wwPDB EM Validation Summary Report (i)

Nov 9, 2022 – 04:51 AM JST

PDB ID	:	6IGZ
EMDB ID	:	EMD-9670
Title	:	Structure of PSI-LHCI
Authors	:	Xiong, P.; Xiaochun, Q.
Deposited on	:	2018-09-27
Resolution	:	3.49 Å(reported)

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

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

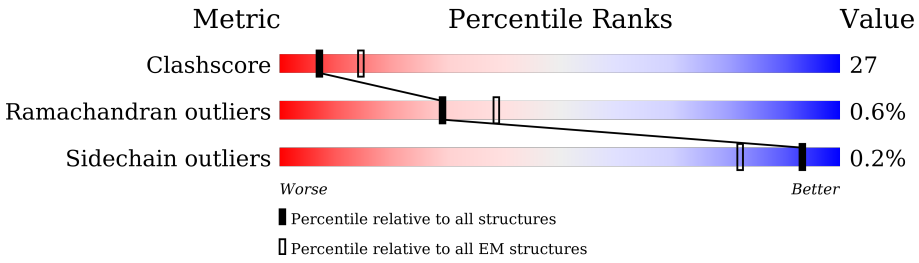
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 3.49 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	7% 58% 40% ··
2	B	734	8% 56% 43%
3	C	81	11% 51% 47% ··
4	D	198	16% 44% 27% ·· 28%
5	E	91	18% 46% 21% 33%
6	F	236	15% 41% 28% 31%
7	G	167	54% 30% 25% 45%
8	H	133	66% 35% 28% · 34%

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Mol	Chain	Length	Quality of chain
9	I	36	33% 56% 33% 11%
10	J	41	24% 71% 29%
11	K	123	28% 37% 26% 35%
12	L	204	59% 47% 27% 24%
13	1	226	22% 48% 37% 15%
13	5	226	35% 48% 37% 14%
14	2	256	6% 51% 32% 17%
15	3	281	6% 51% 28% 20%
16	4	248	15% 50% 34% 17%
16	8	248	21% 44% 38% 17%
17	6	267	13% 47% 39% 14%
18	7	264	12% 47% 39% 14%
19	9	222	38% 49% 33% 18%
20	0	245	68% 47% 35% 18%
21	M	32	28% 75% 22%

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
22	CLA	0	302	X	-	-	-
22	CLA	0	303	X	-	-	-
22	CLA	0	304	X	-	-	-
22	CLA	0	305	X	-	-	-
22	CLA	0	307	X	-	-	-
22	CLA	0	308	X	-	-	-
22	CLA	0	309	X	-	-	-
22	CLA	0	310	X	-	-	-
22	CLA	0	311	X	-	-	-
22	CLA	0	312	X	-	-	-
22	CLA	1	301	X	-	-	-
22	CLA	1	302	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	1	303	X	-	-	-
22	CLA	1	304	X	-	-	-
22	CLA	1	306	X	-	-	-
22	CLA	1	307	X	-	-	-
22	CLA	1	308	X	-	-	-
22	CLA	1	309	X	-	-	-
22	CLA	1	310	X	-	-	-
22	CLA	1	311	X	-	-	-
22	CLA	1	312	X	-	-	-
22	CLA	1	313	X	-	-	-
22	CLA	2	302	X	-	-	-
22	CLA	2	303	X	-	-	-
22	CLA	2	304	X	-	-	-
22	CLA	2	308	X	-	-	-
22	CLA	2	309	X	-	-	-
22	CLA	2	310	X	-	-	-
22	CLA	2	311	X	-	-	-
22	CLA	2	312	X	-	-	-
22	CLA	2	313	X	-	-	-
22	CLA	2	314	X	-	-	-
22	CLA	2	319	X	-	-	-
22	CLA	3	301	X	-	-	-
22	CLA	3	302	X	-	-	-
22	CLA	3	303	X	-	-	-
22	CLA	3	304	X	-	-	-
22	CLA	3	305	X	-	-	-
22	CLA	3	307	X	-	-	-
22	CLA	3	308	X	-	-	-
22	CLA	3	309	X	-	-	-
22	CLA	3	310	X	-	-	-
22	CLA	3	311	X	-	-	-
22	CLA	3	312	X	-	-	-
22	CLA	3	313	X	-	-	-
22	CLA	3	319	X	-	-	-
22	CLA	4	302	X	-	-	-
22	CLA	4	303	X	-	-	-
22	CLA	4	304	X	-	-	-
22	CLA	4	308	X	-	-	-
22	CLA	4	309	X	-	-	-
22	CLA	4	310	X	-	-	-
22	CLA	4	311	X	-	-	-
22	CLA	4	312	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	4	313	X	-	-	-
22	CLA	4	314	X	-	-	-
22	CLA	5	302	X	-	-	-
22	CLA	5	304	X	-	-	-
22	CLA	5	305	X	-	-	-
22	CLA	5	307	X	-	-	-
22	CLA	5	308	X	-	-	-
22	CLA	5	309	X	-	-	-
22	CLA	5	310	X	-	-	-
22	CLA	5	311	X	-	-	-
22	CLA	5	312	X	-	-	-
22	CLA	5	313	X	-	-	-
22	CLA	5	314	X	-	-	-
22	CLA	6	301	X	-	-	-
22	CLA	6	303	X	-	-	-
22	CLA	6	304	X	-	-	-
22	CLA	6	305	X	-	-	-
22	CLA	6	309	X	-	-	-
22	CLA	6	310	X	-	-	-
22	CLA	6	311	X	-	-	-
22	CLA	6	312	X	-	-	-
22	CLA	6	313	X	-	-	-
22	CLA	6	314	X	-	-	-
22	CLA	6	315	X	-	-	-
22	CLA	6	317	X	-	-	-
22	CLA	6	318	X	-	-	-
22	CLA	6	323	X	-	-	-
22	CLA	7	302	X	-	-	-
22	CLA	7	303	X	-	-	-
22	CLA	7	304	X	-	-	-
22	CLA	7	305	X	-	-	-
22	CLA	7	306	X	-	-	-
22	CLA	7	307	X	-	-	-
22	CLA	7	309	X	-	-	-
22	CLA	7	310	X	-	-	-
22	CLA	7	311	X	-	-	-
22	CLA	7	312	X	-	-	-
22	CLA	7	313	X	-	-	-
22	CLA	7	314	X	-	-	-
22	CLA	7	315	X	-	-	-
22	CLA	7	316	X	-	-	-
22	CLA	7	317	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	7	318	X	-	-	-
22	CLA	8	302	X	-	-	-
22	CLA	8	303	X	-	-	-
22	CLA	8	304	X	-	-	-
22	CLA	8	308	X	-	-	-
22	CLA	8	309	X	-	-	-
22	CLA	8	310	X	-	-	-
22	CLA	8	312	X	-	-	-
22	CLA	8	313	X	-	-	-
22	CLA	8	315	X	-	-	-
22	CLA	9	301	X	-	-	-
22	CLA	9	303	X	-	-	-
22	CLA	9	304	X	-	-	-
22	CLA	9	305	X	-	-	-
22	CLA	9	306	X	-	-	-
22	CLA	9	308	X	-	-	-
22	CLA	9	309	X	-	-	-
22	CLA	9	310	X	-	-	-
22	CLA	9	311	X	-	-	-
22	CLA	9	312	X	-	-	-
22	CLA	9	313	X	-	-	-
22	CLA	A	801	X	-	-	-
22	CLA	A	802	X	-	-	-
22	CLA	A	803	X	-	-	-
22	CLA	A	804	X	-	-	-
22	CLA	A	805	X	-	-	-
22	CLA	A	806	X	-	-	-
22	CLA	A	807	X	-	-	-
22	CLA	A	808	X	-	-	-
22	CLA	A	809	X	-	-	-
22	CLA	A	810	X	-	-	-
22	CLA	A	811	X	-	-	-
22	CLA	A	812	X	-	-	-
22	CLA	A	813	X	-	-	-
22	CLA	A	814	X	-	-	-
22	CLA	A	815	X	-	-	-
22	CLA	A	816	X	-	-	-
22	CLA	A	817	X	-	-	-
22	CLA	A	818	X	-	-	-
22	CLA	A	819	X	-	-	-
22	CLA	A	820	X	-	-	-
22	CLA	A	821	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	A	822	X	-	-	-
22	CLA	A	823	X	-	-	-
22	CLA	A	824	X	-	-	-
22	CLA	A	826	X	-	-	-
22	CLA	A	827	X	-	-	-
22	CLA	A	828	X	-	-	-
22	CLA	A	829	X	-	-	-
22	CLA	A	830	X	-	-	-
22	CLA	A	831	X	-	-	-
22	CLA	A	832	X	-	-	-
22	CLA	A	833	X	-	-	-
22	CLA	A	834	X	-	-	-
22	CLA	A	835	X	-	-	-
22	CLA	A	836	X	-	-	-
22	CLA	A	837	X	-	-	-
22	CLA	A	838	X	-	-	-
22	CLA	A	839	X	-	-	-
22	CLA	A	840	X	-	-	-
22	CLA	A	841	X	-	-	-
22	CLA	A	843	X	-	-	-
22	CLA	A	852	X	-	-	-
22	CLA	A	853	X	-	-	-
22	CLA	B	801	X	-	-	-
22	CLA	B	803	X	-	-	-
22	CLA	B	805	X	-	-	-
22	CLA	B	806	X	-	-	-
22	CLA	B	807	X	-	-	-
22	CLA	B	808	X	-	-	-
22	CLA	B	809	X	-	-	-
22	CLA	B	810	X	-	-	-
22	CLA	B	811	X	-	-	-
22	CLA	B	812	X	-	-	-
22	CLA	B	813	X	-	-	-
22	CLA	B	814	X	-	-	-
22	CLA	B	815	X	-	-	-
22	CLA	B	816	X	-	-	-
22	CLA	B	817	X	-	-	-
22	CLA	B	818	X	-	-	-
22	CLA	B	819	X	-	-	-
22	CLA	B	820	X	-	-	-
22	CLA	B	821	X	-	-	-
22	CLA	B	822	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	B	824	X	-	-	-
22	CLA	B	825	X	-	-	-
22	CLA	B	826	X	-	-	-
22	CLA	B	827	X	-	-	-
22	CLA	B	828	X	-	-	-
22	CLA	B	829	X	-	-	-
22	CLA	B	830	X	-	-	-
22	CLA	B	831	X	-	-	-
22	CLA	B	832	X	-	-	-
22	CLA	B	833	X	-	-	-
22	CLA	B	834	X	-	-	-
22	CLA	B	835	X	-	-	-
22	CLA	B	836	X	-	-	-
22	CLA	B	837	X	-	-	-
22	CLA	B	838	X	-	-	-
22	CLA	B	839	X	-	-	-
22	CLA	B	840	X	-	-	-
22	CLA	B	841	X	-	-	-
22	CLA	B	850	X	-	-	-
22	CLA	F	301	X	-	-	-
22	CLA	G	101	X	-	-	-
22	CLA	G	102	X	-	-	-
22	CLA	G	103	X	-	-	-
22	CLA	H	201	X	-	-	-
22	CLA	J	103	X	-	-	-
22	CLA	K	101	X	-	-	-
22	CLA	K	102	X	-	-	-
22	CLA	K	104	X	-	-	-
22	CLA	K	105	X	-	-	-
22	CLA	L	201	X	-	-	-
22	CLA	L	202	X	-	-	-
22	CLA	L	203	X	-	-	-
22	CLA	L	204	X	-	-	-
25	8CT	7	323	-	-	X	-
29	CHL	0	301	X	-	-	-
29	CHL	0	306	X	-	-	-
29	CHL	1	305	X	-	-	-
29	CHL	2	301	X	-	-	-
29	CHL	2	305	X	-	-	-
29	CHL	2	306	X	-	-	-
29	CHL	2	307	X	-	-	-
29	CHL	3	306	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CHL	4	301	X	-	-	-
29	CHL	4	305	X	-	-	-
29	CHL	4	306	X	-	-	-
29	CHL	4	307	X	-	-	-
29	CHL	5	301	X	-	-	-
29	CHL	5	306	X	-	-	-
29	CHL	6	302	X	-	-	-
29	CHL	6	306	X	-	-	-
29	CHL	6	307	X	-	-	-
29	CHL	6	308	X	-	-	-
29	CHL	6	316	X	-	-	-
29	CHL	7	308	X	-	-	-
29	CHL	8	305	X	-	-	-
29	CHL	8	306	X	-	-	-
29	CHL	8	307	X	-	-	-
29	CHL	8	314	X	-	-	-
29	CHL	9	302	X	-	-	-
29	CHL	9	307	X	-	-	-

2 Entry composition (i)

There are 31 unique types of molecules in this entry. The entry contains 51585 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 PsaA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	740	5819	3803	988	1006	22	0	0

- Molecule 2 is a protein called PsaB.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	733	5824	3824	979	1002	19	0	0

- Molecule 3 is a protein called PsaC.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	80	602	370	105	116	11	0	0

- Molecule 4 is a protein called PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	142	1109	709	193	202	5	0	0

- Molecule 5 is a protein called PsaE.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	61	488	308	87	92	1	0	0

- Molecule 6 is a protein called PsaF.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	163	1257	799	219	233	6	0	0

- Molecule 7 is a protein called PsaG.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	92	Total	C	N	O	0	0
			714	462	118	134		

- Molecule 8 is a protein called PsaH.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	88	Total	C	N	O	S	0	0
			677	426	119	131	1		

- Molecule 9 is a protein called PsaI.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	32	Total	C	N	O	S	0	0
			243	168	34	39	2		

- Molecule 10 is a protein called PsaJ.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	41	Total	C	N	O	S	0	0
			336	232	49	54	1		

- Molecule 11 is a protein called PsaK.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	80	Total	C	N	O	S	0	0
			558	363	92	100	3		

- Molecule 12 is a protein called PsaL.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	155	Total	C	N	O	S	0	0
			1139	736	187	212	4		

- Molecule 13 is a protein called Lhca-a.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	1	193	Total	C	N	O	S	0	0
			1466	942	241	271	12		
13	5	195	Total	C	N	O	S	0	0
			1484	956	243	273	12		

- Molecule 14 is a protein called Lhca-c.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	2	212	Total	C	N	O	S	0	0
			1641	1066	265	298	12		

- Molecule 15 is a protein called Lhca-d.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	3	226	Total	C	N	O	S	0	0
			1751	1132	283	326	10		

- Molecule 16 is a protein called Lhca-b.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	4	207	Total	C	N	O	S	0	0
			1589	1046	258	276	9		
16	8	205	Total	C	N	O	S	0	0
			1574	1035	256	274	9		

- Molecule 17 is a protein called Lhca-g.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	6	229	Total	C	N	O	S	0	0
			1797	1182	292	313	10		

- Molecule 18 is a protein called Lhca-h.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	7	228	Total	C	N	O	S	0	0
			1758	1137	291	319	11		

- Molecule 19 is a protein called Lhca-i.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	9	183	Total	C	N	O	S	0	0
			1416	913	235	259	9		

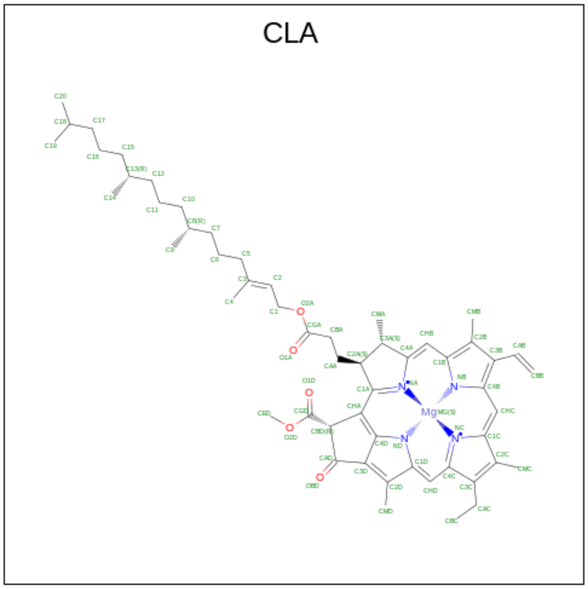
- Molecule 20 is a protein called Lhca-j.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	0	202	Total	C	N	O	S	0	0
			1560	1014	255	280	11		

- Molecule 21 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms	AltConf	Trace
21	M	31	Total C N O 238 158 37 43	0	0

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



Mol	Chain	Residues	Atoms	AltConf
22	A	1	Total C Mg N O 2628 2188 44 176 220	0
22	A	1	Total C Mg N O 2628 2188 44 176 220	0
22	A	1	Total C Mg N O 2628 2188 44 176 220	0
22	A	1	Total C Mg N O 2628 2188 44 176 220	0
22	A	1	Total C Mg N O 2628 2188 44 176 220	0
22	A	1	Total C Mg N O 2628 2188 44 176 220	0
22	A	1	Total C Mg N O 2628 2188 44 176 220	0
22	A	1	Total C Mg N O 2628 2188 44 176 220	0
22	A	1	Total C Mg N O 2628 2188 44 176 220	0
22	A	1	Total C Mg N O 2628 2188 44 176 220	0

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Mol	Chain	Residues	Atoms	AltConf
22	A	1	Total C Mg N O 2628 2188 44 176 220	0
22	A	1	Total C Mg N O 2628 2188 44 176 220	0
22	A	1	Total C Mg N O 2628 2188 44 176 220	0
22	A	1	Total C Mg N O 2628 2188 44 176 220	0
22	A	1	Total C Mg N O 2628 2188 44 176 220	0
22	A	1	Total C Mg N O 2628 2188 44 176 220	0
22	A	1	Total C Mg N O 2628 2188 44 176 220	0
22	A	1	Total C Mg N O 2628 2188 44 176 220	0
22	A	1	Total C Mg N O 2628 2188 44 176 220	0
22	A	1	Total C Mg N O 2628 2188 44 176 220	0
22	A	1	Total C Mg N O 2628 2188 44 176 220	0
22	A	1	Total C Mg N O 2628 2188 44 176 220	0
22	A	1	Total C Mg N O 2628 2188 44 176 220	0
22	A	1	Total C Mg N O 2628 2188 44 176 220	0
22	A	1	Total C Mg N O 2628 2188 44 176 220	0
22	A	1	Total C Mg N O 2628 2188 44 176 220	0
22	A	1	Total C Mg N O 2628 2188 44 176 220	0
22	A	1	Total C Mg N O 2628 2188 44 176 220	0
22	A	1	Total C Mg N O 2628 2188 44 176 220	0
22	A	1	Total C Mg N O 2628 2188 44 176 220	0
22	A	1	Total C Mg N O 2628 2188 44 176 220	0

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Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total 2628	C 2188	Mg 44	N 176	O 220	0
22	A	1	Total 2628	C 2188	Mg 44	N 176	O 220	0
22	A	1	Total 2628	C 2188	Mg 44	N 176	O 220	0
22	A	1	Total 2628	C 2188	Mg 44	N 176	O 220	0
22	A	1	Total 2628	C 2188	Mg 44	N 176	O 220	0
22	A	1	Total 2628	C 2188	Mg 44	N 176	O 220	0
22	A	1	Total 2628	C 2188	Mg 44	N 176	O 220	0
22	A	1	Total 2628	C 2188	Mg 44	N 176	O 220	0
22	A	1	Total 2628	C 2188	Mg 44	N 176	O 220	0
22	A	1	Total 2628	C 2188	Mg 44	N 176	O 220	0
22	A	1	Total 2628	C 2188	Mg 44	N 176	O 220	0
22	A	1	Total 2628	C 2188	Mg 44	N 176	O 220	0
22	A	1	Total 2628	C 2188	Mg 44	N 176	O 220	0
22	B	1	Total 2420	C 2020	Mg 40	N 160	O 200	0
22	B	1	Total 2420	C 2020	Mg 40	N 160	O 200	0
22	B	1	Total 2420	C 2020	Mg 40	N 160	O 200	0
22	B	1	Total 2420	C 2020	Mg 40	N 160	O 200	0
22	B	1	Total 2420	C 2020	Mg 40	N 160	O 200	0
22	B	1	Total 2420	C 2020	Mg 40	N 160	O 200	0
22	B	1	Total 2420	C 2020	Mg 40	N 160	O 200	0
22	B	1	Total 2420	C 2020	Mg 40	N 160	O 200	0

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Mol	Chain	Residues	Atoms	AltConf
22	B	1	Total C Mg N O 2420 2020 40 160 200	0
22	B	1	Total C Mg N O 2420 2020 40 160 200	0
22	B	1	Total C Mg N O 2420 2020 40 160 200	0
22	B	1	Total C Mg N O 2420 2020 40 160 200	0
22	B	1	Total C Mg N O 2420 2020 40 160 200	0
22	B	1	Total C Mg N O 2420 2020 40 160 200	0
22	B	1	Total C Mg N O 2420 2020 40 160 200	0
22	B	1	Total C Mg N O 2420 2020 40 160 200	0
22	B	1	Total C Mg N O 2420 2020 40 160 200	0
22	B	1	Total C Mg N O 2420 2020 40 160 200	0
22	B	1	Total C Mg N O 2420 2020 40 160 200	0
22	B	1	Total C Mg N O 2420 2020 40 160 200	0
22	B	1	Total C Mg N O 2420 2020 40 160 200	0
22	B	1	Total C Mg N O 2420 2020 40 160 200	0
22	B	1	Total C Mg N O 2420 2020 40 160 200	0
22	B	1	Total C Mg N O 2420 2020 40 160 200	0
22	B	1	Total C Mg N O 2420 2020 40 160 200	0
22	B	1	Total C Mg N O 2420 2020 40 160 200	0
22	B	1	Total C Mg N O 2420 2020 40 160 200	0
22	B	1	Total C Mg N O 2420 2020 40 160 200	0
22	B	1	Total C Mg N O 2420 2020 40 160 200	0

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Mol	Chain	Residues	Atoms	AltConf
22	B	1	Total C Mg N O 2420 2020 40 160 200	0
22	B	1	Total C Mg N O 2420 2020 40 160 200	0
22	B	1	Total C Mg N O 2420 2020 40 160 200	0
22	B	1	Total C Mg N O 2420 2020 40 160 200	0
22	B	1	Total C Mg N O 2420 2020 40 160 200	0
22	B	1	Total C Mg N O 2420 2020 40 160 200	0
22	B	1	Total C Mg N O 2420 2020 40 160 200	0
22	B	1	Total C Mg N O 2420 2020 40 160 200	0
22	B	1	Total C Mg N O 2420 2020 40 160 200	0
22	B	1	Total C Mg N O 2420 2020 40 160 200	0
22	B	1	Total C Mg N O 2420 2020 40 160 200	0
22	F	1	Total C Mg N O 45 35 1 4 5	0
22	G	1	Total C Mg N O 141 111 3 12 15	0
22	G	1	Total C Mg N O 141 111 3 12 15	0
22	G	1	Total C Mg N O 141 111 3 12 15	0
22	H	1	Total C Mg N O 65 55 1 4 5	0
22	J	1	Total C Mg N O 42 34 1 4 3	0
22	K	1	Total C Mg N O 187 147 4 16 20	0
22	K	1	Total C Mg N O 187 147 4 16 20	0
22	K	1	Total C Mg N O 187 147 4 16 20	0
22	K	1	Total C Mg N O 187 147 4 16 20	0

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Mol	Chain	Residues	Atoms	AltConf
22	L	1	Total C Mg N O 245 205 4 16 20	0
22	L	1	Total C Mg N O 245 205 4 16 20	0
22	L	1	Total C Mg N O 245 205 4 16 20	0
22	L	1	Total C Mg N O 245 205 4 16 20	0
22	1	1	Total C Mg N O 683 565 12 48 58	0
22	1	1	Total C Mg N O 683 565 12 48 58	0
22	1	1	Total C Mg N O 683 565 12 48 58	0
22	1	1	Total C Mg N O 683 565 12 48 58	0
22	1	1	Total C Mg N O 683 565 12 48 58	0
22	1	1	Total C Mg N O 683 565 12 48 58	0
22	1	1	Total C Mg N O 683 565 12 48 58	0
22	1	1	Total C Mg N O 683 565 12 48 58	0
22	1	1	Total C Mg N O 683 565 12 48 58	0
22	1	1	Total C Mg N O 683 565 12 48 58	0
22	1	1	Total C Mg N O 683 565 12 48 58	0
22	1	1	Total C Mg N O 683 565 12 48 58	0
22	2	1	Total C Mg N O 596 490 11 44 51	0
22	2	1	Total C Mg N O 596 490 11 44 51	0
22	2	1	Total C Mg N O 596 490 11 44 51	0
22	2	1	Total C Mg N O 596 490 11 44 51	0
22	2	1	Total C Mg N O 596 490 11 44 51	0

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Mol	Chain	Residues	Atoms	AltConf
22	2	1	Total C Mg N O 596 490 11 44 51	0
22	2	1	Total C Mg N O 596 490 11 44 51	0
22	2	1	Total C Mg N O 596 490 11 44 51	0
22	2	1	Total C Mg N O 596 490 11 44 51	0
22	2	1	Total C Mg N O 596 490 11 44 51	0
22	2	1	Total C Mg N O 596 490 11 44 51	0
22	3	1	Total C Mg N O 644 520 13 52 59	0
22	3	1	Total C Mg N O 644 520 13 52 59	0
22	3	1	Total C Mg N O 644 520 13 52 59	0
22	3	1	Total C Mg N O 644 520 13 52 59	0
22	3	1	Total C Mg N O 644 520 13 52 59	0
22	3	1	Total C Mg N O 644 520 13 52 59	0
22	3	1	Total C Mg N O 644 520 13 52 59	0
22	3	1	Total C Mg N O 644 520 13 52 59	0
22	3	1	Total C Mg N O 644 520 13 52 59	0
22	3	1	Total C Mg N O 644 520 13 52 59	0
22	3	1	Total C Mg N O 644 520 13 52 59	0
22	3	1	Total C Mg N O 644 520 13 52 59	0
22	3	1	Total C Mg N O 644 520 13 52 59	0
22	4	1	Total C Mg N O 539 439 10 40 50	0
22	4	1	Total C Mg N O 539 439 10 40 50	0

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Mol	Chain	Residues	Atoms	AltConf
22	4	1	Total C Mg N O 539 439 10 40 50	0
22	4	1	Total C Mg N O 539 439 10 40 50	0
22	4	1	Total C Mg N O 539 439 10 40 50	0
22	4	1	Total C Mg N O 539 439 10 40 50	0
22	4	1	Total C Mg N O 539 439 10 40 50	0
22	4	1	Total C Mg N O 539 439 10 40 50	0
22	4	1	Total C Mg N O 539 439 10 40 50	0
22	4	1	Total C Mg N O 539 439 10 40 50	0
22	6	1	Total C Mg N O 785 647 14 56 68	0
22	6	1	Total C Mg N O 785 647 14 56 68	0
22	6	1	Total C Mg N O 785 647 14 56 68	0
22	6	1	Total C Mg N O 785 647 14 56 68	0
22	6	1	Total C Mg N O 785 647 14 56 68	0
22	6	1	Total C Mg N O 785 647 14 56 68	0
22	6	1	Total C Mg N O 785 647 14 56 68	0
22	6	1	Total C Mg N O 785 647 14 56 68	0
22	6	1	Total C Mg N O 785 647 14 56 68	0
22	6	1	Total C Mg N O 785 647 14 56 68	0
22	6	1	Total C Mg N O 785 647 14 56 68	0
22	6	1	Total C Mg N O 785 647 14 56 68	0
22	6	1	Total C Mg N O 785 647 14 56 68	0

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Mol	Chain	Residues	Atoms	AltConf
22	6	1	Total C Mg N O 785 647 14 56 68	0
22	5	1	Total C Mg N O 653 537 12 48 56	0
22	5	1	Total C Mg N O 653 537 12 48 56	0
22	5	1	Total C Mg N O 653 537 12 48 56	0
22	5	1	Total C Mg N O 653 537 12 48 56	0
22	5	1	Total C Mg N O 653 537 12 48 56	0
22	5	1	Total C Mg N O 653 537 12 48 56	0
22	5	1	Total C Mg N O 653 537 12 48 56	0
22	5	1	Total C Mg N O 653 537 12 48 56	0
22	5	1	Total C Mg N O 653 537 12 48 56	0
22	5	1	Total C Mg N O 653 537 12 48 56	0
22	5	1	Total C Mg N O 653 537 12 48 56	0
22	5	1	Total C Mg N O 653 537 12 48 56	0
22	7	1	Total C Mg N O 817 663 16 64 74	0
22	7	1	Total C Mg N O 817 663 16 64 74	0
22	7	1	Total C Mg N O 817 663 16 64 74	0
22	7	1	Total C Mg N O 817 663 16 64 74	0
22	7	1	Total C Mg N O 817 663 16 64 74	0
22	7	1	Total C Mg N O 817 663 16 64 74	0
22	7	1	Total C Mg N O 817 663 16 64 74	0
22	7	1	Total C Mg N O 817 663 16 64 74	0

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Mol	Chain	Residues	Atoms	AltConf
22	7	1	Total C Mg N O 817 663 16 64 74	0
22	7	1	Total C Mg N O 817 663 16 64 74	0
22	7	1	Total C Mg N O 817 663 16 64 74	0
22	7	1	Total C Mg N O 817 663 16 64 74	0
22	7	1	Total C Mg N O 817 663 16 64 74	0
22	7	1	Total C Mg N O 817 663 16 64 74	0
22	7	1	Total C Mg N O 817 663 16 64 74	0
22	7	1	Total C Mg N O 817 663 16 64 74	0
22	8	1	Total C Mg N O 539 439 10 40 50	0
22	8	1	Total C Mg N O 539 439 10 40 50	0
22	8	1	Total C Mg N O 539 439 10 40 50	0
22	8	1	Total C Mg N O 539 439 10 40 50	0
22	8	1	Total C Mg N O 539 439 10 40 50	0
22	8	1	Total C Mg N O 539 439 10 40 50	0
22	8	1	Total C Mg N O 539 439 10 40 50	0
22	8	1	Total C Mg N O 539 439 10 40 50	0
22	8	1	Total C Mg N O 539 439 10 40 50	0
22	8	1	Total C Mg N O 539 439 10 40 50	0
22	9	1	Total C Mg N O 595 487 11 44 53	0
22	9	1	Total C Mg N O 595 487 11 44 53	0
22	9	1	Total C Mg N O 595 487 11 44 53	0

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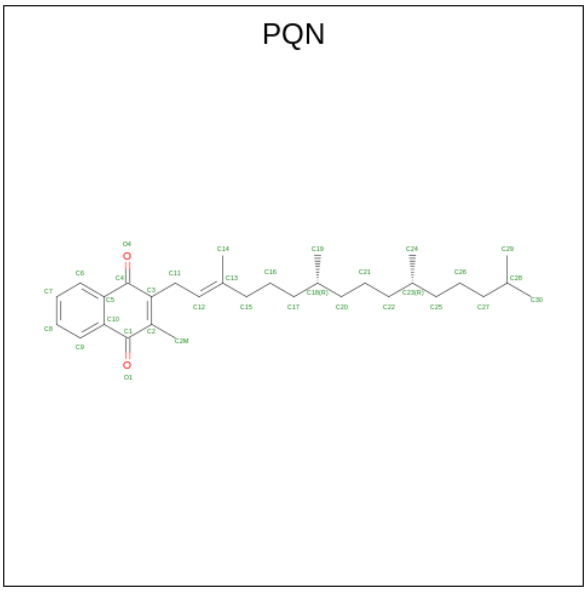
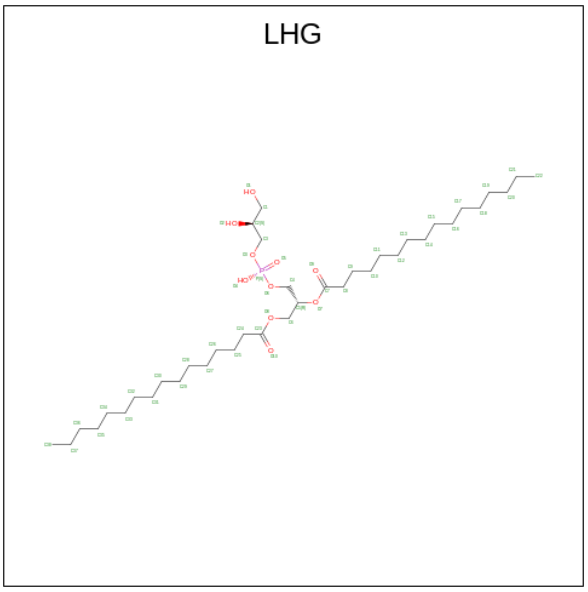
Mol	Chain	Residues	Atoms	AltConf
22	9	1	Total C Mg N O 595 487 11 44 53	0
22	9	1	Total C Mg N O 595 487 11 44 53	0
22	9	1	Total C Mg N O 595 487 11 44 53	0
22	9	1	Total C Mg N O 595 487 11 44 53	0
22	9	1	Total C Mg N O 595 487 11 44 53	0
22	9	1	Total C Mg N O 595 487 11 44 53	0
22	9	1	Total C Mg N O 595 487 11 44 53	0
22	9	1	Total C Mg N O 595 487 11 44 53	0
22	0	1	Total C Mg N O 572 474 10 40 48	0
22	0	1	Total C Mg N O 572 474 10 40 48	0
22	0	1	Total C Mg N O 572 474 10 40 48	0
22	0	1	Total C Mg N O 572 474 10 40 48	0
22	0	1	Total C Mg N O 572 474 10 40 48	0
22	0	1	Total C Mg N O 572 474 10 40 48	0
22	0	1	Total C Mg N O 572 474 10 40 48	0
22	0	1	Total C Mg N O 572 474 10 40 48	0
22	0	1	Total C Mg N O 572 474 10 40 48	0
22	0	1	Total C Mg N O 572 474 10 40 48	0
22	M	1	Total C Mg N O 46 36 1 4 5	0

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



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

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



Mol	Chain	Residues	Atoms				AltConf
24	A	1	Total	C	O	P	0
			76	54	20	2	

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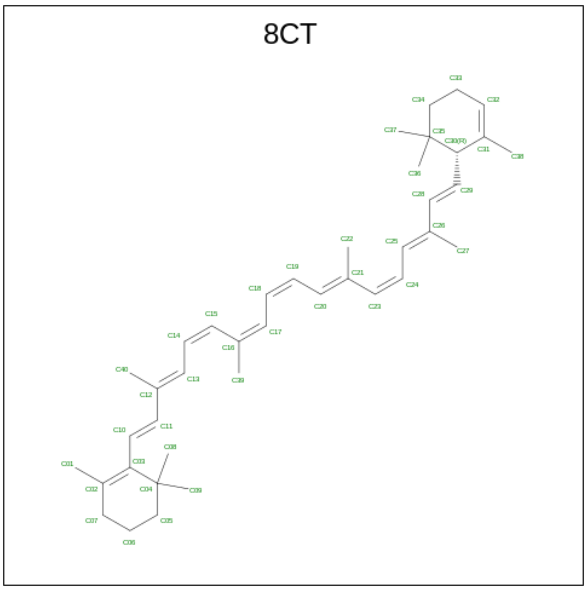
Mol	Chain	Residues	Atoms				AltConf
24	A	1	Total	C	O	P	0
			76	54	20	2	
24	B	1	Total	C	O	P	0
			23	12	10	1	
24	1	1	Total	C	O	P	0
			49	38	10	1	
24	2	1	Total	C	O	P	0
			32	21	10	1	
24	3	1	Total	C	O	P	0
			20	10	9	1	
24	6	1	Total	C	O	P	0
			37	26	10	1	
24	5	1	Total	C	O	P	0
			49	38	10	1	
24	7	1	Total	C	O	P	0
			20	10	9	1	
24	9	1	Total	C	O	P	0
			49	38	10	1	
24	0	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 25 is (6'R,11cis,11'cis,13cis,15cis)-4',5'-didehydro-5',6'-dihydro-beta,beta-carotene (three-letter code: 8CT) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms		AltConf
25	A	1	Total	C	0
			240	240	

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Mol	Chain	Residues	Atoms	AltConf
25	A	1	Total C 240 240	0
25	A	1	Total C 240 240	0
25	A	1	Total C 240 240	0
25	A	1	Total C 240 240	0
25	A	1	Total C 240 240	0
25	B	1	Total C 320 320	0
25	B	1	Total C 320 320	0
25	B	1	Total C 320 320	0
25	B	1	Total C 320 320	0
25	B	1	Total C 320 320	0
25	B	1	Total C 320 320	0
25	B	1	Total C 320 320	0
25	B	1	Total C 320 320	0
25	F	1	Total C 40 40	0
25	G	1	Total C 40 40	0
25	I	1	Total C 40 40	0
25	J	1	Total C 80 80	0
25	J	1	Total C 80 80	0
25	K	1	Total C 40 40	0
25	L	1	Total C 80 80	0
25	L	1	Total C 80 80	0

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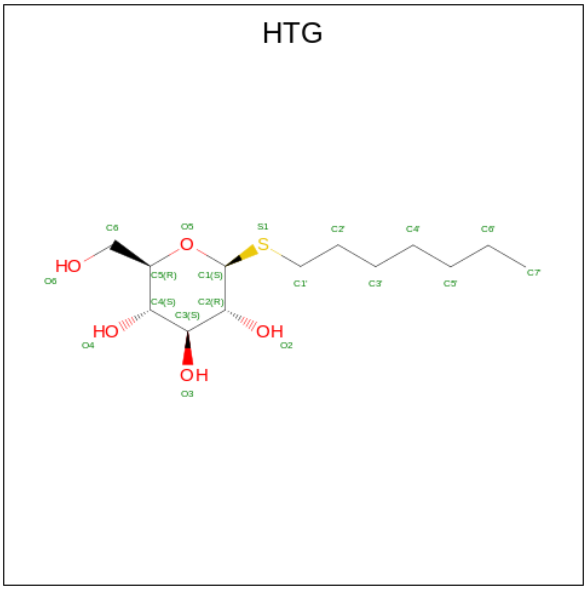
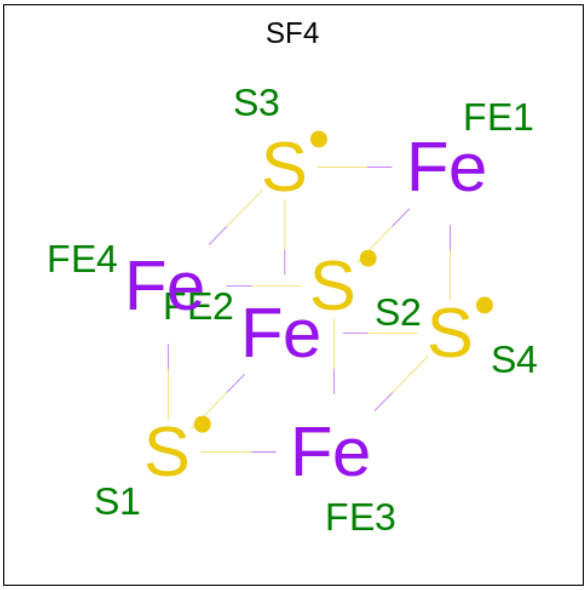
Mol	Chain	Residues	Atoms	AltConf
25	1	1	Total C 40 40	0
25	2	1	Total C 40 40	0
25	3	1	Total C 80 80	0
25	3	1	Total C 80 80	0
25	4	1	Total C 40 40	0
25	6	1	Total C 40 40	0
25	5	1	Total C 40 40	0
25	7	1	Total C 120 120	0
25	7	1	Total C 120 120	0
25	7	1	Total C 120 120	0
25	8	1	Total C 80 80	0
25	8	1	Total C 80 80	0

- Molecule 26 is heptyl 1-thio-beta-D-glucopyranoside (three-letter code: HTG) (formula: $C_{13}H_{26}O_5S$).



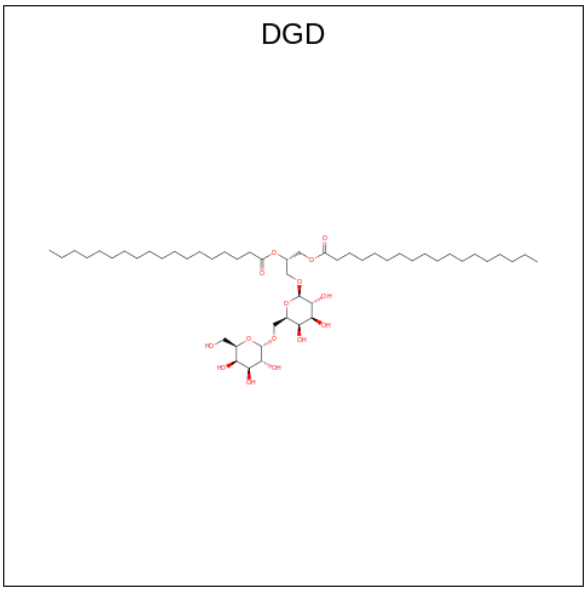
Mol	Chain	Residues	Atoms				AltConf
26	A	1	Total	C	O	S	0
			19	13	5	1	
26	J	1	Total	C	O	S	0
			19	13	5	1	

- Molecule 27 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



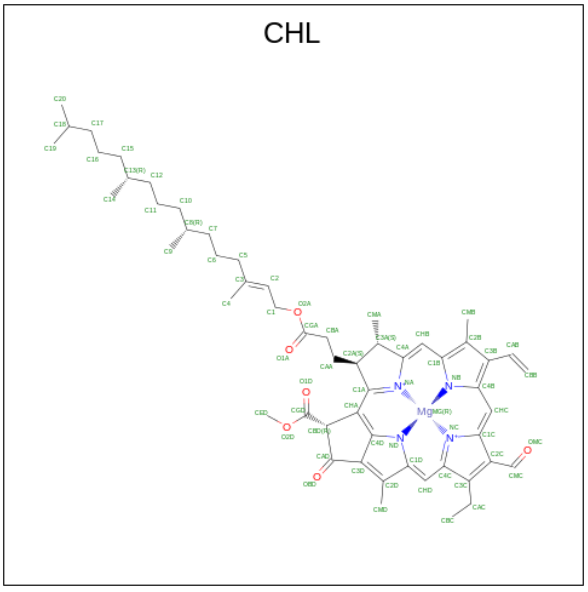
Mol	Chain	Residues	Atoms				AltConf
27	B	1	Total	Fe	S		0
			8	4	4		
27	C	1	Total	Fe	S		0
			16	8	8		
27	C	1	Total	Fe	S		0
			16	8	8		

- Molecule 28 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



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

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



Mol	Chain	Residues	Atoms					AltConf
29	1	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
29	2	1	Total	C	Mg	N	O	0
			203	161	4	16	22	
29	2	1	Total	C	Mg	N	O	0
			203	161	4	16	22	

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Mol	Chain	Residues	Atoms					AltConf
29	2	1	Total	C	Mg	N	O	0
			203	161	4	16	22	
29	2	1	Total	C	Mg	N	O	0
			203	161	4	16	22	
29	3	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
29	4	1	Total	C	Mg	N	O	0
			219	175	4	16	24	
29	4	1	Total	C	Mg	N	O	0
			219	175	4	16	24	
29	4	1	Total	C	Mg	N	O	0
			219	175	4	16	24	
29	4	1	Total	C	Mg	N	O	0
			219	175	4	16	24	
29	6	1	Total	C	Mg	N	O	0
			241	192	5	20	24	
29	6	1	Total	C	Mg	N	O	0
			241	192	5	20	24	
29	6	1	Total	C	Mg	N	O	0
			241	192	5	20	24	
29	6	1	Total	C	Mg	N	O	0
			241	192	5	20	24	
29	6	1	Total	C	Mg	N	O	0
			241	192	5	20	24	
29	5	1	Total	C	Mg	N	O	0
			109	87	2	8	12	
29	5	1	Total	C	Mg	N	O	0
			109	87	2	8	12	
29	7	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
29	8	1	Total	C	Mg	N	O	0
			201	159	4	16	22	
29	8	1	Total	C	Mg	N	O	0
			201	159	4	16	22	
29	8	1	Total	C	Mg	N	O	0
			201	159	4	16	22	
29	8	1	Total	C	Mg	N	O	0
			201	159	4	16	22	
29	9	1	Total	C	Mg	N	O	0
			109	87	2	8	12	
29	9	1	Total	C	Mg	N	O	0
			109	87	2	8	12	

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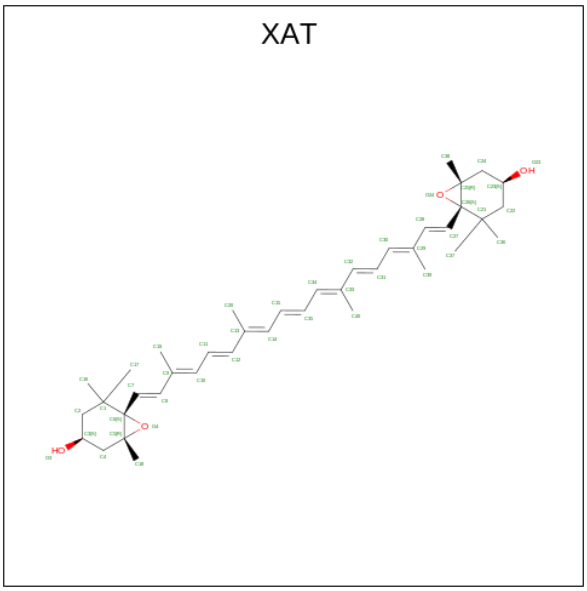
Mol	Chain	Residues	Atoms					AltConf
29	0	1	Total	C	Mg	N	O	0
			109	87	2	8	12	
29	0	1	Total	C	Mg	N	O	0
			109	87	2	8	12	

- Molecule 30 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (three-letter code: XAT) (formula: $C_{40}H_{56}O_4$).



Mol	Chain	Residues	Atoms			AltConf
30	1	1	Total	C	O	0
			88	80	8	
30	1	1	Total	C	O	0
			88	80	8	
30	2	1	Total	C	O	0
			88	80	8	
30	2	1	Total	C	O	0
			88	80	8	
30	3	1	Total	C	O	0
			88	80	8	
30	3	1	Total	C	O	0
			88	80	8	
30	4	1	Total	C	O	0
			88	80	8	
30	4	1	Total	C	O	0
			88	80	8	
30	6	1	Total	C	O	0
			88	80	8	

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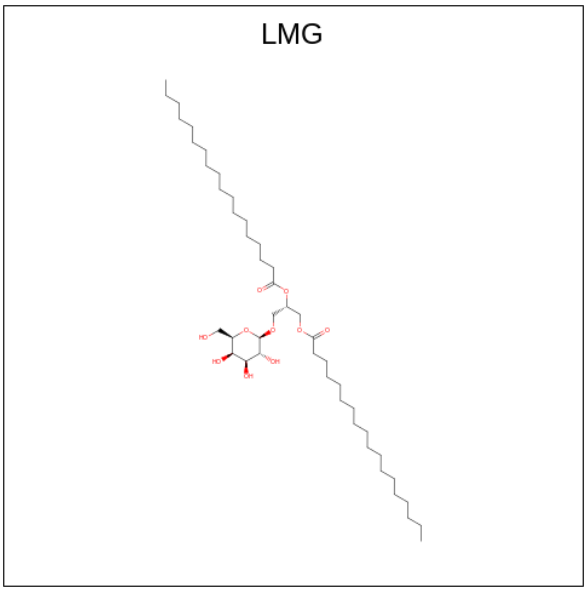
Mol	Chain	Residues	Atoms			AltConf
30	6	1	Total 88	C 80	O 8	0
30	5	1	Total 88	C 80	O 8	0
30	5	1	Total 88	C 80	O 8	0
30	7	1	Total 88	C 80	O 8	0
30	7	1	Total 88	C 80	O 8	0
30	8	1	Total 88	C 80	O 8	0
30	8	1	Total 88	C 80	O 8	0
30	9	1	Total 88	C 80	O 8	0
30	9	1	Total 88	C 80	O 8	0
30	0	1	Total 88	C 80	O 8	0
30	0	1	Total 88	C 80	O 8	0

- Molecule 31 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



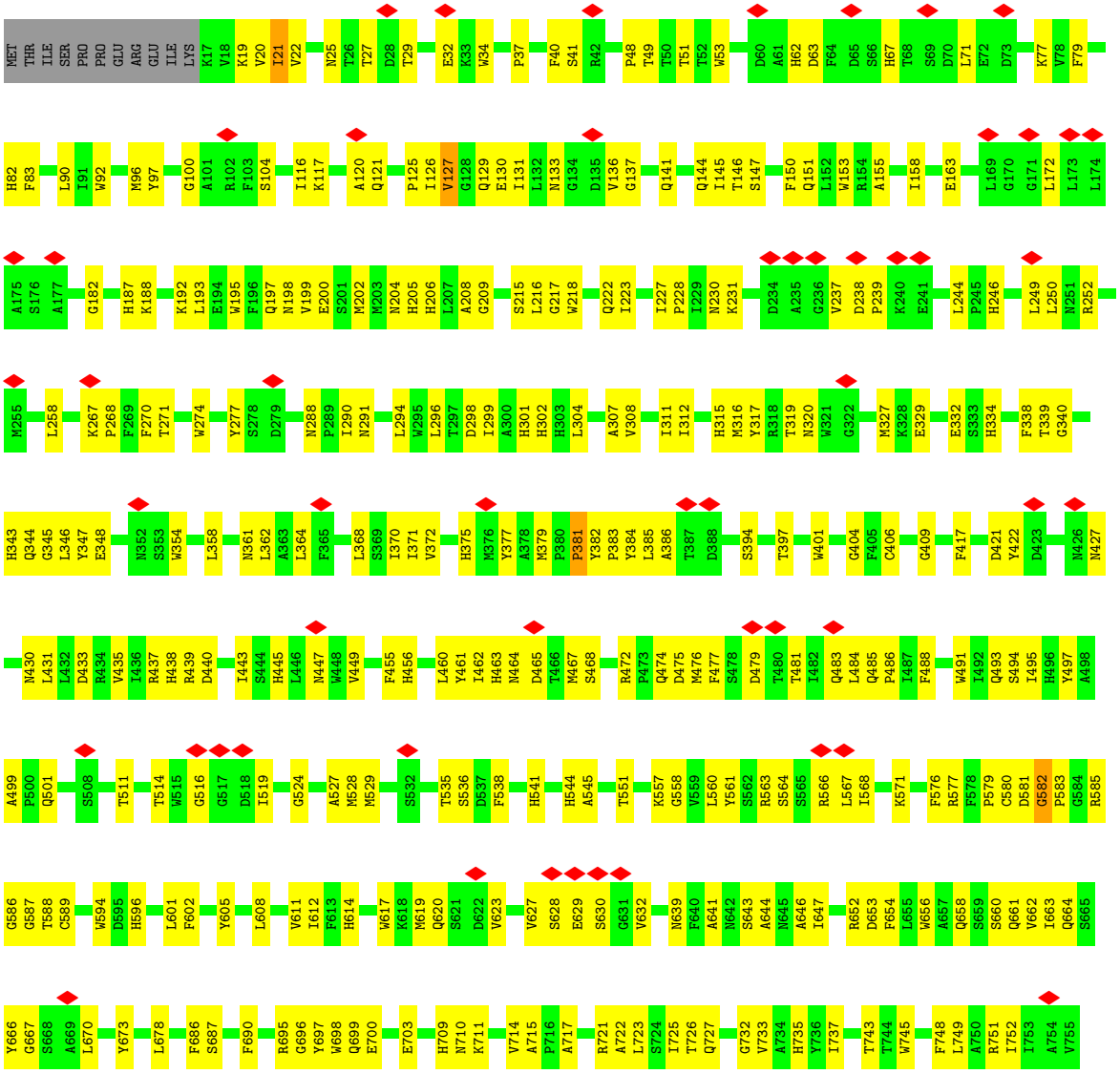
Mol	Chain	Residues	Atoms			AltConf
31	4	1	Total	C	O	0
			44	34	10	
31	5	1	Total	C	O	0
			44	34	10	
31	8	1	Total	C	O	0
			44	34	10	

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: PsaA

Chain A:



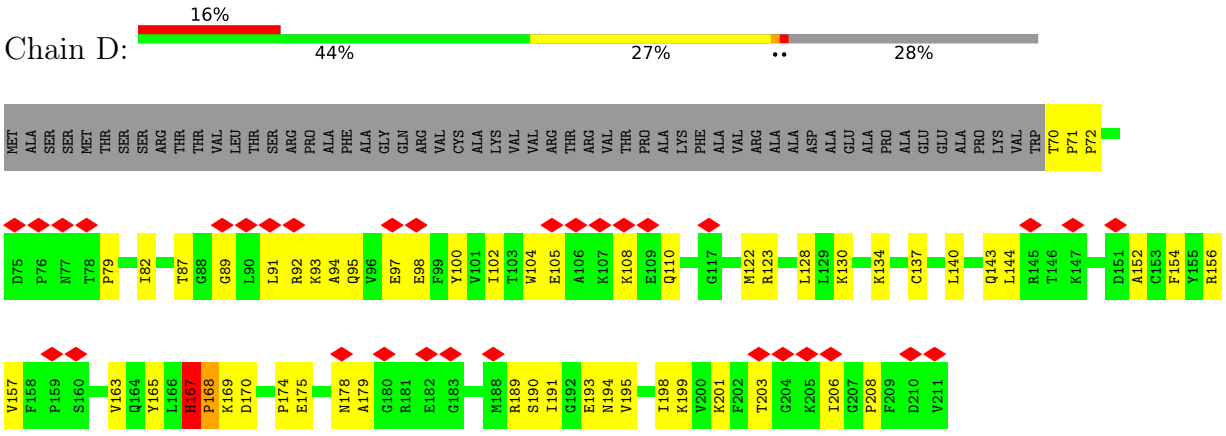
• Molecule 2: PsaB

Chain B:

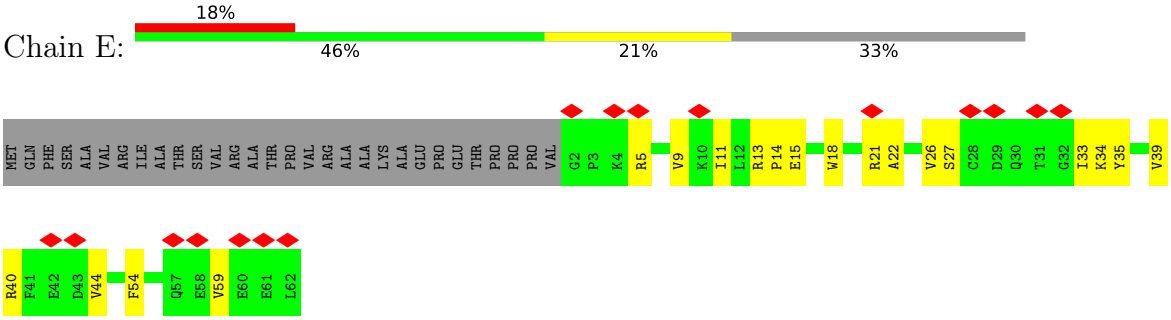
• Molecule 3: PsaC

Chain C:

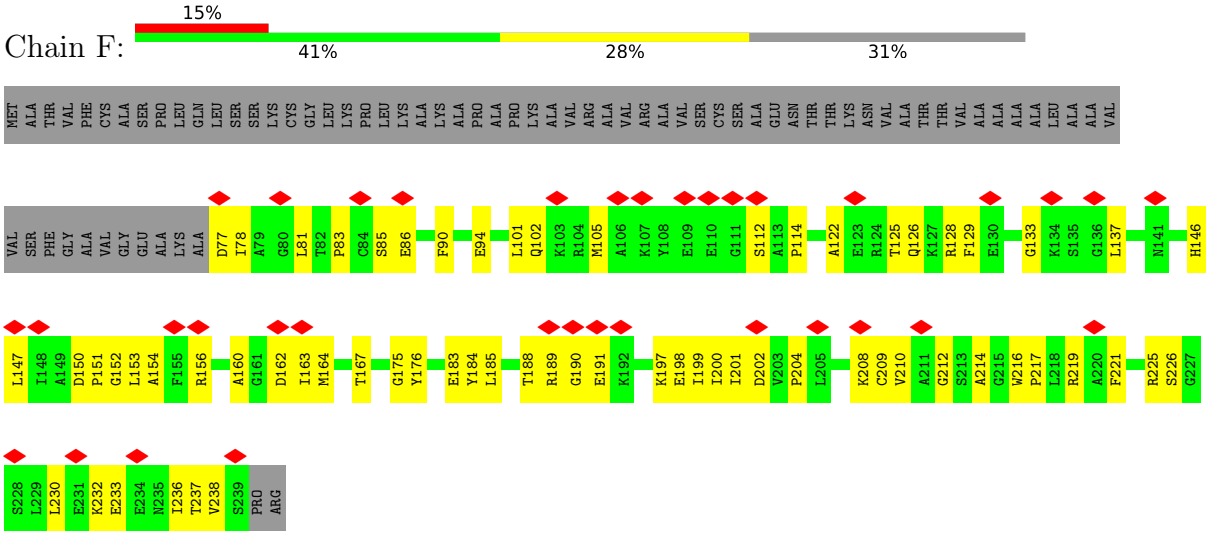
• Molecule 4: PsaD



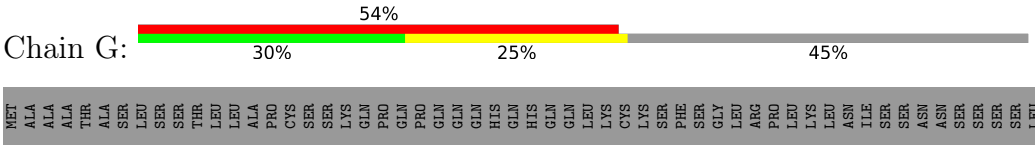
• Molecule 5: PsaE

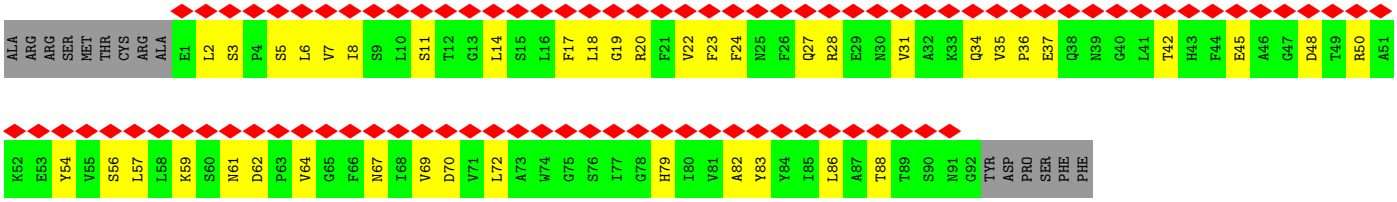


• Molecule 6: PsaF

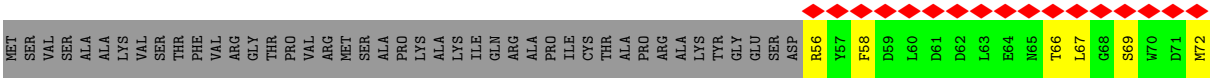


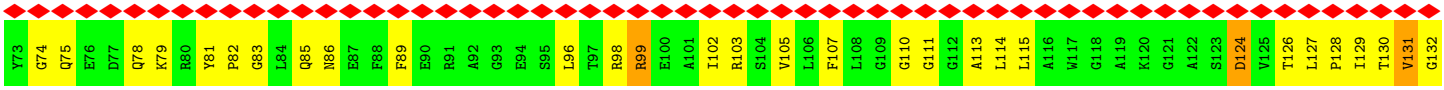
• Molecule 7: PsaG



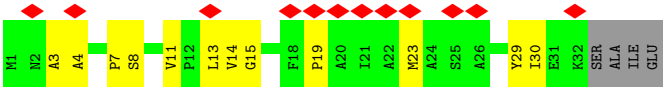


• Molecule 8: PsaH

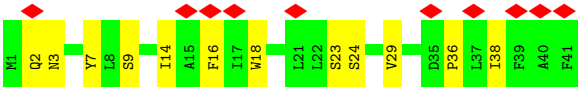




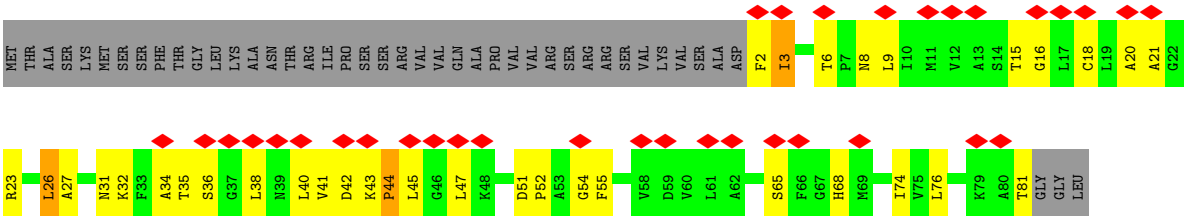
• Molecule 9: PsaI



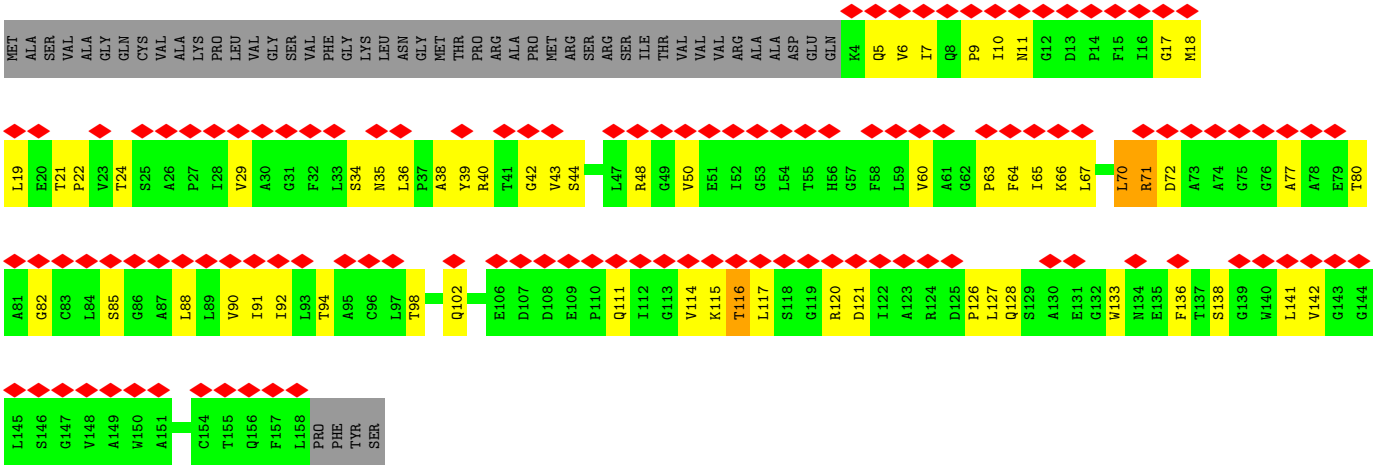
• Molecule 10: PsaJ



• Molecule 11: PsaK

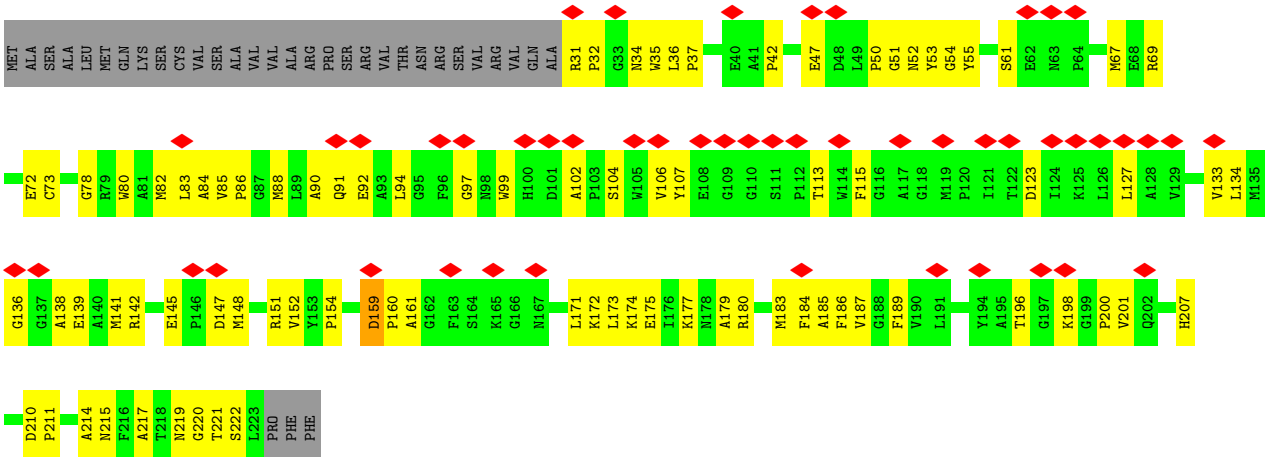


• Molecule 12: PsaL



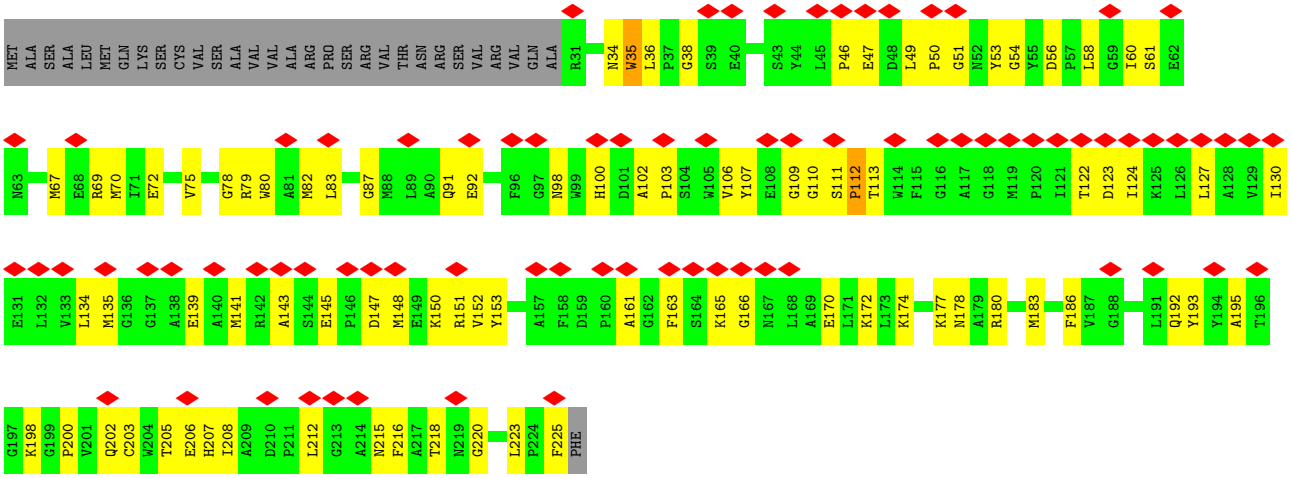
• Molecule 13: Lhca-a

Chain 1:



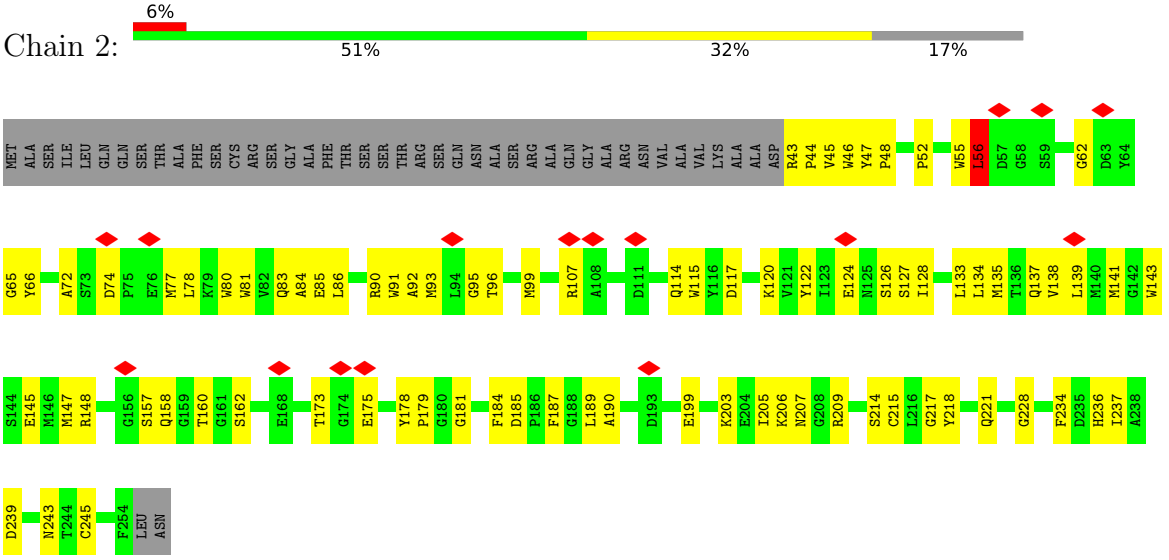
• Molecule 13: Lhca-a

Chain 5:



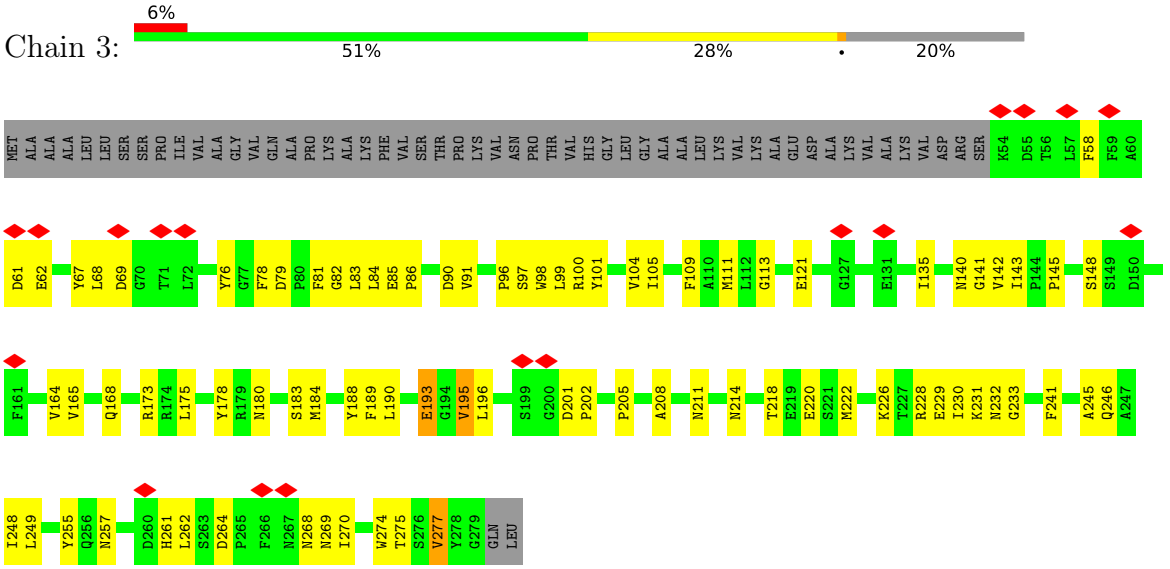
• Molecule 14: Lhca-c

Chain 2:



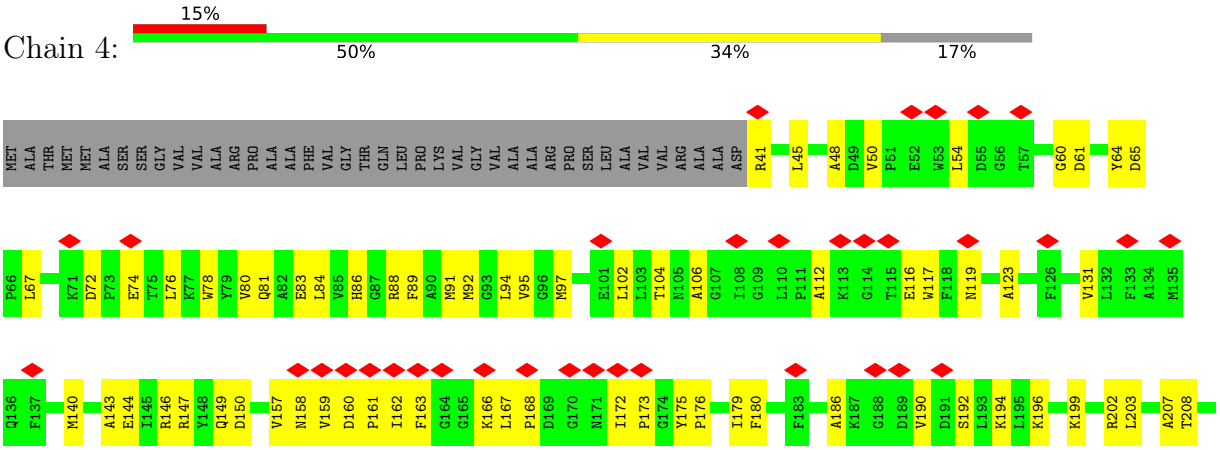
• Molecule 15: Lhca-d

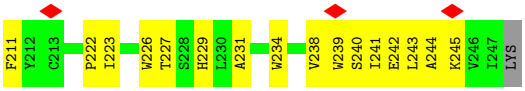
Chain 3:



• Molecule 16: Lhca-b

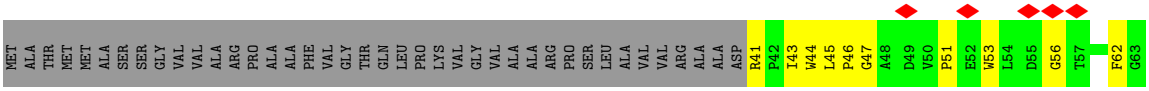
Chain 4:

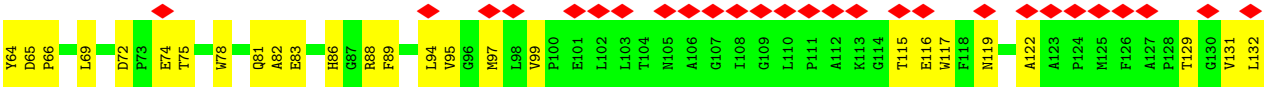


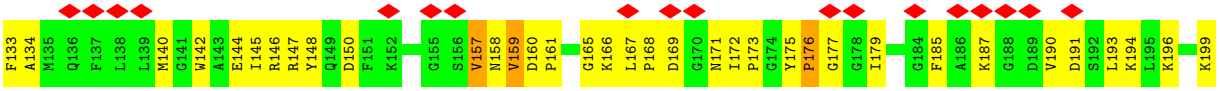


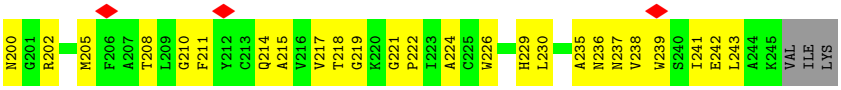
• Molecule 16: Lhca-b

Chain 8:



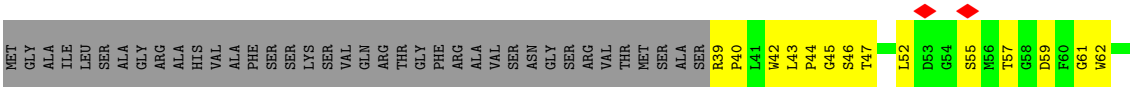


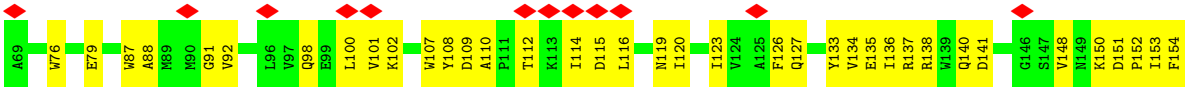


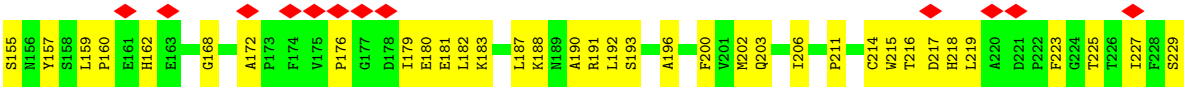


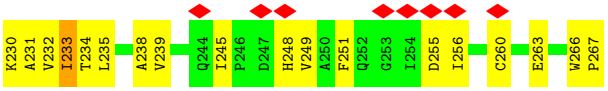
• Molecule 17: Lhca-g

Chain 6:



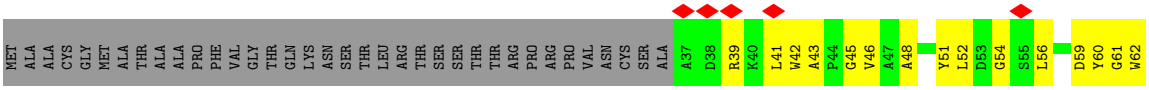


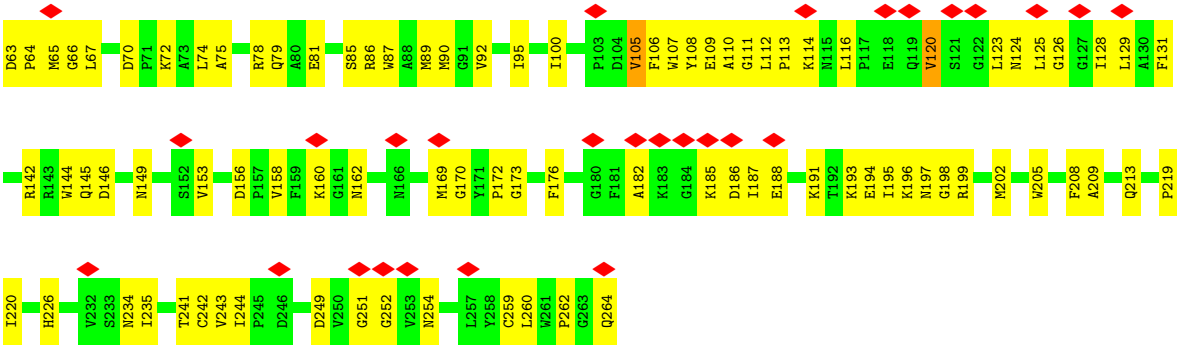




• Molecule 18: Lhca-h

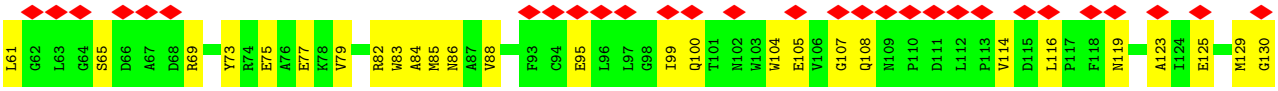
Chain 7:

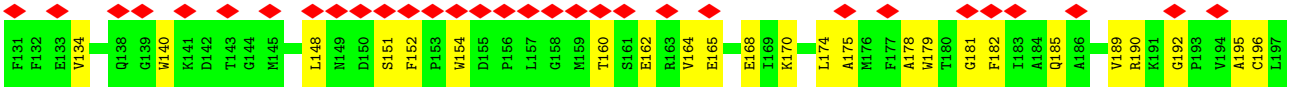


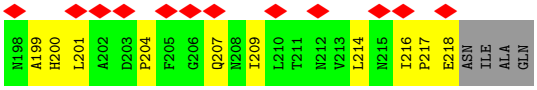


• Molecule 19: Lhca-i

Chain 9:

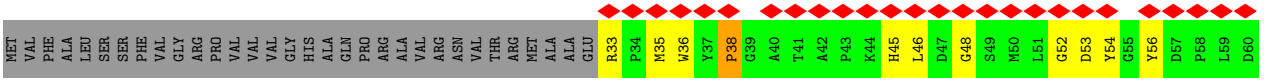


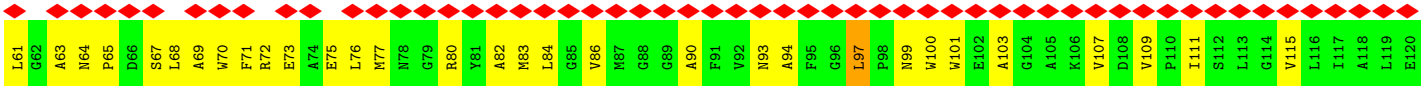


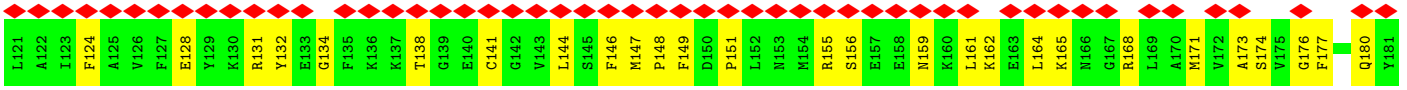


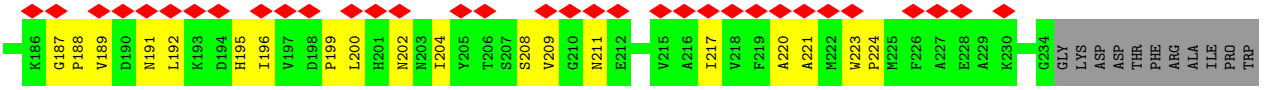
• Molecule 20: Lhca-j

Chain 0:



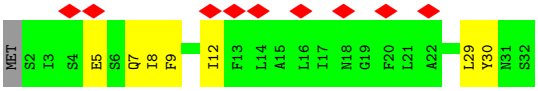






• Molecule 21: Photosystem I reaction center subunit XII

Chain M:


MET
S2
I3
S4
E5
S6
Q7
I8
F9
I12
F13
L14
A15
L16
I17
N18
G19
F20
L21
A22
L29
Y30
N31
S32

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	59525	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.852	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.187	Depositor
Minimum map value	-0.060	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.034	Depositor
Map size (Å)	401.442, 401.442, 401.442	wwPDB
Map dimensions	460, 460, 460	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8727, 0.8727, 0.8727	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, 8CT, PQN, SF4, LMG, HTG, DGD, CHL, XAT, CLA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.51	0/6015	0.53	0/8196
2	B	0.50	0/6034	0.54	0/8239
3	C	0.55	0/612	0.58	0/830
4	D	0.44	0/1135	0.59	0/1533
5	E	0.46	0/498	0.50	0/673
6	F	0.44	0/1281	0.56	0/1724
7	G	0.32	0/730	0.53	0/992
8	H	0.34	0/691	0.52	0/929
9	I	0.45	0/250	0.48	0/341
10	J	0.48	0/346	0.60	0/472
11	K	0.34	0/567	0.68	1/769 (0.1%)
12	L	0.33	0/1165	0.54	0/1591
13	1	0.41	0/1510	0.50	0/2054
13	5	0.40	0/1530	0.56	1/2082 (0.0%)
14	2	0.53	0/1701	0.56	1/2315 (0.0%)
15	3	0.49	0/1801	0.55	0/2444
16	4	0.49	0/1642	0.58	0/2238
16	8	0.43	0/1627	0.56	0/2217
17	6	0.43	0/1862	0.56	0/2542
18	7	0.46	0/1812	0.53	0/2468
19	9	0.39	0/1456	0.58	0/1986
20	0	0.33	0/1603	0.53	0/2174
21	M	0.41	0/241	0.43	0/325
All	All	0.46	0/36109	0.55	3/49134 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
3	C	0	1
4	D	0	1
11	K	0	1
13	1	0	1
14	2	0	2
16	4	0	1
17	6	0	3
20	0	0	3
All	All	0	14

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	5	35	TRP	C-N-CA	-5.90	106.96	121.70
11	K	26	LEU	CA-CB-CG	5.33	127.57	115.30
14	2	56	LEU	CA-CB-CG	5.04	126.90	115.30

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	1	159	ASP	Peptide
1	A	582	GLY	Peptide
3	C	62	PHE	Peptide
4	D	167	HIS	Peptide
11	K	41	VAL	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	5819	0	5659	288	0
2	B	5824	0	5604	363	0
3	C	602	0	591	42	0
4	D	1109	0	1124	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	488	0	480	16	0
6	F	1257	0	1274	60	0
7	G	714	0	708	39	0
8	H	677	0	654	60	0
9	I	243	0	258	10	0
10	J	336	0	355	15	0
11	K	558	0	591	38	0
12	L	1139	0	1147	72	0
13	1	1466	0	1411	83	0
13	5	1484	0	1427	78	0
14	2	1641	0	1537	81	0
15	3	1751	0	1684	91	0
16	4	1589	0	1570	98	0
16	8	1574	0	1550	139	0
17	6	1797	0	1752	116	0
18	7	1758	0	1701	113	0
19	9	1416	0	1367	76	0
20	0	1560	0	1540	91	0
21	M	238	0	248	8	0
22	0	572	0	542	53	0
22	1	683	0	657	79	0
22	2	596	0	548	37	0
22	3	644	0	529	48	0
22	4	539	0	476	38	0
22	5	653	0	599	62	0
22	6	785	0	741	71	0
22	7	817	0	694	80	0
22	8	539	0	477	47	0
22	9	595	0	534	47	0
22	A	2628	0	2677	218	0
22	B	2420	0	2485	239	0
22	F	45	0	33	5	0
22	G	141	0	105	16	0
22	H	65	0	72	18	0
22	J	42	0	31	1	0
22	K	187	0	138	29	0
22	L	245	0	255	26	0
22	M	46	0	33	5	0
23	A	33	0	46	3	0
23	B	33	0	46	3	0
24	0	49	0	72	12	0
24	1	49	0	74	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	2	32	0	34	3	0
24	3	20	0	14	4	0
24	5	49	0	72	8	0
24	6	37	0	44	4	0
24	7	20	0	13	2	0
24	9	49	0	74	8	0
24	A	76	0	98	5	0
24	B	23	0	16	1	0
25	1	40	0	0	13	0
25	2	40	0	0	13	0
25	3	80	0	0	10	0
25	4	40	0	0	12	0
25	5	40	0	0	6	0
25	6	40	0	0	14	0
25	7	120	0	0	36	0
25	8	80	0	0	13	0
25	A	240	0	0	32	0
25	B	320	0	0	40	0
25	F	40	0	0	0	0
25	G	40	0	0	20	0
25	I	40	0	0	0	0
25	J	80	0	0	25	0
25	K	40	0	0	14	0
25	L	80	0	0	0	0
26	A	19	0	26	0	0
26	J	19	0	26	1	0
27	B	8	0	0	1	0
27	C	16	0	0	1	0
28	B	66	0	96	11	0
29	0	109	0	87	18	0
29	1	48	0	33	3	0
29	2	203	0	154	16	0
29	3	47	0	31	4	0
29	4	219	0	176	30	0
29	5	109	0	90	17	0
29	6	241	0	181	22	0
29	7	47	0	31	11	0
29	8	201	0	148	27	0
29	9	109	0	90	6	0
30	0	88	0	104	19	0
30	1	88	0	109	15	0
30	2	88	0	112	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	3	88	0	110	17	0
30	4	88	0	109	16	0
30	5	88	0	107	13	0
30	6	88	0	111	14	0
30	7	88	0	109	15	0
30	8	88	0	109	21	0
30	9	88	0	109	13	0
31	4	44	0	61	1	0
31	5	44	0	61	5	0
31	8	44	0	60	6	0
All	All	51585	0	48901	2693	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 27.

The worst 5 of 2693 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)
22:A:832:CLA:H43	25:B:848:8CT:C27	1.26	1.58
22:1:304:CLA:H3A	25:1:316:8CT:C27	1.31	1.57
22:B:840:CLA:C1C	25:B:848:8CT:C22	1.82	1.57
18:7:251:GLY:HA3	25:7:323:8CT:C01	1.35	1.54
15:3:195:VAL:CG2	15:3:208:ALA:HB3	1.44	1.48

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	738/751 (98%)	680 (92%)	54 (7%)	4 (0%)	29 68
2	B	731/734 (100%)	677 (93%)	53 (7%)	1 (0%)	51 84

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	78/81 (96%)	71 (91%)	7 (9%)	0	100	100
4	D	140/198 (71%)	129 (92%)	9 (6%)	2 (1%)	11	46
5	E	59/91 (65%)	55 (93%)	4 (7%)	0	100	100
6	F	161/236 (68%)	153 (95%)	8 (5%)	0	100	100
7	G	90/167 (54%)	85 (94%)	5 (6%)	0	100	100
8	H	86/133 (65%)	74 (86%)	9 (10%)	3 (4%)	3	27
9	I	30/36 (83%)	27 (90%)	3 (10%)	0	100	100
10	J	39/41 (95%)	36 (92%)	3 (8%)	0	100	100
11	K	78/123 (63%)	69 (88%)	7 (9%)	2 (3%)	5	33
12	L	153/204 (75%)	139 (91%)	13 (8%)	1 (1%)	22	61
13	1	191/226 (84%)	175 (92%)	15 (8%)	1 (0%)	29	68
13	5	193/226 (85%)	173 (90%)	19 (10%)	1 (0%)	29	68
14	2	210/256 (82%)	190 (90%)	20 (10%)	0	100	100
15	3	224/281 (80%)	197 (88%)	26 (12%)	1 (0%)	34	72
16	4	205/248 (83%)	176 (86%)	29 (14%)	0	100	100
16	8	203/248 (82%)	173 (85%)	27 (13%)	3 (2%)	10	45
17	6	227/267 (85%)	200 (88%)	26 (12%)	1 (0%)	34	72
18	7	226/264 (86%)	190 (84%)	31 (14%)	5 (2%)	6	37
19	9	181/222 (82%)	156 (86%)	24 (13%)	1 (1%)	25	64
20	0	200/245 (82%)	175 (88%)	25 (12%)	0	100	100
21	M	29/32 (91%)	29 (100%)	0	0	100	100
All	All	4472/5310 (84%)	4029 (90%)	417 (9%)	26 (1%)	29	64

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	8	157	VAL
4	D	168	PRO
11	K	44	PRO
18	7	110	ALA
18	7	158	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	603/614 (98%)	602 (100%)	1 (0%)	93 98
2	B	600/601 (100%)	599 (100%)	1 (0%)	93 98
3	C	68/69 (99%)	68 (100%)	0	100 100
4	D	119/162 (74%)	119 (100%)	0	100 100
5	E	53/77 (69%)	53 (100%)	0	100 100
6	F	129/180 (72%)	129 (100%)	0	100 100
7	G	78/145 (54%)	78 (100%)	0	100 100
8	H	67/103 (65%)	66 (98%)	1 (2%)	65 84
9	I	25/28 (89%)	25 (100%)	0	100 100
10	J	38/38 (100%)	38 (100%)	0	100 100
11	K	58/94 (62%)	58 (100%)	0	100 100
12	L	118/157 (75%)	116 (98%)	2 (2%)	60 82
13	1	147/175 (84%)	147 (100%)	0	100 100
13	5	149/175 (85%)	149 (100%)	0	100 100
14	2	164/197 (83%)	164 (100%)	0	100 100
15	3	184/225 (82%)	182 (99%)	2 (1%)	73 88
16	4	161/189 (85%)	161 (100%)	0	100 100
16	8	159/189 (84%)	159 (100%)	0	100 100
17	6	188/216 (87%)	188 (100%)	0	100 100
18	7	181/209 (87%)	181 (100%)	0	100 100
19	9	144/173 (83%)	144 (100%)	0	100 100
20	0	160/194 (82%)	160 (100%)	0	100 100
21	M	26/27 (96%)	26 (100%)	0	100 100
All	All	3619/4237 (85%)	3612 (100%)	7 (0%)	93 98

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	L	70	LEU
12	L	71	ARG
15	3	195	VAL
15	3	193	GLU
8	H	124	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 100 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	143	GLN
14	2	114	GLN
20	0	203	ASN
10	J	2	GLN
12	L	128	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

320 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	$\#\|Z\|>2$
29	CHL	8	306	-	51,59,74	2.16	14 (27%)	55,96,114	2.81	23 (41%)
22	CLA	3	301	-	60,68,73	1.49	10 (16%)	70,107,113	1.51	7 (10%)
22	CLA	1	307	-	65,73,73	1.44	9 (13%)	76,113,113	1.40	9 (11%)
22	CLA	L	202	-	65,73,73	1.43	8 (12%)	76,113,113	1.52	9 (11%)
22	CLA	9	304	-	48,56,73	1.67	10 (20%)	55,92,113	1.59	7 (12%)
30	XAT	1	315	-	39,47,47	0.97	2 (5%)	54,74,74	3.10	21 (38%)
22	CLA	2	311	14	52,60,73	1.62	10 (19%)	60,97,113	1.61	7 (11%)
30	XAT	5	316	-	39,47,47	1.04	2 (5%)	54,74,74	3.14	21 (38%)
22	CLA	K	104	-	46,54,73	1.74	9 (19%)	53,90,113	1.56	6 (11%)
29	CHL	1	305	-	48,56,74	2.28	15 (31%)	51,92,114	2.76	22 (43%)
22	CLA	3	305	15	47,55,73	1.68	10 (21%)	54,91,113	1.49	7 (12%)
22	CLA	6	312	-	52,60,73	1.61	9 (17%)	60,97,113	1.51	7 (11%)
22	CLA	4	309	30	60,68,73	1.46	10 (16%)	70,107,113	1.43	9 (12%)
22	CLA	7	307	22	47,55,73	1.69	7 (14%)	54,91,113	1.58	7 (12%)
22	CLA	1	304	-	52,60,73	1.59	9 (17%)	60,97,113	1.50	8 (13%)
22	CLA	9	309	-	60,68,73	1.49	9 (15%)	70,107,113	1.52	9 (12%)
22	CLA	3	309	24	38,45,73	1.79	8 (21%)	43,78,113	1.78	7 (16%)
22	CLA	4	313	-	45,53,73	1.74	10 (22%)	52,89,113	1.68	7 (13%)
22	CLA	3	312	-	45,53,73	1.69	7 (15%)	52,89,113	1.68	9 (17%)
27	SF4	C	101	-	0,12,12	-	-	-		
29	CHL	2	305	-	43,51,74	2.14	14 (32%)	45,86,114	2.99	19 (42%)
22	CLA	B	826	-	65,73,73	1.40	8 (12%)	76,113,113	1.46	7 (9%)
22	CLA	4	304	-	50,58,73	1.61	9 (18%)	58,95,113	1.67	9 (15%)
22	CLA	A	829	-	65,73,73	1.46	10 (15%)	76,113,113	1.45	8 (10%)
22	CLA	1	306	-	65,73,73	1.49	9 (13%)	76,113,113	1.41	8 (10%)
22	CLA	2	319	16	46,54,73	1.70	10 (21%)	53,90,113	1.50	6 (11%)
22	CLA	5	307	-	65,73,73	1.45	7 (10%)	76,113,113	1.38	9 (11%)
22	CLA	6	303	17	65,73,73	1.44	10 (15%)	76,113,113	1.47	8 (10%)
29	CHL	8	305	-	56,64,74	2.04	14 (25%)	61,102,114	2.70	23 (37%)
22	CLA	A	801	-	65,73,73	1.46	10 (15%)	76,113,113	1.36	10 (13%)
22	CLA	3	313	-	46,54,73	1.68	10 (21%)	53,90,113	1.63	6 (11%)
22	CLA	H	201	-	65,73,73	1.42	7 (10%)	76,113,113	1.46	9 (11%)
22	CLA	K	105	-	50,58,73	1.67	9 (18%)	58,95,113	1.64	7 (12%)
24	LHG	9	316	22	48,48,48	0.61	1 (2%)	51,54,54	1.26	6 (11%)
22	CLA	9	301	-	46,54,73	1.79	9 (19%)	57,90,113	1.64	9 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	A	814	-	45,53,73	1.75	10 (22%)	52,89,113	1.54	7 (13%)
22	CLA	4	314	-	65,73,73	1.48	9 (13%)	76,113,113	1.37	8 (10%)
29	CHL	9	307	-	48,56,74	2.27	15 (31%)	51,92,114	2.77	21 (41%)
22	CLA	A	820	-	45,53,73	1.68	8 (17%)	52,89,113	1.71	7 (13%)
22	CLA	A	826	25	65,73,73	1.46	10 (15%)	76,113,113	1.36	5 (6%)
22	CLA	B	830	-	65,73,73	1.42	11 (16%)	76,113,113	1.56	8 (10%)
22	CLA	3	304	-	42,50,73	1.77	10 (23%)	48,85,113	1.56	7 (14%)
25	8CT	6	321	-	40,41,41	4.67	24 (60%)	50,56,56	3.26	18 (36%)
30	XAT	9	314	22	39,47,47	0.95	1 (2%)	54,74,74	4.46	27 (50%)
24	LHG	3	317	22	19,19,48	0.86	0	21,24,54	1.41	2 (9%)
22	CLA	7	302	18	46,54,73	1.69	10 (21%)	53,90,113	1.57	7 (13%)
30	XAT	3	314	25	39,47,47	0.98	3 (7%)	54,74,74	4.62	28 (51%)
22	CLA	B	806	-	65,73,73	1.40	10 (15%)	76,113,113	1.53	9 (11%)
22	CLA	5	305	25	52,60,73	1.66	8 (15%)	60,97,113	1.43	7 (11%)
22	CLA	7	312	30	52,60,73	1.67	9 (17%)	60,97,113	1.43	6 (10%)
29	CHL	2	301	22	61,69,74	1.89	14 (22%)	67,108,114	2.74	22 (32%)
30	XAT	7	319	22	39,47,47	0.98	2 (5%)	54,74,74	3.25	24 (44%)
22	CLA	9	311	-	52,60,73	1.62	7 (13%)	60,97,113	1.59	9 (15%)
22	CLA	2	302	29	65,73,73	1.41	9 (13%)	76,113,113	1.51	11 (14%)
22	CLA	A	821	-	65,73,73	1.42	8 (12%)	76,113,113	1.50	9 (11%)
22	CLA	1	308	13,30	60,68,73	1.50	8 (13%)	70,107,113	1.48	8 (11%)
22	CLA	A	828	-	65,73,73	1.42	9 (13%)	76,113,113	1.51	8 (10%)
22	CLA	0	305	29,22	52,60,73	1.59	7 (13%)	60,97,113	1.58	9 (15%)
22	CLA	A	817	-	65,73,73	1.41	8 (12%)	76,113,113	1.48	8 (10%)
27	SF4	C	102	3	0,12,12	-	-	-		
22	CLA	7	313	-	55,63,73	1.55	10 (18%)	64,101,113	1.62	9 (14%)
25	8CT	4	317	-	40,41,41	4.74	24 (60%)	50,56,56	2.36	15 (30%)
22	CLA	A	835	1	45,53,73	1.75	10 (22%)	52,89,113	1.72	7 (13%)
22	CLA	5	303	-	65,73,73	1.43	9 (13%)	76,113,113	1.36	7 (9%)
22	CLA	8	313	-	45,53,73	1.76	9 (20%)	52,89,113	1.64	8 (15%)
22	CLA	5	302	-	65,73,73	1.44	10 (15%)	76,113,113	1.36	9 (11%)
22	CLA	3	310	-	52,60,73	1.63	9 (17%)	60,97,113	1.50	7 (11%)
22	CLA	G	101	-	45,53,73	1.79	5 (11%)	52,89,113	1.61	8 (15%)
22	CLA	1	313	-	46,54,73	1.71	9 (19%)	53,90,113	1.58	7 (13%)
22	CLA	9	308	-	65,73,73	1.45	10 (15%)	76,113,113	1.42	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	8CT	B	851	22	40,41,41	4.75	25 (62%)	50,56,56	2.52	19 (38%)
22	CLA	8	310	31	55,63,73	1.58	9 (16%)	64,101,113	1.55	6 (9%)
23	PQN	B	842	-	34,34,34	1.47	2 (5%)	42,45,45	1.10	2 (4%)
22	CLA	5	313	-	55,63,73	1.60	8 (14%)	64,101,113	1.40	7 (10%)
30	XAT	6	320	-	39,47,47	0.96	2 (5%)	54,74,74	4.47	21 (38%)
22	CLA	4	312	-	56,64,73	1.56	10 (17%)	65,102,113	1.60	7 (10%)
25	8CT	B	848	-	40,41,41	4.70	24 (60%)	50,56,56	2.60	16 (32%)
24	LHG	5	318	22	48,48,48	0.65	1 (2%)	51,54,54	1.28	6 (11%)
24	LHG	1	317	22	48,48,48	0.68	2 (4%)	51,54,54	1.30	7 (13%)
25	8CT	J	101	-	40,41,41	4.67	24 (60%)	50,56,56	2.99	18 (36%)
22	CLA	B	808	-	65,73,73	1.44	10 (15%)	76,113,113	1.44	9 (11%)
22	CLA	B	823	-	55,63,73	1.58	10 (18%)	64,101,113	1.53	8 (12%)
22	CLA	B	827	-	65,73,73	1.42	8 (12%)	76,113,113	1.48	8 (10%)
24	LHG	A	844	-	48,48,48	0.73	1 (2%)	51,54,54	1.32	6 (11%)
29	CHL	7	308	-	47,55,74	2.15	14 (29%)	50,91,114	2.92	19 (38%)
22	CLA	6	309	17	50,58,73	1.64	8 (16%)	58,95,113	1.56	7 (12%)
22	CLA	B	836	-	60,68,73	1.49	10 (16%)	70,107,113	1.50	8 (11%)
22	CLA	8	311	-	52,60,73	1.67	8 (15%)	60,97,113	1.47	7 (11%)
22	CLA	B	831	-	50,58,73	1.67	10 (20%)	58,95,113	1.63	8 (13%)
22	CLA	2	309	-	60,68,73	1.50	11 (18%)	70,107,113	1.45	7 (10%)
29	CHL	6	308	-	51,59,74	2.11	14 (27%)	55,96,114	2.73	25 (45%)
25	8CT	B	843	-	40,41,41	4.73	25 (62%)	50,56,56	2.87	20 (40%)
22	CLA	B	837	-	65,73,73	1.43	9 (13%)	76,113,113	1.47	9 (11%)
25	8CT	7	321	-	40,41,41	4.66	24 (60%)	50,56,56	3.72	22 (44%)
22	CLA	B	832	-	65,73,73	1.43	10 (15%)	76,113,113	1.49	9 (11%)
22	CLA	B	819	-	60,68,73	1.49	8 (13%)	70,107,113	1.48	9 (12%)
22	CLA	B	850	-	55,63,73	1.57	8 (14%)	64,101,113	1.65	13 (20%)
24	LHG	A	845	22	26,26,48	0.95	1 (3%)	29,32,54	1.38	3 (10%)
22	CLA	A	816	-	45,53,73	1.73	9 (20%)	52,89,113	1.57	6 (11%)
29	CHL	6	302	17,22	61,69,74	1.99	15 (24%)	67,108,114	2.44	24 (35%)
22	CLA	5	310	24	41,49,73	1.76	10 (24%)	47,84,113	1.69	7 (14%)
22	CLA	B	822	-	46,54,73	1.69	10 (21%)	53,90,113	1.63	7 (13%)
22	CLA	0	309	24	41,49,73	1.81	7 (17%)	47,84,113	1.59	8 (17%)
22	CLA	8	302	-	60,68,73	1.51	10 (16%)	70,107,113	1.41	7 (10%)
22	CLA	0	312	29	55,63,73	1.66	7 (12%)	64,101,113	1.53	9 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	XAT	2	315	-	39,47,47	1.14	2 (5%)	54,74,74	5.94	29 (53%)
30	XAT	9	315	-	39,47,47	0.93	2 (5%)	54,74,74	2.88	20 (37%)
22	CLA	7	315	-	46,54,73	1.67	8 (17%)	53,90,113	1.59	7 (13%)
22	CLA	B	824	-	60,68,73	1.53	9 (15%)	70,107,113	1.45	9 (12%)
22	CLA	A	841	25	65,73,73	1.46	11 (16%)	76,113,113	1.40	7 (9%)
22	CLA	B	817	-	55,63,73	1.53	9 (16%)	64,101,113	1.49	8 (12%)
22	CLA	9	303	19	65,73,73	1.43	10 (15%)	76,113,113	1.49	8 (10%)
24	LHG	6	322	22	36,36,48	0.78	1 (2%)	39,42,54	1.26	4 (10%)
22	CLA	6	315	-	65,73,73	1.47	9 (13%)	76,113,113	1.32	7 (9%)
29	CHL	4	306	29	51,59,74	2.23	16 (31%)	55,96,114	2.74	21 (38%)
30	XAT	2	316	-	39,47,47	1.01	2 (5%)	54,74,74	3.14	23 (42%)
22	CLA	A	805	-	65,73,73	1.45	11 (16%)	76,113,113	1.42	9 (11%)
29	CHL	3	306	25	47,55,74	2.08	14 (29%)	50,91,114	2.92	22 (44%)
22	CLA	6	311	24	65,73,73	1.42	10 (15%)	76,113,113	1.41	7 (9%)
22	CLA	K	102	-	46,54,73	1.65	8 (17%)	53,90,113	1.68	8 (15%)
28	DGD	B	849	-	67,67,67	1.01	5 (7%)	81,81,81	1.51	13 (16%)
27	SF4	B	802	-	0,12,12	-	-	-		
22	CLA	3	311	-	55,63,73	1.55	10 (18%)	64,101,113	1.58	8 (12%)
22	CLA	4	302	-	60,68,73	1.50	10 (16%)	70,107,113	1.47	8 (11%)
22	CLA	B	818	-	59,67,73	1.55	11 (18%)	68,105,113	1.68	10 (14%)
22	CLA	8	312	16	56,64,73	1.58	10 (17%)	65,102,113	1.55	7 (10%)
22	CLA	B	805	-	65,73,73	1.44	10 (15%)	76,113,113	1.33	7 (9%)
22	CLA	A	806	-	65,73,73	1.46	10 (15%)	76,113,113	1.42	9 (11%)
30	XAT	8	317	-	39,47,47	0.97	2 (5%)	54,74,74	2.90	21 (38%)
22	CLA	B	814	-	65,73,73	1.46	10 (15%)	76,113,113	1.51	9 (11%)
22	CLA	1	312	29	55,63,73	1.56	8 (14%)	64,101,113	1.56	6 (9%)
22	CLA	0	303	30	65,73,73	1.47	8 (12%)	76,113,113	1.34	7 (9%)
22	CLA	1	301	13	65,73,73	1.49	10 (15%)	76,113,113	1.48	8 (10%)
24	LHG	7	322	22	19,19,48	0.93	0	21,24,54	1.36	2 (9%)
29	CHL	6	307	-	43,51,74	2.33	14 (32%)	45,86,114	2.84	17 (37%)
22	CLA	B	833	-	58,66,73	1.54	10 (17%)	67,104,113	1.58	9 (13%)
22	CLA	B	810	-	65,73,73	1.44	10 (15%)	76,113,113	1.45	9 (11%)
22	CLA	B	829	-	65,73,73	1.43	10 (15%)	76,113,113	1.52	11 (14%)
25	8CT	B	844	-	40,41,41	4.69	24 (60%)	50,56,56	2.90	16 (32%)
22	CLA	5	304	-	52,60,73	1.62	8 (15%)	60,97,113	1.54	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	8CT	F	302	-	40,41,41	4.59	23 (57%)	50,56,56	3.19	20 (40%)
30	XAT	0	314	29,22	39,47,47	0.88	0	54,74,74	3.06	22 (40%)
22	CLA	7	310	18	50,58,73	1.60	9 (18%)	58,95,113	1.77	8 (13%)
22	CLA	7	311	24	38,45,73	1.80	8 (21%)	43,78,113	1.61	7 (16%)
22	CLA	8	308	16	50,58,73	1.66	11 (22%)	58,95,113	1.73	11 (18%)
29	CHL	5	301	13	61,69,74	1.98	14 (22%)	67,108,114	2.53	22 (32%)
29	CHL	0	301	24,22	61,69,74	2.08	16 (26%)	67,108,114	2.42	21 (31%)
25	8CT	A	849	22	40,41,41	4.70	24 (60%)	50,56,56	2.63	18 (36%)
22	CLA	2	303	-	65,73,73	1.46	9 (13%)	76,113,113	1.33	5 (6%)
22	CLA	7	305	-	45,53,73	1.73	10 (22%)	52,89,113	1.52	7 (13%)
22	CLA	A	818	-	65,73,73	1.46	10 (15%)	76,113,113	1.50	8 (10%)
22	CLA	2	308	-	50,58,73	1.62	10 (20%)	58,95,113	1.48	7 (12%)
23	PQN	A	842	-	34,34,34	1.47	2 (5%)	42,45,45	1.31	6 (14%)
22	CLA	B	801	-	65,73,73	1.43	11 (16%)	76,113,113	1.49	8 (10%)
29	CHL	4	307	-	51,59,74	2.04	14 (27%)	55,96,114	2.88	22 (40%)
22	CLA	A	827	-	65,73,73	1.45	10 (15%)	76,113,113	1.49	9 (11%)
22	CLA	6	314	-	43,51,73	1.72	9 (20%)	49,86,113	1.60	6 (12%)
22	CLA	A	839	-	65,73,73	1.44	10 (15%)	76,113,113	1.47	11 (14%)
22	CLA	6	305	-	60,68,73	1.55	8 (13%)	70,107,113	1.36	6 (8%)
29	CHL	5	306	-	48,56,74	2.30	16 (33%)	51,92,114	2.72	20 (39%)
22	CLA	A	810	-	65,73,73	1.47	10 (15%)	76,113,113	1.35	6 (7%)
22	CLA	A	813	-	65,73,73	1.42	9 (13%)	76,113,113	1.58	10 (13%)
22	CLA	0	304	22	52,60,73	1.66	7 (13%)	60,97,113	1.54	7 (11%)
22	CLA	B	825	-	65,73,73	1.45	10 (15%)	76,113,113	1.45	8 (10%)
25	8CT	B	845	-	40,41,41	4.64	24 (60%)	50,56,56	3.16	20 (40%)
22	CLA	4	311	22	52,60,73	1.62	9 (17%)	60,97,113	1.54	7 (11%)
22	CLA	1	303	-	52,60,73	1.60	9 (17%)	60,97,113	1.52	9 (15%)
22	CLA	B	820	-	65,73,73	1.46	10 (15%)	76,113,113	1.39	7 (9%)
25	8CT	A	848	-	40,41,41	4.64	23 (57%)	50,56,56	2.72	15 (30%)
22	CLA	A	811	22	65,73,73	1.50	10 (15%)	76,113,113	1.38	6 (7%)
22	CLA	5	312	30	65,73,73	1.45	7 (10%)	76,113,113	1.46	8 (10%)
22	CLA	J	103	10	42,50,73	1.78	8 (19%)	48,85,113	1.68	6 (12%)
22	CLA	B	816	-	60,68,73	1.51	10 (16%)	70,107,113	1.56	8 (11%)
22	CLA	A	808	1	65,73,73	1.45	9 (13%)	76,113,113	1.45	8 (10%)
25	8CT	L	206	-	40,41,41	4.67	24 (60%)	50,56,56	3.02	19 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	A	832	-	65,73,73	1.43	10 (15%)	76,113,113	1.42	6 (7%)
22	CLA	4	310	-	55,63,73	1.60	10 (18%)	64,101,113	1.51	7 (10%)
30	XAT	0	313	22	39,47,47	1.11	2 (5%)	54,74,74	5.03	22 (40%)
25	8CT	5	317	22	40,41,41	4.75	23 (57%)	50,56,56	3.48	21 (42%)
25	8CT	B	804	-	40,41,41	4.55	23 (57%)	50,56,56	2.90	20 (40%)
22	CLA	B	838	-	47,55,73	1.70	9 (19%)	54,91,113	1.60	6 (11%)
24	LHG	B	852	22	22,22,48	0.84	0	25,28,54	1.21	1 (4%)
22	CLA	3	302	25	50,58,73	1.68	9 (18%)	58,95,113	1.48	6 (10%)
22	CLA	9	306	-	52,60,73	1.62	10 (19%)	60,97,113	1.56	7 (11%)
22	CLA	7	303	18	60,68,73	1.53	10 (16%)	70,107,113	1.51	8 (11%)
22	CLA	5	308	-	42,50,73	1.85	7 (16%)	48,85,113	1.78	8 (16%)
22	CLA	0	308	20	60,68,73	1.50	7 (11%)	70,107,113	1.41	6 (8%)
22	CLA	2	313	-	43,51,73	1.76	10 (23%)	49,86,113	1.59	6 (12%)
25	8CT	3	318	25,22	40,41,41	4.68	25 (62%)	50,56,56	3.66	22 (44%)
22	CLA	A	824	-	55,63,73	1.55	10 (18%)	64,101,113	1.47	8 (12%)
24	LHG	2	318	22	31,31,48	0.81	1 (3%)	34,37,54	1.30	3 (8%)
22	CLA	G	102	-	50,58,73	1.65	7 (14%)	58,95,113	1.59	8 (13%)
29	CHL	0	306	22,30	48,56,74	2.33	16 (33%)	51,92,114	2.69	19 (37%)
22	CLA	B	821	-	50,58,73	1.66	9 (18%)	58,95,113	1.54	8 (13%)
22	CLA	F	301	-	45,53,73	1.74	10 (22%)	52,89,113	1.59	6 (11%)
26	HTG	A	851	-	19,19,19	1.11	2 (10%)	23,24,24	0.73	0
29	CHL	6	306	-	43,51,74	2.17	13 (30%)	45,86,114	2.90	19 (42%)
22	CLA	2	310	24	41,49,73	1.81	10 (24%)	47,84,113	1.66	8 (17%)
22	CLA	6	318	17	52,60,73	1.64	10 (19%)	60,97,113	1.62	9 (15%)
22	CLA	A	804	22	55,63,73	1.55	10 (18%)	64,101,113	1.62	9 (14%)
22	CLA	A	830	-	65,73,73	1.49	10 (15%)	76,113,113	1.52	7 (9%)
22	CLA	A	822	-	49,57,73	1.64	9 (18%)	55,93,113	1.66	10 (18%)
25	8CT	A	854	-	40,41,41	4.68	24 (60%)	50,56,56	2.70	18 (36%)
25	8CT	I	101	-	40,41,41	4.54	23 (57%)	50,56,56	3.13	19 (38%)
22	CLA	1	310	-	52,60,73	1.61	9 (17%)	60,97,113	1.48	7 (11%)
29	CHL	4	301	22,13	61,69,74	1.90	12 (19%)	67,108,114	2.60	24 (35%)
29	CHL	9	302	19	61,69,74	1.94	14 (22%)	67,108,114	2.61	22 (32%)
22	CLA	B	811	-	65,73,73	1.46	10 (15%)	76,113,113	1.46	9 (11%)
22	CLA	9	310	24	41,49,73	1.79	8 (19%)	47,84,113	1.55	7 (14%)
22	CLA	0	311	-	65,73,73	1.46	8 (12%)	76,113,113	1.40	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	0	302	30	65,73,73	1.49	8 (12%)	76,113,113	1.36	9 (11%)
22	CLA	2	304	-	60,68,73	1.49	9 (15%)	70,107,113	1.48	8 (11%)
24	LHG	0	315	29,22	48,48,48	0.58	0	51,54,54	1.24	5 (9%)
22	CLA	9	313	-	55,63,73	1.56	8 (14%)	64,101,113	1.44	7 (10%)
22	CLA	A	833	25	65,73,73	1.44	10 (15%)	76,113,113	1.37	8 (10%)
22	CLA	A	831	-	50,58,73	1.63	10 (20%)	58,95,113	1.64	8 (13%)
22	CLA	L	204	-	50,58,73	1.65	8 (16%)	58,95,113	1.52	8 (13%)
30	XAT	4	315	22	39,47,47	0.95	1 (2%)	54,74,74	3.14	26 (48%)
22	CLA	4	308	16	50,58,73	1.60	10 (20%)	58,95,113	1.67	8 (13%)
30	XAT	4	316	-	39,47,47	1.04	3 (7%)	54,74,74	2.76	21 (38%)
29	CHL	8	307	30	51,59,74	2.11	13 (25%)	55,96,114	2.76	25 (45%)
22	CLA	7	309	22	50,58,73	1.65	10 (20%)	58,95,113	1.43	7 (12%)
25	8CT	3	316	-	40,41,41	4.68	24 (60%)	50,56,56	2.87	20 (40%)
25	8CT	L	205	22	40,41,41	4.65	24 (60%)	50,56,56	3.13	21 (42%)
22	CLA	L	201	-	65,73,73	1.43	10 (15%)	76,113,113	1.35	6 (7%)
22	CLA	A	853	-	65,73,73	1.46	10 (15%)	76,113,113	1.31	9 (11%)
25	8CT	J	104	-	40,41,41	4.70	24 (60%)	50,56,56	2.79	18 (36%)
25	8CT	K	103	-	40,41,41	4.87	24 (60%)	50,56,56	2.64	18 (36%)
29	CHL	6	316	17	43,51,74	2.29	14 (32%)	45,86,114	2.96	19 (42%)
22	CLA	G	103	7	46,54,73	1.67	5 (10%)	53,90,113	1.60	6 (11%)
30	XAT	1	314	22	39,47,47	0.91	1 (2%)	54,74,74	4.66	26 (48%)
22	CLA	A	852	-	49,57,73	1.69	9 (18%)	55,93,113	1.56	6 (10%)
30	XAT	3	315	-	39,47,47	0.98	2 (5%)	54,74,74	2.75	20 (37%)
22	CLA	A	834	-	50,58,73	1.70	10 (20%)	58,95,113	1.53	7 (12%)
22	CLA	3	308	-	50,58,73	1.66	11 (22%)	58,95,113	1.66	9 (15%)
22	CLA	B	835	-	45,53,73	1.69	8 (17%)	52,89,113	1.62	7 (13%)
22	CLA	1	311	-	65,73,73	1.44	10 (15%)	76,113,113	1.44	9 (11%)
22	CLA	8	309	-	60,68,73	1.48	10 (16%)	70,107,113	1.54	9 (12%)
22	CLA	2	312	14	65,73,73	1.40	9 (13%)	76,113,113	1.51	8 (10%)
22	CLA	0	307	22	65,73,73	1.49	7 (10%)	76,113,113	1.45	10 (13%)
22	CLA	7	304	22	47,55,73	1.69	10 (21%)	54,91,113	1.58	8 (14%)
22	CLA	5	314	24	46,54,73	1.73	9 (19%)	53,90,113	1.52	6 (11%)
22	CLA	B	839	25	65,73,73	1.46	8 (12%)	76,113,113	1.37	7 (9%)
22	CLA	M	101	-	46,54,73	1.77	10 (21%)	53,90,113	1.44	7 (13%)
25	8CT	2	317	-	40,41,41	4.70	24 (60%)	50,56,56	2.98	19 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	9	305	-	52,60,73	1.64	9 (17%)	60,97,113	1.64	10 (16%)
22	CLA	B	828	-	65,73,73	1.43	8 (12%)	76,113,113	1.55	9 (11%)
22	CLA	7	306	22	42,50,73	1.78	8 (19%)	48,85,113	1.60	7 (14%)
22	CLA	B	840	-	65,73,73	1.46	9 (13%)	76,113,113	1.45	7 (9%)
22	CLA	A	802	-	65,73,73	1.43	10 (15%)	76,113,113	1.47	7 (9%)
22	CLA	K	101	-	45,53,73	1.74	8 (17%)	52,89,113	1.56	8 (15%)
30	XAT	6	319	22	39,47,47	0.96	2 (5%)	54,74,74	3.23	24 (44%)
22	CLA	2	314	14	49,57,73	1.67	10 (20%)	55,93,113	1.50	8 (14%)
22	CLA	A	809	1	65,73,73	1.44	10 (15%)	76,113,113	1.40	10 (13%)
22	CLA	1	302	-	65,73,73	1.48	10 (15%)	76,113,113	1.43	9 (11%)
22	CLA	6	313	29	65,73,73	1.41	10 (15%)	76,113,113	1.46	10 (13%)
22	CLA	7	316	18	65,73,73	1.48	9 (13%)	76,113,113	1.39	6 (7%)
22	CLA	4	303	-	46,54,73	1.70	9 (19%)	53,90,113	1.60	7 (13%)
22	CLA	5	311	30	45,53,73	1.73	7 (15%)	52,89,113	1.66	7 (13%)
22	CLA	7	314	-	45,53,73	1.71	10 (22%)	52,89,113	1.64	7 (13%)
31	LMG	5	319	22	44,44,55	0.97	3 (6%)	52,52,63	1.33	6 (11%)
22	CLA	8	304	-	50,58,73	1.65	10 (20%)	58,95,113	1.52	6 (10%)
22	CLA	3	319	-	65,73,73	1.50	9 (13%)	76,113,113	1.41	9 (11%)
25	8CT	7	301	29,30	40,41,41	4.63	23 (57%)	50,56,56	2.71	19 (38%)
29	CHL	4	305	29	56,64,74	2.09	16 (28%)	61,102,114	2.53	21 (34%)
22	CLA	6	310	17,30	60,68,73	1.52	9 (15%)	70,107,113	1.47	10 (14%)
25	8CT	8	301	-	40,41,41	4.70	24 (60%)	50,56,56	2.66	18 (36%)
22	CLA	A	843	24	52,60,73	1.62	8 (15%)	60,97,113	1.60	9 (15%)
22	CLA	8	315	-	65,73,73	1.45	7 (10%)	76,113,113	1.34	6 (7%)
22	CLA	6	301	-	52,60,73	1.64	7 (13%)	60,97,113	1.49	8 (13%)
25	8CT	7	323	-	40,41,41	4.70	24 (60%)	50,56,56	2.73	18 (36%)
22	CLA	3	307	15	50,58,73	1.75	10 (20%)	58,95,113	1.55	7 (12%)
31	LMG	4	318	-	44,44,55	0.98	4 (9%)	52,52,63	1.49	9 (17%)
25	8CT	1	316	13	40,41,41	4.73	24 (60%)	50,56,56	2.61	18 (36%)
22	CLA	B	812	2	65,73,73	1.48	10 (15%)	76,113,113	1.41	7 (9%)
22	CLA	A	815	-	47,55,73	1.70	8 (17%)	54,91,113	1.61	8 (14%)
25	8CT	A	847	-	40,41,41	4.60	23 (57%)	50,56,56	2.97	20 (40%)
22	CLA	9	312	30	59,67,73	1.57	9 (15%)	68,105,113	1.40	8 (11%)
22	CLA	A	812	-	54,62,73	1.63	10 (18%)	62,99,113	1.56	8 (12%)
22	CLA	B	815	-	65,73,73	1.41	10 (15%)	76,113,113	1.53	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	HTG	J	102	-	19,19,19	1.12	2 (10%)	23,24,24	0.77	0
22	CLA	A	840	-	65,73,73	1.44	10 (15%)	76,113,113	1.44	9 (11%)
22	CLA	B	809	-	65,73,73	1.47	10 (15%)	76,113,113	1.39	8 (10%)
22	CLA	B	803	-	65,73,73	1.43	10 (15%)	76,113,113	1.44	10 (13%)
22	CLA	0	310	30	52,60,73	1.60	9 (17%)	60,97,113	1.55	7 (11%)
22	CLA	B	813	-	55,63,73	1.58	9 (16%)	64,101,113	1.45	6 (9%)
25	8CT	B	846	-	40,41,41	4.71	24 (60%)	50,56,56	2.91	17 (34%)
22	CLA	A	823	-	51,59,73	1.64	10 (19%)	59,96,113	1.57	8 (13%)
30	XAT	7	320	-	39,47,47	1.01	2 (5%)	54,74,74	2.75	20 (37%)
29	CHL	2	306	-	48,56,74	2.23	15 (31%)	51,92,114	2.75	20 (39%)
22	CLA	7	318	22	65,73,73	1.46	10 (15%)	76,113,113	1.47	9 (11%)
25	8CT	8	318	-	40,41,41	4.69	24 (60%)	50,56,56	2.68	18 (36%)
22	CLA	6	317	-	45,53,73	1.72	10 (22%)	52,89,113	1.62	8 (15%)
22	CLA	8	303	31,22	46,54,73	1.68	10 (21%)	53,90,113	1.57	7 (13%)
31	LMG	8	319	22	44,44,55	0.85	4 (9%)	52,52,63	1.40	5 (9%)
22	CLA	A	803	-	65,73,73	1.43	10 (15%)	76,113,113	1.48	10 (13%)
22	CLA	A	836	-	51,59,73	1.62	10 (19%)	59,96,113	1.58	10 (16%)
22	CLA	B	834	2	65,73,73	1.52	10 (15%)	76,113,113	1.35	8 (10%)
22	CLA	B	841	24	65,73,73	1.43	10 (15%)	76,113,113	1.50	10 (13%)
22	CLA	3	303	-	45,53,73	1.76	9 (20%)	52,89,113	1.59	7 (13%)
25	8CT	A	850	-	40,41,41	4.67	24 (60%)	50,56,56	2.90	18 (36%)
30	XAT	8	316	29	39,47,47	0.92	1 (2%)	54,74,74	3.74	29 (53%)
25	8CT	G	104	-	40,41,41	4.74	24 (60%)	50,56,56	2.59	19 (38%)
22	CLA	A	837	-	65,73,73	1.43	8 (12%)	76,113,113	1.45	8 (10%)
22	CLA	A	825	-	65,73,73	1.46	8 (12%)	76,113,113	1.41	9 (11%)
22	CLA	B	807	-	45,53,73	1.70	10 (22%)	52,89,113	1.84	9 (17%)
22	CLA	5	309	13,30	60,68,73	1.53	9 (15%)	70,107,113	1.42	8 (11%)
30	XAT	5	315	22	39,47,47	0.94	1 (2%)	54,74,74	4.68	23 (42%)
25	8CT	A	846	25	40,41,41	4.64	24 (60%)	50,56,56	2.97	19 (38%)
29	CHL	8	314	-	43,51,74	2.34	15 (34%)	45,86,114	3.01	22 (48%)
25	8CT	B	847	-	40,41,41	4.69	24 (60%)	50,56,56	2.73	18 (36%)
22	CLA	1	309	24	41,49,73	1.79	10 (24%)	47,84,113	1.72	9 (19%)
22	CLA	A	819	-	65,73,73	1.43	9 (13%)	76,113,113	1.53	8 (10%)
22	CLA	7	317	-	65,73,73	1.45	8 (12%)	76,113,113	1.36	7 (9%)
22	CLA	6	323	16	46,54,73	1.68	10 (21%)	53,90,113	1.51	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	6	304	17	65,73,73	1.49	10 (15%)	76,113,113	1.41	8 (10%)
22	CLA	L	203	-	65,73,73	1.44	6 (9%)	76,113,113	1.37	7 (9%)
29	CHL	2	307	-	51,59,74	2.00	13 (25%)	55,96,114	2.87	22 (40%)
22	CLA	A	838	-	65,73,73	1.45	9 (13%)	76,113,113	1.38	9 (11%)
22	CLA	A	807	-	65,73,73	1.44	10 (15%)	76,113,113	1.47	9 (11%)

