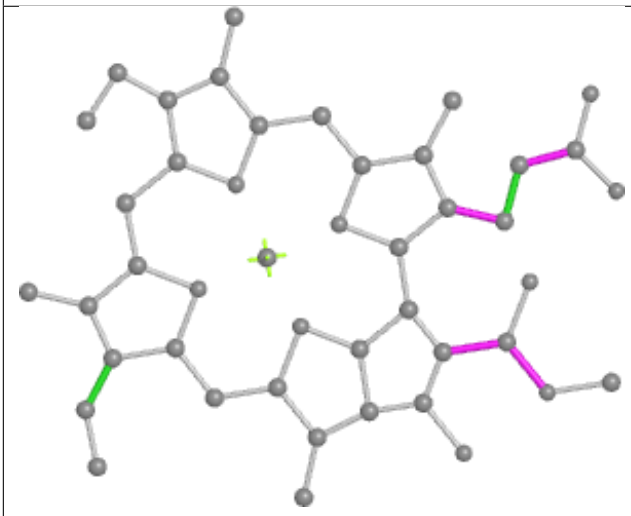


Bond angles



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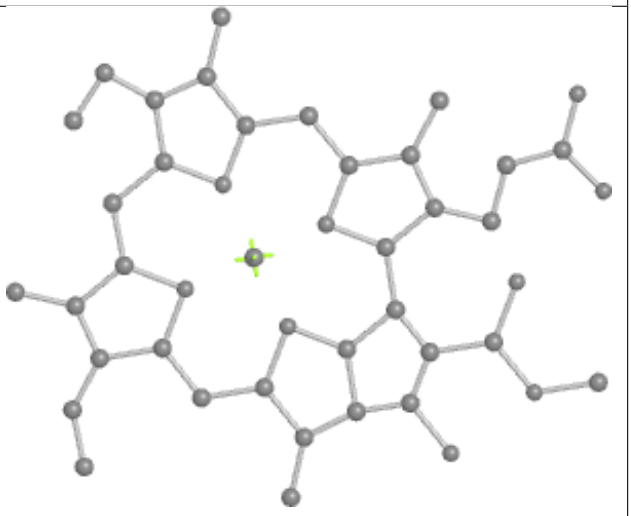
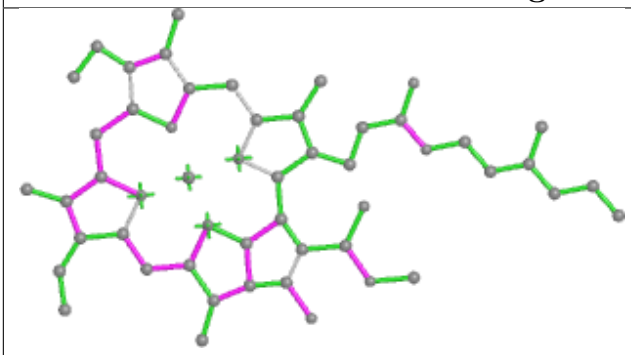
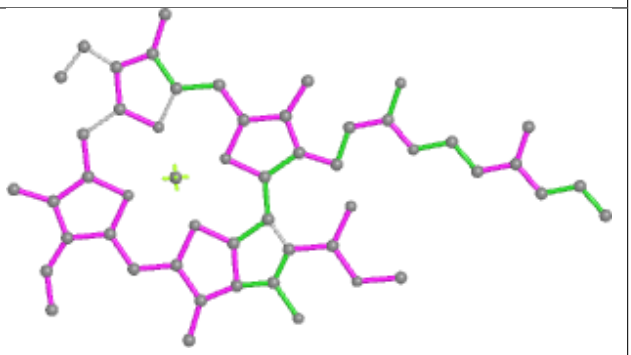
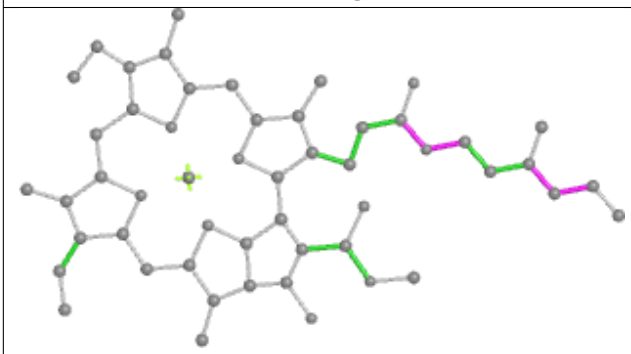
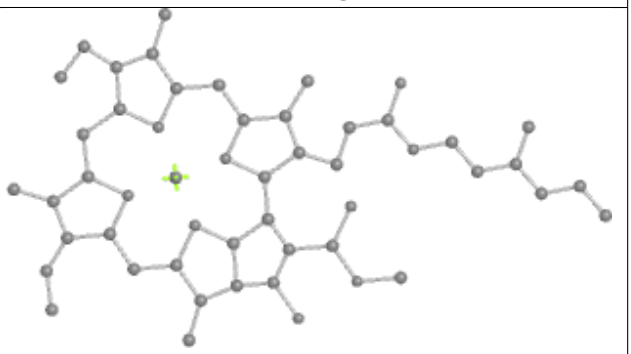


Rings

Ligand CLA 8 612	
 Bond lengths	 Bond angles
 Torsions	 Rings

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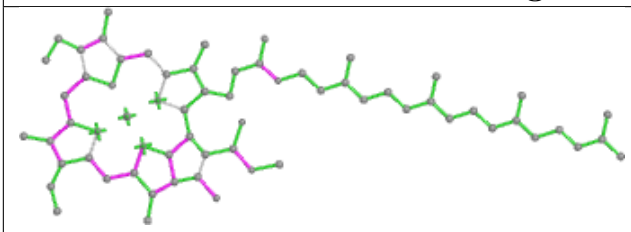
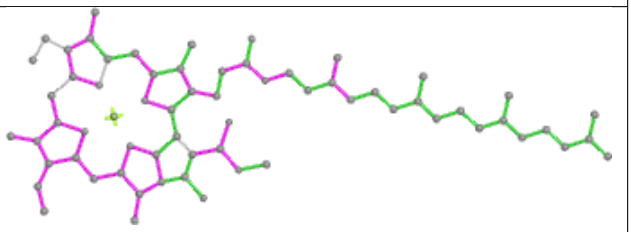
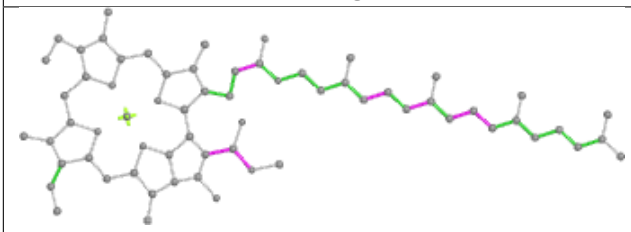
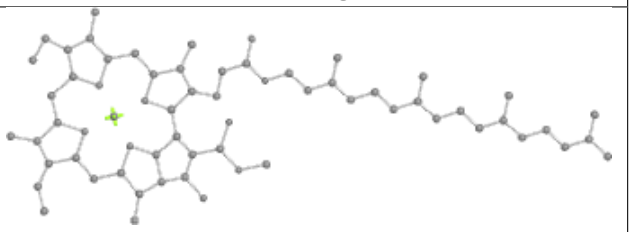
 Bond lengths	 Bond angles
 Torsions	 Rings

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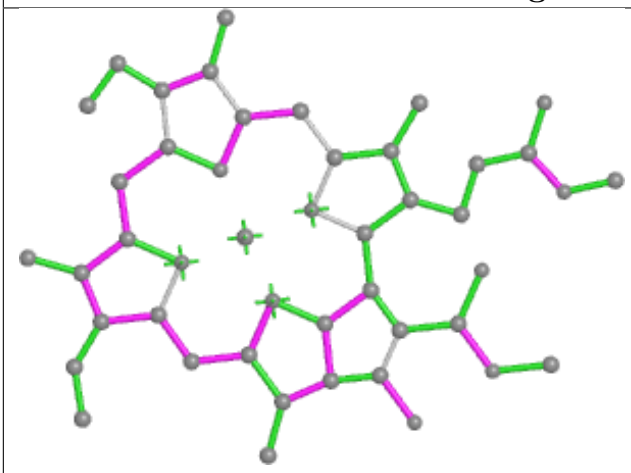

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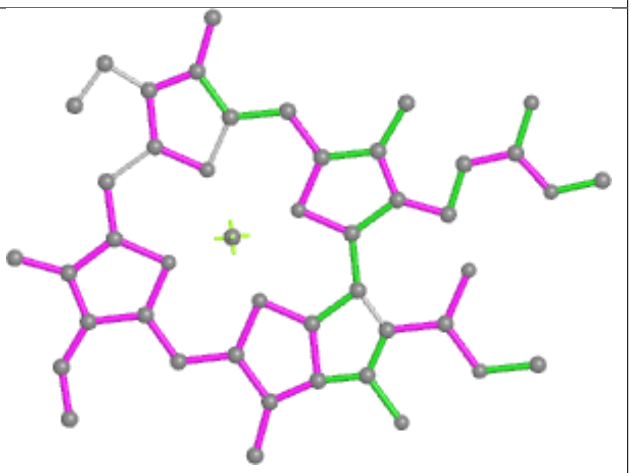
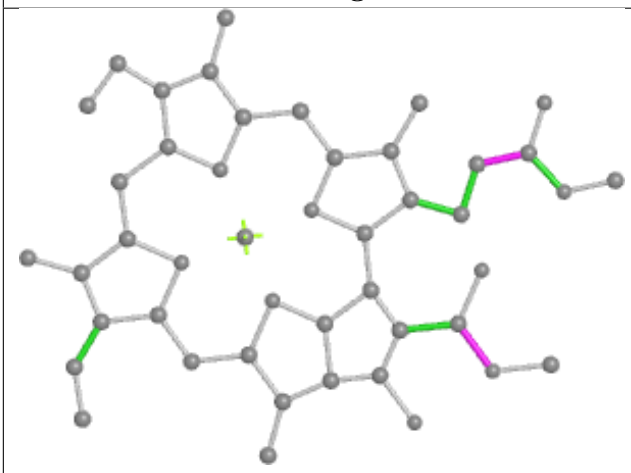
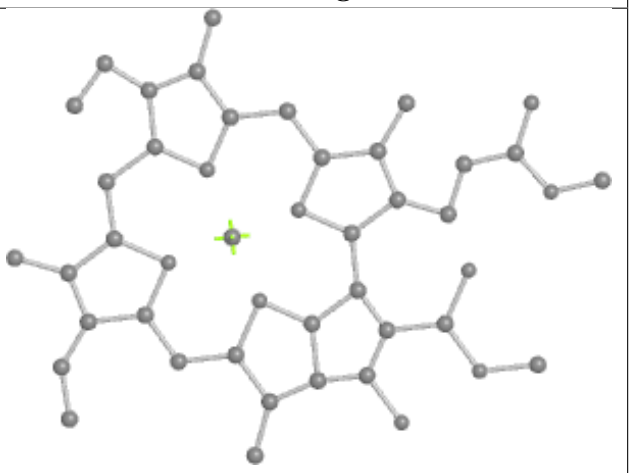


Bond angles

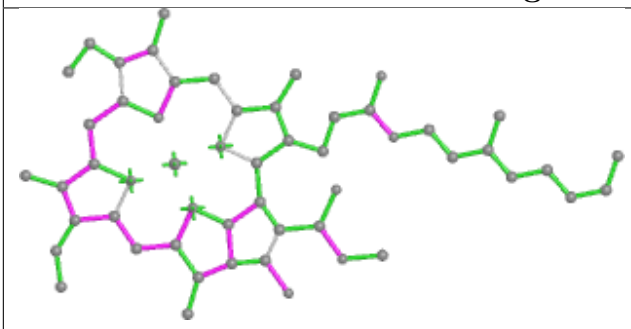


Torsions

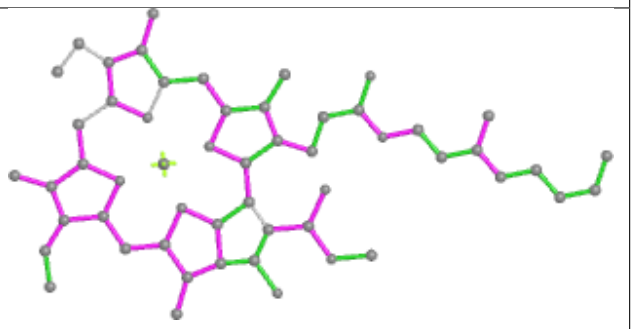


Rings

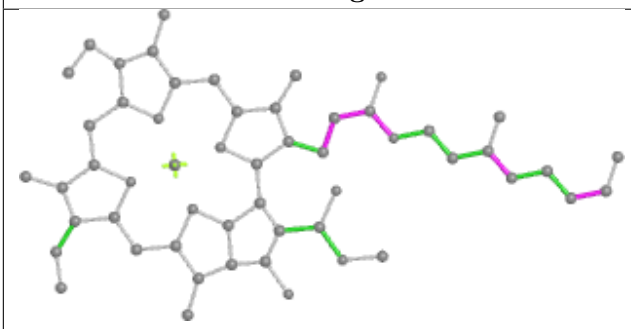
Ligand CLA A 813



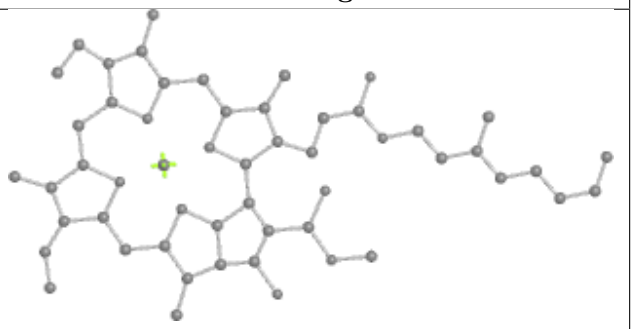
Bond lengths



Bond angles

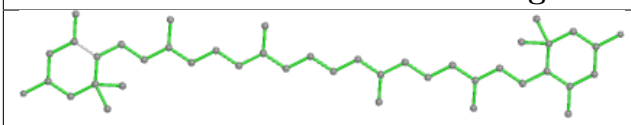


Torsions

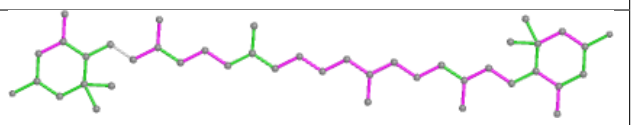


Rings

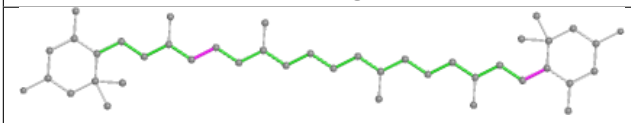
Ligand LUT 5 624



Bond lengths



Bond angles



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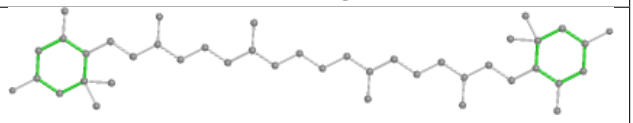
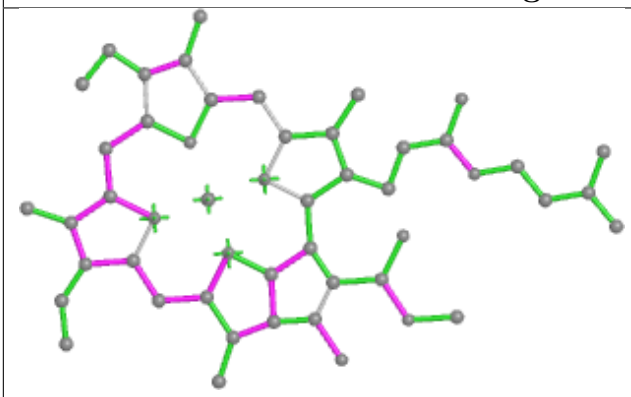


Rings

Ligand CLA G 203



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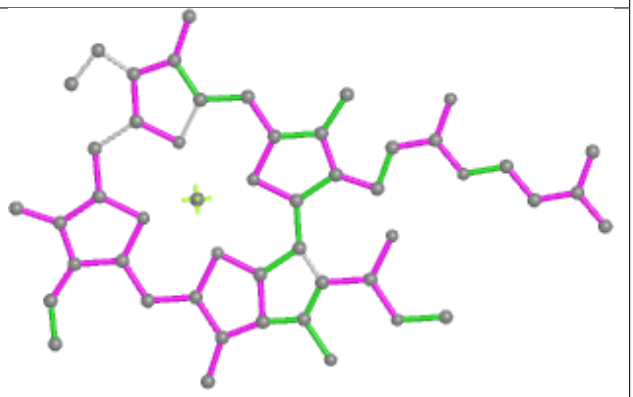
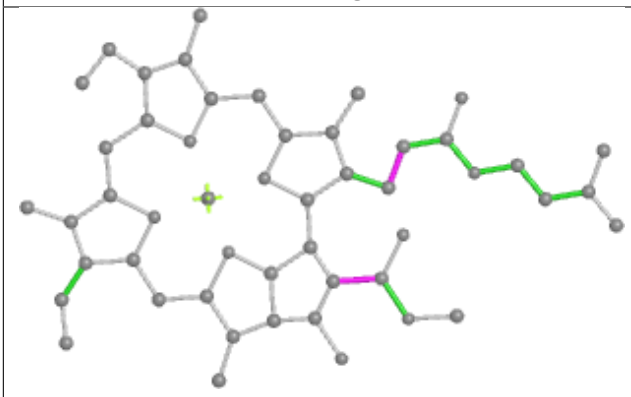


Bond angles



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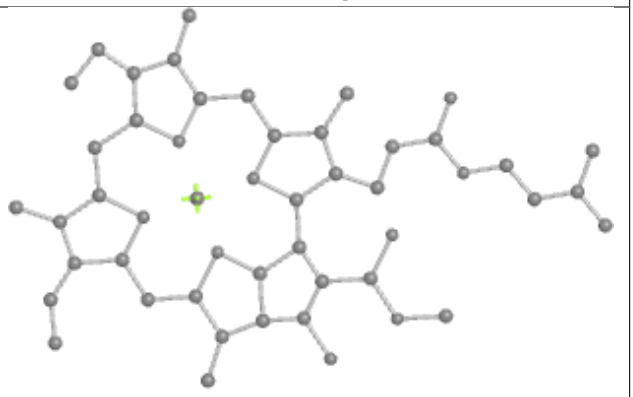
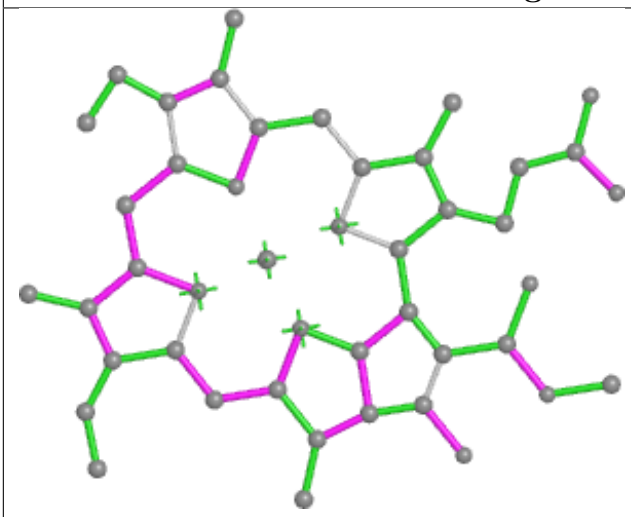
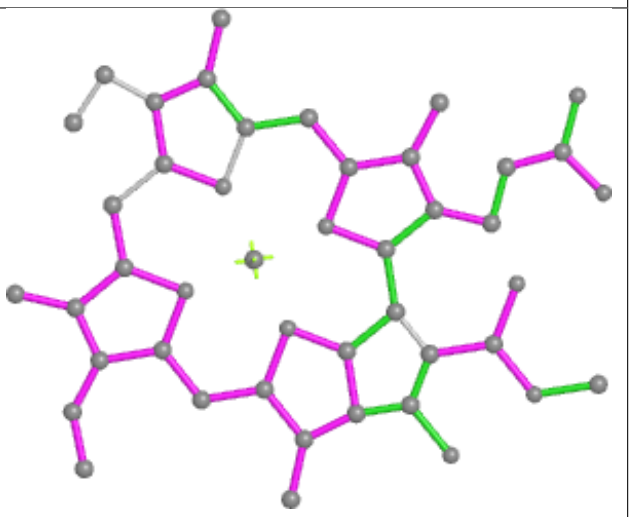


