wwPDB EM Validation Summary Report

Nov 15, 2022 – 01:22 AM JST

PDB ID	:	6JO6
EMDB ID	:	EMD-9854
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:

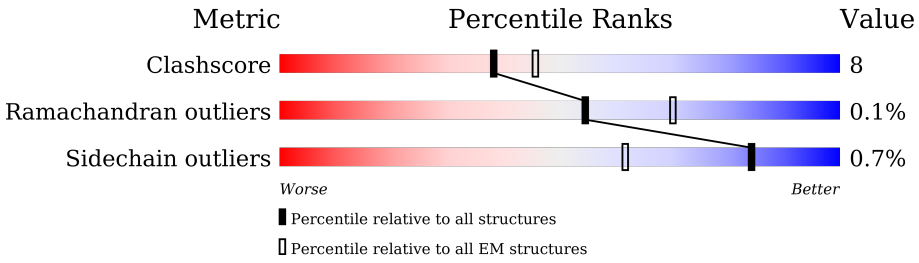
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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	85% 13%
2	B	755	88% 9%
3	C	81	85% 14%
4	D	161	75% 14% 11%
5	E	73	78% 5% 16%
6	F	165	87% 13%
7	G	94	6% 68% 28%
8	I	106	31% 65%

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Mol	Chain	Length	Quality of chain
9	J	41	88% 7% 5%
10	K	87	51% 48%
11	L	156	70% 6% 24%
12	1	194	88% 11%
12	Z	194	7% 91% 8%
13	3	268	62% 13% 25%
14	7	215	83% 15%
15	8	217	77% 21%
16	4	236	74% 12% 14%
17	5	229	85% 12%
18	6	232	84% 15%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CL0	A	801	X	-	-	-
20	CLA	1	602	X	-	-	-
20	CLA	1	603	X	-	-	-
20	CLA	1	604	X	-	-	-
20	CLA	1	606	X	-	-	-
20	CLA	1	608	X	-	-	-
20	CLA	1	609	X	-	-	-
20	CLA	1	610	X	-	-	-
20	CLA	1	611	X	-	-	-
20	CLA	1	612	X	-	-	-
20	CLA	1	613	X	-	-	-
20	CLA	1	614	X	-	-	-
20	CLA	1	616	X	-	-	-
20	CLA	3	602	X	-	-	-
20	CLA	3	603	X	-	-	-
20	CLA	3	604	X	-	-	-
20	CLA	3	606	X	-	-	-
20	CLA	3	607	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	3	609	X	-	-	-
20	CLA	3	610	X	-	-	-
20	CLA	3	611	X	-	-	-
20	CLA	3	612	X	-	-	-
20	CLA	3	617	X	-	-	-
20	CLA	3	620	X	-	-	-
20	CLA	4	601	X	-	-	-
20	CLA	4	603	X	-	-	-
20	CLA	4	609	X	-	-	-
20	CLA	4	610	X	-	-	-
20	CLA	4	611	X	-	-	-
20	CLA	4	612	X	-	-	-
20	CLA	4	614	X	-	-	-
20	CLA	4	616	X	-	-	-
20	CLA	5	601	X	-	-	-
20	CLA	5	603	X	-	-	-
20	CLA	5	606	X	-	-	-
20	CLA	5	609	X	-	-	-
20	CLA	5	610	X	-	-	-
20	CLA	5	611	X	-	-	-
20	CLA	5	612	X	-	-	-
20	CLA	5	613	X	-	-	-
20	CLA	5	614	X	-	-	-
20	CLA	5	616	X	-	-	-
20	CLA	5	617	X	-	-	-
20	CLA	5	621	X	-	-	-
20	CLA	6	601	X	-	-	-
20	CLA	6	602	X	-	-	-
20	CLA	6	603	X	-	-	-
20	CLA	6	604	X	-	-	-
20	CLA	6	609	X	-	-	-
20	CLA	6	610	X	-	-	-
20	CLA	6	611	X	-	-	-
20	CLA	6	612	X	-	-	-
20	CLA	6	613	X	-	-	-
20	CLA	6	614	X	-	-	-
20	CLA	6	616	X	-	-	-
20	CLA	6	617	X	-	-	-
20	CLA	6	622	X	-	-	-
20	CLA	7	601	X	-	-	-
20	CLA	7	602	X	-	-	-
20	CLA	7	603	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	7	604	X	-	-	-
20	CLA	7	606	X	-	-	-
20	CLA	7	609	X	-	-	-
20	CLA	7	610	X	-	-	-
20	CLA	7	611	X	-	-	-
20	CLA	7	612	X	-	-	-
20	CLA	7	613	X	-	-	-
20	CLA	7	614	X	-	-	-
20	CLA	7	616	X	-	-	-
20	CLA	7	620	X	-	-	-
20	CLA	8	601	X	-	-	-
20	CLA	8	602	X	-	-	-
20	CLA	8	603	X	-	-	-
20	CLA	8	604	X	-	-	-
20	CLA	8	606	X	-	-	-
20	CLA	8	608	X	-	-	-
20	CLA	8	609	X	-	-	-
20	CLA	8	610	X	-	-	-
20	CLA	8	611	X	-	-	-
20	CLA	8	612	X	-	-	-
20	CLA	8	613	X	-	-	-
20	CLA	8	614	X	-	-	-
20	CLA	8	616	X	-	-	-
20	CLA	A	802	X	-	-	-
20	CLA	A	803	X	-	-	-
20	CLA	A	804	X	-	-	-
20	CLA	A	805	X	-	-	-
20	CLA	A	806	X	-	-	-
20	CLA	A	807	X	-	-	-
20	CLA	A	808	X	-	-	-
20	CLA	A	809	X	-	-	-
20	CLA	A	810	X	-	-	-
20	CLA	A	811	X	-	-	-
20	CLA	A	812	X	-	-	-
20	CLA	A	813	X	-	-	-
20	CLA	A	814	X	-	-	-
20	CLA	A	815	X	-	-	-
20	CLA	A	816	X	-	-	-
20	CLA	A	817	X	-	-	-
20	CLA	A	820	X	-	-	-
20	CLA	A	821	X	-	-	-
20	CLA	A	822	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	A	824	X	-	-	-
20	CLA	A	826	X	-	-	-
20	CLA	A	827	X	-	-	-
20	CLA	A	828	X	-	-	-
20	CLA	A	829	X	-	-	-
20	CLA	A	830	X	-	-	-
20	CLA	A	831	X	-	-	-
20	CLA	A	832	X	-	-	-
20	CLA	A	833	X	-	-	-
20	CLA	A	834	X	-	-	-
20	CLA	A	835	X	-	-	-
20	CLA	A	837	X	-	-	-
20	CLA	A	838	X	-	-	-
20	CLA	A	839	X	-	-	-
20	CLA	A	840	X	-	-	-
20	CLA	A	841	X	-	-	-
20	CLA	A	842	X	-	-	-
20	CLA	A	843	X	-	-	-
20	CLA	A	854	X	-	-	-
20	CLA	B	802	X	-	-	-
20	CLA	B	803	X	-	-	-
20	CLA	B	804	X	-	-	-
20	CLA	B	805	X	-	-	-
20	CLA	B	806	X	-	-	-
20	CLA	B	807	X	-	-	-
20	CLA	B	808	X	-	-	-
20	CLA	B	809	X	-	-	-
20	CLA	B	810	X	-	-	-
20	CLA	B	811	X	-	-	-
20	CLA	B	812	X	-	-	-
20	CLA	B	813	X	-	-	-
20	CLA	B	814	X	-	-	-
20	CLA	B	815	X	-	-	-
20	CLA	B	816	X	-	-	-
20	CLA	B	817	X	-	-	-
20	CLA	B	818	X	-	-	-
20	CLA	B	819	X	-	-	-
20	CLA	B	820	X	-	-	-
20	CLA	B	822	X	-	-	-
20	CLA	B	823	X	-	-	-
20	CLA	B	824	X	-	-	-
20	CLA	B	825	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	B	826	X	-	-	-
20	CLA	B	827	X	-	-	-
20	CLA	B	828	X	-	-	-
20	CLA	B	829	X	-	-	-
20	CLA	B	831	X	-	-	-
20	CLA	B	832	X	-	-	-
20	CLA	B	833	X	-	-	-
20	CLA	B	834	X	-	-	-
20	CLA	B	835	X	-	-	-
20	CLA	B	836	X	-	-	-
20	CLA	B	837	X	-	-	-
20	CLA	B	838	X	-	-	-
20	CLA	B	839	X	-	-	-
20	CLA	B	841	X	-	-	-
20	CLA	B	852	X	-	-	-
20	CLA	F	301	X	-	-	-
20	CLA	F	303	X	-	-	-
20	CLA	F	304	X	-	-	-
20	CLA	G	203	X	-	-	-
20	CLA	G	204	X	-	-	-
20	CLA	J	3002	X	-	-	-
20	CLA	K	4003	X	-	-	-
20	CLA	Z	602	X	-	-	-
20	CLA	Z	603	X	-	-	-
20	CLA	Z	604	X	-	-	-
20	CLA	Z	606	X	-	-	-
20	CLA	Z	608	X	-	-	-
20	CLA	Z	609	X	-	-	-
20	CLA	Z	610	X	-	-	-
20	CLA	Z	611	X	-	-	-
20	CLA	Z	612	X	-	-	-
20	CLA	Z	613	X	-	-	-
20	CLA	Z	614	X	-	-	-
20	CLA	Z	616	X	-	-	-
27	CHL	1	601	X	-	-	-
27	CHL	1	607	X	-	-	-
27	CHL	3	608	X	-	-	-
27	CHL	4	606	X	-	-	-
27	CHL	4	607	X	-	-	-
27	CHL	4	608	X	-	-	-
27	CHL	4	618	X	-	-	-
27	CHL	5	607	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CHL	5	608	X	-	-	-
27	CHL	5	618	X	-	-	-
27	CHL	6	606	X	-	-	-
27	CHL	6	607	X	-	-	-
27	CHL	6	608	X	-	-	-
27	CHL	6	618	X	-	-	-
27	CHL	7	607	X	-	-	-
27	CHL	8	607	X	-	-	-
27	CHL	Z	601	X	-	-	-
27	CHL	Z	607	X	-	-	-

2 Entry composition (i)

There are 28 unique types of molecules in this entry. The entry contains 45099 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		

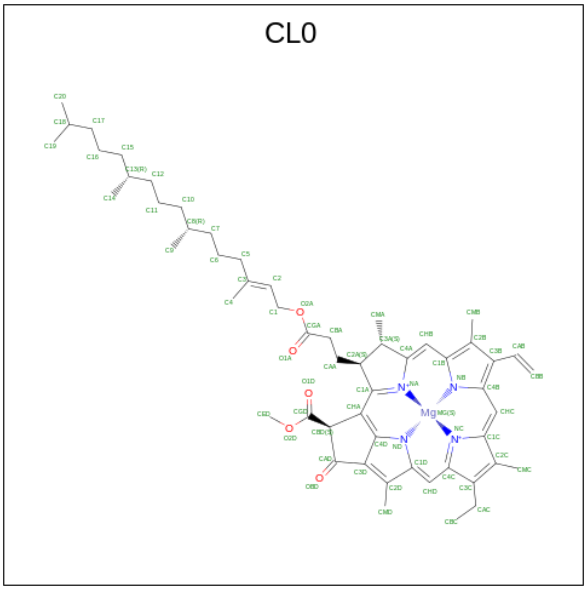
- Molecule 17 is a protein called Chlorophyll a-b binding protein, chloroplastic.

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

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

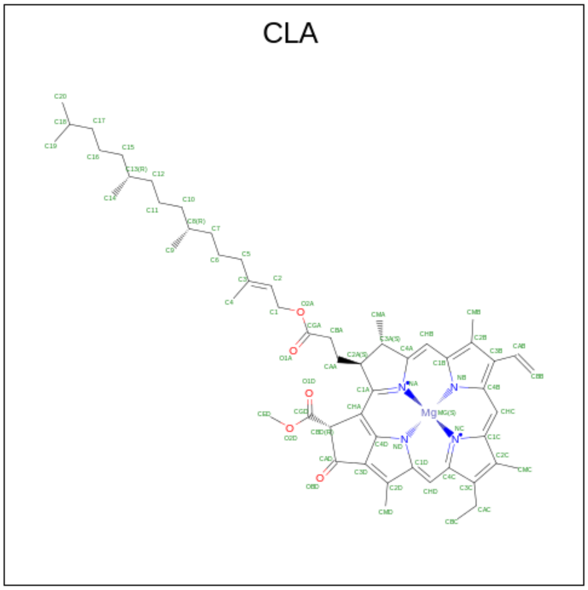
Mol	Chain	Residues	Atoms					AltConf	Trace
18	6	229	Total	C	N	O	S	0	0
			1765	1164	292	303	6		

- Molecule 19 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



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

- Molecule 20 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	
20	A	1	2689	2249	44	176	220	0
20	A	1	2689	2249	44	176	220	0
20	A	1	2689	2249	44	176	220	0
20	A	1	2689	2249	44	176	220	0
20	A	1	2689	2249	44	176	220	0
20	A	1	2689	2249	44	176	220	0
20	A	1	2689	2249	44	176	220	0
20	A	1	2689	2249	44	176	220	0
20	A	1	2689	2249	44	176	220	0
20	A	1	2689	2249	44	176	220	0
20	A	1	2689	2249	44	176	220	0
20	A	1	2689	2249	44	176	220	0
20	A	1	2689	2249	44	176	220	0
20	A	1	2689	2249	44	176	220	0

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

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

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

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Mol	Chain	Residues	Atoms	AltConf
20	B	1	Total C Mg N O 2480 2070 41 164 205	0
20	B	1	Total C Mg N O 2480 2070 41 164 205	0
20	B	1	Total C Mg N O 2480 2070 41 164 205	0
20	B	1	Total C Mg N O 2480 2070 41 164 205	0
20	B	1	Total C Mg N O 2480 2070 41 164 205	0
20	B	1	Total C Mg N O 2480 2070 41 164 205	0
20	B	1	Total C Mg N O 2480 2070 41 164 205	0
20	B	1	Total C Mg N O 2480 2070 41 164 205	0
20	F	1	Total C Mg N O 175 145 3 12 15	0
20	F	1	Total C Mg N O 175 145 3 12 15	0
20	F	1	Total C Mg N O 175 145 3 12 15	0
20	G	1	Total C Mg N O 96 76 2 8 10	0
20	G	1	Total C Mg N O 96 76 2 8 10	0
20	J	1	Total C Mg N O 42 34 1 4 3	0
20	K	1	Total C Mg N O 91 71 2 8 10	0
20	K	1	Total C Mg N O 91 71 2 8 10	0
20	L	1	Total C Mg N O 115 95 2 8 10	0
20	L	1	Total C Mg N O 115 95 2 8 10	0
20	1	1	Total C Mg N O 722 602 12 48 60	0
20	1	1	Total C Mg N O 722 602 12 48 60	0
20	1	1	Total C Mg N O 722 602 12 48 60	0

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Mol	Chain	Residues	Atoms					AltConf
20	1	1	Total 722	C 602	Mg 12	N 48	O 60	0
20	1	1	Total 722	C 602	Mg 12	N 48	O 60	0
20	1	1	Total 722	C 602	Mg 12	N 48	O 60	0
20	1	1	Total 722	C 602	Mg 12	N 48	O 60	0
20	1	1	Total 722	C 602	Mg 12	N 48	O 60	0
20	1	1	Total 722	C 602	Mg 12	N 48	O 60	0
20	1	1	Total 722	C 602	Mg 12	N 48	O 60	0
20	1	1	Total 722	C 602	Mg 12	N 48	O 60	0
20	1	1	Total 722	C 602	Mg 12	N 48	O 60	0
20	3	1	Total 696	C 570	Mg 13	N 52	O 61	0
20	3	1	Total 696	C 570	Mg 13	N 52	O 61	0
20	3	1	Total 696	C 570	Mg 13	N 52	O 61	0
20	3	1	Total 696	C 570	Mg 13	N 52	O 61	0
20	3	1	Total 696	C 570	Mg 13	N 52	O 61	0
20	3	1	Total 696	C 570	Mg 13	N 52	O 61	0
20	3	1	Total 696	C 570	Mg 13	N 52	O 61	0
20	3	1	Total 696	C 570	Mg 13	N 52	O 61	0
20	3	1	Total 696	C 570	Mg 13	N 52	O 61	0
20	3	1	Total 696	C 570	Mg 13	N 52	O 61	0
20	3	1	Total 696	C 570	Mg 13	N 52	O 61	0
20	3	1	Total 696	C 570	Mg 13	N 52	O 61	0

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Mol	Chain	Residues	Atoms					AltConf
20	3	1	Total 696	C 570	Mg 13	N 52	O 61	0
20	7	1	Total 741	C 607	Mg 14	N 56	O 64	0
20	7	1	Total 741	C 607	Mg 14	N 56	O 64	0
20	7	1	Total 741	C 607	Mg 14	N 56	O 64	0
20	7	1	Total 741	C 607	Mg 14	N 56	O 64	0
20	7	1	Total 741	C 607	Mg 14	N 56	O 64	0
20	7	1	Total 741	C 607	Mg 14	N 56	O 64	0
20	7	1	Total 741	C 607	Mg 14	N 56	O 64	0
20	7	1	Total 741	C 607	Mg 14	N 56	O 64	0
20	7	1	Total 741	C 607	Mg 14	N 56	O 64	0
20	7	1	Total 741	C 607	Mg 14	N 56	O 64	0
20	7	1	Total 741	C 607	Mg 14	N 56	O 64	0
20	7	1	Total 741	C 607	Mg 14	N 56	O 64	0
20	7	1	Total 741	C 607	Mg 14	N 56	O 64	0
20	7	1	Total 741	C 607	Mg 14	N 56	O 64	0
20	8	1	Total 680	C 552	Mg 13	N 52	O 63	0
20	8	1	Total 680	C 552	Mg 13	N 52	O 63	0
20	8	1	Total 680	C 552	Mg 13	N 52	O 63	0
20	8	1	Total 680	C 552	Mg 13	N 52	O 63	0
20	8	1	Total 680	C 552	Mg 13	N 52	O 63	0
20	8	1	Total 680	C 552	Mg 13	N 52	O 63	0

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Mol	Chain	Residues	Atoms					AltConf
20	8	1	Total 680	C 552	Mg 13	N 52	O 63	0
20	8	1	Total 680	C 552	Mg 13	N 52	O 63	0
20	8	1	Total 680	C 552	Mg 13	N 52	O 63	0
20	8	1	Total 680	C 552	Mg 13	N 52	O 63	0
20	8	1	Total 680	C 552	Mg 13	N 52	O 63	0
20	8	1	Total 680	C 552	Mg 13	N 52	O 63	0
20	8	1	Total 680	C 552	Mg 13	N 52	O 63	0
20	Z	1	Total 714	C 594	Mg 12	N 48	O 60	0
20	Z	1	Total 714	C 594	Mg 12	N 48	O 60	0
20	Z	1	Total 714	C 594	Mg 12	N 48	O 60	0
20	Z	1	Total 714	C 594	Mg 12	N 48	O 60	0
20	Z	1	Total 714	C 594	Mg 12	N 48	O 60	0
20	Z	1	Total 714	C 594	Mg 12	N 48	O 60	0
20	Z	1	Total 714	C 594	Mg 12	N 48	O 60	0
20	Z	1	Total 714	C 594	Mg 12	N 48	O 60	0
20	Z	1	Total 714	C 594	Mg 12	N 48	O 60	0
20	Z	1	Total 714	C 594	Mg 12	N 48	O 60	0
20	Z	1	Total 714	C 594	Mg 12	N 48	O 60	0
20	Z	1	Total 714	C 594	Mg 12	N 48	O 60	0
20	4	1	Total 576	C 468	Mg 11	N 44	O 53	0
20	4	1	Total 576	C 468	Mg 11	N 44	O 53	0

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Mol	Chain	Residues	Atoms	AltConf
20	4	1	Total C Mg N O 576 468 11 44 53	0
20	4	1	Total C Mg N O 576 468 11 44 53	0
20	4	1	Total C Mg N O 576 468 11 44 53	0
20	4	1	Total C Mg N O 576 468 11 44 53	0
20	4	1	Total C Mg N O 576 468 11 44 53	0
20	4	1	Total C Mg N O 576 468 11 44 53	0
20	4	1	Total C Mg N O 576 468 11 44 53	0
20	4	1	Total C Mg N O 576 468 11 44 53	0
20	4	1	Total C Mg N O 576 468 11 44 53	0
20	5	1	Total C Mg N O 737 597 14 56 70	0
20	5	1	Total C Mg N O 737 597 14 56 70	0
20	5	1	Total C Mg N O 737 597 14 56 70	0
20	5	1	Total C Mg N O 737 597 14 56 70	0
20	5	1	Total C Mg N O 737 597 14 56 70	0
20	5	1	Total C Mg N O 737 597 14 56 70	0
20	5	1	Total C Mg N O 737 597 14 56 70	0
20	5	1	Total C Mg N O 737 597 14 56 70	0
20	5	1	Total C Mg N O 737 597 14 56 70	0
20	5	1	Total C Mg N O 737 597 14 56 70	0
20	5	1	Total C Mg N O 737 597 14 56 70	0
20	5	1	Total C Mg N O 737 597 14 56 70	0

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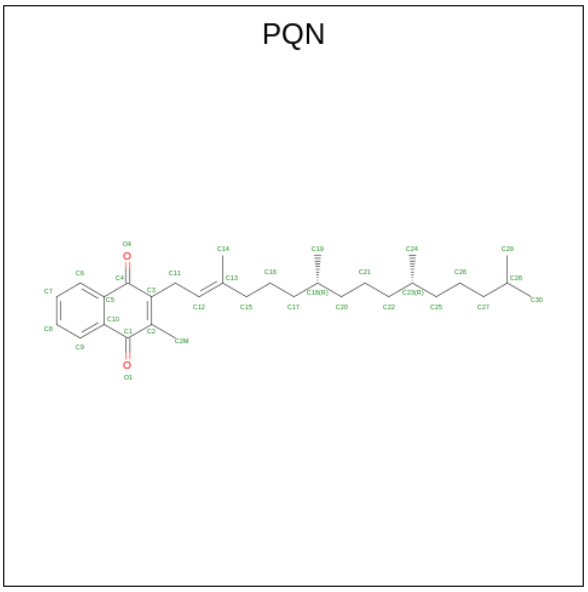
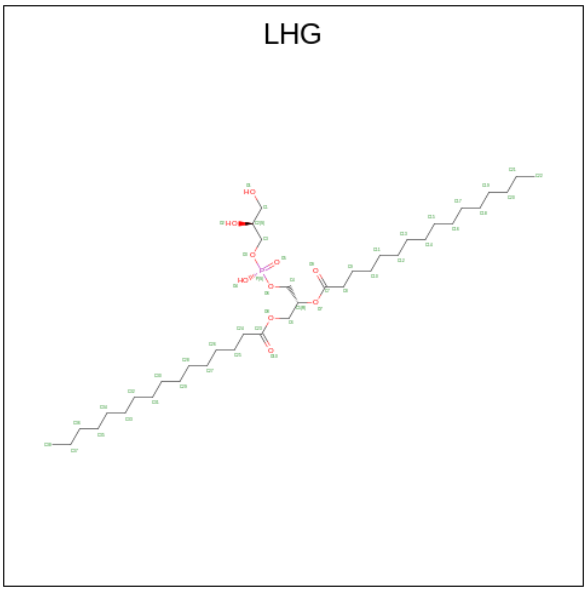
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
20	5	1	737	597	14	56	70	0
20	5	1	737	597	14	56	70	0
20	6	1	696	566	13	52	65	0
20	6	1	696	566	13	52	65	0
20	6	1	696	566	13	52	65	0
20	6	1	696	566	13	52	65	0
20	6	1	696	566	13	52	65	0
20	6	1	696	566	13	52	65	0
20	6	1	696	566	13	52	65	0
20	6	1	696	566	13	52	65	0
20	6	1	696	566	13	52	65	0
20	6	1	696	566	13	52	65	0
20	6	1	696	566	13	52	65	0
20	6	1	696	566	13	52	65	0
20	6	1	696	566	13	52	65	0

- Molecule 21 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



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

- Molecule 22 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



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

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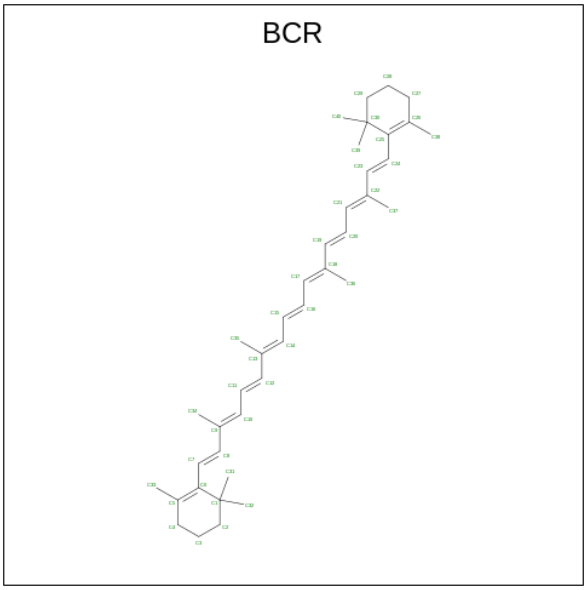
Mol	Chain	Residues	Atoms				AltConf
22	A	1	Total	C	O	P	0
			117	84	30	3	
22	A	1	Total	C	O	P	0
			117	84	30	3	
22	B	1	Total	C	O	P	0
			23	12	10	1	
22	1	1	Total	C	O	P	0
			43	32	10	1	
22	7	1	Total	C	O	P	0
			37	26	10	1	
22	8	1	Total	C	O	P	0
			37	26	10	1	
22	Z	1	Total	C	O	P	0
			43	32	10	1	
22	4	1	Total	C	O	P	0
			81	59	20	2	
22	4	1	Total	C	O	P	0
			81	59	20	2	
22	5	1	Total	C	O	P	0
			37	26	10	1	
22	6	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 23 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	AltConf
23	A	1	Total C 240 240	0
23	A	1	Total C 240 240	0
23	A	1	Total C 240 240	0
23	A	1	Total C 240 240	0
23	A	1	Total C 240 240	0
23	A	1	Total C 240 240	0
23	B	1	Total C 280 280	0
23	B	1	Total C 280 280	0
23	B	1	Total C 280 280	0
23	B	1	Total C 280 280	0
23	B	1	Total C 280 280	0
23	B	1	Total C 280 280	0
23	B	1	Total C 280 280	0
23	F	1	Total C 40 40	0
23	G	1	Total C 40 40	0
23	I	1	Total C 40 40	0
23	J	1	Total C 40 40	0
23	K	1	Total C 80 80	0
23	K	1	Total C 80 80	0
23	L	1	Total C 80 80	0
23	L	1	Total C 80 80	0
23	3	1	Total C 120 120	0

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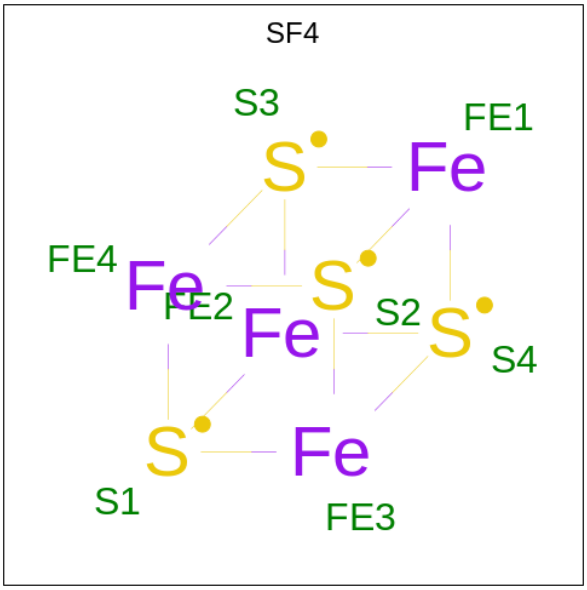
Mol	Chain	Residues	Atoms	AltConf
23	3	1	Total C 120 120	0
23	3	1	Total C 120 120	0
23	7	1	Total C 80 80	0
23	7	1	Total C 80 80	0
23	8	1	Total C 40 40	0
23	4	1	Total C 40 40	0
23	5	1	Total C 80 80	0
23	5	1	Total C 80 80	0
23	6	1	Total C 80 80	0
23	6	1	Total C 80 80	0

- Molecule 24 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

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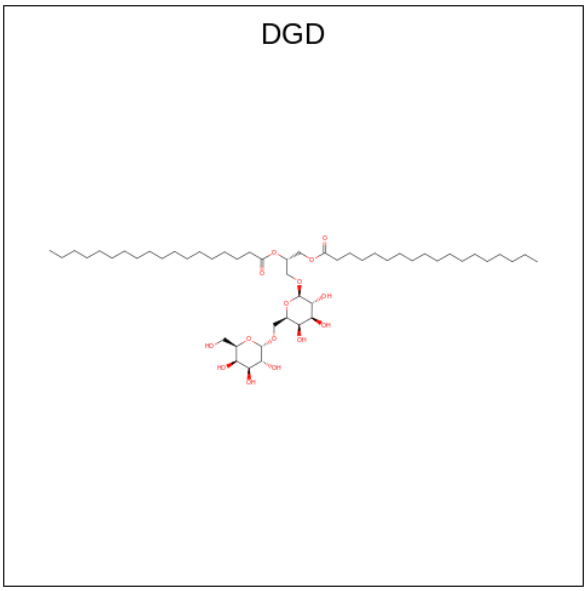
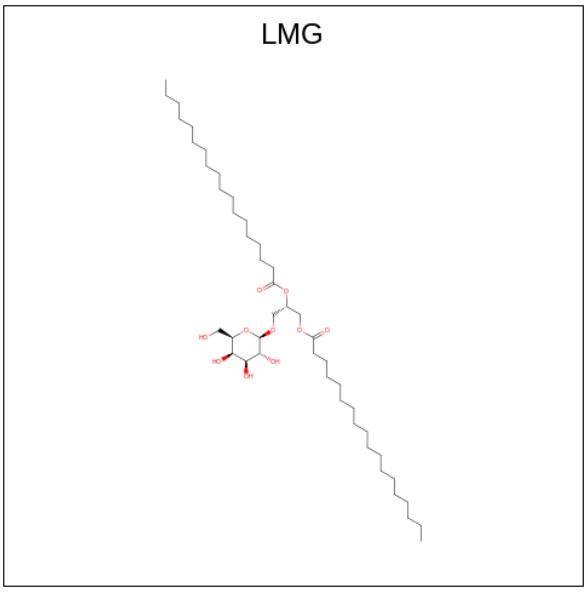
Mol	Chain	Residues	Atoms			AltConf
24	C	1	Total	Fe	S	0
			16	8	8	
24	C	1	Total	Fe	S	0
			16	8	8	

- Molecule 25 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



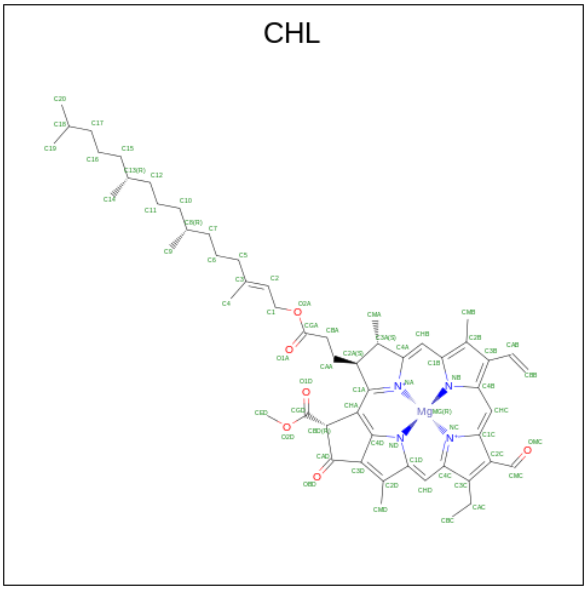
Mol	Chain	Residues	Atoms			AltConf
25	B	1	Total	C	O	0
			66	51	15	

- Molecule 26 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
26	J	1	Total	C	O	0
			35	25	10	

- Molecule 27 is CHLOROPHYLL B (three-letter code: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
27	1	1	Total	C	Mg	N	O	0
			101	79	2	8	12	
27	1	1	Total	C	Mg	N	O	0
			101	79	2	8	12	
27	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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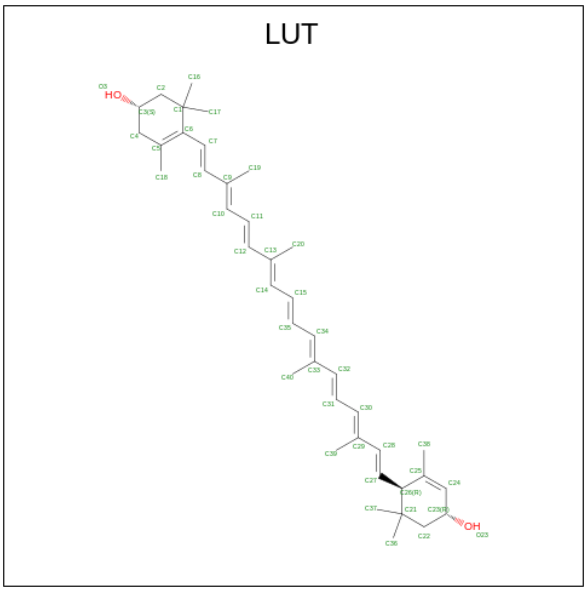
Mol	Chain	Residues	Atoms					AltConf
27	7	1	Total	C	Mg	N	O	0
			54	43	1	4	6	
27	8	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
27	Z	1	Total	C	Mg	N	O	0
			101	79	2	8	12	
27	Z	1	Total	C	Mg	N	O	0
			101	79	2	8	12	
27	4	1	Total	C	Mg	N	O	0
			201	159	4	16	22	
27	4	1	Total	C	Mg	N	O	0
			201	159	4	16	22	
27	4	1	Total	C	Mg	N	O	0
			201	159	4	16	22	
27	4	1	Total	C	Mg	N	O	0
			201	159	4	16	22	
27	5	1	Total	C	Mg	N	O	0
			145	114	3	12	16	
27	5	1	Total	C	Mg	N	O	0
			145	114	3	12	16	
27	5	1	Total	C	Mg	N	O	0
			145	114	3	12	16	
27	6	1	Total	C	Mg	N	O	0
			206	164	4	16	22	
27	6	1	Total	C	Mg	N	O	0
			206	164	4	16	22	
27	6	1	Total	C	Mg	N	O	0
			206	164	4	16	22	
27	6	1	Total	C	Mg	N	O	0
			206	164	4	16	22	

- Molecule 28 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
28	1	1	Total	C	O	0
			126	120	6	
28	1	1	Total	C	O	0
			126	120	6	
28	1	1	Total	C	O	0
			126	120	6	
28	3	1	Total	C	O	0
			84	80	4	
28	3	1	Total	C	O	0
			84	80	4	
28	7	1	Total	C	O	0
			84	80	4	
28	7	1	Total	C	O	0
			84	80	4	
28	8	1	Total	C	O	0
			84	80	4	
28	8	1	Total	C	O	0
			84	80	4	
28	Z	1	Total	C	O	0
			126	120	6	
28	Z	1	Total	C	O	0
			126	120	6	
28	Z	1	Total	C	O	0
			126	120	6	
28	4	1	Total	C	O	0
			84	80	4	
28	4	1	Total	C	O	0
			84	80	4	

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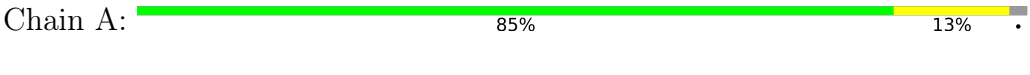
Mol	Chain	Residues	Atoms			AltConf
28	5	1	Total	C	O	0
			84	80	4	
28	5	1	Total	C	O	0
			84	80	4	
28	6	1	Total	C	O	0
			84	80	4	
28	6	1	Total	C	O	0
			84	80	4	

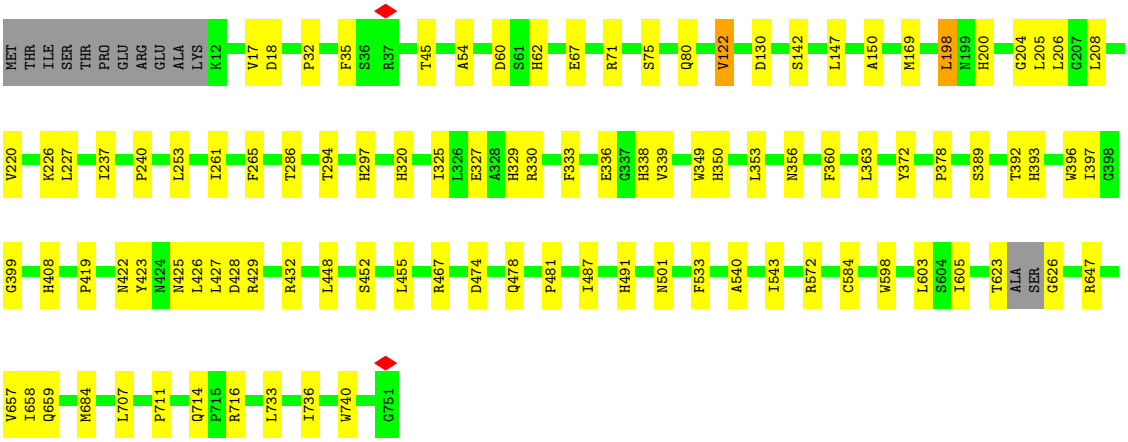
3 Residue-property plots (i)

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

• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

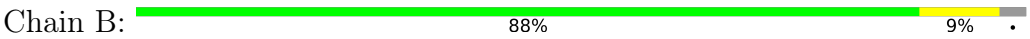
Chain A:

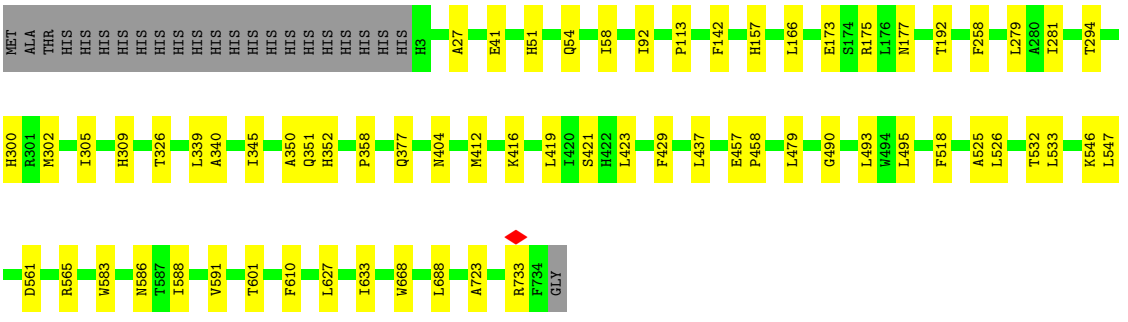




• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

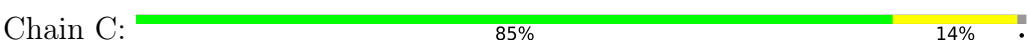
Chain B:

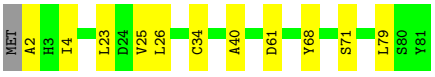




• Molecule 3: Photosystem I iron-sulfur center

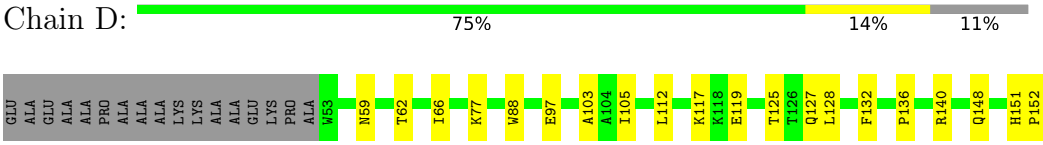
Chain C:





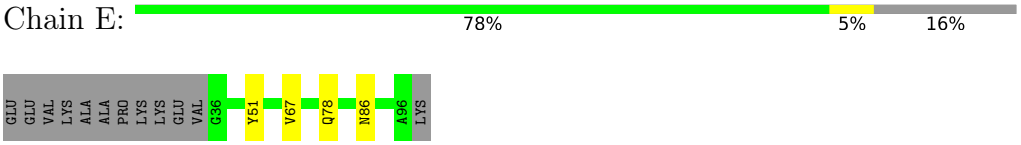
• Molecule 4: Photosystem I reaction center subunit II, chloroplastic

Chain D:



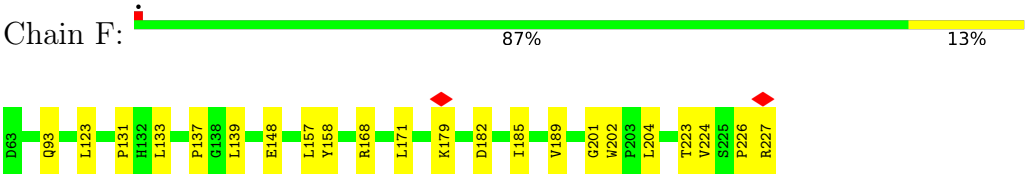
• Molecule 5: Photosystem I reaction center subunit IV, chloroplastic

Chain E:



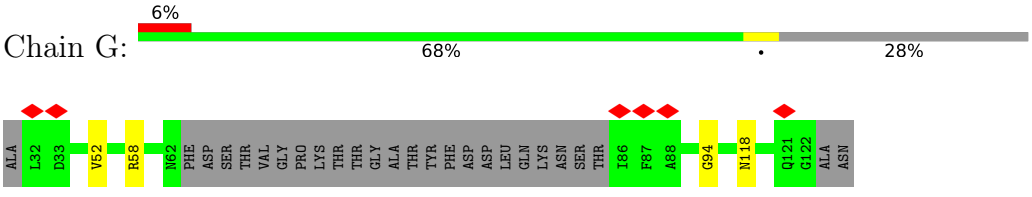
• Molecule 6: Photosystem I reaction center subunit F, Photosystem I reaction center subunit III, chloroplastic

Chain F:



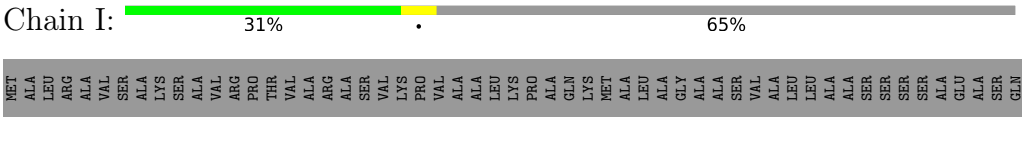
• Molecule 7: Photosystem I reaction center subunit V, chloroplastic

Chain G:



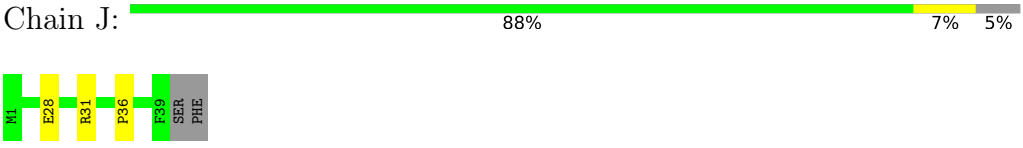
• Molecule 8: Photosystem I reaction center subunit VIII

Chain I:



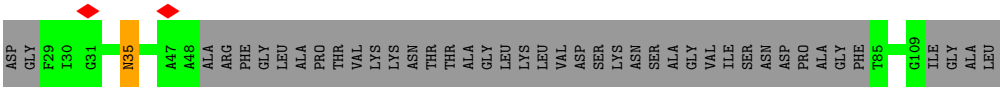
• Molecule 9: Photosystem I reaction center subunit IX

Chain J:



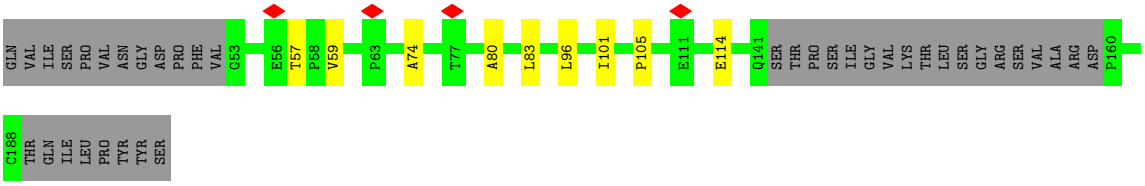
• Molecule 10: Photosystem I reaction center subunit psaK, chloroplastic

Chain K:



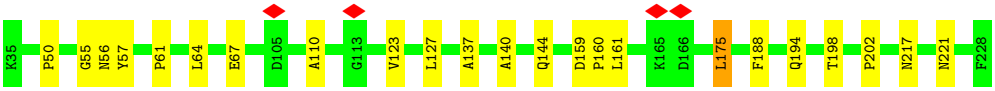
• Molecule 11: Photosystem I reaction center subunit XI

Chain L:



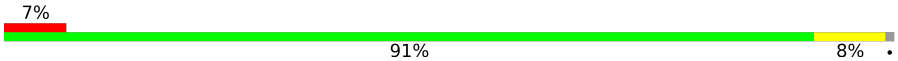
• Molecule 12: Chlorophyll a-b binding protein, chloroplastic

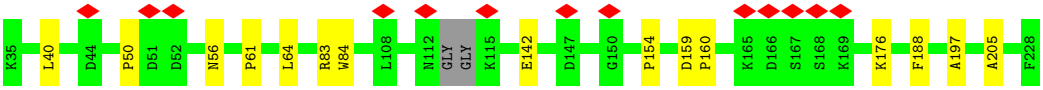
Chain 1:



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

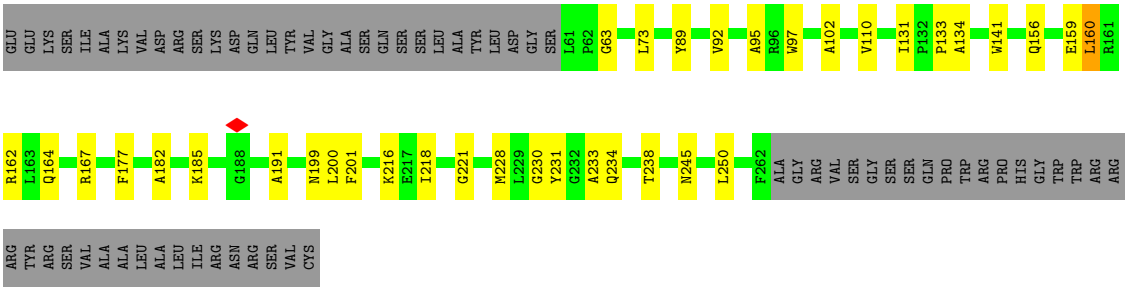
Chain Z:





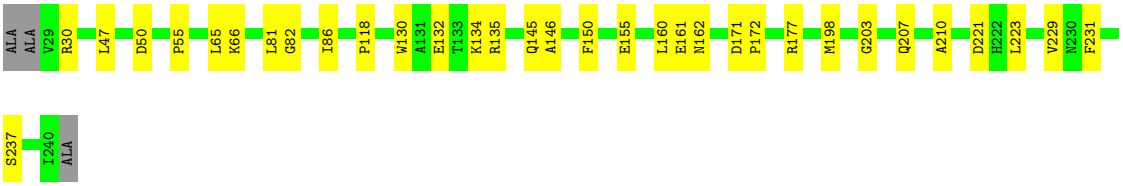
• Molecule 13: Chlorophyll a-b binding protein, chloroplastic

Chain 3:



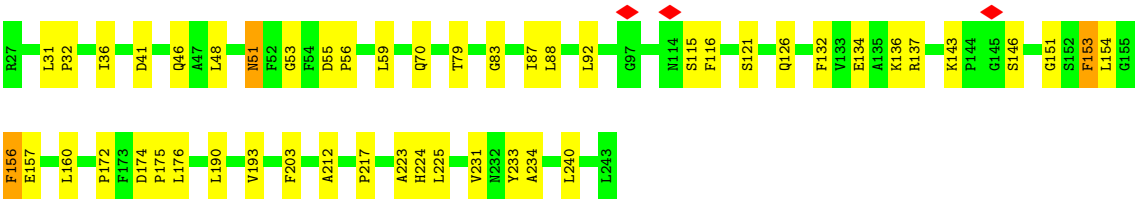
• Molecule 14: Chlorophyll a-b binding protein, chloroplastic

Chain 7:



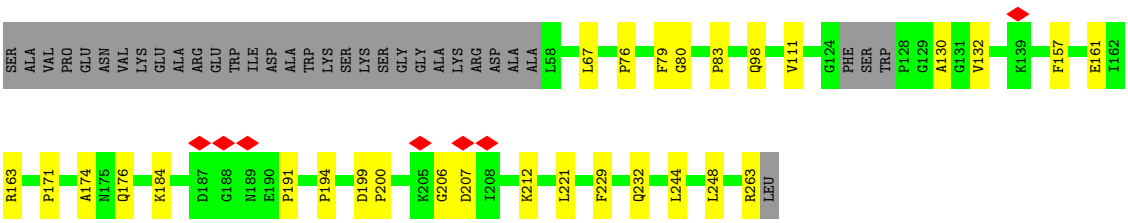
• Molecule 15: Chlorophyll a-b binding protein, chloroplastic

Chain 8:



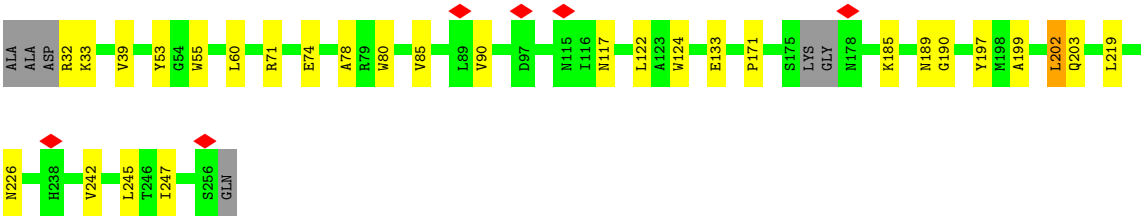
• Molecule 16: Chlorophyll a-b binding protein, chloroplastic

Chain 4:



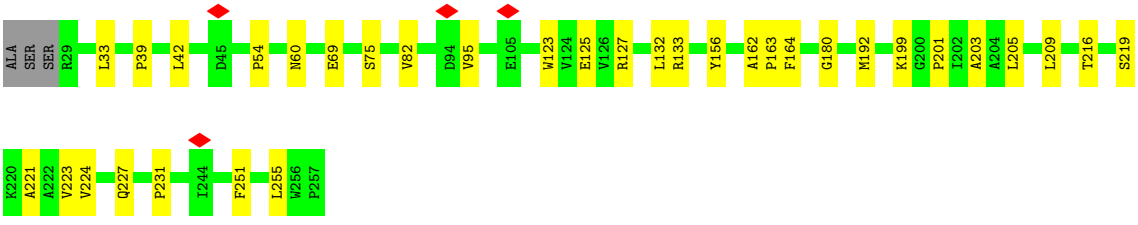
• Molecule 17: Chlorophyll a-b binding protein, chloroplastic

Chain 5:



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

Chain 6:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	379749	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50.0	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	3750	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.460	Depositor
Minimum map value	-0.221	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.011	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: BCR, CLA, PQN, CL0, CHL, DGD, LHG, LMG, LUT, SF4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.35	0/5995	0.59	2/8172 (0.0%)
2	B	0.33	0/6035	0.54	2/8240 (0.0%)
3	C	0.32	0/610	0.60	1/826 (0.1%)
4	D	0.32	0/1160	0.53	0/1567
5	E	0.31	0/490	0.46	0/667
6	F	0.32	0/1291	0.58	0/1747
7	G	0.27	0/513	0.48	0/696
8	I	0.32	0/293	0.59	0/406
9	J	0.33	0/331	0.55	0/454
10	K	0.27	0/297	0.53	0/401
11	L	0.29	0/874	0.57	0/1194
12	1	0.30	0/1490	0.52	1/2028 (0.0%)
12	Z	0.30	0/1481	0.52	0/2015
13	3	0.35	0/1601	0.56	1/2173 (0.0%)
14	7	0.33	0/1696	0.55	0/2303
15	8	0.31	0/1700	0.61	1/2315 (0.0%)
16	4	0.33	0/1621	0.53	0/2209
17	5	0.30	0/1798	0.51	0/2450
18	6	0.30	0/1827	0.54	0/2497
All	All	0.32	0/31103	0.55	8/42360 (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
16	4	0	1
All	All	0	3

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	198	LEU	CA-CB-CG	7.63	132.85	115.30
15	8	240	LEU	CA-CB-CG	7.33	132.16	115.30
2	B	688	LEU	CA-CB-CG	5.74	128.49	115.30
1	A	455	LEU	CA-CB-CG	5.72	128.46	115.30
3	C	23	LEU	CB-CG-CD1	-5.46	101.72	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	4	206	GLY	Peptide
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	73	0
2	B	5822	0	5574	49	0
3	C	600	0	581	7	0
4	D	1132	0	1150	14	0
5	E	480	0	476	4	0
6	F	1265	0	1301	15	0
7	G	503	0	496	2	0
8	I	281	0	292	4	0
9	J	320	0	322	3	0
10	K	297	0	319	1	0
11	L	853	0	864	7	0
12	1	1444	0	1396	18	0
12	Z	1436	0	1389	15	0
13	3	1555	0	1522	26	0
14	7	1644	0	1584	28	0
15	8	1649	0	1629	48	0
16	4	1570	0	1527	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	5	1744	0	1717	32	0
18	6	1765	0	1767	29	0
19	A	65	0	72	1	0
20	1	722	0	735	23	0
20	3	696	0	631	20	0
20	4	576	0	495	22	0
20	5	737	0	638	27	0
20	6	696	0	622	21	0
20	7	741	0	665	22	0
20	8	680	0	593	21	0
20	A	2689	0	2798	122	0
20	B	2480	0	2545	99	0
20	F	175	0	177	8	0
20	G	96	0	72	0	0
20	J	42	0	31	0	0
20	K	91	0	66	3	0
20	L	115	0	111	1	0
20	Z	714	0	716	22	0
21	A	33	0	46	1	0
21	B	33	0	46	1	0
22	1	43	0	56	0	0
22	4	81	0	108	6	0
22	5	37	0	44	1	0
22	6	49	0	73	3	0
22	7	37	0	44	1	0
22	8	37	0	44	0	0
22	A	117	0	153	6	0
22	B	23	0	16	2	0
22	Z	43	0	56	3	0
23	3	120	0	168	15	0
23	4	40	0	56	2	0
23	5	80	0	112	10	0
23	6	80	0	112	9	0
23	7	80	0	112	6	0
23	8	40	0	56	5	0
23	A	240	0	336	20	0
23	B	280	0	392	22	0
23	F	40	0	56	6	0
23	G	40	0	56	4	0
23	I	40	0	56	2	0
23	J	40	0	56	3	0
23	K	80	0	112	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	L	80	0	112	4	0
24	A	8	0	0	0	0
24	C	16	0	0	0	0
25	B	66	0	96	2	0
26	J	35	0	40	0	0
27	1	101	0	74	3	0
27	3	66	0	70	5	0
27	4	201	0	150	1	0
27	5	145	0	103	5	0
27	6	206	0	160	7	0
27	7	54	0	43	0	0
27	8	56	0	47	1	0
27	Z	101	0	74	5	0
28	1	126	0	168	15	0
28	3	84	0	112	6	0
28	4	84	0	112	9	0
28	5	84	0	112	9	0
28	6	84	0	112	11	0
28	7	84	0	112	9	0
28	8	84	0	112	15	0
28	Z	126	0	168	11	0
All	All	45099	0	44862	716	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 716 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)
15:8:156:PHE:CZ	15:8:172:PRO:HG3	1.95	0.99
17:5:185:LYS:O	17:5:189:ASN:ND2	2.01	0.94
15:8:156:PHE:CE1	15:8:172:PRO:HG3	2.06	0.90
17:5:199:ALA:O	17:5:203:GLN:HG3	1.85	0.77
20:3:610:CLA:HBB1	28:3:621:LUT:H32	1.66	0.77

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%)	712 (97%)	21 (3%)	1 (0%)	51	82
2	B	730/755 (97%)	706 (97%)	24 (3%)	0	100	100
3	C	78/81 (96%)	73 (94%)	5 (6%)	0	100	100
4	D	142/161 (88%)	134 (94%)	8 (6%)	0	100	100
5	E	59/73 (81%)	54 (92%)	5 (8%)	0	100	100
6	F	163/165 (99%)	158 (97%)	5 (3%)	0	100	100
7	G	64/94 (68%)	63 (98%)	1 (2%)	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%)	110 (96%)	4 (4%)	0	100	100
12	1	192/194 (99%)	186 (97%)	6 (3%)	0	100	100
12	Z	188/194 (97%)	180 (96%)	8 (4%)	0	100	100
13	3	200/268 (75%)	194 (97%)	6 (3%)	0	100	100
14	7	210/215 (98%)	198 (94%)	12 (6%)	0	100	100
15	8	215/217 (99%)	206 (96%)	9 (4%)	0	100	100
16	4	199/236 (84%)	184 (92%)	14 (7%)	1 (0%)	29	61
17	5	219/229 (96%)	201 (92%)	18 (8%)	0	100	100
18	6	227/232 (98%)	215 (95%)	12 (5%)	0	100	100
All	All	3847/4255 (90%)	3684 (96%)	161 (4%)	2 (0%)	54	82

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	VAL
16	4	207	ASP

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%)	592 (99%)	7 (1%)	71 91
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%)	120 (99%)	1 (1%)	81 94
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%)	85 (100%)	0	100 100
12	1	137/137 (100%)	136 (99%)	1 (1%)	84 95
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%)	160 (98%)	3 (2%)	59 85
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
All	All	3072/3340 (92%)	3049 (99%)	23 (1%)	84 95

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	7	177	ARG
15	8	156	PHE
15	8	153	PHE
16	4	263	ARG

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Mol	Chain	Res	Type
1	A	657	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
17	5	142	ASN
18	6	227	GLN
17	5	226	ASN
13	3	245	ASN
12	Z	221	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

285 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	LHG	8	620	20	36,36,48	1.03	2 (5%)	39,42,54	1.13	2 (5%)
20	CLA	5	612	-	52,60,73	2.30	18 (34%)	60,97,113	3.01	26 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	BCR	8	619	-	41,41,41	0.68	0	56,56,56	1.83	13 (23%)
20	CLA	B	811	-	54,62,73	2.13	16 (29%)	67,100,113	3.04	29 (43%)
20	CLA	F	304	6	65,73,73	2.02	17 (26%)	76,113,113	2.79	28 (36%)
20	CLA	K	4003	-	46,54,73	2.44	15 (32%)	53,90,113	3.15	23 (43%)
20	CLA	B	837	-	65,73,73	2.01	16 (24%)	76,113,113	2.75	30 (39%)
20	CLA	1	608	-	65,73,73	2.04	17 (26%)	76,113,113	2.65	27 (35%)
20	CLA	3	620	-	56,64,73	2.19	17 (30%)	65,102,113	2.86	25 (38%)
20	CLA	Z	613	-	65,73,73	2.05	17 (26%)	76,113,113	2.59	25 (32%)
20	CLA	A	829	-	65,73,73	1.98	16 (24%)	76,113,113	2.74	29 (38%)
20	CLA	A	806	-	65,73,73	1.99	15 (23%)	76,113,113	2.70	25 (32%)
20	CLA	5	603	-	46,54,73	2.40	17 (36%)	53,90,113	3.14	25 (47%)
20	CLA	5	604	17	50,58,73	2.32	15 (30%)	58,95,113	3.05	26 (44%)
21	PQN	A	844	-	34,34,34	1.57	2 (5%)	42,45,45	1.09	3 (7%)
20	CLA	B	813	-	65,73,73	2.01	17 (26%)	76,113,113	2.70	27 (35%)
20	CLA	5	602	17	65,73,73	2.01	15 (23%)	76,113,113	2.76	28 (36%)
20	CLA	B	802	-	65,73,73	1.95	17 (26%)	76,113,113	2.84	27 (35%)
23	BCR	B	801	-	41,41,41	0.73	0	56,56,56	1.93	16 (28%)
27	CHL	5	607	-	51,59,74	2.28	17 (33%)	55,96,114	3.33	30 (54%)
20	CLA	B	841	22	65,73,73	2.03	16 (24%)	76,113,113	2.72	28 (36%)
20	CLA	7	606	-	42,50,73	2.43	16 (38%)	48,85,113	3.43	24 (50%)
28	LUT	6	621	-	42,43,43	0.70	0	51,60,60	1.51	11 (21%)
20	CLA	6	616	18	46,54,73	2.46	16 (34%)	53,90,113	3.13	26 (49%)
23	BCR	A	851	-	41,41,41	0.80	1 (2%)	56,56,56	1.85	13 (23%)
20	CLA	7	612	14	52,60,73	2.25	16 (30%)	60,97,113	3.15	27 (45%)
27	CHL	3	608	-	66,74,74	1.91	16 (24%)	73,114,114	2.92	25 (34%)
26	LMG	J	3001	-	35,35,55	0.96	0	43,43,63	1.23	6 (13%)
20	CLA	8	610	15	60,68,73	2.09	14 (23%)	70,107,113	2.91	31 (44%)
20	CLA	4	613	16	56,64,73	2.20	16 (28%)	65,102,113	2.90	28 (43%)
20	CLA	G	204	7	46,54,73	2.46	16 (34%)	53,90,113	3.15	25 (47%)
20	CLA	B	814	-	60,68,73	2.09	16 (26%)	70,107,113	2.81	28 (40%)
20	CLA	4	616	16	41,49,73	2.55	16 (39%)	47,84,113	3.48	25 (53%)
20	CLA	6	604	-	65,73,73	2.05	17 (26%)	76,113,113	2.64	27 (35%)
20	CLA	B	839	-	65,73,73	2.04	17 (26%)	76,113,113	2.67	26 (34%)
22	LHG	1	620	20	42,42,48	0.99	2 (4%)	45,48,54	1.08	3 (6%)
20	CLA	8	612	15	52,60,73	2.25	17 (32%)	60,97,113	3.03	30 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	LUT	3	622	-	42,43,43	0.79	0	51,60,60	1.71	14 (27%)
20	CLA	A	810	1	65,73,73	1.99	18 (27%)	76,113,113	2.66	27 (35%)
20	CLA	Z	610	12	60,68,73	2.10	15 (25%)	70,107,113	2.88	29 (41%)
20	CLA	A	805	20	55,63,73	2.16	15 (27%)	64,101,113	2.91	26 (40%)
20	CLA	4	614	-	45,53,73	2.44	16 (35%)	52,89,113	3.14	25 (48%)
23	BCR	K	4001	-	41,41,41	0.69	0	56,56,56	2.00	15 (26%)
20	CLA	B	817	-	59,67,73	2.11	16 (27%)	68,105,113	2.84	26 (38%)
20	CLA	8	604	-	46,54,73	2.43	16 (34%)	53,90,113	3.10	25 (47%)
20	CLA	4	612	16	52,60,73	2.26	17 (32%)	60,97,113	3.05	27 (45%)
20	CLA	5	611	22	55,63,73	2.23	18 (32%)	64,101,113	2.87	27 (42%)
23	BCR	B	845	-	41,41,41	0.71	0	56,56,56	1.85	13 (23%)
23	BCR	B	846	-	41,41,41	0.78	0	56,56,56	1.87	15 (26%)
23	BCR	B	843	-	41,41,41	0.71	0	56,56,56	1.59	9 (16%)
20	CLA	B	834	-	65,73,73	2.07	18 (27%)	76,113,113	2.68	28 (36%)
20	CLA	B	804	-	45,53,73	2.43	16 (35%)	52,89,113	3.30	27 (51%)
23	BCR	I	172	-	41,41,41	0.66	0	56,56,56	2.08	15 (26%)
28	LUT	7	622	-	42,43,43	0.74	0	51,60,60	1.58	10 (19%)
20	CLA	8	608	-	50,58,73	2.27	16 (32%)	58,95,113	3.10	26 (44%)
20	CLA	B	832	-	65,73,73	1.98	15 (23%)	76,113,113	2.76	26 (34%)
20	CLA	B	807	-	65,73,73	2.05	16 (24%)	76,113,113	2.74	27 (35%)
20	CLA	L	204	-	50,58,73	2.36	16 (32%)	58,95,113	3.09	25 (43%)
23	BCR	J	3003	-	41,41,41	0.72	0	56,56,56	1.73	12 (21%)
23	BCR	F	305	-	41,41,41	0.70	0	56,56,56	1.92	17 (30%)
20	CLA	7	610	14	60,68,73	2.09	15 (25%)	70,107,113	2.90	29 (41%)
20	CLA	A	838	-	51,59,73	2.30	16 (31%)	59,96,113	3.08	29 (49%)
20	CLA	L	203	-	65,73,73	2.01	16 (24%)	76,113,113	2.73	26 (34%)
27	CHL	4	607	-	51,59,74	2.28	16 (31%)	55,96,114	3.32	24 (43%)
23	BCR	B	847	-	41,41,41	0.77	0	56,56,56	1.92	14 (25%)
20	CLA	A	814	-	65,73,73	1.99	17 (26%)	76,113,113	2.78	27 (35%)
20	CLA	A	831	-	65,73,73	2.00	15 (23%)	76,113,113	2.77	27 (35%)
20	CLA	7	614	-	43,51,73	2.40	15 (34%)	49,86,113	3.33	26 (53%)
20	CLA	8	601	15	65,73,73	2.02	18 (27%)	76,113,113	2.67	28 (36%)
22	LHG	6	619	20	48,48,48	0.93	2 (4%)	51,54,54	1.04	2 (3%)
20	CLA	1	604	-	57,65,73	2.20	16 (28%)	66,103,113	2.85	30 (45%)
20	CLA	A	821	-	45,53,73	2.43	16 (35%)	52,89,113	3.15	25 (48%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	LHG	B	851	20	22,22,48	1.15	2 (9%)	25,28,54	1.24	2 (8%)
20	CLA	6	602	18	65,73,73	2.03	16 (24%)	76,113,113	2.71	27 (35%)
23	BCR	3	717	-	41,41,41	0.73	0	56,56,56	1.82	14 (25%)
28	LUT	Z	618	-	42,43,43	0.75	0	51,60,60	1.59	14 (27%)
23	BCR	L	201	-	41,41,41	0.71	0	56,56,56	1.72	10 (17%)
23	BCR	5	625	-	41,41,41	0.69	0	56,56,56	2.33	20 (35%)
20	CLA	3	614	-	45,53,73	2.48	16 (35%)	52,89,113	3.25	25 (48%)
28	LUT	4	619	-	42,43,43	0.73	0	51,60,60	1.61	13 (25%)
27	CHL	8	607	-	56,64,74	2.15	18 (32%)	61,102,114	3.07	25 (40%)
20	CLA	5	601	17	65,73,73	2.06	17 (26%)	76,113,113	2.69	27 (35%)
20	CLA	5	617	-	46,54,73	2.33	17 (36%)	53,90,113	3.26	23 (43%)
20	CLA	3	607	13	60,68,73	2.14	16 (26%)	70,107,113	2.84	27 (38%)
20	CLA	5	614	-	45,53,73	2.47	16 (35%)	52,89,113	3.19	25 (48%)
23	BCR	A	856	-	41,41,41	0.78	0	56,56,56	1.88	14 (25%)
20	CLA	A	842	-	65,73,73	1.99	17 (26%)	76,113,113	2.82	28 (36%)
20	CLA	B	821	-	46,54,73	2.41	16 (34%)	53,90,113	3.19	23 (43%)
20	CLA	A	815	-	60,68,73	2.14	16 (26%)	70,107,113	2.80	27 (38%)
20	CLA	B	835	-	45,53,73	2.47	17 (37%)	52,89,113	3.07	25 (48%)
20	CLA	3	606	-	42,50,73	2.47	15 (35%)	48,85,113	3.28	23 (47%)
20	CLA	4	611	22	55,63,73	2.25	17 (30%)	64,101,113	2.80	27 (42%)
20	CLA	A	840	-	65,73,73	2.00	17 (26%)	76,113,113	2.84	28 (36%)
20	CLA	B	810	-	65,73,73	2.05	17 (26%)	76,113,113	2.73	27 (35%)
27	CHL	6	618	18	43,51,74	2.38	16 (37%)	45,86,114	3.59	23 (51%)
20	CLA	3	617	13	46,54,73	2.41	17 (36%)	53,90,113	3.18	25 (47%)
27	CHL	Z	601	12	53,61,74	2.25	18 (33%)	57,98,114	3.23	26 (45%)
27	CHL	1	607	-	48,56,74	2.37	19 (39%)	51,92,114	3.07	20 (39%)
20	CLA	A	826	-	65,73,73	1.97	16 (24%)	76,113,113	2.66	24 (31%)
23	BCR	7	623	-	41,41,41	0.70	0	56,56,56	1.99	15 (26%)
20	CLA	7	604	-	56,64,73	2.16	17 (30%)	65,102,113	2.97	26 (40%)
20	CLA	B	820	-	56,64,73	2.19	17 (30%)	65,102,113	2.91	28 (43%)
20	CLA	8	613	15	65,73,73	2.00	15 (23%)	76,113,113	2.68	27 (35%)
20	CLA	F	301	-	65,73,73	2.03	17 (26%)	76,113,113	2.74	28 (36%)
20	CLA	1	616	12	46,54,73	2.43	17 (36%)	53,90,113	3.01	25 (47%)
20	CLA	A	833	-	65,73,73	2.01	16 (24%)	76,113,113	2.74	27 (35%)
20	CLA	5	621	-	46,54,73	2.40	17 (36%)	53,90,113	3.08	26 (49%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	BCR	K	4004	-	41,41,41	0.70	0	56,56,56	1.64	10 (17%)
20	CLA	5	609	17	50,58,73	2.31	17 (34%)	58,95,113	3.12	27 (46%)
20	CLA	A	845	22	52,60,73	2.30	17 (32%)	60,97,113	3.07	24 (40%)
27	CHL	7	607	-	54,62,74	2.20	17 (31%)	58,99,114	3.01	23 (39%)
20	CLA	B	831	-	49,57,73	2.33	16 (32%)	55,93,113	3.19	24 (43%)
28	LUT	7	621	-	42,43,43	0.74	0	51,60,60	1.55	11 (21%)
28	LUT	5	620	-	42,43,43	0.76	0	51,60,60	1.69	13 (25%)
20	CLA	G	203	-	50,58,73	2.34	16 (32%)	58,95,113	3.13	27 (46%)
20	CLA	F	303	-	45,53,73	2.44	18 (40%)	52,89,113	3.20	23 (44%)
20	CLA	3	610	13	65,73,73	2.01	14 (21%)	76,113,113	2.78	29 (38%)
20	CLA	7	608	-	50,58,73	2.29	16 (32%)	58,95,113	3.07	25 (43%)
21	PQN	B	842	-	34,34,34	1.55	2 (5%)	42,45,45	1.05	2 (4%)
20	CLA	3	611	-	41,49,73	2.56	16 (39%)	47,84,113	3.33	25 (53%)
22	LHG	4	623	-	31,31,48	1.15	2 (6%)	34,37,54	1.14	3 (8%)
27	CHL	6	606	-	56,64,74	2.13	16 (28%)	61,102,114	3.16	24 (39%)
28	LUT	3	621	-	42,43,43	0.77	0	51,60,60	1.61	12 (23%)
20	CLA	A	822	-	65,73,73	2.00	16 (24%)	76,113,113	2.56	27 (35%)
20	CLA	A	827	-	65,73,73	2.03	15 (23%)	76,113,113	2.74	27 (35%)
20	CLA	Z	616	12	46,54,73	2.44	17 (36%)	53,90,113	3.04	24 (45%)
27	CHL	6	608	-	51,59,74	2.22	17 (33%)	55,96,114	3.50	25 (45%)
20	CLA	A	818	-	65,73,73	2.00	15 (23%)	76,113,113	2.88	28 (36%)
20	CLA	B	805	-	65,73,73	2.04	17 (26%)	76,113,113	2.76	25 (32%)
23	BCR	L	205	-	41,41,41	0.71	0	56,56,56	1.69	11 (19%)
20	CLA	B	816	-	55,63,73	2.18	16 (29%)	64,101,113	2.97	26 (40%)
20	CLA	J	3002	9	42,50,73	2.45	15 (35%)	48,85,113	3.34	24 (50%)
28	LUT	Z	617	-	42,43,43	0.77	0	51,60,60	1.61	14 (27%)
20	CLA	7	613	14	65,73,73	2.00	18 (27%)	76,113,113	2.64	25 (32%)
28	LUT	Z	619	-	42,43,43	0.72	0	51,60,60	1.71	11 (21%)
20	CLA	5	610	17	60,68,73	2.11	15 (25%)	70,107,113	2.85	29 (41%)
22	LHG	5	623	20	36,36,48	1.06	2 (5%)	39,42,54	1.12	2 (5%)
20	CLA	3	612	13	46,54,73	2.41	17 (36%)	53,90,113	3.22	26 (49%)
27	CHL	6	607	-	56,64,74	2.12	16 (28%)	61,102,114	3.10	27 (44%)
20	CLA	6	617	-	46,54,73	2.42	18 (39%)	53,90,113	3.15	25 (47%)
27	CHL	5	618	17	43,51,74	2.39	16 (37%)	45,86,114	3.63	23 (51%)
20	CLA	A	837	1	45,53,73	2.48	17 (37%)	52,89,113	3.16	25 (48%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	CLA	A	823	-	49,57,73	2.33	17 (34%)	55,93,113	3.14	23 (41%)
20	CLA	B	836	-	60,68,73	2.14	18 (30%)	70,107,113	2.93	29 (41%)
20	CLA	A	843	-	65,73,73	2.01	16 (24%)	76,113,113	2.61	26 (34%)
28	LUT	8	618	-	42,43,43	0.76	0	51,60,60	1.68	13 (25%)
27	CHL	4	606	-	56,64,74	2.13	17 (30%)	61,102,114	3.05	23 (37%)
20	CLA	4	609	16	50,58,73	2.29	18 (36%)	58,95,113	3.16	28 (48%)
28	LUT	1	619	-	42,43,43	0.73	0	51,60,60	1.68	9 (17%)
20	CLA	A	813	-	54,62,73	2.23	16 (29%)	62,99,113	2.93	26 (41%)
20	CLA	8	609	15	46,54,73	2.39	16 (34%)	53,90,113	3.12	25 (47%)
20	CLA	Z	608	-	65,73,73	2.06	17 (26%)	76,113,113	2.64	27 (35%)
20	CLA	Z	603	-	57,65,73	2.18	17 (29%)	66,103,113	2.94	30 (45%)
20	CLA	4	601	16	61,69,73	2.09	16 (26%)	71,108,113	2.77	29 (40%)
23	BCR	3	719	-	41,41,41	0.71	0	56,56,56	1.75	12 (21%)
20	CLA	1	613	-	65,73,73	2.03	16 (24%)	76,113,113	2.62	26 (34%)
28	LUT	1	618	-	42,43,43	0.74	0	51,60,60	1.58	13 (25%)
20	CLA	6	611	22	55,63,73	2.24	18 (32%)	64,101,113	2.84	25 (39%)
20	CLA	6	614	-	45,53,73	2.45	17 (37%)	52,89,113	3.31	26 (50%)
24	SF4	A	853	1,2	0,12,12	-	-	-		
20	CLA	A	811	-	65,73,73	2.00	17 (26%)	76,113,113	2.70	27 (35%)
20	CLA	1	602	12	65,73,73	2.03	16 (24%)	76,113,113	2.71	28 (36%)
22	LHG	4	622	20	48,48,48	0.97	2 (4%)	51,54,54	1.11	3 (5%)
20	CLA	A	828	-	65,73,73	1.96	17 (26%)	76,113,113	2.85	25 (32%)
20	CLA	6	610	18	60,68,73	2.16	16 (26%)	70,107,113	2.81	31 (44%)
23	BCR	B	844	-	41,41,41	0.69	0	56,56,56	1.72	12 (21%)
23	BCR	5	622	-	41,41,41	0.65	0	56,56,56	1.84	16 (28%)
20	CLA	1	609	12	65,73,73	2.05	17 (26%)	76,113,113	2.70	26 (34%)
23	BCR	3	718	-	41,41,41	0.72	0	56,56,56	1.92	16 (28%)
20	CLA	B	833	-	58,66,73	2.14	16 (27%)	67,104,113	2.97	30 (44%)
23	BCR	7	624	-	41,41,41	0.66	0	56,56,56	1.78	13 (23%)
27	CHL	5	608	-	51,59,74	2.20	16 (31%)	55,96,114	3.19	25 (45%)
20	CLA	B	808	-	65,73,73	1.99	18 (27%)	76,113,113	2.77	29 (38%)
20	CLA	A	854	-	65,73,73	1.98	14 (21%)	76,113,113	2.85	31 (40%)
20	CLA	B	818	-	60,68,73	2.08	17 (28%)	70,107,113	2.83	30 (42%)
20	CLA	B	852	-	65,73,73	2.07	16 (24%)	76,113,113	2.62	27 (35%)
20	CLA	5	613	17	56,64,73	2.22	16 (28%)	65,102,113	2.77	26 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	CLA	4	610	16	60,68,73	2.12	16 (26%)	70,107,113	2.82	29 (41%)
20	CLA	A	836	-	50,58,73	2.32	16 (32%)	58,95,113	3.03	29 (50%)
20	CLA	Z	611	22	65,73,73	2.07	16 (24%)	76,113,113	2.61	26 (34%)
20	CLA	A	817	-	57,65,73	2.16	17 (29%)	66,103,113	2.93	27 (40%)
20	CLA	B	803	-	65,73,73	2.00	17 (26%)	76,113,113	2.64	26 (34%)
20	CLA	K	4002	-	45,53,73	2.49	16 (35%)	52,89,113	3.20	25 (48%)
20	CLA	3	609	13	50,58,73	2.33	17 (34%)	58,95,113	3.02	29 (50%)
20	CLA	8	603	-	45,53,73	2.40	17 (37%)	52,89,113	3.29	24 (46%)
27	CHL	4	618	16	43,51,74	2.37	16 (37%)	45,86,114	3.61	22 (48%)
28	LUT	4	620	-	42,43,43	0.73	0	51,60,60	1.54	12 (23%)
20	CLA	A	804	-	65,73,73	1.98	17 (26%)	76,113,113	2.87	32 (42%)
23	BCR	4	621	-	41,41,41	0.68	0	56,56,56	1.77	13 (23%)
20	CLA	A	834	-	65,73,73	2.02	16 (24%)	76,113,113	2.79	29 (38%)
20	CLA	B	829	-	65,73,73	2.00	16 (24%)	76,113,113	2.81	30 (39%)
20	CLA	A	807	1	65,73,73	2.04	18 (27%)	76,113,113	2.77	28 (36%)
20	CLA	1	612	12	52,60,73	2.25	16 (30%)	60,97,113	3.08	29 (48%)
20	CLA	7	601	14	65,73,73	2.02	17 (26%)	76,113,113	2.75	26 (34%)
20	CLA	A	830	-	65,73,73	1.97	17 (26%)	76,113,113	2.63	25 (32%)
20	CLA	3	613	13	55,63,73	2.18	17 (30%)	64,101,113	2.88	26 (40%)
20	CLA	A	808	-	65,73,73	2.02	18 (27%)	76,113,113	2.80	28 (36%)
20	CLA	1	610	12	60,68,73	2.12	15 (25%)	70,107,113	2.90	31 (44%)
20	CLA	A	825	-	55,63,73	2.20	17 (30%)	64,101,113	2.86	25 (39%)
20	CLA	1	611	22	65,73,73	2.06	16 (24%)	76,113,113	2.64	28 (36%)
23	BCR	A	848	-	41,41,41	0.69	0	56,56,56	1.72	13 (23%)
23	BCR	6	625	-	41,41,41	0.66	0	56,56,56	1.99	14 (25%)
20	CLA	8	614	-	55,63,73	2.22	17 (30%)	64,101,113	2.91	29 (45%)
20	CLA	1	614	-	65,73,73	2.05	16 (24%)	76,113,113	2.71	26 (34%)
20	CLA	1	603	-	65,73,73	2.03	17 (26%)	76,113,113	2.74	27 (35%)
20	CLA	6	601	18	65,73,73	2.05	16 (24%)	76,113,113	2.68	28 (36%)
20	CLA	7	603	-	46,54,73	2.41	17 (36%)	53,90,113	3.25	24 (45%)
20	CLA	A	819	-	65,73,73	2.02	16 (24%)	76,113,113	2.70	27 (35%)
20	CLA	7	609	14	50,58,73	2.31	16 (32%)	58,95,113	3.20	30 (51%)
20	CLA	8	602	15	62,70,73	2.05	15 (24%)	72,109,113	2.83	27 (37%)
23	BCR	A	850	-	41,41,41	0.72	0	56,56,56	1.90	10 (17%)
27	CHL	4	608	-	51,59,74	2.17	16 (31%)	55,96,114	3.22	25 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	CLA	Z	614	-	65,73,73	2.06	16 (24%)	76,113,113	2.75	26 (34%)
20	CLA	4	603	16	46,54,73	2.37	16 (34%)	53,90,113	3.16	24 (45%)
20	CLA	3	603	-	65,73,73	1.99	17 (26%)	76,113,113	2.65	27 (35%)
22	LHG	A	847	20	37,37,48	1.05	2 (5%)	40,43,54	1.16	3 (7%)
20	CLA	B	838	-	47,55,73	2.32	17 (36%)	54,91,113	3.21	24 (44%)
25	DGD	B	850	-	67,67,67	0.80	2 (2%)	81,81,81	1.05	4 (4%)
20	CLA	1	606	-	52,60,73	2.29	17 (32%)	60,97,113	3.03	27 (45%)
28	LUT	5	624	-	42,43,43	0.77	0	51,60,60	1.55	13 (25%)
23	BCR	A	852	-	41,41,41	0.72	0	56,56,56	1.91	11 (19%)
20	CLA	A	824	-	51,59,73	2.29	18 (35%)	59,96,113	3.06	24 (40%)
22	LHG	Z	620	20	42,42,48	0.99	2 (4%)	45,48,54	1.12	4 (8%)
28	LUT	8	617	-	42,43,43	0.76	0	51,60,60	1.64	12 (23%)
28	LUT	6	624	-	42,43,43	0.72	0	51,60,60	1.50	12 (23%)
20	CLA	A	802	-	65,73,73	1.99	16 (24%)	76,113,113	2.67	30 (39%)
20	CLA	B	823	-	60,68,73	2.10	16 (26%)	70,107,113	2.71	28 (40%)
20	CLA	A	841	-	65,73,73	2.01	16 (24%)	76,113,113	2.76	29 (38%)
20	CLA	B	815	-	57,65,73	2.18	16 (28%)	66,103,113	2.94	26 (39%)
20	CLA	Z	606	-	52,60,73	2.30	17 (32%)	60,97,113	3.00	27 (45%)
27	CHL	1	601	12	53,61,74	2.20	18 (33%)	57,98,114	3.48	26 (45%)
20	CLA	A	839	-	65,73,73	2.01	17 (26%)	76,113,113	2.80	28 (36%)
20	CLA	4	602	16	60,68,73	2.12	17 (28%)	70,107,113	2.83	27 (38%)
20	CLA	B	840	-	65,73,73	2.06	16 (24%)	76,113,113	2.84	26 (34%)
20	CLA	8	616	15	46,54,73	2.41	18 (39%)	53,90,113	3.00	25 (47%)
20	CLA	5	606	-	55,63,73	2.24	17 (30%)	64,101,113	2.90	27 (42%)
20	CLA	6	612	18	52,60,73	2.25	17 (32%)	60,97,113	3.07	26 (43%)
20	CLA	B	806	2	65,73,73	1.98	15 (23%)	76,113,113	2.70	29 (38%)
20	CLA	B	809	2	65,73,73	1.98	16 (24%)	76,113,113	2.63	27 (35%)
20	CLA	6	613	-	56,64,73	2.20	17 (30%)	65,102,113	2.85	26 (40%)
20	CLA	B	826	-	65,73,73	2.00	17 (26%)	76,113,113	2.81	27 (35%)
20	CLA	8	611	22	46,54,73	2.43	17 (36%)	53,90,113	3.09	25 (47%)
20	CLA	Z	602	12	65,73,73	2.02	17 (26%)	76,113,113	2.72	27 (35%)
20	CLA	Z	609	12	65,73,73	2.04	16 (24%)	76,113,113	2.71	28 (36%)
23	BCR	B	848	-	41,41,41	0.71	0	56,56,56	1.58	10 (17%)
24	SF4	C	101	3	0,12,12	-	-	-		
23	BCR	6	623	-	41,41,41	0.63	0	56,56,56	2.02	16 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	CLA	7	620	-	60,68,73	2.16	16 (26%)	70,107,113	2.80	28 (40%)
20	CLA	6	609	18	50,58,73	2.34	17 (34%)	58,95,113	3.04	26 (44%)
22	LHG	7	625	20	36,36,48	1.03	2 (5%)	39,42,54	1.14	2 (5%)
23	BCR	A	849	-	41,41,41	0.75	0	56,56,56	1.74	14 (25%)
20	CLA	A	835	-	65,73,73	2.04	15 (23%)	76,113,113	2.77	24 (31%)
20	CLA	7	616	14	46,54,73	2.41	16 (34%)	53,90,113	3.05	24 (45%)
22	LHG	A	855	-	29,29,48	1.20	2 (6%)	32,35,54	1.19	3 (9%)
24	SF4	C	102	3	0,12,12	-	-	-		
20	CLA	Z	604	-	57,65,73	2.19	16 (28%)	66,103,113	2.83	28 (42%)
20	CLA	B	828	-	65,73,73	2.00	18 (27%)	76,113,113	2.61	25 (32%)
20	CLA	B	819	-	65,73,73	2.01	15 (23%)	76,113,113	2.59	26 (34%)
20	CLA	A	816	-	65,73,73	2.06	16 (24%)	76,113,113	2.70	27 (35%)
27	CHL	Z	607	-	48,56,74	2.36	17 (35%)	51,92,114	3.18	22 (43%)
28	LUT	1	617	-	42,43,43	0.75	0	51,60,60	1.57	12 (23%)
20	CLA	A	820	-	65,73,73	2.04	17 (26%)	76,113,113	2.79	26 (34%)
20	CLA	B	830	-	50,58,73	2.28	16 (32%)	58,95,113	3.12	28 (48%)
20	CLA	3	602	13	60,68,73	2.11	16 (26%)	70,107,113	2.86	30 (42%)
20	CLA	A	803	-	65,73,73	2.00	16 (24%)	76,113,113	2.85	29 (38%)
20	CLA	B	827	-	65,73,73	2.04	19 (29%)	76,113,113	2.74	27 (35%)
20	CLA	B	825	-	65,73,73	2.04	16 (24%)	76,113,113	2.62	26 (34%)
20	CLA	3	604	-	65,73,73	2.02	15 (23%)	76,113,113	2.65	24 (31%)
20	CLA	B	822	-	59,67,73	2.16	16 (27%)	68,105,113	2.85	27 (39%)
20	CLA	7	602	14	65,73,73	2.02	15 (23%)	76,113,113	2.75	29 (38%)
20	CLA	A	832	-	50,58,73	2.28	16 (32%)	58,95,113	2.98	28 (48%)
20	CLA	4	604	-	50,58,73	2.34	16 (32%)	58,95,113	3.02	27 (46%)
20	CLA	6	603	-	46,54,73	2.39	17 (36%)	53,90,113	3.20	25 (47%)
20	CLA	8	606	-	42,50,73	2.45	17 (40%)	48,85,113	3.26	22 (45%)
20	CLA	A	809	1	65,73,73	2.00	17 (26%)	76,113,113	2.79	27 (35%)
20	CLA	6	622	-	45,53,73	2.43	17 (37%)	52,89,113	3.20	25 (48%)
20	CLA	5	616	17	46,54,73	2.41	18 (39%)	53,90,113	3.11	26 (49%)
20	CLA	B	824	-	65,73,73	2.01	16 (24%)	76,113,113	2.68	30 (39%)
20	CLA	Z	612	-	52,60,73	2.29	17 (32%)	60,97,113	3.01	27 (45%)
20	CLA	B	812	-	65,73,73	2.04	18 (27%)	76,113,113	2.68	27 (35%)
22	LHG	A	846	-	48,48,48	0.91	2 (4%)	51,54,54	1.03	3 (5%)
23	BCR	G	205	-	41,41,41	0.70	0	56,56,56	1.55	13 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	CLA	7	611	22	41,49,73	2.50	18 (43%)	47,84,113	3.45	26 (55%)
19	CL0	A	801	-	65,73,73	1.95	16 (24%)	76,113,113	2.86	29 (38%)
20	CLA	A	812	20	65,73,73	2.00	16 (24%)	76,113,113	2.84	28 (36%)

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	LHG	8	620	20	-	12/41/41/53	-
20	CLA	5	612	-	1/1/12/20	3/22/100/115	-
23	BCR	8	619	-	-	8/29/63/63	0/2/2/2
20	CLA	B	811	-	1/1/13/20	7/25/101/115	-
20	CLA	F	304	6	1/1/15/20	8/37/115/115	-
20	CLA	K	4003	-	1/1/11/20	3/15/93/115	-
20	CLA	B	837	-	1/1/15/20	4/37/115/115	-
20	CLA	1	608	-	1/1/15/20	14/37/115/115	-
20	CLA	3	620	-	1/1/13/20	6/27/105/115	-
20	CLA	Z	613	-	1/1/15/20	11/37/115/115	-
20	CLA	A	829	-	1/1/15/20	22/37/115/115	-
20	CLA	A	806	-	1/1/15/20	17/37/115/115	-
20	CLA	5	603	-	1/1/11/20	4/15/93/115	-
20	CLA	5	604	17	-	2/19/97/115	-
21	PQN	A	844	-	-	7/23/43/43	0/2/2/2
20	CLA	B	813	-	1/1/15/20	13/37/115/115	-
20	CLA	5	602	17	-	11/37/115/115	-
20	CLA	B	802	-	1/1/15/20	14/37/115/115	-
27	CHL	5	607	-	3/3/17/26	8/21/119/137	-
23	BCR	B	801	-	-	6/29/63/63	0/2/2/2
20	CLA	B	841	22	1/1/15/20	8/37/115/115	-
20	CLA	7	606	-	1/1/10/20	7/10/88/115	-
28	LUT	6	621	-	-	4/29/67/67	0/2/2/2
20	CLA	6	616	18	1/1/11/20	4/15/93/115	-
23	BCR	A	851	-	-	4/29/63/63	0/2/2/2
20	CLA	7	612	14	1/1/12/20	5/22/100/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CHL	3	608	-	3/3/20/26	17/39/137/137	-
26	LMG	J	3001	-	-	10/30/50/70	0/1/1/1
20	CLA	8	610	15	1/1/14/20	7/31/109/115	-
20	CLA	4	613	16	-	11/27/105/115	-
20	CLA	G	204	7	1/1/11/20	3/15/93/115	-
20	CLA	B	814	-	1/1/14/20	5/31/109/115	-
20	CLA	4	616	16	1/1/10/20	0/8/86/115	-
20	CLA	6	604	-	1/1/15/20	8/37/115/115	-
20	CLA	B	839	-	1/1/15/20	7/37/115/115	-
22	LHG	1	620	20	-	10/47/47/53	-
20	CLA	8	612	15	1/1/12/20	7/22/100/115	-
28	LUT	3	622	-	-	2/29/67/67	0/2/2/2
20	CLA	A	810	1	1/1/15/20	11/37/115/115	-
20	CLA	Z	610	12	1/1/14/20	12/31/109/115	-
20	CLA	A	805	20	1/1/13/20	7/25/103/115	-
20	CLA	4	614	-	1/1/11/20	2/13/91/115	-
23	BCR	K	4001	-	-	6/29/63/63	0/2/2/2
20	CLA	B	817	-	1/1/13/20	11/30/108/115	-
20	CLA	8	604	-	1/1/11/20	5/15/93/115	-
20	CLA	4	612	16	1/1/12/20	6/22/100/115	-
20	CLA	5	611	22	1/1/13/20	10/25/103/115	-
23	BCR	B	845	-	-	10/29/63/63	0/2/2/2
23	BCR	B	846	-	-	7/29/63/63	0/2/2/2
23	BCR	B	843	-	-	7/29/63/63	0/2/2/2
20	CLA	B	834	-	1/1/15/20	11/37/115/115	-
20	CLA	B	804	-	1/1/11/20	5/13/91/115	-
23	BCR	I	172	-	-	6/29/63/63	0/2/2/2
28	LUT	7	622	-	-	2/29/67/67	0/2/2/2
20	CLA	8	608	-	1/1/12/20	0/19/97/115	-
20	CLA	B	832	-	1/1/15/20	10/37/115/115	-
20	CLA	B	807	-	1/1/15/20	9/37/115/115	-
20	CLA	L	204	-	-	2/19/97/115	-
23	BCR	J	3003	-	-	8/29/63/63	0/2/2/2
20	CLA	7	610	14	1/1/14/20	5/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	A	838	-	1/1/12/20	2/21/99/115	-
20	CLA	L	203	-	-	11/37/115/115	-
27	CHL	4	607	-	3/3/17/26	10/21/119/137	-
23	BCR	B	847	-	-	9/29/63/63	0/2/2/2
20	CLA	A	814	-	1/1/15/20	17/37/115/115	-
20	CLA	A	831	-	1/1/15/20	14/37/115/115	-
20	CLA	7	614	-	1/1/10/20	2/11/89/115	-
20	CLA	8	601	15	1/1/15/20	13/37/115/115	-
22	LHG	6	619	20	-	17/53/53/53	-
20	CLA	1	604	-	1/1/13/20	8/28/106/115	-
20	CLA	A	821	-	1/1/11/20	3/13/91/115	-
22	LHG	B	851	20	-	10/26/26/53	-
20	CLA	6	602	18	1/1/15/20	15/37/115/115	-
23	BCR	3	717	-	-	8/29/63/63	0/2/2/2
28	LUT	Z	618	-	-	5/29/67/67	0/2/2/2
23	BCR	L	201	-	-	6/29/63/63	0/2/2/2
23	BCR	5	625	-	-	7/29/63/63	0/2/2/2
20	CLA	3	614	-	-	2/13/91/115	-
28	LUT	4	619	-	-	2/29/67/67	0/2/2/2
27	CHL	8	607	-	3/3/18/26	11/27/125/137	-
20	CLA	5	601	17	1/1/15/20	9/37/115/115	-
20	CLA	5	617	-	1/1/11/20	2/15/93/115	-
20	CLA	3	607	13	1/1/14/20	16/31/109/115	-
20	CLA	5	614	-	1/1/11/20	4/13/91/115	-
23	BCR	A	856	-	-	8/29/63/63	0/2/2/2
20	CLA	A	842	-	1/1/15/20	14/37/115/115	-
20	CLA	B	821	-	-	7/15/93/115	-
20	CLA	A	815	-	1/1/14/20	8/31/109/115	-
20	CLA	B	835	-	1/1/11/20	5/13/91/115	-
20	CLA	3	606	-	1/1/10/20	0/10/88/115	-
20	CLA	4	611	22	1/1/13/20	8/25/103/115	-
20	CLA	A	840	-	1/1/15/20	9/37/115/115	-
20	CLA	B	810	-	1/1/15/20	12/37/115/115	-
27	CHL	6	618	18	3/3/15/26	8/12/110/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	3	617	13	1/1/11/20	9/15/93/115	-
27	CHL	Z	601	12	3/3/17/26	10/24/122/137	-
27	CHL	1	607	-	3/3/16/26	7/18/116/137	-
20	CLA	A	826	-	1/1/15/20	16/37/115/115	-
23	BCR	7	623	-	-	8/29/63/63	0/2/2/2
20	CLA	7	604	-	1/1/13/20	6/27/105/115	-
20	CLA	B	820	-	1/1/13/20	8/27/105/115	-
20	CLA	8	613	15	1/1/15/20	12/37/115/115	-
20	CLA	B	830	-	-	4/19/97/115	-
20	CLA	F	301	-	1/1/15/20	10/37/115/115	-
20	CLA	1	616	12	1/1/11/20	2/15/93/115	-
20	CLA	A	833	-	1/1/15/20	8/37/115/115	-
20	CLA	5	621	-	1/1/11/20	3/15/93/115	-
23	BCR	K	4004	-	-	6/29/63/63	0/2/2/2
20	CLA	5	609	17	1/1/12/20	6/19/97/115	-
27	CHL	7	607	-	3/3/17/26	8/25/123/137	-
20	CLA	A	845	22	-	13/22/100/115	-
20	CLA	B	831	-	1/1/11/20	4/18/96/115	-
28	LUT	7	621	-	-	5/29/67/67	0/2/2/2
28	LUT	5	620	-	-	2/29/67/67	0/2/2/2
20	CLA	G	203	-	1/1/12/20	1/19/97/115	-
20	CLA	F	303	-	1/1/11/20	2/13/91/115	-
20	CLA	3	610	13	1/1/15/20	13/37/115/115	-
27	CHL	6	606	-	2/2/18/26	4/27/125/137	-
20	CLA	7	608	-	-	4/19/97/115	-
20	CLA	3	611	-	1/1/10/20	2/8/86/115	-
21	PQN	B	842	-	-	4/23/43/43	0/2/2/2
22	LHG	4	623	-	-	10/36/36/53	-
28	LUT	3	621	-	-	2/29/67/67	0/2/2/2
20	CLA	A	822	-	1/1/15/20	11/37/115/115	-
20	CLA	A	827	-	1/1/15/20	6/37/115/115	-
20	CLA	Z	616	12	1/1/11/20	3/15/93/115	-
27	CHL	6	608	-	3/3/17/26	5/21/119/137	-
20	CLA	B	805	-	1/1/15/20	12/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	A	818	-	-	11/37/115/115	-
23	BCR	L	205	-	-	9/29/63/63	0/2/2/2
20	CLA	B	816	-	1/1/13/20	10/25/103/115	-
20	CLA	J	3002	9	1/1/10/20	5/10/88/115	-
28	LUT	Z	617	-	-	4/29/67/67	0/2/2/2
20	CLA	7	613	14	1/1/15/20	6/37/115/115	-
28	LUT	Z	619	-	-	4/29/67/67	0/2/2/2
20	CLA	5	610	17	1/1/14/20	10/31/109/115	-
22	LHG	5	623	20	-	13/41/41/53	-
20	CLA	3	612	13	1/1/11/20	2/15/93/115	-
27	CHL	6	607	-	2/2/18/26	12/27/125/137	-
20	CLA	6	617	-	1/1/11/20	0/15/93/115	-
27	CHL	5	618	17	3/3/15/26	4/12/110/137	-
20	CLA	A	837	1	1/1/11/20	9/13/91/115	-
20	CLA	A	823	-	-	11/18/96/115	-
20	CLA	B	836	-	1/1/14/20	7/31/109/115	-
20	CLA	A	843	-	1/1/15/20	18/37/115/115	-
28	LUT	8	618	-	-	2/29/67/67	0/2/2/2
27	CHL	4	606	-	3/3/18/26	7/27/125/137	-
20	CLA	4	609	16	1/1/12/20	6/19/97/115	-
28	LUT	1	619	-	-	2/29/67/67	0/2/2/2
20	CLA	A	813	-	1/1/12/20	8/24/102/115	-
20	CLA	8	609	15	1/1/11/20	1/15/93/115	-
20	CLA	Z	608	-	1/1/15/20	15/37/115/115	-
20	CLA	Z	603	-	1/1/13/20	9/28/106/115	-
20	CLA	4	601	16	1/1/14/20	10/33/111/115	-
23	BCR	3	719	-	-	8/29/63/63	0/2/2/2
20	CLA	1	613	-	1/1/15/20	12/37/115/115	-
28	LUT	1	618	-	-	2/29/67/67	0/2/2/2
20	CLA	6	611	22	1/1/13/20	7/25/103/115	-
20	CLA	6	614	-	1/1/11/20	4/13/91/115	-
24	SF4	A	853	1,2	-	-	0/6/5/5
20	CLA	A	811	-	1/1/15/20	7/37/115/115	-
20	CLA	1	602	12	1/1/15/20	12/37/115/115	-
22	LHG	4	622	20	-	13/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	A	828	-	1/1/15/20	13/37/115/115	-
20	CLA	6	610	18	1/1/14/20	9/31/109/115	-
23	BCR	B	844	-	-	8/29/63/63	0/2/2/2
23	BCR	5	622	-	-	6/29/63/63	0/2/2/2
24	SF4	C	101	3	-	-	0/6/5/5
20	CLA	1	609	12	1/1/15/20	9/37/115/115	-
23	BCR	3	718	-	-	2/29/63/63	0/2/2/2
20	CLA	B	833	-	1/1/13/20	7/29/107/115	-
27	CHL	5	608	-	2/2/17/26	7/21/119/137	-
23	BCR	7	624	-	-	6/29/63/63	0/2/2/2
20	CLA	B	808	-	1/1/15/20	8/37/115/115	-
20	CLA	A	854	-	1/1/15/20	10/37/115/115	-
20	CLA	B	818	-	1/1/14/20	11/31/109/115	-
20	CLA	B	852	-	1/1/15/20	9/37/115/115	-
20	CLA	5	613	17	1/1/13/20	7/27/105/115	-
20	CLA	4	610	16	1/1/14/20	7/31/109/115	-
20	CLA	A	836	-	-	2/19/97/115	-
20	CLA	Z	611	22	1/1/15/20	10/37/115/115	-
20	CLA	A	817	-	1/1/13/20	4/28/106/115	-
20	CLA	B	803	-	1/1/15/20	9/37/115/115	-
20	CLA	8	603	-	1/1/11/20	2/13/91/115	-
20	CLA	3	609	13	1/1/12/20	5/19/97/115	-
20	CLA	K	4002	-	-	5/13/91/115	-
27	CHL	4	618	16	3/3/15/26	4/12/110/137	-
28	LUT	4	620	-	-	2/29/67/67	0/2/2/2
20	CLA	A	804	-	1/1/15/20	10/37/115/115	-
23	BCR	4	621	-	-	11/29/63/63	0/2/2/2
20	CLA	A	834	-	1/1/15/20	10/37/115/115	-
20	CLA	B	829	-	1/1/15/20	8/37/115/115	-
20	CLA	A	807	1	1/1/15/20	17/37/115/115	-
20	CLA	1	612	12	1/1/12/20	6/22/100/115	-
20	CLA	7	601	14	1/1/15/20	17/37/115/115	-
20	CLA	A	830	-	1/1/15/20	9/37/115/115	-
20	CLA	3	613	13	-	16/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	A	808	-	1/1/15/20	10/37/115/115	-
20	CLA	1	610	12	1/1/14/20	7/31/109/115	-
20	CLA	A	825	-	-	7/25/103/115	-
20	CLA	1	611	22	1/1/15/20	10/37/115/115	-
23	BCR	A	848	-	-	4/29/63/63	0/2/2/2
23	BCR	6	625	-	-	7/29/63/63	0/2/2/2
20	CLA	8	614	-	1/1/13/20	6/25/103/115	-
20	CLA	1	614	-	1/1/15/20	9/37/115/115	-
20	CLA	1	603	-	1/1/15/20	7/37/115/115	-
20	CLA	6	601	18	1/1/15/20	12/37/115/115	-
20	CLA	7	603	-	1/1/11/20	3/15/93/115	-
20	CLA	7	609	14	1/1/12/20	5/19/97/115	-
20	CLA	A	819	-	-	11/37/115/115	-
20	CLA	8	602	15	1/1/14/20	9/34/112/115	-
23	BCR	A	850	-	-	4/29/63/63	0/2/2/2
27	CHL	4	608	-	3/3/17/26	4/21/119/137	-
20	CLA	Z	614	-	1/1/15/20	11/37/115/115	-
20	CLA	4	603	16	1/1/11/20	7/15/93/115	-
20	CLA	3	603	-	1/1/15/20	6/37/115/115	-
22	LHG	A	847	20	-	10/42/42/53	-
20	CLA	B	838	-	1/1/11/20	4/16/94/115	-
25	DGD	B	850	-	-	12/55/95/95	0/2/2/2
20	CLA	1	606	-	1/1/12/20	5/22/100/115	-
28	LUT	5	624	-	-	3/29/67/67	0/2/2/2
23	BCR	A	852	-	-	7/29/63/63	0/2/2/2
20	CLA	A	824	-	1/1/12/20	8/21/99/115	-
22	LHG	Z	620	20	-	17/47/47/53	-
28	LUT	8	617	-	-	3/29/67/67	0/2/2/2
28	LUT	6	624	-	-	3/29/67/67	0/2/2/2
20	CLA	A	802	-	1/1/15/20	7/37/115/115	-
20	CLA	B	823	-	1/1/14/20	7/31/109/115	-
20	CLA	A	841	-	1/1/15/20	10/37/115/115	-
20	CLA	B	815	-	1/1/13/20	4/28/106/115	-
20	CLA	Z	606	-	1/1/12/20	6/22/100/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CHL	1	601	12	3/3/17/26	10/24/122/137	-
20	CLA	A	839	-	1/1/15/20	10/37/115/115	-
20	CLA	4	602	16	-	8/31/109/115	-
20	CLA	B	840	-	-	8/37/115/115	-
20	CLA	8	616	15	1/1/11/20	2/15/93/115	-
20	CLA	5	606	-	1/1/13/20	3/25/103/115	-
20	CLA	6	612	18	1/1/12/20	5/22/100/115	-
20	CLA	B	806	2	1/1/15/20	12/37/115/115	-
20	CLA	B	809	2	1/1/15/20	5/37/115/115	-
20	CLA	6	613	-	1/1/13/20	7/27/105/115	-
20	CLA	B	826	-	1/1/15/20	11/37/115/115	-
20	CLA	8	611	22	1/1/11/20	5/15/93/115	-
20	CLA	Z	602	12	1/1/15/20	12/37/115/115	-
20	CLA	Z	609	12	1/1/15/20	4/37/115/115	-
27	CHL	Z	607	-	3/3/16/26	6/18/116/137	-
23	BCR	B	848	-	-	4/29/63/63	0/2/2/2
23	BCR	6	623	-	-	9/29/63/63	0/2/2/2
20	CLA	7	620	-	1/1/14/20	8/31/109/115	-
20	CLA	6	609	18	1/1/12/20	4/19/97/115	-
22	LHG	7	625	20	-	9/41/41/53	-
23	BCR	A	849	-	-	3/29/63/63	0/2/2/2
20	CLA	A	835	-	1/1/15/20	12/37/115/115	-
20	CLA	7	616	14	1/1/11/20	3/15/93/115	-
22	LHG	A	855	-	-	11/34/34/53	-
24	SF4	C	102	3	-	-	0/6/5/5
20	CLA	Z	604	-	1/1/13/20	6/28/106/115	-
20	CLA	B	828	-	1/1/15/20	9/37/115/115	-
20	CLA	B	819	-	1/1/15/20	13/37/115/115	-
20	CLA	A	816	-	1/1/15/20	9/37/115/115	-
28	LUT	1	617	-	-	2/29/67/67	0/2/2/2
20	CLA	A	820	-	1/1/15/20	16/37/115/115	-
20	CLA	3	602	13	1/1/14/20	9/31/109/115	-
20	CLA	7	602	14	1/1/15/20	13/37/115/115	-
20	CLA	A	803	-	1/1/15/20	5/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	B	827	-	1/1/15/20	15/37/115/115	-
20	CLA	B	825	-	1/1/15/20	6/37/115/115	-
20	CLA	3	604	-	1/1/15/20	8/37/115/115	-
20	CLA	B	822	-	1/1/13/20	12/30/108/115	-
20	CLA	6	603	-	1/1/11/20	3/15/93/115	-
20	CLA	A	832	-	1/1/12/20	2/19/97/115	-
20	CLA	6	622	-	1/1/11/20	3/13/91/115	-
20	CLA	4	604	-	-	4/19/97/115	-
20	CLA	8	606	-	1/1/10/20	4/10/88/115	-
20	CLA	A	809	1	1/1/15/20	16/37/115/115	-
23	BCR	F	305	-	-	8/29/63/63	0/2/2/2
20	CLA	5	616	17	1/1/11/20	7/15/93/115	-
20	CLA	B	824	-	1/1/15/20	11/37/115/115	-
20	CLA	Z	612	-	1/1/12/20	8/22/100/115	-
20	CLA	B	812	-	1/1/15/20	13/37/115/115	-
22	LHG	A	846	-	-	14/53/53/53	-
23	BCR	G	205	-	-	4/29/63/63	0/2/2/2
20	CLA	7	611	22	1/1/10/20	2/8/86/115	-
19	CL0	A	801	-	2/2/20/25	7/37/135/135	-
20	CLA	A	812	20	1/1/15/20	14/37/115/115	-

The worst 5 of 3585 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	844	PQN	C3-C2	7.56	1.49	1.35
21	B	842	PQN	C3-C2	7.40	1.48	1.35
20	B	836	CLA	C3B-C2B	6.65	1.49	1.40
20	B	827	CLA	C3B-C2B	6.11	1.48	1.40
27	1	601	CHL	C3B-C2B	6.02	1.48	1.40

The worst 5 of 6430 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	6	608	CHL	C4A-NA-C1A	-12.36	101.15	106.71
27	1	601	CHL	C4A-NA-C1A	-11.60	101.49	106.71
27	4	608	CHL	C2D-C1D-ND	10.39	117.76	110.10
27	6	618	CHL	C2D-C1D-ND	10.27	117.67	110.10
20	A	818	CLA	C1D-ND-C4D	-10.24	99.06	106.33

5 of 230 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	A	801	CL0	ND
19	A	801	CL0	NC
20	A	802	CLA	ND
20	A	803	CLA	ND
20	A	804	CLA	ND

5 of 2144 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	A	804	CLA	CHA-CBD-CGD-O1D
20	A	804	CLA	CHA-CBD-CGD-O2D
20	A	807	CLA	C1A-C2A-CAA-CBA
20	A	809	CLA	C3A-C2A-CAA-CBA
20	A	812	CLA	C1A-C2A-CAA-CBA

There are no ring outliers.