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
29	CHL	8	306	-	3/3/17/26	9/21/119/137	-
22	CLA	3	301	-	1/1/14/20	11/31/109/115	-
22	CLA	1	307	-	1/1/15/20	16/37/115/115	-
22	CLA	L	202	-	1/1/15/20	15/37/115/115	-
22	CLA	9	304	-	1/1/11/20	8/17/95/115	-
30	XAT	1	315	-	-	1/31/93/93	0/4/4/4
22	CLA	2	311	14	1/1/12/20	7/22/100/115	-
30	XAT	5	316	-	-	2/31/93/93	0/4/4/4
22	CLA	K	104	-	1/1/11/20	5/15/93/115	-
29	CHL	1	305	-	3/3/16/26	7/18/116/137	-
22	CLA	3	305	15	1/1/11/20	8/16/94/115	-
22	CLA	6	312	-	1/1/12/20	9/22/100/115	-
22	CLA	4	309	30	1/1/14/20	14/31/109/115	-
22	CLA	7	307	22	1/1/11/20	3/16/94/115	-
22	CLA	1	304	-	1/1/12/20	6/22/100/115	-
22	CLA	9	309	-	1/1/14/20	15/31/109/115	-
22	CLA	3	309	24	1/1/8/20	0/2/76/115	-
22	CLA	4	313	-	1/1/11/20	6/13/91/115	-
22	CLA	3	312	-	1/1/11/20	7/13/91/115	-
27	SF4	C	101	-	-	-	0/6/5/5
29	CHL	2	305	-	3/3/15/26	3/12/110/137	-
22	CLA	B	826	-	1/1/15/20	13/37/115/115	-
22	CLA	4	304	-	1/1/12/20	4/19/97/115	-
22	CLA	A	829	-	1/1/15/20	10/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	1	306	-	1/1/15/20	12/37/115/115	-
22	CLA	2	319	16	1/1/11/20	9/15/93/115	-
22	CLA	5	307	-	1/1/15/20	16/37/115/115	-
22	CLA	6	303	17	1/1/15/20	16/37/115/115	-
29	CHL	8	305	-	4/4/18/26	9/27/125/137	-
22	CLA	A	801	-	1/1/15/20	8/37/115/115	-
22	CLA	3	313	-	1/1/11/20	7/15/93/115	-
22	CLA	H	201	-	1/1/15/20	16/37/115/115	-
22	CLA	K	105	-	1/1/12/20	9/19/97/115	-
24	LHG	9	316	22	-	22/53/53/53	-
22	CLA	9	301	-	1/1/11/20	6/16/92/115	-
22	CLA	A	814	-	1/1/11/20	10/13/91/115	-
22	CLA	4	314	-	1/1/15/20	18/37/115/115	-
29	CHL	9	307	-	3/3/16/26	10/18/116/137	-
22	CLA	A	820	-	1/1/11/20	4/13/91/115	-
22	CLA	A	826	25	1/1/15/20	13/37/115/115	-
22	CLA	B	830	-	1/1/15/20	9/37/115/115	-
22	CLA	3	304	-	1/1/10/20	3/10/88/115	-
25	8CT	6	321	-	-	9/29/63/63	0/2/2/2
30	XAT	9	314	22	-	4/31/93/93	0/4/4/4
24	LHG	3	317	22	-	12/23/23/53	-
22	CLA	7	302	18	1/1/11/20	7/15/93/115	-
30	XAT	3	314	25	-	4/31/93/93	0/4/4/4
22	CLA	B	806	-	1/1/15/20	17/37/115/115	-
22	CLA	5	305	25	1/1/12/20	6/22/100/115	-
22	CLA	7	312	30	1/1/12/20	3/22/100/115	-
29	CHL	2	301	22	4/4/19/26	13/33/131/137	-
30	XAT	7	319	22	-	7/31/93/93	0/4/4/4
22	CLA	9	311	-	1/1/12/20	4/22/100/115	-
22	CLA	2	302	29	1/1/15/20	17/37/115/115	-
22	CLA	A	821	-	1/1/15/20	9/37/115/115	-
22	CLA	1	308	13,30	1/1/14/20	11/31/109/115	-
22	CLA	A	828	-	1/1/15/20	18/37/115/115	-
22	CLA	0	305	29,22	1/1/12/20	8/22/100/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	A	817	-	1/1/15/20	19/37/115/115	-
27	SF4	C	102	3	-	-	0/6/5/5
22	CLA	7	313	-	1/1/13/20	13/25/103/115	-
25	8CT	4	317	-	-	8/29/63/63	0/2/2/2
22	CLA	A	835	1	1/1/11/20	5/13/91/115	-
22	CLA	5	303	-	-	23/37/115/115	-
22	CLA	8	313	-	1/1/11/20	3/13/91/115	-
22	CLA	5	302	-	1/1/15/20	9/37/115/115	-
22	CLA	3	310	-	1/1/12/20	2/22/100/115	-
22	CLA	G	101	-	1/1/11/20	5/13/91/115	-
22	CLA	1	313	-	1/1/11/20	7/15/93/115	-
22	CLA	9	308	-	1/1/15/20	16/37/115/115	-
25	8CT	B	851	22	-	15/29/63/63	0/2/2/2
22	CLA	8	310	31	1/1/13/20	8/25/103/115	-
23	PQN	B	842	-	-	5/23/43/43	0/2/2/2
22	CLA	5	313	-	1/1/13/20	7/25/103/115	-
30	XAT	6	320	-	-	4/31/93/93	0/4/4/4
22	CLA	4	312	-	1/1/13/20	6/27/105/115	-
25	8CT	B	848	-	-	10/29/63/63	0/2/2/2
24	LHG	5	318	22	-	29/53/53/53	-
24	LHG	1	317	22	-	25/53/53/53	-
25	8CT	J	101	-	-	9/29/63/63	0/2/2/2
22	CLA	B	808	-	1/1/15/20	16/37/115/115	-
22	CLA	B	823	-	-	11/25/103/115	-
22	CLA	B	827	-	1/1/15/20	18/37/115/115	-
24	LHG	A	844	-	-	25/53/53/53	-
29	CHL	7	308	-	3/3/16/26	8/17/115/137	-
22	CLA	6	309	17	1/1/12/20	10/19/97/115	-
22	CLA	B	836	-	1/1/14/20	13/31/109/115	-
22	CLA	8	311	-	-	5/22/100/115	-
22	CLA	B	831	-	1/1/12/20	8/19/97/115	-
22	CLA	2	309	-	1/1/14/20	10/31/109/115	-
29	CHL	6	308	-	3/3/17/26	6/21/119/137	-
25	8CT	B	843	-	-	16/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	837	-	1/1/15/20	17/37/115/115	-
25	8CT	7	321	-	-	10/29/63/63	0/2/2/2
22	CLA	B	832	-	1/1/15/20	14/37/115/115	-
22	CLA	B	819	-	1/1/14/20	19/31/109/115	-
22	CLA	B	850	-	1/1/13/20	11/25/103/115	-
24	LHG	A	845	22	-	16/31/31/53	-
22	CLA	A	816	-	1/1/11/20	4/13/91/115	-
29	CHL	6	302	17,22	4/4/19/26	14/33/131/137	-
22	CLA	5	310	24	1/1/10/20	3/8/86/115	-
22	CLA	B	822	-	1/1/11/20	6/15/93/115	-
22	CLA	0	309	24	1/1/10/20	2/8/86/115	-
22	CLA	8	302	-	1/1/14/20	7/31/109/115	-
22	CLA	0	312	29	1/1/13/20	10/25/103/115	-
30	XAT	2	315	-	-	2/31/93/93	0/4/4/4
30	XAT	9	315	-	-	0/31/93/93	0/4/4/4
22	CLA	7	315	-	1/1/11/20	4/15/93/115	-
22	CLA	B	824	-	1/1/14/20	13/31/109/115	-
22	CLA	A	841	25	1/1/15/20	13/37/115/115	-
22	CLA	B	817	-	1/1/13/20	10/25/103/115	-
22	CLA	9	303	19	1/1/15/20	12/37/115/115	-
24	LHG	6	322	22	-	22/41/41/53	-
22	CLA	6	315	-	1/1/15/20	14/37/115/115	-
29	CHL	4	306	29	3/3/17/26	7/21/119/137	-
30	XAT	2	316	-	-	3/31/93/93	0/4/4/4
22	CLA	A	805	-	1/1/15/20	14/37/115/115	-
29	CHL	3	306	25	3/3/16/26	3/17/115/137	-
22	CLA	6	311	24	1/1/15/20	20/37/115/115	-
22	CLA	K	102	-	1/1/11/20	9/15/93/115	-
28	DGD	B	849	-	-	31/55/95/95	0/2/2/2
27	SF4	B	802	-	-	-	0/6/5/5
22	CLA	3	311	-	1/1/13/20	11/25/103/115	-
22	CLA	4	302	-	1/1/14/20	8/31/109/115	-
22	CLA	B	818	-	1/1/13/20	12/30/108/115	-
22	CLA	8	312	16	1/1/13/20	5/27/105/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	805	-	1/1/15/20	16/37/115/115	-
22	CLA	A	806	-	1/1/15/20	20/37/115/115	-
30	XAT	8	317	-	-	0/31/93/93	0/4/4/4
22	CLA	B	814	-	1/1/15/20	21/37/115/115	-
22	CLA	1	312	29	1/1/13/20	10/25/103/115	-
22	CLA	0	303	30	1/1/15/20	14/37/115/115	-
22	CLA	1	301	13	1/1/15/20	10/37/115/115	-
24	LHG	7	322	22	-	16/23/23/53	-
29	CHL	6	307	-	3/3/15/26	6/12/110/137	-
22	CLA	B	833	-	1/1/13/20	13/29/107/115	-
22	CLA	B	810	-	1/1/15/20	6/37/115/115	-
22	CLA	B	829	-	1/1/15/20	11/37/115/115	-
25	8CT	B	844	-	-	15/29/63/63	0/2/2/2
22	CLA	5	304	-	1/1/12/20	8/22/100/115	-
25	8CT	F	302	-	-	9/29/63/63	0/2/2/2
30	XAT	0	314	29,22	-	8/31/93/93	0/4/4/4
22	CLA	7	310	18	1/1/12/20	7/19/97/115	-
22	CLA	7	311	24	1/1/8/20	0/2/76/115	-
22	CLA	8	308	16	1/1/12/20	6/19/97/115	-
29	CHL	5	301	13	4/4/19/26	14/33/131/137	-
29	CHL	0	301	24,22	4/4/19/26	17/33/131/137	-
25	8CT	A	849	22	-	11/29/63/63	0/2/2/2
22	CLA	2	303	-	1/1/15/20	11/37/115/115	-
22	CLA	7	305	-	1/1/11/20	8/13/91/115	-
22	CLA	A	818	-	1/1/15/20	12/37/115/115	-
22	CLA	2	308	-	1/1/12/20	5/19/97/115	-
23	PQN	A	842	-	-	7/23/43/43	0/2/2/2
22	CLA	B	801	-	1/1/15/20	10/37/115/115	-
29	CHL	4	307	-	3/3/17/26	5/21/119/137	-
22	CLA	A	827	-	1/1/15/20	15/37/115/115	-
22	CLA	6	314	-	1/1/10/20	6/11/89/115	-
22	CLA	A	839	-	1/1/15/20	17/37/115/115	-
22	CLA	6	305	-	1/1/14/20	13/31/109/115	-
29	CHL	5	306	-	3/3/16/26	7/18/116/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	A	810	-	1/1/15/20	11/37/115/115	-
22	CLA	A	813	-	1/1/15/20	16/37/115/115	-
22	CLA	0	304	22	1/1/12/20	11/22/100/115	-
22	CLA	B	825	-	1/1/15/20	17/37/115/115	-
25	8CT	B	845	-	-	12/29/63/63	0/2/2/2
22	CLA	4	311	22	1/1/12/20	8/22/100/115	-
22	CLA	1	303	-	1/1/12/20	8/22/100/115	-
22	CLA	B	820	-	1/1/15/20	9/37/115/115	-
25	8CT	A	848	-	-	6/29/63/63	0/2/2/2
22	CLA	A	811	22	1/1/15/20	18/37/115/115	-
22	CLA	5	312	30	1/1/15/20	12/37/115/115	-
22	CLA	J	103	10	1/1/10/20	8/10/88/115	-
22	CLA	B	816	-	1/1/14/20	13/31/109/115	-
22	CLA	A	808	1	1/1/15/20	20/37/115/115	-
25	8CT	L	206	-	-	15/29/63/63	0/2/2/2
22	CLA	A	832	-	1/1/15/20	16/37/115/115	-
22	CLA	4	310	-	1/1/13/20	7/25/103/115	-
30	XAT	0	313	22	-	16/31/93/93	0/4/4/4
25	8CT	5	317	22	-	10/29/63/63	0/2/2/2
25	8CT	B	804	-	-	15/29/63/63	0/2/2/2
22	CLA	B	838	-	1/1/11/20	4/16/94/115	-
24	LHG	B	852	22	-	10/26/26/53	-
22	CLA	3	302	25	1/1/12/20	2/19/97/115	-
22	CLA	9	306	-	1/1/12/20	8/22/100/115	-
22	CLA	7	303	18	1/1/14/20	17/31/109/115	-
22	CLA	5	308	-	1/1/10/20	2/10/88/115	-
22	CLA	0	308	20	1/1/14/20	16/31/109/115	-
22	CLA	2	313	-	1/1/10/20	2/11/89/115	-
25	8CT	3	318	25,22	-	6/29/63/63	0/2/2/2
22	CLA	A	824	-	1/1/13/20	8/25/103/115	-
24	LHG	2	318	22	-	19/36/36/53	-
22	CLA	G	102	-	1/1/12/20	5/19/97/115	-
29	CHL	0	306	22,30	3/3/16/26	5/18/116/137	-
22	CLA	B	821	-	1/1/12/20	8/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	F	301	-	1/1/11/20	8/13/91/115	-
29	CHL	6	306	-	3/3/15/26	2/12/110/137	-
26	HTG	A	851	-	-	4/10/30/30	0/1/1/1
22	CLA	2	310	24	1/1/10/20	4/8/86/115	-
22	CLA	6	318	17	1/1/12/20	6/22/100/115	-
22	CLA	A	804	22	1/1/13/20	9/25/103/115	-
22	CLA	A	830	-	1/1/15/20	11/37/115/115	-
22	CLA	A	822	-	1/1/11/20	10/18/96/115	-
25	8CT	A	854	-	-	12/29/63/63	0/2/2/2
25	8CT	I	101	-	-	10/29/63/63	0/2/2/2
22	CLA	1	310	-	1/1/12/20	7/22/100/115	-
29	CHL	4	301	22,13	4/4/19/26	11/33/131/137	-
29	CHL	9	302	19	4/4/19/26	11/33/131/137	-
22	CLA	B	811	-	1/1/15/20	11/37/115/115	-
22	CLA	9	310	24	1/1/10/20	4/8/86/115	-
22	CLA	0	311	-	1/1/15/20	14/37/115/115	-
22	CLA	0	302	30	1/1/15/20	16/37/115/115	-
22	CLA	2	304	-	1/1/14/20	16/31/109/115	-
24	LHG	0	315	29,22	-	27/53/53/53	-
22	CLA	9	313	-	1/1/13/20	13/25/103/115	-
22	CLA	A	833	25	1/1/15/20	14/37/115/115	-
22	CLA	A	831	-	1/1/12/20	1/19/97/115	-
22	CLA	L	204	-	1/1/12/20	9/19/97/115	-
30	XAT	4	315	22	-	8/31/93/93	0/4/4/4
22	CLA	4	308	16	1/1/12/20	1/19/97/115	-
30	XAT	4	316	-	-	3/31/93/93	0/4/4/4
29	CHL	8	307	30	3/3/17/26	7/21/119/137	-
22	CLA	7	309	22	1/1/12/20	4/19/97/115	-
25	8CT	3	316	-	-	12/29/63/63	0/2/2/2
25	8CT	L	205	22	-	13/29/63/63	0/2/2/2
22	CLA	L	201	-	1/1/15/20	17/37/115/115	-
22	CLA	A	853	-	1/1/15/20	15/37/115/115	-
25	8CT	J	104	-	-	7/29/63/63	0/2/2/2
25	8CT	K	103	-	-	12/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CHL	6	316	17	3/3/15/26	8/12/110/137	-
22	CLA	G	103	7	1/1/11/20	9/15/93/115	-
30	XAT	1	314	22	-	11/31/93/93	0/4/4/4
22	CLA	A	852	-	1/1/11/20	7/18/96/115	-
30	XAT	3	315	-	-	0/31/93/93	0/4/4/4
22	CLA	A	834	-	1/1/12/20	1/19/97/115	-
22	CLA	3	308	-	1/1/12/20	3/19/97/115	-
22	CLA	B	835	-	1/1/11/20	3/13/91/115	-
22	CLA	1	311	-	1/1/15/20	15/37/115/115	-
22	CLA	8	309	-	1/1/14/20	8/31/109/115	-
22	CLA	2	312	14	1/1/15/20	15/37/115/115	-
22	CLA	0	307	22	1/1/15/20	26/37/115/115	-
22	CLA	7	304	22	1/1/11/20	6/16/94/115	-
22	CLA	5	314	24	1/1/11/20	9/15/93/115	-
22	CLA	B	839	25	1/1/15/20	13/37/115/115	-
22	CLA	M	101	-	-	8/15/93/115	-
25	8CT	2	317	-	-	10/29/63/63	0/2/2/2
22	CLA	9	305	-	1/1/12/20	7/22/100/115	-
22	CLA	B	828	-	1/1/15/20	16/37/115/115	-
22	CLA	7	306	22	1/1/10/20	4/10/88/115	-
22	CLA	B	840	-	1/1/15/20	14/37/115/115	-
22	CLA	A	802	-	1/1/15/20	8/37/115/115	-
22	CLA	K	101	-	1/1/11/20	7/13/91/115	-
30	XAT	6	319	22	-	3/31/93/93	0/4/4/4
22	CLA	2	314	14	1/1/11/20	7/18/96/115	-
22	CLA	A	809	1	1/1/15/20	13/37/115/115	-
22	CLA	1	302	-	1/1/15/20	21/37/115/115	-
22	CLA	6	313	29	1/1/15/20	10/37/115/115	-
22	CLA	7	316	18	1/1/15/20	18/37/115/115	-
22	CLA	4	303	-	1/1/11/20	5/15/93/115	-
22	CLA	5	311	30	1/1/11/20	1/13/91/115	-
22	CLA	7	314	-	1/1/11/20	4/13/91/115	-
31	LMG	5	319	22	-	18/39/59/70	0/1/1/1
22	CLA	8	304	-	1/1/12/20	10/19/97/115	-
22	CLA	3	319	-	1/1/15/20	21/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	8CT	7	301	29,30	-	11/29/63/63	0/2/2/2
29	CHL	4	305	29	4/4/18/26	12/27/125/137	-
22	CLA	6	310	17,30	1/1/14/20	10/31/109/115	-
25	8CT	8	301	-	-	13/29/63/63	0/2/2/2
22	CLA	A	843	24	1/1/12/20	11/22/100/115	-
22	CLA	8	315	-	1/1/15/20	25/37/115/115	-
22	CLA	6	301	-	1/1/12/20	11/22/100/115	-
25	8CT	7	323	-	-	14/29/63/63	0/2/2/2
22	CLA	3	307	15	1/1/12/20	8/19/97/115	-
31	LMG	4	318	-	-	19/39/59/70	0/1/1/1
25	8CT	1	316	13	-	11/29/63/63	0/2/2/2
22	CLA	B	812	2	1/1/15/20	13/37/115/115	-
22	CLA	A	815	-	1/1/11/20	3/16/94/115	-
25	8CT	A	847	-	-	9/29/63/63	0/2/2/2
22	CLA	9	312	30	1/1/13/20	13/30/108/115	-
22	CLA	A	812	-	1/1/12/20	1/24/102/115	-
22	CLA	B	815	-	1/1/15/20	11/37/115/115	-
26	HTG	J	102	-	-	3/10/30/30	0/1/1/1
22	CLA	A	840	-	1/1/15/20	14/37/115/115	-
22	CLA	B	809	-	1/1/15/20	20/37/115/115	-
22	CLA	B	803	-	1/1/15/20	19/37/115/115	-
22	CLA	0	310	30	1/1/12/20	2/22/100/115	-
22	CLA	B	813	-	1/1/13/20	7/25/103/115	-
25	8CT	B	846	-	-	13/29/63/63	0/2/2/2
22	CLA	A	823	-	1/1/12/20	6/21/99/115	-
30	XAT	7	320	-	-	0/31/93/93	0/4/4/4
29	CHL	2	306	-	3/3/16/26	8/18/116/137	-
22	CLA	7	318	22	1/1/15/20	18/37/115/115	-
25	8CT	8	318	-	-	13/29/63/63	0/2/2/2
22	CLA	6	317	-	1/1/11/20	5/13/91/115	-
22	CLA	8	303	31,22	1/1/11/20	3/15/93/115	-
31	LMG	8	319	22	-	17/39/59/70	0/1/1/1
22	CLA	A	803	-	1/1/15/20	17/37/115/115	-
22	CLA	A	836	-	1/1/12/20	11/21/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	834	2	1/1/15/20	16/37/115/115	-
22	CLA	B	841	24	1/1/15/20	13/37/115/115	-
22	CLA	3	303	-	1/1/11/20	5/13/91/115	-
25	8CT	A	850	-	-	11/29/63/63	0/2/2/2
30	XAT	8	316	29	-	7/31/93/93	0/4/4/4
25	8CT	G	104	-	-	13/29/63/63	0/2/2/2
22	CLA	A	837	-	1/1/15/20	19/37/115/115	-
22	CLA	A	825	-	-	15/37/115/115	-
22	CLA	B	807	-	1/1/11/20	5/13/91/115	-
22	CLA	5	309	13,30	1/1/14/20	8/31/109/115	-
30	XAT	5	315	22	-	6/31/93/93	0/4/4/4
25	8CT	A	846	25	-	13/29/63/63	0/2/2/2
29	CHL	8	314	-	3/3/15/26	3/12/110/137	-
25	8CT	B	847	-	-	10/29/63/63	0/2/2/2
22	CLA	1	309	24	1/1/10/20	2/8/86/115	-
22	CLA	A	819	-	1/1/15/20	14/37/115/115	-
22	CLA	7	317	-	1/1/15/20	19/37/115/115	-
22	CLA	6	323	16	1/1/11/20	11/15/93/115	-
22	CLA	6	304	17	1/1/15/20	15/37/115/115	-
22	CLA	L	203	-	1/1/15/20	14/37/115/115	-
29	CHL	2	307	-	3/3/17/26	9/21/119/137	-
22	CLA	A	838	-	1/1/15/20	16/37/115/115	-
22	CLA	A	807	-	1/1/15/20	14/37/115/115	-

The worst 5 of 3250 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	3	318	8CT	C02-C03	14.68	1.59	1.34
25	5	317	8CT	C02-C03	14.38	1.59	1.34
25	K	103	8CT	C32-C31	14.37	1.61	1.32
25	7	301	8CT	C02-C03	14.33	1.59	1.34
25	1	316	8CT	C02-C03	14.33	1.59	1.34

The worst 5 of 3454 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	2	315	XAT	O4-C5-C4	-26.68	93.34	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	0	313	XAT	O24-C25-C24	-23.72	95.57	113.38
30	5	315	XAT	O24-C25-C38	-20.89	90.03	115.06
30	5	315	XAT	O24-C25-C24	-18.04	99.83	113.38
30	2	315	XAT	O4-C5-C18	-18.03	93.46	115.06

5 of 299 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	A	801	CLA	ND
22	A	802	CLA	ND
22	A	803	CLA	ND
22	A	804	CLA	ND
22	A	805	CLA	ND

5 of 3256 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A	803	CLA	CAD-CBD-CGD-O1D
22	A	803	CLA	CAD-CBD-CGD-O2D
22	A	804	CLA	CHA-CBD-CGD-O1D
22	A	804	CLA	CHA-CBD-CGD-O2D
22	A	805	CLA	C14-C13-C15-C16

There are no ring outliers.

302 monomers are involved in 1491 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	8	306	CHL	4	0
22	3	301	CLA	5	0
22	1	307	CLA	6	0
22	L	202	CLA	12	0
22	9	304	CLA	6	0
30	1	315	XAT	5	0
22	2	311	CLA	1	0
30	5	316	XAT	5	0
22	K	104	CLA	6	0
29	1	305	CHL	3	0
22	6	312	CLA	2	0
22	4	309	CLA	8	0
22	7	307	CLA	13	0
22	1	304	CLA	15	0
22	9	309	CLA	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	3	309	CLA	1	0
22	4	313	CLA	5	0
22	3	312	CLA	2	0
27	C	101	SF4	1	0
29	2	305	CHL	8	0
22	B	826	CLA	9	0
22	4	304	CLA	1	0
22	A	829	CLA	6	0
22	1	306	CLA	5	0
22	2	319	CLA	1	0
22	5	307	CLA	3	0
22	6	303	CLA	6	0
29	8	305	CHL	6	0
22	A	801	CLA	7	0
22	3	313	CLA	5	0
22	H	201	CLA	18	0
22	K	105	CLA	14	0
24	9	316	LHG	8	0
22	9	301	CLA	5	0
22	A	814	CLA	4	0
22	4	314	CLA	5	0
29	9	307	CHL	4	0
22	A	820	CLA	4	0
22	A	826	CLA	12	0
22	B	830	CLA	8	0
22	3	304	CLA	1	0
25	6	321	8CT	14	0
30	9	314	XAT	5	0
24	3	317	LHG	4	0
22	7	302	CLA	1	0
30	3	314	XAT	8	0
22	B	806	CLA	10	0
22	5	305	CLA	3	0
22	7	312	CLA	3	0
29	2	301	CHL	3	0
30	7	319	XAT	7	0
22	9	311	CLA	3	0
22	2	302	CLA	8	0
22	A	821	CLA	4	0
22	1	308	CLA	6	0
22	A	828	CLA	11	0
22	0	305	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	817	CLA	7	0
22	7	313	CLA	7	0
25	4	317	8CT	12	0
22	A	835	CLA	2	0
22	5	303	CLA	11	0
22	8	313	CLA	4	0
22	5	302	CLA	8	0
22	3	310	CLA	1	0
22	G	101	CLA	1	0
22	1	313	CLA	1	0
22	9	308	CLA	5	0
25	B	851	8CT	1	0
22	8	310	CLA	9	0
23	B	842	PQN	3	0
22	5	313	CLA	6	0
30	6	320	XAT	7	0
22	4	312	CLA	6	0
25	B	848	8CT	12	0
24	5	318	LHG	8	0
24	1	317	LHG	3	0
25	J	101	8CT	10	0
22	B	808	CLA	10	0
22	B	823	CLA	3	0
22	B	827	CLA	8	0
24	A	844	LHG	3	0
29	7	308	CHL	11	0
22	6	309	CLA	5	0
22	B	836	CLA	2	0
22	8	311	CLA	8	0
22	B	831	CLA	2	0
22	2	309	CLA	6	0
29	6	308	CHL	4	0
25	B	843	8CT	3	0
22	B	837	CLA	6	0
25	7	321	8CT	14	0
22	B	832	CLA	8	0
22	B	819	CLA	4	0
22	B	850	CLA	17	0
24	A	845	LHG	2	0
22	A	816	CLA	3	0
29	6	302	CHL	7	0
22	5	310	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	0	309	CLA	2	0
22	8	302	CLA	4	0
22	0	312	CLA	6	0
30	2	315	XAT	7	0
30	9	315	XAT	8	0
22	7	315	CLA	2	0
22	B	824	CLA	8	0
22	A	841	CLA	6	0
22	B	817	CLA	6	0
22	9	303	CLA	7	0
24	6	322	LHG	4	0
22	6	315	CLA	5	0
29	4	306	CHL	2	0
30	2	316	XAT	7	0
22	A	805	CLA	8	0
29	3	306	CHL	4	0
22	6	311	CLA	5	0
22	K	102	CLA	6	0
28	B	849	DGD	11	0
27	B	802	SF4	1	0
22	3	311	CLA	10	0
22	4	302	CLA	4	0
22	B	818	CLA	6	0
22	8	312	CLA	5	0
22	B	805	CLA	7	0
22	A	806	CLA	4	0
30	8	317	XAT	9	0
22	B	814	CLA	9	0
22	1	312	CLA	8	0
22	0	303	CLA	4	0
22	1	301	CLA	8	0
24	7	322	LHG	2	0
29	6	307	CHL	8	0
22	B	833	CLA	10	0
22	B	810	CLA	8	0
22	B	829	CLA	8	0
22	5	304	CLA	8	0
30	0	314	XAT	11	0
22	7	310	CLA	9	0
22	8	308	CLA	9	0
29	5	301	CHL	12	0
29	0	301	CHL	16	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	A	849	8CT	8	0
22	2	303	CLA	3	0
22	7	305	CLA	3	0
22	A	818	CLA	4	0
22	2	308	CLA	7	0
23	A	842	PQN	3	0
22	B	801	CLA	4	0
29	4	307	CHL	11	0
22	A	827	CLA	9	0
22	6	314	CLA	4	0
22	A	839	CLA	9	0
22	6	305	CLA	11	0
29	5	306	CHL	5	0
22	A	810	CLA	4	0
22	A	813	CLA	14	0
22	0	304	CLA	4	0
22	B	825	CLA	4	0
22	4	311	CLA	5	0
22	1	303	CLA	11	0
22	B	820	CLA	5	0
22	A	811	CLA	5	0
22	5	312	CLA	6	0
22	J	103	CLA	1	0
22	B	816	CLA	5	0
22	A	808	CLA	10	0
22	A	832	CLA	5	0
22	4	310	CLA	1	0
30	0	313	XAT	8	0
25	5	317	8CT	6	0
22	B	838	CLA	1	0
24	B	852	LHG	1	0
22	3	302	CLA	3	0
22	9	306	CLA	5	0
22	7	303	CLA	10	0
22	5	308	CLA	6	0
22	0	308	CLA	4	0
22	2	313	CLA	1	0
22	A	824	CLA	3	0
24	2	318	LHG	3	0
22	G	102	CLA	8	0
29	0	306	CHL	2	0
22	F	301	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	6	306	CHL	2	0
22	6	318	CLA	8	0
22	A	804	CLA	4	0
22	A	830	CLA	3	0
22	A	822	CLA	4	0
25	A	854	8CT	3	0
22	1	310	CLA	6	0
29	4	301	CHL	9	0
29	9	302	CHL	2	0
22	B	811	CLA	4	0
22	9	310	CLA	2	0
22	0	311	CLA	7	0
22	0	302	CLA	15	0
22	2	304	CLA	5	0
24	0	315	LHG	12	0
22	9	313	CLA	3	0
22	A	833	CLA	6	0
22	A	831	CLA	3	0
22	L	204	CLA	5	0
30	4	315	XAT	9	0
22	4	308	CLA	4	0
30	4	316	XAT	7	0
29	8	307	CHL	6	0
22	7	309	CLA	5	0
25	3	316	8CT	10	0
22	L	201	CLA	5	0
22	A	853	CLA	5	0
25	J	104	8CT	16	0
25	K	103	8CT	14	0
29	6	316	CHL	3	0
22	G	103	CLA	7	0
30	1	314	XAT	10	0
22	A	852	CLA	1	0
30	3	315	XAT	9	0
22	A	834	CLA	1	0
22	3	308	CLA	6	0
22	B	835	CLA	1	0
22	1	311	CLA	12	0
22	8	309	CLA	11	0
22	2	312	CLA	5	0
22	0	307	CLA	7	0
22	7	304	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	5	314	CLA	1	0
22	B	839	CLA	4	0
22	M	101	CLA	5	0
25	2	317	8CT	13	0
22	B	828	CLA	7	0
22	7	306	CLA	6	0
22	B	840	CLA	14	0
22	A	802	CLA	4	0
22	K	101	CLA	3	0
30	6	319	XAT	7	0
22	2	314	CLA	1	0
22	A	809	CLA	14	0
22	1	302	CLA	6	0
22	6	313	CLA	5	0
22	7	316	CLA	7	0
22	4	303	CLA	2	0
22	5	311	CLA	6	0
22	7	314	CLA	2	0
31	5	319	LMG	5	0
22	8	304	CLA	2	0
22	3	319	CLA	8	0
29	4	305	CHL	9	0
22	6	310	CLA	9	0
25	8	301	8CT	11	0
22	A	843	CLA	2	0
22	8	315	CLA	3	0
22	6	301	CLA	4	0
25	7	323	8CT	22	0
22	3	307	CLA	9	0
31	4	318	LMG	1	0
25	1	316	8CT	13	0
22	B	812	CLA	4	0
22	A	815	CLA	3	0
25	A	847	8CT	1	0
22	9	312	CLA	9	0
22	A	812	CLA	4	0
22	B	815	CLA	6	0
26	J	102	HTG	1	0
22	A	840	CLA	7	0
22	B	809	CLA	8	0
22	B	803	CLA	18	0
22	0	310	CLA	2	0

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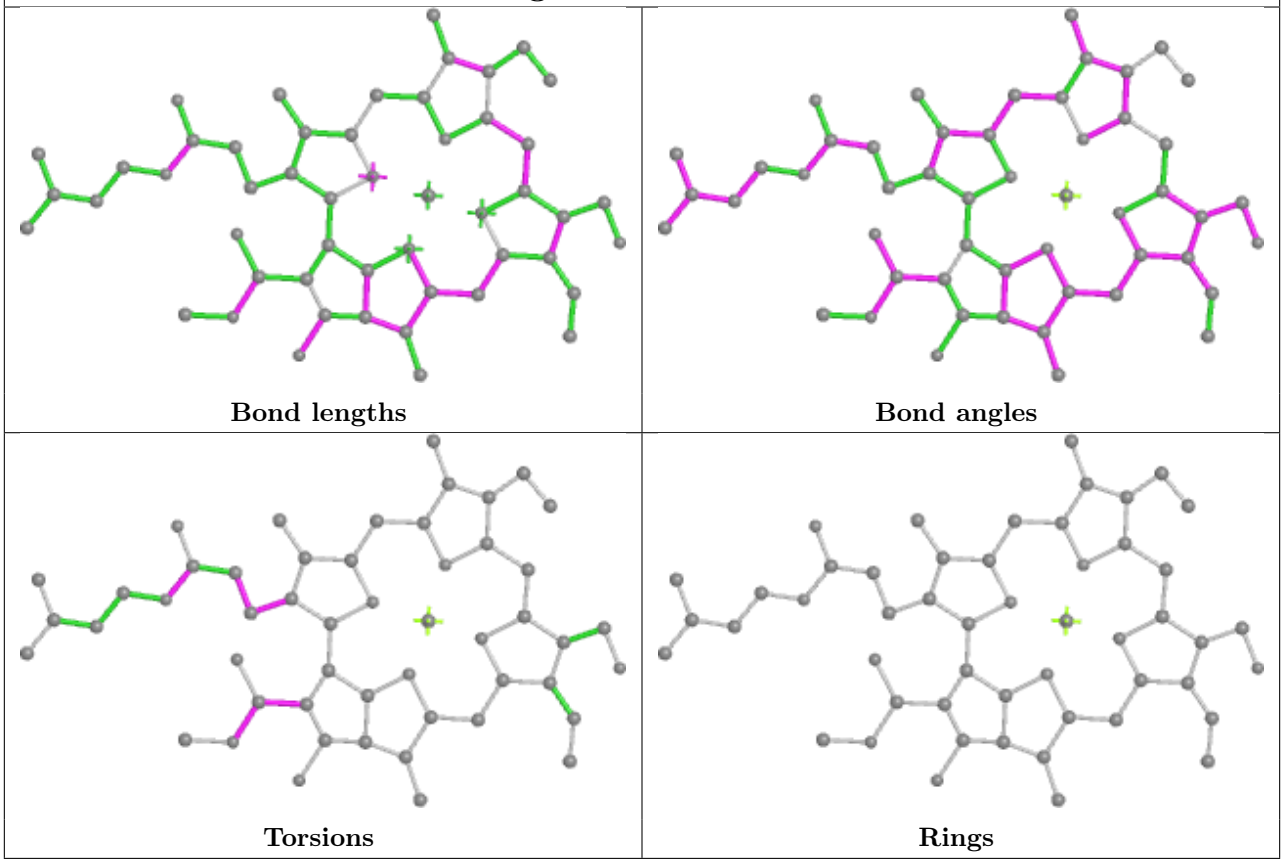
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	813	CLA	10	0
25	B	846	8CT	11	0
22	A	823	CLA	1	0
30	7	320	XAT	8	0
29	2	306	CHL	2	0
22	7	318	CLA	4	0
25	8	318	8CT	2	0
22	6	317	CLA	6	0
22	8	303	CLA	1	0
31	8	319	LMG	6	0
22	A	803	CLA	5	0
22	A	836	CLA	4	0
22	B	834	CLA	5	0
22	B	841	CLA	7	0
22	3	303	CLA	2	0
25	A	850	8CT	20	0
30	8	316	XAT	12	0
25	G	104	8CT	20	0
22	A	837	CLA	6	0
22	A	825	CLA	9	0
22	B	807	CLA	5	0
22	5	309	CLA	10	0
30	5	315	XAT	8	0
25	A	846	8CT	1	0
29	8	314	CHL	11	0
25	B	847	8CT	13	0
22	1	309	CLA	3	0
22	A	819	CLA	6	0
22	7	317	CLA	12	0
22	6	323	CLA	5	0
22	6	304	CLA	5	0
22	L	203	CLA	5	0
29	2	307	CHL	4	0
22	A	838	CLA	3	0
22	A	807	CLA	4	0

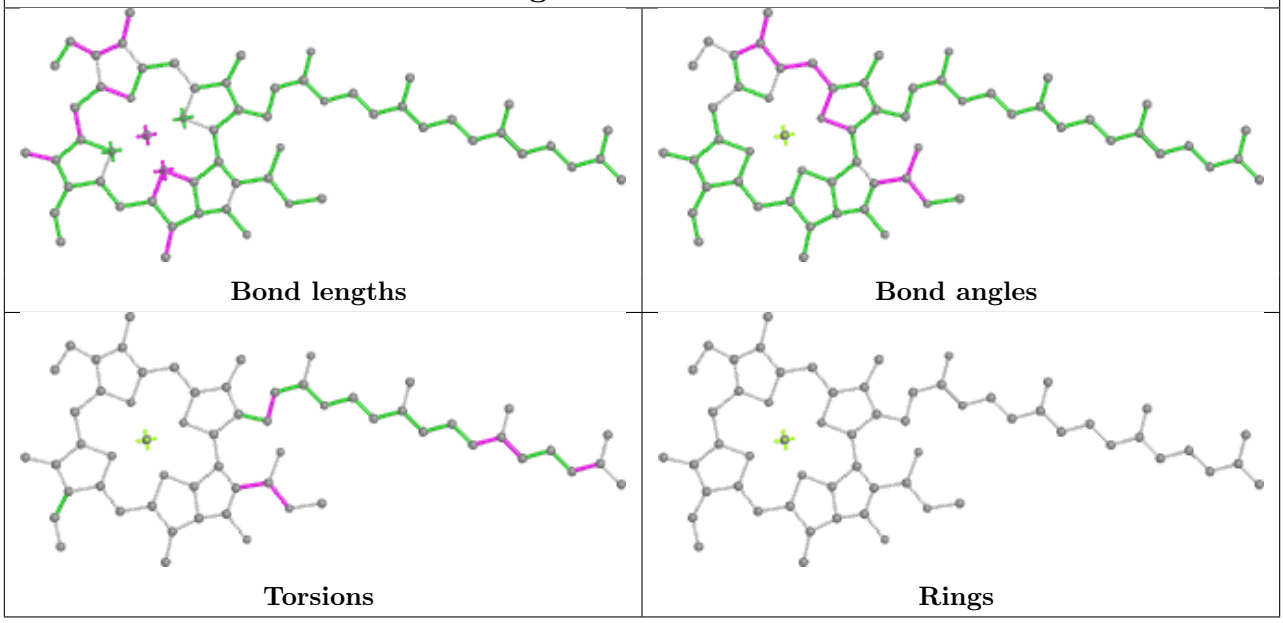
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

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

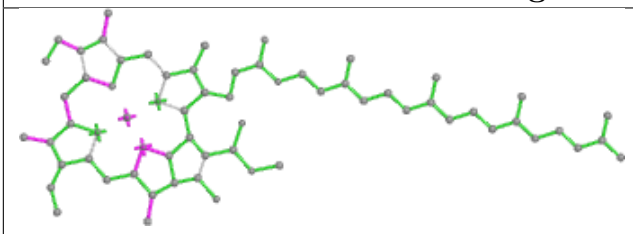
Ligand CHL 8 306



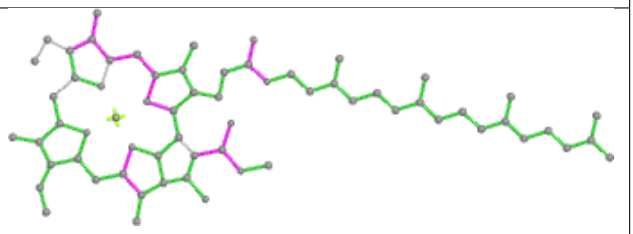
Ligand CLA 3 301



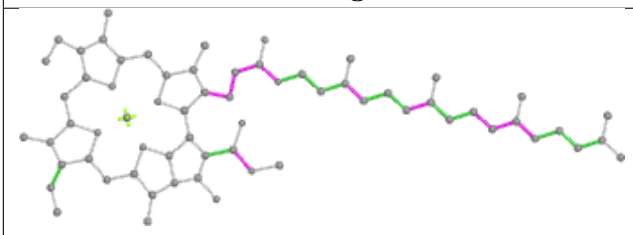
Ligand CLA 1 307



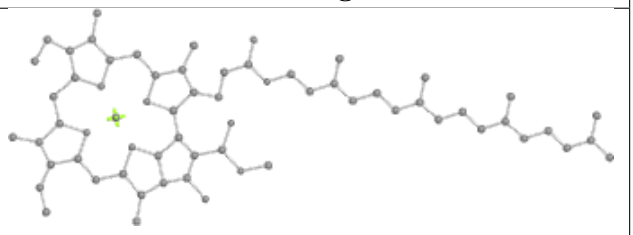
Bond lengths



Bond angles

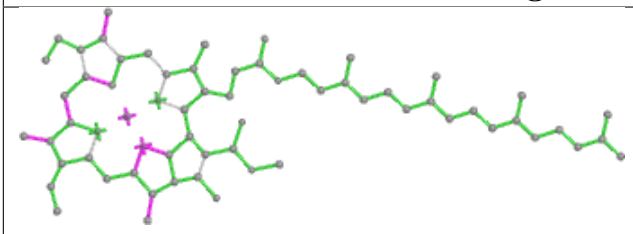


Torsions

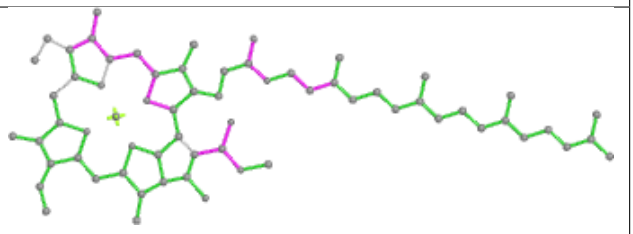


Rings

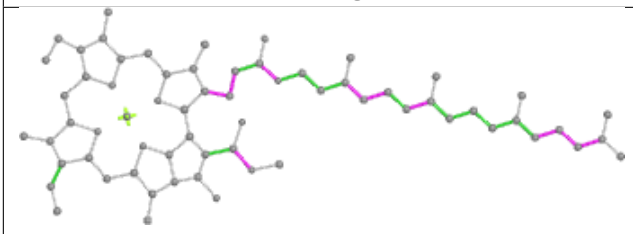
Ligand CLA L 202



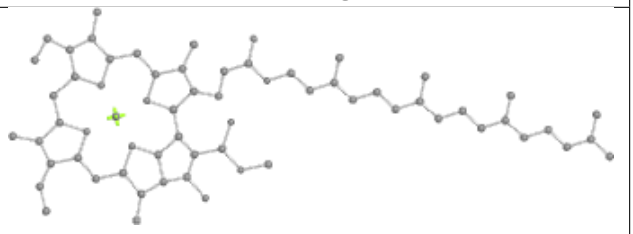
Bond lengths



Bond angles

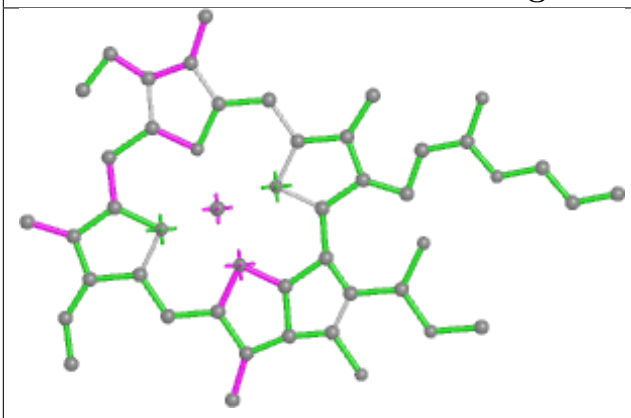


Torsions



Rings

Ligand CLA 9 304



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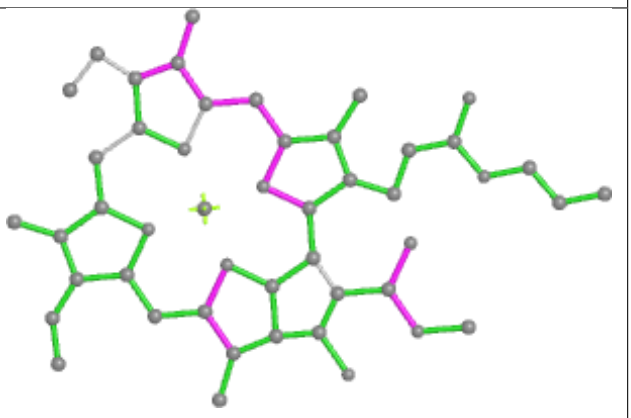
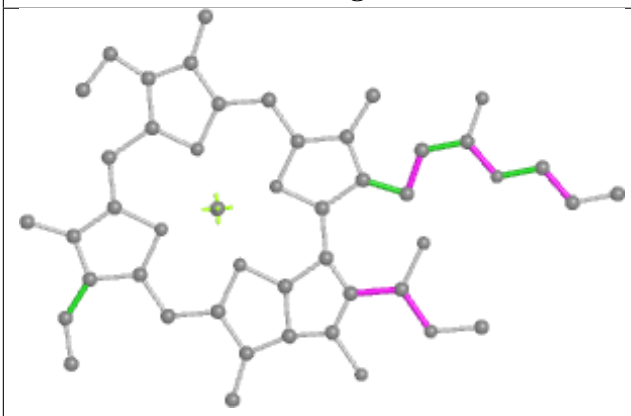
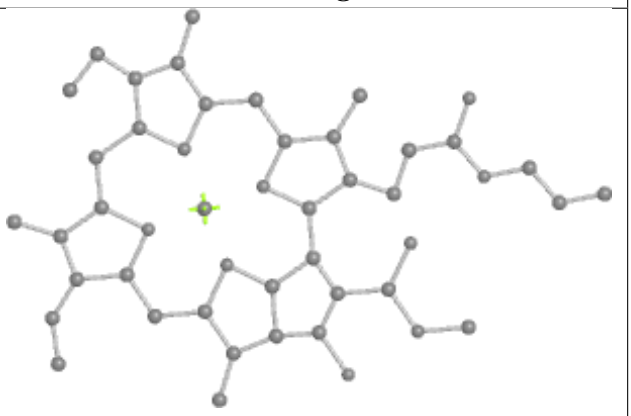


Bond angles

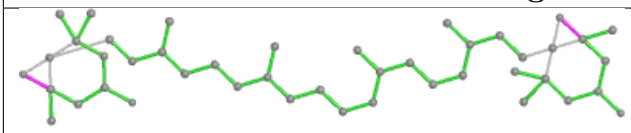


Torsions



Rings

Ligand XAT 1 315



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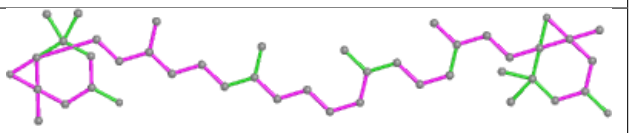
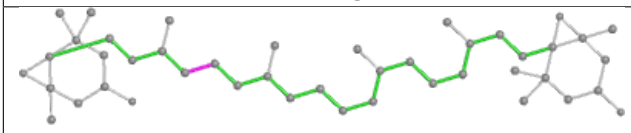
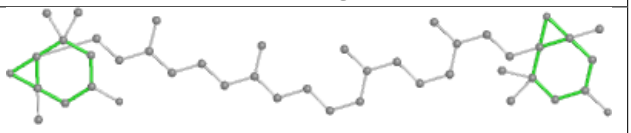


Bond angles

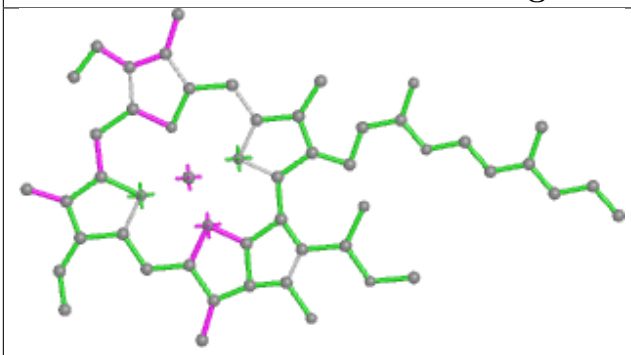


Torsions

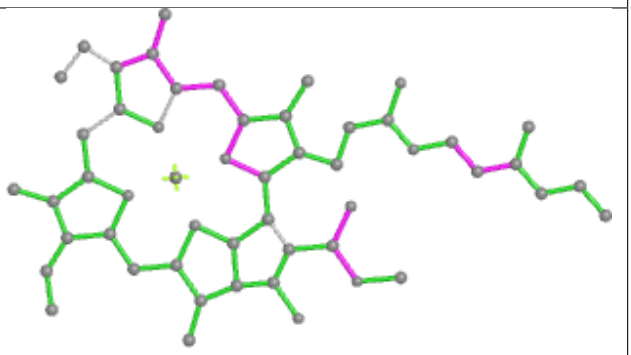


Rings

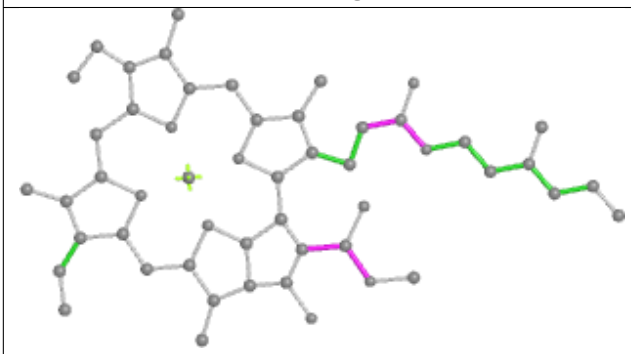
Ligand CLA 2 311



Bond lengths



Bond angles



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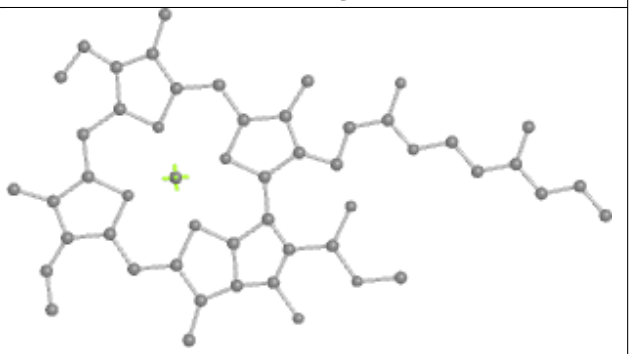
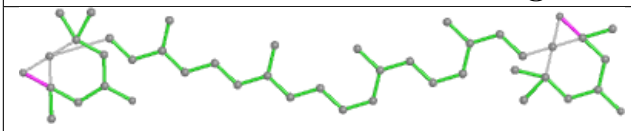
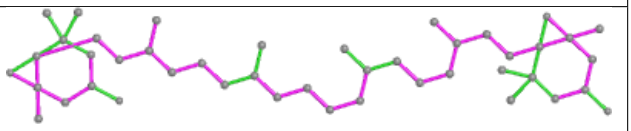


Rings

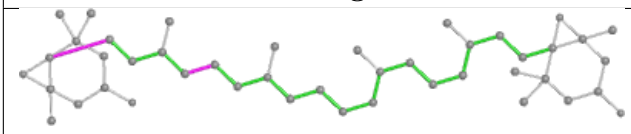
Ligand XAT 5 316



Bond lengths



Bond angles



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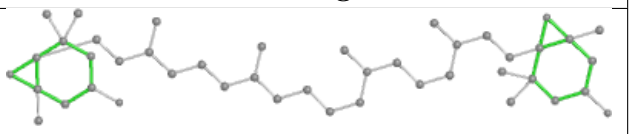
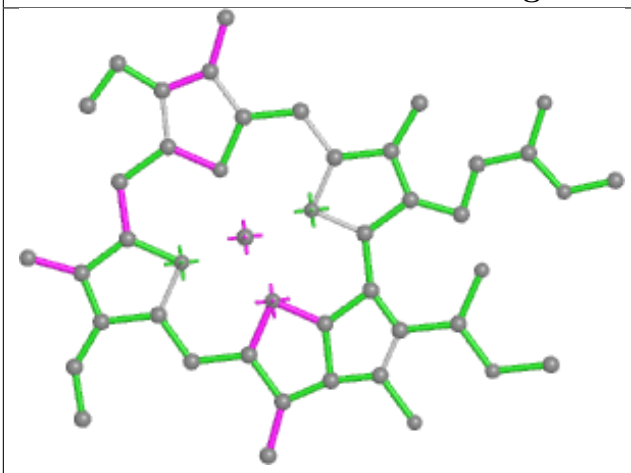


Rings

Ligand CLA K 104



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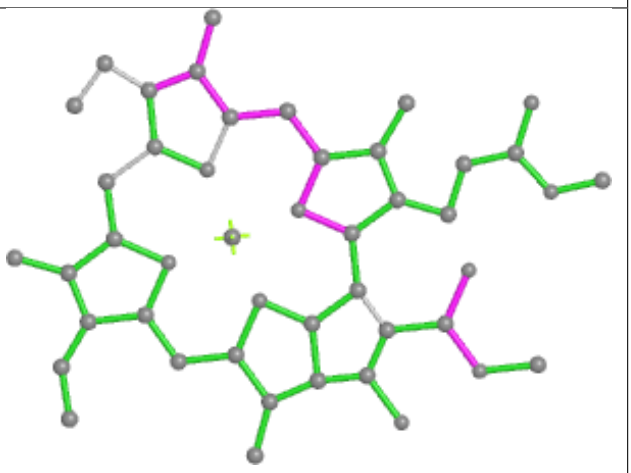
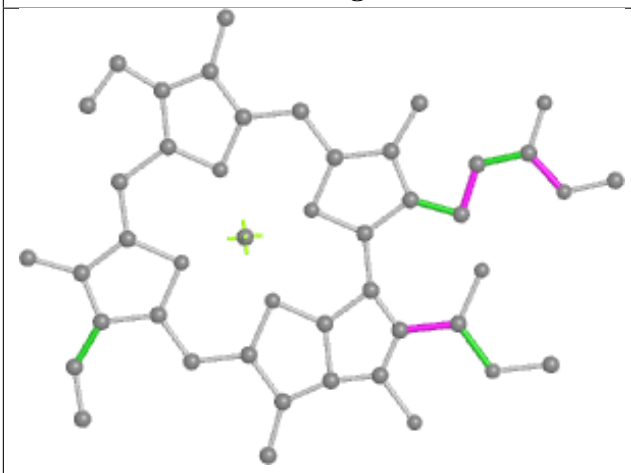


Bond angles



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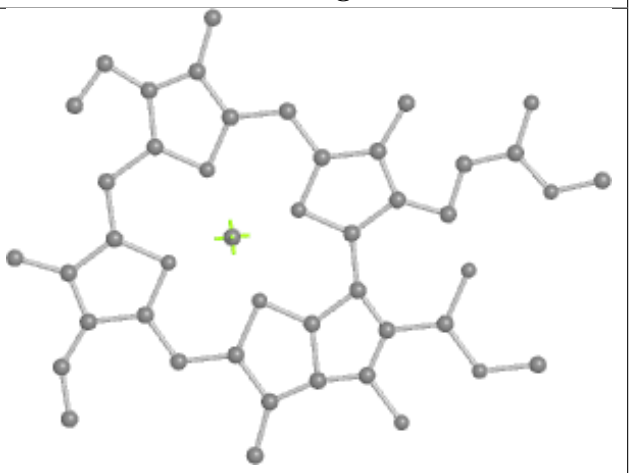
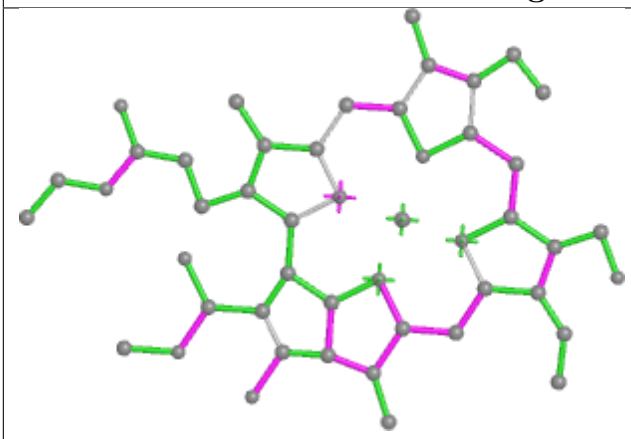


Rings

Ligand CHL 1 305



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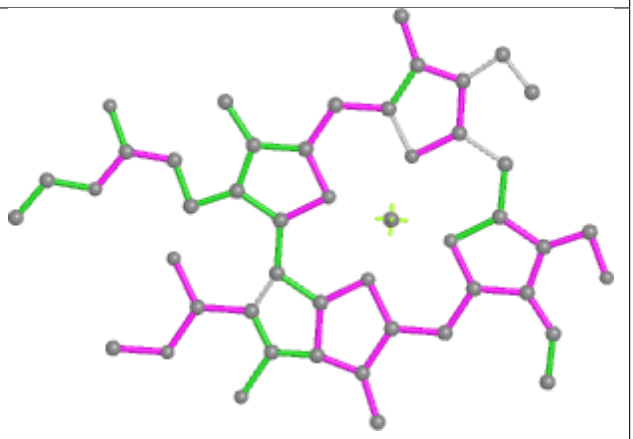
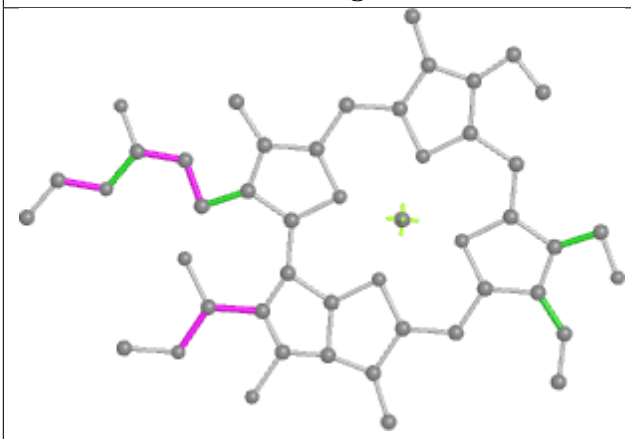


Bond angles



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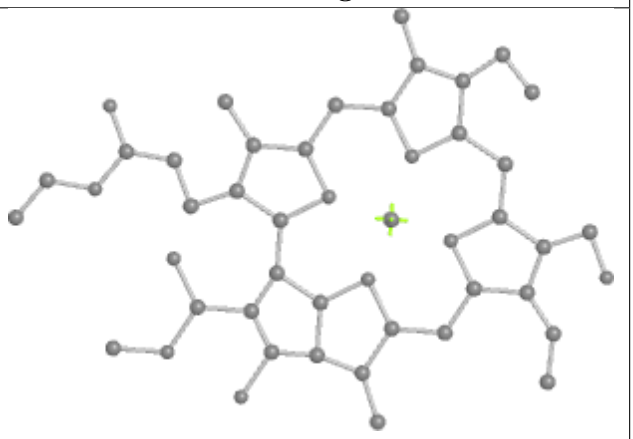
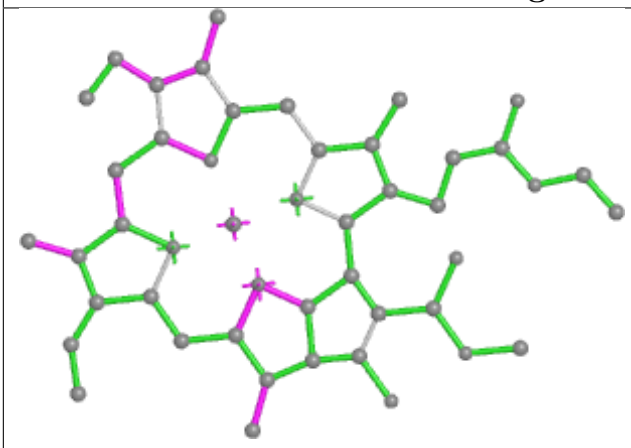


Rings

Ligand CLA 3 305



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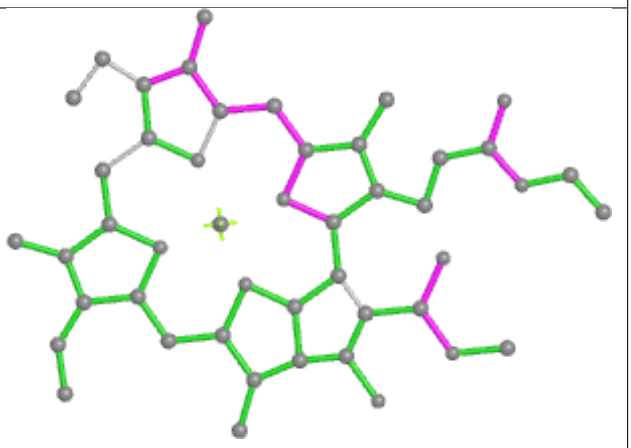
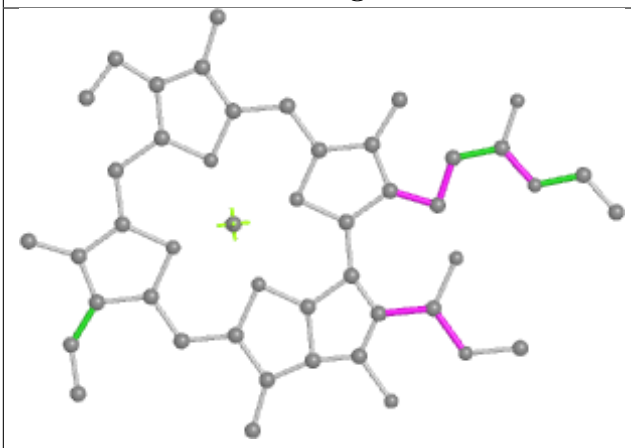


Bond angles



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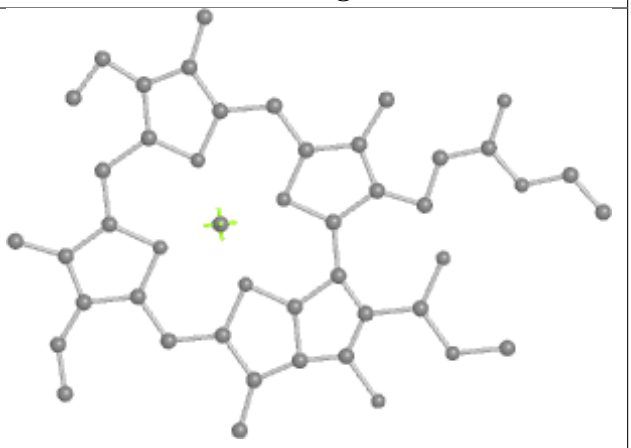
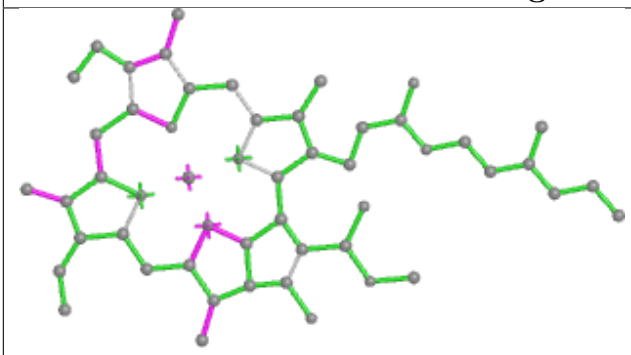


Rings

Ligand CLA 6 312



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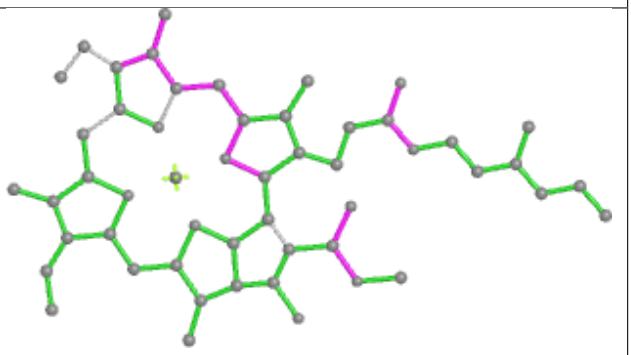
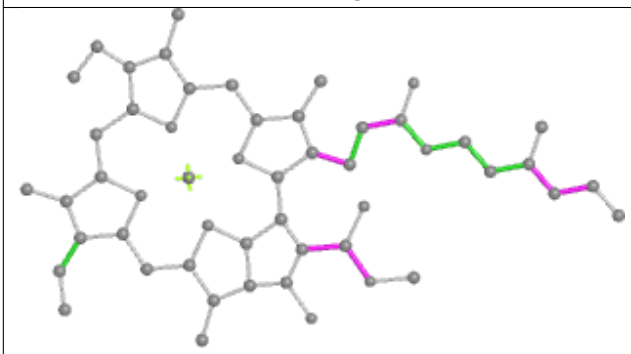


Bond angles



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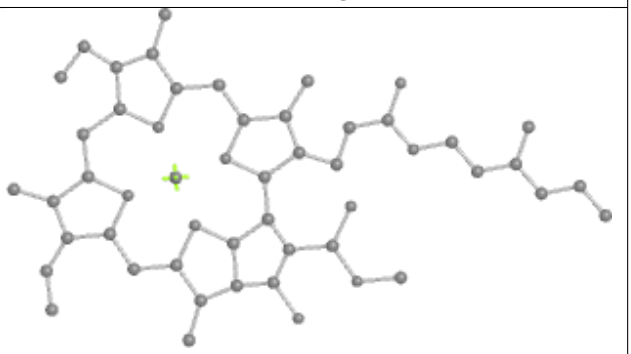
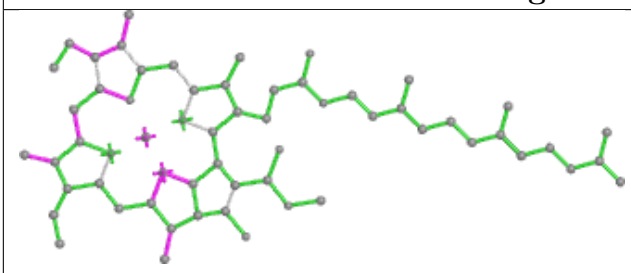


Rings

Ligand CLA 4 309



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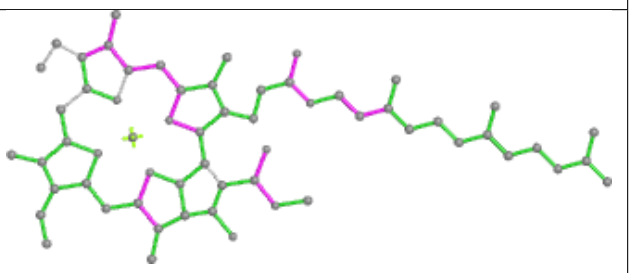

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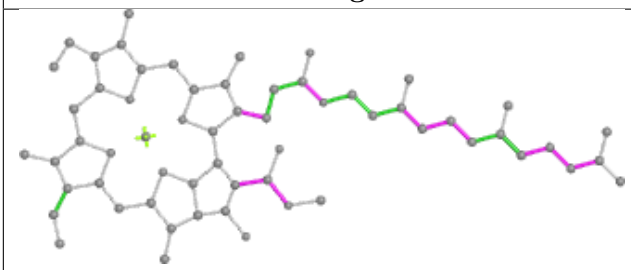

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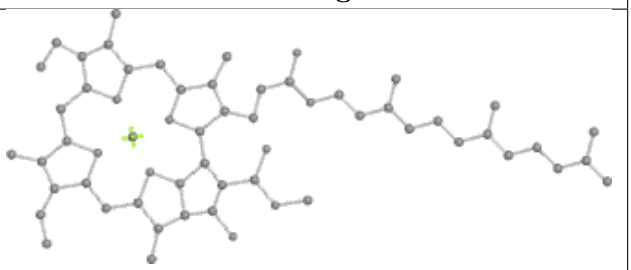
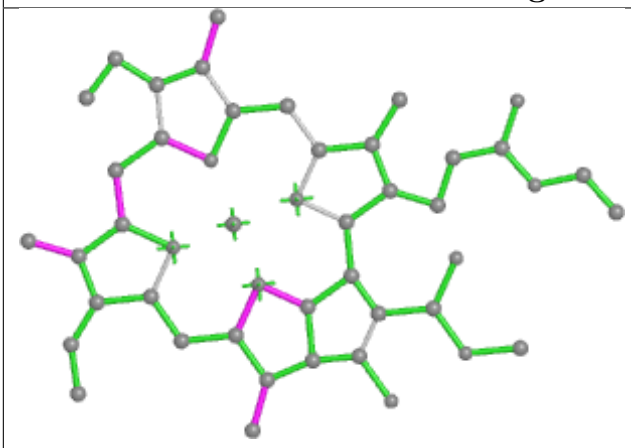


Rings

Ligand CLA 7 307



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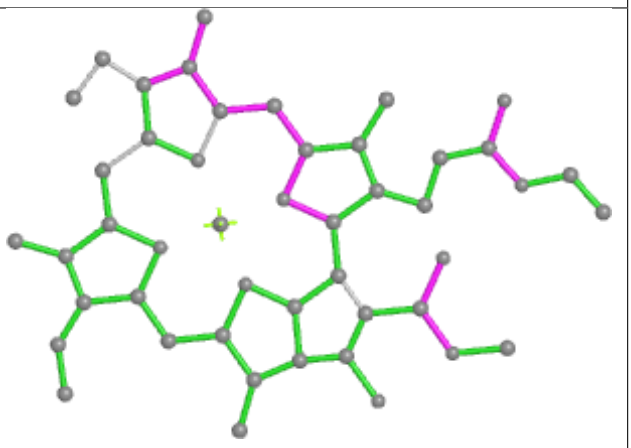

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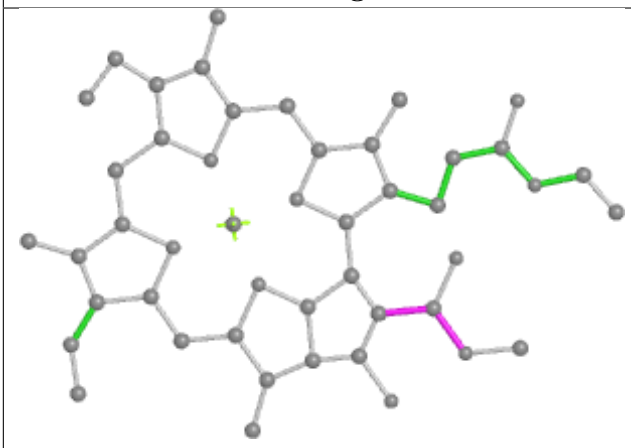

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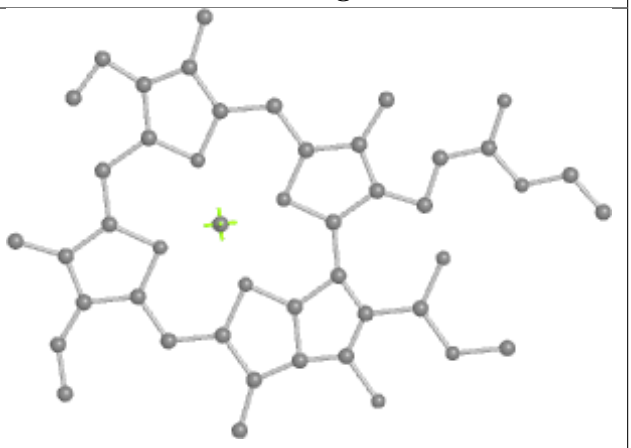
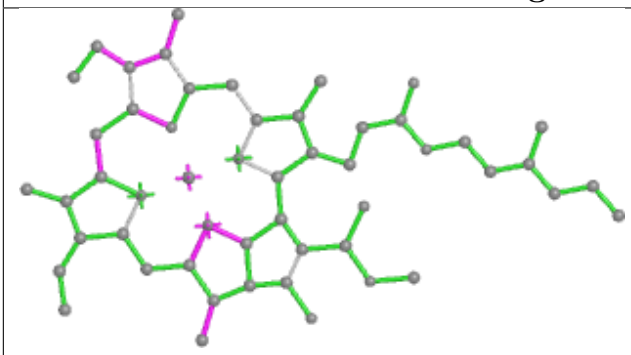
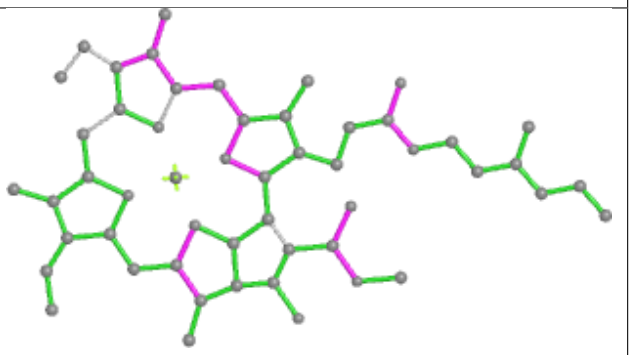
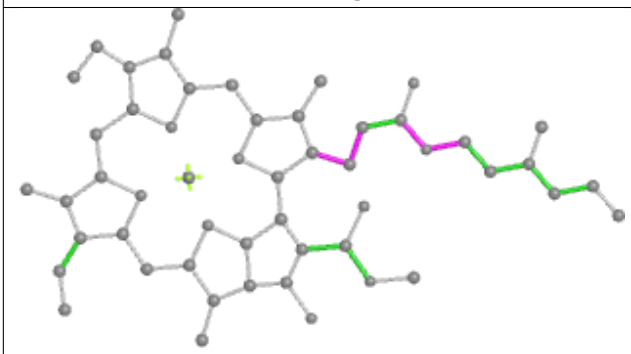
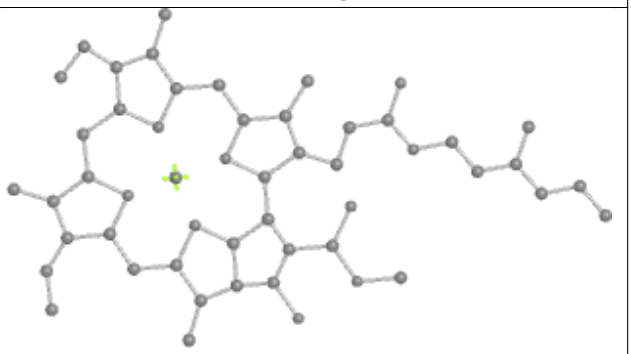
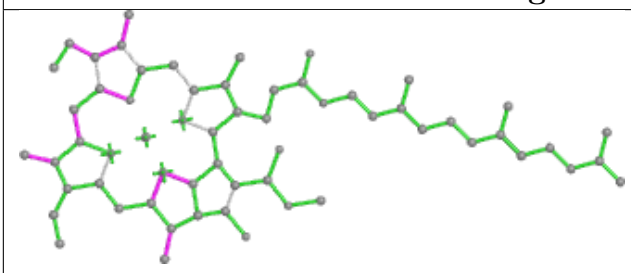
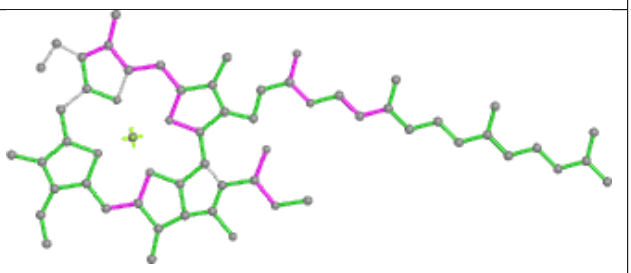
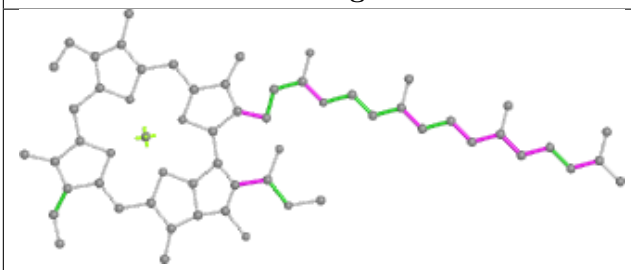
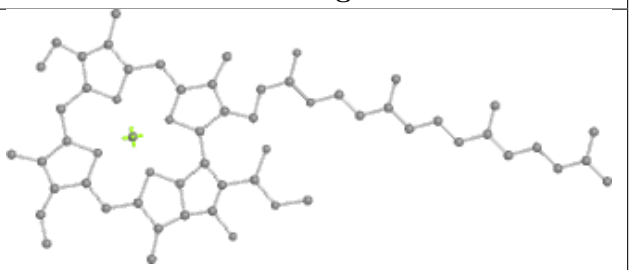
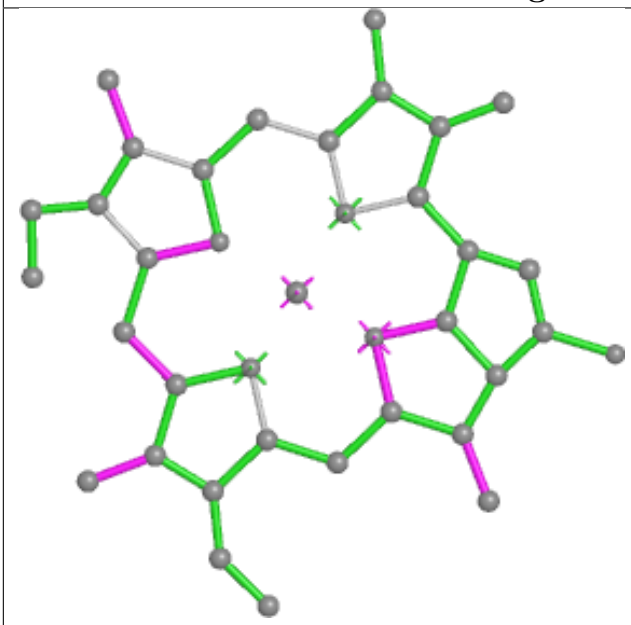


Rings

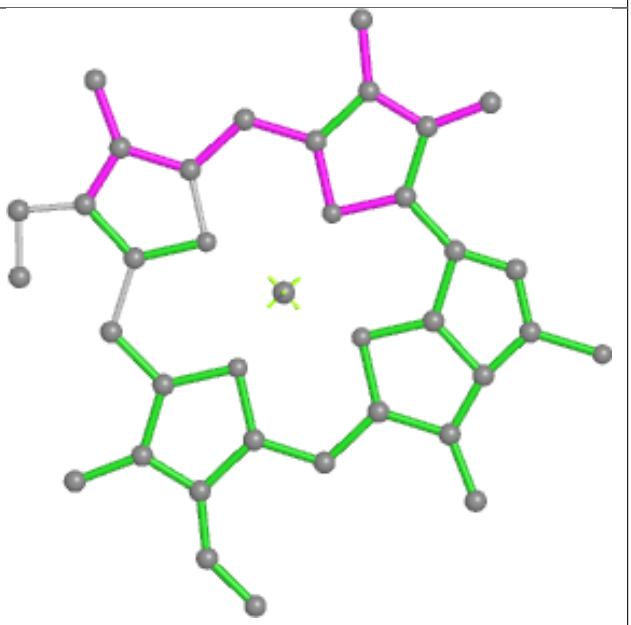
Ligand CLA 1 304	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 9 309	
	
Bond lengths	Bond angles
	
Torsions	Rings

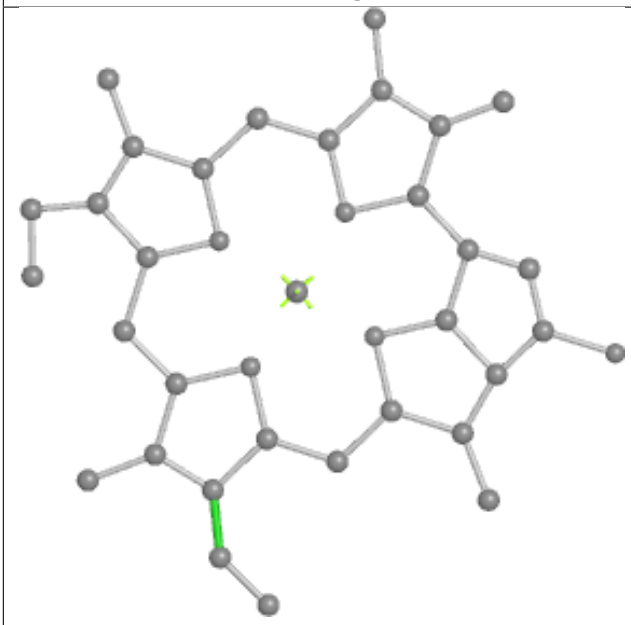
Ligand CLA 3 309



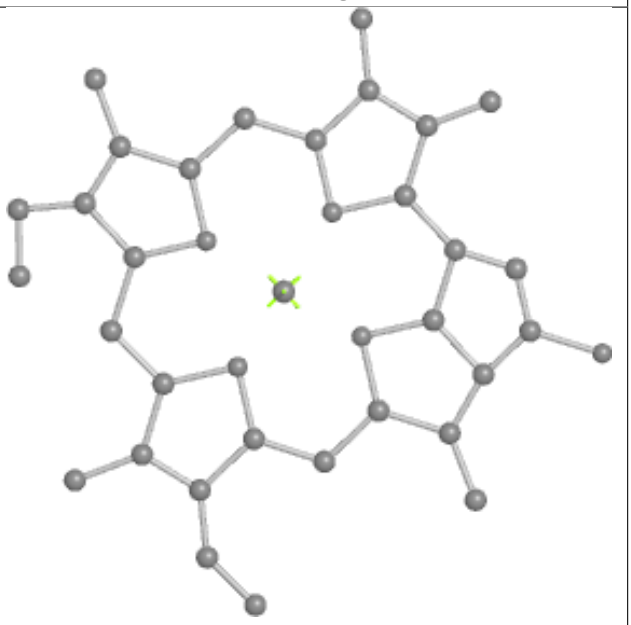
Bond lengths



Bond angles

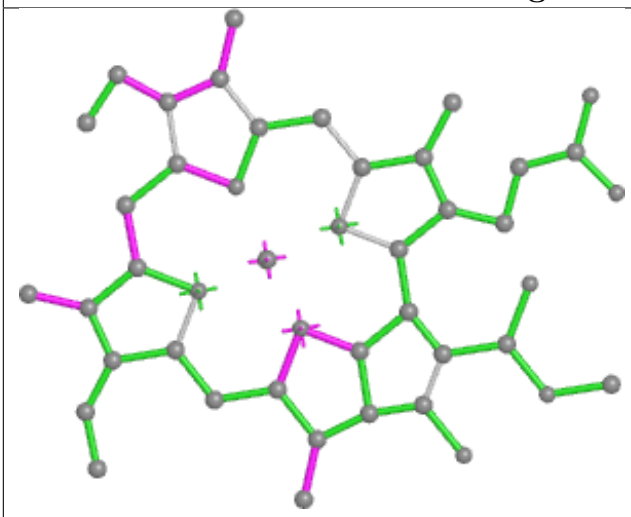


Torsions



Rings

Ligand CLA 4 313



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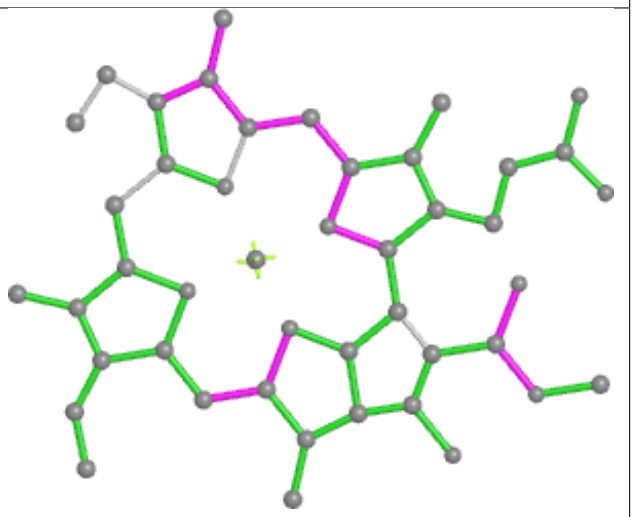
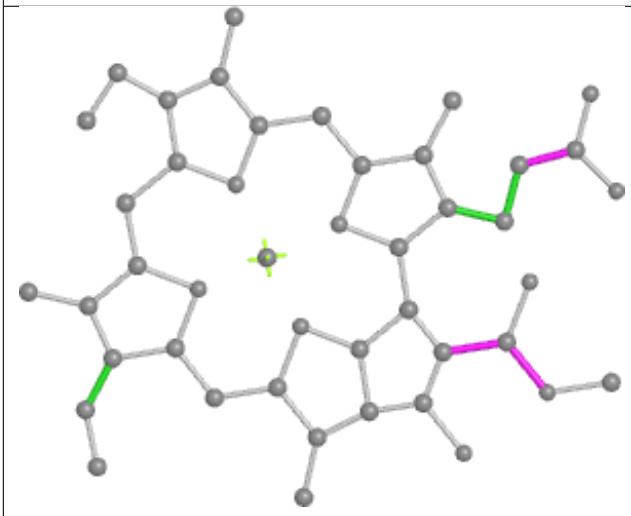
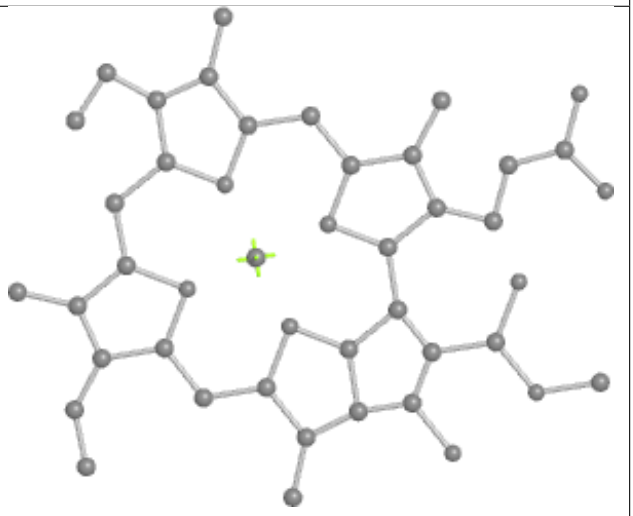


Bond angles

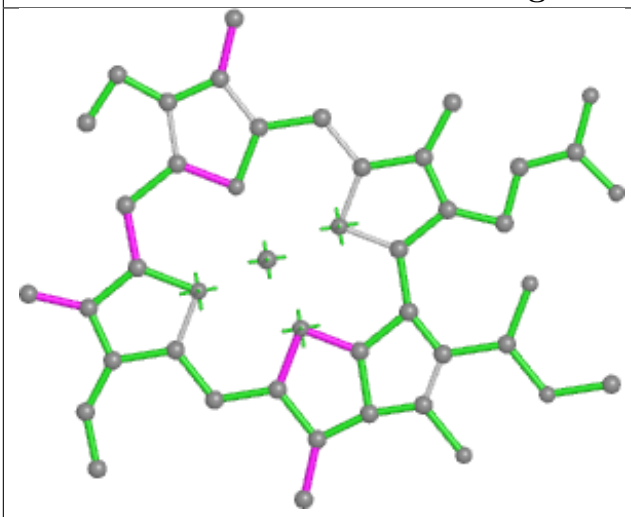


Torsions

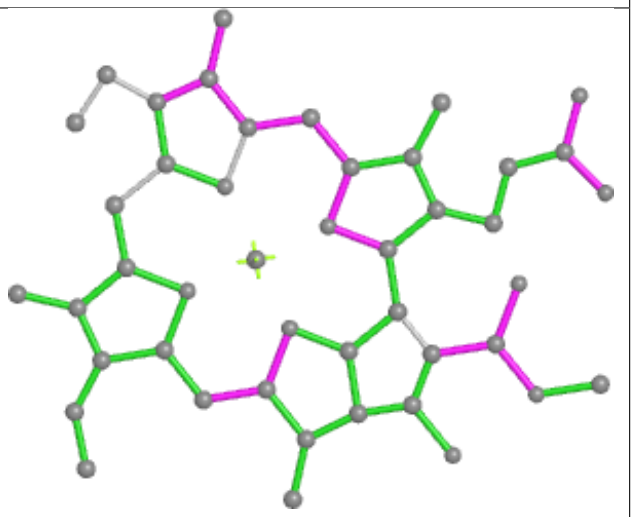


Rings

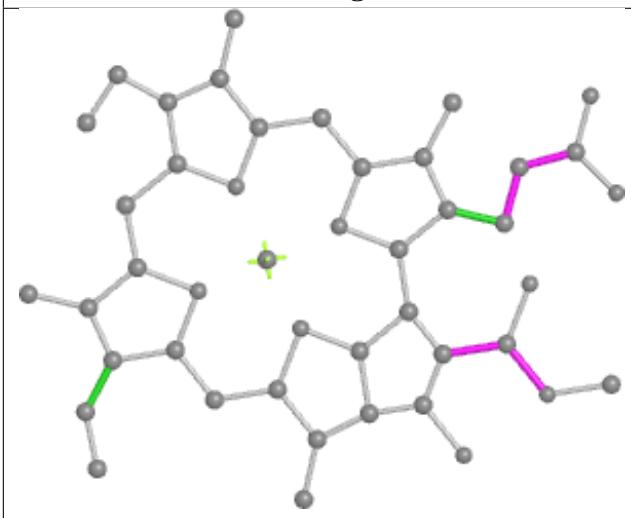
Ligand CLA 3 312



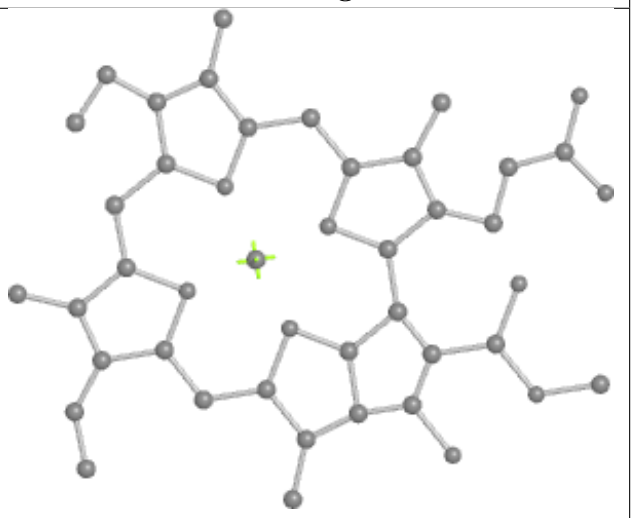
Bond lengths



Bond angles

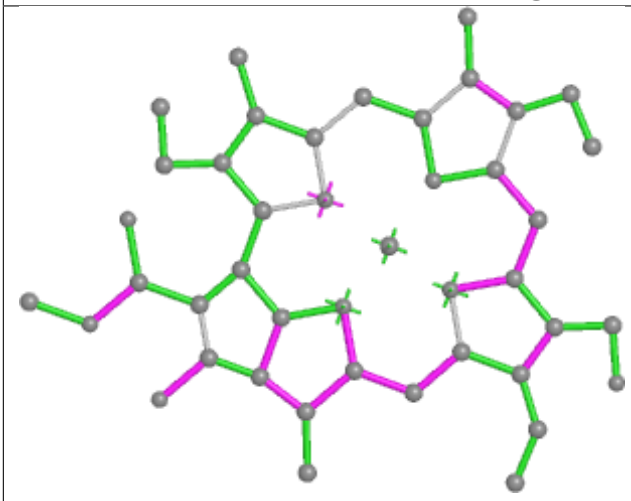


Torsions



Rings

Ligand CHL 2 305



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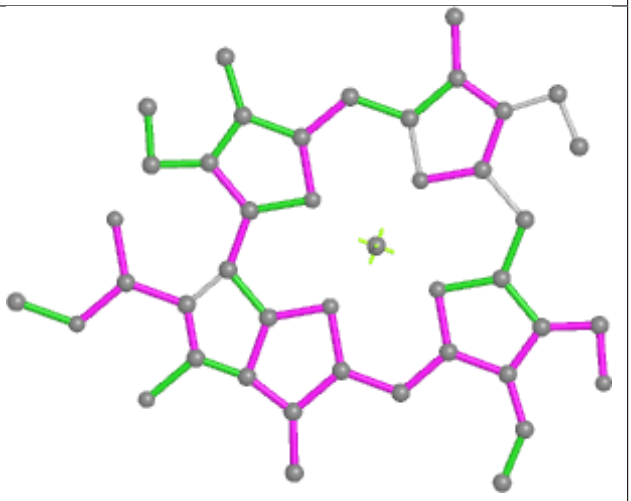
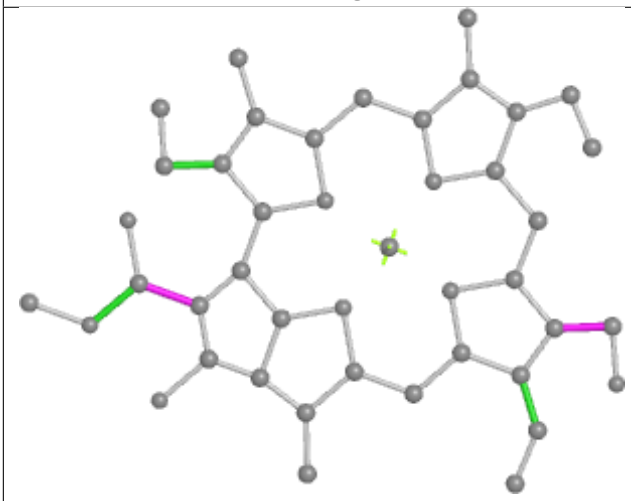
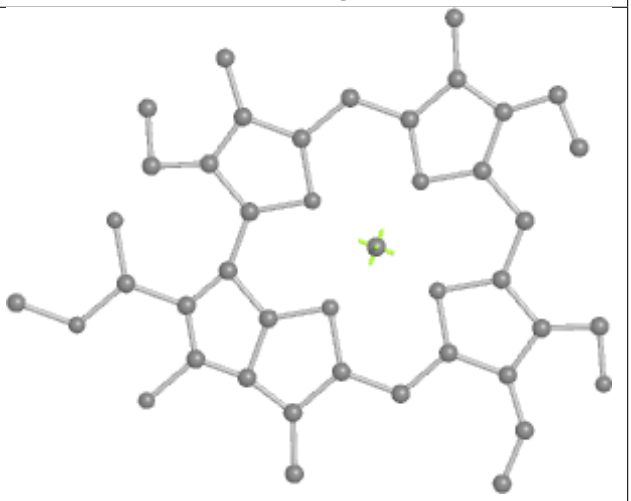


Bond angles

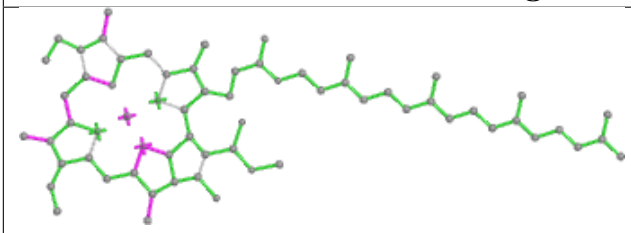


Torsions

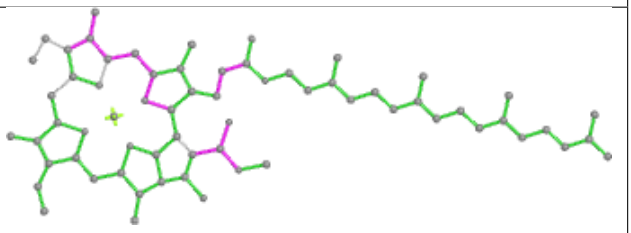


Rings

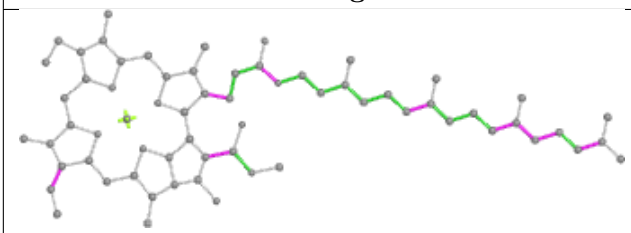
Ligand CLA B 826



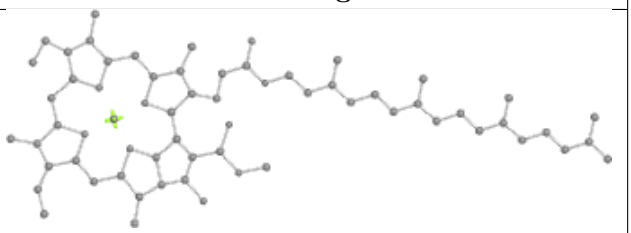
Bond lengths



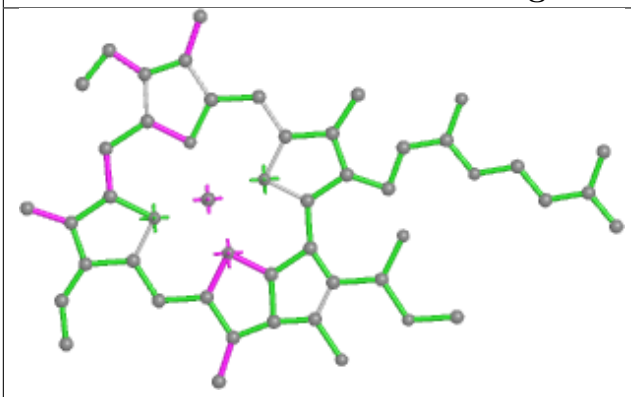
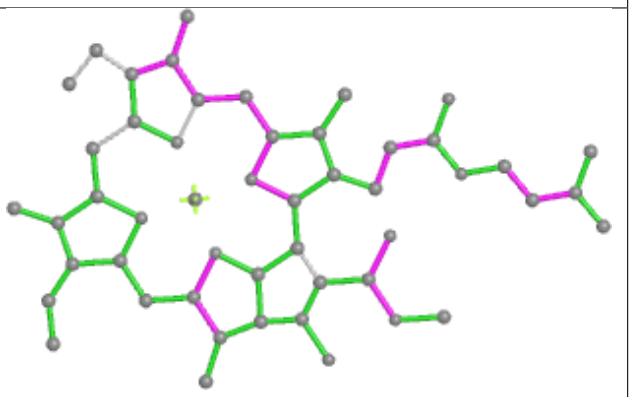
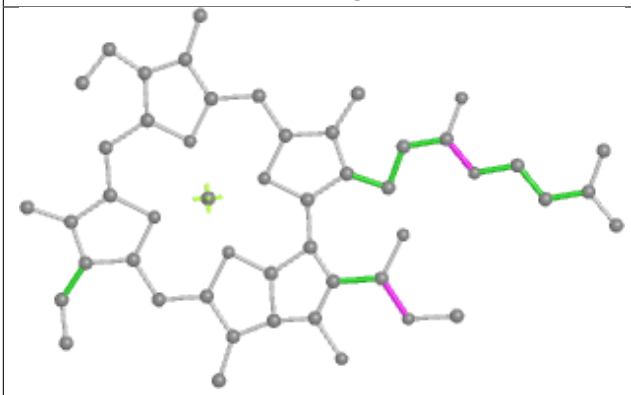
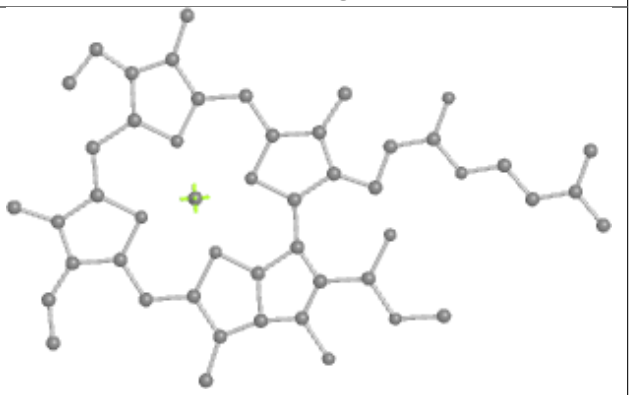
Bond angles

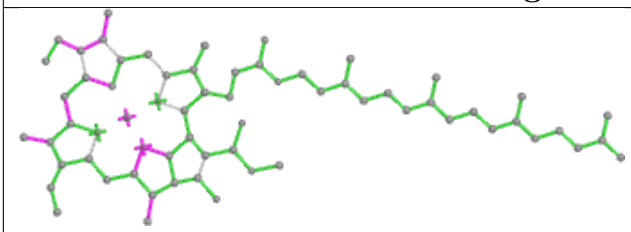
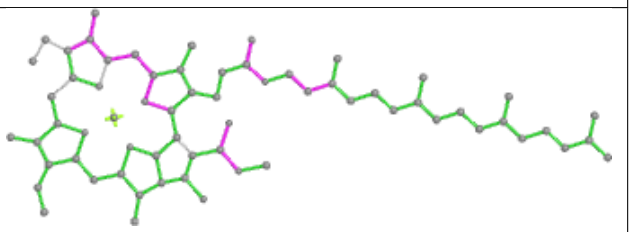
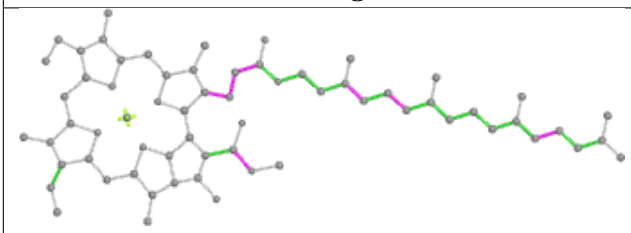
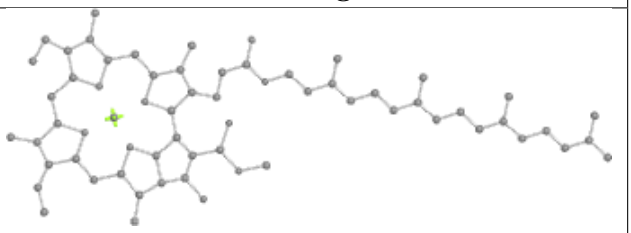


Torsions

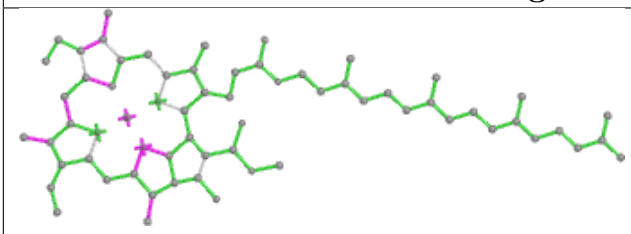


Rings

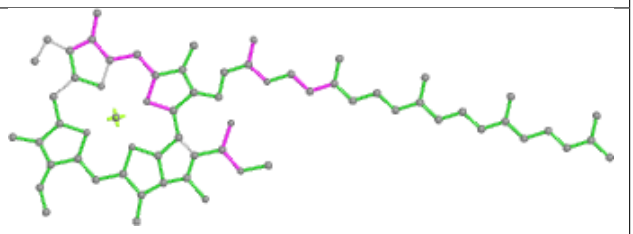
Ligand CLA 4 304	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 829	
	
Bond lengths	Bond angles
	
Torsions	Rings

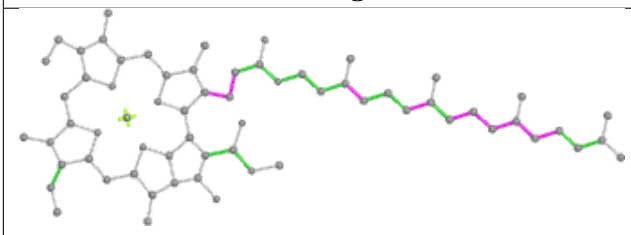
Ligand CLA 1 306



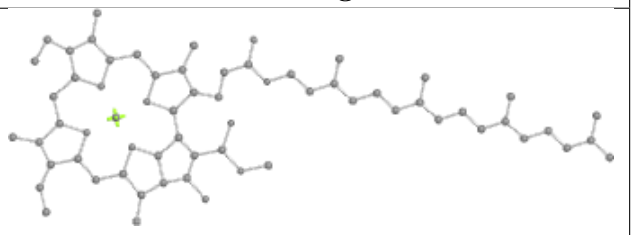
Bond lengths



Bond angles

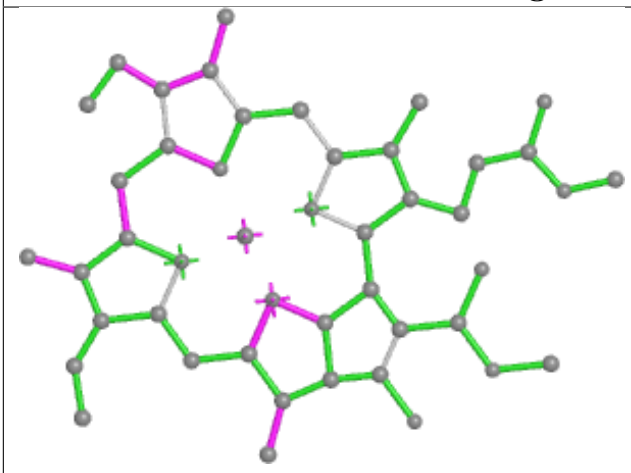


Torsions

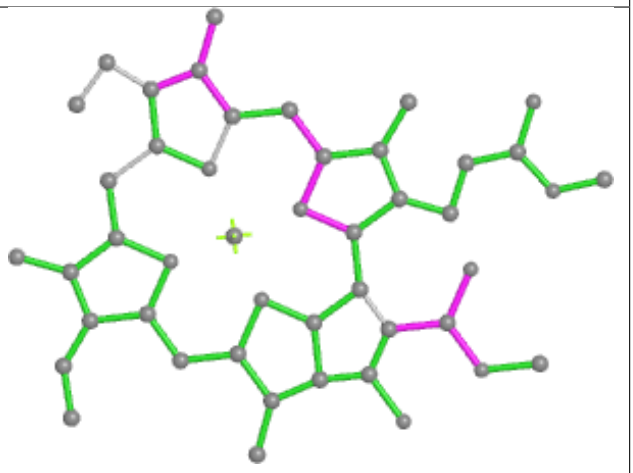


Rings

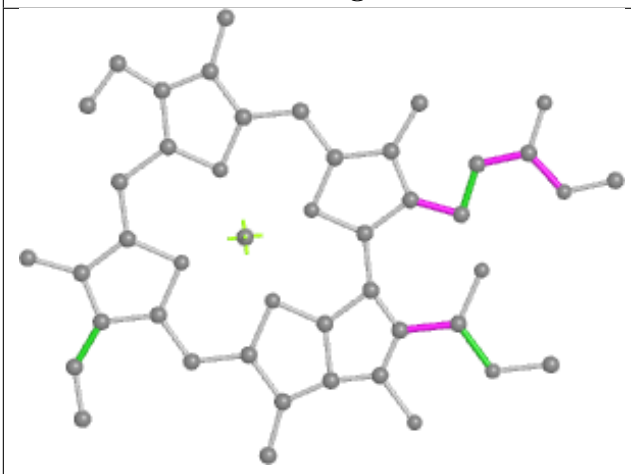
Ligand CLA 2 319



Bond lengths



Bond angles



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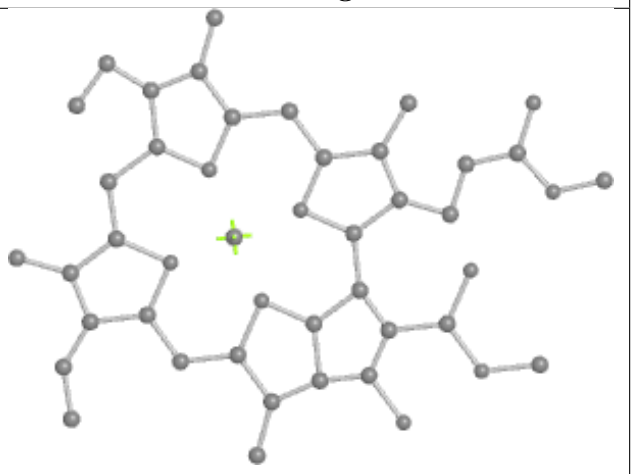
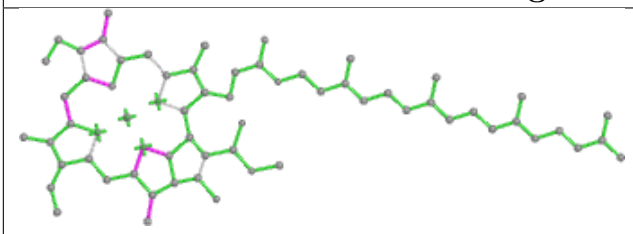
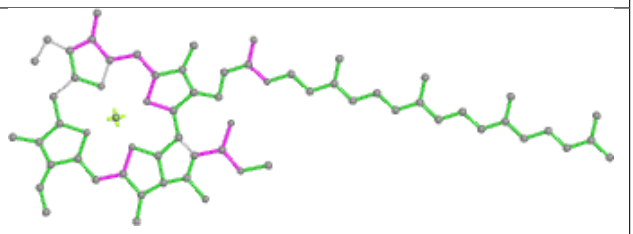


Rings

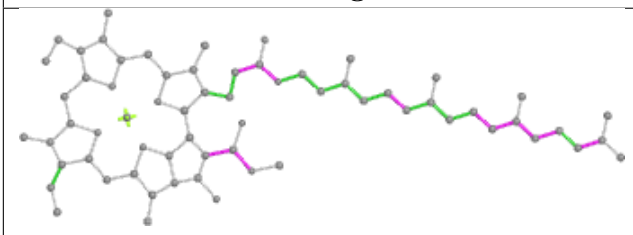
Ligand CLA 5 307



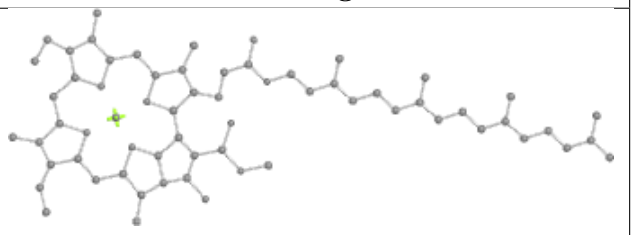
Bond lengths



Bond angles

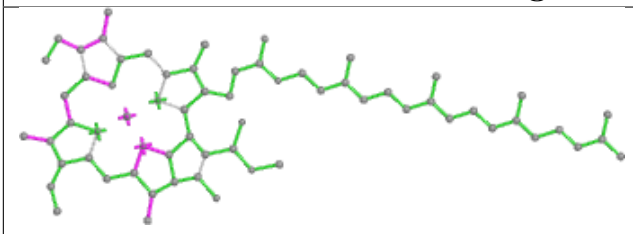


Torsions

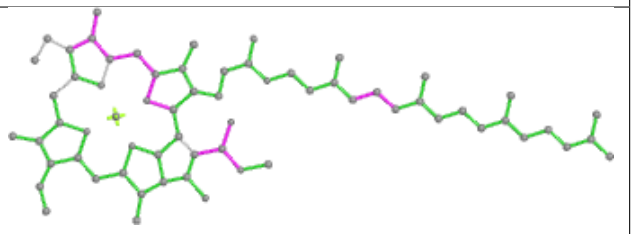


Rings

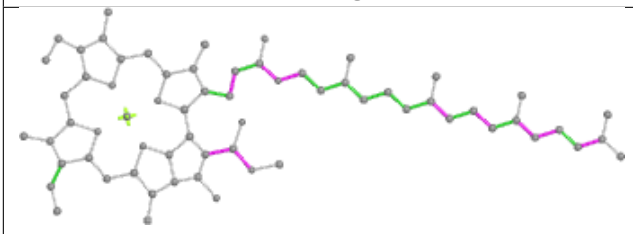
Ligand CLA 6 303



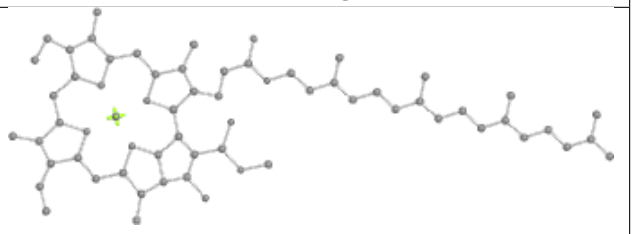
Bond lengths



Bond angles

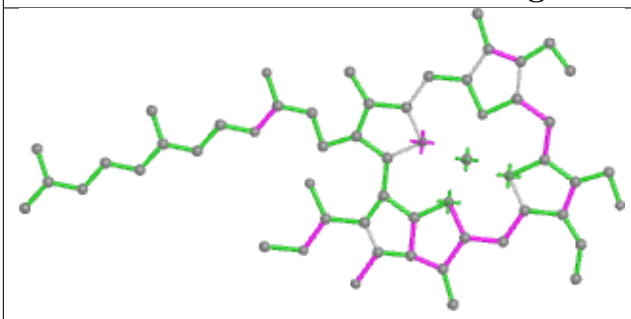


Torsions



Rings

Ligand CHL 8 305



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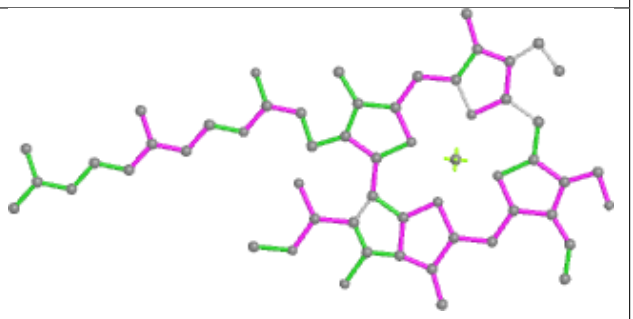
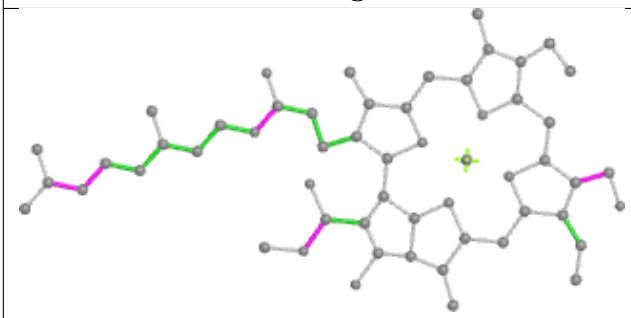


Bond angles



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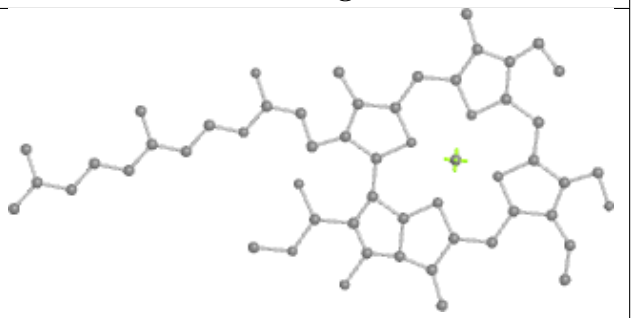
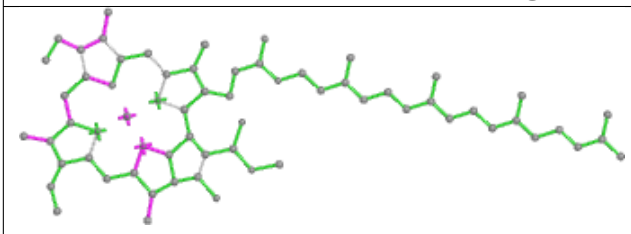


Rings

Ligand CLA A 801



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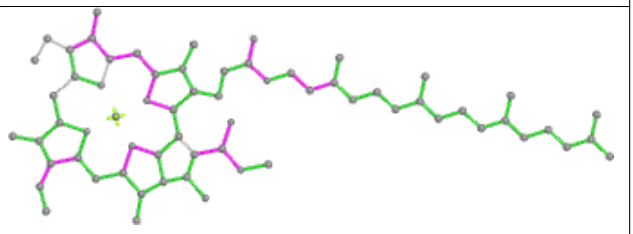
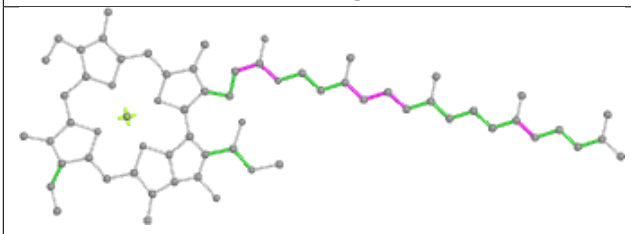
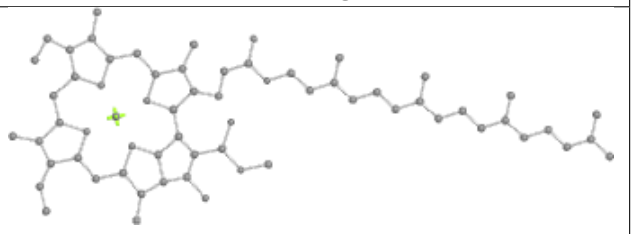


Bond angles

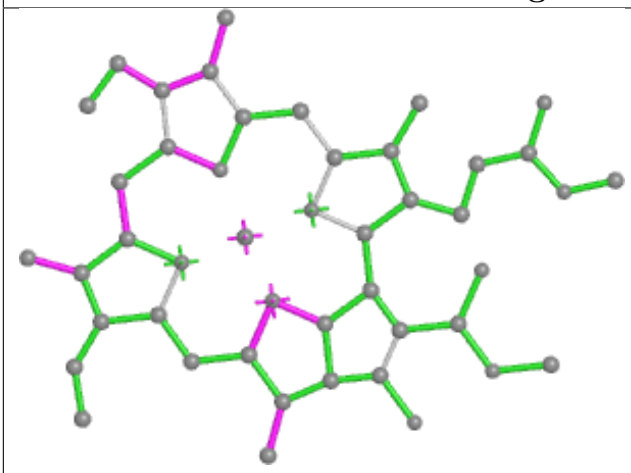


Torsions



Rings

Ligand CLA 3 313



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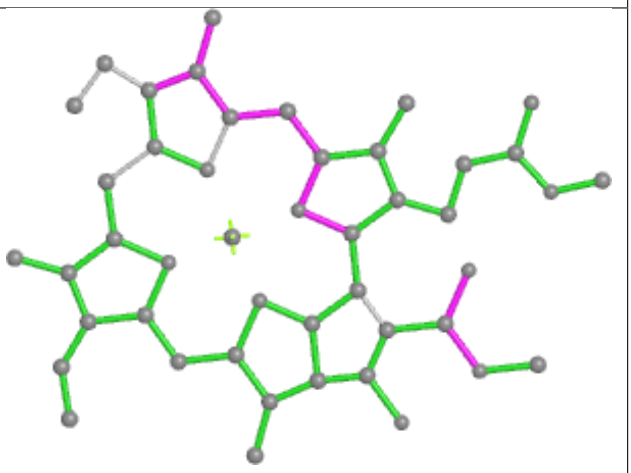
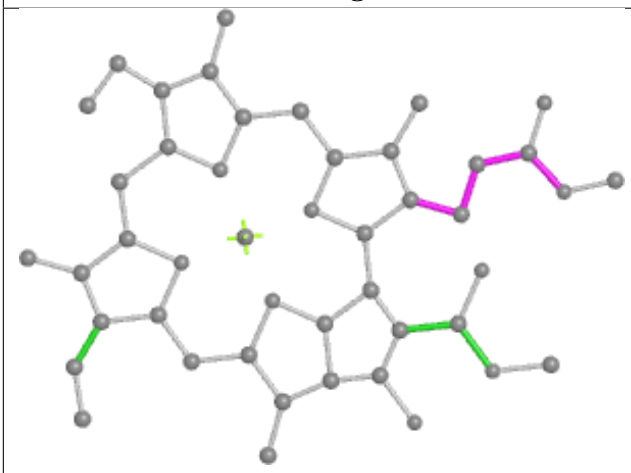
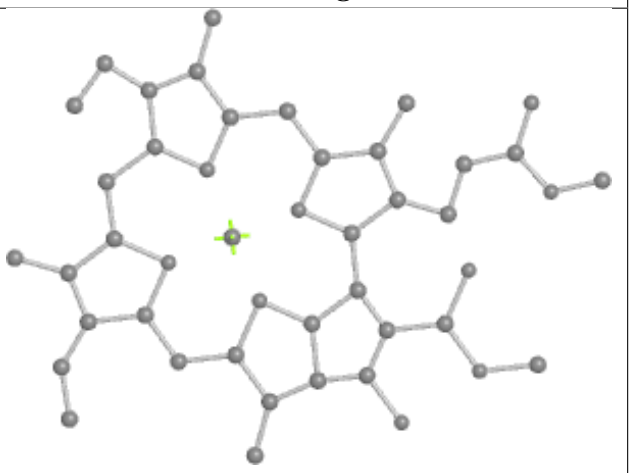


Bond angles

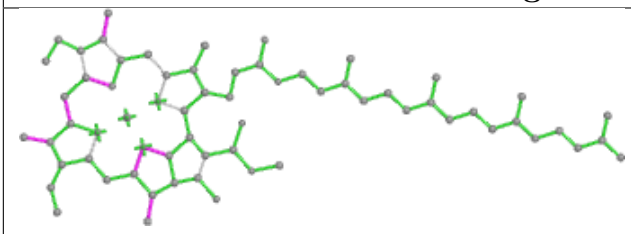


Torsions

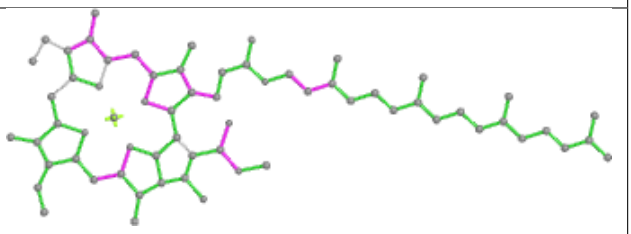


Rings

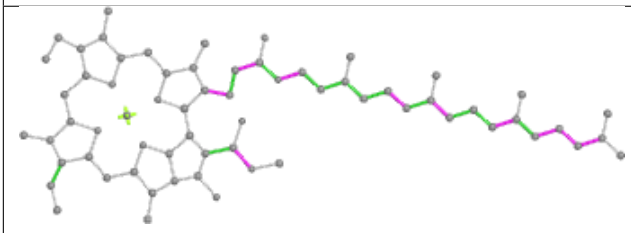
Ligand CLA H 201



Bond lengths



Bond angles



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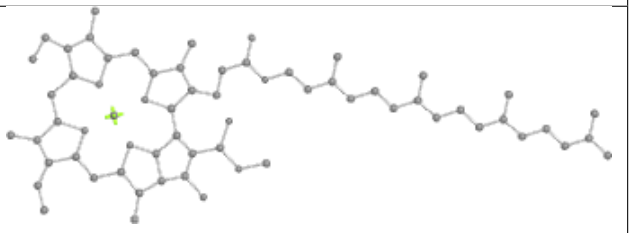
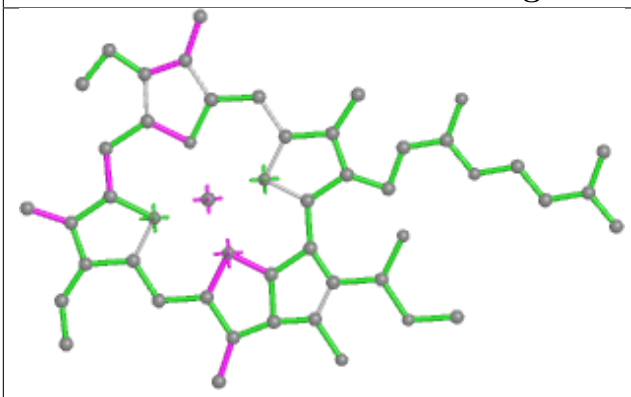
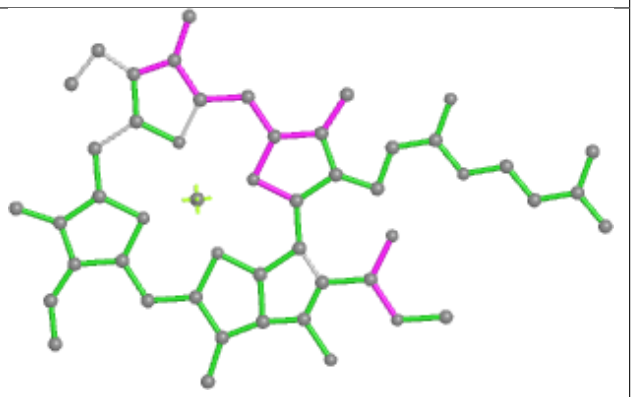


Rings

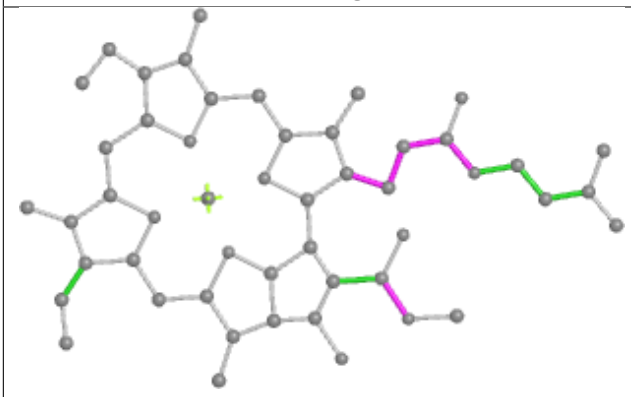
Ligand CLA K 105



Bond lengths



Bond angles



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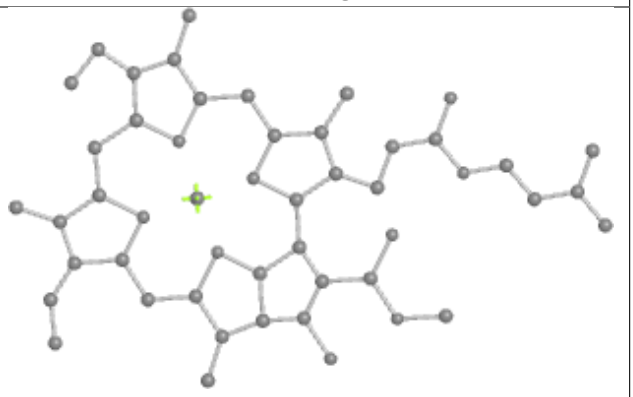
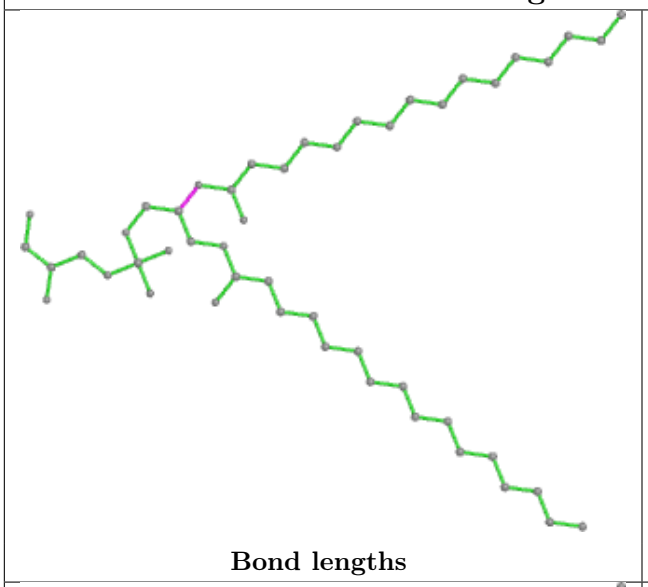
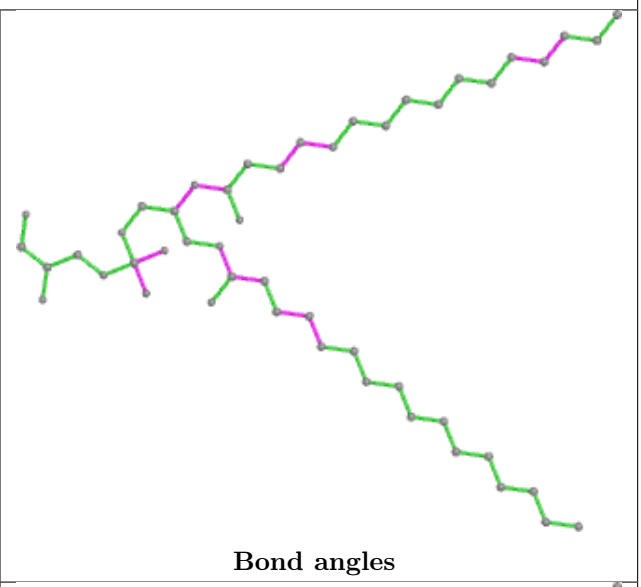