Rings

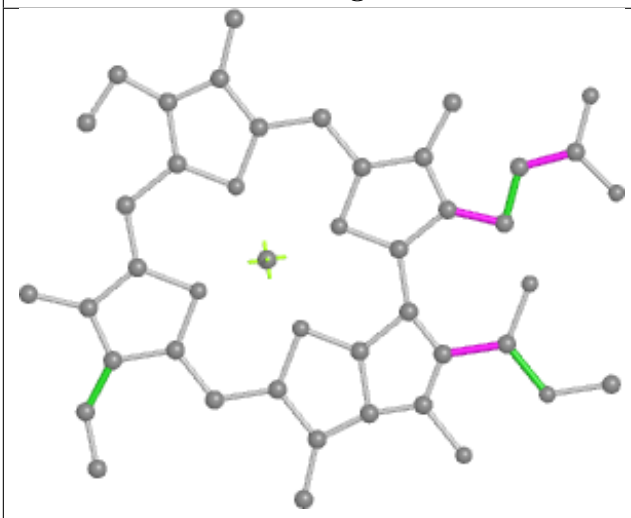
Ligand CLA B 804



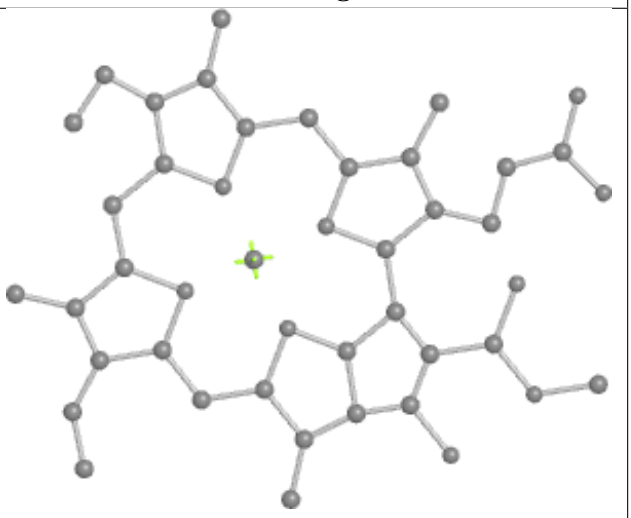
Bond lengths



Bond angles

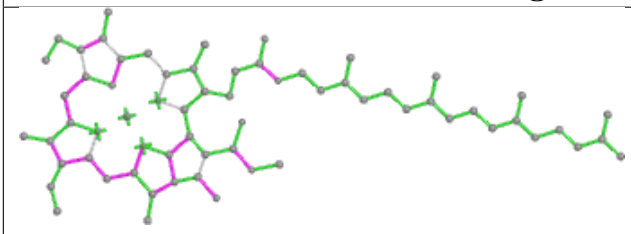


Torsions

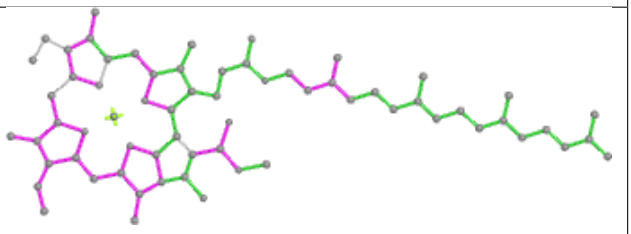


Rings

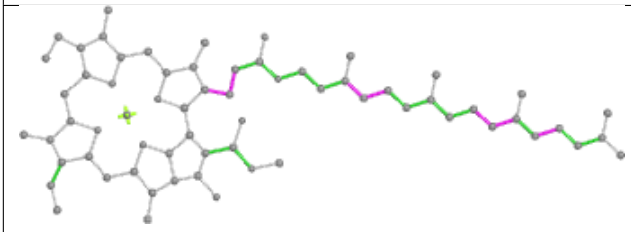
Ligand CLA 3 604



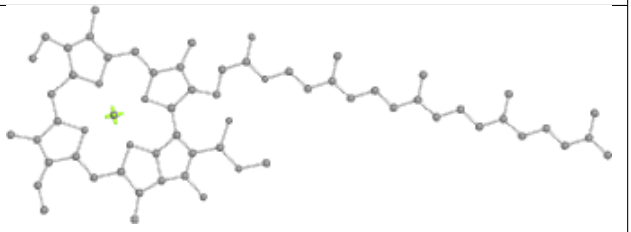
Bond lengths



Bond angles

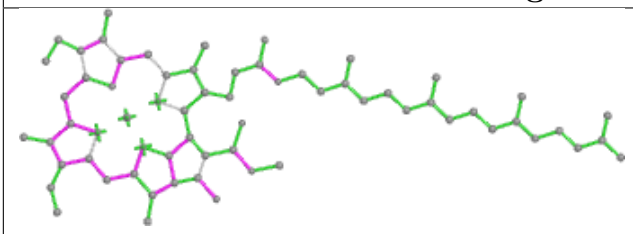


Torsions

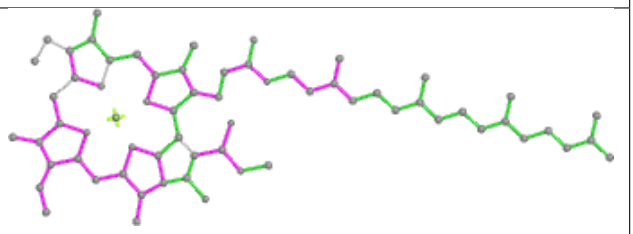


Rings

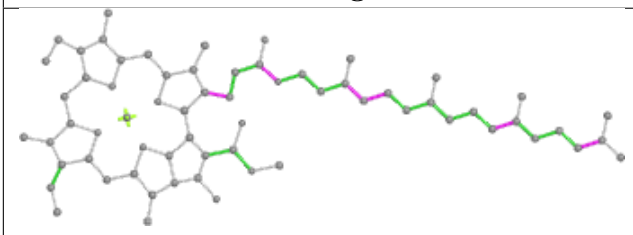
Ligand CLA L 203



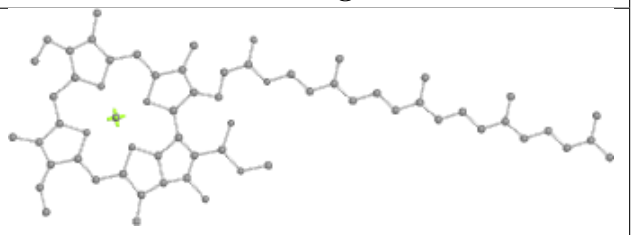
Bond lengths



Bond angles

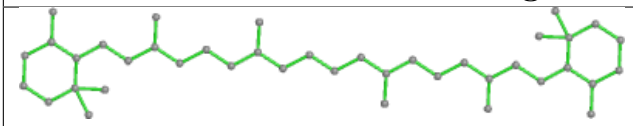


Torsions

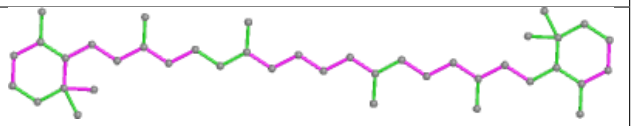


Rings

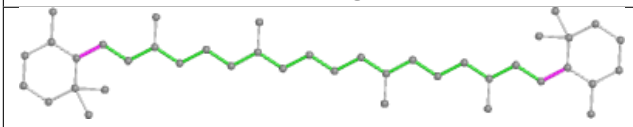
Ligand BCR A 850



Bond lengths



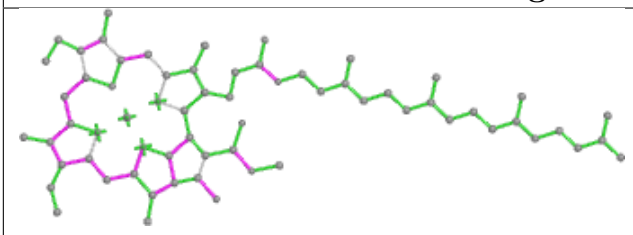
Bond angles



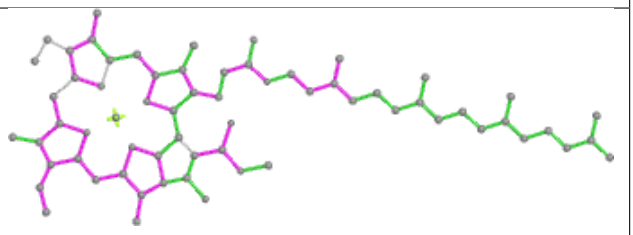
Torsions

Rings

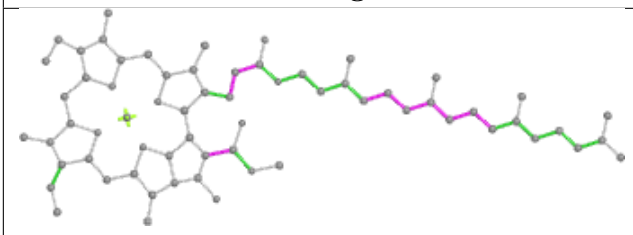
Ligand CLA 6 601



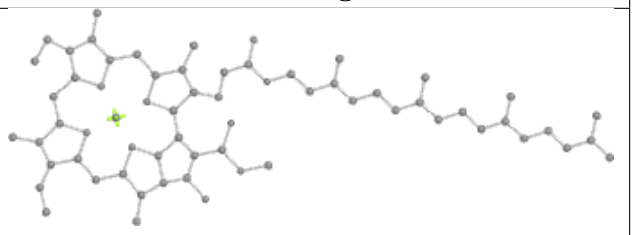
Bond lengths



Bond angles

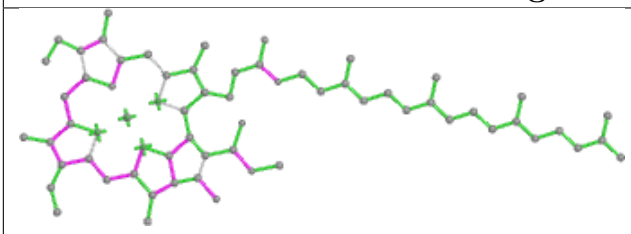


Torsions

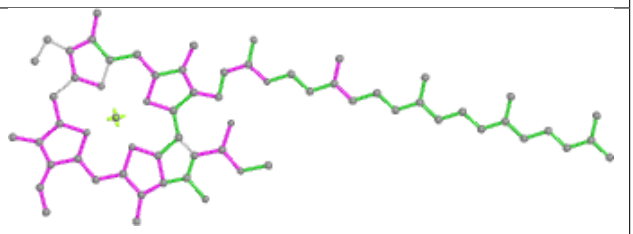


Rings

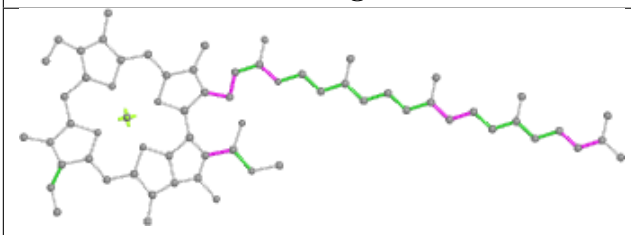
Ligand CLA 7 602



Bond lengths



Bond angles



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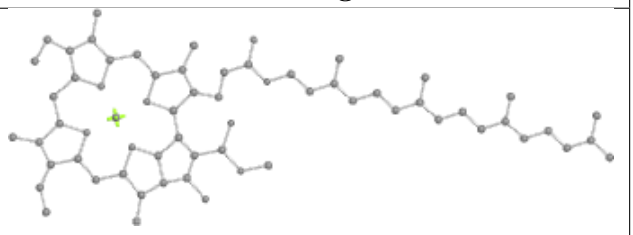
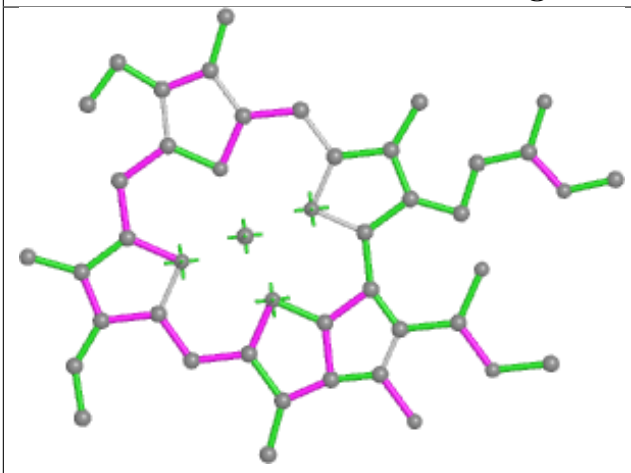


Rings

Ligand CLA 6 616



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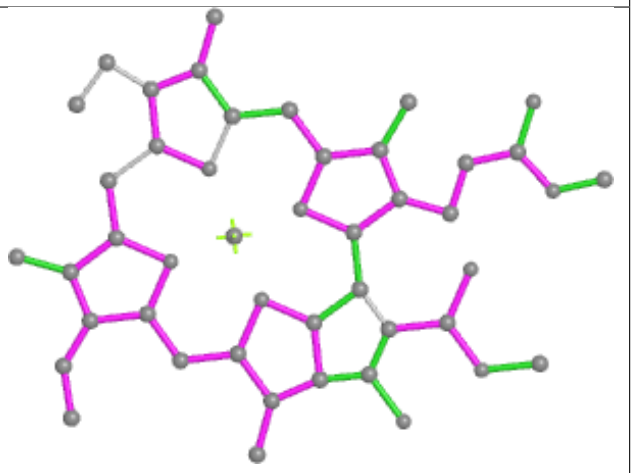
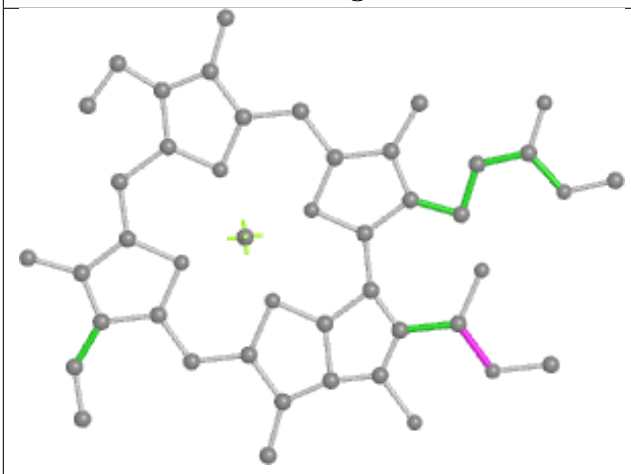
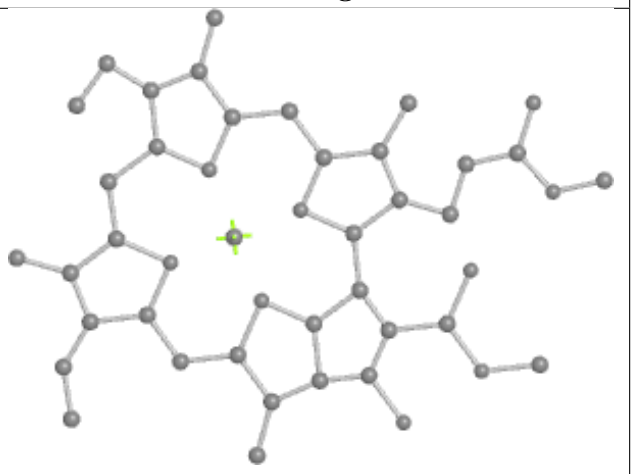


Bond angles

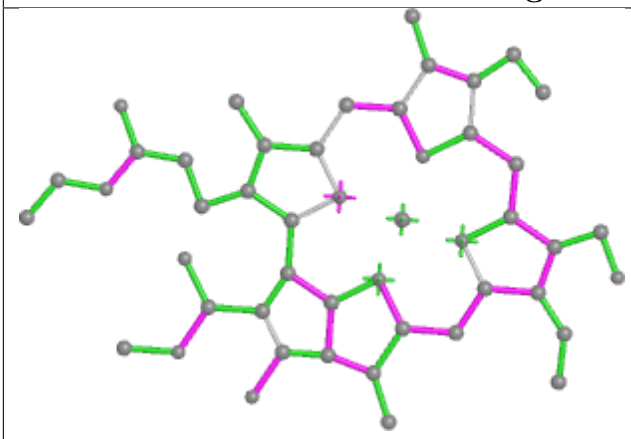


Torsions



Rings

Ligand CHL Z 607



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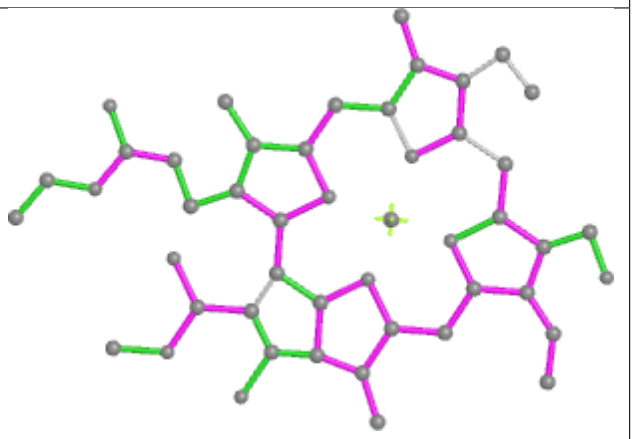
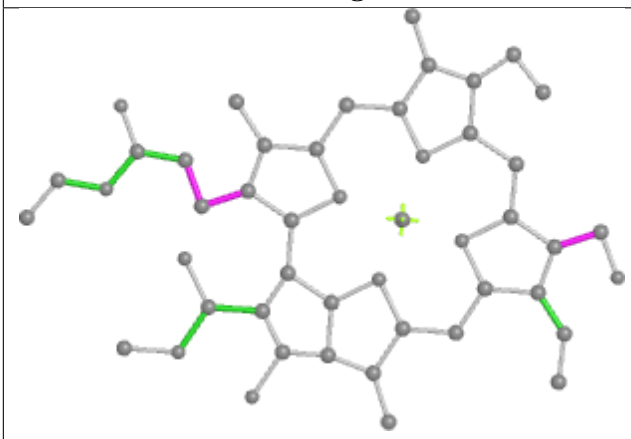
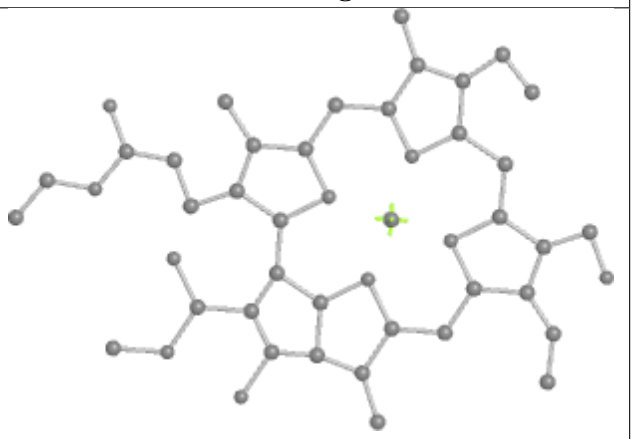


Bond angles

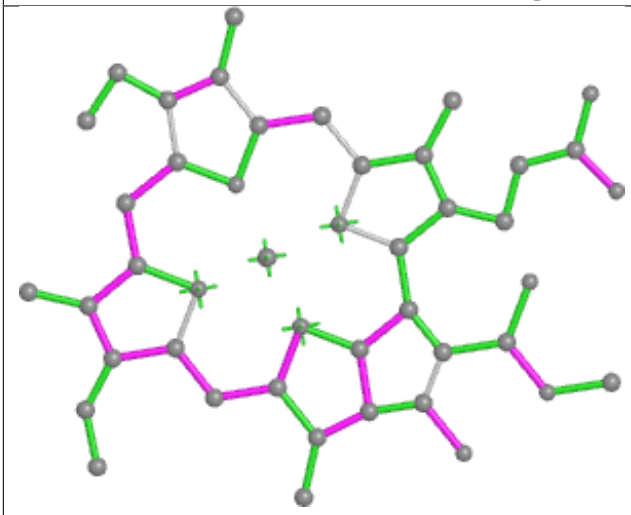


Torsions

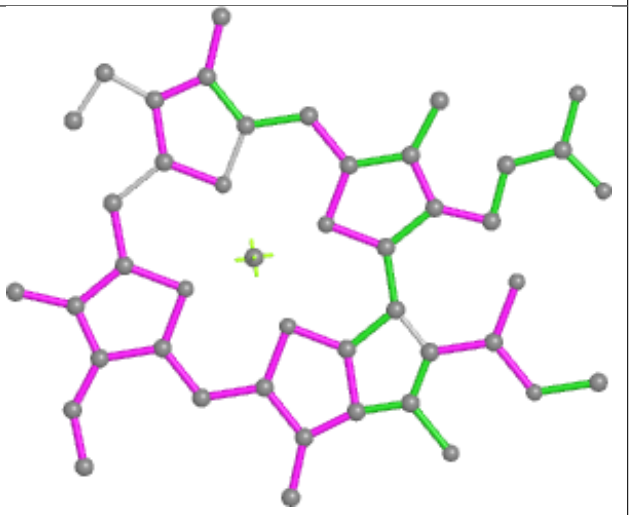


Rings

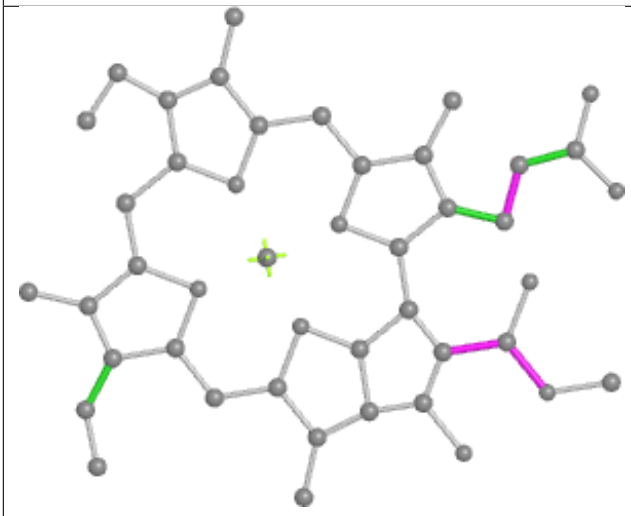
Ligand CLA 2 602



Bond lengths



Bond angles



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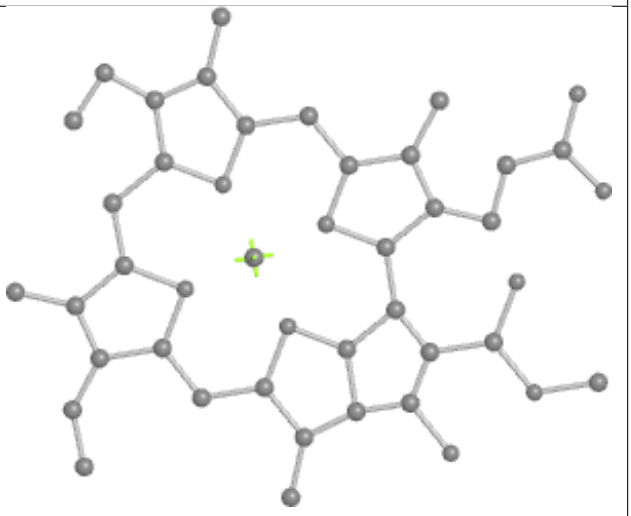
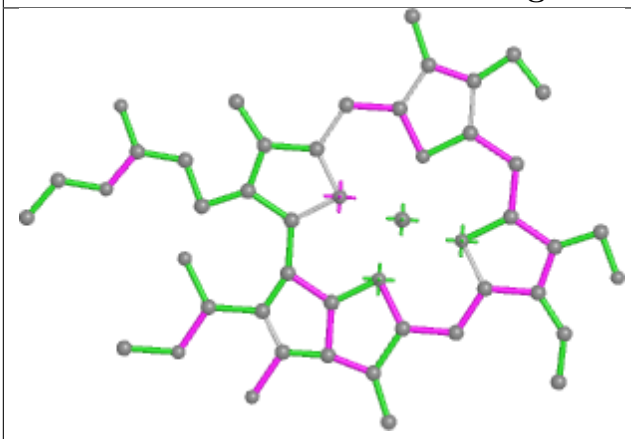


Rings

Ligand CHL 1 607



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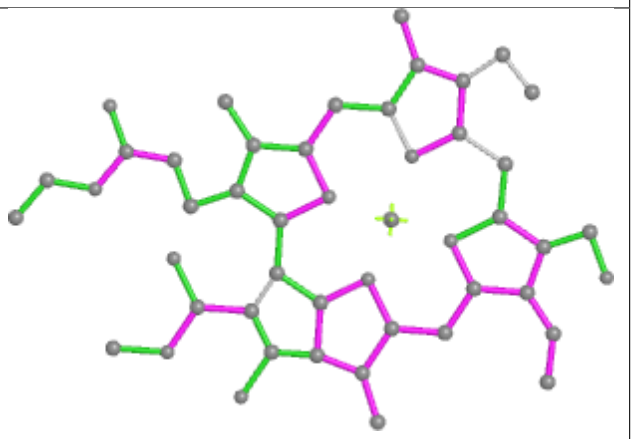

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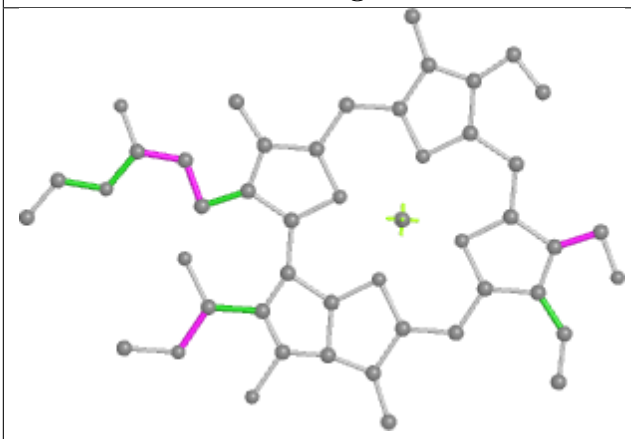

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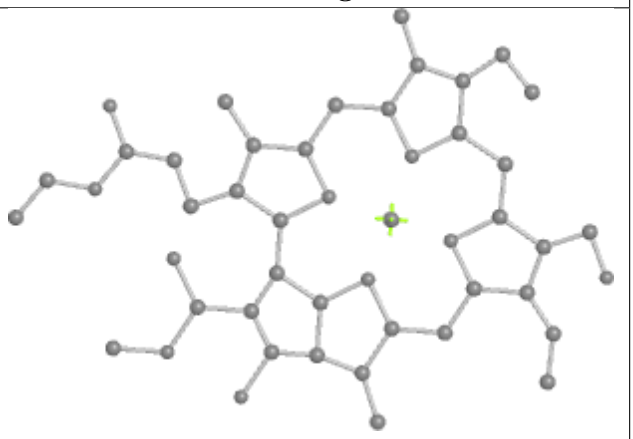

Rings

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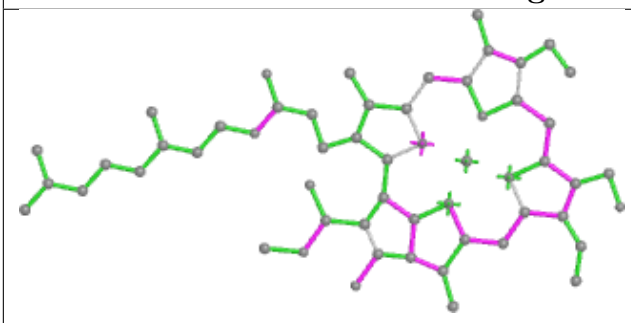