247 monomers are involved in 554 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	8	619	BCR	5	0
20	B	811	CLA	1	0
20	F	304	CLA	2	0
20	K	4003	CLA	2	0
20	B	837	CLA	5	0
20	1	608	CLA	3	0
20	3	620	CLA	1	0
20	Z	613	CLA	2	0
20	A	829	CLA	11	0
20	A	806	CLA	8	0
20	5	603	CLA	1	0
20	5	604	CLA	2	0
21	A	844	PQN	1	0
20	B	813	CLA	5	0
20	5	602	CLA	5	0
20	B	802	CLA	3	0
23	B	801	BCR	4	0
27	5	607	CHL	2	0
20	B	841	CLA	5	0
20	7	606	CLA	1	0
28	6	621	LUT	7	0
20	6	616	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	A	851	BCR	4	0
20	7	612	CLA	1	0
27	3	608	CHL	5	0
20	8	610	CLA	2	0
20	4	613	CLA	3	0
20	B	814	CLA	1	0
20	6	604	CLA	2	0
20	B	839	CLA	4	0
28	3	622	LUT	3	0
20	A	810	CLA	3	0
20	Z	610	CLA	3	0
20	A	805	CLA	4	0
20	4	614	CLA	2	0
23	K	4001	BCR	2	0
20	B	817	CLA	5	0
20	8	604	CLA	1	0
20	4	612	CLA	3	0
20	5	611	CLA	1	0
23	B	846	BCR	4	0
23	B	843	BCR	6	0
20	B	834	CLA	2	0
23	I	172	BCR	2	0
28	7	622	LUT	3	0
20	8	608	CLA	2	0
20	B	832	CLA	5	0
20	B	807	CLA	3	0
23	J	3003	BCR	3	0
23	F	305	BCR	6	0
20	7	610	CLA	3	0
20	A	838	CLA	1	0
20	L	203	CLA	1	0
23	B	847	BCR	2	0
20	A	814	CLA	5	0
20	A	831	CLA	7	0
20	7	614	CLA	1	0
20	8	601	CLA	3	0
22	6	619	LHG	3	0
20	1	604	CLA	1	0
20	A	821	CLA	1	0
22	B	851	LHG	2	0
20	6	602	CLA	1	0
23	3	717	BCR	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	Z	618	LUT	3	0
23	L	201	BCR	3	0
23	5	625	BCR	6	0
20	3	614	CLA	1	0
28	4	619	LUT	7	0
27	8	607	CHL	1	0
20	5	601	CLA	3	0
20	5	617	CLA	2	0
20	3	607	CLA	3	0
20	5	614	CLA	1	0
23	A	856	BCR	3	0
20	A	842	CLA	3	0
20	B	821	CLA	1	0
20	A	815	CLA	3	0
20	B	835	CLA	2	0
20	3	606	CLA	2	0
20	4	611	CLA	4	0
20	A	840	CLA	3	0
27	6	618	CHL	2	0
20	3	617	CLA	2	0
27	Z	601	CHL	5	0
27	1	607	CHL	1	0
20	A	826	CLA	3	0
23	7	623	BCR	5	0
20	7	604	CLA	2	0
20	B	820	CLA	2	0
20	8	613	CLA	5	0
20	F	301	CLA	4	0
20	A	833	CLA	3	0
20	5	621	CLA	1	0
23	K	4004	BCR	1	0
20	5	609	CLA	7	0
20	A	845	CLA	1	0
20	B	831	CLA	1	0
28	7	621	LUT	6	0
28	5	620	LUT	4	0
20	F	303	CLA	2	0
20	3	610	CLA	2	0
20	7	608	CLA	2	0
21	B	842	PQN	1	0
22	4	623	LHG	1	0
27	6	606	CHL	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	3	621	LUT	3	0
20	A	822	CLA	3	0
20	A	827	CLA	2	0
20	Z	616	CLA	1	0
27	6	608	CHL	1	0
20	A	818	CLA	3	0
20	B	805	CLA	8	0
23	L	205	BCR	1	0
20	B	816	CLA	1	0
28	Z	617	LUT	5	0
20	7	613	CLA	3	0
28	Z	619	LUT	3	0
20	5	610	CLA	1	0
22	5	623	LHG	1	0
20	3	612	CLA	2	0
27	6	607	CHL	2	0
27	5	618	CHL	1	0
20	A	837	CLA	1	0
20	A	823	CLA	2	0
20	B	836	CLA	3	0
20	A	843	CLA	6	0
28	8	618	LUT	5	0
20	4	609	CLA	2	0
28	1	619	LUT	3	0
20	A	813	CLA	1	0
20	Z	608	CLA	5	0
20	Z	603	CLA	2	0
20	4	601	CLA	4	0
23	3	719	BCR	6	0
20	1	613	CLA	1	0
28	1	618	LUT	5	0
20	6	611	CLA	2	0
20	6	614	CLA	2	0
20	A	811	CLA	3	0
20	1	602	CLA	6	0
22	4	622	LHG	5	0
20	A	828	CLA	3	0
20	6	610	CLA	5	0
23	B	844	BCR	3	0
23	5	622	BCR	4	0
20	1	609	CLA	2	0
23	3	718	BCR	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	B	833	CLA	4	0
23	7	624	BCR	1	0
27	5	608	CHL	3	0
20	A	854	CLA	5	0
20	B	818	CLA	5	0
20	5	613	CLA	3	0
20	4	610	CLA	1	0
20	A	836	CLA	2	0
20	Z	611	CLA	1	0
20	A	817	CLA	4	0
20	B	803	CLA	1	0
20	K	4002	CLA	1	0
20	3	609	CLA	3	0
28	4	620	LUT	2	0
20	A	804	CLA	2	0
23	4	621	BCR	2	0
20	A	834	CLA	3	0
20	B	829	CLA	5	0
20	A	807	CLA	4	0
20	1	612	CLA	1	0
20	7	601	CLA	6	0
20	A	830	CLA	4	0
20	3	613	CLA	1	0
20	A	808	CLA	2	0
20	1	610	CLA	1	0
20	A	825	CLA	2	0
20	1	611	CLA	1	0
23	A	848	BCR	3	0
23	6	625	BCR	4	0
20	8	614	CLA	4	0
20	1	614	CLA	3	0
20	1	603	CLA	1	0
20	6	601	CLA	1	0
20	A	819	CLA	2	0
20	7	609	CLA	3	0
20	8	602	CLA	3	0
23	A	850	BCR	4	0
27	4	608	CHL	1	0
20	4	603	CLA	1	0
20	3	603	CLA	2	0
22	A	847	LHG	3	0
20	B	838	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	B	850	DGD	2	0
20	1	606	CLA	5	0
28	5	624	LUT	5	0
23	A	852	BCR	3	0
20	A	824	CLA	1	0
22	Z	620	LHG	3	0
28	8	617	LUT	10	0
28	6	624	LUT	4	0
20	A	802	CLA	5	0
20	B	823	CLA	5	0
20	A	841	CLA	8	0
20	B	815	CLA	2	0
27	1	601	CHL	2	0
20	A	839	CLA	2	0
20	4	602	CLA	4	0
20	B	840	CLA	5	0
20	8	616	CLA	1	0
20	5	606	CLA	3	0
20	6	612	CLA	1	0
20	B	806	CLA	4	0
20	B	809	CLA	2	0
20	6	613	CLA	2	0
20	B	826	CLA	3	0
20	Z	602	CLA	4	0
20	Z	609	CLA	1	0
23	B	848	BCR	3	0
23	6	623	BCR	5	0
20	7	620	CLA	1	0
20	6	609	CLA	1	0
22	7	625	LHG	1	0
23	A	849	BCR	4	0
20	A	835	CLA	1	0
20	7	616	CLA	2	0
20	Z	604	CLA	1	0
20	B	828	CLA	3	0
20	B	819	CLA	2	0
20	A	816	CLA	5	0
28	1	617	LUT	7	0
20	A	820	CLA	3	0
20	B	830	CLA	3	0
20	3	602	CLA	1	0
20	A	803	CLA	2	0

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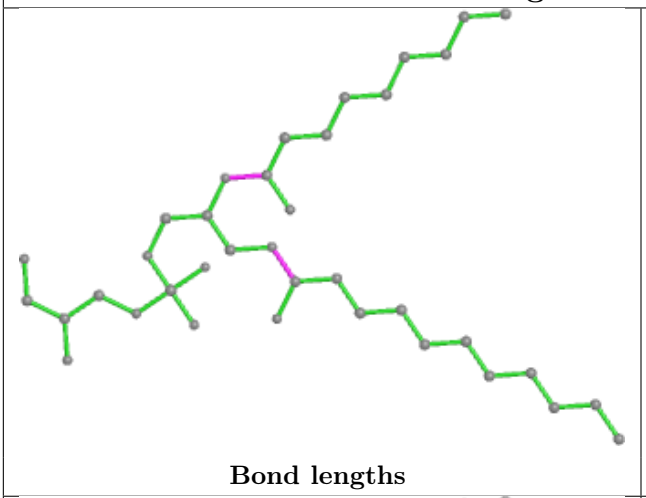
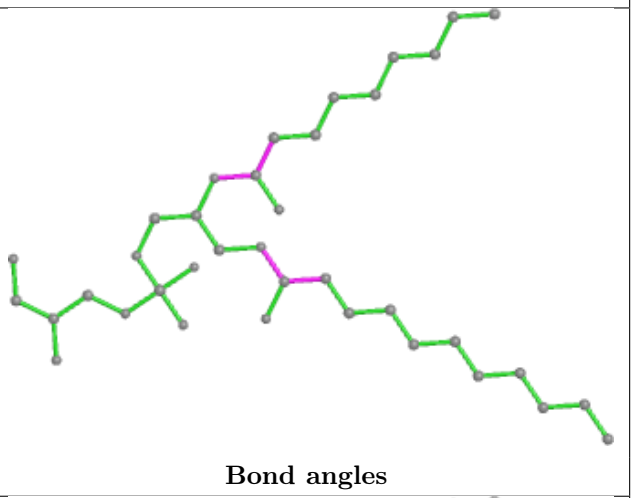
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	B	827	CLA	2	0
20	B	825	CLA	5	0
20	3	604	CLA	2	0
20	B	822	CLA	1	0
20	7	602	CLA	1	0
20	8	606	CLA	2	0
20	A	809	CLA	4	0
20	6	622	CLA	2	0
20	B	824	CLA	4	0
20	Z	612	CLA	2	0
20	B	812	CLA	3	0
22	A	846	LHG	3	0
23	G	205	BCR	4	0
19	A	801	CL0	1	0
20	A	812	CLA	7	0

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.

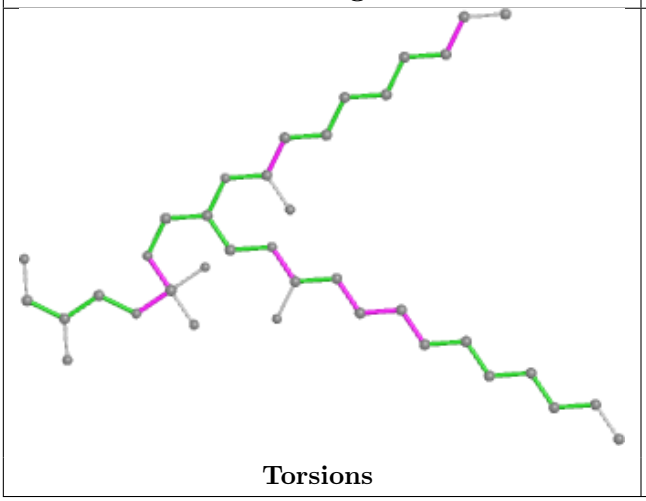
Ligand LHG 8 620



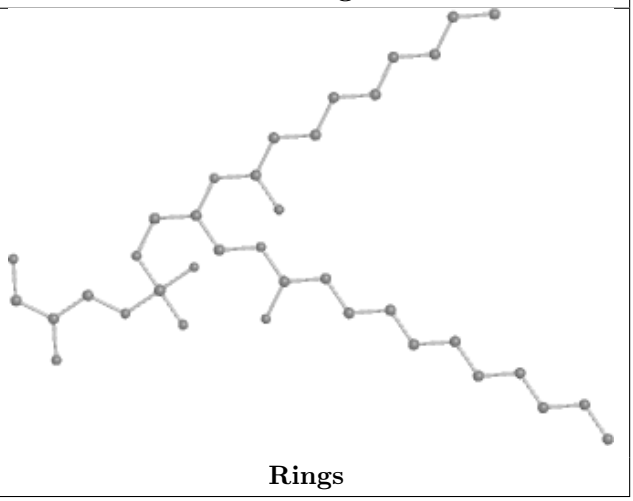
Bond lengths



Bond angles

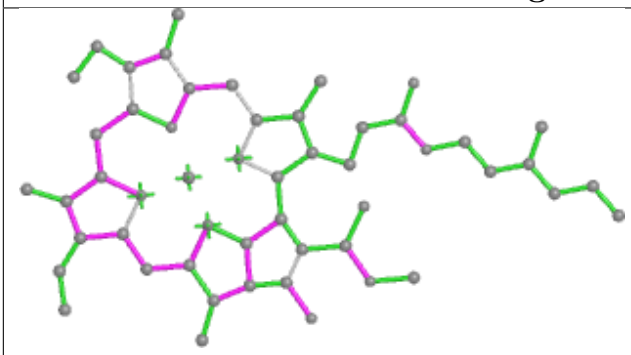


Torsions

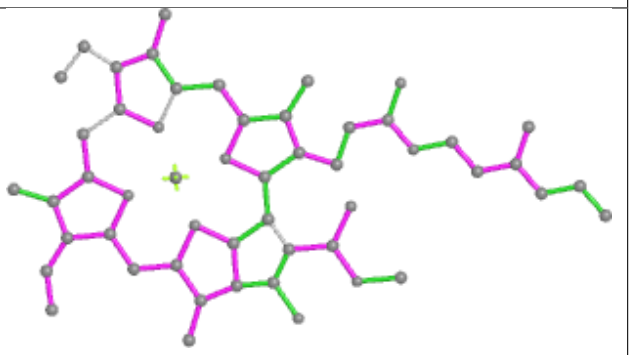


Rings

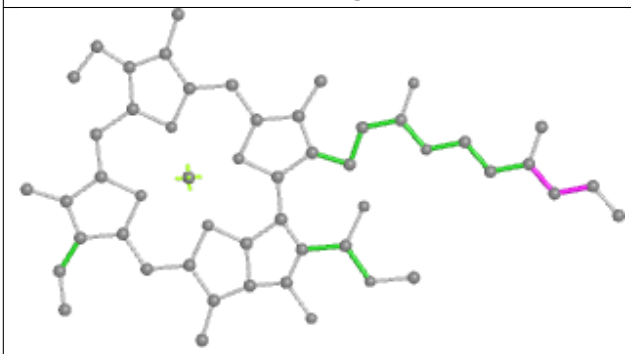
Ligand CLA 5 612



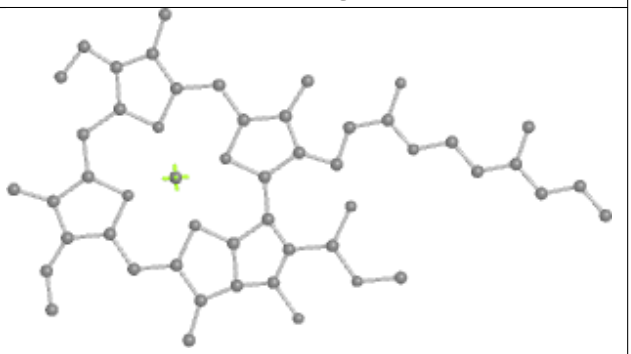
Bond lengths



Bond angles

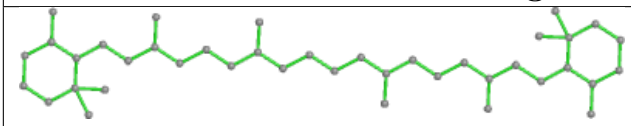


Torsions

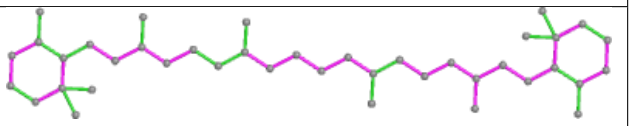


Rings

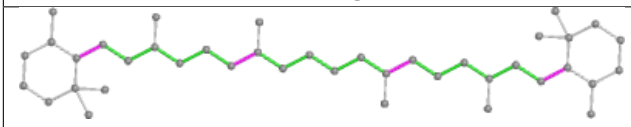
Ligand BCR 8 619



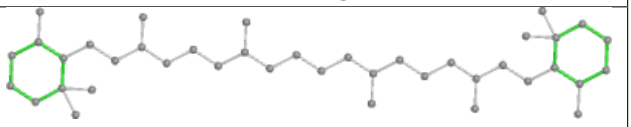
Bond lengths



Bond angles

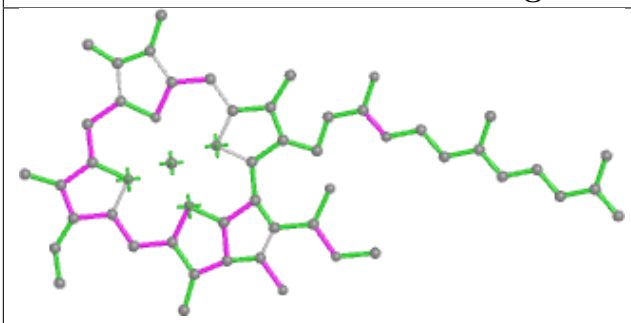


Torsions

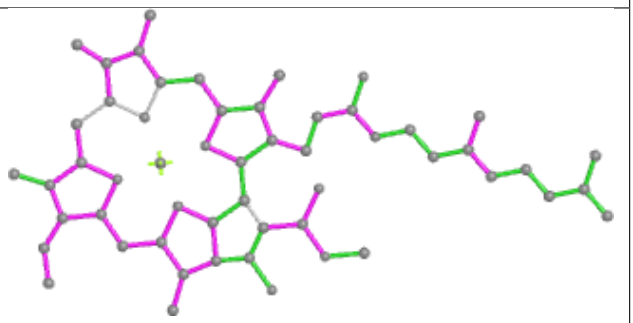


Rings

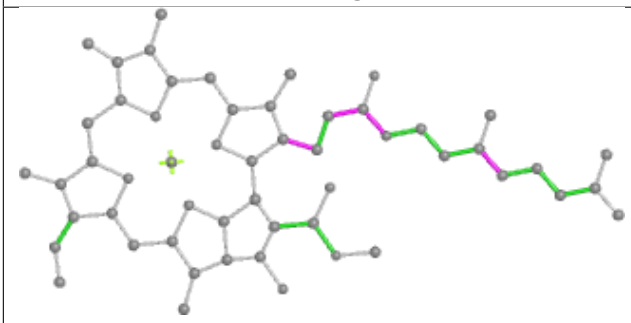
Ligand CLA B 811



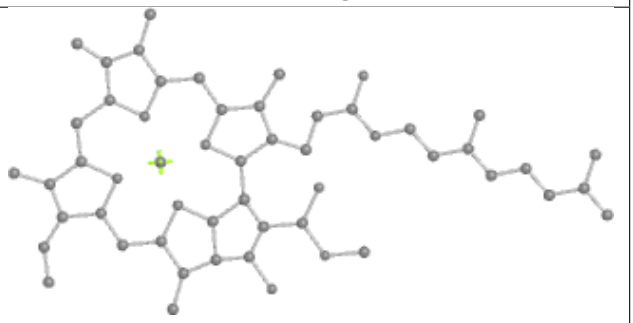
Bond lengths



Bond angles

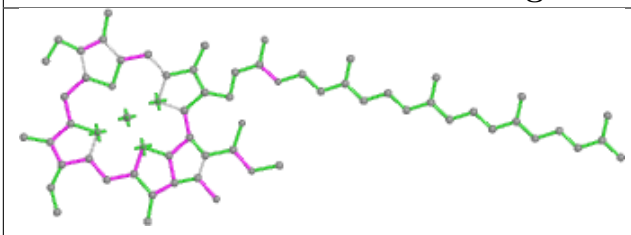


Torsions

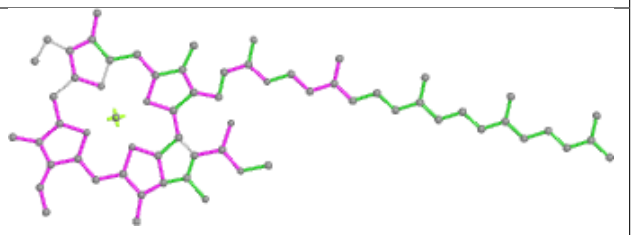


Rings

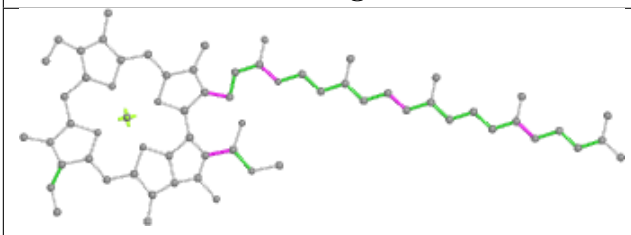
Ligand CLA F 304



Bond lengths



Bond angles



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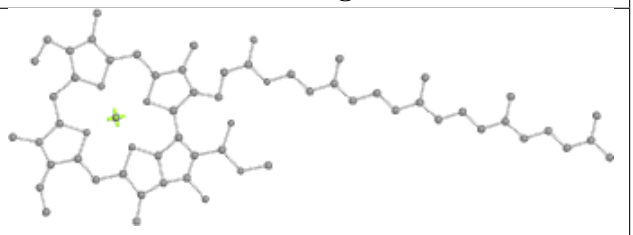
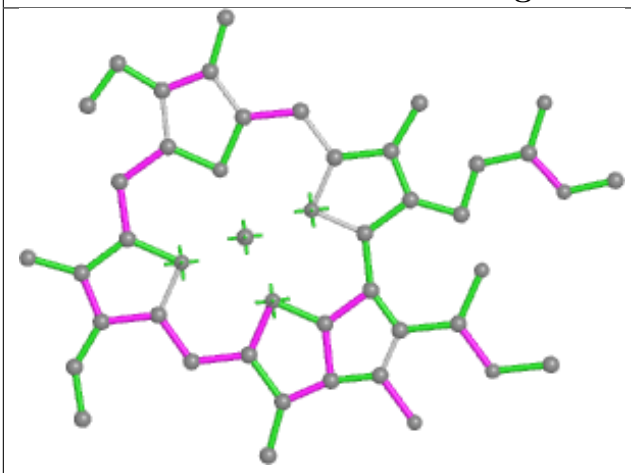


Rings

Ligand CLA K 4003



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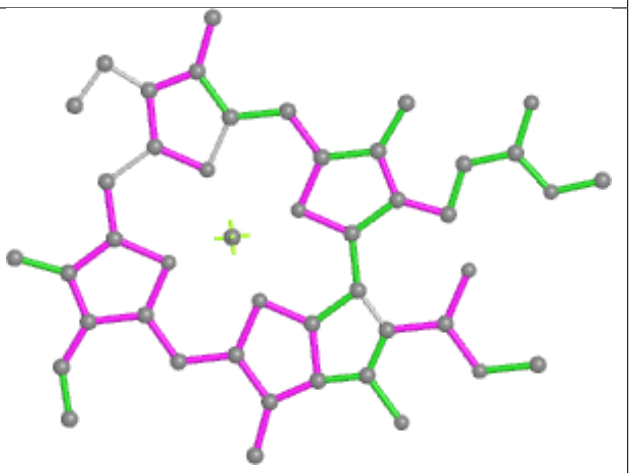

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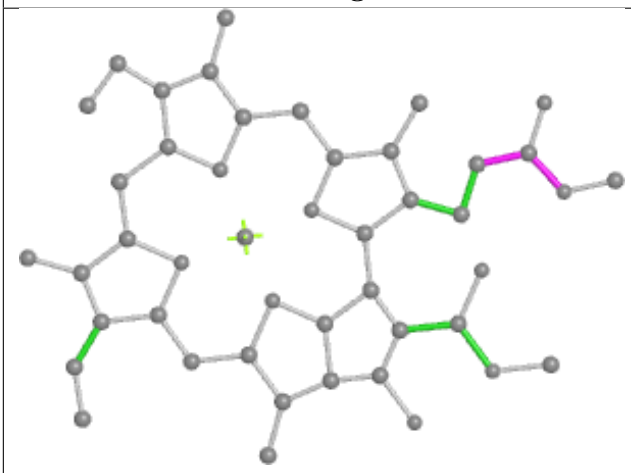

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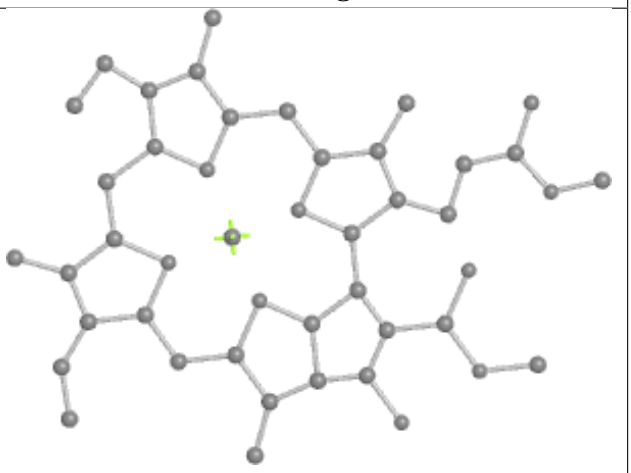
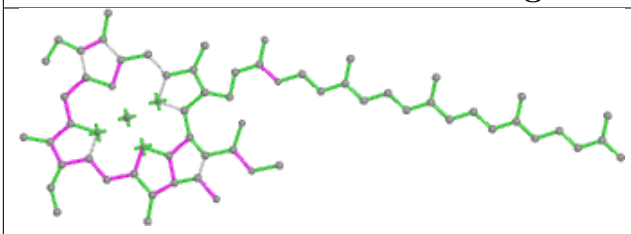


Rings

Ligand CLA B 837



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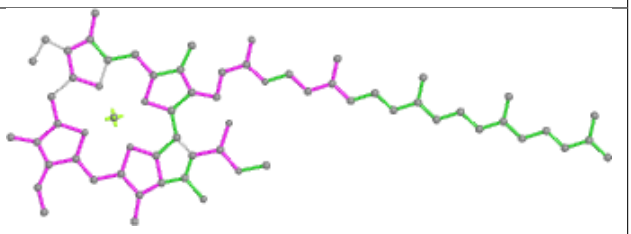

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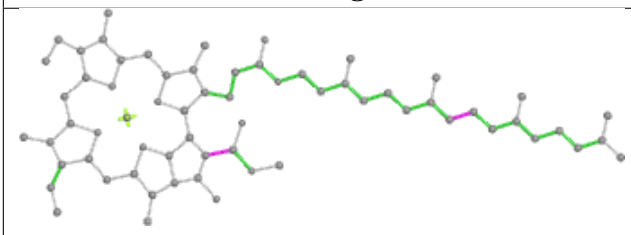

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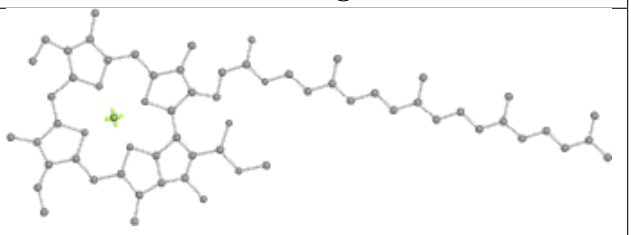
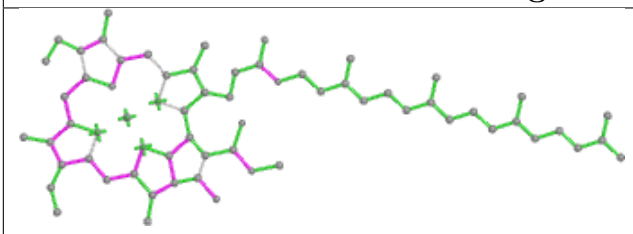


Rings

Ligand CLA 1 608



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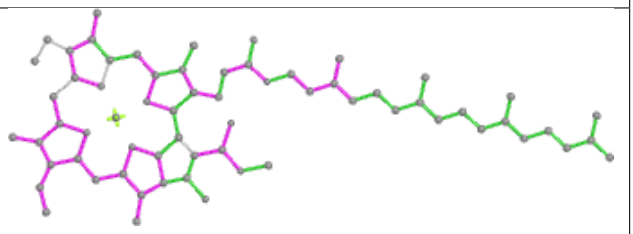

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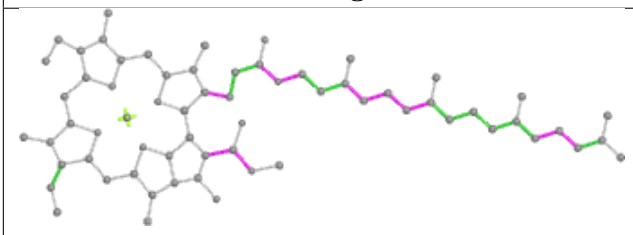

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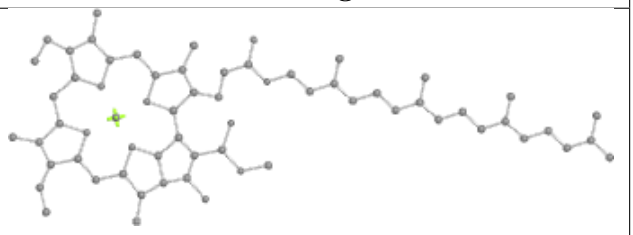
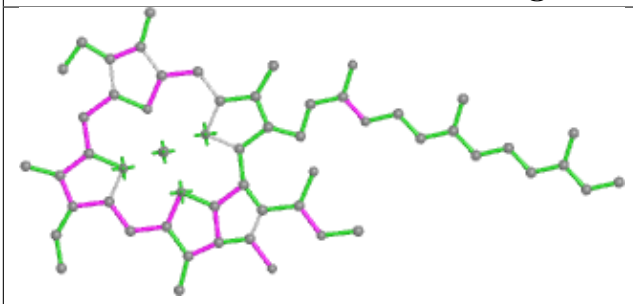


Rings

Ligand CLA 3 620



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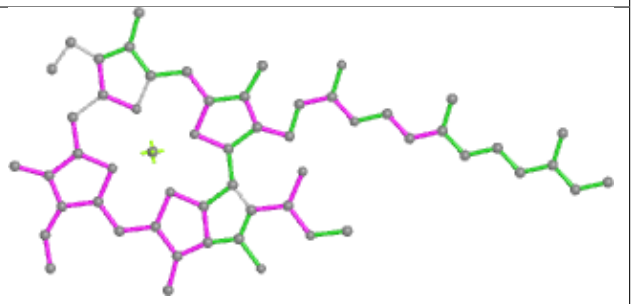

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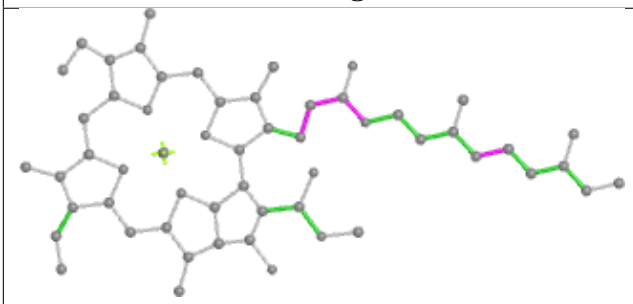

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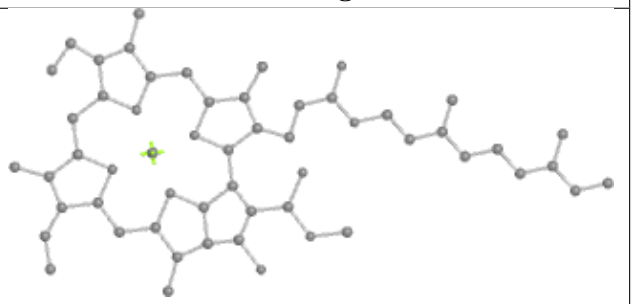
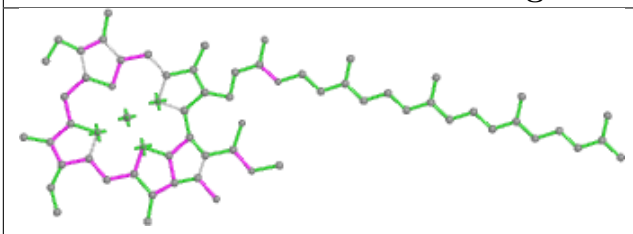


Rings

Ligand CLA Z 613



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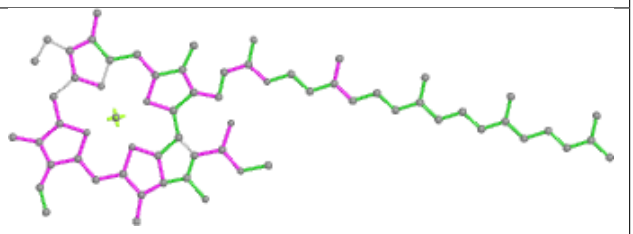

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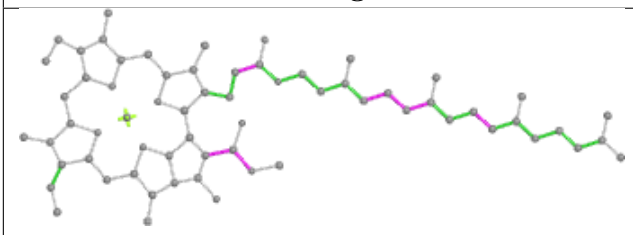

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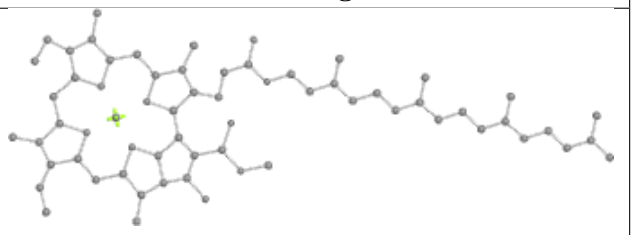
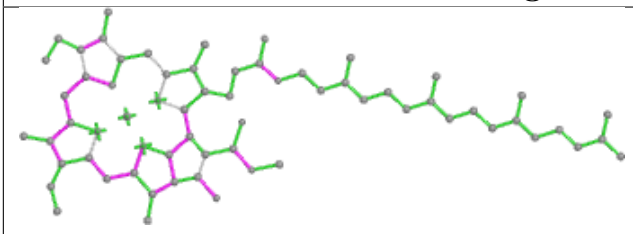


Rings

Ligand CLA A 829



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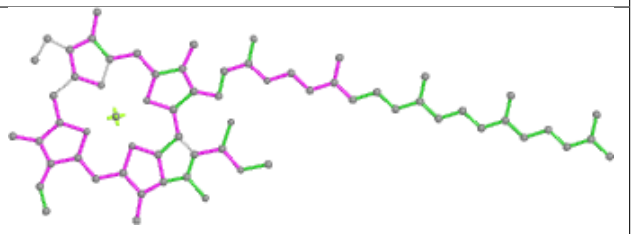

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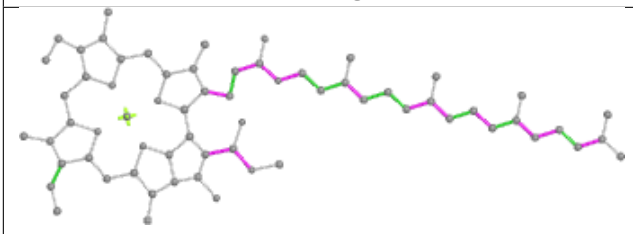

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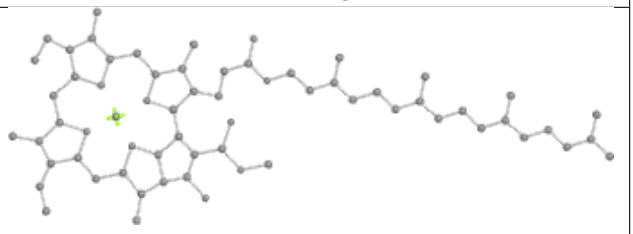
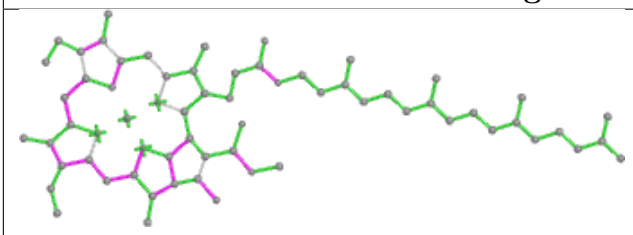
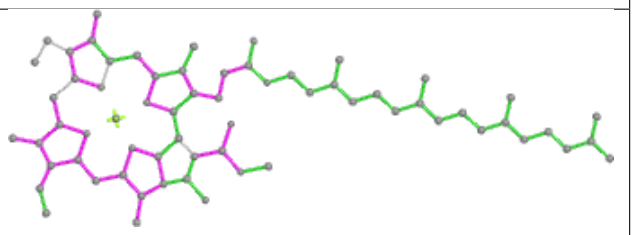


Rings

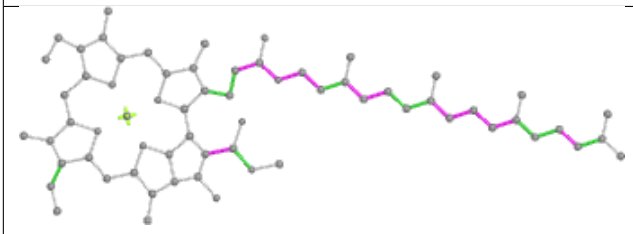
Ligand CLA A 806



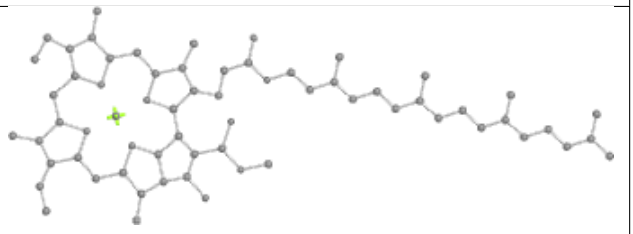
Bond lengths



Bond angles

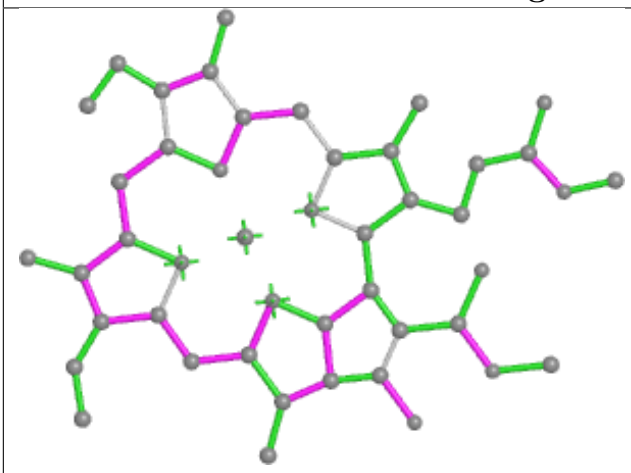


Torsions

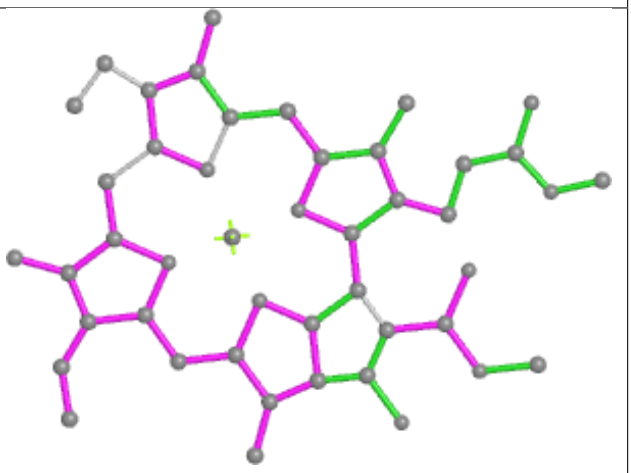


Rings

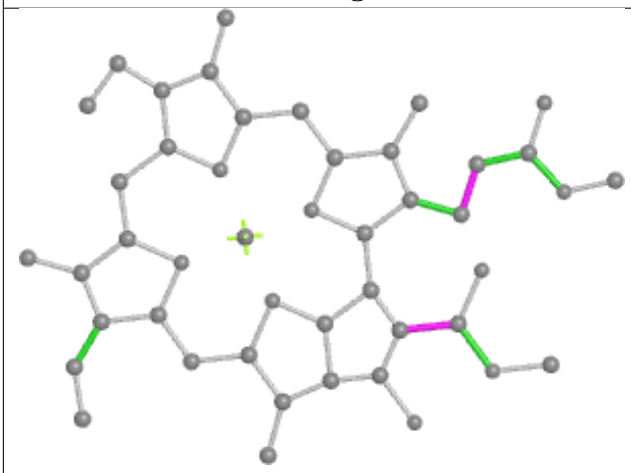
Ligand CLA 5 603



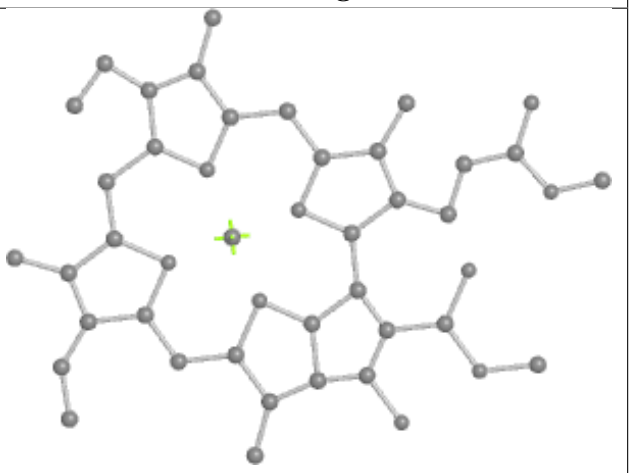
Bond lengths



Bond angles

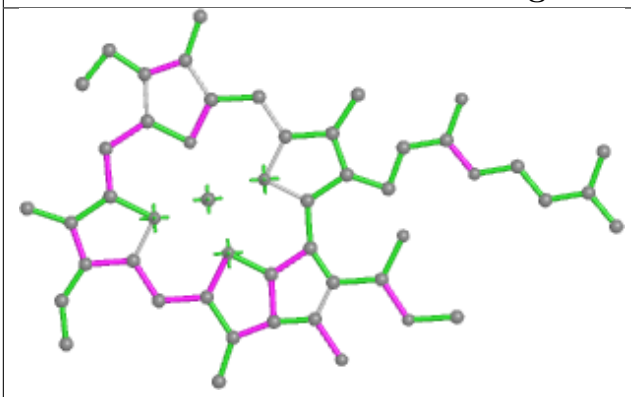


Torsions

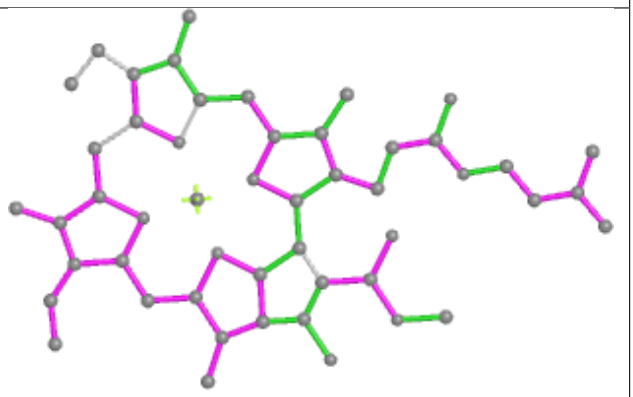


Rings

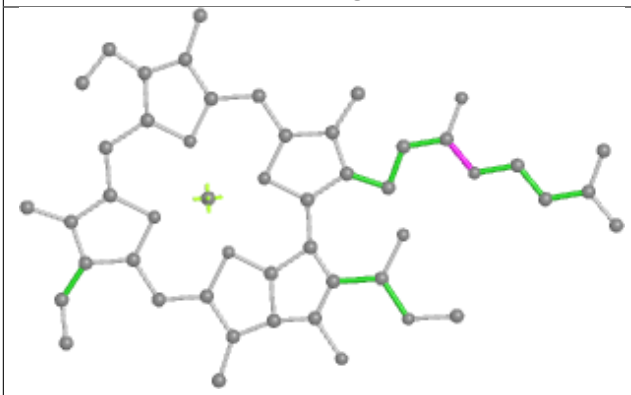
Ligand CLA 5 604



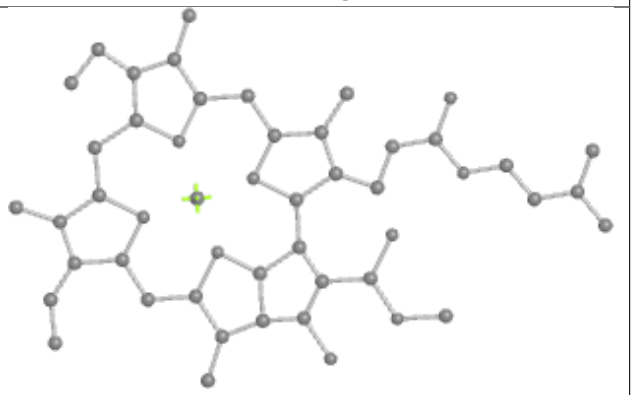
Bond lengths



Bond angles

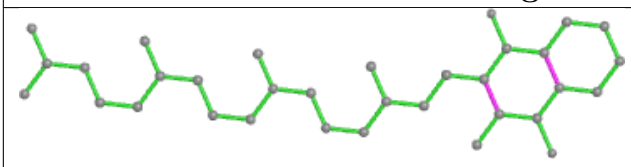


Torsions



Rings

Ligand PQN A 844



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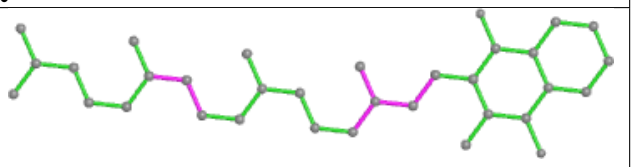
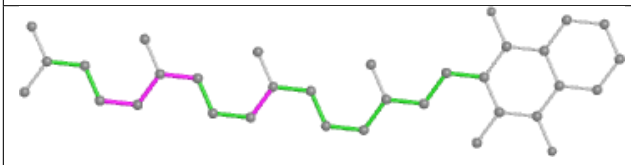
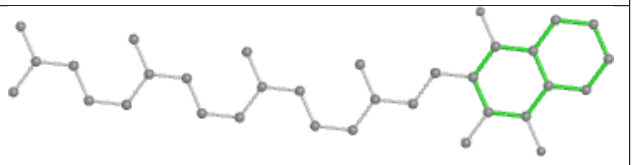


Bond angles

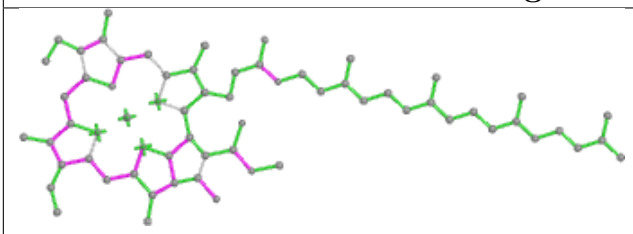


Torsions

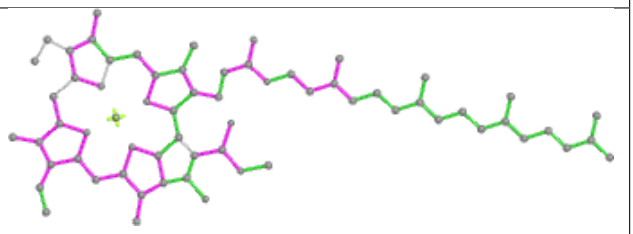


Rings

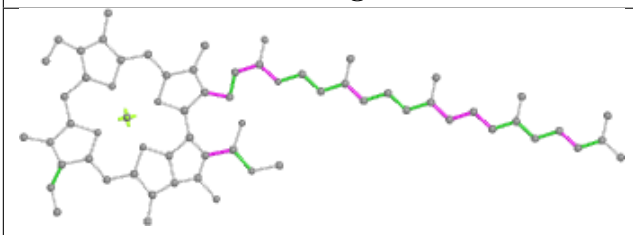
Ligand CLA B 813



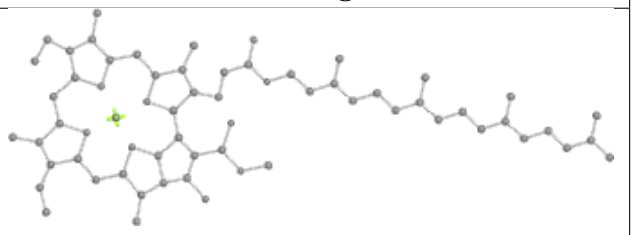
Bond lengths



Bond angles

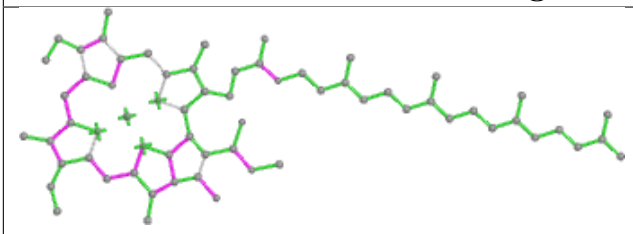


Torsions

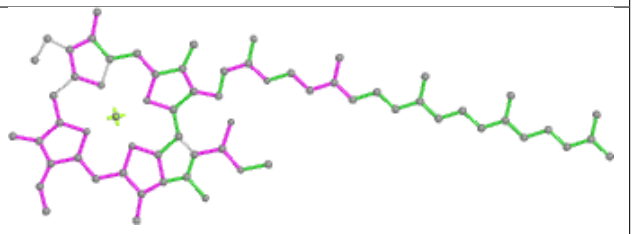


Rings

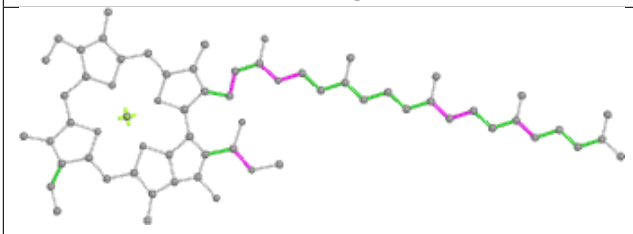
Ligand CLA 5 602



Bond lengths



Bond angles



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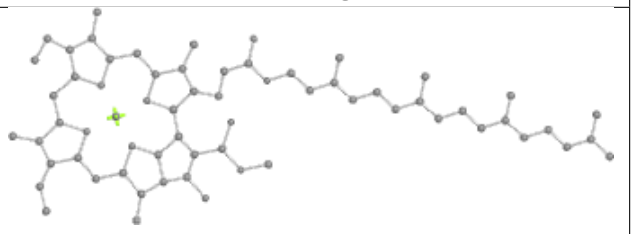
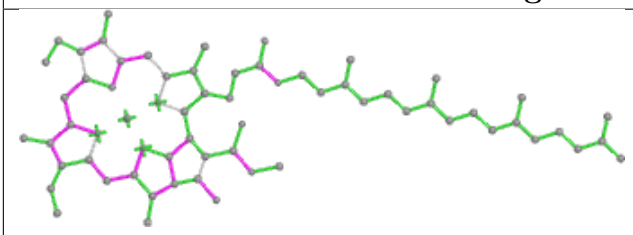


Rings

Ligand CLA B 802



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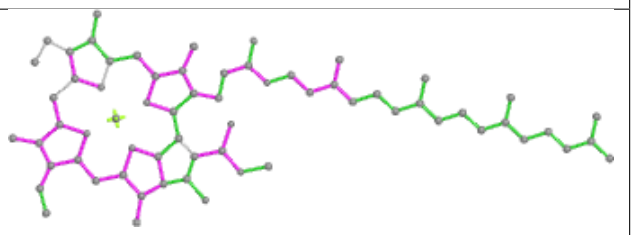
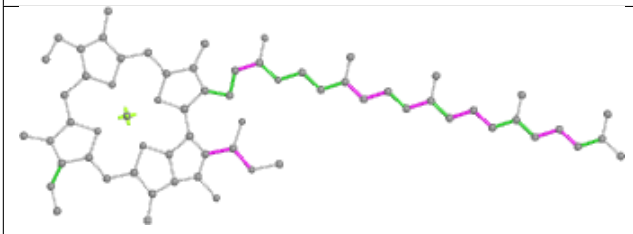


Bond angles



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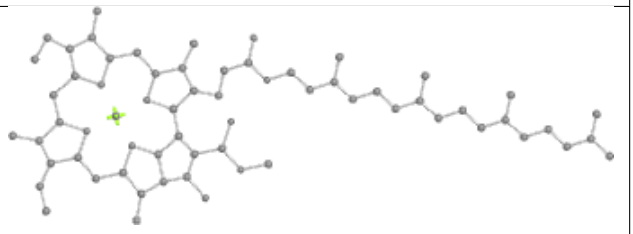
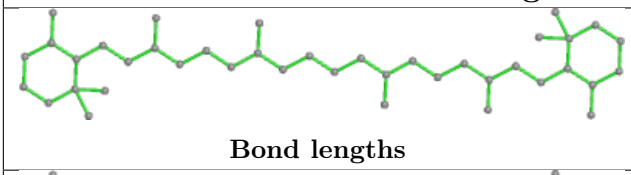


Rings

Ligand BCR B 801



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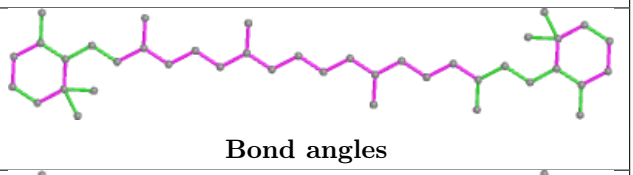
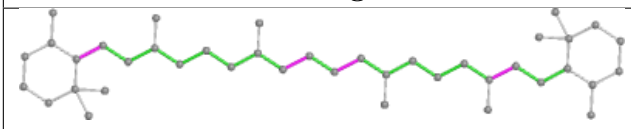


Bond angles



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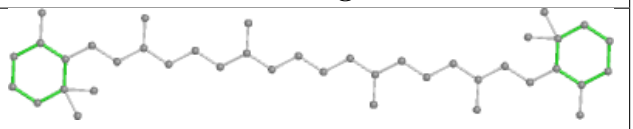
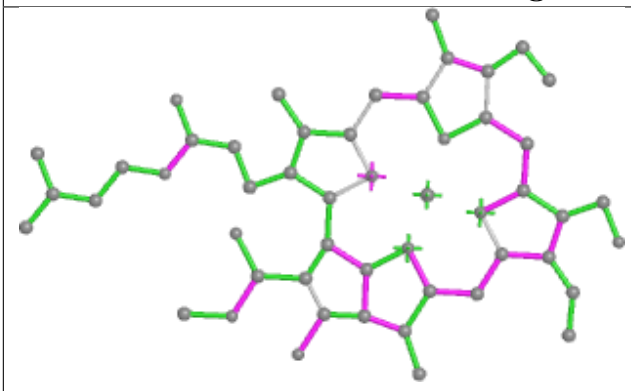


Rings

Ligand CHL 5 607



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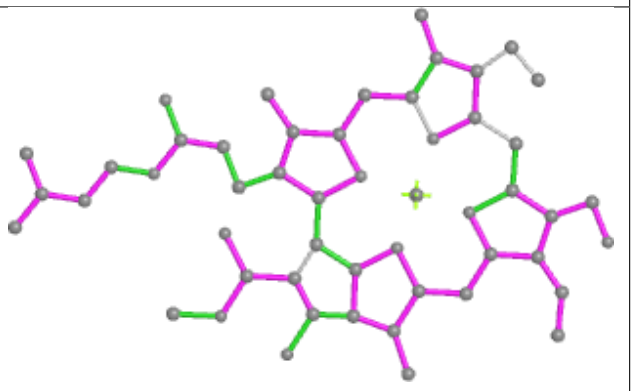
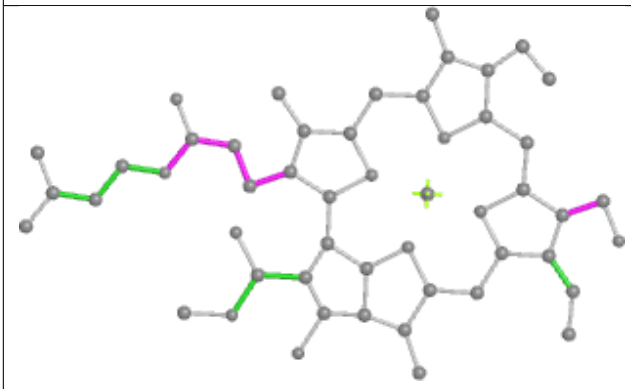


Bond angles



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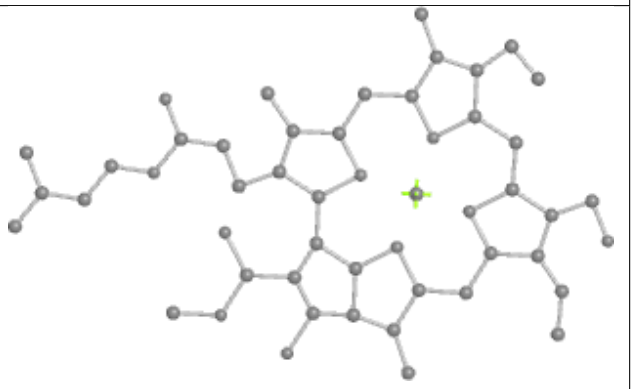
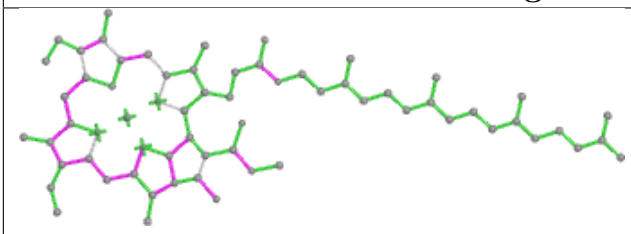


Rings

Ligand CLA B 841



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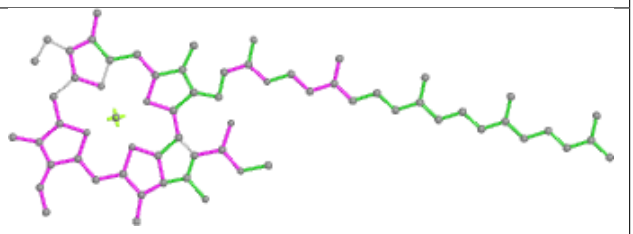
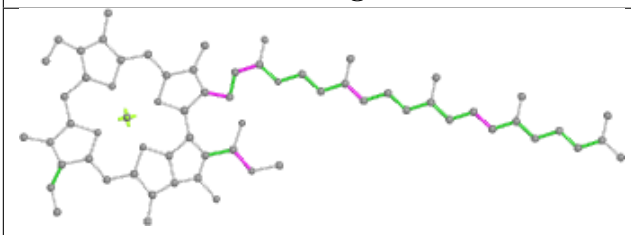


Bond angles



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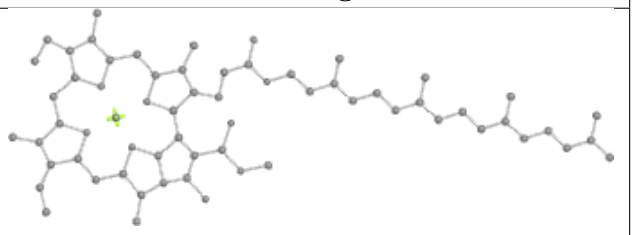
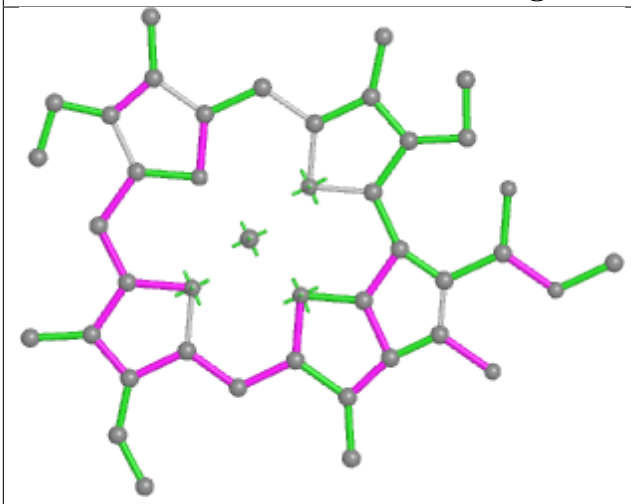


Rings

Ligand CLA 7 606



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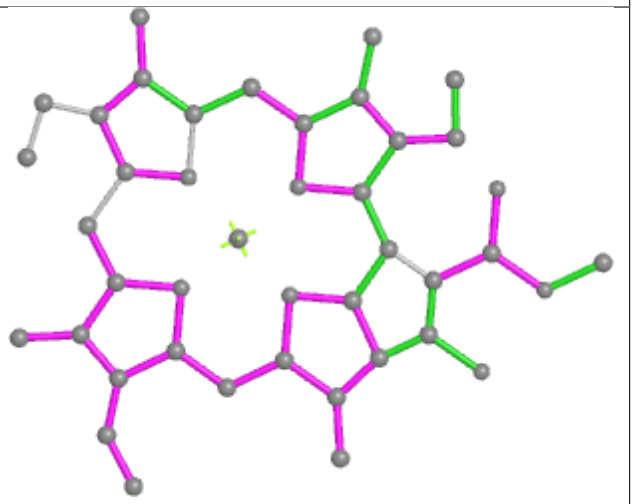
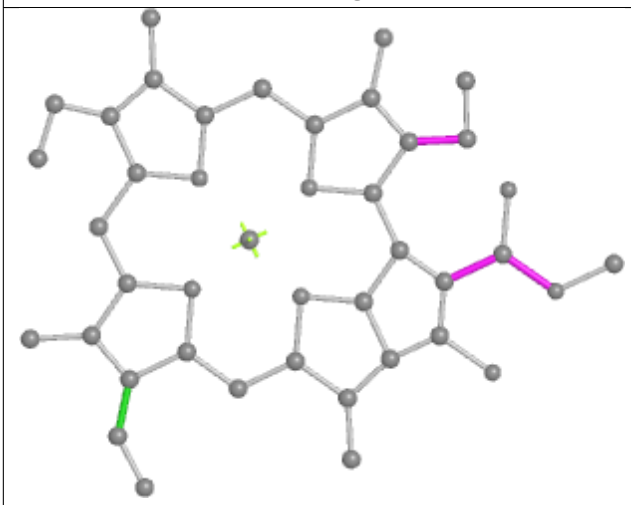


Bond angles



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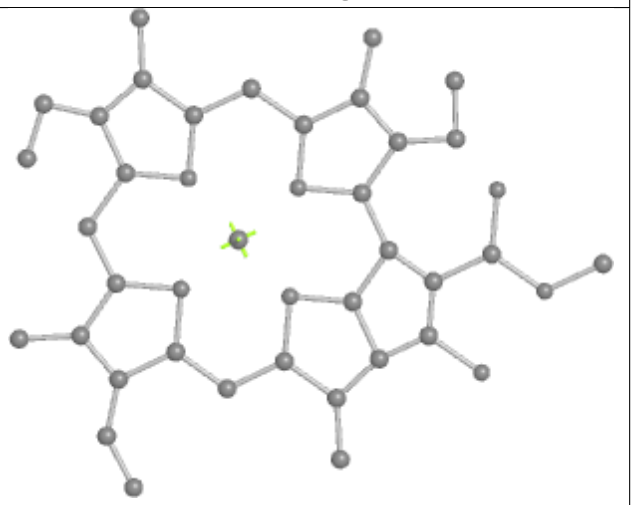
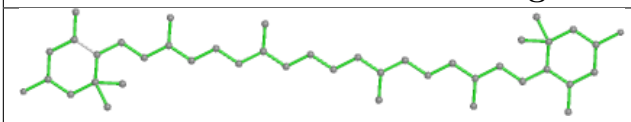


Rings

Ligand LUT 6 621



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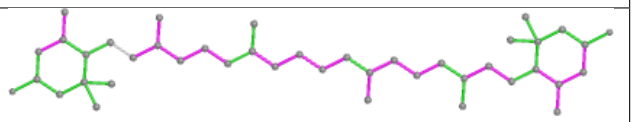
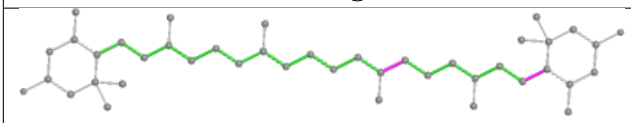


Bond angles



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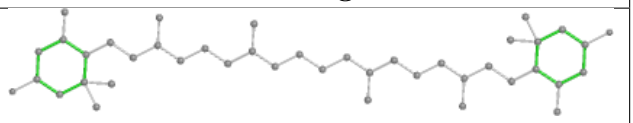
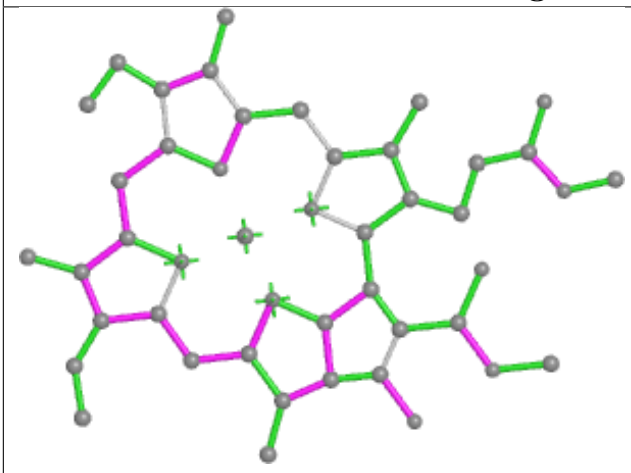


Rings

Ligand CLA 6 616



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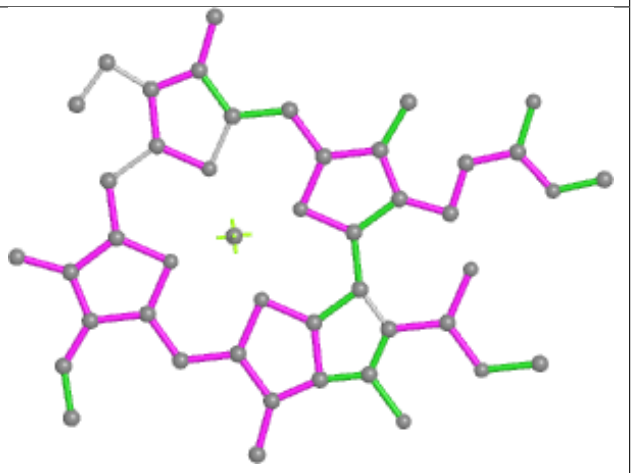
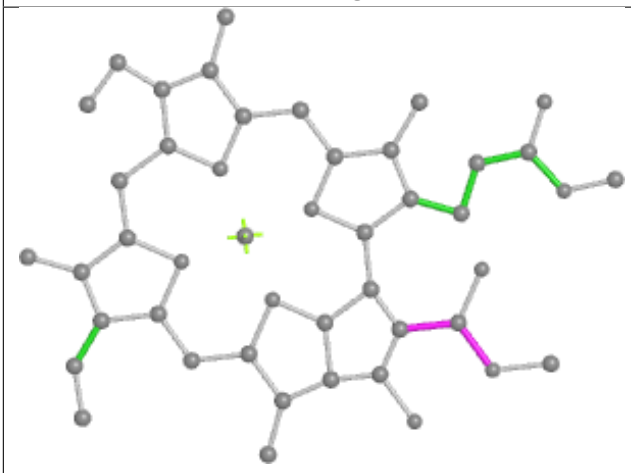


Bond angles



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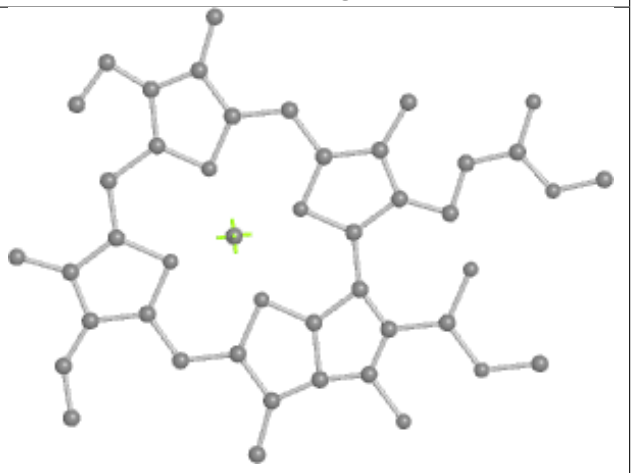
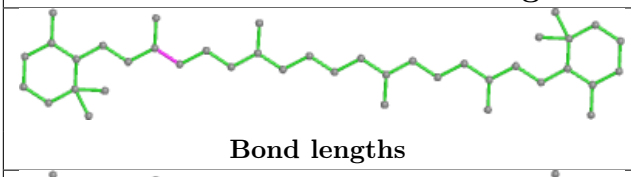


Rings

Ligand BCR A 851



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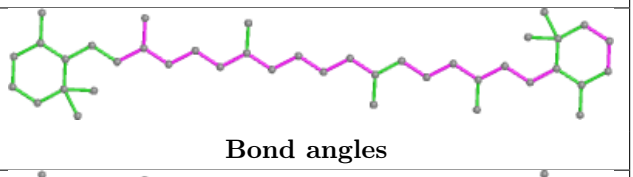
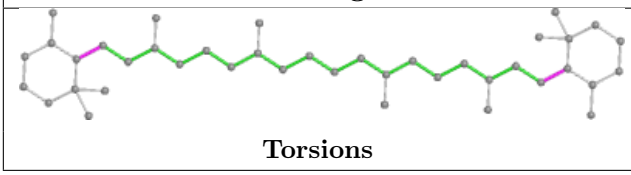
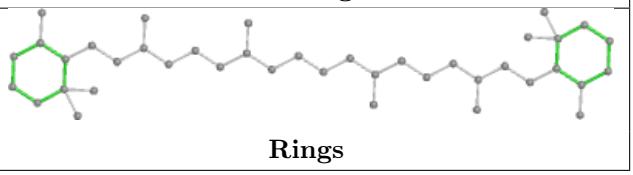


Bond angles

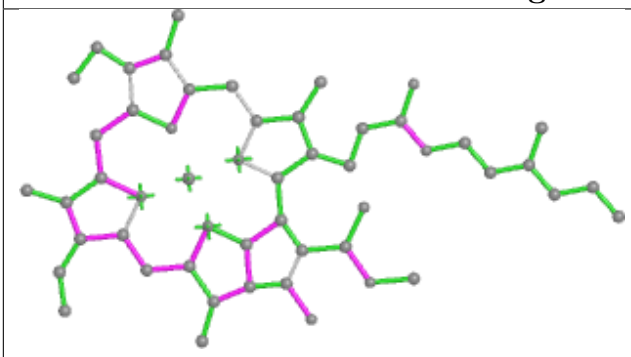


Torsions

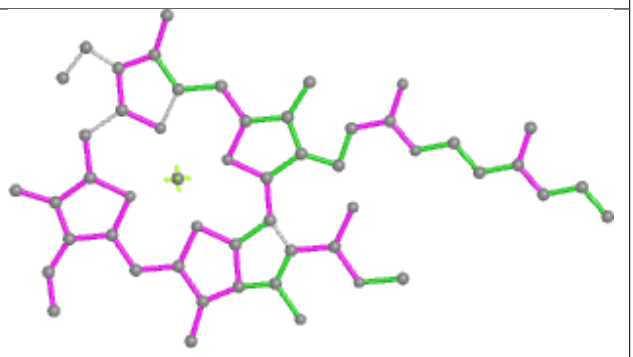


Rings

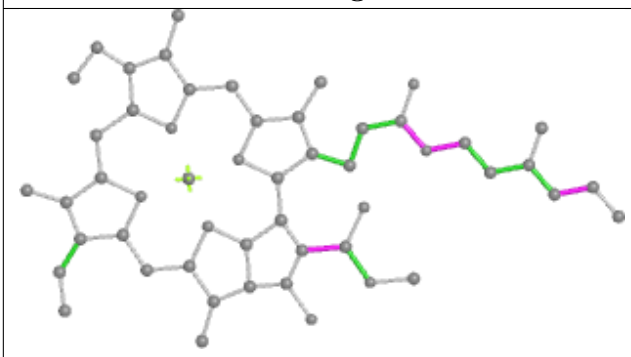
Ligand CLA 7 612



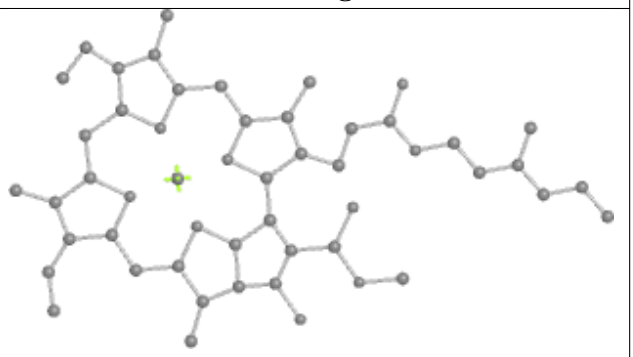
Bond lengths



Bond angles

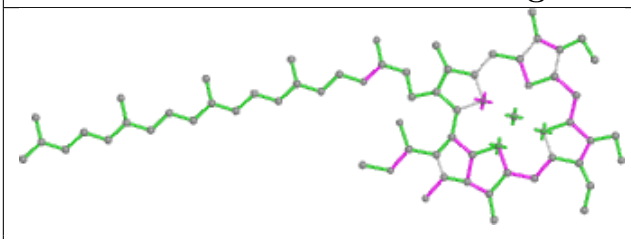


Torsions

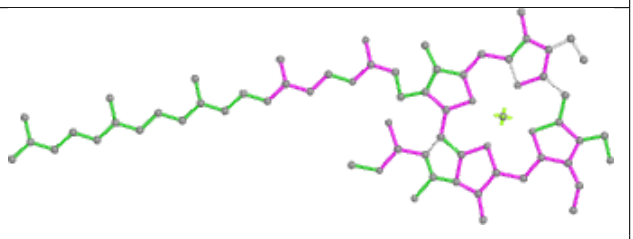


Rings

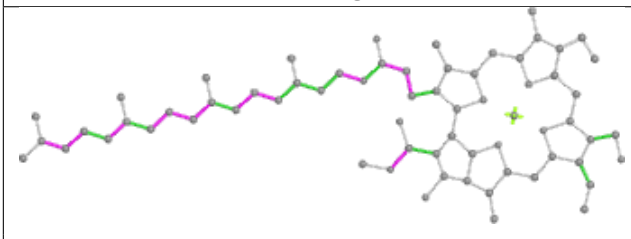
Ligand CHL 3 608



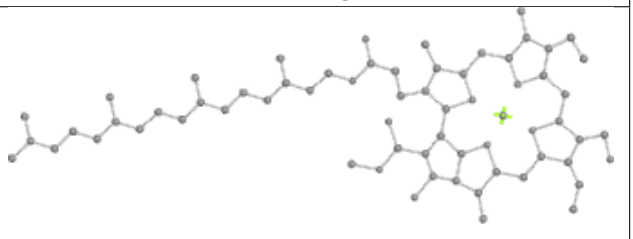
Bond lengths



Bond angles

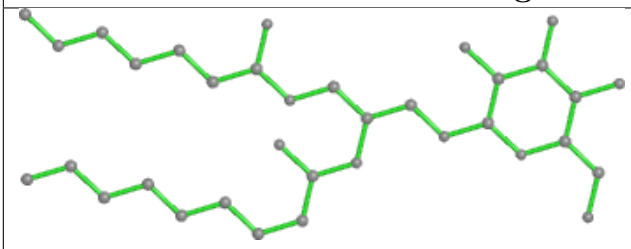


Torsions

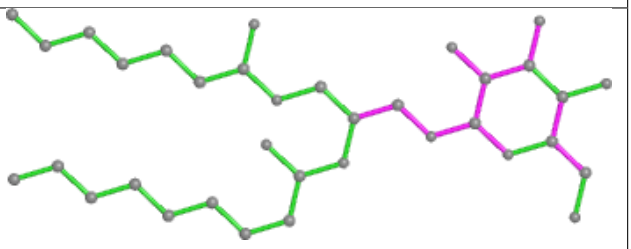


Rings

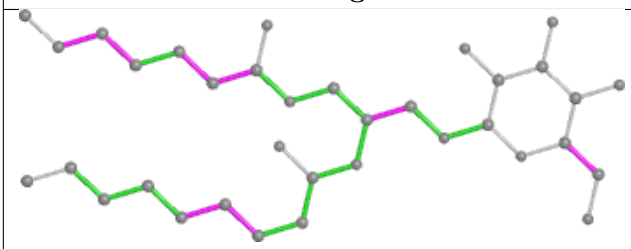
Ligand LMG J 3001



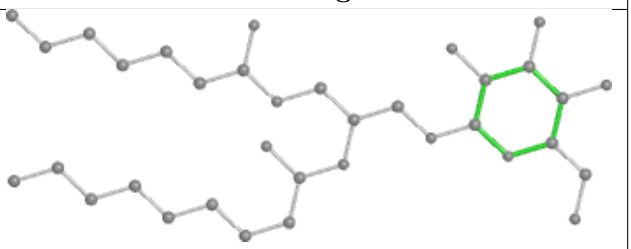
Bond lengths



Bond angles

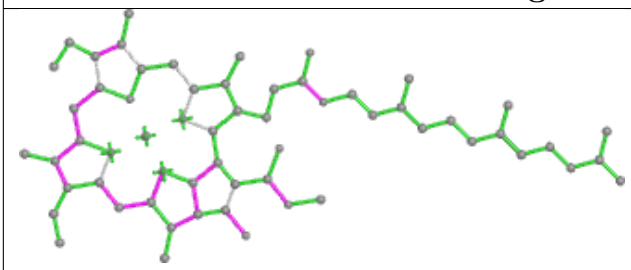


Torsions



Rings

Ligand CLA 8 610



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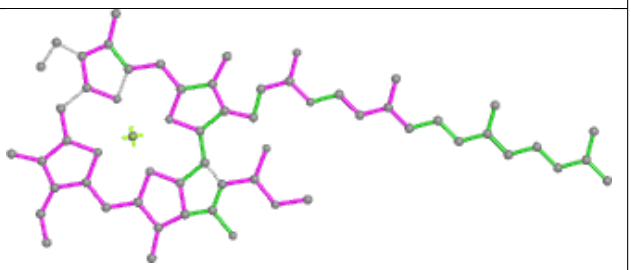
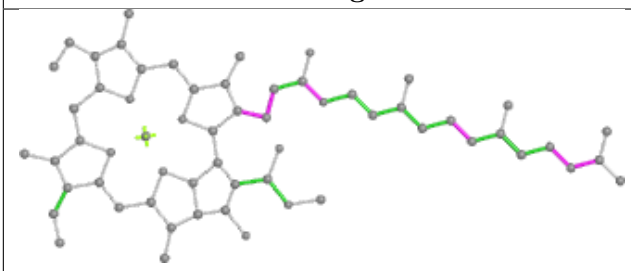


Bond angles



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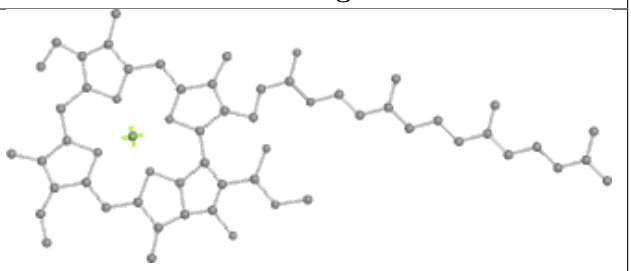
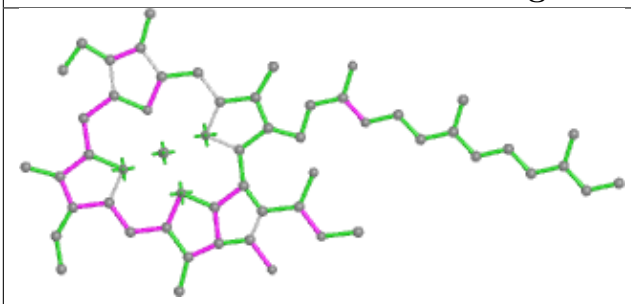


Rings

Ligand CLA 4 613



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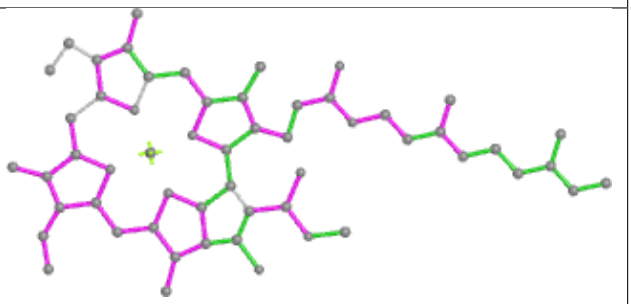

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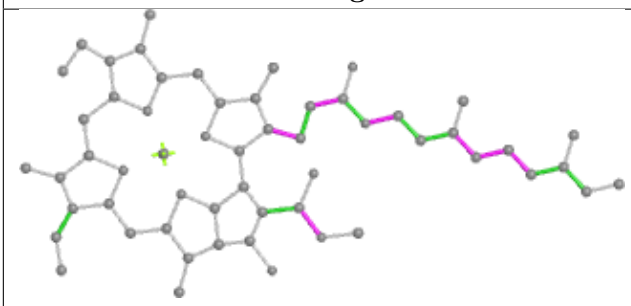
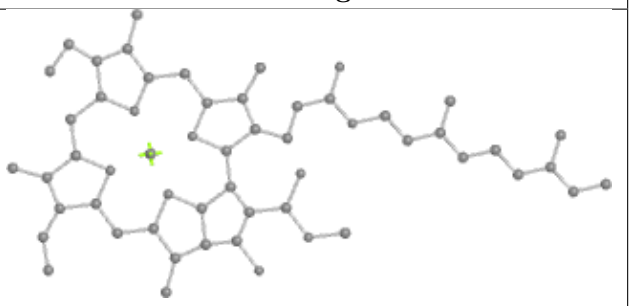
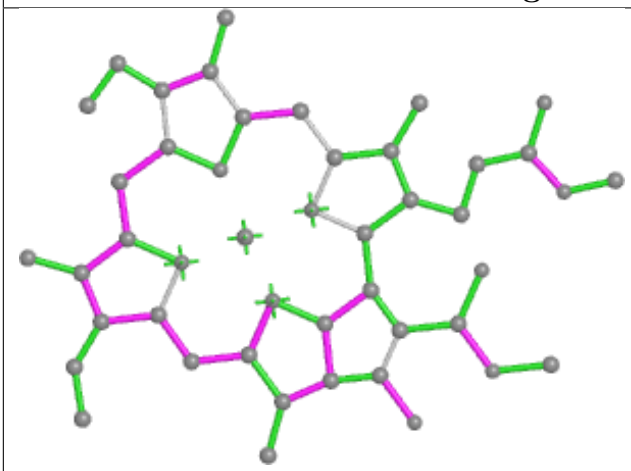


Torsions



Rings

Ligand CLA G 204



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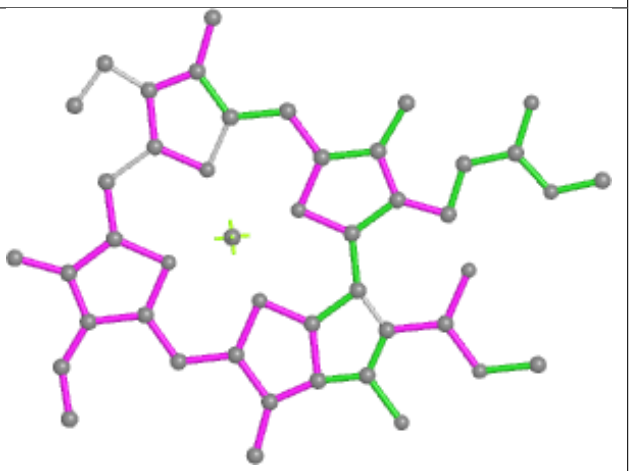
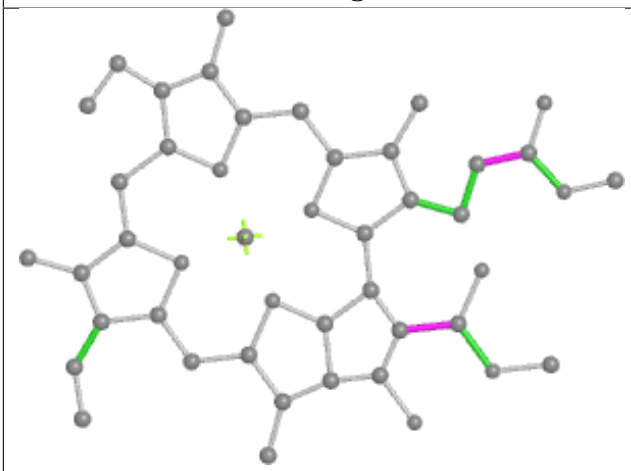
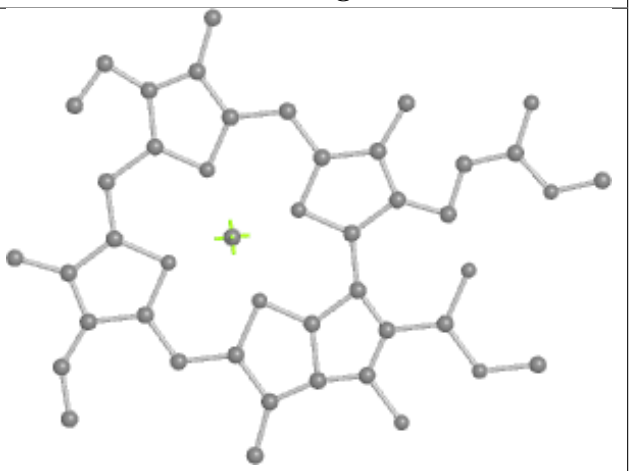


Bond angles

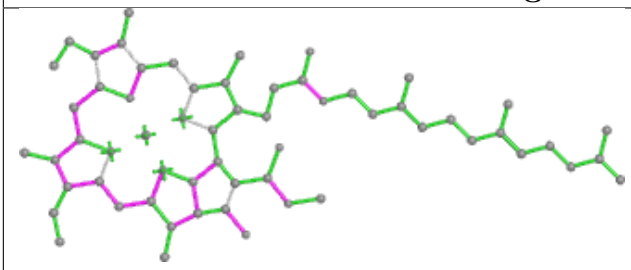


Torsions



Rings

Ligand CLA B 814



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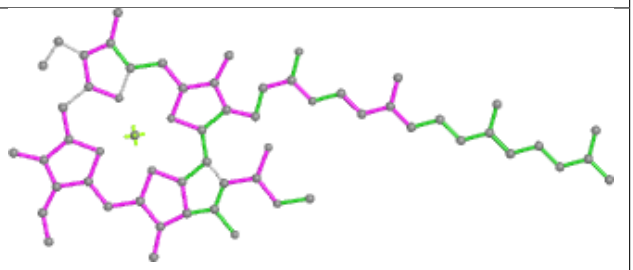
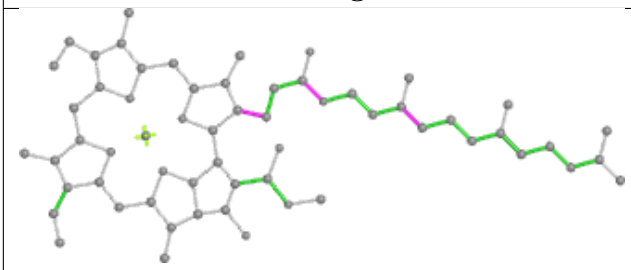


Bond angles



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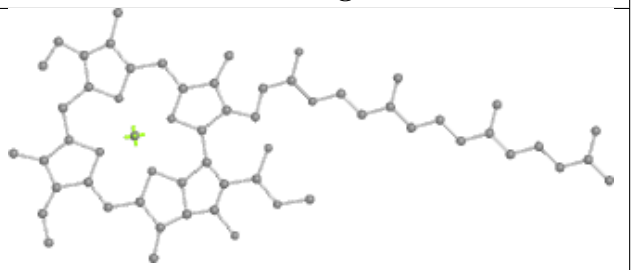
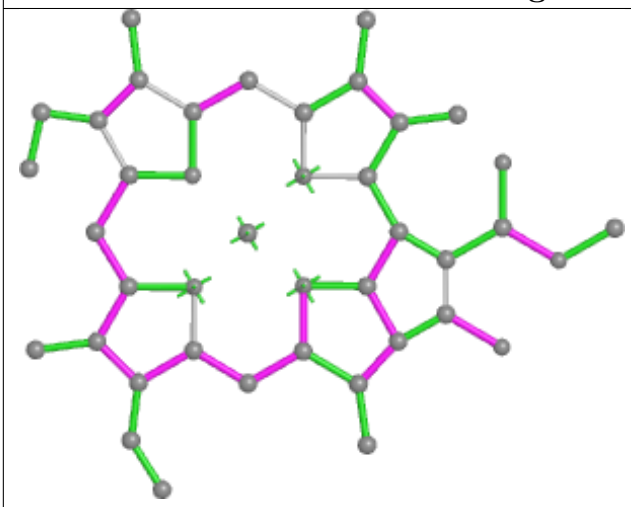


Rings

Ligand CLA 4 616



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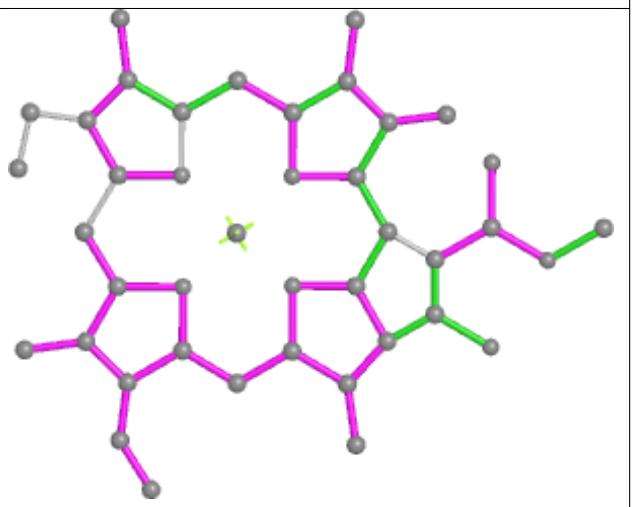
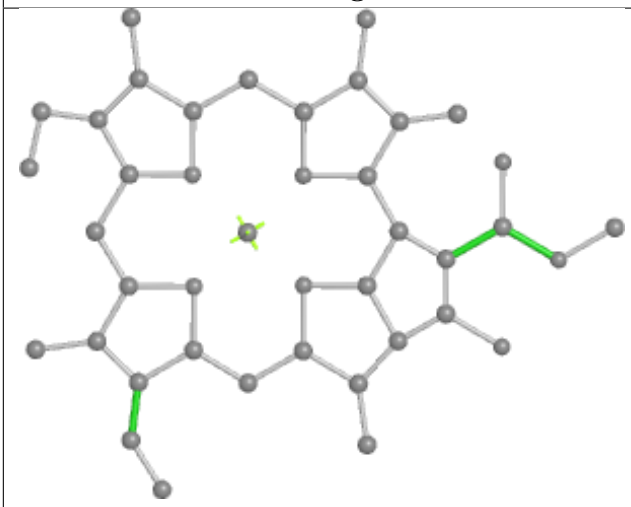


Bond angles



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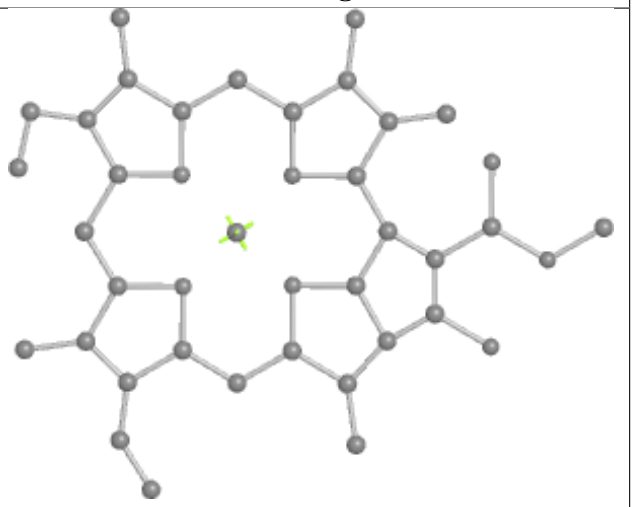
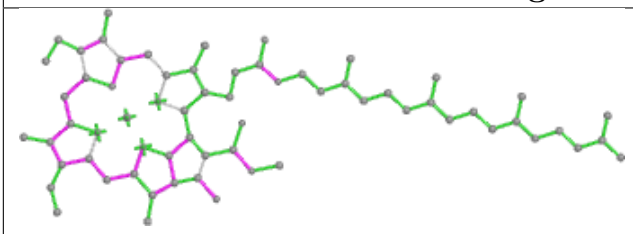


Rings

Ligand CLA 6 604



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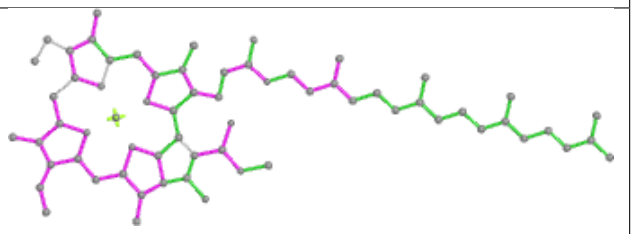
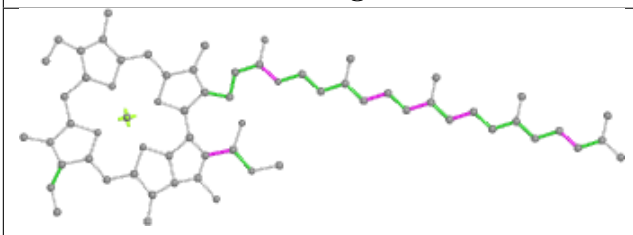


Bond angles



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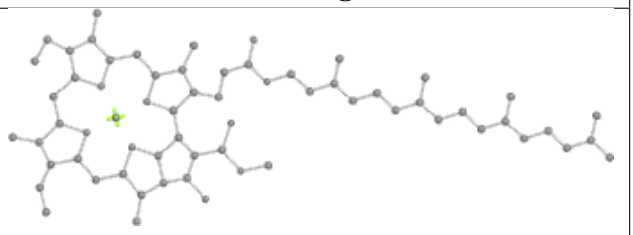
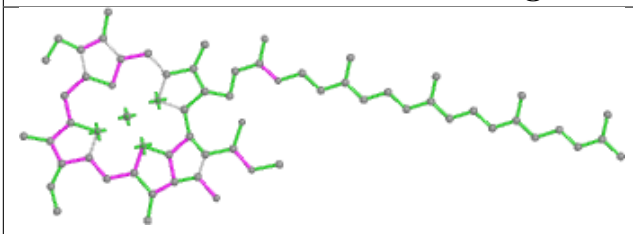


Rings

Ligand CLA B 839



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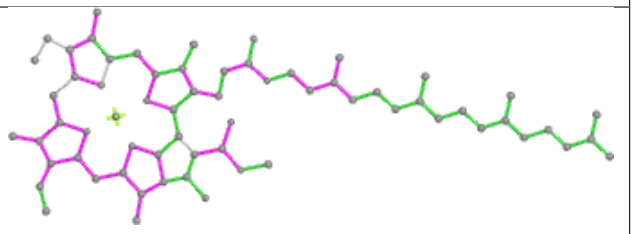
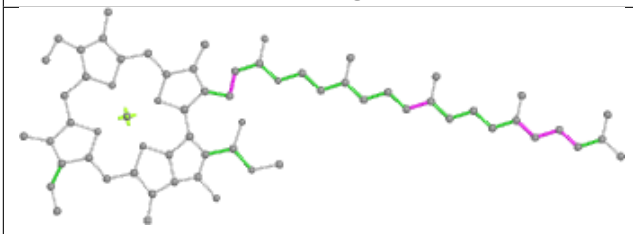


Bond angles



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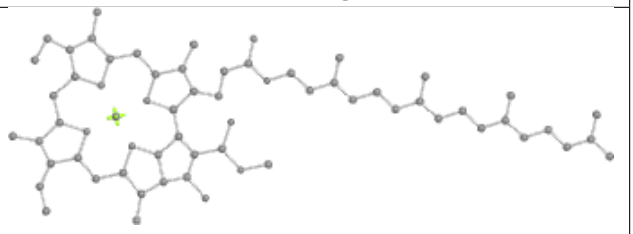
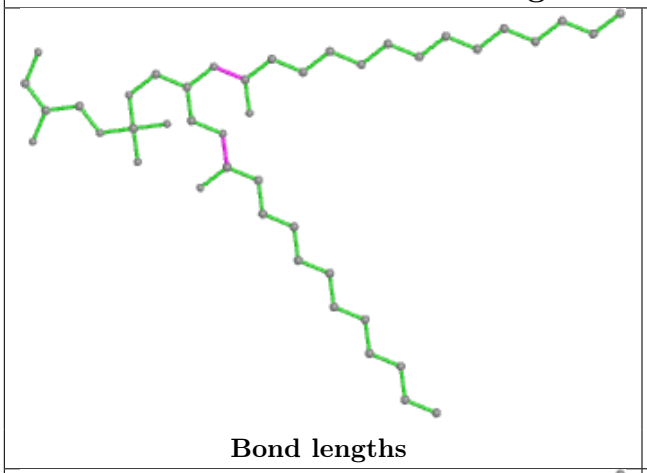


Rings

Ligand LHG 1 620



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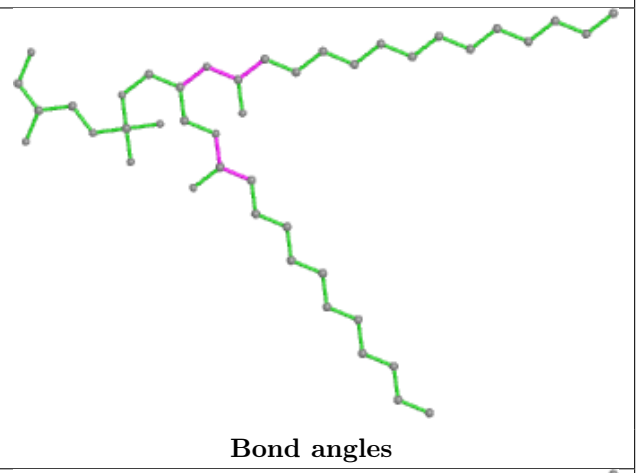
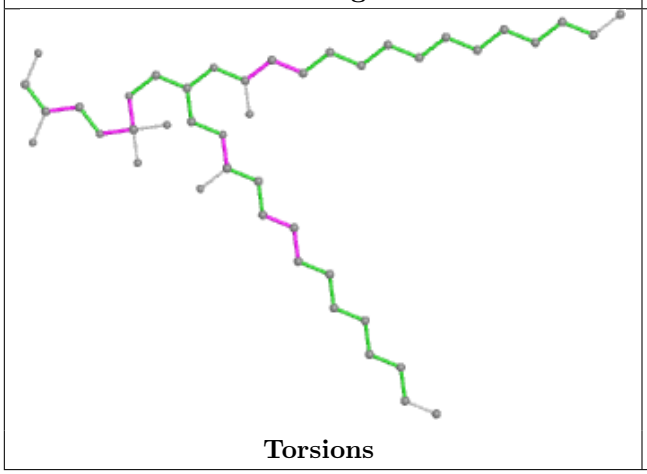


Bond angles



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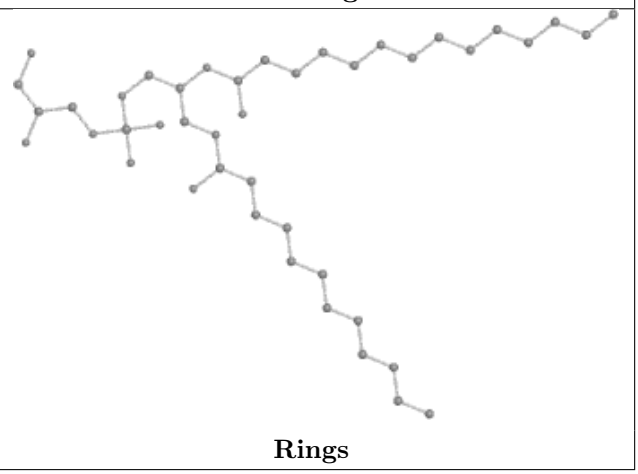
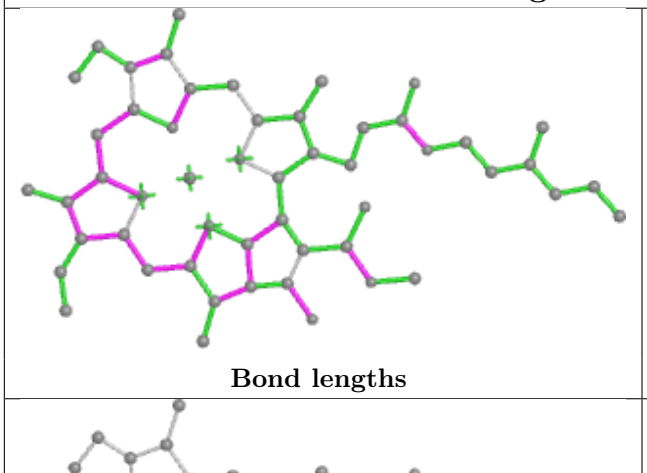


Rings

Ligand CLA 8 612



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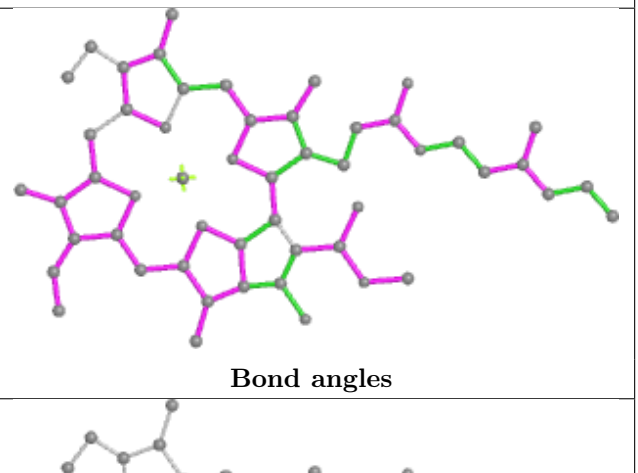
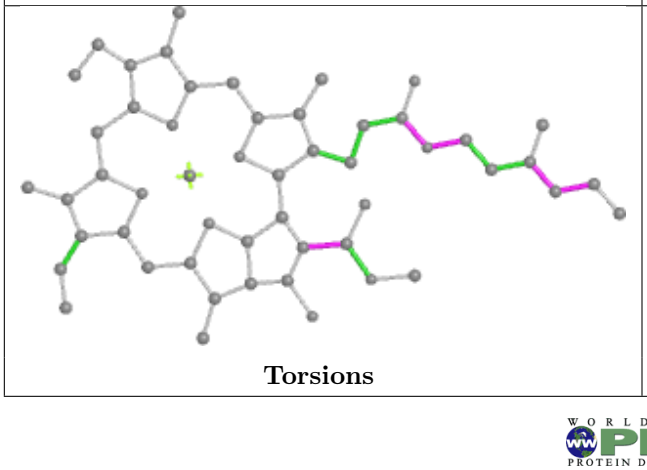