Rings

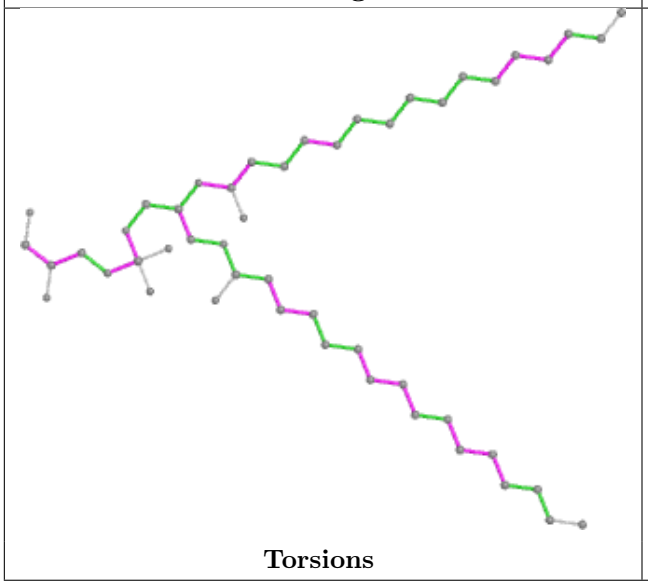
Ligand LHG 9 316



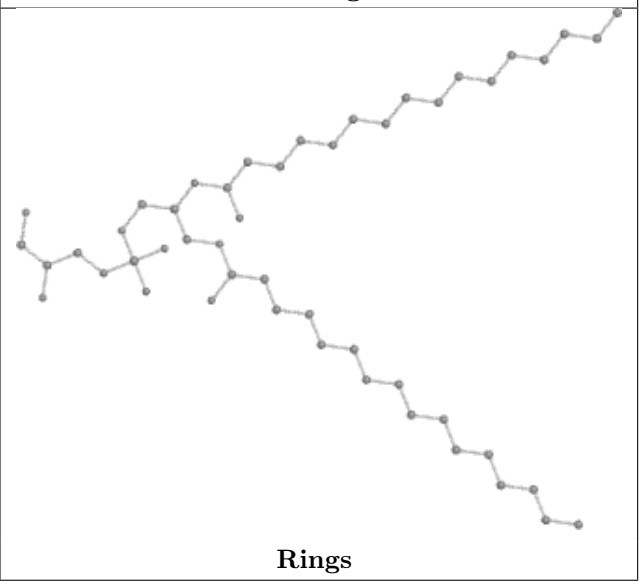
Bond lengths



Bond angles

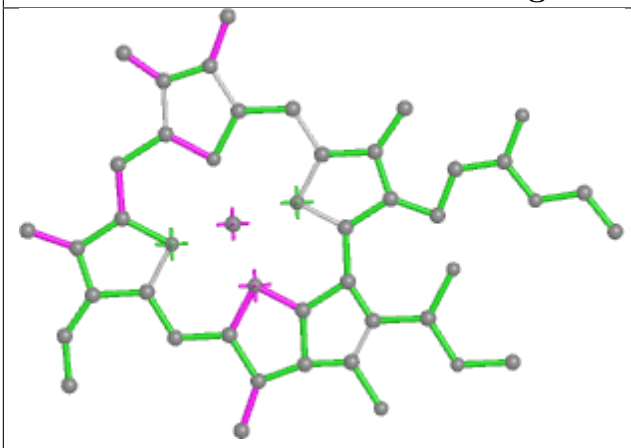


Torsions

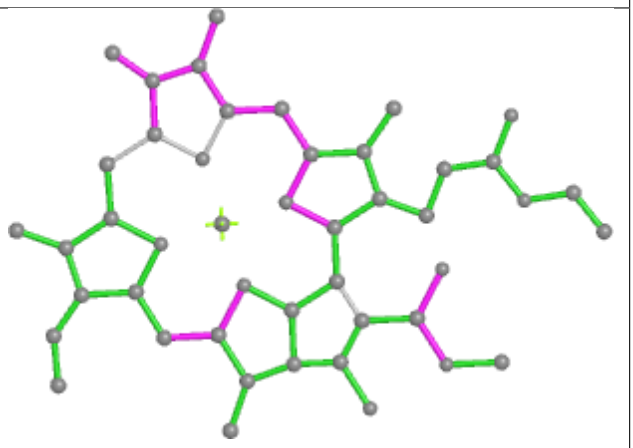


Rings

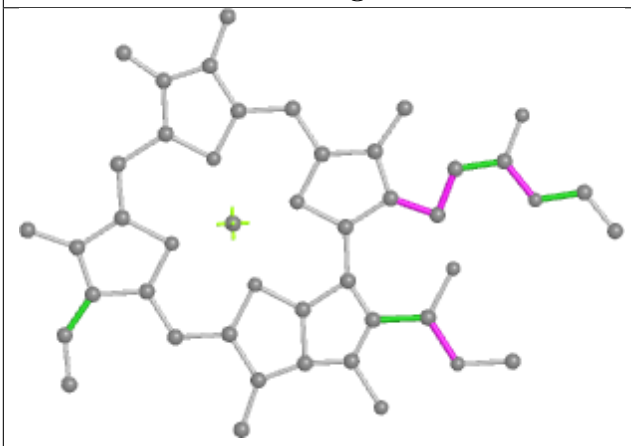
Ligand CLA 9 301



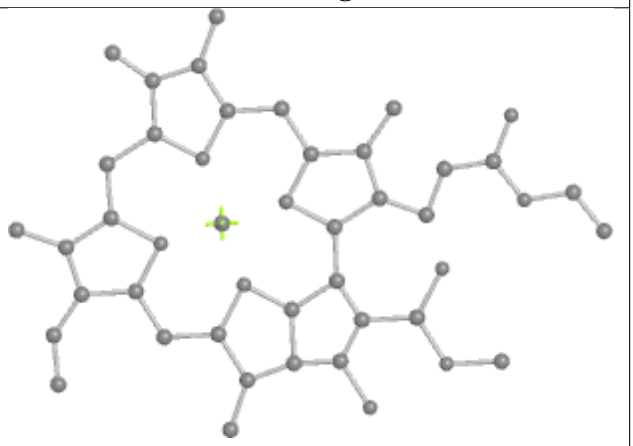
Bond lengths



Bond angles

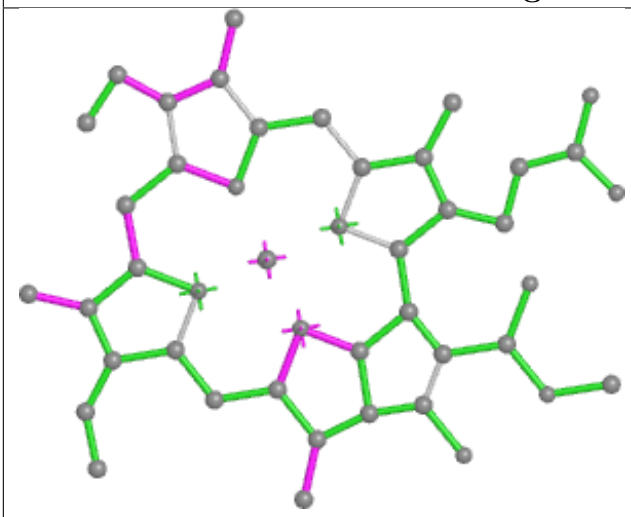


Torsions

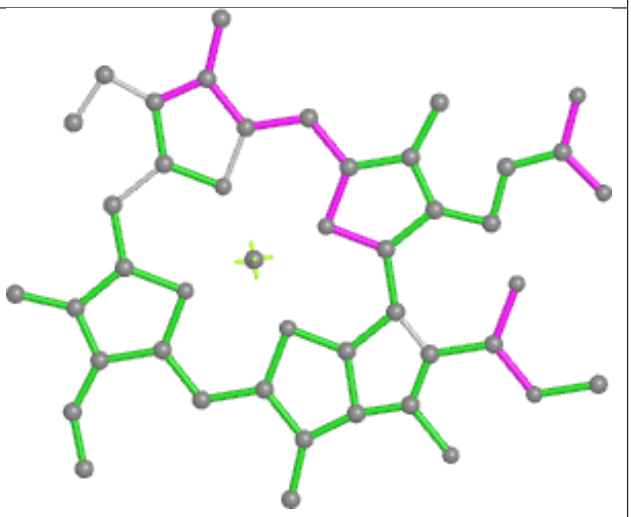


Rings

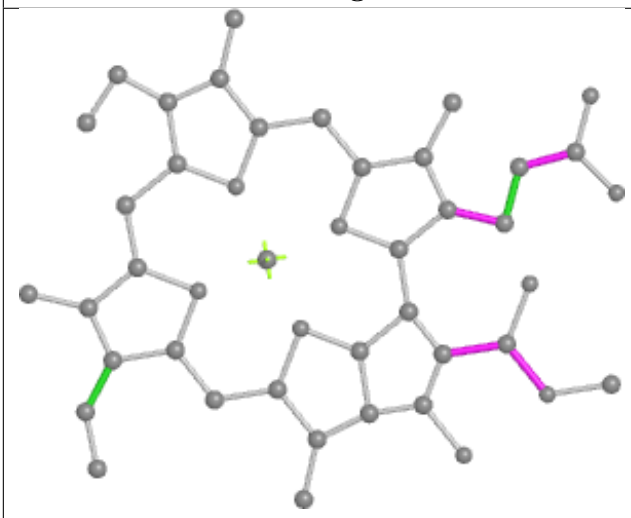
Ligand CLA A 814



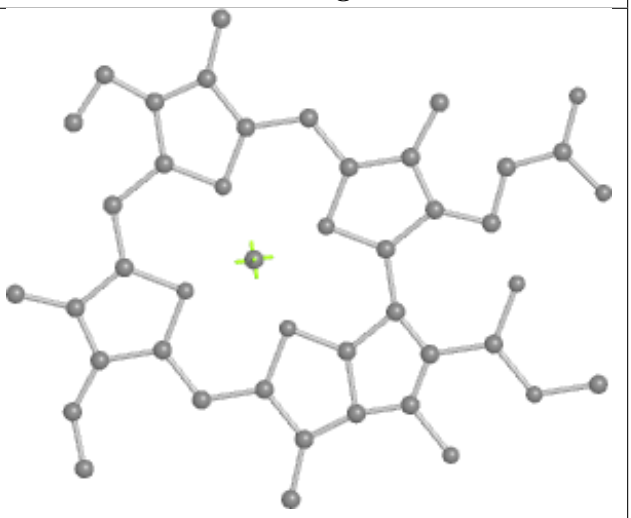
Bond lengths



Bond angles

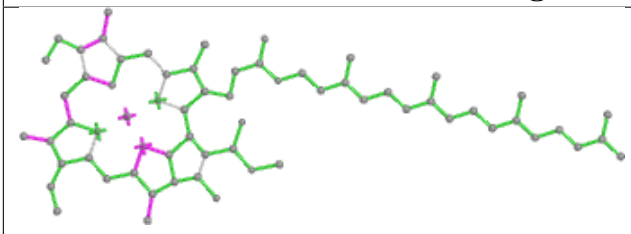


Torsions



Rings

Ligand CLA 4 314



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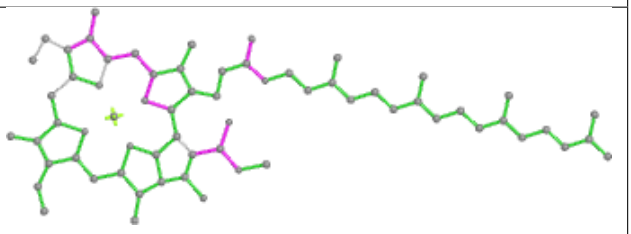
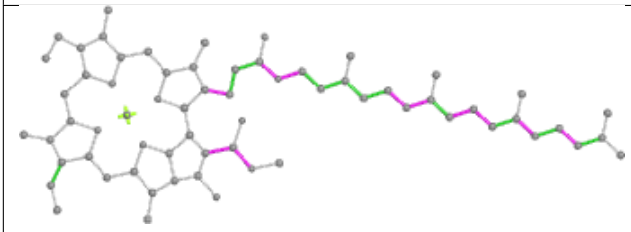
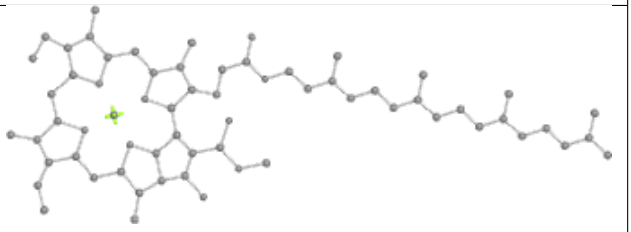


Bond angles

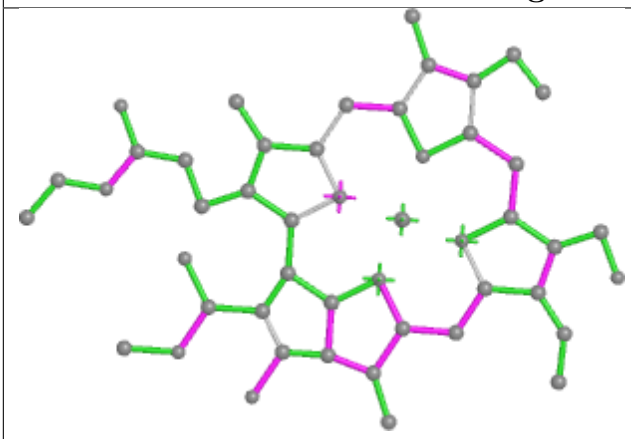


Torsions



Rings

Ligand CHL 9 307



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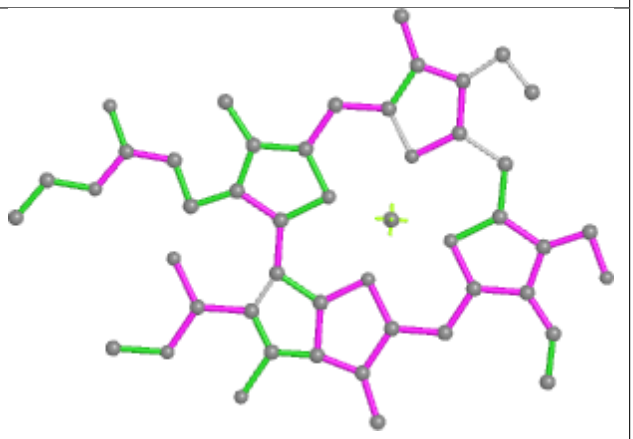
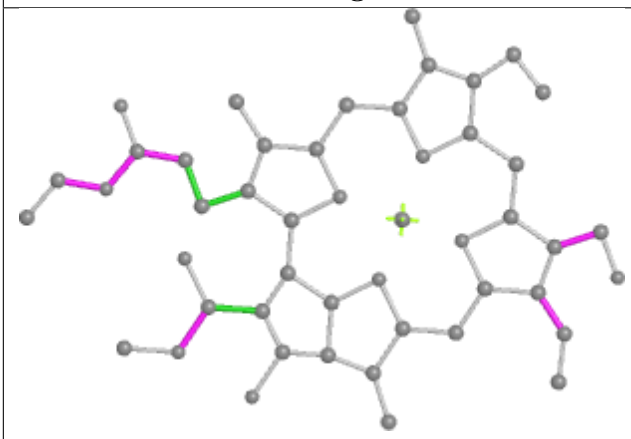
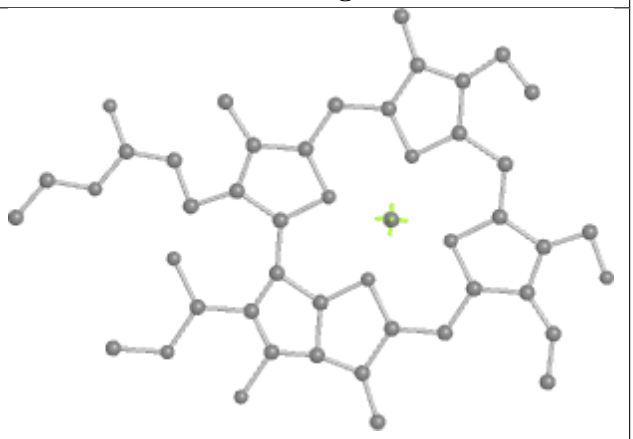


Bond angles

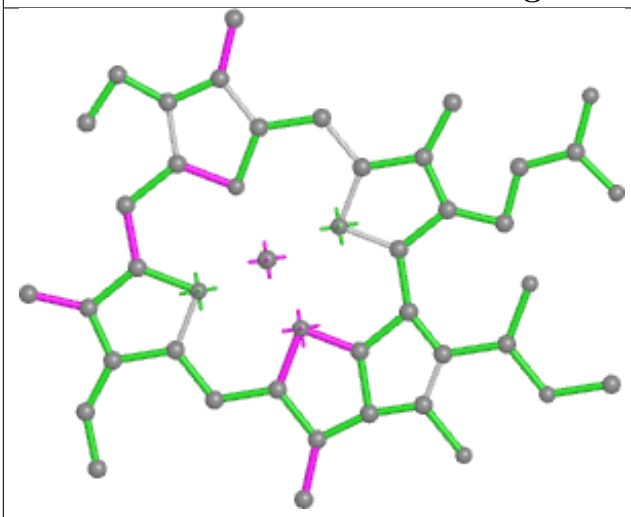


Torsions

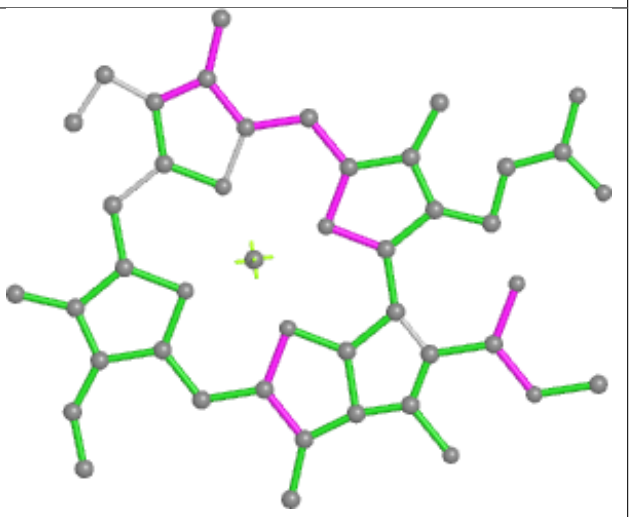


Rings

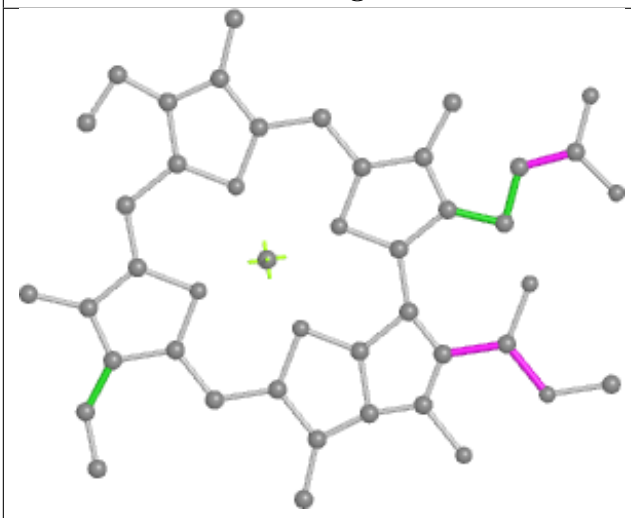
Ligand CLA A 820



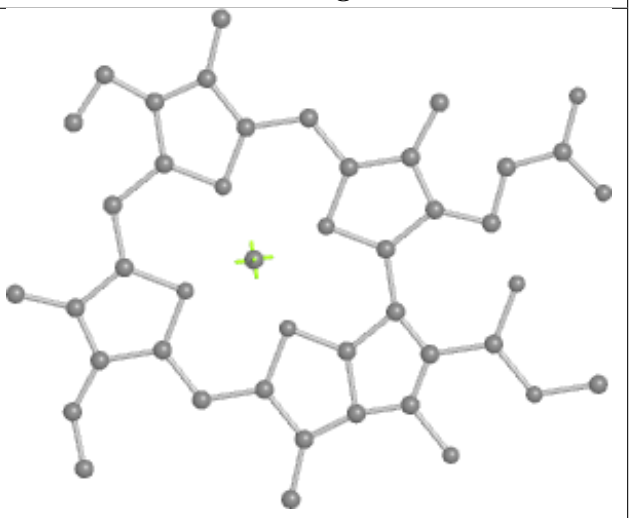
Bond lengths



Bond angles

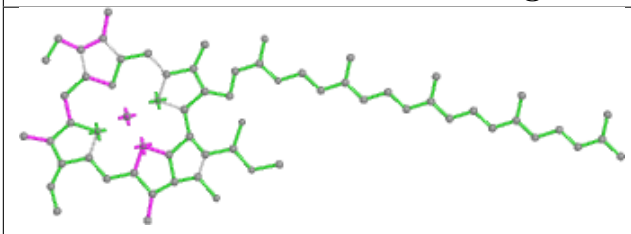


Torsions

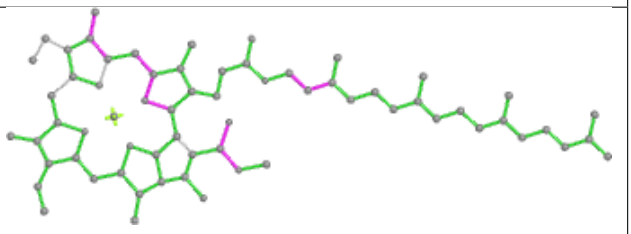


Rings

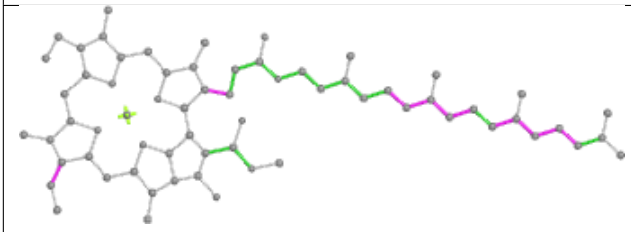
Ligand CLA A 826



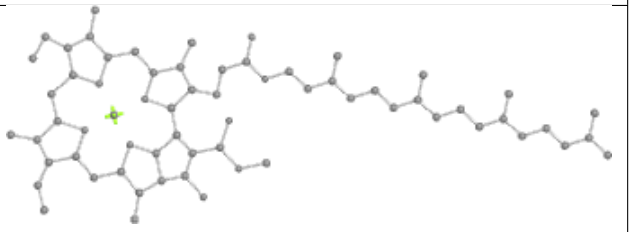
Bond lengths



Bond angles

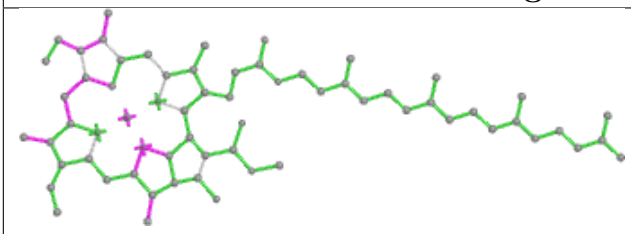


Torsions

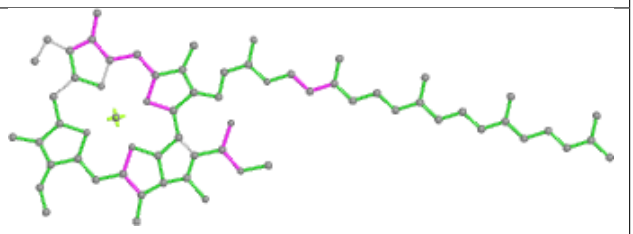


Rings

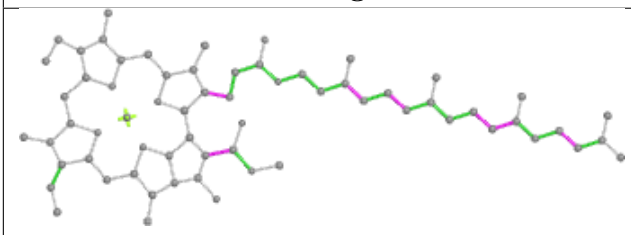
Ligand CLA B 830



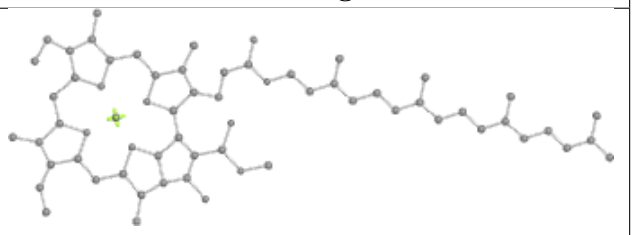
Bond lengths



Bond angles

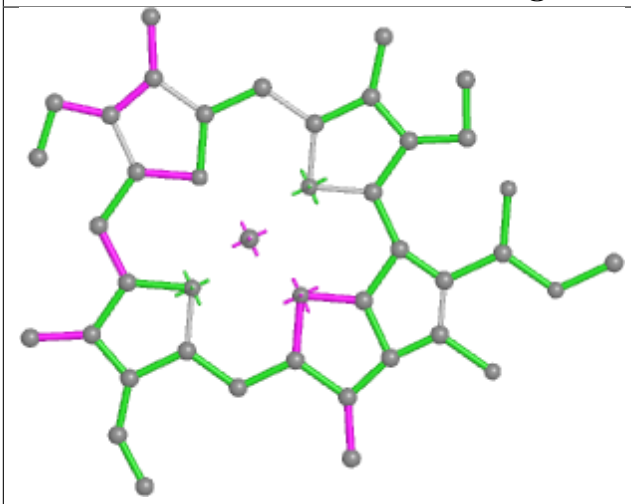


Torsions

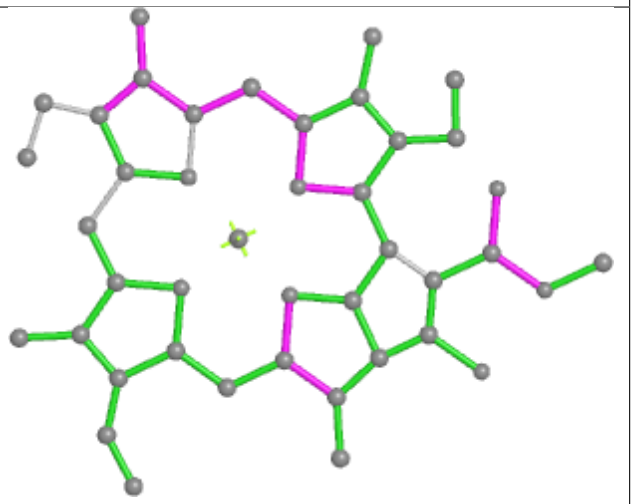


Rings

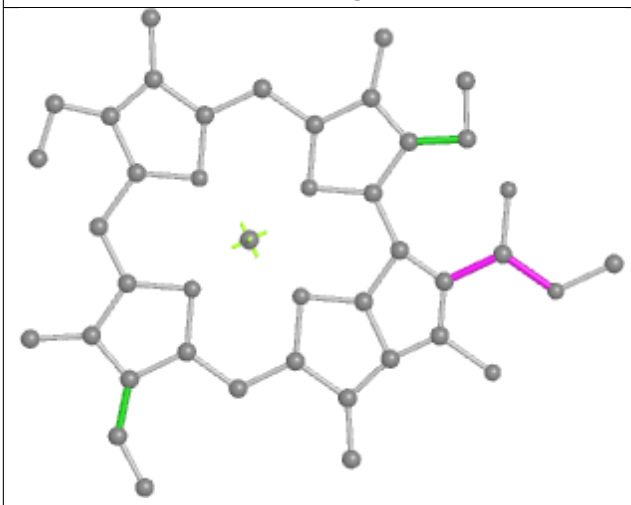
Ligand CLA 3 304



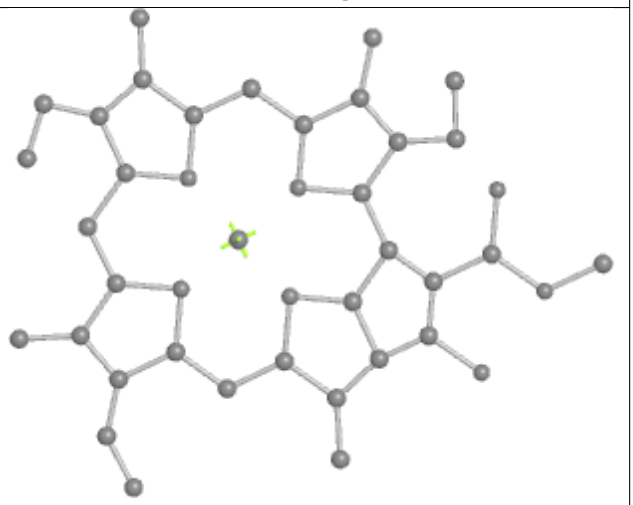
Bond lengths



Bond angles

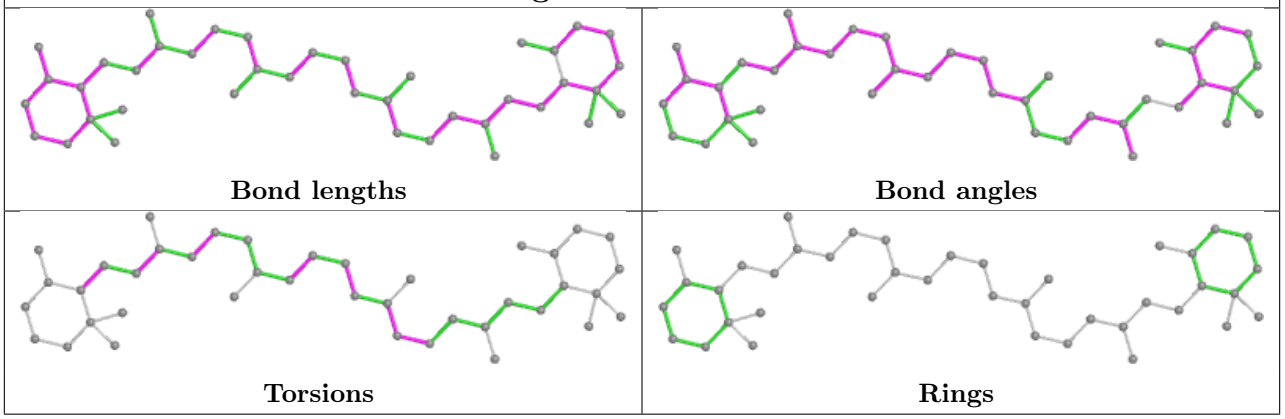


Torsions

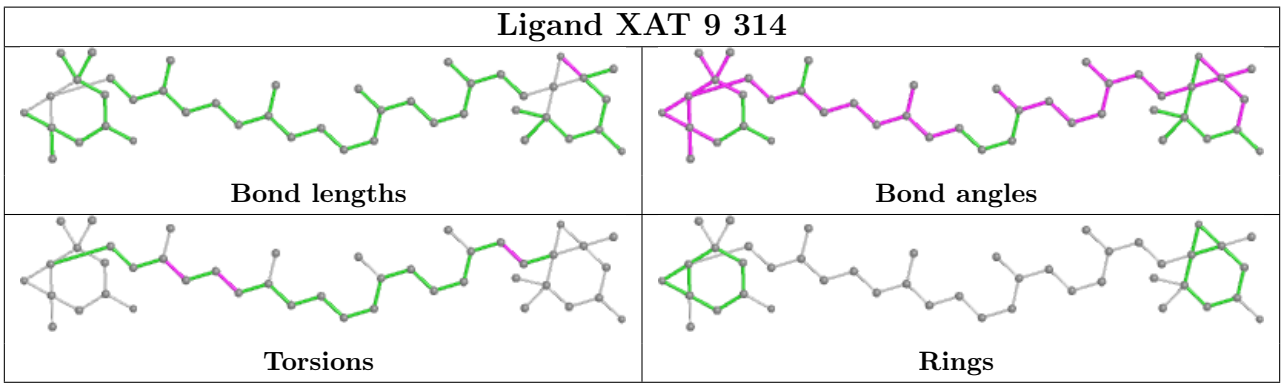


Rings

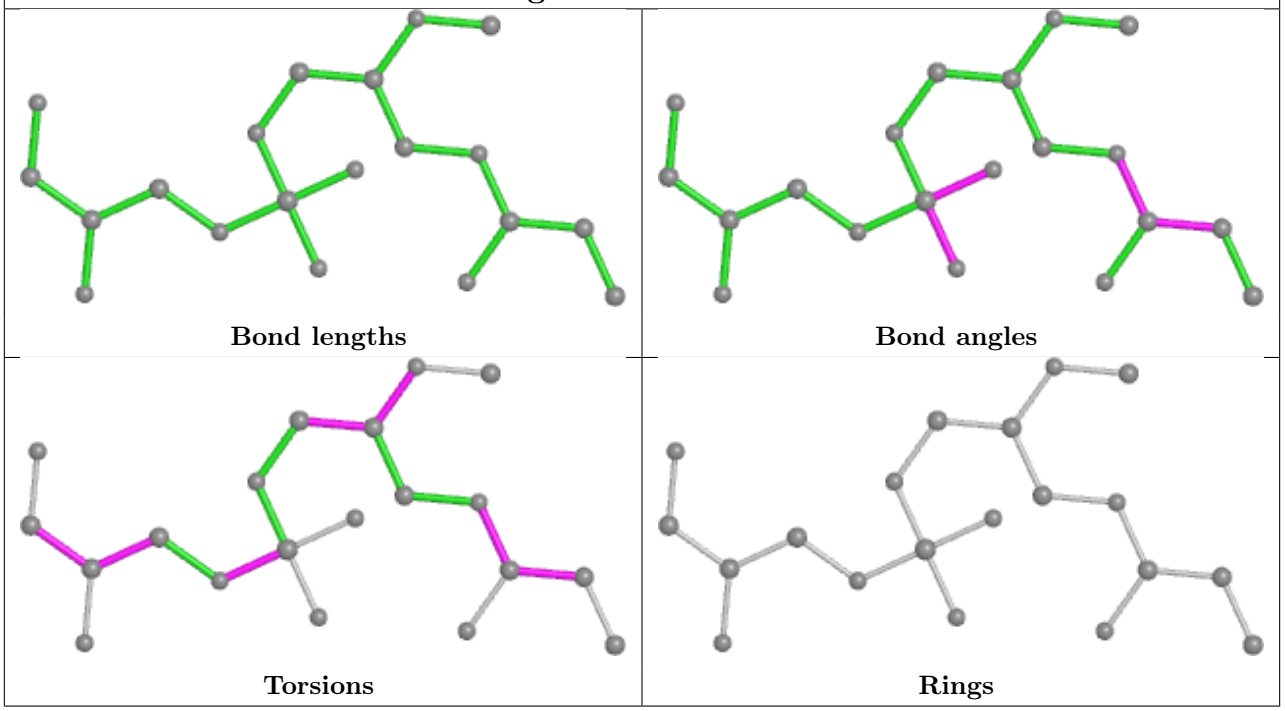
Ligand 8CT 6 321



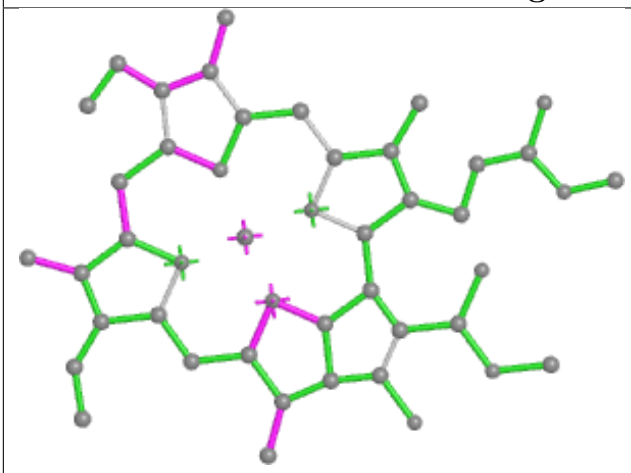
Ligand XAT 9 314



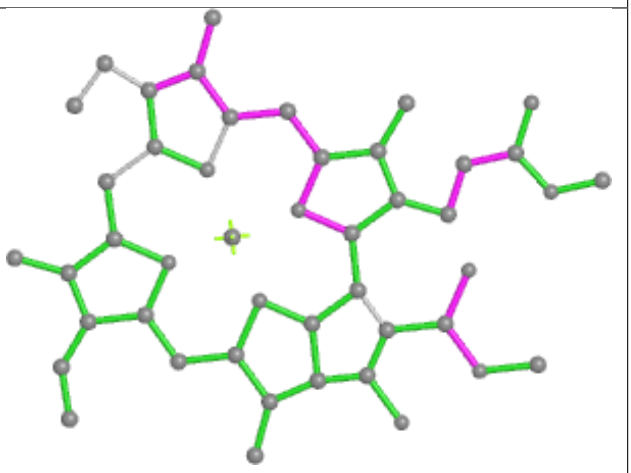
Ligand LHG 3 317



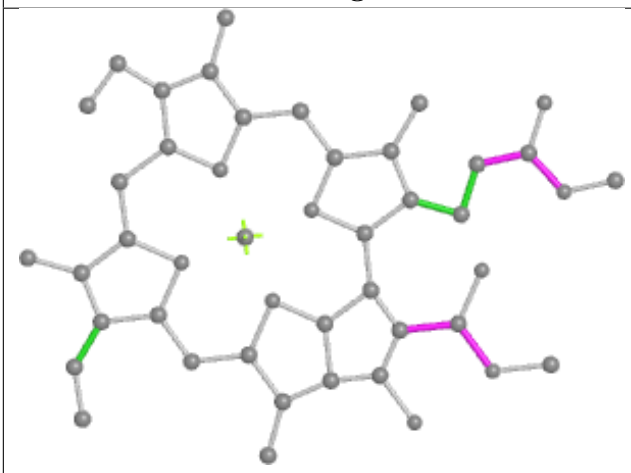
Ligand CLA 7 302



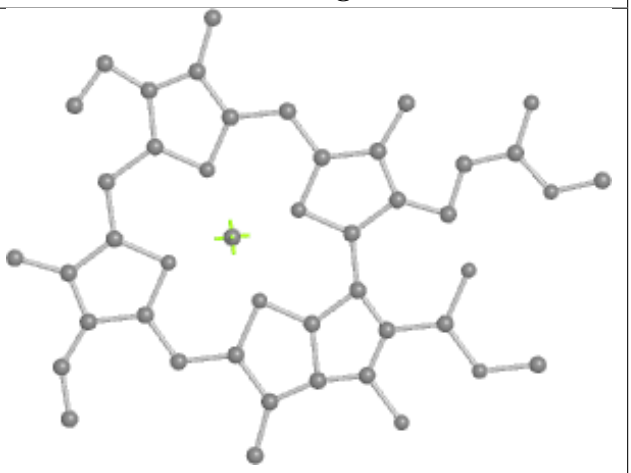
Bond lengths



Bond angles

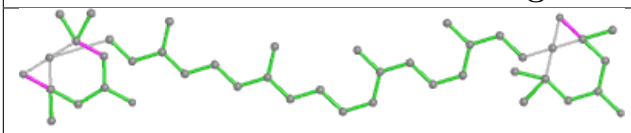


Torsions

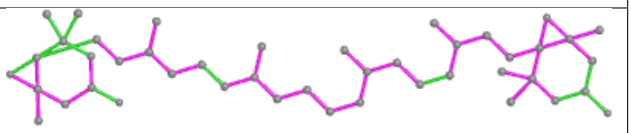


Rings

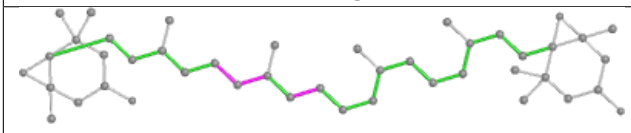
Ligand XAT 3 314



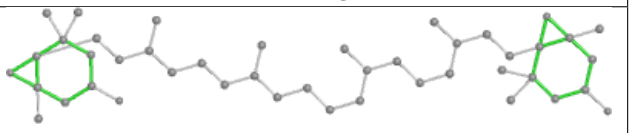
Bond lengths



Bond angles

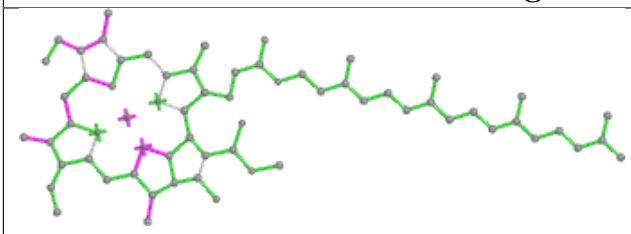


Torsions

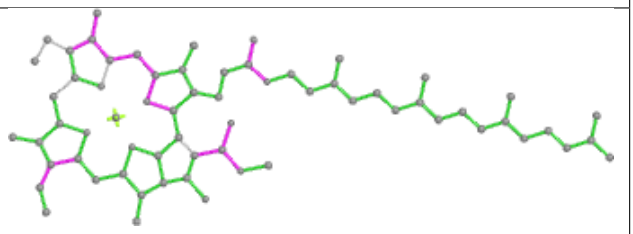


Rings

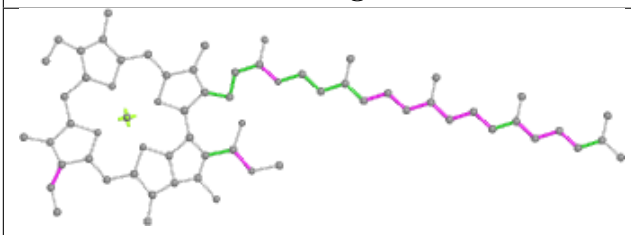
Ligand CLA B 806



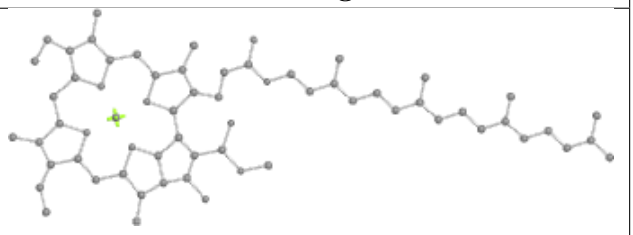
Bond lengths



Bond angles

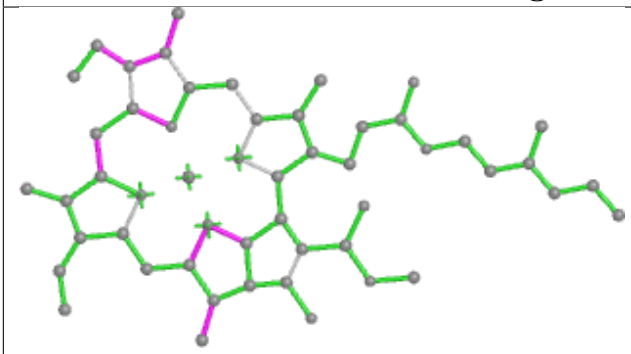


Torsions

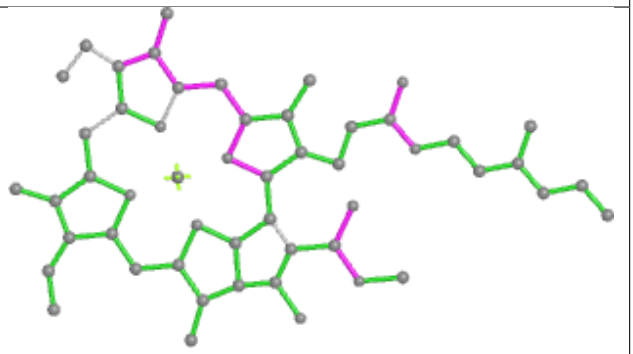


Rings

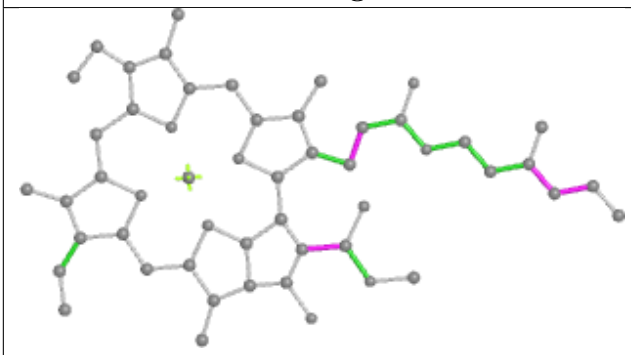
Ligand CLA 5 305



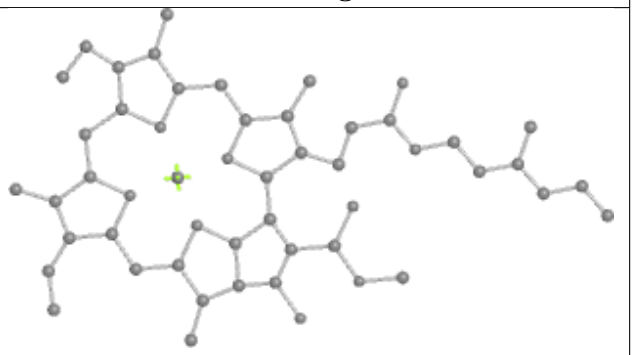
Bond lengths



Bond angles

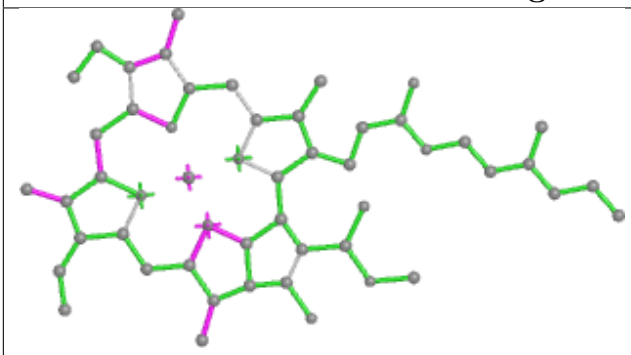


Torsions



Rings

Ligand CLA 7 312



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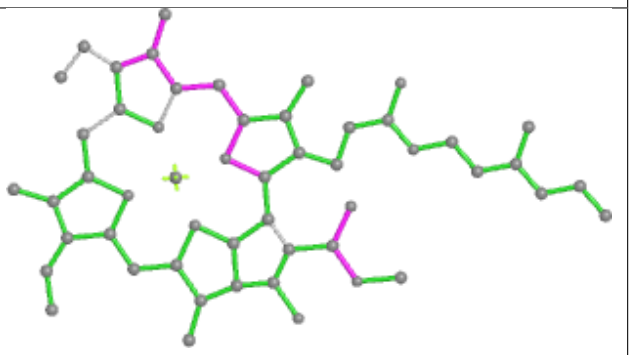
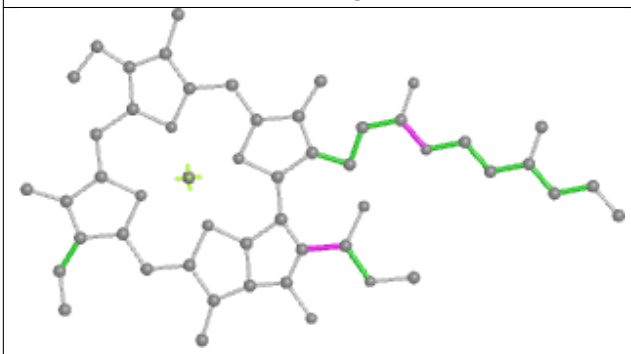


Bond angles



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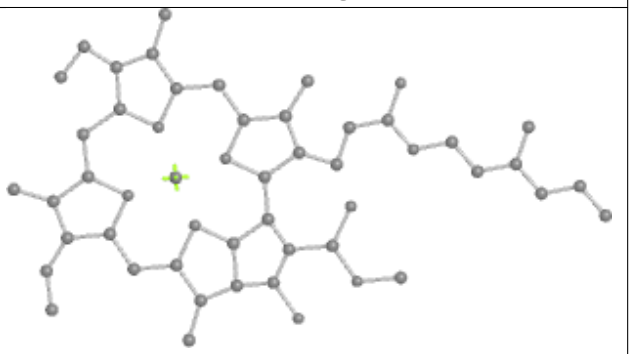
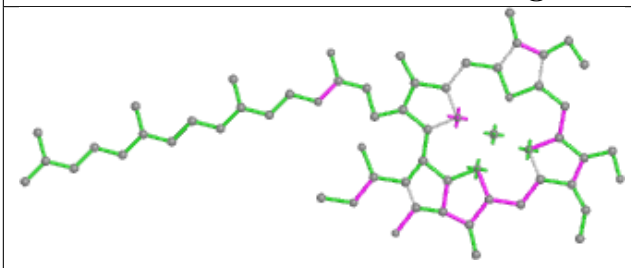
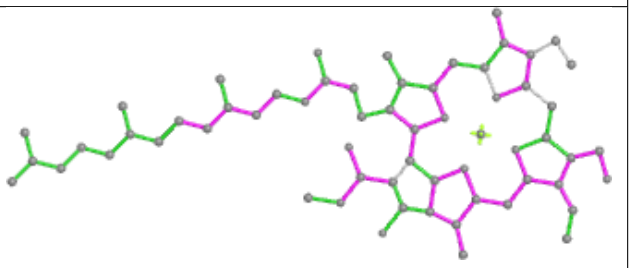


Rings

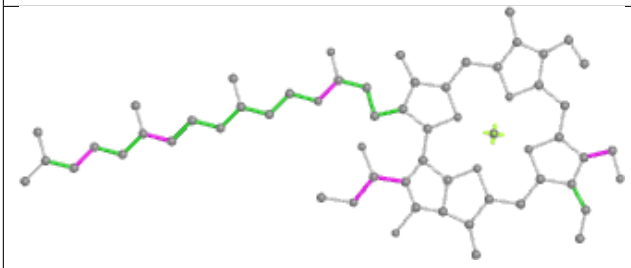
Ligand CHL 2 301



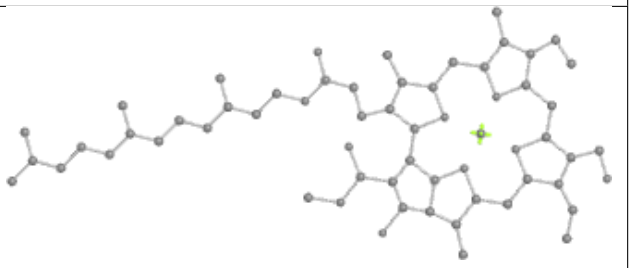
Bond lengths



Bond angles

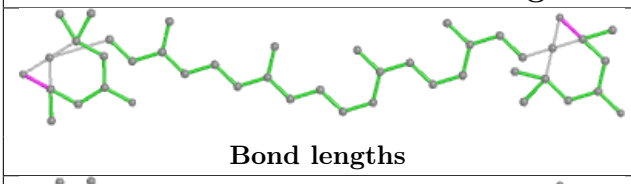


Torsions

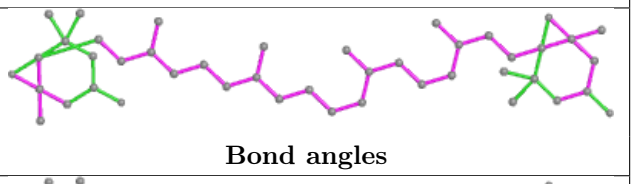


Rings

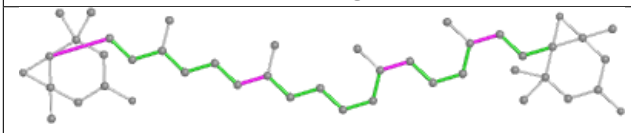
Ligand XAT 7 319



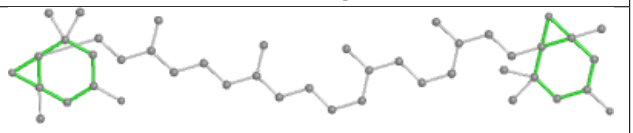
Bond lengths



Bond angles

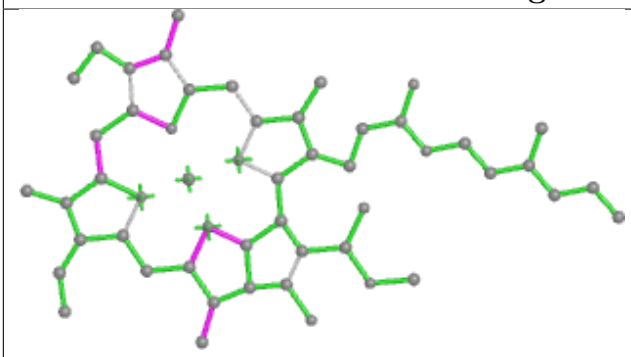


Torsions



Rings

Ligand CLA 9 311



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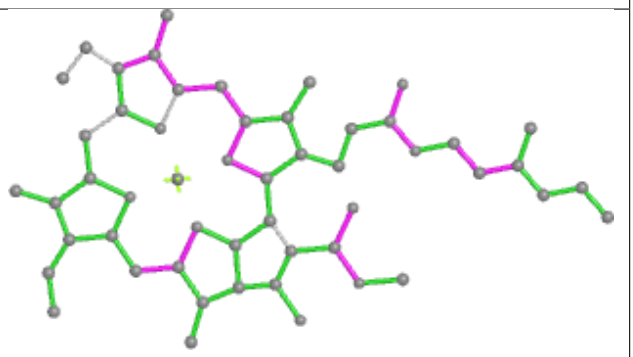

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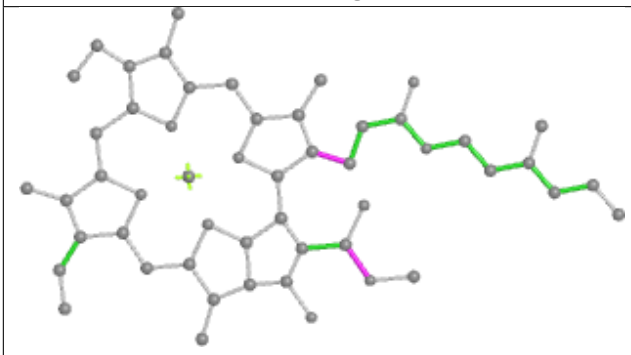
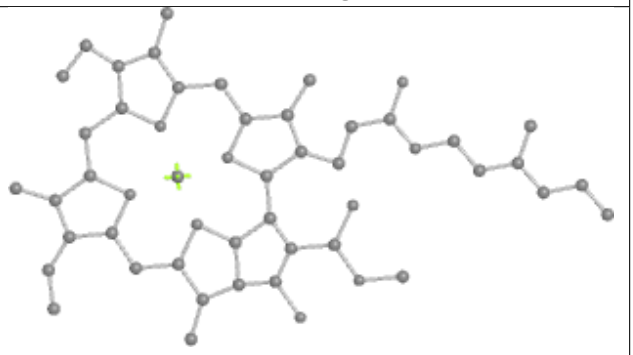
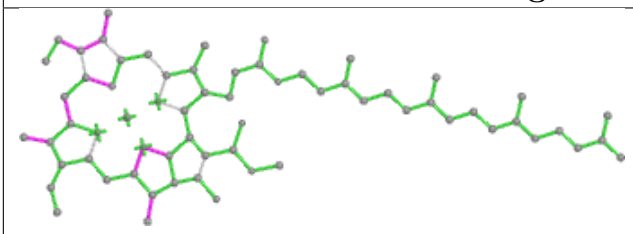


Torsions



Rings

Ligand CLA 2 302



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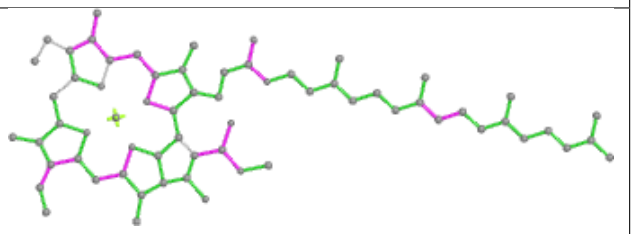
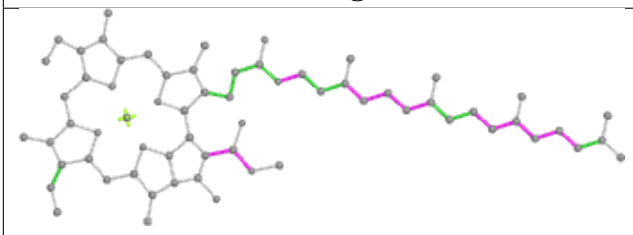


Bond angles



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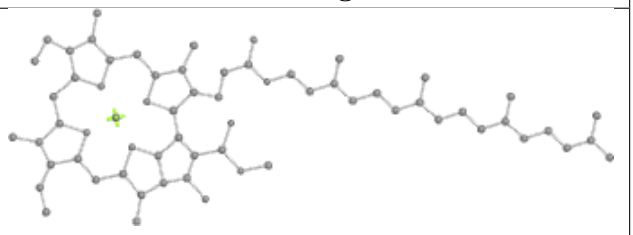
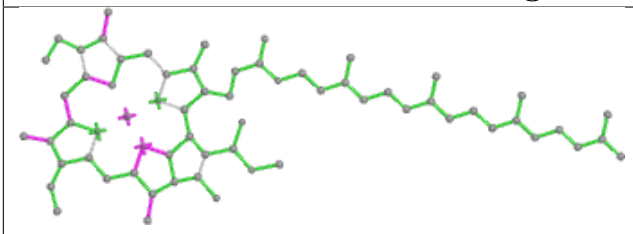


Rings

Ligand CLA A 821



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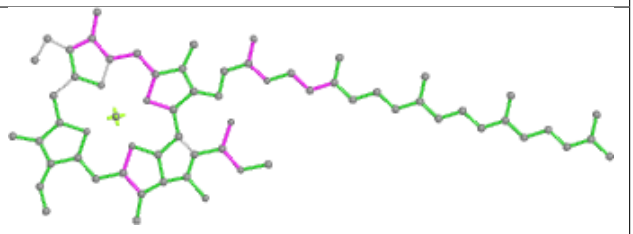
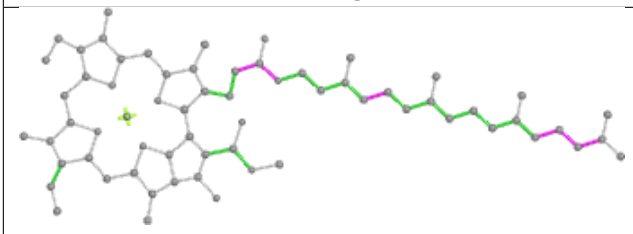
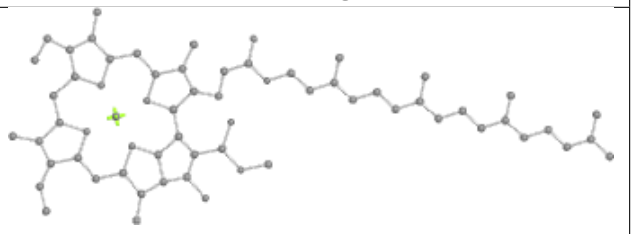


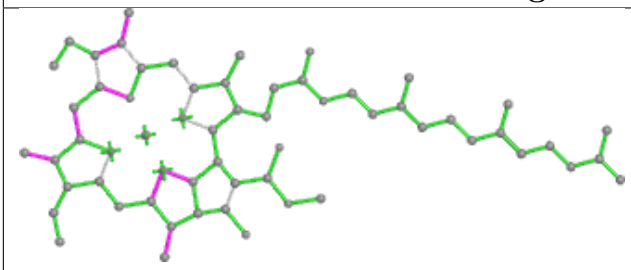
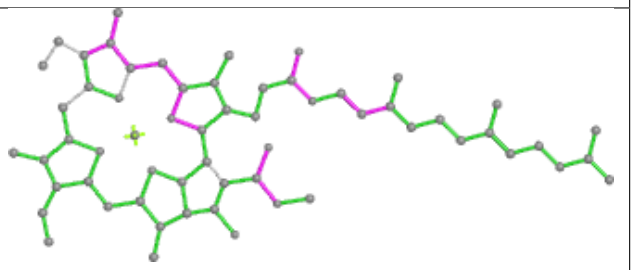
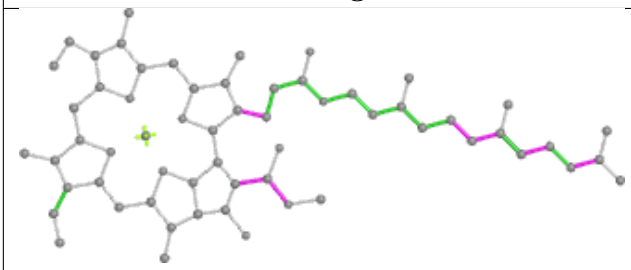
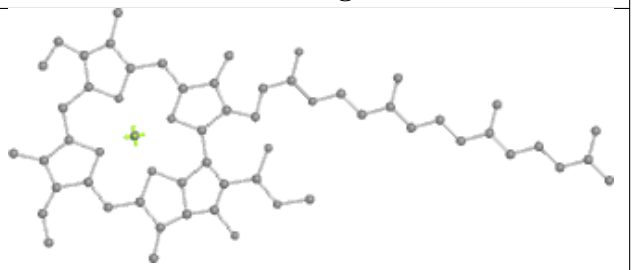
Bond angles



Torsions



Rings

Ligand CLA 1 308	
 Bond lengths	 Bond angles
 Torsions	 Rings

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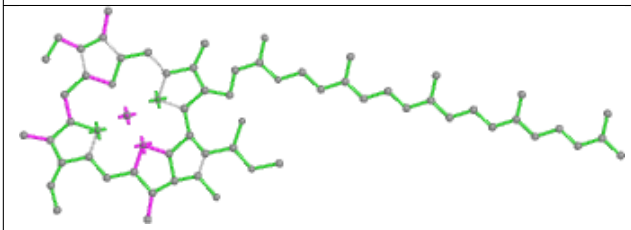
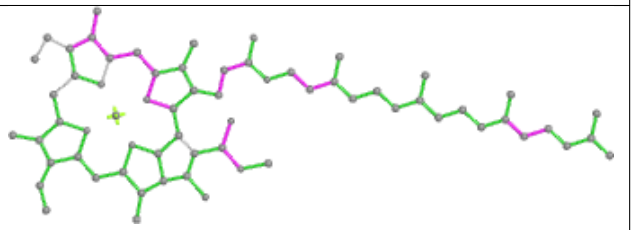
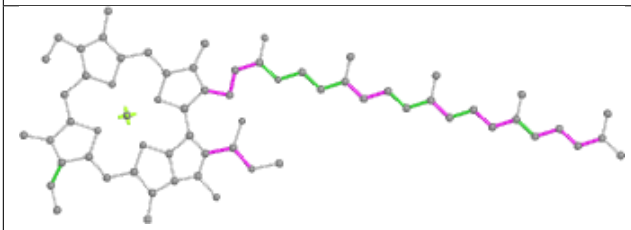
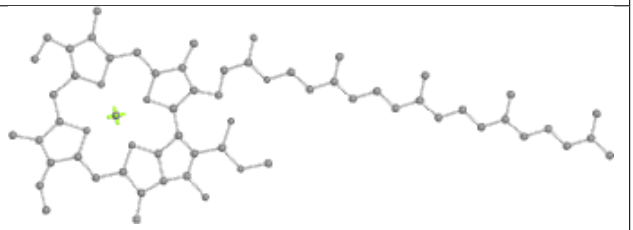
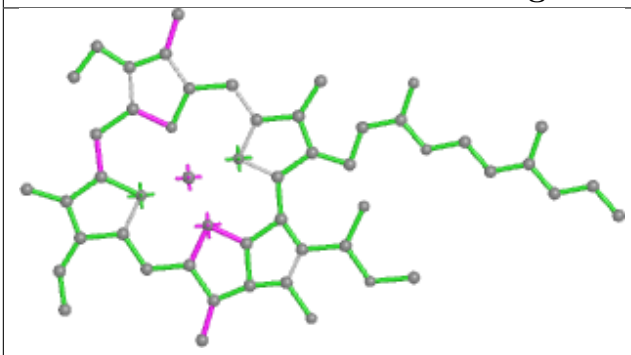
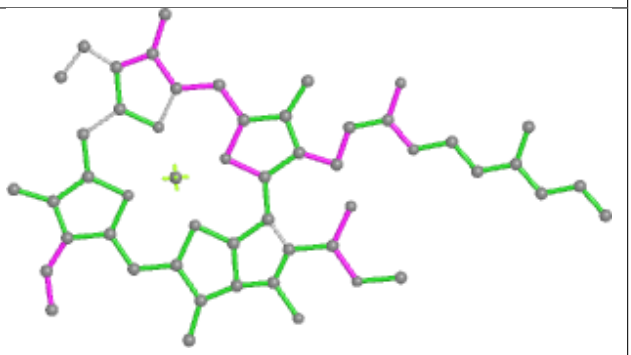
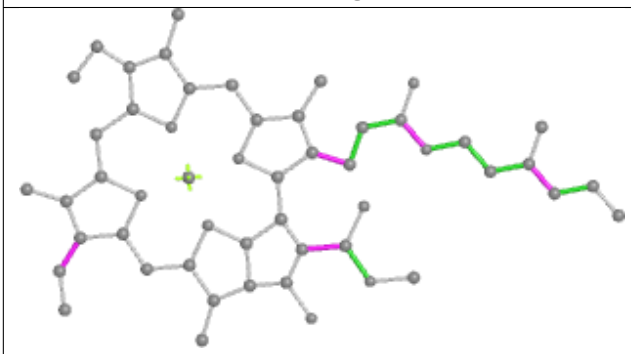
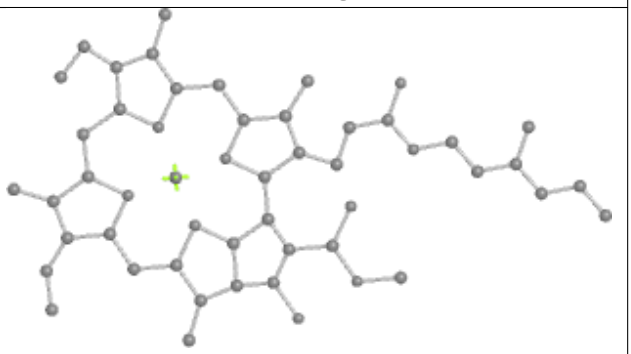
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 0 305	
	
Bond lengths	Bond angles
	
Torsions	Rings

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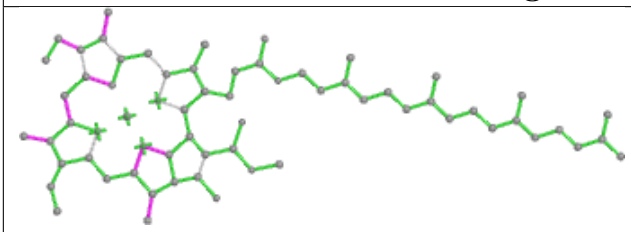
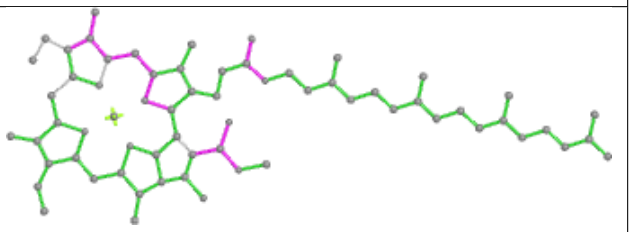
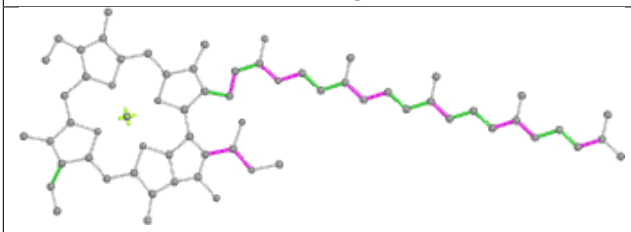
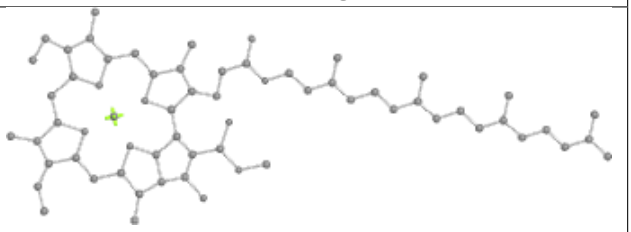
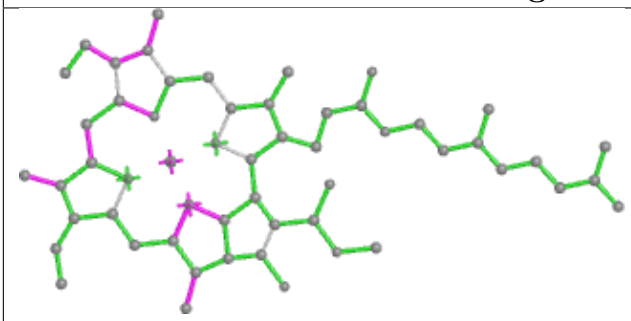
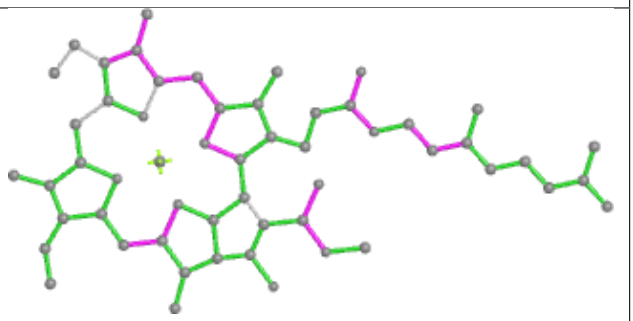
	
Bond lengths	Bond angles
	
Torsions	Rings

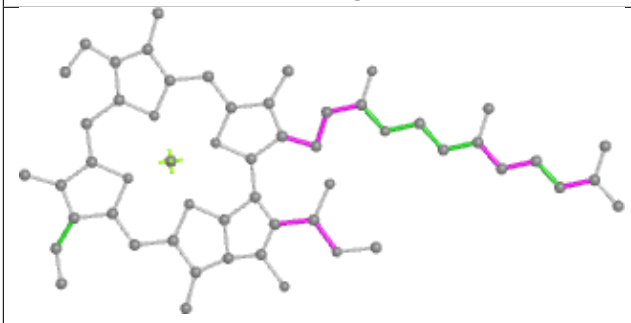
Ligand CLA 7 313



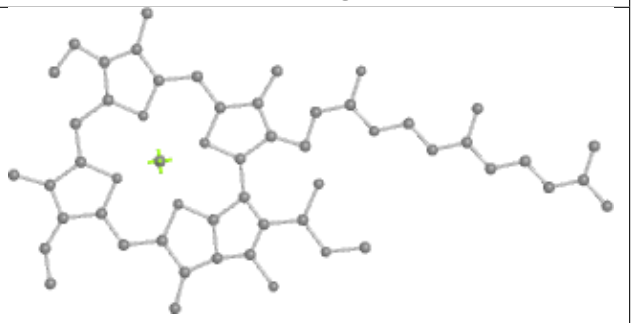
Bond lengths



Bond angles

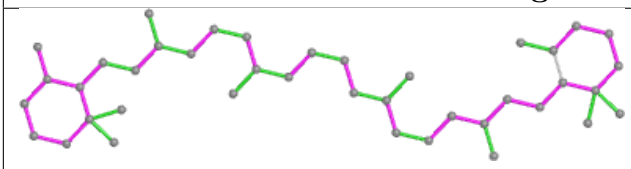


Torsions



Rings

Ligand 8CT 4 317



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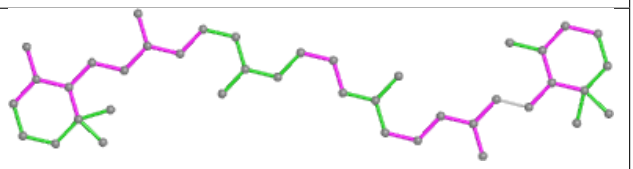
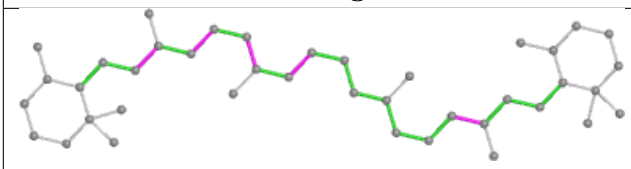


Bond angles



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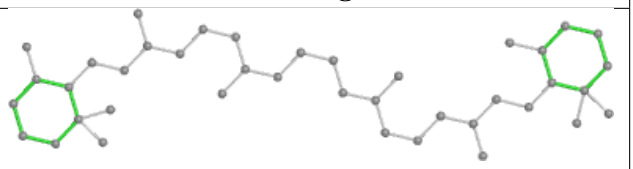
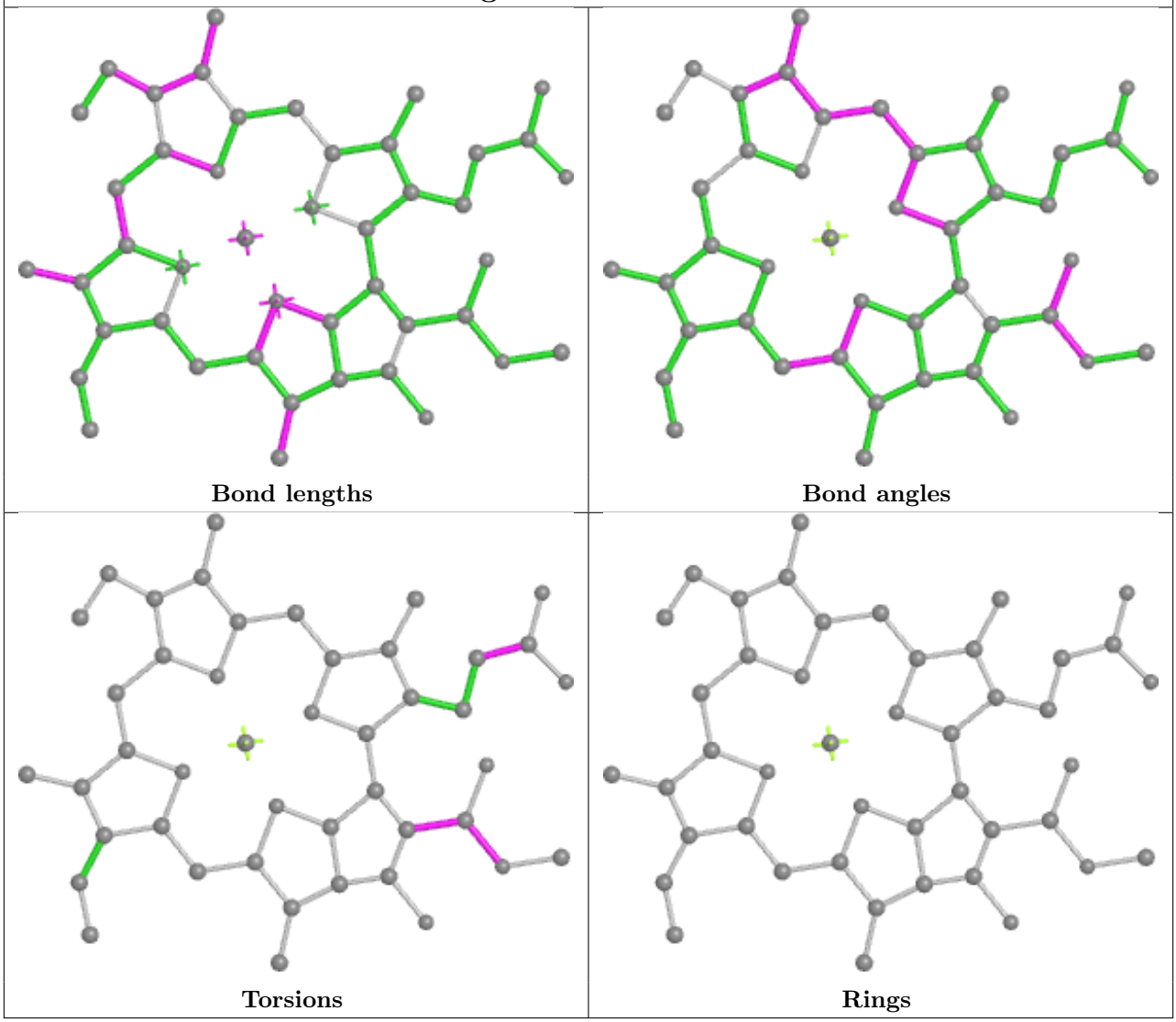


Rings

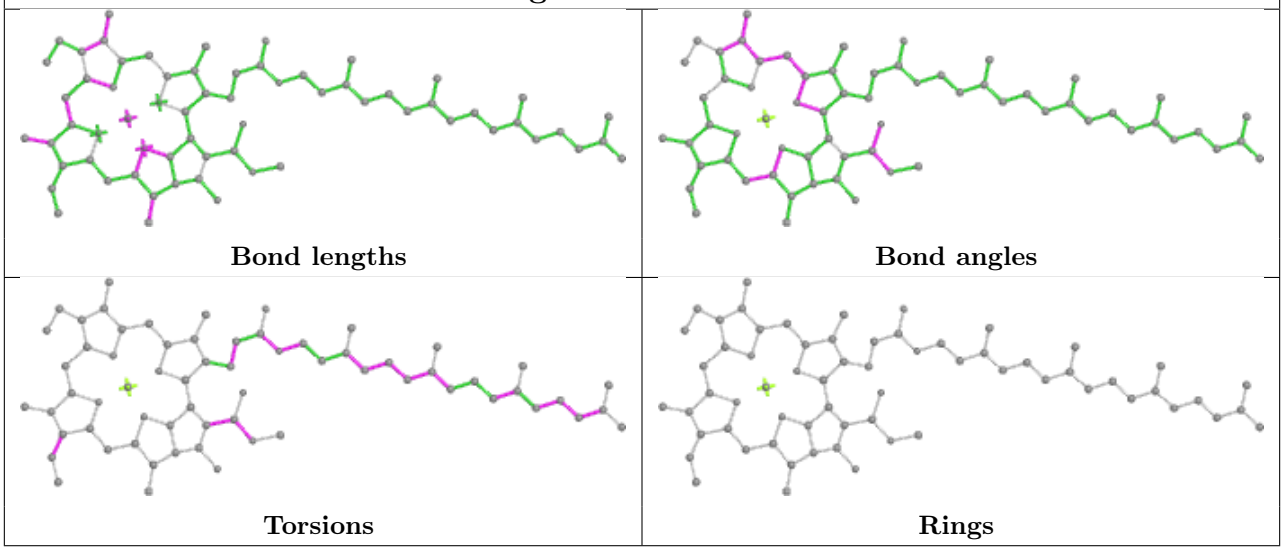
Ligand CLA A 835



Bond lengths | Bond angles

Torsions | Rings

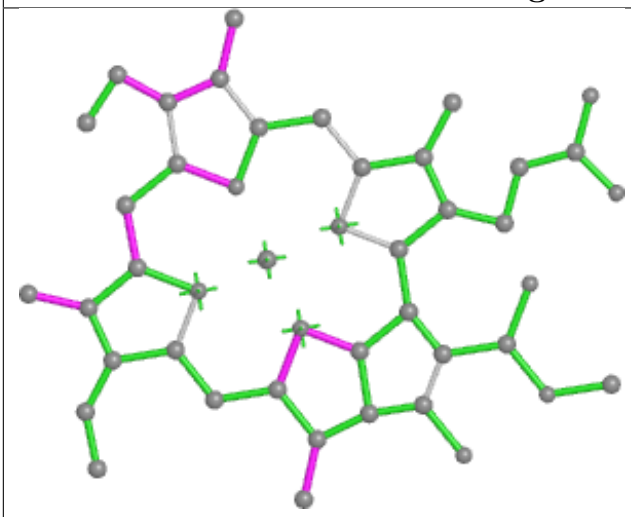
Ligand CLA 5 303



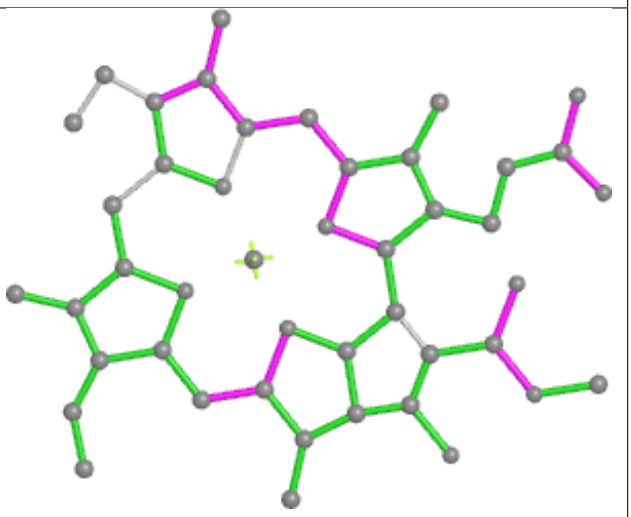
Bond lengths | Bond angles

Torsions | Rings

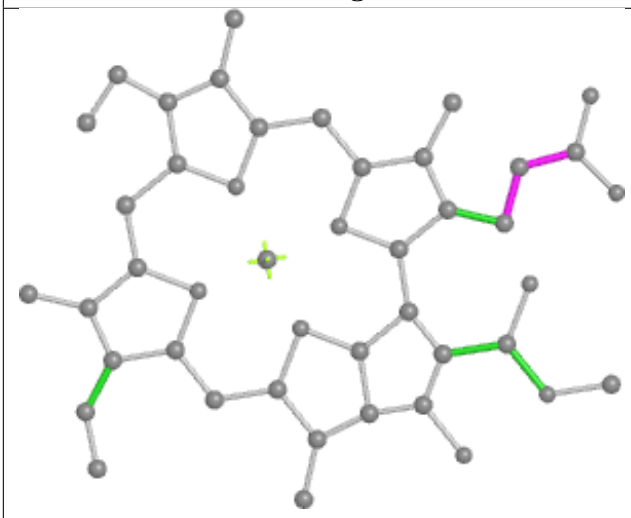
Ligand CLA 8 313



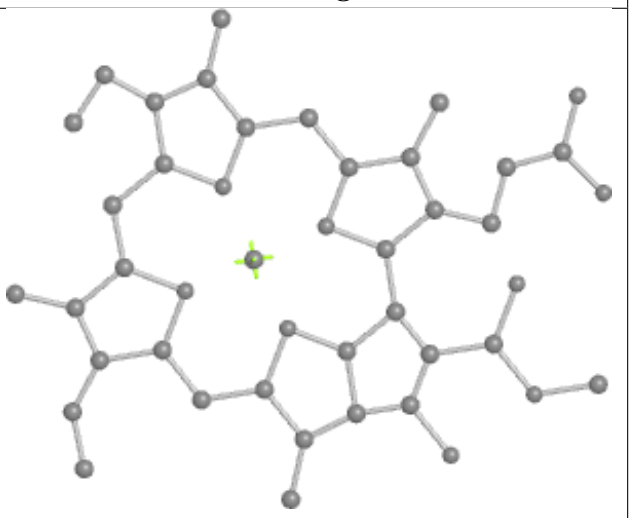
Bond lengths



Bond angles

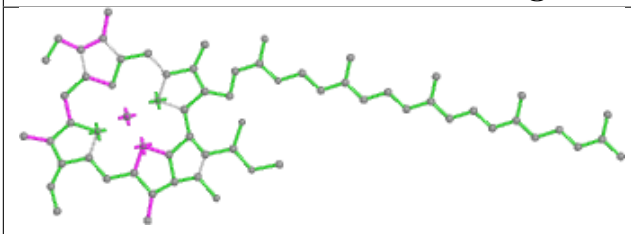


Torsions

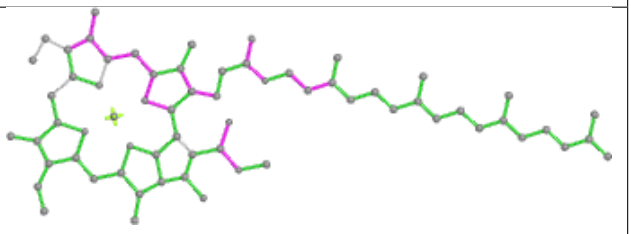


Rings

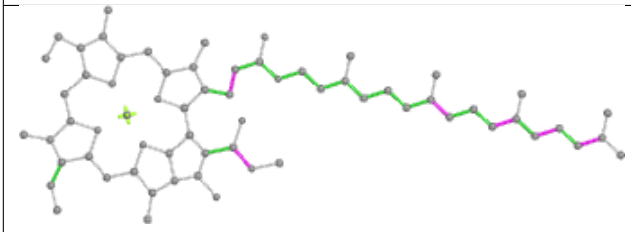
Ligand CLA 5 302



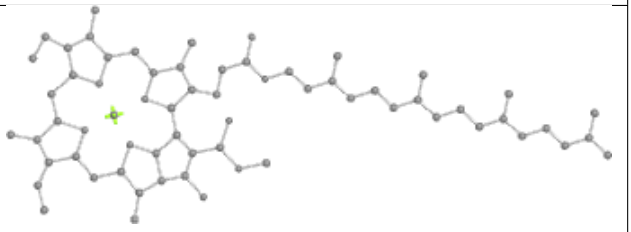
Bond lengths



Bond angles

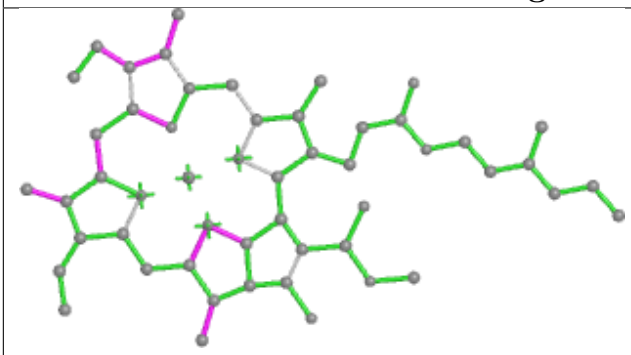


Torsions

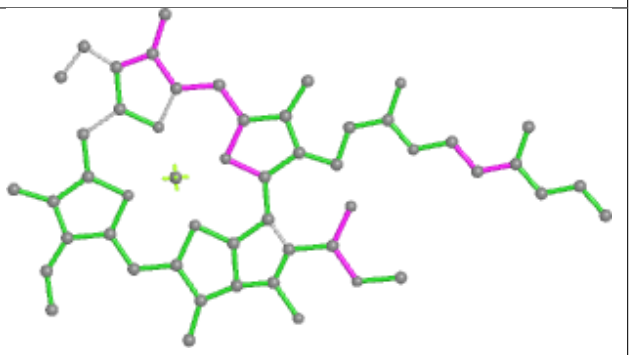


Rings

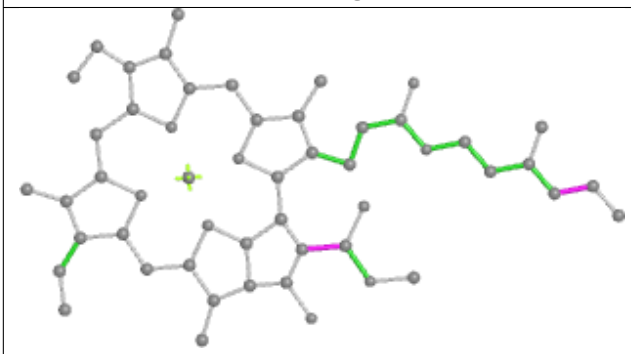
Ligand CLA 3 310



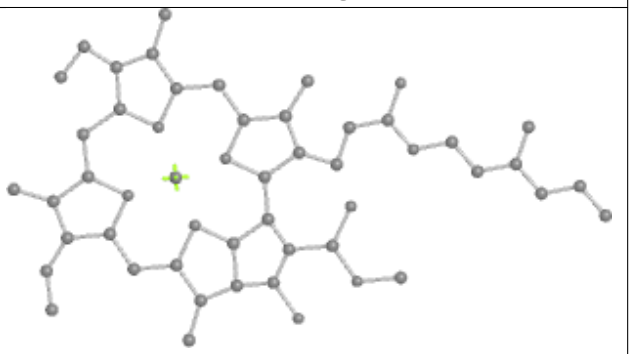
Bond lengths



Bond angles

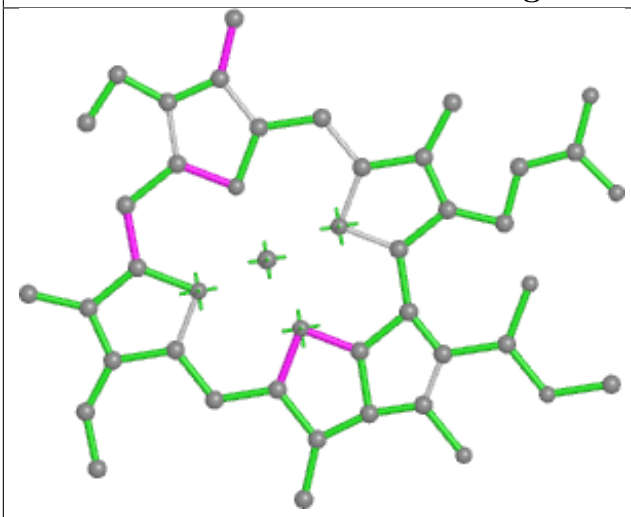


Torsions

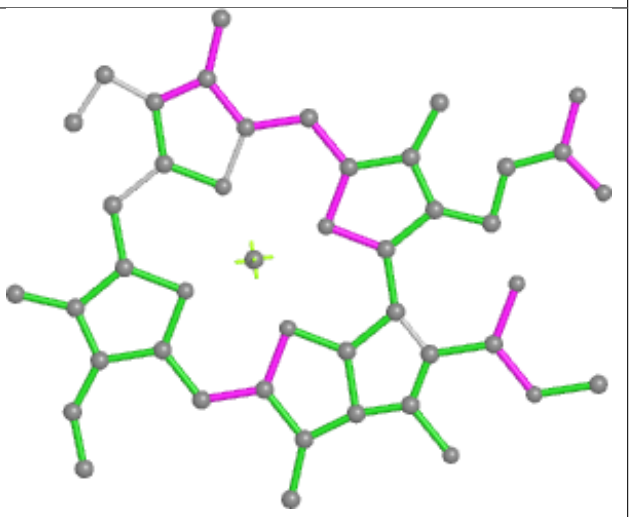


Rings

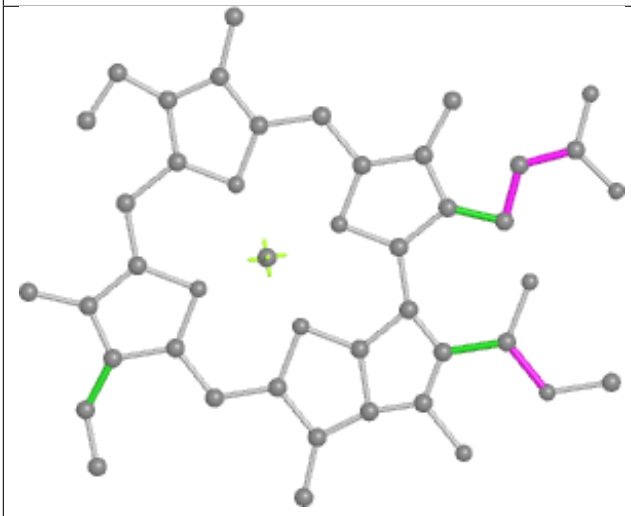
Ligand CLA G 101



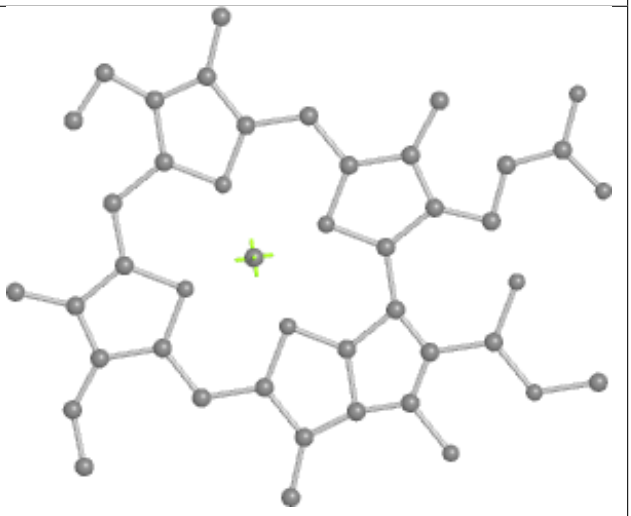
Bond lengths



Bond angles

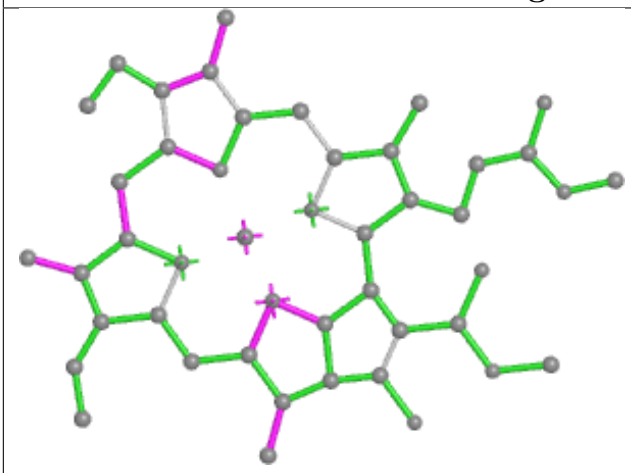


Torsions

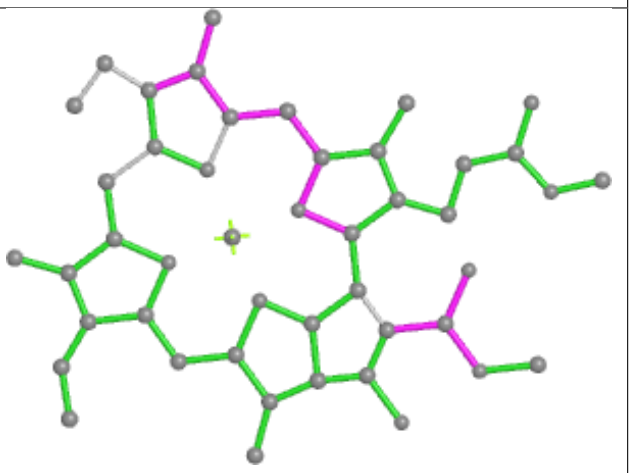


Rings

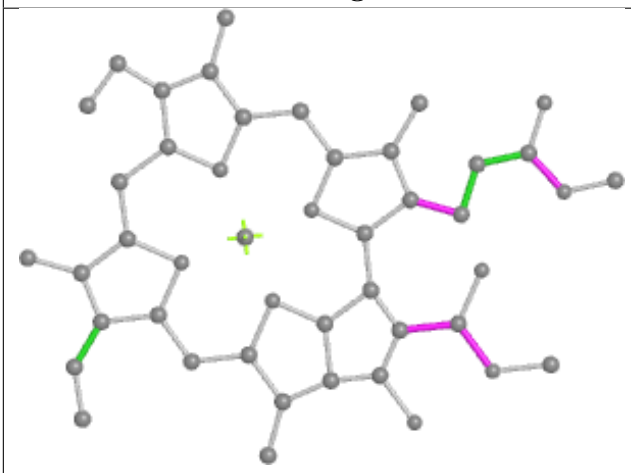
Ligand CLA 1 313



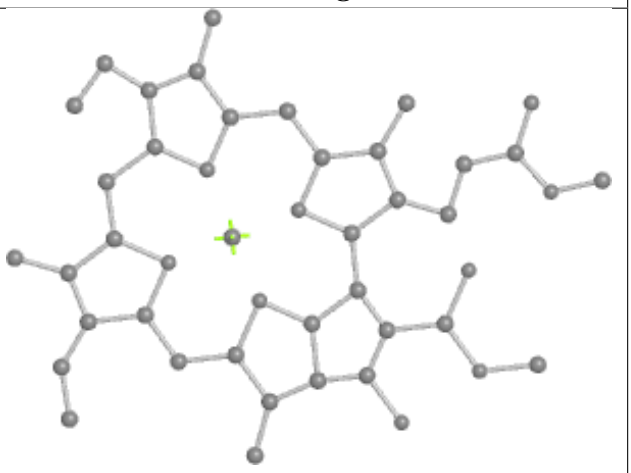
Bond lengths



Bond angles

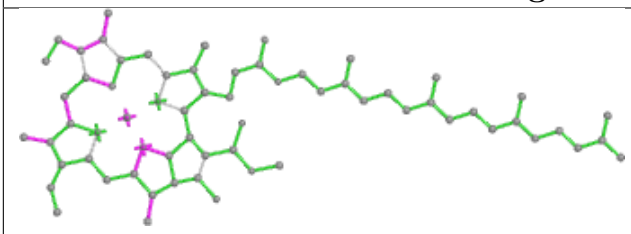


Torsions

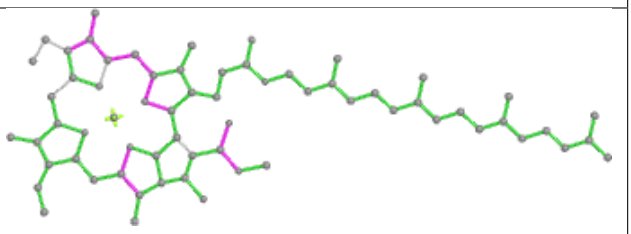


Rings

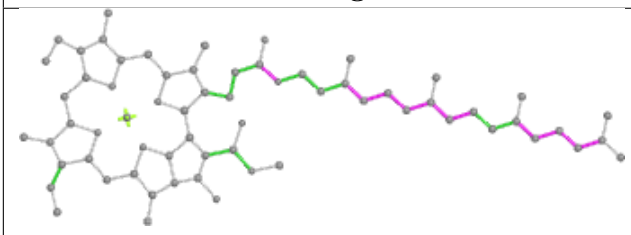
Ligand CLA 9 308



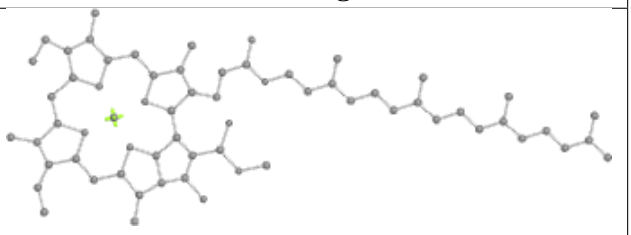
Bond lengths



Bond angles

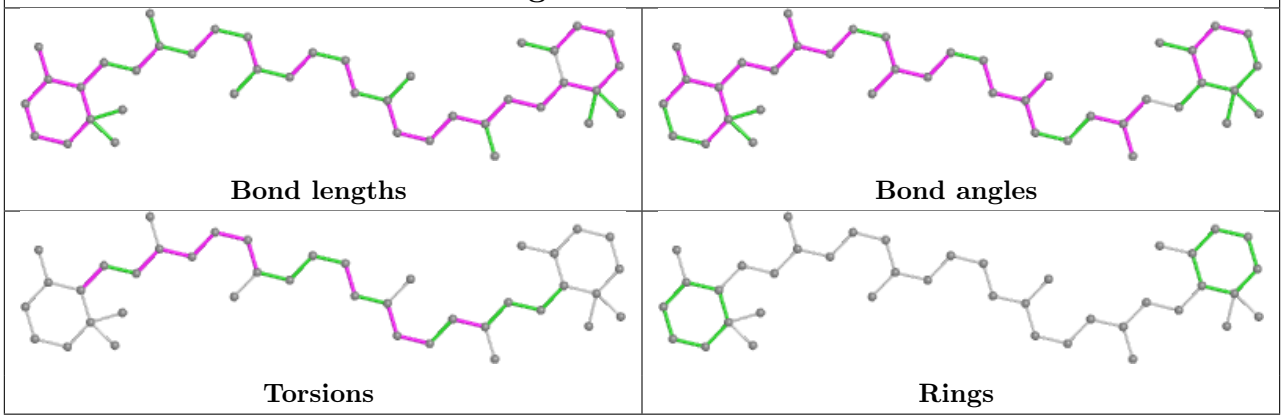


Torsions

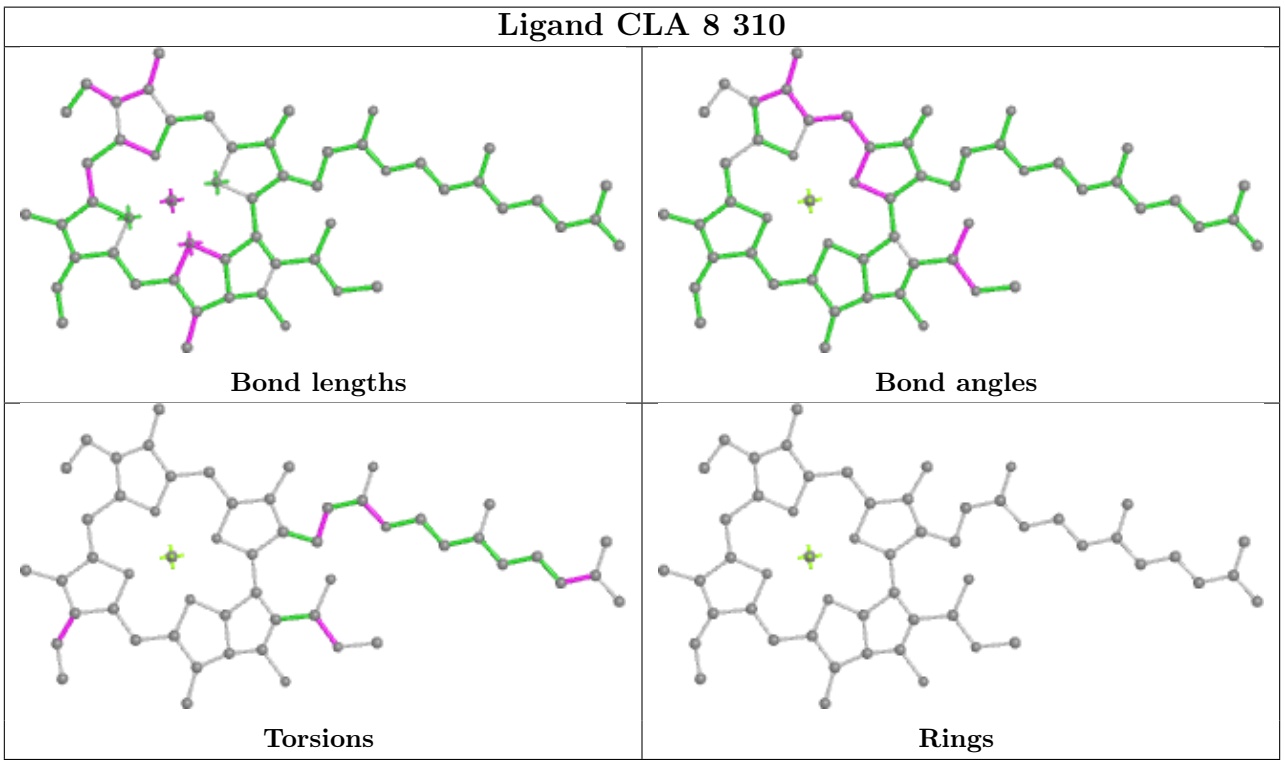


Rings

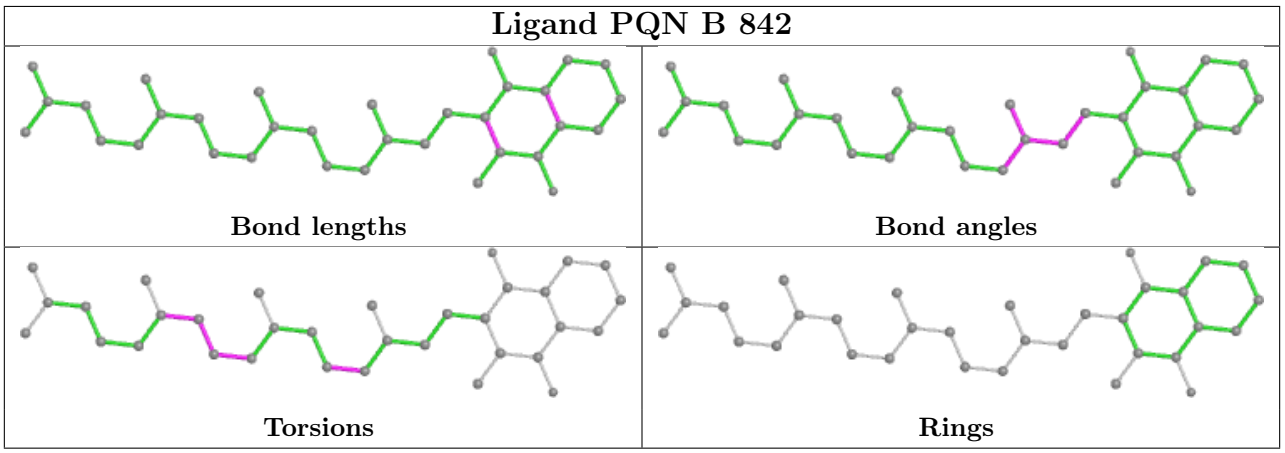
Ligand 8CT B 851



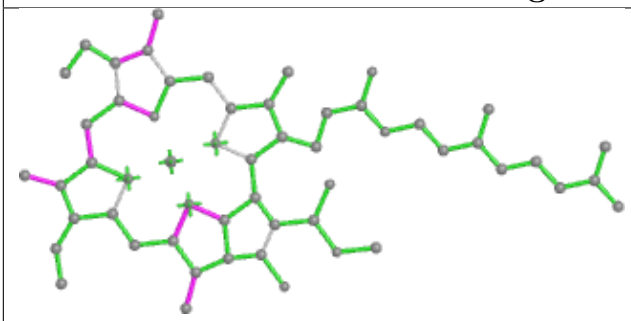
Ligand CLA 8 310



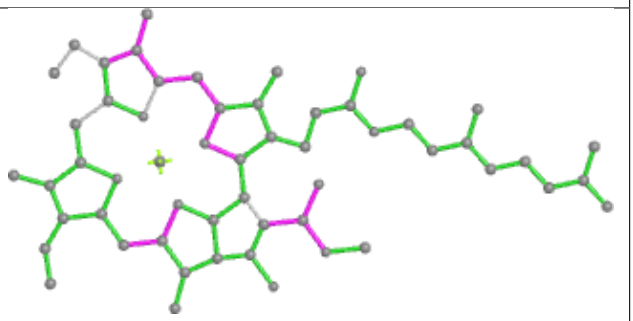
Ligand PQN B 842



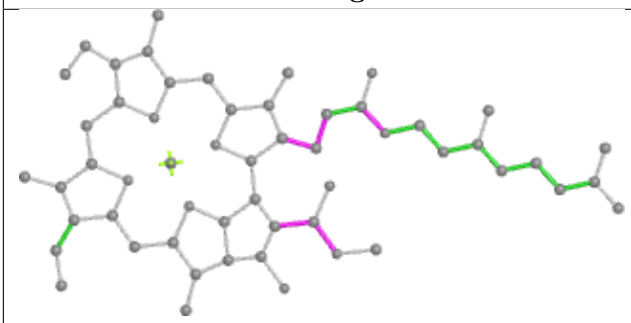
Ligand CLA 5 313



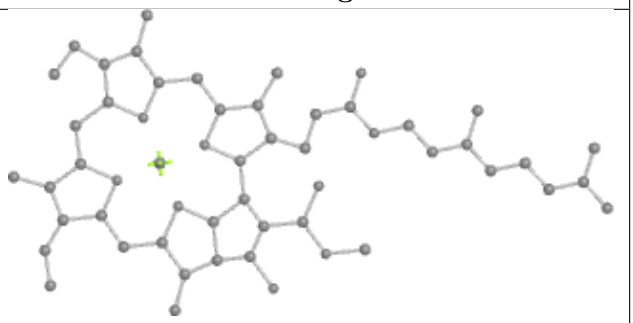
Bond lengths



Bond angles

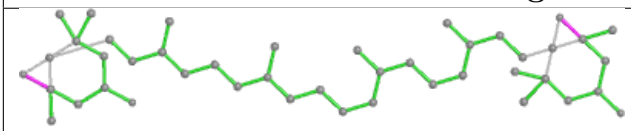


Torsions

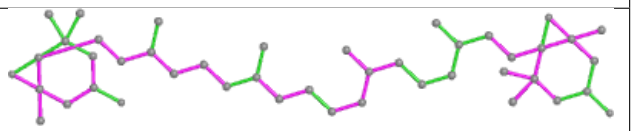


Rings

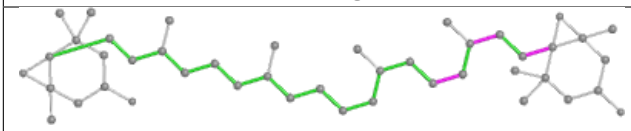
Ligand XAT 6 320



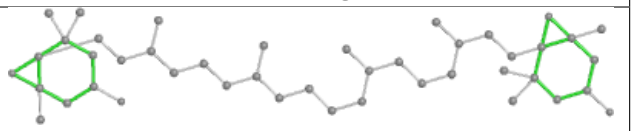
Bond lengths



Bond angles

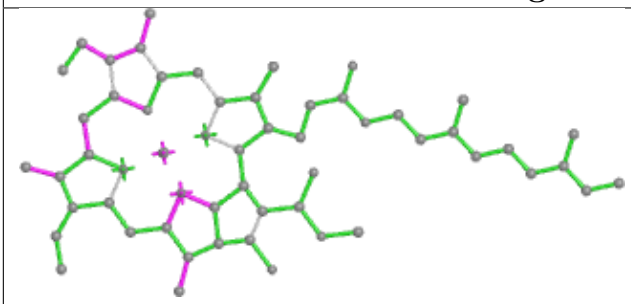


Torsions

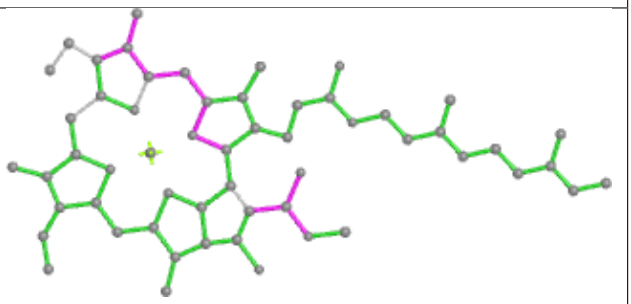


Rings

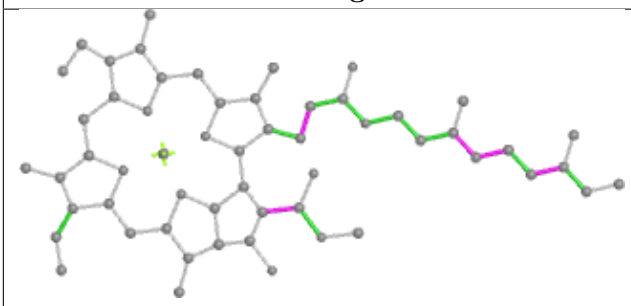
Ligand CLA 4 312



Bond lengths



Bond angles



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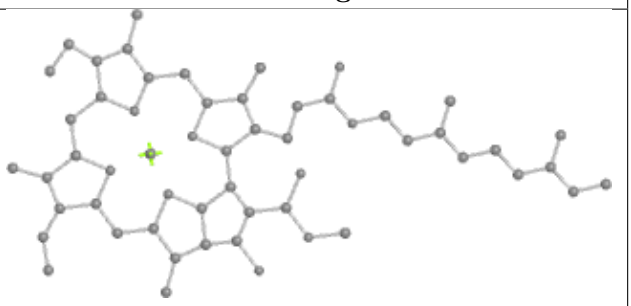
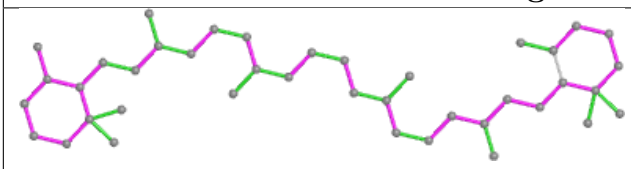
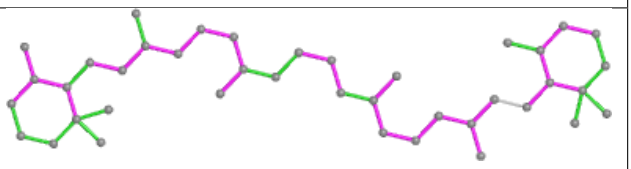


Rings

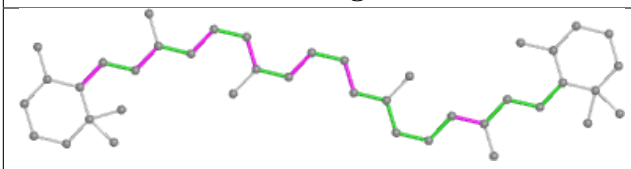
Ligand 8CT B 848



Bond lengths



Bond angles



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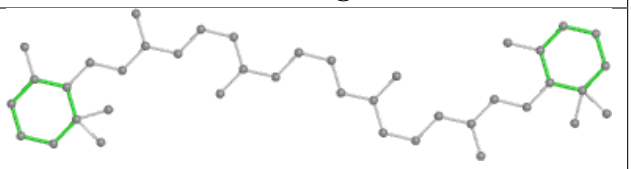
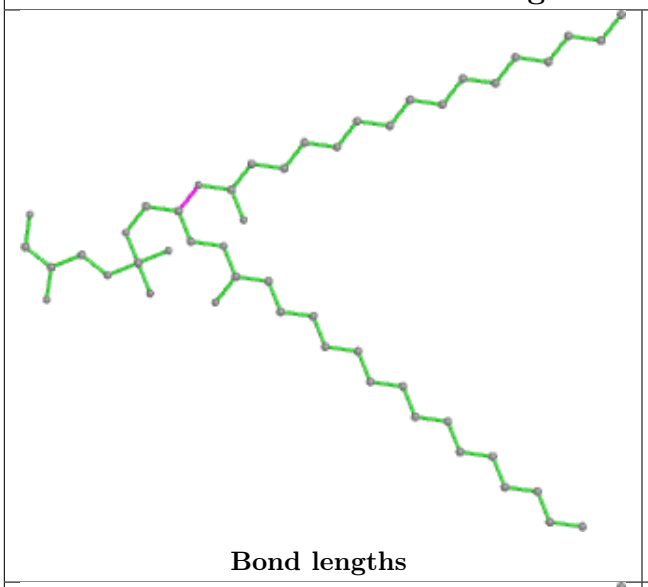
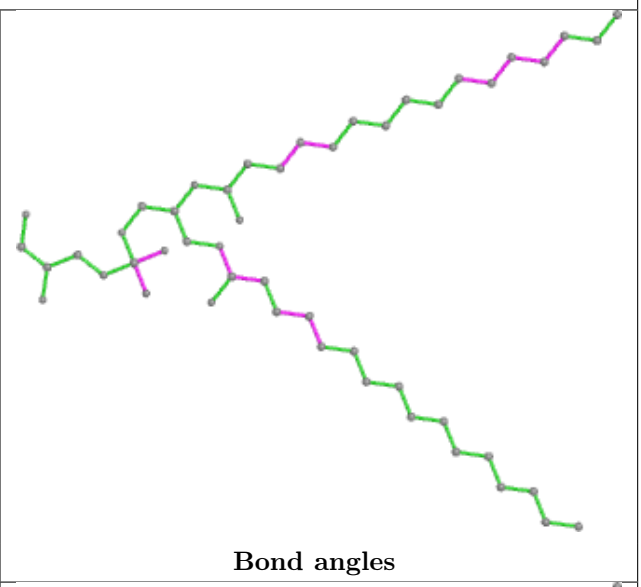