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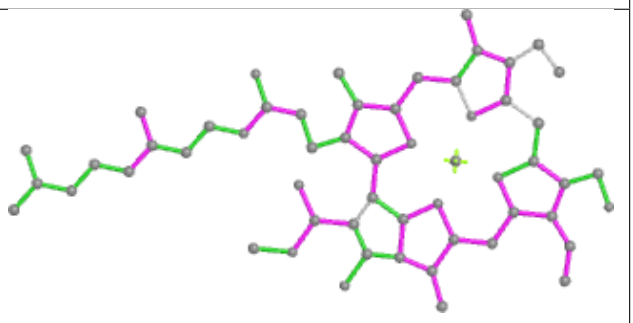
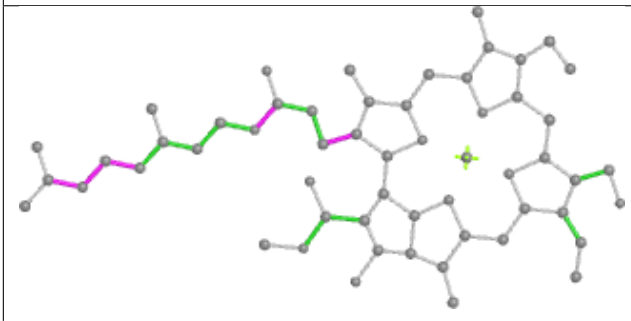


Bond angles



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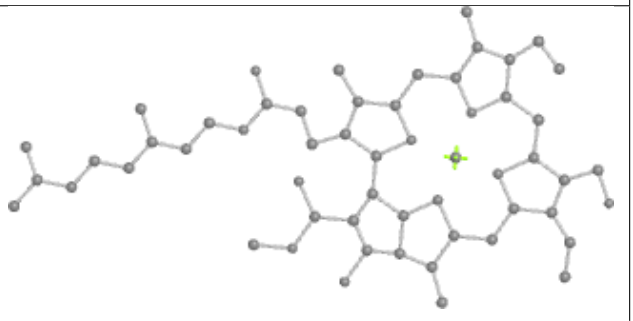
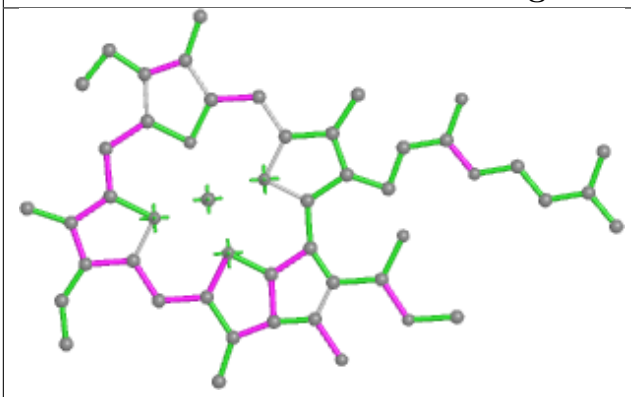
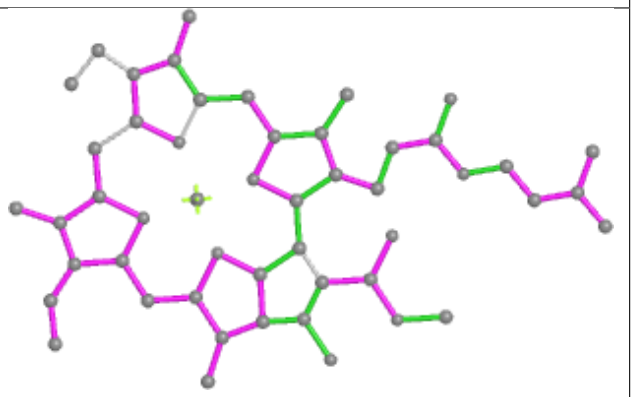


Rings

Ligand CLA 2 607



Bond lengths



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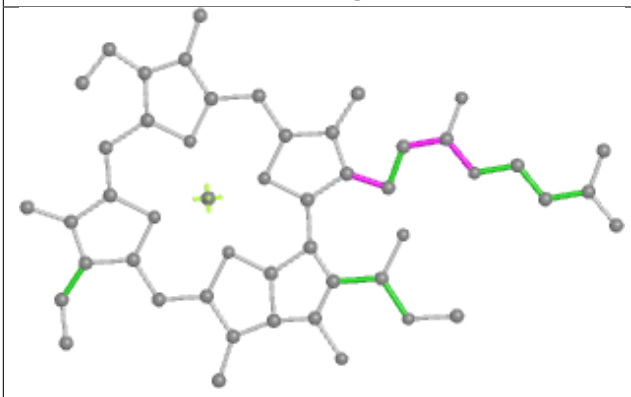

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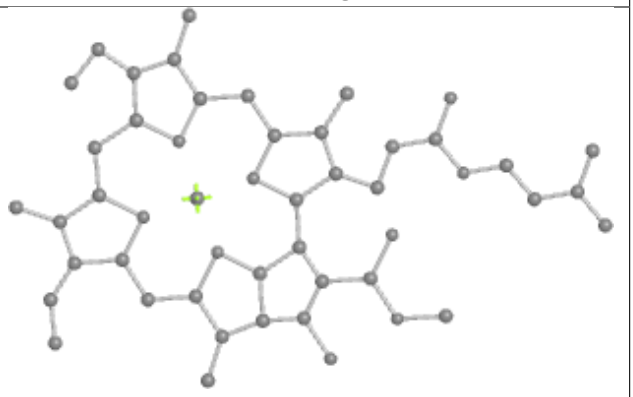
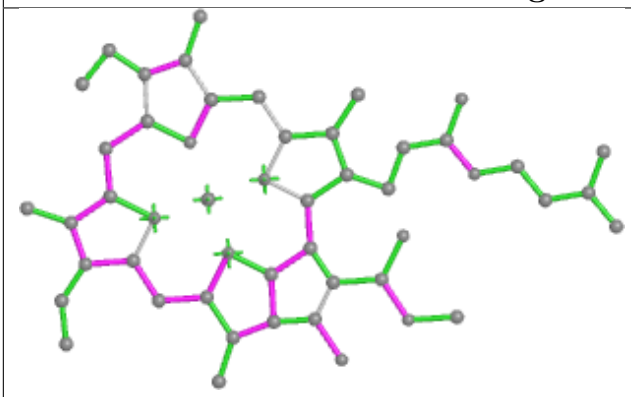
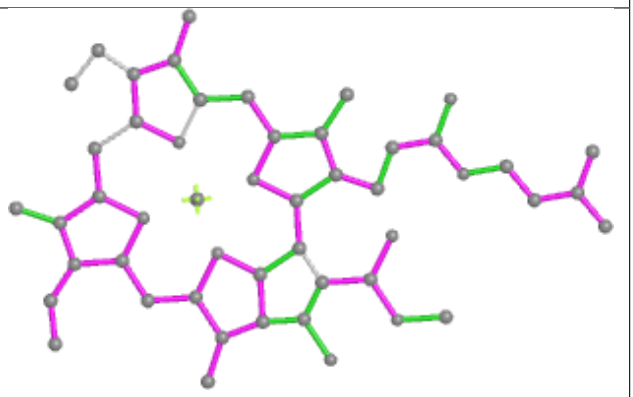


Rings

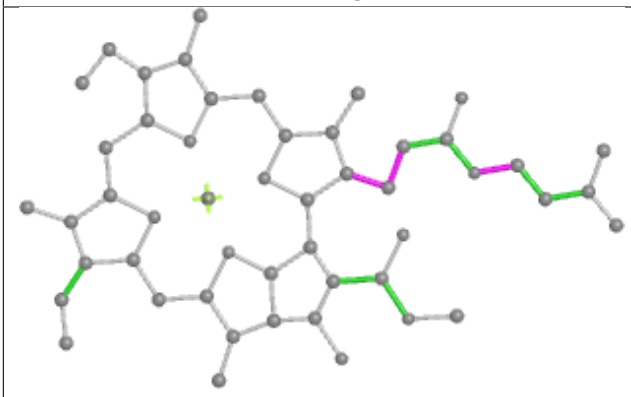
Ligand CLA 5 609



Bond lengths



Bond angles



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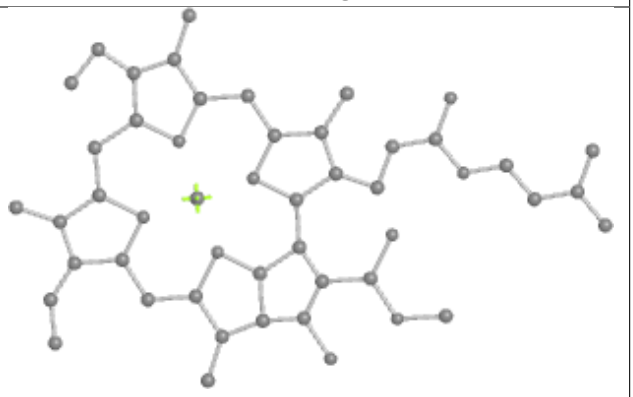
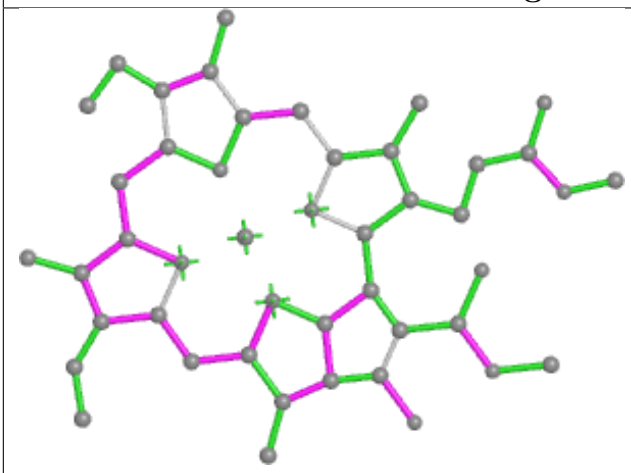
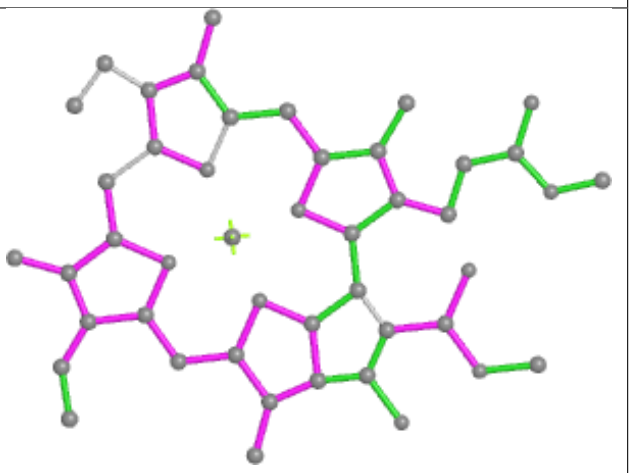


Rings

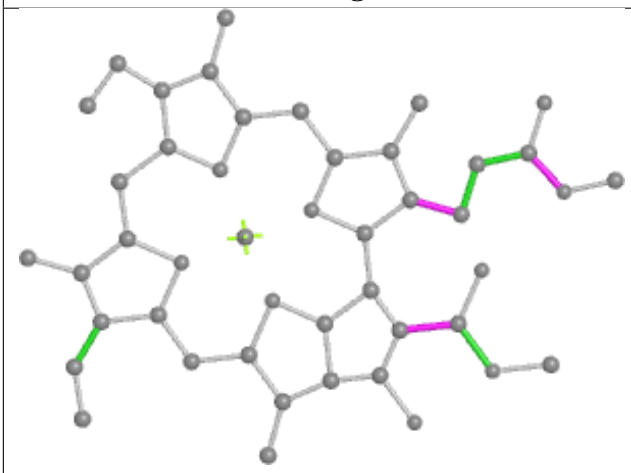
Ligand CLA B 821



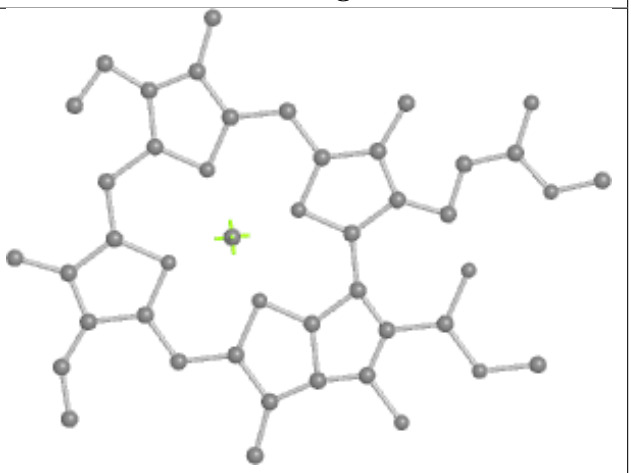
Bond lengths



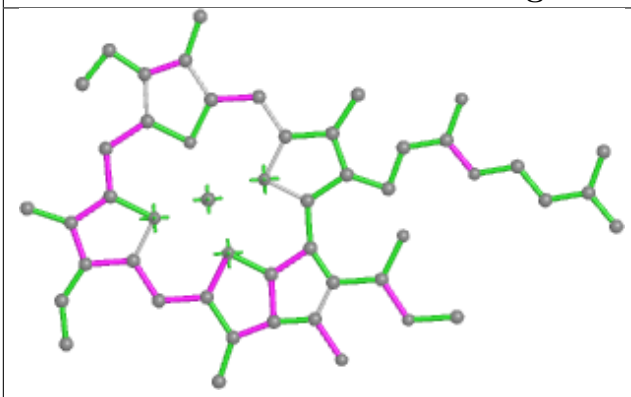
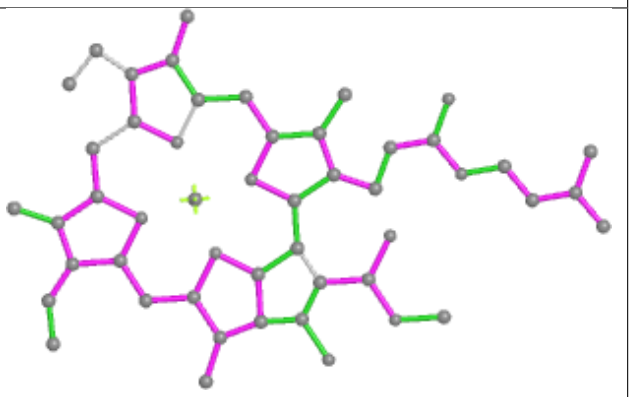
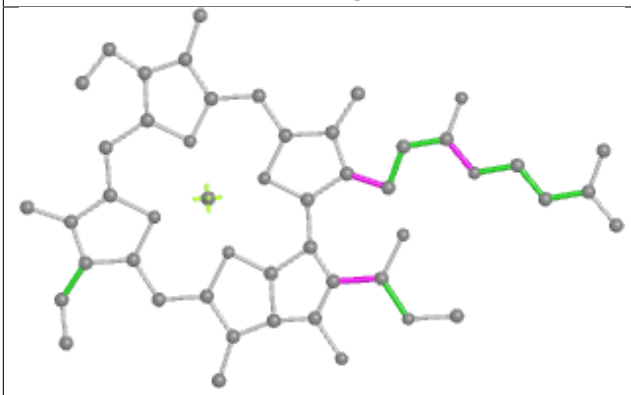
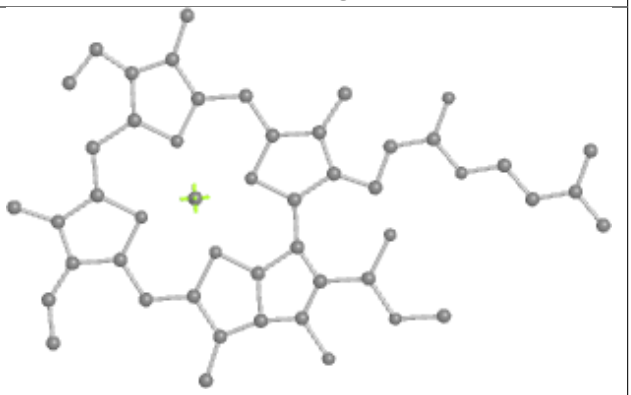
Bond angles

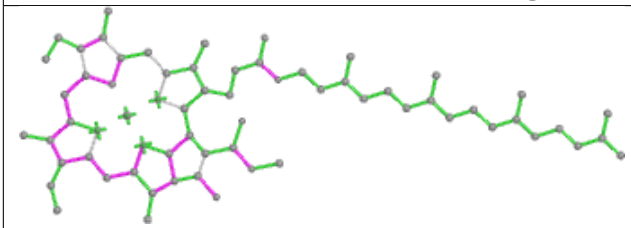
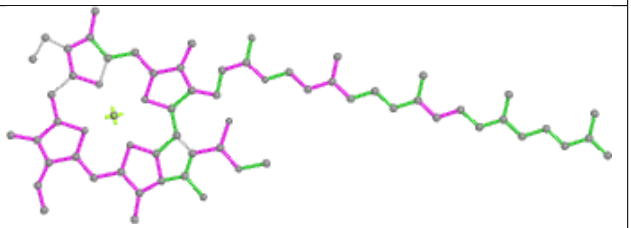
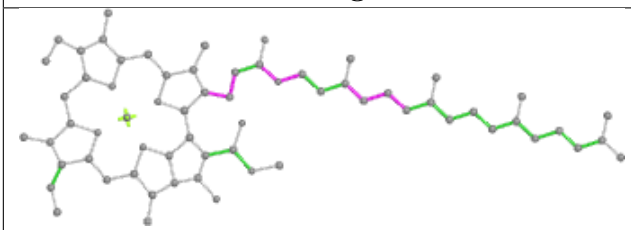
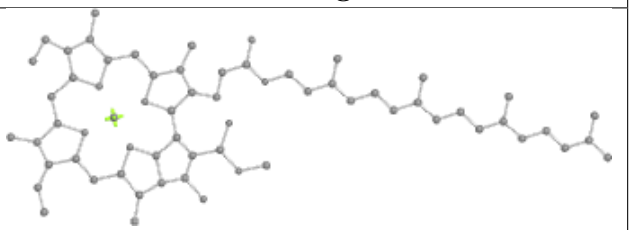


Torsions

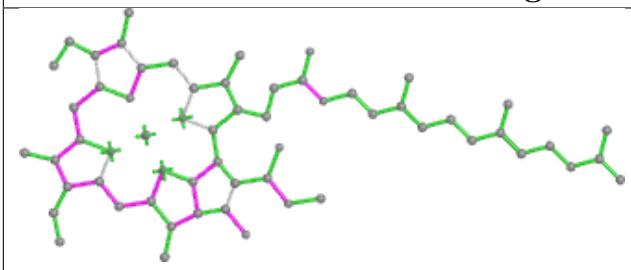


Rings

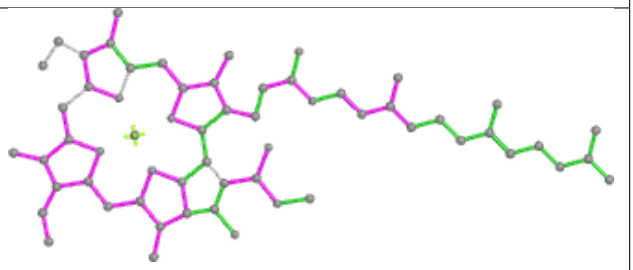
Ligand CLA L 204	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 834	
 Bond lengths	 Bond angles
 Torsions	 Rings

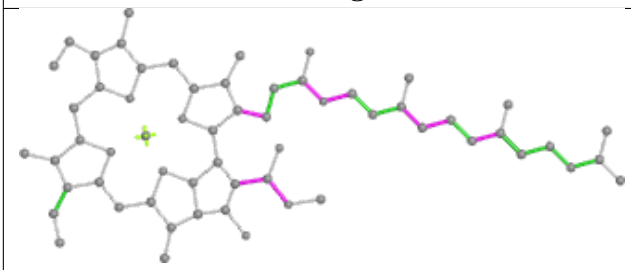
Ligand CLA B 814



Bond lengths



Bond angles



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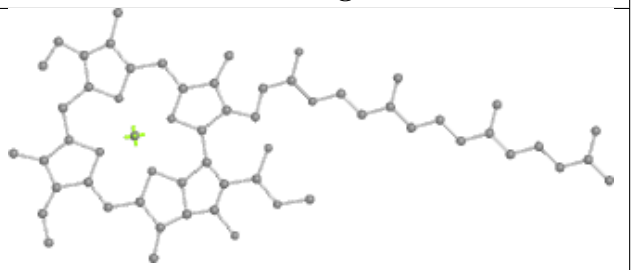
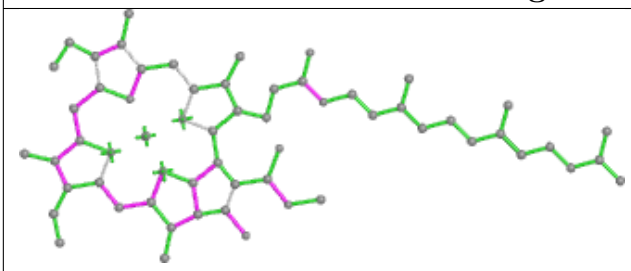
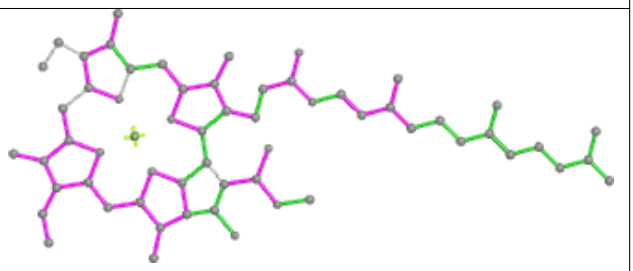


Rings

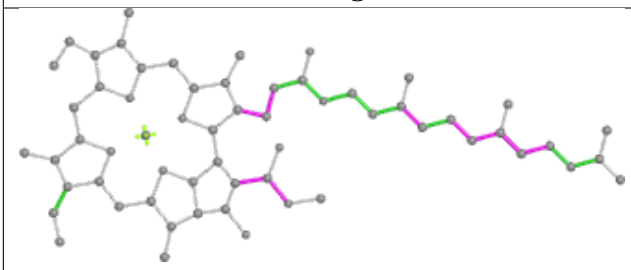
Ligand CLA 1 610



Bond lengths



Bond angles



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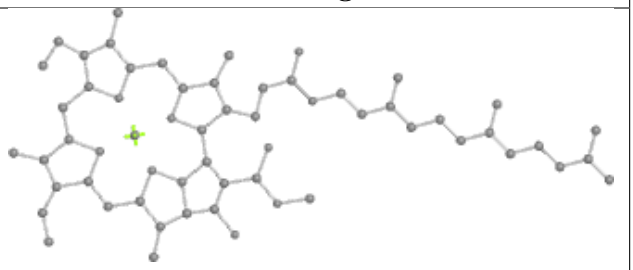
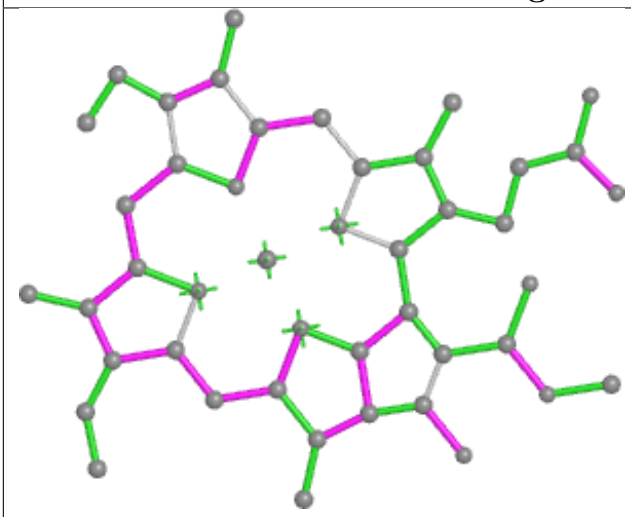
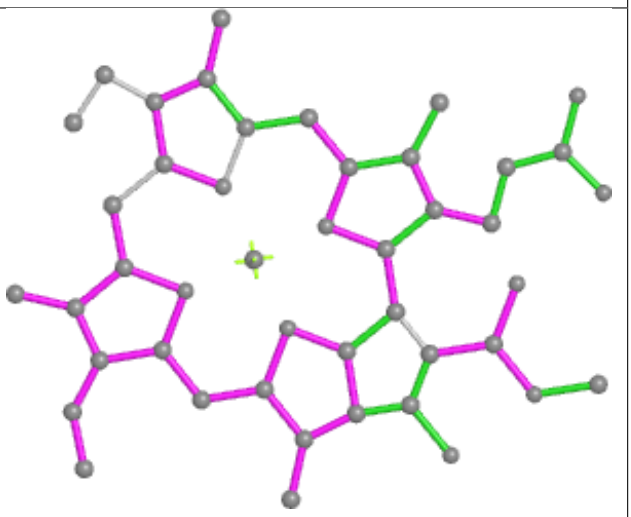