Bond angles



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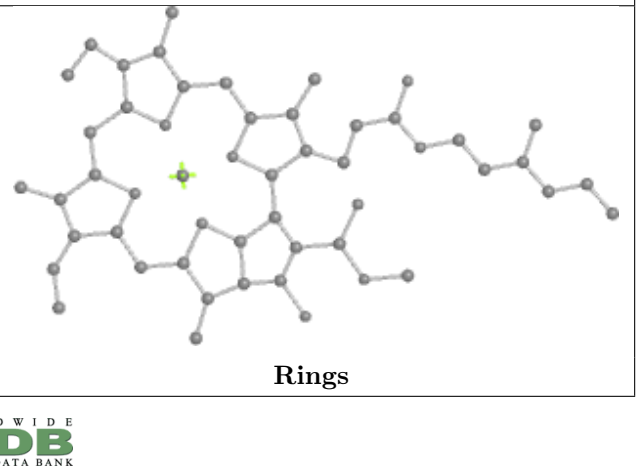
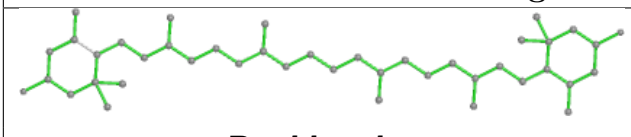


Rings

Ligand LUT 3 622



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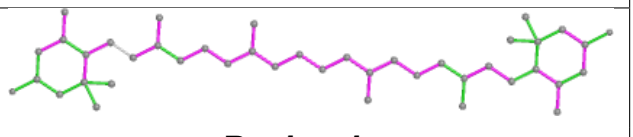
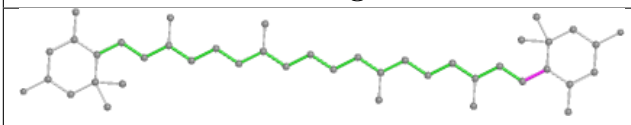


Bond angles



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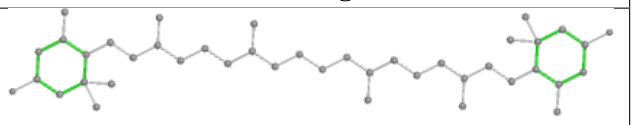
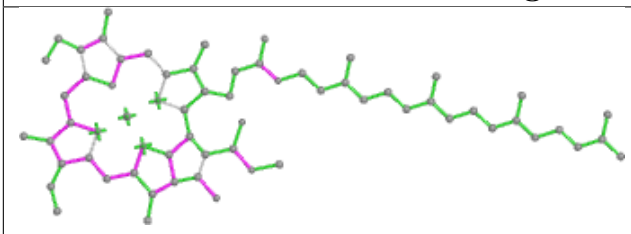


Rings

Ligand CLA A 810



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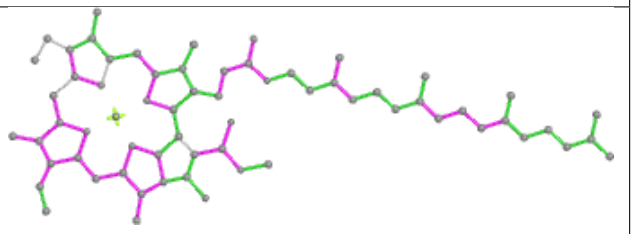
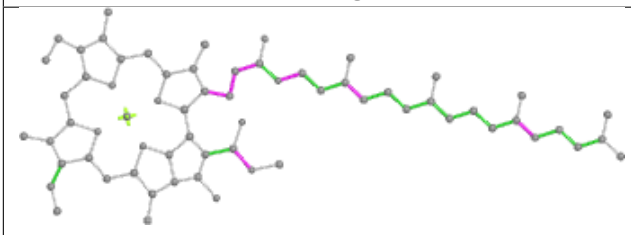
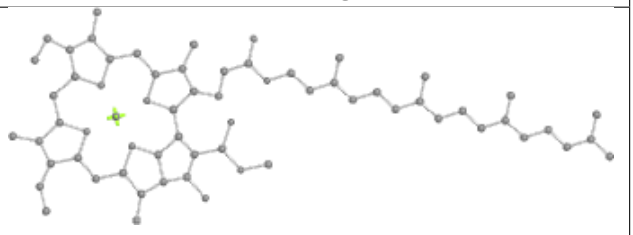


Bond angles

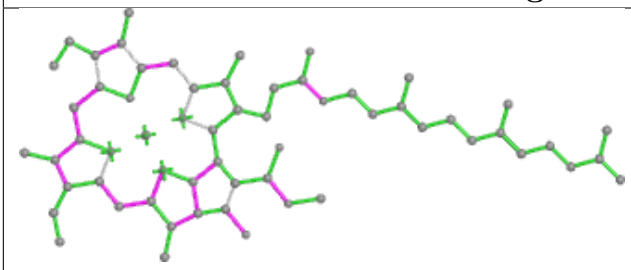


Torsions

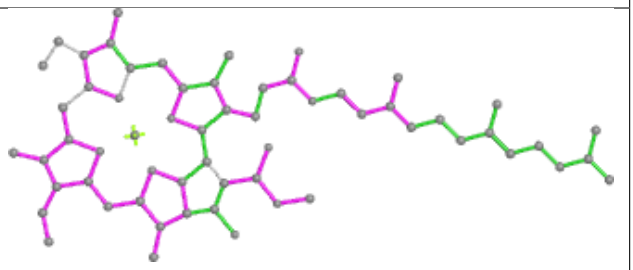


Rings

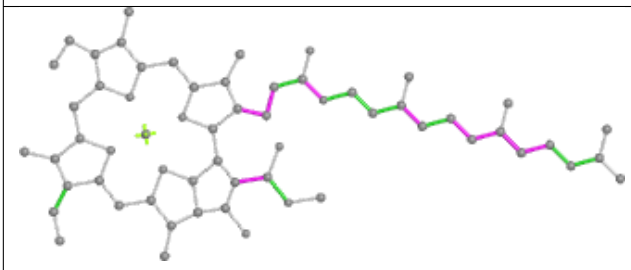
Ligand CLA Z 610



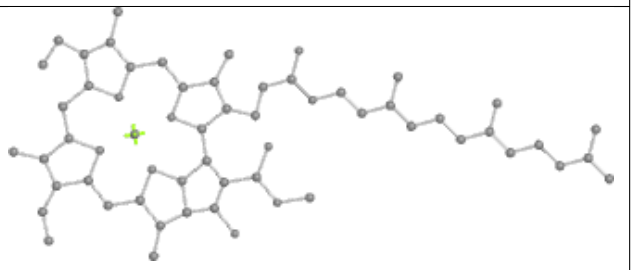
Bond lengths



Bond angles

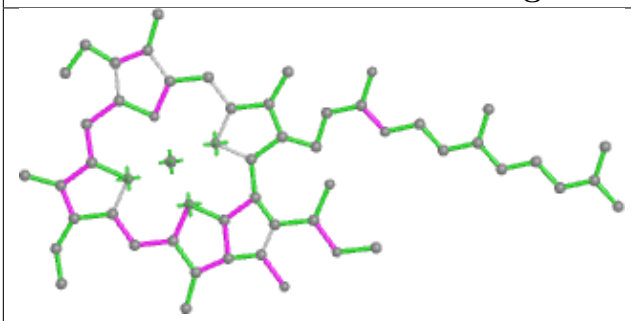


Torsions

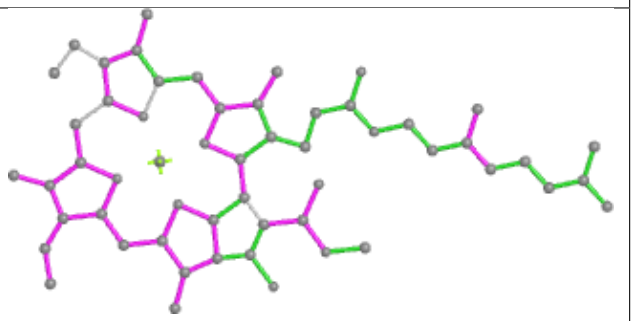


Rings

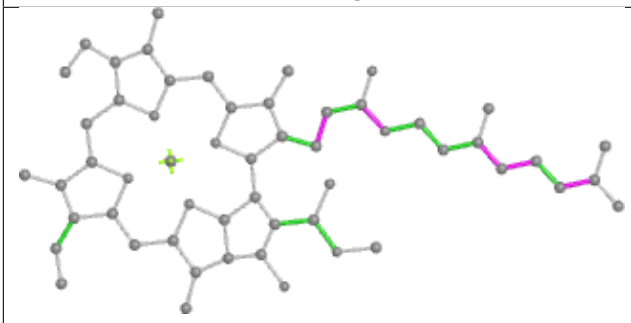
Ligand CLA A 805



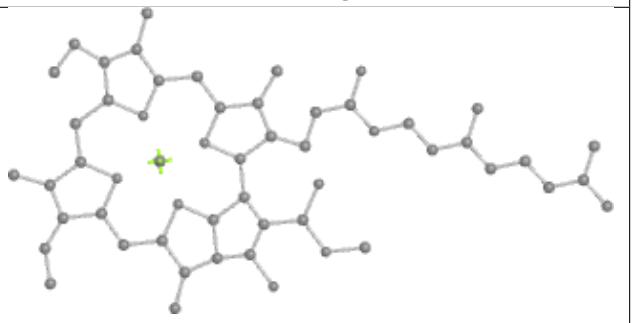
Bond lengths



Bond angles

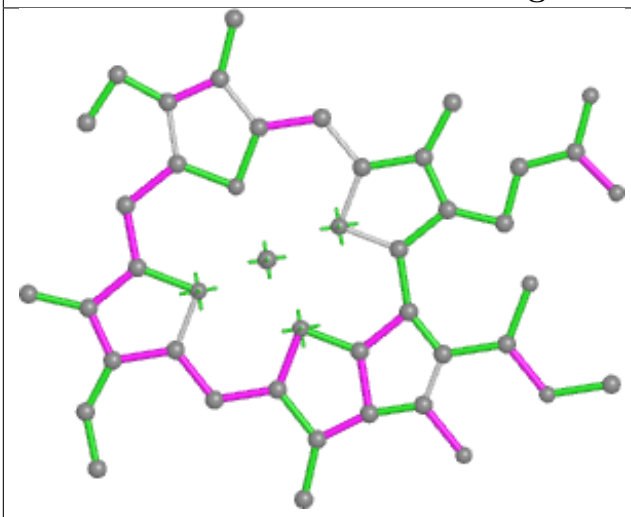


Torsions

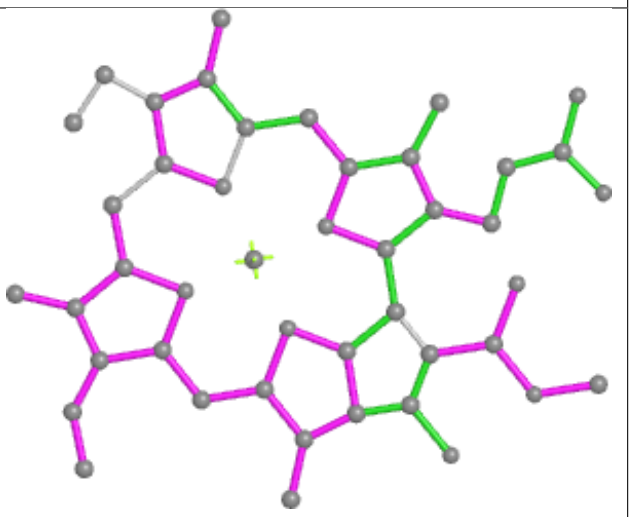


Rings

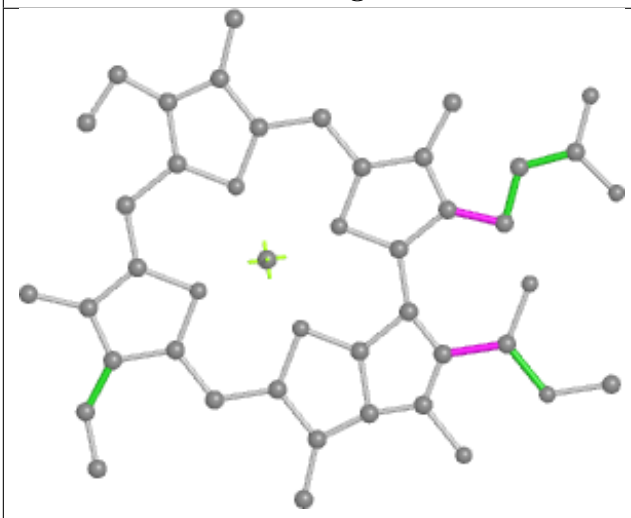
Ligand CLA 4 614



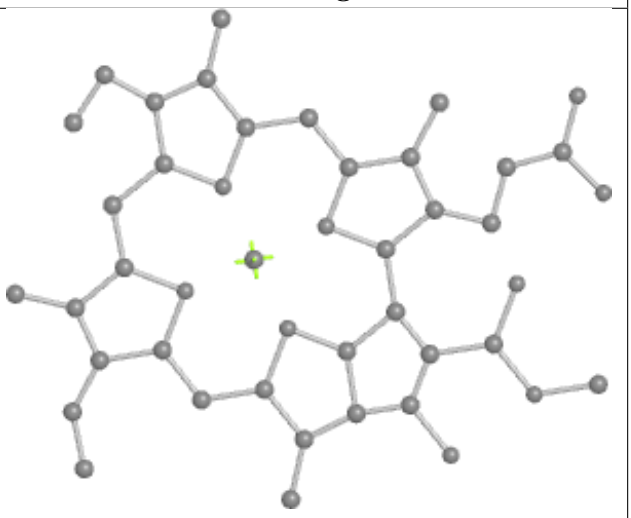
Bond lengths



Bond angles

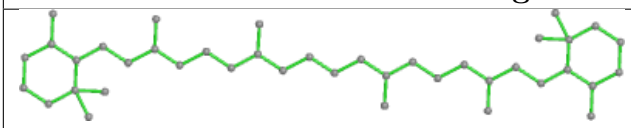


Torsions

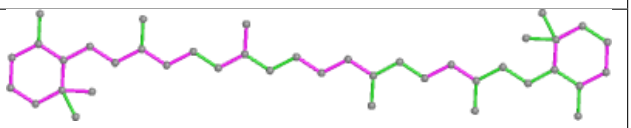


Rings

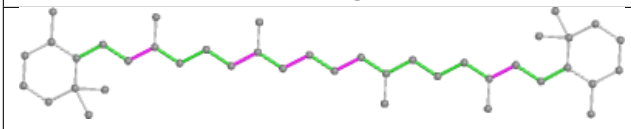
Ligand BCR K 4001



Bond lengths



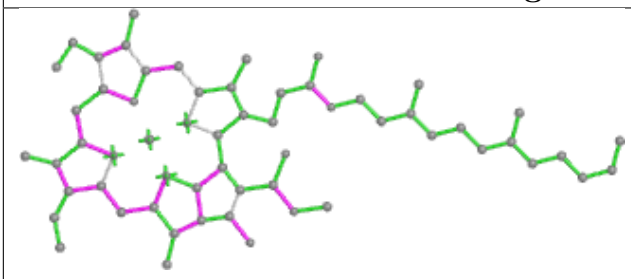
Bond angles



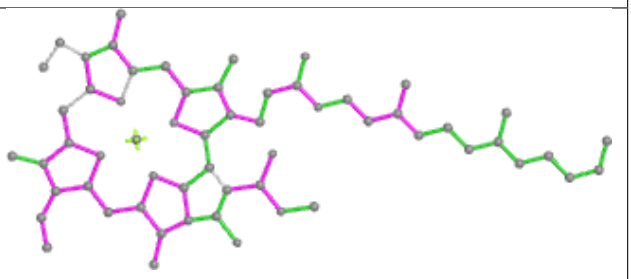
Torsions

Rings

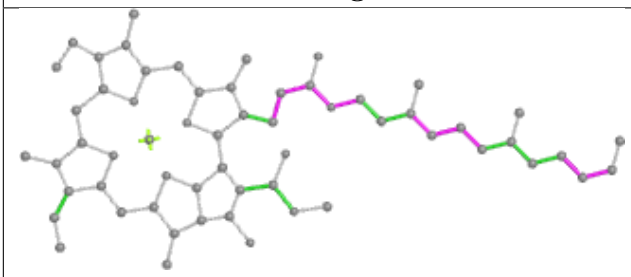
Ligand CLA B 817



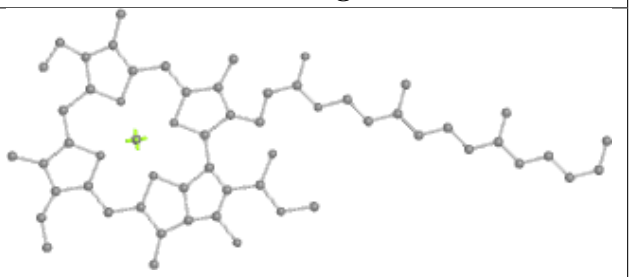
Bond lengths



Bond angles

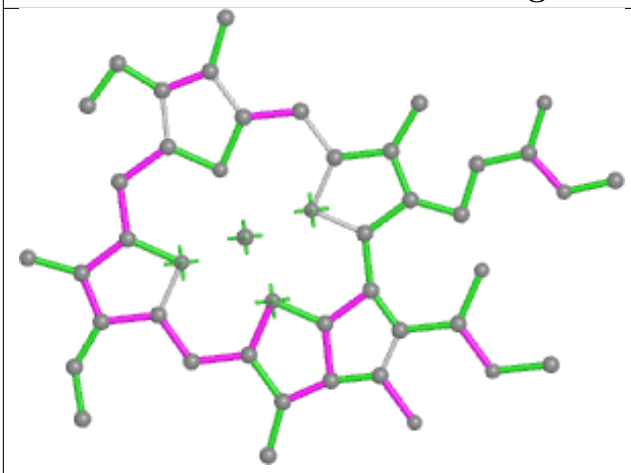


Torsions

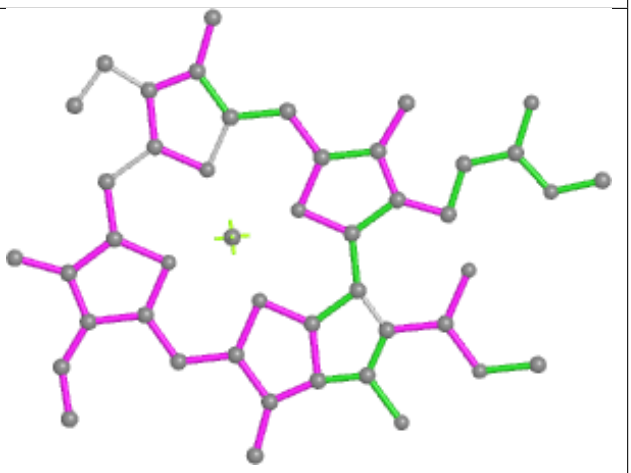


Rings

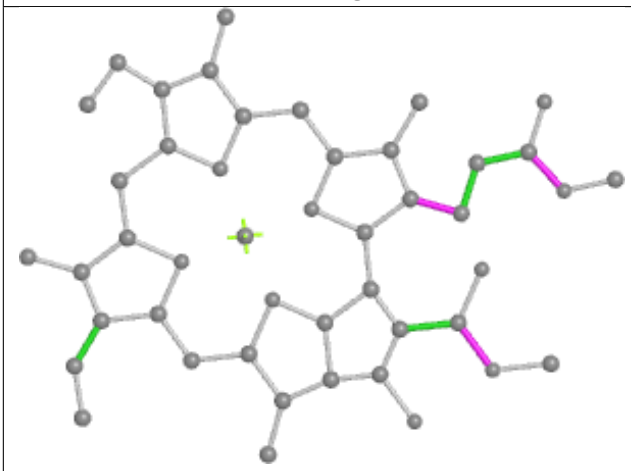
Ligand CLA 8 604



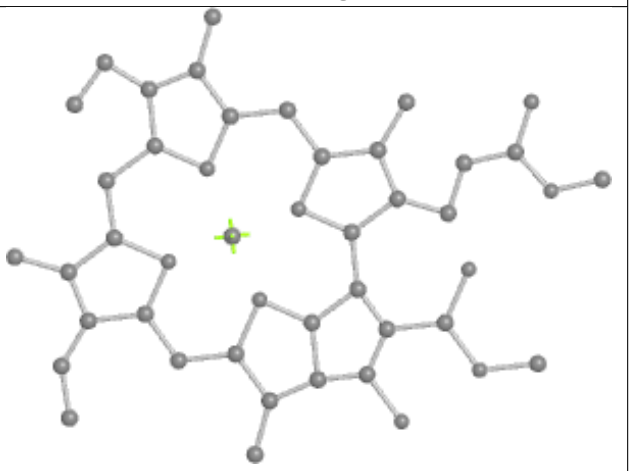
Bond lengths



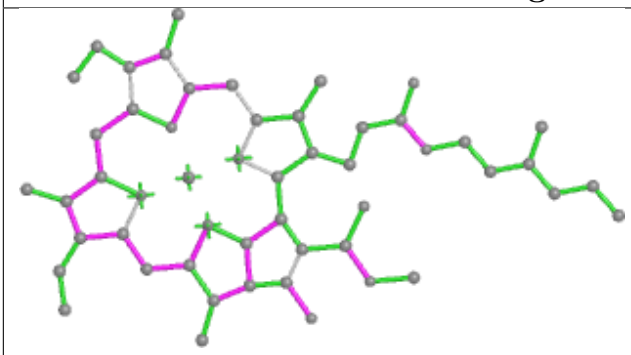
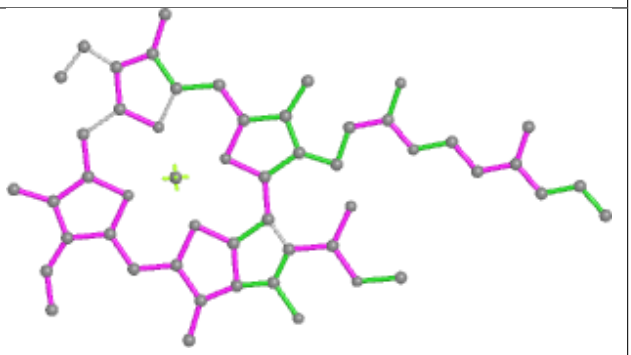
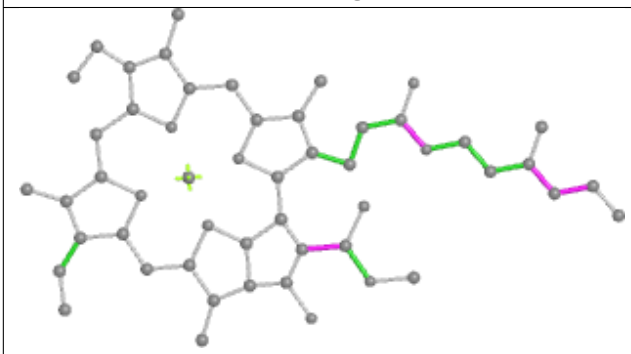
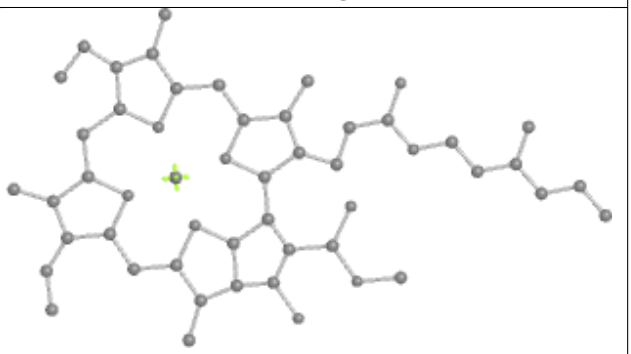
Bond angles

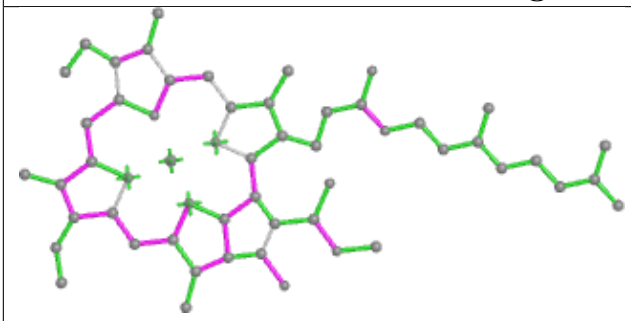
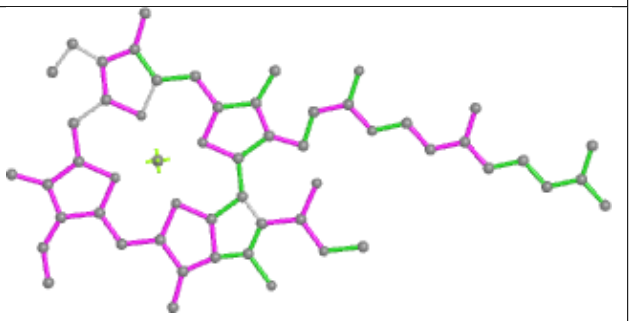
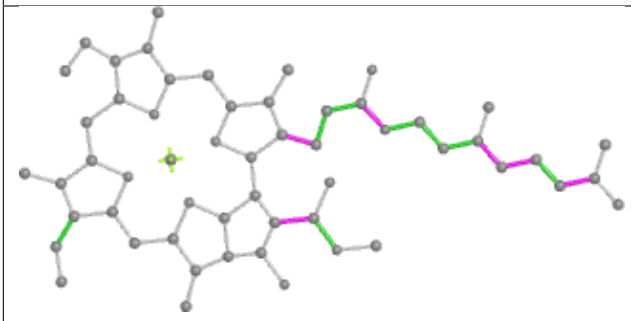
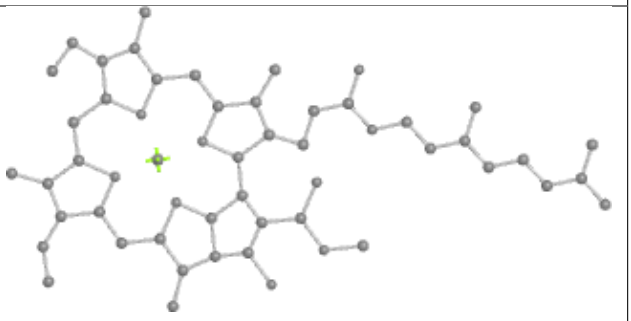


Torsions

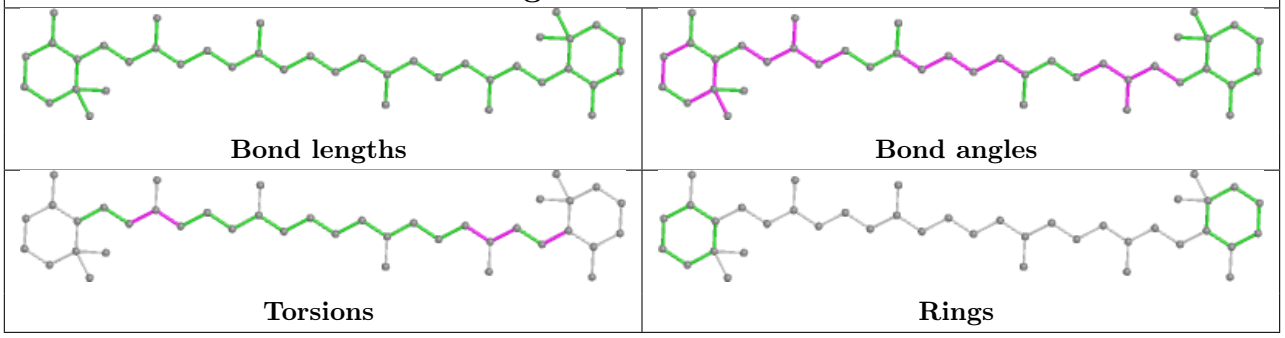


Rings

Ligand CLA 4 612	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 5 611	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR B 845



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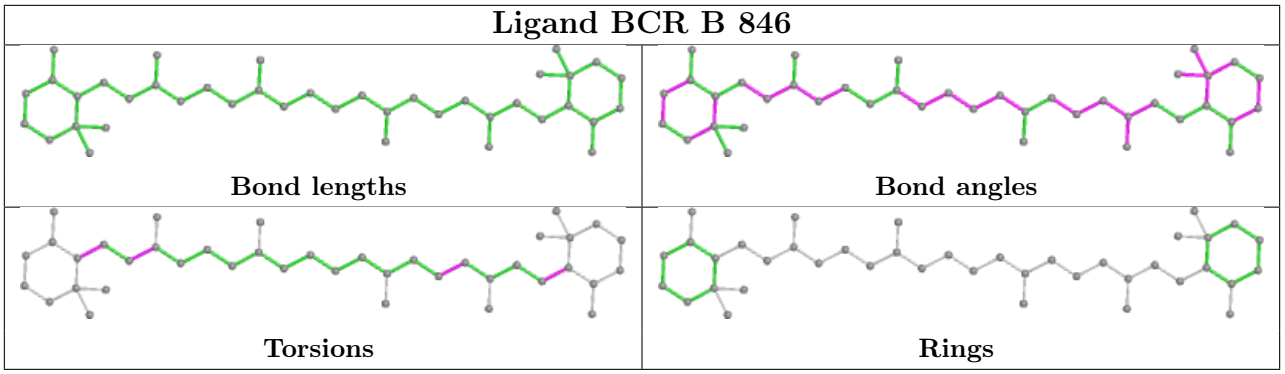

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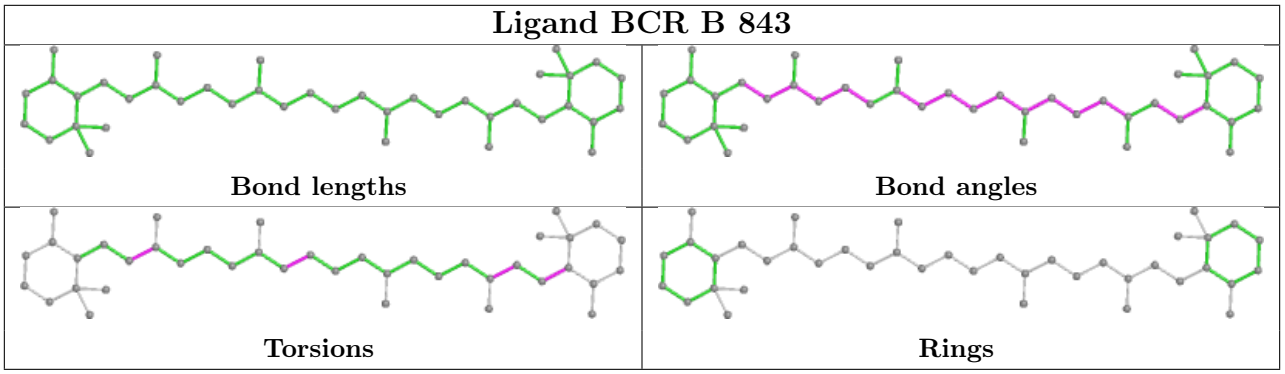
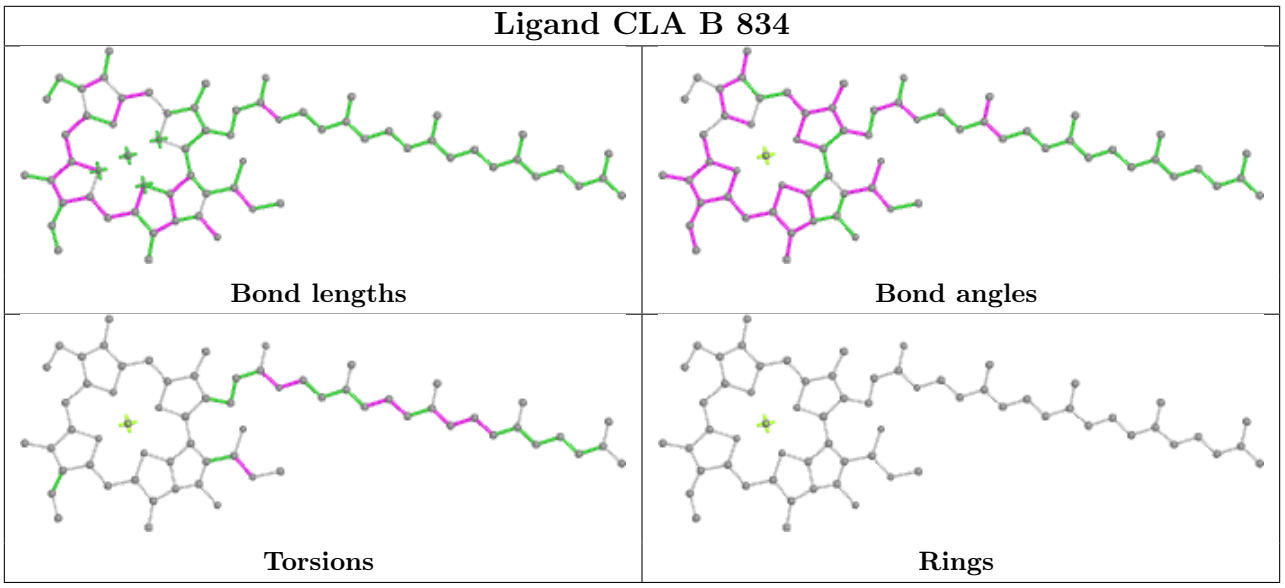
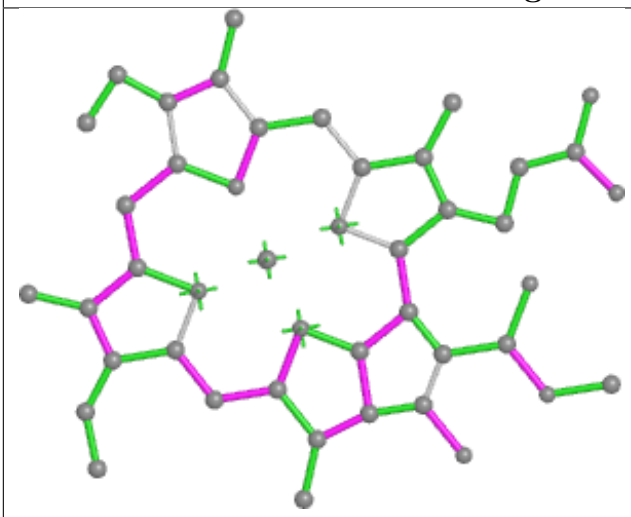


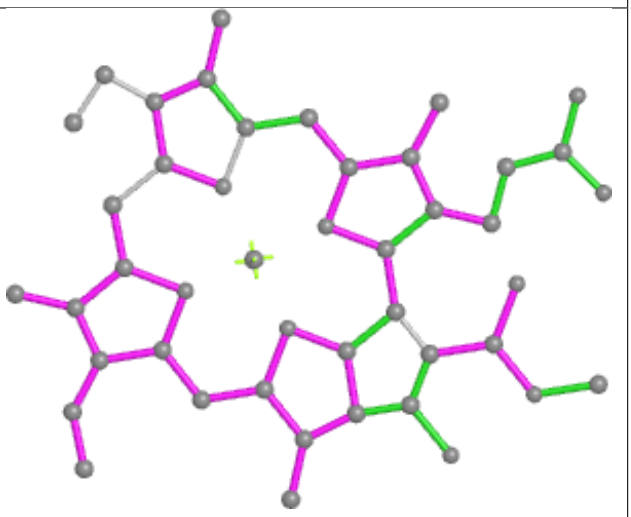
Ligand CLA B 834



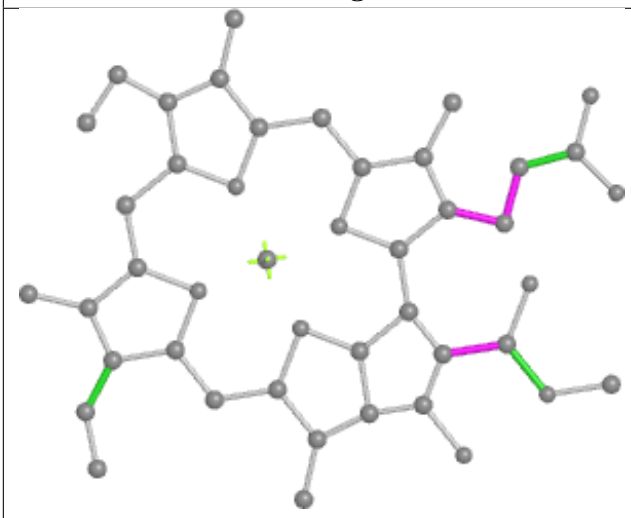
Ligand CLA B 804



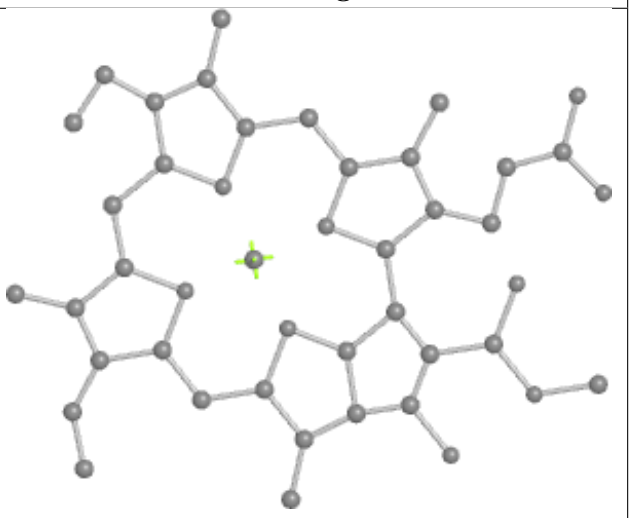
Bond lengths



Bond angles

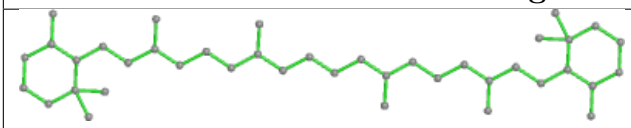


Torsions

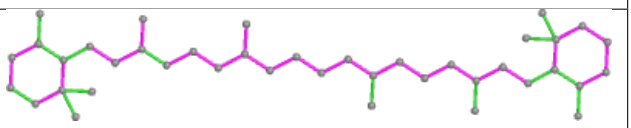


Rings

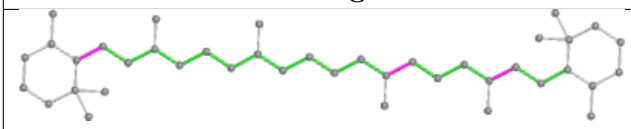
Ligand BCR I 172



Bond lengths



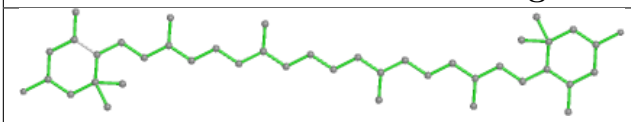
Bond angles



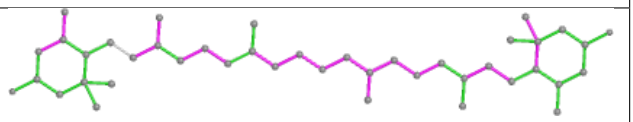
Torsions

Rings

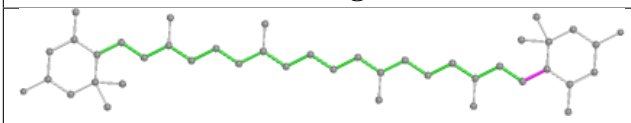
Ligand LUT 7 622



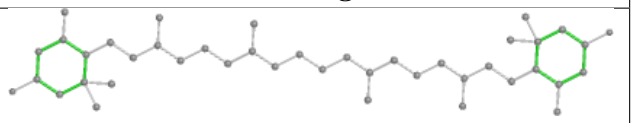
Bond lengths



Bond angles

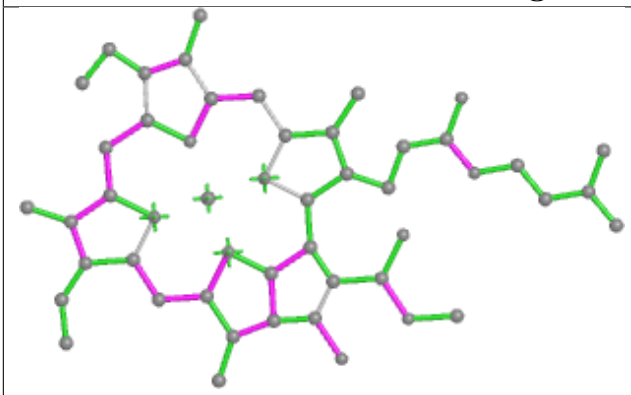


Torsions

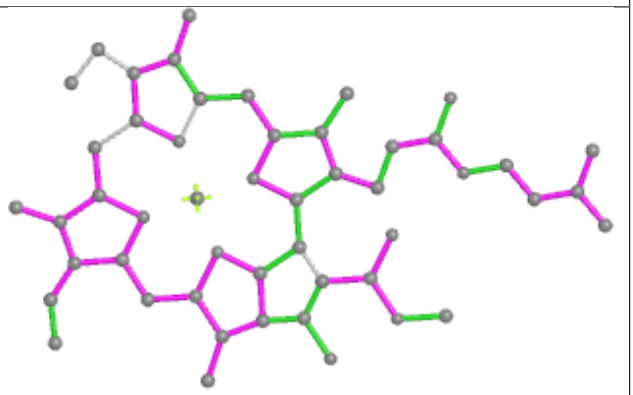


Rings

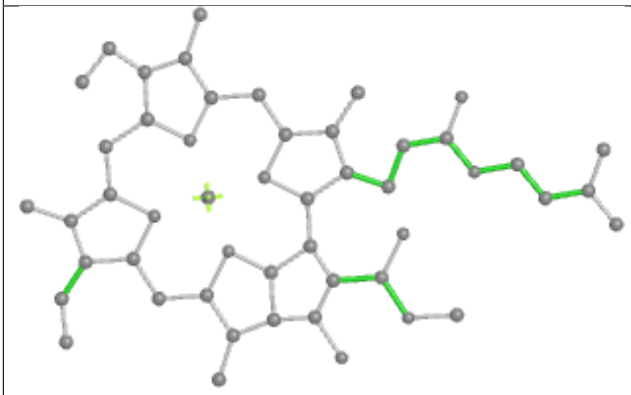
Ligand CLA 8 608



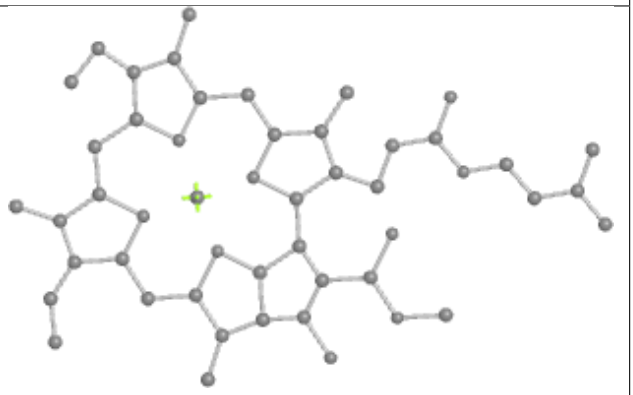
Bond lengths



Bond angles

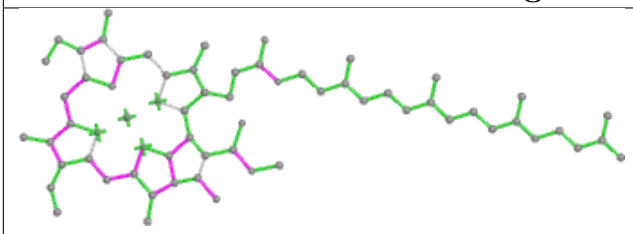


Torsions

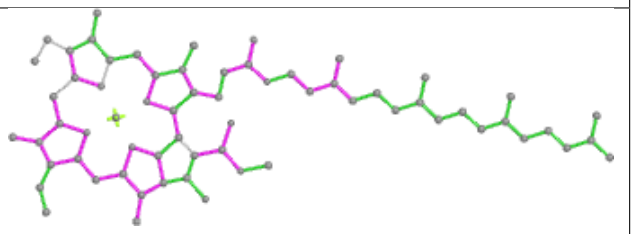


Rings

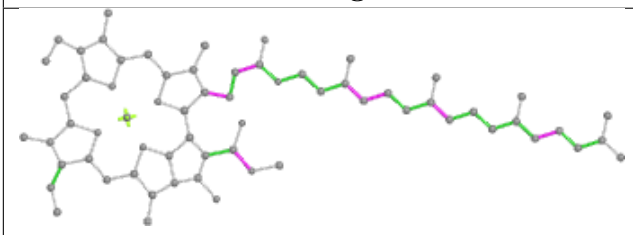
Ligand CLA B 832



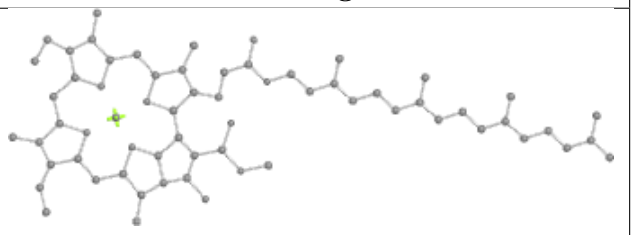
Bond lengths



Bond angles

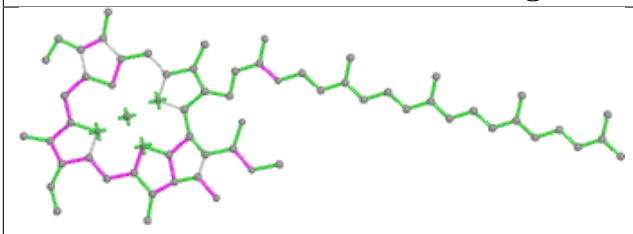


Torsions

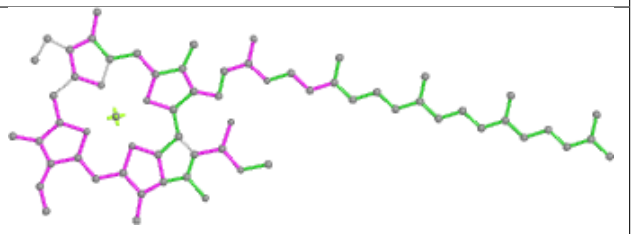


Rings

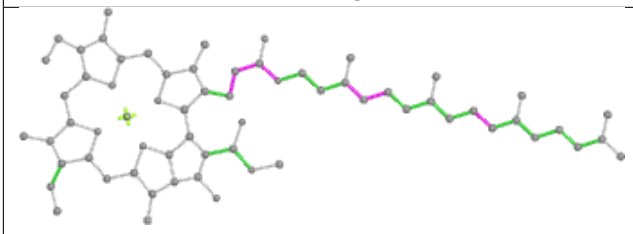
Ligand CLA B 807



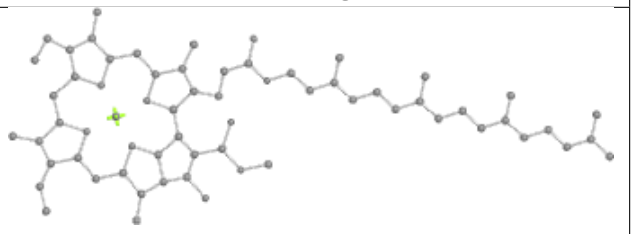
Bond lengths



Bond angles

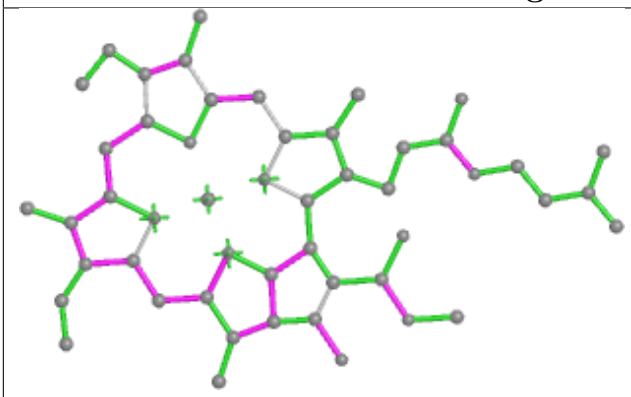


Torsions

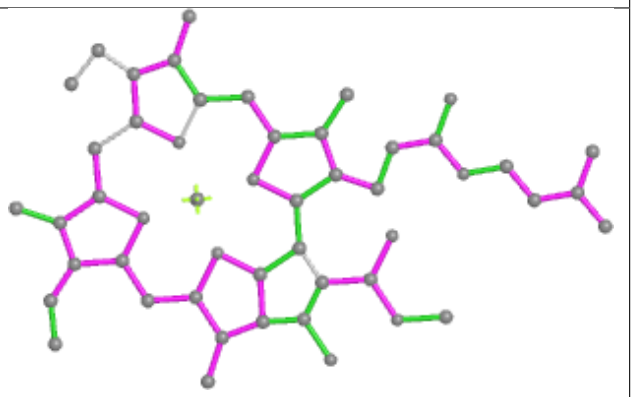


Rings

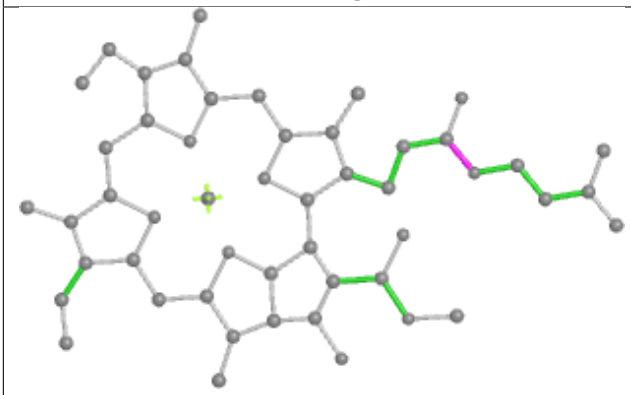
Ligand CLA L 204



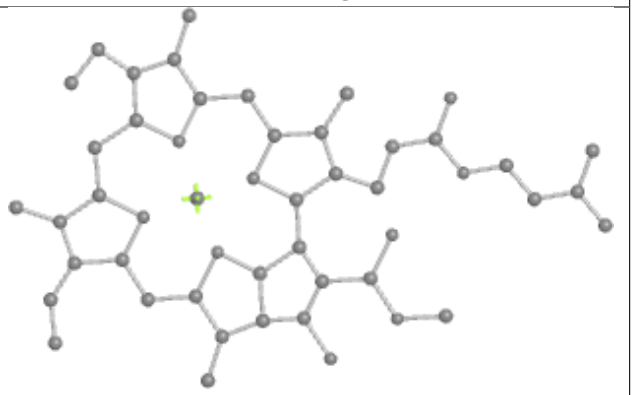
Bond lengths



Bond angles

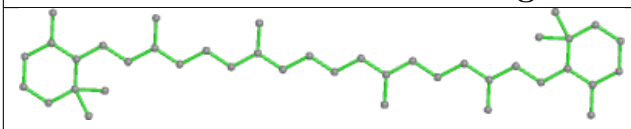


Torsions

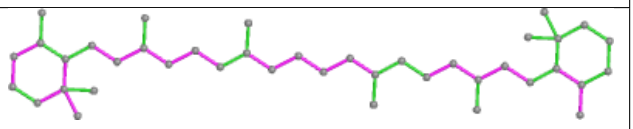


Rings

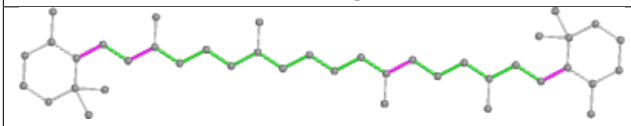
Ligand BCR J 3003



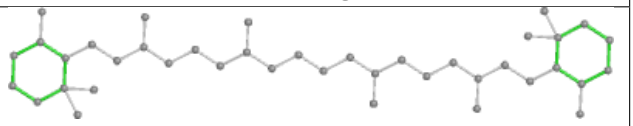
Bond lengths



Bond angles

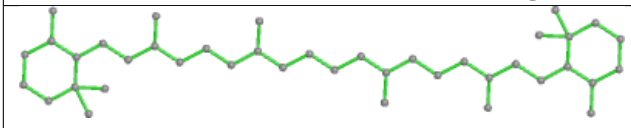


Torsions

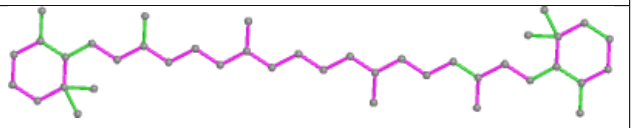


Rings

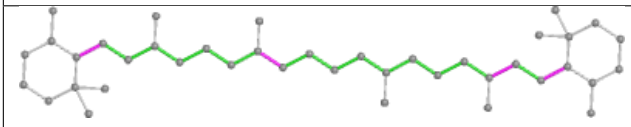
Ligand BCR F 305



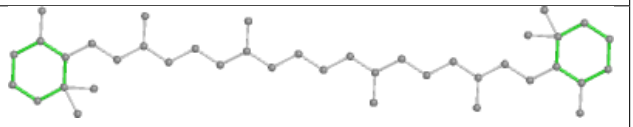
Bond lengths



Bond angles

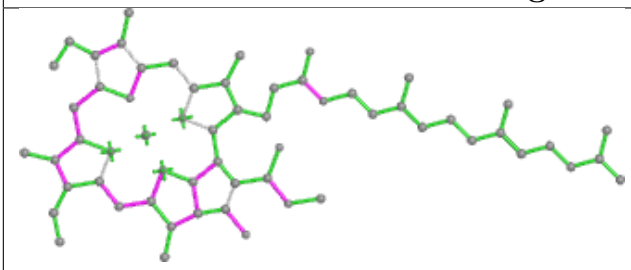


Torsions

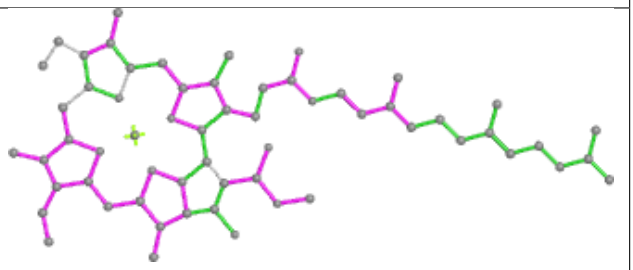


Rings

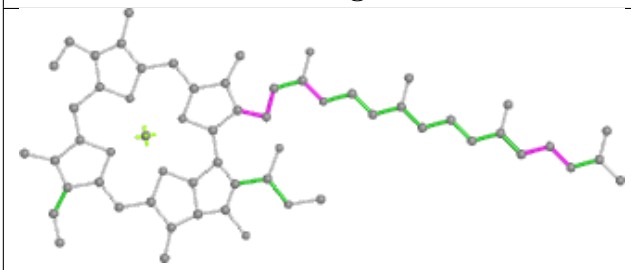
Ligand CLA 7 610



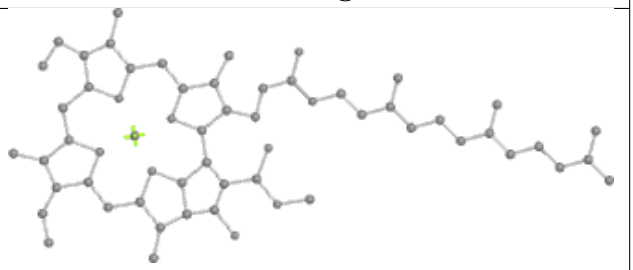
Bond lengths



Bond angles

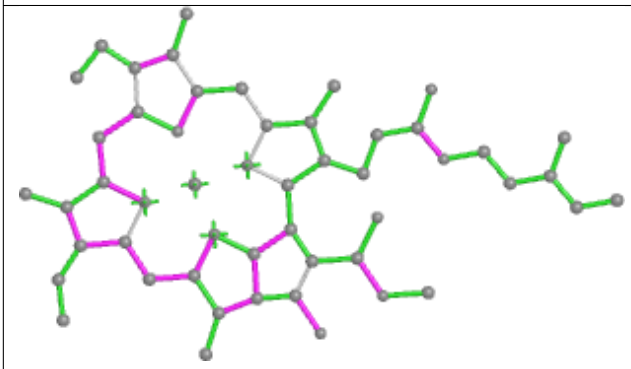


Torsions

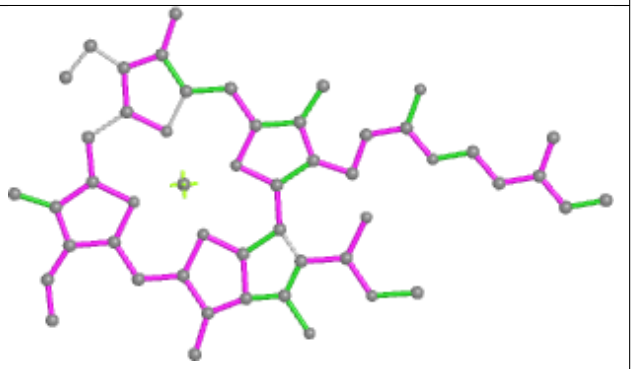


Rings

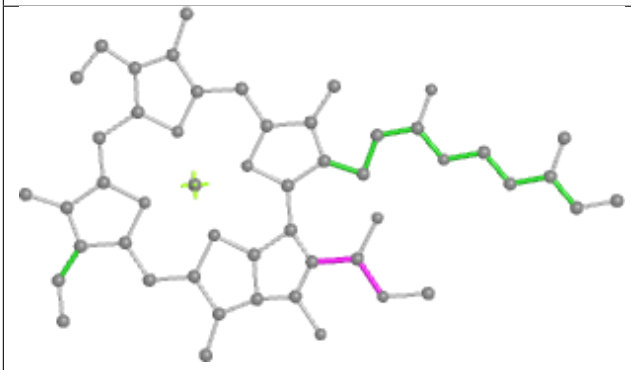
Ligand CLA A 838



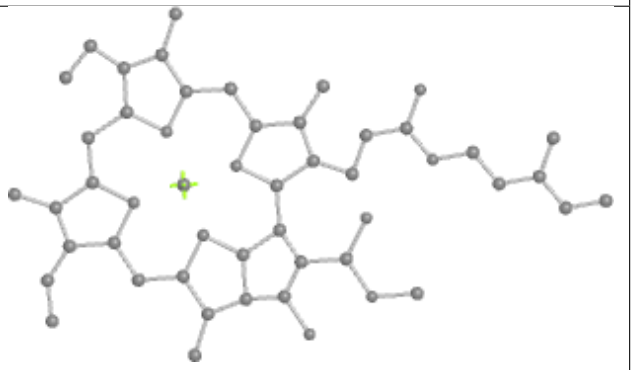
Bond lengths



Bond angles

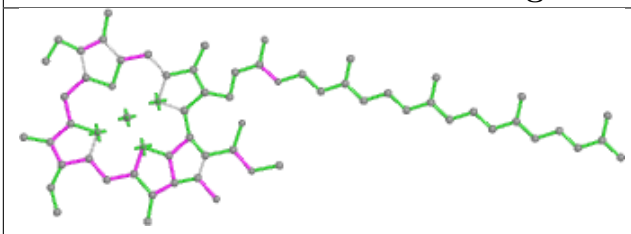


Torsions

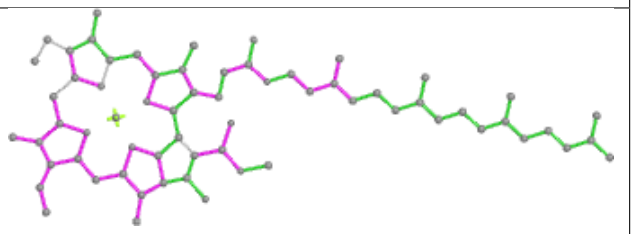


Rings

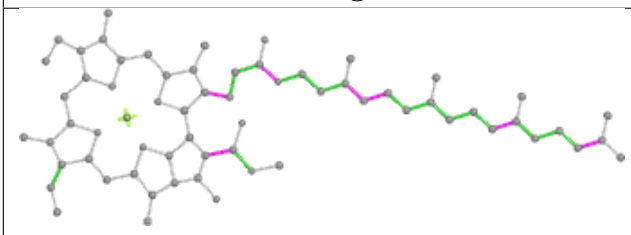
Ligand CLA L 203



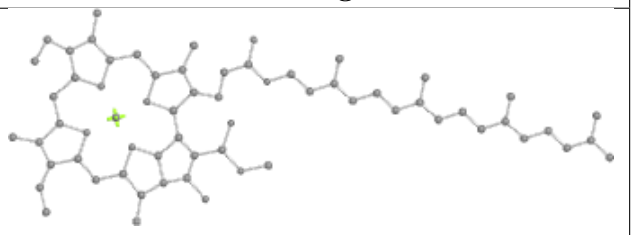
Bond lengths



Bond angles

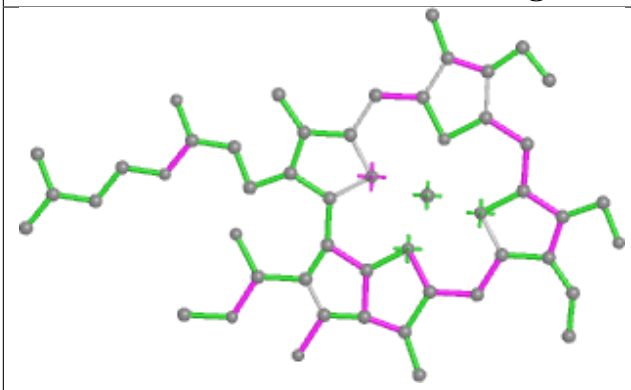


Torsions

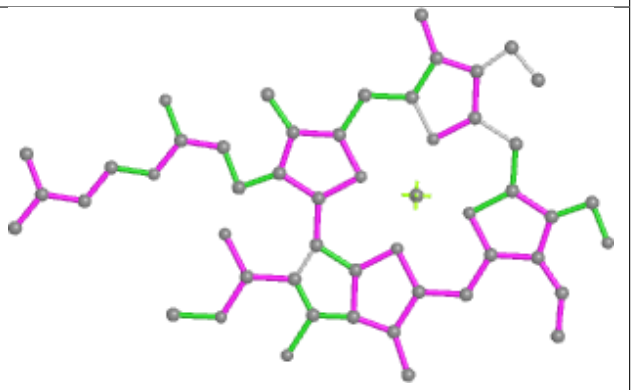


Rings

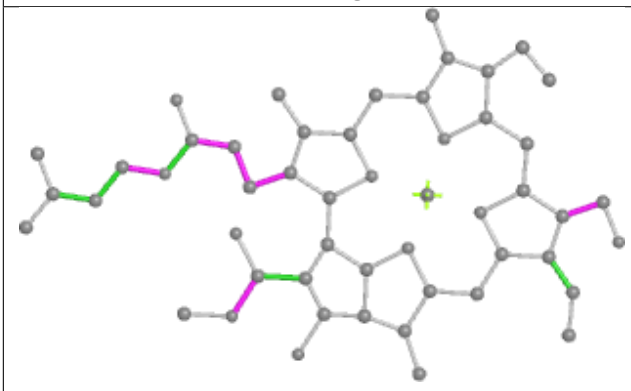
Ligand CHL 4 607



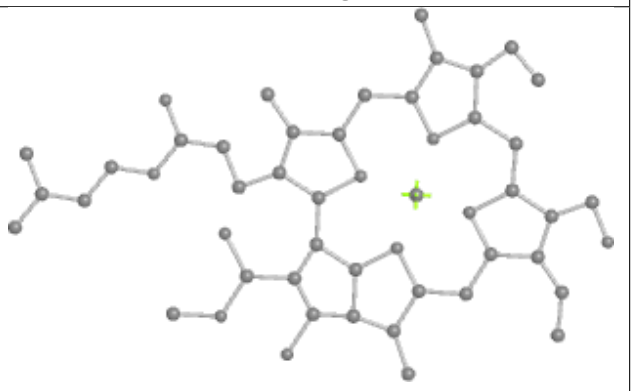
Bond lengths



Bond angles

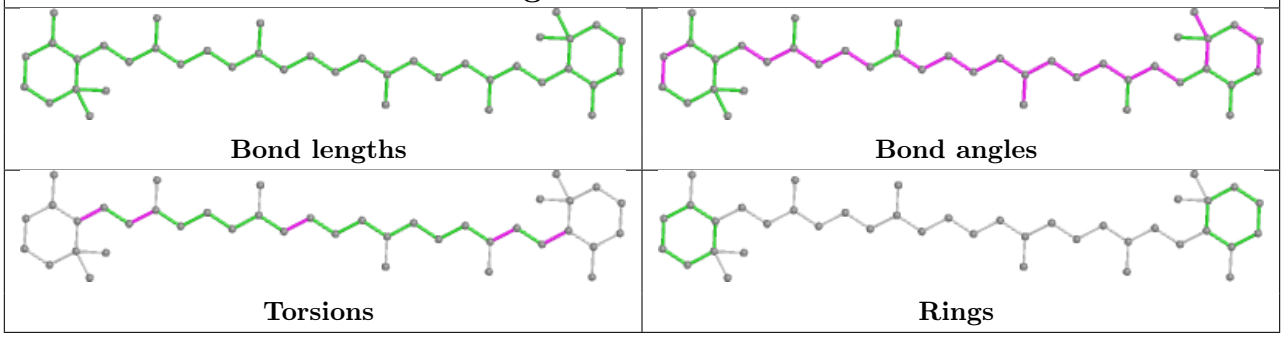


Torsions

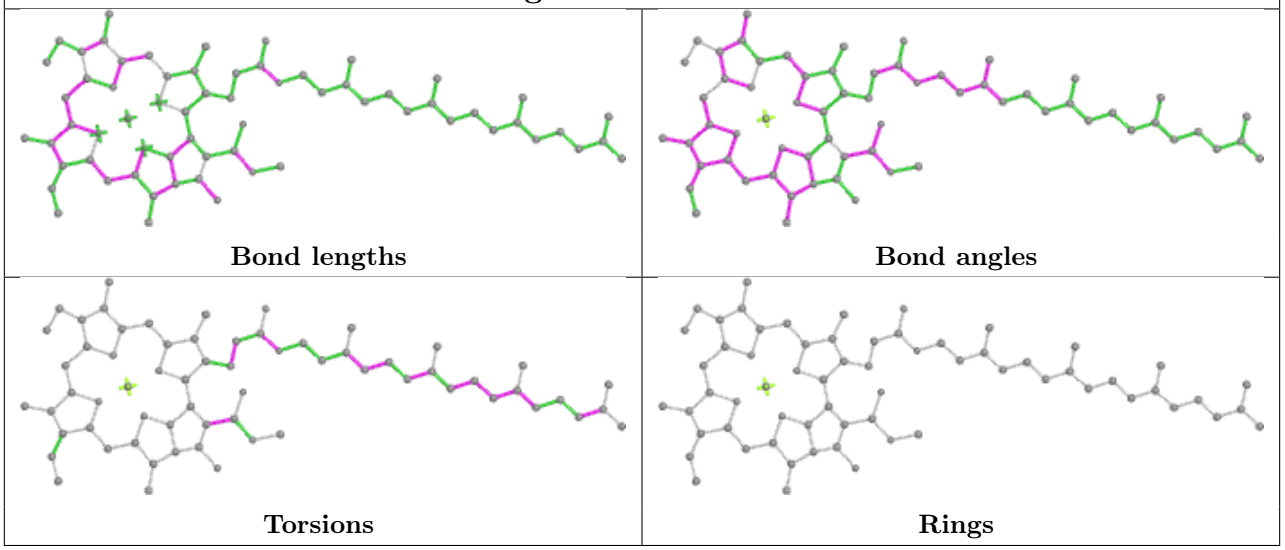


Rings

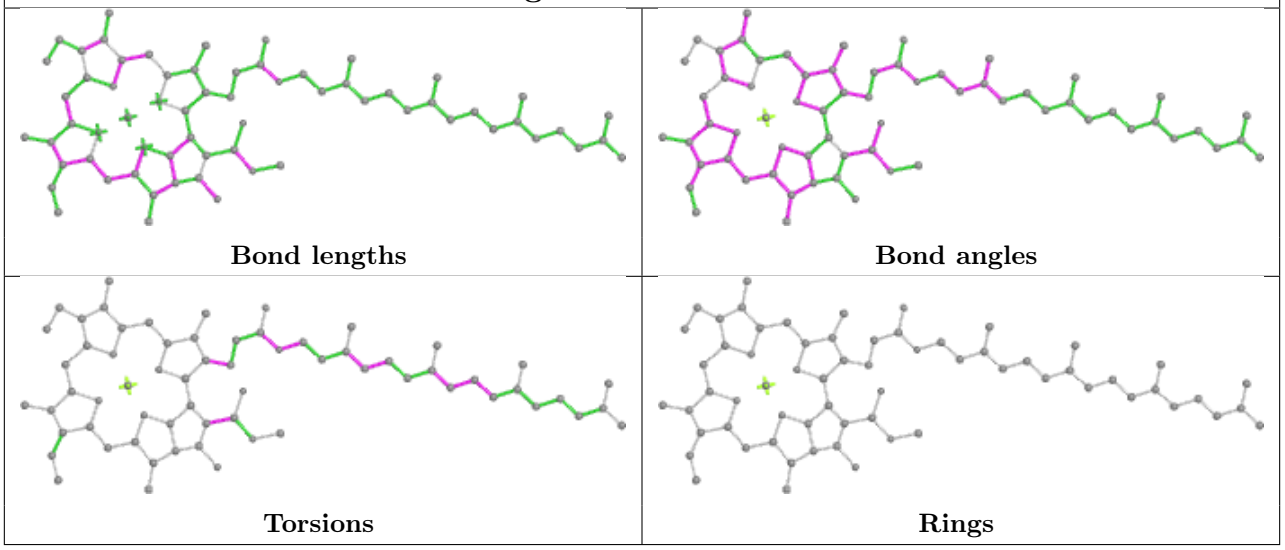
Ligand BCR B 847



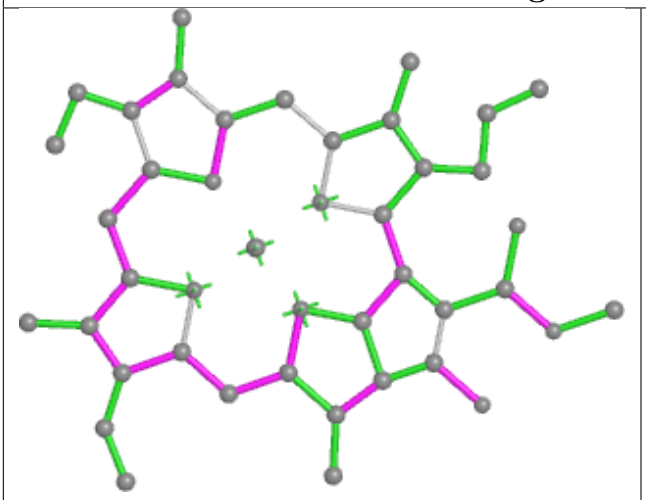
Ligand CLA A 814



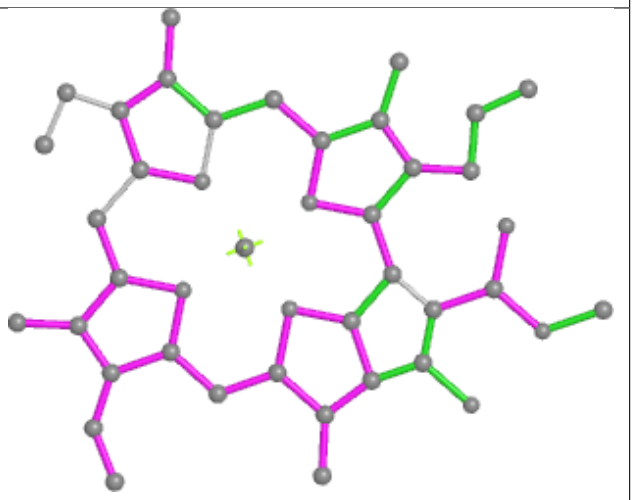
Ligand CLA A 831



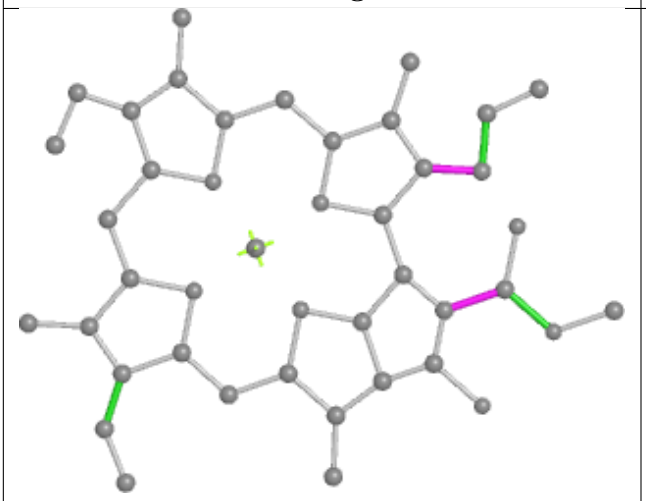
Ligand CLA 7 614



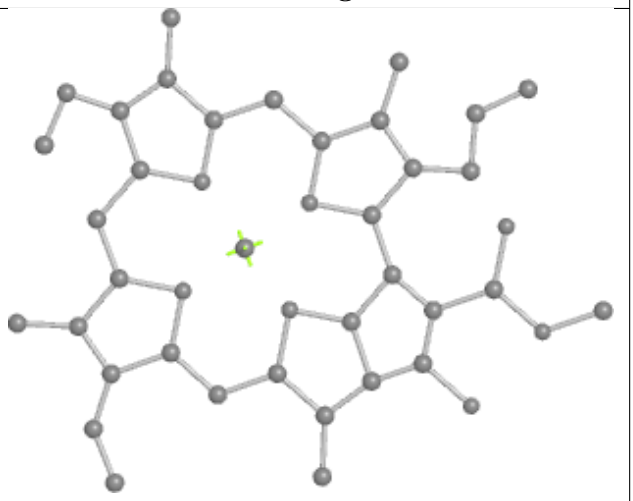
Bond lengths



Bond angles

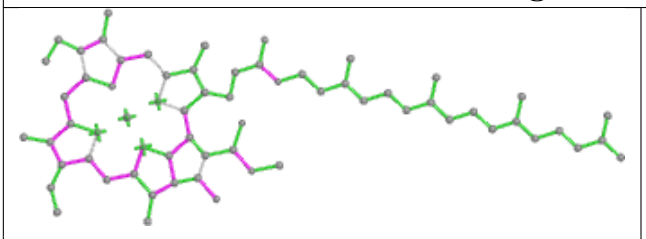


Torsions



Rings

Ligand CLA 8 601



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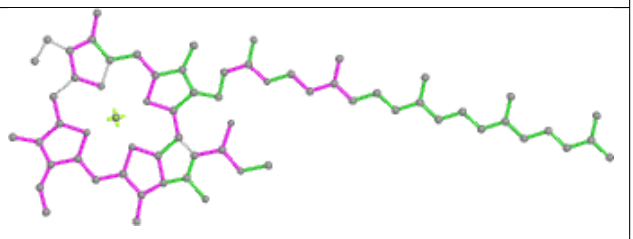
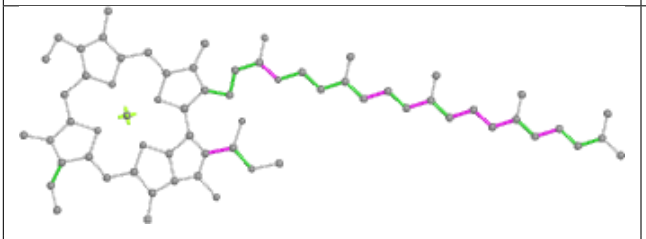
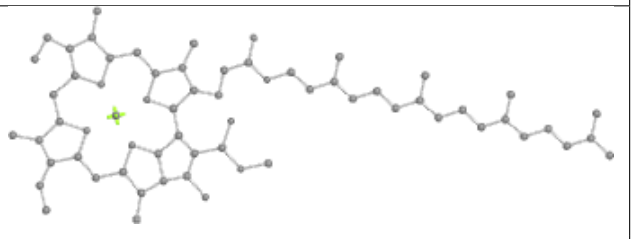


Bond angles

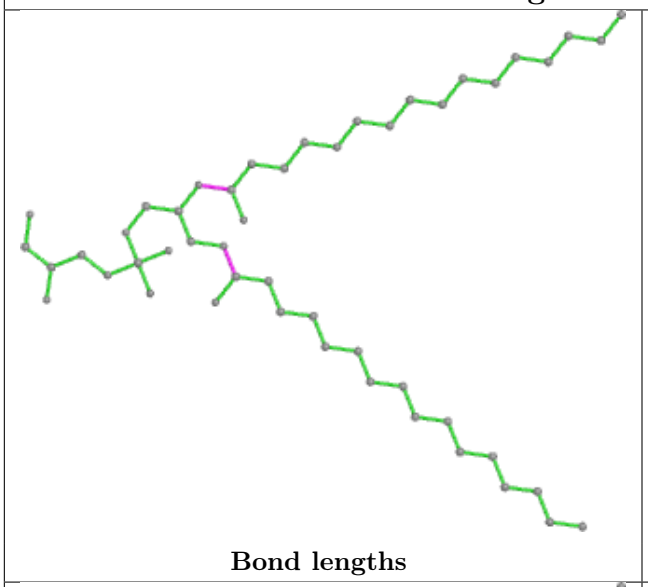


Torsions

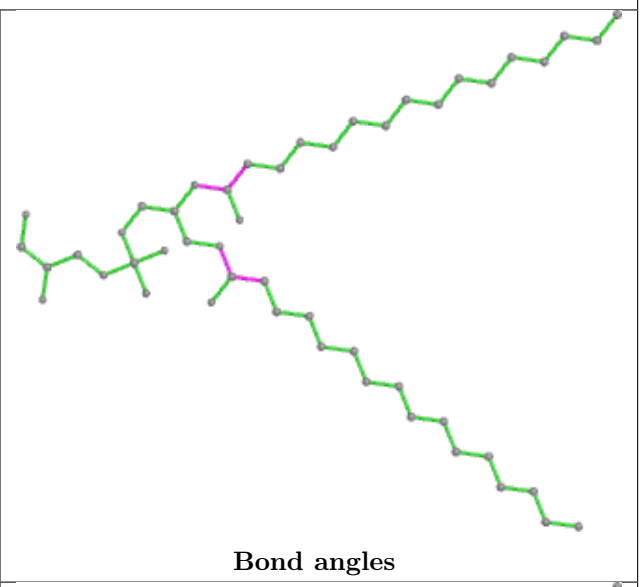


Rings

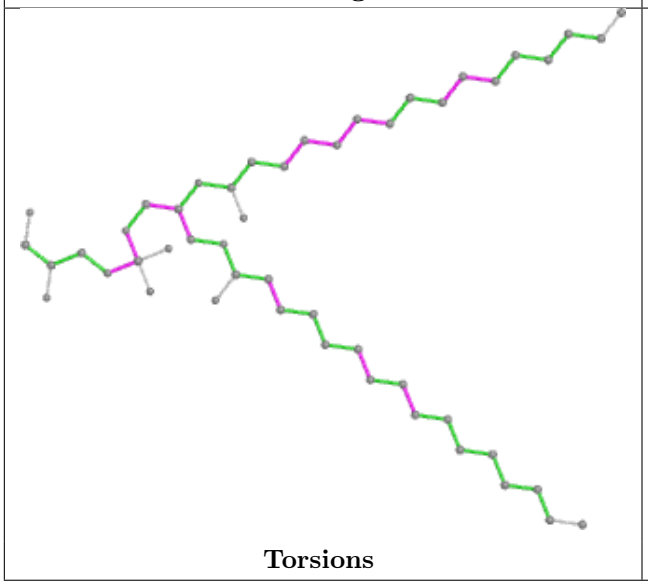
Ligand LHG 6 619



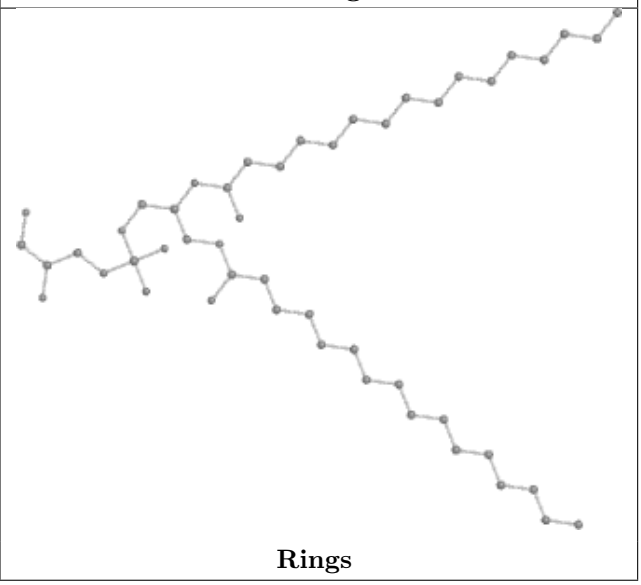
Bond lengths



Bond angles

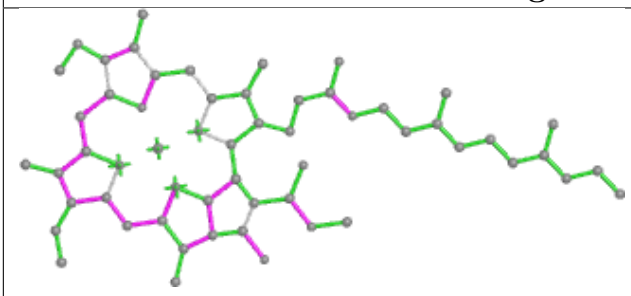


Torsions

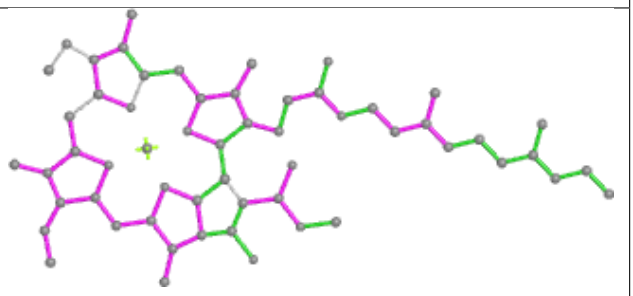


Rings

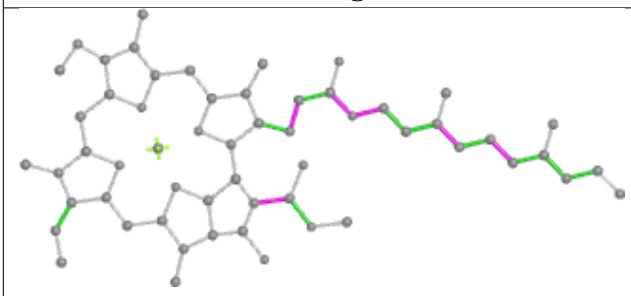
Ligand CLA 1 604



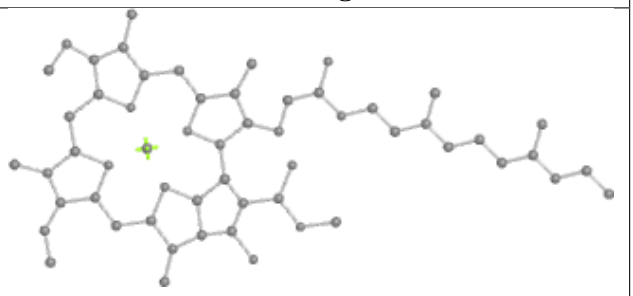
Bond lengths



Bond angles

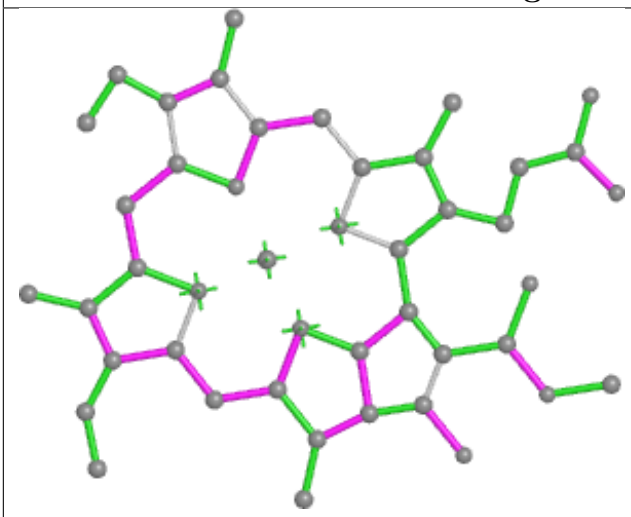


Torsions

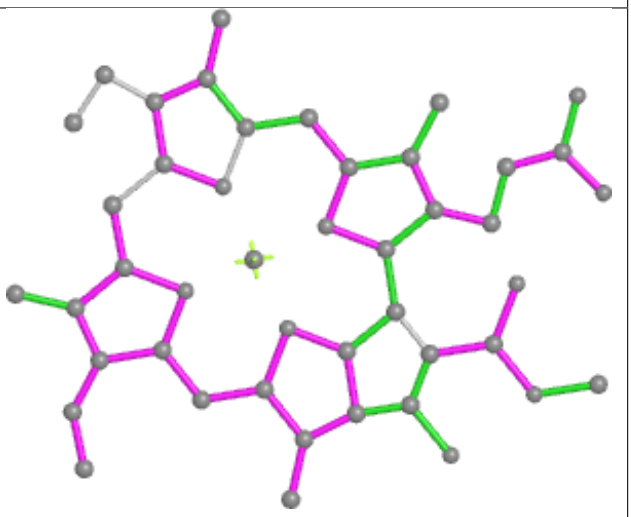


Rings

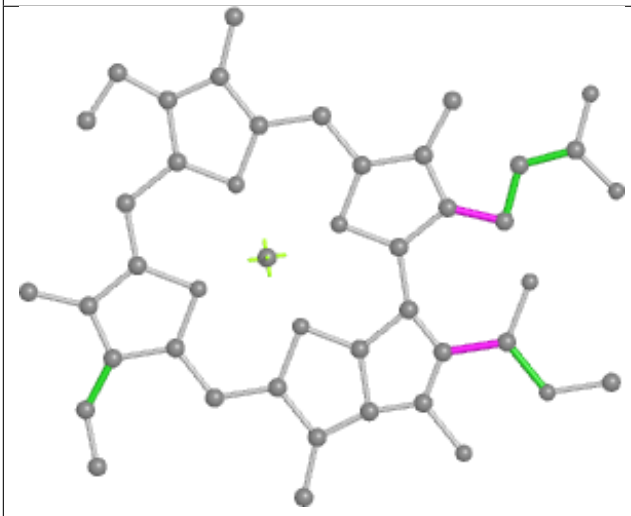
Ligand CLA A 821



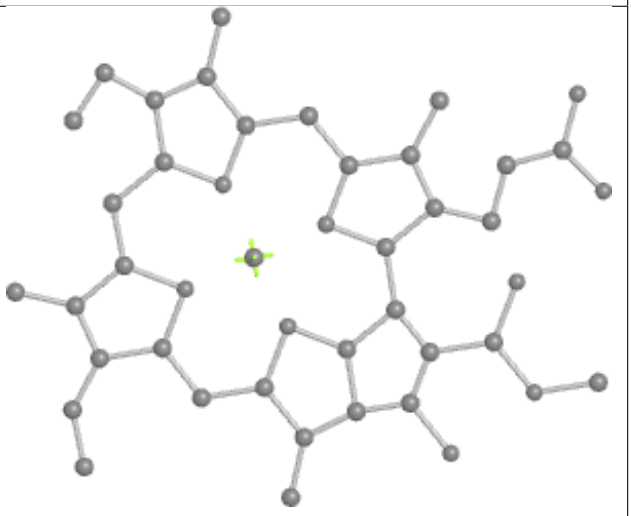
Bond lengths



Bond angles

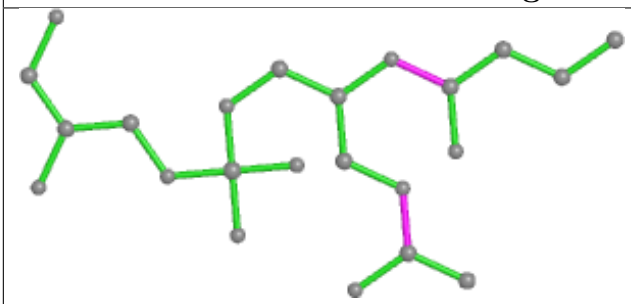


Torsions



Rings

Ligand LHG B 851



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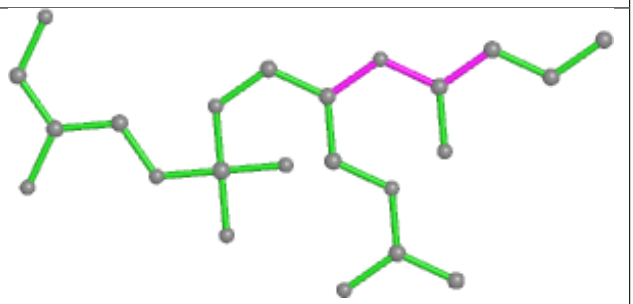
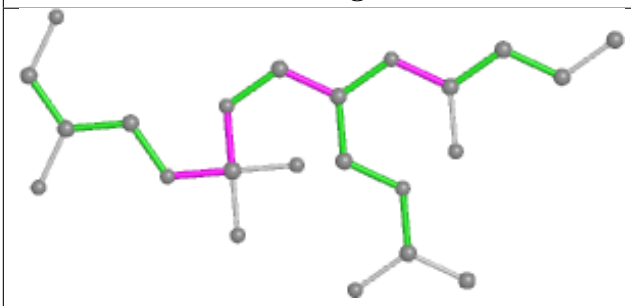
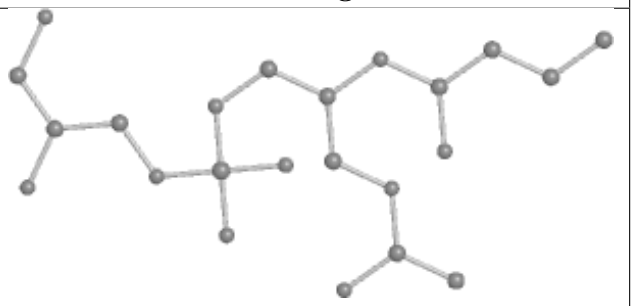


Bond angles

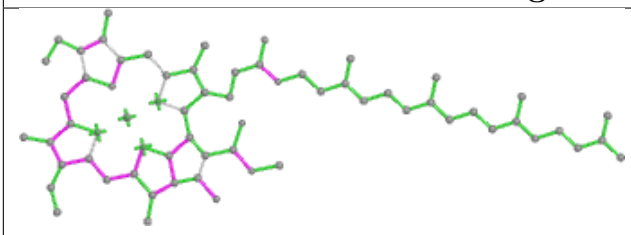


Torsions



Rings

Ligand CLA 6 602



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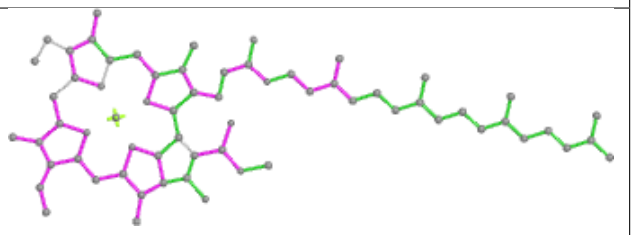
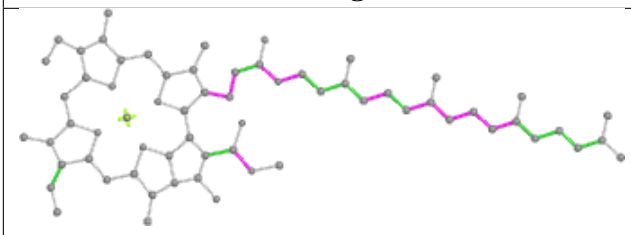


Bond angles



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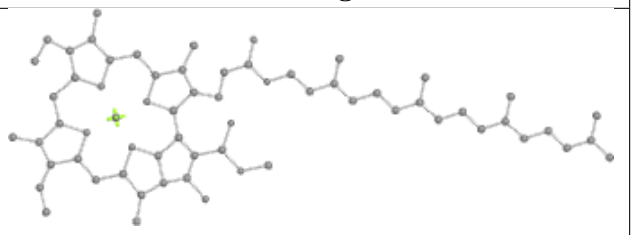
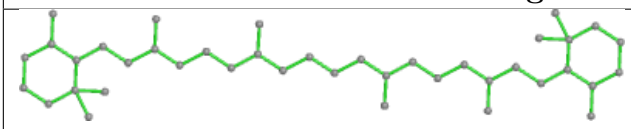
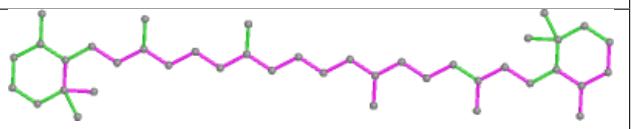


Rings

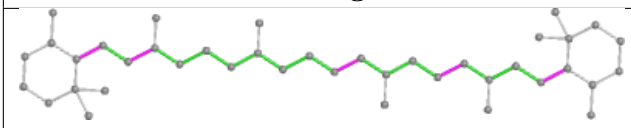
Ligand BCR 3 717



Bond lengths



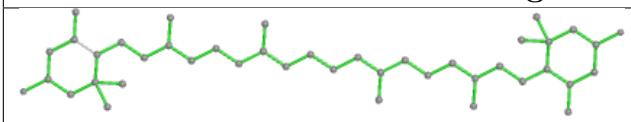
Bond angles



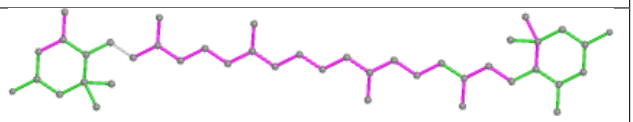
Torsions

Rings

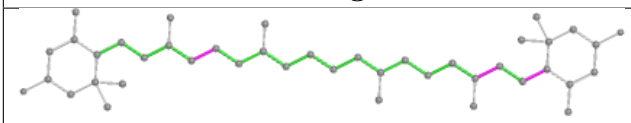
Ligand LUT Z 618



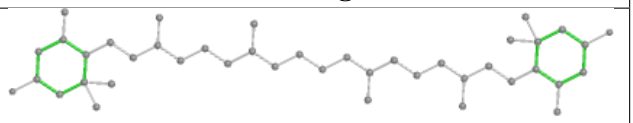
Bond lengths



Bond angles

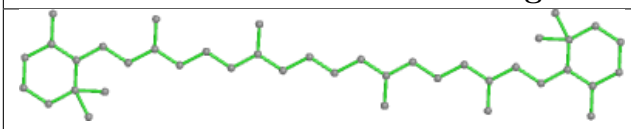


Torsions

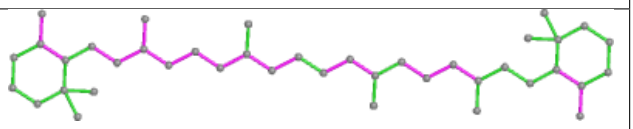


Rings

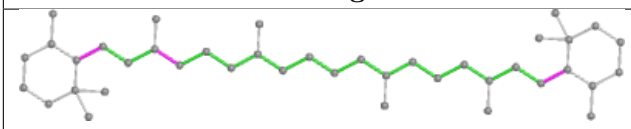
Ligand BCR L 201



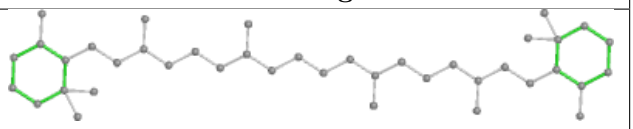
Bond lengths



Bond angles

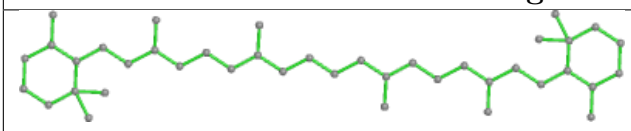


Torsions

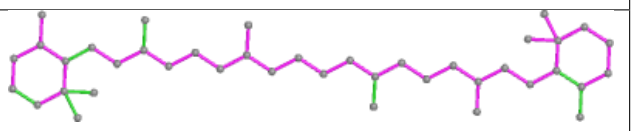


Rings

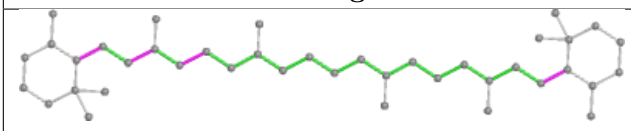
Ligand BCR 5 625



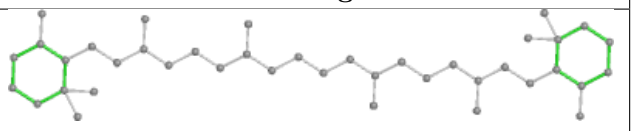
Bond lengths



Bond angles

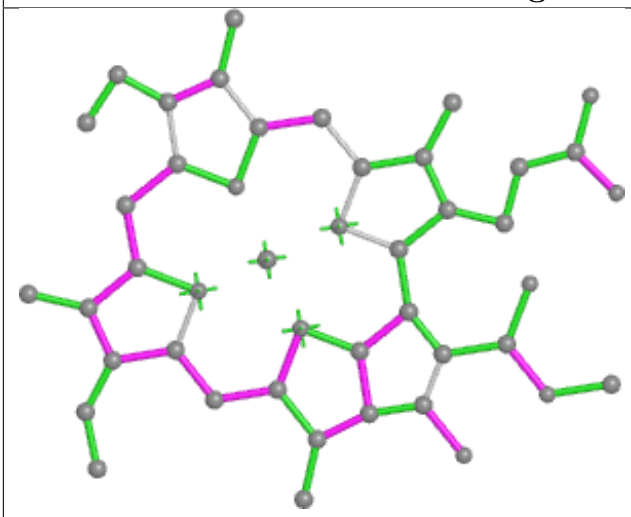


Torsions



Rings

Ligand CLA 3 614



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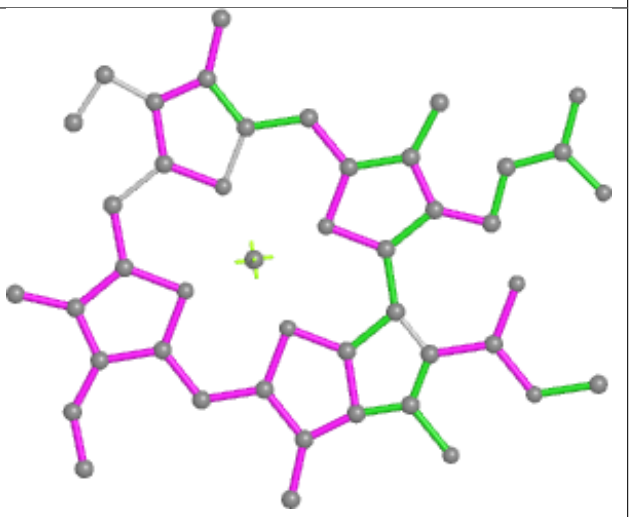

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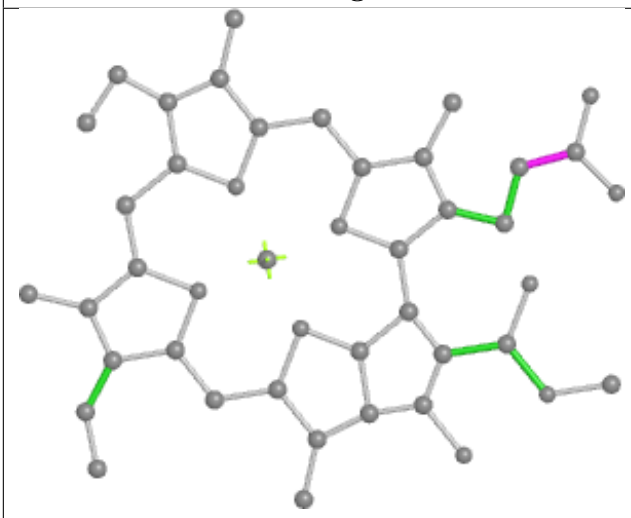

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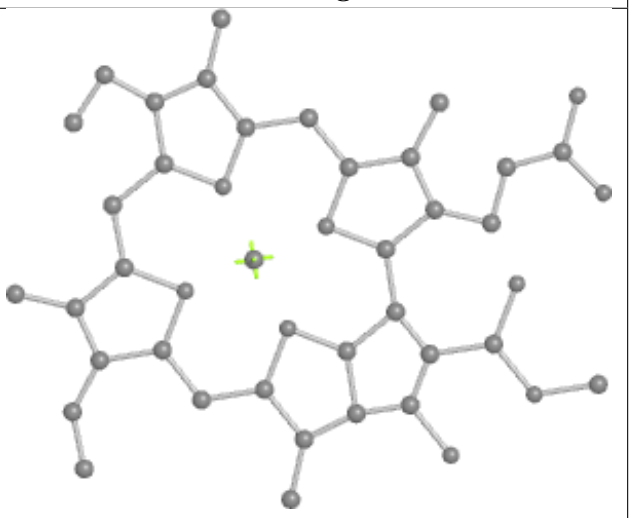
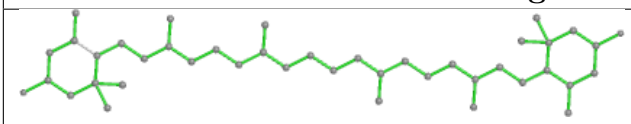


Rings

Ligand LUT 4 619



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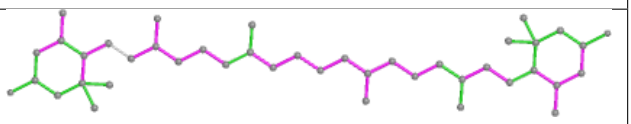
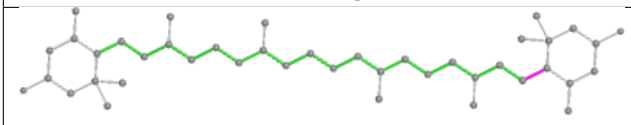


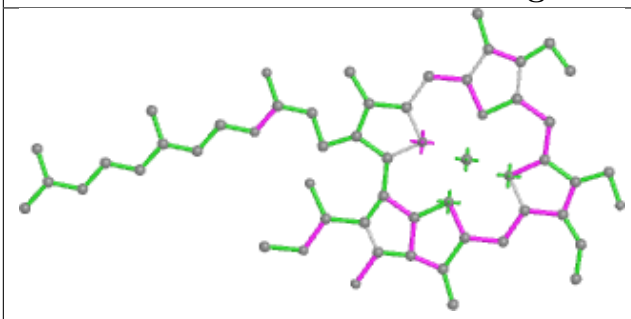
Bond angles



Torsions

Rings

Ligand CHL 8 607



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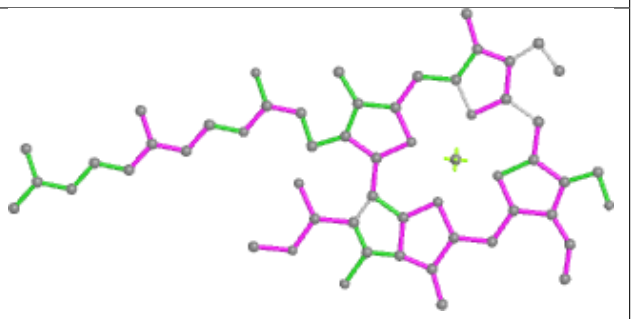
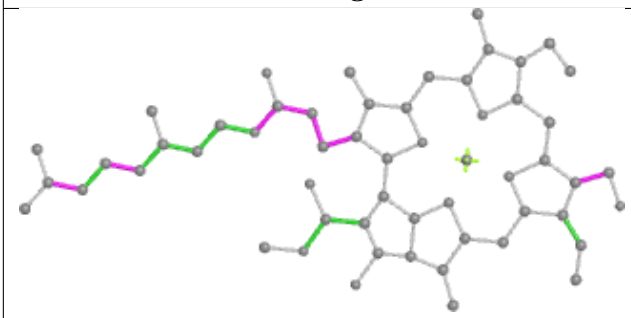
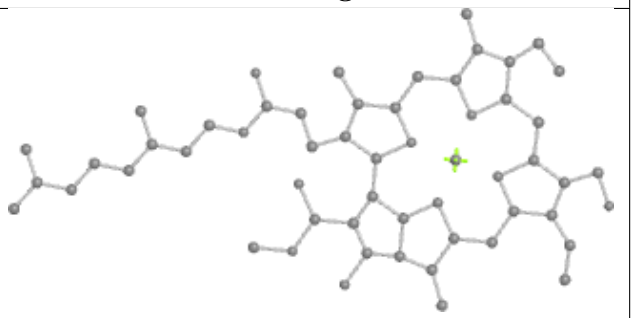


Bond angles

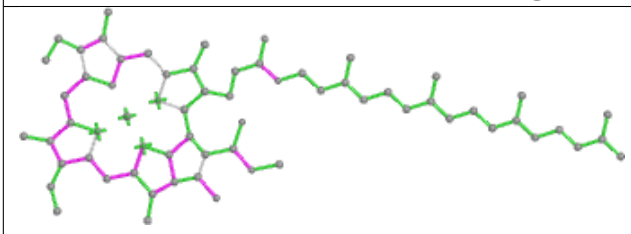


Torsions



Rings

Ligand CLA 5 601



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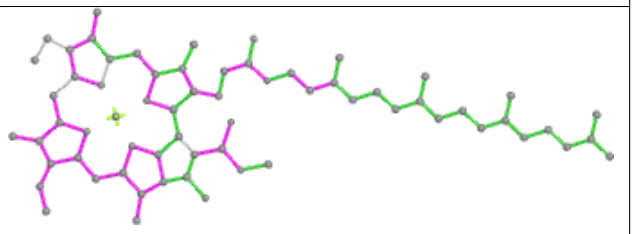
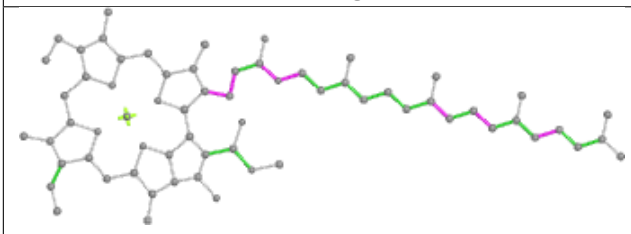