Rings

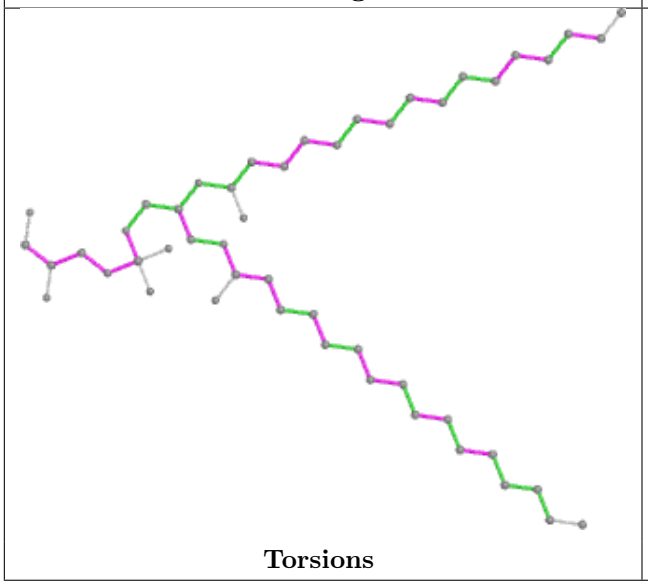
Ligand LHG 5 318



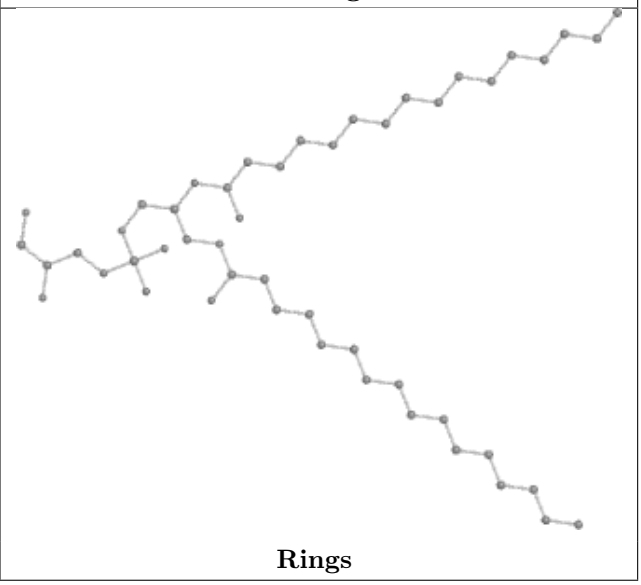
Bond lengths



Bond angles

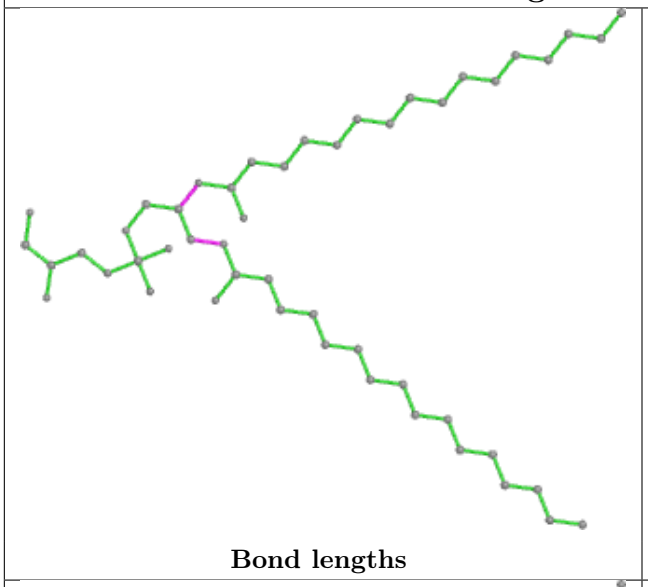


Torsions

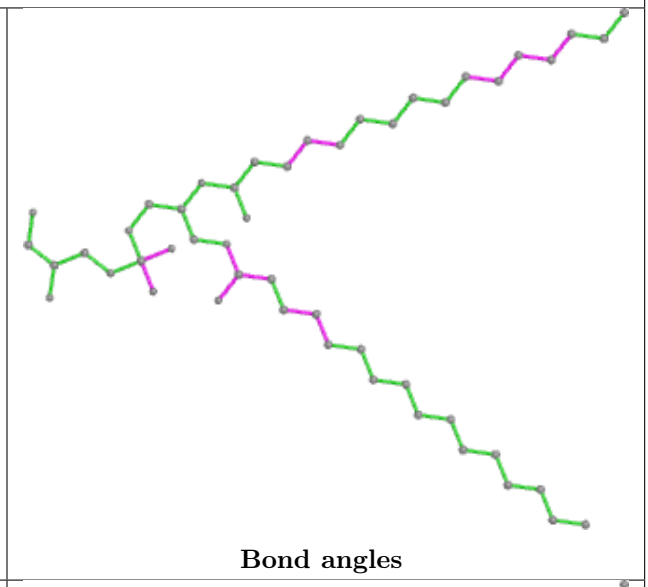


Rings

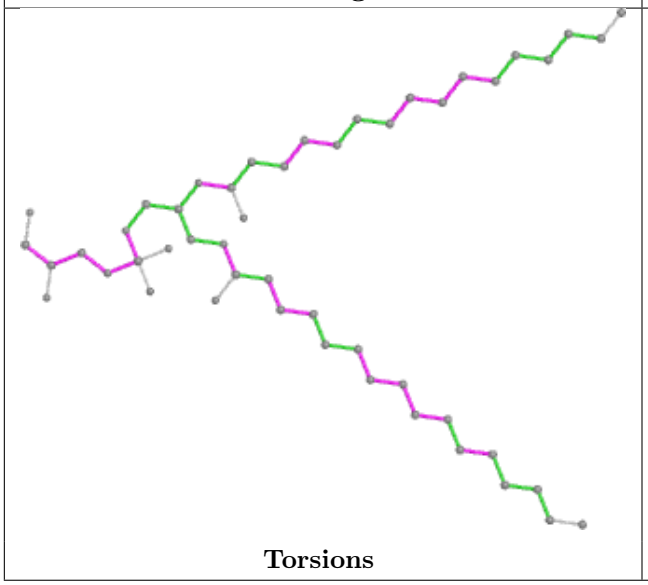
Ligand LHG 1 317



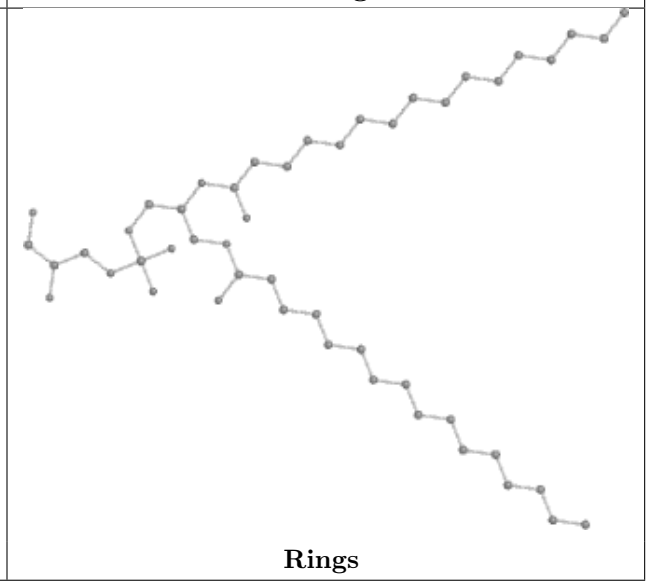
Bond lengths



Bond angles

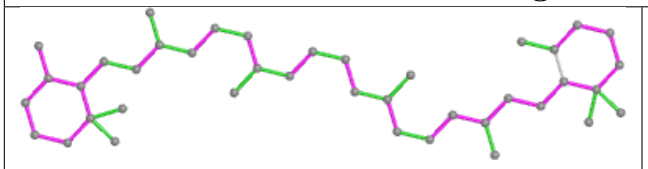


Torsions

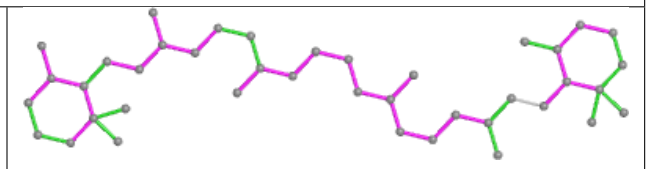


Rings

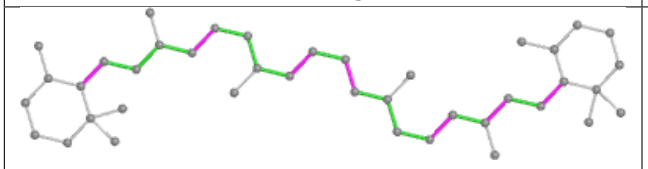
Ligand 8CT J 101



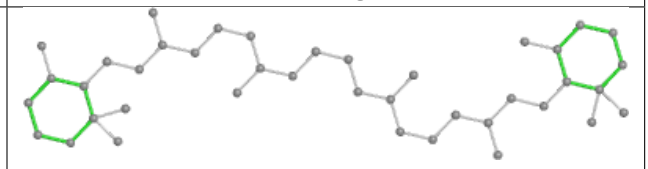
Bond lengths



Bond angles

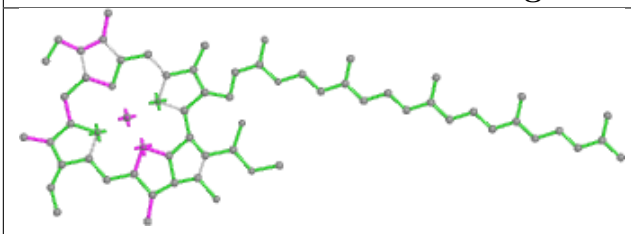


Torsions

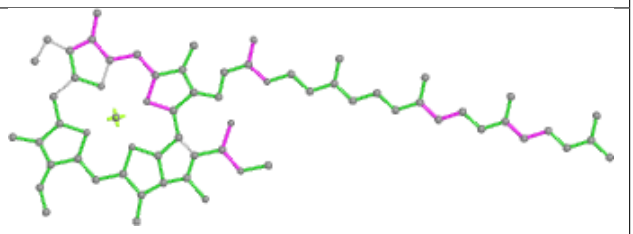


Rings

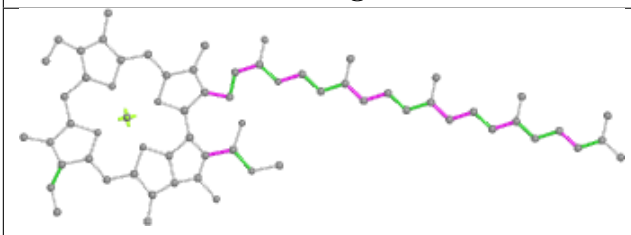
Ligand CLA B 808



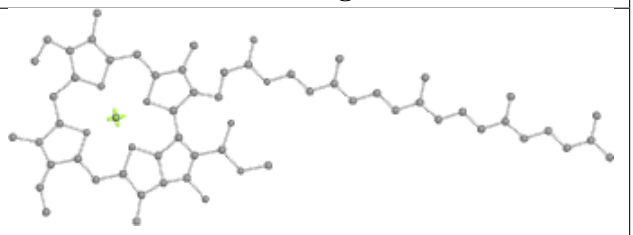
Bond lengths



Bond angles

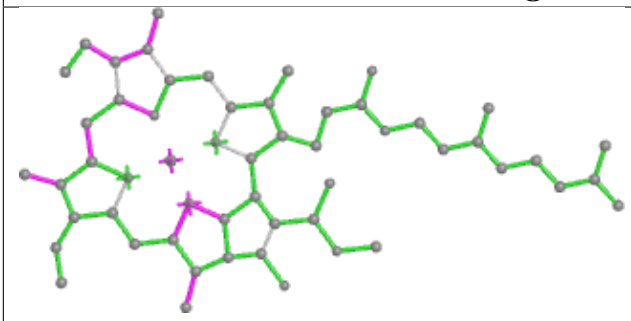


Torsions

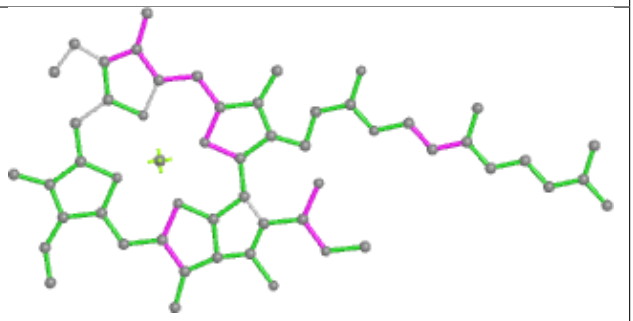


Rings

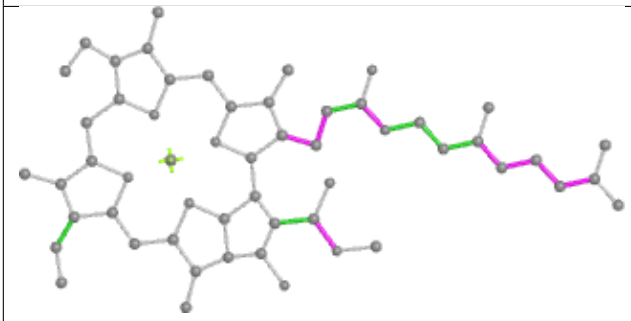
Ligand CLA B 823



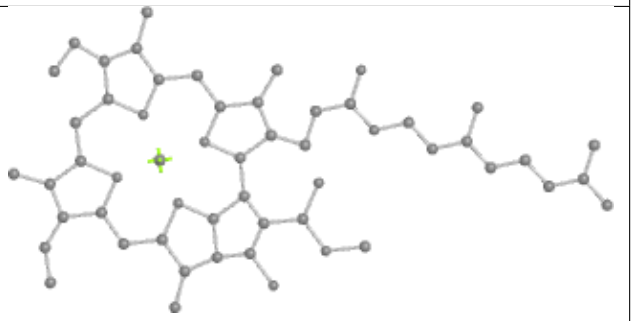
Bond lengths



Bond angles

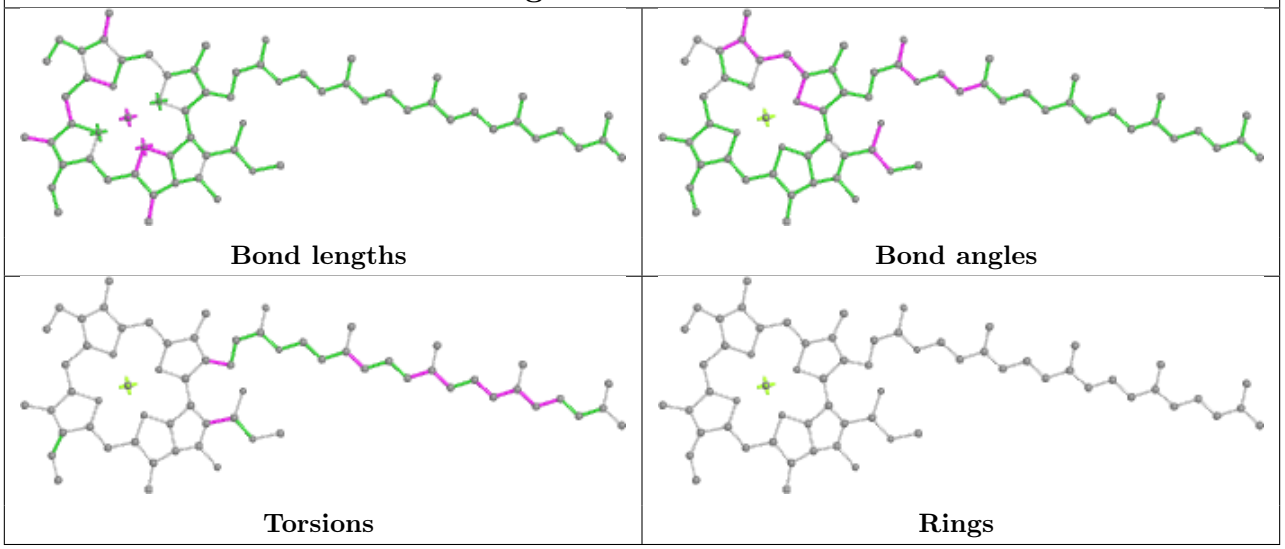


Torsions

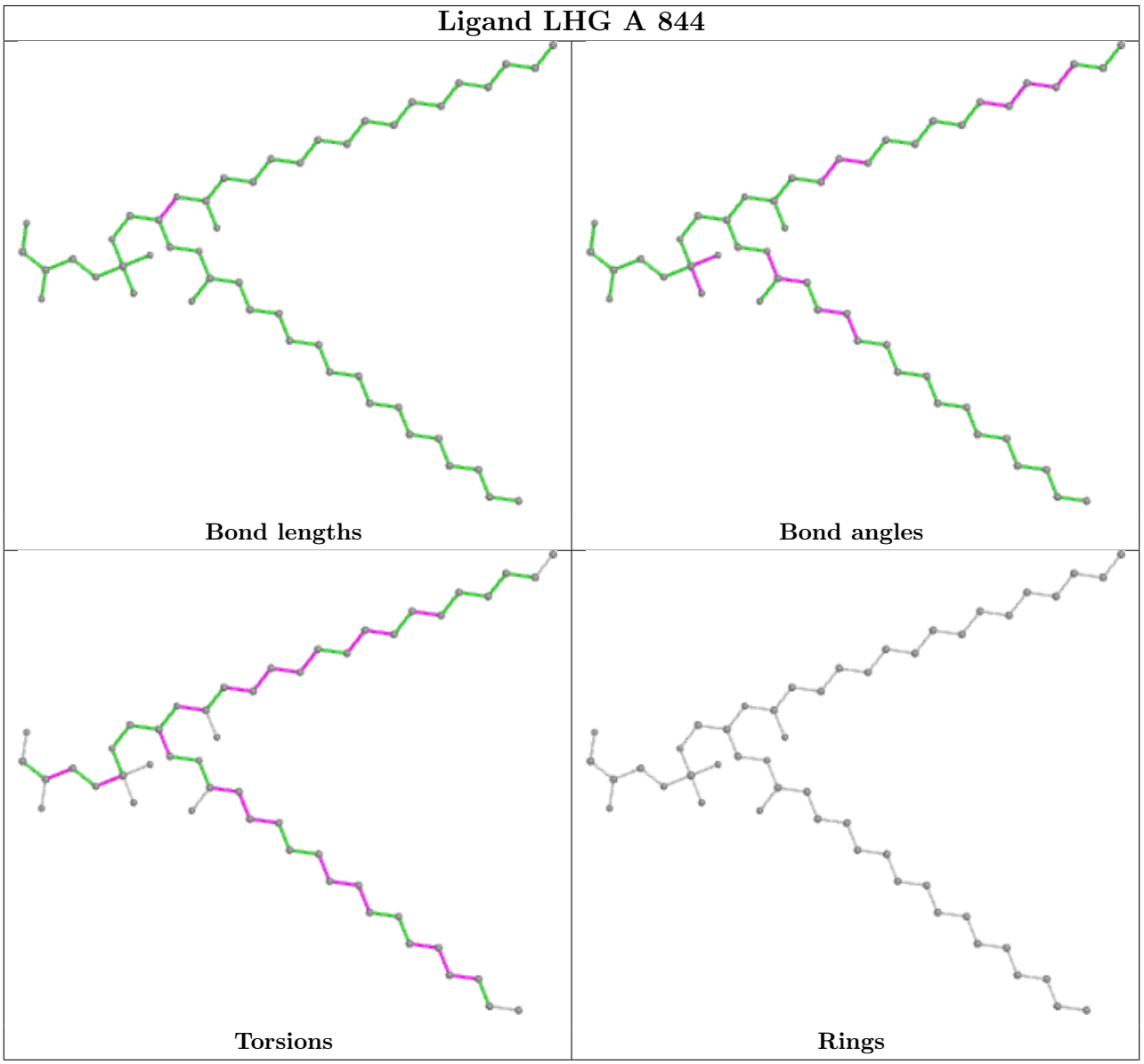


Rings

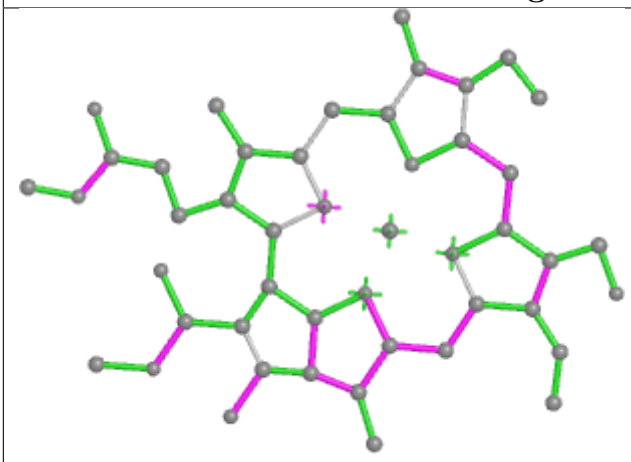
Ligand CLA B 827



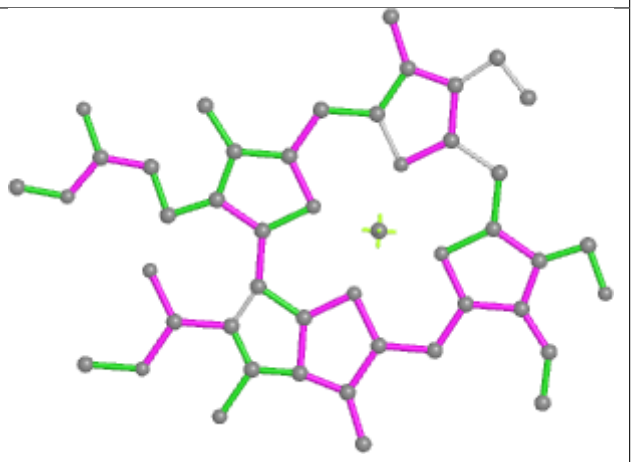
Ligand LHG A 844



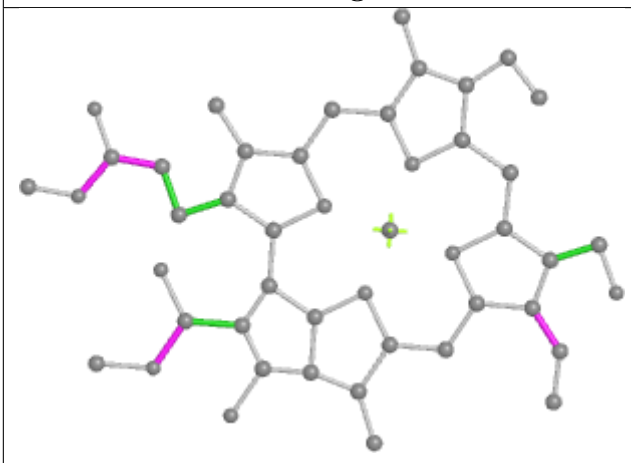
Ligand CHL 7 308



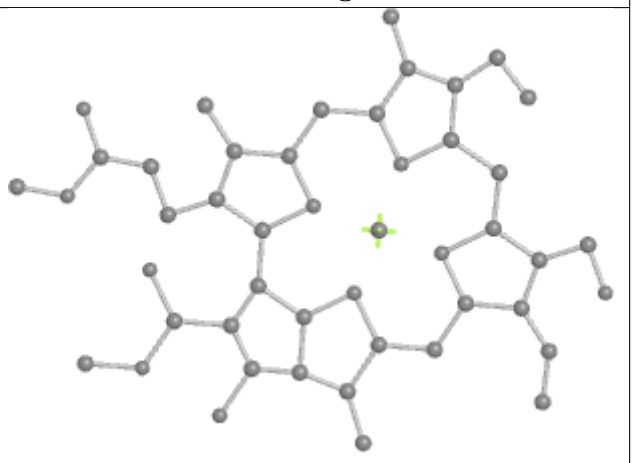
Bond lengths



Bond angles

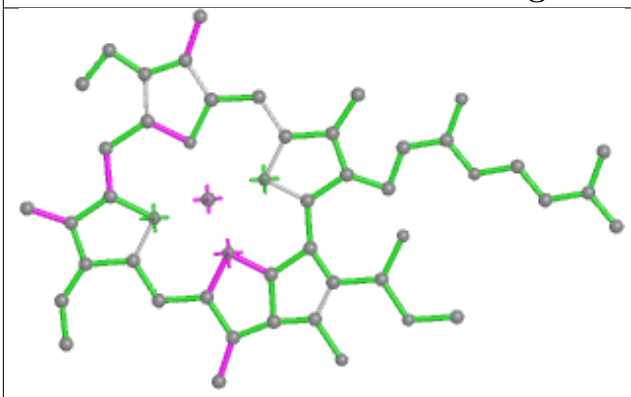


Torsions

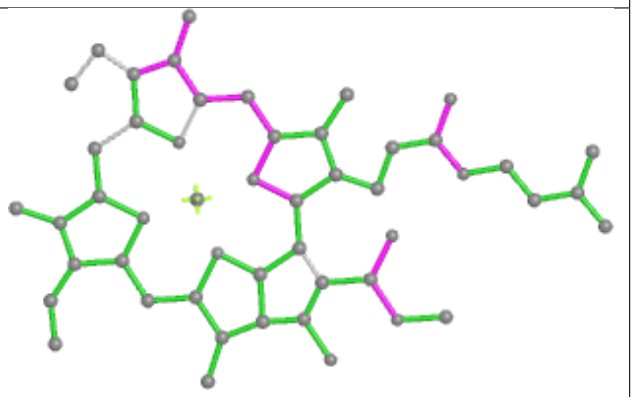


Rings

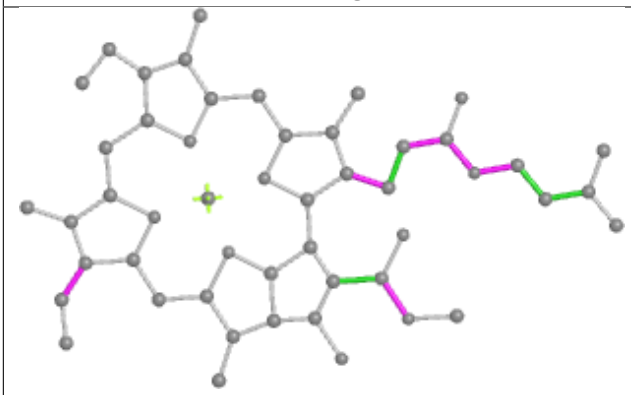
Ligand CLA 6 309



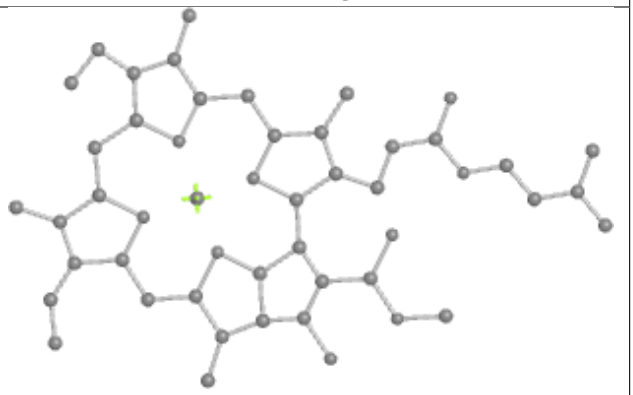
Bond lengths



Bond angles

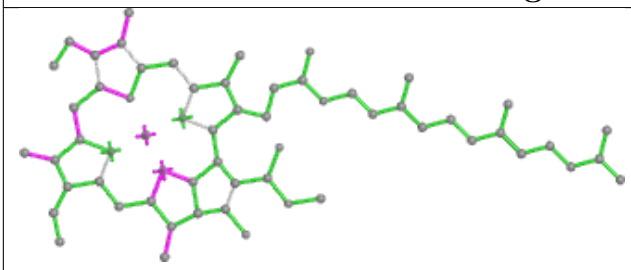


Torsions

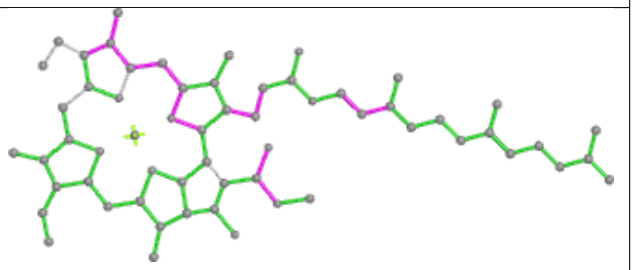


Rings

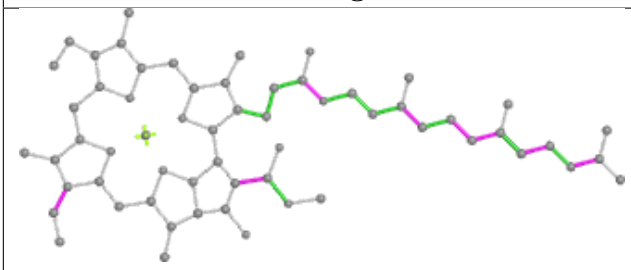
Ligand CLA B 836



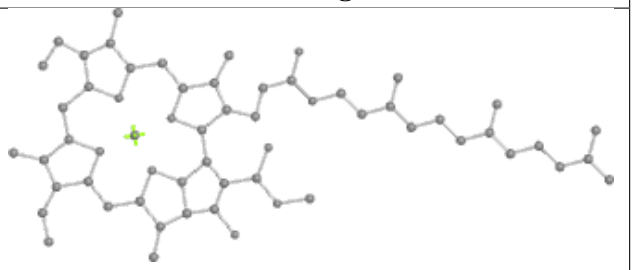
Bond lengths



Bond angles

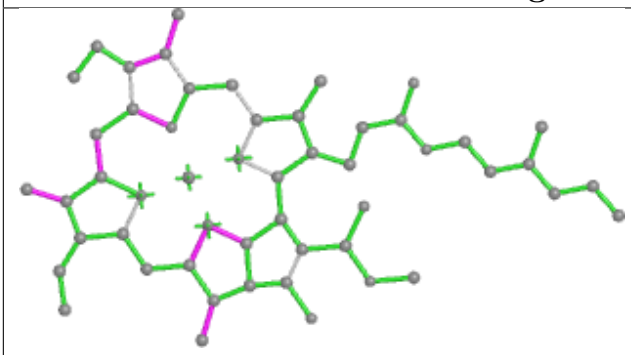


Torsions

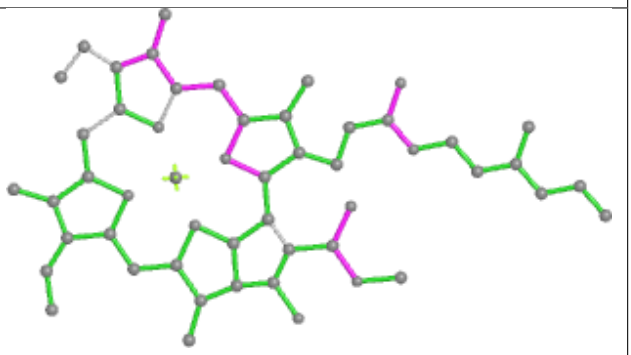


Rings

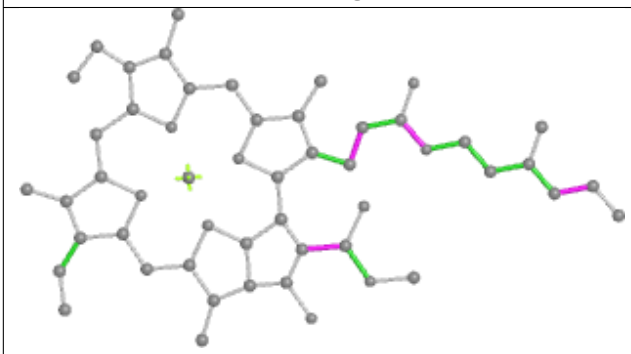
Ligand CLA 8 311



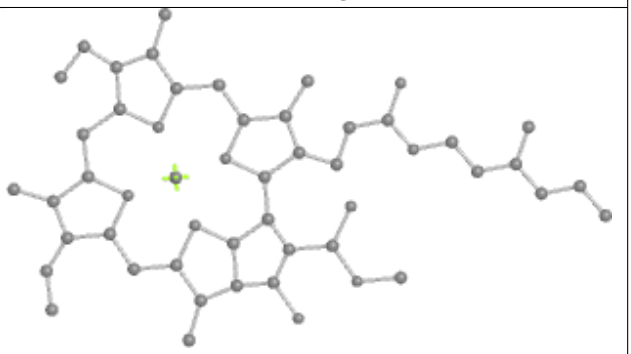
Bond lengths



Bond angles

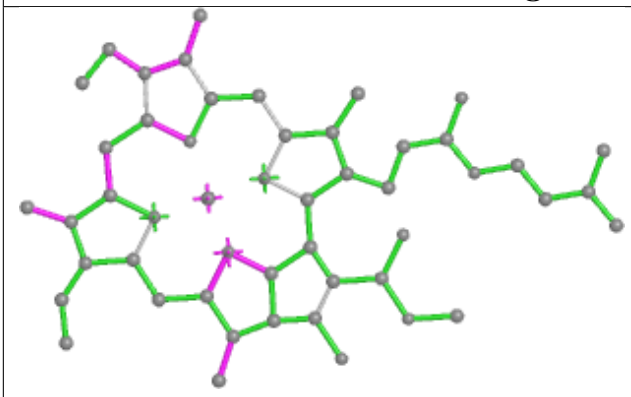


Torsions

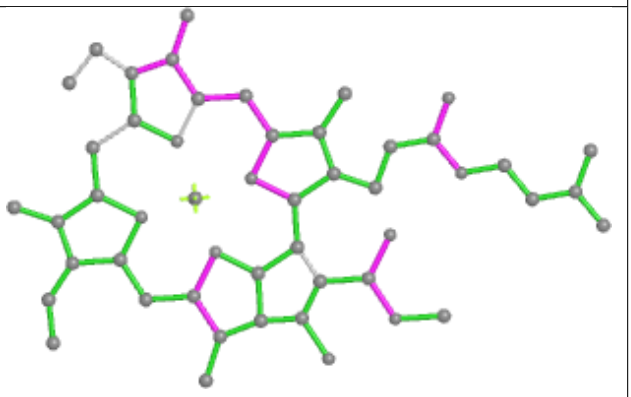


Rings

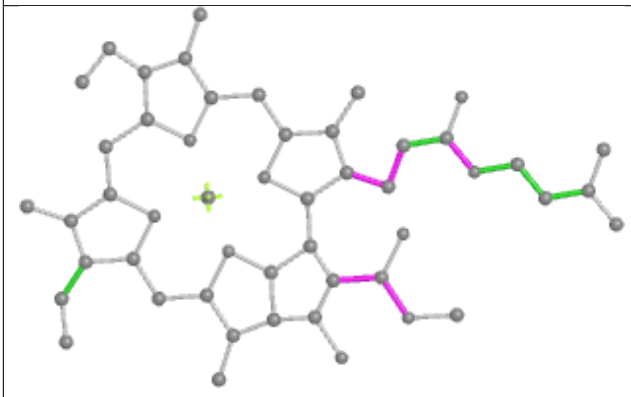
Ligand CLA B 831



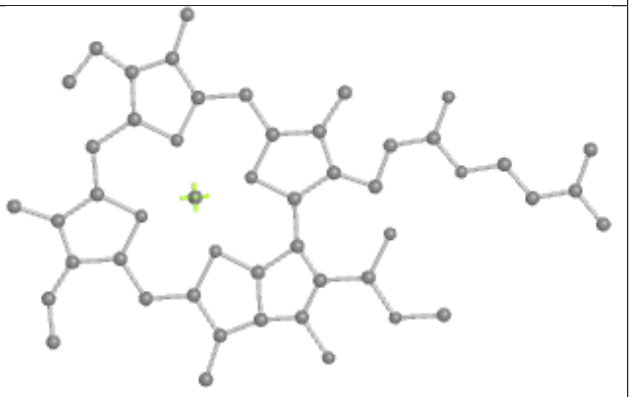
Bond lengths



Bond angles

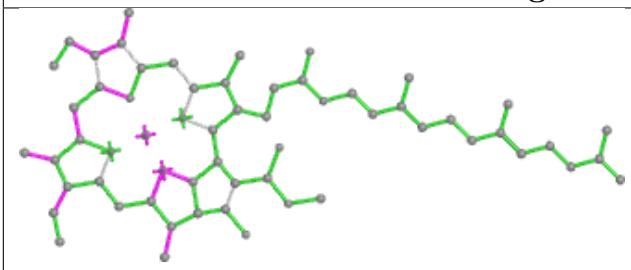


Torsions

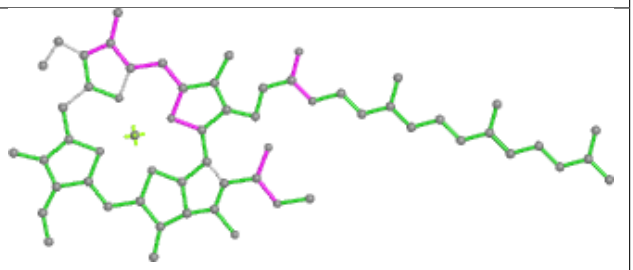


Rings

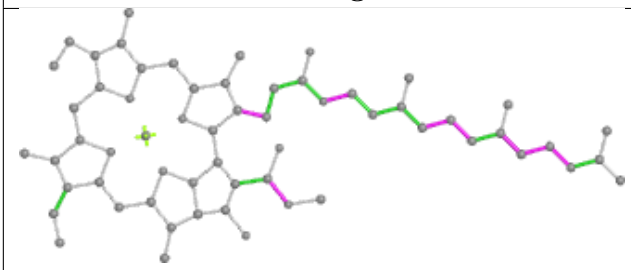
Ligand CLA 2 309



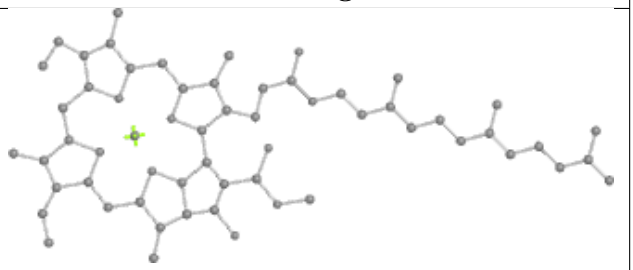
Bond lengths



Bond angles

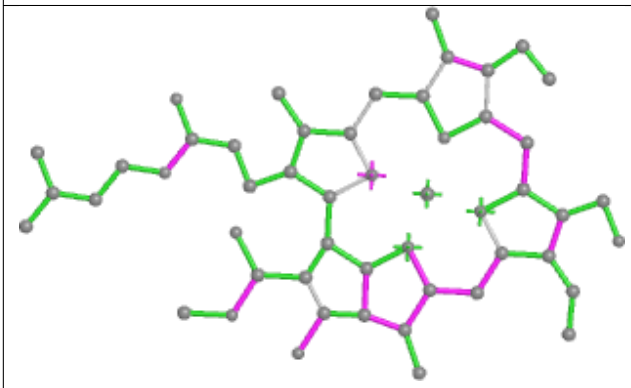


Torsions



Rings

Ligand CHL 6 308



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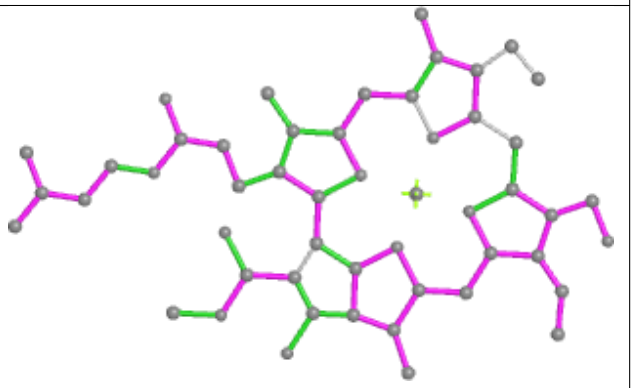
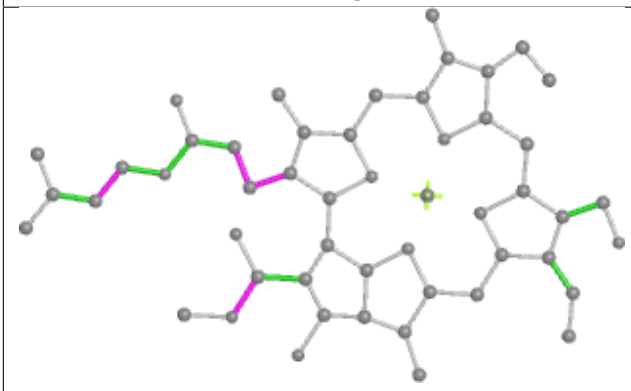
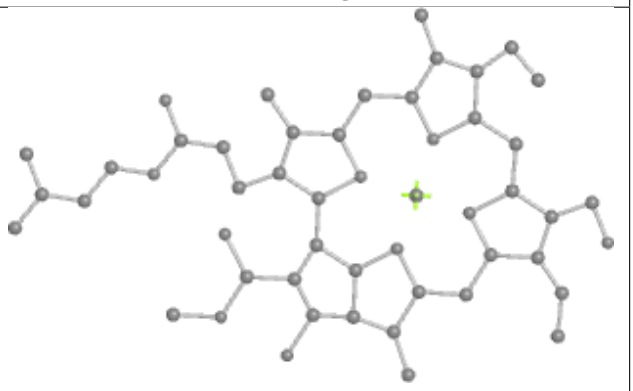


Bond angles

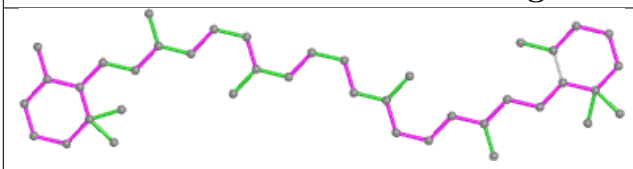


Torsions

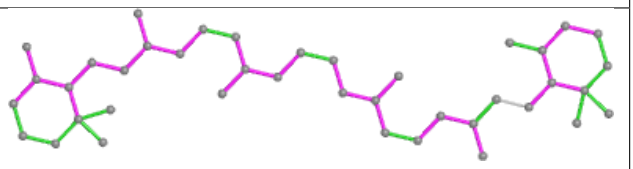


Rings

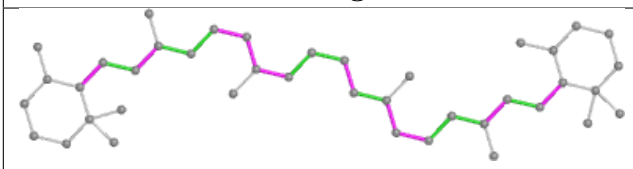
Ligand 8CT B 843



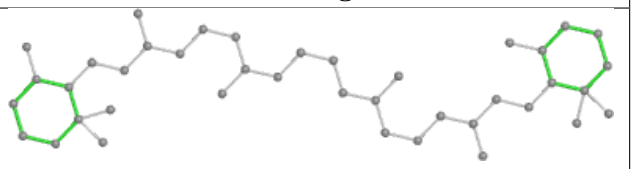
Bond lengths



Bond angles

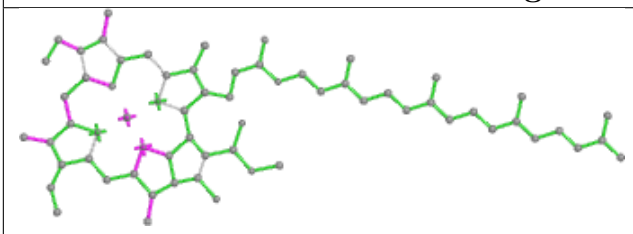


Torsions

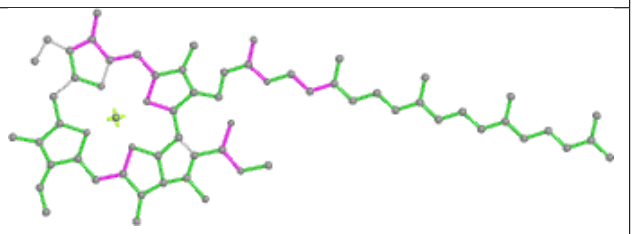


Rings

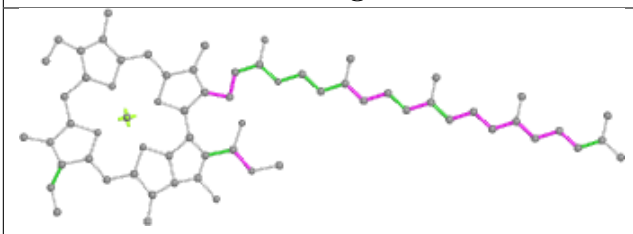
Ligand CLA B 837



Bond lengths



Bond angles



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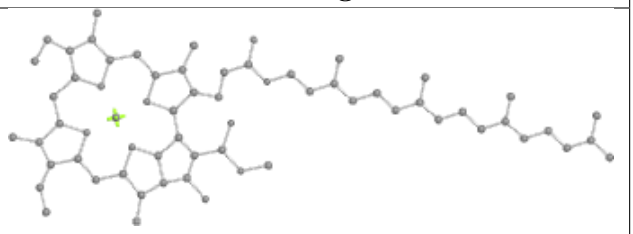
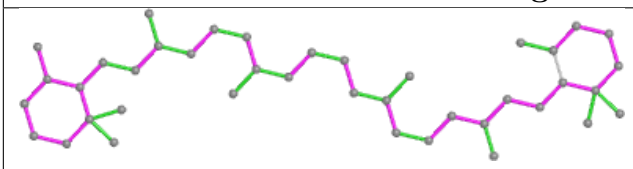
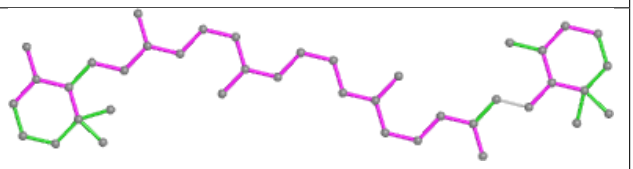


Rings

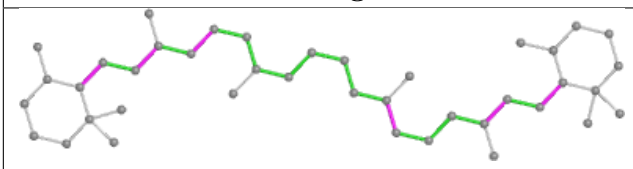
Ligand 8CT 7 321



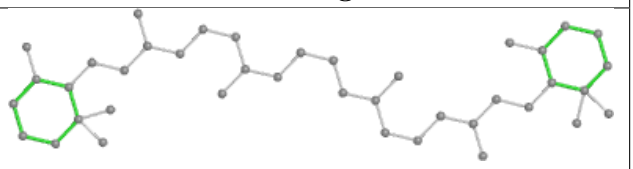
Bond lengths



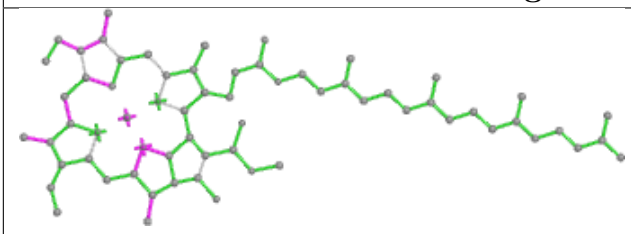
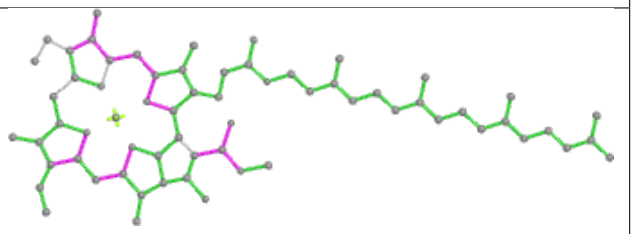
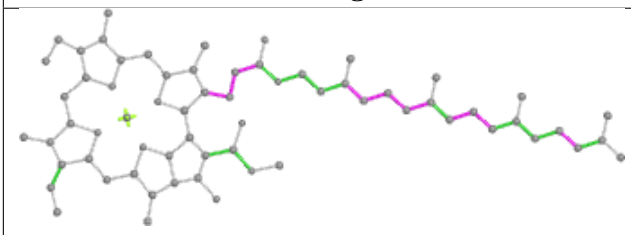
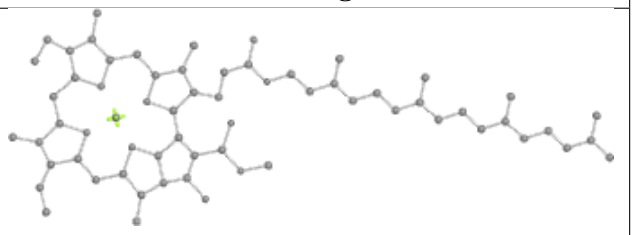
Bond angles

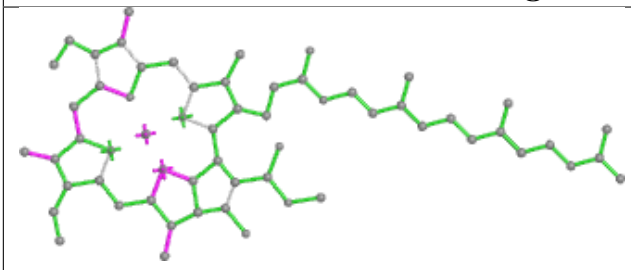
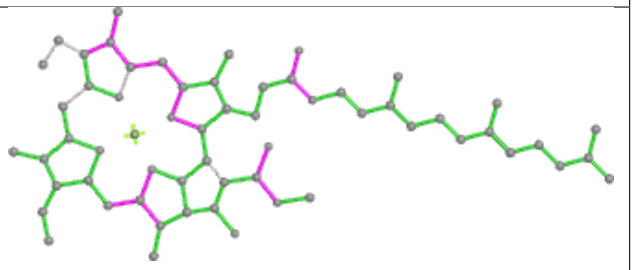
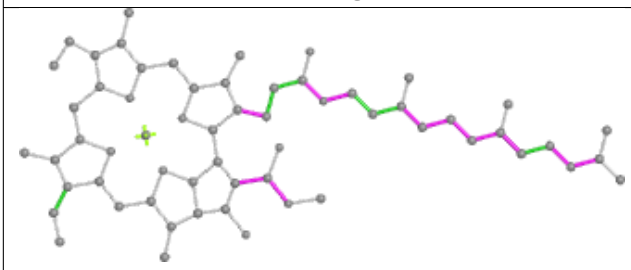
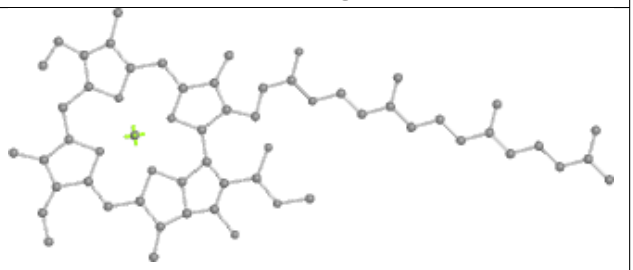


Torsions

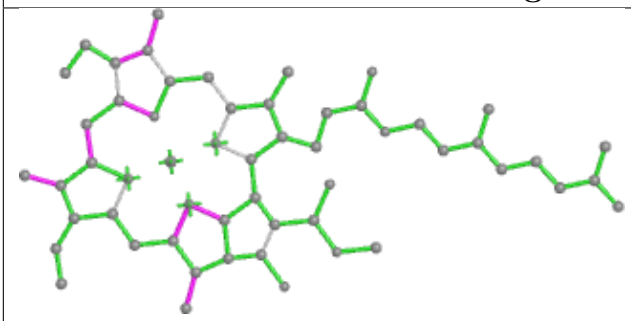


Rings

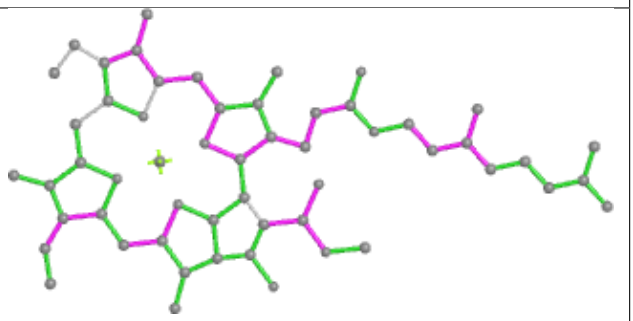
Ligand CLA B 832	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 819	
 Bond lengths	 Bond angles
 Torsions	 Rings

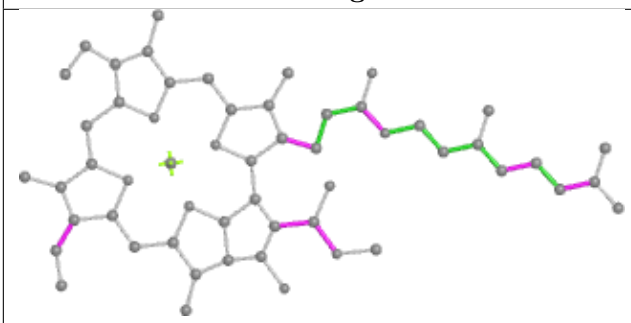
Ligand CLA B 850



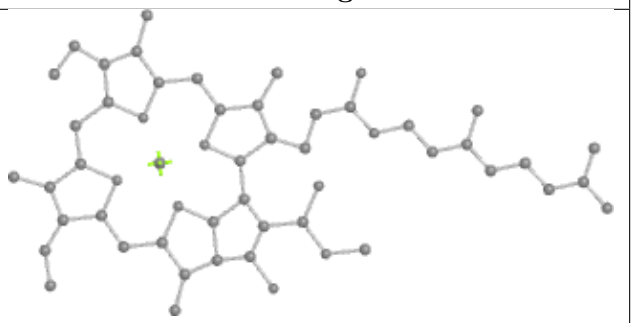
Bond lengths



Bond angles

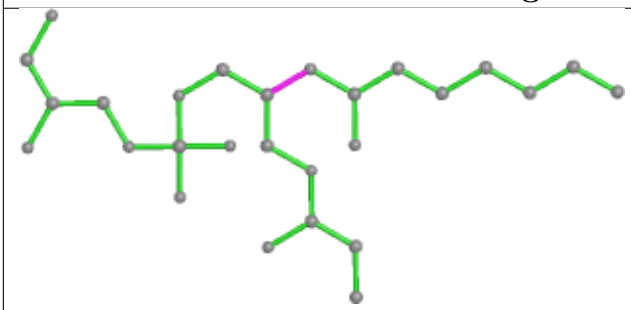


Torsions

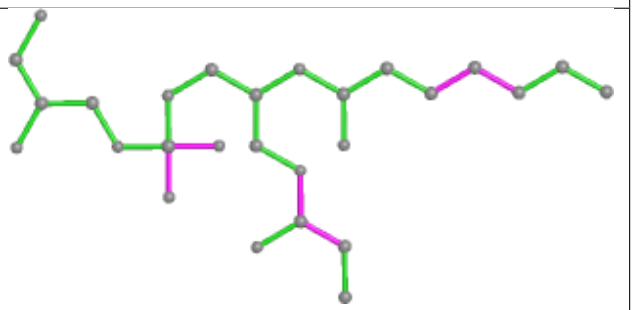


Rings

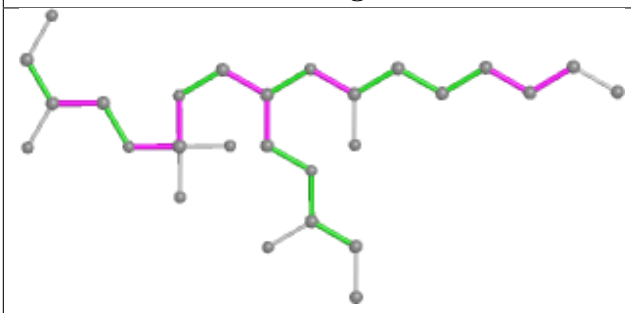
Ligand LHG A 845



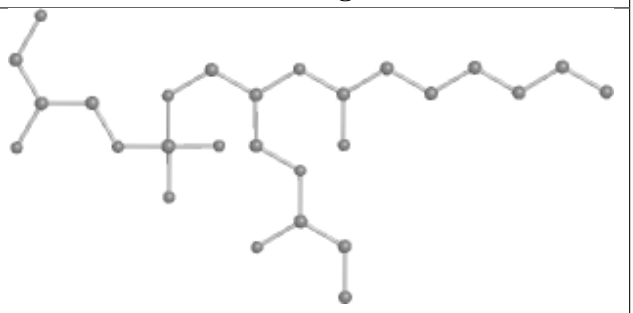
Bond lengths



Bond angles

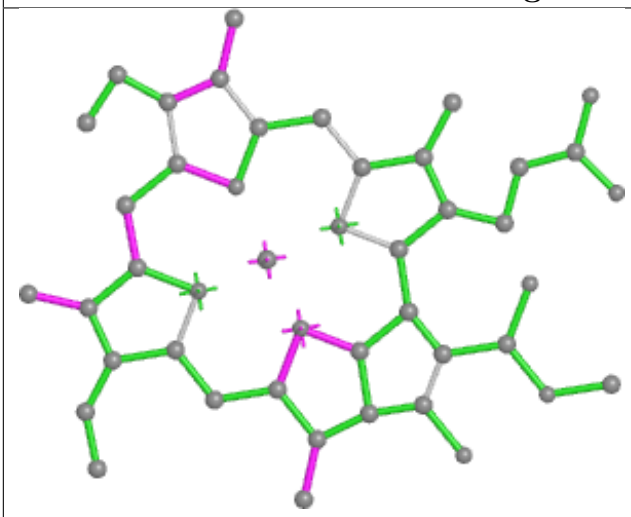


Torsions

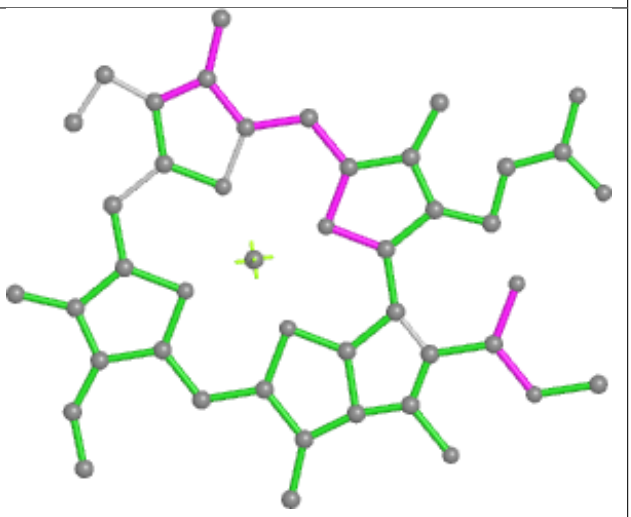


Rings

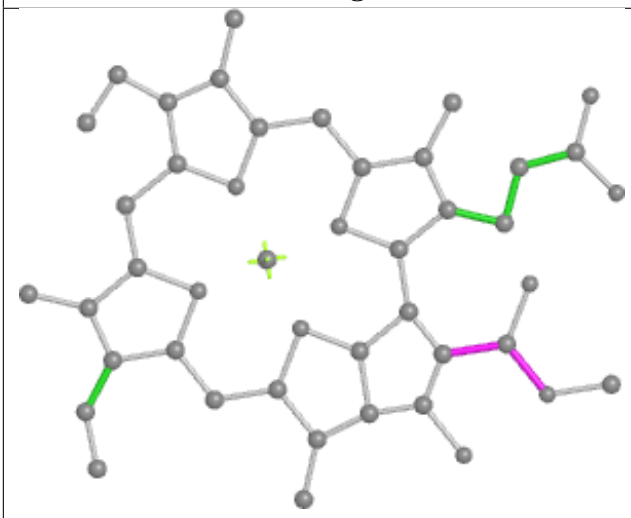
Ligand CLA A 816



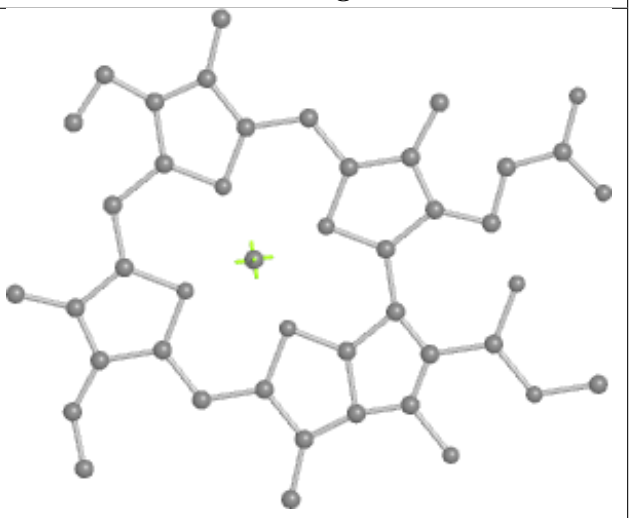
Bond lengths



Bond angles

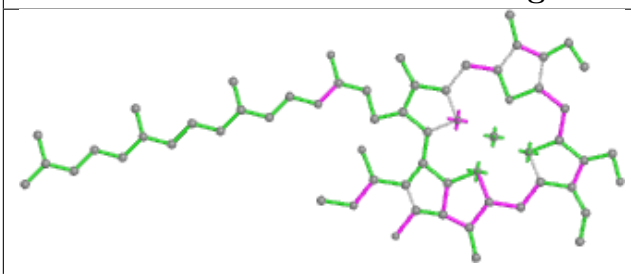


Torsions

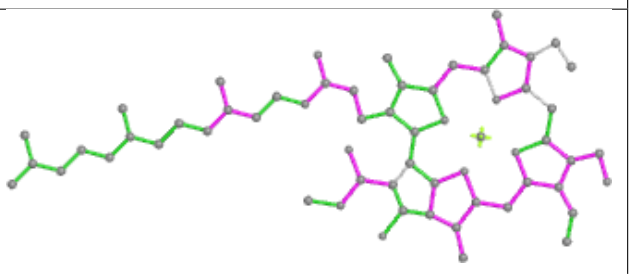


Rings

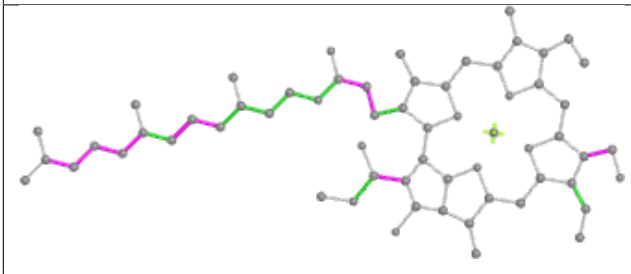
Ligand CHL 6 302



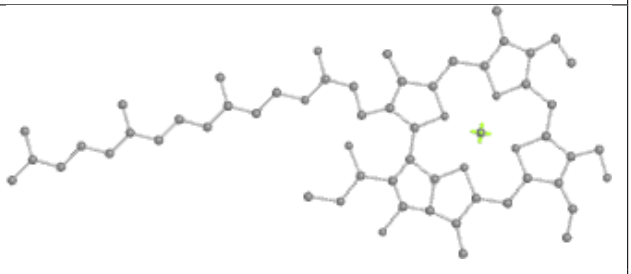
Bond lengths



Bond angles

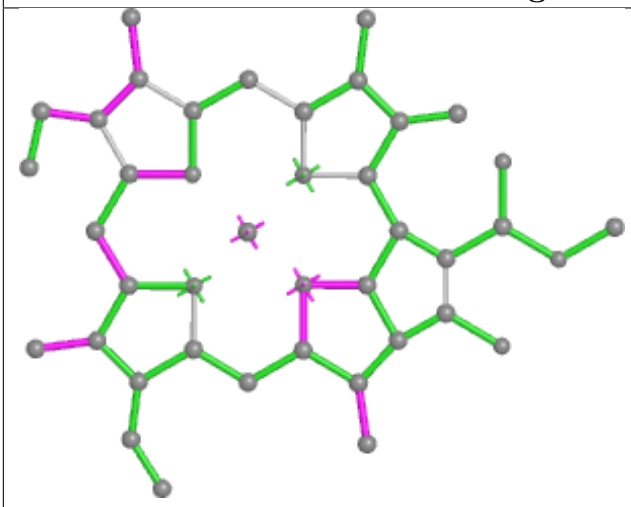


Torsions

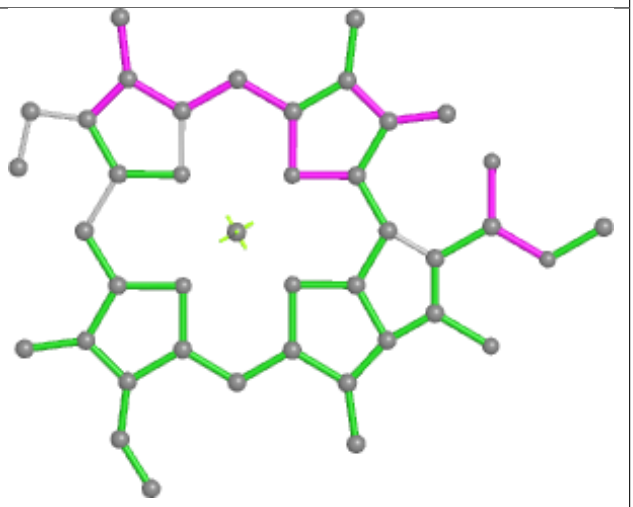


Rings

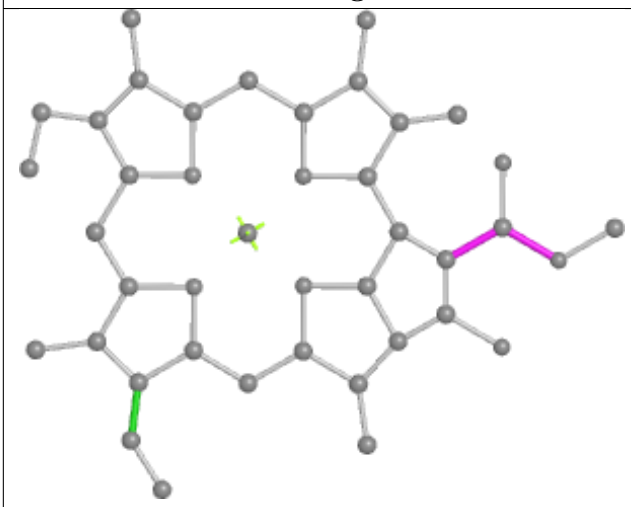
Ligand CLA 5 310



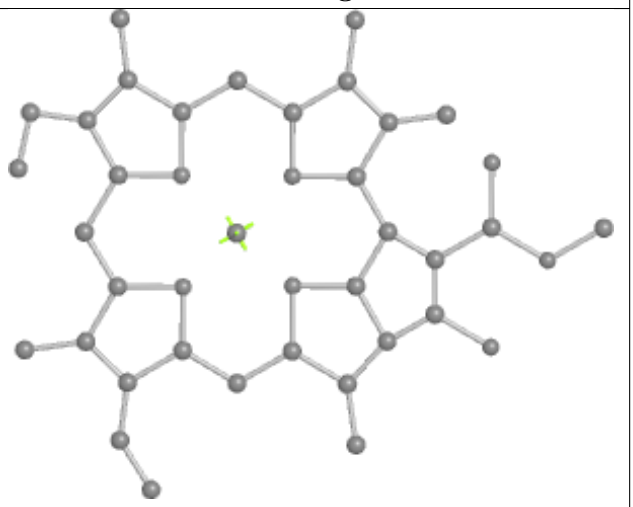
Bond lengths



Bond angles

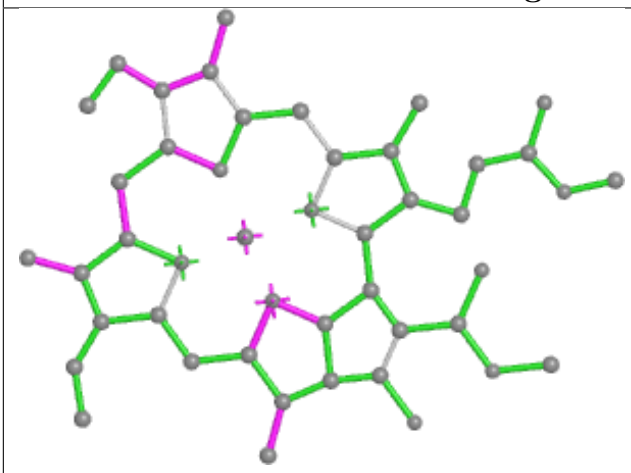


Torsions

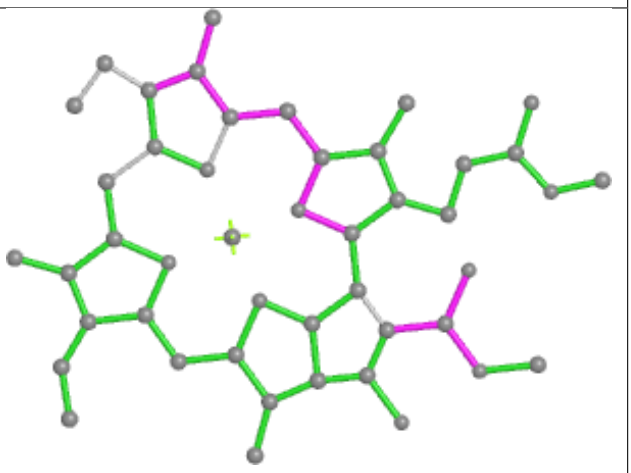


Rings

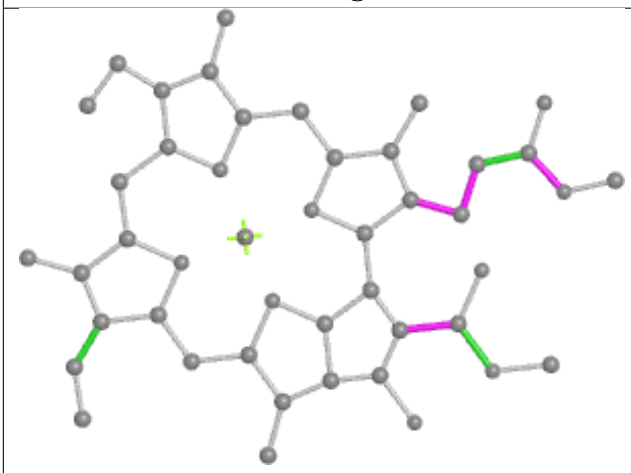
Ligand CLA B 822



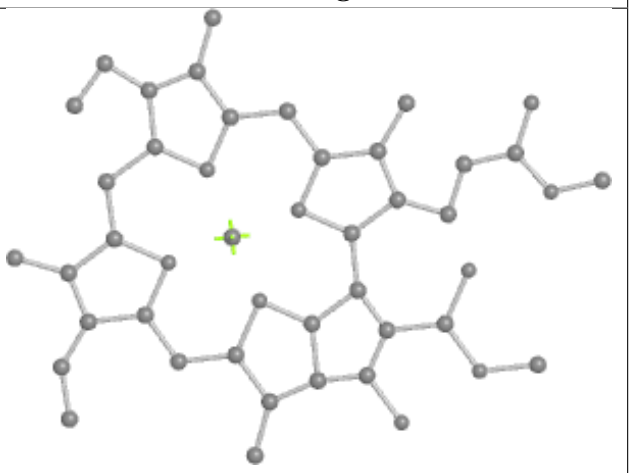
Bond lengths



Bond angles

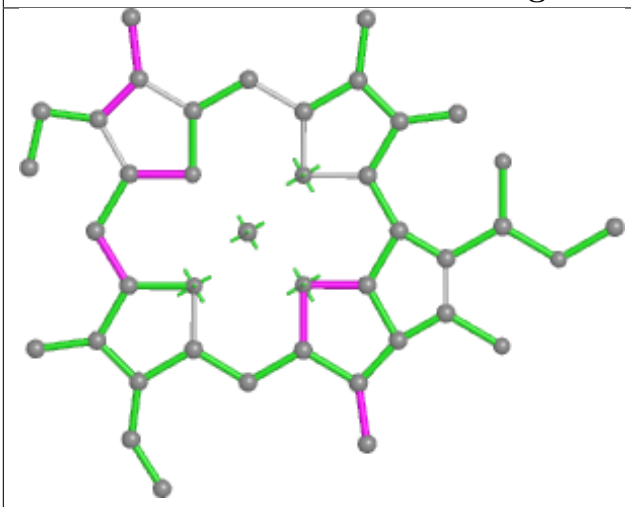


Torsions

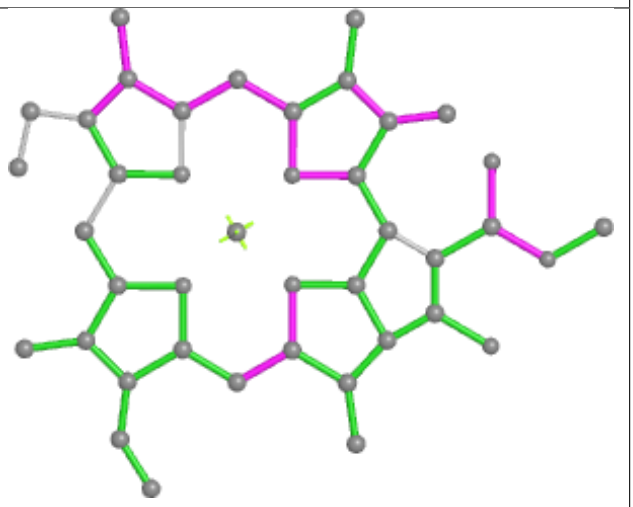


Rings

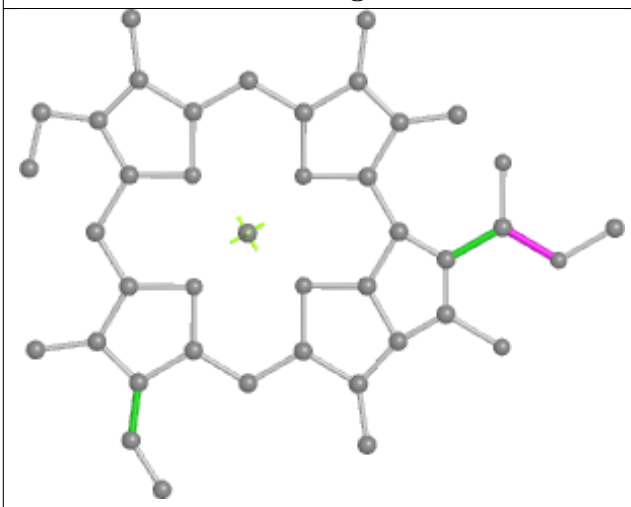
Ligand CLA 0 309



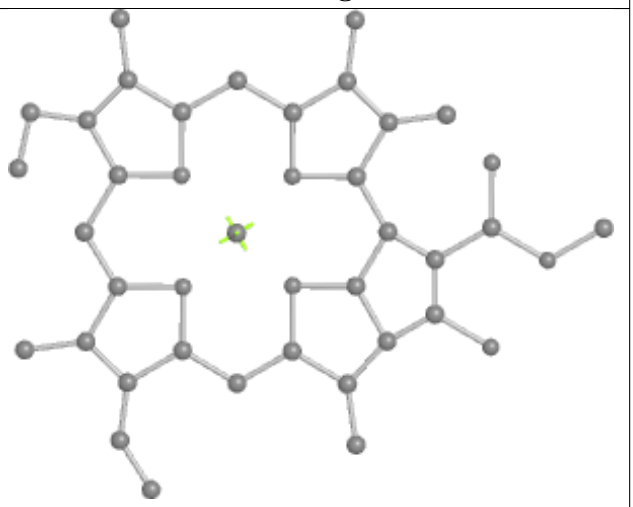
Bond lengths



Bond angles

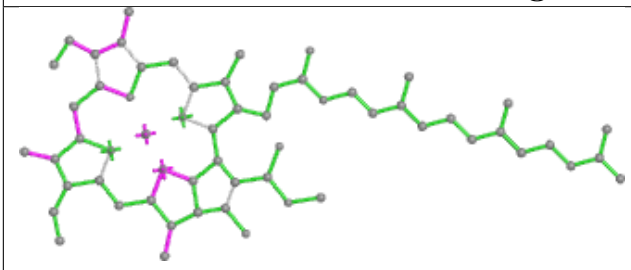


Torsions

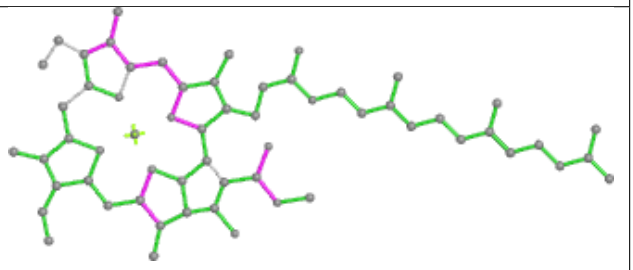


Rings

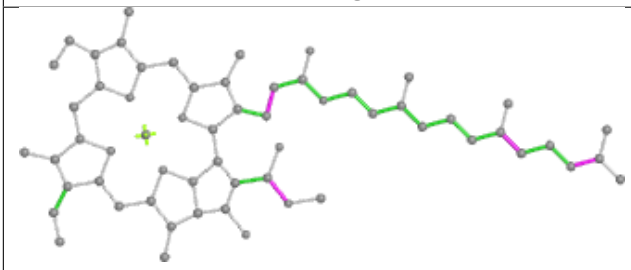
Ligand CLA 8 302



Bond lengths



Bond angles



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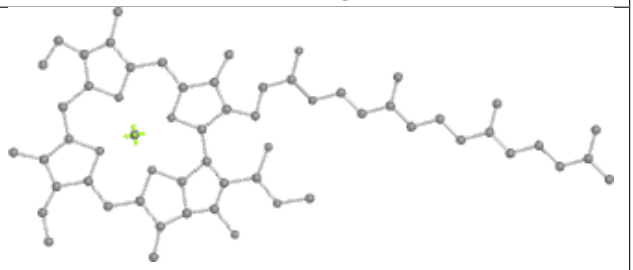
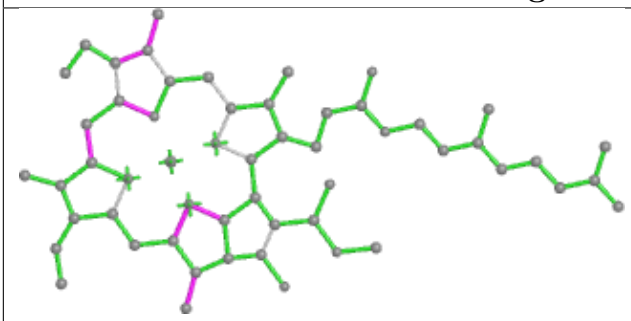


Rings

Ligand CLA 0 312



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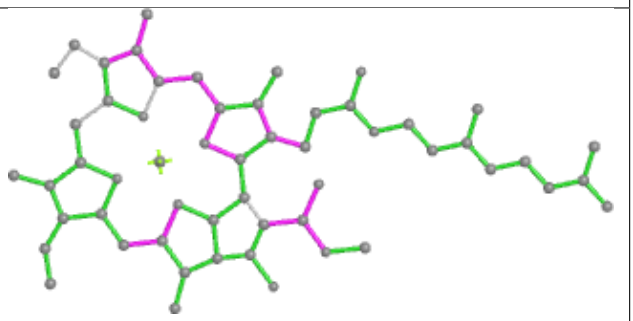
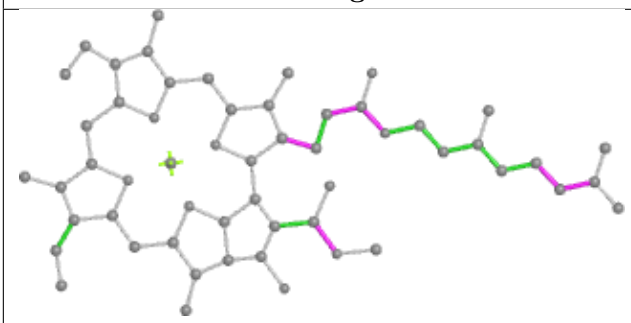
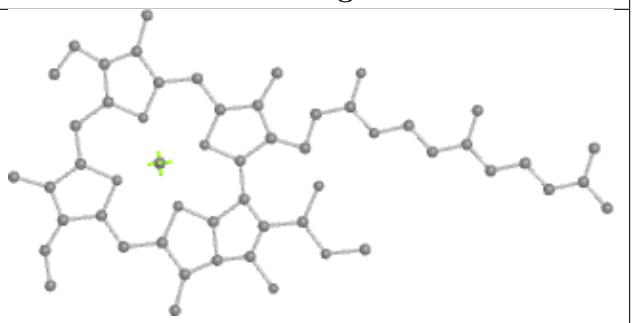


Bond angles

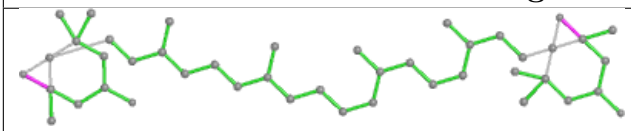


Torsions



Rings

Ligand XAT 2 315



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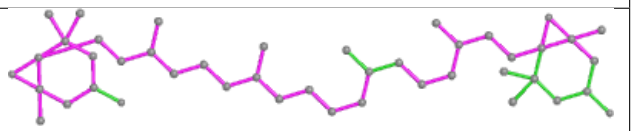
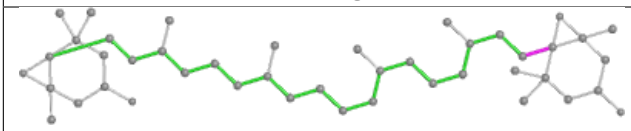
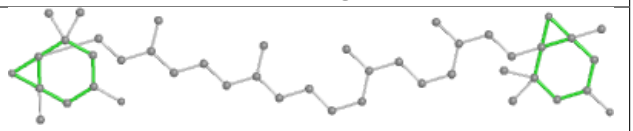


Bond angles

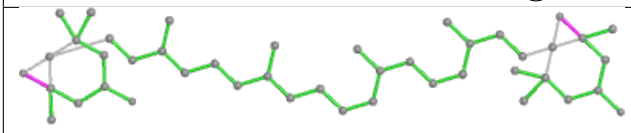


Torsions

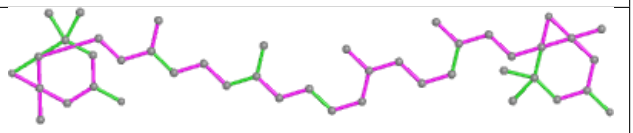


Rings

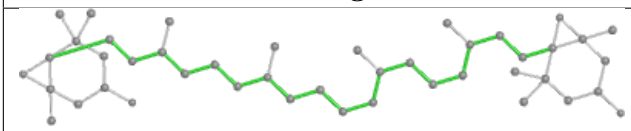
Ligand XAT 9 315



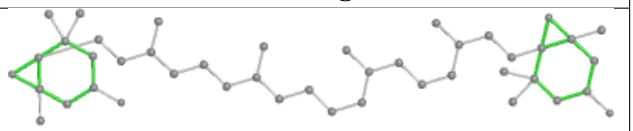
Bond lengths



Bond angles

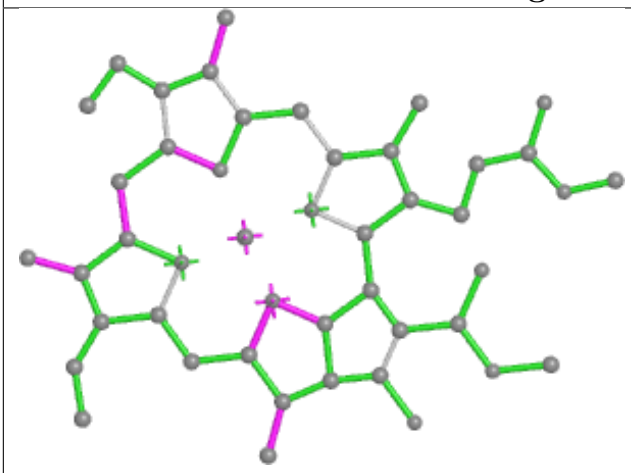


Torsions

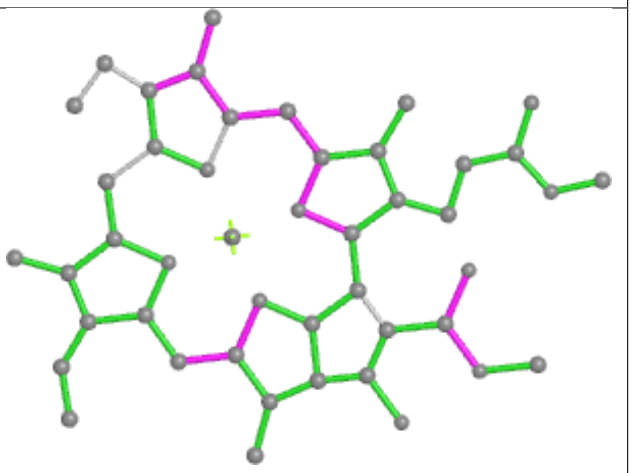


Rings

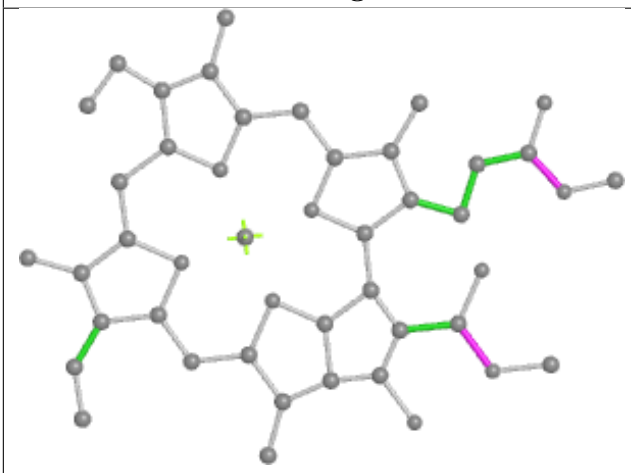
Ligand CLA 7 315



Bond lengths



Bond angles



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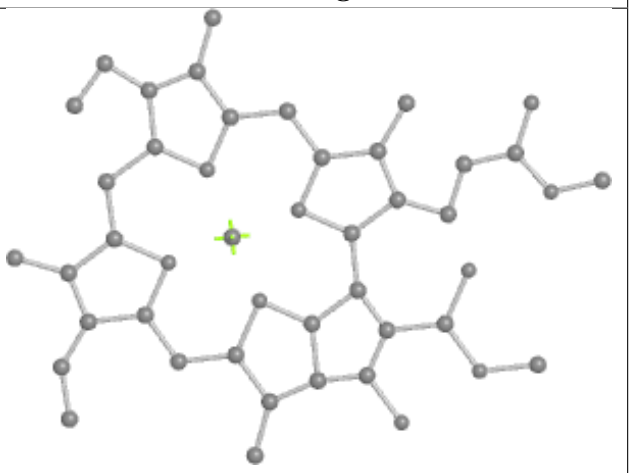
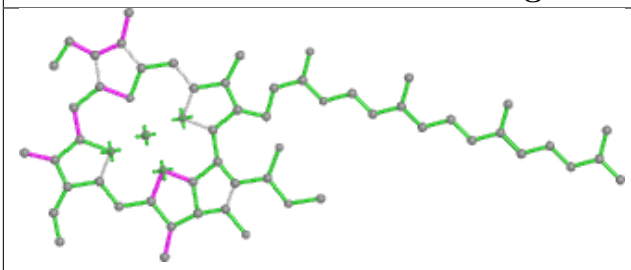
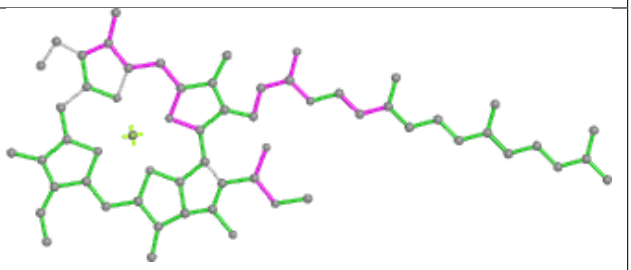


Rings

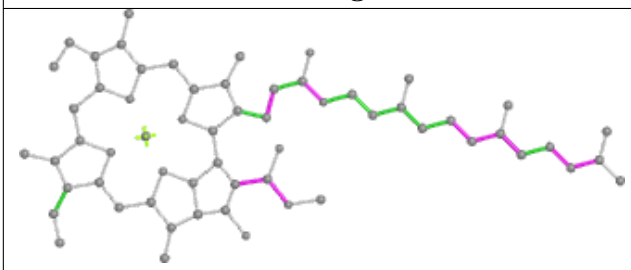
Ligand CLA B 824



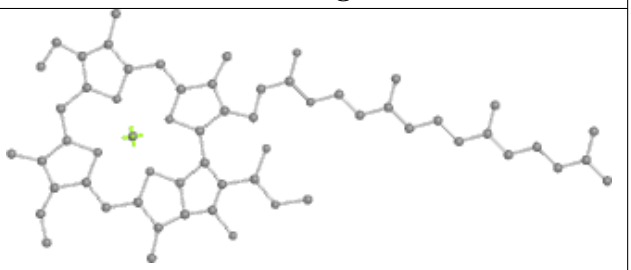
Bond lengths



Bond angles

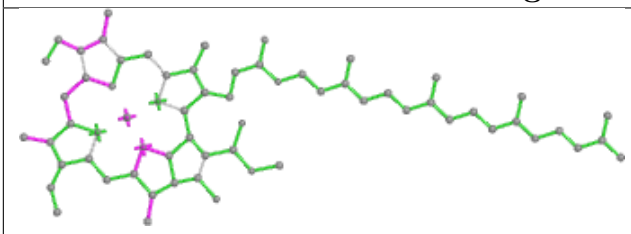


Torsions

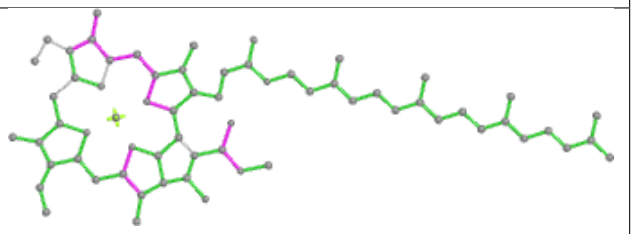


Rings

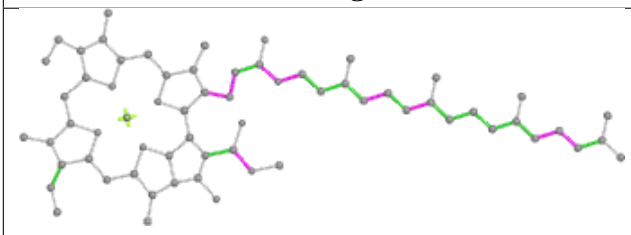
Ligand CLA A 841



Bond lengths



Bond angles



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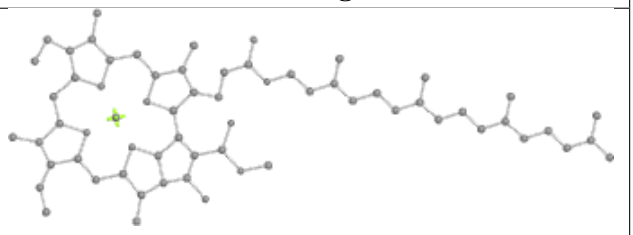
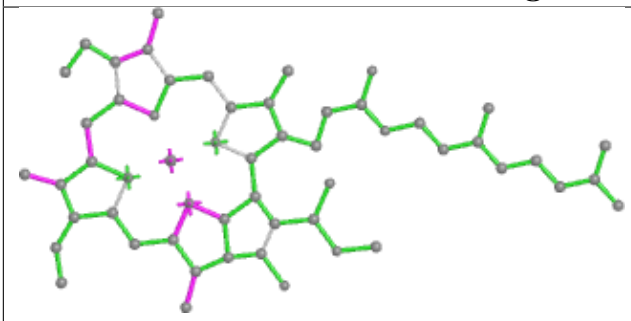
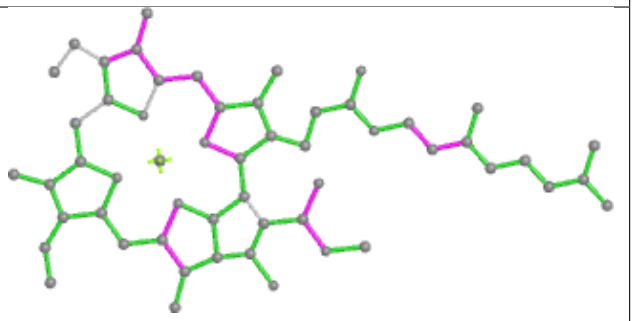


Rings

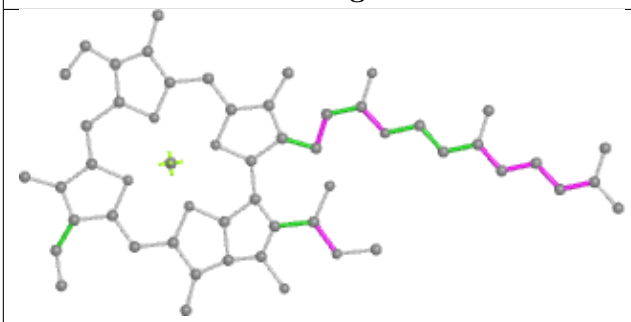
Ligand CLA B 817



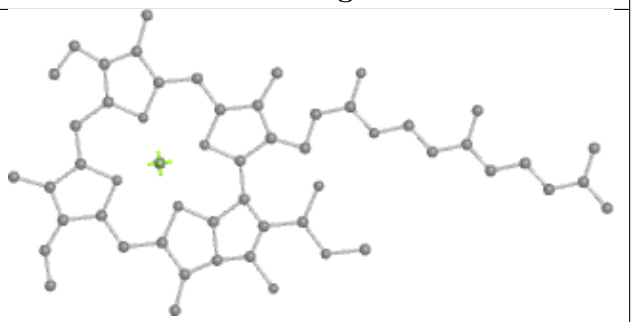
Bond lengths



Bond angles

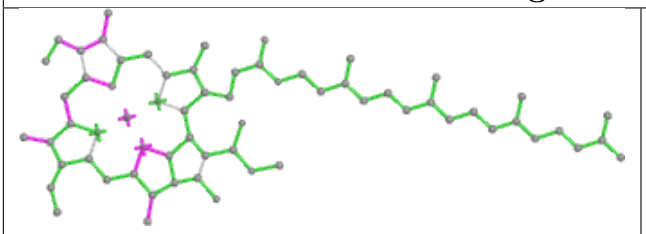


Torsions

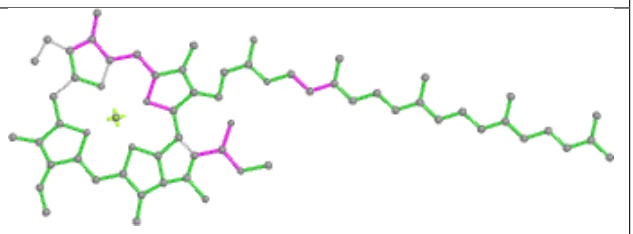


Rings

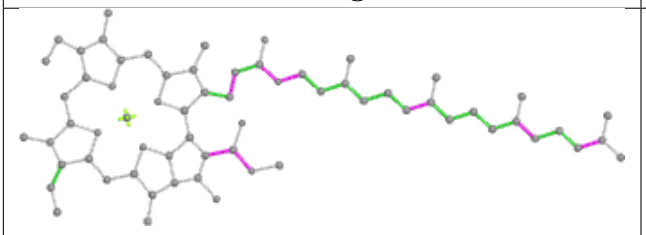
Ligand CLA 9 303



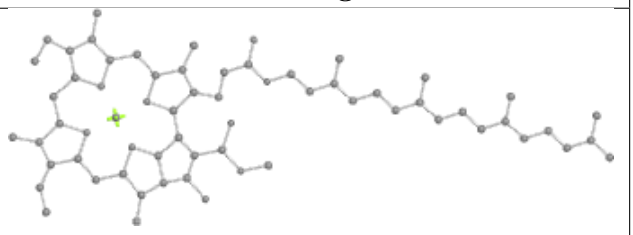
Bond lengths



Bond angles

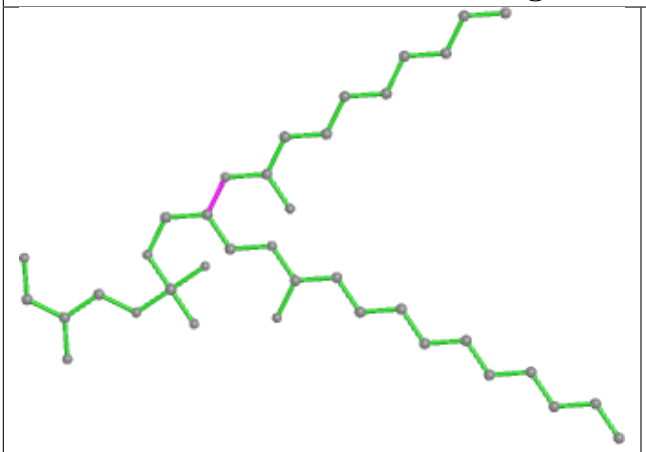


Torsions

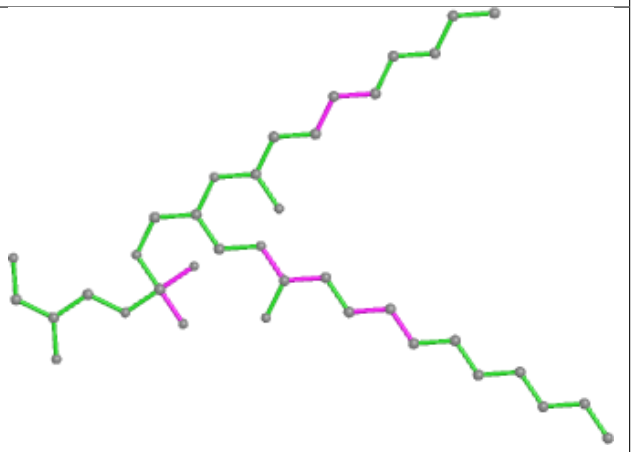


Rings

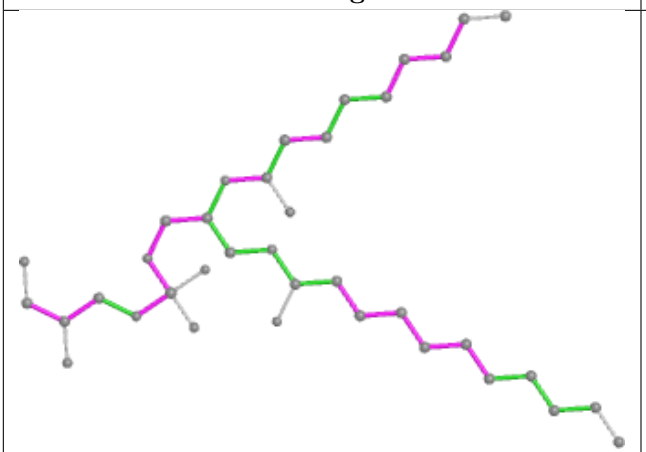
Ligand LHG 6 322



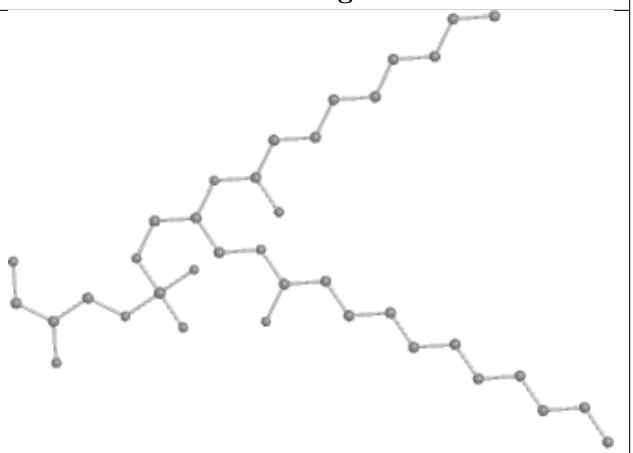
Bond lengths



Bond angles

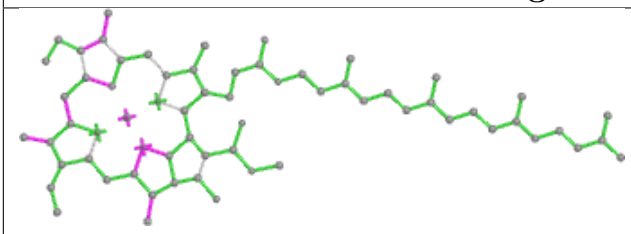


Torsions

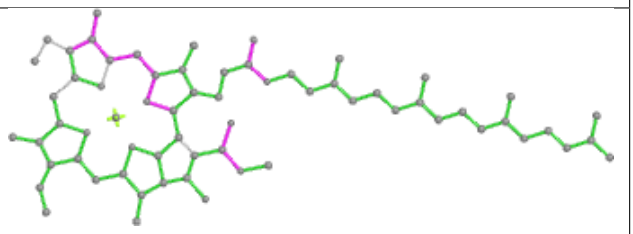


Rings

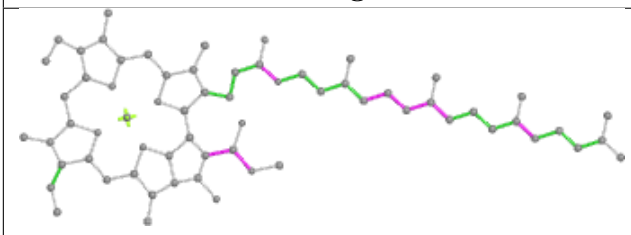
Ligand CLA 6 315



Bond lengths



Bond angles



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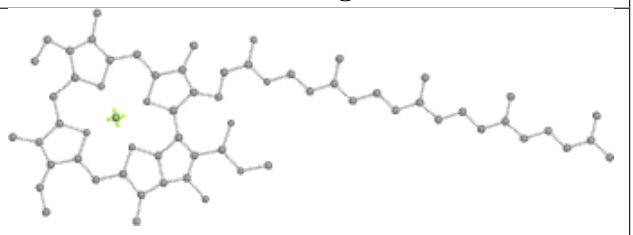
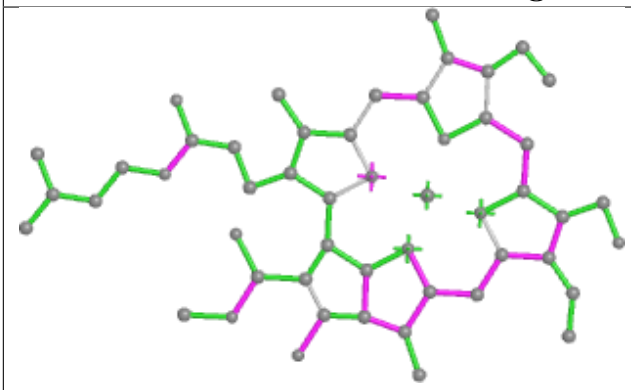


Rings

Ligand CHL 4 306



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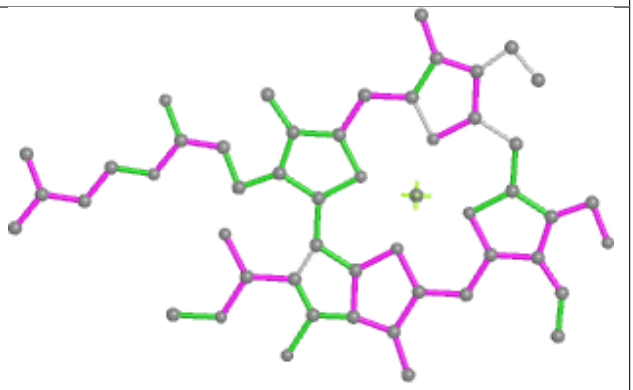
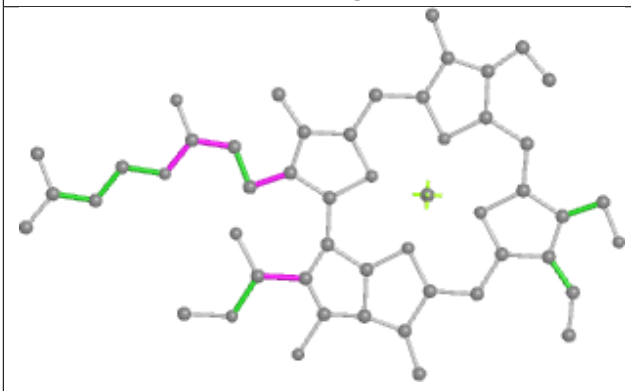
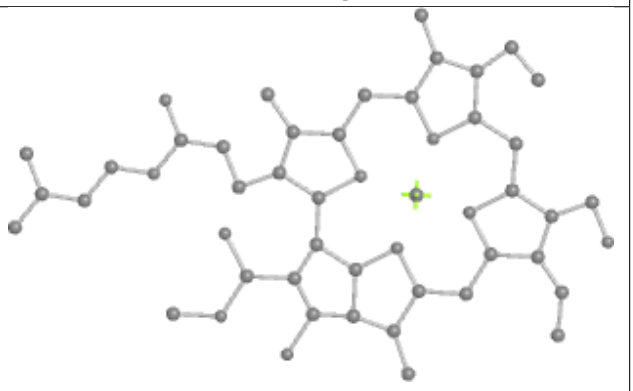


Bond angles

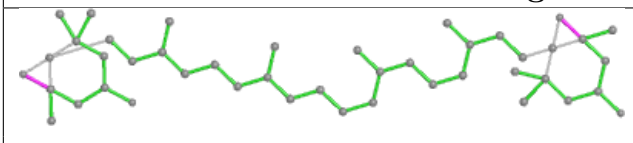


Torsions

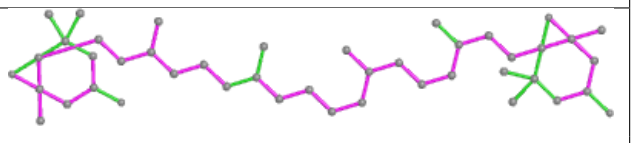


Rings

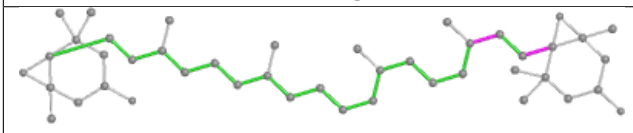
Ligand XAT 2 316



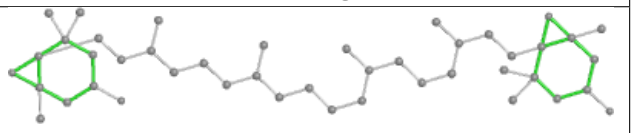
Bond lengths



Bond angles

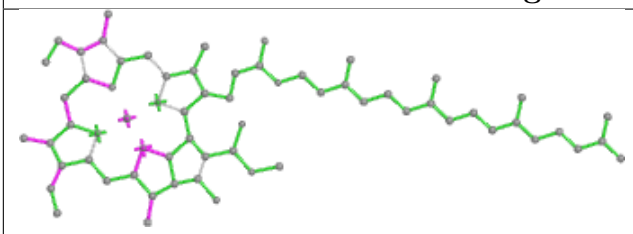


Torsions

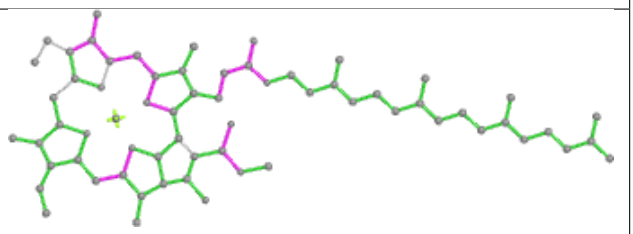


Rings

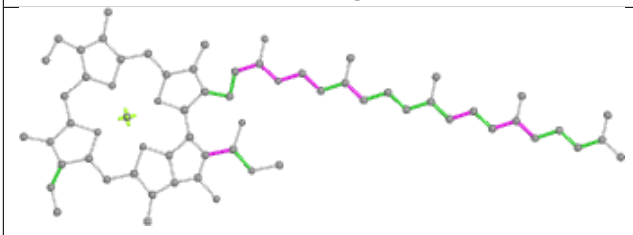
Ligand CLA A 805



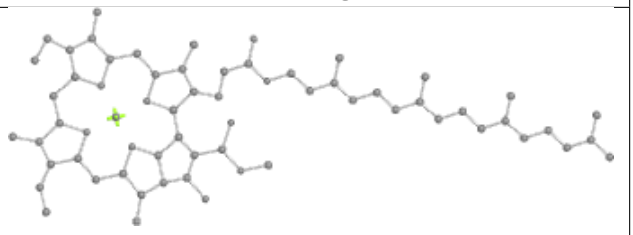
Bond lengths



Bond angles

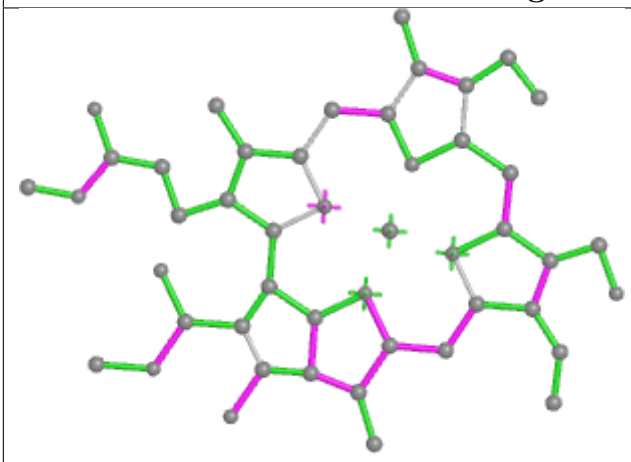


Torsions

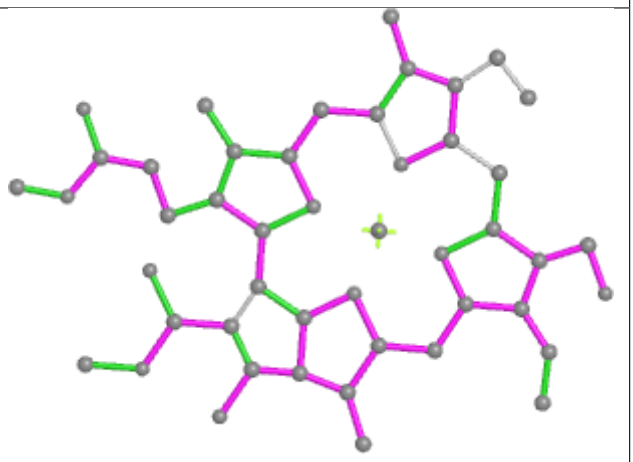


Rings

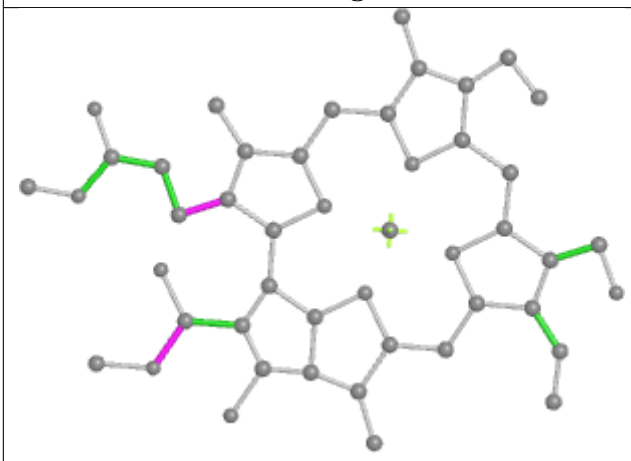
Ligand CHL 3 306



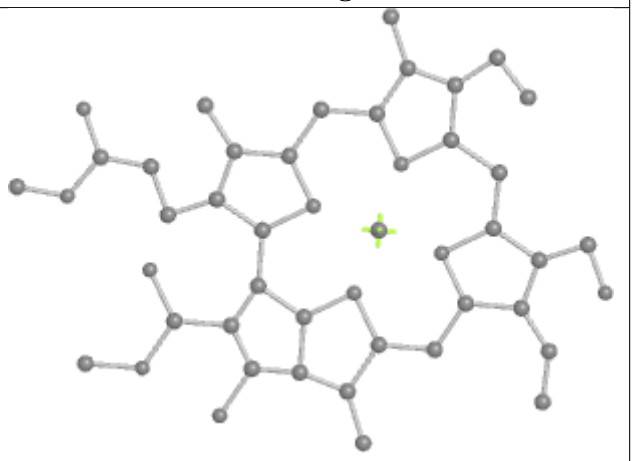
Bond lengths



Bond angles

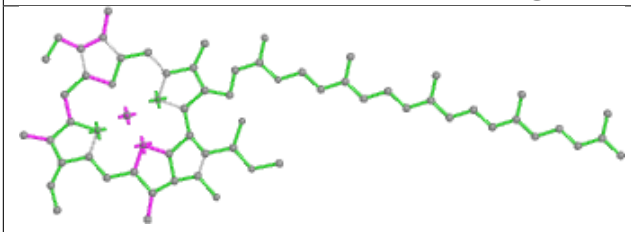


Torsions

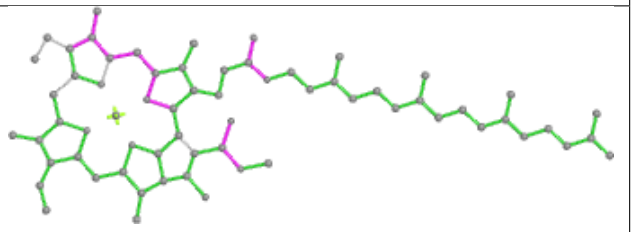


Rings

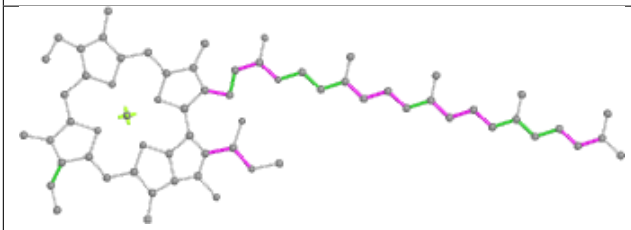
Ligand CLA 6 311



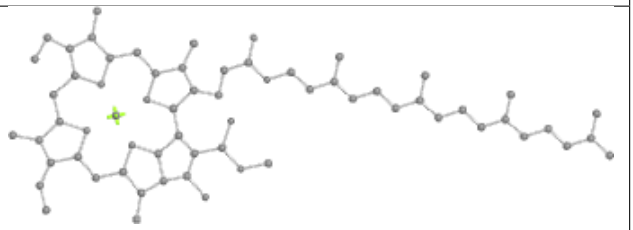
Bond lengths



Bond angles

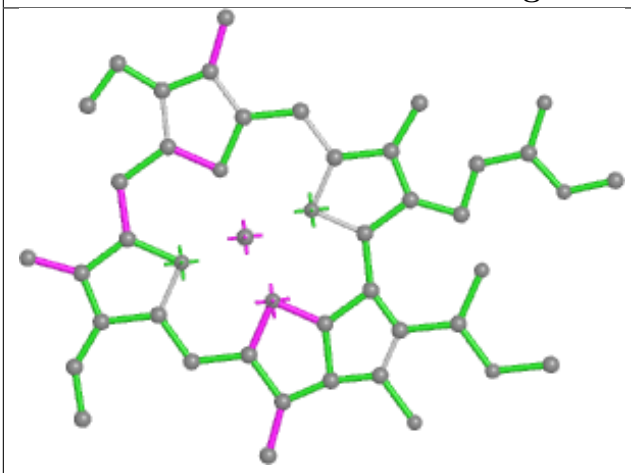


Torsions



Rings

Ligand CLA K 102



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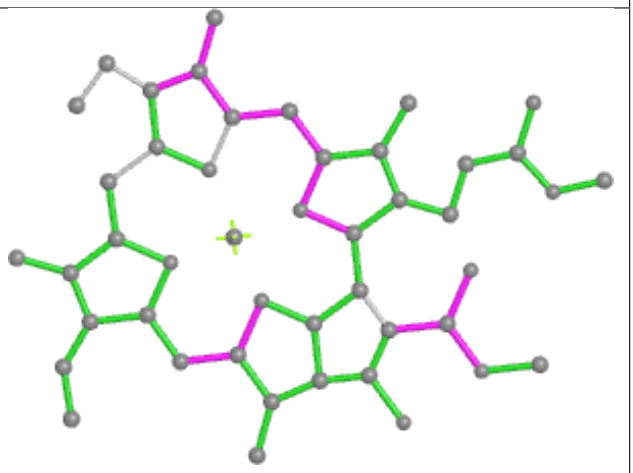
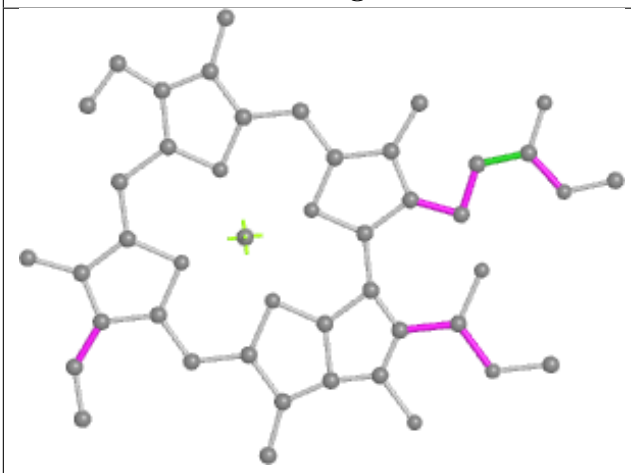
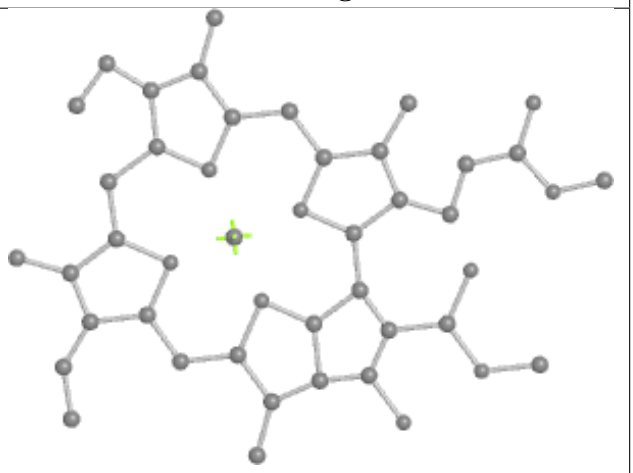


Bond angles

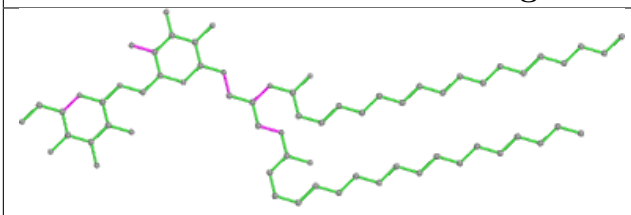


Torsions



Rings

Ligand DGD B 849



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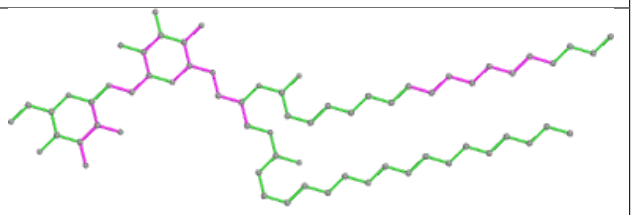
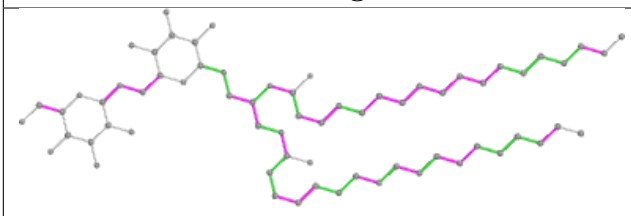
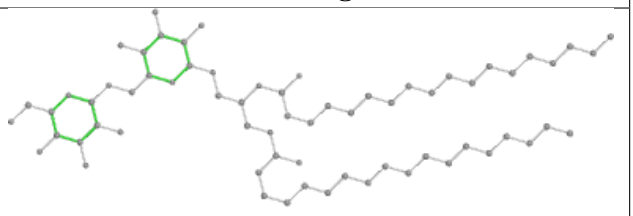


Bond angles

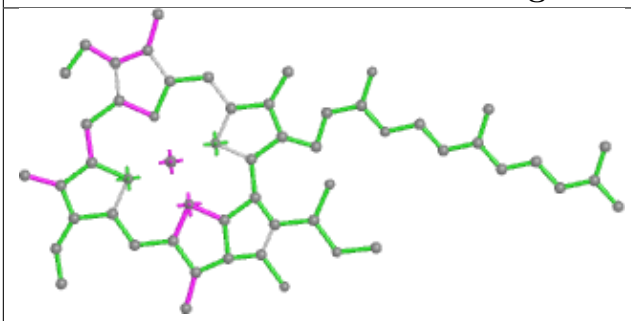


Torsions

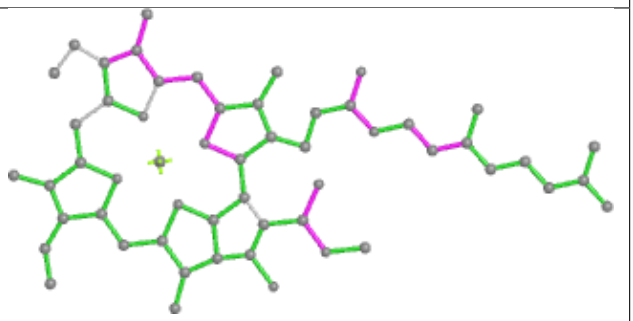


Rings

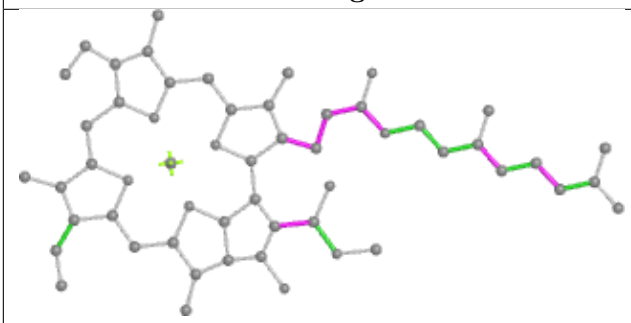
Ligand CLA 3 311



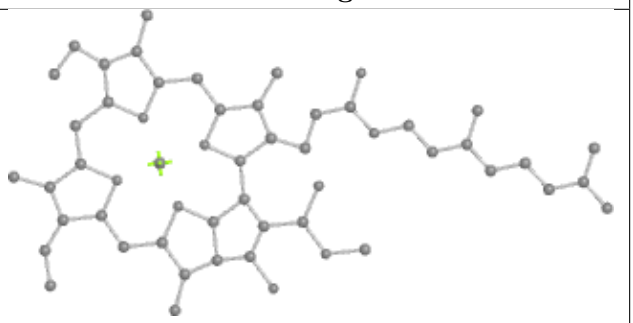
Bond lengths



Bond angles

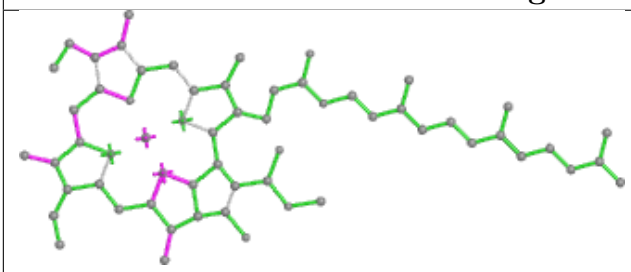


Torsions



Rings

Ligand CLA 4 302



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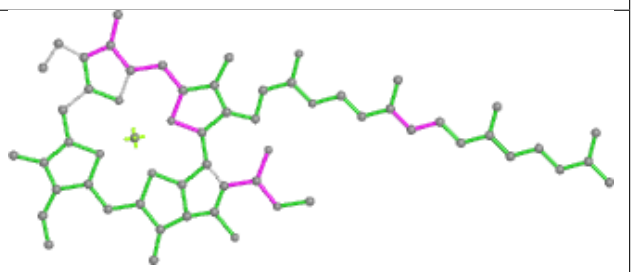
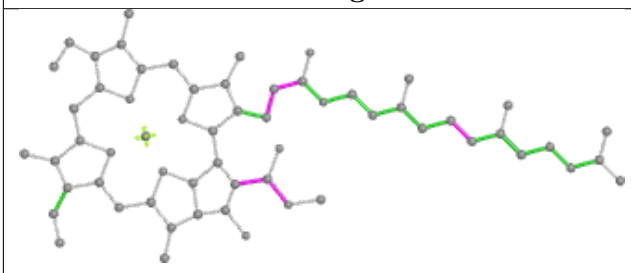


Bond angles



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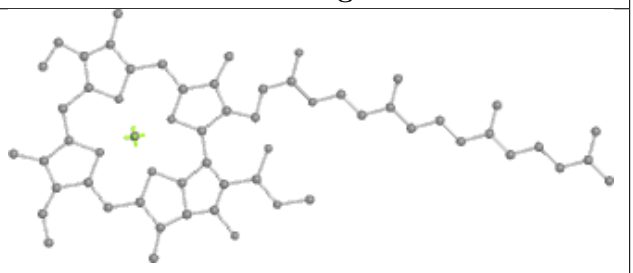
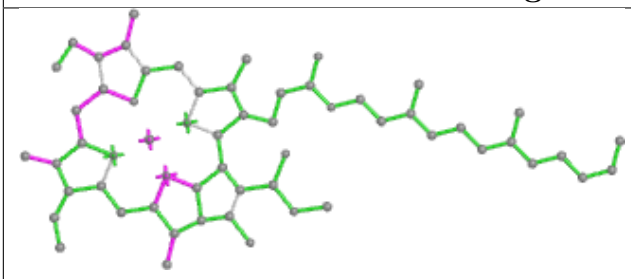


Rings

Ligand CLA B 818



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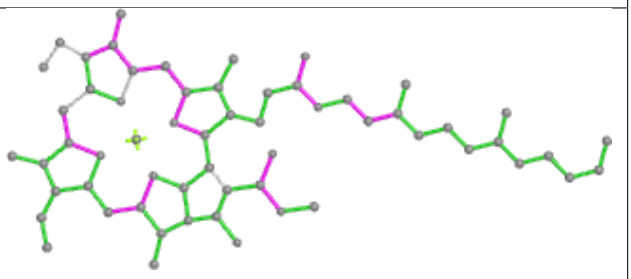
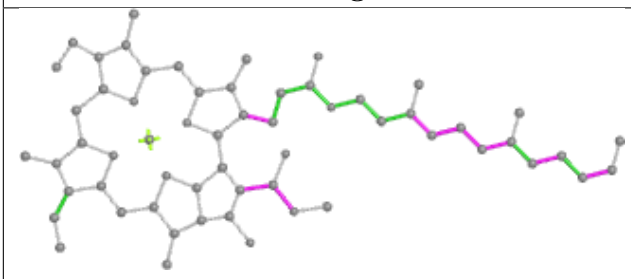
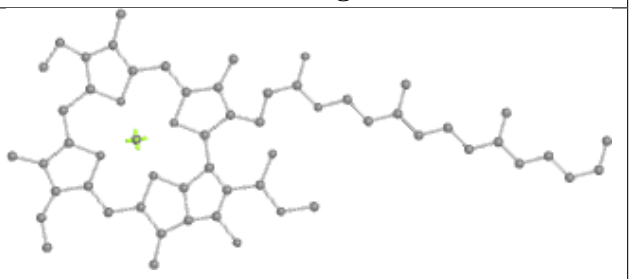


Bond angles

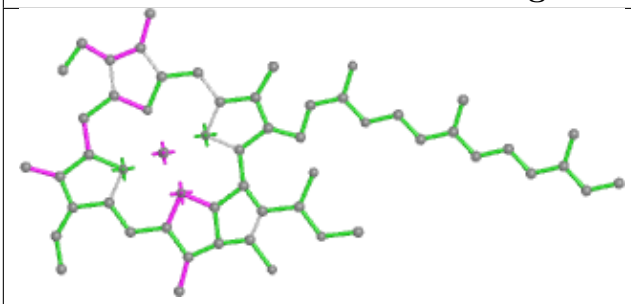


Torsions



Rings

Ligand CLA 8 312



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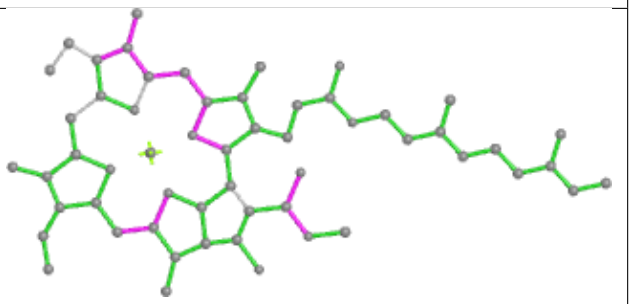
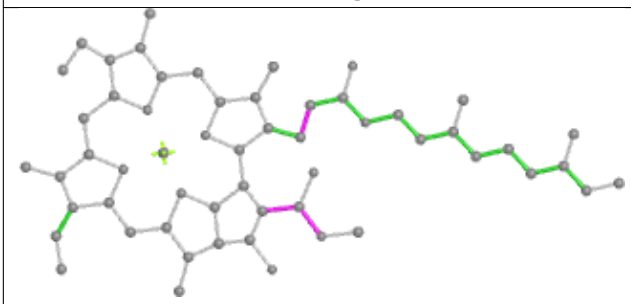


Bond angles



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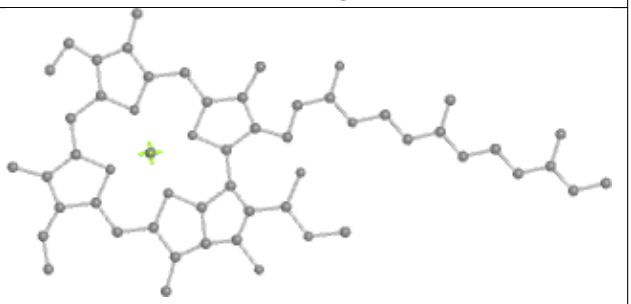
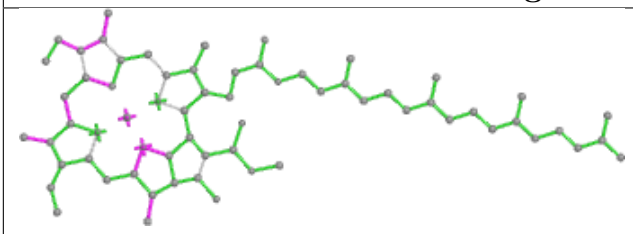
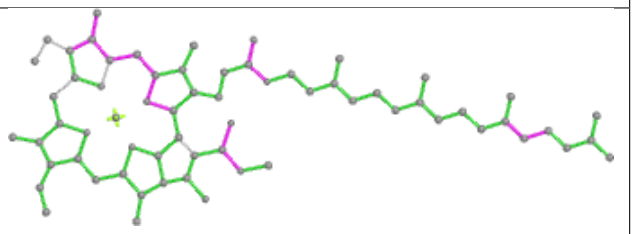


Rings

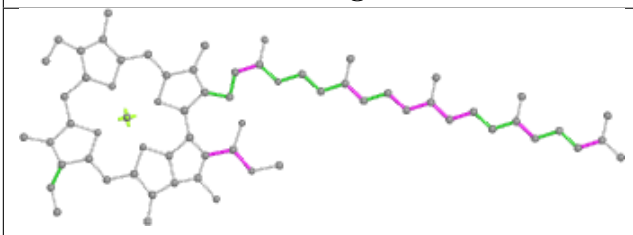
Ligand CLA B 805



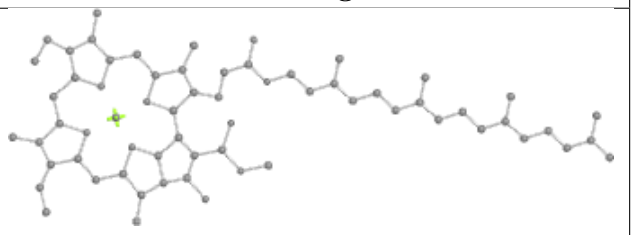
Bond lengths



Bond angles

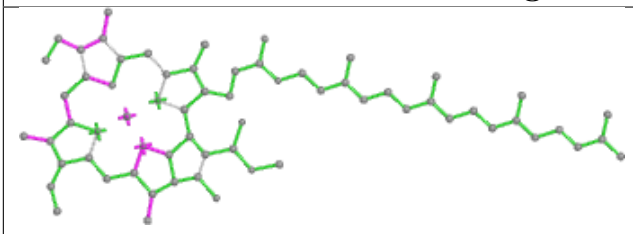


Torsions

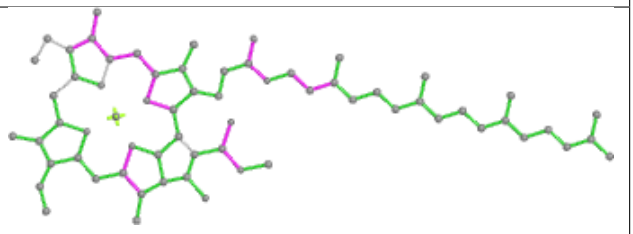


Rings

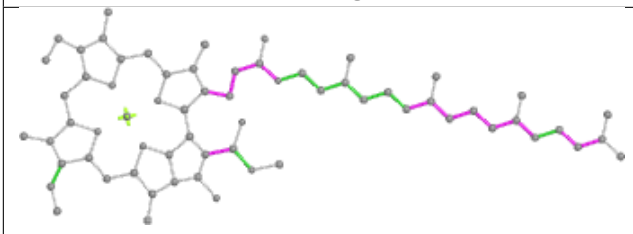
Ligand CLA A 806



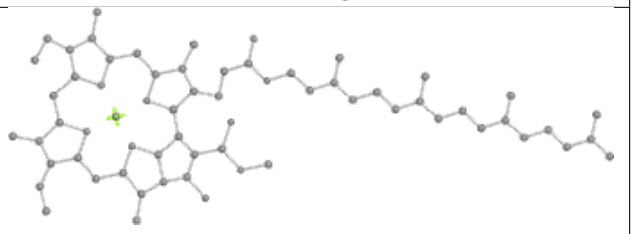
Bond lengths



Bond angles

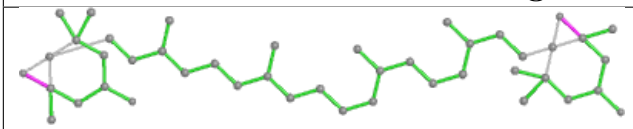


Torsions

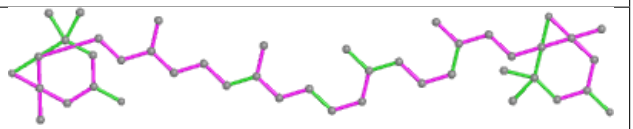


Rings

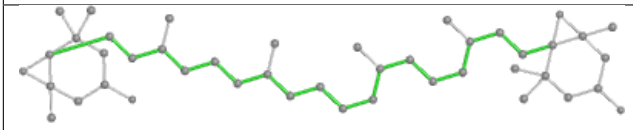
Ligand XAT 8 317



Bond lengths



Bond angles



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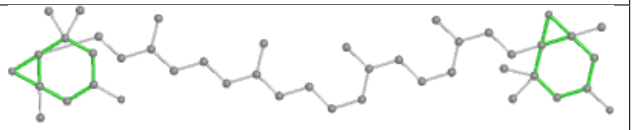
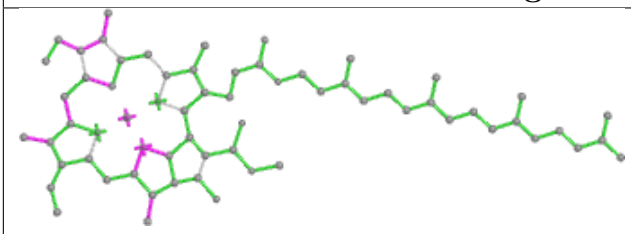


Rings

Ligand CLA B 814



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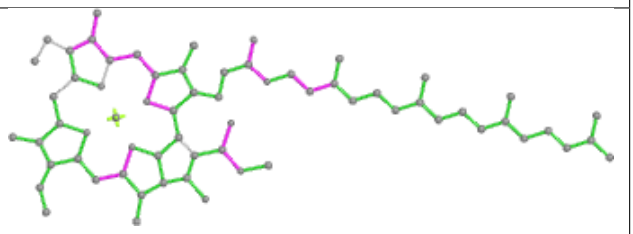
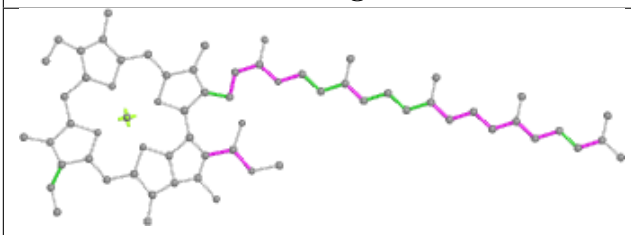


Bond angles



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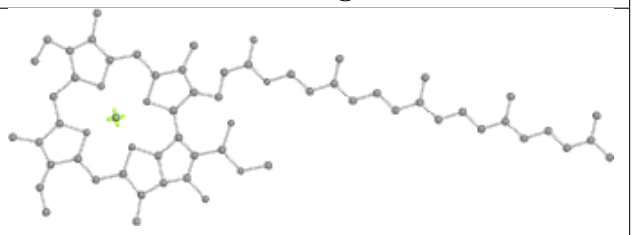
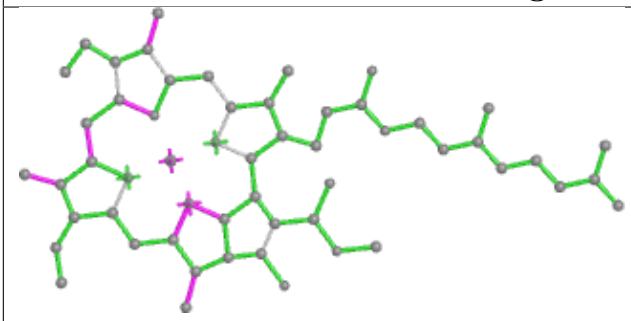


Rings

Ligand CLA 1 312



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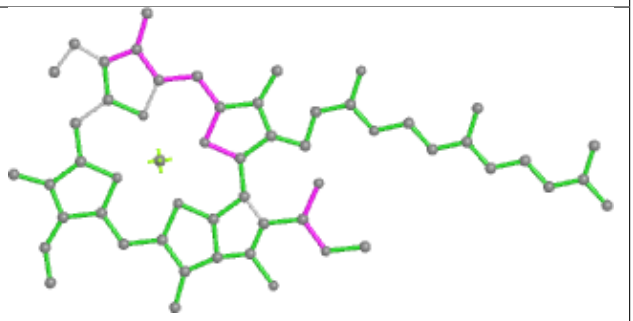
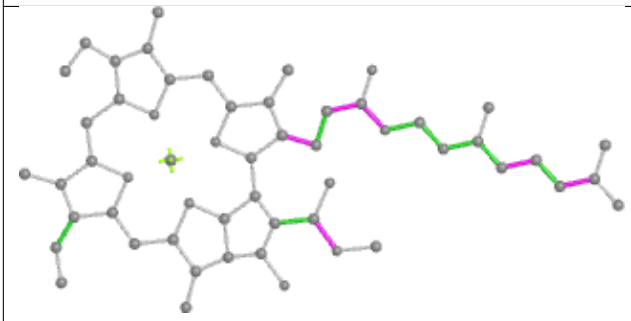


Bond angles



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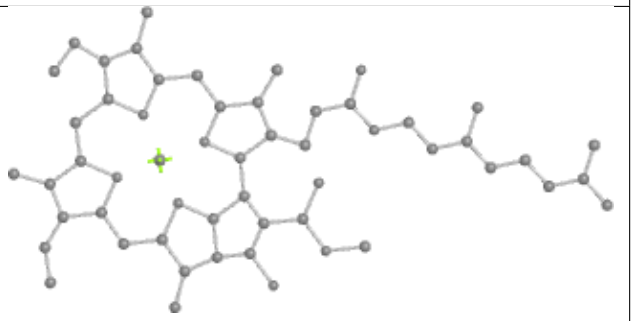
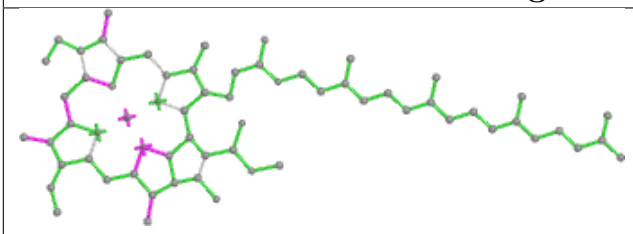
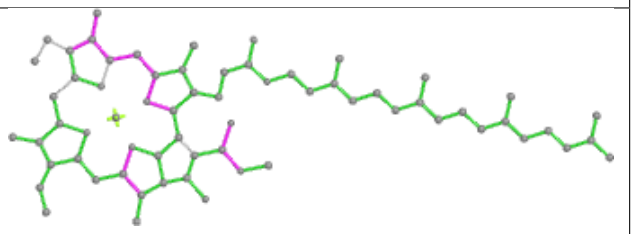