Rings

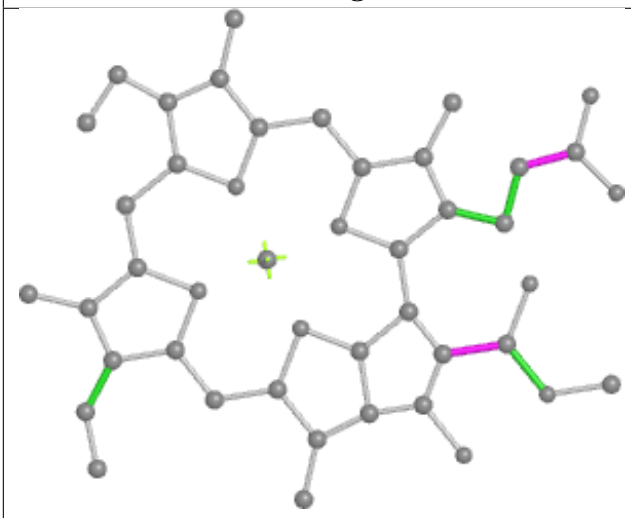
Ligand CLA 6 622



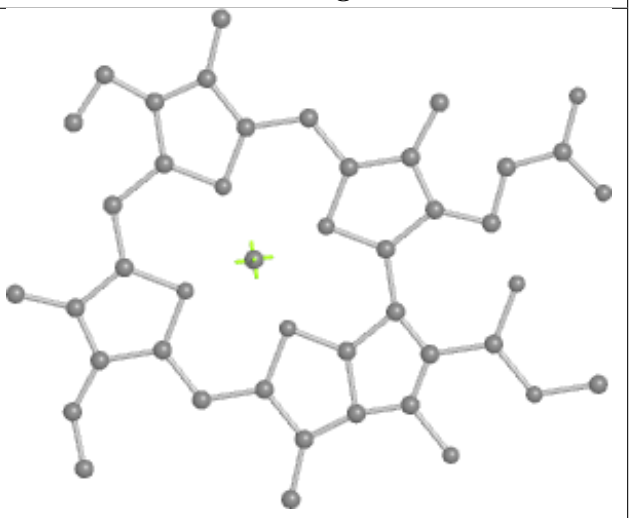
Bond lengths



Bond angles

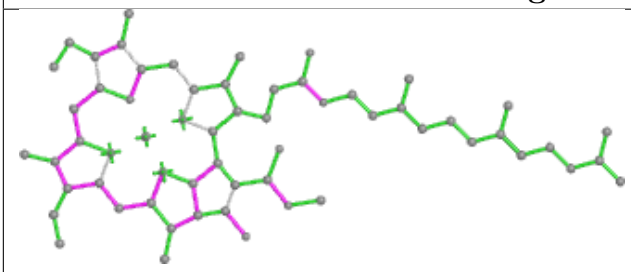


Torsions

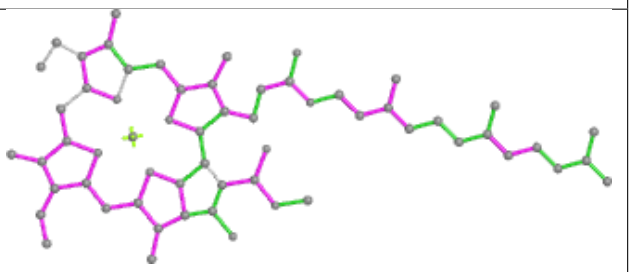


Rings

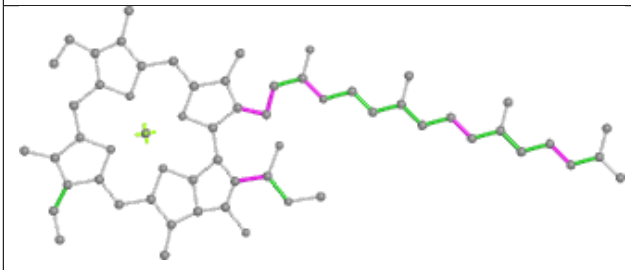
Ligand CLA 5 610



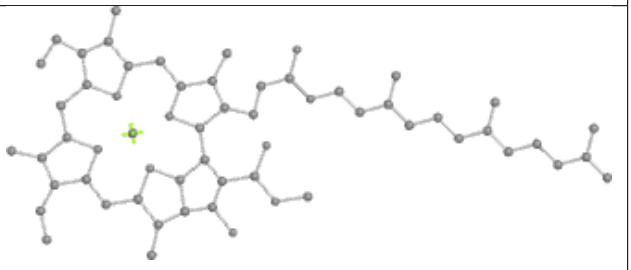
Bond lengths



Bond angles

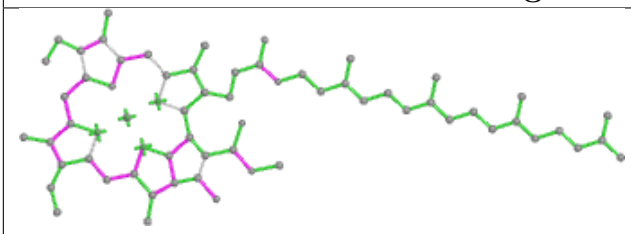


Torsions

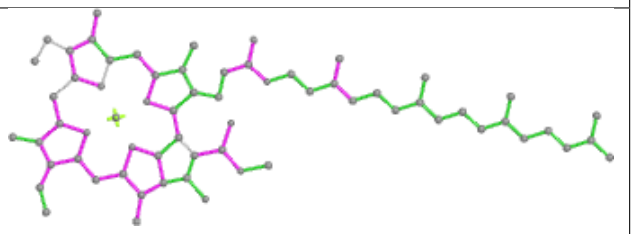


Rings

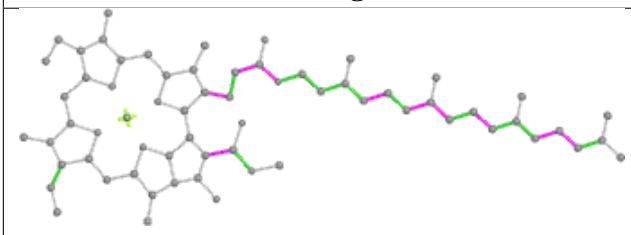
Ligand CLA B 805



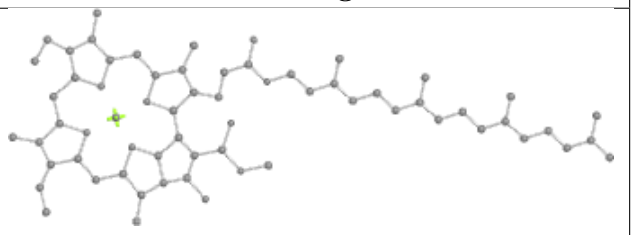
Bond lengths



Bond angles

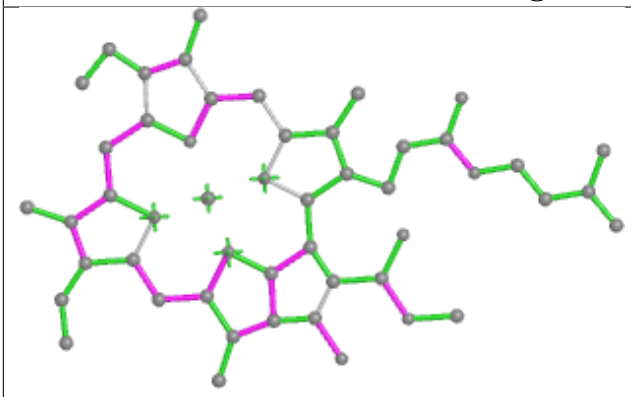


Torsions

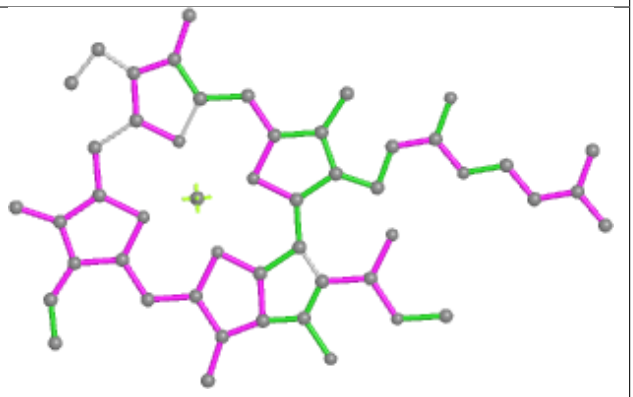


Rings

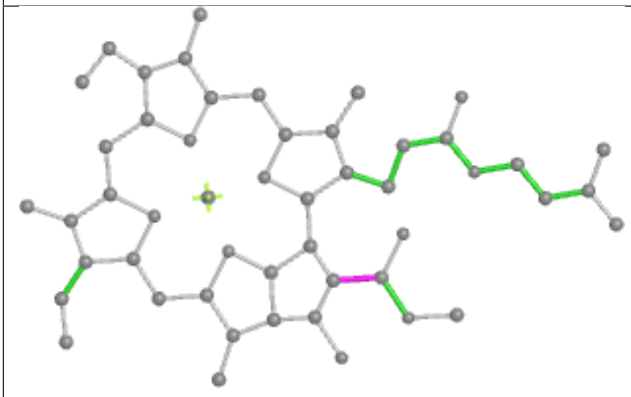
Ligand CLA 8 608



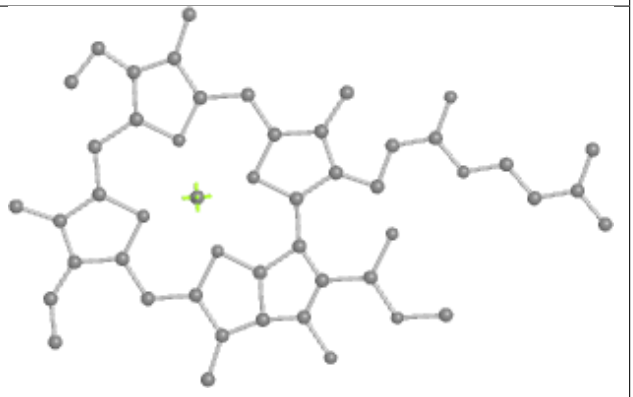
Bond lengths



Bond angles

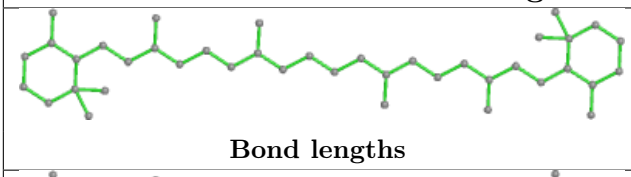


Torsions

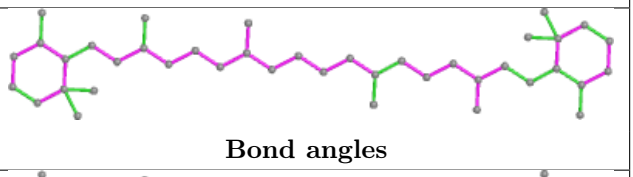


Rings

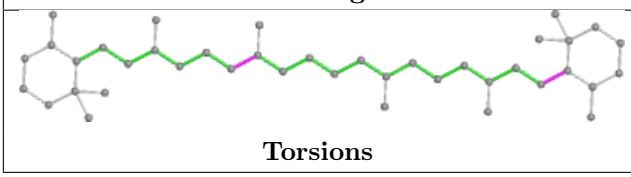
Ligand BCR 3 718



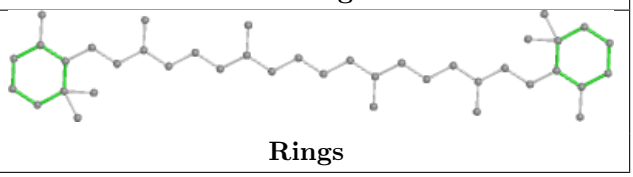
Bond lengths



Bond angles

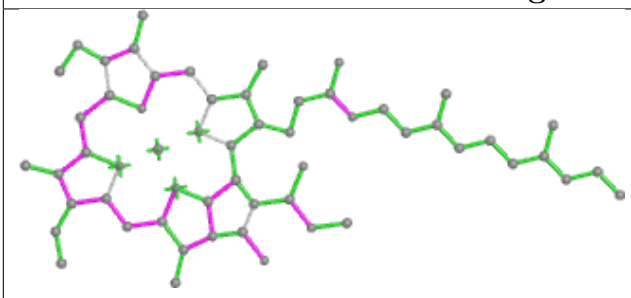


Torsions

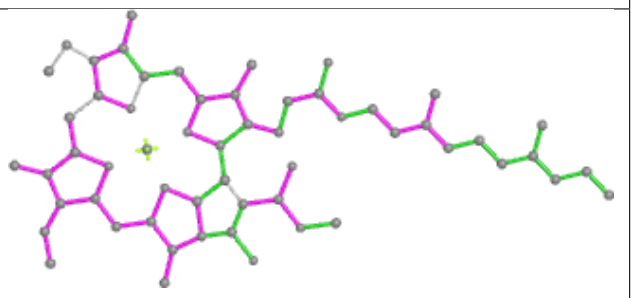


Rings

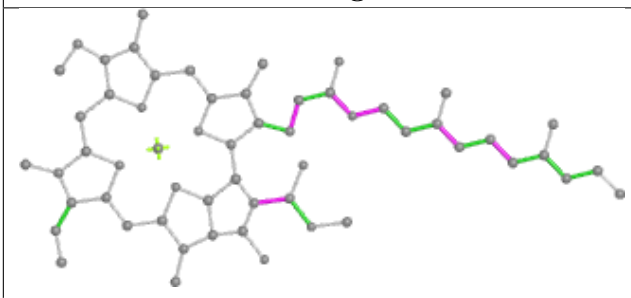
Ligand CLA 1 604



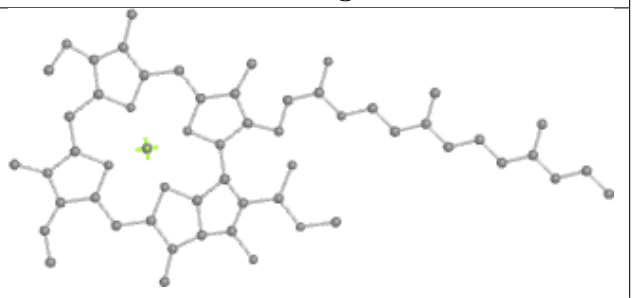
Bond lengths



Bond angles



Torsions



Rings

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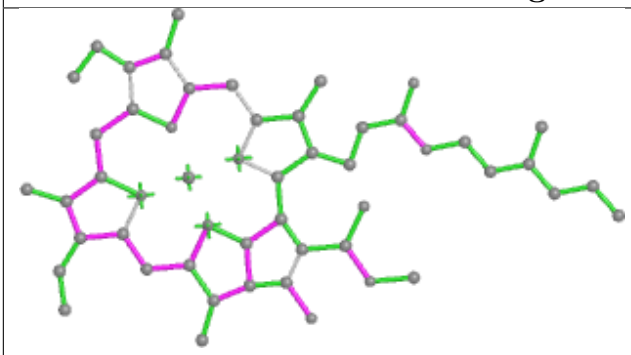
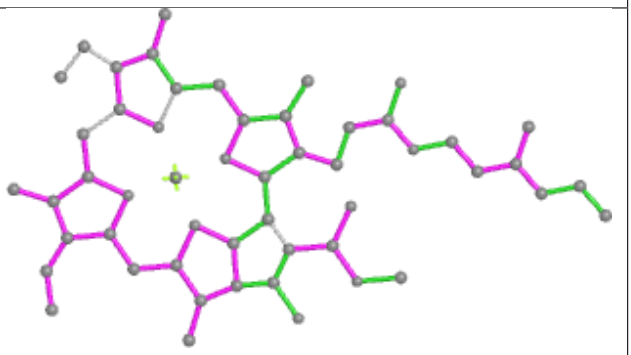
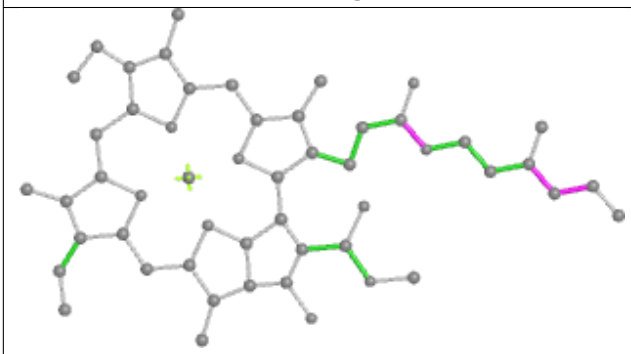


Bond lengths



Bond angles



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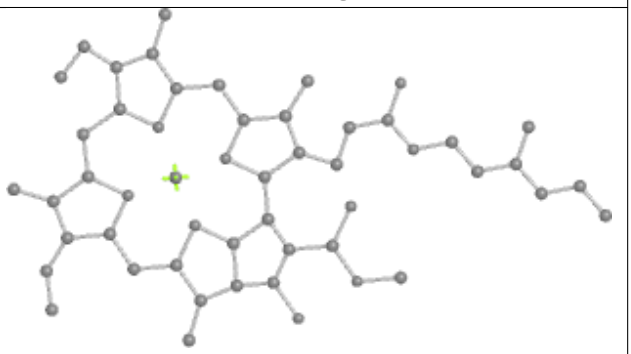
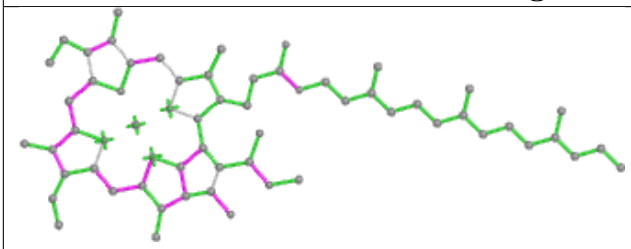
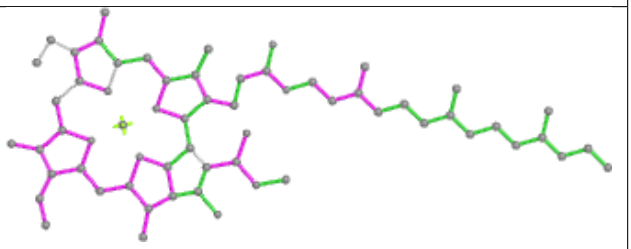


Rings

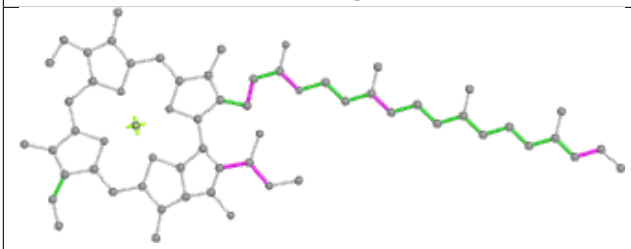
Ligand CLA 8 602



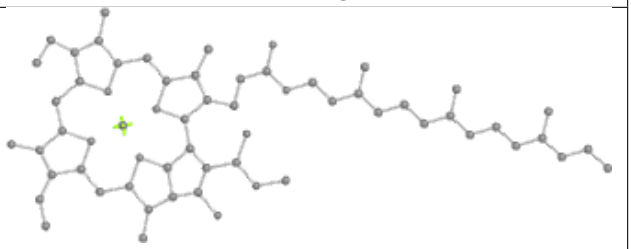
Bond lengths



Bond angles

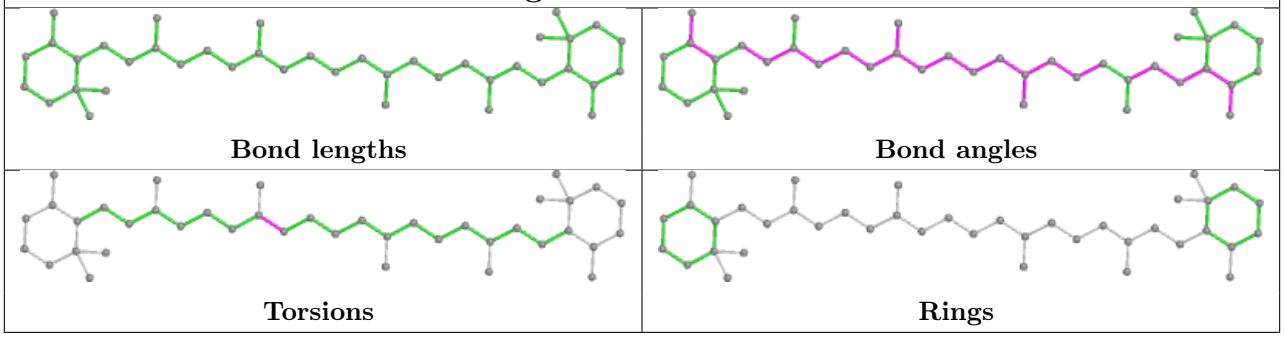


Torsions

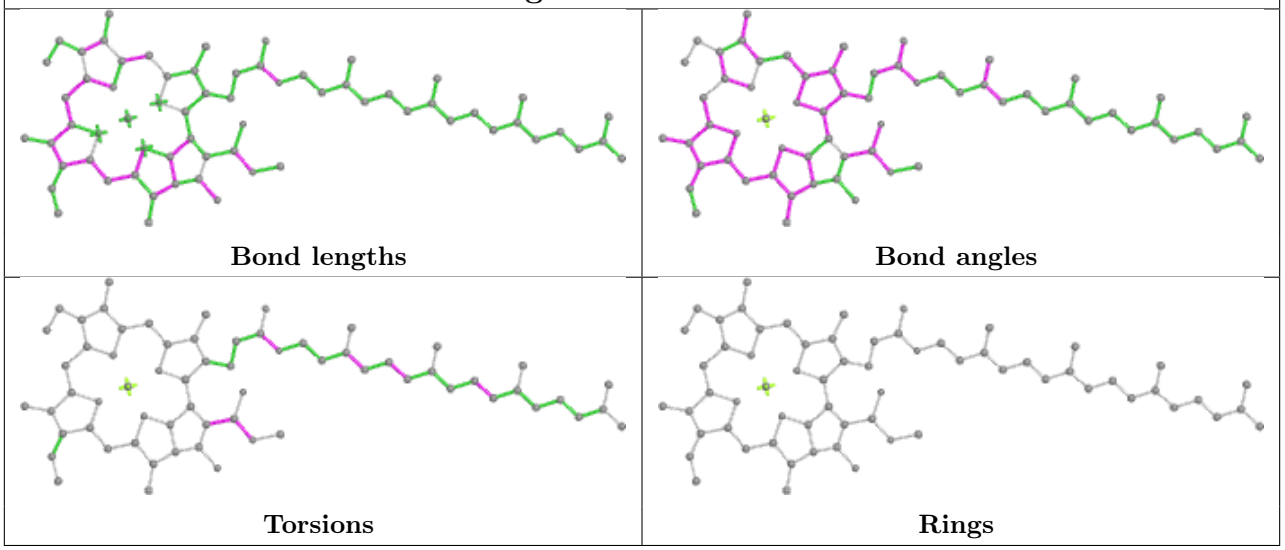


Rings

Ligand BCR F 305



Ligand CLA B 829



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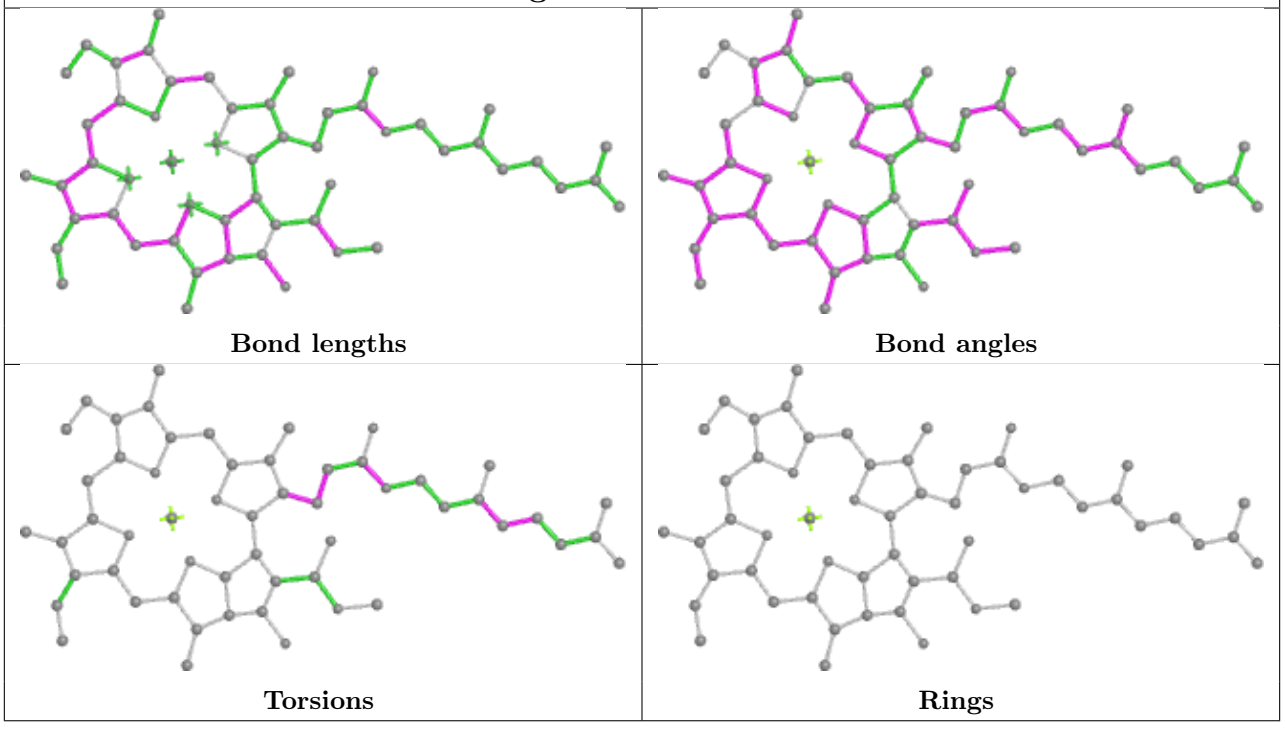