Bond angles



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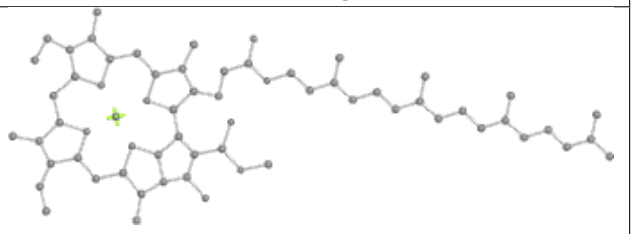
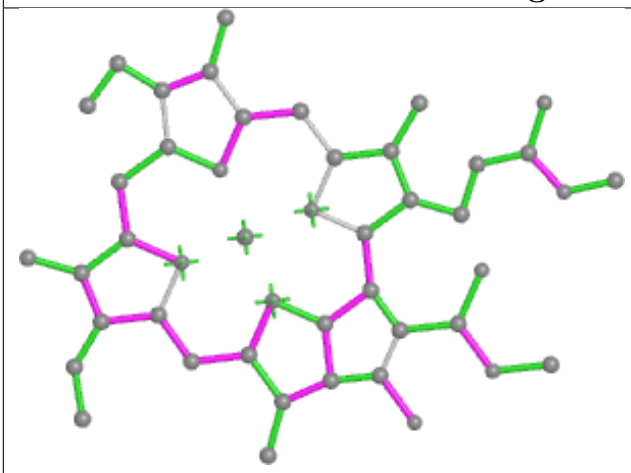


Rings

Ligand CLA 5 617



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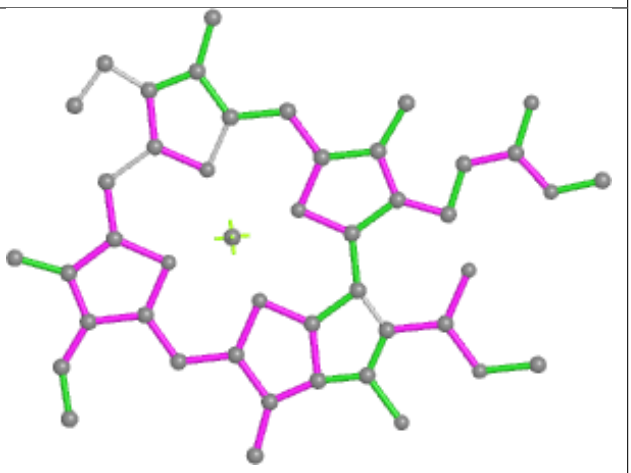
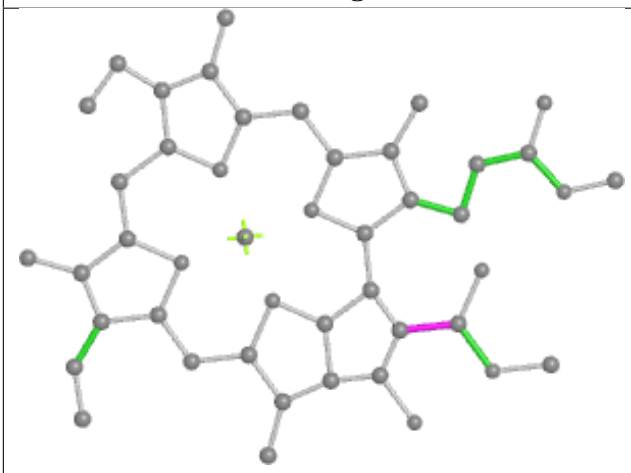


Bond angles



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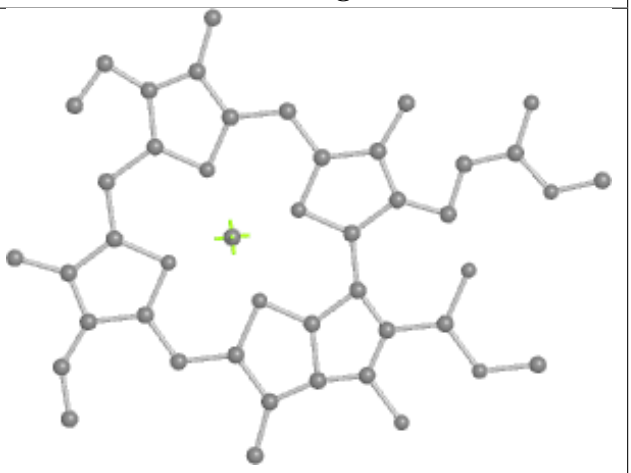
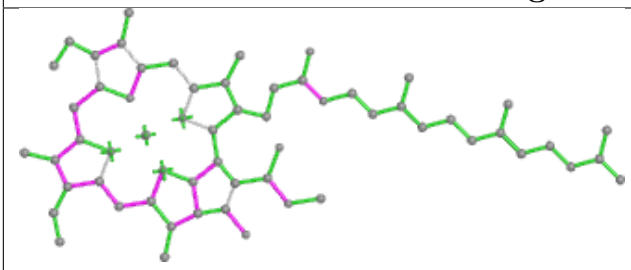


Rings

Ligand CLA 3 607



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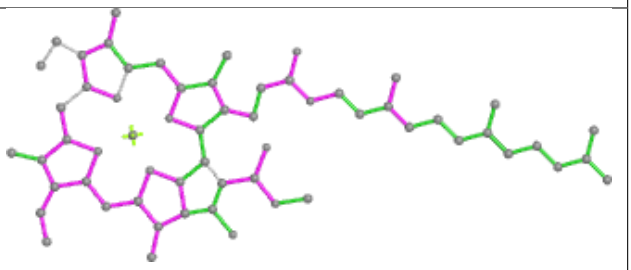
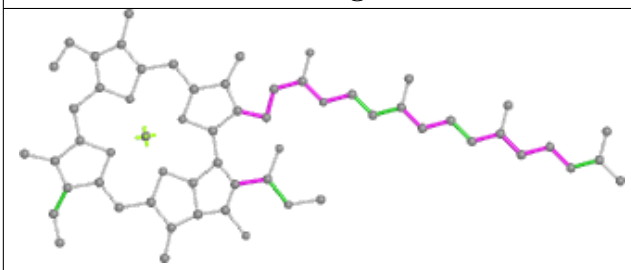


Bond angles



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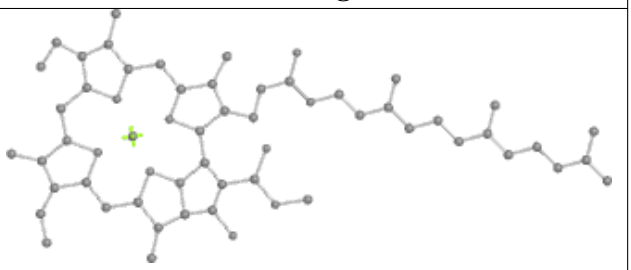
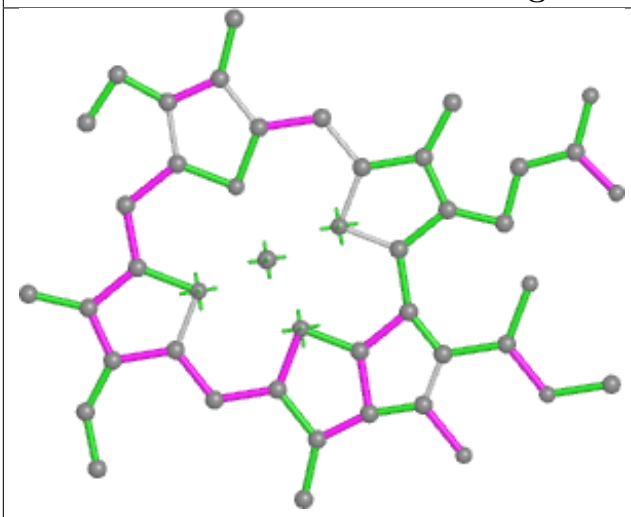


Rings

Ligand CLA 5 614



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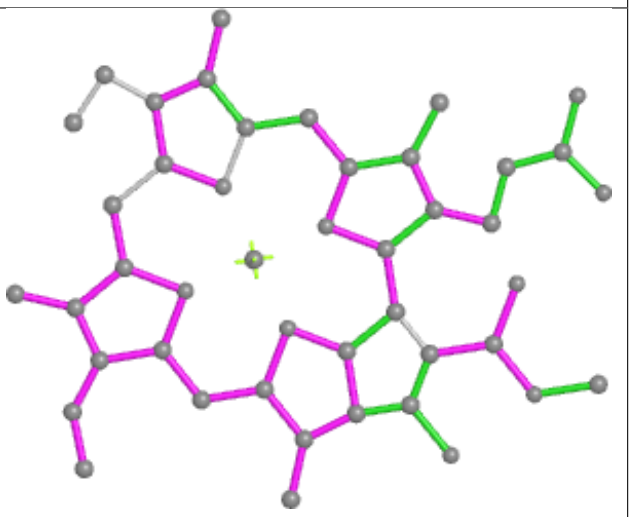

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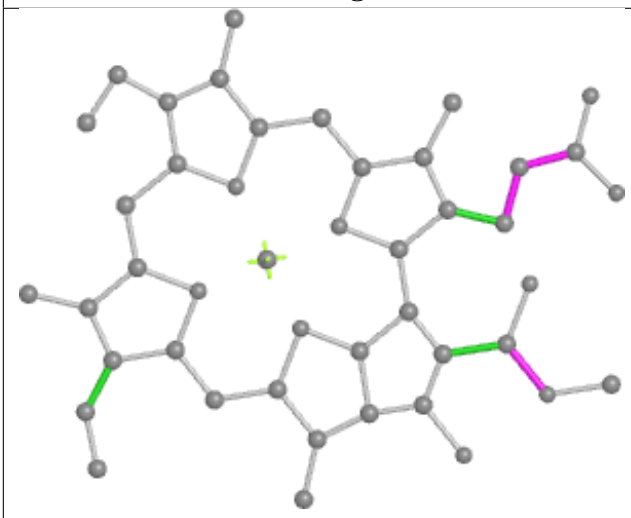

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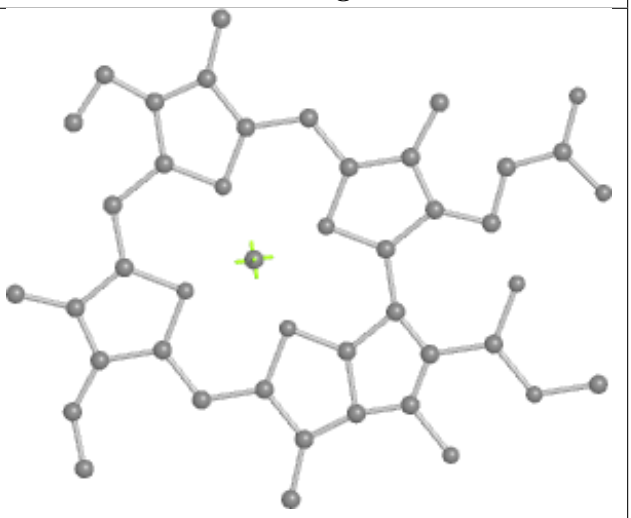
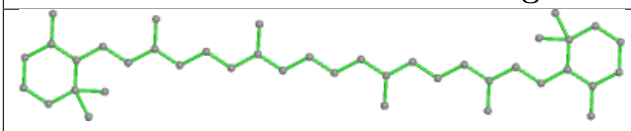


Rings

Ligand BCR A 856



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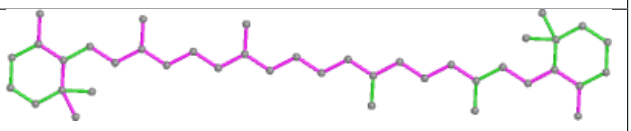
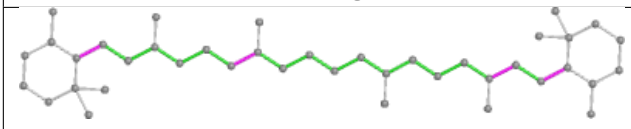


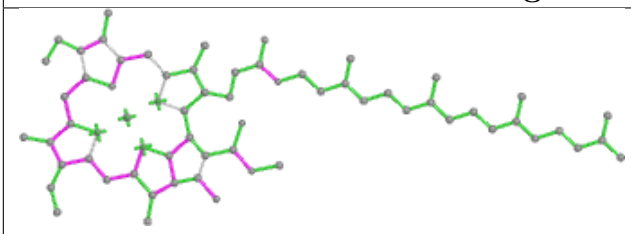
Bond angles



Torsions

Rings

Ligand CLA A 842



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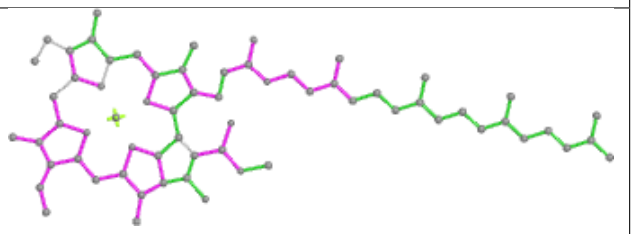
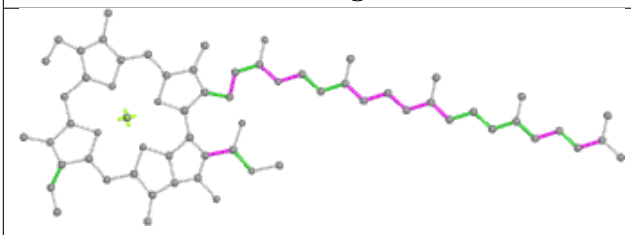


Bond angles



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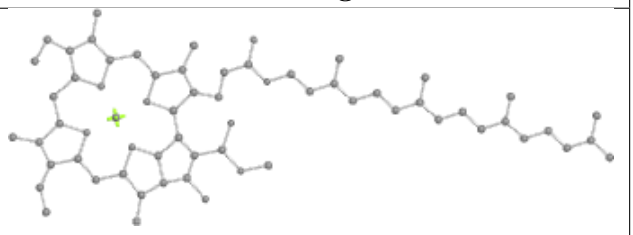
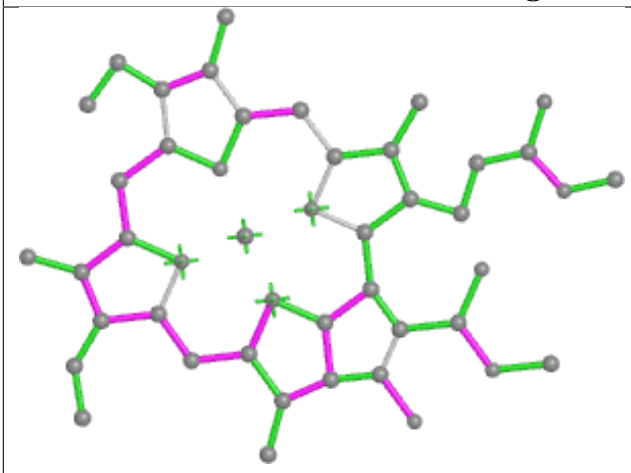


Rings

Ligand CLA B 821



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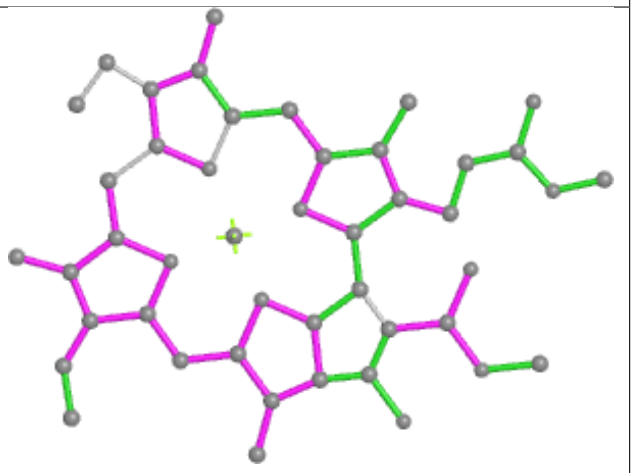
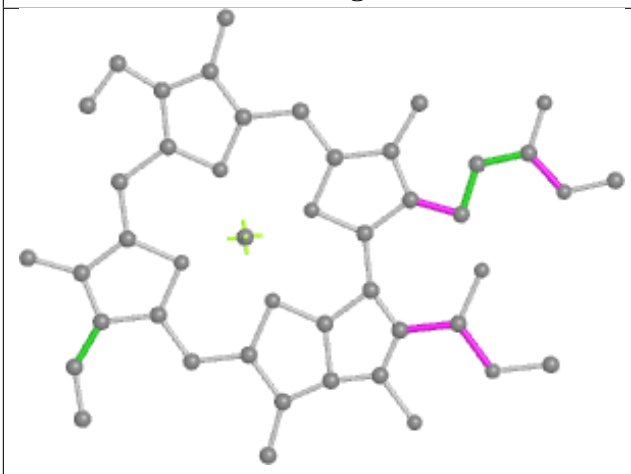


Bond angles



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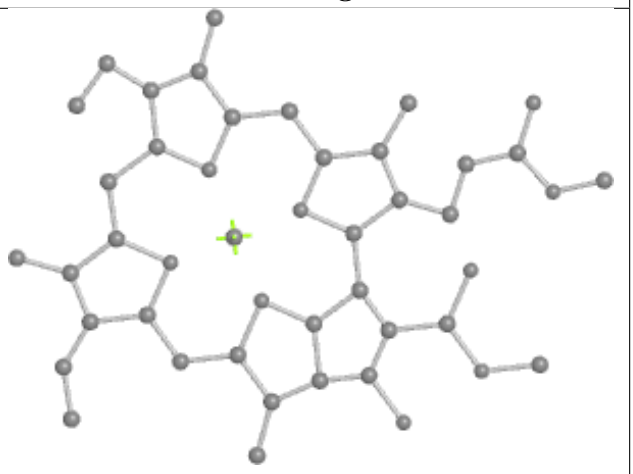
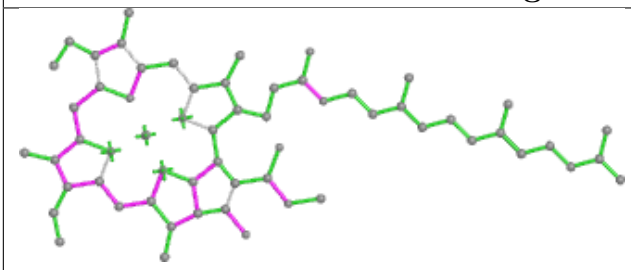


Rings

Ligand CLA A 815



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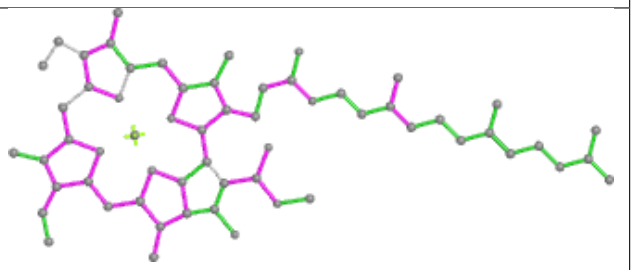
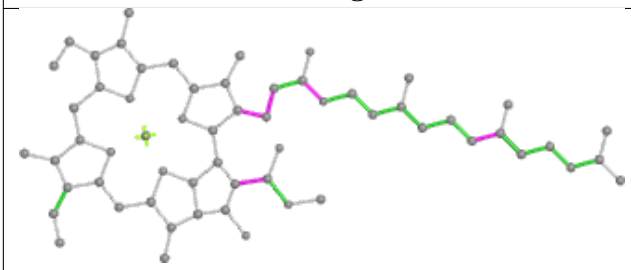


Bond angles



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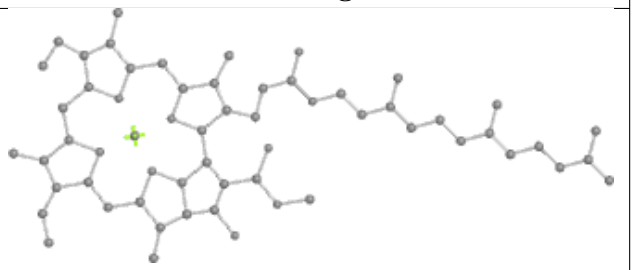
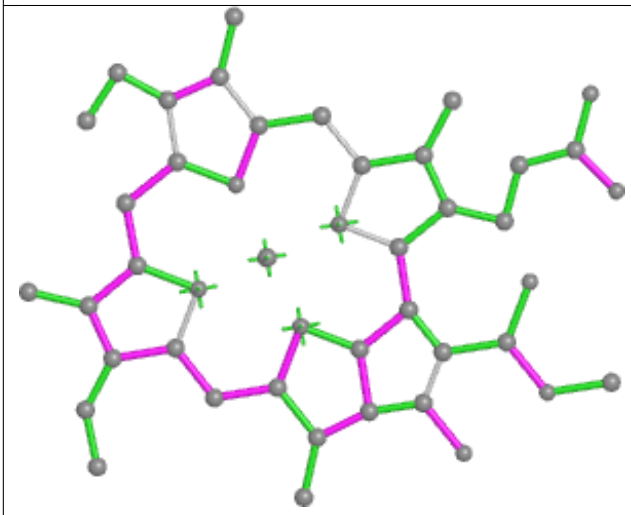


Rings

Ligand CLA B 835



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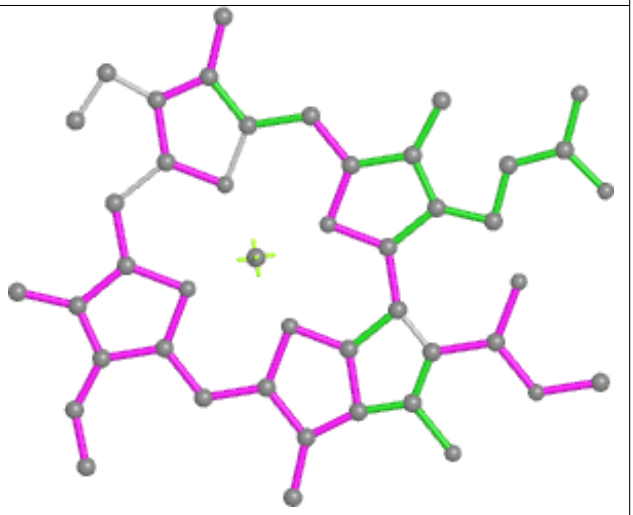
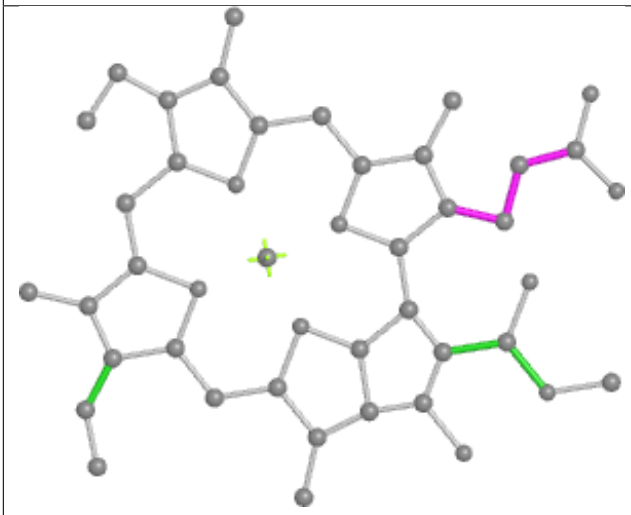


Bond angles



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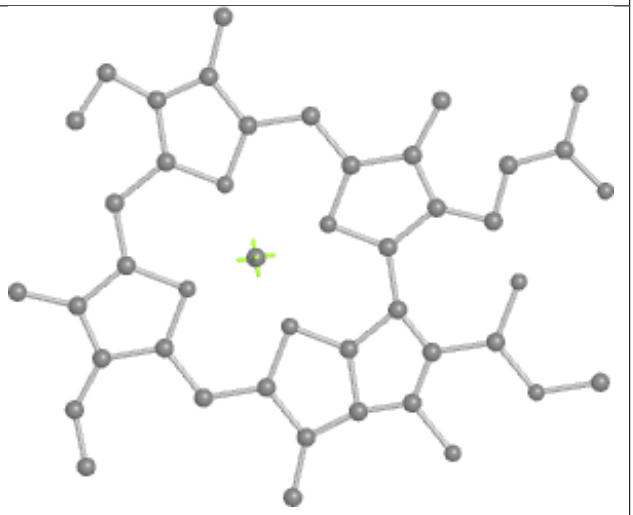
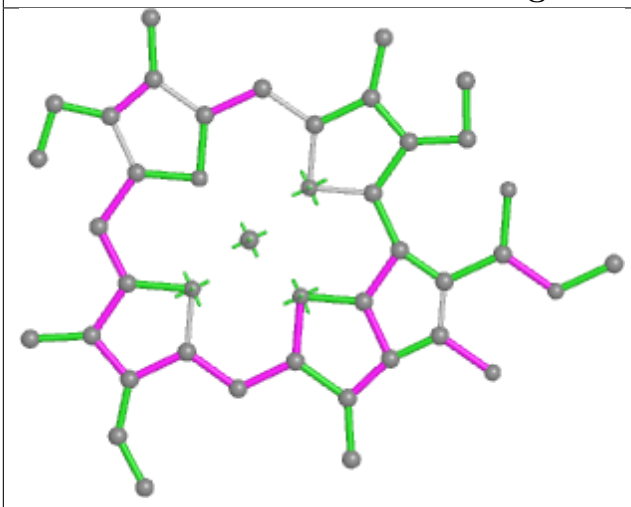
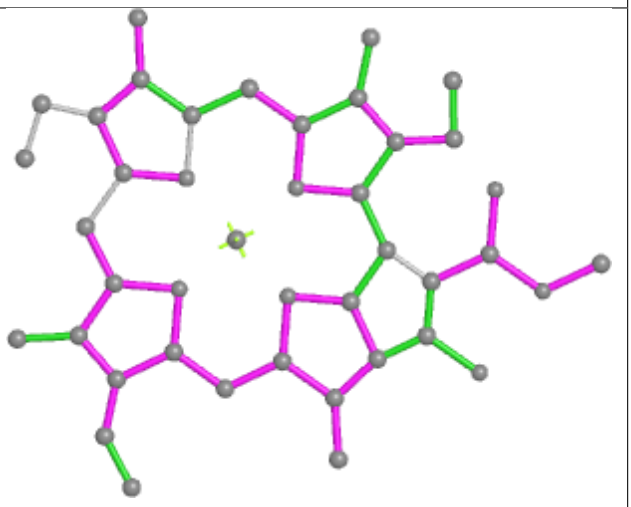


Rings

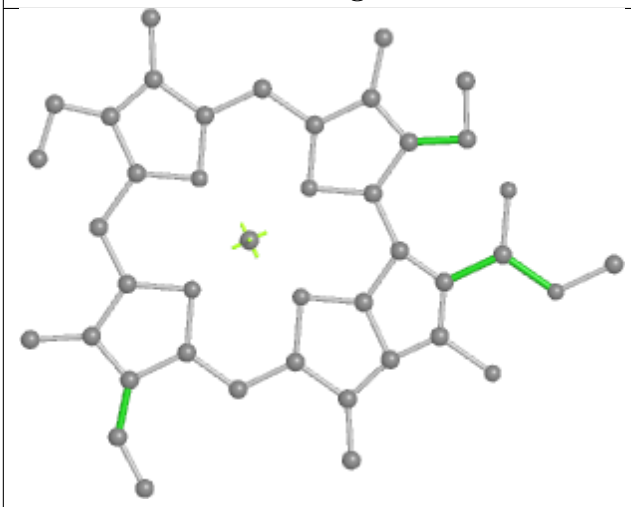
Ligand CLA 3 606



Bond lengths



Bond angles



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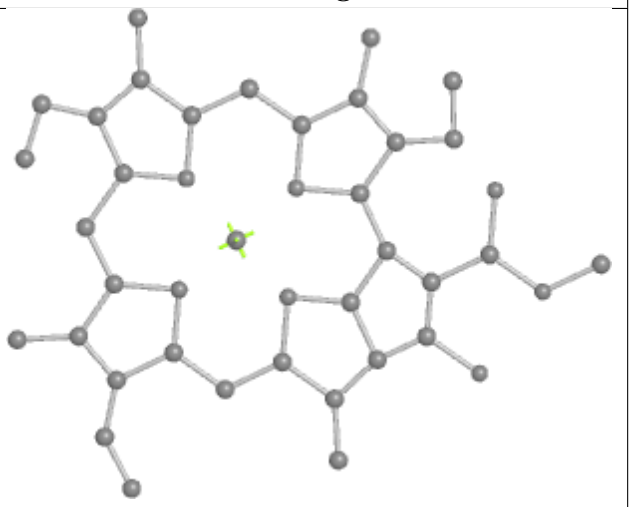
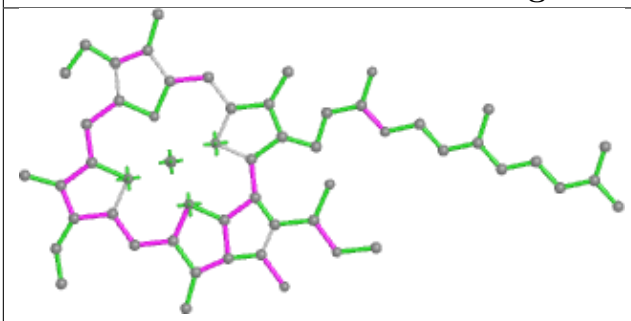


Rings

Ligand CLA 4 611



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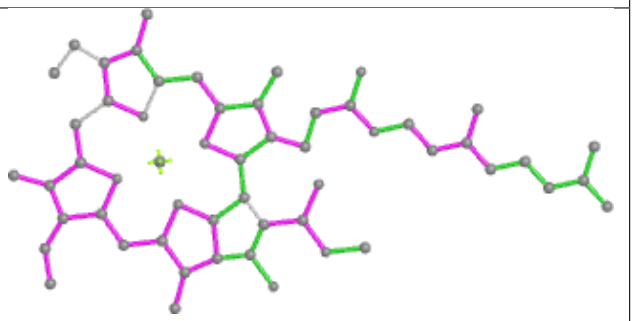
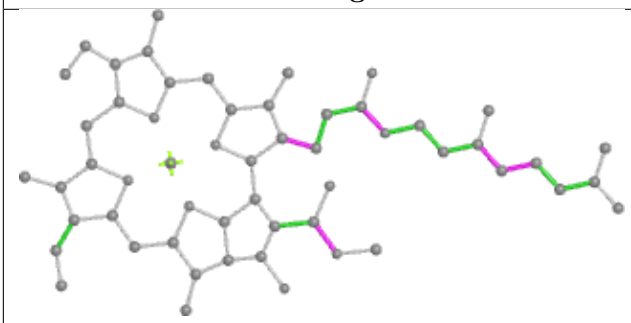


Bond angles



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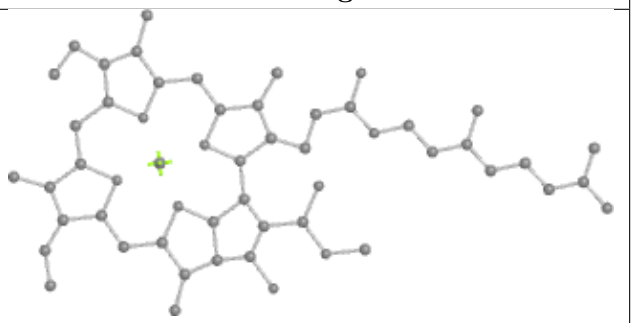
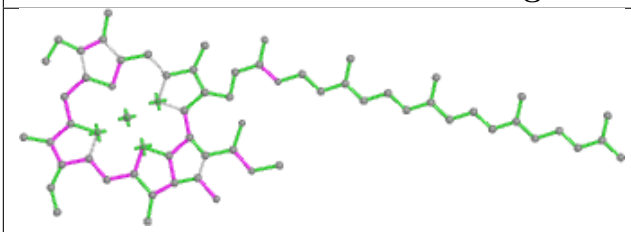
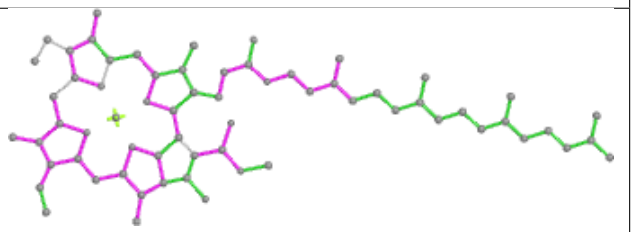


Rings

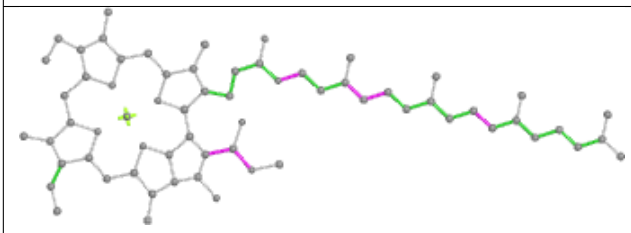
Ligand CLA A 840



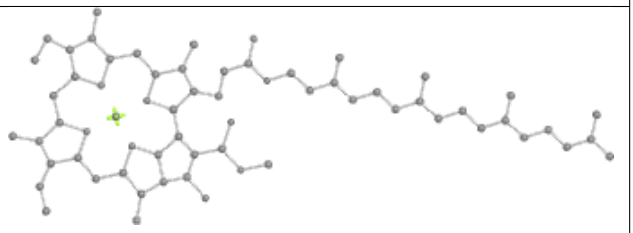
Bond lengths



Bond angles

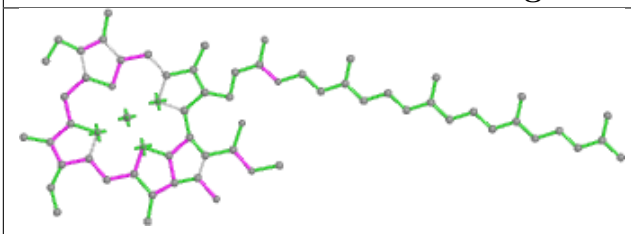


Torsions

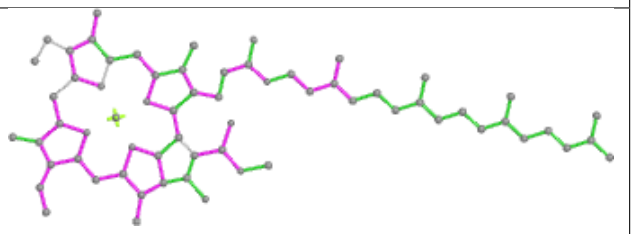


Rings

Ligand CLA B 810



Bond lengths



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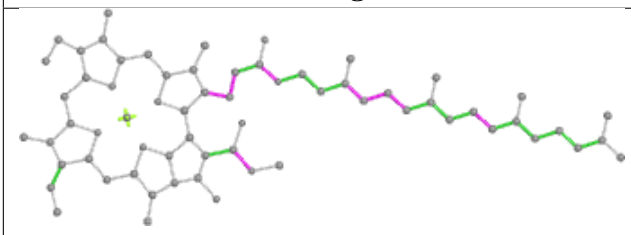

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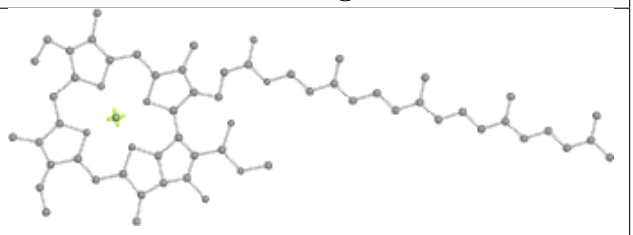
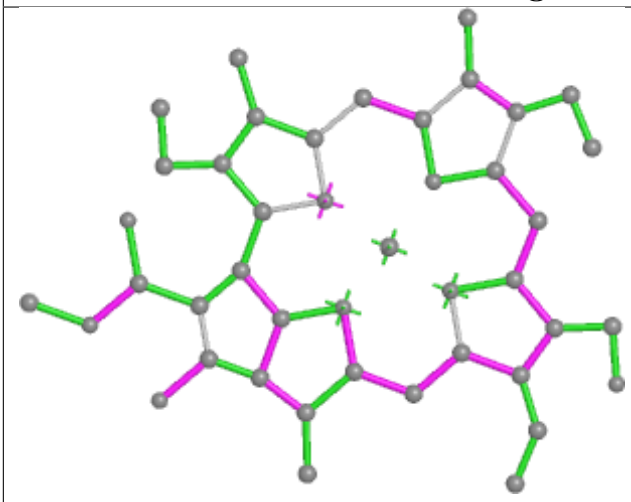


Rings

Ligand CHL 6 618



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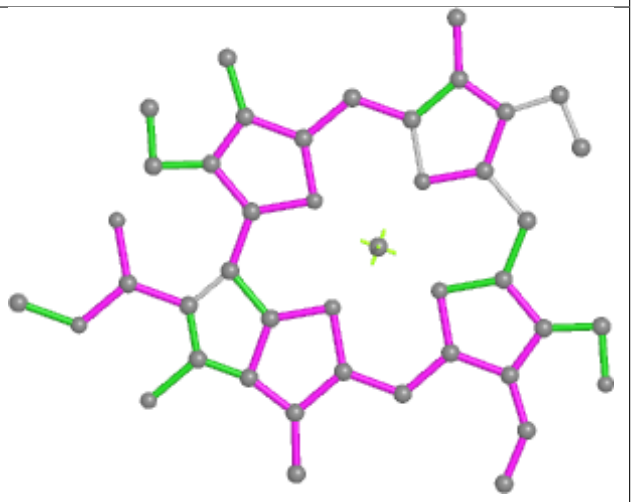
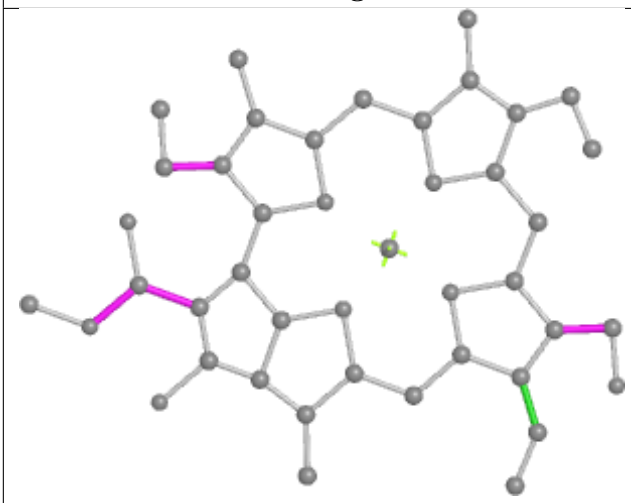


Bond angles



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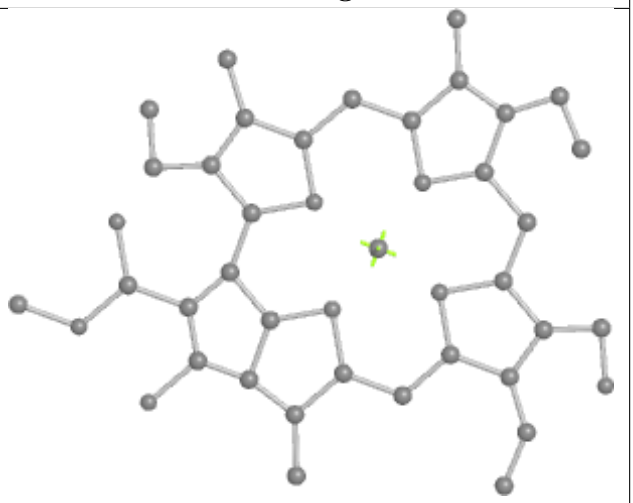
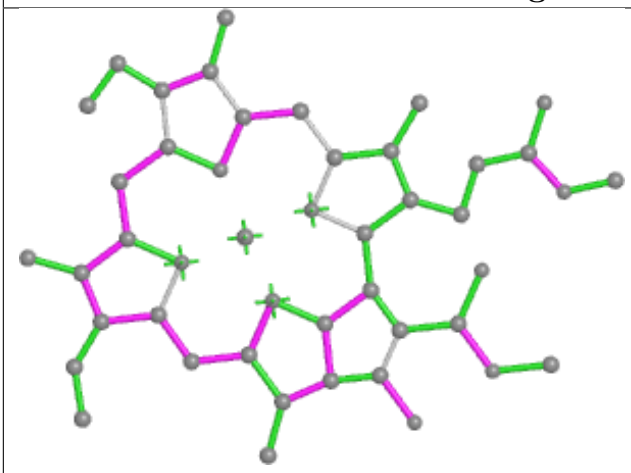


Rings

Ligand CLA 3 617



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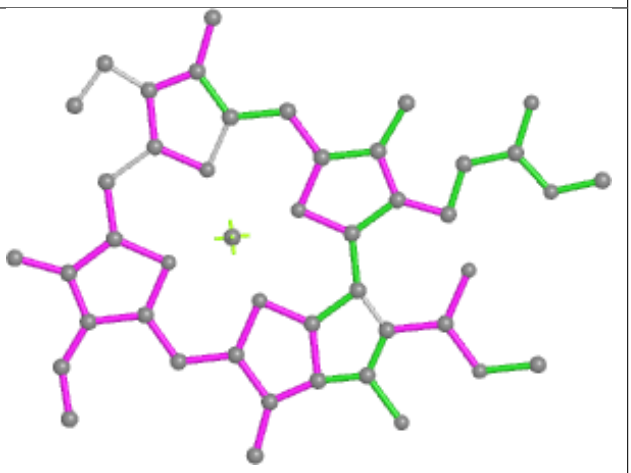
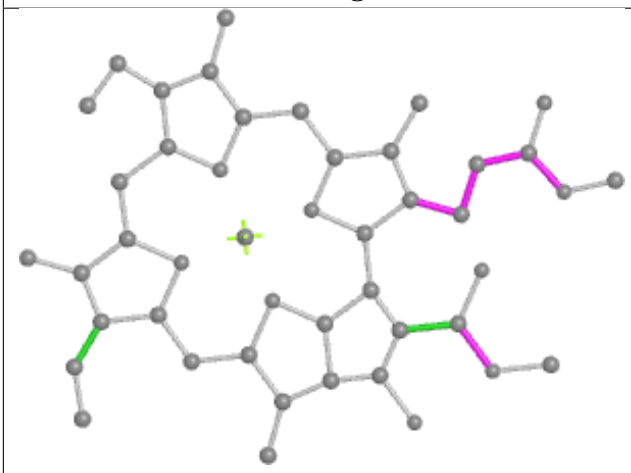


Bond angles



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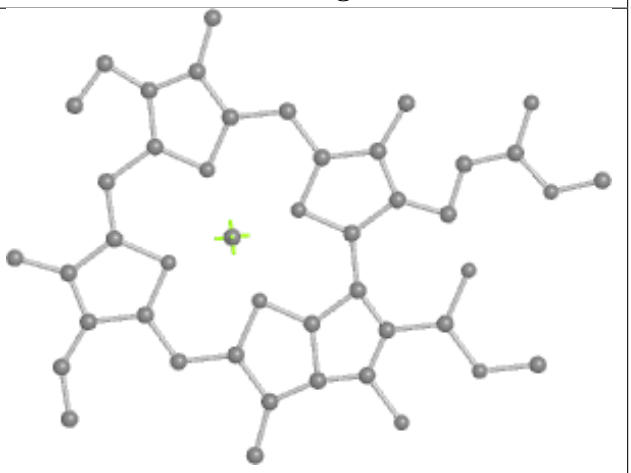
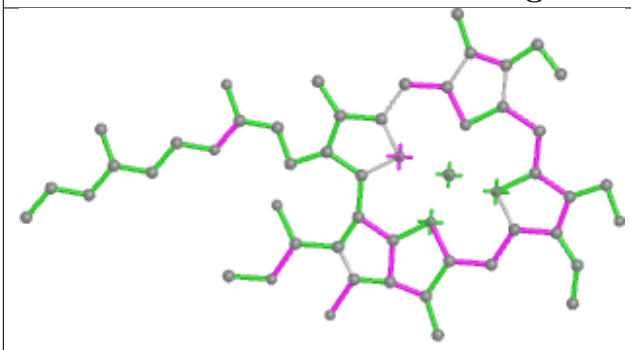


Rings

Ligand CHL Z 601



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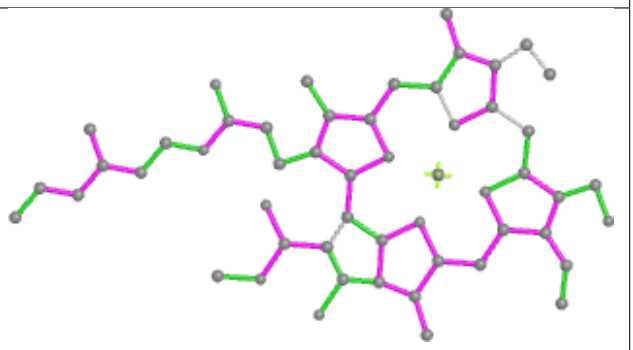
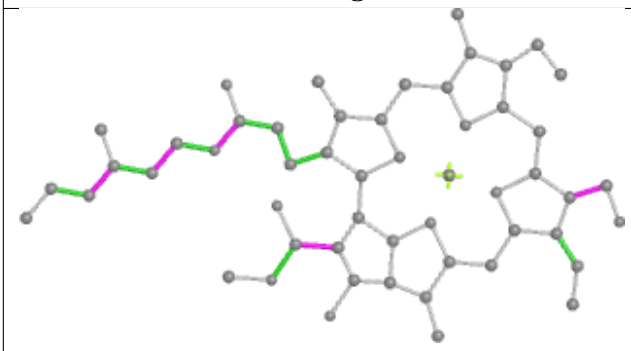


Bond angles



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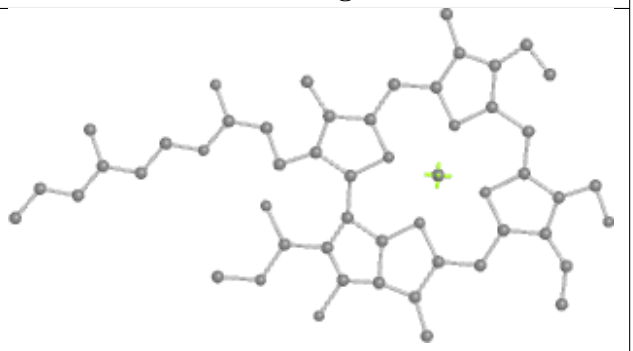

Rings

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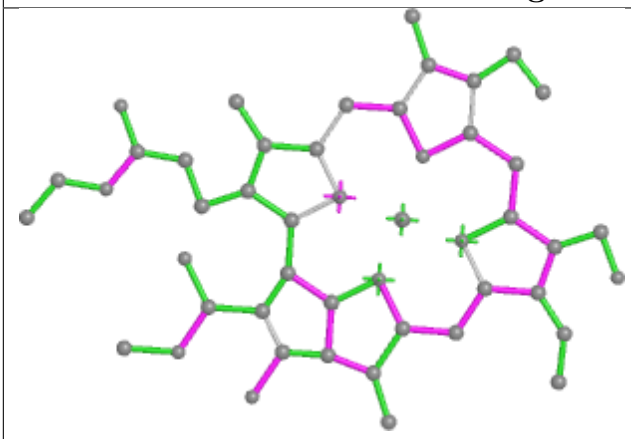

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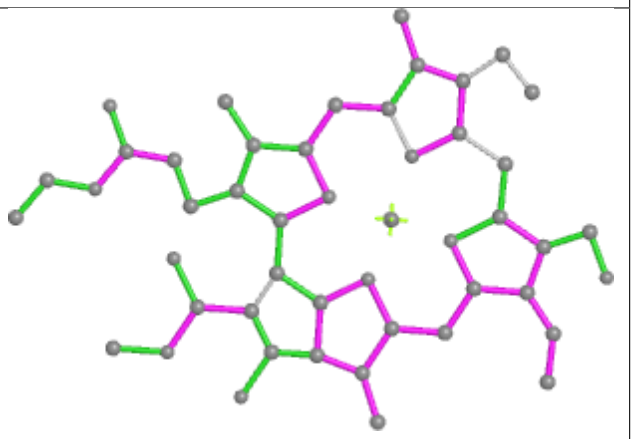

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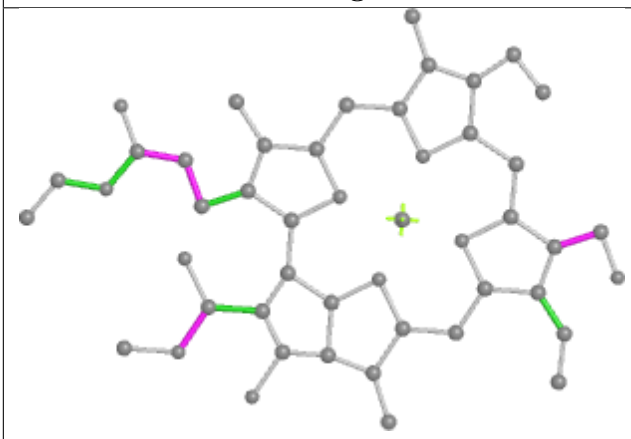

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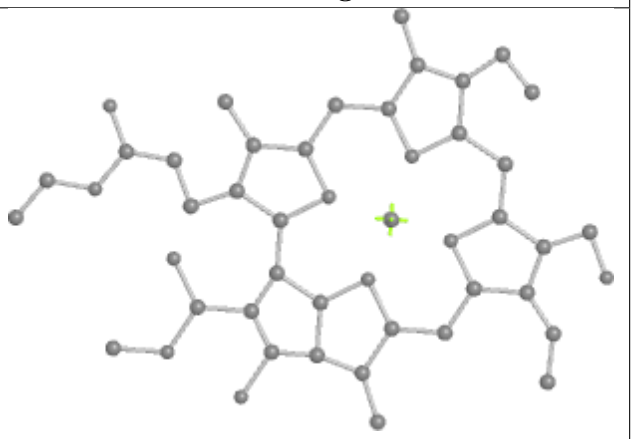
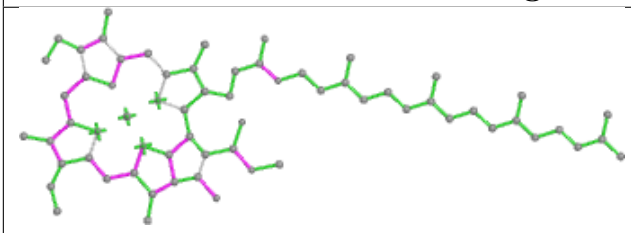


Rings

Ligand CLA A 826



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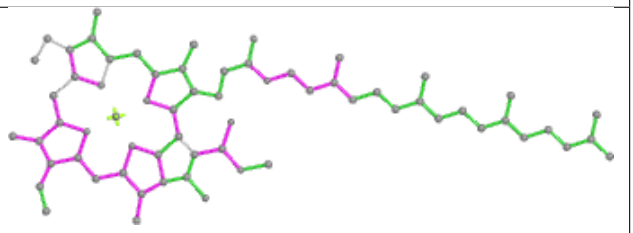
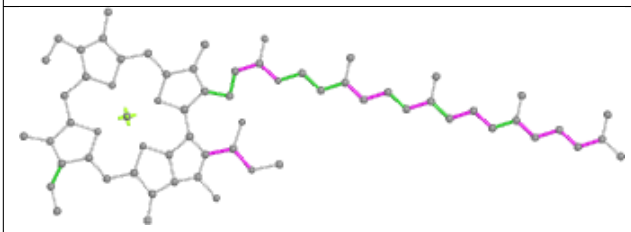


Bond angles



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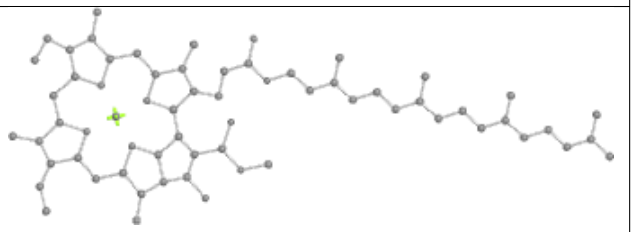
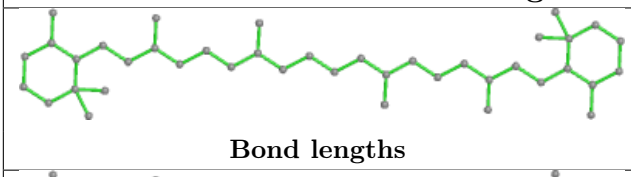


Rings

Ligand BCR 7 623



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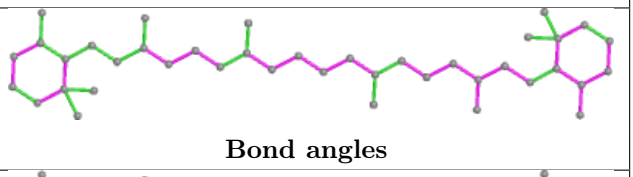
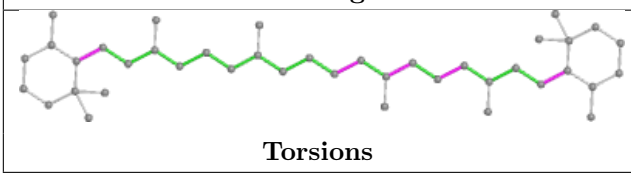


Bond angles



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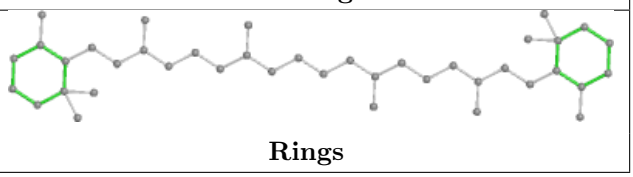
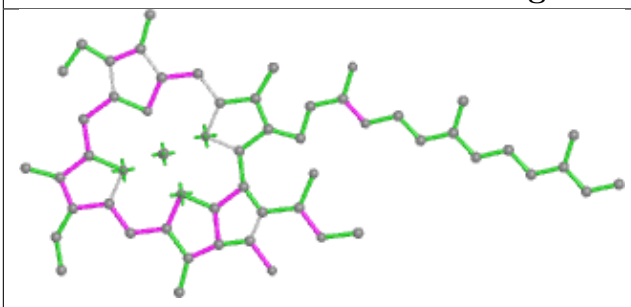


Rings

Ligand CLA 7 604



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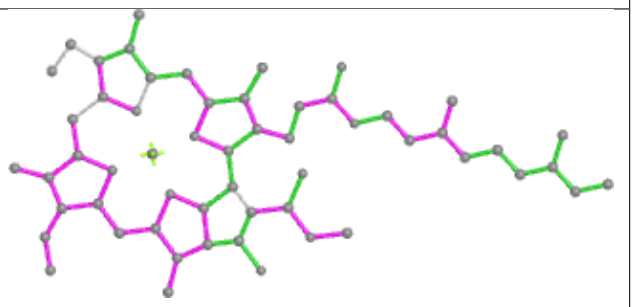
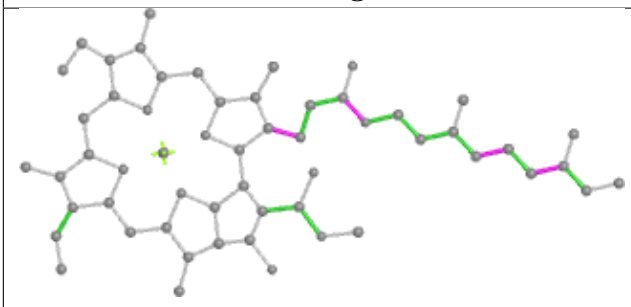


Bond angles



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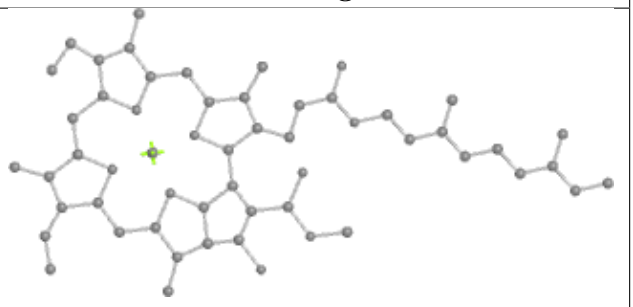
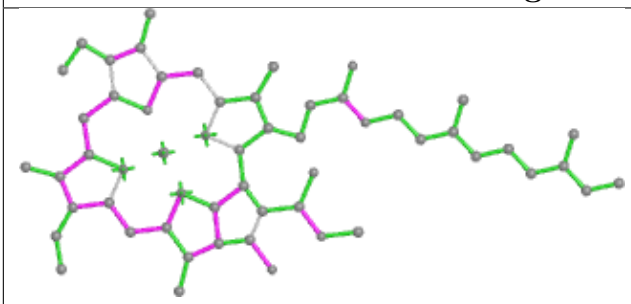


Rings

Ligand CLA B 820



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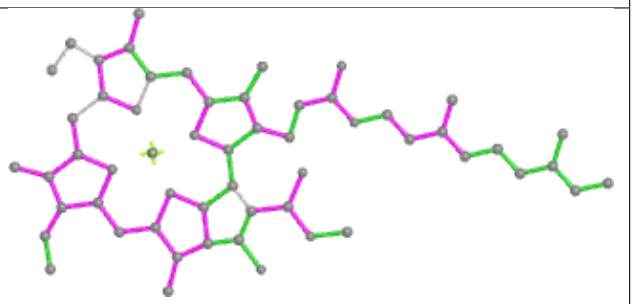
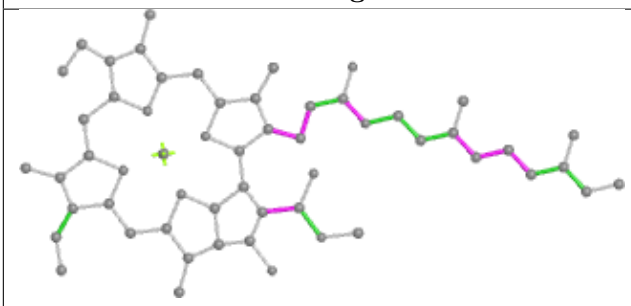


Bond angles



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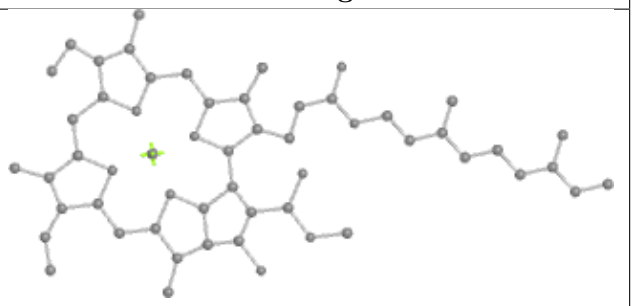
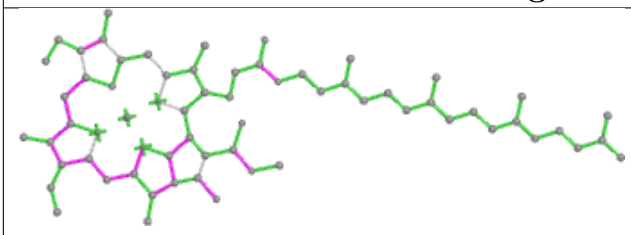


Rings

Ligand CLA 8 613



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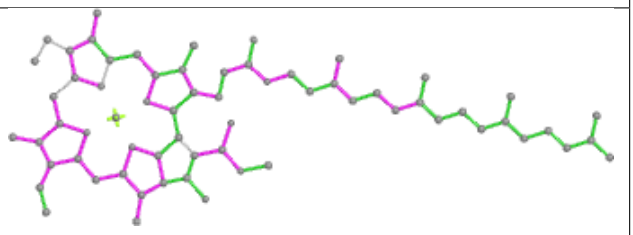

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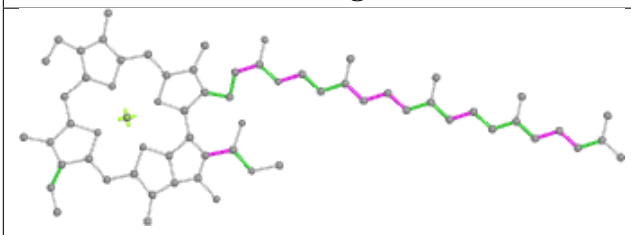

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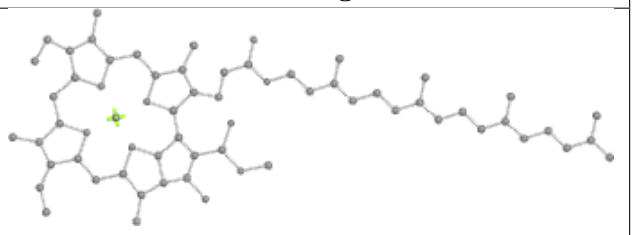
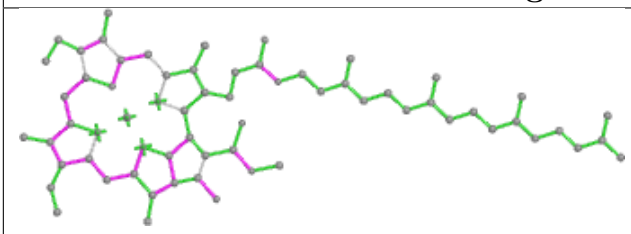


Rings

Ligand CLA F 301



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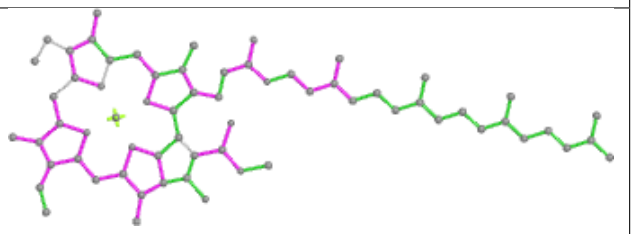
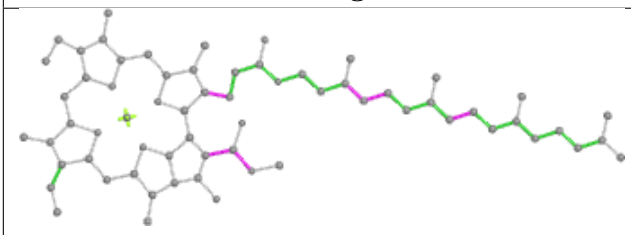


Bond angles



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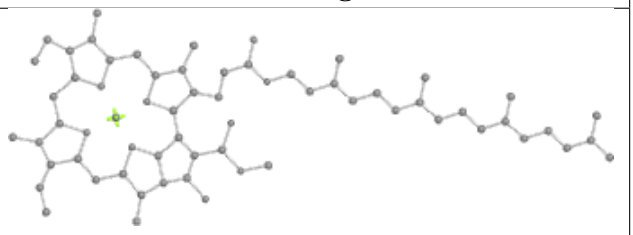
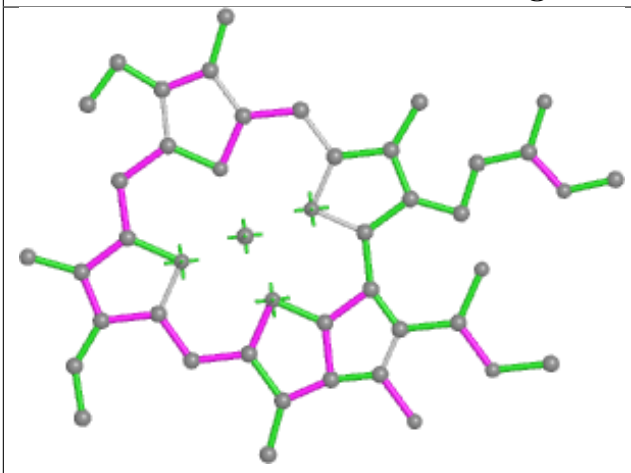


Rings

Ligand CLA 1 616



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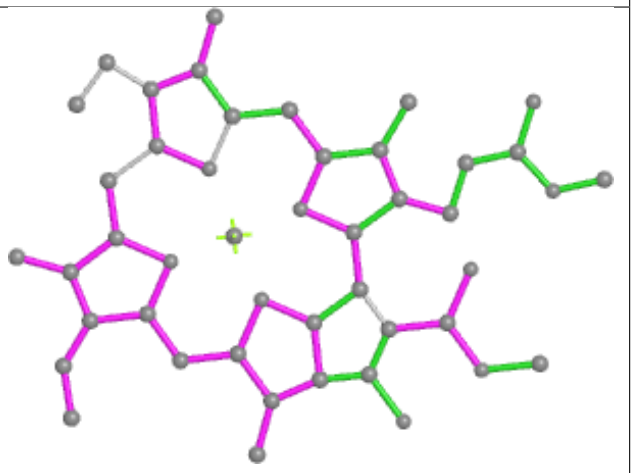
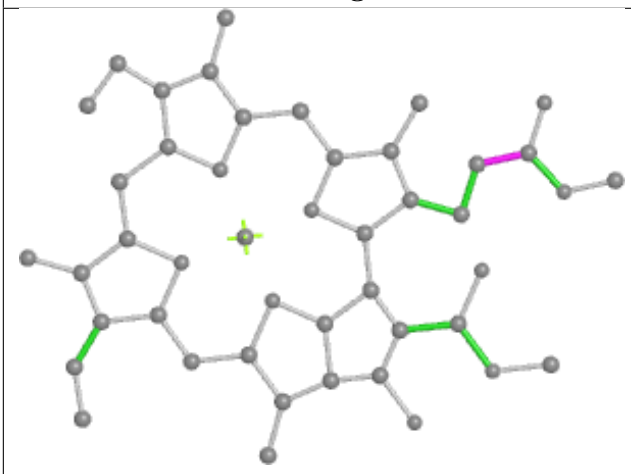


Bond angles



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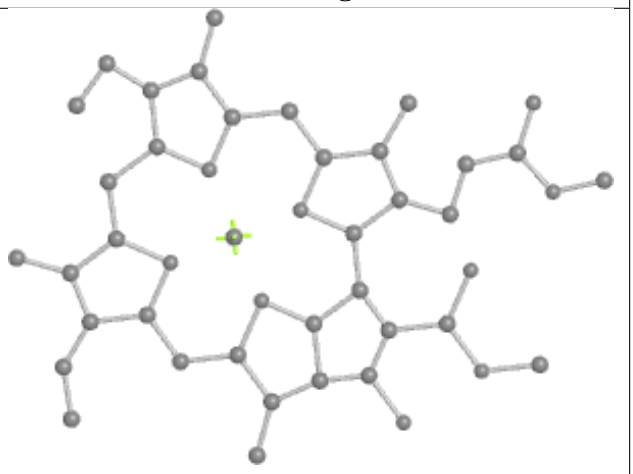
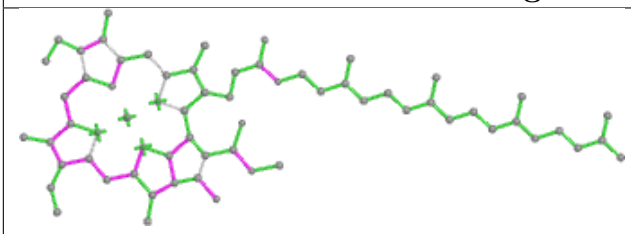
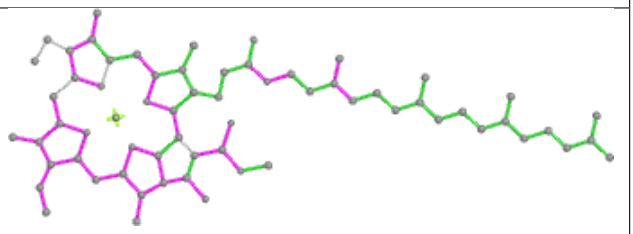


Rings

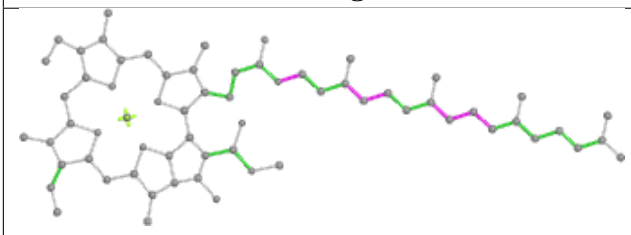
Ligand CLA A 833



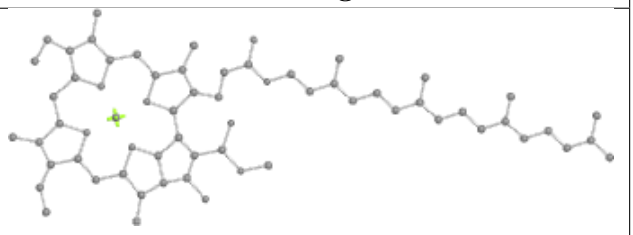
Bond lengths



Bond angles

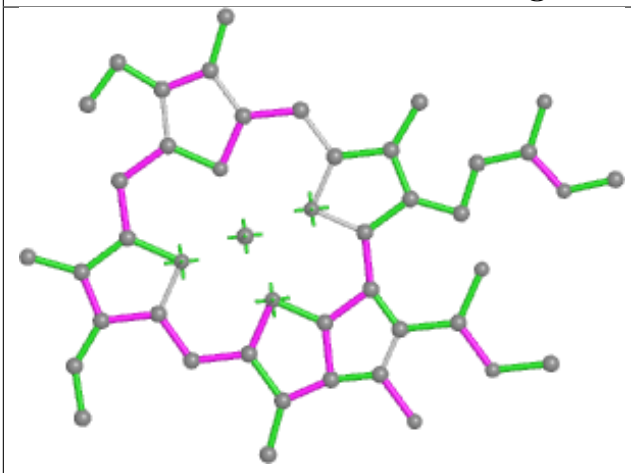


Torsions

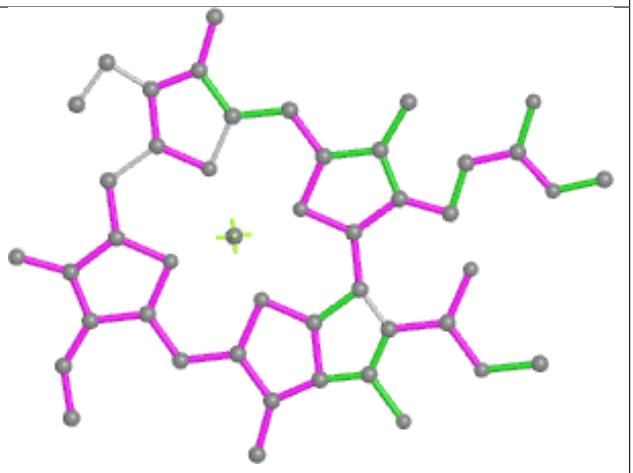


Rings

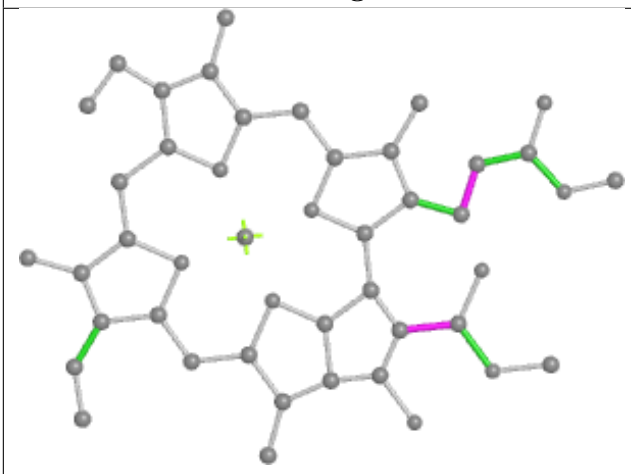
Ligand CLA 5 621



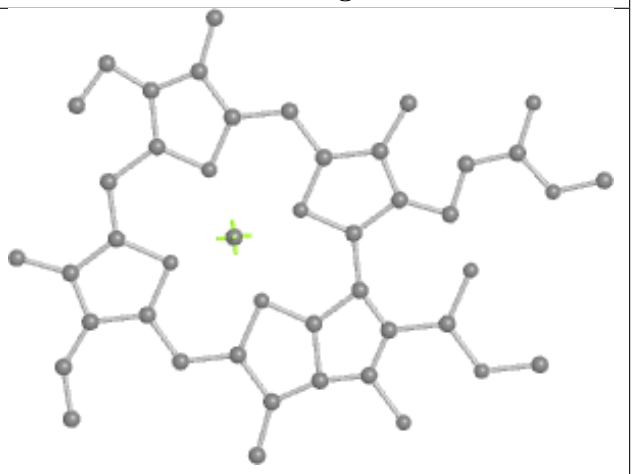
Bond lengths



Bond angles

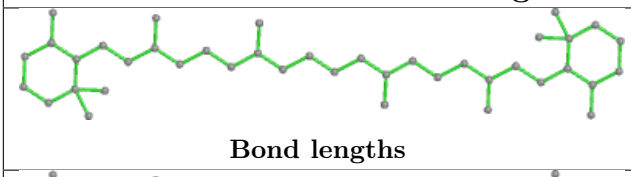


Torsions

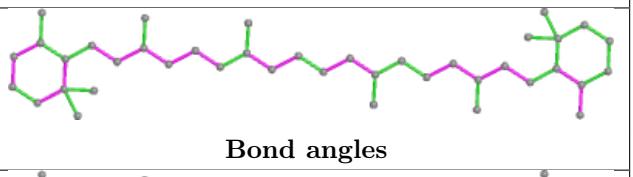


Rings

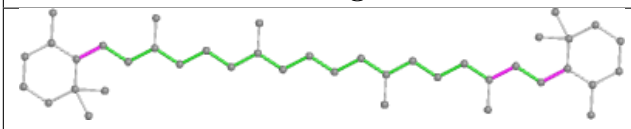
Ligand BCR K 4004



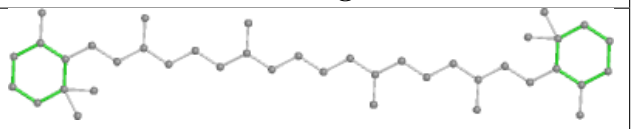
Bond lengths



Bond angles

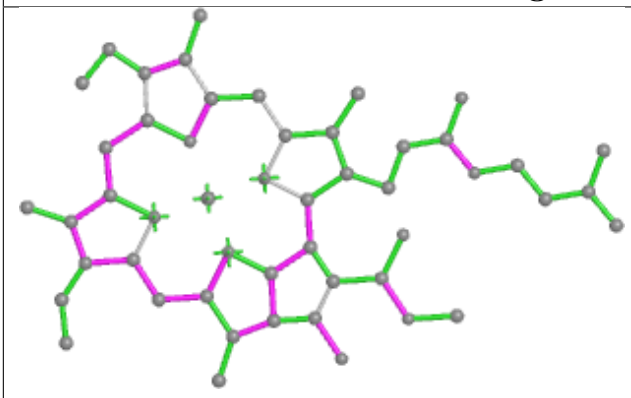


Torsions



Rings

Ligand CLA 5 609



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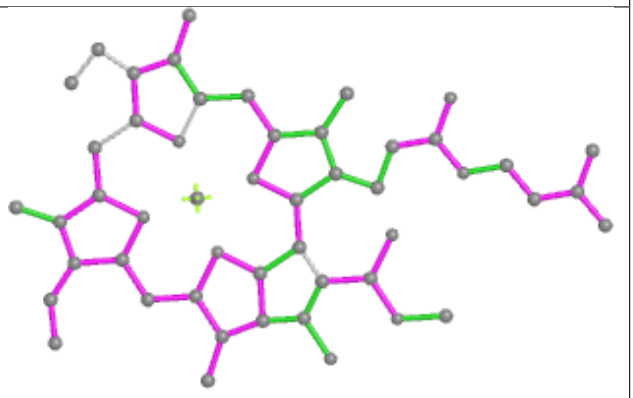

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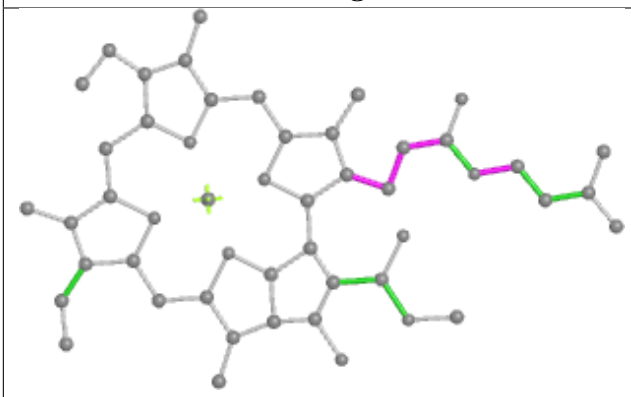

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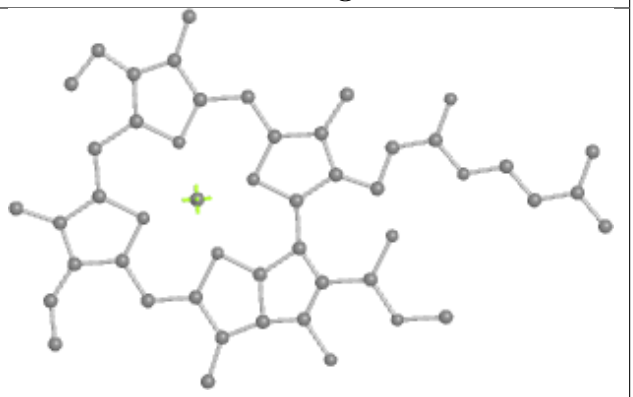
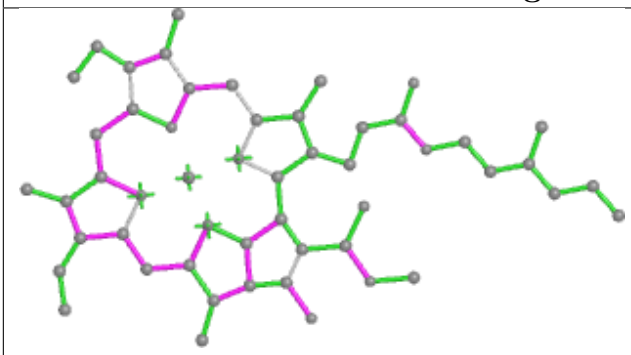


Rings

Ligand CLA A 845



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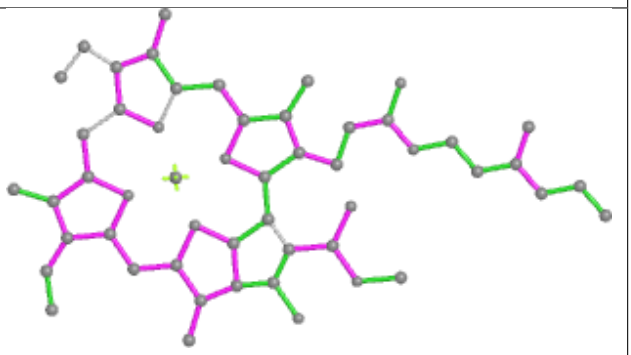
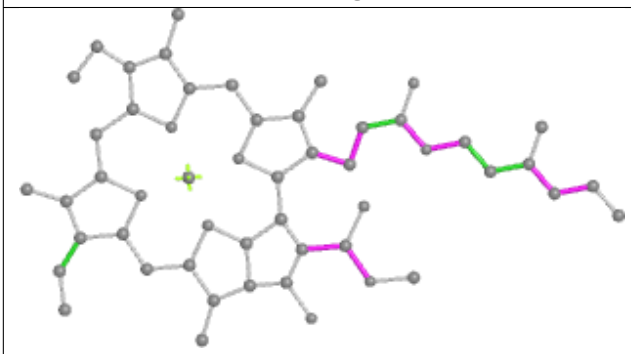


Bond angles



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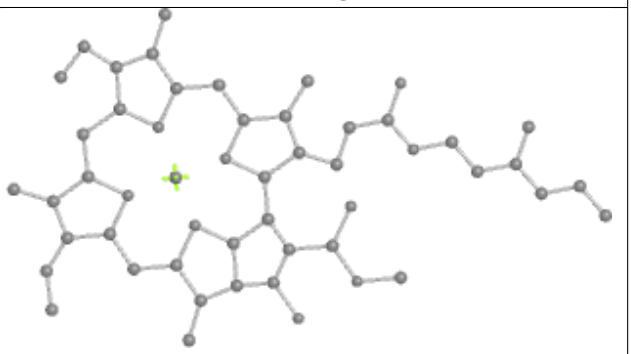
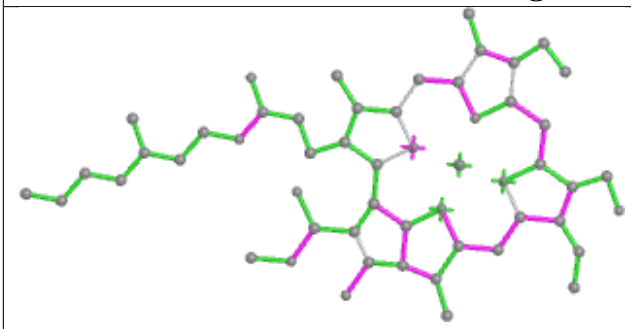


Rings

Ligand CHL 7 607



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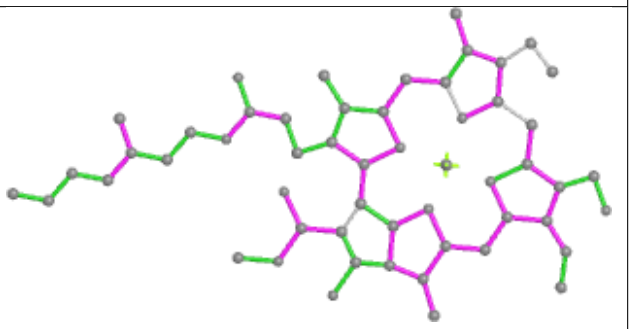
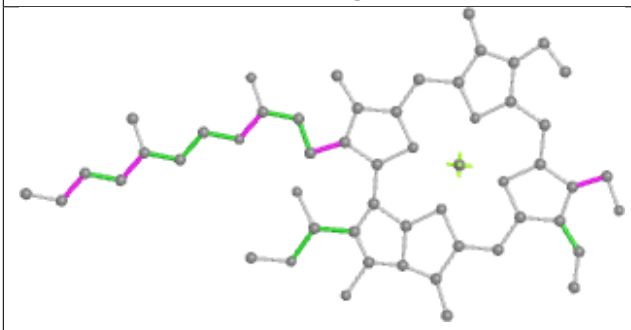


Bond angles



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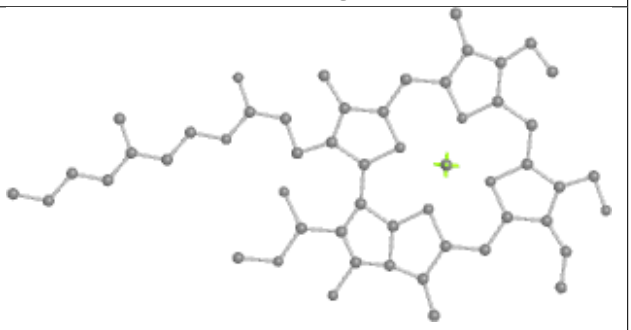
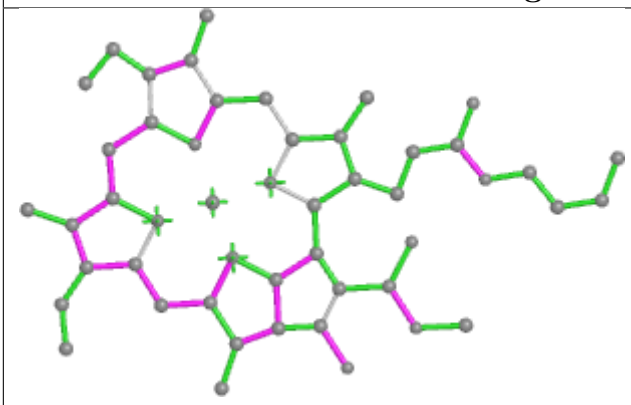


Rings

Ligand CLA B 831



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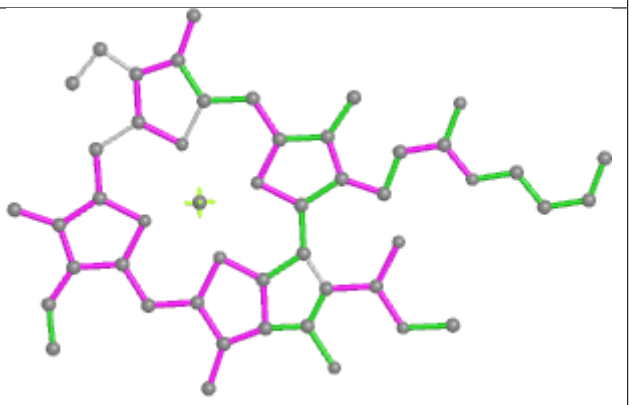
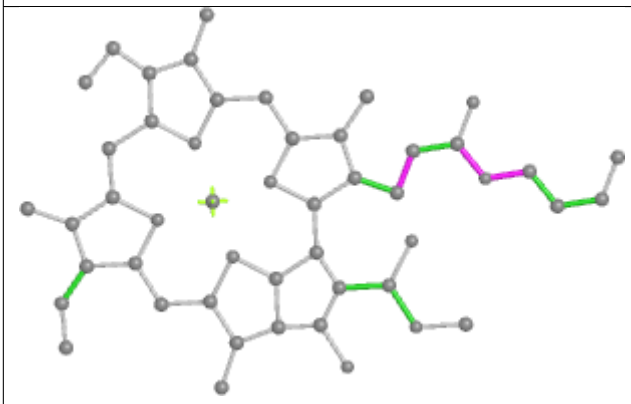


Bond angles



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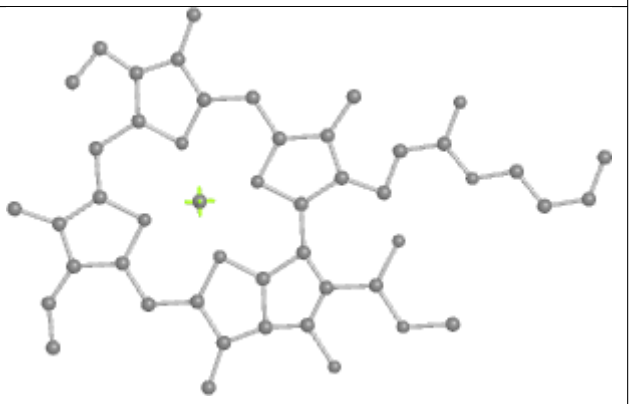
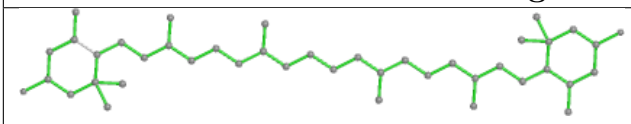


Rings

Ligand LUT 7 621



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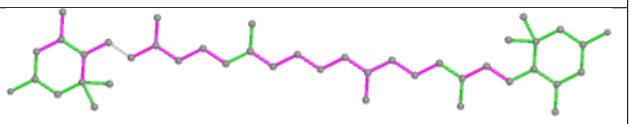
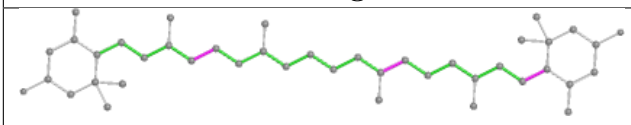


Bond angles



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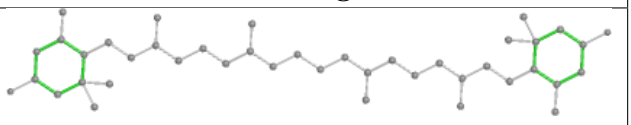
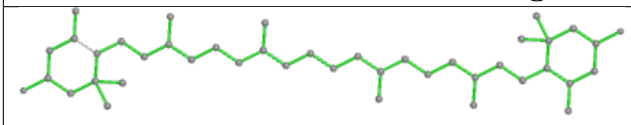


Rings

Ligand LUT 5 620



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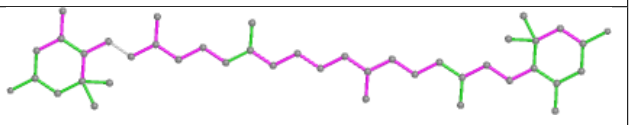
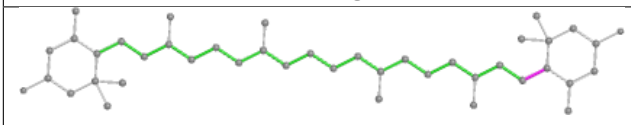


Bond angles



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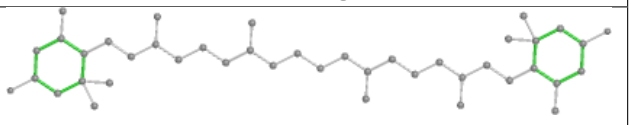
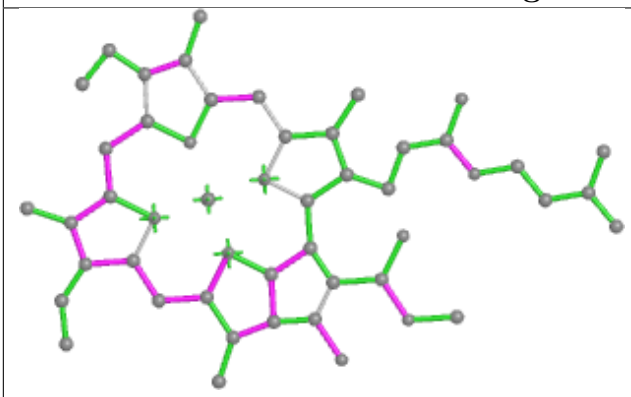


Rings

Ligand CLA G 203



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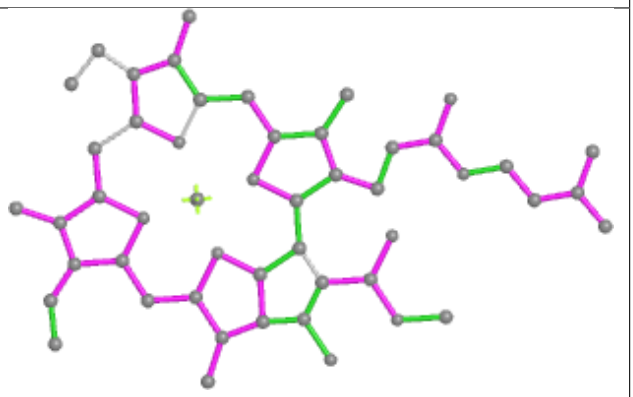

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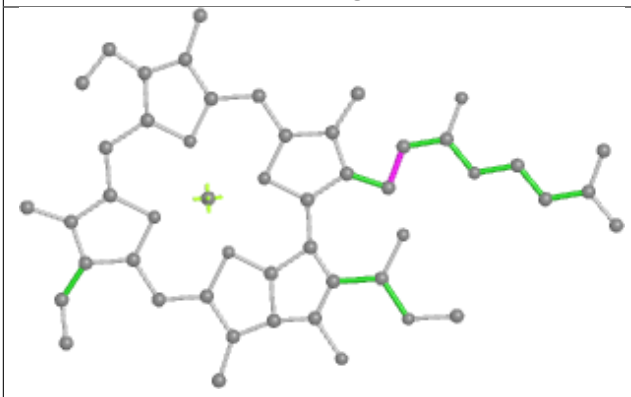

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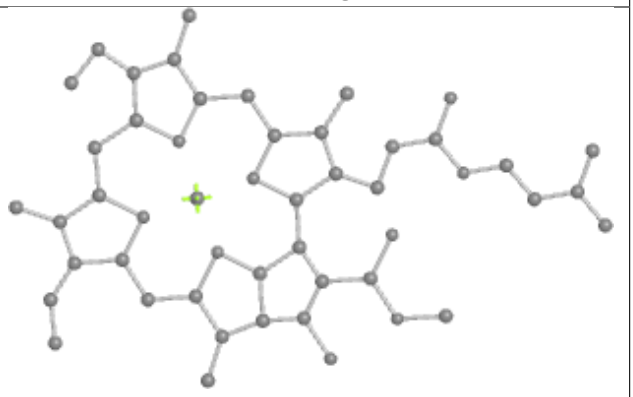
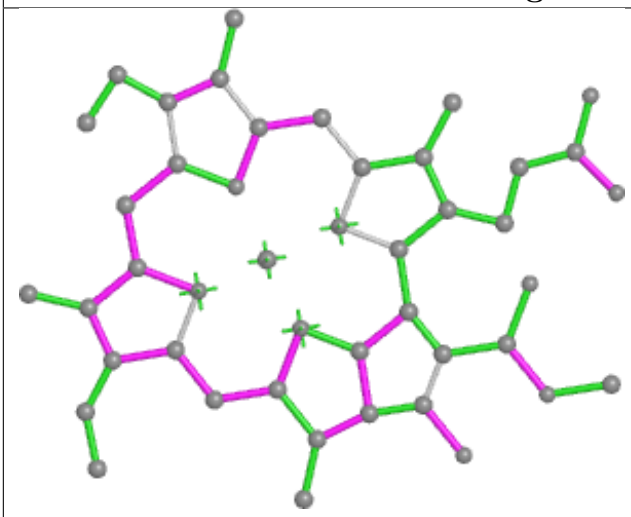


Rings

Ligand CLA F 303



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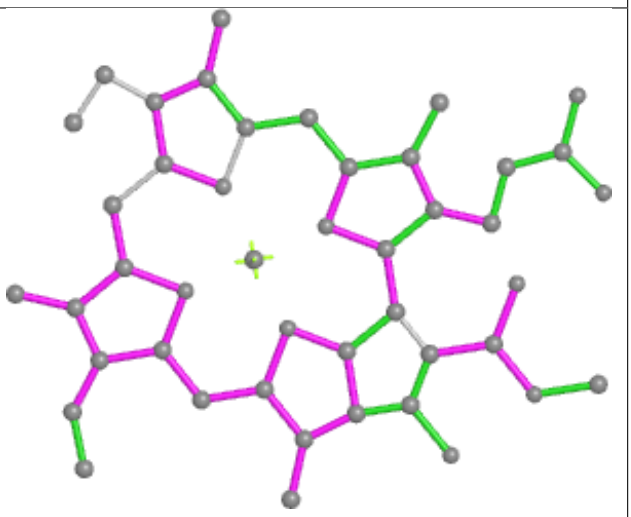
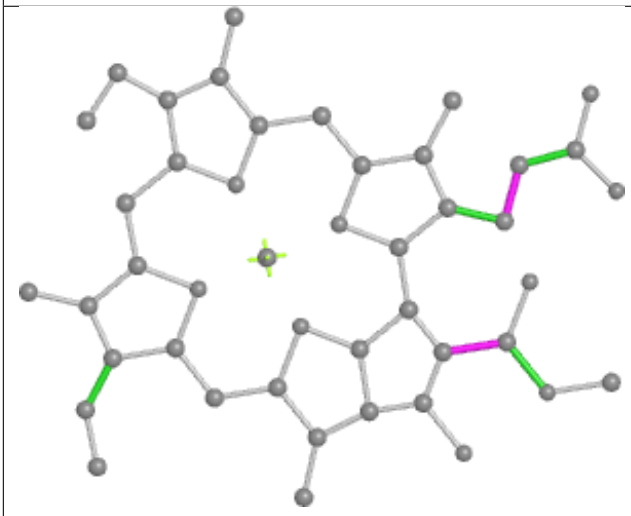


Bond angles



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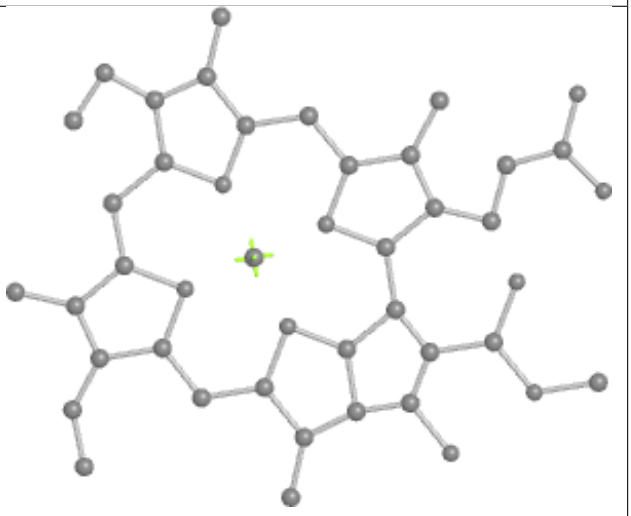
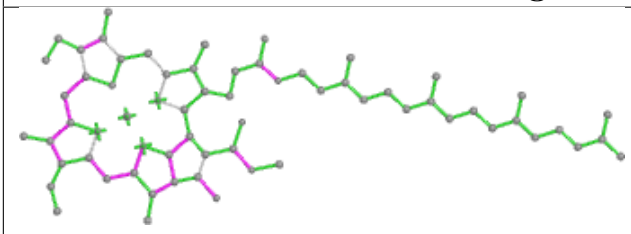


Rings

Ligand CLA 3 610



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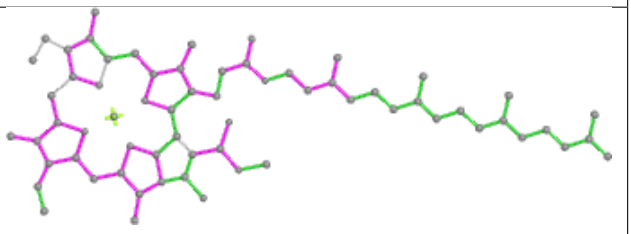
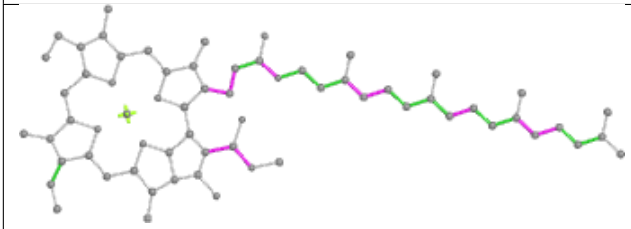


Bond angles



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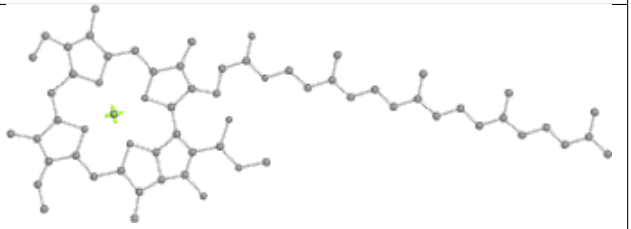
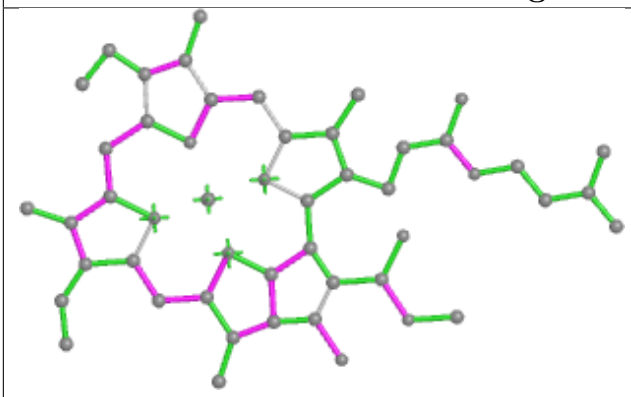


Rings

Ligand CLA 7 608



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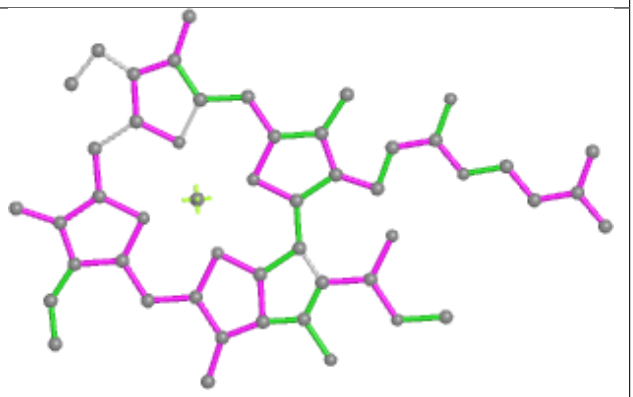
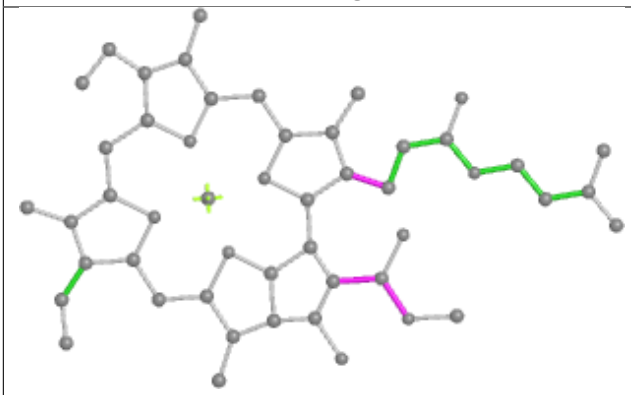


Bond angles



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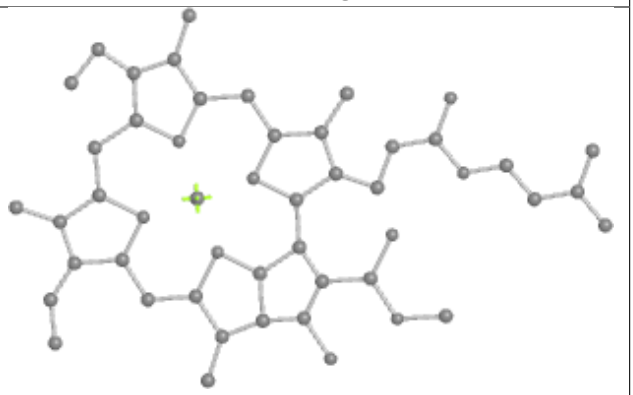
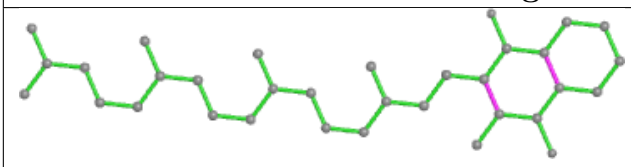


Rings

Ligand PQN B 842



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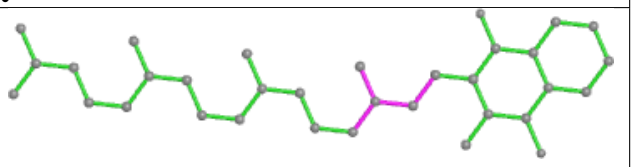
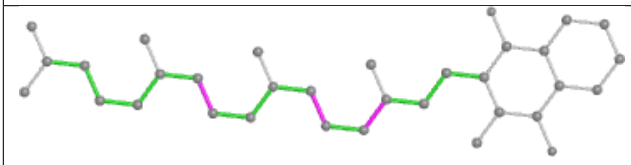


Bond angles



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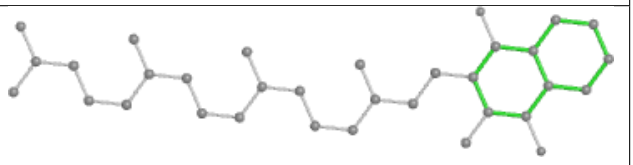
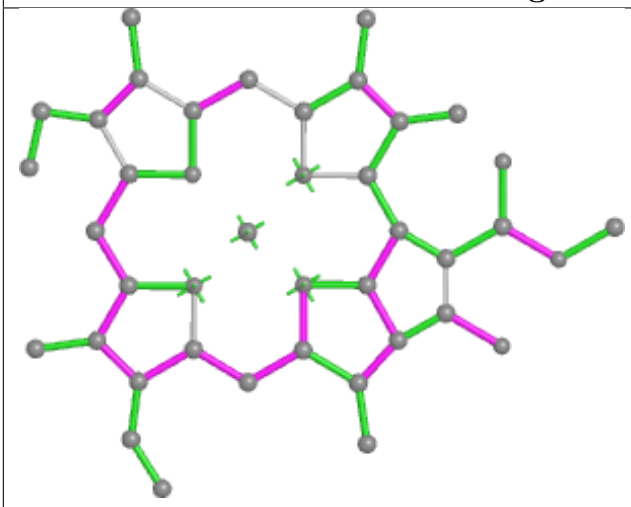


Rings

Ligand CLA 3 611



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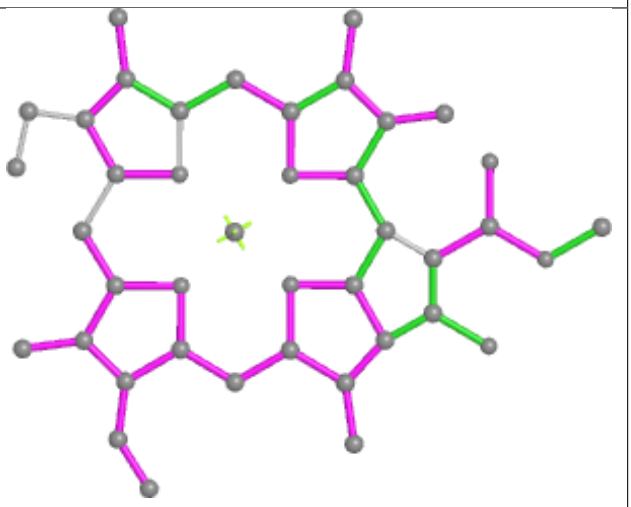
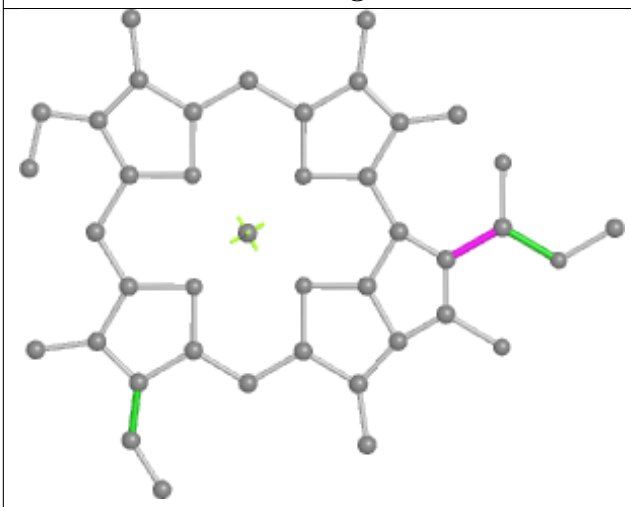


Bond angles



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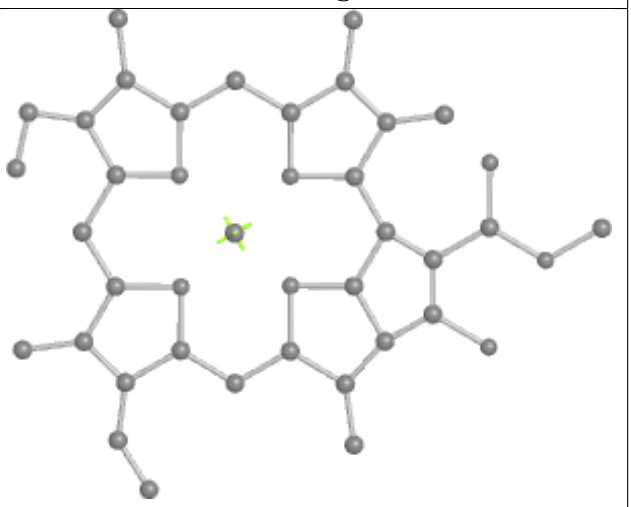
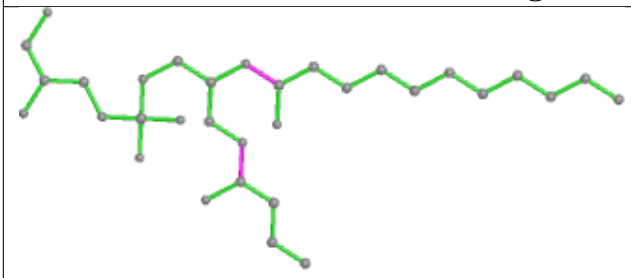