Rings

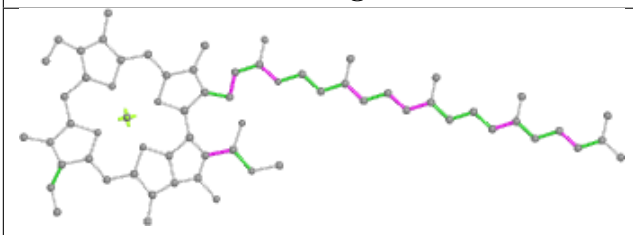
Ligand CLA 0 303



Bond lengths



Bond angles



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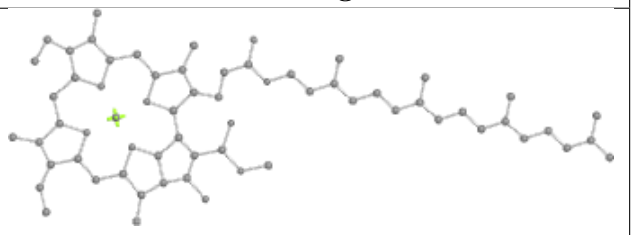
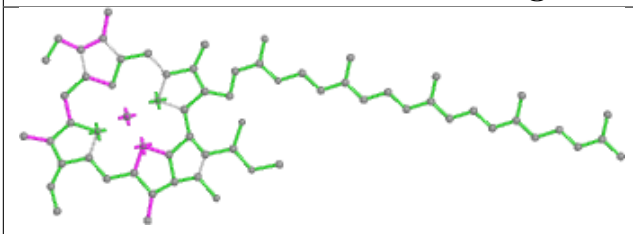
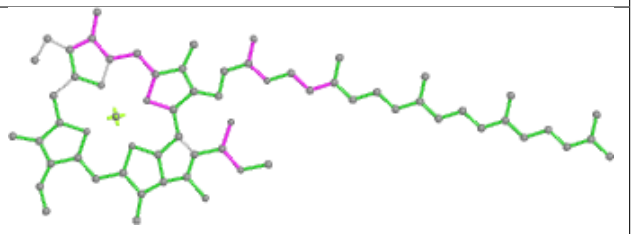


Rings

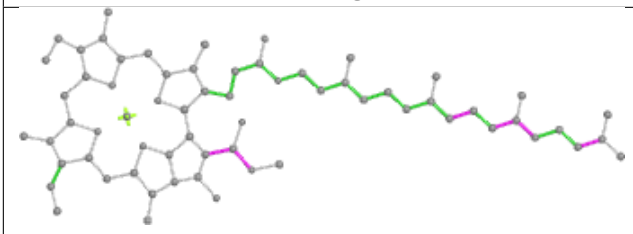
Ligand CLA 1 301



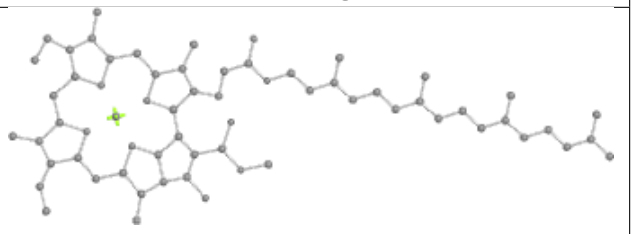
Bond lengths



Bond angles

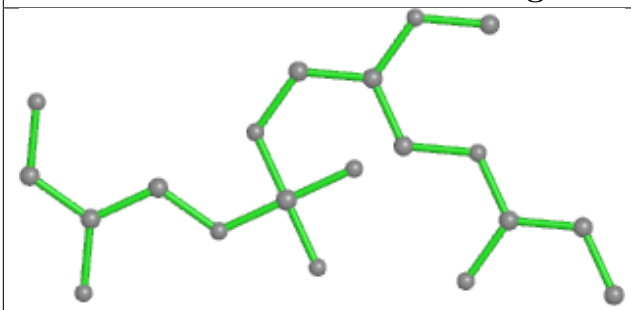


Torsions

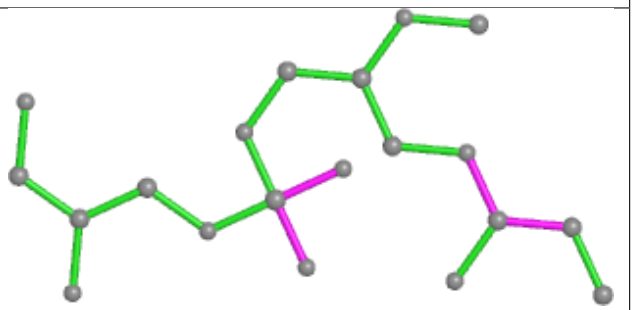


Rings

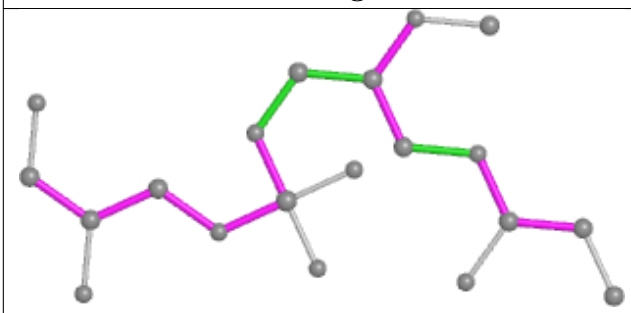
Ligand LHG 7 322



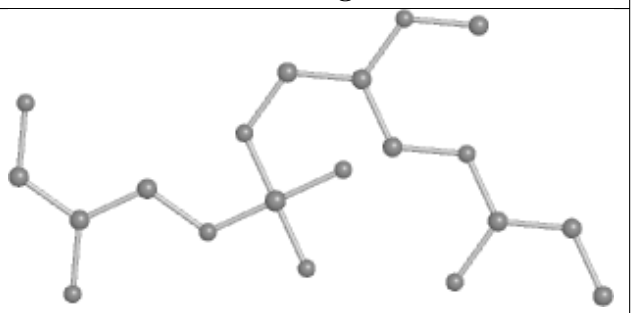
Bond lengths



Bond angles

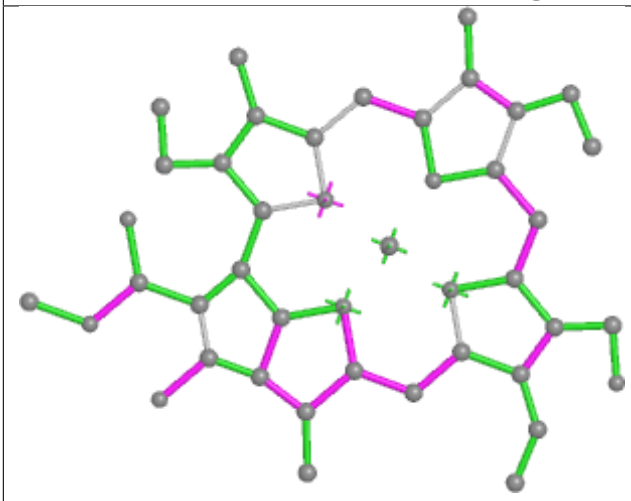


Torsions

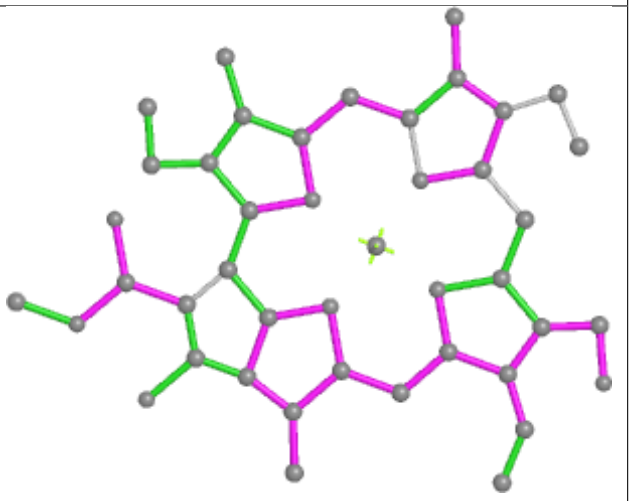


Rings

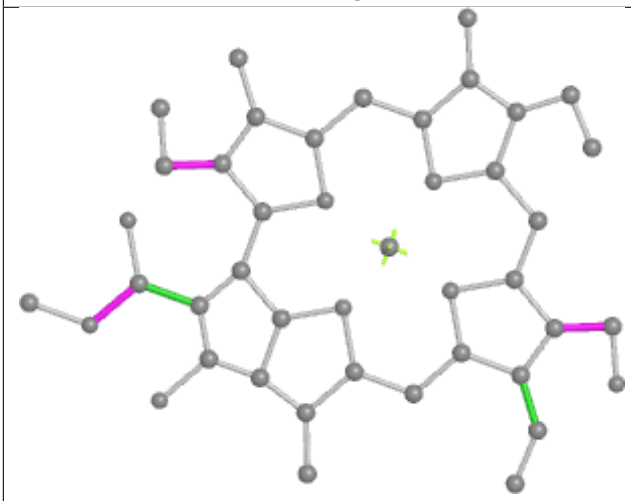
Ligand CHL 6 307



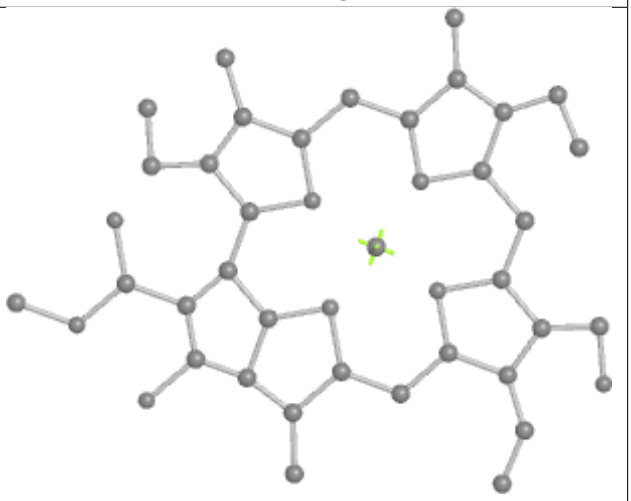
Bond lengths



Bond angles

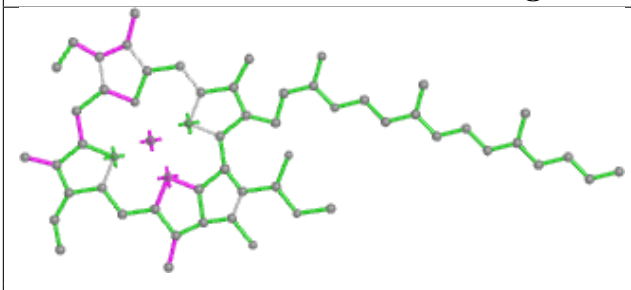


Torsions

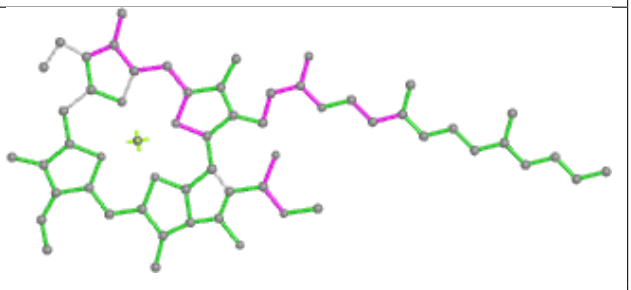


Rings

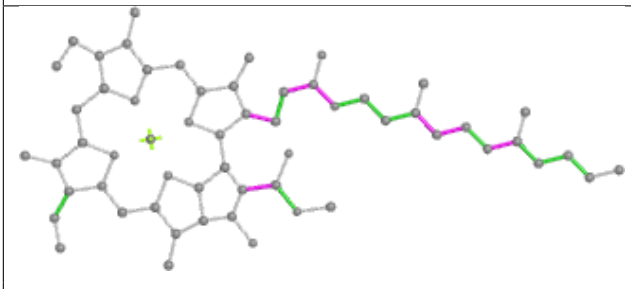
Ligand CLA B 833



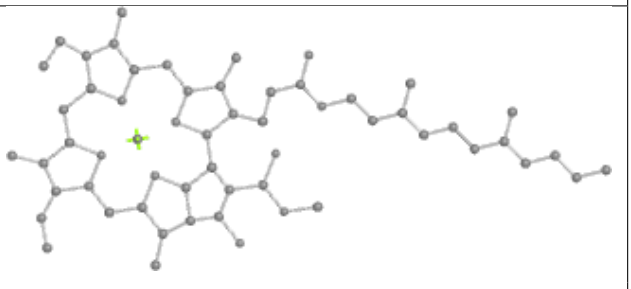
Bond lengths



Bond angles

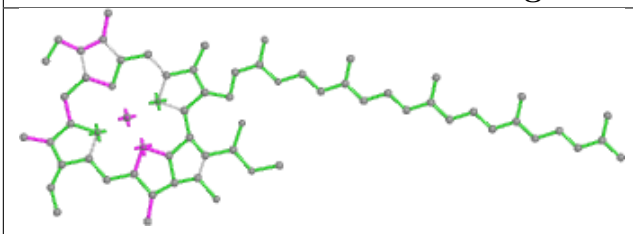


Torsions

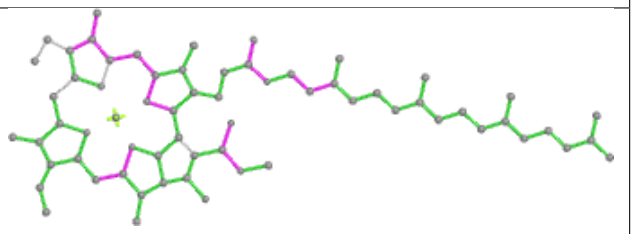


Rings

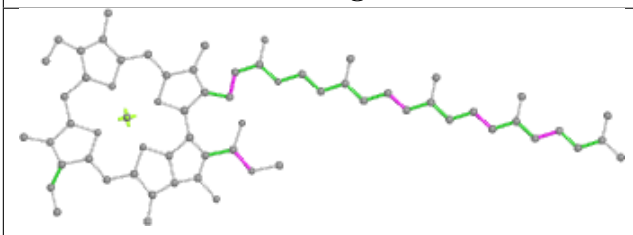
Ligand CLA B 810



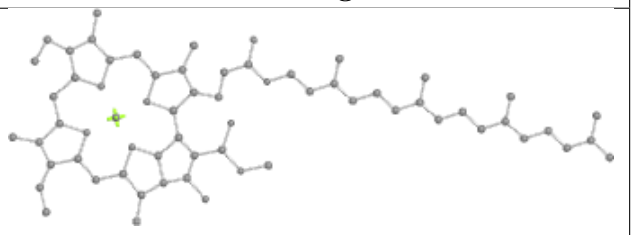
Bond lengths



Bond angles

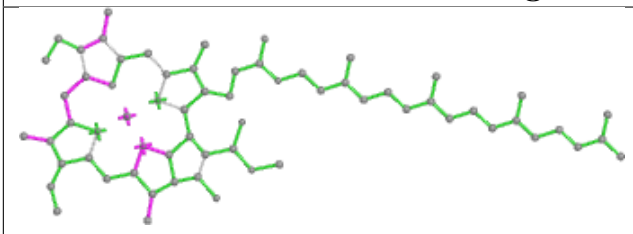


Torsions

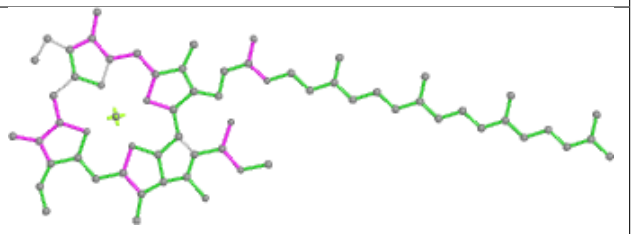


Rings

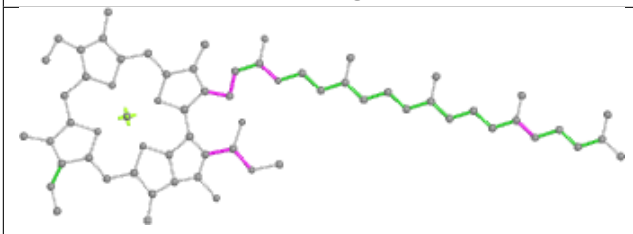
Ligand CLA B 829



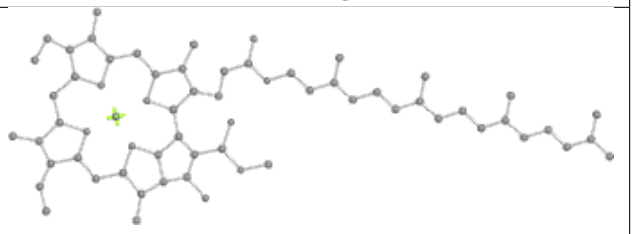
Bond lengths



Bond angles

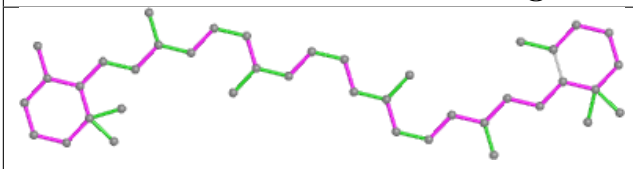


Torsions

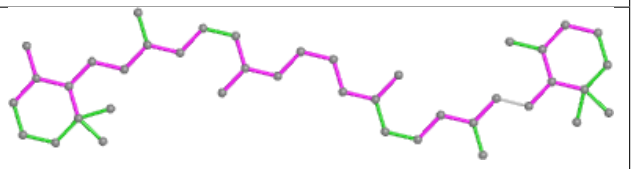


Rings

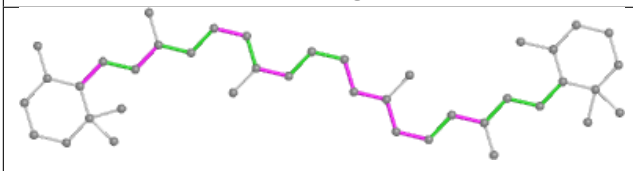
Ligand 8CT B 844



Bond lengths



Bond angles



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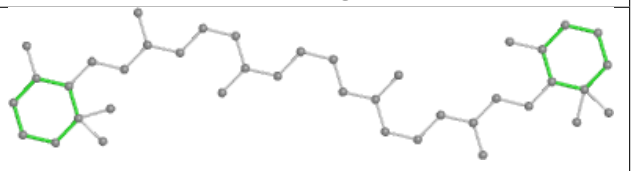
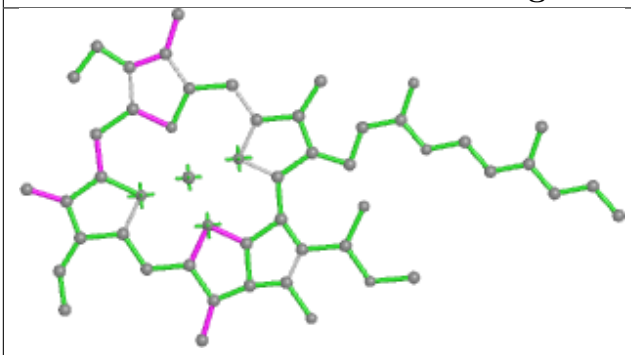


Rings

Ligand CLA 5 304



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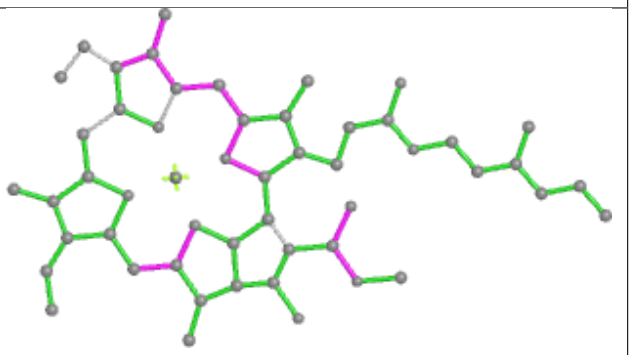
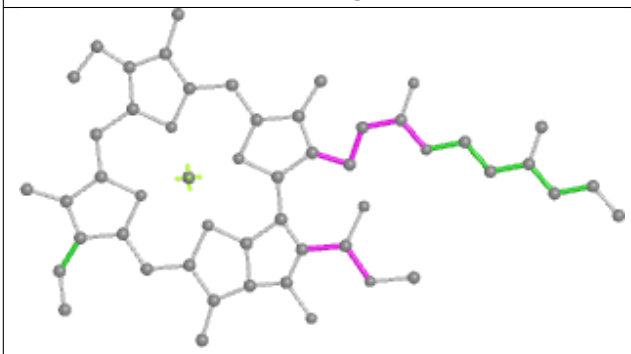


Bond angles



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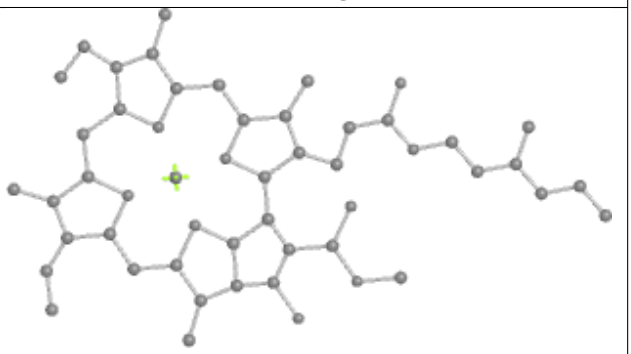
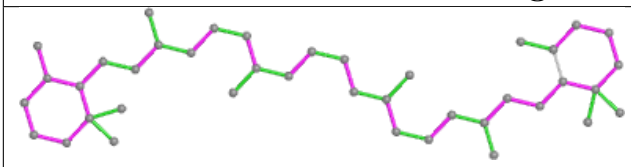
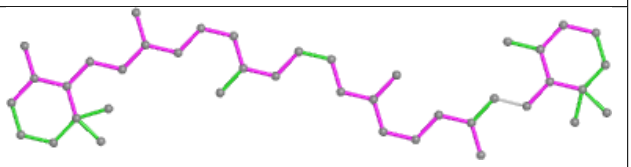


Rings

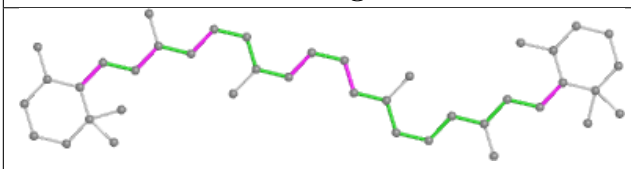
Ligand 8CT F 302



Bond lengths



Bond angles



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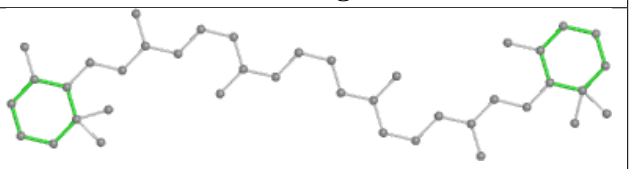
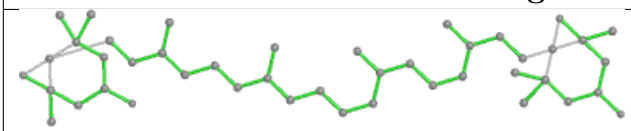
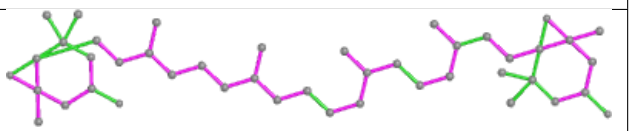


Rings

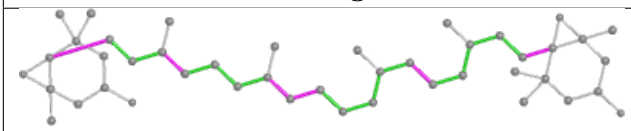
Ligand XAT 0 314



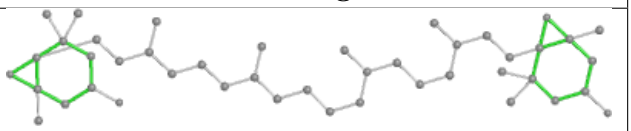
Bond lengths



Bond angles

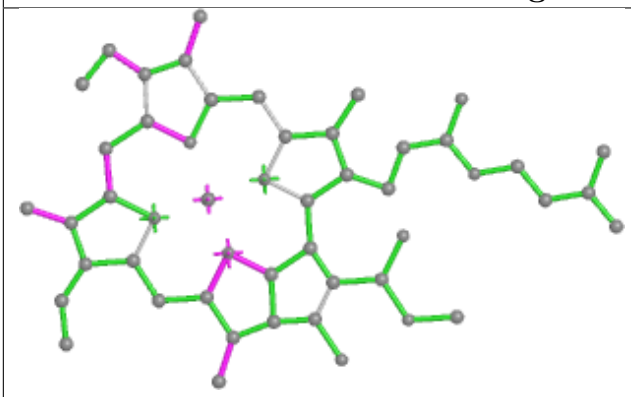


Torsions

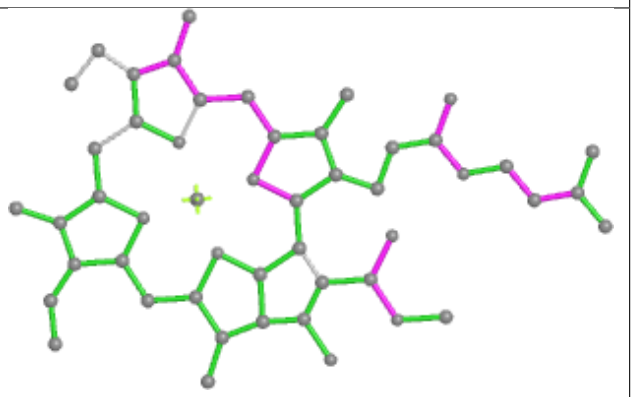


Rings

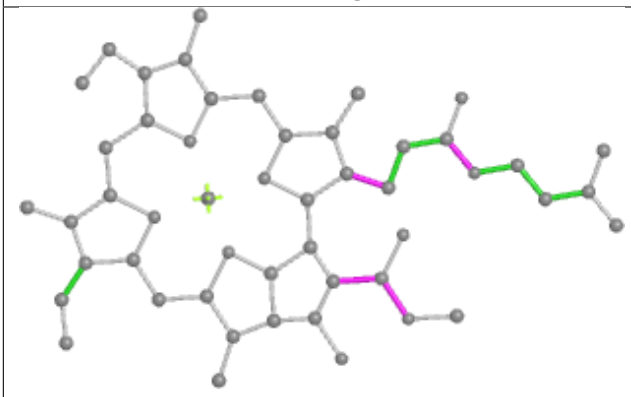
Ligand CLA 7 310



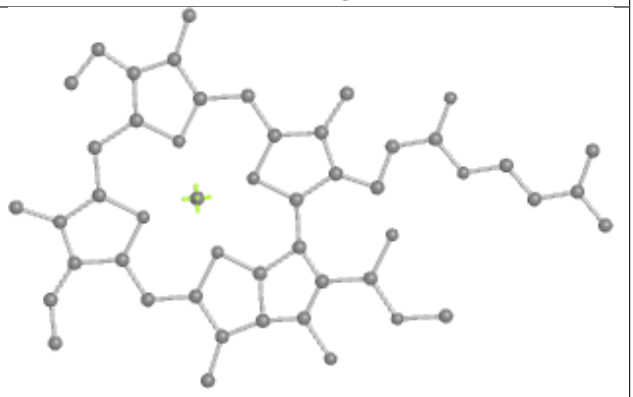
Bond lengths



Bond angles

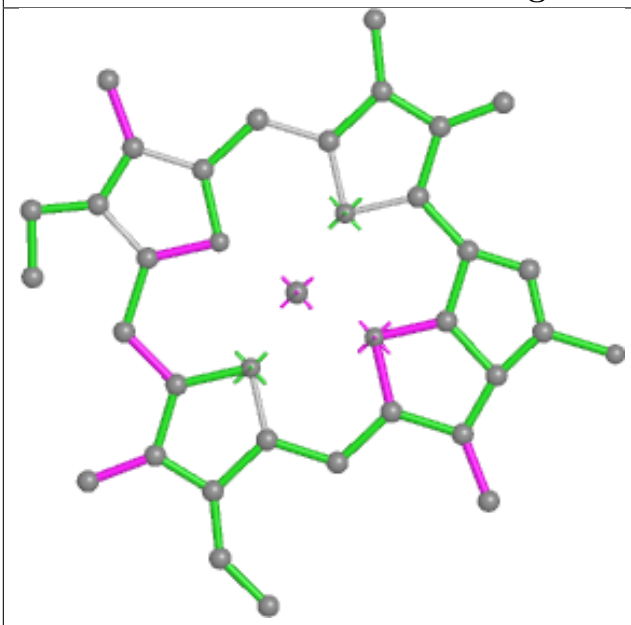


Torsions

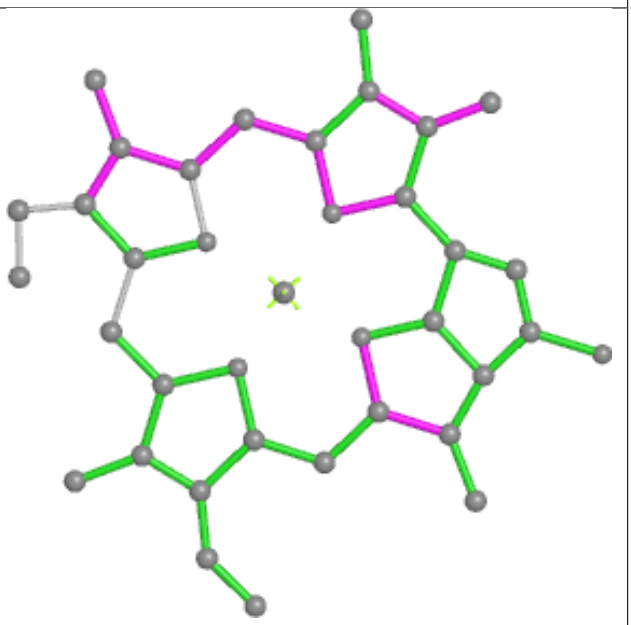


Rings

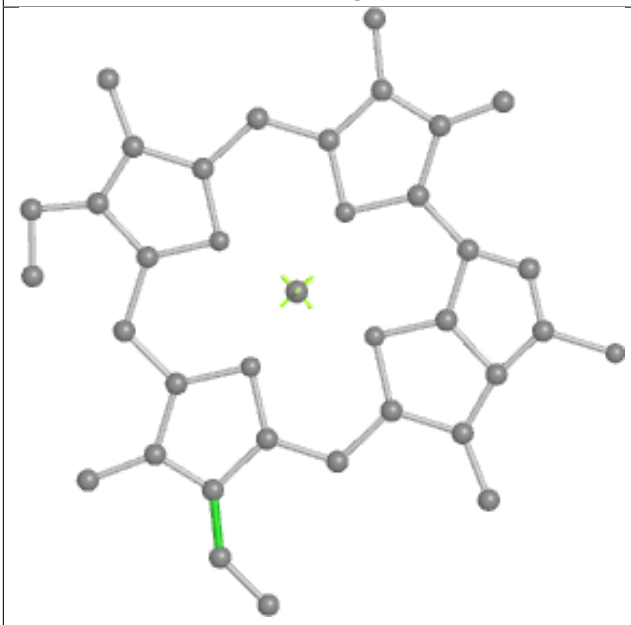
Ligand CLA 7 311



Bond lengths



Bond angles



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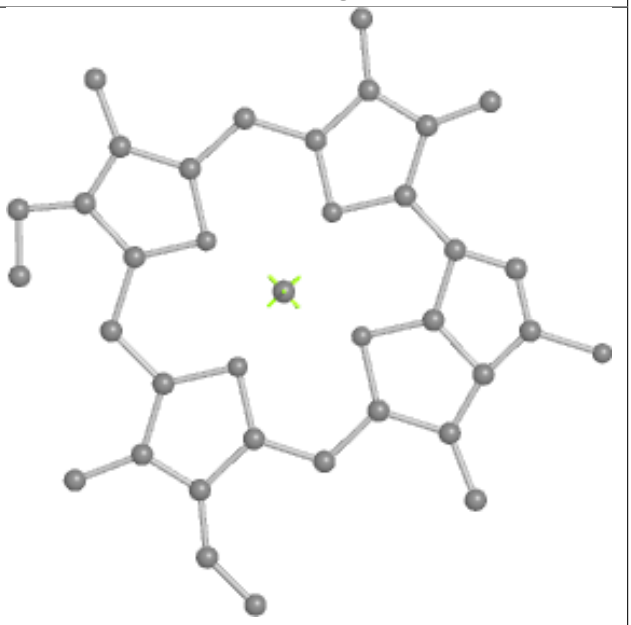
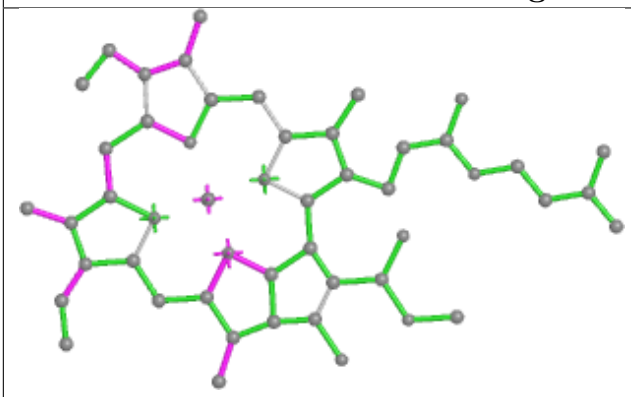


Rings

Ligand CLA 8 308



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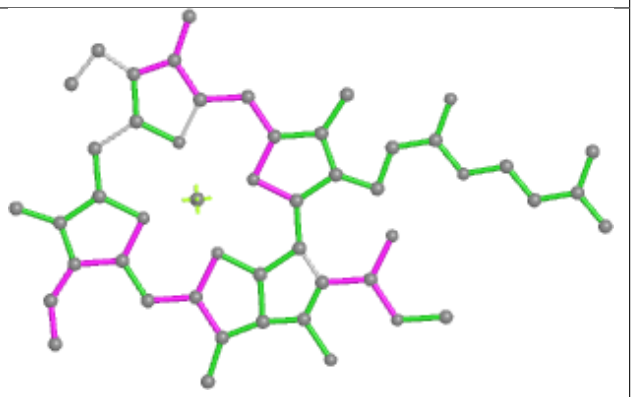
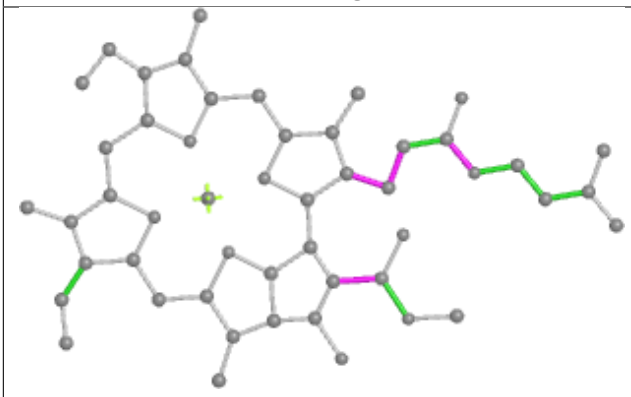


Bond angles



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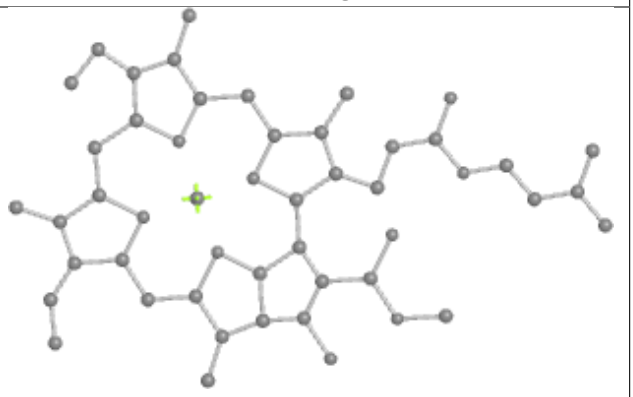
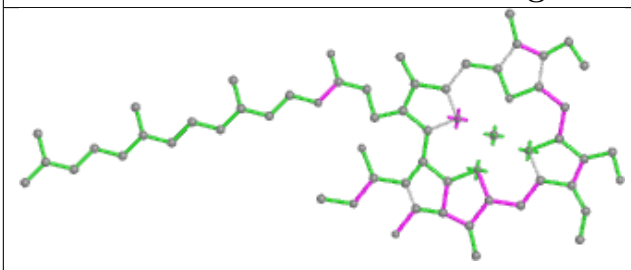


Rings

Ligand CHL 5 301



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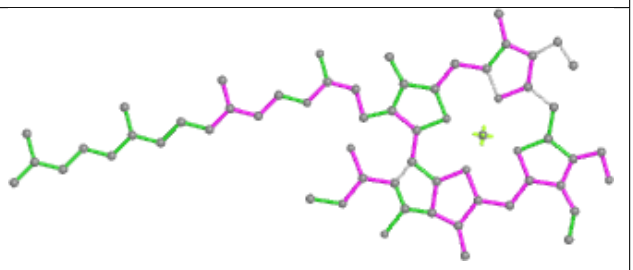
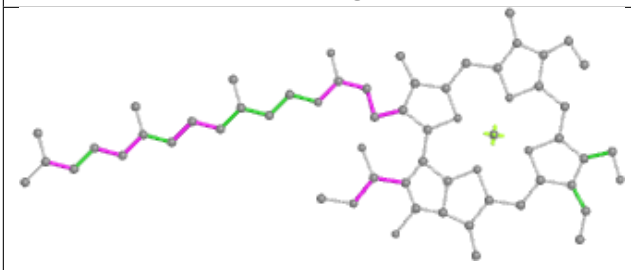


Bond angles



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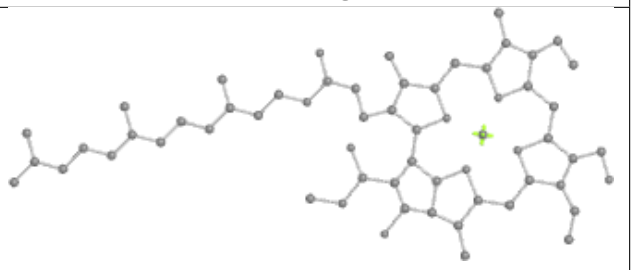
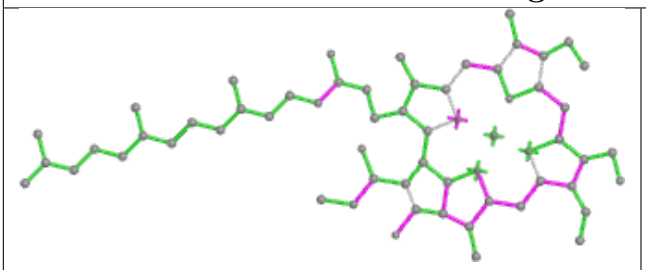
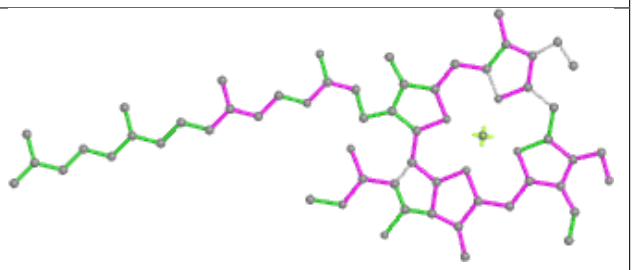


Rings

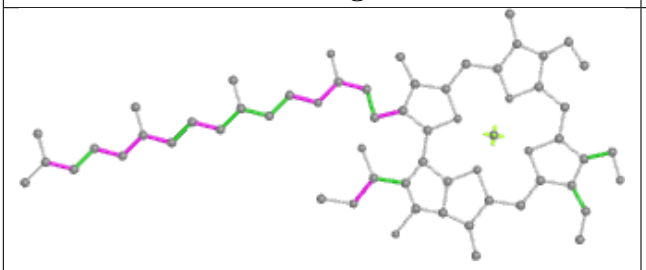
Ligand CHL 0 301



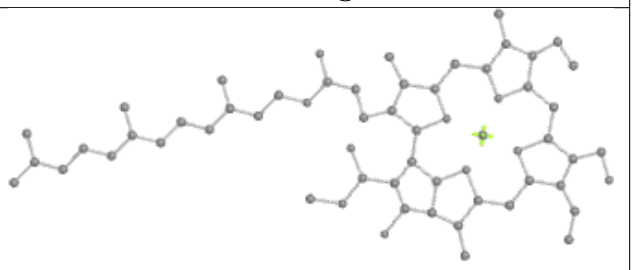
Bond lengths



Bond angles

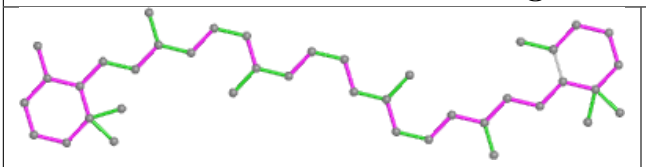


Torsions

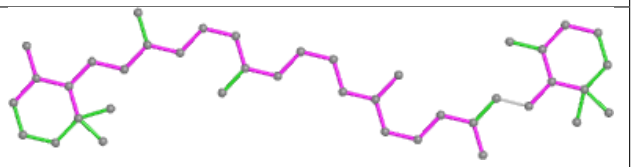


Rings

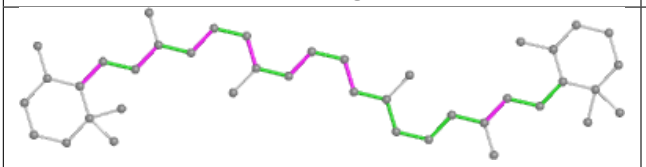
Ligand 8CT A 849



Bond lengths



Bond angles



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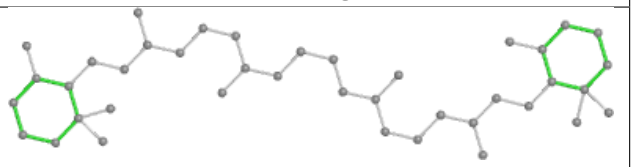
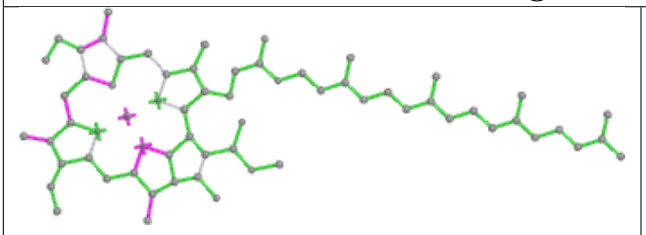
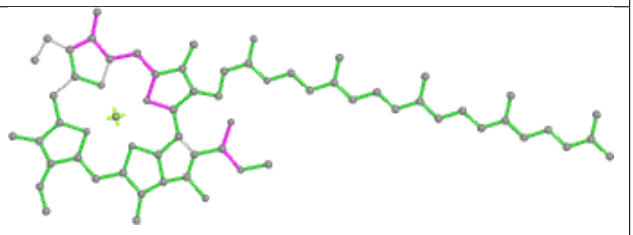


Rings

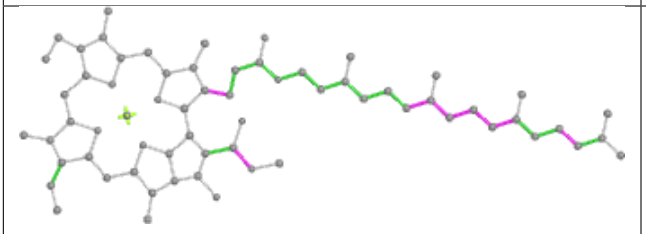
Ligand CLA 2 303



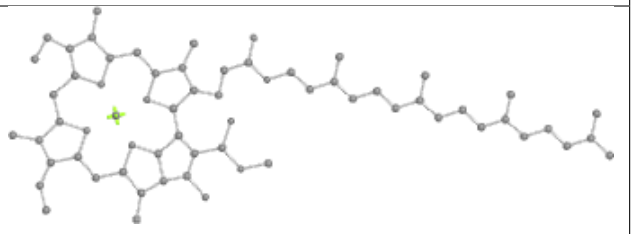
Bond lengths



Bond angles

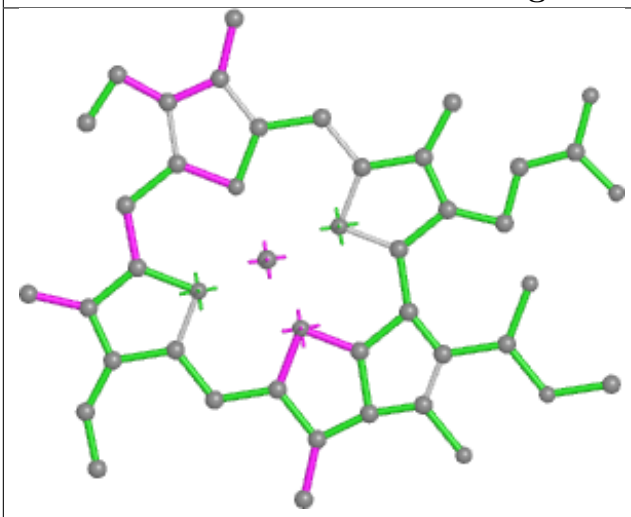


Torsions

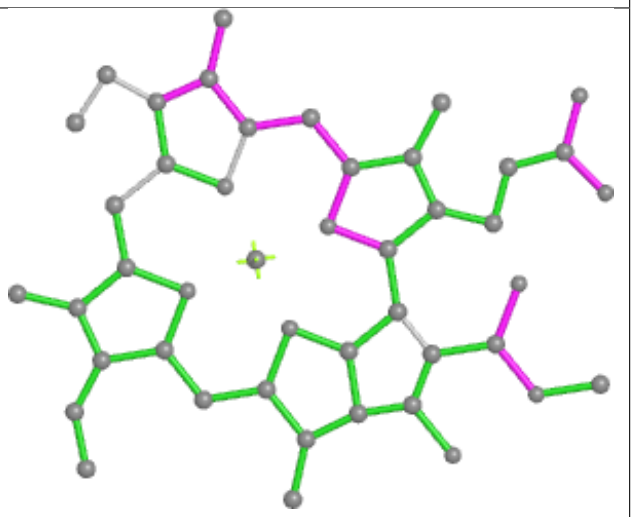


Rings

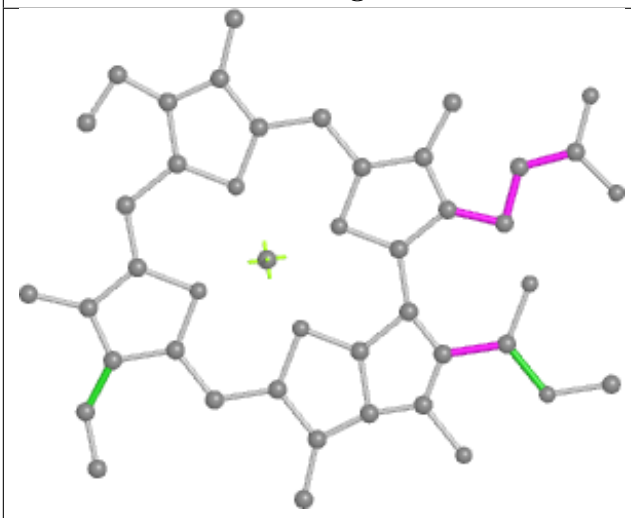
Ligand CLA 7 305



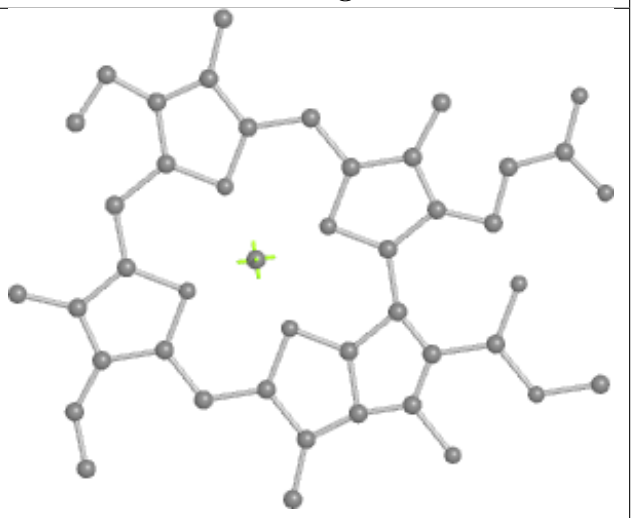
Bond lengths



Bond angles

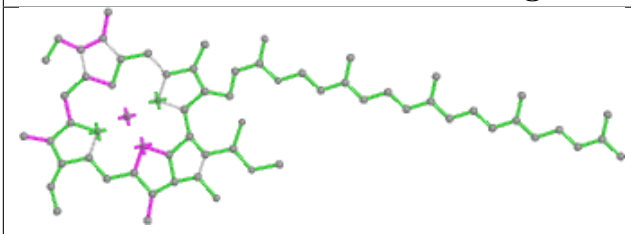


Torsions

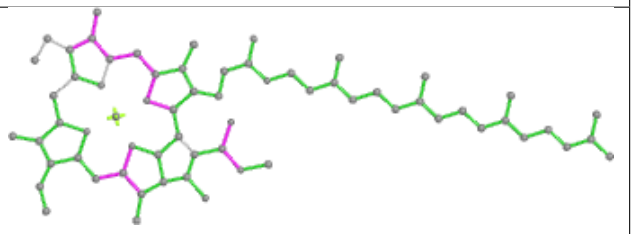


Rings

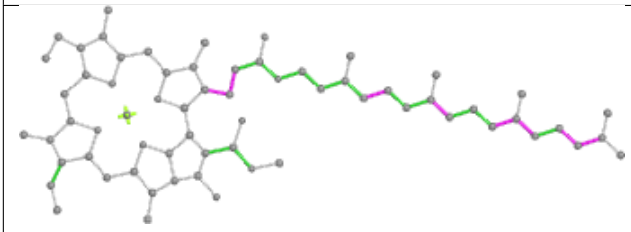
Ligand CLA A 818



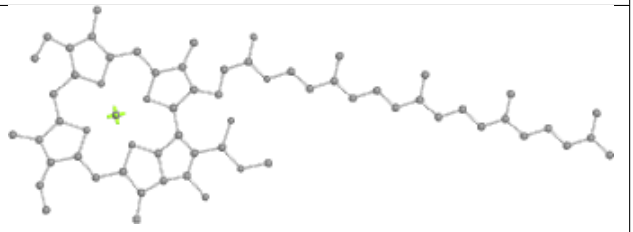
Bond lengths



Bond angles

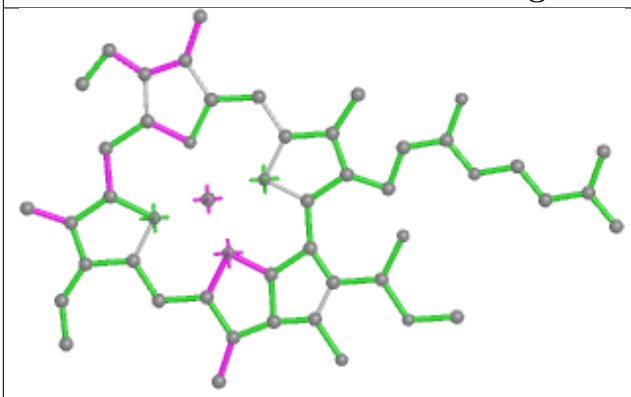


Torsions

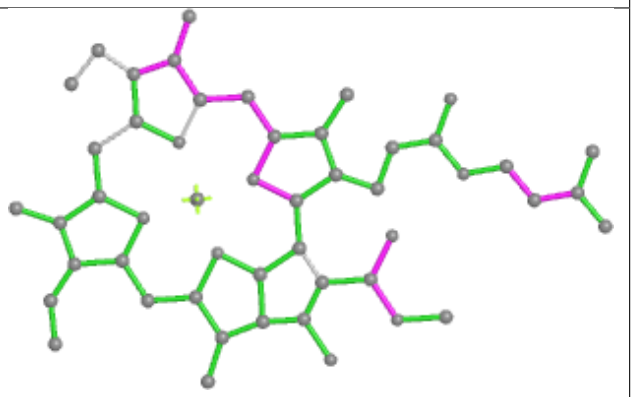


Rings

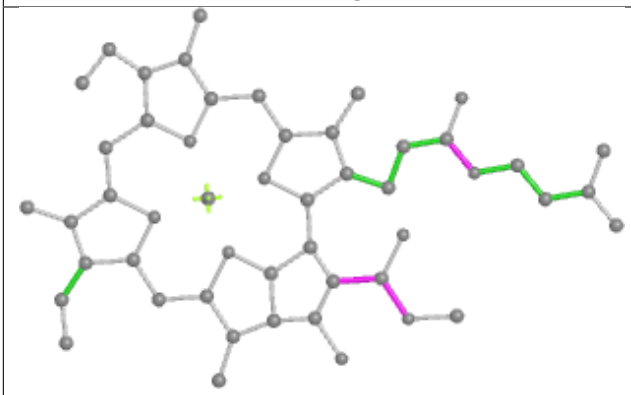
Ligand CLA 2 308



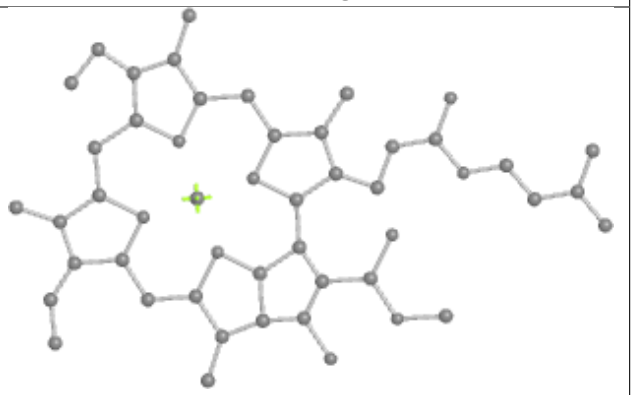
Bond lengths



Bond angles

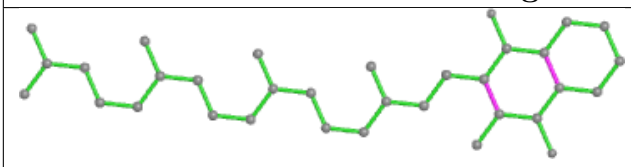


Torsions

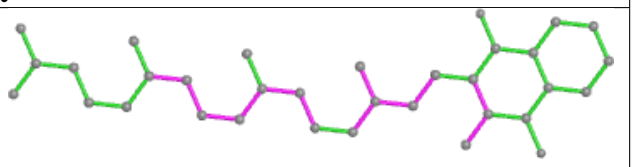


Rings

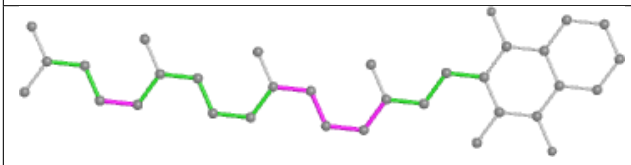
Ligand PQN A 842



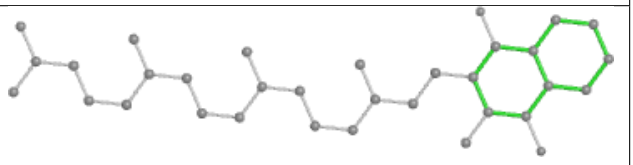
Bond lengths



Bond angles

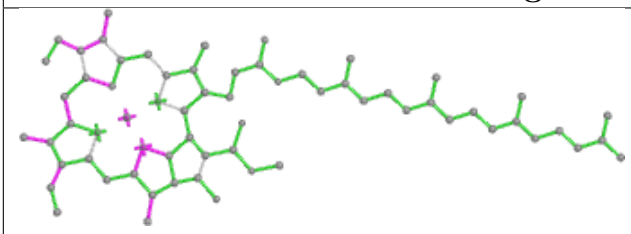


Torsions

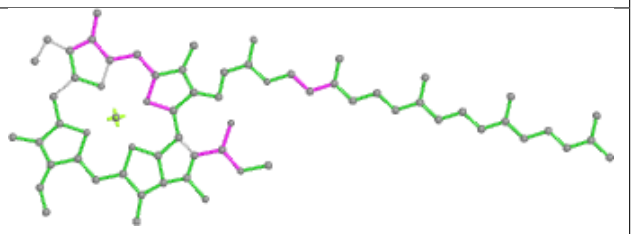


Rings

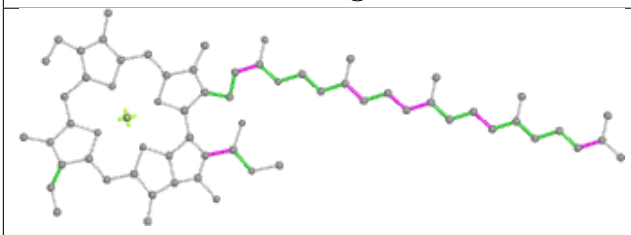
Ligand CLA B 801



Bond lengths



Bond angles



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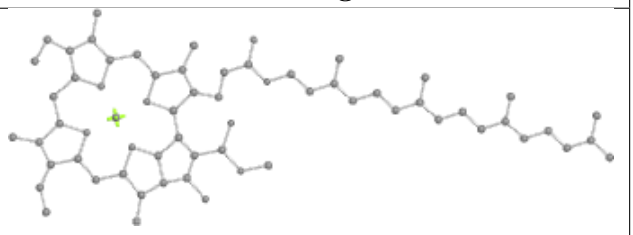
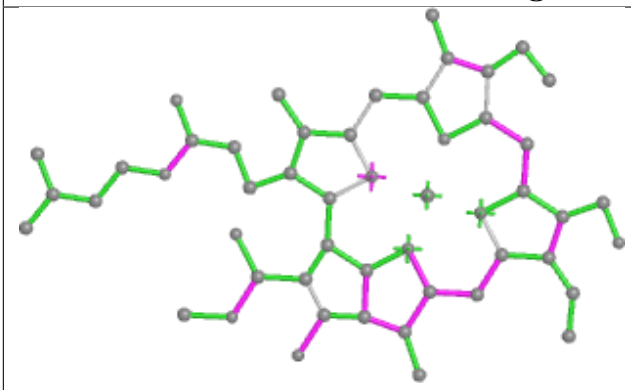


Rings

Ligand CHL 4 307



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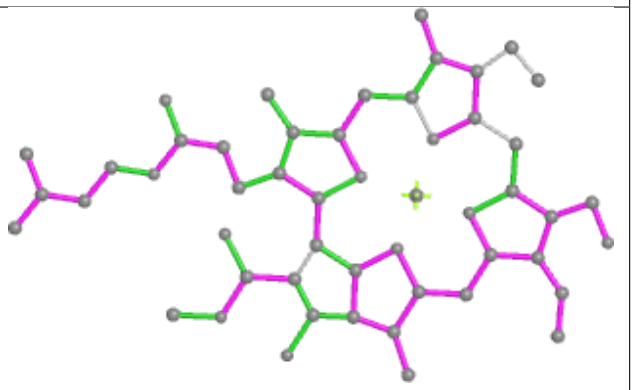
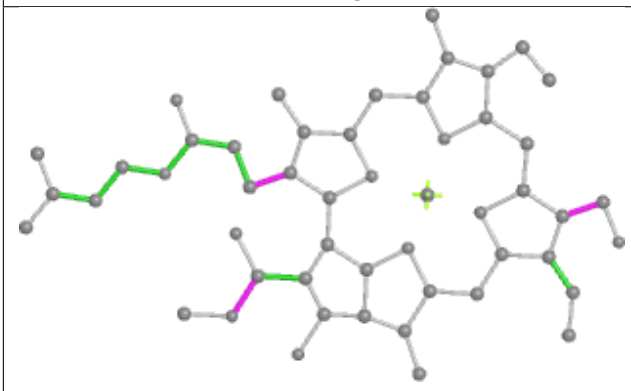


Bond angles



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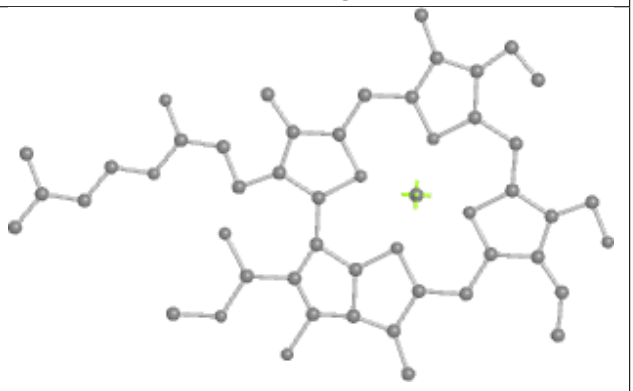
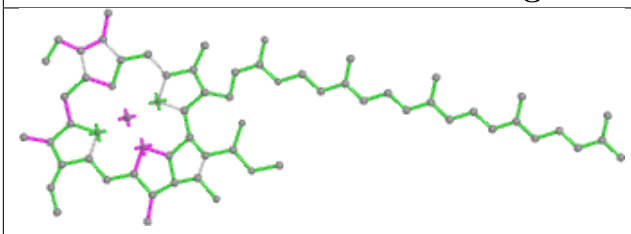
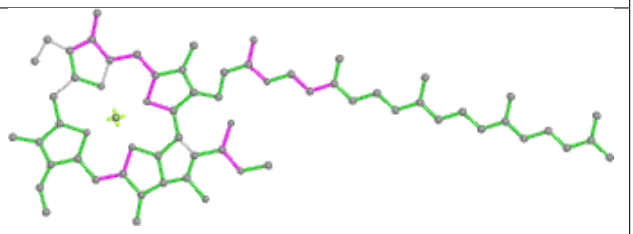


Rings

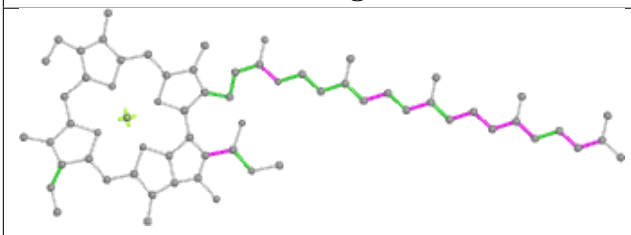
Ligand CLA A 827



Bond lengths



Bond angles



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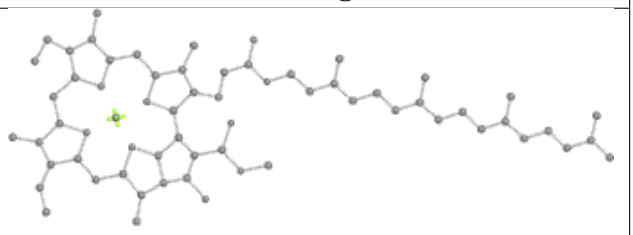
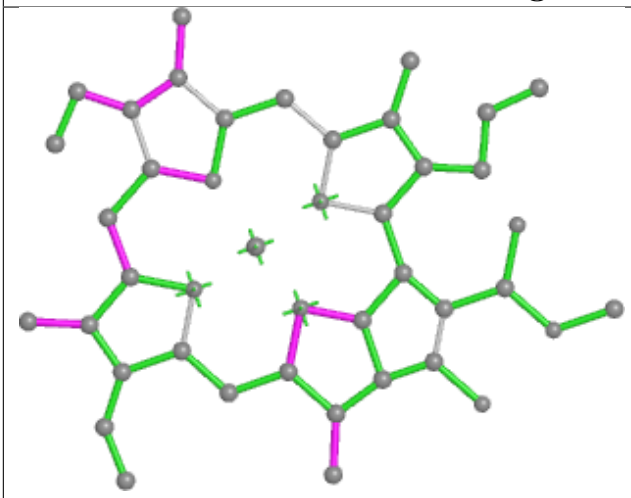
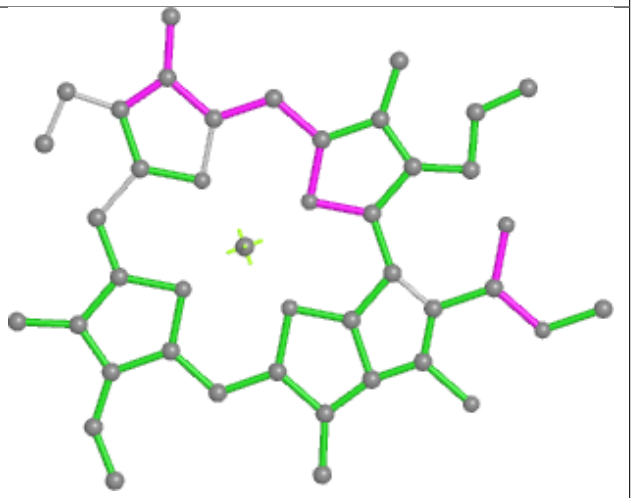


Rings

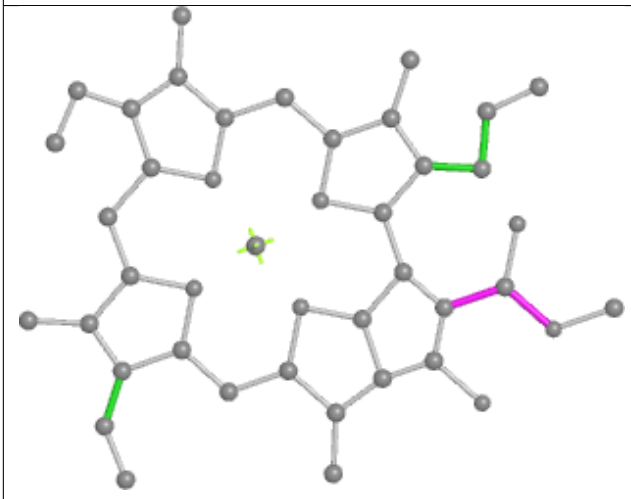
Ligand CLA 6 314



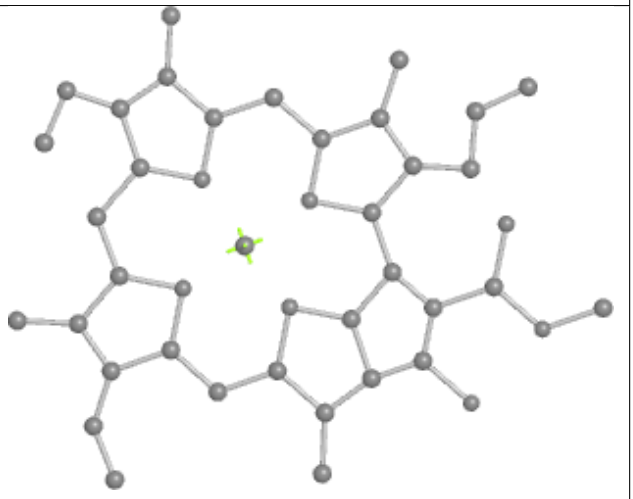
Bond lengths



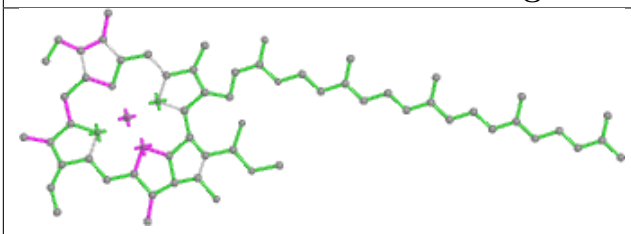
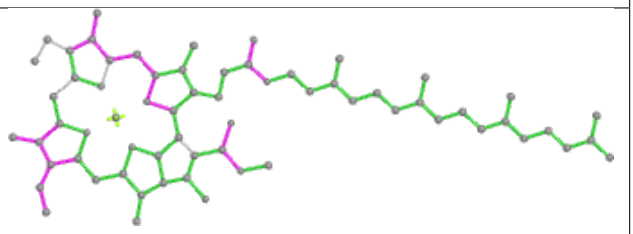
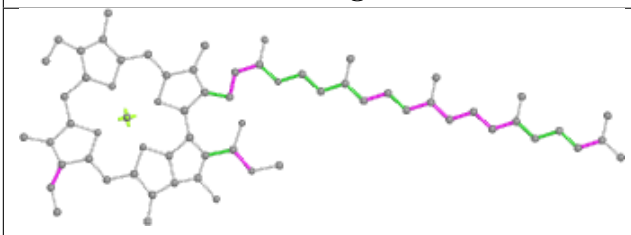
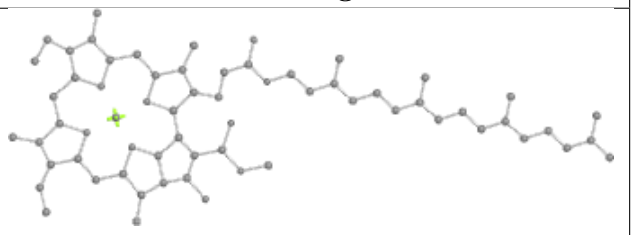
Bond angles

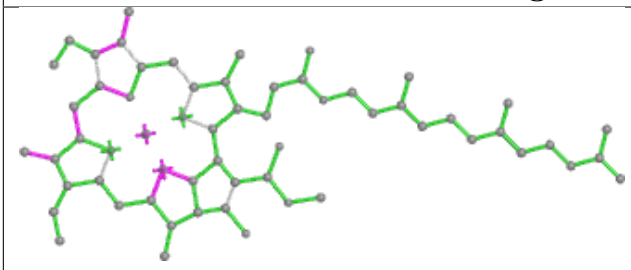
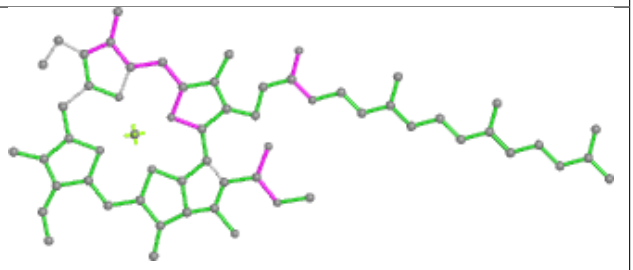
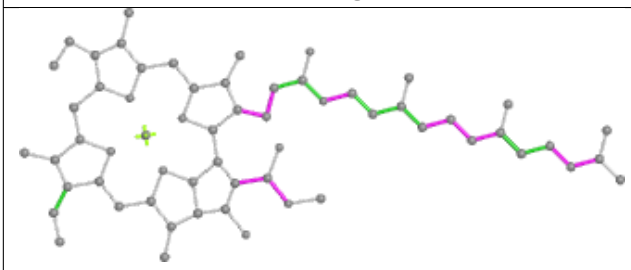
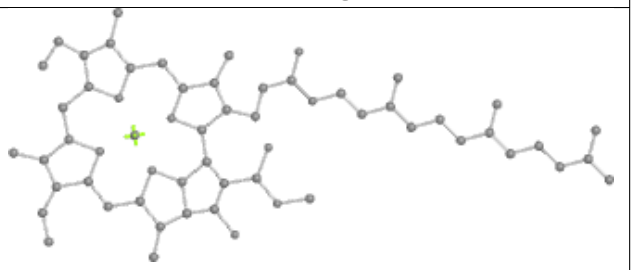


Torsions

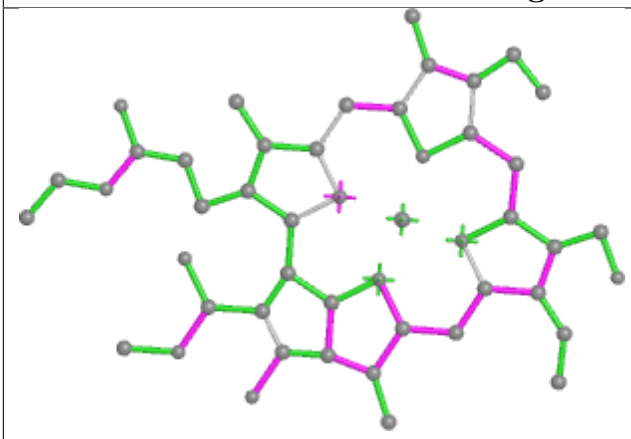


Rings

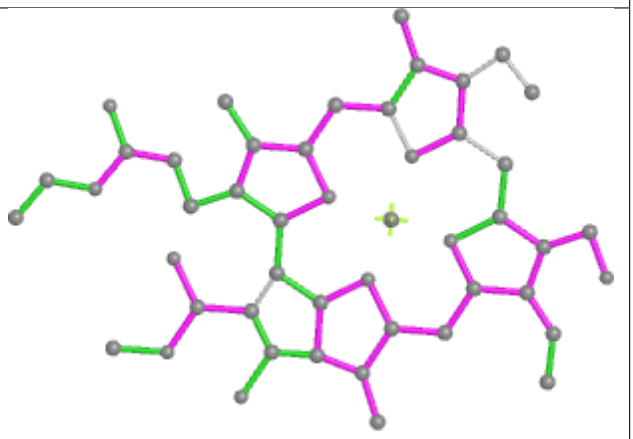
Ligand CLA A 839	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 6 305	
 Bond lengths	 Bond angles
 Torsions	 Rings

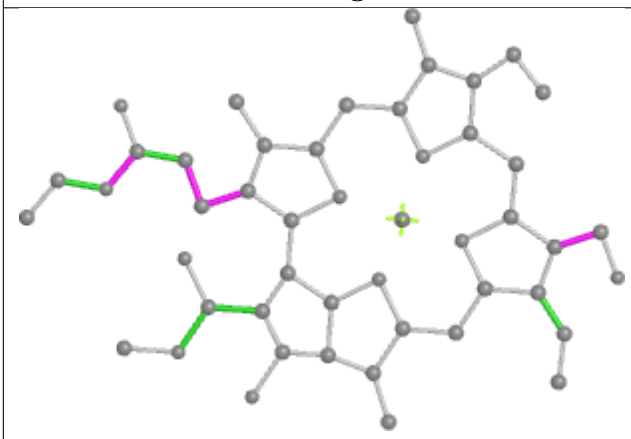
Ligand CHL 5 306



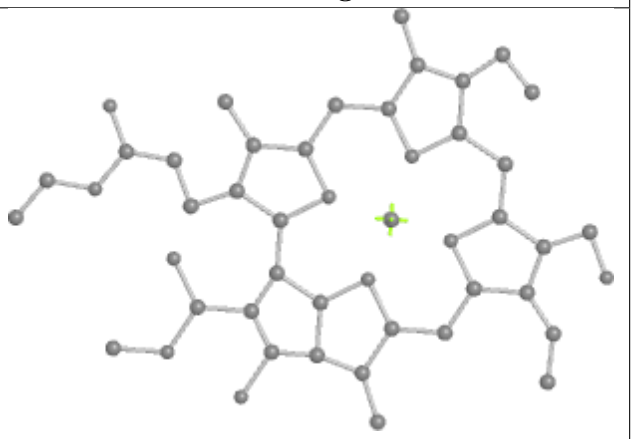
Bond lengths



Bond angles

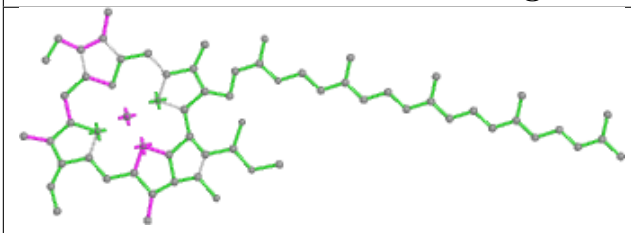


Torsions

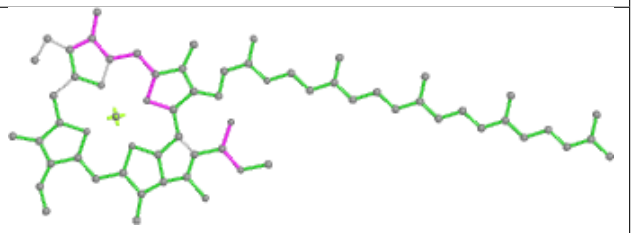


Rings

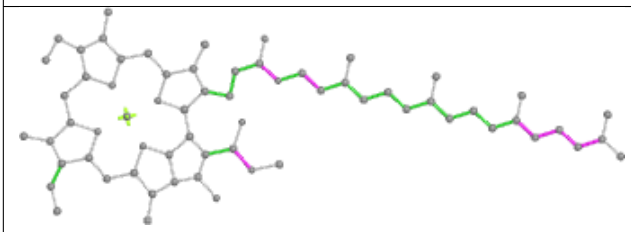
Ligand CLA A 810



Bond lengths



Bond angles



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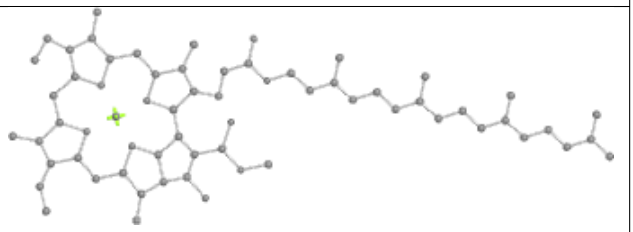
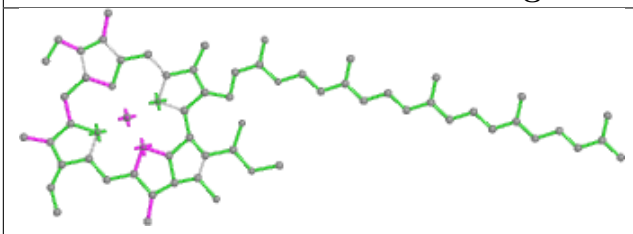
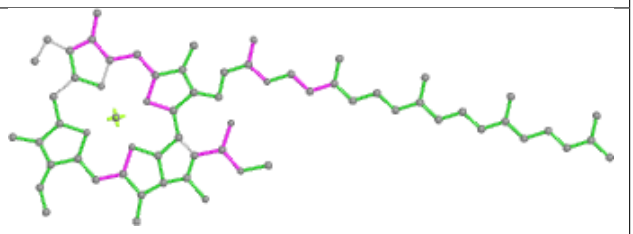


Rings

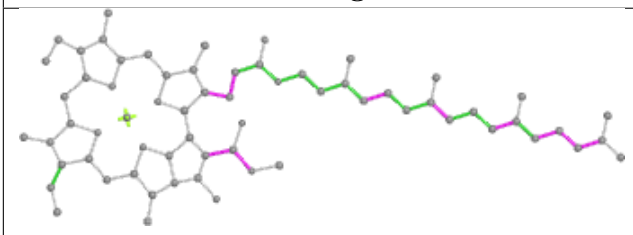
Ligand CLA A 813



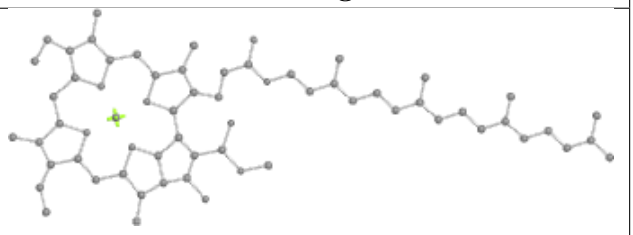
Bond lengths



Bond angles

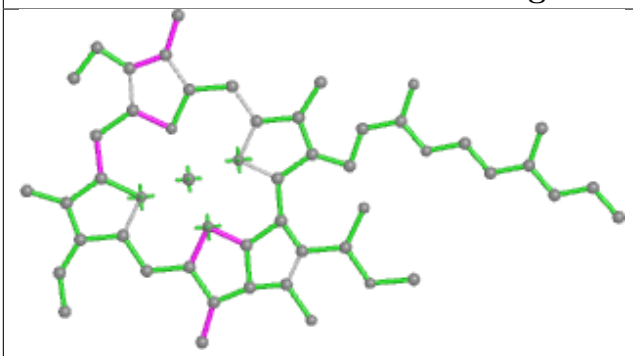


Torsions

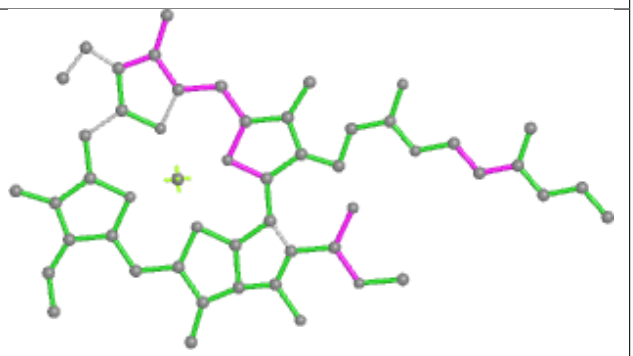


Rings

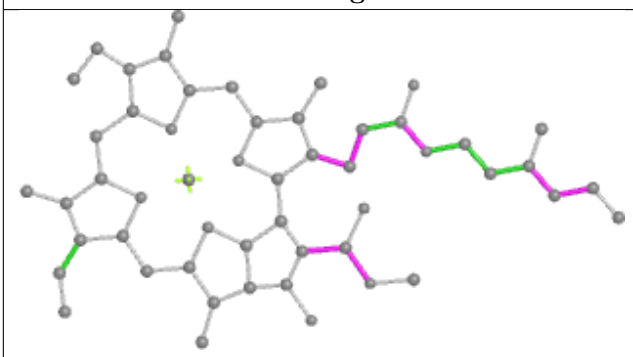
Ligand CLA 0 304



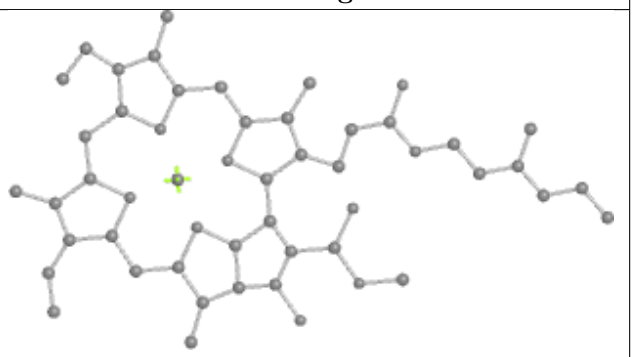
Bond lengths



Bond angles

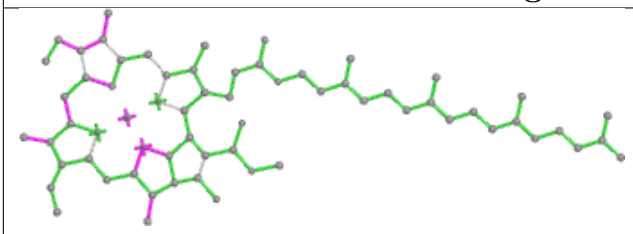


Torsions

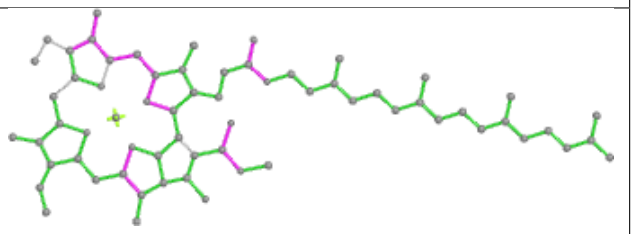


Rings

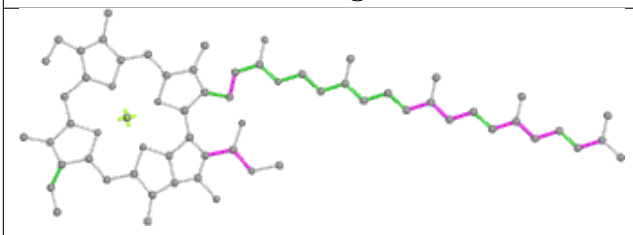
Ligand CLA B 825



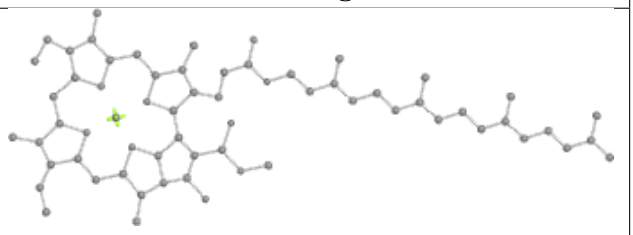
Bond lengths



Bond angles

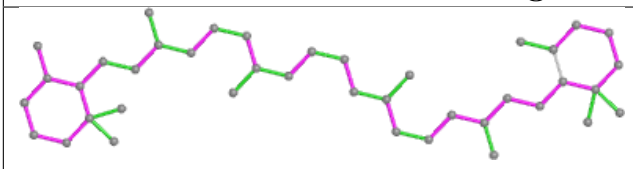


Torsions

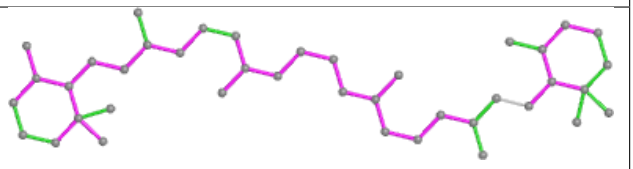


Rings

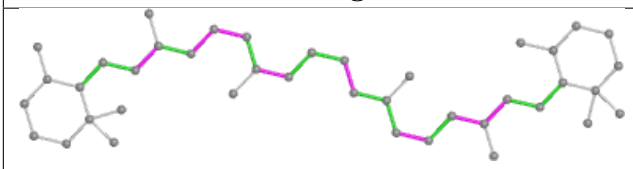
Ligand 8CT B 845



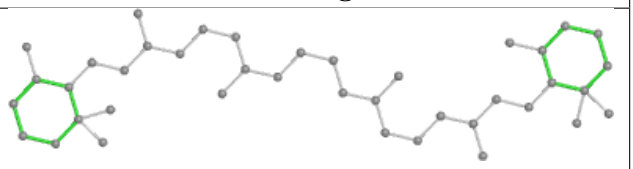
Bond lengths



Bond angles

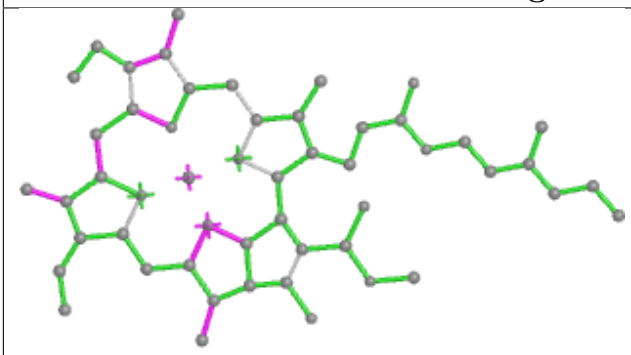


Torsions

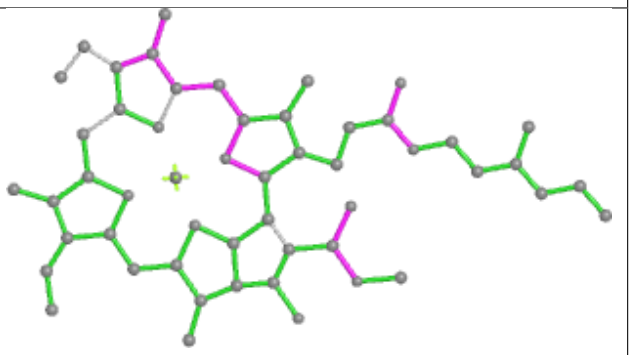


Rings

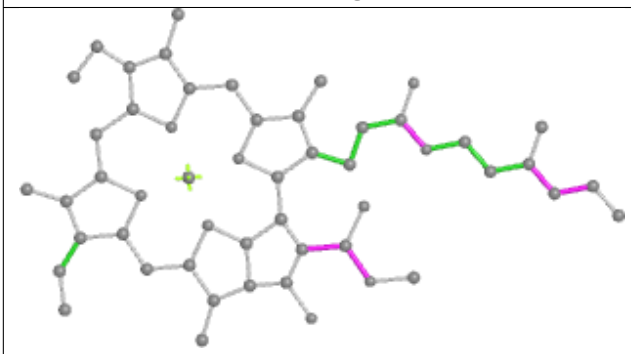
Ligand CLA 4 311



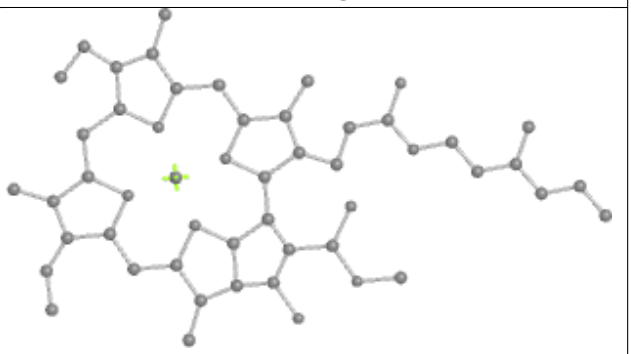
Bond lengths



Bond angles

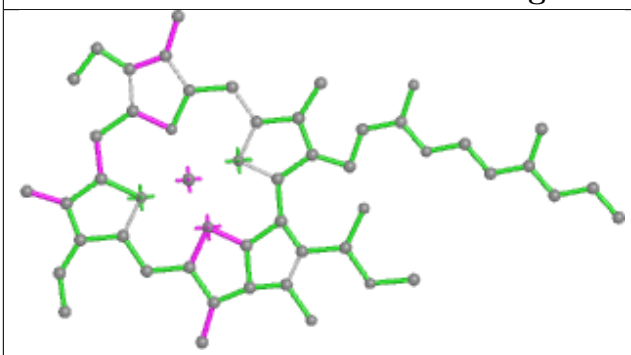


Torsions



Rings

Ligand CLA 1 303



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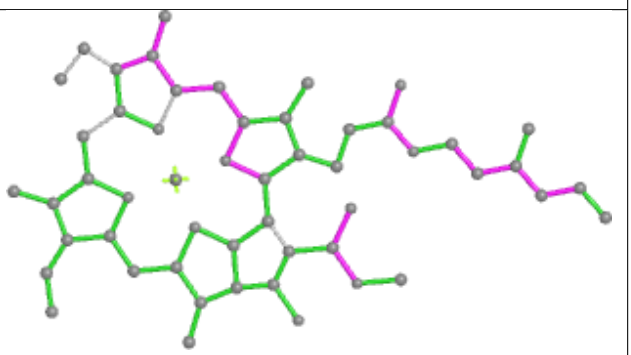
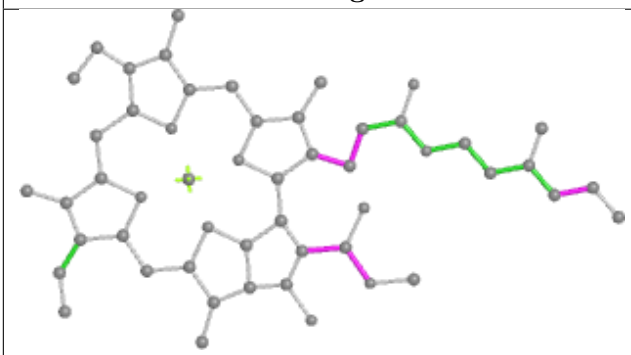
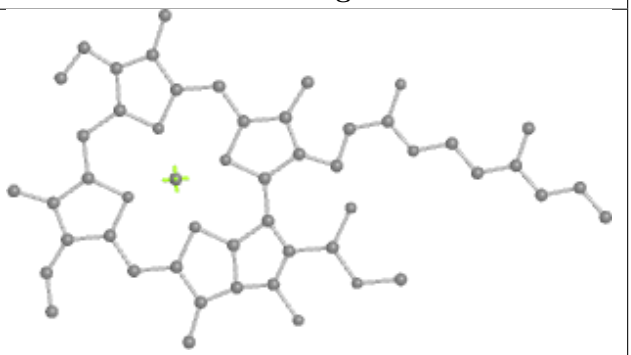


Bond angles

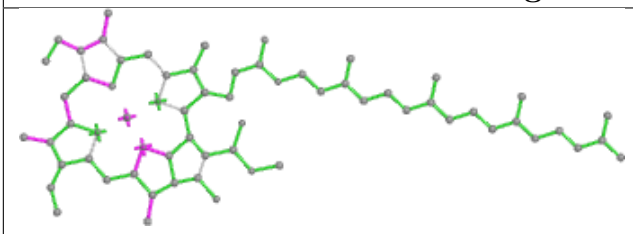


Torsions

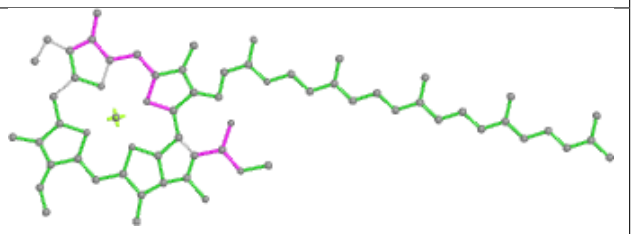


Rings

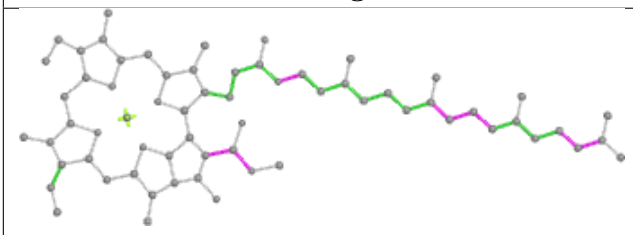
Ligand CLA B 820



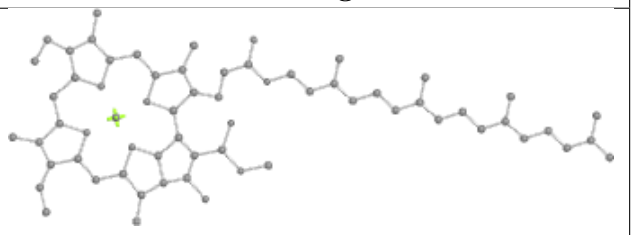
Bond lengths



Bond angles

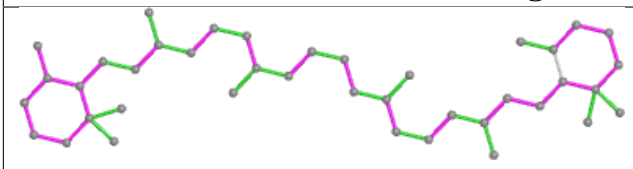


Torsions



Rings

Ligand 8CT A 848



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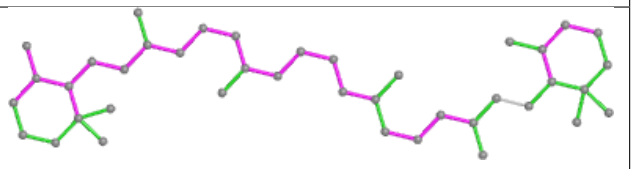
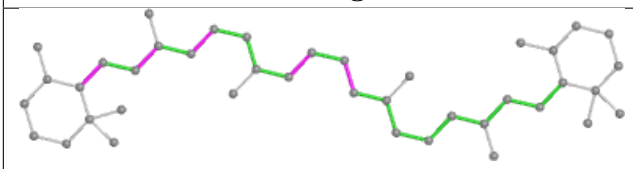


Bond angles



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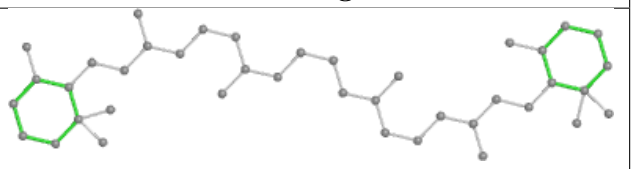
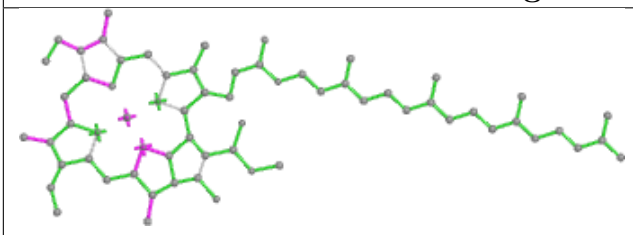


Rings

Ligand CLA A 811



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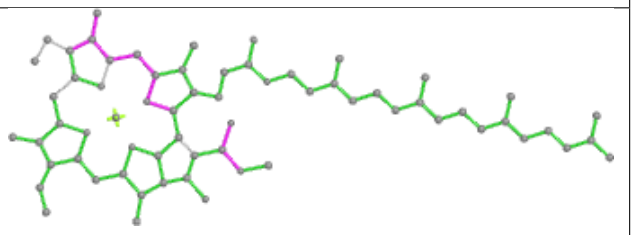
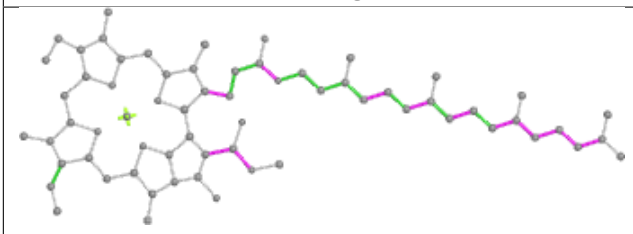
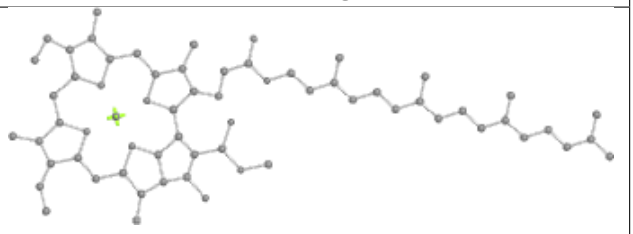


Bond angles

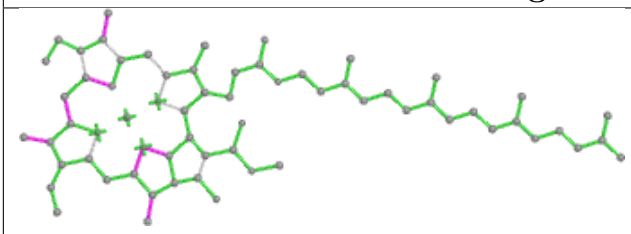


Torsions

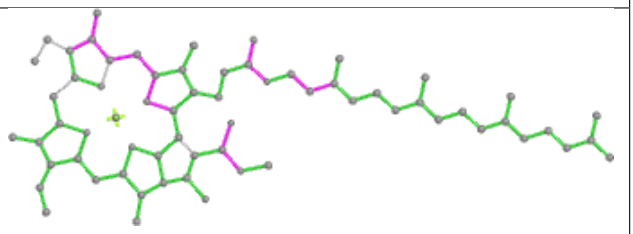


Rings

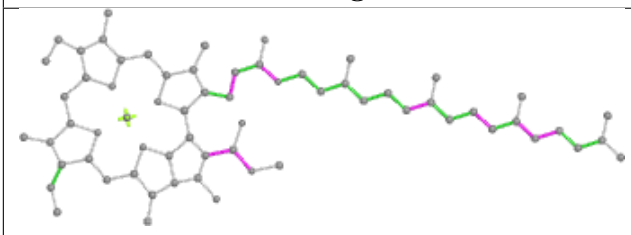
Ligand CLA 5 312



Bond lengths



Bond angles



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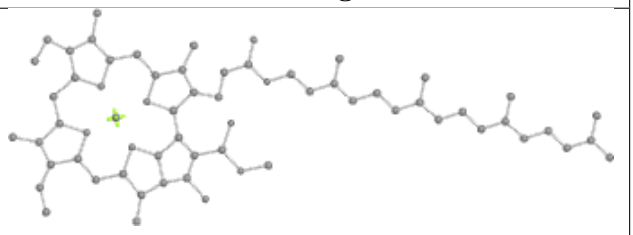
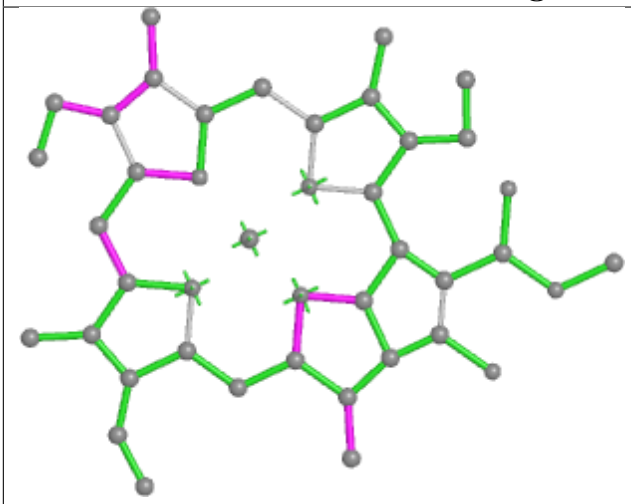
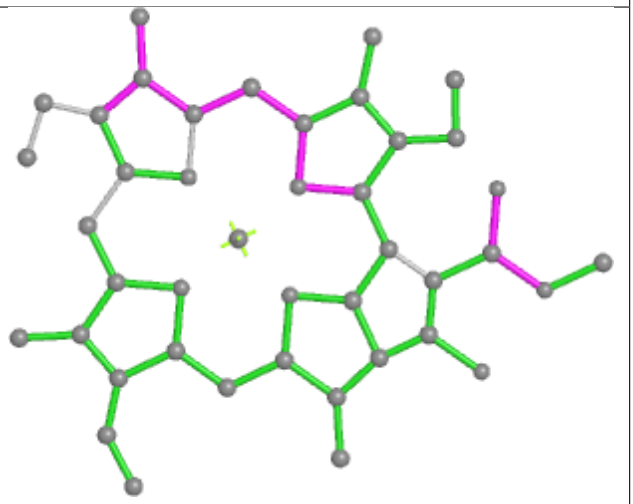


Rings

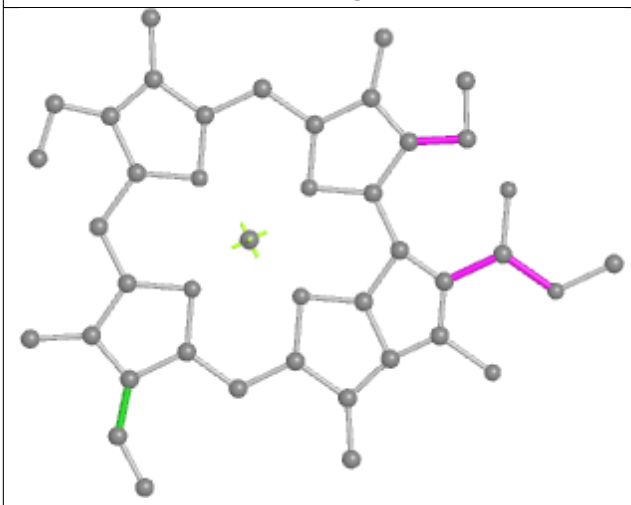
Ligand CLA J 103



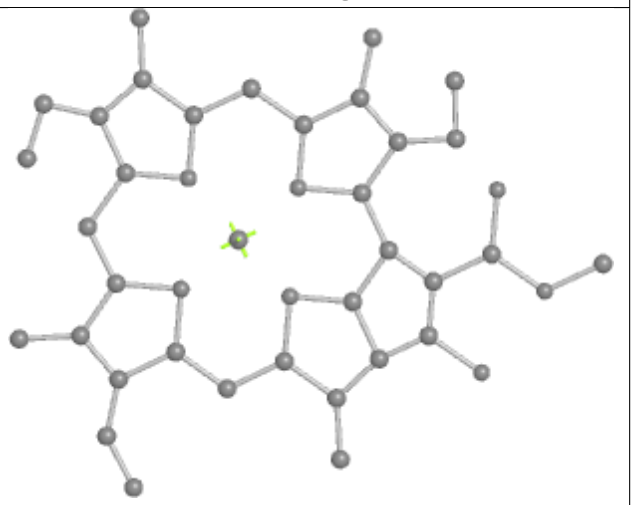
Bond lengths



Bond angles

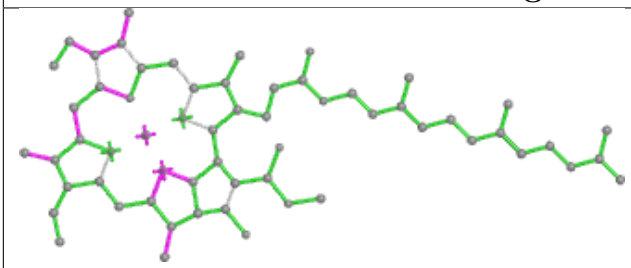


Torsions

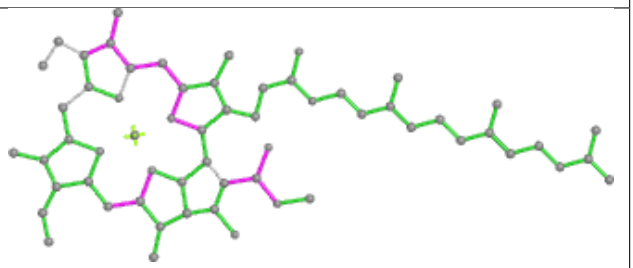


Rings

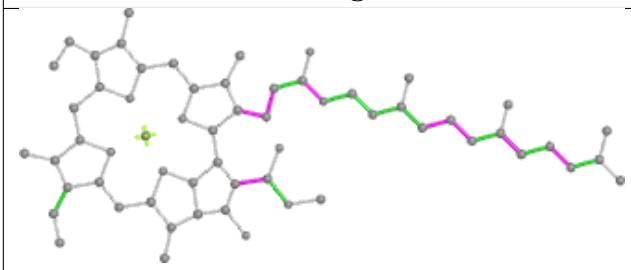
Ligand CLA B 816



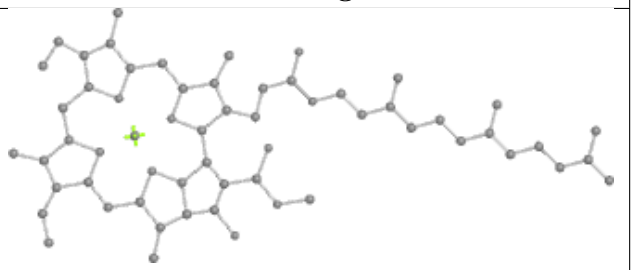
Bond lengths



Bond angles

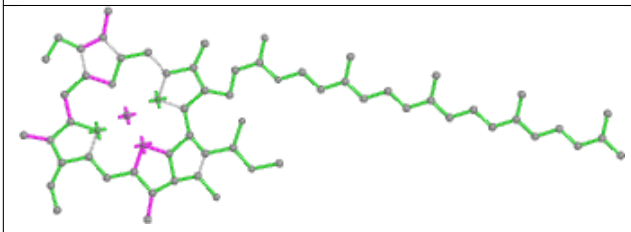


Torsions

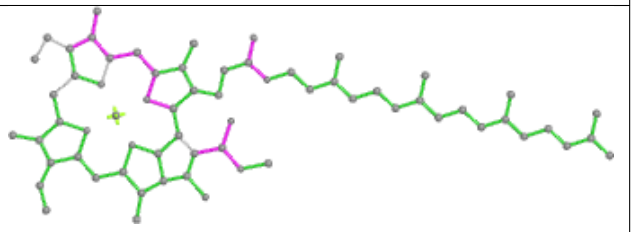


Rings

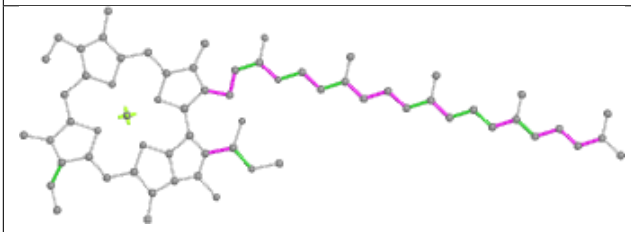
Ligand CLA A 808



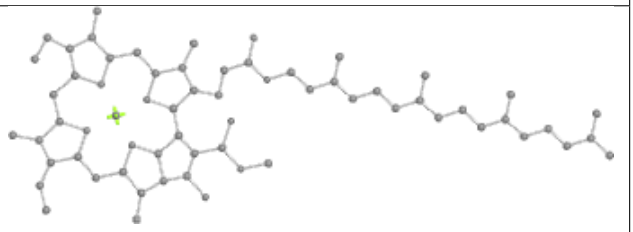
Bond lengths



Bond angles

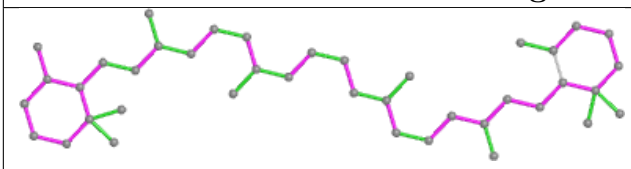


Torsions

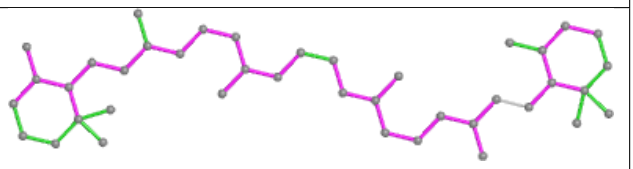


Rings

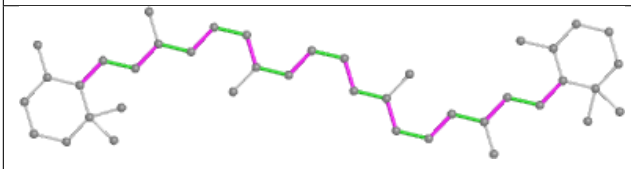
Ligand 8CT L 206



Bond lengths



Bond angles



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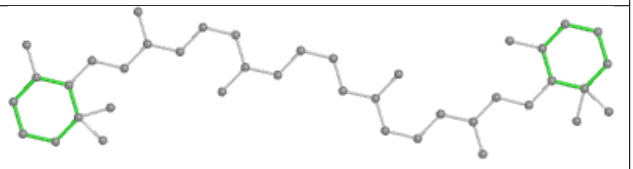
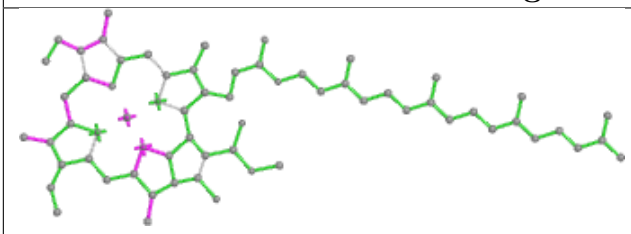
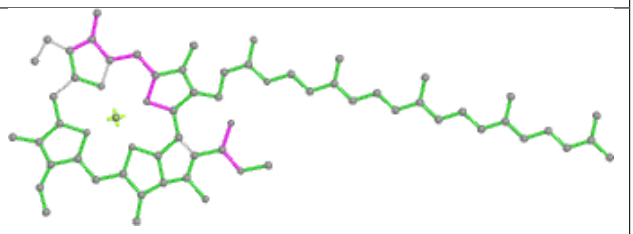


Rings

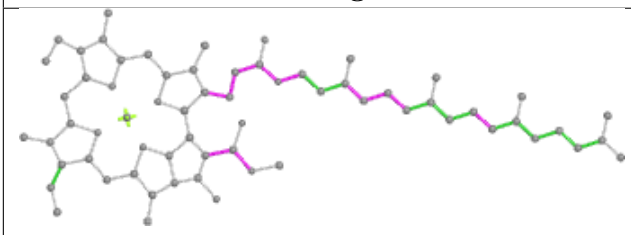
Ligand CLA A 832



Bond lengths



Bond angles



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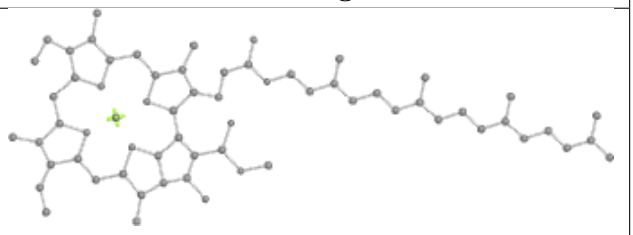
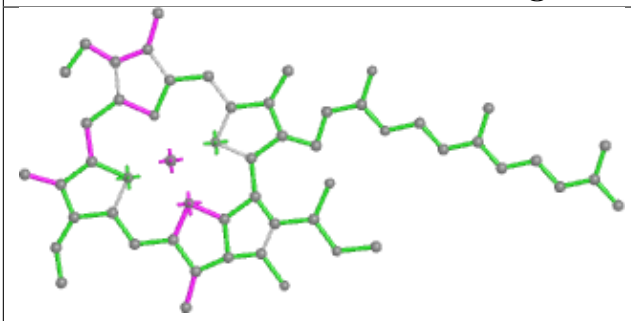
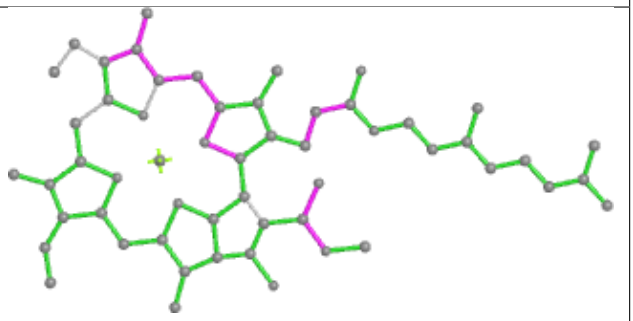


Rings

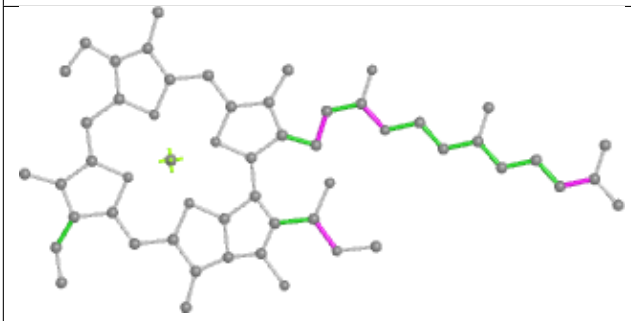
Ligand CLA 4 310



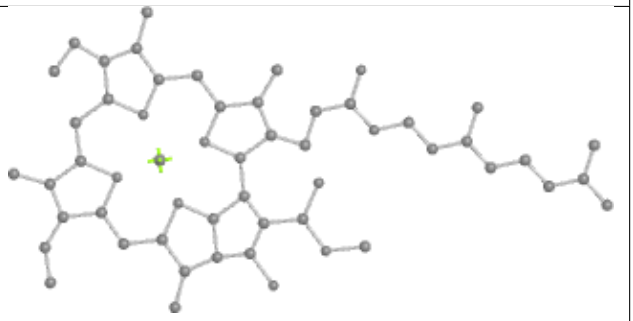
Bond lengths



Bond angles

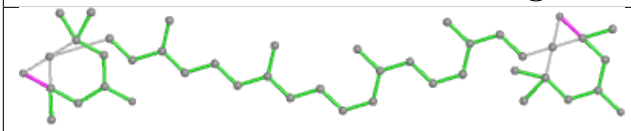


Torsions

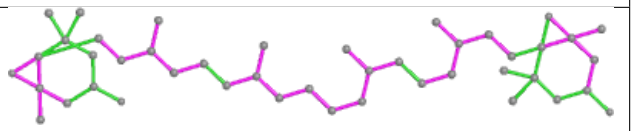


Rings

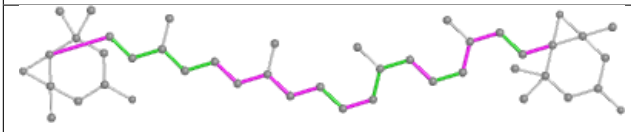
Ligand XAT 0 313



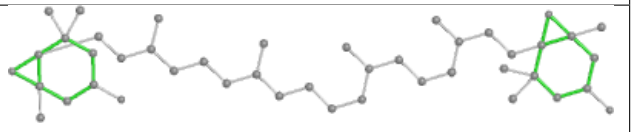
Bond lengths



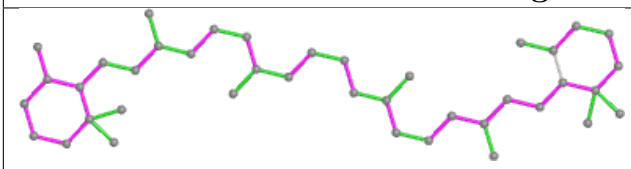
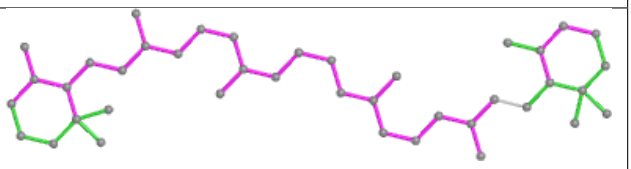
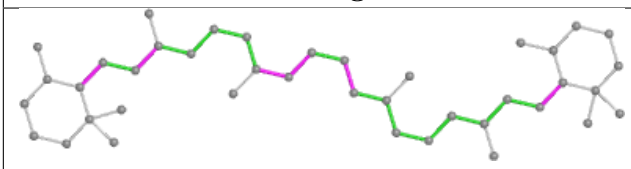
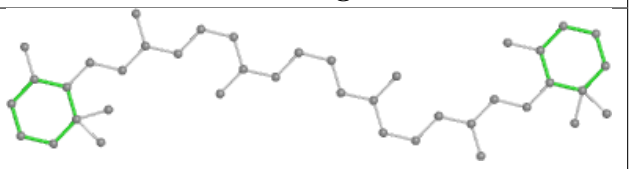
Bond angles

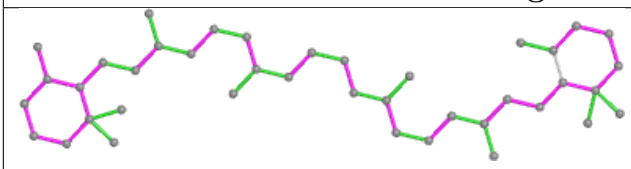
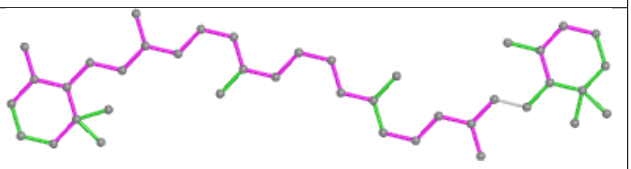
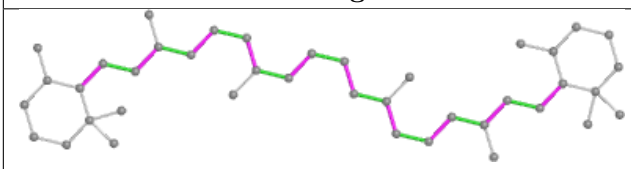
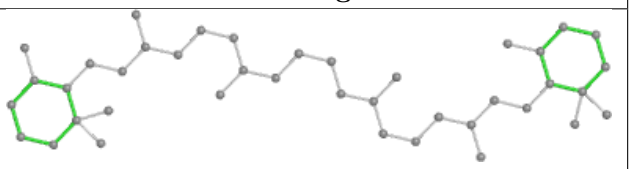


Torsions

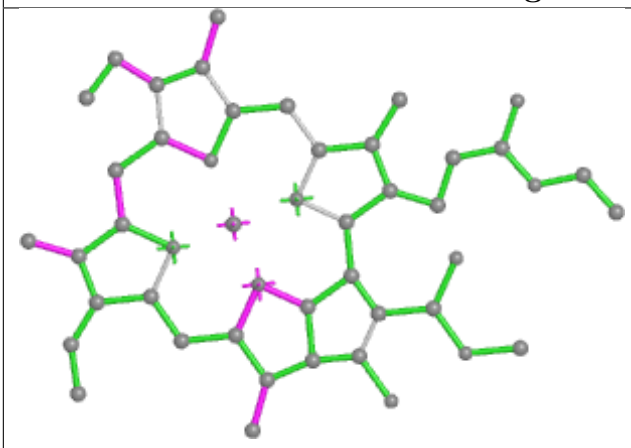


Rings

Ligand 8CT 5 317	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 8CT B 804	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 838



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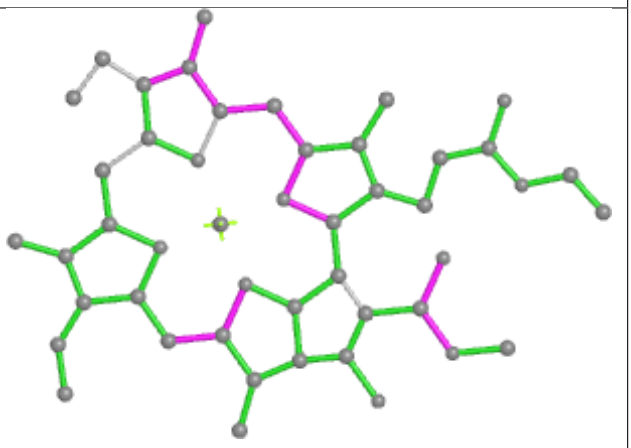

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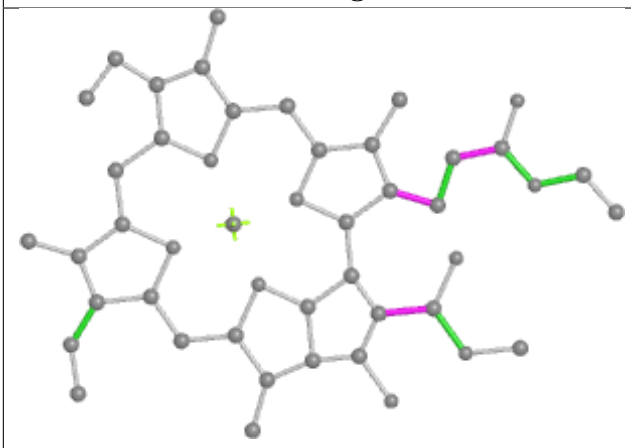

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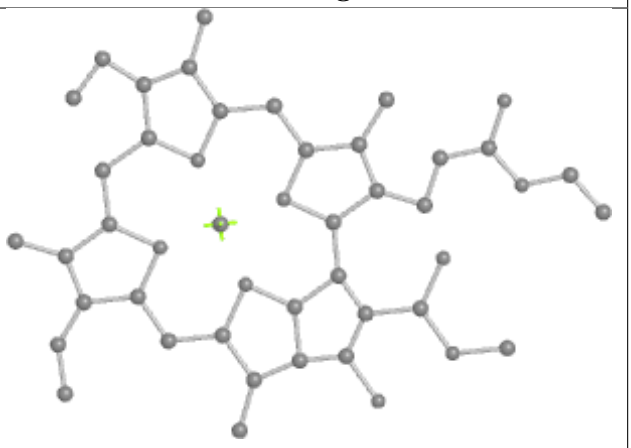
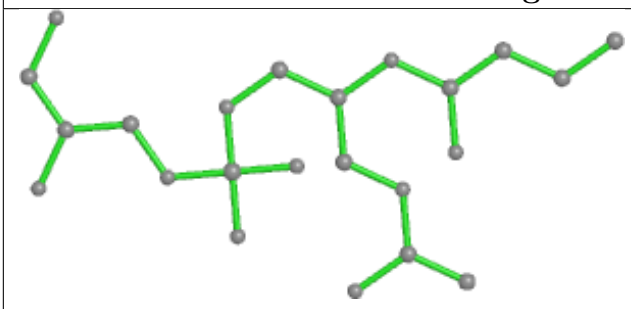


Rings

Ligand LHG B 852



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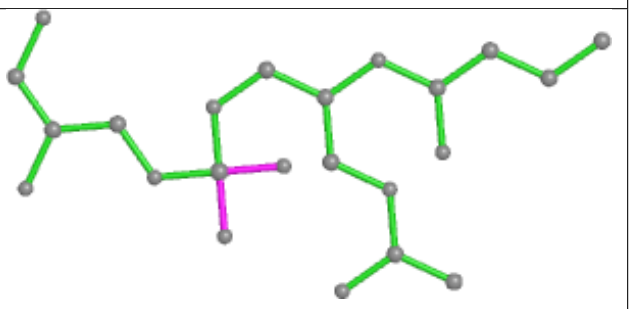

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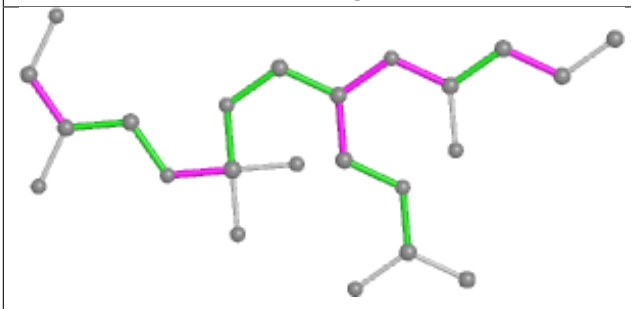

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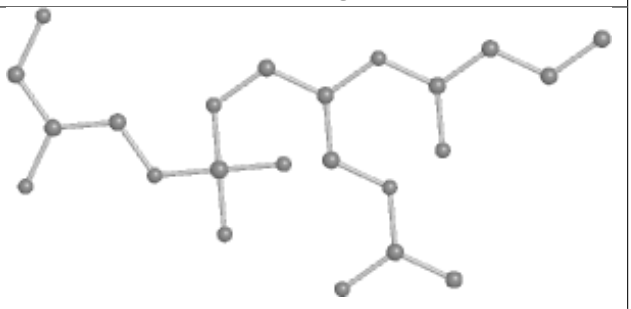
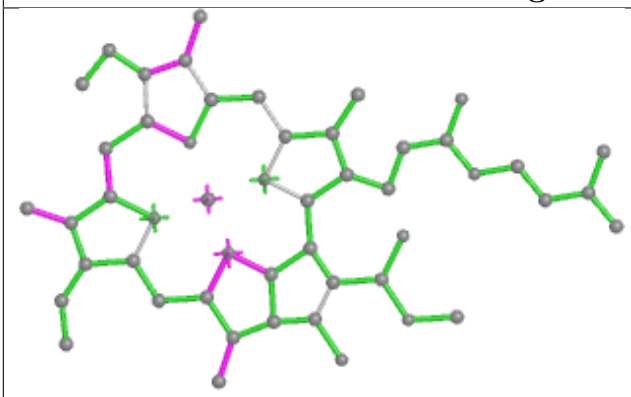


Rings

Ligand CLA 3 302



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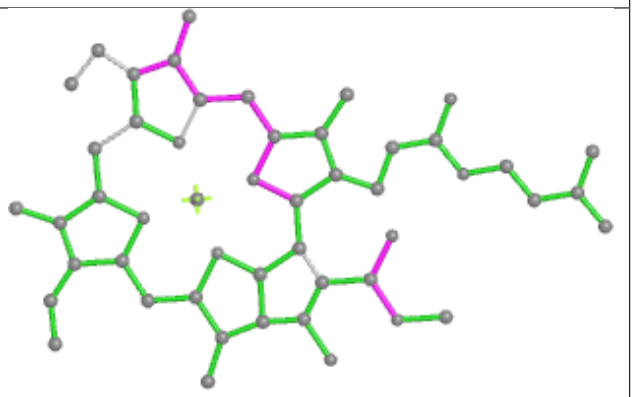
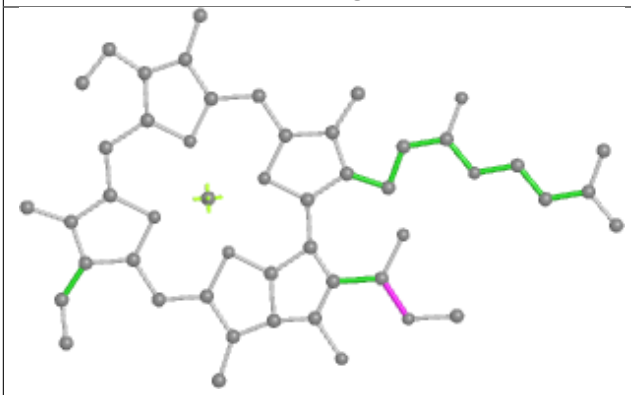


Bond angles



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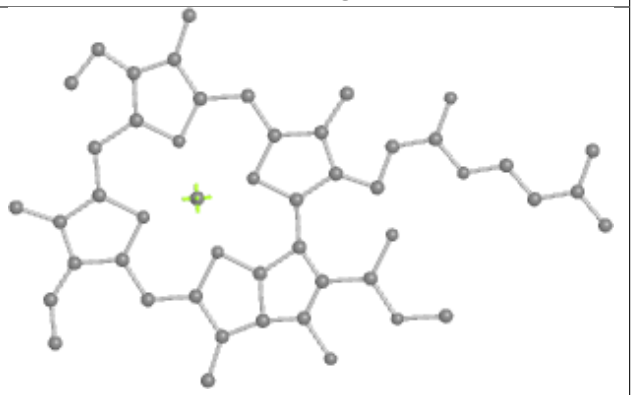
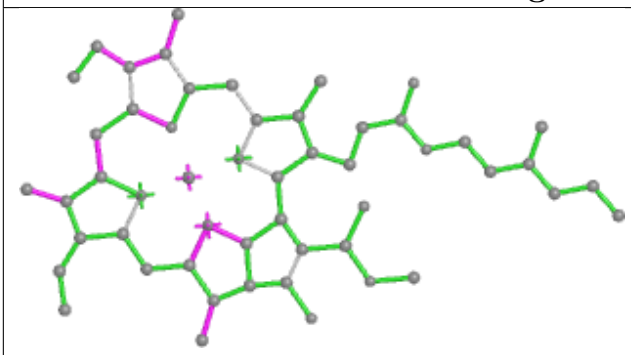