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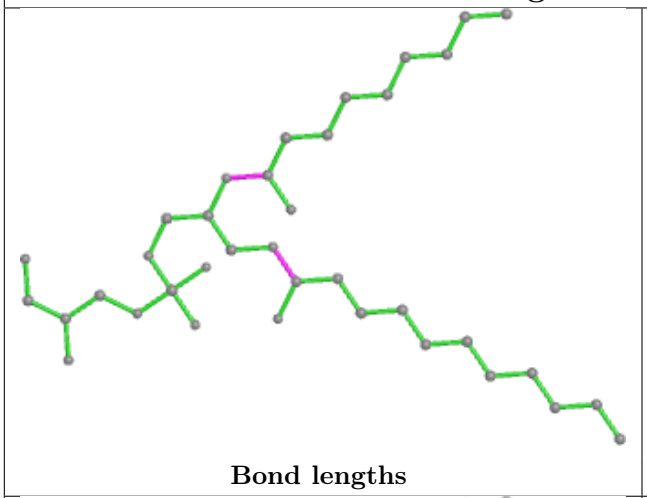
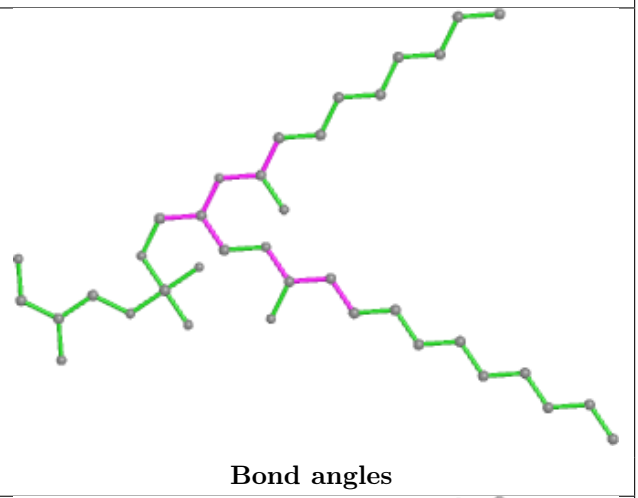
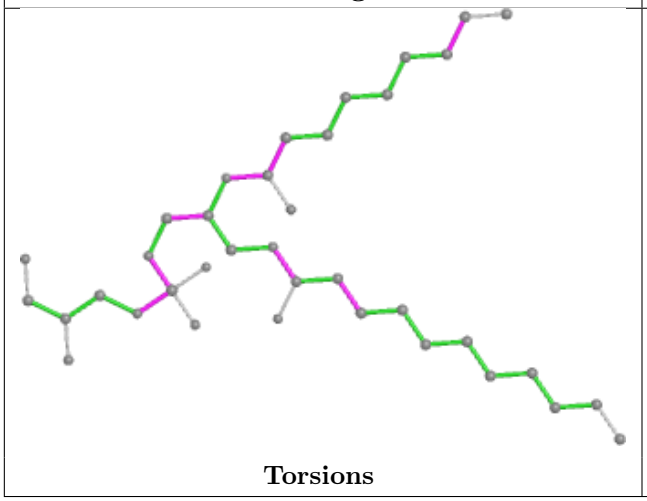


Bond lengths



Bond angles



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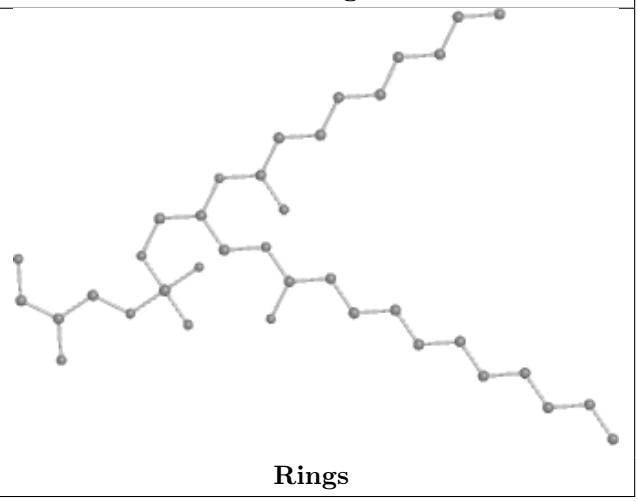
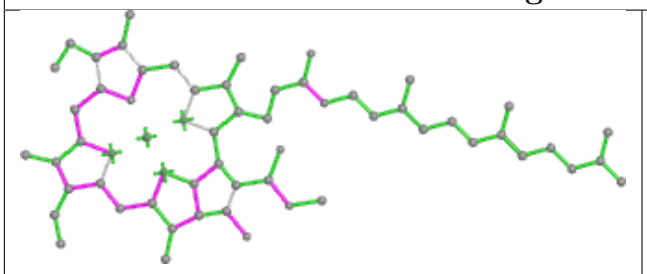
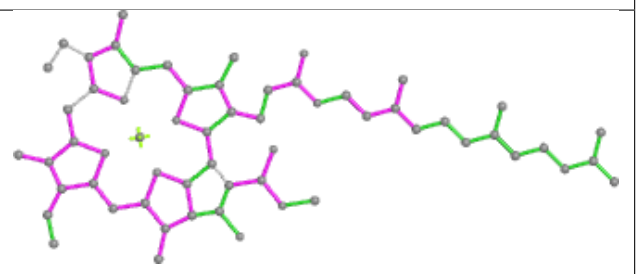


Rings

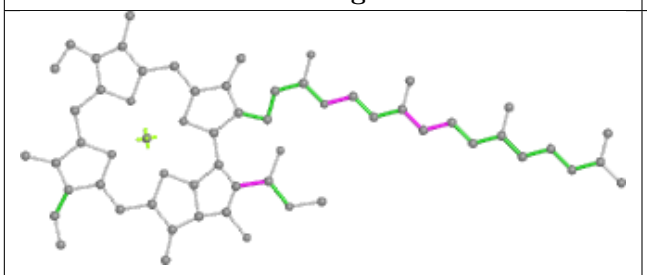
Ligand CLA B 836



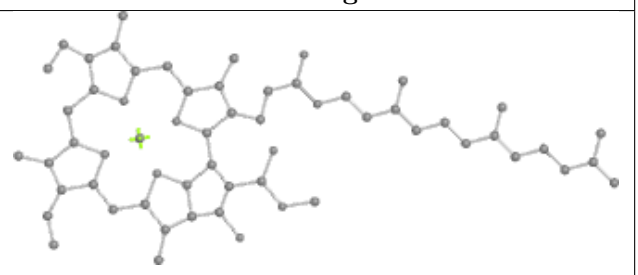
Bond lengths



Bond angles

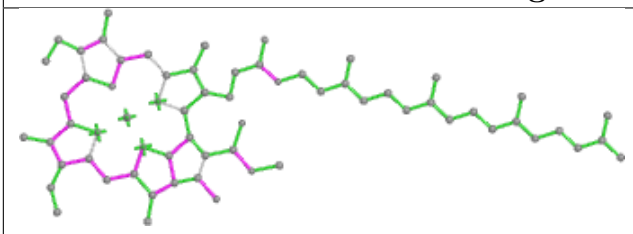


Torsions

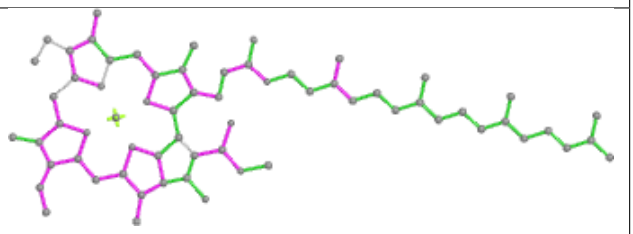


Rings

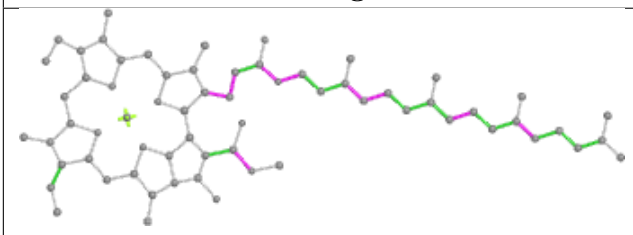
Ligand CLA 1 614



Bond lengths



Bond angles



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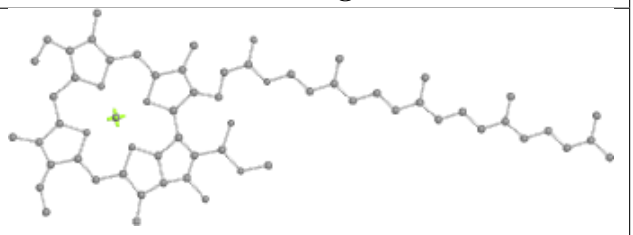
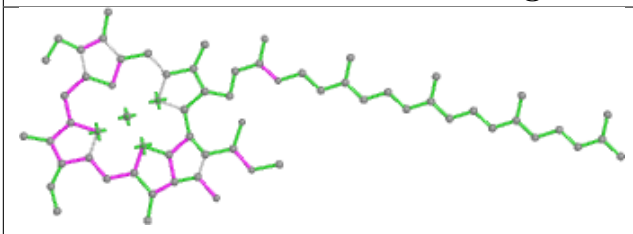
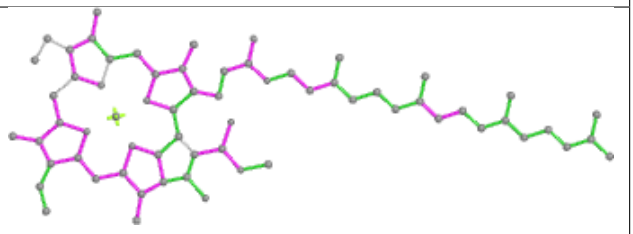


Rings

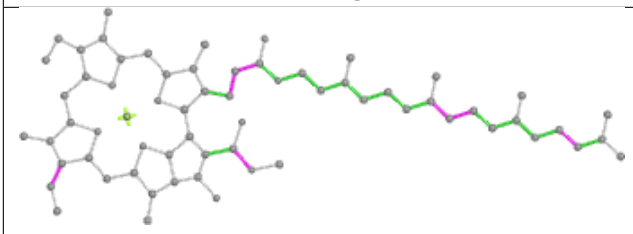
Ligand CLA A 841



Bond lengths



Bond angles



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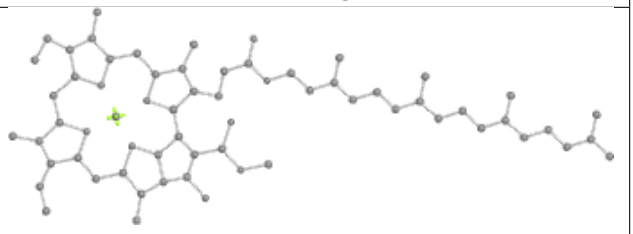
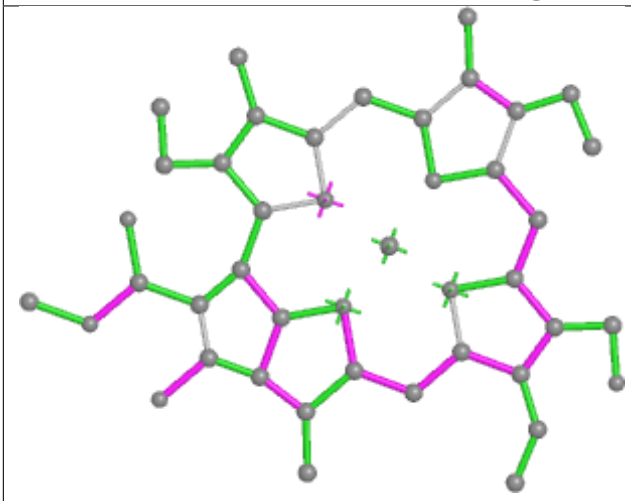


Rings

Ligand CHL 6 618



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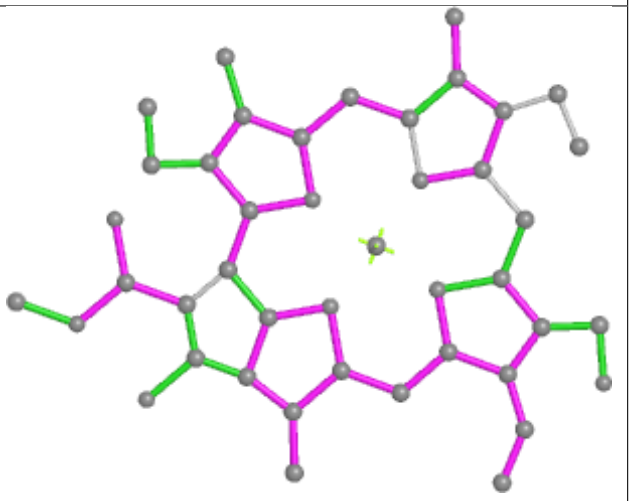
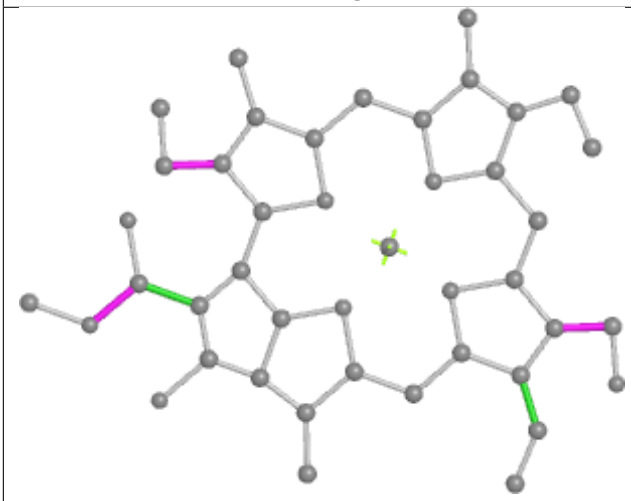
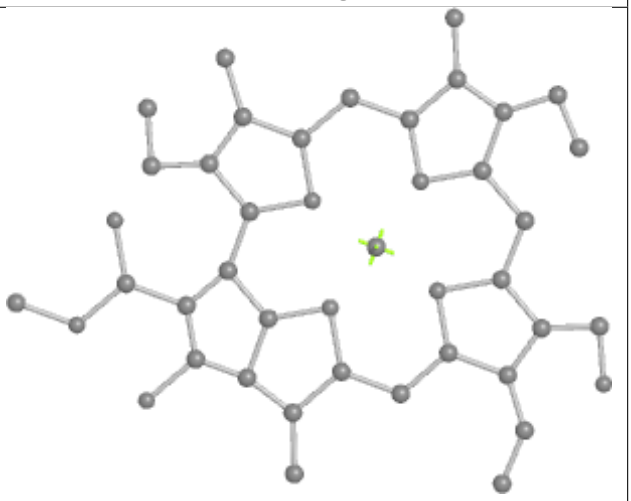


Bond angles

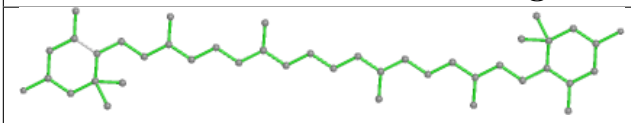


Torsions

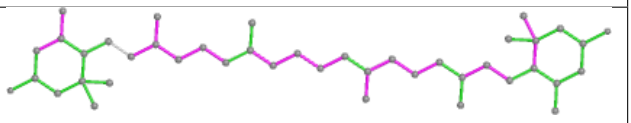


Rings

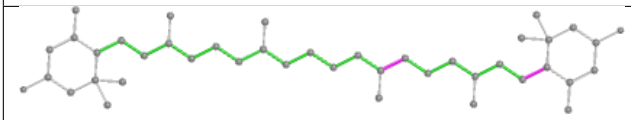
Ligand LUT 7 621



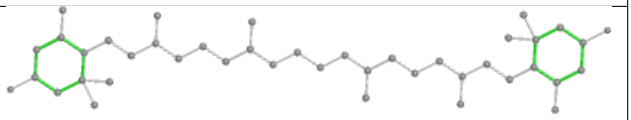
Bond lengths



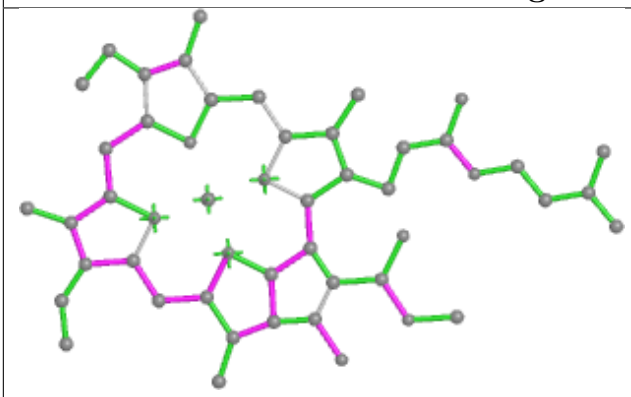
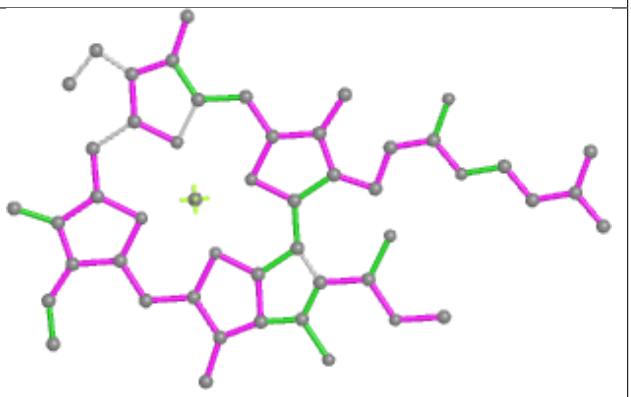
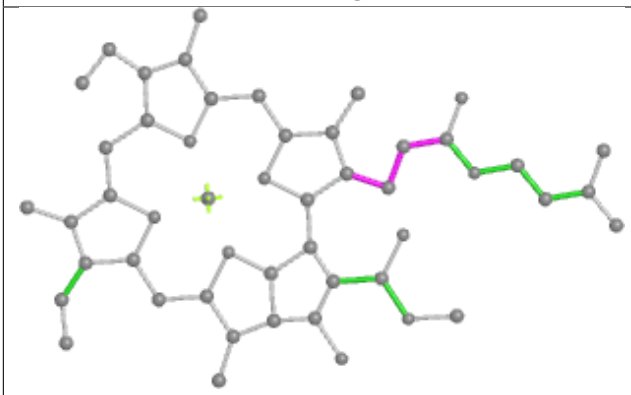
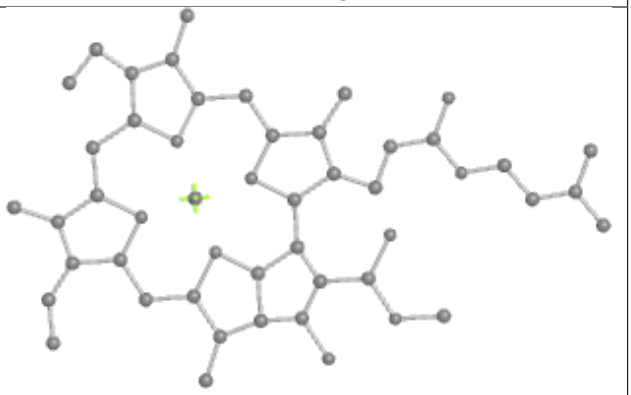
Bond angles

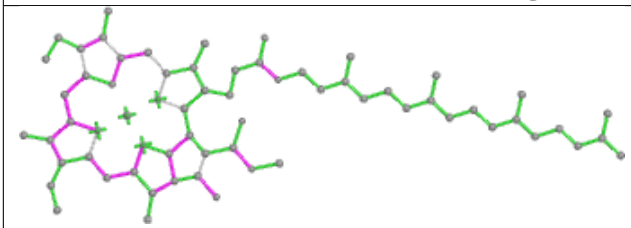
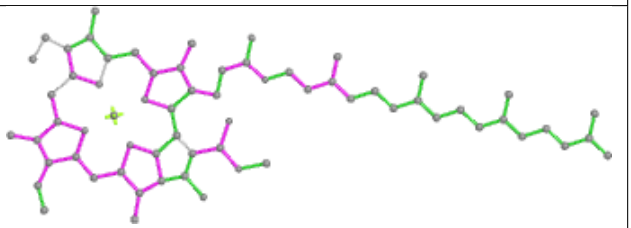
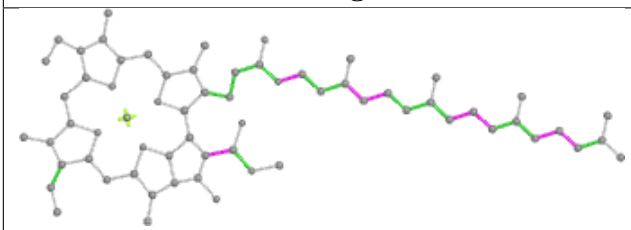
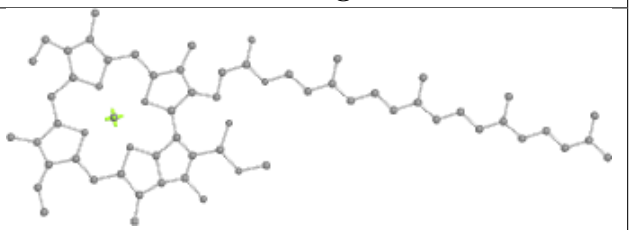