Rings

Ligand LHG 4 623



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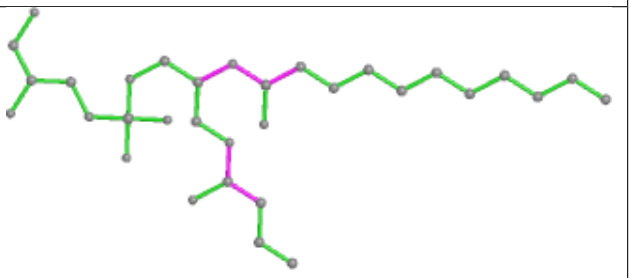
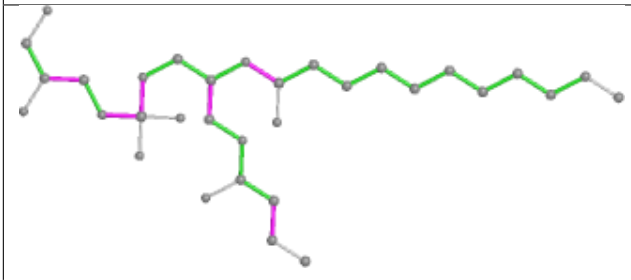


Bond angles



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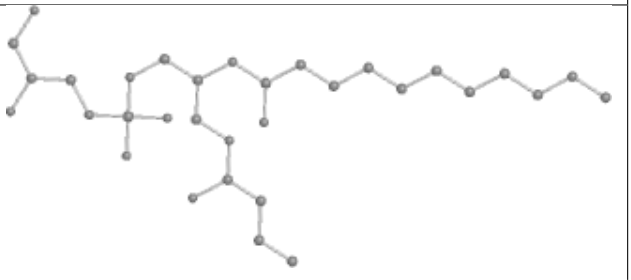
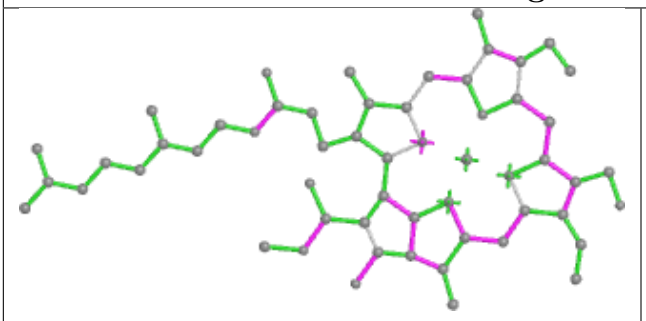
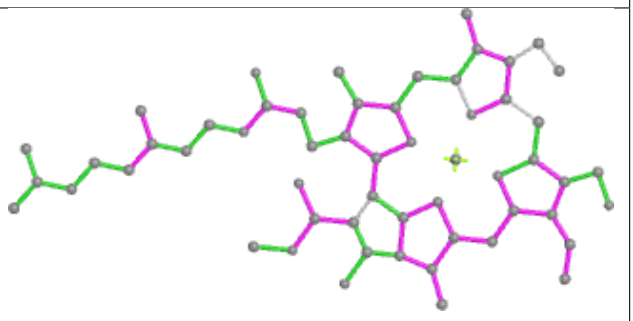


Rings

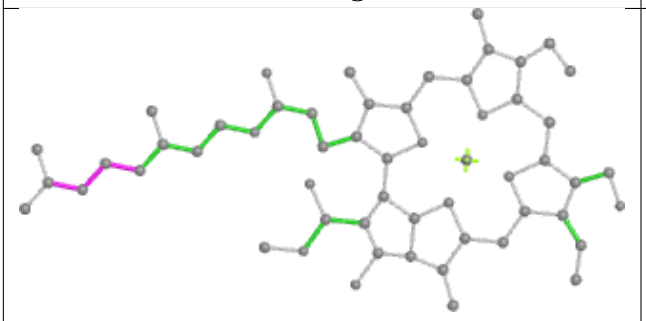
Ligand CHL 6 606



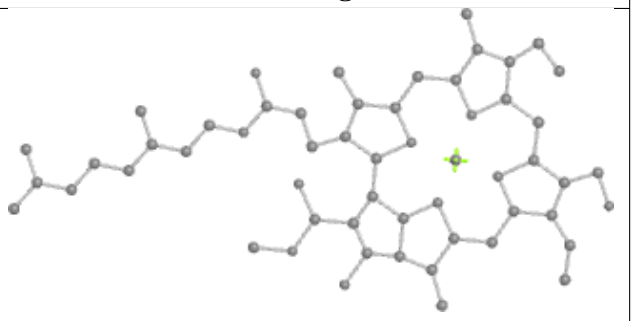
Bond lengths



Bond angles

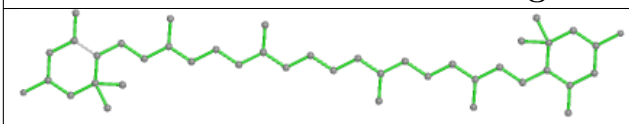


Torsions



Rings

Ligand LUT 3 621



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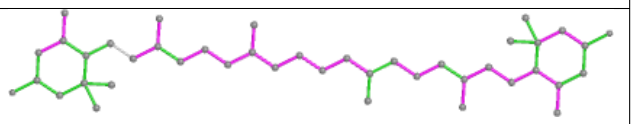
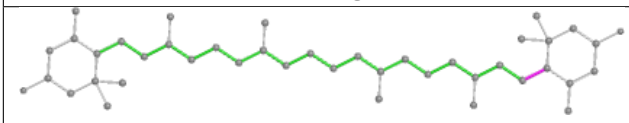


Bond angles



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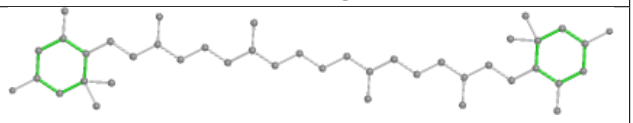
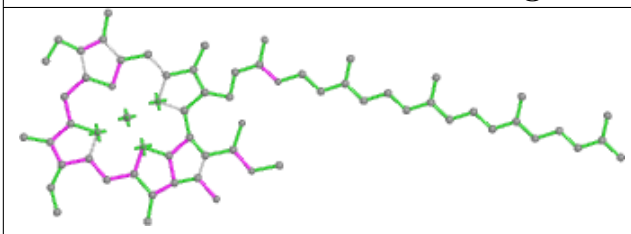


Rings

Ligand CLA A 822



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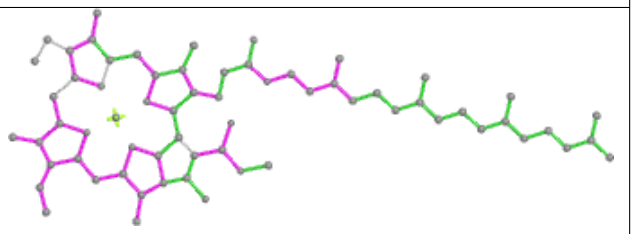
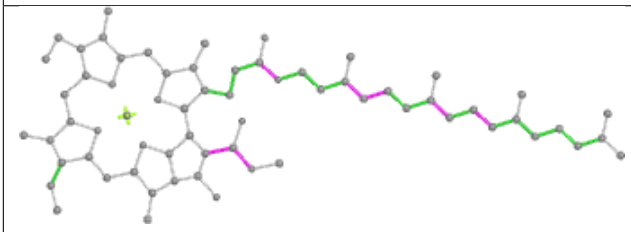


Bond angles



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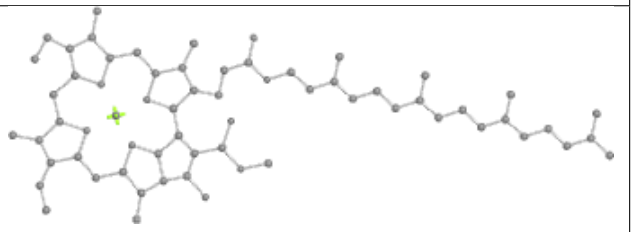
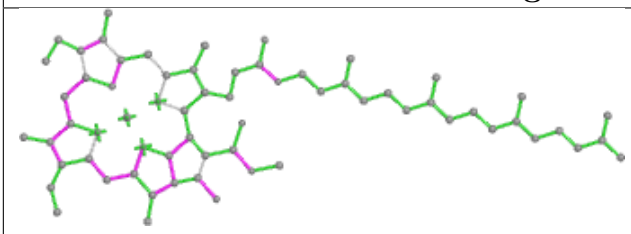


Rings

Ligand CLA A 827



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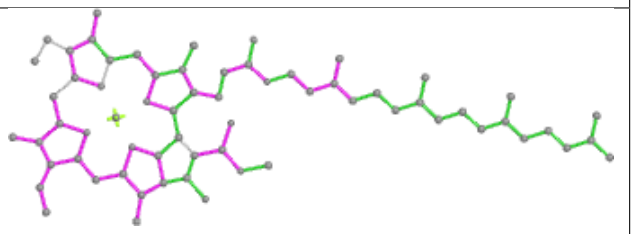
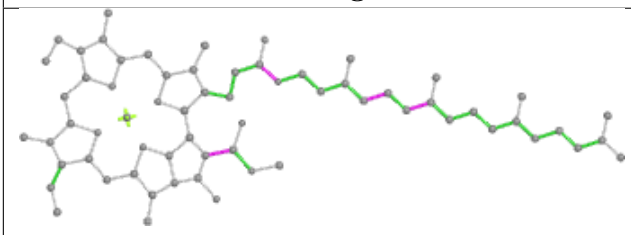


Bond angles



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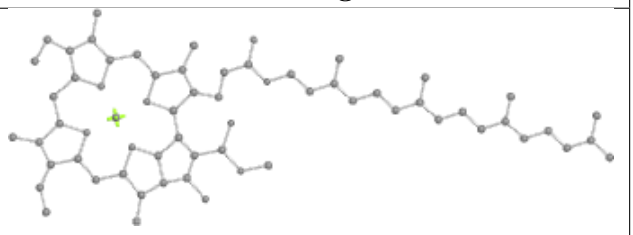
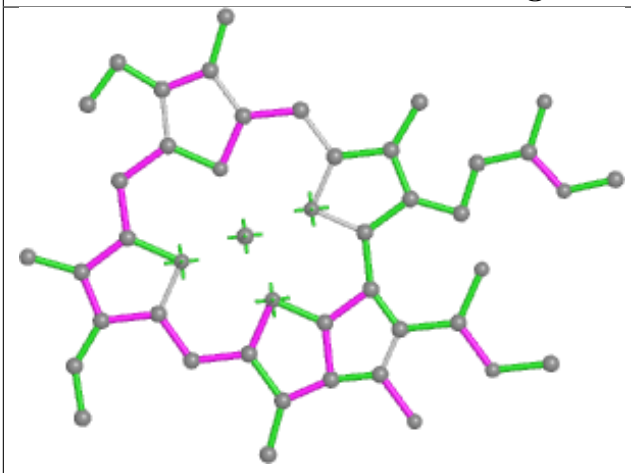


Rings

Ligand CLA Z 616



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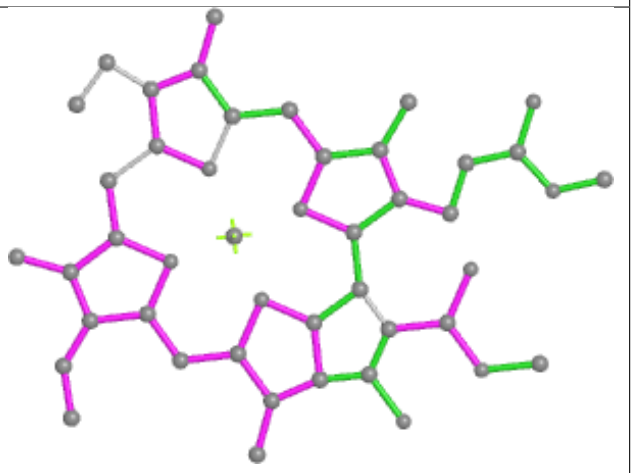
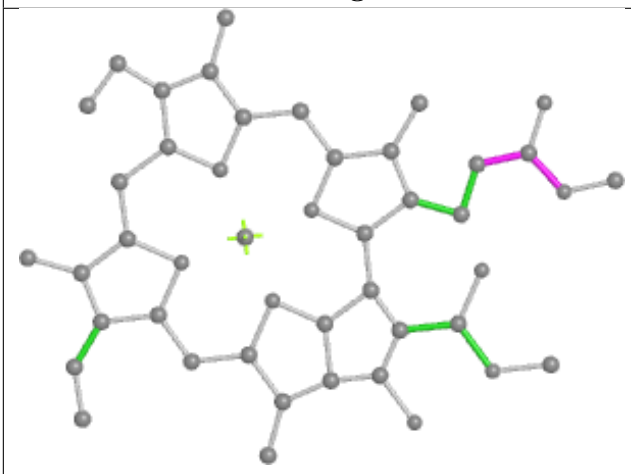


Bond angles



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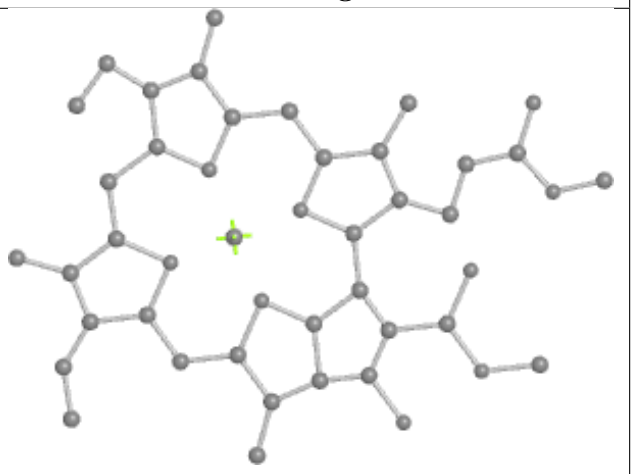
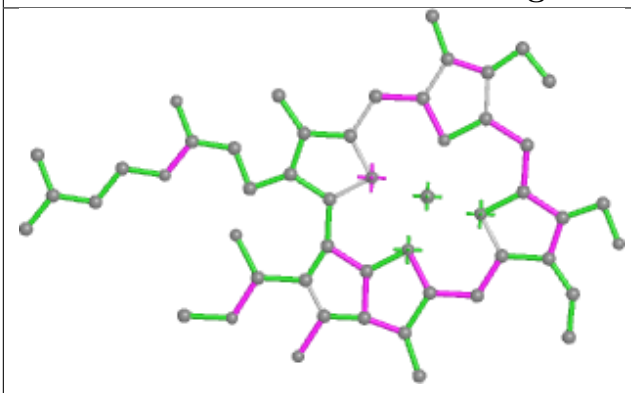


Rings

Ligand CHL 6 608



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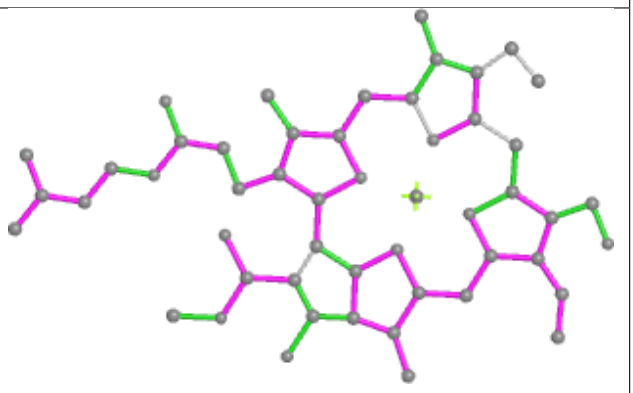
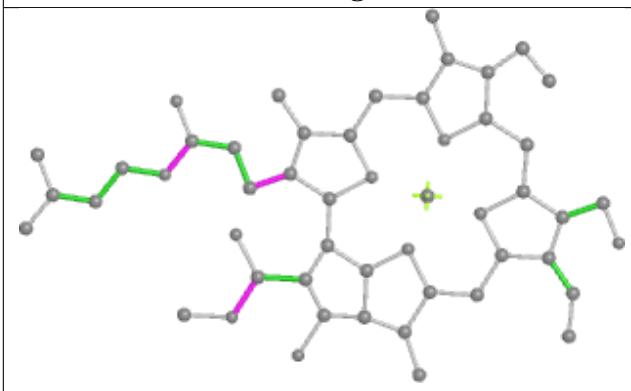


Bond angles



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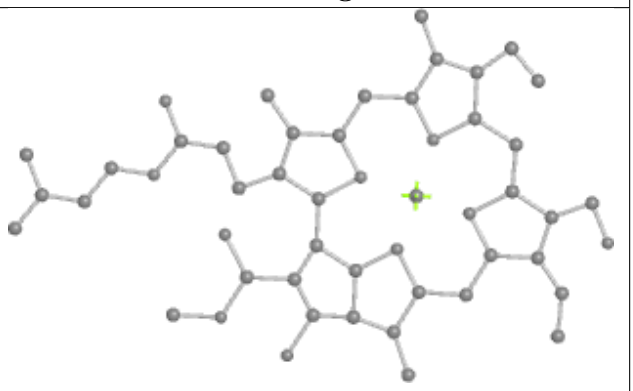
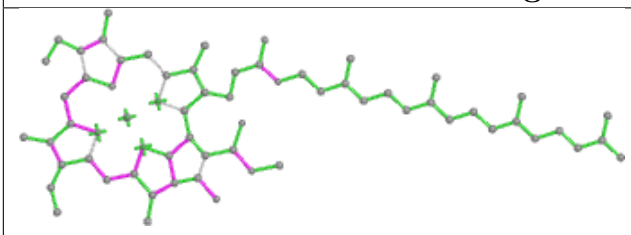


Rings

Ligand CLA A 818



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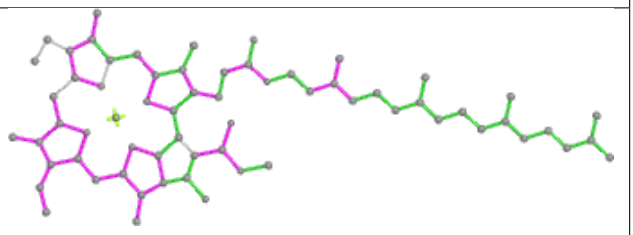
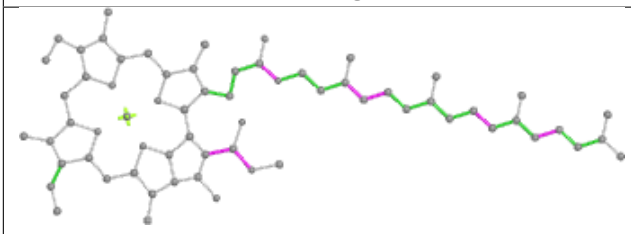


Bond angles



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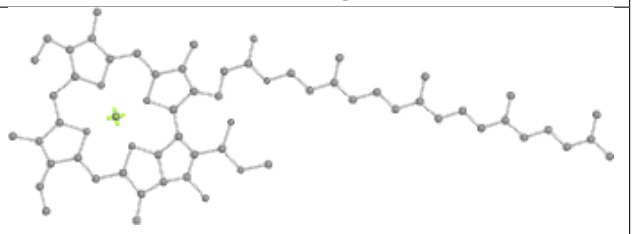
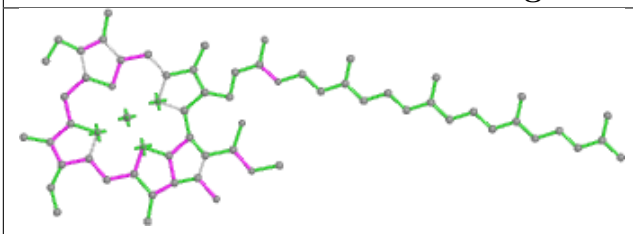


Rings

Ligand CLA B 805



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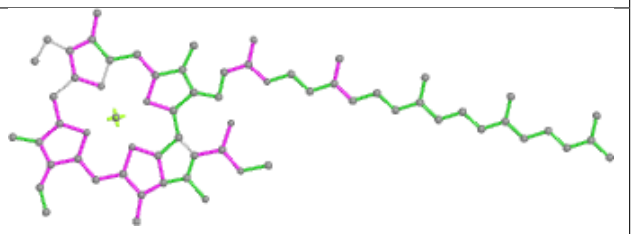
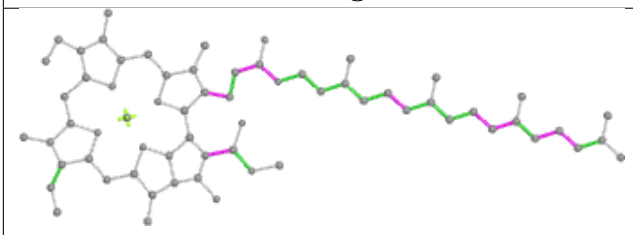


Bond angles



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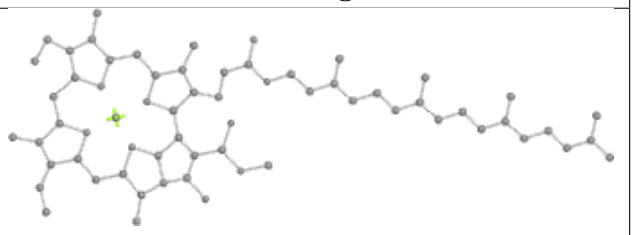
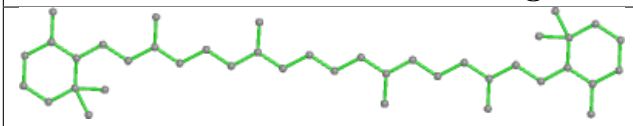


Rings

Ligand BCR L 205



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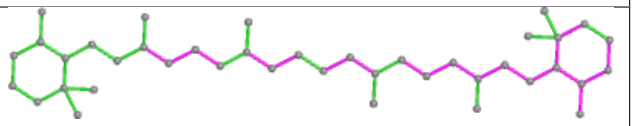
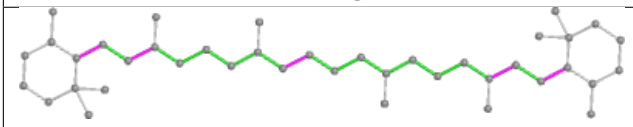


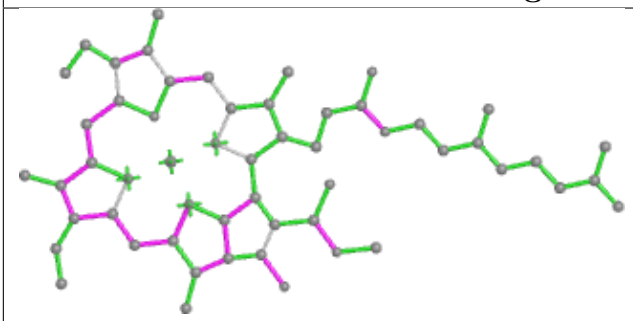
Bond angles



Torsions

Rings

Ligand CLA B 816



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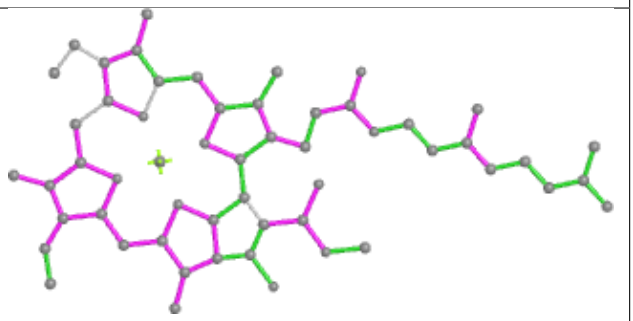

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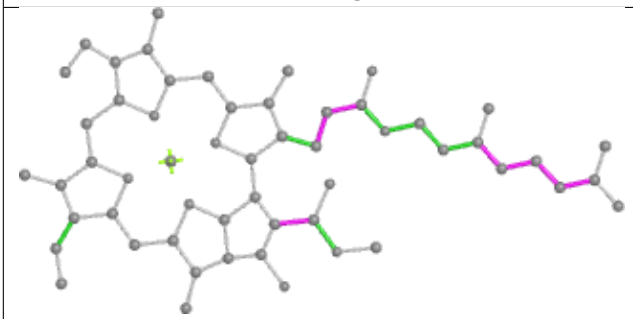

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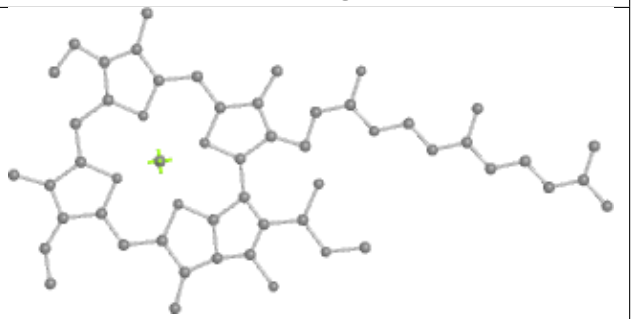
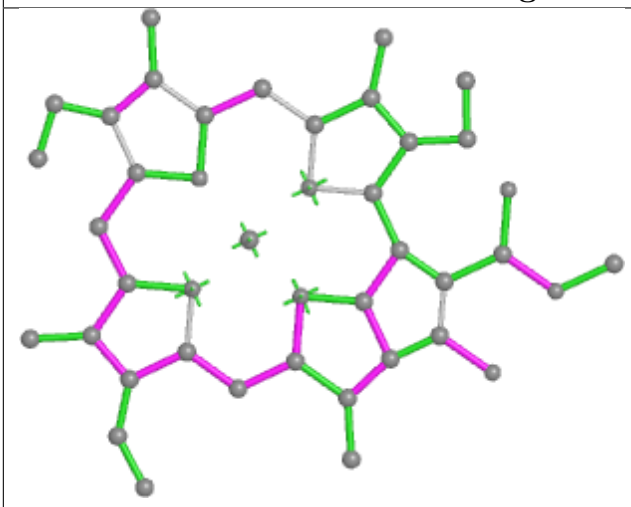


Rings

Ligand CLA J 3002



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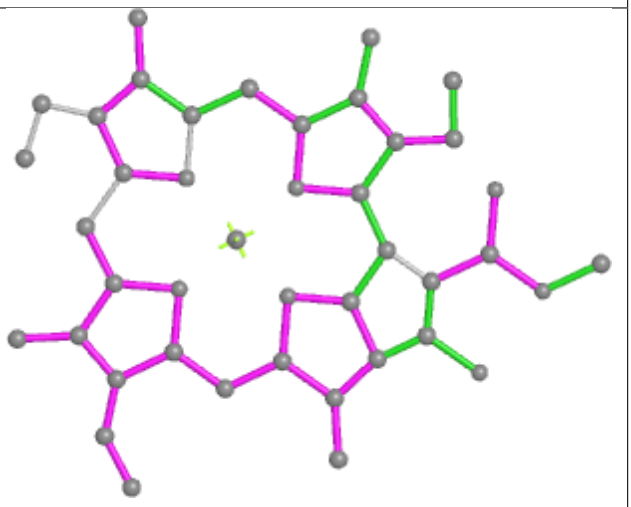

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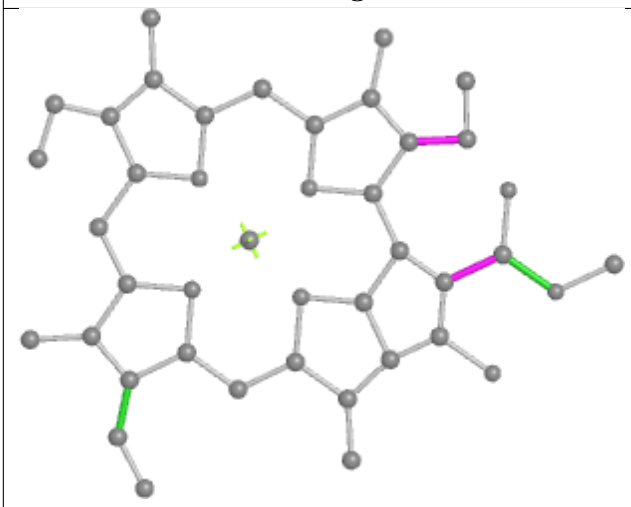

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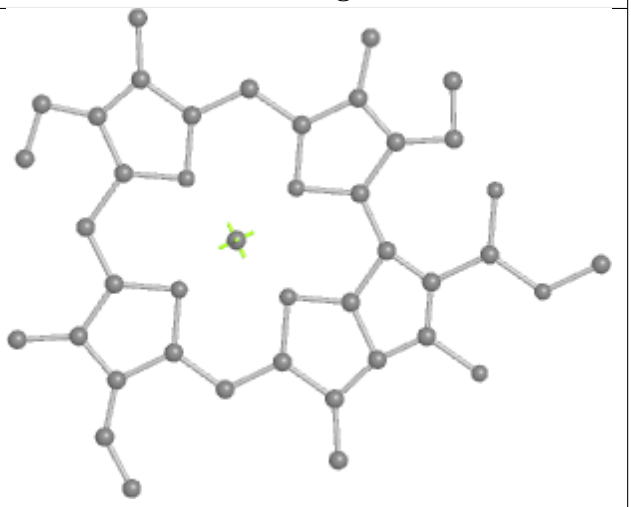
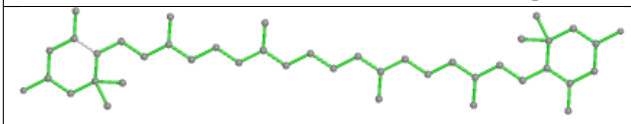


Rings

Ligand LUT Z 617



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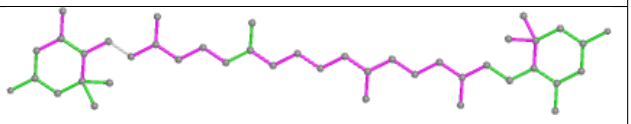

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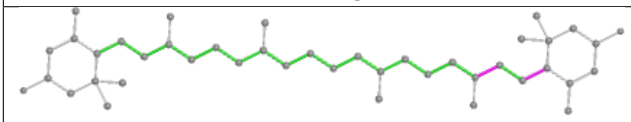

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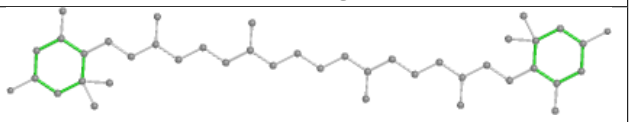
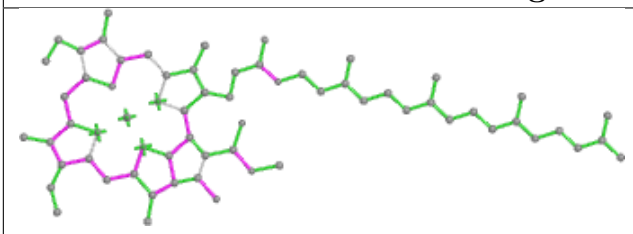
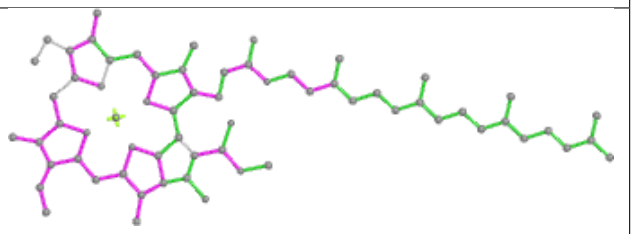


Rings

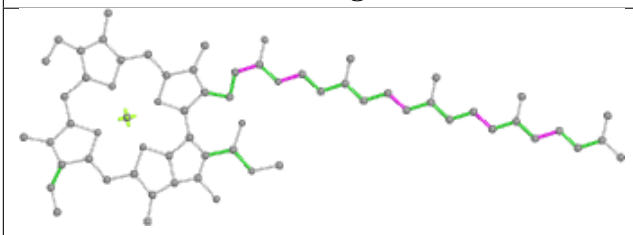
Ligand CLA 7 613



Bond lengths



Bond angles



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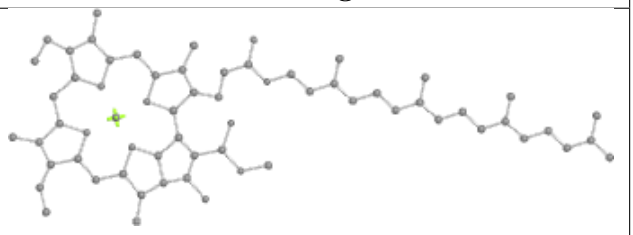
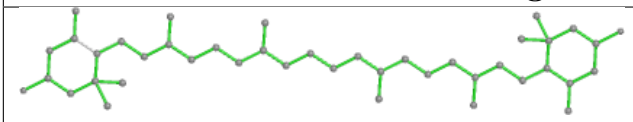
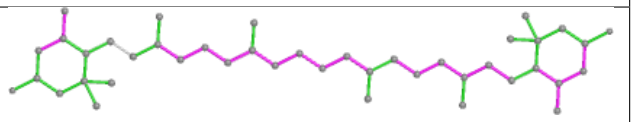


Rings

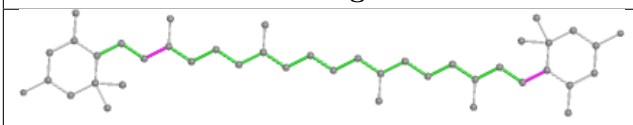
Ligand LUT Z 619



Bond lengths



Bond angles



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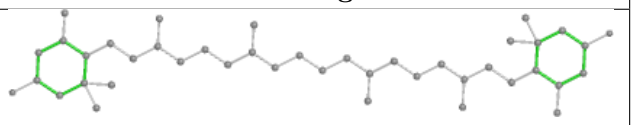
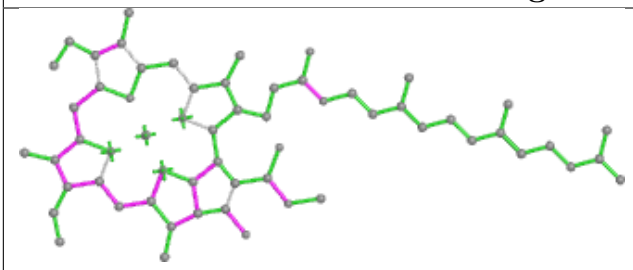
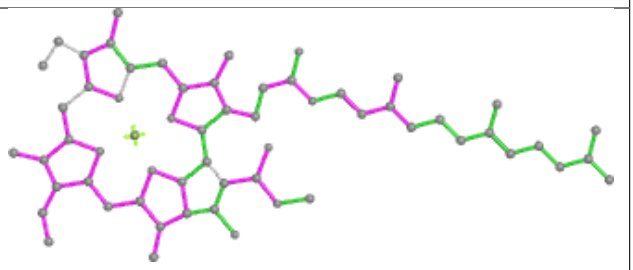


Rings

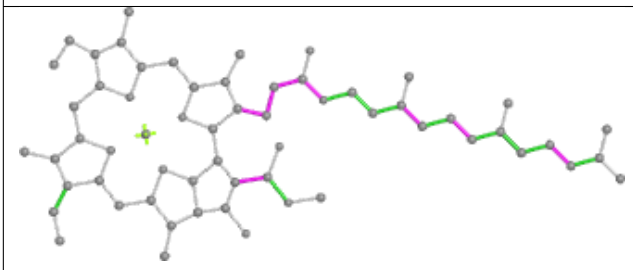
Ligand CLA 5 610



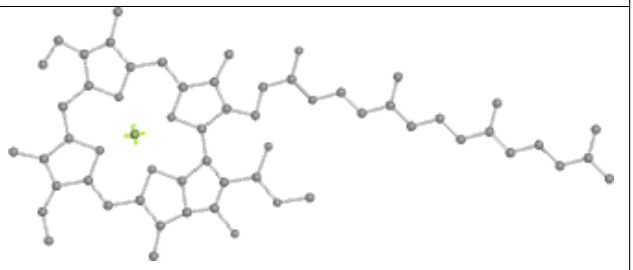
Bond lengths



Bond angles

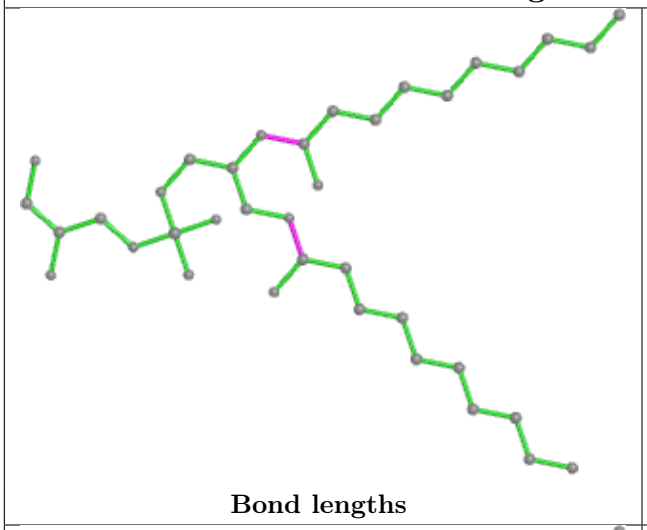


Torsions

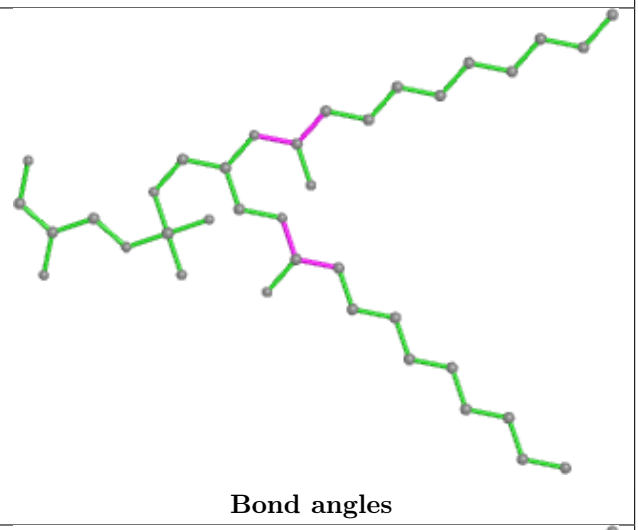


Rings

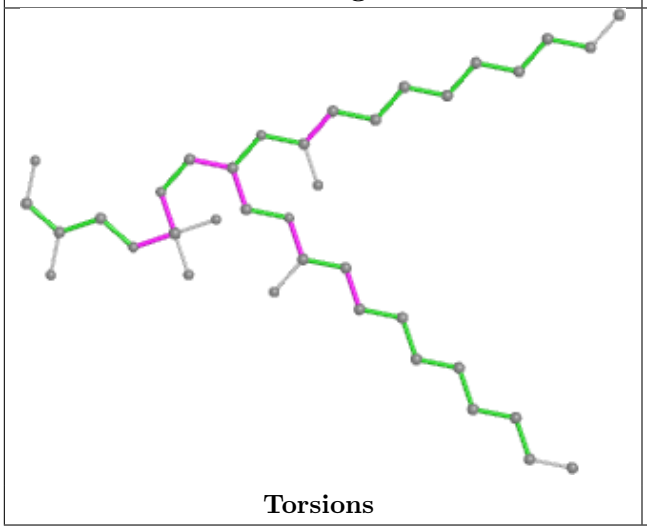
Ligand LHG 5 623



Bond lengths



Bond angles



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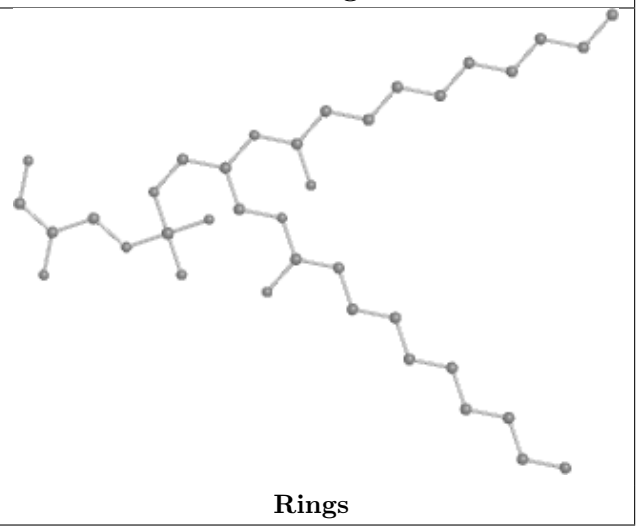
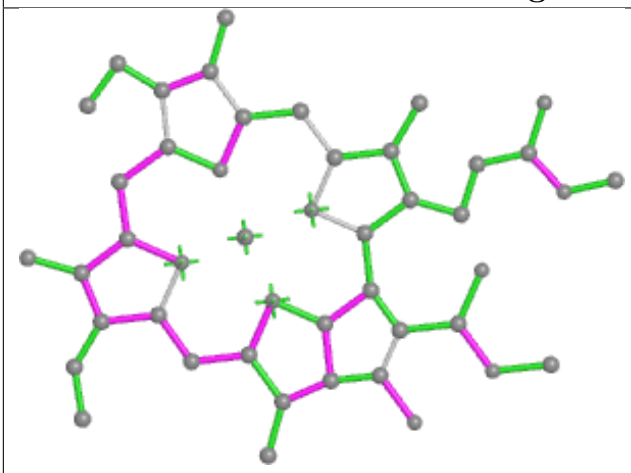


Rings

Ligand CLA 3 612



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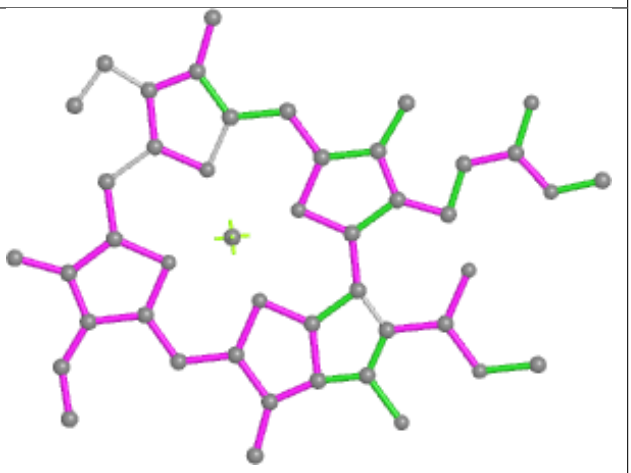

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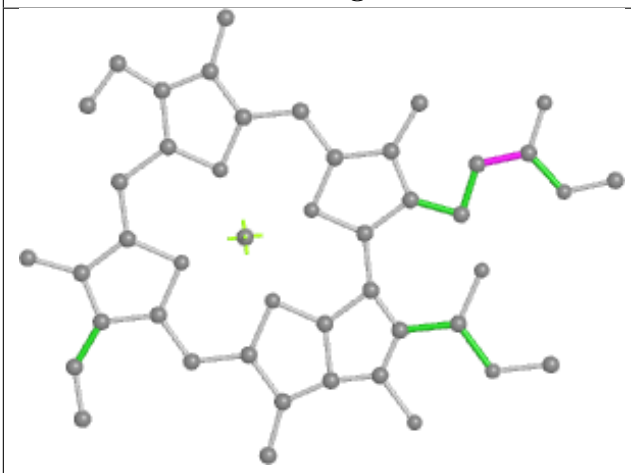

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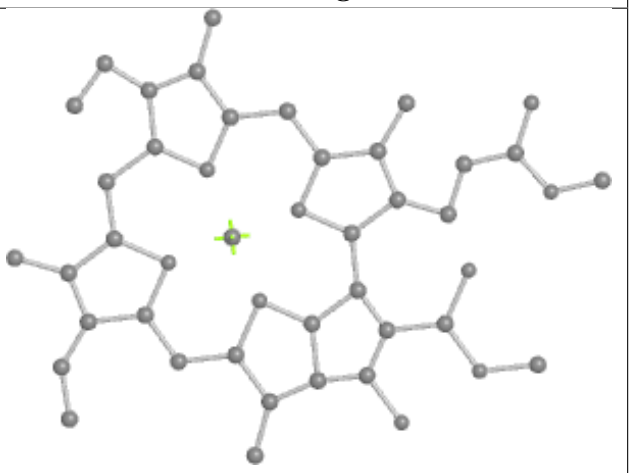
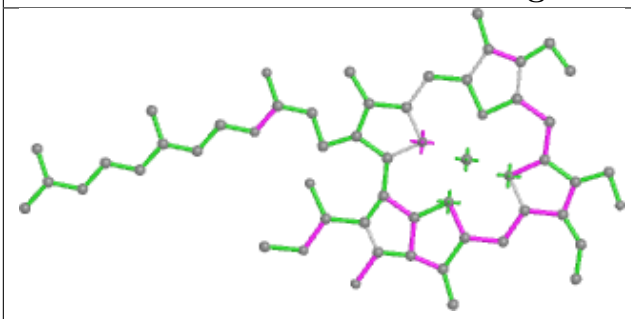


Rings

Ligand CHL 6 607



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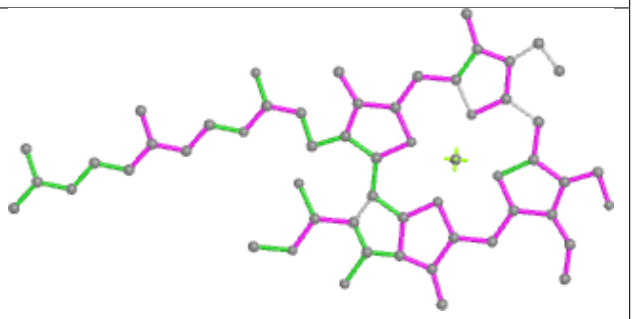
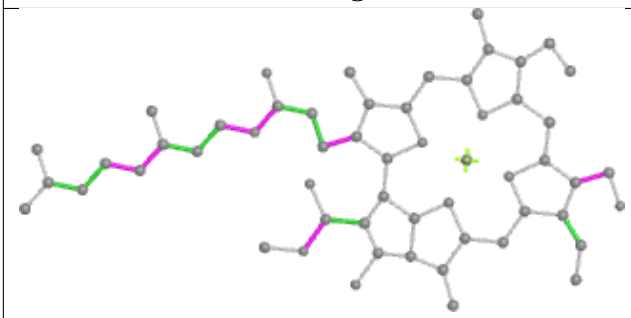


Bond angles



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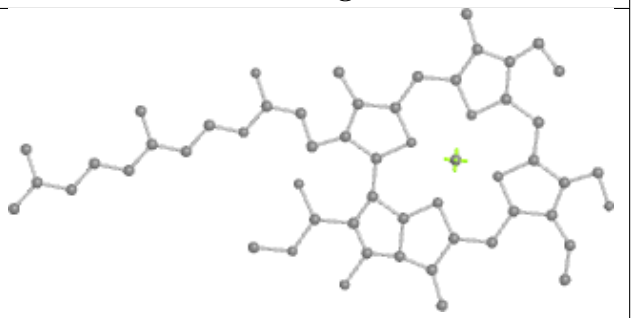
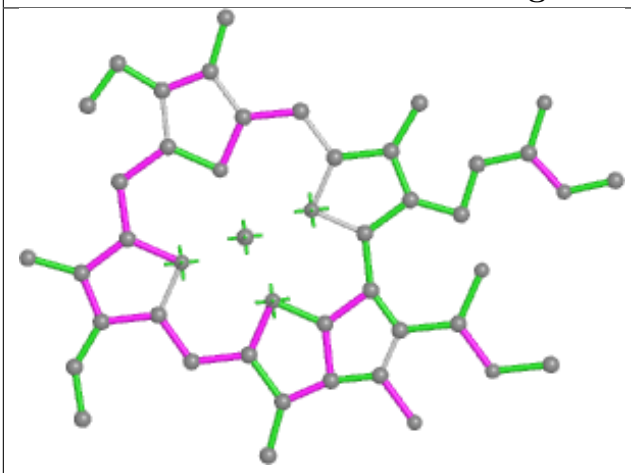


Rings

Ligand CLA 6 617



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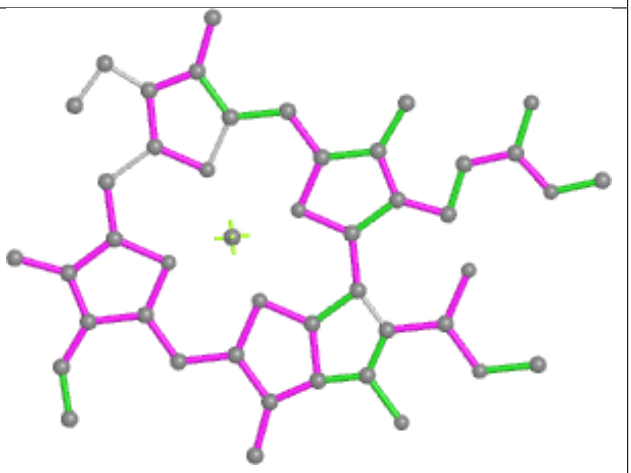

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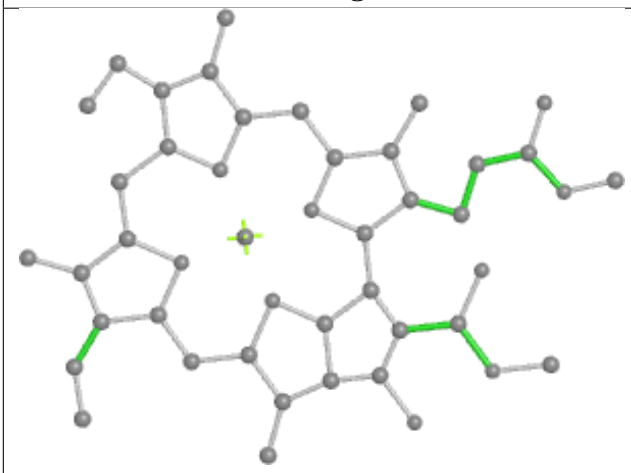

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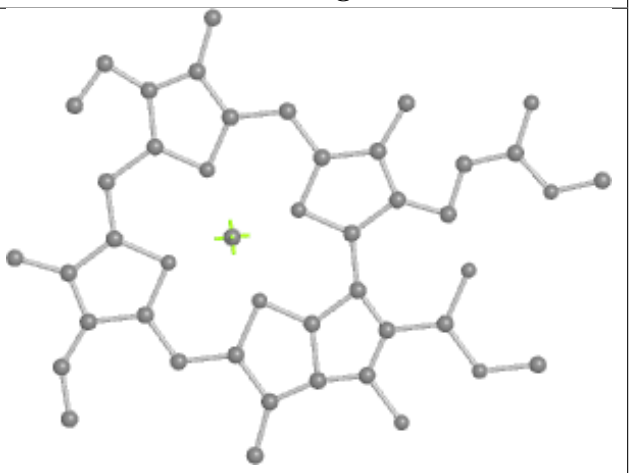
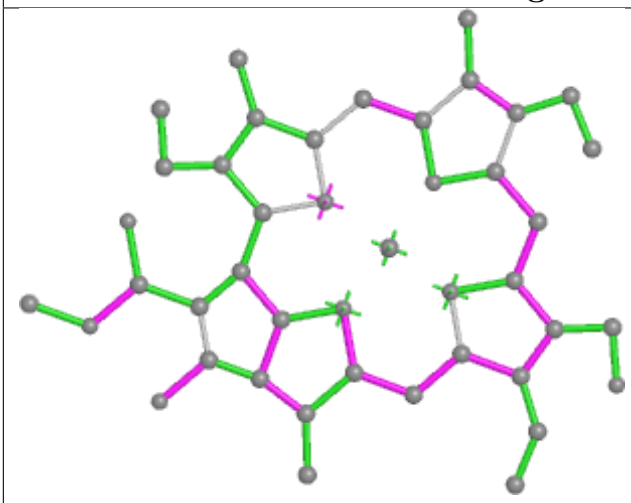


Rings

Ligand CHL 5 618



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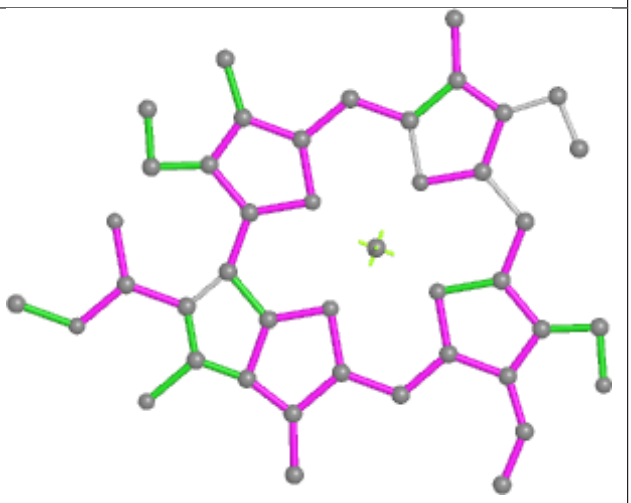
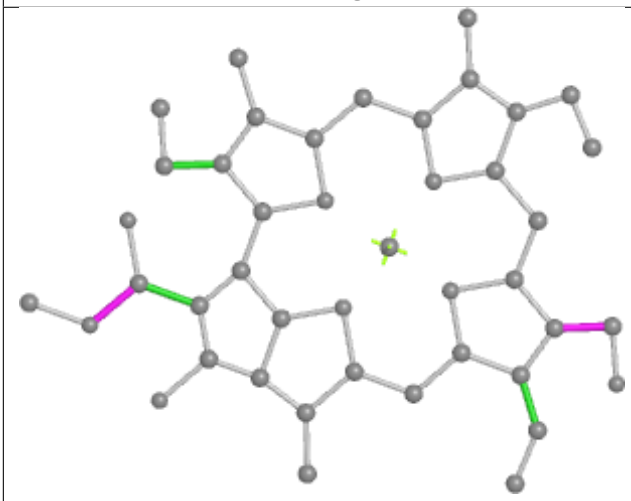


Bond angles



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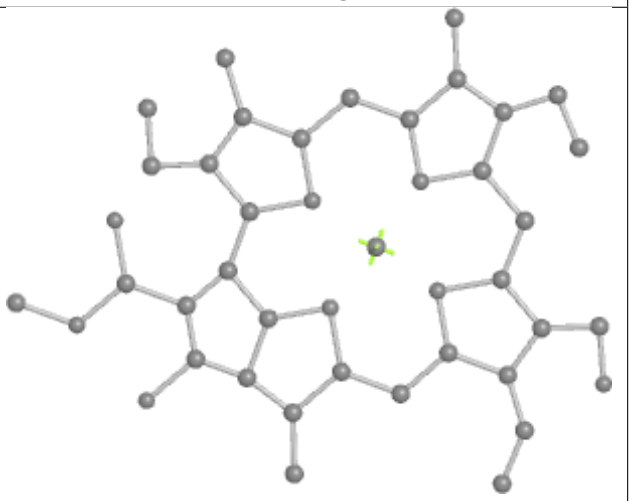
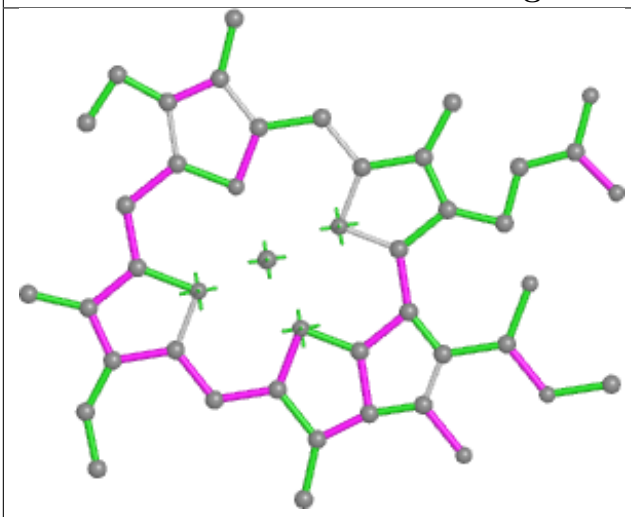


Rings

Ligand CLA A 837



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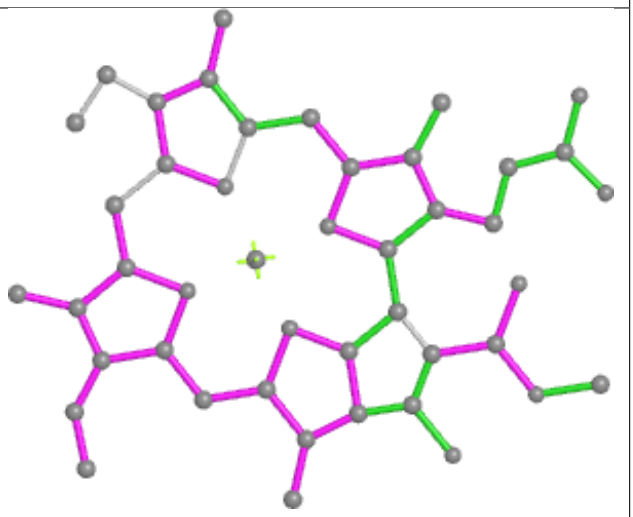

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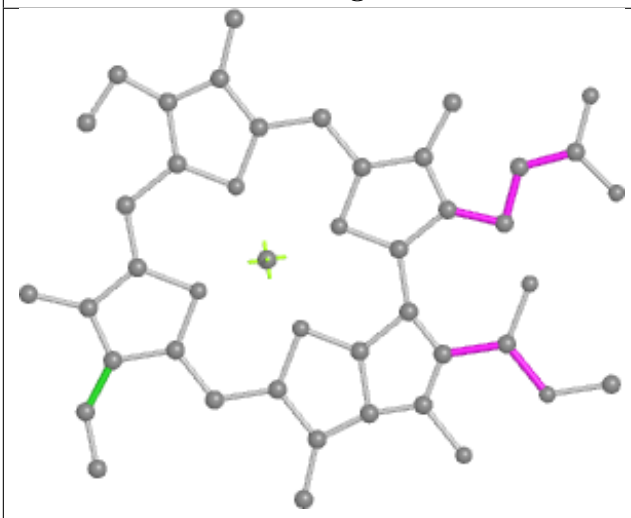

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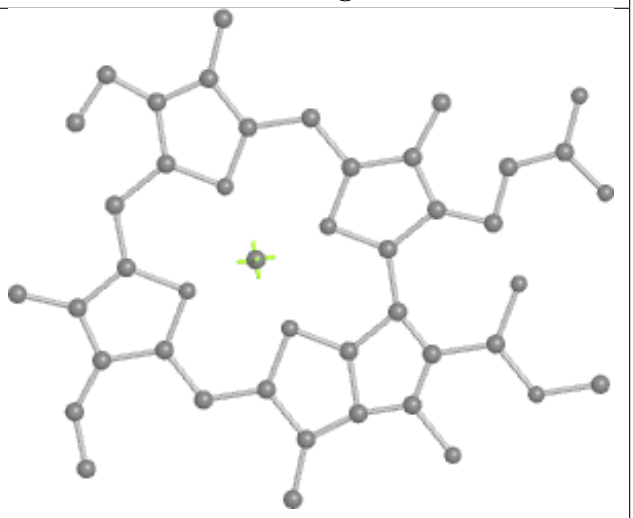
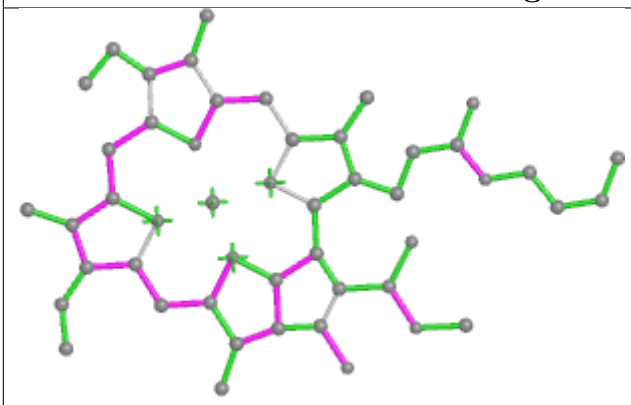


Rings

Ligand CLA A 823



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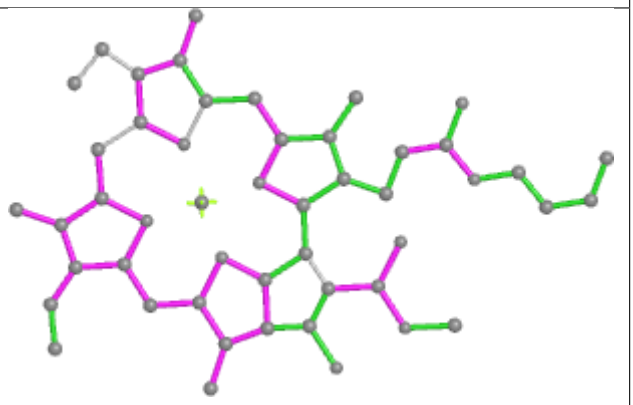

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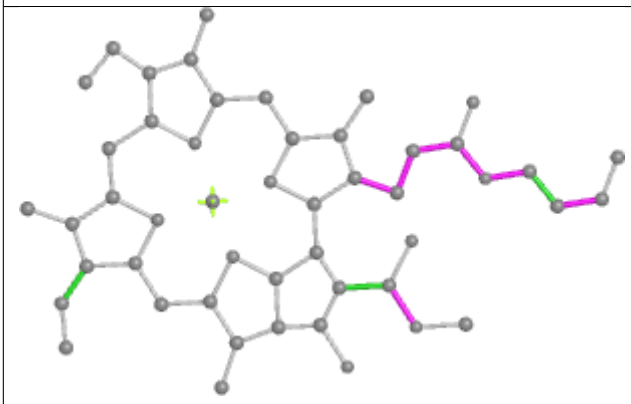

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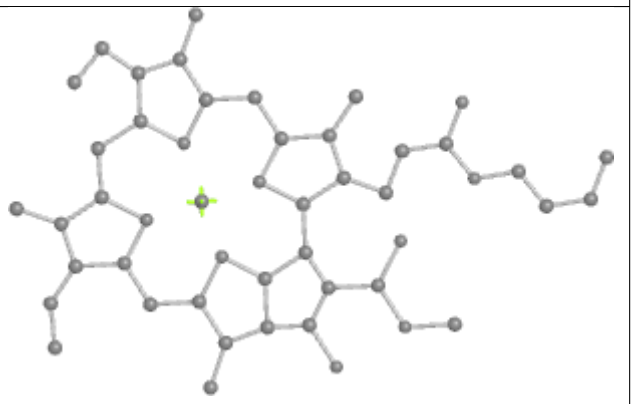
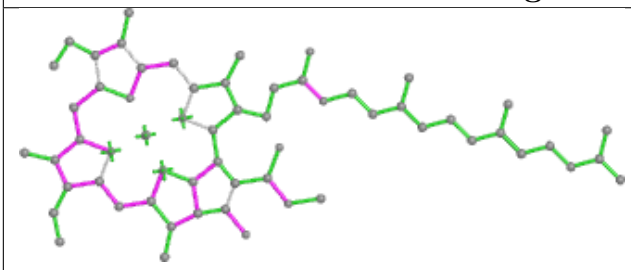


Rings

Ligand CLA B 836



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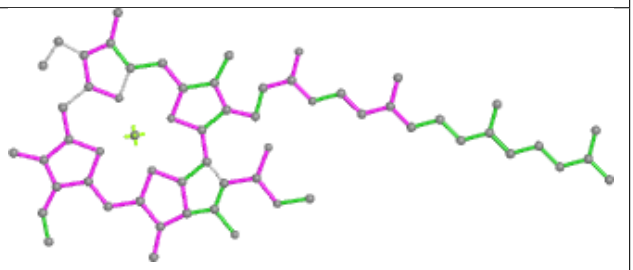

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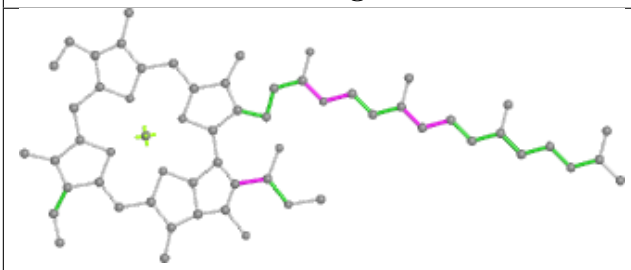

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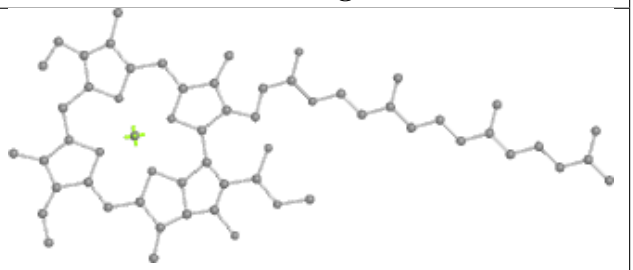
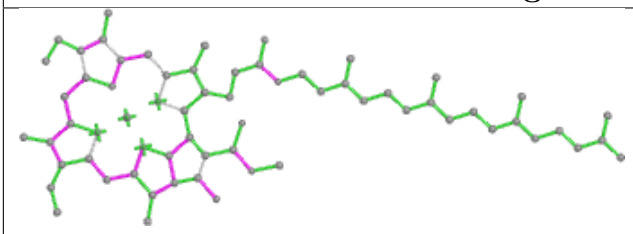


Rings

Ligand CLA A 843



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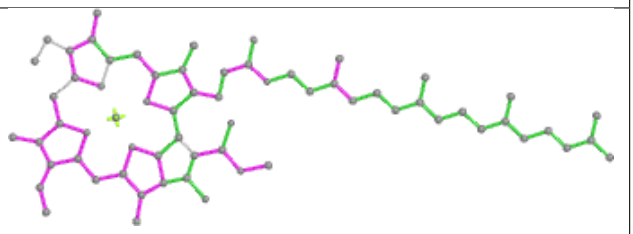

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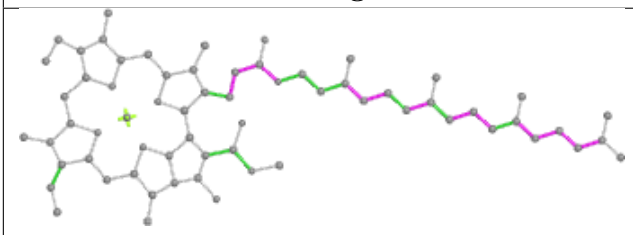

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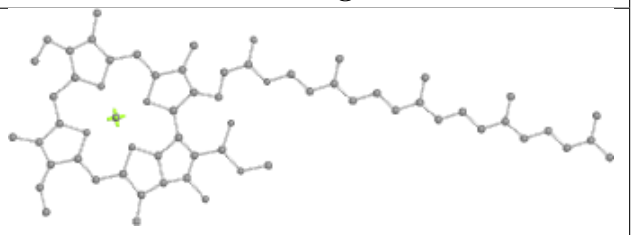
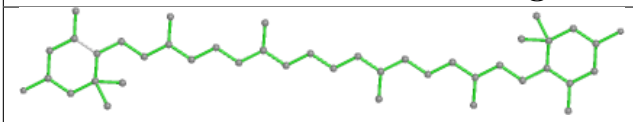


Rings

Ligand LUT 8 618



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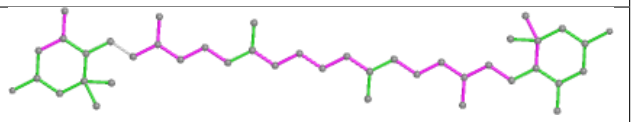
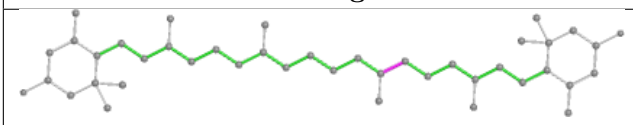


Bond angles



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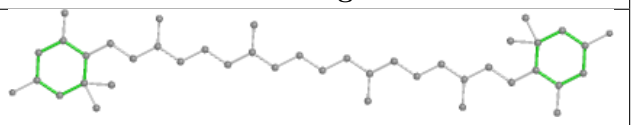
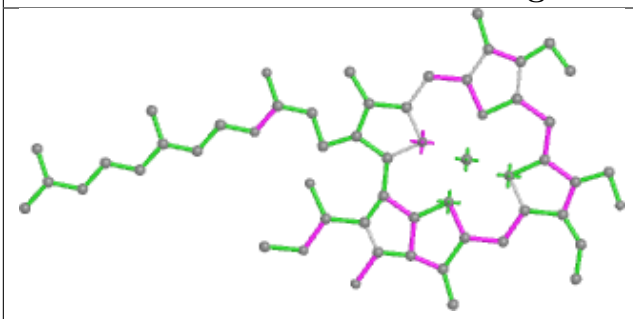


Rings

Ligand CHL 4 606



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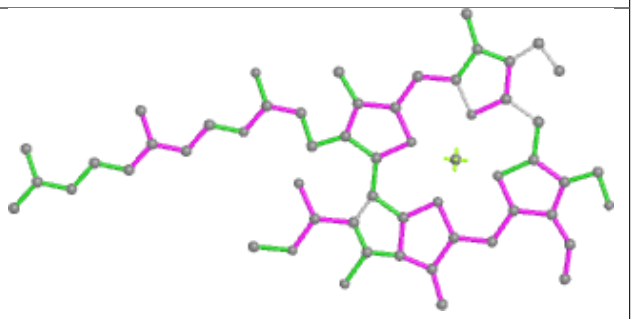
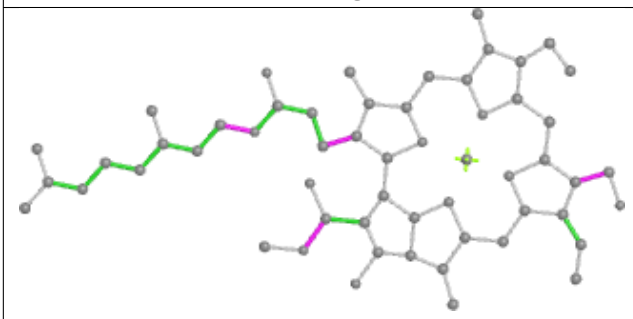


Bond angles



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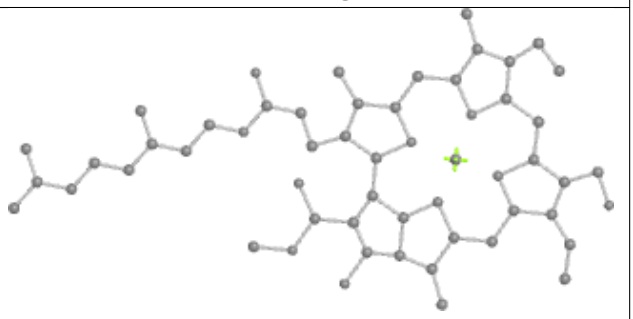
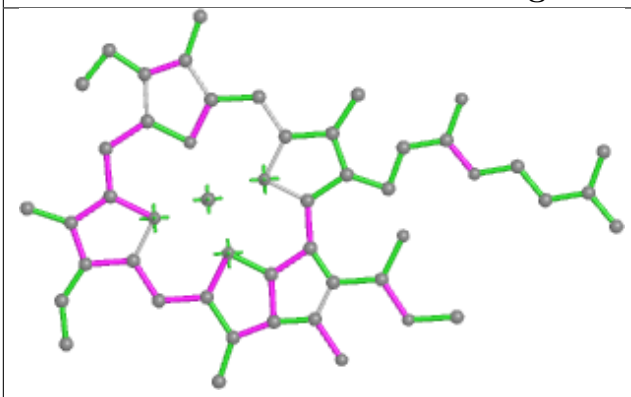


Rings

Ligand CLA 4 609



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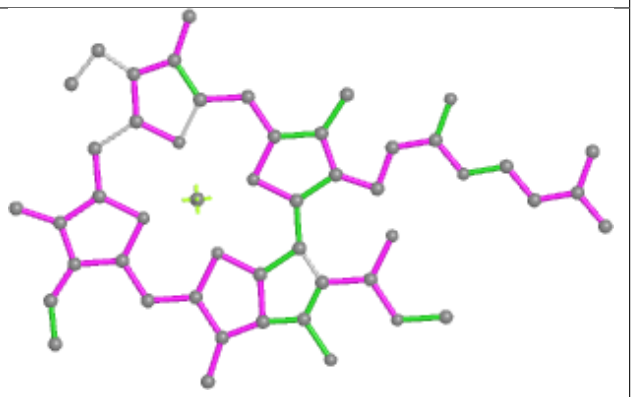
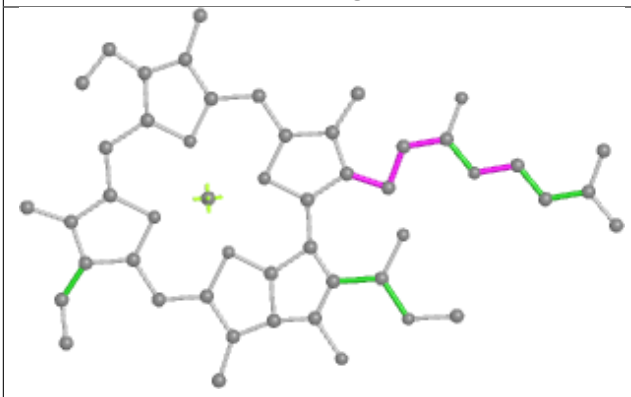


Bond angles



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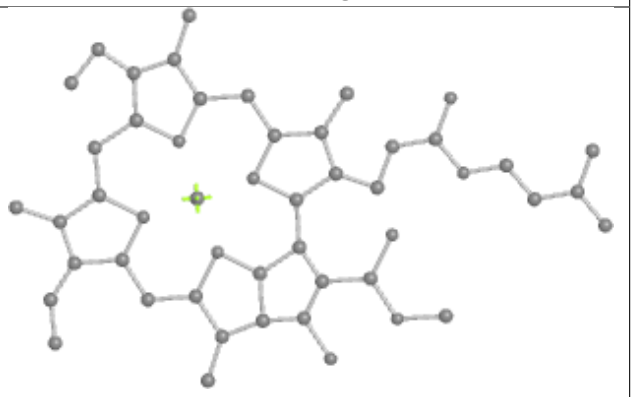
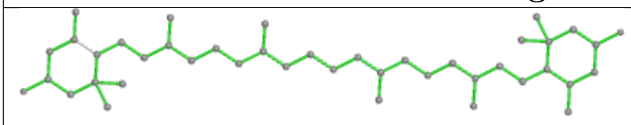


Rings

Ligand LUT 1 619



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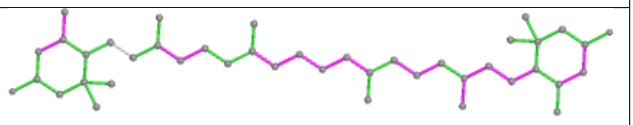
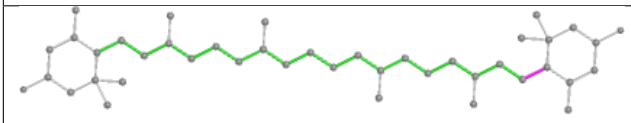


Bond angles



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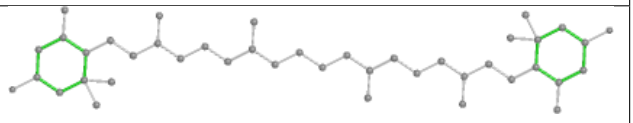
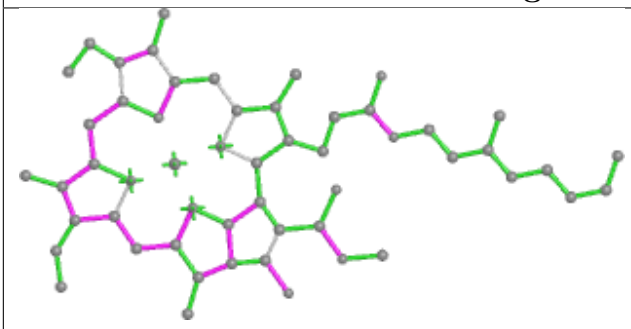


Rings

Ligand CLA A 813



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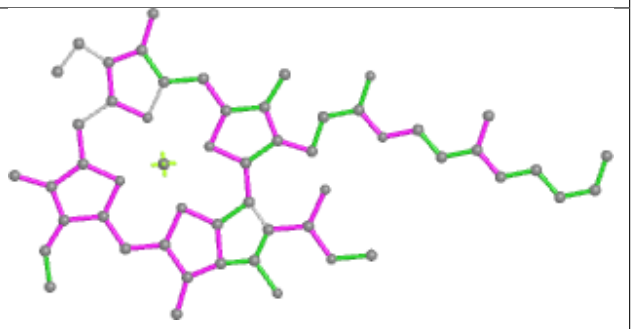
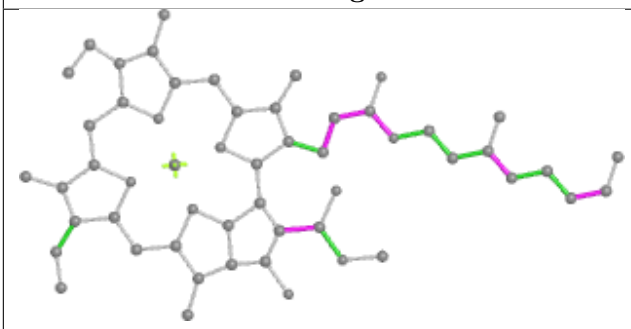
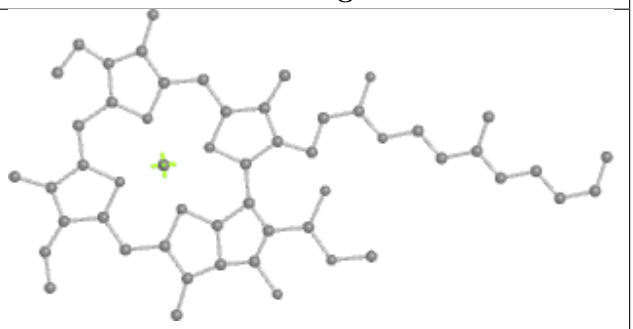


Bond angles

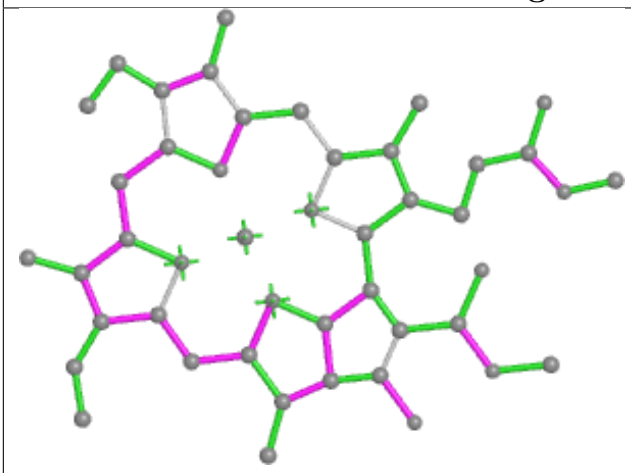


Torsions

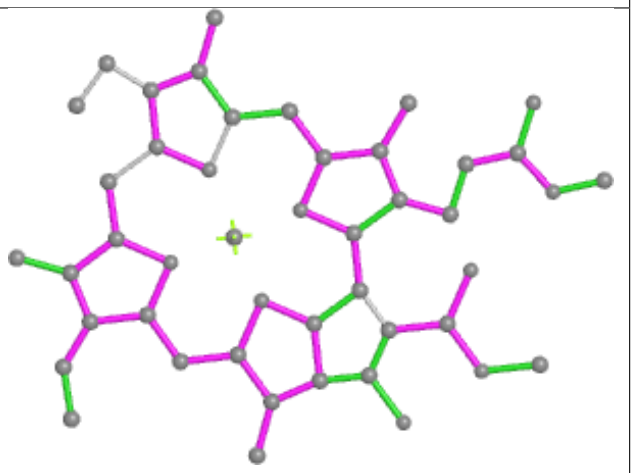


Rings

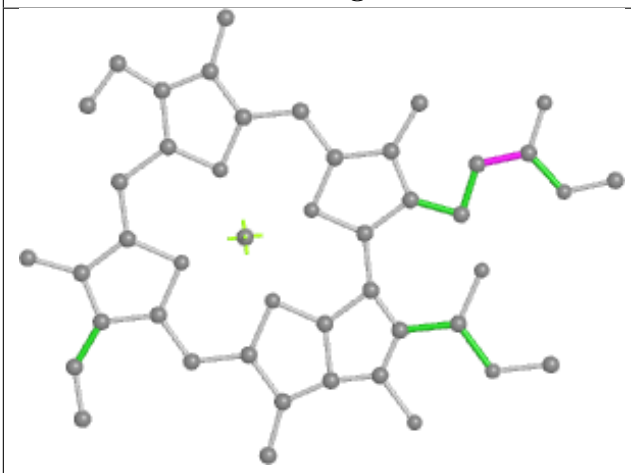
Ligand CLA 8 609



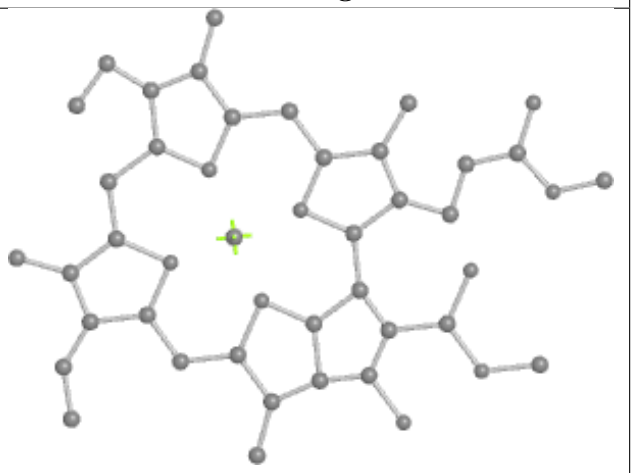
Bond lengths



Bond angles

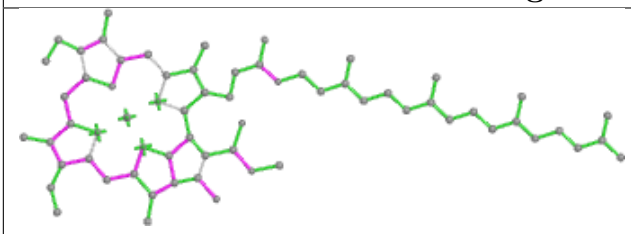


Torsions



Rings

Ligand CLA Z 608



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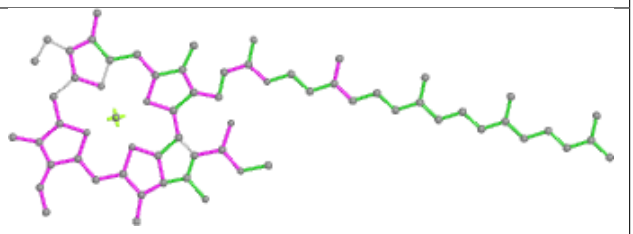
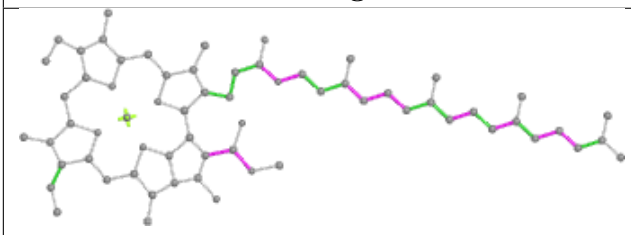
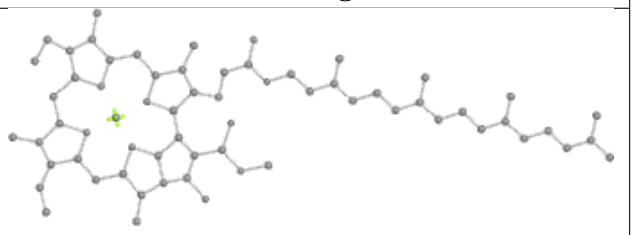


Bond angles

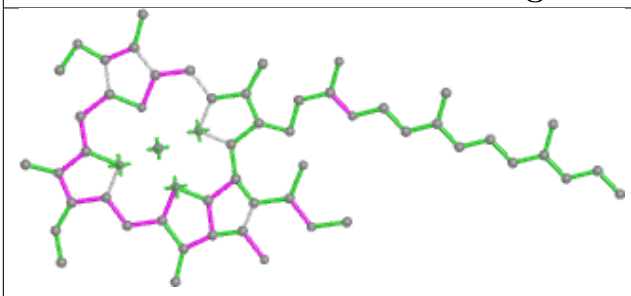


Torsions

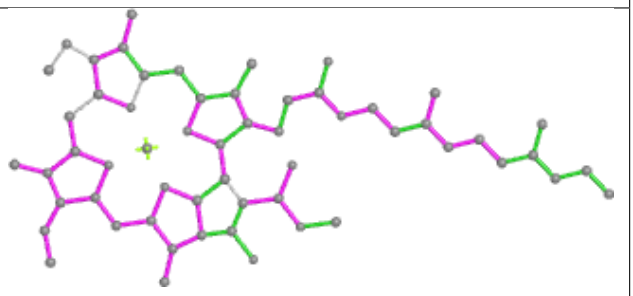


Rings

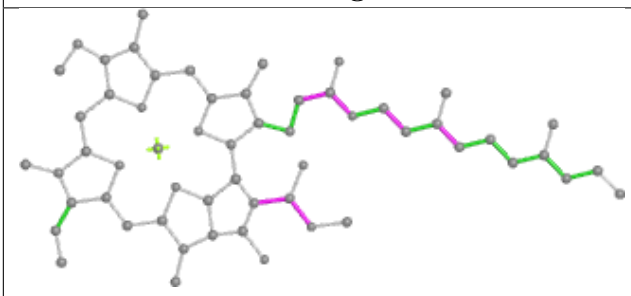
Ligand CLA Z 603



Bond lengths



Bond angles



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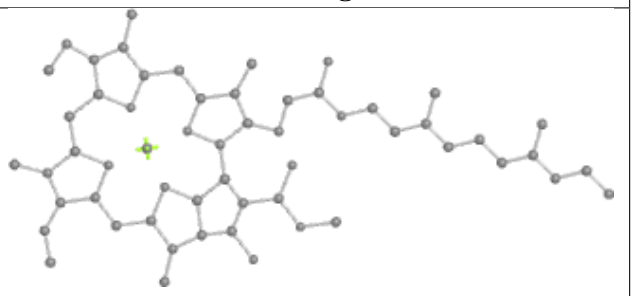
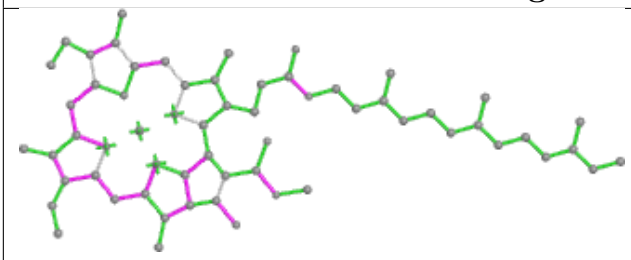


Rings

Ligand CLA 4 601



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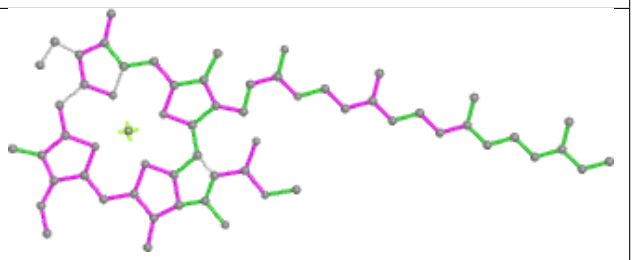
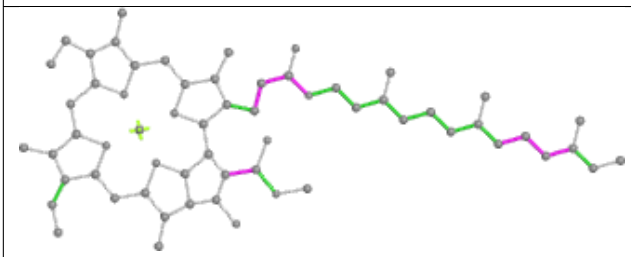


Bond angles



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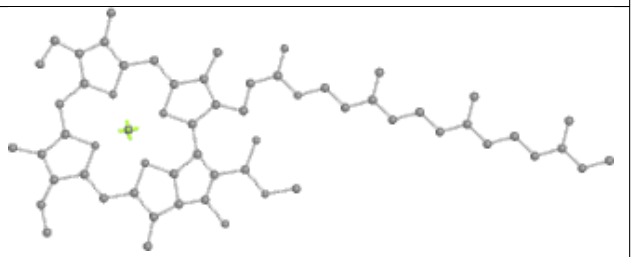
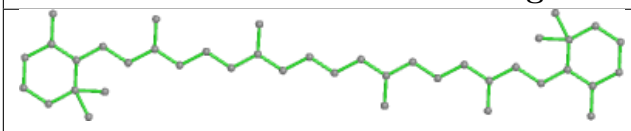


Rings

Ligand BCR 3 719



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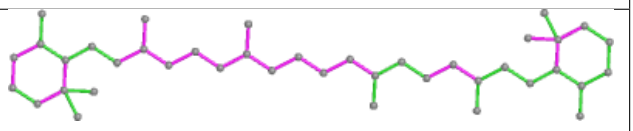

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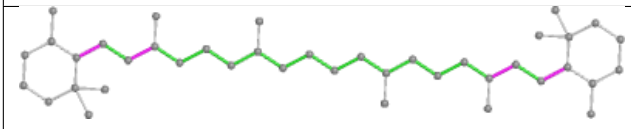
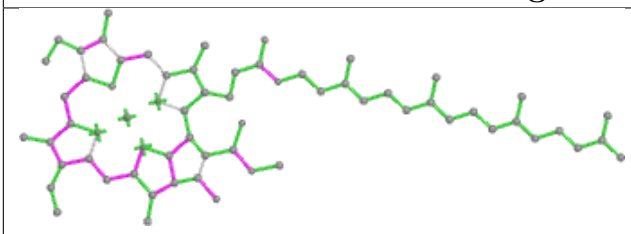


Torsions

Rings

Ligand CLA 1 613



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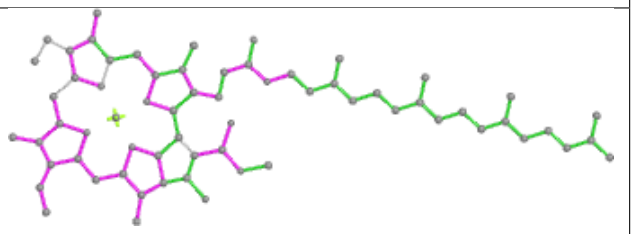
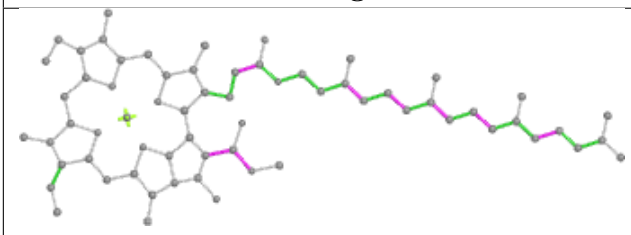


Bond angles



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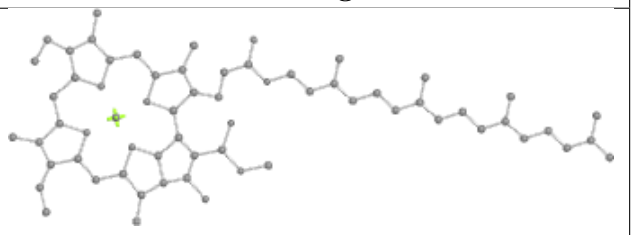

Rings

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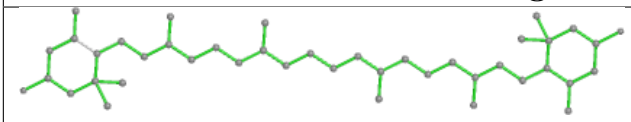

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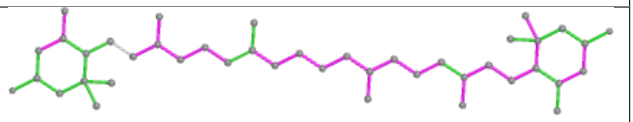
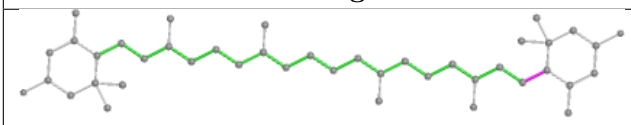


Bond angles



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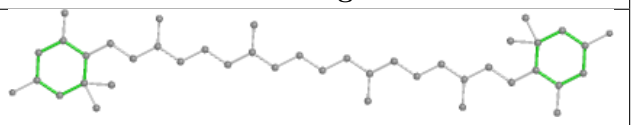
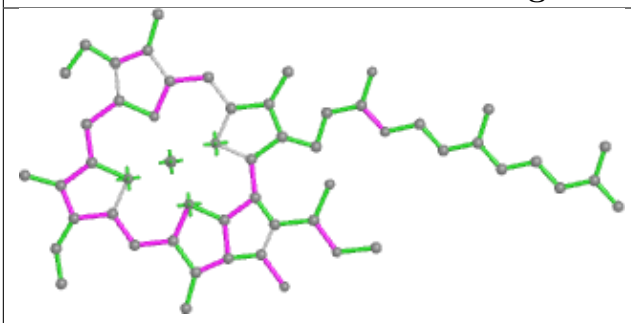


Rings

Ligand CLA 6 611



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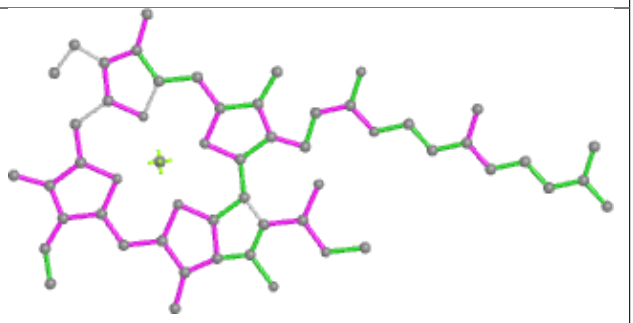
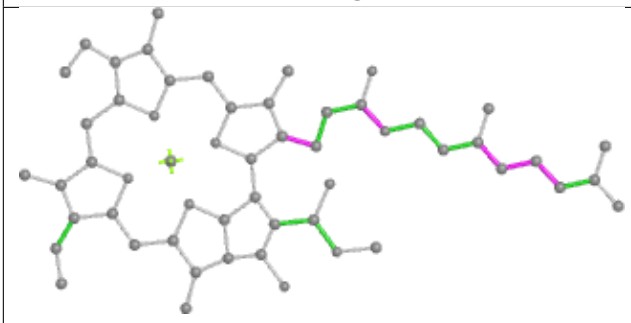


Bond angles



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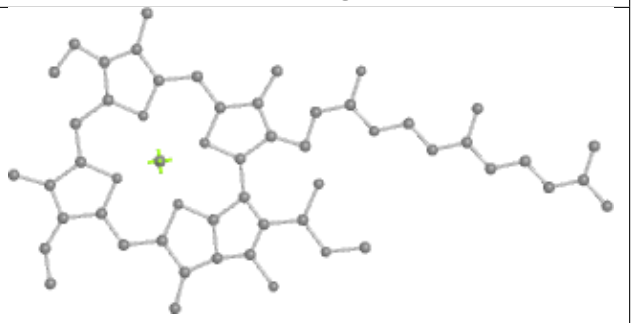

Rings

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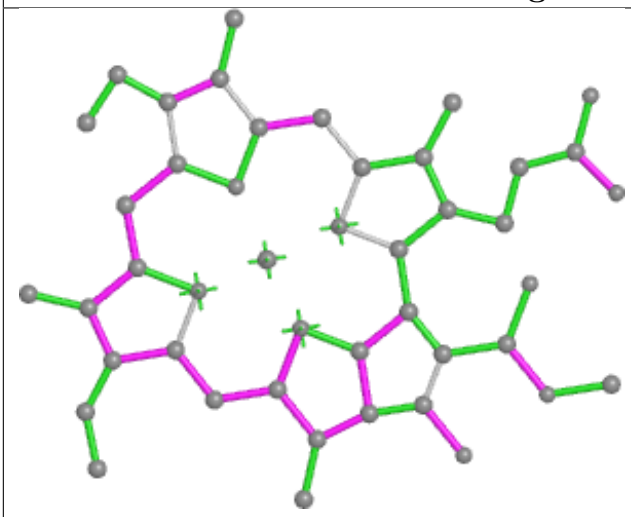

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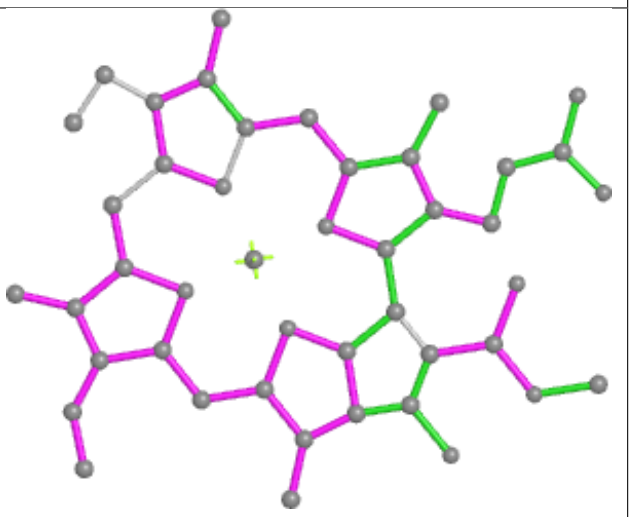
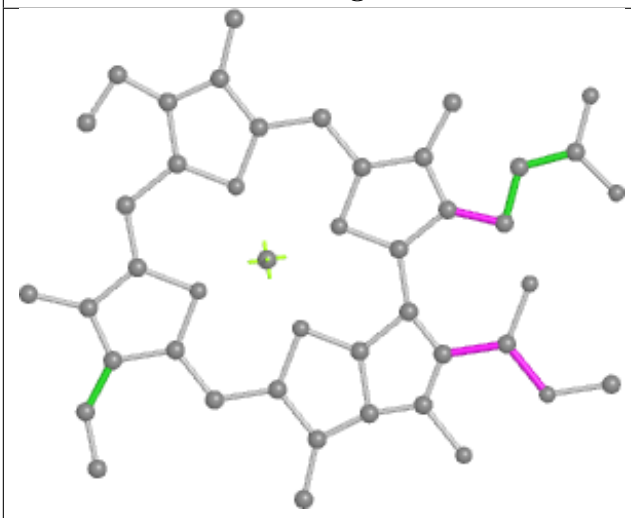
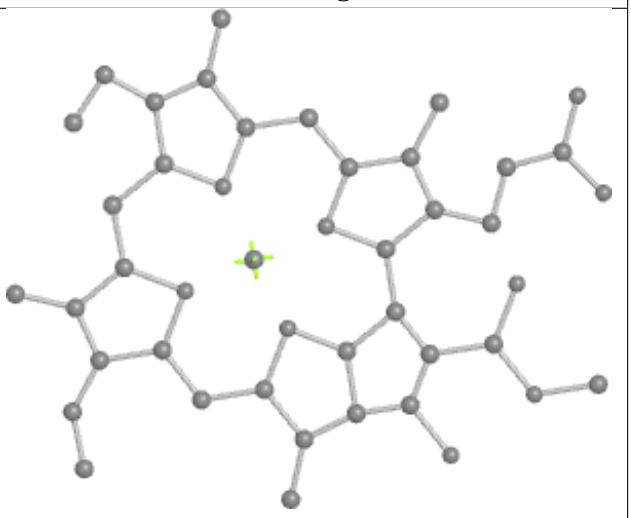


Bond angles

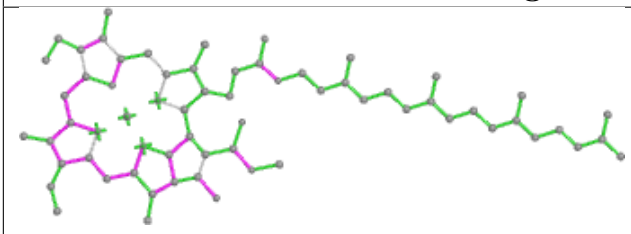


Torsions



Rings

Ligand CLA A 811



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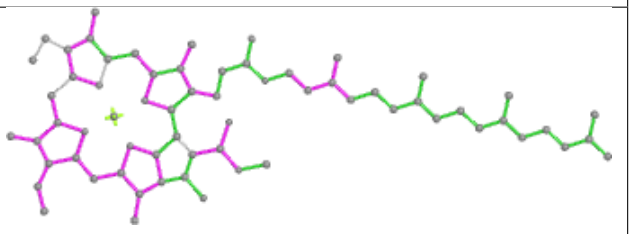
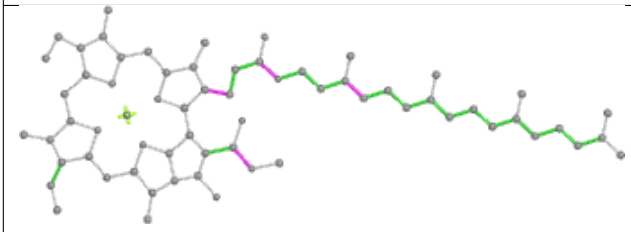


Bond angles



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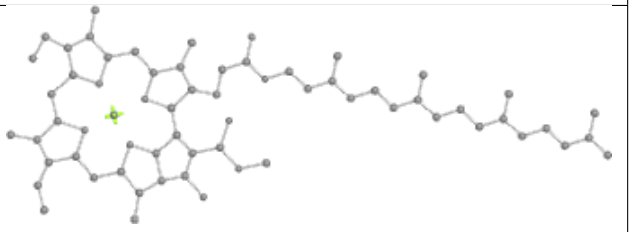
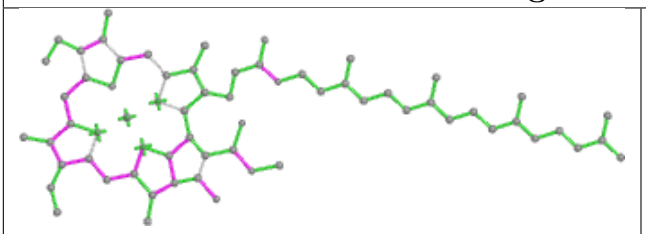


Rings

Ligand CLA 1 602



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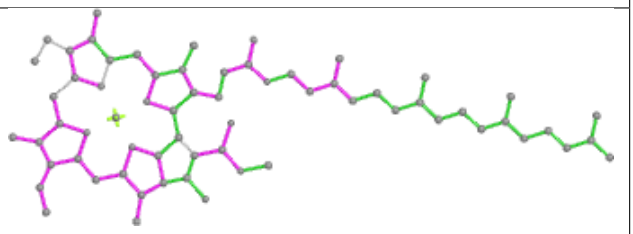
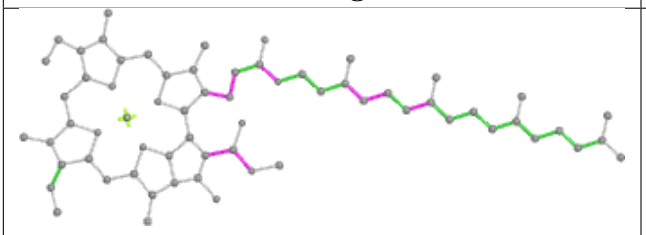


Bond angles



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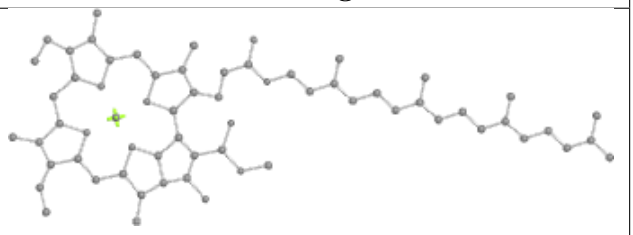
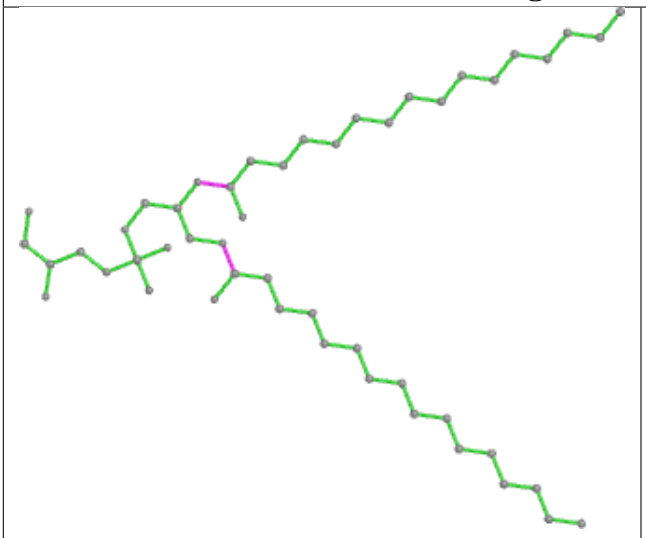


Rings

Ligand LHG 4 622



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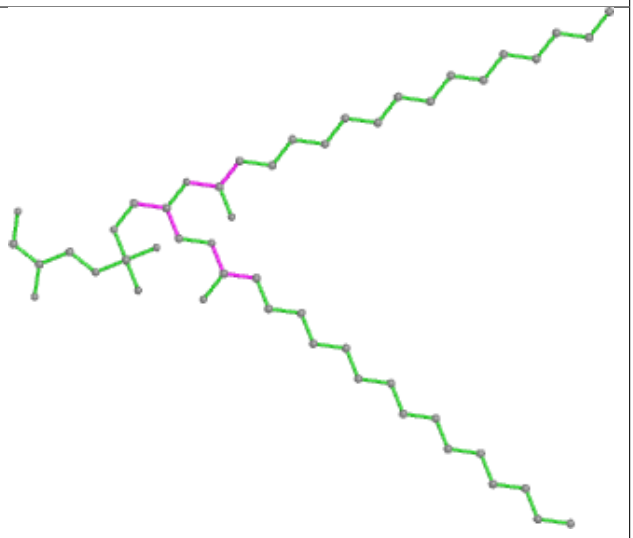
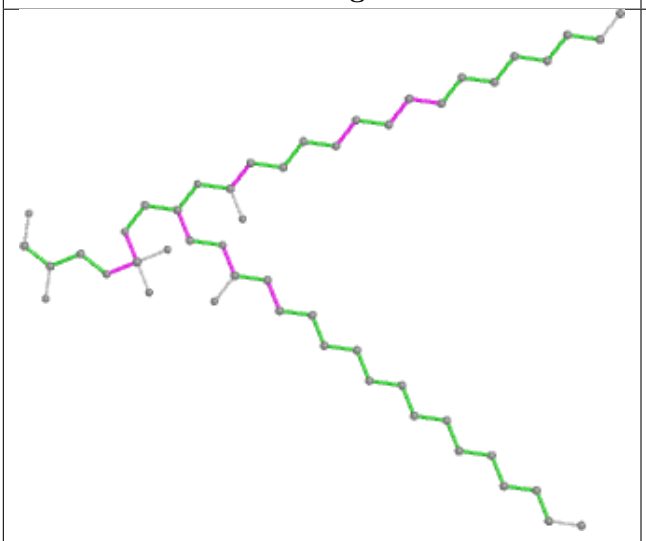