Rings

Ligand CLA 9 306



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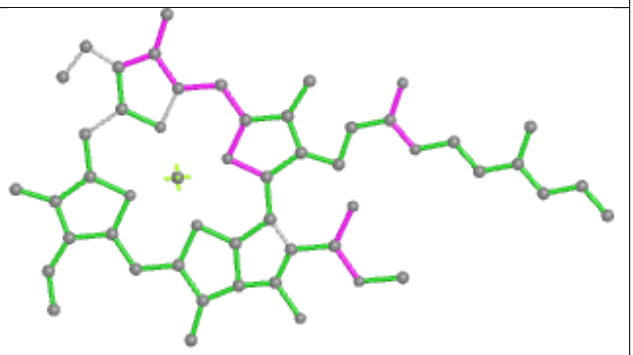

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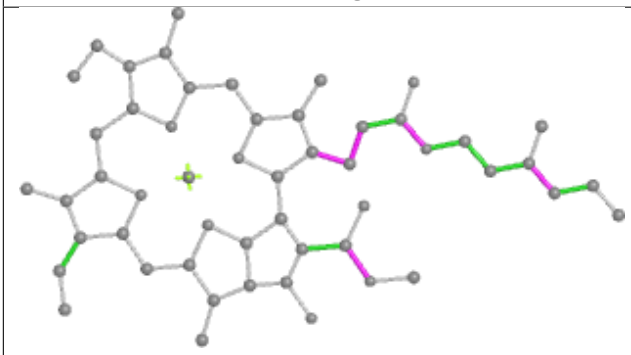

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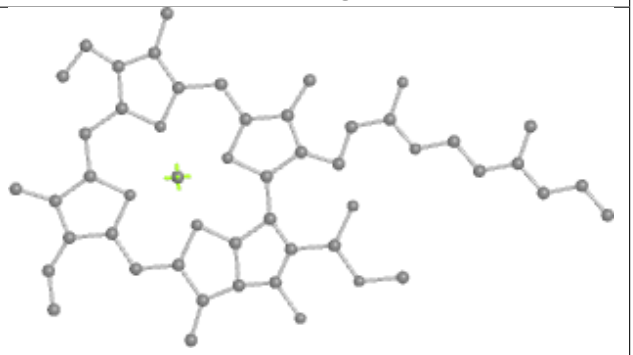
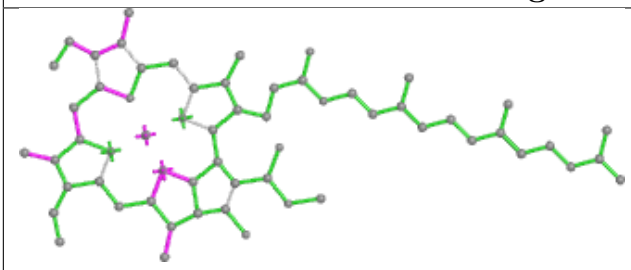


Rings

Ligand CLA 7 303



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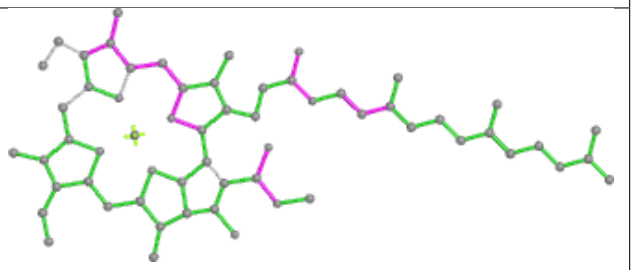

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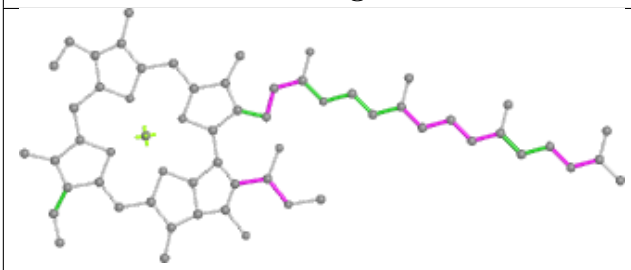

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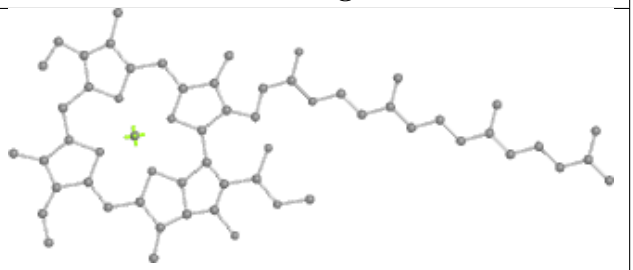
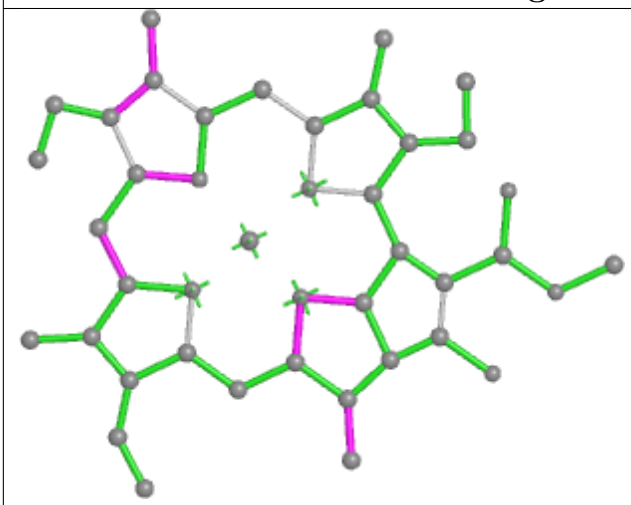


Rings

Ligand CLA 5 308



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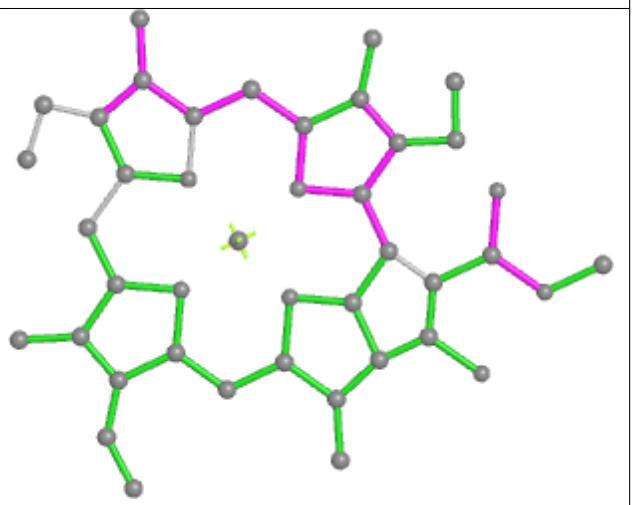
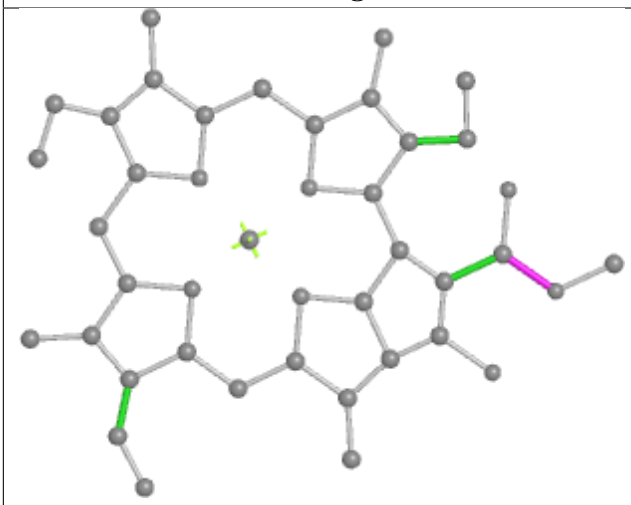


Bond angles



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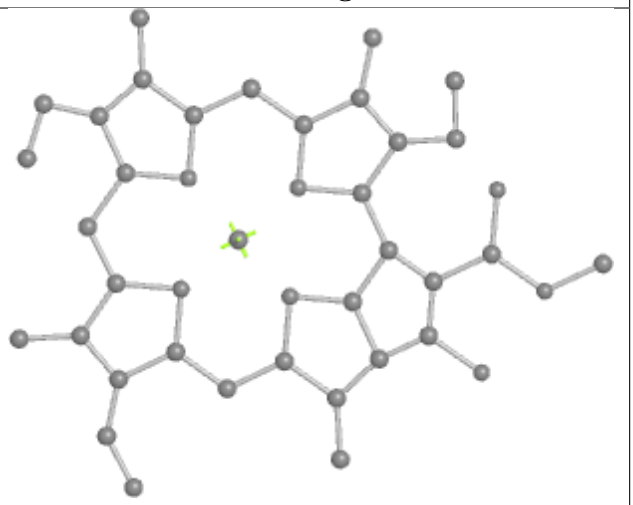
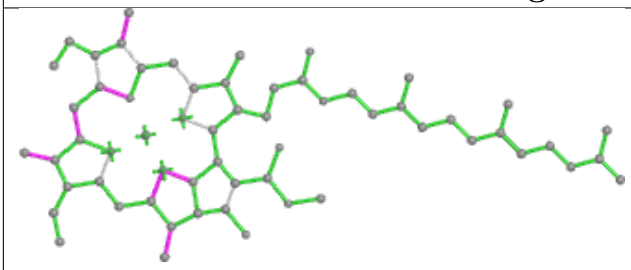


Rings

Ligand CLA 0 308



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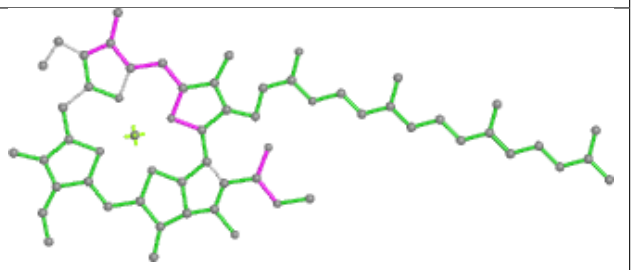

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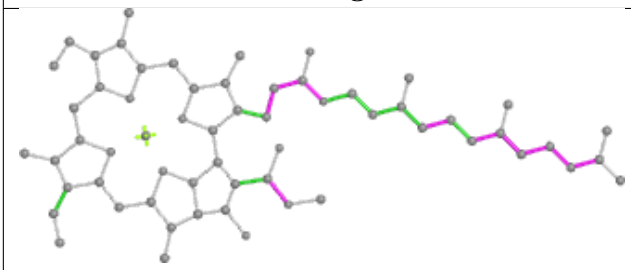

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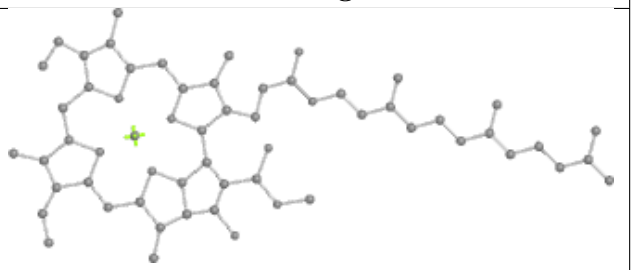
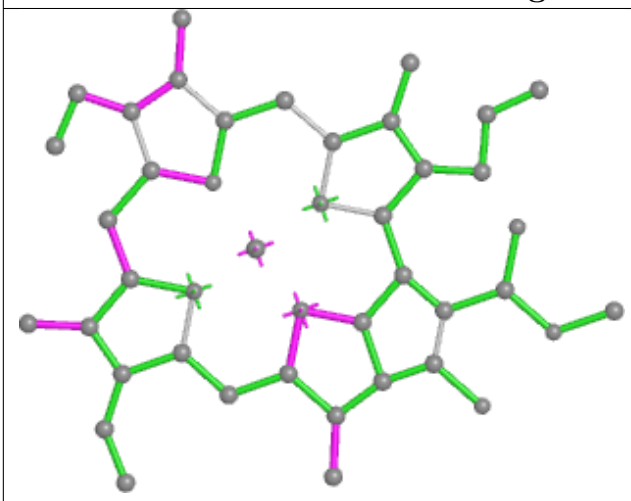


Rings

Ligand CLA 2 313



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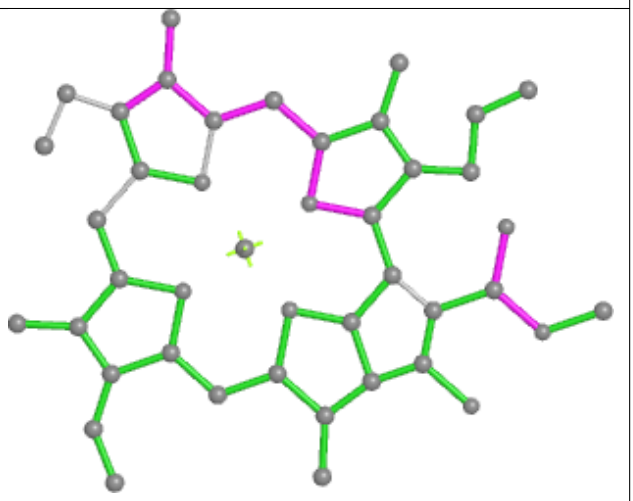

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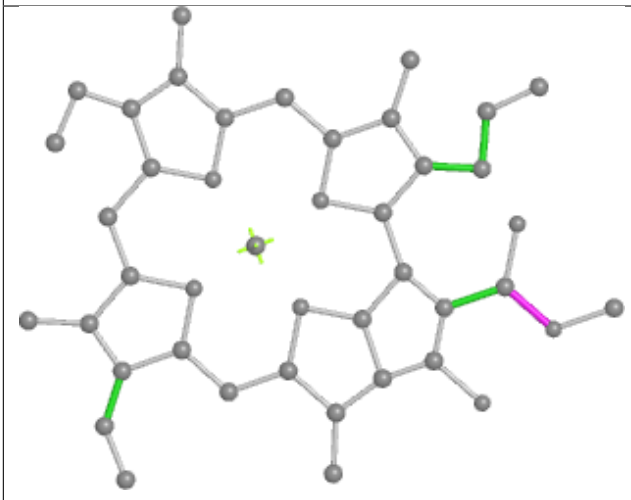

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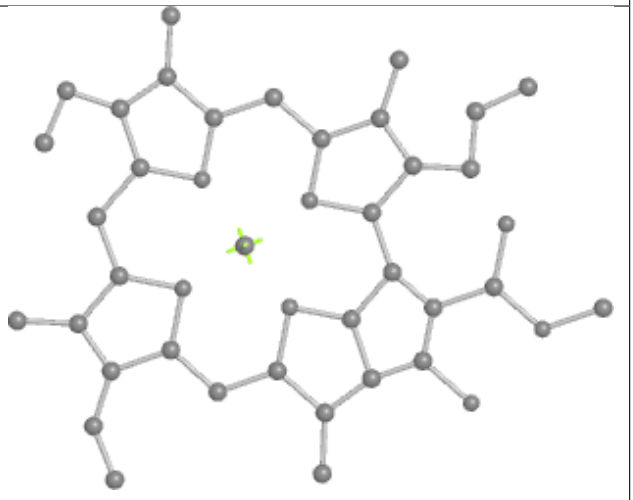
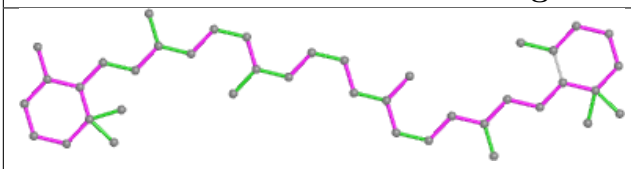
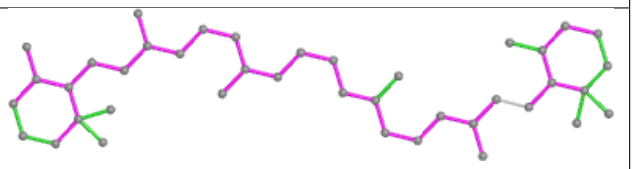
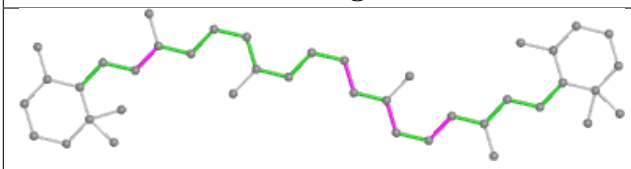
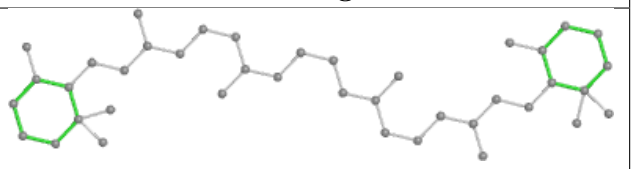
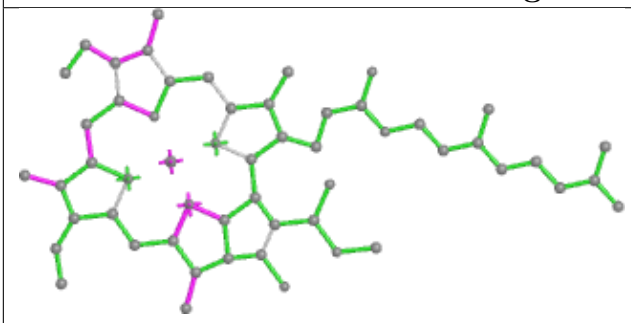
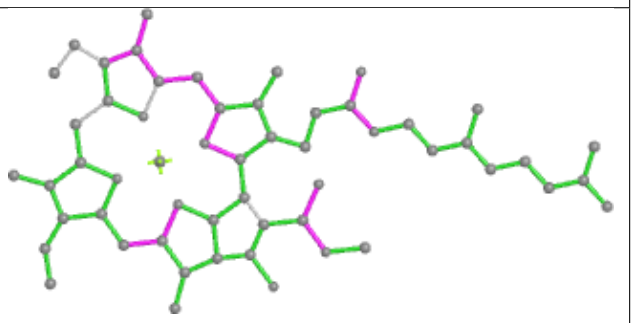
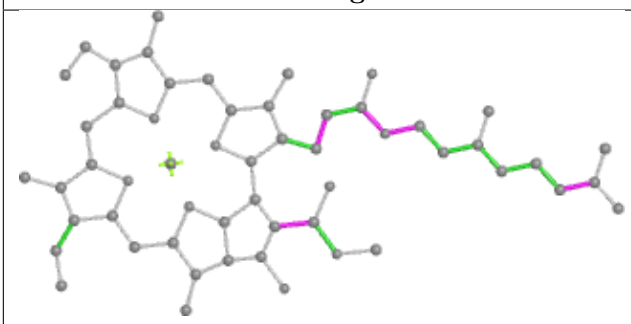
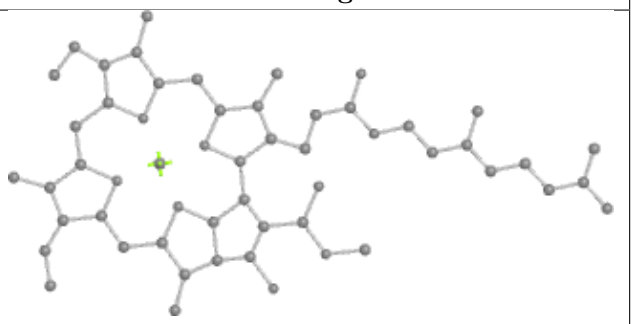
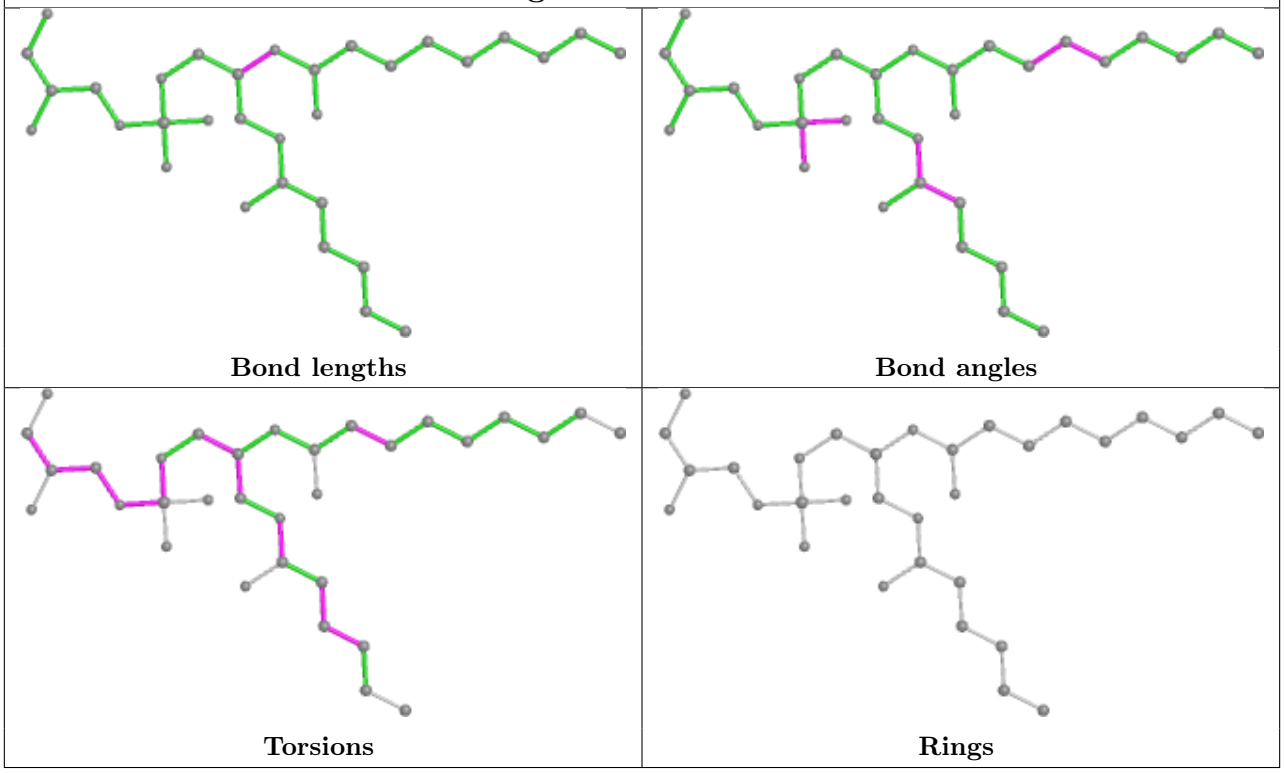


Rings

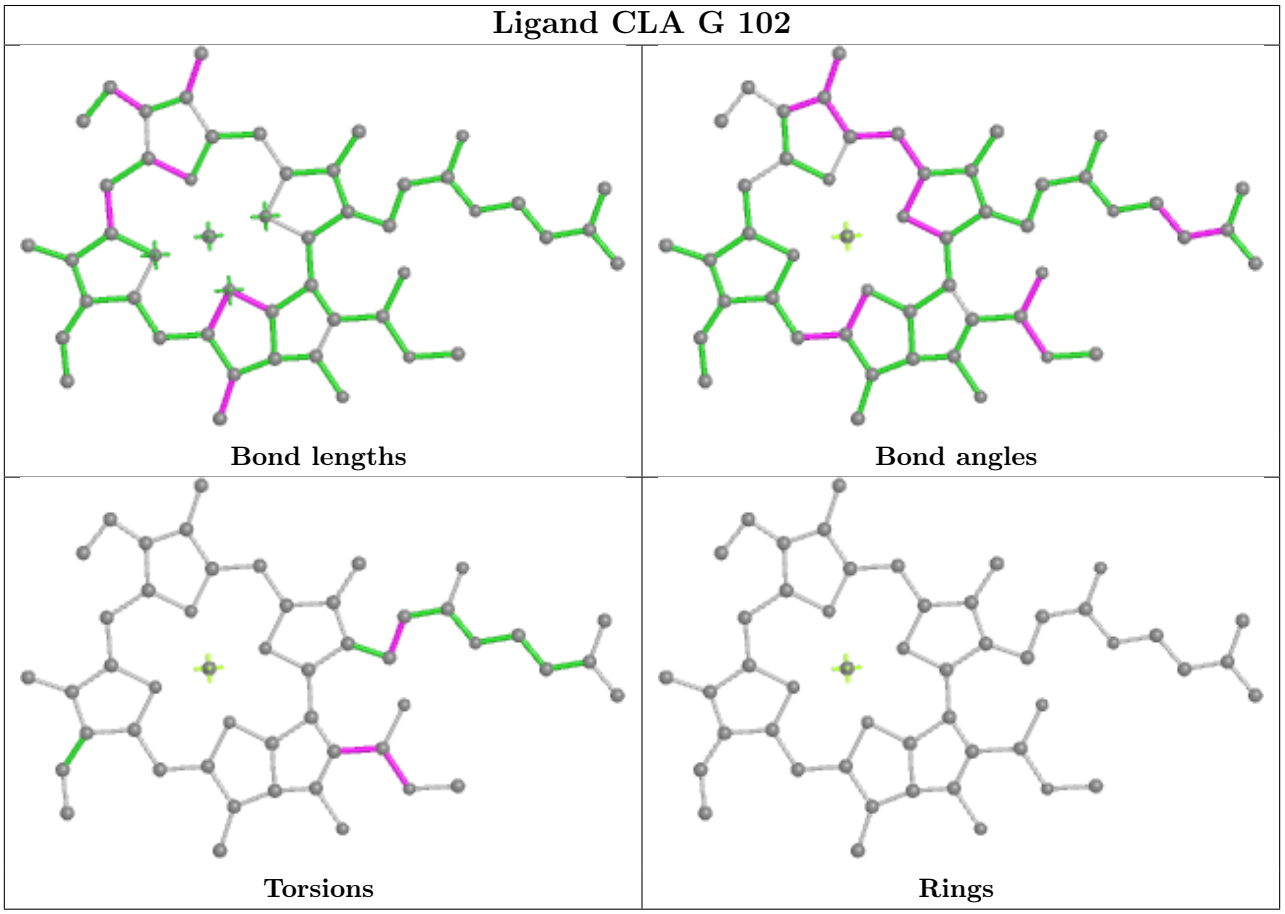
Ligand 8CT 3 318	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 824	
 Bond lengths	 Bond angles
 Torsions	 Rings

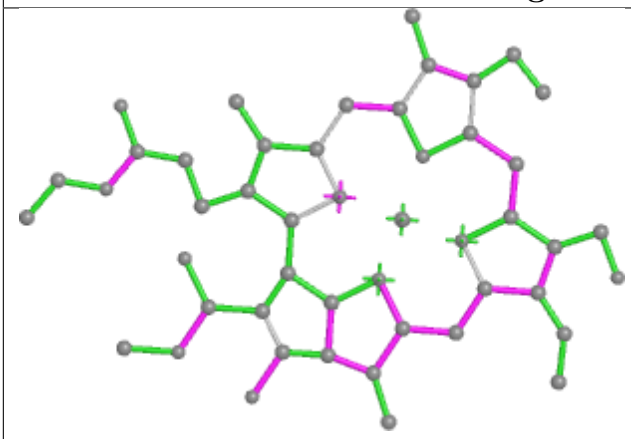
Ligand LHG 2 318



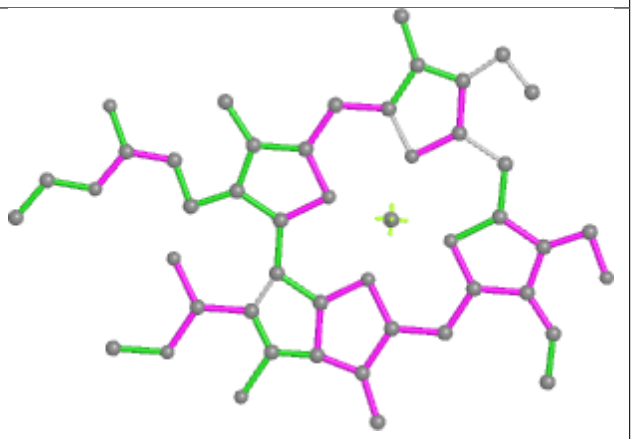
Ligand CLA G 102



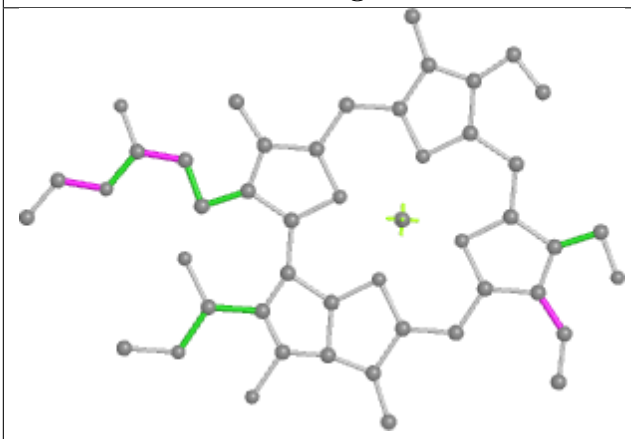
Ligand CHL 0 306



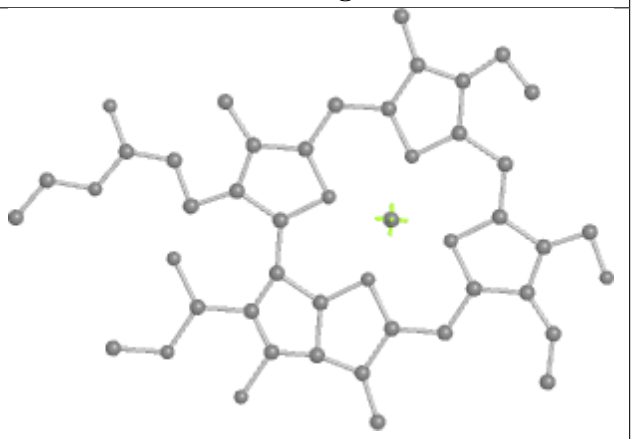
Bond lengths



Bond angles

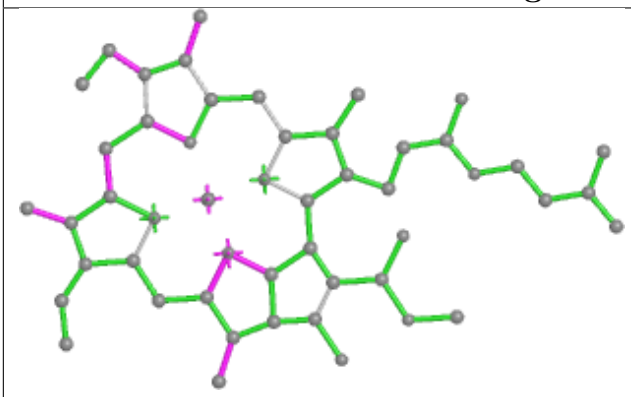


Torsions

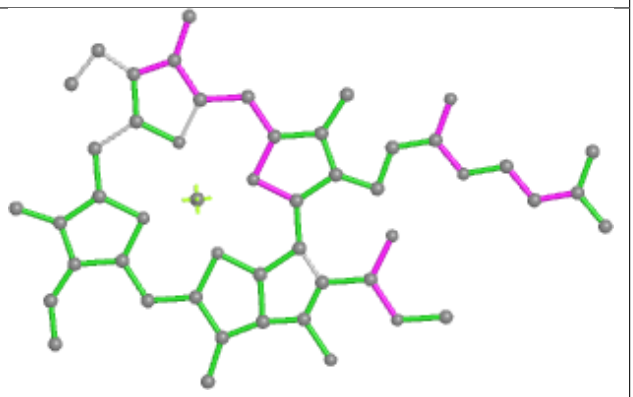


Rings

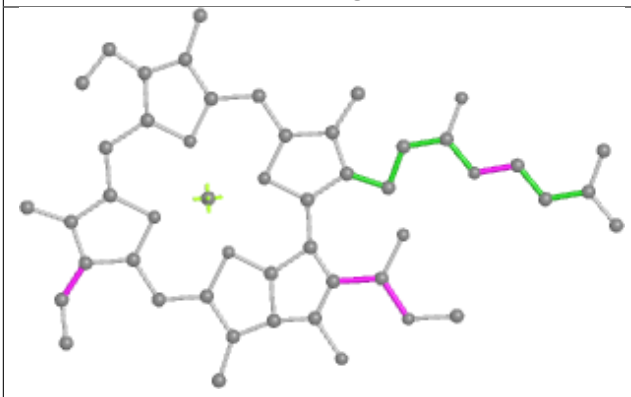
Ligand CLA B 821



Bond lengths



Bond angles



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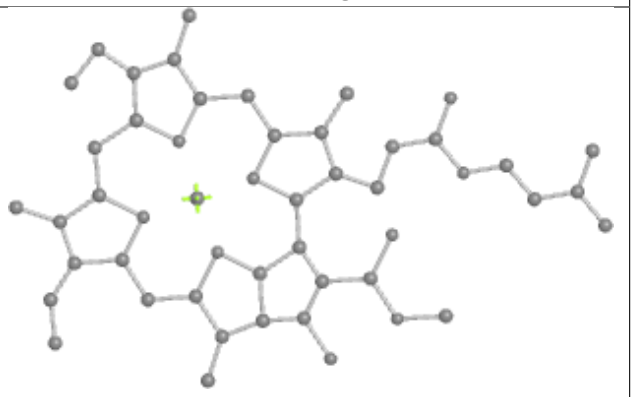
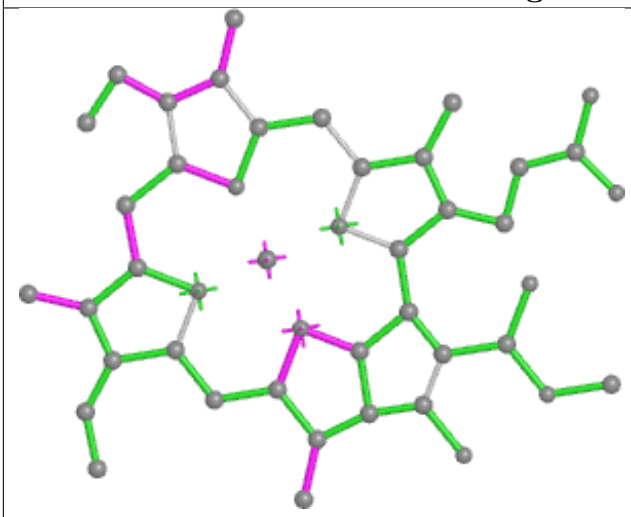
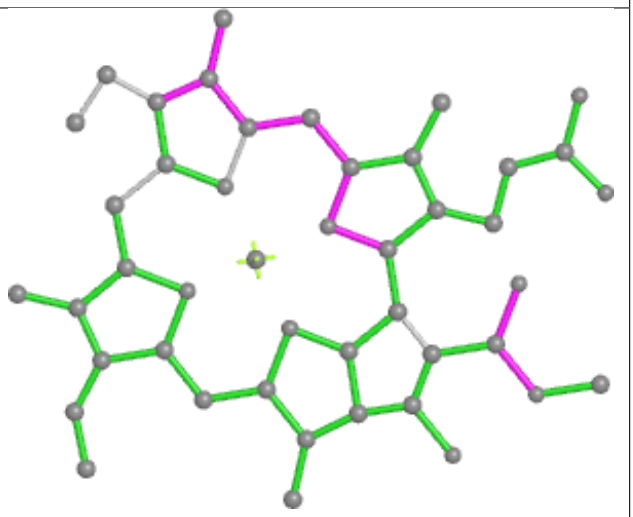


Rings

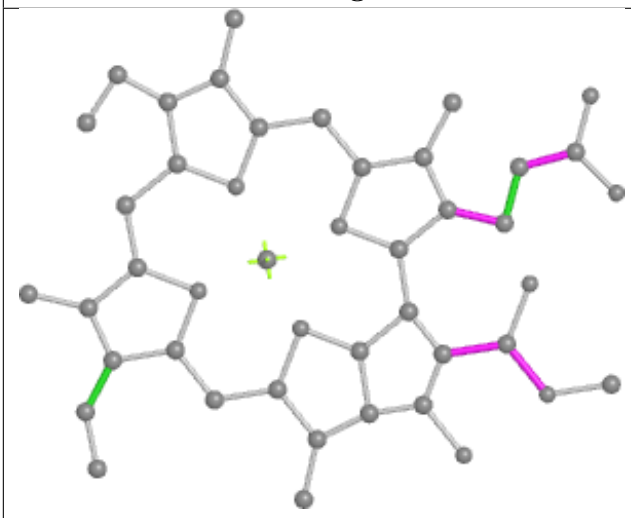
Ligand CLA F 301



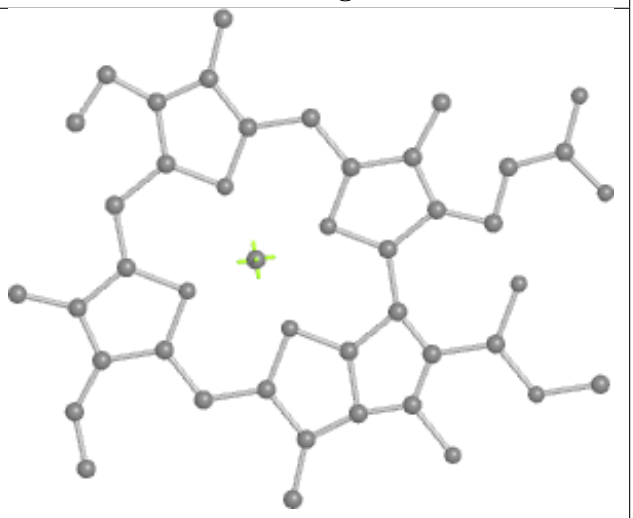
Bond lengths



Bond angles

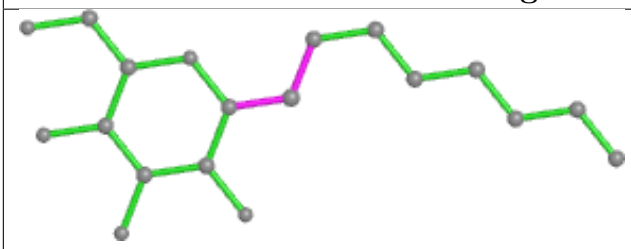


Torsions

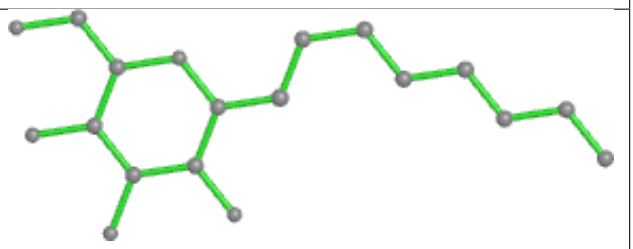


Rings

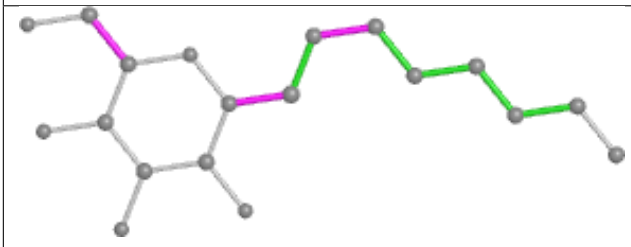
Ligand HTG A 851



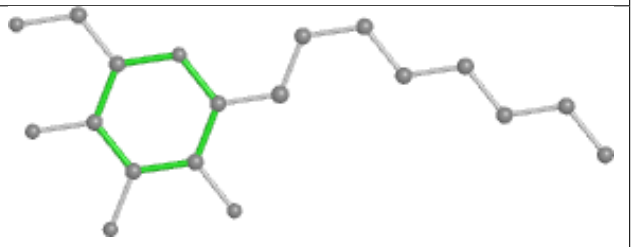
Bond lengths



Bond angles

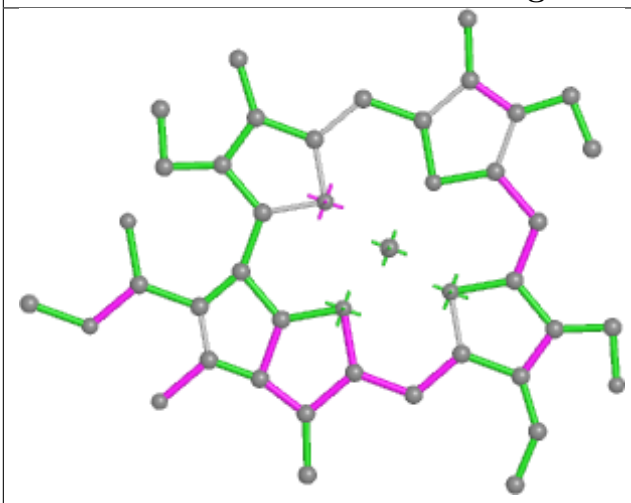


Torsions



Rings

Ligand CHL 6 306



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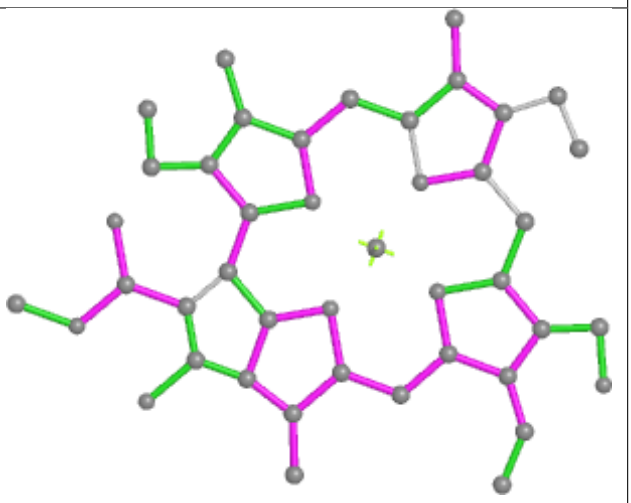
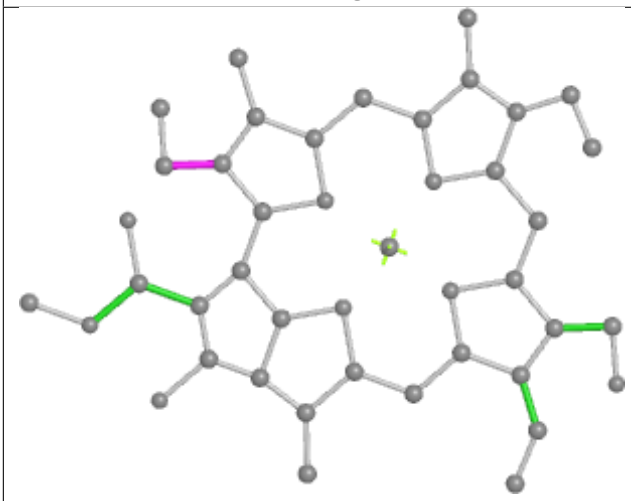
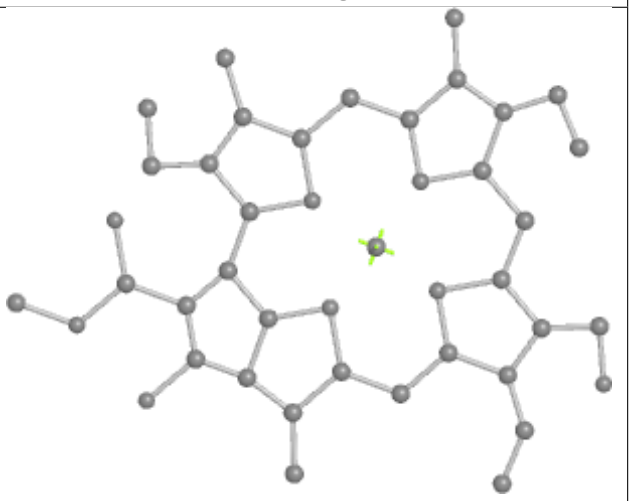


Bond angles

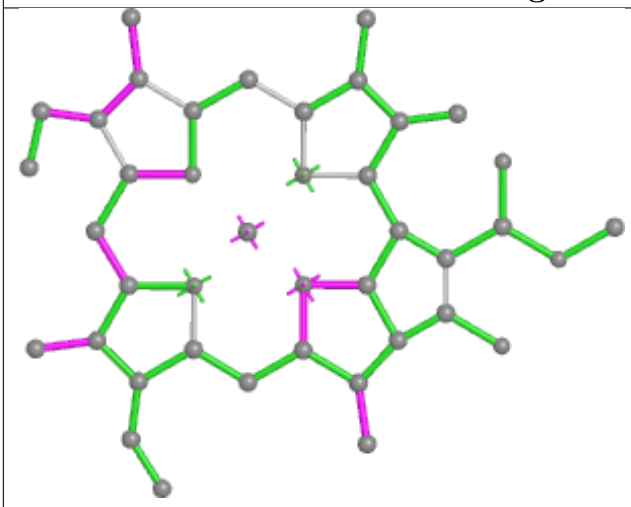


Torsions

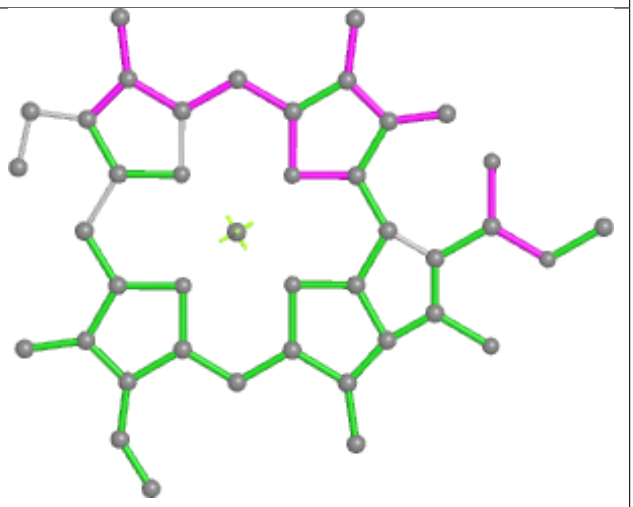


Rings

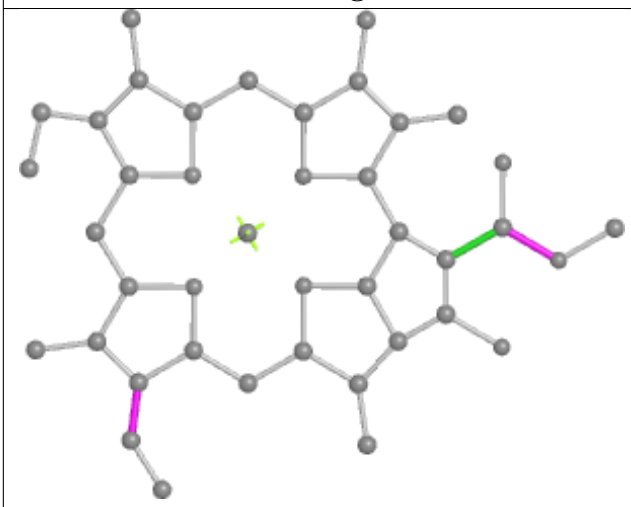
Ligand CLA 2 310



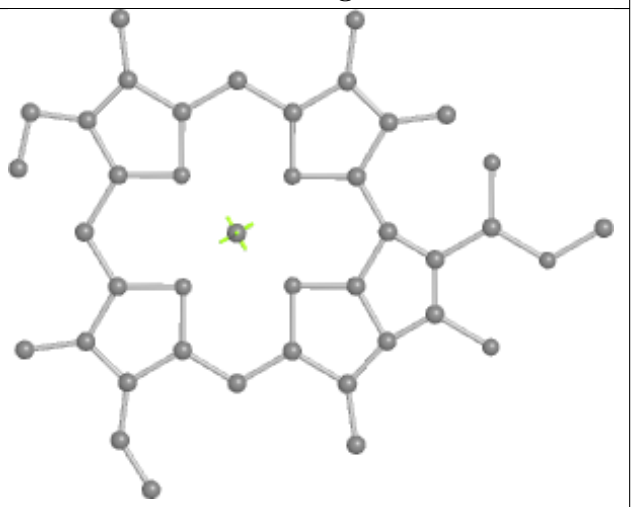
Bond lengths



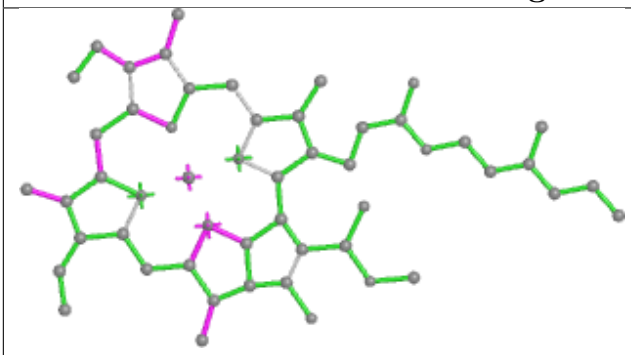
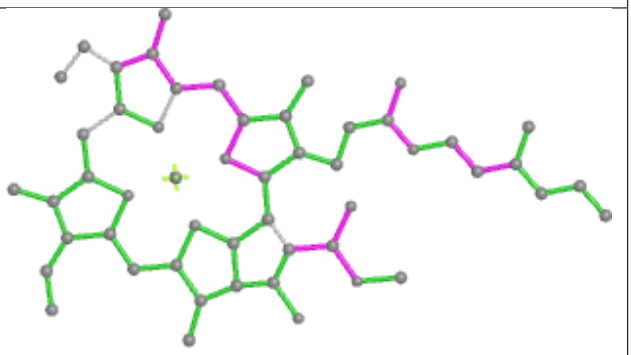
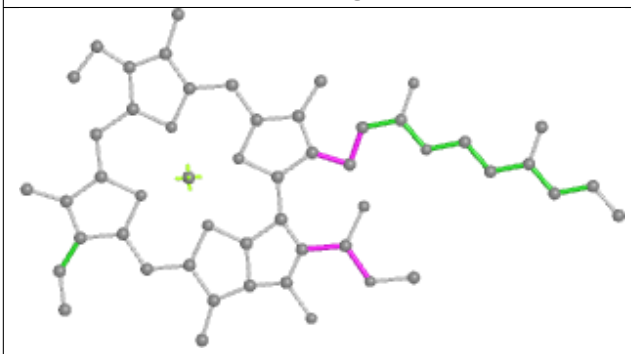
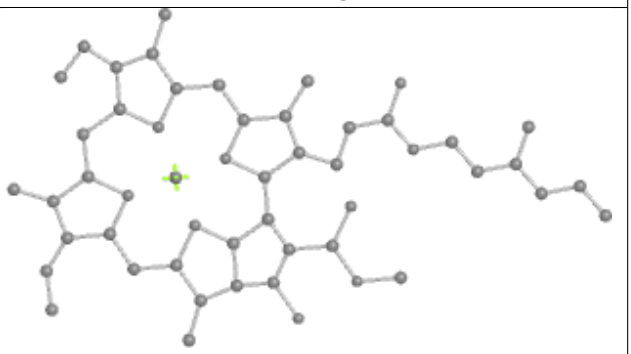
Bond angles

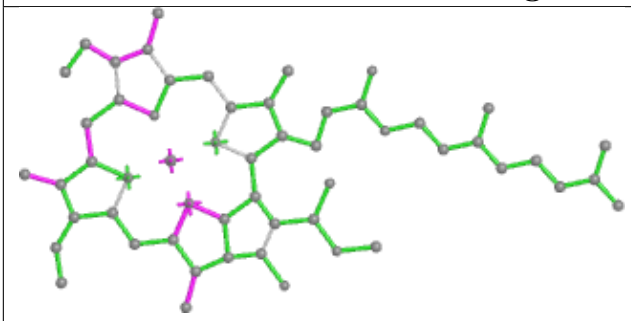
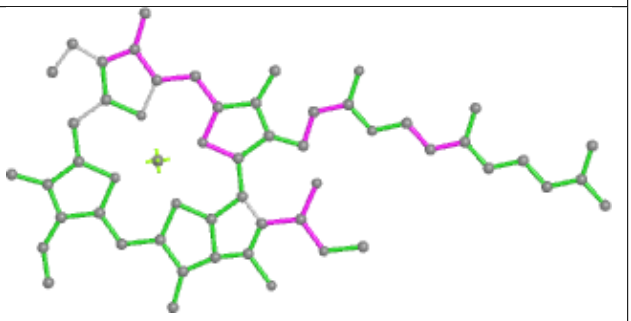
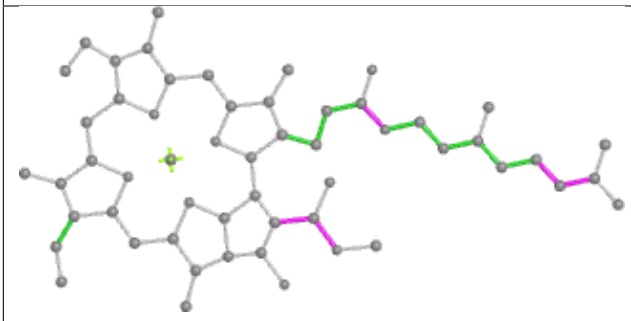
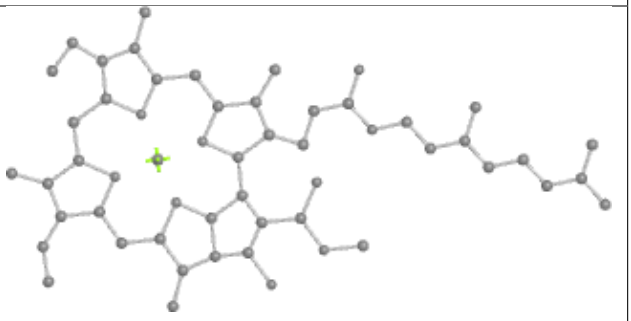


Torsions

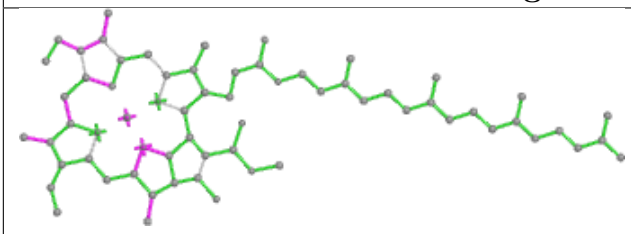


Rings

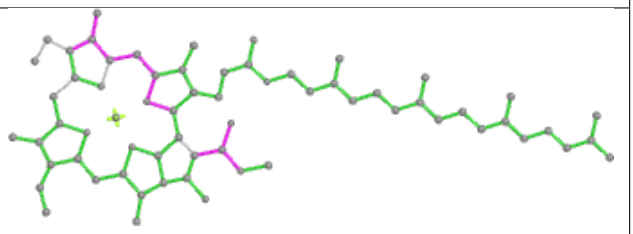
Ligand CLA 6 318	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 804	
	
Bond lengths	Bond angles
	
Torsions	Rings

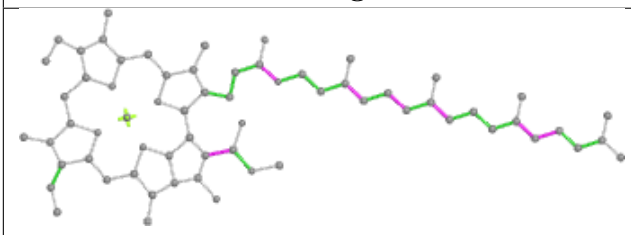
Ligand CLA A 830



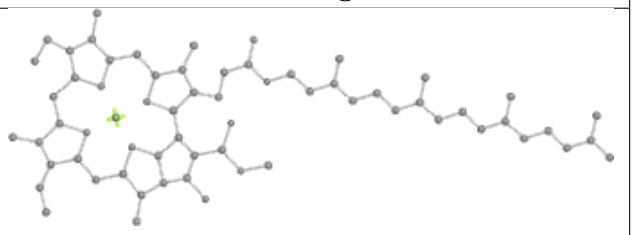
Bond lengths



Bond angles

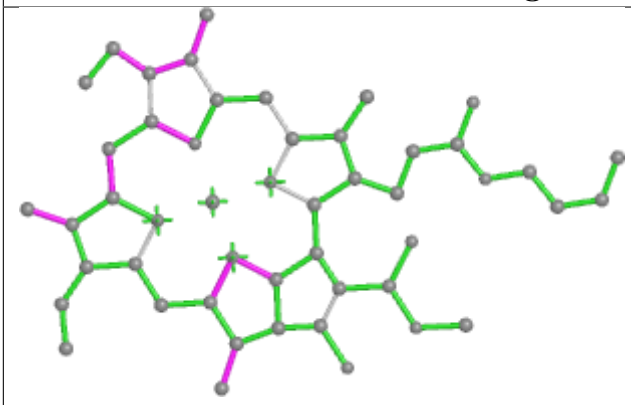


Torsions

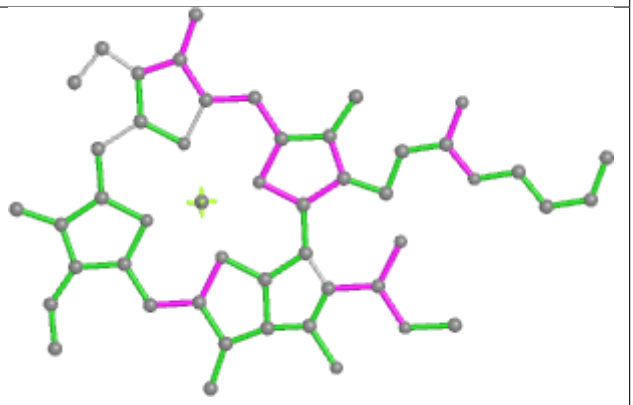


Rings

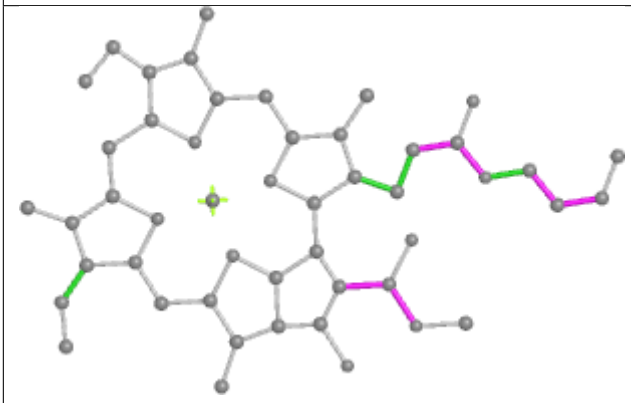
Ligand CLA A 822



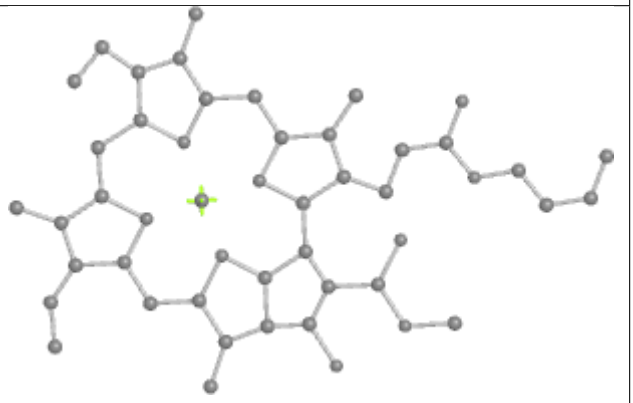
Bond lengths



Bond angles

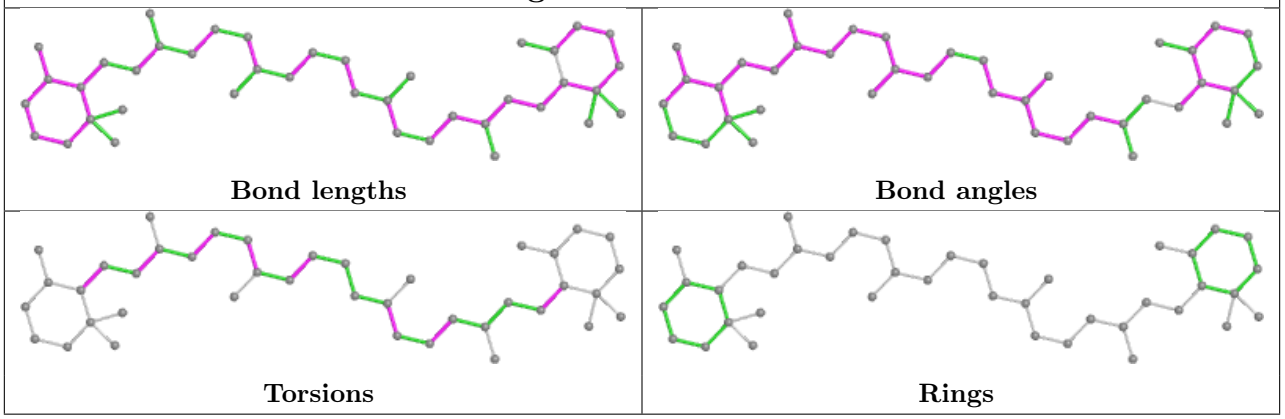


Torsions

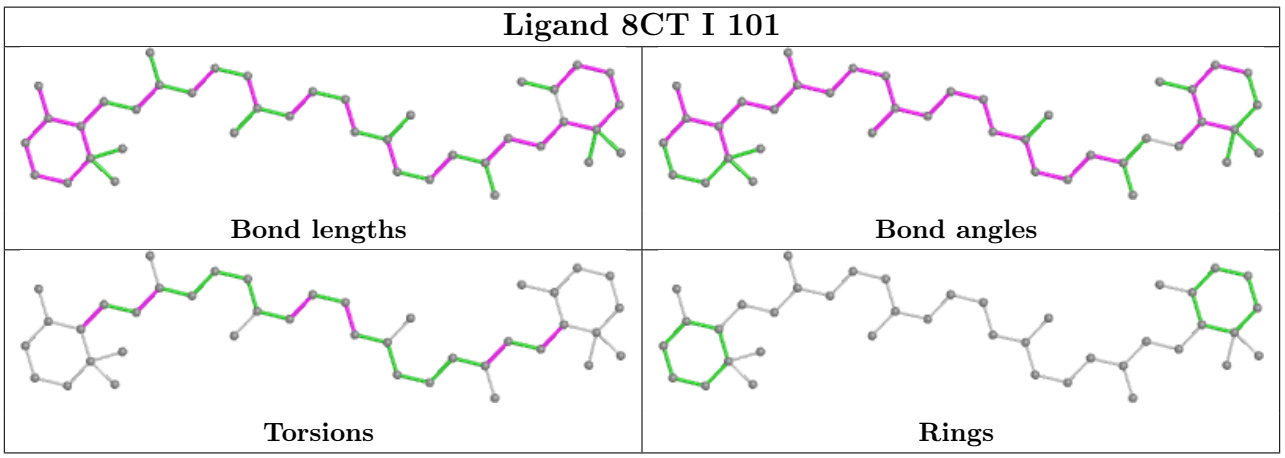


Rings

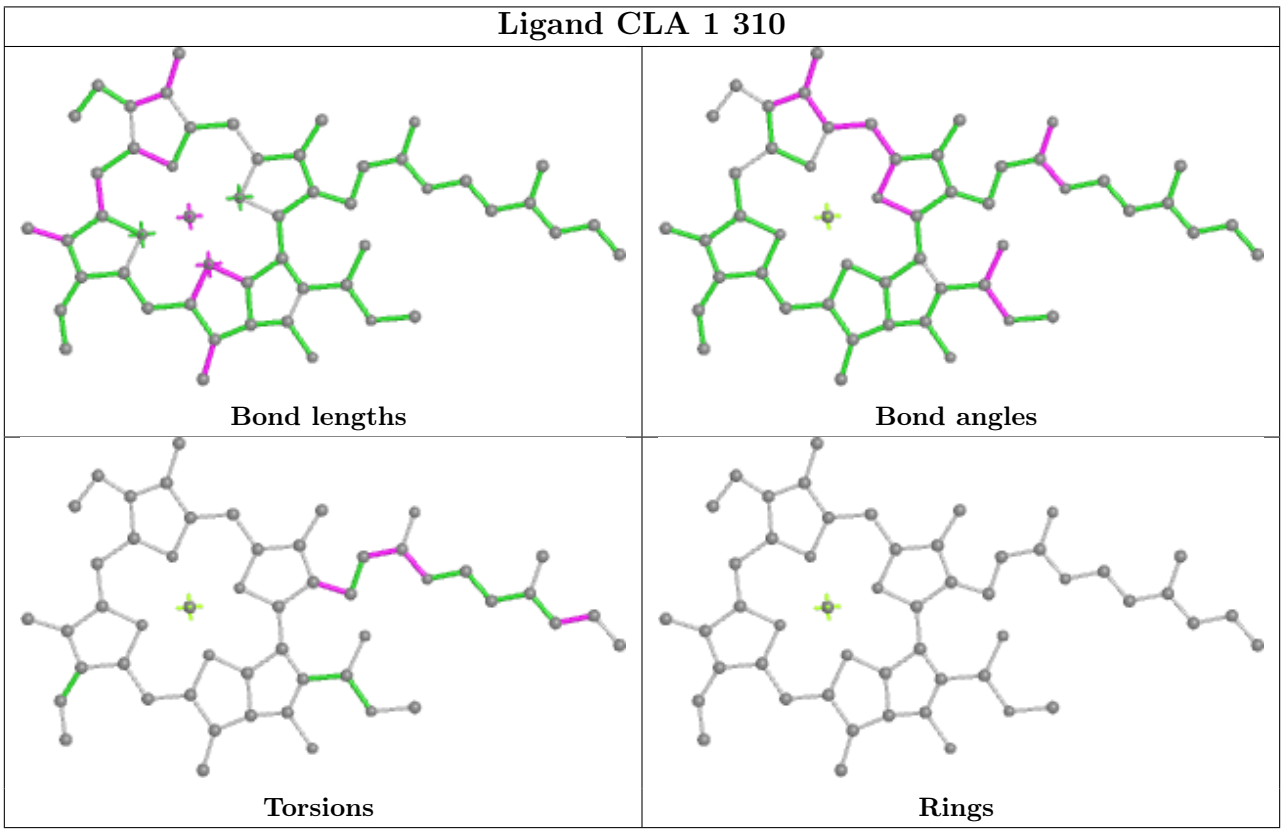
Ligand 8CT A 854



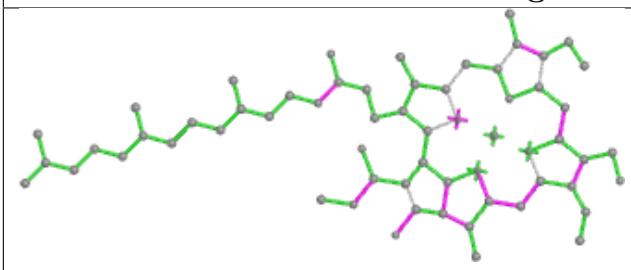
Ligand 8CT I 101



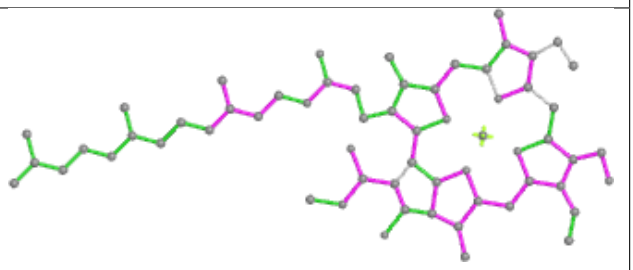
Ligand CLA 1 310



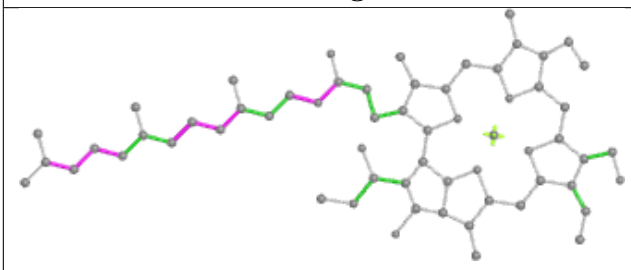
Ligand CHL 4 301



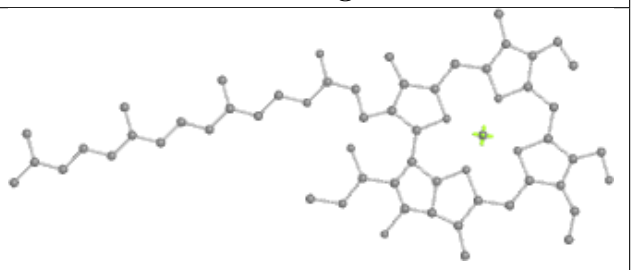
Bond lengths



Bond angles

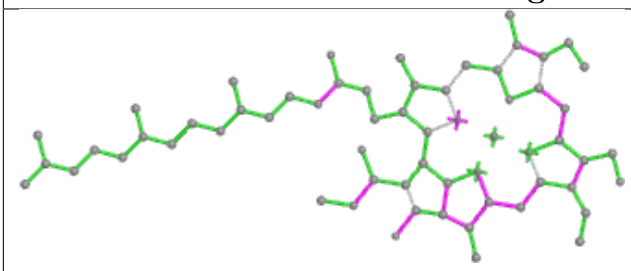


Torsions

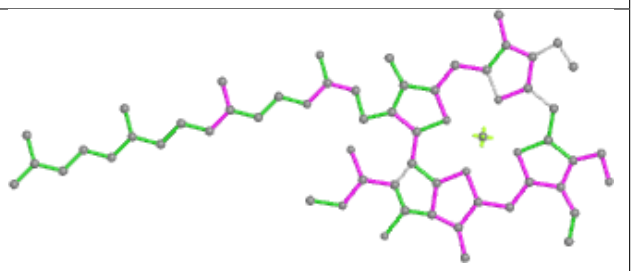


Rings

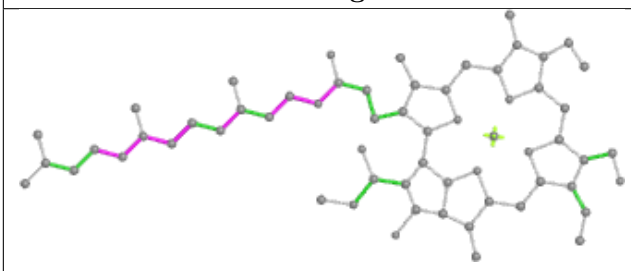
Ligand CHL 9 302



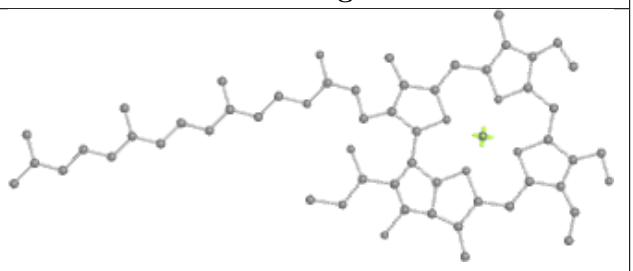
Bond lengths



Bond angles

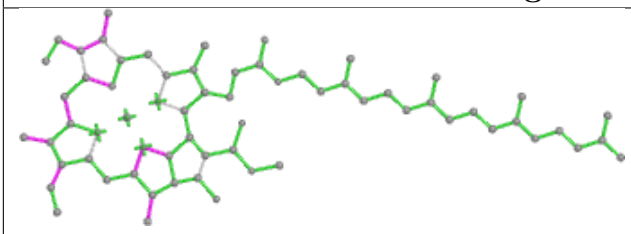


Torsions

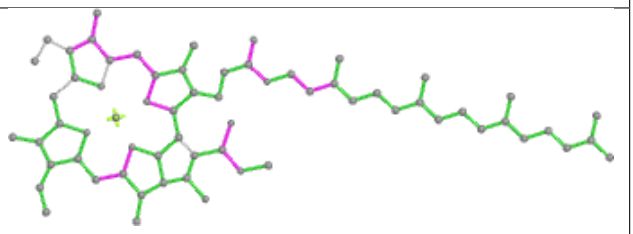


Rings

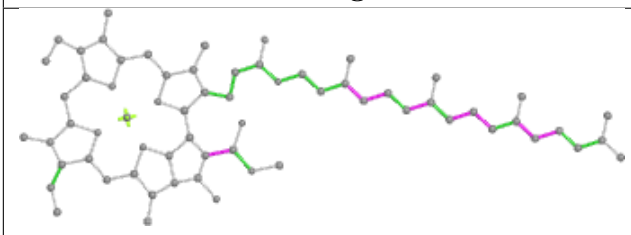
Ligand CLA B 811



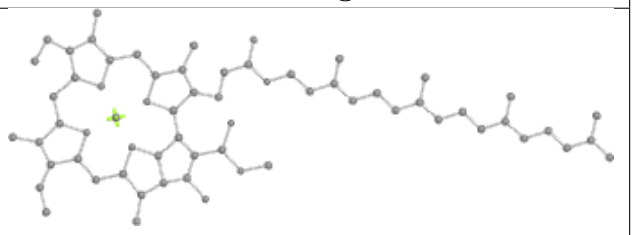
Bond lengths



Bond angles

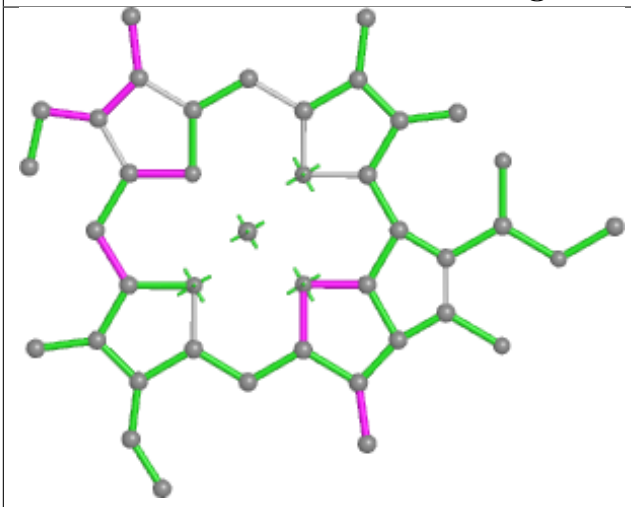


Torsions

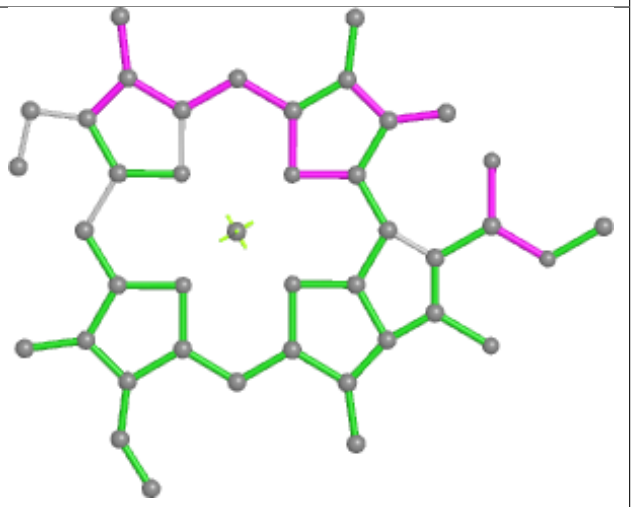


Rings

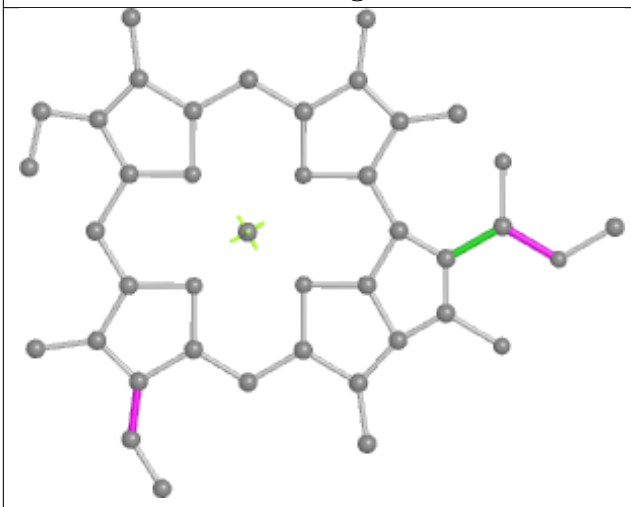
Ligand CLA 9 310



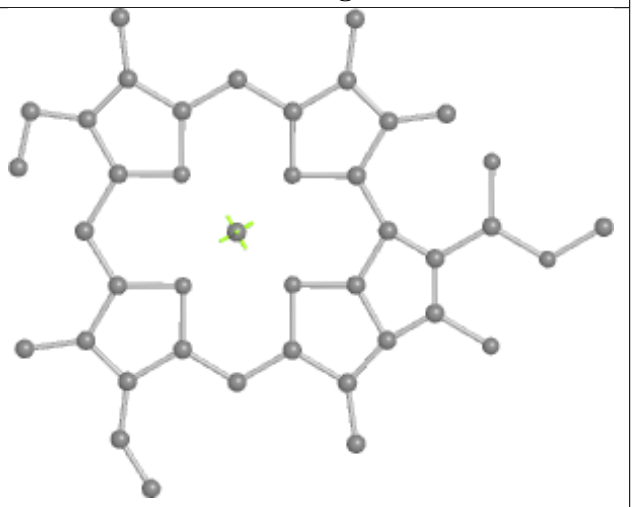
Bond lengths



Bond angles

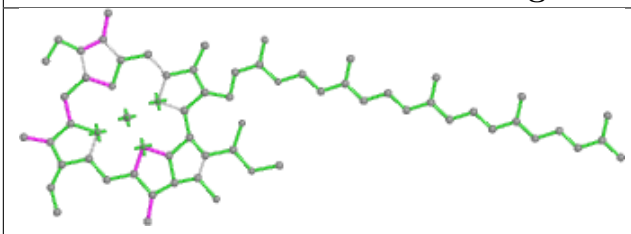


Torsions

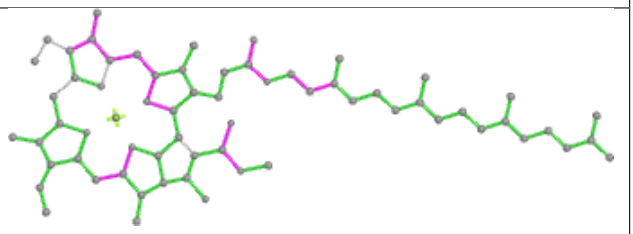


Rings

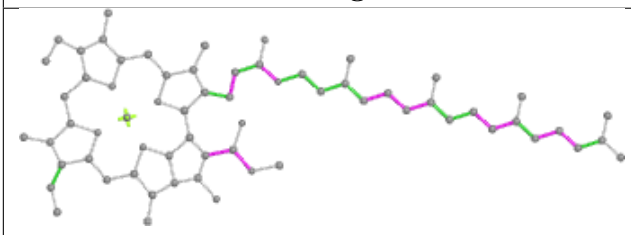
Ligand CLA 0 311



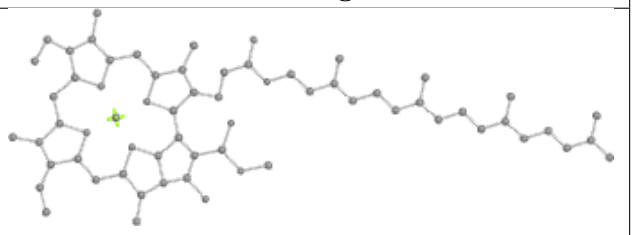
Bond lengths



Bond angles

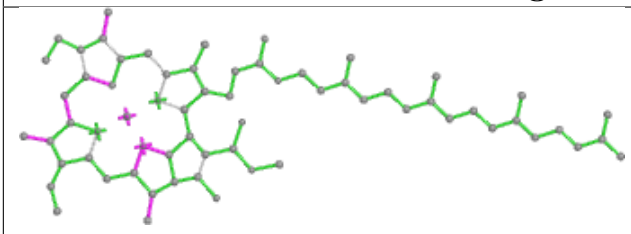


Torsions

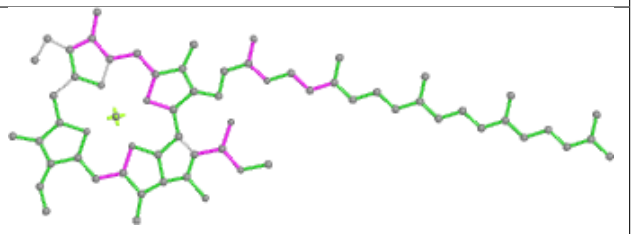


Rings

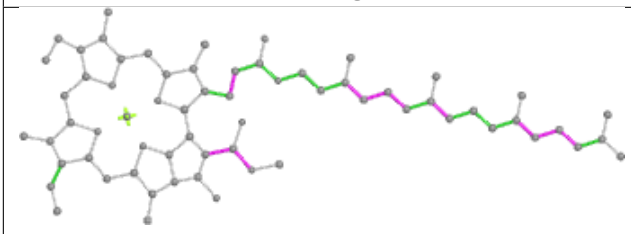
Ligand CLA 0 302



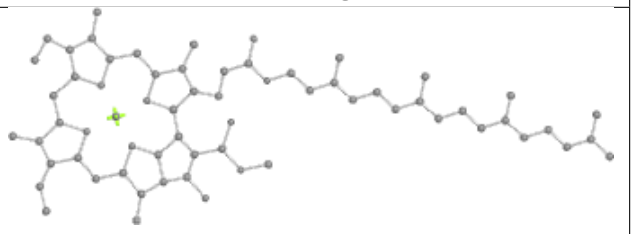
Bond lengths



Bond angles

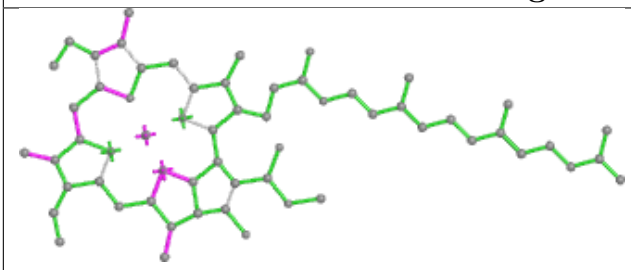


Torsions

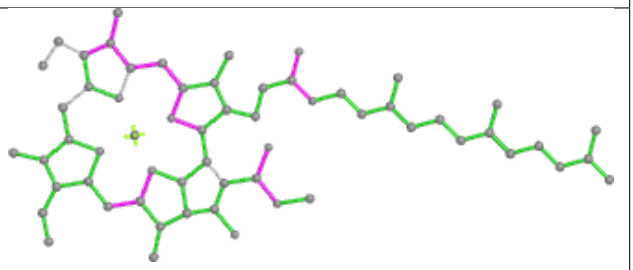


Rings

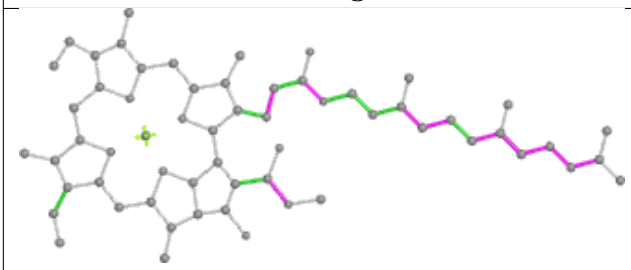
Ligand CLA 2 304



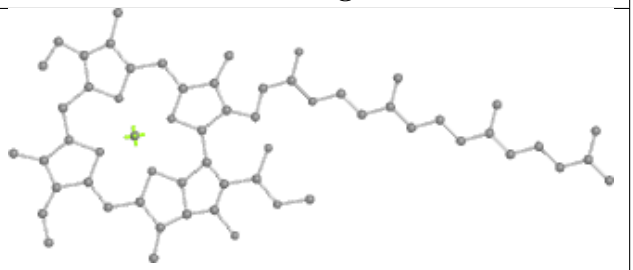
Bond lengths



Bond angles

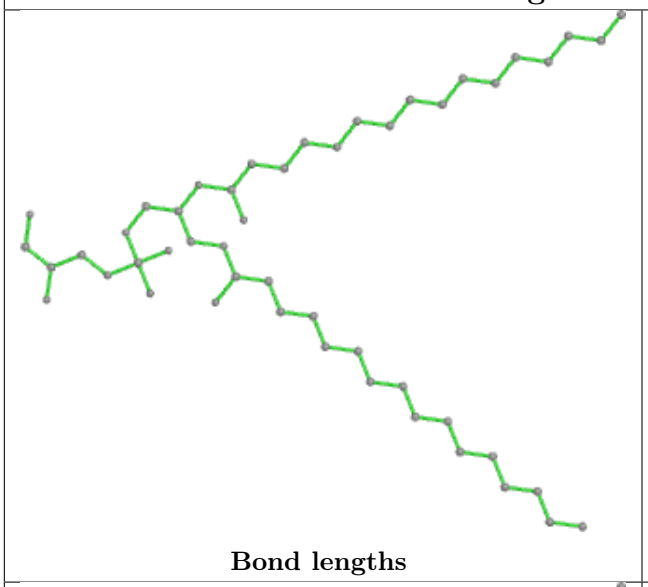


Torsions

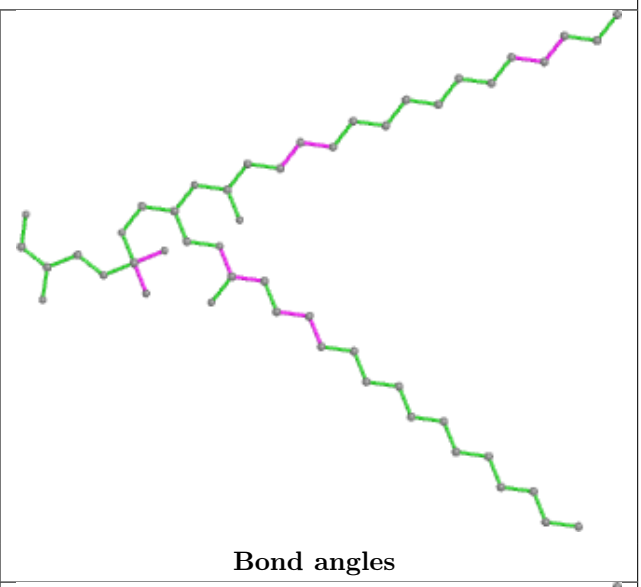


Rings

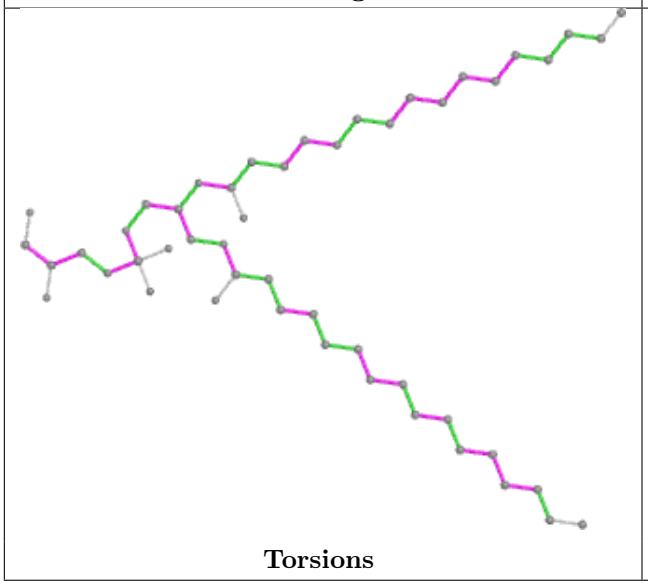
Ligand LHG 0 315



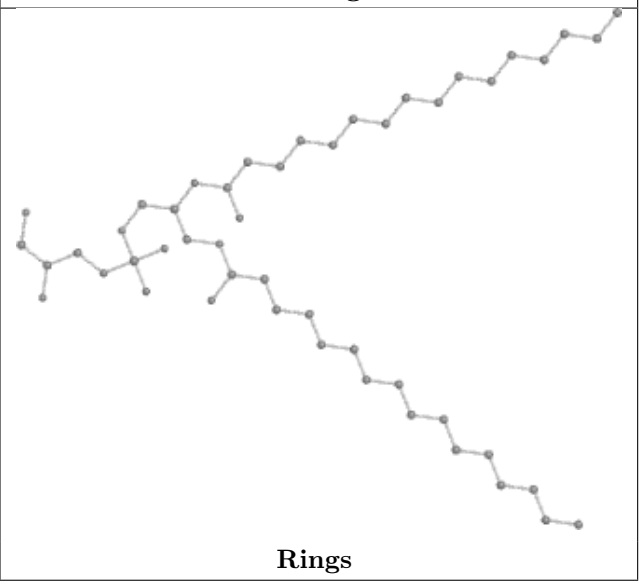
Bond lengths



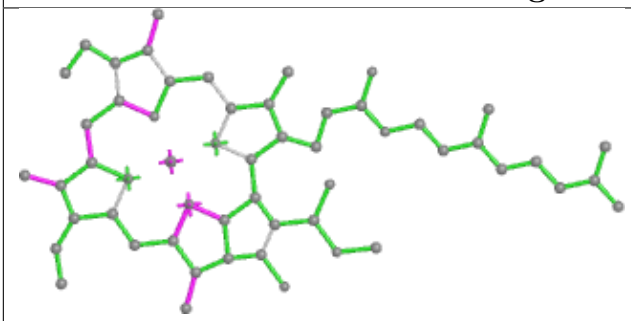
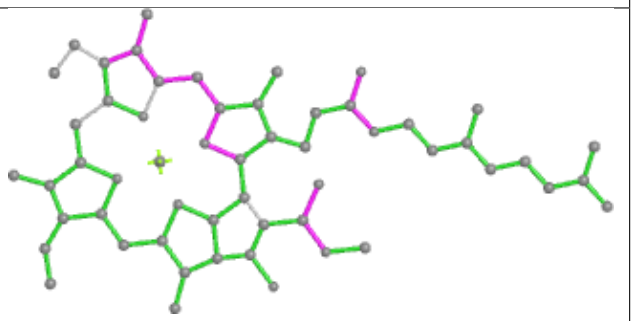
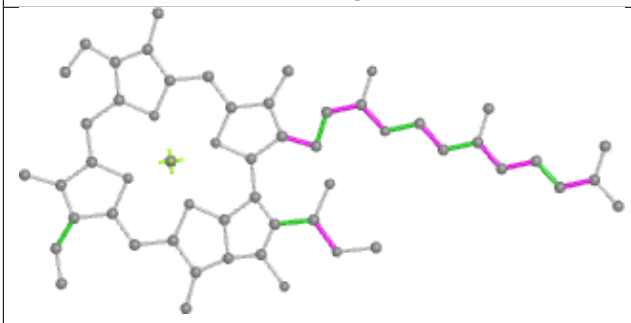
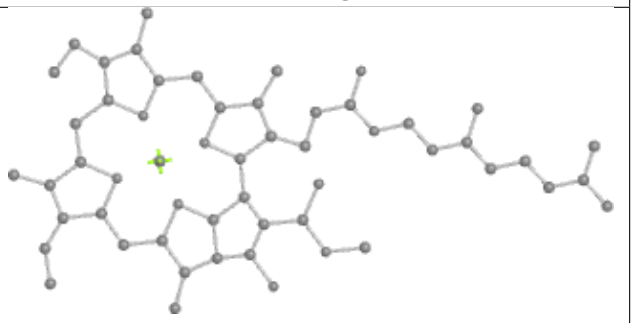
Bond angles

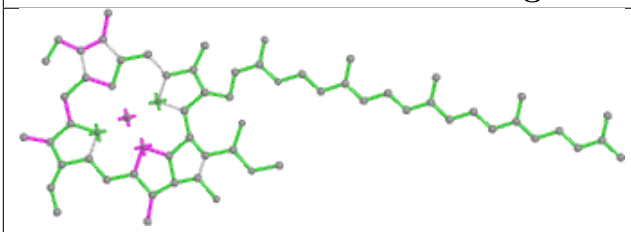
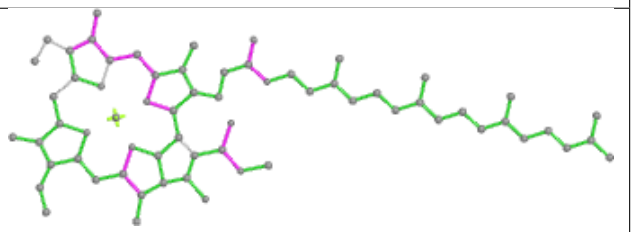
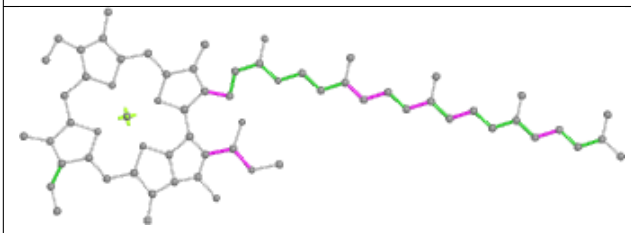
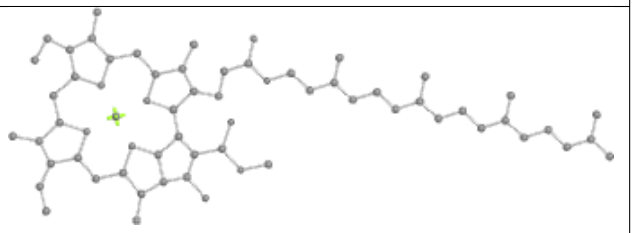


Torsions

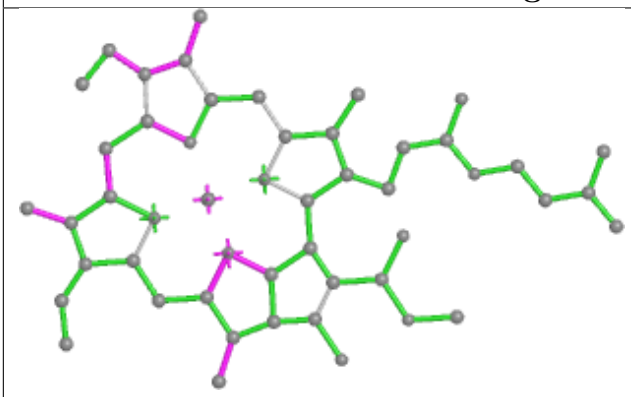


Rings

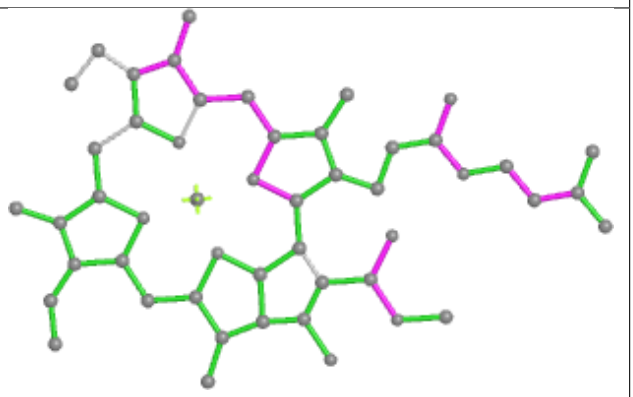
Ligand CLA 9 313	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 833	
 Bond lengths	 Bond angles
 Torsions	 Rings

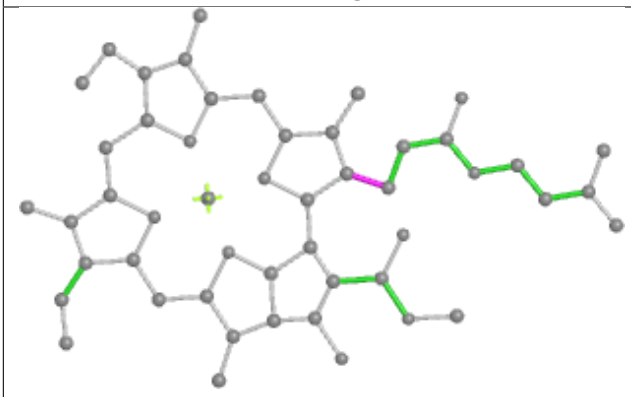
Ligand CLA A 831



Bond lengths



Bond angles



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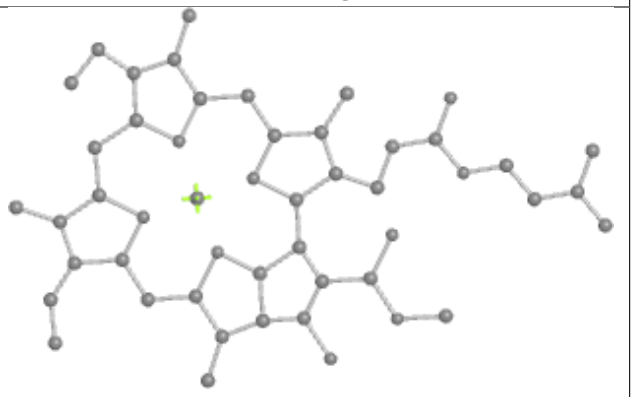
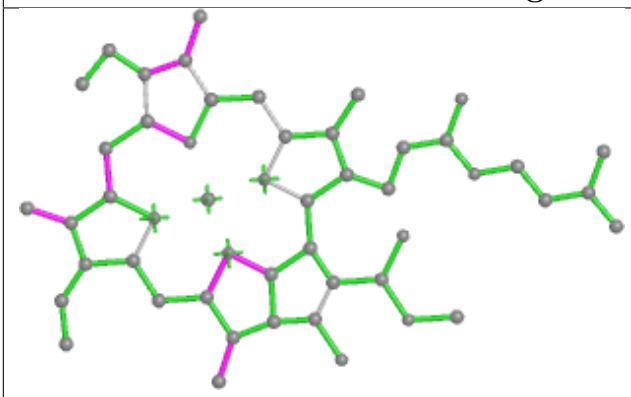
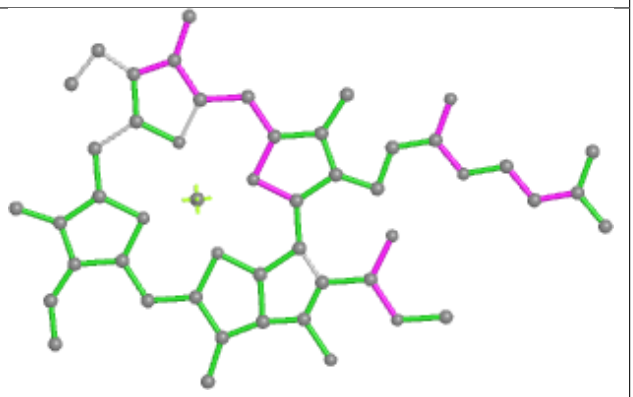


Rings

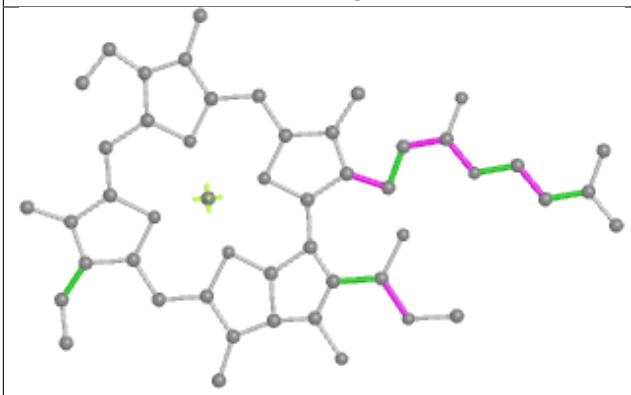
Ligand CLA L 204



Bond lengths



Bond angles



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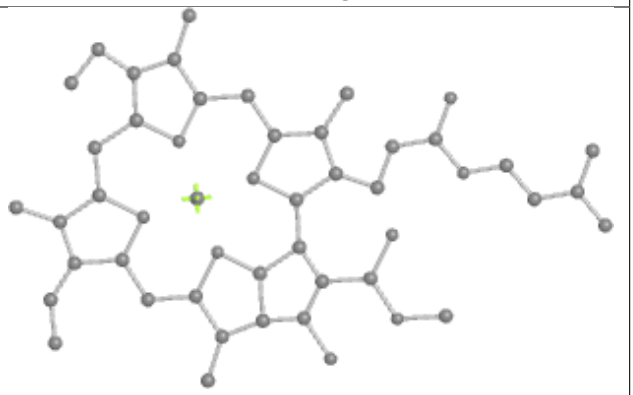
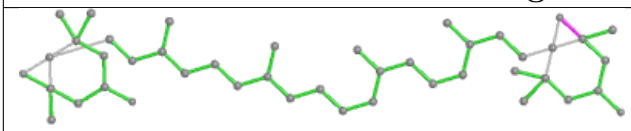


Rings

Ligand XAT 4 315



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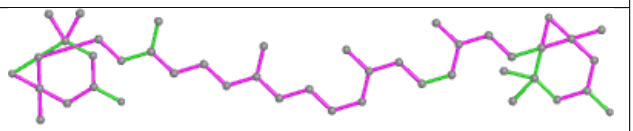
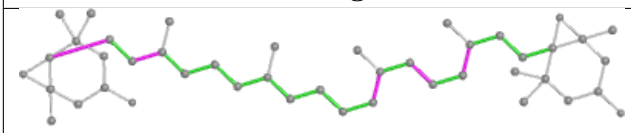


Bond angles



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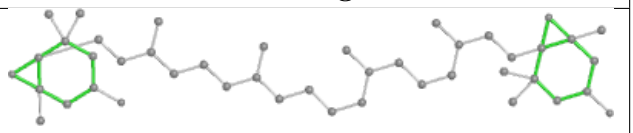
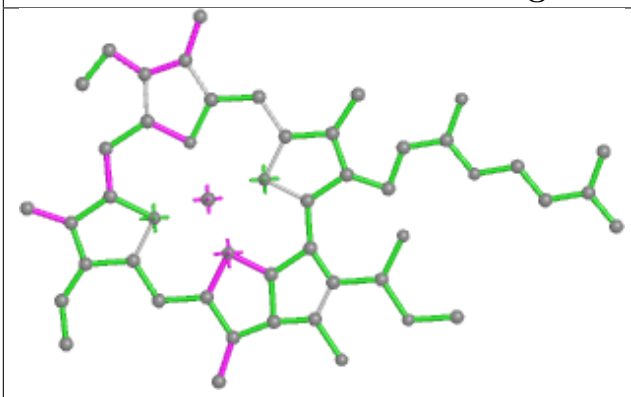


Rings

Ligand CLA 4 308



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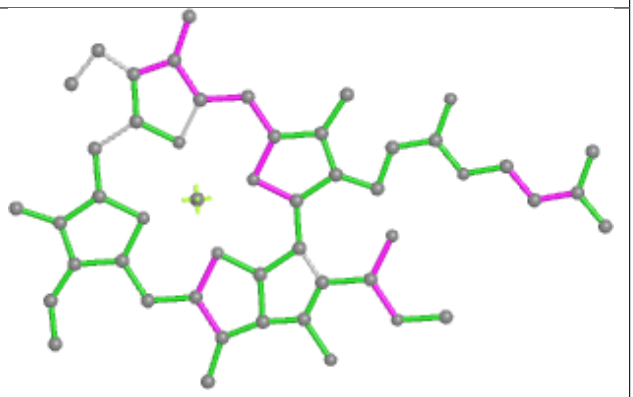
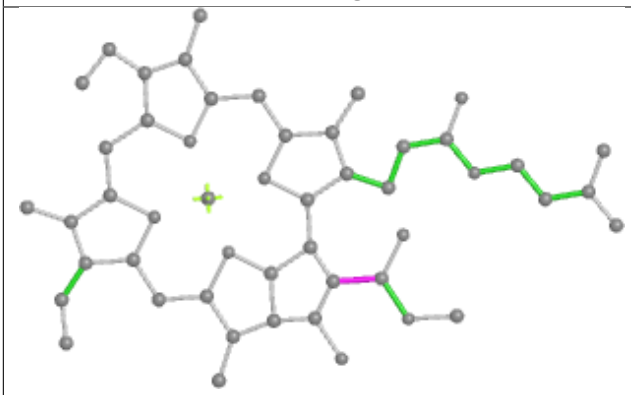


Bond angles



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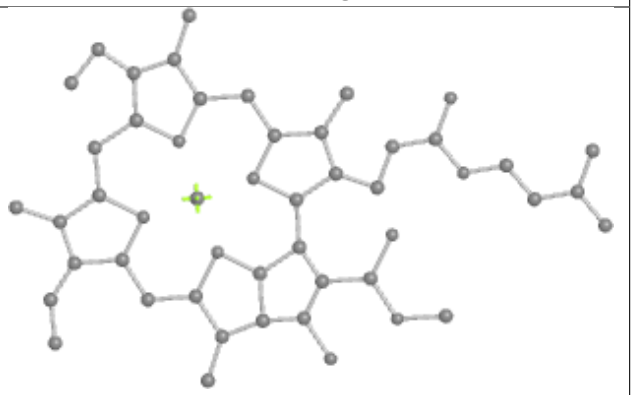
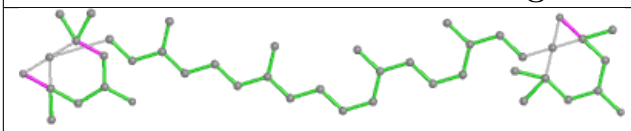


Rings

Ligand XAT 4 316



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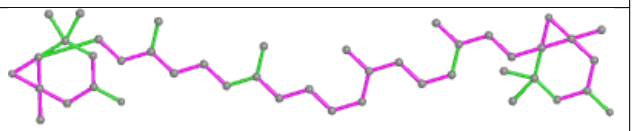
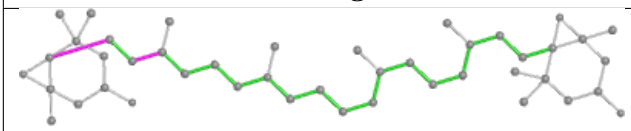


Bond angles



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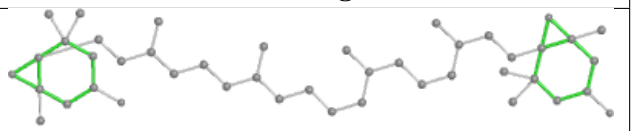
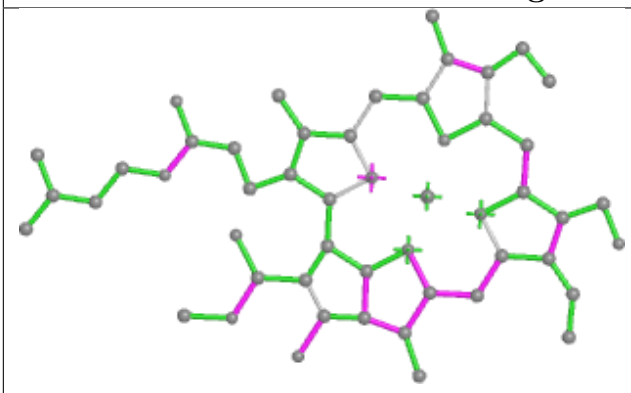


Rings

Ligand CHL 8 307



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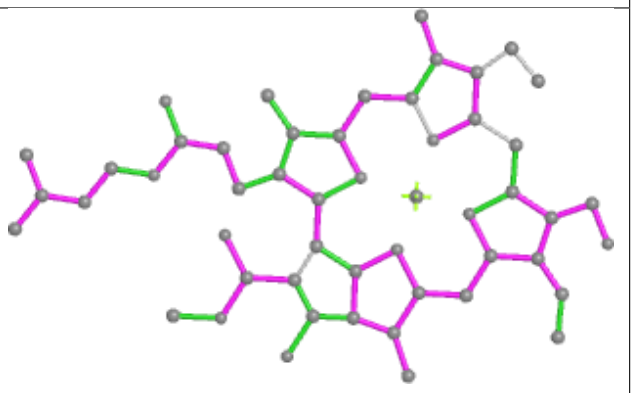
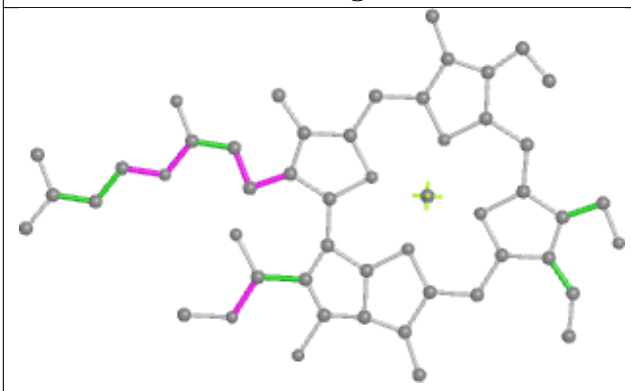


Bond angles



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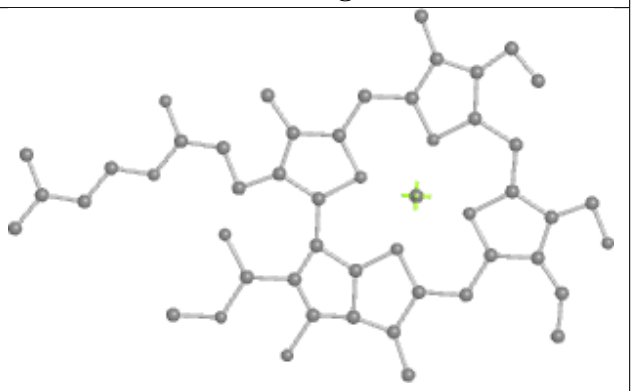
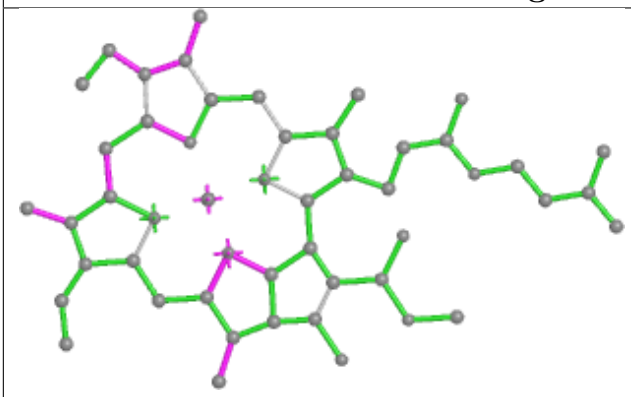


Rings

Ligand CLA 7 309



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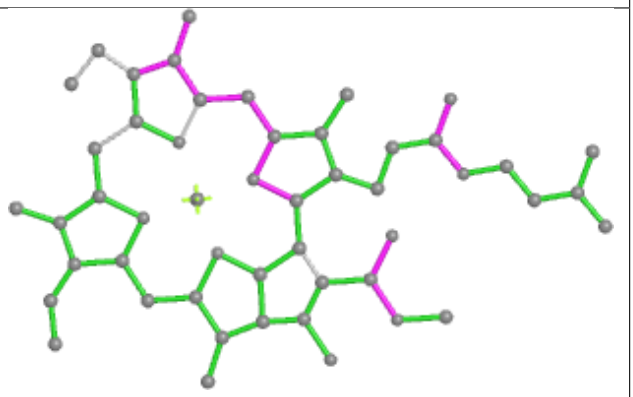
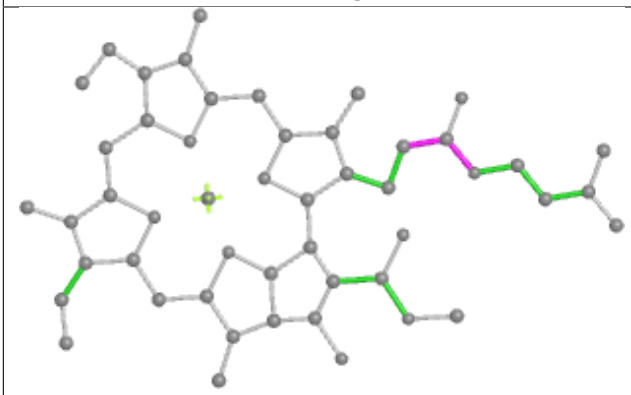


Bond angles



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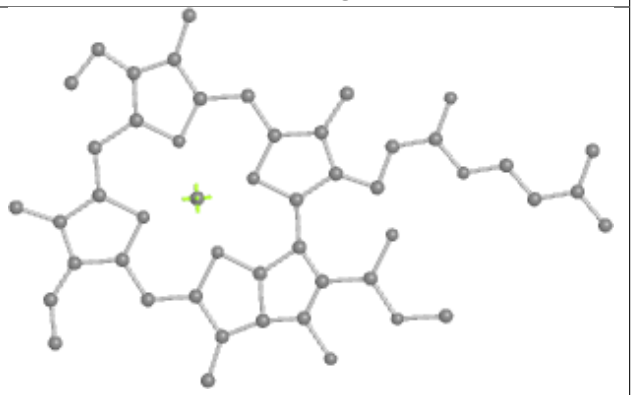
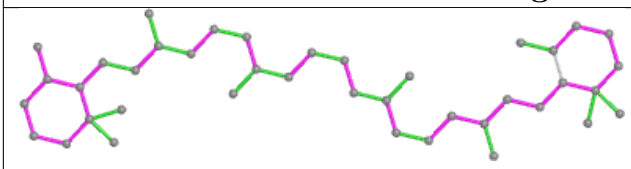


Rings

Ligand 8CT 3 316



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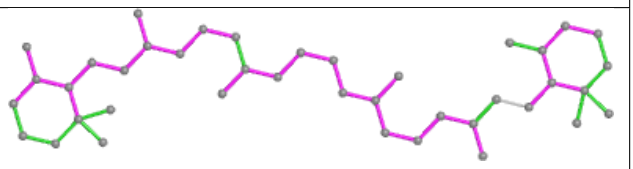
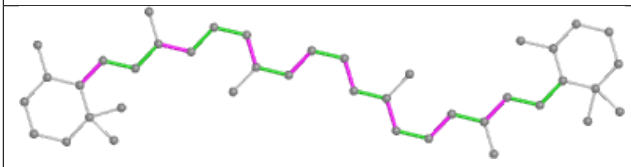


Bond angles



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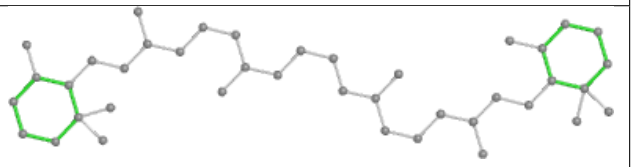
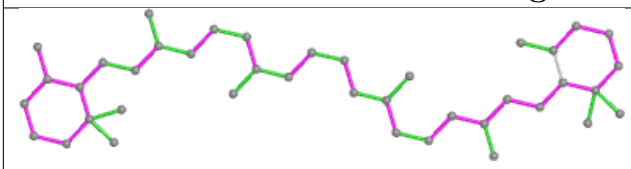


Rings

Ligand 8CT L 205



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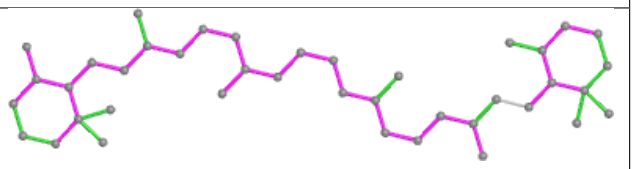
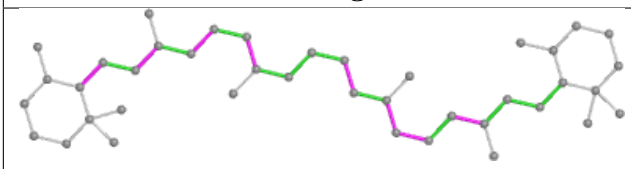


Bond angles



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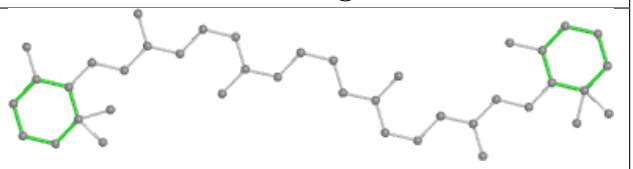
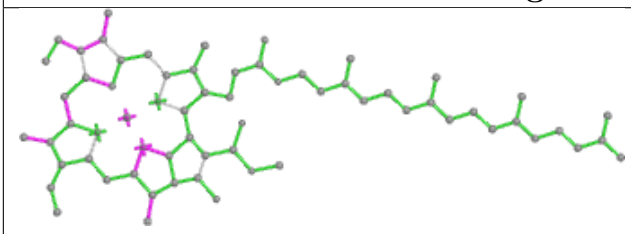
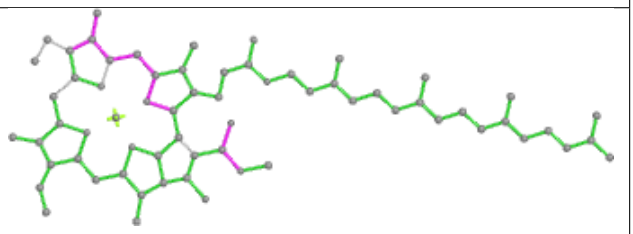


Rings

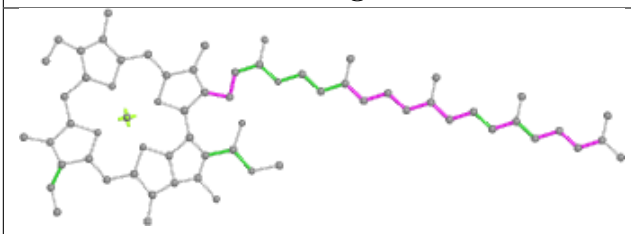
Ligand CLA L 201



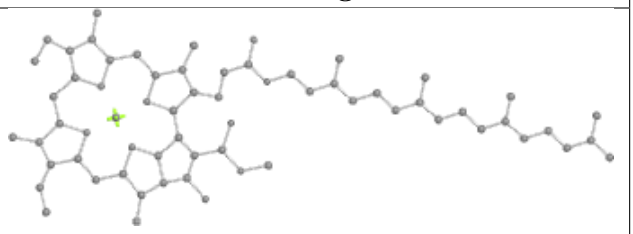
Bond lengths



Bond angles

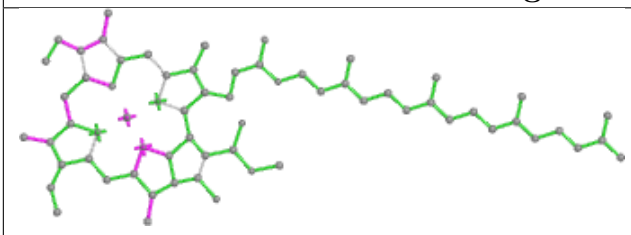


Torsions



Rings

Ligand CLA A 853



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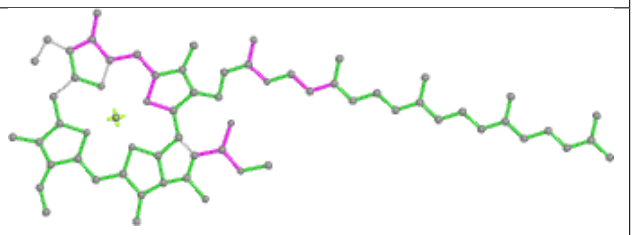
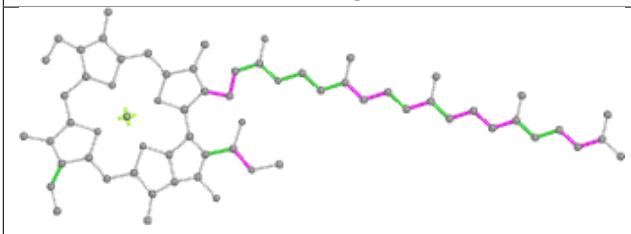
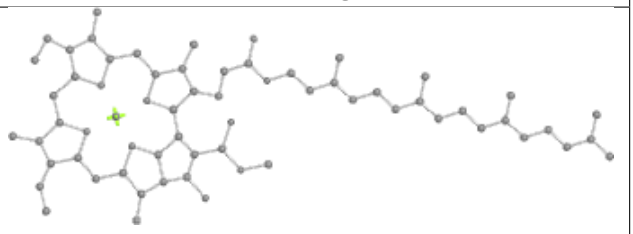


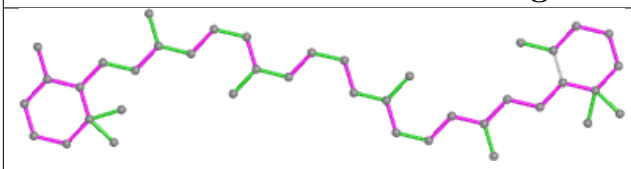
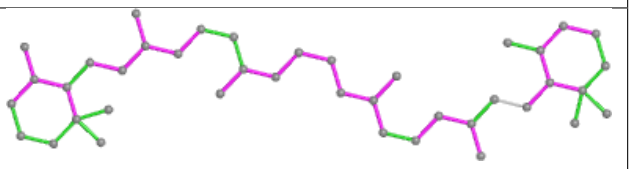
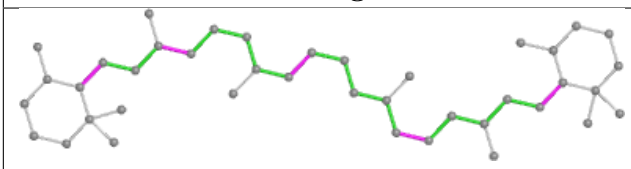
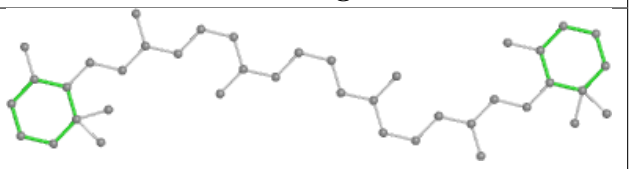
Bond angles

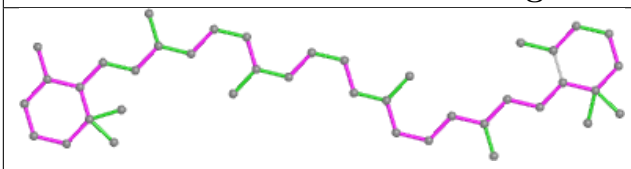
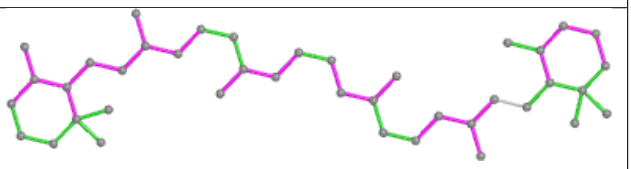
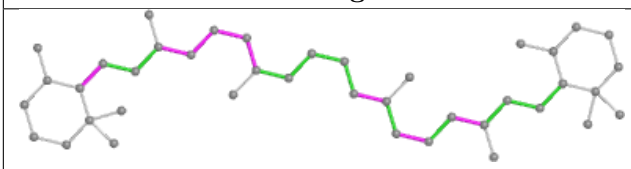
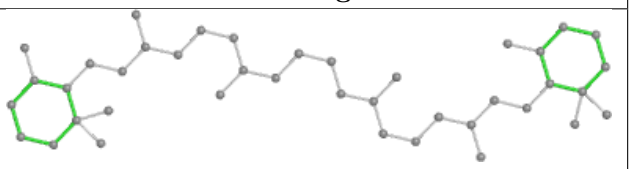


Torsions

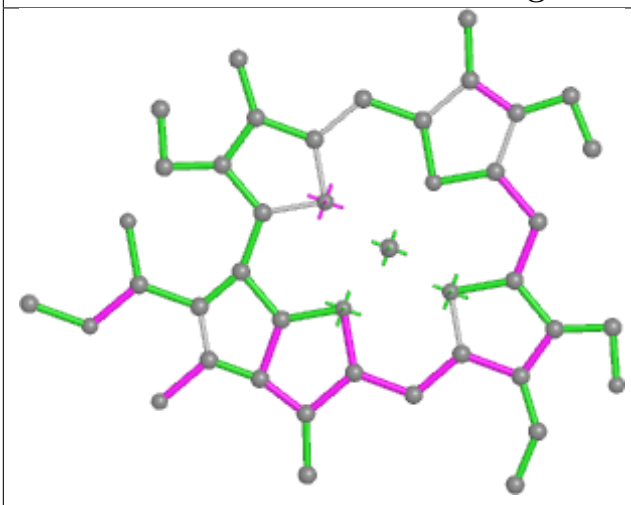


Rings

Ligand 8CT J 104	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 8CT K 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL 6 316



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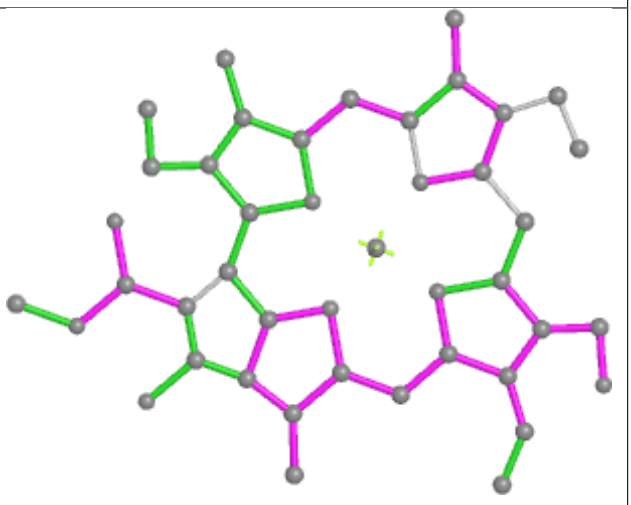

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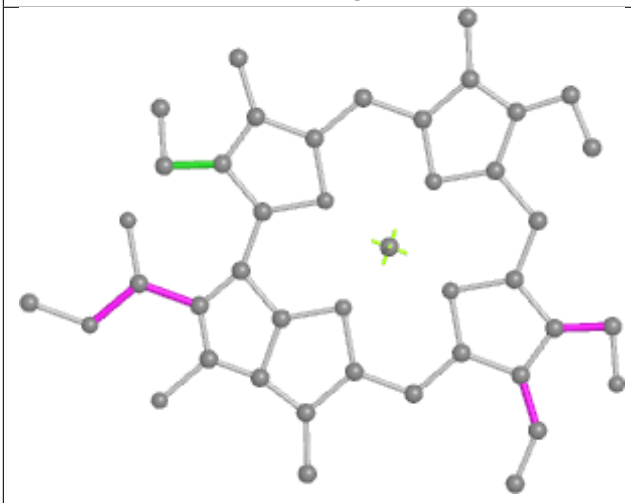

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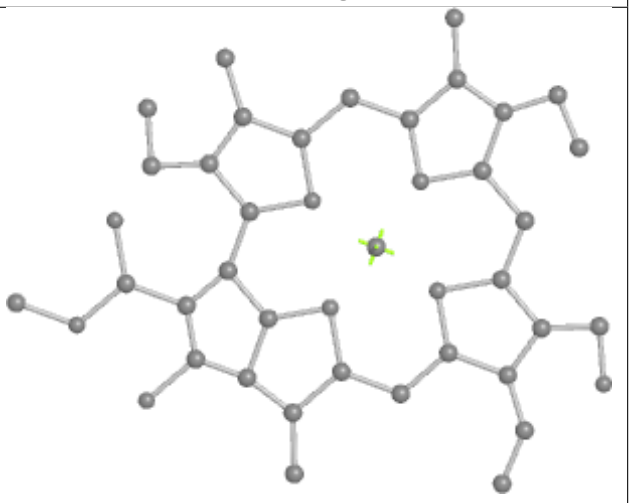
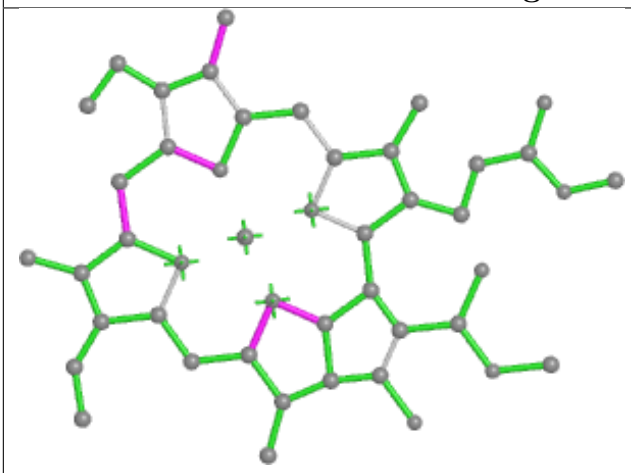