Torsions

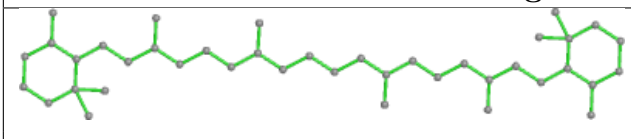


Rings

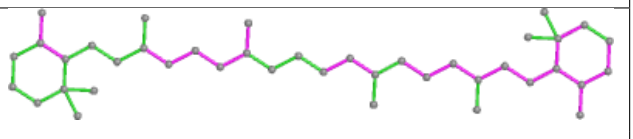
Ligand CLA 7 609	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 802	
 Bond lengths	 Bond angles
 Torsions	 Rings

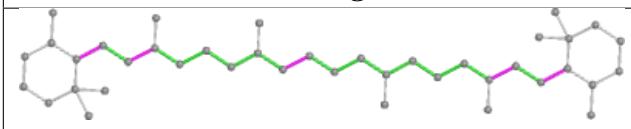
Ligand BCR L 205



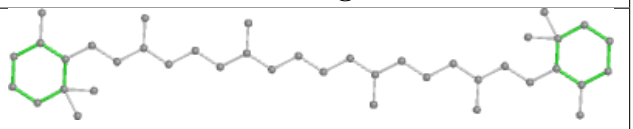
Bond lengths



Bond angles

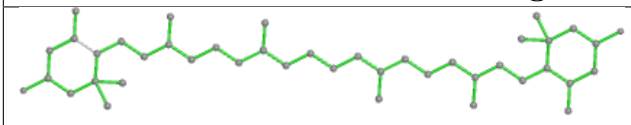


Torsions



Rings

Ligand LUT 3 622



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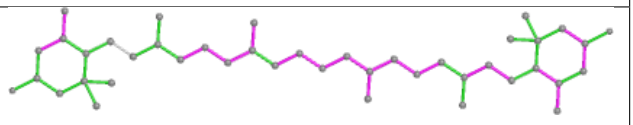
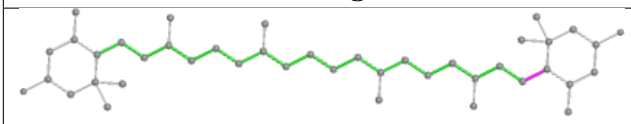


Bond angles



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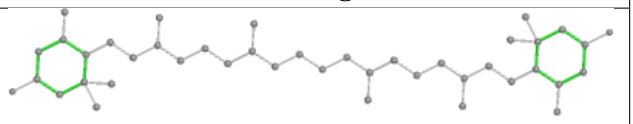
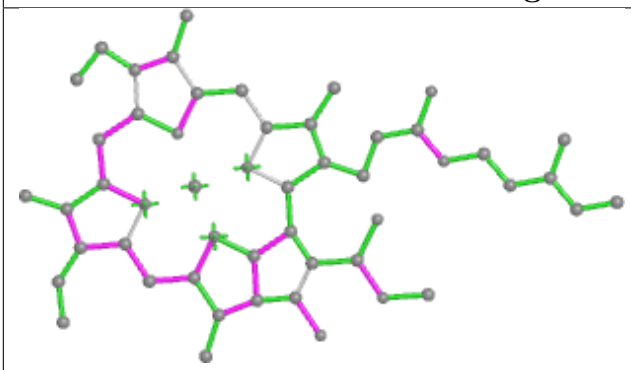


Rings

Ligand CLA A 838



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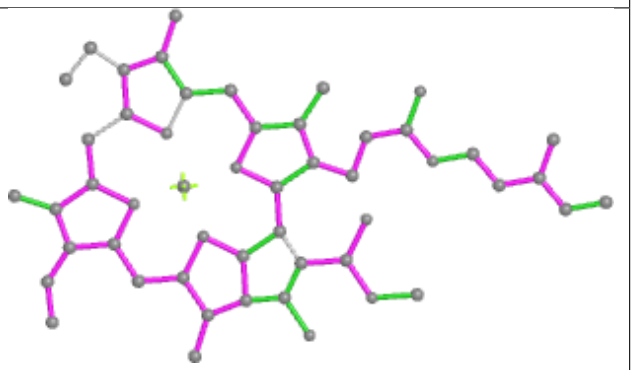

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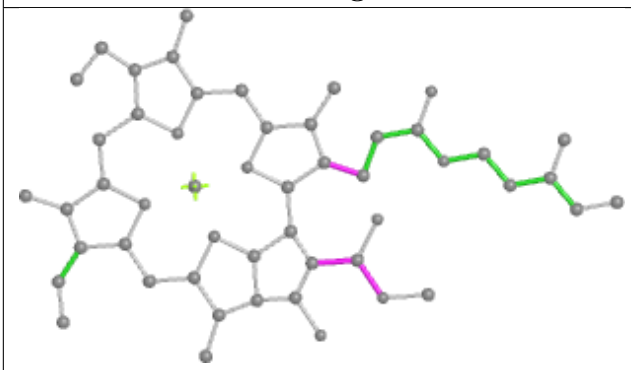

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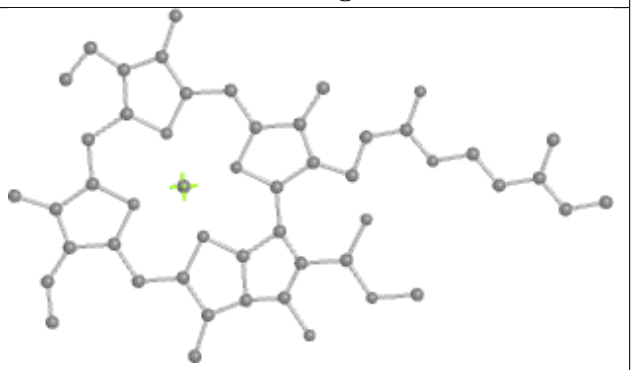
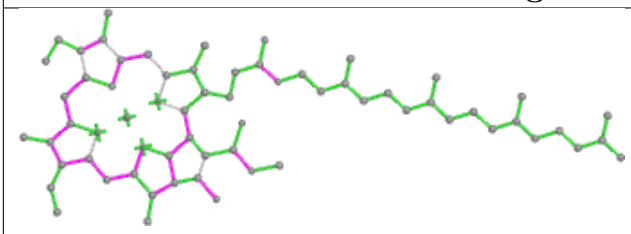
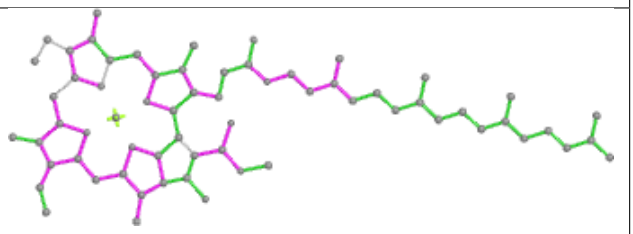


Rings

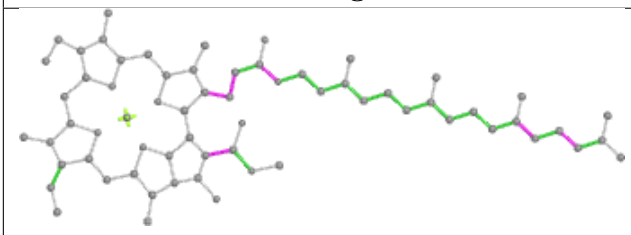
Ligand CLA F 304



Bond lengths



Bond angles



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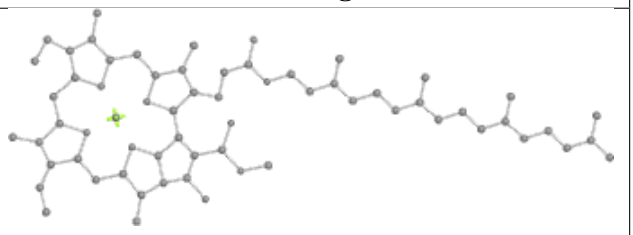
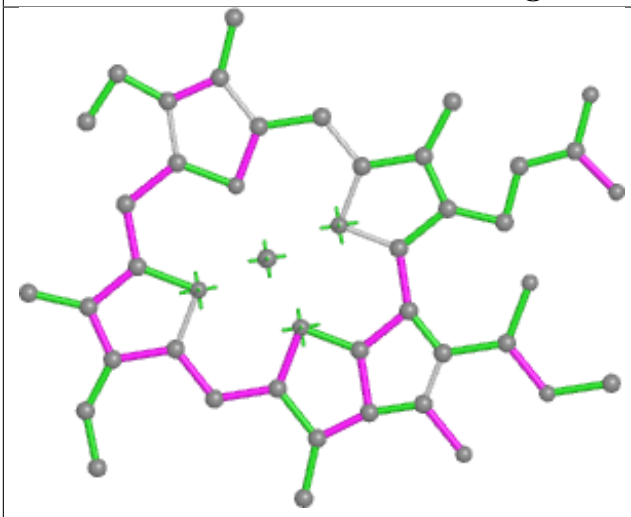


Rings

Ligand CLA B 835



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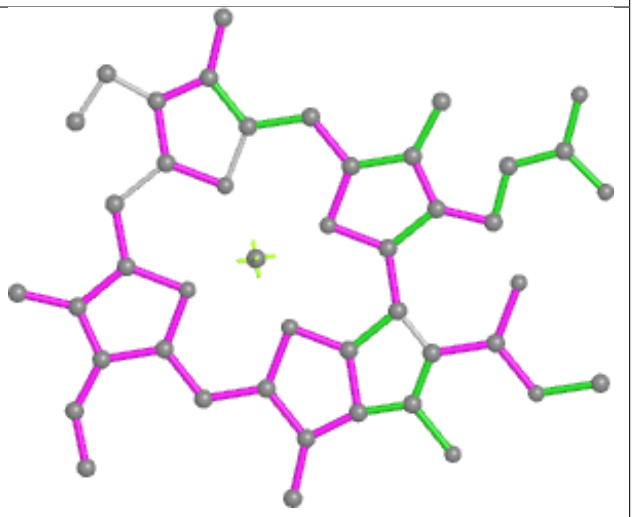
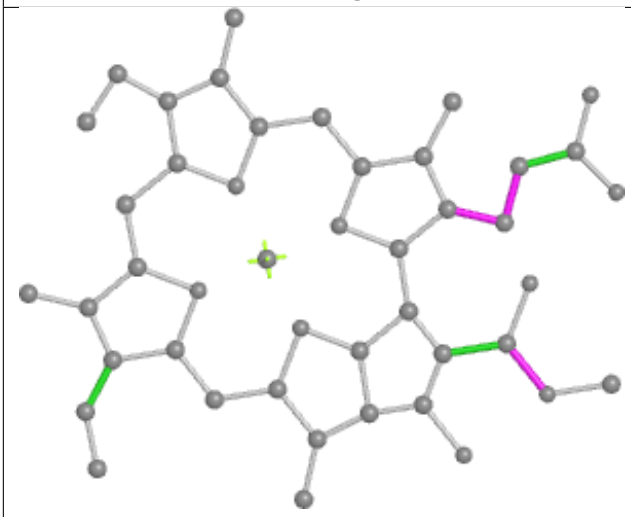


Bond angles



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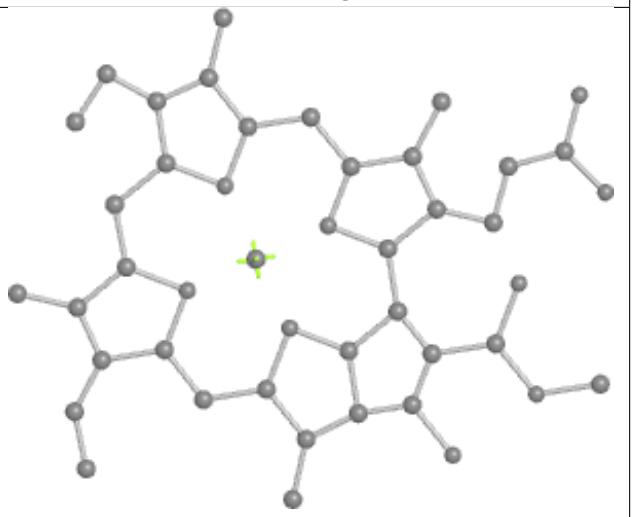
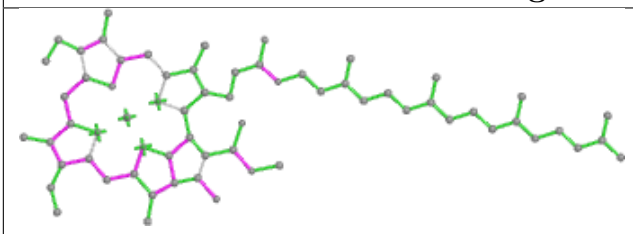


Rings

Ligand CLA 5 601



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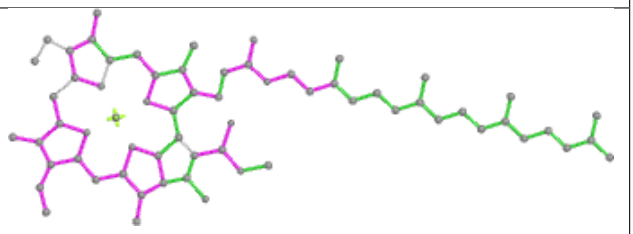
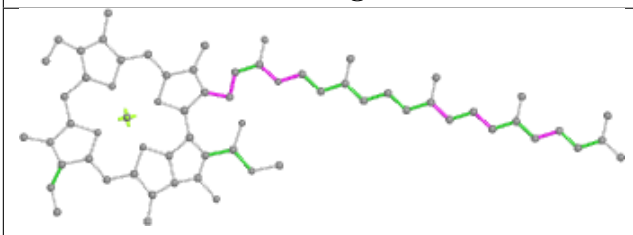


Bond angles



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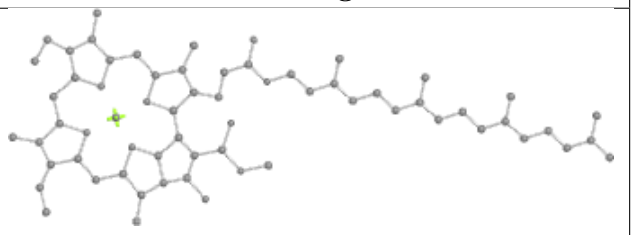
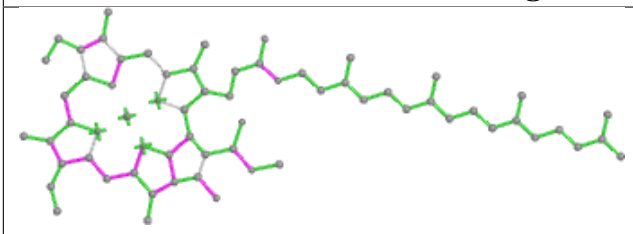


Rings

Ligand CLA B 809



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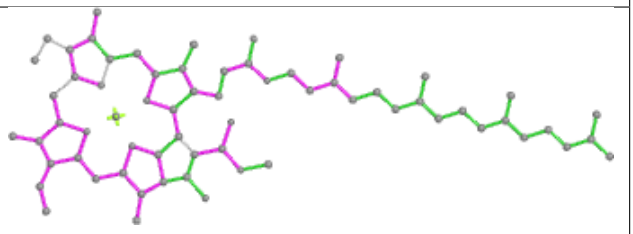
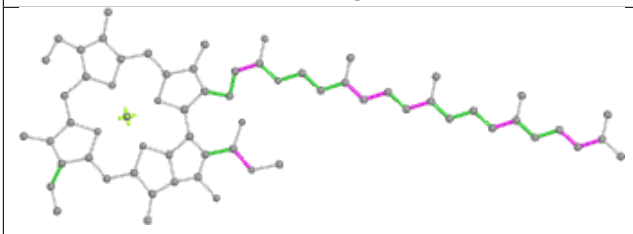


Bond angles



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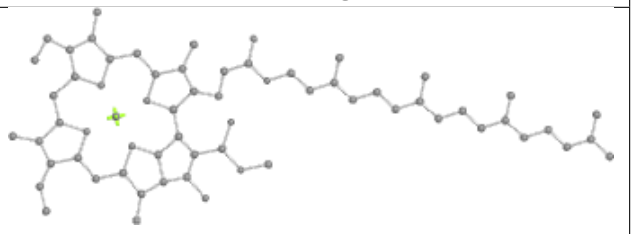
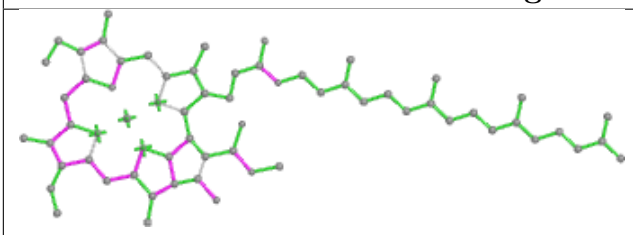


Rings

Ligand CLA B 819



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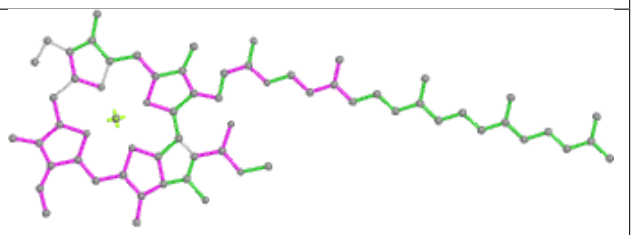
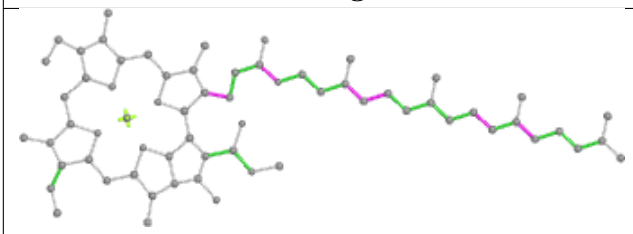


Bond angles



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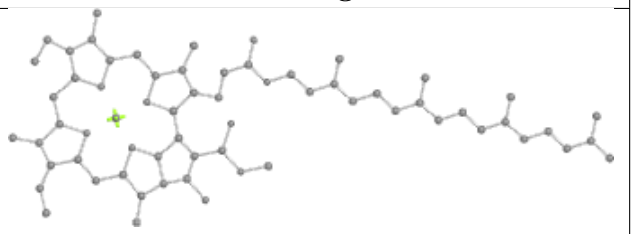
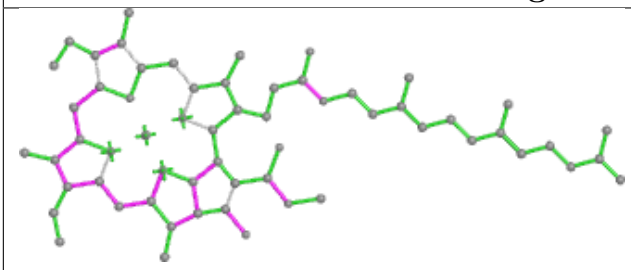
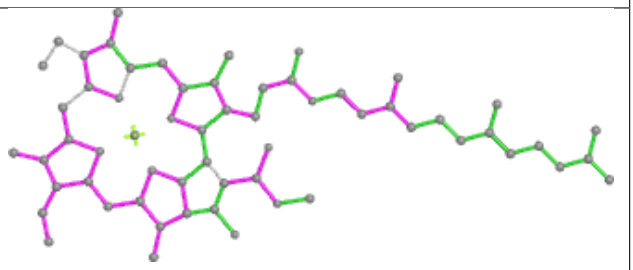


Rings

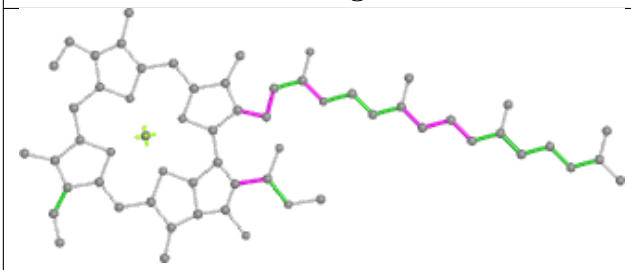
Ligand CLA 9 602



Bond lengths



Bond angles



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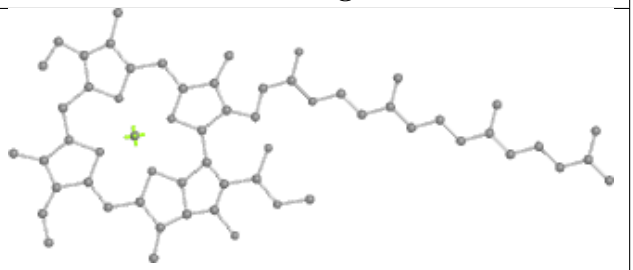
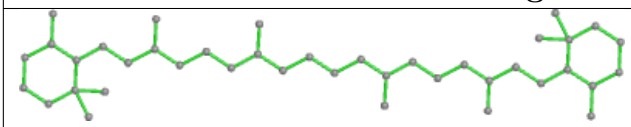


Rings

Ligand BCR 3 717



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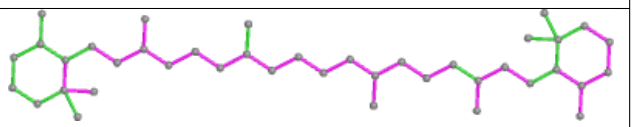
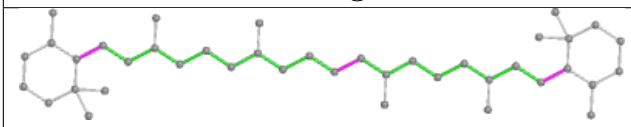


Bond angles



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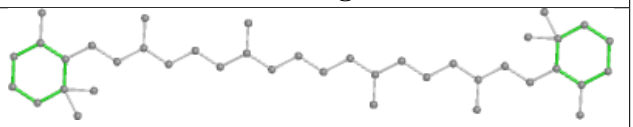
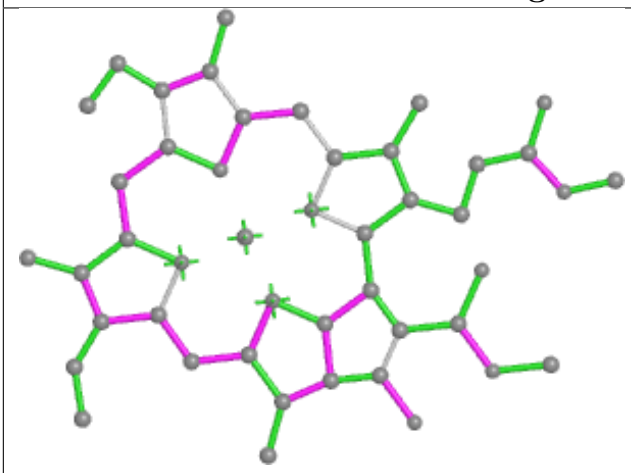


Rings

Ligand CLA 4 603



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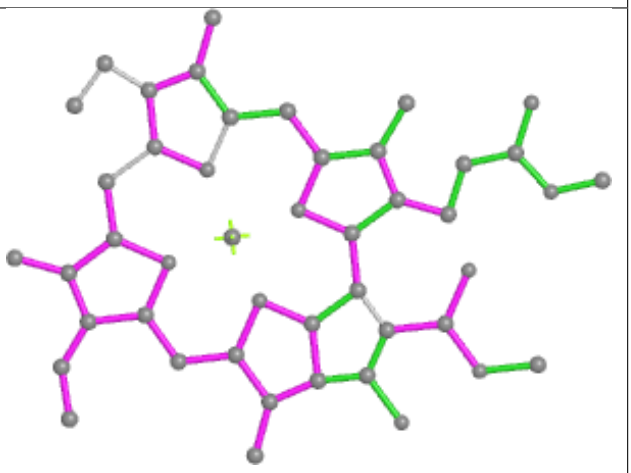
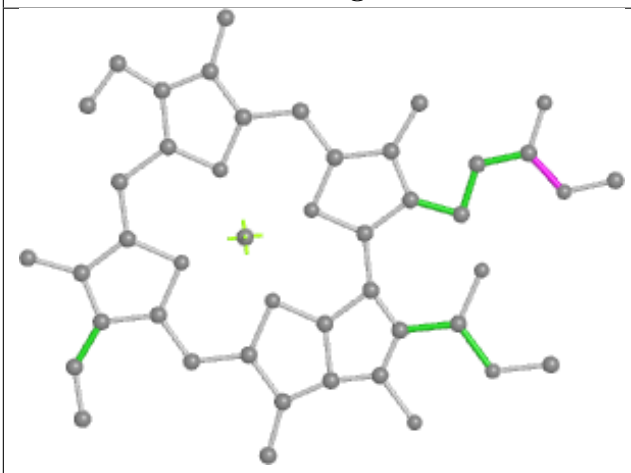