Bond angles



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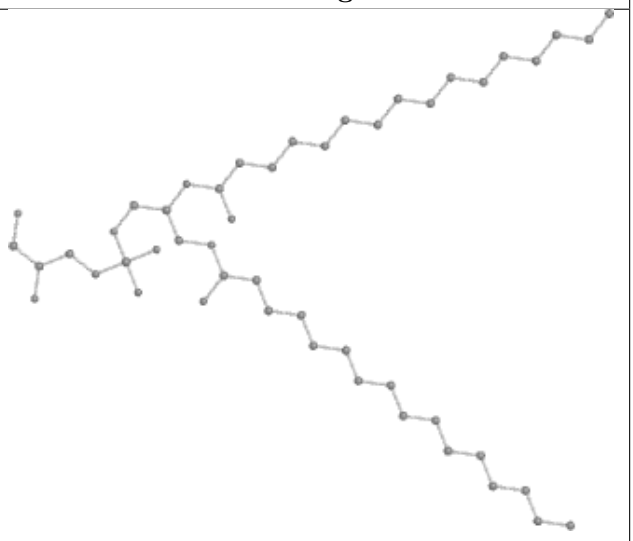
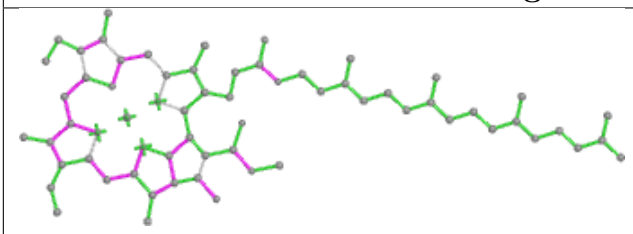
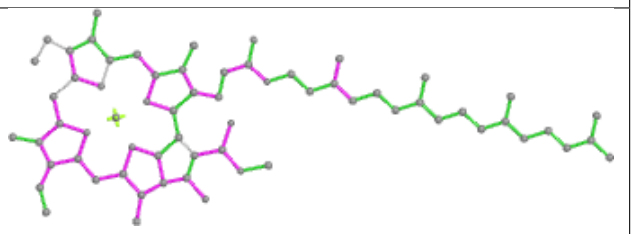


Rings

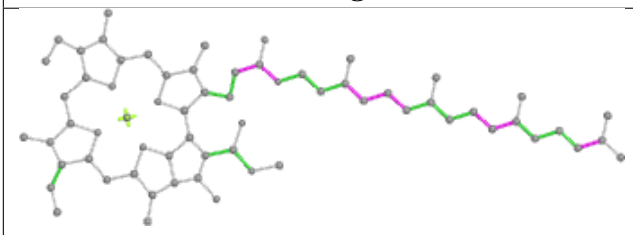
Ligand CLA A 828



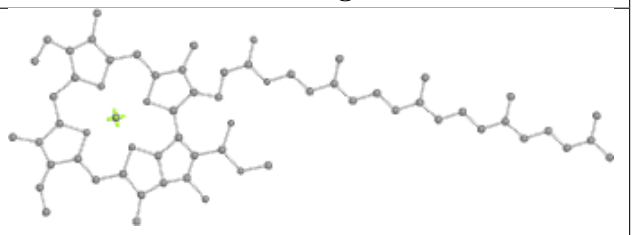
Bond lengths



Bond angles

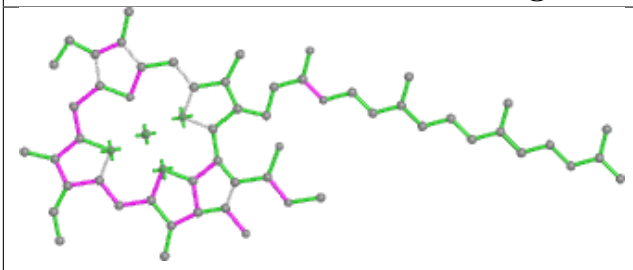


Torsions

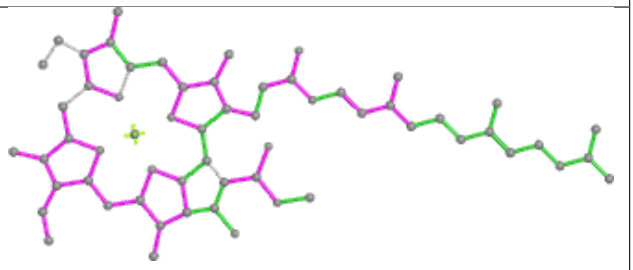


Rings

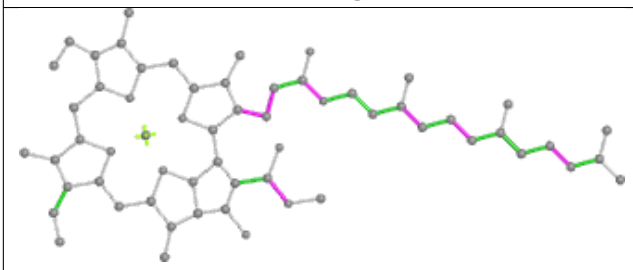
Ligand CLA 6 610



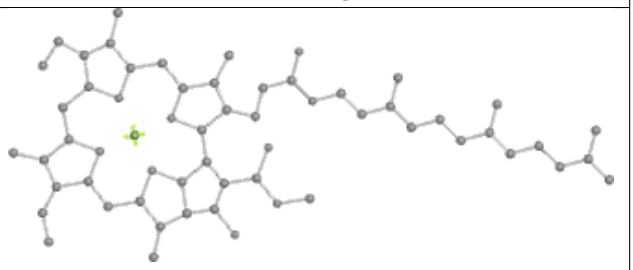
Bond lengths



Bond angles

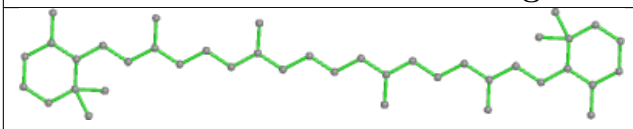


Torsions

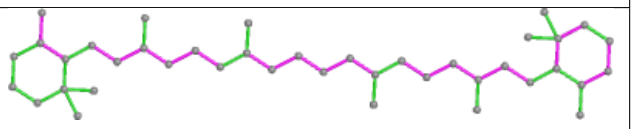


Rings

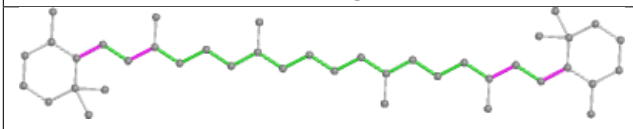
Ligand BCR B 844



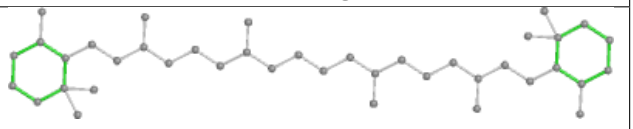
Bond lengths



Bond angles

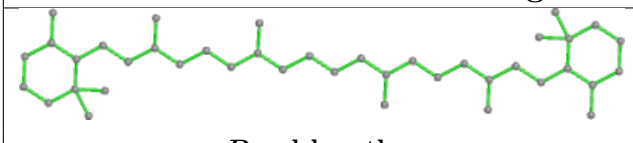


Torsions

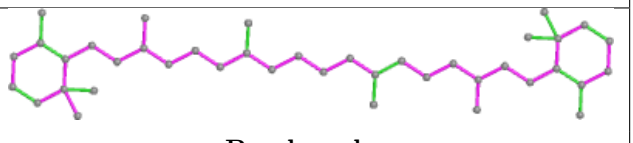


Rings

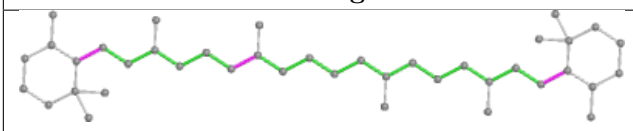
Ligand BCR 5 622



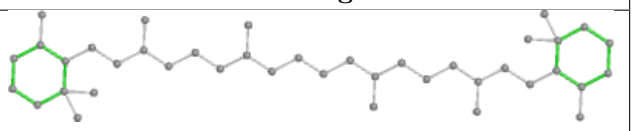
Bond lengths



Bond angles

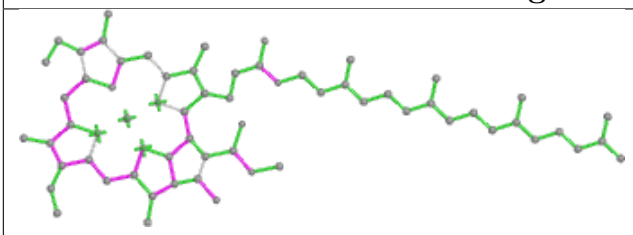


Torsions

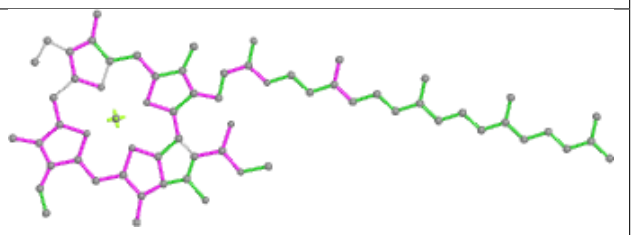


Rings

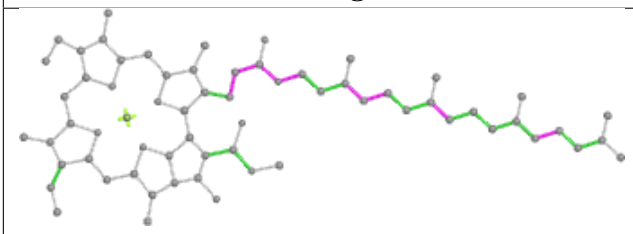
Ligand CLA 1 609



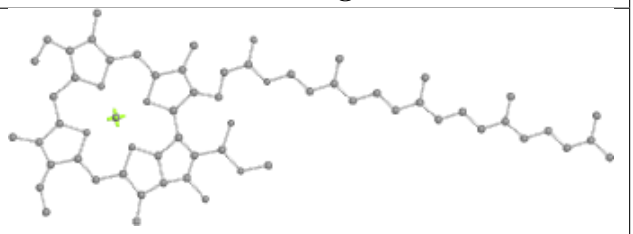
Bond lengths



Bond angles

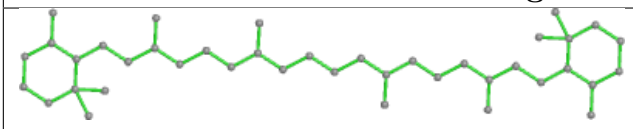


Torsions

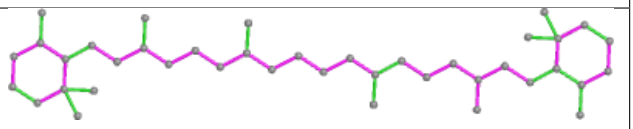


Rings

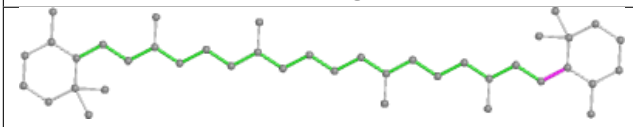
Ligand BCR 3 718



Bond lengths



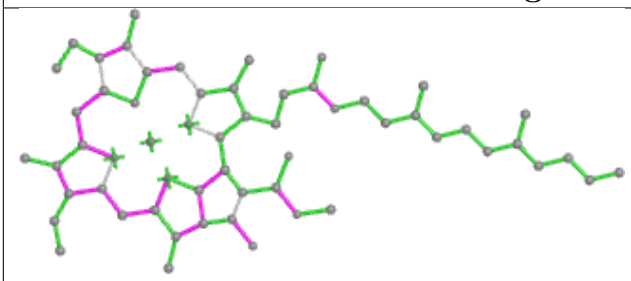
Bond angles



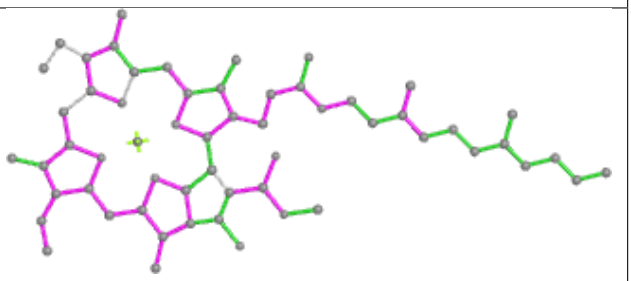
Torsions

Rings

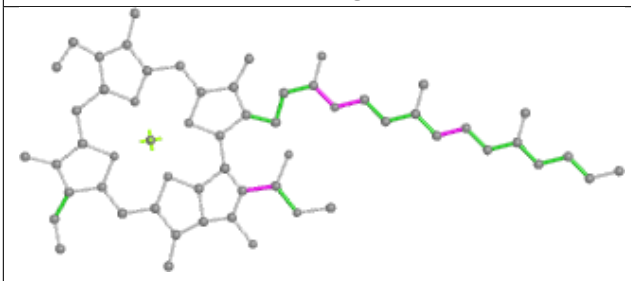
Ligand CLA B 833



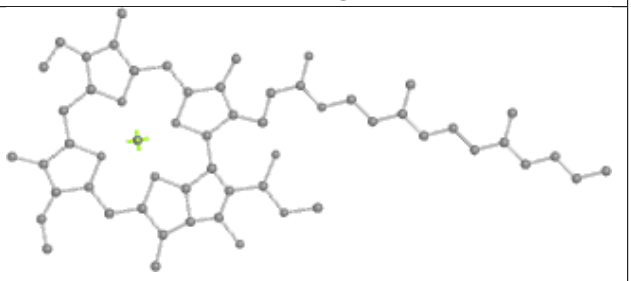
Bond lengths



Bond angles

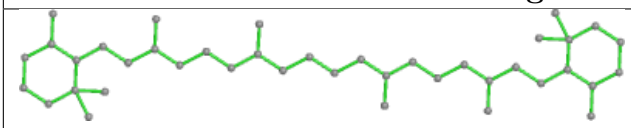


Torsions

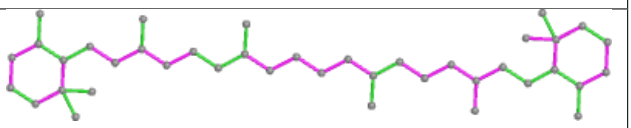


Rings

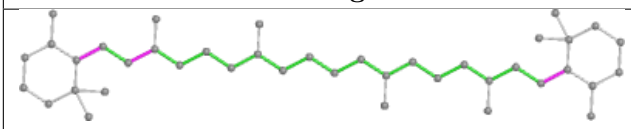
Ligand BCR 7 624



Bond lengths



Bond angles



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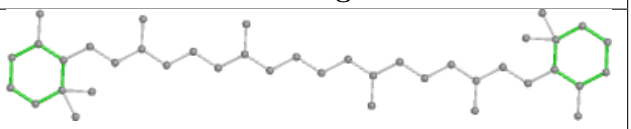
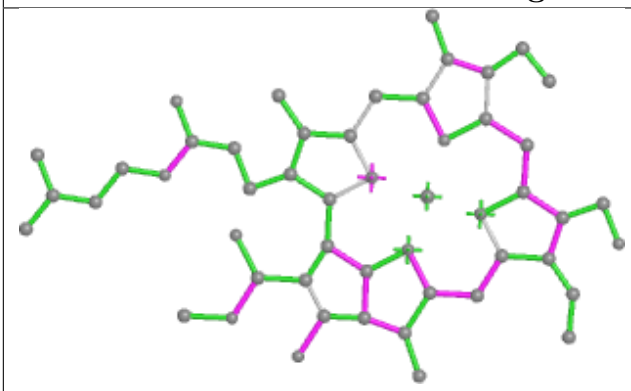
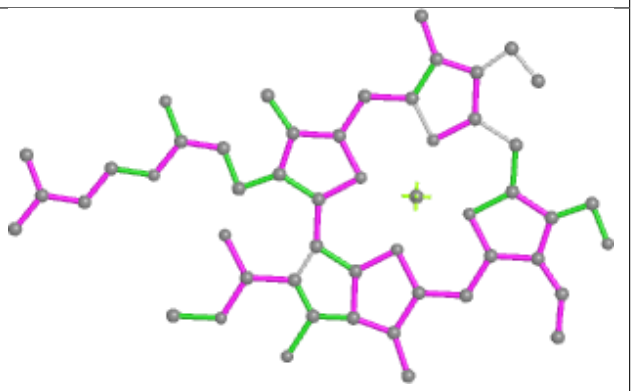


Rings

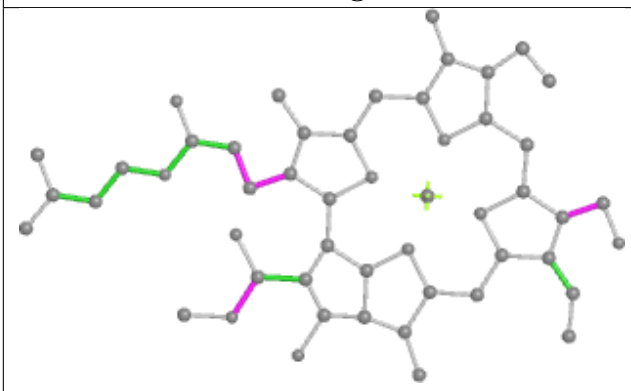
Ligand CHL 5 608



Bond lengths



Bond angles



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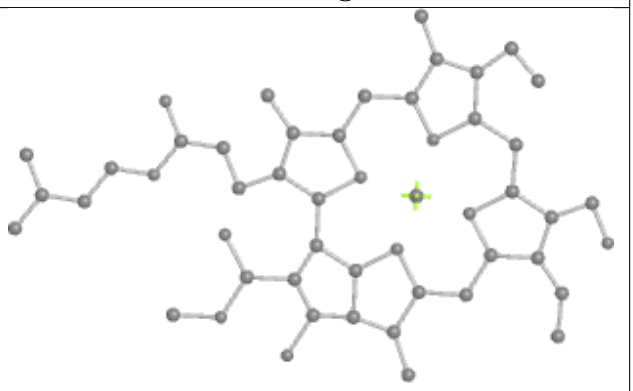
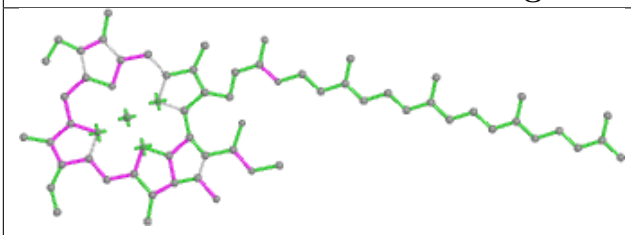
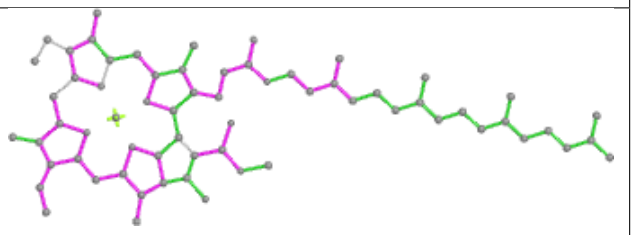


Rings

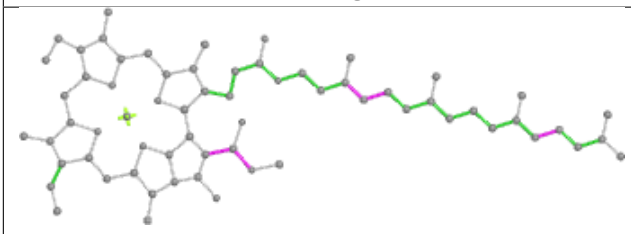
Ligand CLA B 808



Bond lengths



Bond angles



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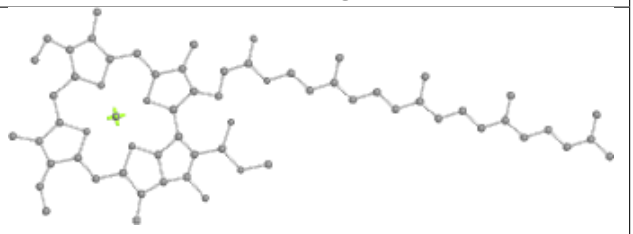
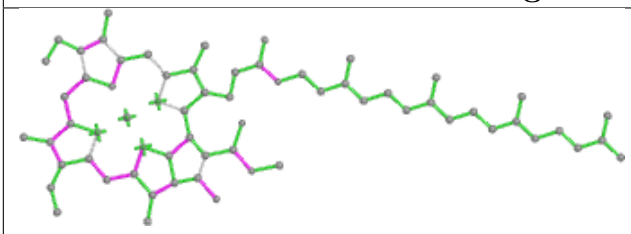
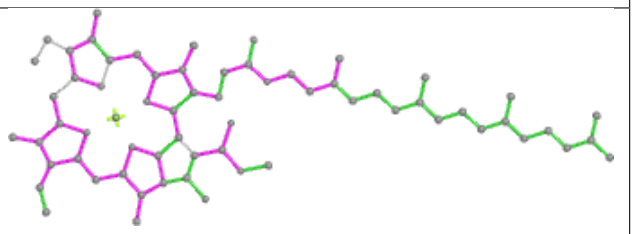
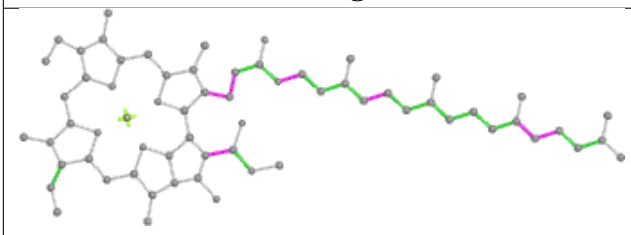
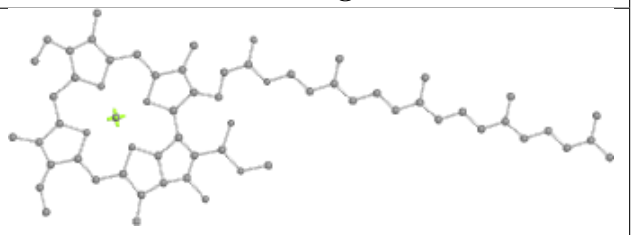
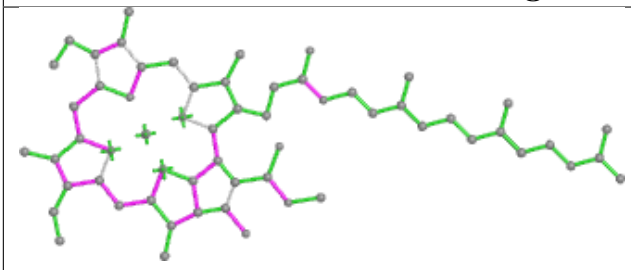
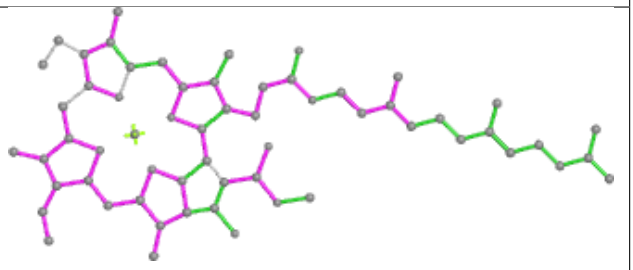
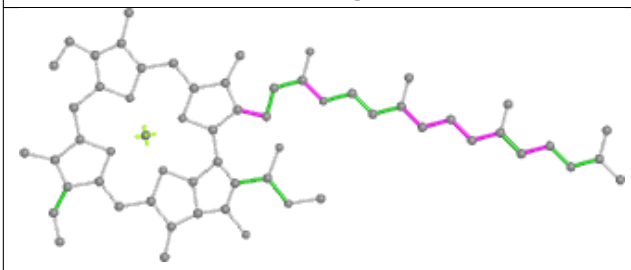
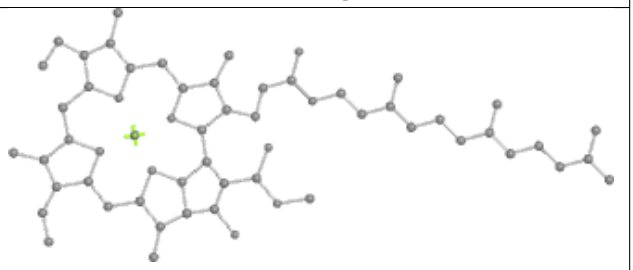
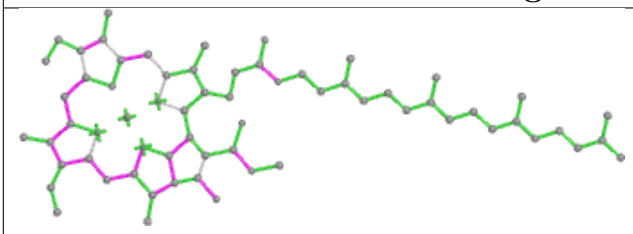


Rings

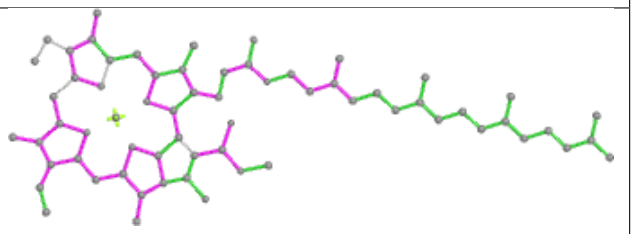
Ligand CLA A 854	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 818	
 Bond lengths	 Bond angles
 Torsions	 Rings

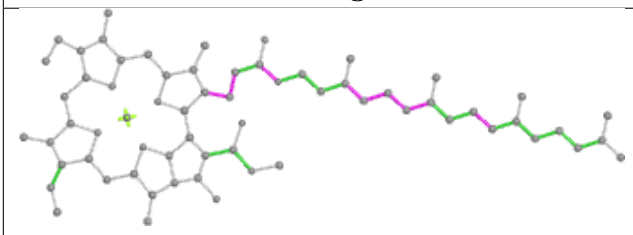
Ligand CLA B 852



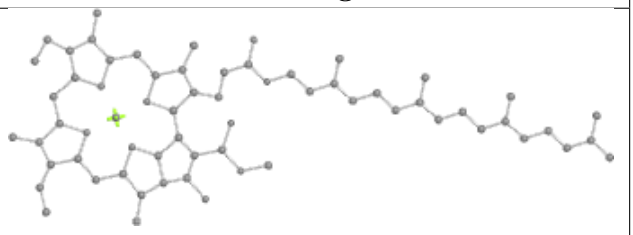
Bond lengths



Bond angles

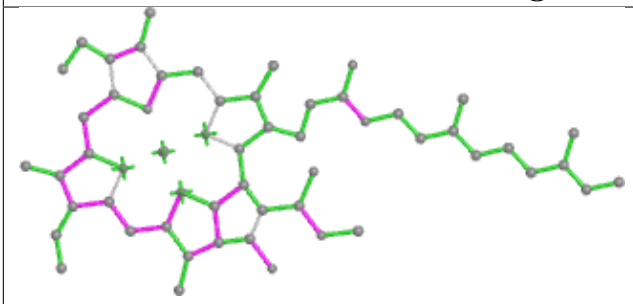


Torsions

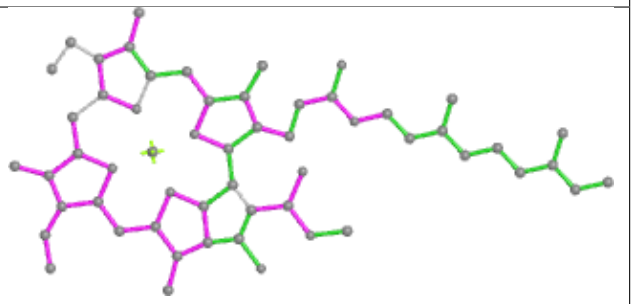


Rings

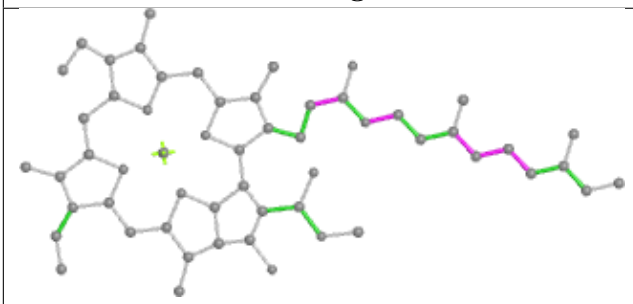
Ligand CLA 5 613



Bond lengths



Bond angles



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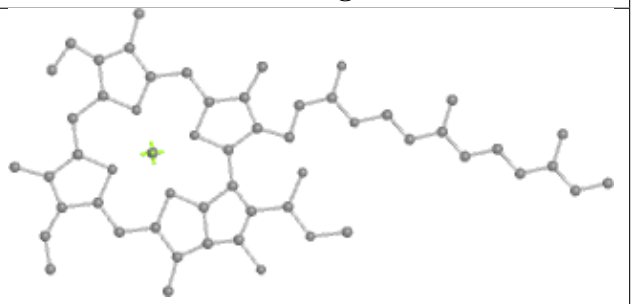
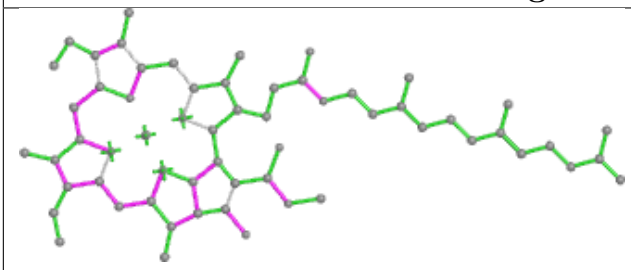
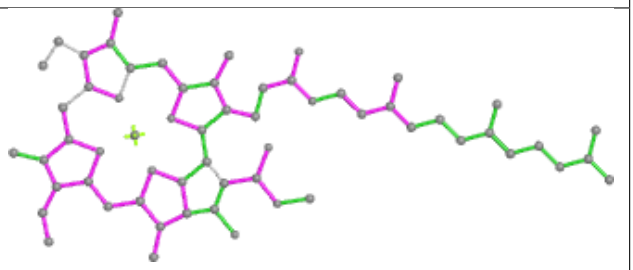


Rings

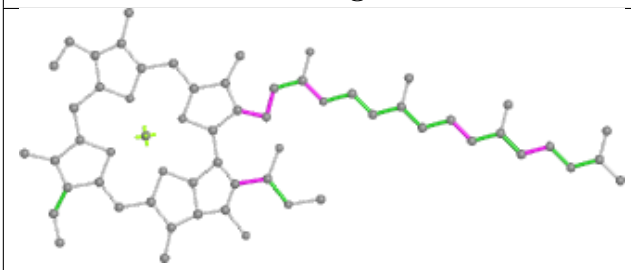
Ligand CLA 4 610



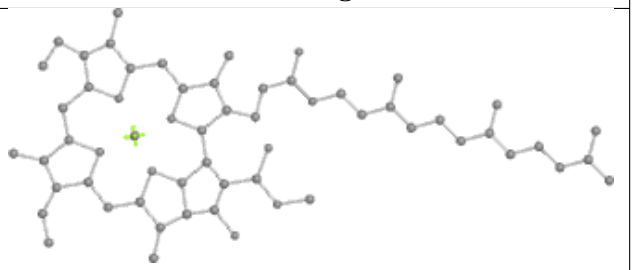
Bond lengths



Bond angles

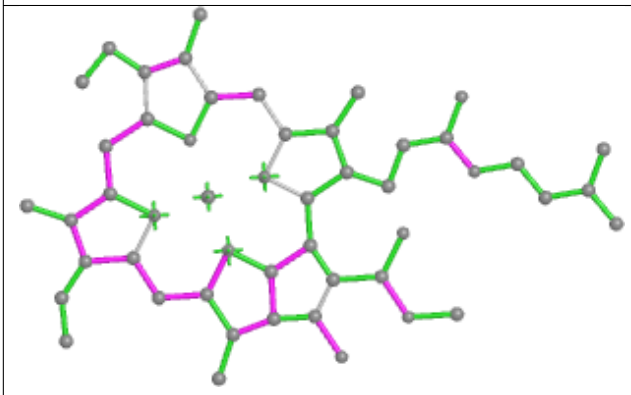


Torsions

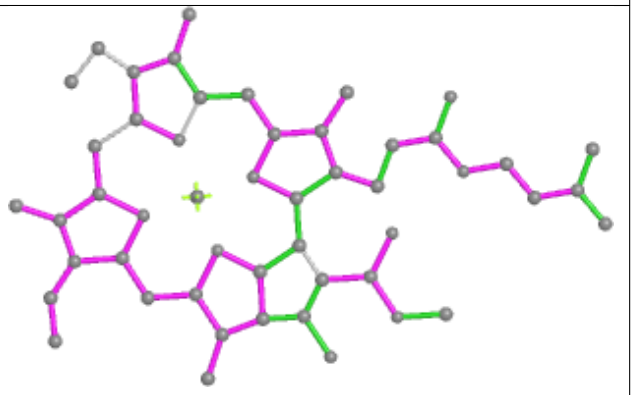


Rings

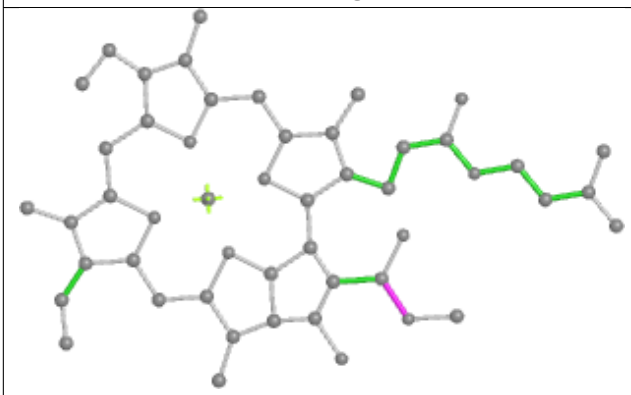
Ligand CLA A 836



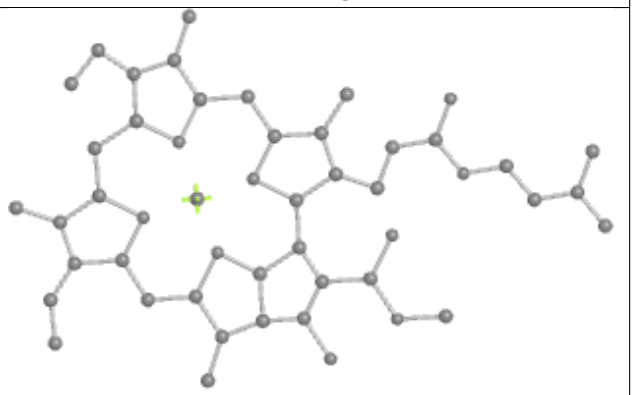
Bond lengths



Bond angles

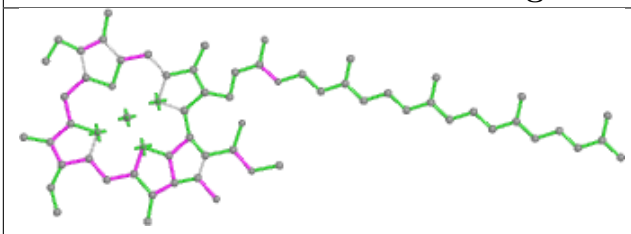


Torsions

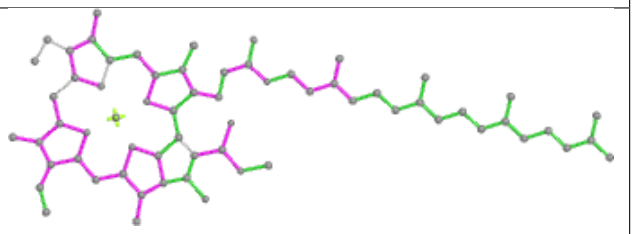


Rings

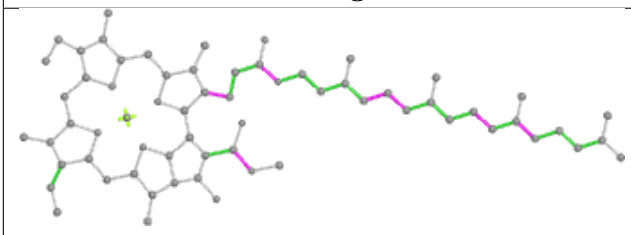
Ligand CLA Z 611



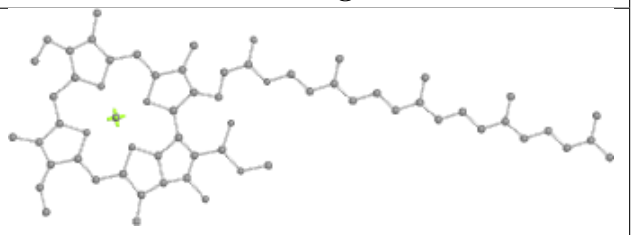
Bond lengths



Bond angles

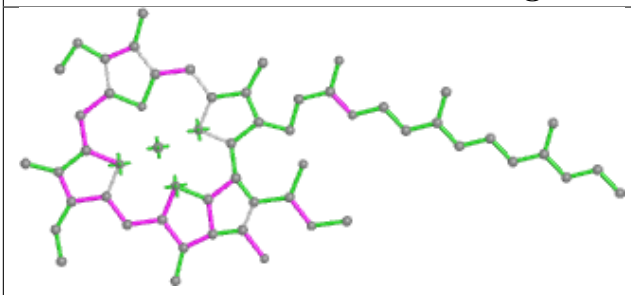


Torsions

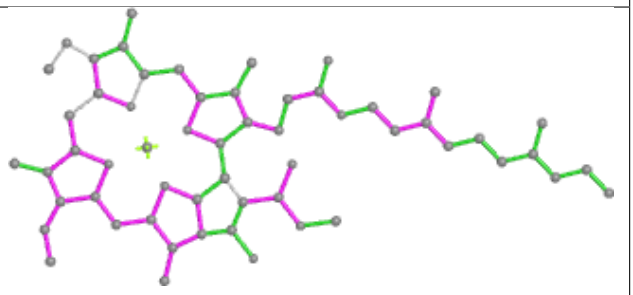


Rings

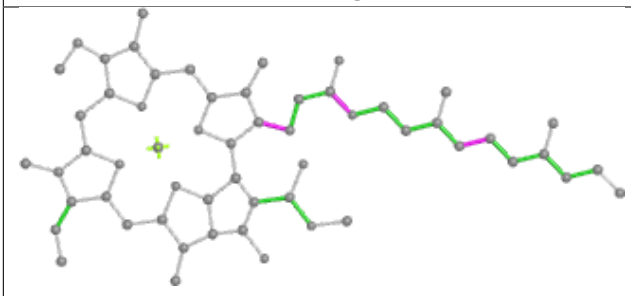
Ligand CLA A 817



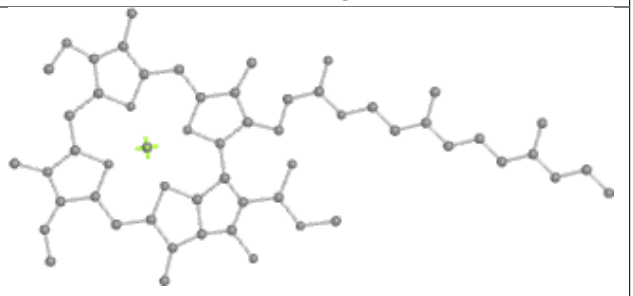
Bond lengths



Bond angles

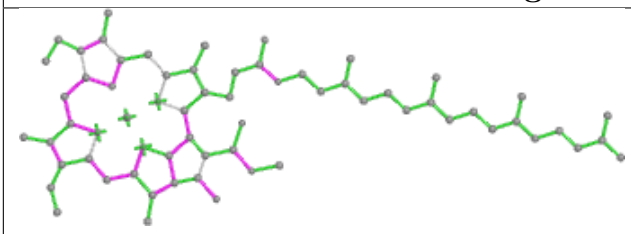


Torsions

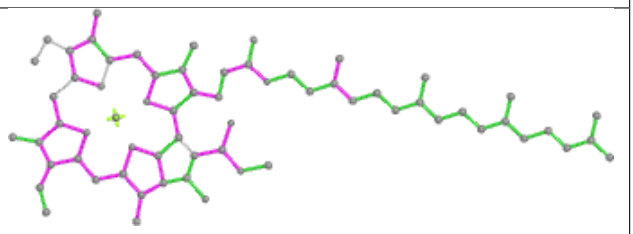


Rings

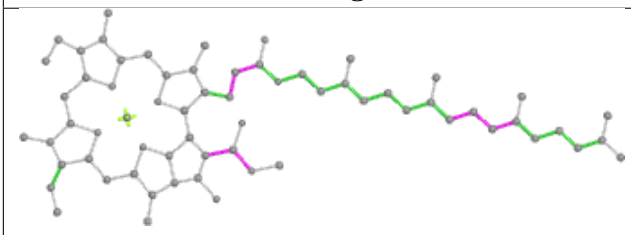
Ligand CLA B 803



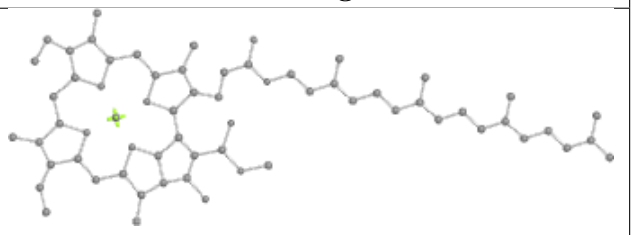
Bond lengths



Bond angles

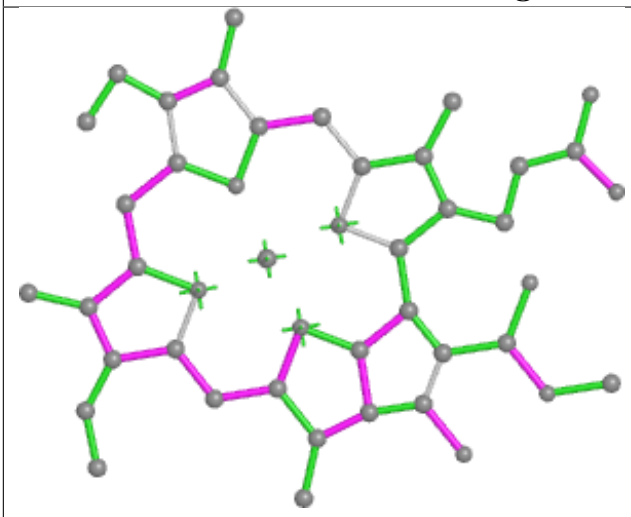


Torsions

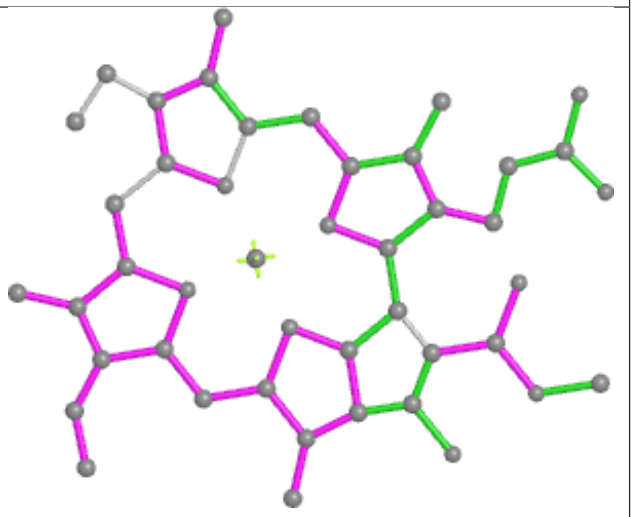


Rings

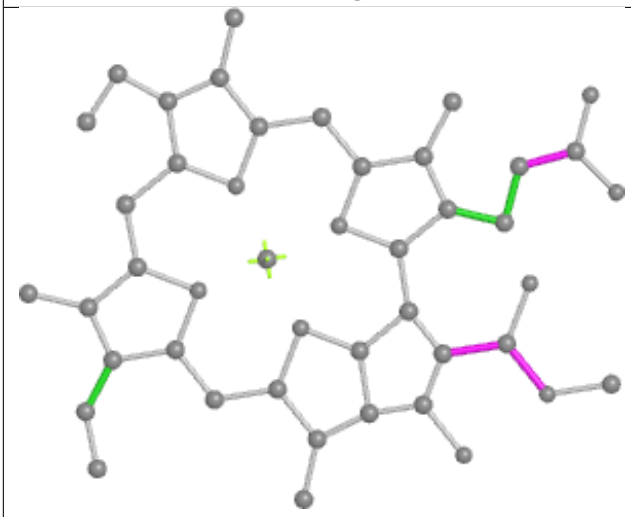
Ligand CLA K 4002



Bond lengths



Bond angles



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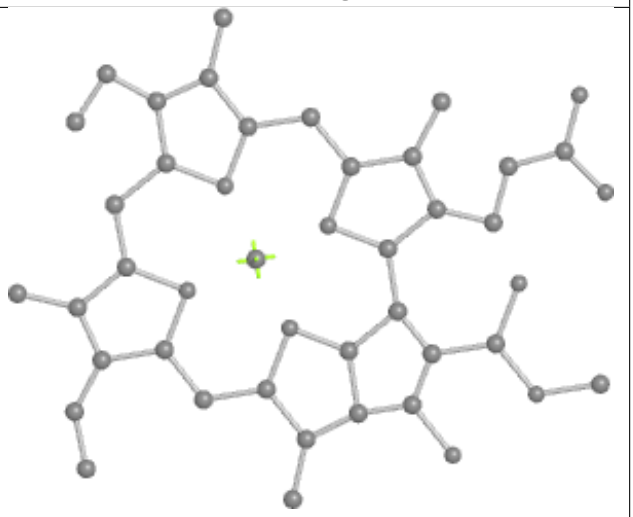
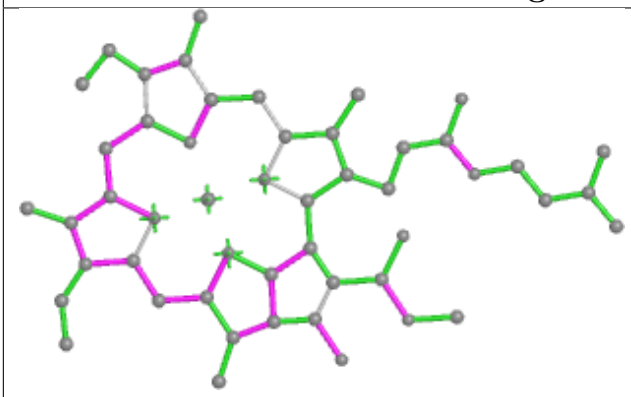


Rings

Ligand CLA 3 609



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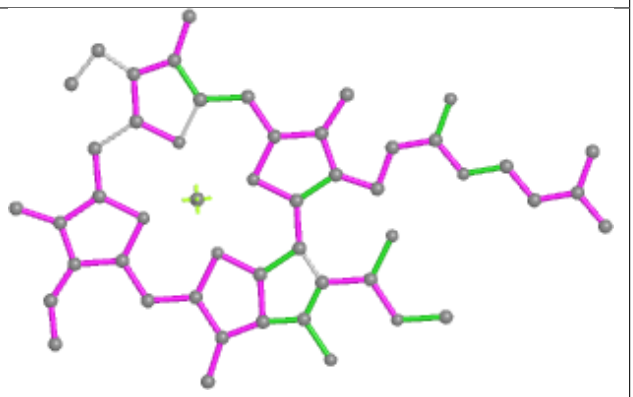
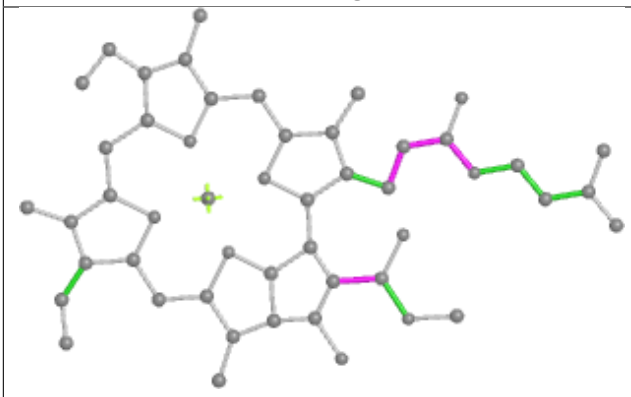


Bond angles



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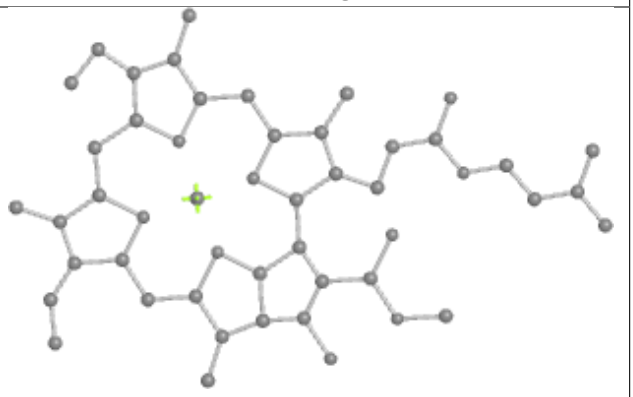
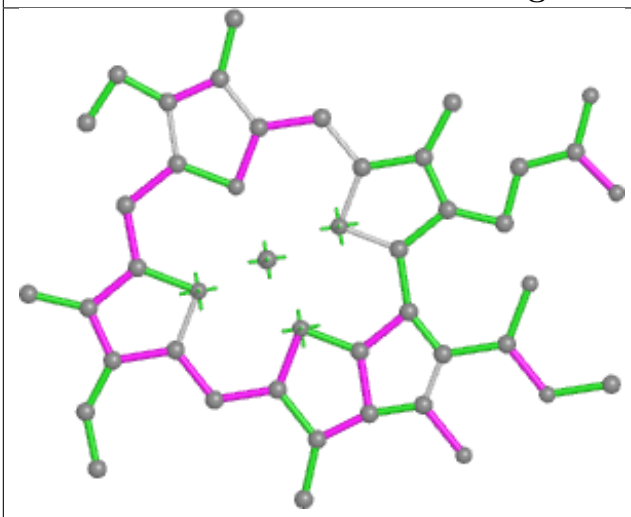


Rings

Ligand CLA 8 603



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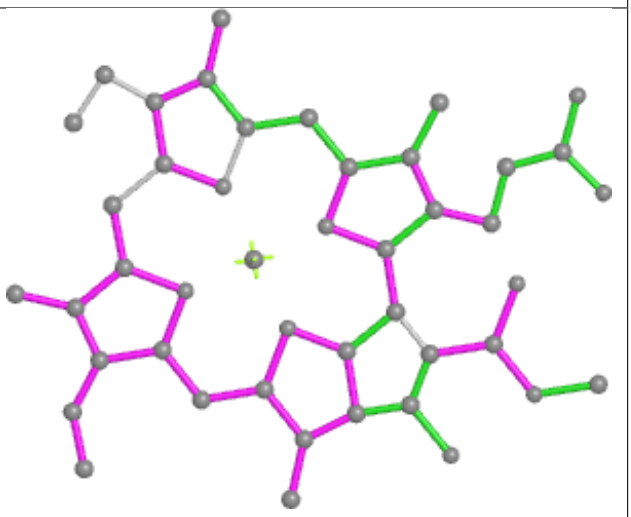
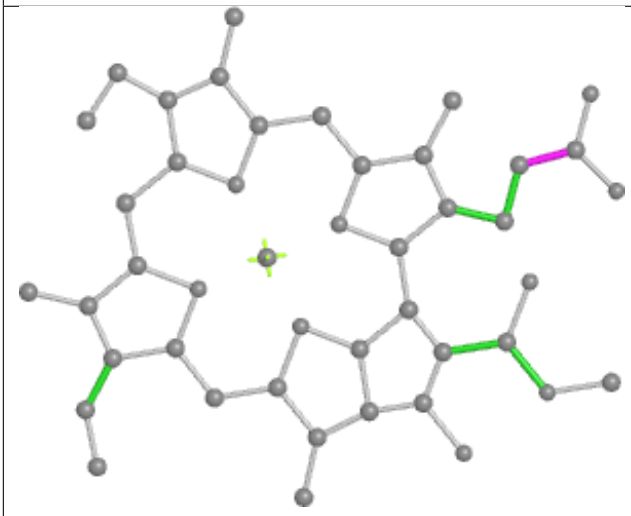


Bond angles



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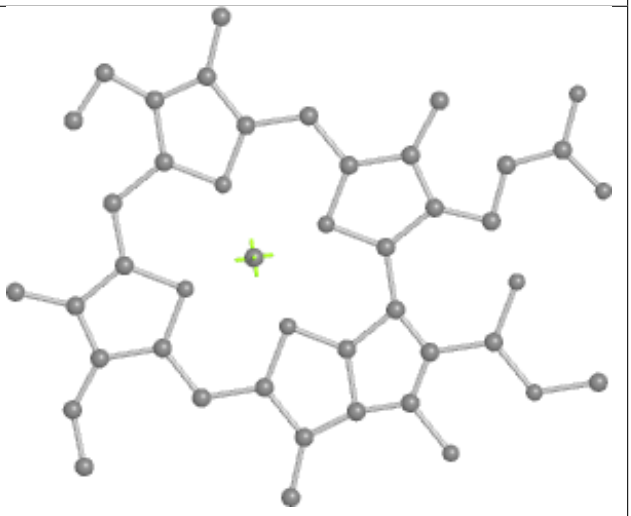
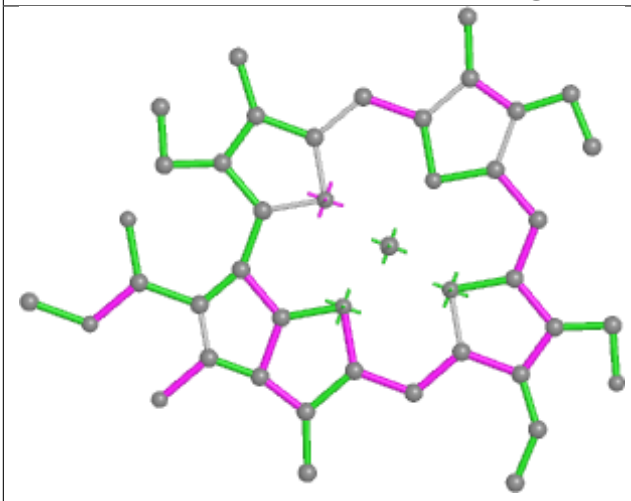


Rings

Ligand CHL 4 618



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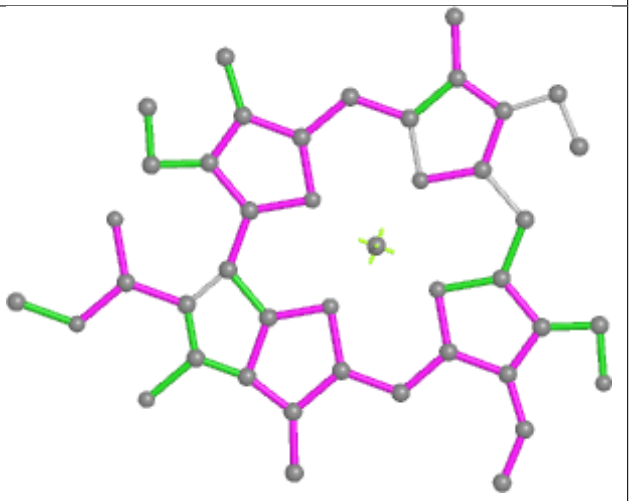
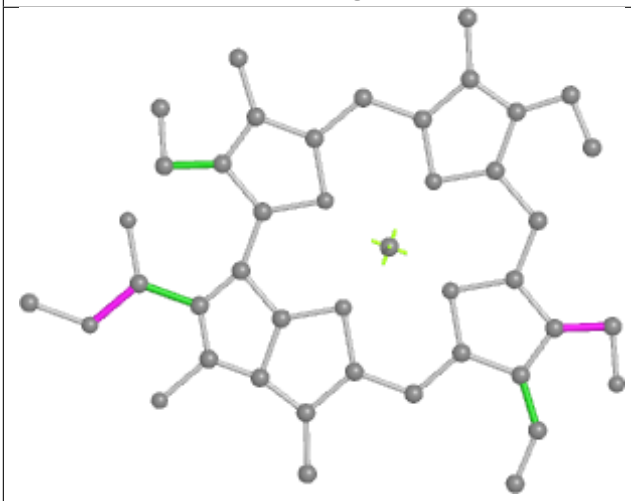


Bond angles



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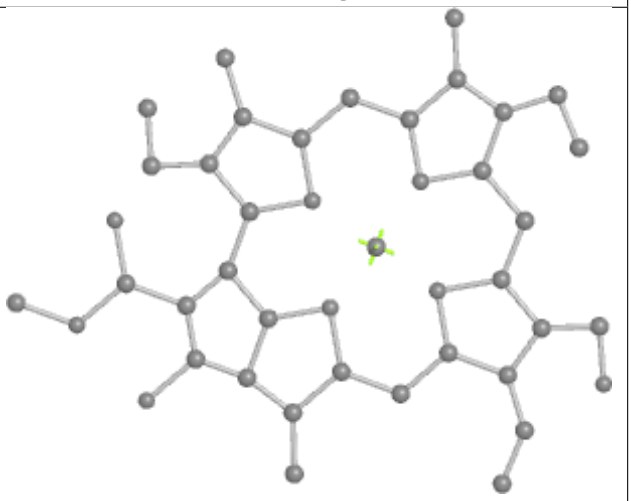

Rings

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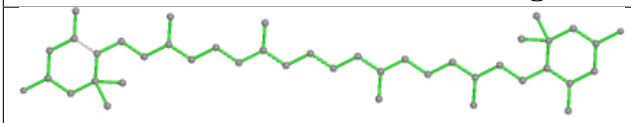

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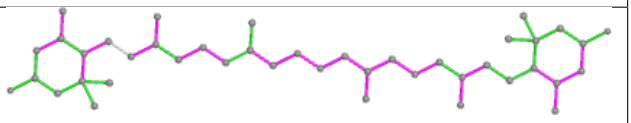
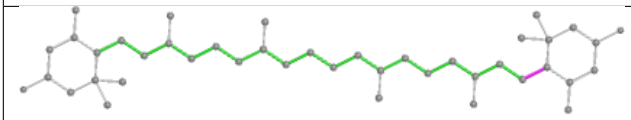


Bond angles



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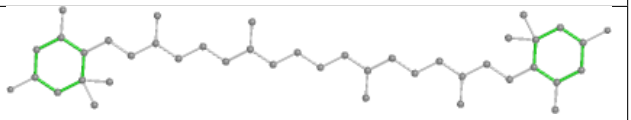
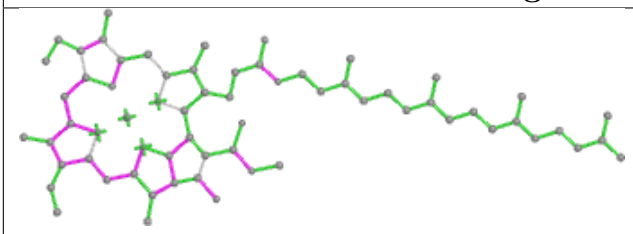


Rings

Ligand CLA A 804



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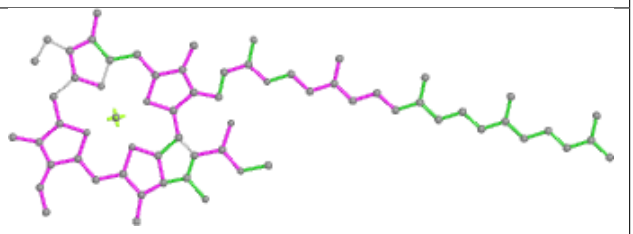
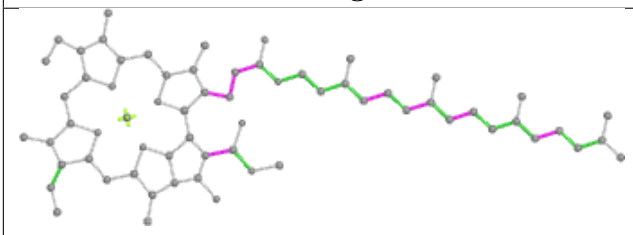
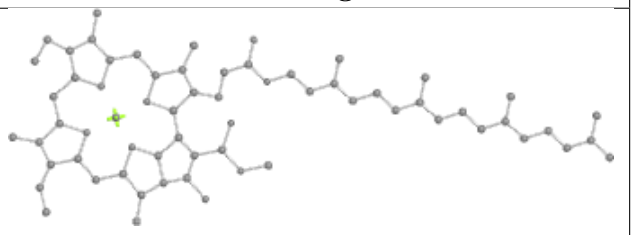


Bond angles

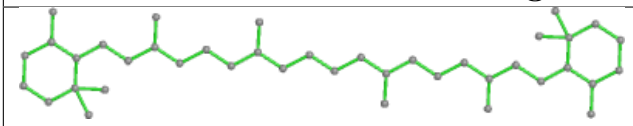


Torsions



Rings

Ligand BCR 4 621



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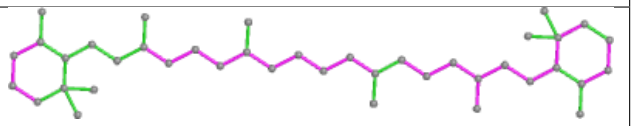
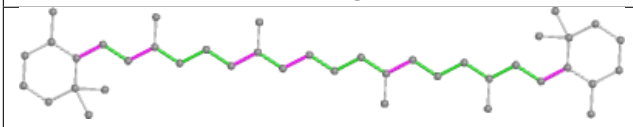


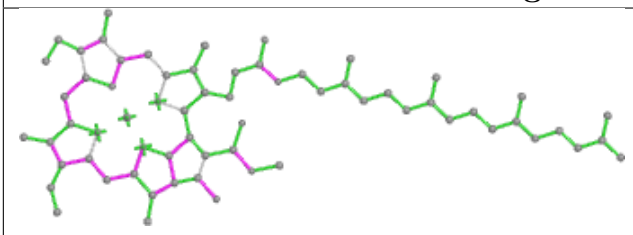
Bond angles



Torsions

Rings

Ligand CLA A 834



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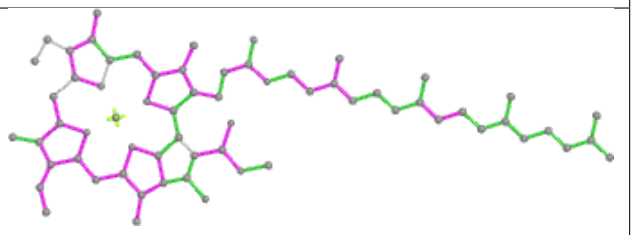
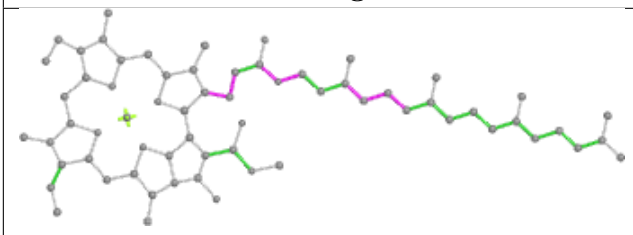


Bond angles



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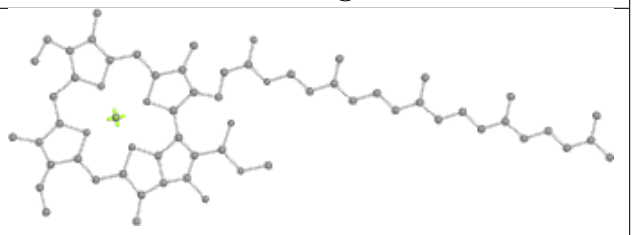
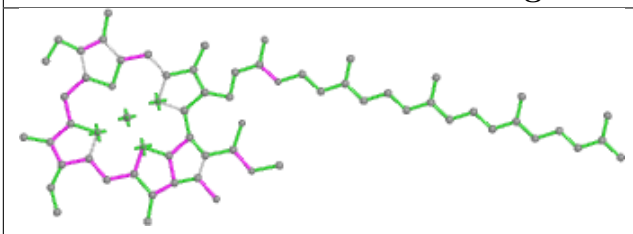


Rings

Ligand CLA B 829



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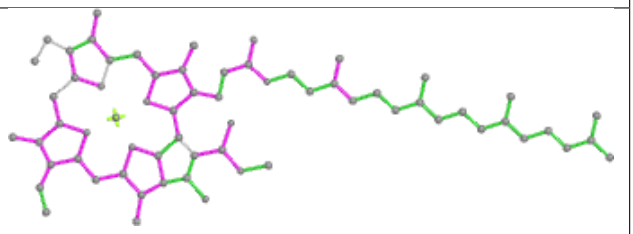
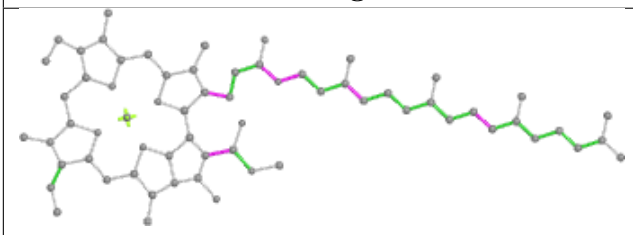


Bond angles



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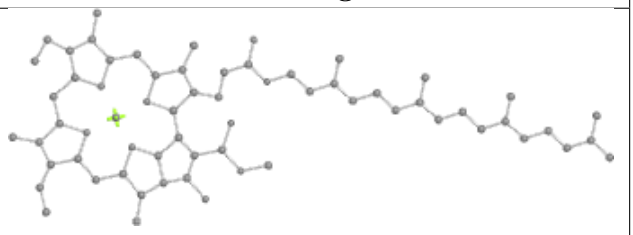
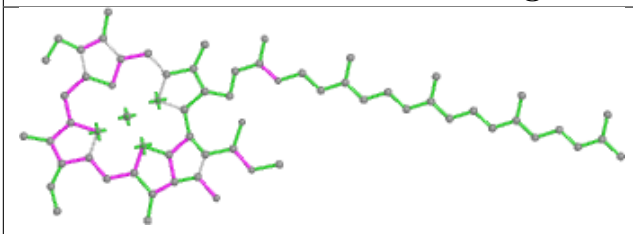
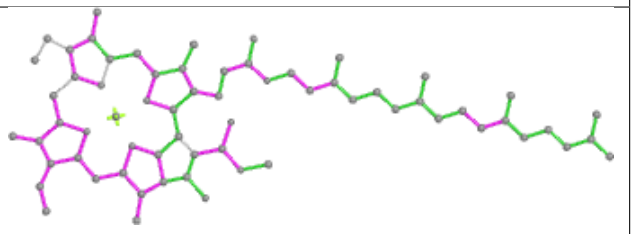


Rings

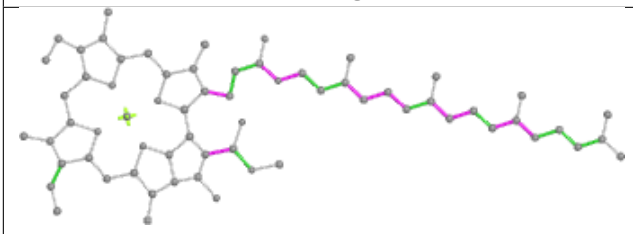
Ligand CLA A 807



Bond lengths



Bond angles



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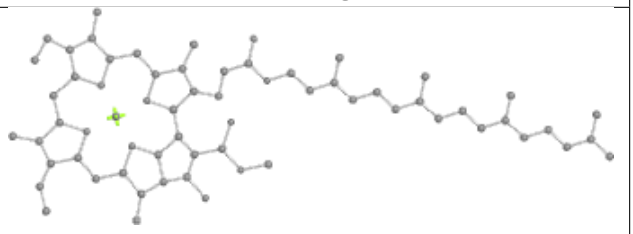
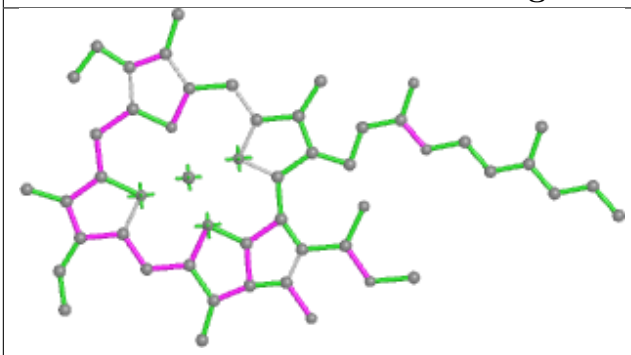
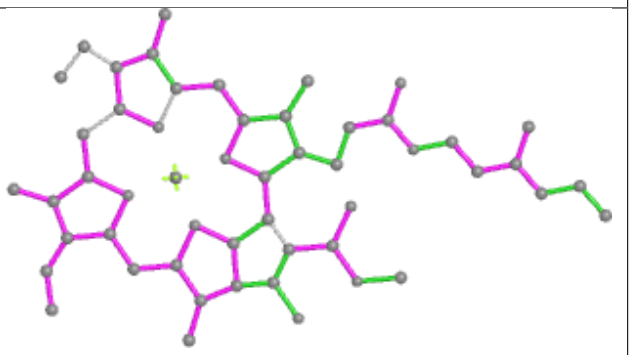
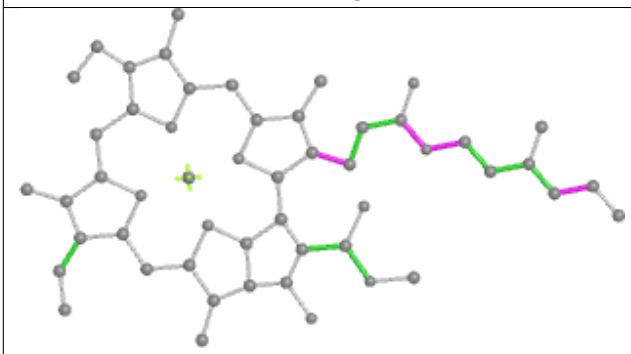
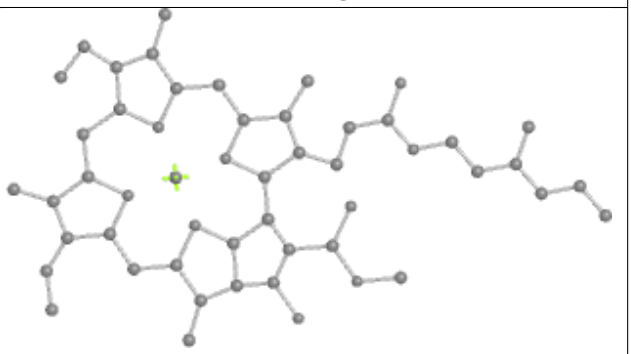
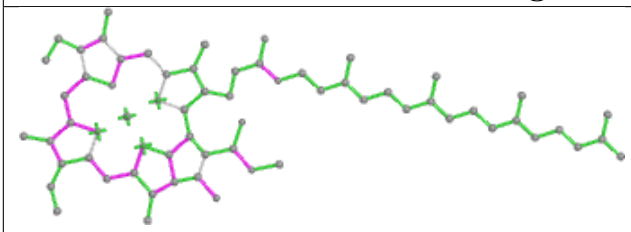
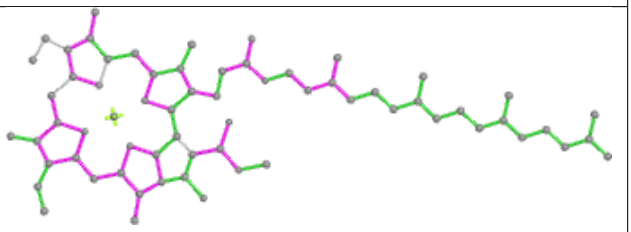
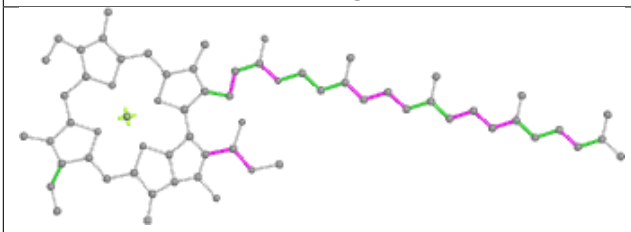
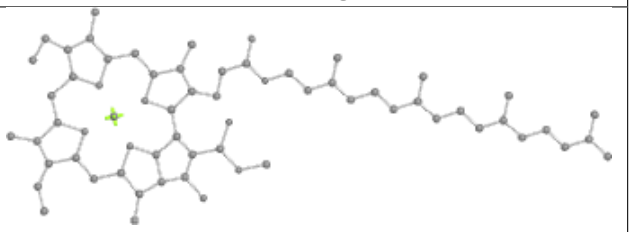
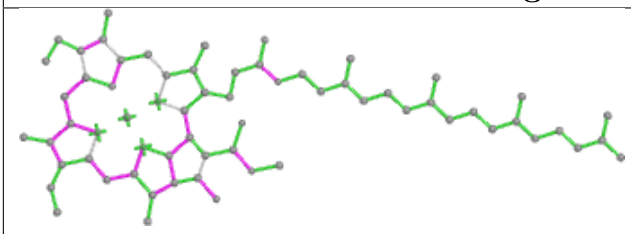


Rings

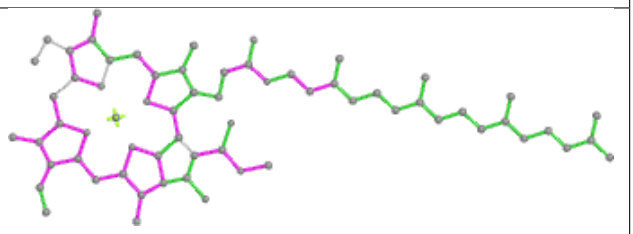
Ligand CLA 1 612	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 7 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

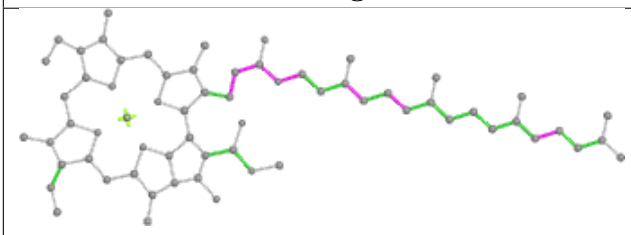
Ligand CLA A 830



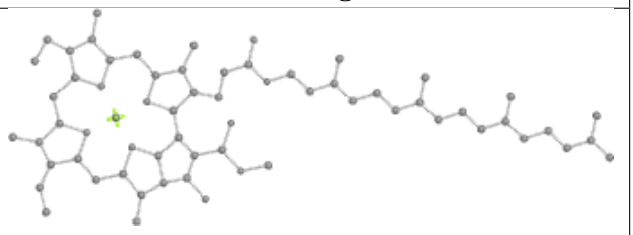
Bond lengths



Bond angles

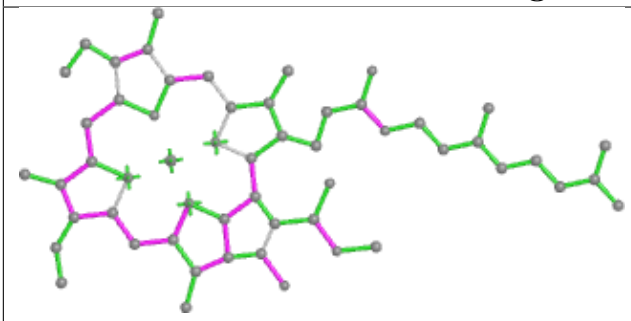


Torsions

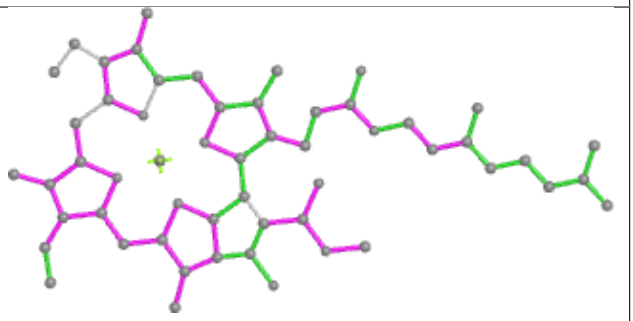


Rings

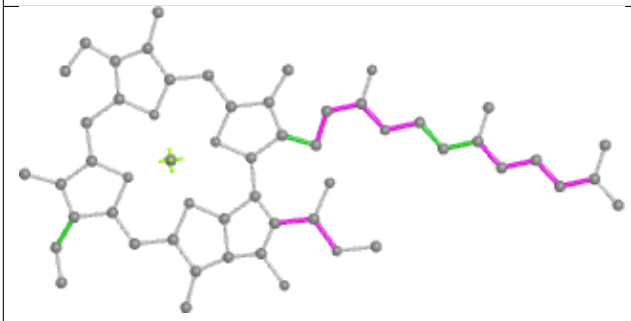
Ligand CLA 3 613



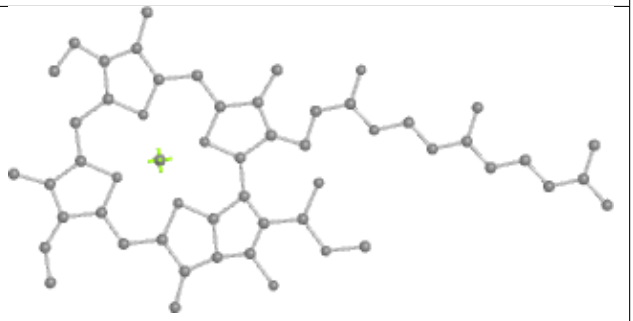
Bond lengths



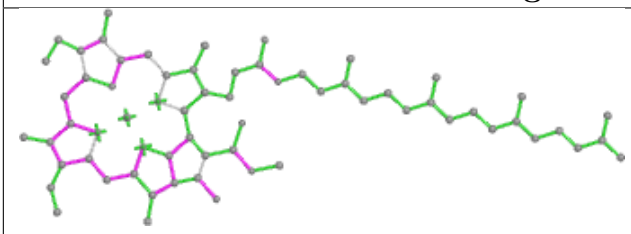
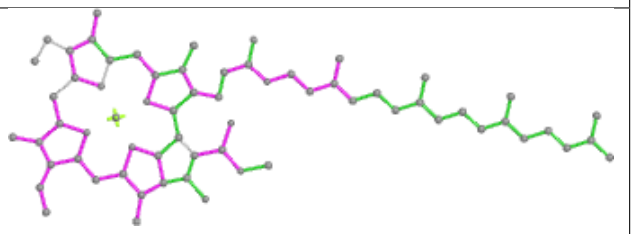
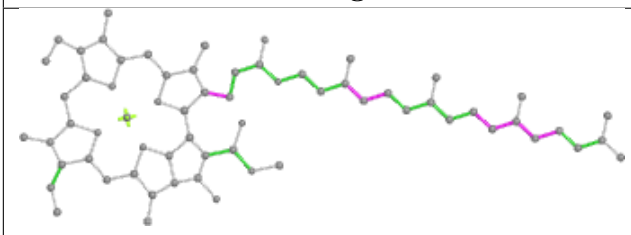
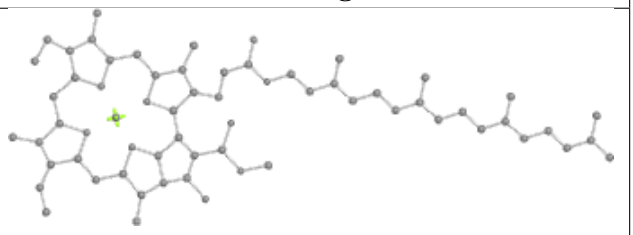
Bond angles

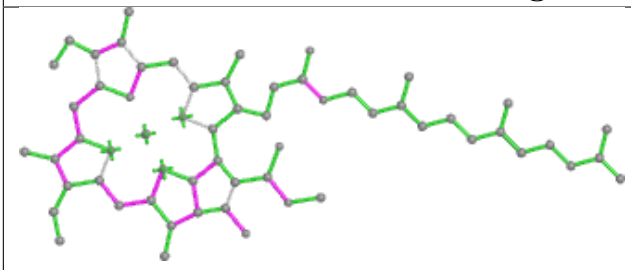
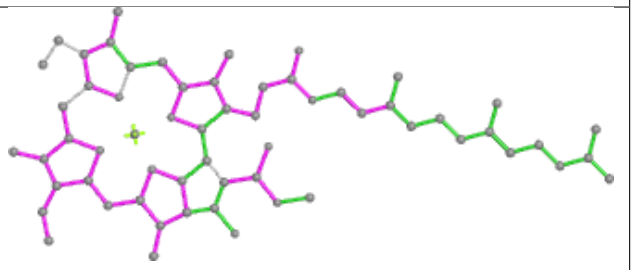
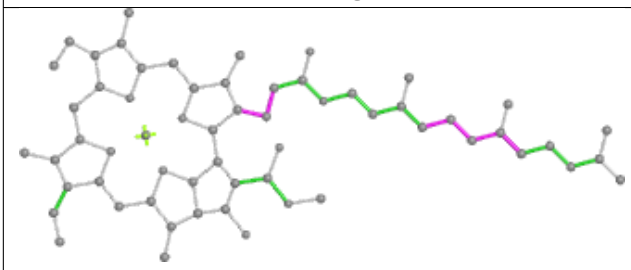
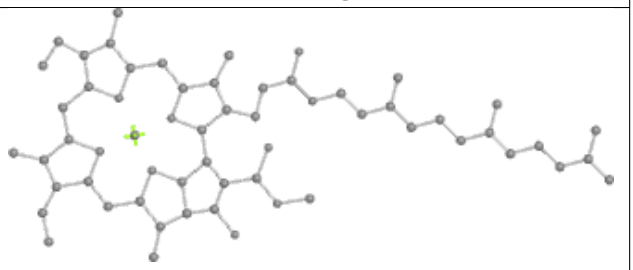


Torsions

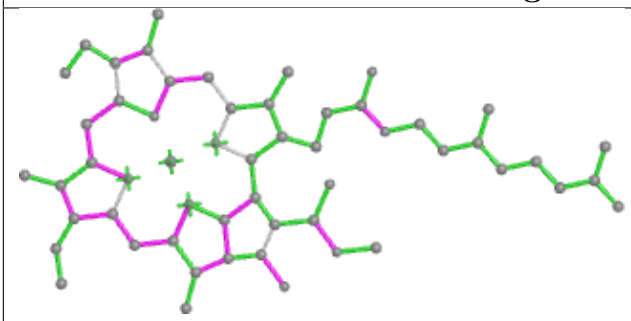


Rings

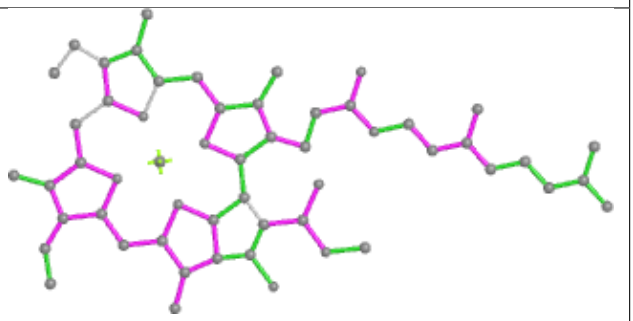
Ligand CLA A 808	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 1 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

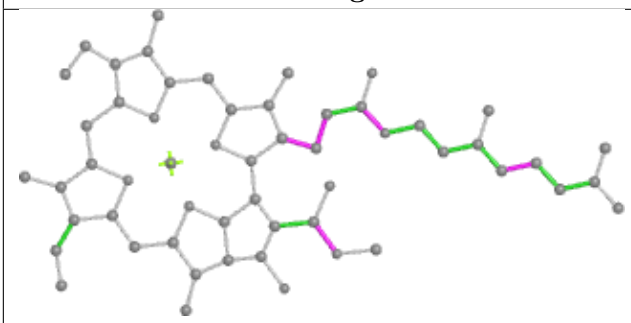
Ligand CLA A 825



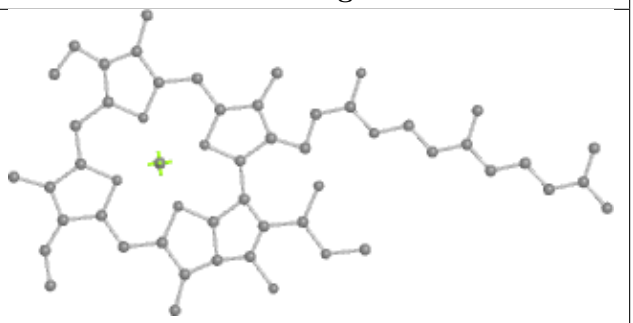
Bond lengths



Bond angles

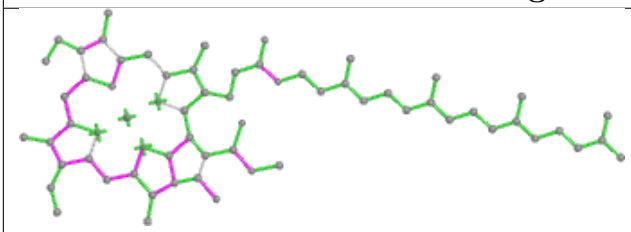


Torsions



Rings

Ligand CLA 1 611



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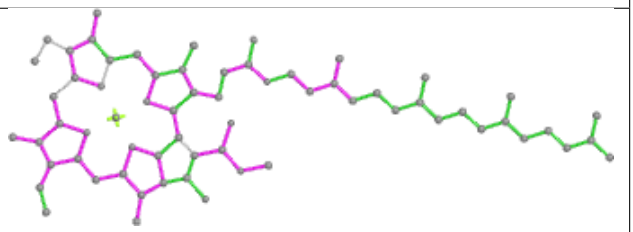
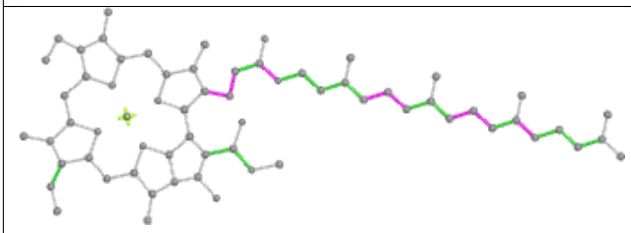


Bond angles



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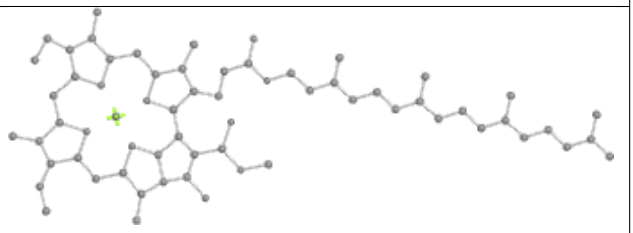
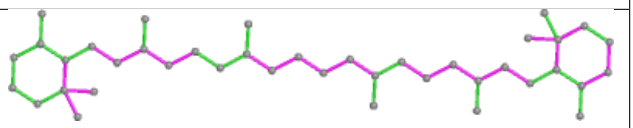


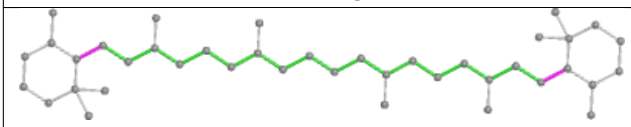
Rings

Ligand BCR A 848

Bond lengths



Bond angles



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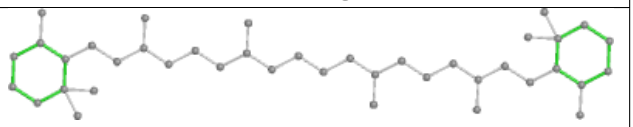
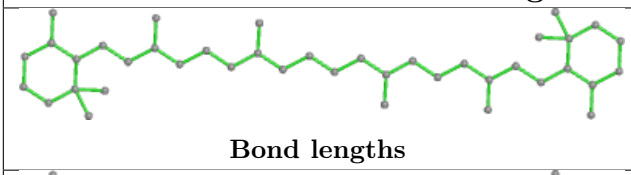


Rings

Ligand BCR 6 625



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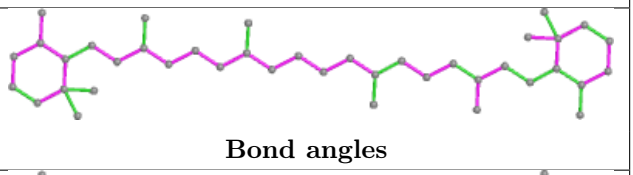
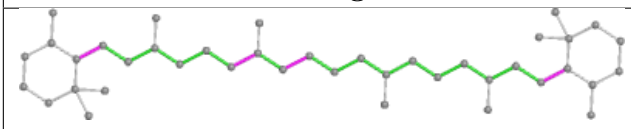


Bond angles



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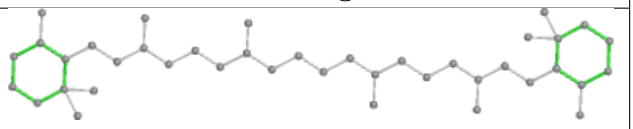
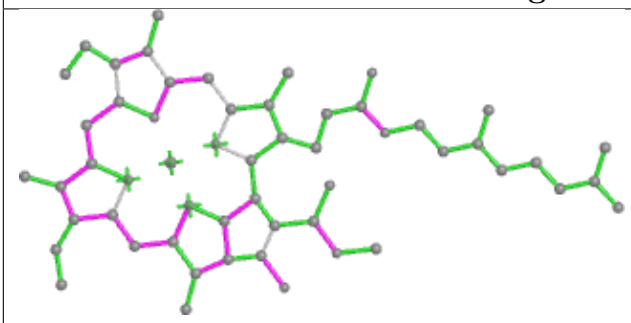


Rings

Ligand CLA 8 614



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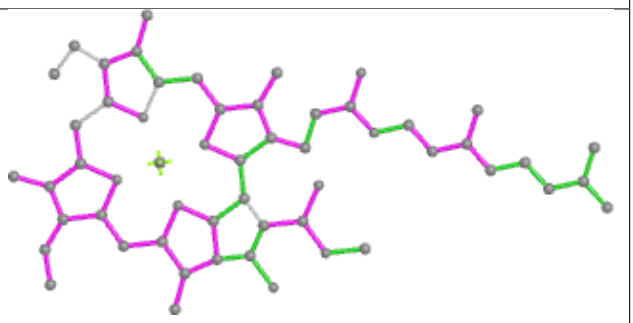
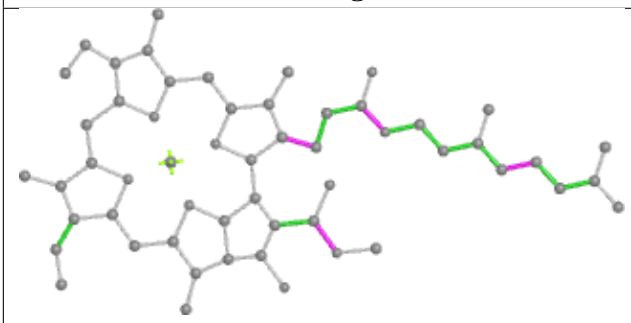


Bond angles



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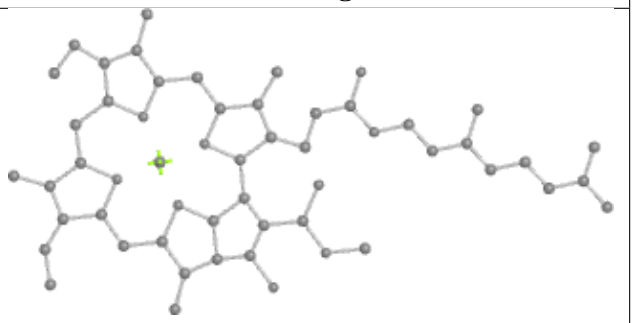
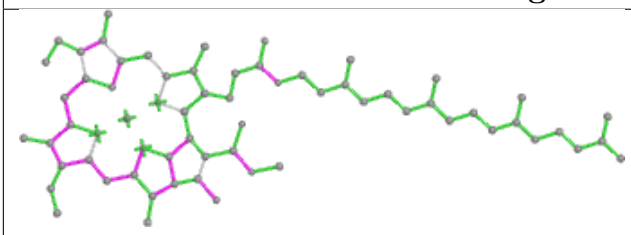


Rings

Ligand CLA 1 614



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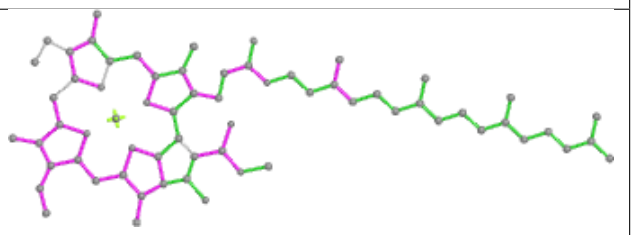

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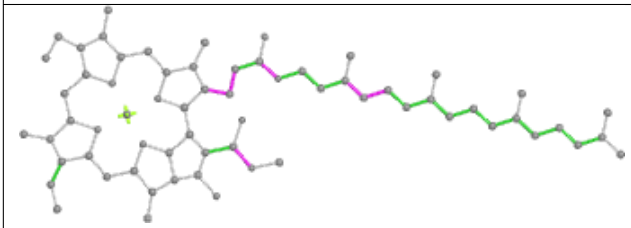

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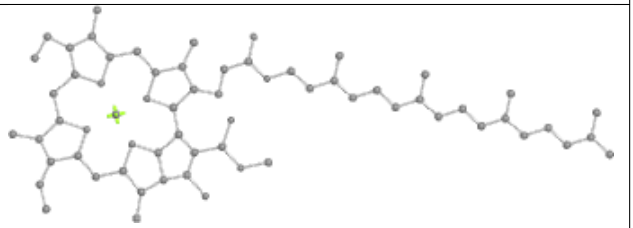
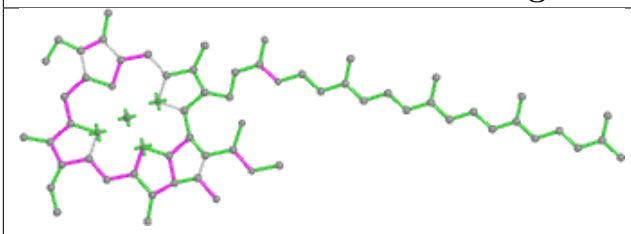
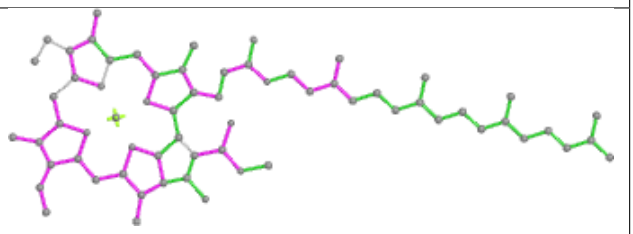


Rings

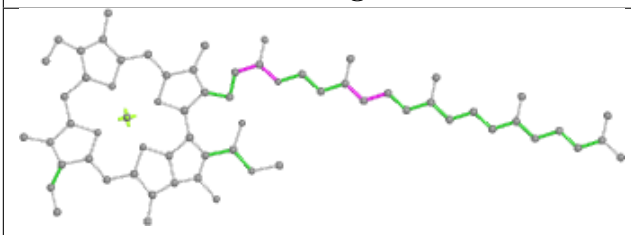
Ligand CLA 1 603



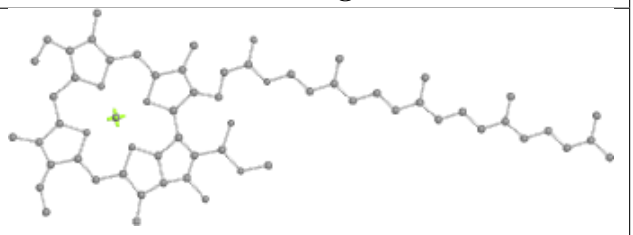
Bond lengths



Bond angles

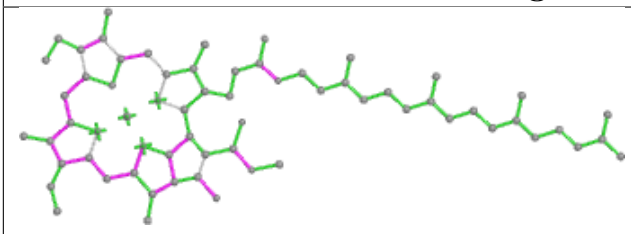


Torsions



Rings

Ligand CLA 6 601



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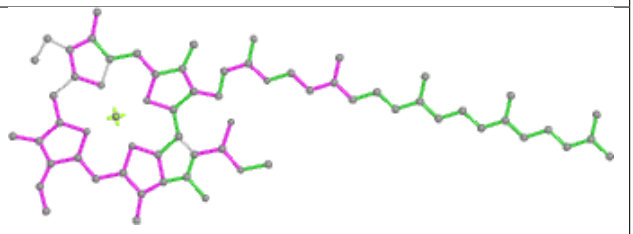
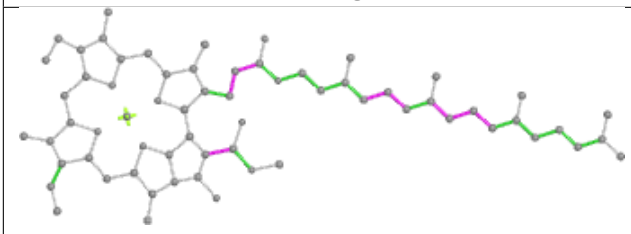


Bond angles



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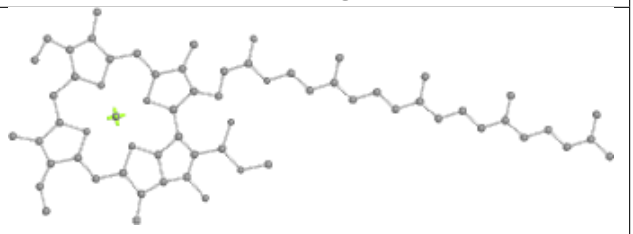
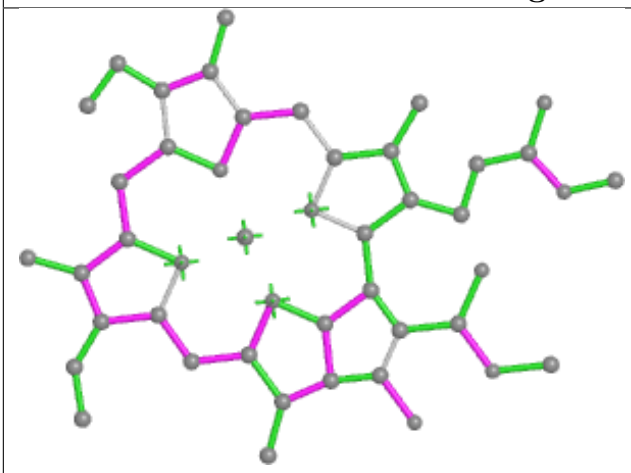


Rings

Ligand CLA 7 603



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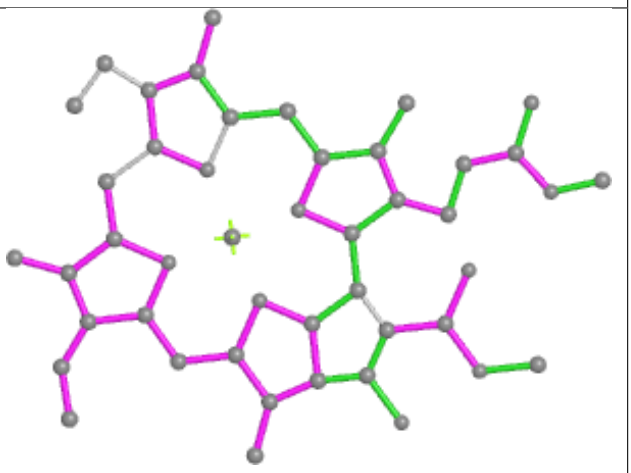

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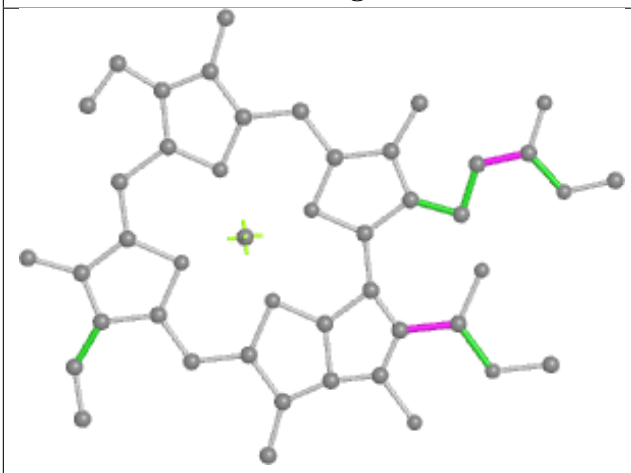

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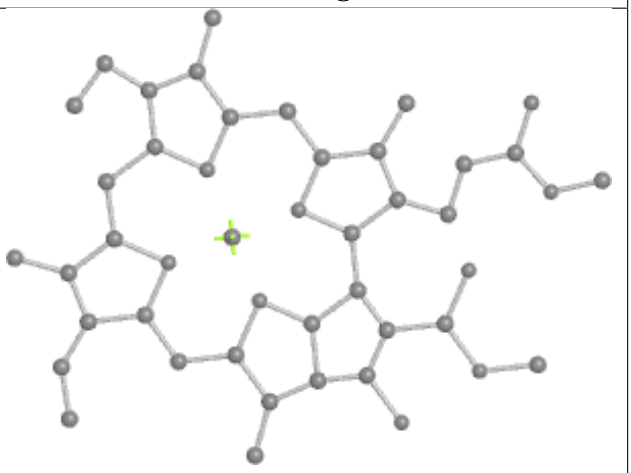
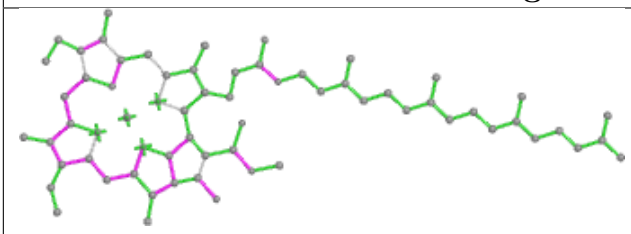


Rings

Ligand CLA A 819



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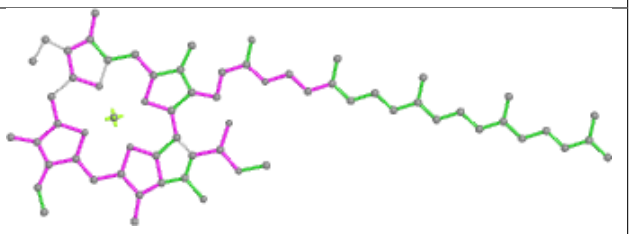
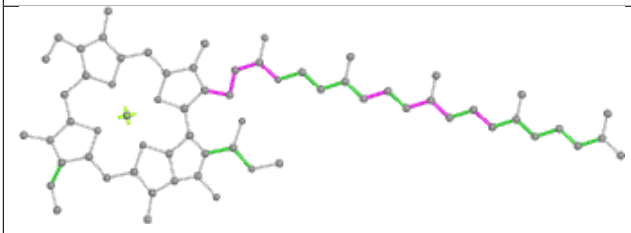


Bond angles



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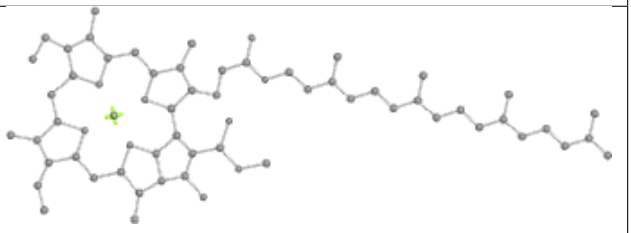
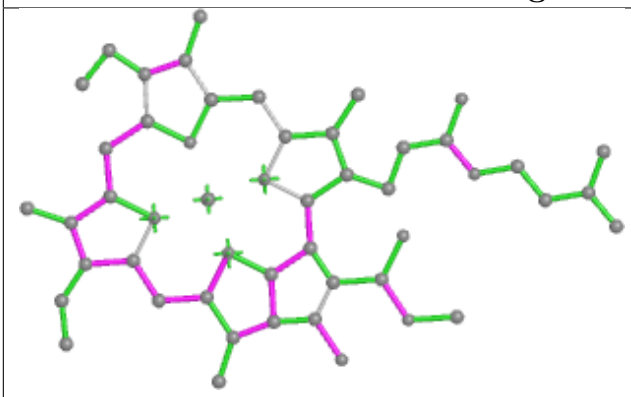
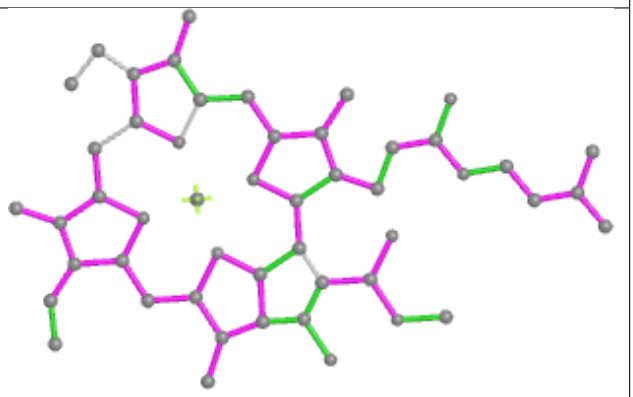