Rings

Ligand CLA G 103



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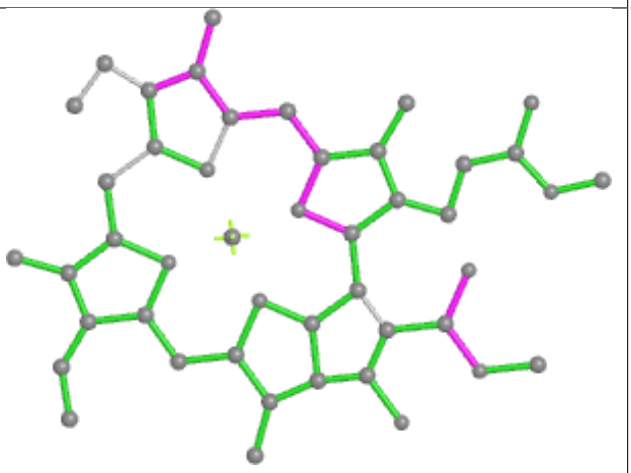

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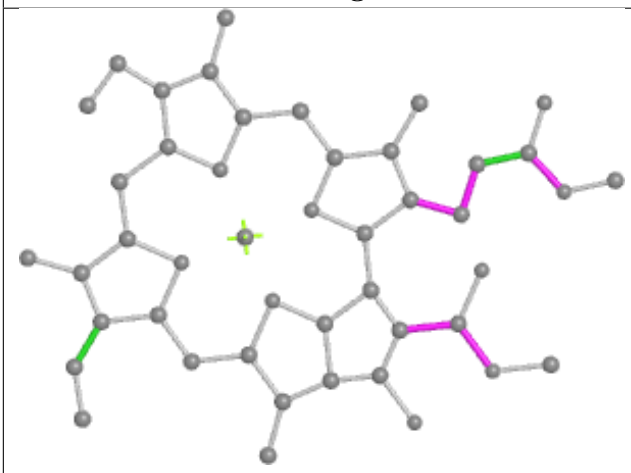

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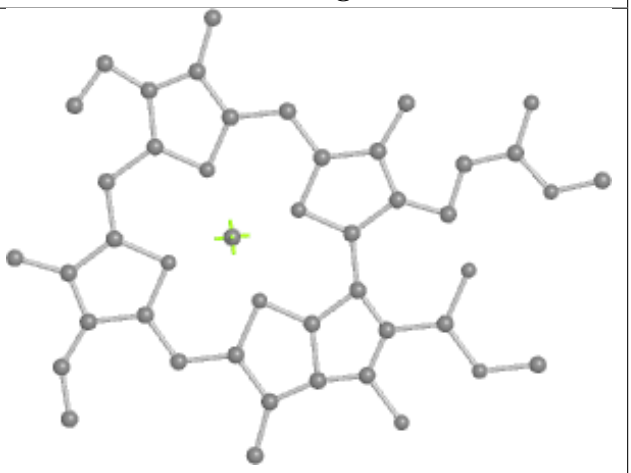
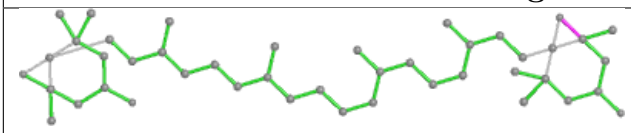


Rings

Ligand XAT 1 314



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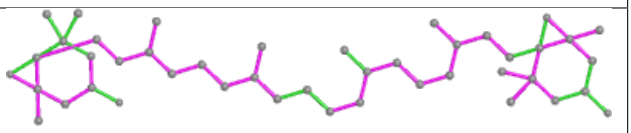

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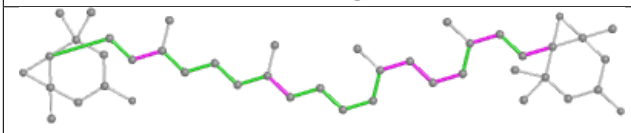

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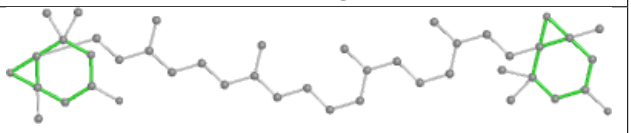
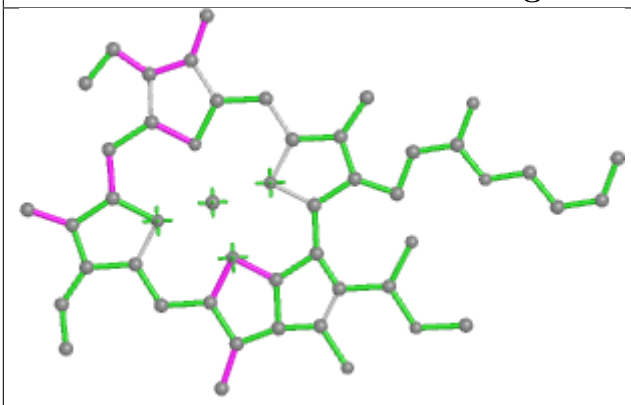


Rings

Ligand CLA A 852



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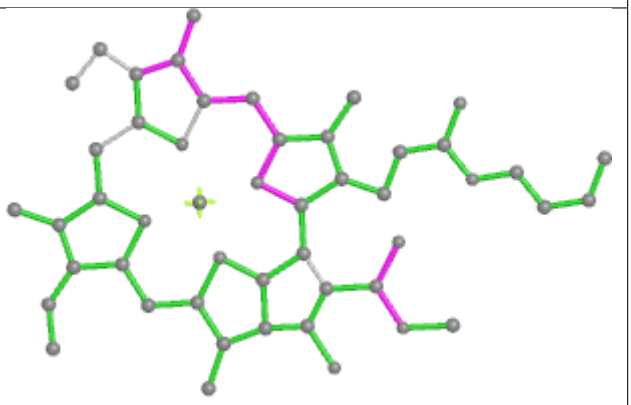
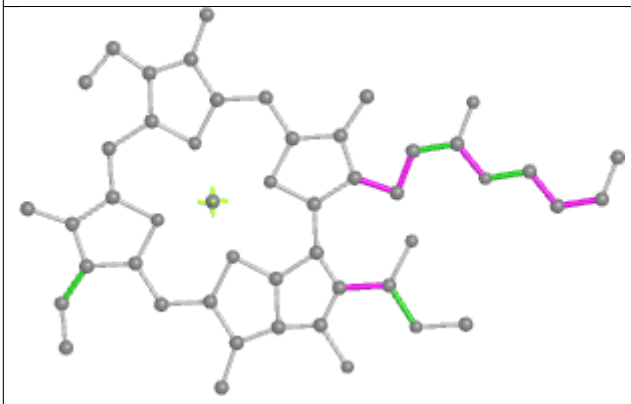


Bond angles



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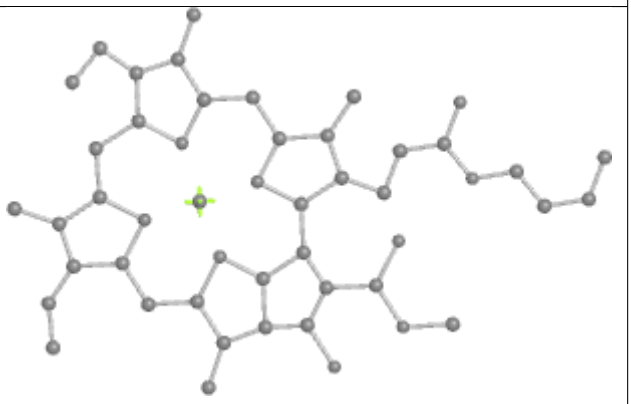
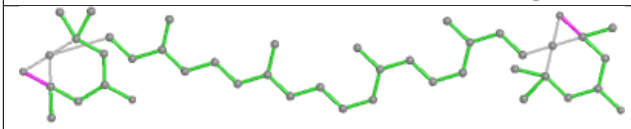


Rings

Ligand XAT 3 315



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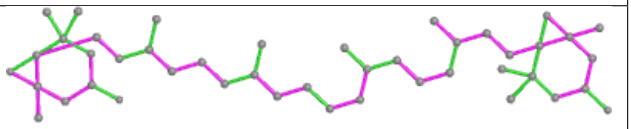

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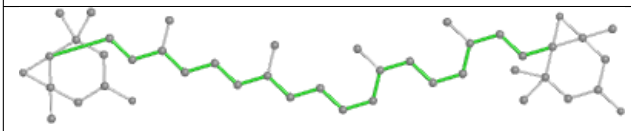

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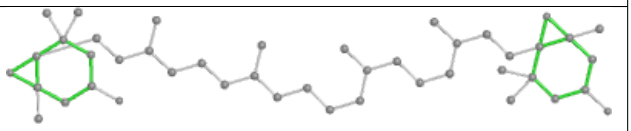
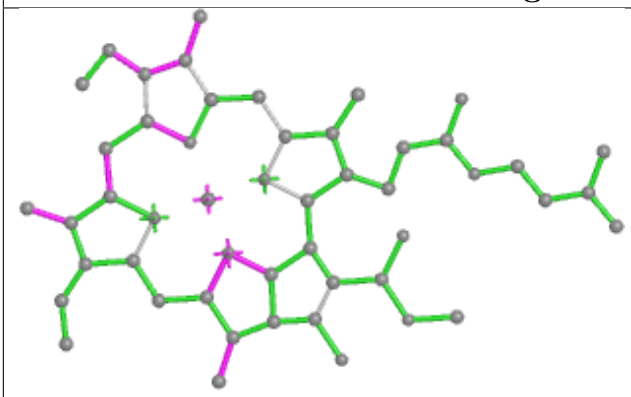


Rings

Ligand CLA A 834



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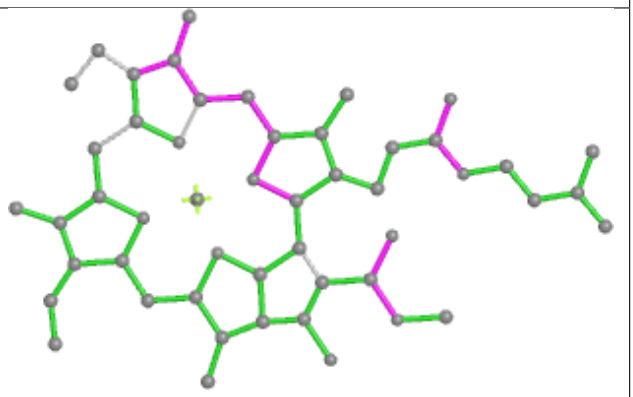

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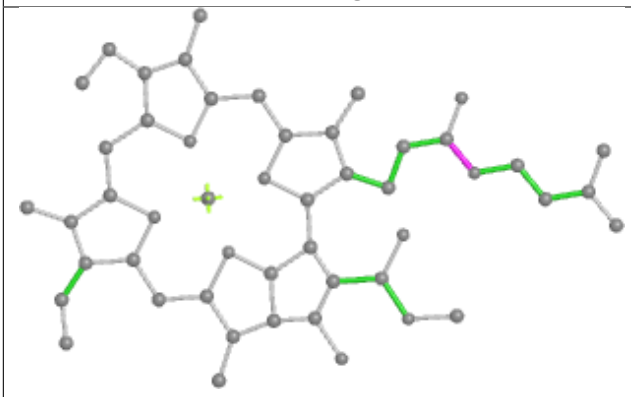

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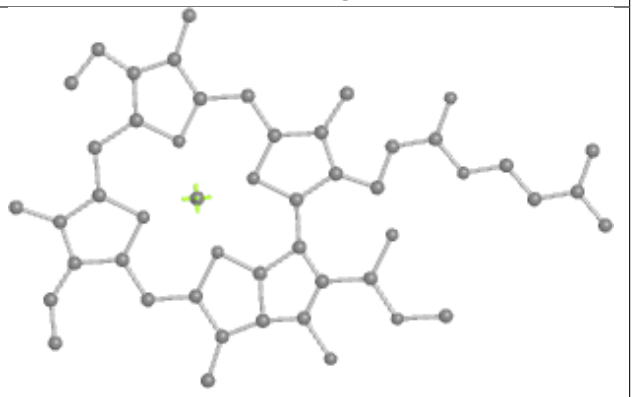
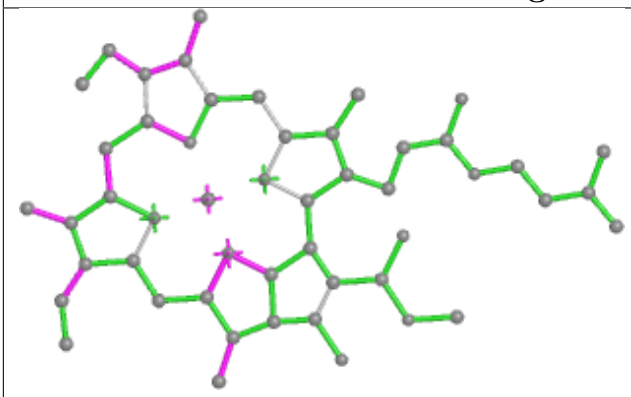


Rings

Ligand CLA 3 308



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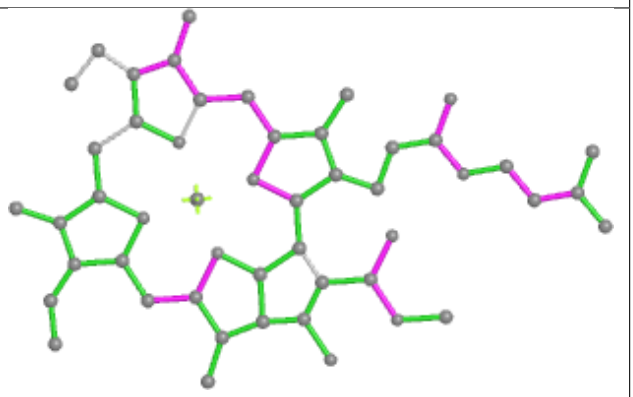
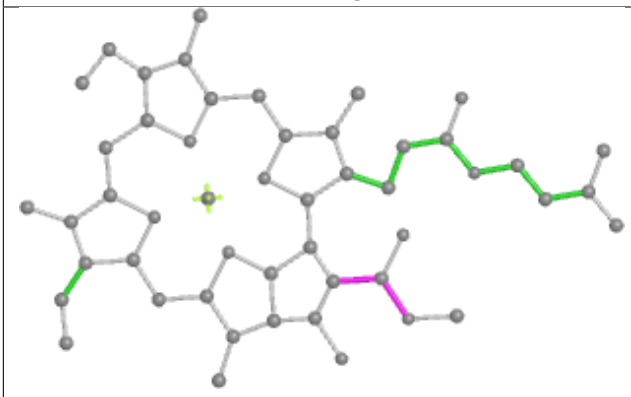


Bond angles



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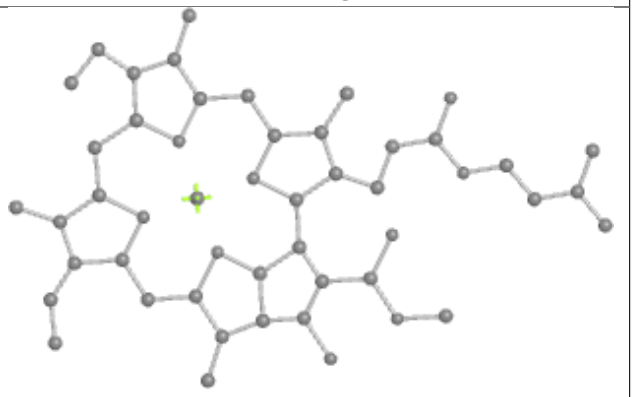
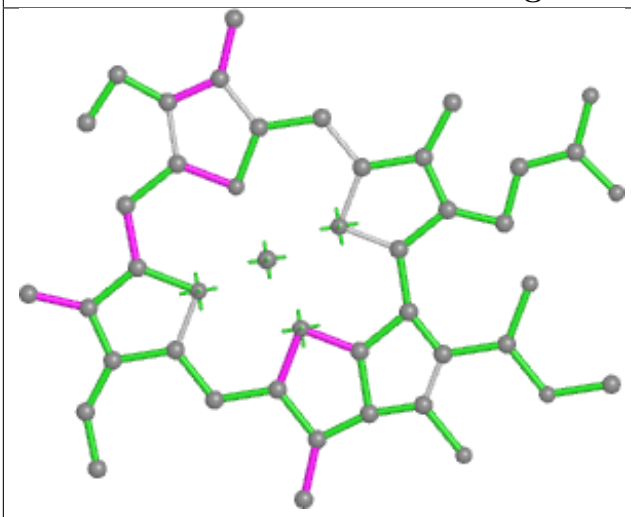


Rings

Ligand CLA B 835



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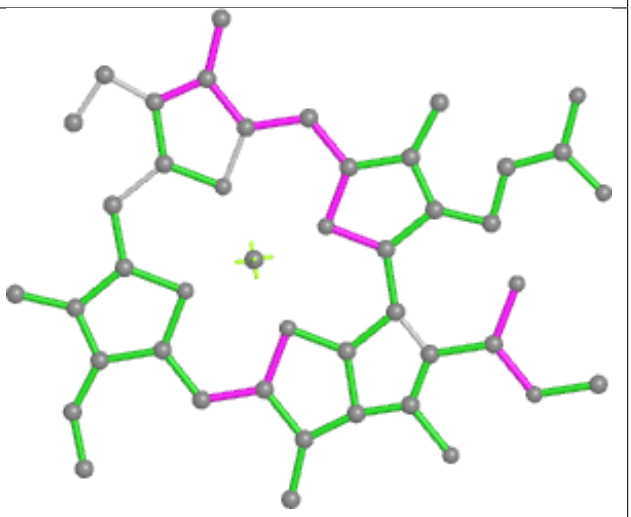

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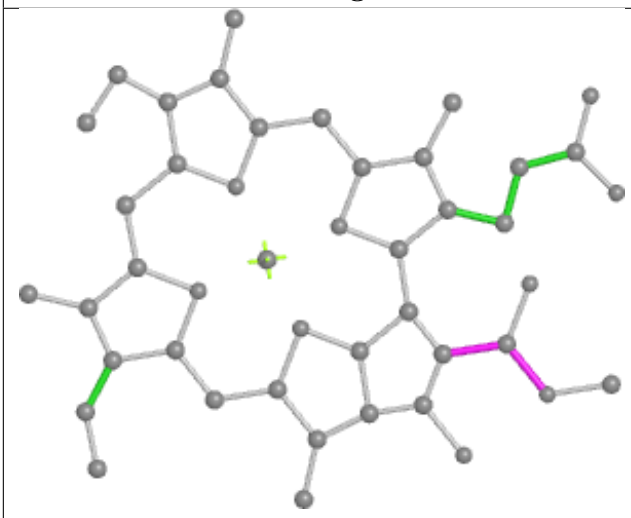

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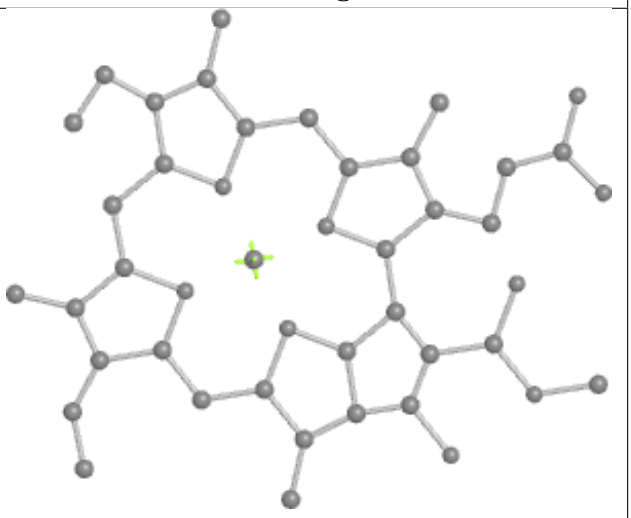
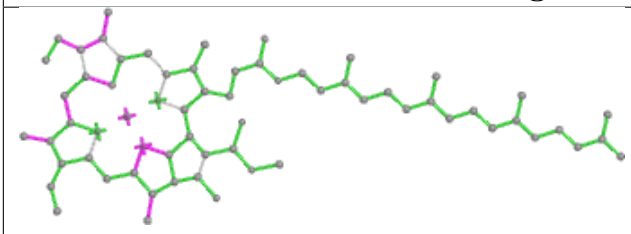


Rings

Ligand CLA 1 311



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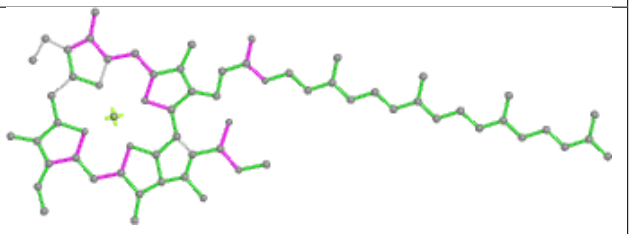

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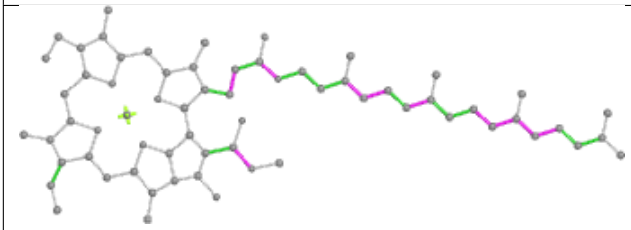

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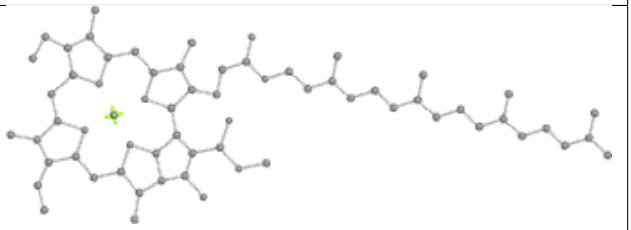
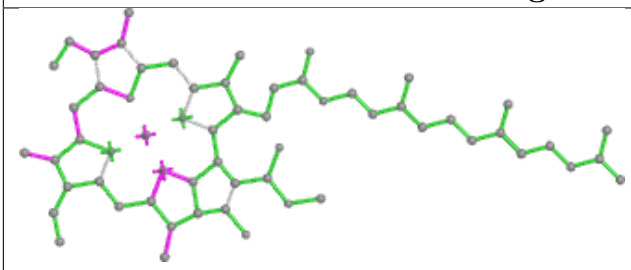


Rings

Ligand CLA 8 309



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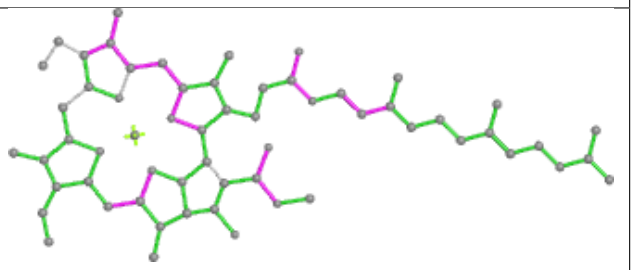

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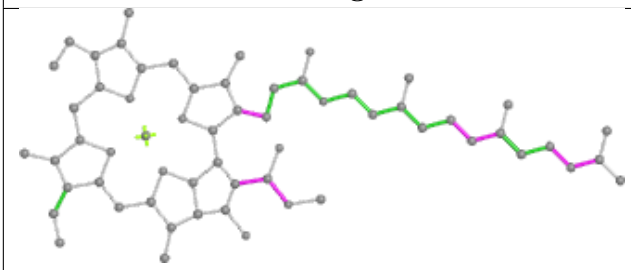

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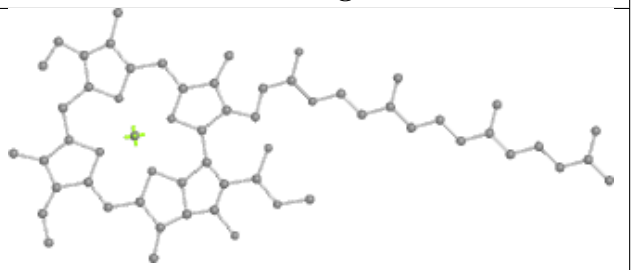
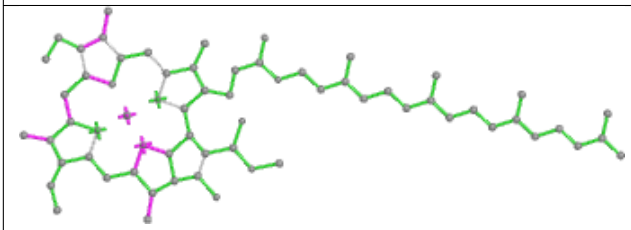


Rings

Ligand CLA 2 312



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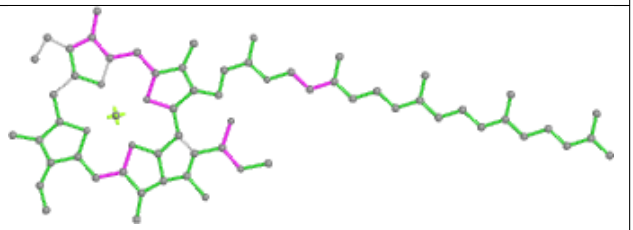

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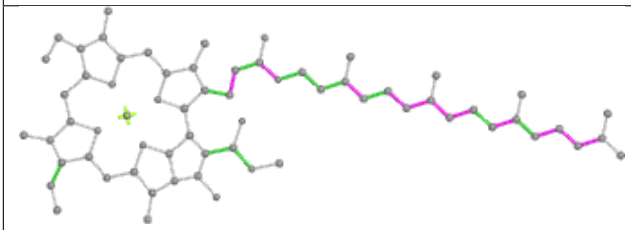

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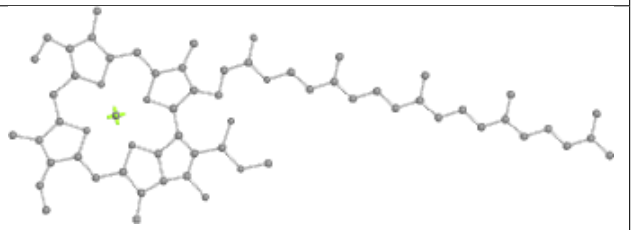
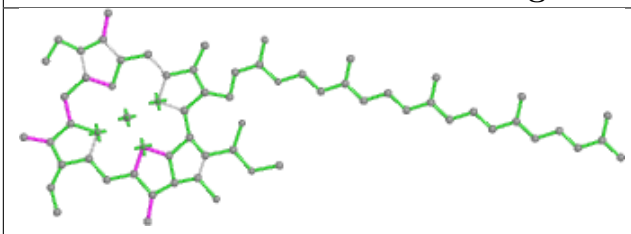


Rings

Ligand CLA 0 307



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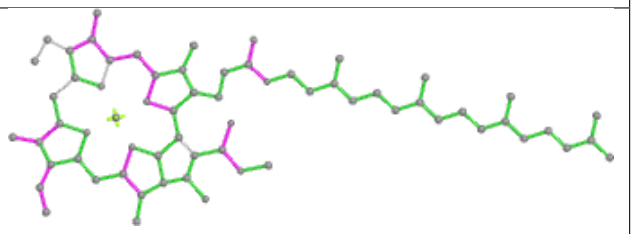

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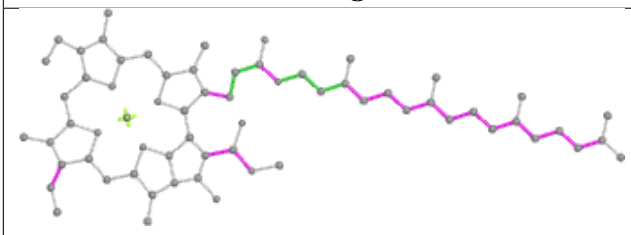

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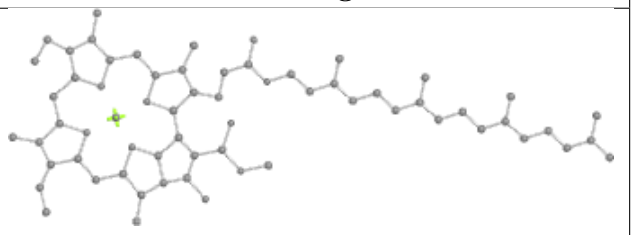
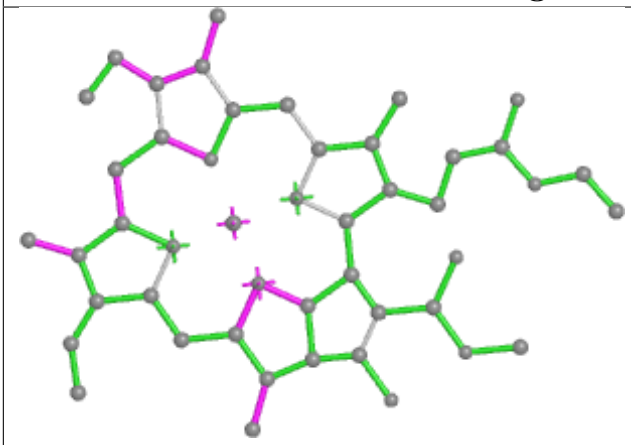


Rings

Ligand CLA 7 304



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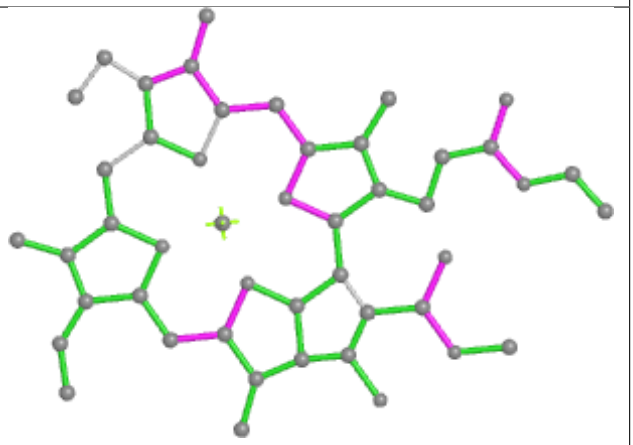
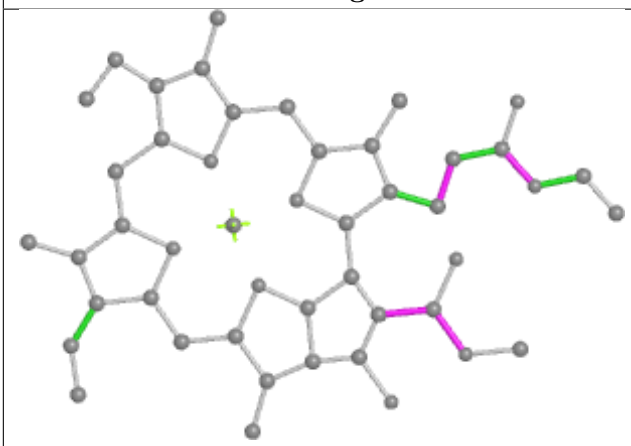


Bond angles



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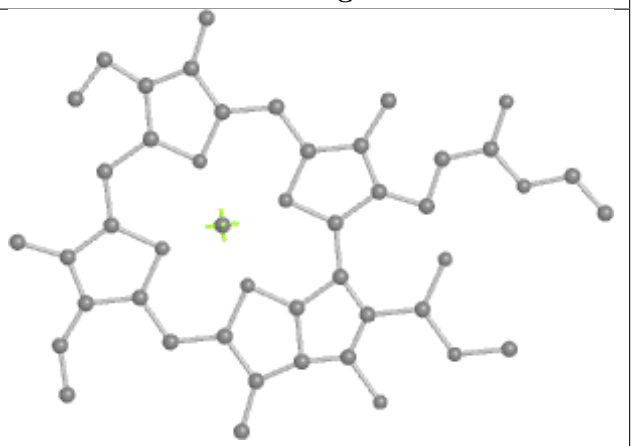
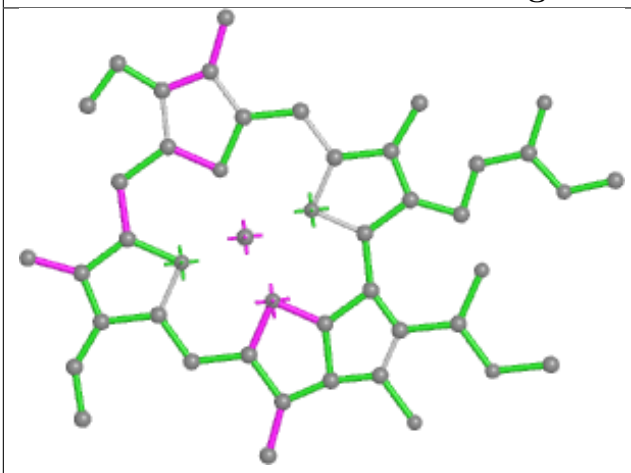
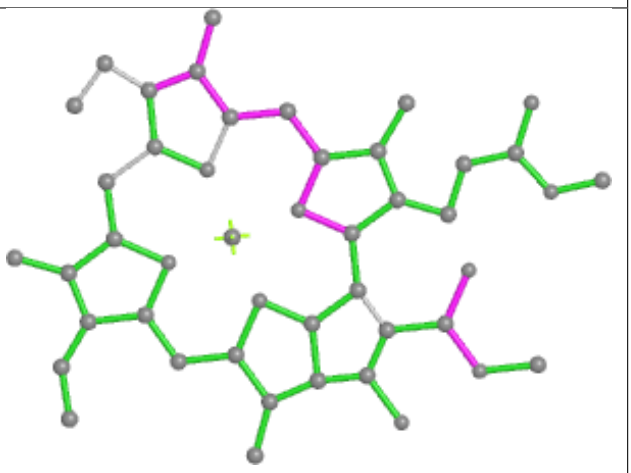


Rings

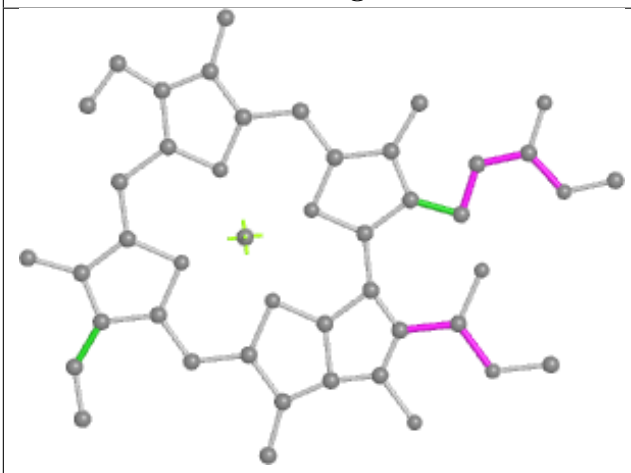
Ligand CLA 5 314



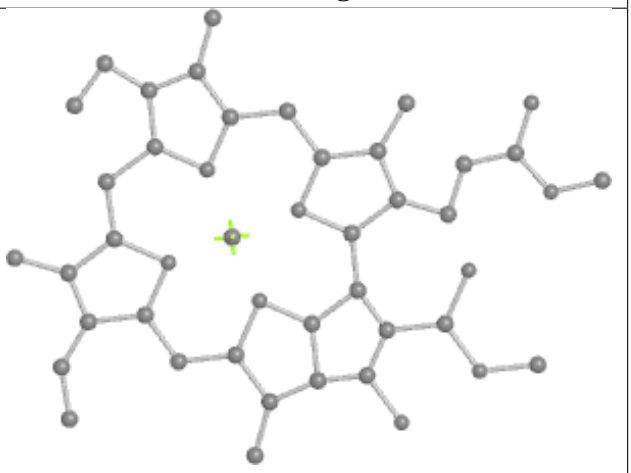
Bond lengths



Bond angles

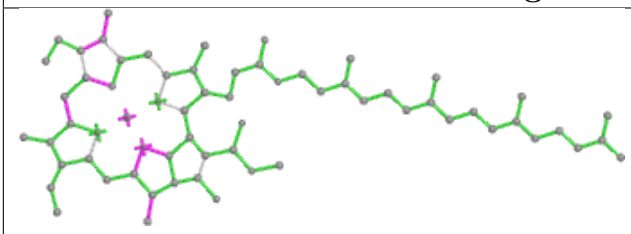


Torsions

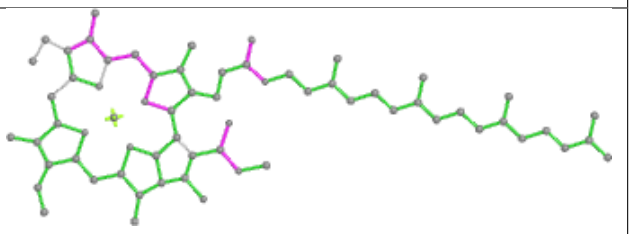


Rings

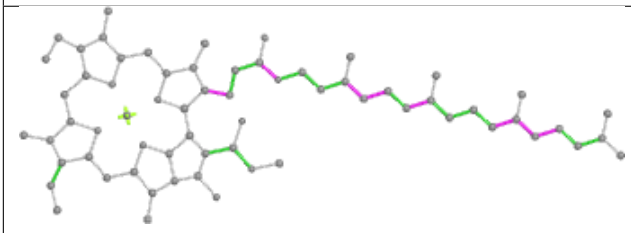
Ligand CLA B 839



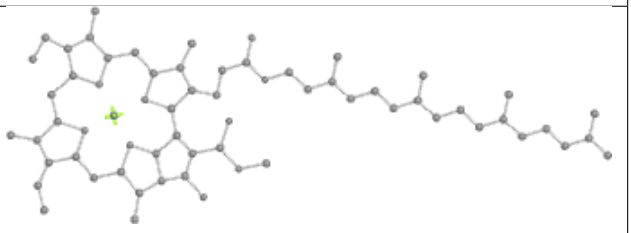
Bond lengths



Bond angles

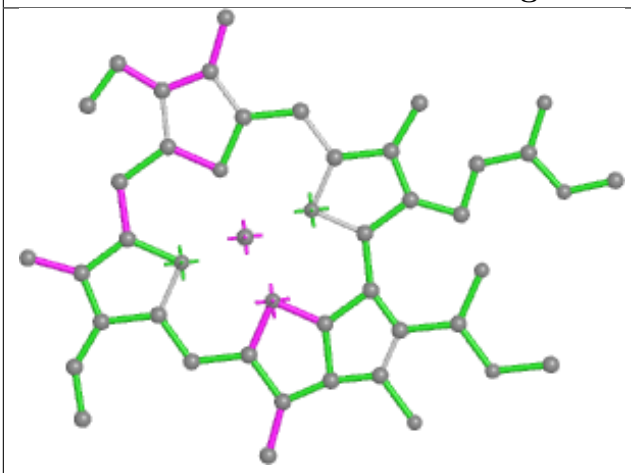


Torsions

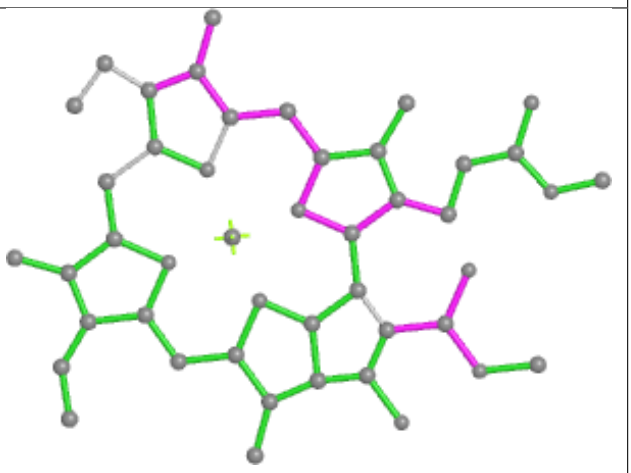


Rings

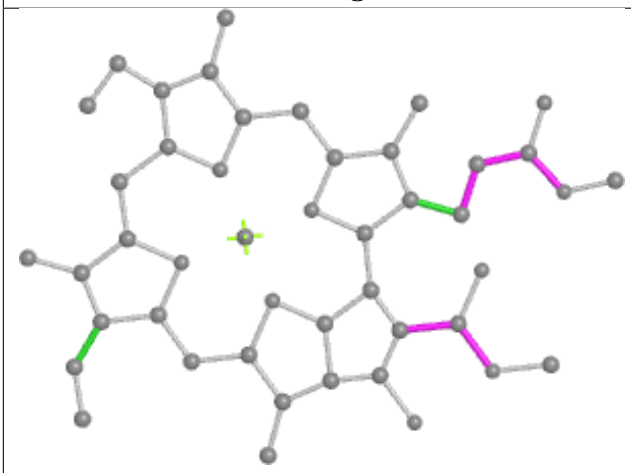
Ligand CLA M 101



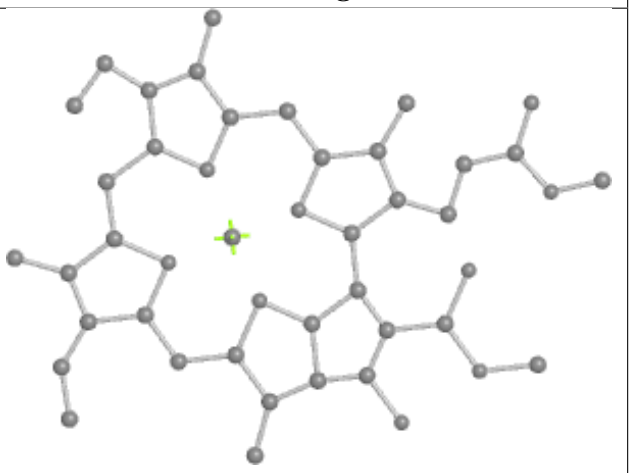
Bond lengths



Bond angles

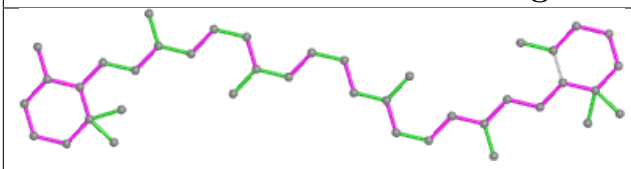


Torsions

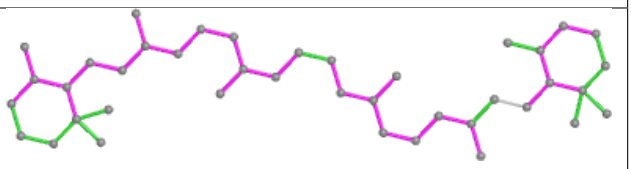


Rings

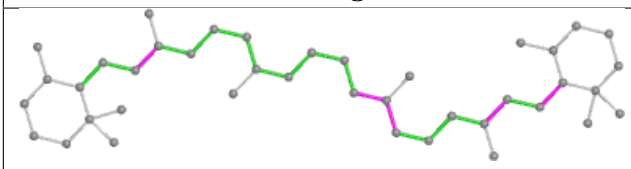
Ligand 8CT 2 317



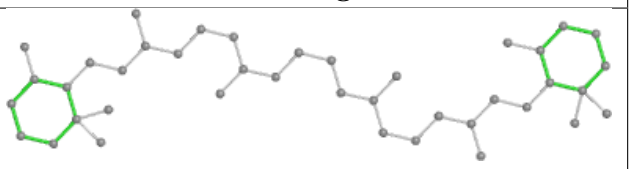
Bond lengths



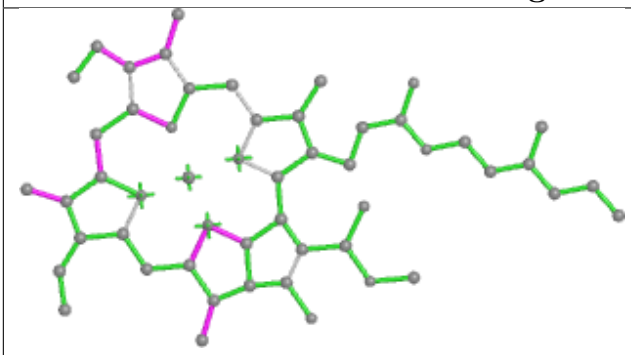
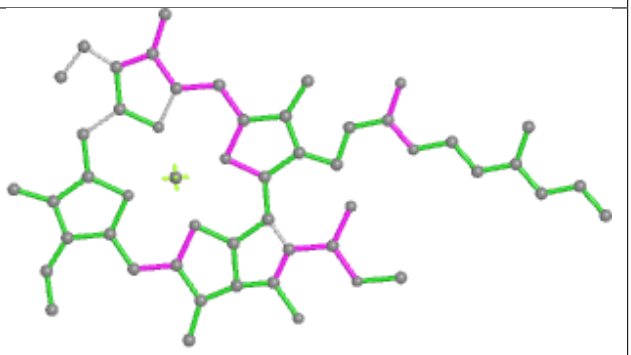
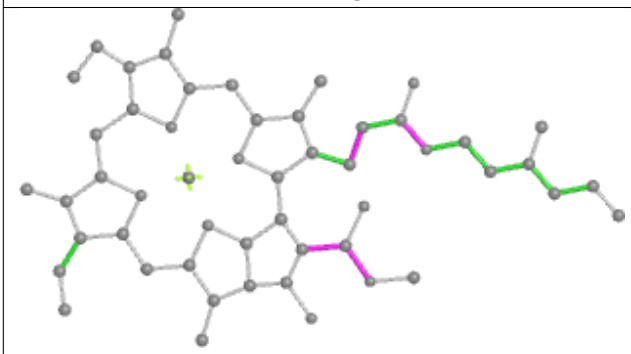
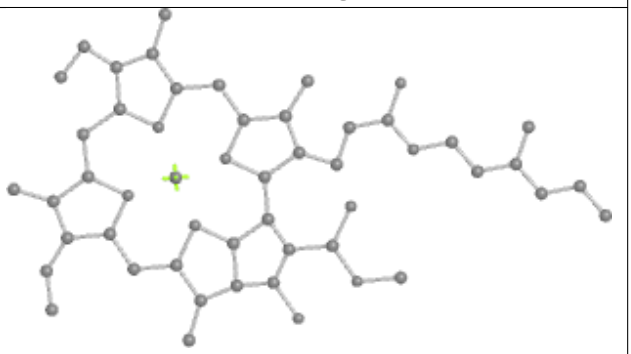
Bond angles

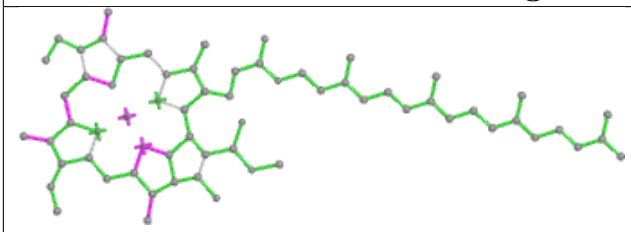
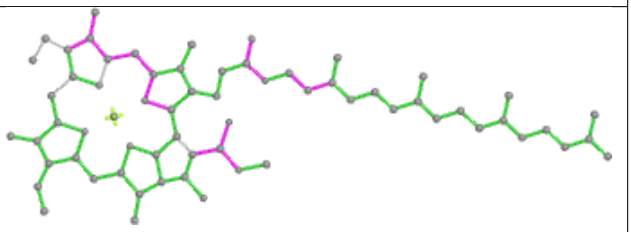
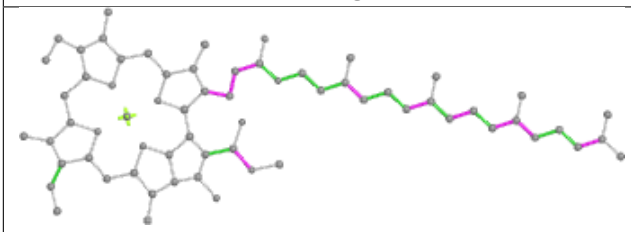
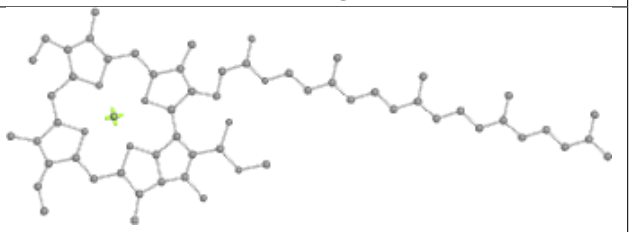


Torsions

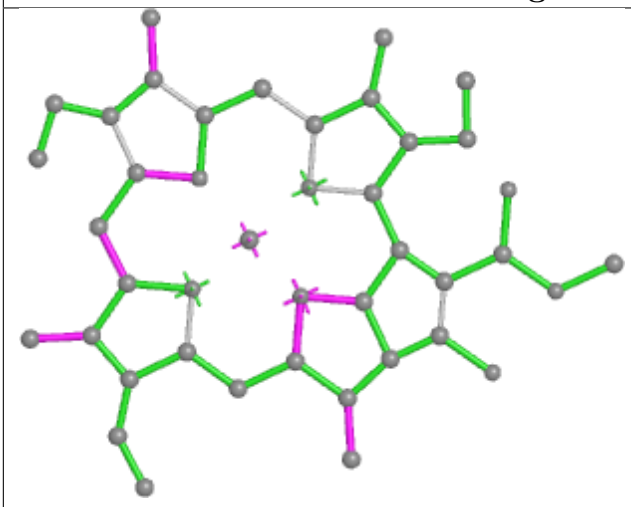


Rings

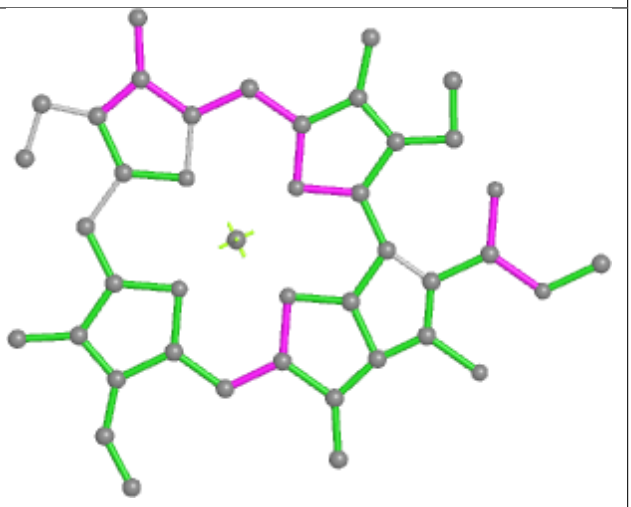
Ligand CLA 9 305	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 828	
	
Bond lengths	Bond angles
	
Torsions	Rings

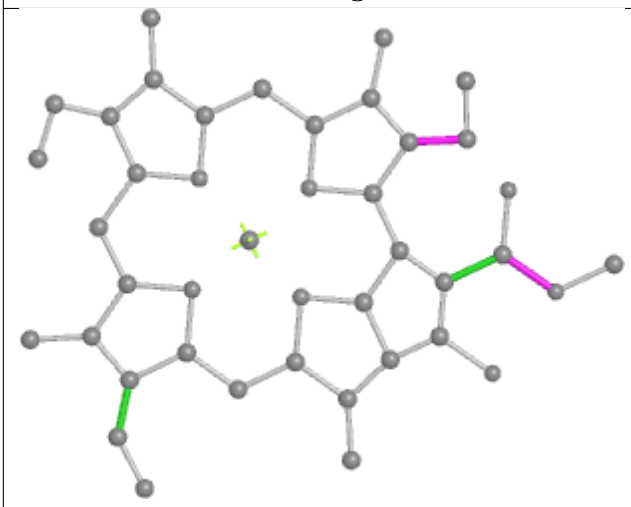
Ligand CLA 7 306



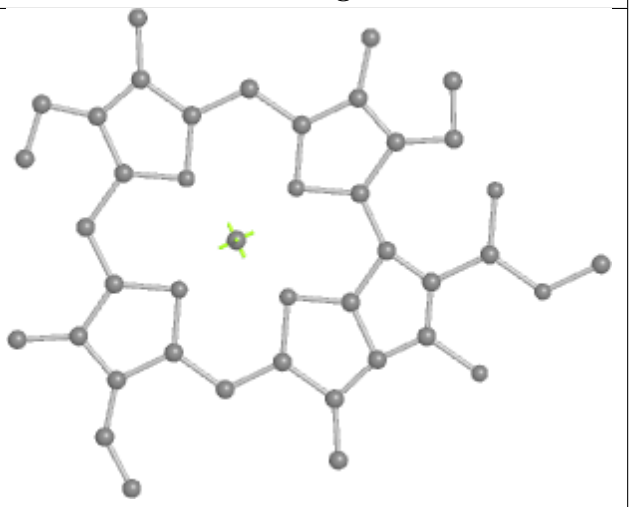
Bond lengths



Bond angles

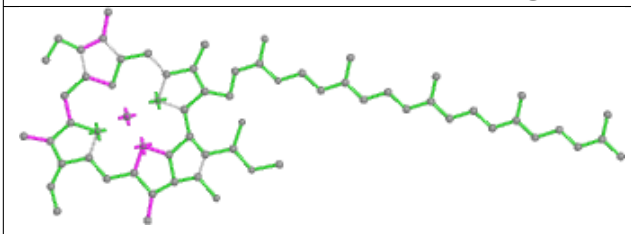


Torsions

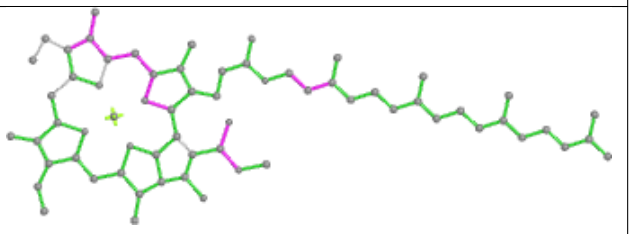


Rings

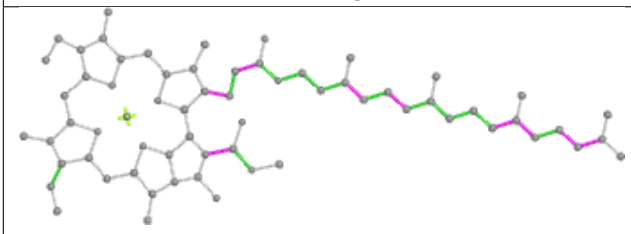
Ligand CLA B 840



Bond lengths



Bond angles



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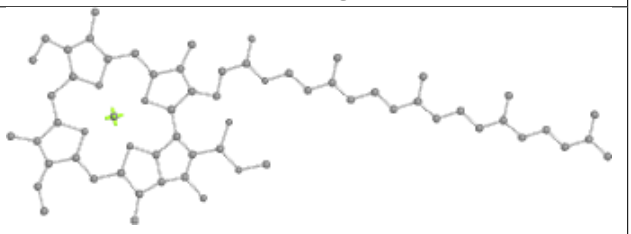
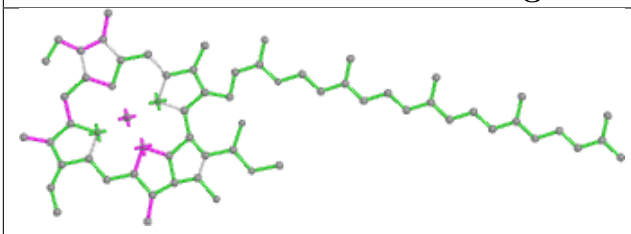
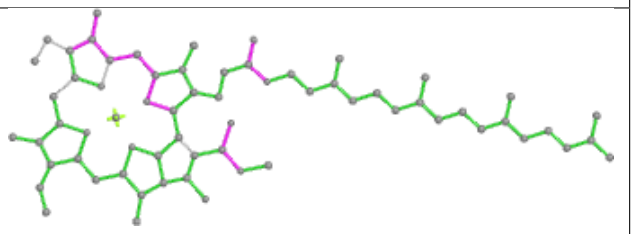


Rings

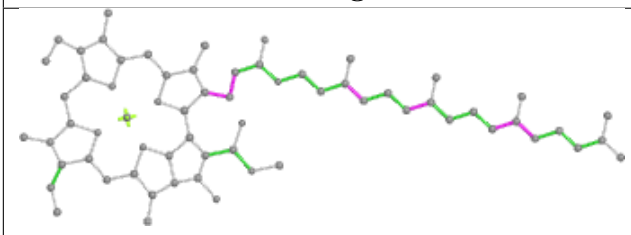
Ligand CLA A 802



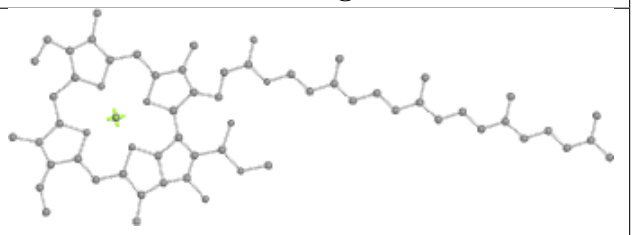
Bond lengths



Bond angles

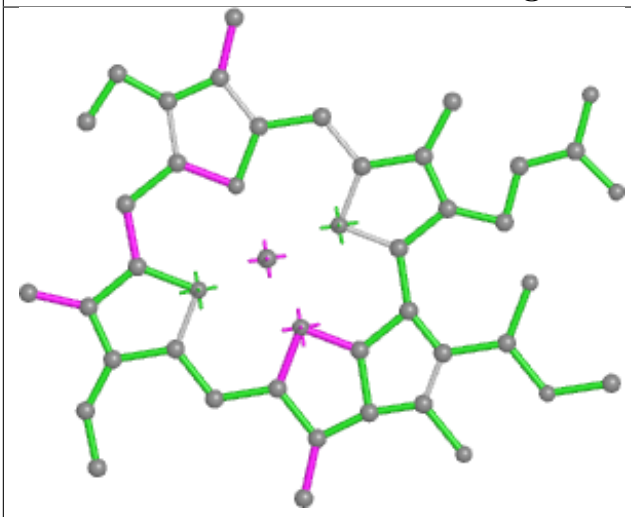


Torsions

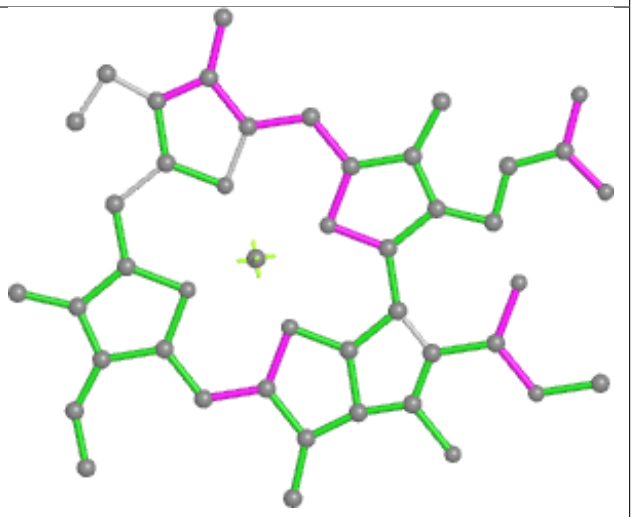


Rings

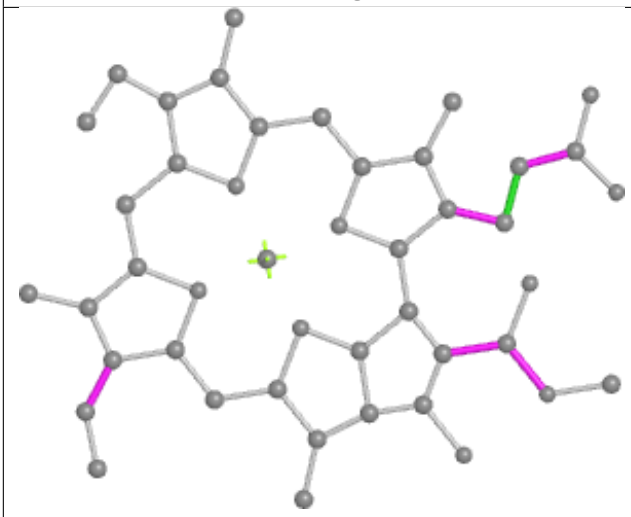
Ligand CLA K 101



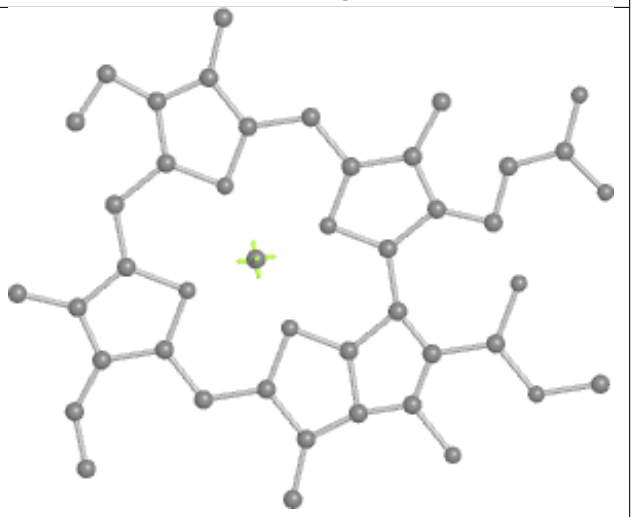
Bond lengths



Bond angles

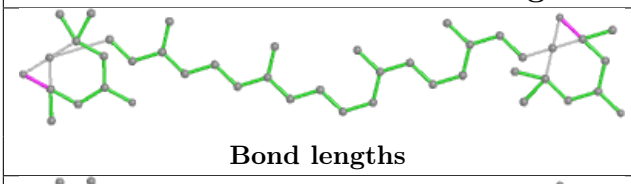


Torsions

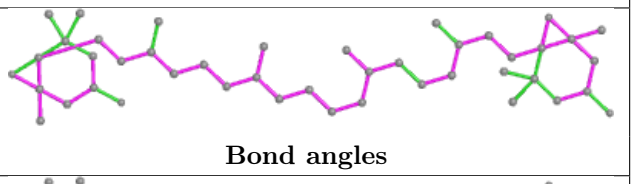


Rings

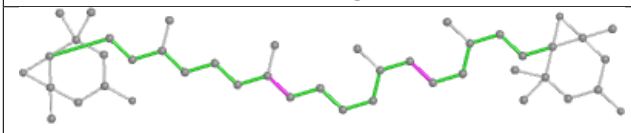
Ligand XAT 6 319



Bond lengths



Bond angles



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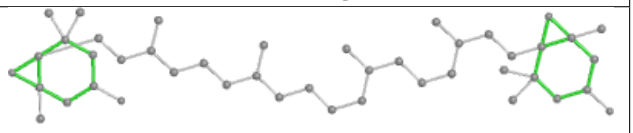
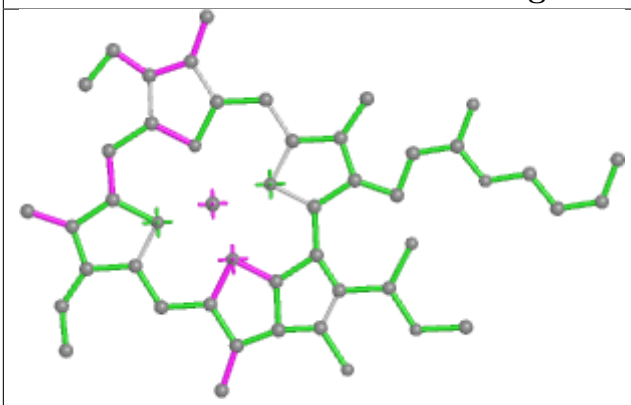


Rings

Ligand CLA 2 314



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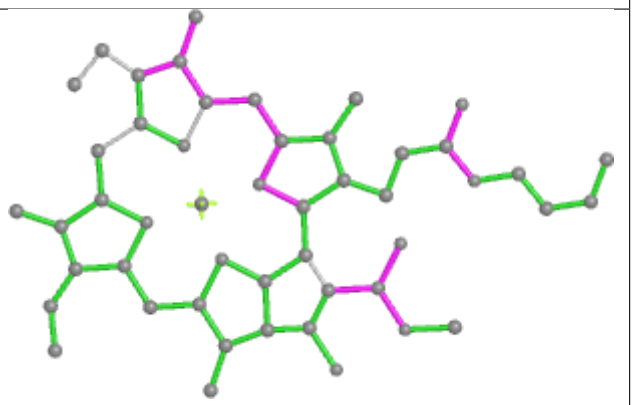
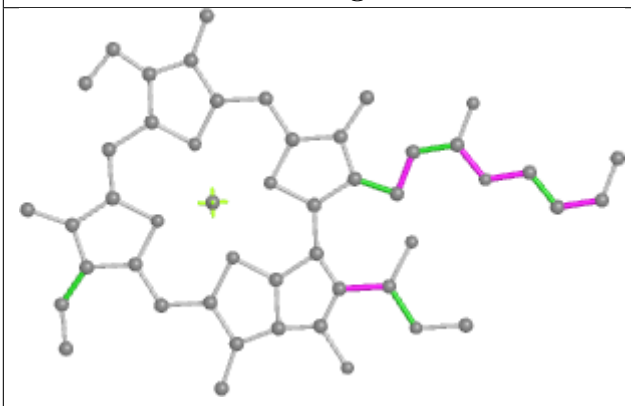


Bond angles



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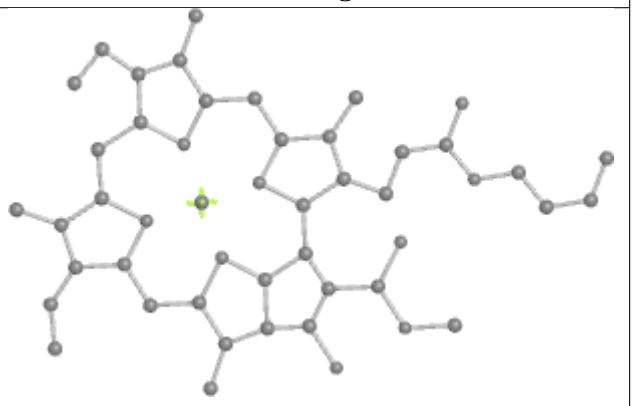
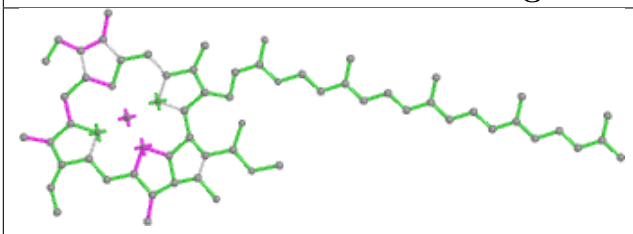
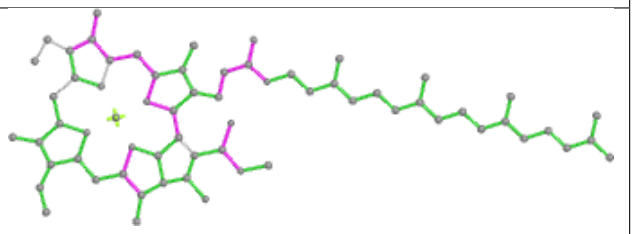


Rings

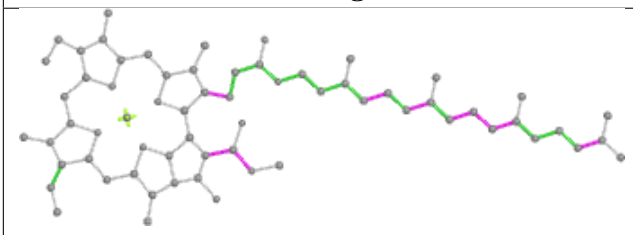
Ligand CLA A 809



Bond lengths



Bond angles



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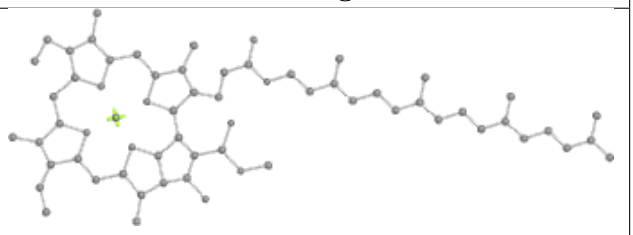
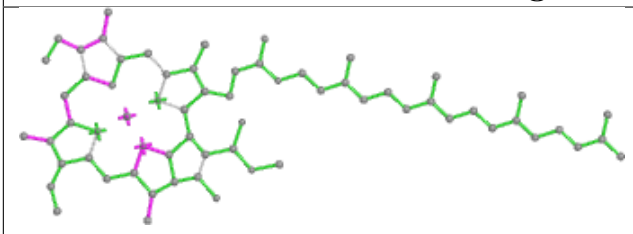
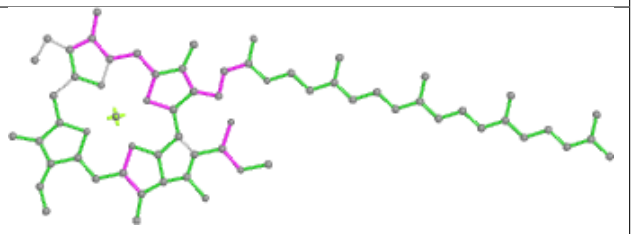


Rings

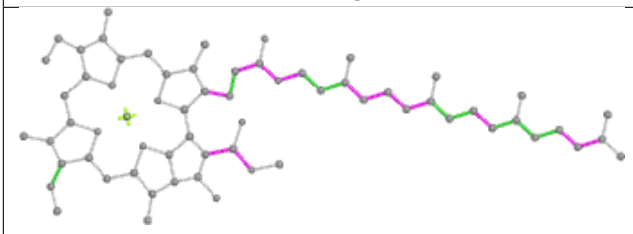
Ligand CLA 1 302



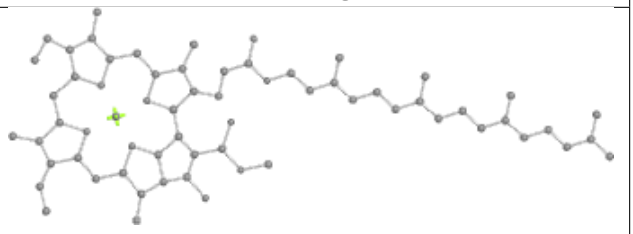
Bond lengths



Bond angles

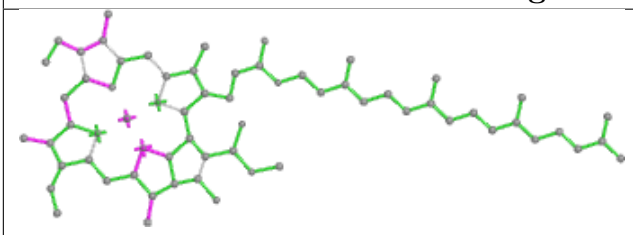


Torsions

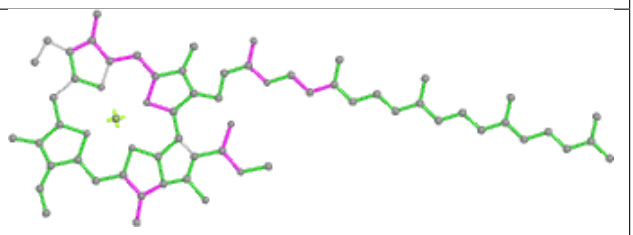


Rings

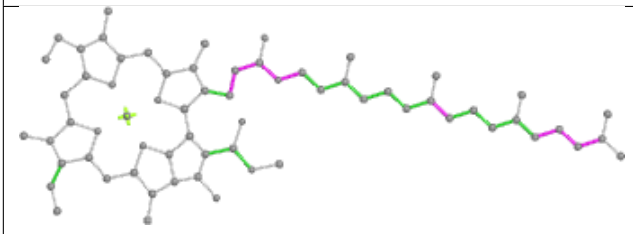
Ligand CLA 6 313



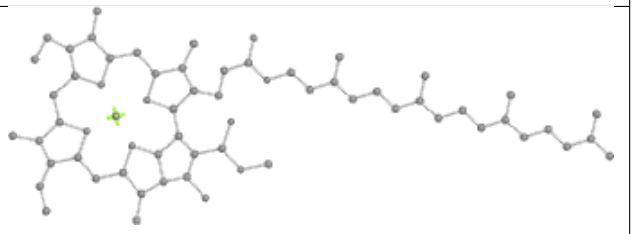
Bond lengths



Bond angles

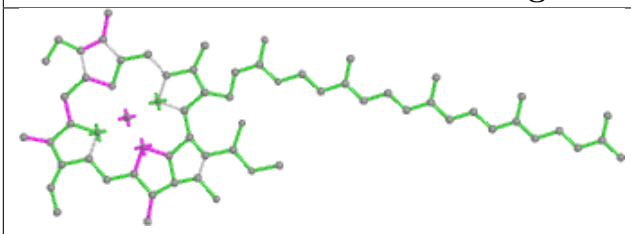


Torsions

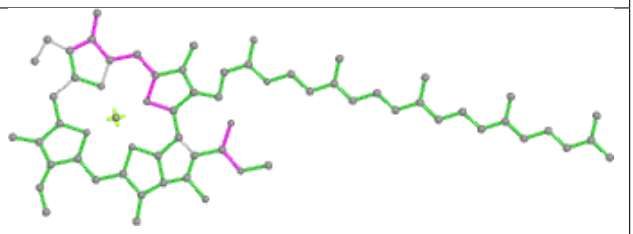


Rings

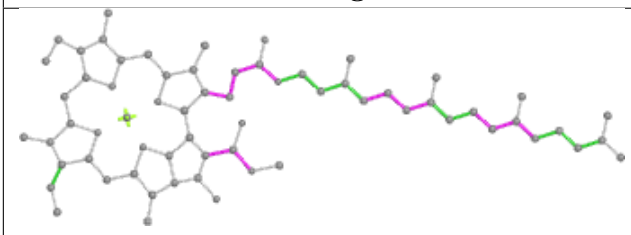
Ligand CLA 7 316



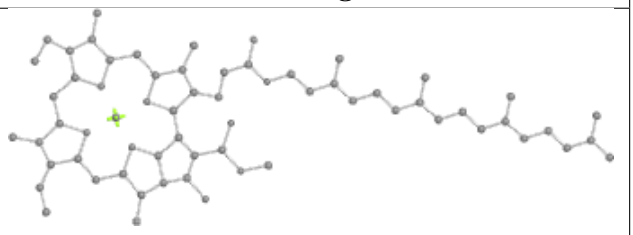
Bond lengths



Bond angles

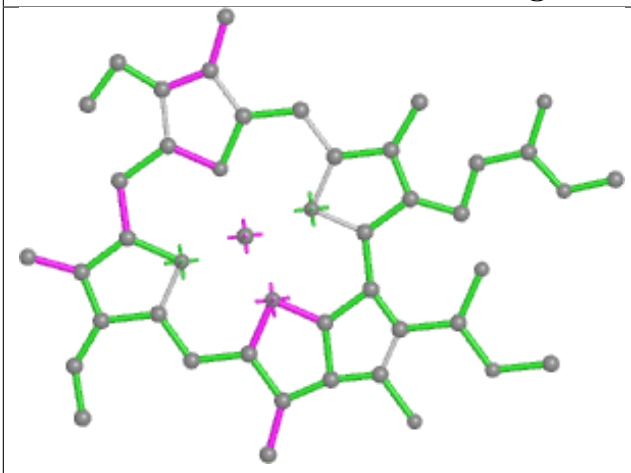


Torsions

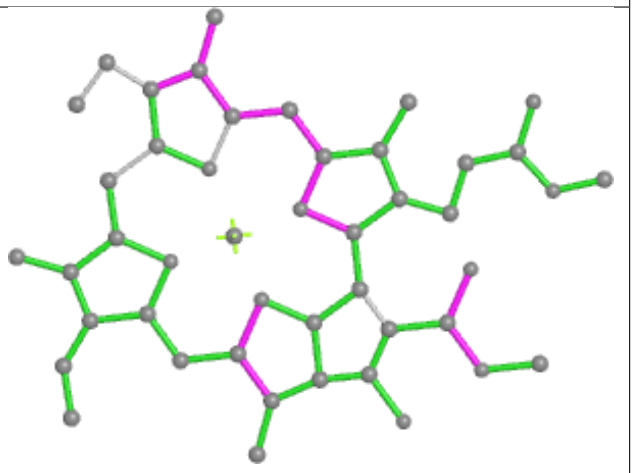


Rings

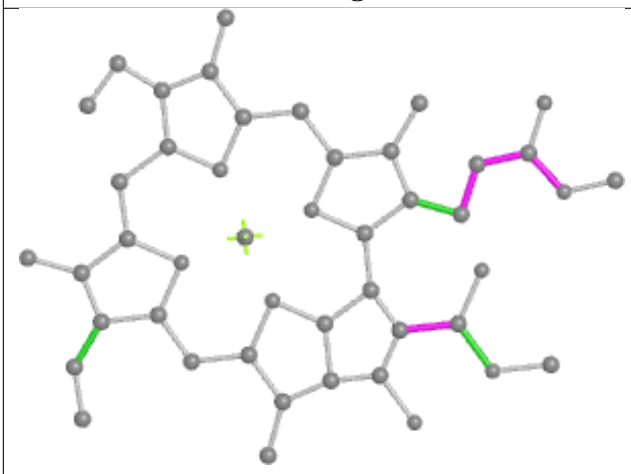
Ligand CLA 4 303



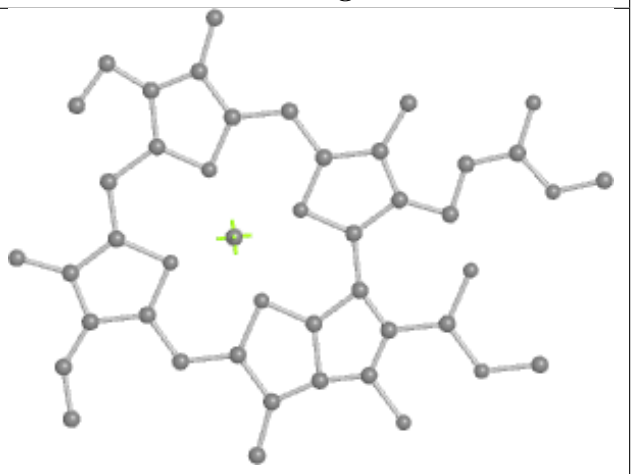
Bond lengths



Bond angles

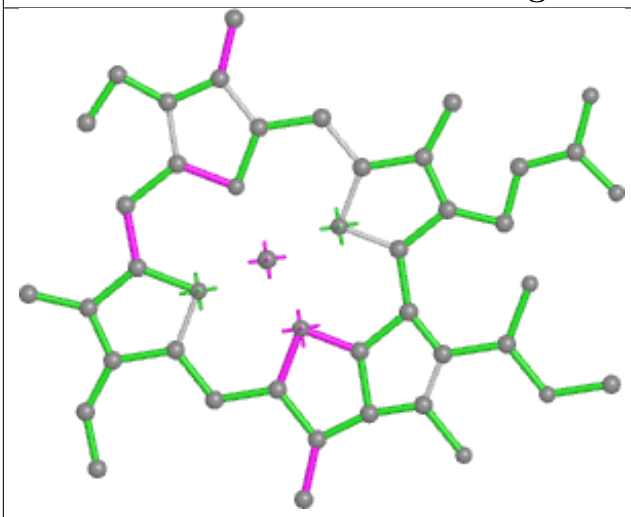


Torsions



Rings

Ligand CLA 5 311



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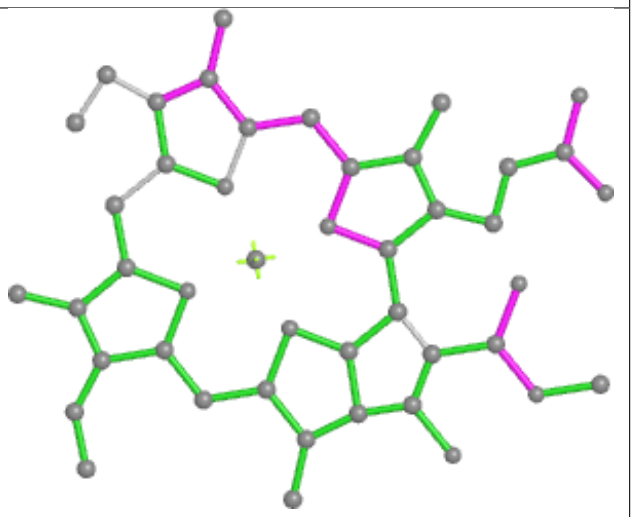
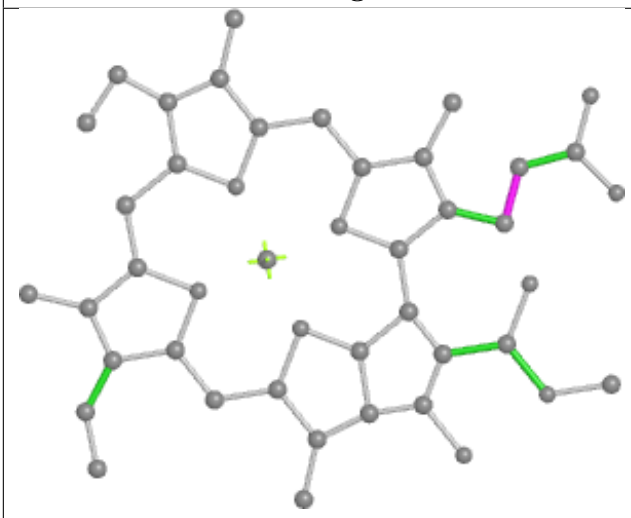


Bond angles



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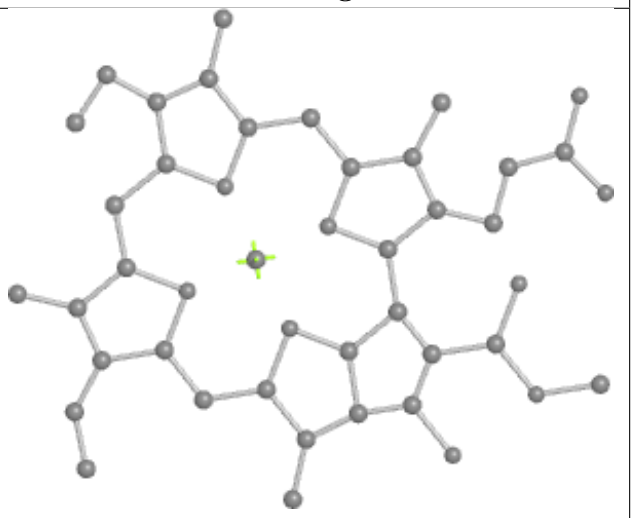
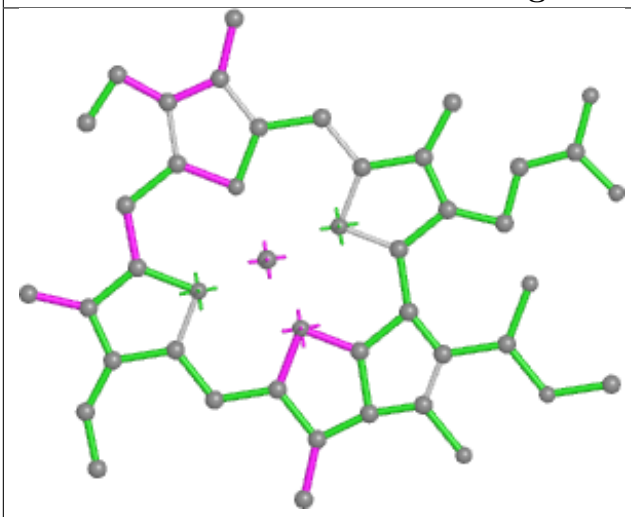
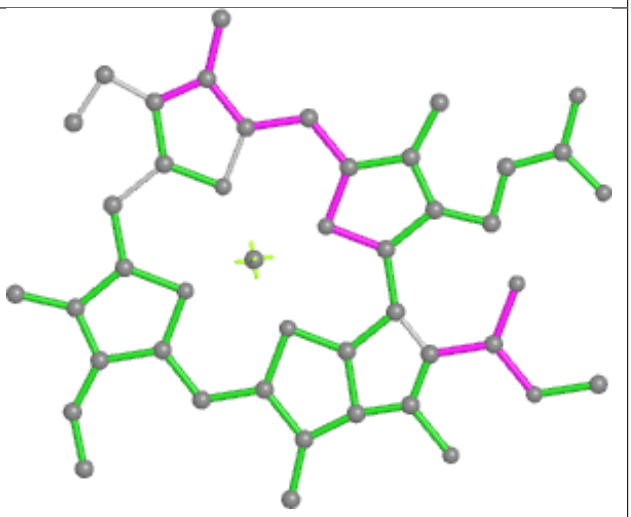


Rings

Ligand CLA 7 314



Bond lengths



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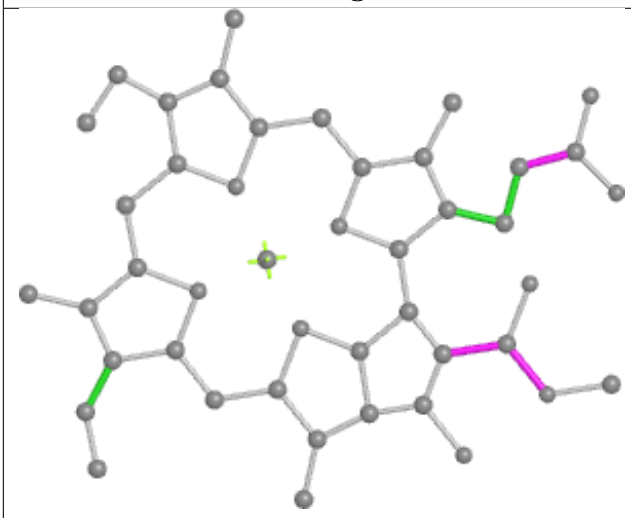
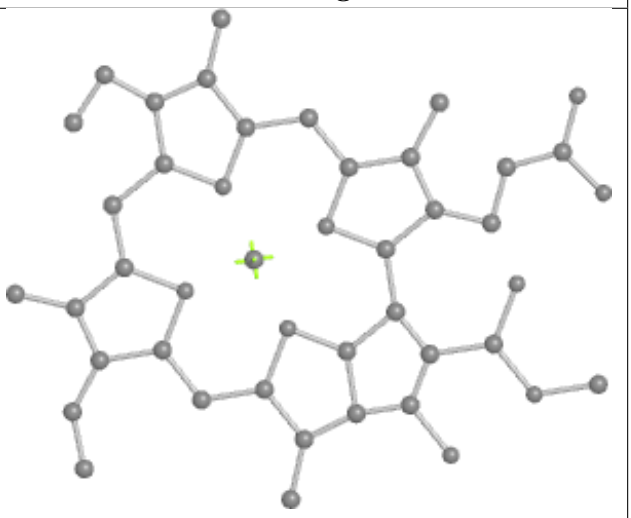
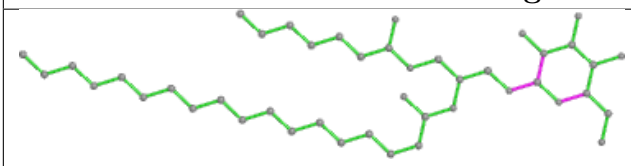


Torsions

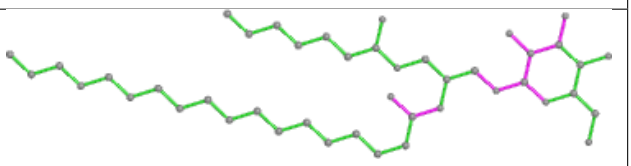


Rings

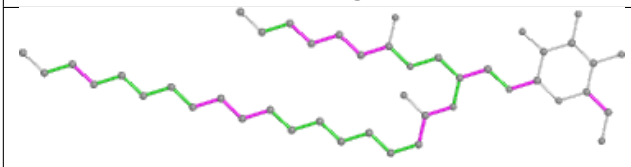
Ligand LMG 5 319



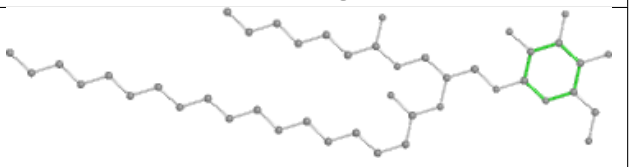
Bond lengths



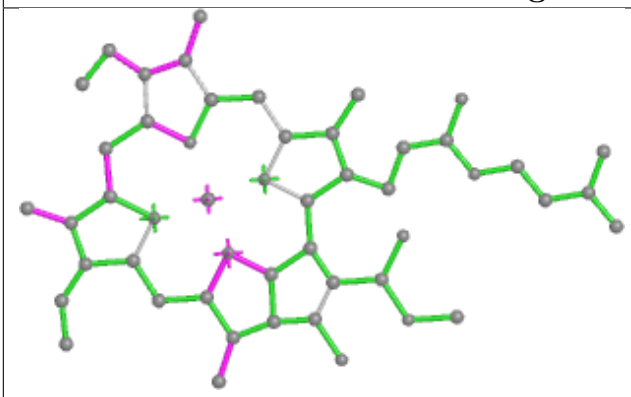
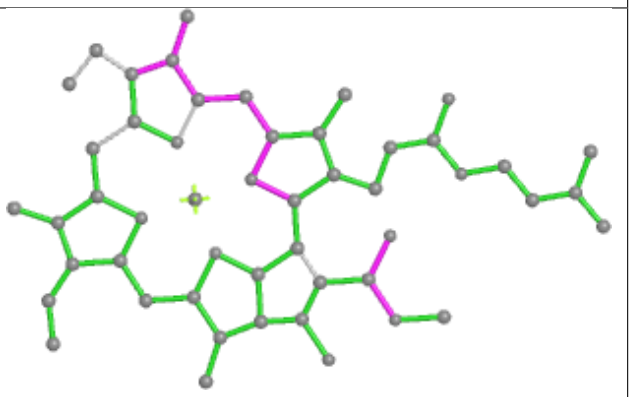
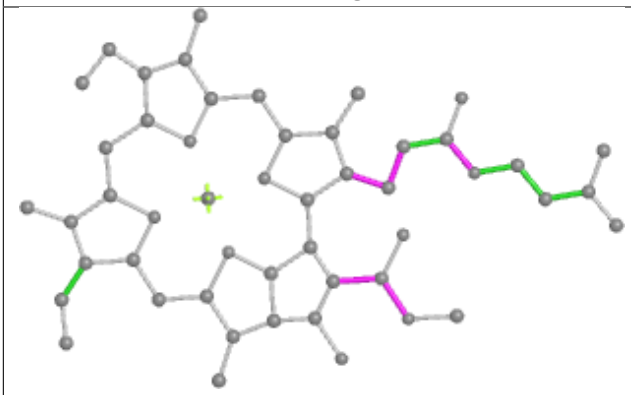
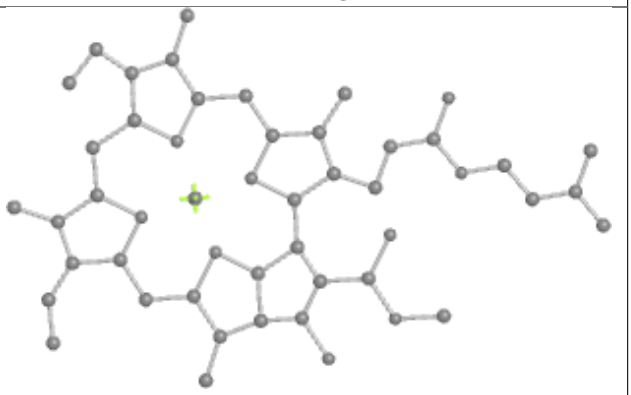
Bond angles



Torsions



Rings

Ligand CLA 8 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

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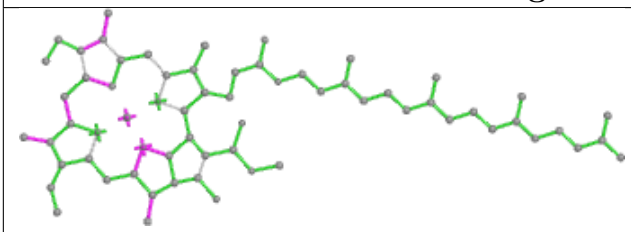
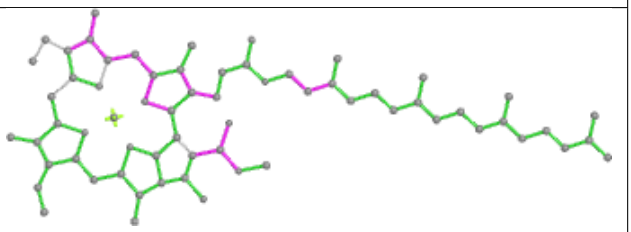
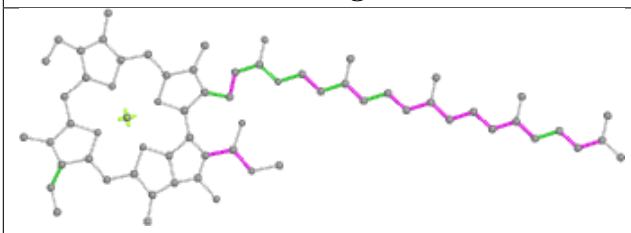
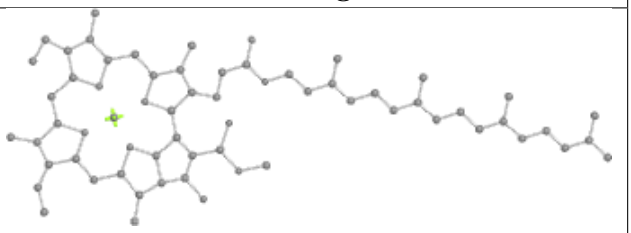
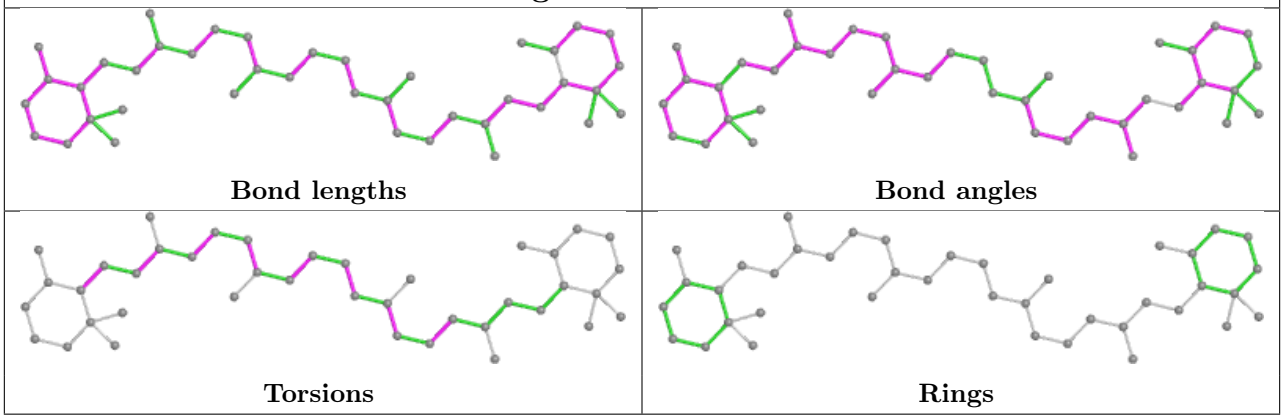
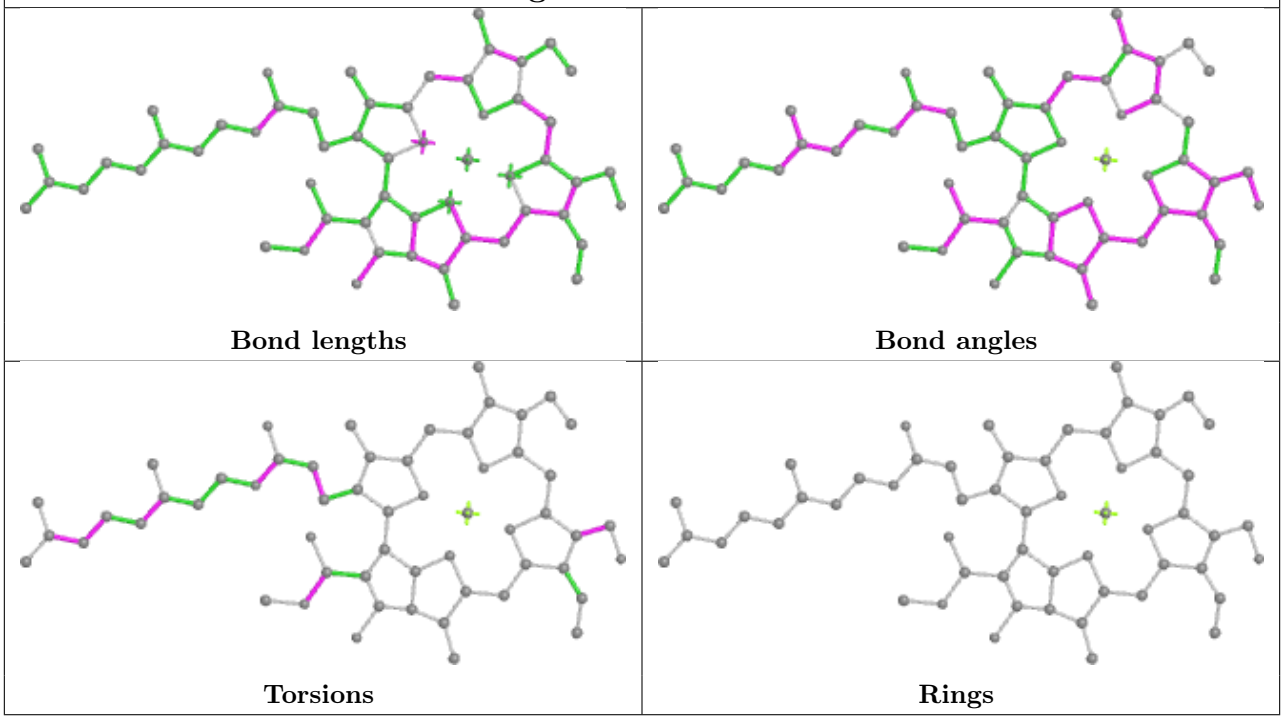
 Bond lengths	 Bond angles
 Torsions	 Rings

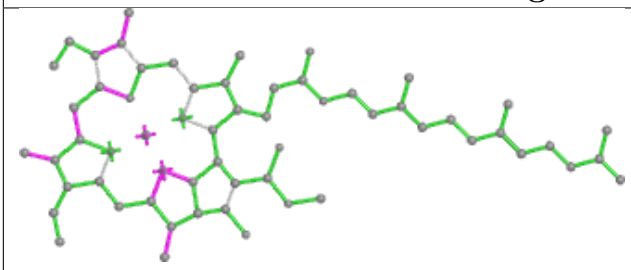
Ligand 8CT 7 301



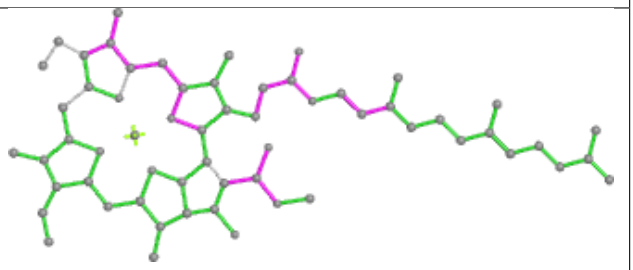
Ligand CHL 4 305



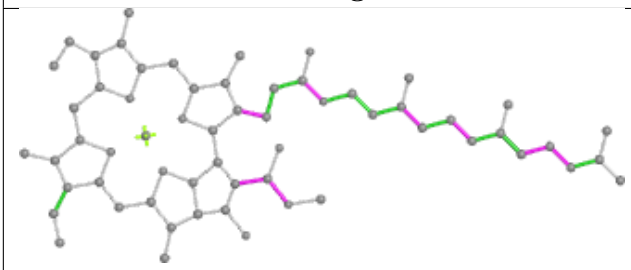
Ligand CLA 6 310



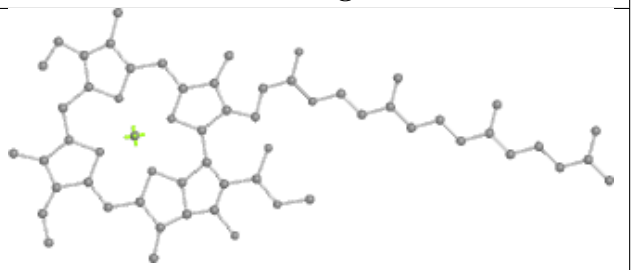
Bond lengths



Bond angles

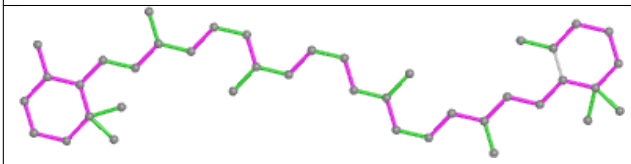


Torsions



Rings

Ligand 8CT 8 301



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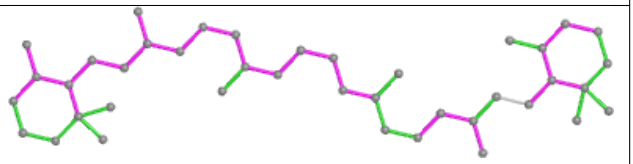
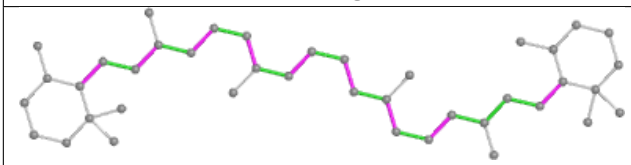


Bond angles



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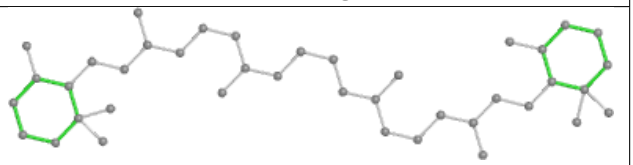
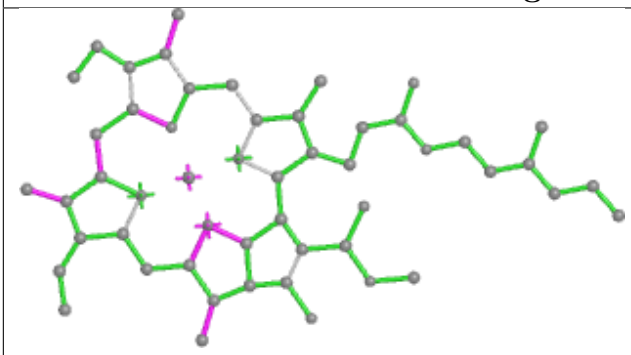
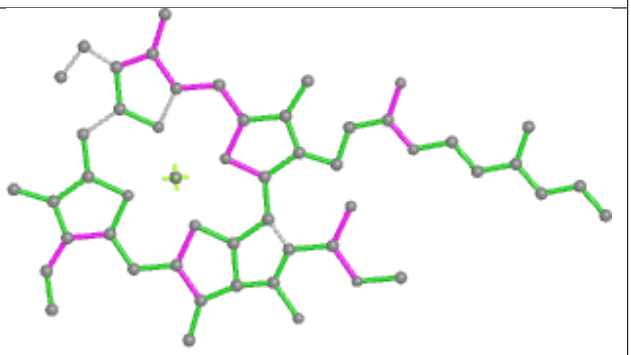


Rings

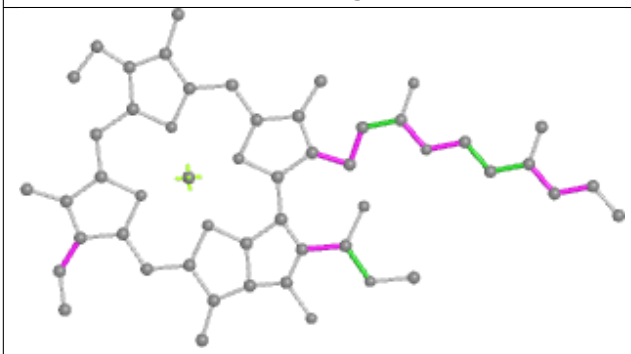
Ligand CLA A 843



Bond lengths



Bond angles



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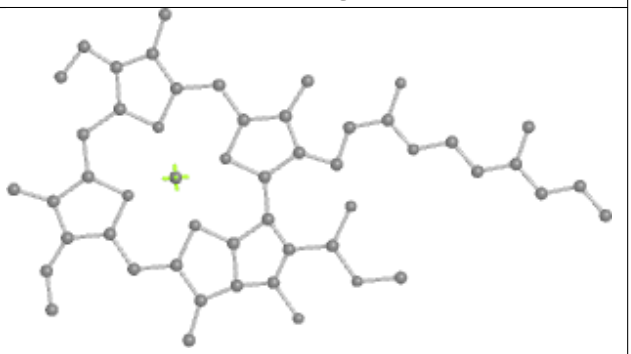
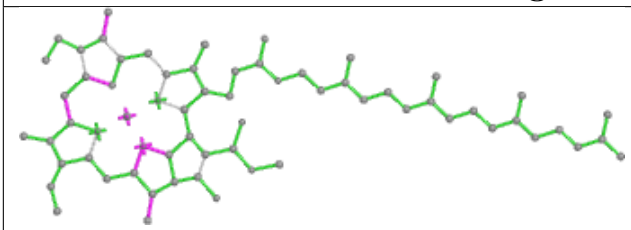


Rings

Ligand CLA 8 315



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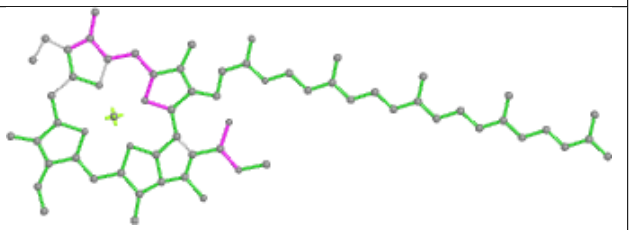
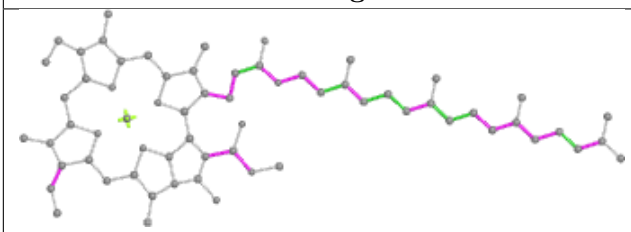


Bond angles



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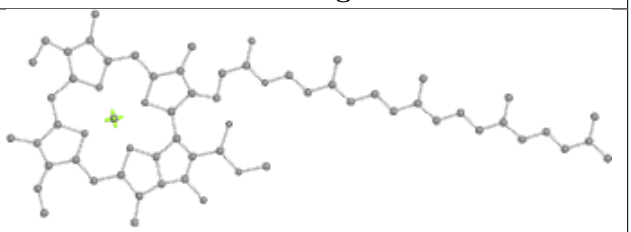
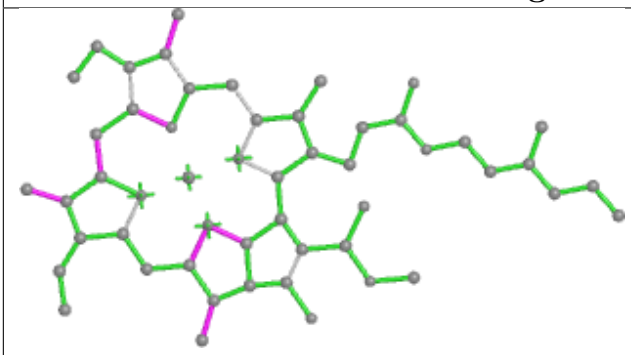
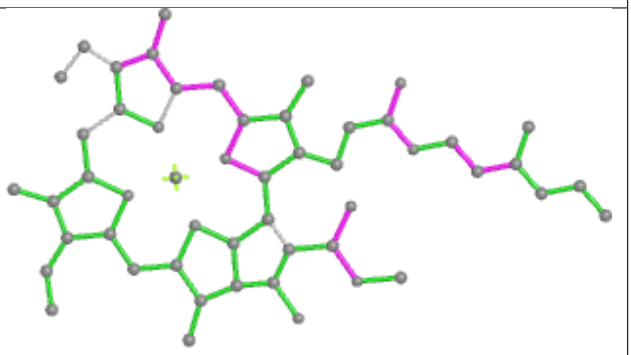
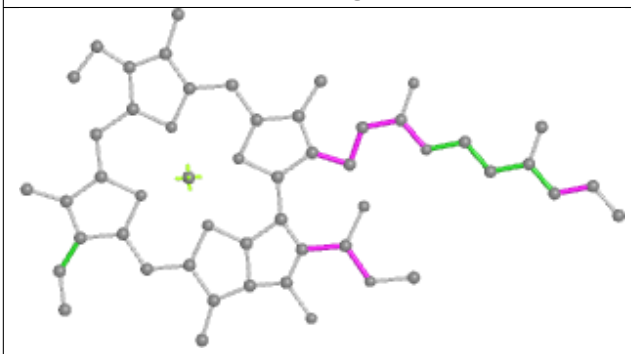
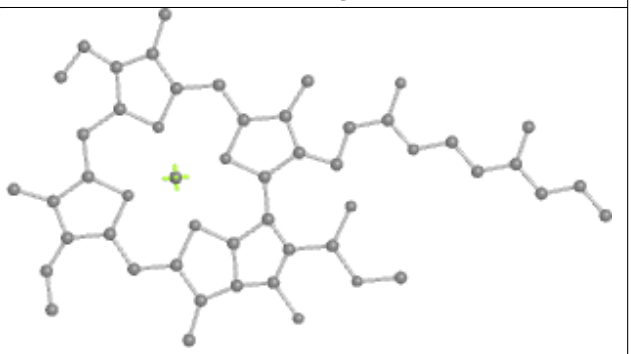
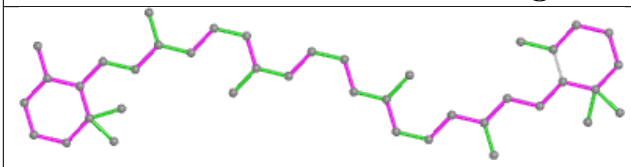
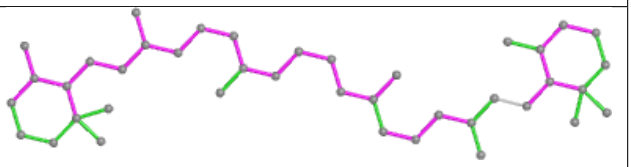
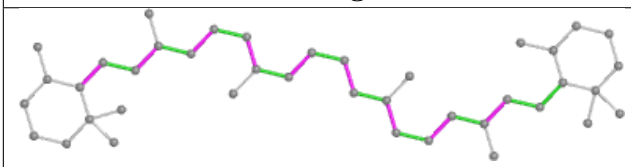
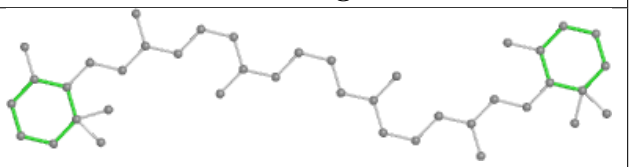
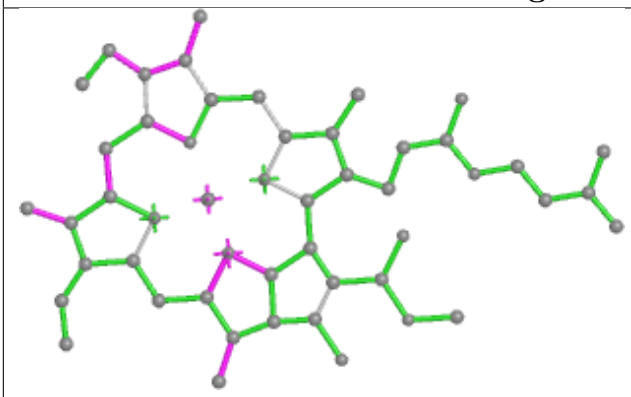


Rings

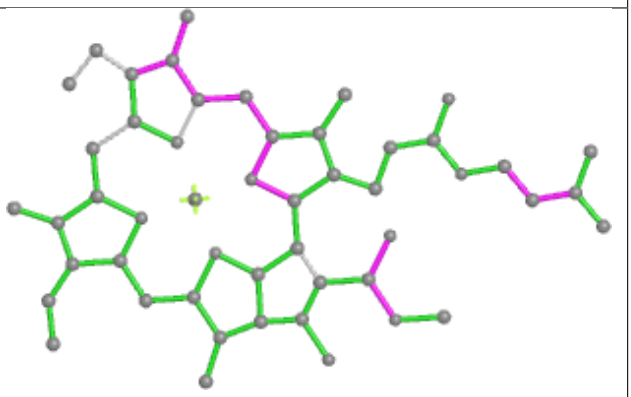
Ligand CLA 6 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand 8CT 7 323	
	
Bond lengths	Bond angles
	
Torsions	Rings

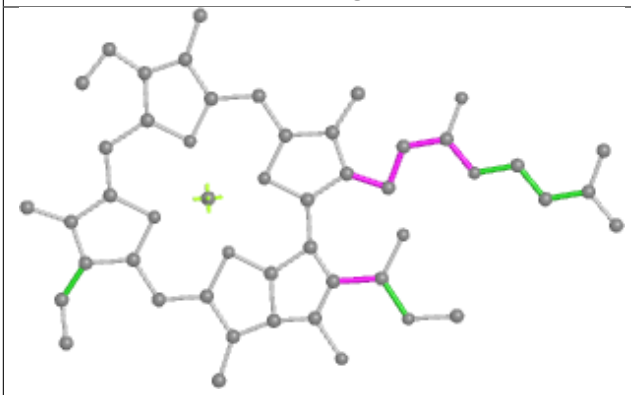
Ligand CLA 3 307



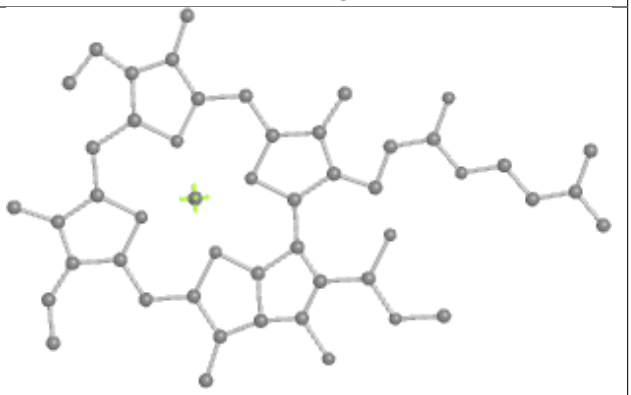
Bond lengths



Bond angles

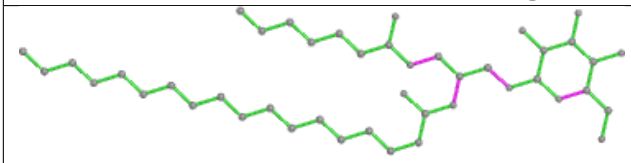


Torsions

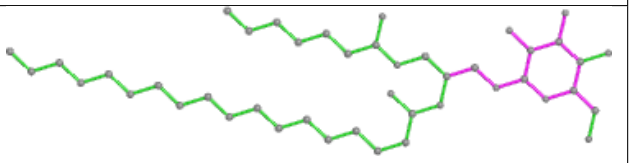


Rings

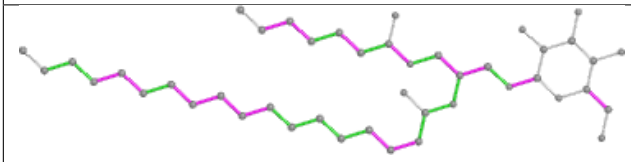
Ligand LMG 4 318



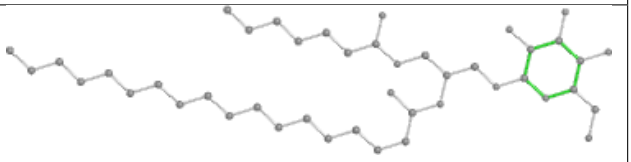
Bond lengths



Bond angles

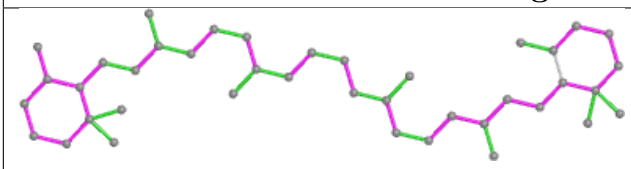


Torsions

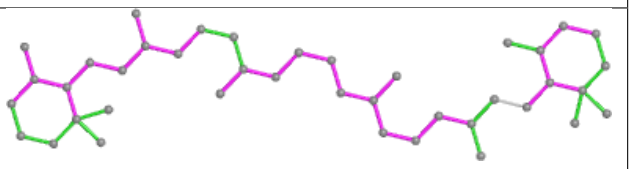


Rings

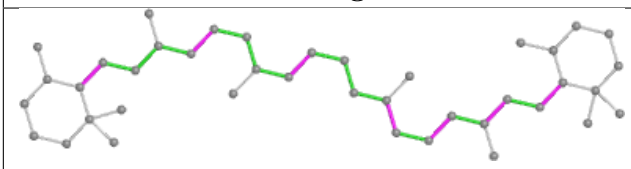
Ligand 8CT 1 316



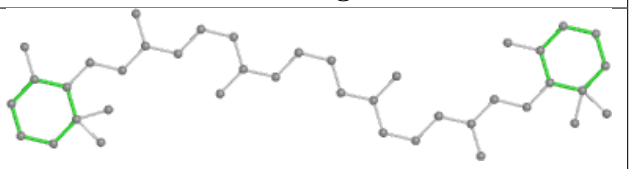
Bond lengths



Bond angles

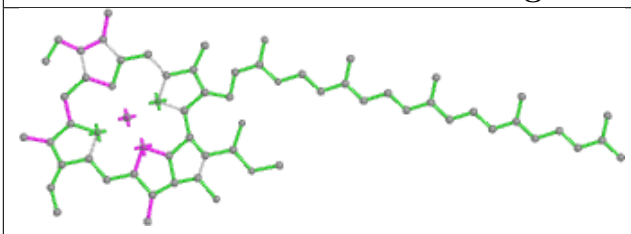


Torsions



Rings

Ligand CLA B 812



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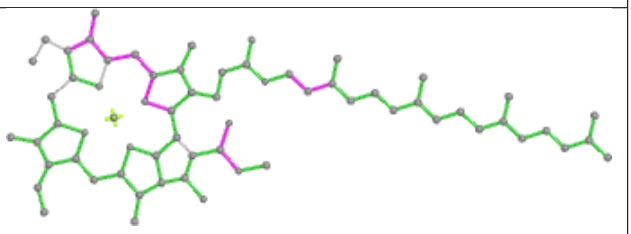
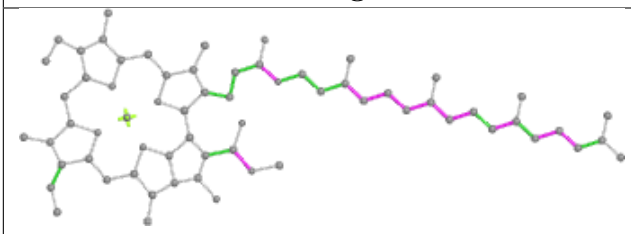
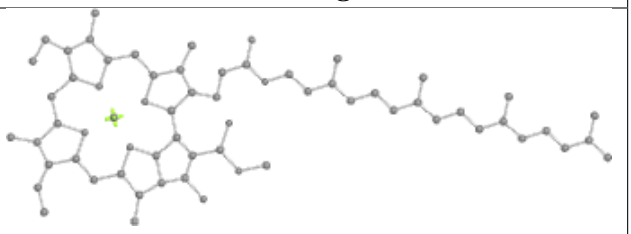


Bond angles

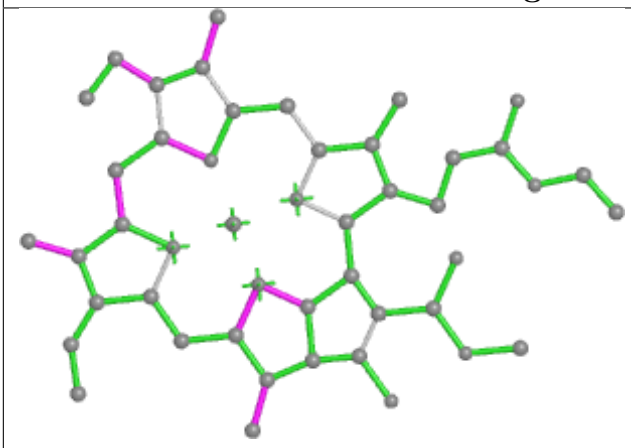


Torsions

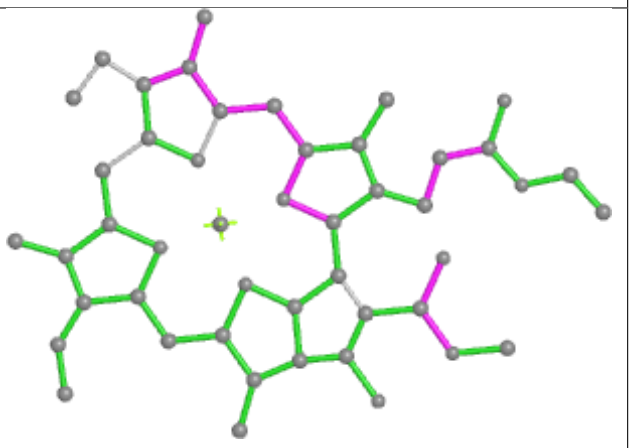


Rings

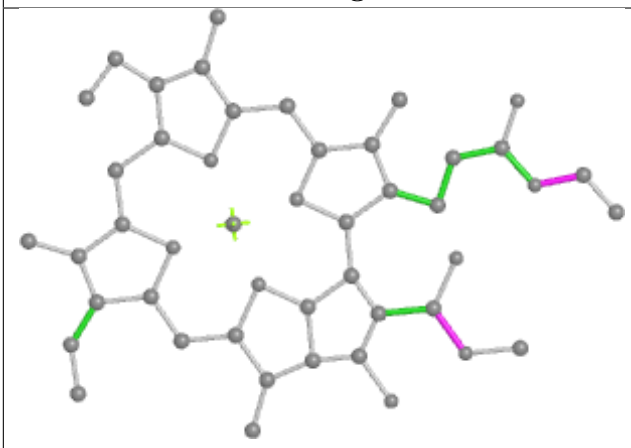
Ligand CLA A 815



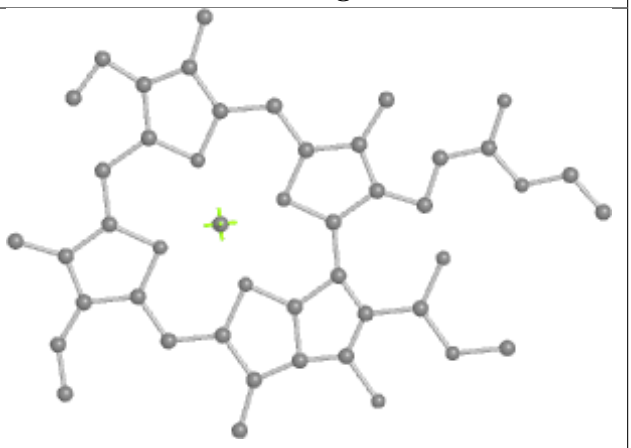
Bond lengths



Bond angles

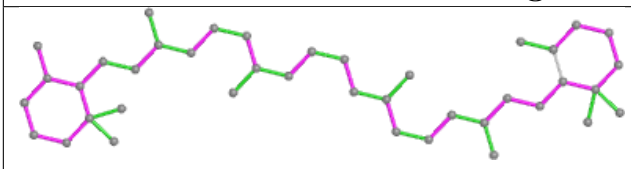


Torsions

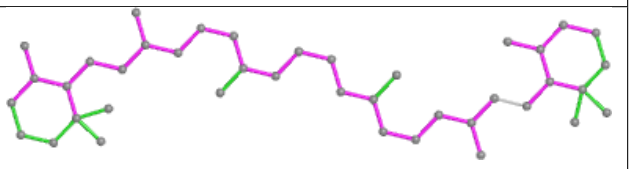


Rings

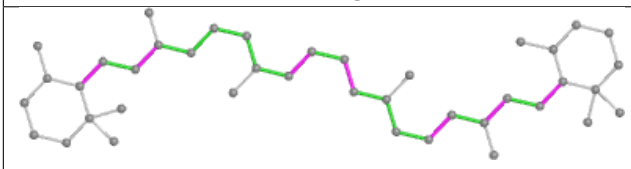
Ligand 8CT A 847



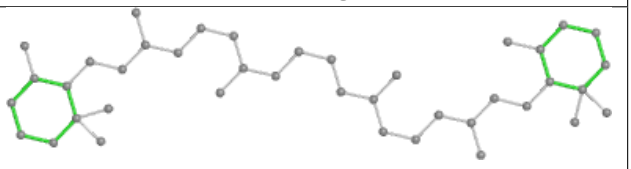
Bond lengths



Bond angles

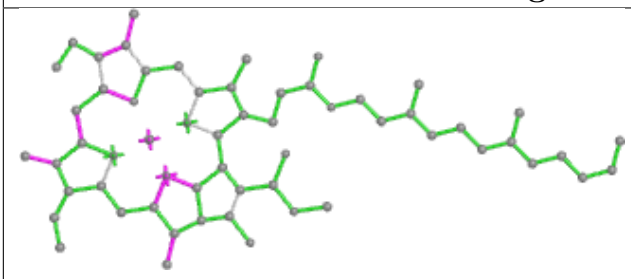


Torsions

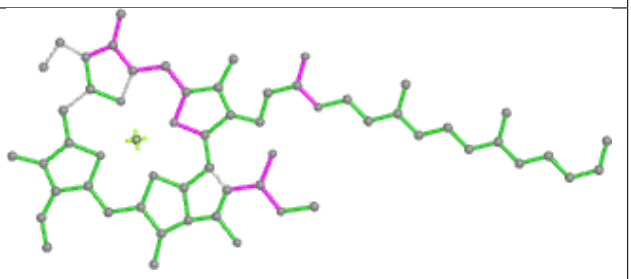


Rings

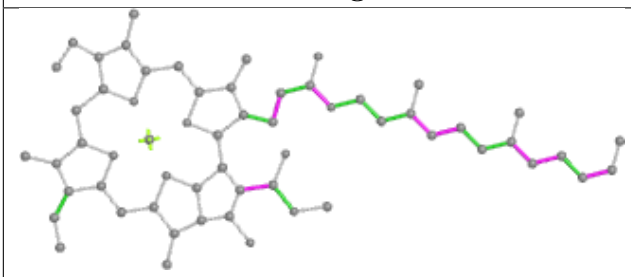
Ligand CLA 9 312



Bond lengths



Bond angles



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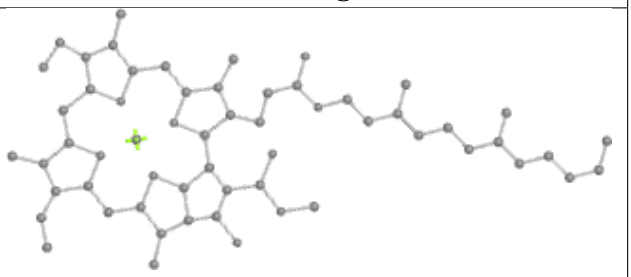
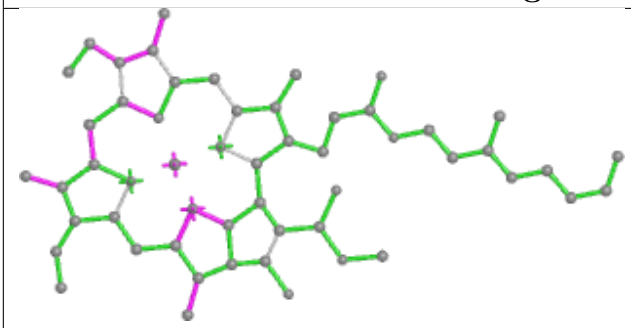
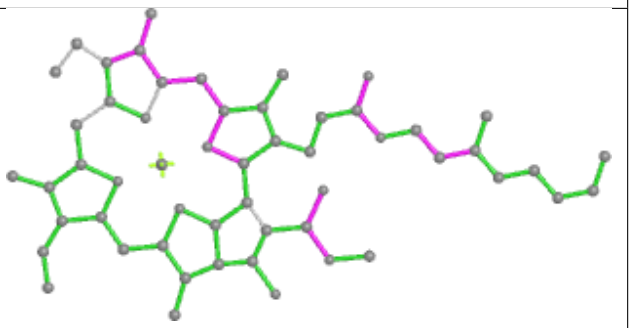