Bond angles



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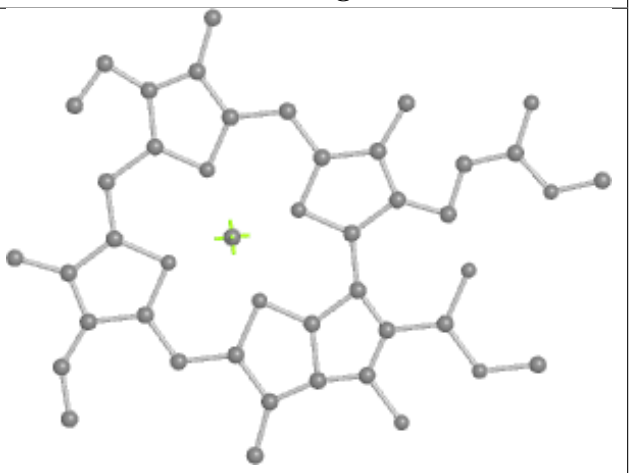
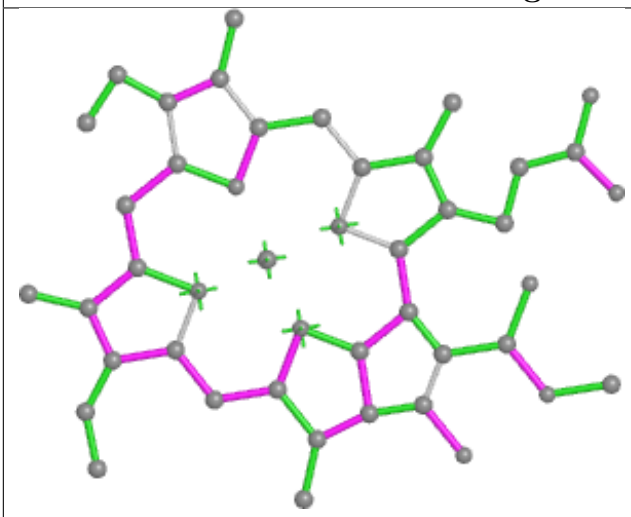


Rings

Ligand CLA A 837



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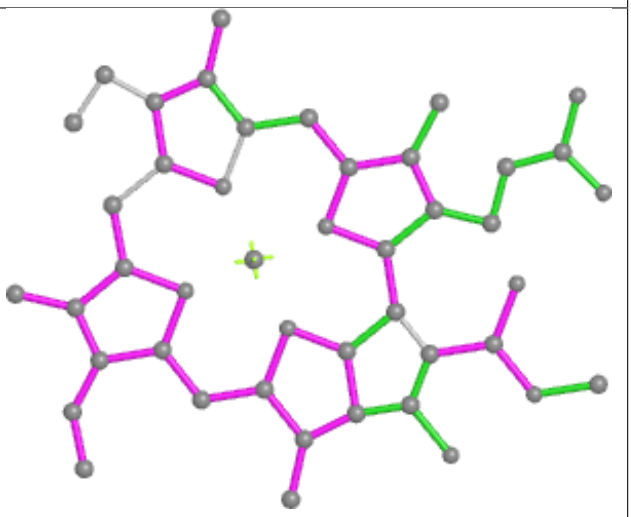
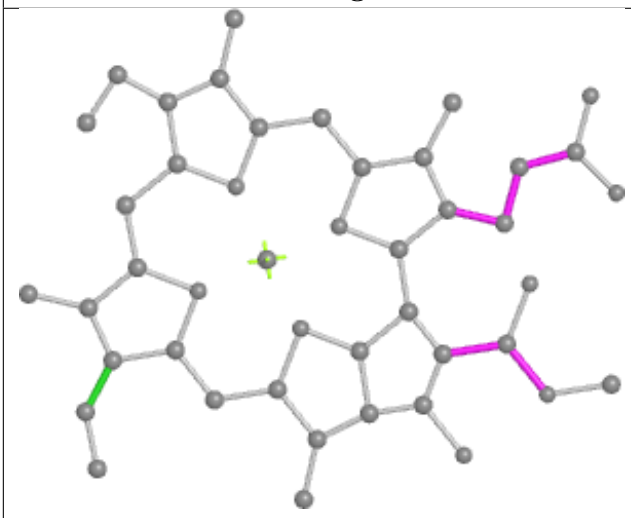


Bond angles



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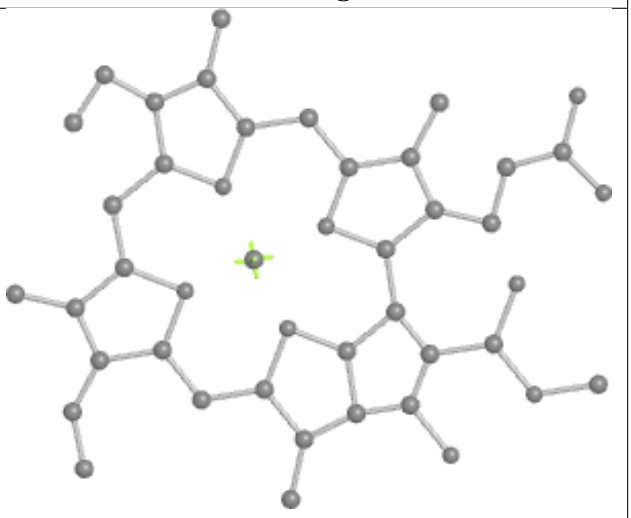
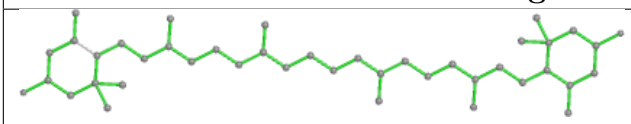
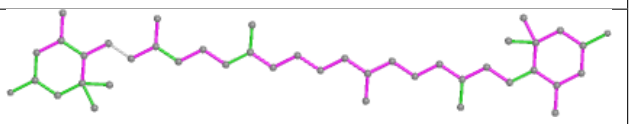


Rings

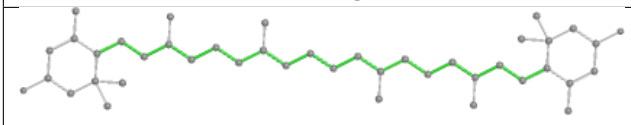
Ligand LUT 2 616



Bond lengths



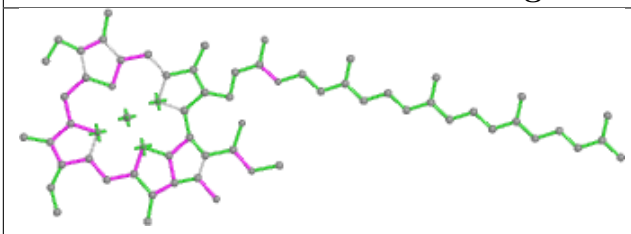
Bond angles



Torsions

Rings

Ligand CLA B 839



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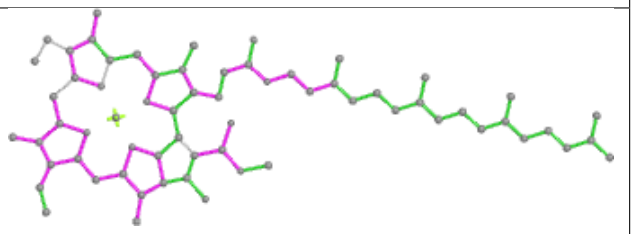
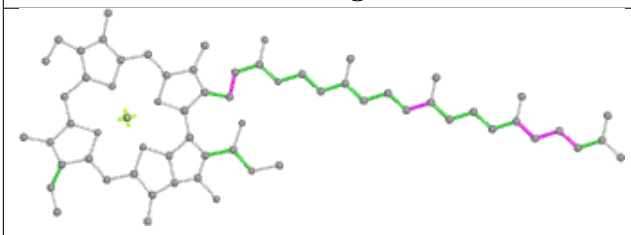
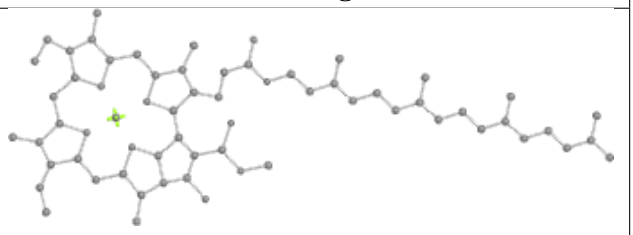


Bond angles

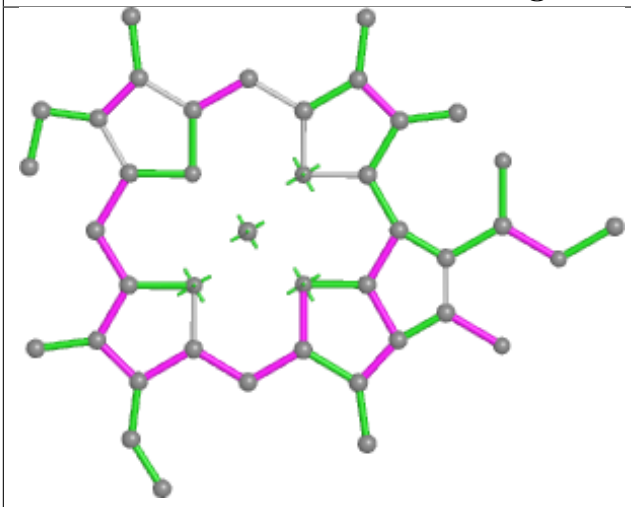


Torsions

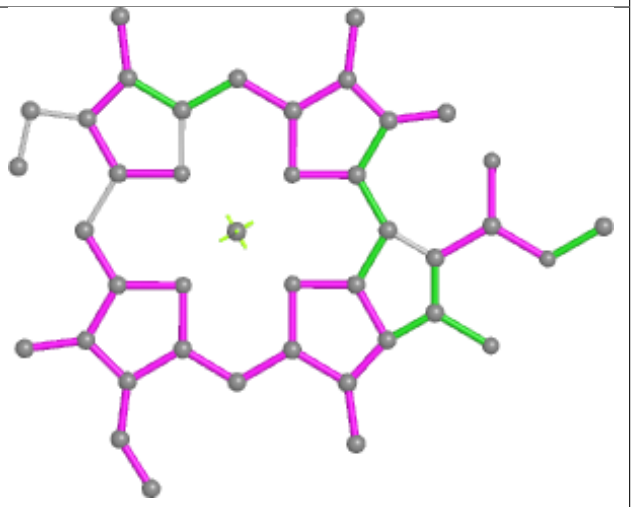


Rings

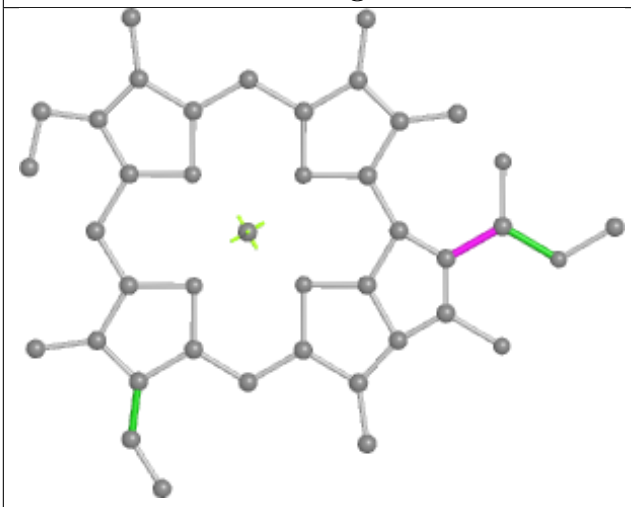
Ligand CLA 2 606



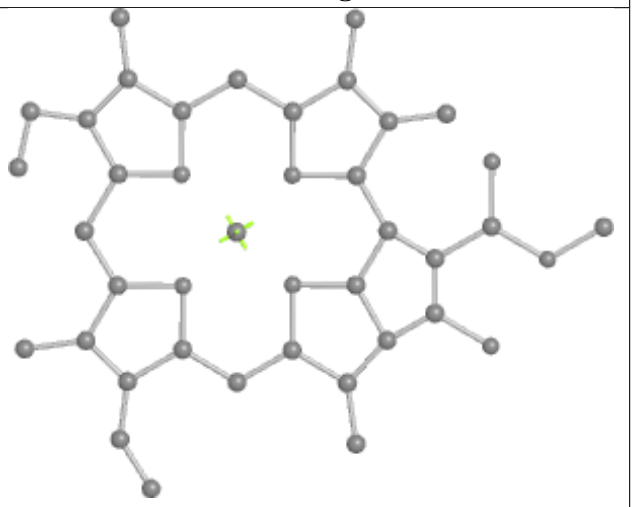
Bond lengths



Bond angles

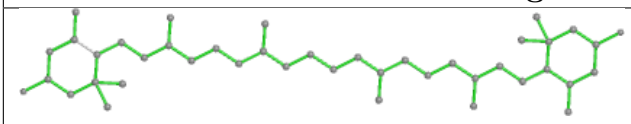


Torsions

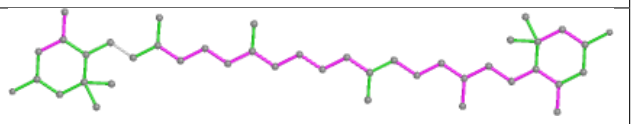


Rings

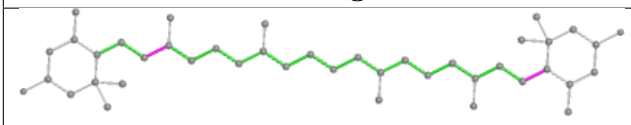
Ligand LUT Z 619



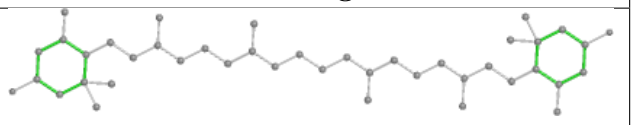
Bond lengths



Bond angles

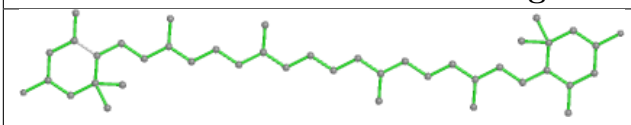


Torsions

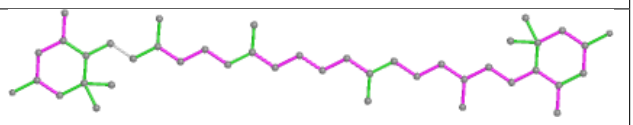


Rings

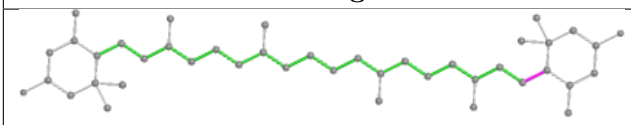
Ligand LUT 1 619



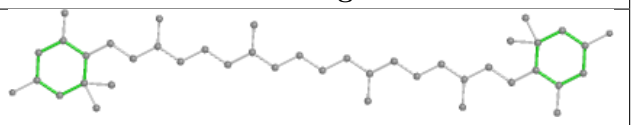
Bond lengths



Bond angles

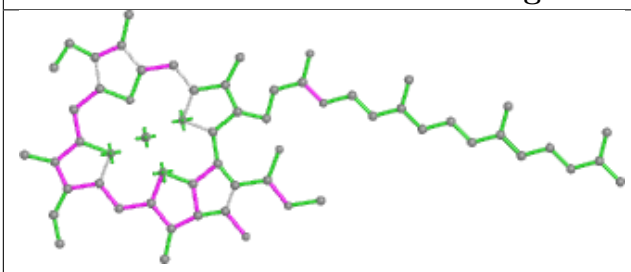


Torsions

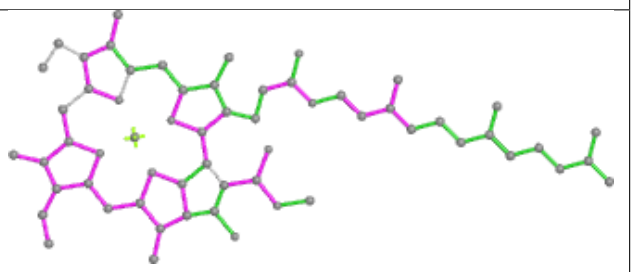


Rings

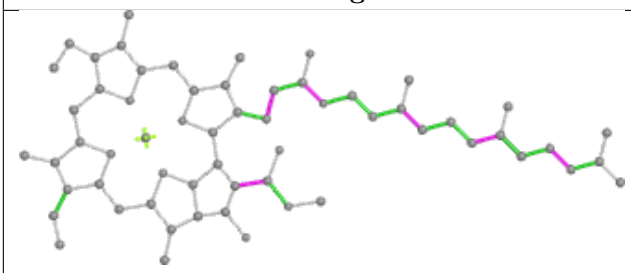
Ligand CLA A 815



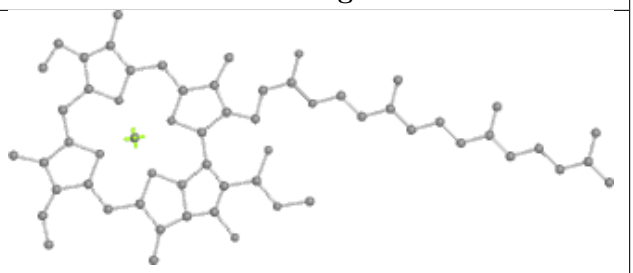
Bond lengths



Bond angles

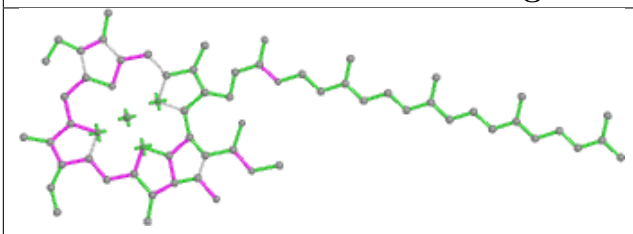


Torsions

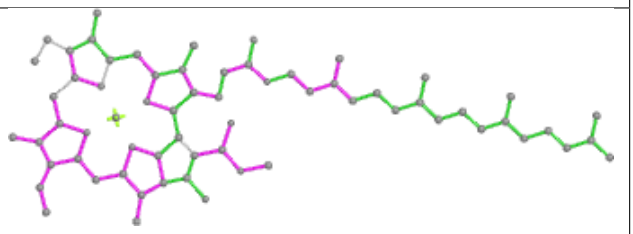


Rings

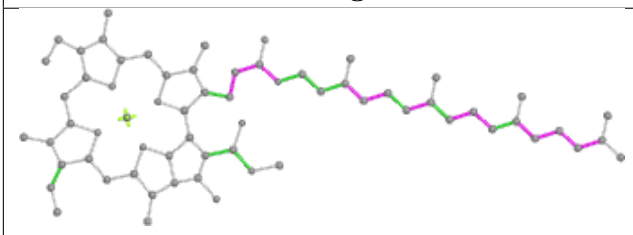
Ligand CLA A 843



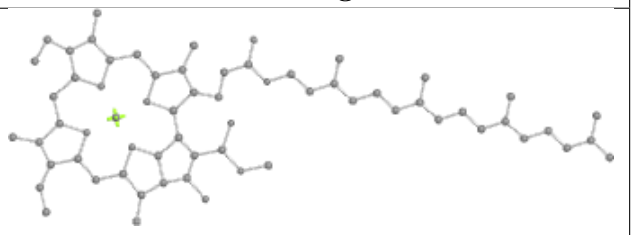
Bond lengths



Bond angles

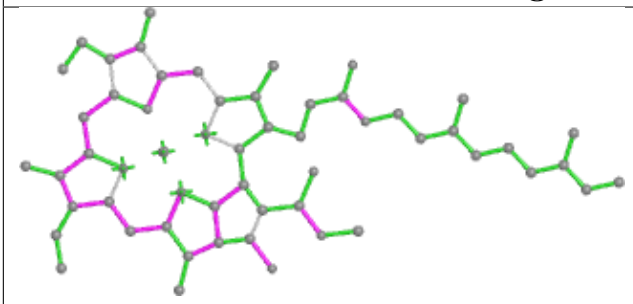


Torsions

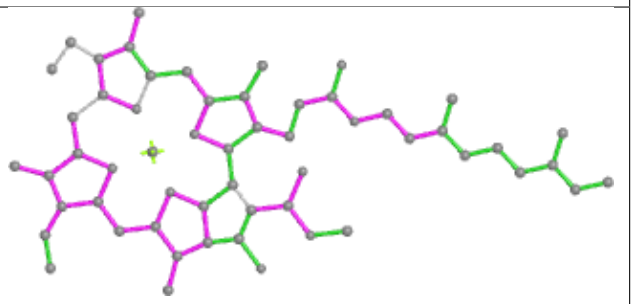


Rings

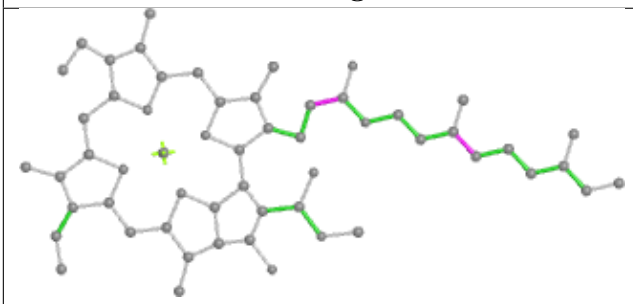
Ligand CLA 6 613



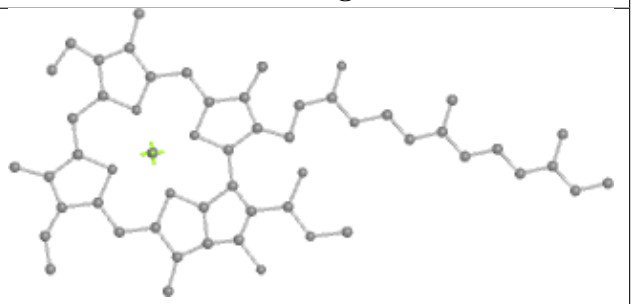
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

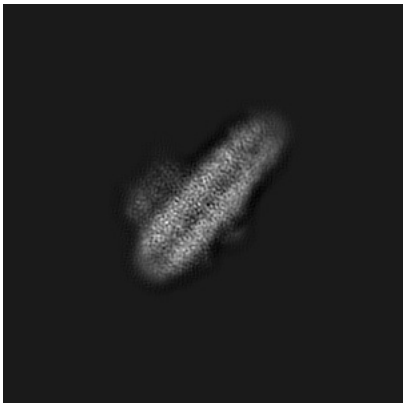
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-9853. These allow visual inspection of the internal detail of the map and identification of artifacts.

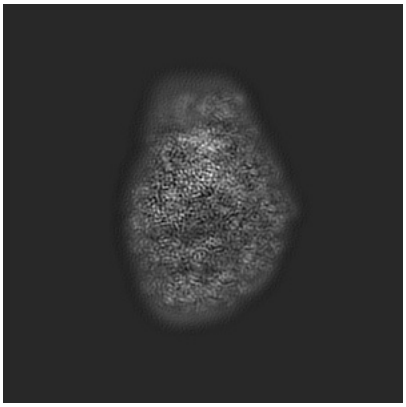
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

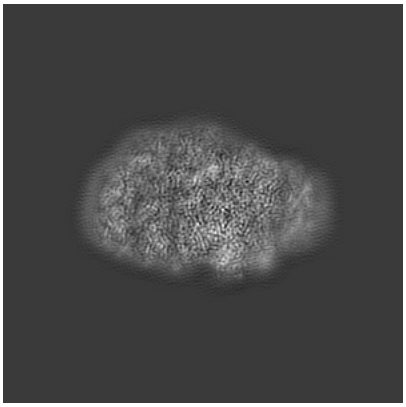
6.1.1 Primary map



X



Y

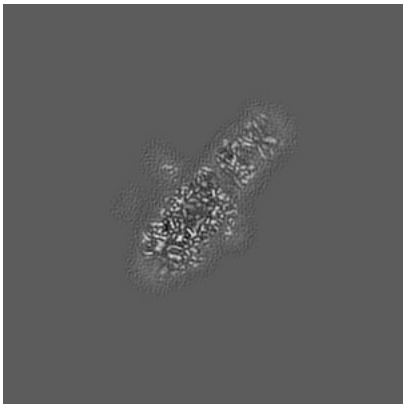


Z

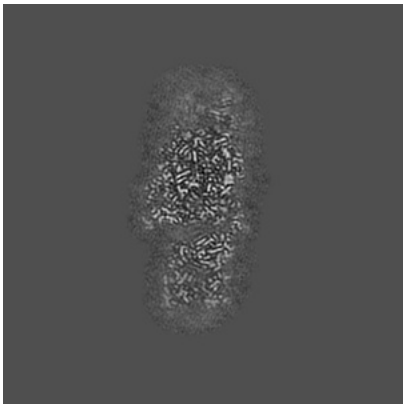
The images above show the map projected in three orthogonal directions.