Rings

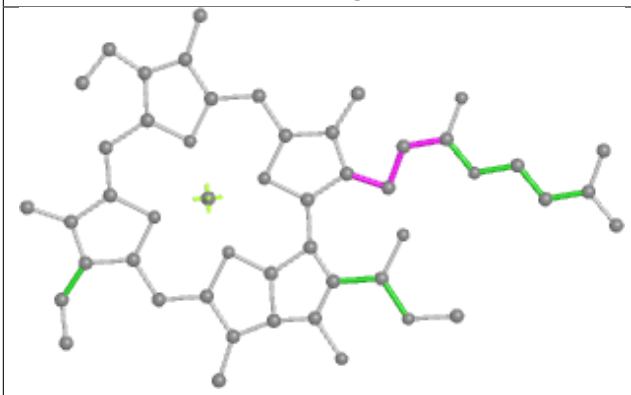
Ligand CLA 7 609



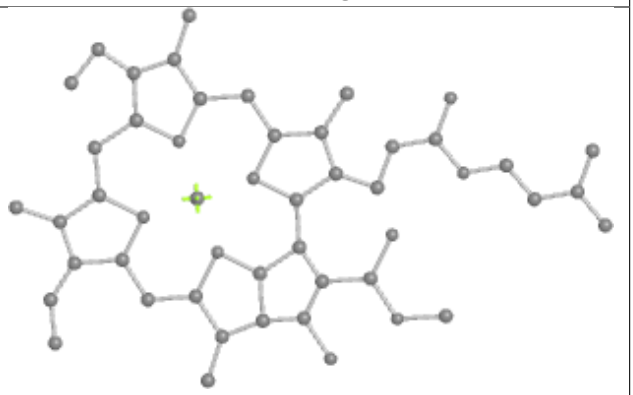
Bond lengths



Bond angles

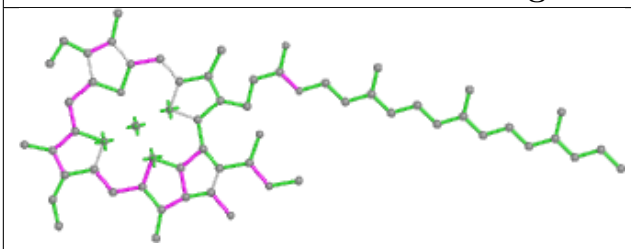


Torsions

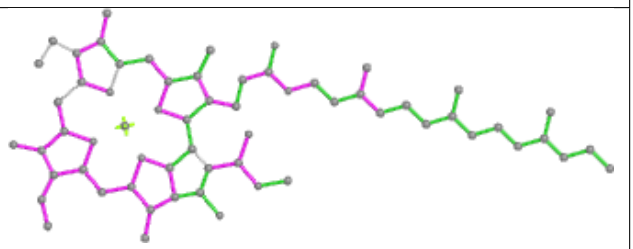


Rings

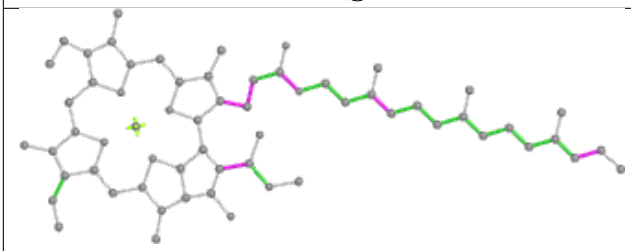
Ligand CLA 8 602



Bond lengths



Bond angles



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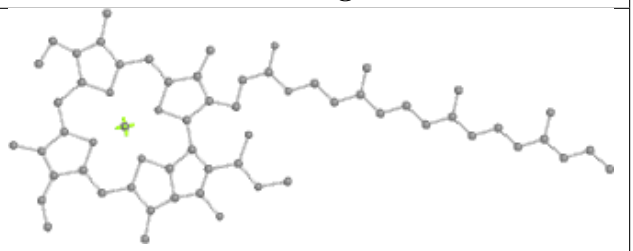
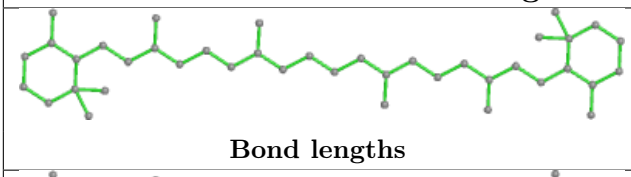
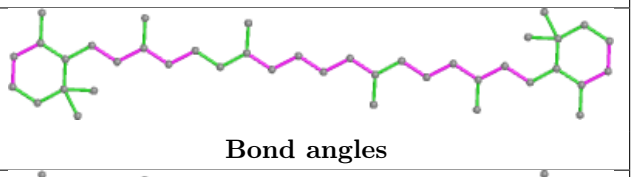


Rings

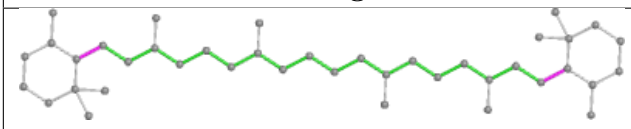
Ligand BCR A 850



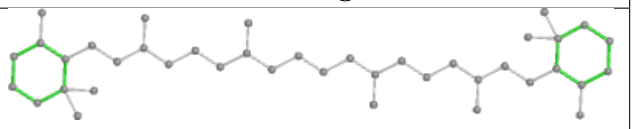
Bond lengths



Bond angles

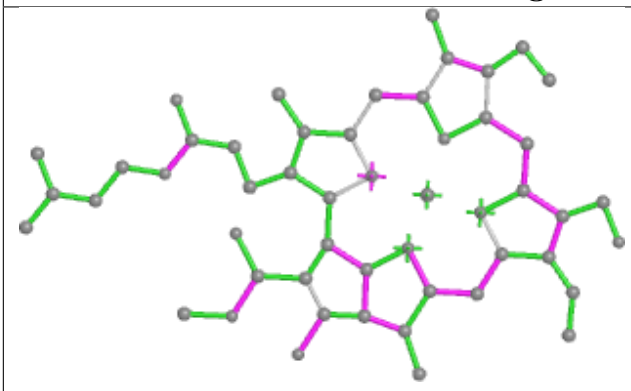


Torsions



Rings

Ligand CHL 4 608



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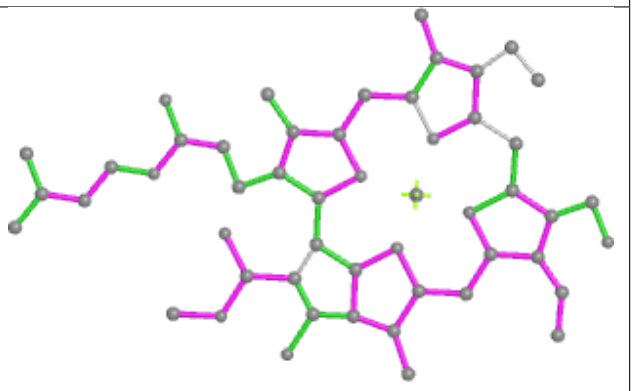

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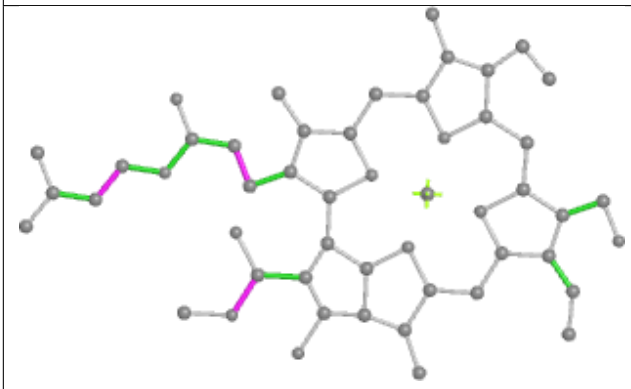

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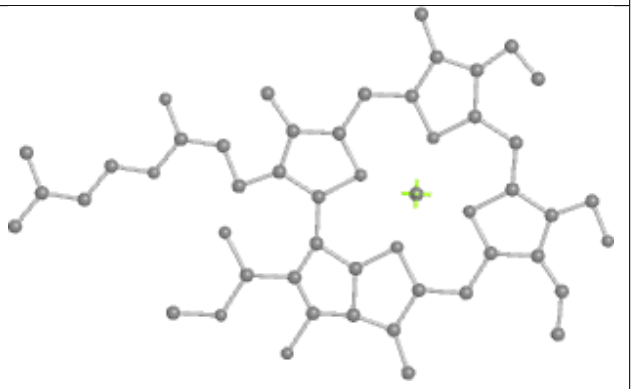
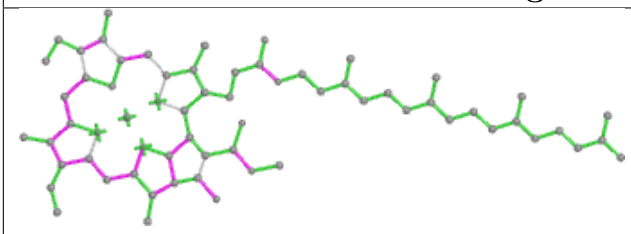


Rings

Ligand CLA Z 614



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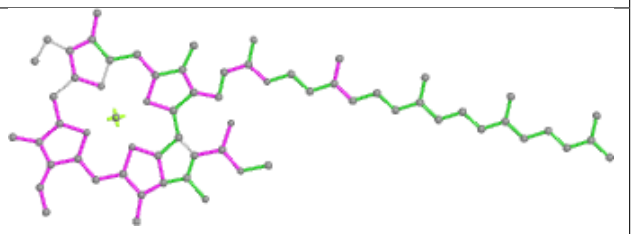
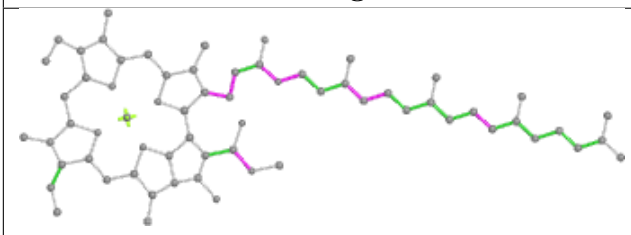


Bond angles



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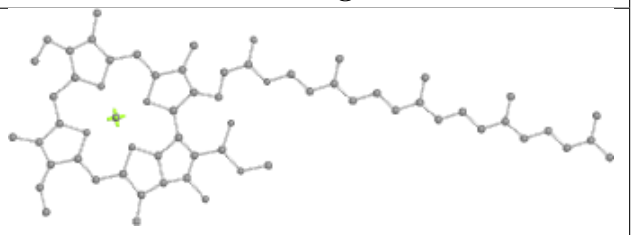
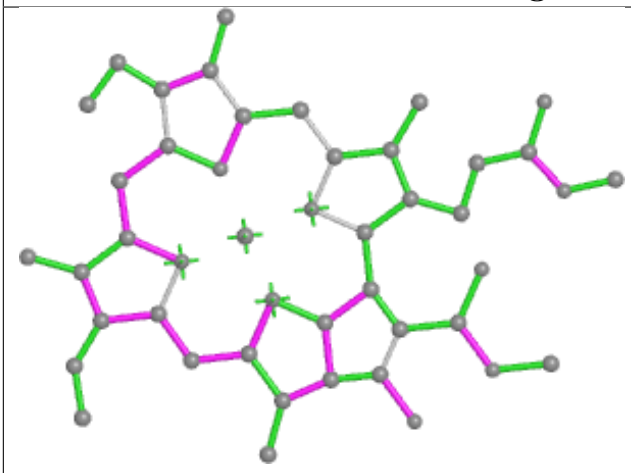


Rings

Ligand CLA 4 603



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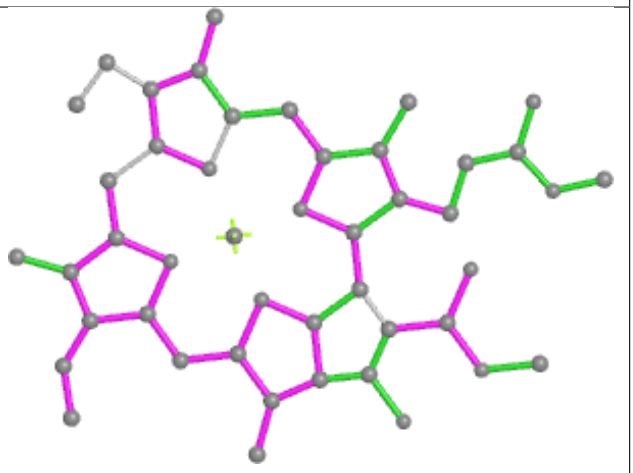

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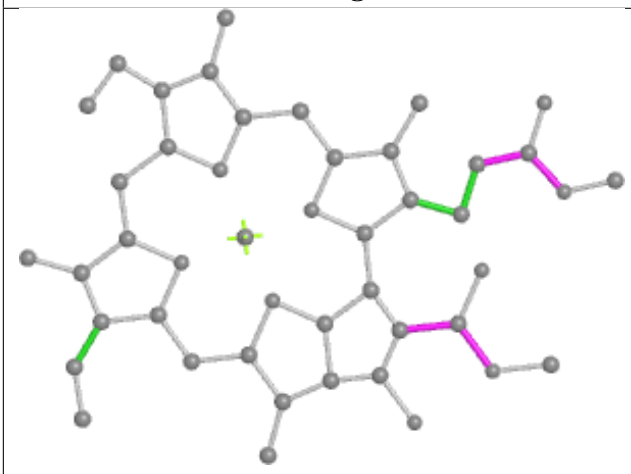

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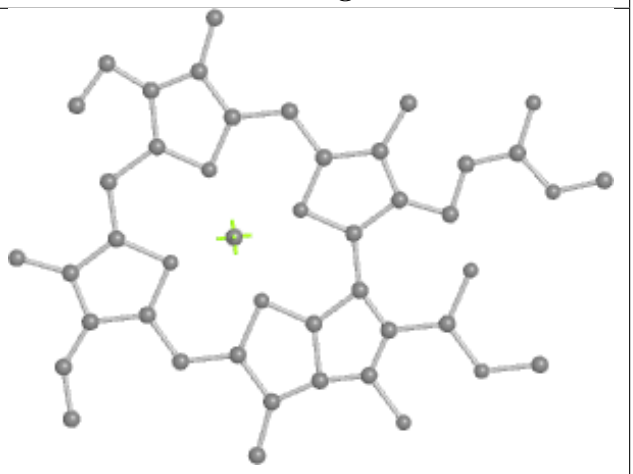
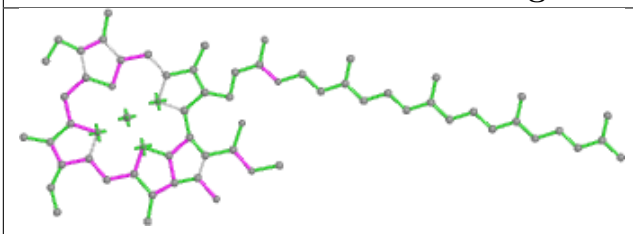


Rings

Ligand CLA 3 603



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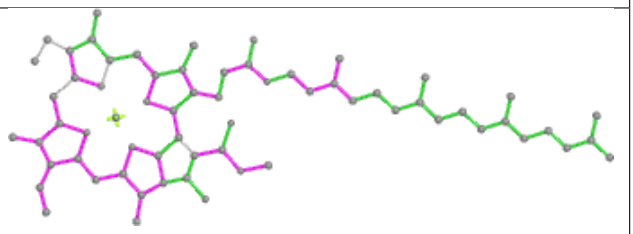

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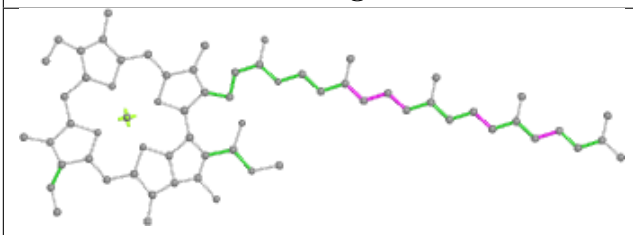

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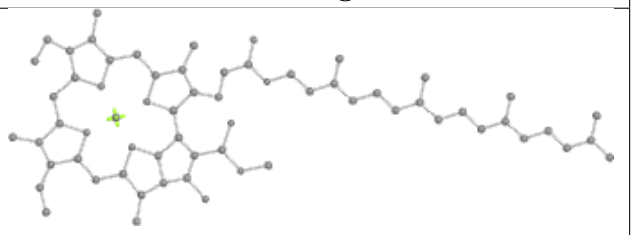
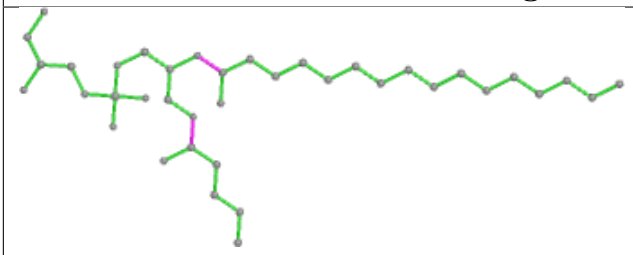


Rings

Ligand LHG A 847



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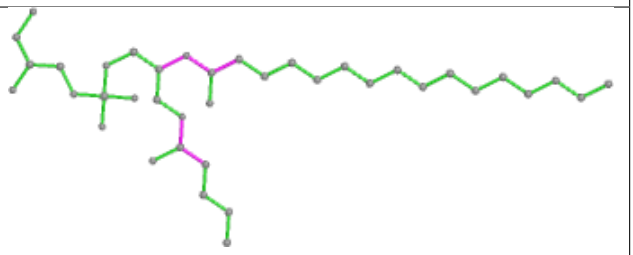
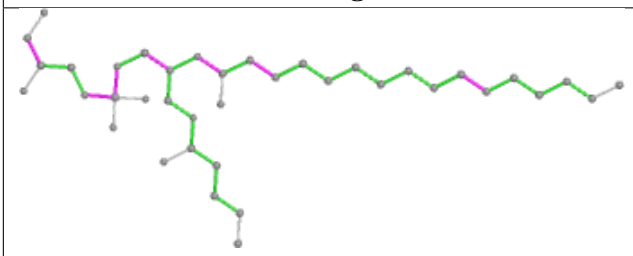


Bond angles



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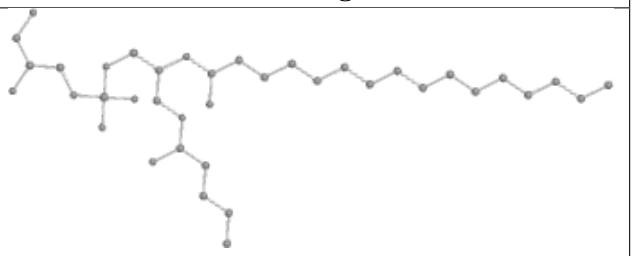
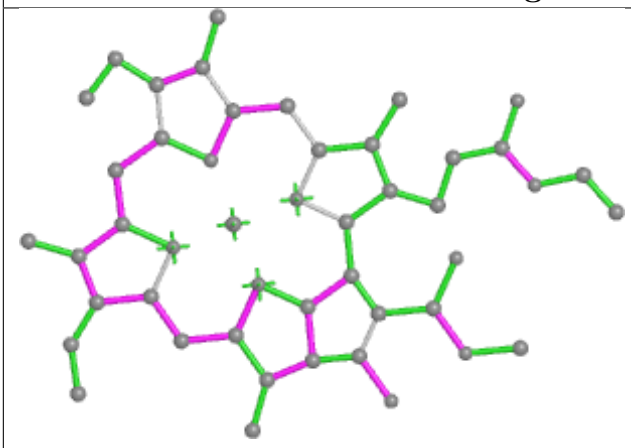


Rings

Ligand CLA B 838



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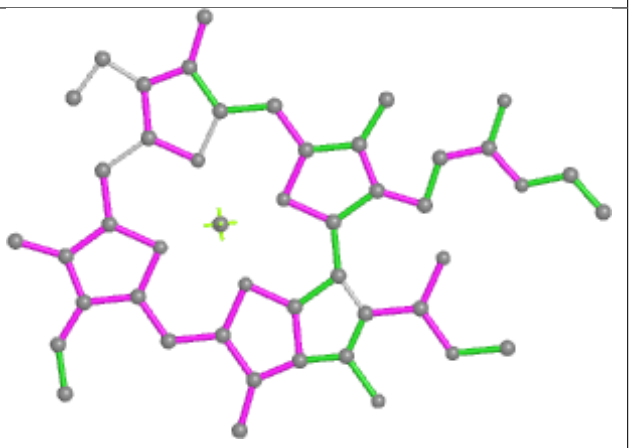

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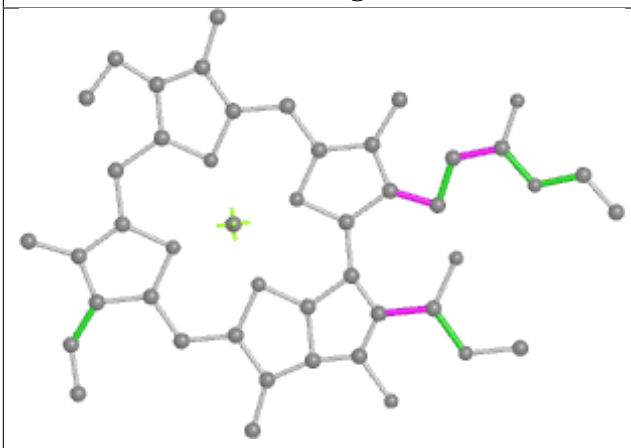

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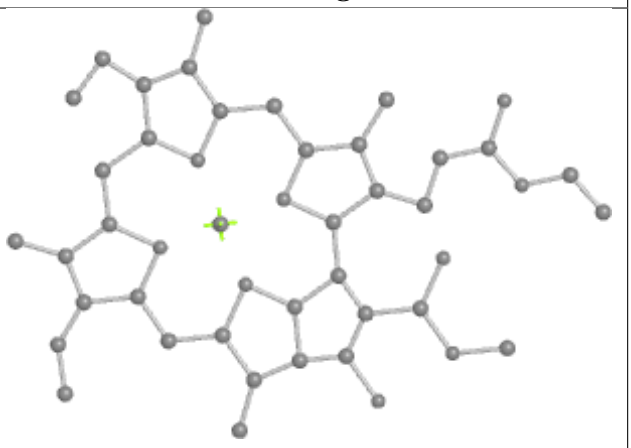
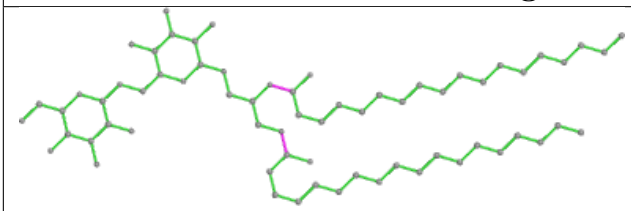


Rings

Ligand DGD B 850



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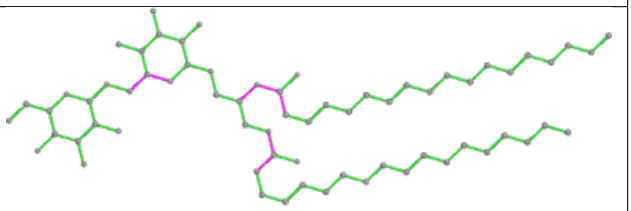
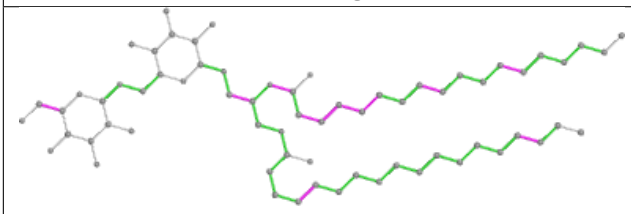


Bond angles



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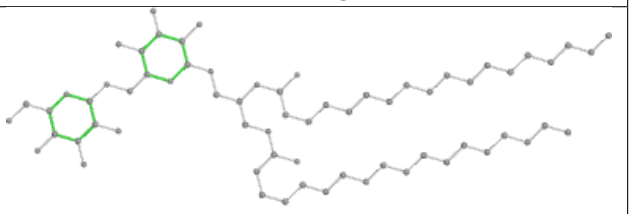
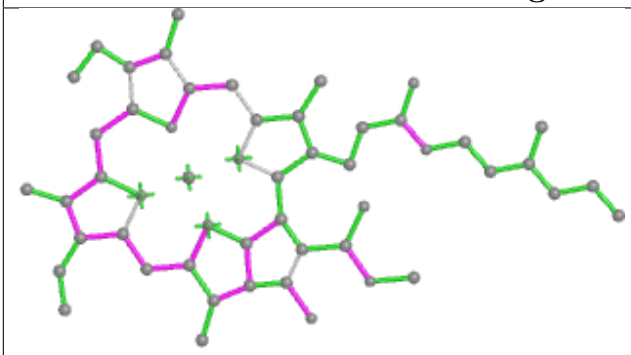


Rings

Ligand CLA 1 606



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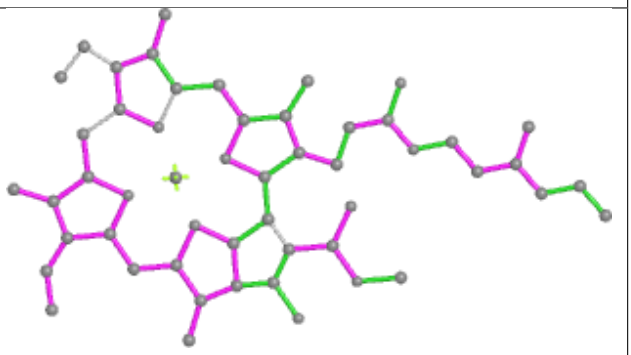
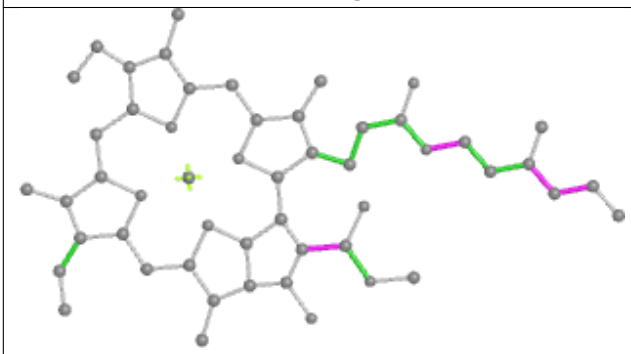


Bond angles



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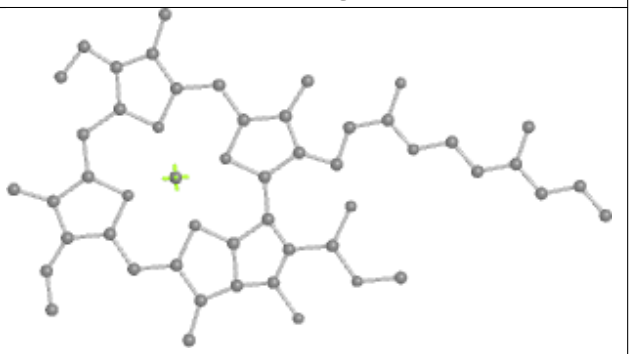
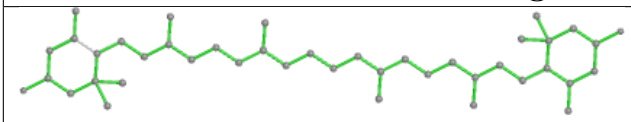


Rings

Ligand LUT 5 624



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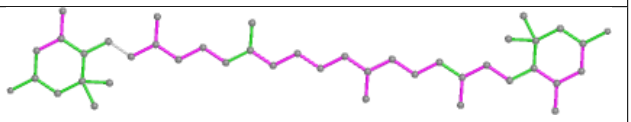

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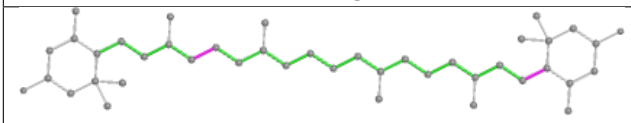

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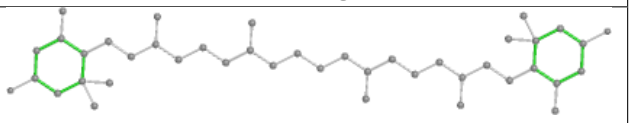
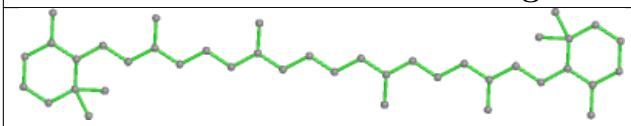


Rings

Ligand BCR A 852



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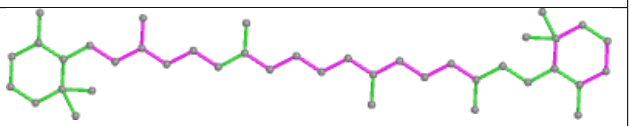

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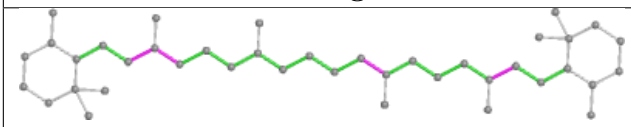

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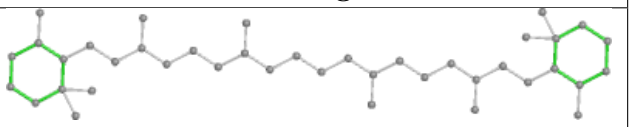
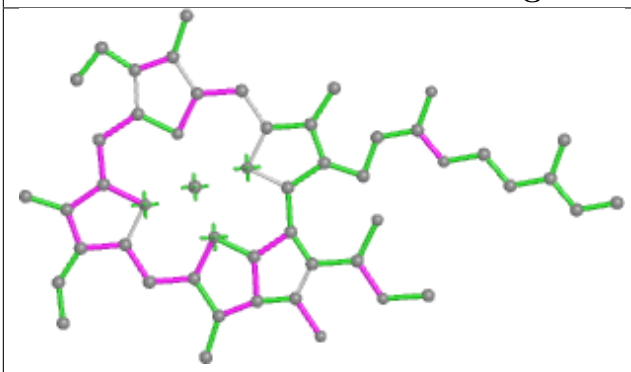


Rings

Ligand CLA A 824



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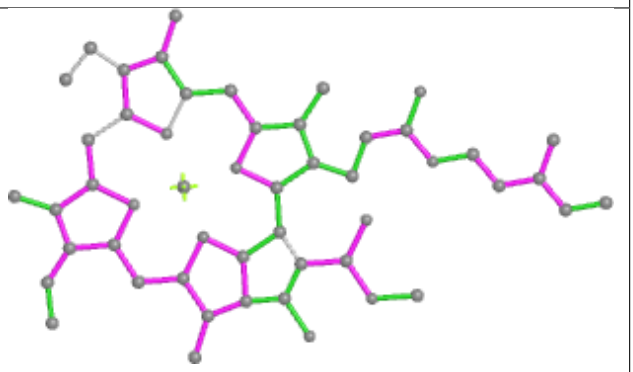
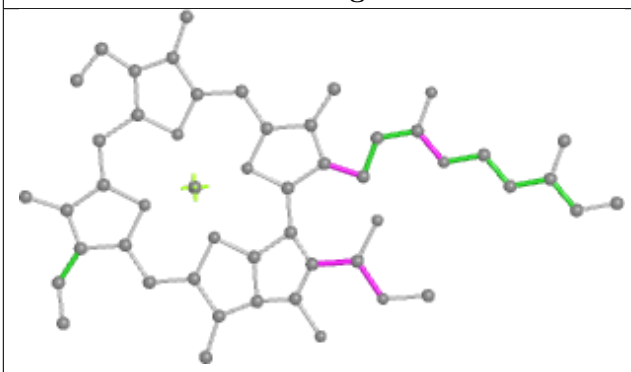


Bond angles



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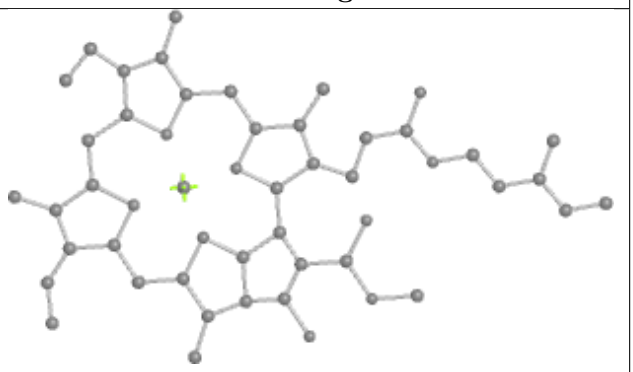
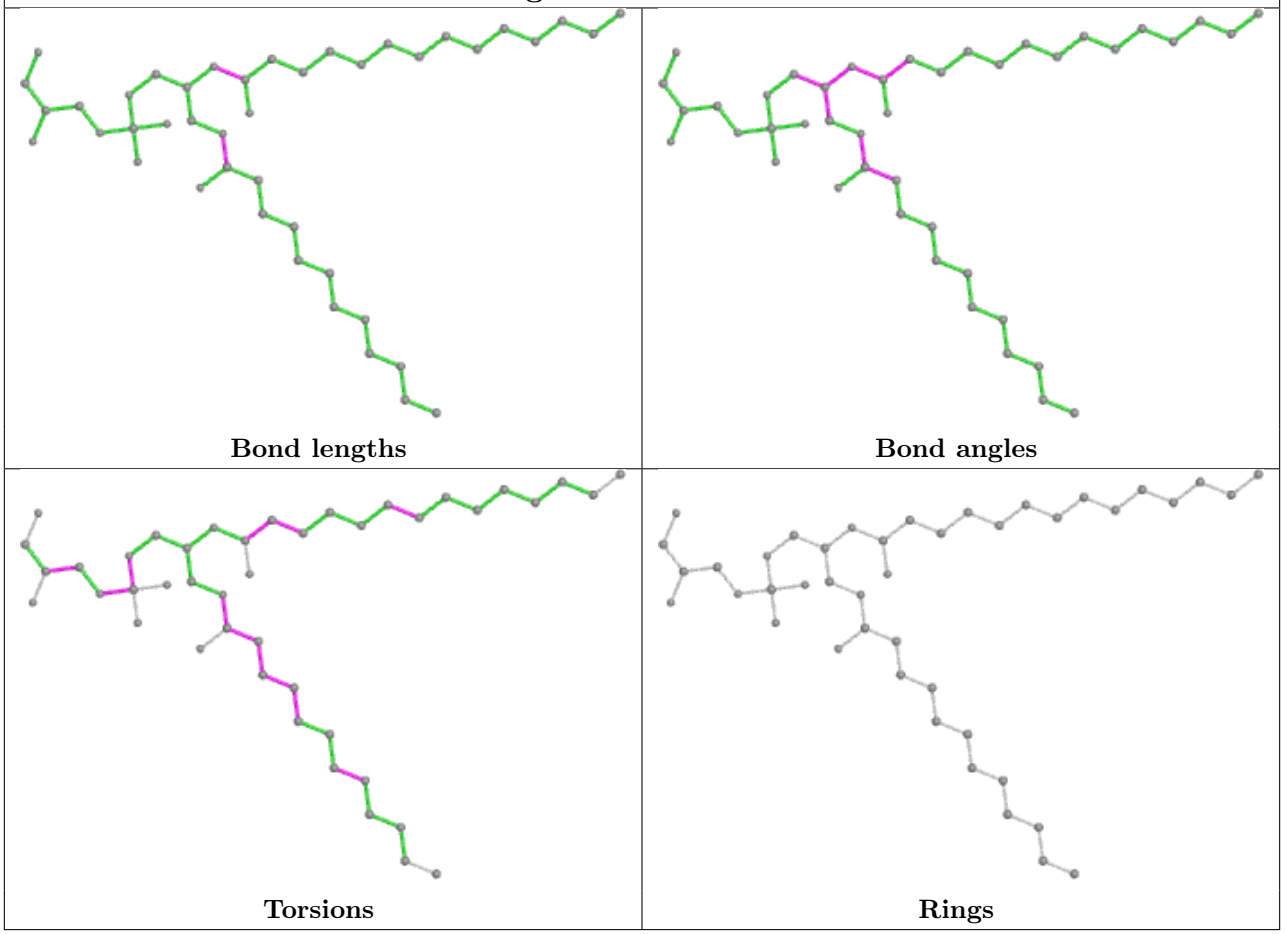


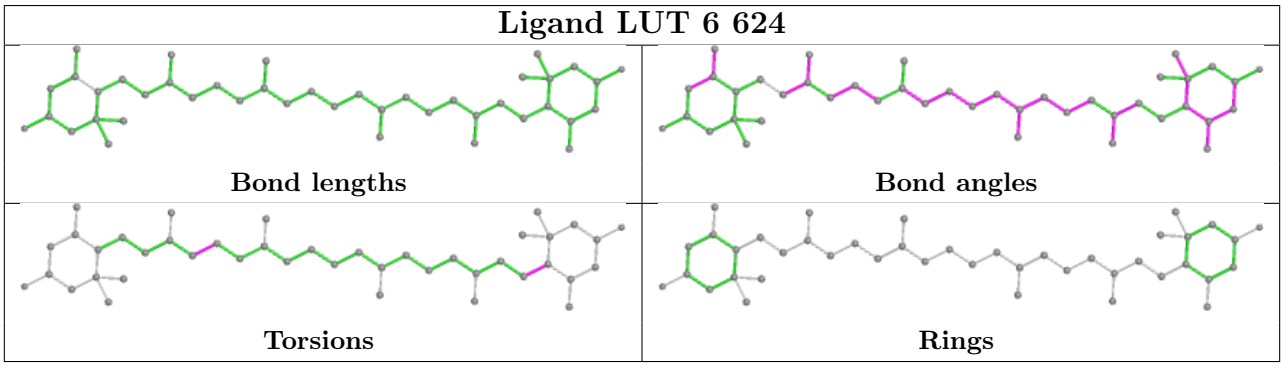
Rings

Ligand LHG Z 620

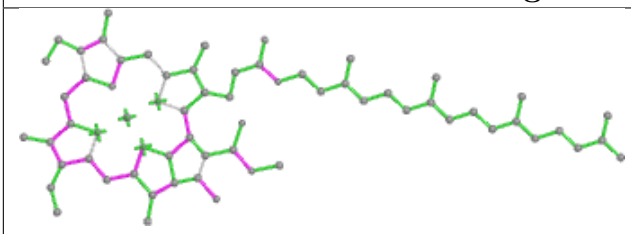


Ligand LUT 8 617

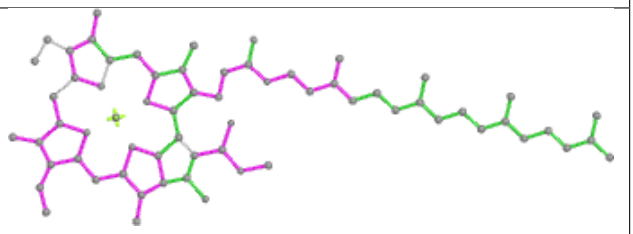
Ligand LUT 6 624



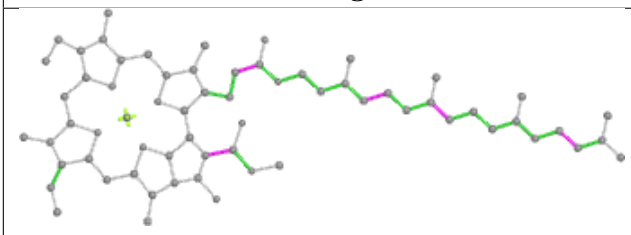
Ligand CLA A 802



Bond lengths



Bond angles



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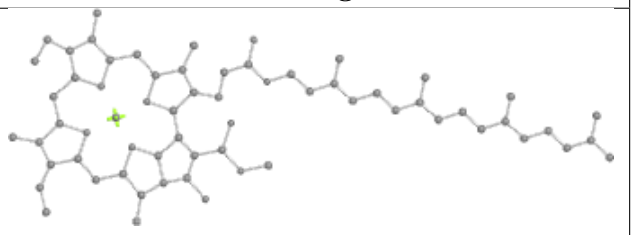
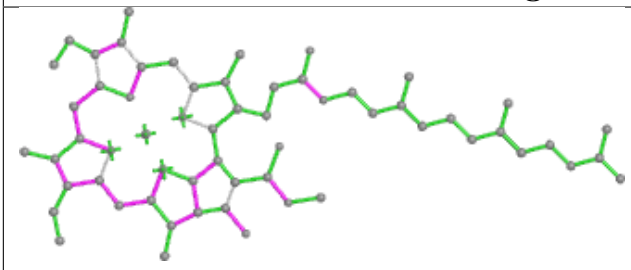


Rings

Ligand CLA B 823



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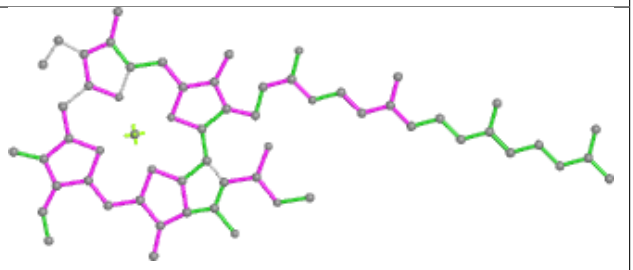
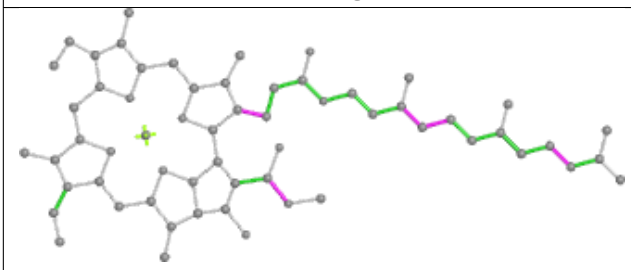
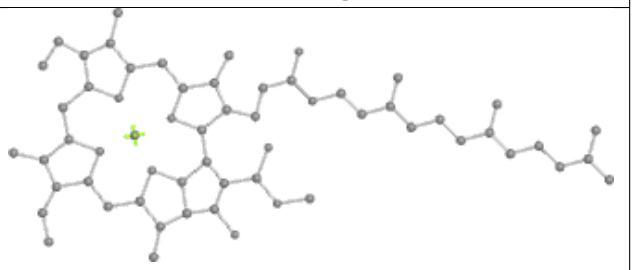


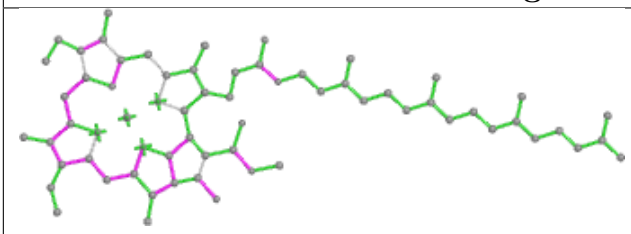
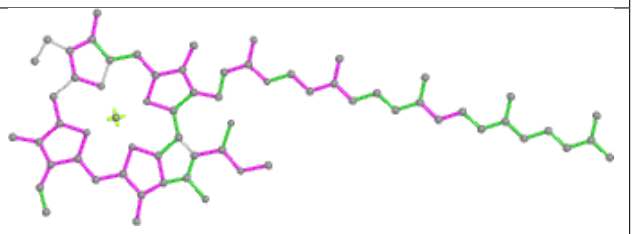
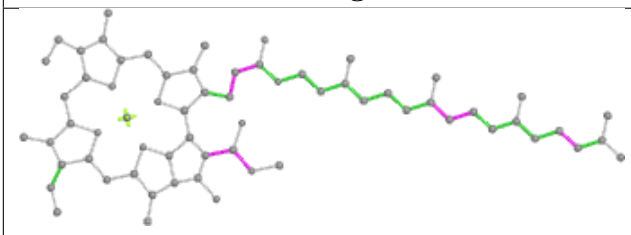
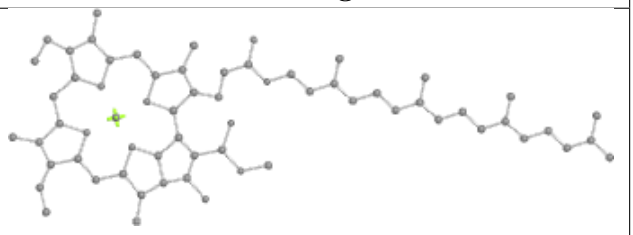
Bond angles

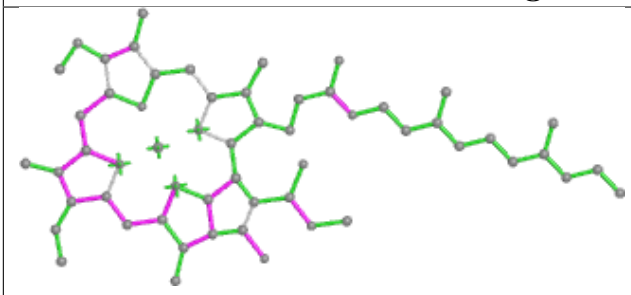
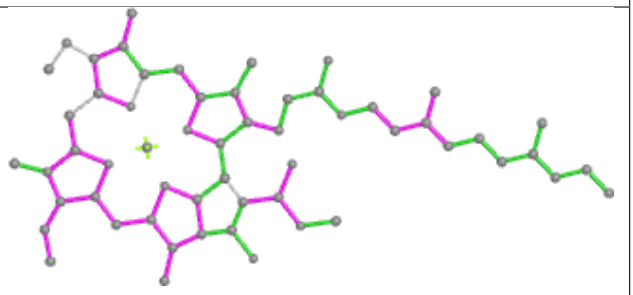
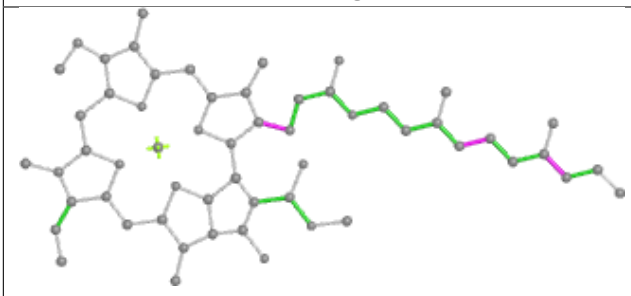
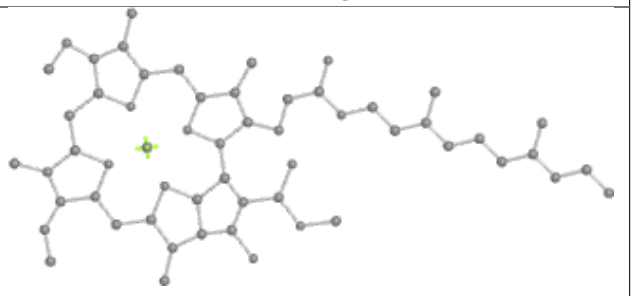


Torsions

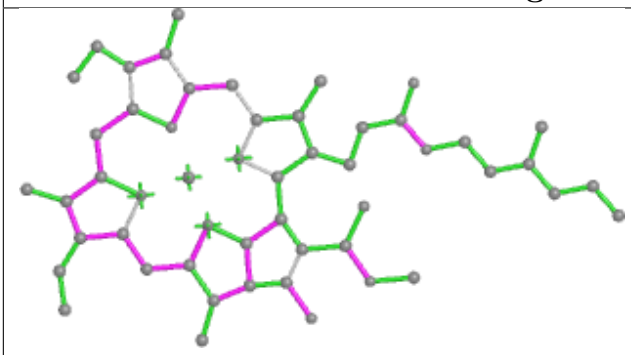


Rings

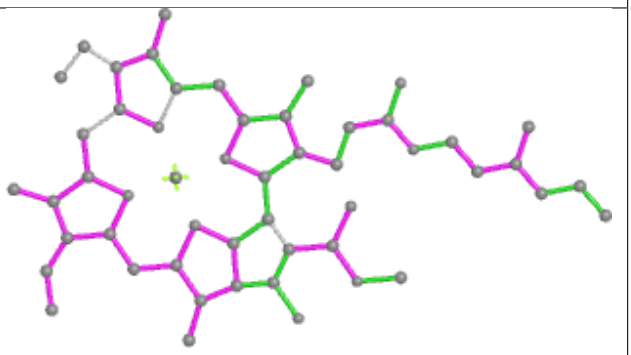
Ligand CLA A 841	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 815	
 Bond lengths	 Bond angles
 Torsions	 Rings

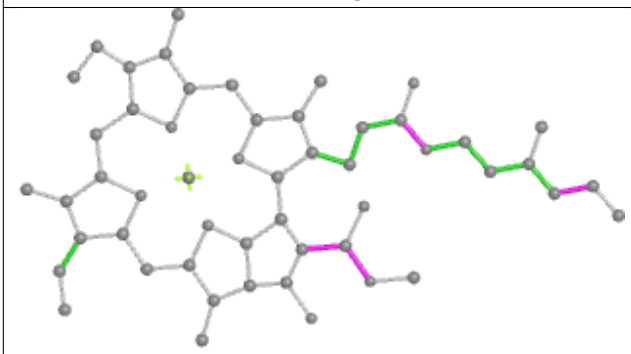
Ligand CLA Z 606



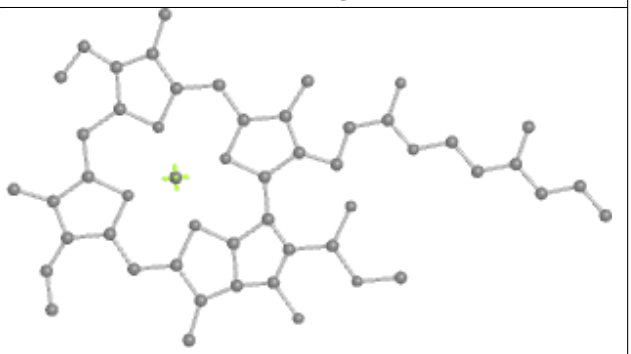
Bond lengths



Bond angles

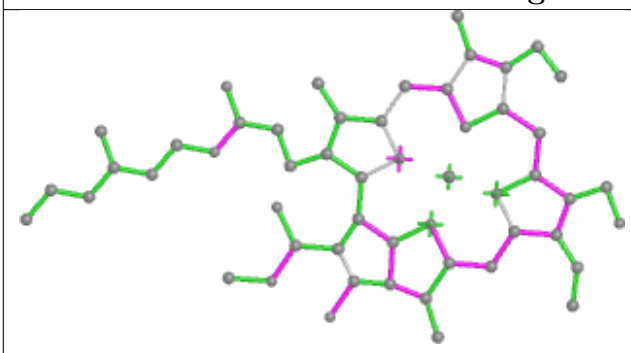


Torsions

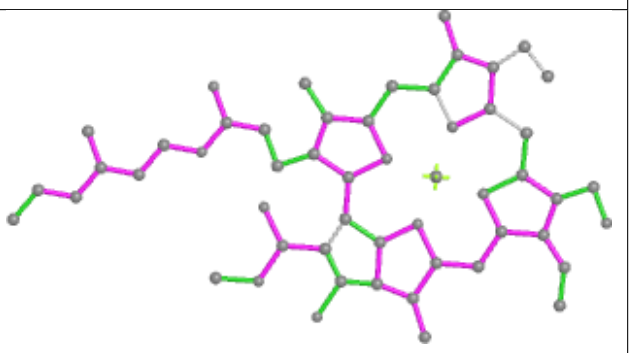


Rings

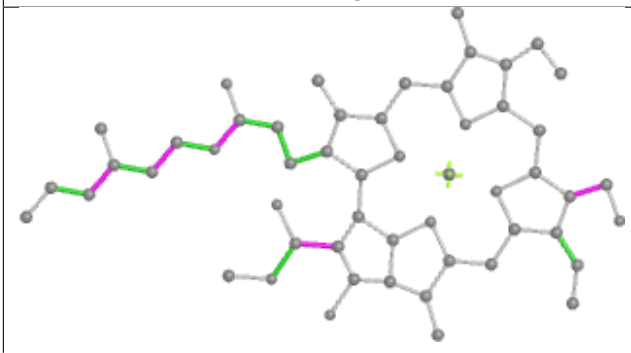
Ligand CHL 1 601



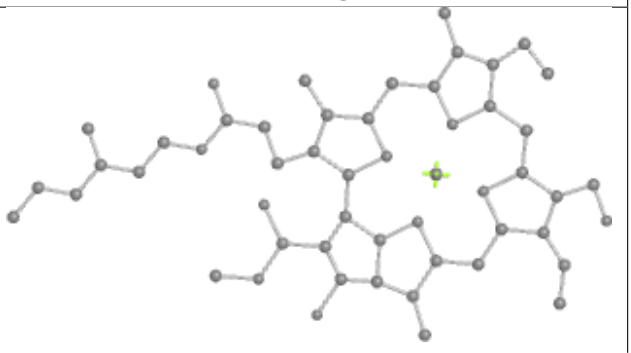
Bond lengths



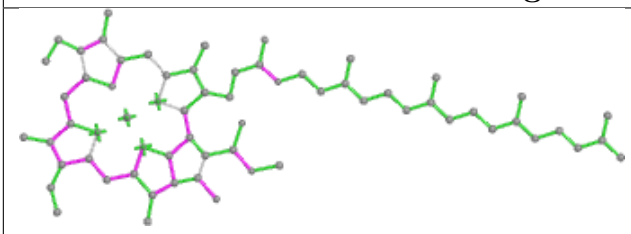
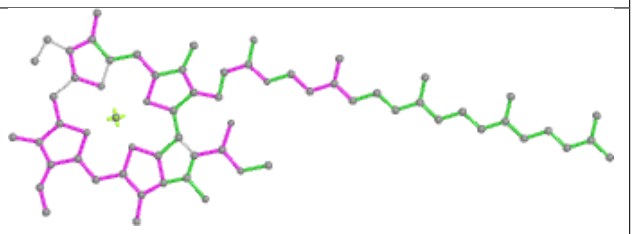
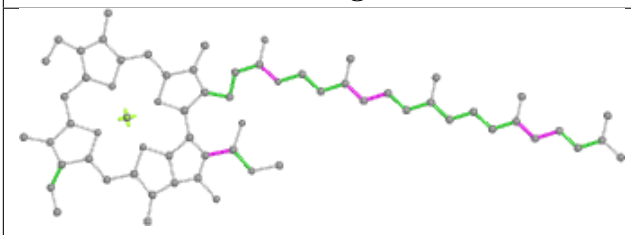
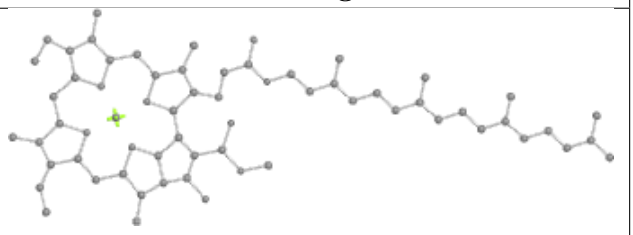
Bond angles

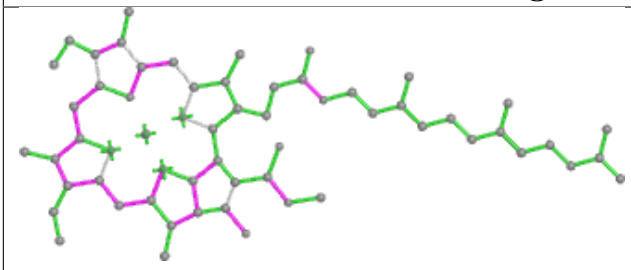
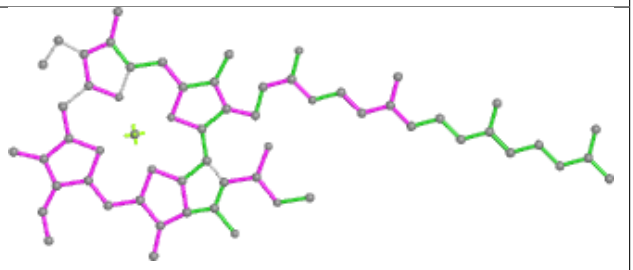
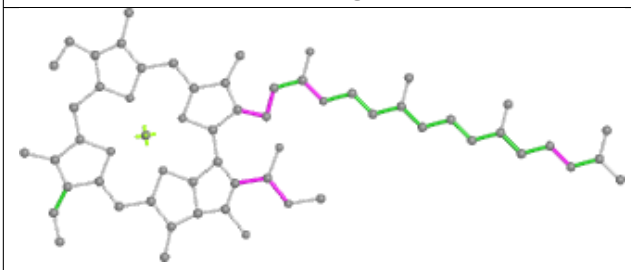
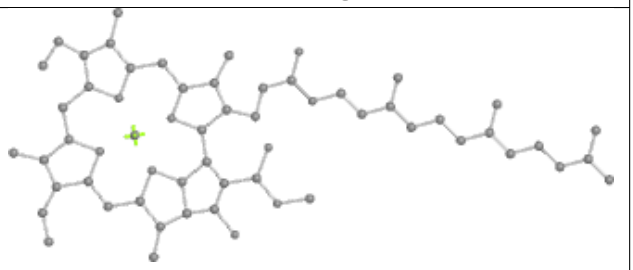


Torsions

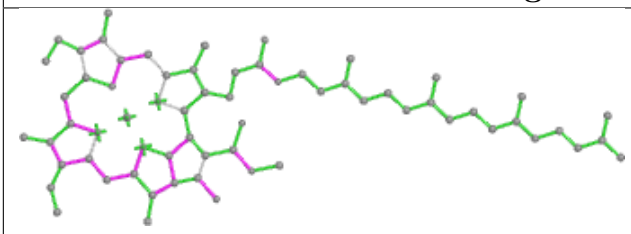


Rings

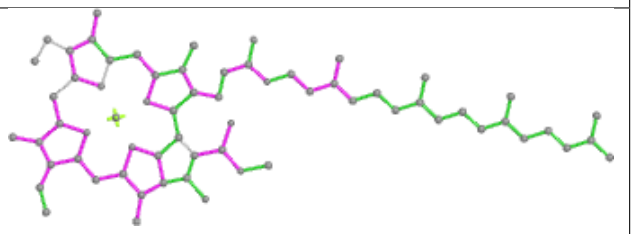
Ligand CLA A 839	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 4 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

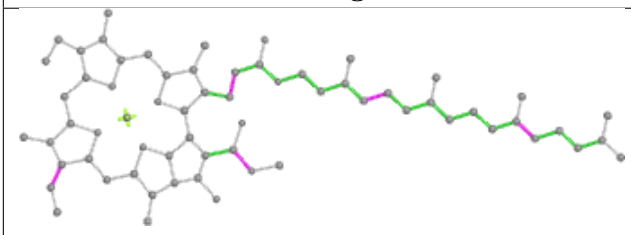
Ligand CLA B 840



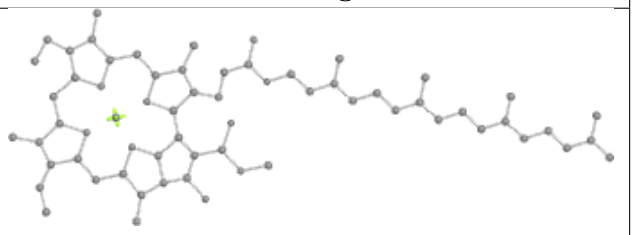
Bond lengths



Bond angles

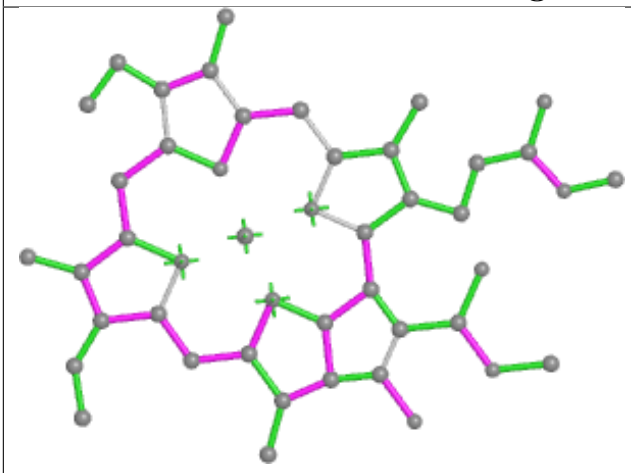


Torsions



Rings

Ligand CLA 8 616



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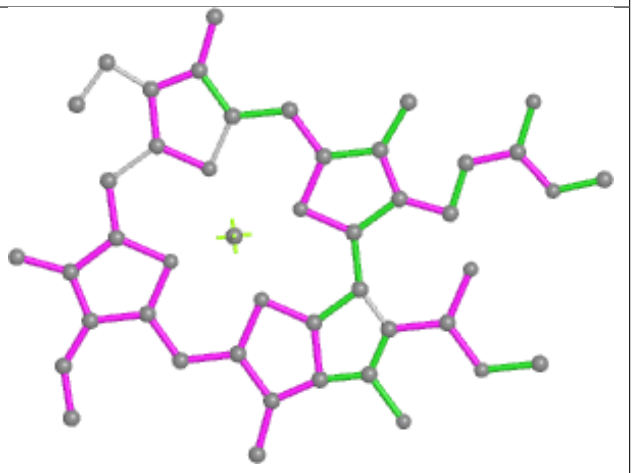
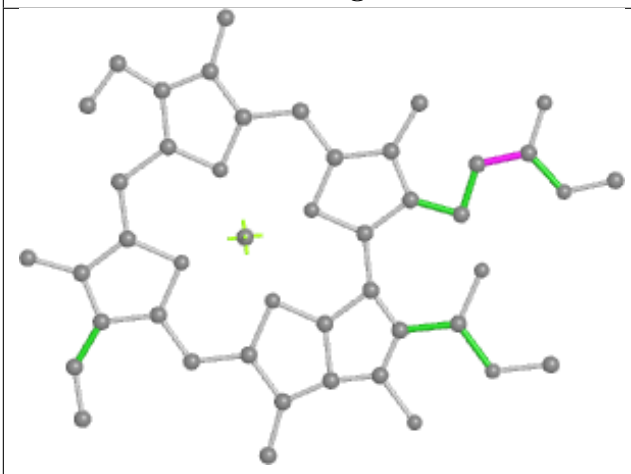


Bond angles



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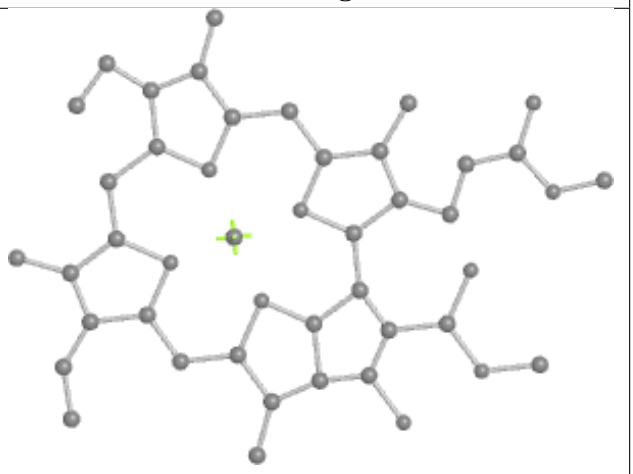
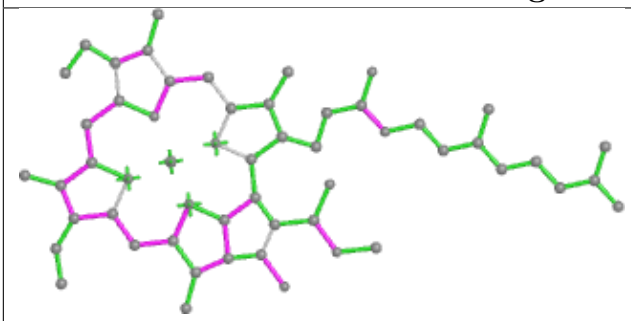


Rings

Ligand CLA 5 606



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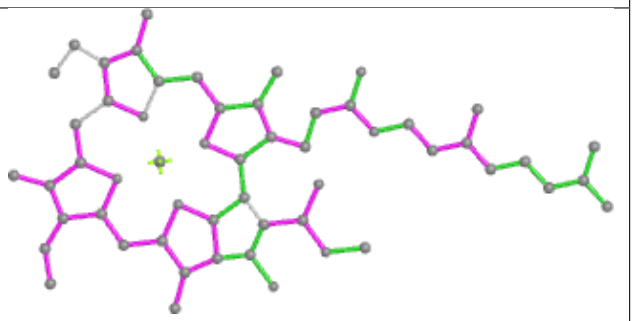
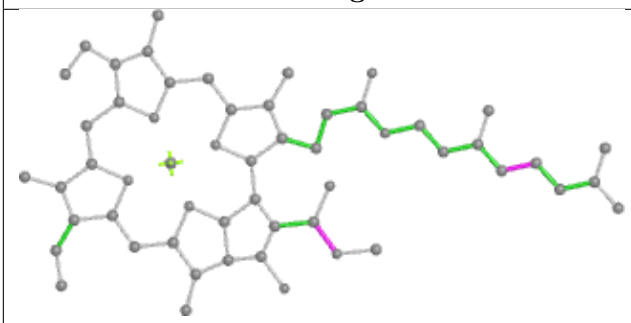


Bond angles



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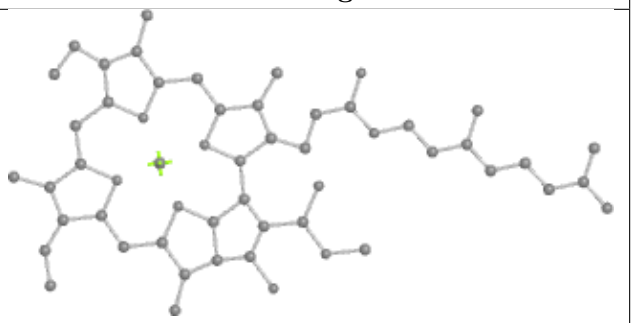
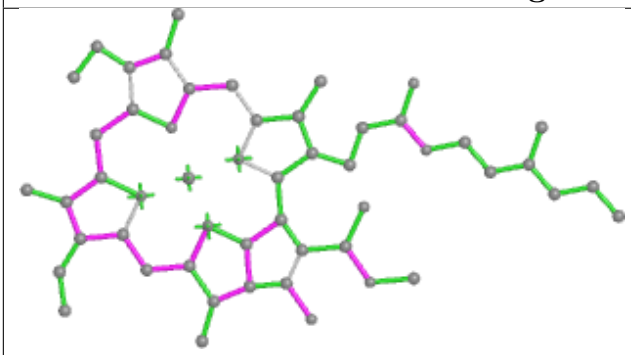


Rings

Ligand CLA 6 612



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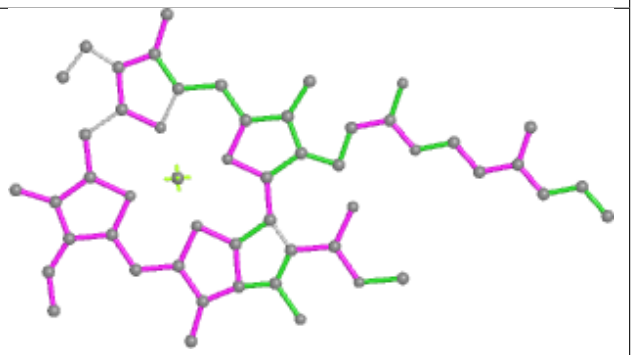
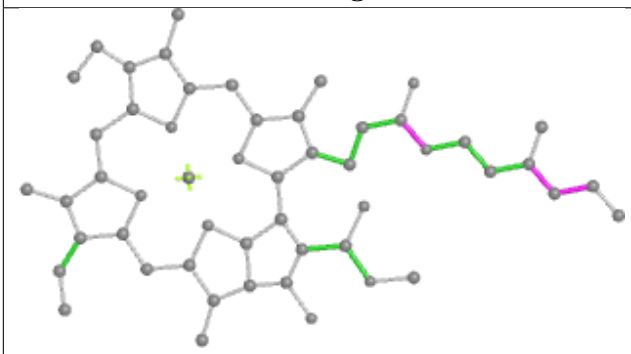
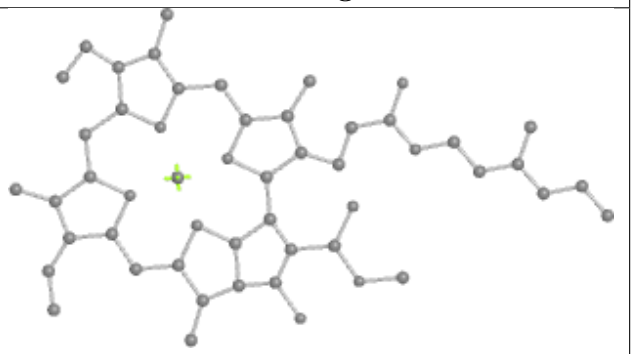


Bond angles

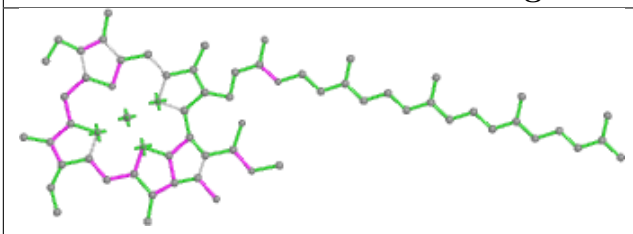


Torsions



Rings

Ligand CLA B 806



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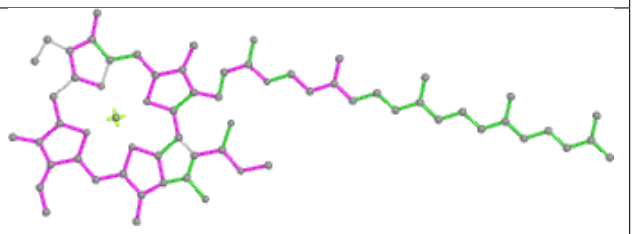
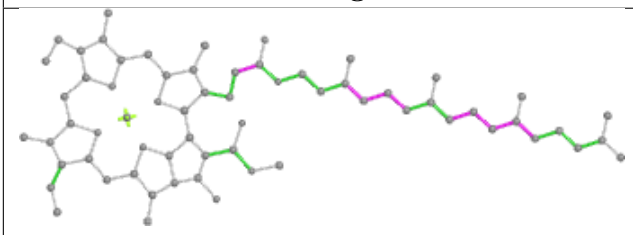


Bond angles



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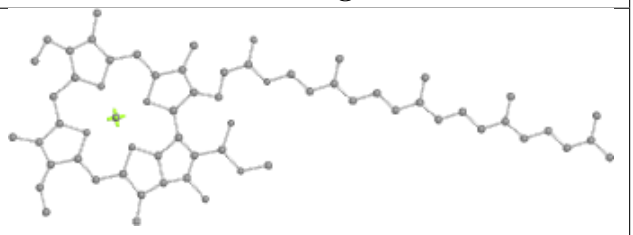
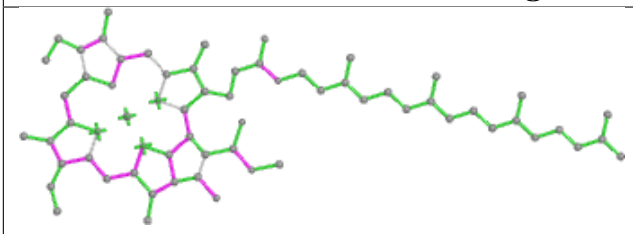


Rings

Ligand CLA B 809



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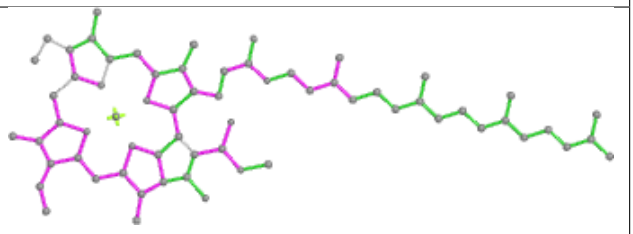
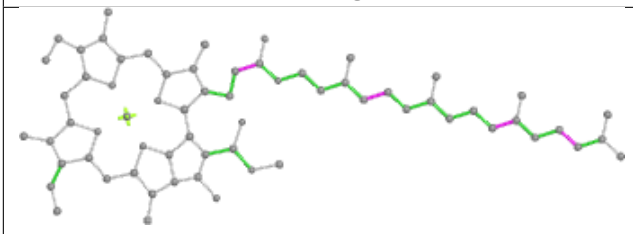
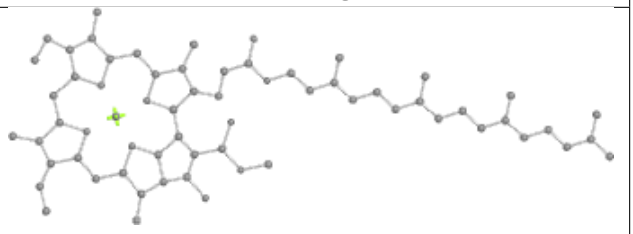


Bond angles

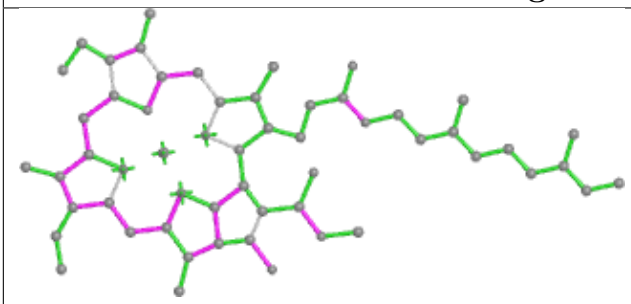


Torsions



Rings

Ligand CLA 6 613



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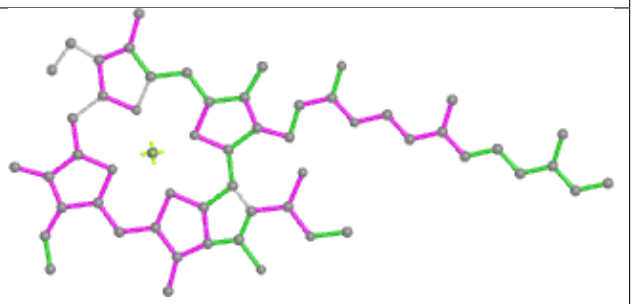
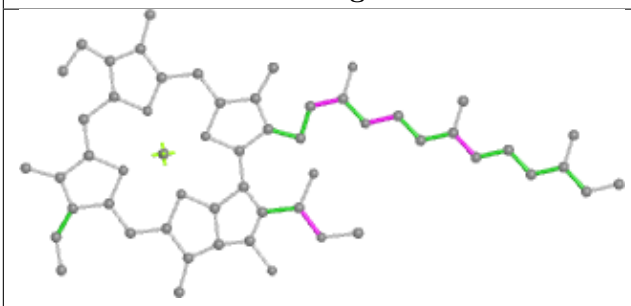
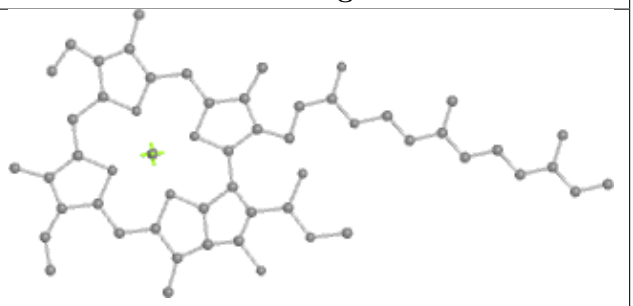


Bond angles

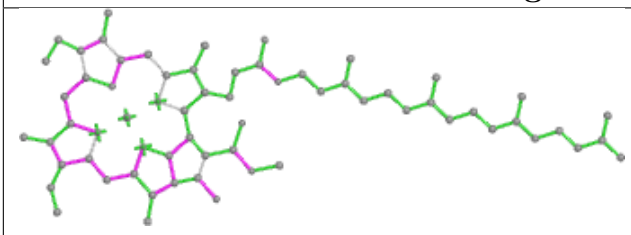


Torsions

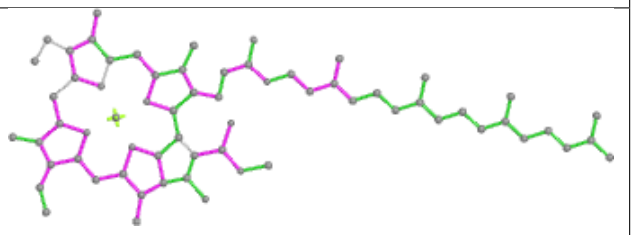


Rings

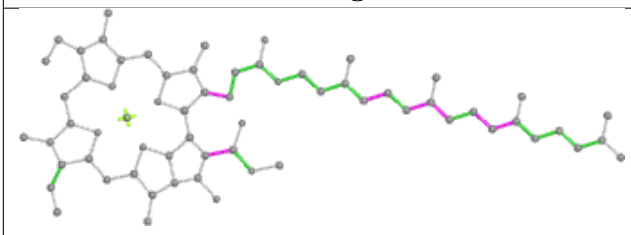
Ligand CLA B 826



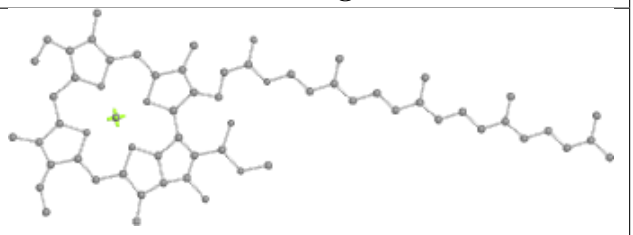
Bond lengths



Bond angles

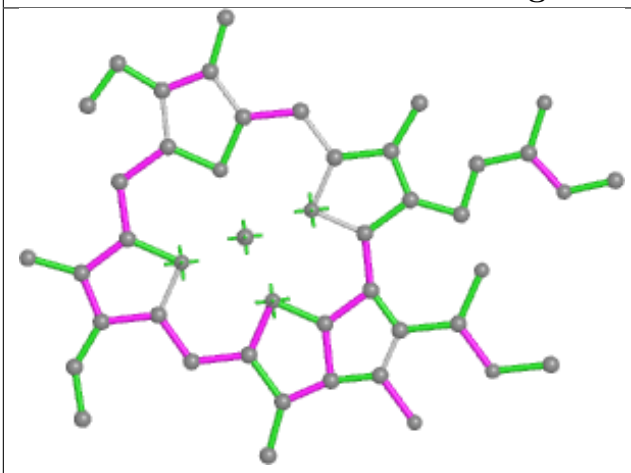


Torsions

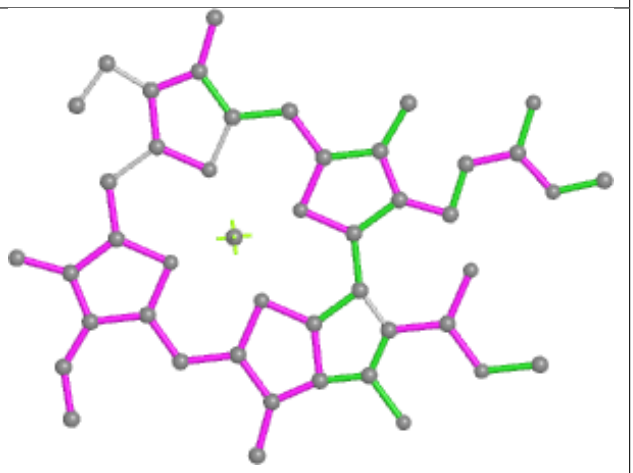


Rings

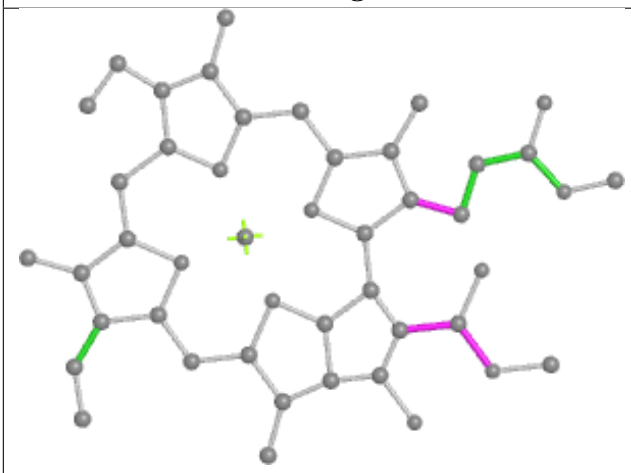
Ligand CLA 8 611



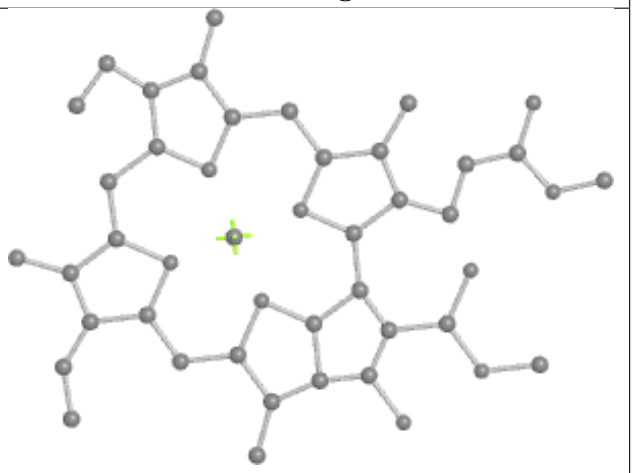
Bond lengths



Bond angles

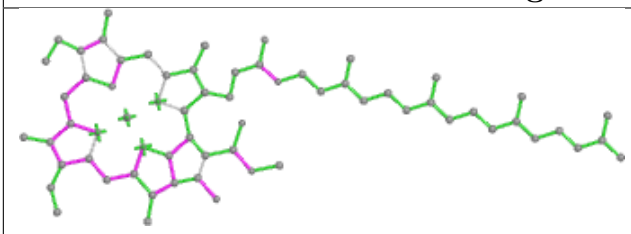


Torsions

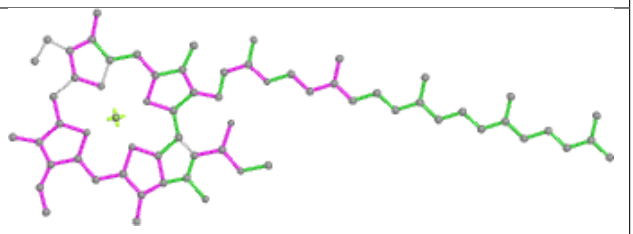


Rings

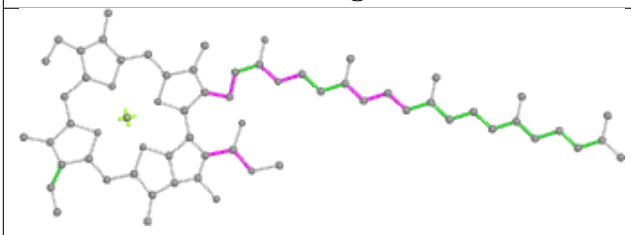
Ligand CLA Z 602



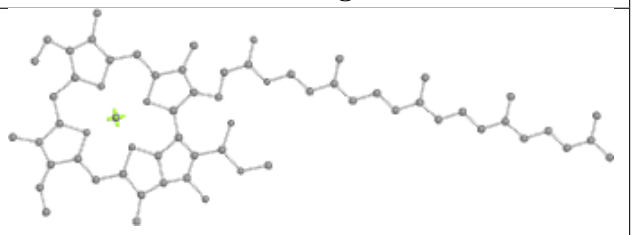
Bond lengths



Bond angles

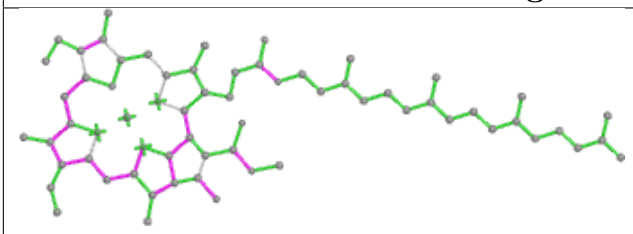


Torsions



Rings

Ligand CLA Z 609



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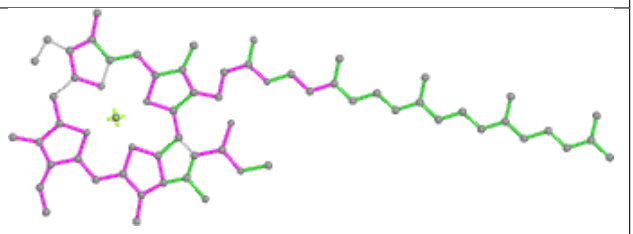
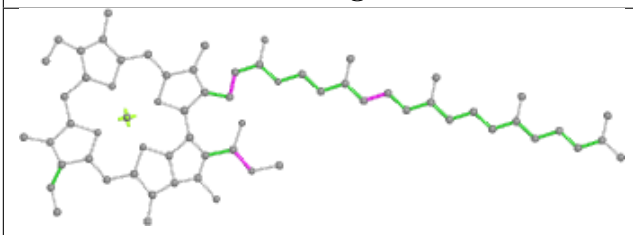
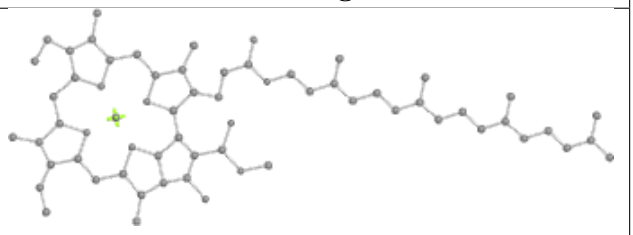


Bond angles

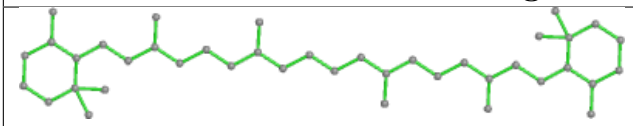


Torsions



Rings

Ligand BCR B 848



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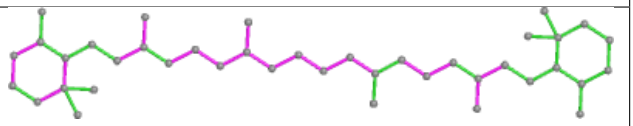
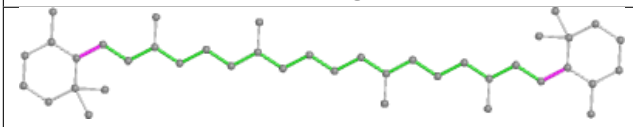


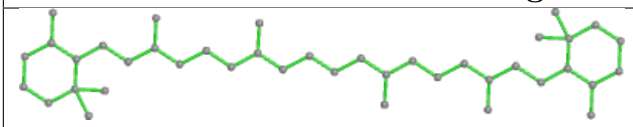
Bond angles



Torsions

Rings

Ligand BCR 6 623



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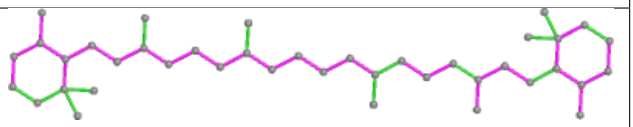
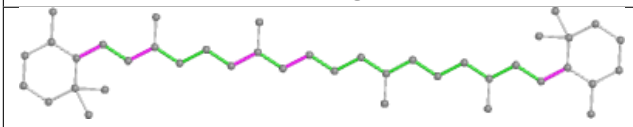


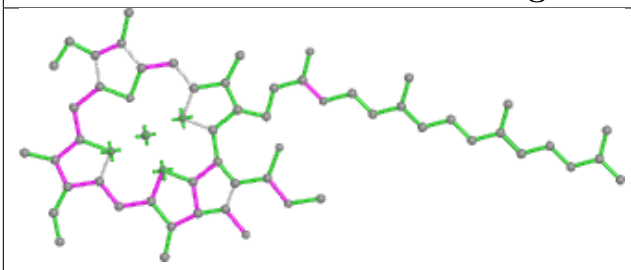
Bond angles



Torsions

Rings

Ligand CLA 7 620



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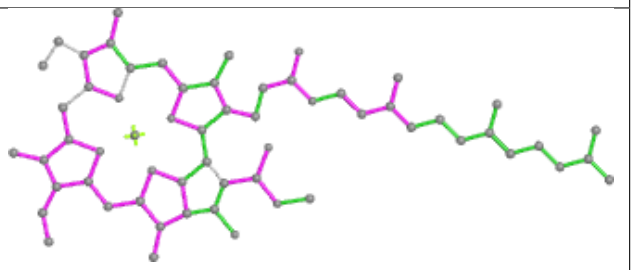
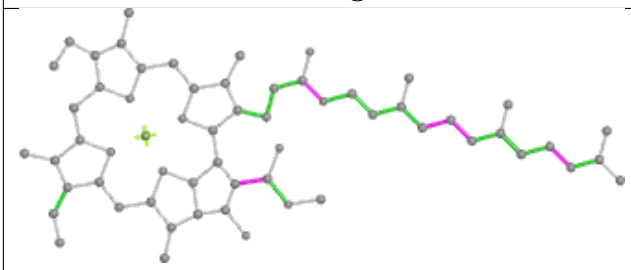
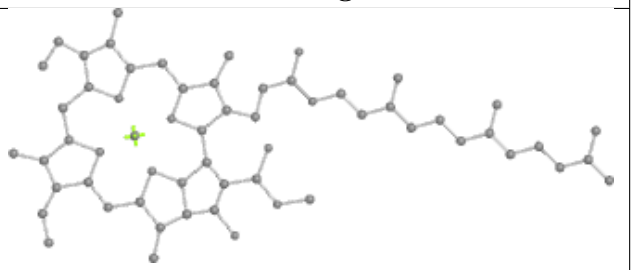


Bond angles

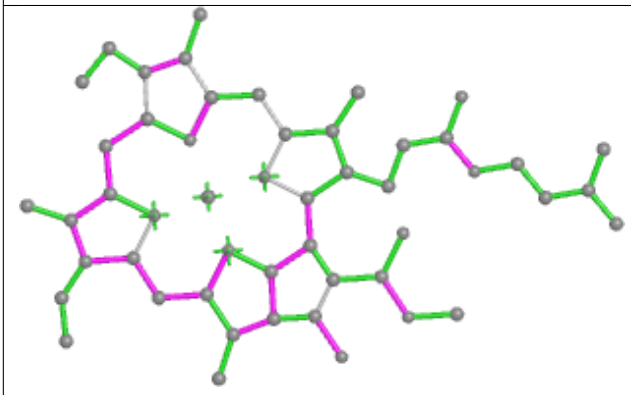


Torsions



Rings

Ligand CLA 6 609



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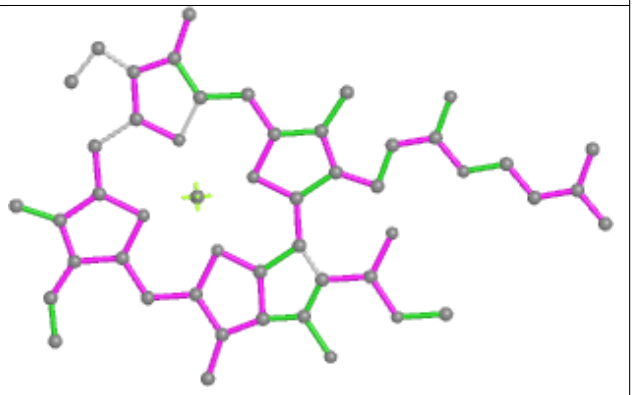
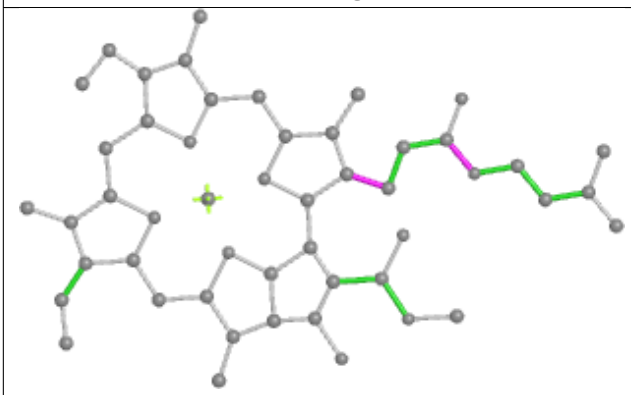


Bond angles



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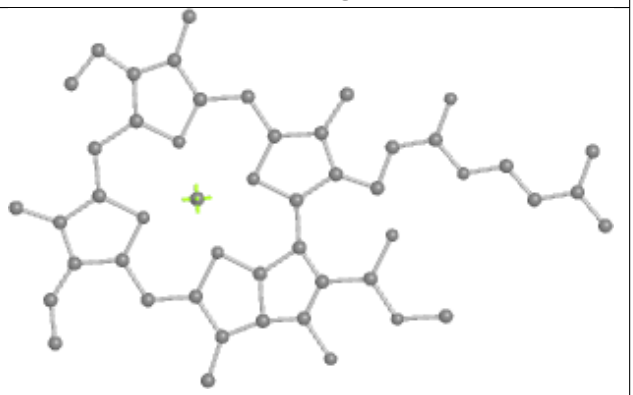
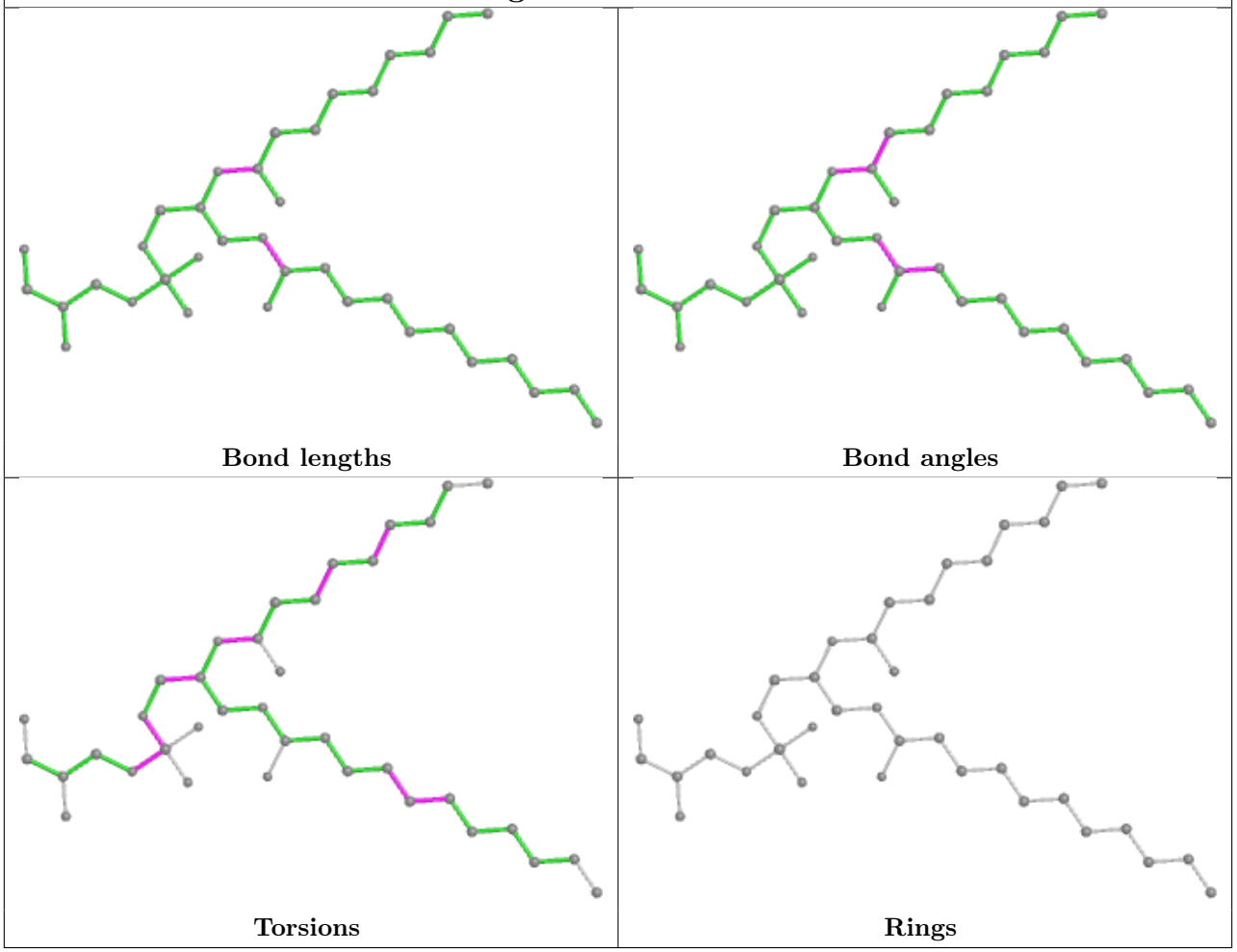
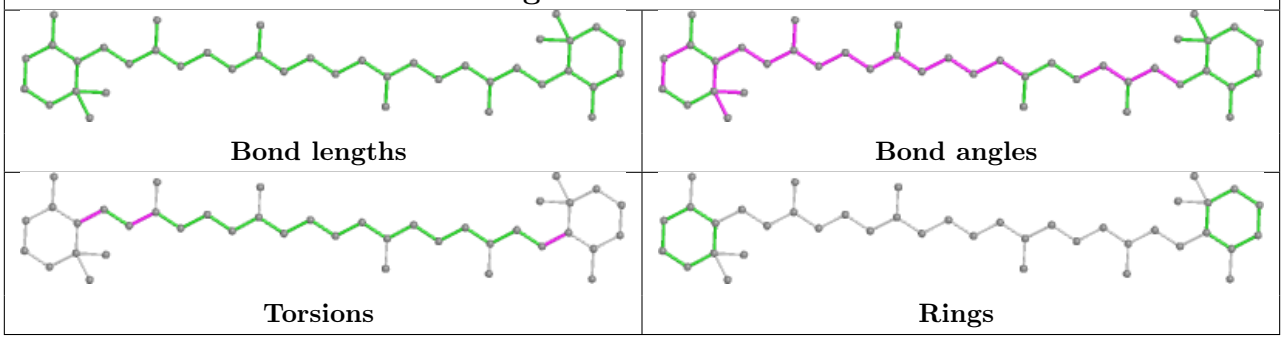


Rings

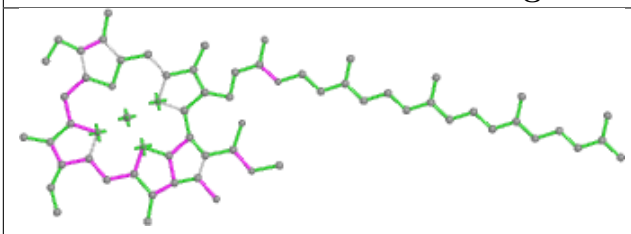
Ligand LHG 7 625



Ligand BCR A 849



Ligand CLA A 835



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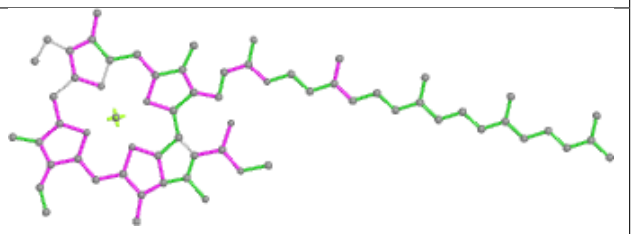
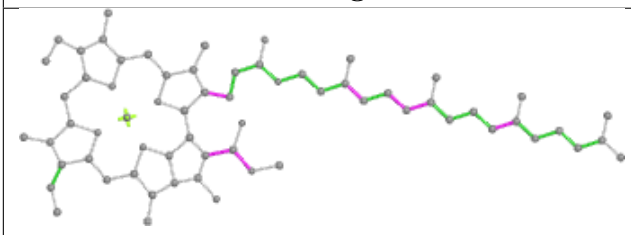


Bond angles



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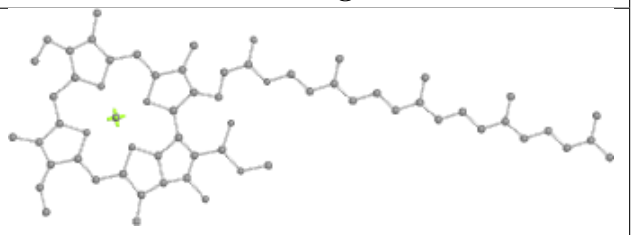
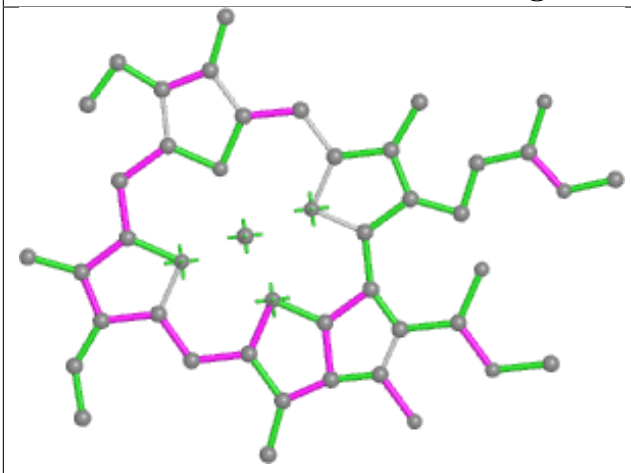


Rings

Ligand CLA 7 616



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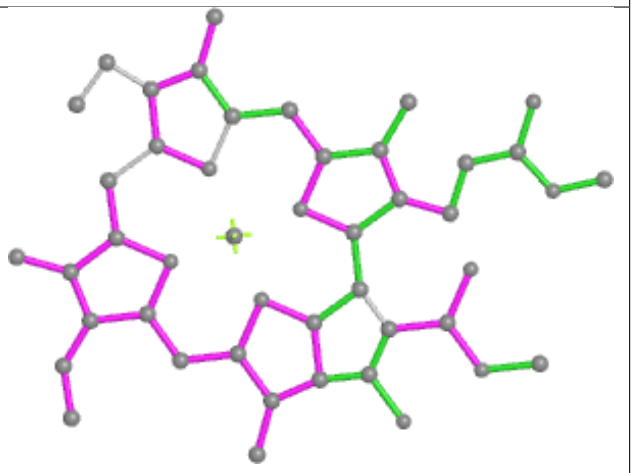
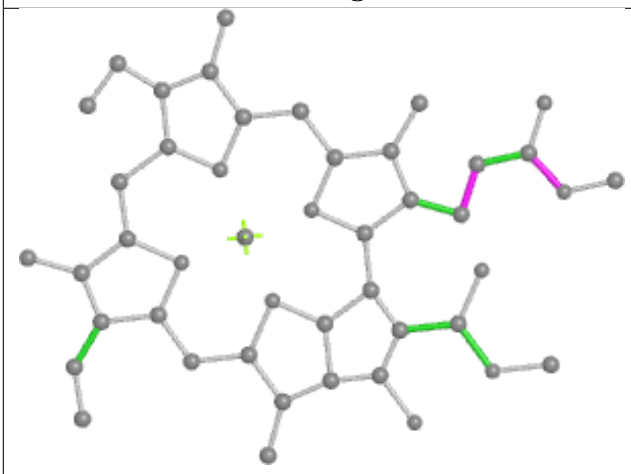


Bond angles



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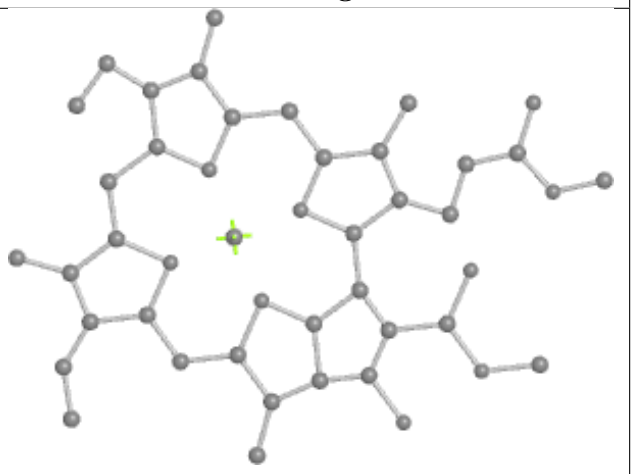
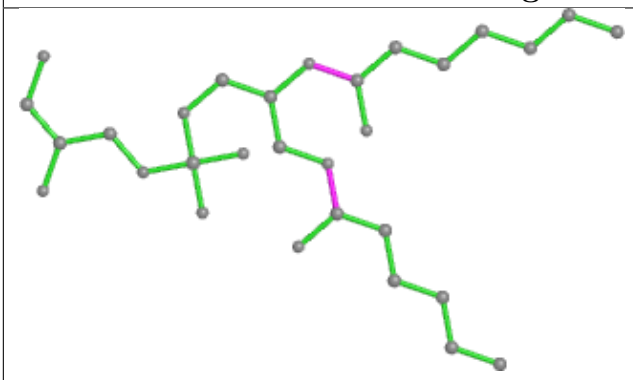


Rings

Ligand LHG A 855



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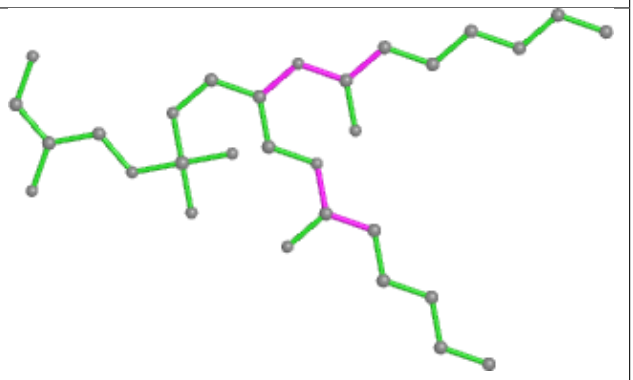
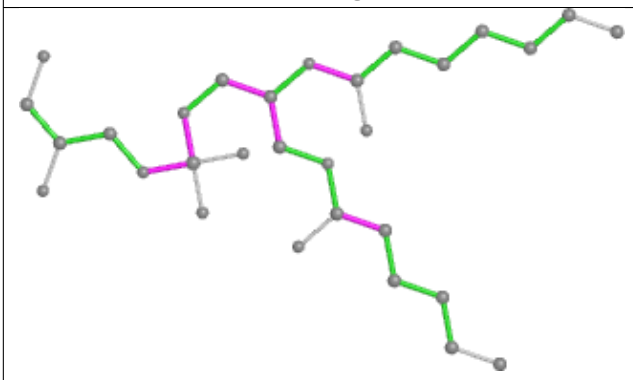
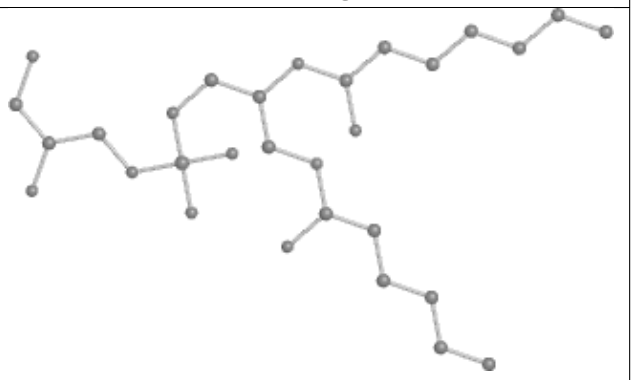