Rings

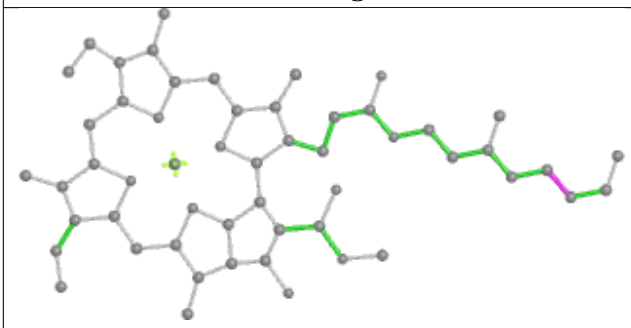
Ligand CLA A 812



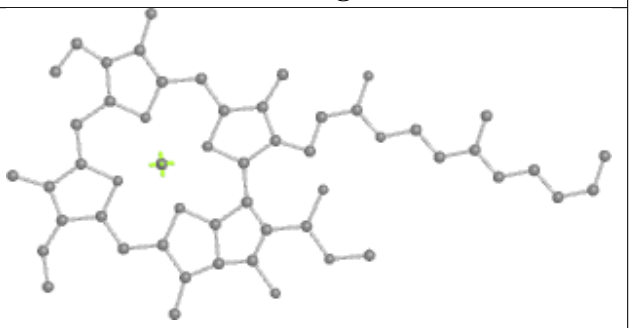
Bond lengths



Bond angles

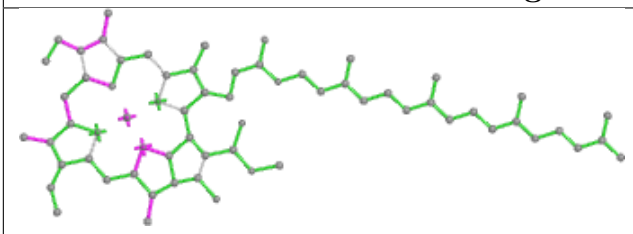


Torsions

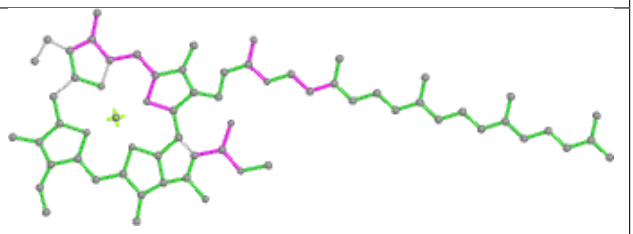


Rings

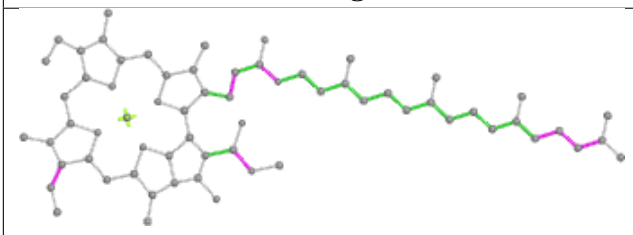
Ligand CLA B 815



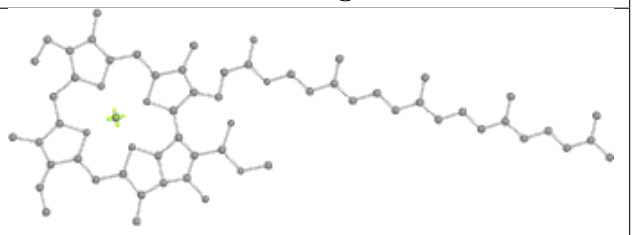
Bond lengths



Bond angles

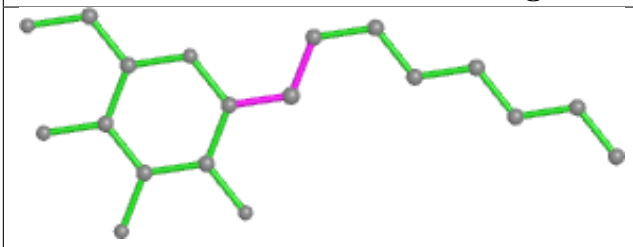


Torsions

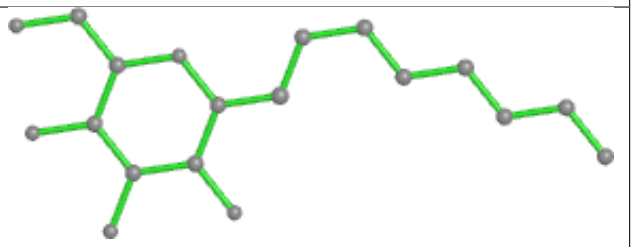


Rings

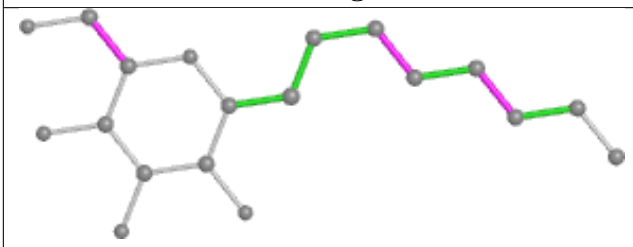
Ligand HTG J 102



Bond lengths



Bond angles



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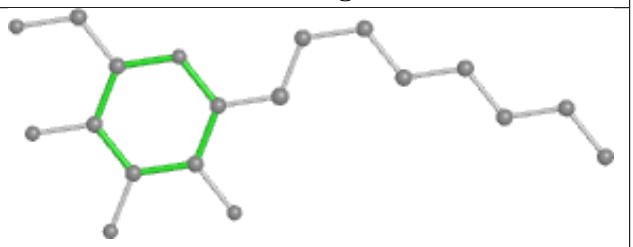
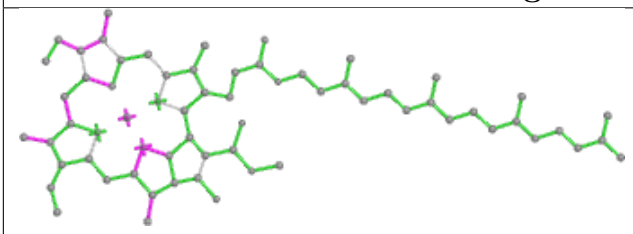
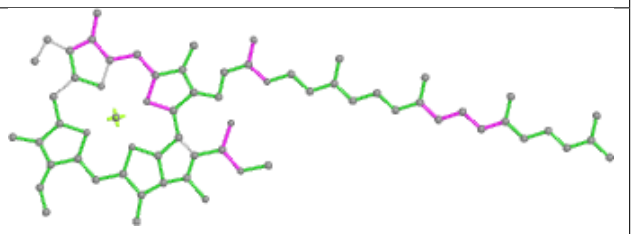


Rings

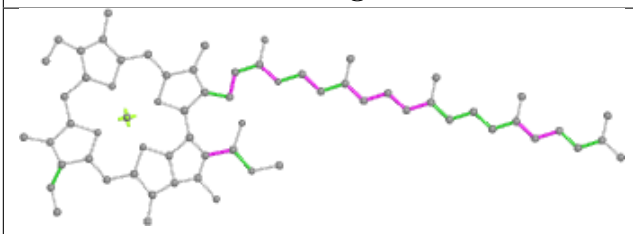
Ligand CLA A 840



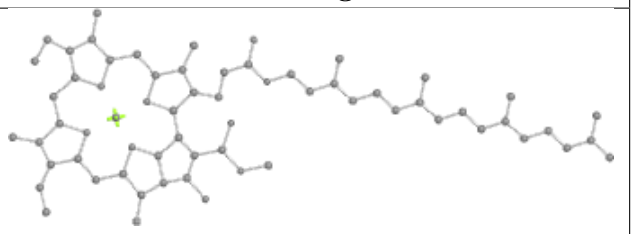
Bond lengths



Bond angles

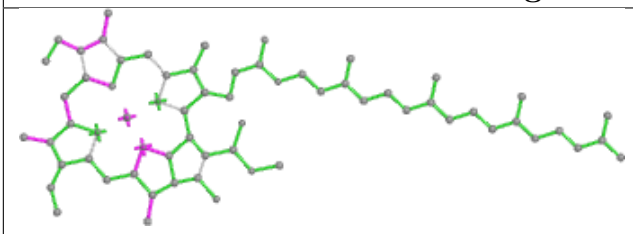


Torsions

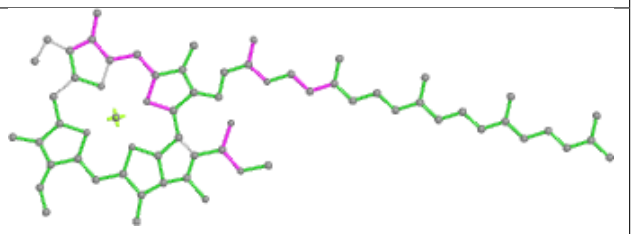


Rings

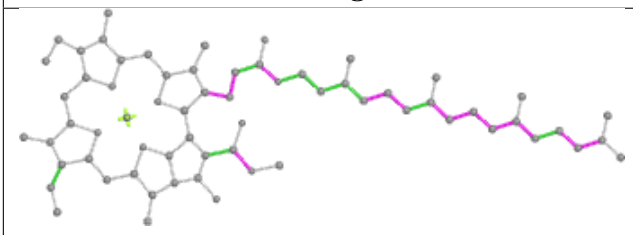
Ligand CLA B 809



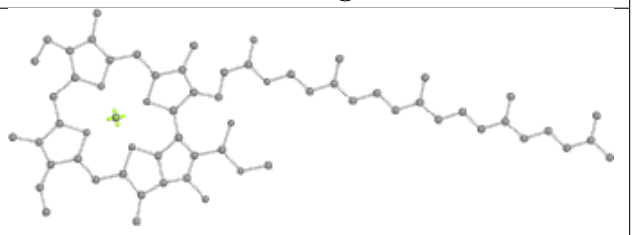
Bond lengths



Bond angles

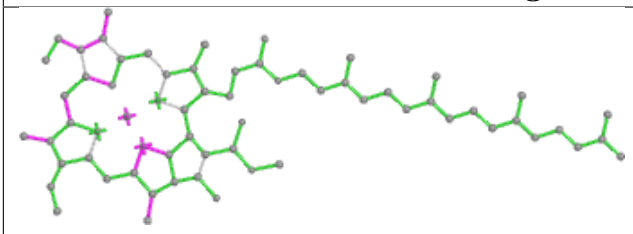


Torsions

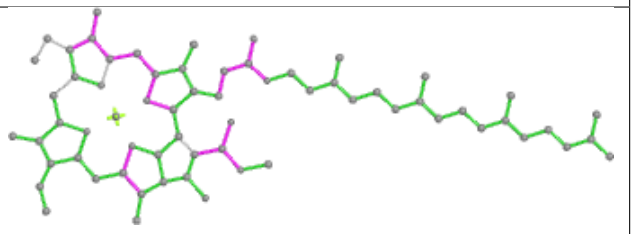


Rings

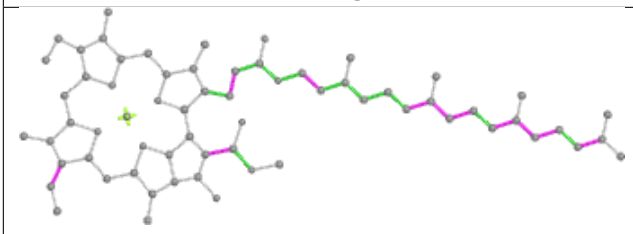
Ligand CLA B 803



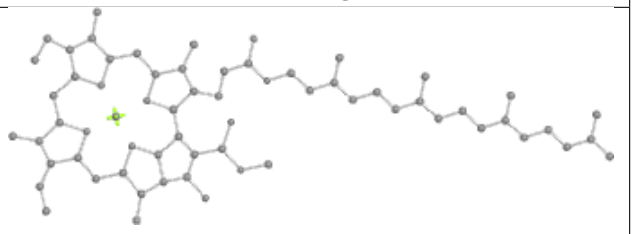
Bond lengths



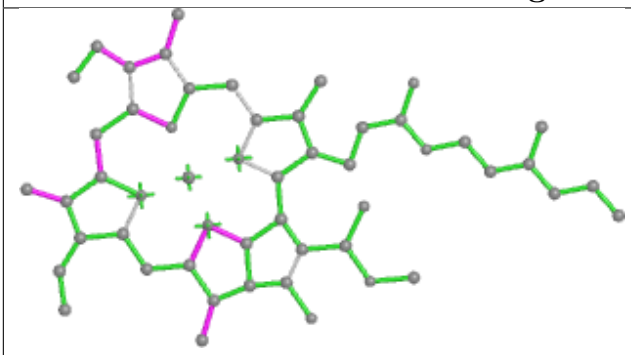
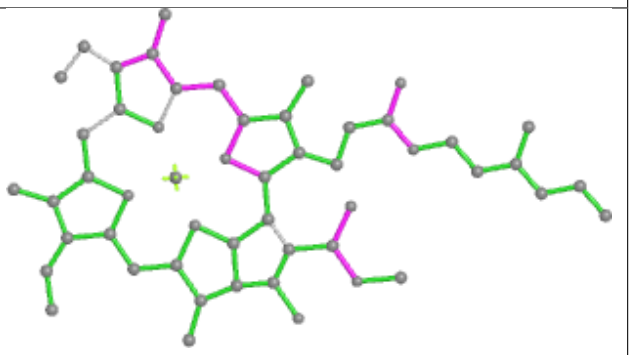
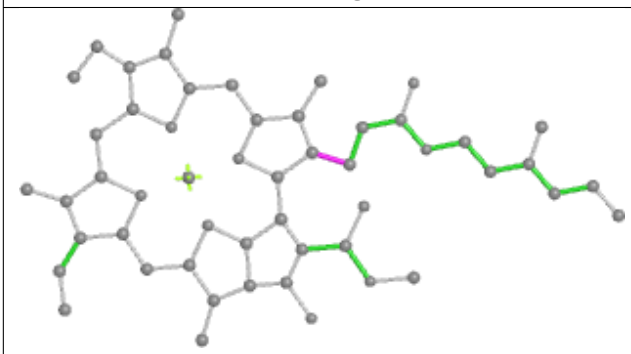
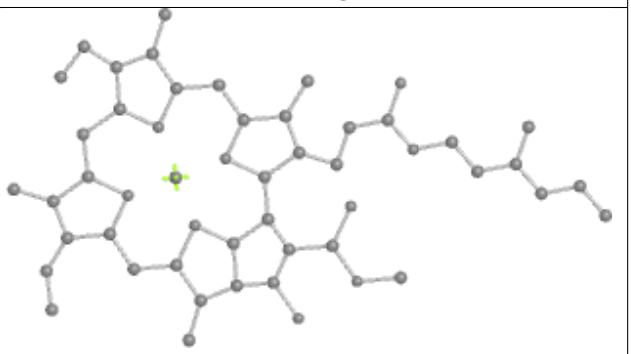
Bond angles

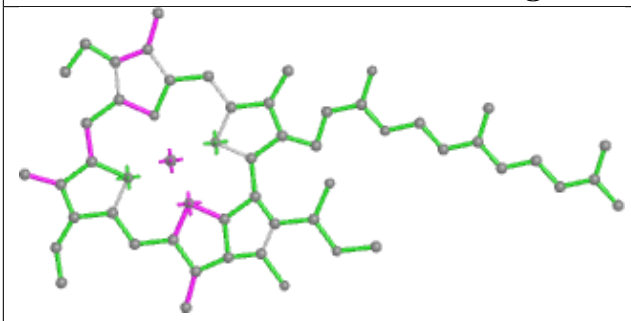
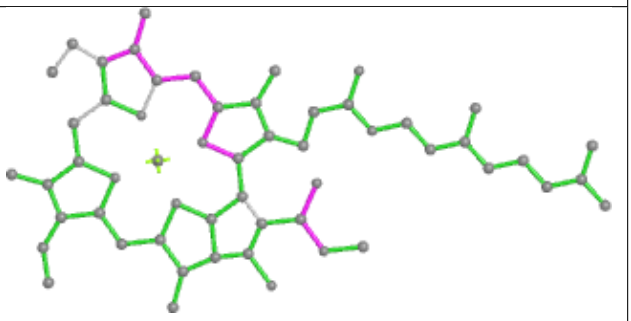
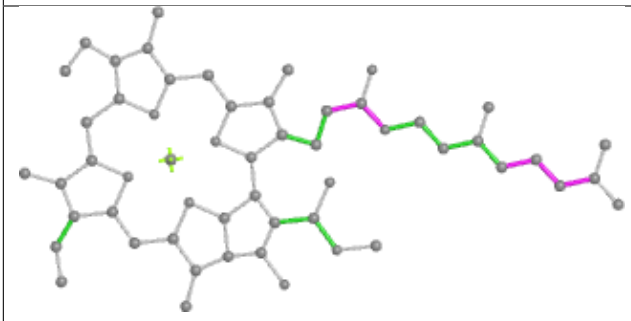
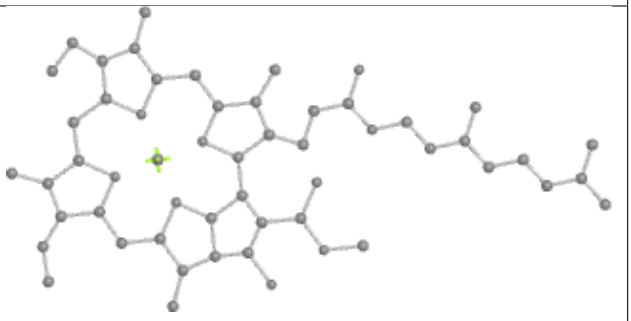


Torsions

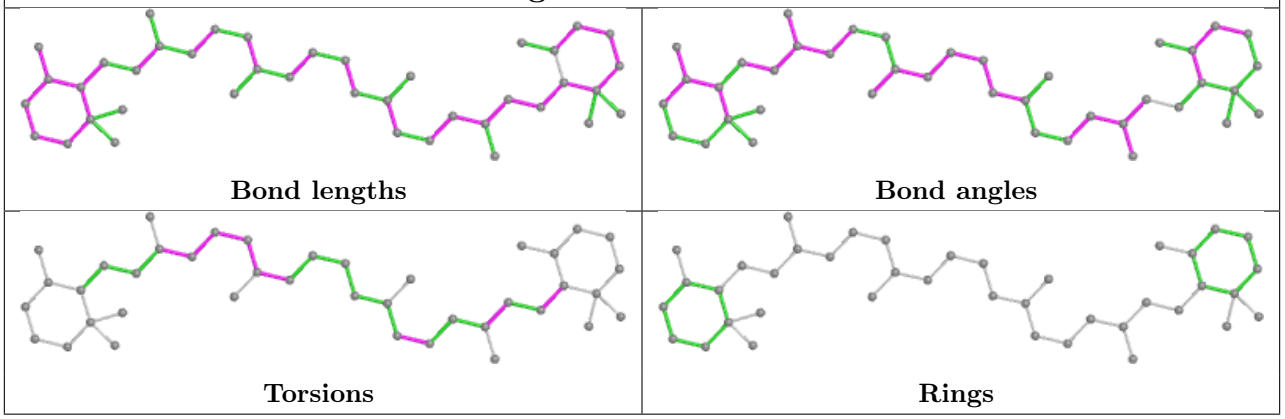


Rings

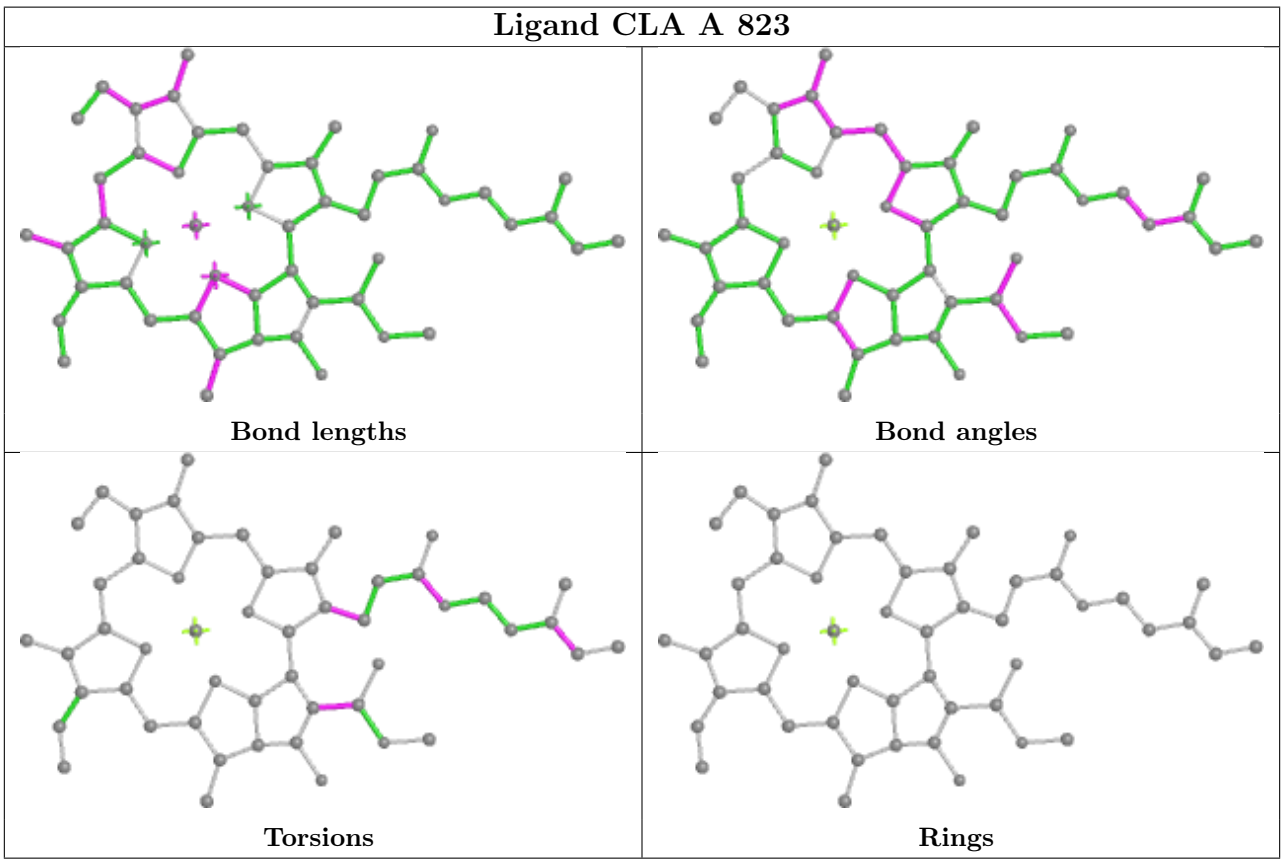
Ligand CLA 0 310	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 813	
	
Bond lengths	Bond angles
	
Torsions	Rings

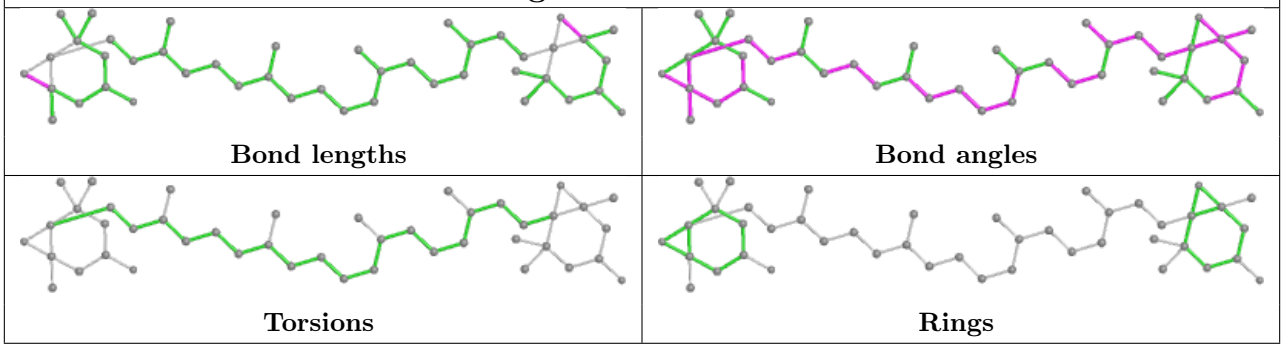
Ligand 8CT B 846



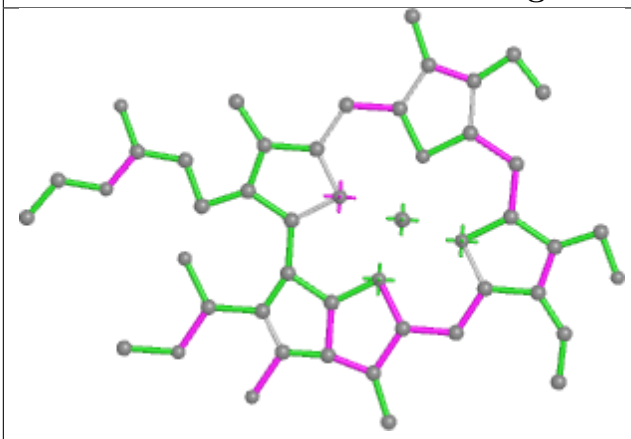
Ligand CLA A 823



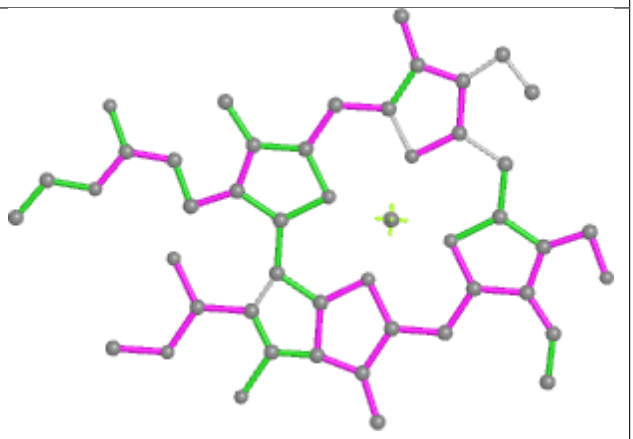
Ligand XAT 7 320



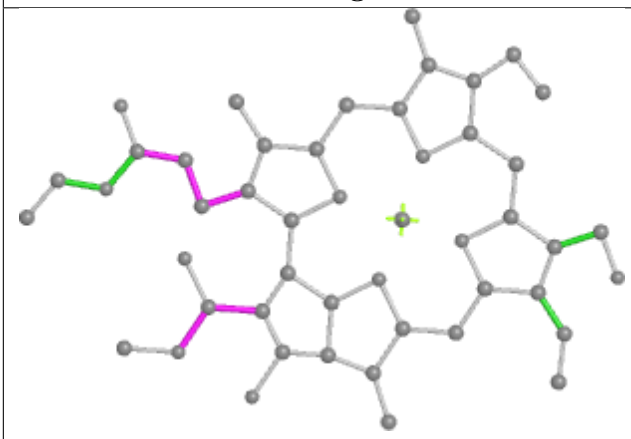
Ligand CHL 2 306



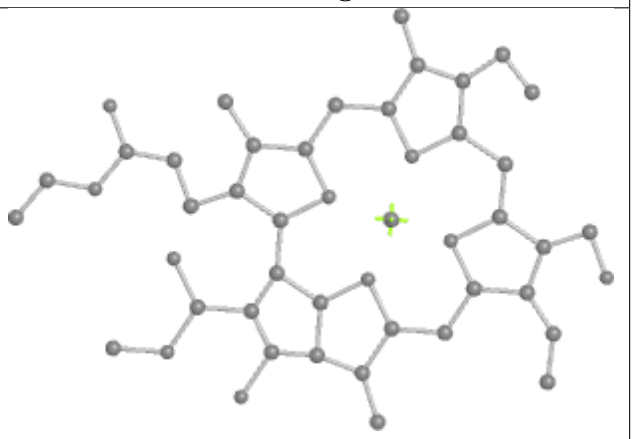
Bond lengths



Bond angles

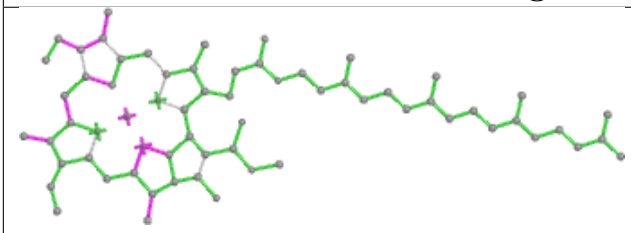


Torsions

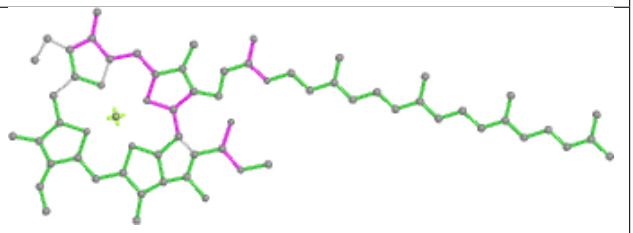


Rings

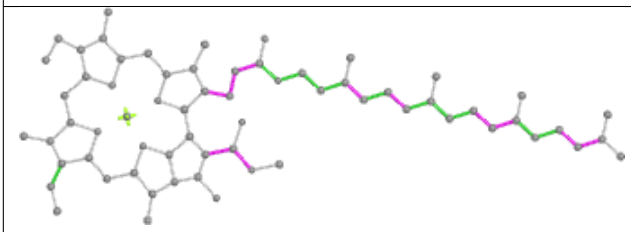
Ligand CLA 7 318



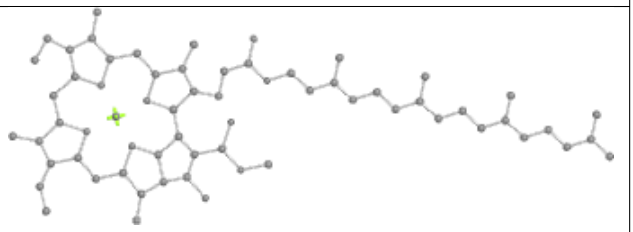
Bond lengths



Bond angles

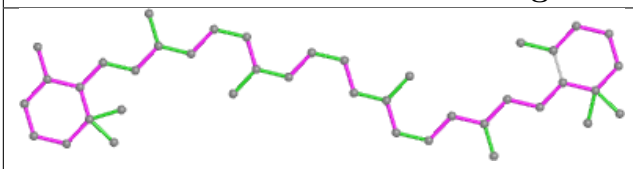


Torsions

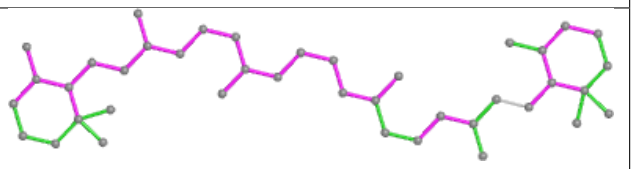


Rings

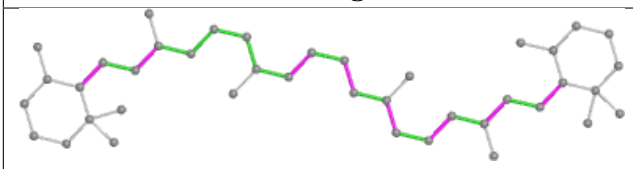
Ligand 8CT 8 318



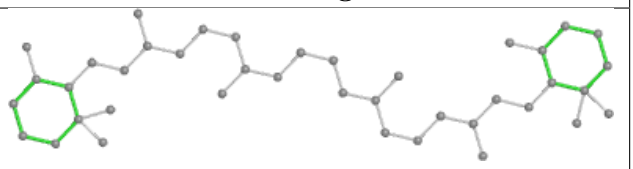
Bond lengths



Bond angles

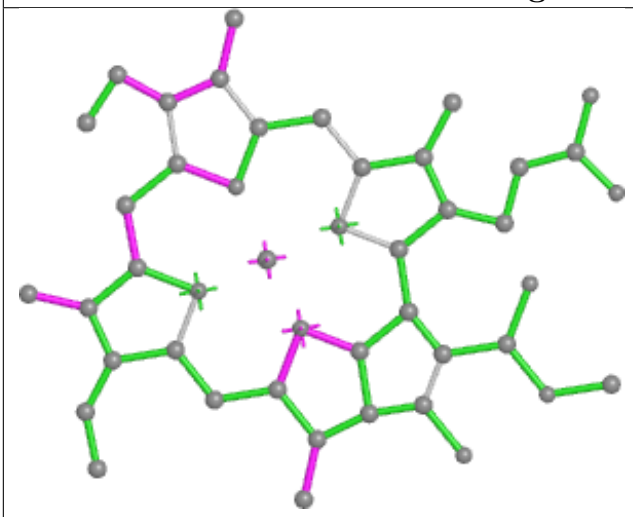


Torsions

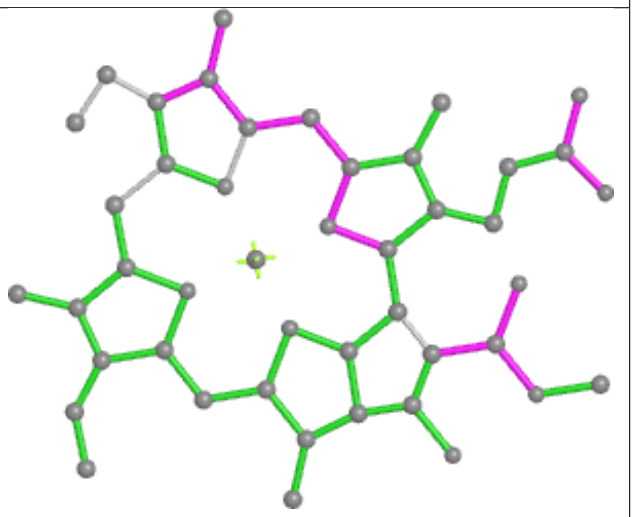


Rings

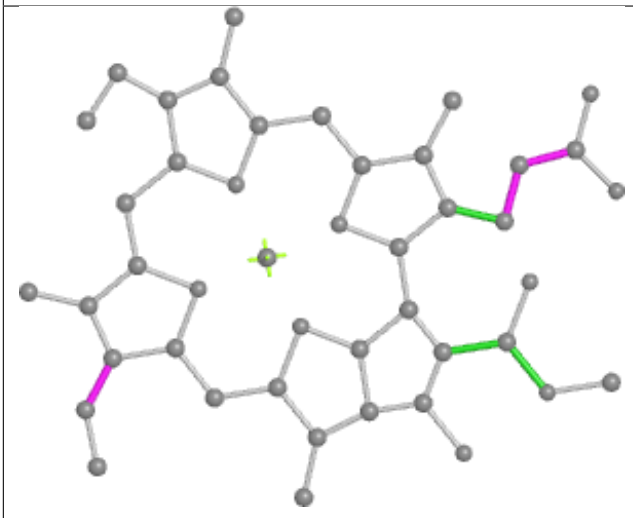
Ligand CLA 6 317



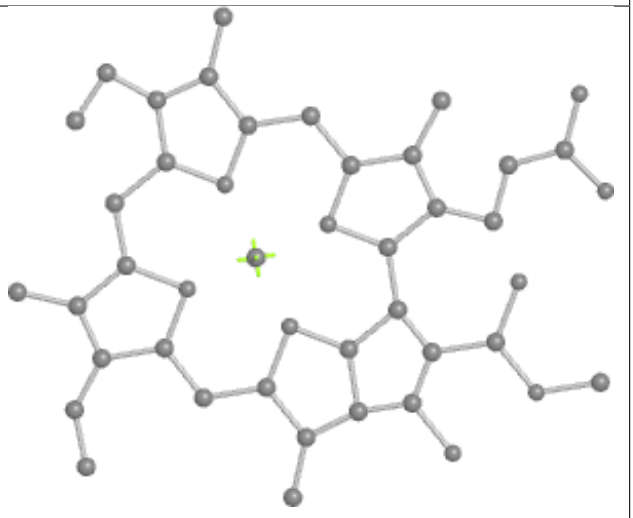
Bond lengths



Bond angles

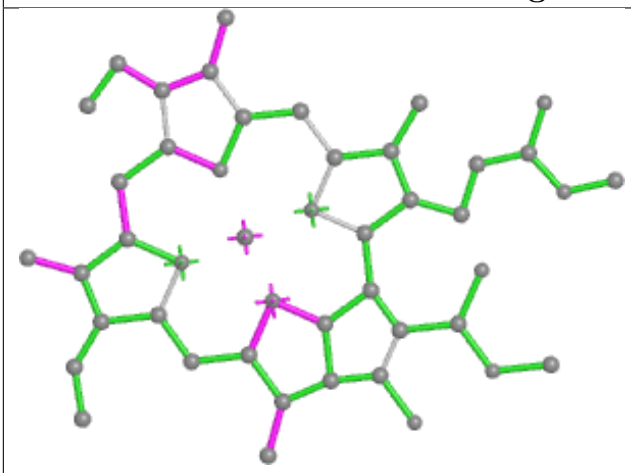


Torsions



Rings

Ligand CLA 8 303



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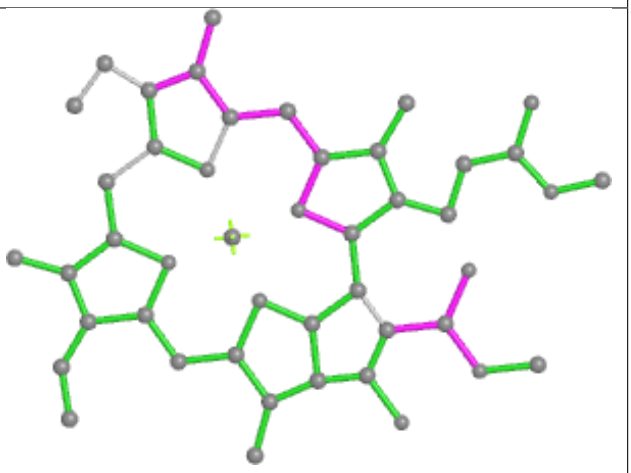
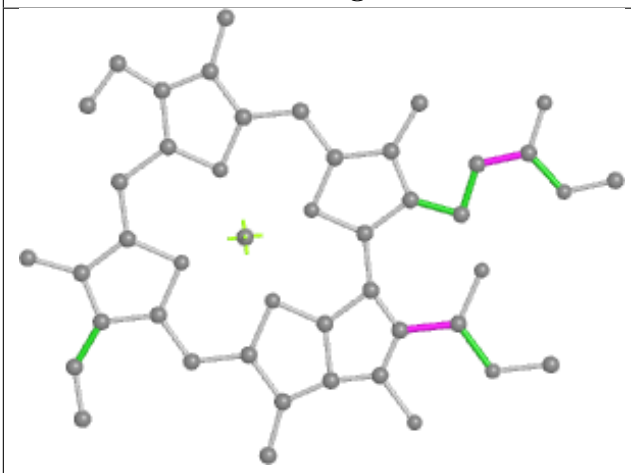
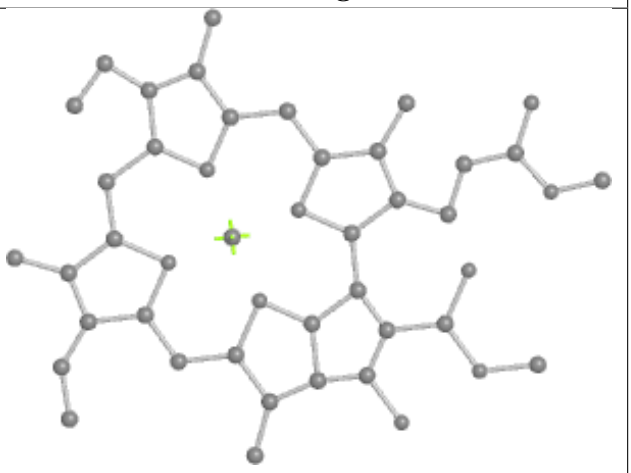


Bond angles

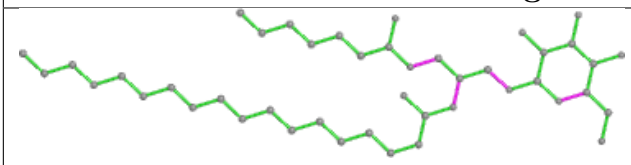


Torsions

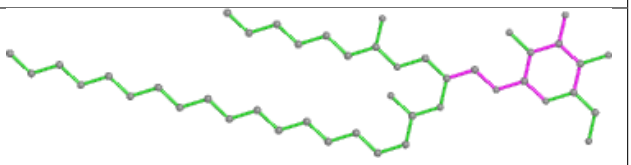


Rings

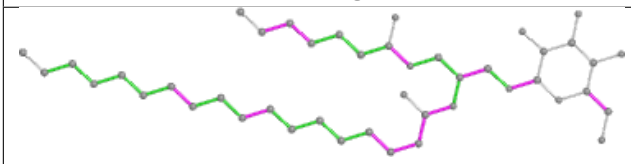
Ligand LMG 8 319



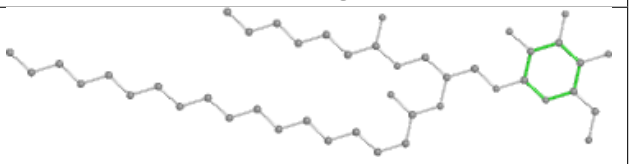
Bond lengths



Bond angles

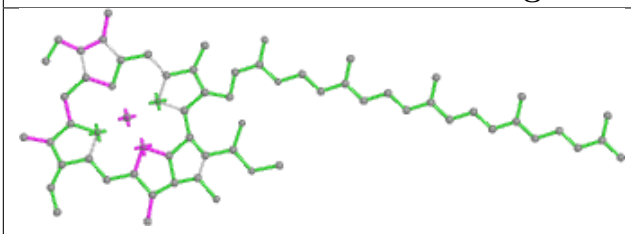


Torsions

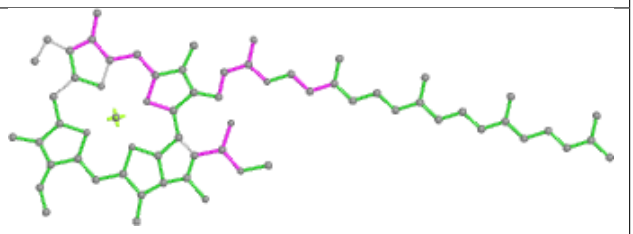


Rings

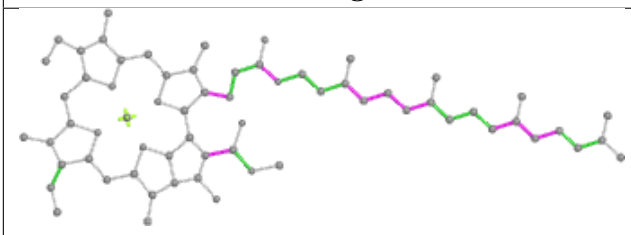
Ligand CLA A 803



Bond lengths



Bond angles



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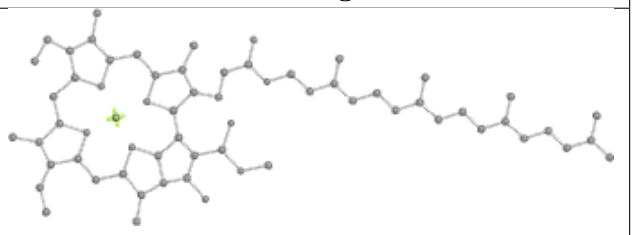
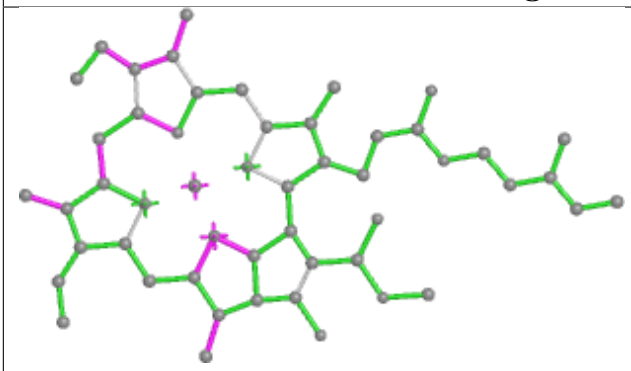


Rings

Ligand CLA A 836



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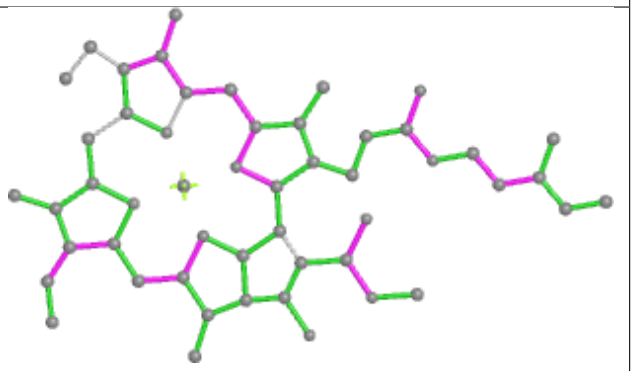
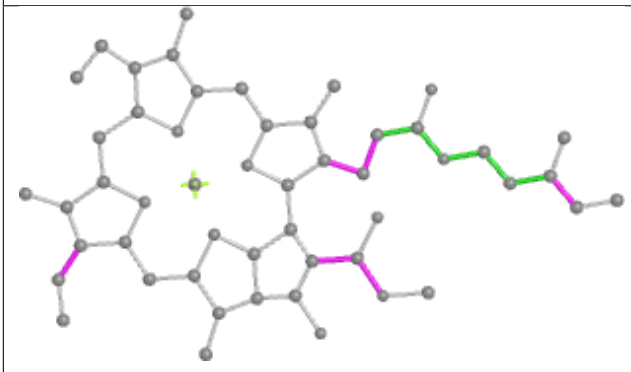
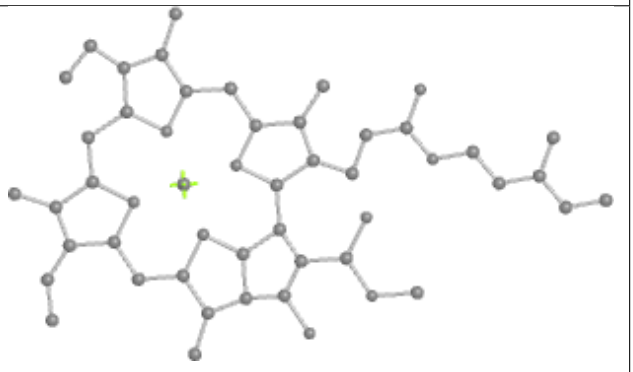


Bond angles

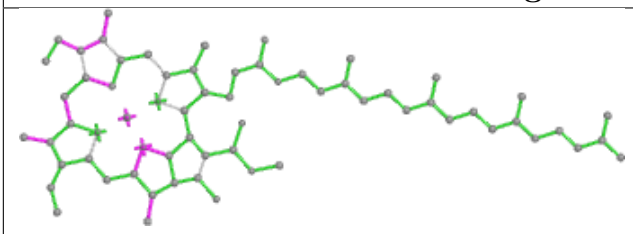


Torsions

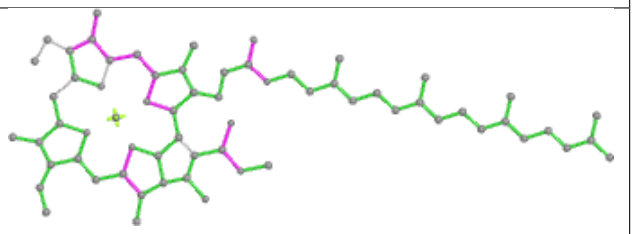


Rings

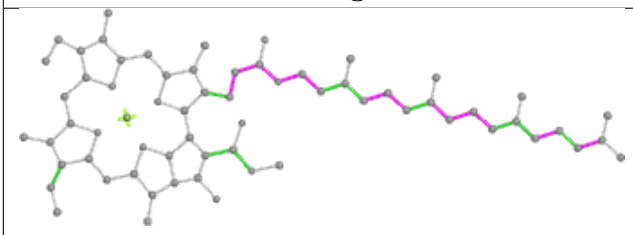
Ligand CLA B 834



Bond lengths



Bond angles



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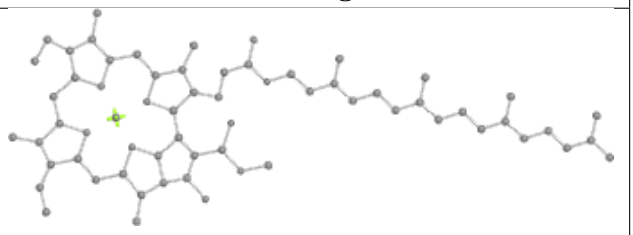
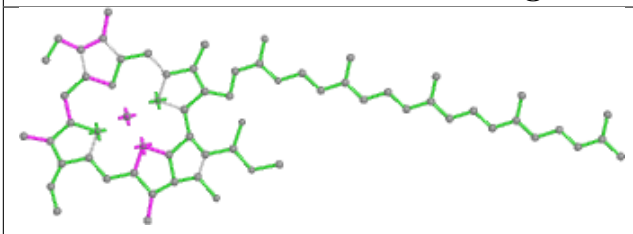
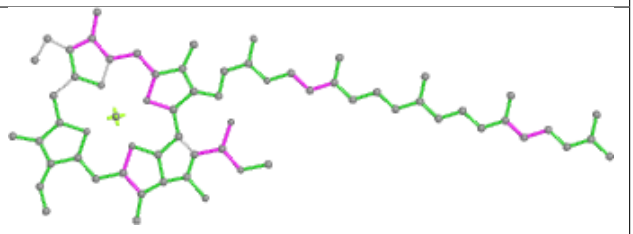


Rings

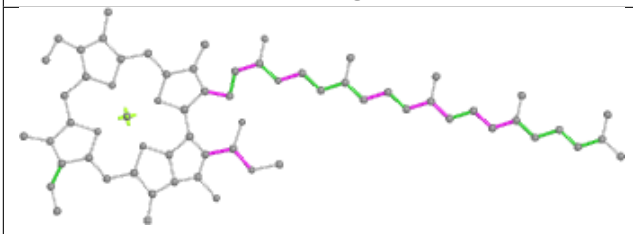
Ligand CLA B 841



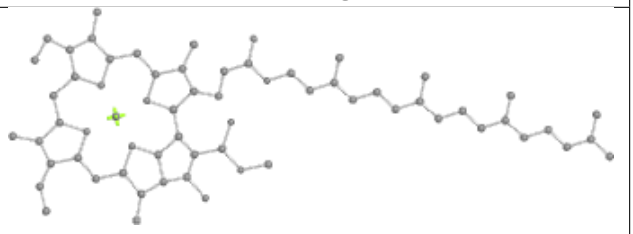
Bond lengths



Bond angles

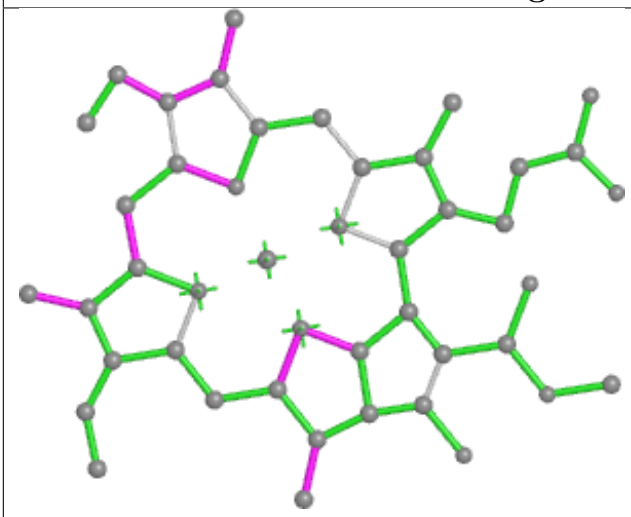


Torsions

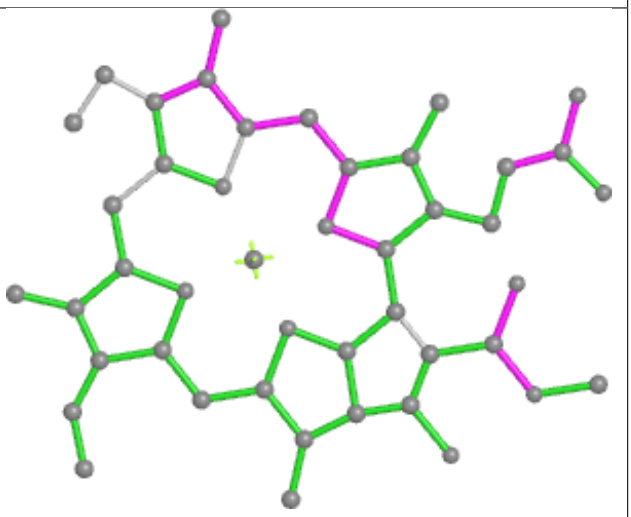


Rings

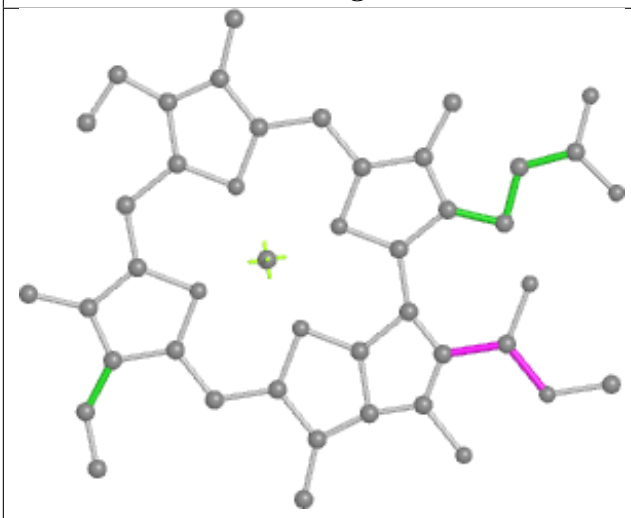
Ligand CLA 3 303



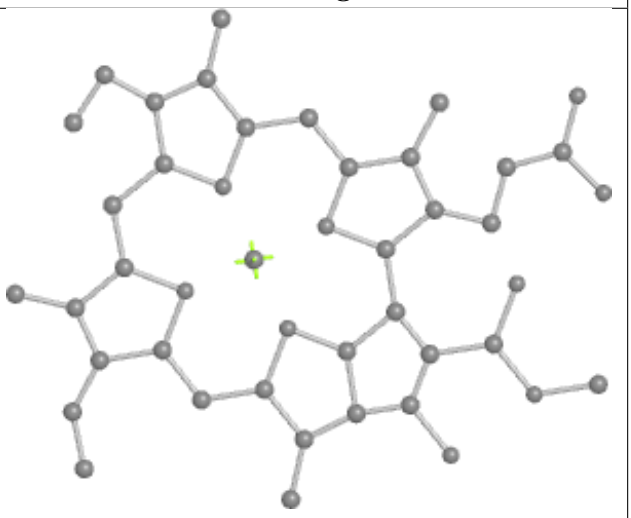
Bond lengths



Bond angles

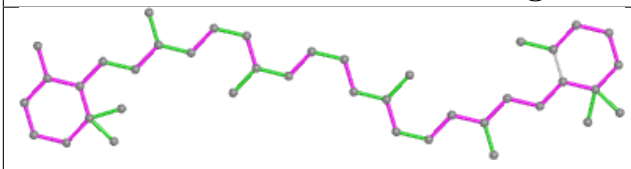


Torsions

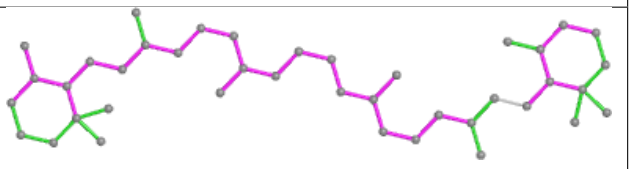


Rings

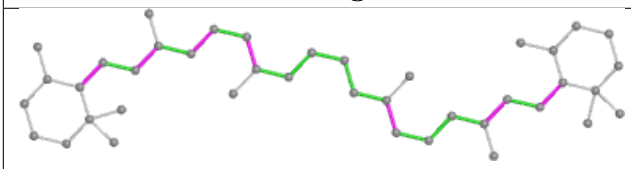
Ligand 8CT A 850



Bond lengths



Bond angles



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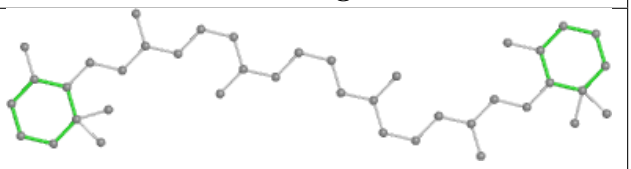
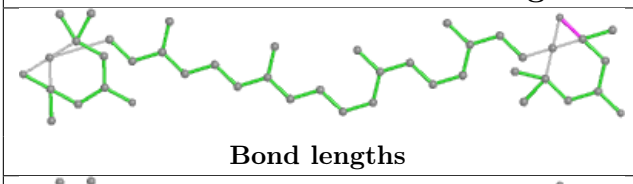
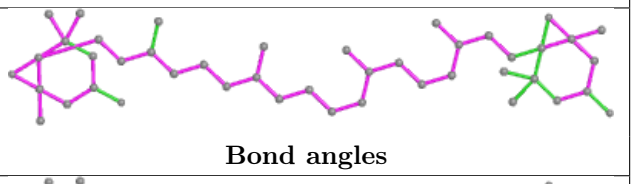


Rings

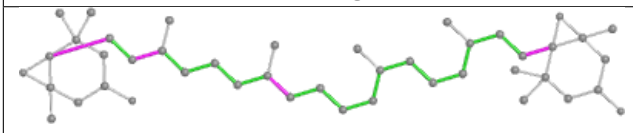
Ligand XAT 8 316



Bond lengths



Bond angles



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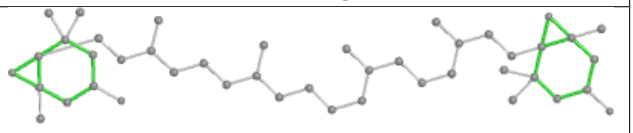
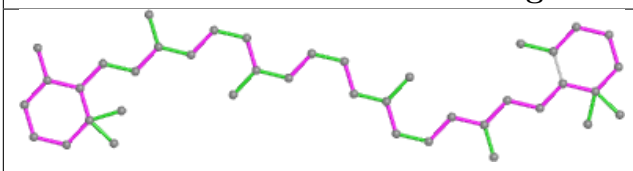
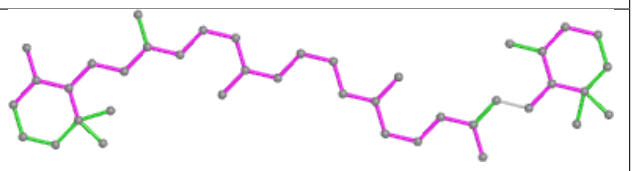


Rings

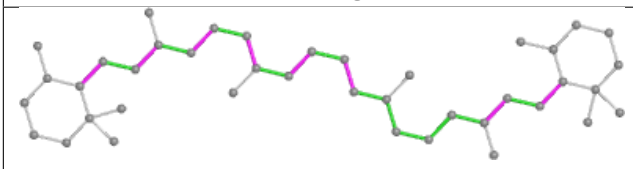
Ligand 8CT G 104



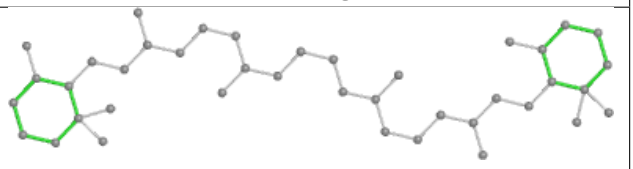
Bond lengths



Bond angles

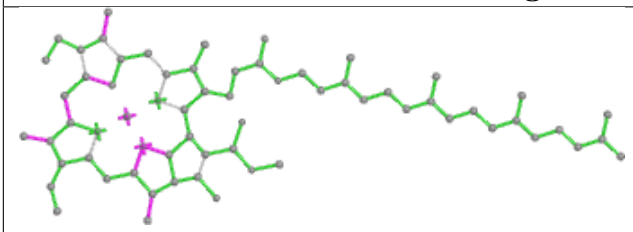


Torsions

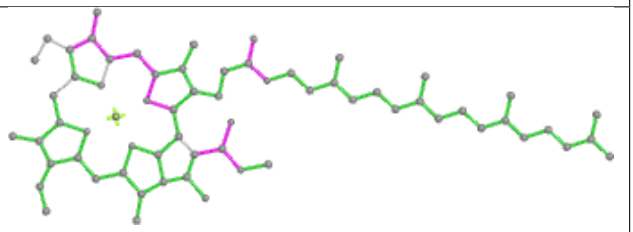


Rings

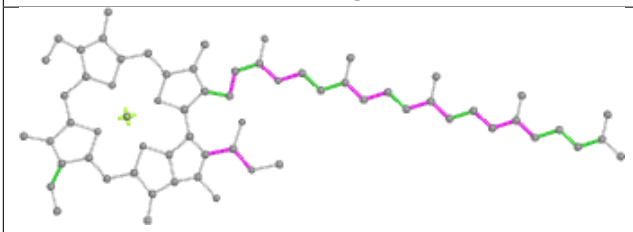
Ligand CLA A 837



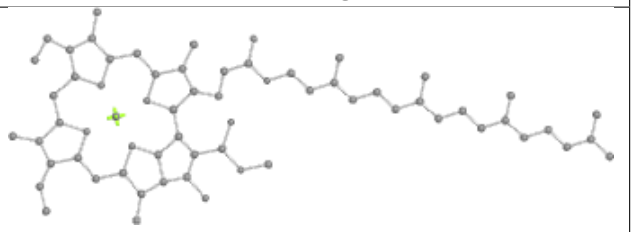
Bond lengths



Bond angles

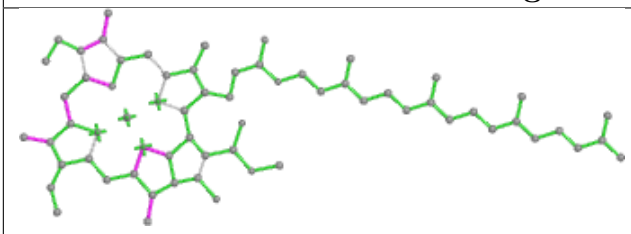


Torsions

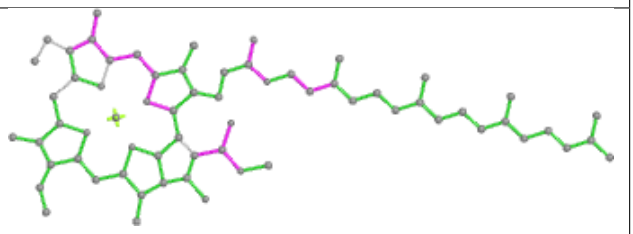


Rings

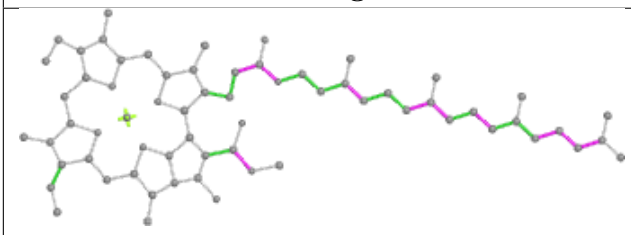
Ligand CLA A 825



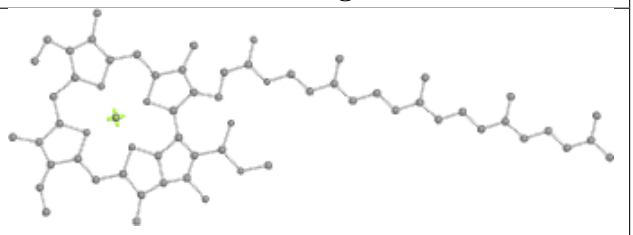
Bond lengths



Bond angles

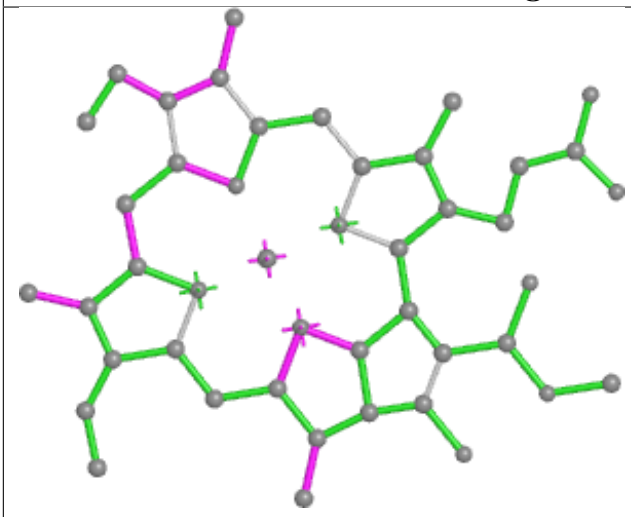


Torsions

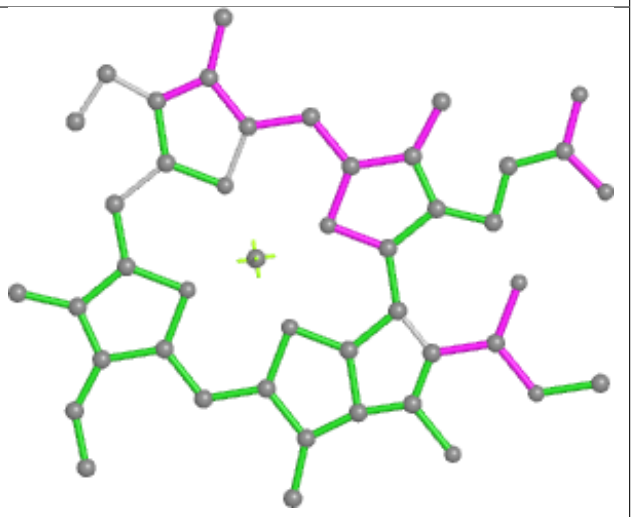


Rings

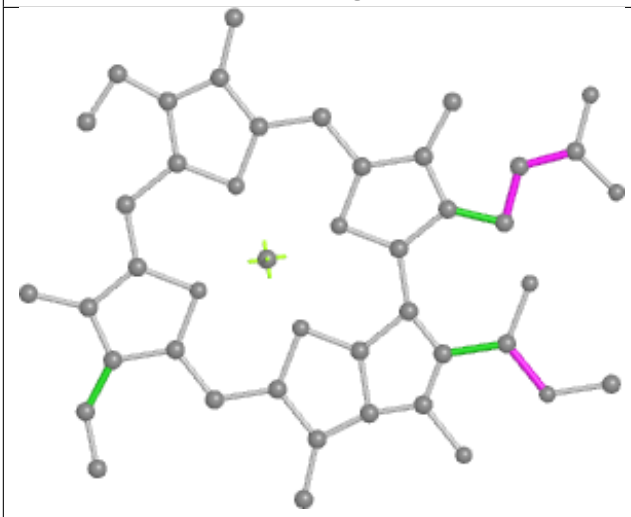
Ligand CLA B 807



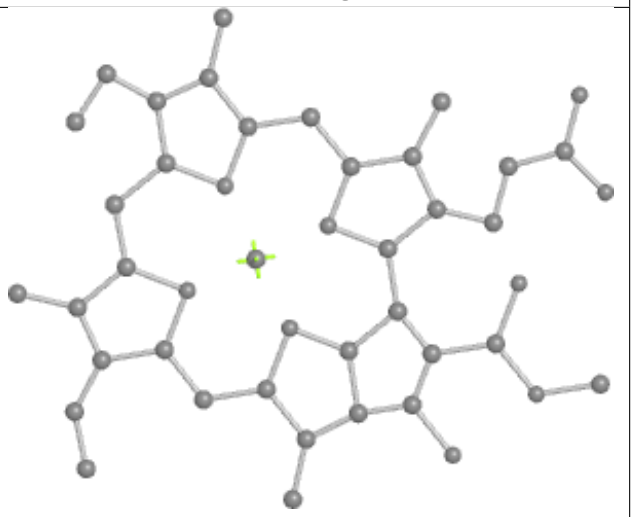
Bond lengths



Bond angles

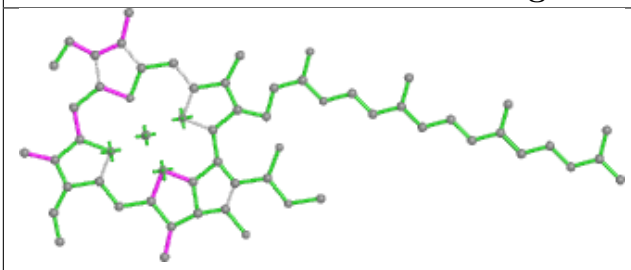


Torsions

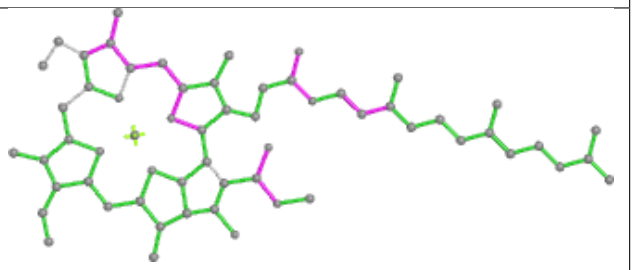


Rings

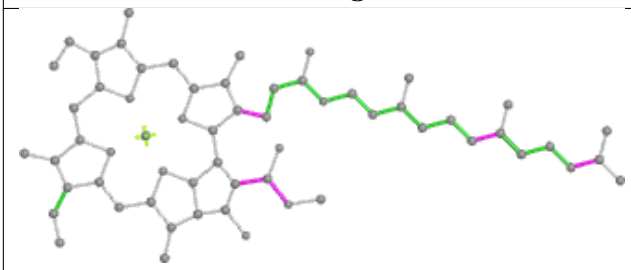
Ligand CLA 5 309



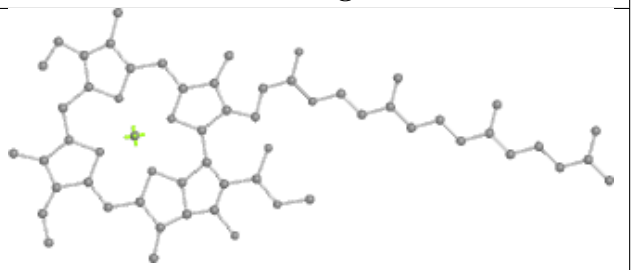
Bond lengths



Bond angles

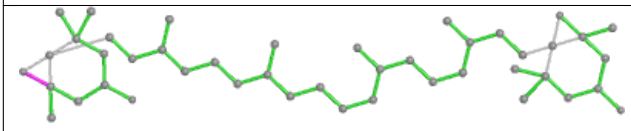


Torsions

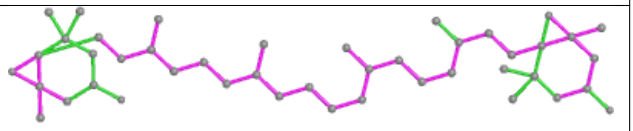


Rings

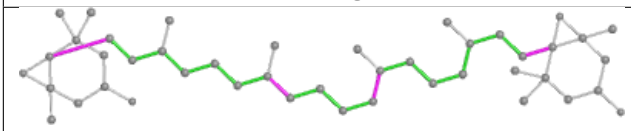
Ligand XAT 5 315



Bond lengths



Bond angles



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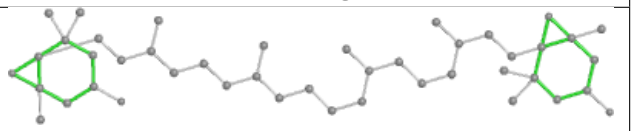
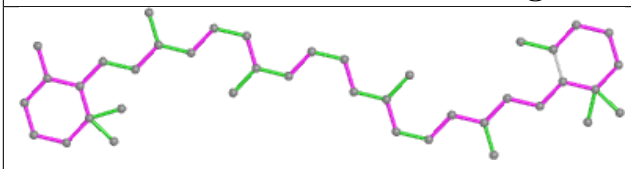
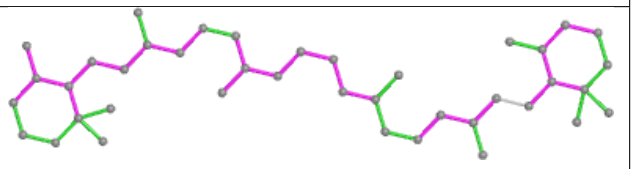


Rings

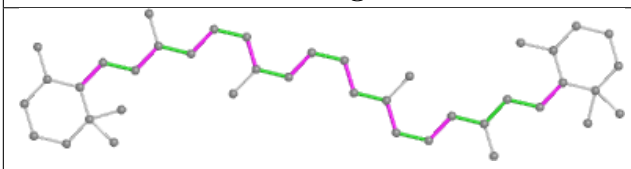
Ligand 8CT A 846



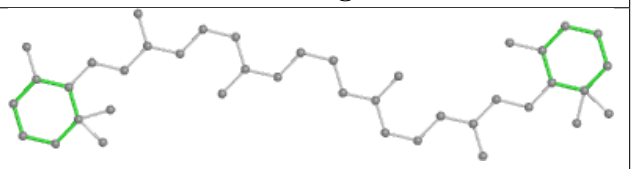
Bond lengths



Bond angles

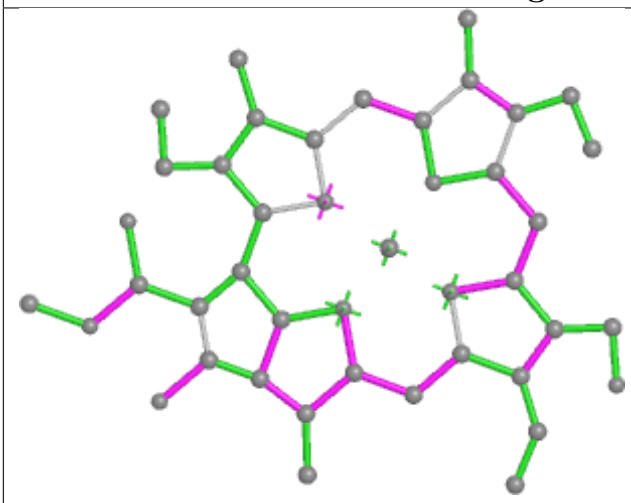


Torsions

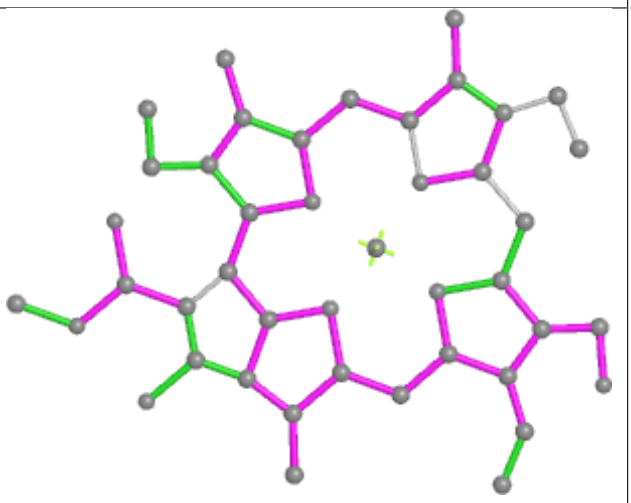


Rings

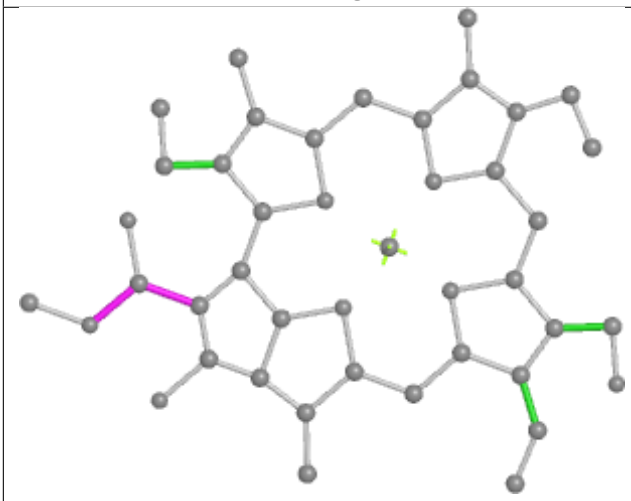
Ligand CHL 8 314



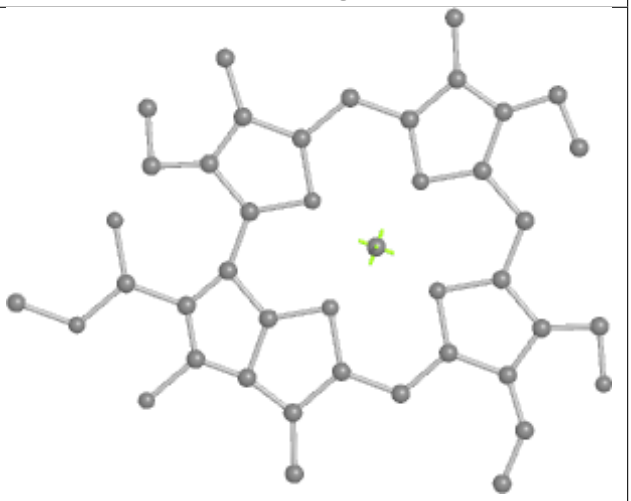
Bond lengths



Bond angles

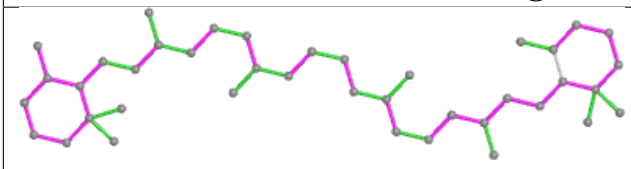


Torsions

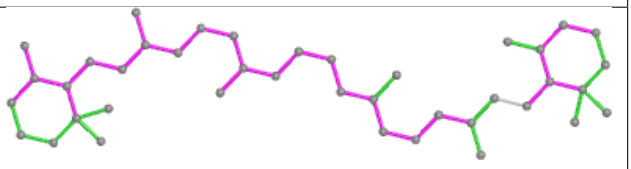


Rings

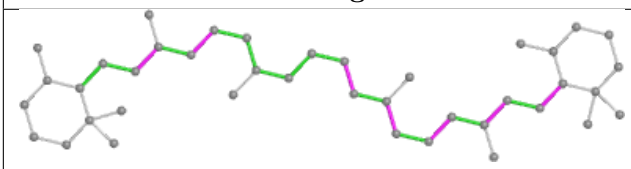
Ligand 8CT B 847



Bond lengths



Bond angles



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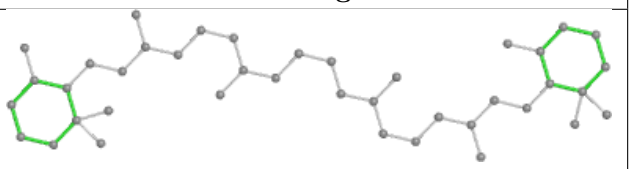
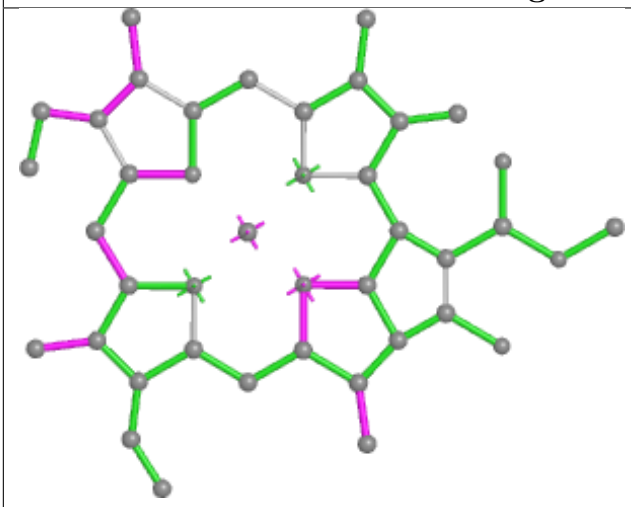
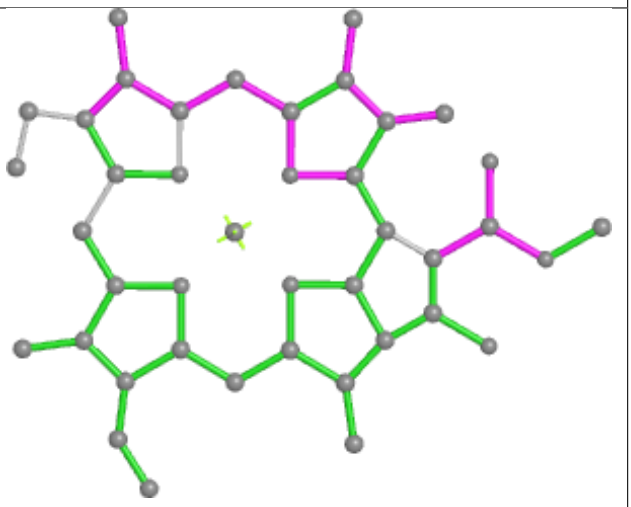


Rings

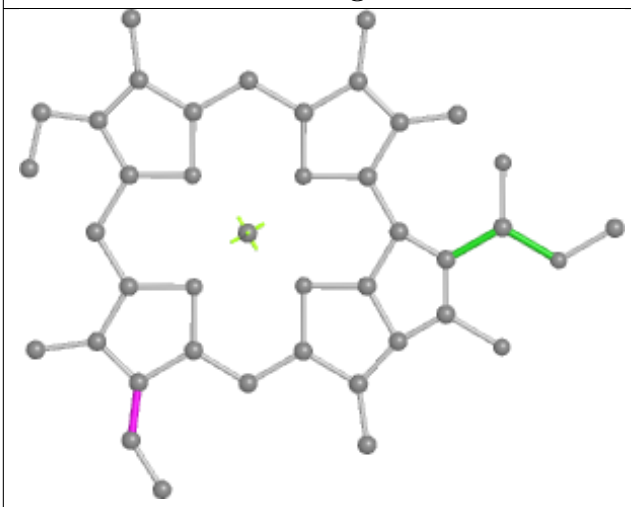
Ligand CLA 1 309



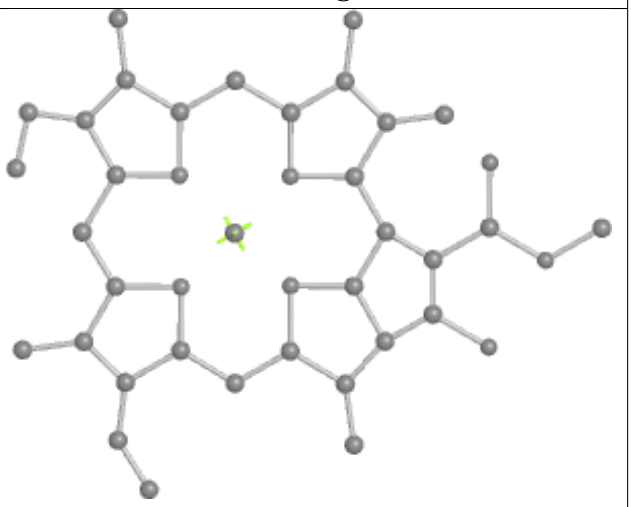
Bond lengths



Bond angles

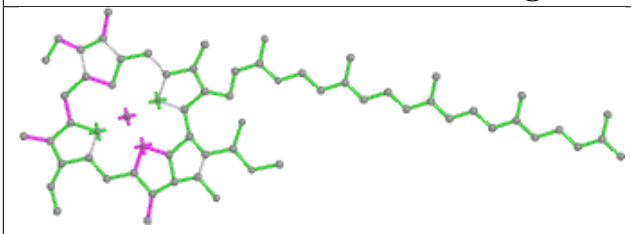


Torsions

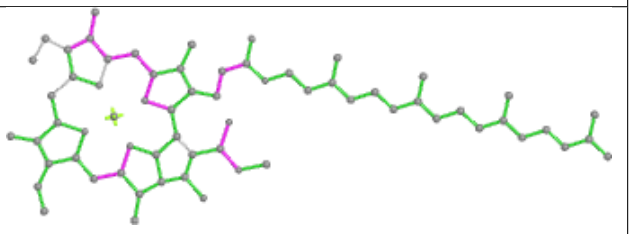


Rings

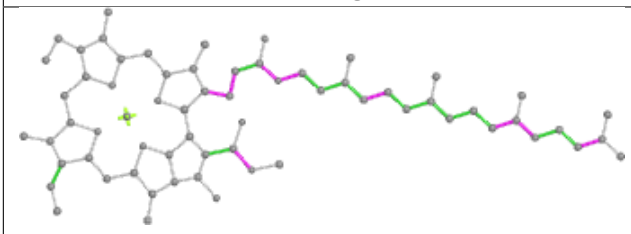
Ligand CLA A 819



Bond lengths



Bond angles



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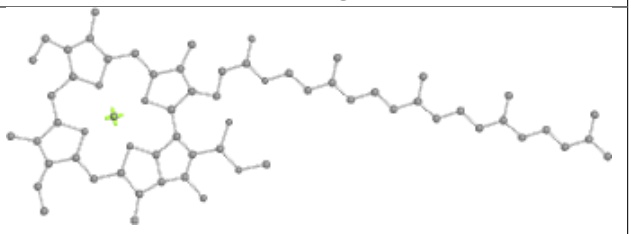
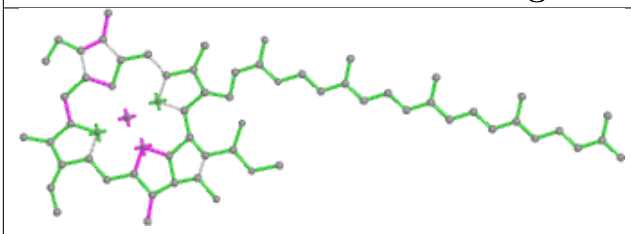
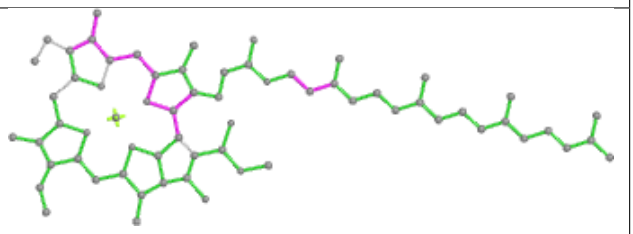


Rings

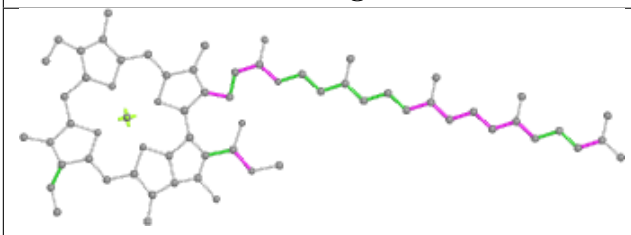
Ligand CLA 7 317



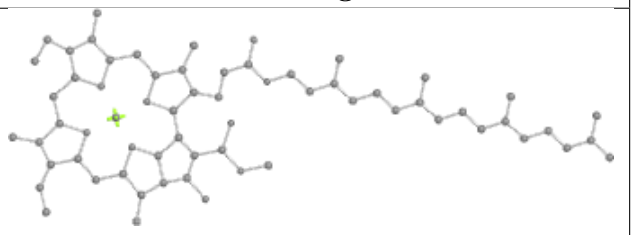
Bond lengths



Bond angles

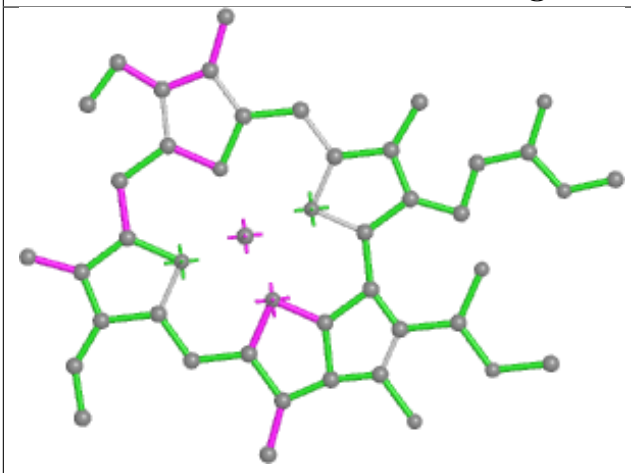


Torsions

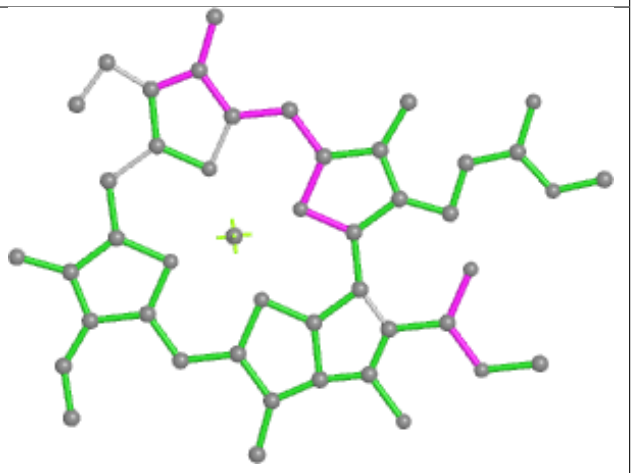


Rings

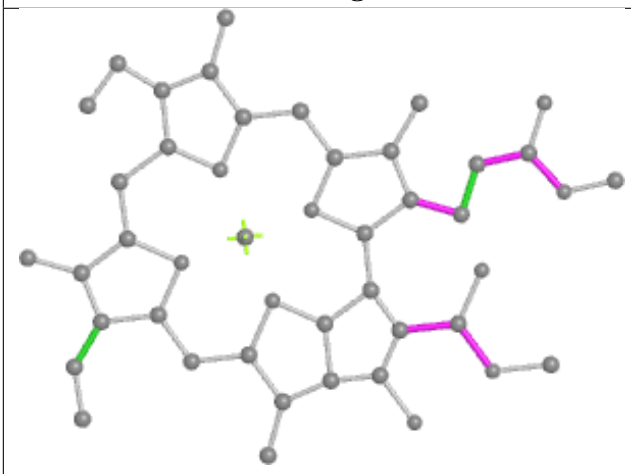
Ligand CLA 6 323



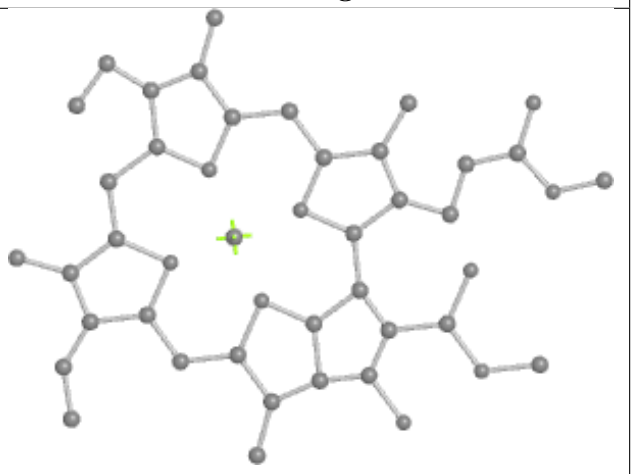
Bond lengths



Bond angles

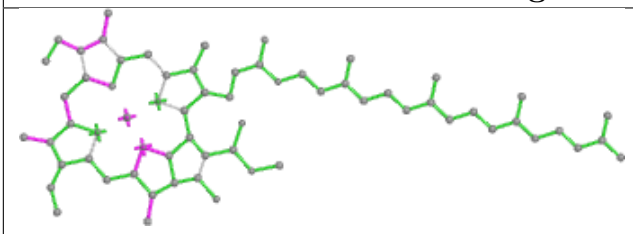


Torsions

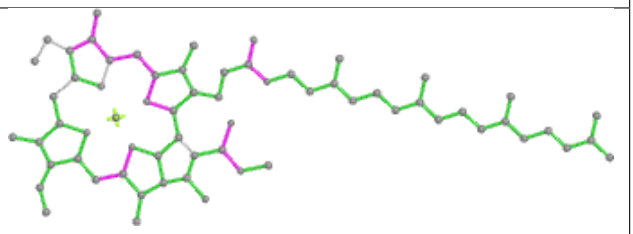


Rings

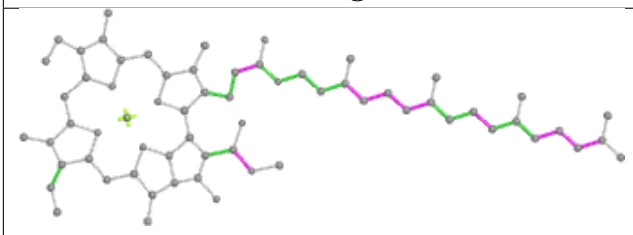
Ligand CLA 6 304



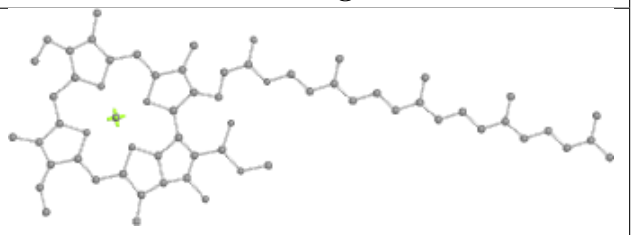
Bond lengths



Bond angles

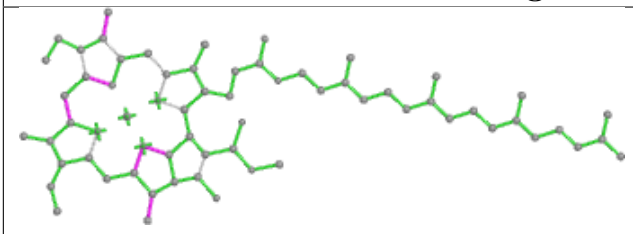


Torsions

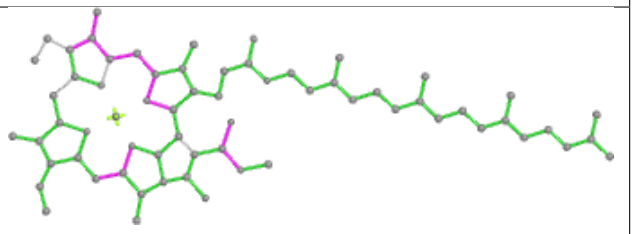


Rings

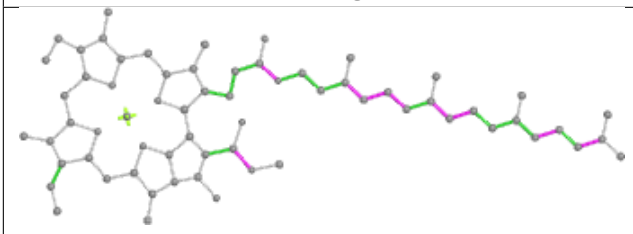
Ligand CLA L 203



Bond lengths



Bond angles



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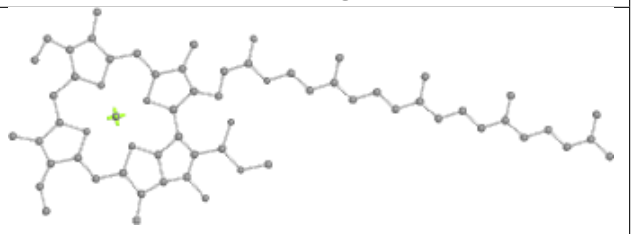
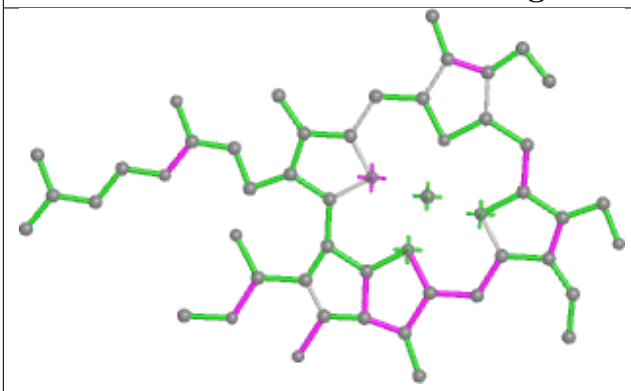
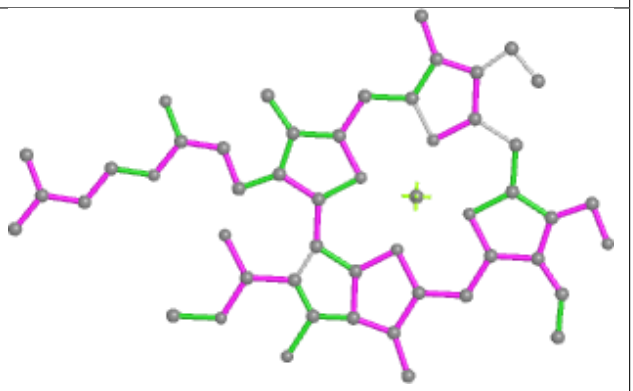


Rings

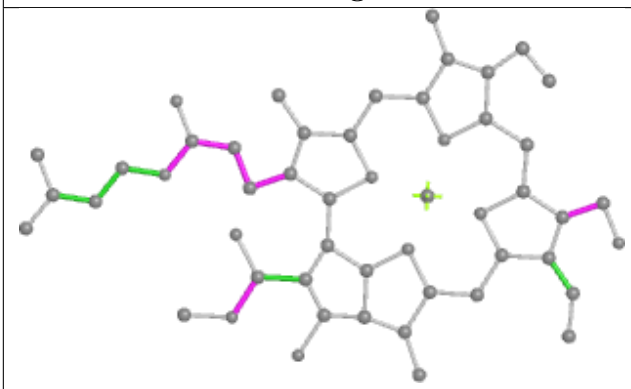
Ligand CHL 2 307



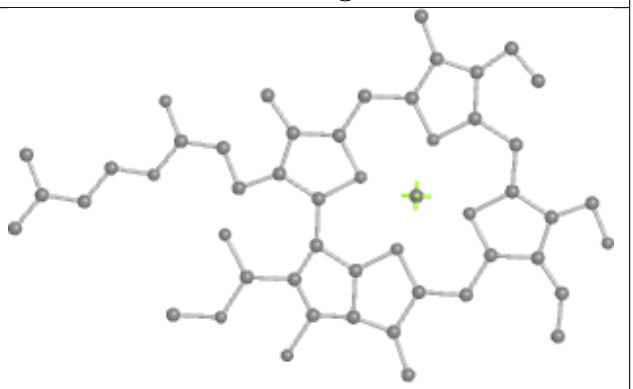
Bond lengths



Bond angles

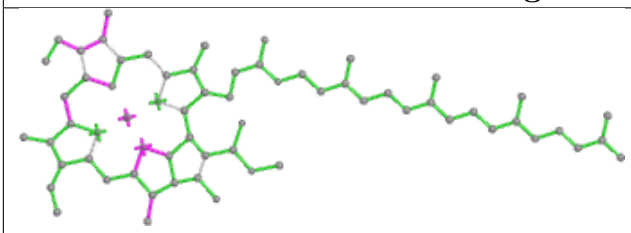


Torsions

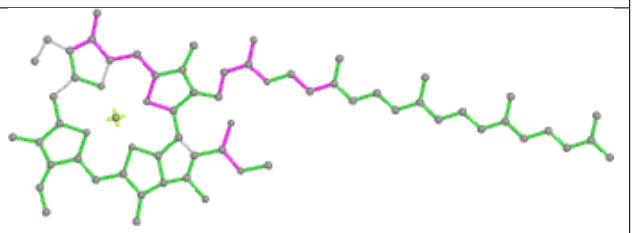


Rings

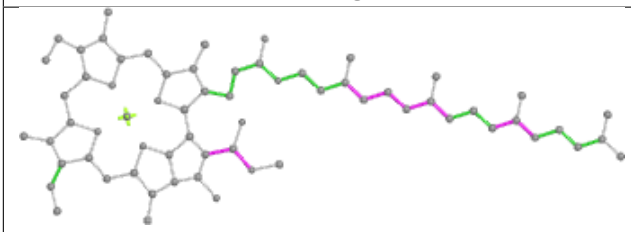
Ligand CLA A 838



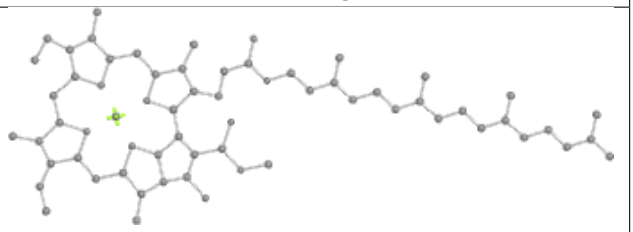
Bond lengths



Bond angles

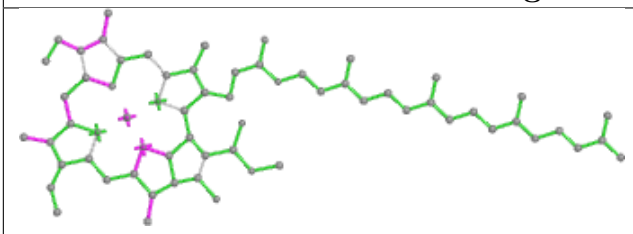


Torsions

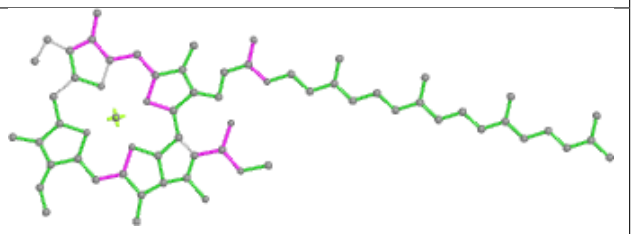


Rings

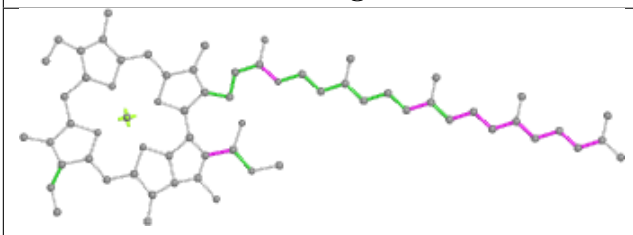
Ligand CLA A 807



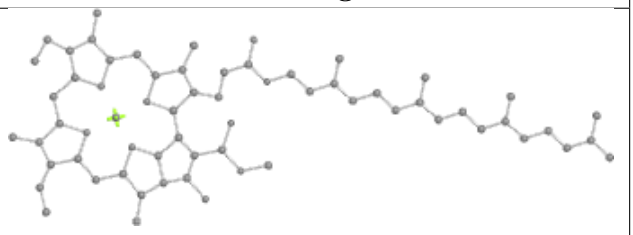
Bond lengths



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.

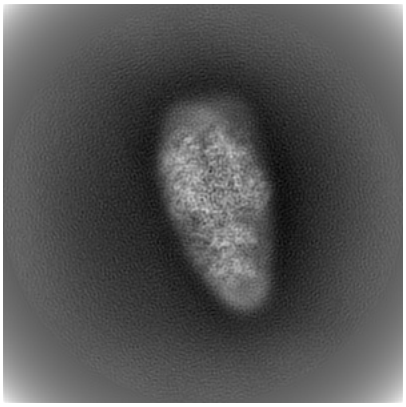
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-9670. These allow visual inspection of the internal detail of the map and identification of artifacts.

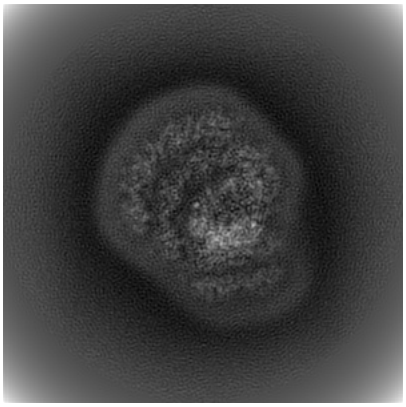
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

6.1.1 Primary map



X



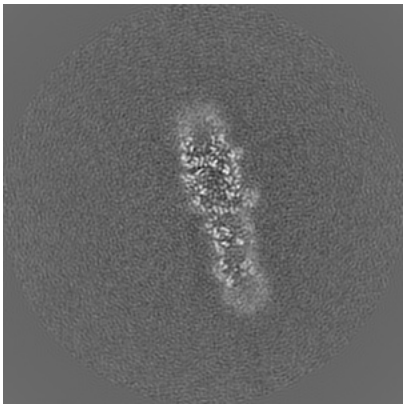
Y

Z

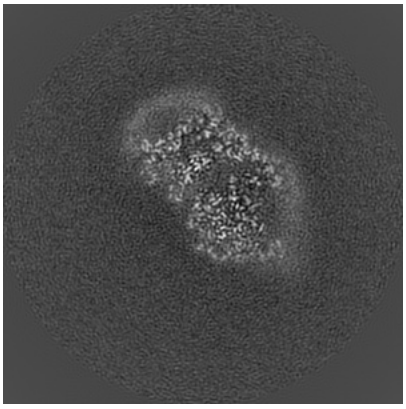
The images above show the map projected in three orthogonal directions.

6.2 Central slices

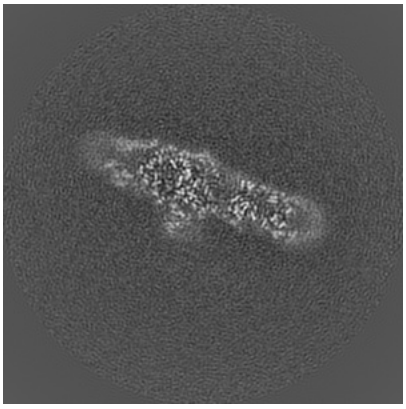
6.2.1 Primary map



X Index: 230



Y Index: 230

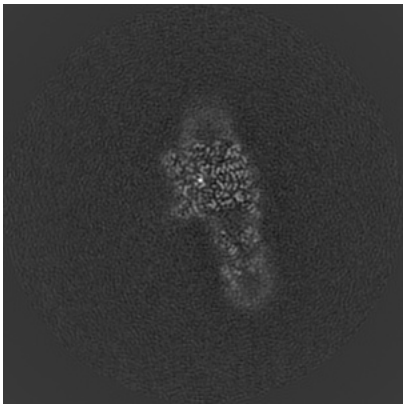


Z Index: 230

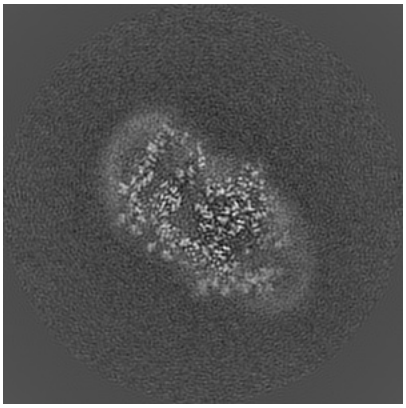
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

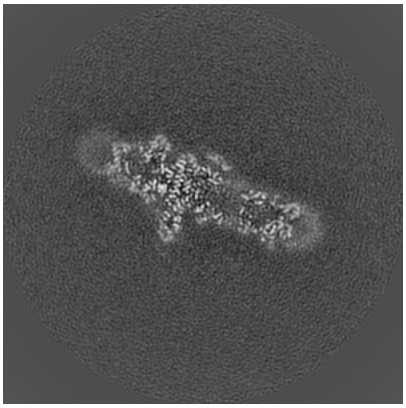
6.3.1 Primary map



X Index: 202



Y Index: 254



Z Index: 250

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 0.034. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

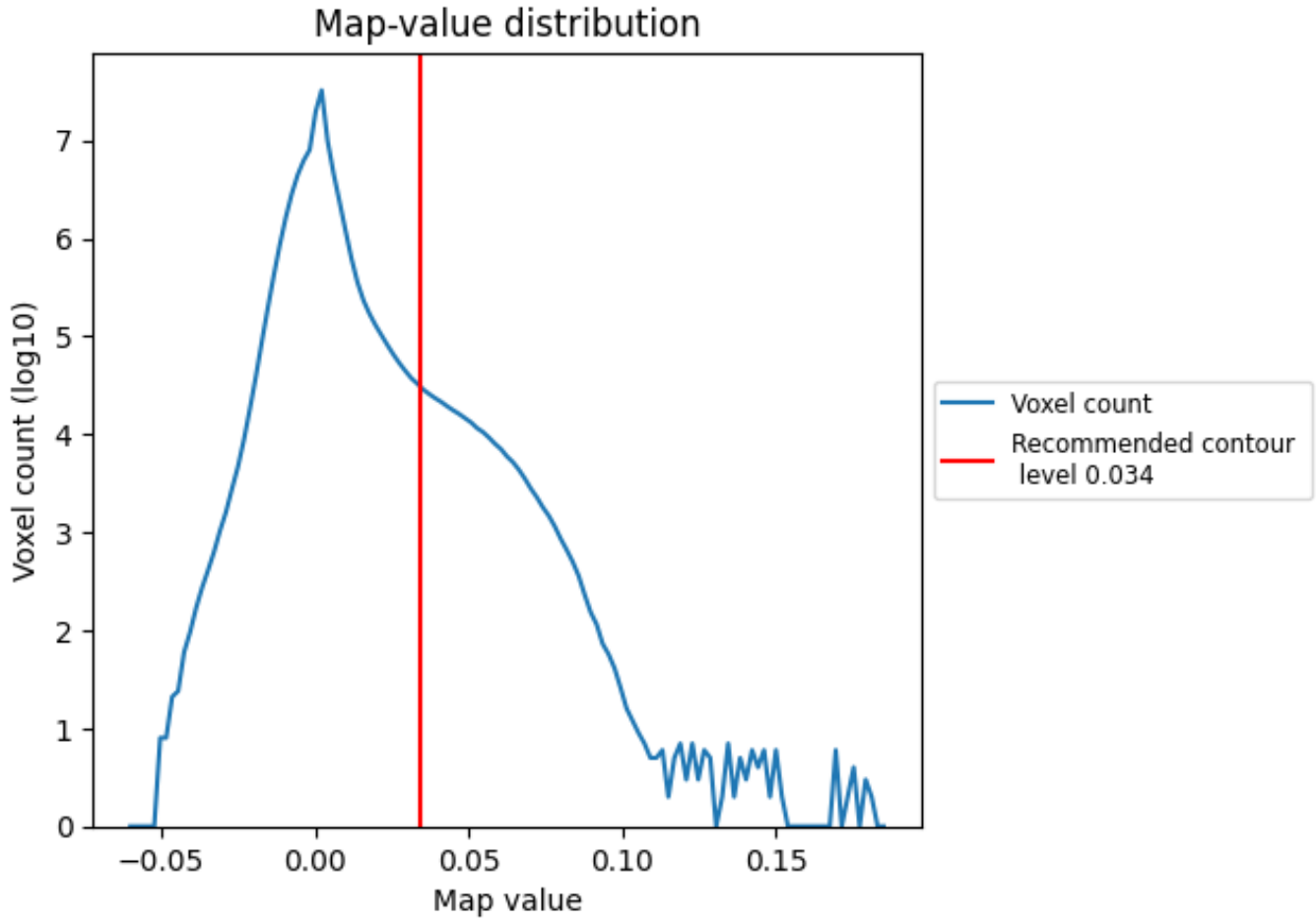
6.5 Mask visualisation (i)

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

7 Map analysis

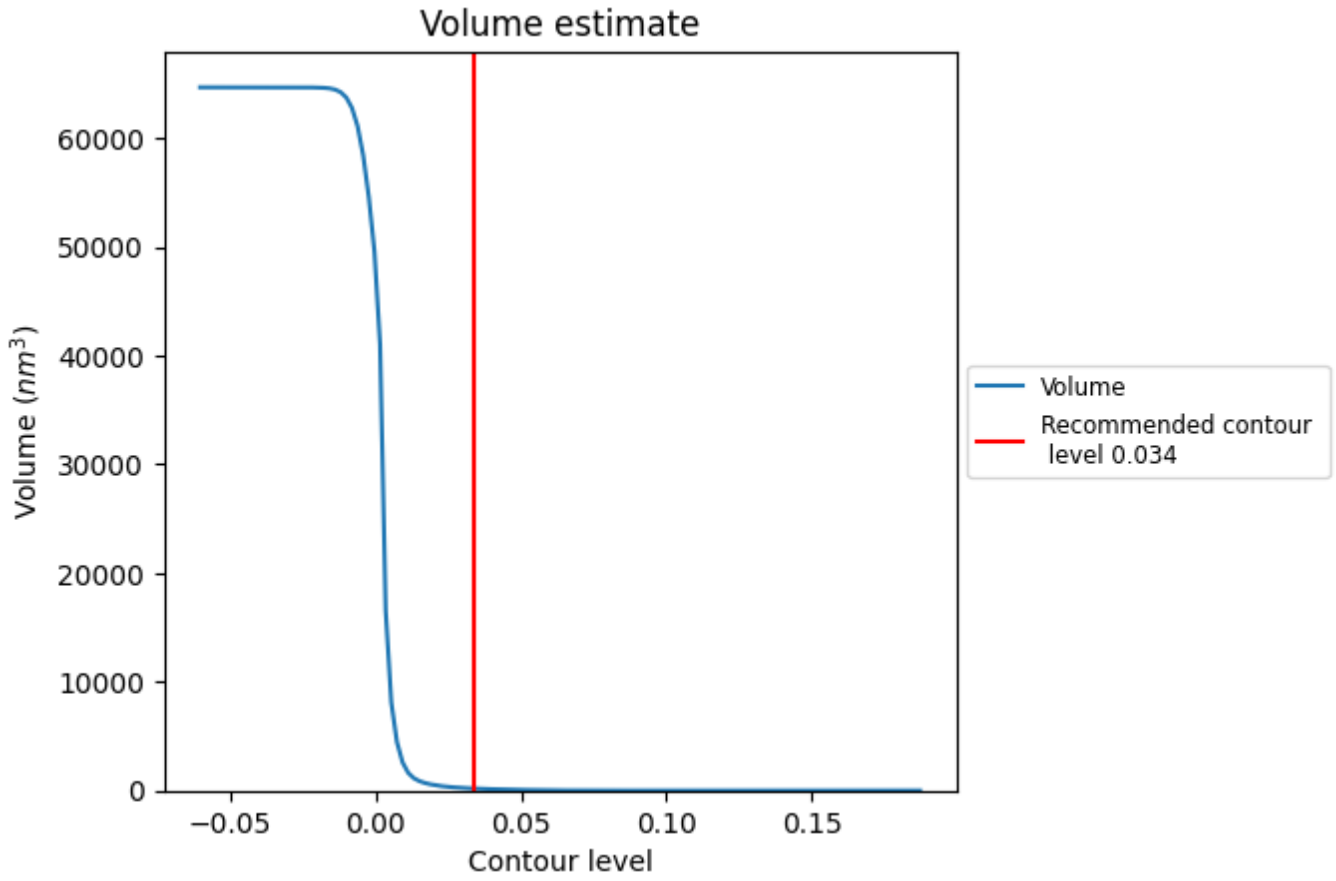
This section contains the results of statistical analysis of the map.

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.

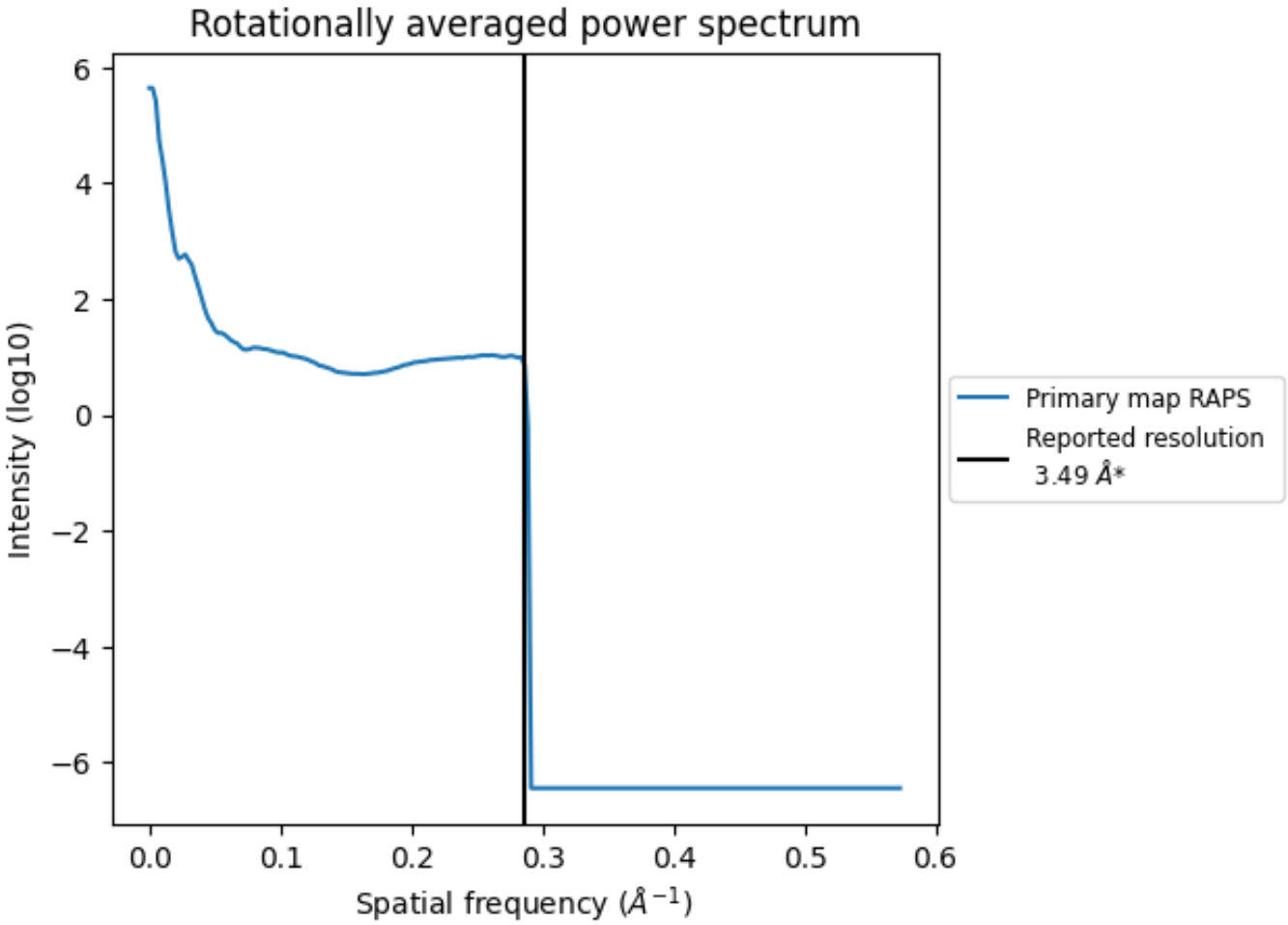
7.2 Volume estimate (i)



The volume at the recommended contour level is 186 nm^3; this corresponds to an approximate mass of 168 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 0.287 Å^{-1}

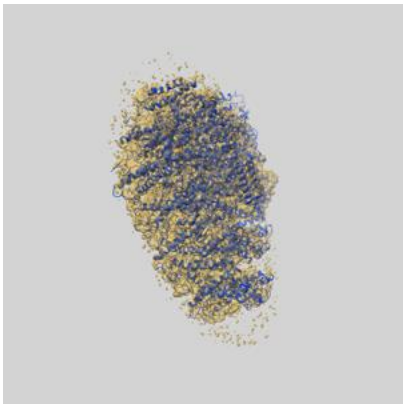
8 Fourier-Shell correlation (i)

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

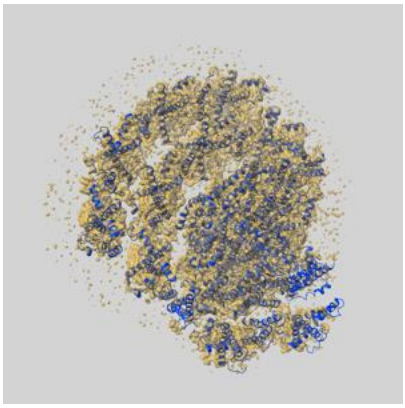
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-9670 and PDB model 6IGZ. Per-residue inclusion information can be found in section 3 on page 34.

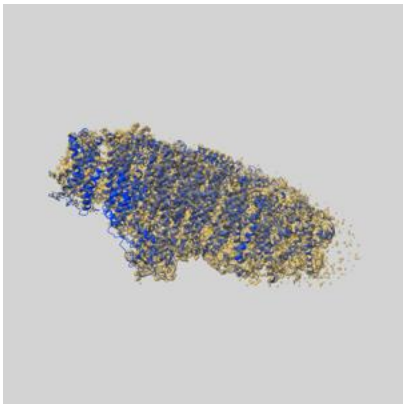
9.1 Map-model overlay



X



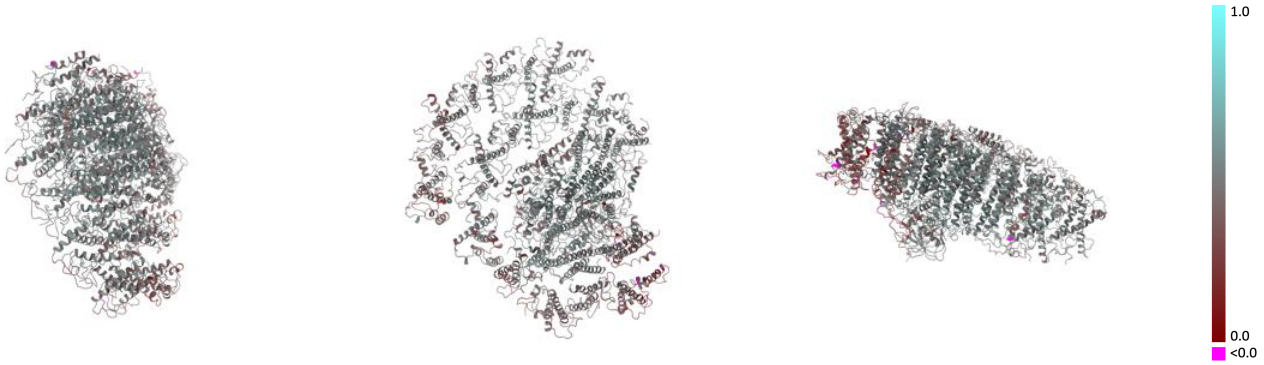
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.034 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

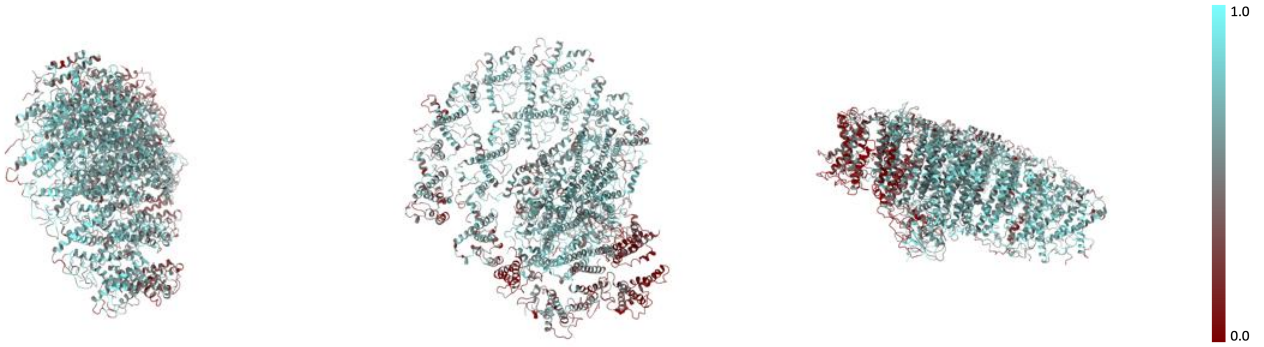
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

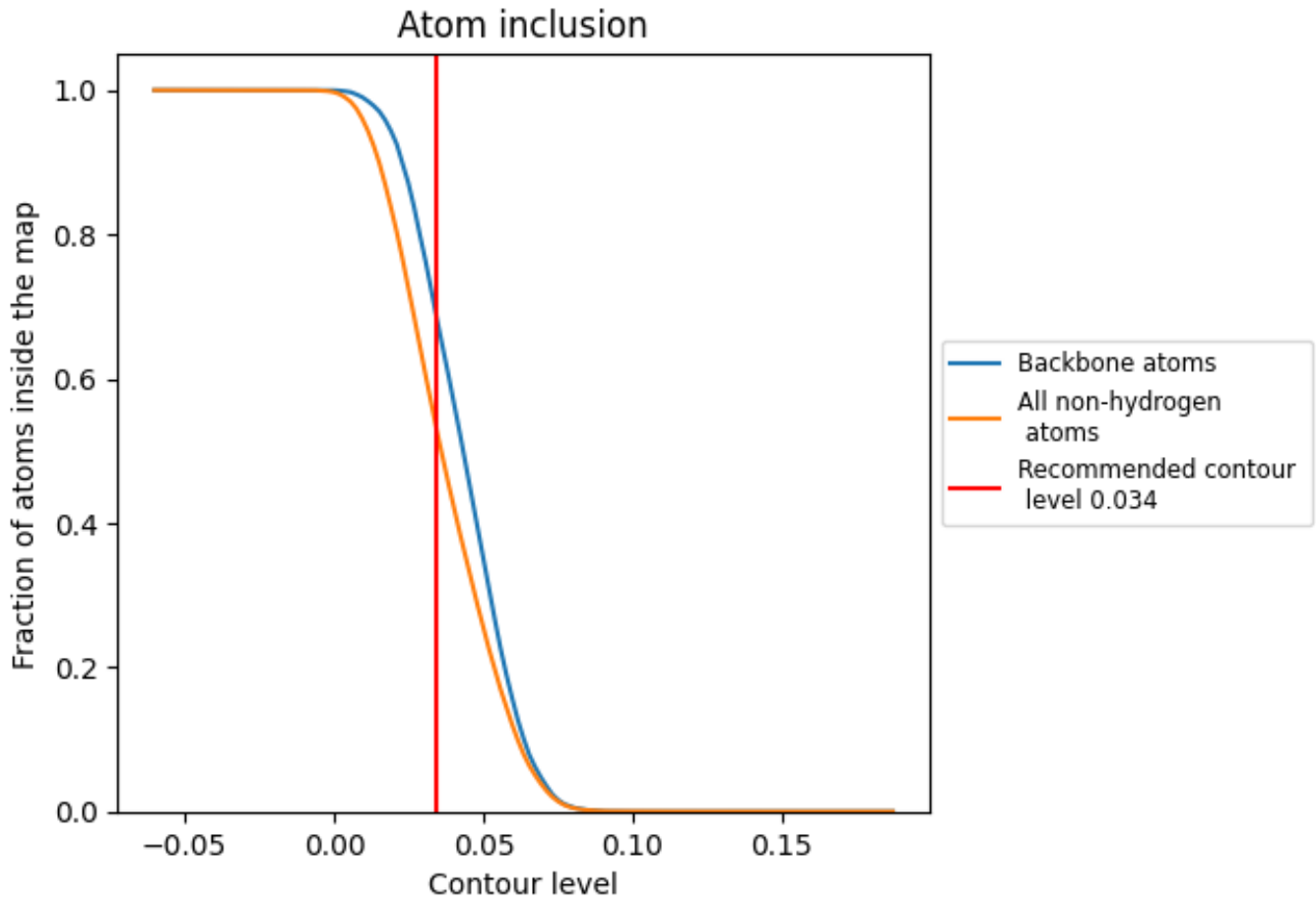
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.034).

9.4 Atom inclusion (i)



At the recommended contour level, 69% of all backbone atoms, 54% 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 (0.034) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5360	0.4750
0	0.2074	0.3440
1	0.5272	0.4620
2	0.6435	0.5160
3	0.6394	0.5010
4	0.5881	0.4810
5	0.4556	0.4250
6	0.5835	0.4770
7	0.5993	0.4760
8	0.5460	0.4490
9	0.4146	0.4280
A	0.6215	0.5250
B	0.6014	0.5160
C	0.7152	0.4740
D	0.5963	0.4680
E	0.5751	0.4740
F	0.5359	0.4700
G	0.1214	0.3640
H	0.0652	0.2890
I	0.4306	0.4880
J	0.4925	0.4980
K	0.4902	0.4400
L	0.2277	0.4030
M	0.5126	0.4760