6.2 Central slices

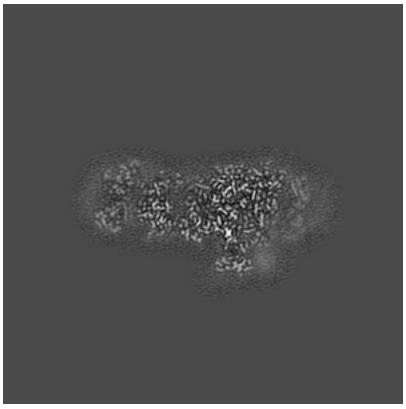
6.2.1 Primary map



X Index: 160



Y Index: 160

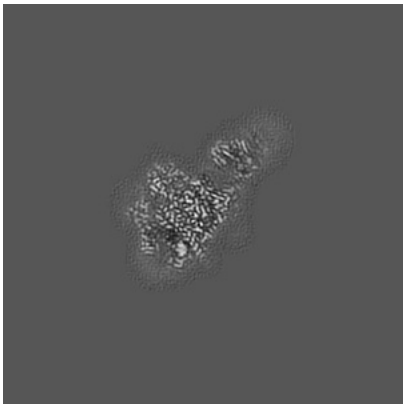


Z Index: 160

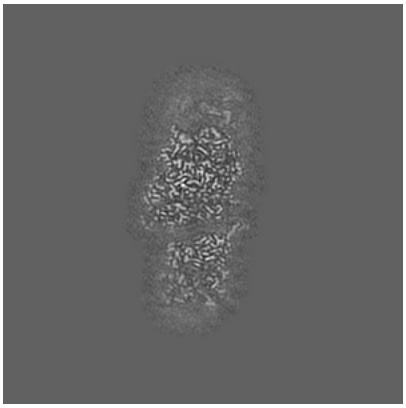
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

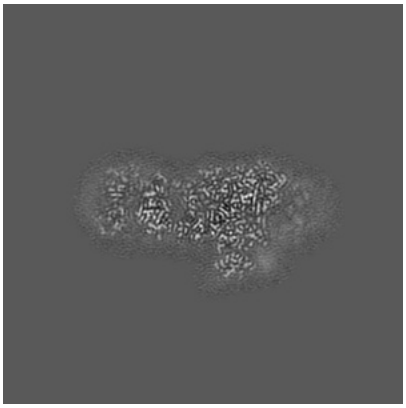
6.3.1 Primary map



X Index: 175



Y Index: 158



Z Index: 157

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

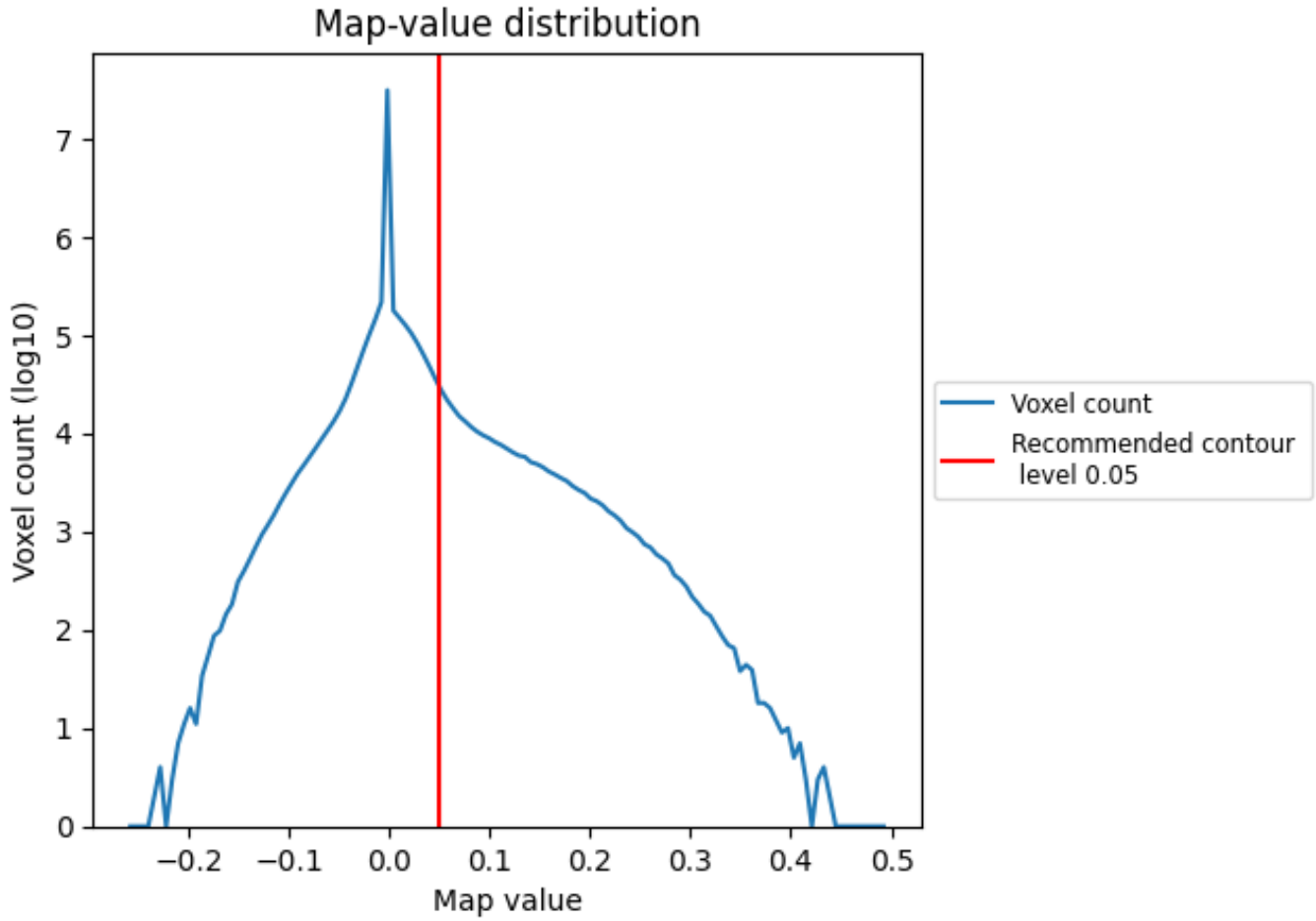
6.5 Mask visualisation (i)

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

7 Map analysis

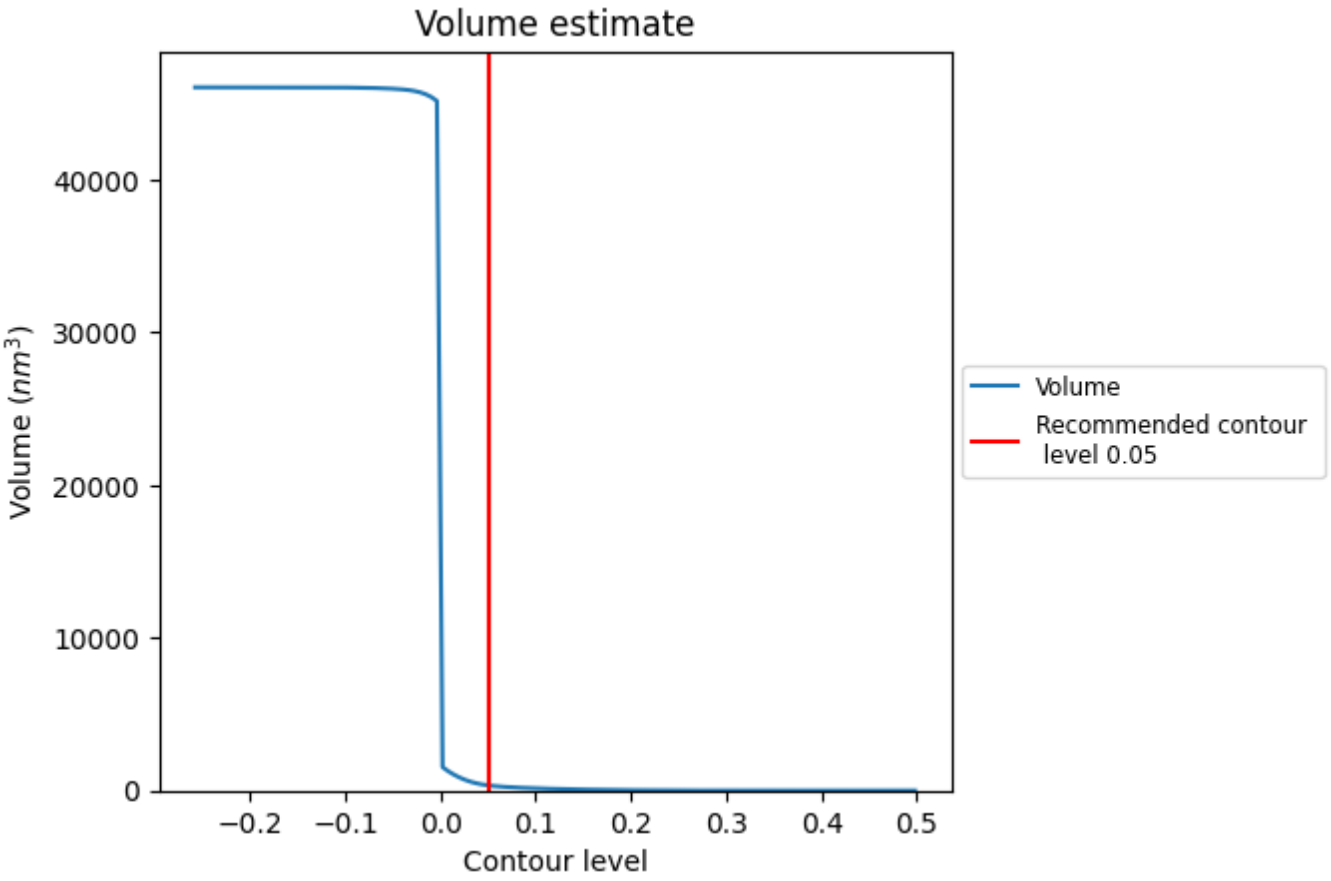
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

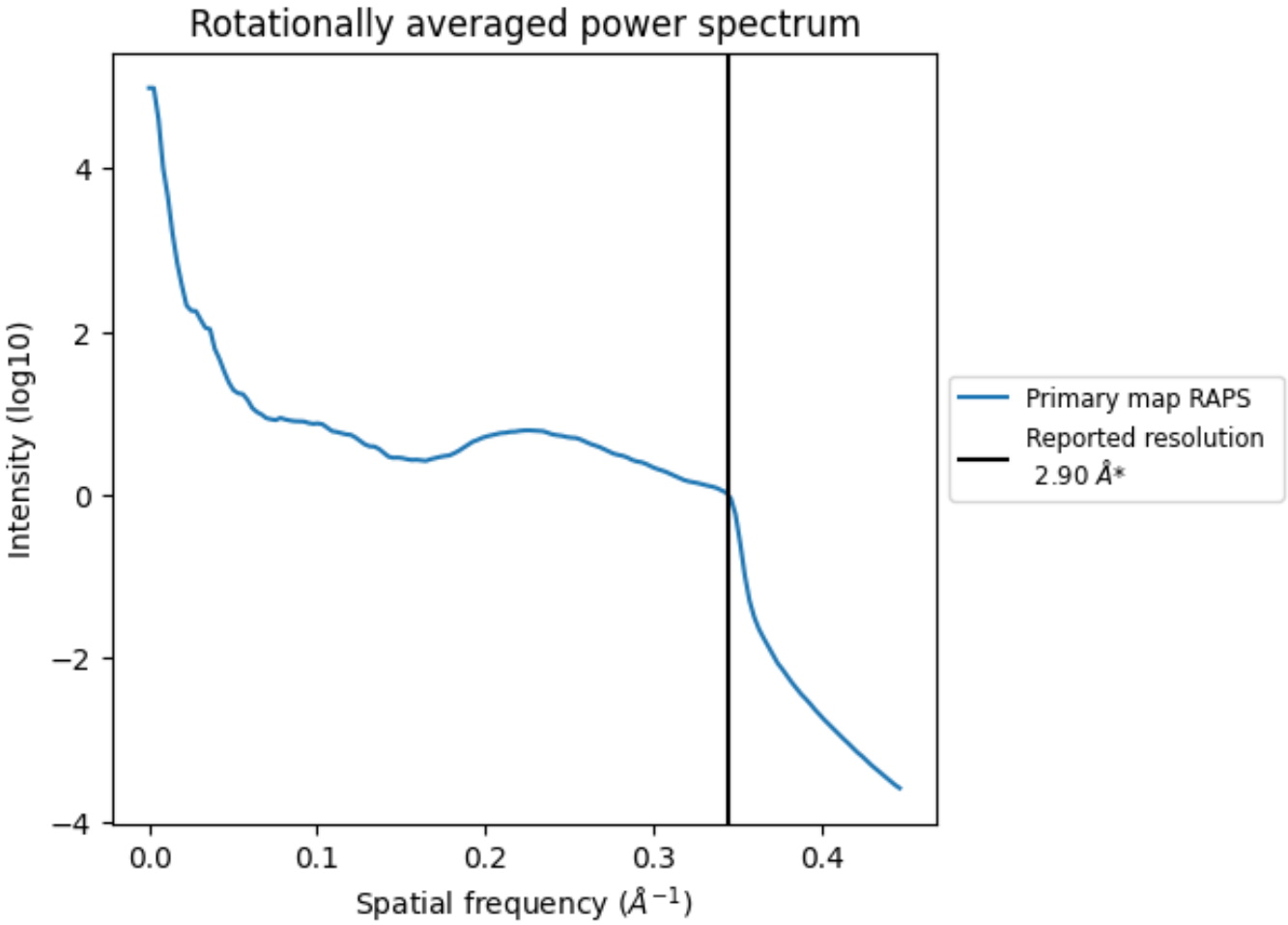
7.2 Volume estimate



The volume at the recommended contour level is 342 nm^3; this corresponds to an approximate mass of 309 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 0.345 $Å^{-1}$

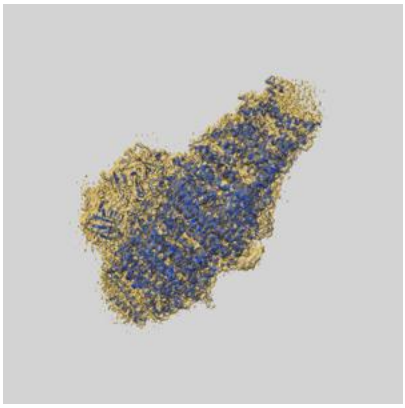
8 Fourier-Shell correlation (i)

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

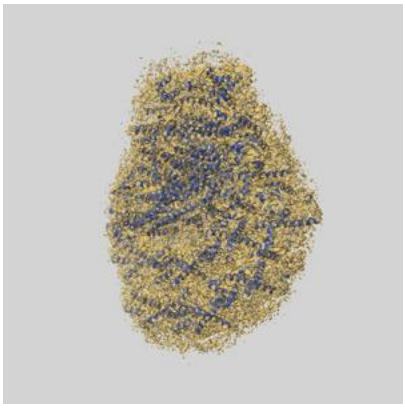
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-9853 and PDB model 6JO5. Per-residue inclusion information can be found in section 3 on page 33.

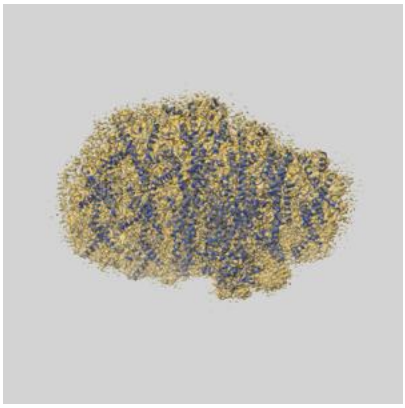
9.1 Map-model overlay



X



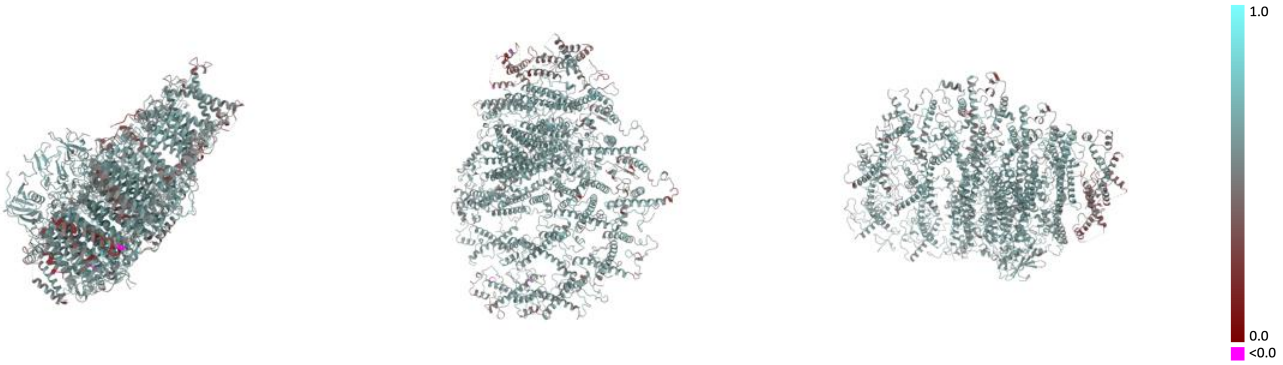
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

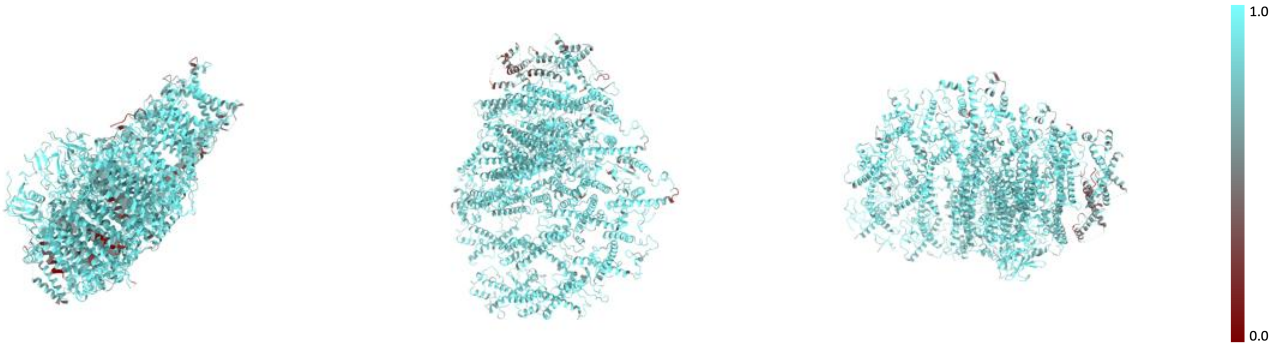
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

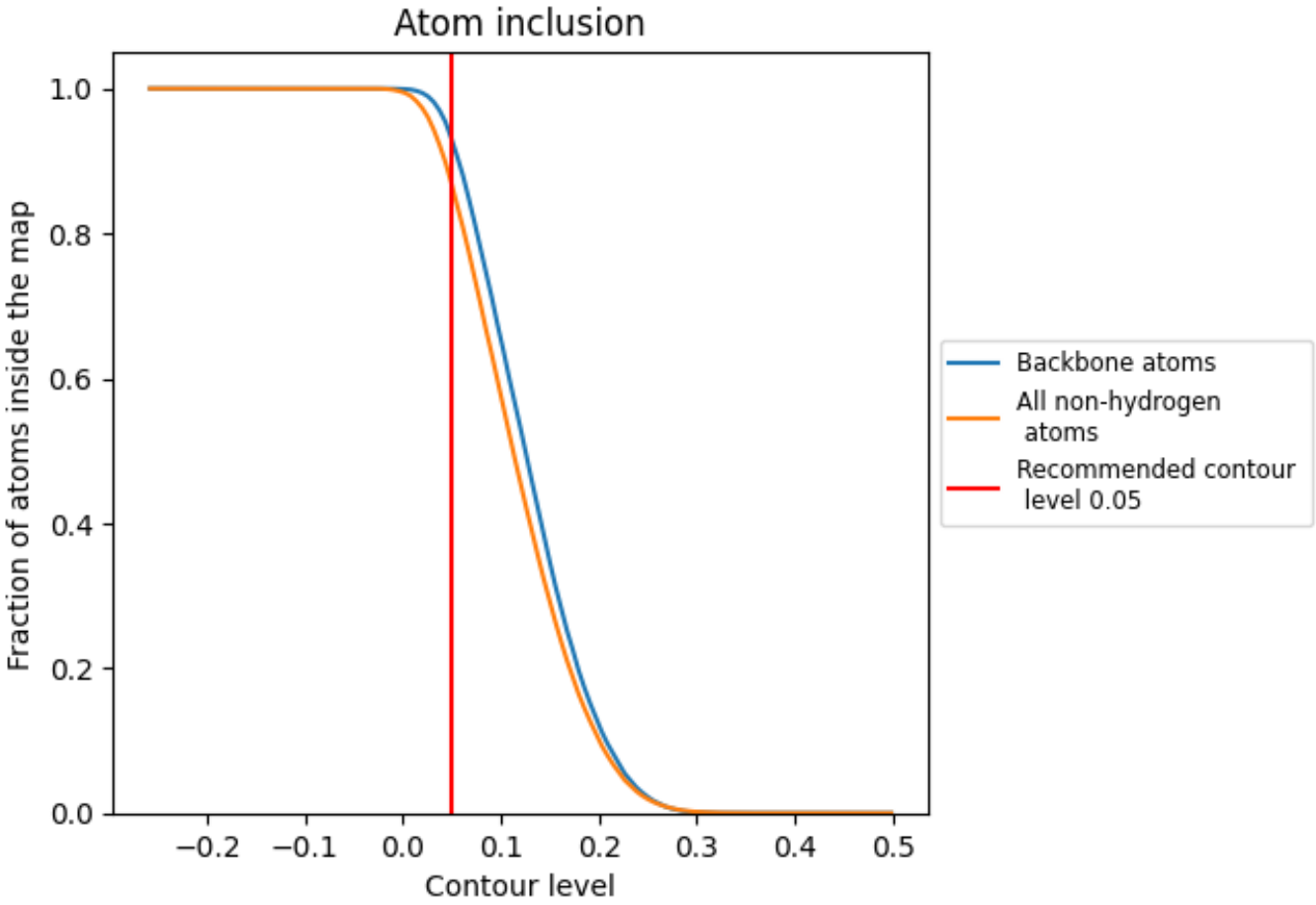
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 87% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8680	0.5670
1	0.8535	0.5660
2	0.5378	0.3290
3	0.8919	0.5820
4	0.8488	0.5440
5	0.8524	0.5470
6	0.8489	0.5510
7	0.8849	0.5860
8	0.8913	0.5830
9	0.6952	0.4490
A	0.9281	0.6080
B	0.9225	0.6090
C	0.9551	0.6010
D	0.9036	0.5730
E	0.8908	0.5830
F	0.8658	0.5660
G	0.8299	0.5500
I	0.8683	0.5680
J	0.9136	0.6010
K	0.7804	0.5270
L	0.8366	0.5420
Z	0.7812	0.5190