Bond angles

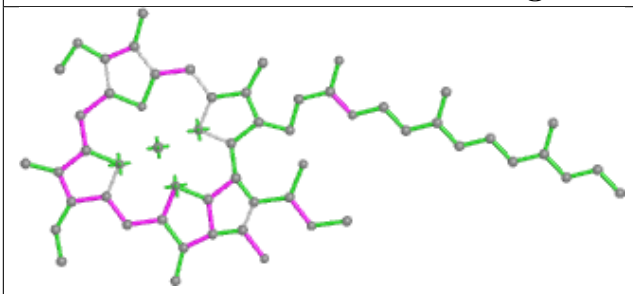


Torsions



Rings

Ligand CLA Z 604



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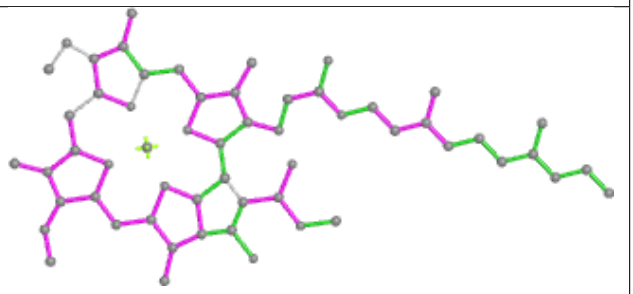
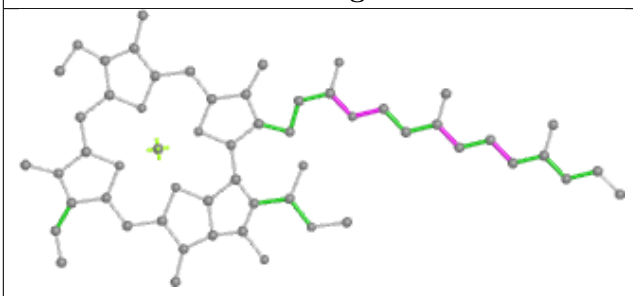


Bond angles



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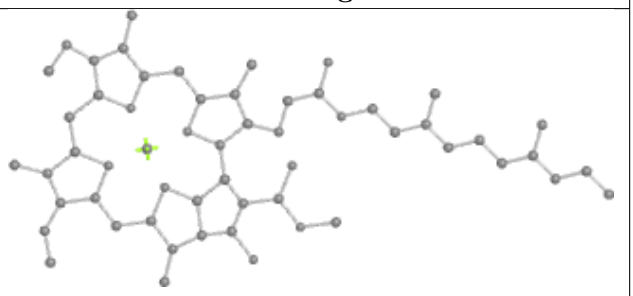
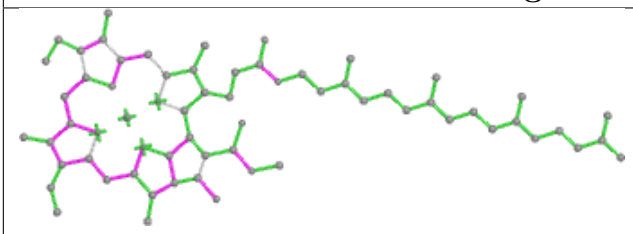


Rings

Ligand CLA B 828



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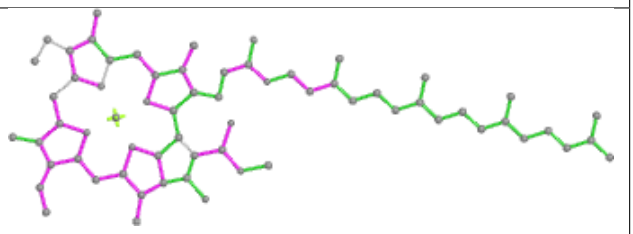
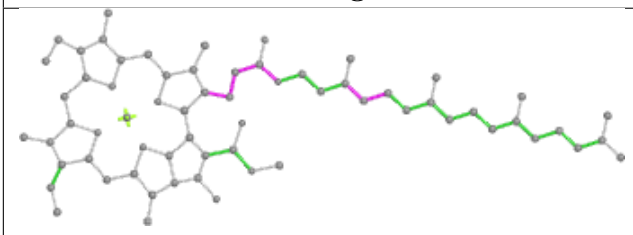


Bond angles



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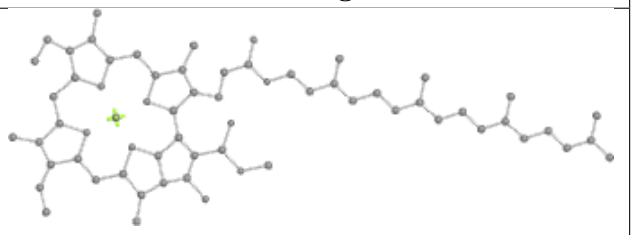
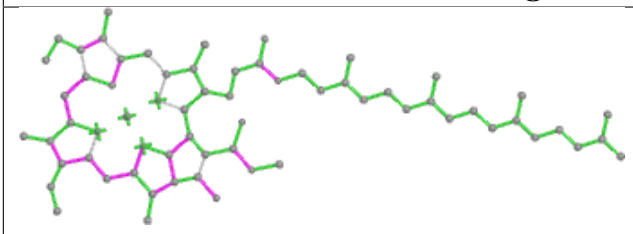
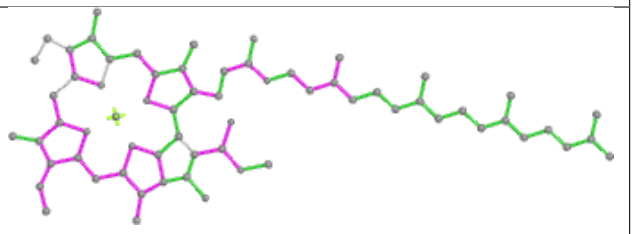


Rings

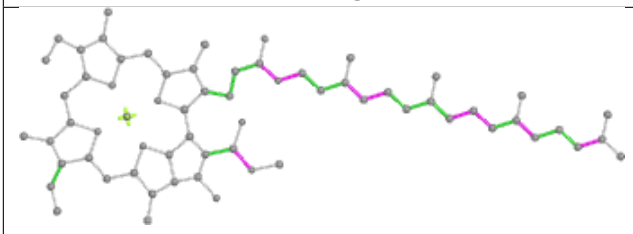
Ligand CLA B 819



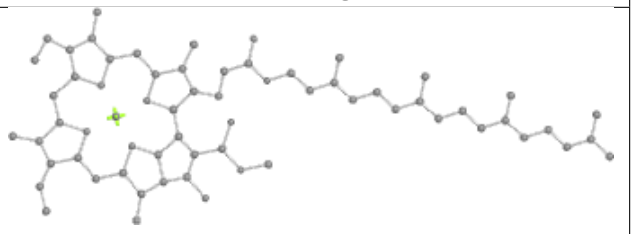
Bond lengths



Bond angles

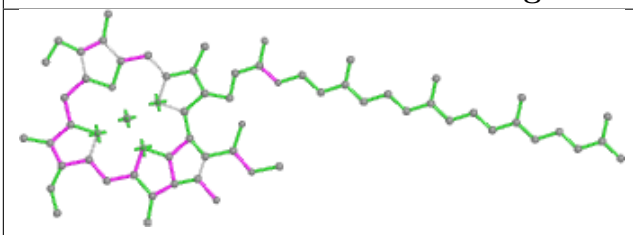


Torsions

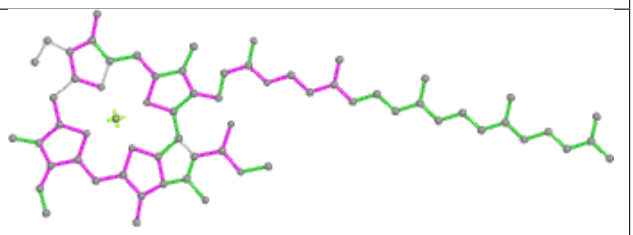


Rings

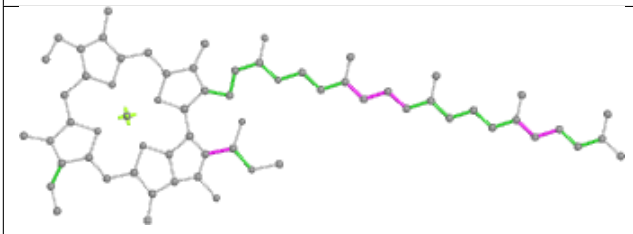
Ligand CLA A 816



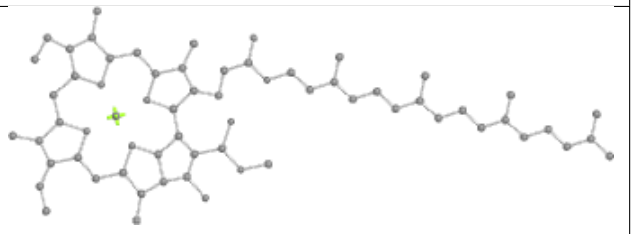
Bond lengths



Bond angles

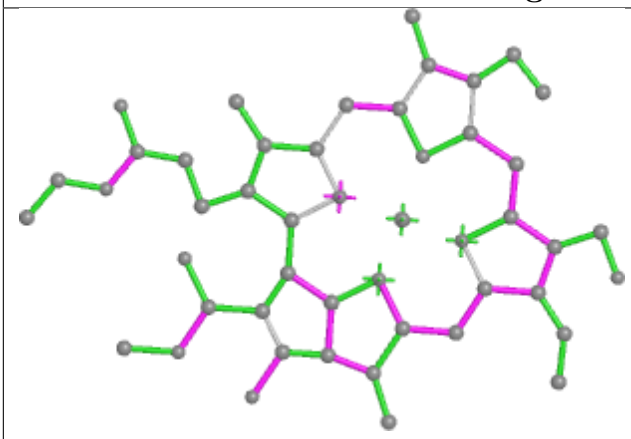


Torsions

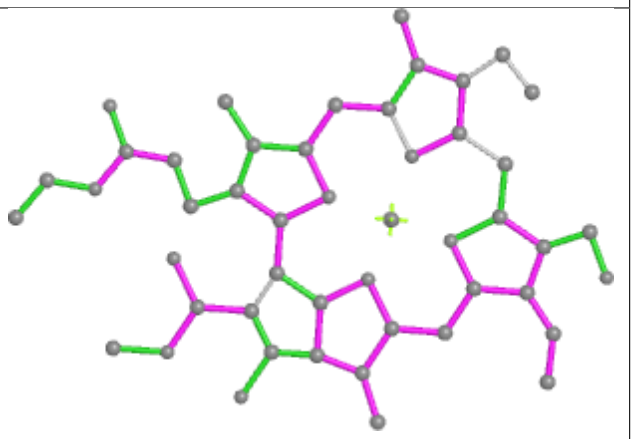


Rings

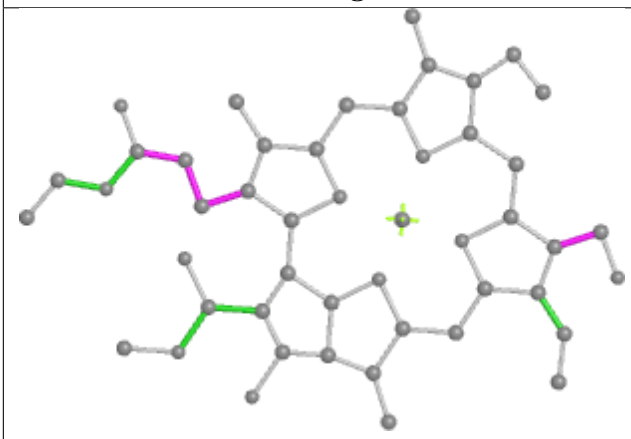
Ligand CHL Z 607



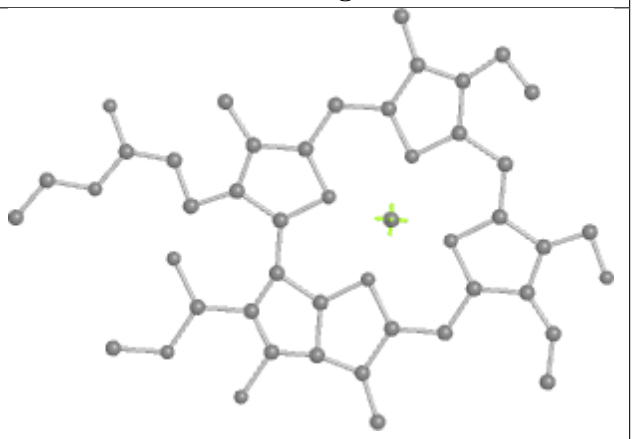
Bond lengths



Bond angles

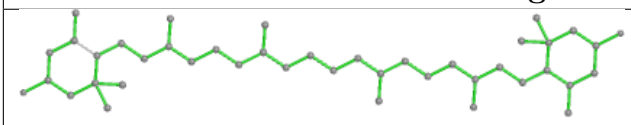


Torsions

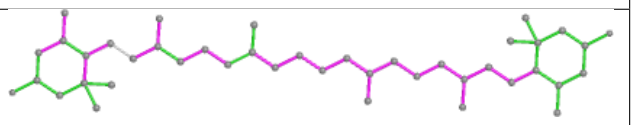


Rings

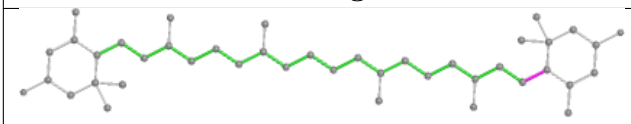
Ligand LUT 1 617



Bond lengths



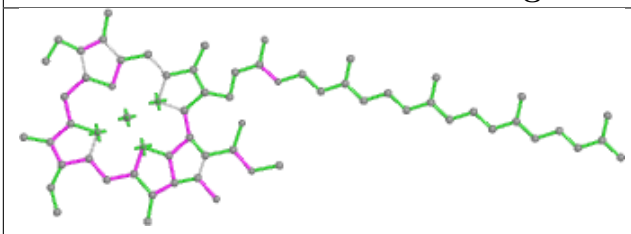
Bond angles



Torsions

Rings

Ligand CLA A 820



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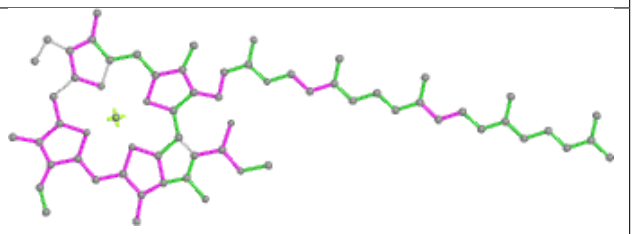
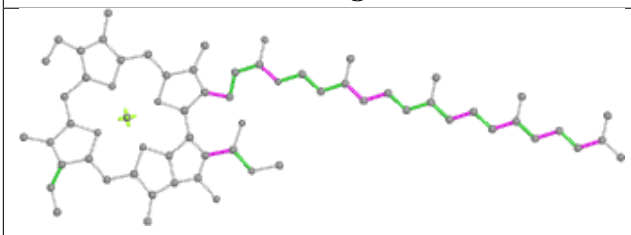
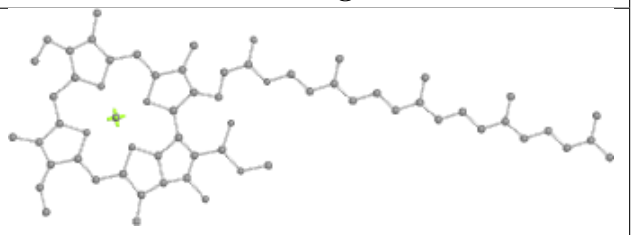


Bond angles

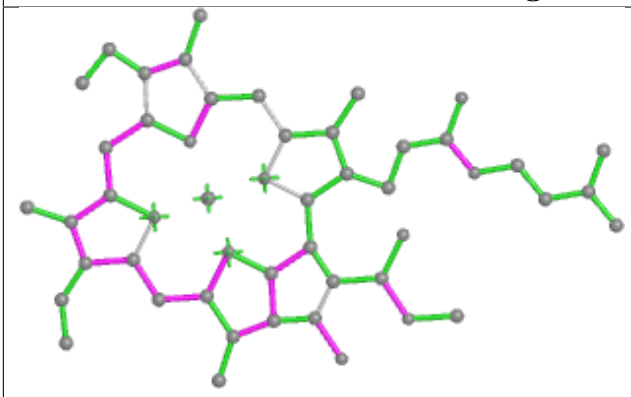


Torsions

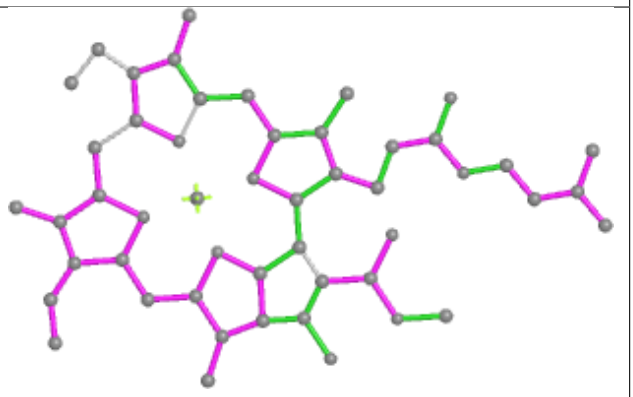


Rings

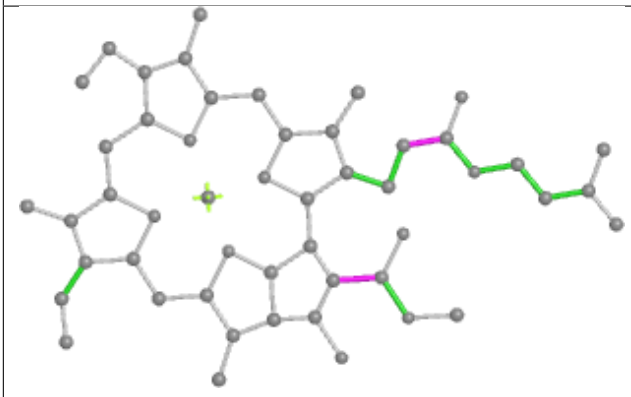
Ligand CLA B 830



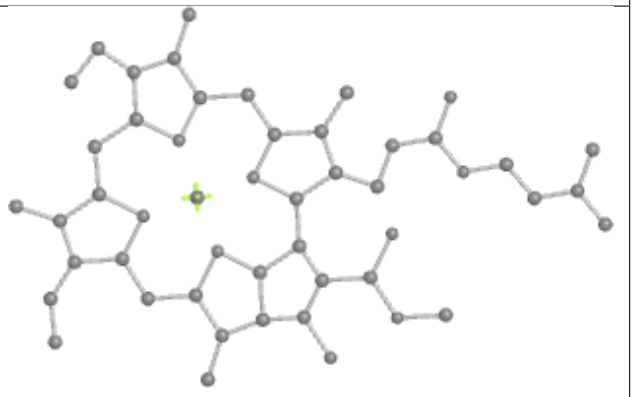
Bond lengths



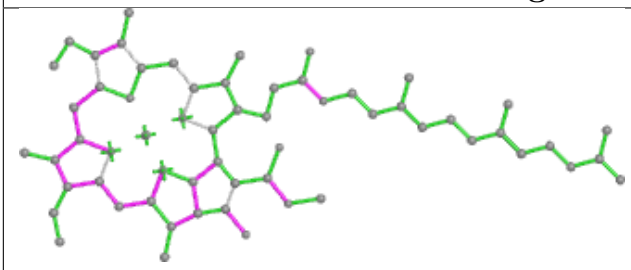
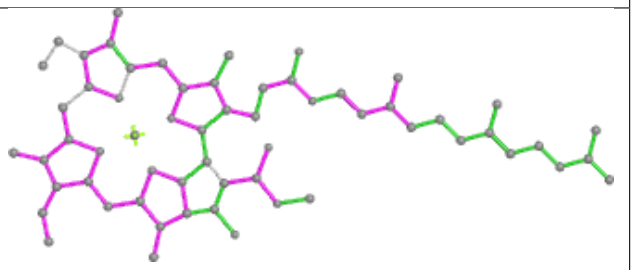
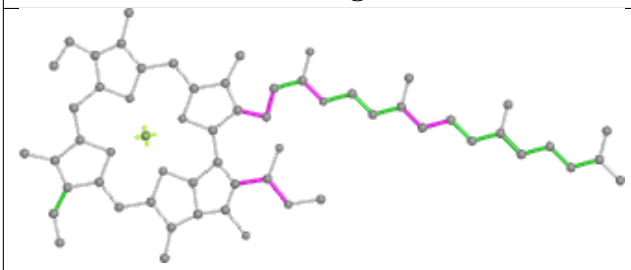
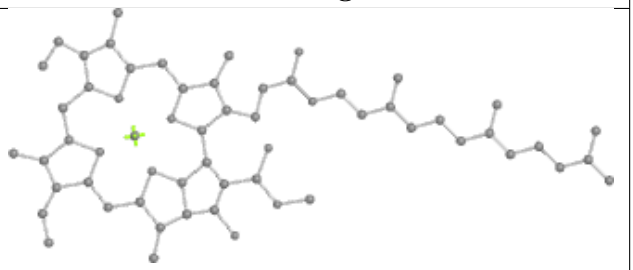
Bond angles

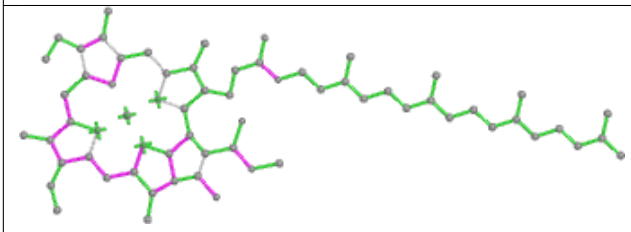
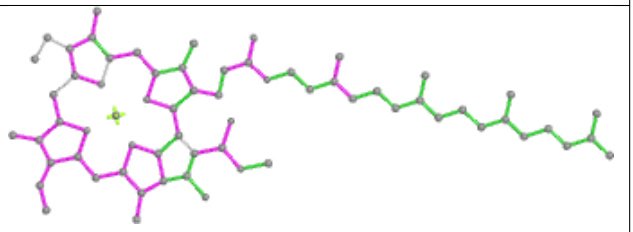
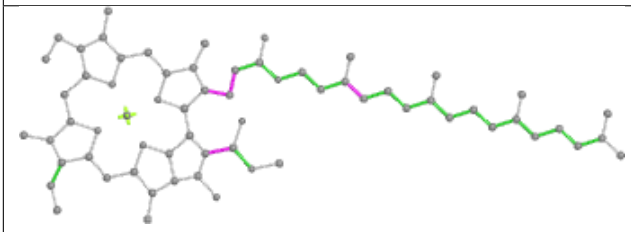
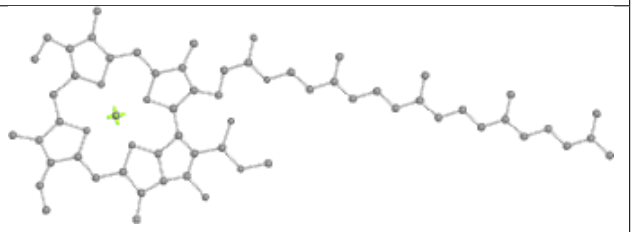


Torsions

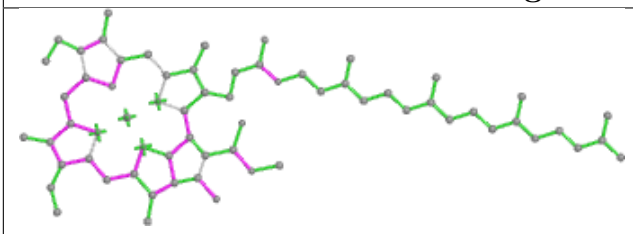


Rings

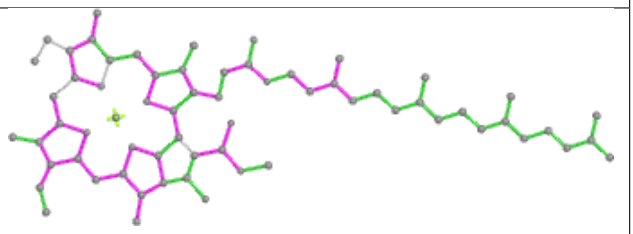
Ligand CLA 3 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 803	
	
Bond lengths	Bond angles
	
Torsions	Rings

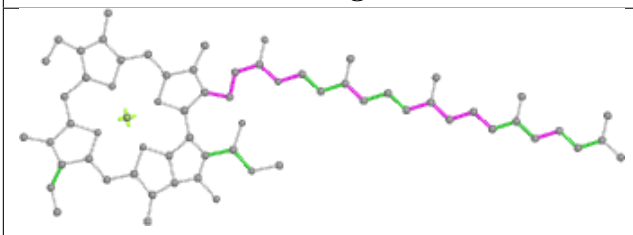
Ligand CLA B 827



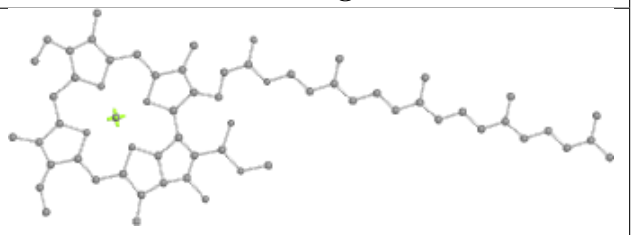
Bond lengths



Bond angles

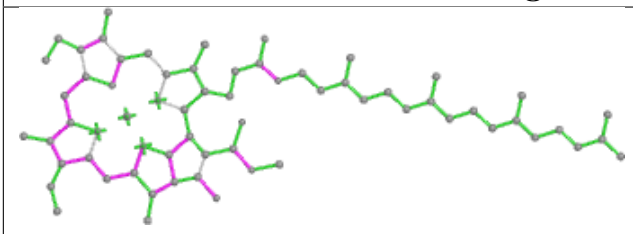


Torsions



Rings

Ligand CLA B 825



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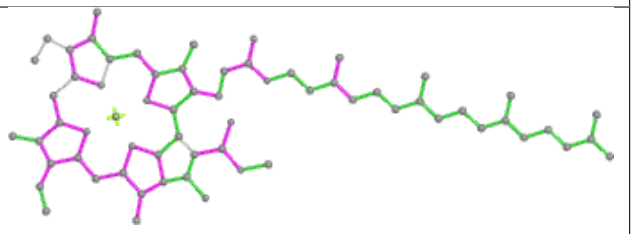
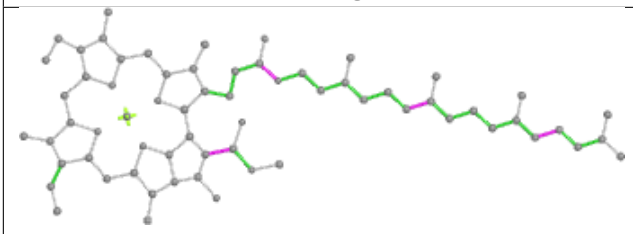


Bond angles



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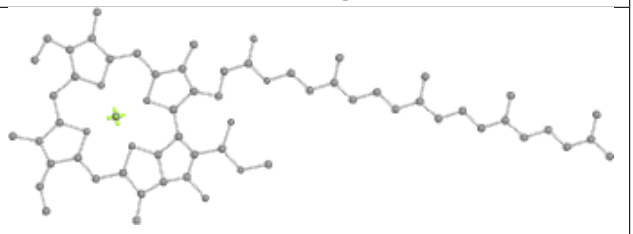
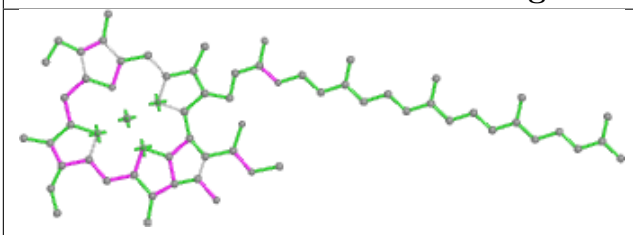


Rings

Ligand CLA 3 604



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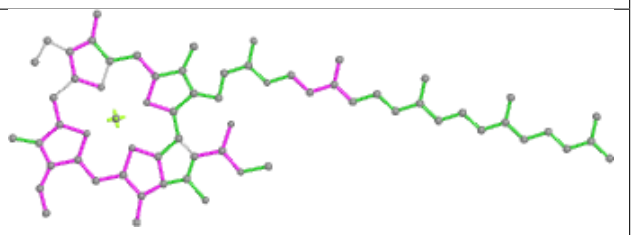
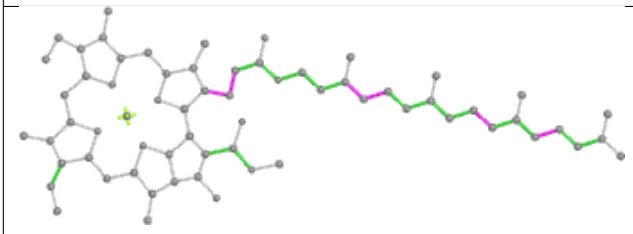
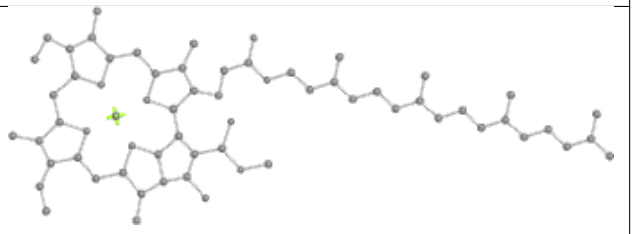


Bond angles

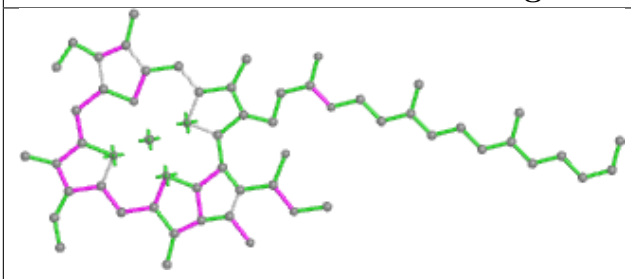


Torsions



Rings

Ligand CLA B 822



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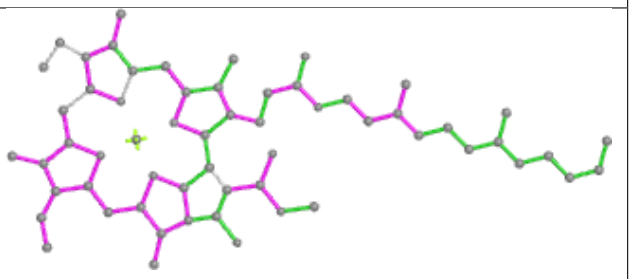
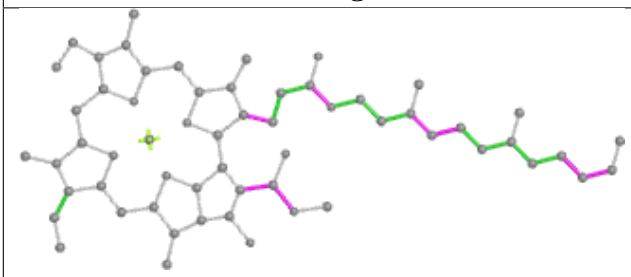
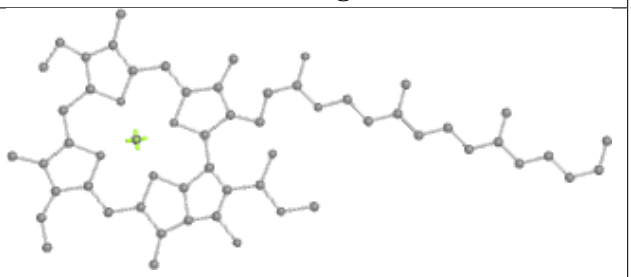


Bond angles

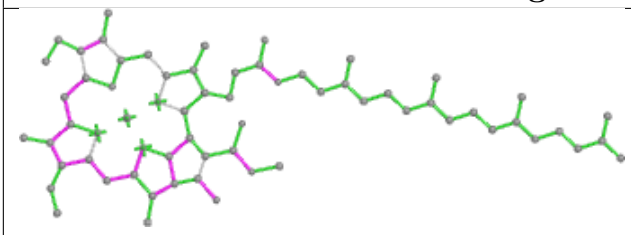


Torsions



Rings

Ligand CLA 7 602



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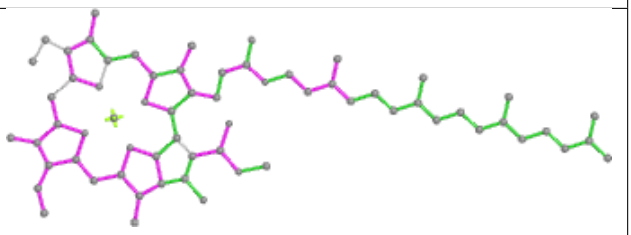
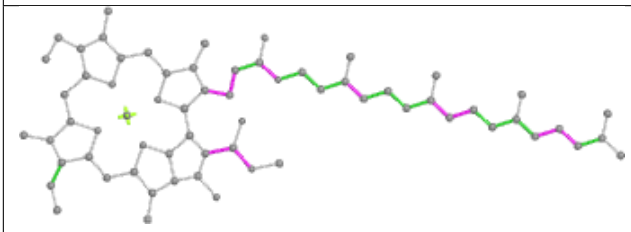


Bond angles



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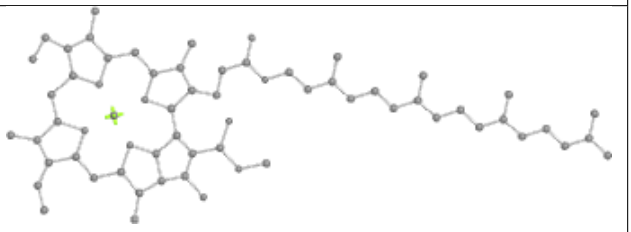
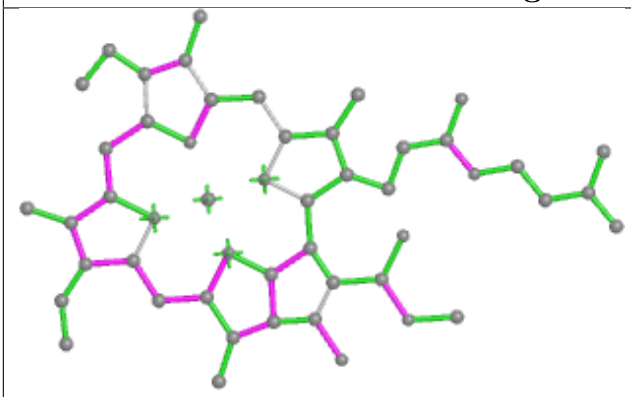


Rings

Ligand CLA A 832



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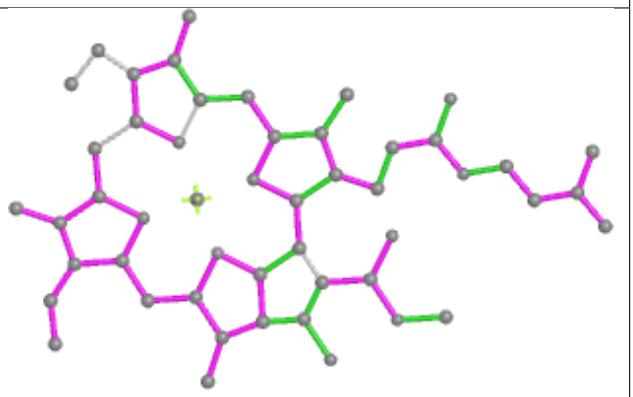
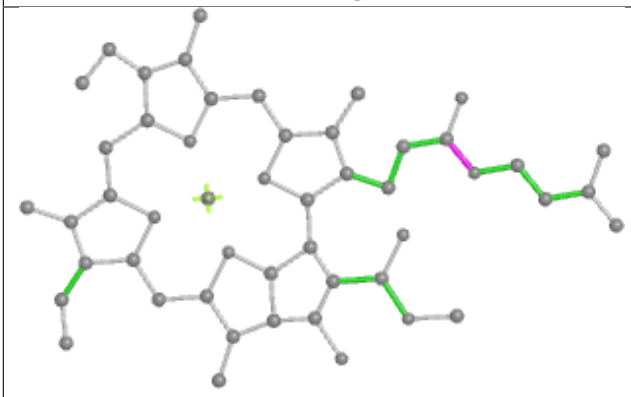


Bond angles



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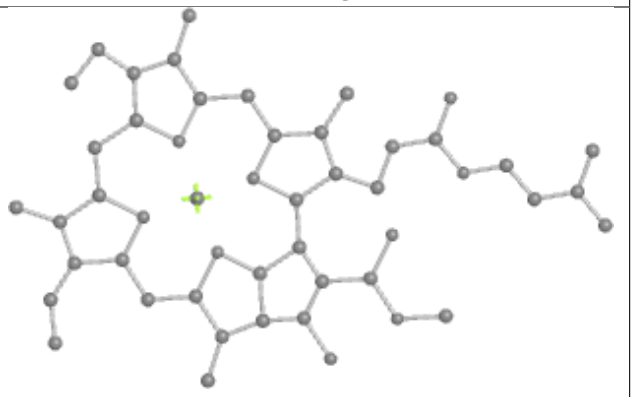
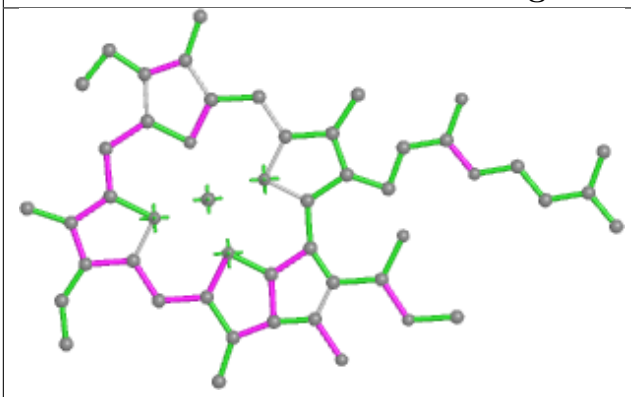


Rings

Ligand CLA 4 604



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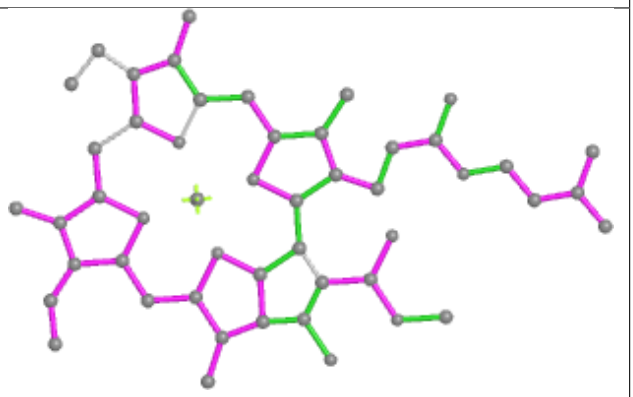
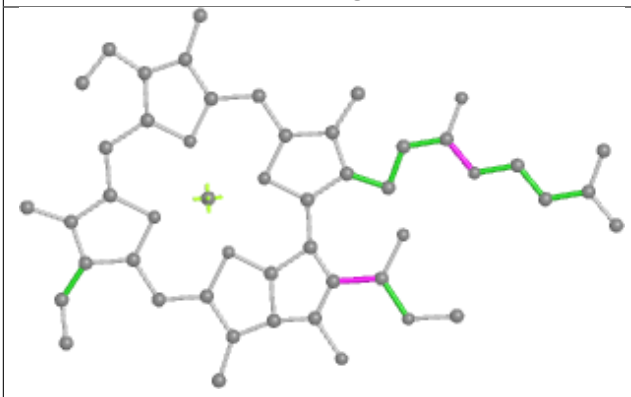
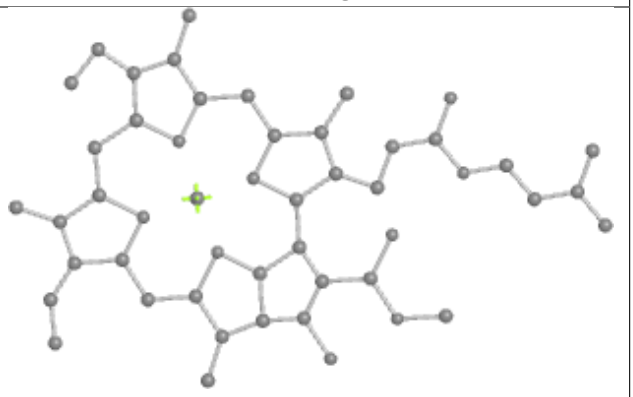


Bond angles

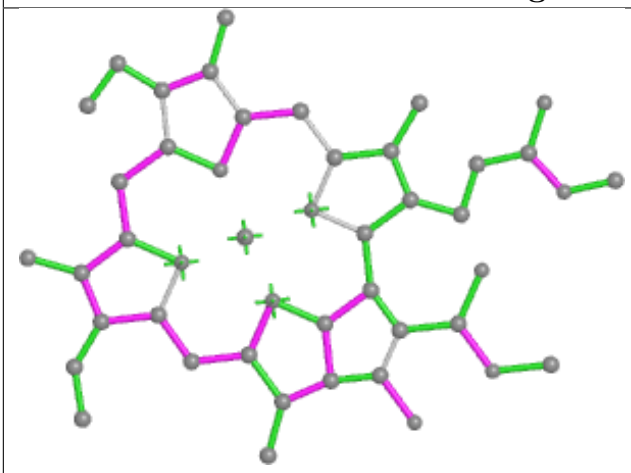


Torsions



Rings

Ligand CLA 6 603



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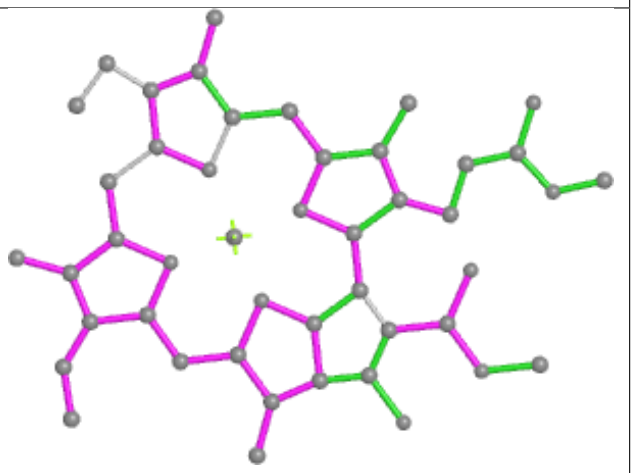
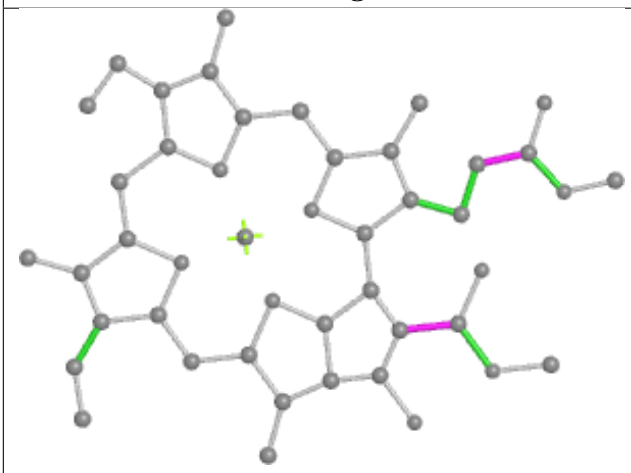
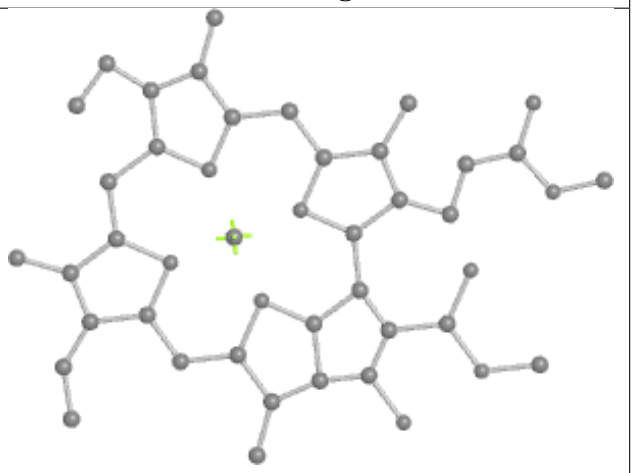


Bond angles

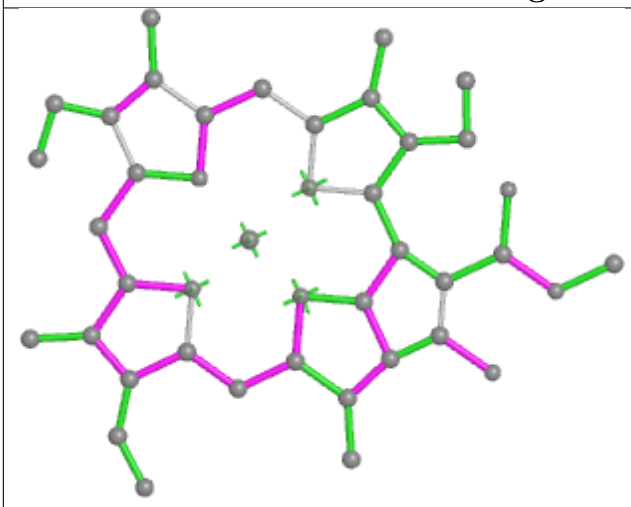


Torsions



Rings

Ligand CLA 8 606



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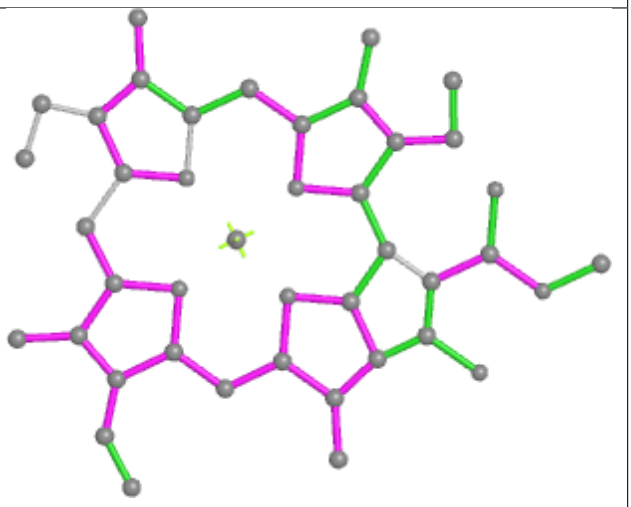
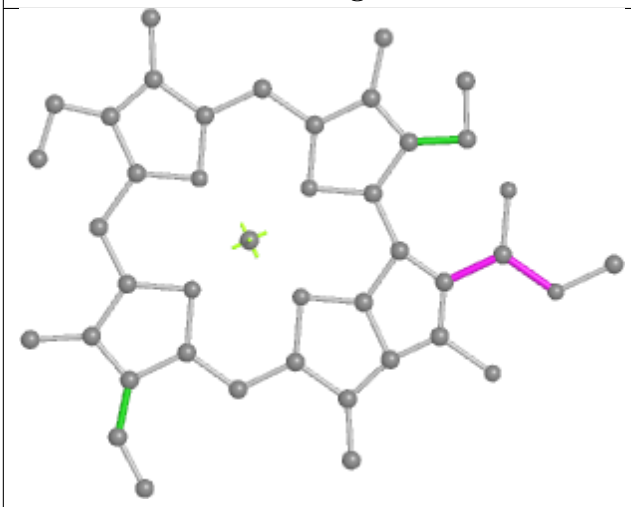
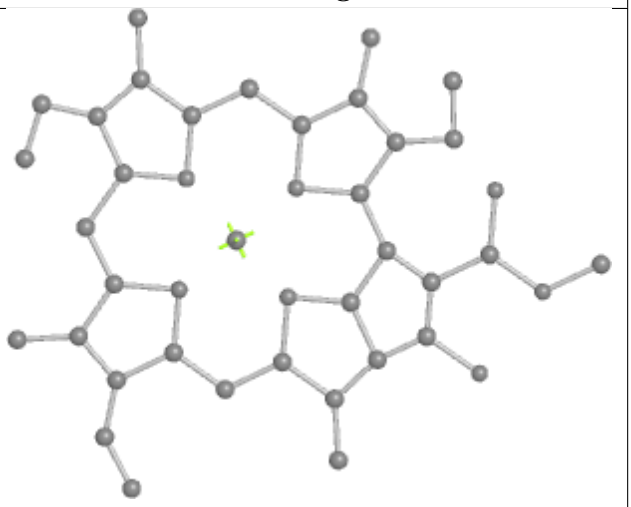


Bond angles

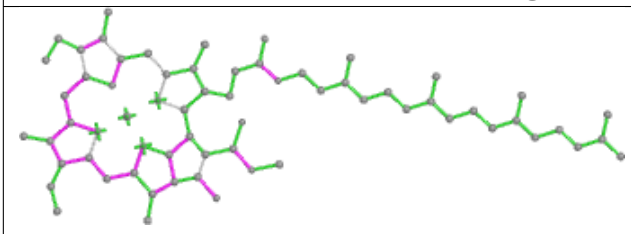


Torsions

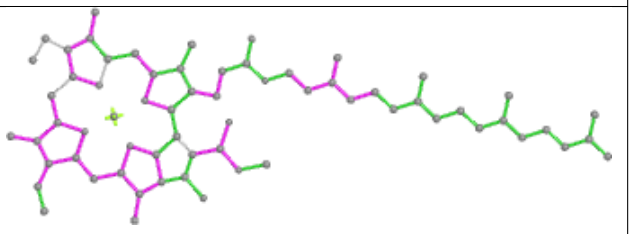


Rings

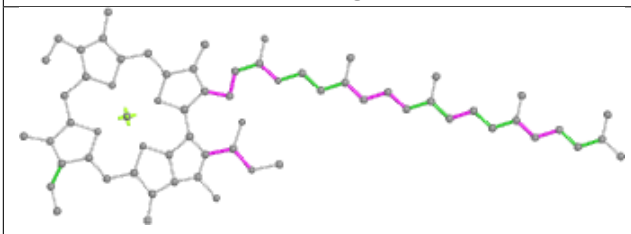
Ligand CLA A 809



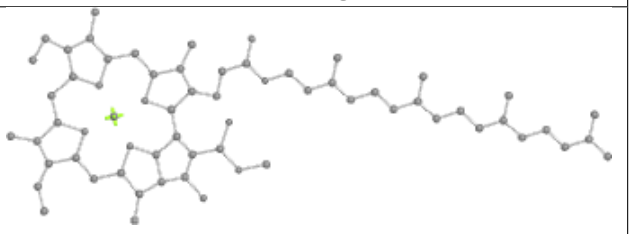
Bond lengths



Bond angles

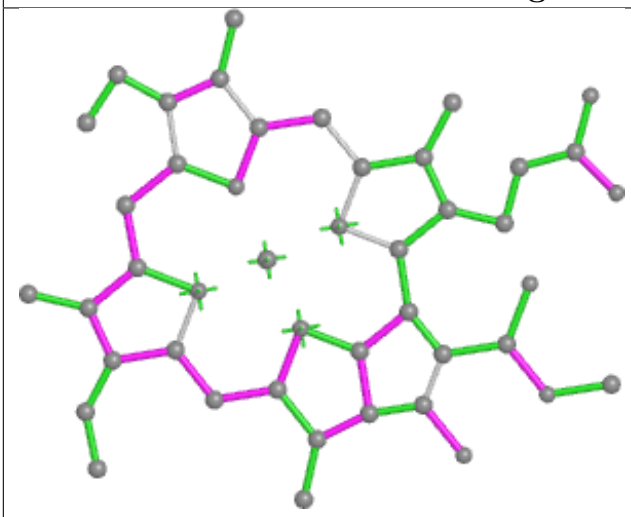


Torsions

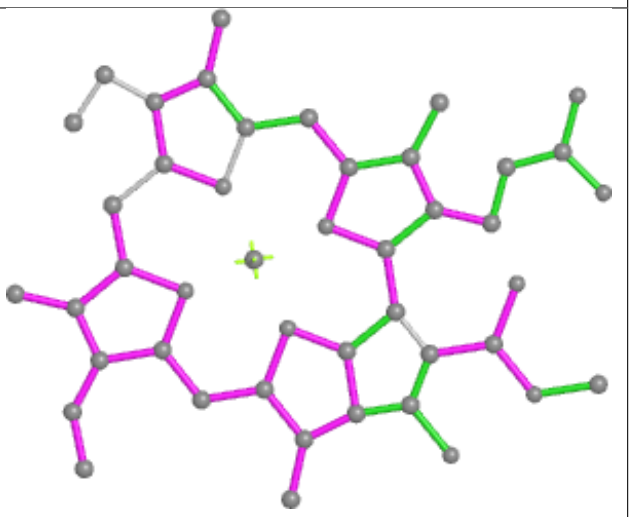


Rings

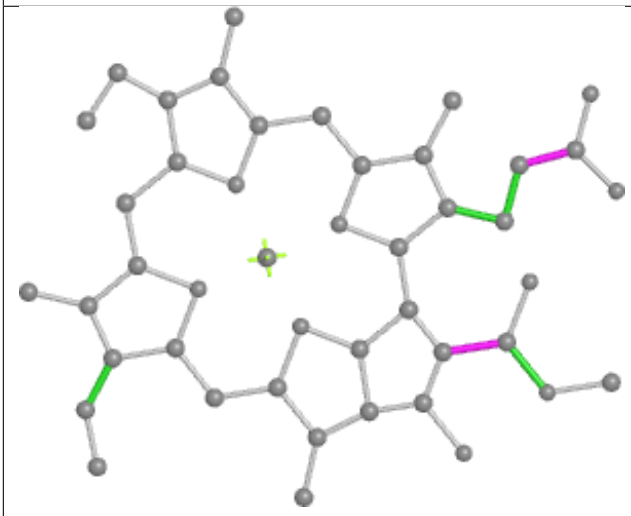
Ligand CLA 6 622



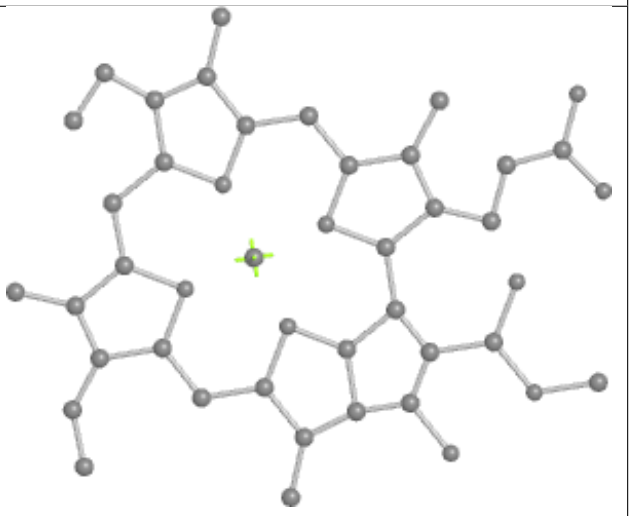
Bond lengths



Bond angles

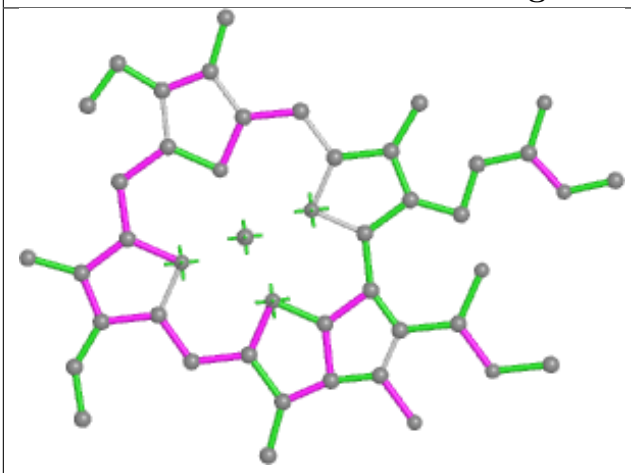


Torsions

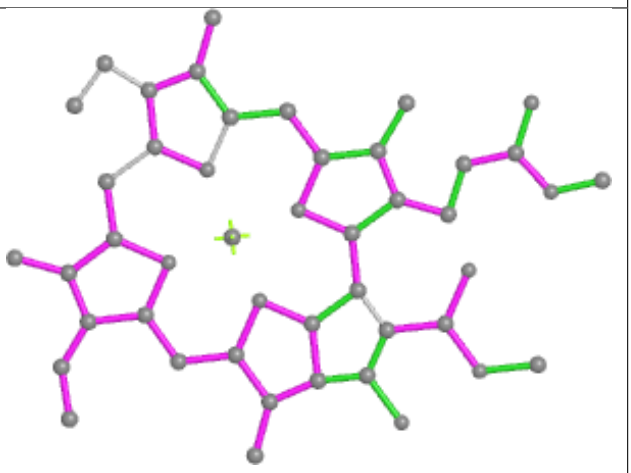


Rings

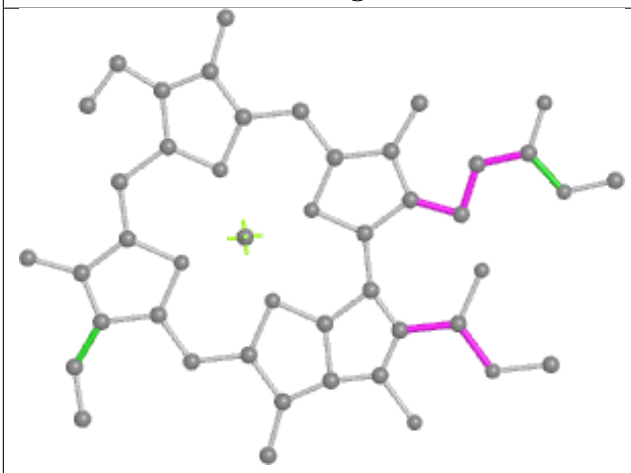
Ligand CLA 5 616



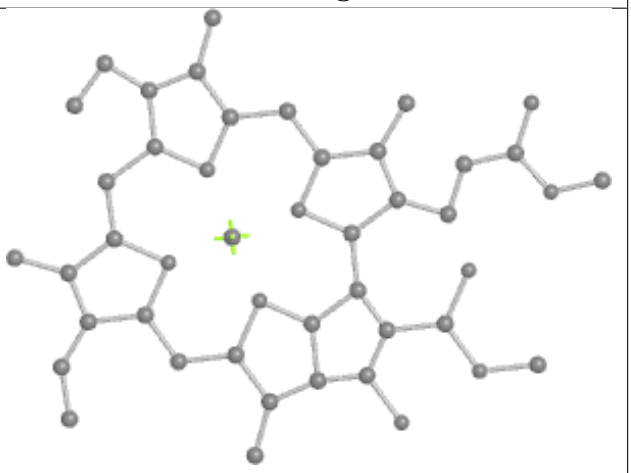
Bond lengths



Bond angles

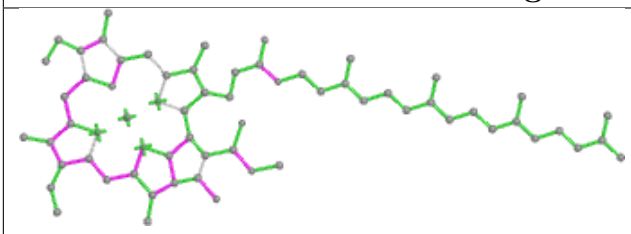


Torsions

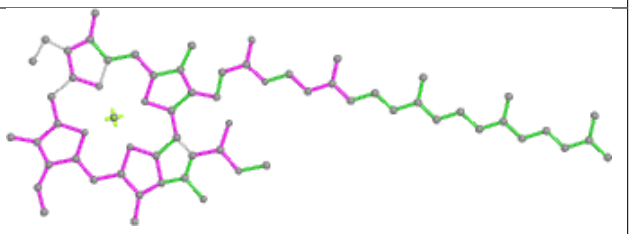


Rings

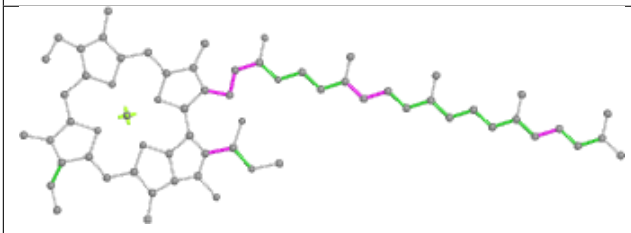
Ligand CLA B 824



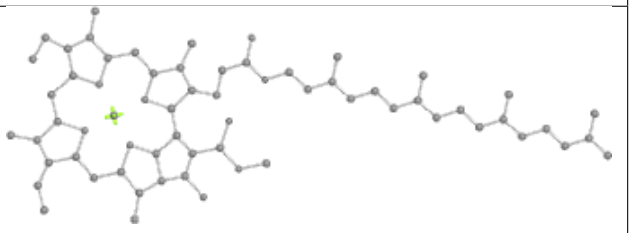
Bond lengths



Bond angles

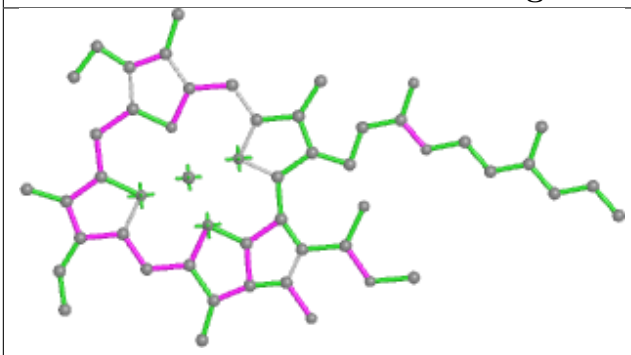


Torsions

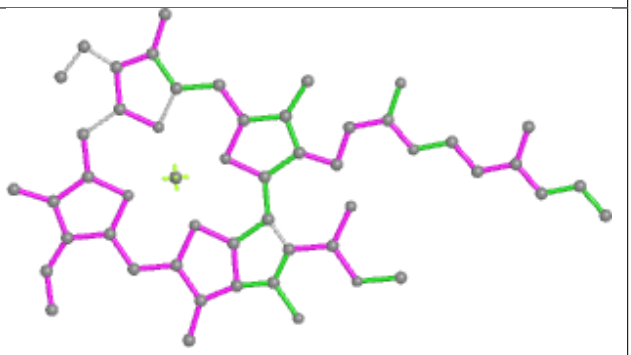


Rings

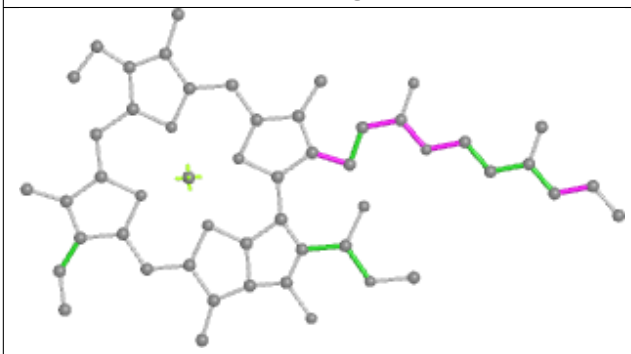
Ligand CLA Z 612



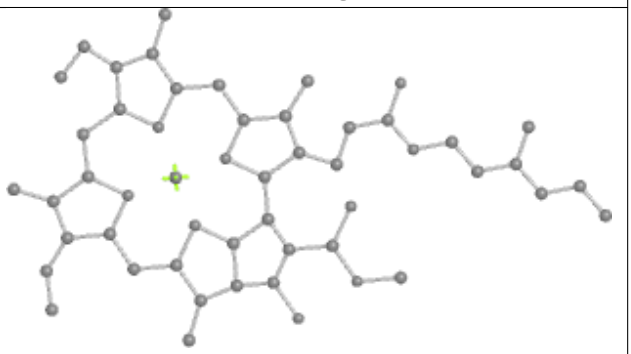
Bond lengths



Bond angles

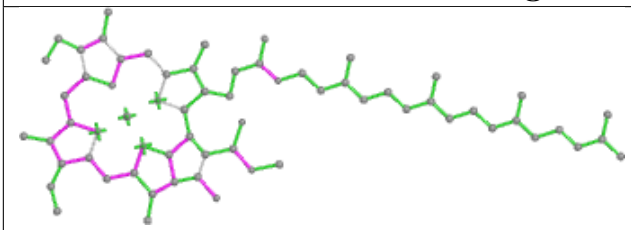


Torsions

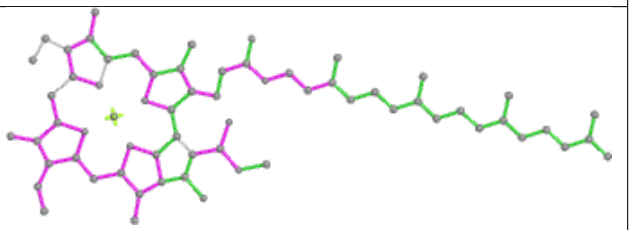


Rings

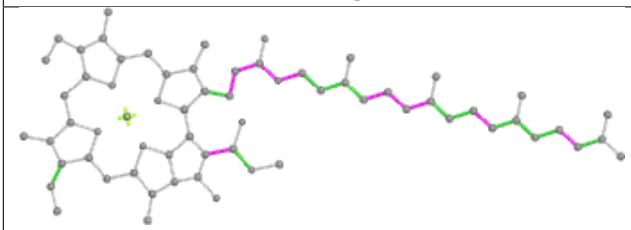
Ligand CLA B 812



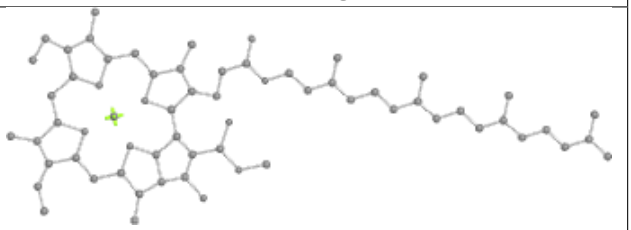
Bond lengths



Bond angles

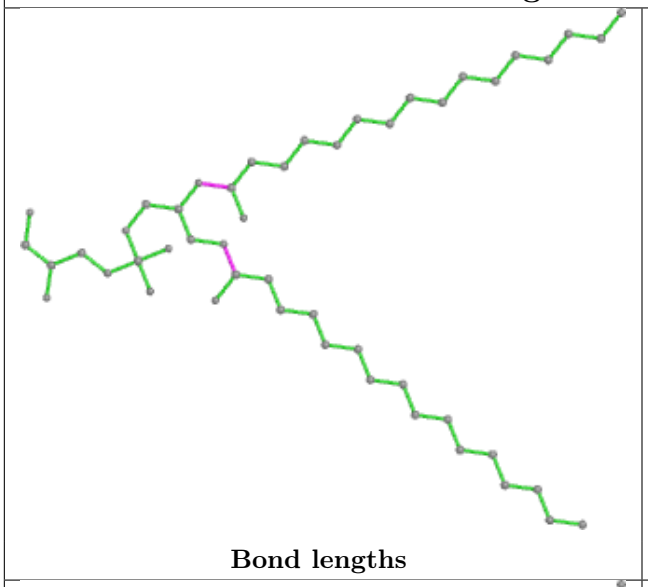


Torsions

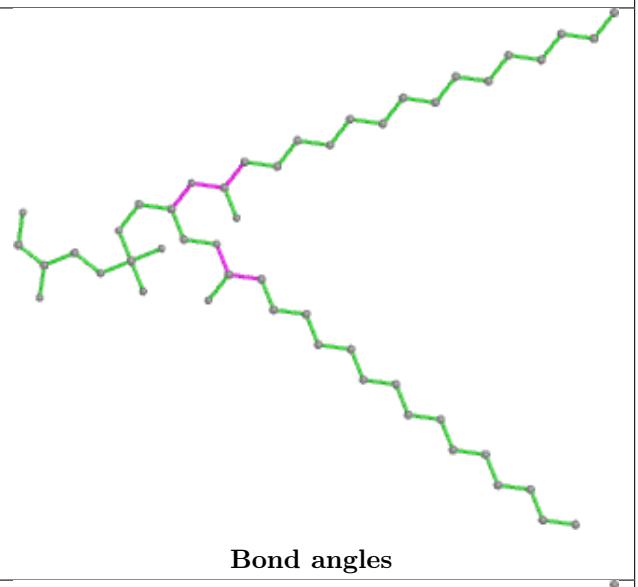


Rings

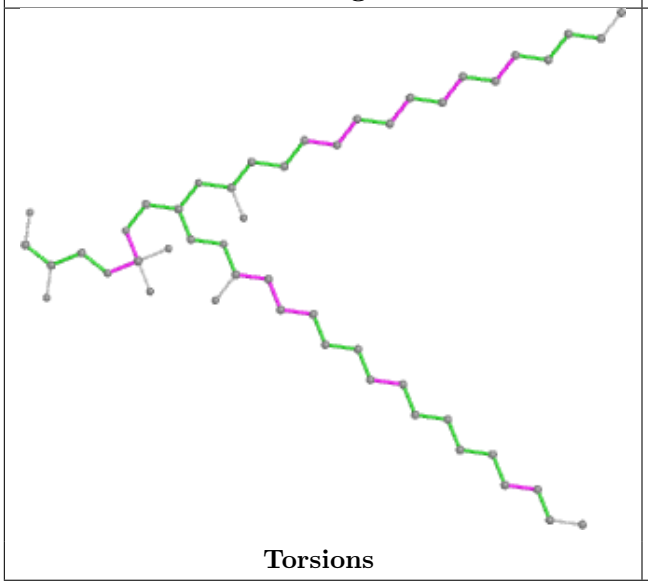
Ligand LHG A 846



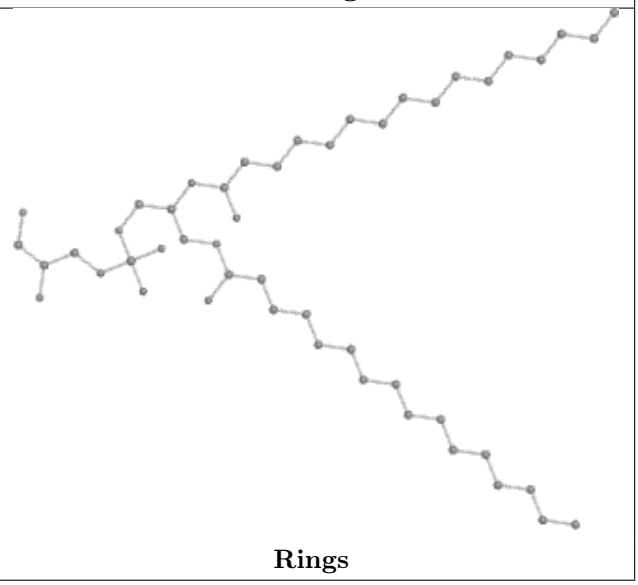
Bond lengths



Bond angles

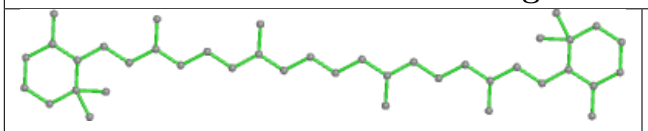


Torsions

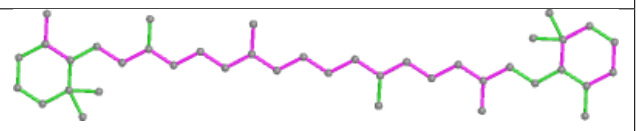


Rings

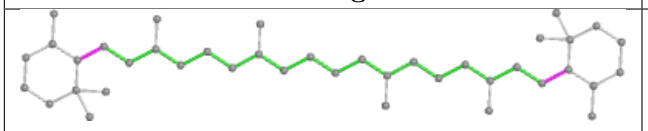
Ligand BCR G 205



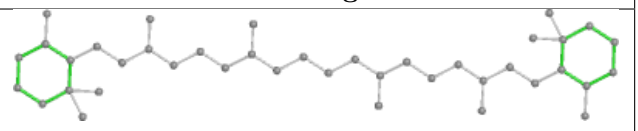
Bond lengths



Bond angles

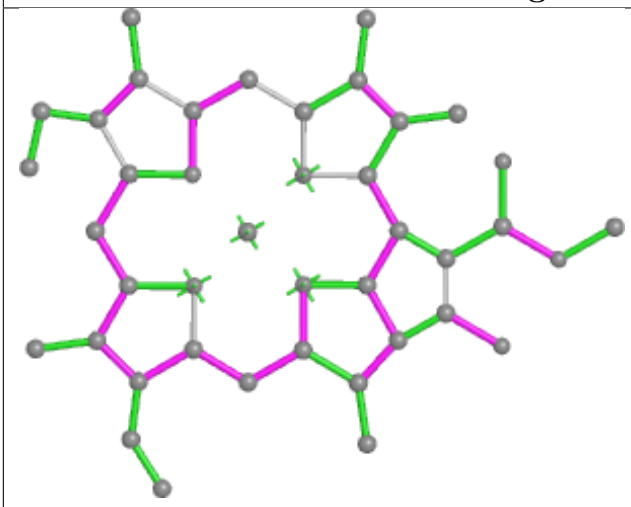


Torsions

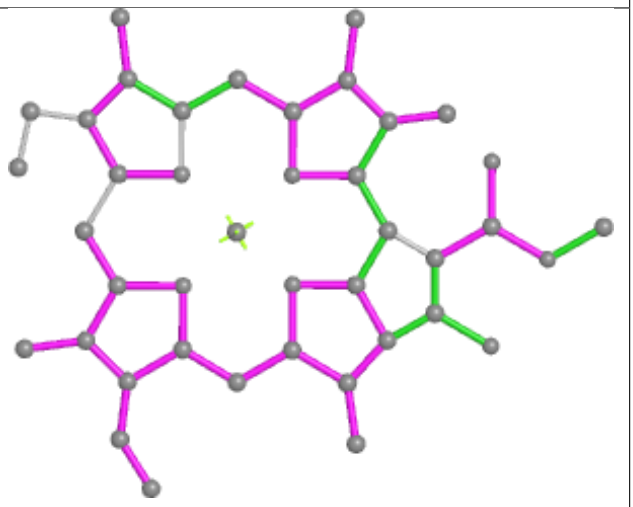


Rings

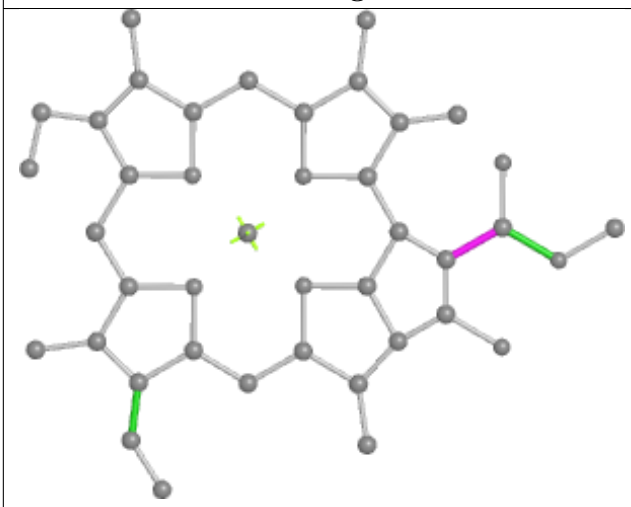
Ligand CLA 7 611



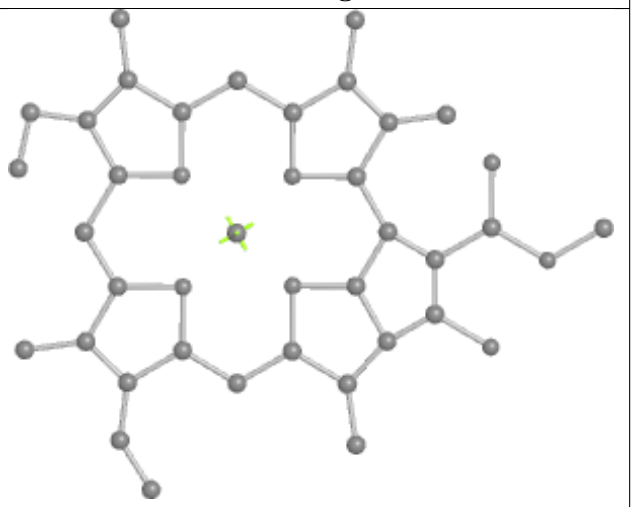
Bond lengths



Bond angles

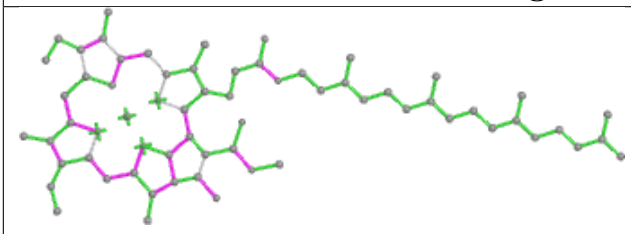


Torsions

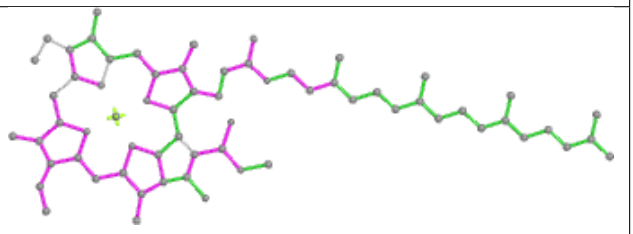


Rings

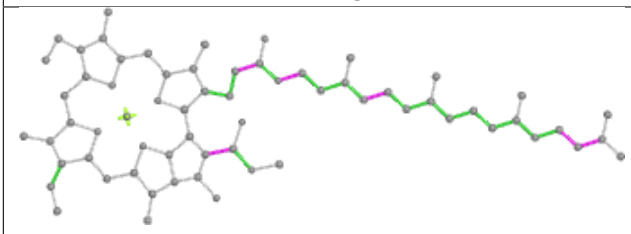
Ligand CL0 A 801



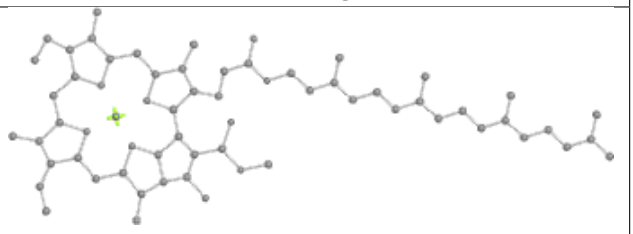
Bond lengths



Bond angles

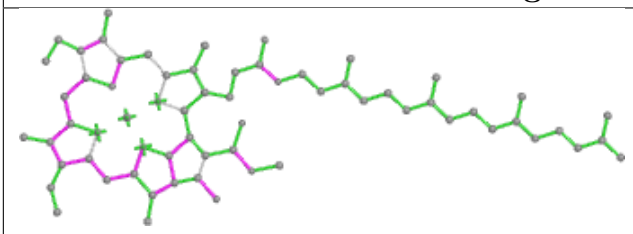


Torsions

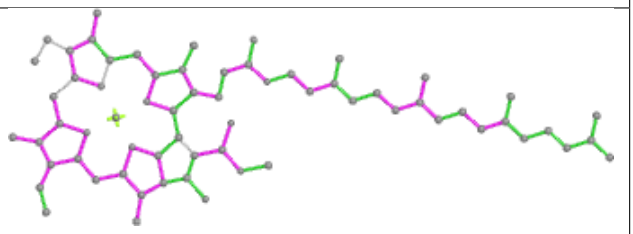


Rings

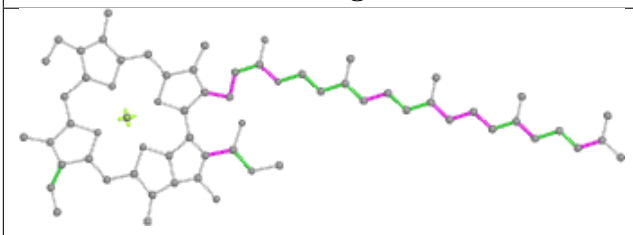
Ligand CLA A 812



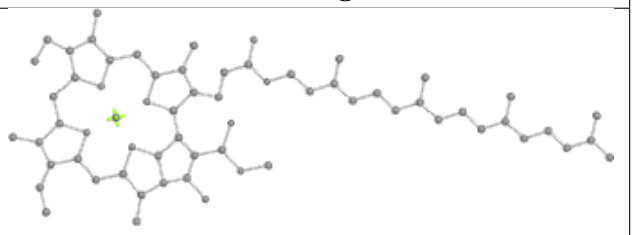
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

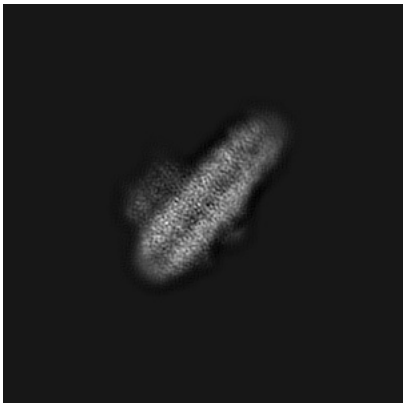
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-9854. These allow visual inspection of the internal detail of the map and identification of artifacts.

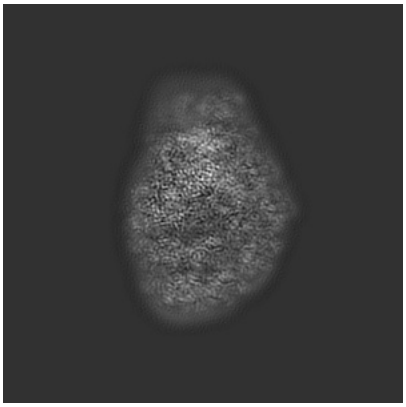
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

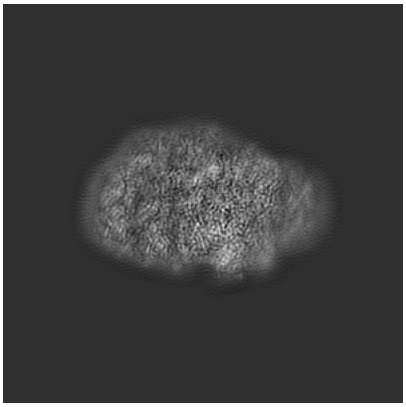
6.1.1 Primary map



X



Y

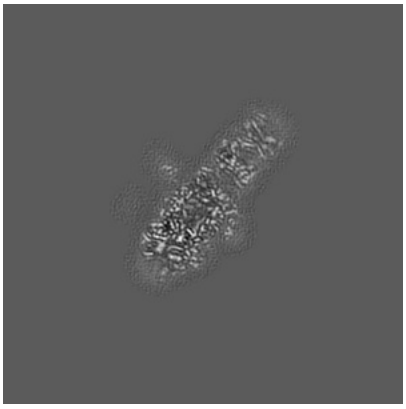


Z

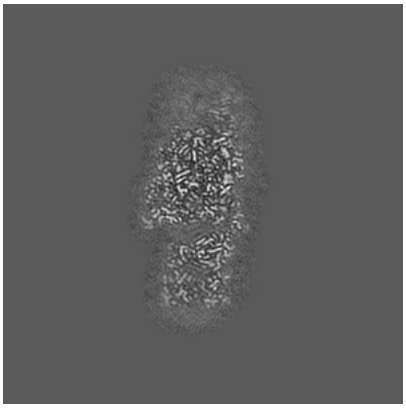
The images above show the map projected in three orthogonal directions.

6.2 Central slices

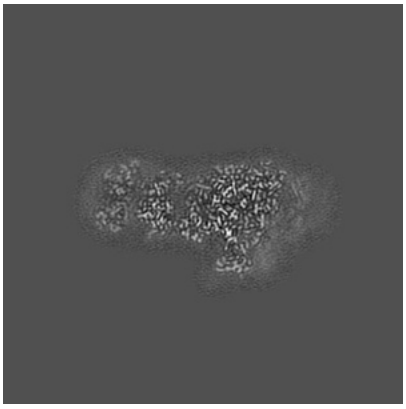
6.2.1 Primary map



X Index: 160



Y Index: 160

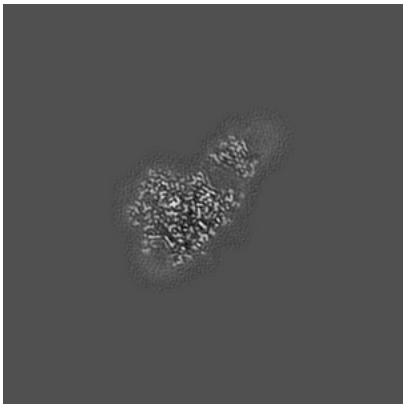


Z Index: 160

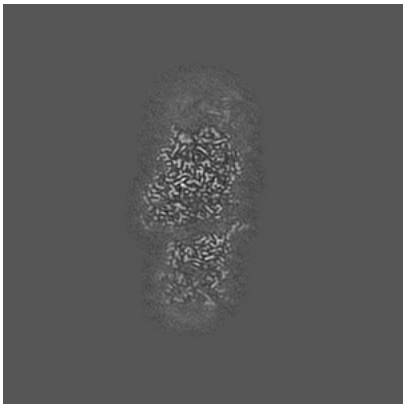
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

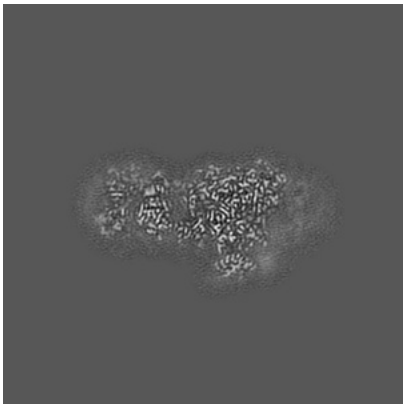
6.3.1 Primary map



X Index: 179



Y Index: 158

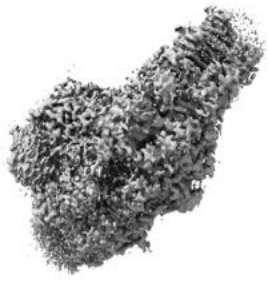


Z Index: 156

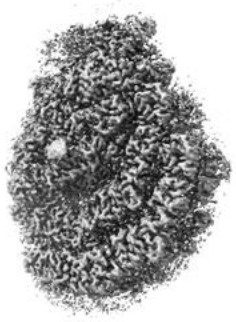
The images above show the largest variance slices of the map in three orthogonal directions.

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.

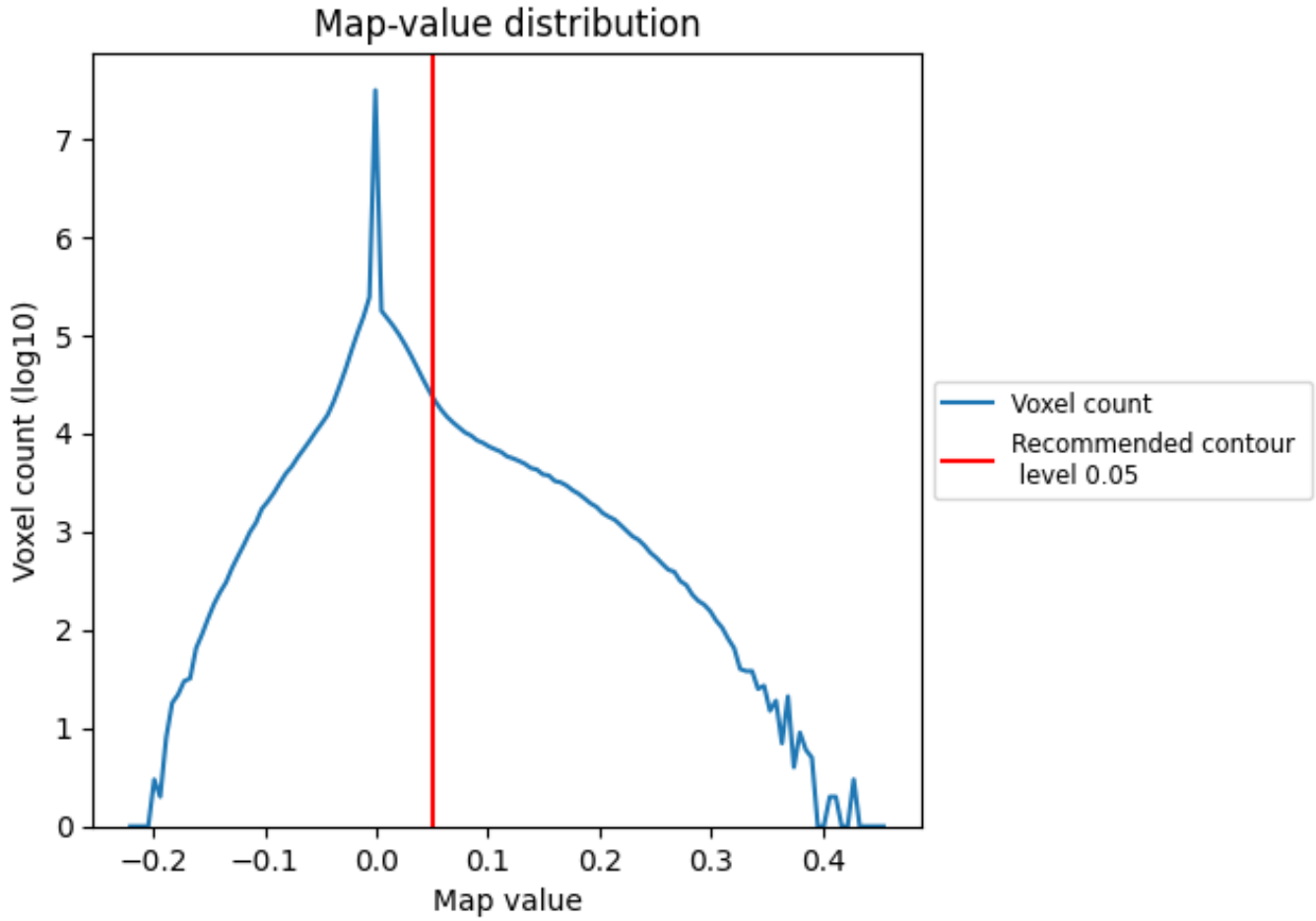
6.5 Mask visualisation (i)

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

7 Map analysis

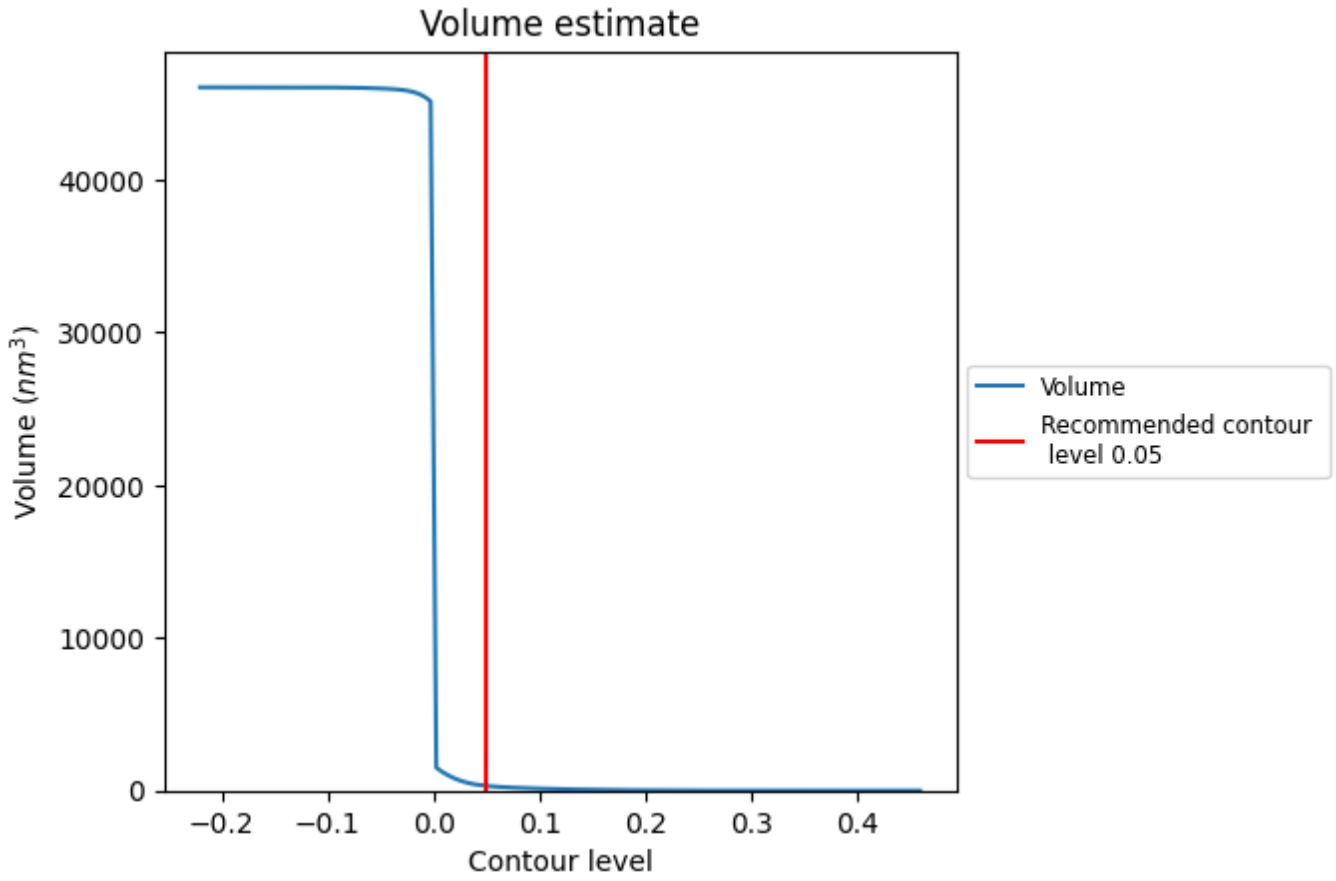
This section contains the results of statistical analysis of the map.

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.

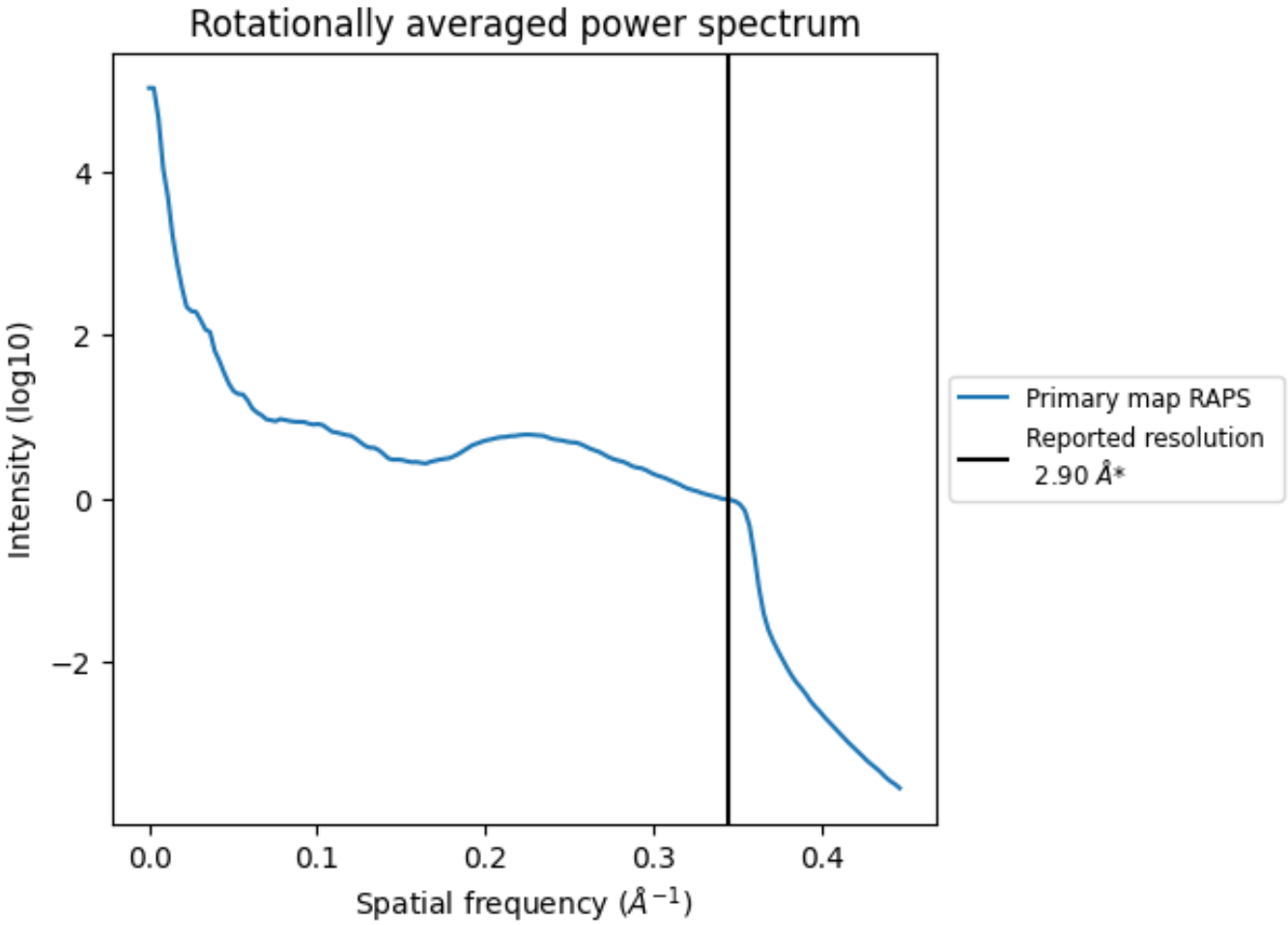
7.2 Volume estimate



The volume at the recommended contour level is 308 nm^3; this corresponds to an approximate mass of 278 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 $Å^{-1}$

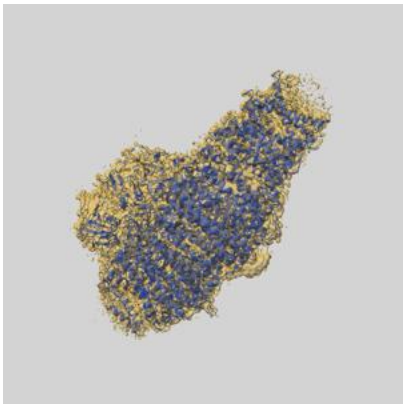
8 Fourier-Shell correlation

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

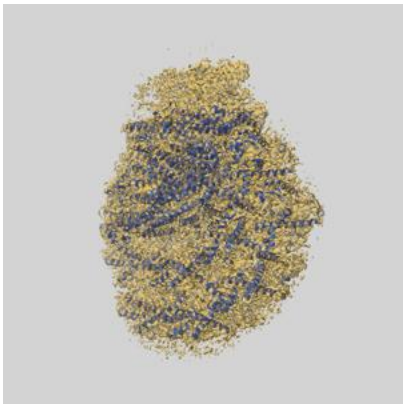
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-9854 and PDB model 6JO6. Per-residue inclusion information can be found in section 3 on page 32.

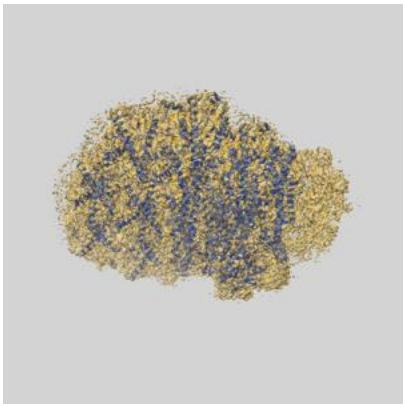
9.1 Map-model overlay



X



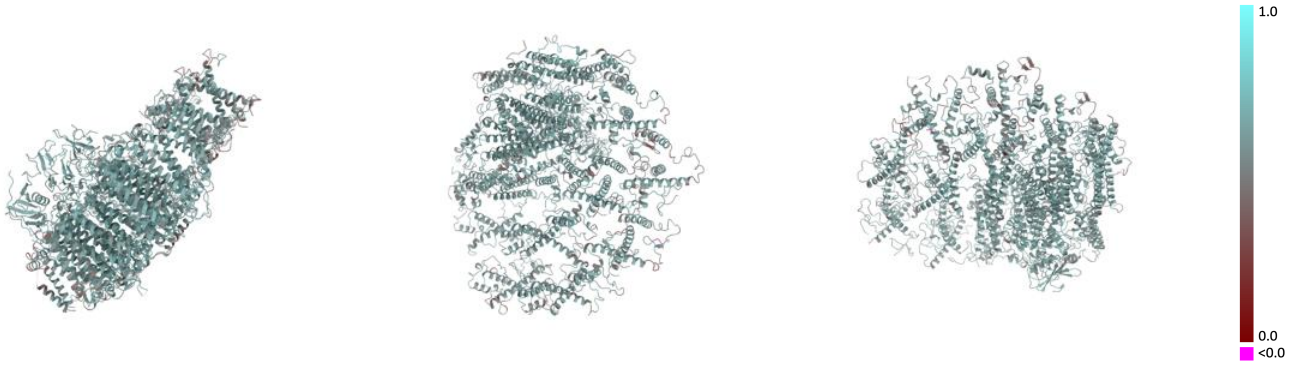
Y



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.

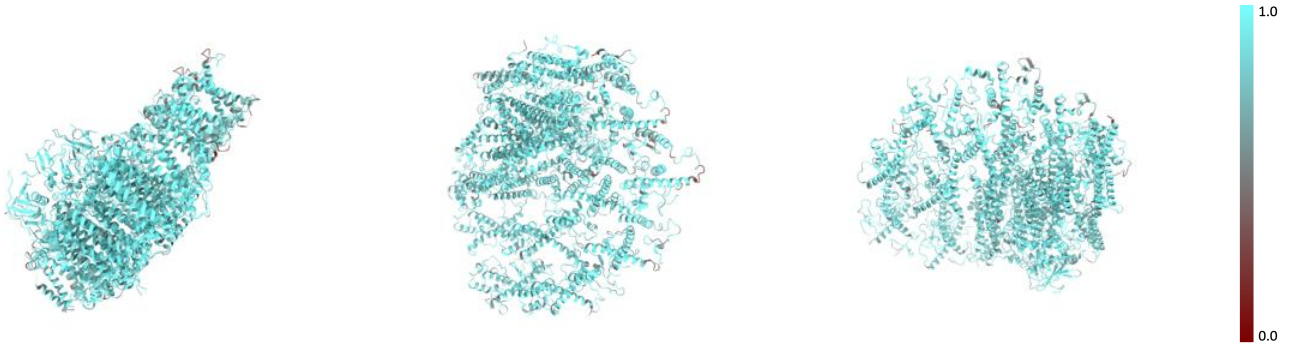
9.2 Q-score mapped to coordinate model



X Y Z

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

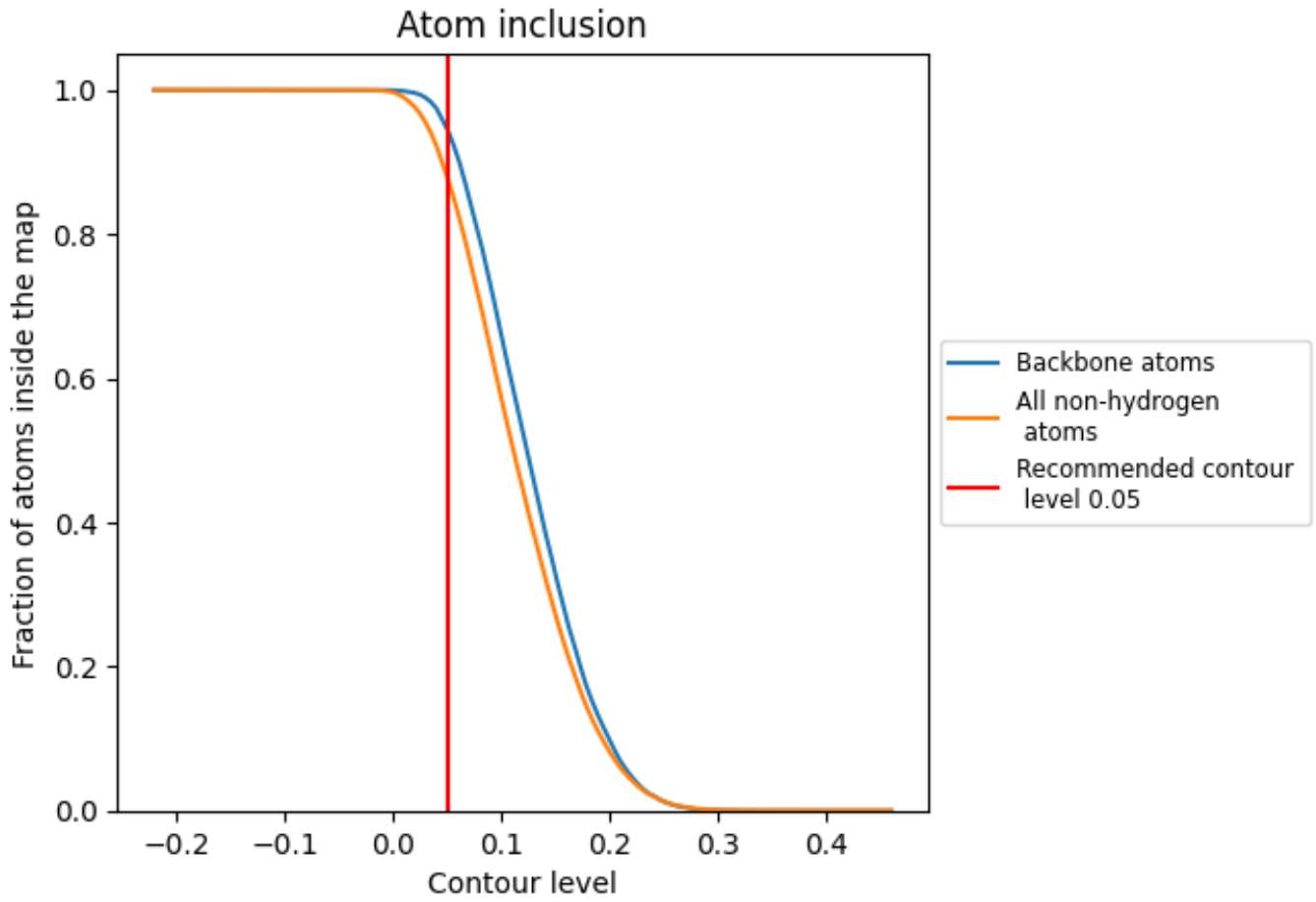
9.3 Atom inclusion mapped to coordinate model



X Y Z

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

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 88% 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	0.8788	0.5910
1	0.8386	0.5770
3	0.8874	0.5890
4	0.8395	0.5540
5	0.8451	0.5630
6	0.8417	0.5630
7	0.8786	0.5960
8	0.8880	0.5940
A	0.9256	0.6190
B	0.9187	0.6180
C	0.9435	0.6050
D	0.9054	0.5830
E	0.8994	0.5890
F	0.8651	0.5780
G	0.7769	0.5650
I	0.8464	0.5720
J	0.9042	0.6080
K	0.7804	0.5480
L	0.7831	0.5440
Z	0.7727	0.5450